BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

Synthesis, structure, ionochromic and cytotoxic properties of new 2-(indolin-2-yl)-1,3-tropolones

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X-ray analysis data of 7b and DFT quantum chemical calculations for 7a, 7b, 8a and 8b

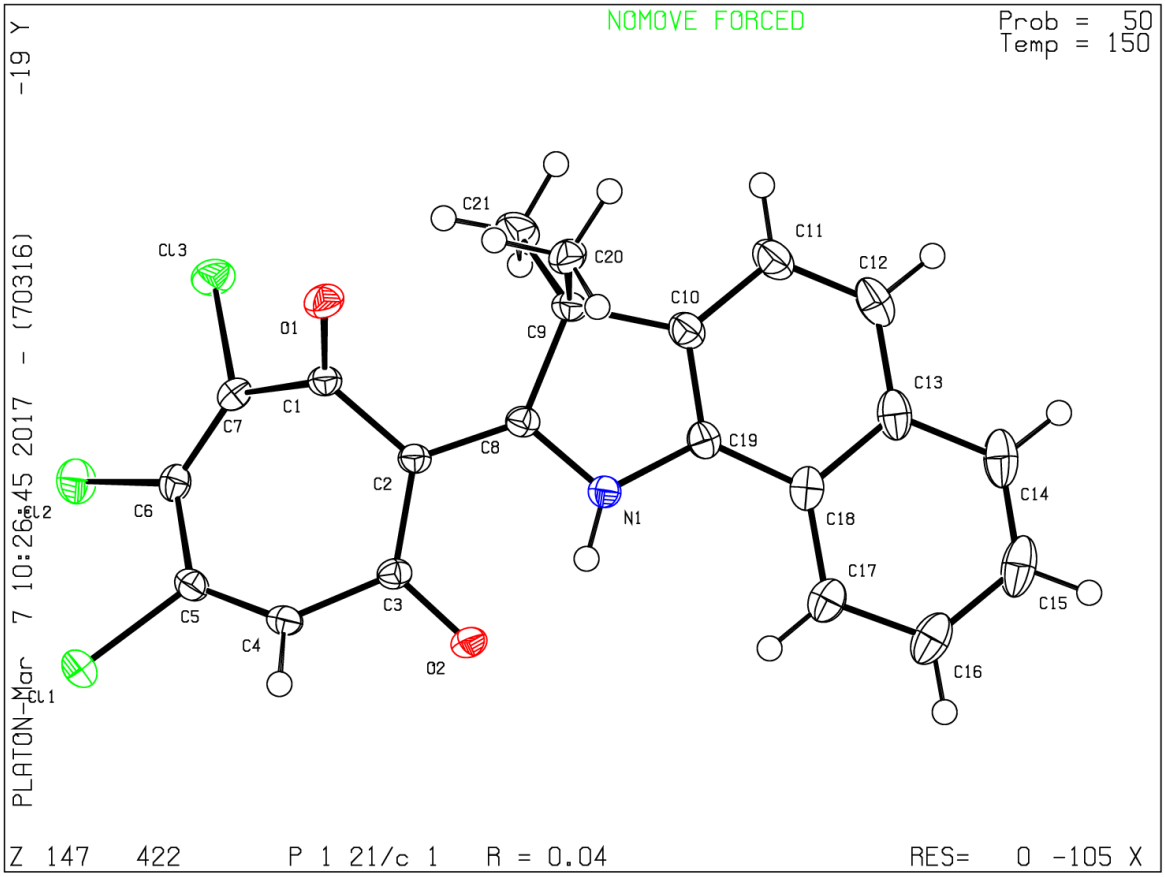
Table S1: Crystal data and structure refinement for **7b**.

CCDC Number	2040907
Empirical formula	$C_{21}H_{14}Cl_3NO_2$
Formula weight	418.68
Temperature/K	150.0(1)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	11.4480(3)
b/Å	7.4883(2)
c/Å	21.7720(6)
α/°	90.00
β/°	102.590(3)
γ/°	90.00
Volume/Å^3	1821.55(9)
Z	4
ρ_{calc} g/cm^3	1.527
μ/mm^{-1}	0.520
F(000)	856
Crystal size/mm^3	0.31 × 0.25 × 0.20
Radiation	MoK\a (λ = 0.7107)
Index ranges	-17 ≤ h ≤ 17, -11 ≤ k ≤8, -32 ≤ l ≤23
Reflections collected	14246
Independent reflections	6352[R_{int} = 0.0214, R_{sigma} = 0.0323]
Data/restraints/parameters	6352/0/247
Goodness-of-fit on F^2	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0385, wR_2 = 0.0928
Final R indexes [all data]	R_1 = 0.0534, wR_2 = 0.1003
Largest diff. peak/hole / e Å^{-3}	0.431/-0.340

Table S2: Bond lengths *d* (Å) and angles *ω* (deg) in **7b**.

Bond	*d*/Å	Bond	*d*/Å	Bond	*d*/Å
Cl(1)-C(5)	1.7393(13)	N(1)-C(8)	1.3381(16)	C(2)-C(8)	1.4139(17)
Cl(2)-C(6)	1.7303(12)	N(1)-C(19)	1.4040(16)	C(2)-C(3)	1.4459(17)
Cl(3)-C(7)	1.7222(13)	N(1)-H(1)	0.857(18)	C(3)-C(4)	1.4783(18)
O(1)-C(1)	1.2194(16)	C(1)-C(2)	1.4702(17)	C(4)-C(5)	1.3391(18)
O(2)-C(3)	1.2543(15)	C(1)-C(7)	1.5170(17)	C(5)-C(6)	1.4636(18)
C(6)-C(7)	1.3407(18)	C(9)-C(20)	1.549(2)	C(12)-C(13)	1.420(2)
C(8)-C(9)	1.5391(18)	C(10)-C(19)	1.3722(19)	C(13)-C(14)	1.423(2)
C(9)-C(10)	1.5156(19)	C(10)-C(11)	1.4064(19)	C(13)-C(18)	1.431(2)
C(9)-C(21)	1.5316(19)	C(11)-C(12)	1.372(2)	C(14)-C(15)	1.364(3)
C(15)-C(16)	1.415(2)	C(16)-C(17)	1.3754(19)	C(17)-C(18)	1.414(2)
Angle	*ω*/deg	Angle	*ω*/deg	Angle	*ω*/deg
C(8)-N(1)-C(19)	112.37(11)	C(3)-C(2)-C(1)	120.92(11)	C(7)-C(6)-C(5)	122.86(11)
C(8)-N(1)-H(1)	115.4(11)	O(2)-C(3)-C(2)	122.75(11)	C(7)-C(6)-Cl(2)	120.01(10)
C(19)-N(1)-H(1)	131.9(11)	O(2)-C(3)-C(4)	114.20(11)	C(5)-C(6)-Cl(2)	117.09(9)
O(1)-C(1)-C(2)	124.45(11)	C(2)-C(3)-C(4)	122.84(11)	C(6)-C(7)-C(1)	127.44(11)
O(1)-C(1)-C(7)	118.05(11)	C(5)-C(4)-C(3)	129.68(12)	C(6)-C(7)-Cl(3)	120.95(10)
C(2)-C(1)-C(7)	117.00(11)	C(4)-C(5)-C(6)	126.57(11)	C(1)-C(7)-Cl(3)	111.61(9)
C(8)-C(2)-C(3)	118.81(11)	C(4)-C(5)-Cl(1)	117.19(10)	N(1)-C(8)-C(2)	120.54(11)
C(8)-C(2)-C(1)	120.26(11)	C(6)-C(5)-Cl(1)	116.22(9)	N(1)-C(8)-C(9)	108.17(11)
C(2)-C(8)-C(9)	131.14(11)	C(19)-C(10)-C(9)	109.60(11)	C(14)-C(15)-C(16)	120.71(14)
C(10)-C(9)-C(21)	111.95(12)	C(11)-C(10)-C(9)	129.96(13)	C(17)-C(16)-C(15)	120.28(15)
C(10)-C(9)-C(8)	100.67(10)	C(12)-C(11)-C(10)	118.44(15)	C(16)-C(17)-C(18)	119.94(14)
C(21)-C(9)-C(8)	114.77(11)	C(11)-C(12)-C(13)	121.75(14)	C(19)-C(18)-C(17)	124.49(13)
C(10)-C(9)-C(20)	107.26(10)	C(12)-C(13)-C(14)	121.86(14)	C(19)-C(18)-C(13)	115.27(13)
C(21)-C(9)-C(20)	111.53(12)	C(12)-C(13)-C(18)	120.38(13)	C(17)-C(18)-C(13)	120.19(12)
C(8)-C(9)-C(20)	109.96(11)	C(14)-C(13)-C(18)	117.74(15)	C(10)-C(19)-N(1)	108.59(11)
C(19)-C(10)-C(11)	120.30(13)	C(15)-C(14)-C(13)	121.04(15)	C(10)-C(19)-C(18)	123.74(12)

7b.cif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C2
C14
CL2
C6
N1
C18
C17
C5
C3
C15
C4
O2
CL1
C16

Table S3: Optimized structure (Cartesian coordinates, Å) of **7a** isomers calculated by the PBE0/6-311+ G(d,p) method in the gas phase.

	7a (NH)				**7a (OH)**		
	X	Y	Z		X	Y	Z
1 C	5.133779	0.740503	-0.465361	1 C	5.127637	0.763631	-0.452105
2 C	4.718896	2.044618	-0.836623	2 C	4.711678	2.098690	-0.696011
3 C	3.405569	2.426372	-0.768508	3 C	3.401830	2.473968	-0.568939
4 C	2.484595	1.466857	-0.321527	4 C	2.474759	1.486270	-0.191937
5 C	2.821386	0.186792	0.047923	5 C	2.824289	0.175580	0.054802
6 C	4.175199	-0.220715	-0.002879	6 C	4.173744	-0.231813	-0.058190
7 C	0.492028	0.537547	0.247733	7 C	0.536502	0.553689	0.314612
8 N	1.110732	1.635309	-0.183904	8 N	1.105218	1.680403	-0.032428
9 C	-0.918267	0.509242	0.335495	9 C	-0.916949	0.517657	0.388851
10 C	-4.075495	0.970710	0.255628	10 C	-4.059442	1.001378	0.128521
11 C	-3.938018	-0.373637	-0.292193	11 C	-3.927985	-0.381749	-0.283608
12 C	-2.826487	-1.106133	-0.105115	12 C	-2.823054	-1.119662	-0.029471
13 C	-1.621048	-0.717034	0.719829	13 C	-1.621388	-0.708613	0.775444
14 O	-1.226861	-1.512804	1.546813	14 O	-1.207729	-1.482650	1.612700
15 C	-1.649466	1.737300	0.090656	15 C	-1.628780	1.706081	0.172635
16 C	-3.081180	1.853713	0.422232	16 C	-3.053509	1.880065	0.314594
17 O	-1.102808	2.801718	-0.252736	17 O	-1.024939	2.843641	-0.060584
18 Cl	-2.666102	-2.681005	-0.778888	18 Cl	-2.722685	-2.756263	-0.547448
19 Cl	-5.260031	-0.986869	-1.216495	19 Cl	-5.259195	-1.080153	-1.131000
20 Cl	-5.679732	1.461429	0.707032	20 Cl	-5.668564	1.602116	0.365924
21 H	0.520277	2.459090	-0.388976	21 H	-0.003660	2.631397	-0.116362
22 C	1.562251	-0.534793	0.507250	22 C	1.572748	-0.568216	0.479452
23 C	1.288335	-1.802797	-0.315092	23 C	1.254213	-1.763236	-0.429965
24 H	1.174077	-1.560648	-1.374884	24 H	1.127402	-1.440472	-1.466863
25 H	2.124108	-2.498028	-0.224136	25 H	2.071905	-2.485731	-0.407442
26 H	0.391642	-2.313645	0.032686	26 H	0.350261	-2.277994	-0.104318
27 C	1.677686	-0.818164	2.019783	27 C	1.728202	-0.972892	1.961057
28 H	2.539811	-1.462043	2.205758	28 H	2.593101	-1.630484	2.071636
29 H	1.834413	0.112262	2.572751	29 H	1.903759	-0.089176	2.580969
30 H	0.774513	-1.302289	2.385794	30 H	0.836022	-1.482619	2.317810
31 C	4.647267	-1.504856	0.371821	31 C	4.643940	-1.547628	0.187012
32 C	6.497694	0.373285	-0.541109	32 C	6.486722	0.397916	-0.588945
33 C	5.978619	-1.823071	0.287273	33 C	5.971136	-1.864131	0.046395
34 C	6.916650	-0.879242	-0.175790	34 C	6.904727	-0.885320	-0.347579
35 H	7.966242	-1.145707	-0.238533	35 H	7.951328	-1.149336	-0.456120
36 H	3.950897	-2.249349	0.736101	36 H	3.948272	-2.318288	0.494217
37 H	6.313352	-2.812431	0.581548	37 H	6.305715	-2.877941	0.240815
38 H	7.212813	1.109794	-0.895640	38 H	7.200001	1.159678	-0.889909
39 H	5.471474	2.747567	-1.179765	39 H	5.462466	2.826177	-0.988880
40 H	3.085582	3.423749	-1.048799	40 H	3.077005	3.492076	-0.752420
41 H	-3.337219	2.843792	0.784215	41 H	-3.327318	2.905075	0.540088

Table S4: Optimized structure (Cartesian coordinates, Å) of **7b** isomers calculated by the PBE0/6-311+ G(d,p) method in the gas phase.

	7b (NH)				**7b (OH)**		
	X	Y	Z		X	Y	Z
1 C	5.069078	-1.474948	-0.117822	1 C	5.063888	-1.488305	-0.242906
2 C	5.172173	-0.072351	-0.301359	2 C	5.167685	-0.076451	-0.338218
3 C	4.006758	0.748304	-0.212961	3 C	4.003997	0.735917	-0.184662
4 C	2.799115	0.071939	0.057713	4 C	2.789751	0.052484	0.056370
5 C	2.712335	-1.285340	0.236668	5 C	2.713423	-1.318793	0.147305
6 C	3.863366	-2.079654	0.151603	6 C	3.860578	-2.109113	0.001546
7 C	0.586682	-0.297093	0.427993	7 C	0.638190	-0.310979	0.418974
8 N	1.525187	0.619493	0.183885	8 N	1.531752	0.627650	0.218511
9 C	-0.774216	0.077286	0.466980	9 C	-0.762111	0.076278	0.471670
10 C	-3.657207	1.431663	0.346529	10 C	-3.612213	1.487486	0.253905
11 C	-3.866099	0.178915	-0.370198	11 C	-3.871211	0.185370	-0.327083
12 C	-3.022905	-0.861707	-0.249053	12 C	-3.040001	-0.870120	-0.165249
13 C	-1.812614	-0.938449	0.651948	13 C	-1.804326	-0.931117	0.688290
14 O	-1.702970	-1.913991	1.365325	14 O	-1.661112	-1.893252	1.413021
15 C	-1.108451	1.484635	0.377329	15 C	-1.086908	1.438012	0.402098
16 C	-2.470188	1.967398	0.664635	16 C	-2.403181	2.005653	0.552976
17 O	-0.256704	2.378678	0.213775	17 O	-0.165064	2.364255	0.320016
18 Cl	-3.274455	-2.324919	-1.117887	18 Cl	-3.400264	-2.388924	-0.886130
19 Cl	-5.242930	0.086408	-1.406686	19 Cl	-5.313269	0.014471	-1.259661
20 Cl	-5.086688	2.307471	0.802867	20 Cl	-4.985852	2.501582	0.556336
21 H	1.202459	1.596970	0.086023	21 H	0.748813	1.864610	0.245897
22 H	3.808468	-3.154491	0.292568	22 H	3.807025	-3.191085	0.075020
23 H	5.972106	-2.072416	-0.193939	23 H	5.965449	-2.080431	-0.367362
24 C	1.281611	-1.660067	0.561672	24 C	1.288925	-1.701209	0.466757
25 C	0.743941	-2.713171	-0.414900	25 C	0.712687	-2.677250	-0.565551
26 H	0.755993	-2.341043	-1.442474	26 H	0.710048	-2.238215	-1.566777
27 H	1.385161	-3.597810	-0.370399	27 H	1.333866	-3.576866	-0.595784
28 H	-0.268487	-3.021263	-0.156309	28 H	-0.301120	-2.982655	-0.305631
29 C	1.240905	-2.164494	2.018857	29 C	1.273760	-2.303531	1.887093
30 H	1.881316	-3.047154	2.102077	30 H	1.903963	-3.197601	1.896569
31 H	1.625998	-1.404457	2.704233	31 H	1.685198	-1.595602	2.611827
32 H	0.223515	-2.424481	2.304738	32 H	0.261756	-2.570855	2.183450
33 H	-2.465958	2.940200	1.144685	33 H	-2.377392	3.032453	0.901523
34 C	6.412010	0.553939	-0.572951	34 C	6.406360	0.562892	-0.583582
35 C	4.116409	2.145419	-0.393660	35 C	4.114671	2.140384	-0.278322
36 C	6.494212	1.911919	-0.744338	36 C	6.488839	1.929162	-0.669984
37 C	5.337489	2.713930	-0.653507	37 C	5.333797	2.723896	-0.515784
38 H	3.231852	2.770971	-0.325200	38 H	3.225794	2.750474	-0.159709
39 H	5.415755	3.787203	-0.790502	39 H	5.412547	3.803780	-0.586218
40 H	7.302900	-0.062970	-0.642650	40 H	7.295335	-0.049533	-0.702101
41 H	7.452807	2.376070	-0.950903	41 H	7.445815	2.404781	-0.857687

Table S5: Optimized structure (Cartesian coordinates, Å) of **8a** isomers calculated by the PBE0/6-311+ G(d,p) method in the gas phase.

8a (NH)				**8a (OH)**			
	X	Y	Z		X	Y	Z
1 C	5.332975	0.752213	-0.546963	1 C	5.300700	0.817420	-0.556830
2 C	4.842979	1.901251	-1.217696	2 C	4.785989	2.035240	-1.073183
3 C	3.502872	2.175061	-1.286602	3 C	3.446309	2.313655	-1.048316
4 C	2.634001	1.264084	-0.667694	4 C	2.591684	1.344402	-0.495284
5 C	3.044057	0.132274	-0.005993	5 C	3.037183	0.144729	0.017160
6 C	4.425002	-0.161516	0.083420	6 C	4.418242	-0.159306	0.011947
7 C	0.687761	0.322596	0.033163	7 C	0.720495	0.366890	0.163822
8 N	1.244183	1.339602	-0.624127	8 N	1.205392	1.445899	-0.396315
9 C	-0.714679	0.218519	0.141803	9 C	-0.723207	0.251692	0.283875
10 C	-3.886301	0.508713	0.158329	10 C	-3.871996	0.481804	0.050361
11 C	-3.656594	-0.830720	-0.377008	11 C	-3.585153	-0.872629	-0.398285
12 C	-2.520203	-1.499530	-0.139081	12 C	-2.459836	-1.530376	-0.062036
13 C	-1.357666	-0.984103	0.681037	13 C	-1.349132	-0.979239	0.788354
14 O	-0.951507	-1.662028	1.599051	14 O	-0.933855	-1.634002	1.716932
15 C	-1.520206	1.337135	-0.306607	15 C	-1.502897	1.358175	-0.073204
16 C	-2.932541	1.456927	0.203011	16 C	-2.945610	1.460937	0.194692
17 O	-1.075673	2.300755	-0.933857	17 O	-0.976837	2.451646	-0.530180
18 Cl	-2.225933	-3.068753	-0.776229	18 Cl	-2.166566	-3.145032	-0.569878
19 Cl	-4.919306	-1.513759	-1.335890	19 Cl	-4.786930	-1.640298	-1.371466
20 Cl	-5.476222	0.818516	0.755019	20 Cl	-5.526245	0.811888	0.408368
21 H	0.625892	2.054577	-1.026464	21 H	0.070892	2.270412	-0.603916
22 C	1.818520	-0.583212	0.543903	22 C	1.835953	-0.612649	0.550108
23 C	1.690765	-2.004126	-0.028925	23 C	1.654005	-1.975173	-0.135213
24 H	1.604926	-1.975551	-1.118308	24 H	1.515351	-1.853808	-1.212956
25 H	2.581268	-2.585014	0.215782	25 H	2.541440	-2.592416	0.014545
26 H	0.827028	-2.523211	0.383786	26 H	0.800759	-2.515177	0.274703
27 C	1.855472	-0.559523	2.085042	27 C	1.953504	-0.729589	2.083802
28 H	2.736113	-1.097765	2.441194	28 H	2.849118	-1.299139	2.340788
29 H	1.925806	0.468878	2.450094	29 H	2.050837	0.261508	2.535653
30 H	0.959539	-1.024112	2.492911	30 H	1.078998	-1.225603	2.500649
31 C	4.969534	-1.288081	0.751420	31 C	4.985364	-1.353506	0.526854
32 C	6.722683	0.495064	-0.486903	32 C	6.689205	0.552130	-0.591553
33 C	6.323552	-1.502490	0.790140	33 C	6.338233	-1.573993	0.477504
34 C	7.212853	-0.606106	0.164802	34 C	7.201920	-0.615515	-0.088476
35 H	8.281259	-0.789341	0.203058	35 H	8.269810	-0.803341	-0.122076
36 H	4.310705	-1.992123	1.243689	36 H	4.344941	-2.105682	0.970558
37 H	6.714360	-2.371820	1.308766	37 H	6.747770	-2.495230	0.878935
38 Cl	-3.260392	3.014654	0.855062	38 Cl	-3.427753	3.035364	0.703884
39 H	7.399587	1.193651	-0.969817	39 H	7.348086	1.298085	-1.026279
40 H	5.558608	2.572475	-1.681901	40 H	5.484860	2.752059	-1.493184
41 H	3.125571	3.054558	-1.796399	41 H	3.046583	3.242620	-1.439260

Table S6: Optimized structure (Cartesian coordinates, Å) of **8b** isomers calculated by the PBE0/6-311+ G(d,p) method in the gas phase.

	8b (NH)				**8b (OH)**		
	X	Y	Z		X	Y	Z
1 C	5.332260	-1.353617	0.283868	1 C	5.313482	-1.400233	0.041366
2 C	5.349437	-0.028216	-0.220110	2 C	5.317864	-0.026927	-0.315025
3 C	4.127323	0.694752	-0.374001	3 C	4.094872	0.708807	-0.331875
4 C	2.956206	0.005097	0.001646	4 C	2.928597	-0.008888	0.017627
5 C	2.951440	-1.276854	0.488598	5 C	2.946905	-1.341248	0.361602
6 C	4.157115	-1.975421	0.636469	6 C	4.151824	-2.055520	0.379850
7 C	0.756095	-0.439513	0.372305	7 C	0.798349	-0.461410	0.416680
8 N	1.641547	0.464256	-0.053613	8 N	1.627445	0.488497	0.056534
9 C	-0.624992	-0.161252	0.342029	9 C	-0.620989	-0.159156	0.433622
10 C	-3.586855	0.975609	0.110609	10 C	-3.536769	1.006261	0.047565
11 C	-3.639617	-0.298981	-0.601237	11 C	-3.602152	-0.312620	-0.564234
12 C	-2.756630	-1.279062	-0.364862	12 C	-2.746001	-1.306804	-0.260232
13 C	-1.614307	-1.206553	0.623527	13 C	-1.607551	-1.211145	0.715573
14 O	-1.506051	-2.082332	1.453315	14 O	-1.470379	-2.072376	1.554458
15 C	-1.047792	1.185264	0.014396	15 C	-1.017396	1.162558	0.196775
16 C	-2.438402	1.618081	0.393979	16 C	-2.391155	1.650454	0.382263
17 O	-0.286636	2.065335	-0.395158	17 O	-0.157293	2.099131	-0.058486
18 Cl	-2.803450	-2.779134	-1.203046	18 Cl	-2.881998	-2.866289	-0.967890
19 Cl	-4.899673	-0.487421	-1.766295	19 Cl	-4.876016	-0.578905	-1.699026
20 Cl	-5.110193	1.629390	0.592434	20 Cl	-5.057218	1.764418	0.342824
21 H	1.280610	1.370025	-0.377066	21 H	0.797396	1.623896	-0.090823
22 H	4.168174	-2.990315	1.021074	22 H	4.174800	-3.106261	0.652210
23 H	6.277110	-1.877674	0.387722	23 H	6.258608	-1.934635	0.042926
24 C	1.531471	-1.687432	0.816936	24 C	1.542638	-1.768399	0.715623
25 C	1.133590	-2.949279	0.038444	25 C	1.076335	-2.948097	-0.146464
26 H	1.197374	-2.783257	-1.039971	26 H	1.079980	-2.688219	-1.208359
27 H	1.826728	-3.754824	0.295801	27 H	1.762543	-3.787754	-0.004688
28 H	0.127137	-3.279039	0.292924	28 H	0.078508	-3.283222	0.137032
29 C	1.415030	-1.898161	2.338826	29 C	1.505196	-2.115676	2.217713
30 H	2.094162	-2.702465	2.635534	30 H	2.188483	-2.949112	2.403883
31 H	1.707199	-0.994410	2.880421	31 H	1.838999	-1.266696	2.820490
32 H	0.395550	-2.167787	2.609621	32 H	0.500036	-2.399485	2.524411
33 C	6.556916	0.614675	-0.583587	33 C	6.512851	0.648470	-0.660680
34 C	4.151260	2.015030	-0.877085	34 C	4.104623	2.075336	-0.686887
35 C	6.555383	1.896335	-1.070555	35 C	6.497260	1.976593	-1.002253
36 C	5.343094	2.602127	-1.218209	36 C	5.283776	2.695484	-1.015216
37 H	3.224387	2.568161	-0.993131	37 H	3.171039	2.627407	-0.696754
38 H	5.355182	3.616034	-1.603676	38 H	5.285490	3.745728	-1.287577
39 H	7.490419	0.071821	-0.469842	39 H	7.447131	0.094934	-0.650608
40 H	7.489917	2.374261	-1.344683	40 H	7.421596	2.480581	-1.264544
41 Cl	-2.447356	3.114805	1.241813	41 Cl	-2.460693	3.231499	1.065182