



Supporting Information

for

Generation of multimillion chemical space based on the parallel Groebke–Blackburn–Bienaymé reaction

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Parallel synthesis of compound library 4

#	ID	Structure	Internal ID	Amine 1		Aldehyde 2		Isonitrile 3		Yield	
				ID	SMILES	ID	SMILES	ID	SMILES	mg	%
<i>Preliminary test experiments, TsOH as the catalyst</i>											
1	4{28,7,4}	CN1N=NC(CNC2=C(N=C3C=C(C=CN23)C2=NOC=N2)C2=CC(CO)=CC(C)=N2)=N1 c:2,11,13,21,28,31,33,t:7,9,18,24	Z8786958949	1{28}	Cl.Nc1cc(ccn1)c2ncon2	2{7}	Cc1cc(CO)cc(C=O)n1	3{4}	Cn1nnc(C[N+][C-])n1	94.4	84
2	4{29,8,5}	COCCCN1=C(N=C2C=CC(OC3CN(C3)C(=O)OC(C)(C)C)=CN12)C1=CON=C1COC c:10,25,33,t:6,8,30	Z8801681836	1{29}	CC(C)(C)OC(=O)N1C(C(C1)O)c2cc(N)n2	2{8}	COCCnocc1C=O	3{5}	COCC[N+][C-]	94.8	72
3	4{30,9,6}	CCOC(=O)CCCN1=C(N=C2C=CC=C(N12)C1=CC=C(C)C=C1)C1=CSC=C1 c:13,15,25,31,t:9,11,20,22,28	Z8784060473	1{30}	Cc1ccc(cc1)c2cccc(N)n2	2{9}	O=Cc1ccsc1	3{6}	CCOC(=O)CC[N+][C-]	79.9	71
4	4{31,10,6}	CCOC(=O)CCCN1=C(N=C2C=CC3=C(CCO3)N12)C1=NC=CC(C)=C1 c:13,26,29,t:9,11,15,24	Z8778277510	1{31}	Nc1ccc2OCc2n1	2{10}	Cc1ccnc(C=O)c1	3{6}	CCOC(=O)CC[N+][C-]	72.0	70
5	4{32,11,7}	CP(C)(=O)C1=CC2=NC(=C(NC3CCOCC3)N2C=C1)C1=NN(CC(F)(F)F)C=C1 c:20,31,t:4,6,8,23	Z8803896935	1{32}	CP(=O)(C)c1ccnc(N)c1	2{11}	FC(F)(F)Cn1ccc(C=O)n1	3{7}	[C-][N+]C1CCOCC1	82.4	69
6	4{33,9,6}	CCCSC1=CC=CC2=NC(=C(NCCCC(=O)OCC)N12)C1=CSC=C1 c:6,27,t:4,8,10,24	Z8797783068	1{33}	CCCSc1ccc(N)n1	2{9}	O=Cc1ccsc1	3{6}	CCOC(=O)CC[N+][C-]	72.0	66
7	4{32,12,7}	COCl=NC=C(C=C1)C1=C(NC2CCOCC2)N2C=CC(=CC2=N1)P(C)(C)=O c:4,6,9,20,22,25,t:2	Z8798985026	1{32}	CP(=O)(C)c1ccnc(N)c1	2{12}	COc1ccc(C=O)n1	3{7}	[C-][N+]C1CCOCC1	70.9	66
8	4{34,13,8}	COC(=O)C(CC1=CC=CC=C1)NC1=C(N=C2C=C(C=CN12)C1=NNC(C)=N1)C1=C(C)NN=N1 c:8,10,18,20,29,32,36,t:6,14,16,25	Z8801681814	1{34}	Cc1nc(n[nH]1)c2ccnc(N)c2	2{13}	Cc1[nH]nnc1C=O	3{8}	COC(=O)C(Cc1cccc1)[N+][C-]	80.1	65
9	4{35,14,6}	CCOC(=O)CCCN1=C(N=C2C=CC(C)=CN12)C1=CC=C(C)C=C1 c:13,16,26,t:9,11,21,23	Z8712546411	1{35}	Cc1ccc(N)n1	2{14}	Cc1ccc(C=O)cc1	3{6}	CCOC(=O)CC[N+][C-]	61.2	64
10	4{36,15,9}	CNC1=C(N=C2C=CC(Br)=CN12)C1=CC=C(OC)C=C1 c:6,9,20,t:2,4,14,16	Z8776690344	1{36}	Nc1ccc(Br)n1	2{15}	COc1ccc(C=O)cc1	3{9}	C[N+][C-]	57.7	64

11	4{37,16,10}	CN1N=CC(CNC(=O)OC(C)(C)C)=C1C1=C(NC2CCOC2)N2C(C=CC=C2C(F)F)=N1 c:2,13,16,27,29,34	Z8810903040	1{37}	Cl.Nc1cccc(n1)C(F)F	2{16}	Cn1ncc(CNC(=O)OC(C)(C)C)c1C=O	3{10}	[C-]#[N+]C1CCOC1	78.9	63
12	4{38,17,9}	CCOC1=CN=C(N=C1)C1=C(NC)N2C=CC(=C2=N1)C#N c:5,7,10,15,17,20,t:3	Z8810902991	1{38}	Nc1cc(C#N)ccn1	2{17}	CCOc1ncc(C=O)nc1	3{9}	C[N+]#[C-]	50.0	63
13	4{39,10,6}	CCOC(=O)CCNC1=C(N=C2N1C=C(Br)C1=C2CCC1)C1=NC=CC(C)=C1 c:11,18,27,30,t:9,15,25	Z8784060925	1{39}	Nc1ncc(Br)c2CCCc21	2{10}	Cc1ccnc(C=O)c1	3{6}	CCOC(=O)C CC[N+]#[C-]	75.9	61
14	4{40,18,4}	CN1N=NC(CNC2=C(N=C3C=C(C=C(C)N23)C(F)(F)F)C2=CN(CCO)N=C2)=N1 c:2,11,29,31,t:7,9,13,23	Z8781341796	1{40}	Cc1cc(cc(N)n1)C(F)(F)F	2{18}	OCCn1cc(C=O)cn1	3{4}	Cn1nnc(C[N+]#[C-])n1	69.7	61
15	4{41,19,11}	COC1=C(N(C)N=C1)C1=C(NCC2=CC(Br)=CC=C2)N2C=C(C)N=CC2=N1 c:6,9,16,18,25,28,t:2,13,22	Z8781341780	1{41}	Cc1cnc(N)c n1	2{19}	COc1enn(C)c1C=O	3{11}	Br1cccc(C[N+]#[C-])c1	70.3	61
16	4{42,20,7}	CCN1C=C(N=N1)C1=C(NC2CCOCC2)N2C=C(SC)C=CC2=N1 c:3,5,8,23,26,t:19	Z8810902980	1{42}	CSc1ccc(N)nc1	2{20}	CCn1cc(C=O)nn1	3{7}	[C-]#[N+]C1CCOCC1	57.5	59
17	4{43,21,12}	CC(C)(C)OC(=O)N1CC2=C(C1)N1C(NCC3COC3)=C(N=C1C=C2)C1=CC2=NC=NN2C=C1 c:9,22,24,27,34,38,t:30,32	Z8798985027	1{43}	CC(C)(C)OC(=O)N1Cc2ccc(N)nc2C1	2{21}	O=Cc1ccn2ncc2c1	3{12}	[C-]#[N+]CC1COC1	74.6	58
18	4{44,22,6}	CCOC(=O)CCNC1=C(N=C2C=NC(CC)=CN12)C1=CC=CC=C1 c:13,17,24,26,t:9,11,22	Z8741907003	1{44}	CCc1cnc(N)cn1	2{22}	O=Cc1cccc1	3{6}	CCOC(=O)C CC[N+]#[C-]	54.9	58
19	4{45,23,10}	FC1=CC2=NC(=C(NC3CCOC3)N2C=C1)C1=C2CCCCN2C(=N1)C(F)(F)F c:16,19,27,t:1,3,5	Z8803896946	1{45}	Cl.Nc1cc(F)ccn1	2{23}	FC(F)(F)c1nc(C=O)c2CCCc12	3{10}	[C-]#[N+]C1CCOC1	62.9	57
20	4{46,18,13}	COC1=CC=C(CNC2=C(N=C3C=CC=CN23)C2=CN(CCO)N=C2)C=C1 c:12,14,25,28,t:2,4,8,10,19	Z8810903006	1{46}	Nc1ccccn1	2{18}	OCCn1cc(C=O)cn1	3{13}	COc1ccc(C[N+]#[C-])cc1	55.8	57
21	4{47,24,14}	COCCNC1=C(N=C2C=C(C=CN12)S(N)(=O)=O)C1=CC(=CC=C1)N(C)C c:9,11,22,24,t:5,7,20	Z8798985048	1{47}	Cl.Nc1cc(ccn1)S(=O)(=O)N	2{24}	CN(C)c1cccc(C=O)c1	3{14}	COCC[N+]#[C-]	59.6	57
22	4{48,25,15}	CCNC1=C(N=C2C=C(C=CN12)S(C)(=O)=O)C1=CN=C(N=C1)C1CCOCC1 c:7,9,20,22,t:3,5,18	Z8781341798	1{48}	CS(=O)(=O)c1ccnc(N)c1	2{25}	O=Cc1cnc(n c1)C2CCOCC2	3{15}	CC[N+]#[C-]	61.4	57

23	4{49,26,7}	OCC1=CC=CC2=NC(CCC3=CC=CC=C3)=C(NC3CCOCC3)N12 c:4,13,15,t:2,6,11,17	Z8741906954	1{49}	Ne1cccc(CO)n1	2{26}	O=CCCc1cccc1	3{7}	[C-]#[N+]C1CCOCC1	53.8	57
24	4{50,27,16}	CN1N=C(N=C1C)C1=C(NC2=C(C)C=CC=C2C)N2C(C=CC=C2P(C)(C)=O)=N1 c:2,4,8,11,14,16,22,24,30	Z8781341789	1{50}	CP(=O)(C)c1cccc(N)n1	2{27}	Cc1nc(C=O)nn1C	3{16}	Cc1cccc(C)c1[N+]#[C-]	62.5	57
25	4{51,22,17}	CC1=C(CI)C=CC2=NC(=C(NCC3CCOCC3)N12)C1=CC=CC=C1 c:1,4,24,26,t:6,8,22	Z8741907089	1{51}	Cc1nc(N)cc1Cl	2{22}	O=Cc1cccc1	3{17}	[C-]#[N+]CC1CCOCC1	54.4	57
26	4{52,28,18}	CC(C)(C)NC1=C(N=C2C=CC(=CN12)C1(CC1)C(F)(F)F)C1=CN(N=C1)C1CCS(=O)(=O)C1 c:9,11,27,t:5,7,24	Z8801681827	1{52}	Ne1ccc(en1)C2(CC2)C(F)(F)F	2{28}	O=Cc1enn(c1)C2CCS(=O)(=O)C2	3{18}	CC(C)(C)[N+]#[C-]	73.6	57
27	4{53,14,17}	CC1=CC=C(C=C1)C1=C(NCC2CCOCC2)N2C=C(CO)C=CC2=N1 c:3,5,8,24,27,t:1,20	Z8776690320	1{53}	Ne1ccc(CO)en1	2{14}	Cc1ccc(C=O)cc1	3{17}	[C-]#[N+]CC1CCOCC1	53.7	57
28	4{36,22,17}	BrC1=CN2C(C=C1)=NC(=C2NCC1CCOCC1)C1=CC=CC=C1 c:5,7,9,23,25,t:1,21	Z8700285600	1{36}	Ne1ccc(Br)en1	2{22}	O=Cc1cccc1	3{17}	[C-]#[N+]CC1CCOCC1	59.0	57
29	4{54,14,6}	CCOC(=O)CCCN1=C(N=C2C=CC(=CN12)C(=O)N(C)C)C1=CC=C(C)C=C1 c:13,15,30,t:9,11,25,27	Z8776690341	1{54}	Cl.CN(C)C(=O)c1ccc(N)nc1	2{14}	Cc1ccc(C=O)cc1	3{6}	CCOC(=O)CC[N+]#[C-]	62.3	56
30	4{55,29,6}	CCOC(=O)CCCN1=C(N=C2C=C(SC)C=CN12)C1=NN(CC)C=C1 c:17,27,t:9,11,13,22	Z8797781157	1{55}	CSc1ccnc(N)c1	2{29}	CCn1ccc(C=O)n1	3{6}	CCOC(=O)CC[N+]#[C-]	58.7	56
31	4{56,9,14}	COCCN1=C(N=C2C=CC(=CN12)C1=NN(C)C=C1)C1=CSC=C1 c:9,11,20,26,t:5,7,16,23	Z8780122427	1{56}	Cn1ccc(n1)c2ccc(N)nc2	2{9}	O=Cc1ccsc1	3{14}	COCC[N+]#[C-]	53.2	56
32	4{57,30,19}	CC(C)OC1=CN2C(C=N1)=NC(C1CCN(CC1)C(C)=O)=C2NCC1=CC=CS1 c:8,10,22,29,t:4,27	Z8786958905	1{57}	CC(C)Oe1cnc(N)en1	2{30}	CC(=O)N1CC(C1)C=O	3{19}	[C-]#[N+]Cc1cccs1	62.2	56
33	4{58,26,7}	C(CC1=CC=CC=C1)C1=C(NC2CCOCC2)N2C=CC(OC3COC3)=CC2=N1 c:4,6,9,20,28,31,t:2	Z8776690336	1{58}	Ne1ccc(OC2COC2)ccn1	2{26}	O=CCCc1cccc1	3{7}	[C-]#[N+]C1CCOCC1	59.1	56
34	4{59,14,17}	CC1=CC=C(C=C1)C1=C(NCC2CCOCC2)N2C=C(CN3CCOCC3)C=CC2=N1 c:3,5,8,30,33,t:1,20	Z8776690335	1{59}	Ne1ccc(CN2CCOCC2)en1	2{14}	Cc1ccc(C=O)cc1	3{17}	[C-]#[N+]CC1CCOCC1	62.8	55
35	4{60,29,14}	CCN1C=CC(=N1)C1=C(NCCOC)N2C=C(OC)C=C(F)C2=N1 c:3,5,8,24,t:16,20	Z8780122035	1{60}	COe1enc(N)c(F)c1	2{29}	CCn1ccc(C=O)n1	3{14}	COCC[N+]#[C-]	49.7	55

36	4{38,15,14}	COCCNC1=C(N=C2C=C(C=CN12)C#N)C1=CC=C(OC)C=C1 c:9,11,24,t:5,7,18,20	Z8711876682	1{38}	Nc1cc(C#N)ccn1	2{15}	COc1ccc(C=O)cc1	3{14}	COCC[N+]#[C-]	48.1	55
37	4{61,26,7}	CCC1=CC=CC2=NC(CCC3=CC=CC=C3)=C(NC3CCOCC3)N12 c:4,13,15,t:2,6,11,17	Z8776690325	1{61}	CCc1cccc(N)n1	2{26}	O=CCCc1ccc1	3{7}	[C-]#[N+]C1CCOCC1	52.1	55
38	4{62,31,20}	COC1=CC(C)=C(NC2=C(N=C3C=C(CO)C=C(N23)C2=CN=CN2)C=C1 c:16,23,27,t:2,5,8,10,12,21	Z8810902966	1{62}	Nc1cc(CO)ccn1	2{31}	O=Cc1cnc[nH]1	3{20}	COc1ccc([N+]#[C-])c(C)c1	52.1	55
39	4{63,32,10}	COC1=C(C)C=CN2C(NC3CCOC3)=C(N=C12)[C@@H]1C[C@H]1C1=CC=NN1C &1:18,20,r,c:2,5,15,27,t:17,25	Z8810903003	1{63}	COc1c(C)ccnc1N	2{32}	Cn1cccc1[C@@H]2C[C@H]2C=O &1:6,8,r	3{10}	[C-]#[N+]C1CCOC1	54.6	55
40	4{62,15,13}	COC1=CC=C(CNC2=C(N=C3C=C(CO)C=CN23)C2=CC=C(OC)C=C2)C=C1 c:16,27,30,t:2,4,8,10,12,21,23	Z8776690332	1{62}	Nc1cc(CO)ccn1	2{15}	COc1ccc(C=O)cc1	3{13}	COc1ccc(C[N+]#[C-])cc1	57.9	55
41	4{37,33,10}	CC(=O)N1CCCC(C1)C1=C(NC2CCOC2)N2C(C=CC=C2C(F)F)=N1 c:10,21,23,28	Z8810903046	1{37}	Cl.Nc1cccc(n1)C(F)F	2{33}	CC(=O)N1C CCC(C1)C=O	3{10}	[C-]#[N+]C1CCOC1	56.2	55
42	4{64,14,17}	CC1=CC=C(C=C1)C1=C(NCC2CCOCC2)N2C=C(C=CC2=N1)N1CCCS1(=O)=O c:3,5,8,20,22,25,t:1	Z8776690346	1{64}	Nc1ccc(n1)N2CCCS2(=O)=O	2{14}	Cc1ccc(C=O)cc1	3{17}	[C-]#[N+]CC1C COCC1	65.3	55
43	4{53,34,21}	CP(C)(=O)C1=CC=C(C=C1)C1=C(NCC2CC2)N2C=C(CO)C=CC2=N1 c:6,8,11,24,27,t:4,20	Z8810902970	1{53}	Nc1ccc(CO)ccn1	2{34}	CP(=O)(C)c1ccc(C=O)cc1	3{21}	[C-]#[N+]CC1C C1	54.7	55
44	4{65,35,5}	CCC1=CN=CC2=NC(=C(NCCCOC)N12)C1=NN(C)C(C)=C1C1 c:4,24,t:2,6,8,19	Z8801681825	1{65}	CCc1cnc(N)n1	2{35}	Cc1c(Cl)c(C=O)nn1C	3{5}	COCCC[N+]#[C-]	53.7	55
45	4{66,36,22}	COCCC1=CC2=NC(=C(NC3COC3)N2C=C1)C1=NC(C)=C(OC(F)F)C=C1 c:18,30,t:4,6,8,21,24	Z8810902992	1{66}	COCCc1cnc(N)c1	2{36}	Cc1nc(C=O)ccc1OC(F)F	3{22}	[C-]#[N+]C1CO C1	59.8	55
46	4{67,15,9}	CNC1=C(N=C2C=CC=C(C)N12)C1=CC=C(OC)C=C1 c:6,20,t:2,4,8,14,16	Z8776690314	1{67}	Cc1cnc(N)n1	2{15}	COc1ccc(C=O)cc1	3{9}	C[N+]#[C-]	39.5	55
47	4{68,37,23}	COC(=O)CCC(NC1=C(N=C2C=C(C=CN12)C#C)C1=NC2=C(CCC2)C=C1)C(=O)OC c:12,14,29,t:8,10,21,23	Z8803896955	1{68}	Nc1cc(C#C)ccn1	2{37}	O=Cc1ccc2C CCc2n1	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	63.6	54
48	4{69,33,24}	CNC(=O)C1=CC2=NC(C3CCCN(C3)C(C)=O)=C(NCC3=CC(OC)=CC=C3)N2C=C1 c:26,28,33,t:4,6,18,22	Z8810903000	1{69}	CNC(=O)c1ccnc(N)c1	2{33}	CC(=O)N1C CCC(C1)C=O	3{24}	COc1cccc(C[N+]#[C-])c1	64.0	54

49	4{70,38,25}	FCCNCN1=C(N=C2N1C=CN=C2C1CC1)C1=NC(=CC=C1)C#C c:7,11,13,22,24,t:5,20	Z8781341774	1{70}	Nc1ncnc1 C2CC2	2{38}	O=Cc1cccc(C#C)n1	3{25}	FCCC[N+]#[C-]	49.2	54
50	4{71,14,17}	CC1=CC=C(C=C1)C1=C(NCC2CCOCC2)N2C=C(I)N=CC2=N1 c:3,5,8,23,26,t:1,20	Z8776690316	1{71}	Nc1nc(I)cn1	2{14}	Cc1ccc(C=O)cc1	3{17}	[C-]#[N+]CC1C COCC1	65.4	54
51	4{36,7,9}	CNC1=C(N=C2C=CC(Br)=CN12)C1=NC(C)=CC(CO)=C1 c:6,9,17,21,t:2,4,14	Z8798985029	1{36}	Nc1ccc(Br)cn1	2{7}	Cc1cc(CO)cc(C=O)n1	3{9}	C[N+]#[C-]	50.7	54
52	4{72,39,12}	COC1=NC(Br)=CN2C(NCC3CCOC3)=C(N=C12)C1=COC=C1 c:5,16,25,t:2,18,22	Z8798985022	1{72}	COc1nc(Br)cnc1N	2{39}	O=Cc1ccoc1	3{12}	[C-]#[N+]CC1C COC1	57.3	54
53	4{73,15,13}	COC1=CC=C(CNC2=C(N=C3C=CC4=NC=C4N23)C2=CC=C(OC)C=C2)C=C1 c:12,16,29,32,t:2,4,8,10,14,23,25	Z8741907043	1{73}	Nc1ccc2nccn2n1	2{15}	COc1ccc(C=O)cc1	3{13}	COc1ccc(C[N+]#[C-])cc1	58.2	54
54	4{74,40,17}	OCC1=CSC(=N1)C1=C(NCC2CCOCC2)N2C(C=CC=C2OC(F)F)=N1 c:5,8,21,23,29,t:2	Z8797782835	1{74}	Nc1cccc(O C(F)F)n1	2{40}	OCc1csc(C=O)n1	3{17}	[C-]#[N+]CC1C COCC1	59.8	54
55	4{75,41,7}	CC(C)(C)OC(=O)N1CCN(CC1)C1=CC=CN2C(NC3CCOCC3)=C(N=C12)C1=NC=CC=C1 c:16,27,35,37,t:14,29,33	Z8797783886	1{75}	CC(C)(C)O C(=O)N1C CN(CC1)c2 ccnc2N	2{41}	O=Cc1ccccn1	3{7}	[C-]#[N+]C1CC OCC1	69.4	54
56	4{76,42,23}	COC(=O)CCC(NC1=C(N=C2C=CC(C)=C(Cl)N12)C1=CN(C)N=C1Cl)C(=O)OC c:12,25,t:8,10,15,21	Z8810903037	1{76}	Cc1ccc(N)nc1Cl	2{42}	Cn1cc(C=O)c(Cl)n1	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	65.5	53
57	4{35,22,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC(C)=CN23)C2=CC=CC=C2)C=C1 c:12,15,22,24,27,t:2,5,8,10,20	Z8712568084	1{35}	Cc1ccc(N)nc1	2{22}	O=Cc1cccc1	3{20}	COc1ccc([N+]#[C-])c(C)c1	49.4	53
58	4{77,41,26}	FC1=CC=C(CNC2=C(N=C3C=CC(=CN23)C2=CN=CC=C2)C2=NC=CC=C2)C=C1 c:11,13,20,22,27,29,32,t:1,3,7,9,18,25	Z8778278038	1{77}	Nc1ccc(en1)c2cccnc2	2{41}	O=Cc1ccccn1	3{26}	Fc1ccc(C[N+]#[C-])cc1	56.9	53
59	4{42,9,27}	CCCCN1=C(N=C2C=CC(SC)=CN12)C1=CS C=C1 c:9,13,21,t:5,7,18	Z8784058856	1{42}	CSc1ccc(N)nc1	2{9}	O=Cc1ccsc1	3{27}	CCCC[N+]#[C-]	45.6	53
60	4{78,43,28}	CCCNC1=C(N=C2C=C(C)C3=NC(C)=CN3N12)C1=CN=C(C=C1)N1CCCCC1 c:14,23,25,t:4,6,8,11,21	Z8801681820	1{78}	Cc1cn2nc(N)cc(C)c2n1	2{43}	O=Cc1ccc(nc1)N2CCCCC2	3{28}	CCC[N+]#[C-]	57.9	53
61	4{79,22,27}	CCCCN1=C(N=C2C=NC=C(C)N12)C1=CC=CC=C1 c:9,19,21,t:5,7,11,17	Z8711872692	1{79}	Cc1nccc(N)n1	2{22}	O=Cc1cccc1	3{27}	CCCC[N+]#[C-]	40.0	53

62	4{80,22,7}	COC1=NC=CN2C(NC3CCOCC3)=C(N=C12)C1=CC=CC=C1 c:4,15,23,25,t:2,17,21	Z8778277285	1{80}	COe1ncnc1N	2{22}	O=Cc1cccc1	3{7}	[C-]#[N+]C1CCOCC1	46.3	53
63	4{81,14,27}	CCCCNC1=C(N=C2C=NC=CN12)C1=CC=C(C)C=C1 c:9,11,21,t:5,7,16,18	Z8700285862	1{81}	Nc1cncn1	2{14}	Cc1ccc(C=O)cc1	3{27}	CCCC[N+]#[C-]	40.0	53
64	4{82,44,7}	CCN1C=C(C=N1)C1=C(NC2CCOCC2)N2C(C=CC3=C2CCCC3)=N1 c:3,5,8,20,22,29	Z8778277692	1{82}	Nc1ccc2CCcC2n1	2{44}	CCn1cc(C=O)cn1	3{7}	[C-]#[N+]C1CCOCC1	52.1	53
65	4{83,45,18}	COC1=C(F)C=CC(=C1)C1=C(NC(C)(C)C)N2C=C(C=CC2=N1)P(C)(C)=O c:2,5,7,10,18,20,23	Z8810903025	1{83}	CP(=O)(C)c1ccc(N)nc1	2{45}	COc1cc(C=O)ccc1F	3{18}	CC(C)(C)[N+]#[C-]	55.5	53
66	4{84,46,7}	COCCCCC1=C(NC2CCOCC2)N2C=CN=C(C(C)C)C2=N1 c:7,18,26,t:20	Z8786958868	1{84}	CC(C)c1cncnc1N	2{46}	COCCCCC=O	3{7}	[C-]#[N+]C1CCOCC1	51.3	53
67	4{61,47,29}	CCOC(=O)CCNC1=C(CCOCC=C)N=C2C=C(C=C(CC)N12) c:8,18,t:16,20	Z8808559858	1{61}	CCc1cccc(N)n1	2{47}	C=CCOCCC=O	3{29}	CCOC(=O)C[C[N+]#[C-]	49.1	53
68	4{85,48,30}	CN1C=C(CNC2=C(N=C3C=C(C=C(C)N23)C#N)C2=CNC(=N2)C2CCC2)C=N1 c:10,23,31,t:2,6,8,12,20	Z8781341795	1{85}	Cc1cc(C#N)cc(N)n1	2{48}	O=Cc1c[nH]c(n1)C2CCC2	3{30}	Cn1cc(C[N+]#[C-])cn1	54.7	52
69	4{47,49,6}	CCOC(=O)CCNC1=C(N=C2C=C(C=CN12)S(N)(=O)=O)C1=CN=C1C c:13,15,27,t:9,11,24	Z8801681821	1{47}	Cl.Nc1cc(ccn1)S(=O)(=O)N	2{49}	Cc1n[nH]cc1C=O	3{6}	CCOC(=O)C[C[N+]#[C-]	57.4	52
70	4{86,50,31}	CSCCNC1=C(N=C2C=C(C(F)F)C(Cl)=CN12)[C@@H]1C[C@H]1C1OCCO1 &1:18,20,r,c:15,t:5,7,9	Z8801681826	1{86}	Nc1cc(C(F)F)c(Cl)cn1	2{50}	O=C[C@@H]1C[C@H]1C2OCCO2 &1:2,4,r	3{31}	CSCC[N+]#[C-]	57.0	52
71	4{87,26,7}	CC1=CC2=NC(CCC3=CC=CC=C3)=C(NC3COCC3)N2C=C1Cl c:10,12,26,t:1,3,8,14	Z8776690323	1{87}	Cc1cc(N)nc1Cl	2{26}	O=CCCc1ccccc1	3{7}	[C-]#[N+]C1CCOCC1	52.1	52
72	4{88,29,7}	CCN1C=CC(=N1)C1=C(NC2CCOCC2)N2C=CC(Br)=C(F)C2=N1 c:3,5,8,19,26,t:22	Z8797786849	1{88}	Nc1nccc(Br)c1F	2{29}	CCn1ccc(C=O)n1	3{7}	[C-]#[N+]C1CCOCC1	57.5	52
73	4{89,51,1}	CC1=C(C=NN1C1CCC1)C1=C(NC2CC2)N2C(C=CC3=C2NN=C3)=N1 c:3,12,21,23,27,29,t:1	Z8801681839	1{89}	Nc1ccc2cn[nH]c2n1	2{51}	Cc1c(C=O)cn1C2CCC2	3{1}	[C-]#[N+]C1CC1	48.9	52

74	4{90,52,15}	CCNC1=C(N=C2C=C(C=CN12)N1C=CC=N1)C1=CN(N=C1)C1CCC1 c:7,9,15,17,23,t:3,5,20	Z8781341788	1{90}	Nc1cc(cen1)n2cccn2	2{52}	O=Cc1enn(c1)C2CCC2	3{15}	CC[N+]#[C-]	48.8	52
75	4{91,53,18}	CC1=NC(C2=C(NC(C)(C)C)N3C=C(C=CC3=N2)C(N)=O)=C(F)C=C1 c:4,12,14,17,25,t:1,22	Z8798985039	1{91}	NC(=O)c1ccc(N)nc1	2{53}	Cc1ccc(F)c(C=O)n1	3{18}	CC(C)(C)[N+]#[C-]	48.0	52
76	4{92,54,32}	COC1=C(C=CS1)C1=C(NC2CCC2)N2C=CC(=CC2=N1)C(N)=O c:4,8,17,19,22,t:2	Z8808559893	1{92}	NC(=O)c1ccc(N)c1	2{54}	COc1secc1C=O	3{32}	[C-]#[N+]C1CC C1	48.0	52
77	4{92,41,17}	NC(=O)C1=CC2=NC(=C(NCC3CCOCC3)N2C=C1)C1=NC=CC=C1 c:20,25,27,t:3,5,7,23	Z8784059425	1{92}	NC(=O)c1ccc(N)c1	2{41}	O=Cc1ccccn1	3{17}	[C-]#[N+]CC1C COCC1	49.1	52
78	4{93,55,33}	COC1=CN2C(C=N1)=NC(=C2NCC1=C(OC)C=CC=C1)C1=CC(=NC=C1)P(C)(C)=O c:6,8,10,15,19,21,26,28,t:2,24	Z8798985018	1{93}	COc1cnc(N)c1	2{55}	CP(=O)(C)c1ccc(C=O)ccn1	3{33}	COc1cccc1C[N+]#[C-]	61.2	52
79	4{94,14,17}	CC1=CC=C(C=C1)C1=C(NCC2CCOCC2)N2N=C(F)C=CC2=N1 c:3,5,8,23,26,t:1,20	Z8776690309	1{94}	Nc1ccc(F)n1	2{14}	Cc1ccc(C=O)cc1	3{17}	[C-]#[N+]CC1C COCC1	47.4	52
80	4{76,56,23}	COC(=O)CCC(NC1=C(N=C2C=CC(C)=C(C1)N12)C1=C(C)C=NC(F)=C1)C(=O)OC c:12,21,24,27,t:8,10,15	Z8810903005	1{76}	Cc1ccc(N)nc1Cl	2{56}	Cc1cnc(F)cc1C=O	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	62.5	52
81	4{95,46,25}	COCCCCC1=C(NCCCF)N2C=C(C=CC2=N1)C(F)F c:7,15,17,20	Z8781341784	1{95}	Nc1ccc(en1)C(F)F	2{46}	COCCCCC=O	3{25}	FCCC[N+]#[C-]	47.8	52
82	4{96,14,17}	COCCN(C)CC1=CC2=NC(=C(NCC3CCOCC3)N2C=C1)C1=CC=C(C)C=C1 c:24,32,t:7,9,11,27,29	Z8776690343	1{96}	COCCN(C)Cc1cnc(N)c1	2{14}	Cc1ccc(C=O)cc1	3{17}	[C-]#[N+]CC1C COCC1	58.6	51
83	4{97,57,10}	CC1=CC(F)=CN2C(NC3CCOC3)=C(N=C12)C1CCOC1 c:4,14,t:1,16	Z8798985034	1{97}	Cc1cc(F)cn1	2{57}	O=CC1CCO C1	3{10}	[C-]#[N+]C1CC OC1	42.2	51
84	4{98,58,27}	CCCCNC1=C(N=C2C=CC=C(OC(F)(F)F)N12)C1=NSN=C1 c:9,24,t:5,7,11,21	Z8797783281	1{98}	Nc1cccc(O C(F)(F)F)n1	2{58}	O=Cc1ensn1	3{27}	CCCC[N+]#[C-]	49.3	51
85	4{99,59,34}	COC1=C(Br)C=C(C=N1)C1=C(NCC2CCCO2)N2C=C(C=CC2=N1)S(N)(=O)=O c:2,5,7,10,21,23,26	Z8808559882	1{99}	Nc1ccc(en1)S(=O)(=O)N	2{59}	COc1ncc(C=O)cc1Br	3{34}	[C-]#[N+]CC1C CCO1	66.6	51
86	4{100,29,14}	CCN1C=CC(=N1)C1=C(NCCOC)N2C(C=NC3=C2C=CC=C3)=N1 c:3,5,8,17,19,22,24,26	Z8778277663	1{100}	Nc1enc2ccc cc2n1	2{29}	CCn1ccc(C=O)n1	3{14}	COCC[N+]#[C-]	46.3	51

87	4{95,60,35}	CSCCCNC1=C(N=C2C=CC(=CN12)C(F)F)C(C)C1CCOC1 c:10,12,t:6,8	Z8810903012	1{95}	Nc1ccc(en1)C(F)F	2{60}	CC(C=O)C1CCOC1	3{35}	CSCCC[N+]#[C-]	50.5	51
88	4{70,61,32}	CS(=O)C1=CC=C(C=C1)C1=C(NC2CCC2)N2C=CN=C(C3CC3)C2=N1 c:5,7,10,19,28,t:3,21	Z8810903026	1{70}	Nc1ncnc1C2CC2	2{61}	CS(=O)c1ccc(C=O)cc1	3{32}	[C-]#[N+]C1CC1	49.9	50
89	4{81,14,17}	CC1=CC=C(C=C1)C1=C(NCC2CCOCC2)N2C=CN=CC2=N1 c:3,5,8,20,22,25,t:1	Z8781341793	1{81}	Nc1cncn1	2{14}	Cc1ccc(C=O)cc1	3{17}	[C-]#[N+]CC1C1COCC1	43.8	50
90	4{92,31,36}	COC(=O)[C@@H]1CC(CN1C(=O)OC(C)(C)C)NC1=C(N=C2C=C(C=CN12)C(N)=O)C1=CN=CN1 c:22,24,34,t:18,20,32	Z8798985053	1{92}	NC(=O)c1cnc(N)c1	2{31}	O=Cc1cnc[nH]1	3{36}	COC(=O)[C@@H]1C[C@@H](CN1C(=O)OC(C)(C)C)[N+]#[C-]	63.7	50
91	4{46,15,9}	CNC1=C(N=C2C=CC=CN12)C1=CC=C(OC)C=C1 c:6,8,19,t:2,4,13,15	Z8776690321	1{46}	Nc1cccen1	2{15}	COc1ccc(C=O)cc1	3{9}	C[N+]#[C-]	34.4	50
92	4{101,62,14}	COCCNC1=C(N=C2N1C=C(CO)C=C2C1)C1C11CCOCC1 c:7,15,t:5,11	Z8810902961	1{101}	Nc1ncc(CO)cc1Cl	2{62}	O=CC1CC21CCOCC2	3{14}	COCC[N+]#[C-]	49.6	50
93	4{102,63,37}	COCN1N=CC=C1C1=C(NC2CC(C2)C(=O)OC)N2C=CC(=CC2=N1)C(=O)N(C)C c:4,6,9,22,24,27	Z8781341782	1{102}	CN(C)C(=O)c1cnc(N)c1	2{63}	COCn1ccc1C=O	3{37}	COC(=O)C1CC(C1)[N+]#[C-]	57.8	50
94	4{46,22,14}	COCCNC1=C(N=C2C=CC=CN12)C1=CC=C(C=C1) c:9,11,18,20,t:5,7,16	Z8711876379	1{46}	Nc1cccen1	2{22}	O=Cc1cccc1	3{14}	COCC[N+]#[C-]	36.2	50
95	4{50,64,26}	CP(C)(=O)C1=CC=CC2=NC(=C(NCC3=CC=C(F)C=C3)N12)C1=CC=C(C=C1)N1C=CN=C1 c:6,19,27,29,33,35,t:4,8,10,14,16,25	Z8810902997	1{50}	CP(=O)(C)c1cccc(N)n1	2{64}	O=Cc1ccc(cc1)n2ccnc2	3{26}	Fe1ccc(C[N+]#[C-])cc1	62.0	50
96	4{103,65,38}	CC(C)(C)OC(=O)NC1CC2(C1)CC(C2)C1=C(NC2=CC3=C(OCO3)C=C2)N2C(C=NC=C2CO)=N1 c:17,28,33,35,39,t:20,22	Z8803896970	1{103}	Nc1cnc(CO)n1	2{65}	CC(C)(C)OC(=O)NC1CC2(C1)CC(C2)C=O	3{38}	[C-]#[N+]c1ccc2OCOc2c1	66.4	50
97	4{104,66,39}	CCOCCNC1=C(N=C2C=CC3=C(COCC3)N12)C1=C(C)N(CC)N=C1C c:10,22,28,t:6,8,12	Z8810903028	1{104}	Nc1ccc2CCOCc2n1	2{66}	CCn1nc(C)c(C=O)c1C	3{39}	CCOCC[N+]#[C-]	51.6	50
98	4{103,67,40}	CCOC(=O)C1=CC=C(NC2=C(N=C3C=NC=C(CO)N23)C2CCCSC2)C=C1 c:14,30,t:5,7,10,12,16	Z8798985062	1{103}	Nc1cnc(CO)n1	2{67}	O=CC1CCCSC1	3{40}	CCOC(=O)c1ccc([N+]#[C-])cc1	55.5	50

99	4{105,68,41}	COC1=CC=C(NC2=C(N=C3C=CC=C(N23)C(N)=O)C2=NC=C(S2)C(C)O)C=C1 c:11,13,23,30,t:2,4,7,9,21	Z8810902972	1{105}	NC(=O)c1c ccc(N)n1	2{68}	CC(O)c1enc(C=O)s1	3{41}	COc1ccc([N +]#[C-])cc1	54.5	49
100	4{36,40,13}	COC1=CC=C(CNC2=C(N=C3C=CC(Br)=CN2 3)C2=NC(CO)=CS2)C=C1 c:12,15,24,28,t:2,4,8,10,20	Z8808559864	1{36}	Nc1ccc(Br) cn1	2{40}	OCc1esc(C= O)n1	3{13}	COc1ccc(C[N+]#[C-])cc1	59.3	49
101	4{47,69,6}	CCOC(=O)CCNC1=C(N=C2C=C(C=CN12)S (N)(=O)=O)C1=NN(C)C(C)=C1 c:13,15,29,t:9,11,24	Z8808559899	1{47}	Cl.Nc1cc(cc n1)S(=O)(= O)N	2{69}	Cc1cc(C=O) mn1C	3{6}	CCOC(=O)C CC[N+]#[C-]	55.9	49
102	4{45,70,12}	CC(F)(F)C1=NC(=CS1)C1=C(NCC2CCOC2) N2C=CC(F)=CC2=N1 c:6,10,21,24,27,t:4	Z8801681810	1{45}	Cl.Nc1cc(F) ccn1	2{70}	CC(F)(F)c1n c(C=O)cs1	3{12}	[C-]#[N+]CC1C COC1	50.8	49
103	4{106,15,13}	COC1=CC=C(CNC2=C(N=C3C=CC(OC)=NN 23)C2=CC=C(OC)C=C2)C=C1 c:12,16,27,30,t:2,4,8,10,21,23	Z8776690338	1{106}	COc1ccc(N) nn1	2{15}	COc1ccc(C= O)cc1	3{13}	COc1ccc(C[N+]#[C-])cc1	51.9	49
104	4{59,71,42}	CN1C=C(C=N1)[C@@H]1OCC[C@H]1C1=C (NC2=C(C)C=CC=C2)N2C=C(CN3CCOCC3) C=CC2=N1 &1:6,10,r;c:2,4,13,16,19,21,35,38,t:25	Z8810903017	1{59}	Nc1ccc(CN 2CCOCC2) cn1	2{71}	Cn1cc(cn1)[C@@H]2OC C[C@H]2C= O &1:6,10,r	3{42}	Cc1ccccc1[N +]#[C-]	62.6	49
105	4{104,72,39}	CCOCCNC1=C(C[C@@H](C)NC(=O)OCC2= CC=CC=C2)N=C2C=CC3=C(COCC3)N12 c:6,18,20,25,t:16,23,27	Z8808559855	1{104}	Nc1ccc2CC OCc2n1	2{72}	C[C@H](CC =O)NC(=O) OCc1ccccc1	3{39}	CCOCC[N+] #[C-]	59.9	49
106	4{107,16,10}	CN1N=CC(CNC(=O)OC(C)(C)C)=C1C1=C(N C2CCOC2)N2C=C(OCCO)C=CC2=N1 c:2,13,16,32,35,t:26	Z8808559898	1{107}	Nc1ccc(OC CO)cn1	2{16}	Cn1ncc(CNC (=O)OC(C)(C)C)c1C=O	3{10}	[C-]#[N+]C1CC OC1	62.6	49
107	4{108,73,12}	CCCOC1=CN2C(NCC3CCOC3)=C(N=C2C=C 1)C1=C(C)C=NN1C c:15,17,20,23,26,t:4	Z8810902969	1{108}	CCCOc1ccc (N)nc1	2{73}	Cc1cnn(C)c1 C=O	3{12}	[C-]#[N+]CC1C COC1	48.8	49
108	4{109,74,41}	COC1=CC=C(NC2=C(N=C3C=CC=C(N23)S(N)(=O)=O)C2=C(CI)N(C)C=N2)C=C1 c:11,13,22,27,30,t:2,4,7,9	Z8810902958	1{109}	Cl.Nc1cccc (n1)S(=O)(= O)N	2{74}	Cn1enc(C=O)c1Cl	3{41}	COc1ccc([N +]#[C-])cc1	57.1	49
109	4{67,26,27}	CCCCNC1=C(CCC2=CC=CC=C2)N=C2C=C C=C(C)N12 c:5,11,13,18,t:9,16,20	Z8711876474	1{67}	Cc1ccccc(N) n1	2{26}	O=CCCc1cc ccc1	3{27}	CCCC[N+]#[C-]	40.6	49

110	4{110,44,7}	CCN1C=C(C=N1)C1=C(NC2CCOCC2)N2C=C(C(C)=CC2=N1)S(N)(=O)=O c:3,5,8,19,22,25	Z8780122393	1{110}	Cc1cc(N)nc1S(=O)(=O)N	2{44}	CCn1cc(C=O)cn1	3{7}	[C-]#[N+]C1CCOCC1	53.3	49
111	4{22,26,16}	CC1=CC=CC(C)=C1NC1=C(CCC2=CC=CC=C2)N=C2C=CC(CI)=NN12 c:3,6,10,16,18,23,26,t:1,14,21	Z8741907012	1{22}	Nc1ccc(Cl)nn1	2{26}	O=CCCc1ccc1	3{16}	Cc1cccc(C)c1[N+]#[C-]	49.6	49
112	4{36,15,11}	COC1=CC=C(C=C1)C1=C(NCC2=CC(Br)=C=C2)N2C=C(Br)C=CC2=N1 c:4,6,9,16,18,25,28,t:2,13,22	Z8712552581	1{36}	Nc1ccc(Br)cn1	2{15}	COc1ccc(C=O)cc1	3{11}	Br1cccc(C[N+]#[C-])c1	63.4	48
113	4{53,75,33}	COCC1=CC=C(O1)C1=C(NCC2=C(OC)C=CC=C2)N2C=C(CO)C=CC2=N1 c:5,9,13,17,19,27,30,t:3,23	Z8803896929	1{53}	Nc1ccc(CO)cn1	2{75}	COc1ccc(C=O)o1	3{33}	COc1cccc1C[N+]#[C-]	51.2	48
114	4{50,76,26}	CCC1=NN(C)C=C1)C1=C(NCC2=CC=C(F)C=C2)N2C(C=CC=C2P(C)(C)=O)=N1 c:6,9,18,23,25,31,t:2,13,15	Z8803896928	1{50}	CP(=O)(C)c1cccc(N)n1	2{76}	CCc1cc(C=O)n(C)n1	3{26}	Fc1ccc(C[N+]#[C-])cc1	55.3	48
115	4{111,18,43}	COC(=O)C1=CN2C(NC3CCN(CC3)C(=O)OC(C)(C)C)=C(N=C2C(C)=C1)C1=CN(CCO)N=C1 c:22,24,28,37,t:4,31	Z8786958933	1{111}	COC(=O)c1cnc(N)c(C)c1	2{18}	OCCn1cc(C=O)cn1	3{43}	CC(C)(C)OC(=O)N1CCCC(C1)[N+]#[C-]	64.7	48
116	4{112,77,10}	COC1=CN=CC2=NC(CC3CCCC3)=C(NC3CCOC3)N12 c:4,t:2,6,15	Z8781341791	1{112}	COc1cnc(N)n1	2{77}	O=CCC1CC1	3{10}	[C-]#[N+]C1CCOC1	40.6	48
117	4{113,78,14}	COCCNC1=C(N=C2N1C=CC=C2N1CCOCC1)C1COC(C)C1 c:7,11,13,t:5	Z8810903019	1{113}	Nc1ncccc1N2CCOCC2	2{78}	CC1CC(CO1)C=O	3{14}	COCC[N+]#[C-]	46.3	48
118	4{114,40,7}	COCC1=CC2=NC(=C(NC3CCOCC3)N2C=C1)C1=NC(CO)=CS1 c:19,26,t:3,5,7,22	Z8786958883	1{114}	COc1ccnc(N)c1	2{40}	OCc1csc(C=O)n1	3{7}	[C-]#[N+]C1CCOCC1	48.0	48
119	4{46,7,9}	CNC1=C(N=C2C=CC=CN12)C1=NC(C)=CC(CO)=C1 c:6,8,16,20,t:2,4,13	Z8803896924	1{46}	Nc1cccnc1	2{7}	Cc1cc(CO)cc(C=O)n1	3{9}	C[N+]#[C-]	34.4	47
120	4{62,15,27}	CCCCNC1=C(N=C2C=C(CO)C=CN12)C1=C(C=C(OC)C=C1) c:13,24,t:5,7,9,18,20	Z8741907001	1{62}	Nc1cc(CO)cn1	2{15}	COc1ccc(C=O)cc1	3{27}	CCCC[N+]#[C-]	41.5	47
121	4{44,79,13}	CCC1=CN2C(NCC3=CC=C(OC)C=C3)=C(N=C2C=N1)C1=NC=CO1 c:14,16,18,21,26,t:2,8,10,24	Z8803896965	1{44}	CCc1cnc(N)cn1	2{79}	O=Cc1ncco1	3{13}	COc1ccc(C[N+]#[C-])cc1	44.4	47
122	4{115,26,26}	OCC1=CN2C(C=N1)=NC(CCC1=CC=CC=C1)=C2NCC1=CC=C(F)C=C1 c:6,8,15,17,19,29,t:2,13,24,26	Z8776690347	1{115}	Nc1cnc(CO)cn1	2{26}	O=CCCc1ccc1	3{26}	Fc1ccc(C[N+]#[C-])cc1	47.8	47

123	4{116,15,9}	CNC1=C(N=C2C=CC(C)=C(C#N)N12)C1=CC=C(OC)C=C1 c:6,22,t:2,4,9,16,18	Z8776690312	1{116}	Cc1ccc(N)nc1C#N	2{15}	COc1ccc(C=O)cc1	3{9}	C[N+]#[C-]	36.9	47
124	4{117,80,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC=C(N23)C2(CCC2)C(F)(F)F)C2=NC=C(C)S2)C=C1 c:12,14,35,t:2,5,8,10,28,30	Z8797785072	1{117}	Nc1cccc(n1)C2(CCC2)C(F)(F)F	2{80}	Cc1cnc(C=O)s1	3{20}	COc1ccc([N+]#[C-])c(C)c1	58.8	46
125	4{34,81,23}	COC(=O)CCC(NC1=C(N=C2C=C(C=CN12)C1=NNC(C)=N1)C1=NC(=CC=C1)C(F)F)C(=O)OC c:12,14,23,28,30,t:8,10,19,26	Z8810902953	1{34}	Cc1nc(n[nH]1)c2ccnc(N)c2	2{81}	FC(F)c1cccc(C=O)n1	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	62.1	46
126	4{118,82,32}	COC1=C(C=CC=C1F)C1=C(NC2CCC2)N2C(C=CC=C2C(C)O)=N1 c:4,6,10,20,22,27,t:2	Z8801681833	1{118}	Cl.CC(O)c1cccc(N)n1	2{82}	COc1c(F)ccc1C=O	3{32}	[C-]#[N+]C1CC C1	44.2	46
127	4{119,14,17}	CC1=CC=C(C=C1)C1=C(NCC2CCOCC2)N2C=C(C=CC2=N1)C#N c:3,5,8,20,22,25,t:1	Z8776690318	1{119}	Nc1ccc(C#N)cn1	2{14}	Cc1ccc(C=O)cc1	3{17}	[C-]#[N+]CC1C COCC1	43.0	46
128	4{120,83,5}	COCCCN1=C(N=C2C=C(C=CN12)C1=CN(C)N=C1)C1=CC(=CC=C1)S(N)(=O)=O c:10,12,21,26,28,t:6,8,17,24	Z8798985044	1{120}	Cn1cc(cn1)c2ccnc(N)c2	2{83}	NS(=O)(=O)c1cccc(C=O)c1	3{5}	COCCC[N+]#[C-]	54.4	46
129	4{65,84,7}	CCC1=CN=CC2=NC(CCSC)=C(NC3CCOCC3)N12 c:4,t:2,6,12	Z8778278039	1{65}	CCc1cnc(N)n1	2{84}	CSCCC=O	3{7}	[C-]#[N+]C1CC OCC1	39.0	45
130	4{104,85,44}	CC(C)(C)OC(=O)NCCCCN1=C(N=C2C=CC3=C(COCC3)N12)C1=CN=NS1 c:17,31,t:13,15,19,29	Z8810903041	1{104}	Nc1ccc2CCOCc2n1	2{85}	O=Cc1cnns1	3{44}	CC(C)(C)OC(=O)NCCCC [N+]#[C-]	53.8	45
131	4{121,39,10}	BrC1=CC2=NC(C3=COC=C3)=C(NC3CCOC3)N2C=C1 c:9,22,t:1,3,6,11	Z8808559862	1{121}	Nc1cc(Br)cn1	2{39}	O=Cc1ccoc1	3{10}	[C-]#[N+]C1CC OC1	42.0	45
132	4{81,46,13}	COCCCCC1=C(NCC2=CC=C(OC)C=C2)N2C=CN=CC2=N1 c:7,17,21,23,26,t:11,13	Z8808559867	1{81}	Nc1cncn1	2{46}	COCCCCC=O	3{13}	COc1ccc(C[N+]#[C-])cc1	42.4	44
133	4{122,10,7}	CC(=O)NC1=CC=CN2C(NC3CCOCC3)=C(N=C12)C1=NC=CC(C)=C1 c:6,17,25,28,t:4,19,23	Z8784059625	1{122}	Cl.CC(=O)Nc1ccnc1N	2{10}	Cc1cnc(C=O)c1	3{7}	[C-]#[N+]C1CC OCC1	43.7	44
134	4{32,86,35}	CSCCCN1=C(N=C2C=C(C=CN12)P(C)(C)=O)C1CCN(C(=O)OC(C)(C)C)C1(C)C c:10,12,t:6,8	Z8803896948	1{32}	CP(=O)(C)c1ccnc(N)c1	2{86}	CC(C)(C)OC(=O)N1CCC(C=O)C1(C)C	3{35}	CSCCC[N+]#[C-]	59.1	44

135	4{123,87,22}	CC(C)(C)OC(=O)[C@@H]1C[C@H]1C1=C(NC2OC2)N2C=CC(OCCO)=CC2=N1 &1:7,9,r,c:11,20,26,29	Z8810903001	1{123}	Cl.Nc1cc(OCCO)ccn1	2{87}	CC(C)(C)OC(=O)[C@@H]1C[C@H]1C=O &1:7,9,r	3{22}	[C-]#[N+]C1CO C1	46.5	44
136	4{38,19,9}	CNC1=C(N=C2C=C(C=CN12)C#N)C1=C(OC)C=NN1C c:6,8,15,19,t:2,4	Z8801681823	1{38}	Nc1cc(C#N)ccn1	2{19}	COc1cnn(C)c1C=O	3{9}	C[N+]#[C-]	33.7	44
137	4{73,88,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC4=NC=CN4N23)C2=CC3=C(C=CC=N3)C=C2)C=C1 c:12,16,27,29,32,35,t:2,5,8,10,14,23,25	Z8810903009	1{73}	Nc1ccc2nccn2n1	2{88}	O=Cc1ccc2ccnc2c1	3{20}	COc1ccc([N+]#[C-])c(C)c1	49.7	44
138	4{70,89,35}	CCC1=NC=C(C=N1)C1=C(NCCCC)N2C=C(N=C(C3CC3)C2=N1 c:4,6,9,18,27,t:2,20	Z8798985038	1{70}	Nc1cncnc1C2CC2	2{89}	CCc1ncc(C=O)cn1	3{35}	CSCCC[N+]#[C-]	43.3	43
139	4{109,90,41}	COC1=CC=C(NC2=C(N=C3C=CC=C(N23)S(N)(=O)=O)C2=COC(C)=N2)C=C1 c:11,13,26,29,t:2,4,7,9,22	Z8808559860	1{109}	Cl.Nc1cccc(n1)S(=O)(=O)N	2{90}	Cc1nc(C=O)co1	3{41}	COc1ccc([N+]#[C-])cc1	46.6	43
140	4{124,91,14}	COCCNC1=C(N=C2N1C=CC=C2CO)C1=CC2=C(OCCC2)C=C1 c:7,11,13,27,t:5,18,20	Z8778278032	1{124}	Nc1ncccc1CO	2{91}	O=Cc1ccc2OCCCc2c1	3{14}	COCC[N+]#[C-]	41.0	43
141	4{50,92,7}	CC1=NOC(=C1)C1=C(NC2CCOCC2)N2C(C=CC=C2P(C)(C)=O)=N1 c:4,7,19,21,27,t:1	Z8810903002	1{50}	CP(=O)(C)c1cccc(N)n1	2{92}	Cc1cc(C=O)on1	3{7}	[C-]#[N+]C1CCOCC1	43.4	43
142	4{54,93,3}	CN(C)C(=O)C1=CN2C(C=C1)=NC(=C2NC1=C(F)C=C(Cl)C=C1)C1=NC(CO)=CC=C1 c:9,11,13,17,23,30,32,t:5,20,26	Z8798985024	1{54}	Cl.CN(C)C(=O)c1ccc(N)nc1	2{93}	OCc1cccc(C=O)n1	3{3}	Fc1cc(Cl)ccc1[N+]#[C-]	50.9	43
143	4{125,50,26}	OCCC1=CN2C(C=C1)=NC([C@@H]1C[C@H]1C1OCCO1)=C2NCC1=CC=C(F)C=C1 &1:11,13,r,c:7,9,21,31,t:3,26,28	Z8803896967	1{125}	Nc1ccc(CC(O)cn1	2{50}	O=C[C@@H]1C[C@H]1C2OCCO2 &1:2,4,r	3{26}	Fc1ccc(C[N+]#[C-])cc1	46.0	43
144	4{126,94,45}	COC1=C(F)N2C(NCC=C)=C(N=C2C=C1)C1=NC=CN=C1 c:2,10,12,15,20,22,t:18	Z8781341797	1{126}	COc1ccc(N)nc1F	2{94}	O=Cc1cncn1	3{45}	C=CC[N+]#[C-]	34.6	43
145	4{127,9,27}	CCCCNC1=C(N=C2N1C=CC=C2F)C1=CSC=C1 c:7,11,13,20,t:5,17	Z8780121542	1{127}	Nc1ncccc1F	2{9}	O=Cc1ccsc1	3{27}	CCCC[N+]#[C-]	33.0	42
146	4{67,95,9}	CNC1=C(N=C2C=CC=C(C)N12)C1=CC(=NC=C1)N(C)C c:6,16,18,t:2,4,8,14	Z8810903035	1{67}	Cc1cccc(N)n1	2{95}	CN(C)c1cc(C=O)ccn1	3{9}	C[N+]#[C-]	32.1	42

147	4{128,26,7}	COCCN(C)C1=CN2C(C=C1)=NC(CCC1=CC=CC=C1)=C2NC1CCOCC1 c:10,12,19,21,23,t:6,17	Z8776690315	1{128}	COCCN(C) c1ccc(N)nc 1	2{26}	O=CCCc1cc ccc1	3{7}	[C-] #[N+]C1CC OCC1	46.5	42
148	4{50,96,26}	CP(C)(=O)C1=CC=CC2=NC(C3=CC(=NO3)C3=CC=CC=C3)=C(NCC3=CC=C(F)C=C3)N12 c:6,13,19,21,32,t:4,8,11,17,23,27,29	Z8810902990	1{50}	CP(=O)(C)c 1cccc(N)n1	2{96}	O=Cc1cc(no 1)c2ccccc2	3{26}	Fc1ccc(C[N+] #[C-])cc1	52.0	42
149	4{40,25,22}	CC1=CC(=CC2=NC(=C(NC3COCC3)N12)C1=CN=C(N=C1)C1CCOCC1)C(F)(F)F c:3,20,22,t:1,5,7,18	Z8786958875	1{40}	Cc1cc(cc(N) n1)C(F)(F) F	2{25}	O=Cc1ene(n c1)C2CCOC C2	3{22}	[C-] #[N+]C1CO C1	48.9	42
150	4{129,97,17}	CSC1=CC=CC2=NC(=C(NCC3CCOCC3)N12)C1=CC=C(F)C=C1 c:4,27,t:2,6,8,22,24	Z8797781065	1{129}	CSc1cccc(N) n1	2{97}	Fc1ccc(C=O) cc1	3{17}	[C-] #[N+]CC1C COCC1	41.7	42
151	4{130,77,27}	CCCCNC1=C(CC2CCCC2)N=C2N1C=C(F)C=C2C1 c:5,14,21,t:18	Z8780121734	1{130}	Nc1ncc(F)c c1Cl	2{77}	O=CCC1CC CC1	3{27}	CCCC[N+]# C-]	35.9	41
152	4{131,26,7}	C(CC1=CC=CC=C1)C1=C(NC2CCOCC2)N2N=C(C=CC2=N1)C1=CC=CC=C1 c:4,6,9,20,22,25,30,32,t:2,28	Z8776690317	1{131}	Nc1ccc(nn1) c2ccccc2	2{26}	O=CCCc1cc ccc1	3{7}	[C-] #[N+]C1CC OCC1	44.1	41
153	4{76,26,7}	CC1=C(Cl)N2C(C=C1)=NC(CCC1=CC=CC=C1)=C2NC1CCOCC1 c:1,6,8,15,17,19,t:13	Z8776690313	1{76}	Cc1ccc(N)n c1Cl	2{26}	O=CCCc1cc ccc1	3{7}	[C-] #[N+]C1CC OCC1	40.4	40
154	4{132,15,13}	CNS(=O)(=O)C1=CC2=NC(=C(NCC3=CC=C(OC)C=C3)N2C=C1)C1=CC=C(OC)C=C1 c:19,24,33,t:5,7,9,13,15,27,29	Z8776690328	1{132}	Cl.NNS(=O) (=O)c1ccnc(N)c1	2{15}	COc1ccc(C= O)cc1	3{13}	COc1ccc(C[N+]#[C-])cc1	49.4	40
155	4{91,94,6}	CCOC(=O)CCCN1=C(N=C2C=CC(=CN12)C(N)=O)C1=NC=CN=C1 c:13,15,25,27,t:9,11,23	Z8784059427	1{91}	NC(=O)c1c cc(N)nc1	2{94}	O=Cc1cncn 1	3{6}	CCOC(=O)C CC[N+]#[C-]	40.2	40
156	4{133,41,14}	COCCNC1=C(N=C2N1C=C(F)C=C2Br)C1=NC=CC=C1 c:7,14,20,22,t:5,11,18	Z8786838536	1{133}	Nc1ncc(F)c c1Br	2{41}	O=Cc1cccc 1	3{14}	COCC[N+]# C-]	39.6	40
157	4{134,77,27}	CCCCNC1=C(CC2CCCC2)N=C2N1C=CC=C2OC1CCOCC1 c:5,14,18,20	Z8778277289	1{134}	Nc1ncccc1 OC2CCOC C2	2{77}	O=CCC1CC CC1	3{27}	CCCC[N+]# C-]	40.0	40
158	4{124,98,46}	COC1=NC=C(N=C1)C1=C(NCC(C)=C)N2C=CC=C(CO)C2=N1 c:4,6,9,17,24,t:2,19	Z8781341794	1{124}	Nc1ncccc1 CO	2{98}	COc1cnc(C= O)cn1	3{46}	CC(=C)C[N+] #[C-]	35.0	40
159	4{135,99,35}	CCCC1=NC=CN2C(NCCCSC)=C(N=C12)C1=COC=N1 c:5,14,23,t:3,16,20	Z8803896937	1{135}	CCCc1cnc c1N	2{99}	O=Cc1coen 1	3{35}	CSCCC[N+] #[C-]	35.6	40
160	4{35,15,9}	CNC1=C(N=C2C=CC(C)=CN12)C1=CC=C(OC)C=C1 c:6,9,20,t:2,4,14,16	Z8712537091	1{35}	Cc1ccc(N)n c1	2{15}	COc1ccc(C= O)cc1	3{9}	C[N+]#[C-]	28.7	40

161	4{96,100,47}	CCN1C=C(C=N1)[C@@H]1OCC[C@H]1C1=C(NC(C)C)N2C=CC(CN(C)CCOC)=CC2=N1 &1:7,11,r,c:3,5,14,21,30,33	Z8801681818	1{96}	COCCN(C)Cclccnc(N)c1	2{100}	CCn1cc(cn1)[C@@H]2OCC[C@H]2C=O &1:7,11,r	3{47}	CC(C)[N+]#[C-]	47.3	40
162	4{36,26,7}	BrC1=CN2C(C=C1)=NC(CCC1=CC=CC=C1)=C2NC1CCOCC1 c:5,7,14,16,18,t:1,12	Z8712587521	1{36}	Nc1ccc(Br)cn1	2{26}	O=CCCc1ccc1	3{7}	[C-]#[N+]C1CCOCC1	42.6	39
163	4{136,101,14}	COCCNC1=C(N=C2N1C=C(C)C=C2Br)C1=C(CO)C=CS1 c:7,14,18,22,t:5,11	Z8810903027	1{136}	Cc1cnc(N)c(Br)c1	2{101}	OCc1ccsc1C=O	3{14}	COCC[N+]#[C-]	41.9	39
164	4{137,15,17}	COC1=CC=C(C=C1)C1=C(NCC2CCOCC2)N2N=C(C)C=CC2=N1 c:4,6,9,24,27,t:2,21	Z8741907028	1{137}	Cc1ccc(N)cn1	2{15}	COc1ccc(C=O)cc1	3{17}	[C-]#[N+]CC1C COCC1	37.2	39
165	4{32,102,31}	CSCCNC1=C(N=C2C=C(C=CN12)P(C)(C)=O)C1=C(Br)C(C)=CC(Cl)=N1 c:9,11,20,24,27,t:5,7	Z8801681845	1{32}	CP(=O)(C)c1ccnc(N)c1	2{102}	Cc1cc(Cl)nc(C=O)c1Br	3{31}	CSCC[N+]#[C-]	51.2	39
166	4{138,103,48}	CC(C)(C)OC(=O)N1CCCC(C1)NC1=C(N=C2C=CC=C(F)N12)C1CCC2(COC2)OC1 c:19,t:15,17,21	Z8798985030	1{138}	Nc1cccc(F)n1	2{103}	O=CC1CCC2(COC2)OC1	3{48}	CC(C)(C)OC(=O)N1CCCC(C1)[N+]#[C-]	48.4	39
167	4{139,104,24}	COC1=CC(CNC2=C(N=C3C=C(C=CN23)C(F)F)C2=NC(C)=CO2)=CC=C1 c:11,13,24,27,29,t:2,7,9,21	Z8810902993	1{139}	Nc1cc(cen1)C(F)F	2{104}	Cc1coc(C=O)n1	3{24}	COc1cccc(C[N+]#[C-])c1	40.0	39
168	4{109,105,34}	CN1N=NC2=C1C(=CC=C2)C1=C(NCC2CCC(O2)N2C(C=CC=C2S(N)(=O)=O)=N1 c:2,4,7,9,12,24,26,32	Z8803896953	1{109}	Cl.Nc1cccc(n1)S(=O)(=O)N	2{105}	Cn1nc2cccc(C=O)c12	3{34}	[C-]#[N+]CC1C CCO1	44.4	38
169	4{140,106,49}	COC1=C(N=CC=N1)C1=C(NC2CC(F)(F)C2)N2C(C=NC(I)=C2Cl)=N1 c:4,6,9,21,24,27,t:2	Z8781341776	1{140}	Nc1cnc(I)c(Cl)n1	2{106}	COc1cncnc1C=O	3{49}	FC1(F)CC(C1)[N+]#[C-]	50.9	38
170	4{36,26,16}	CC1=CC=CC(C)=C1NC1=C(CCC2=CC=CC=C2)N=C2C=CC(Br)=CN12 c:3,6,10,16,18,23,26,t:1,14,21	Z8712537093	1{36}	Nc1ccc(Br)cn1	2{26}	O=CCCc1ccc1	3{16}	Cc1cccc(C)c1[N+]#[C-]	43.5	38
171	4{125,107,31}	CSCCNC1=C(N=C2C=CC(CCO)=CN12)C1=NC(C)=CS1 c:9,14,22,t:5,7,19	Z8810902950	1{125}	Nc1ccc(CC(O)cn1)	2{107}	Cc1csc(C=O)n1	3{31}	CSCC[N+]#[C-]	36.0	38
172	4{80,108,23}	COC(=O)CCC(NC1=C(N=C2N1C=CN=C2OC)C1=CN=C(N=C1)N1CCOCC1)C(=O)OC c:10,14,16,23,25,t:8,21	Z8801681842	1{80}	COc1cncnc1N	2{108}	O=Cc1cnc(nc1)N2CCOCC2	3{23}	COC(=O)CC(C[N+]#[C-])C(=O)OC	49.5	38

173	4{81,26,13}	COC1=CC=C(CNC2=C(CCC3=CC=CC=C3)N=C3C=NC=CN23)C=C1 c:8,14,16,21,23,28,t:2,4,12,19	Z8712562312	1{81}	Ne1cncen1	2{26}	O=CCCc1ccc1	3{13}	COc1ccc(C[N+]#[C-])cc1	36.5	38
174	4{141,109,32}	CN1C=C(C)C(=N1)C1=C(NC2CCC2)N2C=C(C(NC(C)=O)=CC2=N1 c:5,8,17,23,26,t:2	Z8786958863	1{141}	CC(=O)Nc1ccnc(N)c1	2{109}	Cc1cn(C)nc1C=O	3{32}	[C-]#[N+]C1CC C1	34.4	38
175	4{109,110,50}	CP(C)(=O)C1=NC=C(C=C1)C1=C(NC2=CC3=C(OCCO3)C=C2)N2C(C=CC=C2S(N)(=O)=O)=N1 c:6,8,11,23,28,30,36,t:4,14,16	Z8803896963	1{109}	Cl.Nc1cccc(n1)S(=O)(=O)N	2{110}	CP(=O)(C)c1ccc(C=O)cn1	3{50}	[C-]#[N+]c1ccc2OCCOc2e1	50.5	37
176	4{48,93,35}	CSCCNC1=C(N=C2C=C(C=CN12)S(C)(=O)=O)C1=NC(CO)=CC=C1 c:10,12,25,27,t:6,8,21	Z8801681824	1{48}	CS(=O)(=O)c1ccnc(N)c1	2{93}	OCc1cccc(C=O)n1	3{35}	CSCCC[N+]#[C-]	41.1	37
177	4{142,111,51}	CC(C)(C)OC(=O)NCCNC1=C(N=C2N1C=CC=C2OCCS(C)(=O)=O)C1CCCC1 c:13,17,19,t:11	Z8808559876	1{142}	CS(=O)(=O)CCOc1ccnc1N	2{111}	O=CC1CCC C1	3{51}	CC(C)(C)OC(=O)NCC[N+]#[C-]	47.2	37
178	4{83,112,52}	CP(C)(=O)C1=CN2C(C=C1)=NC(=C2NCCOC C1CC1)C1=C2C=CC=NN2N=C1 c:8,10,12,24,26,28,32,t:4	Z8786958945	1{83}	CP(=O)(C)c1ccc(N)nc1	2{112}	O=Cc1cnn2nccc12	3{52}	[C-]#[N+]CCOC C1CC1	42.8	37
179	4{143,113,10}	CCC1=NN2C(C=C1)=NC(=C2NC1CCOC1)C1=CC(COC)=C(OC)C=C1 c:6,8,10,29,t:2,20,25	Z8801681837	1{143}	CCc1ccc(N)nn1	2{113}	COCc1cc(C=O)ccc1OC	3{10}	[C-]#[N+]C1CC OC1	38.6	37
180	4{37,114,39}	CCOCCNC1=C(N=C2C=CC=C(C(F)F)N12)[C@@@H]1CC[C@@H](C1)C(=O)OC &1:18,21,r,c:10,t:6,8,12	Z8801681838	1{37}	Cl.Nc1cccc(n1)C(F)F	2{114}	COC(=O)[C@@@H]1CC[C@@H](C1)C=O &1:4,7,r	3{39}	CCOCC[N+]#[C-]	38.4	37
181	4{144,115,15}	CCNC1=C(N=C2C=CC(=CN12)S(=O)(=O)NC)C1=CC(OC)=NN1C c:7,9,23,t:3,5,19	Z8808559877	1{144}	CNS(=O)(=O)c1ccc(N)nc1	2{115}	COc1cc(C=O)n(C)n1	3{15}	CC[N+]#[C-]	36.4	37
182	4{145,116,17}	CS(=O)(=O)C1=CC=CC2=NC(=C(NCC3CCO CC3)N12)C1=CN(CCC=C)N=N1 c:6,31,t:4,8,10,24	Z8778278046	1{145}	CS(=O)(=O)c1cccc(N)n1	2{116}	C=CCcn1cc(C=O)nn1	3{17}	[C-]#[N+]CC1C COCC1	42.0	36
183	4{146,117,12}	CS(=O)(=O)C1=CN2C(C=C1)=NC(C1CCCC1 CC1)=C2NCC1CCOC1 c:8,10,21,t:4	Z8810903032	1{146}	CS(=O)(=O)c1ccc(N)nc1	2{117}	O=CC1CCC C21CC2	3{12}	[C-]#[N+]CC1C COC1	37.9	36

184	4{147,118,17}	CC1=NC=CC(=C1)C1=C(NCC2CCOCC2)N2 C3=C(CCC3)C=CC2=N1 c:3,5,8,26,29,t:1,20	Z8778277442	1{147}	Ne1ccc2CC Cc2n1	2{118}	Cc1cc(C=O) ccn1	3{17}	[C-] #[N+]CC1C COCC1	35.2	36
185	4{148,14,14}	COCCNC1=C(N=C2C=CC(=CN12)S(=O)(=O) N1CCCCC1)C1=CC=C(C)C=C1 c:9,11,31,t:5,7,26,28	Z8776690322	1{148}	Ne1ccc(cn1))S(=O)(=O) N2CCCCC2	2{14}	Cc1ccc(C=O))cc1	3{14}	COCC[N+]#[C-]	41.5	36
186	4{149,77,17}	C1C1=CN2C(NCC3CCOCC3)=C(CC3CCCC3) N=C2C(Br)=C1 c:22,26,t:1,13	Z8786845282	1{149}	Ne1ncc(Cl) cc1Br	2{77}	O=CCC1CC CC1	3{17}	[C-] #[N+]CC1C COCC1	41.3	36
187	4{150,119,53}	CCOC(=O)C1=NN=C(N1)C1=C(NCCOCC2= CC=CC=C2)N2C=CC(=CC2=N1)C1CCOC1 c:7,11,20,22,26,28,31,t:5,18	Z8801681847	1{150}	Ne1cc(cen1))C2CCOC2	2{119}	CCOC(=O)c 1nnc(C=O)[n H]1	3{53}	[C-] #[N+]CCOC c1cccc1	46.1	36
188	4{81,48,13}	COC1=CC=C(CNC2=C(N=C3C=NC=CN23)C 2=CNC(=N2)C2CCC2)C=C1 c:12,14,22,30,t:2,4,8,10,19	Z8810903030	1{81}	Ne1cncen1	2{48}	O=Cc1c[nH] c(n1)C2CCC 2	3{13}	COc1ccc(C[N+]#[C-])cc1	36.0	36
189	4{36,14,18}	CC1=CC=C(C=C1)C1=C(NC(C)(C)C)N2C=C(Br)C=CC2=N1 c:3,5,8,19,22,t:1,16	Z3220348675	1{36}	Ne1ccc(Br) cn1	2{14}	Cc1ccc(C=O))cc1	3{18}	CC(C)(C)[N +]#[C-]	34.4	36
190	4{151,14,14}	COCCNC1=C(N=C2C=NC=C(C1)N12)C1=CC =C(C)C=C1 c:9,22,t:5,7,11,17,19	Z8711872648	1{151}	Ne1cnc(Cl) n1	2{14}	Cc1ccc(C=O))cc1	3{14}	COCC[N+]#[C-]	29.6	35
191	4{35,26,54}	CC1=CN2C(C=C1)=NC(CCC1=CC=CC=C1)= C2NC1=CC=CC=C1 c:5,7,14,16,18,24,26,t:1,12,22	Z8700285742	1{35}	Cc1ccc(N)n c1	2{26}	O=CCc1cc ccc1	3{54}	[C-] #[N+]c1cccc c1	30.6	35
192	4{145,120,22}	CS(=O)(=O)C1=CC=CC2=NC(=C(NC3COC3) N12)C1=NC2=C(C=CC=C2)C=N1 c:6,25,27,30,t:4,8,10,21,23	Z8808559874	1{145}	CS(=O)(=O) c1cccc(N)n 1	2{120}	O=Cc1ncc2c cccc2n1	3{22}	[C-] #[N+]C1CO C1	36.8	34
193	4{152,29,7}	CCN1C=CC(=N1)C1=C(NC2CCOCC2)N2C= C(N=C(Cl)C2=N1)C1=CC=CC=C1 c:3,5,8,19,25,30,32,t:21,28	Z8786927263	1{152}	Ne1ncc(nc1 Cl)c2cccc2	2{29}	CCn1ccc(C= O)n1	3{7}	[C-] #[N+]C1CC OCC1	38.9	34
194	4{141,121,55}	CCC1=CON=C1C1=C(NCCC#N)N2C=CC(N C(C)=O)=CC2=N1 c:5,8,16,22,25,t:2	Z8786958870	1{141}	CC(=O)Ne1 ccnc(N)c1	2{121}	CCc1cnc1C =O	3{55}	[C-] #[N+]CCC# N	31.1	34
195	4{153,122,15}	CCNC1=C(N=C2C=CC=C(N12)C(C)(C)O)C1 =CN=C(N=C1)C1=CC=CS1 c:7,9,20,22,27,t:3,5,18,25	Z8798985031	1{153}	CC(C)(O)c1 cccc(N)n1	2{122}	O=Cc1cnc(n c1)c2cccs2	3{15}	CC[N+]#[C-]	34.3	33
196	4{143,103,33}	CCC1=NN2C(NCC3=C(OC)C=CC=C3)=C(N= C2C=C1)C1CCC2(COC2)OC1 c:8,12,14,16,18,21,t:2	Z8798985020	1{143}	CCc1ccc(N) nn1	2{103}	O=CC1CCC 2(COC2)OC 1	3{33}	COc1cccc1 C[N+]#[C-]	36.8	33

197	4{154,123,49}	CC1=NC=C(N=C1)C1=C(NC2CC(F)(F)C2)N2 C=CC(=CC2=N1)[N+](=[O-])=O c:3,5,8,19,21,24,t:1	Z8803896961	1{154}	Nc1cc(cen1))[N+](=O)[O-]	2{123}	Cc1cnc(C=O))cn1	3{49}	FC1(F)CC(C 1)[N+]#[C-]	32.3	33
198	4{92,124,7}	COC1=C(OCC2=C(C)ON=C2C)C=CC(=C1)C 1=C(NC2CCOCC2)N2C=CC(=CC2=N1)C(N) =O c:2,6,10,14,16,19,30,32,35	Z8810903018	1{92}	NC(=O)c1c cnc(N)c1	2{124}	COc1cc(C=O))ccc1OCc2c(C)noc2C	3{7}	[C-]#[N+]C1CC OCC1	43.0	32
199	4{155,125,7}	COC1=NC=NC(=C1)C1=C(NC2CCOCC2)N2 C=CC=C(C1)C2=N1 c:4,6,9,20,26,t:2,22	Z8810902988	1{155}	Ne1ncecc1 Cl	2{125}	COc1cc(C=O))ncn1	3{7}	[C-]#[N+]C1CC OCC1	31.3	32
200	4{156,9,14}	COCCNC1=C(N=C2N1C(Cl)=CC=C2Cl)C1= CSC=C1 c:7,12,14,21,t:5,18	Z8786838532	1{156}	Ne1nc(Cl)c cc1Cl	2{9}	O=Cc1ccsc1	3{14}	COCC[N+]#[C-]	29.8	32
201	4{157,19,9}	CNC1=C(N=C2C=C(C)C=C(Br)N12)C1=C(O C)C=NN1C c:15,19,t:2,4,6,9	Z8808559897	1{157}	Cc1cc(N)nc (Br)c1	2{19}	COc1cnn(C) c1C=O	3{9}	C[N+]#[C-]	30.3	32
202	4{94,126,10}	COC1=CC(=CC(F)=C1)C1=C(NC2CCOC2)N2 N=C(F)C=CC2=N1 c:4,7,10,23,26,t:2,20	Z8801681829	1{94}	Ne1ccc(F)n n1	2{126}	COc1cc(F)cc (C=O)c1	3{10}	[C-]#[N+]C1CC OC1	29.7	32
203	4{41,127,9}	CNC1=C(N=C2C=NC(C)=CN12)C1=CC(OC) =NS1 c:6,9,18,t:2,4,14	Z8798985021	1{41}	Cc1cnc(N)c n1	2{127}	COc1cc(C=O))sn1	3{9}	C[N+]#[C-]	23.5	32
204	4{158,128,18}	CC1=CC(C)=C(C2=C(NC(C)(C)C)N3C=C(N= CC3=N2)P(C)(C)=O)C(C)=C1 c:6,14,16,19,27,t:1,4	Z8798985019	1{158}	CP(=O)(C)c 1cnc(N)cn1	2{128}	Cc1cc(C)c(C =O)c(C)c1	3{18}	CC(C)(C)[N +]#[C-]	32.7	32
205	4{38,129,13}	COC1=CC=C(CNC2=C(N=C3C=C(C=CN23) C#N)C2=CC=CC3=NC=NN23)C=C1 c:12,14,23,27,32,t:2,4,8,10,21,25	Z8801681835	1{38}	Ne1cc(C#N))cen1	2{129}	O=Cc1cccc2 ncmn12	3{13}	COc1ccc(C[N+]#[C-])cc1	33.6	31
206	4{106,15,9}	CNC1=C(N=C2C=CC(OC)=NN12)C1=CC=C(OC)C=C1 c:6,10,21,t:2,4,15,17	Z8776690310	1{106}	COc1ccc(N) nn1	2{15}	COc1ccc(C= O)cc1	3{9}	C[N+]#[C-]	23.9	31
207	4{41,15,9}	CNC1=C(N=C2C=NC(C)=CN12)C1=CC=C(O C)C=C1 c:6,9,20,t:2,4,14,16	Z8776690348	1{41}	Cc1cnc(N)c n1	2{15}	COc1ccc(C= O)cc1	3{9}	C[N+]#[C-]	22.4	31
208	4{159,9,7}	NC(=O)C1=CC=C(C1)N2C(NC3CCOCC3)=C(N=C12)C1=CSC=C1 c:17,26,t:3,5,19,23	Z8780122422	1{159}	NC(=O)c1c cc(Cl)nc1N	2{9}	O=Cc1ccsc1	3{7}	[C-]#[N+]C1CC OCC1	31.3	31
209	4{160,77,27}	CCCCNC1=C(CC2CCCC2)N=C2N1C=C(Br)C =C2C#C c:5,14,21,t:18	Z8784059428	1{160}	Ne1ncc(Br) cc1C#C	2{77}	O=CCC1CC CC1	3{27}	CCCC[N+]#[C-]	31.1	31
210	4{85,130,35}	COC1=NN=C(C=C1)C1=C(NCCCSC)N2C(C= C(C=C2C)C#N)=N1 c:4,6,9,19,21,26,t:2	Z8810902989	1{85}	Cc1cc(C#N) cc(N)n1	2{130}	COc1ccc(C= O)nn1	3{35}	CSCCC[N+] #[C-]	30.6	31

211	4{150,131,22}	C1CC1C1=NNC(=N1)C1=C(NC2COC2)N2C=CC(=CC2=N1)C1CCOC1 c:7,10,19,21,24,t:4	Z8801681805	1{150}	Nc1cc(cen1)C2CCOC2	2{131}	O=Ce1nc(n[nH]1)C2CC2	3{22}	[C-]#[N+]C1CO C1	30.4	31
212	4{83,132,18}	COC1=C(C2=C(NC(C)(C)C)N3C=C(C=CC3=N2)P(C)(C)=O)C(Br)=C(F)C=C1 c:2,4,12,14,17,28,t:25	Z8801681816	1{83}	CP(=O)(C)c1ccc(N)nc1	2{132}	COc1ccc(F)c(Br)c1C=O	3{18}	CC(C)(C)[N+]#[C-]	38.4	30
213	4{161,133,7}	C(C1CCC=CC1)C1=C(NC2CCOCC2)N2N=C=C=CC2=N1 c:4,8,19,21,24	Z8808559853	1{161}	Ne1cccenn1	2{133}	O=CCC1CC=C=CC1	3{7}	[C-]#[N+]C1CCOCC1	25.6	30
214	4{81,22,26}	FC1=CC=C(CNC2=C(N=C3C=NC=CN23)C2=CC=CC=C2)C=C1 c:11,13,20,22,25,t:1,3,7,9,18	Z8712538668	1{81}	Ne1cncen1	2{22}	O=Cc1cccc1	3{26}	Fe1ccc(C[N+]#[C-])cc1	25.9	30
215	4{162,134,12}	CCNC(=O)C1=CC2=NC(=C(NCC3CCOC3)N2C2=C1C=CC=C2)C1=NC(OC)=CC=N1 c:21,24,26,33,35,t:5,7,9,29	Z8810902973	1{162}	CCNC(=O)c1cc(N)nc2cccc12	2{134}	COc1ccnc(C=O)n1	3{12}	[C-]#[N+]CC1C COC1	35.9	30
216	4{163,97,27}	CCCCNC1=C(N=C2C=CC3=C(C=CC=C3)N12)C1=CC=C(F)C=C1 c:9,13,15,26,t:5,7,11,21,23	Z8778277625	1{163}	Ne1ccc2ccc cc2n1	2{97}	Fe1ccc(C=O) cc1	3{27}	CCCC[N+]#[C-]	26.7	30
217	4{164,135,21}	CN(C)CC1=CC2=NC(=C(NCC3CC3)N2C=C1)C1=C(C)N(C)N=C1C c:18,21,26,t:4,6,8	Z8798985065	1{164}	CN(C)Cc1c cnc(N)c1	2{135}	Cc1nn(C)c(C) c1C=O	3{21}	[C-]#[N+]CC1C C1	27.5	29
218	4{153,136,22}	COC1=CC(OC)=C(Br)C(C)=C1C1=C(NC2CO C2)N2C(C=CC=C2C(C)(C)O)=N1 c:10,13,23,25,31,t:2,6	Z8810903033	1{153}	CC(C)(O)c1 cccc(N)n1	2{136}	COc1cc(OC) c(C=O)c(C)c 1Br	3{22}	[C-]#[N+]C1CO C1	37.0	29
219	4{93,79,14}	COCCNC1=C(N=C2C=NC(OC)=CN12)C1=NC=CO1 c:9,13,20,t:5,7,18	Z8778278042	1{93}	COc1cnc(N) cn1	2{79}	O=Cc1ncco1	3{14}	COCC[N+]#[C-]	22.3	29
220	4{165,40,17}	OCC1=CSC(=N1)C1=C(NCC2CCOCC2)N2C=CC=C(C2=N1)C1=CC=CC=C1 c:5,8,20,22,25,30,32,t:2,28	Z8780122087	1{165}	Ne1ncccc1c 2cccc2	2{40}	OCc1csc(C=O)n1	3{17}	[C-]#[N+]CC1C COCC1	32.2	28
221	4{62,137,11}	CC1=C(C(C)=NO1)C1=C(NCC2=CC(Br)=CC=C2)N2C=CC(CO)=CC2=N1 c:4,8,15,17,21,25,28,t:1,12	Z8810902983	1{62}	Ne1cc(CO)c en1	2{137}	Cc1noc(C)c1 C=O	3{11}	Bre1cccc(C[N+]#[C-])c1	32.4	28
222	4{144,138,37}	CNS(=O)(=O)C1=CN2C(C=C1)=NC(=C2NC1CC(C1)C(=O)OC)C1=NC(C)=NC(C)=C1 c:9,11,13,29,32,t:5,26	Z8810903016	1{144}	CNS(=O)(=O)c1ccc(N) nc1	2{138}	Cc1cc(C=O) nc(C)n1	3{37}	COC(=O)C1 CC(C1)[N+]#[C-]	33.3	28
223	4{164,139,24}	COC1=CC(CNC2=C(N=C3C=C(CN(C)C)C=C N23)C2=C(C)N(CCO)N=C2C)=CC=C1 c:17,22,29,32,34,t:2,7,9,11	Z8810903038	1{164}	CN(C)Cc1c cnc(N)c1	2{139}	Cc1nn(CCO) c(C)c1C=O	3{24}	COc1cccc(C[N+]#[C-])c1	33.3	27

224	4{31,140,22}	COCCCC(NC(=O)OC(C)(C)C)C1=C(NC2COC2)N2C3=C(OCC3)C=CC2=N1 c:13,28,31,t:22	Z8810903043	1{31}	Nc1ccc2OC Cc2n1	2{140}	COCCCC(NC(=O)OC(C)(C)C)C=O	3{22}	[C-] #[N+]C1CO C1	30.8	27
225	4{166,141,22}	COC1=NC(CI)=CC(=C1)C1=C(NC2COC2)N2C=CC(CSCCO)=CC2=N1 c:5,7,10,19,26,29,t:2	Z8801681806	1{166}	Nc1cc(CSCCO)ccn1	2{141}	COc1cc(C=O)cc(CI)n1	3{22}	[C-] #[N+]C1CO C1	31.0	27
226	4{106,142,9}	CNC1=C(N=C2C=CC(OC)=NN12)C1=C(CCC=C)C=CC=C1 c:6,10,15,21,23,t:2,4	Z8778278045	1{106}	COc1ccc(N)nn1	2{142}	C=CCCc1ccc cc1C=O	3{9}	C[N+]#[C-]	22.4	27
227	4{167,110,56}	CC1=CN=C(C)C2=NC(=C(NC3=CC=C(OCC4=CC=CC=C4)C=C3)N12)C1=CN=C(C=C1)P(C)(C)O c:19,21,24,32,34,t:1,3,6,8,11,13,17,30	Z8803896947	1{167}	Cc1cnc(C)c(N)n1	2{110}	CP(=O)(C)c1ccc(C=O)cn1	3{56}	[C-] #[N+]c1ccc(OCC2cccc2)cc1	35.9	27
228	4{168,14,17}	CC1=CC=C(C=C1)C1=C(NCC2CCOCC2)N2C(C=NC=C2C#N)=N1 c:3,5,8,21,23,27,t:1	Z8776690324	1{168}	Nc1cnc(C#N)n1	2{14}	Cc1ccc(C=O)cc1	3{17}	[C-] #[N+]CC1C COCC1	25.0	27
229	4{169,143,13}	CNC(=O)C1=NN2C(C=C1)=NC(=C2NCC1=C(C=C(OC)C=C1)C1=CC(OC)=C(OC)C=C1 c:8,10,12,23,34,t:4,17,19,26,30	Z8810902954	1{169}	CNC(=O)c1ccc(N)nn1	2{143}	COc1ccc(C=O)cc1OC	3{13}	COc1ccc(C[N+]#[C-])cc1	32.1	27
230	4{170,94,6}	CCOC(=O)CCNC1=C(N=C2N1C=CC(C)=C2Br)C1=NC=CN=C1 c:11,15,18,24,26,t:9,22	Z8780121700	1{170}	Cc1cnc(N)c1Br	2{94}	O=Cc1cncn1	3{6}	CCOC(=O)C CC[N+]#[C-]	29.9	26
231	4{171,115,15}	CCNC1=C(N=C2C=C(C=CN12)N1C=CN=C1)C1=CC(OC)=NN1C c:7,9,15,17,24,t:3,5,20	Z8808559875	1{171}	Nc1cc(ccn1)n2ccnc2	2{115}	COc1cc(C=O)n(C)n1	3{15}	CC[N+]#[C-]	23.7	26
232	4{121,144,10}	BrC1=CC2=NC(C3=NOC(=C3)C3CC3)=C(NC3CCOC3)N2C=C1 c:9,26,t:1,3,6,15	Z8810902956	1{121}	Nc1cc(Br)cn1	2{144}	O=Cc1cc(on1)C2CC2	3{10}	[C-] #[N+]C1CC OC1	26.8	26
233	4{172,145,29}	CCOC(=O)CCNC1=C(N=C2N1C=CC1=C2CCO1)C1=CN(C)C(=O)C2=C1N=CC=C2 c:10,14,16,29,32,34,t:8,23	Z8810902987	1{172}	Nc1nccc2O CCc21	2{145}	Cn1cc(C=O)c2ncccc2e1=O	3{29}	CCOC(=O)C C[N+]#[C-]	29.7	25
234	4{32,146,7}	C[C@@H]1C[C@@H]1CCCC1=C(NC2CCOC2)N2C=CC(=CC2=N1)P(C)(C)O &l:1,3,r,c:7,18,20,23	Z8810903008	1{32}	CP(=O)(C)c1ccnc(N)c1	2{146}	C[C@@H]1C[C@@H]1CCC=O &l:1,3,r	3{7}	[C-] #[N+]C1CC OCC1	25.7	25
235	4{173,147,57}	COCCCCC1=C(NCC2=CC=CC=C2)N2C=C(C=C(Br)C2=N1)C(=O)N(C)C c:6,12,14,18,24,t:10,20	Z8808559883	1{173}	CN(C)C(=O)c1cnc(N)c(Br)c1	2{147}	COCCCCC=O	3{57}	[C-] #[N+]Cc1cc ccc1	31.4	25

236	4{174,14,17}	CC1=CC=C(C=C1)C1=C(NCC2CCOCC2)N2C(C=CC=C2C#N)=N1 c:3,5,8,21,23,27,t:1	Z8776690319	1{174}	Nc1cccc(C#N)n1	2{14}	Cc1ccc(C=O)cc1	3{17}	[C-]#[N+]CC1C COCC1	23.3	25
237	4{175,148,24}	COC1=C(C(C)=NN1C)C1=C(NCC2=CC(OC)=CC=C2)N2C=CC=C(OCCF)C2=N1 c:5,10,18,20,24,33,t:2,14,26	Z8803896932	1{175}	Nc1ncccc1 OCCF	2{148}	COc1c(C=O)c(C)nn1C	3{24}	COc1cccc(C[N+]#[C-])c1	29.5	25
238	4{176,29,6}	CCOC(=O)CCCN1=C(N=C2N1C=CN=C2N1CCCC1)C1=NN(CC)C=C1 c:11,15,17,31,t:9,26	Z8784060255	1{176}	Nc1ncnc1 N2CCCC2	2{29}	CCn1ccc(C=O)n1	3{6}	CCOC(=O)C CC[N+]#[C-]	27.6	25
239	4{141,149,22}	COC1=C(OC)C(=CC(Br)=C1)C1=C(NC2COC2)N2C=CC(NC(C)=O)=CC2=N1 c:2,6,9,12,21,27,30	Z8808559892	1{141}	CC(=O)Nc1 cnc(N)c1	2{149}	COc1cc(Br)c c(C=O)c1OC	3{22}	[C-]#[N+]C1CO C1	30.9	25
240	4{177,69,17}	CN1N=C(C=C1C)C1=C(NCC2CCOCC2)N2C=CC3=C(C=CC=N3)C2=N1 c:2,4,8,20,24,26,30,t:22	Z8778277872	1{177}	Nc1nccc2nc ccc12	2{69}	Cc1cc(C=O) nn1C	3{17}	[C-]#[N+]CC1C COCC1	25.2	25
241	4{54,150,49}	CN(C)C(=O)C1=CN2C(C=C1)=NC(C1CCC(C1)OCC1=CC=CC=C1)=C2NC1CC(F)(F)C1 c:9,11,25,27,29,t:5,23	Z8801681834	1{54}	Cl.CN(C)C(=O)c1ccc(N)n1	2{150}	O=CC1CCC(CC1)OCc2cc ccc2	3{49}	FC1(F)CC(C1)[N+]#[C-]	32.3	25
242	4{178,9,6}	CCOC(=O)CCCN1=C(N=C2N1C=C(C=C2C#C)C(F)(F)F)C1=CSC=C1 c:11,15,17,29,t:9,26	Z8780122088	1{178}	Nc1ncc(cc1 C#C)C(F)(F)F	2{9}	O=Cc1ccsc1	3{6}	CCOC(=O)C CC[N+]#[C-]	28.1	25
243	4{139,151,39}	CCOCCN1=C(N=C2C=C(C=CN12)C(F)F)C1=CC(C)=NN1 c:10,12,23,t:6,8,20	Z8781341768	1{139}	Nc1cc(cen1)C(F)F	2{151}	Cc1cc(C=O)[nH]n1	3{39}	CCOCC[N+]#[C-]	22.1	24
244	4{54,14,58}	CN(C)C(=O)C1=CN2C(C=C1)=NC(=C2NC1(C)CC1)C1=CC=C(C)C=C1 c:9,11,13,27,t:5,22,24	Z8776690331	1{54}	Cl.CN(C)C(=O)c1ccc(N)n1	2{14}	Cc1ccc(C=O)cc1	3{58}	CC1(CC1)[N+]#[C-]	22.7	24
245	4{41,15,54}	COC1=CC=C(C=C1)C1=C(NC2=CC=CC=C2)N2C=C(C)N=CC2=N1 c:4,6,9,14,16,23,26,t:2,12,20	Z8711872689	1{41}	Cc1cnc(N)c n1	2{15}	COc1ccc(C=O)cc1	3{54}	[C-]#[N+]c1cccc c1	21.4	24
246	4{61,81,23}	CCC1=CC=CC2=NC(=C(NC(CCC(=O)OC)C(=O)OC)N12)C1=NC(=CC=C1)C(F)F c:4,27,29,t:2,6,8,25	Z8810903044	1{61}	CCc1cccc(N)n1	2{81}	FC(F)c1cccc(C=O)n1	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	28.7	24
247	4{179,152,23}	COC(=O)CCC(C)C1=C(NC(CCC(=O)OC)C(=O)OC)N2C=CC(OC)=CC2=N1 c:8,23,27,30	Z8801681822	1{179}	COc1ccnc(N)c1	2{152}	COC(=O)CC C(C)C=O	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	27.6	23
248	4{158,153,18}	CC(C)(C)NC1=C(N=C2C=NC(=CN12)P(C)(C)=O)C1=CN(CC(F)(F)F)N=N1 c:9,11,28,t:5,7,20	Z8803896925	1{158}	CP(=O)(C)c 1cnc(N)en1	2{153}	FC(F)(F)Cn1 cc(C=O)nn1	3{18}	CC(C)(C)[N+]#[C-]	26.1	23

249	4{73,15,9}	CNC1=C(N=C2C=CC3=NC=CN3N12)C1=CC=C(OC)C=C1 c:6,10,23,t:2,4,8,17,19	Z8776690333	1{73}	Nc1ccc2nccn2n1	2{15}	COc1ccc(C=O)cc1	3{9}	C[N+][C-]	18.1	23
250	4{167,154,29}	CCOC(=O)CCNC1=C(N=C2N1C(C)=CN=C2C)C1N(CC11CCOCC1)C(=O)OC(C)(C)C c:10,15,17,t:8	Z8810902967	1{167}	Cc1cnc(C)c(N)n1	2{154}	CC(C)(C)OC(=O)N1CC2(CCOCC2)C1C=O	3{29}	CCOC(=O)C[C[N+][C-]	30.0	23
251	4{180,155,53}	COC(=O)C1=CC2=NC(=C(NCCOCC3=CC=C(C=C3)N2C=C1C)C1=CN=CN=C1 c:17,19,24,30,32,t:4,6,8,15,28	Z8803896942	1{180}	COC(=O)c1cc(N)ncc1C	2{155}	O=Cc1cncnc1	3{53}	[C-][N+]CCOCc1cccc1	25.1	22
252	4{47,137,6}	CCOC(=O)CCNC1=C(N=C2C=C(C=CN12)S(N)(=O)=O)C1=C(C)ON=C1C c:13,15,24,28,t:9,11	Z8803896968	1{47}	Cl.Nc1cc(ccn1)S(=O)(=O)N	2{137}	Cc1noc(C)c1C=O	3{6}	CCOC(=O)C[C[N+][C-]	25.0	22
253	4{181,77,6}	CCOC(=O)CCNC1=C(CC2CCCC2)N=C2N1C=CC1=C2N=CC=N1 c:9,18,22,24,27,29	Z8784060825	1{181}	Nc1nccc2nccnc12	2{77}	O=CCC1CC1	3{6}	CCOC(=O)C[C[N+][C-]	22.6	22
254	4{182,14,7}	CC1=CC=C(C=C1)C1=C(NC2CCOCC2)N2C=C(C=C(I)C2=N1)C(F)(F)F c:3,5,8,19,25,t:1,21	Z8797786219	1{182}	Nc1ncc(cc1I)C(F)(F)F	2{14}	Cc1ccc(C=O)cc1	3{7}	[C-][N+]C1CCOCC1	29.7	22
255	4{183,156,10}	COC1=CC=C(C)N2C(NC3CCOC3)=C(N=C12)C1=C(CI)N=CN1C c:15,21,24,t:2,4,17	Z8801681815	1{183}	COc1ccc(C)nc1N	2{156}	Cn1cnc(Cl)c1C=O	3{10}	[C-][N+]C1CCOC1	21.0	21
256	4{184,22,7}	NC(=S)C1=CN2C(C=C1)=NC(=C2NC1CCOCC1)C1=CC=CC=C1 c:7,9,11,24,26,t:3,22	Z8784059422	1{184}	NC(=S)c1ccc(N)nc1	2{22}	O=Cc1cccc1	3{7}	[C-][N+]C1CCOCC1	20.1	21
257	4{185,26,7}	CC1=C(C=CC2=NC(CCC3=CC=CC=C3)=C(NC3CCOCC3)N12)S(C)(=O)=O c:3,12,14,t:1,5,10,16	Z8776690329	1{185}	Cc1nc(N)cc1S(=O)(=O)C	2{26}	O=CCCc1ccc1	3{7}	[C-][N+]C1CCOCC1	23.5	21
258	4{46,157,9}	CNC1=C(N=C2C=CC=CN12)C1=NC2=C(C=C1)N=CC=C2 c:6,8,15,17,20,22,t:2,4,13	Z8798985061	1{46}	Nc1ccccn1	2{157}	O=Cc1ccc2ncccc2n1	3{9}	C[N+][C-]	15.5	21
259	4{161,14,26}	CC1=CC=C(C=C1)C1=C(NCC2=CC=C(F)C=C2)N2N=CC=CC2=N1 c:3,5,8,17,21,23,26,t:1,12,14	Z8741907011	1{161}	Nc1cccnn1	2{14}	Cc1ccc(C=O)cc1	3{26}	Fe1ccc(C[N+][C-])cc1	18.6	21
260	4{28,158,31}	CSCCNC1=C(N=C2C=C(C=CN12)C1=NOC=N1)C1=CN(C=C)N=C1 c:9,11,19,27,t:5,7,16,22	Z8798985032	1{28}	Cl.Nc1cc(ccn1)c2ncon2	2{158}	C=Cn1cc(C=O)cn1	3{31}	CSCC[N+][C-]	20.0	20

261	4{19,22,7}	N#CC1=CC=CN2C(NC3CCOCC3)=C(N=C12)C1=CC=CC=C1 c:4,15,23,25,t:2,17,21	Z8780121582	1{19}	Nc1ncccc1 C#N	2{22}	O=Cc1cccc 1	3{7}	[C-] #[N+]C1CC OCC1	17.2	20
262	4{32,58,16}	CC1=CC=CC(C)=C1NC1=C(N=C2C=C(C=C N12)P(C)(C)=O)C1=NSN=C1 c:3,6,14,16,28,t:1,10,12,25	Z8781341783	1{32}	CP(=O)(C)c 1ccnc(N)c1	2{58}	O=Cc1cnsn1	3{16}	Cc1cccc(C)c 1[N+]#[C-]	21.4	20
263	4{38,129,9}	CNC1=C(N=C2C=C(C=CN12)C#N)C1=CC=C C2=NC=NN12 c:6,8,17,21,t:2,4,15,19	Z8798985023	1{38}	Nc1cc(C#N)ccn1	2{129}	O=Cc1cccc2 ncnn12	3{9}	C[N+]#[C-]	15.5	20
264	4{186,159,1}	CN(C)S(=O)(=O)C1=CC2=NC(=C(NC3CC3)N 2C=C1)C1=NNC2=C1C=CC(F)=C2 c:19,25,28,31,t:6,8,10,22	Z8810903045	1{186}	Cl.CN(C)S(=O)(=O)c1c cnc(N)c1	2{159}	Fc1ccc2c(C= O)n[nH]c2c1	3{1}	[C-] #[N+]C1CC 1	22.0	20
265	4{123,160,49}	CN1N=C(C=C1C1=C(NC2CC(F)(F)C2)N2C= CC(OCCO)=CC2=N1)C1CC1 c:2,4,7,18,24,27	Z8803896943	1{123}	Cl.Nc1cc(O CCO)ccn1	2{160}	Cn1nc(cc1C =O)C2CC2	3{49}	FC1(F)CC(C 1)[N+]#[C-]	21.0	19
266	4{97,161,14}	CCN1C=NC=C1C1=C(NCCOC)N2C=C(F)C= C(C)C2=N1 c:3,5,8,23,t:16,19	Z8778278036	1{97}	Cc1cc(F)cn c1N	2{161}	CCn1cnc1C =O	3{14}	COCC[N+]#/ C-]	16.4	19
267	4{46,162,9}	CNC1=C(N=C2C=CC=CN12)C1=CC(OC)=N C(C)=C1 c:6,8,17,20,t:2,4,13	Z8810902981	1{46}	Nc1ccccn1	2{162}	COc1cc(C=O)cc(C)n1	3{9}	C[N+]#[C-]	13.8	19
268	4{70,163,22}	FC1=C(C2=C(NC3COC3)N3C=CN=C(C4CC4)C3=N2)C(I)=CN=C1 c:1,3,12,21,25,27,t:14	Z8801681849	1{70}	Nc1ncncn1 C2CC2	2{163}	Fc1cnc(I)c1 C=O	3{22}	[C-] #[N+]C1CO C1	23.2	19
269	4{187,164,46}	CN1N=C(C2=C1CCOC2)C1=C(NCC(C)=C)N 2C=C(Cl)C(=CC2=N1)C#N c:2,4,12,23,26,t:20	Z8810903034	1{187}	Nc1cc(C#N)c(Cl)cn1	2{164}	Cn1nc(C=O) c2COCCc21	3{46}	CC(=C)C[N+] #[C-]	19.6	19
270	4{188,165,59}	COC(=O)[C@H]1C[C@@H](C1)NIC=CC(=N 1)C1=C(NCCC2=CC(F)=CC=C2)N2C(C=NC= C2C(=O)OC)=N1 r,c:10,12,15,23,25,30,32,38,t:20	Z8810902960	1{188}	COC(=O)c1 cnc(N)n1	2{165}	COC(=O)[C @H]1C[C@ @H](C1)n2c cc(C=O)n2	3{59}	Fc1cccc(CC[N+]#[C-])c1	25.2	19
271	4{189,44,27}	CCCCNC1=C(N=C2N1C=CC=C2N(C)C)C1= CN(CC)N=C1 c:7,11,13,24,t:5,19	Z8797781359	1{189}	CN(C)c1ccc nc1N	2{44}	CCn1cc(C=O)cn1	3{27}	CCCC[N+]#/ C-]	16.7	19
272	4{190,166,12}	C(NC1=C(N=C2C=C3C=CC=CC3=NN12)C1= NC(=CS1)C1CC1)C1CCOC1 c:8,10,13,20,t:2,4,6,18	Z8786958851	1{190}	Nc1cc2cccc c2nn1	2{166}	O=Cc1nc(es1)C2CC2	3{12}	[C-] #[N+]CC1C COC1	19.7	19
273	4{186,167,29}	CCOC(=O)CCNC1=C(N=C2C=C(C=CN12)S(=O)(=O)N(C)C)C1=NN=CN1 c:12,14,27,t:8,10,25	Z8808559859	1{186}	Cl.CN(C)S(=O)(=O)c1c cnc(N)c1	2{167}	O=Cc1nnc[n H]1	3{29}	CCOC(=O)C C[N+]#[C-]	20.4	19
274	4{118,46,25}	COCCCCC1=C(NCCCF)N2C(C=CC=C2C(C)O)=N1 c:7,16,18,23	Z8781341799	1{118}	Cl.CC(O)c1 cccc(N)n1	2{46}	COCCCCC =O	3{25}	FCCC[N+]#/ C-]	16.7	18

275	4{191,168,22}	CC(C)(C)C1=CN2C(NC3COC3)=C(N=C2C=C1)C1=NOC=C1 c:13,15,18,24,t:4,21	Z8810902975	1{191}	CC(C)(C)c1ccc(N)nc1	2{168}	O=Cc1cccon1	3{22}	[C-] #[N+]C1CO C1	15.3	18
276	4{114,40,25}	COCC1=CC2=NC(=C(NCCCCF)N2C=C1)C1=NC(CO)=CS1 c:16,23,t:3,5,7,19	Z8781341790	1{114}	COCC1ccnc(N)c1	2{40}	OCc1csc(C=O)n1	3{25}	FCCC[N+]#[C-]	16.5	17
277	4{157,14,54}	CC1=CC=C(C=C1)C1=C(NC2=CC=CC=C2)N2C(C=C(C)C=C2Br)=N1 c:3,5,8,13,15,23,26,t:1,11,20	Z8741907090	1{157}	Cc1cc(N)nc(Br)c1	2{14}	Cc1ccc(C=O)cc1	3{54}	[C-] #[N+]c1cccc c1	18.3	17
278	4{192,22,27}	CCCCNC1=C(N=C2N1C(F)=CC=C2Cl)C1=CC=CC=C1 c:7,12,14,20,22,t:5,18	Z8786838535	1{192}	Nc1nc(F)cc1Cl	2{22}	O=Cc1cccc1	3{27}	CCCC[N+]#[C-]	14.4	17
279	4{22,19,13}	COC1=C(N(C)N=C1)C1=C(NCC2=CC=C(OC)C=C2)N2N=C(Cl)C=CC2=N1 c:6,9,19,26,29,t:2,13,15,23	Z8798985042	1{22}	Nc1ccc(Cl)nn1	2{19}	COc1cnn(C)c1C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	18.0	17
280	4{193,169,12}	CNC(=O)C1=CN2C(C=C1)=NC(=C2NCC1CCOC1)C1=NNC2=C1N=CC=C2 c:8,10,12,26,29,31,t:4,23	Z8803896944	1{193}	CNC(=O)c1ccc(N)nc1	2{169}	O=Cc1n[nH]c2cccnc12	3{12}	[C-] #[N+]CC1C COC1	16.3	15
281	4{73,151,13}	COC1=CC=C(CNC2=C(N=C3C=CC4=NC=C4N423)C2=CC(C)=NN2)C=C1 c:12,16,26,30,t:2,4,8,10,14,23	Z8810902952	1{73}	Nc1ccc2nccn2n1	2{151}	Cc1cc(C=O)[nH]n1	3{13}	COc1ccc(C[N+]#[C-])cc1	15.4	15
282	4{169,15,13}	CNC(=O)C1=NN2C(C=C1)=NC(=C2NCC1=C(C=C(OC)C=C1)C1=CC=C(OC)C=C1 c:8,10,12,23,32,t:4,17,19,26,28	Z8776690339	1{169}	CNC(=O)c1ccc(N)nn1	2{15}	COc1ccc(C=O)cc1	3{13}	COc1ccc(C[N+]#[C-])cc1	16.9	15
283	4{194,170,7}	CCN1N=NC(=N1)C1=C(NC2CCOCC2)N2C=CN=C(N3C=CC=N3)C2=N1 c:3,5,8,19,24,26,30,t:21	Z8780122086	1{194}	Nc1nccnc1n2cccn2	2{170}	CCn1nnc(C=O)n1	3{7}	[C-] #[N+]C1CC OCC1	15.1	15
284	4{73,19,13}	COC1=C(N(C)N=C1)C1=C(NCC2=CC=C(OC)C=C2)N2N3C=CN=C3C=CC2=N1 c:6,9,19,24,26,29,32,t:2,13,15	Z8798985040	1{73}	Nc1ccc2nccn2n1	2{19}	COc1cnn(C)c1C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	15.8	15
285	4{195,118,7}	CC1=NC=CC(=C1)C1=C(NC2CCOCC2)N2C=C(Br)C=C(NS(C)(=O)=O)C2=N1 c:3,5,8,30,t:1,19,22	Z8780122346	1{195}	CS(=O)(=O)Nc1cc(Br)nc1N	2{118}	Cc1cc(C=O)ccn1	3{7}	[C-] #[N+]C1CC OCC1	18.5	14
286	4{196,171,43}	COC1CC(C(OC)O1)C1=C(NC2CCN(CC2)C(=O)OC(C)(C)C)N2C=C(C)C=C(C#N)C2=N1 c:10,36,t:28,31	Z8808559881	1{196}	Cc1cnc(N)c(C#N)c1	2{171}	COC1CC(C=O)C(OC)O1	3{43}	CC(C)(C)OC(=O)N1CCC(CC1)[N+]#[C-]	18.5	14
287	4{73,172,11}	BrC1=CC(CNC2=C(N=C3C=CC4=NC=CN4N23)C2=CNC(=N2)C2CC2)=CC=C1 c:10,14,24,30,32,t:1,6,8,12,21	Z8808559861	1{73}	Nc1ccc2nccn2n1	2{172}	O=Cc1c[nH]c(n1)C2CC2	3{11}	Br1cccc(C[N+]#[C-])c1	16.9	14

288	4{197,29,45}	CCN1C=CC(=N1)C1=C(NCC=C)N2C=C(C=C C2=N1)S(=O)(=O)CC(C)C c:3,5,8,15,17,20	Z8786958927	1{197}	CC(C)CS(=O)(=O)c1ccc(N)nc1	2{29}	CCn1ccc(C=O)n1	3{45}	C=CC[N+]#[C-]	14.2	14
289	4{180,173,15}	CCNC1=C(N=C2C=C(C(=O)OC)C(C)=CN12) C1=NC(=NN1C)C(F)(F)F c:14,21,t:3,5,7,19	Z8810902977	1{180}	COC(=O)c1ccc(N)nc1C	2{173}	Cn1nc(nc1C=O)C(F)(F)F	3{15}	CC[N+]#[C-]	13.5	13
290	4{198,174,31}	CSCCNC1=C(N=C2C=NC(C#C)=C(Cl)N12)C 1=CN(CC2CCCO2)N=N1 c:9,29,t:5,7,13,19	Z8801681832	1{198}	Ne1cnc(C#C)c(Cl)n1	2{174}	O=Cc1cn(CC2CCCO2)nn1	3{31}	CSCC[N+]#[C-]	14.3	13
291	4{113,170,7}	CCN1N=NC(=N1)C1=C(NC2CCOCC2)N2C= CC=C(N3CCOCC3)C2=N1 c:3,5,8,19,31,t:21	Z8784060348	1{113}	Ne1ncccc1N2CCOCC2	2{170}	CCn1nnc(C=O)n1	3{7}	[C-] #[N+]C1CCOCC1	13.0	12
292	4{79,109,9}	CNC1=C(N=C2C=NC=C(C)N12)C1=NN(C)C =C1C c:6,18,t:2,4,8,14	Z8803896951	1{79}	Cc1cnc(N)n1	2{109}	Cc1cn(C)nc1C=O	3{9}	C[N+]#[C-]	8.4	12
293	4{194,175,60}	COC(=O)C1=CC(NC2=C(N=C3N2C=CN=C3 N2C=CC=N2)C2=NNC=C2)=CC=C1 c:10,14,16,20,22,28,30,32,t:4,8,25	Z8803896952	1{194}	Ne1ncnc1n2ccn2	2{175}	O=Cc1cc[nH]n1	3{60}	COC(=O)c1ccc([N+]#[C-])c1	12.9	12
294	4{104,176,12}	COC(=O)C1=C(Cl)SC(=C1)C1=C(NCC2CCO C2)N2C(C=CC3=C2COCC3)=N1 c:4,8,11,23,25,32	Z8810902978	1{104}	Ne1ccc2CCOCe2n1	2{176}	COC(=O)c1cc(C=O)sc1Cl	3{12}	[C-] #[N+]CC1C COC1	13.6	11
295	4{199,77,6}	CCOC(=O)CCNC1=C(CC2CCCC2)N=C2N1 C=CC=C2C(C)(F)F c:9,18,22,24	Z8797784767	1{199}	CC(F)(F)c1ccnc1N	2{77}	O=CCC1CC CC1	3{6}	CCOC(=O)C CC[N+]#[C-]	12.0	11
296	4{200,15,9}	CNC1=C(N=C2C=C(C)C=C(OC)N12)C1=CC =C(OC)C=C1 c:22,t:2,4,6,9,16,18	Z8776690326	1{200}	Cl.COC1cc(C)cc(N)n1	2{15}	COc1ccc(C=O)cc1	3{9}	C[N+]#[C-]	9.0	11
297	4{201,108,5}	COCCNC1=C(N=C2C=C(C=CN12)C(F)(F)F)C1=CN=C(N=C1)N1CCOCC1 c:10,12,23,25,t:6,8,21	Z8803896939	1{201}	Ne1cc(ccn1)C(F)(F)F	2{108}	O=Cc1cnc(nc1)N2CCOC C2	3{5}	COCCC[N+]#[C-]	12.9	11
298	4{161,98,6}	CCOC(=O)CCNC1=C(N=C2C=CC=NN12)C 1=NC=C(OC)N=C1 c:13,15,26,t:9,11,20,22	Z8801681809	1{161}	Ne1cccenn1	2{98}	COc1cnc(C=O)en1	3{6}	CCOC(=O)C CC[N+]#[C-]	10.3	11
299	4{135,130,32}	CCCC1=NC=CN2C(NC3CCC3)=C(N=C12)C1 =NN=C(OC)C=C1 c:5,14,26,t:3,16,20,22	Z8801681840	1{135}	CCCc1ncnc1N	2{130}	COc1ccc(C=O)nn1	3{32}	[C-] #[N+]C1CC C1	9.8	11
300	4{179,177,5}	COCCNC1=C(CC2CC(C2)C(=O)OC)N=C2C =C(OC)C=CN12 c:6,24,t:18,20	Z8808559865	1{179}	COc1cnc(N)c1	2{177}	COC(=O)C1 CC(CC=O)C 1	3{5}	COCCC[N+]#[C-]	10.3	11

301	4{202,69,14}	COCCNC1=C(N=C2N1C=C(Br)C=C2C(C)(C)C)C1=NN(C)C(C)=C1 c:7,14,26,t:5,11,21	Z8780122084	1{202}	CC(C)(C)c1cc(Br)enc1N	2{69}	Cc1cc(C=O)nn1C	3{14}	COCC[N+]#[C-]	11.8	10
302	4{123,178,22}	COC1=CC2=C(OC(=C2)C2=C(NC3COC3)N3C=CC(OCCO)=CC3=N2)C=C1 c:7,10,19,25,28,31,t:2,4	Z8810903015	1{123}	Cl.Nc1cc(OCCO)ccn1	2{178}	COc1ccc2oc(C=O)cc2c1	3{22}	[C-]#[N+]C1CO C1	10.9	10
303	4{101,179,14}	COCCNC1=C(N=C2N1C=C(CO)C=C2C1)C1=CC=C(OC2CCOC2)C=C1 c:7,15,30,t:5,11,19,21	Z8801681830	1{101}	Nc1ncc(CO)cc1Cl	2{179}	O=Cc1ccc(O C2CCOC2)cc1	3{14}	COCC[N+]#[C-]	11.5	10
304	4{78,180,2}	CC1=CN2N3C(C=C(C)C2=N1)=NC(CCCCCF)=C3NC1=CC=C(F)C=C1 c:10,12,20,29,t:1,6,24,26	Z8808559869	1{78}	Cc1en2nc(N)cc(C)c2n1	2{180}	FCCCCC=O	3{2}	Fc1ccc([N+]#[C-])cc1	10.0	10
305	4{203,22,14}	COCCNC1=C(N=C2N1C1=C(C=CC=C1)N=C2N1CCCC1)C1=CC=CC=C1 c:7,13,15,18,29,31,t:5,11,27	Z8797783649	1{203}	Nc1nc2ccc c2nc1N3CC CC3	2{22}	O=Cc1cccc1	3{14}	COCC[N+]#[C-]	9.8	9
306	4{73,181,13}	COC1=CC=C(CNC2=C(N=C3C=CC4=NC=C4N23)C2=CN=C3CCCN23)C=C1 c:12,16,33,t:2,4,8,10,14,23,25	Z8801681846	1{73}	Nc1ccc2ncc n2n1	2{181}	O=Cc1cnc2C CCn12	3{13}	COc1ccc(C[N+]#[C-])cc1	9.7	9
307	4{73,19,58}	COC1=C(N(C)N=C1)C1=C(NC2(C)CC2)N2N3C=CN=C3C=CC2=N1 c:6,9,19,21,24,27,t:2	Z8781341775	1{73}	Nc1ccc2ncc n2n1	2{19}	COc1cnn(C) c1C=O	3{58}	CC1(CC1)[N+]#[C-]	8.0	9
308	4{204,14,27}	CCCCNC1=C(N=C2N1C=CC(Cl)=C2I)C1=CC=C(C)C=C1 c:7,11,14,23,t:5,18,20	Z8786897242	1{204}	Nc1nccc(Cl)c1I	2{14}	Cc1ccc(C=O)cc1	3{27}	CCCC[N+]#[C-]	10.1	8
309	4{145,182,37}	COC(=O)C1CC(C1)NC1=C(N=C2C=CC=C(N12)S(C)(=O)=O)C1=NC=CN1CC#C c:14,16,27,t:10,12,25	Z8781341787	1{145}	CS(=O)(=O)c1cccc(N)n1	2{182}	O=Cc1cncn1 CC#C	3{37}	COC(=O)C1 CC(C1)[N+]#[C-]	9.3	8
310	4{169,49,13}	CNC(=O)C1=NN2C(NCC3=CC=C(OC)C=C3)=C(N=C2C=C1)C1=CN=C1C c:16,18,20,23,29,t:4,10,12,26	Z8808559891	1{169}	CNC(=O)c1ccc(N)nn1	2{49}	Cc1n[nH]cc1 C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	8.0	8
311	4{205,9,27}	CCCCNC1=C(N=C2N1C=CN=C2C#C)C1=CS C=C1 c:7,11,13,21,t:5,18	Z8778277313	1{205}	Nc1ncnc1 C#C	2{9}	O=Cc1ccsc1	3{27}	CCCC[N+]#[C-]	5.8	7
312	4{124,183,12}	COC(=O)C(C)OC1=CC=C(C=C1)C1=C(NCC2CCOC2)N2C=CC=C(CO)C2=N1 c:9,11,14,25,32,t:7,27	Z8798985043	1{124}	Nc1ncccc1 CO	2{183}	COC(=O)C(C)Oc1ccc(C=O)cc1	3{12}	[C-]#[N+]CC1C COC1	8.2	7
313	4{206,80,6}	CCOC(=O)CCCNC1=C(N=C2N1C=CC(I)=C2F)C1=NC=C(C)S1 c:11,15,18,t:9,22,24	Z8786849399	1{206}	Nc1nccc(I)c1F	2{80}	Cc1enc(C=O)s1	3{6}	CCOC(=O)C CC[N+]#[C-]	9.4	7

314	4{106,22,54}	COC1=NN2C(C=C1)=NC(=C2NC1=CC=CC=C1)C1=CC=CC=C1 c:6,8,10,16,18,23,25,t:2,14,21	Z8741907033	1{106}	COc1ccc(N)nn1	2{22}	O=Cc1cccc1	3{54}	[C-] #[N+]c1cccc1	6.0	7
315	4{207,184,14}	COCCNC1=C(N=C2C=CC(=CN12)N1CCN(C1)C(=O)C1CC1)C1CC1 c:9,11,t:5,7	Z8780122426	1{207}	Nc1ccc(en1)N2CCN(C2)C(=O)C3CC3	2{184}	O=CC1CC1	3{14}	COCC[N+]#[C-]	7.1	7
316	4{137,58,13}	COC1=CC=C(CNC2=C(N=C3C=CC(C)=NN23)C2=NSN=C2)C=C1 c:12,15,23,26,t:2,4,8,10,20	Z8798985035	1{137}	Cc1ccc(N)nn1	2{58}	O=Cc1cnsn1	3{13}	COc1ccc(C[N+]#[C-])cc1	6.4	7
317	4{208,94,6}	CCOC(=O)CCCN1=C(N=C2N1C=CN=C2OC1CCCC1)C1=NC=CN=C1 c:11,15,17,29,31,t:9,27	Z8778277288	1{208}	Nc1cncnc1OC2CCCC2	2{94}	O=Cc1cncn1	3{6}	CCOC(=O)CC[N+]#[C-]	7.1	6
318	4{209,40,17}	OCC1=CSC(=N1)C1=C(NCC2CCOCC2)N2C=CC=C(N3CCCC3)C2=N1 c:5,8,20,32,t:2,22	Z8784060440	1{209}	Nc1cncnc1N2CCCC2	2{40}	OCc1csc(C=O)n1	3{17}	[C-] #[N+]CC1C COCC1	7.3	6
319	4{161,15,13}	COC1=CC=C(CNC2=C(N=C3C=CC=NN23)C2=CC=C(OC)C=C2)C=C1 c:12,14,25,28,t:2,4,8,10,19,21	Z8776690334	1{161}	Nc1ccenn1	2{15}	COc1ccc(C=O)cc1	3{13}	COc1ccc(C[N+]#[C-])cc1	6.2	6
320	4{210,185,34}	CN1C=NC(=C1)C1=C(NCC2CCCO2)N2C(=N1)C(Br)=CC=C2F c:2,4,7,18,22,24	Z8810903013	1{210}	Nc1nc(F)cc1Br	2{185}	Cn1cnc(C=O)c1	3{34}	[C-] #[N+]CC1C CCO1	6.6	6
321	4{169,53,13}	CNC(=O)C1=NN2C(C=C1)=NC(=C2NCC1=C=C(OC)C=C1)C1=C(F)C=CC(C)=N1 c:8,10,12,23,26,29,32,t:4,17,19	Z8803896966	1{169}	CNC(=O)c1ccc(N)nn1	2{53}	Cc1ccc(F)c(C=O)n1	3{13}	COc1ccc(C[N+]#[C-])cc1	7.0	6
322	4{211,59,34}	COC1=C(Br)C=C(C=N1)C1=C(NCC2CCCO2)N2C=CC=C(C3=NN=NN3)C2=N1 c:2,5,7,10,21,27,32,t:23,25	Z8808559885	1{211}	Nc1cncnc1c2n[nH]2	2{59}	COc1ncc(C=O)cc1Br	3{34}	[C-] #[N+]CC1C CCO1	7.7	6
323	4{104,186,12}	FC1=C2SC(=NC2=CC=C1)C1=C(NCC2CCOC2)N2C(C=CC3=C2COCC3)=N1 c:1,4,7,9,12,24,26,33	Z8810902982	1{104}	Nc1ccc2CCOCc2n1	2{186}	Fe1cccc2nc(C=O)sc12	3{12}	[C-] #[N+]CC1C COC1	7.0	6
324	4{212,187,49}	CCOC(=O)C1=NC(=C2C=CC=CN12)C1=C(NC2CC(F)(F)C2)N2C=C(COC)C=CC2=N1 c:9,11,16,32,35,t:5,7,27	Z8803896960	1{212}	Cl.COCc1ccc(N)nc1	2{187}	CCOC(=O)c1nc(C=O)c2ccccn12	3{49}	FC1(F)CC(C1)[N+]#[C-]	7.2	6
325	4{213,15,9}	CNC1=C(N=C2N1C(OC)=CC=C2F)C1=CC=C(OC)C=C1 c:4,10,12,22,t:2,16,18	Z8776690311	1{213}	COc1ccc(F)c(N)n1	2{15}	COc1ccc(C=O)cc1	3{9}	C[N+]#[C-]	4.5	5

326	4{214,188,12}	<chem>COC1=CC(Br)=C(C)N2C(NCC3CCOC3)=C(CCC3(CC3)C#N)N=C12</chem> t:2,5,17,27	Z8798985054	1{214}	<chem>COc1cc(Br)c(C)nc1N</chem>	2{188}	<chem>O=CCCC1(C1)C#N</chem>	3{12}	[C-]#[N+]CC1COC1	6.4	5
327	4{215,84,7}	<chem>CSCCC1=C(NC2CCOCC2)N2N=C(Cl)C=C(C)C2=N1</chem> c:4,22,t:15,18	Z8778278037	1{215}	<chem>Cl.Cc1cc(Cl)nn1N</chem>	2{84}	<chem>CSCCC=O</chem>	3{7}	[C-]#[N+]C1CCOCC1	4.7	5
328	4{156,103,47}	<chem>CC(C)NC1=C(N=C2N1C(Cl)=CC=C2Cl)C1CC2(COC2)OC1</chem> c:6,11,13,t:4	Z8810903010	1{156}	<chem>Nc1nc(Cl)ccc1Cl</chem>	2{103}	<chem>O=CC1CCC2(COC2)OC1</chem>	3{47}	CC(C)[N+]#[C-]	4.5	4
329	4{47,118,14}	<chem>COCCNC1=C(N=C2C=C(C=CN12)S(N)(=O)=O)C1=CC(C)=NC=C1</chem> c:9,11,23,25,t:5,7,20	Z8784059519	1{47}	<chem>Cl.Nc1cc(ccn1)S(=O)(=O)N</chem>	2{118}	<chem>Cc1cc(C=O)ccn1</chem>	3{14}	COCC[N+]#[C-]	4.3	4
330	4{198,189,31}	<chem>CSCCNC1=C(N=C2C=NC(C#C)=C(Cl)N12)C1=CN(N=N1)C1CCOCC1</chem> c:9,22,t:5,7,13,19	Z8801681831	1{198}	<chem>Nc1cnc(C#C)c(Cl)n1</chem>	2{189}	<chem>O=Cc1cn(nn1)C2CCOCC2</chem>	3{31}	CSCC[N+]#[C-]	4.7	4
331	4{73,161,20}	<chem>CCN1C=NC=C1C1=C(NC2=C(C)C=C(OC)C=C2)N2N3C=CN=C3C=CC2=N1</chem> c:3,5,8,11,18,23,25,28,31,t:14	Z8801681850	1{73}	<chem>Nc1ccc2nccn2n1</chem>	2{161}	<chem>CCn1cnc1C=O</chem>	3{20}	COc1ccc([N+]#[C-])c(C)c1	4.3	4
332	4{216,190,10}	<chem>CC1=CC2=NC(C3=CC(=NN3)C3=NC=CC=C3)=C(NC3CCOC3)N2N=C1C</chem> c:8,14,16,29,t:1,3,6,12,18	Z8801681808	1{216}	<chem>Cc1cc(N)nn1C</chem>	2{190}	<chem>O=Cc1cc(n[nH]1)c2cccn2</chem>	3{10}	[C-]#[N+]C1CCOC1	4.1	4
333	4{217,14,7}	<chem>CN1C(=O)NC2=C1C=CN1C(NC3CCOCC3)=C(N=C21)C1=CC=C(C)C=C1</chem> c:5,8,19,30,t:21,25,27	Z8784060908	1{217}	<chem>Cn1c(=O)[nH]e2c(N)nc1c2</chem>	2{14}	<chem>Cc1ccc(C=O)cc1</chem>	3{7}	[C-]#[N+]C1CCOCC1	3.9	4
334	4{218,34,61}	<chem>CC(C)(C)OC(=O)NCCCNC1=C(N=C2C=CC(=NN12)C(C)(C)C)C1=CC=C(C=C1)P(C)(C)=O</chem> c:16,18,29,31,t:12,14,27	Z8803896931	1{218}	<chem>CC(C)(C)c1ccc(N)nn1</chem>	2{34}	<chem>CP(=O)(C)c1ccc(C=O)cc1</chem>	3{61}	CC(C)(C)OC(=O)NCCC[N+]#[C-]	5.1	4
335	4{219,14,27}	<chem>CCCCNC1=C(N=C2N1C=C(Br)C1=C2N=CC=C1)C1=CC=C(C)C=C1</chem> c:7,14,17,19,27,t:5,11,22,24	Z8797778731	1{219}	<chem>Nc1ncc(Br)c2ccnc12</chem>	2{14}	<chem>Cc1ccc(C=O)cc1</chem>	3{27}	CCCC[N+]#[C-]	4.1	4
336	4{220,191,7}	<chem>CCN1C=NN=C1C1=C(NC2CCOCC2)N2C=C=C(C3CC3)C2=N1</chem> c:3,5,8,19,28,t:21	Z8803896959	1{220}	<chem>Cl.Nc1nccc1C2CC2</chem>	2{191}	<chem>CCn1cnc1C=O</chem>	3{7}	[C-]#[N+]C1CCOCC1	3.5	4
337	4{38,58,9}	<chem>CNC1=C(N=C2C=C(C=CN12)C#N)C1=NSN=C1</chem> c:6,8,18,t:2,4,15	Z8786958823	1{38}	<chem>Nc1cc(C#N)ccn1</chem>	2{58}	<chem>O=Cc1cnsn1</chem>	3{9}	C[N+]#[C-]	2.6	4
338	4{221,192,14}	<chem>COCCNC1=C(N=C2N1C(C)=CC=C2C#N)C1=NC(OC)=CC=C1</chem> c:7,12,14,23,25,t:5,19	Z8798985058	1{221}	<chem>Cc1ccc(C#N)c(N)n1</chem>	2{192}	<chem>COc1cccc(C=O)n1</chem>	3{14}	COCC[N+]#[C-]	3.3	4

339	4{161,27,13}	COC1=CC=C(CNC2=C(N=C3C=CC=NN23)C2=NN(C)C(C)=N2)C=C1 c:12,14,24,27,t:2,4,8,10,19	Z8786958899	1{161}	Nc1cccnn1	2{27}	Cc1nc(C=O)nn1C	3{13}	COc1ccc(C[N+]#[C-])cc1	3.4	4
340	4{222,193,62}	COC(=O)C1=CN2C(NC3(CCCC3)C(=O)OC)=C(N=C2C=N1)C1=NN2CCCCOC2=C1 c:18,20,23,35,t:4,26	Z8808559886	1{222}	Cl.COC(=O)c1cnc(N)cn1	2{193}	O=Cc1cc2OCCCCn2n1	3{62}	COC(=O)C1(CCCC1)[N+]#[C-]	4.3	4
341	4{24,26,14}	COCCNC1=C(CCC2=CC=CC=C2)N=C2N1C=CN=C2C1 c:5,11,13,16,20,22,t:9	Z8741907130	1{24}	Nc1ncnc1Cl	2{26}	O=CCc1ccc1	3{14}	COCC[N+]#[C-]	3.2	4
342	4{223,194,29}	CCOC(=O)CCNC1=C(N=C2C=CC(=NN12)C(N)=O)C1=CC=C(N1C)C(=O)OC c:12,14,24,t:8,10,22	Z8798985052	1{223}	NC(=O)c1ccc(N)nn1	2{194}	COC(=O)c1ccc(C=O)nn1C	3{29}	CCOC(=O)C[N+]#[C-]	3.9	4
343	4{161,94,11}	BrC1=CC(CNC2=C(N=C3C=CC=NN23)C2=N=C=CN=C2)=CC=C1 c:10,12,19,21,23,25,t:1,6,8,17	Z8803896956	1{161}	Nc1cccnn1	2{94}	O=Cc1cncn1	3{11}	Br1cccc(C[N+]#[C-])c1	3.6	3
344	4{224,95,63}	CN(C)C1=NC=CC(=C1)C1=C(NCC(F)F)N2N=C(C=CC2=N1)C1CC1 c:5,7,10,18,20,23,t:3	Z8781341778	1{224}	Nc1ccc(nn1)C2CC2	2{95}	CN(C)c1cc(C=O)ccn1	3{63}	FC(F)C[N+]#[C-]	3.2	3
345	4{225,195,27}	CCCCNC1=C(N=C2C=C(Cl)C=NN12)C1=CC(F)=C(OC)N=C1 c:12,24,t:5,7,9,17,20	Z8778278044	1{225}	Nc1cc(Cl)ccnn1	2{195}	COc1ncc(C=O)cc1F	3{27}	CCCC[N+]#[C-]	3.0	3
346	4{226,97,17}	CC(C)(C)C1=CC=CC2=NC(=C(NCC3CCOCC3)N12)C1=CC=C(F)C=C1 c:6,29,t:4,8,10,24,26	Z8784060117	1{226}	CC(C)(C)c1cccc(N)n1	2{97}	Fc1ccc(C=O)cc1	3{17}	[C-]#[N+]CC1C COCC1	3.2	3
347	4{227,135,47}	CC(C)NC1=C(N=C2C=NC(Br)=C(Cl)N12)C1=C(C)N(C)N=C1C c:8,17,22,t:4,6,11	Z8810903047	1{227}	Nc1enc(Br)c(Cl)n1	2{135}	Cc1nn(C)c(C)c1C=O	3{47}	CC(C)[N+]#[C-]	3.2	3
348	4{228,14,7}	CC1=CC=C(C=C1)C1=C(NC2CCOCC2)N2C=CN3C=CN=C3C2=N1 c:3,5,8,19,22,24,28,t:1	Z8778277397	1{228}	Nc1ncn2ccnc12	2{14}	Cc1ccc(C=O)cc1	3{7}	[C-]#[N+]C1CC OCC1	2.6	3
349	4{229,196,64}	COC(=O)[C@@H]1CC[C@@H](C1)NC1=C(N=C2C=CC(=CN12)S(O)(=O)=O)C1=C(C)C=C(C=C1)N1C=CN=C1 &1:4,7,r,c:15,17,26,29,31,35,37,t:11,13	Z8810903023	1{229}	Nc1ccc(en1)S(=O)(=O)O	2{196}	Cc1ccc(ccc1C=O)n2ccnc2	3{64}	COC(=O)[C@@H]1CC[C@@H](C1)[N+]#[C-] &1:4,7,r	3.4	3
350	4{176,197,14}	COCCNC1=C(N=C2N1C=CN=C2N1CCCC1)C1=NN(C)C(=C1)C(=O)OC c:7,11,13,26,t:5,22	Z8798985046	1{176}	Nc1ncnc1N2CCCC2	2{197}	COC(=O)c1ccc(C=O)nn1C	3{14}	COCC[N+]#[C-]	2.4	2
351	4{230,198,34}	CCC1=NN(C)C=C1C1=C(NCC2CCCO2)N2C=C(Br)C=C(C(C)O)C2=N1 c:6,9,29,t:2,20,23	Z8810902957	1{230}	CC(O)c1cc(Br)cn1N	2{198}	CCc1nn(C)cc1C=O	3{34}	[C-]#[N+]CC1C COO1	2.6	2

352	4{231,63,37}	COCN1N=CC=C1C1=C(NC2CC(C2)C(=O)O)C)N2N=C(C=CC2=N1)C(F)(F)F c:4,6,9,22,24,27	Z8781341773	1{231}	Nc1ccc(nn1)C(F)(F)F	2{63}	COCn1nccc1 C=O	3{37}	COC(=O)C1 CC(C1)[N+] #[C-]	2.4	2
353	4{232,41,17}	COC1=CC=NN2C(NCC3CCOCC3)=C(N=C12)C1=NC=CC=C1 c:4,16,24,26,t:2,18,22	Z8778277287	1{232}	COc1ccnnc1N	2{41}	O=Cc1cccc1	3{17}	[C-] #[N+]CC1C COCC1	1.8	2
354	4{233,97,27}	CCCCN1=C(N=C2N1C=C(Cl)C(Cl)=C2Cl)C1=CC=C(F)C=C1 c:7,15,24,t:5,11,19,21	Z8780122034	1{233}	Nc1ncc(Cl)c(Cl)c1Cl	2{97}	Fc1ccc(C=O)cc1	3{27}	CCCC[N+]#[C-]	2.0	2
355	4{234,199,10}	O=C1N(CC2=C(NC3CCOC3)N3C=CN=C(OC4CCC4)C3=N2)C(=O)C2=C1C=CC=C2 c:4,14,25,30,33,35,t:16	Z8810903007	1{234}	Nc1ncnc1OC2CCC2	2{199}	O=CCN1C(=O)c2cccc2C1=O	3{10}	[C-] #[N+]C1CC OC1	2.2	2
356	4{128,200,23}	COCCN(C)C1=CN2C(C=C1)=NC(CCCC#CC)=C2NC(CCC(=O)OC)C(=O)OC c:10,12,20,t:6	Z8808559870	1{128}	COCCN(C)c1ccc(N)nc1	2{200}	CC#CCCC=O	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	1.6	1
357	4{229,201,64}	COC(=O)[C@@H]1CC[C@@H](C1)NC1=C(N=C2C=CC(=CN12)S(O)(=O)=O)C1=CC(F)=C(C)C=C1 &1:4,7,r,c:15,17,32,t:11,13,26,29	Z8803896930	1{229}	Nc1ccc(en1)S(=O)(=O)O	2{201}	Cc1ccc(C=O)cc1F	3{64}	COC(=O)[C@@H]1CC[C@@H](C1)[N+]#[C-] &1:4,7,r	1.4	1
358	4{235,77,27}	CCCCN1=C(CC2CCCC2)N=C2N1C=CC1=C2C=CC=C1 c:5,14,18,20,23,25	Z8797776760	1{235}	Nc1nccc2ccc12	2{77}	O=CCC1CC CC1	3{27}	CCCC[N+]#[C-]	0.0	0
359	4{236,94,6}	CCOC(=O)CCCN1=C(N=C2N1C=CC1=C2C=NC=C1)C1=NC=CN=C1 c:11,15,17,20,22,27,29,t:9,25	Z8797775788	1{236}	Nc1nccc2ccncc12	2{94}	O=Cc1cncn1	3{6}	CCOC(=O)C CC[N+]#[C-]	0.0	0
360	4{237,58,14}	COCCN1=C(N=C2C=C3C=CC=C(Br)C3=CN12)C1=NSN=C1 c:11,17,25,t:5,7,9,13,22	Z8797774930	1{237}	Nc1cc2cccc(Br)c2cn1	2{58}	O=Cc1cnsn1	3{14}	COCC[N+]#[C-]	0.0	0
361	4{23,202,21}	FC1=CN=CC(F)=C1C1=C(NCC2CC2)N2C(C=NC=C2Br)=N1 c:3,6,9,19,21,24,t:1	Z8808559895	1{23}	Nc1cnc(Br)n1	2{202}	Fc1cnc(F)c1C=O	3{21}	[C-] #[N+]CC1C C1	0.0	0
362	4{238,203,6}	CCOC(=O)CCCN1=C(N=C2N1C=CC(OC)=C2C#N)C1=NN(CC(F)F)C=C1 c:11,15,19,31,t:9,24	Z8808559887	1{238}	COc1cnc(N)c1C#N	2{203}	FC(F)Cn1ccc(C=O)n1	3{6}	CCOC(=O)C CC[N+]#[C-]	0.0	0
363	4{184,204,7}	CSC1=NC=C(N1C)C1=C(NC2CCOCC2)N2C=C(C=CC2=N1)C(N)=S c:4,9,20,22,25,t:2	Z8808559884	1{184}	NC(=S)c1ccc(N)nc1	2{204}	CSc1ncc(C=O)n1C	3{7}	[C-] #[N+]C1CC OCC1	0.0	0

364	4{111,55,3}	COC(=O)C1=CN2C(NC3=C(F)C=C(Cl)C=C3)=C(N=C2C(C)=C1)C1=CC(=NC=C1)P(C)(C)=O c:9,15,17,19,23,28,30,t:4,12,26	Z8808559857	1{111}	COC(=O)c1cnc(N)c(C)c1	2{55}	CP(=O)(C)c1cc(C=O)cen1	3{3}	Fe1cc(Cl)ccc1[N+]#[C-]	0.0	0
365	4{211,90,65}	CC1=NC(=CO1)C1=C(NC2CCCC2)N2C=CC=C(C3=NN=NN3)C2=N1 c:3,7,17,23,28,t:1,19,21	Z8808559854	1{211}	Nc1ncccc1c2nnn[nH]2	2{90}	Cc1nc(C=O)col	3{65}	[C-]#[N+]C1CC1	0.0	0
366	4{239,123,22}	CC1=NC=C(N=C1)C1=C(NC2COC2)N2C=C(C=CC2=N1)N1CCCC1 c:3,5,8,17,19,22,t:1	Z8810903042	1{239}	Cl.Cl.Nc1ccc(en1)N2CCCC2	2{123}	Cc1cnc(C=O)en1	3{22}	[C-]#[N+]C1CO1	0.0	0
367	4{63,205,10}	COC(=O)C1=C2COCCN2C(=C1)C1=C(NC2COC2)N2C=CC(C)=C(OC)C2=N1 c:4,12,15,25,33,t:28	Z8810902998	1{63}	COc1c(C)ccnc1N	2{205}	COC(=O)c1cc(C=O)n2CCOCc12	3{10}	[C-]#[N+]C1CCOC1	0.0	0
368	4{240,206,15}	CCNC1=C(C[C@H](C)NC(=O)OC(C)(C)C)N=C2C=CC(=CN12)C1=NNN=N1 c:3,18,20,28,t:16,25	Z8810902974	1{240}	Nc1ccc(en1)c2nn[nH]n2	2{206}	C[C@@H](CC=O)NC(=O)OC(C)(C)C	3{15}	CC[N+]#[C-]	0.0	0
369	4{241,199,21}	BrC1=NN2C(C=C1)=NC(CN1C(=O)C3=C(C=CC=C3)C1=O)=C2NCC1CC1 c:5,7,16,18,23,t:1,14	Z8810902971	1{241}	Nc1ccc(Br)nn1	2{199}	O=CCN1C(=O)c2ccccc2C1=O	3{21}	[C-]#[N+]CC1C1	0.0	0
370	4{242,10,27}	CCCCNC1=C(N=C2N1C=C(C=C2Cl)C(N)=O)C1=NC=CC(C)=C1 c:7,11,13,22,25,t:5,20	Z8786904184	1{242}	NC(=O)c1cnc(N)c(Cl)c1	2{10}	Cc1cnc(C=O)c1	3{27}	CCCC[N+]#[C-]	0.0	0
371	4{243,40,20}	COC1=CC(C)=C(NC2=C(N=C3N2N=C(Cl)C2=C3C=CC=C2)C2=NC(CO)=CS2)C=C1 c:10,17,20,22,29,33,t:2,5,8,14,25	Z8778277875	1{243}	Nc1nnc(Cl)c2ccccc12	2{40}	OCc1csc(C=O)n1	3{20}	COc1ccc([N+]#[C-])c(C)c1	0.0	0
372	4{244,84,66}	CSCCC1=C(NC(C)C2=CC=CC=C2)N2C=C(N=CC2=N1)C#N c:4,11,13,17,19,22,t:9	Z8781341800	1{244}	Nc1cnc(C#N)en1	2{84}	CSCCC=O	3{66}	CC([N+]#[C-])c1ccccc1	0.0	0
373	4{245,207,37}	COC(=O)C1CC(C1)NC1=C(N=C2C=CC=C(N12)C(C)(F)F)C1=CC(=NN1C)C(=O)OC c:14,16,27,t:10,12,25	Z8781341781	1{245}	Cl.CC(F)(F)c1cccc(N)n1	2{207}	COC(=O)c1cc(C=O)n(C)n1	3{37}	COC(=O)C1CC(C1)[N+]#[C-]	0.0	0
374	4{246,97,20}	COC(=O)C1=C2N(C=CN3C(NC4=C(C)C=C(OC)C=C4)=C(N=C23)C2=CC=C(F)C=C2)N=C1 c:7,12,19,21,32,35,t:4,15,23,27,29	Z8784060942	1{246}	COC(=O)c1cmn2ccnc(N)c12	2{97}	Fe1ccc(C=O)cc1	3{20}	COc1ccc([N+]#[C-])c(C)c1	0.0	0
375	4{247,41,7}	C1CC(CCO1)NC1=C(N=C2N1C=CN1N=CN=C21)C1=NC=CC=C1 c:10,14,17,25,27,t:8,19,23	Z8784060639	1{247}	Nc1nccn2ncnc12	2{41}	O=Cc1ccccn1	3{7}	[C-]#[N+]C1CCOCC1	0.0	0

376	4{248,22,14}	COCCNC1=C(N=C2N1C=CC1=C2SC=C1)C1=CC=CC=C1 c:7,11,13,17,22,24,t:5,20	Z8784060579	1{248}	Nc1nccc2ccsc12	2{22}	O=Cc1cccc1	3{14}	COCC[N+][#C-]	0.0	0
377	4{20,170,6}	CCOC(=O)CCCNC1=C(N=C2N1C(C)=CC(C)=C2C(N)=O)C1=NN(CC)N=N1 c:11,16,19,30,t:9,25	Z8780122411	1{20}	Cl.Cc1cc(C)c(C(=O)N)c(N)n1	2{170}	CCn1nnc(C=O)n1	3{6}	CCOC(=O)CC[N+][#C-]	0.0	0
378	4{249,10,17}	CC1=CC(=NC=C1)C1=C(NCC2CCOCC2)N2N=C(C)C=C(C2=N1)C(F)(F)F c:3,5,8,23,26,t:1,20	Z8780122347	1{249}	Cc1cc(c(N)nn1)C(F)(F)F	2{10}	Cc1ccnc(C=O)c1	3{17}	[C-][#N+]CC1C COCC1	0.0	0
379	4{250,14,14}	COCCNC1=C(N=C2N1C=C(Br)C=C2S(=O)(=O)N1CCCC1)C1=CC=C(C)C=C1 c:7,14,31,t:5,11,26,28	Z8780122344	1{250}	Nc1ncc(Br)cc1S(=O)(=O)N2CCCC2	2{14}	Cc1ccc(C=O)cc1	3{14}	COCC[N+][#C-]	0.0	0
380	4{14,26,54}	COC1=NC=CC2=NC(CCC3=CC=CC=C3)=C(NC3=CC=CC=C3)N12 c:4,13,15,22,24,t:2,6,11,17,20	Z8711876243	1{14}	COc1nccc(N)n1	2{26}	O=CCCc1cccc1	3{54}	[C-][#N+]c1cccc1	0.0	0
381	4{9,14,17}	CC1=CC=C(C=C1)C1=C(NCC2CCOCC2)N2C=C(Cl)C=NC2=N1 c:3,5,8,23,26,t:1,20	Z8711871953	1{9}	Nc1ncc(Cl)cn1	2{14}	Cc1ccc(C=O)cc1	3{17}	[C-][#N+]CC1C COCC1	0.0	0
382	4{251,208,23}	CCC1=CN=C(S1)C1=C(NC(CCC(=O)OC)C(=O)OC)N2C(C=CC3=C2NC(=O)C=C3)=N1 c:4,8,24,26,32,34,t:2	Z8801681813	1{251}	Nc1ccc2ccc(=O)[nH]c2n1	2{208}	CCc1enc(C=O)s1	3{23}	COC(=O)CC C([N+][#C-])C(=O)OC	0.0	0
383	4{252,97,20}	COC1=CC(C)=C(NC2=C(N=C3N2C=CC(F)=C3)C2=CC=C(F)C=C2)C=C1 c:10,14,17,26,29,t:2,5,8,21,23	Z8797786651	1{252}	Nc1nccc(F)c11	2{97}	Fc1ccc(C=O)cc1	3{20}	COc1ccc([N+][#C-])c(C)c1	0.0	0
384	4{253,69,14}	COCCNC1=C(N=C2C=CC=C(N12)C(N)=S)C1=NN(C)C(C)=C1 c:9,11,24,t:5,7,19	Z8797781693	1{253}	NC(=S)c1ccc(N)n1	2{69}	Cc1cc(C=O)nn1C	3{14}	COCC[N+][#C-]	0.0	0
385	4{254,182,54}	COC(=O)C1=CN2C(C=C1C)=NC(=C2NC1=C C=CC=C1)C1=NC=CN1CC#C c:8,11,13,19,21,26,t:4,17,24	Z8778278035	1{254}	COC(=O)c1cnc(N)cc1C	2{182}	O=Cc1nccn1CC#C	3{54}	[C-][#N+]c1cccc1	0.0	0
386	4{22,207,13}	COC(=O)C1=NN(C)C(=C1)C1=C(NCC2=CC=C(OC)C=C2)N2N=C(Cl)C=CC2=N1 c:8,11,21,28,31,t:4,15,17,25	Z8803896962	1{22}	Nc1ccc(Cl)nn1	2{207}	COC(=O)c1cc(C=O)n(C)n1	3{13}	COc1ccc(C[N+][#C-])cc1	0.0	0
387	4{220,209,22}	C1CC1C1=CC=CN2C(NC3COC3)=C(N=C12)C1=NN=C2CCCCN12 c:6,15,t:4,17,21,23	Z8803896927	1{220}	Cl.Nc1nccc1C2CC2	2{209}	O=Cc1nnc2C CCCn12	3{22}	[C-][#N+]C1CO C1	0.0	0

388	4{255,210,39}	CCOCCNC1=C(N=C2C=CC3=NC=C(Br)N3N12)C1=C(F)C=C(C=C1)C1=CC=NC=C1 c:10,22,25,27,32,34,t:6,8,12,14,30	Z8803896923	1{255}	Nc1ccc2ncc(Br)n2n1	2{210}	Fe1cc(ccc1C=O)c2ccncc2	3{39}	CCOCC[N+]#[C-]	0.0	0
389	4{256,211,67}	CCC(C)NC1=C(N=C2C=CC3=NN=NN3N12)C1=C(Br)C=CC(Cl)=C1F c:9,13,20,23,26,t:5,7,11	Z8803896957	1{256}	Nc1ccc2nnn2n1	2{211}	Fe1c(Cl)ccc(Br)c1C=O	3{67}	CCC(C)[N+]#[C-]	0.0	0
390	4{125,212,15}	CCNC1=C(N=C2C=CC(CCO)=CN12)C1=NO C(=C1)C(F)F c:7,12,20,t:3,5,17	Z8808559873	1{125}	Nc1ccc(CC(O)n1	2{212}	FC(F)c1cc(C=O)no1	3{15}	CC[N+]#[C-]	0.0	0
391	4{257,213,28}	CCCNC1=C(N=C2N1C=CN=C2OCC(F)F)C1=C2COCCN2N=N1 c:6,10,12,20,28,t:4	Z8808559872	1{257}	Nc1ncnc1OCC(F)F	2{213}	O=Cc1nm2COCc12	3{28}	CCC[N+]#[C-]	0.0	0
392	4{92,214,14}	COCCNC1=C(N=C2C=C(C=CN12)C(N)=O)C1=CC=NN1CC(C)C c:9,11,21,t:5,7,19	Z8810903048	1{92}	NC(=O)c1cnc(N)c1	2{214}	CC(C)Cn1ncc1C=O	3{14}	COCC[N+]#[C-]	0.0	0
393	4{78,215,39}	CCOCCNC1=C(N=C2C=C(C)C3=NC(C)=CN3N12)C1=NC(=CS1)C1=CC=CC=C1 c:16,25,31,33,t:6,8,10,13,23,29	Z8810903022	1{78}	Cc1cn2nc(N)cc(C)c2n1	2{215}	O=Cc1nc(cs1)c2ccccc2	3{39}	CCOCC[N+]#[C-]	0.0	0
394	4{111,216,22}	COC(=O)C1=NC=C(S1)C1=C(NC2COC2)N2 C=C(C=C(C)C2=N1)C(=O)OC c:6,10,19,25,t:4,21	Z8810902995	1{111}	COC(=O)c1cnc(N)c(C)c1	2{216}	COC(=O)c1ncc(C=O)s1	3{22}	[C-]#[N+]C1CO C1	0.0	0
395	4{169,207,13}	CNC(=O)C1=NN2C(C=C1)=NC(=C2NCC1=C C=C(OC)C=C1)C1=CC(=NN1C)C(=O)OC c:8,10,12,23,28,t:4,17,19,26	Z8810902985	1{169}	CNC(=O)c1ccc(N)nn1	2{207}	COC(=O)c1cc(C=O)n(C)n1	3{13}	COc1ccc(C[N+]#[C-])cc1	0.0	0
396	4{258,217,67}	CCC(C)NC1=C(N=C2C=CC3=C(N=CC=N3)N12)C1=CC(=O)N(C)C=C1 c:9,13,15,27,t:5,7,11,21	Z8810902984	1{258}	Nc1ccc2nccnc2n1	2{217}	Cn1ccc(C=O)cc1=O	3{67}	CCC(C)[N+]#[C-]	0.0	0
397	4{259,11,7}	FC(F)(F)CN1C=CC(=N1)C1=C(NC2CCOCC2)N2C(=N1)C(=CC1=C2CCC(F)(F)C1)C#N c:6,8,11,22,25,27	Z8810902976	1{259}	Nc1nc2CC(C(F)(F)C)c2cc1C#N	2{11}	FC(F)(F)Cn1ccc(C=O)n1	3{7}	[C-]#[N+]C1CCOCC1	0.0	0
398	4{260,218,14}	COCCNC1=C(N=C2N1C=CC=C2N1CCCC1)C1CC(C1)OC c:7,11,13,t:5	Z8810902962	1{260}	Nc1ncccc1N2CCCC2	2{218}	COC1CC(C1)C=O	3{14}	COCC[N+]#[C-]	0.0	0
399	4{261,21,39}	CCOCCNC1=C(N=C2C=CC(=CN12)N1CCC(C1)N(C)C)C1=CC2=NC=NN2C=C1 c:10,12,31,35,t:6,8,27,29	Z8798985033	1{261}	CN(C)C1C CN(CC1)c2ccc(N)nc2	2{21}	O=Cc1cn2nccnc2c1	3{39}	CCOCC[N+]#[C-]	0.0	0
400	4{262,181,28}	CCCNC1=C(N=C2C=CC(NC(C)=O)=CN12)C1=CN=C2CCCN12 c:8,14,t:4,6,19,21	Z8786958954	1{262}	CC(=O)Nc1ccc(N)nc1	2{181}	O=Cc1cnc2C CCn12	3{28}	CCC[N+]#[C-]	0.0	0
401	4{263,121,25}	CCC1=CON=C1C1=C(NCCCF)N2C=CC=C(C(F)F)C2=N1 c:5,8,16,24,t:2,18	Z8781341772	1{263}	Nc1ncccc1C(F)F	2{121}	CCc1cnc1C=O	3{25}	FCCC[N+]#[C-]	0.0	0

402	4{264,44,27}	CCCCNC1=C(N=C2C=NC=C(N3CCCC3)N12)C1=CN(CC)N=C1 c:9,27,t:5,7,11,22	Z8784060344	1{264}	Nc1ncce(n1)N2CCCC2	2{44}	CCn1cc(C=O)cn1	3{27}	CCCC[N+][#][C-]	0.0	0
403	4{18,40,20}	COC1=CC(C)=C(NC2=C(N=C3C=C(Br)C(=CN23)[N+][O-])=O)C2=NC(CO)=CS2)C=C1 c:15,27,31,t:2,5,8,10,12,23	Z8780122420	1{18}	Nc1cc(Br)c(c1)[N+](=O)[O-]	2{40}	OCc1csc(C=O)n1	3{20}	COc1ccc([N+][#][C-])c(C)c1	0.0	0
404	4{17,14,7}	CC1=CC=C(C=C1)C1=C(NC2CCOCC2)N2C=CC=C(C2=N1)[N+][O-]=O c:3,5,8,19,21,24,t:1	Z8780122033	1{17}	Nc1ncce1[N+](=O)[O-]	2{14}	Cc1ccc(C=O)cc1	3{7}	[C-][#][N+]C1CCOCC1	0.0	0
405	4{265,80,14}	COCCNC1=C(N=C2N1C(F)=CC=C2F)C1=NC=C(C)S1 c:7,12,14,t:5,18,20	Z8780121774	1{265}	Nc1nc(F)cc1F	2{80}	Cc1cnc(C=O)s1	3{14}	COCC[N+][#][C-]	0.0	0
406	4{3,26,17}	C(CC1=CC=CC=C1)C1=C(NCC2CCOCC2)N2C=CSC2=N1 c:4,6,9,21,25,t:2	Z8711876688	1{3}	Nc1ncs1	2{26}	O=CCCc1ccc1	3{17}	[C-][#][N+]CC1C COCC1	0.0	0
407	4{266,22,13}	COC1=CC=C(CNC2=C(N=C3N2C=CN=C3C#N)C2=CC=CC=C2)C=C1 c:10,14,16,23,25,28,t:2,4,8,21	Z8741907203	1{266}	Nc1ncnc1C#N	2{22}	O=Cc1cccc1	3{13}	COc1ccc(C[N+][#][C-])cc1	0.0	0
408	4{267,219,1}	CN1C=C(C=C1C#N)C1=C(NC2CC2)N2C(C=CC=C2C#C)=N1 c:2,4,9,18,20,24	Z8801681851	1{267}	Nc1cccc(C#C)n1	2{219}	Cn1cc(C=O)cc1C#N	3{1}	[C-][#][N+]C1CC1	0.0	0
409	4{174,220,51}	CC1=C(C(C)=NN1)C1=C(NCCNC(=O)OC(C)(C)C)N2C(C=CC=C2C#N)=N1 c:4,8,23,25,29,t:1	Z8801681843	1{174}	Nc1cccc(C#N)n1	2{220}	Cc1n[nH]c(C)c1C=O	3{51}	CC(C)(C)OC(=O)NCC[N+][#][C-]	0.0	0
410	4{99,68,41}	COC1=CC=C(NC2=C(N=C3C=CC(=CN23)S(N)(=O)=O)C2=NC=C(S2)C(C)O)C=C1 c:11,13,24,31,t:2,4,7,9,22	Z8801681811	1{99}	Nc1ccc(c1)S(=O)(=O)N	2{68}	CC(O)c1nc(C=O)s1	3{41}	COc1ccc([N+][#][C-])cc1	0.0	0
411	4{268,94,17}	NC(=O)C1=CC(OC2=CN3C(C=C2)=NC(=C3)NCC2CCOCC2)C2=NC=CN=C2)=CC=C1 c:11,13,15,29,31,33,35,t:3,7,27	Z8797784545	1{268}	NC(=O)c1ccc(Oc2ccc(N)nc2)c1	2{94}	O=Cc1cncn1	3{17}	[C-][#][N+]CC1C COCC1	0.0	0
412	4{269,9,27}	CCCCNC1=C(N=C2C=C3C=CNC3=CN12)C1=CSC=C1 c:11,15,23,t:5,7,9,20	Z8797773920	1{269}	Nc1cc2cc[nH]c2cn1	2{9}	O=Cc1ccsc1	3{27}	CCCC[N+][#][C-]	0.0	0
413	4{270,112,13}	COC1=CC=C(CNC2=C(N=C3C=CC4=NC=NN4N23)C2=C3C=CC=NN3N=C2)C=C1 c:12,16,23,25,27,31,34,t:2,4,8,10,14	Z8778278047	1{270}	Nc1ccc2ncn2n1	2{112}	O=Cc1cmn2ncccc12	3{13}	COc1ccc(C[N+][#][C-])cc1	0.0	0
414	4{76,84,18}	CSCCC1=C(NC(C)(C)C)N2C(C=CC(C)=C2C1)=N1 c:4,13,16,19	Z8778278030	1{76}	Cc1ccc(N)nc1Cl	2{84}	CSCCC=O	3{18}	CC(C)(C)[N+][#][C-]	0.0	0

415	4{151,157,9}	CNC1=C(N=C2C=NC=C(Cl)N12)C1=NC2=C(C=C1)N=CC=C2 c:6,16,18,21,23,t:2,4,8,14	Z8803896945	1{151}	Nc1cnc(Cl)n1	2{157}	O=Cc1ccc2ncccc2n1	3{9}	C[N+]#[C-]	0.0	0
416	4{222,221,5}	COCCNC1=C(N=C2C=NC(=CN12)C(=O)OC)C1=NC(OC)=C(C)S1 c:10,12,t:6,8,21,25	Z8803896936	1{222}	Cl.COC(=O)c1cnc(N)cn1	2{221}	COc1nc(C=O)sc1C	3{5}	COCCC[N+]#[C-]	0.0	0
417	4{262,222,10}	COC1=C(OCCN2CCOCC2)C=CC(=C1)C1=C(NC2CCOC2)N2C=C(NC(C)=O)C=CC2=N1 c:2,14,16,19,35,38,t:29	Z8808559889	1{262}	CC(=O)Nc1ccc(N)nc1	2{222}	COc1cc(C=O)ccc1OCCN2CCOCC2	3{10}	[C-]#[N+]C1CCOC1	0.0	0
418	4{145,223,3}	COC(=O)C1=NC=C(C=C1)C1=C(NC2=C(F)C=C(C1)C=C2)N2C(C=CC=C2S(C)(=O)=O)=N1 c:6,8,11,14,20,25,27,33,t:4,17	Z8808559871	1{145}	CS(=O)(=O)c1cccc(N)n1	2{223}	Cl.COC(=O)c1ccc(C=O)cn1	3{3}	Fe1cc(Cl)ccc1[N+]#[C-]	0.0	0
419	4{105,224,66}	CC(NC1=C(N=C2C=CC=C(N12)C(N)=O)C1COC1C)C1=CC=CC=C1 c:7,9,26,28,t:3,5,24	Z8810903039	1{105}	NC(=O)c1ccc(N)n1	2{224}	CC1OCCC1C=O	3{66}	CC([N+]#[C-])c1ccccc1	0.0	0
420	4{158,225,18}	CC(C)(C)NC1=C(N=C2C=NC(=CN12)P(C)(C)=O)C1=C2C=NNC2=CC(Cl)=C1 c:9,11,20,22,26,29,t:5,7	Z8810903021	1{158}	CP(=O)(C)c1cnc(N)cn1	2{225}	Clc1cc(C=O)c2cn[nH]c2c1	3{18}	CC(C)(C)[N+]#[C-]	0.0	0
421	4{271,226,67}	CCC(C)NC1=C(N=C2C=CC(C(=O)OC)=C(F)N12)C1=C(C)N(CC(F)(F)F)N=C1 c:9,21,30,t:5,7,15	Z8810903011	1{271}	COC(=O)c1ccc(N)nc1F	2{226}	Cc1c(C=O)cn1CC(F)(F)F	3{67}	CCC(C)[N+]#[C-]	0.0	0
422	4{144,227,37}	CNS(=O)(=O)C1=CN2C(NC3CC(C3)C(=O)OC)=C(N=C2C=C1)C1=NC=CS1 c:18,20,23,28,t:5,26	Z8810902996	1{144}	CNS(=O)(=O)c1ccc(N)nc1	2{227}	O=Cc1nccs1	3{37}	COC(=O)C1CC(C1)[N+]#[C-]	0.0	0
423	4{158,228,32}	CC(C)(C)OC(=O)N1CCC(C1)C1=C(NC2CCC2)N2C=C(N=CC2=N1)P(C)(C)=O c:13,22,24,27	Z8798985055	1{158}	CP(=O)(C)c1cnc(N)cn1	2{228}	CC(C)(C)OC(=O)N1CCC(C1)C=O	3{32}	[C-]#[N+]C1CCOC1	0.0	0
424	4{272,229,29}	CCOC(=O)CCNC1=C(N=C2C=CC(CN3CCCC3)=CN12)C1=CN=C(OCCO)C=C1 c:12,21,34,t:8,10,26,28	Z8798985037	1{272}	Nc1ccc(CN2CCCC2)cn1	2{229}	OCCOc1ccc(C=O)cn1	3{29}	CCOC(=O)C[N+]#[C-]	0.0	0
425	4{273,230,64}	COC(=O)[C@@H]1CC[C@@H](C1)NC1=C(N=C2C=C3C=NNC3=CN12)C1=CC(OC)=CN=C1 &1:4,7,r,c:17,21,30,32,t:11,13,15,26	Z8786958894	1{273}	Nc1cc2cn[nH]c2cn1	2{230}	COc1cnc(C=O)c1	3{64}	COC(=O)[C@@H]1CC[C@@H](C1)[N+]#[C-] &1:4,7,r	0.0	0

426	4{274,69,6}	CCOC(=O)CCCNC1=C(N=C2N1C=C(C=C2F)C(=O)OC)C1=NN(C)C(C)=C1 c:11,15,17,30,t:9,25	Z8786938003	1{274}	COC(=O)c1cnc(N)c(F)c1	2{69}	Cc1cc(C=O)nn1C	3{6}	CCOC(=O)C CC[N+]#[C-]	0.0	0
427	4{275,58,7}	FC1=CC=C(Cl)N2C(NC3CCOCC3)=C(N=C12)C1=NSN=C1 c:15,24,t:1,3,17,21	Z8786838534	1{275}	Nc1nc(Cl)cc1F	2{58}	O=Cc1cnsn1	3{7}	[C-] #[N+]C1CC OCC1	0.0	0
428	4{276,48,7}	N#CCC1=CC=CC2=NC(=C(NC3CCOCC3)N12)C1=CNC(=N1)C1CCC1 c:5,25,t:3,7,9,22	Z8781341802	1{276}	Nc1cccc(C#N)n1	2{48}	O=Cc1c[nH]c(n1)C2CCC2	3{7}	[C-] #[N+]C1CC OCC1	0.0	0
429	4{137,112,14}	COCCNC1=C(N=C2C=CC(C)=NN12)C1=C2C=CC=NN2N=C1 c:9,12,17,19,21,25,t:5,7	Z8781341792	1{137}	Cc1ccc(N)n1	2{112}	O=Cc1cnn2ncccc12	3{14}	COCC[N+]#[C-]	0.0	0
430	4{277,231,4}	CCOC1=NN2C(C=C1)=NC(C1=NC3=C(CC(C)CC3)S1)=C2NCC1=NN(C)N=N1 c:7,9,23,32,t:3,12,14,28	Z8781341786	1{277}	CCOCc1ccc(N)n1	2{231}	CC1CCc2nc(C=O)sc2C1	3{4}	Cn1nnc(C[N+]#[C-])n1	0.0	0
431	4{213,232,27}	CCCCNC1=C(N=C2N1C(OC)=CC=C2F)C1=NOCC1 c:7,13,15,t:5,19	Z8780122425	1{213}	COc1ccc(F)c(N)n1	2{232}	O=CC1=NOCC1	3{27}	CCCC[N+]#[C-]	0.0	0
432	4{278,80,27}	CCCCNC1=C(N=C2C=CC(C#N)=C(F)N12)C1=NC=C(C)S1 c:9,t:5,7,13,19,21	Z8780122343	1{278}	Nc1ccc(C#N)c(F)n1	2{80}	Cc1cnc(C=O)s1	3{27}	CCCC[N+]#[C-]	0.0	0
433	4{279,77,6}	CCOC(=O)CCCNC1=C(CC2CCCC2)N=C2N1C=C(Br)C=C2S(=O)(=O)NC c:9,18,25,t:22	Z8780122340	1{279}	CNS(=O)(=O)c1cc(Br)cn1N	2{77}	O=CCC1CCCC1	3{6}	CCOC(=O)C CC[N+]#[C-]	0.0	0
434	4{279,58,27}	CCCCNC1=C(N=C2N1C=C(Br)C=C2S(=O)(=O)NC)C1=NSN=C1 c:7,14,25,t:5,11,22	Z8780122268	1{279}	CNS(=O)(=O)c1cc(Br)cn1N	2{58}	O=Cc1cnsn1	3{27}	CCCC[N+]#[C-]	0.0	0
435	4{280,26,7}	BrC1=C2N=CC=CC2=CC2=NC(CCC3=CC=C(C=C3)=C(NC3CCOCC3)N12 c:1,3,5,8,17,19,t:10,15,21	Z8776690337	1{280}	Nc1cc2cccn2c(Br)n1	2{26}	O=CCCc1ccc1	3{7}	[C-] #[N+]C1CC OCC1	0.0	0
436	4{244,26,26}	FC1=CC=C(CNC2=C(CCC3=CC=CC=C3)N=C3C=NC(=CN23)C#N)C=C1 c:7,13,15,20,22,29,t:1,3,11,18	Z8776690340	1{244}	Nc1cnc(C#N)n1	2{26}	O=CCCc1ccc1	3{26}	Fc1ccc(C[N+]#[C-])cc1	0.0	0
437	4{15,15,27}	CCCCNC1=C(N=C2C=CN=C(F)N12)C1=CC=C(OC)C=C1 c:9,23,t:5,7,11,17,19	Z8711876135	1{15}	Nc1cnc(F)n1	2{15}	COc1ccc(C=O)cc1	3{27}	CCCC[N+]#[C-]	0.0	0
438	4{281,14,54}	CC1=CC=C(C=C1)C1=C(NC2=CC=CC=C2)N2C=CN=C(F)C2=N1 c:3,5,8,13,15,19,25,t:1,11,21	Z8711876133	1{281}	Nc1cncnc1F	2{14}	Cc1ccc(C=O)cc1	3{54}	[C-] #[N+]c1cccc1	0.0	0
439	4{282,26,14}	COCCNC1=C(CCC2=CC=CC=C2)N=C2C=N=C(C(O)N12 c:5,11,13,18,t:9,16,20	Z8711875965	1{282}	Nc1cnc(O)n1	2{26}	O=CCCc1ccc1	3{14}	COCC[N+]#[C-]	0.0	0

440	4{8,26,17}	CC1=NC2=NC(CCC3=CC=CC=C3)=C(NCC3CCOCC3)N2C(C)=C1 c:10,12,28,t:1,3,8,14	Z8711872601	1{8}	Cc1cc(C)nc(N)n1	2{26}	O=CCCc1ccc1	3{17}	[C-]#[N+]CC1C COCC1	0.0	0
441	4{283,233,39}	CCOCCNC1=C(CCCOCC=C)N=C2C=CC3=C(N=CC(=C3)C(=O)OC)N12 c:6,17,21,23,t:15,19	Z8801681852	1{283}	COC(=O)c1cnc2nc(N)ccc2c1	2{233}	C=CCOCCC C=O	3{39}	CCOCC[N+]#[C-]	0.0	0
442	4{284,234,32}	N#CCC1=CC2=NC(=C(NC3CCCC3)N2C=C1)C1=NN=C2CCCCCN12 c:17,t:3,5,7,20,22	Z8801681812	1{284}	Nc1cc(CC#N)ccn1	2{234}	O=Cc1nnc2CCCCn12	3{32}	[C-]#[N+]C1CC C1	0.0	0
443	4{285,10,7}	CC1=CC(=NC=C1)C1=C(NC2CCOCC2)N2C(=N1)C1=C(C=C(Br)C=C1)C=C2C c:3,5,8,19,27,30,t:1,22,24	Z8797779857	1{285}	Cc1cc2cc(Br)ccc2c(N)n1	2{10}	Cc1ccnc(C=O)c1	3{7}	[C-]#[N+]C1CC OCC1	0.0	0
444	4{284,157,11}	BrC1=CC(CNC2=C(N=C3C=C(CC#N)C=CN23)C2=NC3=C(C=C2)N=CC=C3)=CC=C1 c:15,22,24,27,29,31,33,t:1,6,8,10,20	Z8778278043	1{284}	Nc1cc(CC#N)ccn1	2{157}	O=Cc1ccc2ncccc2n1	3{11}	Br1cccc(C[N+]#[C-])c1	0.0	0
445	4{94,79,27}	CCCCNC1=C(N=C2C=CC(F)=NN12)C1=NC=CO1 c:9,12,19,t:5,7,17	Z8778278041	1{94}	Nc1ccc(F)n1	2{79}	O=Cc1ncco1	3{27}	CCCC[N+]#[C-]	0.0	0
446	4{81,129,9}	CNC1=C(N=C2C=NC=CN12)C1=CC=CC2=NC=NN12 c:6,8,15,19,t:2,4,13,17	Z8808559888	1{81}	Nc1cncn1	2{129}	O=Cc1cccc2ncnn12	3{9}	C[N+]#[C-]	0.0	0
447	4{286,235,23}	COC(=O)CCC(NC1=C(N=C2C=CC(=CN12)C1=NC=CC=C1)C1=CSC(=C1)C#N)C(=O)OC c:12,14,21,23,29,t:8,10,19,26	Z8808559878	1{286}	Cl.Cl.Nc1cc(cn1)c2ccc cn2	2{235}	O=Cc1csc(C#N)c1	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	0.0	0
448	4{287,236,21}	C1C1=CC2=NC(CCC3OCCO3)=C(NCC3CC3)N2C=C1 c:23,t:1,3,13	Z8810903029	1{287}	Nc1cc(Cl)cc n1	2{236}	O=CCCC1O CCO1	3{21}	[C-]#[N+]CC1C C1	0.0	0
449	4{288,148,39}	CCOCCNC1=C(N=C2C=C(NC(=O)OC(C)(C)C)C=CN12)C1=C(OC)N(C)N=C1C c:20,25,31,t:6,8,10	Z8810903014	1{288}	CC(C)(C)OC(=O)Nc1cnc(N)c1	2{148}	COc1c(C=O)c(C)nn1C	3{39}	CCOCC[N+]#[C-]	0.0	0
450	4{238,237,26}	COC1=C(C#N)C2=NC(C3CCCOCC3)=C(NC3=CC=C(F)C=C3)N2C=C1 c:2,25,30,t:6,16,20,22	Z8810902986	1{238}	COc1cnc(N)c1C#N	2{237}	O=CC1CCC OCC1	3{26}	Fc1ccc(C[N+]#[C-])cc1	0.0	0
451	4{158,2,31}	CSCCNC1=C(N=C2C=NC(=CN12)P(C)(C)=O)C1=C(F)C=NC(Cl)=C1 c:9,11,20,23,26,t:5,7	Z8798985045	1{158}	CP(=O)(C)c1cnc(N)cn1	2{2}	Fc1cnc(Cl)cc 1C=O	3{31}	CSCC[N+]#[C-]	0.0	0
452	4{284,95,30}	CN(C)C1=NC=CC(=C1)C1=C(NCC2=CN(C)N=C2)N2C=CC(CC#N)=CC2=N1 c:5,7,10,18,22,27,30,t:3,14	Z8781341770	1{284}	Nc1cc(CC#N)ccn1	2{95}	CN(C)c1cc(C=O)ccn1	3{30}	Cn1cc(C[N+]#[C-])cn1	0.0	0

453	4{21,69,17}	CN1N=C(C=C1C)C1=C(NCC2CCOCC2)N2C(=N1)C(=CC=C2Cl)S(N)(=O)=O c:2,4,8,20,23,25	Z8780122404	1{21}	Nc1nc(Cl)ccc1S(=O)(=O)N	2{69}	Cc1cc(C=O)nn1C	3{17}	[C-]#[N+]CC1C COCC1	0.0	0
454	4{289,97,6}	CCOC(=O)CCCN1=C(N=C2N1C=CC=C2C(F)(F)C(F)(F)F)C1=CC=C(F)C=C1 c:11,15,17,32,t:9,27,29	Z8780122348	1{289}	Cl.Nc1nccc1C(F)(F)C(F)(F)F	2{97}	Fc1ccc(C=O)cc1	3{6}	CCOC(=O)C CC[N+]#[C-]	0.0	0
455	4{290,41,7}	COC(=O)C1=CC=C(Br)N2C(NC3CCOCC3)=C(N=C12)C1=NC=CC=C1 c:18,26,28,t:4,6,20,24	Z8780122335	1{290}	COC(=O)c1ccc(Br)nc1N	2{41}	O=Cc1ccccn1	3{7}	[C-]#[N+]C1CC OCC1	0.0	0
456	4{5,26,17}	C(NC1=C(CCC2=CC=CC=C2)N=C2NN=NN12)C1CCOCC1 c:2,8,10,16,t:6,13	Z8711892497	1{5}	Nc1nnn[nH]1	2{26}	O=CCCc1ccc1	3{17}	[C-]#[N+]CC1C COCC1	0.0	0
457	4{291,22,54}	C1C1=CN2C(NC3=CC=CC=C3)=C(N=C2C(Cl)=C1)C1=CC=CC=C1 c:8,10,12,14,18,23,25,t:1,6,21	Z8711876685	1{291}	Nc1ncc(Cl)cc1Cl	2{22}	O=Cc1cccc1	3{54}	[C-]#[N+]c1cccc1	0.0	0
458	4{10,26,27}	CCCCN1=C(CCC2=CC=CC=C2)N=C2N=C(C(Br)=CN12) c:5,11,13,18,21,t:9,16	Z8711871783	1{10}	Nc1ncc(Br)cn1	2{26}	O=CCCc1ccc1	3{27}	CCCC[N+]#[C-]	0.0	0
459	4{292,130,32}	CCOC1=CN=CC2=NC(=C(NC3CCC3)N12)C1=NN=C(OC)C=C1 c:5,26,t:3,7,9,20,22	Z8801681848	1{292}	CCOc1nccc(N)n1	2{130}	COc1ccc(C=O)nn1	3{32}	[C-]#[N+]C1CC C1	0.0	0
460	4{293,156,10}	COC1=CC(C)=CN2C(NC3CCOC3)=C(N=C12)C1=C(Cl)N=CN1C c:5,15,21,24,t:2,17	Z8801681819	1{293}	COc1cc(C)cnc1N	2{156}	Cn1enc(Cl)c1C=O	3{10}	[C-]#[N+]C1CC OC1	0.0	0
461	4{234,238,39}	CCOCCN1=C(N=C2N1C=CN=C2OC1CCC1)C1=C(Br)N=C2COCCN12 c:8,12,14,23,t:6,26	Z8801681807	1{234}	Nc1nccnc1OC2CCC2	2{238}	Brc1nc2COCn2c1C=O	3{39}	CCOCC[N+]#[C-]	0.0	0
462	4{294,10,6}	CCOC(=O)CCCN1=C(N=C2N1C=C(C=C2Cl)S(C)(=O)=O)C1=NC=CC(C)=C1 c:11,15,17,27,30,t:9,25	Z8797786418	1{294}	CS(=O)(=O)c1enc(N)c(Cl)c1	2{10}	Cc1ccnc(C=O)c1	3{6}	CCOC(=O)C CC[N+]#[C-]	0.0	0
463	4{229,170,7}	CCN1N=NC(=N1)C1=C(NC2CCOCC2)N2C=C(C=C2=N1)S(O)(=O)=O c:3,5,8,19,21,24	Z8797781947	1{229}	Nc1ccc(en1)S(=O)(=O)O	2{170}	CCn1nnc(C=O)n1	3{7}	[C-]#[N+]C1CC OCC1	0.0	0
464	4{295,80,14}	COCCN1=C(N=C2N1C(C)=CC1=C2C=CC=C1)C1=NC=C(C)S1 c:7,12,14,17,19,t:5,22,24	Z8797778300	1{295}	Cc1cc2cccc2c(N)n1	2{80}	Cc1enc(C=O)s1	3{14}	COCC[N+]#[C-]	0.0	0
465	4{296,22,7}	BrC1=CC2=CC3=NC(=C(NC4CCOCC4)N3=C2C=C1)C1=CC=CC=C1 c:19,22,27,29,t:1,3,5,7,25	Z8797775351	1{296}	Nc1cc2cc(Br)ccc2en1	2{22}	O=Cc1cccc1	3{7}	[C-]#[N+]C1CC OCC1	0.0	0

466	4{123,239,6}	CCOC(=O)CCNC1=C(N=C2C=C(OCCO)C=CN12)C1=NOC2=C1CCCC2 c:19,27,t:9,11,13,24	Z8778278033	1{123}	Cl.Nc1cc(OCCO)ccn1	2{239}	O=Cc1noc2CCCCc12	3{6}	CCOC(=O)CC[N+]#[C-]	0.0	0
467	4{46,240,9}	CCN1N=C(Br)C=C1C1=C(NC)N2C=CC=CC2=N1 c:6,9,14,16,19,t:3	Z8803896938	1{46}	Nc1cccn1	2{240}	CCn1nc(Br)cc1C=O	3{9}	C[N+]#[C-]	0.0	0
468	4{99,241,41}	COC1=CC=C(NC2=C(N=C3C=CC(=CN23)S(N)(=O)=O)C2=C(Br)C=NN2C)C=C1 c:11,13,22,25,30,t:2,4,7,9	Z8808559900	1{99}	Nc1ccc(en1)S(=O)(=O)N	2{241}	Cn1ncc(Br)cc1C=O	3{41}	COc1ccc([N+]#[C-])cc1	0.0	0
469	4{121,242,10}	BrC1=CC2=NC(=C(NC3CCOC3)N2C=C1)C1=CN2N=CC(C#N)=C2N=C1 c:16,22,26,29,t:1,3,5,19	Z8808559894	1{121}	Nc1cc(Br)ccn1	2{242}	O=Cc1cnc2c(C#N)enn2c1	3{10}	[C-]#[N+]C1CCOC1	0.0	0
470	4{297,243,7}	CCC1=NOC=C1C1=C(NC2CCOCC2)N2C(=N1)C(C#N)=C(C)C1=C2C=CC=C1 c:5,8,19,27,30,32,t:2,24	Z8808559868	1{297}	Cc1c(C#N)cc(N)nc2cccc12	2{243}	CCc1nocc1C=O	3{7}	[C-]#[N+]C1CCOCC1	0.0	0
471	4{298,244,62}	COC(=O)C1(CCCC1)NC1=C(N=C2C=CC3=C(N=C(Cl)C=C3)N12)C1=CN(C)C(=O)C=C1 c:15,22,34,t:11,13,17,19,28	Z8810903004	1{298}	Nc1ccc2ccc(Cl)nc2n1	2{244}	Cn1cc(C=O)ccc1=O	3{62}	COC(=O)C1(CCCC1)[N+]#[C-]	0.0	0
472	4{125,245,31}	COC(=O)C1=CSC(=C1)C1=C(NCCSC)N2C=C(CCO)C=CC2=N1 c:7,10,23,26,t:4,18	Z8810902968	1{125}	Nc1ccc(CC)cc1	2{245}	COC(=O)c1csc(C=O)c1	3{31}	CSCC[N+]#[C-]	0.0	0
473	4{260,246,14}	COCCNC1=C(N=C2N1C=CC=C2N1CCCC1)C1CC1CCOC1 c:7,11,13,t:5	Z8810902964	1{260}	Nc1ncccc1N2CCCC2	2{246}	O=CC1CC21CCCOC2	3{14}	COCC[N+]#[C-]	0.0	0
474	4{101,247,6}	CCOC1CC(C1)C1=C(NCCCC(=O)OCC)N2C=C(CO)C=C(Cl)C2=N1 c:8,28,t:20,24	Z8810902959	1{101}	Nc1ncc(CO)cc1Cl	2{247}	CCOC1CC(C1)C=O	3{6}	CCOC(=O)CC[N+]#[C-]	0.0	0
475	4{24,27,13}	COC1=CC=C(CNC2=C(N=C3N2C=CN=C3Cl)C2=NN(C)C(C)=N2)C=C1 c:10,14,16,25,28,t:2,4,8,20	Z8798985028	1{24}	Nc1ncnc1Cl	2{27}	Cc1nc(C=O)nn1C	3{13}	COc1ccc(C[N+]#[C-])cc1	0.0	0
476	4{22,232,9}	CNC1=C(N=C2C=CC(Cl)=NN12)C1=NOCC1 c:6,9,t:2,4,14	Z8786958907	1{22}	Nc1ccc(Cl)nn1	2{232}	O=CC1=NOCC1	3{9}	C[N+]#[C-]	0.0	0
477	4{299,170,27}	CCCCNC1=C(N=C2N1C(OC)=CC=C2[N+]([O-])=O)C1=NN(CC)N=N1 c:7,13,15,26,t:5,21	Z8786939735	1{299}	COc1ccc([N+](=O)[O-])c(N)n1	2{170}	CCn1nnc(C=O)n1	3{27}	CCCC[N+]#[C-]	0.0	0
478	4{300,97,14}	COCCNC1=C(N=C2N1C1=C(C=CC=C1)N=C2Cl)C1=CC=C(F)C=C1 c:7,13,15,18,27,t:5,11,22,24	Z8786917530	1{300}	Nc1nc2cccc2nc1Cl	2{97}	Fc1ccc(C=O)cc1	3{14}	COCC[N+]#[C-]	0.0	0

479	4{301,94,7}	FC1=CC(Cl)=CN2C(NC3CCOCC3)=C(N=C12)C1=NC=CN=C1 c:4,15,23,25,t:1,17,21	Z8786838538	1{301}	Nc1ncc(Cl)cc1F	2{94}	O=Cc1cncn1	3{7}	[C-] #[N+]C1CCOCC1	0.0	0
480	4{241,79,12}	BrC1=NN2C(C=C1)=NC(C1=NC=CO1)=C2NCC1CCOC1 c:5,7,12,15,t:1,10	Z8781341779	1{241}	Nc1ccc(Br)nn1	2{79}	O=Cc1ncco1	3{12}	[C-] #[N+]CC1CCOC1	0.0	0
481	4{302,49,38}	CC1=NNC=C1C1=C(NC2=CC3=C(OCO3)C=C2)N2N=CC(=CC2=N1)C#N c:4,7,18,22,24,27,t:1,10,12	Z8781341777	1{302}	Nc1cc(C#N)cnn1	2{49}	Cc1n[nH]cc1C=O	3{38}	[C-] #[N+]c1ccc2OCOc2c1	0.0	0
482	4{303,94,17}	C(NC1=C(N=C2N1N=CC1=C2C=CC=C1)C1=NC=CN=C1)C1CCOCC1 c:4,8,10,13,15,20,22,t:2,18	Z8784060785	1{303}	Nc1nccc2ccc12	2{94}	O=Cc1cncn1	3{17}	[C-] #[N+]CC1CCOCC1	0.0	0
483	4{304,10,6}	CCOC(=O)CCCN1=C(N=C2N1C=C(Br)C=C2C#N)C1=NC=CC(C)=C1 c:11,18,25,28,t:9,15,23	Z8780121875	1{304}	Nc1ncc(Br)cc1C#N	2{10}	Cc1ccnc(C=O)c1	3{6}	CCOC(=O)C CC[N+]#[C-]	0.0	0
484	4{196,118,17}	CC1=CN2C(NCC3CCOCC3)=C(N=C2C(=C1)C#N)C1=CC(C)=NC=C1 c:13,15,18,26,28,t:1,23	Z8780121777	1{196}	Cc1cnc(N)c(C#N)c1	2{118}	Cc1cc(C=O)ccn1	3{17}	[C-] #[N+]CC1CCOCC1	0.0	0
485	4{305,14,14}	CCN1CCN(CC1)C(=O)C1=CN2C(C=C1)=NC(=C2NCCOC)C1=CC=C(C)C=C1 c:15,17,19,32,t:11,27,29	Z8776690327	1{305}	Cl.C1.CCN1CCN(CC1)C(=O)c2ccc(N)nc2	2{14}	Cc1ccc(C=O)cc1	3{14}	COCC[N+]#[C-]	0.0	0
486	4{102,14,58}	CN(C)C(=O)C1=CC2=NC(=C(NC3(C)CC3)N2C=C1)C1=CC=C(C)C=C1 c:19,27,t:5,7,9,22,24	Z8776690342	1{102}	CN(C)C(=O)c1ccnc(N)c1	2{14}	Cc1ccc(C=O)cc1	3{58}	CC1(CC1)[N+]#[C-]	0.0	0
487	4{4,14,14}	COCCNC1=C(N=C2SC=NN12)C1=CC=C(C)C=C1 c:10,20,t:5,7,15,17	Z8711891697	1{4}	Nc1nncs1	2{14}	Cc1ccc(C=O)cc1	3{14}	COCC[N+]#[C-]	0.0	0
488	4{6,15,14}	COCCNC1=C(N=C2N=CC=CN12)C1=CC=C(OC)C=C1 c:9,11,22,t:5,7,16,18	Z8700285979	1{6}	Nc1nccn1	2{15}	COc1ccc(C=O)cc1	3{14}	COCC[N+]#[C-]	0.0	0
489	4{81,15,58}	COC1=CC=C(C=C1)C1=C(NC2(C)CC2)N2C=CN=CC2=N1 c:4,6,9,18,20,23,t:2	Z8712581562	1{81}	Nc1cncn1	2{15}	COc1ccc(C=O)cc1	3{58}	CC1(CC1)[N+]#[C-]	0.0	0
490	4{223,248,34}	COC1=CC(Cl)=C(C2=C(NCC3CCCO3)N3N=C(C=CC3=N2)C(N)=O)C(F)=C1 c:7,18,20,23,30,t:2,5	Z8801681817	1{223}	NC(=O)c1ccc(N)nn1	2{248}	COc1cc(F)c(C=O)c(Cl)c1	3{34}	[C-] #[N+]CC1CCCO1	0.0	0
491	4{306,118,17}	CC1=NC=CC(=C1)C1=C(NCC2CCOCC2)N2C=CC(=C(Cl)C2=N1)C(F)(F)F c:3,5,8,20,26,t:1,22	Z8797785420	1{306}	Nc1nccc(c1Cl)C(F)(F)F	2{118}	Cc1cc(C=O)ccn1	3{17}	[C-] #[N+]CC1CCOCC1	0.0	0

492	4{307,118,14}	COCCNC1=C(N=C2N1C=C(Br)C1=C2C=CC=C1)C1=CC(C)=NC=C1 c:7,14,17,19,25,27,t:5,11,22	Z8797779551	1{307}	Nc1ncc(Br) c2cccc12	2{118}	Cc1cc(C=O) ccn1	3{14}	COCC[N+][#] C-]	0.0	0
493	4{308,18,58}	CCOC1=CC2=NC(C3=CN(CCO)N=C3)=C(N C3(C)CC3)N2C=C1 c:14,26,t:3,5,8,16	Z8778278040	1{308}	CCOc1ccnc (N)c1	2{18}	OCCn1cc(C= O)cn1	3{58}	CC1(CC1)[N +][#][C-]	0.0	0
494	4{309,249,14}	CCN1N=CC=C1C1=C(NCCOC)N2C(C=NC= C2C(F)(F)F)=N1 c:3,5,8,17,19,25	Z8778278031	1{309}	Nc1nccc(n1)C(F)(F)F	2{249}	CCn1nccc1C =O	3{14}	COCC[N+][#] C-]	0.0	0
495	4{210,167,65}	FC1=CC=C(Br)C2=NC(C3=NN=CN3)=C(NC3 CCCC3)N12 c:11,t:1,3,6,9,14	Z8803896971	1{210}	Nc1nc(F)cc c1Br	2{167}	O=Cc1nnc[n H]1	3{65}	[C-]#[N+]C1CC CC1	0.0	0
496	4{310,250,66}	CC(NC1=C(N=C2N1C=CC1=C2N(C)C(=O)N 1C)C1=CN(C)N=C1Br)C1=CC=CC=C1 c:5,9,11,25,31,33,t:3,21,29	Z8803896958	1{310}	Cn1c(=O)n(C)c2c(N)nc cc12	2{250}	Cn1cc(C=O) c(Br)n1	3{66}	CC([N+][#][C-])c1cccc1	0.0	0
497	4{119,251,10}	N#CC1=CN2C(NC3CCOC3)=C(N=C2C=C1)C 1=CC(=NN1)C1=CC=NC=C1 c:12,14,17,22,28,30,t:2,20,26	Z8803896950	1{119}	Nc1ccc(C# N)n1	2{251}	O=Cc1cc(n[n H]1)c2ccncc 2	3{10}	[C-]#[N+]C1CC OC1	0.0	0
498	4{77,13,1}	CC1=C(N=NN1)C1=C(NC2CC2)N2C=C(C=C C2=N1)C1=CN=CC=C1 c:3,7,15,17,20,25,27,t:1,23	Z8803896941	1{77}	Nc1ccc(en1)c2ccncc2	2{13}	Cc1[nH]nnc1 C=O	3{1}	[C-]#[N+]C1CC 1	0.0	0
499	4{176,252,14}	COCCNC1=C(N=C2N1C=CN=C2N1CCCC1) C1=CC(F)=C(C=C1)C#N c:7,11,13,25,27,t:5,22	Z8803896922	1{176}	Nc1ncnc1 N2CCCC2	2{252}	Fc1cc(C=O)c cc1C#N	3{14}	COCC[N+][#] C-]	0.0	0
500	4{229,253,68}	CCC1CC1C1=C(NC2CCCC2)N2C=C(C=CC 2=N1)S(O)(=O)=O c:6,17,19,22	Z8803896954	1{229}	Nc1ccc(en1)S(=O)(=O) O	2{253}	CCC1CC1C= O	3{68}	[C-]#[N+]C1CC CCC1	0.0	0
501	4{164,104,24}	COC1=CC(CNC2=C(N=C3C=C(CN(C)C)C=C N23)C2=NC(C)=CO2)=CC=C1 c:17,25,28,30,t:2,7,9,11,22	Z8808559890	1{164}	CN(C)Cc1c cnc(N)c1	2{104}	Cc1coc(C=O) n1	3{24}	COc1cccc(C[N+][#][C-])c1	0.0	0
502	4{261,254,39}	CCOCCNC1=C(CCCCC#C)N=C2C=CC(=CN 12)N1CCC(CC1)N(C)C c:6,16,18,t:14	Z8808559879	1{261}	CN(C)C1C CN(CC1)c2 ccc(N)nc2	2{254}	O=CCCCC #C	3{39}	CCOCC[N+] #[C-]	0.0	0
503	4{297,89,7}	CCC1=NC=C(C=N1)C1=C(NC2CCOCC2)N2 C(=N1)C(C#N)=C(C)C1=C2C=CC=C1 c:4,6,9,20,28,31,33,t:2,25	Z8808559866	1{297}	Cc1c(C#N)c (N)nc2cccc 12	2{89}	CCc1ncc(C= O)cn1	3{7}	[C-]#[N+]C1CC OCC1	0.0	0
504	4{311,255,10}	FC1=CC2=NC(=C(NC3CCOC3)N2C=C1)C1= CC2=C(NC=N2)C=C1 c:16,24,27,t:1,3,5,19,21	Z8808559856	1{311}	Nc1cc(F)cc n1	2{255}	O=Cc1ccc2[nH]enc2c1	3{10}	[C-]#[N+]C1CC OC1	0.0	0

505	4{312,256,39}	CCOCCNC1=C(N=C2C=CC3=C(NC(=O)NC3=O)N12)C1=CN(CCCl)N=C1 c:10,30,t:6,8,12,24	Z8810903024	1{312}	Nc1ccc2c(=O)[nH]c(=O)[nH]c2n1	2{256}	ClCCn1cc(C=O)cn1	3{39}	CCOCC[N+]#[C-]	0.0	0
506	4{151,257,9}	CNC1=C(N=C2C=NC=C(Cl)N12)C1CC(C1)N C(=O)OC(C)(C)C c:6,t:2,4,8	Z8810902999	1{151}	Nc1cncc(Cl)n1	2{257}	CC(C)(C)OC(=O)NC1CC(C1)C=O	3{9}	C[N+]#[C-]	0.0	0
507	4{271,258,67}	CCC(C)NC1=C(N=C2C=CC(C(=O)OC)=C(F)N12)C1=NN=C(S1)C1CC1 c:9,23,t:5,7,15,21	Z8810902994	1{271}	COC(=O)c1ccc(N)nc1F	2{258}	O=Cc1nnc(s1)C2CC2	3{67}	CCC(C)[N+]#[C-]	0.0	0
508	4{168,205,21}	COC(=O)C1=C2COCCN2C(=C1)C1=C(NCC2CC2)N2C(C=NC=C2C#N)=N1 c:4,12,15,25,27,31	Z8810902955	1{168}	Nc1cncc(C#N)n1	2{205}	COC(=O)c1cc(C=O)n2CCOCc12	3{21}	[C-]#[N+]CC1CC1	0.0	0
509	4{109,259,34}	COC1=C(C=C(C=C1)C1=CN=CN=C1)C1=C(NCC2CCCO2)N2C(C=CC=C2S(N)(=O)=O)=N1 c:4,6,11,13,16,28,30,36,t:2,9	Z8798985063	1{109}	Cl.Nc1cccc(n1)S(=O)(=O)N	2{259}	COc1ccc(cc1C=O)c2ennc2	3{34}	[C-]#[N+]CC1CCO1	0.0	0
510	4{313,260,14}	COCCNC1=C(N=C2N1C1=C(CCCC1)C=C2C#N)C1=NOC(C)=C1 c:7,18,27,t:5,11,23	Z8798985060	1{313}	Nc1nc2CCCCc2cc1C#N	2{260}	Cc1cc(C=O)no1	3{14}	COCC[N+]#[C-]	0.0	0
511	4{271,261,44}	COC(=O)C1=C(F)N2C(NCCCCNC(=O)OC(C)(C)C)=C(N=C2C=C1)C1=NC=C(C)N1C c:4,21,23,26,t:29,31	Z8798985025	1{271}	COC(=O)c1ccc(N)nc1F	2{261}	Cc1enc(C=O)n1C	3{44}	CC(C)(C)OC(=O)NCCCC[N+]#[C-]	0.0	0
512	4{314,262,22}	CCC1=NN(C)C(=C1C1)C1=C(NC2COC2)N2C(C=CC=C2CC(=O)OC)=N1 c:6,10,20,22,29,t:2	Z8786958839	1{314}	COC(=O)C1cccc(N)n1	2{262}	CCc1nn(C)c(C=O)c1Cl	3{22}	[C-]#[N+]C1CO1	0.0	0
513	4{23,263,46}	CC(=C)CNC1=C(N=C2C=NC=C(Br)N12)C1=CN=C2C=NC=CN12 c:9,21,23,t:5,7,11,17,19	Z8786958792	1{23}	Nc1cncc(Br)n1	2{263}	O=Cc1enc2cncn12	3{46}	CC(=C)C[N+]#[C-]	0.0	0
514	4{315,264,14}	COCCNC1=C(N=C2C=NC(Br)=C(F)N12)C1=NC(Br)=CN1 c:9,21,t:5,7,12,18	Z8781341801	1{315}	Nc1enc(Br)c(F)n1	2{264}	Br1c[nH]c(C=O)n1	3{14}	COCC[N+]#[C-]	0.0	0
515	4{316,14,27}	CCCCNC1=C(N=C2C=CC=C(N12)C(N)=N)C1=CC=C(C)C=C1 c:9,11,24,t:5,7,19,21	Z8784060088	1{316}	Cl.Cl.NC(=N)c1cccc(N)n1	2{14}	Cc1ccc(C=O)cc1	3{27}	CCCC[N+]#[C-]	0.0	0
516	4{317,29,20}	CCN1C=CC(=N1)C1=C(NC2=C(C)C=C(OC)C=C2)N2C=C(C=C(C2=N1)C(F)(F)C(F)(F)F) c:3,5,8,11,18,22,24,27,t:14	Z8780122386	1{317}	Nc1ncc(cc1C(F)(F)F)C(F)(F)F	2{29}	CCn1ccc(C=O)n1	3{20}	COc1ccc([N+]#[C-])c(C)c1	0.0	0

517	4{13,14,27}	CCCCNC1=C(N=C2C=C(C)N=C(C)N12)C1=CC=C(C)C=C1 c:23,t:5,7,9,12,18,20	Z8711876248	1{13}	Cc1ccc(N)nc(C)n1	2{14}	Cc1ccc(C=O)cc1	3{27}	CCCC[N+][C-]	0.0	0
518	4{169,14,14}	CNC(=O)C1=NN2C(C=C1)=NC(=C2NCCOC)C1=CC=C(C)C=C1 c:8,10,12,25,t:4,20,22	Z8741907038	1{169}	CNC(=O)c1ccc(N)nn1	2{14}	Cc1ccc(C=O)cc1	3{14}	COCC[N+][C-]	0.0	0
519	4{267,177,34}	COC(=O)C1CC(CC2=C(NCC3CCCO3)N3C(C=CC=C3C#C)=N2)C1 c:8,20,22,26	Z8801681841	1{267}	Nc1cccc(C#C)n1	2{177}	COC(=O)C1CC(CC=O)C1	3{34}	[C-][N+]CC1C=CCO1	0.0	0
520	4{229,265,64}	COC(=O)[C@@H]1CC[C@@H](C1)NC1=C(N=C2C=CC(=CN12)S(O)(=O)=O)C1CCCC1 &1:4,7,r,c:15,17,t:11,13	Z8803896964	1{229}	Nc1ccc(en1)S(=O)(=O)O	2{265}	O=CC1CCC=CC1	3{64}	COC(=O)[C@@H]1CC[C@@H](C1)[N+]#[C-] &1:4,7,r	0.0	0
521	4{38,266,9}	CNC1=C(N=C2C=C(C=CN12)C#N)C1=CC(=CC=C1)C1=CN=C(C=C1)C#N c:6,8,17,19,24,26,t:2,4,15,22	Z8803896949	1{38}	Nc1cc(C#N)ccn1	2{266}	O=Cc1cccc(c1)c2ccc(C#N)nc2	3{9}	C[N+]#[C-]	0.0	0
522	4{48,267,15}	CCNC1=C(N=C2C=C(C=CN12)S(C)(=O)=O)[C@H](CCC(=O)OC(C)(C)C)NC(=O)OC(C)(C)C c:7,9,t:3,5	Z8803896934	1{48}	CS(=O)(=O)c1ccnc(N)c1	2{267}	CC(C)(C)OC(=O)CC[C@H](NC(=O)OC(C)(C)C)C=O	3{15}	CC[N+]#[C-]	0.0	0
523	4{238,268,7}	CC[C@@H](NC(=O)OC(C)(C)C)C1=C(NC2C=COCC2)N2C=CC(OC)=C(C#N)C2=N1 c:11,22,31,t:26	Z8808559880	1{238}	COc1ccnc(N)c1C#N	2{268}	CC[C@@H](NC(=O)OC(C)(C)C)C=O	3{7}	[C-][N+]C1CC=OCC1	0.0	0
524	4{31,269,22}	C1CC(C1)C1=CC(=NN1)C1=C(NC2COC2)N2C3=C(OCC3)C=CC2=N1 c:7,11,26,29,t:5,20	Z8810903036	1{31}	Nc1ccc2OC=Cc2n1	2{269}	O=Cc1cc([N+][H])n1C2CCC2	3{22}	[C-][N+]C1CO=C1	0.0	0
525	4{145,270,15}	CCNC1=C(N=C2C=CC=C(N12)S(C)(=O)=O)C1[C@H]2CC[C@H](C2)[C@@H]1NC(=O)OC(C)(C)C &1:17,20,22,r,c:7,9,t:3,5	Z8810903031	1{145}	CS(=O)(=O)c1cccc(N)n1	2{270}	CC(C)(C)OC(=O)N[C@@H]1C(C=O)[C@H]2CC[C@@H]1C2 &1:8,12,15,r	3{15}	CC[N+]#[C-]	0.0	0

526	4{258,271,67}	CCC(C)NC1=C(N=C2C=CC3=C(N=CC=N3)N12)C1=NN(C)N=N1 c:9,13,15,25,t:5,7,11,21	Z8810902979	1{258}	Nc1ccc2nccnc2n1	2{271}	Cn1nnc(C=O)n1	3{67}	CCC(C)[N+]#[C-]	0.0	0
527	4{211,3,66}	CC(NC1=C(N=C2N1C=CC=C2C1=NN=NN1)C1=NC=C(C=C1)C#N)C1=CC=CC=C1 c:5,9,11,16,22,24,31,33,t:3,14,20,29	Z8798985051	1{211}	Nc1ncccc1c2nnn[nH]2	2{3}	O=Cc1ccc(C#N)cn1	3{66}	CC([N+]#[C-])c1cccc1	0.0	0
528	4{275,182,14}	COCCNC1=C(N=C2N1C(Cl)=CC=C2F)C1=NC=CN1CC#C c:7,12,14,20,t:5,18	Z8798985050	1{275}	Nc1nc(Cl)ccc1F	2{182}	O=Cc1nccn1CC#C	3{14}	COCC[N+]#[C-]	0.0	0
529	4{318,273,12}	COC(=O)C1=CN2C(NCC3CCOC3)=C(N=C2C(OC)=N1)C1=C(Br)N(C)N=C1C c:15,17,22,25,30,t:4	Z8798985049	1{318}	COC(=O)c1cnc(N)c(OC)n1	2{273}	Cc1m(C)c(Br)c1C=O	3{12}	[C-]#[N+]CC1COC1	0.0	0
530	4{198,118,31}	CSCCNC1=C(N=C2C=NC(C#C)=C(Cl)N12)C1=CC(C)=NC=C1 c:9,22,24,t:5,7,13,19	Z8798985041	1{198}	Nc1nc(C#C)c(Cl)n1	2{118}	Cc1cc(C=O)ccn1	3{31}	CSCC[N+]#[C-]	0.0	0
531	4{35,129,9}	CNC1=C(N=C2C=CC(C)=CN12)C1=CC=CC2=NC=NN12 c:6,9,16,20,t:2,4,14,18	Z8798985036	1{35}	Cc1ccc(N)nc1	2{129}	O=Cc1cccc2ncm12	3{9}	C[N+]#[C-]	0.0	0
532	4{314,231,4}	COC(=O)CC1=CC=CC2=NC(C3=NC4=C(CC(C)CC4)S3)=C(NCC3=NN(C)N=N3)N12 c:7,31,t:5,9,12,14,23,27	Z8786958826	1{314}	COC(=O)C1cccc(N)n1	2{231}	CC1CCc2nc(C=O)sc2C1	3{4}	Cn1nnc(C[N+]#[C-])n1	0.0	0
533	4{25,274,25}	CN(C)C1=CC=CC2=NC(CC3(CCOCC3)C#N)=C(NCCCF)N12 c:5,t:3,7,19	Z8781341785	1{25}	CN(C)c1ccc(N)n1	2{274}	O=CCC1(CCOC1)C#N	3{25}	FCCC[N+]#[C-]	0.0	0
534	4{319,275,25}	CN1C=C(C)N=C1C1=C(NCCCF)N2C(C=CC(Br)=C2C#N)=N1 c:5,8,17,20,24,t:2	Z8781341771	1{319}	Nc1ccc(Br)c(C#N)n1	2{275}	Cc1cn(C)c(C=O)n1	3{25}	FCCC[N+]#[C-]	0.0	0
535	4{320,29,7}	CCN1C=CC(=N1)C1=C(NC2CCOCC2)N2C=CN3N=CC(=C3C2=N1)[N+][[O-]]=O c:3,5,8,19,22,24,28	Z8784060976	1{320}	Nc1nccn2ncc([N+](=O)[O-])c12	2{29}	CCn1ccc(C=O)n1	3{7}	[C-]#[N+]C1CCOCC1	0.0	0
536	4{321,80,20}	COC1=CC(C)=C(NC2=C(N=C3N2C=CC2=C3C=NC=N2)C2=NC=C(C)S2)C=C1 c:10,14,16,19,21,31,t:2,5,8,24,26	Z8784060875	1{321}	Nc1nccc2ncc12	2{80}	Cc1nc(C=O)s1	3{20}	COc1ccc([N+]#[C-])c(C)c1	0.0	0
537	4{260,69,14}	COCCNC1=C(N=C2N1C=CC=C2N1CCCC1)C1=NN(C)C(C)=C1 c:7,11,13,27,t:5,22	Z8784060346	1{260}	Nc1ncccc1N2CCCC2	2{69}	Cc1cc(C=O)mn1C	3{14}	COCC[N+]#[C-]	0.0	0
538	4{322,58,14}	COCCNC1=C(N=C2N1C=CN=C2Br)C1=NSN=C1 c:7,11,13,20,t:5,17	Z8780121564	1{322}	Nc1nccnc1Br	2{58}	O=Cc1cnsn1	3{14}	COCC[N+]#[C-]	0.0	0
539	4{22,15,9}	CNC1=C(N=C2C=CC(Cl)=NN12)C1=CC=C(OC)C=C1 c:6,9,20,t:2,4,14,16	Z8776690345	1{22}	Nc1ccc(Cl)nn1	2{15}	COc1ccc(C=O)cc1	3{9}	C[N+]#[C-]	0.0	0

540	4{323,14,17}	CC1=CC=C(C=C1)C1=C(NCC2CCOCC2)N2C(C=CC=C2O)=N1 c:3,5,8,21,23,26,t:1	Z8711876680	1{323}	Nc1cccc(O)n1	2{14}	Cc1ccc(C=O)cc1	3{17}	[C-]#[N+]CC1C COCC1	0.0	0
541	4{12,15,17}	CCC1=CC2=NC(=C(NCC3CCOCC3)N2C=N1)C1=CC=C(OC)C=C1 c:19,28,t:2,4,6,22,24	Z8711876287	1{12}	CCc1cc(N)n cn1	2{15}	COc1ccc(C=O)cc1	3{17}	[C-]#[N+]CC1C COCC1	0.0	0
542	4{16,22,17}	FC1=CN=CN2C(NCC3CCOCC3)=C(N=C12)C1=CC=CC=C1 c:3,15,23,25,t:1,17,21	Z8711876147	1{16}	Nc1ncnc1F	2{22}	O=Cc1cccc1	3{17}	[C-]#[N+]CC1C COCC1	0.0	0
543	4{7,22,54}	CC1=CN2C(NC3=CC=CC=C3)=C(N=C2N=C1)C1=CC=CC=C1 c:8,10,12,14,17,22,24,t:1,6,20	Z8711872483	1{7}	Cc1nc(N)n c1	2{22}	O=Cc1cccc1	3{54}	[C-]#[N+]c1cccc1	0.0	0
544	4{11,15,14}	COCCNC1=C(N=C2N=C(Cl)C=C(Cl)N12)C1=CC=C(OC)C=C1 c:24,t:5,7,9,12,18,20	Z8711872231	1{11}	Nc1nc(Cl)c c(Cl)n1	2{15}	COc1ccc(C=O)cc1	3{14}	COCC[N+]#[C-]	0.0	0
545	4{270,26,9}	CNC1=C(CCC2=CC=CC=C2)N=C2C=CC3=N C=NN3N12 c:2,8,10,15,19,t:6,13,17	Z8741907041	1{270}	Nc1ccc2nnc n2n1	2{26}	O=CCCc1ccc1	3{9}	C[N+]#[C-]	0.0	0
546	4{324,14,11}	CC1=CC=C(C=C1)C1=C(NCC2=CC(Br)=CC=C2)N2C=CC(N)=CC2=N1 c:3,5,8,15,17,21,24,27,t:1,12	Z8741906951	1{324}	Cl.Nc1ccnc(N)c1	2{14}	Cc1ccc(C=O)cc1	3{11}	BrC1cccc(C[N+]#[C-])c1	0.0	0
547	4{325,22,20}	COC1=CC(C)=C(NC2=C(N=C3C=C(O)C=CN23)C2=CC=CC=C2)C=C1 c:15,22,24,27,t:2,5,8,10,12,20	Z8741906950	1{325}	Nc1cc(O)cc n1	2{22}	O=Cc1cccc1	3{20}	COc1ccc([N+]#[C-])c(C)c1	0.0	0
548	4{326,276,47}	COC(OC)C1=C(NC(C)C)N2C=C(Cl)C(Br)=C2=N1 c:5,16,19,t:12	Z8801681844	1{326}	Nc1cc(Br)c(Cl)n1	2{276}	COC(OC)C=O	3{47}	CC(C)[N+]#[C-]	0.0	0
549	4{240,277,37}	COC(=O)C1CC(C1)NC1=C(CC(NC(=O)OC(C)(C)C)C2CC2)N=C2C=CC(=CN12)C1=NNN=N1 c:10,28,30,38,t:26,35	Z8801681828	1{240}	Nc1ccc(cn1)c2nn[nH]n2	2{277}	CC(C)(C)OC(=O)NC(CC(=O)C1CC1	3{37}	COC(=O)C1CC(C1)[N+]#[C-]	0.0	0
550	4{327,170,27}	CCCCNC1=C(N=C2N1C=CC(C(=O)OC)=C2F)C1=NN(CC)N=N1 c:7,11,17,26,t:5,21	Z8797787109	1{327}	COC(=O)c1ccnc(N)c1F	2{170}	CCn1nnc(C=O)n1	3{27}	CCCC[N+]#[C-]	0.0	0
551	4{328,41,17}	BrC1=C2C=CNC2=CN2C(NCC3CCOCC3)=C(N=C12)C1=NC=CC=C1 c:1,3,7,19,27,29,t:21,25	Z8797775508	1{328}	Nc1ncc2[nH]ccc2c1Br	2{41}	O=Cc1ccccn1	3{17}	[C-]#[N+]CC1C COCC1	0.0	0
552	4{113,278,6}	CCOC(=O)CCNC1=C(N=C2N1C=CC=C2N1CCOCC1)C1=C(Br)N=NN1C c:11,15,17,27,30,t:9	Z8803896969	1{113}	Nc1ncccc1N2CCOCC2	2{278}	Cn1nnc(Br)c1C=O	3{6}	CCOC(=O)C CC[N+]#[C-]	0.0	0

553	4{329,107,7}	COC1=CC=C(C)C2=NC(=C(NC3CCOCC3)N12)C1=NC(C)=CS1 c:25,t:2,4,7,9,22	Z8803896940	1{329}	Cl.COc1ccc(C)c(N)n1	2{107}	Cc1csc(C=O)n1	3{7}	[C-]#[N+]C1CCOCC1	0.0	0
554	4{154,279,33}	COC1=C(CNC2=C(N=C3C=C(C=CN23)[N+]([O-])=O)[C@@H]2CCCO[C@H]2C2=NC=CN2C)C=CC=C1 &1:18,23,r,c:2,10,12,29,34,36,t:6,8,27	Z8808559896	1{154}	Nc1cc(cen1)[N+](=O)[O-]	2{279}	Cn1ccnc1[C@@H]2OCC[C@H]2C=O &1:6,11,r	3{33}	COc1ccccc1C[N+]#[C-]	0.0	0
555	4{330,250,1}	CN(C)S(=O)(=O)C1=CN2C(C=C1)=NC(=C2N1CC1)C1=CN(C)N=C1Br c:10,12,14,26,t:6,22	Z8808559863	1{330}	CN(C)S(=O)(=O)c1ccc(N)nc1	2{250}	Cn1cc(C=O)c(Br)n1	3{1}	[C-]#[N+]C1CC1	0.0	0
556	4{331,280,49}	CN(C)CCN(C)CC1=CN2C(NC3CC(F)(F)C3)=C(N=C2C=C1)C1=NSC(=C1)[N+]([O-])=O c:19,21,24,30,t:8,27	Z8810903020	1{331}	Cl.Cl.Cl.CN(C)CCN(C)Cc1ccc(N)nc1	2{280}	[O-][N+](=O)c1cc(C=O)ns1	3{49}	FC1(F)CC(C1)[N+]#[C-]	0.0	0
557	4{332,281,21}	CCC1=CC=CN2C(NCC3CC3)=C(N=C12)C1=NN=C(C=C1)C(=O)OC c:4,13,21,23,t:2,15,19	Z8810902965	1{332}	CCc1cccn1N	2{281}	COC(=O)c1ccc(C=O)nn1	3{21}	[C-]#[N+]CC1CC1	0.0	0
558	4{41,266,9}	CNC1=C(N=C2C=NC(C)=CN12)C1=CC(=CC=C1)C1=CN=C(C=C1)C#N c:6,9,16,18,23,25,t:2,4,14,21	Z8810902963	1{41}	Cc1cnc(N)c n1	2{266}	O=Cc1cccc(c1)c2ccc(C#N)nc2	3{9}	C[N+]#[C-]	0.0	0
559	4{35,79,9}	CNC1=C(N=C2C=CC(C)=CN12)C1=NC=CO1 c:6,9,16,t:2,4,14	Z8810902951	1{35}	Cc1ccc(N)nc1	2{79}	O=Cc1ncco1	3{9}	C[N+]#[C-]	0.0	0
560	4{256,126,44}	COC1=CC(=CC(F)=C1)C1=C(NCCCCNC(=O)OC(C)(C)N2N3N=NN=C3C=CC2=N1 c:4,7,10,27,29,32,35,t:2	Z8798985064	1{256}	Nc1ccc2nnn n2n1	2{126}	COc1cc(F)cc(C=O)c1	3{44}	CC(C)(C)OC(=O)NCCCC[N+]#[C-]	0.0	0
561	4{333,282,8}	COC(=O)C(CC1=CC=CC=C1)NC1=C(N=C2C=CC=C(N12)C1=CC=NC=C1)C1CC2(C1)OC CO2 c:8,10,18,20,27,29,t:6,14,16,25	Z8798985059	1{333}	Nc1cccc(n1)c2cnc2	2{282}	O=CC1CC2(C1)OCCO2	3{8}	COC(=O)C(Cc1ccccc1)[N+]#[C-]	0.0	0
562	4{146,283,12}	CS(=O)(=O)C1=CN2C(C=C1)=NC(=C2NCC1CCO1)C1=C2N=CC=CC2=CC=C1 c:8,10,12,23,25,27,30,32,t:4	Z8798985057	1{146}	CS(=O)(=O)c1ccc(N)nc1	2{283}	O=Cc1cccc2ccnc12	3{12}	[C-]#[N+]CC1CCOCC1	0.0	0
563	4{192,182,14}	COCCNC1=C(N=C2N1C(F)=CC=C2C1)C1=NC=CN1CC#C c:7,12,14,20,t:5,18	Z8798985056	1{192}	Nc1nc(F)cc1Cl	2{182}	O=Cc1cncn1CC#C	3{14}	COCC[N+]#[C-]	0.0	0

564	4{334,284,7}	CC1=C(N=CC=N1)C1=C(NC2CCOCC2)N2C=C3COCCC3=C(C#N)C2=N1 c:3,5,8,31,t:1,19,26	Z8798985047	1{334}	Nc1ncc2CO CCc2c1C# N	2{284}	Cc1nccnc1C =O	3{7}	[C-]]#[N+]C1CC OCC1	0.0	0
565	4{335,27,58}	CN1N=C(N=C1C)C1=C(NC2(C)CC2)N2C3=C(NC=C3)C=C(Br)C2=N1 c:2,4,8,20,27,t:17,23	Z8786958812	1{335}	Nc1nc2cc[n H]c2cc1Br	2{27}	Cc1nc(C=O) nn1C	3{58}	CC1(CC1)[N +]#[C-]	0.0	0
566	4{336,44,17}	CCN1C=C(C=N1)C1=C(NCC2CCOCC2)N2C(=N1)C(C1)=NC1=C2C=CC(=C1)[N+](=[O-])=O c:3,5,8,20,24,26,29,31	Z8786935772	1{336}	Nc1nc2ccc(cc2nc1Cl)[N+](=O)[O-]	2{44}	CCn1cc(C=O))cn1	3{17}	[C-]]#[N+]CC1C COCC1	0.0	0
567	4{337,118,14}	COCCNC1=C(N=C2N1C=CC(Br)=C2Cl)C1=CC(C)=NC=C1 c:7,11,14,21,23,t:5,18	Z8786901713	1{337}	Nc1nccc(Br))c1Cl	2{118}	Cc1cc(C=O) ccn1	3{14}	COCC[N+]#[C-]	0.0	0
568	4{338,170,6}	CCOC(=O)CCCNC1=C(N=C2N1C=CC1=C2C=CN=C1)C1=NN(CC)N=N1 c:11,15,17,20,22,30,t:9,25	Z8778277874	1{338}	Nc1nccc2cn ccc12	2{170}	CCn1nnc(C= O)n1	3{6}	CCOC(=O)C CC[N+]#[C-]	0.0	0
569	4{339,80,14}	COCCNC1=C(N=C2N1C=CC1=C2C=CS1)C1=NC=C(C)S1 c:7,11,13,16,t:5,20,22	Z8778277362	1{339}	Nc1nccc2sc cc12	2{80}	Cc1enc(C=O))s1	3{14}	COCC[N+]#[C-]	0.0	0
570	4{340,58,14}	CCOC1=CC=CN2C(NCCOC)=C(N=C12)C1=NSN=C1 c:5,13,22,t:3,15,19	Z8778277284	1{340}	CCOc1cccn c1N	2{58}	O=Cc1cnsn1	3{14}	COCC[N+]#[C-]	0.0	0
571	4{341,80,39}	CCOCCNC1=C(N=C2C=CC(CN(C)C)=CN12)C1=NC=C(C)S1 c:10,16,t:6,8,21,23	Z8781341769	1{341}	CN(C)Cc1c cc(N)nc1	2{80}	Cc1enc(C=O))s1	3{39}	CCOCC[N+] #[C-]	0.0	0
572	4{342,118,17}	CC1=NC=CC(=C1)C1=C(NCC2CCOCC2)N2C=CC3=C(C=CC(=C3)[N+](=[O-])=O)C2=N1 c:3,5,8,20,24,26,33,t:1,22	Z8784060910	1{342}	Nc1nccc2cc (ccc12)[N+] (=O)[O-]	2{118}	Cc1cc(C=O) ccn1	3{17}	[C-]]#[N+]CC1C COCC1	0.0	0
573	4{343,58,27}	CCCCNC1=C(N=C2N1C=CC1=C2C=CO1)C1=NSN=C1 c:7,11,13,16,23,t:5,20	Z8784060493	1{343}	Nc1nccc2oc cc12	2{58}	O=Cc1cnsn1	3{27}	CCCC[N+]#[C-]	0.0	0
574	4{344,58,14}	COCCNC1=C(N=C2N1C=CC=C2SC)C1=NSN=C1 c:7,11,13,21,t:5,18	Z8784059177	1{344}	CSc1ccnc1 N	2{58}	O=Cc1cnsn1	3{14}	COCC[N+]#[C-]	0.0	0
575	4{26,22,14}	COCCNC1=C(N=C2C=CC=C(N3CCCC3)N12)C1=CC=CC=C1 c:9,24,26,t:5,7,11,22	Z8780122312	1{26}	Nc1cccc(n1))N2CCCC2	2{22}	O=Cc1cccc 1	3{14}	COCC[N+]#[C-]	0.0	0
576	4{345,41,17}	BrC1=CN2C(NCC3CCOCC3)=C(N=C2C(Br)=N1)C1=NC=CC=C1 c:13,15,19,24,26,t:1,22	Z8780121691	1{345}	Nc1ncc(Br) nc1Br	2{41}	O=Cc1cccn 1	3{17}	[C-]]#[N+]CC1C COCC1	0.0	0
577	4{188,14,14}	COCCNC1=C(N=C2C=NC=C(N12)C(=O)OC)C1=CC=C(C)C=C1 c:9,11,25,t:5,7,20,22	Z8776690330	1{188}	COC(=O)c1 cncc(N)n1	2{14}	Cc1ccc(C=O))cc1	3{14}	COCC[N+]#[C-]	0.0	0

578	4{1,22,27}	CCCCNC1=C(N=C2C=CN12)C1=CC=CC=C1 c:9,17,19,t:5,7,15	Z8711892168	1{1}	Nc1cc[nH]n1	2{22}	O=Cc1cccc1	3{27}	CCCC[N+][C-]	0.0	0
579	4{2,15,54}	COC1=CC=C(C=C1)C1=C(NC2=CC=CC=C2)N2OC=CC2=N1 c:4,6,9,14,16,21,24,t:2,12	Z8711891895	1{2}	Nc1ccn1	2{15}	COc1ccc(C=O)cc1	3{54}	[C-][N+]c1cccc1	0.0	0
580	4{346,15,9}	CNC1=C(N=C2N1C=CN=C2C)C1=CC=C(OC)C=C1 c:4,8,10,20,t:2,14,16	Z8741907202	1{346}	Cc1ncnc1N	2{15}	COc1ccc(C=O)cc1	3{9}	C[N+][C-]	0.0	0
<i>Preliminary test experiments, Sc(OTf)₃ as the catalyst</i>											
581	4{347,242,24}	COC1=CC(CNC2=C(N=C3C=CC(C1)=CN23)C2=CN3N=CC(C#N)=C3N=C2)=CC=C1 c:11,14,22,26,29,31,33,t:2,7,9,19	Z8878918808	1{347}	Nc1ccc(Cl)cn1	2{242}	O=Cc1cnc2c(C#N)cnn2c1	3{24}	COc1ccc(C[N+][C-])c1	114.9	99
582	4{54,285,53}	CN(C)C(=O)C1=CN2C(NCCOCC3=CC=CC=C3)=C(N=C2C=C1)C1=CSC(=C1)[N+](O)=O c:16,18,20,22,25,31,t:5,14,28	Z8878918446	1{54}	Cl.CN(C)C(=O)c1ccc(N)nc1	2{285}	[O-][N+](=O)c1cc(C=O)cs1	3{53}	[C-][N+]CCOCc1cccc1	99.6	79
583	4{105,286,34}	NC(=O)C1=CC=CC2=NC(=C(NCC3CCCO3)N12)C1=NC=CC(=C1)C(F)(F)F c:5,24,26,t:3,7,9,22	Z8878918833	1{105}	NC(=O)c1cccc(N)n1	2{286}	FC(F)(F)c1ccnc(C=O)c1	3{34}	[C-][N+]CC1COCO1	81.8	75
584	4{69,287,12}	CNC(=O)C1=CC2=NC(=C(NCC3CCOC3)N2C=C1)C1=CC(OCCOC)=CC=C1 c:20,31,33,t:4,6,8,23	Z8878918860	1{69}	CNC(=O)c1ccnc(N)c1	2{287}	COCCCOc1cccc(C=O)c1	3{12}	[C-][N+]CC1COCO1	82.5	70
585	4{348,288,39}	CCOCCNC1=C(N=C2C=NC(F)=CN12)C1=C(C=CCF)C=C1 c:10,13,25,t:6,8,18,20	Z8878918639	1{348}	Nc1cnc(F)cn1	2{288}	FCCc1ccc(C=O)cc1	3{39}	CCOCC[N+][C-]	60.2	68
586	4{349,110,69}	COC1=C(NC2=C(N=C3C=CC(Br)=C(C)N23)C2=CN=C(C=C2)P(C)(C)O)C=CC=C1 c:2,9,20,22,29,31,t:5,7,12,18	Z8846492345	1{349}	Cc1nc(N)ccc1Br	2{110}	CP(=O)(C)c1cccc(C=O)cn1	3{69}	COc1cccc1[N+][C-]	88.3	67
587	4{153,289,22}	COC1=C(OCC#C)C=C(C=C1)C1=C(NC2COC2)N2C(C=CC=C2C(C)O)=N1 c:2,8,10,13,23,25,31	Z8873684876	1{153}	CC(C)(O)c1cccc(N)n1	2{289}	COc1ccc(C=O)cc1OCC#C	3{22}	[C-][N+]C1COC1	71.8	65
588	4{28,174,7}	C(C1CCCO1)N1C=C(N=N1)C1=C(NC2CCOC2)N2C=CC(=CC2=N1)C1=NOC=N1 c:8,10,13,24,26,29,35,t:32	Z8878918438	1{28}	Cl.Nc1cc(ccn1)c2ncon2	2{174}	O=Cc1cn(CC2CCCO2)nn1	3{7}	[C-][N+]C1CCOCC1	76.3	65
589	4{193,290,10}	CNC(=O)C1=CN2C(C=C1)=NC(=C2NC1CCO)C1=CC(OC2=NC=CC=C2)=CC=C1 c:8,10,12,28,30,32,34,t:4,22,26	Z8878918325	1{193}	CNC(=O)c1cccc(N)nc1	2{290}	O=Cc1cccc(Oc2cccn2)c1	3{10}	[C-][N+]C1CCOC1	74.8	65

590	4{41,30,13}	COC1=CC=C(CNC2=C(N=C3C=NC(C)=CN2)3)C2CCN(CC2)C(C)=O)C=C1 c:12,15,30,t:2,4,8,10	Z8873684727	1{41}	Cc1cnc(N)c n1	2{30}	CC(=O)NIC CC(CC1)C= O	3{13}	COc1ccc(C[N+]#[C-])cc1	67.7	64
591	4{107,291,24}	COC1=CC(CNC2=C(N=C3C=CC(OCCO)=CN2)3)C2=C(C)C(OC)=CN=C2)=CC=C1 c:11,17,22,27,29,31,33,t:2,7,9	Z8878918508	1{107}	Nc1ccc(OC CO)cn1	2{291}	COc1cnc(C =O)c1C	3{24}	COc1cccc(C[N+]#[C-])c1	74.7	64
592	4{107,292,21}	CC1=C(SC=N1)C1=C(NCC2CC2)N2C=C(OC CO)C=CC2=N1 c:4,7,22,25,t:1,16	Z8873684602	1{107}	Nc1ccc(OC CO)cn1	2{292}	Cc1ncsc1C= O	3{21}	[C-]#[N+]CC1C C1	57.6	62
593	4{108,139,21}	CCCOC1=CN2C(C=C1)=NC(=C2NCC1CC1) C1=C(C)N(CCO)N=C1C c:8,10,12,21,28,t:4	Z8873684946	1{108}	CCCOc1ccc (N)cn1	2{139}	Cc1nn(CCO) c(C)c1C=O	3{21}	[C-]#[N+]CC1C C1	63.0	61
594	4{347,171,49}	COC1CC(C(OC)O1)C1=C(NC2CC(F)(F)C2)N 2C=C(Cl)C=CC2=N1 c:10,24,27,t:21	Z8873685323	1{347}	Nc1ccc(Cl)c n1	2{171}	COC1CC(C= O)C(OC)O1	3{49}	FC1(F)CC(C 1)[N+]#[C-]	60.9	58
595	4{350,293,5}	COCCNC1=C(N=C2C=NC(=CN12)C1=CC= CC=C1)C1=C(F)N(C)N=C1 c:10,12,19,21,24,29,t:6,8,17	Z8873684623	1{350}	Nc1cnc(en1) c2ccccc2	2{293}	Cn1ccc(C=O)c1F	3{5}	COCCC[N+] #[C-]	59.7	58
596	4{267,294,23}	COC(=O)CCC(NC1=C(N=C2C=CC=C(C#C)N 12)C1=C(OC)C(=O)C=CO1)C(=O)OC c:12,21,27,t:8,10,14	Z8878918868	1{267}	Nc1cccc(C# C)n1	2{294}	COc1c(C=O) occc1=O	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	68.7	58
597	4{81,112,9}	CNC1=C(N=C2C=NC=CN12)C1=C2C=CC=N N2N=C1 c:6,8,13,15,17,21,t:2,4	Z8873685319	1{81}	Nc1cncn1	2{112}	O=Cc1cnn2n cccc12	3{9}	C[N+]#[C-]	41.3	58
598	4{95,295,31}	CSCCNC1=C(N=C2C=CC(=CN12)C(F)F)C1= CSC(C)=N1 c:9,11,23,t:5,7,19	Z8873684632	1{95}	Nc1ccc(en1) C(F)F	2{295}	Cc1nc(C=O) cs1	3{31}	CSCC[N+]#[C-]	55.0	57
599	4{351,296,44}	CC(C)(C)OC(=O)NCCCCNC1=C(N=C2C=CC 3=C(C(O)CC3)N12)C1=CN(CCF)N=C1 c:17,35,t:13,15,19,29	Z8878918517	1{351}	Nc1ccc2CC C(O)c2n1	2{296}	FCCn1cc(C= O)cn1	3{44}	CC(C)(C)OC (=O)NCCCC [N+]#[C-]	72.7	57
600	4{118,124,31}	COC1=C(OCC2=C(C)ON=C2)C=CC(=C1)C 1=C(NCCSC)N2C(C=CC=C2C(C)O)=N1 c:2,6,10,14,16,19,28,30,35	Z8854581141	1{118}	Cl.CC(O)c1 cccc(N)n1	2{124}	COc1cc(C=O)ccc1OCc2c(C)noc2C	3{31}	CSCC[N+]#[C-]	73.8	57
601	4{28,297,26}	CCN1N=C(C)C(=N1)C1=C(NCC2=CC=C(F)C =C2)N2C=CC(=CC2=N1)C1=NOC=N1 c:6,9,18,22,24,27,33,t:3,13,15,30	Z8846491885	1{28}	Cl.Nc1cc(cc n1)c2ncon2	2{297}	CCn1nc(C)c(C=O)n1	3{26}	Fc1ccc(C[N+] #[C-])cc1	64.0	57
602	4{142,298,12}	CS(=O)(=O)CCOC1=CC=CN2C(NCC3CCOC 3)=C(CCCC3=CC=CC=C3)N=C12 c:9,27,29,t:7,20,25,32	Z8873684783	1{142}	CS(=O)(=O) CCOc1ccc nc1N	2{298}	O=CCCCc1c cccc1	3{12}	[C-]#[N+]CC1C COC1	69.9	57

603	4{153,299,15}	CCNC1=C(N=C2C=CC=C(N12)C(C)(C)O)C1=C(OC)C(OC)=CC=C1F c:7,9,18,24,26,t:3,5	Z8873684819	1{153}	CC(C)(O)c1cccc(N)n1	2{299}	COc1ccc(F)c(C=O)c1OC	3{15}	CC[N+]#[C-]	56.6	56
604	4{105,300,29}	CCOC(=O)CCNC1=C(CC2CN(C2)C(=O)OC(C)(C)C)N=C2C=CC=C(N12)C(N)=O c:8,25,27,t:23	Z8855739218	1{105}	NC(=O)c1cccc(N)n1	2{300}	CC(C)(C)OC(=O)N1CC(C=C=O)C1	3{29}	CCOC(=O)C[C[N+]#[C-]	67.3	56
605	4{352,301,49}	CNC(=O)C1=C(F)C=CC(=C1)C1=C(NC2CC(F)(F)C2)N2C=C(C=CC2=N1)N1CCN(C)C(=O)C1 c:4,7,9,12,23,25,28	Z8873684938	1{352}	CN1CCN(C1=O)c2ccc(N)nc2	2{301}	CNC(=O)c1cc(C=O)ccc1F	3{49}	FC1(F)CC(C1)[N+]#[C-]	73.5	56
606	4{91,302,7}	NC(=O)C1=CN2C(C=C1)=NC([C@@H]1C[C@@H]1C1=CC=C(F)C=C1)=C2NC1CCOCC1 &1:11,13,r,c:7,9,21,23,t:3,16,18	Z8829498723	1{91}	NC(=O)c1ccc(N)nc1	2{302}	Fc1ccc(cc1)[C@@H]2C[C@@H]2C=O &1:7,9,r	3{7}	[C-]#[N+]C1CCOCC1	59.4	56
607	4{67,284,13}	COC1=CC=C(CNC2=C(N=C3C=CC=C(C)N23)C2=C(C)N=CC=N2)C=C1 c:12,20,23,25,28,t:2,4,8,10,14	Z8878918440	1{67}	Cc1cccc(N)n1	2{284}	Cc1cccnc1C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	53.6	55
608	4{267,303,23}	COC(=O)CCC(NC1=C(N=C2C=CC=C(C#C)N12)C1=C(C)C(=C(OC)C=C1)[N+][[O-]]=O)C(=O)OC c:12,21,28,t:8,10,14,24	Z8854581183	1{267}	Nc1cccc(C#C)n1	2{303}	COc1ccc(C=O)c(C)c1[N+](=O)[O-]	3{23}	COC(=O)CC(C([N+]#[C-])C(=O)OC	71.7	55
609	4{124,304,43}	CC1=C(C=NN1CC(F)F)C1=C(NC2CCN(CC2)C(=O)OC(C)(C)C)N2C=CC=C(CO)C2=N1 c:3,11,29,36,t:1,31	Z8878918512	1{124}	Nc1cccc1CO	2{304}	Cc1c(C=O)cnn1CC(F)F	3{43}	CC(C)(C)OC(=O)N1CCC(CC1)[N+]#[C-]	73.1	55
610	4{52,189,7}	FC(F)(F)C1(CC1)C1=CN2C(C=C1)=NC(C1=CN(N=N1)C1CCOCC1)=C2NC1CCOCC1 c:12,14,20,29,t:8,17	Z8878918380	1{52}	Nc1ccc(cn1)C2(CC2)C(F)(F)F	2{189}	O=Cc1cn(nn1)C2CCOCC2	3{7}	[C-]#[N+]C1CCOCC1	71.0	55
611	4{353,223,15}	CCNC1=C(N=C2C=CC(NS(C)(=O)=O)=CN12)C1=CN=C(C=C1)C(=O)OC c:7,14,21,23,t:3,5,19	Z8878918898	1{353}	Cl.CS(=O)(=O)Nc1ccc(N)nc1	2{223}	Cl.COC(=O)c1ccc(C=O)c1n1	3{15}	CC[N+]#[C-]	57.9	55
612	4{354,305,70}	COCC1=NC(=CN1)C1=C(NC2CCN(C2)C(=O)OC(C)(C)C)N2C=C(C=CC2=N1)C(=O)OC c:5,9,26,28,31,t:3	Z8855619579	1{354}	COC(=O)c1ccc(N)nc1	2{305}	COCC1nc(C=O)c[nH]1	3{70}	CC(C)(C)OC(=O)N1CCC(C1)[N+]#[C-]	69.9	55
613	4{144,306,47}	CNS(=O)(=O)C1=CN2C(C=C1)=NC(=C2NC(C)C)C1=CC=C(C=C1)N(C)CCO c:9,11,13,22,24,t:5,20	Z8855739270	1{144}	CNS(=O)(=O)c1ccc(N)nc1	2{306}	CN(CCO)c1ccc(C=O)cc1	3{47}	CC(C)[N+]#[C-]	61.8	55

614	4{41,307,9}	CNC1=C(N=C2C=NC(C)=CN12)C1=CN=C(C)N1C c:6,9,t:2,4,14,16	Z8849597811	1{41}	Cc1cnc(N)c n1	2{307}	Cn1c(Cl)ncc 1C=O	3{9}	C[N+]#[C-]	40.9	55
615	4{50,308,31}	CSCCNC1=C(CCC2CCCC2)N=C2C=CC=C(N12)P(C)(C)=O c:5,17,19,t:15	Z8873685271	1{50}	CP(=O)(C)c 1cccc(N)n1	2{308}	O=CCCC1C CCC1	3{31}	CSCC[N+]#[C-]	56.1	55
616	4{54,309,47}	CC(C)NC1=C(N=C2C=CC(=CN12)C(=O)N(C)C)C1=CC=C(C=C1)N1C=CC=N1 c:8,10,22,24,28,30,t:4,6,20	Z8829498465	1{54}	Cl.CN(C)C(=O)c1ccc(N)nc1	2{309}	O=Cc1ccc(cc 1)n2cccn2	3{47}	CC(C)[N+]#[C-]	57.4	55
617	4{52,310,7}	FC(F)(F)C1(CC1)C1=CN2C(C=C1)=NC(C1C)COC3(CCC3)C1)=C2NC1CCOCC1 c:12,14,27,t:8	Z8878918339	1{52}	Nc1ccc(en1)C2(CC2)C(F)(F)F	2{310}	O=CC1CCO C2(CCC2)C1	3{7}	[C-]#[N+]C1CC OCC1	66.2	55
618	4{49,84,13}	COC1=CC=C(CNC2=C(CCSC)N=C3C=CC=C(CO)N23)C=C1 c:8,16,25,t:2,4,14,18	Z8855739168	1{49}	Nc1cccc(C O)n1	2{84}	CSCCC=O	3{13}	COc1ccc(C[N+]#[C-])cc1	52.5	54
619	4{355,93,22}	CC(C)C1=CC=CC2=NC(=C(NC3COC3)N12)C1=NC(CO)=CC=C1 c:5,24,26,t:3,7,9,20	Z8873684910	1{355}	CC(C)c1ccc c(N)n1	2{93}	OCc1cccc(C =O)n1	3{22}	[C-]#[N+]C1CO C1	49.6	54
620	4{351,311,39}	CCOCCNC1=C(N=C2C=CC3=C(C(O)CC3)N12)C1=NN(CC(F)(F)F)C=C1Br c:10,30,t:6,8,12,22	Z8855739266	1{351}	Nc1ccc2CC C(O)c2n1	2{311}	FC(F)(F)Cn1 cc(Br)c(C=O)n1	3{39}	CCOCC[N+]# [C-]	71.5	54
621	4{356,312,8}	COC(=O)C(CC1=CC=CC=C1)NC1=C(N=C2C=CC(C1)=C(N12)C(=O)N(C)C)C1CCOC1(C)C c:8,10,18,21,t:6,14,16	Z8846491967	1{356}	CN(C)C(=O) c1nc(N)ccc 1Cl	2{312}	CC1(C)OCC C1C=O	3{8}	COC(=O)C(Cc1cccc1)[N+]#[C-]	72.5	54
622	4{357,175,49}	OCC1CCN(CC1)C1=CN2C(NC3CC(F)(F)C3)=C(N=C2C=C1)C1=NNC=C1 c:20,22,25,31,t:9,28	Z8873685388	1{357}	Nc1ccc(en1)N2CCC(C O)CC2	2{175}	O=Cc1cc[nH]n1	3{49}	FC1(F)CC(C 1)[N+]#[C-]	58.4	54
623	4{53,236,42}	CC1=C(NC2=C(CCC3OCCO3)N=C3C=CC(CO)=CN23)C=CC=C1 c:1,4,16,20,25,27,t:14	Z8837933178	1{53}	Nc1ccc(CO) cn1	2{236}	O=CCCC1O CCO1	3{42}	Cc1cccc1[N +]#[C-]	51.0	53
624	4{48,313,22}	COC1=CC2=C(C=C1)N(C)C=C2C1=C(NC2C)OC2)N2C=CC(=CC2=N1)S(C)(=O)=O c:4,6,11,14,23,25,28,t:2	Z8878918334	1{48}	CS(=O)(=O) c1ccnc(N)c 1	2{313}	COc1ccc2n(C)cc(C=O)c2 c1	3{22}	[C-]#[N+]C1CO C1	62.4	53
625	4{69,314,46}	CNC(=O)C1=CC2=NC(C3=CN=C3)=C(NCC(C)=C)N2C=C1 c:12,23,t:4,6,9,14	Z8878918522	1{69}	CNC(=O)c1 ccnc(N)c1	2{314}	O=Cc1cn[nH]c1	3{46}	CC(=C)C[N+]]#[C-]	44.3	53
626	4{118,82,18}	COC1=C(C=CC=C1F)C1=C(NC(C)(C)C)N2C(C=CC=C2C(C)O)=N1 c:4,6,10,19,21,26,t:2	Z8873685369	1{118}	Cl.CC(O)c1 cccc(N)n1	2{82}	COc1c(F)ccc c1C=O	3{18}	CC(C)(C)[N +]#[C-]	51.0	53

627	4{49,52,13}	COC1=CC=C(CNC2=C(N=C3C=CC=C(CO)N23)C2=CN(N=C2)C2CCC2)C=C1 c:12,24,32,t:2,4,8,10,14,21	Z8873684618	1{49}	Nc1cccc(CO)n1	2{52}	O=Cc1enn(c1)C2CCC2	3{13}	COc1cccc(C[N+]#[C-])cc1	57.4	53
628	4{193,4,12}	CNC(=O)C1=CN2C(C=C1)=NC(=C2NCC1CCOC1)C1=C(C1)C=CC=C1C1 c:8,10,12,23,26,28,t:4	Z8855739153	1{193}	CNC(=O)c1ccc(N)nc1	2{4}	Clc1cccc(Cl)c1C=O	3{12}	[C-]#[N+]CC1COC1	59.6	53
629	4{193,315,12}	CCCN1C=CC(=N1)C1=C(NCC2CCOC2)N2C=C(C=CC2=N1)C(=O)NC c:4,6,9,20,22,25	Z8854581159	1{193}	CNC(=O)c1ccc(N)nc1	2{315}	CCCN1ccc(C=O)n1	3{12}	[C-]#[N+]CC1COC1	54.3	53
630	4{358,316,22}	COC(=O)C1=CC2=C(C=C1)N=C(C=C2)C1=C(NC2COC2)N2C=CC(=CC2=N1)C(C)(C)O c:6,8,11,13,16,25,27,30,t:4	Z8846491841	1{358}	CC(C)(O)c1ccnc(N)c1	2{316}	COC(=O)c1ccc2nc(C=O)ccc2c1	3{22}	[C-]#[N+]C1CO C1	61.4	53
631	4{92,317,14}	CCN1N=CC(=N1)C1=C(NCCOC)N2C=CC(=CC2=N1)C(N)=O c:3,5,8,16,18,21	Z8873685381	1{92}	NC(=O)c1ccnc(N)c1	2{317}	CCN1ccc(C=O)n1	3{14}	COCC[N+]#[C-]	46.7	53
632	4{359,318,22}	FC(F)OC1=CN2C(C=C1)=NC(C1CC11CC1(F)F)=C2NC1COC1 c:8,10,21,t:4	Z8878918410	1{359}	Nc1ccc(OC(F)F)cn1	2{318}	FC1(F)CC21CC2C=O	3{22}	[C-]#[N+]C1CO C1	49.9	53
633	4{71,319,10}	CC1=C(C=CC(OCC#N)=C1)C1=C(NC2CCOC2)N2C=C(I)N=CC2=N1 c:3,9,12,25,28,t:1,22	Z8855739134	1{71}	Nc1cnc(I)en1	2{319}	Cc1cc(OCC#N)ccc1C=O	3{10}	[C-]#[N+]C1CCOC1	67.2	52
634	4{113,62,14}	COCCNC1=C(N=C2N1C=CC=C2N1CCOCC1)C1CC11CCOCC1 c:7,11,13,t:5	Z8878918357	1{113}	Nc1ncccc1N2CCOCC2	2{62}	O=CC1CC21CCOCC2	3{14}	COCC[N+]#[C-]	54.6	52
635	4{360,320,29}	CCOC(=O)CCNC1=C(N=C2C=C(C(=O)OC)C(Br)=CN12)C1=NN(C)C=N1 c:19,28,t:8,10,12,24	Z8878918308	1{360}	COC(=O)c1cc(N)nc1Br	2{320}	Cn1cnc(C=O)n1	3{29}	CCOC(=O)C[C[N+]#[C-]	63.7	52
636	4{352,103,47}	CC(C)NC1=C(N=C2C=CC(=CN12)N1CCN(C)C(=O)C1)C1CCC2(COC2)OC1 c:8,10,t:4,6	Z8849597817	1{352}	CN1CCN(C1=O)c2ccc(N)nc2	2{103}	O=CC1CCC2(COC2)OC1	3{47}	CC(C)[N+]#[C-]	58.4	52
637	4{261,321,12}	CN(C)C1CCN(CC1)C1=CN2C(C=C1)=NC(C1CC11CCC(F)(F)CC1)=C2NCC1CCOC1 c:14,16,30,t:10	Z8873685382	1{261}	CN(C)C1CCN(CC1)c2ccc(N)nc2	2{321}	FC1(F)CCC2((CC2C=O)C1	3{12}	[C-]#[N+]CC1COC1	68.6	52
638	4{37,139,24}	COC1=CC(CNC2=C(N=C3C=CC=C(C(F)F)N23)C2=C(C)N(CCO)N=C2C)=CC=C1 c:11,21,28,31,33,t:2,7,9,13	Z8878918891	1{37}	Cl.Nc1cccc(n1)C(F)F	2{139}	Cc1nn(CCO)c(C)c1C=O	3{24}	COc1cccc(C[N+]#[C-])c1	62.1	52
639	4{180,155,53}	COC(=O)C1=CC2=NC(=C(NCCOCC3=CC=C(C=C3)N2C=C1C)C1=CN=CN=C1 c:17,19,24,30,32,t:4,6,8,15,28	Z8803896942	1{180}	COC(=O)c1cc(N)nc1C	2{155}	O=Cc1cncnc1	3{53}	[C-]#[N+]CCOCC1cccc1	58.7	52

640	4{87,322,23}	COC(=O)CCC(NC1=C(N=C2C=C(C)C(Cl)=C(N12)C1=CC(NC(C)=O)=CC=C1)C(=O)OC c:16,27,29,t:8,10,12,21	Z8873684717	1{87}	Cc1cc(N)nc1Cl	2{322}	CC(=O)Nc1ccc(C=O)c1	3{23}	COC(=O)CC(C[N+]#[C-])C(=O)OC	66.5	52
641	4{311,220,61}	CC1=C(C(C)=NN1)C1=C(NCCCNC(=O)OC(C)(C)C)N2C=CC(F)=CC2=N1 c:4,8,23,26,29,t:1	Z8878918419	1{311}	Nc1cc(F)ccn1	2{220}	Cc1n[nH]c(C)c1C=O	3{61}	CC(C)(C)OC(=O)NCCC[N+]#[C-]	56.6	52
642	4{361,323,12}	CC(C)OC1=CC=CN2C(NCC3CCOC3)=C(N=C12)[C@@H]1C[C@@H](C1)NC(=O)OC(C)(C)C r,c:6,17,t:4,19	Z8846492360	1{361}	Cl.CC(C)Oc1ccnc1N	2{323}	CC(C)(C)OC(=O)N[C@H]1C[C@H](C1)C=O	3{12}	[C-]#[N+]CC1COC1	62.2	52
643	4{120,324,70}	CN1C=C(C=N1)C1=CC2=NC(C3CC4(C3)CCCO4)=C(NC3CCN(C3)C(=O)OC(C)(C)C)N2C=C1 c:2,4,39,t:7,9,21	Z8829498458	1{120}	Cn1cc(en1)c2ccnc(N)c2	2{324}	O=CC1CC2(C1)CCCO2	3{70}	CC(C)(C)OC(=O)N1CCC(C1)[N+]#[C-]	68.6	52
644	4{193,325,21}	CNC(=O)C1=CN2C(C=C1)=NC(CCN1C(=O)C3=C(C=CC=C3)C1=O)=C2NCC1CC1 c:8,10,20,22,27,t:4,18	Z8878918490	1{193}	CNC(=O)c1ccc(N)nc1	2{325}	O=CCCN1C(=O)c2ccccc2C1=O	3{21}	[C-]#[N+]CC1CC1	58.1	52
645	4{362,326,10}	CNC(=O)C1=CC=CC2=NC(=C(NC3CCOC3)N12)C1=CC=NN1C c:6,24,t:4,8,10,22	Z8873684581	1{362}	CNC(=O)c1cccc(N)n1	2{326}	Cn1cccc1C=O	3{10}	[C-]#[N+]C1CCOC1	47.3	51
646	4{109,327,29}	CCOC(=O)CCNC1=C(N=C2C=CC=C(N12)S(N)(=O)=O)C1=NC(Cl)=CC(Cl)=C1 c:12,14,26,29,t:8,10,23	Z8855739173	1{109}	Cl.Nc1cccc(n1)S(=O)(=O)N	2{327}	Clc1cc(Cl)nc(C=O)c1	3{29}	CCOC(=O)CC[N+]#[C-]	63.4	51
647	4{107,328,43}	CCC1=NNC=C1C1=C(NC2CCN(CC2)C(=O)OC(C)(C)C)N2C=C(OCCO)C=CC2=N1 c:5,8,32,35,t:2,26	Z8873685371	1{107}	Nc1ccc(OCO)en1	2{328}	Cl.CCc1n[nH]cc1C=O	3{43}	CC(C)(C)OC(=O)N1CCC(CC1)[N+]#[C-]	65.0	51
648	4{363,329,62}	COC(=O)C1=CC2=NC(=C(NC3(CCCC3)C(=O)OC)N2C=C1)C1=C(C)N(CCC1)N=C1C c:23,26,33,t:4,6,8	Z8878918904	1{363}	COC(=O)c1ccnc(N)c1	2{329}	Cc1nn(CCC1)c(C)c1C=O	3{62}	COC(=O)C1(CCCC1)[N+]#[C-]	65.4	51
649	4{364,330,62}	COC(=O)C1(CCCC1)NC1=C(N=C2C=CC(=C(N12)N1CCNC(=O)C1)C1=C(OC)C(Cl)=NC=C1 c:15,17,30,35,37,t:11,13	Z8849597816	1{364}	Nc1ccc(en1)N2CCNC(=O)C2	2{330}	COc1c(Cl)nc1C=O	3{62}	COC(=O)C1(CCCC1)[N+]#[C-]	68.8	51
650	4{48,331,35}	CSCCCNC1=C(N=C2C=C(C=CN12)S(C)(=O)=O)C1=CC2=C(OCCNC2=O)C=C1 c:10,12,32,t:6,8,21,23	Z8873685336	1{48}	CS(=O)(=O)c1ccnc(N)c1	2{331}	O=Cc1ccc2OCCNC(=O)c2c1	3{35}	CSCCC[N+]#[C-]	63.4	51

651	4{113,246,14}	COCCNC1=C(N=C2N1C=CC=C2N1CCOCC1)C1CC11CCCOC1 c:7,11,13,t:5	Z8878918399	1{113}	Nc1ncccc1 N2CCOCC2	2{246}	O=CC1CC21 CCCOC2	3{14}	COCC[N+]#[C-]	53.2	51
652	4{36,46,9}	CNC1=C(CCCCOCC)N=C2C=CC(Br)=CN12 c:2,13,16,t:11	Z8873684758	1{36}	Nc1ccc(Br) cn1	2{46}	COCCCCC =O	3{9}	C[N+]#[C-]	44.7	51
653	4{327,332,34}	COC(=O)C1=C(F)C2=NC(=C(NCC3CCCO3)N2C=C1)C1=CN(CC2CC2)N=C1 c:4,21,32,t:7,9,24	Z8878918569	1{327}	COC(=O)c1 ccnc(N)c1F	2{332}	O=Cc1cnn(C C2CC2)c1	3{34}	[C-] #[N+]CC1C CCO1	56.6	51
654	4{358,333,15}	CCNC1=C(N=C2C=C(C=CN12)C(C)(C)O)C1CCC2(CC(C2)(OC)OC)CC1 c:7,9,t:3,5	Z8878918336	1{358}	CC(C)(O)c1 ccnc(N)c1	2{333}	COCC1(CC2(C1)CCC(CC2)C=O)OC	3{15}	CC[N+]#[C-]	54.5	50
655	4{66,99,22}	COCCC1=CC2=NC(=C(NC3COC3)N2C=C1)C1=COC=N1 c:18,24,t:4,6,8,21	Z8873684845	1{66}	COCCc1ccn c(N)c1	2{99}	O=Cc1cocn1	3{22}	[C-] #[N+]C1CO C1	42.4	50
656	4{365,334,10}	CC1=C(N=CO1)C1=C(NC2CCOC2)N2C(C=C(C)C=C2C)=N1 c:3,7,21,24,t:1,18	Z8878918832	1{365}	Cc1cc(C)nc (N)c1	2{334}	Cc1ocnc1C= O	3{10}	[C-] #[N+]C1CC OC1	42.0	50
657	4{366,134,12}	COCC1=NC(=NC=C1)C1=C(NCC2CCOC2)N2C=CC=C(OC)C2=N1 c:4,6,9,20,27,t:2,22	Z8873684742	1{366}	COc1ccnc 1N	2{134}	COc1ccnc(C =O)n1	3{12}	[C-] #[N+]CC1C COC1	47.8	50
658	4{367,335,34}	CC1=CN2C(NCC3CCCO3)=C(N=C2C(=C1)C#C)C1=CN(N=C1)C1CCOCC1 c:12,14,17,25,t:1,22	Z8873685329	1{367}	Cc1cnc(N)c (C#C)c1	2{335}	O=Cc1cnn(c 1)C2CCOCC 2	3{34}	[C-] #[N+]CC1C CCO1	54.5	50
659	4{166,336,32}	COCC1=NSC=C1C1=C(NC2CCC2)N2C=CC(CSCCO)=CC2=N1 c:5,8,17,24,27,t:2	Z8873684839	1{166}	Nc1cc(CSC CO)ccn1	2{336}	COc1nsc1C =O	3{32}	[C-] #[N+]C1CC C1	52.5	50
660	4{368,337,49}	CN1C=C(C=N1)C1=C(C)N2C(C=C1)=NC(=C2N1CC(F)(F)C1)C1=CN(C)C(=O)N(C)C1=O c:2,4,7,12,14,16,t:27	Z8873684788	1{368}	Cc1nc(N)cc c1c2cnn(C) c2	2{337}	Cn1cc(C=O) c(=O)n(C)c1 =O	3{49}	FC1(F)CC(C 1)[N+]#[C-]	61.1	50
661	4{92,338,7}	CC1=C(OC=C1)C1=C(NC2CCOCC2)N2C=C(C=CC2=N1)C(N)=O c:4,7,18,20,23,t:1	Z8878918819	1{92}	NC(=O)c1c cnc(N)c1	2{338}	Cc1ccoc1C= O	3{7}	[C-] #[N+]C1CC OCC1	45.6	50
662	4{164,328,24}	CCC1=NNC=C1C1=C(NCC2=CC(OC)=CC=C2)N2C=CC(CN(C)C)=CC2=N1 c:5,8,16,18,22,28,31,t:2,12	Z8873684947	1{164}	CN(C)Cc1c cnc(N)c1	2{328}	Cl.CCC1n[nH]]cc1C=O	3{24}	COc1cccc(C N+)#[C-]c1	54.1	50

663	4{351,339,67}	CCC(C)NC1=C(N=C2C=CC3=C(C(O)CC3)N12)C1=NN=C(N1)C(F)(F)F c:9,23,t:5,7,11,21	Z8878918810	1{351}	Nc1ccc2CC(O)c2n1	2{339}	FC(F)(F)c1nnc(C=O)[nH]1	3{67}	CCC(C)[N+]#[C-]	50.9	50
664	4{103,165,40}	CCOC(=O)C1=CC=C(NC2=C(N=C3C=NC=C(CO)N23)C2=NN(C=C2)[C@H]2[C@@H](C2)C(=O)OC)C=C1 r,c:14,26,38,t:5,7,10,12,16,23	Z8878918652	1{103}	Nc1cnc(CO)n1	2{165}	COC(=O)[C@H]1C[C@@H](C1)n2cc(C=O)n2	3{40}	CCOC(=O)c1ccc([N+]#[C-])cc1	65.6	50
665	4{369,340,18}	CCN1C=NC(=N1)C1=C(NC(C)(C)C)N2C=C(C=CC2=N1)C(F)C(F)(F)F c:3,5,8,16,18,21	Z8878918892	1{369}	Cl.Nc1ccc(cn1)C(F)C(F)(F)F	2{340}	CCn1cnc(C=O)n1	3{18}	CC(C)(C)[N+]#[C-]	51.1	49
666	4{348,341,39}	CCOCCNC1=C(N=C2C=NC(F)=CN12)C1=CN=C(S1)C(C)O c:10,13,20,t:6,8,18	Z8878918626	1{348}	Nc1cnc(F)c n1	2{341}	CC(O)c1ncc(C=O)s1	3{39}	CCOCC[N+]#[C-]	51.1	49
667	4{54,36,22}	CN(C)C(=O)C1=CN2C(C=C1)=NC(=C2NC1COC1)C1=NC(C)=C(OC(F)F)C=C1 c:9,11,13,31,t:5,22,25	Z8846491870	1{54}	Cl.CN(C)C(=O)c1ccc(N)nc1	2{36}	Cc1nc(C=O)ccc1OC(F)F	3{22}	[C-]#[N+]C1COC1	55.1	49
668	4{366,342,12}	COC1=CC=CN2C(NCC3CCOC3)=C(N=C12)C1=CN=C(S1)C1=NC=CC=C1 c:4,15,23,29,31,t:2,17,21,27	Z8873684850	1{366}	COc1cccnc1N	2{342}	O=Cc1cnc(s1)c2cccn2	3{12}	[C-]#[N+]CC1COC1	53.7	49
669	4{370,343,10}	COC1=C(Br)C=CN2C(NC3CCOC3)=C(N=C12)C1C(C)C1Cl c:2,5,15,t:17	Z8854581178	1{370}	COc1c(N)nc cclBr	2{343}	CC1C(Cl)C1C=O	3{10}	[C-]#[N+]C1CCOC1	52.7	49
670	4{113,344,6}	CCOC(=O)CCNC1=C(N=C2N1C=CC=C2N1CCOCC1)C1=C(C)C=NN1COC c:11,15,17,27,30,t:9	Z8873685396	1{113}	Nc1ncccc1N2CCOCC2	2{344}	COc1nccc(C)c1C=O	3{6}	CCOC(=O)C CC[N+]#[C-]	59.8	49
671	4{50,174,7}	CP(C)(=O)C1=CC=CC2=NC(=C(NC3CCOCC3)N12)C1=CN(CC2CCCO2)N=N1 c:6,33,t:4,8,10,23	Z8849597810	1{50}	CP(=O)(C)c1ccc(N)n1	2{174}	O=Cc1cn(CC2CCCO2)nn1	3{7}	[C-]#[N+]C1CCOCC1	58.2	49
672	4{105,300,34}	CC(C)(C)OC(=O)N1CC(CC2=C(NCC3CCCO3)N3C(C=CC=C3C(N)=O)=N2)C1 c:11,23,25,30	Z8878918635	1{105}	NC(=O)c1c ccc(N)n1	2{300}	CC(C)(C)OC(=O)N1CC(C=C=O)C1	3{34}	[C-]#[N+]CC1COCO1	55.9	48
673	4{54,138,53}	CN(C)C(=O)C1=CN2C(C=C1)=NC(=C2NCCOCC1=CC=CC=C1)C1=NC(C)=NC(C)=C1 c:9,11,13,23,25,31,34,t:5,21,28	Z8873684825	1{54}	Cl.CN(C)C(=O)c1ccc(N)nc1	2{138}	Cc1cc(C=O)nc(C)n1	3{53}	[C-]#[N+]CCOCC1cccc1	57.5	48
674	4{369,203,7}	FC(F)CN1C=CC(=N1)C1=C(NC2CCOCC2)N2C=C(C=CC2=N1)C(F)C(F)(F)F c:5,7,10,21,23,26	Z8878918909	1{369}	Cl.Nc1ccc(cn1)C(F)C(F)(F)F	2{203}	FC(F)Cn1ccc(C=O)n1	3{7}	[C-]#[N+]C1CCOCC1	57.7	48

675	4{48,345,22}	COC1=CC(C2=C(NC3COC3)N3C=CC(=CC3=N2)S(C)(=O)=O)=C(F)C=C1 c:5,14,16,19,28,t:2,25	Z8878918335	1{48}	CS(=O)(=O)c1ccnc(N)c1	2{345}	COc1ccc(F)c(C=O)c1	3{22}	[C-] #[N+]C1CO C1	49.4	48
676	4{371,164,10}	CN1N=C(C2=C1CCOC2)C1=C(NC2CCOC2)N2C=CC=C(OCCCC#N)C2=N1 c:2,4,12,22,33,t:24	Z8873685339	1{371}	Nc1ncccc1OCCCC#N	2{164}	Cn1nc(C=O)c2COCCc21	3{10}	[C-] #[N+]C1CC OC1	54.4	48
677	4{327,346,34}	CCN(C)C(=O)C1=CC=C(C=C1)C1=C(NCC2C CCO2)N2C=CC(C(=O)OC)=C(F)C2=N1 c:8,10,13,24,34,t:6,30	Z8878918338	1{327}	COC(=O)c1ccnc(N)c1F	2{346}	CCN(C)C(=O)c1ccc(C=O)cc1	3{34}	[C-] #[N+]CC1C CCO1	58.5	48
678	4{187,70,12}	CC(F)(F)C1=NC(=CS1)C1=C(NCC2CCOC2)N2C=C(Cl)C(=CC2=N1)C#N c:6,10,24,27,t:4,21	Z8878918511	1{187}	Nc1cc(C#N)c(Cl)cn1	2{70}	CC(F)(F)c1nc(C=O)cs1	3{12}	[C-] #[N+]CC1C COC1	54.6	48
679	4{125,122,31}	CSCCNC1=C(N=C2C=CC(CCO)=CN12)C1=CN=C(N=C1)C1=CC=CS1 c:9,14,21,23,28,t:5,7,19,26	Z8873684811	1{125}	Nc1ccc(CC O)cn1	2{122}	O=Cc1enc(n c1)c2cccs2	3{31}	CSCC[N+]#[C-]	53.0	48
680	4{92,347,18}	CCCN1C=C(N=N1)C1=C(NC(C)(C)C)N2C=C(C=CC2=N1)C(N)=O c:4,6,9,17,19,22	Z8855739156	1{92}	NC(=O)c1ccnc(N)c1	2{347}	CCCN1cc(C=O)nn1	3{18}	CC(C)(C)[N+]#[C-]	43.9	48
681	4{347,139,21}	CC1=NN(CCO)C(C)=C1C1=C(NCC2CC2)N2C=C(Cl)C=CC2=N1 c:8,11,23,26,t:1,20	Z8873685465	1{347}	Nc1ccc(Cl)cn1	2{139}	Cc1nn(CCO)c(C)c1C=O	3{21}	[C-] #[N+]CC1C C1	46.2	48
682	4{372,314,46}	CC(=C)CNC1=C(N=C2N1C=CC=C2OCC1=C C=NC=C1)C1=CNN=C1 c:7,11,13,20,22,28,t:5,18,25	Z8873684836	1{372}	Nc1ncccc1OCe2ccncc2	2{314}	O=Cc1cn[nH]c1	3{46}	CC(=C)C[N+]#[C-]	46.0	47
683	4{79,30,13}	COC1=CC=C(CNC2=C(N=C3C=NC=C(C)N23)C2CCN(CC2)C(C)=O)C=C1 c:12,30,t:2,4,8,10,14	Z8878918306	1{79}	Cc1cncc(N)n1	2{30}	CC(=O)N1C CC(CC1)C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	50.0	47
684	4{48,348,22}	CC(C)(C)OC(=O)N1CC2CCC1C(C2)C1=C(NC2COC2)N2C=CC(=CC2=N1)S(C)(=O)=O c:17,26,28,31	Z8878918482	1{48}	CS(=O)(=O)c1ccnc(N)c1	2{348}	CC(C)(C)OC(=O)N1CC2CCC1C(C2)C=O	3{22}	[C-] #[N+]C1CO C1	64.6	47
685	4{48,345,15}	CCNC1=C(N=C2C=C(C=CN12)S(C)(=O)=O)C1=C(F)C=CC(OC)=C1 c:7,9,18,21,25,t:3,5	Z8878918575	1{48}	CS(=O)(=O)c1ccnc(N)c1	2{345}	COc1ccc(F)c(C=O)c1	3{15}	CC[N+]#[C-]	46.0	47
686	4{367,349,34}	CC1=CN2C(NCC3CCCO3)=C(N=C2C(=C1)C#C)C1C[C@H]2OC(C)(C)O[C@H]2C1 c:12,14,17,t:1	Z8873684754	1{367}	Cc1cnc(N)c(C#C)c1	2{349}	CC1(C)O[C@@@H]2CC(C[C@@@H]2O1)C=O	3{34}	[C-] #[N+]CC1C CCO1	50.0	47

687	4{293,350,12}	COC1=CC(C)=CN2C(NCC3CCOC3)=C(N=C12)C1C2CCOCC12 c:5,16,t:2,18	Z8873684691	1{293}	COc1cc(C)cnc1N	2{350}	O=CC1C2CCOCC12	3{12}	[C-]#[N+]CC1COC1	44.9	47
688	4{373,351,39}	CCOCCNC1=C(CCCSC)N=C2C=CC(CNC(=O)OC(C)(C)C)=CN12 c:6,15,26,t:13	Z8878918621	1{373}	CC(C)(C)OC(=O)NCc1ccc(N)nc1	2{351}	CSCCCC=O	3{39}	CCOCC[N+]#[C-]	54.2	46
689	4{230,198,34}	CCC1=NN(C)C=C1C1=C(NCC2CCCO2)N2C=C(Br)C=C(C(C)O)C2=N1 c:6,9,29,t:2,20,23	Z8810902957	1{230}	CC(O)c1cc(Br)cnc1N	2{198}	CCc1nn(C)cc1C=O	3{34}	[C-]#[N+]CC1COCO1	56.1	46
690	4{374,352,70}	COCCCC1=C(NC2CCN(C2)C(=O)OC(C)(C)C)N2C(C=CC=C2C(=O)OC)=N1 c:5,23,25,31	Z8878918489	1{374}	COC(=O)c1cccc(N)n1	2{352}	COCCCC=O	3{70}	CC(C)(C)OC(=O)N1CCCC(C1)[N+]#[C-]	54.0	46
691	4{375,139,10}	CC(C)OC1=CN=CC2=NC(=C(NC3CCOC3)N12)C1=C(C)N(CCO)N=C1C c:6,22,29,t:4,8,10	Z8873684781	1{375}	CC(C)Oe1cncc(N)n1	2{139}	Cc1nn(CCO)c(C)c1C=O	3{10}	[C-]#[N+]C1CCOC1	50.0	46
692	4{150,223,35}	COC(=O)C1=NC=C(C=C1)C1=C(NCCCSC)N2C=CC(=CC2=N1)C1CCOC1 c:6,8,11,20,22,25,t:4	Z8855619591	1{150}	Nc1cc(cen1)C2CCOC2	2{223}	Cl.COC(=O)c1ccc(C=O)cnc1	3{35}	CSCCC[N+]#[C-]	53.0	46
693	4{167,353,23}	COC(=O)CCC(NC1=C(N=C2N1C(C)=CN=C2C)C1=C(CF)C=CC=C1)C(=O)OC c:10,15,17,21,25,27,t:8	Z8878918618	1{167}	Cc1enc(C)c(N)n1	2{353}	FCc1cccc1C=O	3{23}	COC(=O)CC(C([N+]#[C-]))C(=O)OC	53.2	46
694	4{77,354,5}	COCCNC1=C(N=C2C=CC(=CN12)C1=CN=CC=C1)C1=C(C=CC=C1)P(C)(C)=O c:10,12,19,21,26,28,t:6,8,17,24	Z8873684627	1{77}	Nc1ccc(en1)c2cccn2	2{354}	CP(=O)(C)c1cccc1C=O	3{5}	COCCC[N+]#[C-]	53.8	46
695	4{206,62,14}	COCCNC1=C(N=C2N1C=CC(I)=C2F)C1CC11CCOCC1 c:7,11,14,t:5	Z8873684638	1{206}	Nc1nccc(I)c1F	2{62}	O=CC1CC21CCOCC2	3{14}	COCC[N+]#[C-]	55.1	46
696	4{353,355,15}	CCNC1=C(N=C2C=CC(NS(C)=O)=O)=CN12)C1=C(CCNC(=O)OC(C)(C)OC)=N1 c:7,14,19,32,t:3,5	Z8873684671	1{353}	Cl.CS(=O)(=O)Nc1ccc(N)nc1	2{355}	CC(C)(C)OC(=O)NCCc1ocnc1C=O	3{15}	CC[N+]#[C-]	57.1	46
697	4{69,242,61}	CNC(=O)C1=CC2=NC(=C(NCCCNC(=O)OC(C)(C)C)N2C=C1)C1=CN2N=CC(C#N)=C2N=C1 c:24,30,34,37,t:4,6,8,27	Z8873685295	1{69}	CNC(=O)c1ccnc(N)c1	2{242}	O=Cc1cnc2c(C#N)cnn2c1	3{61}	CC(C)(C)OC(=O)NCCC[N+]#[C-]	60.0	45
698	4{50,356,18}	CC(C)CN1C=C(N=N1)C1=C(NC(C)(C)C)N2C(C=CC=C2P(C)(C)=O)=N1 c:5,7,10,19,21,27	Z8873684868	1{50}	CP(=O)(C)c1cccc(N)n1	2{356}	CC(C)Cn1cc(C=O)nn1	3{18}	CC(C)(C)[N+]#[C-]	47.5	45

699	4{109,357,50}	CCC1=C(C(C)=NO1)C1=C(NC2=CC3=C(OC CO3)C=C2)N2C(C=CC=C2S(N)(=O)=O)=N1 c:5,9,21,26,28,34,t:2,12,14	Z8878918305	1{109}	Cl.Nc1cccc(n1)S(=O)(= O)N	2{357}	CCc1onc(C)c 1C=O	3{50}	[C-]#[N+]c1ccc 2OCCOc2c1	55.6	45
700	4{113,358,14}	COCCNC1=C(N=C2N1C=CC=C2N1CCOCC1)C1CC11CCN(C1)C(=O)OC(C)(C)C c:7,11,13,t:5	Z8878918398	1{113}	Nc1cccc1 N2CCOCC2	2{358}	CC(C)(C)OC (=O)N1CCC 2(CC2C=O) C1	3{14}	COCC[N+]# C-]	57.4	45
701	4{48,359,22}	COC1=CC(=CC(=C1)C1=C(NC2COC2)N2C= CC(=CC2=N1)S(C)(=O)=O)C(F)(F)F c:4,6,9,18,20,23,t:2	Z8873684872	1{48}	CS(=O)(=O)c1ccnc(N)c 1	2{359}	COc1cc(C=O)cc(c1)C(F)(F)F	3{22}	[C-]#[N+]C1CO C1	53.3	45
702	4{47,195,26}	COC1=C(F)C=C(C=N1)C1=C(NCC2=CC=C(F))C=C2)N2C=CC(=CC2=N1)S(N)(=O)=O c:2,5,7,10,19,23,25,28,t:14,16	Z8849597834	1{47}	Cl.Nc1cc(cc n1)S(=O)(= O)N	2{195}	COc1ncc(C= O)cc1F	3{26}	Fc1ccc(C[N+]#[C-])cc1	53.5	44
703	4{376,360,12}	COC1=NC(Cl)=CN2C(NCC3CCOC3)=C(N=C 12)C1=C2N=CN(C)C2=CC=C1 c:5,16,22,24,29,31,t:2,18	Z8873684704	1{376}	COc1nc(Cl) cnc1N	2{360}	Cn1enc2c(C =O)cccc12	3{12}	[C-]#[N+]CC1C COC1	49.4	44
704	4{38,7,9}	CNC1=C(N=C2C=C(C=CN12)C#N)C1=NC(C)=CC(CO)=C1 c:6,8,18,22,t:2,4,15	Z8873685471	1{38}	Nc1cc(C#N)ccn1	2{7}	Cc1cc(CO)cc (C=O)n1	3{9}	C[N+]#[C-]	35.0	44
705	4{91,361,7}	NC(=O)C1=CN2C(C=C1)=NC(=C2NC1CCOC C1)C1=C(Br)C=CC(Br)=N1 c:7,9,11,22,25,28,t:3	Z8873685278	1{91}	NC(=O)c1c cc(N)nc1	2{361}	Brc1ccc(Br)c (C=O)n1	3{7}	[C-]#[N+]C1CC OCC1	59.0	44
706	4{104,362,39}	CCOCCNC1=C(N=C2C=CC3=C(COCC3)N12)C1=CC(OC)=C(OC)C(OC)=C1 c:10,32,t:6,8,12,22,26	Z8846492263	1{104}	Nc1ccc2CC OCc2n1	2{362}	COc1cc(C=O)cc(OC)c1O C	3{39}	CCOCC[N+] #[C-]	50.3	44
707	4{54,93,22}	CN(C)C(=O)C1=CN2C(C=C1)=NC(=C2NC1C OC1)C1=NC(CO)=CC=C1 c:9,11,13,26,28,t:5,22	Z8829498567	1{54}	Cl.CN(C)C(=O)c1ccc(N)nc1	2{93}	OCc1cccc(C =O)n1	3{22}	[C-]#[N+]C1CO C1	43.0	43
708	4{193,169,12}	CNC(=O)C1=CN2C(C=C1)=NC(=C2NCC1CC OC1)C1=NNC2=C1N=CC=C2 c:8,10,12,26,29,31,t:4,23	Z8803896944	1{193}	CNC(=O)c1 ccc(N)nc1	2{169}	O=Cc1n[nH] c2cccnc12	3{12}	[C-]#[N+]CC1C COC1	45.8	43
709	4{79,307,13}	COC1=CC=C(CNC2=C(N=C3C=NC=C(C)N2 3)C2=CN=C(Cl)N2C)C=C1 c:12,28,t:2,4,8,10,14,20,22	Z8855739194	1{79}	Cc1nccc(N n1)	2{307}	Cn1c(Cl)ncc 1C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	44.3	43
710	4{62,363,6}	CCOC(=O)CCNC1=C(N=C2C=C(CO)C=CN 12)C1=CNC(C)=N1 c:17,26,t:9,11,13,22	Z8878918835	1{62}	Nc1cc(CO)c cn1	2{363}	Cc1nc(C=O) c[nH]1	3{6}	CCOC(=O)C CC[N+]#[C-]	41.0	42

711	4{99,364,66}	CC(NC1=C(CCC2CCCO2)N=C2C=CC(=CN12)S(N)(=O)=O)C1=CC=CC=C1 c:3,15,17,28,30,t:13,26	Z8873685354	1{99}	Nc1ccc(en1)S(=O)(=O)N	2{364}	O=CCCC1C CCO1	3{66}	CC([N+]#[C-])c1cccc1	47.5	42
712	4{139,365,10}	FC(F)C1=CC2=NC(=C(NC3CCOC3)N2C=C1)C1=NNC2=C1C=NC=C2 c:18,24,27,29,t:3,5,7,21	Z8873684877	1{139}	Nc1cc(ccn1)C(F)F	2{365}	O=Cc1n[nH]c2ccncc12	3{10}	[C-]#[N+]C1CCOC1	41.9	42
713	4{92,366,26}	CCN1C=NC(=C1)C1=C(NCC2=CC=C(F)C=C2)N2C=CC(=CC2=N1)C(N)=O c:3,5,8,17,21,23,26,t:12,14	Z8878918679	1{92}	NC(=O)c1ccnc(N)c1	2{366}	CCn1cnc(C=O)c1	3{26}	Fc1ccc(C[N+]#[C-])cc1	42.6	42
714	4{101,89,6}	CCOC(=O)CCCN1=C(N=C2N1C=C(CO)C=C2C1)C1=CN=C(CC)N=C1 c:11,19,29,t:9,15,23,25	Z8873685362	1{101}	Nc1ncc(CO)cc1C1	2{89}	CCc1ncc(C=O)cn1	3{6}	CCOC(=O)C CC[N+]#[C-]	46.8	41
715	4{179,42,5}	COCCCN1=C(N=C2C=C(OC)C=CN12)C1=CN(C)N=C1C1 c:14,23,t:6,8,10,19	Z8878918672	1{179}	COc1ccnc(N)c1	2{42}	Cn1cc(C=O)c(Cl)n1	3{5}	COCCC[N+]#[C-]	39.2	41
716	4{377,367,12}	NC(=O)C1=CC(=CC=C1)C1=C(NCC2CCOC2)N2C=CC=C(OCC(F)F)C2=N1 c:5,7,10,21,31,t:3,23	Z8854581151	1{377}	Nc1ncccc1OCC(F)F	2{367}	NC(=O)c1ccc(C=O)c1	3{12}	[C-]#[N+]CC1C COC1	46.6	41
717	4{127,320,29}	CCOC(=O)CCNC1=C(N=C2N1C=CC=C2F)C1=NN(C)C=N1 c:10,14,16,24,t:8,20	Z8878918360	1{127}	Nc1ncccc1F	2{320}	Cn1cnc(C=O)n1	3{29}	CCOC(=O)C C[N+]#[C-]	37.2	41
718	4{32,11,18}	CC(C)(C)NC1=C(N=C2C=C(C=CN12)P(C)(C)=O)C1=NN(CC(F)(F)F)C=C1 c:9,11,28,t:5,7,20	Z8878918527	1{32}	CP(=O)(C)c1ccnc(N)c1	2{11}	FC(F)(F)Cn1ccc(C=O)n1	3{18}	CC(C)(C)[N+]#[C-]	46.2	41
719	4{377,368,12}	CC1=C(C)N=NC(=C1)C1=C(NCC2CCOC2)N2C=CC=C(OCC(F)F)C2=N1 c:1,4,6,9,20,30,t:22	Z8846492294	1{377}	Nc1ncccc1OCC(F)F	2{368}	Cc1cc(C=O)mc1C	3{12}	[C-]#[N+]CC1C COC1	45.1	41
720	4{378,369,24}	COC1=CC(CNC2=C(N=C3N2C=CC=C3OCC2=CN=CC=C2)C2=CON=C2C)=CC=C1 c:9,13,15,22,24,30,33,35,t:2,7,20,27	Z8878918644	1{378}	Nc1ncccc1OCc2ccncc2	2{369}	Cc1nocc1C=O	3{24}	COc1cccc(C[N+]#[C-])c1	49.2	41
721	4{73,370,20}	CNC(=O)C1=CC=C(C=C1)C1=C(NC2=C(C)C=C(OC)C=C2)N2N3C=CN=C3C=CC2=N1 c:6,8,11,14,21,26,28,31,34,t:4,17	Z8873684621	1{73}	Nc1ccc2nccn2n1	2{370}	CNC(=O)c1ccc(C=O)cc1	3{20}	COc1ccc([N+]#[C-])c(C)c1	47.2	41
722	4{267,371,23}	COC(=O)CCC(NC1=C(N=C2C=CC=C(C#C)N12)C1=C(C)C(OC)=CC=N1)C(=O)OC c:12,21,26,28,t:8,10,14	Z8878918809	1{267}	Nc1cccc(C#C)n1	2{371}	COc1ccnc(C=O)c1C	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	48.3	41
723	4{50,11,18}	CC(C)(C)NC1=C(N=C2C=CC=C(N12)P(C)(C)=O)C1=NN(CC(F)(F)F)C=C1 c:9,11,28,t:5,7,20	Z8878918561	1{50}	CP(=O)(C)c1cccc(N)n1	2{11}	FC(F)(F)Cn1ccc(C=O)n1	3{18}	CC(C)(C)[N+]#[C-]	45.7	41

724	4{105,185,41}	COC1=CC=C(NC2=C(N=C3C=CC=C(N23)C(N)=O)C2=CN(C)C=N2)C=C1 c:11,13,25,28,t:2,4,7,9,21	Z8855619757	1{105}	NC(=O)c1c ccc(N)n1	2{185}	Cn1cnc(C=O) c1	3{41}	COc1ccc([N+] #[C-])cc1	40.1	41
725	4{188,372,62}	COC(=O)C1=CN=CC2=NC(=C(NC3(CCCC3)C(=O)OC)N12)C1=NN(C)N=C1C c:6,30,t:4,8,10,26	Z8873684844	1{188}	COC(=O)c1 cncc(N)n1	2{372}	Cc1nn(C)nc1 C=O	3{62}	COC(=O)C1(CCCC1)[N+] #[C-]	45.3	41
726	4{92,204,26}	CSC1=NC=C(N1C)C1=C(NCC2=CC=C(F)C=C2)N2C=CC(=CC2=N1)C(N)=O c:4,9,18,22,24,27,t:2,13,15	Z8854581172	1{92}	NC(=O)c1c cnc(N)c1	2{204}	CSc1ncc(C= O)n1C	3{26}	Fc1ccc(C[N+] #[C-])cc1	44.8	40
727	4{113,373,14}	COCCNC1=C(N=C2N1C=CC=C2N1CCOCC1) [C@@H]1[C@@H](C)C1(F)F &1:20,21,r,c:7,11,13,t:5	Z8855619505	1{113}	Nc1ncccc1 N2CCOCC2	2{373}	C[C@@H]1[C@@H](C= O)C1(F)F &1:1,2,r	3{14}	COCC[N+] #[C-]	39.9	40
728	4{28,374,7}	C(C1CC1)N1C=C(N=N1)C1=C(NC2CCOCC2) N2C=CC(=CC2=N1)C1=NOC=N1 c:6,8,11,22,24,27,33,t:30	Z8878918456	1{28}	Cl.Nc1cc(cc n1)c2ncon2	2{374}	O=Cc1cn(CC 2CC2)nn1	3{7}	[C-] #[N+]C1CC OCC1	44.3	40
729	4{142,375,24}	COCC1=C(N=CO1)C1=C(NCC2=CC(OC)=C C=C2)N2C=CC=C(OCCS(C)(=O)=O)C2=N1 c:5,9,17,19,23,35,t:3,13,25	Z8873684680	1{142}	CS(=O)(=O))CCOc1ccc nc1N	2{375}	COc1ocnc1 C=O	3{24}	COc1cccc(C[N+] #[C-])c1	53.0	40
730	4{103,376,5}	COCCNC1=C(N=C2C=NC=C(CO)N12)C1= C(Br)SC(=N1)C1CC1 c:10,19,23,t:6,8,12	Z8873684652	1{103}	Nc1cnc(C O)n1	2{376}	Br1sc(nc1C =O)C2CC2	3{5}	COCCC[N+] #[C-]	47.7	40
731	4{369,340,31}	CCN1C=NC(=N1)C1=C(NCCSC)N2C=C(C=C C2=N1)C(F)C(F)F c:3,5,8,16,18,21	Z8873685474	1{369}	Cl.Nc1ccc(c n1)C(F)C(F) (F)F	2{340}	CCn1cnc(C= O)n1	3{31}	CSCC[N+] #[C-]	43.6	40
732	4{50,295,18}	CC1=NC(=CS1)C1=C(NC(C)(C)C)N2C(C=CC =C2P(C)(C)=O)=N1 c:3,7,16,18,24,t:1	Z8846492023	1{50}	CP(=O)(C)c 1cccc(N)n1	2{295}	Cc1nc(C=O) cs1	3{18}	CC(C)(C)[N +] #[C-]	39.1	40
733	4{379,377,7}	CC1=CN=C1C1=C(NC2CCOCC2)N2C=CC =C(Br)C2=N1 c:4,7,18,24,t:1,20	Z8835022881	1{379}	Nc1ncccc1 Br	2{377}	Cl.Cc1c[nH] nc1C=O	3{7}	[C-] #[N+]C1CC OCC1	40.4	40
734	4{179,378,5}	COCCNC1=C(N=C2C=C(OC)C=CN12)C1= NC(=CC(Cl)=C1)C(=O)OC c:14,21,24,t:6,8,10,19	Z8878918656	1{179}	COc1ccnc(N)c1	2{378}	COC(=O)c1c c(Cl)cc(C=O) n1	3{5}	COCCC[N+] #[C-]	43.4	40
735	4{81,116,13}	COC1=CC=C(CNC2=C(N=C3C=NC=CN23)C 2=CN(CCC=C)N=N2)C=C1 c:12,14,26,29,t:2,4,8,10,19	Z8878918775	1{81}	Nc1cncn1	2{116}	C=CCcn1cc(C=O)nn1	3{13}	COc1ccc(C[N+] #[C-])cc1	40.2	40

736	4{48,379,22}	CC1=C(Br)SC(=C1)C1=C(NC2COC2)N2C=C C(=CC2=N1)S(C)(=O)=O c:1,5,8,17,19,22	Z8878918403	1{48}	CS(=O)(=O) c1ccnc(N)c 1	2{379}	Cc1cc(C=O)s c1Br	3{22}	[C-] #[N+]C1CO C1	43.1	40
737	4{36,40,9}	CNC1=C(N=C2C=CC(Br)=CN12)C1=NC(CO) =CS1 c:6,9,18,t:2,4,14	Z8849597803	1{36}	Nc1ccc(Br) cn1	2{40}	OCc1csc(C= O)n1	3{9}	C[N+]#[C-]	36.1	39
738	4{375,334,43}	CC(C)OC1=CN=CC2=NC(=C(NC3CCN(CC3) C(=O)OC(C)(C)C)N12)C1=C(C)OC=N1 c:6,30,34,t:4,8,10	Z8873684703	1{375}	CC(C)Oe1c ncc(N)n1	2{334}	Cc1ocnc1C= O	3{43}	CC(C)(C)OC (=O)N1CCC(CC1)[N+]#[C-]	48.4	39
739	4{81,257,13}	COC1=CC=C(CNC2=C(N=C3C=NC=CN23)C 2CC(C2)NC(=O)OC(C)(C)C)C=C1 c:12,14,32,t:2,4,8,10	Z8873684711	1{81}	Nc1cncn1	2{257}	CC(C)(C)OC (=O)N1CCC(C1)C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	44.8	39
740	4{41,116,13}	COC1=CC=C(CNC2=C(N=C3C=NC(C)=CN2 3)C2=CN(CCC=C)N=N2)C=C1 c:12,15,27,30,t:2,4,8,10,20	Z8878918374	1{41}	Cc1cnc(N)c n1	2{116}	C=CCCn1cc(C=O)nn1	3{13}	COc1ccc(C[N+]#[C-])cc1	41.2	39
741	4{91,380,7}	CC(C)(C)OC(=O)N1CCC(C)(CC2=C(NC3CC OCC3)N3C=C(C=CC3=N2)C(N)=O)C1 c:13,24,26,29	Z8878918828	1{91}	NC(=O)c1c cc(N)nc1	2{380}	CC(C)(C)OC (=O)N1CCC(C)(CC=O)C1	3{7}	[C-] #[N+]C1CC OCC1	47.7	39
742	4{142,326,21}	CN1N=CC=C1C1=C(NCC2CC2)N2C=CC=C(OCCS(C)(=O)=O)C2=N1 c:2,4,7,16,28,t:18	Z8878918680	1{142}	CS(=O)(=O))CCOc1ccc nc1N	2{326}	Cn1ncce1C= O	3{21}	[C-] #[N+]CC1C C1	40.5	39
743	4{146,139,10}	CC1=NN(CCO)C(C)=C1C1=C(NC2CCOC2)N 2C=C(C=CC2=N1)S(C)(=O)=O c:8,11,21,23,26,t:1	Z8878918388	1{146}	CS(=O)(=O) c1ccc(N)nc 1	2{139}	Cc1m(CCO) c(C)c1C=O	3{10}	[C-] #[N+]C1CC OC1	43.6	38
744	4{65,381,5}	CCC1=CN=CC2=NC(=C(NCCCOC)N12)C1= C2N(C)C=NC2=CC=C1 c:4,19,23,26,28,t:2,6,8	Z8855619749	1{65}	CCc1cnc(N)n1	2{381}	Cn1cnc2cccc (C=O)c12	3{5}	COCCC[N+] #[C-]	37.8	38
745	4{199,382,34}	COC(C)(C)CC1=C(NCC2CCCO2)N2C=CC=C (C2=N1)C(C)(F)F c:6,17,19,22	Z8873685428	1{199}	CC(F)(F)c1 ccnc1N	2{382}	COC(C)(C)C C=O	3{34}	[C-] #[N+]CC1C CCO1	38.0	38
746	4{181,62,14}	COCCNC1=C(N=C2N1C=CC1=C2N=CC=N1) C1CC1CCOCC1 c:7,11,13,16,18,t:5	Z8878918816	1{181}	Nc1nccc2nc cnc12	2{62}	O=CC1CC21 CCOCC2	3{14}	COCC[N+]#[C-]	36.3	38
747	4{380,383,5}	COCCNC1=C(N=C2N1C=C(Cl)N=C2C)C1= NC=C(C)C=C1 c:8,15,24,t:6,12,19,21	Z8878918328	1{380}	Cc1nc(Cl)c nc1N	2{383}	Cc1ccc(C=O)nc1	3{5}	COCCC[N+] #[C-]	35.3	38

748	4{218,384,10}	CN1N=C(C=C1C(F)F)C1=C(NC2CCOC2)N2 N=C(C=CC2=N1)C(C)(C)C c:2,4,10,20,22,25	Z8878918504	1{218}	CC(C)(C)c1 ccc(N)nn1	2{384}	Cn1nc(C=O) cc1C(F)F	3{10}	[C-] #[N+]C1CC OC1	39.9	38
749	4{78,385,44}	CC1=CN2N3C(NCCCCNC(=O)OC(C)(C)C)= C(N=C3C=C(C)C2=N1)C1=CC(=CC=C1)[N+] ([O-])=O c:18,20,27,32,34,t:1,23,30	Z8855739078	1{78}	Cc1cn2nc(N) cc(C)c2n1	2{385}	[O-]][N+](=O)c1 cccc(C=O)c1	3{44}	CC(C)(C)OC (=O)NCCCC [N+]#[C-]	50.3	38
750	4{381,378,5}	COCCCN1=C(N=C2C=NC=C(OCC(F)(F)F) N12)C1=NC(=CC(Cl)=C1)C(=O)OC c:10,25,28,t:6,8,12,23	Z8878918804	1{381}	Ne1cncc(O) CC(F)(F)F n1	2{378}	COC(=O)c1c c(Cl)cc(C=O) n1	3{5}	COCCCN1+ #[C-]	48.2	38
751	4{185,386,23}	COC(=O)CCC(NC1=C(N=C2C=CC(=C(C)N1 2)S(C)(=O)=O)[C@H]1CC1(C)C)C(=O)OC c:12,t:8,10,14	Z8878918777	1{185}	Cc1nc(N)cc c1S(=O)(=O) C	2{386}	CC1(C)C[C @@H]1C=O	3{23}	COC(=O)CC C([N+]#[C-]])C(=O)OC	45.9	38
752	4{371,114,12}	COC(=O)[C@@H]1CC[C@@H](C1)C1=C(N CC2CCOC2)N2C=CC=C(OCCCC#N)C2=N1 &1:4,7,r,c:10,21,32,t:23	Z8873684896	1{371}	Ne1ncccc1 OCCCC#N	2{114}	COC(=O)[C @@H]1CC[C@@H](C1) C=O &1:4,7,r	3{12}	[C-] #[N+]CC1C COC1	43.1	37
753	4{50,387,14}	CCN1N=C(C)C=C1C1=C(NCCOC)N2C(C=C C=C2P(C)(C)=O)=N1 c:6,9,18,20,26,t:3	Z8829498583	1{50}	CP(=O)(C)c 1cccc(N)n1	2{387}	CCn1nc(C)cc 1C=O	3{14}	COCC[N+]#[C-]	37.6	37
754	4{382,233,62}	COC(=O)C1(CCCC1)NC1=C(CCCOCC=C)N= C2C=NC(=CN12)C(F)(F)F c:11,22,24,t:20	Z8849597830	1{382}	Ne1enc(en1)C(F)(F)F	2{233}	C=CCOCCC C=O	3{62}	COC(=O)C1(CCCC1)[N+] #[C-]	42.6	37
755	4{187,16,10}	CN1N=CC(CNC(=O)OC(C)(C)C)=C1C1=C(N C2CCOC2)N2C=C(Cl)C(=CC2=N1)C#N c:2,13,16,29,32,t:26	Z8873684856	1{187}	Ne1cc(C#N)c(Cl)cn1	2{16}	Cn1ncc(CNC (=O)OC(C)(C)C)c1C=O	3{10}	[C-] #[N+]C1CC OC1	47.1	37
756	4{144,99,53}	CNS(=O)(=O)C1=CN2C(NCCOCC3=CC=CC =C3)=C(N=C2C=C1)C1=COC=N1 c:16,18,20,22,25,31,t:5,14,28	Z8873684634	1{144}	CNS(=O)(=O) c1ccc(N) nc1	2{99}	O=Cc1coen1	3{53}	[C-] #[N+]CCOC c1cccc1	42.0	36
757	4{383,388,69}	COC1=NN(C)C=C1C1=C(NC2=C(OC)C=CC= C2)N2N=C(C=CC2=N1)C1=NC=CC=C1 c:6,9,12,16,18,22,24,27,32,34,t:2,30	Z8854581142	1{383}	Ne1ccc(nn1)c2cccn2	2{388}	COc1nn(C)c c1C=O	3{69}	COc1cccc1[N+]#[C-]	42.0	36
758	4{119,236,61}	CC(C)(C)OC(=O)NCCCN1=C(CCC2OCCO2)N=C2C=CC(=CN12)C#N c:12,24,26,t:22	Z8878918645	1{119}	Ne1ccc(C# N)en1	2{236}	O=CCCC1O CCO1	3{61}	CC(C)(C)OC (=O)NCCC[N+]#[C-]	40.7	36

759	4{384,104,10}	CCOC1=C(C)N2C(NC3CCOC3)=C(N=C2C=C1)C1=NC(C)=CO1 c:3,14,16,19,25,t:22	Z8873684881	1{384}	CCOe1ccc(N)nc1C	2{104}	Cc1coc(C=O)n1	3{10}	[C-]#[N+]C1CCOC1	33.6	36
760	4{48,389,22}	CS(=O)(=O)C1=CC2=NC(=C(NC3COC3)N2C=C1)C1=C(F)C(CI)=C(F)C=C1 c:18,21,28,t:4,6,8,25	Z8873684750	1{48}	CS(=O)(=O)c1ccnc(N)c1	2{389}	Fc1ccc(C=O)c(F)c1Cl	3{22}	[C-]#[N+]C1COCl	40.6	36
761	4{385,282,67}	CCC(C)NC1=C(N=C2C=C(C#N)C3=C(C=CC=C3)N12)C1CC2(C1)OCCO2 c:15,17,t:5,7,9,13	Z8878918363	1{385}	Nc1cc(C#N)c2ccccc2n1	2{282}	O=CC1CC2(C1)OCCO2	3{67}	CCC(C)[N+]#[C-]	36.9	36
762	4{92,125,26}	COC1=NC=NC(=C1)C1=C(NCC2=CC=C(F)C=C2)N2C=CC(=CC2=N1)C(N)=O c:4,6,9,18,22,24,27,t:2,13,15	Z8878918302	1{92}	NC(=O)c1cnc(N)c1	2{125}	COc1cc(C=O)ncn1	3{26}	Fc1ccc(C[N+]#[C-])cc1	38.1	36
763	4{46,40,13}	COC1=CC=C(CNC2=C(N=C3C=CC=CN23)C2=NC(CO)=CS2)C=C1 c:12,14,23,27,t:2,4,8,10,19	Z8873685476	1{46}	Nc1ccccn1	2{40}	OCc1csc(C=O)n1	3{13}	COc1ccc(C[N+]#[C-])cc1	35.4	36
764	4{99,286,34}	NS(=O)(=O)C1=CN2C(C=C1)=NC(=C2NCC1CCCO1)C1=NC=CC(=C1)C(F)(F)F c:8,10,12,25,27,t:4,23	Z8878918636	1{99}	Nc1ccc(en1)S(=O)(=O)N	2{286}	FC(F)(F)c1ccnc(C=O)c1	3{34}	[C-]#[N+]CC1COCO1	42.7	36
765	4{386,390,5}	COCCCN1=C(N=C2C=C(C)C=CN12)C1CC2C(C1)C2(F)F c:13,t:6,8,10	Z8878918859	1{386}	Cc1ccnc(N)c1	2{390}	FC1(F)C2CC(C21)C=O	3{5}	COCC[N+]#[C-]	32.4	36
766	4{109,391,29}	CCOC(=O)CCNC1=C(CCC(C)(C)C(=O)OCC)N=C2C=CC=C(N12)S(N)(=O)=O c:8,22,24,t:20	Z8878918665	1{109}	Cl.Nc1cccc(n1)S(=O)(=O)N	2{391}	CCOC(=O)C(C)(C)CCC=O	3{29}	CCOC(=O)C[N+]#[C-]	43.9	36
767	4{193,328,10}	CCC1=NNC=C1C1=C(NC2CCOC2)N2C=C(C=CC2=N1)C(=O)NC c:5,8,18,20,23,t:2	Z8873684878	1{193}	CNC(=O)c1ccc(N)nc1	2{328}	Cl.CCc1n[nH]cc1C=O	3{10}	[C-]#[N+]C1CCOC1	34.2	36
768	4{371,365,12}	N#CCCCOC1=CC=CN2C(NCC3CCOC3)=C(N=C12)C1=NNC2=C1C=NC=C2 c:8,19,28,31,33,t:6,21,25	Z8837933140	1{371}	Nc1ncccc1OCCCC#N	2{365}	O=Cc1n[nH]c2ccccc12	3{12}	[C-]#[N+]CC1COC1	40.0	35
769	4{387,375,46}	COCC1=C(N=CO1)C1=C(NCC(C)=C)N2C=C(C=C(OC(F)F)C2=N1) c:5,9,17,26,t:3,19	Z8873684838	1{387}	Nc1ncccc1OC(F)F	2{375}	COc1ocnc1C=O	3{46}	CC(=C)C[N+]#[C-]	34.9	35
770	4{146,392,46}	CC(=C)CNC1=C(N=C2C=CC(=CN12)S(C)(=O)=O)C1CCOCC1 c:9,11,t:5,7	Z8878918503	1{146}	CS(=O)(=O)c1ccc(N)nc1	2{392}	O=CC1CCOCC1	3{46}	CC(=C)C[N+]#[C-]	32.9	35

771	4{32,393,18}	CC(C)(C)NC1=C(N=C2C=C(C=CN12)P(C)(C)=O)C1=CC(Br)=C(F)C=C1 c:9,11,26,t:5,7,20,23	Z8878918310	1{32}	CP(=O)(C)c1ccnc(N)c1	2{393}	Fc1ccc(C=O)cc1Br	3{18}	CC(C)(C)[N+][C-]	40.8	34
772	4{327,90,65}	COC(=O)C1=C(F)C2=NC(=C(NC3CCCC3)N2C=C1)C1=COC(C)=N1 c:4,20,27,t:7,9,23	Z8855739109	1{327}	COC(=O)c1ccnc(N)c1F	2{90}	Cc1nc(C=O)col	3{65}	[C-][N+][C1CC1]CC1	33.0	34
773	4{380,312,5}	COCCNC1=C(N=C2N1C=C(Cl)N=C2C)C1COC1(C)C c:8,15,t:6,12	Z8873685390	1{380}	Cc1nc(Cl)cnc1N	2{312}	CC1(C)OCC1C=O	3{5}	COCC[N+][C-]	32.4	34
774	4{142,394,24}	COC1=CC(CNC2=C(N=C3N2C=CC=C3OCCS(C)(=O)=O)C2=NOC=C2C)=CC=C1 c:9,13,15,28,31,33,t:2,7,25	Z8878918913	1{142}	CS(=O)(=O)CCOc1ccnc1N	2{394}	Cc1conc1C=O	3{24}	COc1cccc(C[N+][C-])c1	41.8	34
775	4{348,258,44}	CC(C)(C)OC(=O)NCCCCNC1=C(N=C2C=NC(F)=CN12)C1=NN=C(S1)C1CC1 c:17,20,27,t:13,15,25	Z8873684733	1{348}	Nc1nc(F)cnc1	2{258}	O=Cc1nnc(s1)C2CC2	3{44}	CC(C)(C)OC(=O)NCCCC[N+][C-]	40.9	34
776	4{146,395,10}	CC(C)(C)OC(=O)N[C@H]1C[C@@H](C1)C1=C(NC2CCOC2)N2C=C(C=CC2=N1)S(C)(=O)=O r,c:13,23,25,28	Z8873684865	1{146}	CS(=O)(=O)c1ccc(N)nc1	2{395}	CC(C)(C)OC(=O)N[C@H]1C[C@@H](C1)C=O	3{10}	[C-][N+][C1CC1]OC1	41.1	34
777	4{41,396,13}	COC1=CC=C(CNC2=C(N=C3C=NC(C)=CN23)C2=CN=C3COCCN23)C=C1 c:12,15,31,t:2,4,8,10,20,22	Z8873684595	1{41}	Cc1nc(N)cnc1	2{396}	O=Cc1enc2COCc1n2	3{13}	COc1ccc(C[N+][C-])cc1	35.6	34
778	4{356,397,1}	COC1=C(C2=C(NC3CC3)N3C(C=CC(Cl)=C3C(=O)N(C)C)=N2)C(C)=CC(C)=N1 c:2,4,13,16,23,27,30	Z8846492036	1{356}	CN(C)C(=O)c1nc(N)ccc1Cl	2{397}	COc1nc(C)cc(C)c1C=O	3{1}	[C-][N+][C1CC1]	37.4	33
779	4{181,358,14}	COCCNC1=C(N=C2N1C=CC1=C2N=CC=N1)C1CC1CCN(C1)C(=O)OC(C)(C)C c:7,11,13,16,18,t:5	Z8878918434	1{181}	Nc1nccc2nccnc12	2{358}	CC(C)(C)OC(=O)N1CCC2(CC2C=O)C1	3{14}	COCC[N+][C-]	39.6	33
780	4{286,383,23}	COC(=O)CCC(NC1=C(N=C2C=CC(=CN12)C1=NC=CC=C1)C1=NC=C(C)C=C1)C(=O)OC c:12,14,21,23,31,t:8,10,19,26,28	Z8855739252	1{286}	Cl.Cl.Nc1ccc(en1)c2cccn2	2{383}	Cc1ccc(C=O)nc1	3{23}	COC(=O)CC(C[N+][C-])C(=O)OC	41.5	33
781	4{214,32,10}	COC1=CC(Br)=C(C)N2C(NC3CCOC3)=C(N=C12)[C@@H]1C[C@H]1C1=CC=NN1C &1:19,21,r,c:16,28,t:2,5,18,26	Z8873684886	1{214}	COc1cc(Br)c(C)nc1N	2{32}	Cn1nccc1[C@@H]2C[C@H]2C=O &1:6,8,r	3{10}	[C-][N+][C1CC1]OC1	40.3	33

782	4{81,19,9}	CNC1=C(N=C2C=NC=CN12)C1=C(OC)C=N N1C c:6,8,13,17,t:2,4	Z8855619682	1{81}	Ne1cncn1	2{19}	COc1enn(C) c1C=O	3{9}	C[N+]#[C-]	23.3	33
783	4{78,398,28}	CCCNC1=C(N=C2C=C(C)C3=NC(C)=CN3N1 2)C1=CC2=C(CCCC2)O1 c:14,t:4,6,8,11,21,23	Z8878918628	1{78}	Cc1cn2nc(N) cc(C)c2n1	2{398}	O=Cc1cc2C CCCc2o1	3{28}	CCC[N+]#[C-]]	32.7	33
784	4{286,235,23}	COC(=O)CCC(NC1=C(N=C2C=CC(=CN12)C 1=NC=CC=C1)C1=CSC(=C1)C#N)C(=O)OC c:12,14,21,23,29,t:8,10,19,26	Z8808559878	1{286}	Cl.Cl.Nc1cc c(en1)c2ccc cn2	2{235}	O=Cc1csc(C #N)c1	3{23}	COC(=O)CC C([N+]#[C-]])C(=O)OC	42.3	33
785	4{361,399,12}	CC(C)OC1=CC=CN2C(NCC3CCOC3)=C(N= C12)C1=CN(N=C1C)C1CC1 c:6,17,26,t:4,19,23	Z8878918330	1{361}	Cl.CC(C)Oc 1ccnc1N	2{399}	Cc1nn(cc1C =O)C2CC2	3{12}	[C-] #[N+]CC1C COC1	35.0	33
786	4{118,400,35}	CSCCCNC1=C(N=C2C=CC=C(C(C)O)N12)C 1=CN(N=N1)C1CCCC1 c:10,23,t:6,8,12,20	Z8873684919	1{118}	Cl.CC(O)c1 cccc(N)n1	2{400}	O=Cc1cn(nn 1)C2CCCC2	3{35}	CSCCC[N+] #[C-]	35.3	33
787	4{111,206,22}	COC(=O)C1=CN2C(NC3COC3)=C(C[C@H](C)NC(=O)OC(C)(C)C)N=C2C(C)=C1 c:26,30,t:4,13	Z8873684805	1{111}	COC(=O)c1 cnc(N)c(C)c 1	2{206}	C[C@@H](CC=O)NC(= O)OC(C)(C) C	3{22}	[C-] #[N+]C1CO C1	36.7	33
788	4{79,106,13}	COC1=CC=C(CNC2=C(N=C3C=NC=C(C)N2 3)C2=C(OC)N=CC=N2)C=C1 c:12,20,24,26,29,t:2,4,8,10,14	Z8835022911	1{79}	Cc1cncc(N) n1	2{106}	COc1cnccn1 C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	32.8	32
789	4{187,401,12}	CN1N=C(Br)C(=N1)C1=C(NCC2CCOC2)N2C =C(Cl)C(=CC2=N1)C#N c:5,8,22,25,t:2,19	Z8873684795	1{187}	Ne1cc(C#N) c(Cl)cn1	2{401}	Cn1nc(Br)c(C=O)n1	3{12}	[C-] #[N+]CC1C COC1	37.8	32
790	4{350,56,23}	COC(=O)CCC(NC1=C(N=C2C=NC(=CN12)C 1=CC=CC=C1)C1=C(C)C=NC(F)=C1)C(=O)O C c:12,14,21,23,26,29,32,t:8,10,19	Z8849597821	1{350}	Ne1cnc(en1) c2cccc2	2{56}	Cc1cnc(F)cc 1C=O	3{23}	COC(=O)CC C([N+]#[C-]])C(=O)OC	40.7	32
791	4{73,402,13}	COC1=CC=C(CNC2=C(N=C3C=CC4=NC=C N4N23)C2=C(F)C(C)=CC=C2)C=C1 c:12,16,23,27,29,32,t:2,4,8,10,14	Z8878918874	1{73}	Ne1ccc2ncc n2n1	2{402}	Cc1cccc(C= O)c1F	3{13}	COc1ccc(C[N+]#[C-])cc1	33.9	31
792	4{127,403,29}	CCOC(=O)CCNC1=C(N=C2N1C=CC=C2F)C 1=CN=C(Cl)N1 c:10,14,16,t:8,20,22	Z8873684670	1{127}	Ne1ncccc1F	2{403}	Clc1ncc(C= O)[nH]1	3{29}	CCOC(=O)C C[N+]#[C-]	29.6	31
793	4{388,404,67}	CCC(C)NC1=C(N=C2C=C3CCCOC3=CN12) C1=NN=C(C)N1 c:16,t:5,7,9,21,23	Z8873685425	1{388}	Cl.Nc1cc2C CCOc2cn1	2{404}	Cc1nnc(C=O) [nH]1	3{67}	CCC(C)[N+] #[C-]	27.2	31

794	4{81,157,9}	CNC1=C(N=C2C=NC=CN12)C1=NC2=C(C=C1)N=CC=C2 c:6,8,15,17,20,22,t:2,4,13	Z8835022913	1{81}	Nc1cncn1	2{157}	O=Cc1ccc2ncccc2n1	3{9}	C[N+]#[C-]	22.9	31
795	4{81,396,13}	COC1=CC=C(CNC2=C(N=C3C=NC=CN23)C2=CN=C3COCCN23)C=C1 c:12,14,30,t:2,4,8,10,19,21	Z8878918856	1{81}	Nc1cncn1	2{396}	O=Cc1cnc2C OCCn12	3{13}	COc1ccc(C[N+]#[C-])cc1	30.9	30
796	4{187,405,12}	CC(F)(F)C1=NC=C(S1)C1=C(NCC2CCOC2)N2C=C(Cl)C(=CC2=N1)C#N c:6,10,24,27,t:4,21	Z8878918560	1{187}	Nc1cc(C#N)c(Cl)cn1	2{405}	CC(F)(F)c1ncc(C=O)s1	3{12}	[C-]#[N+]CC1C COC1	34.6	30
797	4{186,406,8}	COC(=O)C(CC1=CC=CC=C1)NC1=C(N=C2C=C(C=CN12)S(=O)(=O)N(C)C)C1=CC=NS1 c:8,10,18,20,33,t:6,14,16,31	Z8873684677	1{186}	Cl.CN(C)S(=O)(=O)c1cnc(N)c1	2{406}	O=Cc1ccns1	3{8}	COC(=O)C(Cc1cccc1)[N+]#[C-]	39.2	30
798	4{68,371,23}	COC(=O)CCC(NC1=C(N=C2C=C(C=CN12)C#C)C1=C(C)C(OC)=CC=N1)C(=O)OC c:12,14,21,26,28,t:8,10	Z8878918811	1{68}	Nc1cc(C#C)ccn1	2{371}	COc1cnc(C=O)c1C	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	35.2	30
799	4{348,407,2}	CCC1=NN=C(N1)C1=C(NC2=CC=C(F)C=C2)N2C=C(F)N=CC2=N1 c:4,8,16,23,26,t:2,11,13,20	Z8873684930	1{348}	Nc1cnc(F)cn1	2{407}	CCc1nnc(C=O)[nH]1	3{2}	Fc1ccc([N+]#[C-])cc1	27.3	30
800	4{96,408,60}	COCCN(C)CC1=CC2=NC(CCN3CCOC3=O)=C(NC3=CC(=CC=C3)C(=O)OC)N2C=C1 c:25,27,36,t:7,9,20,23	Z8849597825	1{96}	COCCN(C)Cc1cnc(N)c1	2{408}	O=CCCN1C COC1=O	3{60}	COC(=O)c1cccc([N+]#[C-])c1	38.4	30
801	4{359,409,22}	CC(C)(C)OC(=O)NC1=NC=C(N=C1)C1=C(NC2COC2)N2C=C(OC(F)F)C=CC2=N1 c:10,12,15,30,33,t:8,24	Z8854581143	1{359}	Nc1ccc(OC(F)F)cn1	2{409}	CC(C)(C)OC(=O)Nc1cnc(C=O)cn1	3{22}	[C-]#[N+]C1CO C1	35.7	29
802	4{61,320,23}	CCC1=CC=CC2=NC(=C(NC(CCC(=O)OC)C(=O)OC)N12)C1=NN(C)C=N1 c:4,29,t:2,6,8,25	Z8873685304	1{61}	CCc1cccc(N)n1	2{320}	Cn1cnc(C=O)n1	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	31.7	29
803	4{188,410,67}	CCC(C)NC1=C(N=C2C=NC=C(N12)C(=O)OC)C1=CSC(=N1)C1=NC=CC=N1 c:9,11,23,28,30,t:5,7,20,26	Z8873685325	1{188}	COC(=O)c1cnc(N)n1	2{410}	O=Cc1esc(n1)c2nccn2	3{67}	CCC(C)[N+]#[C-]	32.4	29
804	4{70,92,31}	CSCCN1=C(N=C2N1C=CN=C2C1CC1)C1=CC(C)=NO1 c:7,11,13,23,t:5,20	Z8873684624	1{70}	Nc1cncn1 C2CC2	2{92}	Cc1cc(C=O)on1	3{31}	CSCC[N+]#[C-]	26.0	29
805	4{128,320,29}	CCOC(=O)CCNC1=C(N=C2C=CC(=CN12)N(C)CCOC)C1=NN(C)C=N1 c:12,14,29,t:8,10,25	Z8878918844	1{128}	COCCN(C)c1ccc(N)nc1	2{320}	Cn1cnc(C=O)n1	3{29}	CCOC(=O)C C[N+]#[C-]	31.5	29
806	4{83,411,7}	CP(C)(=O)C1=CN2C(C=C1)=NC(=C2NC1CC OCC1)C1=CC2=C(CCC2)N=C1 c:8,10,12,31,t:4,23,25	Z8835022873	1{83}	CP(=O)(C)c1ccc(N)nc1	2{411}	O=Cc1cnc2C CCc2c1	3{7}	[C-]#[N+]C1CC OCC1	31.6	29

807	4{239,223,37}	COC(=O)C1CC(C1)NC1=C(N=C2C=CC(=CN12)N1CCCC1)C1=CN=C(C=C1)C(=O)OC c:14,16,29,31,t:10,12,27	Z8855619681	1{239}	Cl.Cl.Nc1cc c(en1)N2C CCC2	2{223}	Cl.COC(=O) c1ccc(C=O)c n1	3{37}	COC(=O)C1 CC(C1)[N+] #[C-]	34.6	28
808	4{83,412,31}	CSCCNC1=C(N=C2C=CC(=CN12)P(C)(C)=O) C1=CC(SC)=CC=C1 c:9,11,24,26,t:5,7,20	Z8878918765	1{83}	CP(=O)(C)c 1ccc(N)nc1	2{412}	CSclcccc(C= O)c1	3{31}	CSCC[N+]#[C-]	30.7	28
809	4{311,413,12}	FC1=CC2=NC(C3=CN=C(S3)C3=CC=NC=C3)=C(NCC3CCOC3)N2C=C1 c:8,14,16,30,t:1,3,6,12,18	Z8849597805	1{311}	Nc1cc(F)cc n1	2{413}	O=Cc1cnc(s1 c2ccncc2	3{12}	[C-]#[N+]CC1C COC1	29.9	28
810	4{32,5,31}	CSCCNC1=C(N=C2C=C(C=CN12)P(C)(C)=O) C1=C(C)C=NC=C1C c:9,11,20,23,25,t:5,7	Z8878918836	1{32}	CP(=O)(C)c 1ccnc(N)c1	2{5}	Cc1cnc(C)c 1C=O	3{31}	CSCC[N+]#[C-]	29.2	28
811	4{154,414,49}	CCC1=C(N=CC=C1)C1=C(NC2CC(F)(F)C2)N 2C=CC(=CC2=N1)[N+](=[O-])=O c:4,6,9,20,22,25,t:2	Z8873685281	1{154}	Nc1cc(ccn1)[N+](=O)[O-]	2{414}	CCc1ccnc1 C=O	3{49}	FC1(F)CC(C 1)[N+]#[C-]	27.8	28
812	4{348,415,67}	CCC(C)NC1=C(N=C2C=NC(F)=CN12)C1=N C=NN1CC c:9,12,19,t:5,7,17	Z8873685461	1{348}	Nc1cnc(F)c n1	2{415}	CCn1ncn1C =O	3{67}	CCC(C)[N+] #[C-]	22.5	27
813	4{28,416,7}	COCC1=CC(F)=C(C2=C(NC3CCOCC3)N3C= CC(=CC3=N2)C2=NOC=N2)C(F)=C1 c:8,19,21,24,30,34,t:3,6,27	Z8873685350	1{28}	Cl.Nc1cc(cc n1)c2ncon2	2{416}	COCc1cc(F) c(C=O)c(F)c 1	3{7}	[C-]#[N+]C1CC OCC1	32.7	27
814	4{103,293,40}	CCOC(=O)C1=CC=C(NC2=C(N=C3C=NC=C(CO)N23)C2=C(F)N(C)N=C2)C=C1 c:14,23,28,31,t:5,7,10,12,16	Z8878918658	1{103}	Nc1cnc(C O)n1	2{293}	Cn1ncc(C=O c1F	3{40}	CCOC(=O)c 1ccc([N+]#[C-])cc1	30.4	27
815	4{85,417,31}	CSCCNC1=C(N=C2C=C(C=C(C)N12)C#N)C1 =C2N=NN(C)C2=CC=C1 c:9,19,21,26,28,t:5,7,11	Z8873684768	1{85}	Cc1cc(C#N) cc(N)n1	2{417}	Cn1nnc2c(C =O)cccc12	3{31}	CSCC[N+]#[C-]	27.4	27
816	4{50,418,15}	CCNC1=C(N=C2C=CC=C(N12)P(C)(C)=O)C 1=NC2=C(C=CC=C2C1)C=C1 c:7,9,22,24,28,t:3,5,18,20	Z8846492148	1{50}	CP(=O)(C)c 1cccc(N)n1	2{418}	Clc1cccc2ccc (C=O)nc12	3{15}	CC[N+]#[C-]	28.9	27
817	4{72,375,24}	COCC1=C(N=CO1)C1=C(NCC2=CC(OC)=C C=C2)N2C=C(Br)N=C(OC)C2=N1 c:5,9,17,19,31,t:3,13,23,26	Z8855619691	1{72}	COc1nc(Br) cnc1N	2{375}	COCc1ocn1 C=O	3{24}	COc1cccc(C N+)#[C-]c1	34.0	27
818	4{185,419,8}	COC(=O)C(CC1=CC=CC=C1)NC1=C(N=C2C =CC(=C(C)N12)S(C)(=O)=O)C1=NC=CC(OC)=C1 c:8,10,18,32,36,t:6,14,16,20,30	Z8878918452	1{185}	Cc1nc(N)cc c1S(=O)(=O)C	2{419}	COc1cnc(C =O)c1	3{8}	COC(=O)C(Cc1cccc1)[N+]#[C-]	35.4	27
819	4{81,420,9}	CNC1=C(CC(C)(C)C#N)N=C2C=NC=CN12 c:2,12,14,t:10	Z8878918348	1{81}	Nc1cncn1	2{420}	CC(C)(CC= O)C#N	3{9}	C[N+]#[C-]	16.1	26

820	4{41,421,9}	CNC1=C(N=C2C=NC(C)=CN12)C1=CN=C(S1)C1=CC=CO1 c:6,9,16,22,t:2,4,14,20	Z8873685445	1{41}	Cc1cnc(N)c n1	2{421}	O=Cc1cnc(s1) c2cccc2	3{9}	C[N+]#[C-]	21.8	26
821	4{176,377,14}	COCCNC1=C(N=C2N1C=CN=C2N1CCCC1)C1=NNC=C1C c:7,11,13,25,t:5,22	Z8878918326	1{176}	Nc1cncnc1 N2CCCC2	2{377}	Cl.Cc1c[nH] nc1C=O	3{14}	COCC[N+]#[C-]	23.8	26
822	4{85,422,35}	CSCCCNC1=C(N=C2C=C(C=C(C)N12)C#N)C1CC1CCOC1 c:10,t:6,8,12	Z8855739119	1{85}	Cc1cc(C#N) cc(N)n1	2{422}	O=CC1CC21 CCOC2	3{35}	CSCCC[N+]#[C-]	24.8	26
823	4{28,92,18}	CC1=NOC(=C1)C1=C(NC(C)(C)C)N2C=CC(=CC2=N1)C1=NOC=N1 c:4,7,15,17,20,26,t:1,23	Z8878918344	1{28}	Cl.Nc1cc(cc n1)c2ncon2	2{92}	Cc1cc(C=O) on1	3{18}	CC(C)(C)[N+]#[C-]	23.2	25
824	4{362,423,10}	CNC(=O)C1=CC=CC2=NC(=C(NC3CCOC3)N12)C1=CC2=C(C=CN2C)C=C1 c:6,26,31,t:4,8,10,22,24	Z8855619560	1{362}	CNC(=O)c1 cccc(N)n1	2{423}	Cn1ccc2ccc(C=O)cc12	3{10}	[C-]]#[N+]C1CC OC1	26.6	25
825	4{356,353,1}	CN(C)C(=O)C1=C(CI)C=CC2=NC(=C(NC3C3)N12)C1=C(CF)C=CC=C1 c:5,8,22,26,28,t:10,12	Z8846492014	1{356}	CN(C)C(=O) c1nc(N)ccc 1Cl	2{353}	FCc1cccc1 C=O	3{1}	[C-]]#[N+]C1CC 1	26.1	25
826	4{389,424,5}	COCCNC1=C(N=C2N1C=C(C)C=C2)C1=NN(C)C(=N1)C(F)(F)F c:8,15,23,t:6,12,19	Z8873684934	1{389}	Cc1cnc(N)c (C)c1	2{424}	Cn1nc(C=O) nc1C(F)(F)F	3{5}	COCC[N+]#[C-]	25.8	25
827	4{141,209,35}	CSCCCNC1=C(N=C2C=C(NC(C)=O)C=CN12)C1=NN=C2CCCCN12 c:16,t:6,8,10,21,23	Z8878918331	1{141}	CC(=O)Nc1 ccnc(N)c1	2{209}	O=Cc1nnc2C CCCN12	3{35}	CSCCC[N+]#[C-]	26.8	25
828	4{390,191,31}	CCN1C=NN=C1C1=C(NCCSC)N2C(C=CC(C)C)=C2Cl=N1 c:3,5,8,17,21,24	Z8878918633	1{390}	CCc1ccc(N) nc1Cl	2{191}	CCn1enne1C =O	3{31}	CSCC[N+]#[C-]	24.2	25
829	4{391,425,49}	CS(=O)(=O)N1CCCC(C1)C1=C(NC2CC(F)(F)C2)N2N=C(C=CC2=N1)C1=C(F)C=CC=C1 c:11,22,24,27,30,33,35	Z8873684675	1{391}	Nc1ccc(nn1) c2cccc2F	2{425}	CS(=O)(=O) N1CCCC(C1) C=O	3{49}	FC1(F)CC(C1)[N+]#[C-]	31.5	24
830	4{392,258,67}	CCC(C)NC1=C(N=C2C=CC3=C(NC(C)=N3)N12)C1=NN=C(S1)C1CC1 c:9,15,23,t:5,7,11,21	Z8878918394	1{392}	Cl.Cc1nc2c cc(N)nc2[n H]1	2{258}	O=Cc1nnc(s1) C2CC2	3{67}	CCC(C)[N+]#[C-]	24.1	24
831	4{123,426,22}	CCOC(=O)COC1=CC=C(C=C1)C1=C(NC2COC2)N2C=CC(OCCO)=CC2=N1 c:9,11,14,23,29,32,t:7	Z8878918409	1{123}	Cl.Nc1cc(O CCO)ccn1	2{426}	CCOC(=O)C Oc1ccc(C=O) cc1	3{22}	[C-]]#[N+]C1CO C1	28.4	24
832	4{46,112,9}	CNC1=C(N=C2C=CC=CN12)C1=C2C=CC=N2N=C1 c:6,8,13,15,17,21,t:2,4	Z8873684790	1{46}	Nc1cccn1	2{112}	O=Cc1cmn2n cccc12	3{9}	C[N+]#[C-]	17.3	24
833	4{142,427,24}	COC1=CC(CNC2=C(N=C3N2C=CC=C3OCCS(C)(=O)=O)C2=NOC3=C2COCC3)=CC=C1 c:9,13,15,28,35,37,t:2,7,25	Z8873685374	1{142}	CS(=O)(=O) CCOc1ccc nc1N	2{427}	O=Cc1noc2C COCc12	3{24}	COc1ccc(C[N+]#[C-])c1	32.5	24

834	4{54,130,53}	COC1=NN=C(C=C1)C1=C(NCCOCC2=CC=C(C=C2)N2C=C(C=CC2=N1)C(=O)N(C)C c:4,6,9,18,20,24,26,29,t:2,16	Z8849597837	1{54}	Cl.CN(C)C(=O)c1ccc(N)nc1	2{130}	COc1ccc(C=O)nn1	3{53}	[C-]#[N+]CCOCc1cccc1	29.1	24
835	4{78,428,28}	CCCNC1=C(N=C2C=C(C)C3=NC(C)=CN3N12)C1=CC(OCC2CC2)=C(OC)C=C1 c:14,33,t:4,6,8,11,21,29	Z8873684682	1{78}	Cc1cn2nc(N)cc(C)c2n1	2{428}	COc1ccc(C=O)cc1OCC2CC2	3{28}	CCC[N+]#[C-]	27.3	24
836	4{59,279,42}	CN1C=CN=C1[C@@H]1OCCC[C@H]1C1=C(NC2=C(C)C=CC=C2)N2C=C(CN3CCOCC3)C=CC2=N1 &1:6,11,r,c:2,4,14,17,20,22,36,39,t:26	Z8878918314	1{59}	Nc1ccc(CN2CCOCC2)cn1	2{279}	Cn1ccnc1[C@@H]2OCC[C@H]2C=O &1:6,11,r	3{42}	Cc1cccc1[N+]#[C-]	31.5	24
837	4{291,30,9}	CNC1=C(N=C2N1C=C(Cl)C=C2Cl)C1CCN(CCl)C(C)=O c:4,11,t:2,8	Z8829498779	1{291}	Nc1ncc(Cl)cc1Cl	2{30}	CC(=O)N1C(CC(Cl)C=O	3{9}	C[N+]#[C-]	21.8	24
838	4{158,429,31}	CSCCNC1=C(N=C2C=NC(=CN12)P(C)(C)=O)C1=C(CCCC1)SC1=CC=CC=C1 c:9,11,30,32,t:5,7,20,28	Z8835022878	1{158}	CP(=O)(C)c1nc(N)en1	2{429}	O=CC1=C(CCCC1)Sc2ccccc2	3{31}	CSCC[N+]#[C-]	30.1	24
839	4{73,430,13}	COC1=CC=C(CNC2=C(N=C3C=CC4=NC=C(N4N23)C2=C(C)N=C(OC)C=C2)C=C1 c:12,16,23,30,33,t:2,4,8,10,14,26	Z8873685436	1{73}	Nc1ccc2nccn2n1	2{430}	COc1ccc(C=O)c(C)n1	3{13}	COc1ccc(C[N+]#[C-])cc1	26.4	24
840	4{172,110,29}	CCOC(=O)CCNC1=C(N=C2N1C=CC1=C2CCO1)C1=CN=C(C=C1)P(C)(C)=O c:10,14,16,25,27,t:8,23	Z8873684941	1{172}	Nc1nccc2OCCc21	2{110}	CP(=O)(C)c1ccc(C=O)en1	3{29}	CCOC(=O)C[C[N+]#[C-]	27.3	24
841	4{353,431,15}	CCNC1=C(N=C2C=CC(NS(C)(=O)=O)=CN12)C1CC(Cl)N(C)C(=O)OC(C)(C)C c:7,14,t:3,5	Z8878918906	1{353}	Cl.CS(=O)(=O)Nc1ccc(N)nc1	2{431}	CN(C1CC(C1)C=O)C(=O)OC(C)(C)C	3{15}	CC[N+]#[C-]	27.6	23
842	4{92,432,7}	NC(=O)C1=CC2=NC(=C(NC3CCOCC3)N2C=C1)C1=CSC(=N1)C1=CC=C(Cl)C=C1 c:19,25,33,t:3,5,7,22,28,30	Z8873685470	1{92}	NC(=O)c1cnc(N)c1	2{432}	Clc1ccc(cc1)c2nc(C=O)es2	3{7}	[C-]#[N+]C1CCOCC1	28.4	23
843	4{181,433,14}	COCCNC1=C(N=C2N1C=CC1=C2N=CC=N1)C1=CN(N=C1)C1=C(F)C=CC=C1 c:7,11,13,16,18,24,27,30,32,t:5,21	Z8878918573	1{181}	Nc1nccc2nccn2	2{433}	Fe1cccc1n2cc(C=O)en2	3{14}	COCC[N+]#[C-]	25.1	23
844	4{109,434,34}	COC1=CC(=NC(C)=C1)C1=C(NCC2CCCO2)N2C(C=CC=C2S(N)(=O)=O)=N1 c:4,7,10,22,24,30,t:2	Z8873685267	1{109}	Cl.Nc1cccc(n1)S(=O)(=O)N	2{434}	COc1cc(C)nc(C=O)c1	3{34}	[C-]#[N+]CC1COCO1	25.8	23
845	4{393,13,5}	COCCNC1=C(N=C2C=CC(Cl)=C(Cl)N12)C1=C(C)NN=N1 c:10,19,23,t:6,8,13	Z8878918379	1{393}	Nc1ccc(Cl)c(Cl)n1	2{13}	Cc1[nH]nn1C=O	3{5}	COCCC[N+]#[C-]	21.8	23

846	4{387,435,12}	CCOC(=O)C1=NOC(=C1)C1=C(NCC2CCOC2)N2C=CC=C(OC(F)F)C2=N1 c:8,11,22,31,t:5,24	Z8878918785	1{387}	Nc1ncccc1 OC(F)F	2{435}	CCOC(=O)c 1cc(C=O)on1	3{12}	[C-]]#[N+]CC1C COC1	25.6	22
847	4{47,436,6}	CCCCC1=NC(=CN1)C1=C(NCCCC(=O)OCC)N2C=CC(=CC2=N1)S(N)(=O)=O c:6,10,22,24,27,t:4	Z8854581177	1{47}	Cl.Nc1cc(cc n1)S(=O)(=O)N	2{436}	CCCCc1nc(C =O)c[nH]1	3{6}	CCOC(=O)C CC[N+]#[C-]	27.0	22
848	4{123,437,15}	CCNC1=C(N=C2C=C(OCCO)C=CN12)C1=C N(CC)N=C1C c:13,23,t:3,5,7,18	Z8878918598	1{123}	Cl.Nc1cc(O CCO)ccn1	2{437}	CCn1cc(C=O)c(C)n1	3{15}	CC[N+]#[C-]	19.6	22
849	4{386,438,5}	COCCCN1=C(N=C2C=C(C)C=CN12)C1=N C(C)=NC(=C1)C(F)F c:13,21,23,t:6,8,10,18	Z8873684622	1{386}	Cc1ccnc(N) c1	2{438}	Cc1nc(C=O) cc(n1)C(F)F	3{5}	COCCC[N+] #[C-]	21.4	22
850	4{50,439,31}	COC1=C(C=CC(=C1)C1=C(NCCSC)N2C(C= CC=C2P(C)(C)=O)=N1)S(C)(=O)=O c:4,6,9,18,20,26,t:2	Z8873684911	1{50}	CP(=O)(C)c 1cccc(N)n1	2{439}	COc1cc(C=O)ccc1S(=O)(=O)C	3{31}	CSCC[N+]#[C-]	27.6	22
851	4{48,440,22}	CS(=O)(=O)C1=CC2=NC(=C(NC3COC3)N2C =C1)C1=CC=C(C=C1)N1C=C(Br)C=N1 c:18,23,25,32,t:4,6,8,21,29	Z8873684765	1{48}	CS(=O)(=O) c1ccnc(N)c 1	2{440}	Br1enn(c1)c 2ccc(C=O)cc 2	3{22}	[C-]]#[N+]C1CO C1	28.9	22
852	4{83,441,31}	CCC(C)C(OC)C1=C(NCCSC)N2C=C(C=CC2 =N1)P(C)(C)=O c:7,15,17,20	Z8837933137	1{83}	CP(=O)(C)c 1ccc(N)nc1	2{441}	CCC(C)C(O C)C=O	3{31}	CSCC[N+]#[C-]	22.5	22
853	4{146,164,51}	CN1N=C(C2=C1CCOC2)C1=C(NCCNC(=O) OC(C)(C)C)N2C=C(C=CC2=N1)S(C)(=O)=O c:2,4,12,26,28,31	Z8855619628	1{146}	CS(=O)(=O) c1ccc(N)nc 1	2{164}	Cn1nc(C=O) c2COCCc21	3{51}	CC(C)(C)OC (=O)NCC[N +]#[C-]	28.0	21
854	4{187,375,46}	COCC1=C(N=CO1)C1=C(NCC(C)=C)N2C=C (Cl)C(=CC2=N1)C#N c:5,9,20,23,t:3,17	Z8873684920	1{187}	Nc1cc(C#N)c(Cl)cn1	2{375}	COCC1ocnc1 C=O	3{46}	CC(=C)C[N+]]#[C-]	20.0	21
855	4{83,442,37}	COC(=O)C1CC(C1)NC1=C(N=C2C=CC(=CN 12)P(C)(C)=O)C1=CC2=C(COC2)C=C1 c:14,16,33,t:10,12,25,27	Z8846492124	1{83}	CP(=O)(C)c 1ccc(N)nc1	2{442}	O=Cc1ccc2C OCc2c1	3{37}	COC(=O)C1 CC(C1)[N+] #[C-]	24.6	21
856	4{166,443,22}	OCCSCC1=CC2=NC(=C(NC3COC3)N2C=C1)C1=C2N=CC=CC2=C(F)C=C1 c:19,22,24,26,32,t:5,7,9,29	Z8873685480	1{166}	Nc1cc(CSC CO)ccn1	2{443}	Fc1ccc(C=O) c2ncccc12	3{22}	[C-]]#[N+]C1CO C1	23.7	21
857	4{181,344,14}	COCCNC1=C(N=C2N1C=CC1=C2N=CC=N1) C1=C(C)C=NN1COC c:7,11,13,16,18,21,24,t:5	Z8873684762	1{181}	Nc1nccc2nc cnc12	2{344}	COc1nccc(C)c1C=O	3{14}	COCC[N+]#[C-]	20.3	20

858	4{95,444,35}	CSCCCNC1=C(N=C2C=CC(=CN12)C(F)F)C1=C(O)C=CN=C1 c:10,12,20,23,25,t:6,8	Z8873685420	1{95}	Nc1ccc(en1)C(F)F	2{444}	Oc1ccncc1C=O	3{35}	CSCCC[N+]#[C-]	20.1	20
859	4{330,445,29}	CCOC(=O)CCNC1=C(N=C2C=CC(=CN12)S(=O)(=O)N(C)C)C1=NOC(=C1)C(C)(C)C c:12,14,28,t:8,10,25	Z8873685490	1{330}	CN(C)S(=O)(=O)c1ccc(N)nc1	2{445}	CC(C)(C)c1cc(C=O)no1	3{29}	CCOC(=O)C[N+]#[C-]	25.5	20
860	4{22,307,13}	COC1=CC=C(CNC2=C(N=C3C=CC(CI)=NN23)C2=CN=C(CI)N2C)C=C1 c:12,15,28,t:2,4,8,10,20,22	Z8835022916	1{22}	Nc1ccc(CI)nn1	2{307}	Cn1c(CI)ncc1C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	22.0	20
861	4{351,446,28}	CCCNC1=C(N=C2C=CC3=C(C(O)CC3)N12)C1=CC(=CC=C1)C(=O)NC c:8,22,24,t:4,6,10,20	Z8873684684	1{351}	Nc1ccc2CC(C(O)c2n1	2{446}	CNC(=O)c1ccc(C=O)c1	3{28}	CCC[N+]#[C-]	19.8	20
862	4{101,260,6}	CCOC(=O)CCCNC1=C(N=C2N1C=C(CO)C=C2CI)C1=NOC(C)=C1 c:11,19,27,t:9,15,23	Z8873685370	1{101}	Nc1ncc(CO)cc1Cl	2{260}	Cc1cc(C=O)no1	3{6}	CCOC(=O)C[N+]#[C-]	21.1	20
863	4{181,447,6}	CCOC(=O)CCCNC1=C(N=C2N1C=CC1=C2N=CC=N1)C1=CC=C(C=C1)C#CC(C)(C)O c:11,15,17,20,22,27,29,t:9,25	Z8873684692	1{181}	Nc1nccc2ncnc12	2{447}	CC(C)(O)C#Cc1ccc(C=O)cc1	3{6}	CCOC(=O)C[N+]#[C-]	24.4	20
864	4{28,448,7}	COC1=C2OCOC2=CC(=C1)C1=C(NC2CCOC2)N2C=CC(=CC2=N1)C1=NOC=N1 c:2,8,10,13,24,26,29,35,t:32	Z8878918875	1{28}	Cl.Nc1cc(ccn1)c2ncon2	2{448}	COc1cc(C=O)cc2OCOC21	3{7}	[C-]#[N+]C1CCOCC1	23.2	20
865	4{218,34,61}	CC(C)(C)OC(=O)NCCCNC1=C(N=C2C=CC(=NN12)C(C)(C)C)C1=CC=C(C=C1)P(C)(C)=O c:16,18,29,31,t:12,14,27	Z8803896931	1{218}	CC(C)(C)c1ccc(N)nn1	2{34}	CP(=O)(C)c1ccc(C=O)cc1	3{61}	CC(C)(C)OC(=O)NCCC[N+]#[C-]	26.6	20
866	4{46,58,9}	CNC1=C(N=C2C=CC=CN12)C1=NSN=C1 c:6,8,16,t:2,4,13	Z8855739152	1{46}	Nc1cccn1	2{58}	O=Cc1cnsn1	3{9}	C[N+]#[C-]	12.2	19
867	4{155,449,14}	COCCNC1=C(N=C2N1C=CC=C2CI)C1=C(C)C=C(S1)C(N)=O c:7,11,13,17,20,t:5	Z8878918329	1{155}	Nc1ncccc1Cl	2{449}	Cc1cc(sc1C=O)C(=O)N	3{14}	COCC[N+]#[C-]	19.1	19
868	4{176,450,14}	COCCNC1=C(N=C2N1C=CN=C2N1CCCC1)C1=CC(=CC=C1)S(=O)(=O)N(C)C c:7,11,13,24,26,t:5,22	Z8846491730	1{176}	Nc1ncnc1N2CCCC2	2{450}	CN(C)S(=O)(=O)c1cccc(C=O)c1	3{14}	COCC[N+]#[C-]	23.1	19
869	4{213,92,31}	COC1=CC=C(F)C2=NC(C3=CC(C)=NO3)=C(NCCSC)N12 c:13,t:2,4,7,10,16	Z8873684810	1{213}	COc1ccc(F)c(N)n1	2{92}	Cc1cc(C=O)on1	3{31}	CSCC[N+]#[C-]	17.3	19
870	4{46,27,9}	CNC1=C(N=C2C=CC=CN12)C1=NN(C)C(C)=N1 c:6,8,18,t:2,4,13	Z8855739086	1{46}	Nc1cccn1	2{27}	Cc1nc(C=O)nn1C	3{9}	C[N+]#[C-]	12.4	19
871	4{330,229,69}	COC1=C(NC2=C(N=C3C=CC(=CN23)S(=O)(=O)N(C)C)C2=CN=C(OCCO)C=C2)C=CC=C1 c:2,9,11,30,33,35,t:5,7,22,24	Z8878918769	1{330}	CN(C)S(=O)(=O)c1ccc(N)nc1	2{229}	OCCOCc1ccc(C=O)en1	3{69}	COc1cccc1[N+]#[C-]	24.3	19

872	4{327,451,34}	COC(=O)C1=C(F)C2=NC(=C(NCC3CCCO3)N2C=C1)C1=NC=CC(=C1)C(F)F c:4,21,26,28,t:7,9,24	Z8878918780	1{327}	COC(=O)c1ccnc(N)c1F	2{451}	FC(F)c1ccnc(C=O)c1	3{34}	[C-]]#[N+]CC1C CCO1	20.8	18
873	4{218,334,21}	CC1=C(N=CO1)C1=C(NCC2CC2)N2N=C(C=CC2=N1)C(C)(C)C c:3,7,16,18,21,t:1	Z8837933146	1{218}	CC(C)(C)c1ccc(N)nn1	2{334}	Cc1ocnc1C=O	3{21}	[C-]]#[N+]CC1C C1	16.0	18
874	4{331,452,49}	CN(C)CCN(C)CC1=CN2C(C=C1)=NC(=C2N1)CC(F)(F)C1)C1=CC=C(C=C1)C(N)=O c:12,14,16,29,31,t:8,27	Z8878918445	1{331}	Cl.Cl.Cl.CN(C)CCN(C)Cc1ccc(N)nc1	2{452}	NC(=O)c1ccc(C=O)cc1	3{49}	FC1(F)CC(C1)[N+]#[C-]	22.4	18
875	4{81,453,9}	CNC1=C(N=C2C=NC=CN12)C1=CC(C=C)=CN=C1 c:6,8,17,19,t:2,4,13	Z8873684792	1{81}	Nc1cncn1	2{453}	Cl.C=Cc1cnc(C=O)c1	3{9}	C[N+]#[C-]	12.3	18
876	4{394,169,10}	FC1=C(C=C)C=CC2=NC(=C(NC3CCOC3)N12)C1=NNC2=C1N=CC=C2 c:1,5,24,27,29,t:7,9,21	Z8878918526	1{394}	Nc1ccc(C=C)c(F)n1	2{169}	O=Cc1n[nH]c2ccnc12	3{10}	[C-]]#[N+]C1CC OC1	17.7	18
877	4{93,454,61}	COC(C)CC1=C(NCCCNC(=O)OC(C)(C)C)N2C=C(OC)N=CC2=N1 c:5,24,27,t:20	Z8878918849	1{93}	COc1cnc(N)c1	2{454}	COC(C)CC=O	3{61}	CC(C)(C)OC(=O)NCCC[N+]#[C-]	18.6	18
878	4{103,455,59}	CC1=C(C(Br)=NO1)C1=C(NCCC2=CC(F)=C(C=C2)N2C(C=NC=C2CO)=N1 c:4,8,16,18,23,25,29,t:1,13	Z8878918462	1{103}	Nc1cnc(CO)n1	2{455}	Cc1onc(Br)c1C=O	3{59}	Fe1cccc(CC[N+]#[C-])c1	21.0	17
879	4{171,216,53}	COC(=O)C1=NC=C(S1)C1=C(NCCOCC2=CC=CC=C2)N2C=CC(=CC2=N1)N1C=CN=C1 c:6,10,19,21,25,27,30,34,36,t:4,17	Z8878918572	1{171}	Nc1cc(cen1)n2cnc2	2{216}	COC(=O)c1ncc(C=O)s1	3{53}	[C-]]#[N+]CCOC c1cccc1	22.2	17
880	4{120,456,71}	COC1=CC(NC2=C(N=C3C=C(C=CN23)C2=C(N(C)N=C2)C2=CC(=CO2)S(N)(=O)=O)=CC=C1 c:10,12,21,26,33,35,t:2,6,8,17,24	Z8873685316	1{120}	Cn1cc(en1)c2cnc(N)c2	2{456}	NS(=O)(=O)c1coc(C=O)c1	3{71}	COc1cccc([N+]#[C-])c1	21.7	17
881	4{186,457,29}	CCOC(=O)CCNC1=C(N=C2C=C(C=CN12)S(=O)(=O)N(C)C)C1=NN=C(C=C1)C(F)(F)F c:12,14,27,29,t:8,10,25	Z8878918863	1{186}	Cl.CN(C)S(=O)(=O)c1ccnc(N)c1	2{457}	FC(F)(F)c1ccc(C=O)nn1	3{29}	CCOC(=O)C[N+]#[C-]	22.6	17
882	4{78,458,51}	COC1=C(C)C=CC(=N1)C1=C(NCCNC(=O)OC(C)(C)C)N2N3C=C(C)N=C3C(C)=CC2=N1 c:2,5,7,10,28,32,35,t:25	Z8878918675	1{78}	Cc1cn2nc(N)cc(C)c2n1	2{458}	COc1nc(C=O)ccc1C	3{51}	CC(C)(C)OC(=O)NCC[N+]#[C-]	21.1	17
883	4{363,459,62}	COC(=O)C1=CC2=NC(=C(NC3(CCCC3)C(=O)OC)N2C=C1)C1=NNC(C)=C1C c:23,30,t:4,6,8,26	Z8873684726	1{363}	COC(=O)c1ccnc(N)c1	2{459}	Cc1[nH]nc(C=O)c1C	3{62}	COC(=O)C1(CCCC1)[N+]#[C-]	18.5	17

884	4{35,396,13}	COC1=CC=C(CNC2=C(N=C3C=CC(C)=CN23)C2=CN=C3COCCN23)C=C1 c:12,15,31,t:2,4,8,10,20,22	Z8873684635	1{35}	Cc1ccc(N)nc1	2{396}	O=Cc1cnc2COCc1n2	3{13}	COc1ccc(C[N+]#[C-])cc1	17.3	16
885	4{193,460,60}	CNC(=O)C1=CN2C(NC3=CC(=CC=C3)C(=O)OC)=C(N=C2C=C1)C1=NC=C(C)O1 c:11,13,19,21,24,t:4,9,27,29	Z8835022877	1{193}	CNC(=O)c1ccc(N)nc1	2{460}	Cc1cnc(C=O)o1	3{60}	COC(=O)c1ccc([N+]#[C-])c1	17.9	16
886	4{395,461,7}	CCN1N=CC(=C1F)C1=C(NC2CCOCC2)N2N=C(C=C(C)C2=N1)C(F)(F)F c:3,5,9,20,26,t:22	Z8878918396	1{395}	Cc1cc(nnc1N)C(F)(F)F	2{461}	CCn1ncc(C=O)c1F	3{7}	[C-]#[N+]C1CCOCC1	18.1	16
887	4{137,284,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC(C)=NN23)C2=C(C)N=CC=N2)C=C1 c:12,15,20,23,25,28,t:2,5,8,10	Z8873684616	1{137}	Cc1ccc(N)nc1	2{284}	Cc1nccnc1C=O	3{20}	COc1ccc([N+]#[C-])c(C)c1	15.7	16
888	4{99,229,50}	NS(=O)(=O)C1=CN2C(NC3=CC4=C(OCCO4)C=C3)=C(N=C2C=C1)C1=CN=C(OCCO)C=C1 c:18,20,22,25,36,t:4,9,11,28,30	Z8837933134	1{99}	Nc1ccc(en1)S(=O)(=O)N	2{229}	OCCOc1ccc(C=O)en1	3{50}	[C-]#[N+]c1ccc2OCCOc2c1	21.0	16
889	4{103,354,40}	CCOC(=O)C1=CC=C(NC2=C(N=C3C=NC=C(CO)N23)C2=C(C=CC=C2)P(C)(C)=O)C=C1 c:14,25,27,34,t:5,7,10,12,16,23	Z8878918669	1{103}	Nc1cnc(C)Onc1	2{354}	CP(=O)(C)c1cccc1C=O	3{40}	CCOC(=O)c1ccc([N+]#[C-])cc1	20.1	16
890	4{78,462,39}	CCOCCNC1=C(N=C2C=C(C)C3=NC(C)=CN3N12)C1=C(Br)C=CC(C)=C1F c:16,23,26,29,t:6,8,10,13	Z8873685495	1{78}	Cc1en2nc(N)cc(C)c2n1	2{462}	Cc1ccc(Br)c(C=O)c1F	3{39}	CCOCC[N+]#[C-]	19.7	16
891	4{291,274,13}	COC1=CC=C(CNC2=C(CC3(CCOCC3)C#N)N=C3N2C=C(Cl)C=C3Cl)C=C1 c:8,20,27,31,t:2,4,24	Z8873685489	1{291}	Nc1ncc(Cl)cc1Cl	2{274}	O=CCC1(CCOC1)C#N	3{13}	COc1ccc(C[N+]#[C-])cc1	18.8	16
892	4{167,463,5}	COCCNC1=C(N=C2N1C(C)=CN=C2C)C1=C(C)C(I)=NN1C c:8,13,15,19,23,t:6	Z8873684713	1{167}	Cc1cnc(C)c(N)nc1	2{463}	Cc1c(I)nn(C)c1C=O	3{5}	COCC[N+]#[C-]	18.9	15
893	4{50,464,31}	CSCCNC1=C(N=C2C=CC=C(N12)P(C)(C)=O)C1=CC2=C(C=CC=C2)N2N=NN=C12 c:9,11,24,26,30,t:5,7,20,22,32	Z8873685251	1{50}	CP(=O)(C)c1ccc(N)nc1	2{464}	O=Cc1ccccc2n3nnnc13	3{31}	CSCC[N+]#[C-]	17.7	14
894	4{230,349,34}	CC(O)C1=CC(Br)=CN2C(NCC3CCCO3)=C(N=C12)C1C[C@H]2OC(C)(C)O[C@H]2C1 c:6,17,t:3,19	Z8873685493	1{230}	CC(O)c1cc(Br)nc1N	2{349}	CC1(C)O[C@@@H]2CC(C)[C@@@H]2O1)C=O	3{34}	[C-]#[N+]CC1CCO1	18.8	14
895	4{79,129,13}	COC1=CC=C(CNC2=C(N=C3C=NC=C(C)N23)C2=CC=CC3=NC=NN23)C=C1 c:12,22,26,31,t:2,4,8,10,14,20,24	Z8878918798	1{79}	Cc1nccc(N)nc1	2{129}	O=Cc1cccc2ncnn12	3{13}	COc1ccc(C[N+]#[C-])cc1	15.0	14

896	4{382,305,71}	COCC1=NC(=CN1)C1=C(NC2=CC(OC)=CC=C2)N2C=C(N=CC2=N1)C(F)(F)F c:5,9,16,18,22,24,27,t:3,12	Z8878918670	1{382}	Nc1cnc(en1)C(F)(F)F	2{305}	COCC1nc(C=O)c[nH]1	3{71}	COc1cccc([N+][C-])c1	16.1	14
897	4{179,465,23}	COC(=O)CCC(NC1=C(N=C2C=C(OC)C=CN12)C1=C(C1)C=C(C)C=N1)C(=O)OC c:16,21,27,t:8,10,12,24	Z8878918401	1{179}	COc1ccnc(N)c1	2{465}	Cc1cnc(C=O)c(Cl)c1	3{23}	COC(=O)CC(C([N+][C-])C(=O)OC	17.2	14
898	4{396,466,23}	COC(=O)CCC(NC1=C(N=C2C=CC(=NN12)C1=CN(C)N=C1)C1=CC(Cl)=C(C)N=C1)C(=O)OC c:12,14,23,32,t:8,10,19,26,29	Z8829498618	1{396}	Cn1cc(en1)c2ccc(N)nn2	2{466}	Cc1ncc(C=O)cc1Cl	3{23}	COC(=O)CC(C([N+][C-])C(=O)OC	19.0	14
899	4{181,467,14}	COCCNC1=C(N=C2N1C=CC1=C2N=CC=N1)C1=C(C)SC(Br)=N1 c:7,11,13,16,18,21,26,t:5	Z8855739274	1{181}	Nc1nccc2ncnc12	2{467}	Cc1sc(Br)nc1C=O	3{14}	COCC[N+][C-]	15.9	14
900	4{54,468,37}	COC(=O)C1CC(C1)NC1=C(CC(C)SC)N=C2C=CC(=CN12)C(=O)N(C)C c:10,19,21,t:17	Z8873685443	1{54}	Cl.CN(C)C(=O)c1ccc(N)nc1	2{468}	CSC(C)CC=O	3{37}	COC(=O)C1CC(C1)[N+][C-]	15.2	14
901	4{169,469,11}	CNC(=O)C1=NN2C(C=C1)=NC(C1CCSC1)=C2NCC1=CC(Br)=CC=C1 c:8,10,18,26,28,t:4,23	Z8829498482	1{169}	CNC(=O)c1ccc(N)nn1	2{469}	O=CC1CCSC1	3{11}	Br1cccc(C[N+][C-])c1	16.5	14
902	4{72,470,12}	COC1=NC(Br)=CN2C(NCC3CCOC3)=C(N=C12)C1=COC(Br)=N1 c:5,16,26,t:2,18,22	Z8878918789	1{72}	COc1nc(Br)nc1N	2{470}	Br1nc(C=O)co1	3{12}	[C-][N+][C]C1COC1	17.5	14
903	4{251,471,62}	COC(=O)C1(CCCC1)NC1=C(N=C2C=CC3=C(NC(=O)C=C3)N12)C1=NC=C2OCOC2=C1 c:15,22,36,t:11,13,17,28,30	Z8873684899	1{251}	Nc1ccc2ccc(=O)[nH]c2n1	2{471}	O=Cc1cc2OCoc2en1	3{62}	COC(=O)C1(CCCC1)[N+][C-]	16.4	14
904	4{73,94,11}	BrC1=CC(CNC2=C(N=C3C=CC4=NC=CN4N23)C2=NC=CN=C2)=CC=C1 c:10,14,23,25,27,29,t:1,6,8,12,21	Z8873685473	1{73}	Nc1ccc2nccn2n1	2{94}	O=Cc1cncn1	3{11}	Br1cccc(C[N+][C-])c1	15.3	13
905	4{83,472,26}	COC(=O)C1=CC2=C(C=NN2C=C1)C1=C(NC2=CC=C(F)C=C2)N2C=C(C=CC2=N1)P(C)(C)=O c:8,12,15,24,28,30,33,t:4,6,19,21	Z8846491855	1{83}	CP(=O)(C)c1ccc(N)nc1	2{472}	COC(=O)c1cnc2ncc(C=O)c2c1	3{26}	Fe1ccc(C[N+][C-])cc1	17.9	13
906	4{397,177,5}	COCCNC1=C(CC2CC(C2)C(=O)OC)N=C2N1C=CC(C)=C2C c:6,18,22,25	Z8873684719	1{397}	Cl.Cc1ccnc(N)c1C	2{177}	COC(=O)C1CC(CC=O)C1	3{5}	COCCC[N+][C-]	13.1	13
907	4{229,473,68}	COC1=CC(C)=C(C=C1)C1=C(NC2CCCCC2)N2C=C(C=CC2=N1)S(O)(=O)=O c:5,7,10,21,23,26,t:2	Z8829498563	1{229}	Nc1ccc(en1)S(=O)(=O)O	2{473}	COc1ccc(C=O)c(C)c1	3{68}	[C-][N+][C]1CCCCC1	15.0	13

908	4{222,193,62}	COC(=O)C1=CN2C(NC3(CCCC3)C(=O)OC)=C(N=C2C=N1)C1=NN2CCCCOC2=C1 c:18,20,23,35,t:4,26	Z8808559886	1{222}	Cl.COC(=O)c1cnc(N)cn1	2{193}	O=Cc1cc2OCCCCn2n1	3{62}	COC(=O)C1(CCCC1)[N+]#[C-]	16.3	13
909	4{78,474,51}	CC1=CN2N3C(NCCNC(=O)OC(C)(C)C)=C(N=C3C=C(C)C2=N1)C1=NNC2=C1C=CC=N2 c:16,18,25,31,34,36,t:1,21,28	Z8878918667	1{78}	Cc1cn2nc(N)cc(C)c2n1	2{474}	O=Cc1n[nH]c2ncccc12	3{51}	CC(C)(C)OC(=O)NCC[N+]#[C-]	16.5	13
910	4{167,475,5}	COCCNC1=C(N=C2N1C(C)=CN=C2C)C1=CC2=C(O1)C(F)=NC=C2 c:8,13,15,21,26,28,t:6,19	Z8878918907	1{167}	Cc1cnc(C)c(N)n1	2{475}	Fe1nccc2cc(C=O)oc12	3{5}	COCCC[N+]#[C-]	12.8	13
911	4{398,130,32}	COC1=NN=C(C=C1)C1=C(NC2CCC2)N2C=CC(=CC2=N1)C(C)(F)F c:4,6,9,18,20,23,t:2	Z8854581139	1{398}	Cl.CC(F)(F)c1cnc(N)c1	2{130}	COc1ccc(C=O)nn1	3{32}	[C-]#[N+]C1CC1	12.4	13
912	4{27,368,21}	COC1=CC=CC2=NC(=C(NCC3CC3)N12)C1=NN=C(C)C(C)=C1 c:4,25,t:2,6,8,19,21	Z8855739205	1{27}	COc1cccc(N)n1	2{368}	Cc1cc(C=O)nnc1C	3{21}	[C-]#[N+]CC1C1	10.9	13
913	4{99,476,57}	COC(=O)CCC1=NOC=C1C1=C(NCC2=CC=C(C=C2)N2C=C(C=CC2=N1)S(N)(=O)=O c:9,12,18,20,24,26,29,t:6,16	Z8854581136	1{99}	Nc1ccc(en1)S(=O)(=O)N	2{476}	COC(=O)CCc1nocc1C=O	3{57}	[C-]#[N+]Cc1ccc1	15.4	13
914	4{399,477,37}	COC(=O)C1CC(C1)NC1=C(N=C2C=CC(OC(C)C)=NN12)C(NC(=O)OC(C)(C)C)C1COC1 c:14,20,t:10,12	Z8846492223	1{399}	CC(C)Oc1ccc(N)nn1	2{477}	CC(C)(C)OC(=O)NC(C=O)C1COC1	3{37}	COC(=O)C1CC(C1)[N+]#[C-]	16.5	12
915	4{77,478,5}	COCCNC1=C(N=C2C=CC(=CN12)C1=CN=CC=C1)C1=CN(C)C(=O)C2=C1C=CN=C2 c:10,12,19,21,30,33,35,t:6,8,17,24	Z8873684782	1{77}	Nc1ccc(en1)c2cccnc2	2{478}	Cn1cc(C=O)c2ccncc2c1=O	3{5}	COCCC[N+]#[C-]	14.9	12
916	4{181,479,14}	COCCNC1=C(N=C2N1C=CC1=C2N=CC=N1)C1=CN(N=C1)C1=CC(C)=CC=C1 c:7,11,13,16,18,24,30,32,t:5,21,27	Z8878918565	1{181}	Nc1nccc2ncnc12	2{479}	Cc1cccc(c1)n2cc(C=O)cn2	3{14}	COCC[N+]#[C-]	13.4	12
917	4{67,396,9}	CNC1=C(N=C2C=CC=C(C)N12)C1=CN=C2C OCCN12 c:6,t:2,4,8,14,16	Z8873685379	1{67}	Cc1cccc(N)n1	2{396}	O=Cc1cnc2C OCCn12	3{9}	C[N+]#[C-]	9.5	12
918	4{169,25,13}	CNC(=O)C1=NN2C(C=C1)=NC(=C2NCC1=C(C=OC)C=C1)C1=CN=C(N=C1)C1CCOCC1 c:8,10,12,23,28,30,t:4,17,19,26	Z8855619638	1{169}	CNC(=O)c1ccc(N)nn1	2{25}	O=Cc1cnc(nc1)C2CCOCC2	3{13}	COc1ccc(C[N+]#[C-])cc1	15.6	12
919	4{198,189,31}	CSCCNC1=C(N=C2C=NC(C#C)=C(C1)N12)C1=CN(N=N1)C1CCOCC1 c:9,22,t:5,7,13,19	Z8801681831	1{198}	Nc1cnc(C#C)c(Cl)n1	2{189}	O=Cc1cn(nn1)C2CCOCC2	3{31}	CSCC[N+]#[C-]	13.2	12

920	4{88,480,34}	FC1=C(Br)C=CN2C(NCC3CCCO3)=C(N=C12)C1=CC2=C(CCOC2)N=C1 c:1,4,15,30,t:17,21,23	Z8878918389	1{88}	Nc1ncce(Br)c1F	2{480}	O=Cc1cnc2C COCc2c1	3{34}	[C-] #[N+]CC1C CCO1	14.0	12
921	4{150,481,22}	CC1=NNC2=C1C=CC(=C2)C1=C(NC2COC2)N2C=CC(=CC2=N1)C1CCOC1 c:4,7,9,12,21,23,26,t:1	Z8873685244	1{150}	Nc1cc(ccn1)C2CCOC2	2{481}	Cc1n[nH]c2cc(C=O)ccc12	3{22}	[C-] #[N+]C1CO C1	11.8	11
922	4{370,281,10}	COC(=O)C1=NN=C(C=C1)C1=C(NC2CCOC2)N2C=CC(Br)=C(OC)C2=N1 c:6,8,11,21,29,t:4,24	Z8878918604	1{370}	COc1c(N)nccc1Br	2{281}	COC(=O)c1ccc(C=O)nn1	3{10}	[C-] #[N+]C1CC OC1	13.5	11
923	4{158,482,7}	CP(C)(=O)C1=CN2C(C=N1)=NC(=C2NC1CCOCC1)C1=CC(=CC(C1)=C1)C(F)(F)F c:8,10,12,25,28,t:4,23	Z8855739184	1{158}	CP(=O)(C)c1cnc(N)cn1	2{482}	FC(F)(F)c1cc(C1)cc(C=O)c1	3{7}	[C-] #[N+]C1CC OCC1	13.7	11
924	4{351,483,71}	COC1=CC(NC2=C(N=C3C=CC4=C(C(O)CC4)N23)C2=CN(C=N2)C2CC2)=CC=C1 c:10,25,31,33,t:2,6,8,12,22	Z8849597808	1{351}	Nc1ccc2CC(C(O)c2n1	2{483}	Cl.O=Cc1cn(Cn1)C2CC2	3{71}	COc1cccc([N+])#[C-]c1	11.5	11
925	4{99,484,50}	NS(=O)(=O)C1=CN2C(NC3=CC4=C(OCCO4)C=C3)=C(N=C2C=C1)C1=CC(=CS1)C#N c:18,20,22,25,30,t:4,9,11,28	Z8873685404	1{99}	Nc1ccc(en1)S(=O)(=O)N	2{484}	O=Cc1cc(C#N)cs1	3{50}	[C-] #[N+]c1ccc2OCCOc2c1	12.8	10
926	4{166,173,32}	CN1N=C(N=C1C1=C(NC2CCC2)N2C=CC(CSCCO)=CC2=N1)C(F)(F)F c:2,4,7,16,23,26	Z8878918387	1{166}	Nc1cc(CSCCO)cn1	2{173}	Cn1nc(nc1C=O)C(F)(F)F	3{32}	[C-] #[N+]C1CC C1	11.9	10
927	4{79,485,13}	COC1=CC=C(CNC2=C(N=C3C=NC=C(C)N23)C2=NOC3=C2CCC3)C=C1 c:12,23,30,t:2,4,8,10,14,20	Z8873684741	1{79}	Cc1cnc(N)n1	2{485}	O=Cc1noc2C CCc12	3{13}	COc1ccc(C[N+])#[C-]cc1	10.2	10
928	4{146,486,46}	CN1C(Cl)=NC(Cl)=C1C1=C(NCC(C)=C)N2C=C(C=CC2=N1)S(C)(=O)=O c:3,6,9,17,19,22	Z8878918499	1{146}	CS(=O)(=O)c1ccc(N)nc1	2{486}	Cn1c(Cl)nc(Cl)c1C=O	3{46}	CC(=C)C[N+] #[C-]	11.1	10
929	4{112,487,61}	COC1=CN=CC2=NC(=C(NCCCNC(=O)OC(C)(C)C)N12)C1=C(Cl)C=NN1C c:4,25,28,t:2,6,8	Z8873684760	1{112}	COc1cnc(N)n1	2{487}	Cn1nc(Cl)c1C=O	3{61}	CC(C)(C)OC(=O)NCCC[N+] #[C-]	11.0	9
930	4{400,488,15}	CCNC1=C(N=C2C=CC(COC(C)C)=CN12)C1=CC2=C(NC(=O)CC2)N=C1 c:7,14,29,t:3,5,19,21	Z8878918822	1{400}	CC(C)OCc1ccc(N)nc1	2{488}	O=Cc1cnc2N C(=O)CCc2c1	3{15}	CC[N+] #[C-]	9.5	9
931	4{399,489,22}	CC(C)OC1=NN2C(NC3COC3)=C(N=C2C=C1)C1=NOC(=C1)C1CCC1 c:13,15,18,24,t:4,21	Z8854581166	1{399}	CC(C)Oc1ccc(N)nn1	2{489}	O=Cc1cc(on1)C2CCC2	3{22}	[C-] #[N+]C1CO C1	9.1	9

932	4{401,296,39}	CCOCCNC1=C(N=C2C=CC3=C(N=CC=C3C1)N12)C1=CN(CCF)N=C1 c:10,14,16,29,t:6,8,12,23	Z8873684628	1{401}	Nc1ccc2c(C)ccnc2n1	2{296}	FCCn1cc(C=O)en1	3{39}	CCOCC[N+]#[C-]	9.9	9
933	4{83,490,18}	CC(C)(C)NC1=C(N=C2C=CC(=CN12)P(C)(C)=O)C1=CC(OC(F)(F)CF)=CC=C1 c:9,11,28,30,t:5,7,20	Z8878918343	1{83}	CP(=O)(C)c1ccc(N)nc1	2{490}	FCC(F)(F)Oc1cccc(C=O)c1	3{18}	CC(C)(C)[N+]#[C-]	10.5	9
934	4{79,129,9}	CNC1=C(N=C2C=NC=C(C)N12)C1=CC=CC2=NC=NN12 c:6,16,20,t:2,4,8,14,18	Z8849597841	1{79}	Cc1cnc(N)n1	2{129}	O=Cc1cccc2ncnn12	3{9}	C[N+]#[C-]	6.3	8
935	4{125,212,15}	CCNC1=C(N=C2C=CC(CCO)=CN12)C1=NO C(=C1)C(F)F c:7,12,20,t:3,5,17	Z8808559873	1{125}	Nc1ccc(CC)Oen1	2{212}	FC(F)c1cc(C=O)no1	3{15}	CC[N+]#[C-]	7.1	8
936	4{291,27,9}	CNC1=C(N=C2N1C=C(C1)C=C2C1)C1=NN(C)C(C)=N1 c:4,11,20,t:2,8,15	Z8878918327	1{291}	Nc1ncc(Cl)cc1Cl	2{27}	Cc1nc(C=O)nn1C	3{9}	C[N+]#[C-]	6.5	8
937	4{402,491,49}	CC(C)(C)OC(=O)N1CCC2CC12CC1=C(NC2C(C(F)(F)C2)N2C(C=NC=C2F)=N1 c:16,28,30,33	Z8835022917	1{402}	Nc1cnc(F)n1	2{491}	CC(C)(C)OC(=O)N1CCC2CC21CC=O	3{49}	FC1(F)CC(C1)[N+]#[C-]	8.8	7
938	4{216,190,10}	CC1=CC2=NC(C3=CC(=NN3)C3=NC=CC=C3)=C(NC3CCOC3)N2N=C1C c:8,14,16,29,t:1,3,6,12,18	Z8801681808	1{216}	Cc1cc(N)nn1C	2{190}	O=Cc1cc(n[nH]1)c2ccccn2	3{10}	[C-]#[N+]C1CCOC1	7.5	7
939	4{251,492,70}	CC1=NC(C)=C(C)N=C1C1=C(NC2CCN(C2)C(=O)OC(C)(C)C)N2C(C=CC3=C2NC(=O)C=C3)=N1 c:7,10,28,30,36,38,t:1,4	Z8873684809	1{251}	Nc1ccc2ccc(=O)[nH]c2n1	2{492}	Cc1nc(C)c(C=O)nc1C	3{70}	CC(C)(C)OC(=O)N1CCC(C1)[N+]#[C-]	8.9	7
940	4{240,277,22}	CC(C)(C)OC(=O)NC(CC1=C(NC2COC2)N2C=C(C=CC2=N1)C1=NNN=N1)C1CC1 c:10,19,21,24,30,t:27	Z8878918548	1{240}	Nc1ccc(en1)c2nn[nH]n2	2{277}	CC(C)(C)OC(=O)NC(CC=O)C1CC1	3{22}	[C-]#[N+]C1CO C1	8.7	7
941	4{73,493,13}	COC1=CC=C(CNC2=C(N=C3C=CC4=NC=C4N23)C2=C(F)C=CC=N2)C=C1 c:12,16,23,26,28,31,t:2,4,8,10,14	Z8878918871	1{73}	Nc1ccc2nccn2n1	2{493}	Fe1cccnc1C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	6.6	6
942	4{92,310,18}	CC(C)(C)NC1=C(N=C2C=C(C=CN12)C(N)=O)C1CCOC2(CCC2)C1 c:9,11,t:5,7	Z8855619753	1{92}	NC(=O)c1ccnc(N)c1	2{310}	O=CC1CCOC2(CCC2)C1	3{18}	CC(C)(C)[N+]#[C-]	6.0	6
943	4{158,448,31}	COC1=C2OCOC2=CC(=C1)C1=C(NCCSC)N2C=C(N=CC2=N1)P(C)(C)=O c:2,8,10,13,21,23,26	Z8835022883	1{158}	CP(=O)(C)c1cnc(N)cn1	2{448}	COc1cc(C=O)cc2OCOC21	3{31}	CSCC[N+]#[C-]	7.0	6

944	4{330,250,1}	CN(C)S(=O)(=O)C1=CN2C(C=C1)=NC(=C2N1)C1=CN(C)N=C1Br c:10,12,14,26,t:6,22	Z8808559863	1{330}	CN(C)S(=O)(=O)c1ccc(N)nc1	2{250}	Cn1cc(C=O)c(Br)n1	3{1}	[C-]#[N+]C1CC1	7.0	6
945	4{197,404,2}	CC(C)CS(=O)(=O)C1=CN2C(C=C1)=NC(C1=NN=C(C)N1)=C2NC1=CC=C(F)C=C1 c:11,13,22,31,t:7,16,18,26,28	Z8878918439	1{197}	CC(C)CS(=O)(=O)c1ccc(N)nc1	2{404}	Cc1nnc(C=O)[nH]1	3{2}	Fc1ccc([N+]#[C-])cc1	6.4	6
946	4{73,494,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC4=NC=CN4N23)C2=C(C1)N=CS2)C=C1 c:12,16,23,26,30,t:2,5,8,10,14	Z8878918470	1{73}	Nc1ccc2nccn2n1	2{494}	Clc1ncsc1C=O	3{20}	COc1ccc([N+]#[C-])c(C)c1	5.6	5
947	4{28,11,26}	FC1=CC=C(CNC2=C(N=C3C=C(C=CN23)C2=NOC=N2)C2=NN(CC(F)(F)F)C=C2)C=C1 c:11,13,21,32,35,t:1,3,7,9,18,24	Z8873685392	1{28}	Cl.Nc1cc(ccn1)c2ncon2	2{11}	FC(F)(F)Cn1ccc(C=O)n1	3{26}	Fc1ccc(C[N+]#[C-])cc1	6.2	5
948	4{403,495,26}	COC(=O)C1=NN2C(C=C1)=NC(=C2NCC1=C(C=C(F)C=C1)C1=C(C1)C=CC=N1 c:8,10,12,22,25,28,30,t:4,17,19	Z8778278034	1{403}	COC(=O)c1ccc(N)mn1	2{495}	Clc1cccnc1C=O	3{26}	Fc1ccc(C[N+]#[C-])cc1	5.5	5
949	4{188,496,62}	COC(=O)C1=CC(=CC(=C1)[N+])([O-])=O)C1=C(NC2(CCCC2)C(=O)OC)N2C(C=N)C=C2C(=O)OC)=N1 c:6,8,14,29,31,37,t:4	Z8854581134	1{188}	COC(=O)c1cnc(N)n1	2{496}	COC(=O)c1cc(C=O)cc(c1)[N+](=O)[O-]	3{62}	COC(=O)C1(CCCC1)[N+]#[C-]	6.1	5
950	4{94,497,43}	CCN1N=CC(C)=C1C1=C(NC2CCN(CC2)C(=O)OC(C)(C)C)N2N=C(F)C=CC2=N1 c:3,6,9,30,33,t:27	Z8878918795	1{94}	Nc1ccc(F)n1	2{497}	CCn1ncc(C)c1C=O	3{43}	CC(C)(C)OC(=O)N1CCC(CC1)[N+]#[C-]	5.3	4
951	4{354,108,71}	COC(=O)C1=CN2C(C=C1)=NC(=C2NC1=CC(OC)=CC=C1)C1=CN=C(N=C1)N1CCOCC1 c:8,10,12,20,22,27,29,t:4,16,25	Z8878918649	1{354}	COC(=O)c1ccc(N)nc1	2{108}	O=Cc1enc(nc1)N2CCOCC2	3{71}	COc1cccc([N+]#[C-])c1	5.5	4
952	4{267,498,23}	COC(=O)CCC(NC1=C(N=C2C=CC=C(C#C)N12)C1=C(Br)N=CS1)C(=O)OC c:12,21,24,t:8,10,14	Z8854581160	1{267}	Nc1cccc(C#C)n1	2{498}	BrC1ncsc1C=O	3{23}	COC(=O)CC(C[N+]#[C-])C(=O)OC	5.5	4
953	4{181,499,14}	COCCNC1=C(N=C2N1C=CC1=C2N=CC=N1)C1=C(OC)C(F)=C(I)C=C1 c:7,11,13,16,18,21,29,t:5,26	Z8878918786	1{181}	Nc1nccc2ncnc12	2{499}	COc1c(F)c(I)ccc1C=O	3{14}	COCC[N+]#[C-]	5.5	4
954	4{251,500,62}	COC(=O)C1(CCCC1)NC1=C(N=C2C=CC3=C(NC(=O)C=C3)N12)C1=CN=CS1 c:15,22,30,t:11,13,17,28	Z8878918867	1{251}	Nc1ccc2ccc(=O)[nH]c2n1	2{500}	O=Cc1cnsc1	3{62}	COC(=O)C1(CCCC1)[N+]#[C-]	4.3	4
955	4{223,501,34}	NC(=O)C1=NN2C(C=C1)=NC(=C2NCC1CCC(O)C1)C1=CC=C(C=C1)N1CCC1 c:7,9,11,24,26,t:3,22	Z8829498718	1{223}	NC(=O)c1ccc(N)mn1	2{501}	O=Cc1ccc(cc1)N2CCCC2	3{34}	[C-]#[N+]CC1CCC(O)1	3.9	4

956	4{194,502,49}	FC1(F)CC(C1)NC1=C(N=C2N1C=CN=C2N1C=CC=N1)C1=CC=C(C=C1)C1=CN=C1 c:10,14,16,20,22,27,29,35,t:8,25,32	Z8855739082	1{194}	Nc1ncnc1n2cccn2	2{502}	Cl.O=Cc1ccc(cc1)c2cn[nH]c2	3{49}	FC1(F)CC(C1)[N+]#[C-]	4.3	4
957	4{181,503,14}	COCCNC1=C(N=C2N1C=CC1=C2N=CC=N1)C1=CSC(Br)=N1 c:7,11,13,16,18,25,t:5,21	Z8878918553	1{181}	Nc1nccc2ncnc12	2{503}	BrC1nc(C=O)cs1	3{14}	COCC[N+]#[C-]	3.9	4
958	4{83,504,31}	CSCCNC1=C(N=C2C=CC(=CN12)P(C)(C)=O)C1=C(F)C(F)=C(Br)C=C1 c:9,11,20,27,t:5,7,24	Z8878918772	1{83}	CP(=O)(C)c1ccc(N)nc1	2{504}	Fc1c(F)c(C=O)ccc1Br	3{31}	CSCC[N+]#[C-]	4.5	4
959	4{73,137,11}	CC1=C(C(C)=NO1)C1=C(NCC2=CC(Br)=CC=C2)N2N3C=CN=C3C=CC2=N1 c:4,8,15,17,22,24,27,30,t:1,12	Z8878918842	1{73}	Nc1ccc2ncn2n1	2{137}	Cc1noc(C)c1C=O	3{11}	Br1cccc(C[N+]#[C-])c1	4.1	4
960	4{22,207,9}	CNC1=C(N=C2C=CC(Cl)=NN12)C1=CC(=N1)C(=O)OC c:6,9,16,t:2,4,14	Z8846491866	1{22}	Nc1ccc(Cl)nn1	2{207}	COC(=O)c1cc(C=O)n(C)n1	3{9}	C[N+]#[C-]	3.0	3
961	4{389,505,23}	COC(=O)CCC(NC1=C(N=C2N1C=C(C)C=C2)C1=CC=CN2N=CC=C12)C(=O)OC c:10,17,23,26,t:8,14,21,28	Z8878918448	1{389}	Cc1nc(N)c(C)c1	2{505}	O=Cc1cccn2nccc12	3{23}	COC(=O)CC(C[N+]#[C-])C(=O)OC	3.6	3
962	4{329,50,18}	COC1=CC=C(C)C2=NC([C@@H]3C[C@H]3C3OCCO3)=C(NC(C)(C)C)N12 &1:10,12,r,t:2,4,7,19	Z8873684730	1{329}	Cl.COc1ccc(C)c(N)n1	2{50}	O=C[C@@H]1C[C@H]1C2OCCO2 &1:2,4,r	3{18}	CC(C)(C)[N+]#[C-]	2.6	3
963	4{158,506,18}	CC(C)(C)NC1=C(N=C2C=NC(=CN12)P(C)(C)=O)C1=CC2=C(C=C1)N=CC(Br)=C2 c:9,11,22,24,27,30,t:5,7,20	Z8855739253	1{158}	CP(=O)(C)c1cnc(N)en1	2{506}	Br1enc2ccc(C=O)cc2c1	3{18}	CC(C)(C)[N+]#[C-]	3.4	3
964	4{193,319,10}	CNC(=O)C1=CN2C(NC3CCOC3)=C(N=C2C=C1)C1=C(C)C=C(OCC#N)C=C1 c:14,16,19,22,31,t:4,25	Z8878918349	1{193}	CNC(=O)c1ccc(N)nc1	2{319}	Cc1cc(OCC#N)ccc1C=O	3{10}	[C-]#[N+]C1CCOC1	2.8	3
965	4{288,148,39}	CCOCCNC1=C(N=C2C=C(NC(=O)OC(C)(C)C)C=CN12)C1=C(OC)N(C)N=C1C c:20,25,31,t:6,8,10	Z8810903014	1{288}	CC(C)(C)OC(=O)Nc1ccnc(N)c1	2{148}	COc1c(C=O)c(C)nn1C	3{39}	CCOCC[N+]#[C-]	3.0	2
966	4{404,110,29}	CCOC(=O)CCNC1=C(N=C2C=CC=C(OC(C)CC)N12)C1=CN=C(C=C1)P(C)(C)=O c:12,26,28,t:8,10,14,24	Z8878918631	1{404}	CCC(C)Oc1cccc(N)n1	2{110}	CP(=O)(C)c1ccc(C=O)cn1	3{29}	CCOC(=O)C[N+]#[C-]	3.0	2
967	4{334,363,11}	CC1=NC(=CN1)C1=C(NCC2=CC(Br)=CC=C2)N2C=C3COCCC3=C(C#N)C2=N1 c:3,7,14,16,32,t:1,11,20,27	Z8837933173	1{334}	Nc1ncc2COCCc2c1C#N	2{363}	Cc1nc(C=O)c[nH]1	3{11}	Br1cccc(C[N+]#[C-])c1	2.2	2

968	4{227,135,47}	CC(C)NC1=C(N=C2C=NC(Br)=C(Cl)N12)C1=C(C)N(C)N=C1C c:8,17,22,t:4,6,11	Z8810903047	1{227}	Nc1enc(Br)c(Cl)n1	2{135}	Cc1nm(C)c(C)c1C=O	3{47}	CC(C)[N+]#[C-]	1.4	1
969	4{19,227,37}	COC(=O)C1CC(C1)NC1=C(N=C2N1C=CC=C2C#N)C1=NC=CS1 c:12,16,18,25,t:10,23	Z8878918900	1{19}	Nc1ncccc1C#N	2{227}	O=Cc1nccs1	3{37}	COC(=O)C1CC(C1)[N+]#[C-]	0.0	0
970	4{376,507,12}	COC1=NC(Cl)=CN2C(NCC3CCOC3)=C(N=C12)C1=CC2=CN=CN2C=C1 c:5,16,26,30,t:2,18,22,24	Z8878918603	1{376}	COc1nc(Cl)cnc1N	2{507}	O=Cc1ccn2cncc2c1	3{12}	[C-]#[N+]CC1COC1	0.0	0
971	4{366,507,12}	COC1=CC=CN2C(NCC3CCOC3)=C(N=C12)C1=CC2=CN=CN2C=C1 c:4,15,25,29,t:2,17,21,23	Z8878918592	1{366}	COc1ccnc1N	2{507}	O=Cc1ccn2cncc2c1	3{12}	[C-]#[N+]CC1COC1	0.0	0
972	4{181,508,14}	COCCNC1=C(N=C2N1C=CC1=C2N=CC=N1)C1=CC=C(CN2CCOCC2)C=C1 c:7,11,13,16,18,33,t:5,21,23	Z8878918550	1{181}	Nc1nccc2nccnc12	2{508}	O=Cc1ccc(CN2CCOCC2)cc1	3{14}	COCC[N+]#[C-]	0.0	0
973	4{197,509,2}	CC(C)CS(=O)(=O)C1=CN2C(C=C1)=NC(=C2)NC1=CC=C(F)C=C1)C1=NN=CN1C c:11,13,15,24,29,t:7,19,21,27	Z8878918495	1{197}	CC(C)CS(=O)(=O)c1ccc(N)n1	2{509}	Cn1cnnc1C=O	3{2}	Fc1ccc([N+]#[C-])cc1	0.0	0
974	4{179,424,23}	COC(=O)CCC(NC1=C(N=C2C=C(OC)C=CN12)C1=NN(C)C(=N1)C(F)(F)C(=O)OC c:16,25,t:8,10,12,21	Z8878918337	1{179}	COc1ccnc(N)c1	2{424}	Cn1nc(C=O)nc1C(F)(F)F	3{23}	COC(=O)CC([N+]#[C-])C(=O)OC	0.0	0
975	4{389,510,23}	COC(=O)CCC(NC1=C(N=C2N1C=C(C)C=C2)C1=C(C)SC2=CN=CN12)C(=O)OC c:10,17,21,27,t:8,14,25	Z8878918322	1{389}	Cc1enc(N)c(C)c1	2{510}	Cc1sc2cnnc2c1C=O	3{23}	COC(=O)CC([N+]#[C-])C(=O)OC	0.0	0
976	4{179,81,23}	COC(=O)CCC(NC1=C(N=C2C=C(OC)C=CN12)C1=NC(=CC=C1)C(F)F)C(=O)OC c:16,23,25,t:8,10,12,21	Z8873684674	1{179}	COc1ccnc(N)c1	2{81}	FC(F)c1cccc(C=O)n1	3{23}	COC(=O)CC([N+]#[C-])C(=O)OC	0.0	0
977	4{213,191,31}	CCN1C=NN=C1C1=C(NCCSC)N2C(=N1)C(F)=CC=C2OC c:3,5,8,16,20,22	Z8873685469	1{213}	COc1ccc(F)c(N)n1	2{191}	CCn1cnnc1C=O	3{31}	CSCC[N+]#[C-]	0.0	0
978	4{405,511,1}	CC(NC(=O)OC(C)C)C1=C(NC2CC2)N2C=C(C=CC2=N1)N1CCCC1=O c:10,18,20,23	Z8829498661	1{405}	Nc1ccc(en1)N2CCCC2=O	2{511}	CC(NC(=O)OC(C)C)C=O	3{1}	[C-]#[N+]C1CC1	0.0	0
979	4{221,512,14}	COCCNC1=C(N=C2N1C(C)=CC=C2C#N)C1=NC=C(CN(C)C)S1 c:7,12,14,t:5,19,21	Z8829498460	1{221}	Cc1ccc(C#N)c(N)n1	2{512}	CN(C)Cc1ncc(C=O)s1	3{14}	COCC[N+]#[C-]	0.0	0
980	4{251,324,70}	CC(C)(C)OC(=O)N1CCC(C1)NC1=C(N=C2C=CC3=C(NC(=O)C=C3)N12)C1CC2(C1)CCO2 c:18,25,t:14,16,20	Z8854581157	1{251}	Nc1ccc2ccc(=O)[nH]c2n1	2{324}	O=CC1CC2(C1)CCCO2	3{70}	CC(C)(C)OC(=O)N1CCC(C1)[N+]#[C-]	0.0	0

981	4{198,464,14}	COCCNC1=C(N=C2C=NC(C#C)=C(Cl)N12)C1=CC2=C(C=CC=C2)N2N=NN=C12 c:9,23,25,29,t:5,7,13,19,21,31	Z8835022894	1{198}	Ne1cnc(C#C)c(Cl)n1	2{464}	O=Cc1cc2ccc2n3nnnc13	3{14}	COCC[N+][#][C-]	0.0	0
982	4{406,356,31}	CSCCNC1=C(N=C2C=CC=C(N12)C1=NN=N1)C1=CN(CC(C)C)N=N1 c:9,11,19,29,t:5,7,16,22	Z8855739251	1{406}	Ne1cccc(n1)c2nn[nH]n2	2{356}	CC(C)Cn1cc(C=O)nn1	3{31}	CSCC[N+][#][C-]	0.0	0
983	4{113,278,6}	CCOC(=O)CCNC1=C(N=C2N1C=CC=C2N1CCOCC1)C1=C(Br)N=NN1C c:11,15,17,27,30,t:9	Z8803896969	1{113}	Ne1ncccc1N2CCOCC2	2{278}	Cn1nnc(Br)c1C=O	3{6}	CCOC(=O)C CC[N+][#][C-]	0.0	0
984	4{318,273,12}	COC(=O)C1=CN2C(NCC3CCOC3)=C(N=C2C(OC)=N1)C1=C(Br)N(C)N=C1C c:15,17,22,25,30,t:4	Z8798985049	1{318}	COC(=O)c1cnc(N)c(OC)n1	2{273}	Cc1nn(C)c(Br)c1C=O	3{12}	[C-]][N+]CC1C COC1	0.0	0
985	4{340,513,23}	CCOC1=CC=CN2C(NC(CCC(=O)OC)C(=O)OC)=C(N=C12)C1=C(F)C=NC(F)=C1 c:5,20,26,29,32,t:3,22	Z8846492252	1{340}	CCOC1cccn1N	2{513}	Fc1cc(C=O)c(F)en1	3{23}	COC(=O)CC C([N+][#][C-])C(=O)OC	0.0	0
986	4{179,445,23}	COC(=O)CCC(NC1=C(N=C2C=C(OC)C=CN12)C1=NOC(=C1)C(C)C(C)C(=O)OC c:16,24,t:8,10,12,21	Z8846491733	1{179}	COc1ccnc(N)c1	2{445}	CC(C)(C)c1cc(C=O)no1	3{23}	COC(=O)CC C([N+][#][C-])C(=O)OC	0.0	0
987	4{211,47,41}	COC1=CC=C(NC2=C(CCOCC=C)N=C3N2C=CC=C3C2=NN=NN2)C=C1 c:7,15,19,21,26,30,t:2,4,24	Z8837933183	1{211}	Ne1ncccc1c2nnn[nH]2	2{47}	C=CCOCCC=O	3{41}	COc1ccc([N+][#][C-])cc1	0.0	0
988	4{262,139,12}	CC(=O)NC1=CN2C(C=C1)=NC(=C2NCC1CCOC1)C1=C(C)N(CCO)N=C1C c:8,10,12,23,30,t:4	Z8837933180	1{262}	CC(=O)Ne1ccc(N)nc1	2{139}	Cc1nn(CCO)c(C)c1C=O	3{12}	[C-]][N+]CC1C COC1	0.0	0
989	4{312,514,12}	O=C1NC(=O)C2=C(N1)N1C(C=C2)=NC(=C1NCC1CCOC1)C1=CC2=C3N(CCCC3=C1)CC2 c:5,11,13,15,35,t:26,28	Z8837933160	1{312}	Ne1ccc2c(=O)[nH]c(=O)[nH]c2n1	2{514}	O=Cc1cc2CCN3CCCc(c1)c32	3{12}	[C-]][N+]CC1C COC1	0.0	0
990	4{407,435,12}	CCCOC1=NC=CN2C(NCC3CCOC3)=C(N=C12)C1=CC(=NO)C(=O)OCC c:6,17,25,t:4,19,23	Z8837933152	1{407}	CCCOc1nccnc1N	2{435}	CCOC(=O)c1cc(C=O)on1	3{12}	[C-]][N+]CC1C COC1	0.0	0
991	4{144,515,53}	CNS(=O)(=O)C1=CN2C(NCCOCC3=CC=CC=C3)=C(N=C2C=C1)C1=NOC(CN(C)C)=C1 c:16,18,20,22,25,35,t:5,14,28	Z8837933145	1{144}	CNS(=O)(=O)c1ccc(N)nc1	2{515}	CN(C)Cc1cc(C=O)no1	3{53}	[C-]][N+]CCOC c1cccc1	0.0	0
992	4{5,26,17}	C(NC1=C(CCC2=CC=CC=C2)N=C2NN=NN12)C1CCOCC1 c:2,8,10,16,t:6,13	Z8711892497	1{5}	Ne1nnn[nH]1	2{26}	O=CCCc1ccc1	3{17}	[C-]][N+]CC1C COCC1	0.0	0

993	4{408,516,10}	COC1=C(Br)C=CC2=NC(=C(NC3CCOC3)N12)C1=NN(C)C(=N1)C1CC1 c:2,5,25,t:7,9,21	Z8878918788	1{408}	COc1nc(N)ccc1Br	2{516}	Cn1nc(C=O)nc1C2CC2	3{10}	[C-]#[N+]C1CCOC1	0.0	0
994	4{409,517,38}	CN1C=NN=C1C1=CC2=NC(C3=CC(=CS3)S(N)(=O)=O)=C(NC3=CC4=C(OCO4)C=C3)N2C=C1 c:2,4,14,32,37,t:7,9,12,21,24,26	Z8878918632	1{409}	Cn1cnn1c2ccnc(N)c2	2{517}	NS(=O)(=O)c1csc(C=O)c1	3{38}	[C-]#[N+]c1ccc2OCOc2c1	0.0	0
995	4{410,518,62}	COC(=O)C1(CCCC1)NC1=C(N=C2C=CC3=C(N=CC(Cl)=C3)N12)C1=C(C)N=CN1 c:15,19,22,28,31,t:11,13,17	Z8878918579	1{410}	Nc1ccc2cc(Cl)nc2n1	2{518}	Cc1nc[nH]c1C=O	3{62}	COC(=O)C1(CCCC1)[N+]#[C-]	0.0	0
996	4{408,519,12}	COC1=C(Br)C=CC2=NC(=C(NCC3CCOC3)N12)C1=CN=C(S1)C(F)F c:2,5,24,t:7,9,22	Z8878918551	1{408}	COc1nc(N)ccc1Br	2{519}	FC(F)c1ncc(C=O)s1	3{12}	[C-]#[N+]CC1CCOC1	0.0	0
997	4{251,271,71}	COC1=CC(NC2=C(N=C3C=CC4=C(NC(=O)C=C4)N23)C2=NN(C)N=N2)=CC=C1 c:10,17,27,29,31,t:2,6,8,12,23	Z8878918383	1{251}	Nc1ccc2ccc(=O)[nH]c2n1	2{271}	Cn1nnc(C=O)n1	3{71}	COc1cccc([N+]#[C-])c1	0.0	0
998	4{411,103,37}	COC(=O)C1CC(C1)NC1=C(N=C2C=C(Br)C=C(F)N12)C1CCC2(COC2)OC1 t:10,12,14,17	Z8873684672	1{411}	Nc1cc(Br)cc(F)n1	2{103}	O=CC1CCC2(COC2)OC1	3{37}	COC(=O)C1CC(C1)[N+]#[C-]	0.0	0
999	4{412,520,10}	COC1=C(C=NN=C1)C1=C(NC2CCOC2)N2C=C(Br)C(CO)=CC2=N1 c:4,6,9,24,27,t:2,19	Z8873684643	1{412}	Nc1cc(CO)cc(Br)n1	2{520}	COc1cnncc1C=O	3{10}	[C-]#[N+]C1CCOC1	0.0	0
1000	4{340,478,5}	CCOC1=CC=CN2C(NCCCOC)=C(N=C12)C1=CN(C)C(=O)C2=C1C=CN=C2 c:5,14,26,29,31,t:3,16,20	Z8873685464	1{340}	CCOc1cccn1N	2{478}	Cn1cc(C=O)c2ccncc2c1=O	3{5}	COCCC[N+]#[C-]	0.0	0
1001	4{413,521,22}	FC(F)(F)C1=CC2=NC(=C(NC3COC3)N2N=C1)C1=C(Br)C=NC(Br)=C1 c:18,21,24,27,t:4,6,8	Z8873685394	1{413}	Nc1cc(cnn1)C(F)(F)F	2{521}	Brcc1cc(C=O)c(Br)n1	3{22}	[C-]#[N+]C1COC1	0.0	0
1002	4{329,191,7}	CCN1C=NN=C1C1=C(NC2CCOCC2)N2C(=N1)C(C)=CC=C2OC c:3,5,8,19,23,25	Z8873685376	1{329}	Cl.COc1ccc(C)c(N)n1	2{191}	CCn1cnn1C=O	3{7}	[C-]#[N+]C1CCOCC1	0.0	0
1003	4{37,520,24}	COC1=CC(CNC2=C(N=C3C=CC=C(C(F)F)N23)C2=C(OC)C=NN=C2)=CC=C1 c:11,21,25,27,29,31,t:2,7,9,13	Z8873684890	1{37}	Cl.Nc1cccc(n1)C(F)F	2{520}	COc1cnncc1C=O	3{24}	COc1cccc(C[N+]#[C-])c1	0.0	0
1004	4{48,173,15}	CCNC1=C(N=C2C=C(C=CN12)S(C)(=O)=O)C1=NC(=NN1C)C(F)(F)F c:7,9,20,t:3,5,18	Z8873684636	1{48}	CS(=O)(=O)c1cnc(N)c1	2{173}	Cn1nc(nc1C=O)C(F)(F)F	3{15}	CC[N+]#[C-]	0.0	0

1005	4{348,404,2}	CC1=NN=C(N1)C1=C(NC2=CC=C(F)C=C2)N2C=C(F)N=CC2=N1 c:3,7,15,22,25,t:1,10,12,19	Z8873684580	1{348}	Nc1cnc(F)c n1	2{404}	Cc1mnc(C=O) [nH]1	3{2}	Fe1ccc([N+] #[C-])cc1	0.0	0
1006	4{251,522,70}	COC1=C(C=C(C)C=N1)C1=C(NC2CCN(C2)C(=O)OC(C)(C)C)N2C(C=CC3=C2NC(=O)C=C3)=N1 c:7,10,28,30,36,38,t:2,4	Z8873684826	1{251}	Nc1ccc2ccc (=O)[nH]c2 n1	2{522}	COc1ncc(C)c c1C=O	3{70}	CC(C)(C)OC (=O)N1CCCC (C1)[N+]#[C-]	0.0	0
1007	4{169,523,13}	CNC(=O)C1=NN2C(C=C1)=NC(=C2NCC1=C C=C(OC)C=C1)C1=C(F)C(OC)=CC=C1 c:8,10,12,23,26,31,33,t:4,17,19	Z8829498665	1{169}	CNC(=O)c1 ccc(N)nn1	2{523}	COc1cccc(C =O)c1F	3{13}	COc1ccc(C[N+]#[C-])cc1	0.0	0
1008	4{378,524,12}	FC1=NC(F)=C(F)C(=C1)C1=C(NCC2CCOC2) N2C=CC=C(OCC3=CN=CC=C3)C2=N1 c:7,10,21,29,31,35,t:1,4,23,27	Z8829498545	1{378}	Nc1ncccc1 OCc2ccnc 2	2{524}	Fe1cc(C=O)c (F)c(F)n1	3{12}	[C-]#[N+]CC1C COC1	0.0	0
1009	4{223,382,50}	COC(C)(C)CC1=C(NC2=CC3=C(OCCO3)C=C2)N2N=C(C=CC2=N1)C(N)=O c:6,18,22,24,27,t:9,11	Z8829498488	1{223}	NC(=O)c1c cc(N)nn1	2{382}	COC(C)(C)C C=O	3{50}	[C-]#[N+]c1ccc 2OCCOc2c1	0.0	0
1010	4{223,525,66}	CC(NC1=C(N=C2C=CC(=NN12)C(N)=O)C1=C (Br)C=NC=C1F)C1=CC=CC=C1 c:7,9,17,20,22,28,30,t:3,5,26	Z8835022910	1{223}	NC(=O)c1c cc(N)nn1	2{525}	Fe1cncc(Br)c 1C=O	3{66}	CC([N+]#[C-)c1cccc1	0.0	0
1011	4{69,526,21}	CNC(=O)C1=CC2=NC(=C(NCC3CC3)N2C=C1) C1=CN2N=CC(C(N)=O)=C2N=C1 c:18,24,29,32,t:4,6,8,21	Z8835022893	1{69}	CNC(=O)c1 ccnc(N)c1	2{526}	NC(=O)c1en n2cc(C=O)en c12	3{21}	[C-]#[N+]CC1C C1	0.0	0
1012	4{231,408,33}	COC1=C(CNC2=C(CCN3CCOC3=O)N=C3C=CC(=NN23)C(F)(F)F)C=CC=C1 c:2,6,19,21,30,32,t:17	Z8855739158	1{231}	Nc1ccc(nn1) C(F)(F)F	2{408}	O=CCCN1C COC1=O	3{33}	COc1cccc1 C[N+]#[C-]	0.0	0
1013	4{158,527,7}	CC(C)(C)OC(=O)N1CC[C@@H](CC2=C(NC3CCOCC3)N3C=C(N=CC3=N2)P(C)(C)=O)C1 c:12,23,25,28	Z8846492320	1{158}	CP(=O)(C)c 1cnc(N)en1	2{527}	CC(C)(C)OC (=O)N1CC[C @@H](CC=O)C1	3{7}	[C-]#[N+]C1CC OCC1	0.0	0
1014	4{383,528,1}	CN1N=C(C)C(Cl)=C1C1=C(NC2CC2)N2N=C (C=CC2=N1)C1=NC=CC=C1 c:6,9,17,19,22,27,29,t:2,25	Z8837933181	1{383}	Nc1ccc(nn1) c2cccn2	2{528}	Cc1m(C)c(C =O)c1Cl	3{1}	[C-]#[N+]C1CC 1	0.0	0
1015	4{399,477,22}	CC(C)OC1=NN2C(C=C1)=NC(C(NC(=O)OC(C)(C)C)C1COC1)=C2NC1COC1 c:8,10,26,t:4	Z8837933163	1{399}	CC(C)Oc1c cc(N)nn1	2{477}	CC(C)(C)OC (=O)NC(C=O)C1COC1	3{22}	[C-]#[N+]C1CO C1	0.0	0

1016	4{2,15,54}	COC1=CC=C(C=C1)C1=C(NC2=CC=CC=C2)N2OC=CC2=N1 c:4,6,9,14,16,21,24,t:2,12	Z8711891895	1{2}	Nc1cccon1	2{15}	COc1ccc(C=O)cc1	3{54}	[C-] #[N+]c1cccc1	0.0	0
1017	4{181,529,6}	CCOC(=O)CCCN1=C(N=C2N1C=CC1=C2N=CC=N1)C1=CC(CI)=C(C=C1)S(N)(=O)=O c:11,15,17,20,22,28,30,t:9,25	Z8878918889	1{181}	Nc1nccc2ncenc12	2{529}	NS(=O)(=O)c1ccc(C=O)c1Cl	3{6}	CCOC(=O)C CC[N+]#[C-]	0.0	0
1018	4{414,281,48}	COC(=O)C1=NN=C(C=C1)C1=C(NC2CCCN(C2)C(=O)OC(C)(C)C)N2C=C(CI)N=CC2=N1 c:6,8,11,32,35,t:4,29	Z8878918817	1{414}	Nc1enc(Cl)en1	2{281}	COC(=O)c1ccc(C=O)nn1	3{48}	CC(C)(C)OC (=O)N1CCC C(C1)[N+]#[C-]	0.0	0
1019	4{388,530,39}	CCOCCN1=C(N=C2C=C3CCOC3=CN12)C1CC2(CC(C2)OC)C1 c:17,t:6,8,10	Z8878918764	1{388}	Cl.Nc1cc2C CCOc2en1	2{530}	COC1CC2(C1)CC(C2)C=O	3{39}	CCOCC[N+]# [C-]	0.0	0
1020	4{415,531,10}	CC1=NC=C(C=N1)C1=C(NC2CCOC2)N2C(=N1)C(CCl)=CC=C2Br c:3,5,8,18,23,25,t:1	Z8878918581	1{415}	Cl.Nc1nc(Br)ccc1CC1	2{531}	Cc1ncc(C=O)en1	3{10}	[C-] #[N+]C1CC OC1	0.0	0
1021	4{416,532,23}	COC(=O)CCC(NC1=C(N=C2C=C(CCl)C=CN12)C1=C(OC)C(OC)=NC=N1)C(=O)OC c:16,21,27,29,t:8,10,12	Z8873684772	1{416}	Cl.Nc1cc(CCl)ccn1	2{532}	COc1ncc(C=O)c1OC	3{23}	COC(=O)CC C([N+]#[C-]) C(=O)OC	0.0	0
1022	4{83,464,7}	CP(C)(=O)C1=CN2C(C=C1)=NC(=C2NC1CCOCC1)C1=CC2=C(C=CC=C2)N2N=NN=C12 c:8,10,12,27,29,33,t:4,23,25,35	Z8873684678	1{83}	CP(=O)(C)c1ccc(N)nc1	2{464}	O=Cc1cc2ccc2n3nnc13	3{7}	[C-] #[N+]C1CC OCC1	0.0	0
1023	4{409,533,38}	CCC1=CC(=NO1)C1=C(NC2=CC3=C(OCO3)C=C2)N2C=CC(=CC2=N1)C1=NN=CN1C c:4,8,19,23,25,28,33,t:2,11,13,31	Z8873685397	1{409}	Cn1ennc1c2cenc(N)c2	2{533}	CCc1cc(C=O)no1	3{38}	[C-] #[N+]c1cccc 2OCOc2c1	0.0	0
1024	4{329,534,7}	COC1=CC=C(C)C2=NC(C3=NN(C=C3)C(C)C)=C(NC3CCOCC3)N12 c:13,t:2,4,7,10,18	Z8873685344	1{329}	Cl.COc1ccc(C)c(N)n1	2{534}	CC(C)n1ccc(C=O)n1	3{7}	[C-] #[N+]C1CC OCC1	0.0	0
1025	4{179,535,5}	COCCCN1=C(N=C2C=C(OC)C=CN12)C1=NOC(=C1)C(C)C)O c:14,22,t:6,8,10,19	Z8873685310	1{179}	COc1cenc(N)c1	2{535}	CC(C)(O)c1ccc(C=O)no1	3{5}	COCCC[N+]# [C-]	0.0	0
1026	4{89,271,71}	COC1=CC(NC2=C(N=C3C=CC4=C(NN=C4)N23)C2=NN(C)N=N2)=CC=C1 c:10,15,25,27,29,t:2,6,8,12,21	Z8873684617	1{89}	Nc1ccc2cn[nH]c2n1	2{271}	Cn1nnc(C=O)n1	3{71}	COc1cccc([N+]# [C-])c1	0.0	0
1027	4{408,536,12}	COC1=C(Br)C=CC2=NC(C3=CN=C(O3)C3COCC3)=C(NCC3CCOC3)N12 c:2,5,12,t:7,10,22	Z8873684800	1{408}	COc1nc(N)ccc1Br	2{536}	O=Cc1enc(o1)C2CCOCC2	3{12}	[C-] #[N+]CC1C COC1	0.0	0

1028	4{68,537,1}	COC(=O)C1=CN=C(C=C1)C1=C(NC2CC2)N2C=CC(=CC2=N1)C#C c:6,8,11,19,21,24,t:4	Z8829498778	1{68}	Nc1cc(C#C)ccn1	2{537}	COC(=O)c1ccc(C=O)nc1	3{1}	[C-]#[N+]C1CC1	0.0	0
1029	4{151,17,9}	CCOC1=CN=C(N=C1)C1=C(NC)N2C(C=NC=C2C1)=N1 c:5,7,10,16,18,21,t:3	Z8829498592	1{151}	Nc1cnc(C1)n1	2{17}	CCOc1cnc(C=O)nc1	3{9}	C[N+]#[C-]	0.0	0
1030	4{181,538,11}	CN1C=NC=C1C1=C(NCC2=CC(Br)=CC=C2)N2C=CC3=C(N=CC=N3)C2=N1 c:2,4,7,14,16,20,24,26,30,t:11,22	Z8854581173	1{181}	Nc1nccc2nccnc12	2{538}	Cn1cnc1C=O	3{11}	Br1cccc(C[N+]#[C-])c1	0.0	0
1031	4{334,98,13}	COC1=CC=C(CNC2=C(N=C3N2C=C2COCC2=C3C#N)C2=NC=C(OC)N=C2)C=C1 c:10,21,32,35,t:2,4,8,14,26,28	Z8835022915	1{334}	Nc1ncc2COCCc2c1C#N	2{98}	COc1cnc(C=O)nc1	3{13}	COc1ccc(C[N+]#[C-])cc1	0.0	0
1032	4{223,539,50}	NC(=O)C1=NN2C(C=C1)=NC([C@@H]1CC[C@H]1C(F)(F)F)=C2NC1=CC2=C(OCCO2)C=C1 &l:11,16,r,c:7,9,22,35,t:3,26,28	Z8835022898	1{223}	NC(=O)c1ccc(N)nn1	2{539}	FC(F)(F)[C@@H]1CCC[C@H]1C=O &l:4,9,r	3{50}	[C-]#[N+]c1ccc2OCCOc2c1	0.0	0
1033	4{223,540,66}	CC(NC1=C(N=C2C=CC(=NN12)C(N)=O)C1C)CC2CN(CC12)C(=O)OC(C)(C)C1=CC=CC=C1 c:7,9,36,38,t:3,5,34	Z8835022885	1{223}	NC(=O)c1ccc(N)nn1	2{540}	CC(C)(C)OC(=O)N1CC2CCC(C=O)C2C1	3{66}	CC([N+]#[C-])c1cccc1	0.0	0
1034	4{417,515,49}	CN(C)CC1=CC(=NO1)C1=C(NC2CC(F)(F)C2)N2C=C(Cl)C(=CC2=N1)C(F)(F)F c:6,10,24,27,t:4,21	Z8849597801	1{417}	Cl.Nc1cc(c(Cl)cn1)C(F)(F)F	2{515}	CN(C)Cc1cc(C=O)no1	3{49}	FC1(F)CC(C1)[N+]#[C-]	0.0	0
1035	4{406,541,35}	CSCCCNC1=C(N=C2C=CC=C(N12)C1=NNN=N1)C1=C(C)N(N=C1C)C(C)C c:10,12,20,23,27,t:6,8,17	Z8855739120	1{406}	Nc1cccc(n1)c2nn[nH]n2	2{541}	CC(C)n1nc(C)c(C=O)c1C	3{35}	CSCCC[N+]#[C-]	0.0	0
1036	4{128,200,23}	COCCN(C)C1=CN2C(C=C1)=NC(CCCC#CC)=C2NC(CCC(=O)OC)C(=O)OC c:10,12,20,t:6	Z8808559870	1{128}	COCCN(C)c1ccc(N)nc1	2{200}	CC#CCCCC=O	3{23}	COC(=O)CC(C[N+]#[C-])C(=O)OC	0.0	0
1037	4{223,194,29}	CCOC(=O)CCNC1=C(N=C2C=CC(=NN12)C(N)=O)C1=CC=C(N1C)C(=O)OC c:12,14,24,t:8,10,22	Z8798985052	1{223}	NC(=O)c1ccc(N)nn1	2{194}	COC(=O)c1ccc(C=O)n1C	3{29}	CCOC(=O)C(C[N+]#[C-])	0.0	0
1038	4{73,79,9}	CNC1=C(N=C2C=CC3=NC=CN3N12)C1=NC=CO1 c:6,10,19,t:2,4,8,17	Z8846491979	1{73}	Nc1ccc2nccn2n1	2{79}	O=Cc1ncco1	3{9}	C[N+]#[C-]	0.0	0
1039	4{312,522,38}	COC1=C(C=C(C)C=N1)C1=C(NC2=CC3=C(OCO3)C=C2)N2C(C=CC3=C2NC(=O)NC3=O)=N1 c:7,10,21,26,28,37,t:2,4,13,15	Z8837933184	1{312}	Nc1ccc2c(=O)[nH]c(=O)[nH]c2n1	2{522}	COc1ncc(C)c1C=O	3{38}	[C-]#[N+]c1ccc2OCOc2c1	0.0	0

1040	4{83,542,18}	CC(C)(C)NC1=C(N=C2C=CC(=CN12)P(C)(C)=O)C1N(CC1CCC1)C(=O)OC(C)(C)C c:9,11,t:5,7	Z8837933158	1{83}	CP(=O)(C)c1ccc(N)nc1	2{542}	CC(C)(C)OC(=O)N1CC2(CCC2)C1C=O	3{18}	CC(C)(C)[N+][C-]	0.0	0
1041	4{271,8,62}	COCC1=NOC=C1C1=C(NC2(CCCC2)C(=O)OC)N2C(C=CC(C(=O)OC)=C2F)=N1 c:6,9,24,30,33,t:3	Z8837933155	1{271}	COC(=O)c1ccc(N)nc1F	2{8}	COCc1nocclC=O	3{62}	COC(=O)C1(CCCC1)[N+][C-]	0.0	0
1042	4{181,340,14}	CCN1C=NC(=N1)C1=C(NCCOC)N2C=CC3=C(N=CC=N3)C2=N1 c:3,5,8,16,20,22,26,t:18	Z8855619535	1{181}	Nc1nccc2ncnc12	2{340}	CCn1enc(C=O)n1	3{14}	COCC[N+][C-]	0.0	0
1043	4{111,543,15}	CCNC1=C(N=C2N1C=C(C=C2C)C(=O)OC)C(=O)OCC c:5,9,11,t:3	Z8878918801	1{111}	COC(=O)c1cnc(N)c(C)c1	2{543}	CCOC(=O)C=O	3{15}	CC[N+][C-]	0.0	0
1044	4{176,512,14}	COCCNC1=C(N=C2N1C=CN=C2N1CCCC1)C1=NC=C(CN(C)C)S1 c:7,11,13,t:5,22,24	Z8878918774	1{176}	Nc1ncnc1N2CCCC2	2{512}	CN(C)Cc1enc(C=O)s1	3{14}	COCC[N+][C-]	0.0	0
1045	4{188,329,71}	COC(=O)C1=CN=CC2=NC(=C(NC3=CC(OC)=CC=C3)N12)C1=C(C)N(CCC1)N=C1C c:6,17,19,25,32,t:4,8,10,13	Z8878918673	1{188}	COC(=O)c1cnc(N)n1	2{329}	Cc1nn(CCC1)c(C)c1C=O	3{71}	COC1cccc([N+][C-])c1	0.0	0
1046	4{193,544,72}	CNC(=O)C1=CN2C(C=C1)=NC(=C2NC1=C(C)C=C(F)C=C1)C1=NN=C2CCCN12 c:8,10,12,16,22,t:4,19,25,27	Z8878918671	1{193}	CNC(=O)c1ccc(N)nc1	2{544}	O=Cc1nnc2C(Cc1)N2	3{72}	Cc1cc(F)ccc1[N+][C-]	0.0	0
1047	4{240,545,32}	COCCN1N=C(C)C(=C1C)C1=C(NC2CCC2)N2C=C(C=CC2=N1)C1=NN=N1 c:8,12,21,23,26,32,t:5,29	Z8878918647	1{240}	Nc1ccc(en1)c2nn[nH]n2	2{545}	COCCn1nc(C)c(C=O)c1C	3{32}	[C-][N+]C1CC1	0.0	0
1048	4{251,546,62}	COC(=O)C1(CCCC1)NC1=C(N=C2C=CC3=C(NC(=O)C=C3)N12)C1=C(C)N(C)C(C)=C1C c:15,22,28,34,t:11,13,17	Z8878918476	1{251}	Nc1ccc2ccc(=O)[nH]c2n1	2{546}	Cc1c(C)n(C)c(C)c1C=O	3{62}	COC(=O)C1(CCCC1)[N+][C-]	0.0	0
1049	4{413,547,22}	FC(F)(F)C1=NC(Br)=C(S1)C1=C(NC2COC2)N2N=CC(=CC2=N1)C(F)(F)F c:7,11,20,22,25,t:4	Z8873684720	1{413}	Nc1cc(cnn1)C(F)(F)F	2{547}	FC(F)(F)c1nc(Br)c(C=O)s1	3{22}	[C-][N+]C1CO1	0.0	0
1050	4{404,320,29}	CCOC(=O)CCNC1=C(N=C2C=CC=C(OC(C)CC)N12)C1=NN(C)C=N1 c:12,28,t:8,10,14,24	Z8873684653	1{404}	CCC(C)Oc1cccc(N)n1	2{320}	Cn1enc(C=O)n1	3{29}	CCOC(=O)C[N+][C-]	0.0	0
1051	4{418,293,23}	COC(=O)CCC(NC1=C(N=C2C=C(CBr)C=CN12)C1=C(F)N(C)N=C1)C(=O)OC c:16,21,26,t:8,10,12	Z8829498702	1{418}	Br.Nc1cc(CBr)ccn1	2{293}	Cn1ncc(C=O)c1F	3{23}	COC(=O)CC([N+][C-])C(=O)OC	0.0	0

1052	4{283,548,2}	COC(=O)C1=CC2=C(N=C1)N1C(C=C2)=NC(CCC2=NC=CN=C2)=C1NC1=CC=C(F)C=C1 c:6,8,13,15,22,24,26,35,t:4,20,30,32	Z8829498469	1{283}	COC(=O)c1cnc2nc(N)ccc2c1	2{548}	O=CCCc1cnccn1	3{2}	Fc1ccc([N+]#[C-])cc1	0.0	0
1053	4{107,520,21}	COC1=C(C=NN=C1)C1=C(NCC2CC2)N2C=C(OCCO)C=CC2=N1 c:4,6,9,24,27,t:2,18	Z8854581165	1{107}	Nc1ccc(OC CO)cn1	2{520}	COc1cnncc1C=O	3{21}	[C-]#[N+]CC1CC1	0.0	0
1054	4{419,425,21}	CS(=O)(=O)N1CCCC(C1)C1=C(NCC2CC2)N2C(C=CC(C#C)=C2F)=N1 c:11,21,25,28	Z8854581152	1{419}	Nc1ccc(C#C)c(F)n1	2{425}	CS(=O)(=O)N1CCCC(C1)C=O	3{21}	[C-]#[N+]CC1CC1	0.0	0
1055	4{62,278,6}	CCOC(=O)CCCNC1=C(N=C2C=C(CO)C=CN12)C1=C(Br)N=NN1C c:17,22,25,t:9,11,13	Z8835022869	1{62}	Nc1cc(CO)ccn1	2{278}	Cn1nnc(Br)c1C=O	3{6}	CCOC(=O)CC[N+]#[C-]	0.0	0
1056	4{262,323,12}	CC(=O)NC1=CN2C(NCC3CCOC3)=C(N=C2C=C1)[C@@H]1C[C@@H](C1)NC(=O)OC(C)(C)C r,c:15,17,20,t:4	Z8837933177	1{262}	CC(=O)Nc1ccc(N)nc1	2{323}	CC(C)(C)OC(=O)N[C@H]1C[C@H](C1)C=O	3{12}	[C-]#[N+]CC1CCOC1	0.0	0
1057	4{364,478,5}	COCCCN1=C(N=C2C=CC(=CN12)N1CCNC(=O)C1)C1=CN(C)C(=O)C2=C1C=CN=C2 c:10,12,31,34,36,t:6,8,25	Z8837933150	1{364}	Nc1ccc(en1)N2CCNC(=O)C2	2{478}	Cn1cc(C=O)c2ccncc2c1=O	3{5}	COCCC[N+]#[C-]	0.0	0
1058	4{409,549,73}	COC(=O)C1=NC=C(C2=C(NC3=C(OC)C=C(OC)C=C3)N3C=CC(=CC3=N2)C2=NN=CN2C)C(C)=C1 c:8,11,19,23,25,28,33,39,t:4,6,15,31	Z8837933147	1{409}	Cn1cnncc2ccnc(N)c2	2{549}	COC(=O)c1cc(C)c(C=O)cn1	3{73}	COc1ccc([N+]#[C-])c(OC)c1	0.0	0
1059	4{179,550,1}	COC1=CC2=NC(=C(NC3CC3)N2C=C1)C1=NC(Br)=NN1C c:15,21,t:2,4,6,18	Z8855619768	1{179}	COc1ccnc(N)c1	2{550}	Cn1nc(Br)nc1C=O	3{1}	[C-]#[N+]C1CC1	0.0	0
1060	4{420,324,70}	CC(C)(C)OC(=O)N1CCC(C1)NC1=C(N=C2C=CC3=C(NC=N3)N12)C1CC2(C1)CCCO2 c:18,23,t:14,16,20	Z8878918829	1{420}	Cl.Cl.Nc1cc2nc[nH]c2n1	2{324}	O=CC1CC2(C1)CCCO2	3{70}	CC(C)(C)OC(=O)N1CCC(C1)[N+]#[C-]	0.0	0
1061	4{376,435,12}	CCOC(=O)C1=NOC(=C1)C1=C(NCC2CCOC2)N2C=C(C1)N=C(OC)C2=N1 c:8,11,30,t:5,22,25	Z8878918770	1{376}	COc1nc(Cl)cnc1N	2{435}	CCOC(=O)c1cc(C=O)on1	3{12}	[C-]#[N+]CC1CCOC1	0.0	0
1062	4{141,551,35}	CSCCCN1=C(N=C2C=C(NC(C)=O)C=CN12)C1CC1(Br)Br c:16,t:6,8,10	Z8878918596	1{141}	CC(=O)Nc1ccnc(N)c1	2{551}	BrC1(Br)CC1C=O	3{35}	CSCCC[N+]#[C-]	0.0	0

1063	4{187,507,12}	C1C1=CN2C(C=C1C#N)=NC(=C2NCC1CCO C1)C1=CC2=CN=CN2C=C1 c:5,9,11,26,30,t:1,22,24	Z8878918538	1{187}	Nc1cc(C#N)(Cl)cn1	2{507}	O=Cc1ccn2c ncc2c1	3{12}	[C-]#[N+]CC1C COC1	0.0	0
1064	4{401,341,39}	CCOCCNC1=C(N=C2C=CC3=C(N=CC=C3Cl N12)C1=CN=C(S1)C(C)O c:10,14,16,25,t:6,8,12,23	Z8878918509	1{401}	Nc1ccc2c(C l)ccnc2n1	2{341}	CC(O)c1ncc(C=O)s1	3{39}	CCOCC[N+] #[C-]	0.0	0
1065	4{19,552,37}	COC(=O)C1CC(C1)NC1=C(N=C2N1C=CC=C 2C#N)C1=CN=C(C=C1)C#C c:12,16,18,25,27,t:10,23	Z8878918485	1{19}	Nc1ncccc1 C#N	2{552}	O=Cc1ccc(C #C)nc1	3{37}	COC(=O)C1 CC(C1)[N+] #[C-]	0.0	0
1066	4{251,217,62}	COC(=O)C1(CCCC1)NC1=C(N=C2C=CC3=C (NC(=O)C=C3)N12)C1=CC(=O)N(C)C=C1 c:15,22,34,t:11,13,17,28	Z8878918355	1{251}	Nc1ccc2ccc (=O)[nH]c2 n1	2{217}	Cn1ccc(C=O)cc1=O	3{62}	COC(=O)C1(CCCC1)[N+] #[C-]	0.0	0
1067	4{411,55,37}	COC(=O)C1CC(C1)NC1=C(N=C2C=C(Br)C= C(F)N12)C1=CC(=NC=C1)P(C)(C)=O c:25,27,t:10,12,14,17,23	Z8873684748	1{411}	Nc1cc(Br)c c(F)n1	2{55}	CP(=O)(C)c1 cc(C=O)cn1	3{37}	COC(=O)C1 CC(C1)[N+] #[C-]	0.0	0
1068	4{72,553,12}	COC1=NC(Br)=CN2C(NCC3CCOC3)=C(N=C 12)C1=CSC(=C1)C1OCCO1 c:5,16,25,t:2,18,22	Z8873684745	1{72}	COc1nc(Br) cnc1N	2{553}	O=Cc1esc(c1)C2OCCO2	3{12}	[C-]#[N+]CC1C COC1	0.0	0
1069	4{421,543,15}	CCNC1=C(N=C2C=CC(C(=O)OC)=C(C1)N12) C(=O)OCC c:7,t:3,5,13	Z8873684725	1{421}	COC(=O)c1 ccc(N)nc1C 1	2{543}	CCOC(=O)C =O	3{15}	CC[N+]#[C-]	0.0	0
1070	4{188,492,71}	COC(=O)C1=CN=CC2=NC(=C(NC3=CC(OC) =CC=C3)N12)C1=C(C)N=C(C)C(C)=N1 c:6,17,19,25,32,t:4,8,10,13,28	Z8873684709	1{188}	COC(=O)c1 cncc(N)n1	2{492}	Cc1nc(C)c(C =O)nc1C	3{71}	COc1cccc([N +]#[C-])c1	0.0	0
1071	4{251,372,71}	COC1=CC(NC2=C(N=C3C=CC4=C(NC(=O)C =C4)N23)C2=NN(C)N=C2C)=CC=C1 c:10,17,27,30,32,t:2,6,8,12,23	Z8873685367	1{251}	Nc1ccc2ccc (=O)[nH]c2 n1	2{372}	Cc1nn(C)nc1 C=O	3{71}	COc1cccc([N +]#[C-])c1	0.0	0
1072	4{372,526,46}	CC(=C)CNC1=C(N=C2N1C=CC=C2OCC1=C C=NC=C1)C1=CN2N=CC(C(N)=O)=C2N=C1 c:7,11,13,20,22,28,33,36,t:5,18,25	Z8873684842	1{372}	Nc1ncccc1 OCc2ccncc 2	2{526}	NC(=O)c1cn n2cc(C=O)cn c12	3{46}	CC(=C)C[N+] #[C-]	0.0	0
1073	4{119,544,72}	CC1=C(NC2=C(N=C3C=CC(=CN23)C#N)C2 =NN=C3CCCN23)C=CC(F)=C1 c:1,8,10,27,30,t:4,6,17,19	Z8873684824	1{119}	Nc1ccc(C# N)cn1	2{544}	O=Cc1mnc2C CCn12	3{72}	Cc1cc(F)ccc 1[N+]#[C-]	0.0	0
1074	4{329,92,31}	COC1=CC=C(C)C2=NC(C3=CC(C)=NO3)=C(NCCSC)N12 c:13,t:2,4,7,10,16	Z8873684801	1{329}	Cl.COc1ccc (C)c(N)n1	2{92}	Cc1cc(C=O) on1	3{31}	CSCC[N+]#[C-]	0.0	0
1075	4{213,340,31}	CCN1C=NC(=N1)C1=C(NCCSC)N2C(=N1)C(F)=CC=C2OC c:3,5,8,16,20,22	Z8829498705	1{213}	COc1ccc(F) c(N)n1	2{340}	CCn1cnc(C= O)n1	3{31}	CSCC[N+]#[C-]	0.0	0

1076	4{128,554,1}	COCCN(C)C1=CN2C(C=C1)=NC(=C2NC1CC1)C1=C(CO)C=CC=C1 c:10,12,14,22,26,28,t:6	Z8829498587	1{128}	COCCN(C) c1ccc(N)nc 1	2{554}	OCc1cccc1 C=O	3{1}	[C-] #[N+]C1CC 1	0.0	0
1077	4{158,555,7}	CC1=NN(C(C)=C1C1=C(NC2CCOCC2)N2C=C(N=CC2=N1)P(C)(C)=O)C1=NC=CC=C1 c:5,8,19,21,24,33,35,t:1,31	Z8854581148	1{158}	CP(=O)(C)c 1cnc(N)cn1	2{555}	Cc1nn(c(C)c 1C=O)c2cccc n2	3{7}	[C-] #[N+]C1CC OCC1	0.0	0
1078	4{234,520,12}	COC1=C(C=NN=C1)C1=C(NCC2CCOC2)N2C=CN=C(OC3CCC3)C2=N1 c:4,6,9,20,31,t:2,22	Z8849597838	1{234}	Ne1ncnc1 OC2CCC2	2{520}	COc1cnccc1 C=O	3{12}	[C-] #[N+]CC1C COC1	0.0	0
1079	4{158,556,35}	COC1=CC2=C(NN=C2C2=C(NCCCSC)N3C=C(N=CC3=N2)P(C)(C)=O)C=C1 c:7,10,19,21,24,31,t:2,4	Z8849597799	1{158}	CP(=O)(C)c 1cnc(N)cn1	2{556}	COc1ccc2[n H]nc(C=O)c 2c1	3{35}	CSCCC[N+] #[C-]	0.0	0
1080	4{419,164,46}	CN1N=C(C2=C1CCOC2)C1=C(NCC(C)=C)N2C(C=CC(C#C)=C2F)=N1 c:2,4,12,21,25,28	Z8855739188	1{419}	Ne1ccc(C# C)c(F)n1	2{164}	Cn1nc(C=O) c2COCCc21	3{46}	CC(=C)C[N+] #[C-]	0.0	0
1081	4{35,129,9}	CNC1=C(N=C2C=CC(C)=CN12)C1=CC=CC2=NC=NN12 c:6,9,16,20,t:2,4,14,18	Z8798985036	1{35}	Cc1ccc(N)n c1	2{129}	O=Cc1cccc2 ncnm12	3{9}	C[N+]#[C-]	0.0	0
1082	4{397,532,1}	COC1=C(OC)C(=NC=N1)C1=C(NC2CC2)N2C=CC(C)=C(C)C2=N1 c:2,6,8,11,19,26,t:22	Z8846492153	1{397}	Cl.Cc1ccnc(N)c1C	2{532}	COc1ncnc(C =O)c1OC	3{1}	[C-] #[N+]C1CC 1	0.0	0
1083	4{84,173,32}	CC(C)C1=NC=CN2C(NC3CCC3)=C(N=C12)C1=NC(=NN1C)C(F)(F)F c:5,14,22,t:3,16,20	Z8846491988	1{84}	CC(C)c1ncc nc1N	2{173}	Cn1nc(nc1C =O)C(F)(F)F	3{32}	[C-] #[N+]C1CC C1	0.0	0
1084	4{422,480,29}	CCOC(=O)CCNC1=C(N=C2N1C(F)=CC=C2C#C)C1=CC2=C(CCOC2)N=C1 c:10,15,17,31,t:8,22,24	Z8846491751	1{422}	Ne1nc(F)cc c1C#C	2{480}	O=Cc1cnc2C COCCc2c1	3{29}	CCOC(=O)C C[N+]#[C-]	0.0	0
1085	4{223,557,50}	COC1=NC=C(F)C(=C1)C1=C(NC2=CC3=C(OCCO3)C=C2)N2N=C(C=CC2=N1)C(N)=O c:7,10,22,26,28,31,t:2,4,13,15	Z8837933142	1{223}	NC(=O)c1c cc(N)nn1	2{557}	COc1cc(C=O) c(F)cn1	3{50}	[C-] #[N+]c1ccc 2OCCOc2c1	0.0	0
1086	4{169,558,9}	CNC(=O)C1=NN2C(C=C1)=NC(=C2NC)C1=CC(Cl)=NC(C)=C1 c:8,10,12,20,23,t:4,17	Z8837933138	1{169}	CNC(=O)c1 ccc(N)nn1	2{558}	Cc1cc(C=O) cc(Cl)n1	3{9}	C[N+]#[C-]	0.0	0
1087	4{251,108,62}	COC(=O)C1(CCCC1)NC1=C(N=C2C=CC3=C(NC(=O)C=C3)N12)C1=CN=C(N=C1)N1CCOCC1 c:15,22,30,32,t:11,13,17,28	Z8878918895	1{251}	Ne1ccc2ccc (=O)[nH]c2 n1	2{108}	O=Cc1cnc(n c1)N2CCOC C2	3{62}	COC(=O)C1(CCCC1)[N+] #[C-]	0.0	0

1088	4{416,559,23}	COC(=O)CCC(NC1=C(CC2CCOC(C)(C)C2)N=C2C=C(CCl)C=CN12)C(=O)OC c:8,26,t:20,22	Z8878918846	1{416}	Cl.Nc1cc(CCl)ccn1	2{559}	CC1(C)CC(C=C=O)CCO1	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	0.0	0
1089	4{181,560,14}	COCCNC1=C(N=C2N1C=CC1=C2N=CC=N1)C1=NC2=C(CCCC2)S1 c:7,11,13,16,18,t:5,21,23	Z8878918501	1{181}	Nc1nccc2ncnc12	2{560}	O=Cc1nc2C CCCc2s1	3{14}	COCC[N+]#[C-]	0.0	0
1090	4{181,450,6}	CCOC(=O)CCNC1=C(N=C2N1C=CC1=C2N=CC=N1)C1=CC(=CC=C1)S(=O)(=O)N(C)C c:11,15,17,20,22,27,29,t:9,25	Z8878918356	1{181}	Nc1nccc2ncnc12	2{450}	CN(C)S(=O)(=O)c1cccc(C=O)c1	3{6}	CCOC(=O)C CC[N+]#[C-]	0.0	0
1091	4{423,123,22}	CC(C)OC1=CC=CC2=NC(=C(NC3COC3)N12)C1=NC=C(C)N=C1 c:6,26,t:4,8,10,21,23	Z8873684718	1{423}	Cl.CC(C)Oc1cccc(N)n1	2{123}	Cc1nc(C=O)cn1	3{22}	[C-] #[N+]C1CO C1	0.0	0
1092	4{251,108,67}	CCC(C)NC1=C(N=C2C=CC3=C(NC(=O)C=C3)N12)C1=CN=C(N=C1)N1CCOCC1 c:9,16,24,26,t:5,7,11,22	Z8873685341	1{251}	Nc1ccc2ccc(=O)[nH]c2n1	2{108}	O=Cc1nc(n c1)N2CCOC C2	3{67}	CCC(C)[N+] #[C-]	0.0	0
1093	4{240,561,15}	CCNC1=C(N=C2C=CC(=CN12)C1=NNN=N1)C1=C(F)C=C(C=C1)C1=NC=CO1 c:7,9,17,20,23,25,30,t:3,5,14,28	Z8873685268	1{240}	Nc1ccc(en1)c2nn[nH]n2	2{561}	Fe1cc(ccc1C=O)c2ncco2	3{15}	CC[N+]#[C-]	0.0	0
1094	4{415,139,21}	CC1=NN(CCO)C(C)=C1C1=C(NCC2CC2)N2C(=N1)C(CCl)=CC=C2Br c:8,11,20,25,27,t:1	Z8873684925	1{415}	Cl.Nc1nc(Br)ccc1CCl	2{139}	Cc1nn(CCO)c(C)c1C=O	3{21}	[C-] #[N+]CC1C C1	0.0	0
1095	4{424,562,39}	CCOCCNC1=C(N=C2C=CC3=C(NC(=O)CO3)N12)C1=C(OC)C=C(C)C=C1 c:10,23,30,t:6,8,12,27	Z8873684903	1{424}	Nc1ccc2OC C(=O)Nc2n1	2{562}	COc1cc(C)cc c1C=O	3{39}	CCOCC[N+] #[C-]	0.0	0
1096	4{211,563,41}	COC1=CC=C(NC2=C(N=C3N2C=CC=C3C2=NN=NN2)C2=CN=C(NC(C)=O)C=C2)C=C1 c:9,13,15,20,32,35,t:2,4,7,18,24,26	Z8829498711	1{211}	Nc1ncccc1c2n[nH]2	2{563}	CC(=O)Nc1c cc(C=O)cn1	3{41}	COc1ccc([N+]#[C-])cc1	0.0	0
1097	4{425,524,12}	CC(C)OC1=NC=CN2C(NCC3CCOC3)=C(N=C12)C1=C(F)C(F)=NC(F)=C1 c:6,17,23,27,30,t:4,19	Z8829498569	1{425}	CC(C)Oc1nccnc1N	2{524}	Fe1cc(C=O)c(F)c(F)n1	3{12}	[C-] #[N+]CC1C COC1	0.0	0
1098	4{167,564,1}	CN1N=NC=C1C1=C(NC2CC2)N2C(=N1)C(C)=NC=C2C c:2,4,7,15,19,21	Z8835022914	1{167}	Cc1nc(C)(N)n1	2{564}	Cn1nccc1C=O	3{1}	[C-] #[N+]C1CC 1	0.0	0
1099	4{422,565,50}	COC1(CC(C1)C1=C(NC2=CC3=C(OCCO3)C=C2)N2C(=N1)C(=CC=C2F)C#C)OC c:7,19,23,26,28,t:10,12	Z8835022909	1{422}	Nc1nc(F)cc1C#C	2{565}	COC1(CC(C1)C=O)OC	3{50}	[C-] #[N+]c1ccc 2OCCOc2c1	0.0	0

1100	4{198,60,32}	CC(C1CCOC1)C1=C(NC2CCC2)N2C(C=NC(C#C)=C2Cl)=N1 c:8,18,22,25	Z8835022907	1{198}	Ne1cnc(C#C)c(Cl)n1	2{60}	CC(C=O)C1CCOC1	3{32}	[C-]#[N+]C1CC1	0.0	0
1101	4{61,388,1}	CCC1=CC=CC2=NC(=C(NC3CC3)N12)C1=C(N(C)N=C1OC c:4,22,t:2,6,8,18	Z8855739210	1{61}	CCc1cccc(N)n1	2{388}	COc1nn(C)c1C=O	3{1}	[C-]#[N+]C1CC1	0.0	0
1102	4{231,515,33}	COC1=C(CNC2=C(N=C3C=CC(=NN23)C(F)(F)F)C2=NO(CN(C)C)=C2)C=CC=C1 c:2,10,12,28,31,33,t:6,8,21	Z8855739129	1{231}	Ne1ccc(nn1)C(F)(F)F	2{515}	CN(C)Cc1cc(C=O)no1	3{33}	COc1cccc1C[N+]#[C-]	0.0	0
1103	4{260,534,14}	COCCNC1=C(N=C2N1C=CC=C2N1CCCC1)C1=NN(C=C1)C(C)C c:7,11,13,25,t:5,22	Z8855739106	1{260}	Ne1ncccc1N2CCCC2	2{534}	CC(C)n1ccc(C=O)n1	3{14}	COCC[N+]#[C-]	0.0	0
1104	4{271,226,67}	CCC(C)NC1=C(N=C2C=CC(C(=O)OC)=C(F)N12)C1=C(C)N(CC(F)(F)F)N=C1 c:9,21,30,t:5,7,15	Z8810903011	1{271}	COC(=O)c1ccc(N)nc1F	2{226}	Cc1c(C=O)cnn1CC(F)(F)F	3{67}	CCC(C)[N+]#[C-]	0.0	0
1105	4{169,207,13}	CNC(=O)C1=NN2C(C=C1)=NC(=C2NCC1=C(C=C(OC)C=C1)C1=CC(=NN1C)C(=O)OC c:8,10,12,23,28,t:4,17,19,26	Z8810902985	1{169}	CNC(=O)c1ccc(N)nn1	2{207}	COC(=O)c1cc(C=O)n(C)n1	3{13}	COc1ccc(C[N+]#[C-])cc1	0.0	0
1106	4{260,246,14}	COCCNC1=C(N=C2N1C=CC=C2N1CCCC1)C1CC1CCOC1 c:7,11,13,t:5	Z8810902964	1{260}	Ne1ncccc1N2CCCC2	2{246}	O=CC1CC21CCCOC2	3{14}	COCC[N+]#[C-]	0.0	0
1107	4{211,3,66}	CC(NC1=C(N=C2N1C=CC=C2C1=NN=NN1)C1=NC=C(C=C1)C#N)C1=CC=CC=C1 c:5,9,11,16,22,24,31,33,t:3,14,20,29	Z8798985051	1{211}	Ne1ncccc1c2nnn[nH]2	2{3}	O=Cc1ccc(C#N)en1	3{66}	CC([N+]#[C-])c1cccc1	0.0	0
1108	4{92,566,32}	NC(=O)C1=CC2=NC(=C(NC3CCC3)N2C=C1)C1=C(Cl)N=C2SC=CN12 c:17,20,26,t:3,5,7,23	Z8846492139	1{92}	NC(=O)c1ccnc(N)c1	2{566}	Clc1nc2scn2c1C=O	3{32}	[C-]#[N+]C1CC1	0.0	0
1109	4{151,170,13}	CCN1N=NC(=N1)C1=C(NCC2=CC=C(OC)C=C2)N2C(C=NC=C2Cl)=N1 c:3,5,8,18,23,25,28,t:12,14	Z8837933149	1{151}	Ne1cnc(Cl)n1	2{170}	CCn1nnc(C=O)n1	3{13}	COc1ccc(C[N+]#[C-])cc1	0.0	0
1110	4{419,236,21}	FC1=C(C=CC2=NC(CCC3OCCO3)=C(NCC3CC3)N12)C#C c:3,t:1,5,15	Z8855619583	1{419}	Ne1ccc(C#C)c(F)n1	2{236}	O=CCCC1OCCO1	3{21}	[C-]#[N+]CC1C1	0.0	0
1111	4{419,567,10}	CN1N=C2CCCC2=C1C1=C(NC2CCOC2)N2C(C=CC(C#C)=C2F)=N1 c:8,11,22,26,29,t:2	Z8855619516	1{419}	Ne1ccc(C#C)c(F)n1	2{567}	Cn1nc2CCc2c1C=O	3{10}	[C-]#[N+]C1CCOC1	0.0	0
1112	4{179,42,1}	COC1=CC2=NC(=C(NC3CC3)N2C=C1)C1=C(N(C)N=C1Cl c:15,22,t:2,4,6,18	Z8855619513	1{179}	COc1cnc(N)c1	2{42}	Cn1cc(C=O)c(Cl)n1	3{1}	[C-]#[N+]C1CC1	0.0	0

1113	4{181,512,26}	CN(C)CC1=CN=C(S1)C1=C(NCC2=CC=C(F)C=C2)N2C=CC3=C(N=CC=N3)C2=N1 c:6,10,19,23,27,29,33,t:4,14,16,25	Z8878918854	1{181}	Nc1nccc2ncnc12	2{512}	CN(C)Cc1enc(C=O)s1	3{26}	Fc1ccc(C[N+][C-])cc1	0.0	0
1114	4{392,530,67}	CCC(C)NC1=C(N=C2C=CC3=C(NC(C)=N3)N12)C1CC2(CC(C2)OC)C1 c:9,15,t:5,7,11	Z8878918595	1{392}	Cl.Cc1nc2ccc(N)nc2[nH]1	2{530}	COC1CC2(C1)CC(C2)C=O	3{67}	CCC(C)[N+][C-]	0.0	0
1115	4{251,568,71}	COC1=CC(NC2=C(N=C3C=CC4=C(NC(=O)C=C4)N23)C2=CN=C(S2)C2=NC=CN=C2)=CC=C1 c:10,17,25,31,33,35,37,t:2,6,8,12,23,29	Z8878918353	1{251}	Nc1ccc2ccc(=O)[nH]c2n1	2{568}	O=Cc1enc(s1)c2cncnc2	3{71}	COc1cccc([N+][C-])c1	0.0	0
1116	4{410,217,62}	COC(=O)C1(CCCC1)NC1=C(N=C2C=CC3=C(N=CC(Cl)=C3)N12)C1=CC(=O)N(C)C=C1 c:15,19,22,34,t:11,13,17,28	Z8873684787	1{410}	Nc1ccc2cc(Cl)nc2n1	2{217}	Cn1ccc(C=O)cc1=O	3{62}	COC(=O)C1(CCCC1)[N+][C-]	0.0	0
1117	4{420,569,67}	CCC(C)NC1=C(CC2CCOC2=O)N=C2C=CC3=C(NC=N3)N12 c:5,17,22,t:15,19	Z8873685393	1{420}	Cl.Cl.Nc1cc2nc[nH]c2n1	2{569}	O=CCC1CCOC1=O	3{67}	CCC(C)[N+][C-]	0.0	0
1118	4{19,316,22}	COC(=O)C1=CC2=C(C=C1)N=C(C=C2)C1=C(NC2COC2)N2C=CC=C(C#N)C2=N1 c:6,8,11,13,16,25,32,t:4,27	Z8873685313	1{19}	Nc1ncccc1C#N	2{316}	COC(=O)c1ccc2nc(C=O)ccc2c1	3{22}	[C-][N+]#C1CO C1	0.0	0
1119	4{392,530,39}	CCOCCNC1=C(N=C2C=CC3=C(NC(C)=N3)N12)C1CC2(CC(C2)OC)C1 c:10,16,t:6,8,12	Z8873685309	1{392}	Cl.Cc1nc2ccc(N)nc2[nH]1	2{530}	COC1CC2(C1)CC(C2)C=O	3{39}	CCOCC[N+][C-]	0.0	0
1120	4{292,444,32}	CCOC1=CN=CC2=NC(=C(NC3CCC3)N12)C1=C(O)C=CN=C1 c:5,20,23,25,t:3,7,9	Z8873684915	1{292}	CCOc1cnc(N)n1	2{444}	Oc1cncnc1C=O	3{32}	[C-][N+]#C1CC C1	0.0	0
1121	4{151,453,9}	CNC1=C(N=C2C=NC=C(Cl)N12)C1=CC(C=C)=CN=C1 c:6,18,20,t:2,4,8,14	Z8829498655	1{151}	Nc1cnc(Cl)n1	2{453}	Cl.C=Cc1cnc(C=O)c1	3{9}	C[N+][C-]	0.0	0
1122	4{99,224,41}	COC1=CC=C(NC2=C(N=C3C=CC(=CN23)S(N)(=O)=O)C2CCOC2C)C=C1 c:11,13,29,t:2,4,7,9	Z8854581182	1{99}	Nc1ccc(en1)S(=O)(=O)N	2{224}	CC1OCCC1C=O	3{41}	COc1ccc([N+][C-])cc1	0.0	0
1123	4{262,399,43}	CC(=O)NC1=CN2C(C=C1)=NC(=C2NC1CCN(CC1)C(=O)OC(C)(C)C)C1=CN(N=C1C)C1C c:8,10,12,33,t:4,30	Z8835022897	1{262}	CC(=O)Nc1ccc(N)nc1	2{399}	Cc1nn(cc1C=O)C2CC2	3{43}	CC(C)(C)OC(=O)N1CCC(CC1)[N+][C-]	0.0	0
1124	4{144,477,47}	CNS(=O)(=O)C1=CN2C(C=C1)=NC(C(NC(=O)OC(C)(C)C)C1COC1)=C2NC(C)C c:9,11,27,t:5	Z8855739262	1{144}	CNS(=O)(=O)c1ccc(N)nc1	2{477}	CC(C)(C)OC(=O)NC(C=O)C1COC1	3{47}	CC(C)[N+][C-]	0.0	0

1125	4{174,202,61}	CC(C)(C)OC(=O)NCCCNC1=C(N=C2C=CC=C(C#N)N12)C1=C(F)C=NC=C1F c:16,25,28,30,t:12,14,18	Z8846492017	1{174}	Nc1cccc(C#N)n1	2{202}	Fc1cnc(F)c1C=O	3{61}	CC(C)(C)OC(=O)NCCC[N+][C-]	0.0	0
1126	4{169,570,14}	CNC(=O)C1=NN2C(C=C1)=NC(C1CCN(CC1C)C(=O)OC(C)(C)C)=C2NCCOC c:8,10,27,t:4	Z8855619678	1{169}	CNC(=O)c1ccc(N)nn1	2{570}	CC1CN(CCC1C=O)C(=O)OC(C)(C)C	3{14}	COCC[N+][C-]	0.0	0
1127	4{426,571,67}	CCC(C)NC1=C(N=C2C=C(C=CN12)C1=NN=NN1)C1CC2(CCC2(OC)OC)C1 c:9,11,18,t:5,7,16	Z8855619619	1{426}	Nc1cc(cen1)e2nn[nH]2	2{571}	COC1(CCC21CC(C2)C=O)OC	3{67}	CCC(C)[N+][C-]	0.0	0
1128	4{1,22,27}	CCCCNC1=C(N=C2C=CN12)C1=CC=CC=C1 c:9,17,19,t:5,7,15	Z8711892168	1{1}	Nc1cc[nH]n1	2{22}	O=Cc1cccc1	3{27}	CCCC[N+][C-]	0.0	0
1129	4{427,572,5}	COCCNC1=C(N=C2C=C3C=CC=NC3=C(O)C)N12)C1=NC(=CC(OC)=C1)C(=O)OC c:12,14,26,30,t:6,8,10,17,24	Z8878918797	1{427}	COc1nc(N)cc2ccnc12	2{572}	COC(=O)c1c(O)cc(C=O)n1	3{5}	COCC[N+][C-]	0.0	0
1130	4{251,573,62}	COC(=O)C1(CCCC1)NC1=C(N=C2C=CC3=C(NC(=O)C=C3)N12)C1=C(C)SN=C1C c:15,22,28,32,t:11,13,17	Z8878918589	1{251}	Nc1ccc2ccc(=O)[nH]c2n1	2{573}	Cc1nsc(C)c1C=O	3{62}	COC(=O)C1(CCCC1)[N+][C-]	0.0	0
1131	4{240,574,22}	CC(C)(C)OC(=O)N[C@H](CC1=C(NC2COC2)N2C=C(C=CC2=N1)C1=NNN=N1)C(C)(C)C c:10,19,21,24,30,t:27	Z8878918571	1{240}	Nc1ccc(en1)c2nn[nH]n2	2{574}	CC(C)(C)OC(=O)N[C@H](CC(=O)C(C)(C)C)	3{22}	[C-][N+][C1CO]C1	0.0	0
1132	4{240,575,22}	CC(C)(C)OC(=O)NC(CC1=C(NC2COC2)N2C=C(C=CC2=N1)C1=NNN=N1)C(F)(F)F c:10,19,21,24,30,t:27	Z8878918544	1{240}	Nc1ccc(en1)c2nn[nH]n2	2{575}	CC(C)(C)OC(=O)NC(CC(=O)C(F)(F)F)	3{22}	[C-][N+][C1CO]C1	0.0	0
1133	4{424,576,39}	CCOCCNC1=C(N=C2C=CC3=C(NC(=O)CO3)N12)C1=C(OC)C=CC=N1 c:10,23,27,29,t:6,8,12	Z8878918477	1{424}	Nc1ccc2OC(C(=O)Nc2n1	2{576}	COc1ccnc1C=O	3{39}	CCOCC[N+][C-]	0.0	0
1134	4{428,544,60}	COC(=O)C1=CC(NC2=C(N=C3C=NC(Br)=CN23)C2=NN=C3CCCN23)=CC=C1 c:12,15,29,31,t:4,8,10,20,22	Z8878918461	1{428}	Nc1cnc(Br)cn1	2{544}	O=Cc1mnc2CCn12	3{60}	COC(=O)c1ccc([N+][C-])c1	0.0	0
1135	4{424,577,39}	CCOCCNC1=C(N=C2C=CC3=C(NC(=O)CO3)N12)C1=CC(=CC(F)=C1)C#N c:10,25,28,t:6,8,12,23	Z8878918450	1{424}	Nc1ccc2OC(C(=O)Nc2n1	2{577}	Fc1cc(C=O)c(C#N)c1	3{39}	CCOCC[N+][C-]	0.0	0
1136	4{19,55,3}	CP(C)(=O)C1=NC=CC(=C1)C1=C(NC2=C(F)C=C(C1)C=C2)N2C=CC=C(C#N)C2=N1 c:6,8,11,14,20,24,31,t:4,17,26	Z8878918414	1{19}	Nc1ncccc1C#N	2{55}	CP(=O)(C)c1cc(C=O)cn1	3{3}	Fc1cc(Cl)ccc1[N+][C-]	0.0	0

1137	4{425,281,46}	COC(=O)C1=NN=C(C=C1)C1=C(NCC(C)=C)N2C=CN=C(OC(C)C)C2=N1 c:6,8,11,19,28,t:4,21	Z8878918359	1{425}	CC(C)Oe1nccnc1N	2{281}	COC(=O)c1ccc(C=O)nn1	3{46}	CC(=C)C[N+]#[C-]	0.0	0
1138	4{353,547,15}	CCNC1=C(N=C2C=CC(NS(C)(=O)=O)=CN12)C1=C(Br)N=C(S1)C(F)(F)F c:7,14,19,22,t:3,5	Z8873684737	1{353}	Cl.CS(=O)(=O)Nc1ccc(N)nc1	2{547}	FC(F)(F)c1nc(Br)c(C=O)s1	3{15}	CC[N+]#[C-]	0.0	0
1139	4{420,578,67}	CCC(C)NC1=C(N=C2C=CC3=C(NC=N3)N12)C1=CC(=CC(=C1)C#N)C#N c:9,14,22,24,t:5,7,11,20	Z8873684712	1{420}	Cl.Cl.Nc1cc2nc[nH]c2n1	2{578}	O=Cc1cc(C#N)cc(C#N)c1	3{67}	CCC(C)[N+]#[C-]	0.0	0
1140	4{411,188,37}	COC(=O)C1CC(C1)NC1=C(CCC2(CC2)C#N)N=C2C=C(Br)C=C(F)N12 c:10,t:20,22,25	Z8873684705	1{411}	Nc1cc(Br)cc(F)n1	2{188}	O=CCCC1(C1)C#N	3{37}	COC(=O)C1CC(C1)[N+]#[C-]	0.0	0
1141	4{54,543,15}	CCNC1=C(N=C2C=CC(=CN12)C(=O)N(C)C)C(=O)OCC c:7,9,t:3,5	Z8873684702	1{54}	Cl.CN(C)C(=O)c1ccc(N)nc1	2{543}	CCOC(=O)C=O	3{15}	CC[N+]#[C-]	0.0	0
1142	4{251,579,67}	CCCN1C=C(C=N1)C1=C(NC(C)CC)N2C(C=CC3=C2NC(=O)C=C3)=N1 c:4,6,9,18,20,26,28	Z8873685293	1{251}	Nc1ccc2ccc(=O)[nH]c2n1	2{579}	CCCN1cc(C=O)en1	3{67}	CCC(C)[N+]#[C-]	0.0	0
1143	4{348,509,2}	CN1C=NN=C1C1=C(NC2=CC=C(F)C=C2)N2C=C(F)N=CC2=N1 c:2,4,7,15,22,25,t:10,12,19	Z8873684897	1{348}	Nc1cnc(F)c1n1	2{509}	Cn1cnc1C=O	3{2}	Fc1ccc([N+]#[C-])cc1	0.0	0
1144	4{193,520,10}	CNC(=O)C1=CN2C(C=C1)=NC(=C2NC1CCO)C1)C1=C(OC)C=NN=C1 c:8,10,12,22,26,28,t:4	Z8873684606	1{193}	CNC(=O)c1ccc(N)nc1	2{520}	COc1cnc1C=O	3{10}	[C-]#[N+]C1CCOC1	0.0	0
1145	4{89,217,71}	COC1=CC(NC2=C(N=C3C=CC4=C(NN=C4)N23)C2=CC(=O)N(C)C=C2)=CC=C1 c:10,15,27,29,31,t:2,6,8,12,21	Z8873684593	1{89}	Nc1ccc2cn[nH]c2n1	2{217}	Cn1ccc(C=O)cc1=O	3{71}	COc1cccc([N+]#[C-])c1	0.0	0
1146	4{187,281,12}	COC(=O)C1=NN=C(C=C1)C1=C(NCC2CCO)C2)N2C=C(Cl)C(=CC2=N1)C#N c:6,8,11,25,28,t:4,22	Z8873684820	1{187}	Nc1cc(C#N)c(Cl)en1	2{281}	COC(=O)c1ccc(C=O)nn1	3{12}	[C-]#[N+]CC1COC1	0.0	0
1147	4{73,1,13}	COC1=CC=C(CNC2=C(N=C3C=CC4=NC=C4)N23)C2=C(Cl)C=NC=C2)C=C1 c:12,16,23,26,28,32,t:2,4,8,10,14	Z8854581154	1{73}	Nc1ccc2cncn2n1	2{1}	Clc1cnc(Cl)c1C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	0.0	0
1148	4{169,97,14}	CNC(=O)C1=NN2C(C=C1)=NC(=C2NCCOC)C1=CC=C(F)C=C1 c:8,10,12,25,t:4,20,22	Z8835022906	1{169}	CNC(=O)c1ccc(N)nn1	2{97}	Fc1ccc(C=O)cc1	3{14}	COCC[N+]#[C-]	0.0	0

1149	4{166,580,22}	OCCSCC1=CC2=NC(=C(NC3COC3)N2C=C1)C1=C(F)C(Cl)=NC(Cl)=C1 c:19,22,26,29,t:5,7,9	Z8835022900	1{166}	Nc1cc(CSCCO)ccn1	2{580}	Fc1c(Cl)nc(Cl)cc1C=O	3{22}	[C-]]#[N+]C1CO C1	0.0	0
1150	4{330,581,1}	CCC1=CN=C(O)C1=C(NC2CC2)N2C=C(C=CC2=N1)S(=O)(=O)N(C)C c:4,8,16,18,21,t:2	Z8835022884	1{330}	CN(C)S(=O)(=O)c1ccc(N)nc1	2{581}	CCc1cnc(C=O)o1	3{1}	[C-]]#[N+]C1CC 1	0.0	0
1151	4{399,582,35}	CSCCCNC1=C(N=C2C=CC(OC(C)C)=NN12)C(CC(F)F)NC(=O)OC(C)C c:10,16,t:6,8	Z8849597814	1{399}	CC(C)Oe1c1cc(N)nn1	2{582}	CC(C)(C)OC(=O)NC(CC(F)F)C=O	3{35}	CSCCC[N+] #[C-]	0.0	0
1152	4{406,146,7}	C[C@@H]1C[C@@H]1CCC1=C(NC2CCOC2)N2C(C=CC=C2C2=NNN=N2)=N1 &1:1,3,r,c:7,19,21,27,29,t:24	Z8849597813	1{406}	Nc1cccc(n1)c2nn[nH]n2	2{146}	C[C@@H]1C[C@@H]1CCC=O &1:1,3,r	3{7}	[C-]]#[N+]C1CC OCC1	0.0	0
1153	4{50,268,7}	CC[C@@H](NC(=O)OC(C)C)C1=C(NC2CCOCC2)N2C(C=CC=C2P(C)C)=O=N1 c:11,23,25,31	Z8855739264	1{50}	CP(=O)(C)c1cccc(N)n1	2{268}	CC[C@@H](NC(=O)OC(C)C)C=O	3{7}	[C-]]#[N+]C1CC OCC1	0.0	0
1154	4{429,200,23}	COC(=O)CCC(NC1=C(CCCC#CC)N=C2N1C=CC=C2CBr)C(=O)OC c:8,16,20,22	Z8846492230	1{429}	Br.Nc1nccc1CBr	2{200}	CC#CCCCC=O	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	0.0	0
1155	4{334,137,11}	CC1=C(C(C)=NO1)C1=C(NCC2=CC(Br)=CC=C2)N2C=C3COCCC3=C(C#N)C2=N1 c:4,8,15,17,33,t:1,12,21,28	Z8837933169	1{334}	Nc1ncc2COCCc2c1C#N	2{137}	Cc1noc(C)c1C=O	3{11}	Br1cccc(C[N+]#[C-])c1	0.0	0
1156	4{283,8,71}	COCC1=NOC=C1C1=C(NC2=CC(OC)=CC=C2)N2C(C=CC3=C2N=CC(=C3)C(=O)OC)=N1 c:6,9,16,18,23,25,28,30,36,t:3,12	Z8837933153	1{283}	COC(=O)c1cnc2nc(N)cc2c1	2{8}	COCC1nocc1C=O	3{71}	COc1cccc([N+]#[C-])c1	0.0	0
1157	4{169,30,9}	CNC(=O)C1=NN2C(C=C1)=NC(C1CCN(CC1)C(C)=O)=C2NC c:8,10,22,t:4	Z8855619766	1{169}	CNC(=O)c1ccc(N)nn1	2{30}	CC(=O)N1C CC(CC1)C=O	3{9}	C[N+]#[C-]	0.0	0
1158	4{167,550,1}	CN1N=C(Br)N=C1C1=C(NC2CC2)N2C(=N1)C(C)=NC=C2C c:5,8,16,20,22,t:2	Z8855619760	1{167}	Cc1cnc(C)(N)n1	2{550}	Cn1nc(Br)nc1C=O	3{1}	[C-]]#[N+]C1CC 1	0.0	0
1159	4{430,583,34}	CC1=C(N2C=CC(Cl)=CC2=N1)C1=C(NCC2C CCO2)N2C=CC3=C(C2=N1)S(=O)(=O)NC3=O c:4,7,10,13,24,26,29,t:1	Z8855619649	1{430}	Nc1nccc2C(=O)NS(=O)(=O)c21	2{583}	Cc1nc2cc(Cl)ccn2c1C=O	3{34}	[C-]]#[N+]CC1C CCO1	0.0	0
1160	4{192,79,14}	COCCNC1=C(N=C2N1C(F)=CC=C2Cl)C1=N C=CO1 c:7,12,14,20,t:5,18	Z8855619641	1{192}	Nc1nc(F)cc1Cl	2{79}	O=Cc1ncco1	3{14}	COCC[N+]#[C-]	0.0	0

Parallel synthesis of compound library 4, main experiment

1161	4{28,189,7}	C1CC(CCO1)NC1=C(N=C2C=C(C=CN12)C1=NOC=N1)C1=CN(N=N1)C1CCOCC1 c:12,14,22,28,t:8,10,19,25	Z8878918418	1{28}	Cl.Nc1cc(ccn1)c2ncon2	2{189}	O=Cc1cn(nn1)C2CCOCC2	3{7}	[C-] #[N+]C1CCOCC1	105.1	89
1162	4{180,336,32}	COC(=O)C1=CC2=NC(=C(NC3CCC3)N2C=C1C)C1=CSN=C1OC c:18,25,t:4,6,8,22	Z8878918612	1{180}	COC(=O)c1cc(N)ncc1C	2{336}	COc1nscclC=O	3{32}	[C-] #[N+]C1CCOCC1	83.5	83
1163	4{76,584,23}	COC(=O)CCC(NC1=C(N=C2C=CC(C)=C(C1)N12)C1=C(OC)C=C(C)N=C1)C(=O)OC c:12,21,28,t:8,10,15,25	Z8873684644	1{76}	Cc1ccc(N)nc1Cl	2{584}	COc1cc(C)nc1C=O	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	100.6	81
1164	4{180,545,35}	COCCN1N=C(C)C(=C1C)C1=C(NCCCSC)N2C=C(C)C(=CC2=N1)C(=O)OC c:8,12,24,27,t:5,21	Z8878918407	1{180}	COC(=O)c1cc(N)ncc1C	2{545}	COCCn1nc(C)c(C=O)c1C	3{35}	CSCCC[N+]#[C-]	96.9	81
1165	4{405,585,5}	COCCCN1=C(CC2CC2(Cl)Cl)N=C2C=CC(=CN12)N1CCCC1=O c:6,17,19,t:15	Z8855739175	1{405}	Nc1ccc(cn1)N2CCCC2=O	2{585}	ClC1(Cl)CC1CC=O	3{5}	COCCCN1#[C-]	86.6	78
1166	4{392,586,67}	CCC(C)NC1=C(N=C2C=CC3=C(NC(C)=N3)N12)C1=CC2=C(COC2)N=C1 c:9,15,29,t:5,7,11,21,23	Z8878918627	1{392}	Cl.Cc1nc2ccc(N)nc2[nH]1	2{586}	O=Cc1cnc2COCc2c1	3{67}	CCC(C)[N+]#[C-]	75.2	77
1167	4{374,587,5}	COCCCN1=C(N=C2C=CC=C(N12)C(=O)OC)C1=C(C)ON=C1OC c:10,12,21,25,t:6,8	Z8835022866	1{374}	COC(=O)c1cccc(N)n1	2{587}	COc1noc(C)c1C=O	3{5}	COCCCN1#[C-]	76.2	75
1168	4{431,588,61}	CN1C=C(C(C)=N1)C1=C(NCCCNC(=O)OC(C)(C)C)N2C=C(F)C=CC2=N1 c:2,5,8,26,29,t:23	Z8878918395	1{431}	Nc1ccc(F)cn1	2{588}	Cc1nn(C)cc1C=O	3{61}	CC(C)(C)OC(=O)NCCC[N+]#[C-]	80.5	74
1169	4{64,589,49}	CN1N=C(C)C(=C1Cl)C1=C(NC2CC(F)(F)C2)N2C=C(C=CC2=N1)N1CCCS1(=O)=O c:5,9,20,22,25,t:2	Z8878918677	1{64}	Nc1ccc(cn1)N2CCCS2(=O)=O	2{589}	Cc1nn(C)c(C1)c1C=O	3{49}	FC1(F)CC(C1)[N+]#[C-]	91.5	72
1170	4{153,336,53}	COC1=NSC=C1C1=C(NCCOCC2=CC=CC=C2)N2C(C=CC=C2C(C)O)=N1 c:5,8,17,19,24,26,32,t:2,15	Z8855619615	1{153}	CC(C)(O)c1cccc(N)n1	2{336}	COc1nscclC=O	3{53}	[C-] #[N+]CCOCC1CCCC1	84.8	72
1171	4{103,590,59}	OCC1=CN=CC2=NC(=C(NCCC3=CC(F)=CC=C3)N12)C1=CN=C(C=C1)C1=CSC=N1 c:4,16,18,26,28,34,t:2,6,8,13,24,31	Z8878918413	1{103}	Nc1cncc(CO)n1	2{590}	O=Cc1ccc(nc1)c2cscn2	3{59}	Fc1cccc(CC[N+]#[C-])c1	86.3	72

1172	4{362,326,21}	CNC(=O)C1=CC=CC2=NC(=C(NCC3CC3)N12)C1=CC=NN1C c:6,23,t:4,8,10,21	Z8878918629	1{362}	CNC(=O)c1cccc(N)n1	2{326}	Cn1ncccc1C=O	3{21}	[C-] #[N+]CC1C C1	61.3	70
1173	4{105,591,29}	CCOC(=O)CCNC1=C(N=C2C=CC=C(N12)C(N)=O)C1=CC=C(C=C1)N1CCOCC1 c:12,14,24,26,t:8,10,22	Z8878918651	1{105}	NC(=O)c1cccc(N)n1	2{591}	O=Cc1ccc(cc1)N2CCOCC2	3{29}	CCOC(=O)C C[N+]#[C-]	82.0	69
1174	4{365,592,10}	COC(=O)C1=CC(=CN1C)C1=C(NC2CCOC2)N2C(C=C(C)C=C2C)=N1 c:6,11,25,28,t:4,22	Z8878918853	1{365}	Cc1cc(C)nc(N)c1	2{592}	COC(=O)c1cc(C=O)en1C	3{10}	[C-] #[N+]C1CC OC1	68.9	69
1175	4{62,593,6}	CCOC(=O)CCNC1=C(N=C2C=C(CO)C=CN12)C1=CC=C(NC(C)=O)C=C1 c:17,30,t:9,11,13,22,24	Z8873685260	1{62}	Nc1cc(CO)ccn1	2{593}	CC(=O)Nc1ccc(C=O)cc1	3{6}	CCOC(=O)C CC[N+]#[C-]	76.2	69
1176	4{28,461,7}	CCN1N=CC(=C1F)C1=C(NC2CCOCC2)N2C=CC(=CC2=N1)C1=NOC=N1 c:3,5,9,20,22,25,31,t:28	Z8873684724	1{28}	Cl.Nc1cc(ccn1)c2ncon2	2{461}	CCn1ncc(C=O)c1F	3{7}	[C-] #[N+]C1CC OCC1	73.7	69
1177	4{362,594,12}	CNC(=O)C1=CC=CC2=NC(=C(NCC3CCOC3)N12)C1=CC=C(C=C1)N(C)C c:6,25,27,t:4,8,10,23	Z8855739195	1{362}	CNC(=O)c1cccc(N)n1	2{594}	CN(C)c1ccc(C=O)cc1	3{12}	[C-] #[N+]CC1C COC1	72.9	69
1178	4{50,595,7}	CN1C=C2C=C(C=CC2=N1)C1=C(NC2CCOC2)N2C(C=CC=C2P(C)(C)=O)=N1 c:4,6,9,12,24,26,32,t:2	Z8878918460	1{50}	CP(=O)(C)c1cccc(N)n1	2{595}	Cn1cc2cc(C=O)ccc2n1	3{7}	[C-] #[N+]C1CC OCC1	77.4	68
1179	4{109,335,41}	COC1=CC=C(NC2=C(N=C3C=CC=C(N23)S(N)(=O)=O)C2=CN(N=C2)C2CCOCC2)C=C1 c:11,13,25,35,t:2,4,7,9,22	Z8855739105	1{109}	Cl.Nc1cccc(n1)S(=O)(=O)N	2{335}	O=Cc1cnn(cc1)C2CCOCC2	3{41}	COc1ccc([N+]#[C-])cc1	84.6	67
1180	4{37,596,12}	CN1N=C(C)C2=C1N=CC(=C2)C1=C(NCC2COC2)N2C(C=CC=C2C(F)F)=N1 c:5,8,10,13,25,27,32,t:2	Z8873685247	1{37}	Cl.Nc1cccc(n1)C(F)F	2{596}	Cc1nn(C)c2ncc(C=O)cc12	3{12}	[C-] #[N+]CC1C COC1	73.7	66
1181	4{42,192,7}	COC1=NC(=CC=C1)C1=C(NC2CCOCC2)N2C=C(SC)C=CC2=N1 c:4,6,9,24,27,t:2,20	Z8855619653	1{42}	CSc1ccc(N)nc1	2{192}	COc1cccc(C=O)n1	3{7}	[C-] #[N+]C1CC OCC1	65.2	65
1182	4{125,597,7}	CC1=C(C)N=C(O1)C1=C(NC2CCOCC2)N2C=C(CCO)C=CC2=N1 c:1,4,8,24,27,t:19	Z8873685318	1{125}	Nc1ccc(CC)ocn1	2{597}	Cc1nc(C=O)oc1C	3{7}	[C-] #[N+]C1CC OCC1	62.6	65
1183	4{333,152,29}	CCOC(=O)CCNC1=C(N=C2C=CC=C(N12)C1=CC=NC=C1)C(C)CCC(=O)OC c:12,14,21,23,t:8,10,19	Z8878918843	1{333}	Nc1cccc(n1)c2ccncc2	2{152}	COC(=O)CC(C)C=O	3{29}	CCOC(=O)C C[N+]#[C-]	73.1	64

1184	4{432,452,22}	CC1=CC2=NC(=C(NC3COC3)N2C=C1I)C1=CC=C(C=C1)C(N)=O c:15,21,23,t:1,3,5,19	Z8835022888	1{432}	Cc1cc(N)nc1	2{452}	NC(=O)c1ccc(C=O)cc1	3{22}	[C-]]#[N+]C1CO C1	76.9	64
1185	4{414,598,10}	COC1=CC(OC)=C(C2=C(NC3CCOC3)N3C=C(CI)N=CC3=N2)C(C)=C1 c:8,21,24,28,t:2,6,18	Z8878918855	1{414}	Nc1cnc(Cl)cn1	2{598}	COc1cc(C)c(C=O)c(OC)c1	3{10}	[C-]]#[N+]C1CC OC1	66.7	64
1186	4{50,599,7}	CC1=CC(=CC(C)=C1OC(F)F)C1=C(NC2CCOCC2)N2C(C=CC=C2P(C)(C)=O)=N1 c:3,6,13,25,27,33,t:1	Z8873684592	1{50}	CP(=O)(C)c1cccc(N)n1	2{599}	Cc1cc(C=O)cc(C)c1OC(F)F	3{7}	[C-]]#[N+]C1CC OCC1	79.2	63
1187	4{36,30,13}	COC1=CC=C(CNC2=C(N=C3C=CC(Br)=CN23)C2CCN(CC2)C(C)=O)C=C1 c:12,15,30,t:2,4,8,10	Z8835022908	1{36}	Nc1ccc(Br)cn1	2{30}	CC(=O)N1C CC(CC1)C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	77.7	63
1188	4{105,600,50}	CS(=O)(=O)CCN1C=C(C=N1)C1=C(NC2=CC3=C(OCCO3)C=C2)N2C(C=CC=C2C(N)=O)=N1 c:7,9,12,24,29,31,36,t:15,17	Z8829498490	1{105}	NC(=O)c1cccc(N)n1	2{600}	CS(=O)(=O) CCn1cc(C=O) cn1	3{50}	[C-]]#[N+]c1ccc 2OCCOc2c1	81.3	62
1189	4{73,24,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC4=NC=CN4N23)C2=CC(=CC=C2)N(C)C)C=C1 c:12,16,25,27,33,t:2,5,8,10,14,23	Z8873685335	1{73}	Nc1ccc2nccn2n1	2{24}	CN(C)c1cccc(C=O)c1	3{20}	COc1ccc([N +]#[C-])c(C)c1	69.5	62
1190	4{50,601,7}	CC1=C(C=CC(=C1)C1=C(NC2CCOCC2)N2C(C=CC=C2P(C)(C)=O)=N1)C1CC1 c:3,5,8,20,22,28,t:1	Z8873684736	1{50}	CP(=O)(C)c1cccc(N)n1	2{601}	Cc1cc(C=O)ccc1C2CC2	3{7}	[C-]]#[N+]C1CC OCC1	67.6	62
1191	4{118,422,32}	CC(O)C1=CC=CC2=NC(C3CC33CCOC3)=C(NC3CCC3)N12 c:5,t:3,7,18	Z8855739136	1{118}	Cl.CC(O)c1cccc(N)n1	2{422}	O=CC1CC21 CCOC2	3{32}	[C-]]#[N+]C1CC C1	54.4	62
1192	4{369,54,7}	COC1=C(C=CS1)C1=C(NC2CCOCC2)N2C=C(C=CC2=N1)C(F)C(F)(F)F c:4,8,19,21,24,t:2	Z8873684631	1{369}	Cl.Nc1ccc(cn1)C(F)C(F)(F)F	2{54}	COc1sccc1C=O	3{7}	[C-]]#[N+]C1CC OCC1	71.3	61
1193	4{118,602,31}	CSCCN1=C(N=C2C=CC=C(C(C)O)N12)C1=CC=C(C=C1)C(=O)NC1CC1 c:9,21,23,t:5,7,11,19	Z8878918307	1{118}	Cl.CC(O)c1cccc(N)n1	2{602}	O=Cc1ccc(cc1)C(=O)NC2 CC2	3{31}	CSCC[N+]#[C-]	67.9	61
1194	4{394,603,12}	COC(=O)C1=CC(=NS1)C1=C(NCC2CCOC2)N2C(C=CC(C=C)=C2F)=N1 c:6,10,22,26,29,t:4	Z8873685487	1{394}	Nc1ccc(C=C)c(F)n1	2{603}	COC(=O)c1cc(C=O)ns1	3{12}	[C-]]#[N+]CC1C COC1	66.3	61
1195	4{50,604,7}	CCN1N=C(C2=C1C=CC=C2)C1=C(NC2CCOCC2)N2C(C=CC=C2P(C)(C)=O)=N1 c:3,5,8,10,13,25,27,33	Z8873684666	1{50}	CP(=O)(C)c1cccc(N)n1	2{604}	CCn1nc(C=O)c2cccc12	3{7}	[C-]]#[N+]C1CC OCC1	71.3	60

1196	4{28,340,18}	CCN1C=NC(=N1)C1=C(NC(C)(C)C)N2C=CC(=CC2=N1)C1=NOC=N1 c:3,5,8,16,18,21,27,t:24	Z8878918333	1{28}	Cl.Nc1cc(ccn1)c2ncon2	2{340}	CCn1cnc(C=O)n1	3{18}	CC(C)(C)[N+][C-]	57.4	60
1197	4{142,605,10}	COC1=C(C=CC(=C1)C(F)F)C1=C(NC2CCOC2)N2C=CC=C(OCCS(C)(=O)=O)C2=N1 c:4,6,12,22,34,t:2,24	Z8878918427	1{142}	CS(=O)(=O)CCOc1cccn1N	2{605}	COc1ccc(cc1C=O)C(F)F	3{10}	[C-]#[N+]C1CCOC1	78.3	60
1198	4{431,16,10}	CN1N=CC(CNC(=O)OC(C)(C)C)=C1C1=C(NC2CCOC2)N2C=C(F)C=CC2=N1 c:2,13,16,29,32,t:26	Z8878918826	1{431}	Nc1ccc(F)c n1	2{16}	Cn1ncc(CNC(=O)OC(C)(C)C)c1C=O	3{10}	[C-]#[N+]C1CCOC1	69.8	60
1199	4{431,606,10}	CC(C)(C)OC(=O)N1CC(C2=C(NC3CCOC3)N3C=C(F)C=CC3=N2)C2(CC2)C1 c:10,23,26,t:20	Z8878918807	1{431}	Nc1ccc(F)c n1	2{606}	CC(C)(C)OC(=O)N1CC(C=O)C2(CC2)C1	3{10}	[C-]#[N+]C1CCOC1	67.5	60
1200	4{125,64,31}	CSCNC1=C(N=C2C=CC(CCO)=CN12)C1=CC=C(C=C1)N1C=CN=C1 c:9,14,21,23,27,29,t:5,7,19	Z8873684773	1{125}	Nc1ccc(CCO)n1	2{64}	O=Cc1ccc(cc1)n2ccnc2	3{31}	CSCC[N+][C-]	63.7	60
1201	4{69,328,21}	CCC1=NNC=C1C1=C(NCC2CC2)N2C=CC(=CC2=N1)C(=O)NC c:5,8,17,19,22,t:2	Z8878918912	1{69}	CNC(=O)c1ccnc(N)c1	2{328}	Cl.CCc1n[nH]cc1C=O	3{21}	[C-]#[N+]CC1CC1	54.7	60
1202	4{73,607,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC4=NC=CN4N23)C2=CN(N=C2)C(C)(C)C)C=C1 c:12,16,26,33,t:2,5,8,10,14,23	Z8878918447	1{73}	Nc1ccc2nccn2n1	2{607}	CC(C)(C)n1cc(C=O)c n1	3{20}	COc1ccc([N+][C-])c(C)c1	66.8	60
1203	4{142,608,10}	CS(=O)(=O)CCOC1=CC=CN2C(NC3CCOC3)=C(CC3(CCC3)C#N)N=C12 c:9,t:7,19,29	Z8878918597	1{142}	CS(=O)(=O)CCOc1cccn1N	2{608}	O=CCC1(CC1)C#N	3{10}	[C-]#[N+]C1CCOC1	66.7	59
1204	4{164,609,43}	CN(C)CC1=CC2=NC(=C(NC3CCN(CC3)C(=O)OC(C)(C)C)N2C=C1)C1=CSC=N1 c:27,33,t:4,6,8,30	Z8878918897	1{164}	CN(C)Cc1ccnc(N)c1	2{609}	O=Cc1csen1	3{43}	CC(C)(C)OC(=O)N1CCC(CC1)[N+][C-]	72.6	59
1205	4{353,610,15}	CCNC1=C(N=C2C=CC(NS(C)(=O)=O)=CN12)C1=C(F)C(F)=C(C=C1)C(=O)OC c:7,14,19,23,25,t:3,5	Z8873684834	1{353}	Cl.CS(=O)(=O)Nc1ccc(N)n1	2{610}	COC(=O)c1ccc(C=O)c(F)c1F	3{15}	CC[N+][C-]	67.4	59
1206	4{52,297,7}	CCN1N=C(C)C(=N1)C1=C(NC2CCOCC2)N2C=C(C=CC2=N1)C1(CC1)C(F)(F)F c:6,9,20,22,25,t:3	Z8878918531	1{52}	Nc1ccc(cn1)C2(CC2)C(F)(F)F	2{297}	CCn1nc(C)c(C=O)n1	3{7}	[C-]#[N+]C1CCOCC1	68.9	59

1207	4{125,124,31}	COC1=C(OCC2=C(C)ON=C2C)C=CC(=C1)C1=C(NCCSC)N2C=C(CCO)C=CC2=N1 c:2,6,10,14,16,19,32,35,t:27	Z8873684793	1{125}	Nc1ccc(CC O)cn1	2{124}	COc1cc(C=O))ccc1OCc2c(C)noc2C	3{31}	CSCC[N+]#[C-]	75.9	58
1208	4{64,611,49}	COC1=CC(=CC(OC)=C1)C1=C(NC2CC(F)(F) C2)N2C=C(C=CC2=N1)N1CCCS1(=O)=O c:4,8,11,22,24,27,t:2	Z8878918362	1{64}	Nc1ccc(cn1)N2CCCS2(=O)=O	2{611}	COc1cc(OC) cc(C=O)c1	3{49}	FC1(F)CC(C 1)[N+]#[C-]	75.1	58
1209	4{350,165,5}	COCCNC1=C(N=C2C=NC(=CN12)C1=CC= CC=C1)C1=NN(C=C1)[C@H]1C[C@H](C1)C(=O)OC r,c:10,12,19,21,27,t:6,8,17,24	Z8873684588	1{350}	Nc1enc(cn1)c2ccccc2	2{165}	COC(=O)[C @H]1C[C@ @H](C1)n2c cc(C=O)n2	3{5}	COCC[N+] #[C-]	72.2	58
1210	4{125,612,7}	CN(C)C1=C(F)C=C(C2=C(NC3CCOCC3)N3C =C(CCO)C=CC3=N2)C(F)=C1 c:3,8,24,27,31,t:6,19	Z8873685302	1{125}	Nc1ccc(CC O)cn1	2{612}	CN(C)c1cc(F))c(C=O)cc1F	3{7}	[C-]#[N+]C1CC OCC1	65.2	58
1211	4{433,472,7}	COC(=O)C1=CC2=C(C=NN2C=C1)C1=C(NC 2CCOCC2)N2C(C=CC(C#C)=C2C)=N1 c:8,12,15,27,31,34,t:4,6	Z8873685352	1{433}	Cc1nc(N)cc c1C#C	2{472}	COC(=O)c1c cn2ncc(C=O) c2c1	3{7}	[C-]#[N+]C1CC OCC1	67.2	58
1212	4{50,613,7}	CN1C=C2C=CC=C(C2=N1)C1=C(NC2CCOC C2)N2C(C=CC=C2P(C)(C)=O)=N1 c:4,6,9,12,24,26,32,t:2	Z8878918464	1{50}	CP(=O)(C)c 1cccc(N)n1	2{613}	Cn1cc2cccc(C=O)c2n1	3{7}	[C-]#[N+]C1CC OCC1	65.9	58
1213	4{371,614,12}	CC(C)CN1C=C(C=N1)C1=C(NCC2CCOC2)N 2C=CC=C(OCCCC#N)C2=N1 c:5,7,10,21,32,t:23	Z8878918368	1{371}	Nc1ncccc1 OCCCC#N	2{614}	CC(C)Cn1cc(C=O)cn1	3{12}	[C-]#[N+]CC1C COC1	65.7	58
1214	4{362,486,12}	CNC(=O)C1=CC=CC2=NC(=C(NCC3CCOC3)N12)C1=C(Cl)N=C(Cl)N1C c:6,23,t:4,8,10,26	Z8878918802	1{362}	CNC(=O)c1c cccc(N)n1	2{486}	Cn1c(Cl)nc(Cl)c1C=O	3{12}	[C-]#[N+]CC1C COC1	65.8	58
1215	4{71,615,21}	IC1=CN2C(C=N1)=NC(C1=CN(N=C1)C1=NC =CC=C1)=C2NCC1CC1 c:5,7,13,18,20,22,t:1,10,16	Z8878918800	1{71}	Nc1nc(I)cn 1	2{615}	O=Cc1nnc(1)c2ccccn2	3{21}	[C-]#[N+]CC1C C1	71.0	58
1216	4{92,616,7}	CCOC1=C(OC(F)F)C=CC(=C1)C1=C(NC2CC OCC2)N2C=CC(=CC2=N1)C(N)=O c:3,9,11,14,25,27,30	Z8873685472	1{92}	NC(=O)c1c cnc(N)c1	2{616}	CCOc1cc(C= O)ccc1OC(F) F	3{7}	[C-]#[N+]C1CC OCC1	69.3	57
1217	4{64,617,49}	CC(C)C1=NNC(=C1)C1=C(NC2CC(F)(F)C2) N2C=C(C=CC2=N1)N1CCCS1(=O)=O c:6,9,20,22,25,t:3	Z8846491763	1{64}	Nc1ccc(cn1)N2CCCS2(=O)=O	2{617}	CC(C)c1cc(C =O)[nH]n1	3{49}	FC1(F)CC(C 1)[N+]#[C-]	69.7	57
1218	4{362,618,10}	CNC(=O)C1=CC=CC2=NC(=C(NC3CCOC3) N12)C1=C(C)C=C(C=C1)C(F)F c:6,22,25,27,t:4,8,10	Z8835022880	1{362}	CNC(=O)c1c cccc(N)n1	2{618}	Cc1cc(ccc1C =O)C(F)F	3{10}	[C-]#[N+]C1CC OC1	61.9	57

1219	4{164,619,12}	COC1=C(SC)C=CC(=C1)C1=C(NCC2CCOC2)N2C=CC(CN(C)C)=CC2=N1 c:2,6,8,11,22,28,31	Z8878918823	1{164}	CN(C)Cc1ccnc(N)c1	2{619}	COe1ccc(C=O)ccc1SC	3{12}	[C-]#[N+]CC1COC1	65.9	57
1220	4{412,531,12}	CC1=NC=C(C=N1)C1=C(NCC2CCOC2)N2C=C(Br)C(CO)=CC2=N1 c:3,5,8,24,27,t:1,19	Z8873685276	1{412}	Nc1cc(CO)c(Br)cn1	2{531}	Cc1nccc(C=O)cn1	3{12}	[C-]#[N+]CC1COC1	64.5	57
1221	4{69,33,51}	CNC(=O)C1=CC2=NC(C3CCCN(C3)C(C)=O)=C(NCCNC(=O)OC(C)(C)C)N2C=C1 c:33,t:4,6,18	Z8829498629	1{69}	CNC(=O)c1ccnc(N)c1	2{33}	CC(=O)N1C CCC(C1)C=O	3{51}	CC(C)(C)OC(=O)NCC[N+]#[C-]	70.7	57
1222	4{386,42,5}	COCCCN1=C(N=C2C=C(C)C=CN12)C1=CN(C)N=C1Cl c:13,22,t:6,8,10,18	Z8855739213	1{386}	Cc1ccnc(N)c1	2{42}	Cn1cc(C=O)c(Cl)n1	3{5}	COCCCN[+]#[C-]	51.3	57
1223	4{286,620,5}	COCCCN1=C(N=C2C=CC(=CN12)C1=NC=CC=C1)C1=C(Cl)N(C)N=C1 c:10,12,19,21,24,29,t:6,8,17	Z8873684813	1{286}	Cl.Cl.Nc1ccc(en1)c2cccn2	2{620}	Cn1nccc(C=O)c1Cl	3{5}	COCCCN[+]#[C-]	61.0	57
1224	4{107,621,43}	CC1=C(N=CC=C1)C1=C(NC2CCN(CC2)C(=O)OC(C)(C)C)N2C=C(OCCO)C=CC2=N1 c:3,5,8,32,35,t:1,26	Z8878918760	1{107}	Nc1ccc(OC CO)cn1	2{621}	Cc1cccnc1C=O	3{43}	CC(C)(C)OC(=O)N1CCC(CC1)[N+]#[C-]	71.8	57
1225	4{333,219,23}	COC(=O)CCC(NC1=C(N=C2C=CC=C(N12)C1=CC=NC=C1)C1=CN(C)C(=C1)C#N)C(=O)OC c:12,14,21,23,30,t:8,10,19,26	Z8878918787	1{333}	Nc1cccc(n1)c2ccncc2	2{219}	Cn1cc(C=O)cc1C#N	3{23}	COC(=O)CC(C[N+]#[C-])C(=O)OC	72.6	57
1226	4{434,54,7}	COC1=C(C=CS1)C1=C(NC2CCOCC2)N2C=C(C=CC2=N1)C(C)(F)F c:4,8,19,21,24,t:2	Z8878918451	1{434}	CC(F)(F)c1ccc(N)nc1	2{54}	COc1secc1C=O	3{7}	[C-]#[N+]C1CCOCC1	60.2	57
1227	4{371,622,12}	CCNC(=O)COC1=CC=C(C=C1)C1=C(NCC2CCOC2)N2C=CC=C(OCCCC#N)C2=N1 c:9,11,14,25,36,t:7,27	Z8873684585	1{371}	Nc1ncccc1OCCCC#N	2{622}	CCNC(=O)COc1ccc(C=O)cc1	3{12}	[C-]#[N+]CC1COC1	73.0	57
1228	4{167,623,5}	COCCCN1=C(N=C2N1C(C)=CN=C2C)C1=C(OC)C=C(OCC#N)C=C1 c:8,13,15,19,29,t:6,23	Z8878918766	1{167}	Cc1enc(C)c(N)n1	2{623}	COe1cc(OC C#N)ccc1C=O	3{5}	COCCCN[+]#[C-]	60.5	57
1229	4{48,624,15}	CCNC1=C(N=C2C=C(C=CN12)S(C)(=O)=O)C1=C(C)NN=C1Br c:7,9,18,22,t:3,5	Z8846492000	1{48}	CS(=O)(=O)c1ccnc(N)c1	2{624}	Cc1[nH]nc(Br)c1C=O	3{15}	CC[N+]#[C-]	60.9	57
1230	4{187,164,12}	CN1N=C(C2=C1CCOC2)C1=C(NCC2CCOC2)N2C=C(Cl)C(=CC2=N1)C#N c:2,4,12,26,29,t:23	Z8878918577	1{187}	Nc1cc(C#N)c(Cl)cn1	2{164}	Cn1nc(C=O)c2COCCc21	3{12}	[C-]#[N+]CC1COC1	63.1	57

1231	4{357,452,49}	NC(=O)C1=CC=C(C=C1)C1=C(NC2CC(F)(F)C2)N2C=C(C=CC2=N1)N1CCCC(CO)CC1 c:5,7,10,21,23,26,t:3	Z8873685383	1{357}	Nc1ccc(en1)N2CCC(CO)CC2	2{452}	NC(=O)c1ccc(C=O)cc1	3{49}	FC1(F)CC(C1)[N+]#[C-]	69.6	57
1232	4{92,361,7}	NC(=O)C1=CC2=NC(=C(NC3CCOCC3)N2C=C1)C1=C(Br)C=CC(Br)=N1 c:19,22,25,28,t:3,5,7	Z8837933172	1{92}	NC(=O)c1cnc(N)c1	2{361}	Br1ccc(Br)c(C=O)n1	3{7}	[C-]#[N+]C1CCOCC1	75.7	57
1233	4{212,425,49}	COCC1=CN2C(C=C1)=NC(C1CCCN(C1)S(C)(=O)=O)=C2NC1CC(F)(F)C1 c:7,9,22,t:3	Z8878918794	1{212}	Cl.COCc1ccc(N)nc1	2{425}	CS(=O)(=O)N1CCCC(C1)C=O	3{49}	FC1(F)CC(C1)[N+]#[C-]	65.5	57
1234	4{435,219,23}	COC(=O)CCC(NC1=C(N=C2N1C=C(Br)C=C2)C1=CN(C)C(=C1)C#N)C(=O)OC c:10,17,25,t:8,14,21	Z8873685363	1{435}	Cc1ccc(Br)cn1N	2{219}	Cn1cc(C=O)cc1C#N	3{23}	COC(=O)CC(C([N+]#[C-])C(=O)OC	74.6	57
1235	4{118,625,31}	COC1=C(OCC2=CN=CC=C2)C=C(C=C1)C1=C(NCCSC)N2C(C=CC=C2C(C)O)=N1 c:2,8,10,13,15,18,27,29,34,t:6	Z8878918332	1{118}	Cl.CC(O)c1cccc(N)n1	2{625}	COc1ccc(C=O)cc1OCc2ccnc2	3{31}	CSCC[N+]#[C-]	70.8	56
1236	4{69,392,46}	CNC(=O)C1=CC2=NC(C3CCOCC3)=C(NCC(C)=C)N2C=C1 c:24,t:4,6,15	Z8878918588	1{69}	CNC(=O)c1ccnc(N)c1	2{392}	O=CC1CCOCC1	3{46}	CC(=C)C[N+]#[C-]	49.8	56
1237	4{62,243,6}	CCOC(=O)CCCN1=C(N=C2C=C(CO)C=CN12)C1=CON=C1CC c:17,25,t:9,11,13,22	Z8835022875	1{62}	Nc1cc(CO)cn1	2{243}	CCc1nocc1C=O	3{6}	CCOC(=O)CC[N+]#[C-]	56.5	56
1238	4{436,585,23}	CCC1=CC2=NC(CC3CC3(C1)C1)=C(NC(CCC(=O)OC)C(=O)OC)N2C=C1 c:29,t:2,4,13	Z8878918311	1{436}	CCc1ccnc(N)c1	2{585}	ClC1(Cl)CC1CC=O	3{23}	COC(=O)CC(C([N+]#[C-])C(=O)OC	67.1	56
1239	4{40,626,22}	CC(=O)N1CCC2=C(C1)C=C(S2)C1=C(NC2COC2)N2C(C=C(C=C2)C(F)(F)F)=N1 c:6,10,14,24,26,33	Z8878918861	1{40}	Cc1cc(cc(N)n1)C(F)(F)F	2{626}	CC(=O)N1CCe2sc(C=O)cc2C1	3{22}	[C-]#[N+]C1COC1	63.3	56
1240	4{107,627,61}	CCC1=NC(C)=C(N1)C1=C(NCCCNC(=O)OC(C)(C)C)N2C=C(OCCO)C=CC2=N1 c:5,9,30,33,t:2,24	Z8878918682	1{107}	Nc1ccc(OC)CO)cn1	2{627}	CCc1nc(C)c(C=O)[nH]1	3{61}	CC(C)(C)OC(=O)NCCC[N+]#[C-]	69.3	56
1241	4{187,628,10}	COCC1=C(C=CC=C1)C1=C(NC2CCOC2)N2C=C(Cl)C(=CC2=N1)C#N c:5,7,10,23,26,t:3,20	Z8878918779	1{187}	Nc1cc(C#N)c(Cl)cn1	2{628}	COc1cccc1C=O	3{10}	[C-]#[N+]C1CCOC1	57.7	56
1242	4{351,629,39}	CCOCCN1=C(N=C2C=CC3=C(C(O)CC3)N12)C1=C(C)C=C(C)C=N1 c:10,22,28,t:6,8,12,25	Z8873684794	1{351}	Nc1ccc2CC(C(O)c2n1	2{629}	Cc1cnc(C=O)c(C)c1	3{39}	CCOCC[N+]#[C-]	55.2	56
1243	4{76,630,23}	COCCN1C=C(C=N1)C1=C(NC(CCC(=O)OC)C(=O)OC)N2C(C=CC(C)=C2Cl)=N1 c:5,7,10,26,29,32	Z8855739199	1{76}	Cc1ccc(N)nc1Cl	2{630}	COCCn1cc(C=O)cn1	3{23}	COC(=O)CC(C([N+]#[C-])C(=O)OC	69.8	56

1244	4{437,586,67}	CCC(C)NC1=C(N=C2C=CC3=C(NC(=N3)C(F)(F)F)N12)C1=CC2=C(COC2)N=C1 c:9,14,32,t:5,7,11,24,26	Z8835022891	1{437}	Cl.Nc1ccc2nc([nH]c2n1)C(F)(F)F	2{586}	O=Cc1cnc2COCc2c1	3{67}	CCC(C)[N+]#[C-]	62.7	56
1245	4{112,304,61}	COC1=CN=CC2=NC(=C(NCCCNC(=O)OC(C)(C)C)N12)C1=C(C)N(CC(F)F)N=C1 c:4,25,33,t:2,6,8	Z8829498762	1{112}	COc1cnc(N)n1	2{304}	Cc1c(C=O)cnn1CC(F)F	3{61}	CC(C)(C)OC(=O)NCCC[N+]#[C-]	70.0	56
1246	4{180,206,22}	COC(=O)C1=CC2=NC(C[C@H](C)NC(=O)OC(C)(C)C)=C(NC3COC3)N2C=C1C c:29,t:4,6,19	Z8878918791	1{180}	COC(=O)c1cc(N)nc1C	2{206}	C[C@@H](CC=O)NC(=O)OC(C)(C)C	3{22}	[C-]#[N+]C1CO C1	59.5	56
1247	4{109,631,34}	COC1=NC=C(C2=C(NCC3CCCO3)N3C(C=C)C=C3S(N)(=O)=O=N2)C(OC)=C1 c:6,18,20,26,31,t:2,4	Z8837933179	1{109}	Cl.Nc1cccc(n1)S(=O)(=O)N	2{631}	COc1cc(OC)c(C=O)cn1	3{34}	[C-]#[N+]CC1C CCO1	65.0	56
1248	4{363,305,38}	COCC1=NC(=CN1)C1=C(NC2=CC3=C(OCO3)C=C2)N2C=CC(=CC2=N1)C(=O)OC c:5,9,20,24,26,29,t:3,12,14	Z8849597828	1{363}	COC(=O)c1ccnc(N)c1	2{305}	COCC1nc(C=O)c[nH]1	3{38}	[C-]#[N+]c1ccc2OCOc2c1	63.0	55
1249	4{384,399,10}	CCOC1=C(C)N2C(NC3CCOC3)=C(N=C2C=C1)C1=CN(N=C1C)C1CC1 c:3,14,16,19,25,t:22	Z8878918784	1{384}	CCOc1ccc(N)nc1C	2{399}	Cc1nn(cc1C=O)C2CC2	3{10}	[C-]#[N+]C1CCOC1	57.1	55
1250	4{212,632,49}	COCC1=CN2C(C=C1)=NC(=C2NC1CC(F)F)C1)C1=C(OC)C=CC(F)=C1 c:7,9,11,22,26,29,t:3	Z8855739201	1{212}	Cl.COCC1ccc(N)nc1	2{632}	COc1ccc(F)c1C=O	3{49}	FC1(F)CC(C1)[N+]#[C-]	58.5	55
1251	4{105,357,34}	CCC1=C(C(C)=NO1)C1=C(NCC2CCCO2)N2C(C=CC=C2C(N)=O)=N1 c:5,9,21,23,28,t:2	Z8837933175	1{105}	NC(=O)c1ccc(N)n1	2{357}	CCc1onc(C)c1C=O	3{34}	[C-]#[N+]CC1C CCO1	55.2	55
1252	4{327,633,41}	COC(=O)C1=C(F)C2=NC(=C(NC3=CC=C(OC)C=C3)N2C=C1)C1=CN=C1OC c:4,18,23,29,t:7,9,12,14,26	Z8878918608	1{327}	COC(=O)c1ccnc(N)c1F	2{633}	COc1n[nH]c1C=O	3{41}	COc1ccc([N+]#[C-])cc1	61.5	55
1253	4{42,153,7}	CSC1=CN2C(NC3CCOCC3)=C(N=C2C=C1)C1=CN(CC(F)F)N=N1 c:13,15,18,29,t:2,21	Z8855619755	1{42}	CSc1ccc(N)nc1	2{153}	FC(F)(F)Cn1cc(C=O)nn1	3{7}	[C-]#[N+]C1CCOCC1	61.6	55
1254	4{187,314,51}	CC(C)(C)OC(=O)NCCNC1=C(N=C2C=C(C#N)C(CI)=CN12)C1=CN=C1 c:20,28,t:11,13,15,25	Z8873685419	1{187}	Nc1cc(C#N)c(Cl)cn1	2{314}	O=Cc1cn[nH]c1	3{51}	CC(C)(C)OC(=O)NCC[N+]#[C-]	59.9	55
1255	4{368,425,49}	CN1C=C(C=N1)C1=C(C)N2C(C=C1)=NC(C1CCCN(C1)S(C)(=O)=O)=C2NC1CC(F)(F)C1 c:2,4,7,12,14,27	Z8878918422	1{368}	Cc1nc(N)cc1c2cnn(C)c2	2{425}	CS(=O)(=O)N1CCCC(C1)C=O	3{49}	FC1(F)CC(C1)[N+]#[C-]	71.4	55

1256	4{118,634,31}	CSCCNC1=C(N=C2C=CC=C(C(C)O)N12)C(C)C1CCOCC1 c:9,t:5,7,11	Z8873684888	1{118}	Cl.CC(O)c1cccc(N)n1	2{634}	CC(C=O)C1CCOCC1	3{31}	CSCC[N+][C-]	54.2	55
1257	4{109,635,34}	CCOC(=O)C1=COC(=C1)C1=C(NCC2CCCO2)N2C(C=CC=C2S(N)(=O)=O)=N1 c:8,11,23,25,31,t:5	Z8878918497	1{109}	Cl.Nc1cccc(n1)S(=O)(=O)N	2{635}	CCOC(=O)c1coc(C=O)c1	3{34}	[C-]#[N+]CC1COCO1	64.7	55
1258	4{28,310,18}	CC(C)(C)NC1=C(N=C2C=C(C=CN12)C1=NO)C=N1)C1CCOC2(CCC2)C1 c:9,11,19,t:5,7,16	Z8878918576	1{28}	Cl.Nc1cc(ccn1)c2ncon2	2{310}	O=CC1CCOC2(CCC2)C1	3{18}	CC(C)(C)[N+][C-]	56.8	55
1259	4{80,233,62}	COC(=O)C1(CCCC1)NC1=C(CCCOCC=C)N=C2N1C=CN=C2OC c:11,20,24,26	Z8855739111	1{80}	COc1ncnc1N	2{233}	C=CCOCCC=O	3{62}	COC(=O)C1(CCCC1)[N+][C-]	57.9	55
1260	4{353,138,53}	CC1=NC(C)=NC(=C1)C1=C(NCCOCC2=CC=CC=C2)N2C=C(NS(C)(=O)=O)C=CC2=N1 c:4,6,9,18,20,31,34,t:1,16,24	Z8878918620	1{353}	Cl.CS(=O)(=O)Nc1ccc(N)nc1	2{138}	Cc1cc(C=O)nc(C)n1	3{53}	[C-]#[N+]CCOCc1cccc1	69.5	55
1261	4{64,636,33}	COC1=C(CNC2=C(N=C3C=CC(=CN23)N2CCS2(=O)=O)C2=CN(C)N=C2)C=CC=C1 c:2,10,12,29,32,34,t:6,8,25	Z8878918493	1{64}	Nc1ccc(en1)N2CCCS2(=O)=O	2{636}	Cn1cc(C=O)cn1	3{33}	COc1cccc1C[N+][C-]	67.3	55
1262	4{104,637,46}	CC(=C)CNC1=C(N=C2C=CC3=C(COCC3)N12)C1=CC2=C(C=C1)S(=O)(=O)CCC2 c:9,23,25,t:5,7,11,21	Z8835022899	1{104}	Nc1ccc2CCOCc2n1	2{637}	O=Cc1ccc2c(CCCS2(=O)=O)c1	3{46}	CC(=C)C[N+][C-]	63.0	55
1263	4{438,314,12}	CCC1=C(Br)C=CC2=NC(C3=CNN=C3)=C(NCC3CCOC3)N12 c:2,5,13,t:7,10,15	Z8878918792	1{438}	CCc1nc(N)ccc1Br	2{314}	O=Cc1cn[nH]c1	3{12}	[C-]#[N+]CC1COC1	58.0	55
1264	4{99,638,34}	NS(=O)(=O)C1=CN2C(NCC3CCCO3)=C(N=C2C=C1)C1=CN(CC2CCOCC2)N=C1 c:15,17,20,34,t:4,23	Z8855739112	1{99}	Nc1ccc(en1)S(=O)(=O)N	2{638}	O=Cc1cnn(C2CCOCC2)c1	3{34}	[C-]#[N+]CC1COCO1	68.4	55
1265	4{123,277,22}	CC(C)(C)OC(=O)NC(CC1=C(NC2COC2)N2C=CC(OCCO)=CC2=N1)C1CC1 c:10,19,25,28	Z8878918908	1{123}	Cl.Nc1cc(OCCO)ccn1	2{277}	CC(C)(C)OC(=O)NC(CC(=O)C1CC1	3{22}	[C-]#[N+]C1COC1	59.2	55
1266	4{91,639,7}	CC1=NN=C(O1)C1=CC(=CC=C1)C1=C(NC2CCOCC2)N2C=C(C=CC2=N1)C(N)=O c:3,9,11,14,25,27,30,t:1,7	Z8873684799	1{91}	NC(=O)c1ccc(N)nc1	2{639}	Cc1nnc(o1)c2cccc(C=O)c2	3{7}	[C-]#[N+]C1CCOCC1	62.1	55
1267	4{49,63,13}	COCN1N=CC=C1C1=C(NCC2=CC=C(OC)C=C2)N2C(C=CC=C2CO)=N1 c:4,6,9,19,24,26,30,t:13,15	Z8873684609	1{49}	Nc1cccc(CO)n1	2{63}	COc1ncccc1C=O	3{13}	COc1ccc(C[N+][C-])cc1	58.4	55

1268	4{97,280,49}	CC1=CC(F)=CN2C(NC3CC(F)(F)C3)=C(N=C12)C1=NSC(=C1)[N+](=[O-])=O c:4,15,24,t:1,17,21	Z8837933162	1{97}	Cc1cc(F)cn c1N	2{280}	[O-]][N+](=O)c1 cc(C=O)ns1	3{49}	FC1(F)CC(C 1)[N+]#[C-]	56.9	55
1269	4{69,596,61}	CNC(=O)C1=CC2=NC(=C(NCCCNC(=O)OC(C) (C)C)N2C=C1)C1=CC2=C(N=C1)N(C)N=C 2C c:24,29,31,36,t:4,6,8,27	Z8873685321	1{69}	CNC(=O)c1 ccnc(N)c1	2{596}	Cc1nn(C)c2n cc(C=O)cc12	3{61}	CC(C)(C)OC (=O)NCCC[N+]#[C-]	73.1	55
1270	4{32,640,7}	CC(C)N1C=C(N=N1)C1=C(NC2CCOCC2)N2 C=CC(=CC2=N1)P(C)(C)=O c:4,6,9,20,22,25	Z8878918430	1{32}	CP(=O)(C)c 1ccnc(N)c1	2{640}	CC(C)n1cc(C =O)nn1	3{7}	[C-]]#[N+]C1CC OCC1	59.6	55
1271	4{37,641,10}	CC1=NC(C)=C(S1)C1=C(NC2CCOC2)N2C(C =CC=C2C(F)F)=N1 c:4,8,19,21,26,t:1	Z8878918319	1{37}	Cl.Nc1cccc(n1)C(F)F	2{641}	Cc1nc(C)c(C =O)s1	3{10}	[C-]]#[N+]C1CC OC1	54.0	55
1272	4{77,35,23}	COC(=O)CCC(NC1=C(N=C2C=CC(=CN12)C 1=CN=CC=C1)C1=NN(C)C(C)=C1Cl)C(=O)O C c:12,14,21,23,31,t:8,10,19,26	Z8854581168	1{77}	Nc1ccc(en1)c2cccnc2	2{35}	Cc1c(Cl)c(C =O)nn1C	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	73.5	55
1273	4{49,112,6}	CCOC(=O)CCCNC1=C(N=C2C=CC=C(CO)N 12)C1=C2C=CC=NN2N=C1 c:13,22,24,26,30,t:9,11,15	Z8849597835	1{49}	Nc1cccc(C O)n1	2{112}	O=Cc1cnn2n cccc12	3{6}	CCOC(=O)C CC[N+]#[C-]	58.3	55
1274	4{92,642,7}	CC1=C(C=C(Br)S1)C1=C(NC2CCOCC2)N2C =CC(=CC2=N1)C(N)=O c:8,19,21,24,t:1,3	Z8837933167	1{92}	NC(=O)c1c cnc(N)c1	2{642}	Cc1sc(Br)cc1 C=O	3{7}	[C-]]#[N+]C1CC OCC1	64.4	55
1275	4{439,164,12}	CN1N=C(C2=C1CCOC2)C1=C(NCC2CCOC2)N2C=CC=C(OCC3=CC=CC=C3)C2=N1 c:2,4,12,23,31,33,37,t:25,29	Z8878918613	1{439}	Nc1ncccc1 OCc2cccc2	2{164}	Cn1nc(C=O) c2COCCc21	3{12}	[C-]]#[N+]CC1C COC1	67.9	55
1276	4{125,643,7}	CC1=C(Br)C=C(O1)C1=C(NC2CCOCC2)N2C =C(CCO)C=CC2=N1 c:1,4,8,24,27,t:19	Z8873685294	1{125}	Nc1ccc(CC O)cn1	2{643}	Cc1oc(C=O) cc1Br	3{7}	[C-]]#[N+]C1CC OCC1	62.1	55
1277	4{50,644,7}	CP(C)(=O)C1=CC=CC2=NC(=C(NC3CCOCC 3)N12)C1=CC(F)=C(OCC#C)C=C1 c:6,32,t:4,8,10,23,26	Z8878918412	1{50}	CP(=O)(C)c 1cccc(N)n1	2{644}	Fc1cc(C=O)c cc1OCC#C	3{7}	[C-]]#[N+]C1CC OCC1	65.2	55
1278	4{105,382,50}	COC(C)(C)CC1=C(NC2=CC3=C(OCCO3)C= C2)N2C(C=CC=C2C(N)=O)=N1 c:6,18,23,25,30,t:9,11	Z8878918605	1{105}	NC(=O)c1c ccc(N)n1	2{382}	COC(C)(C)C C=O	3{50}	[C-]]#[N+]c1ccc 2OCCOc2c1	58.5	55
1279	4{267,353,23}	COC(=O)CCC(NC1=C(N=C2C=CC=C(C#C)N 12)C1=C(CF)C=CC=C1)C(=O)OC c:12,21,25,27,t:8,10,14	Z8878918888	1{267}	Nc1cccc(C# C)n1	2{353}	FCc1cccc1 C=O	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	62.4	55

1280	4{66,299,22}	COCCC1=CC2=NC(=C(NC3COC3)N2C=C1)C1=C(OC)C(OC)=CC=C1F c:18,21,27,29,t:4,6,8	Z8873684894	1{66}	COCCc1ccn c(N)c1	2{299}	COc1ccc(F)c (C=O)c1OC	3{22}	[C-] #[N+]C1CO C1	59.0	54
1281	4{405,535,23}	COC(=O)CCC(NC1=C(N=C2C=CC(=CN12)N1CCCC1=O)C1=NOC(=C1)C(C)(C)O)C(=O)OC c:12,14,29,t:8,10,26	Z8835022904	1{405}	Nc1ccc(cn1))N2CCCC2 =O	2{535}	CC(C)(O)c1c c(C=O)no1	3{23}	COC(=O)CC C([N+]#[C-]) C(=O)OC	73.4	54
1282	4{125,645,36}	COC(=O)[C@@H]1CC(CN1C(=O)OC(C)(C)C)NC1=C(N=C2C=CC(CCO)=CN12)C1=CCN=N1 c:22,27,35,t:18,20,32	Z8873685427	1{125}	Nc1ccc(CC O)cn1	2{645}	O=Cc1c[nH] nn1	3{36}	COC(=O)[C @@H]1C[C @@H](CN1 C(=O)OC(C) (C)C)[N+]# C-]	69.3	54
1283	4{62,49,13}	COC1=CC=C(CNC2=C(N=C3C=C(CO)C=CN23)C2=CCN=C2C)C=C1 c:16,24,28,t:2,4,8,10,12,21	Z8873685386	1{62}	Nc1cc(CO)c cn1	2{49}	Cc1n[nH]cc1 C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	53.4	54
1284	4{377,622,12}	CCNC(=O)COC1=CC=C(C=C1)C1=C(NCC2COC2)N2C=CC=C(OCC(F)F)C2=N1 c:9,11,14,25,35,t:7,27	Z8873684829	1{377}	Nc1ncccc1 OCC(F)F	2{622}	CCNC(=O)C Oc1ccc(C=O)cc1	3{12}	[C-] #[N+]CC1C COC1	69.7	54
1285	4{69,646,12}	CNC(=O)C1=CC2=NC(=C(NCC3CCOC3)N2C=C1)C1=CNC(=N1)C1=CC=CC=C1 c:20,26,31,33,t:4,6,8,23,29	Z8854581158	1{69}	CNC(=O)c1 ccnc(N)c1	2{646}	O=Cc1c[nH] c(n1)c2cccc 2	3{12}	[C-] #[N+]CC1C COC1	61.1	54
1286	4{353,123,53}	CC1=NC=C(N=C1)C1=C(NCCOCC2=CC=CC=C2)N2C=C(NS(C)(=O)=O)C=CC2=N1 c:3,5,8,17,19,30,33,t:1,15,23	Z8878918609	1{353}	Cl.CS(=O)(=O)Nc1ccc(N)nc1	2{123}	Cc1nc(C=O)cn1	3{53}	[C-] #[N+]CCOC c1cccc1	66.3	54
1287	4{193,647,10}	CNC(=O)C1=CN2C(C=C1)=NC(=C2NC1CCO)C1)C1=CC2=C(OC=C2)C=C1 c:8,10,12,27,30,t:4,22,24	Z8878918315	1{193}	CNC(=O)c1 ccc(N)nc1	2{647}	O=Cc1ccc2o ccc2c1	3{10}	[C-] #[N+]C1CC OC1	55.2	54
1288	4{400,648,22}	CCC(CC1=C(NC2COC2)N2C=C(COC(C)C)C=CC2=N1)NC(=O)OC(C)(C)C c:4,20,23,t:13	Z8878918564	1{400}	CC(C)OCc1 ccc(N)nc1	2{648}	CCC(CC=O) NC(=O)OC(C)(C)C	3{22}	[C-] #[N+]C1CO C1	60.4	54
1289	4{440,649,10}	CN1N=C(C=C1)C1=C(NC2CCOC2)N2C(C=C)C=C2C1=N1)C(F)F c:2,4,7,18,20,23	Z8855739124	1{440}	Nc1cccc(Cl) n1	2{649}	Cn1nc(cc1C =O)C(F)F	3{10}	[C-] #[N+]C1CC OC1	53.8	54
1290	4{129,110,29}	CCOC(=O)CCNC1=C(N=C2C=CC=C(SC)N12)C1=CN=C(C=C1)P(C)(C)=O c:12,23,25,t:8,10,14,21	Z8873685433	1{129}	CSc1cccc(N) n1	2{110}	CP(=O)(C)c1 ccc(C=O)cn1	3{29}	CCOC(=O)C C[N+]#[C-]	63.3	54

1291	4{49,94,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC=C(CO)N23)C2=NC=CN=C2)C=C1 c:12,23,25,28,t:2,5,8,10,14,21	Z8878918384	1{49}	Ne1cccc(CO)n1	2{94}	O=Cc1cncn1	3{20}	COc1ccc([N+][C-])c(C)c1	52.9	54
1292	4{378,650,12}	C(NC1=C(N=C2N1C=CC=C2OCC1=CN=CC=C1)C1=CC2=C(CCOC2)C=C1)C1CCOC1 c:4,8,10,17,19,31,t:2,15,22,24	Z8878918324	1{378}	Ne1ncccc1OCc2ccnc2	2{650}	O=Cc1ccc2COCc2c1	3{12}	[C-][N+]CC1COC1	66.8	54
1293	4{41,651,14}	COCCNC1=C(N=C2C=NC(C)=CN12)C1=C(C)OC(C)=C1 c:9,12,17,22,t:5,7	Z8846492117	1{41}	Cc1cnc(N)c1	2{651}	Cc1cc(C=O)c(C)o1	3{14}	COCC[N+][C-]	43.9	54
1294	4{79,116,13}	COC1=CC=C(CNC2=C(N=C3C=NC=C(C)N23)C2=CN(CCC=C)N=N2)C=C1 c:12,27,30,t:2,4,8,10,14,20	Z8878918467	1{79}	Cc1cnc(N)n1	2{116}	C=CCcn1cc(C=O)nn1	3{13}	COc1ccc(C[N+][C-])cc1	56.8	54
1295	4{441,534,7}	CC(C)N1C=CC(=N1)C1=C(NC2CCOCC2)N2C=C(F)C(=CC2=N1)C(C)(F)F c:4,6,9,23,26,t:20	Z8878918385	1{441}	CC(F)(F)c1cc(N)ccc1F	2{534}	CC(C)n1ccc(C=O)n1	3{7}	[C-][N+]C1CCOCC1	59.4	54
1296	4{153,575,15}	CCNC1=C(CC(NC(=O)OC(C)(C)C(F)(F)F)N=C2C=CC=C(N12)C(C)(C)O c:3,21,23,t:19	Z8873684649	1{153}	CC(C)(O)c1cccc(N)n1	2{575}	CC(C)(C)OC(=O)NC(CC=O)C(F)(F)F	3{15}	CC[N+][C-]	62.7	54
1297	4{50,11,7}	CP(C)(=O)C1=CC=CC2=NC(=C(NC3CCOCC3)N12)C1=NN(CC(F)(F)F)C=C1 c:6,31,t:4,8,10,23	Z8878918428	1{50}	CP(=O)(C)c1cccc(N)n1	2{11}	FC(F)(F)Cn1ccc(C=O)n1	3{7}	[C-][N+]C1CCOCC1	64.3	54
1298	4{28,11,7}	FC(F)(F)CN1C=CC(=N1)C1=C(NC2CCOCC2)N2C=CC(=CC2=N1)C1=NOC=N1 c:6,8,11,22,24,27,33,t:30	Z8849597824	1{28}	Cl.Nc1cc(ccn1)c2ncon2	2{11}	FC(F)(F)Cn1ccc(C=O)n1	3{7}	[C-][N+]C1CCOCC1	63.0	54
1299	4{35,420,13}	COC1=CC=C(CNC2=C(CC(C)(C)C#N)N=C3C=CC(C)=CN23)C=C1 c:8,18,21,26,t:2,4,16	Z8837933159	1{35}	Cc1ccc(N)nc1	2{420}	CC(C)(CC=O)C#N	3{13}	COc1ccc(C[N+][C-])cc1	50.6	54
1300	4{50,652,31}	CSCCNC1=C(N=C2C=CC=C(N12)P(C)(C)=O)C1=CSC2=C1C(F)=CC=C2 c:9,11,23,27,29,t:5,7,20	Z8878918839	1{50}	CP(=O)(C)c1cccc(N)n1	2{652}	Fe1cccc2ccc(C=O)c12	3{31}	CSCC[N+][C-]	62.8	54
1301	4{362,497,10}	CCN1N=CC(C)=C1C1=C(NC2CCOCC2)N2C(C)=CC=C2C(=O)NC)=N1 c:3,6,9,20,22,28	Z8855619571	1{362}	CNC(=O)c1cccc(N)n1	2{497}	CCn1ccc(C)c1C=O	3{10}	[C-][N+]C1CCOC1	53.1	53
1302	4{104,144,46}	CC(=C)CNC1=C(N=C2C=CC3=C(COCC3)N12)C1=NOC(=C1)C1CC1 c:9,24,t:5,7,11,21	Z8829498719	1{104}	Ne1ccc2CCOCc2n1	2{144}	O=Cc1cc(on1)C2CC2	3{46}	CC(=C)C[N+][C-]	50.4	53

1303	4{46,181,13}	COC1=CC=C(CNC2=C(N=C3C=CC=CN23)C2=CN=C3CCCN23)C=C1 c:12,14,29,t:2,4,8,10,19,21	Z8829498470	1{46}	Nc1ccccn1	2{181}	O=Cc1cnc2CCn12	3{13}	COc1cccc([N+]#[C-])c1	51.7	53
1304	4{77,653,23}	COC(=O)CCC(NC1=C(N=C2C=CC(=CN12)C1=CN=CC=C1)C1C2CCC(F)(F)C12)C(=O)OC c:12,14,21,23,t:8,10,19	Z8835022901	1{77}	Nc1ccc(cn1)c2ccccc2	2{653}	FC1(F)CCC2C(C=O)C21	3{23}	COC(=O)CC([N+]#[C-])C(=O)OC	69.6	53
1305	4{367,600,34}	CC1=CN2C(NCC3CCCO3)=C(N=C2C(=C1)C#C)C1=CN(CCS(C)(=O)=O)N=C1 c:12,14,17,31,t:1,22	Z8873685409	1{367}	Cc1cnc(N)c(C#C)c1	2{600}	CS(=O)(=O)CCn1cc(C=O)cn1	3{34}	[C-]#[N+]CC1COCO1	61.4	53
1306	4{164,596,24}	COC1=CC(CNC2=C(N=C3C=C(CN(C)C)C=C N23)C2=CC3=C(N=C2)N(C)N=C3C)=CC=C1 c:17,24,26,31,34,36,t:2,7,9,11,22	Z8873684817	1{164}	CN(C)Cc1cnc(N)c1	2{596}	Cc1nn(C)c2ncc(C=O)cc12	3{24}	COc1cccc([N+]#[C-])c1	65.4	53
1307	4{50,374,26}	CP(C)(=O)C1=CC=CC2=NC(C3=CN(CC4CC4)N=N3)=C(NCC3=CC=C(F)C=C3)N12 c:6,19,30,t:4,8,11,21,25,27	Z8846492347	1{50}	CP(=O)(C)c1cccc(N)n1	2{374}	O=Cc1cn(CC2CC2)nn1	3{26}	Fc1ccc(C[N+]#[C-])c1	62.6	53
1308	4{372,6,12}	CC1=C(C2=C(NCC3CCOC3)N3C=CC=C(OC C4=CC=NC=C4)C3=N2)C(C)=NC=C1 c:1,3,14,22,24,28,32,34,t:16,20	Z8878918442	1{372}	Nc1ncccc1OCc2ccccc2	2{6}	Cc1ccnc(C)c1C=O	3{12}	[C-]#[N+]CC1COCO1	61.3	53
1309	4{107,334,24}	COC1=CC(CNC2=C(N=C3C=CC(OCCO)=CN23)C2=C(C)OC=N2)=CC=C1 c:11,17,22,26,28,30,t:2,7,9	Z8846491955	1{107}	Nc1ccc(OC CO)cn1	2{334}	Cc1ocnc1C=O	3{24}	COc1cccc([N+]#[C-])c1	56.3	53
1310	4{142,596,21}	CN1N=C(C)C2=C1N=CC(=C2)C1=C(NCC2C C2)N2C=CC=C(OCCS(C)(=O)=O)C2=N1 c:5,8,10,13,22,34,t:2,24	Z8878918663	1{142}	CS(=O)(=O)CCOc1cccn1N	2{596}	Cc1nn(C)c2ncc(C=O)cc12	3{21}	[C-]#[N+]CC1CC1	64.9	53
1311	4{105,654,50}	NC(=O)C1=CC=CC2=NC(CCC3=CN=CO3)=C(NC3=CC4=C(OCCO4)C=C3)N12 c:5,14,29,t:3,7,12,17,20,22	Z8873684669	1{105}	NC(=O)c1cccc(N)n1	2{654}	O=CCCc1cnco1	3{50}	[C-]#[N+]c1cccc2OCCO2c1	57.8	53
1312	4{193,655,12}	CNC(=O)C1=CN2C(NCC3CCOC3)=C(N=C2 C=C1)C1=C(Cl)C=CC=C1F c:15,17,20,23,26,28,t:4	Z8855739170	1{193}	CNC(=O)c1cccc(N)nc1	2{655}	Fc1cccc(Cl)c1C=O	3{12}	[C-]#[N+]CC1COCO1	57.4	53
1313	4{103,656,59}	CC1=NC(=C(C)S1)C1=C(NCCC2=CC(F)=CC= C2)N2C(C=NC=C2CO)=N1 c:8,16,18,23,25,29,t:1,3,13	Z8878918303	1{103}	Nc1cnc(C O)n1	2{656}	Cc1nc(C=O)c(C)s1	3{59}	Fc1cccc(CC[N+]#[C-])c1	56.6	53
1314	4{73,69,11}	CN1N=C(C=C1C)C1=C(NCC2=CC(Br)=CC=C2)N2N3C=CN=C3C=CC2=N1 c:2,4,8,15,17,22,24,27,30,t:12	Z8878918812	1{73}	Nc1ccc2ccn2n1	2{69}	Cc1cc(C=O)nn1C	3{11}	Br1cccc([N+]#[C-])c1	62.1	53

1315	4{442,294,5}	COCNC1=C(N=C2N1C=C(Cl)C=C2C)C1=C(OC)C(=O)C=CO1 c:8,15,19,25,t:6,12	Z8878918660	1{442}	Cc1cc(Cl)cn c1N	2{294}	COc1c(C=O) occc1=O	3{5}	COCNC1=C(N=C2N1C=C(Cl)C=C2C)C1=C(OC)C(=O)C=CO1	53.7	53
1316	4{50,153,7}	CP(C)(=O)C1=CC=CC2=NC(=C(NC3CCOCC3)N12)C1=CN(CC(F)(F)F)N=N1 c:6,31,t:4,8,10,23	Z8873684656	1{50}	CP(=O)(C)c 1cccc(N)n1	2{153}	FC(F)(F)Cn1 cc(C=O)nn1	3{7}	[C-] #[N+]C1CC OCC1	62.8	53
1317	4{50,639,26}	CC1=NN=C(O1)C1=CC(=CC=C1)C1=C(NCC2=CC=C(F)C=C2)N2C(C=CC=C2P(C)(C)=O)=N1 c:3,9,11,14,23,28,30,36,t:1,7,18,20	Z8873685338	1{50}	CP(=O)(C)c 1cccc(N)n1	2{639}	Cc1nnc(o1)c 2cccc(C=O)c 2	3{26}	Fe1ccc(C[N+] #[C-])cc1	67.5	53
1318	4{353,273,31}	CSCNC1=C(N=C2C=CC(NS(C)(=O)=O)=C N12)C1=C(Br)N(C)N=C1C c:9,16,21,26,t:5,7	Z8835022896	1{353}	Cl.CS(=O)(=O)Nc1ccc(N)nc1	2{273}	Cc1nn(C)c(B r)c1C=O	3{31}	CSCC[N+]#[C-]	67.2	53
1319	4{92,441,7}	CCC(C)C(OC)C1=C(NC2CCOCC2)N2C=CC(=CC2=N1)C(N)=O c:7,18,20,23	Z8873684751	1{92}	NC(=O)c1c cnc(N)c1	2{441}	CCC(C)C(O C)C=O	3{7}	[C-] #[N+]C1CC OCC1	51.1	52
1320	4{73,607,11}	CC(C)(C)N1C=C(C=N1)C1=C(NCC2=CC(Br)=CC=C2)N2N3C=CN=C3C=CC2=N1 c:5,7,10,17,19,24,26,29,32,t:14	Z8829498713	1{73}	Nc1ccc2ncc n2n1	2{607}	CC(C)(C)n1c c(C=O)cn1	3{11}	Br1cccc(C[N+]#[C-])c1	65.7	52
1321	4{357,657,49}	CC(C)N1C=C(C(C)=N1)C1=C(NC2CC(F)(F)C2)N2C=C(C=CC2=N1)N1CCC(CO)CC1 c:4,7,10,21,23,26	Z8873685401	1{357}	Nc1ccc(en1)N2CCC(C O)CC2	2{657}	CC(C)n1cc(C =O)c(C)n1	3{49}	FC1(F)CC(C 1)[N+]#[C-]	64.8	52
1322	4{362,658,21}	CNC(=O)C1=CC=CC2=NC(C3=CN=C(CNC(=O)OC(C)(C)C)S3)=C(NCC3CC3)N12 c:6,t:4,8,11,13,25	Z8878918429	1{362}	CNC(=O)c1 cccc(N)n1	2{658}	CC(C)(C)OC (=O)NCc1nc c(C=O)s1	3{21}	[C-] #[N+]CC1C C1	64.5	52
1323	4{50,659,6}	CCOC(=O)CCNC1=C(N=C2C=CC=C(N12)P(C)(C)=O)C1=CC=CC2=NN(C)C=C12 c:13,15,26,t:9,11,24,28,32	Z8835022890	1{50}	CP(=O)(C)c 1cccc(N)n1	2{659}	Cn1cc2c(C= O)cccc2n1	3{6}	CCOC(=O)C CC[N+]#[C-]	64.0	52
1324	4{69,660,10}	CNC(=O)C1=CC2=NC(=C(NC3CCOC3)N2C=C1)C1=NSC=C1 c:19,25,t:4,6,8,22	Z8873684835	1{69}	CNC(=O)c1 ccnc(N)c1	2{660}	O=Cc1ccsn1	3{10}	[C-] #[N+]C1CC OC1	48.4	52
1325	4{32,308,31}	CSCNC1=C(CCC2CCCC2)N=C2C=C(C=CN12)P(C)(C)=O c:5,17,19,t:15	Z8873685265	1{32}	CP(=O)(C)c 1ccnc(N)c1	2{308}	O=CCCC1C CCC1	3{31}	CSCC[N+]#[C-]	53.5	52
1326	4{443,135,49}	CN1N=C(C)C(=C1C)C1=C(NC2CC(F)(F)C2)N2C=C(Br)C(Cl)=CC2=N1 c:5,9,24,27,t:2,20	Z8878918557	1{443}	Nc1cc(Cl)c(Br)cn1	2{135}	Cc1nn(C)c(C)c1C=O	3{49}	FC1(F)CC(C 1)[N+]#[C-]	62.6	52

1327	4{444,326,10}	CN1N=CC=C1C1=C(NC2CCOC2)N2C=C3CC CCC3=CC2=N1 c:2,4,7,24,27,t:17	Z8878918320	1{444}	Nc1cc2CCC Cc2cn1	2{326}	Cn1ncce1C= O	3{10}	[C-]#[N+]C1CC OC1	47.5	52
1328	4{121,314,10}	BrC1=CC2=NC(C3=CN=C3)=C(NC3CCOC 3)N2C=C1 c:9,22,t:1,3,6,11	Z8855619525	1{121}	Nc1cc(Br)c cn1	2{314}	O=Cc1cn[nH]c1	3{10}	[C-]#[N+]C1CC OC1	49.0	52
1329	4{153,61,35}	CSCCNC1=C(N=C2C=CC=C(N12)C(C)(C)O)C1=CC=C(C=C1)S(C)=O c:10,12,23,25,t:6,8,21	Z8873685333	1{153}	CC(C)(O)c1 cccc(N)n1	2{61}	CS(=O)c1ccc (C=O)cc1	3{35}	CSCCC[N+] #[C-]	58.7	52
1330	4{153,437,15}	CCNC1=C(N=C2C=CC=C(N12)C(C)(C)O)C1 =CN(CC)N=C1C c:7,9,23,t:3,5,18	Z8873684807	1{153}	CC(C)(O)c1 cccc(N)n1	2{437}	CCn1cc(C=O)c(C)n1	3{15}	CC[N+]#[C-]	46.0	52
1331	4{311,169,10}	FC1=CC2=NC(=C(NC3CCOC3)N2C=C1)C1= NNC2=C1N=CC=C2 c:16,22,25,27,t:1,3,5,19	Z8873685463	1{311}	Nc1cc(F)cc n1	2{169}	O=Cc1n[nH] c2ccnc12	3{10}	[C-]#[N+]C1CC OC1	47.6	52
1332	4{32,356,18}	CC(C)CN1C=C(N=N1)C1=C(NC(C)(C)C)N2C =CC(=CC2=N1)P(C)(C)=O c:5,7,10,18,20,23	Z8878918506	1{32}	CP(=O)(C)c 1ccnc(N)c1	2{356}	CC(C)Cn1cc (C=O)nn1	3{18}	CC(C)(C)[N +]#[C-]	54.6	52
1333	4{362,291,10}	CNC(=O)C1=CC=CC2=NC(=C(NC3CCOC3) N12)C1=C(C)C(OC)=CN=C1 c:6,22,27,29,t:4,8,10	Z8873684583	1{362}	CNC(=O)c1 cccc(N)n1	2{291}	COc1ncce(C =O)c1C	3{10}	[C-]#[N+]C1CC OC1	53.4	52
1334	4{186,630,69}	COCCN1C=C(C=N1)C1=C(NC2=C(OC)C=C C=C2)N2C=CC(=CC2=N1)S(=O)(=O)N(C)C c:5,7,10,13,17,19,23,25,28	Z8878918547	1{186}	Cl.CN(C)S (=O)(=O)c1c cnc(N)c1	2{630}	COCCn1cc (C=O)en1	3{69}	COc1cccc[N+]#[C-]	65.8	52
1335	4{120,661,62}	COC(=O)C1(CCCC1)NC1=C(N=C2C=C(C=C N12)C1=CN(C)N=C1)C1=CN(CC(F)(F)F)N=C 1 c:15,17,26,37,t:11,13,22,29	Z8837933168	1{120}	Cn1cc(en1) c2ccnc(N)c 2	2{661}	FC(F)(F)Cn1 cc(C=O)en1	3{62}	COC(=O)C1(CCCC1)[N+] #[C-]	68.2	52
1336	4{48,437,15}	CCNC1=C(N=C2C=C(C=CN12)S(C)(=O)=O) C1=CN(CC)N=C1C c:7,9,23,t:3,5,18	Z8878918641	1{48}	CS(=O)(=O) c1ccnc(N)c 1	2{437}	CCn1cc(C=O)c(C)n1	3{15}	CC[N+]#[C-]	48.6	52
1337	4{387,446,39}	CCOCCNC1=C(N=C2N1C=CC=C2OC(F)F)C 1=CC(=CC=C1)C(=O)NC c:8,12,14,23,25,t:6,21	Z8878918827	1{387}	Nc1ncce1 OC(F)F	2{446}	CNC(=O)c1c ccc(C=O)c1	3{39}	CCOCC[N+] #[C-]	59.4	52
1338	4{142,662,10}	CP(C)(=O)C1=CC(=CC=C1)C1=C(NC2CCOC 2)N2C=CC=C(OCCS(C)(=O)=O)C2=N1 c:6,8,11,21,33,t:4,23	Z8878918611	1{142}	CS(=O)(=O))CCOc1ccc nc1N	2{662}	CP(=O)(C)c1 cccc(C=O)c1	3{10}	[C-]#[N+]C1CC OC1	66.8	52
1339	4{141,60,35}	CSCCNC1=C(N=C2C=C(NC(C)=O)C=CN12)C(C)C1CCOC1 c:16,t:6,8,10	Z8878918520	1{141}	CC(=O)Nc1 ccnc(N)c1	2{60}	CC(C=O)C1 CCOC1	3{35}	CSCCC[N+] #[C-]	52.6	52

1340	4{154,663,37}	COC(=O)C1CC(C1)NC1=C(N=C2C=C(C=CN12)[N+](O-))=O)C1=CC(OCC(N)=O)=C(OC)C=C1 c:14,16,35,t:10,12,24,31	Z8873684657	1{154}	Nc1cc(cen1)[N+](=O)[O-]	2{663}	COc1ccc(C=O)cc1OCC(=O)N	3{37}	COC(=O)C1CC(C1)[N+]#[C-]	65.6	52
1341	4{49,370,13}	CNC(=O)C1=CC=C(C=C1)C1=C(NCC2=CC=C(OC)C=C2)N2C(C=CC=C2CO)=N1 c:6,8,11,21,26,28,32,t:4,15,17	Z8873684755	1{49}	Nc1cccc(CO)n1	2{370}	CNC(=O)c1ccc(C=O)cc1	3{13}	COc1ccc(C[N+]#[C-])cc1	58.1	52
1342	4{351,67,44}	CC(C)(C)OC(=O)NCCCCNC1=C(N=C2C=CC3=C(C(O)CC3)N12)C1CCCSC1 c:17,t:13,15,19	Z8878918545	1{351}	Nc1ccc2CC(CO)c2n1	2{67}	O=CC1CCCSC1	3{44}	CC(C)(C)OC(=O)NCCCC[N+]#[C-]	64.2	52
1343	4{127,664,34}	COC1=C(OC)C(=CC=C1)C1=C(NCC2CCCO2)N2C=CC=C(F)C2=N1 c:2,6,8,11,22,28,t:24	Z8878918847	1{127}	Nc1ncccc1F	2{664}	COc1cccc(C=O)c1OC	3{34}	[C-]#[N+]CC1COCO1	51.7	52
1344	4{412,291,10}	COC1=C(C)C(=CN=C1)C1=C(NC2CCOC2)N2C=C(Br)C(CO)=CC2=N1 c:2,5,7,10,25,28,t:20	Z8878918318	1{412}	Nc1cc(CO)c(Br)cn1	2{291}	COc1nccc(C=O)c1C	3{10}	[C-]#[N+]C1CCOC1	60.2	51
1345	4{35,307,9}	CNC1=C(N=C2C=CC(C)=CN12)C1=CN=C(C1)N1C c:6,9,t:2,4,14,16	Z8855619567	1{35}	Cc1ccc(N)nc1	2{307}	Cn1c(Cl)ncc1C=O	3{9}	C[N+]#[C-]	38.2	51
1346	4{146,665,46}	CN1N=NC(=C1C)C1=C(NCC(C)=C)N2C=C(C=CC2=N1)S(C)(=O)=O c:2,4,8,16,18,21	Z8873684789	1{146}	CS(=O)(=O)c1ccc(N)nc1	2{665}	Cc1c(C=O)nn1C	3{46}	CC(=C)C[N+]#[C-]	49.9	51
1347	4{166,666,22}	COC1=C(OC)C=C(C2=C(NC3COC3)N3C=CC(CSCCO)=CC3=N2)C(F)=C1 c:2,8,17,24,27,31,t:6	Z8878918601	1{166}	Nc1cc(CSCCO)cn1	2{666}	COc1cc(F)c(C=O)cc1OC	3{22}	[C-]#[N+]C1COC1	56.1	51
1348	4{366,567,12}	COC1=CC=CN2C(NCC3CCOC3)=C(N=C12)C1=C2CCCC2=NN1C c:4,15,21,27,t:2,17	Z8878918600	1{366}	COc1cccnc1N	2{567}	Cn1nc2CCCc2c1C=O	3{12}	[C-]#[N+]CC1COC1	50.8	51
1349	4{62,49,11}	CC1=NNC=C1C1=C(NCC2=CC(Br)=CC=C2)N2C=CC(CO)=CC2=N1 c:4,7,14,16,20,24,27,t:1,11	Z8878918555	1{62}	Nc1cc(CO)cn1	2{49}	Cc1n[nH]cc1C=O	3{11}	Brc1cccc(C[N+]#[C-])c1	57.0	51
1350	4{32,356,7}	CC(C)CN1C=C(N=N1)C1=C(NC2CCOCC2)N2C=CC(=CC2=N1)P(C)(C)=O c:5,7,10,21,23,26	Z8878918404	1{32}	CP(=O)(C)c1ccnc(N)c1	2{356}	CC(C)Cn1ccc(C=O)nn1	3{7}	[C-]#[N+]C1CCOCC1	57.5	51
1351	4{142,567,10}	CN1N=C2CCCC2=C1C1=C(NC2CCOC2)N2C=CC=C(OCCS(C)(=O)=O)C2=N1 c:8,11,21,33,t:2,23	Z8873684708	1{142}	CS(=O)(=O)CCOc1cccnc1N	2{567}	Cn1nc2CCCc2c1C=O	3{10}	[C-]#[N+]C1CCOC1	61.5	51

1352	4{442,42,23}	COC(=O)CCC(NC1=C(N=C2N1C=C(Cl)C=C2C)C1=CN(C)N=C1Cl)C(=O)OC c:10,17,25,t:8,14,21	Z8878918525	1{442}	Cc1cc(Cl)en c1N	2{42}	Cn1cc(C=O) c(Cl)n1	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	62.7	51
1353	4{230,667,29}	CCOC(=O)CCNC1=C(N=C2N1C=C(Br)C=C2C(C)O)C1=C2N=CC=CN2N=C1C c:10,17,23,25,27,31,t:8,14	Z8878918668	1{230}	CC(O)c1cc(Br)enc1N	2{667}	Cc1nn2cccnc 2c1C=O	3{29}	CCOC(=O)C C[N+]#[C-]	67.2	51
1354	4{103,668,5}	COCCCN1=C(CC2CCCC(C)(C)O2)N=C2C=NC=C(CO)N12 c:6,20,t:18,22	Z8878918885	1{103}	Ne1cncc(C O)n1	2{668}	CC1(C)CCC C(CC=O)O1	3{5}	COCCC[N+] #[C-]	50.0	51
1355	4{373,352,62}	COCCCC1=C(NC2(CCCC2)C(=O)OC)N2C=C(CNC(=O)OC(C)(C)C)C=CC2=N1 c:5,30,33,t:19	Z8829498753	1{373}	CC(C)(C)O C(=O)NCc1 ccc(N)nc1	2{352}	COCCCC=O	3{62}	COC(=O)C1(CCCC1)[N+] #[C-]	63.5	51
1356	4{214,536,10}	COC1=CC(Br)=C(C)N2C(NC3CCOC3)=C(N=C12)C1=CN=C(O1)C1CCOCC1 c:16,24,t:2,5,18,22	Z8873684853	1{214}	COc1cc(Br) c(C)nc1N	2{536}	O=Cc1enc(o 1)C2CCOCC 2	3{10}	[C-]#[N+]C1CC OC1	65.8	51
1357	4{445,320,29}	CCOC(=O)CCNC1=C(N=C2C=NC(SC)=CN12)C1=NN(C)C=N1 c:12,16,25,t:8,10,21	Z8873684837	1{445}	CSc1enc(N) cn1	2{320}	Cn1enc(C=O) n1	3{29}	CCOC(=O)C C[N+]#[C-]	49.7	51
1358	4{153,277,15}	CCNC1=C(CC(NC(=O)OC(C)(C)C)C2CC2)N=C2C=CC=C(N12)C(C)(C)O c:3,21,23,t:19	Z8873684594	1{153}	CC(C)(O)c1 cccc(N)n1	2{277}	CC(C)(C)OC (=O)NC(CC =O)C1CC1	3{15}	CC[N+]#[C-]	55.3	51
1359	4{154,669,47}	CC(C)NC1=C(N=C2C=C(C=CN12)[N+]([O-])=O)C1=C(Br)N(C)N=C1 c:8,10,18,23,t:4,6	Z8855619636	1{154}	Ne1cc(cen1)[N+](=O)[O-]	2{669}	Cn1ncc(C=O) c1Br	3{47}	CC(C)[N+]#[C-]	52.0	51
1360	4{359,437,22}	CCN1C=C(C(C)=N1)C1=C(NC2COC2)N2C=C(OC(F)F)C=CC2=N1 c:3,6,9,24,27,t:18	Z8873684884	1{359}	Ne1ccc(OC(F)F)cn1	2{437}	CCn1cc(C=O) c(C)n1	3{22}	[C-]#[N+]C1CO C1	49.7	51
1361	4{105,349,66}	CC(NC1=C(N=C2C=CC=C(N12)C(N)=O)C1C[C@H]2OC(C)(C)O[C@H]2C1)C1=CC=CC=C1 c:7,9,31,33,t:3,5,29	Z8873684852	1{105}	NC(=O)c1c ccc(N)n1	2{349}	CC1(C)O[C @@H]2CC(C[C@@H]2 O1)C=O	3{66}	CC([N+]#[C-])c1cccc1	57.4	51
1362	4{91,670,26}	CN(C)C(=O)C1=NN(C=C1)C1=CC=C(C=C1)C1=C(NCC2=CC=C(F)C=C2)N2C=C(C=CC2=N1)C(N)=O c:8,13,15,18,27,31,33,36,t:5,11,22,24	Z8846491744	1{91}	NC(=O)c1c cc(N)nc1	2{670}	CN(C)C(=O) c1ccn(n1)c2c cc(C=O)cc2	3{26}	Fc1ccc(C[N+] #[C-])cc1	67.9	51

1363	4{446,671,38}	COCCCC=C(NC2=CC3=C(OCO3)C=C2)N2C=CC(=CC2=N1)C1=CN=CC=C1 c:4,15,19,21,24,29,31,t:7,9,27	Z8878918659	1{446}	Nc1cc(cen1)c2cccnc2	2{671}	COCCCC=O	3{38}	[C-]]#[N+]c1ccc 2OCOe2c1	53.0	51
1364	4{44,672,9}	CCC1=CN2C(C=N1)=NC(=C2NC)C1=C(C)S C=N1 c:6,8,10,15,19,t:2	Z8846491880	1{44}	CCc1cnc(N) cn1	2{672}	Cc1scnc1C= O	3{9}	C[N+]#[C-]	37.3	51
1365	4{356,673,34}	CN(C)C(=O)C1=C(C1)C=CC2=NC(=C(NCC3 CCCO3)N12)C1=NC=CC(C1)=C1 c:5,8,27,30,t:10,12,25	Z8837933144	1{356}	CN(C)C(=O) c1nc(N)ccc 1C1	2{673}	Clc1ccnc(C= O)c1	3{34}	[C-]]#[N+]CC1C CCO1	59.1	50
1366	4{371,350,28}	CCCNC1=C(N=C2N1C=CC=C2OCCCC#N)C 1C2CCOCC12 c:6,10,12,t:4	Z8855739193	1{371}	Nc1ncccc1 OCCCC#N	2{350}	O=CC1C2C COCC12	3{28}	CCC[N+]#[C-]]	48.1	50
1367	4{105,674,66}	CC(NC1=C(N=C2C=CC=C(N12)C(N)=O)C1= C(C)NN=C1C1)C1=CC=CC=C1 c:7,9,17,21,27,29,t:3,5,25	Z8878918771	1{105}	NC(=O)c1c ccc(N)n1	2{674}	Cc1[nH]nc(C l)c1C=O	3{66}	CC([N+]#[C-])c1cccc1	53.6	50
1368	4{47,495,6}	CCOC(=O)CCCNC1=C(N=C2C=C(C=CN12)S (N)(=O)=O)C1=C(C1)C=CC=N1 c:13,15,24,27,29,t:9,11	Z8855739260	1{47}	Cl.Nc1cc(cc n1)S(=O)(= O)N	2{495}	Clc1ccnc1C =O	3{6}	CCOC(=O)C CC[N+]#[C-]	59.4	50
1369	4{447,675,49}	CN(C)C1=CN2C(C=C1)=NC(C1COCCN1C(= O)OC(C)(C)C)=C2NC1CC(F)(F)C1 c:7,9,25,t:3	Z8846492240	1{447}	CN(C)c1ccc (N)nc1	2{675}	CC(C)(C)OC (=O)N1CCO CC1C=O	3{49}	FC1(F)CC(C 1)[N+]#[C-]	61.3	50
1370	4{107,676,10}	OCCOC1=CN2C(C=C1)=NC(=C2NC1CCOC1)C1=CC=CC2=NON=C12 c:8,10,12,24,t:4,22,26,29	Z8837933182	1{107}	Nc1ccc(OC CO)cn1	2{676}	O=Cc1cccc2 nonc12	3{10}	[C-]]#[N+]C1CC OC1	51.7	50
1371	4{103,677,5}	COCCCN1=C(N=C2C=NC=C(CO)N12)C1= NN(C=C1)C1CN(C1)C(=O)OC(C)(C)C c:10,22,t:6,8,12,19	Z8873685498	1{103}	Nc1cnc(C O)n1	2{677}	CC(C)(C)OC (=O)N1CC(C 1)n2ccc(C=O)n2	3{5}	COCCC[N+] #[C-]	62.1	50
1372	4{431,603,10}	COC(=O)C1=CC(=NS1)C1=C(NC2CCOC2)N 2C=C(F)C=CC2=N1 c:6,10,23,26,t:4,20	Z8873685422	1{431}	Nc1ccc(F)c n1	2{603}	COC(=O)c1c c(C=O)ns1	3{10}	[C-]]#[N+]C1CC OC1	49.1	50
1373	4{448,645,31}	CSCCN1=C(N=C2C=C(F)C(C=C)=CN12)C1 =CNN=N1 c:14,22,t:5,7,9,19	Z8878918630	1{448}	Nc1cc(F)c(C=C)cn1	2{645}	O=Cc1c[nH] nn1	3{31}	CSCC[N+]#[C-]	43.2	50
1374	4{154,160,47}	CC(C)NC1=C(N=C2C=C(C=CN12)[N+])([O-])=O)C1=CC(=NN1C)C1CC1 c:8,10,20,t:4,6,18	Z8873684929	1{154}	Nc1cc(cen1)N+](=O)[O-]	2{160}	Cn1nc(cc1C =O)C2CC2	3{47}	CC(C)[N+]#[C-]	46.1	50

1375	4{83,393,18}	CC(C)(C)NC1=C(N=C2C=CC(=CN12)P(C)(C)=O)C1=CC(Br)=C(F)C=C1 c:9,11,26,t:5,7,20,23	Z8878918877	1{83}	CP(=O)(C)c1ccc(N)nc1	2{393}	Fc1ccc(C=O)cc1Br	3{18}	CC(C)(C)[N+][C-]	59.3	50
1376	4{153,318,53}	CC(C)(O)C1=CC=CC2=NC(C3CC3CC3(F)F)=C(NCCOCC3=CC=CC=C3)N12 c:6,28,30,t:4,8,19,26	Z8873685482	1{153}	CC(C)(O)c1cccc(N)n1	2{318}	FC1(F)CC21CC2C=O	3{53}	[C-][N+]CCOCc1ccccc1	57.8	50
1377	4{38,15,9}	CNC1=C(N=C2C=C(C=CN12)C#N)C1=CC=C(OC)C=C1 c:6,8,21,t:2,4,15,17	Z8873684862	1{38}	Nc1cc(C#N)ccn1	2{15}	COc1ccc(C=O)cc1	3{9}	C[N+][C-]	37.6	50
1378	4{366,164,12}	COC1=CC=CN2C(NCC3CCOC3)=C(N=C12)C1=NN(C)C2=C1COCC2 c:4,15,25,t:2,17,21	Z8873684843	1{366}	COc1ccccc1N	2{164}	Cn1nc(C=O)c2COCCc21	3{12}	[C-][N+]CC1CCOC1	51.8	50
1379	4{428,678,10}	COC1=CC(OC)=C(C1)C=C1C1=C(NC2CCOC2)N2C=C(Br)N=CC2=N1 c:9,12,25,28,t:2,6,22	Z8873685486	1{428}	Nc1cnc(Br)cn1	2{678}	COc1cc(OC)c(C=O)cc1Cl	3{10}	[C-][N+]C1CCOC1	61.3	50
1380	4{349,312,23}	COC(=O)CCC(NC1=C(N=C2C=CC(Br)=C(C)N12)C1CCOC1(C)C(=O)OC c:12,t:8,10,15	Z8878918386	1{349}	Cc1nc(N)ccc1Br	2{312}	CC1(C)OCC1C=O	3{23}	COC(=O)CC(C[N+][C-])C(=O)OC	65.1	50
1381	4{32,679,7}	CP(C)(=O)C1=CC2=NC(=C(NC3CCOCC3)N2C=C1)C1=CC(=CC=C1)C1CCC1 c:20,25,27,t:4,6,8,23	Z8846492376	1{32}	CP(=O)(C)c1ccnc(N)c1	2{679}	O=Cc1cccc(c1)C2CCC2	3{7}	[C-][N+]C1CCOCC1	57.0	50
1382	4{69,33,46}	CNC(=O)C1=CC2=NC(C3CCCN(C3)C(C)=O)=C(NCC(C)=C)N2C=C1 c:27,t:4,6,18	Z8873684791	1{69}	CNC(=O)c1ccnc(N)c1	2{33}	CC(=O)N1C(CCC(C1)C=O)	3{46}	CC(=C)C[N+][C-]	49.7	50
1383	4{81,17,13}	CCOC1=CN=C(N=C1)C1=C(NCC2=CC=C(OC)C=C2)N2C=CN=CC2=N1 c:5,7,10,20,24,26,29,t:3,14,16	Z8873684723	1{81}	Nc1cncn1	2{17}	CCOc1cnc(C=O)nc1	3{13}	COc1ccc(C[N+][C-])cc1	50.6	50
1384	4{175,33,46}	CC(=C)CNC1=C(N=C2N1C=CC=C2OCCF)C1CCCN(C1)C(C)=O c:7,11,13,t:5	Z8878918376	1{175}	Nc1ncccc1OCCF	2{33}	CC(=O)N1C(CCC(C1)C=O)	3{46}	CC(=C)C[N+][C-]	50.4	50
1385	4{103,668,59}	CC1(C)CCCC(CC2=C(NCCC3=CC(F)=CC=C3)N3C(C=NC=C3CO)=N2)O1 c:8,16,18,23,25,29,t:13	Z8873685368	1{103}	Nc1cnc(C)cn1	2{668}	CC1(C)CCC(C(CC=O)O1)	3{59}	Fc1cccc(CC[N+][C-])c1	55.5	50
1386	4{49,284,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC=C(CO)N23)C2=C(C)N=CC=N2)C=C1 c:12,21,24,26,29,t:2,5,8,10,14	Z8873684918	1{49}	Nc1cccc(C)cn1	2{284}	Cc1cncnc1C=O	3{20}	COc1ccc([N+][C-])c(C)c1	50.5	50
1387	4{109,680,34}	CC(C)(C)C1=NC(=CC=C1)C1=C(NCC2CCC(O2)N2C(C=CC=C2S(N)(=O)=O)=N1 c:6,8,11,23,25,31,t:4	Z8873684828	1{109}	Cl.Nc1cccc(n1)S(=O)(=O)N	2{680}	CC(C)(C)c1cccc(C=O)n1	3{34}	[C-][N+]CC1CCO1	57.7	50

1388	4{91,681,7}	NC(=O)C1=CN2C(C=C1)=NC(=C2NC1CCOC C1)C1=C(Br)C=CC(Cl)=N1 c:7,9,11,22,25,28,t:3	Z8855739117	1{91}	NC(=O)c1c cc(N)nc1	2{681}	Clc1ccc(Br)c (C=O)n1	3{7}	[C-]#[N+]C1CC OCC1	60.6	50
1389	4{360,320,66}	COC(=O)C1=CC2=NC(=C(NC(C)C3=CC=CC =C3)N2C=C1Br)C1=NN(C)C=N1 c:15,17,22,30,t:4,6,8,13,26	Z8873684804	1{360}	COC(=O)c1 cc(N)nc1Br	2{320}	Cn1cnc(C=O n1	3{66}	CC([N+]#[C-)c1ccccc1	61.2	50
1390	4{330,653,29}	CCOC(=O)CCNC1=C(N=C2C=CC(=CN12)S(=O)(=O)N(C)C)C1C2CCC(F)(F)C12 c:12,14,t:8,10	Z8878918876	1{330}	CN(C)S(=O) (=O)c1ccc(N)nc1	2{653}	FC1(F)CCC2 C(C=O)C21	3{29}	CCOC(=O)C C[N+]#[C-]	61.3	50
1391	4{142,608,24}	COC1=CC(CNC2=C(CC3(CCC3)C#N)N=C3N 2C=CC=C3OCCS(C)(=O)=O)=CC=C1 c:7,17,21,23,32,34,t:2	Z8846491945	1{142}	CS(=O)(=O)CCOc1ccc nc1N	2{608}	O=CCC1(CC C1)C#N	3{24}	COc1cccc(C[N+]#[C-])c1	62.9	50
1392	4{292,634,31}	CCOC1=CN=CC2=NC(C(C)C3CCOCC3)=C(NCCSC)N12 c:5,t:3,7,18	Z8878918654	1{292}	CCOc1cnc (N)n1	2{634}	CC(C=O)C1 CCOCC1	3{31}	CSCC[N+]#[C-]	48.9	50
1393	4{357,283,49}	OCC1CCN(CC1)C1=CN2C(C=C1)=NC(=C2N C1CC(F)(F)C1)C1=C2N=CC=CC2=CC=C1 c:13,15,17,28,30,32,35,37,t:9	Z8878918884	1{357}	Nc1ccc(en1)N2CCC(C O)CC2	2{283}	O=Cc1cccc2 ccnc12	3{49}	FC1(F)CC(C 1)[N+]#[C-]	62.1	50
1394	4{128,229,29}	CCOC(=O)CCNC1=C(N=C2C=CC(=CN12)N(C)CCOC)C1=CN=C(OCCO)C=C1 c:12,14,33,t:8,10,25,27	Z8873684803	1{128}	COCCN(C) c1ccc(N)nc 1	2{229}	OCCOc1ccc(C=O)cn1	3{29}	CCOC(=O)C C[N+]#[C-]	61.2	50
1395	4{32,338,18}	CC1=C(OC=C1)C1=C(NC(C)(C)C)N2C=CC(= CC2=N1)P(C)(C)=O c:4,7,15,17,20,t:1	Z8878918367	1{32}	CP(=O)(C)c 1cnc(N)c1	2{338}	Cc1ccoc1C= O	3{18}	CC(C)(C)[N +]#[C-]	46.2	50
1396	4{414,326,21}	CN1N=CC=C1C1=C(NCC2CC2)N2C=C(Cl)N =CC2=N1 c:2,4,7,19,22,t:16	Z8873684909	1{414}	Nc1cnc(Cl) cn1	2{326}	Cn1ncclC= O	3{21}	[C-]#[N+]CC1C C1	40.5	50
1397	4{412,682,10}	OCC1=CC2=NC(=C(NC3CCOC3)N2C=C1Br) C1=C(Cl)C(F)=NC=C1 c:17,21,25,27,t:2,4,6	Z8878918351	1{412}	Nc1cc(CO)c (Br)cn1	2{682}	Fc1nccl(C= O)c1Cl	3{10}	[C-]#[N+]C1CC OC1	59.1	50
1398	4{435,312,23}	COC(=O)CCC(NC1=C(N=C2N1C=C(Br)C=C 2C)C1CCOC1(C)C)C(=O)OC c:10,17,t:8,14	Z8878918352	1{435}	Cc1cc(Br)c nc1N	2{312}	CC1(C)OCC C1C=O	3{23}	COC(=O)CC C([N+]#[C-)C(=O)OC	64.3	49
1399	4{50,297,26}	CCN1N=C(C)C(=N1)C1=C(NCC2=CC=C(F)C =C2)N2C(C=CC=C2P(C)(C)=O)=N1 c:6,9,18,23,25,31,t:3,13,15	Z8849597820	1{50}	CP(=O)(C)c 1cccc(N)n1	2{297}	CCn1nc(C)c(C=O)n1	3{26}	Fc1ccc(C[N+]#[C-])cc1	56.8	49
1400	4{40,545,22}	COCCN1N=C(C)C(=C1C)C1=C(NC2COC2)N 2C(C=C(C=C2)C(F)(F)F)=N1 c:8,12,22,24,31,t:5	Z8873684600	1{40}	Cc1cc(cc(N)n1)C(F)(F) F	2{545}	COCCn1nc(C)c(C=O)c1 C	3{22}	[C-]#[N+]C1CO C1	56.4	49

1401	4{449,683,14}	COCCNC1=C(N=C2N1C=CC=C2)C1=C(C)N(C)N=C1Br c:7,11,13,17,22,t:5	Z8873684661	1{449}	Nc1ncccc1I	2{683}	Cc1c(C=O)c(Br)nn1C	3{14}	COCC[N+][#C-]	65.2	49
1402	4{450,33,21}	CCC1=CC(Br)=CN2C(NCC3CC3)=C(N=C12)C1CCCN(C1)C(C)=O c:5,14,t:2,16	Z8878918411	1{450}	CCc1cc(Br)nc1N	2{33}	CC(=O)N1C CCC(C1)C=O	3{21}	[C-][#N+]CC1C C1	55.8	49
1403	4{32,684,18}	CC(C)(C)NC1=C(N=C2C=C(C=CN12)P(C)(C)=O)C1=CN(N=N1)C1CCCC1 c:9,11,23,t:5,7,20	Z8873685458	1{32}	CP(=O)(C)c1ccnc(N)c1	2{684}	O=Cc1cn(nn1)C2CCCC2	3{18}	CC(C)(C)[N+][#C-]	55.1	49
1404	4{49,494,13}	COC1=CC=C(CNC2=C(N=C3C=CC=C(CO)N23)C2=C(Cl)N=CS2)C=C1 c:12,21,24,28,t:2,4,8,10,14	Z8878918773	1{49}	Nc1cccc(C)O)n1	2{494}	Clc1ncsc1C=O	3{13}	COc1ccc(C[N+][#C-])cc1	53.3	49
1405	4{142,531,21}	CC1=NC=C(C=N1)C1=C(NCC2CC2)N2C=CC=C(OCCS(C)(=O)=O)C2=N1 c:3,5,8,17,29,t:1,19	Z8835022872	1{142}	CS(=O)(=O)CCOc1ccnc1N	2{531}	Cc1ncc(C=O)cn1	3{21}	[C-][#N+]CC1C C1	53.3	49
1406	4{389,584,23}	COC(=O)CCC(NC1=C(N=C2N1C=C(C)C=C2)C)C1=C(OC)C=C(C)N=C1)C(=O)OC c:10,17,21,28,t:8,14,25	Z8878918437	1{389}	Cc1cnc(N)c(C)c1	2{584}	COc1cc(C)nc1C=O	3{23}	COC(=O)CC C([N+][#C-])C(=O)OC	58.5	49
1407	4{451,352,62}	COCCCC1=C(NC2(CCCC2)C(=O)OC)N2C(C=CC3=C2C=CC=N3)=N1 c:5,20,22,25,27,29	Z8835022895	1{451}	Nc1ccc2nccc2n1	2{352}	COCCCC=O	3{62}	COC(=O)C1(CCCC1)[N+][#C-]	50.6	49
1408	4{119,304,46}	CC(=C)CNC1=C(N=C2C=CC(=CN12)C#N)C1=C(C)N(CC(F)F)N=C1 c:9,11,18,26,t:5,7	Z8829498647	1{119}	Nc1ccc(C#N)cn1	2{304}	Cc1c(C=O)cnn1CC(F)F	3{46}	CC(=C)C[N+][#C-]	47.1	49
1409	4{36,420,9}	CNC1=C(CC(C)(C)C#N)N=C2C=CC(Br)=CN12 c:2,12,15,t:10	Z8873684797	1{36}	Nc1ccc(Br)cn1	2{420}	CC(C)(CC=O)C#N	3{9}	C[N+][#C-]	40.6	49
1410	4{136,78,14}	COCCNC1=C(N=C2N1C=C(C)C=C2Br)C1CO C(C)C1 c:7,14,t:5,11	Z8878918455	1{136}	Cc1cnc(N)c(Br)c1	2{78}	CC1CC(CO1)C=O	3{14}	COCC[N+][#C-]	48.6	49
1411	4{161,31,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC=NN23)C2=CN=CN2)C=C1 c:12,14,21,25,t:2,5,8,10,19	Z8878918346	1{161}	Nc1cccenn1	2{31}	O=Cc1cnc[nH]1	3{20}	COc1ccc([N+][#C-])c(C)c1	42.2	49
1412	4{452,350,74}	CC(C)(C)OC(=O)N1CCCC(C1)NC1=C(N=C2C=CC3=C(C=NC=C3)N12)C1C2CCOCC12 c:19,23,25,t:15,17,21	Z8878918350	1{452}	Nc1ccc2ccncc2n1	2{350}	O=CC1C2C COCC12	3{74}	CC(C)(C)OC(=O)N1CCC[C@H](C1)[N+][#C-]	61.0	49
1413	4{83,417,31}	CSCCNC1=C(N=C2C=CC(=CN12)P(C)(C)=O)C1=C2N=NN(C)C2=CC=C1 c:9,11,20,22,27,29,t:5,7	Z8873685242	1{83}	CP(=O)(C)c1ccc(N)nc1	2{417}	Cn1nnc2c(C=O)cccc12	3{31}	CSCC[N+][#C-]	54.5	49

1414	4{209,62,14}	COCCNC1=C(N=C2N1C=CC=C2N1CCCC1)C1CC11CCOCC1 c:7,11,13,t:5	Z8878918420	1{209}	Ne1ncccc1 N2CCCCC2	2{62}	O=CC1CC21 CCOCC2	3{14}	COCC[N+]#[C-]	50.6	49
1415	4{91,639,18}	CC1=NN=C(O1)C1=CC(=CC=C1)C1=C(NC(C)(C)C)N2C=C(C=CC2=N1)C(N)=O c:3,9,11,14,22,24,27,t:1,7	Z8873685279	1{91}	NC(=O)c1c cc(N)nc1	2{639}	Cc1nnc(o1)c 2cccc(C=O)c 2	3{18}	CC(C)(C)[N +]#[C-]	51.1	49
1416	4{155,685,7}	ClC1=CC=CN2C(NC3CCOCC3)=C(N=C12)C1=CN(CC2CCOC2)N=N1 c:3,14,30,t:1,16,20	Z8849597800	1{155}	Ne1ncccc1 Cl	2{685}	O=Cc1cn(CC 2CCOC2)nn1	3{7}	[C-]#[N+]C1CC OCC1	52.6	48
1417	4{93,171,43}	COC1CC(C(OC)O1)C1=C(NC2CCN(CC2)C(=O)OC(C)(C)C)N2C=C(OC)N=CC2=N1 c:10,32,35,t:28	Z8854581175	1{93}	COc1cnc(N)cn1	2{171}	COC1CC(C= O)C(OC)O1	3{43}	CC(C)(C)OC (=O)N1CCC(CC1)[N+]#[C-]	62.4	48
1418	4{36,274,13}	COC1=CC=C(CNC2=C(CC3(CCOCC3)C#N)N=C3C=CC(Br)=CN23)C=C1 c:8,22,25,30,t:2,4,20	Z8873684625	1{36}	Ne1ccc(Br) cn1	2{274}	O=CCC1(CC OCC1)C#N	3{13}	COc1ccc(C[N+]#[C-])cc1	59.4	48
1419	4{193,325,24}	CNC(=O)C1=CN2C(C=C1)=NC(CCN1C(=O)C3=C(C=CC=C3)C1=O)=C2NCC1=CC(OC)=CC=C1 c:8,10,20,22,27,36,38,t:4,18,32	Z8878918431	1{193}	CNC(=O)c1 ccc(N)nc1	2{325}	O=CCCN1C(=O)c2cccc2 C1=O	3{24}	COc1cccc(C[N+]#[C-])c1	63.0	48
1420	4{93,425,60}	COC(=O)C1=CC(NC2=C(N=C3C=NC(OC)=CN23)C2CCCN(C2)S(C)(=O)=O)=CC=C1 c:12,16,31,33,t:4,8,10	Z8873684614	1{93}	COc1cnc(N)cn1	2{425}	CS(=O)(=O) N1CCCC(C1)C=O	3{60}	COC(=O)c1c ccc([N+]#[C-)c1	59.8	48
1421	4{373,83,39}	CCOCCNC1=C(N=C2C=CC(CNC(=O)OC(C)(C)C)=CN12)C1=CC(=CC=C1)S(N)(=O)=O c:10,21,28,30,t:6,8,26	Z8878918606	1{373}	CC(C)(C)O C(=O)NCc1 ccc(N)nc1	2{83}	NS(=O)(=O) c1cccc(C=O) c1	3{39}	CCOCC[N+]# #[C-]	69.0	48
1422	4{99,686,34}	CCNC(=O)C1=CC=C(C=C1)C1=C(NCC2CCC(O2)N2C=C(C=CC2=N1)S(N)(=O)=O c:7,9,12,23,25,28,t:5	Z8878918473	1{99}	Ne1ccc(en1)S(=O)(=O) N	2{686}	CCNC(=O)c 1ccc(C=O)cc 1	3{34}	[C-]#[N+]CC1C CCO1	57.7	48
1423	4{363,687,62}	COC(=O)C1=CC2=NC(=C(NC3(CCCC3)C(=O)OC)N2C=C1)C1=C2CSCCC2=NN1C c:23,26,33,t:4,6,8	Z8873684689	1{363}	COC(=O)c1 ccnc(N)c1	2{687}	Cn1nc2CCS Cc2c1C=O	3{62}	COC(=O)C1(CCCC1)[N+]# #[C-]	61.1	48
1424	4{107,688,10}	COC1=C(C2=C(NC3CCOC3)N3C=C(OCCO)C=CC3=N2)C(C)=C(Br)C=N1 c:2,4,20,23,30,t:14,27	Z8873685266	1{107}	Ne1ccc(OC CO)cn1	2{688}	COc1ncc(Br) c(C)c1C=O	3{10}	[C-]#[N+]C1CC OC1	60.3	48

1425	4{153,689,22}	CC(=O)OCCN1C=C(C=N1)C1=C(NC2COC2)N2C(C=CC=C2C(C)O)=N1 c:7,9,12,22,24,30	Z8873684893	1{153}	CC(C)(O)c1cccc(N)n1	2{689}	CC(=O)OCCn1cc(C=O)cn1	3{22}	[C-] #[N+]C1CO C1	52.0	48
1426	4{366,296,39}	CCOCCNC1=C(N=C2N1C=CC=C2OC)C1=C(N(CCF)N=C1 c:8,12,14,25,t:6,19	Z8849597807	1{366}	COc1ccnc1N	2{296}	FCCn1cc(C=O)cn1	3{39}	CCOCC[N+]#[C-]	45.2	48
1427	4{174,588,61}	CN1C=C(C(C)=N1)C1=C(NCCCNC(=O)OC(C)(C)C)N2C(C=CC=C2C#N)=N1 c:2,5,8,24,26,30	Z8878918523	1{174}	Nc1cccc(C#N)n1	2{588}	Cc1nn(C)cc1C=O	3{61}	CC(C)(C)OC(=O)NCCC[N+]#[C-]	53.3	48
1428	4{193,690,10}	CNC(=O)C1=CN2C(C=C1)=NC(CCC1(CCN(C1)C(=O)OC(C)(C)C)C#N)=C2NC1CCOC1 c:8,10,30,t:4	Z8873684584	1{193}	CNC(=O)c1ccc(N)nc1	2{690}	CC(C)(C)OC(=O)N1CCC(CCC=O)(CC1)C#N	3{10}	[C-] #[N+]C1CCOC1	64.6	48
1429	4{41,25,13}	COC1=CC=C(CNC2=C(N=C3C=NC(C)=CN23)C2=CN=C(N=C2)C2CCOCC2)C=C1 c:12,15,22,24,34,t:2,4,8,10,20	Z8878918532	1{41}	Cc1cnc(N)cn1	2{25}	O=Cc1cnc(nc1)C2CCOCC2	3{13}	COc1ccc(C[N+]#[C-])cc1	56.0	48
1430	4{167,386,23}	COC(=O)CCC(NC1=C(N=C2N1C(C)=CN=C2C)[C@H]1CC1(C)C)C(=O)OC c:10,15,17,t:8	Z8878918593	1{167}	Cc1cnc(C)c(N)n1	2{386}	CC1(C)C[C@@H]1C=O	3{23}	COC(=O)CC(C[N+]#[C-])C(=O)OC	50.3	48
1431	4{70,60,31}	CSCCNC1=C(N=C2N1C=CN=C2C1CC1)C(C)C1CCOC1 c:7,11,13,t:5	Z8873685406	1{70}	Nc1cncnc1C2CC2	2{60}	CC(C=O)C1CCOC1	3{31}	CSCC[N+]#[C-]	44.8	48
1432	4{139,369,46}	CC(=C)CNC1=C(N=C2C=C(C=CN12)C(F)F)C1=CON=C1C c:9,11,22,t:5,7,19	Z8873684771	1{139}	Nc1cc(cen1)C(F)F	2{369}	Cc1noc1C=O	3{46}	CC(=C)C[N+]#[C-]	41.2	48
1433	4{453,312,23}	CCC1=CN2C(C=C1)=NC(C1CCOC1(C)C)=C2NC(CCC(=O)OC)C(=O)OC c:6,8,18,t:2	Z8878918617	1{453}	CCc1ccc(N)nc1	2{312}	CC1(C)OCC1C=O	3{23}	COC(=O)CC(C[N+]#[C-])C(=O)OC	53.8	48
1434	4{330,674,29}	CCOC(=O)CCNC1=C(N=C2C=CC(=CN12)S(=O)(=O)N(C)C)C1=C(C)NN=C1C1 c:12,14,25,29,t:8,10	Z8878918825	1{330}	CN(C)S(=O)(=O)c1ccc(N)nc1	2{674}	Cc1[nH]nc(C1)c1C=O	3{29}	CCOC(=O)C(C[N+]#[C-])	58.6	48
1435	4{454,103,37}	COC(=O)C1CC(C1)NC1=C(N=C2C=C(OC(C)C(F)(F)F)C=CN12)C1CCC2(COC2)OC1 c:23,t:10,12,14	Z8873685311	1{454}	CC(Oc1ccnc(N)c1)C(F)(F)F	2{103}	O=CC1CCC2(COC2)OC1	3{37}	COC(=O)C1CC(C1)[N+]#[C-]	62.3	48
1436	4{53,691,60}	COC(=O)C1=CC(NC2=C(N=C3C=CC(CO)=CN23)C2=CC(=C(C)O2)S(C)(=O)=O)=CC=C1 c:12,16,31,33,t:4,8,10,21,23	Z8873684605	1{53}	Nc1ccc(CO)cn1	2{691}	Cc1oc(C=O)cc1S(=O)(=O)C	3{60}	COC(=O)c1ccc([N+]#[C-])c1	58.6	48
1437	4{91,439,7}	COC1=C(C=CC(=C1)C1=C(NC2CCOCC2)N2C=C(C=CC2=N1)C(N)=O)S(C)(=O)=O c:4,6,9,20,22,25,t:2	Z8878918831	1{91}	NC(=O)c1ccc(N)nc1	2{439}	COc1cc(C=O)ccc1S(=O)(=O)C	3{7}	[C-] #[N+]C1CCOCC1	57.1	48

1438	4{47,158,26}	NS(=O)(=O)C1=CC2=NC(C3=CN(C=C)N=C3)=C(NCC3=CC=C(F)C=C3)N2C=C1 c:14,25,30,t:4,6,9,16,20,22	Z8849597833	1{47}	Cl.Nc1cc(ccn1)S(=O)(=O)N	2{158}	C=Cn1cc(C=O)en1	3{26}	Fc1ccc(C[N+][C-])cc1	53.0	48
1439	4{327,47,41}	COC(=O)C1=C(F)C2=NC(CCOCC=C)=C(NC3=CC=C(OC)C=C3)N2C=C1 c:4,24,29,t:7,15,18,20	Z8849597797	1{327}	COC(=O)c1ccnc(N)c1F	2{47}	C=CCOCCC=O	3{41}	COc1ccc([N+][C-])cc1	51.2	47
1440	4{173,147,64}	COCCCCC1=C(N[C@@H]2CC[C@@H](C2)C(=O)OC)N2C=C(C=C(Br)C2=N1)C(=O)N(C)C &1:9,12,r,c:6,20,26,t:22	Z8873684645	1{173}	CN(C)C(=O)c1cnc(N)c(Br)c1	2{147}	COCCCCC=O	3{64}	COC(=O)[C@@H]1CC[C@@H](C1)[N+][C-] &1:4,7,r	63.5	47
1441	4{139,692,10}	CN1N=C(C2=C1CCN(C2)C(=O)OC(C)(C)C)C1=C(NC2CCOC2)N2C=CC(=CC2=N1)C(F)F c:2,4,19,29,31,34	Z8854581147	1{139}	Nc1cc(ccn1)C(F)F	2{692}	Cn1nc(C=O)c2CN(CCc21)C(=O)OC(C)(C)C	3{10}	[C-][N+]C1CCOC1	62.3	47
1442	4{107,139,72}	CC1=NN(CCO)C(C)=C1C1=C(NC2=C(C)C=C(F)C=C2)N2C=C(OCCO)C=CC2=N1 c:8,11,14,20,30,33,t:1,17,24	Z8854581169	1{107}	Nc1ccc(OC)COen1	2{139}	Cc1m(CCO)c(C)c1C=O	3{72}	Cc1cc(F)ccc1[N+][C-]	55.8	47
1443	4{50,693,14}	CCC1=C(SC=C1)C1=C(NCCOC)N2C(C=CC=C2P(C)(C)=O)=N1 c:5,8,17,19,25,t:2	Z8855739084	1{50}	CP(=O)(C)c1cccc(N)n1	2{693}	CCc1ccsc1C=O	3{14}	COCC[N+][C-]	47.9	47
1444	4{455,403,23}	COC(=O)CCC(NC1=C(N=C2C=C(Cl)C=C(Cl)N12)C1=CN=C(Cl)N1)C(=O)OC t:8,10,12,15,21,23	Z8873685301	1{455}	Nc1cc(Cl)cc(Cl)n1	2{403}	Clc1ncc(C=O)[nH]1	3{23}	COC(=O)CC(C[N+][C-])C(=O)OC	58.5	47
1445	4{369,441,7}	CCC(C)C(OC)C1=C(NC2CCOCC2)N2C=C(C=CC2=N1)C(F)C(F)(F)F c:7,18,20,23	Z8873684615	1{369}	Cl.Nc1ccc(cn1)C(F)C(F)(F)F	2{441}	CCC(C)C(OC)C=O	3{7}	[C-][N+]C1CCOCC1	53.0	47
1446	4{66,694,22}	COCCC1=CC2=NC(C3CCCN(C3)C(=O)OC(C)(C)C)=C(NC3COC3)N2C=C1 c:32,t:4,6,22	Z8873684777	1{66}	COCCc1ccnc(N)c1	2{694}	CC(C)(C)OC(=O)N1CCC(C(C1)C=O	3{22}	[C-][N+]C1COC1	54.7	47
1447	4{42,695,7}	COC(=O)COC1=C(OC)C=CC(=C1)C1=C(NC2CCOCC2)N2C=C(SC)C=CC2=N1 c:6,10,12,15,30,33,t:26	Z8873685254	1{42}	CSc1ccc(N)nc1	2{695}	COC(=O)COc1cc(C=O)ccc1OC	3{7}	[C-][N+]C1CCOCC1	58.1	47
1448	4{69,111,21}	CNC(=O)C1=CC2=NC(C3CCCC3)=C(NCC3C3)N2C=C1 c:24,t:4,6,14	Z8873684662	1{69}	CNC(=O)c1ccnc(N)c1	2{111}	O=CC1CCC1	3{21}	[C-][N+]CC1C1	39.6	47

1449	4{209,246,14}	COCCNC1=C(N=C2N1C=CC=C2N1CCCC1)C1CC11CCOC1 c:7,11,13,t:5	Z8873684821	1{209}	Ne1ncccc1 N2CCCCC2	2{246}	O=CC1CC21 CCOC2	3{14}	COCC[N+]#[C-]	48.8	47
1450	4{456,597,7}	CC1=C(C)N=C(O1)C1=C(NC2CCOCC2)N2C=CC(OCCNC(=O)OC(C)(C)C)=CC2=N1 c:1,4,8,19,32,35	Z8878918453	1{456}	CC(C)(C)O C(=O)NCC Oc1cnc(N) c1	2{597}	Cc1nc(C=O) oc1C	3{7}	[C-] #[N+]C1CC OCC1	59.7	47
1451	4{351,156,44}	CN1C=NC(Cl)=C1C1=C(NCCCCNC(=O)OC(C)(C)C)N2C(C=CC3=C2C(O)CC3)=N1 c:2,5,8,25,27,34	Z8878918530	1{351}	Ne1ccc2CC C(O)c2n1	2{156}	Cn1cnc(Cl)c 1C=O	3{44}	CC(C)(C)OC (=O)NCCCC [N+]#[C-]	60.1	47
1452	4{28,639,7}	CC1=NN=C(O1)C1=CC(=CC=C1)C1=C(NC2CCOCC2)N2C=CC(=CC2=N1)C1=NOC=N1 c:3,9,11,14,25,27,30,36,t:1,7,33	Z8873684579	1{28}	Cl.Nc1cc(cc n1)c2ncon2	2{639}	Cc1nnc(o1)c 2cccc(C=O)c 2	3{7}	[C-] #[N+]C1CC OCC1	56.0	47
1453	4{28,153,18}	CC(C)(C)NC1=C(N=C2C=C(C=CN12)C1=NO C=N1)C1=CN(CC(F)(F)F)N=N1 c:9,11,19,30,t:5,7,16,22	Z8878918566	1{28}	Cl.Nc1cc(cc n1)c2ncon2	2{153}	FC(F)(F)Cn1 cc(C=O)nn1	3{18}	CC(C)(C)[N +]#[C-]	51.3	47
1454	4{193,392,10}	CNC(=O)C1=CN2C(C=C1)=NC(C1CCOCC1)=C2NC1CCOC1 c:8,10,19,t:4	Z8837933148	1{193}	CNC(=O)c1 ccc(N)nc1	2{392}	O=CC1CCO CC1	3{10}	[C-] #[N+]C1CC OC1	43.5	47
1455	4{367,480,34}	CC1=CN2C(NCC3CCCO3)=C(N=C2C(=C1)C #C)C1=CC2=C(CCOC2)N=C1 c:12,14,17,31,t:1,22,24	Z8878918521	1{367}	Cc1cnc(N)c (C#C)c1	2{480}	O=Cc1cnc2C COCc2c1	3{34}	[C-] #[N+]CC1C CCO1	49.0	47
1456	4{388,509,67}	CCC(C)NC1=C(N=C2C=C3CCCO3=CN12) C1=NN=CN1C c:16,23,t:5,7,9,21	Z8878918886	1{388}	Cl.Nc1cc2C CCOc2cn1	2{509}	Cn1cnc1C= O	3{67}	CCC(C)[N+] #[C-]	41.1	47
1457	4{78,629,75}	CC1=CN2N3C(C=C(C)C2=N1)=NC(=C3NCC 1=C(Br)C=CC=C1)C1=C(C)C=C(C)C=N1 c:10,12,14,19,22,24,27,33,t:1,6,30	Z8878918790	1{78}	Cc1cn2nc(N) cc(C)c2n1	2{629}	Cc1cnc(C=O) c(C)c1	3{75}	Br1ccccc1C [N+]#[C-]	59.8	47
1458	4{457,99,15}	CCNC1=C(N=C2C=C(C(F)F)C(Br)=CN12)C1 =COC=N1 c:13,21,t:3,5,7,18	Z8878918390	1{457}	Ne1cc(C(F) F)c(Br)cn1	2{99}	O=Cc1cocn1	3{15}	CC[N+]#[C-]	44.8	46
1459	4{374,696,62}	COCCC1=NC=C(S1)C1=C(NC2(CCCC2)C(=O) OC)N2C(C=CC=C2C(=O)OC)=N1 c:6,10,25,27,33,t:4	Z8878918657	1{374}	COC(=O)c1 cccc(N)n1	2{696}	COCCc1ncc(C=O)s1	3{62}	COC(=O)C1(CCCC1)[N+] #[C-]	57.4	46
1460	4{81,30,6}	CCOC(=O)CCNC1=C(N=C2C=NC=CN12)C 1CCN(CC1)C(C)=O c:13,15,t:9,11	Z8846492161	1{81}	Ne1cncn1	2{30}	CC(=O)N1C CC(CC1)C= O	3{6}	CCOC(=O)C CC[N+]#[C-]	46.4	46

1461	4{155,246,14}	COCCNC1=C(N=C2N1C=CC=C2Cl)C1CC11 CCCOC1 c:7,11,13,t:5	Z8878918901	1{155}	Ne1ncecc1 Cl	2{246}	O=CC1CC21 CCCOC2	3{14}	COCC[N+][# C-]	41.7	46
1462	4{79,697,13}	CCC1=NC=C(N1)C1=C(NCC2=CC=C(OC)C=C2) N2C(C=NC=C2C)=N1 c:4,8,18,23,25,28,t:2,12,14	Z8873685303	1{79}	Cc1ncce(N) n1	2{697}	CCc1nce(C= O)[nH]1	3{13}	COc1ccc(C[N+][#C-])cc1	44.9	46
1463	4{436,294,23}	CCC1=CC2=NC(=C(NC(CCC(=O)OC)C(=O) OC)N2C=C1)C1=C(OC)C(=O)C=CO1 c:22,25,31,t:2,4,6	Z8873684864	1{436}	CCc1cenc(N)c1	2{294}	COc1c(C=O) occc1=O	3{23}	COC(=O)CC C([N+][#C-])C(=O)OC	54.6	46
1464	4{166,698,22}	CC(C)(C)OC(=O)N1CCC(CC1)C1=C(NC2CO C2)N2C=CC(CSCCO)=CC2=N1 c:14,23,30,33	Z8878918872	1{166}	Ne1cc(CSC CO)ccn1	2{698}	CC(C)(C)OC (=O)N1CCC(CC1)C=O	3{22}	[C-][N+]C1CO C1	61.8	45
1465	4{348,699,39}	CCOCCNC1=C(N=C2C=NC(F)=CN12)C1=C C=C(C=C1)C1(F)COC1 c:10,13,20,22,t:6,8,18	Z8873684846	1{348}	Ne1enc(F)c n1	2{699}	FC1(COC1)c 2ccc(C=O)cc 2	3{39}	CCOCC[N+] #[C-]	45.9	45
1466	4{359,700,22}	CC(C)(C)OC(=O)N1CC(C1)C1=C(NC2COC2) N2C=C(OC(F)F)C=CC2=N1 c:12,27,30,t:21	Z8878918370	1{359}	Ne1ccc(OC(F)F)cn1	2{700}	CC(C)(C)OC (=O)N1CC(C 1)C=O	3{22}	[C-][N+]C1CO C1	48.6	45
1467	4{458,662,46}	CC(=C)CNC1=C(N=C2C=CC=C(Br)N12)C1=C CC(=CC=C1)P(C)(C)=O c:9,19,21,t:5,7,11,17	Z8849597795	1{458}	Ne1cccc(Br) n1	2{662}	CP(=O)(C)c1 cccc(C=O)c1	3{46}	CC(=C)C[N+] #[C-]	51.0	45
1468	4{378,701,10}	C(OC1=CC=CN2C(NC3CCOC3)=C(N=C12)C 1=CN=CC=C1)C1=CN=CC=C1 c:4,14,22,24,29,31,t:2,16,20,27	Z8873685385	1{378}	Ne1ncecc1 OCe2ccenc 2	2{701}	O=Cc1ccenc 1	3{10}	[C-][N+]C1CC OC1	47.2	45
1469	4{66,700,22}	COCCC1=CC2=NC(C3CN(C3)C(=O)OC(C)(C) C)=C(NC3COC3)N2C=C1 c:30,t:4,6,20	Z8878918304	1{66}	COCCc1ccn c(N)c1	2{700}	CC(C)(C)OC (=O)N1CC(C 1)C=O	3{22}	[C-][N+]C1CO C1	45.9	45
1470	4{50,604,18}	CCN1N=C(C2=C1C=CC=C2)C1=C(NC(C)(C) C)N2C(C=CC=C2P(C)(C)=O)=N1 c:3,5,8,10,13,22,24,30	Z8873684874	1{50}	CP(=O)(C)c 1cccc(N)n1	2{604}	CCn1nc(C=O) c2cccc12	3{18}	CC(C)(C)[N +][#C-]	49.8	45
1471	4{445,564,29}	CCOC(=O)CCNC1=C(N=C2C=NC(SC)=CN12) C1=CN=NN1C c:12,16,23,t:8,10,21	Z8873684880	1{445}	CSc1enc(N) cn1	2{564}	Cn1ncc1C= O	3{29}	CCOC(=O)C C[N+][#C-]	43.8	45
1472	4{378,702,12}	CC(C)CC1=C(NCC2CCOC2)N2C=CC=C(OC C3=CN=CC=C3)C2=N1 c:4,15,23,25,29,t:17,21	Z8873684951	1{378}	Ne1ncecc1 OCe2ccenc 2	2{702}	CC(C)CC=O	3{12}	[C-][N+]CC1C COC1	45.9	45

1473	4{425,32,46}	CC(C)OC1=NC=CN2C(NCC(C)=C)=C(N=C12)[C@@H]1C[C@H]1C1=CC=NN1C &1:18,20,r,c:6,14,26,t:4,16,24	Z8878918354	1{425}	CC(C)Oe1nccnc1N	2{32}	Cn1nccc1[C@@H]2C[C@H]2C=O &1:6,8,r	3{46}	CC(=C)C[N+]#[C-]	44.1	45
1474	4{141,331,35}	CSCCCNC1=C(N=C2C=C(NC(C)=O)C=CN12)C1=CC2=C(OCCNC2=O)C=C1 c:16,32,t:6,8,10,21,23	Z8878918507	1{141}	CC(=O)Nc1ccnc(N)c1	2{331}	O=Cc1ccc2OCCNC(=O)c2c1	3{35}	CSCCC[N+]#[C-]	52.9	45
1475	4{50,703,35}	CSCCCNC1=C(N=C2C=CC=C(N12)P(C)(C)=O)C1=NC2=C(C=CC(C1)=C2)C=C1 c:10,12,25,28,31,t:6,8,21,23	Z8829498499	1{50}	CP(=O)(C)c1cccc(N)n1	2{703}	Clc1ccc2ccc(C=O)nc2c1	3{35}	CSCCC[N+]#[C-]	55.1	44
1476	4{348,704,39}	CCOCCNC1=C(N=C2C=NC(F)=CN12)C1=NC(=NN1C)C1CC1 c:10,13,20,t:6,8,18	Z8878918625	1{348}	Nc1cnc(F)c1n1	2{704}	Cn1nc(nc1C=O)C2CC2	3{39}	CCOCC[N+]#[C-]	47.4	44
1477	4{88,382,34}	COC(C)(C)CC1=C(NCC2CCCO2)N2C=CC(Br)=C(F)C2=N1 c:6,17,24,t:20	Z8878918372	1{88}	Nc1nccc(Br)c1F	2{382}	COC(C)(C)C=C=O	3{34}	[C-]#[N+]CC1C=CCO1	48.1	44
1478	4{104,705,39}	CCOCCNC1=C(CCCCC#C)N=C2C=CC3=C(COCC3)N12 c:6,17,t:15,19	Z8855739223	1{104}	Nc1ccc2CCOCc2n1	2{705}	O=CCCCC#C	3{39}	CCOCC[N+]#[C-]	42.7	44
1479	4{371,395,21}	CC(C)(C)OC(=O)N[C@H]1C[C@@H](C1)C1=C(NCC2CC2)N2C=CC=C(OCCCC#N)C2=N1 r,c:13,22,33,t:24	Z8855619719	1{371}	Nc1ncccc1OCCCC#N	2{395}	CC(C)(C)OC(=O)N[C@H]1C[C@@H](C1)C=O	3{21}	[C-]#[N+]CC1C=C1	52.7	44
1480	4{330,706,29}	CCOC(=O)CCNC1=C(N=C2C=CC(=CN12)S(=O)(=O)N(C)C)C1=CC(=NN1CC)C1CC1 c:12,14,27,t:8,10,25	Z8878918881	1{330}	CN(C)S(=O)(=O)c1ccc(N)nc1	2{706}	CCn1nc(cc1C=O)C2CC2	3{29}	CCOC(=O)C[N+]#[C-]	56.8	44
1481	4{70,61,35}	CSCCCNC1=C(N=C2N1C=CN=C2C1CC1)C1=CC=C(C=C1)S(C)=O c:8,12,14,23,25,t:6,21	Z8829498725	1{70}	Nc1ncnc1C2CC2	2{61}	CS(=O)c1ccc(C=O)cc1	3{35}	CSCCC[N+]#[C-]	47.9	44
1482	4{437,217,67}	CCC(C)NC1=C(N=C2C=CC3=C(NC(=N3)C(F)(F)F)N12)C1=CC(=O)N(C)C=C1 c:9,14,30,t:5,7,11,24	Z8873684902	1{437}	Cl.Nc1ccc2nc([nH]c2n1)C(F)(F)F	2{217}	Cn1ccc(C=O)cc1=O	3{67}	CCC(C)[N+]#[C-]	48.3	44
1483	4{113,707,6}	CCOC(=O)CCNC1=C(N=C2N1C=CC=C2N1CCOCC1)C1=NC(=NC=C1)N(C)C c:11,15,17,29,31,t:9,27	Z8873684707	1{113}	Nc1ncccc1N2CCOCC2	2{707}	CN(C)c1nccc(C=O)n1	3{6}	CCOC(=O)C[N+]#[C-]	54.2	44
1484	4{73,430,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC4=NC=CN4N23)C2=C(C)N=C(OC)C=C2)C=C1 c:12,16,23,30,33,t:2,5,8,10,14,26	Z8873684873	1{73}	Nc1ccc2nccn2n1	2{430}	COc1ccc(C=O)c(C)n1	3{20}	COc1ccc([N+]#[C-])c(C)c1	49.5	44

1485	4{333,535,34}	CC(C)(O)C1=CC(=NO1)C1=C(NCC2CCCO2)N2C(C=CC=C2C2=CC=NC=C2)=N1 c:6,10,22,24,29,31,33,t:4,27	Z8837933154	1{333}	Nc1cccc(n1)c2cnc2	2{535}	CC(C)(O)c1c(C=O)no1	3{34}	[C-] #[N+]CC1C CCO1	50.1	44
1486	4{99,349,50}	CC1(C)O[C@@H]2CC(C[C@@H]2O1)C1=C(NC2=CC3=C(OCCO3)C=C2)N2C=C(C=CC2=N1)S(N)(=O)=O c:12,24,28,30,33,t:15,17	Z8873684900	1{99}	Nc1ccc(en1)S(=O)(=O)N	2{349}	CC1(C)O[C@@H]2CC(C[C@@H]2O1)C=O	3{50}	[C-] #[N+]c1ccc 2OCCOc2c1	58.0	44
1487	4{155,344,14}	COCCNC1=C(N=C2N1C=CC=C2Cl)C1=C(C)C=NN1COC c:7,11,13,17,20,t:5	Z8854581167	1{155}	Nc1ncccc1Cl	2{344}	COcN1ccc(C)c1C=O	3{14}	COCC[N+]#[C-]	41.5	44
1488	4{123,299,22}	COC1=C(OC)C(C2=C(NC3COC3)N3C=CC(O)CCO)=CC3=N2=C(F)C=C1 c:2,7,16,22,25,30,t:27	Z8878918466	1{123}	Cl.Nc1cc(O)CCO)ccn1	2{299}	COc1ccc(F)c(C=O)c1OC	3{22}	[C-] #[N+]C1CO C1	41.2	44
1489	4{139,708,12}	CC1=NC(C)=C(C=C1)C1=C(NCC2CCOC2)N2C=CC(=CC2=N1)C(F)F c:4,6,9,20,22,25,t:1	Z8829498785	1{139}	Nc1cc(en1)C(F)F	2{708}	Cc1ccc(C=O)c(C)n1	3{12}	[C-] #[N+]CC1C COC1	43.9	44
1490	4{433,340,18}	CCN1C=NC(=N1)C1=C(NC(C)(C)C)N2C(C=CC(C#C)=C2C)=N1 c:3,5,8,17,21,24	Z8873684740	1{433}	Cc1nc(N)cc1C#C	2{340}	CCn1cnc(C=O)n1	3{18}	CC(C)(C)[N+]#[C-]	37.8	43
1491	4{95,709,31}	CSCCNC1=C(N=C2C=CC(=CN12)C(F)F)C1=CC=C(OCCO)C=C1 c:9,11,27,t:5,7,19,21	Z8878918594	1{95}	Nc1ccc(en1)C(F)F	2{709}	OCCOc1ccc(C=O)cc1	3{31}	CSCC[N+]#[C-]	46.0	43
1492	4{69,710,46}	CNC(=O)C1=CC2=NC(=C(NCC(C)=C)N2C=C1)C1=C(C)N=CC(F)=C1 c:17,20,23,26,t:4,6,8	Z8873684779	1{69}	CNC(=O)c1ccnc(N)c1	2{710}	Cc1ncc(F)cc1C=O	3{46}	CC(=C)C[N+]#[C-]	40.9	43
1493	4{99,382,34}	COC(C)(C)CC1=C(NCC2CCCO2)N2C=C(C=CC2=N1)S(N)(=O)=O c:6,17,19,22	Z8878918441	1{99}	Nc1ccc(en1)S(=O)(=O)N	2{382}	COC(C)(C)C=C=O	3{34}	[C-] #[N+]CC1C CCO1	44.2	43
1494	4{431,711,10}	CC1=C(N=C2C=CC=CC2=N1)C1=C(NC2CCOC2)N2C=C(F)C=CC2=N1 c:5,7,10,13,26,29,t:1,3,23	Z8855619764	1{431}	Nc1ccc(F)c1n1	2{711}	Cc1nc2ccccc2nc1C=O	3{10}	[C-] #[N+]C1CC OC1	42.0	43
1495	4{32,356,14}	COCCNC1=C(N=C2C=C(C=CN12)P(C)(C)=O)C1=CN(CC(C)C)N=N1 c:9,11,27,t:5,7,20	Z8835022892	1{32}	CP(=O)(C)c1ccnc(N)c1	2{356}	CC(C)Cn1cc(C=O)nn1	3{14}	COCC[N+]#[C-]	45.1	43
1496	4{459,424,5}	COCCNC1=C(N=C2C=CC(OC3=CN=CC=C3)=CN12)C1=NN(C)C(=N1)C(F)F c:10,16,18,20,29,t:6,8,14,25	Z8855739211	1{459}	Nc1ccc(Oc2ccnc2)cn1	2{424}	Cn1nc(C=O)nc1C(F)F	3{5}	COCCC[N+]#[C-]	51.5	43
1497	4{113,538,6}	CCOC(=O)CCNC1=C(N=C2N1C=CC=C2N1CCOCC1)C1=CN=CN1C c:11,15,17,29,t:9,27	Z8873684619	1{113}	Nc1ncccc1N2CCOCC2	2{538}	Cn1cnc1C=O	3{6}	CCOC(=O)C CC[N+]#[C-]	47.5	43

1498	4{62,469,6}	CCOC(=O)CCNC1=C(N=C2C=C(CO)C=CN12)C1CCSC1 c:17,t:9,11,13	Z8873684937	1{62}	Nc1cc(CO)c cn1	2{469}	O=CC1CCS C1	3{6}	CCOC(=O)C CC[N+]#[C-]	41.8	43
1499	4{103,293,5}	COCCNC1=C(N=C2C=NC=C(CO)N12)C1=C(F)N(C)N=C1 c:10,19,24,t:6,8,12	Z8873684766	1{103}	Nc1cncc(C O)n1	2{293}	Cn1ncc(C=O)c1F	3{5}	COCCC[N+] #[C-]	38.1	42
1500	4{125,712,31}	CSCCNC1=C(N=C2C=CC(CCO)=CN12)C1C COC2(CCOC2)C1 c:9,14,t:5,7	Z8855739254	1{125}	Nc1ccc(CC O)cn1	2{712}	O=CC1CCO C2(CCOC2)C1	3{31}	CSCC[N+]#[C-]	46.2	42
1501	4{46,17,9}	CCOC1=CN=C(N=C1)C1=C(NC)N2C=CC=C C2=N1 c:5,7,10,15,17,20,t:3	Z8873684778	1{46}	Nc1cccn1	2{17}	CCOc1ncc(C =O)nc1	3{9}	C[N+]#[C-]	30.7	42
1502	4{153,155,49}	CC(C)(O)C1=CC=CC2=NC(=C(NC3CC(F)(F) C3)N12)C1=CN=CN=C1 c:6,25,27,t:4,8,10,23	Z8855739103	1{153}	CC(C)(O)c1 cccc(N)n1	2{155}	O=Cc1cnnc 1	3{49}	FC1(F)CC(C 1)[N+]#[C-]	40.9	42
1503	4{119,34,48}	CC(C)(C)OC(=O)N1CCCC(C1)NC1=C(N=C2 C=CC(=CN12)C#N)C1=CC=C(C=C1)P(C)(C) =O c:19,21,30,32,t:15,17,28	Z8878918824	1{119}	Nc1ccc(C# N)cn1	2{34}	CP(=O)(C)c1 ccc(C=O)cc1	3{48}	CC(C)(C)OC (=O)N1CCC C(C1)[N+]#[C-]	56.1	42
1504	4{103,713,73}	CCN1N=C(Br)C(=N1)C1=C(NC2=C(OC)C=C (OC)C=C2)N2C(C=NC=C2CO)=N1 c:6,9,12,20,25,27,31,t:3,16	Z8873684774	1{103}	Nc1cncc(C O)n1	2{713}	CCn1nc(Br)c (C=O)n1	3{73}	COc1ccc([N +]#[C-]])c(OC)c1	53.7	42
1505	4{327,185,65}	COC(=O)C1=C(F)C2=NC(C3=CN(C)C=N3)= C(NC3CCCC3)N2C=C1 c:4,14,27,t:7,10,16	Z8854581146	1{327}	COC(=O)c1 ccnc(N)c1F	2{185}	Cn1ncc(C=O)c1	3{65}	[C-]]#[N+]C1CC CC1	40.4	42
1506	4{118,417,31}	CSCCNC1=C(N=C2C=CC=C(C(C)O)N12)C1 =C2N=NN(C)C2=CC=C1 c:9,19,21,26,28,t:5,7,11	Z8873684753	1{118}	Cl.CC(O)c1 cccc(N)n1	2{417}	Cn1nnc2c(C =O)cccc12	3{31}	CSCC[N+]#[C-]	43.2	42
1507	4{185,56,8}	COC(=O)C(CC1=CC=CC=C1)NC1=C(N=C2C =CC(=C(C)N12)S(C)(=O)=O)C1=C(C)C=NC(F)=C1 c:8,10,18,30,33,36,t:6,14,16,20	Z8873684859	1{185}	Cc1nc(N)cc c1S(=O)(=O)C	2{56}	Cc1ncc(F)cc 1C=O	3{8}	COC(=O)C(Cc1cccc1)[N+]#[C-]	56.1	42
1508	4{50,153,18}	CC(C)(C)NC1=C(N=C2C=CC=C(N12)P(C)(C) =O)C1=CN(CC(F)(F)F)N=N1 c:9,11,28,t:5,7,20	Z8873684854	1{50}	CP(=O)(C)c 1cccc(N)n1	2{153}	FC(F)(F)Cn1 cc(C=O)nn1	3{18}	CC(C)(C)[N +]#[C-]	46.8	42
1509	4{32,714,18}	CC(C)OC1=C(F)C=C(C=C1)C1=C(NC(C)(C) C)N2C=CC(=CC2=N1)P(C)(C)=O c:4,7,9,12,20,22,25	Z8878918552	1{32}	CP(=O)(C)c 1ccnc(N)c1	2{714}	CC(C)Oc1cc c(C=O)cc1F	3{18}	CC(C)(C)[N +]#[C-]	47.1	42

1510	4{358,223,15}	CCNC1=C(N=C2C=C(C=CN12)C(C)(C)O)C1=CN=C(C=C1)C(=O)OC c:7,9,20,22,t:3,5,18	Z8873684855	1{358}	CC(C)(O)c1ccnc(N)c1	2{223}	Cl.COC(=O)c1ccc(C=O)c n1	3{15}	CC[N+]#[C-]	40.0	42
1511	4{386,549,5}	COCCNC1=C(N=C2C=C(C)C=CN12)C1=C(C)C=C(N=C1)C(=O)OC c:13,18,21,23,t:6,8,10	Z8873685491	1{386}	Cc1ccnc(N)c1	2{549}	COC(=O)c1cc(C)(C=C(O)c n1	3{5}	COCC[N+]#[C-]	41.4	42
1512	4{180,212,32}	COC(=O)C1=CC2=NC(=C(NC3CCC3)N2C=C1C)C1=NOC(=C1)C(F)F c:18,25,t:4,6,8,22	Z8878918640	1{180}	COC(=O)c1cc(N)nc1C	2{212}	FC(F)c1cc(C=O)no1	3{32}	[C-]#[N+]C1CC C1	42.2	41
1513	4{105,715,57}	NC(=O)C1=CC=CC2=NC(CC3CCOCC3)=C(NCC3=CC=CC=C3)N12 c:5,23,25,t:3,7,17,21	Z8854581144	1{105}	NC(=O)c1ccc(N)n1	2{715}	O=CCC1CC OCC1	3{57}	[C-]#[N+]Cc1ccc ccl	40.8	41
1514	4{83,716,18}	CC(C)N(C)C1=NC=C(C=C1)C1=C(NC(C)(C)C)N2C=C(C=CC2=N1)P(C)(C)=O c:7,9,12,20,22,25,t:5	Z8878918500	1{83}	CP(=O)(C)c1ccc(N)nc1	2{716}	CC(C)N(C)c1ccc(C=O)en 1	3{18}	CC(C)(C)[N+]#[C-]	46.3	41
1515	4{28,153,7}	FC(F)(F)CN1C=C(N=N1)C1=C(NC2CCOCC2)N2C=CC(=CC2=N1)C1=NOC=N1 c:6,8,11,22,24,27,33,t:30	Z8878918496	1{28}	Cl.Nc1cc(cc n1)c2ncon2	2{153}	FC(F)(F)Cn1 cc(C=O)nn1	3{7}	[C-]#[N+]C1CC OCC1	48.6	41
1516	4{32,717,18}	COC1=CC(=CC=C1)C1=NC(=CS1)C1=C(NC(C)(C)C)N2C=CC(=CC2=N1)P(C)(C)=O c:4,6,11,15,23,25,28,t:2,9	Z8837933157	1{32}	CP(=O)(C)c1ccnc(N)c1	2{717}	COc1cccc(c1)c2nc(C=O)c s2	3{18}	CC(C)(C)[N+]#[C-]	50.7	41
1517	4{183,148,51}	COC1=C(C(C)=NN1C)C1=C(NCCNC(=O)OC(C)(C)C)N2C(=N1)C(OC)=CC=C2C c:5,10,24,29,31,t:2	Z8835022879	1{183}	COc1ccc(C)nc1N	2{148}	COc1c(C=O)c(C)nn1C	3{51}	CC(C)(C)OC(=O)NCC[N+]#[C-]	49.6	41
1518	4{79,26,9}	CNC1=C(CCC2=CC=CC=C2)N=C2C=NC=C(C)N12 c:2,8,10,15,t:6,13,17	Z8837933185	1{79}	Cc1nccc(N)n1	2{26}	O=CCCc1ccc ccl	3{9}	C[N+]#[C-]	29.5	41
1519	4{52,683,14}	COCCNC1=C(N=C2C=CC(=CN12)C1(CC1)C(F)(F)F)C1=C(C)N(C)N=C1Br c:9,11,24,29,t:5,7	Z8854581180	1{52}	Nc1ccc(en1)C2(CC2)C(F)(F)F	2{683}	Cc1c(C=O)c(Br)nn1C	3{14}	COCC[N+]#[C-]	52.3	41
1520	4{149,317,7}	CCN1N=CC(=N1)C1=C(NC2CCOCC2)N2C=C(Cl)C=C(Br)C2=N1 c:3,5,8,26,t:19,22	Z8878918369	1{149}	Nc1ncc(Cl)cc1Br	2{317}	CCn1ncc(C=O)n1	3{7}	[C-]#[N+]C1CC OCC1	47.1	41
1521	4{101,707,14}	COCCNC1=C(N=C2N1C=C(CO)C=C2Cl)C1=NC(=NC=C1)N(C)C c:7,15,21,23,t:5,11,19	Z8878918821	1{101}	Nc1ncc(CO)cc1Cl	2{707}	CN(C)c1nccc(C=O)n1	3{14}	COCC[N+]#[C-]	41.7	41
1522	4{187,567,12}	CN1N=C2CCCC2=C1C1=C(NCC2CCOC2)N2C=C(Cl)C(=CC2=N1)C#N c:8,11,25,28,t:2,22	Z8878918514	1{187}	Nc1cc(C#N)c(Cl)en1	2{567}	Cn1nc2CCCCc2c1C=O	3{12}	[C-]#[N+]CC1C COC1	43.9	41

1523	4{142,319,21}	CC1=C(C=CC(OCC#N)=C1)C1=C(NCC2CC2)N2C=CC=C(OCCS(C)(=O)=O)C2=N1 c:3,9,12,21,33,t:1,23	Z8878918666	1{142}	CS(=O)(=O)CCOc1cccnc1N	2{319}	Cc1cc(OCC#N)ccc1C=O	3{21}	[C-]#[N+]CC1C C1	50.3	41
1524	4{32,604,18}	CCN1N=C(C2=C1C=CC=C2)C1=C(NC(C)(C)C)N2C=CC(=CC2=N1)P(C)(C)=O c:3,5,8,10,13,21,23,26	Z8837933166	1{32}	CP(=O)(C)c1ccnc(N)c1	2{604}	CCn1nc(C=O)c2cccc12	3{18}	CC(C)(C)[N+]]#[C-]	45.3	41
1525	4{460,690,10}	CC1=CC=CN2C(NC3CCOC3)=C(CCC3(CCN(C)C3)C(=O)OC(C)(C)C)C#N)N=C12 c:3,t:1,13,33	Z8873685453	1{460}	Cc1ccnc1N	2{690}	CC(C)(C)OC(=O)N1CCC(CCC=O)(CC1)C#N	3{10}	[C-]#[N+]C1CC OC1	50.0	41
1526	4{461,217,62}	COC(=O)C1(CCCC1)NC1=C(N=C2C=C(C#N)C(Br)=CN12)C1=CC(=O)N(C)C=C1 c:20,31,t:11,13,15,25	Z8878918323	1{461}	Nc1cc(C#N)c(Br)cn1	2{217}	Cn1ccc(C=O)cc1=O	3{62}	COC(=O)C1(CCCC1)[N+] #[C-]	51.7	41
1527	4{377,662,24}	COC1=CC(CNC2=C(N=C3N2C=CC=C3OCC(F)F)C2=CC(=CC=C2)P(C)(C)=O)=CC=C1 c:9,13,15,25,27,33,35,t:2,7,23	Z8878918896	1{377}	Nc1ncccc1OCC(F)F	2{662}	CP(=O)(C)c1cccc(C=O)c1	3{24}	COc1cccc(C[N+] #[C-])c1	53.2	41
1528	4{172,320,29}	CCOC(=O)CCNC1=C(N=C2N1C=CC1=C2CCO1)C1=NN(C)C=N1 c:10,14,16,27,t:8,23	Z8873684906	1{172}	Nc1nccc2OCCc21	2{320}	Cn1enc(C=O)n1	3{29}	CCOC(=O)C C[N+] #[C-]	39.0	41
1529	4{396,324,70}	CN1C=C(C=N1)C1=NN2C(C=C1)=NC(C1CC3(C1)CCCO3)=C2NC1CCN(C1)C(=O)OC(C)(C)C c:2,4,11,13,25,t:7	Z8873684660	1{396}	Cn1cc(en1)c2ccc(N)nm2	2{324}	O=CC1CC2(C1)CCCO2	3{70}	CC(C)(C)OC(=O)N1CCC(C1)[N+] #[C-]	54.0	41
1530	4{68,13,38}	CC1=C(N=NN1)C1=C(NC2=CC3=C(OCO3)C=C2)N2C=CC(=CC2=N1)C#C c:3,7,18,22,24,27,t:1,10,12	Z8837933156	1{68}	Nc1cc(C#C)ccn1	2{13}	Cc1[nH]nnc1C=O	3{38}	[C-]#[N+]c1ccc 2OCOc2c1	39.3	40
1531	4{54,718,37}	COC(=O)C1CC(C1)NC1=C(N=C2C=CC(=CN12)C(=O)N(C)C)C1=C(Br)C=CS1 c:14,16,26,29,t:10,12	Z8878918615	1{54}	Cl.CN(C)C(=O)c1ccc(N)nc1	2{718}	Brclccsc1C=O	3{37}	COC(=O)C1CC(C1)[N+] #[C-]	52.1	40
1532	4{327,47,34}	COC(=O)C1=C(F)C2=NC(CCOCC=C)=C(NC3CCCO3)N2C=C1 c:4,27,t:7,15	Z8855739171	1{327}	COC(=O)c1ccnc(N)c1F	2{47}	C=CCOCCC=O	3{34}	[C-]#[N+]CC1C CCO1	41.1	40
1533	4{73,29,11}	CCN1C=CC(=N1)C1=C(NCC2=CC(Br)=CC=C2)N2N3C=CN=C3C=CC2=N1 c:3,5,8,15,17,22,24,27,30,t:12	Z8873685497	1{73}	Nc1ccc2nccn2n1	2{29}	CCn1ccc(C=O)n1	3{11}	Brclcccc(C[N+] #[C-])c1	47.5	40
1534	4{434,189,26}	CC(F)(F)C1=CN2C(NCC3=CC=C(F)C=C3)=C(N=C2C=C1)C1=CN(N=N1)C1CCOCC1 c:15,17,19,22,28,t:4,10,12,25	Z8878918893	1{434}	CC(F)(F)c1ccc(N)nc1	2{189}	O=Cc1en(nn1)C2CCOCC2	3{26}	Fc1ccc(C[N+] #[C-])cc1	49.6	40

1535	4{101,192,14}	COCCNC1=C(N=C2N1C=C(CO)C=C2Cl)C1=NC(OC)=CC=C1 c:7,15,23,25,t:5,11,19	Z8878918840	1{101}	Nc1ncc(CO)cc1Cl	2{192}	COc1cccc(C=O)n1	3{14}	COCC[N+]#[C-]	39.3	40
1536	4{38,420,9}	CNC1=C(CC(C)(C)C#N)N=C2C=C(C=CN12)C#N c:2,12,14,t:10	Z8854581149	1{38}	Nc1cc(C#N)ccn1	2{420}	CC(C)(CC=O)C#N	3{9}	C[N+]#[C-]	27.3	40
1537	4{327,638,34}	COC(=O)C1=C(F)C2=NC(=C(NCC3CCCO3)N2C=C1)C1=CN(CC2CCOCC2)N=C1 c:4,21,35,t:7,9,24	Z8878918578	1{327}	COC(=O)c1ccnc(N)c1F	2{638}	O=Cc1cnn(C2CCOCC2)c1	3{34}	[C-]#[N+]CC1COCO1	49.3	40
1538	4{456,189,18}	CC(C)(C)NC1=C(N=C2C=C(OCCNC(=O)OC(C)(C)C)C=CN12)C1=CN(N=N1)C1CCOCC1 c:22,30,t:5,7,9,27	Z8878918782	1{456}	CC(C)(C)OC(=O)NCCOc1cnc(N)c1	2{189}	O=Cc1cn(nn1)C2CCOCC2	3{18}	CC(C)(C)[N+]#[C-]	53.7	40
1539	4{105,434,29}	CCOC(=O)CCNC1=C(N=C2C=CC=C(N12)C(N)=O)C1=NC(C)=CC(OC)=C1 c:12,14,25,29,t:8,10,22	Z8878918662	1{105}	NC(=O)c1cccc(N)n1	2{434}	COc1cc(C)nc(C=O)c1	3{29}	CCOC(=O)C[N+]#[C-]	42.7	40
1540	4{83,50,18}	CC(C)(C)NC1=C(N=C2C=CC(=CN12)P(C)(C)=O)[C@@H]1C[C@H]1C1OCCO1 &1:18,20,r,c:9,11,t:5,7	Z8878918397	1{83}	CP(=O)(C)c1ccc(N)nc1	2{50}	O=C[C@@H]1C[C@H]1C2OCCO2 &1:2,4,r	3{18}	CC(C)(C)[N+]#[C-]	40.5	40
1541	4{73,142,13}	COC1=CC=C(CNC2=C(N=C3C=CC4=NC=C(N4N23)C2=C(CCC=C)C=CC=C2)C=C1 c:12,16,23,29,31,34,t:2,4,8,10,14	Z8855739261	1{73}	Nc1ccc2nccn2n1	2{142}	C=CCCc1ccc(C=O)cc1	3{13}	COc1ccc(C[N+]#[C-])cc1	45.4	40
1542	4{360,564,29}	CCOC(=O)CCNC1=C(N=C2C=C(C(=O)OC)C(Br)=CN12)C1=CN=NN1C c:19,26,t:8,10,12,24	Z8878918408	1{360}	COC(=O)c1cc(N)nc1Br	2{564}	Cn1ncc1C=O	3{29}	CCOC(=O)C[N+]#[C-]	48.3	40
1543	4{36,170,9}	CCN1N=NC(=N1)C1=C(NC)N2C=C(Br)C=C2=N1 c:3,5,8,16,19,t:13	Z8873685407	1{36}	Nc1ccc(Br)cn1	2{170}	CCn1nnc(C=O)n1	3{9}	C[N+]#[C-]	34.4	40
1544	4{48,719,22}	CS(=O)(=O)C1=CC2=NC(=C(NC3COC3)N2C=C1)C1=C(Cl)C=C(Br)C=C1 c:18,21,27,t:4,6,8,24	Z8873684833	1{48}	CS(=O)(=O)c1ccnc(N)c1	2{719}	Clc1cc(Br)cc1C=O	3{22}	[C-]#[N+]C1CO1	48.6	39
1545	4{83,720,26}	CC[C@@H]1C[C@H]1C1=C(NCC2=CC=C(F)C=C2)N2C=C(C=CC2=N1)P(C)(C)=O &1:2,4,r,c:6,15,19,21,24,t:10,12	Z8837933151	1{83}	CP(=O)(C)c1ccc(N)nc1	2{720}	CC[C@@H]1C[C@H]1C=O &1:2,4,r	3{26}	Fe1ccc(C[N+]#[C-])cc1	40.9	39
1546	4{175,405,12}	CC(F)(F)C1=NC=C(S1)C1=C(NCC2CCOC2)N2C=CC=C(OCFF)C2=N1 c:6,10,21,30,t:4,23	Z8878918883	1{175}	Nc1ncccc1OCCF	2{405}	CC(F)(F)c1ncc(C=O)s1	3{12}	[C-]#[N+]CC1COCO1	45.3	39

1547	4{32,640,18}	CC(C)N1C=C(N=N1)C1=C(NC(C)(C)C)N2C=CC(=CC2=N1)P(C)(C)=O c:4,6,9,17,19,22	Z8837933170	1{32}	CP(=O)(C)c1ccnc(N)c1	2{640}	CC(C)n1cc(C=O)nn1	3{18}	CC(C)(C)[N+][C-]	39.7	39
1548	4{462,352,70}	COCCCC1=C(NC2CCN(C2)C(=O)OC(C)(C)C)N2C=C(Br)C=C(CO)C2=N1 c:5,30,t:22,25	Z8873684582	1{462}	Nc1ncc(Br)cc1CO	2{352}	COCCCC=O	3{70}	CC(C)(C)OC(=O)N1CCCC(C1)[N+][C-]	51.3	39
1549	4{32,439,7}	COC1=C(C=CC(=C1)C1=C(NC2CCOCC2)N2C=CC(=CC2=N1)P(C)(C)=O)S(C)(=O)=O c:4,6,9,20,22,25,t:2	Z8873684658	1{32}	CP(=O)(C)c1ccnc(N)c1	2{439}	COe1cc(C=O)ccc1S(=O)(=O)C	3{7}	[C-][N+]C1CCOCC1	50.7	39
1550	4{372,721,12}	COC(=O)C1=CC(=CN=C1)C1=C(NCC2CCOC2)N2C=CC=C(OCC3=CC=NC=C3)C2=N1 c:6,8,11,22,30,32,36,t:4,24,28	Z8878918479	1{372}	Nc1ncccc1OCc2ccncc2	2{721}	COC(=O)c1cncc(C=O)c1	3{12}	[C-][N+]CC1COC1	48.7	39
1551	4{193,722,12}	CNC(=O)C1=CN2C(C=C1)=NC(=C2NCC1CCOC1)C1=CC=C(C=C1)N1CCN(C)CC1 c:8,10,12,25,27,t:4,23	Z8849597829	1{193}	CNC(=O)c1ccc(N)nc1	2{722}	CN1CCN(C1)c2ccc(C=O)cc2	3{12}	[C-][N+]CC1COC1	47.6	39
1552	4{123,689,22}	CC(=O)OCCN1C=C(C=N1)C1=C(NC2COC2)N2C=CC(OCCO)=CC2=N1 c:7,9,12,21,27,30	Z8878918424	1{123}	Cl.Nc1cc(OCCO)ccn1	2{689}	CC(=O)OCCn1cc(C=O)en1	3{22}	[C-][N+]C1CO C1	38.9	39
1553	4{73,723,13}	CCCC(C)C1=C(NCC2=CC=C(OC)C=C2)N2N3C=CN=C3C=CC2=N1 c:5,15,20,22,25,28,t:9,11	Z8854581156	1{73}	Nc1ccc2nccn2n1	2{723}	CCCC(C)C=O	3{13}	COe1ccc(C[N+][C-])cc1	38.4	39
1554	4{83,340,18}	CCN1C=NC(=N1)C1=C(NC(C)(C)C)N2C=C(C=CC2=N1)P(C)(C)=O c:3,5,8,16,18,21	Z8878918361	1{83}	CP(=O)(C)c1ccc(N)nc1	2{340}	CCn1cnc(C=O)n1	3{18}	CC(C)(C)[N+][C-]	38.1	39
1555	4{144,724,15}	CCNC1=C(N=C2C=CC(=CN12)S(=O)(=O)NC)C1=C(OC)C=CC=C1F c:7,9,19,23,25,t:3,5	Z8873684668	1{144}	CNS(=O)(=O)c1ccc(N)nc1	2{724}	COc1cccc(F)c1C=O	3{15}	CC[N+][C-]	40.0	39
1556	4{133,61,22}	CS(=O)C1=CC=C(C=C1)C1=C(NC2COC2)N2C=C(F)C=C(Br)C2=N1 c:5,7,10,26,t:3,19,22	Z8873684901	1{133}	Nc1ncc(F)cc1Br	2{61}	CS(=O)c1ccc(C=O)cc1	3{22}	[C-][N+]C1CO C1	44.5	39
1557	4{393,725,5}	CCN1N=NC=C1C1=C(NCCCOC)N2C(C=CC(Cl)=C2Cl)=N1 c:3,5,8,18,21,24	Z8878918309	1{393}	Nc1ccc(Cl)c(Cl)n1	2{725}	CCn1ncc1C=O	3{5}	COCCC[N+][C-]	38.6	39
1558	4{372,726,12}	CS(=O)(=O)C1=CC(=CC=C1)C1=C(NCC2CCOC2)N2C=CC=C(OCC3=CC=NC=C3)C2=N1 c:6,8,11,22,30,32,36,t:4,24,28	Z8878918471	1{372}	Nc1ncccc1OCc2ccncc2	2{726}	CS(=O)(=O)c1cccc(C=O)c1	3{12}	[C-][N+]CC1COC1	49.9	39

1559	4{347,536,46}	CC(=C)CNC1=C(N=C2C=CC(Cl)=CN12)C1=CN=C(O1)C1CCOCC1 c:9,12,19,t:5,7,17	Z8849597802	1{347}	Nc1ccc(Cl)cn1	2{536}	O=Cc1enc(o1)C2CCOCC2	3{46}	CC(=C)C[N+][C-]	38.6	38
1560	4{366,721,10}	COC(=O)C1=CC(=CN=C1)C1=C(NC2CCOC2)N2C=CC=C(OC)C2=N1 c:6,8,11,21,28,t:4,23	Z8849597815	1{366}	COc1cccnc1N	2{721}	COC(=O)c1cncc(C=O)c1	3{10}	[C-][N+]C1CCOC1	38.1	38
1561	4{212,155,76}	COCC1=CN2C(C=C1)=NC(=C2NC1CN(C1)C(=O)OC(C)(C)C)C1=CN=CN=C1 c:7,9,11,29,31,t:3,27	Z8873684912	1{212}	Cl.COCc1ccc(N)nc1	2{155}	O=Cc1encnc1	3{76}	CC(C)(C)OC(=O)N1CC(C1)[N+]#[C-]	42.4	38
1562	4{146,180,51}	CC(C)(C)OC(=O)NCCNC1=C(CCCCCF)N=C2C=CC(=CN12)S(C)(=O)=O c:11,21,23,t:19	Z8878918796	1{146}	CS(=O)(=O)c1ccc(N)nc1	2{180}	FCCCCC=O	3{51}	CC(C)(C)OC(=O)NCC[N+]#[C-]	45.7	38
1563	4{79,25,20}	COC1=CC(C)=C(NC2=C(N=C3C=NC=C(C)N23)C2=CN=C(N=C2)C2CCOCC2)C=C1 c:12,22,24,34,t:2,5,8,10,14,20	Z8878918845	1{79}	Cc1encnc(N)n1	2{25}	O=Cc1enc(nc1)C2CCOCC2	3{20}	COc1ccc([N+]#[C-])c(C)c1	44.3	38
1564	4{47,727,6}	CCOC(=O)CCNC1=C(N=C2C=C(C=CN12)S(N)(=O)=O)C1=CN=C(N=C1)C(C)C c:13,15,26,28,t:9,11,24	Z8849597798	1{47}	Cl.Nc1cc(ccn1)S(=O)(=O)N	2{727}	CC(C)c1ncc(C=O)cn1	3{6}	CCOC(=O)CC[N+]#[C-]	45.9	38
1565	4{79,728,9}	CNC1=C(N=C2C=NC=C(C)N12)C1=CN=C(S1)C1CCC1 c:6,16,t:2,4,8,14	Z8878918882	1{79}	Cc1encnc(N)n1	2{728}	O=Cc1enc(s1)C2CCC2	3{9}	C[N+]#[C-]	30.6	38
1566	4{91,555,26}	CC1=NN(C(C)=C1)C1=C(NCC2=CC=C(F)C=C2)N2C=C(C=CC2=N1)C(N)=O)C1=NC=CC=C1 c:5,8,17,21,23,26,34,36,t:1,12,14,32	Z8873684863	1{91}	NC(=O)c1ccc(N)nc1	2{555}	Cc1nn(c(C)c1C=O)e2ccccn2	3{26}	Fe1ccc(C[N+]#[C-])cc1	46.6	38
1567	4{59,729,49}	COC1=C(C=CC=C1C#N)C1=C(NC2CC(F)(F)C2)N2C=C(CN3CCOCC3)C=CC2=N1 c:4,6,11,32,35,t:2,22	Z8873684701	1{59}	Nc1ccc(CN2CCOCC2)cn1	2{729}	COc1c(C=O)cccc1C#N	3{49}	FC1(F)CC(C1)[N+]#[C-]	46.2	38
1568	4{239,119,37}	CCOC(=O)C1=NN=C(N1)C1=C(NC2CC(C2)C(=O)OC)N2C=C(C=CC2=N1)N1CCCC1 c:7,11,24,26,29,t:5	Z8873684590	1{239}	Cl.Cl.Nc1ccc(en1)N2CCCC2	2{119}	CCOC(=O)c1nncc(C=O)[nH]1	3{37}	COC(=O)C1CC(C1)[N+]#[C-]	46.1	38
1569	4{351,730,28}	CCCNC1=C(N=C2C=CC3=C(C(O)CC3)N12)C1=CN(N=C1C)C(C)(C)C c:8,23,t:4,6,10,20	Z8873684849	1{351}	Nc1ccc2CC(C(O)c2)n1	2{730}	Cc1nn(cc1C=O)C(C)(C)C	3{28}	CCC[N+]#[C-]	37.4	38
1570	4{49,197,13}	COC(=O)C1=CC(=NN1C)C1=C(NCC2=CC=C(OC)C=C2)N2C(C=CC=C2CO)=N1 c:6,11,21,26,28,32,t:4,15,17	Z8873684639	1{49}	Nc1cccc(CO)n1	2{197}	COC(=O)c1ccc(C=O)nn1C	3{13}	COc1ccc(C[N+]#[C-])cc1	42.9	38

1571	4{463,135,49}	CN1N=C(C)C(=C1C)C1=C(NC2CC(F)(F)C2)N2C=C(C=CC2=N1)C(=O)OC(C)(C)C c:5,9,20,22,25,t:2	Z8849597818	1{463}	CC(C)(C)O C(=O)c1ccc (N)nc1	2{135}	Cc1nn(C)c(C) c1C=O	3{49}	FC1(F)CC(C 1)[N+]#[C-]	43.9	38
1572	4{83,731,31}	COC1=C(C=CC(Br)=C1)C1=C(NCCSC)N2C=C(C=CC2=N1)P(C)(C)=O c:4,7,10,18,20,23,t:2	Z8873685488	1{83}	CP(=O)(C)c 1ccc(N)nc1	2{731}	COc1cc(Br)c cc1C=O	3{31}	CSCC[N+]#[C-]	47.6	38
1573	4{139,375,51}	COCC1=C(N=CO1)C1=C(NCCNC(=O)OC(C) (C)C)N2C=CC(=CC2=N1)C(F)F c:5,9,23,25,28,t:3	Z8878918813	1{139}	Nc1cc(ccn1)C(F)F	2{375}	COCc1ocnc1 C=O	3{51}	CC(C)(C)OC (=O)NCC[N +]#[C-]	44.4	38
1574	4{358,732,15}	CCNC1=C(N=C2C=C(C=CN12)C(C)(C)O)[C @@H]1C[C@H]1C1CC1 &1:16,18,r,c:7,9,t:3,5	Z8878918454	1{358}	CC(C)(O)c1 ccnc(N)c1	2{732}	O=C[C@@H]1C[C@H]1 C2CC2 &1:2,4,r	3{15}	CC[N+]#[C-]	30.3	37
1575	4{41,733,13}	COC1=CC=C(CNC2=C(N=C3C=NC(C)=CN2 3)C2=NN(N=N2)C(C)(C)C=C1 c:12,15,23,30,t:2,4,8,10,20	Z8855739216	1{41}	Cc1cnc(N)c n1	2{733}	CC(C)(C)n1n nc(C=O)n1	3{13}	COc1ccc(C[N+]#[C-])cc1	39.7	37
1576	4{83,146,18}	C[C@@H]1C[C@@H]1CCCC1=C(NC(C)(C)C) N2C=C(C=CC2=N1)P(C)(C)=O &1:1,3,r,c:7,15,17,20	Z8878918375	1{83}	CP(=O)(C)c 1ccc(N)nc1	2{146}	C[C@@H]1 C[C@@H]1 CCC=O &1:1,3,r	3{18}	CC(C)(C)[N +]#[C-]	35.1	37
1577	4{41,95,9}	CNC1=C(N=C2C=NC(C)=CN12)C1=CC(=NC =C1)N(C)C c:6,9,16,18,t:2,4,14	Z8855739107	1{41}	Cc1cnc(N)c n1	2{95}	CN(C)c1cc(C=O)ccn1	3{9}	C[N+]#[C-]	28.5	37
1578	4{188,734,62}	COC(=O)C1=CN=CC2=NC(=C(NC3(CCCC3) C(=O)OC)N12)C1=C(C)C(=NN1)C(F)(F)F c:6,26,29,t:4,8,10	Z8835022882	1{188}	COC(=O)c1 cnc(N)n1	2{734}	Cc1c(C=O)[n H]nc1C(F)(F)F	3{62}	COC(=O)C1(CCCC1)[N+] #[C-]	47.0	37
1579	4{62,94,11}	OCC1=CC2=NC(=C(NCC3=CC(Br)=CC=C3) N2C=C1)C1=NC=CN=C1 c:13,15,20,25,27,t:2,4,6,10,23	Z8873684641	1{62}	Nc1cc(CO)c cn1	2{94}	O=Cc1cncn 1	3{11}	Brc1cccc(C[N+]#[C-])c1	41.0	37
1580	4{69,369,24}	CNC(=O)C1=CC2=NC(=C(NCC3=CC(OC)=C C=C3)N2C=C1)C1=CON=C1C c:16,18,23,29,t:4,6,8,12,26	Z8878918887	1{69}	CNC(=O)c1 ccnc(N)c1	2{369}	Cc1noc1C= O	3{24}	COc1cccc(C[N+]#[C-])c1	38.7	37
1581	4{359,735,22}	COC(=O)C1=CN=C(S1)C1=C(NC2COC2)N2 C=C(OC(F)F)C=CC2=N1 c:6,10,25,28,t:4,19	Z8854581181	1{359}	Nc1ccc(OC(F)F)cn1	2{735}	COC(=O)c1c nc(C=O)s1	3{22}	[C-]#[N+]C1CO C1	39.2	37
1582	4{174,21,43}	CC(C)(C)OC(=O)N1CCC(CC1)NC1=C(N=C2 C=CC=C(C#N)N12)C1=CC2=NC=NN2C=C1 c:19,32,36,t:15,17,21,28,30	Z8873685273	1{174}	Nc1cccc(C# N)n1	2{21}	O=Cc1cn2n cnc2c1	3{43}	CC(C)(C)OC (=O)N1CCC(CC1)[N+]#[C-]	45.0	36

1583	4{166,168,35}	CSCCCNC1=C(N=C2C=C(CSCCO)C=CN12)C1=NOC=C1 c:17,25,t:6,8,10,22	Z8854581179	1{166}	Nc1cc(CSCCO)ccn1	2{168}	O=Cc1ccn1	3{35}	CSCCC[N+]#[C-]	36.8	36
1584	4{99,736,34}	CC1(C)CC(C1)C1=C(NCC2CCCO2)N2C=C(C=CC2=N1)S(N)(=O)=O c:7,18,20,23	Z8835022874	1{99}	Nc1ccc(en1)S(=O)(=O)N	2{736}	CC1(C)CC(C1)C=O	3{34}	[C-]#[N+]CC1CCO1	36.8	36
1585	4{28,737,7}	FC1=C(C=CC(=C1)C1=C(NC2CCOCC2)N2C=CC(=CC2=N1)C1=NOC=N1)C#C c:3,5,8,19,21,24,30,t:1,27	Z8873684597	1{28}	Cl.Nc1cc(ccn1)c2ncon2	2{737}	Fc1cc(C=O)cc1C#C	3{7}	[C-]#[N+]C1CCOCC1	39.0	36
1586	4{180,168,32}	COC(=O)C1=CC2=NC(=C(NC3CCC3)N2C=C1C)C1=NOC=C1 c:18,25,t:4,6,8,22	Z8878918534	1{180}	COC(=O)c1cc(N)nc1C	2{168}	O=Cc1ccn1	3{32}	[C-]#[N+]C1CC1	31.4	36
1587	4{464,390,5}	COCCNC1=C(N=C2C=CC(=CN12)N1CCN(C)CC1)C1CC2C(C1)C2(F)F c:10,12,t:6,8	Z8855619556	1{464}	CN1CCN(C1)c2ccc(N)nc2	2{390}	FC1(F)C2CC(CC21)C=O	3{5}	COCC[N+]#[C-]	40.3	36
1588	4{367,364,34}	CC1=CN2C(NCC3CCCO3)=C(CCC3CCCO3)N=C2C(=C1)C#C c:22,25,t:1,12	Z8878918416	1{367}	Cc1enc(N)c(C#C)c1	2{364}	O=CCCC1CCO1	3{34}	[C-]#[N+]CC1CCO1	33.8	35
1589	4{73,53,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC4=NC=CN4N23)C2=C(F)C=CC(C)=N2)C=C1 c:12,16,23,26,29,32,t:2,5,8,10,14	Z8878918602	1{73}	Nc1ccc2nccn2n1	2{53}	Cc1ccc(F)c(C=O)n1	3{20}	COc1ccc([N+]#[C-])c(C)c1	38.5	35
1590	4{48,99,15}	CCNC1=C(N=C2C=C(C=CN12)S(C)(=O)=O)C1=COC=N1 c:7,9,21,t:3,5,18	Z8873685462	1{48}	CS(=O)(=O)c1cenc(N)c1	2{99}	O=Cc1ccn1	3{15}	CC[N+]#[C-]	29.2	35
1591	4{439,148,10}	COC1=C(C(C)=NN1C)C1=C(NC2CCOC2)N2C=CC=C(OCC3=CC=CC=C3)C2=N1 c:5,10,20,28,30,34,t:2,22,26	Z8849597809	1{439}	Nc1ncccc1OCc2cccc2	2{148}	COc1c(C=O)c(C)nn1C	3{10}	[C-]#[N+]C1CCOC1	41.3	35
1592	4{73,88,11}	BrC1=CC(CNC2=C(N=C3C=CC4=NC=CN4N23)C2=CC3=C(C=CC=N3)C=C2)=CC=C1 c:10,14,25,27,30,32,34,t:1,6,8,12,21,23	Z8873684895	1{73}	Nc1ccc2nccn2n1	2{88}	O=Cc1ccc2ccnc2c1	3{11}	Br1cccc(C[N+]#[C-])c1	44.5	35
1593	4{36,672,14}	COCCNC1=C(N=C2C=CC(Br)=CN12)C1=C(C)SC=N1 c:9,12,17,21,t:5,7	Z8846492100	1{36}	Nc1ccc(Br)cn1	2{672}	Cc1scnc1C=O	3{14}	COCC[N+]#[C-]	34.5	35
1594	4{405,587,38}	COC1=NOC(C)=C1C1=C(NC2=CC3=C(OCO3)C=C2)N2C=C(C=CC2=N1)N1CCCC1=O c:6,9,20,24,26,29,t:2,12,14	Z8878918646	1{405}	Nc1ccc(en1)N2CCCC2=O	2{587}	COc1noc(C)c1C=O	3{38}	[C-]#[N+]c1ccc2OCOc2c1	42.0	35
1595	4{371,486,12}	CN1C(C1)=NC(C1)=C1C1=C(NCC2CCOC2)N2C=CC=C(OCCCC#N)C2=N1 c:3,6,9,20,31,t:22	Z8873684601	1{371}	Nc1ncccc1OCCCC#N	2{486}	Cn1c(Cl)nc(Cl)c1C=O	3{12}	[C-]#[N+]CC1CCOC1	42.1	35

1596	4{185,738,29}	CCOC(=O)CCNC1=C(N=C2C=CC(=C(C)N12)S(C)(=O)=O)C1=CC(CI)=CN=C1 c:12,27,29,t:8,10,14,24	Z8855739080	1{185}	Cc1nc(N)cc1S(=O)(=O)C	2{738}	Clc1encc(C=O)c1	3{29}	CCOC(=O)C[C[N+][C-]]	40.9	35
1597	4{47,116,26}	NS(=O)(=O)C1=CC2=NC(=C(NCC3=CC=C(F)C=C3)N2C=C1)C1=CN(CCC=C)N=N1 c:17,22,32,t:4,6,8,12,14,25	Z8849597831	1{47}	Cl.Nc1cc(ccn1)S(=O)(=O)N	2{116}	C=CCcn1cc(C=O)nn1	3{26}	Fc1ccc(C[N+][C-])cc1	41.3	35
1598	4{129,550,29}	CCOC(=O)CCNC1=C(N=C2C=CC=C(SC)N12)C1=NC(Br)=NN1C c:12,24,t:8,10,14,21	Z8873684879	1{129}	CSc1cccc(N)n1	2{550}	Cn1nc(Br)nc1C=O	3{29}	CCOC(=O)C[C[N+][C-]]	41.0	35
1599	4{206,344,14}	COCCNC1=C(N=C2N1C=CC(I)=C2F)C1=C(C)C=NN1COC c:7,11,14,18,21,t:5	Z8873684648	1{206}	Nc1nccc(I)c1F	2{344}	COc1nccc(C)c1C=O	3{14}	COCC[N+][C-]	42.9	35
1600	4{41,161,13}	CCN1C=NC=C1C1=C(NCC2=CC=C(OC)C=C2)N2C=C(C)N=CC2=N1 c:3,5,8,18,25,28,t:12,14,22	Z8855739127	1{41}	Cc1enc(N)c1n1	2{161}	CCn1encc1C=O	3{13}	COc1ccc(C[N+][C-])cc1	33.8	35
1601	4{359,689,15}	CCNC1=C(N=C2C=CC(OC(F)F)=CN12)C1=CN(CCOC(C)=O)N=C1 c:7,13,27,t:3,5,18	Z8873685423	1{359}	Nc1ccc(OC(F)F)c1n1	2{689}	CC(=O)OCCn1cc(C=O)cn1	3{15}	CC[N+][C-]	35.3	34
1602	4{119,454,61}	COC(C)CC1=C(NCCCNC(=O)OC(C)(C)C)N2C=C(C=CC2=N1)C#N c:5,20,22,25	Z8878918653	1{119}	Nc1ccc(C#N)c1n1	2{454}	COC(C)CC=O	3{61}	CC(C)(C)OC(=O)NCCC[N+][C-]	35.6	34
1603	4{109,357,41}	CCC1=C(C(C)=NO1)C1=C(NC2=CC=C(OC)C=C2)N2C(C=CC=C2S(N)(=O)=O)=N1 c:5,9,18,23,25,31,t:2,12,14	Z8854581176	1{109}	Cl.Nc1cccc(n1)S(=O)(=O)N	2{357}	CCc1onc(C)c1C=O	3{41}	COc1ccc([N+][C-])cc1	39.0	34
1604	4{73,739,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC4=NC=CN4N23)C2=CC3=C(C=NN3C)C=C2)C=C1 c:12,16,27,32,35,t:2,5,8,10,14,23,25	Z8855619518	1{73}	Nc1ccc2nccn2n1	2{739}	Cn1ncc2ccc(C=O)cc12	3{20}	COc1ccc([N+][C-])c(C)c1	38.6	34
1605	4{286,740,23}	COC(=O)CCC(NC1=C(N=C2C=CC(=CN12)C1=NC=CC=C1)C1=CN(N=C1)C(F)F)C(=O)OC c:12,14,21,23,29,t:8,10,19,26	Z8829498781	1{286}	Cl.Cl.Nc1ccc(en1)c2cccen2	2{740}	FC(F)n1cc(C=O)c1n1	3{23}	COC(=O)CC(C([N+][C-])C(=O)OC	44.1	34
1606	4{287,603,10}	COC(=O)C1=CC(=NS1)C1=C(NC2CCOC2)N2C=CC(CI)=CC2=N1 c:6,10,20,23,26,t:4	Z8873685424	1{287}	Nc1cc(Cl)ccn1	2{603}	COC(=O)c1cc(C=O)ns1	3{10}	[C-][N+][C1CCOC1	34.3	34
1607	4{36,257,9}	CNC1=C(N=C2C=CC(Br)=CN12)C1CC(C1)NC(=O)OC(C)(C)C c:6,9,t:2,4	Z8873685342	1{36}	Nc1ccc(Br)c1n1	2{257}	CC(C)(C)OC(=O)NC1CC(C1)C=O	3{9}	C[N+][C-]	35.7	33

1608	4{465,741,49}	FC1(F)CC(C1)NC1=C(N=C2C=CC(=CN12)S(=O)(=O)NC1CC1)C1=CC=C(C=C1)N1C=NC=N1 c:12,14,29,31,35,37,t:8,10,27	Z8829498651	1{465}	Nc1ccc(en1)S(=O)(=O)NC2CC2	2{741}	O=Cc1ccc(cc1)n2cncn2	3{49}	FC1(F)CC(C1)[N+]#[C-]	43.8	33
1609	4{146,328,24}	CCC1=NNC=C1C1=C(NCC2=CC(OC)=CC=C2)N2C=C(C=CC2=N1)S(C)(=O)=O c:5,8,16,18,22,24,27,t:2,12	Z8878918638	1{146}	CS(=O)(=O)c1ccc(N)nc1	2{328}	Cl.CCCc1n[nH]cc1C=O	3{24}	COc1cccc(C[N+]#[C-])c1	38.3	33
1610	4{447,135,37}	COC(=O)C1CC(C1)NC1=C(N=C2C=CC(=CN12)N(C)C)C1=C(C)N(C)N=C1C c:14,16,24,29,t:10,12	Z8873684739	1{447}	CN(C)c1ccc(N)nc1	2{135}	Cc1nn(C)c(C)c1C=O	3{37}	COC(=O)C1CC(C1)[N+]#[C-]	35.6	33
1611	4{166,626,15}	CCNC1=C(N=C2C=C(CSCCO)C=CN12)C1=CC2=C(CCN(C2)C(C)=O)S1 c:14,t:3,5,7,19,21	Z8873684916	1{166}	Nc1cc(CSCCO)ccn1	2{626}	CC(=O)N1CCc2sc(C=O)c2C1	3{15}	CC[N+]#[C-]	38.7	33
1612	4{460,369,21}	CC1=NOC=C1C1=C(NCC2CC2)N2C=CC=C(C)C2=N1 c:4,7,16,22,t:1,18	Z8855619657	1{460}	Cc1cccnc1N	2{369}	Cc1noc1C=O	3{21}	[C-]#[N+]CC1C1	25.4	33
1613	4{48,742,22}	CS(=O)(=O)C1=CC2=NC(=C(NC3COC3)N2C=C1)C1=C(F)C(Br)=CC=C1F c:18,21,25,27,t:4,6,8	Z8873684860	1{48}	CS(=O)(=O)c1ccnc(N)c1	2{742}	Fe1ccc(Br)c(F)c1C=O	3{22}	[C-]#[N+]C1CO1	41.1	33
1614	4{41,672,13}	COC1=CC=C(CNC2=C(N=C3C=NC(C)=CN23)C2=C(C)SC=N2)C=C1 c:12,15,20,24,27,t:2,4,8,10	Z8878918776	1{41}	Cc1cnc(N)c1	2{672}	Cc1scnc1C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	32.7	33
1615	4{49,29,13}	CCN1C=CC(=N1)C1=C(NCC2=CC=C(OC)C=C2)N2C(C=CC=C2CO)=N1 c:3,5,8,18,23,25,29,t:12,14	Z8878918879	1{49}	Nc1cccc(C)O1	2{29}	CCn1ccc(C=O)n1	3{13}	COc1ccc(C[N+]#[C-])cc1	33.3	33
1616	4{48,115,35}	COC1=NN(C)C(=C1)C1=C(NCCCSC)N2C=C(C=CC2=N1)S(C)(=O)=O c:6,9,18,20,23,t:2	Z8873685307	1{48}	CS(=O)(=O)c1ccnc(N)c1	2{115}	COc1cc(C=O)n(C)n1	3{35}	CSCCC[N+]#[C-]	36.1	33
1617	4{62,49,6}	CCOC(=O)CCNC1=C(N=C2C=C(CO)C=CN12)C1=CN=C1C c:17,25,t:9,11,13,22	Z8873684869	1{62}	Nc1cc(CO)c1	2{49}	Cc1n[nH]cc1C=O	3{6}	CCOC(=O)CC[N+]#[C-]	31.5	33
1618	4{358,87,15}	CCNC1=C(N=C2C=C(C=CN12)C(C)(C)O)[C@@H]1C[C@H]1C(=O)OC(C)(C)C &1:16,18,r,c:7,9,t:3,5	Z8878918449	1{358}	CC(C)(O)c1ccnc(N)c1	2{87}	CC(C)(C)OC(=O)[C@@H]1C[C@H]1C=O &1:7,9,r	3{15}	CC[N+]#[C-]	31.5	32
1619	4{166,60,32}	CC(C1CCOC1)C1=C(NC2CCC2)N2C=CC(CS)CCO)=CC2=N1 c:8,17,24,27	Z8878918678	1{166}	Nc1cc(CSCCO)ccn1	2{60}	CC(C=O)C1CCOC1	3{32}	[C-]#[N+]C1CC1	32.9	32

1620	4{125,92,18}	CC1=NOC(=C1)C1=C(NC(C)(C)C)N2C=C(CO)C=CC2=N1 c:4,7,20,23,t:1,15	Z8873684676	1{125}	Nc1ccc(CC)cn1	2{92}	Cc1cc(C=O)on1	3{18}	CC(C)(C)[N+]#[C-]	27.5	32
1621	4{109,743,34}	CCC1=NC=CC(=C1)C1=C(NCC2CCCO2)N2C(C=CC=C2S(N)(=O)=O)=N1 c:4,6,9,21,23,29,t:2	Z8873684764	1{109}	Cl.Nc1cccc(n1)S(=O)(=O)N	2{743}	CCc1cc(C=O)ccn1	3{34}	[C-]#[N+]CC1CCO1	35.0	32
1622	4{32,744,31}	CSCCNC1=C(N=C2C=C(C=CN12)P(C)(C)=O)C1=C(F)C=CC(=C1)C#C c:9,11,20,23,25,t:5,7	Z8873684898	1{32}	CP(=O)(C)c1ccnc(N)c1	2{744}	Fc1ccc(C#C)cc1C=O	3{31}	CSCC[N+]#[C-]	35.0	32
1623	4{153,745,15}	CCNC1=C(N=C2C=CC=C(N12)C(C)(C)O)C1=C(C)C=NC=C1 c:7,9,18,21,23,t:3,5	Z8878918516	1{153}	CC(C)(O)c1cccc(N)n1	2{745}	Cc1cncnc1C=O	3{15}	CC[N+]#[C-]	27.0	32
1624	4{466,294,5}	COCCNC1=C(N=C2C=CC(OCCC(C)C)=NN12)C1=C(OC)C(=O)C=CO1 c:10,18,23,29,t:6,8	Z8878918834	1{466}	CC(C)CCOc1ccc(N)nn1	2{294}	COc1c(C=O)occc1=O	3{5}	COCCC[N+]#[C-]	36.1	32
1625	4{186,746,8}	COC(=O)C(CC1=CC=CC=C1)NC1=C(N=C2C=C(C=CN12)S(=O)(=O)N(C)C)C1=C(C)C=C N=C1 c:8,10,18,20,31,34,36,t:6,14,16	Z8873684706	1{186}	Cl.CN(C)S(=O)(=O)c1ccnc(N)c1	2{746}	Cc1cncnc1C=O	3{8}	COC(=O)C(Cc1cccc1)[N+]#[C-]	42.8	32
1626	4{438,747,10}	CCOC(=O)C1=COC(=N1)C1=C(NC2CCOC2)N2C(C=CC(Br)=C2CC)=N1 c:8,11,22,25,29,t:5	Z8855619574	1{438}	CCc1nc(N)ccc1Br	2{747}	CCOC(=O)c1coc(C=O)n1	3{10}	[C-]#[N+]C1CCOC1	39.0	32
1627	4{46,19,9}	CNC1=C(N=C2C=CC=CN12)C1=C(OC)C=N N1C c:6,8,13,17,t:2,4	Z8873684646	1{46}	Nc1ccccn1	2{19}	COc1cnn(C)c1C=O	3{9}	C[N+]#[C-]	22.2	32
1628	4{105,480,50}	NC(=O)C1=CC=CC2=NC(=C(NC3=CC4=C(O)CCO4)C=C3)N12)C1=CC2=C(CCO2)N=C1 c:5,21,36,t:3,7,9,12,14,27,29	Z8829498452	1{105}	NC(=O)c1cccc(N)n1	2{480}	O=Cc1cnc2COCc2c1	3{50}	[C-]#[N+]c1cccc2OCCO2c1	38.1	32
1629	4{171,318,15}	CCNC1=C(N=C2C=C(C=CN12)N1C=CN=C1)C1CC1CC1(F)F c:7,9,15,17,t:3,5	Z8878918910	1{171}	Nc1cc(ccn1)n2ccnc2	2{318}	FC1(F)CC21CC2C=O	3{15}	CC[N+]#[C-]	28.3	32
1630	4{353,748,32}	CN1N=C(C=C1)C1=C(NC2CCCC2)N2C=C(NS(C)(=O)=O)C=CC2=N1)C(F)(F)F c:2,4,7,23,26,t:16	Z8873685348	1{353}	Cl.CS(=O)(=O)Nc1ccc(N)nc1	2{748}	Cn1nc(cc1C=O)C(F)(F)F	3{32}	[C-]#[N+]C1CC1	36.5	32
1631	4{92,749,14}	COCCNC1=C(N=C2C=C(C=CN12)C(N)=O)[C@H]1C[C@H]1C1=CC=CC=C1 &1:17,19,r,c:9,11,25,27,t:5,7,23	Z8854581153	1{92}	NC(=O)c1ccnc(N)c1	2{749}	O=C[C@@H]1C[C@H]1c2ccccc2 &1:2,4,r	3{14}	COCC[N+]#[C-]	29.8	32
1632	4{83,203,26}	CP(C)(=O)C1=CN2C(C=C1)=NC(C1=NN(CC(F)F)C=C1)=C2NCC1=CC=C(F)C=C1 c:8,10,20,22,32,t:4,13,27,29	Z8846491831	1{83}	CP(=O)(C)c1ccc(N)nc1	2{203}	FC(F)Cn1ccc(C=O)n1	3{26}	Fc1ccc(C[N+]#[C-])cc1	37.8	31

1633	4{187,662,12}	CP(C)(=O)C1=CC(=CC=C1)C1=C(NCC2CCOC2)N2C=C(Cl)C(=CC2=N1)C#N c:6,8,11,25,28,t:4,22	Z8873684757	1{187}	Nc1cc(C#N)c(Cl)cn1	2{662}	CP(=O)(C)c1cccc(C=O)c1	3{12}	[C-]#[N+]CC1COC1	36.1	31
1634	4{377,665,46}	CN1N=NC(=C1C)C1=C(NCC(C)=C)N2C=CC=C(OCC(F)F)C2=N1 c:2,4,8,16,26,t:18	Z8878918373	1{377}	Nc1ncccc1OCC(F)F	2{665}	Cc1c(C=O)nn1C	3{46}	CC(=C)C[N+]#[C-]	30.5	31
1635	4{84,645,31}	CSCCNC1=C(N=C2N1C=CN=C2C(C)C)C1=CN=N1 c:7,11,13,22,t:5,19	Z8873684861	1{84}	CC(C)c1nccnc1N	2{645}	O=Cc1c[nH]nn1	3{31}	CSCC[N+]#[C-]	26.7	31
1636	4{41,262,9}	CCC1=NN(C)C(=C1Cl)C1=C(NC)N2C=C(C)N=CC2=N1 c:6,10,18,21,t:2,15	Z8878918869	1{41}	Cc1cnc(N)cn1	2{262}	CCc1nn(C)c(C=O)c1Cl	3{9}	C[N+]#[C-]	25.5	31
1637	4{92,101,7}	NC(=O)C1=CC2=NC(=C(NC3CCOCC3)N2C=C1)C1=C(CO)C=CS1 c:19,22,26,t:3,5,7	Z8829498636	1{92}	NC(=O)c1cnc(N)c1	2{101}	OCc1ccsc1C=O	3{7}	[C-]#[N+]C1CCOCC1	31.2	31
1638	4{73,750,13}	CCOC1=CC(=CC=C1)C1=C(NCC2=CC=C(O)C)C=C2)N2N3C=CN=C3C=CC2=N1 c:5,7,10,20,25,27,30,33,t:3,14,16	Z8878918873	1{73}	Nc1ccc2nccn2n1	2{750}	CCOc1cccc(C=O)c1	3{13}	COc1ccc(C[N+]#[C-])cc1	34.6	31
1639	4{467,751,47}	COC1=CC2=C(C=C1)C=C(CO2)C1=C(NC(C)C)N2C=C(C=CC2=N1)C(=O)N1CCOCC1 c:4,6,9,14,21,23,26,t:2	Z8873685299	1{467}	Nc1ccc(en1)C(=O)N2C COCC2	2{751}	COc1ccc2C=C(COc2c1)C=O	3{47}	CC(C)[N+]#[C-]	37.4	31
1640	4{352,752,49}	CN1CCN(CC1=O)C1=CN2C(C=C1)=NC(=C2)NC1CC(F)(F)C1)C1=CC(=CC=C1)C#N c:13,15,17,30,32,t:9,28	Z8873684814	1{352}	CN1CCN(C)C1=O)c2ccc(N)nc2	2{752}	O=Cc1cccc(C#N)c1	3{49}	FC1(F)CC(C1)[N+]#[C-]	36.3	31
1641	4{69,753,10}	CNC(=O)C1=CC2=NC([C@@H]3CCCC[C@H](C)N3C(=O)OC(C)(C)C)=C(NC3CCOC3)N2C=C1 &1:9,13,r;c:34,t:4,6,23	Z8878918622	1{69}	CNC(=O)c1cnc(N)c1	2{753}	C[C@@H]1CCC[C@H](C=O)N1C(=O)OC(C)(C)C &1:1,5,r	3{10}	[C-]#[N+]C1CCOC1	38.0	31
1642	4{28,115,7}	COC1=NN(C)C(=C1)C1=C(NC2CCOCC2)N2C=CC(=CC2=N1)C1=NOC=N1 c:6,9,20,22,25,31,t:2,28	Z8855739208	1{28}	Cl.Nc1cc(ccn1)c2ncon2	2{115}	COc1cc(C=O)n(C)n1	3{7}	[C-]#[N+]C1CCOCC1	32.8	31
1643	4{83,754,18}	CC(C)(C)NC1=C(N=C2C=CC(=CN12)P(C)(C)=O)C1CC2CC2C1 c:9,11,t:5,7	Z8878918486	1{83}	CP(=O)(C)c1ccc(N)nc1	2{754}	O=CC1CC2CC2C1	3{18}	CC(C)(C)[N+]#[C-]	28.7	31
1644	4{183,392,28}	CCCNC1=C(N=C2N1C(C)=CC=C2OC)C1CCOCC1 c:6,11,13,t:4	Z8849597822	1{183}	COc1ccc(C)nc1N	2{392}	O=CC1CCOCC1	3{28}	CCC[N+]#[C-]	25.2	31

1645	4{350,354,5}	COCCNC1=C(N=C2C=NC(=CN12)C1=CC=CC=C1)C1=C(C=CC=C1)P(C)(C)=O c:10,12,19,21,26,28,t:6,8,17,24	Z8878918587	1{350}	Nc1cnc(en1) c2ccccc2	2{354}	CP(=O)(C)c1 ccccc1C=O	3{5}	COCCC[N+] #[C-]	36.1	31
1646	4{154,468,47}	CSC(C)CC1=C(NC(C)C)N2C=CC(=CC2=N1)[N+][O-]=O c:5,12,14,17	Z8854581155	1{154}	Nc1cc(ccn1) [N+](=O)[O-]	2{468}	CSC(C)CC=O	3{47}	CC(C)[N+]#[C-]	25.6	31
1647	4{85,755,15}	CCNC1=C(N=C2C=C(C=C(C)N12)C#N)C1=C2=C(C=C1)N(C)C(=O)O2 c:7,19,21,t:3,5,9,17	Z8849597804	1{85}	Cc1cc(C#N) cc(N)n1	2{755}	Cn1c(=O)oc2 cc(C=O)ccc1 2	3{15}	CC[N+]#[C-]	28.8	31
1648	4{79,137,13}	COC1=CC=C(CNC2=C(N=C3C=NC=C(C)N23)C2=C(C)ON=C2C)C=C1 c:12,20,24,28,t:2,4,8,10,14	Z8854581163	1{79}	Cc1cncc(N) n1	2{137}	Cc1noc(C)c1 C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	30.0	31
1649	4{72,536,46}	COC1=NC(Br)=CN2C(NCC(C)=C)=C(N=C12)C1=CN=C(O1)C1CCOCC1 c:5,13,21,t:2,15,19	Z8835022870	1{72}	COc1nc(Br) cnc1N	2{536}	O=Cc1cnc(o1) C2CCOCC 2	3{46}	CC(=C)C[N+]#[C-]	36.9	30
1650	4{186,756,69}	COC1=C(NC2=C(N=C3C=C(C=CN23)S(=O)(=O)N(C)C)C2=CC(=CO2)S(C)(=O)=O)C=CC=C1 c:2,9,11,24,32,34,t:5,7,22	Z8878918381	1{186}	Cl.CN(C)S(=O)(=O)c1c cnc(N)c1	2{756}	CS(=O)(=O) c1coc(C=O)c 1	3{69}	COc1ccccc1[N+]#[C-]	40.3	30
1651	4{41,757,13}	CCCN1N=CN=C1C1=C(NCC2=CC=C(OC)C=C2)N2C=C(C)N=CC2=N1 c:4,6,9,19,26,29,t:13,15,23	Z8878918313	1{41}	Cc1cnc(N)c n1	2{757}	CCCN1ncnc1 C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	31.0	30
1652	4{109,539,34}	NS(=O)(=O)C1=CC=CC2=NC([C@@H]3CCCC[C@H]3C(F)(F)F)=C(NCC3CCCO3)N12 &1:11,16,r,c:6,t:4,8,21	Z8835022889	1{109}	Cl.Nc1cccc(n1) S(=O)(=O)N	2{539}	FC(F)(F)[C@@H]1CCCC[C@H]1C=O &1:4,9,r	3{34}	[C-] #[N+]CC1C CCO1	36.6	30
1653	4{68,354,59}	CP(C)(=O)C1=C(C=CC=C1)C1=C(NCCC2=C(C(F)=CC=C2)N2C=CC(=CC2=N1)C#C c:6,8,11,19,21,25,27,30,t:4,16	Z8873684914	1{68}	Nc1cc(C#C) ccn1	2{354}	CP(=O)(C)c1 ccccc1C=O	3{59}	Fc1cccc(CC[N+]#[C-])c1	35.3	30
1654	4{46,396,9}	CNC1=C(N=C2C=CC=CN12)C1=CN=C2COCN12 c:6,8,t:2,4,13,15	Z8849597823	1{46}	Nc1ccccn1	2{396}	O=Cc1cnc2C OCCn12	3{9}	C[N+]#[C-]	22.1	30
1655	4{377,413,10}	FC(F)COC1=CC=CN2C(NC3CCOC3)=C(N=C12)C1=CN=C(S1)C1=CC=NC=C1 c:7,17,25,31,33,t:5,19,23,29	Z8873684699	1{377}	Nc1cccc1 OCC(F)F	2{413}	O=Cc1cnc(s1) c2ccccc2	3{10}	[C-] #[N+]C1CC OC1	36.2	30
1656	4{353,626,35}	CSCCCNC1=C(N=C2C=CC(NS(C)(=O)=O)=CN12)C1=CC2=C(CCN(C2)C(C)=O)S1 c:10,17,t:6,8,22,24	Z8873685326	1{353}	Cl.CS(=O)(=O) Nc1ccc(N)nc1	2{626}	CC(=O)N1C Cc2sc(C=O)c c2C1	3{35}	CSCCC[N+]#[C-]	40.1	30

1657	4{83,595,7}	CN1C=C2C=C(C=CC2=N1)C1=C(NC2CCOC2)N2C=C(C=CC2=N1)P(C)(C)=O c:4,6,9,12,23,25,28,t:2	Z8849597826	1{83}	CP(=O)(C)c1ccc(N)nc1	2{595}	Cn1cc2cc(C=O)ccc2n1	3{7}	[C-] #[N+]C1CC OCC1	34.4	30
1658	4{433,50,18}	CC1=C(C=CC2=NC([C@@H]3C[C@H]3C3OCCO3)=C(NC(C)(C)C)N12)C#C &1:8,10,r,c:3,t:1,5,17	Z8873684729	1{433}	Cc1nc(N)ccc1C#C	2{50}	O=C[C@@H]1C[C@H]1C2OCCO2 &1:2,4,r	3{18}	CC(C)(C)[N+] #[C-]	27.5	30
1659	4{32,758,26}	CP(C)(=O)C1=CC2=NC(=C(NCC3=CC=C(F)C=C3)N2C=C1)C1=C(F)C=C(C=C1)C(F)F c:17,22,25,28,30,t:4,6,8,12,14	Z8873685331	1{32}	CP(=O)(C)c1ccnc(N)c1	2{758}	FC(F)c1ccc(C=O)c(F)c1	3{26}	Fc1ccc(C[N+] #[C-])cc1	37.4	30
1660	4{68,673,23}	COC(=O)CCC(NC1=C(N=C2C=C(C=CN12)C#C)C1=NC=CC(C1)=C1)C(=O)OC c:12,14,23,26,t:8,10,21	Z8878918805	1{68}	Nc1cc(C#C)ccn1	2{673}	Clc1ccnc(C=O)c1	3{23}	COC(=O)CC C([N+] #[C-])C(=O)OC	34.4	30
1661	4{171,408,15}	CCNC1=C(CCN2CCOC2=O)N=C2C=C(C=C N12)N1C=CN=C1 c:3,16,18,24,26,t:14	Z8846491754	1{171}	Nc1cc(ccn1)n2ccnc2	2{408}	O=CCCN1C COC1=O	3{15}	CC[N+] #[C-]	27.4	30
1662	4{428,665,24}	COC1=CC(CNC2=C(N=C3C=NC(Br)=CN23)C2=C(C)N(C)N=N2)=CC=C1 c:11,14,19,24,26,28,t:2,7,9	Z8855739182	1{428}	Nc1cnc(Br)cn1	2{665}	Cc1c(C=O)nn1C	3{24}	COc1cccc(C [N+] #[C-])c1	34.5	30
1663	4{234,519,10}	FC(F)C1=NC=C(S1)C1=C(NC2CCOC2)N2C=CN=C(OC3CCC3)C2=N1 c:5,9,19,30,t:3,21	Z8878918457	1{234}	Nc1ncnc1OC2CCC2	2{519}	FC(F)c1ncc(C=O)s1	3{10}	[C-] #[N+]C1CC OC1	32.7	30
1664	4{54,216,53}	COC(=O)C1=NC=C(S1)C1=C(NCCOCC2=CC=CC=C2)N2C=C(C=CC2=N1)C(=O)N(C)C c:6,10,19,21,25,27,30,t:4,17	Z8878918850	1{54}	Cl.CN(C)C(=O)c1ccc(N)nc1	2{216}	COC(=O)c1ncc(C=O)s1	3{53}	[C-] #[N+]CCOC c1cccc1	38.5	30
1665	4{83,759,18}	COCC1=CC=C(S1)C1=C(NC(C)(C)C)N2C=C(C=CC2=N1)P(C)(C)=O c:5,9,17,19,22,t:3	Z8846492332	1{83}	CP(=O)(C)c1ccc(N)nc1	2{759}	COCC1ccc(C=O)s1	3{18}	CC(C)(C)[N+] #[C-]	31.2	30
1666	4{197,407,67}	CCC(C)NC1=C(N=C2C=CC(=CN12)S(=O)(=O)CC(C)C)C1=NN=C(CC)N1 c:9,11,t:5,7,23,25	Z8873685459	1{197}	CC(C)CS(=O)(=O)c1ccc(N)nc1	2{407}	CCc1nnc(C=O)[nH]1	3{67}	CCC(C)[N+] #[C-]	32.1	29
1667	4{65,35,23}	CCC1=CN=CC2=NC(=C(NC(CCC(=O)OC)C(=O)OC)N12)C1=NN(C)C(C)=C1C1 c:4,30,t:2,6,8,25	Z8878918830	1{65}	CCc1cnc(N)nc1	2{35}	Cc1c(Cl)c(C=O)nn1C	3{23}	COC(=O)CC C([N+] #[C-])C(=O)OC	35.6	29
1668	4{76,294,23}	COC(=O)CCC(NC1=C(N=C2C=CC(C)=C(C1)N12)C1=C(OC)C(=O)C=CO1)C(=O)OC c:12,21,27,t:8,10,15	Z8878918563	1{76}	Cc1ccc(N)nc1Cl	2{294}	COc1c(C=O)occc1=O	3{23}	COC(=O)CC C([N+] #[C-])C(=O)OC	36.7	29

1669	4{83,760,31}	CSCCNC1=C(N=C2C=CC(=CN12)P(C)(C)=O)C1=CC(F)=C(C=C1)C1CC1 c:9,11,23,25,t:5,7,20	Z8873685439	1{83}	CP(=O)(C)c1ccc(N)nc1	2{760}	Fc1cc(C=O)ccc1C2CC2	3{31}	CSCC[N+]#[C-]	32.9	29
1670	4{186,386,23}	COC(=O)CCC(NC1=C(N=C2C=C(C=CN12)S(=O)(=O)N(C)C)[C@H]1CC1(C)C)C(=O)OC c:12,14,t:8,10	Z8873685446	1{186}	Cl.CN(C)S(=O)(=O)c1cnc(N)c1	2{386}	CC1(C)C[C@@H]1C=O	3{23}	COC(=O)CC(C([N+]#[C-])C(=O)OC	36.5	29
1671	4{32,761,7}	CP(C)(=O)C1=CC2=NC(=C(NC3CCOCC3)N2C=C1)C1=C(C1)C=C(C=C1)C#C c:20,23,26,28,t:4,6,8	Z8873684640	1{32}	CP(=O)(C)c1ccnc(N)c1	2{761}	Clc1cc(C#C)ccc1C=O	3{7}	[C-]#[N+]C1CCOCC1	33.3	29
1672	4{83,760,18}	CC(C)(C)NC1=C(N=C2C=CC(=CN12)P(C)(C)=O)C1=CC(F)=C(C=C1)C1CC1 c:9,11,23,25,t:5,7,20	Z8878918433	1{83}	CP(=O)(C)c1ccc(N)nc1	2{760}	Fc1cc(C=O)ccc1C2CC2	3{18}	CC(C)(C)[N+]#[C-]	31.1	29
1673	4{431,762,10}	FC1=CN2C(C=C1)=NC(C1CC1(F)F)=C2NC1CCOC1 c:5,7,15,t:1	Z8849597836	1{431}	Nc1ccc(F)cn1	2{762}	FC1(F)CC1C=O	3{10}	[C-]#[N+]C1CCOC1	23.1	29
1674	4{28,373,18}	C[C@@H]1[C@@H](C2=C(NC(C)(C)C)N3C=CC(=CC3=N2)C2=NOC=N2)C1(F)F &1:1,2,r,c:3,11,13,16,22,t:19	Z8846492415	1{28}	Cl.Nc1cc(ccn1)c2ncon2	2{373}	C[C@@H]1[C@@H](C=O)C1(F)F &1:1,2,r	3{18}	CC(C)(C)[N+]#[C-]	26.9	29
1675	4{54,763,37}	COC(=O)C1CC(C1)NC1=C(N=C2C=CC(=CN12)C(=O)N(C)C)C1=NNC2=C1C=C(C=C2)C(=O)OC c:14,16,29,32,34,t:10,12,26	Z8873684933	1{54}	Cl.CN(C)C(=O)c1ccc(N)nc1	2{763}	COC(=O)c1cc2[nH]nc(C=O)c2c1	3{37}	COC(=O)C1CC(C1)[N+]#[C-]	38.0	29
1676	4{73,764,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC4=NC=CN4N23)C2=C(OC)C(C1)=CC=C2)C=C1 c:12,16,23,28,30,33,t:2,5,8,10,14	Z8878918364	1{73}	Nc1ccc2nccn2n1	2{764}	COc1c(Cl)ccc1C=O	3{20}	COc1ccc([N+]#[C-])c(C)c1	33.4	29
1677	4{113,447,14}	COCCNC1=C(N=C2N1C=CC=C2N1CCOCC1)C1=CC=C(C=C1)C#CC(C)(C)O c:7,11,13,25,27,t:5,23	Z8878918558	1{113}	Nc1ncccc1N2CCOCC2	2{447}	CC(C)(O)C#Cc1ccc(C=O)cc1	3{14}	COCC[N+]#[C-]	33.3	28
1678	4{81,274,13}	COC1=CC=C(CNC2=C(CC3(CCOCC3)C#N)N=C3C=NC=CN23)C=C1 c:8,22,24,29,t:2,4,20	Z8878918599	1{81}	Nc1cncn1	2{274}	O=CCC1(CCOC1)C#N	3{13}	COc1ccc(C[N+]#[C-])cc1	28.9	28
1679	4{356,746,8}	COC(=O)C(CC1=CC=CC=C1)NC1=C(N=C2C=CC(C1)=C(N12)C(=O)N(C)C)C1=C(C)C=CN=C1 c:8,10,18,21,31,34,36,t:6,14,16	Z8878918444	1{356}	CN(C)C(=O)c1nc(N)ccc1Cl	2{746}	Cc1cncnc1C=O	3{8}	COC(=O)C(Cc1cccc1)[N+]#[C-]	37.7	28

1680	4{77,725,5}	CCN1N=NC=C1C1=C(NCCCOC)N2C=C(C=CC2=N1)C1=CN=CC=C1 c:3,5,8,17,19,22,27,29,t:25	Z8878918529	1{77}	Nc1ccc(en1) c2cccnc2	2{725}	CCn1nnc1C =O	3{5}	COCCC[N+] #[C-]	28.8	28
1681	4{54,575,32}	CN(C)C(=O)C1=CN2C(C=C1)=NC(CC(NC(=O)OC(C)(C)C)C(F)(F)F)=C2NC1CCC1 c:9,11,27,t:5	Z8873685300	1{54}	Cl.CN(C)C(=O)c1ccc(N) nc1	2{575}	CC(C)(C)OC(=O)NC(CC(=O)C(F)(F)F	3{32}	[C-] #[N+]C1CC C1	35.8	28
1682	4{199,563,34}	CC(=O)NC1=NC=C(C=C1)C1=C(NCCC2CCC O2)N2C=CC=C(C2=N1)C(C)(F)F c:6,8,11,22,24,27,t:4	Z8878918377	1{199}	CC(F)(F)c1 ccnc1N	2{563}	CC(=O)Nc1c cc(C=O)en1	3{34}	[C-] #[N+]CC1C CCO1	31.6	28
1683	4{81,420,13}	COC1=CC=C(CNC2=C(CC(C)(C)C#N)N=C3 C=NC=CN23)C=C1 c:8,18,20,25,t:2,4,16	Z8878918554	1{81}	Nc1cncn1	2{420}	CC(C)(CC= O)C#N	3{13}	COc1ccc(C[N+]#[C-])cc1	25.3	28
1684	4{79,396,13}	COC1=CC=C(CNC2=C(N=C3C=NC=C(C)N2 3)C2=CN=C3COCCN23)C=C1 c:12,31,t:2,4,8,10,14,20,22	Z8878918546	1{79}	Cc1cnc(N) n1	2{396}	O=Cc1cnc2C OCCn12	3{13}	COc1ccc(C[N+]#[C-])cc1	29.4	28
1685	4{105,654,66}	CC(NC1=C(CCC2=CN=CO2)N=C2C=CC=C(N12)C(N)=O)C1=CC=CC=C1 c:3,9,15,17,27,29,t:7,13,25	Z8878918902	1{105}	NC(=O)c1c ccc(N)n1	2{654}	O=CCCc1cn co1	3{66}	CC([N+]#[C-])c1cccc1	28.1	28
1686	4{154,552,49}	[O-]][N+](=O)C1=CC2=NC(=C(NC3CC(F)(F)C3) N2C=C1)C1=CN=C(C=C1)C#C c:19,24,26,t:3,5,7,22	Z8873685272	1{154}	Nc1cc(en1))[N+](=O)[O-]	2{552}	O=Cc1ccc(C #C)nc1	3{49}	FC1(F)CC(C 1)[N+]#[C-]	27.7	28
1687	4{50,744,7}	CP(C)(=O)C1=CC=CC2=NC(=C(NC3CCOCC 3)N12)C1=C(F)C=CC(=C1)C#C c:6,23,26,28,t:4,8,10	Z8846492306	1{50}	CP(=O)(C)c 1cccc(N)n1	2{744}	Fe1ccc(C#C) cc1C=O	3{7}	[C-] #[N+]C1CC OCC1	30.8	28
1688	4{468,756,69}	COC1=C(NC2=C(N=C3C=CC=C(N23)C2=CN (C)N=C2)C2=CC(=CO2)S(C)(=O)=O)C=CC= C1 c:2,9,11,20,25,33,35,t:5,7,16,23	Z8878918317	1{468}	Cl.Cl.Cn1cc (en1)c2cccc (N)n2	2{756}	CS(=O)(=O) c1coc(C=O)c 1	3{69}	COc1cccc1[N+]#[C-]	34.5	28
1689	4{48,765,22}	CS(=O)(=O)C1=CC2=NC(=C(NC3COC3)N2C =C1)C1=CN=C(OC2=CC=C(F)C=C2)C=C1 c:18,31,34,t:4,6,8,21,23,26,28	Z8873684798	1{48}	CS(=O)(=O) c1ccnc(N)c 1	2{765}	Fe1ccc(Oc2c cc(C=O)cn2) cc1	3{22}	[C-] #[N+]C1CO C1	33.7	27
1690	4{95,61,37}	COC(=O)C1CC(C1)NC1=C(N=C2C=CC(=CN 12)C(F)F)C1=CC=C(C=C1)S(C)=O c:14,16,26,28,t:10,12,24	Z8849597796	1{95}	Nc1ccc(en1) C(F)F	2{61}	CS(=O)c1ccc (C=O)cc1	3{37}	COC(=O)C1 CC(C1)[N+] #[C-]	32.2	27

1691	4{73,88,13}	COC1=CC=C(CNC2=C(N=C3C=CC4=NC=C N4N23)C2=CC3=C(C=CC=N3)C=C2)C=C1 c:12,16,27,29,32,35,t:2,4,8,10,14,23,25	Z8829498653	1{73}	Nc1ccc2ncc n2n1	2{88}	O=Cc1ccc2c ccnc2c1	3{13}	COc1ccc(C[N+]#[C-])cc1	31.2	27
1692	4{142,766,46}	CC1CC1C1=C(NCC(C)=C)N2C=CC=C(OCCS (C)(=O)=O)C2=N1 c:5,13,25,t:15	Z8873684943	1{142}	CS(=O)(=O)CCOc1ccc nc1N	2{766}	CC1CC1C= O	3{46}	CC(=C)C[N+]#[C-]	27.0	27
1693	4{103,354,5}	COCCCN1=C(N=C2C=NC=C(CO)N12)C1= C(C=CC=C1)P(C)(C)=O c:10,21,23,t:6,8,12,19	Z8873685481	1{103}	Nc1cncc(C O)n1	2{354}	CP(=O)(C)c1 ccccc1C=O	3{5}	COCCC[N+] #[C-]	28.8	27
1694	4{464,438,5}	COCCCN1=C(N=C2C=CC(=CN12)N1CCN(C)CC1)C1=NC(C)=NC(=C1)C(F)F c:10,12,28,30,t:6,8,25	Z8878918570	1{464}	CN1CCN(C C1)c2ccc(N)nc2	2{438}	Cc1nc(C=O) cc(n1)C(F)F	3{5}	COCCC[N+] #[C-]	32.9	27
1695	4{46,257,9}	CNC1=C(N=C2C=CC=CN12)C1CC(C1)NC(= O)OC(C)(C)C c:6,8,t:2,4	Z8878918515	1{46}	Nc1ccccn1	2{257}	CC(C)(C)OC (=O)NC1CC(C1)C=O	3{9}	C[N+]#[C-]	23.3	27
1696	4{123,149,15}	CCNC1=C(N=C2C=C(OCCO)C=CN12)C1=C(OC)C(OC)=CC(Br)=C1 c:13,18,24,27,t:3,5,7	Z8878918634	1{123}	Cl.Nc1cc(O CCO)ccn1	2{149}	COc1cc(Br)c c(C=O)c1OC	3{15}	CC[N+]#[C-]	32.0	27
1697	4{81,46,9}	CNC1=C(CCCCO)N=C2C=NC=CN12 c:2,13,15,t:11	Z8873684589	1{81}	Nc1cnccn1	2{46}	COCCCCC =O	3{9}	C[N+]#[C-]	18.2	27
1698	4{434,92,31}	CSCCN1=C(N=C2C=CC(=CN12)C(C)(F)F C1=CC(C)=NO1 c:9,11,23,t:5,7,20	Z8878918864	1{434}	CC(F)(F)c1 ccc(N)nc1	2{92}	Cc1cc(C=O) on1	3{31}	CSCCN[+]# [C-]	25.8	27
1699	4{81,25,13}	COC1=CC=C(CNC2=C(N=C3C=NC=CN23)C 2=CN=C(N=C2)C2CCOCC2)C=C1 c:12,14,21,23,33,t:2,4,8,10,19	Z8878918423	1{81}	Nc1cnccn1	2{25}	O=Cc1enc(n c1)C2CCOC C2	3{13}	COc1ccc(C[N+]#[C-])cc1	30.4	27
1700	4{386,725,5}	CCN1N=NC=C1C1=C(NCCCOC)N2C=CC(C) =CC2=N1 c:3,5,8,17,20,23	Z8873684786	1{386}	Cc1cncc(N) c1	2{725}	CCn1ncc1C =O	3{5}	COCCC[N+] #[C-]	22.8	27
1701	4{99,767,73}	CCCC(OC)C1=C(NC2=C(OC)C=C(OC)C=C2) N2C=C(C=CC2=N1)S(N)(=O)=O c:6,9,17,21,23,26,t:13	Z8855619704	1{99}	Nc1ccc(en1)S(=O)(=O) N	2{767}	CCCC(OC)C =O	3{73}	COc1ccc([N +]#[C-])c(OC)c1	31.6	27
1702	4{103,768,5}	COCCCN1=C(N=C2C=NC=C(CO)N12)C1= C(F)C(Br)=C(F)C=C1 c:10,19,26,t:6,8,12,23	Z8873685426	1{103}	Nc1cncc(C O)n1	2{768}	Fc1ccc(C=O) c(F)c1Br	3{5}	COCCC[N+] #[C-]	30.9	27
1703	4{91,125,26}	COC1=NC=NC(=C1)C1=C(NCC2=CC=C(F)C =C2)N2C=C(C=CC2=N1)C(N)=O c:4,6,9,18,22,24,27,t:2,13,15	Z8878918391	1{91}	NC(=O)c1c cc(N)nc1	2{125}	COc1cc(C=O)ncn1	3{26}	Fc1ccc(C[N+] #[C-])cc1	28.3	27

1704	4{124,769,43}	CN1N=CN=C1C1=C(NC2CCN(CC2)C(=O)O C(C)(C)C)N2C=CC=C(CO)C2=N1 c:2,4,7,25,32,t:27	Z8878918536	1{124}	Ne1ncccc1 CO	2{769}	Cn1ncnc1C= O	3{43}	CC(C)(C)OC (=O)N1CCCC (CC1)[N+]# C-]	30.8	27
1705	4{78,770,39}	CCOCCNC1=C(N=C2C=C(C)C3=NC(C)=CN 3N12)C1=C(OC)C=CC(Cl)=C1C1 c:16,23,27,30,t:6,8,10,13	Z8873684775	1{78}	Cc1cn2nc(N)cc(C)c2n1	2{770}	COc1ccc(Cl) c(Cl)c1C=O	3{39}	CCOCC[N+] #[C-]	32.3	27
1706	4{155,450,14}	COCCNC1=C(N=C2N1C=CC=C2Cl)C1=CC(= CC=C1)S(=O)(=O)N(C)C c:7,11,13,19,21,t:5,17	Z8873684599	1{155}	Ne1ncccc1 Cl	2{450}	CN(C)S(=O) (=O)c1cccc(C=O)c1	3{14}	COCC[N+]# C-]	29.4	27
1707	4{48,216,15}	CCNC1=C(N=C2C=C(C=CN12)S(C)(=O)=O) C1=CN=C(S1)C(=O)OC c:7,9,20,t:3,5,18	Z8878918866	1{48}	CS(=O)(=O))c1ccnc(N)c 1	2{216}	COC(=O)c1n cc(C=O)s1	3{15}	CC[N+]#[C-]	27.2	27
1708	4{175,516,46}	CN1N=C(N=C1C1CC1)C1=C(NCC(C)=C)N2 C=CC=C(OCCF)C2=N1 c:2,4,11,19,28,t:21	Z8873684651	1{175}	Ne1ncccc1 OCCF	2{516}	Cn1nc(C=O) nc1C2CC2	3{46}	CC(=C)C[N+] #[C-]	26.5	26
1709	4{32,771,15}	CCNC1=C(N=C2C=C(C=CN12)P(C)(C)=O)C 1=CC=C(C=C1)C(F)(F)Cl c:7,9,20,22,t:3,5,18	Z8846492144	1{32}	CP(=O)(C)c 1ccnc(N)c1	2{771}	FC(F)(Cl)c1c cc(C=O)cc1	3{15}	CC[N+]#[C-]	28.1	26
1710	4{103,772,5}	COCCNC1=C(N=C2C=NC=C(CO)N12)C1= NC=C(OC(F)(F)C(F)(F)F)C=C1 c:10,31,t:6,8,12,19,21	Z8873684802	1{103}	Ne1cncc(C O)n1	2{772}	FC(F)(F)C(F) (F)Oc1ccc(C =O)nc1	3{5}	COCCC[N+] #[C-]	31.6	26
1711	4{123,119,32}	CCOC(=O)C1=NN=C(N1)C1=C(NC2CCC2)N 2C=CC(OCCO)=CC2=N1 c:7,11,20,26,29,t:5	Z8855739092	1{123}	Cl.Nc1cc(O CCO)ccn1	2{119}	CCOC(=O)c 1nnc(C=O)[n H]1	3{32}	[C-]#[N+]C1CC C1	27.3	26
1712	4{28,773,7}	CC(C)CN1N=C(C)C(=C1Cl)C1=C(NC2CCOC C2)N2C=CC(=CC2=N1)C1=NOC=N1 c:8,12,23,25,28,34,t:5,31	Z8878918880	1{28}	Cl.Nc1cc(cc n1)c2ncon2	2{773}	CC(C)Cn1nc (C)c(C=O)c1 Cl	3{7}	[C-]#[N+]C1CC OCC1	32.1	26
1713	4{91,774,35}	CSCCCNC1=C(N=C2C=CC(=CN12)C(N)=O) C1=NC(Br)=CS1 c:10,12,23,t:6,8,20	Z8835022912	1{91}	NC(=O)c1c cc(N)nc1	2{774}	Br1csc(C=O)n1	3{35}	CSCCC[N+] #[C-]	30.0	26
1714	4{46,48,9}	CNC1=C(N=C2C=CC=CN12)C1=CNC(=N1)C 1CCC1 c:6,8,16,t:2,4,13	Z8878918425	1{46}	Ne1cccn1	2{48}	O=Cc1c[nH] c(n1)C2CCC 2	3{9}	C[N+]#[C-]	18.8	26
1715	4{186,775,66}	COC(=O)C1=NC(C)=C(S1)C1=C(NC(C)C2=C C=CC=C2)N2C=CC(=CC2=N1)S(=O)(=O)N(C)C c:7,11,18,20,24,26,29,t:4,16	Z8855739085	1{186}	Cl.CN(C)S(=O)(=O)c1c cnc(N)c1	2{775}	COC(=O)c1n c(C)c(C=O)s 1	3{66}	CC([N+]#[C-)c1cccc1	35.0	26

1716	4{28,225,7}	C1C1=CC2=C(C=NN2)C(=C1)C1=C(NC2CCOCC2)N2C=CC(=CC2=N1)C1=NOC=N1 c:5,9,12,23,25,28,34,t:1,3,31	Z8835022876	1{28}	Cl.Nc1cc(ccn1)c2ncon2	2{225}	Clc1cc(C=O)c2cn[nH]c2c1	3{7}	[C-] #[N+]C1CCOCC1	30.4	26
1717	4{144,776,22}	CNS(=O)(=O)C1=CN2C(C=C1)=NC(=C2NC1COC1)C1=C(F)C=C(C=C1F)C#C c:9,11,13,22,25,27,t:5	Z8837933171	1{144}	CNS(=O)(=O)c1ccc(N)nc1	2{776}	Fc1cc(C#C)c(F)c1C=O	3{22}	[C-] #[N+]C1COCC1	29.1	26
1718	4{187,777,12}	COC(C1CCCC1)C1=C(NCC2CCOC2)N2C=C(C1)C(=CC2=N1)C#N c:9,23,26,t:20	Z8878918559	1{187}	Nc1cc(C#N)c(Cl)cn1	2{777}	COC(C=O)C1CCCC1	3{12}	[C-] #[N+]CC1CCOC1	27.0	26
1719	4{380,406,23}	COC(=O)CCC(NC1=C(N=C2N1C=C(Cl)N=C2C)C1=CC=NS1)C(=O)OC c:10,17,23,t:8,14,21	Z8878918820	1{380}	Cc1nc(Cl)cn1N	2{406}	O=Cc1ccns1	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	29.3	26
1720	4{47,469,6}	CCOC(=O)CCCN1=C(N=C2C=C(C=CN12)S(N)(=O)=O)C1CCSC1 c:13,15,t:9,11	Z8878918614	1{47}	Cl.Nc1cc(ccn1)S(=O)(=O)N	2{469}	O=CC1CCSC1	3{6}	CCOC(=O)C CC[N+]#[C-]	28.2	25
1721	4{49,116,13}	COC1=CC=C(CNC2=C(N=C3C=CC=C(CO)N23)C2=CN(CCC=C)N=N2)C=C1 c:12,28,31,t:2,4,8,10,14,21	Z8854581145	1{49}	Nc1cccc(CO)n1	2{116}	C=CCCN1cc(C=O)nn1	3{13}	COc1ccc(C[N+]#[C-])cc1	27.6	25
1722	4{49,284,13}	COC1=CC=C(CNC2=C(N=C3C=CC=C(CO)N23)C2=C(C)N=CC=N2)C=C1 c:12,21,24,26,29,t:2,4,8,10,14	Z8873684722	1{49}	Nc1cccc(CO)n1	2{284}	Cc1ncnc1C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	25.4	25
1723	4{50,760,18}	CC(C)(C)NC1=C(N=C2C=CC=C(N12)P(C)(C)=O)C1=CC(F)=C(C=C1)C1CC1 c:9,11,23,25,t:5,7,20	Z8873684866	1{50}	CP(=O)(C)c1cccc(N)n1	2{760}	Fc1cc(C=O)c1c2cc2	3{18}	CC(C)(C)[N+]#[C-]	26.9	25
1724	4{428,710,10}	CC1=C(C=C(F)C=N1)C1=C(NC2CCOC2)N2C=C(Br)N=CC2=N1 c:6,9,22,25,t:1,3,19	Z8855739115	1{428}	Nc1nc(Br)cn1	2{710}	Cc1ncc(F)cc1C=O	3{10}	[C-] #[N+]C1CCOCC1	26.4	25
1725	4{79,420,13}	COC1=CC=C(CNC2=C(CC(C)(C)C#N)N=C3C=NC=C(C)N23)C=C1 c:8,18,26,t:2,4,16,20	Z8873684695	1{79}	Cc1ncc(N)n1	2{420}	CC(C)(CC=O)C#N	3{13}	COc1ccc(C[N+]#[C-])cc1	23.5	25
1726	4{36,396,9}	CNC1=C(N=C2C=CC(Br)=CN12)C1=CN=C2COCCN12 c:6,9,t:2,4,14,16	Z8855739232	1{36}	Nc1ccc(Br)cn1	2{396}	O=Cc1cnc2COCCn12	3{9}	C[N+]#[C-]	23.1	25
1727	4{120,778,38}	CCOC(=O)C1=NN(C)C(=N1)C1=C(NC2=CC3=C(OCO3)C=C2)N2C=CC(=CC2=N1)C1=CN(C)N=C1 c:9,12,23,27,29,32,39,t:5,15,17,35	Z8878918472	1{120}	Cn1cc(cn1)c2ccnc(N)c2	2{778}	CCOC(=O)c1nc(C=O)n(C)n1	3{38}	[C-] #[N+]c1ccc2OCOc2c1	32.2	24
1728	4{139,104,46}	CC(=C)CNC1=C(N=C2C=C(C=CN12)C(F)F)C1=NC(C)=CO1 c:9,11,22,t:5,7,19	Z8873684776	1{139}	Nc1cc(cen1)C(F)F	2{104}	Cc1coc(C=O)n1	3{46}	CC(=C)C[N+]#[C-]	21.0	24

1729	4{41,25,9}	CNC1=C(N=C2C=NC(C)=CN12)C1=CN=C(N=C1)C1CCOCC1 c:6,9,16,18,t:2,4,14	Z8837933133	1{41}	Cc1enc(N)c n1	2{25}	O=Cc1enc(n c1)C2CCOC C2	3{9}	C[N+]#[C-]	21.4	24
1730	4{146,608,72}	CC1=C(NC2=C(CC3(CCC3)C#N)N=C3C=CC (=CN23)S(C)(=O)=O)C=CC(F)=C1 c:1,4,16,18,27,30,t:14	Z8835022903	1{146}	CS(=O)(=O) c1ccc(N)nc 1	2{608}	O=CCC1(CC C1)C#N	3{72}	Cc1cc(F)ccc 1[N+]#[C-]	27.2	24
1731	4{397,312,23}	COC(=O)CCC(NC1=C(N=C2N1C=CC(C)=C2 C)C1CCOC1(C)C)C(=O)OC c:10,14,17,t:8	Z8873684611	1{397}	Cl.Cc1ccnc(N)c1C	2{312}	CC1(C)OCC C1C=O	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	27.4	24
1732	4{70,115,32}	COC1=NN(C)C(=C1)C1=C(NC2CCC2)N2C= CN=C(C3CC3)C2=N1 c:6,9,18,27,t:2,20	Z8873685440	1{70}	Nc1ncnc1 C2CC2	2{115}	COc1cc(C=O)n(C)n1	3{32}	[C-]#[N+]C1CC C1	22.1	24
1733	4{138,236,61}	CC(C)(C)OC(=O)NCCCNC1=C(CCC2OCCO2 N)=C2C=CC=C(F)N12 c:12,24,t:22,26	Z8878918528	1{138}	Nc1cccc(F) n1	2{236}	O=CCCC1O CCO1	3{61}	CC(C)(C)OC (=O)NCCC[N+]#[C-]	26.7	24
1734	4{428,334,10}	CC1=C(N=CO1)C1=C(NC2CCOC2)N2C=C(B r)N=CC2=N1 c:3,7,20,23,t:1,17	Z8878918814	1{428}	Nc1enc(Br) cn1	2{334}	Cc1ocnc1C= O	3{10}	[C-]#[N+]C1CC OC1	23.7	24
1735	4{230,320,50}	CC(O)C1=CC(Br)=CN2C(NC3=CC4=C(OCC O4)C=C3)=C(N=C12)C1=NN(C)C=N1 c:6,20,22,32,t:3,11,13,24,28	Z8873685280	1{230}	CC(O)c1cc(Br)enc1N	2{320}	Cn1enc(C=O)n1	3{50}	[C-]#[N+]c1ccc 2OCCOc2c1	30.7	24
1736	4{150,131,15}	CCNC1=C(N=C2C=C(C=CN12)C1CCOC1)C1 =NC(=NN1)C1CC1 c:7,9,22,t:3,5,20	Z8855619710	1{150}	Nc1cc(ccn1)C2CCOC2	2{131}	O=Cc1nc(n[n H]1)C2CC2	3{15}	CC[N+]#[C-]	22.0	24
1737	4{38,697,9}	CCC1=NC=C(N1)C1=C(NC)N2C=CC(=CC2= N1)C#N c:4,8,13,15,18,t:2	Z8837933174	1{38}	Nc1cc(C#N)ccn1	2{697}	CCc1ncc(C= O)[nH]1	3{9}	C[N+]#[C-]	17.3	24
1738	4{361,164,28}	CCCNC1=C(N=C2N1C=CC=C2OC(C)C)C1= NN(C)C2=C1COCC2 c:6,10,12,23,t:4,19	Z8855739088	1{361}	Cl.CC(C)Oc 1ccnc1N	2{164}	Cn1nc(C=O) c2COCCc21	3{28}	CCC[N+]#[C-]	23.9	24
1739	4{161,49,11}	CC1=NNC=C1C1=C(NCC2=CC(Br)=CC=C2) N2N=CC=CC2=N1 c:4,7,14,16,20,22,25,t:1,11	Z8873685264	1{161}	Nc1ccenn1	2{49}	Cc1n[nH]cc1 C=O	3{11}	Brc1cccc(C[N+]#[C-])c1	24.8	24
1740	4{399,779,22}	COC1=C2NC=NC2=CC(=C1)C1=C(NC2COC 2)N2N=C(OC(C)C)C=CC2=N1 c:2,5,8,10,13,28,31,t:22	Z8854581138	1{399}	CC(C)Oc1c cc(N)nn1	2{779}	COc1cc(C=O)cc2nc[nH]c1 2	3{22}	[C-]#[N+]C1CO C1	25.1	24

1741	4{124,460,61}	CC1=CN=C(O1)C1=C(NCCCNC(=O)OC(C)(C)C)N2C=CC=C(CO)C2=N1 c:3,7,22,29,t:1,24	Z8873684796	1{124}	Ne1ncccc1 CO	2{460}	Cc1cnc(C=O) o1	3{61}	CC(C)(C)OC (=O)NCCC[N+]#[C-]	25.4	23
1742	4{436,235,23}	CCC1=CC2=NC(C3=CSC(=C3)C#N)=C(NC(C CC(=O)OC)C(=O)OC)N2C=C1 c:10,30,t:2,4,7,14	Z8873684840	1{436}	CCc1cncnc(N)c1	2{235}	O=Cc1csc(C #N)c1	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	26.8	23
1743	4{54,780,37}	COC(=O)C1CC(C1)NC1=C(N=C2C=CC(=CN 12)C(=O)N(C)C)[C@@H]1C[C@H]1C1=CSC =C1 &1:23,25,r,c:14,16,33,t:10,12,30	Z8873684637	1{54}	Cl.CN(C)C(=O)c1ccc(N)nc1	2{780}	O=C[C@@H]1C[C@H]1c 2ccsc2 &1:2,4,r	3{37}	COC(=O)C1 CC(C1)[N+] #[C-]	27.0	23
1744	4{32,744,7}	CP(C)(=O)C1=CC2=NC(=C(NC3CCOCC3)N2 C=C1)C1=C(F)C=CC(=C1)C#C c:20,23,26,28,t:4,6,8	Z8873684685	1{32}	CP(=O)(C)c 1cnc(N)c1	2{744}	Fc1ccc(C#C) cc1C=O	3{7}	[C-]#[N+]C1CC OCC1	25.3	23
1745	4{89,569,67}	CCC(C)NC1=C(CC2CCOC2=O)N=C2C=CC3 =C(NN=C3)N12 c:5,17,22,t:15,19	Z8873684913	1{89}	Ne1ccc2en[nH]c2n1	2{569}	O=CCC1CC OC1=O	3{67}	CCC(C)[N+] #[C-]	20.1	23
1746	4{78,629,44}	CC1=CN2N3C(C=C(C)C2=N1)=NC(=C3NCC CCNC(=O)OC(C)(C)C)C1=C(C)C=C(C)C=N1 c:10,12,14,30,36,t:1,6,33	Z8878918890	1{78}	Cc1cn2nc(N)cc(C)c2n1	2{629}	Cc1cnc(C=O)c(C)c1	3{44}	CC(C)(C)OC (=O)NCCCC [N+]#[C-]	29.2	23
1747	4{32,439,31}	COC1=C(C=CC(=C1)C1=C(NCCSC)N2C=CC (=CC2=N1)P(C)(C)=O)S(C)(=O)=O c:4,6,9,17,19,22,t:2	Z8873684927	1{32}	CP(=O)(C)c 1cnc(N)c1	2{439}	COc1cc(C=O)ccc1S(=O)(=O)C	3{31}	CSCC[N+]#[C-]	28.2	22
1748	4{50,781,18}	CC(C)(C)NC1=C(N=C2C=CC=C(N12)P(C)(C) =O)C1=CC(Cl)=C(OCCBr)C=C1 c:9,11,29,t:5,7,20,23	Z8873685421	1{50}	CP(=O)(C)c 1cccc(N)n1	2{781}	Clc1cc(C=O) ccc1OCCBr	3{18}	CC(C)(C)[N +]#[C-]	30.1	22
1749	4{101,538,7}	CN1C=NC=C1C1=C(NC2CCOCC2)N2C=C(C O)C=C(Cl)C2=N1 c:2,4,7,26,t:18,22	Z8854581140	1{101}	Ne1ncc(CO)cc1Cl	2{538}	Cn1cnc1C= O	3{7}	[C-]#[N+]C1CC OCC1	21.8	22
1750	4{161,84,20}	COC1=CC(C)=C(NC2=C(CCSC)N=C3C=CC= NN23)C=C1 c:8,16,18,23,t:2,5,14	Z8878918342	1{161}	Ne1cccenn1	2{84}	CSCCC=O	3{20}	COc1ccc([N +]#[C-])c(C)c1	19.8	22
1751	4{118,782,35}	CSCCNC1=C(N=C2C=CC=C(C(C)O)N12)C 1=C2N(C)C(=O)N(C)C2=CC=C1 c:10,20,29,31,t:6,8,12	Z8873684944	1{118}	Cl.CC(O)c1 cccc(N)n1	2{782}	Cn1c(=O)n(C)c2c(C=O)c cc12	3{35}	CSCC[N+] #[C-]	25.5	22
1752	4{400,155,15}	CCNC1=C(N=C2C=CC(COC(C)C)=CN12)C1 =CN=CN=C1 c:7,14,21,23,t:3,5,19	Z8855739166	1{400}	CC(C)OCc1 ccc(N)nc1	2{155}	O=Cc1cncnc 1	3{15}	CC[N+]#[C-]	18.6	22

1753	4{377,34,46}	CC(=C)CNC1=C(N=C2N1C=CC=C2OCC(F)F)C1=CC=C(C=C1)P(C)(C)=O c:7,11,13,23,25,t:5,21	Z8873684633	1{377}	Nc1ncccc1 OCC(F)F	2{34}	CP(=O)(C)c1 ccc(C=O)cc1	3{46}	CC(=C)C[N+] #[C-]	25.0	22
1754	4{414,236,60}	COC(=O)C1=CC(NC2=C(CCC3OCCO3)N=C3C=NC(Cl)=CN23)=CC=C1 c:8,20,23,27,29,t:4,18	Z8878918661	1{414}	Nc1cnc(Cl) cn1	2{236}	O=CCCC1O CCO1	3{60}	COC(=O)c1c ccc([N+]#[C-])c1	23.8	22
1755	4{56,783,23}	COC(=O)CCC(NC1=C(N=C2C=CC(=CN12)C1=NN(C)C=C1)C1=NOC(=C1)C(C)C)C(=O)OC c:12,14,23,29,t:8,10,19,26	Z8829498623	1{56}	Cn1ccc(n1) c2ccc(N)nc 2	2{783}	CC(C)c1cc(C =O)no1	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	28.3	22
1756	4{150,488,35}	CSCCCNC1=C(N=C2C=C(C=CN12)C1CCOC1)C1=CC2=C(NC(=O)CC2)N=C1 c:10,12,33,t:6,8,23,25	Z8855739215	1{150}	Nc1cc(cen1) C2CCOC2	2{488}	O=Cc1cnc2N C(=O)CCc2c 1	3{35}	CSCCC[N+] #[C-]	25.6	22
1757	4{301,93,32}	OCC1=NC(=CC=C1)C1=C(NC2CCC2)N2C=C(Cl)C=C(F)C2=N1 c:4,6,9,25,t:2,18,21	Z8878918582	1{301}	Nc1ncc(Cl) cc1F	2{93}	OCc1cccc(C =O)n1	3{32}	[C-] #[N+]C1CC C1	20.1	21
1758	4{351,784,39}	CCOCCNC1=C(N=C2C=CC3=C(C(O)CC3)N12)C1=C(Cl)N=C(OC)N1C c:10,22,t:6,8,12,25	Z8873685475	1{351}	Nc1ccc2CC C(O)c2n1	2{784}	COc1nc(Cl)c (C=O)n1C	3{39}	CCOCC[N+] #[C-]	23.4	21
1759	4{442,177,23}	COC(=O)CCC(NC1=C(CC2CC(C2)C(=O)OC)N=C2N1C=C(Cl)C=C2C)C(=O)OC c:8,20,27,t:24	Z8878918316	1{442}	Cc1cc(Cl)cn c1N	2{177}	COC(=O)C1 CC(CC=O)C 1	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	26.8	21
1760	4{469,745,22}	CC1=C(C=CN=C1)C1=C(NC2COC2)N2C=C(OC(F)(F)F)C=CC2=N1 c:3,5,8,24,27,t:1,17	Z8878918481	1{469}	Nc1ccc(OC(F)(F)F)cn1	2{745}	Cc1cncccc1C =O	3{22}	[C-] #[N+]C1CO C1	19.9	21
1761	4{99,785,66}	CCN1N=C(Br)N=C1C1=C(NC(C)C2=CC=CC=C2)N2C=C(C=CC2=N1)S(N)(=O)=O c:6,9,16,18,22,24,27,t:3,14	Z8873685434	1{99}	Nc1ccc(en1) S(=O)(=O) N	2{785}	CCn1nc(Br)n c1C=O	3{66}	CC([N+]#[C-])c1cccc1	28.1	21
1762	4{103,786,5}	COCCNC1=C(N=C2C=NC=C(CO)N12)C1=C(F)C(F)=C(Cl)C=C1 c:10,19,26,t:6,8,12,23	Z8873684818	1{103}	Nc1cnc(C O)n1	2{786}	Fe1c(F)c(C=O)ccc1Cl	3{5}	COCCC[N+] #[C-]	21.9	21
1763	4{188,787,62}	COC(=O)C1=CN=CC2=NC(=C(NC3(CCCC3)C(=O)OC)N12)C1=CC2=C(C=C1)N(C)C(C)=N2 c:6,28,30,36,t:4,8,10,26	Z8873684885	1{188}	COC(=O)c1 cnc(N)n1	2{787}	Cc1nc2cc(C=O)ccc2n1C	3{62}	COC(=O)C1(CCCC1)[N+]#[C-]	26.2	21
1764	4{35,25,13}	COC1=CC=C(CNC2=C(N=C3C=CC(C)=CN23)C2=CN=C(N=C2)C2CCOCC2)C=C1 c:12,15,22,24,34,t:2,4,8,10,20	Z8873685250	1{35}	Cc1ccc(N)n c1	2{25}	O=Cc1cnc(n c1)C2CCOC C2	3{13}	COc1ccc(C[N+]#[C-])cc1	24.3	21

1765	4{138,729,49}	COC1=C(C=CC=C1C#N)C1=C(NC2CC(F)(F)C2)N2C(C=CC=C2F)=N1 c:4,6,11,23,25,28,t:2	Z8873685330	1{138}	Nc1cccc(F)n1	2{729}	COc1c(C=O)cccc1C#N	3{49}	FC1(F)CC(C1)[N+]#[C-]	20.9	21
1766	4{396,587,59}	COC1=NOC(C)=C1C1=C(NCCC2=CC(F)=CC=C2)N2N=C(C=CC2=N1)C1=CN(C)N=C1 c:6,9,17,19,23,25,28,35,t:2,14,31	Z8873685432	1{396}	Cn1cc(en1)c2ccc(N)nn2	2{587}	COc1noc(C)c1C=O	3{59}	Fe1cccc(CC[N+]#[C-])c1	24.9	21
1767	4{128,653,34}	COCCN(C)C1=CN2C(C=C1)=NC(C1C3CCC(F)(F)C13)=C2NCC1CCCO1 c:10,12,24,t:6	Z8829498615	1{128}	COCCN(C)c1ccc(N)nc1	2{653}	FC1(F)CCC2C(C=O)C21	3{34}	[C-]#[N+]CC1COCO1	23.4	21
1768	4{421,306,22}	COC(=O)C1=C(CI)N2C(C=C1)=NC(=C2NC1COC1)C1=CC=C(C=C1)N(C)CCO c:4,9,11,13,24,26,t:22	Z8837933165	1{421}	COC(=O)c1ccc(N)nc1C1	2{306}	CN(CCO)c1ccc(C=O)cc1	3{22}	[C-]#[N+]C1CO C1	23.9	21
1769	4{351,788,39}	CCOCCNC1=C(CC2(CCCC2)NC(=O)OC(C)(C)C)N=C2C=CC3=C(C(O)CC3)N12 c:6,25,t:23,27	Z8873685499	1{351}	Nc1ccc2CC(C(O)c2n1	2{788}	CC(C)(C)OC(=O)NC1(CC=O)CCCC1	3{39}	CCOCC[N+]#[C-]	25.2	20
1770	4{254,57,37}	COC(=O)C1CC(C1)NC1=C(N=C2C=C(C)C(=CN12)C(=O)OC)C1CCOC1 c:17,t:10,12,14	Z8878918642	1{254}	COC(=O)c1cnc(N)cc1C	2{57}	O=CC1CCOC1	3{37}	COC(=O)C1CC(C1)[N+]#[C-]	21.2	20
1771	4{50,789,18}	CC(C)(C)NC1=C(N=C2C=CC=C(N12)P(C)(C)=O)C1=CC(F)=C(C=C1)C(F)(F)F c:9,11,23,25,t:5,7,20	Z8878918803	1{50}	CP(=O)(C)c1cccc(N)n1	2{789}	Fe1cc(C=O)c1cc1C(F)(F)F	3{18}	CC(C)(C)[N+]#[C-]	23.3	20
1772	4{356,110,69}	COC1=C(NC2=C(N=C3C=CC(CI)=C(N23)C(=O)N(C)C)C2=CN=C(C=C2)P(C)(C)=O)C=CC=C1 c:2,9,12,24,26,33,35,t:5,7,22	Z8849597827	1{356}	CN(C)C(=O)c1nc(N)ccc1C1	2{110}	CP(=O)(C)c1ccc(C=O)cn1	3{69}	COc1cccc1[N+]#[C-]	27.0	20
1773	4{91,790,7}	COC(=O)C1=C(F)C=C(C=C1F)C1=C(NC2CCOCC2)N2C=C(C=CC2=N1)C(N)=O c:4,7,9,13,24,26,29	Z8873684767	1{91}	NC(=O)c1ccc(N)nc1	2{790}	COC(=O)c1cc(F)cc(C=O)c1F	3{7}	[C-]#[N+]C1CCOCC1	23.3	20
1774	4{112,627,24}	CCC1=NC(C)=C(N1)C1=C(NCC2=CC(OC)=CC=C2)N2C(C=NC=C2OC)=N1 c:5,9,17,19,24,26,30,t:2,13	Z8873685496	1{112}	COc1cnc(N)n1	2{627}	CCc1nc(C)c(C=O)[nH]1	3{24}	COc1cccc(C1[N+]#[C-])c1	20.9	20
1775	4{199,654,34}	CC(F)(F)C1=CC=CN2C(NCC3CCCC3)=C(CC3=CN=CO3)N=C12 c:6,23,t:4,17,21,27	Z8873684785	1{199}	CC(F)(F)c1cccnc1N	2{654}	O=CCCc1cnco1	3{34}	[C-]#[N+]CC1COCO1	20.0	20
1776	4{50,791,7}	CC1=CN2C=CC=C(C2=N1)C1=C(NC2CCOCC2)N2C(C=CC=C2P(C)(C)=O)=N1 c:4,6,9,12,24,26,32,t:1	Z8854581150	1{50}	CP(=O)(C)c1cccc(N)n1	2{791}	Cc1cn2cccc(C=O)c2n1	3{7}	[C-]#[N+]C1CCOCC1	22.5	20

1777	4{209,153,14}	COCCNC1=C(N=C2N1C=CC=C2N1CCCC1)C1=CN(CC(F)(F)F)N=N1 c:7,11,13,31,t:5,23	Z8855739191	1{209}	Nc1ncccc1 N2CCCCC2	2{153}	FC(F)(F)Cn1 cc(C=O)nn1	3{14}	COCC[N+][# C-]	22.5	20
1778	4{166,748,15}	CCNC1=C(N=C2C=C(CSCCO)C=CN12)C1=CC(=NN1C)C(F)(F)F c:14,21,t:3,5,7,19	Z8873684936	1{166}	Nc1cc(CSC CO)ccn1	2{748}	Cn1nc(cc1C =O)C(F)(F)F	3{15}	CC[N+][#C-]	21.1	20
1779	4{73,77,20}	COC1=CC(C)=C(NC2=C(CC3CCCC3)N=C3C=CC4=NC=CN4N23)C=C1 c:8,19,23,30,t:2,5,17,21	Z8873684830	1{73}	Nc1ccc2ncc n2n1	2{77}	O=CCC1CC CC1	3{20}	COc1ccc([N +][#C-])c(C)c1	19.8	19
1780	4{470,704,39}	CCOCCNC1=C(N=C2C=CC3=C(C=C(C=C3)C(=O)OC)N12)C1=NC(=NN1C)C1CC1 c:10,14,16,28,t:6,8,12,26	Z8878918435	1{470}	COC(=O)c1 ccc2ccc(N)n c2c1	2{704}	Cn1nc(nc1C =O)C2CC2	3{39}	CCOCC[N+] #[C-]	22.1	19
1781	4{87,81,23}	COC(=O)CCC(NC1=C(N=C2C=C(C)C(CI)=CN12)C1=NC(=CC=C1)C(F)F)C(=O)OC c:16,23,25,t:8,10,12,21	Z8873684939	1{87}	Cc1cc(N)nc c1Cl	2{81}	FC(F)c1cccc C=O)n1	3{23}	COC(=O)CC C([N+][#C-])C(=O)OC	23.8	19
1782	4{83,412,18}	CSC1=CC(=CC=C1)C1=C(NC(C)(C)C)N2C=C(C=CC2=N1)P(C)(C)O c:4,6,9,17,19,22,t:2	Z8878918865	1{83}	CP(=O)(C)c 1ccc(N)nc1	2{412}	CSelcccc(C= O)c1	3{18}	CC(C)(C)[N +][#C-]	19.7	19
1783	4{99,767,50}	CCCC(OC)C1=C(NC2=CC3=C(OCCO3)C=C2)N2C=C(C=CC2=N1)S(N)(=O)=O c:6,18,22,24,27,t:9,11	Z8873684922	1{99}	Nc1ccc(en1)S(=O)(=O) N	2{767}	CCCC(OC)C =O	3{50}	[C-][#N+]c1ccc 2OCCOc2c1	21.5	18
1784	4{184,695,14}	COCCNC1=C(N=C2C=CC(=CN12)C(N)=S)C1=CC(OCC(=O)OC)=C(OC)C=C1 c:9,11,31,t:5,7,19,27	Z8878918894	1{184}	NC(=S)c1cc c(N)nc1	2{695}	COC(=O)CO c1cc(C=O)cc c1OC	3{14}	COCC[N+][# C-]	22.0	18
1785	4{275,172,14}	COCCNC1=C(N=C2N1C(CI)=CC=C2F)C1=CN(C=N1)C1CC1 c:7,12,14,21,t:5,18	Z8835022886	1{275}	Nc1nc(Cl)c cc1F	2{172}	O=Cc1c[nH] c(n1)C2CC2	3{14}	COCC[N+][# C-]	17.3	18
1786	4{455,42,23}	COC(=O)CCC(NC1=C(N=C2C=C(CI)C=C(CI)N12)C1=CN(C)N=C1Cl)C(=O)OC c:25,t:8,10,12,15,21	Z8873684883	1{455}	Nc1cc(Cl)cc (Cl)n1	2{42}	Cn1cc(C=O) c(Cl)n1	3{23}	COC(=O)CC C([N+][#C-])C(=O)OC	23.2	18
1787	4{379,792,14}	COCCNC1=C(N=C2N1C=CC=C2Br)C1=NN(C)N=C1 c:7,11,13,21,t:5,17	Z8878918465	1{379}	Nc1ncccc1 Br	2{792}	Cn1ncc(C=O)n1	3{14}	COCC[N+][# C-]	17.1	18
1788	4{103,455,5}	COCCNC1=C(N=C2C=NC=C(CO)N12)C1=C(C)ON=C1Br c:10,19,23,t:6,8,12	Z8873684822	1{103}	Nc1cncc(C O)n1	2{455}	Cc1onc(Br)c 1C=O	3{5}	COCCC[N+] #[C-]	19.3	18
1789	4{371,721,28}	CCCNC1=C(N=C2N1C=CC=C2OCCCC#N)C1=CC(=CN=C1)C(=O)OC c:6,10,12,23,25,t:4,21	Z8878918541	1{371}	Nc1ncccc1 OCCCC#N	2{721}	COC(=O)c1c ncc(C=O)c1	3{28}	CCC[N+][#C]	19.1	18

1790	4{186,746,69}	COC1=C(NC2=C(N=C3C=C(C=CN23)S(=O)(=O)N(C)C)C2=C(C)C=CN=C2)C=CC=C1 c:2,9,11,22,25,27,30,32,t:5,7	Z8855619586	1{186}	Cl.CN(C)S(=O)(=O)c1ccnc(N)c1	2{746}	Cc1ccnc1C=O	3{69}	COc1cccc1[N+][C-]	21.2	18
1791	4{50,644,18}	CC(C)(C)NC1=C(N=C2C=CC=C(N12)P(C)(C)=O)C1=CC(F)=C(OCC#C)C=C1 c:9,11,29,t:5,7,20,23	Z8878918524	1{50}	CP(=O)(C)c1cccc(N)n1	2{644}	Fc1cc(C=O)ccc1OCC#C	3{18}	CC(C)(C)[N+][C-]	20.0	18
1792	4{32,793,31}	CSCCNC1=C(N=C2C=C(C=CN12)P(C)(C)=O)C1=NC=C(S1)C(C)C c:9,11,22,t:5,7,20	Z8873684907	1{32}	CP(=O)(C)c1ccnc(N)c1	2{793}	CC(C)c1nc(C=O)s1	3{31}	CSCC[N+][C-]	19.7	18
1793	4{101,260,14}	COCCNC1=C(N=C2N1C=C(CO)C=C2C1)C1=NOC(C)=C1 c:7,15,23,t:5,11,19	Z8873684928	1{101}	Nc1ncc(CO)cc1Cl	2{260}	Cc1cc(C=O)no1	3{14}	COCC[N+][C-]	16.1	18
1794	4{99,736,29}	CCOC(=O)CCNC1=C(N=C2C=CC(=CN12)S(N)(=O)=O)C1CC(C)(C)C1 c:12,14,t:8,10	Z8878918655	1{99}	Nc1ccc(en1)S(=O)(=O)N	2{736}	CC1(C)CC(C1)C=O	3{29}	CCOC(=O)C[N+][C-]	18.8	18
1795	4{137,69,13}	COC1=CC=C(CNC2=C(N=C3C=CC(C)=NN23)C2=NN(C)C(C)=C2)C=C1 c:12,15,25,28,t:2,4,8,10,20	Z8873684693	1{137}	Cc1ccc(N)n1	2{69}	Cc1cc(C=O)nn1C	3{13}	COc1ccc(C[N+][C-])cc1	17.0	17
1796	4{36,27,9}	CNC1=C(N=C2C=CC(Br)=CN12)C1=NN(C)C(C)=N1 c:6,9,19,t:2,4,14	Z8873685408	1{36}	Nc1ccc(Br)cn1	2{27}	Cc1nc(C=O)nn1C	3{9}	C[N+][C-]	15.1	17
1797	4{101,727,14}	COCCNC1=C(N=C2N1C=C(CO)C=C2C1)C1=CN=C(N=C1)C(C)C c:7,15,21,23,t:5,11,19	Z8873684769	1{101}	Nc1ncc(CO)cc1Cl	2{727}	CC(C)c1ncc(C=O)cn1	3{14}	COCC[N+][C-]	17.4	17
1798	4{386,419,23}	COC(=O)CCC(NC1=C(N=C2C=C(C)C=CN12)C1=NC=CC(OC)=C1)C(=O)OC c:15,22,26,t:8,10,12,20	Z8854581171	1{386}	Cc1ccnc(N)c1	2{419}	COc1ccnc(C=O)c1	3{23}	COC(=O)CC(C[N+][C-])C(=O)OC	18.7	17
1799	4{171,763,22}	COC(=O)C1=CC2=C(NN=C2C2=C(NC3COC3)N3C=CC(=CC3=N2)N2C=CN=C2)C=C1 c:9,12,21,23,26,30,32,35,t:4,6	Z8873685413	1{171}	Nc1cc(ccn1)n2ccnc2	2{763}	COC(=O)c1ccc2[nH]nc(C=O)c2c1	3{22}	[C-][N+]C1CO C1	19.4	17
1800	4{37,794,10}	CC(C)(C)OC(=O)NCCC1=NC(=CS1)C1=C(NC2CCOC2)N2C(C=CC=C2C(F)F)=N1 c:12,16,27,29,34,t:10	Z8873684613	1{37}	Cl.Nc1cccc(en1)C(F)F	2{794}	CC(C)(C)OC(=O)NCCc1nc(C=O)cs1	3{10}	[C-][N+]C1CCOC1	21.4	17
1801	4{103,795,5}	COCCNC1=C(N=C2C=NC=C(CO)N12)C1=C(Br)C=C(Cl)C=C1 c:10,19,25,t:6,8,12,22	Z8873685437	1{103}	Nc1cnc(CO)n1	2{795}	Clc1ccc(C=O)c(Br)c1	3{5}	COCCC[N+][C-]	18.9	16
1802	4{184,189,26}	NC(=S)C1=CN2C(NCC3=CC=C(F)C=C3)=C(N=C2C=C1)C1=CN(N=N1)C1CCOCC1 c:14,16,18,21,27,t:3,9,11,24	Z8878918818	1{184}	NC(=S)c1ccc(N)n1	2{189}	O=Cc1cn(nn1)C2CCOCC2	3{26}	Fc1ccc(C[N+][C-])cc1	20.0	16

1803	4{382,459,62}	COC(=O)C1(CCCC1)NC1=C(N=C2C=NC(=C N12)C(F)(F)F)C1=NNC(C)=C1C c:15,17,30,t:11,13,26	Z8873684931	1{382}	Nc1cnc(en1)C(F)(F)F	2{459}	Cc1[nH]nc(C =O)c1C	3{62}	COC(=O)C1(CCCC1)[N+] #[C-]	18.1	16
1804	4{124,796,43}	COC(=O)C1=C(F)C=C(C=N1)C1=C(NC2CCN (CC2)C(=O)OC(C)(C)C)N2C=CC=C(CO)C2= N1 c:4,7,9,12,30,37,t:32	Z8878918505	1{124}	Nc1ncccc1 CO	2{796}	COC(=O)c1n cc(C=O)cc1F	3{43}	CC(C)(C)OC (=O)N1CCCC (CC1)[N+]# C-]	21.3	16
1805	4{373,85,39}	CCOCCNC1=C(N=C2C=CC(CNC(=O)OC(C) (C)C)=CN12)C1=CN=NS1 c:10,21,28,t:6,8,26	Z8878918358	1{373}	CC(C)(C)O C(=O)NCc1 ccc(N)nc1	2{85}	O=Cc1cnns1	3{39}	CCOCC[N+] #[C-]	19.0	16
1806	4{142,242,21}	CS(=O)(=O)CCOC1=CC=CN2C(NCC3CC3)= C(N=C12)C1=CN2N=CC(C#N)=C2N=C1 c:9,18,27,31,34,t:7,20,24	Z8878918674	1{142}	CS(=O)(=O)CCOc1ccc nc1N	2{242}	O=Cc1cnc2c (C#N)cnn2c1	3{21}	[C-]#[N+]CC1C C1	19.0	16
1807	4{101,538,14}	COCCNC1=C(N=C2N1C=C(CO)C=C2C1)C1= CN=CN1C c:7,15,21,t:5,11,19	Z8878918498	1{101}	Nc1ncc(CO)cc1Cl	2{538}	Cn1cncclC= O	3{14}	COCC[N+]# C-]	14.1	16
1808	4{375,375,51}	COCC1=C(N=CO1)C1=C(NCCNC(=O)OC(C) (C)C)N2C(C=NC=C2OC(C)C)=N1 c:5,9,24,26,32,t:3	Z8855619770	1{375}	CC(C)Oclc ncc(N)n1	2{375}	COCC1ocnc1 C=O	3{51}	CC(C)(C)OC (=O)NCC[N +]#[C-]	18.7	15
1809	4{79,733,13}	COC1=CC=C(CNC2=C(N=C3C=NC=C(C)N2 3)C2=NN(N=N2)C(C)(C)C)C=C1 c:12,23,30,t:2,4,8,10,14,20	Z8854581174	1{79}	Cc1cnc(N) n1	2{733}	CC(C)(C)n1n nc(C=O)n1	3{13}	COc1ccc(C[N+]#[C-])cc1	15.8	15
1810	4{48,797,22}	CS(=O)(=O)C1=CC2=NC(=C(NC3COC3)N2C =C1)C1=C(F)C=NC=C1 c:18,21,24,26,t:4,6,8	Z8878918421	1{48}	CS(=O)(=O)c1ccnc(N)c 1	2{797}	Fc1cncclC= O	3{22}	[C-]#[N+]C1CO C1	14.9	15
1811	4{54,689,53}	CN(C)C(=O)C1=CN2C(C=C1)=NC(C1=CN(C COC(C)=O)N=C1)=C2NCCOCC1=CC=CC=C 1 c:9,11,23,25,35,37,t:5,14,33	Z8878918851	1{54}	Cl.CN(C)C(=O)c1ccc(N)nc1	2{689}	CC(=O)OCC n1cc(C=O)cn 1	3{53}	[C-]#[N+]CCOC c1cccc1	19.5	15
1812	4{464,271,70}	CN1N=NC(=N1)C1=C(NC2CCN(C2)C(=O)O C(C)(C)C)N2C=C(C=CC2=N1)N1CCN(C)CC 1 c:2,4,7,24,26,29	Z8837933135	1{464}	CN1CCN(C C1)c2ccc(N)nc2	2{271}	Cn1nnc(C=O)n1	3{70}	CC(C)(C)OC (=O)N1CCCC (C1)[N+]# [C-]	18.9	15
1813	4{433,340,31}	CCN1C=NC(=N1)C1=C(NCCSC)N2C(C=CC(C#C)=C2C)=N1 c:3,5,8,17,21,24	Z8878918539	1{433}	Cc1nc(N)cc c1C#C	2{340}	CCn1cnc(C= O)n1	3{31}	CSCC[N+]# [C-]	13.3	14
1814	4{78,798,51}	CN1C=C(N=N1)C1=C(NCCNC(=O)OC(C)(C) C)N2N3C=C(C)N=C3C(C)=CC2=N1 c:2,4,7,25,29,32,t:22	Z8878918911	1{78}	Cc1cn2nc(N)cc(C)c2n1	2{798}	Cn1cc(C=O) nn1	3{51}	CC(C)(C)OC (=O)NCC[N +]#[C-]	16.6	14

1815	4{340,725,5}	CCOC1=CC=CN2C(NCCCCO)=C(N=C12)C1=CN=NN1CC c:5,14,22,t:3,16,20	Z8873685248	1{340}	CCOc1cccn c1N	2{725}	CCn1nnc1C =O	3{5}	COCCC[N+] #[C-]	13.3	14
1816	4{185,799,8}	COC(=O)C(CC1=CC=CC=C1)NC1=C(N=C2C=CC(=C(C)N12)S(C)(=O)=O)C1=NN=C(C)C=C1 c:8,10,18,35,t:6,14,16,20,30,32	Z8878918436	1{185}	Cc1nc(N)cc c1S(=O)(=O))C	2{799}	Cc1ccc(C=O))nn1	3{8}	COC(=O)C(Cc1cccc1)[N+]#[C-]	18.4	14
1817	4{154,800,47}	CC(C)NC1=C(N=C2C=C(C=CN12)[N+](=[O-])=O)C1=CC2=C(NC(=O)CO)C=C1 c:8,10,28,t:4,6,18,20	Z8873684917	1{154}	Nc1cc(ccn1))N+](=O)[O-]	2{800}	O=Cc1ccc2N C(=O)COc2c 1	3{47}	CC(C)[N+]#[C-]	14.1	14
1818	4{48,277,31}	CSCCNC1=C(CC(NC(=O)OC(C)(C)C)C2CC2)N=C2C=C(C=CN12)S(C)(=O)=O c:5,23,25,t:21	Z8835022868	1{48}	CS(=O)(=O) c1ccnc(N)c 1	2{277}	CC(C)(C)OC (=O)NC(CC =O)C1CC1	3{31}	CSCC[N+]#[C-]	17.9	14
1819	4{462,801,39}	CCOCCNC1=C(N=C2N1C=C(Br)C=C2CO)C1=CN=C(S1)C1=CN(C)N=C1 c:8,15,22,30,t:6,12,20,26	Z8855619696	1{462}	Nc1ncc(Br) cc1CO	2{801}	Cn1cc(en1)c 2ncc(C=O)s2	3{39}	CCOCC[N+] #[C-]	18.1	14
1820	4{99,802,34}	NS(=O)(=O)C1=CN2C(NCC3CCCO3)=C(N=C2C=C1)C1=CN2C=CN=C2S1 c:15,17,20,26,28,t:4,23	Z8878918406	1{99}	Nc1ccc(en1))S(=O)(=O) N	2{802}	O=Cc1en2cc nc2s1	3{34}	[C-]]#[N+]CC1C CCO1	15.8	14
1821	4{79,421,9}	CNC1=C(N=C2C=NC=C(C)N12)C1=CN=C(S1)C1=CC=CO1 c:6,16,22,t:2,4,8,14,20	Z8873685441	1{79}	Cc1cncc(N) n1	2{421}	O=Cc1cnc(s1) c2cccc2	3{9}	C[N+]#[C-]	11.7	14
1822	4{445,803,29}	CCOC(=O)CCNC1=C(N=C2C=NC(SC)=CN12)C1=CC=C(C=C1)C1=NN=C(C)N=N1 c:12,16,23,25,33,t:8,10,21,28,30	Z8873684851	1{445}	CSc1cnc(N) cn1	2{803}	Cc1nnc(nn1) c2ccc(C=O)c c2	3{29}	CCOC(=O)C C[N+]#[C-]	16.7	14
1823	4{414,804,46}	CN1C=NC(Br)=C1C1=C(NCC(C)=C)N2C=C(Cl)N=CC2=N1 c:2,5,8,19,22,t:16	Z8873685477	1{414}	Nc1cnc(Cl) cn1	2{804}	Cn1cnc(Br)c 1C=O	3{46}	CC(=C)C[N+]]#[C-]	14.1	14
1824	4{452,134,51}	COC1=NC(=NC=C1)C1=C(NCCNC(=O)OC(C)(C)C)N2C(C=CC3=C2C=NC=C3)=N1 c:4,6,9,24,26,29,31,33,t:2	Z8878918681	1{452}	Nc1ccc2ccn cc2n1	2{134}	COc1ccnc(C =O)n1	3{51}	CC(C)(C)OC (=O)NCC[N +]#[C-]	16.0	14
1825	4{471,538,14}	COCCNC1=C(N=C2N1C=C(C)C=C2)C1=CN=CN1C c:7,14,20,t:5,11,18	Z8873684926	1{471}	Cc1cnc(N)c (I)c1	2{538}	Cn1cncc1C= O	3{14}	COCC[N+]#[C-]	15.1	14
1826	4{154,805,47}	CC(C)NC1=C(N=C2C=C(C=CN12)[N+](=[O-])=O)C1=CC=C(C=C1)S(=O)(=O)N(C)C c:8,10,20,22,t:4,6,18	Z8878918643	1{154}	Nc1cc(ccn1))N+](=O)[O-]	2{805}	CN(C)S(=O) (=O)c1ccc(C =O)cc1	3{47}	CC(C)[N+]#[C-]	14.7	14
1827	4{176,538,14}	COCCNC1=C(N=C2N1C=CN=C2N1CCCC1)C1=CN=CN1C c:7,11,13,24,t:5,22	Z8837933141	1{176}	Nc1ncnc1 N2CCCC2	2{538}	Cn1cncc1C= O	3{14}	COCC[N+]#[C-]	12.4	13

1828	4{91,806,7}	NC(=O)C1=CN2C(C=C1)=NC(=C2NC1CCOC C1)C1=NC2=C(C=C1)C(F)=CC(F)=C2 c:7,9,11,24,26,30,33,t:3,22	Z8873684756	1{91}	NC(=O)c1c cc(N)nc1	2{806}	Fc1cc(F)c2cc c(C=O)nc2c1	3{7}	[C-]#[N+]C1CC OCC1	15.3	13
1829	4{472,685,6}	CCOC(=O)CCCNC1=C(N=C2N1C=C(C=C2C #N)C(C)C)C1=CN(CC2CCOC2)N=N1 c:11,15,17,35,t:9,25	Z8855619511	1{472}	CC(C)c1enc (N)c(C#N)c 1	2{685}	O=Cc1cn(CC 2CCOC2)nn1	3{6}	CCOC(=O)C CC[N+]#[C-]	16.8	13
1830	4{47,172,6}	CCOC(=O)CCCNC1=C(N=C2C=C(C=CN12)S (N)(=O)=O)C1=CNC(=N1)C1CC1 c:13,15,27,t:9,11,24	Z8878918607	1{47}	Cl.Nc1cc(cc n1)S(=O)(=O) N	2{172}	O=Cc1c[nH] c(n1)C2CC2	3{6}	CCOC(=O)C CC[N+]#[C-]	15.5	13
1831	4{137,94,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC(C)=NN 23)C2=NC=CN=C2)C=C1 c:12,15,22,24,27,t:2,5,8,10,20	Z8873685256	1{137}	Cc1ccc(N)n n1	2{94}	O=Cc1cncn 1	3{20}	COc1ccc([N +]#[C-]]c(C)c1	12.4	13
1832	4{22,151,13}	COC1=CC=C(CNC2=C(N=C3C=CC(CI)=NN2 3)C2=CC(C)=NN2)C=C1 c:12,15,23,27,t:2,4,8,10,20	Z8878918393	1{22}	Nc1ccc(Cl) nn1	2{151}	Cc1cc(C=O)[nH]n1	3{13}	COc1ccc(C[N+]#[C-])cc1	12.9	13
1833	4{390,189,22}	CCC1=C(Cl)N2C(NC3COC3)=C(N=C2C=C1) C1=CN(N=N1)C1CCOCC1 c:2,12,14,17,23,t:20	Z8849597832	1{390}	CCc1ccc(N) nc1Cl	2{189}	O=Cc1cn(nn 1)C2CCOCC 2	3{22}	[C-]#[N+]C1CO C1	14.1	13
1834	4{354,704,62}	COC(=O)C1=CN2C(C=C1)=NC(=C2NC1(CC CC1)C(=O)OC)C1=NC(=NN1C)C1CC1 c:8,10,12,28,t:4,26	Z8837933143	1{354}	COC(=O)c1c ccc(N)nc1	2{704}	Cn1nc(nc1C =O)C2CC2	3{62}	COC(=O)C1(CCCC1)[N+] #[C-]	15.2	13
1835	4{193,199,21}	CNC(=O)C1=CN2C(C=C1)=NC(CN1C(=O)C3 =C(C=CC=C3)C1=O)=C2NCC1CC1 c:8,10,19,21,26,t:4,17	Z8873684696	1{193}	CNC(=O)c1c ccc(N)nc1	2{199}	O=CCN1C(= O)c2ccccc2C 1=O	3{21}	[C-]#[N+]CC1C C1	13.7	13
1836	4{118,347,35}	CCCN1C=C(N=N1)C1=C(NCCCSC)N2C(C= CC=C2C(C)O)=N1 c:4,6,9,19,21,26	Z8873684940	1{118}	Cl.CC(O)c1c cccc(N)n1	2{347}	CCCN1cc(C= O)nn1	3{35}	CSCCC[N+] #[C-]	12.6	12
1837	4{391,425,47}	CC(C)NC1=C(N=C2C=CC(=NN12)C1=C(F)C =CC=C1)C1CCCN(C1)S(C)(=O)=O c:8,10,15,18,20,t:4,6	Z8837933176	1{391}	Nc1ccc(nn1) c2ccccc2F	2{425}	CS(=O)(=O) N1CCCC(C1)C=O	3{47}	CC(C)[N+]#[C-]	14.5	12
1838	4{119,647,10}	N#CC1=CN2C(C=C1)=NC(=C2NC1CCOC1)C 1=CC2=C(OC=C2)C=C1 c:6,8,10,25,28,t:2,20,22	Z8878918848	1{119}	Nc1ccc(C# N)cn1	2{647}	O=Cc1ccc2o ccc2c1	3{10}	[C-]#[N+]C1CC OC1	11.2	12
1839	4{146,111,12}	CS(=O)(=O)C1=CN2C(C=C1)=NC(C1CCCC1)=C2NCC1CCOC1 c:8,10,18,t:4	Z8878918852	1{146}	CS(=O)(=O) c1ccc(N)nc 1	2{111}	O=CC1CCC C1	3{12}	[C-]#[N+]CC1C COC1	11.4	12
1840	4{32,659,18}	CN1C=C2C(C=CC=C2C2=C(NC(C)(C)C)N3C =CC(=CC3=N2)P(C)(C)=O)=N1 c:2,5,7,10,18,20,23,29	Z8878918543	1{32}	CP(=O)(C)c 1ccnc(N)c1	2{659}	Cn1cc2c(C= O)cccc2n1	3{18}	CC(C)(C)[N +]#[C-]	12.1	11

1841	4{83,807,18}	CC(C)(C)NC1=C(N=C2C=CC(=CN12)P(C)(C)=O)C1=C2N=CC=CC2=CC(F)=C1 c:9,11,20,22,24,27,30,t:5,7	Z8855739224	1{83}	CP(=O)(C)c1ccc(N)nc1	2{807}	Fc1cc(C=O)c2ncccc2c1	3{18}	CC(C)(C)[N+][C-]	12.5	11
1842	4{46,170,9}	CCN1N=NC(=N1)C1=C(NC)N2C=CC=CC2=N1 c:3,5,8,13,15,18	Z8873684867	1{46}	Nc1ccccn1	2{170}	CCn1nnc(C=O)n1	3{9}	C[N+][C-]	7.3	11
1843	4{28,790,7}	COC(=O)C1=C(F)C=C(C=C1F)C1=C(NC2CCOCC2)N2C=CC(=CC2=N1)C1=NOC=N1 c:4,7,9,13,24,26,29,35,t:32	Z8873684576	1{28}	Cl.Nc1cc(ccn1)c2ncon2	2{790}	COC(=O)c1c(F)cc(C=O)c1F	3{7}	[C-][N+]C1CCOCC1	13.5	11
1844	4{83,808,18}	CC1=C(Cl)N=C(C2=C(NC(C)(C)C)N3C=C(C=CC3=N2)P(C)(C)=O)C(F)=C1 c:1,6,14,16,19,27,t:4	Z8855619564	1{83}	CP(=O)(C)c1ccc(N)nc1	2{808}	Cc1cc(F)c(C=O)nc1Cl	3{18}	CC(C)(C)[N+][C-]	11.8	11
1845	4{473,809,15}	CCNC1=C(N=C2C=CC=C(N12)C(=O)OCC)C1=CN=C(S1)C(=O)OCC c:7,9,21,t:3,5,19	Z8854581170	1{473}	Cl.CCOC(=O)c1cccc(N)n1	2{809}	CCOC(=O)c1ncc(C=O)s1	3{15}	CC[N+][C-]	11.1	11
1846	4{22,44,13}	CCN1C=C(C=N1)C1=C(NCC2=CC=C(OC)C=C2)N2N=C(Cl)C=CC2=N1 c:3,5,8,18,25,28,t:12,14,22	Z8878918382	1{22}	Nc1ccc(Cl)nn1	2{44}	CCn1cc(C=O)en1	3{13}	COc1ccc(C[N+][C-])cc1	10.9	11
1847	4{141,234,32}	CC(=O)NC1=CC2=NC(=C(NC3CCC3)N2C=C1)C1=NN=C2CCCCN12 c:18,t:4,6,8,21,23	Z8873684816	1{141}	CC(=O)Nc1ccnc(N)c1	2{234}	O=Cc1nnc2CCCCn12	3{32}	[C-][N+]C1CC1	10.7	10
1848	4{394,328,12}	CCC1=NNC=C1C1=C(NCC2CCOC2)N2C(C=CC(C=C)=C2F)=N1 c:5,8,20,24,27,t:2	Z8873685500	1{394}	Nc1ccc(C=C)cc(F)n1	2{328}	Cl.CCc1n[nH]cc1C=O	3{12}	[C-][N+]CC1COC1	10.0	10
1849	4{474,66,51}	CCN1N=C(C)C(=C1C)C1=C(NCCNC(=O)OC(C)(C)C)N2N=C(Cl)C=C(OC)C2=N1 c:6,10,32,t:3,24,27	Z8829498507	1{474}	COc1cc(Cl)nn1N	2{66}	CCn1nc(C)c(C=O)c1C	3{51}	CC(C)(C)OC(=O)NCC[N+][C-]	13.0	10
1850	4{113,810,14}	COCCNC1=C(N=C2N1C=CC=C2N1CCOCC1)C1=CN=C(NC(=O)OC(C)(C)C)S1 c:7,11,13,t:5,23,25	Z8878918584	1{113}	Nc1ncccc1N2CCOCC2	2{810}	CC(C)(C)OC(=O)Nc1ncc(C=O)s1	3{14}	COCC[N+][C-]	13.0	10
1851	4{176,529,14}	COCCNC1=C(N=C2N1C=CN=C2N1CCCC1)C1=CC(Cl)=C(C=C1)S(N)(=O)=O c:7,11,13,25,27,t:5,22	Z8878918347	1{176}	Nc1ncnc1N2CCCC2	2{529}	NS(=O)(=O)c1ccc(C=O)c1Cl	3{14}	COCC[N+][C-]	12.3	10
1852	4{78,811,10}	CC1=CN2N3C(C=C(C)C2=N1)=NC(=C3NC1CCOC1)C1=CC=C(C=C1)C1=CC=CC=C1 c:10,12,14,26,28,33,35,t:1,6,24,31	Z8855619702	1{78}	Cc1cn2nc(N)cc(C)c2n1	2{811}	O=Cc1ccc(cc1)c2ccccc2	3{10}	[C-][N+]C1CCOC1	11.5	10
1853	4{78,812,39}	CCOCCNC1=C(N=C2C=C(C)C3=NC(C)=CN3N12)C1=CC2=C(O1)C=C(C=C2)C(=O)OC c:16,25,29,31,t:6,8,10,13,23	Z8855739169	1{78}	Cc1cn2nc(N)cc(C)c2n1	2{812}	COC(=O)c1ccc2cc(C=O)oc2c1	3{39}	CCOCC[N+][C-]	11.9	10

1854	4{141,545,22}	COCCN1N=C(C)C(=C1C)C1=C(NC2COC2)N2C=CC(NC(C)=O)=CC2=N1 c:8,12,21,27,30,t:5	Z8873684905	1{141}	CC(=O)Nc1ccnc(N)c1	2{545}	COCCn1nc(C)c(C=O)c1C	3{22}	[C-] #[N+]C1CO C1	10.4	10
1855	4{164,292,21}	CN(C)CC1=CC2=NC(=C(NCC3CC3)N2C=C1)C1=C(C)N=CS1 c:18,21,24,t:4,6,8	Z8878918341	1{164}	CN(C)Cc1ccnc(N)c1	2{292}	Cc1ncsc1C=O	3{21}	[C-] #[N+]CC1C C1	8.9	10
1856	4{48,813,22}	CS(=O)(=O)C1=CC2=NC(=C(NC3COC3)N2C=C1)C1=C(Cl)C(F)=CC=C1F c:18,21,25,27,t:4,6,8	Z8878918903	1{48}	CS(=O)(=O)c1ccnc(N)c1	2{813}	Fc1ccc(F)c(C=O)c1Cl	3{22}	[C-] #[N+]C1CO C1	11.2	10
1857	4{188,687,62}	COC(=O)C1=CN=CC2=NC(=C(NC3(CCCC3)C(=O)OC)N12)C1=C2CSCCC2=NN1C c:6,26,33,t:4,8,10	Z8873684948	1{188}	COC(=O)c1cncc(N)n1	2{687}	Cn1nc2CCSCc2c1C=O	3{62}	COC(=O)C1(CCCC1)[N+]#[C-]	11.9	9
1858	4{43,814,39}	CCOCCNC1=C(CCCC(=O)OC)N=C2C=CC3=C(CN(C3)C(=O)OC(C)(C)C)N12 c:6,17,t:15,19	Z8873684823	1{43}	CC(C)(C)OC(=O)N1Cc2ccc(N)nc2C1	2{814}	COC(=O)CCCC=O	3{39}	CCOCC[N+]#[C-]	11.2	9
1859	4{112,815,12}	COC1=NC(Cl)=C(S1)C1=C(NCC2CCOC2)N2C(C=NC=C2OC)=N1 c:5,9,21,23,27,t:2	Z8846492110	1{112}	COc1cncc(N)n1	2{815}	COc1nc(Cl)c(C=O)s1	3{12}	[C-] #[N+]CC1C COC1	9.9	9
1860	4{161,593,14}	COCCNC1=C(N=C2C=CC=NN12)C1=CC=C(NC(C)=O)C=C1 c:9,11,24,t:5,7,16,18	Z8854581137	1{161}	Nc1cccn1	2{593}	CC(=O)Nc1ccc(C=O)cc1	3{14}	COCC[N+]#[C-]	8.0	9
1861	4{54,168,22}	CN(C)C(=O)C1=CN2C(NC3COC3)=C(N=C2C=C1)C1=NOC=C1 c:14,16,19,25,t:5,22	Z8829498572	1{54}	Cl.CN(C)C(=O)c1ccc(N)nc1	2{168}	O=Cc1ccn1	3{22}	[C-] #[N+]C1CO C1	8.0	9
1862	4{146,816,46}	COC1=C(OCCCC#N)C=C(C=C1)C1=C(NCC(C)=C)N2C=C(C=CC2=N1)S(C)(=O)=O c:2,10,12,15,23,25,28	Z8878918537	1{146}	CS(=O)(=O)c1ccc(N)nc1	2{816}	COc1ccc(C=O)cc1OCCCC#N	3{46}	CC(=C)C[N+]#[C-]	11.0	9
1863	4{79,239,9}	CNC1=C(N=C2C=NC=C(C)N12)C1=NOC2=C1CCCC2 c:6,17,t:2,4,8,14	Z8873685460	1{79}	Cc1cncc(N)n1	2{239}	O=Cc1noc2CCCCc12	3{9}	C[N+]#[C-]	6.8	9
1864	4{119,70,10}	CC(F)(F)C1=NC(=CS1)C1=C(NC2CCOC2)N2C=C(C=CC2=N1)C#N c:6,10,20,22,25,t:4	Z8855619533	1{119}	Nc1ccc(C#N)nc1	2{70}	CC(F)(F)c1nc(C=O)cs1	3{10}	[C-] #[N+]C1CC OC1	8.4	8
1865	4{99,349,29}	CCOC(=O)CCNC1=C(N=C2C=CC(=CN12)S(N)(=O)=O)C1C[C@H]2OC(C)(C)O[C@H]2C1 c:12,14,t:8,10	Z8878918664	1{99}	Nc1ccc(en1)S(=O)(=O)N	2{349}	CC1(C)O[C@@@H]2CC(C[C@@@H]2O1)C=O	3{29}	CCOC(=O)C[C[N+]#[C-]	10.7	8

1866	4{81,58,13}	COC1=CC=C(CNC2=C(N=C3C=NC=CN23)C2=NSN=C2)C=C1 c:12,14,22,25,t:2,4,8,10,19	Z8829498707	1{81}	Nc1cncn1	2{58}	O=Cc1cnsn1	3{13}	COc1ccc(C[N+]#[C-])cc1	7.4	8
1867	4{22,106,13}	COC1=CC=C(CNC2=C(N=C3C=CC(CI)=NN23)C2=C(OC)N=CC=N2)C=C1 c:12,15,20,24,26,29,t:2,4,8,10	Z8873684759	1{22}	Nc1ccc(Cl)nn1	2{106}	COc1cncn1C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	8.6	8
1868	4{475,212,22}	CC1=C(C=CC2=NC(=C(NC3COC3)N12)C1=NOC(=C1)C(F)F)C(F)F c:3,21,t:1,5,7,18	Z8873685492	1{475}	Cc1nc(N)ccc1C(F)F	2{212}	FC(F)c1cc(C=O)no1	3{22}	[C-]#[N+]C1CO C1	8.4	8
1869	4{378,427,28}	CCCNC1=C(N=C2N1C=CC=C2OCC1=CN=C(C=C1)C1=NOC2=C1COCC2 c:6,10,12,19,21,27,t:4,17,24	Z8855739093	1{378}	Nc1cccc1OCc2ccnc2	2{427}	O=Cc1noc2C COCc12	3{28}	CCC[N+]#[C-]]	8.6	8
1870	4{83,102,31}	CSCCNC1=C(N=C2C=CC(=CN12)P(C)(C)=O)C1=C(Br)C(C)=CC(CI)=N1 c:9,11,20,24,27,t:5,7	Z8878918762	1{83}	CP(=O)(C)c1ccc(N)nc1	2{102}	Cc1cc(Cl)nc(C=O)c1Br	3{31}	CSCC[N+]#[C-]]	10.3	8
1871	4{376,134,12}	COC1=NC(=NC=C1)C1=C(NCC2CCOC2)N2C=C(Cl)N=C(OC)C2=N1 c:4,6,9,28,t:2,20,23	Z8873685405	1{376}	COc1nc(Cl)cnc1N	2{134}	COc1cnc(C=O)n1	3{12}	[C-]#[N+]CC1C COC1	8.2	8
1872	4{50,817,18}	CC(C)(C)NC1=C(N=C2C=CC=C(N12)P(C)(C)=O)C1=C(Br)C=CC(OC(F)F)=C1 c:9,11,20,23,29,t:5,7	Z8873684848	1{50}	CP(=O)(C)c1cccc(N)n1	2{817}	FC(F)Oc1ccc(Br)c(C=O)c1	3{18}	CC(C)(C)[N+]#[C-]	10.1	8
1873	4{354,818,39}	CCOCCNC1=C(N=C2C=CC(=CN12)C(=O)OC)C1=C(F)C(F)=NC=C1 c:10,12,21,25,27,t:6,8	Z8855619720	1{354}	COC(=O)c1ccc(N)nc1	2{818}	Fc1cnc(C=O)c1F	3{39}	CCOCC[N+]#[C-]	7.8	8
1874	4{331,819,49}	CN(C)CCN(C)CC1=CN2C(C=C1)=NC(=C2N1)CC(F)(F)C1)C1=NN(C)C=C1Br c:12,14,16,31,t:8,27	Z8878918459	1{331}	Cl.Cl.Cl.CN(C)CCN(C)Cc1ccc(N)nc1	2{819}	Cn1cc(Br)c(C=O)n1	3{49}	FC1(F)CC(C1)[N+]#[C-]	10.3	8
1875	4{73,166,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC4=NC=CN4N23)C2=NC(=CS2)C2CC2)C=C1 c:12,16,25,33,t:2,5,8,10,14,23	Z8878918637	1{73}	Nc1ccc2nccn2n1	2{166}	O=Cc1nc(cs1)C2CC2	3{20}	COc1ccc([N+]#[C-])c(C)c1	8.4	7
1876	4{109,686,50}	CCNC(=O)C1=CC=C(C=C1)C1=C(NC2=CC3=C(OCCO3)C=C2)N2C(C=CC=C2S(N)(=O)=O)=N1 c:7,9,12,24,29,31,37,t:5,15,17	Z8873684650	1{109}	Cl.Nc1cccc(n1)S(=O)(=O)N	2{686}	CCNC(=O)c1ccc(C=O)cc1	3{50}	[C-]#[N+]c1ccc2OCCOc2c1	9.4	7
1877	4{79,262,9}	CCC1=NN(C)C(=C1Cl)C1=C(NC)N2C(C=NC=C2)=N1 c:6,10,16,18,21,t:2	Z8837933139	1{79}	Cc1cnc(N)n1	2{262}	CCc1nn(C)c(C=O)c1Cl	3{9}	C[N+]#[C-]	5.8	7

1878	4{400,820,22}	CCN(CC)CCC1=NC(=CS1)C1=C(NC2COC2)N2C=C(COC(C)C)C=CC2=N1 c:9,13,29,32,t:7,22	Z8878918616	1{400}	CC(C)OCc1ccc(N)nc1	2{820}	CCN(CC)CCc1nc(C=O)cs1	3{22}	[C-] #[N+]C1CO C1	7.9	7
1879	4{87,821,23}	COC(=O)CCC(NC1=C(N=C2C=C(C)C(Cl)=CN12)C1=CN=C(N=C1)C1CC1)C(=O)OC c:16,23,25,t:8,10,12,21	Z8873684681	1{87}	Cc1cc(N)nc1Cl	2{821}	O=Cc1cnc(nc1)C2CC2	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	8.5	7
1880	4{161,137,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC=NN23)C2=C(C)ON=C2C)C=C1 c:12,14,19,23,27,t:2,5,8,10	Z8878918648	1{161}	Ne1cccnn1	2{137}	Cc1noc(C)c1C=O	3{20}	COc1ccc([N+]#[C-])c(C)c1	6.3	7
1881	4{389,822,23}	COC(=O)CCC(NC1=C(N=C2N1C=C(C)C=C2C)C1=NN(CC(F)(F)F)N=C1)C(=O)OC c:10,17,29,t:8,14,21	Z8878918365	1{389}	Cc1cnc(N)c(C)c1	2{822}	FC(F)(F)Cn1ncc(C=O)n1	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	8.1	6
1882	4{85,823,35}	CSCCCNC1=C(N=C2C=C(C=C(C)N12)C#N)C1=NN(C)C2=C1C=CC=N2 c:10,24,27,29,t:6,8,12,20	Z8873684904	1{85}	Cc1cc(C#N)cc(N)n1	2{823}	Cn1nc(C=O)c2cccnc12	3{35}	CSCCC[N+]#[C-]	6.7	6
1883	4{375,242,21}	CC(C)OC1=CN=CC2=NC(=C(NCC3CC3)N12)C1=CN2N=CC(C#N)=C2N=C1 c:6,24,28,31,t:4,8,10,21	Z8873684892	1{375}	CC(C)Oe1cnc(N)n1	2{242}	O=Cc1cnc2c(C#N)enn2c1	3{21}	[C-] #[N+]CC1C C1	6.6	6
1884	4{161,824,6}	CCOC(=O)CCCN1=C(N=C2C=CC=NN12)C1=NC(Br)=CC=C1 c:13,15,23,25,t:9,11,20	Z8873684923	1{161}	Ne1cccnn1	2{824}	Br1c1ccc(C=O)n1	3{6}	CCOC(=O)C CC[N+]#[C-]	6.8	6
1885	4{146,104,46}	CC(=C)CNC1=C(N=C2C=CC(=CN12)S(C)(=O)=O)C1=NC(C)=CO1 c:9,11,23,t:5,7,20	Z8873684784	1{146}	CS(=O)(=O)c1ccc(N)nc1	2{104}	Cc1coc(C=O)n1	3{46}	CC(=C)C[N+]#[C-]	5.8	6
1886	4{50,825,18}	CC(C)C1=NC=C(N1C)C1=C(NC(C)(C)C)N2C(C=CC=C2P(C)(C)=O)=N1 c:5,10,19,21,27,t:3	Z8878918793	1{50}	CP(=O)(C)c1ccc(N)n1	2{825}	CC(C)c1ncc(C=O)n1C	3{18}	CC(C)(C)[N+]#[C-]	6.4	6
1887	4{46,274,9}	CNC1=C(CC2(CCOCC2)C#N)N=C2C=CC=C N12 c:2,16,18,t:14	Z8878918469	1{46}	Ne1cccnn1	2{274}	O=CCC1(CC OCC1)C#N	3{9}	C[N+]#[C-]	4.5	6
1888	4{395,101,7}	CC1=CC(=NN2C(NC3CCOCC3)=C(N=C12)C1=C(CO)C=CS1)C(F)(F)F c:3,14,20,24,t:1,16	Z8878918535	1{395}	Cc1cc(mnc1N)C(F)(F)F	2{101}	OCc1ccc1C=O	3{7}	[C-] #[N+]C1CC OCC1	6.6	6
1889	4{79,826,9}	CNC1=C(N=C2C=NC=C(C)N12)C1=NC(Cl)=CS1 c:6,17,t:2,4,8,14	Z8878918870	1{79}	Cc1cnc(N)n1	2{826}	Clc1csc(C=O)n1	3{9}	C[N+]#[C-]	4.5	6
1890	4{54,827,37}	CCN(CCO)C1=CC(C)=C(C=C1)C1=C(NC2C(C(C2)C(=O)OC)N2C=C(C=CC2=N1)C(=O)N(C)C c:9,11,14,27,29,32,t:6	Z8854581161	1{54}	Cl.CN(C)C(=O)c1ccc(N)nc1	2{827}	CCN(CCO)c1ccc(C=O)c(C)c1	3{37}	COC(=O)C1 CC(C1)[N+]#[C-]	7.8	6

1891	4{91,828,26}	CC(N1C(=O)C2=C(C=CC=C2)C1=O)C1=C(NCC2=CC=C(F)C=C2)N2C=C(C=CC2=N1)C(N)=O c:7,9,15,24,28,30,33,t:5,19,21	Z8878918519	1{91}	NC(=O)c1ccc(N)nc1	2{828}	CC(C=O)N1C(=O)c2cccc2C1=O	3{26}	Fc1ccc(C[N+][C-])cc1	7.2	6
1892	4{73,307,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC4=NC=CN4N23)C2=CN=C(Cl)N2C)C=C1 c:12,16,31,t:2,5,8,10,14,23,25	Z8855739267	1{73}	Nc1ccc2nccn2n1	2{307}	Cn1c(Cl)ncc1C=O	3{20}	COc1ccc([N+][C-])c(C)c1	6.0	5
1893	4{73,829,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC4=NC=CN4N23)C2=CC(Cl)=C(OC)N=C2)C=C1 c:12,16,30,33,t:2,5,8,10,14,23,26	Z8878918518	1{73}	Nc1ccc2nccn2n1	2{829}	COc1ncc(C=O)cc1Cl	3{20}	COc1ccc([N+][C-])c(C)c1	6.4	5
1894	4{331,741,49}	CN(C)CCN(C)CC1=CN2C(C=C1)=NC(=C2N1)CC(F)(F)C1)C1=CC=C(C=C1)N1C=NC=N1 c:12,14,16,29,31,35,37,t:8,27	Z8873684908	1{331}	Cl.C1.C1.CN(C)CCN(C)C1ccc(N)nc1	2{741}	O=Cc1ccc(cc1)n2cncn2	3{49}	FC1(F)CC(C1)[N+][C-]	7.0	5
1895	4{141,209,32}	CC(=O)NC1=CC2=NC(=C(NC3CCC3)N2C=C1)C1=NN=C2CCCCN12 c:18,t:4,6,8,21,23	Z8873684831	1{141}	CC(=O)Nc1ccnc(N)c1	2{209}	O=Cc1nnc2CCCCn12	3{32}	[C-][N+]C1CC1	5.3	5
1896	4{99,241,34}	CN1N=CC(Br)=C1C1=C(NCC2CCCO2)N2C=C(C=CC2=N1)S(N)(=O)=O c:2,5,8,19,21,24	Z8829498789	1{99}	Nc1ccc(en1)S(=O)(=O)N	2{241}	Cn1ncc(Br)c1C=O	3{34}	[C-][N+]CC1CCCCO1	6.2	5
1897	4{137,94,13}	COC1=CC=C(CNC2=C(N=C3C=CC(C)=NN23)C2=NC=CN=C2)C=C1 c:12,15,22,24,27,t:2,4,8,10,20	Z8873685365	1{137}	Cc1ccc(N)nn1	2{94}	O=Cc1cncn1	3{13}	COc1ccc(C[N+][C-])cc1	4.5	5
1898	4{73,307,13}	COC1=CC=C(CNC2=C(N=C3C=CC4=NC=CN4N23)C2=CN=C(Cl)N2C)C=C1 c:12,16,31,t:2,4,8,10,14,23,25	Z8837933161	1{73}	Nc1ccc2nccn2n1	2{307}	Cn1c(Cl)ncc1C=O	3{13}	COc1ccc(C[N+][C-])cc1	4.7	4
1899	4{22,170,9}	CCN1N=NC(=N1)C1=C(NC)N2N=C(Cl)C=C2=N1 c:3,5,8,16,19,t:13	Z8846491739	1{22}	Nc1ccc(Cl)nn1	2{170}	CCn1nnc(C=O)n1	3{9}	C[N+][C-]	3.1	4
1900	4{81,170,9}	CCN1N=NC(=N1)C1=C(NC)N2C=CN=CC2=N1 c:3,5,8,13,15,18	Z8855739229	1{81}	Nc1cncn1	2{170}	CCn1nnc(C=O)n1	3{9}	C[N+][C-]	2.7	4
1901	4{389,572,23}	COC(=O)CCC(NC1=C(N=C2N1C=C(C)C=C2)C)C1=NC(=CC(OC)=C1)C(=O)OC)C(=O)OC c:10,17,23,27,t:8,14,21	Z8878918405	1{389}	Cc1cnc(N)c(C)c1	2{572}	COC(=O)c1cc(OC)cc(C=O)n1	3{23}	COC(=O)CC(C[N+][C-])C(=O)OC	5.3	4
1902	4{476,279,47}	CC(C)NC1=C(N=C2C=CC=C(CC3=NC=CC=C3)N12)[C@@H]1CCCO[C@H]1C1=NC=CN1C &1:20,25,r,c:8,15,17,32,t:4,6,10,13,30	Z8873685372	1{476}	Nc1cccc(Cc2ccccn2)n1	2{279}	Cn1cnc1[C@@H]2OCC[C@H]2C=O &1:6,11,r	3{47}	CC(C)[N+][C-]	4.7	4

1903	4{187,427,46}	CC(=C)CNC1=C(N=C2C=C(C#N)C(Cl)=CN12)C1=NOC2=C1COCC2 c:14,22,t:5,7,9,19	Z8873684945	1{187}	Nc1cc(C#N)c(Cl)cn1	2{427}	O=Cc1noc2COCc12	3{46}	CC(=C)C[N+]#[C-]	3.9	4
1904	4{161,116,13}	COC1=CC=C(CNC2=C(N=C3C=CC=NN23)C2=CN(CCC=C)N=N2)C=C1 c:12,14,26,29,t:2,4,8,10,19	Z8837933164	1{161}	Nc1cccn1	2{116}	C=CCcn1cc(C=O)nn1	3{13}	COc1ccc(C[N+]#[C-])cc1	3.7	4
1905	4{380,830,5}	COCCNC1=C(N=C2N1C=C(Cl)N=C2C)C1=NC(=CC=C1)C(=O)OC c:8,15,21,23,t:6,12,19	Z8878918321	1{380}	Cc1nc(Cl)cn1N	2{830}	COC(=O)c1ccc(C=O)n1	3{5}	COCCC[N+]#[C-]	3.4	3
1906	4{78,85,74}	CC1=CN2N3C(NC4CCCN(C4)C(=O)OC(C)(C)C)=C(N=C3C=C(C)C2=N1)C1=CN=NS1 c:20,22,29,34,t:1,25,32	Z8873684642	1{78}	Cc1cn2nc(N)cc(C)c2n1	2{85}	O=Cc1cnns1	3{74}	CC(C)(C)OC(=O)N1CCCC[C@H](C1)[N+]#[C-]	4.0	3
1907	4{477,235,23}	COC(=O)CCC(NC1=C(N=C2C=C(F)C(Br)=CN12)C1=CSC(=C1)C#N)C(=O)OC c:16,24,t:8,10,12,21	Z8878918562	1{477}	Nc1cc(F)c(Br)cn1	2{235}	O=Cc1csc(C#N)c1	3{23}	COC(=O)CC(C[N+]#[C-])C(=O)OC	4.0	3
1908	4{79,485,9}	CNC1=C(N=C2C=NC=C(C)N12)C1=NOC2=C1CCC2 c:6,17,t:2,4,8,14	Z8873685257	1{79}	Cc1cncc(N)n1	2{485}	O=Cc1noc2C CCc12	3{9}	C[N+]#[C-]	2.0	3
1909	4{73,137,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC4=NC=CN4N23)C2=C(C)ON=C2C)C=C1 c:12,16,23,27,31,t:2,5,8,10,14	Z8878918340	1{73}	Nc1ccc2nccn2n1	2{137}	Cc1noc(C)c1C=O	3{20}	COc1ccc([N+]#[C-])c(C)c1	2.8	3
1910	4{87,235,23}	COC(=O)CCC(NC1=C(N=C2C=C(C)C(Cl)=CN12)C1=CSC(=C1)C#N)C(=O)OC c:16,24,t:8,10,12,21	Z8873685450	1{87}	Cc1cc(N)nc1Cl	2{235}	O=Cc1csc(C#N)c1	3{23}	COC(=O)CC(C[N+]#[C-])C(=O)OC	3.2	3
1911	4{164,831,10}	CN(C)CC1=CC2=NC(C3=CN=C(S3)C3CN(C3)C(=O)OC(C)(C)C)=C(NC3CCOC3)N2C=C1 c:11,37,t:4,6,9,26	Z8878918533	1{164}	CN(C)Cc1cnc(N)c1	2{831}	CC(C)(C)OC(=O)N1CC(C1)c2ncc(C=O)s2	3{10}	[C-]#[N+]C1CCOC1	3.4	3
1912	4{209,260,14}	COCCNC1=C(N=C2N1C=CC=C2N1CCCCC1)C1=NOC(C)=C1 c:7,11,13,27,t:5,23	Z8878918510	1{209}	Nc1ncccc1N2CCCCC2	2{260}	Cc1cc(C=O)no1	3{14}	COCC[N+]#[C-]	2.4	2
1913	4{369,101,7}	OCC1=C(SC=C1)C1=C(NC2CCOCC2)N2C=C(C=CC2=N1)C(F)C(F)(F)F c:5,8,19,21,24,t:2	Z8873684604	1{369}	Cl.Nc1ccc(cn1)C(F)C(F)(F)F	2{101}	OCc1ccsc1C=O	3{7}	[C-]#[N+]C1CCOCC1	2.8	2
1914	4{141,832,22}	CC1OC2=C(NC1=O)C=C(C=C2)C1=C(NC2COC2)N2C=CC(NC(C)=O)=CC2=N1 c:3,9,11,14,23,29,32	Z8878918783	1{141}	CC(=O)Nc1ccnc(N)c1	2{832}	CC1Oe2ccc(C=O)cc2NC1=O	3{22}	[C-]#[N+]C1CO C1	2.8	2

1915	4{61,756,23}	CCC1=CC=CC2=NC(C3=CC(=CO3)S(C)(=O)=O)=C(NC(CCC(=O)OC)C(=O)OC)N12 c:4,11,t:2,6,9,18	Z8873685377	1{61}	CCc1cccc(N)n1	2{756}	CS(=O)(=O)c1coc(C=O)c1	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	2.8	2
1916	4{478,769,21}	CN1N=CN=C1C1=C(NCC2CC2)N2C(C=C(Br)C=C2C)=N1 c:2,4,7,20,23,t:17	Z8873684620	1{478}	Cc1cc(Br)cc(N)n1	2{769}	Cn1ncnc1C=O	3{21}	[C-] #[N+]CC1C C1	2.0	2
1917	4{479,408,47}	CC(C)NC1=C(CCN2CCOC2=O)N=C2C=CC(CI)=C(Br)N12 c:4,17,t:15,20	Z8878918400	1{479}	Nc1ccc(Cl)c(Br)n1	2{408}	O=CCCN1C COC1=O	3{47}	CC(C)[N+]#[C-]	1.8	2
1918	4{113,260,6}	CCOC(=O)CCCN1=C(N=C2N1C=CC=C2N1CCOCC1)C1=NOC(C)=C1 c:11,15,17,31,t:9,27	Z8873685448	1{113}	Nc1ncccc1 N2CCOCC2	2{260}	Cc1cc(C=O) no1	3{6}	CCOC(=O)C CC[N+]#[C-]	1.8	2
1919	4{395,439,7}	COC1=C(C=CC(=C1)C1=C(NC2CCOCC2)N2N=C(C=C(C)C2=N1)C(F)(F)F)S(C)(=O)=O c:4,6,9,20,26,t:2,22	Z8878918392	1{395}	Cc1cc(nnc1N)C(F)(F)F	2{439}	COc1cc(C=O))ccc1S(=O)(=O)C	3{7}	[C-] #[N+]C1CC OCC1	2.0	2
1920	4{187,413,12}	C1C1=CN2C(NCC3CCOC3)=C(N=C2C=C1C#N)C1=CN=C(S1)C1=CC=NC=C1 c:12,14,17,24,30,32,t:1,22,28	Z8878918513	1{187}	Nc1cc(C#N)c(Cl)cn1	2{413}	O=Cc1nc(s1)c2ccncc2	3{12}	[C-] #[N+]CC1C COC1	1.6	1
1921	4{327,833,34}	COC(=O)C1=C(F)C2=NC(C3=CC=C(S3)C#N)=C(NCC3CCCO3)N2C=C1 c:4,12,29,t:7,10,17	Z8878918899	1{327}	COC(=O)c1ccnc(N)c1F	2{833}	O=Cc1ccc(C#N)s1	3{34}	[C-] #[N+]CC1C CCO1	0.0	0
1922	4{480,168,22}	CC1=C(C)C(CI)=NN2C(NC3COC3)=C(N=C12)C1=NOC=C1 c:1,5,14,23,t:16,20	Z8878918862	1{480}	Cc1c(C)c(Cl)nnc1N	2{168}	O=Cc1ccon1	3{22}	[C-] #[N+]C1CO C1	0.0	0
1923	4{91,472,18}	COC(=O)C1=CC2=C(C=NN2C=C1)C1=C(NC(C)(C)C)N2C=C(C=CC2=N1)C(N)=O c:8,12,15,23,25,28,t:4,6	Z8878918837	1{91}	NC(=O)c1ccc(N)nc1	2{472}	COC(=O)c1c cn2ncc(C=O) c2c1	3{18}	CC(C)(C)[N+]#[C-]	0.0	0
1924	4{421,488,37}	COC(=O)C1CC(C1)NC1=C(N=C2C=CC(C(=O)OC)=C(CI)N12)C1=CC2=C(NC(=O)CC2)N=C1 c:14,36,t:10,12,20,26,28	Z8878918610	1{421}	COC(=O)c1ccc(N)nc1C1	2{488}	O=Cc1cnc2N C(=O)CCc2c1	3{37}	COC(=O)C1 CC(C1)[N+]#[C-]	0.0	0
1925	4{218,649,10}	CN1N=C(C=C1C1=C(NC2CCOC2)N2N=C(C=CC2=N1)C(C)(C)C)C(F)F c:2,4,7,17,19,22	Z8878918586	1{218}	CC(C)(C)c1ccc(N)mn1	2{649}	Cn1nc(cc1C=O)C(F)F	3{10}	[C-] #[N+]C1CC OC1	0.0	0
1926	4{94,21,60}	COC(=O)C1=CC(NC2=C(N=C3C=CC(F)=NN23)C2=CC3=NC=NN3C=C2)=CC=C1 c:12,15,24,28,30,32,t:4,8,10,20,22	Z8878918540	1{94}	Nc1ccc(F)nn1	2{21}	O=Cc1ccn2n cnc2c1	3{60}	COC(=O)c1c ccc([N+]#[C-])c1	0.0	0
1927	4{123,289,22}	COC1=C(OCC#C)C=C(C=C1)C1=C(NC2COC2)N2C=CC(OCCO)=CC2=N1 c:2,8,10,13,22,28,31	Z8878918484	1{123}	Cl.Nc1cc(OCCO)ccn1	2{289}	COc1ccc(C=O)cc1OCC#C	3{22}	[C-] #[N+]C1CO C1	0.0	0

1928	4{457,119,22}	CCOC(=O)C1=NN=C(N1)C1=C(NC2COC2)N2C=C(Br)C(=CC2=N1)C(F)F c:7,11,23,26,t:5,20	Z8878918474	1{457}	Nc1cc(C(F)F)c(Br)cn1	2{119}	CCOC(=O)c1nnc(C=O)[nH]1	3{22}	[C-] #[N+]C1CO C1	0.0	0
1929	4{267,834,5}	COCCNC1=C(CC2CCC(C)(C)O2)N=C2C=C C=C(C#C)N12 c:6,19,t:17,21	Z8878918458	1{267}	Nc1cccc(C#C)n1	2{834}	CC1(C)CCC(C=O)O1	3{5}	COCC[N+] #[C-]	0.0	0
1930	4{185,799,69}	COC1=C(NC2=C(N=C3C=CC(=C(C)N23)S(C)(=O)=O)C2=NN=C(C)C=C2)C=CC=C1 c:2,9,26,29,31,t:5,7,11,21,23	Z8878918417	1{185}	Cc1nc(N)ccc1S(=O)(=O)C	2{799}	Cc1ccc(C=O)nn1	3{69}	COc1cccc1[N+]#[C-]	0.0	0
1931	4{267,383,5}	COCCNC1=C(N=C2C=CC=C(C#C)N12)C1=NC=C(C)C=C1 c:10,24,t:6,8,12,19,21	Z8878918371	1{267}	Nc1cccc(C#C)n1	2{383}	Cc1ccc(C=O)nc1	3{5}	COCC[N+] #[C-]	0.0	0
1932	4{47,179,6}	CCOC(=O)CCNC1=C(N=C2C=C(C=CN12)S(N)(=O)=O)C1=CC=C(OC2CCOC2)C=C1 c:13,15,35,t:9,11,24,26	Z8873684752	1{47}	Cl.Nc1cc(ccn1)S(=O)(=O)N	2{179}	O=Cc1ccc(O C2CCOC2)c c1	3{6}	CCOC(=O)C CC[N+]#[C-]	0.0	0
1933	4{28,189,26}	FC1=CC=C(CNC2=C(N=C3C=C(C=CN23)C2=NOC=N2)C2=CN(N=N2)C2CCOCC2)C=C1 c:11,13,21,27,37,t:1,3,7,9,18,24	Z8873685403	1{28}	Cl.Nc1cc(ccn1)c2ncon2	2{189}	O=Cc1cn(nn1)C2CCOCC2	3{26}	Fc1ccc(C[N+] #[C-])cc1	0.0	0
1934	4{42,835,14}	COCCNC1=C(N=C2C=CC(SC)=CN12)C1=CS C(=N1)N(C(C)=O)C1=CC=CC=C1 c:9,13,21,30,32,t:5,7,18,28	Z8873685375	1{42}	CSc1ccc(N)nc1	2{835}	CC(=O)N(c1nc(C=O)cs1)c2cccc2	3{14}	COCC[N+]#[C-]	0.0	0
1935	4{172,403,29}	CCOC(=O)CCNC1=C(N=C2N1C=CC1=C2CCO1)C1=CN=C(C1)N1 c:10,14,16,t:8,23,25	Z8873684921	1{172}	Nc1nccc2OCCc21	2{403}	Clc1ncc(C=O)[nH]1	3{29}	CCOC(=O)C C[N+]#[C-]	0.0	0
1936	4{38,170,9}	CCN1N=NC(=N1)C1=C(NC)N2C=CC(=CC2=N1)C#N c:3,5,8,13,15,18	Z8873684882	1{38}	Nc1cc(C#N)ccn1	2{170}	CCn1nnc(C=O)n1	3{9}	C[N+]#[C-]	0.0	0
1937	4{184,28,26}	NC(=S)C1=CN2C(NCC3=CC=C(F)C=C3)=C(N=C2C=C1)C1=CN(N=C1)C1CCS(=O)(=O)C1 c:14,16,18,21,27,t:3,9,11,24	Z8873684871	1{184}	NC(=S)c1ccc(N)nc1	2{28}	O=Cc1cnn(c1)C2CCS(=O)(=O)C2	3{26}	Fc1ccc(C[N+] #[C-])cc1	0.0	0
1938	4{28,439,18}	COC1=C(C=CC(=C1)C1=C(NC(C)(C)C)N2C=CC(=CC2=N1)C1=NOC=N1)S(C)(=O)=O c:4,6,9,17,19,22,28,t:2,25	Z8873684857	1{28}	Cl.Nc1cc(ccn1)c2ncon2	2{439}	COc1cc(C=O)ccc1S(=O)(=O)C	3{18}	CC(C)(C)[N+] #[C-]	0.0	0
1939	4{73,98,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC4=NC=CN4N23)C2=NC=C(OC)N=C2)C=C1 c:12,16,29,32,t:2,5,8,10,14,23,25	Z8873684847	1{73}	Nc1ccc2nccn2n1	2{98}	COc1cnc(C=O)cn1	3{20}	COc1ccc([N+] #[C-])c(C)c1	0.0	0
1940	4{209,377,14}	COCCNC1=C(N=C2N1C=CC=C2N1CCCC1)C1=NN=C1C c:7,11,13,26,t:5,23	Z8873684812	1{209}	Nc1ncccc1N2CCCC2	2{377}	Cl.Cc1c[nH]nc1C=O	3{14}	COCC[N+]#[C-]	0.0	0

1941	4{101,62,6}	CCOC(=O)CCNC1=C(N=C2N1C=C(CO)C=C2C1)C1CC1CCOCC1 c:11,19,t:9,15	Z8829498700	1{101}	Ne1ncc(CO)cc1Cl	2{62}	O=CC1CC21CCOCC2	3{6}	CCOC(=O)C CC[N+]#[C-]	0.0	0
1942	4{111,119,15}	CCNC1=C(N=C2N1C=C(C=C2C)C(=O)OC)C1=NN=C(N1)C(=O)OCC c:5,9,11,21,t:3,19	Z8878918878	1{111}	COC(=O)c1cnc(N)c(C)c1	2{119}	CCOC(=O)c1nnc(C=O)[nH]1	3{15}	CC[N+]#[C-]	0.0	0
1943	4{225,588,60}	COC(=O)C1=CC(NC2=C(N=C3C=C(C1)C=N23)C2=CN(C)N=C2C)=CC=C1 c:15,24,27,29,t:4,8,10,12,20	Z8878918841	1{225}	Ne1cc(Cl)cnm1	2{588}	Cc1nm(C)cc1C=O	3{60}	COC(=O)c1cccc([N+]#[C-])c1	0.0	0
1944	4{146,766,51}	CC1CC1C1=C(NCCNC(=O)OC(C)(C)C)N2C=C(C=CC2=N1)S(C)(=O)O c:5,19,21,24	Z8878918806	1{146}	CS(=O)(=O)c1ccc(N)nc1	2{766}	CC1CC1C=O	3{51}	CC(C)(C)OC(=O)NCC[N+]#[C-]	0.0	0
1945	4{292,212,35}	CCOC1=CN=CC2=NC(=C(NCCCSC)N12)C1=NOC(=C1)C(F)F c:5,23,t:3,7,9,20	Z8878918799	1{292}	CCOc1cncc(N)n1	2{212}	FC(F)c1cc(C=O)no1	3{35}	CSCCC[N+]#[C-]	0.0	0
1946	4{301,735,22}	COC(=O)C1=CN=C(S1)C1=C(NC2COC2)N2C=C(Cl)C=C(F)C2=N1 c:6,10,26,t:4,19,22	Z8878918778	1{301}	Ne1ncc(Cl)cc1F	2{735}	COC(=O)c1cnc(C=O)s1	3{22}	[C-]#[N+]C1CO C1	0.0	0
1947	4{73,558,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC4=NC=CN4N23)C2=CC(Cl)=NC(C)=C2)C=C1 c:12,16,26,29,32,t:2,5,8,10,14,23	Z8878918591	1{73}	Ne1ccc2nccn2n1	2{558}	Cc1cc(C=O)cc(Cl)n1	3{20}	COc1ccc([N+]#[C-])c(C)c1	0.0	0
1948	4{394,395,10}	CC(C)(C)OC(=O)N[C@H]1C[C@@H](C1)C1=C(NC2CCOC2)N2C(C=CC(C=C)=C2F)=N1 r,c:13,24,28,31	Z8878918567	1{394}	Ne1ccc(C=C)c(F)n1	2{395}	CC(C)(C)OC(=O)N[C@H]1C[C@@H](C1)C=O	3{10}	[C-]#[N+]C1CCOC1	0.0	0
1949	4{399,216,15}	CCNC1=C(N=C2C=CC(OC(C)C)=NN12)C1=CN=C(S1)C(=O)OC c:7,13,20,t:3,5,18	Z8878918443	1{399}	CC(C)Oc1ccc(N)nm1	2{216}	COC(=O)c1ncc(C=O)s1	3{15}	CC[N+]#[C-]	0.0	0
1950	4{150,212,32}	FC(F)C1=CC(=NO1)C1=C(NC2CCC2)N2C=C(C(=CC2=N1)C1CCOC1 c:5,9,18,20,23,t:3	Z8878918415	1{150}	Ne1cc(cen1)C2CCOC2	2{212}	FC(F)c1cc(C=O)no1	3{32}	[C-]#[N+]C1CC C1	0.0	0
1951	4{78,134,77}	COC1=NC(=NC=C1)C1=C(NC2CCCN(C2)C(=O)OC(C)(C)C)N2N3C=C(C)N=C3C(C)=CC2=N1 c:4,6,9,31,35,38,t:2,28	Z8878918312	1{78}	Cc1en2nc(N)cc(C)c2n1	2{134}	COc1ccnc(C=O)n1	3{77}	CC(C)(C)OC(=O)N1CCC[C@@H](C1)[N+]#[C-]	0.0	0
1952	4{78,836,28}	CCCNC1=C(N=C2C=C(C)C3=NC(C)=CN3N12)C1=C(Cl)NN=C1CC c:14,21,25,t:4,6,8,11	Z8873684738	1{78}	Cc1en2nc(N)cc(C)c2n1	2{836}	CCc1n[nH]c(Cl)c1C=O	3{28}	CCC[N+]#[C-]	0.0	0

1953	4{59,837,49}	CC(C)(C)OC(=O)N1C=NC(=C1)C1=C(NC2C C(F)(F)C2)N2C=C(CN3CCOCC3)C=CC2=N1 c:8,10,13,34,37,t:24	Z8873684673	1{59}	Nc1ccc(CN 2CCOCC2) cn1	2{837}	CC(C)(C)OC (=O)n1cnc(C =O)c1	3{49}	FC1(F)CC(C 1)[N+]#[C-]	0.0	0
1954	4{73,838,13}	COC1=CC=C(CNC2=C(N=C3C=CC4=NC=C N4N23)C2=CN=C(N=C2)C(C)(C)C=C1 c:12,16,25,27,34,t:2,4,8,10,14,23	Z8873685389	1{73}	Nc1ccc2ncc n2n1	2{838}	CC(C)(C)c1n cc(C=O)cn1	3{13}	COc1ccc(C[N+]#[C-])cc1	0.0	0
1955	4{171,123,22}	CC1=NC=C(N=C1)C1=C(NC2COC2)N2C=C C(=CC2=N1)N1C=CN=C1 c:3,5,8,17,19,22,26,28,t:1	Z8873685373	1{171}	Nc1cc(cen1)n2ccnc2	2{123}	Cc1cnc(C=O)cn1	3{22}	[C-]#[N+]C1CO C1	0.0	0
1956	4{81,40,9}	CNC1=C(N=C2C=NC=CN12)C1=NC(CO)=C S1 c:6,8,17,t:2,4,13	Z8873685259	1{81}	Nc1cncn1	2{40}	OCc1csc(C= O)n1	3{9}	C[N+]#[C-]	0.0	0
1957	4{49,757,13}	CCCN1N=CN=C1C1=C(NCC2=CC=C(OC)C= C2)N2C(C=CC=C2CO)=N1 c:4,6,9,19,24,26,30,t:13,15	Z8873684630	1{49}	Nc1cccc(C O)n1	2{757}	CCCN1cnc1 C=O	3{13}	COc1ccc(C[N+]#[C-])cc1	0.0	0
1958	4{81,240,9}	CCN1N=C(Br)C=C1C1=C(NC)N2C=CN=CC2 =N1 c:6,9,14,16,19,t:3	Z8854581135	1{81}	Nc1cncn1	2{240}	CCN1nc(Br)c c1C=O	3{9}	C[N+]#[C-]	0.0	0
1959	4{481,654,69}	COC(=O)C1=C(Br)N2C(NC3=C(OC)C=CC=C 3)=C(CCC3=CN=CO3)N=C2C=C1 c:4,10,14,16,24,28,31,t:18,22	Z8855619774	1{481}	COC(=O)c1 ccc(N)nc1B r	2{654}	O=CCCc1cn co1	3{69}	COc1cccc1[N+]#[C-]	0.0	0
1960	4{172,550,29}	CCOC(=O)CCNC1=C(N=C2N1C=CC1=C2CC O1)C1=NC(Br)=NN1C c:10,14,16,26,t:8,23	Z8878918905	1{172}	Nc1nccc2O CCc21	2{550}	Cn1nc(Br)nc 1C=O	3{29}	CCOC(=O)C C[N+]#[C-]	0.0	0
1961	4{482,131,22}	COC(=O)C1=C(C)C=CC2=NC(C3=NC(=NN3) C3CC3)=C(NC3COC3)N12 c:4,7,14,t:9,12,21	Z8878918858	1{482}	COC(=O)c1 nc(N)ccc1C	2{131}	O=Cc1nc(n[n H]1)C2CC2	3{22}	[C-]#[N+]C1CO C1	0.0	0
1962	4{375,516,46}	CC(C)OC1=CN=CC2=NC(C3=NN(C)C(=N3) C3CC3)=C(NCC(C)=C)N12 c:6,15,t:4,8,11,21	Z8878918857	1{375}	CC(C)Oc1c ncc(N)n1	2{516}	Cn1nc(C=O) nc1C2CC2	3{46}	CC(=C)C[N+] #[C-]	0.0	0
1963	4{288,350,28}	CCCN1C1=C(N=C2C=C(NC(=O)OC(C)(C)C) =CN12)C1C2CCOCC12 c:18,t:4,6,8	Z8878918619	1{288}	CC(C)(C)O C(=O)Nc1c cnc(N)c1	2{350}	O=CC1C2C COCC12	3{28}	CCC[N+]#[C-]	0.0	0
1964	4{187,342,12}	C1C1=CN2C(NCC3CCOC3)=C(N=C2C=C1C# N)C1=CN=C(S1)C1=NC=CC=C1 c:12,14,17,24,30,32,t:1,22,28	Z8878918585	1{187}	Nc1cc(C#N)c(Cl)cn1	2{342}	O=Cc1cnc(s1)c2cccn2	3{12}	[C-]#[N+]CC1C COC1	0.0	0
1965	4{353,306,15}	CCNC1=C(N=C2C=CC(NS(C)(=O)=O)=CN12)C1=CC=C(C=C1)N(C)CCO c:7,14,21,23,t:3,5,19	Z8878918483	1{353}	Cl.CS(=O)(=O)Nc1ccc(N)nc1	2{306}	CN(CCO)c1c cc(C=O)cc1	3{15}	CC[N+]#[C-]	0.0	0

1966	4{261,148,28}	CCCNC1=C(N=C2C=CC(=CN12)N1CCC(CC1)N(C)C)C1=C(OC)N(C)N=C1C c:8,10,25,31,t:4,6	Z8878918402	1{261}	CN(C)C1C CN(CC1)c2 ccc(N)nc2	2{148}	COc1c(C=O) c(C)nn1C	3{28}	CCC[N+]#[C-]]	0.0	0
1967	4{79,197,13}	COC(=O)C1=CC(=NN1C)C1=C(NCC2=CC=C(OC)C=C2)N2C(C=NC=C2C)=N1 c:6,11,21,26,28,31,t:4,15,17	Z8878918378	1{79}	Cc1cncc(N) n1	2{197}	COC(=O)c1c c(C=O)nn1C	3{13}	COc1ccc(C[N+]#[C-])cc1	0.0	0
1968	4{78,839,28}	CCCNC1=C(N=C2C=C(C)C3=NC(C)=CN3N12)C1=CN(C=N1)C1=CC=CC=C1 c:14,24,29,31,t:4,6,8,11,21,27	Z8873684735	1{78}	Cc1cn2nc(N) cc(C)c2n1	2{839}	O=Cc1cn(cn 1)c2ccccc2	3{28}	CCC[N+]#[C-]]	0.0	0
1969	4{73,161,13}	CCN1C=NC=C1C1=C(NCC2=CC=C(OC)C=C2)N2N3C=CN=C3C=CC2=N1 c:3,5,8,18,23,25,28,31,t:12,14	Z8873684734	1{73}	Nc1ccc2ncc n2n1	2{161}	CCn1cncc1C =O	3{13}	COc1ccc(C[N+]#[C-])cc1	0.0	0
1970	4{397,424,5}	COCCNC1=C(N=C2N1C=CC(C)=C2C)C1=NN(C)C(=N1)C(F)(F)F c:8,12,15,23,t:6,19	Z8873684721	1{397}	Cl.Cc1cncc(N)c1C	2{424}	Cn1nc(C=O) nc1C(F)(F)F	3{5}	COCCC[N+]# #[C-]	0.0	0
1971	4{91,840,7}	NC(=O)C1=CN2C(C=C1)=NC(C1=CN(N=C1)C1=CC=C(C=C1)[N+])([O-])=O=C2NC1CCOCC1 c:7,9,15,20,22,27,t:3,12,18	Z8873685479	1{91}	NC(=O)c1c cc(N)nc1	2{840}	[O-]][N+](=O)c1 ccc(cc1)n2cc (C=O)cn2	3{7}	[C-]]#[N+]C1CC OCC1	0.0	0
1972	4{22,262,9}	CCC1=NN(C)C(=C1C1)C1=C(NC)N2N=C(Cl)C=CC2=N1 c:6,10,18,21,t:2,15	Z8873685395	1{22}	Nc1ccc(Cl) nn1	2{262}	CCc1nn(C)c(C=O)c1Cl	3{9}	C[N+]#[C-]	0.0	0
1973	4{184,792,14}	COCCNC1=C(N=C2C=CC(=CN12)C(N)=S)C1=NN(C)N=C1 c:9,11,23,t:5,7,19	Z8873685314	1{184}	NC(=S)c1cc c(N)nc1	2{792}	Cn1ncc(C=O) n1	3{14}	COCC[N+]#[C-]	0.0	0
1974	4{62,184,6}	CCOC(=O)CCCNC1=C(N=C2C=C(CO)C=CN12)C1CC1 c:17,t:9,11,13	Z8873685245	1{62}	Nc1cc(CO)c cn1	2{184}	O=CC1CC1	3{6}	CCOC(=O)C CC[N+]#[C-]	0.0	0
1975	4{436,572,23}	CCC1=CC2=NC(=C(NC(CCC(=O)OC)C(=O)OC)N2C=C1)C1=NC(=CC(OC)=C1)C(=O)OC c:22,27,31,t:2,4,6,25	Z8873684935	1{436}	CCc1cncc(N)c1	2{572}	COC(=O)c1c c(OC)cc(C= O)n1	3{23}	COC(=O)CC C([N+]#[C-]])C(=O)OC	0.0	0
1976	4{103,841,5}	COCCNC1=C(N=C2C=NC=C(CO)N12)C1=C(Br)C(=NN1C)C(F)(F)F c:10,19,22,t:6,8,12	Z8873684832	1{103}	Nc1cncc(C O)n1	2{841}	Cn1nc(c(Br)c 1C=O)C(F)(F) F	3{5}	COCCC[N+]# #[C-]	0.0	0
1977	4{375,531,10}	CC(C)OC1=CN=CC2=NC(=C(NC3CCOC3)N12)C1=CN=C(C)N=C1 c:6,27,t:4,8,10,22,24	Z8873684827	1{375}	CC(C)Oc1c ncc(N)n1	2{531}	Cc1ncc(C=O) cn1	3{10}	[C-]]#[N+]C1CC OC1	0.0	0
1978	4{187,682,12}	FC1=C(Cl)C(=CC=N1)C1=C(NCC2CCOC2)N2C=C(Cl)C(=CC2=N1)C#N c:1,4,6,9,23,26,t:20	Z8849597819	1{187}	Nc1cc(C#N) c(Cl)cn1	2{682}	Fc1nccc(C= O)c1Cl	3{12}	[C-]]#[N+]CC1C COC1	0.0	0

1979	4{46,842,9}	CNC1=C(N=C2C=CC=CN12)C1=C(Br)C=C(O)C(=O)OC c:6,8,13,16,t:2,4	Z8846491863	1{46}	Ne1ccccn1	2{842}	COC(=O)c1c c(Br)c(C=O) o1	3{9}	C[N+]#[C-]	0.0	0
1980	4{50,843,18}	CC(C)(C)NC1=C(N=C2C=CC=C(N12)P(C)(C)=O)C1=C(Br)C(F)=CC(F)=C1 c:9,11,20,24,27,t:5,7	Z8878918768	1{50}	CP(=O)(C)c 1cccc(N)n1	2{843}	Fc1cc(F)c(Br) c(C=O)c1	3{18}	CC(C)(C)[N +]#[C-]	0.0	0
1981	4{81,844,9}	CNC1=C(N=C2C=NC=CN12)C1=NN2C=CC=CC2=C1 c:6,8,16,18,21,t:2,4,13	Z8878918767	1{81}	Ne1cncen1	2{844}	O=Cc1cc2cc ccn2n1	3{9}	C[N+]#[C-]	0.0	0
1982	4{172,775,29}	CCOC(=O)CCNC1=C(N=C2N1C=CC1=C2CCO1)C1=C(C)N=C(S1)C(=O)OC c:10,14,16,23,26,t:8	Z8878918761	1{172}	Ne1nccc2O CCc21	2{775}	COC(=O)c1n c(C)c(C=O)s 1	3{29}	CCOC(=O)C C[N+]#[C-]	0.0	0
1983	4{70,845,31}	CSCCNC1=C(N=C2N1C=CN=C2C1CC1)C1=CC=CN2C=CN=C12 c:7,11,13,22,25,t:5,20,27	Z8878918676	1{70}	Ne1ncnc1 C2CC2	2{845}	O=Cc1cccn2 ccnc12	3{31}	CSCC[N+]#[C-]	0.0	0
1984	4{94,846,60}	COC(=O)C1=CC(NC2=C(N=C3C=CC(F)=NN23)C2=C(C)N=NS2)=CC=C1 c:12,15,20,23,26,28,t:4,8,10	Z8878918568	1{94}	Ne1ccc(F)n n1	2{846}	Cc1nnsc1C= O	3{60}	COC(=O)c1c ccc[N+]#[C-]c1	0.0	0
1985	4{161,137,11}	CC1=C(C(C)=NO1)C1=C(NCC2=CC(Br)=CC=C2)N2N=CC=CC2=N1 c:4,8,15,17,21,23,26,t:1,12	Z8878918542	1{161}	Ne1ccenn1	2{137}	Cc1noc(C)c1 C=O	3{11}	Br1cccc(C[N+]#[C-])c1	0.0	0
1986	4{150,735,32}	COC(=O)C1=CN=C(S1)C1=C(NC2CCC2)N2C=CC(=CC2=N1)C1CCOC1 c:6,10,19,21,24,t:4	Z8878918432	1{150}	Ne1cc(cen1)C2CCOC2	2{735}	COC(=O)c1c nc(C=O)s1	3{32}	[C-]#[N+]C1CC C1	0.0	0
1987	4{73,195,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC4=NC=CN4N23)C2=CC(F)=C(OC)N=C2)C=C1 c:12,16,30,33,t:2,5,8,10,14,23,26	Z8873684780	1{73}	Ne1ccc2ncc n2n1	2{195}	COc1ncc(C= O)cc1F	3{20}	COc1ccc([N +]#[C-])c(C)c1	0.0	0
1988	4{28,847,7}	CC1CC(CN1C(=O)OC(C)(C)C)C1=C(NC2CCOCC2)N2C=CC(=CC2=N1)C1=NOC=N1 c:14,25,27,30,36,t:33	Z8873684679	1{28}	Cl.Ne1cc(cc n1)c2ncon2	2{847}	CC1CC(CN1 C(=O)OC(C) (C)C)C=O	3{7}	[C-]#[N+]C1CC OCC1	0.0	0
1989	4{267,354,59}	CP(C)(=O)C1=C(C=CC=C1)C1=C(NCCC2=C(C(F)=CC=C2)N2C(C=CC=C2#C)=N1 c:6,8,11,19,21,26,28,32,t:4,16	Z8873684664	1{267}	Ne1cccc(C# C)n1	2{354}	CP(=O)(C)c1 cccc1C=O	3{59}	Fc1cccc(CC[N+]#[C-])c1	0.0	0
1990	4{99,767,66}	CCCC(OC)C1=C(NC(C)C2=CC=CC=C2)N2C=C(C=CC2=N1)S(N)(=O)=O c:6,13,15,19,21,24,t:11	Z8873684891	1{99}	Ne1ccc(en1)S(=O)(=O) N	2{767}	CCCC(OC)C =O	3{66}	CC([N+]#[C-])c1cccc1	0.0	0

1991	4{164,804,21}	CN(C)CC1=CC2=NC(=C(NCC3CC3)N2C=C1)C1=C(Br)N=CN1C c:18,21,24,t:4,6,8	Z8873684889	1{164}	CN(C)Cc1ccnc(N)c1	2{804}	Cn1cnc(Br)c1C=O	3{21}	[C-]#[N+]CC1C1	0.0	0
1992	4{81,95,9}	CNC1=C(N=C2C=NC=CN12)C1=CC(=NC=C1)N(C)C c:6,8,15,17,t:2,4,13	Z8873684629	1{81}	Nc1cncn1	2{95}	CN(C)c1cc(C=O)ccn1	3{9}	C[N+]#[C-]	0.0	0
1993	4{78,848,28}	CCCNC1=C(N=C2C=C(C)C3=NC(C)=CN3N12)C1=CN(N=C1C)C1=CC=C(C)C=C1 c:14,24,33,t:4,6,8,11,21,28,30	Z8873684841	1{78}	Cc1cn2nc(N)cc(C)c2n1	2{848}	Cc1nn(cc1C=O)c2ccc(C)cc2	3{28}	CCC[N+]#[C-]	0.0	0
1994	4{340,13,5}	CCOC1=CC=CN2C(NCCCOC)=C(N=C12)C1=C(C)NN=N1 c:5,14,20,24,t:3,16	Z8873684808	1{340}	CCOC1cccn1N	2{13}	Cc1[nH]mnc1C=O	3{5}	COCCC[N+]#[C-]	0.0	0
1995	4{483,55,33}	COC1=C(CNC2=C(N=C3C=CC(=CN23)N2C(C)=CC=C2C)C2=CC(=NC=C2)P(C)(C)=O)C=CC=C1 c:2,10,12,19,21,27,29,36,38,t:6,8,25	Z8854581164	1{483}	Cc1ccc(C)n1c2ccc(N)nc2	2{55}	CP(=O)(C)c1cc(C=O)ccn1	3{33}	COc1cccc1C[N+]#[C-]	0.0	0
1996	4{452,849,51}	CC(C)(C)OC(=O)NCCNC1=C(CN2C(=O)CO3=C2C=CC=C3)N=C2C=CC3=C(C=NC=C3)N12 c:11,19,22,24,29,33,35,t:27,31	Z8835022887	1{452}	Nc1ccc2ccncc2n1	2{849}	O=CCN1C(=O)COc2cccc12	3{51}	CC(C)(C)OC(=O)NCC[N+]#[C-]	0.0	0
1997	4{123,779,31}	COC1=C2NC=NC2=CC(=C1)C1=C(NCCSC)N2C=CC(OCCO)=CC2=N1 c:2,5,8,10,13,21,27,30	Z8835022867	1{123}	Cl.Nc1cc(OCCO)ccn1	2{779}	COc1cc(C=O)cc2nc[nH]c12	3{31}	CSCC[N+]#[C-]	0.0	0
1998	4{73,284,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC4=NC=CN4N23)C2=C(C)N=CC=N2)C=C1 c:12,16,23,26,28,31,t:2,5,8,10,14	Z8849597812	1{73}	Nc1ccc2nccn2n1	2{284}	Cc1ncnc1C=O	3{20}	COc1ccc([N+]#[C-])c(C)c1	0.0	0
1999	4{397,740,23}	COC(=O)CCC(NC1=C(N=C2N1C=CC(C)=C2)C)C1=CN(N=C1)C(F)F)C(=O)OC c:10,14,17,24,t:8,21	Z8855739214	1{397}	Cl.Cc1ccnc(N)c1C	2{740}	FC(F)n1cc(C=O)cn1	3{23}	COC(=O)CC(C([N+]#[C-])C(=O)OC	0.0	0
2000	4{65,850,23}	CCC1=CN=CC2=NC(C3=NN(C=C3)C(F)F)=C(NC(CCC(=O)OC)C(=O)OC)N12 c:4,12,t:2,6,9,17	Z8846491975	1{65}	CCc1cnc(N)n1	2{850}	FC(F)n1ccc(C=O)n1	3{23}	COC(=O)CC(C([N+]#[C-])C(=O)OC	0.0	0
2001	4{433,191,31}	CCN1C=NN=C1C1=C(NCCSC)N2C(C=CC(C#C)=C2C)=N1 c:3,5,8,17,21,24	Z8878918624	1{433}	Cc1nc(N)cc1C#C	2{191}	CCn1cnc1C=O	3{31}	CSCC[N+]#[C-]	0.0	0
2002	4{46,46,9}	CNC1=C(CCCCCOC)N=C2C=CC=CN12 c:2,13,15,t:11	Z8878918468	1{46}	Nc1cccn1	2{46}	COCCCCC=O	3{9}	C[N+]#[C-]	0.0	0
2003	4{393,177,23}	COC(=O)CCC(NC1=C(CC2CC(C2)C(=O)OC)N=C2C=CC(Cl)=C(Cl)N12)C(=O)OC c:8,22,t:20,25	Z8873684763	1{393}	Nc1ccc(Cl)c(Cl)n1	2{177}	COC(=O)C1CC(CC=O)C1	3{23}	COC(=O)CC(C([N+]#[C-])C(=O)OC	0.0	0

2004	4{80,258,67}	CCC(C)NC1=C(N=C2N1C=CN=C2OC)C1=N N=C(S1)C1CC1 c:7,11,13,20,t:5,18	Z8873685494	1{80}	COc1ncnc 1N	2{258}	O=Cc1nnc(s 1)C2CC2	3{67}	CCC(C)[N+] #[C-]	0.0	0
2005	4{22,197,13}	COC(=O)C1=CC(=NN1C)C1=C(NCC2=CC=C (OC)C=C2)N2N=C(Cl)C=CC2=N1 c:6,11,21,28,31,t:4,15,17,25	Z8873685384	1{22}	Nc1ccc(Cl) nn1	2{197}	COC(=O)c1c c(C=O)nn1C	3{13}	COc1ccc(C[N+]#[C-])cc1	0.0	0
2006	4{156,119,22}	CCOC(=O)C1=NN=C(N1)C1=C(NC2COC2)N 2C(=N1)C(Cl)=CC=C2Cl c:7,11,20,24,26,t:5	Z8873685327	1{156}	Nc1nc(Cl)c cc1Cl	2{119}	CCOC(=O)c 1nnc(C=O)[n H]1	3{22}	[C-]#[N+]C1CO C1	0.0	0
2007	4{79,121,13}	CCC1=CON=C1C1=C(NCC2=CC=C(OC)C=C 2)N2C(C=NC=C2C)=N1 c:5,8,18,23,25,28,t:2,12,14	Z8873684603	1{79}	Cc1nccc(N) n1	2{121}	CCc1conc1C =O	3{13}	COc1ccc(C[N+]#[C-])cc1	0.0	0
2008	4{28,851,7}	COC1=C(SC)C=C(C=C1)C1=C(NC2CCOCC2)N2C=CC(=CC2=N1)C1=NOC=N1 c:2,6,8,11,22,24,27,33,t:30	Z8855739220	1{28}	Cl.Nc1cc(cc n1)c2ncon2	2{851}	COc1ccc(C= O)cc1SC	3{7}	[C-]#[N+]C1CC OCC1	0.0	0
2009	4{94,762,21}	FC1=NN2C(C=C1)=NC(C1CC1(F)F)=C2NCC 1CC1 c:5,7,15,t:1	Z8855739147	1{94}	Nc1ccc(F)n n1	2{762}	FC1(F)CC1C =O	3{21}	[C-]#[N+]CC1C C1	0.0	0
2010	4{484,569,78}	CC(C)(C)OC(=O)NCC1=CC=C(NC2=C(CC3C COC3=O)N=C3C=CC4=C(N=CC=C4)N23)C= C1 c:14,26,30,32,38,t:9,11,24,28	Z8878918838	1{484}	Br.Nc1ccc2 ccnc2n1	2{569}	O=CCC1CC OC1=O	3{78}	CC(C)(C)OC (=O)NCc1cc c([N+]#[C-])cc1	0.0	0
2011	4{398,689,15}	CCNC1=C(N=C2C=C(C=CN12)C(C)(F)F)C1= CN(CCOC(C)=O)N=C1 c:7,9,27,t:3,5,18	Z8878918781	1{398}	Cl.CC(F)(F) c1cnc(N)c 1	2{689}	CC(=O)OCC n1cc(C=O)en 1	3{15}	CC[N+]#[C-]	0.0	0
2012	4{103,455,40}	CCOC(=O)C1=CC=C(NC2=C(N=C3C=NC=C(CO)N23)C2=C(C)ON=C2Br)C=C1 c:14,23,27,31,t:5,7,10,12,16	Z8878918650	1{103}	Nc1cnc(C O)n1	2{455}	Cc1onc(Br)c 1C=O	3{40}	CCOC(=O)c 1ccc([N+]#[C-])cc1	0.0	0
2013	4{188,352,38}	COCCCC1=C(NC2=CC3=C(OCO3)C=C2)N2 C(C=NC=C2C(=O)OC)=N1 c:5,16,21,23,29,t:8,10	Z8878918549	1{188}	COC(=O)c1 cnc(N)n1	2{352}	COCCCC=O	3{38}	[C-]#[N+]c1ccc 2OCOc2c1	0.0	0
2014	4{234,427,10}	C1CC(C1)OC1=NC=CN2C(NC3CCOC3)=C(N =C12)C1=NOC2=C1COCC2 c:8,18,27,t:6,20,24	Z8873684715	1{234}	Nc1ncnc1 OC2CCCC2	2{427}	O=Cc1noc2C COCc12	3{10}	[C-]#[N+]C1CC OC1	0.0	0
2015	4{436,852,23}	CCC1=CC2=NC(=C(NC(CCC(=O)OC)C(=O) OC)N2C=C1)C1=CC(=CN=C1)C(F)F c:22,27,29,t:2,4,6,25	Z8873684687	1{436}	CCc1cnc(N)c1	2{852}	FC(F)c1cnc (C=O)c1	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	0.0	0

2016	4{332,454,21}	CCC1=CC=CN2C(NCC3CC3)=C(CC(C)OC)N=C12 c:4,t:2,13,20	Z8873685478	1{332}	CCc1cccn1 N	2{454}	COC(C)CC=O	3{21}	[C-] #[N+]CC1C C1	0.0	0
2017	4{448,50,31}	CSCCNC1=C(N=C2C=C(F)C(C=C)=CN12)[C@@@H]1C[C@H]1C1OCCO1 &1:17,19,r,c:14,t:5,7,9	Z8873684887	1{448}	Nc1cc(F)c(C=C)cn1	2{50}	O=C[C@@H]1C[C@H]1C2OCCO2 &1:2,4,r	3{31}	CSCC[N+]#[C-]	0.0	0
2018	4{73,838,20}	COC1=CC(C)=C(NC2=C(N=C3C=CC4=NC=CN4N23)C2=CN=C(N=C2)C(C)(C)C)C=C1 c:12,16,25,27,34,t:2,5,8,10,14,23	Z8873684626	1{73}	Nc1ccc2nccn2n1	2{838}	CC(C)(C)c1ncc(C=O)cn1	3{20}	COc1ccc([N+]#[C-])c(C)c1	0.0	0
2019	4{48,131,15}	CCNC1=C(N=C2C=C(C=CN12)S(C)(=O)=O)C1=NC(=NN1)C1CC1 c:7,9,20,t:3,5,18	Z8873684591	1{48}	CS(=O)(=O)c1ccnc(N)c1	2{131}	O=Cc1nc(n[nH]1)C2CC2	3{15}	CC[N+]#[C-]	0.0	0
2020	4{78,853,46}	CC(=C)CNC1=C(N=C2C=C(C)C3=NC(C)=CN3N12)C1=CN=C(N=C1)N1CCCC1 c:15,24,26,t:5,7,9,12,22	Z8835022902	1{78}	Cc1cn2nc(N)cc(C)c2n1	2{853}	O=Cc1cnc(ncl)N2CCCC2	3{46}	CC(=C)C[N+]#[C-]	0.0	0
2021	4{161,727,6}	CCOC(=O)CCNC1=C(N=C2C=CC=NN12)C1=CN=C(N=C1)C(C)C c:13,15,22,24,t:9,11,20	Z8835022871	1{161}	Nc1ccenn1	2{727}	CC(C)c1ncc(C=O)cn1	3{6}	CCOC(=O)CC[N+]#[C-]	0.0	0
2022	4{73,162,13}	COC1=CC=C(CNC2=C(N=C3C=CC4=NC=CN4N23)C2=CC(OC)=NC(C)=C2)C=C1 c:12,16,27,30,33,t:2,4,8,10,14,23	Z8855739268	1{73}	Nc1ccc2nccn2n1	2{162}	COc1cc(C=O)cc(C)n1	3{13}	COc1ccc(C[N+]#[C-])cc1	0.0	0
2023	4{78,854,28}	CCCNC1=C(N=C2C=C(C)C3=NC(C)=CN3N12)C1=CN(C)N=C1CN1C(=O)C2=C(C=CC=C2)C1=O c:14,25,34,36,t:4,6,8,11,21,32	Z8878918623	1{78}	Cc1cn2nc(N)cc(C)c2n1	2{854}	Cn1cc(C=O)c(CN2C(=O)c3ccccc3C2=O)n1	3{28}	CCC[N+]#[C-]	0.0	0
2024	4{397,585,23}	COC(=O)CCC(NC1=C(CC2CC2(C1)Cl)N=C2N1C=CC(C)=C2)C(=O)OC c:8,17,21,24	Z8878918590	1{397}	Cl.Cc1ccnc(N)c1C	2{585}	ClC1(C1)CC1CC=O	3{23}	COC(=O)CC(C[N+]#[C-])C(=O)OC	0.0	0
2025	4{103,855,59}	OCC1=CN=CC2=NC(C3=CC(=NO3)C3CCC3)=C(NCCC3=CC(F)=CC=3)N12 c:4,11,27,29,t:2,6,9,19,24	Z8878918366	1{103}	Nc1cncc(CO)n1	2{855}	O=Cc1cc(no1)C2CCC2	3{59}	Fe1cccc(CC[N+]#[C-])c1	0.0	0
2026	4{22,69,13}	COC1=CC=C(CNC2=C(N=C3C=CC(C1)=NN23)C2=NN(C)C(C)=C2)C=C1 c:12,15,25,28,t:2,4,8,10,20	Z8878918345	1{22}	Nc1ccc(Cl)nn1	2{69}	Cc1cc(C=O)nn1C	3{13}	COc1ccc(C[N+]#[C-])cc1	0.0	0
2027	4{85,191,31}	CCN1C=NN=C1C1=C(NCCSC)N2C(C=C(C=C2)C#N)=N1 c:3,5,8,17,19,24	Z8873684761	1{85}	Cc1cc(C#N)cc(N)n1	2{191}	CCn1cnnc1C=O	3{31}	CSCC[N+]#[C-]	0.0	0

2028	4{73,91,13}	COC1=CC=C(CNC2=C(N=C3C=CC4=NC=C N4N23)C2=CC3=C(OCCC3)C=C2)C=C1 c:12,16,32,35,t:2,4,8,10,14,23,25	Z8873684728	1{73}	Nc1ccc2ncc n2n1	2{91}	O=Cc1ccc2O CCCc2c1	3{13}	COc1ccc(C[N+]#[C-])cc1	0.0	0
2029	4{261,856,12}	CCC1=C(N(C)N=C1)C1=C(NCC2CCOC2)N2 C=C(C=CC2=N1)N1CCC(CC1)N(C)C c:6,9,20,22,25,t:2	Z8873685402	1{261}	CN(C)C1C CN(CC1)c2 ccc(N)nc2	2{856}	CCc1cnn(C)c 1C=O	3{12}	[C-]#[N+]CC1C COC1	0.0	0
2030	4{119,291,21}	COC1=C(C)C(=CN=C1)C1=C(NCC2CC2)N2 C=C(C=CC2=N1)C#N c:2,5,7,10,19,21,24	Z8873684942	1{119}	Ne1ccc(C# N)cn1	2{291}	COc1cnc(C =O)c1C	3{21}	[C-]#[N+]CC1C C1	0.0	0
2031	4{333,857,23}	COC(=O)CCC(NC1=C(N=C2C=CC=C(N12)C 1=CC=NC=C1)C1=C(F)C(OC)=NC=C1)C(=O) OC c:12,14,21,23,26,31,33,t:8,10,19	Z8873684932	1{333}	Ne1cccc(n1 c2cncnc2	2{857}	COc1cnc(C =O)c1F	3{23}	COC(=O)CC C([N+]#[C-])C(=O)OC	0.0	0
2032	4{164,242,10}	CN(C)CC1=CC2=NC(=C(NC3CCOC3)N2C=C 1)C1=CN2N=CC(C#N)=C2N=C1 c:19,25,29,32,t:4,6,8,22	Z8873684815	1{164}	CN(C)Cc1c cnc(N)c1	2{242}	O=Cc1cnc2c (C#N)enn2c1	3{10}	[C-]#[N+]C1CC OC1	0.0	0
2033	4{100,408,37}	COC(=O)C1CC(C1)NC1=C(CCN2CCOC2=O) N=C2C=NC3=C(C=CC=C3)N12 c:10,23,27,29,t:21,25	Z8846491960	1{100}	Ne1cnc2ccc cc2n1	2{408}	O=CCCN1C COC1=O	3{37}	COC(=O)C1 CC(C1)[N+] #[C-]	0.0	0
2034	4{160,247,14}	CCOC1CC(C1)C1=C(NCCOC)N2C=C(Br)C= C(C#C)C2=N1 c:8,24,t:16,19	Z8878918815	1{160}	Ne1ncc(Br) cc1C#C	2{247}	CCOC1CC(C 1)C=O	3{14}	COCC[N+]#[C-]	0.0	0
2035	4{167,294,5}	COCCNC1=C(N=C2N1C(C)=CN=C2C)C1= C(OC)C(=O)C=CO1 c:8,13,15,19,25,t:6	Z8878918763	1{167}	Cc1cnc(C)c (N)n1	2{294}	COc1c(C=O) occc1=O	3{5}	COCCC[N+] #[C-]	0.0	0
2036	4{452,858,44}	COC1=CC(=O)OC(=C1)C1=C(NCCCCNC(=O))OC(C)(C)N2C(C=CC3=C2C=NC=C3)=N1 c:7,10,27,29,32,34,36,t:2	Z8878918580	1{452}	Ne1ccc2ccn cc2n1	2{858}	COc1cc(C=O))oc(=O)c1	3{44}	CC(C)(C)OC (=O)NCCCC [N+]#[C-]	0.0	0
2037	4{81,826,13}	COC1=CC=C(CNC2=C(N=C3C=NC=CN23)C 2=NC(CI)=CS2)C=C1 c:12,14,22,26,t:2,4,8,10,19	Z8878918556	1{81}	Ne1cncn1	2{826}	C1c1csc(C=O)n1	3{13}	COc1ccc(C[N+]#[C-])cc1	0.0	0
2038	4{46,859,9}	CNC1=C(N=C2C=CC=CN12)C1=CN2C=CC= C(F)C2=N1 c:6,8,16,22,t:2,4,13,18	Z8878918480	1{46}	Ne1ccccn1	2{859}	Fc1ccn2cc(C=O)nc12	3{9}	C[N+]#[C-]	0.0	0
2039	4{267,860,5}	CCOC(=O)C1=NC(=NN1C)C1=C(NCCCCOC) N2C(C=CC=C2C#C)=N1 c:7,12,22,24,28,t:5	Z8878918426	1{267}	Ne1cccc(C# C)n1	2{860}	CCOC(=O)c 1nc(C=O)nn 1C	3{5}	COCCC[N+] #[C-]	0.0	0

2040	4{103,861,5}	COCNC1=C(N=C2C=NC=C(CO)N12)C1=C(OC)C(CI)=CC=C1Cl c:10,19,24,26,t:6,8,12	Z8873684770	1{103}	Nc1cncc(CO)n1	2{861}	COc1c(Cl)cc(Cl)c1C=O	3{5}	COCCC[N+]#[C-]	0.0	0
2041	4{352,862,47}	CC(C)NC1=C(N=C2C=CC(=CN12)N1CCN(C)C(=O)C1)C1=CSC(=N1)N(C)C(C)=O c:8,10,27,t:4,6,24	Z8873684746	1{352}	CN1CCN(C1=O)c2ccc(N)nc2	2{862}	CN(C(=O)C)c1nc(C=O)cs1	3{47}	CC(C)[N+]#[C-]	0.0	0
2042	4{78,863,28}	CCCNC1=C(N=C2C=C(C)C3=NC(C)=CN3N12)C1=CC2=C(OC(C)(C)C2)C=C1 c:14,31,t:4,6,8,11,21,23	Z8873684710	1{78}	Cc1cn2nc(N)cc(C)c2n1	2{863}	CC1(C)Ce2cc(C=O)ccc2O1	3{28}	CCC[N+]#[C-]	0.0	0
2043	4{125,864,18}	COC(=O)C1=CN2C(C=C1)=NC=C2C1=C(NC(C)(C)C)N2C=C(CCO)C=CC2=N1 c:8,10,12,15,28,31,t:4,23	Z8873684647	1{125}	Nc1ccc(CC)cn1	2{864}	COC(=O)c1ccc2ncc(C=O)n2c1	3{18}	CC(C)(C)[N+]#[C-]	0.0	0
2044	4{327,865,34}	COC(=O)C1=C(F)C2=NC(=C(NCC3CCCO3)N2C=C1)C1=NN2CCCCC2=C1 c:4,21,32,t:7,9,24	Z8873685355	1{327}	COC(=O)c1ccnc(N)c1F	2{865}	O=Cc1cc2C CCCn2n1	3{34}	[C-]#[N+]CC1C CCO1	0.0	0
2045	4{485,564,29}	CCOC(=O)CCNC1=C(N=C2N1C=CC1=C2CN(CC1)C(=O)OC(C)(C)C1=CN=NN1C c:10,14,16,33,t:8,31	Z8873684924	1{485}	CC(C)(C)OC(=O)N1C Cc2ccnc(N)c2C1	2{564}	Cn1nccc1C=O	3{29}	CCOC(=O)C C[N+]#[C-]	0.0	0
2046	4{161,363,11}	CC1=NC(=CN1)C1=C(NCC2=CC(Br)=CC=C2)N2N=CC=CC2=N1 c:3,7,14,16,20,22,25,t:1,11	Z8873684806	1{161}	Nc1cccnn1	2{363}	Cc1nc(C=O)c[nH]1	3{11}	Br1cccc(C[N+]#[C-])c1	0.0	0
2047	4{364,866,38}	FC(F)(F)COCCC1=C(NC2=CC3=C(OCO3)C=C2)N2C=C(C=CC2=N1)N1CCNC(=O)C1 c:8,19,23,25,28,t:11,13	Z8854581162	1{364}	Nc1ccc(en1)N2CCNC(=O)C2	2{866}	FC(F)(F)CO CCC=O	3{38}	[C-]#[N+]c1ccc2OCoc2c1	0.0	0
2048	4{78,867,46}	COC(=O)C1=NC=CC(=C1)C1=C(NCC(C)=C)N2N3C=C(C)N=C3C(C)=CC2=N1 c:6,8,11,23,27,30,t:4,20	Z8835022905	1{78}	Cc1cn2nc(N)cc(C)c2n1	2{867}	COC(=O)c1cc(C=O)ccn1	3{46}	CC(=C)C[N+]#[C-]	0.0	0
2049	4{143,862,43}	CCC1=NN2C(C=C1)=NC(=C2NC1CCN(CC1)C(=O)OC(C)(C)C1=CSC(=N1)N(C)C(C)=O c:6,8,10,31,t:2,28	Z8849597840	1{143}	CCc1ccc(N)nn1	2{862}	CN(C(=O)C)c1nc(C=O)cs1	3{43}	CC(C)(C)OC(=O)N1CCC(CC1)[N+]#[C-]	0.0	0
2050	4{121,272,10}	CC(C)C1=NN=C(S1)C1=C(NC2CCOC2)N2C=CC(Br)=CC2=N1 c:5,9,19,22,25,t:3	Z8849597839	1{121}	Nc1cc(Br)cn1	2{272}	CC(C)c1nnc(C=O)s1	3{10}	[C-]#[N+]C1CCOC1	0.0	0
2051	4{73,161,11}	CCN1C=NC=C1C1=C(NCC2=CC(Br)=CC=C2)N2N3C=CN=C3C=CC2=N1 c:3,5,8,15,17,22,24,27,30,t:12	Z8849597806	1{73}	Nc1ccc2nccn2n1	2{161}	CCn1cncc1C=O	3{11}	Br1cccc(C[N+]#[C-])c1	0.0	0

2052	4{91,447,7}	CC(C)(O)C#CC1=CC=C(C=C1)C1=C(NC2CCOCC2)N2C=C(C=CC2=N1)C(N)=O c:8,10,13,24,26,29,t:6	Z8837933136	1{91}	NC(=O)c1ccc(N)nc1	2{447}	CC(C)(O)C#Cc1ccc(C=O)cc1	3{7}	[C-]][N+]C1CCOCC1	0.0	0
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