



Supporting Information

for

Thiadiazino-indole, thiadiazino-carbazole and benzothiadiazino-carbazole dioxides: synthesis, physicochemical and early ADME characterization of representatives of new tri-, tetra- and pentacyclic ring systems and their intermediates

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Experimental procedures and characterization of compounds (E)-7a, 7b, (E)-7c, (Z)-7c, 7d, (E)-7f, 7g, 7i, 7j, (E)-9a, (E)-9b, 3a–d, 3f, 3g, 3i, 3j, 10a, 10b. Kinetic solubility of compounds 7a–j, 3a–j, (E)-9a, (E)-9b, 10a and 10b; permeability and membrane retention of compounds (E)-7a, (E)-7c, (Z)-7c, 7d, 7e, 3b, 3c and 3e

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Table S1. Calculated physicochemical properties of the compounds (ACD Labs/Percepta^a)

Compound	Molecular weight (Da)	clog <i>P</i> (-)	cp <i>K</i> _a (basic)	No of rings	TPSA (Å ²)	No of hydrogen donors	No of hydrogen acceptors
(<i>E</i>)- 7a	294.37	2.13	3.37	2	82.51	1	6
7b	308.4	2.44	3.37	2	82.51	1	6
(<i>E</i>)- 7c	280.35	1.75	2.46	2	82.51	1	6
(<i>Z</i>)- 7c	280.35	1.75	2.46	2	82.51	1	6
7d	306.38	1.75	3.37	3	82.51	1	6
7e	320.41	2.28	3.11	3	82.51	1	6
(<i>E</i>)- 7f	356.44	3.26	3.29	3	82.51	1	6
7g	370.47	3.57	3.29	3	82.51	1	6
crude 7h	342.42	2.89	2.38	3	82.51	1	6
7i	370.47	2.94	3.72	4	82.18	2	6
7j	384.5	3.15	3.72	4	82.18	2	6
3a	277.34	1.93	-	3	73.91	1	5
3b	291.37	2.28	-	3	73.91	1	5
3c	263.32	1.55	-	3	73.91	1	5
3d	289.35	1.86	-	4	73.91	1	5
3e	303.38	2.26	-	4	73.91	1	5
3f	339.41	3.26	-	4	73.91	1	5
3g	353.44	2.94	-	4	73.91	1	5
3h	325.39	2.49	-	4	73.91	1	5
3i	351.42	3.62	-	5	73.91	1	5
3j	365.45	3.77	-	5	73.91	1	5
(<i>E</i>)- 9a	368.45	2.96	1.49	4	82.51	1	6
(<i>E</i>)- 9b	430.52	4.11	1.41	5	82.51	1	6
10a	351.42	3.56	-	5	73.91	1	5
10b	413.49	4.91	-	6	73.91	1	5

^aACD/Labs Percepta, version: 2019.1.0; <https://www.acdlabs.com/products/percepta/> Accessed: Jan 08, 2025

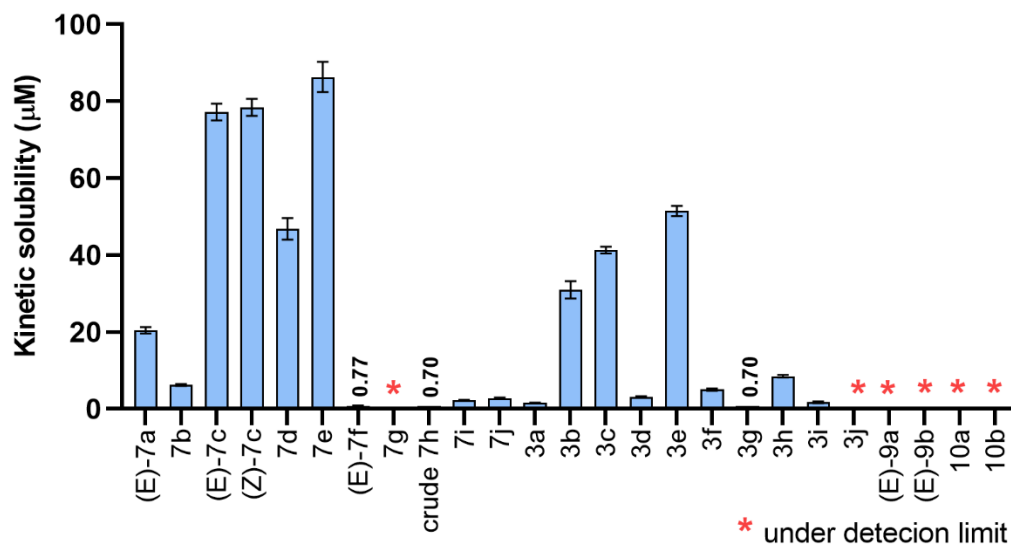


Figure S1. Kinetic solubility of the compounds (PBS pH 7.4, 1–10% DMSO, 2 h, 37 °C; $n = 3$).

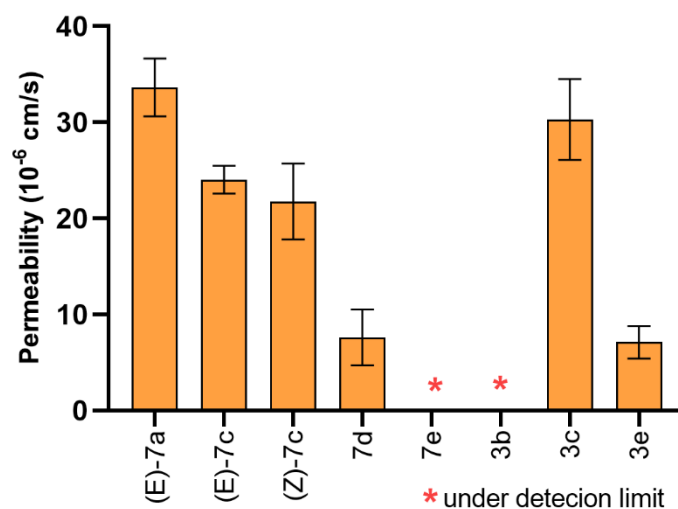


Figure S2. GI PAMPA permeability of the compounds with a minimal kinetic solubility of 10 μM. (membrane PC:chol 4:1; 1% DMSO, donor pH 6.5, acceptor pH 7.4; 4 h, 37 °C; $n = 3$).

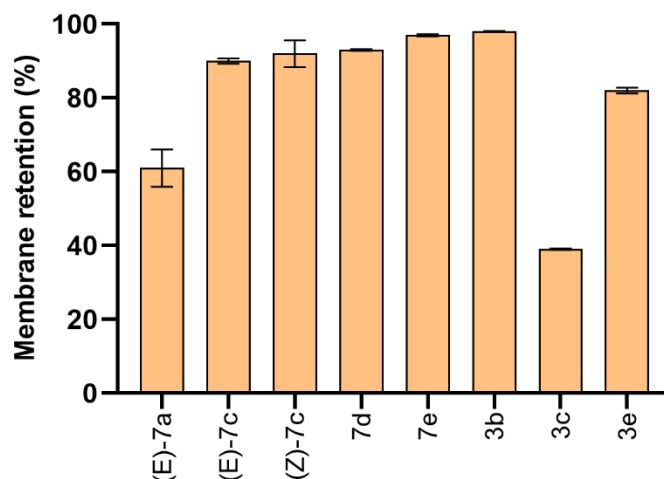


Figure S3. GI PAMPA membrane retention of the compounds with a minimal kinetic solubility of 10 μ M. (membrane PC:chol 4:1; 1% DMSO, donor pH 6.5, acceptor pH 7.4; 4 h, 37 $^{\circ}$ C; n=3)

Experimental procedures and characterization of compounds (E)-7a, 7b, (E)-7c, (Z)-7c, 7d, (E)-7f, 7g, 7i, 7j, (E)-9a, (E)-9b, 3a–d, 3f, 3g, 3i, 3j, 10a, 10b

2,4-Dimethyl-8-[(2E)-2-(1-methylpropylidene)hydrazino]-2H-1,2,3-benzothiadiazine 1,1-dioxide [(E)-7a]. Prepared according to the general procedure, using **5a** and **6a** as the starting materials. Yield: 121.0 mg (99%), crude **7a**, mixture of *E* and *Z* isomers in a 96:4 ratio (according to LC–MS). Pure (E)-**7a** was obtained by purification using flash chromatography (hexane–EtOAc). Yield: 115.0 mg (94%), yellow powder. Mp 99–100 $^{\circ}$ C (EtOH). ^1H NMR (600 MHz, DMSO- d_6): 9.04 (br s, 1H), 7.81 (d, J = 8.5 Hz, 1H), 7.72 (m, 1H), 7.20 (d, J = 7.7 Hz, 1H), 3.38 (s, 3H), 2.44 (s, 3H), 2.34 (q, J = 7.4 Hz, 2H), 1.88 (s, 3H), 1.10 (t, J = 7.4 Hz, 3H). $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, DMSO- d_6): 153.0, 149.9, 141.2, 134.6, 129.2, 116.7 (2C), 113.3, 34.8, 31.5, 20.4, 15.1, 10.8. IR (KBr): 3363, 1570, 1472, 1301, 1151; HRMS (EI) m/z : M^{++} calcd for $\text{C}_{13}\text{H}_{19}\text{N}_4\text{O}_2\text{S}$ 295.1229; found: 295.1228.

8-[2-(1-Ethylpropylidene)hydrazino]-2,4-dimethyl-2H-1,2,3-benzothiadiazine 1,1-dioxide (7b). Prepared according to the general procedure, using **5a** and **6b** as the starting materials. Yield: 106.5 mg (83%), yellow crystals. Mp 94–95 $^{\circ}$ C (EtOH). ^1H NMR (600 MHz, DMSO- d_6): 9.20 (br s, 1H), 7.82 (d, J = 8.4 Hz, 1H), 7.73 (m, 1H), 7.20 (d, J = 7.7 Hz, 1H), 3.38 (s, 3H), 2.44 (s, 3H), 2.35 (q, J = 7.3 Hz, 2H), 2.27 (q, J = 7.7 Hz, 2H), 1.11 (t, J = 7.3 Hz, 3H), 1.10 (t, J = 7.7 Hz, 3H). $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, DMSO- d_6): 157.1, 149.8, 141.3, 134.7,

129.2, 116.7, 116.6, 113.2, 34.8, 29.2, 22.3, 20.4, 10.7, 9.3. IR (KBr): 3355, 1570, 1475, 1297, 1150; HRMS (EI) m/z : M^{+} calcd for $C_{14}H_{20}N_4O_2S$ 308.1301; found: 308.1306.

2,4-Dimethyl-8-[(2*E*)-2-propylidenehydrazino]-2*H*-1,2,3-benzothiadiazine 1,1-dioxide

[(*E*)-7c]. Prepared according to the general procedure, using **5a** and **6c** as the starting materials. Yield: 85 mg (74%), crude **7c**, mixture of *E* and *Z* isomers in a 2:1 ratio (according to LC–MS). Pure (*E*)-**7c** was obtained by purification using flash chromatography (hexane–EtOAc). Yield: 55 mg (48%), colorless crystals. Mp 90–91 °C (EtOH). 1H NMR (600 MHz, DMSO- d_6): 9.40 (br s, 1H), 7.77 (d, J = 8.6 Hz, 1H), 7.69 (m, 1H), 7.57 (t, J = 5.0 Hz, 1H), 7.18 (d, J = 7.6 Hz, 1H), 3.36 (s, 3H), 2.43 (s, 3H), 2.29 (m, 2H), 1.08 (t, J = 7.4 Hz, 3H). $^{13}C\{^1H\}$ NMR (150 MHz, DMSO- d_6): 149.9, 148.8, 141.0, 134.4, 129.3, 117.0, 116.6, 113.2, 34.8, 25.5, 20.4, 10.9. IR (KBr): 3324, 1599, 1472, 1333, 1311, 1156; HRMS (EI) m/z : M^{+} calcd for $C_{12}H_{16}N_4O_2S$ 280.0998; found: 280.0993.

2,4-Dimethyl-8-[(2*Z*)-2-propylidenehydrazino]-2*H*-1,2,3-benzothiadiazine 1,1-dioxide

[(*Z*)-7c]. Prepared according to the general procedure, using **5a** and **6c** as the starting materials. Yield: 85 mg (74%), crude **7c**, mixture of *E* and *Z* isomers in a 2:1 ratio (according to LC–MS). Pure (*Z*)-**7c** was obtained by purification using flash chromatography (hexane–EtOAc). Yield: 26 mg (23%), pale yellow crystals. Mp 110–111 °C (EtOH). 1H NMR (600 MHz, DMSO- d_6): 9.32 (br s, 1H), 7.80 (d, J = 8.4 Hz, 1H), 7.75 (m, 1H), 7.27 (d, J = 7.6 Hz, 1H), 6.74 (t, J = 5.1 Hz, 1H), 3.38 (s, 3H), 2.45 (s, 3H), 2.23 (m, 2H), 1.14 (t, J = 7.5 Hz, 3H). $^{13}C\{^1H\}$ NMR (150 MHz, DMSO- d_6): 149.9, 147.6, 140.8, 134.7, 129.2, 117.5, 116.8, 113.8, 34.8, 20.4, 19.9, 10.3. IR (KBr): 3337, 1601, 1477, 1292, 1157; HRMS (EI) m/z : M^{+} calcd for $C_{12}H_{16}N_4O_2S$ 280.0998; found: 280.0993.

8-(2-Cyclopentylidenehydrazino)-2,4-dimethyl-2*H*-1,2,3-benzothiadiazine 1,1-dioxide

(7d). Prepared according to the general procedure, using **5a** and **6d** as the starting materials. Yield: 117.5 mg (92%), yellow crystals. Mp 121–122 °C (EtOH). 1H NMR (600 MHz, DMSO- d_6): 8.84 (br s, 1H), 7.75 (d, J = 8.5 Hz, 1H), 7.70 (m, 1H), 7.18 (d, J = 7.5 Hz, 1H), 3.37 (s, 3H), 2.44 (s, 3H), 2.42 (t, J = 7.3 Hz, 2H), 2.28 (t, J = 7.3 Hz, 2H), 1.84 (m, 2H), 1.73 (m, 2H). $^{13}C\{^1H\}$ NMR (150 MHz, DMSO- d_6): 161.8, 149.8, 141.1, 134.6, 129.2, 116.6, 116.5, 113.1, 34.8, 32.8, 27.2, 24.7, 24.6, 20.4. IR (KBr): 3337, 1598, 1473, 1297, 1154; HRMS (EI) m/z : M^{+} calcd for $C_{14}H_{18}N_4O_2S$ 306.1150; found: 306.1145.

8-[(2*E*)-2-(3,4-Dihydronaphthalen-1(2*H*)-ylidene)hydrazino]-2,4-dimethyl-2*H*-1,2,3-

benzothiadiazine 1,1-dioxide [(*E*)-9a]. Prepared according to the general procedure, using **5a** and **8** as the starting materials. Yield: 145.5 mg (95%), yellow crystals. Mp 180–181 °C (EtOH).

¹H NMR (600 MHz, DMSO-*d*₆): 9.46 (br s, 1H), 8.12 (m, 1H), 8.05 (d, *J* = 8.5 Hz, 1H), 7.80 (m, 1H), 7.28 (m, 3H), 7.21 (m, 1H), 3.41 (s, 3H), 2.76 (m, 2H), 2.63 (t, *J* = 6.4 Hz, 2H), 2.47 (s, 3H), 1.92 (m, 2H). ¹³C{¹H} NMR (150 MHz, DMSO-*d*₆): 150.0, 146.6, 140.7, 139.5, 134.8, 132.5, 129.3, 128.8, 128.7, 126.6, 124.3, 117.5, 117.1, 114.1, 34.8, 28.9, 24.8, 21.3, 20.4. IR (KBr): 3346, 1572, 1473, 1311, 1293, 1104; HRMS (EI) *m/z*: M⁺ calcd for C₁₉H₂₀N₄O₂S 368.1307; found: 368.1296.

2-Methyl-8-[(2*E*)-2-(1-methylpropylidene)hydrazino]-4-phenyl-2*H*-1,2,3-

benzothiadiazine 1,1-dioxide [(*E*)-7f]. Prepared according to the general procedure, using **5b** and **6a** as the starting materials. Yield: 110.0 mg (93%), crude **7f**, mixture of *E* and *Z* isomers in a 9:1 ratio (according to LC–MS). Pure (*E*)-**7f** was obtained by purification using flash chromatography (hexane–EtOAc). Yield: 100.3 mg (84%), yellow crystals. Mp 123–124 °C (EtOH). ¹H NMR (600 MHz, DMSO-*d*₆): 9.11 (br s, 1H), 7.84 (d, *J* = 8.5 Hz, 1H), 7.66 (m, 1H), 7.58 (m, 2H), 7.54 (m, 3H), 6.74 (d, *J* = 7.6 Hz, 1H), 3.49 (s, 3H), 2.35 (q, *J* = 7.4 Hz, 2H), 1.92 (s, 3H), 1.11 (t, *J* = 7.4 Hz, 3H). ¹³C{¹H} NMR (150 MHz, DMSO-*d*₆): 153.4, 152.7, 141.4, 134.9, 134.5, 130.0, 129.1 (2C), 128.9 (2C), 128.8, 118.5, 117.0, 114.0, 35.3, 31.5, 15.1, 10.8. IR (KBr): 3359, 1592, 1469, 1315, 1299, 1151; HRMS (EI) *m/z*: M⁺ calcd for C₁₈H₂₀N₄O₂S 356.1310; found: 356.1304.

8-[2-(1-Ethylpropylidene)hydrazino]-2-methyl-4-phenyl-2*H*-1,2,3-benzothiadiazine 1,1-dioxide (7g). Prepared according to the general procedure, using **5b** and **6b** as the starting materials. Yield: 108.0 mg (88%), yellow crystals. Mp 160–161 °C (EtOH). ¹H NMR (600 MHz, DMSO-*d*₆): 9.26 (br s, 1H), 7.85 (d, *J* = 8.5 Hz, 1H), 7.66 (m, 1H), 7.58 (m, 2H), 7.55 (m, 1H), 7.54 (m, 2H), 6.74 (d, *J* = 8.5 Hz, 1H), 3.50 (s, 3H), 2.37 (q, *J* = 7.3 Hz, 2H), 2.31 (q, *J* = 7.7 Hz, 2H), 1.13 (t, *J* = 7.7 Hz, 3H), 1.12 (t, *J* = 7.3 Hz, 3H). ¹³C{¹H} NMR (150 MHz, DMSO-*d*₆): 157.4, 152.7, 141.4, 134.9, 134.5, 130.0, 129.1 (2C), 128.9 (2C), 128.7, 118.5, 116.9, 113.9, 35.3, 29.2, 22.4, 10.1, 9.3. IR (KBr): 3367, 1594, 1471, 1317, 1299, 1152; HRMS (EI) *m/z*: M⁺ calcd for C₁₉H₂₂N₄O₂S 370.1463; found: 370.1465.

8-(2-Cyclopentylidenehydrazino)-2-methyl-4-phenyl-2*H*-1,2,3-benzothiadiazine 1,1-dioxide (7i). Prepared according to the general procedure, using **5b** and **6d** as the starting materials. Yield: 114.6 mg (94%), yellow crystals. Mp 151–152 °C (EtOH). ¹H NMR (600 MHz, DMSO-*d*₆): 8.91 (br s, 1H), 7.78 (d, *J* = 8.5 Hz, 1H), 7.64 (m, 1H), 7.58 (m, 2H), 7.55 (m, 1H), 7.54 (m, 2H), 6.73 (d, *J* = 7.7 Hz, 1H), 3.49 (s, 3H), 2.44 (t, *J* = 7.1 Hz, 2H), 2.32 (t, *J* = 7.1 Hz, 2H), 1.86 (m, 2H), 1.74 (m, 2H). ¹³C{¹H} NMR (150 MHz, DMSO-*d*₆): 162.1, 152.7, 141.3, 134.9, 134.5, 130.0, 129.1 (2C), 128.9 (2C), 128.8, 118.5, 116.8, 113.8, 35.2, 32.9,

27.3, 24.7, 24.6. IR (KBr): 3343, 1591, 1469, 1348, 1153, 1106, 692; HRMS (ESI) m/z : $[M+H]^+$ calcd for $C_{19}H_{21}N_4O_2S$ 369.1380; found: 369.1381.

8-(2-Cyclohexylidenehydrazino)-2-methyl-4-phenyl-2*H*-1,2,3-benzothiadiazine 1,1-dioxide (7j). Prepared according to the general procedure, using **5b** and **6e** as the starting materials. Yield: 116.4 mg (92%), yellow crystals. Mp 175–176 °C (EtOH). 1H NMR (600 MHz, DMSO- d_6): 9.26 (br s, 1H), 7.83 (d, J = 8.6 Hz, 1H), 7.64 (m, 1H), 7.58 (m, 2H), 7.55 (m, 1H), 7.54 (m, 2H), 6.73 (d, J = 7.7 Hz, 1H), 3.49 (s, 3H), 2.35 (m, 4H), 1.67 (m, 4H), 1.62 (m, 2H). $^{13}C\{^1H\}$ NMR (150 MHz, DMSO- d_6): 155.2, 152.7, 141.5, 134.9, 134.5, 130.0, 129.1 (2C), 128.9 (2C), 128.8, 118.4, 116.8, 113.9, 35.3, 34.9, 26.7, 26.1, 25.4, 25.2. IR (KBr): 3367, 1593, 1472, 1299, 1152, 733; HRMS (EI) m/z : M^{+} calcd for $C_{20}H_{22}N_4O_2S$ 382.1463; found: 382.1467.

8-[(2*E*)-2-(3,4-Dihydronaphthalen-1(2*H*)-ylidene)hydrazino]-2-methyl-4-phenyl-2*H*-1,2,3-benzothiadiazine 1,1-dioxide [(*E*)-9b]. Prepared according to the general procedure, using **5b** and **8** as the starting materials. Yield: 145.0 mg (95%), orange crystals. Mp 235–236 °C (EtOH). 1H NMR (600 MHz, DMSO- d_6): 9.53 (br s, 1H), 8.15 (m, 1H), 8.09 (d, J = 8.5 Hz, 1H), 7.74 (m, 1H), 7.61 (m, 2H), 7.57 (m, 1H), 7.56 (m, 2H), 7.29 (m, 1H), 7.28 (m, 1H), 7.22 (m, 1H), 6.83 (m, 1H), 3.52 (s, 3H), 2.78 (m, 2H), 2.68 (t, J = 6.5 Hz, 2H), 1.94 (m, 2H). $^{13}C\{^1H\}$ NMR (150 MHz, DMSO- d_6): 152.8, 146.9, 140.9, 139.6, 134.8, 134.7, 132.5, 130.1, 129.1 (2C), 128.9 (3C), 128.8, 128.7, 126.6, 124.4, 119.3, 117.5, 114.6, 35.3, 28.9, 24.9, 21.3. 1H NMR (600 MHz, $CDCl_3$): 9.63 (br s, 1H), 8.18 (m, 1H), 8.07 (d, J = 8.4 Hz, 1H), 7.62 (m, 2H), 7.52 (m, 1H), 7.48 (m, 3H), 7.25 (m, 2H*, overlapping with the solvent signal), 7.16 (m, 1H), 6.81 (d, J = 7.8 Hz, 1H), 3.61 (s, 3H), 2.81 (m, 2H), 2.72 (t, J = 6.6 Hz, 2H), 2.03 (m, 2H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$): 153.1, 146.0, 141.3, 139.2, 135.3, 133.4, 132.9, 129.6, 129.4, 129.1 (2C), 128.5 (3C), 128.4, 126.5, 124.4, 119.0, 117.2, 114.9, 35.4, 29.6, 25.1, 21.6. IR (KBr): 3329, 1589, 1465, 1315, 1153, 1105, 721; HRMS (EI) m/z : M^{+} calcd for $C_{24}H_{22}N_4O_2S$ 430.1463; found: 430.1467.

2,4,7,8-Tetramethyl-2,9-dihydro[1,2,3]thiadiazino[5,6-*g*]indole 1,1-dioxide (3a). Prepared according to Method A, using crude **7a** as the starting material. Yield: 70 mg (65%). Prepared according to Method B, using **5a** and **6a** as the starting materials. Yield: 102.0 mg (47%), yellow crystals. Mp 188–189 °C. 1H NMR (600 MHz, DMSO- d_6): 11.35 (br s, 1H), 7.87 (d, J = 8.4 Hz, 1H), 7.42 (d, J = 8.4 Hz, 1H), 3.40 (s, 3H), 2.51 (s, 3H), 2.44 (s, 3H), 2.23 (s, 3H). $^{13}C\{^1H\}$ NMR (150 MHz, DMSO- d_6): 150.1, 138.9, 133.3, 125.4, 122.4, 120.8, 116.6, 114.9, 107.8,

34.5, 20.7, 11.7, 8.2. IR (KBr): 3373, 1304, 1185, 1153, 1123; HRMS (EI) m/z : M^{+} calcd for $C_{13}H_{15}N_3O_2S$ 277.0879; found: 277.0883.

8-Ethyl-2,4,7-trimethyl-2,9-dihydro[1,2,3]thiadiazino[5,6-g]indole 1,1-dioxide (3b).

Prepared according to Method A, using crude **7b** as the starting material. Yield: 88.0 mg (92%).

Prepared according to Method B, using **5a** and **6b** as the starting materials. Yield: 61.0 mg (50%), off-white crystals. Mp 190–191 °C. 1H NMR (600 MHz, DMSO- d_6): 11.32 (br s, 1H), 7.89 (d, J = 8.4 Hz, 1H), 7.43 (d, J = 8.4 Hz, 1H), 3.41 (s, 3H), 2.85 (q, J = 7.5 Hz, 2H), 2.51 (s, 3H), 2.25 (s, 3H), 1.20 (t, J = 7.5 Hz, 3H). $^{13}C\{^1H\}$ NMR (150 MHz, DMSO- d_6): 150.1, 144.7, 133.4, 125.4, 122.6, 121.0, 116.6, 115.1, 107.0, 34.6, 20.7, 19.1, 14.7, 8.1. IR (KBr): 3388, 3363, 1303, 1186, 1123; HRMS (EI) m/z : M^{+} calcd for $C_{14}H_{18}N_3O_2S$ 292.1120; found: 292.1110.

2,4,7-Trimethyl-2,9-dihydro[1,2,3]thiadiazino[5,6-g]indole 1,1-dioxide (3c).

Prepared according to Method A, using crude **7c** as the starting material. Yield: 42.5 mg (46%). Prepared according to Method B, using **5a** and **6c** as the starting materials. Yield: 33.0 mg (30%), yellow crystals. Mp 192–193 °C (EtOH). 1H NMR (600 MHz, DMSO- d_6): 11.42 (br s, 1H), 8.01 (d, J = 8.4 Hz, 1H), 7.48 (d, J = 8.4 Hz, 1H), 7.44 (br s, 1H), 3.42 (s, 3H), 2.53 (s, 3H), 2.34 (s, 3H). $^{13}C\{^1H\}$ NMR (150 MHz, DMSO- d_6): 149.9, 132.4, 128.9, 126.3, 123.8, 122.0, 116.5, 115.5, 111.6, 34.6, 20.7, 9.3. IR (KBr): 3377, 1305, 1187, 1140, 1081; HRMS (ESI) m/z : $[M+H]^+$ calcd for $C_{12}H_{13}N_3O_2S$: 263.0723; found: 263.0727.

2,4-Dimethyl-7,8,9,10-tetrahydro-2H-cyclopenta[b][1,2,3]thiadiazino[5,6-g]indole 1,1-dioxide (3d).

Prepared according to Method A, using crude **7d** as the starting material. Yield: 30.2 mg (33%). Prepared according to Method B, using **5a** and **6d** as the starting materials. Yield: 30.0 mg (25%), yellow crystals. Mp 198–199 °C (decomp). 1H NMR (600 MHz, DMSO- d_6): 11.51 (br s, 1H), 7.80 (d, J = 8.4 Hz, 1H), 7.42 (d, J = 8.4 Hz, 1H), 3.41 (s, 3H), 2.91 (t, J = 7.2 Hz, 2H), 2.81 (t, J = 7.0 Hz, 2H), 2.50 (s, 3H), 2.50 (m, 2H). $^{13}C\{^1H\}$ NMR (150 MHz, DMSO- d_6): 151.9, 150.1, 130.5, 128.2, 122.8, 120.4, 119.6, 117.1, 115.8, 34.6, 28.4, 26.2, 23.9, 20.6. IR (KBr): 3373, 1310, 1136, 1102; HRMS (EI) m/z : M^{+} calcd for $C_{14}H_{15}N_3O_2S$ 289.0885; found: 289.0884.

2,7,8-Trimethyl-4-phenyl-2,9-dihydro[1,2,3]thiadiazino[5,6-g]indole 1,1-dioxide (3f).

Prepared according to Method A, using crude **7f** as the starting material. Yield: 6.07 mg (70%).

Prepared according to Method B, using **5b** and **6a** as the starting materials. Yield: 75.0 mg (67%), yellow crystals. Mp 122–123 °C (EtOH). 1H NMR (600 MHz, DMSO- d_6): 11.50 (br s, 1H), 7.80 (d, J = 8.5 Hz, 1H), 7.61 (m, 2H), 7.55 (m, 3H), 7.00 (d, J = 8.5 Hz, 1H), 3.52 (s,

3H), 2.47 (s, 3H), 2.21 (s, 3H). $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, DMSO- d_6): 153.1, 139.4, 135.7, 133.4, 129.8, 129.3 (2C), 128.8 (2C), 125.5, 122.2, 120.0, 118.3, 115.7, 108.0, 35.0, 11.7, 8.2. IR (KBr): 3389, 1357, 1312, 1123, 696, 592; HRMS (EI) m/z : M^{+} calcd for $\text{C}_{18}\text{H}_{17}\text{N}_3\text{O}_2\text{S}$ 339.1041; found: 339.1034.

8-Ethyl-2,7-dimethyl-4-phenyl-2,9-dihydro[1,2,3]thiadiazino[5,6-g]indole 1,1-dioxide

(3g). Prepared according to Method A, using crude **7g** as the starting material. Yield: 71.0 mg (75%). Prepared according to Method B, using **5b** and **6b** as the starting materials. Yield: 70.0 mg (60%), yellow crystals. Mp 133–134 °C (EtOH). ^1H NMR (600 MHz, DMSO- d_6): 11.47 (br s, 1H), 7.82 (d, $J = 8.5$ Hz, 1H), 7.61 (m, 2H), 7.55 (m, 3H), 7.01 (d, $J = 8.5$ Hz, 1H), 3.53 (s, 3H), 2.88 (q, $J = 7.6$ Hz, 2H), 2.24 (s, 3H), 1.23 (t, $J = 7.6$ Hz, 3H). $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, DMSO- d_6): 153.2, 145.1, 135.7, 133.5, 129.8, 129.2 (2C), 128.8 (2C), 125.5, 122.3, 120.2, 118.3, 116.0, 107.2, 35.0, 19.1, 14.7, 8.0. IR (KBr): 3367, 1360, 1309, 1124; HRMS (EI) m/z : M^{+} calcd for $\text{C}_{19}\text{H}_{19}\text{N}_3\text{O}_2\text{S}$ 353.1198; found: 353.1196.

2-Methyl-4-phenyl-7,8,9,10-tetrahydro-2H-cyclopenta[b][1,2,3]thiadiazino[5,6-g]indole 1,1-dioxide (3i).

Prepared according to Method A, using crude **7i** as the starting material. Yield: 43.0 mg (45%). Prepared according to Method B, using **5b** and **6d** as the starting materials. Yield: 41.0 mg (35%), yellow crystals. Mp 150–151 °C (EtOH). ^1H NMR (600 MHz, DMSO- d_6): 11.65 (br s, 1H), 7.74 (d, $J = 8.4$ Hz, 1H), 7.60 (m, 2H), 7.55 (m, 3H), 7.00 (d, $J = 8.4$ Hz, 1H), 3.52 (s, 3H), 3.94 (m, 2H), 2.80 (m, 2H), 2.51 (m, 2H). $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, DMSO- d_6): 153.1, 152.4, 135.7, 130.6, 129.8, 129.3 (2C), 128.8 (2C), 128.2, 122.6, 119.8, 119.6, 118.8, 116.7, 35.0, 28.4, 26.2, 23.9. IR (KBr): 3438, 1347, 1316, 1135, 1105, 694; HRMS (EI) m/z : M^{+} calcd for $\text{C}_{19}\text{H}_{17}\text{N}_3\text{O}_2\text{S}$ 351.1041; found: 351.1042.

2-Methyl-4-phenyl-2,7,8,9,10,11-hexahydro[1,2,3]thiadiazino[6,5-a]carbazole 1,1-dioxide

(3j). Prepared according to Method A, using crude **7j** as the starting material. Yield: 63.5 mg (66%). Prepared according to Method B, using **5b** and **6e** as the starting materials. Yield: 81.0 mg (67%), yellow crystals. Mp 190 °C (decomp). ^1H NMR (600 MHz, DMSO- d_6): 11.52 (br s, 1H), 7.78 (d, $J = 8.4$ Hz, 1H), 7.60 (m, 2H), 7.55 (m, 1H), 7.54 (m, 2H), 7.00 (d, $J = 8.4$ Hz, 1H), 3.52 (s, 3H), 2.85 (m, 2H), 2.68 (m, 2H), 1.86 (m, 2H), 1.82 (m, 2H). $^{13}\text{C}\{^1\text{H}\}$ NMR (150 MHz, DMSO- d_6): 153.1, 142.2, 135.7, 131.9, 129.8, 129.3 (2C), 128.8 (2C), 126.0, 122.0, 120.1, 118.3, 116.0, 110.7, 35.0, 23.4, 22.7, 22.6, 20.4. IR (KBr): 3385, 1305, 1163, 1123, 697; HRMS (EI) m/z : M^{+} calcd for $\text{C}_{20}\text{H}_{19}\text{N}_3\text{O}_2\text{S}$ 365.1198; found: 365.1195.

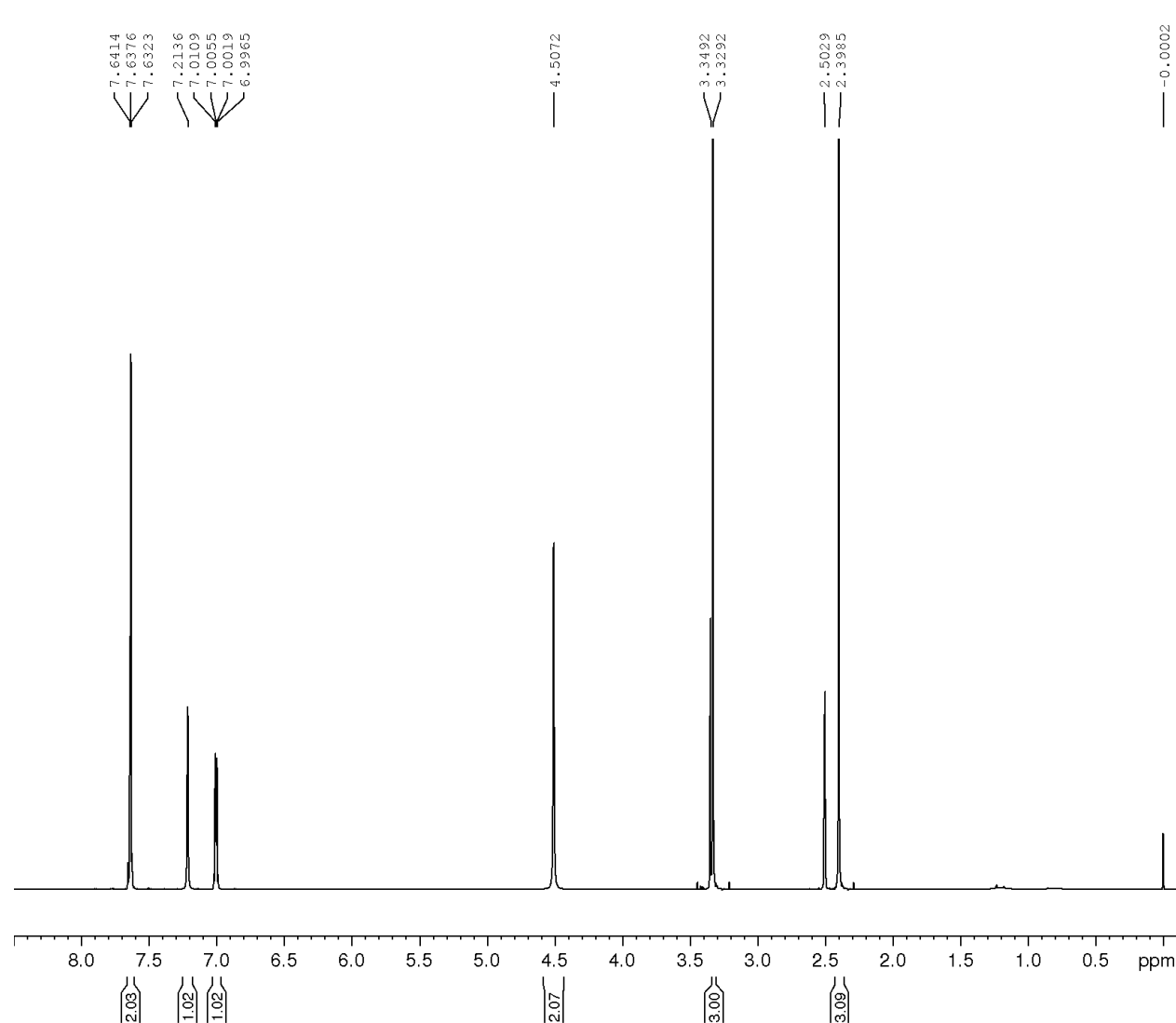
2,4-Dimethyl-2,13-dihydrobenzo[a][1,2,3]thiadiazino[5,6-i]carbazole 1,1-dioxide (10a).

Prepared according to Method A, using crude (*E*)-**9a** as the starting material. Yield: 76 mg

(80%), yellow crystals. Mp 223–224 °C (EtOH). ¹H NMR (600 MHz, DMSO-*d*₆): 12.31 (br s, 1H), 9.12 (d, *J* = 8.0 Hz, 1H), 8.74 (d, *J* = 8.0 Hz, 1H), 8.38 (d, *J* = 8.0 Hz, 1H), 8.11 (d, *J* = 7.6 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.70 (m, 1H), 7.66 (m, 1H), 3.50 (s, 3H), 2.62 (s, 3H). ¹³C{¹H} NMR (150 MHz, DMSO-*d*₆): 150.2, 138.1, 133.2, 129.7, 128.8, 128.1, 126.8, 126.2, 124.8, 124.6, 123.9, 121.9, 121.5, 119.3, 117.9, 117.1, 115.9, 34.8, 20.8. IR (KBr): 3366, 1313, 1137, 801; HRMS (EI) *m/z*: M⁺ calcd for C₁₉H₁₅N₃O₂S 349.0889; found: 349.0883.

2-Methyl-4-phenyl-2,13-dihydrobenzo[*a*][1,2,3]thiadiazino[5,6-*i*]carbazole 1,1-dioxide (10b). Prepared according to Method A, using crude (*E*)-**9b** as the starting material. Yield: 80 mg (84%), orange crystals. Mp 259–260 °C (EtOH). ¹H NMR (600 MHz, DMSO-*d*₆): 12.48 (br s, 1H), 9.13 (d, *J* = 8.0 Hz, 1H), 8.66 (d, *J* = 8.3 Hz, 1H), 8.34 (d, *J* = 8.5 Hz, 1H), 8.11 (d, *J* = 8.0 Hz, 1H), 7.82 (d, *J* = 8.5 Hz, 1H), 7.72 (m, 1H), 7.70 (m, 2H), 7.67 (m, 1H), 7.60 (m, 1H), 7.59 (m, 2H), 7.30 (d, *J* = 8.3 Hz, 1H), 3.62 (s, 3H). ¹³C{¹H} NMR (150 MHz, DMSO-*d*₆): 153.0, 138.4, 135.5, 133.3, 130.0, 129.8, 129.3 (2C), 128.9 (2C), 128.8, 128.2, 126.9, 126.3, 124.6, 123.9, 123.8, 122.0, 121.5, 119.5, 119.2, 117.0, 116.9, 35.2. IR (KBr): 3453, 2923, 1315, 1299, 1135, 797, 727, 693; HRMS (EI) *m/z*: M⁺ calcd for C₂₄H₁₇N₃O₂S 411.1047; found: 411.1037.

¹H NMR spectrum of **5a**



Standard 1H
142437
PGY0668_1
Pusztai Gyongyver
2024.04.11. (KP)

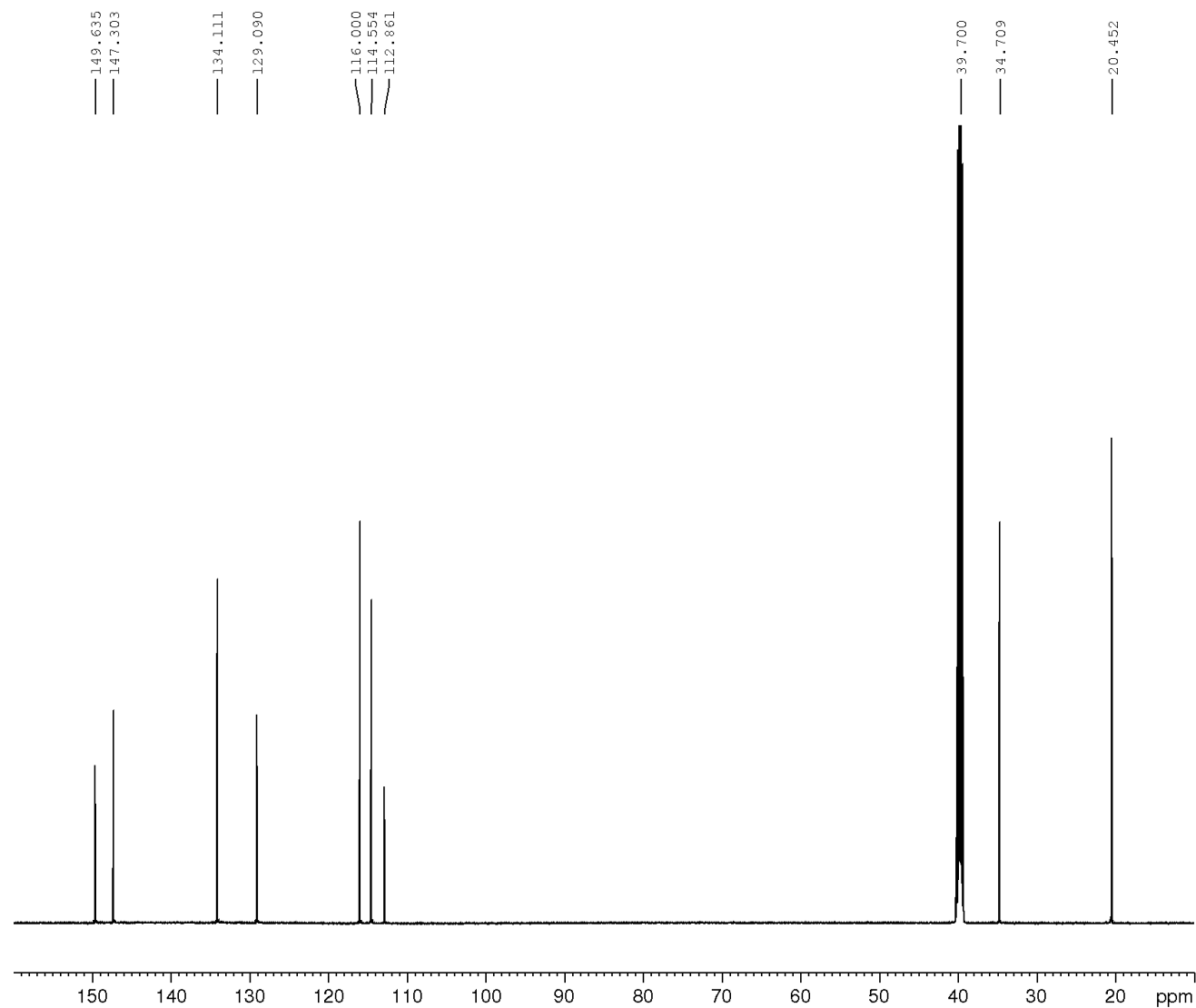
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EXPNO 21
PROCNO 1

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PULPROG zg30
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SOLVENT DMSO
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DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000031 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of **5a**



Standard 13C
142437
PGY0668_1
Pusztai Gyongyver
2024.04.11. (KP)

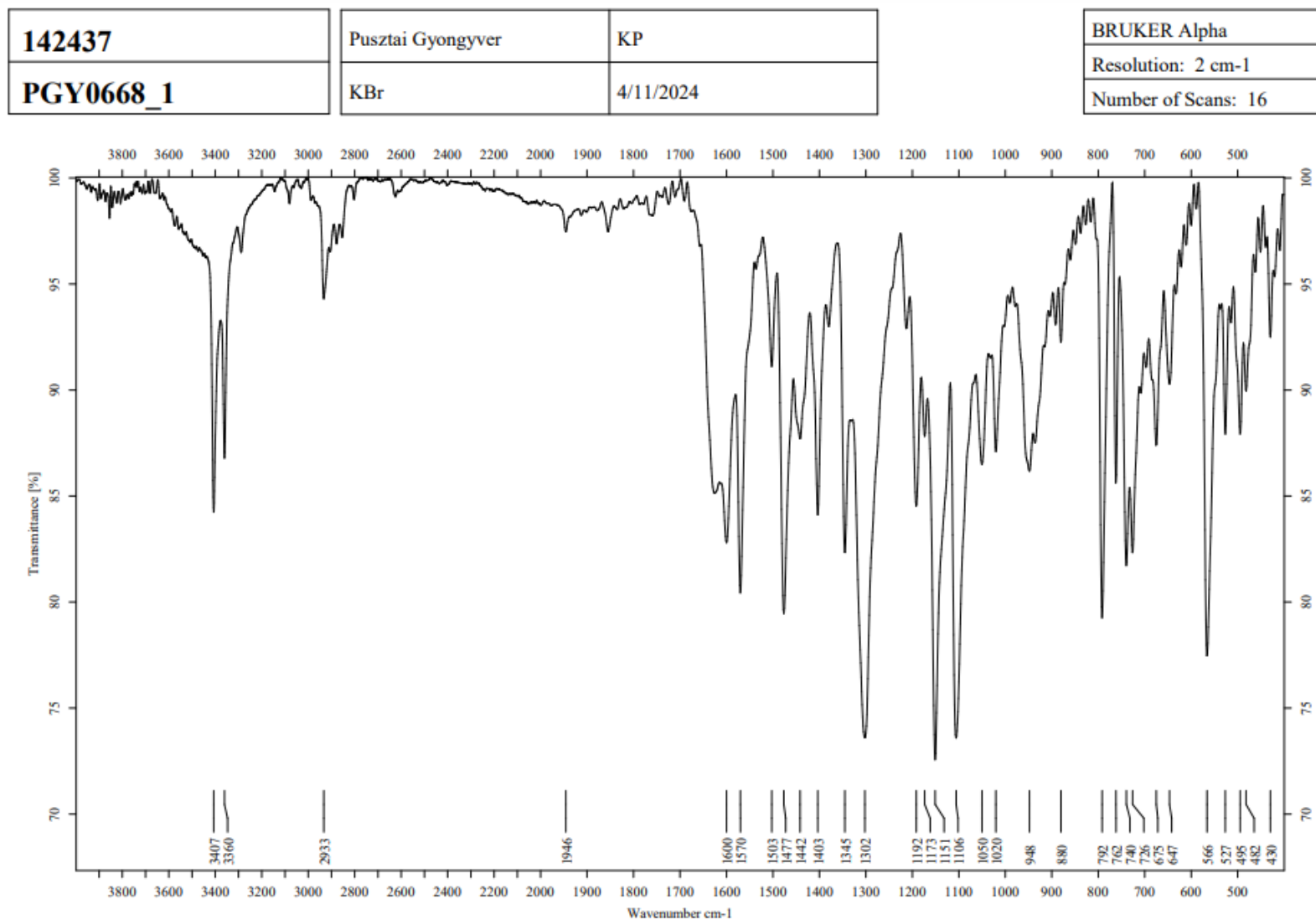
Current Data Parameters
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EXPNO 22
PROCNO 1

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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of 5a

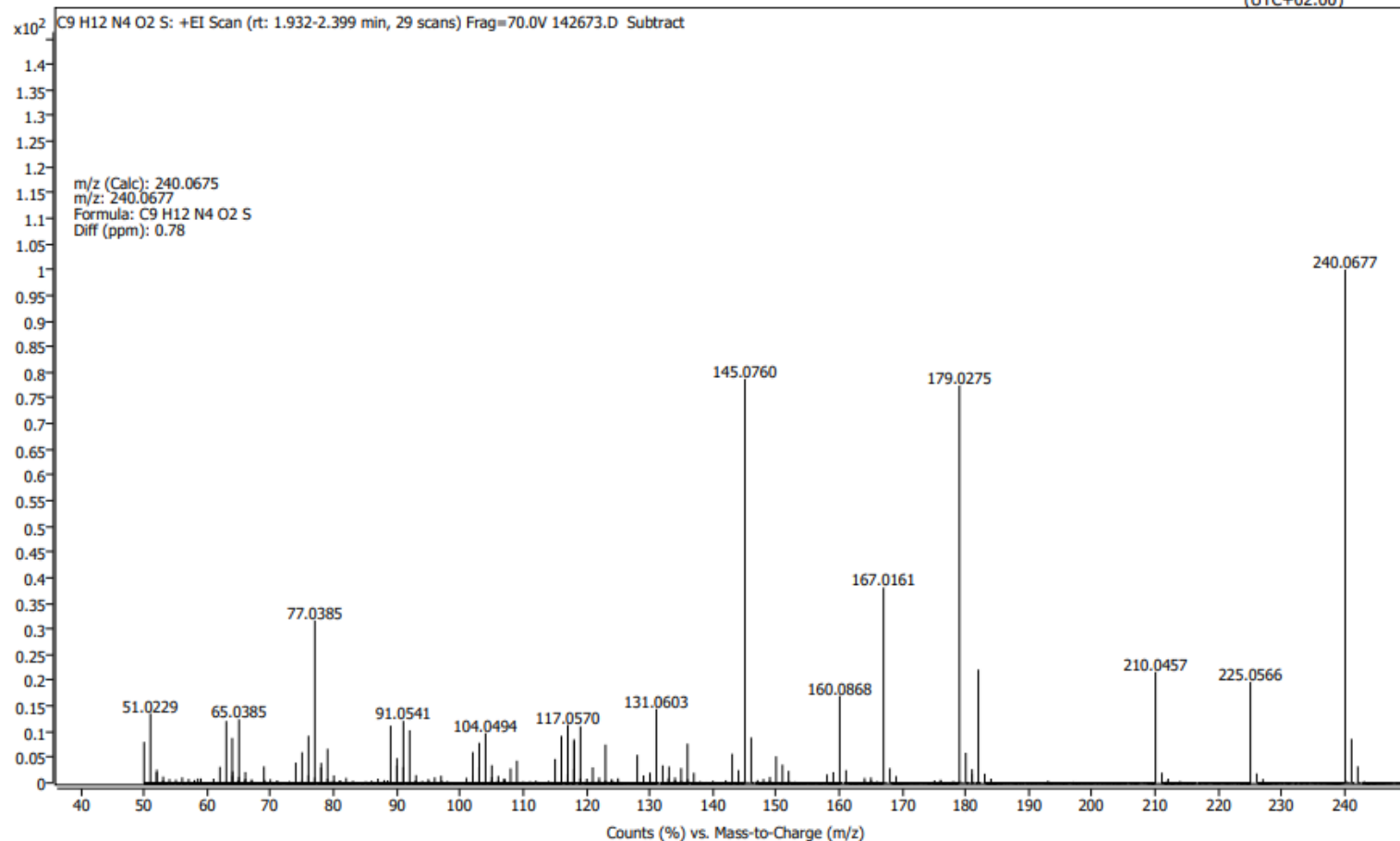


HRMS spectrum of 5a

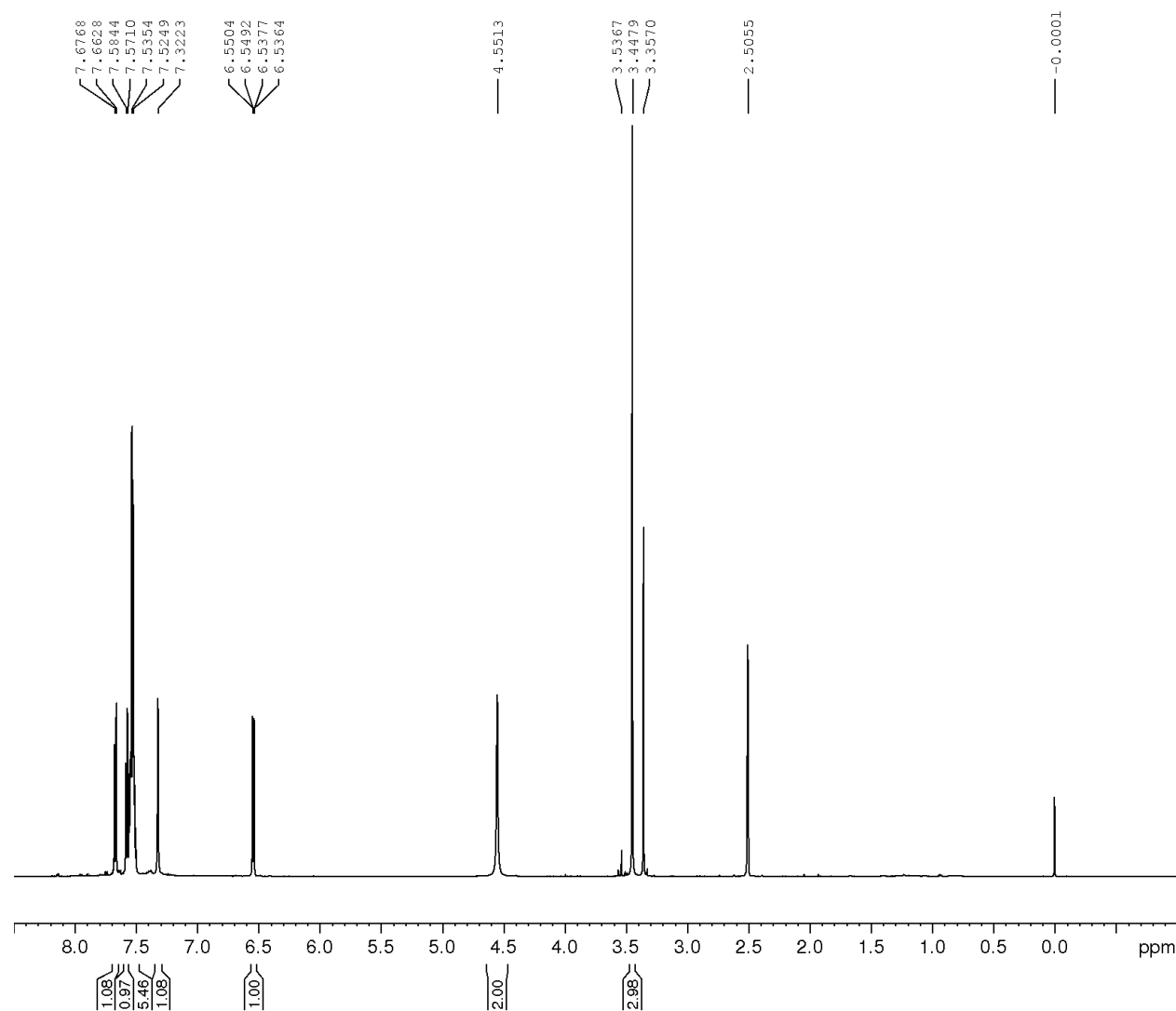
Spectrum Plot Report



Name	PGY0668_1, Pusztai Gyongyver	Rack Pos.	Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	Plate Pos.	IRM Status	Success	Acq. Time (Local)	4/16/2024 2:29:07 PM
Data File	142437.D	Method (Acq)	DIP_70eV.M	Comment		(UTC+02:00)



¹H NMR spectrum of **5b**



Standard 1H
143047
PGY0747_1
Pusztai Gyongyver
2024.09.13. (KP)

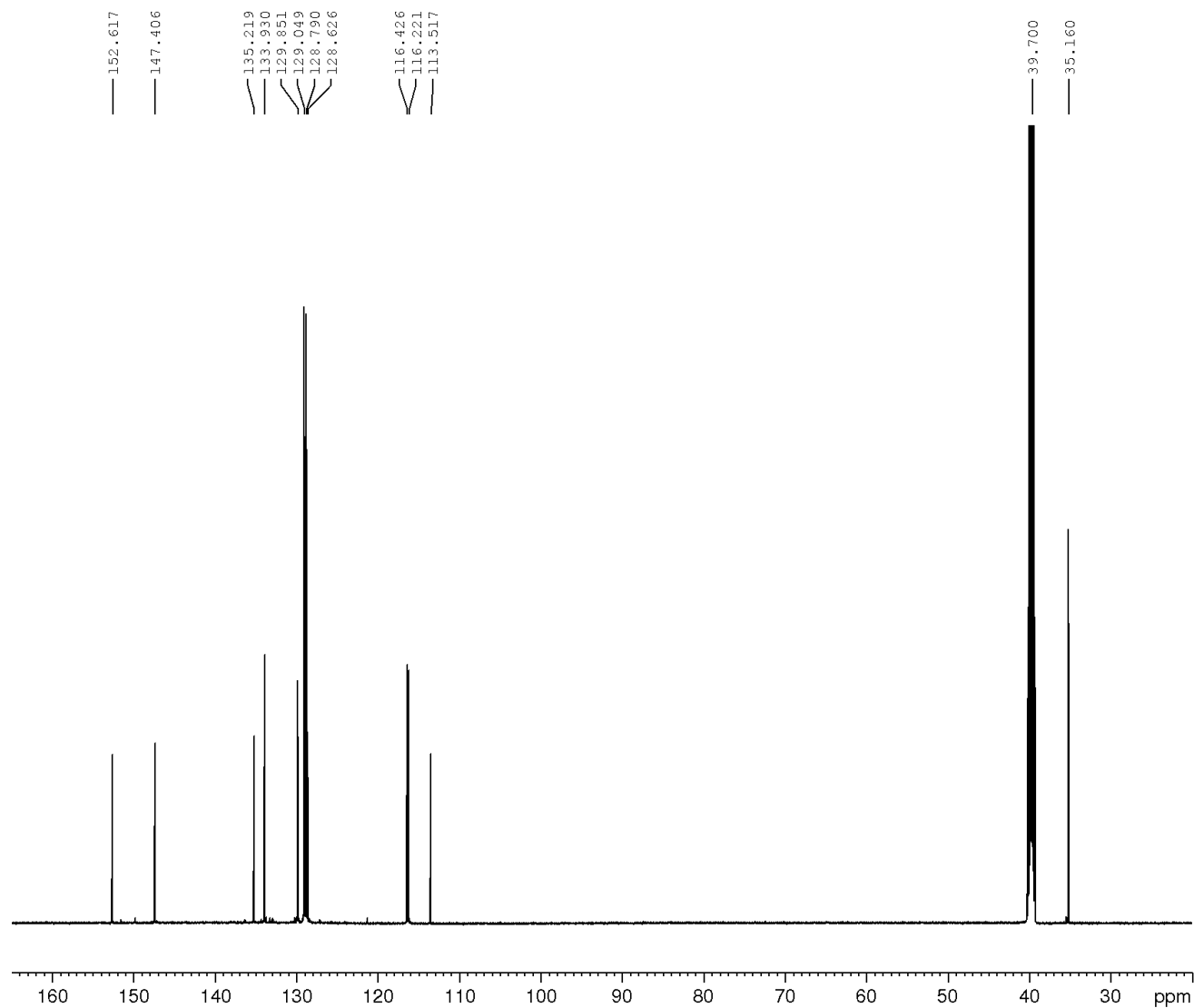
Current Data Parameters
NAME 143047
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
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Time 22.52 h
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 133.88
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000016 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of **5b**



Standard 13C
143047
PGY0747_1
Pusztai Gyongyver
2024.09.13. (KP)

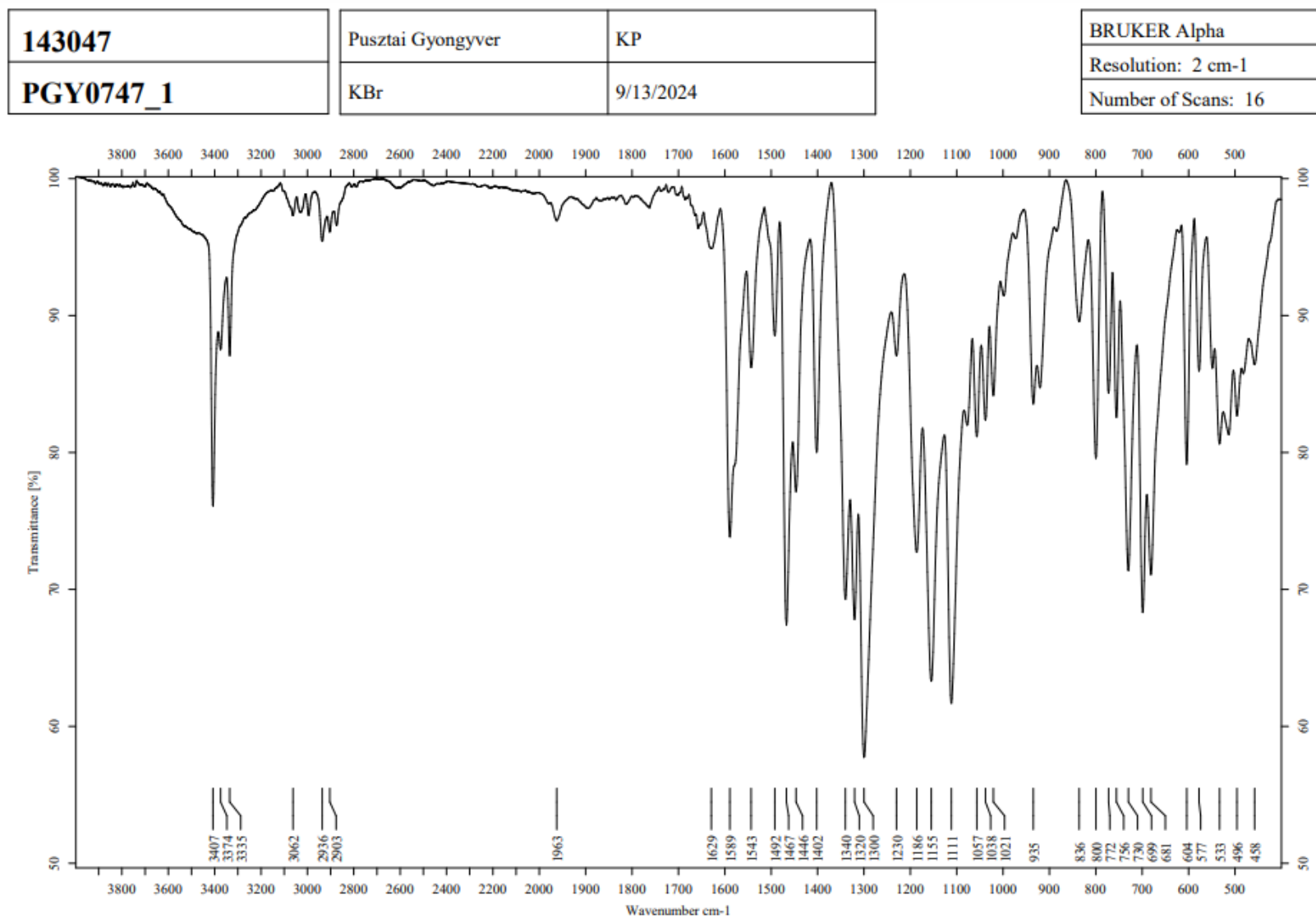
Current Data Parameters
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EXPNO 22
PROCNO 1

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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of **5b**

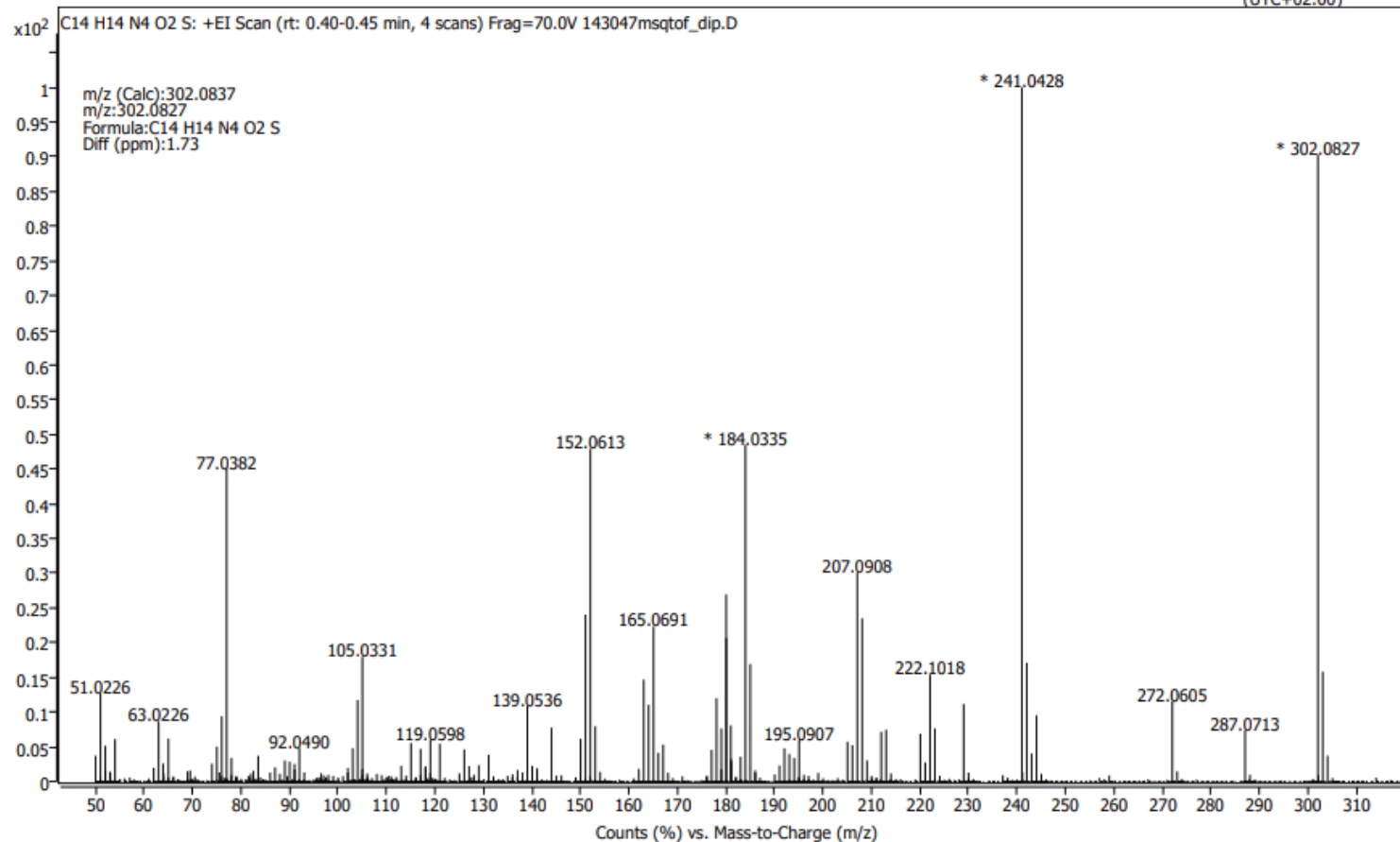


HRMS spectrum of **5b**

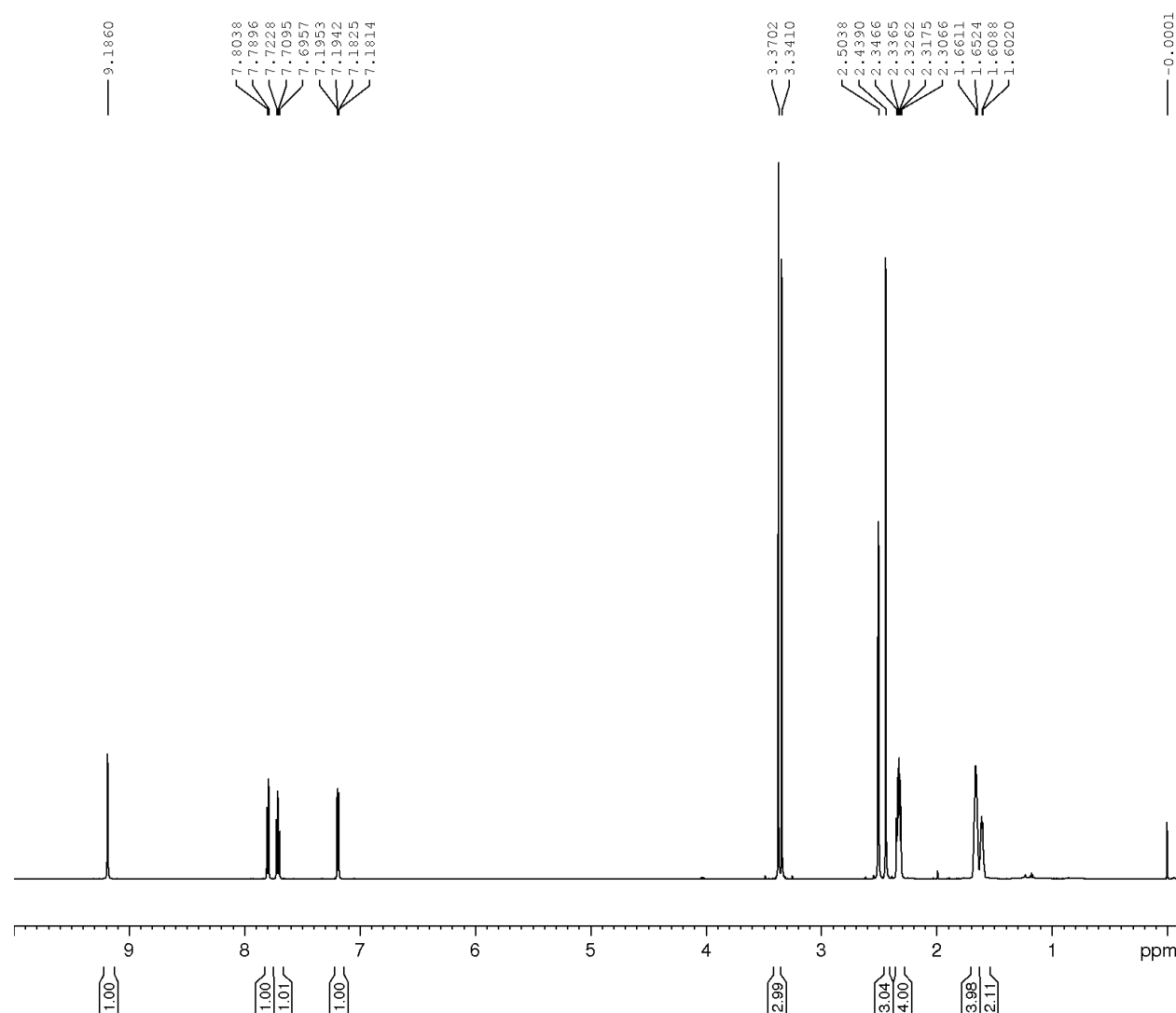
Spectrum Plot Report



Name	PGY0747_1, Pusztai Gyongyver	Rack Pos.	Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	Plate Pos.	IRM Status	Success	Acq. Time (Local)	9/30/2024 1:08:59 PM (UTC+02:00)
Data File	143047msqtof_dip.D	Method (Acq)	DIP_70eV.M	Comment		



¹H NMR spectrum of 7e



Standard 1H
142695
PGY0537_1A
Pusztai Gyongyver
2024.04.19. (KP)

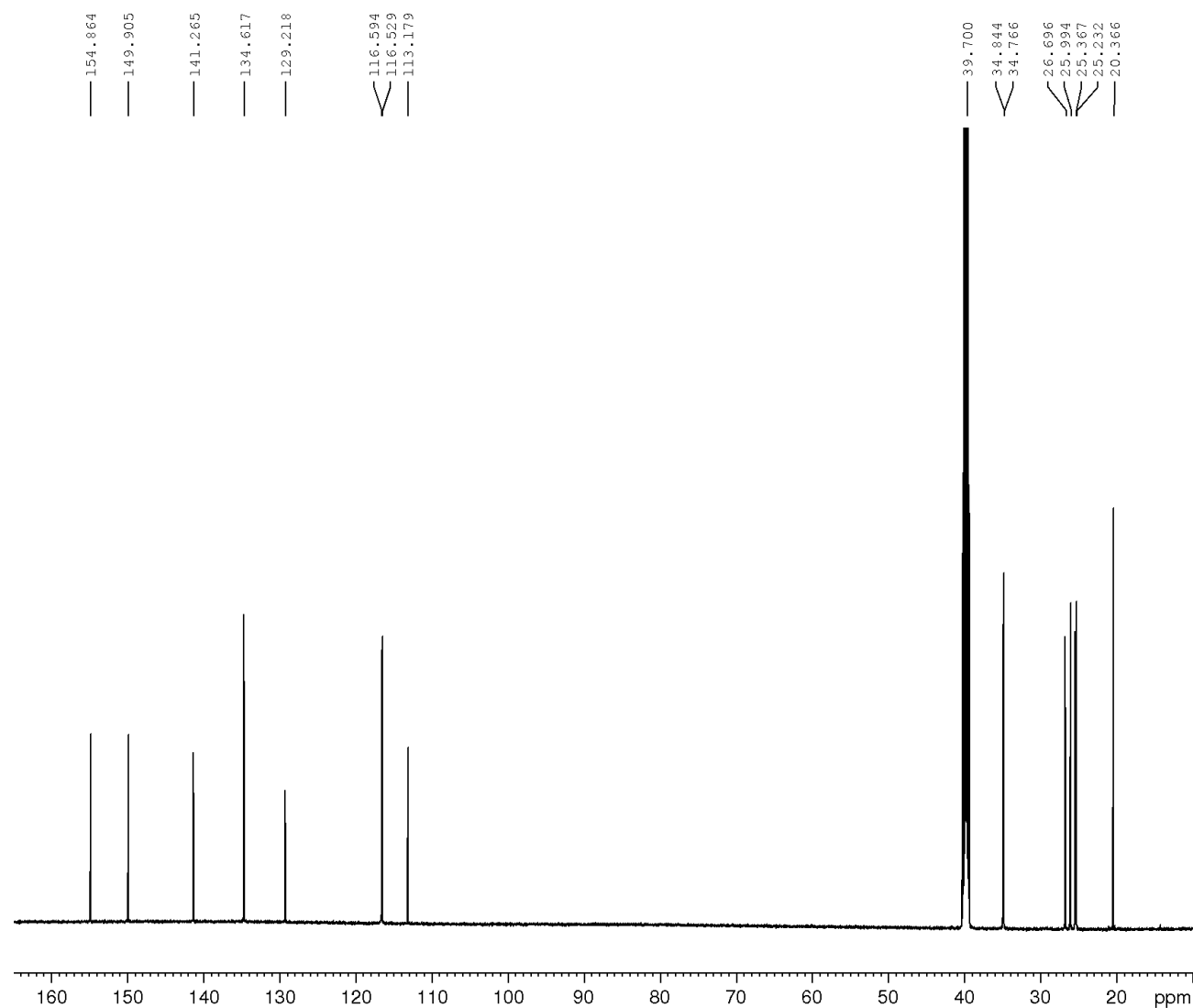
Current Data Parameters
NAME 142695
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
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INSTRUM spect
PROBHD Z145856_0002 (zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000026 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of 7e



Standard 13C
142695
PGY0537_1A
Pusztai Gyongyver
2024.04.22. (KP)

Current Data Parameters
NAME 142695
EXPNO 22
PROCNO 1

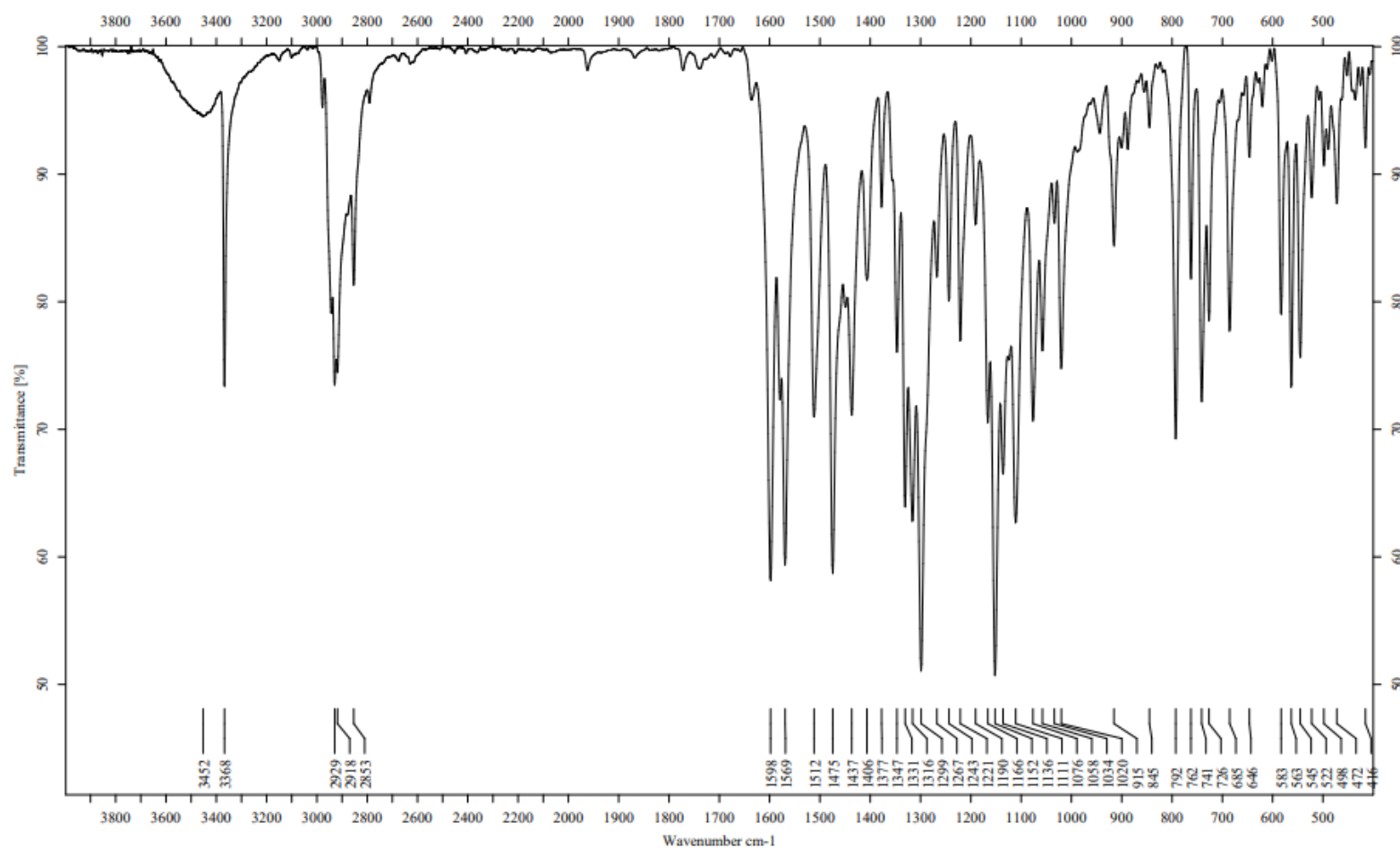
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SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
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F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



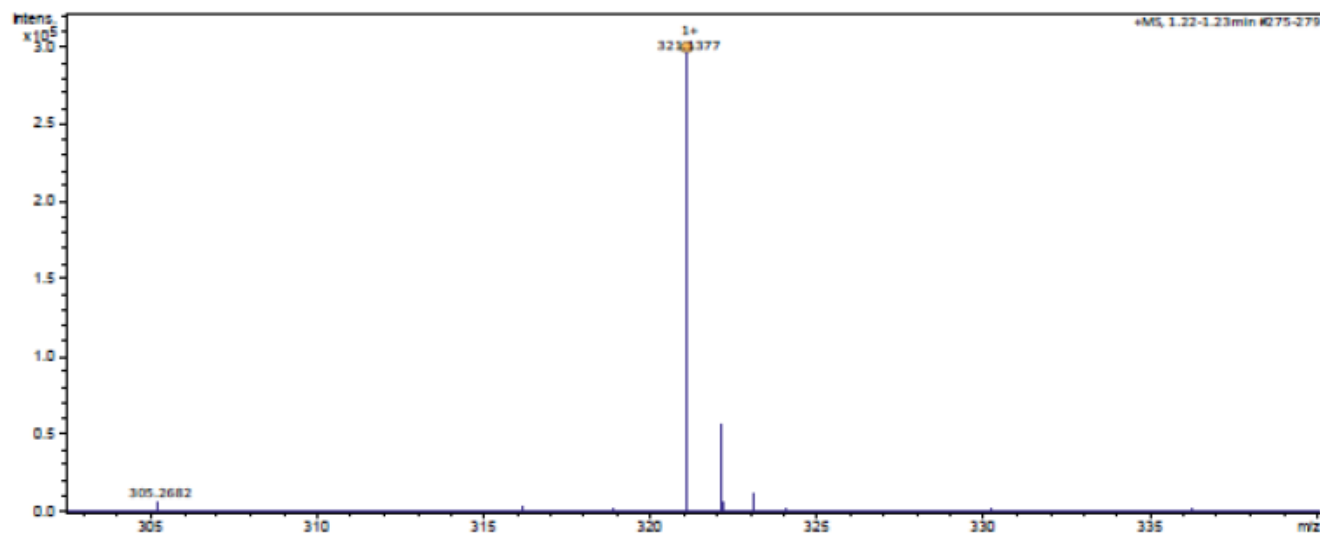
IR spectrum of 7e

142695	Pusztai Gyongyver	KP	BRUKER Alpha
PGY0537_1A	KBr	4/23/2024	Resolution: 2 cm-1
			Number of Scans: 16



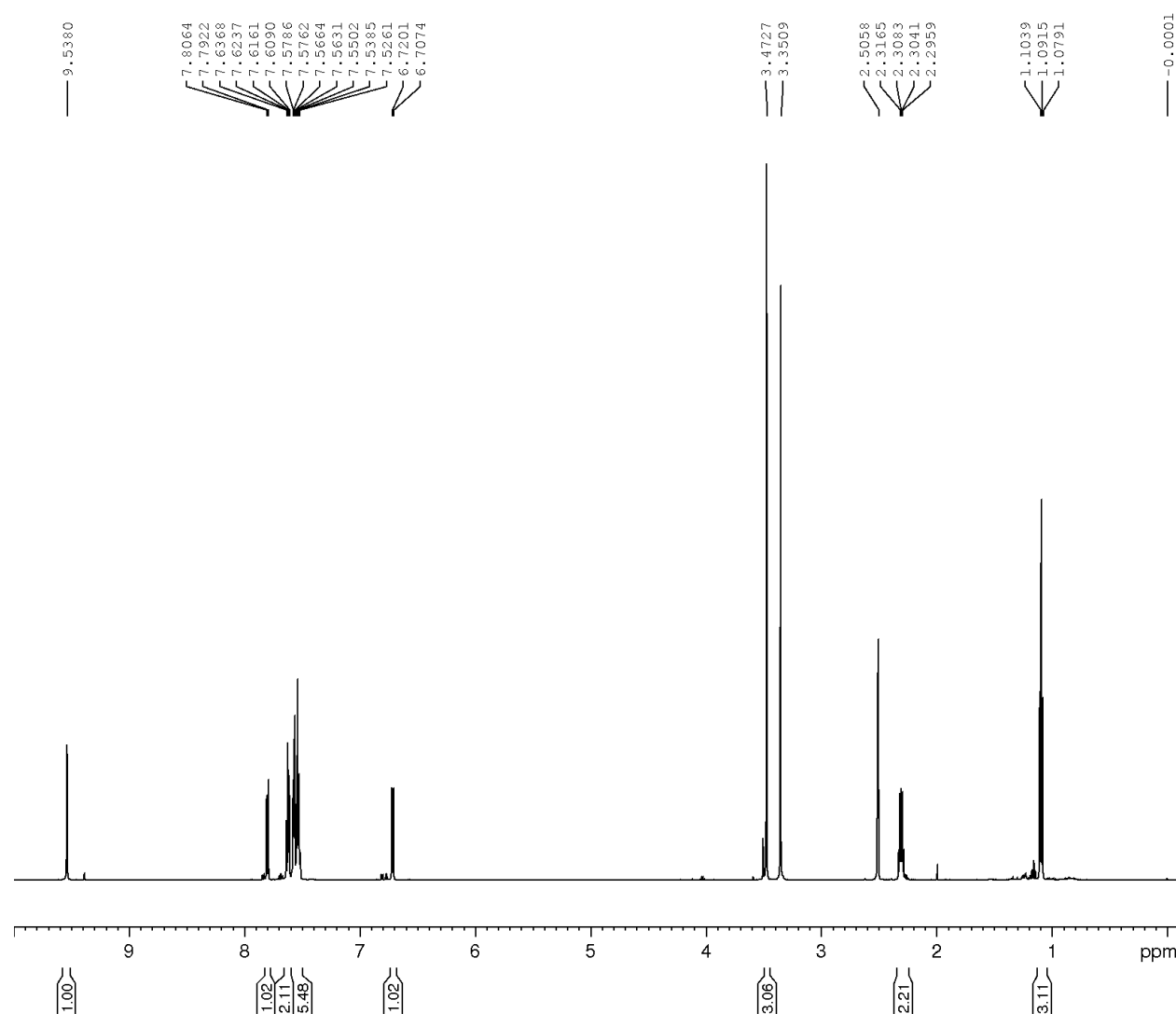
HRMS spectrum of 7e

Sample: PGY0537_1A	Lab code: Nsz - 28997
Submitter: Pusztai Gyongyve	Project: Other



Meas. m/z	Ion Formula	m/z	err [ppm]
321.1377	C ₁₅ H ₂₁ N ₄ O ₂ S	321.1385	1.0

¹H NMR spectrum of (*E*)-7h



Standard 1H
144031
PGY0841_1A
Pusztai Gyongyver
2024.12.13. (KP)

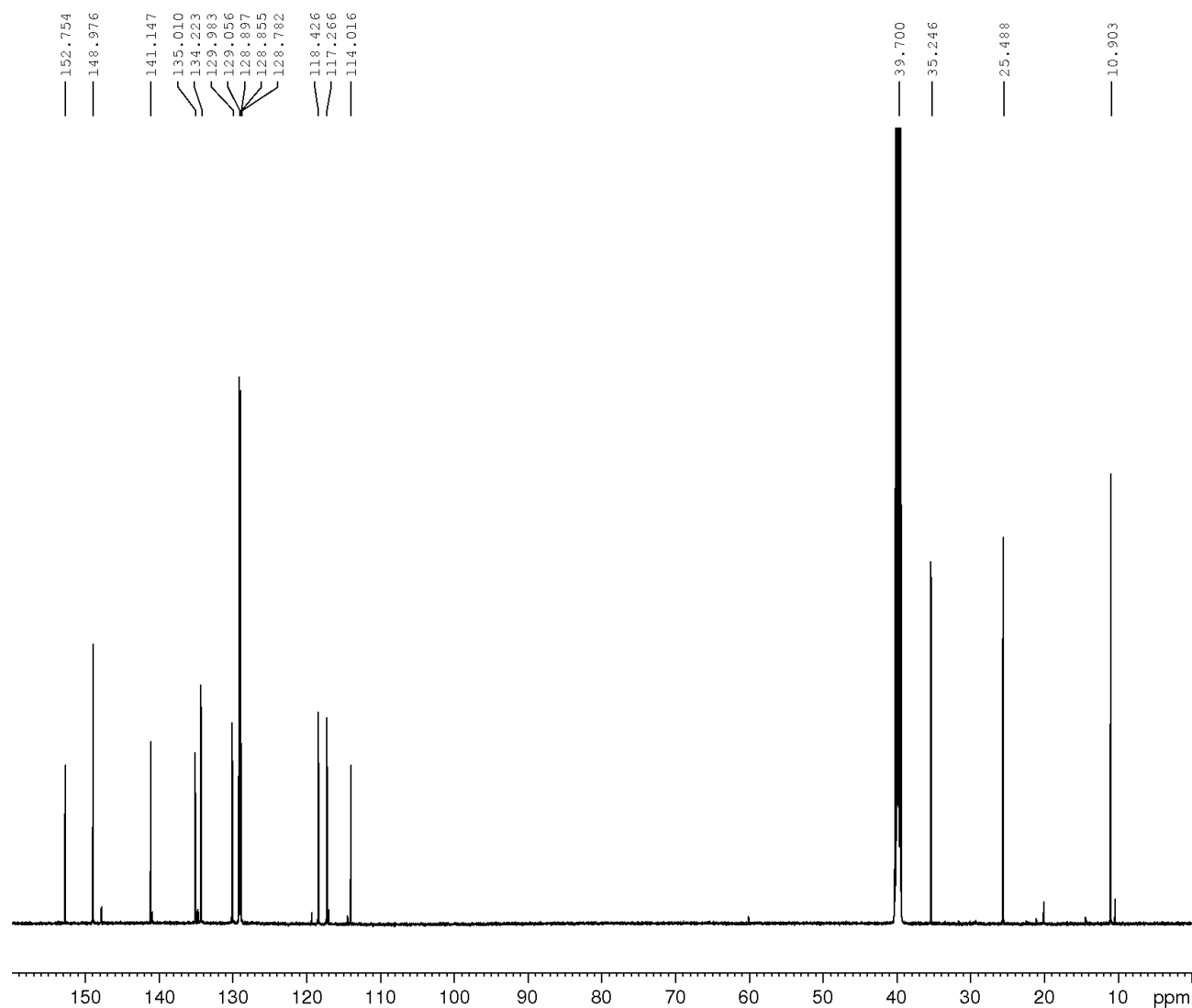
Current Data Parameters
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EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000015 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of (*E*)-7h



Standard 13C
144031
PGY0841_1A
Pusztai Gyongyver
2024.12.13. (KP)

Current Data Parameters
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EXPNO 12
PROCNO 1

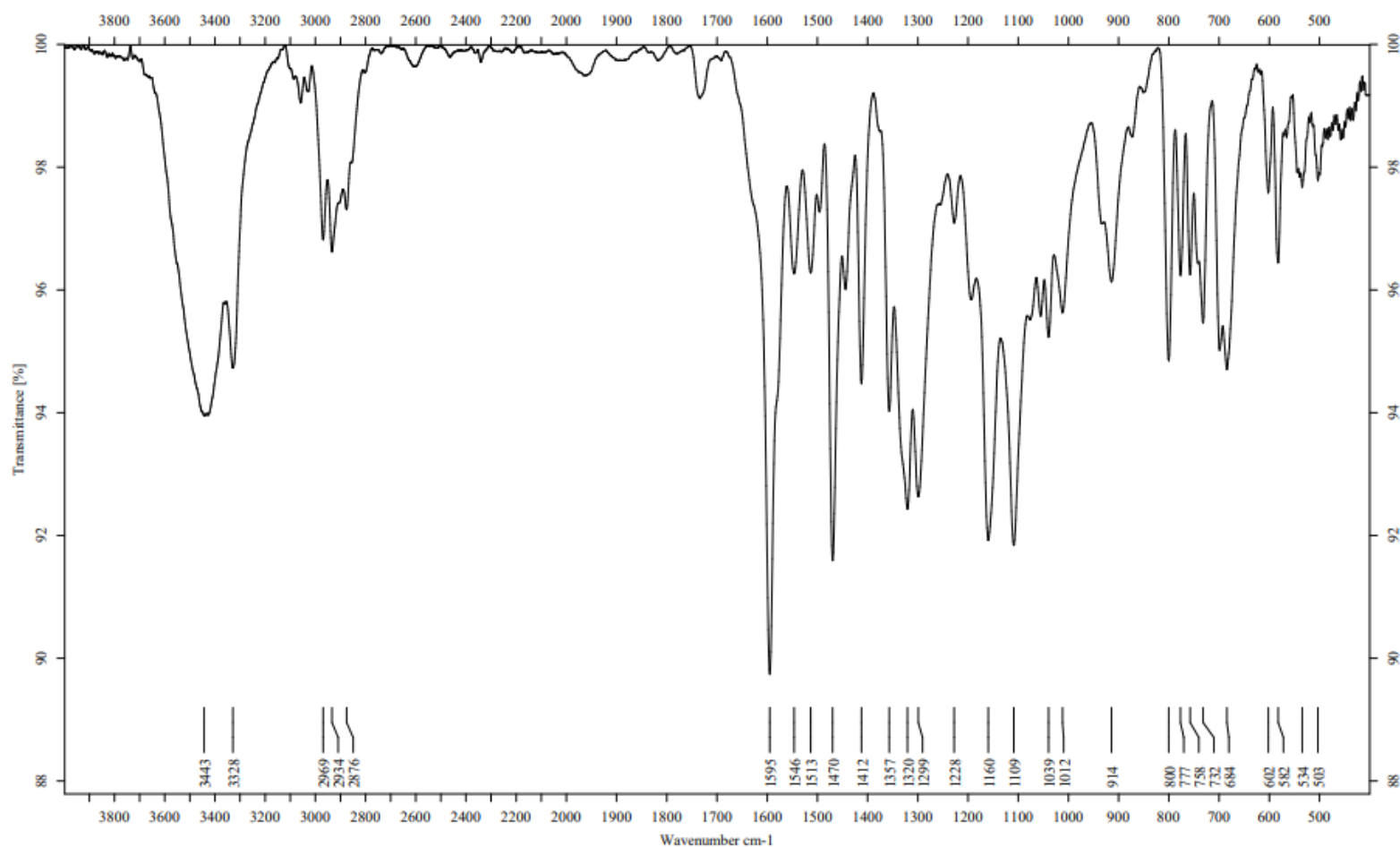
F2 - Acquisition Parameters
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Time 21.24 h
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701603 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of (*E*)-7h

144031	Pusztai Gyongyver	KP	BRUKER Alpha
PGY0841_1A	KBr	12/16/2024	Resolution: 2 cm-1
			Number of Scans: 16

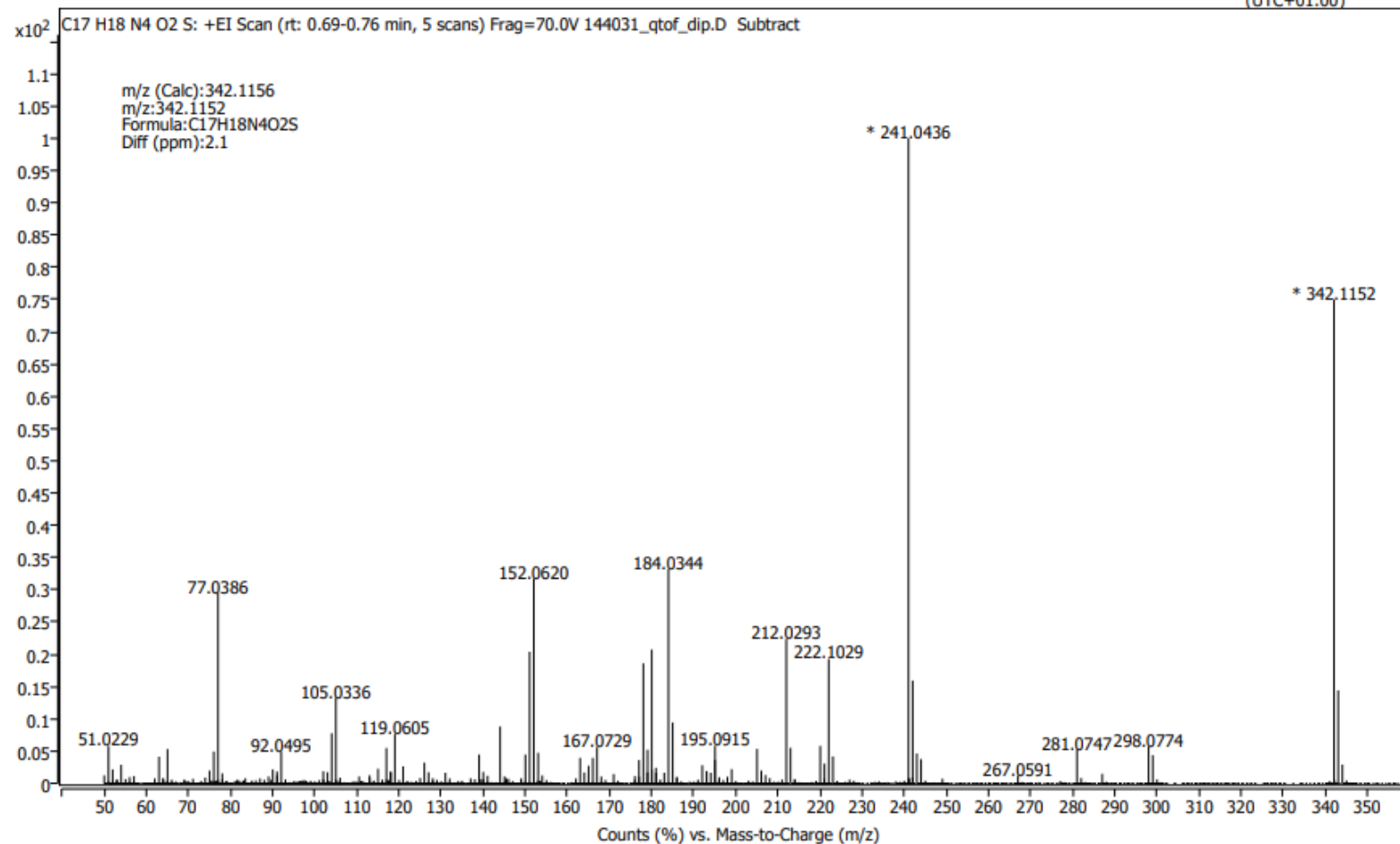


HRMS spectrum of (E)-7h

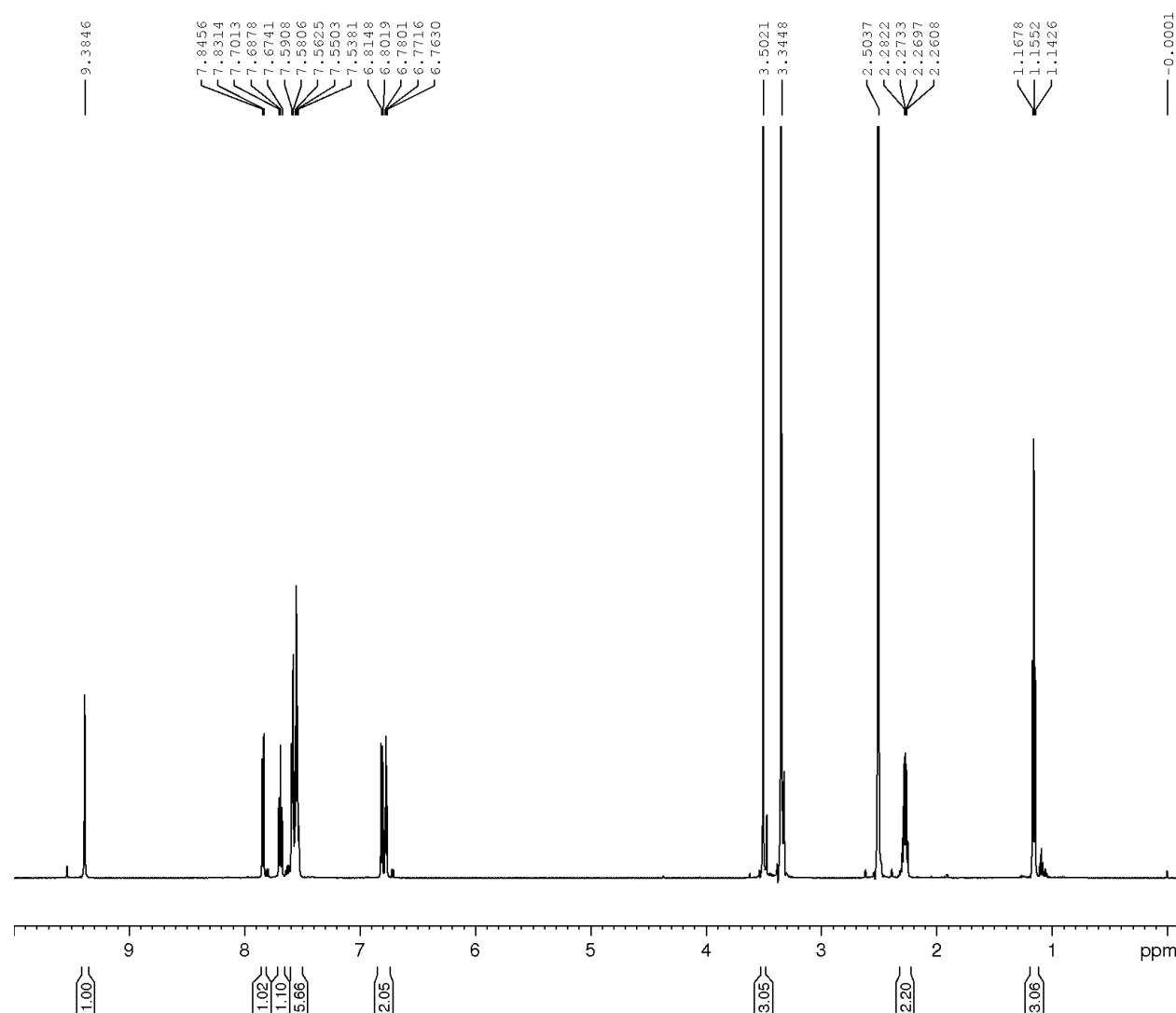
Spectrum Plot Report



Name	PGY0841_1A, Pusztai Gyongyver	Rack Pos.		Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	Plate Pos.		IRM Status	Success		
Data File	144031_qtof_dip.D	Method (Acq)	DIP_70eV.M	Comment		Acq. Time (Local)	1/3/2025 11:33:10 AM (UTC+01:00)



¹H NMR spectrum of (Z)-7h



Standard 1H
144038
PGY0792_1A
Pusztai Gyongyver
2024.12.17. (KP)

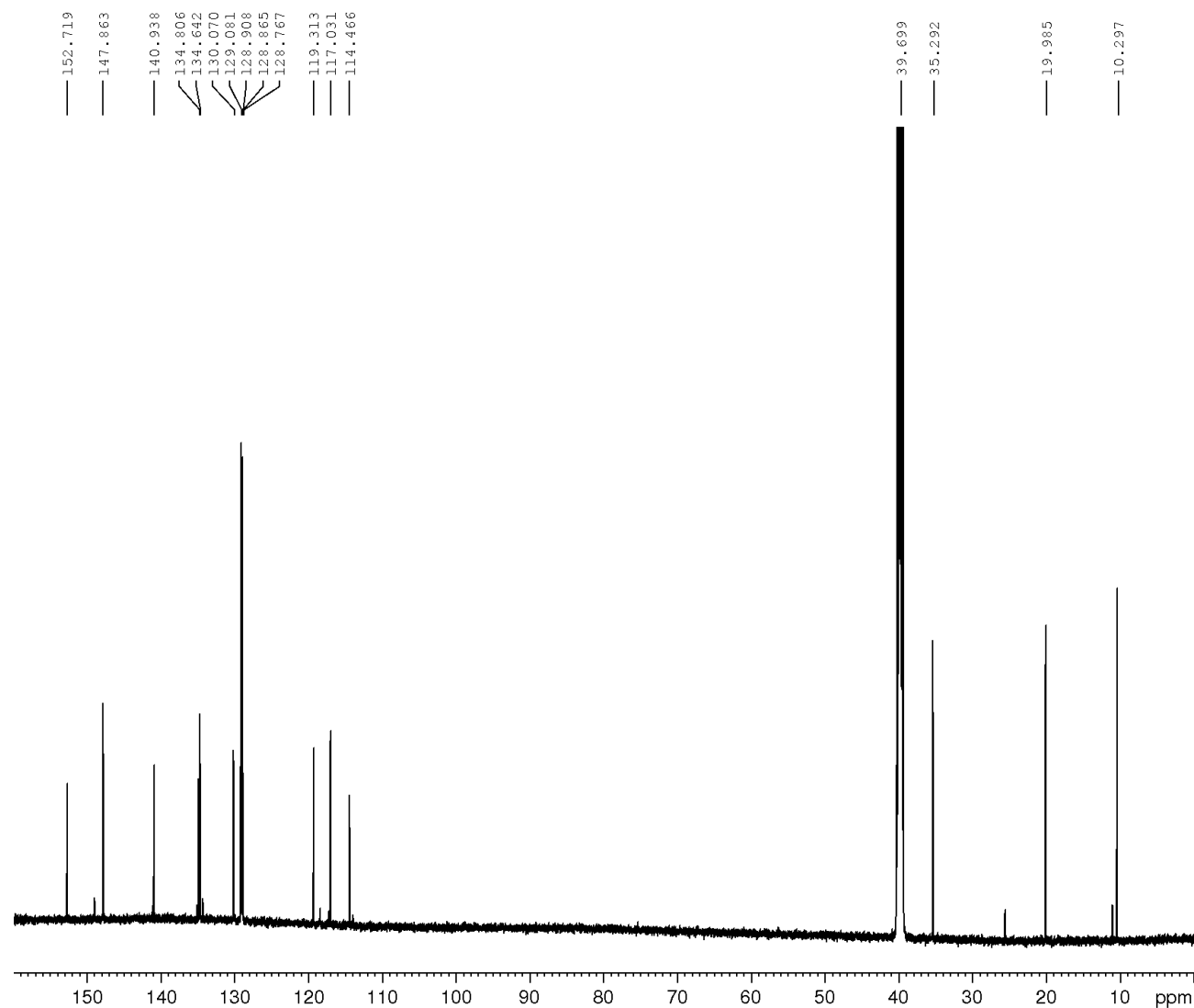
Current Data Parameters
NAME 144038
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241217
Time 13.20 h
INSTRUM spect
PROBHD Z145856_0002 (zg30)
PULPROG 65536
TD 16
SOLVENT DMSO
NS 2
DS 12019.230 Hz
SWH 0.366798 Hz
FIDRES 2.7262976 sec
AQ 196.07
RG 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000028 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of (Z)-7h



Standard 13C
144038
PGY0792_1A
Pusztai Gyongyver
2024.12.18. (KP)

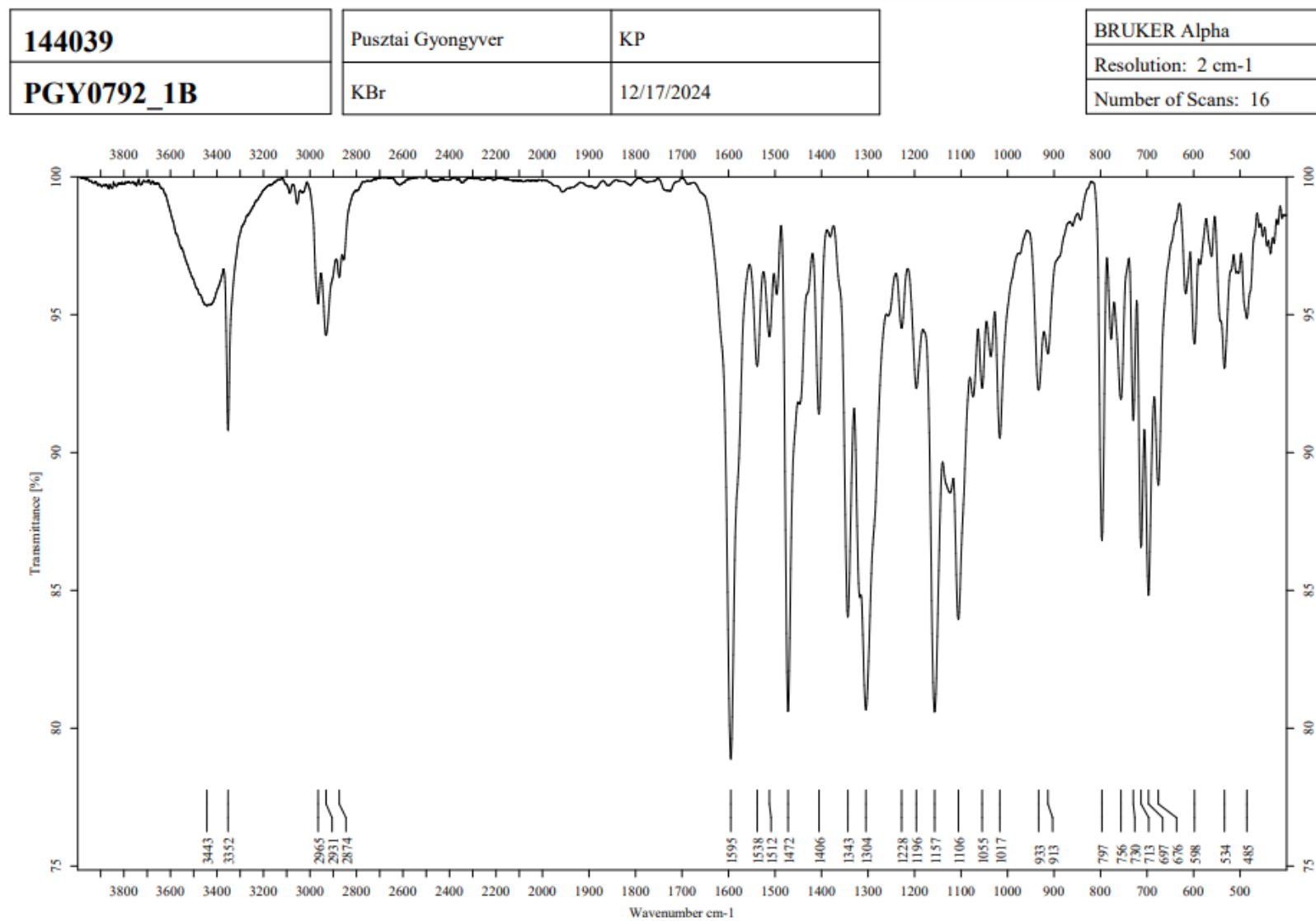
Current Data Parameters
NAME 144038
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241218
Time 18.21 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701601 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of (Z)-7h

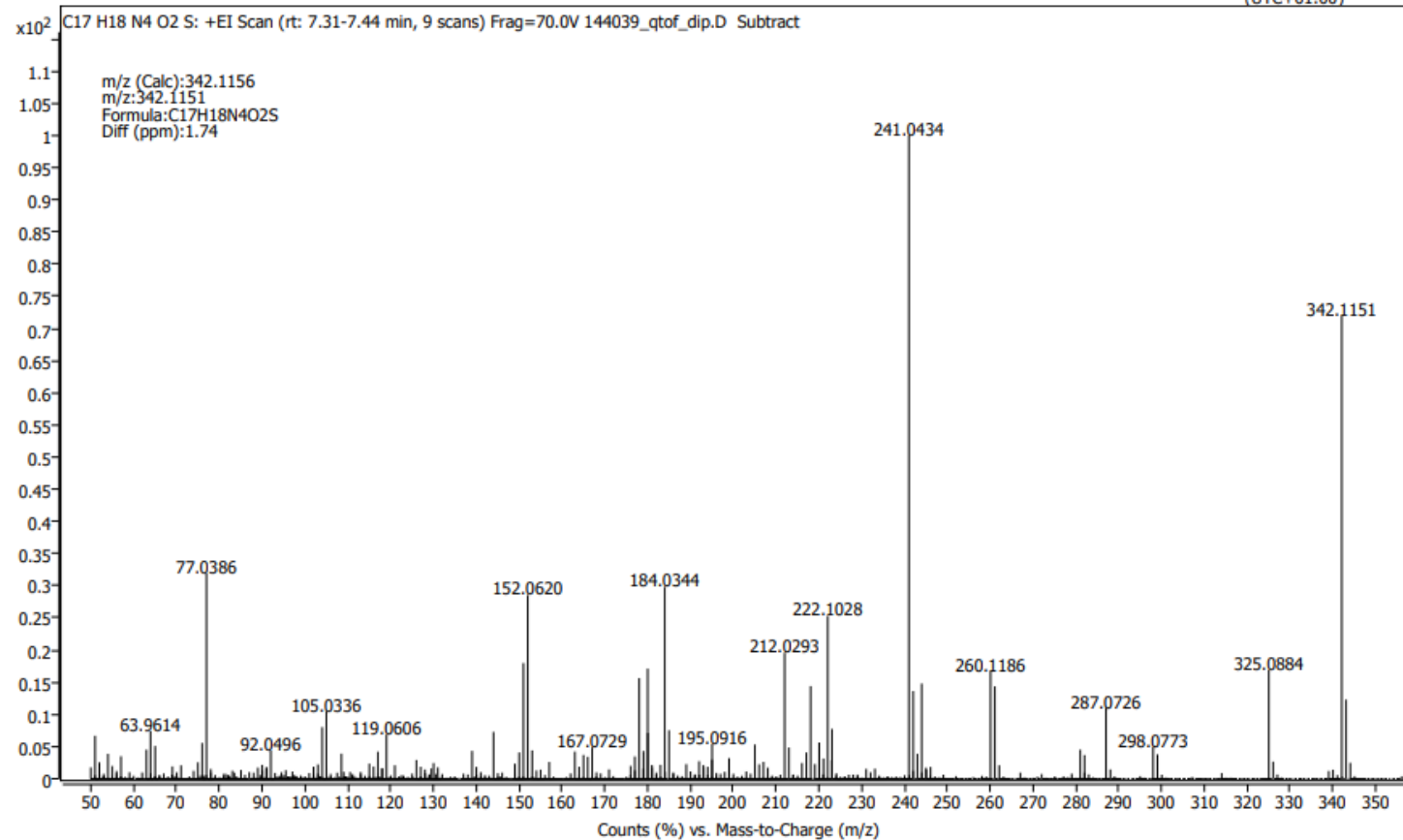


HRMS spectrum of (Z)-7h

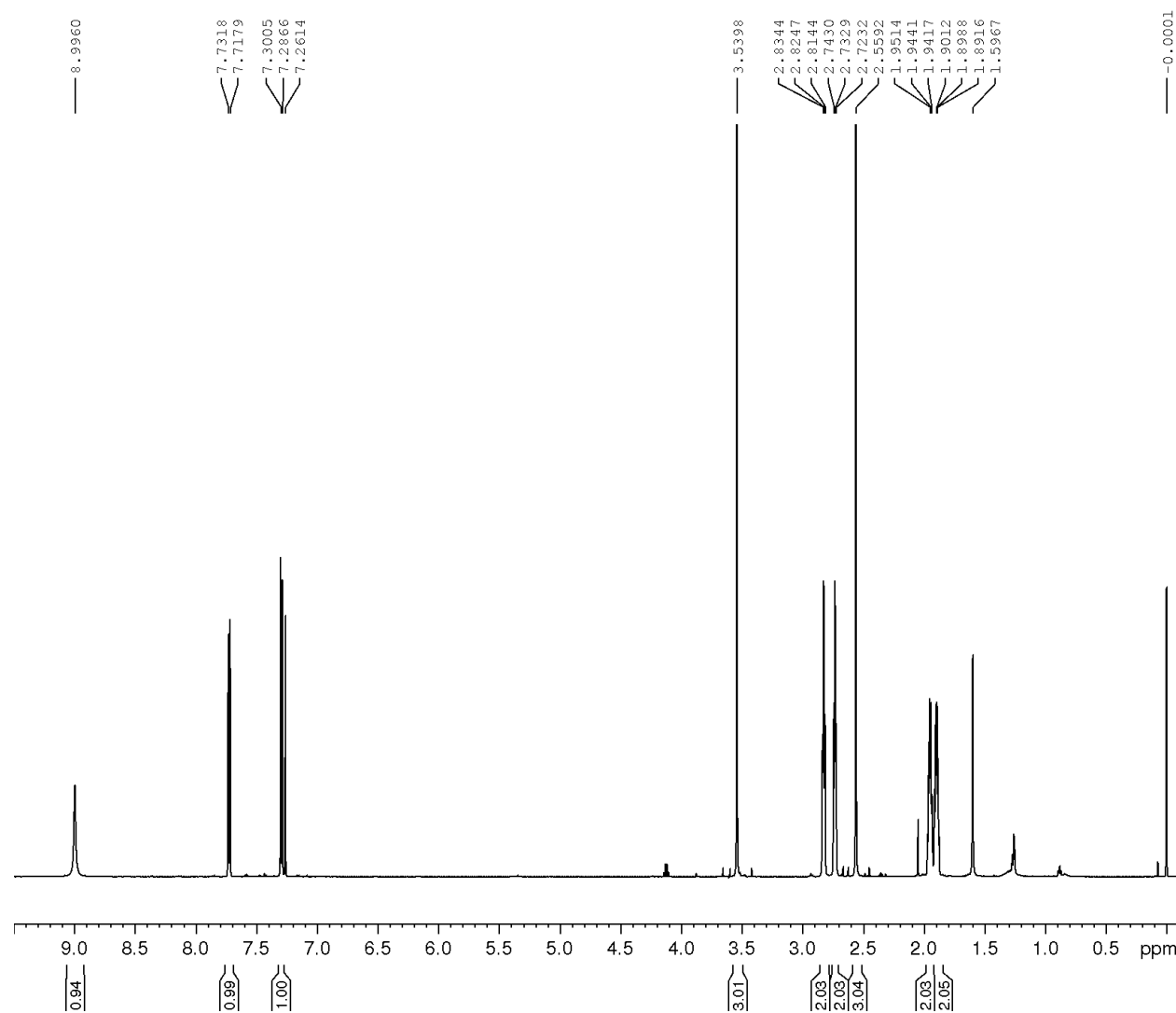
Spectrum Plot Report



Name	PGY0792_1B, Pusztai Gyongyver	Rack Pos.	Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	Plate Pos.	IRM Status	Success	Acq. Time (Local)	1/3/2025 11:12:27 AM (UTC+01:00)
Data File	144039_qtof_dip.D	Method (Acq)	DIP_70eV.M	Comment		



¹H NMR spectrum of **3e**



Standard 1H
142501
PGY0676_1A
Pusztai Gyongyver
2024.03.01. (KP)

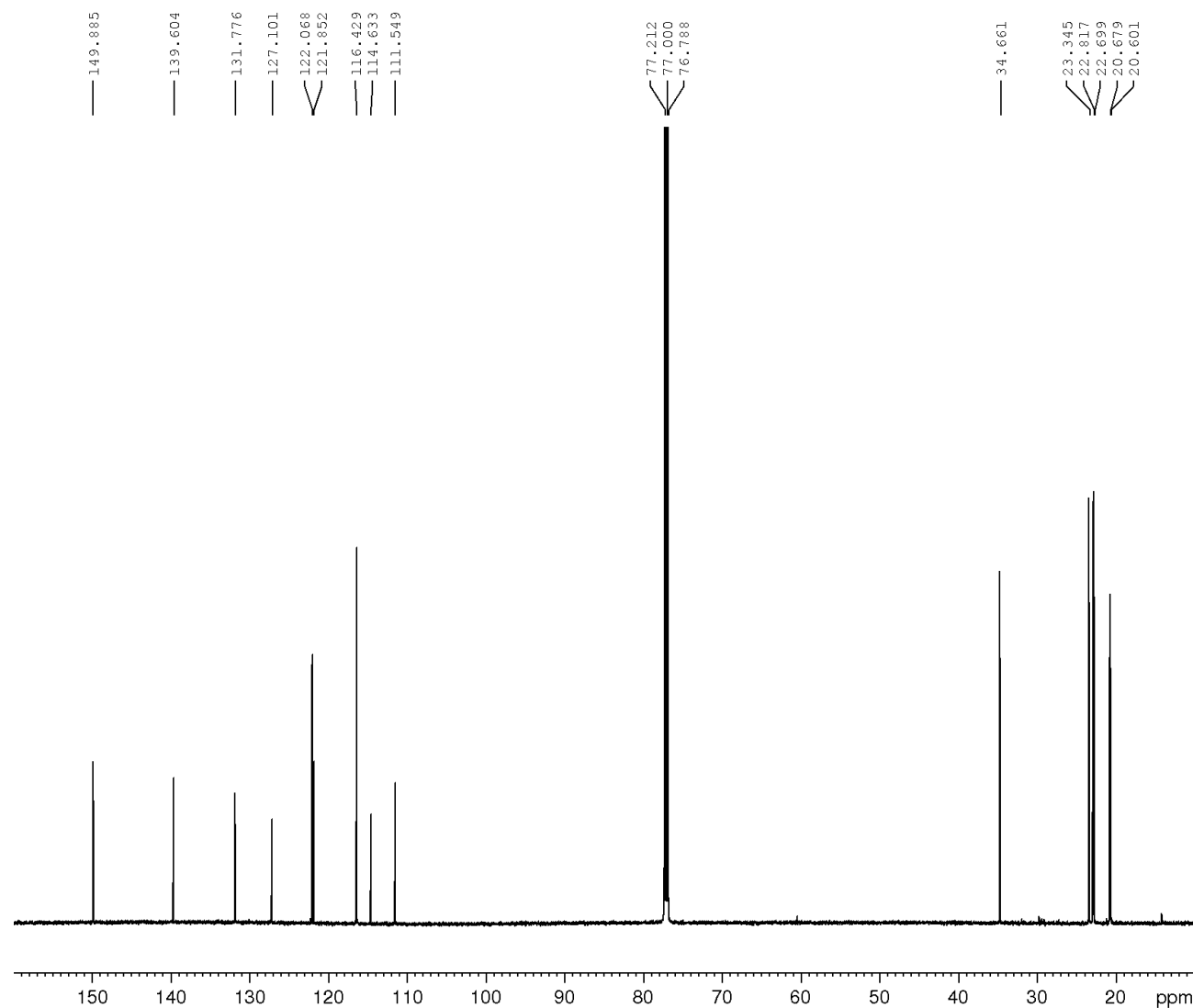
Current Data Parameters
NAME 142501
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240302
Time 2.36 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of **3e**



Standard 13C
142501
PGY0676_1A
Pusztai Gyongyver
2024.03.01. (KP)

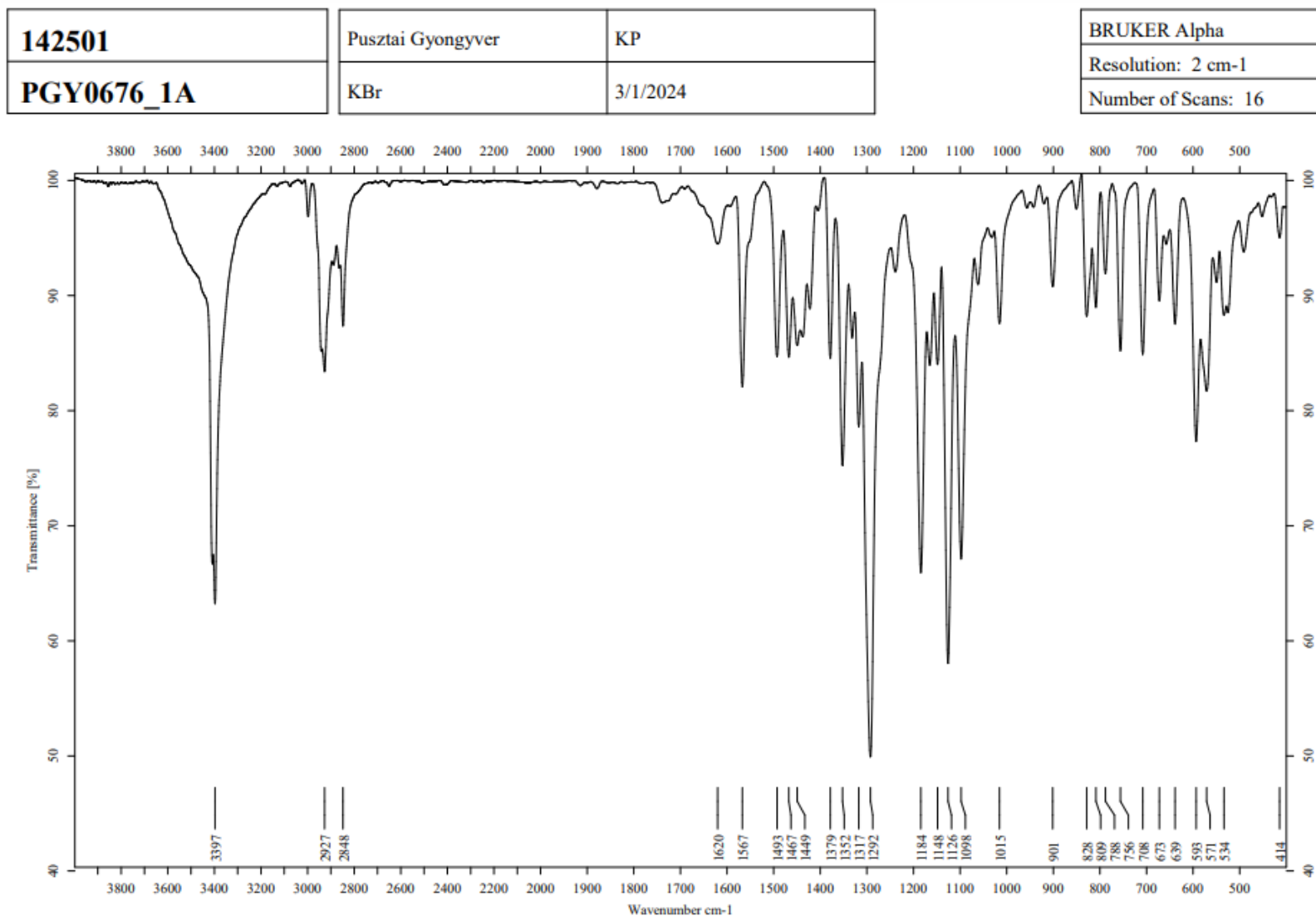
Current Data Parameters
NAME 142501
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240302
Time 3.45 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 32768
SF 150.8701265 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of **3e**

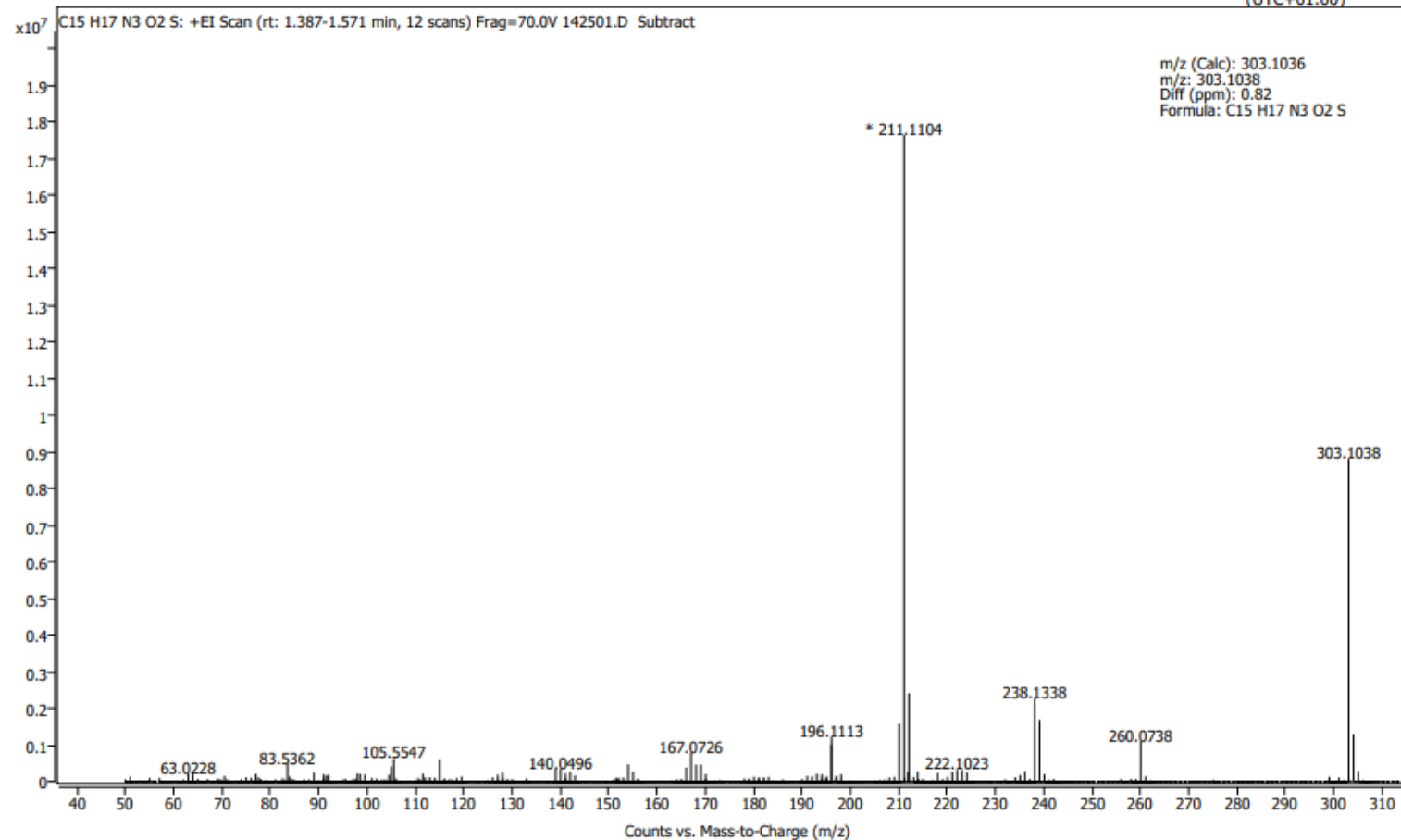


HRMS spectrum of 3e

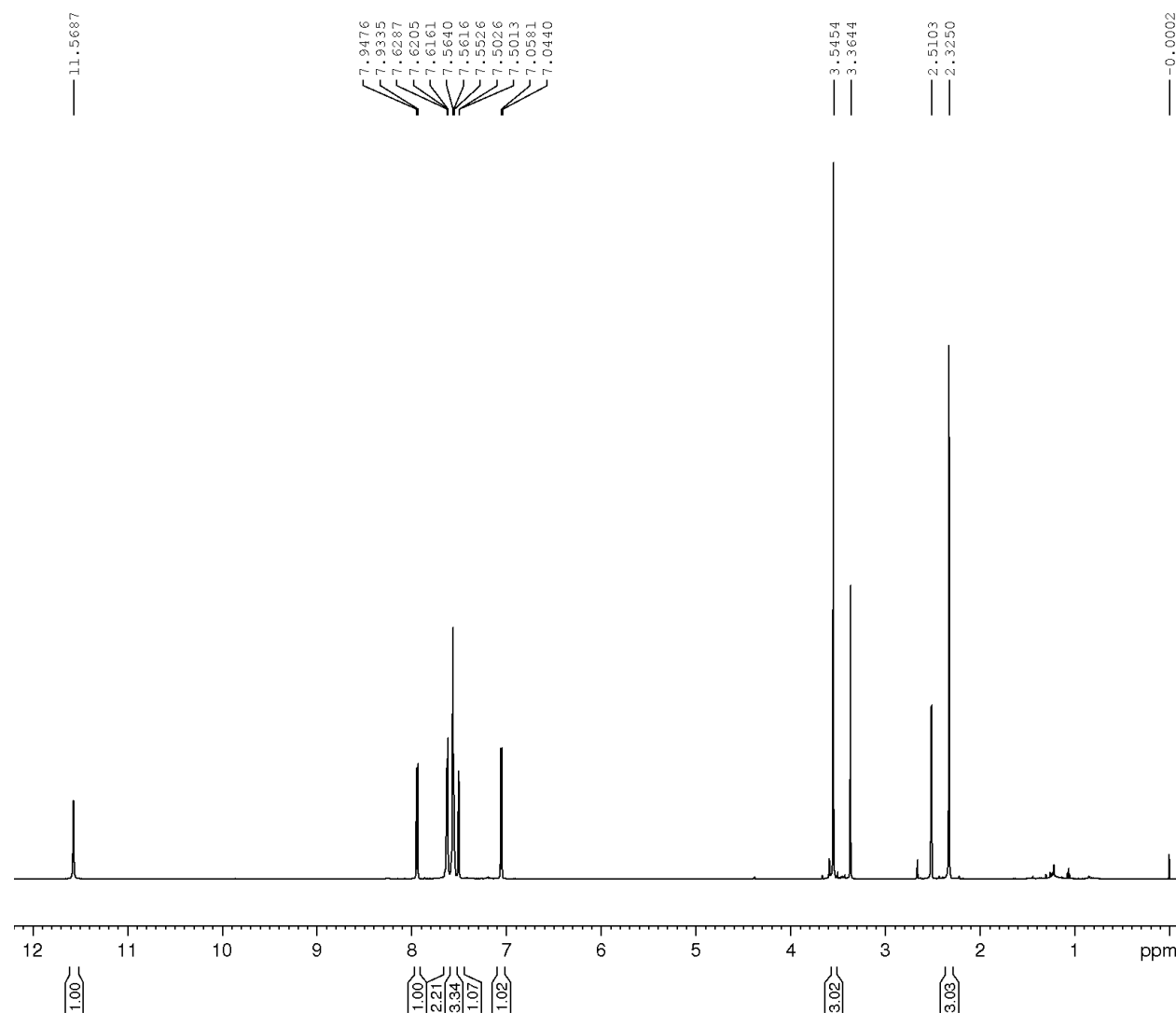
Spectrum Plot Report



Name	PGY0676_1A, Pusztai Gyongyver	Rack Pos.	Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	Plate Pos.	IRM Status	Success	Acq. Time (Local)	3/5/2024 10:57:51 AM (UTC+01:00)
Data File	142501.D	Method (Acq)	DIP_70eV.M	Comment		



¹H NMR spectrum of **3h**



Standard 1H
143660
PGY0765_1A
Pusztai Gyongyver
2024.10.09. (KP)

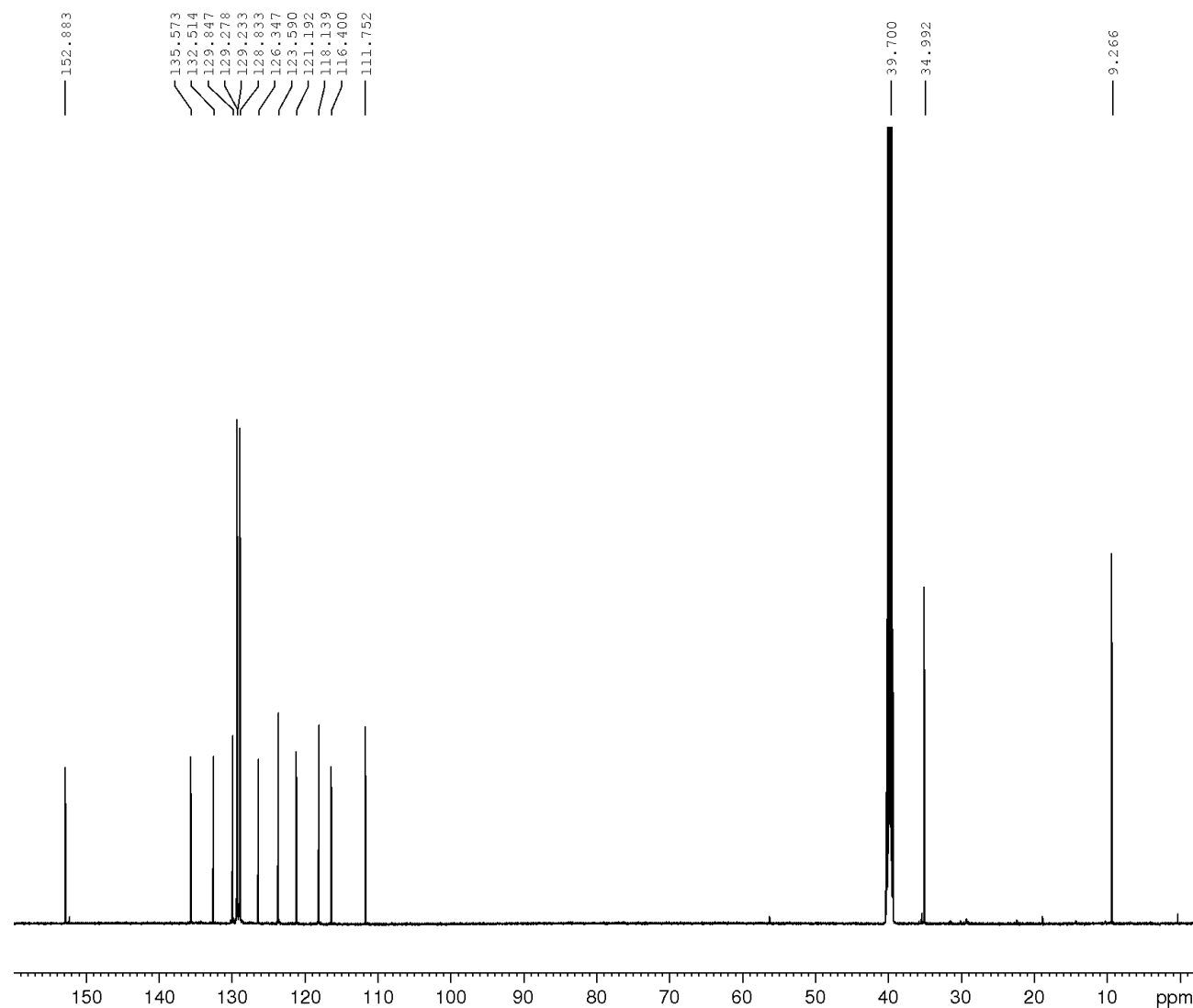
Current Data Parameters
NAME 143660
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241009
Time 19.11 h
INSTRUM spect
PROBHD Z145856_0002 (zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 599.9999985 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of **3h**



Standard 13C
143660
PGY0765_1A
Pusztai Gyongyver
2024.10.09. (KP)

Current Data Parameters
NAME 143660
EXPNO 13
PROCNO 1

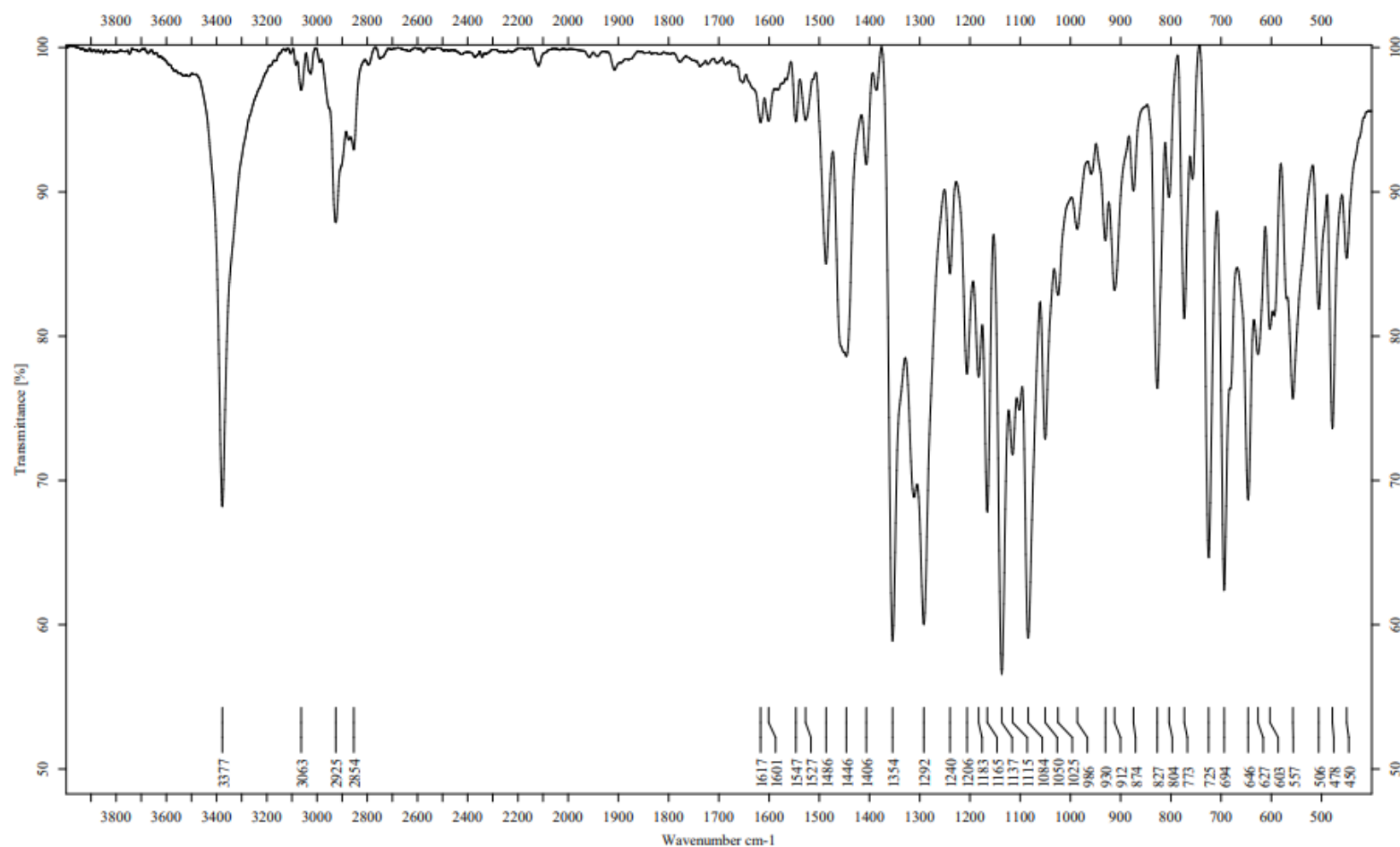
F2 - Acquisition Parameters
Date_ 20241009
Time 20.21 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701601 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of **3h**

143660	Pusztai Gyongyver	KP	BRUKER Alpha
PGY0765_1A	KBr	10/9/2024	Resolution: 2 cm-1
			Number of Scans: 16

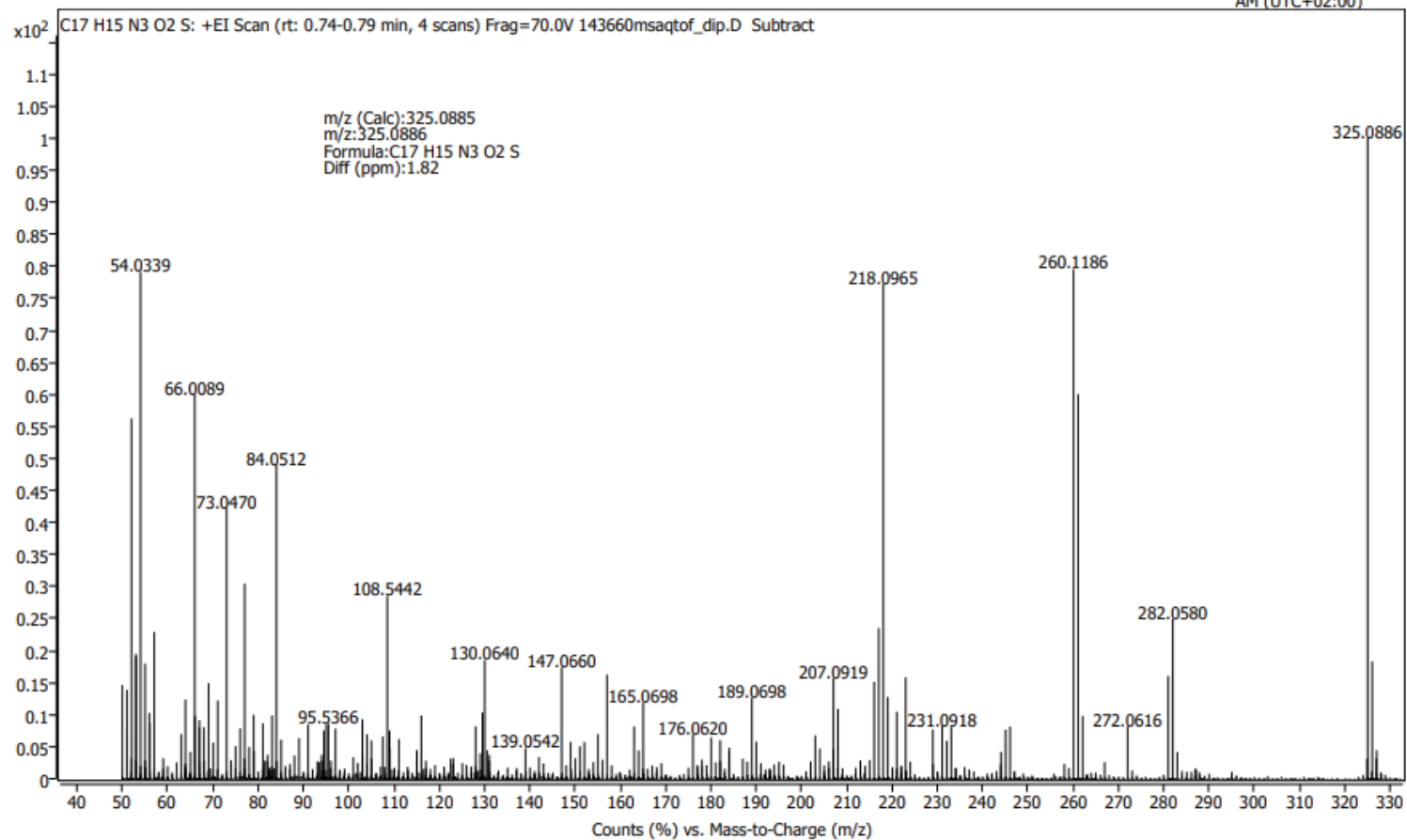


HRMS spectrum of **3h**

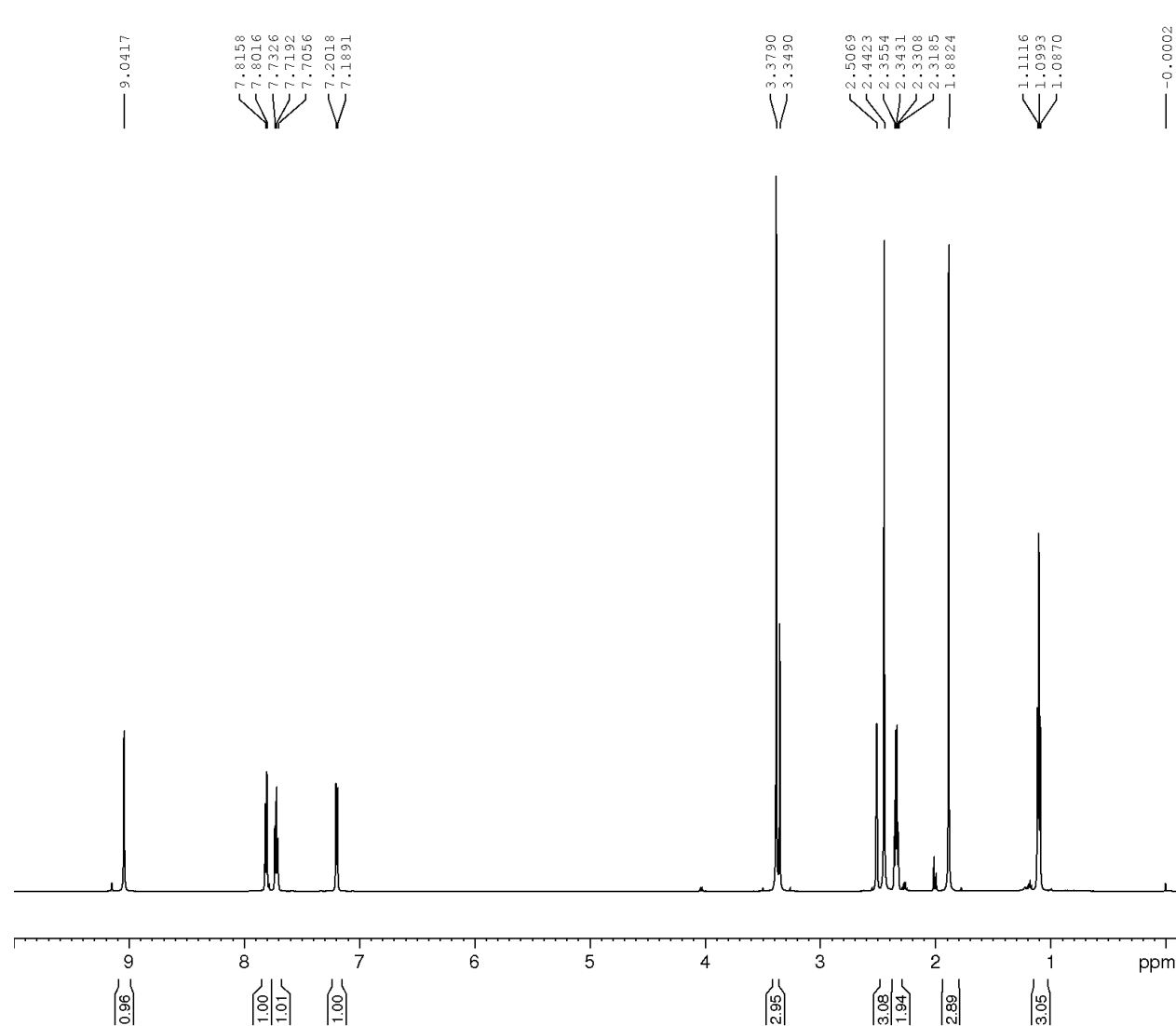
Spectrum Plot Report



Name	PGY0765_1A, Pusztai Gyongyver	Rack Pos.	Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	Plate Pos.	IRM Status	Success		
Data File	143660msaqtod_dip.D	Method (Acq)	DIP_70eV.M	Comment	Acq. Time (Local)	10/24/2024 8:35:54 AM (UTC+02:00)



¹H NMR spectrum of (*E*)-**7a**



Standard 1H
142698
PGY0530_1C
Pusztai Gyongyver
2024.04.23. (KP)

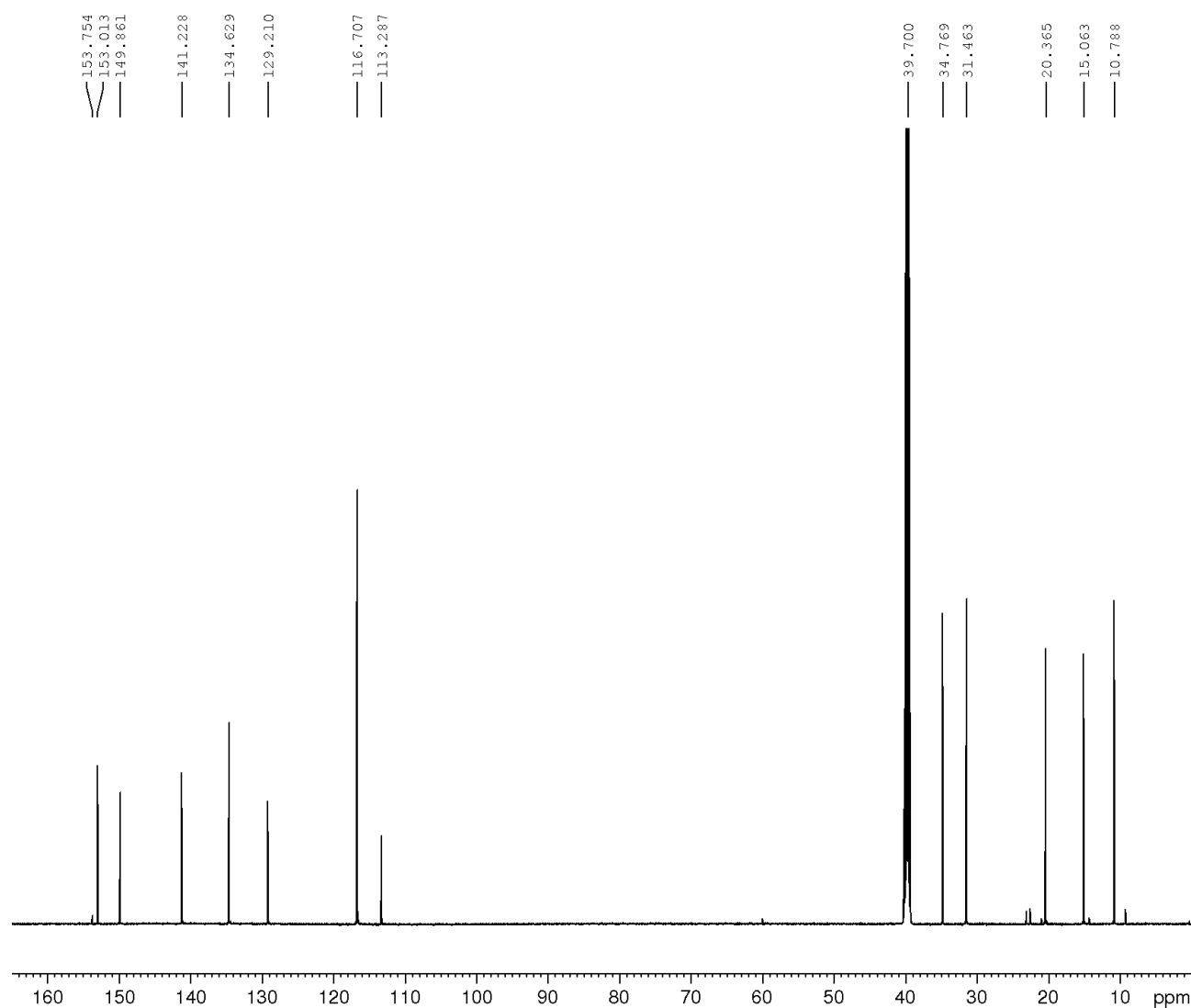
Current Data Parameters
NAME 142698
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240423
Time 16.28 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 111.4
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000005 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of (*E*)-7a



Standard 13C
142698
PGY0530_1C
Pusztai Gyongyver
2024.04.23. (KP)

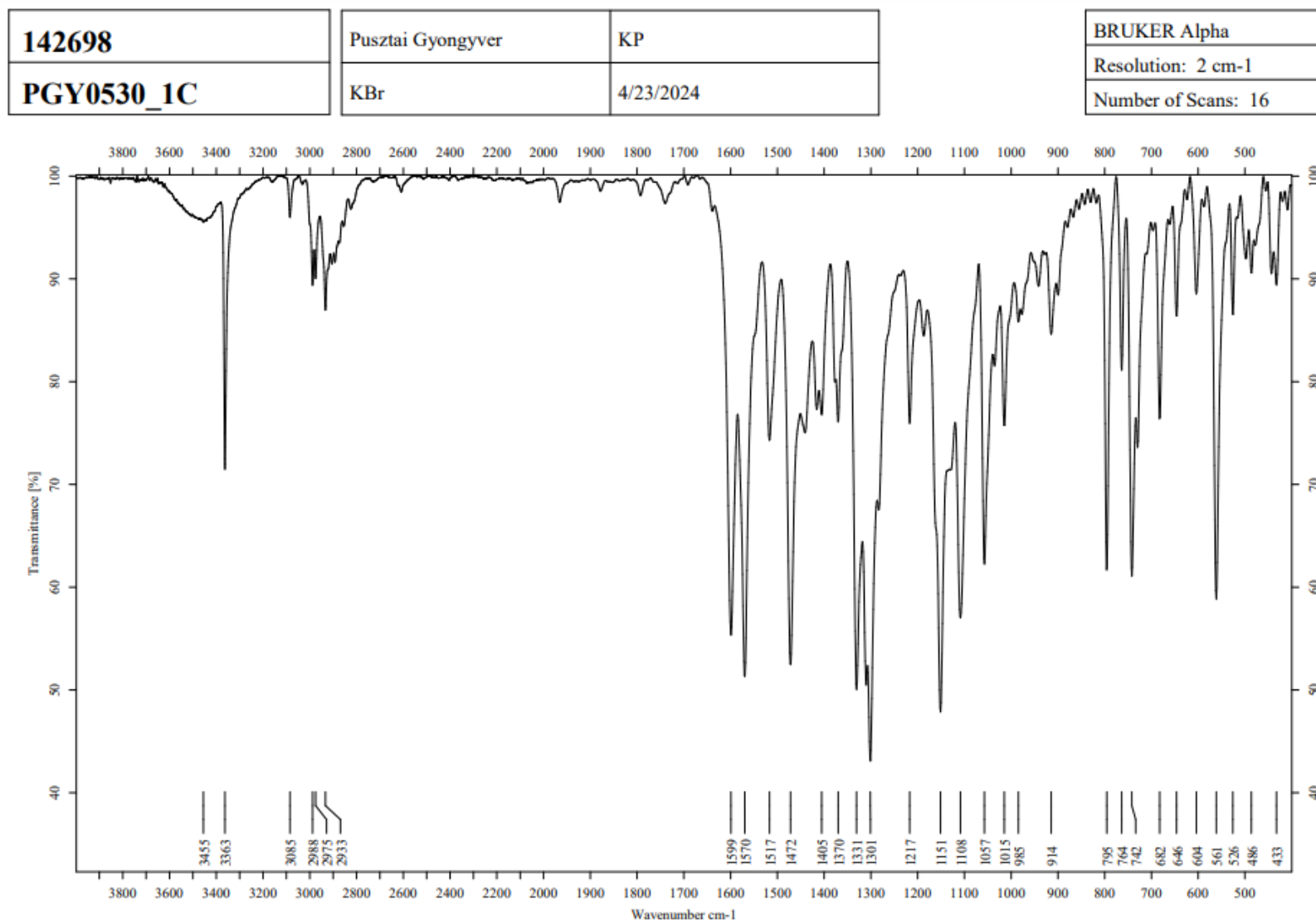
Current Data Parameters
NAME 142698
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240423
Time 17.36 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 32768
SF 150.8701599 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

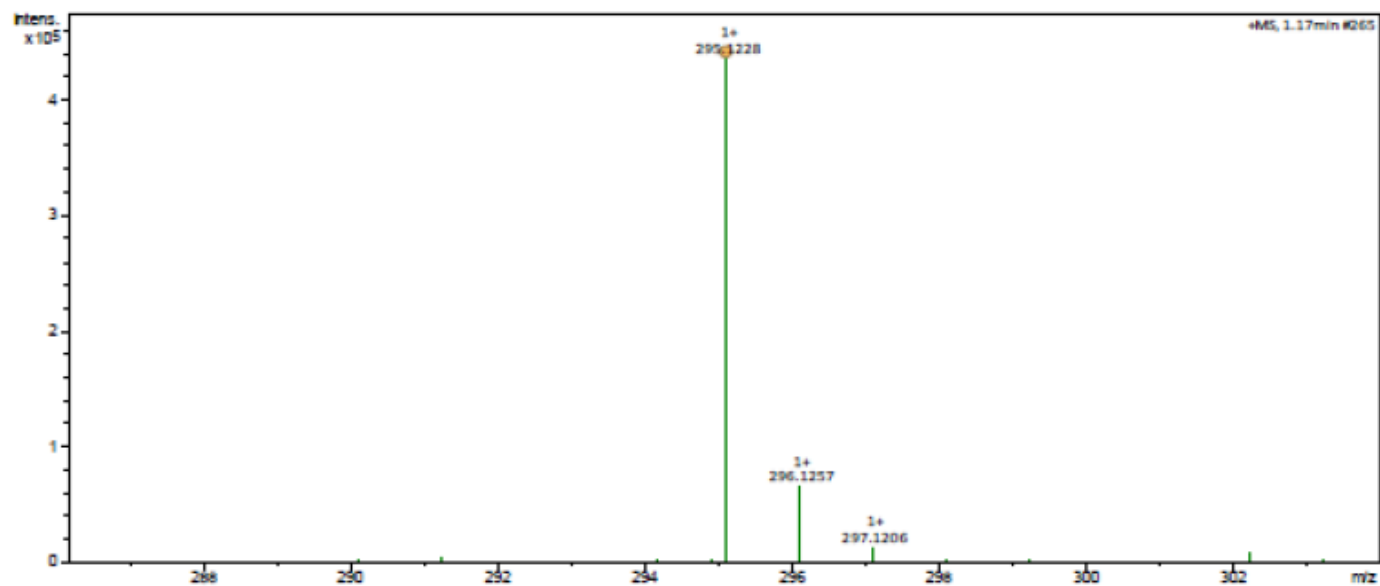


IR spectrum of (*E*)-7a



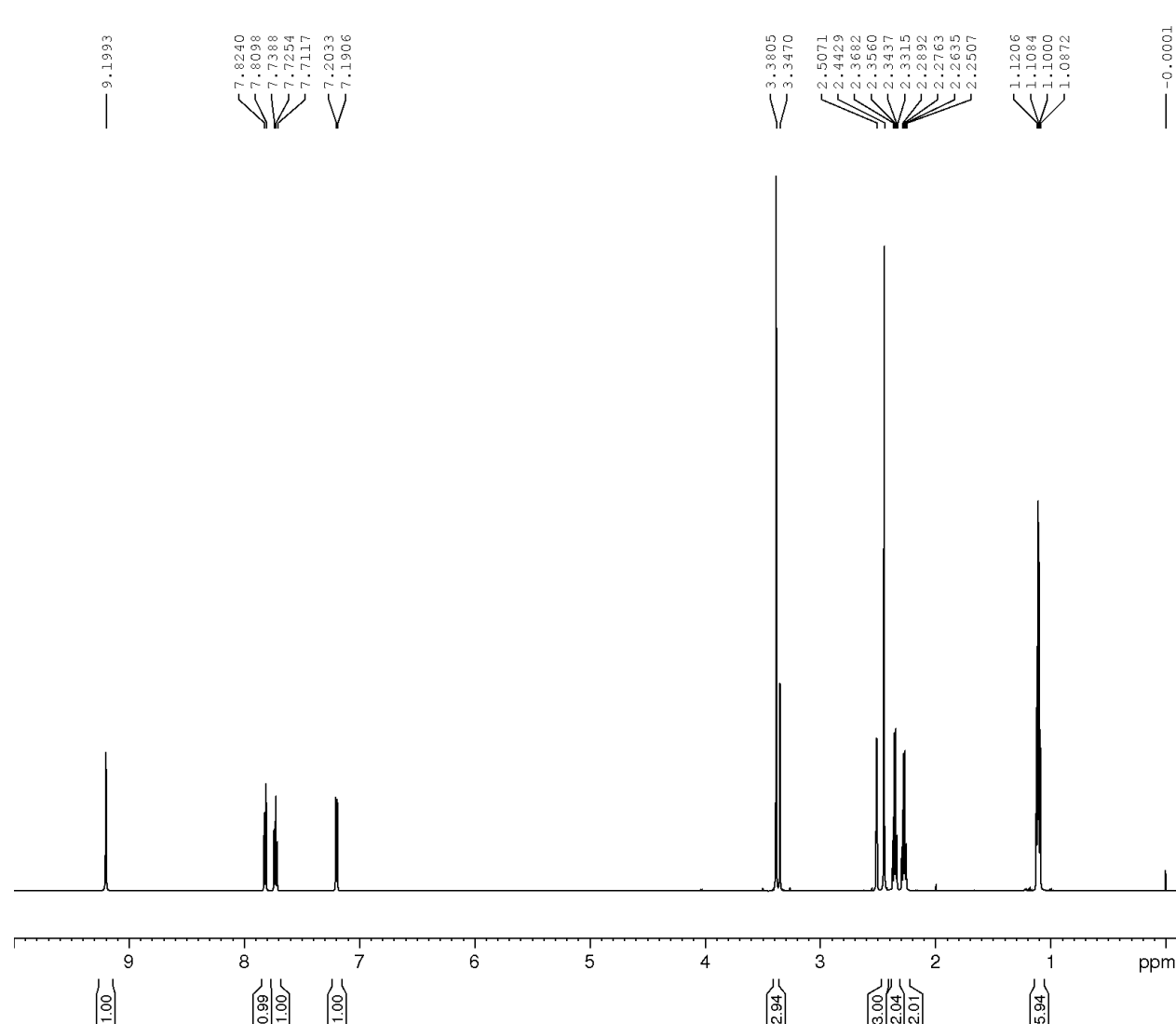
HRMS spectrum of (*E*)-7a

Sample: PGY0530_1C	Lab code: Nsz - 28996
Submitter: Pusztai Gyongyve	Project: Other



Meas. m/z	Ion Formula	m/z	err [ppm]
295.1228	C ₁₃ H ₁₉ N ₄ O ₂ S	295.1229	1.5

¹H NMR spectrum of 7b



Standard 1H
142657
PGY0538_1A
Pusztai Gyongyver
2024.04.11. (KP)

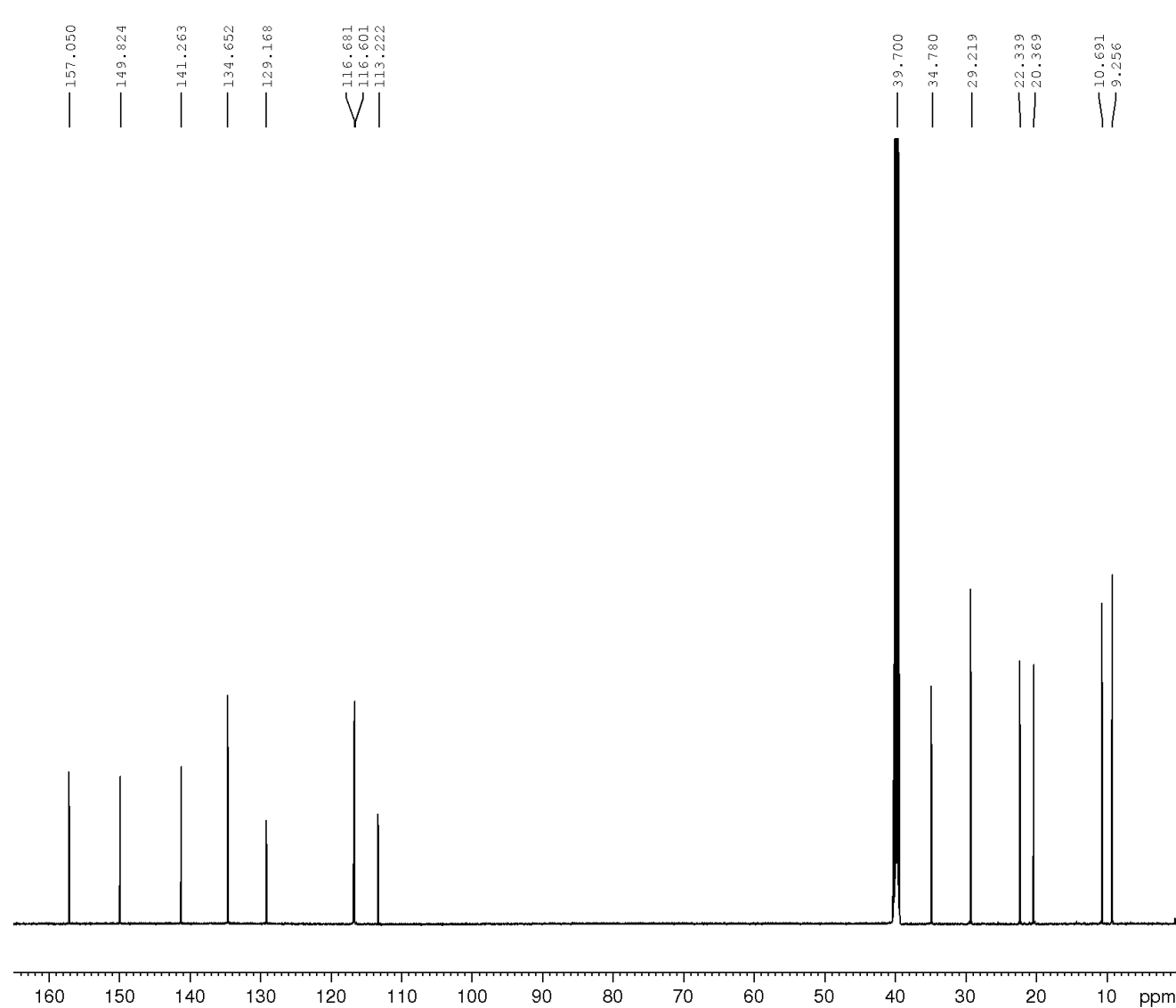
Current Data Parameters
NAME 142657
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240411
Time 21.02 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 119.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000004 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of **7b**



Standard 13C
142657
PGY0538_1A
Pusztai Gyongyver
2024.04.11. (KP)

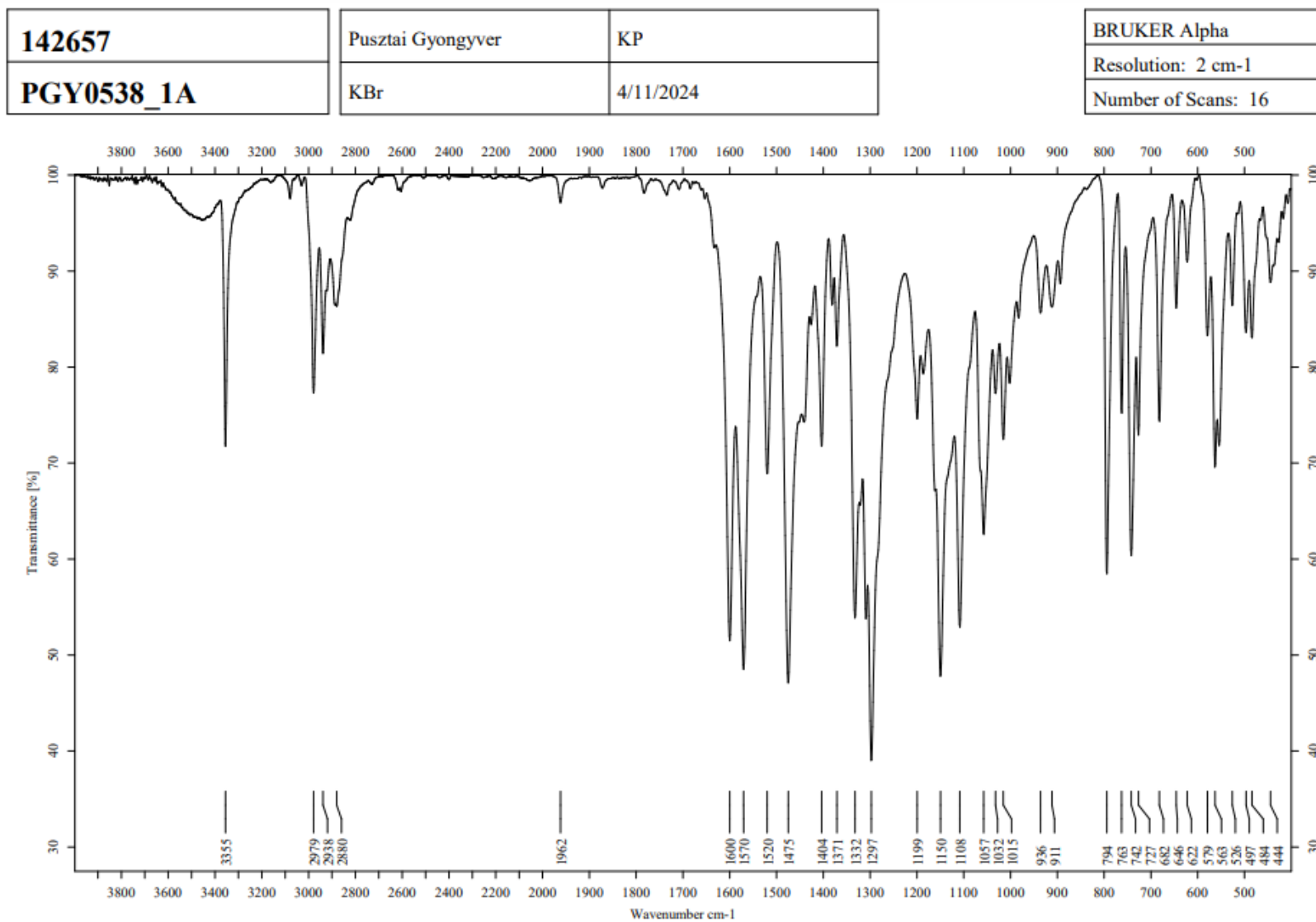
Current Data Parameters
NAME 142657
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240411
Time 22.12 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 32768
SF 150.8701601 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of **7b**

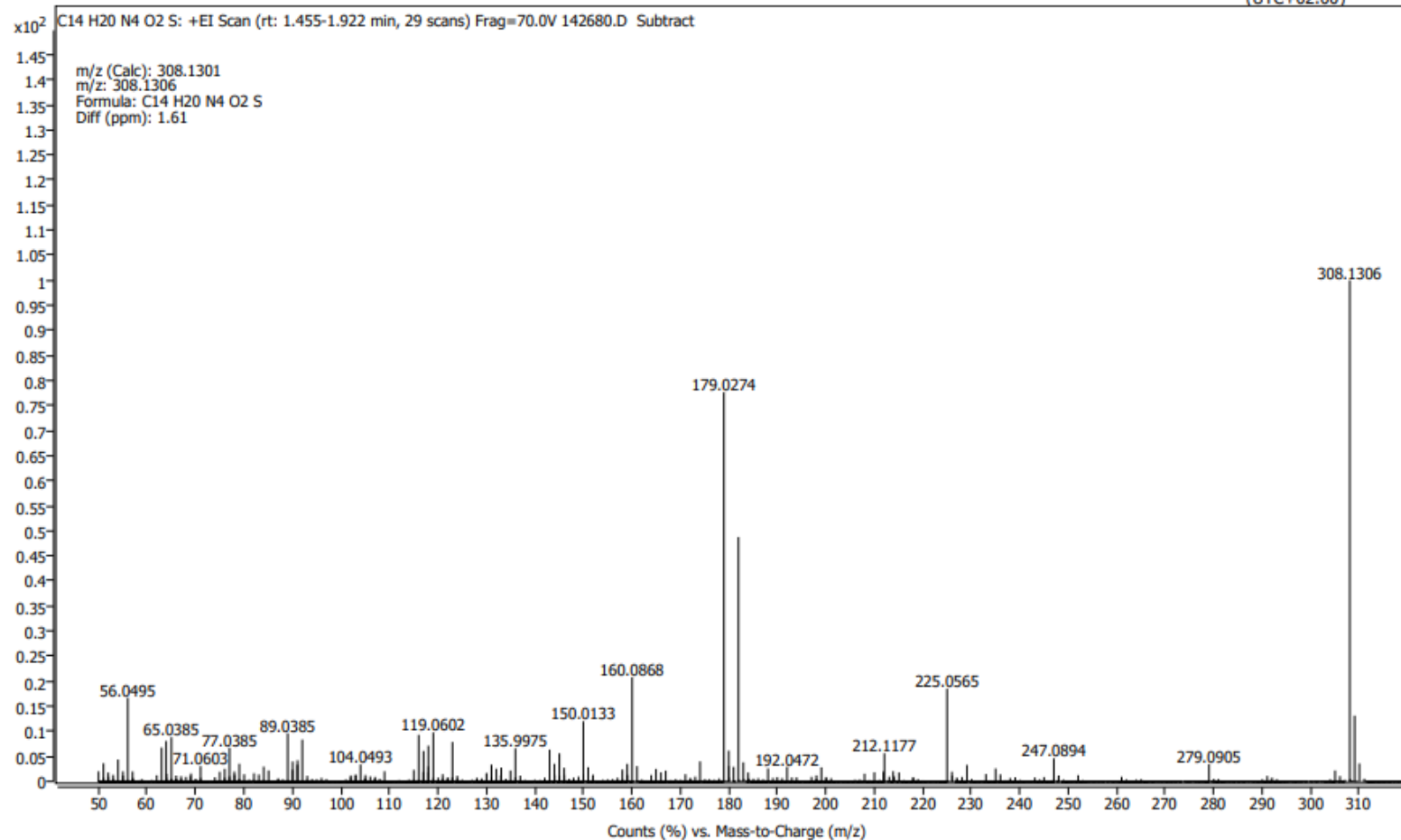


HRMS spectrum of **7b**

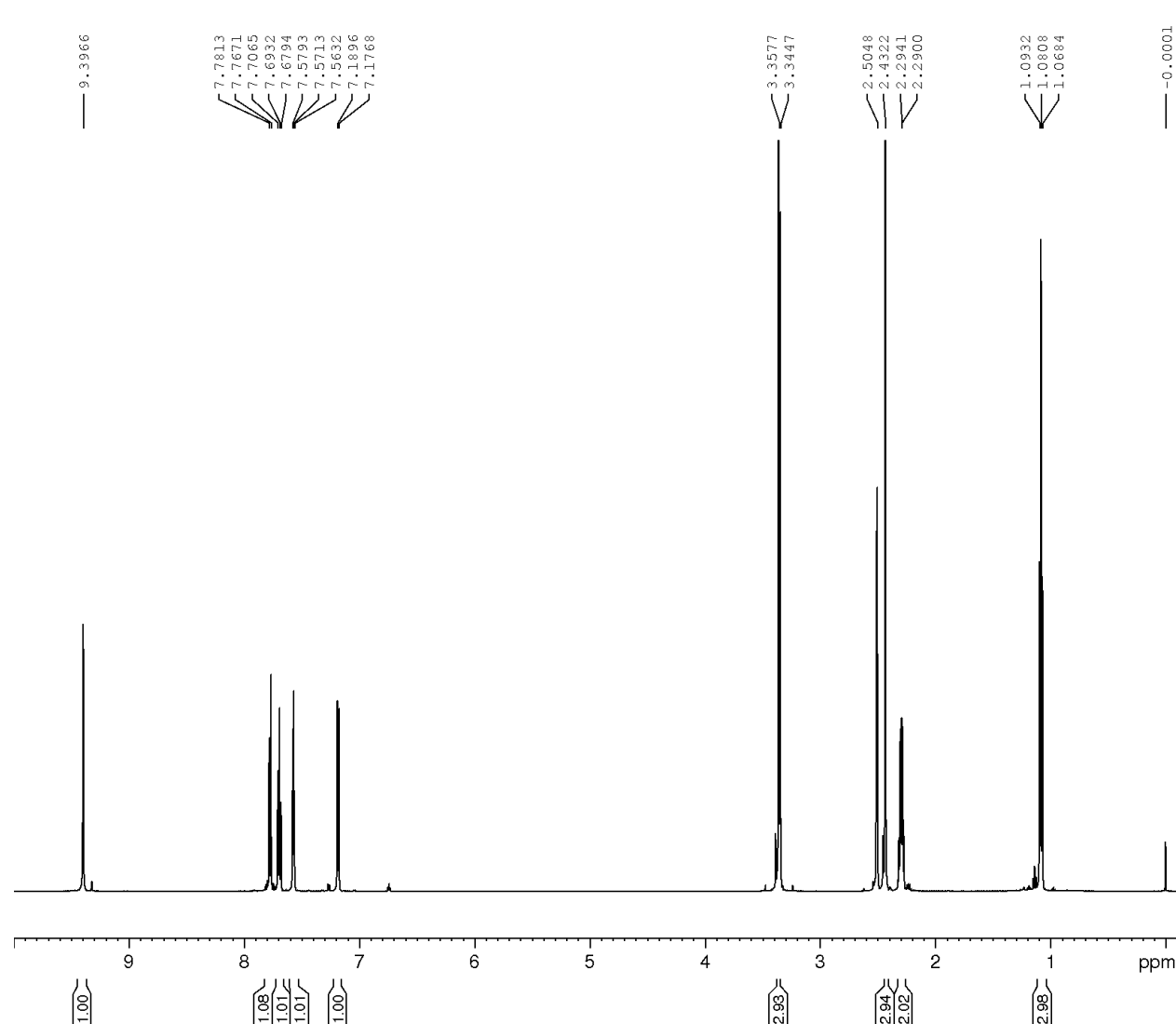
Spectrum Plot Report



Name	PGY0538_1A, Pusztai Gyongyver	Rack Pos.		Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	Plate Pos.		IRM Status	Success		
Data File	142657.D	Method (Acq)	DIP_70eV.M	Comment		Acq. Time (Local)	4/16/2024 2:01:53 PM (UTC+02:00)



¹H NMR spectrum of (*E*)-7c



Standard 1H
143707
PGY0790_1A
Pusztai Gyongyver
2024.10.24. (KP)

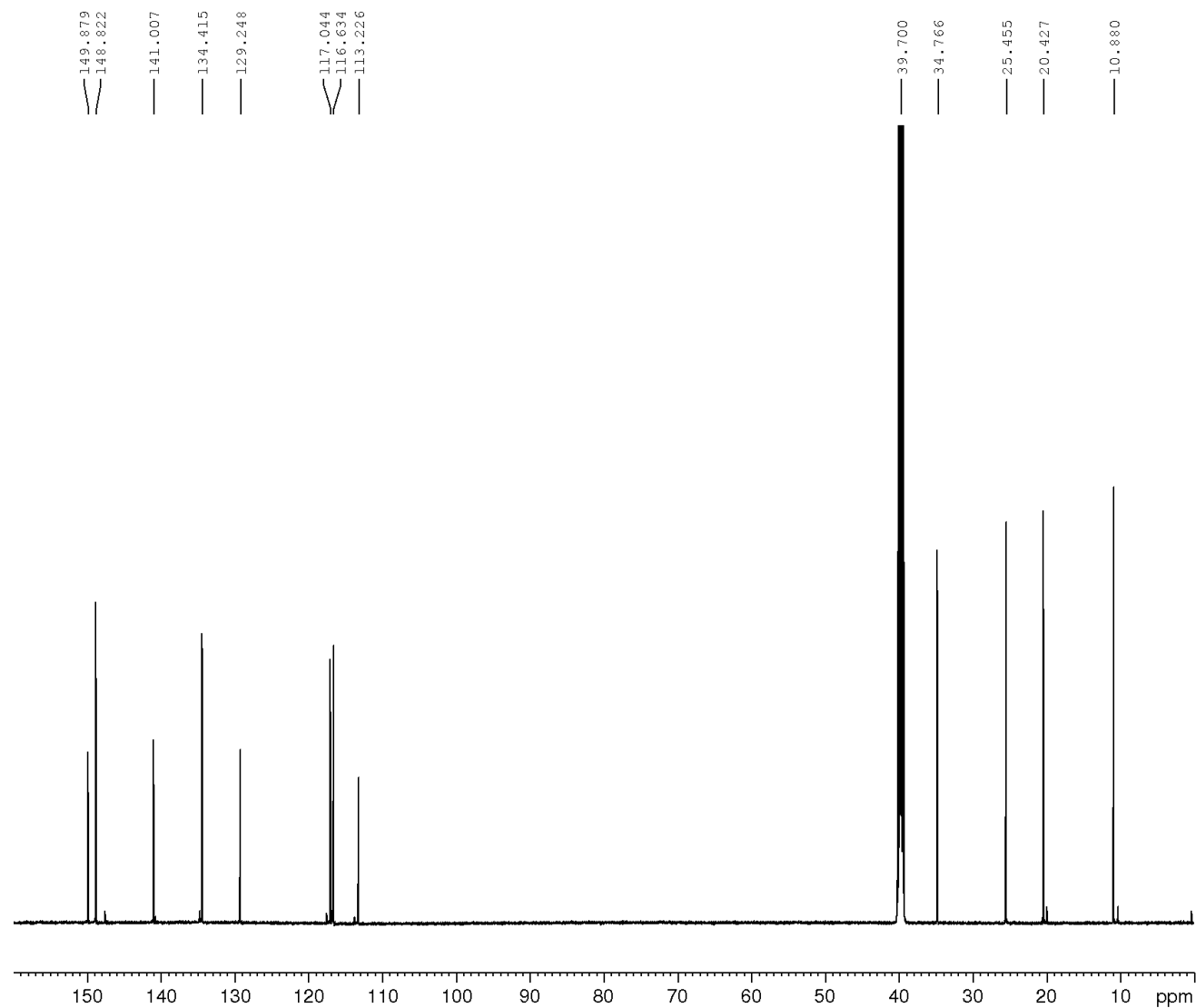
Current Data Parameters
NAME 143707
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241024
Time 15.44 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000018 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of (*E*)-7c



Standard 13C
143707
PGY0790_1A
Pusztai Gyongyver
2024.10.24. (KP)

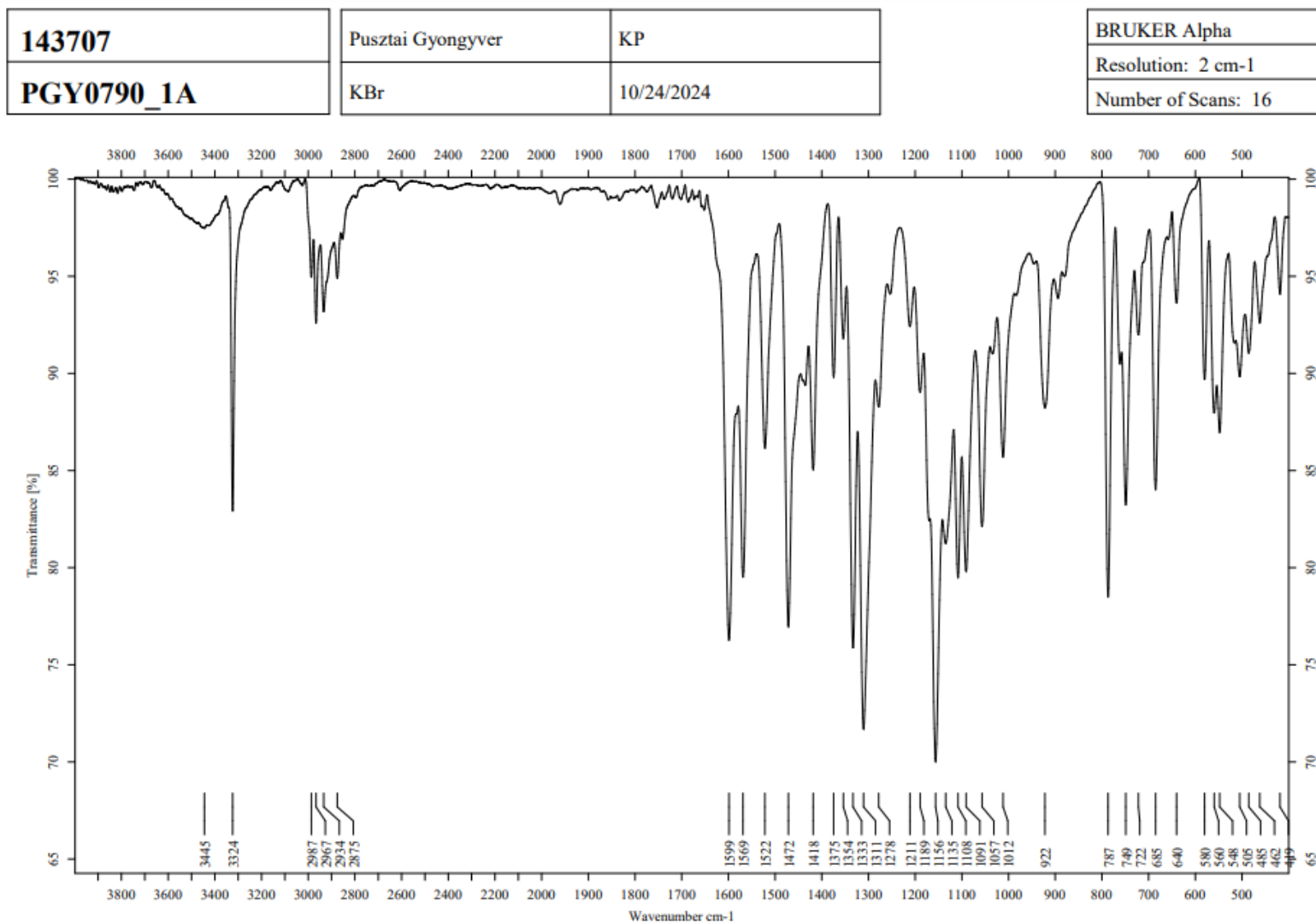
Current Data Parameters
NAME 143707
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241024
Time 16.53 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701603 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of (*E*)-7c

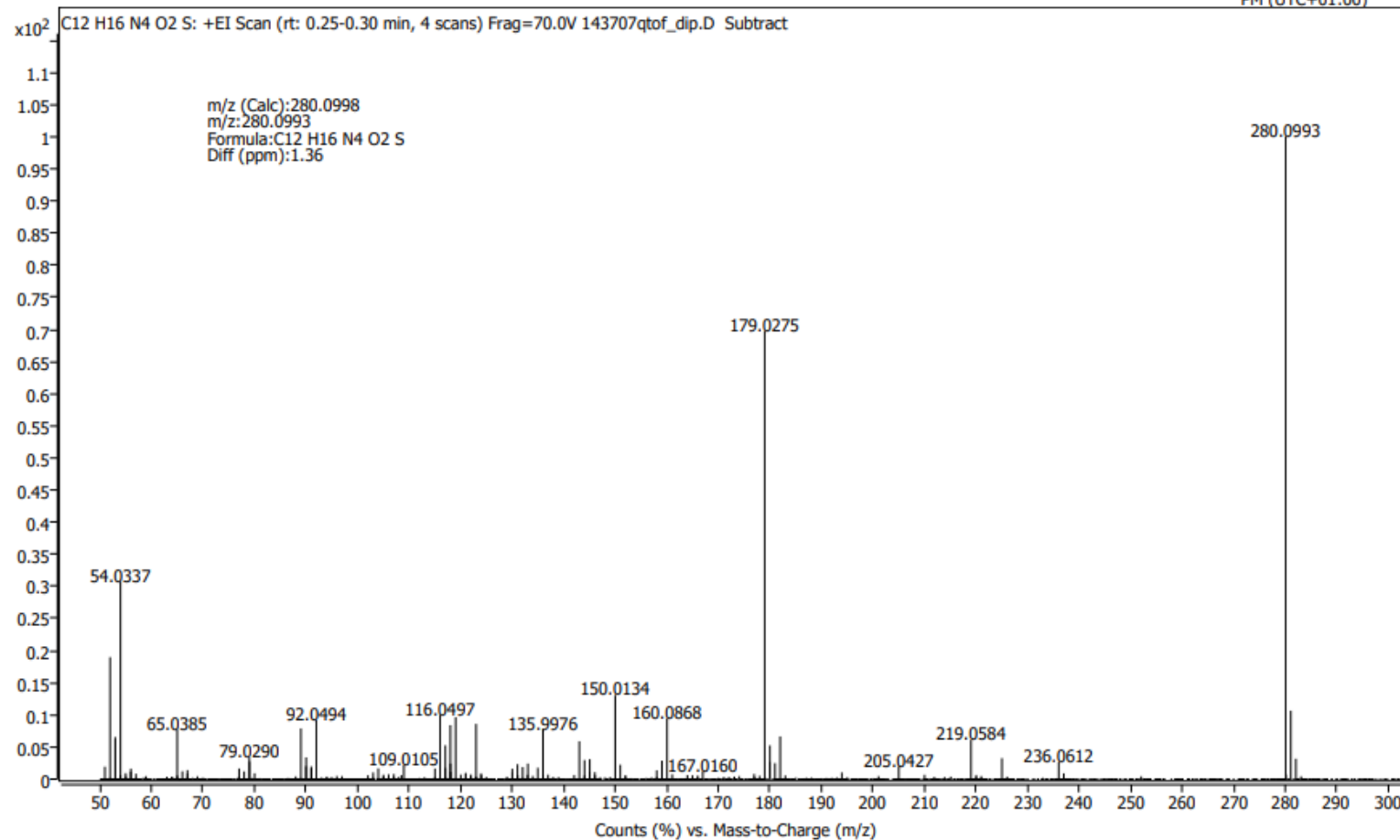


HRMS spectrum of (E)-7c

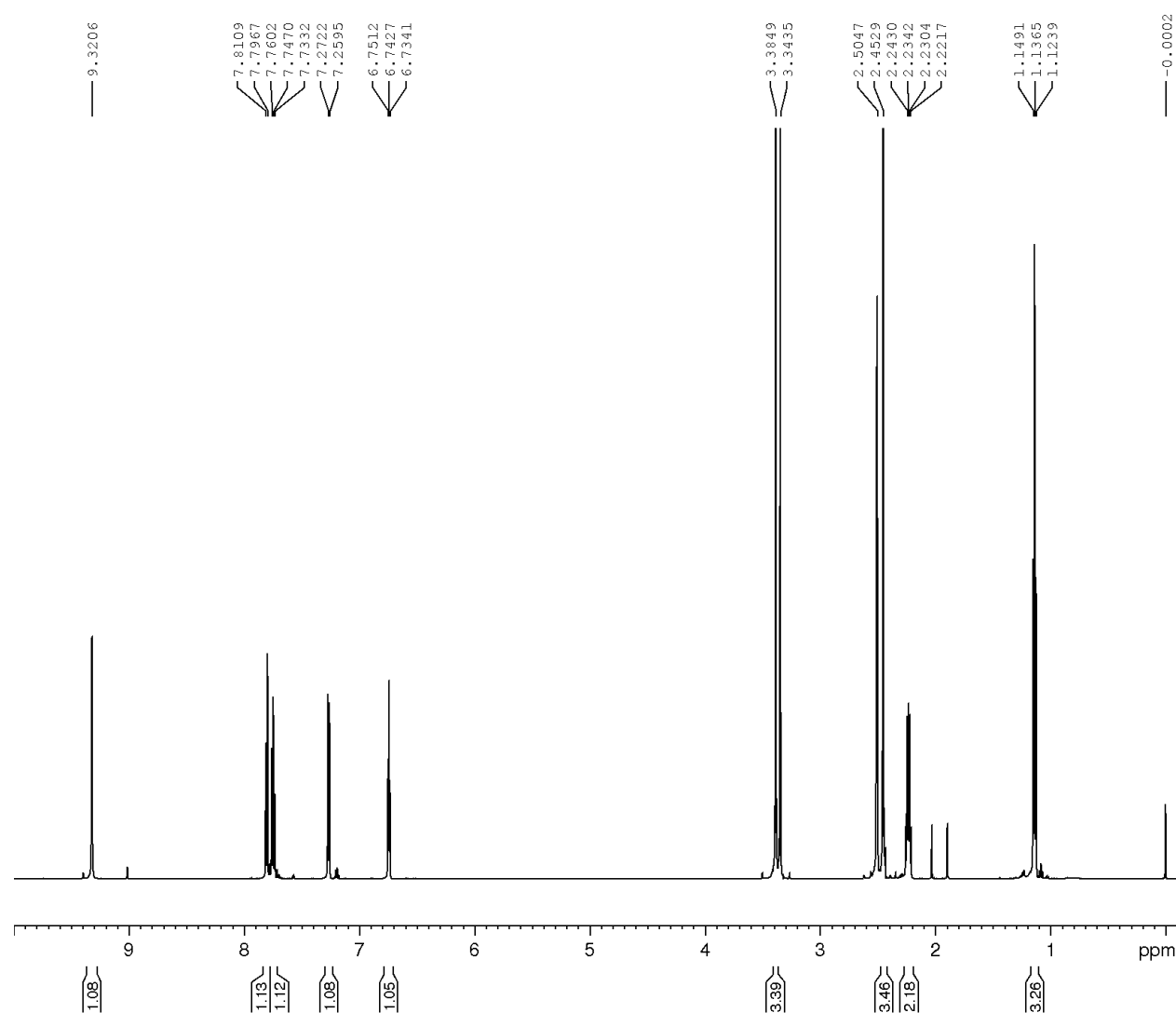
Spectrum Plot Report



Name	PGZ0790_1A, Pusztai Gyongyver	Rack Pos.	Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	1	Plate Pos.	IRM Status	Success		
Data File	143707qtof_dip.D	Method (Acq)	DIP_70eV_4min.M	Comment	Acq. Time (Local)	11/21/2024 5:33:16 PM (UTC+01:00)



¹H NMR spectrum of (Z)-7c



Standard 1H
143697
PGY0790_1B
Pusztai Gyongyver
2024.10.24. (KP)

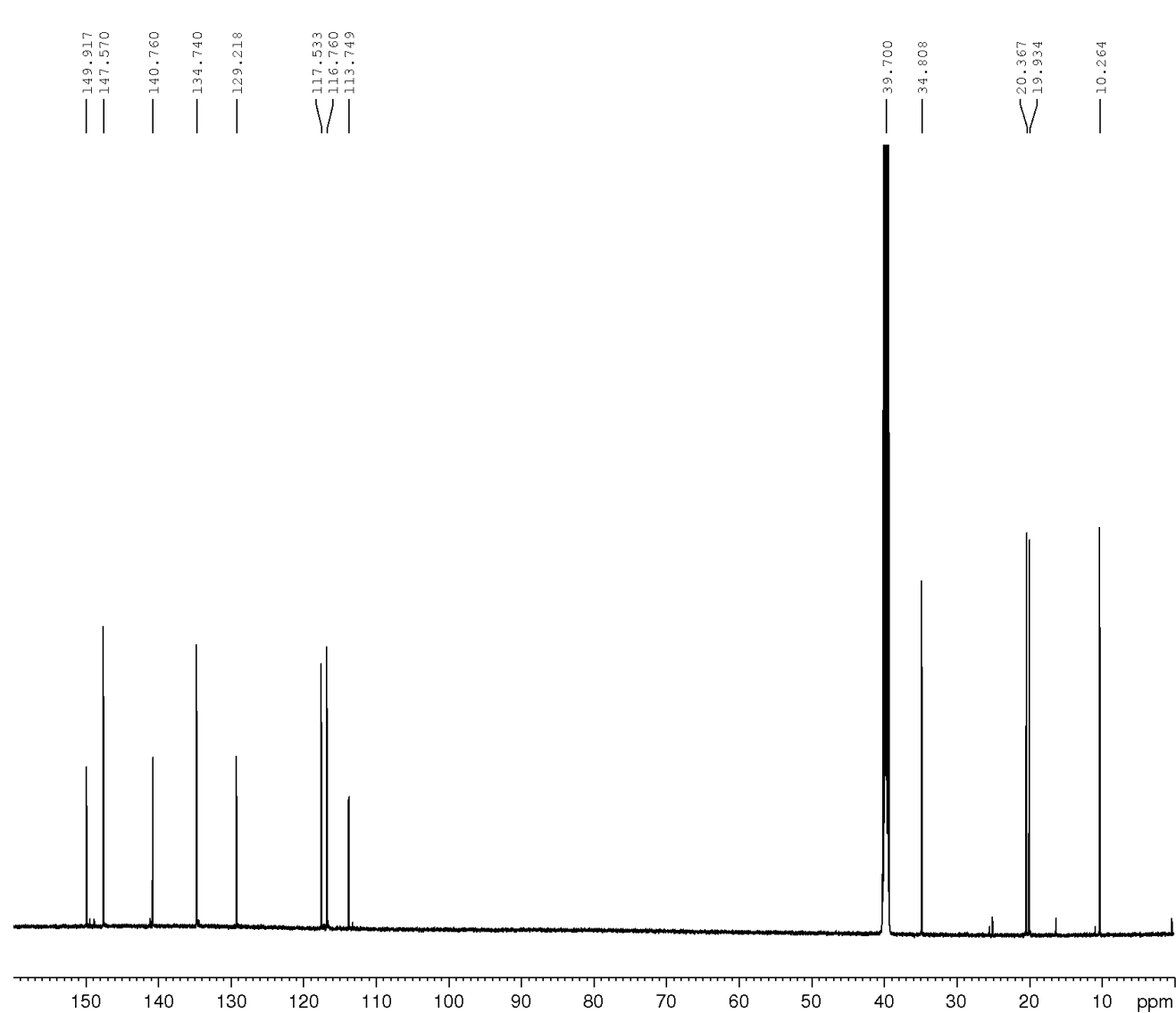
Current Data Parameters
NAME 143697
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241024
Time 19.40 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000019 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of (Z)-7c



Standard 13C
143697
PGY0790_1B
Pusztai Gyongyver
2024.10.24. (KP)

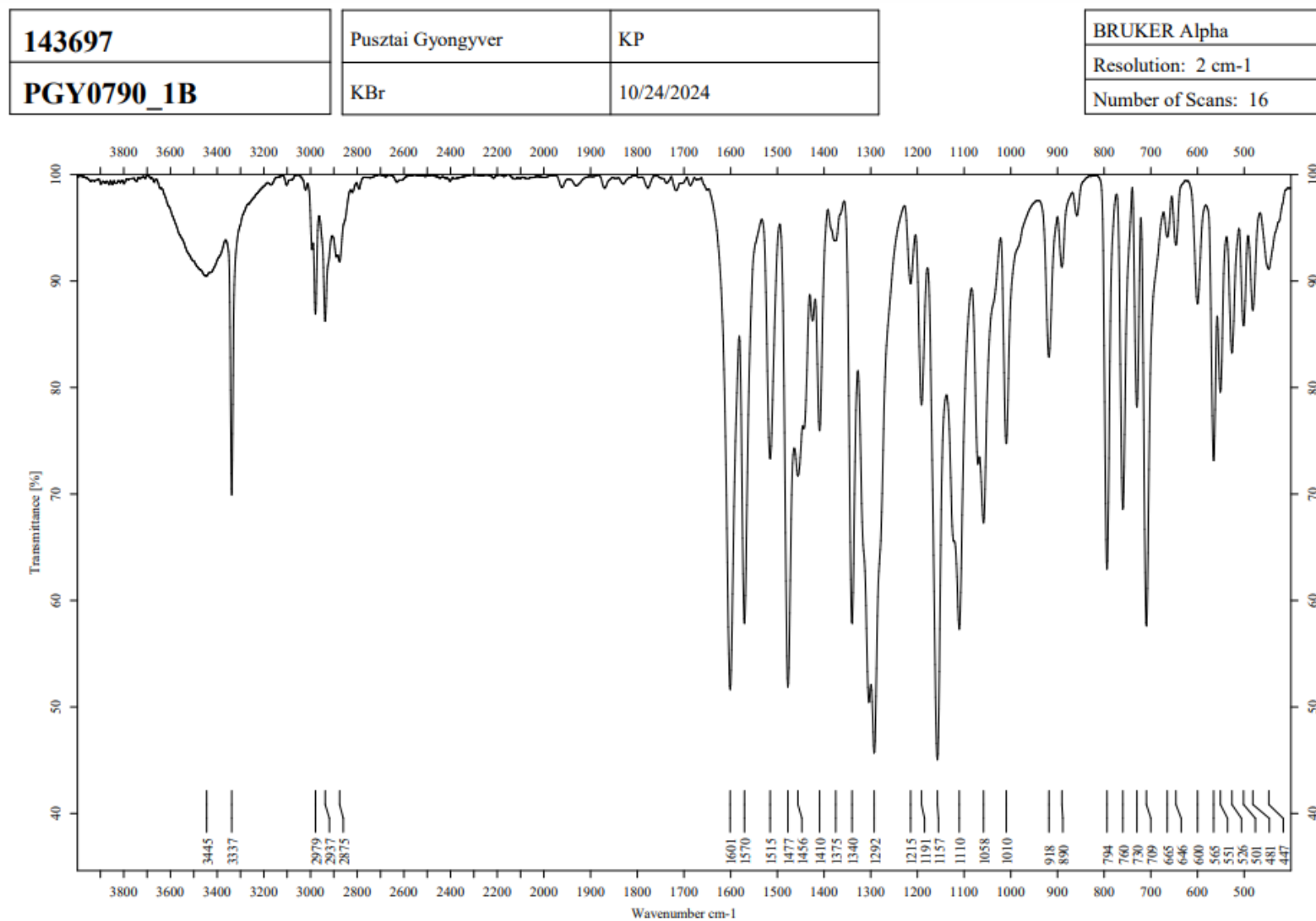
Current Data Parameters
NAME 143697
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241024
Time 20.48 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701603 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of (Z)-7c

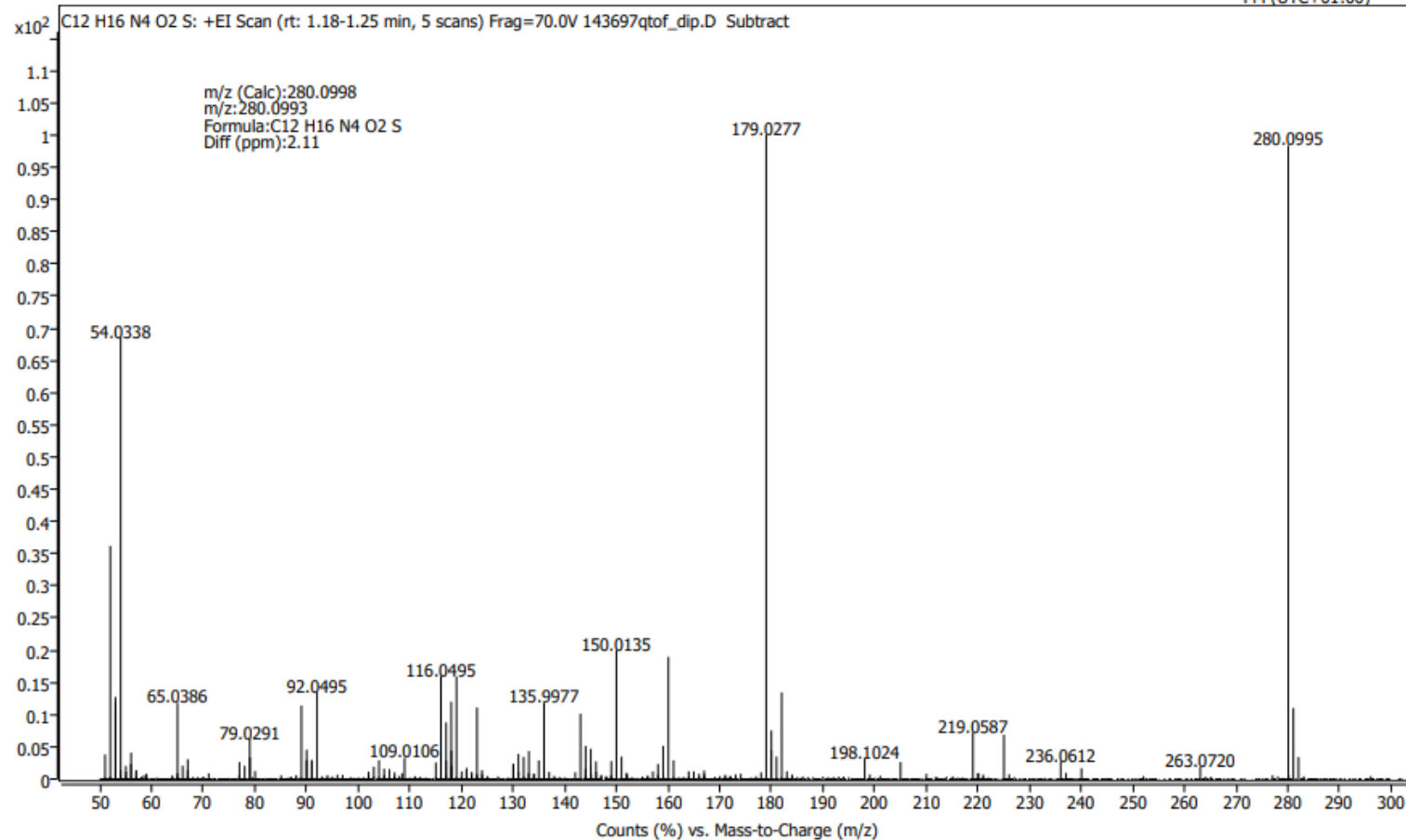


HRMS spectrum of (Z)-7c

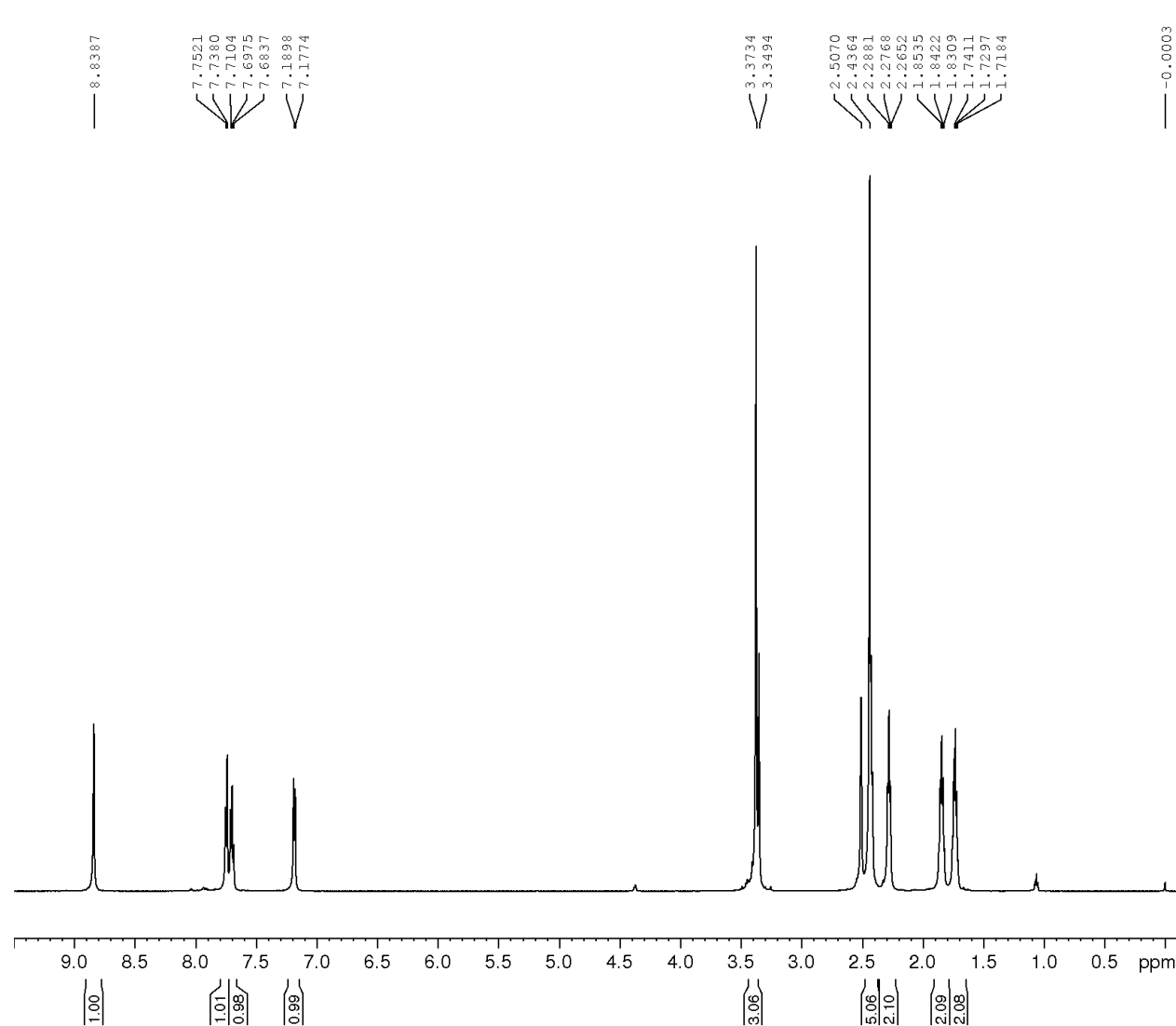
Spectrum Plot Report



Name	PGZ0790_1B, Pusztai Gyongyver	Rack Pos.	Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	1	Plate Pos.	IRM Status	Success	Acq. Time (Local)	11/21/2024 5:41:17 PM (UTC+01:00)
Data File	143697qtof_dip.D	Method (Acq)	DIP_70eV_4min.M	Comment		



¹H NMR spectrum of **7d**



Standard 1H
143739
PGY0808_1
Pusztai Gyongyver
2024.10.21. (DA)

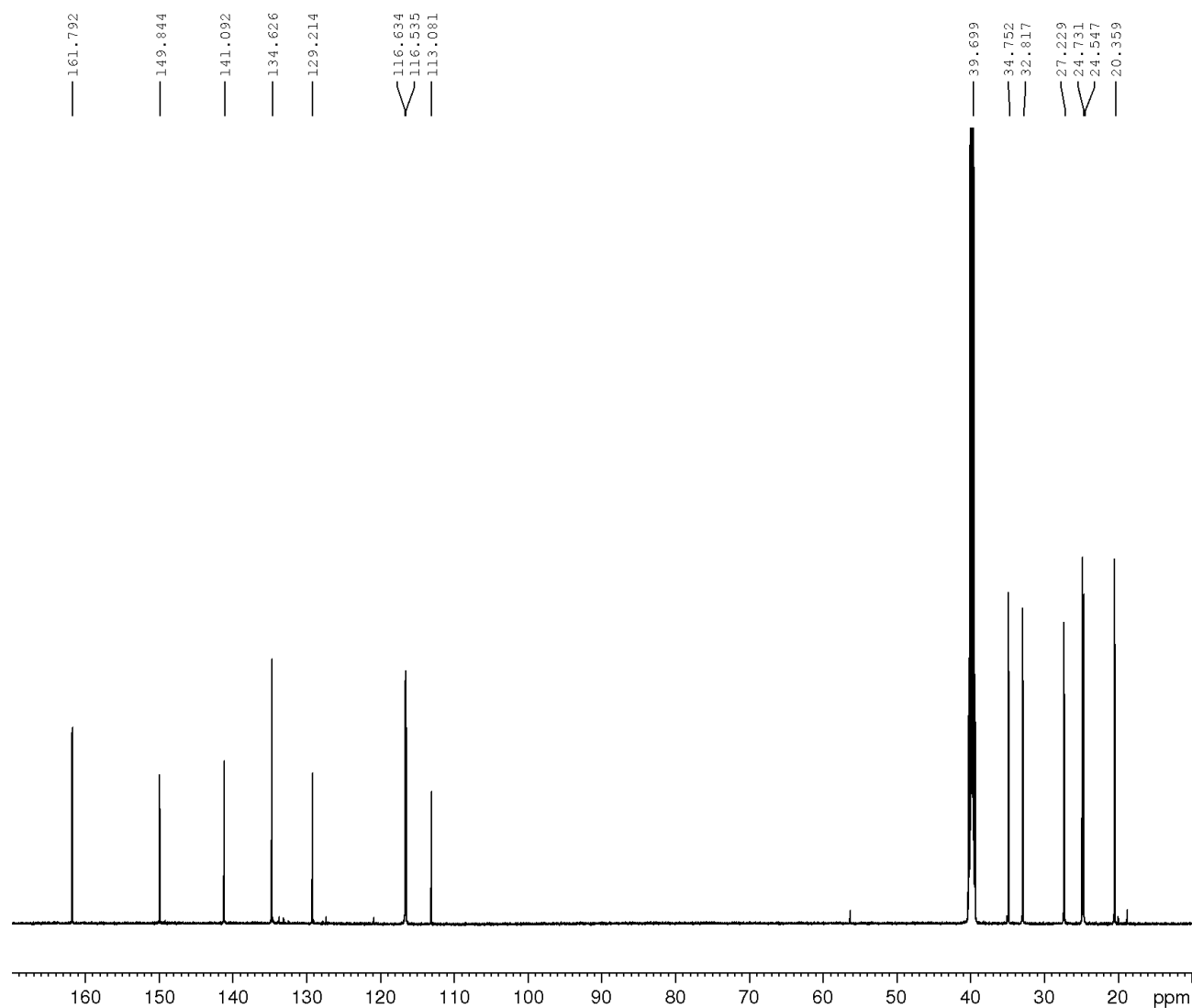
Current Data Parameters
NAME 143739
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241021
Time 17.52 h
INSTRUM spect
PROBHD Z145856_0002 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 111.4
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000012 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



¹³C NMR spectrum of **7d**



Standard 13C
143739
PGY0808_1
Pusztai Gyongyver
2024.10.21. (DA)

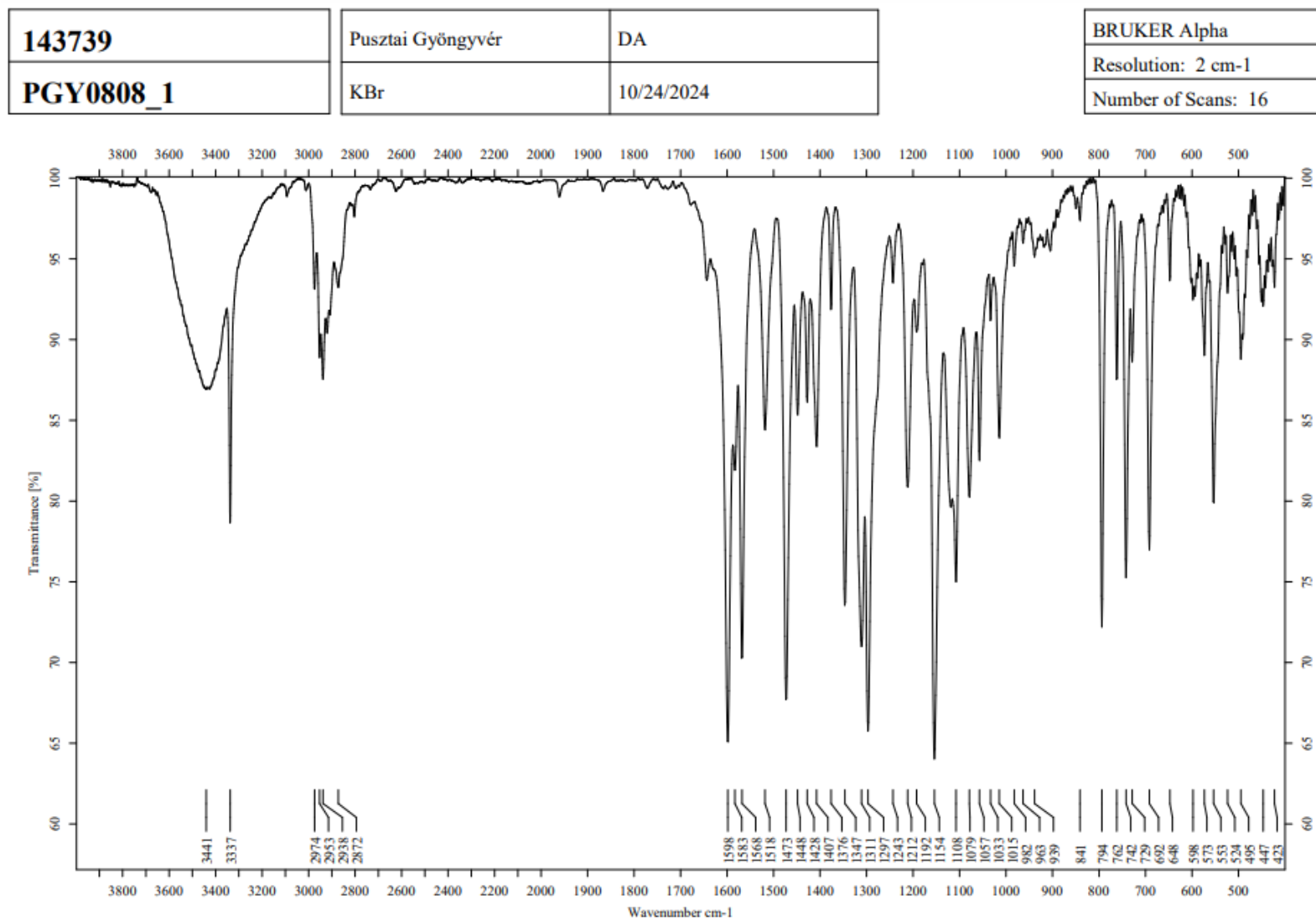
Current Data Parameters
NAME 143739
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241021
Time 19.01 h
INSTRUM spect
PROBHD z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701608 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of 7d

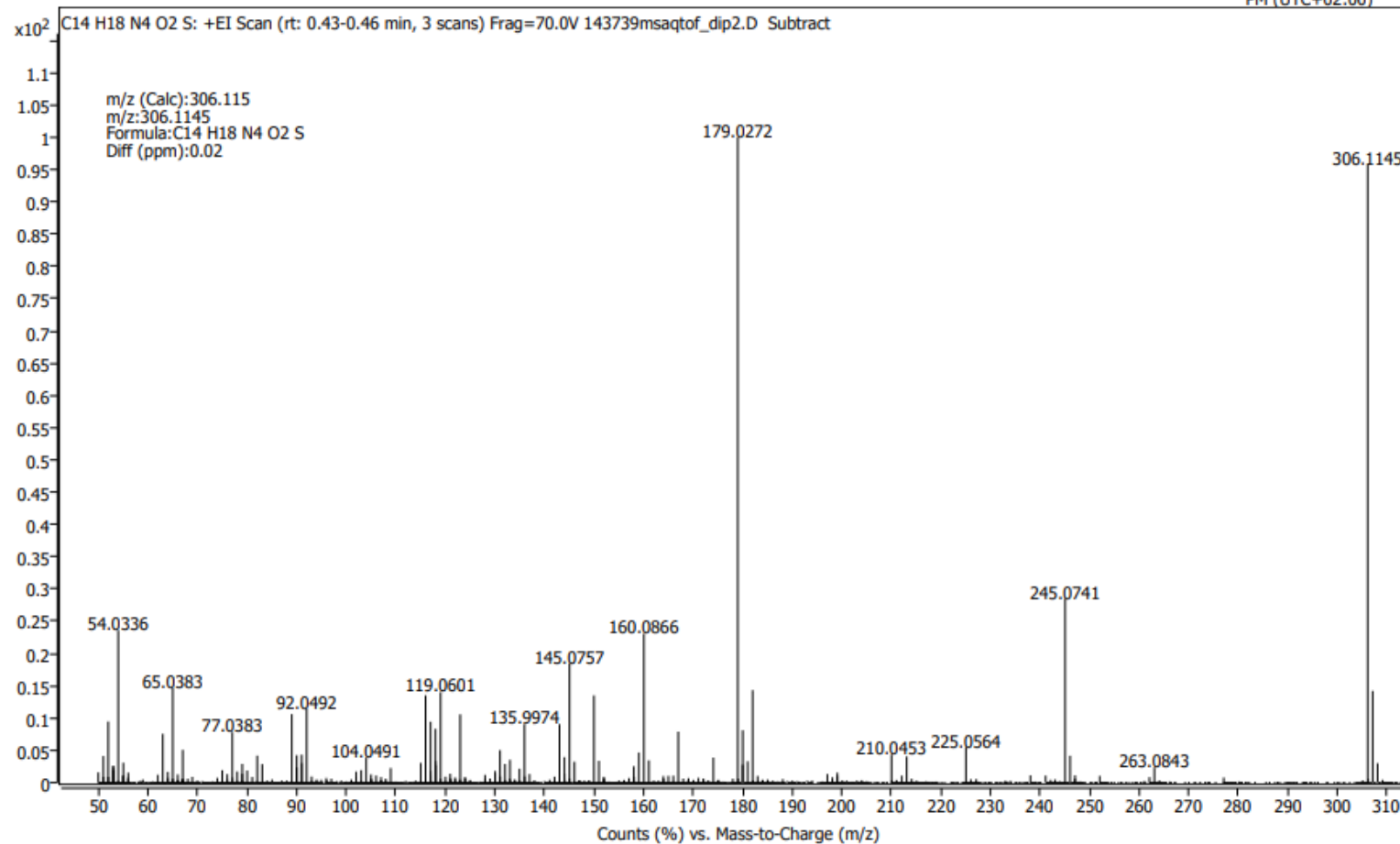


HRMS spectrum of **7d**

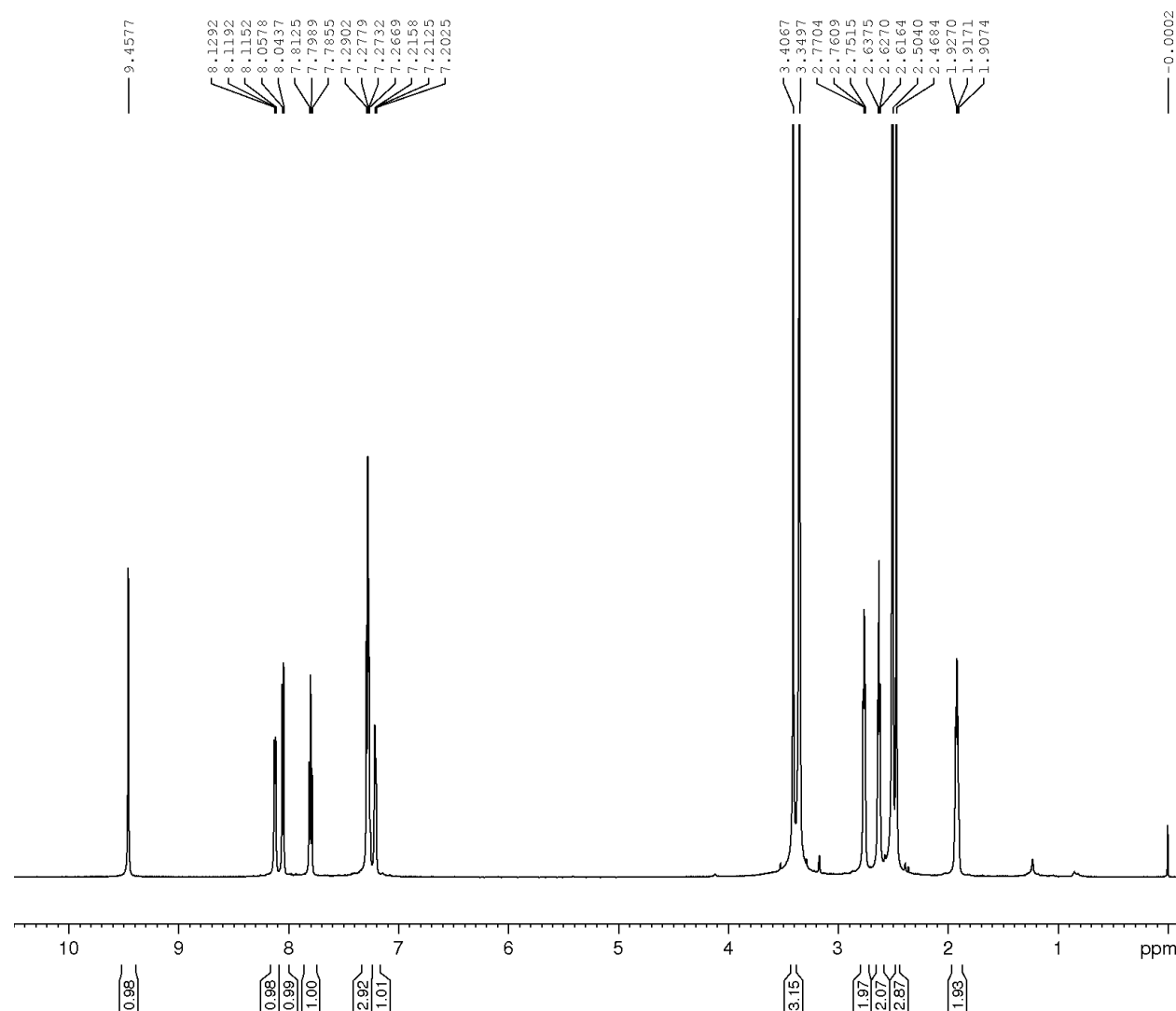
Spectrum Plot Report



Name	PGY00808_1, Pusztai Gyongyver	Rack Pos.	Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	Plate Pos.	IRM Status	Success	Acq. Time (Local)	10/24/2024 1:41:44 PM (UTC+02:00)
Data File	143739msaqtod_dip2.D Method (Acq)	DIP_70eV_4min.M	Comment			



¹H NMR spectrum of (*E*)-**9a**



Standard 1H
143519
PGY0782_1
Pusztai Gyongyver
2024.09.17. (DA)

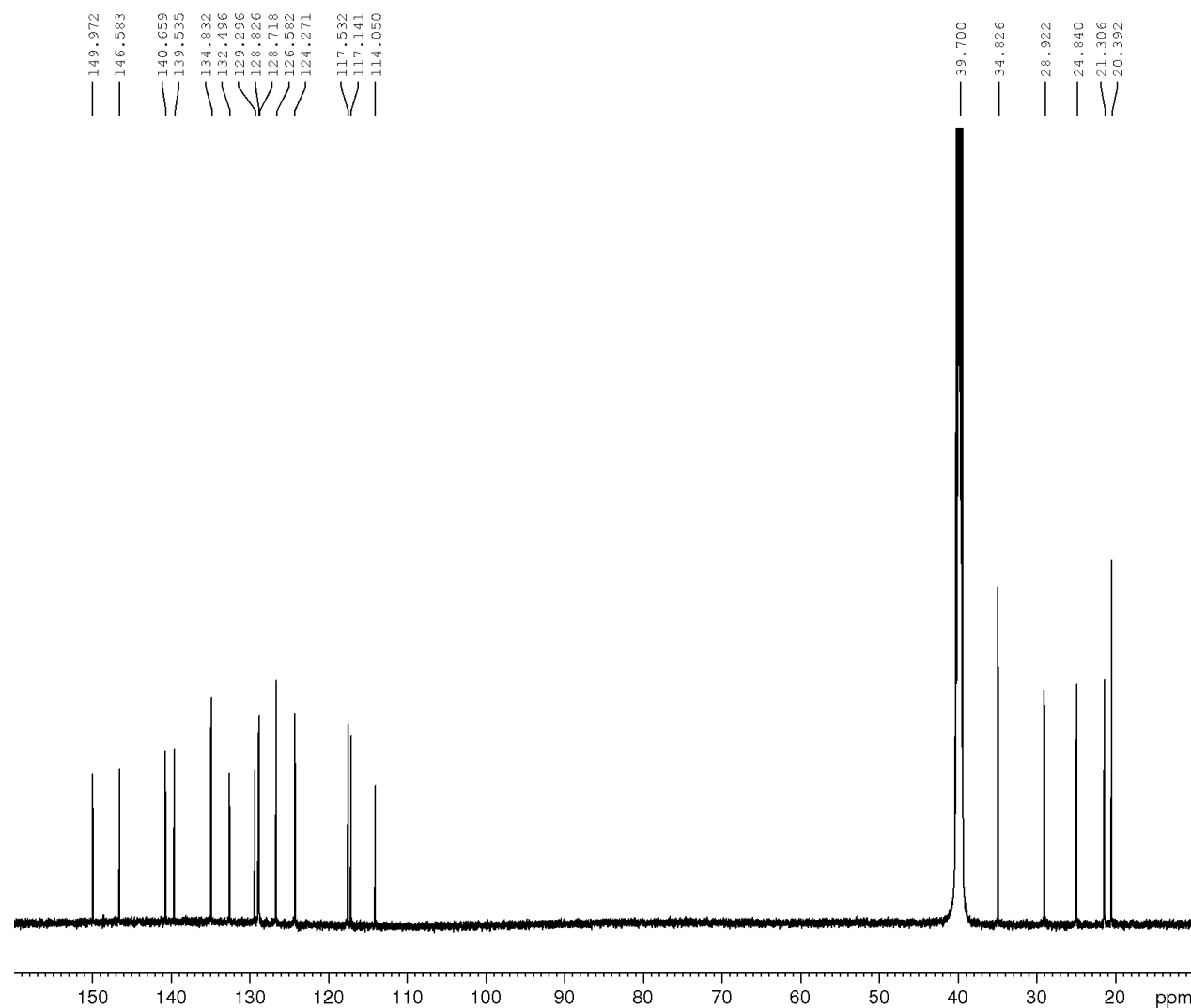
Current Data Parameters
NAME 143519
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240918
Time 10.56 h
INSTRUM spect
PROBHD Z145856_0002 (zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000025 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of (*E*)-**9a**



Standard 13C
143519
PGY0782_1
Pusztai Gyongyver
2024.09.17. (DA)

Current Data Parameters
NAME 143519
EXPNO 22
PROCNO 1

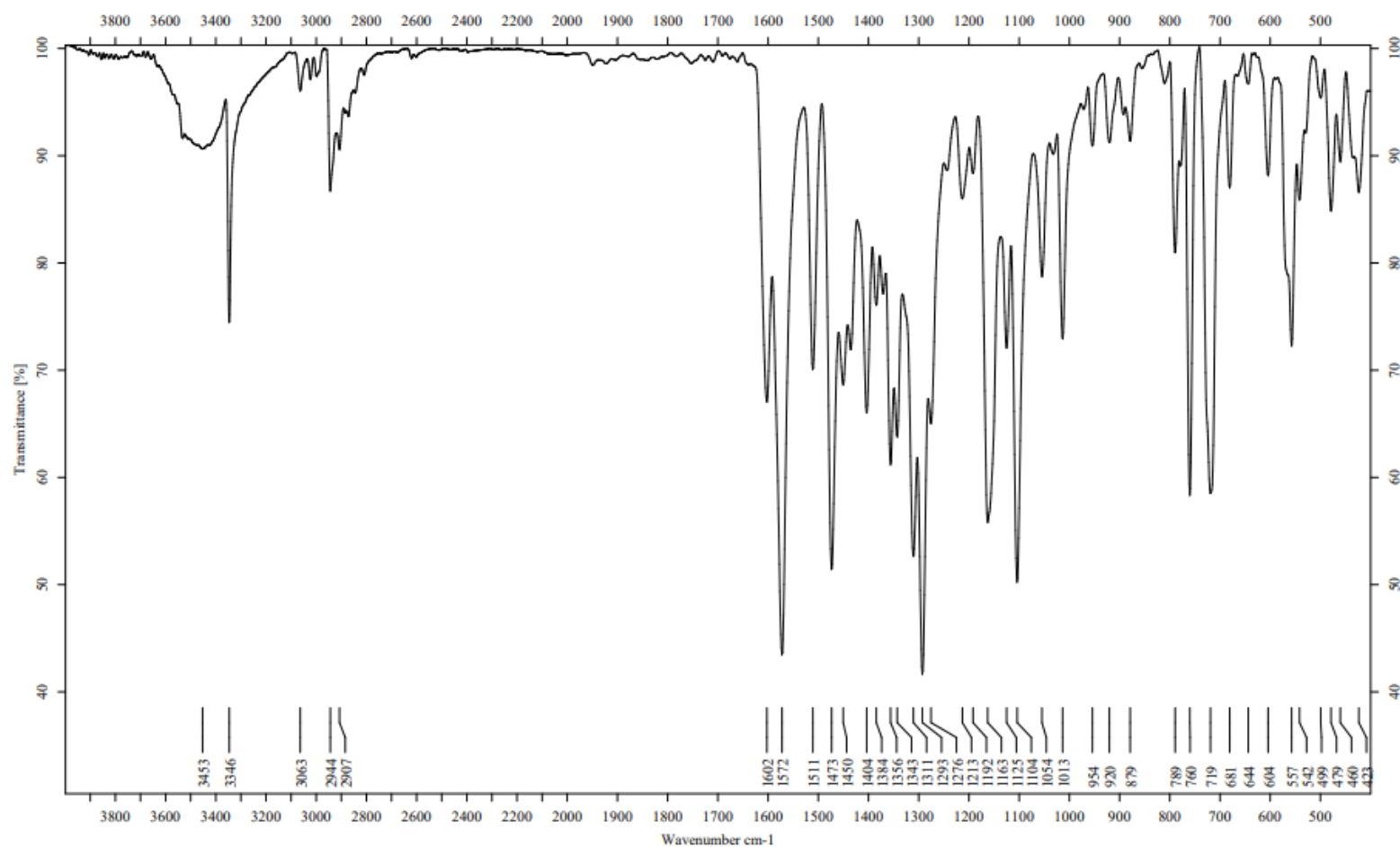
F2 - Acquisition Parameters
Date_ 20240918
Time 12.05 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701594 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of (*E*)-**9a**

143519	Pusztai Gyongyver	KP	BRUKER Alpha
PGY0782_1	KBr	9/17/2024	Resolution: 2 cm-1
			Number of Scans: 16

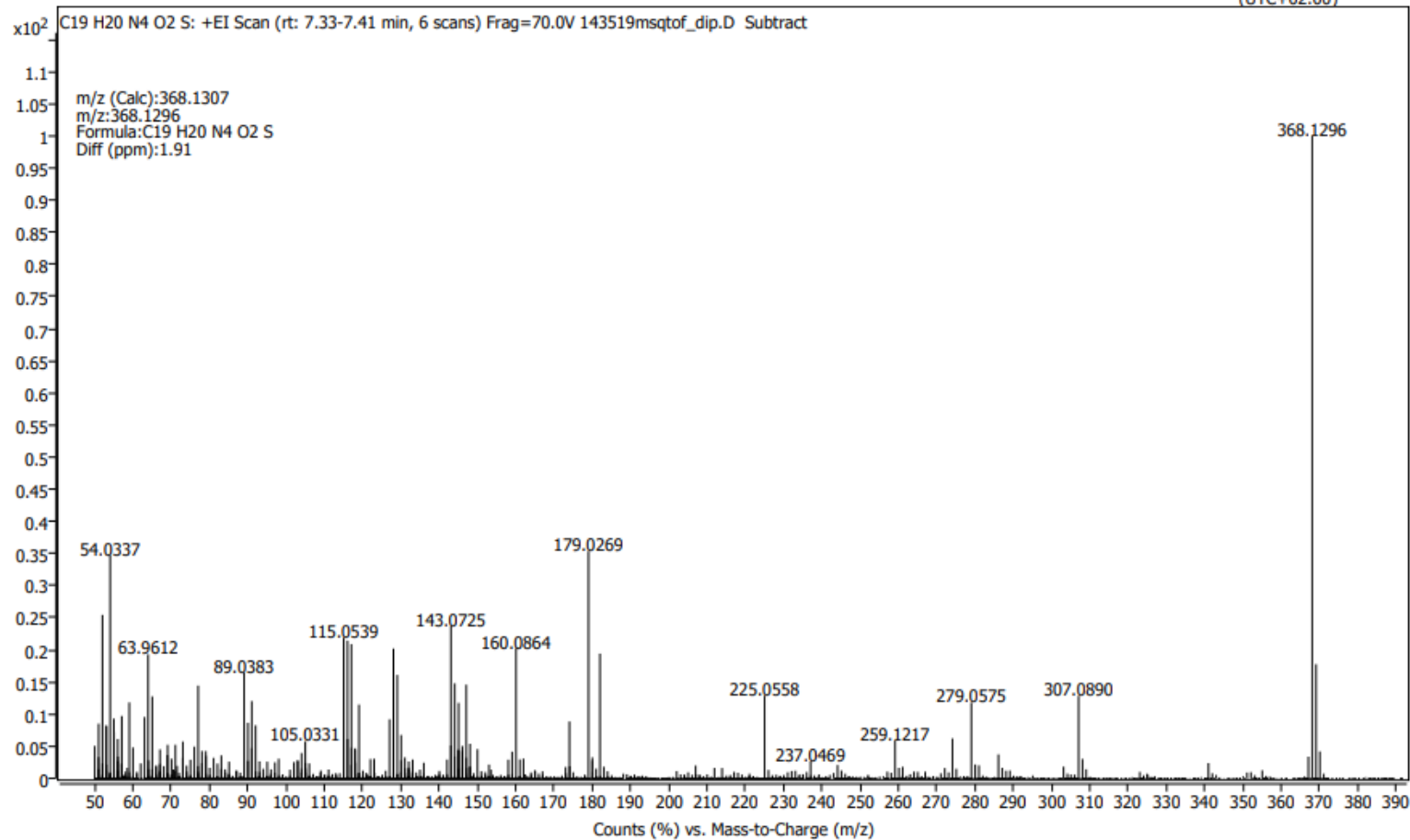


HRMS spectrum of (*E*)-9a

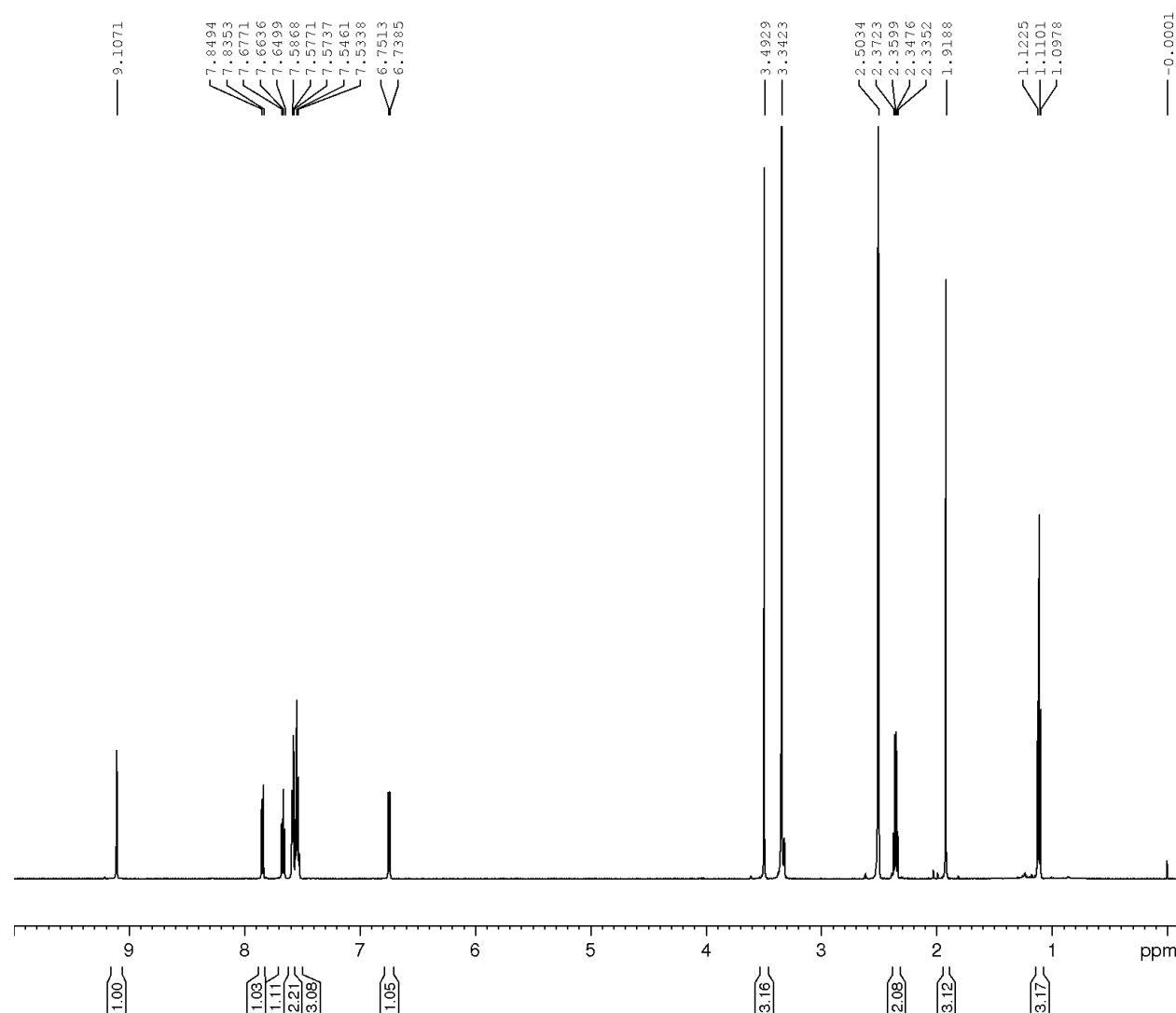
Spectrum Plot Report



Name	PGY0782_1, Pusztai Gyongyver	Rack Pos.	Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	Plate Pos.	IRM Status	Success	Acq. Time (Local)	9/30/2024 1:27:33 PM (UTC+02:00)
Data File	143519msqtof_dip.D	Method (Acq)	DIP_70eV.M	Comment		



¹H NMR spectrum of (*E*)-**7f**



Standard 1H
144013
PGY0791_1A
Pusztai Gyongyver
2024.12.12. (KP)

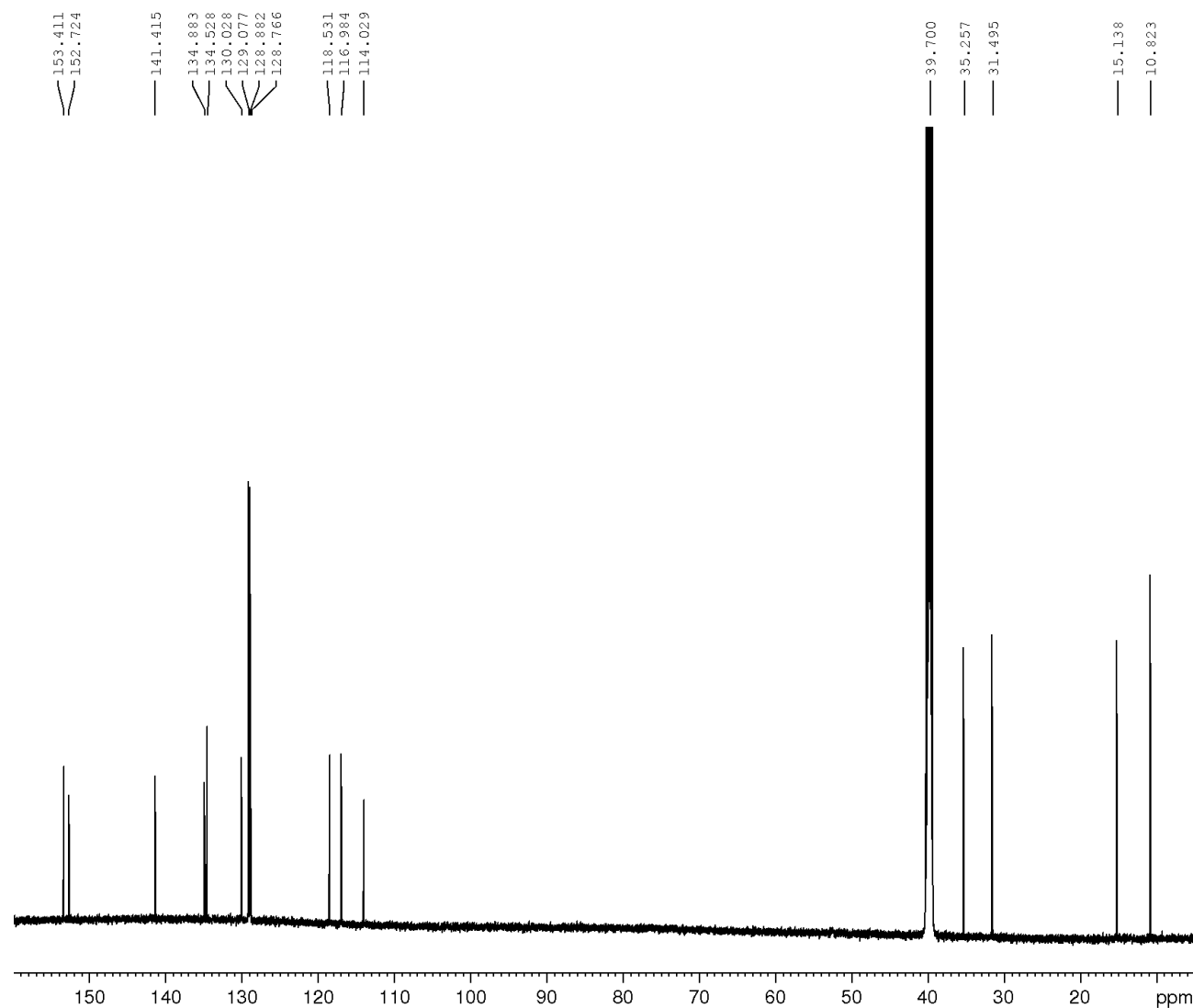
Current Data Parameters
NAME 144013
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241212
Time 18.06 h
INSTRUM spect
PROBHD Z145856_0002 (zg30)
PULPROG 65536
TD 16
SOLVENT DMSO
NS 2
DS 12019.230 Hz
SWH 0.366798 Hz
FIDRES 2.7262976 sec
AQ 196.07
RG 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000031 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of (*E*)-7f



Standard 13C
144013
PGY0791_1A
Pusztai Gyongyver
2024.12.12. (KP)

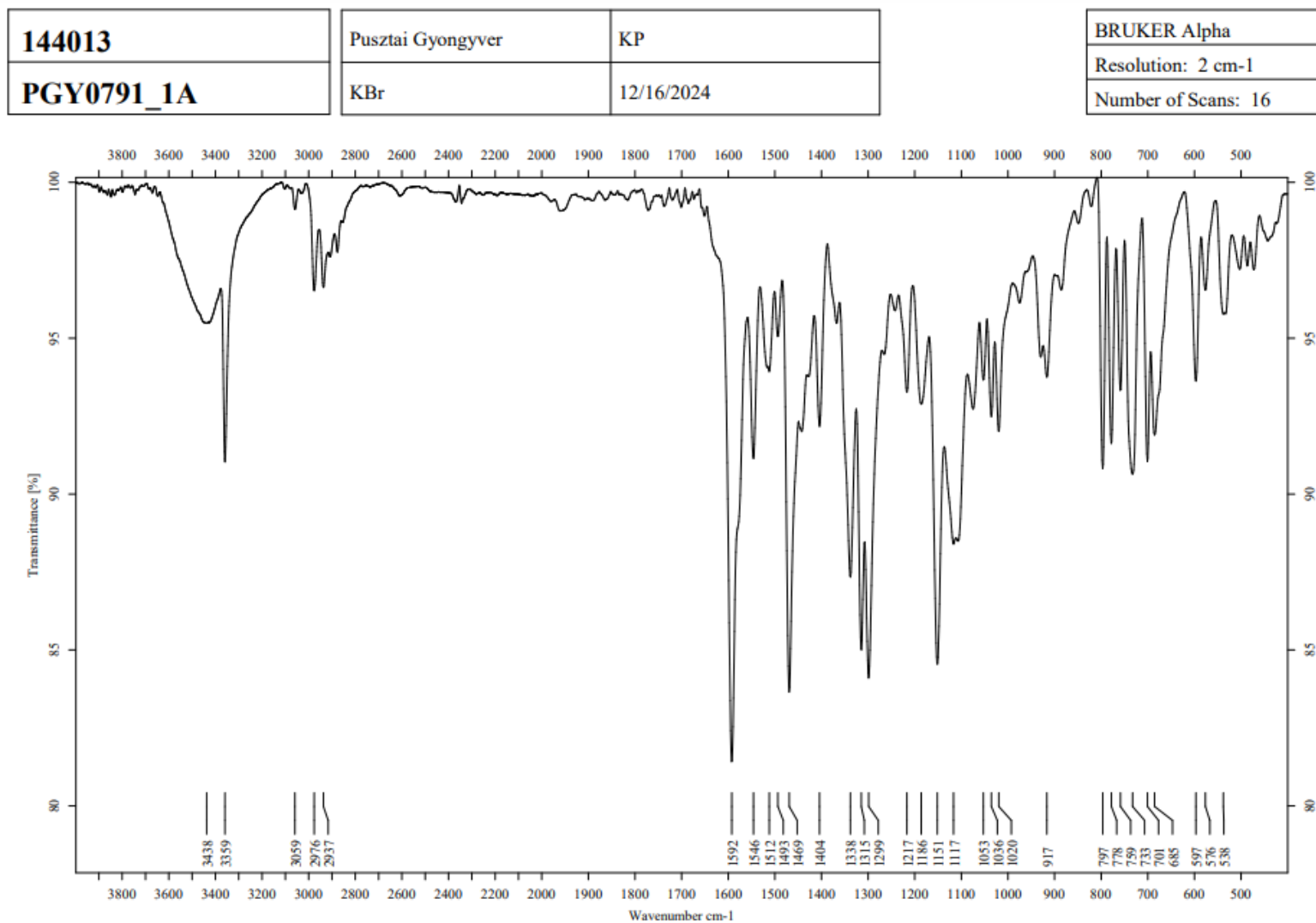
Current Data Parameters
NAME 144013
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241212
Time 19.14 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701604 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of (*E*)-**7f**

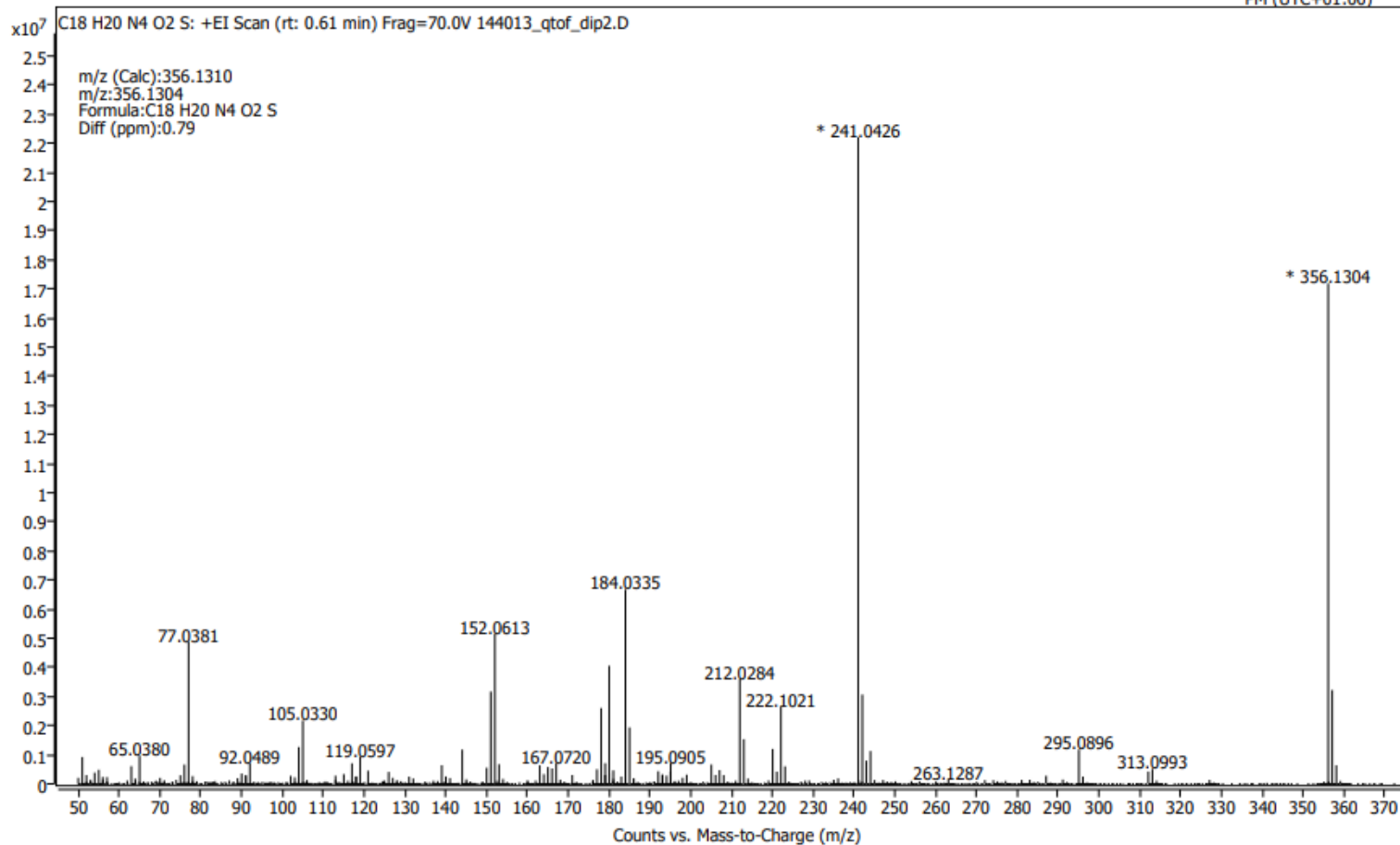


HRMS spectrum of (*E*)-7f

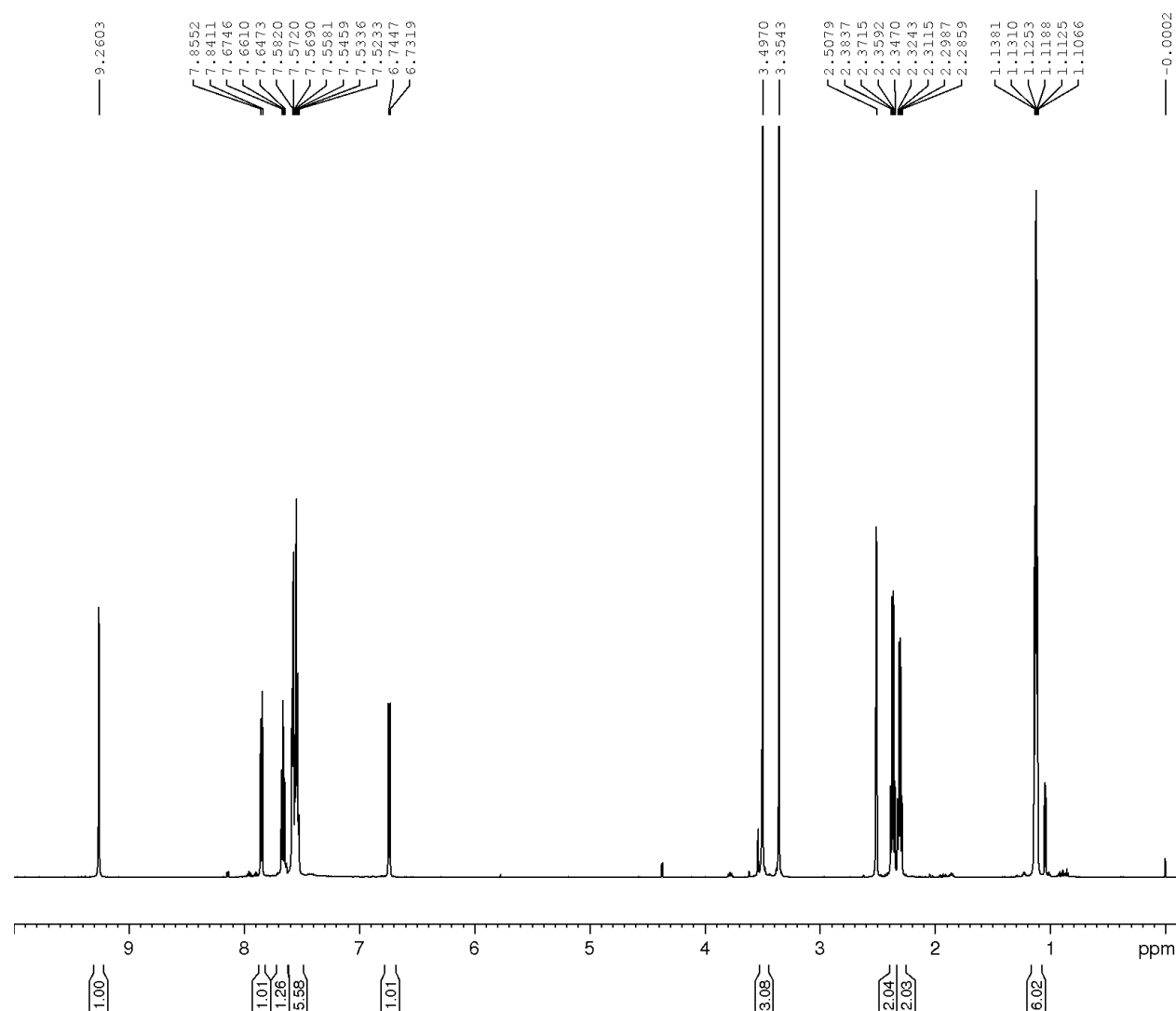
Spectrum Plot Report



Name	PGZ0791_1A, Pusztai Gyongyver	Rack Pos.	Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	Plate Pos.	IRM Status	Success	Acq. Time (Local)	12/13/2024 12:41:35 PM (UTC+01:00)
Data File	144013_qtof_dip2.D	Method (Acq)	DIP_70eV.M	Comment		



¹H NMR spectrum of 7g



Standard 1H
143537
PGY0777_1A
Pusztai Gyongyver
2024.09.23. (KP)

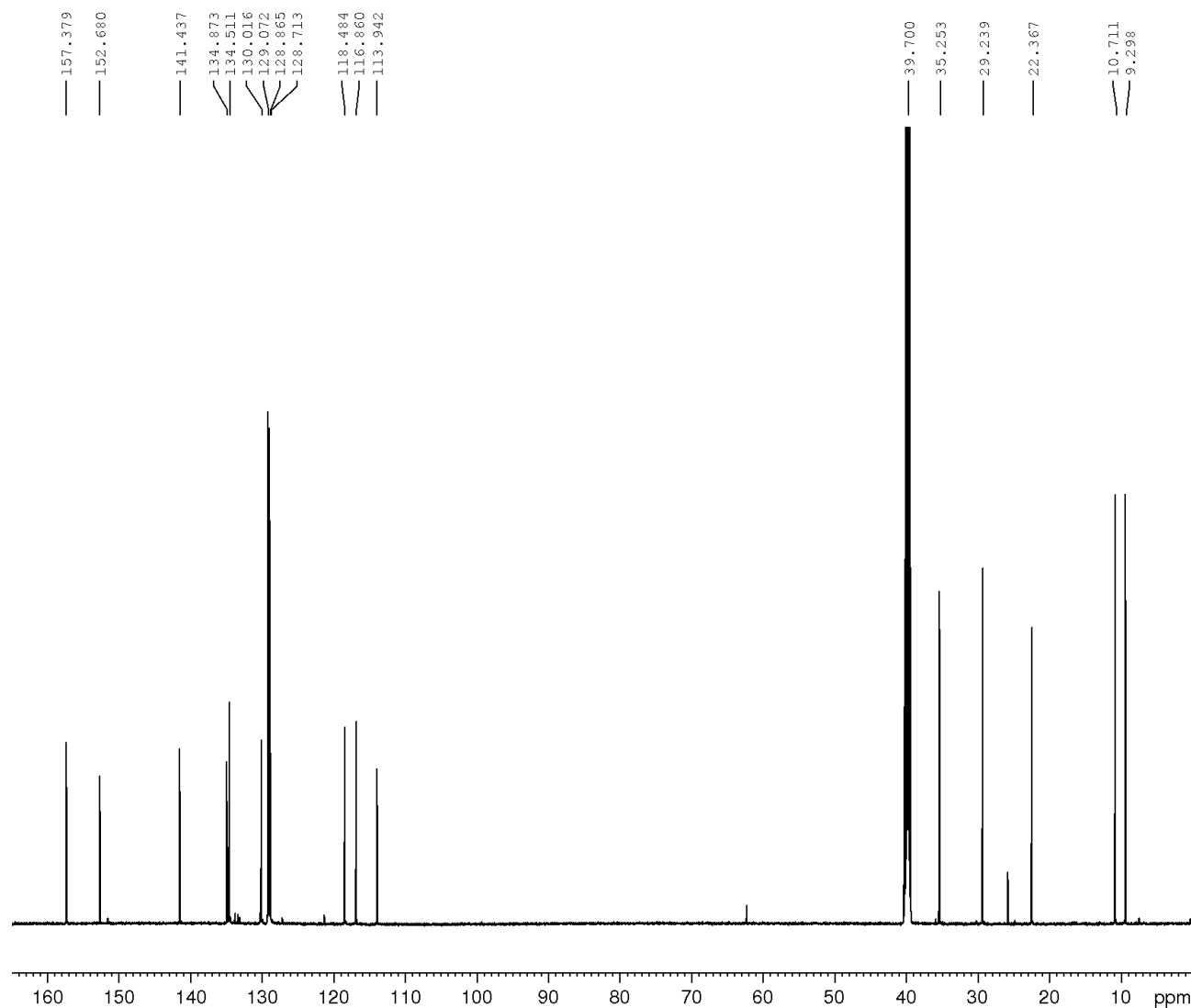
Current Data Parameters
NAME 143537
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240924
Time 3.00 h
INSTRUM spect
PROBHD Z145856_0002 (zg30)
PULPROG 65536
TD 16
SOLVENT DMSO
NS 2
DS 12019.230 Hz
SWH 0.366798 Hz
FIDRES 2.7262976 sec
AQ 119.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of **7g**



Standard 13C
143537
PGY0777_1A
Pusztai Gyongyver
2024.09.23. (KP)

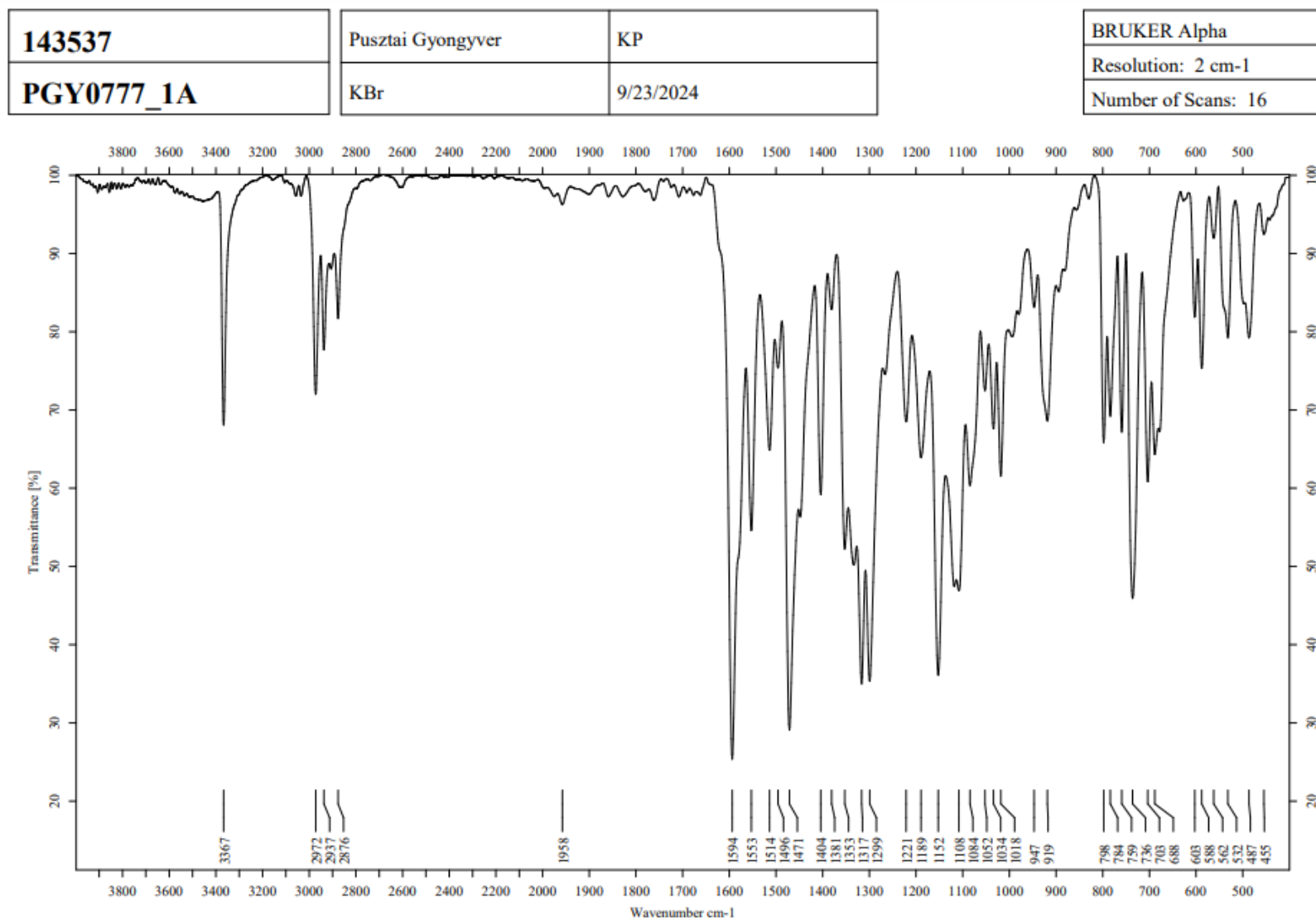
Current Data Parameters
NAME 143537
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240924
Time 4.09 h
INSTRUM spect
PROBHD z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

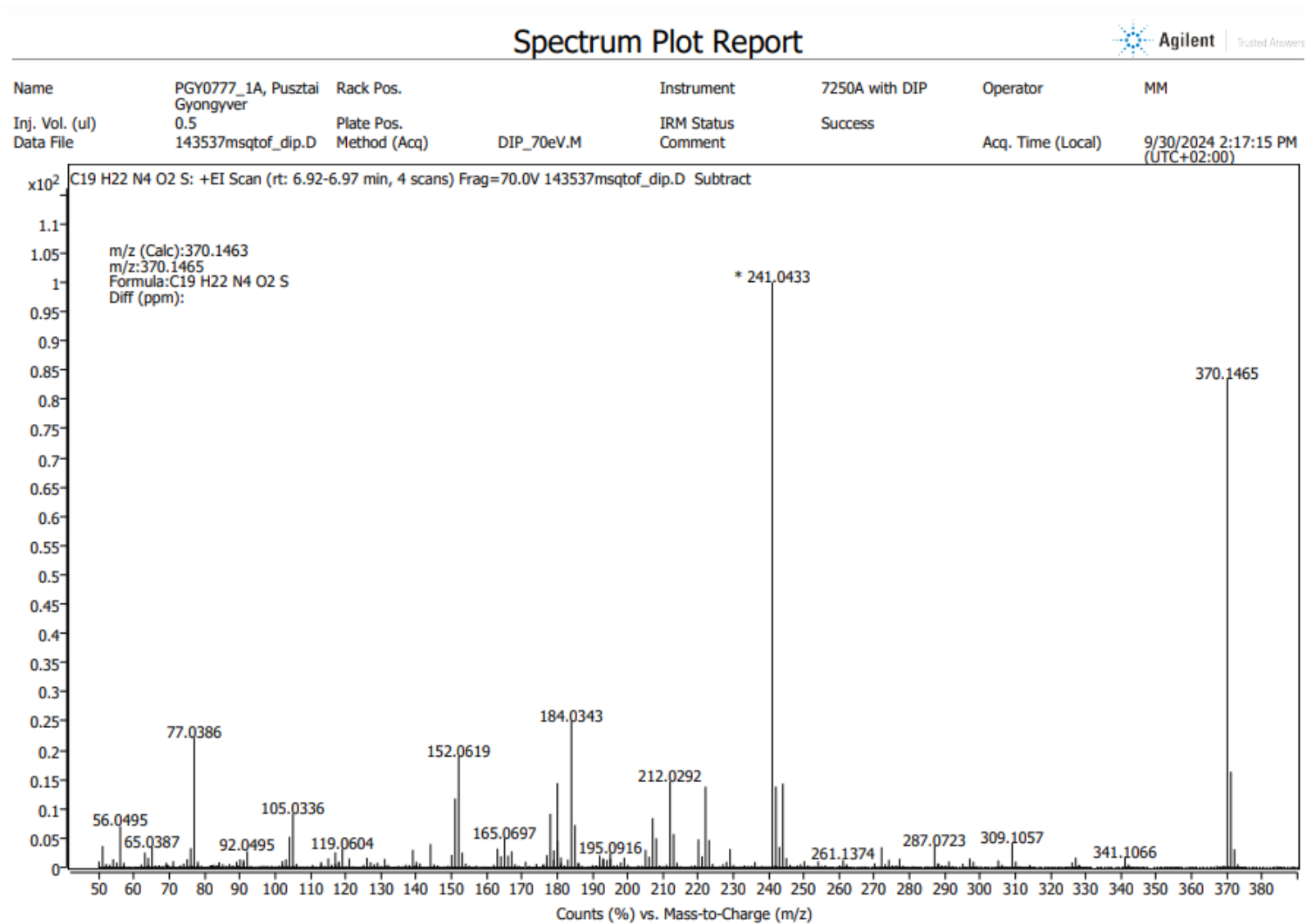
F2 - Processing parameters
SI 131072
SF 150.8701604 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



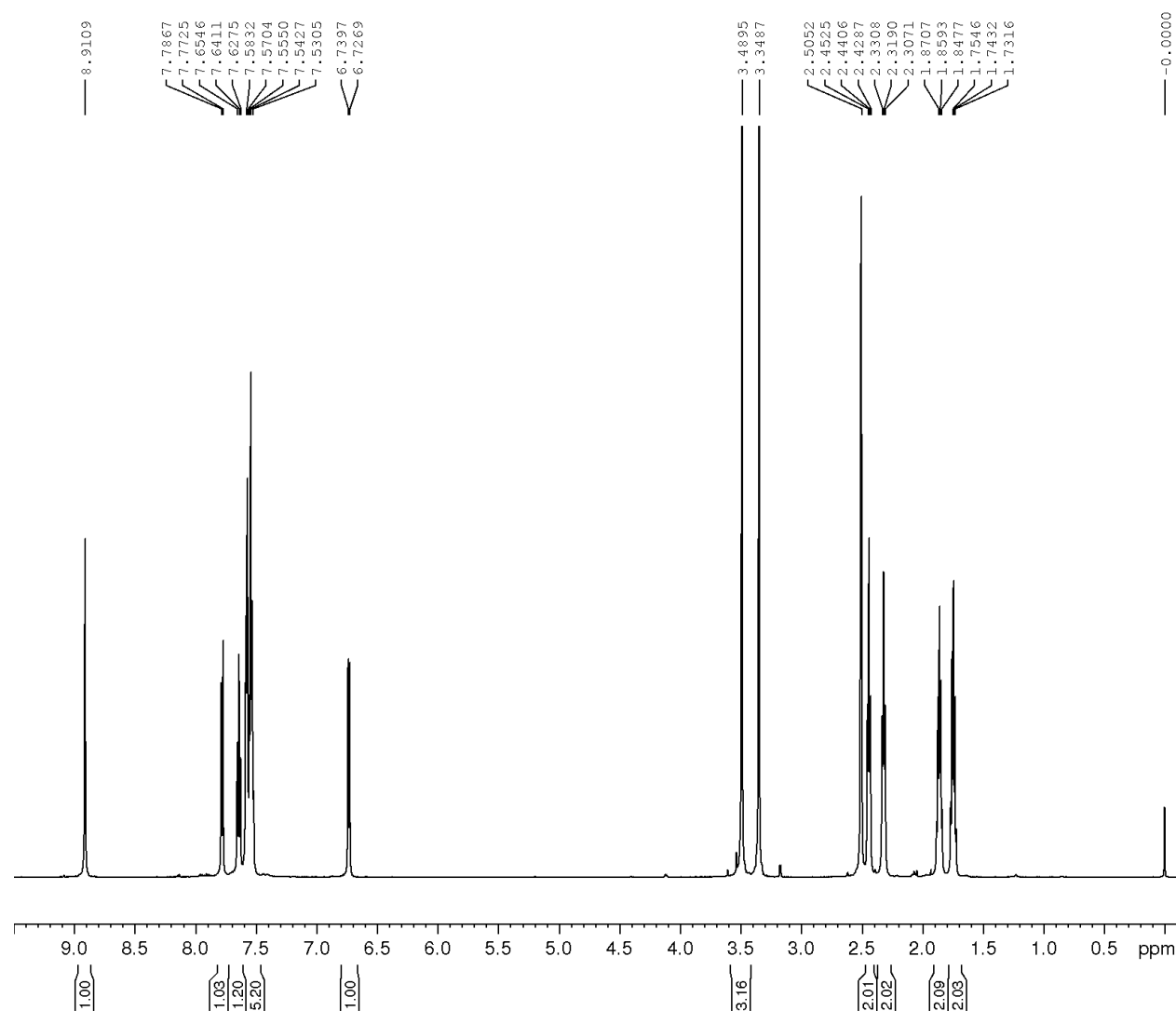
IR spectrum of **7g**



HRMS spectrum of 7g



¹H NMR spectrum of **7i**



Standard 1H
143675
PGY0789_1A
Pusztai Gyongyver
2024.10.09. (KP)

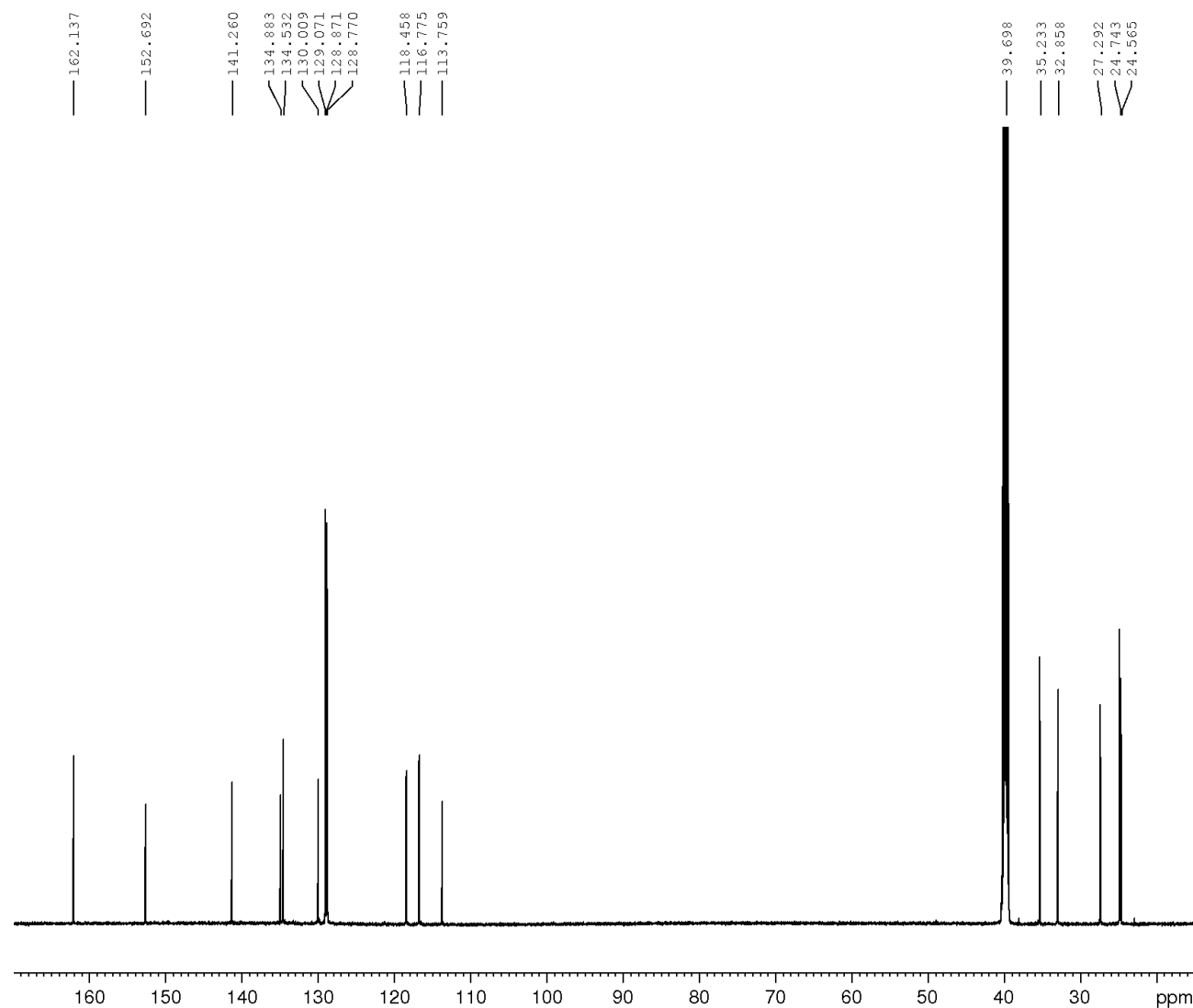
Current Data Parameters
NAME 143675
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241009
Time 15.56 h
INSTRUM spect
PROBHD Z145856_0002 (zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000016 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of 7i



Standard 13C
143675
PGY0789_1A
Pusztai Gyongyver
2024.10.09. (KP)

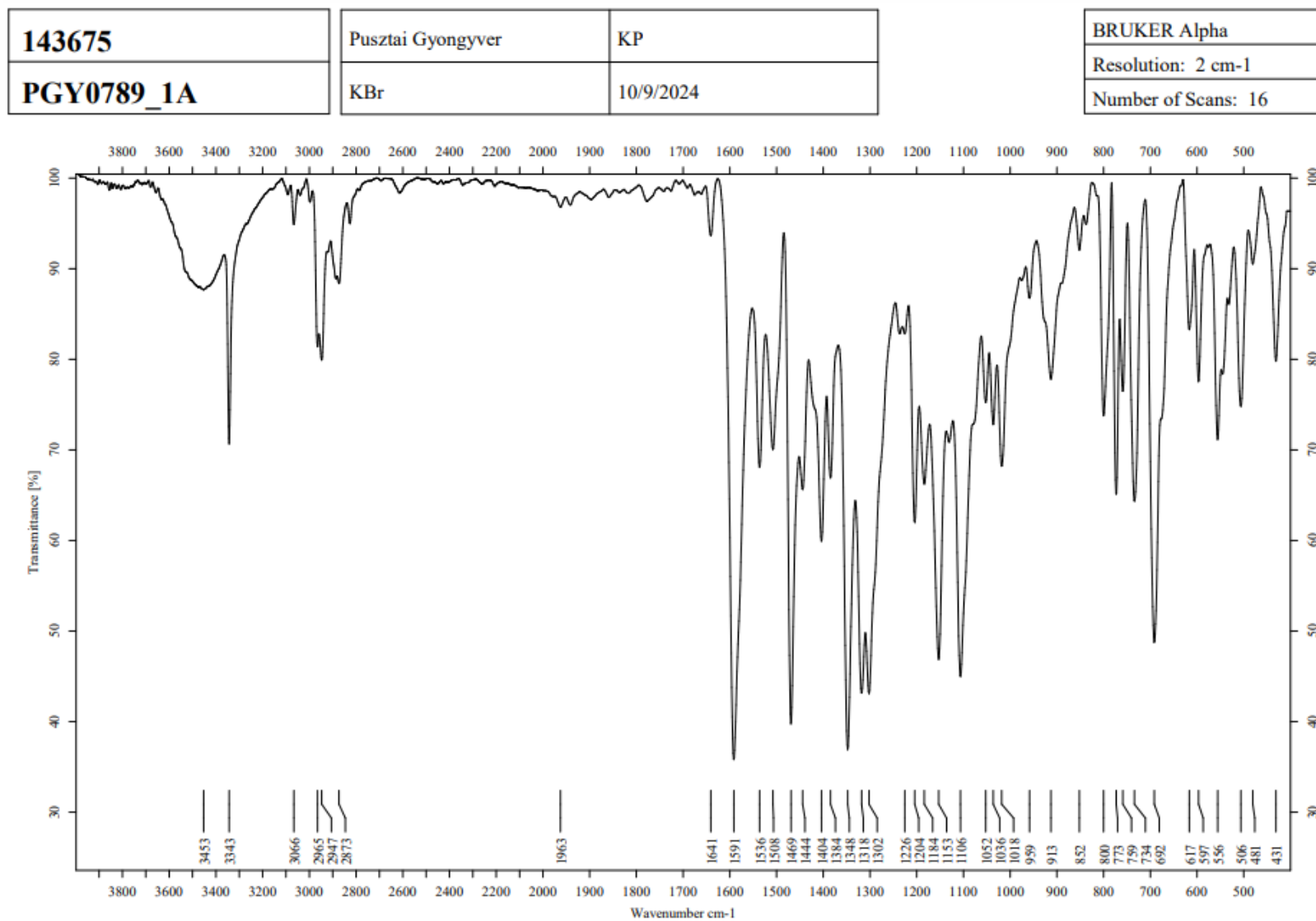
Current Data Parameters
NAME 143675
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241009
Time 17.05 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701607 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

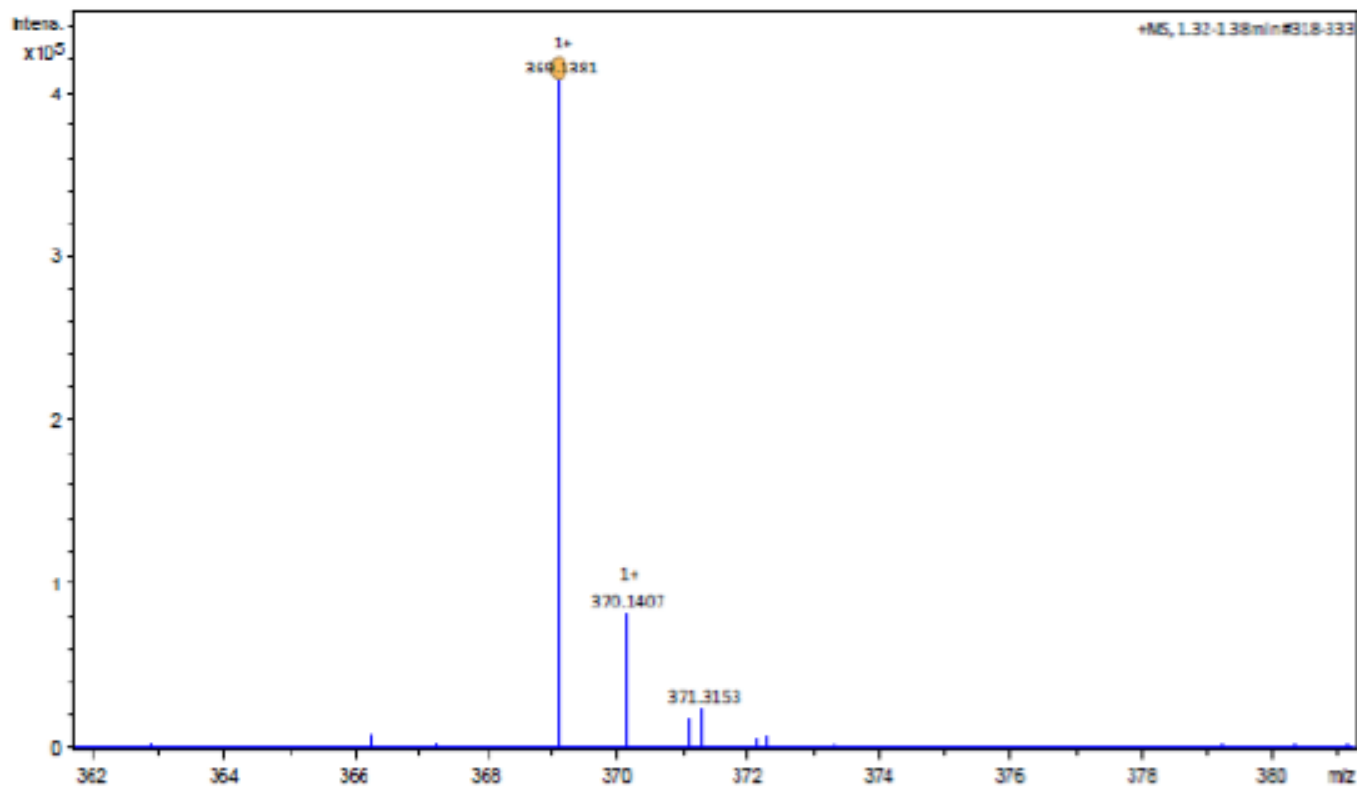


IR spectrum of **7i**



HRMS spectrum of **7i**

Sample: PGY0789_1A	Lab code: Nsz - 29676
Submitter: Pusztai Gyongyve	Project: Other

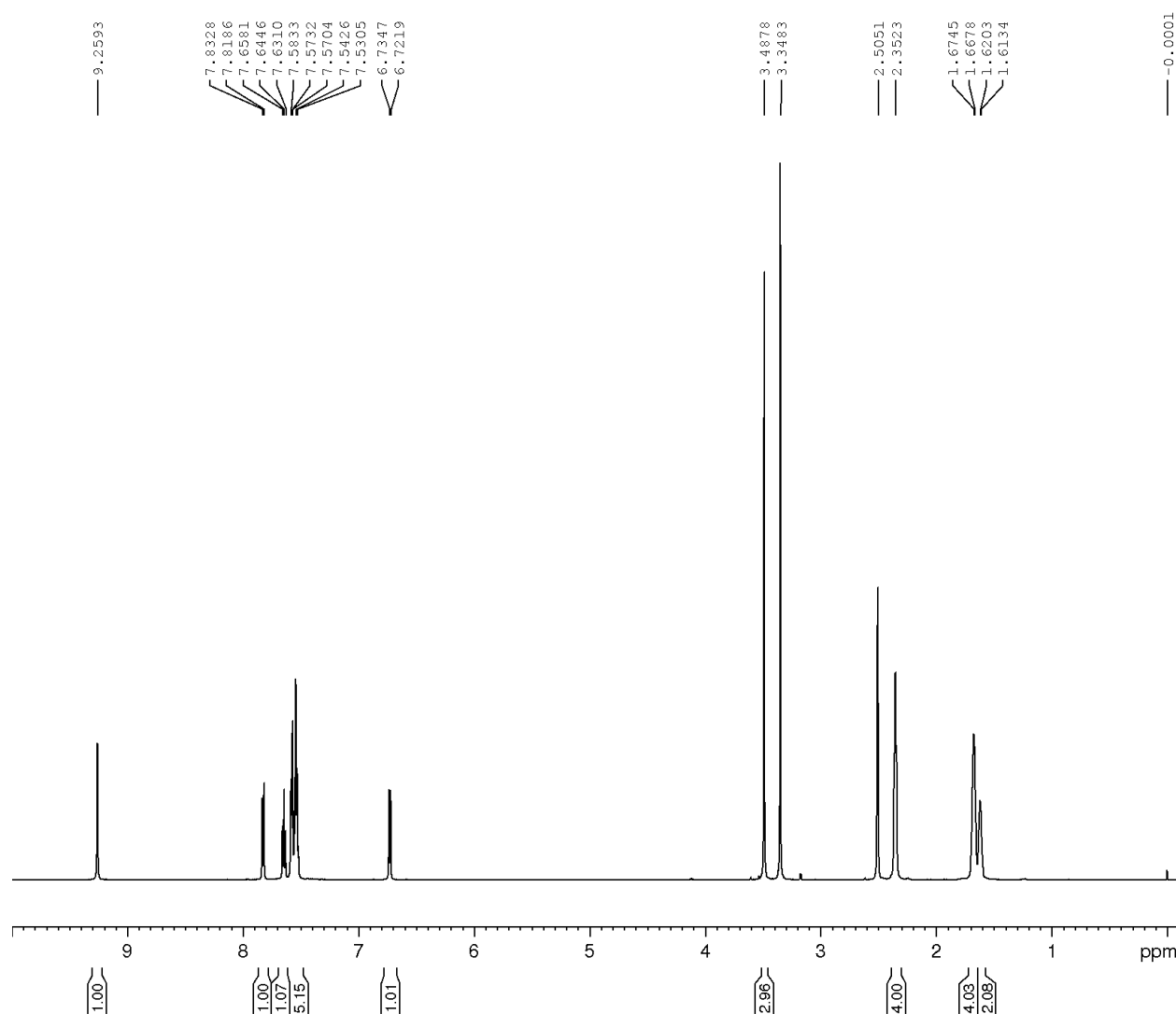


Minta: 29676_PGY0789_1A

Spektrum: MS_1.32-1.38min

Measured	Intens	Formula	Theoretical	[ppm]	[mmu]
369.1381	100	C ₁₉ H ₂₁ N ₄ O ₂ S ₁	369.1380	0.3	-0.1

¹H NMR spectrum of 7j



Standard 1H
143440
PGY0778_1
Pusztai Gyongyver
2024.09.19. (KP)

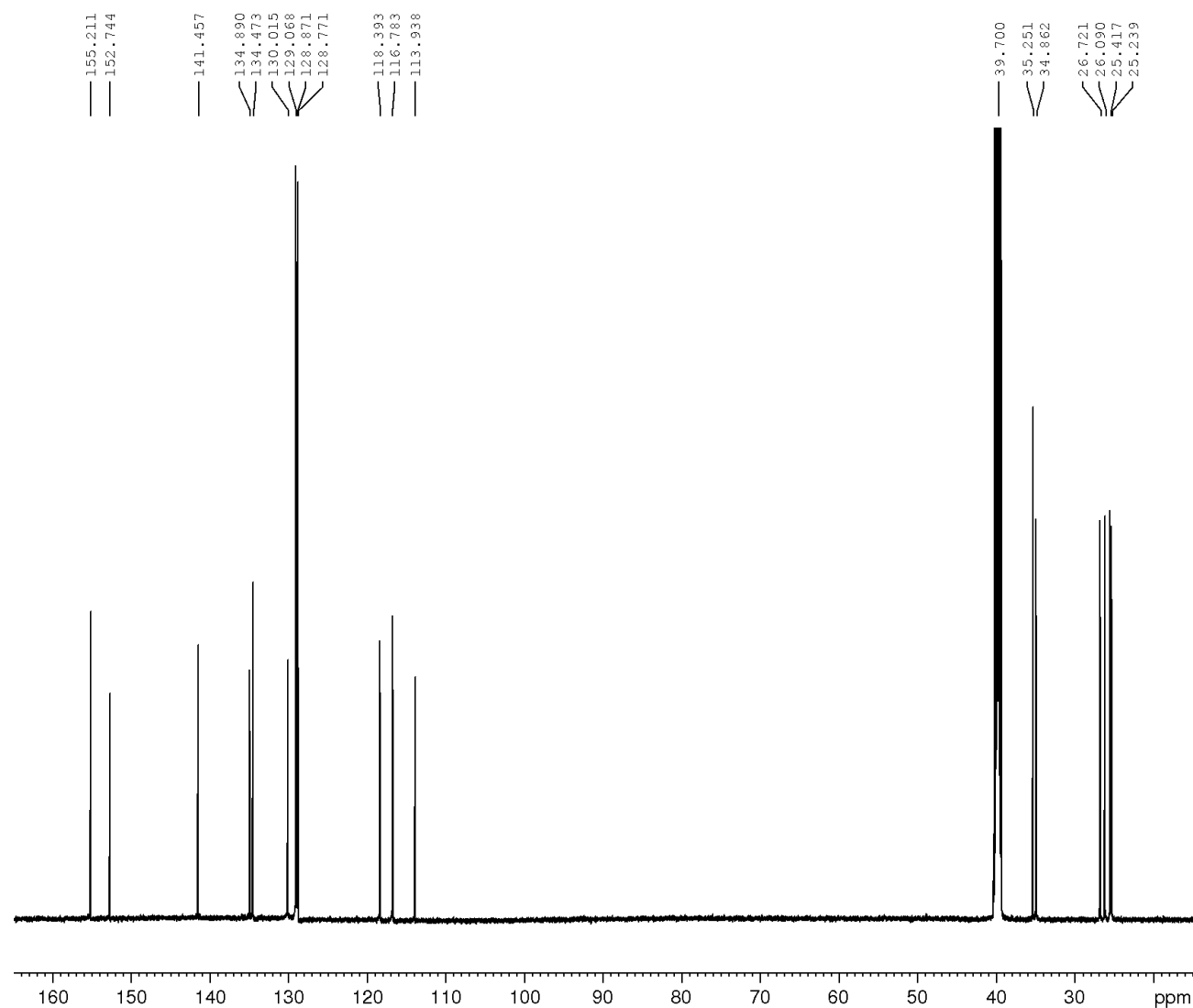
Current Data Parameters
NAME 143440
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240919
Time 15.53 h
INSTRUM spect
PROBHD Z145856_0002 (zg30)
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000018 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of 7j



Standard 13C
143440
PGY0778_1
Pusztai Gyongyver
2024.09.19. (KP)

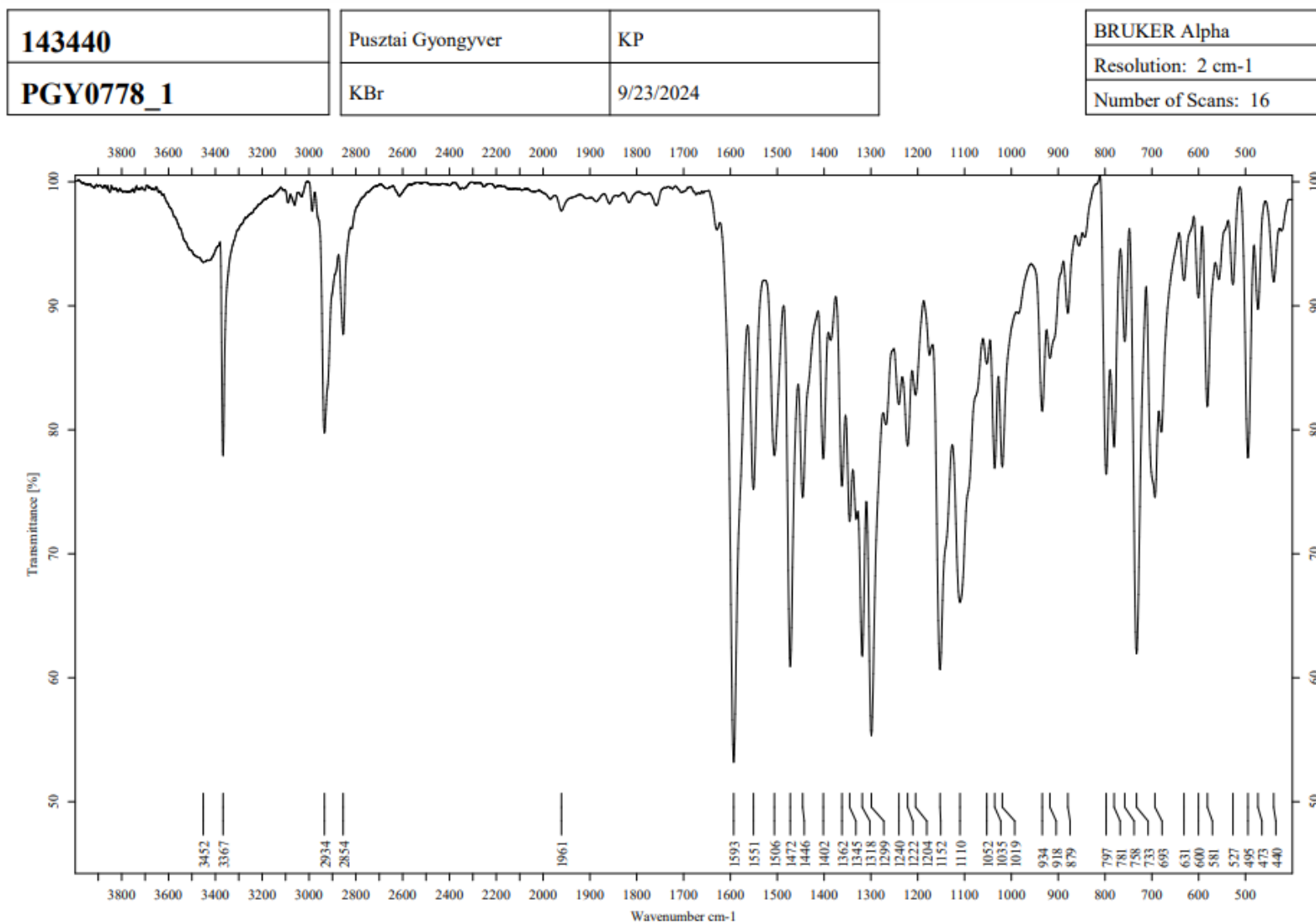
Current Data Parameters
NAME 143440
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240919
Time 20.27 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701604 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of 7j

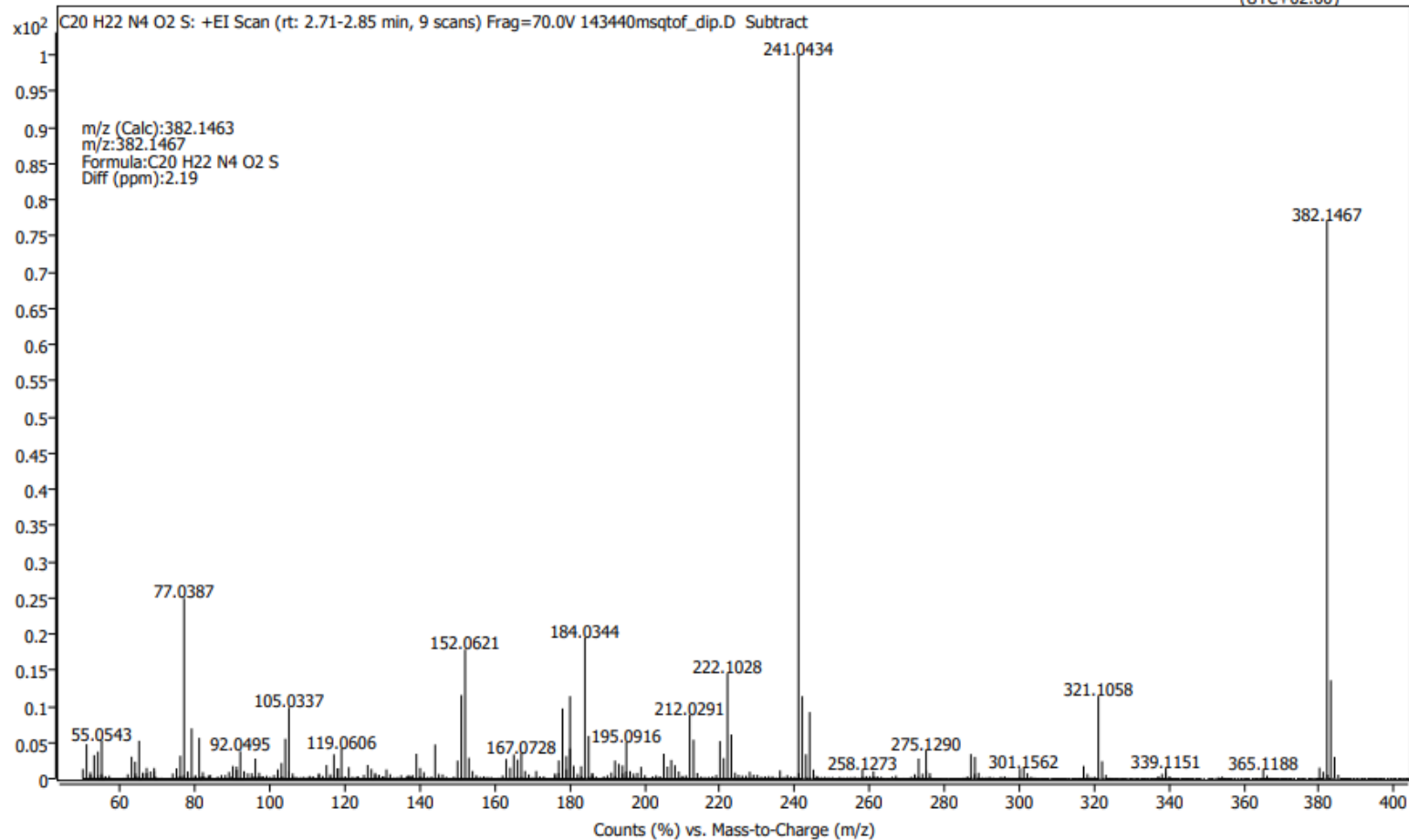


HRMS spectrum of 7j

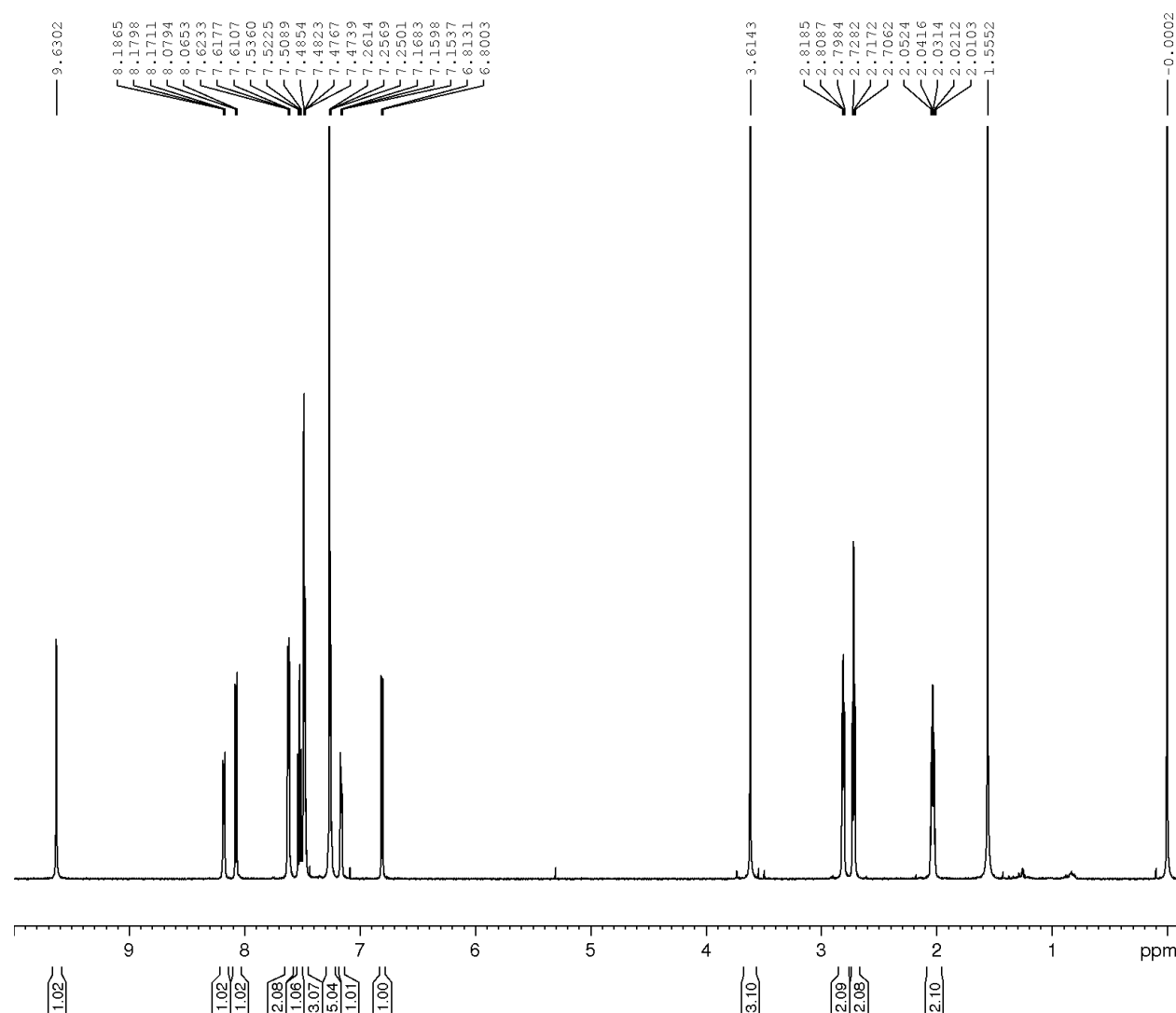
Spectrum Plot Report



Name	PGY0778_1, Pusztai Gyongyver	Rack Pos.	Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	Plate Pos.	IRM Status	Success	Acq. Time (Local)	9/30/2024 2:33:23 PM
Data File	143440msqtof_dip.D	Method (Acq)	DIP_70eV.M	Comment		(UTC+02:00)



¹H NMR spectrum of (*E*)-**9b**



Standard 1H
144148
PGY0788_1A
Pusztai Gyongyver
2025.01.21. (KP)

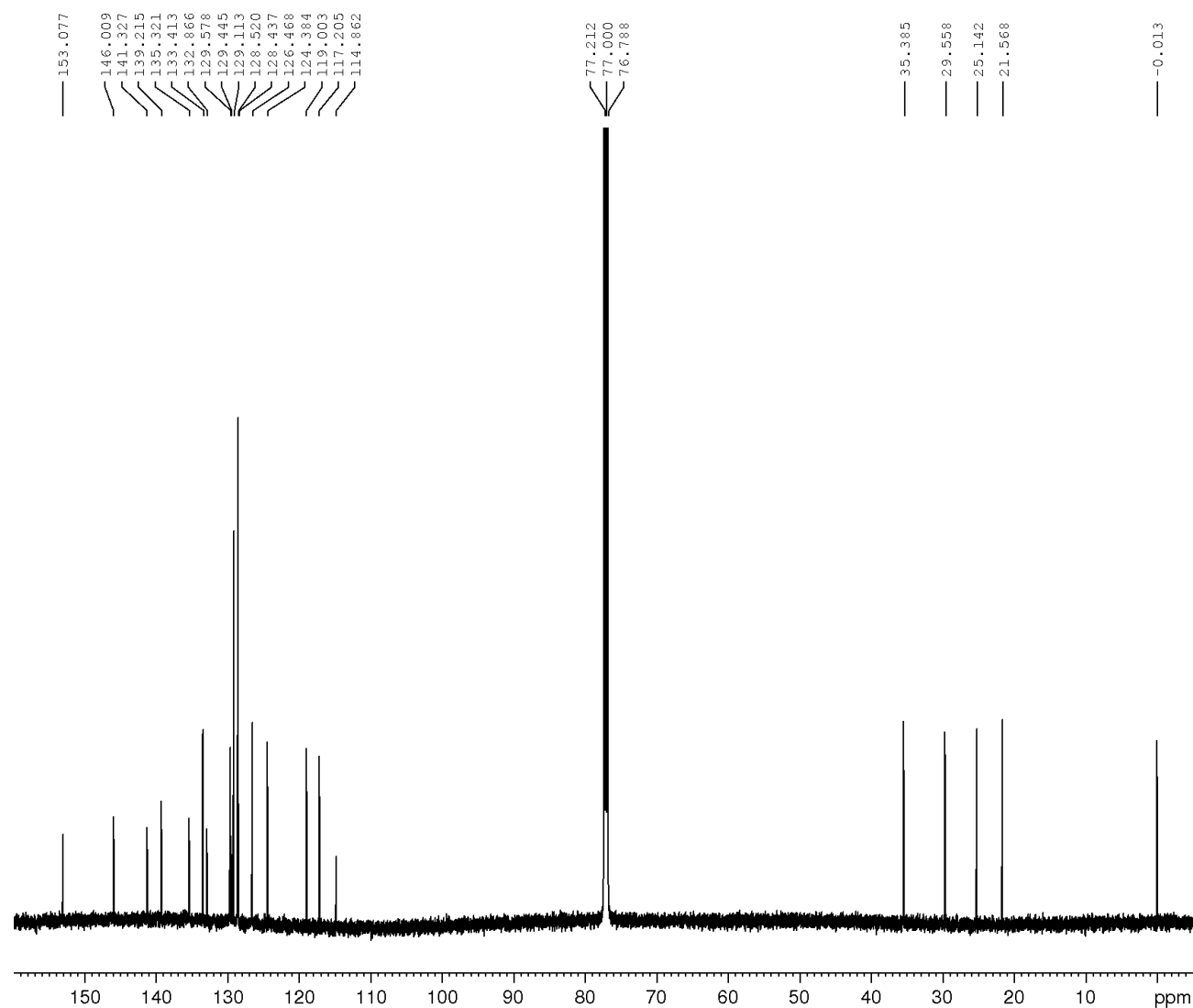
Current Data Parameters
NAME 144148
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250122
Time 4.10 h
INSTRUM spect
PROBHD Z145856_0002 (Z145856_0002)
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of (*E*)-9b



Standard 13C
144148
PGY0788_1A
Pusztai Gyongyver
2025.01.21. (KP)

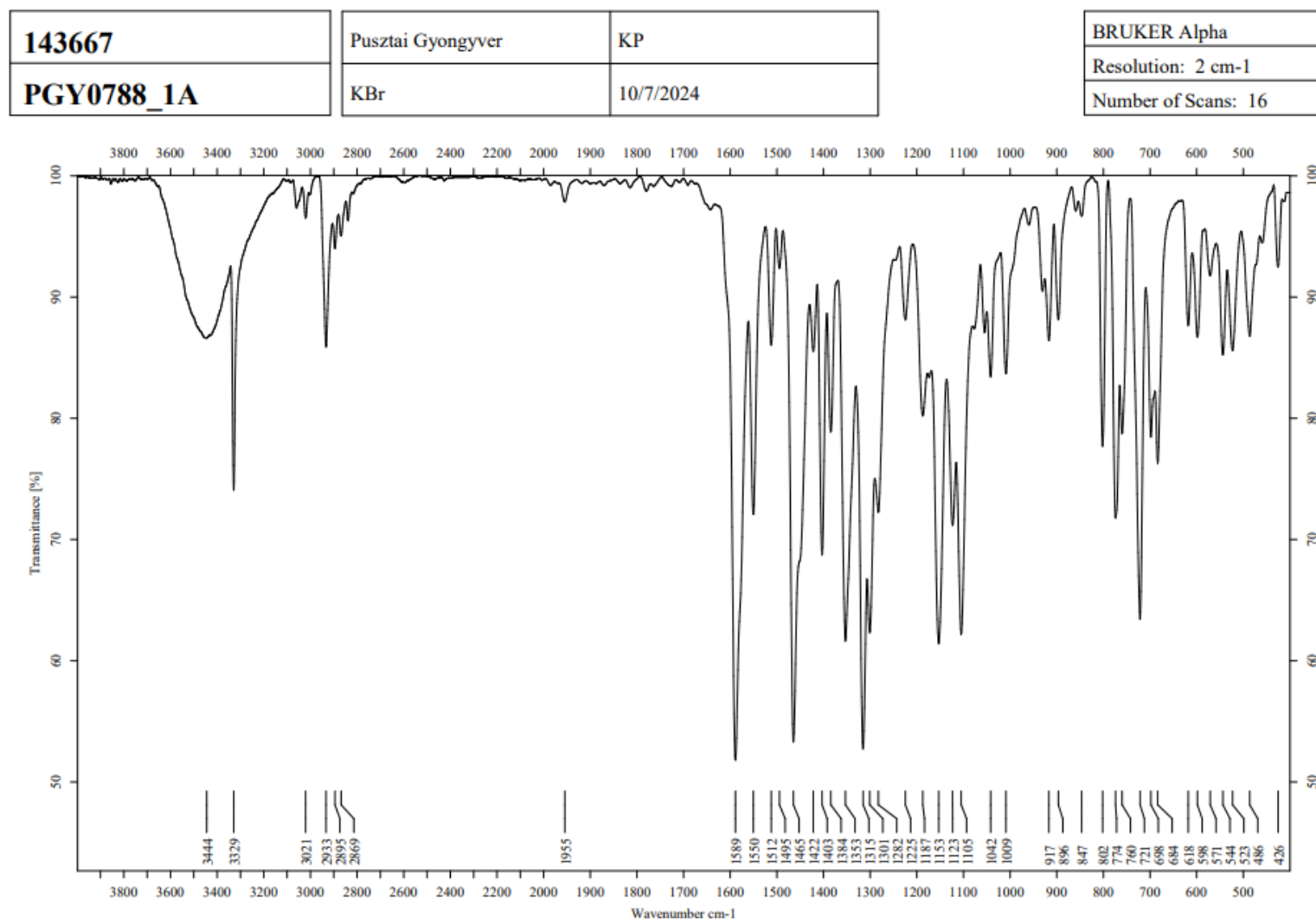
Current Data Parameters
NAME 144148
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250122
Time 5.19 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701254 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of (*E*)-**9b**

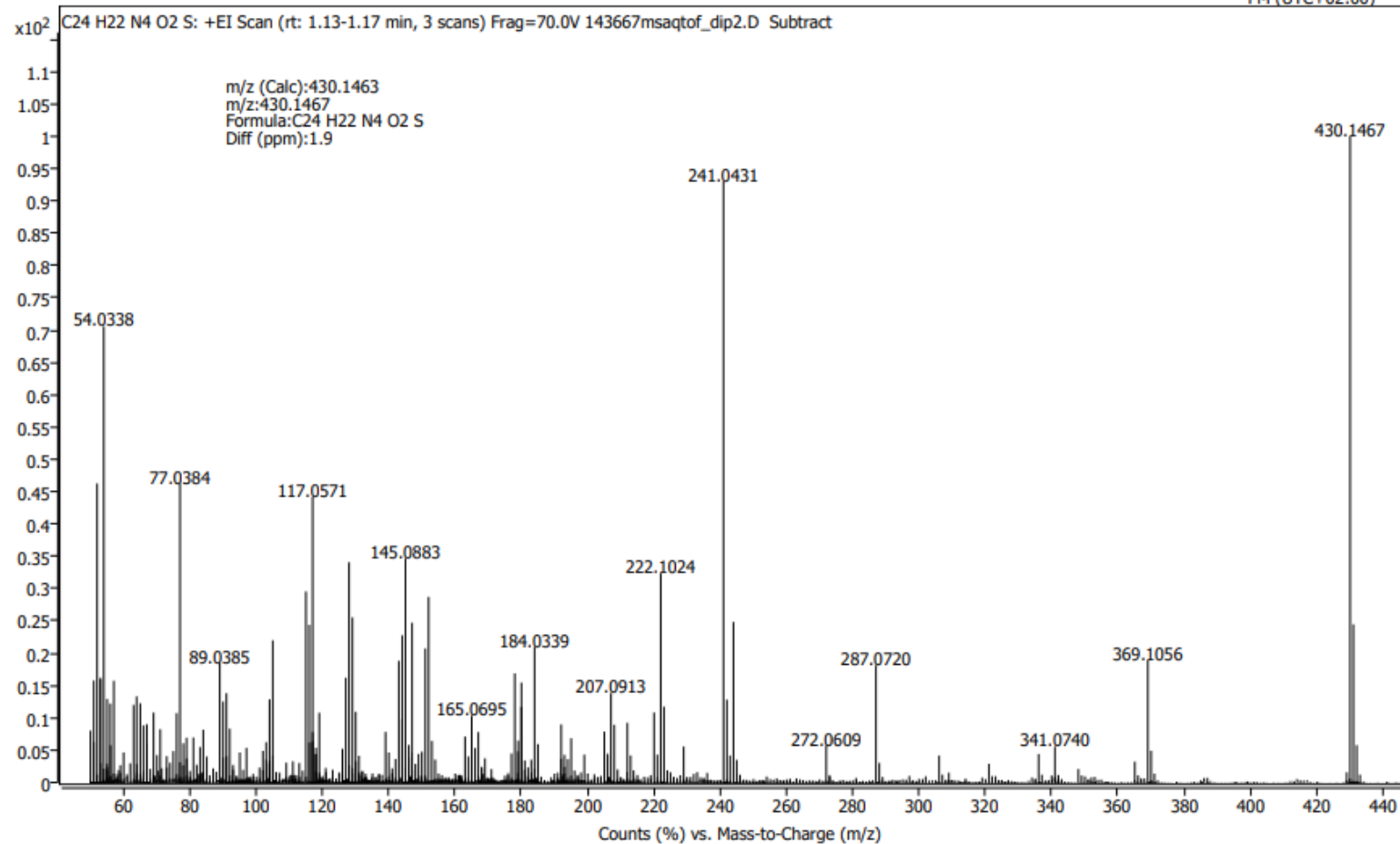


HRMS spectrum of (E)-9b

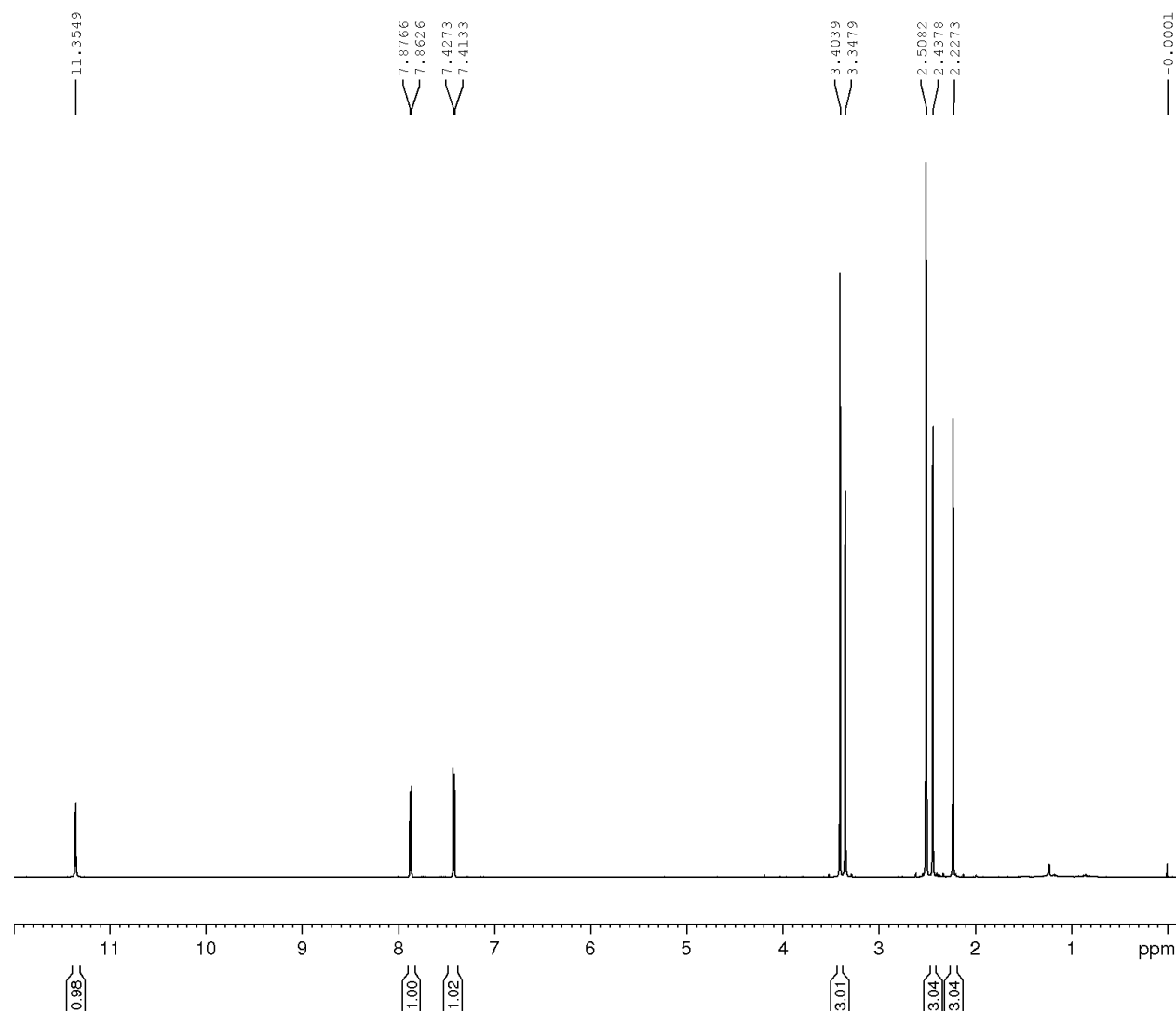
Spectrum Plot Report



Name	PGY0788_1A, Pusztai	Rack Pos.	Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	Plate Pos.	IRM Status	Success	Acq. Time (Local)	10/24/2024 1:24:33 PM (UTC+02:00)
Data File	143667msaqtodip2.D Method (Acq)	DIP_70eV_4min.M	Comment			



¹H NMR spectrum of **3a**



Standard 1H
142718
PGY0685_1A
Pusztai Gyongyver
2024.04.29. (KP)

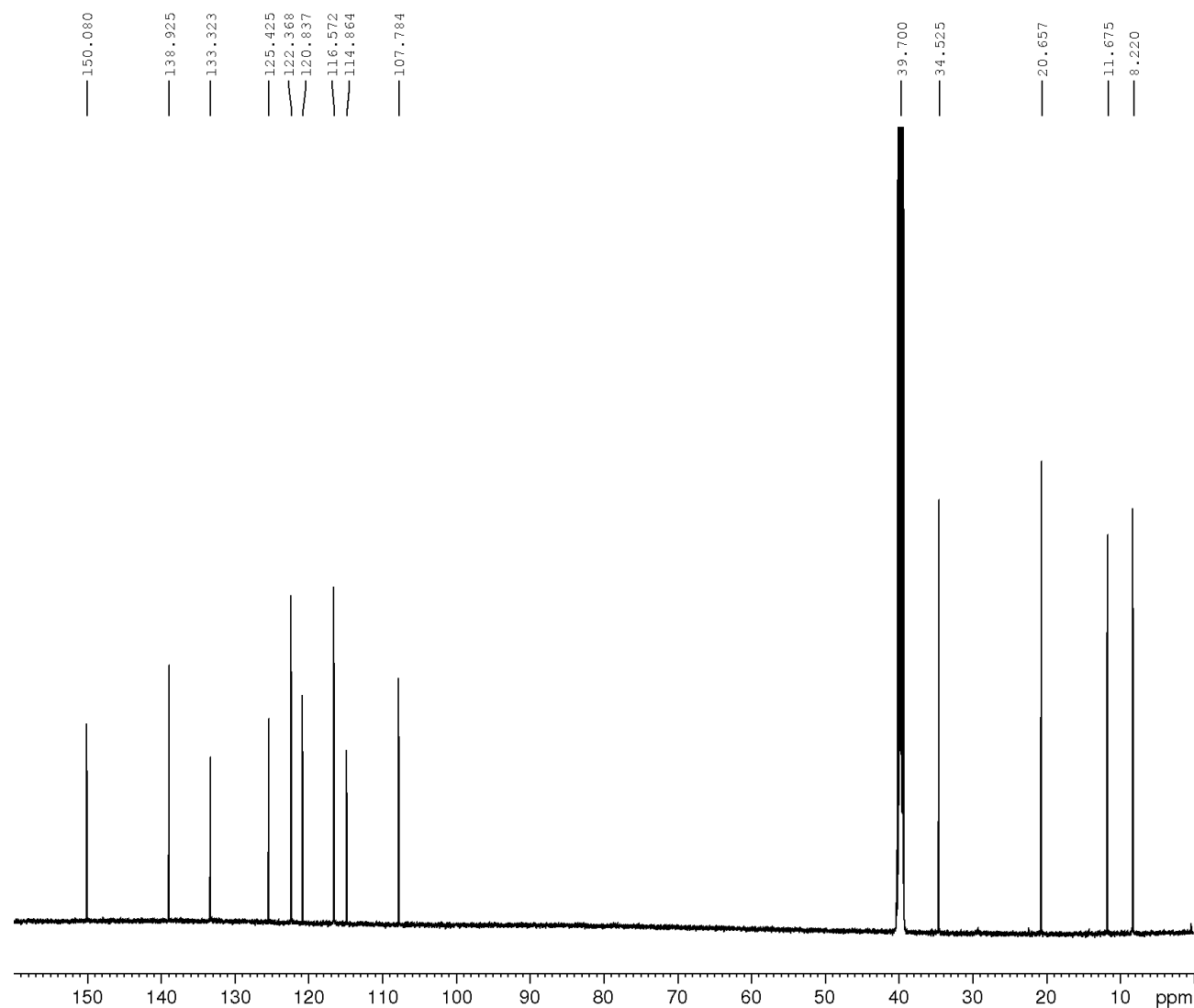
Current Data Parameters
NAME 142718
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240429
Time 20.46 h
INSTRUM spect
PROBHD Z145856_0002 (Z145856)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000021 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of **3a**



Standard ¹³C
142718
PGY0685_1A
Pusztai Gyongyver
2024.04.29. (KP)

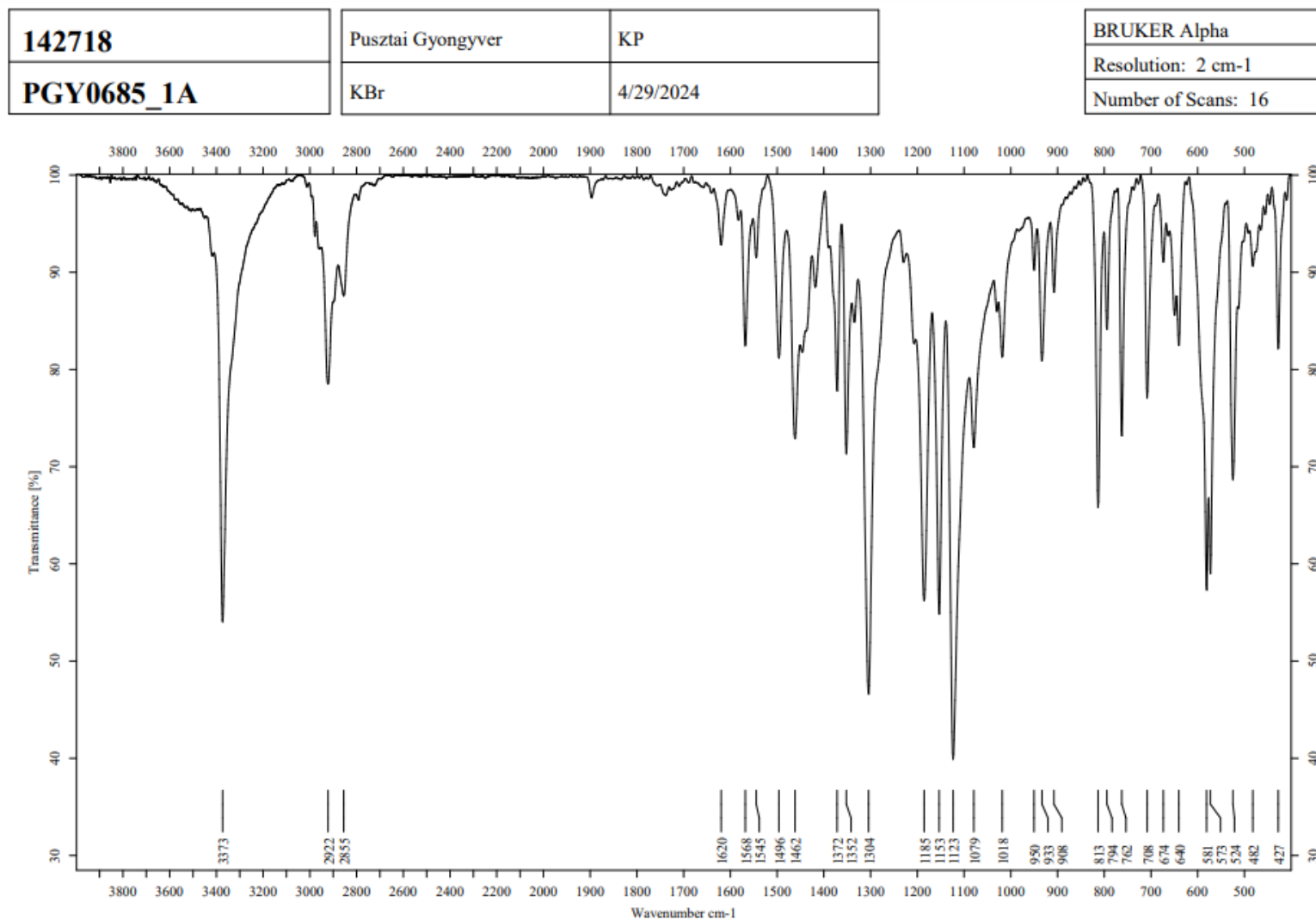
Current Data Parameters
NAME 142718
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240429
Time 21.54 h
INSTRUM spect
PROBHD z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 32768
SF 150.8701591 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of **3a**

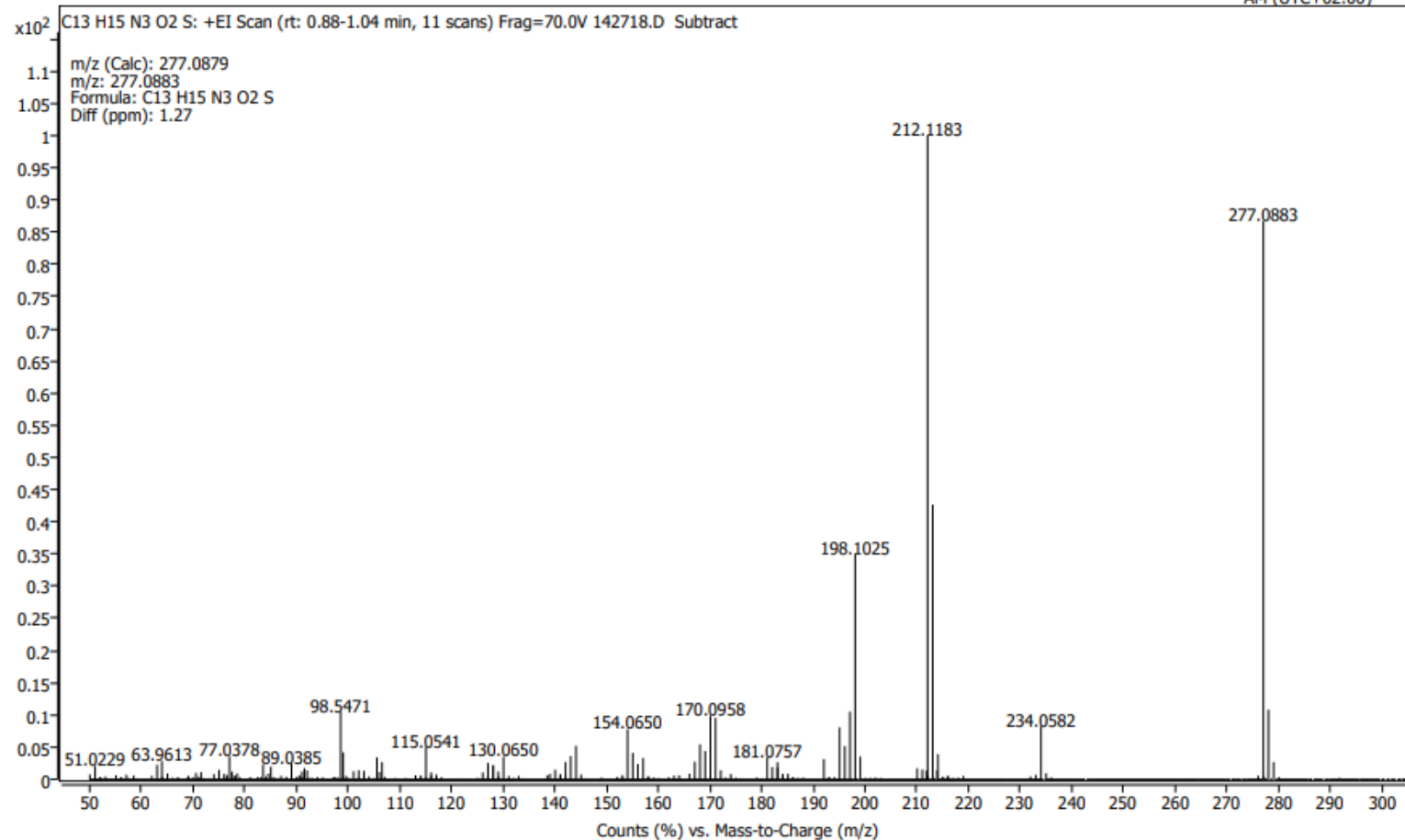


HRMS spectrum of **3a**

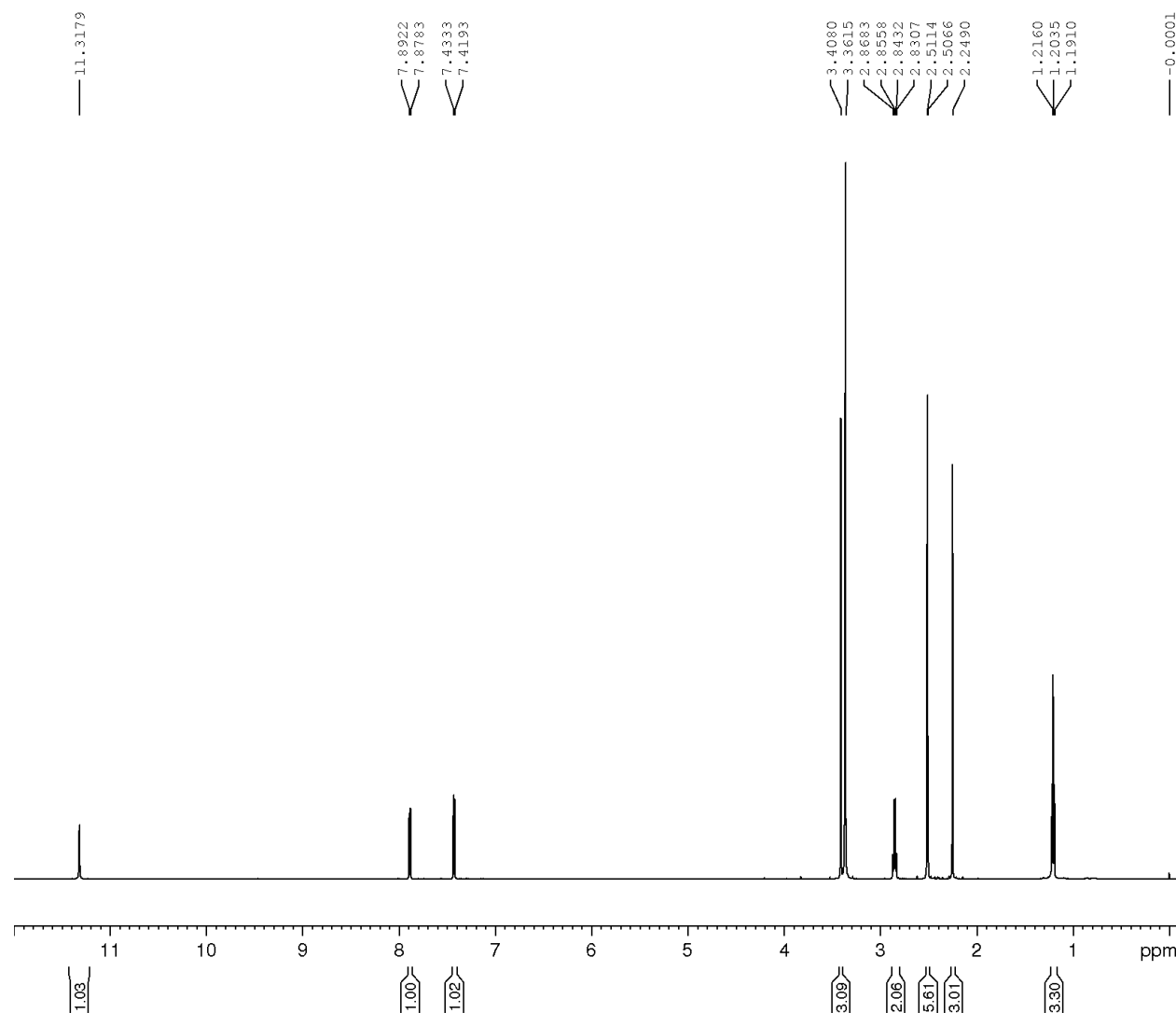
Spectrum Plot Report



Name	PGY0685_1A, Pusztai	Rack Pos.	Instrument	7250A with DIP	Operator
Inj. Vol. (ul)	0.5	Plate Pos.	IRM Status	Success	
Data File	142718.D	Method (Acq)	DIP_70eV.M	Comment	Acq. Time (Local)
					4/30/2024 11:53:20 AM (UTC+02:00)



¹H NMR spectrum of **3b**



Standard 1H
142611
PGY0686_1B
Pusztai Gyongyver
2024.04.08. (KP)

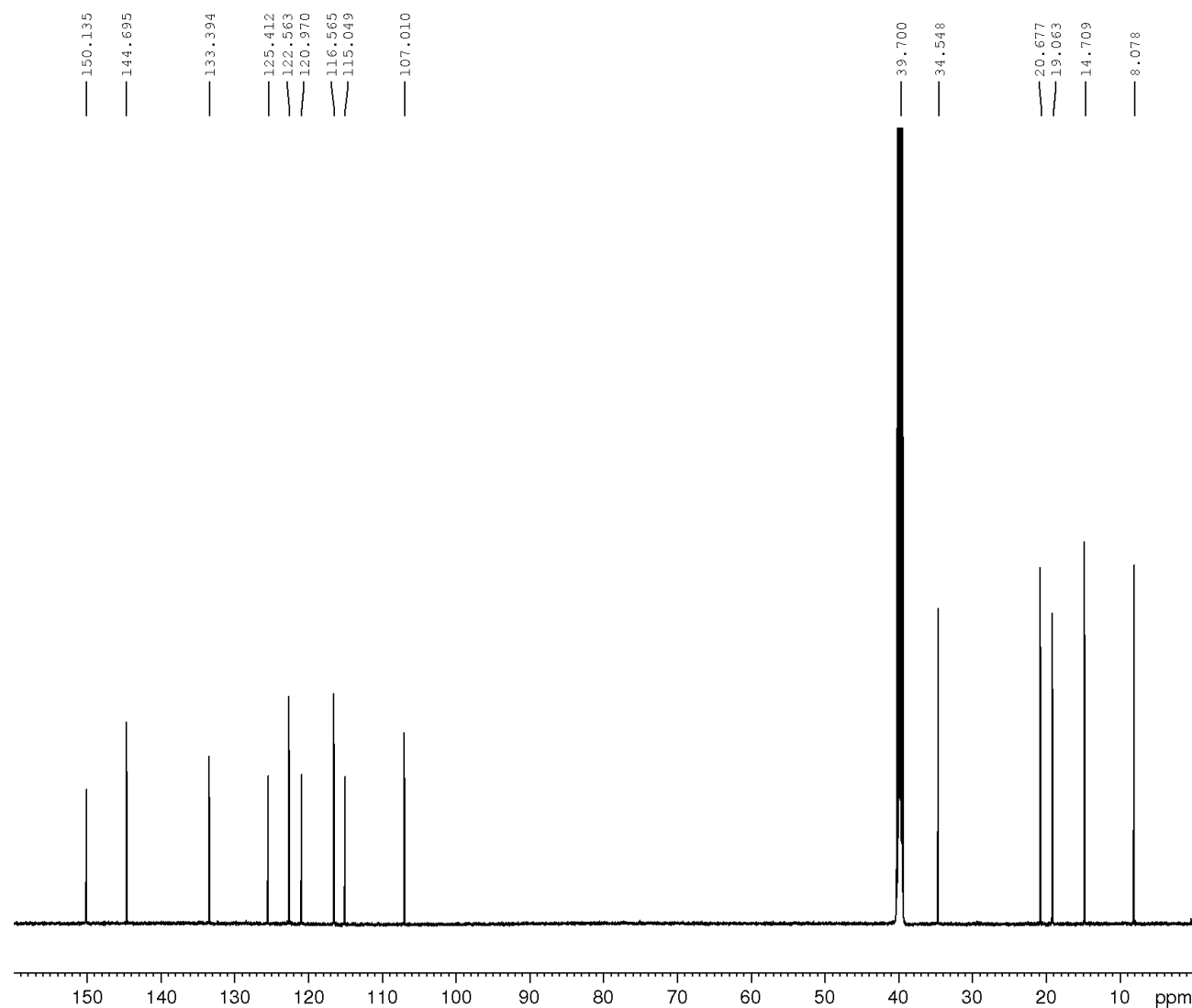
Current Data Parameters
NAME 142611
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240408
Time 16.49 h
INSTRUM spect
PROBHD Z145856_0002 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000012 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of **3b**



Standard 13C
142611
PGY0686_1B
Pusztai Gyongyver
2024.04.08. (KP)

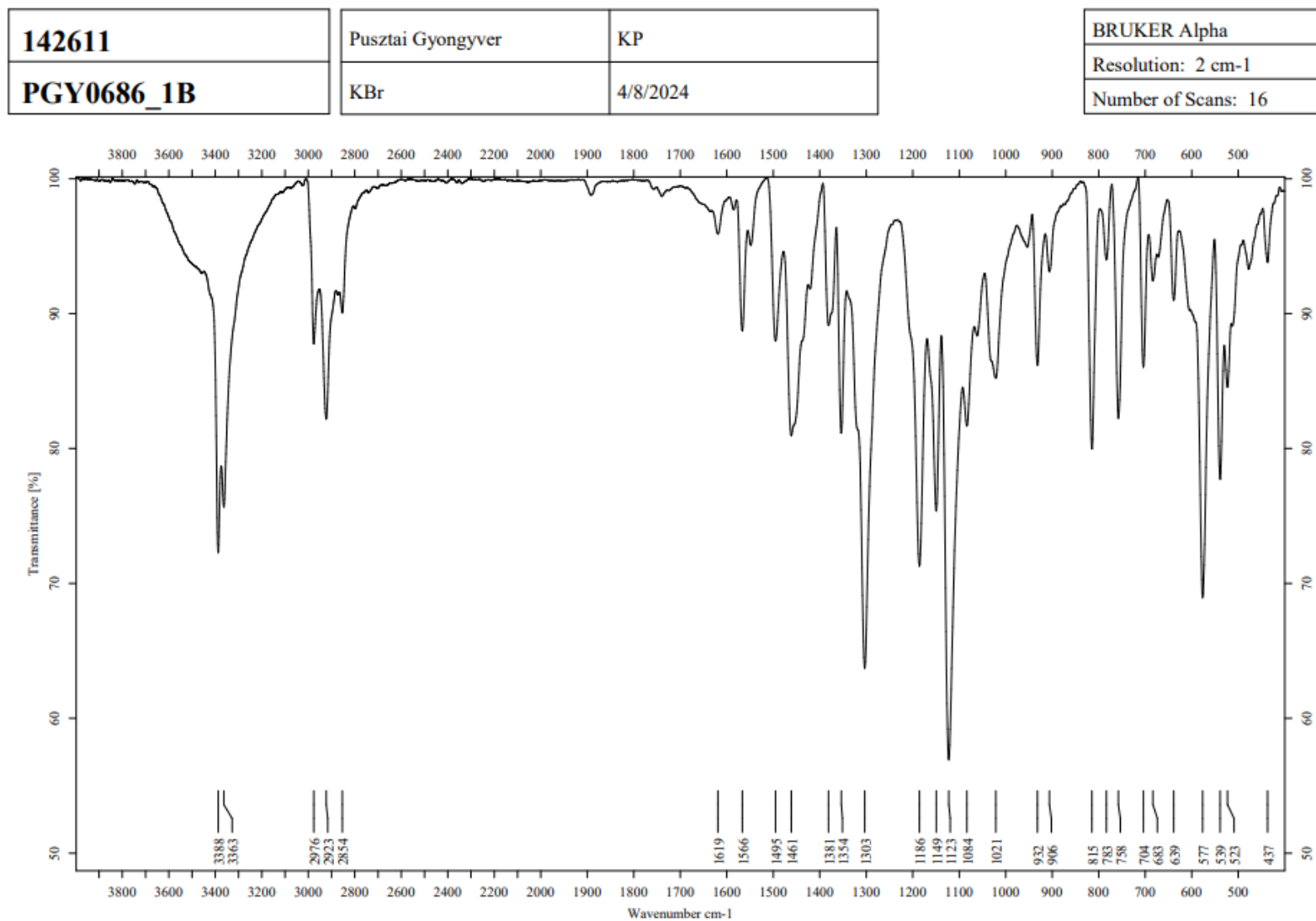
Current Data Parameters
NAME 142611
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240408
Time 17.58 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 32768
SF 150.8701576 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

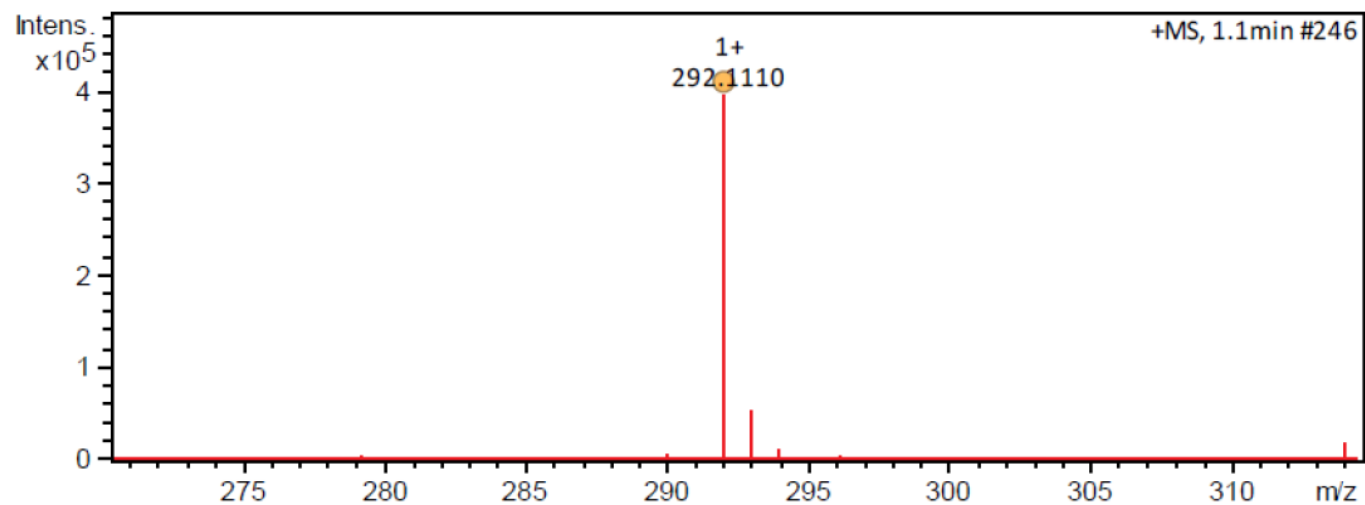


IR spectrum of **3b**



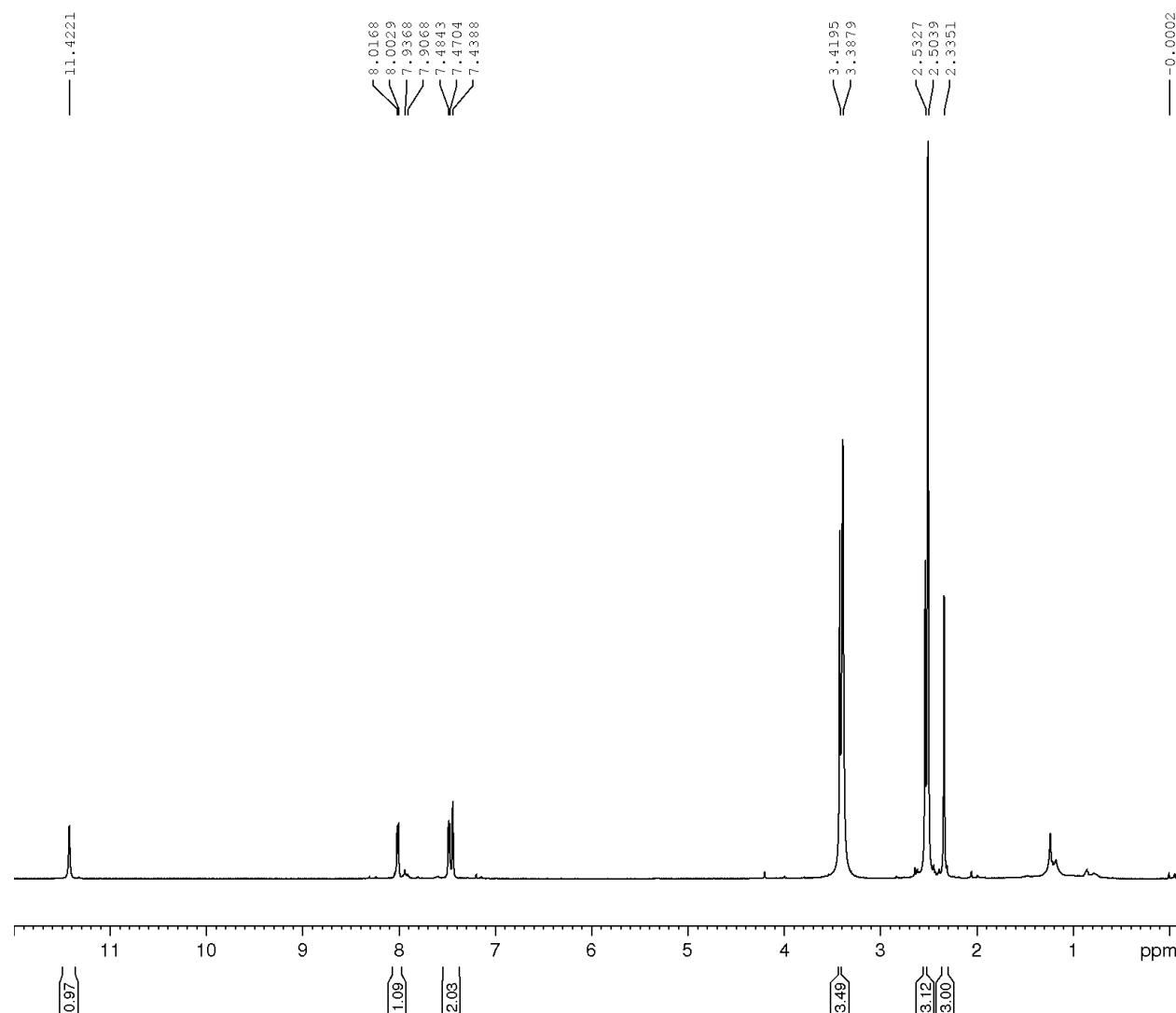
HRMS spectrum of **3b**

Sample: PGY00686_1B	Lab code: Nsz - 28962
Submitter: Pusztai Gyongyve	Project: Other



Meas. m/z	m/z	Ion Formula	err [ppm]
292.1110	292.1120	C ₁₄ H ₁₈ N ₃ O ₂ S	1.6

¹H NMR spectrum of **3c**



Standard 1H
142823
PGY0719_3C
Pusztai Gyongyver
2024.05.30. (KP)

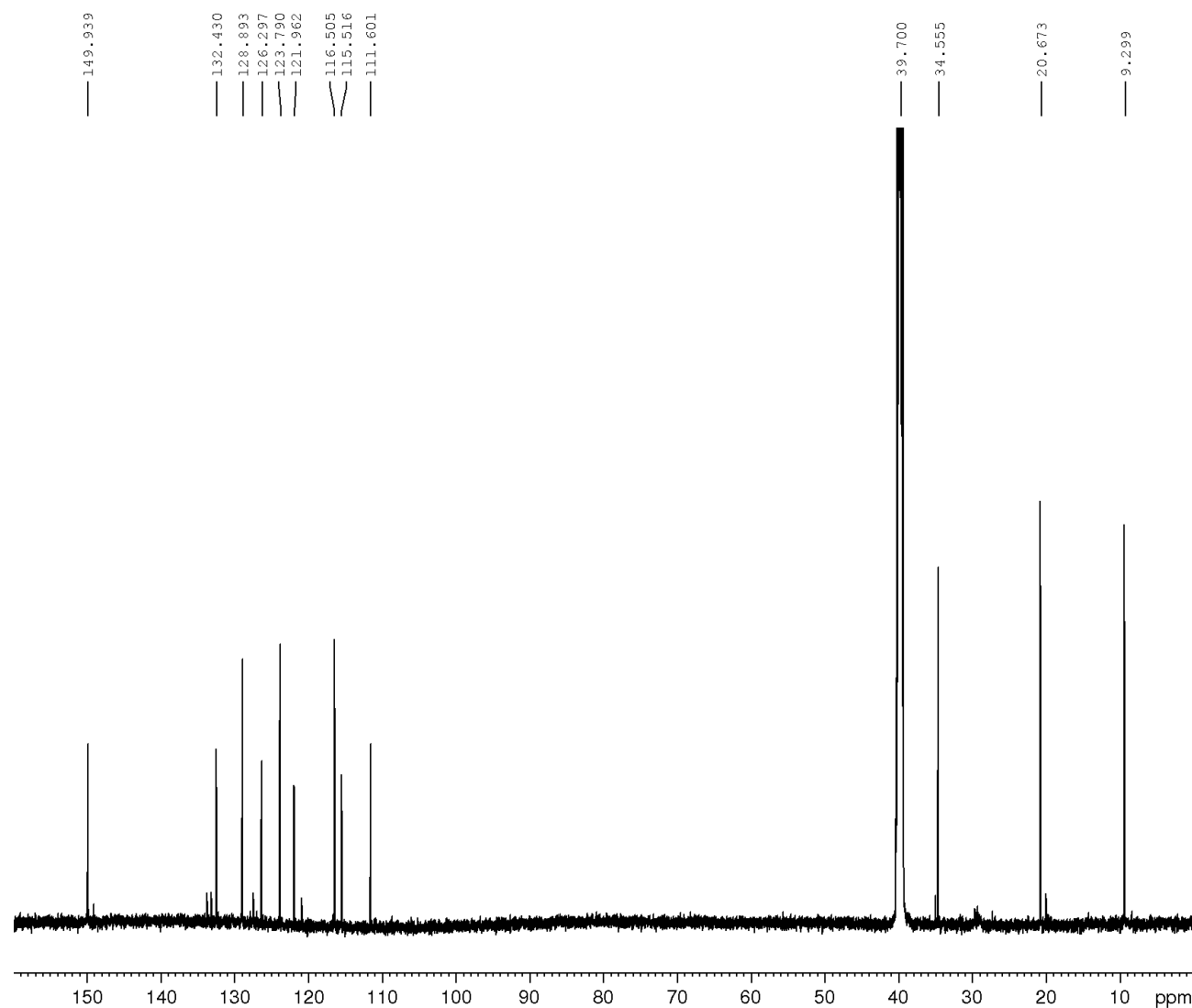
Current Data Parameters
NAME 142823
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240530
Time 16.05 h
INSTRUM spect
PROBHD Z145856_0002 (zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000027 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of **3c**



Standard 13C
142823
PGY0719_3C
Pusztai Gyongyver
2024.05.30. (KP)

Current Data Parameters
NAME 142823
EXPNO 22
PROCNO 1

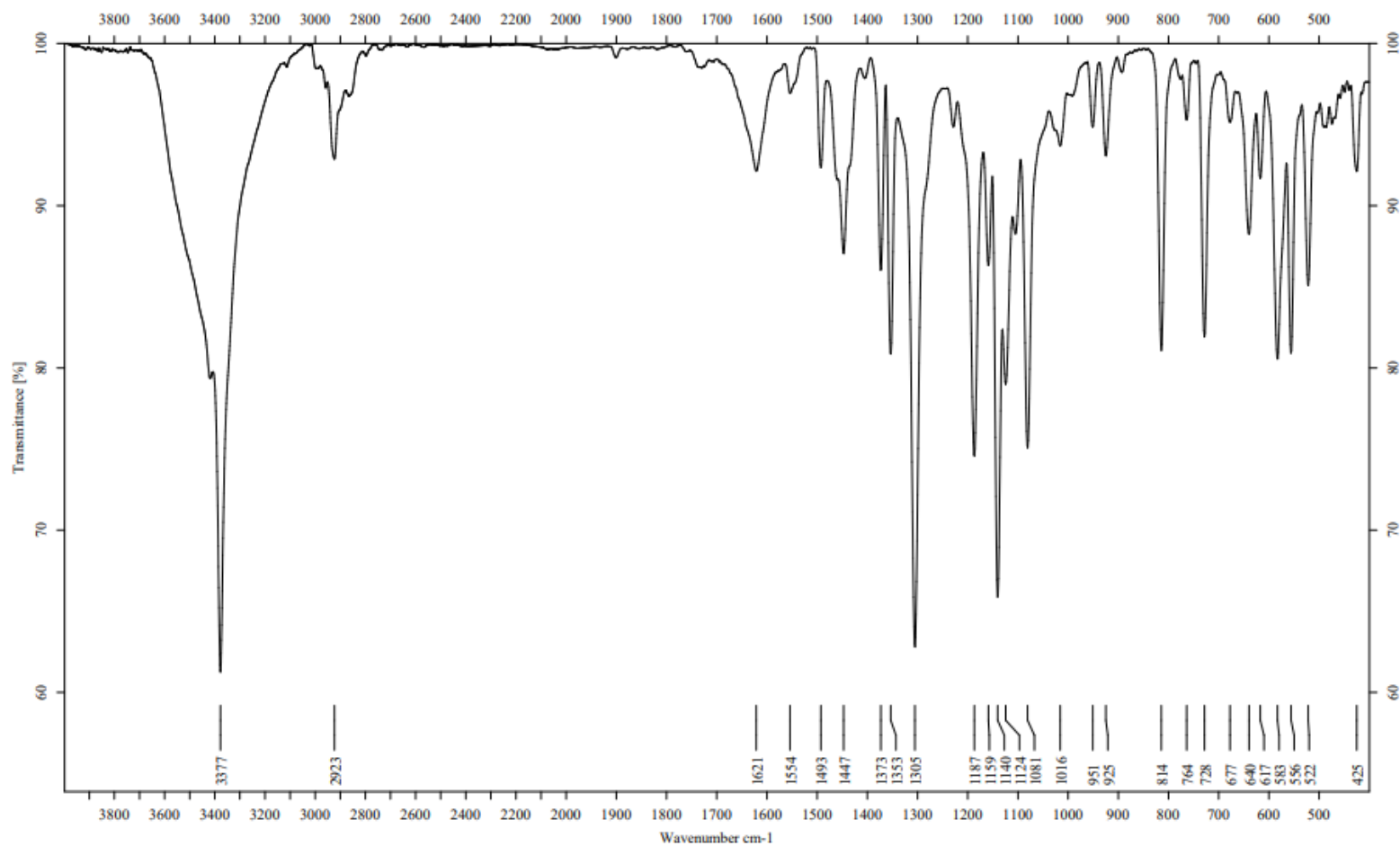
F2 - Acquisition Parameters
Date_ 20240530
Time 17.15 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 32768
SF 150.8701592 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of **3c**

143608	Pusztai Gyongyver	KP	BRUKER Alpha
PGY0786_1A	KBr	9/30/2024	Resolution: 2 cm-1
			Number of Scans: 16

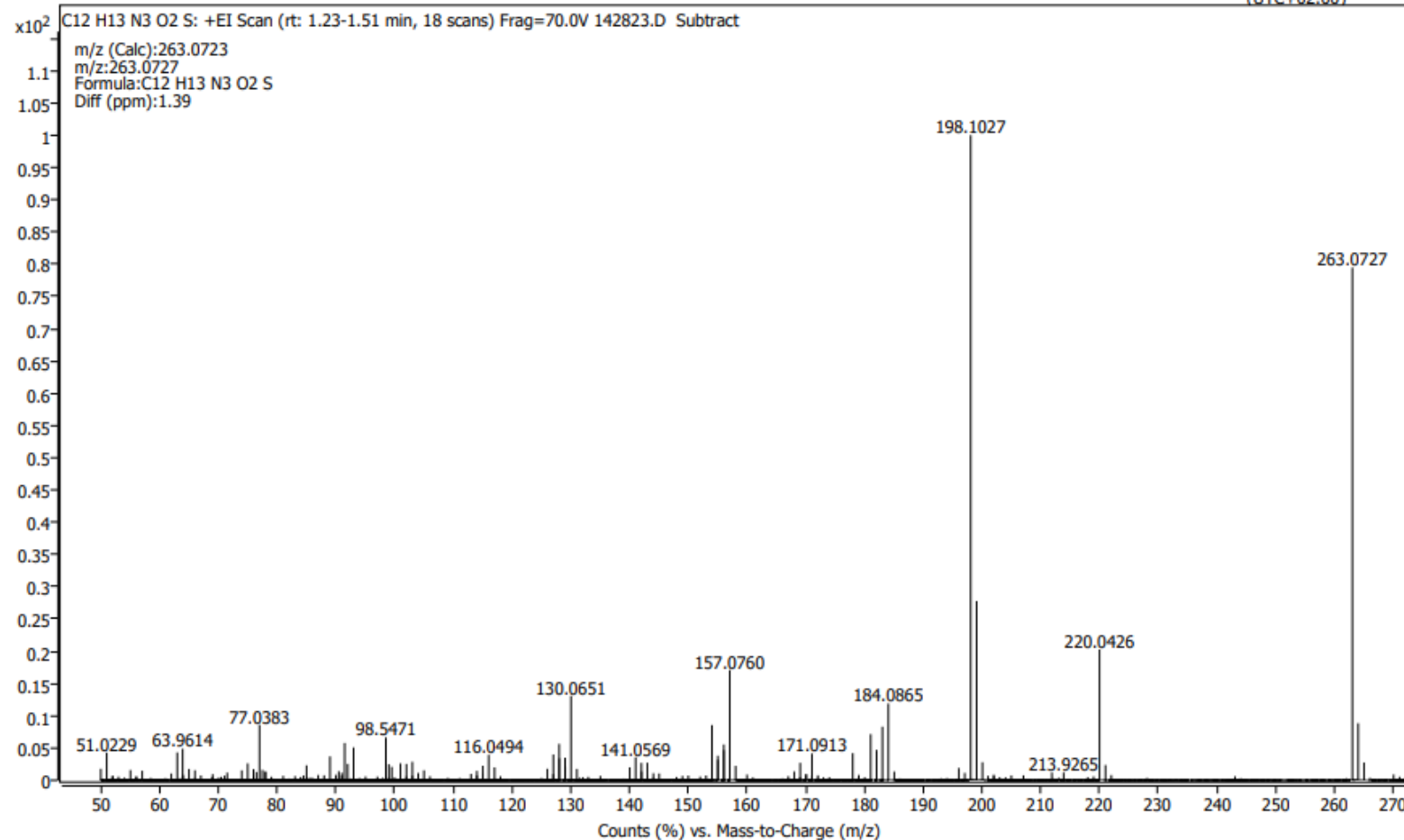


HRMS spectrum of 3c

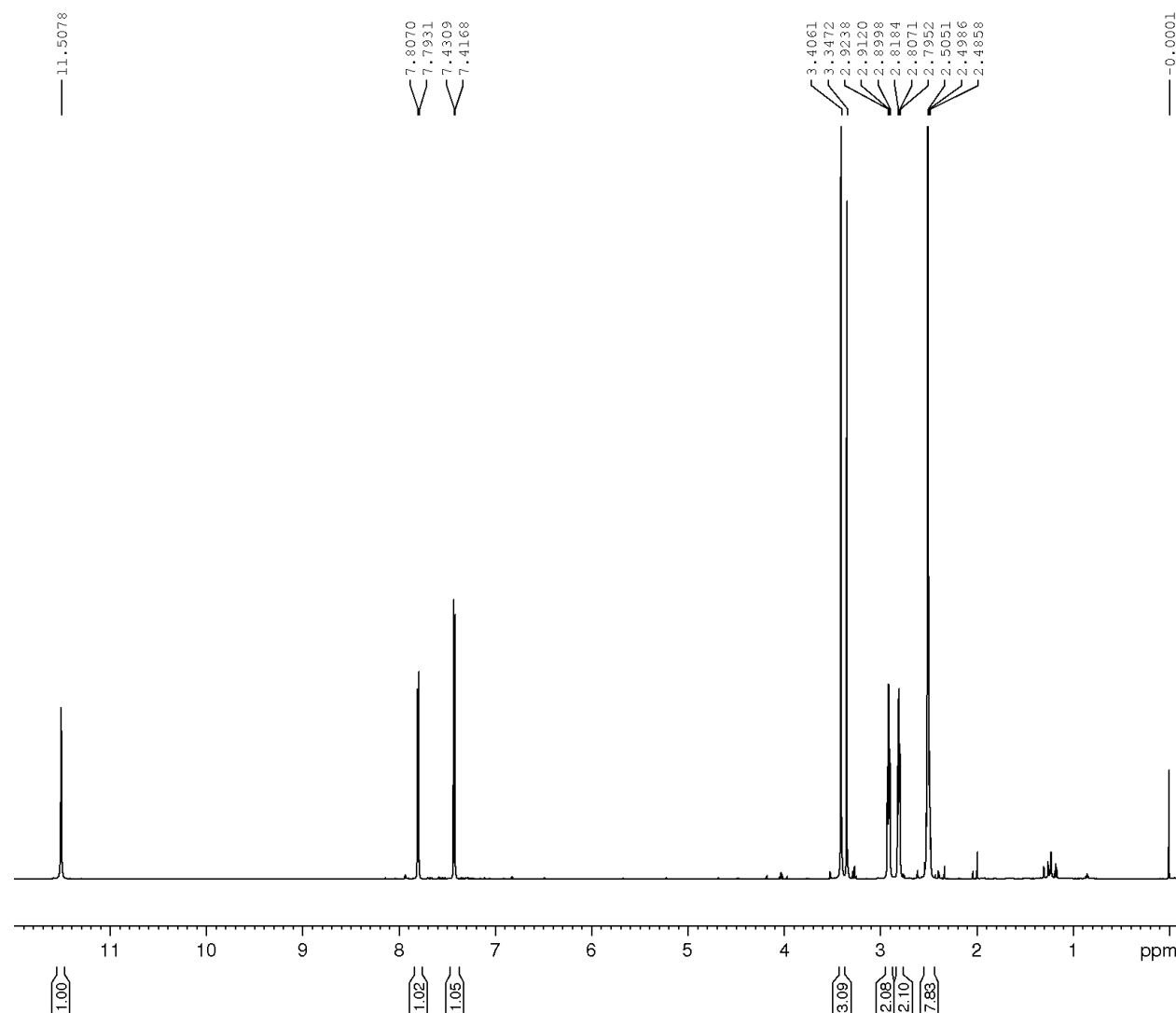
Spectrum Plot Report



Name	PGY0719_3C	Rack Pos.		Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	Plate Pos.		IRM Status	Success		
Data File	142823.D	Method (Acq)	DIP_70eV.M	Comment		Acq. Time (Local)	5/22/2024 2:18:41 PM (UTC+02:00)



¹H NMR spectrum of 3d



Standard 1H
143628
PGY0784_1A
Pusztai Gyongyver
2024.10.02. (KP)

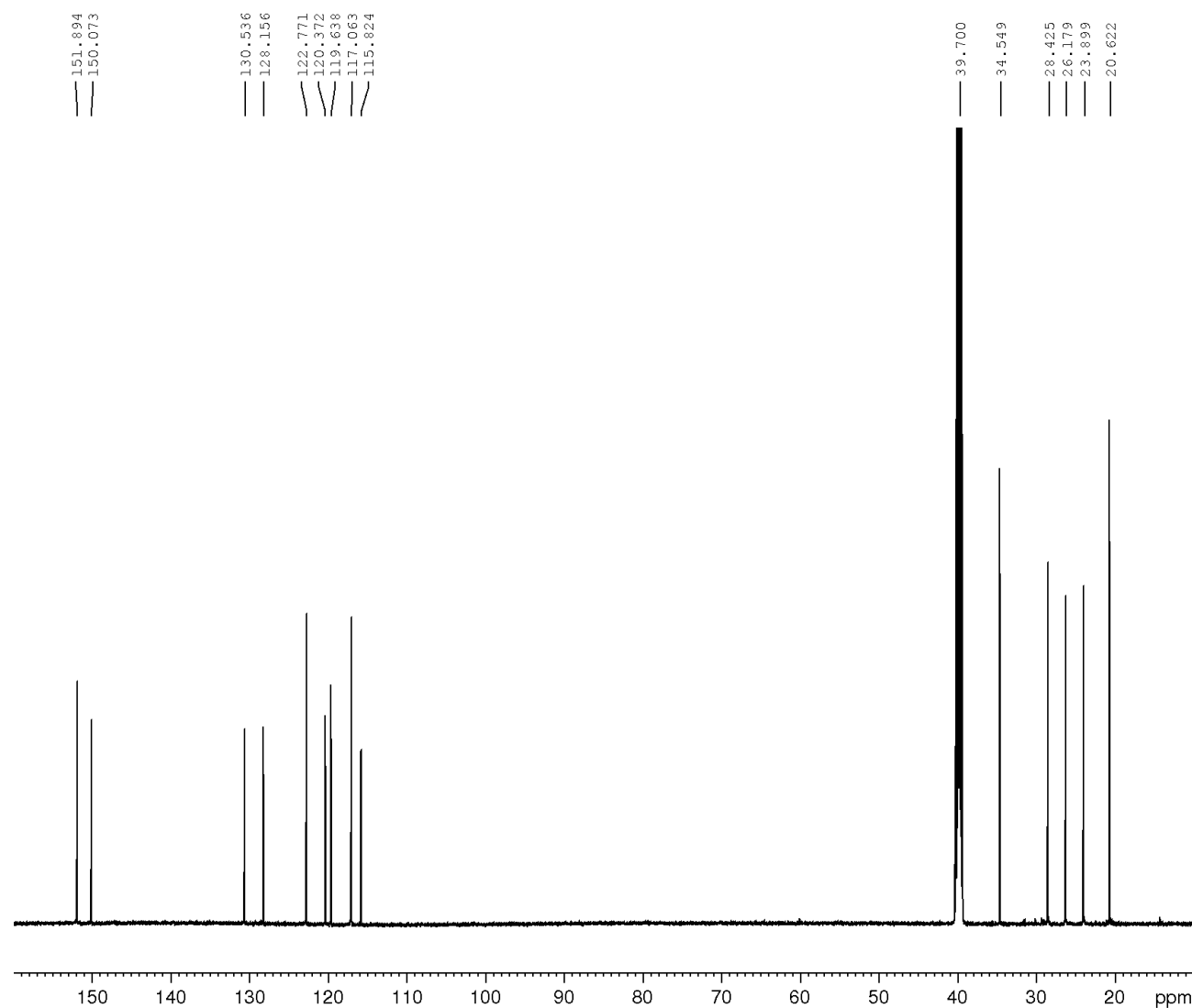
Current Data Parameters
NAME 143628
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241003
Time 4.12 h
INSTRUM spect
PROBHD Z145856_0002 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000021 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of **3d**



Standard 13C
143628
PGY0784_1A
Pusztai Gyongyver
2024.10.02. (KP)

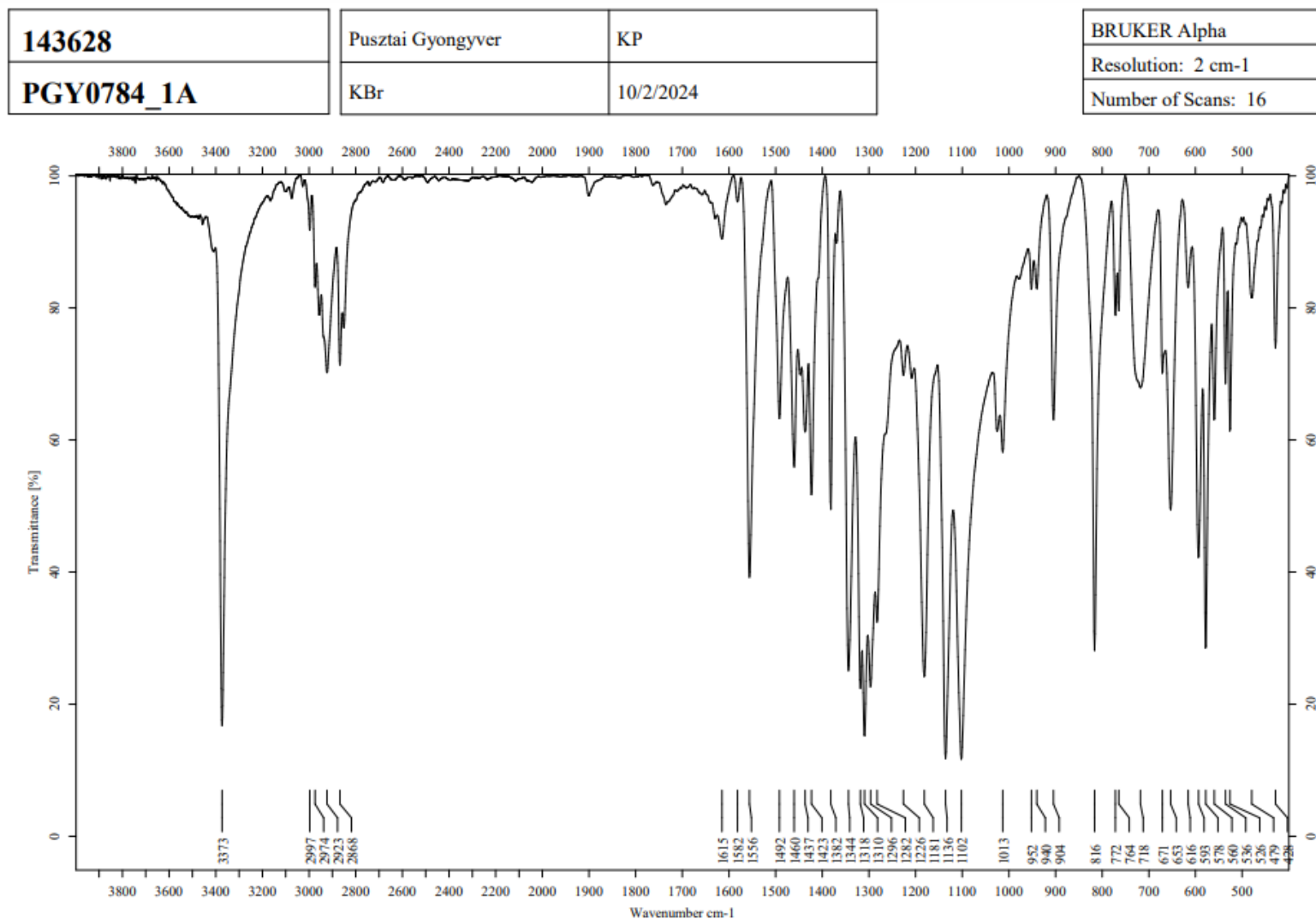
Current Data Parameters
NAME 143628
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241003
Time 5.20 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701600 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of **3d**

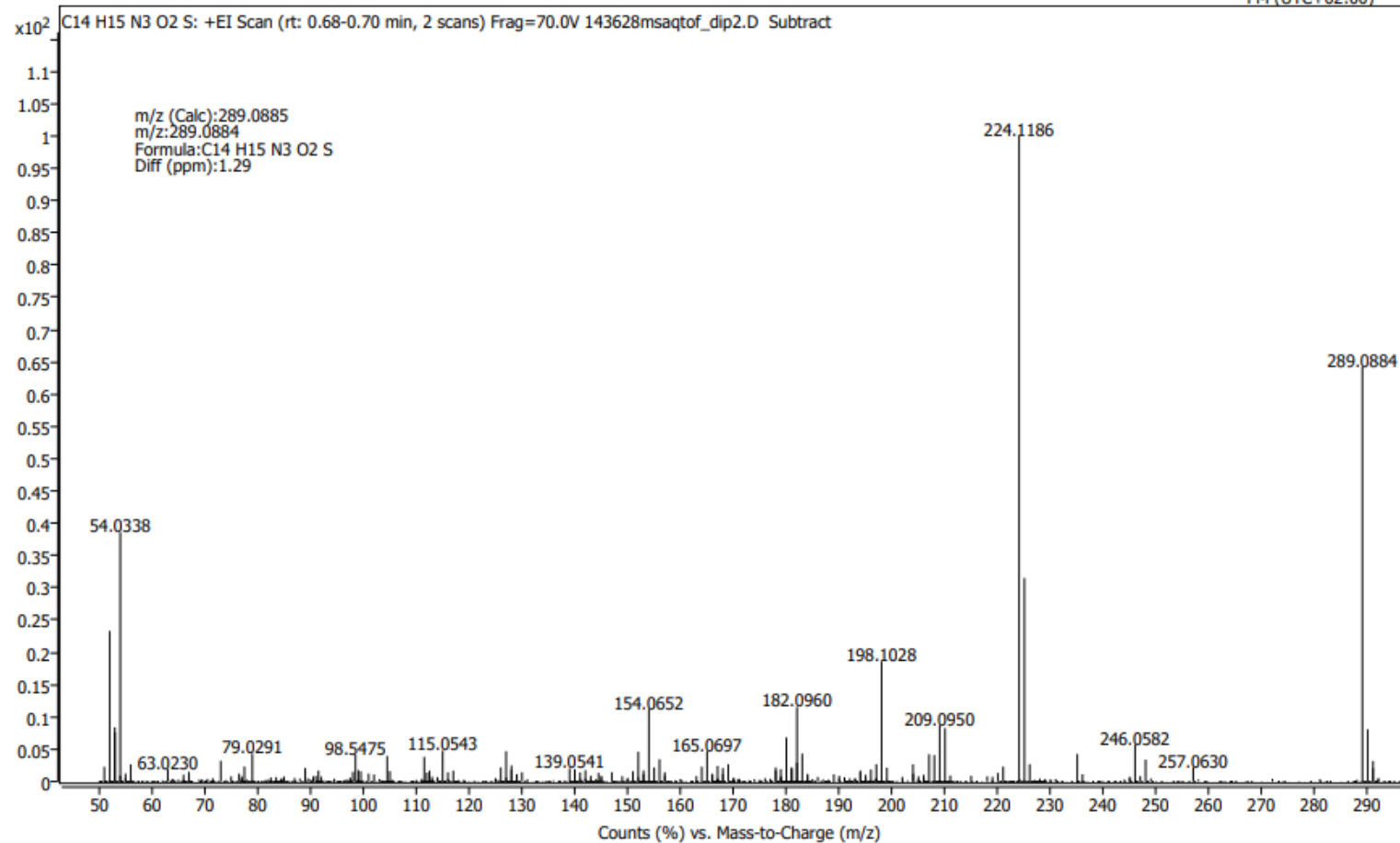


HRMS spectrum of **3d**

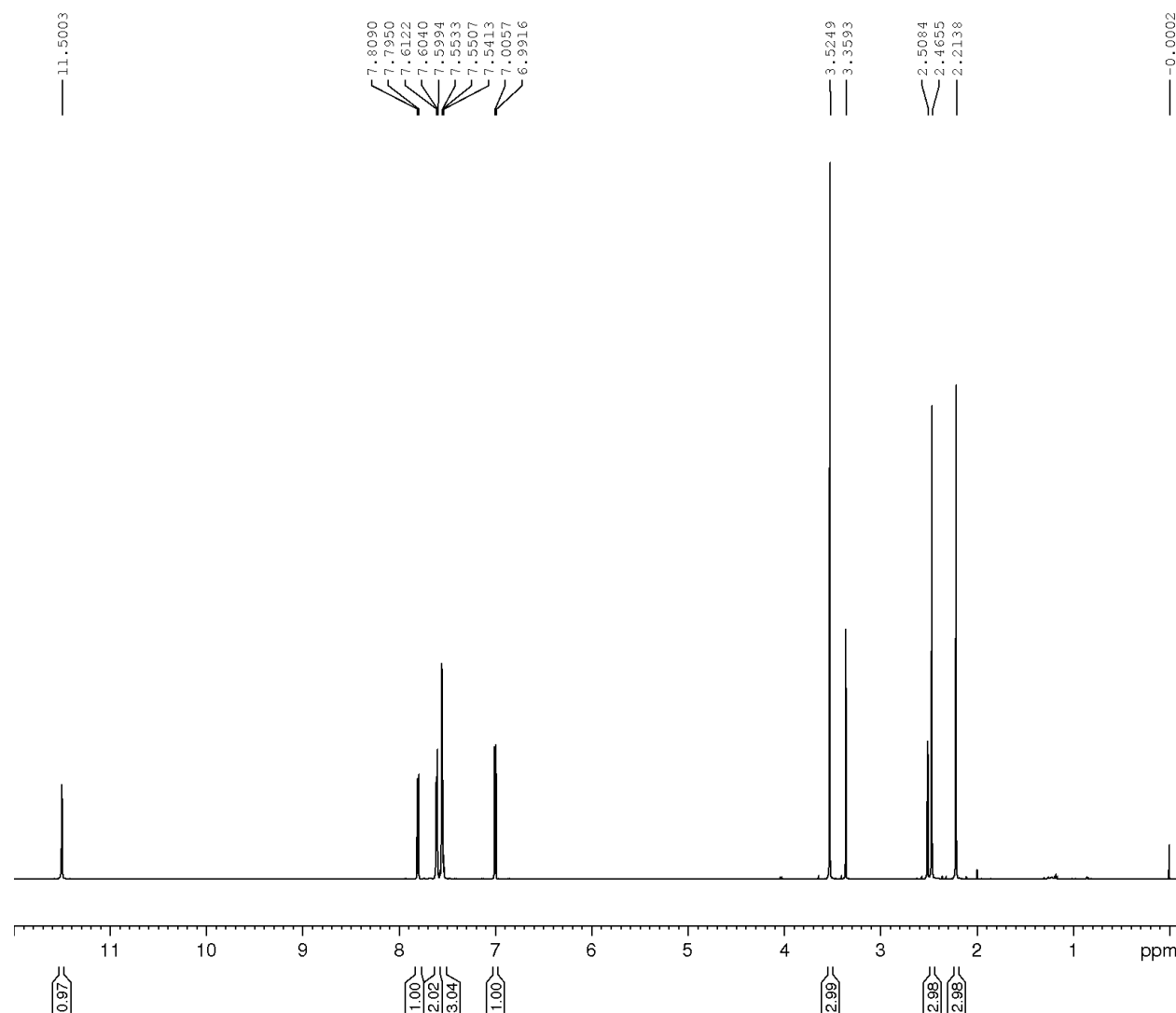
Spectrum Plot Report



Name	PGY0784_1A, Pusztai Rack Pos.	Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	IRM Status	Success		
Data File	143628msaqtod_dip2.D Method (Acq)	DIP_70eV_4min.M	Comment	Acq. Time (Local)	10/24/2024 1:31:58 PM (UTC+02:00)



¹H NMR spectrum of **3f**



Standard 1H
143417
PGY0766_1A
Pusztai Gyongyver
2024.09.11. (KP)

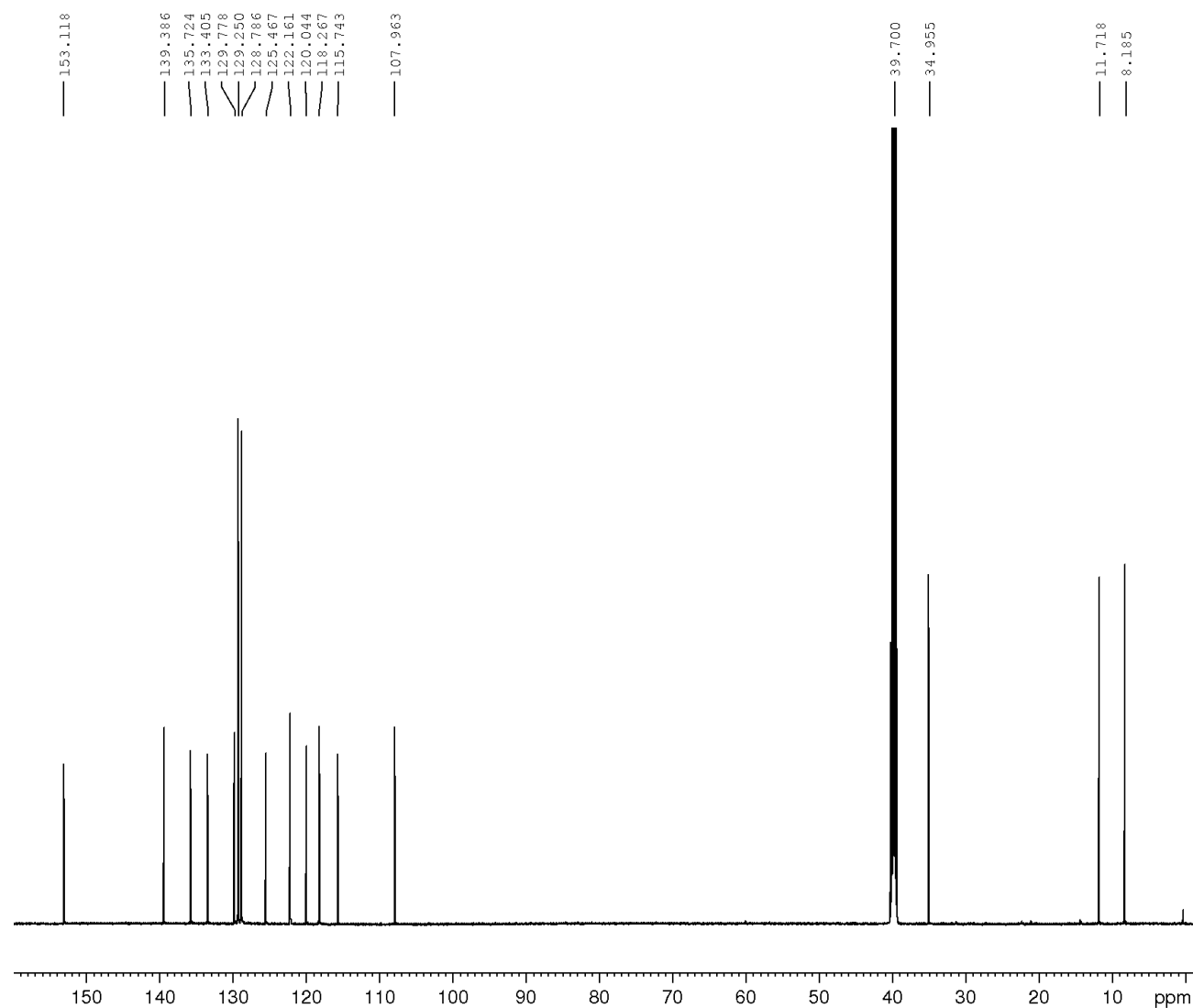
Current Data Parameters
NAME 143417
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240911
Time 22.21 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 599.9999998 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of **3f**



Standard 13C
143417
PGY0766_1A
Pusztai Gyongyver
2024.09.11. (KP)

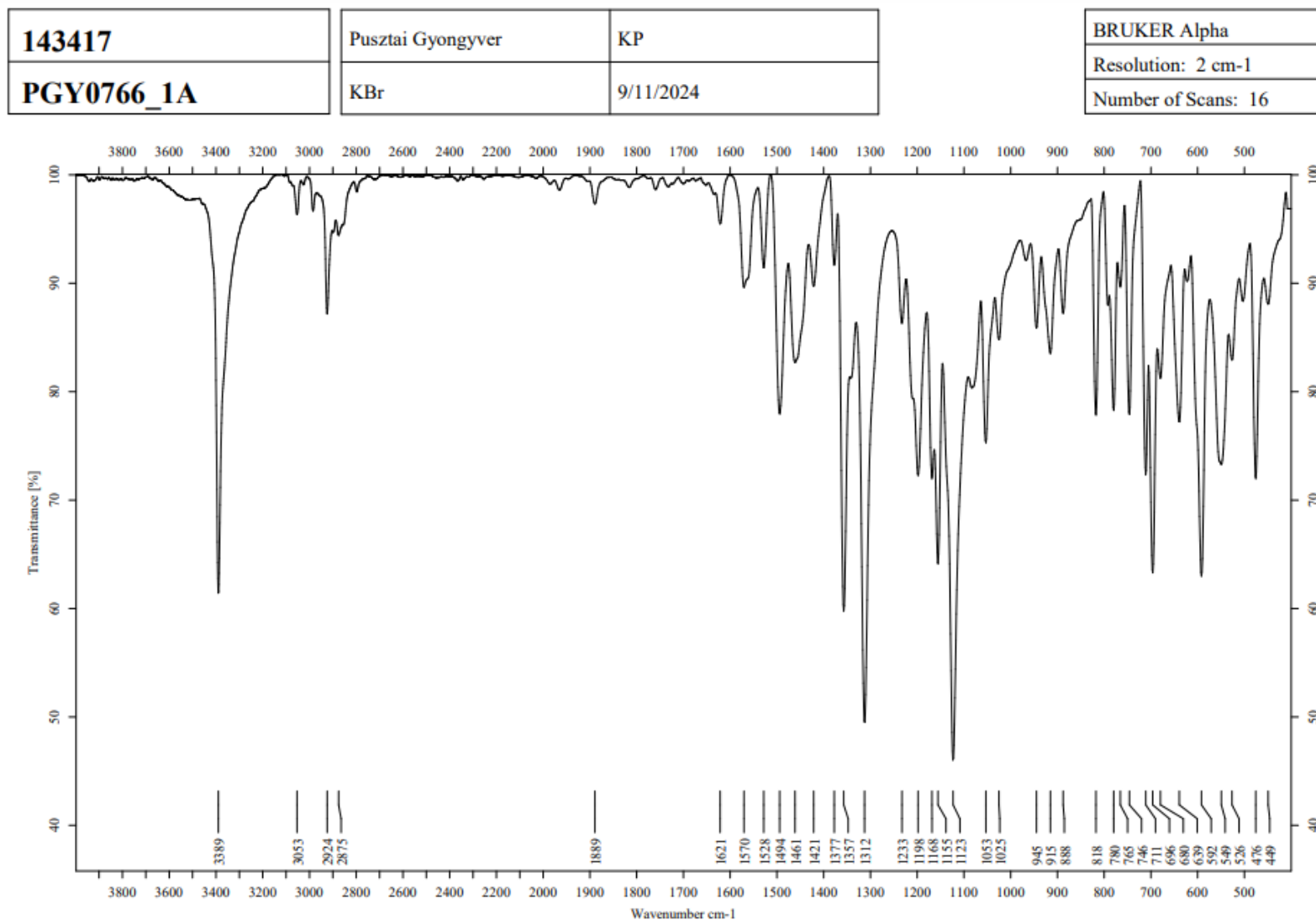
Current Data Parameters
NAME 143417
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240911
Time 23.30 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701601 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of **3f**

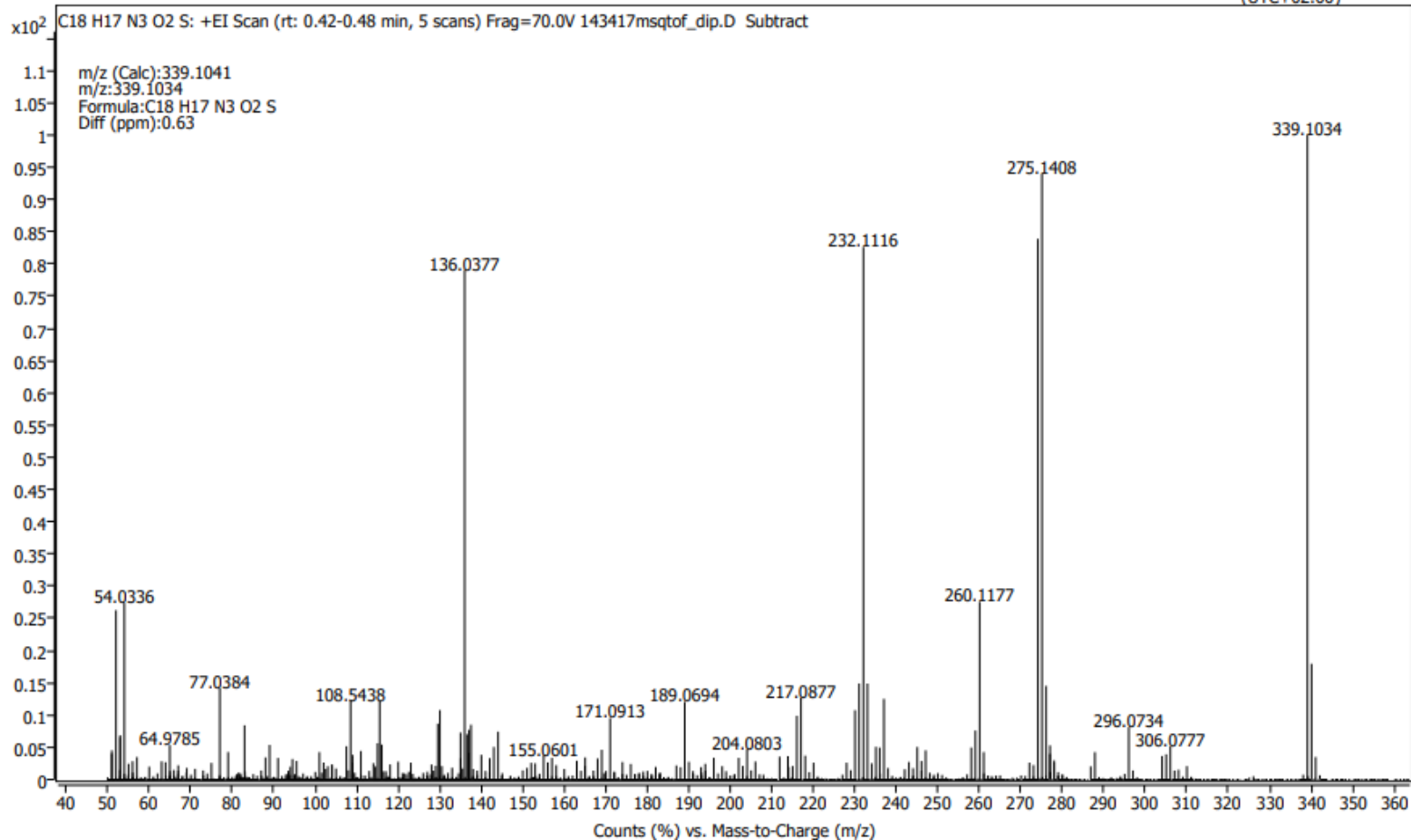


HRMS spectrum of **3f**

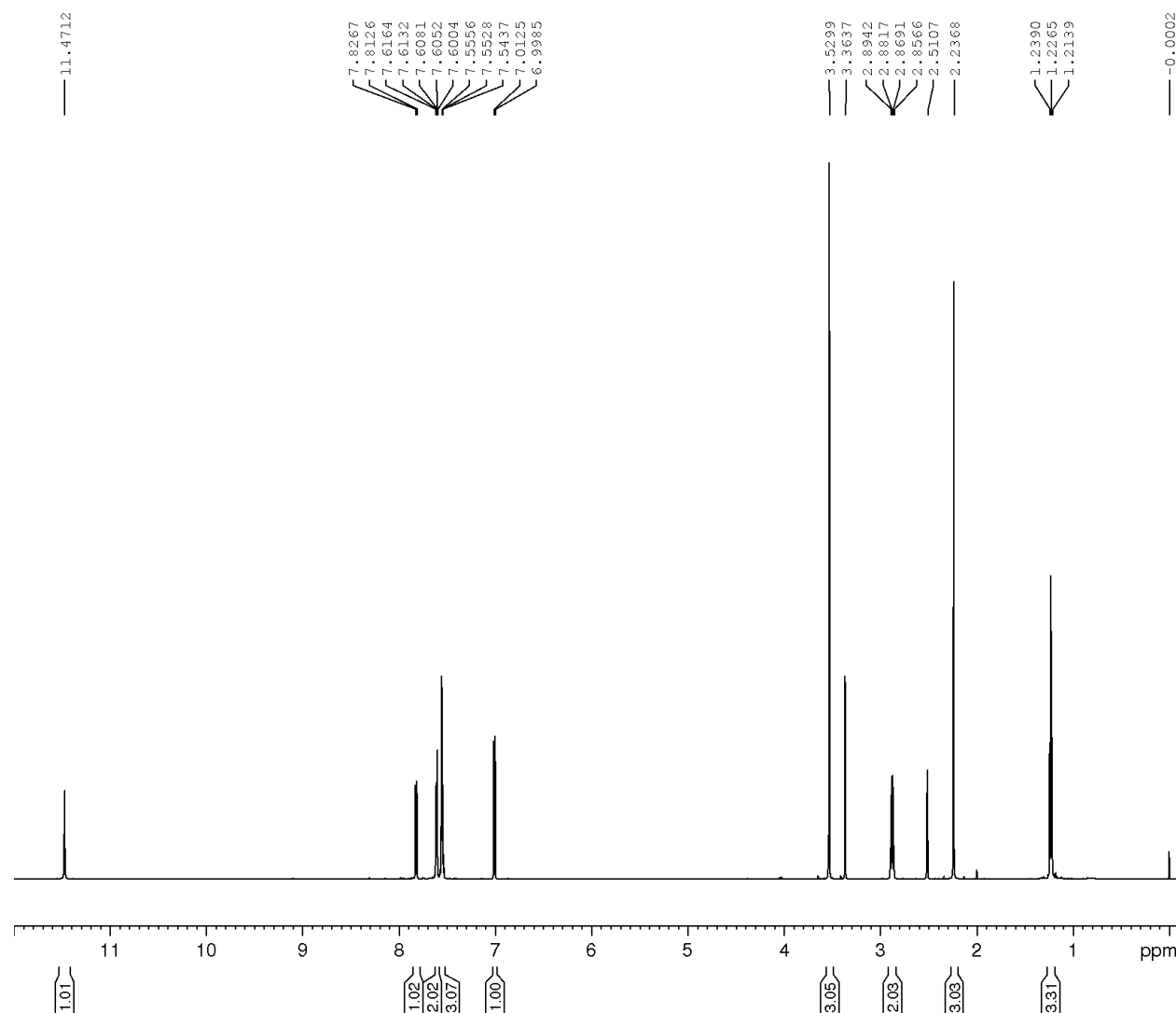
Spectrum Plot Report



Name	PGY0766_1A, Pusztai Gyongyver	Rack Pos.	Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	Plate Pos.	IRM Status	Success		
Data File	143417msqtof_dip.D	Method (Acq)	DIP_70eV.M	Comment	Acq. Time (Local)	9/18/2024 8:57:11 AM (UTC+02:00)



¹H NMR spectrum of **3g**



Standard 1H
143497
PGY0767_1A
Pusztai Gyongyver
2024.09.11. (KP)

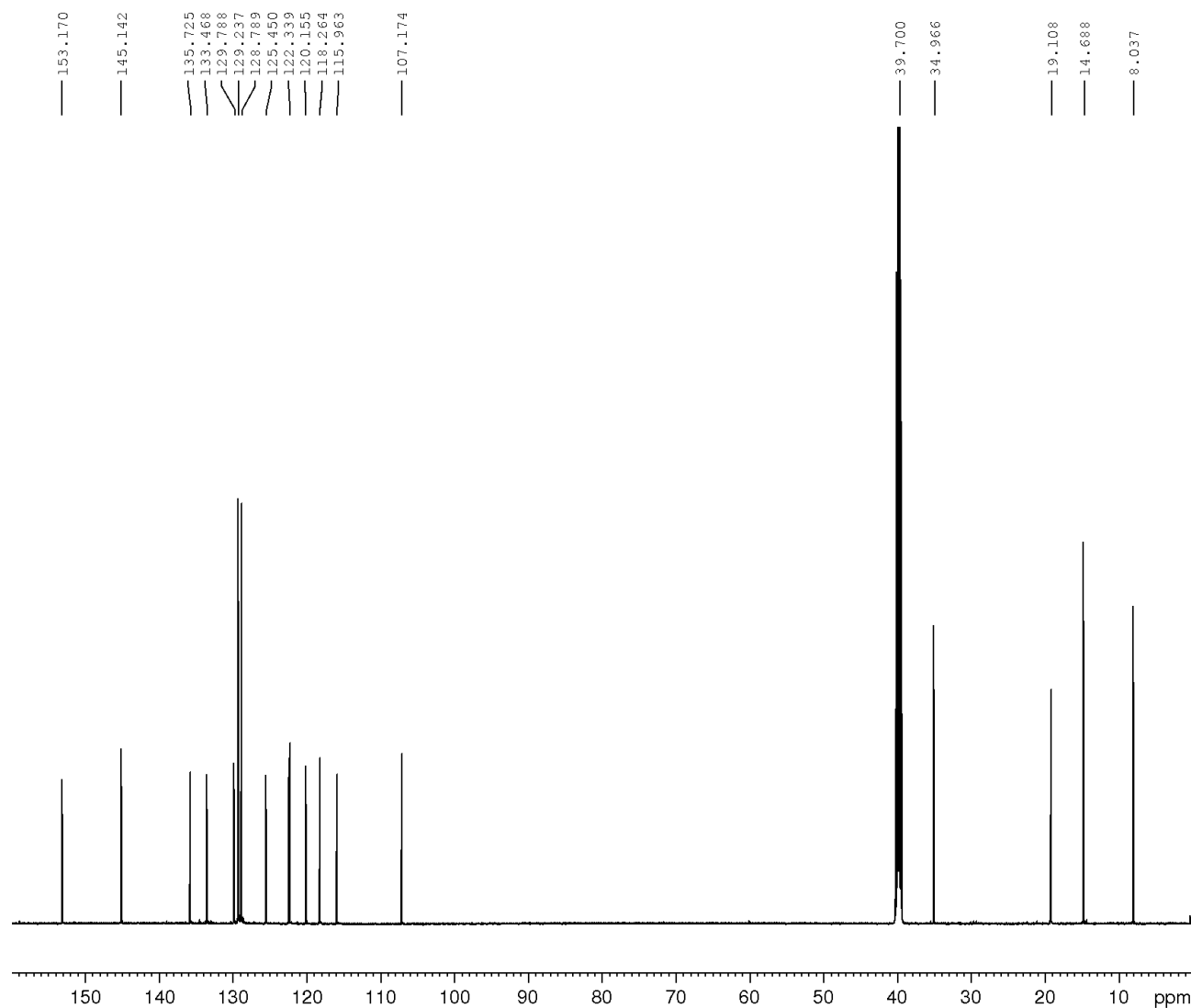
Current Data Parameters
NAME 143497
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240912
Time 0.56 h
INSTRUM spect
PROBHD Z145856_0002 (zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 119.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 599.9999984 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of **3g**



Standard 13C
143497
PGY0767_1A
Pusztai Gyongyver
2024.09.11. (KP)

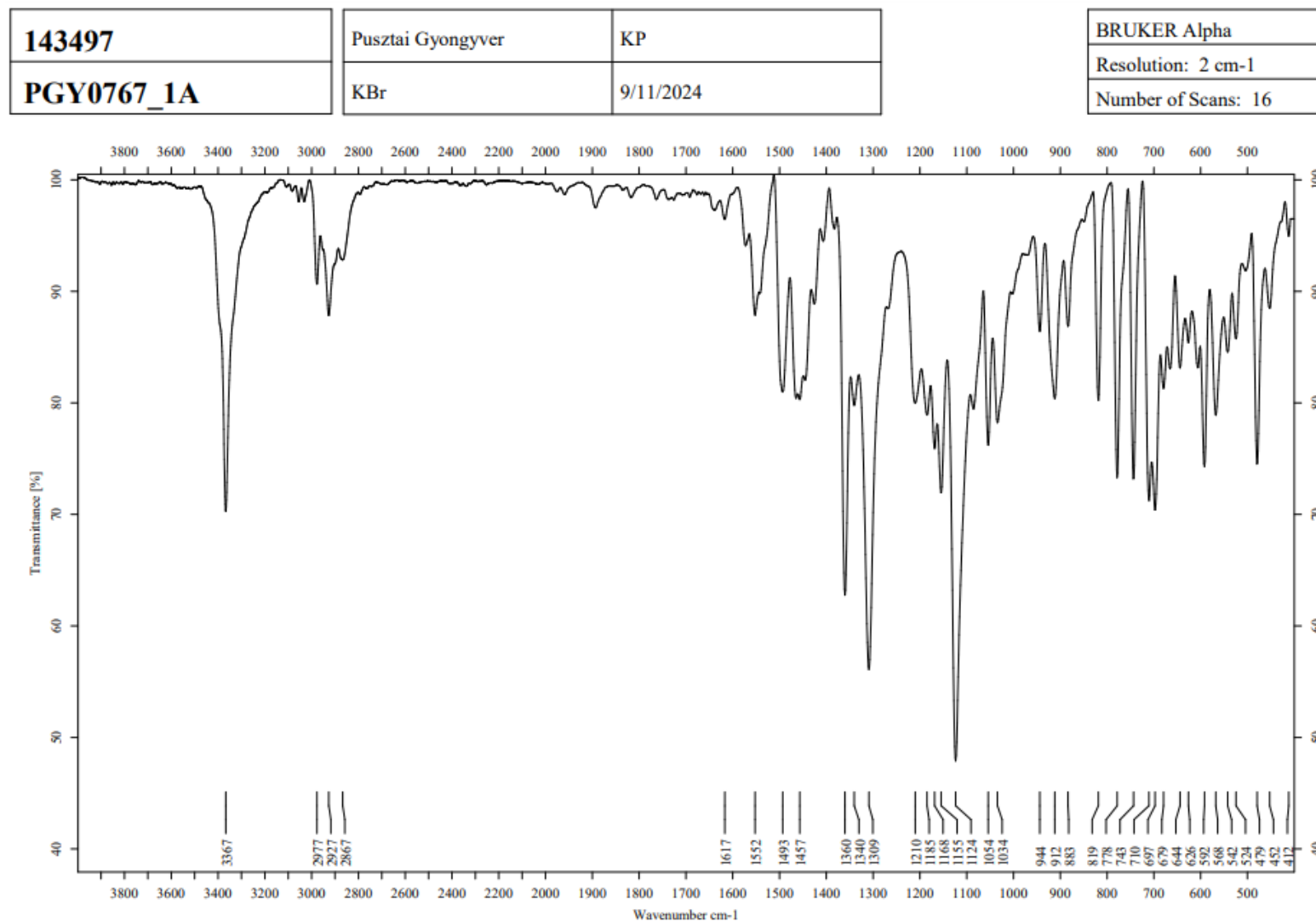
Current Data Parameters
NAME 143497
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240912
Time 2.04 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701600 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of **3g**

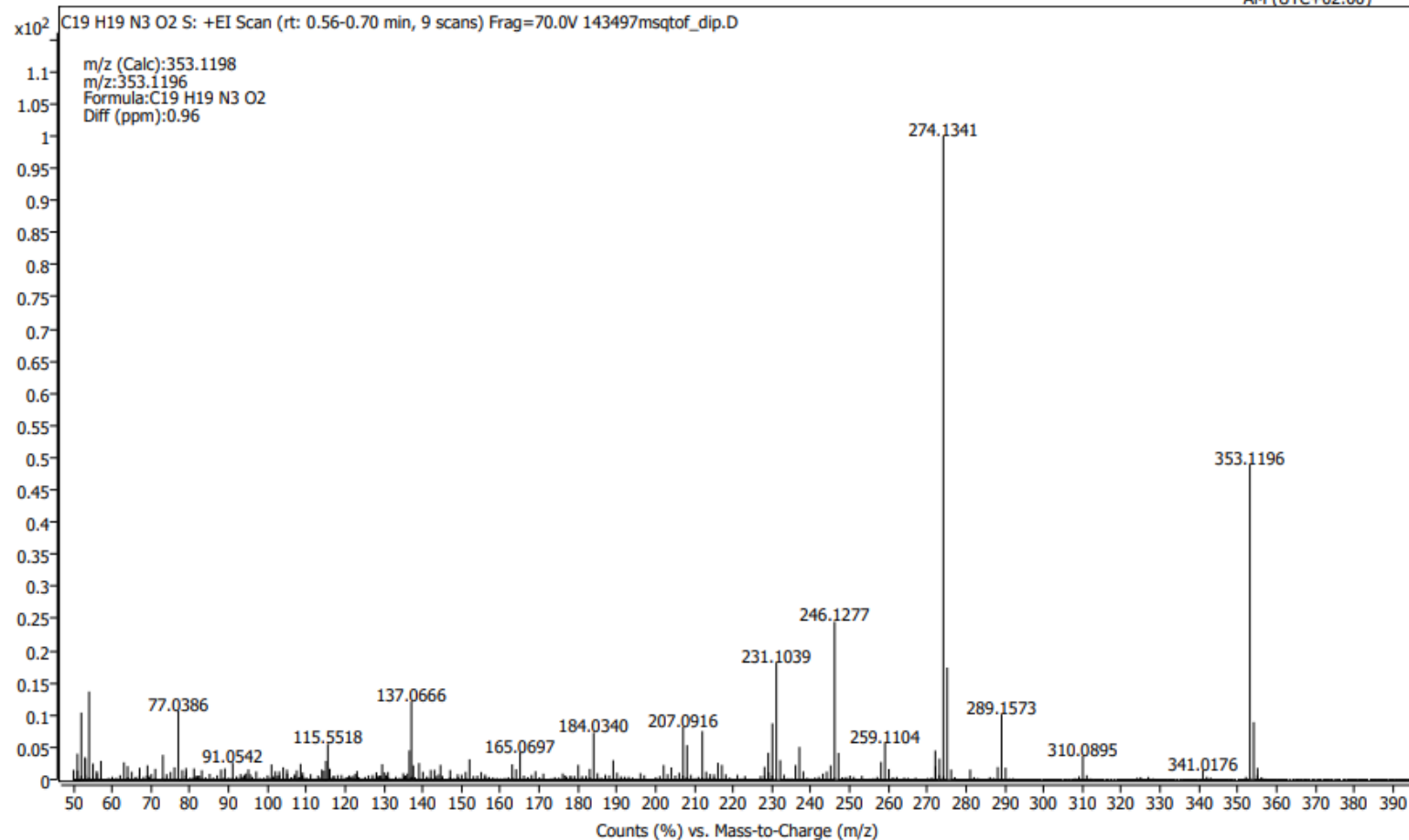


HRMS spectrum of **3g**

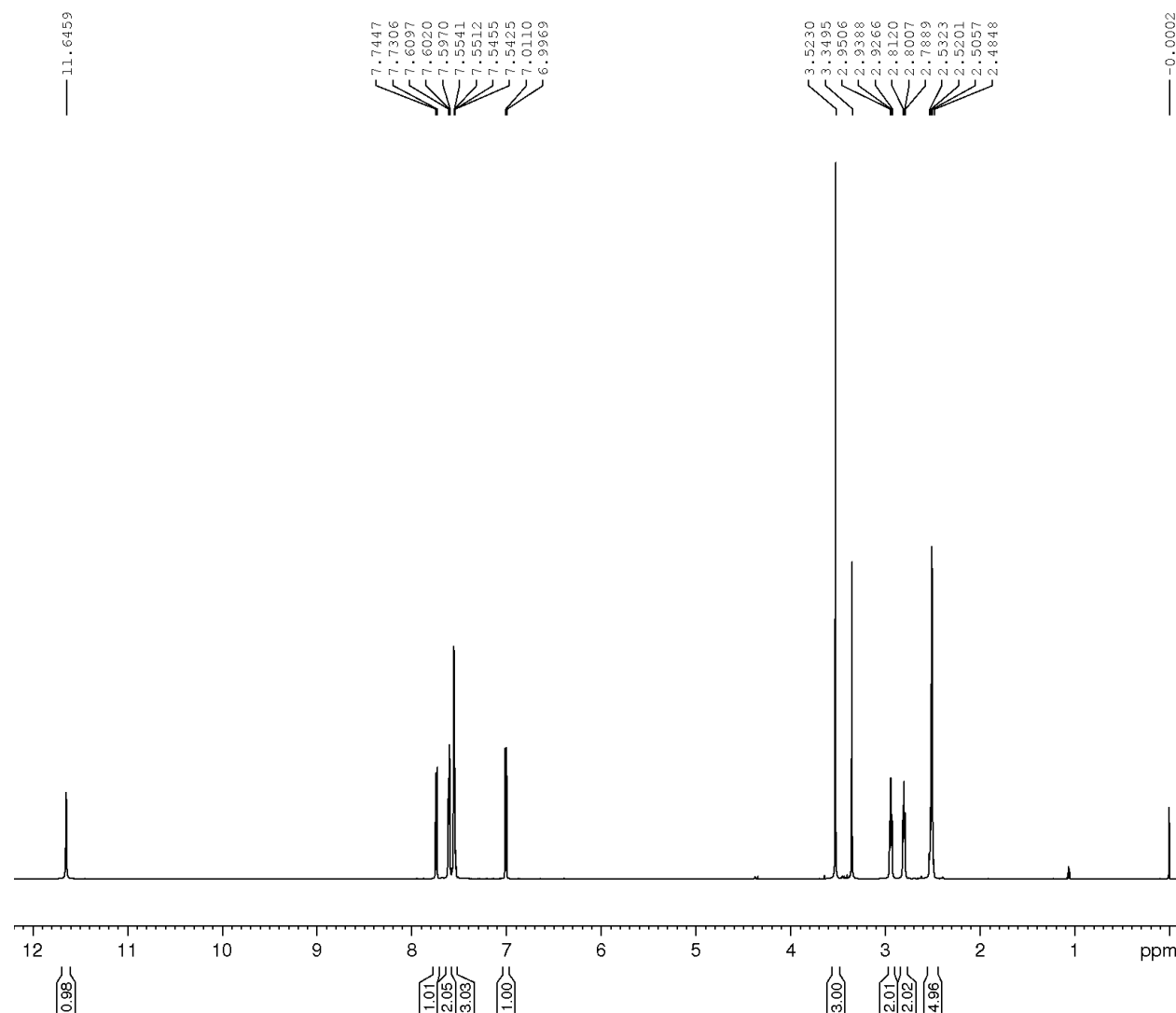
Spectrum Plot Report



Name	PGY0767_1A, Pusztai Gyongyver	Rack Pos.		Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	Plate Pos.		IRM Status	Success	Acq. Time (Local)	9/18/2024 10:07:07 AM (UTC+02:00)
Data File	143497msqtof_dip.D	Method (Acq)	DIP_70eV.M	Comment			



¹H NMR spectrum of **3i**



Standard 1H
143568
PGY0758_1C
Pusztai Gyongyver
2024.10.04. (KP)

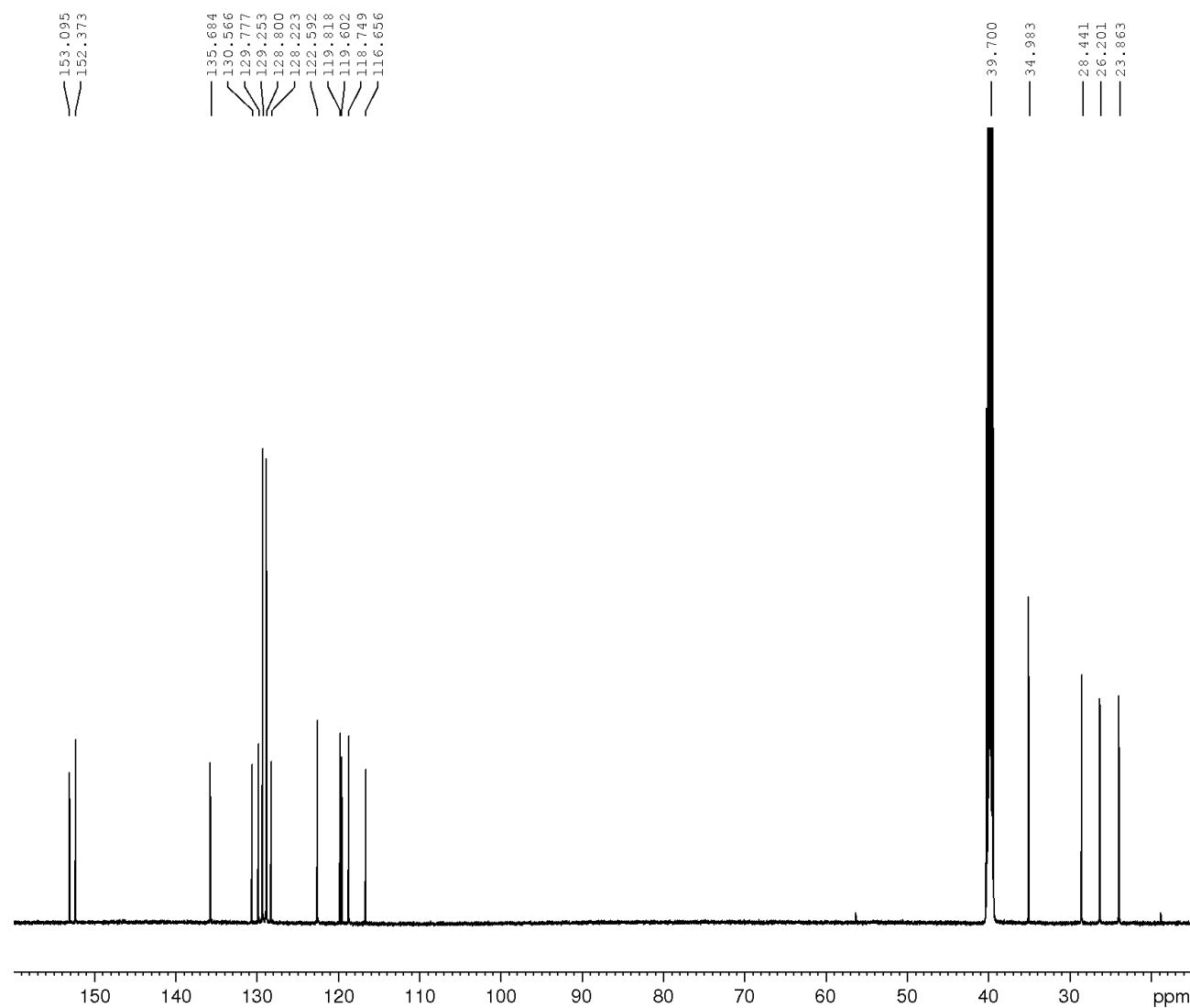
Current Data Parameters
NAME 143568
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241004
Time 22.39 h
INSTRUM spect
PROBHD Z145856_0002 (zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000014 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of **3i**



Standard 13C
143568
PGY0758_1C
Pusztai Gyongyver
2024.10.04. (KP)

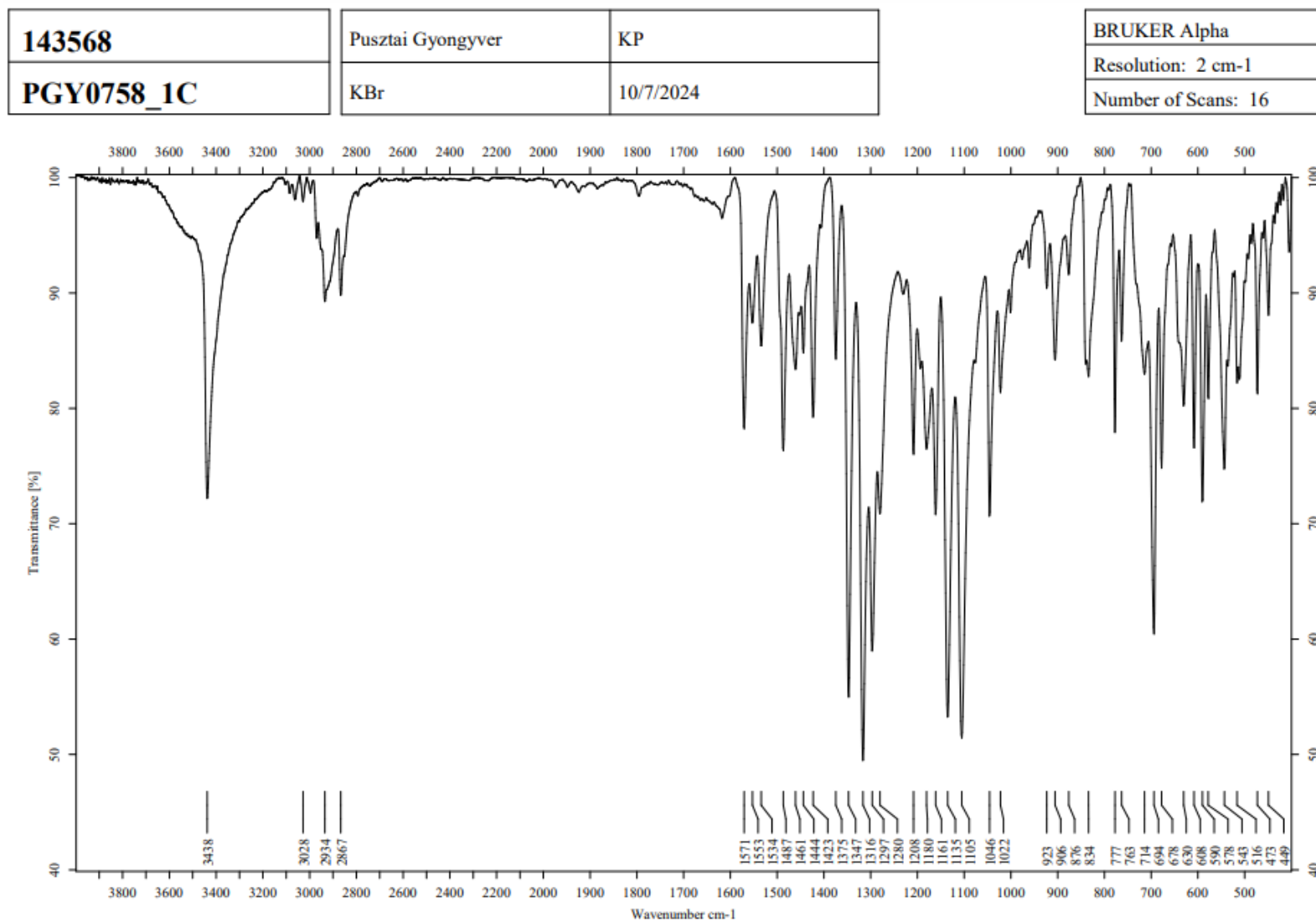
Current Data Parameters
NAME 143568
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241004
Time 23.48 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701603 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of **3i**

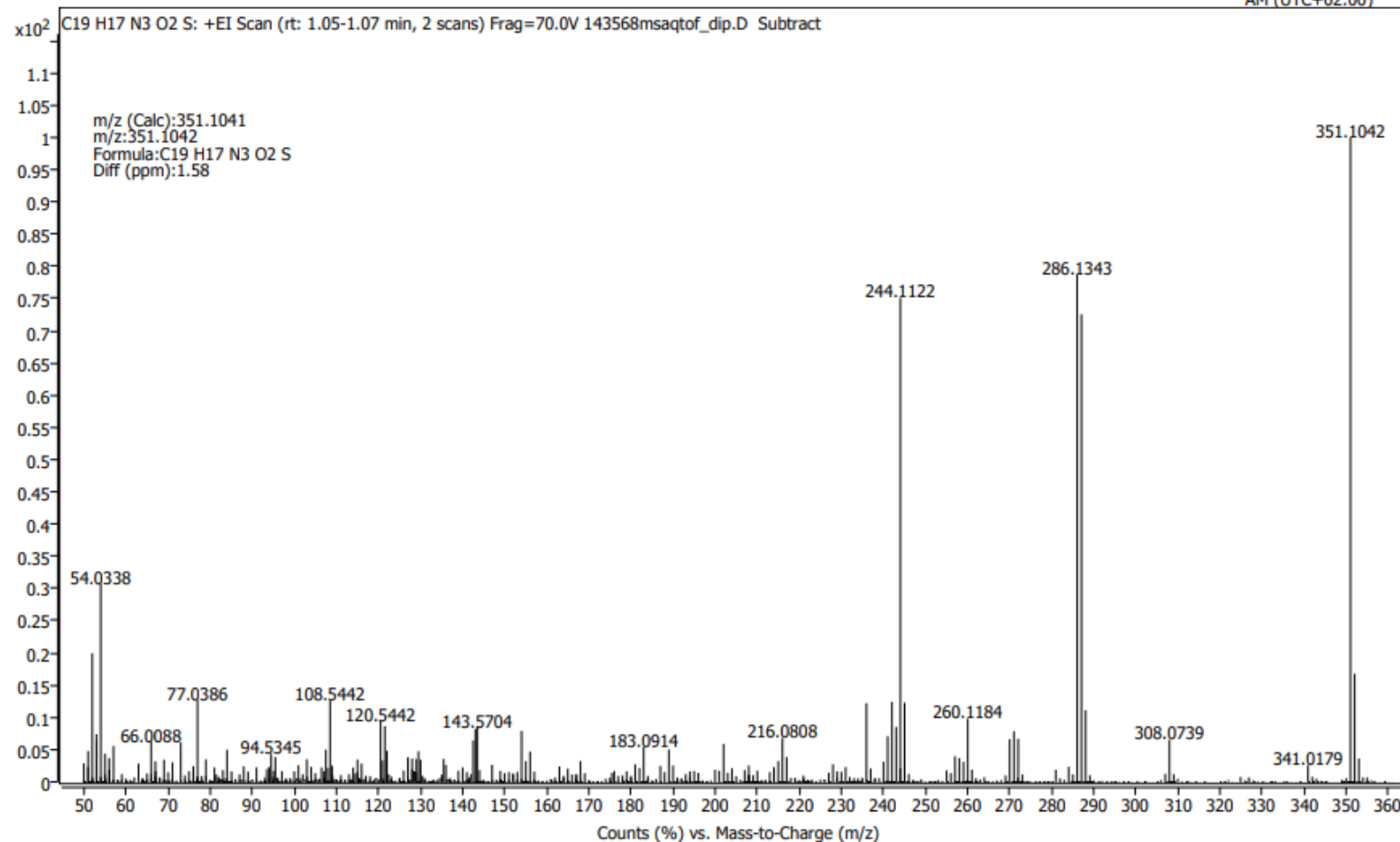


HRMS spectrum of 3i

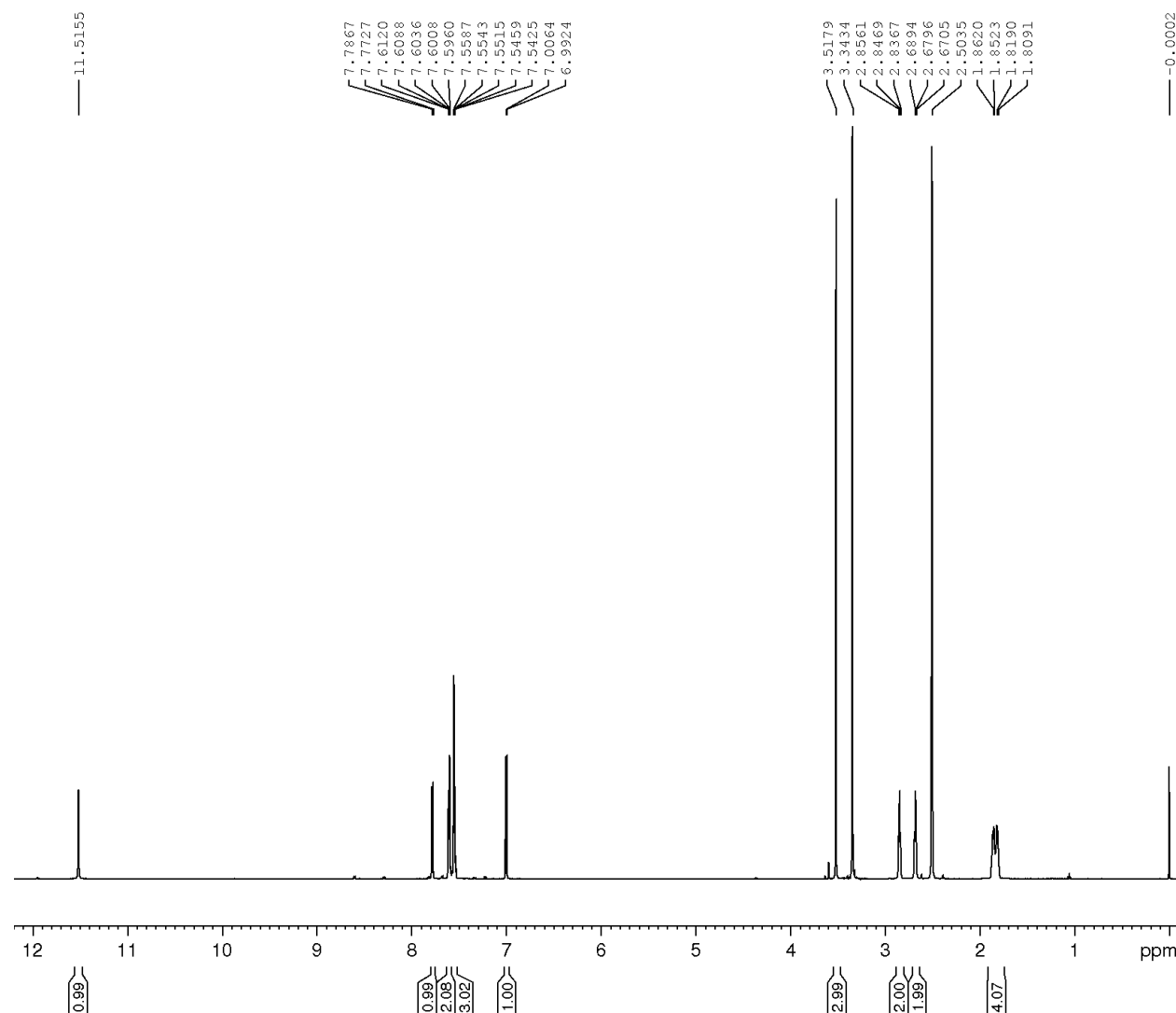
Spectrum Plot Report



Name	PGY0758_1C, Pusztai Gyongyver	Rack Pos.		Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	Plate Pos.		IRM Status	Success		
Data File	143568msaqtod_dip.D	Method (Acq)	DIP_70eV.M	Comment		Acq. Time (Local)	10/24/2024 8:22:46 AM (UTC+02:00)



¹H NMR spectrum of **3j**



Standard 1H
143569
PGY0768_1A
Pusztai Gyongyver
2024.09.20. (KP)

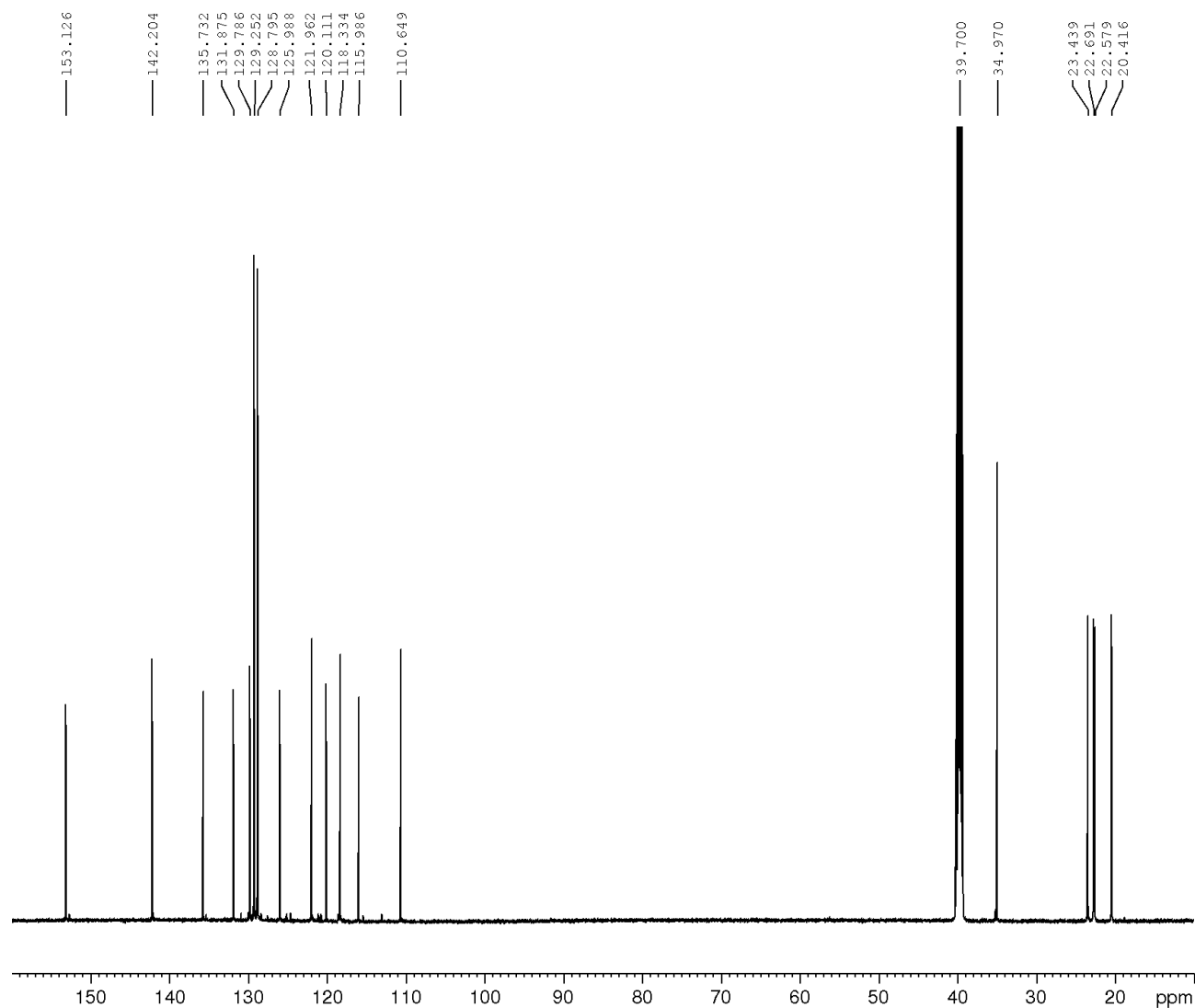
Current Data Parameters
NAME 143569
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240920
Time 11.44 h
INSTRUM spect
PROBHD Z145856_0002 (zg30)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000027 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of **3j**



Standard 13C
143569
PGY0768_1A
Pusztai Gyongyver
2024.09.30. (KP)

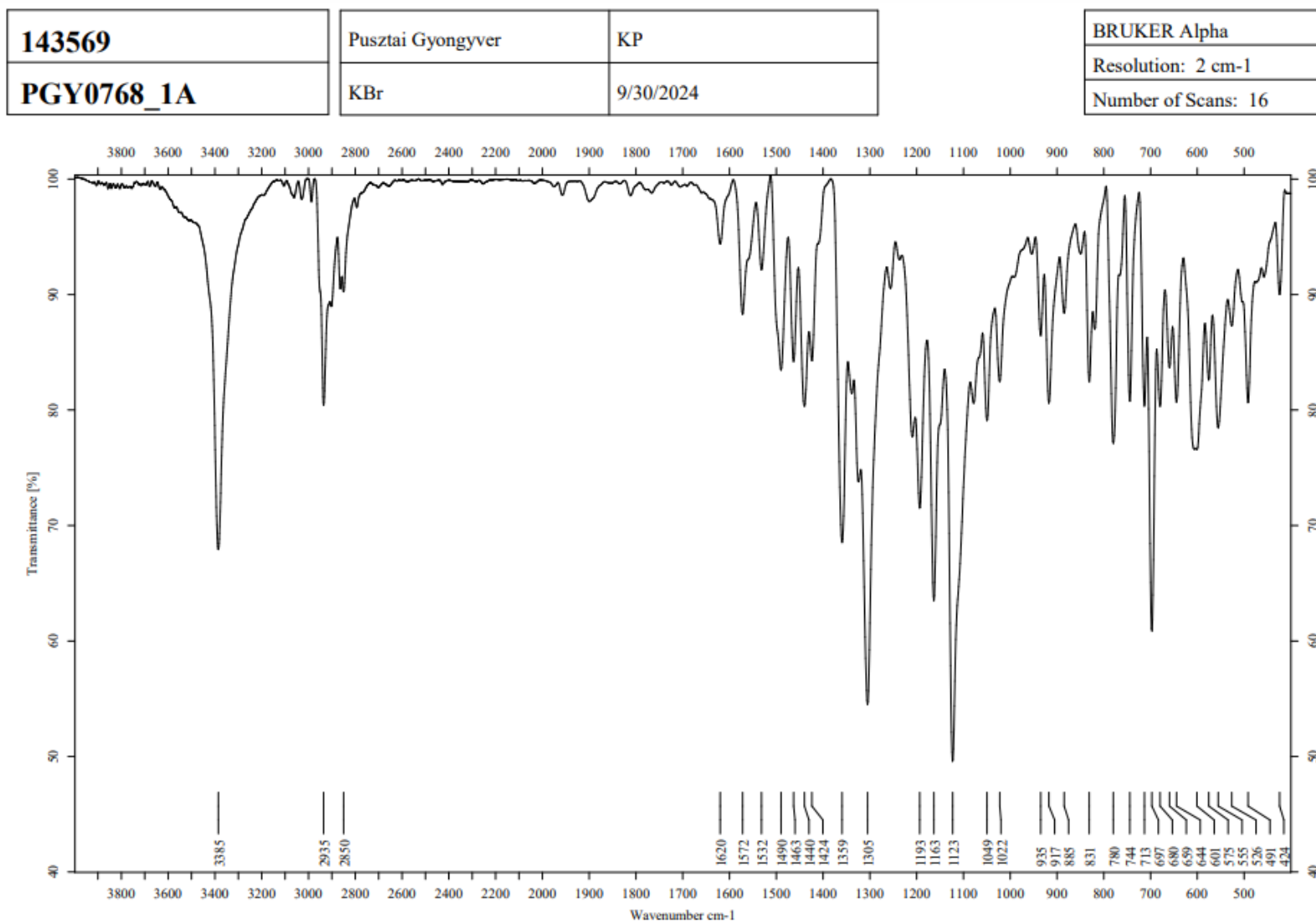
Current Data Parameters
NAME 143569
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240930
Time 16.44 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701587 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of **3j**

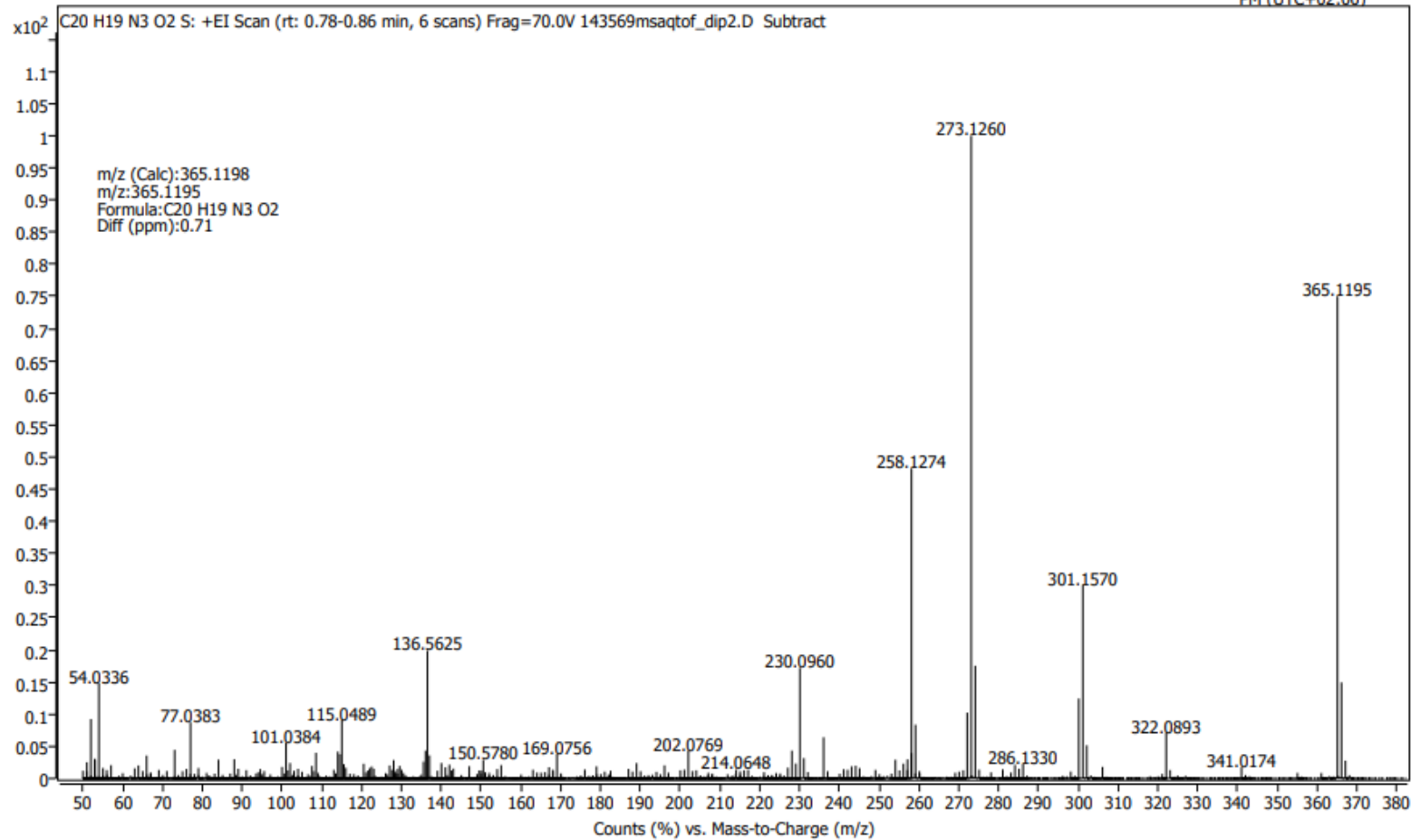


HRMS spectrum of 3j

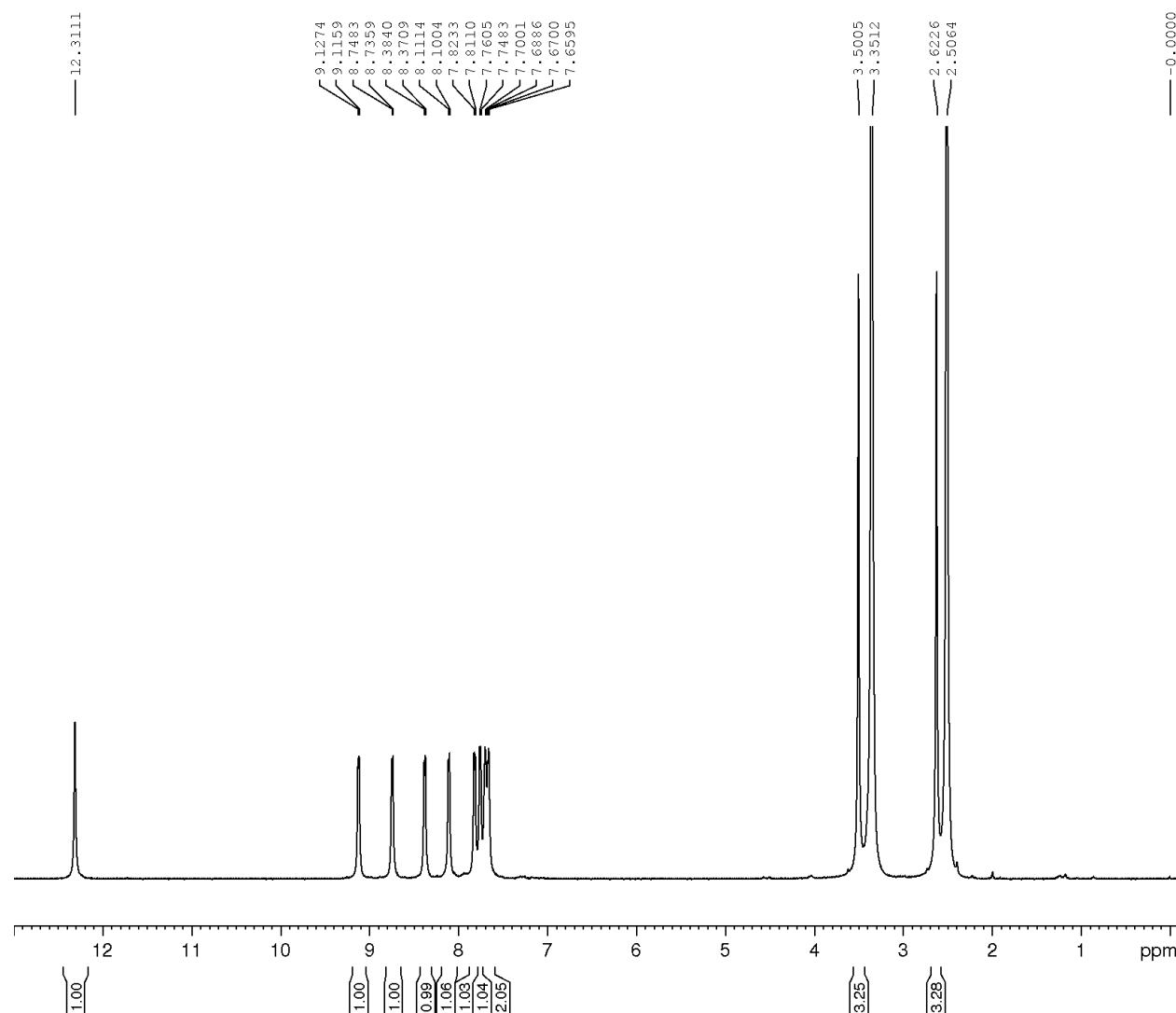
Spectrum Plot Report



Name	Rack Pos.	Instrument	Success	Operator
Inj. Vol. (ul)	Plate Pos.	IRM Status		
Data File	143569msaqtod_dip2.D Method (Acq)	Comment		
				Acq. Time (Local)
				10/24/2024 1:11:43 PM (UTC+02:00)



¹H NMR spectrum of **10a**



Standard 1H
144057
PGY0835_2A
Pusztai Gyongyver
2024.01.07. (KP)

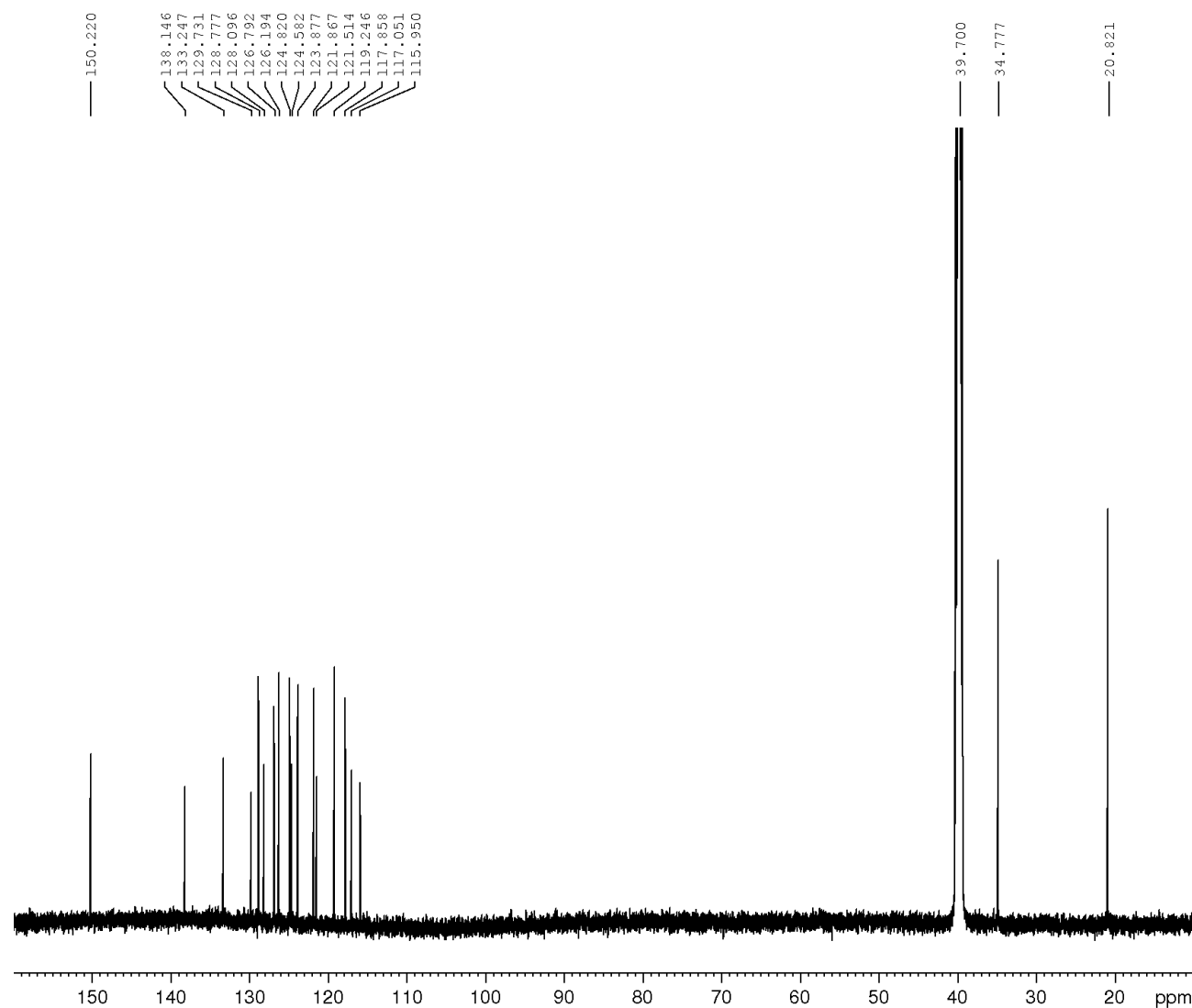
Current Data Parameters
NAME 144057
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250107
Time 14.28 h
INSTRUM spect
PROBHD Z145856_0002 (zg30)
PULPROG 65536
TD DMSO
SOLVENT 16
NS 2
DS 12019.230 Hz
SWH 0.366798 Hz
FIDRES 2.7262976 sec
AQ 196.07
RG 41.600 usec
DW 25.00 usec
DE 295.0 K
TE 1.00000000 sec
D1 1
TD0 600.0037050 MHz
SFO1 1H
NUC1 11.50 usec
P1 28.00000000 W
PLW1

F2 - Processing parameters
SI 65536
SF 600.0000012 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of **10a**



Standard 13C
144057
PGY0835_2A
Pusztai Gyongyver
2025.01.07. (KP)

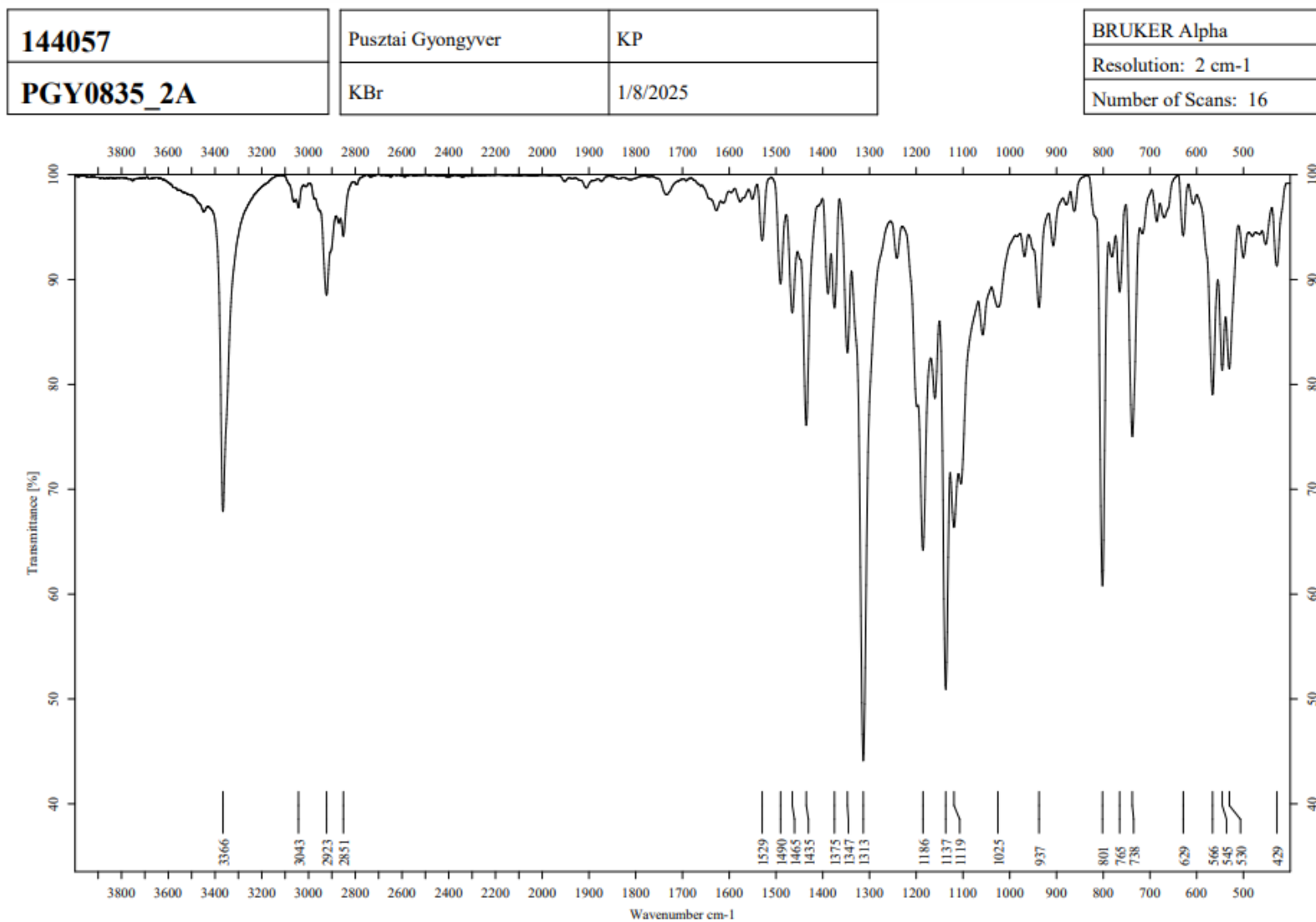
Current Data Parameters
NAME 144057
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20250107
Time 16.03 h
INSTRUM spect
PROBHD z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701597 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of **10a**

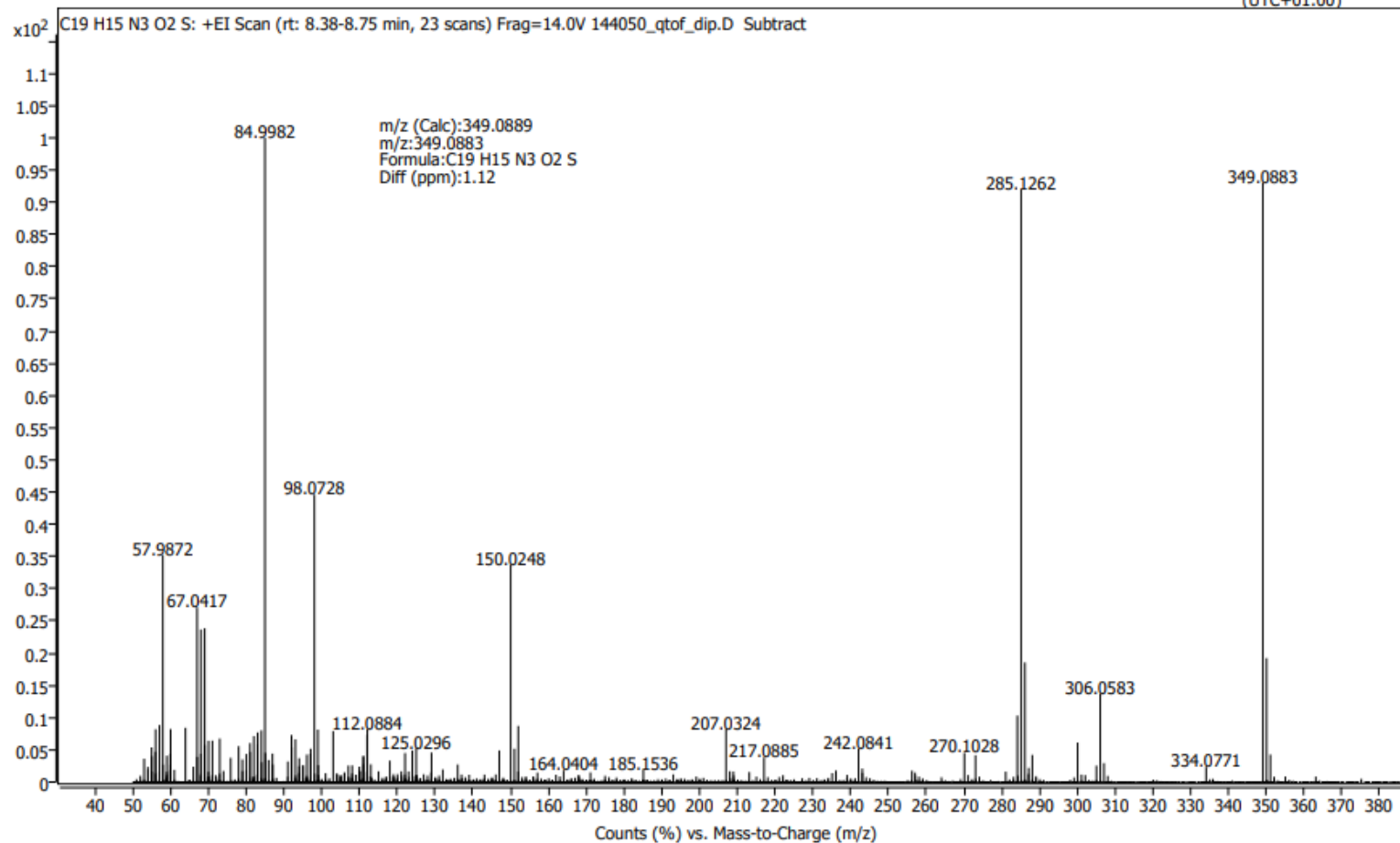


HRMS spectrum of **10a**

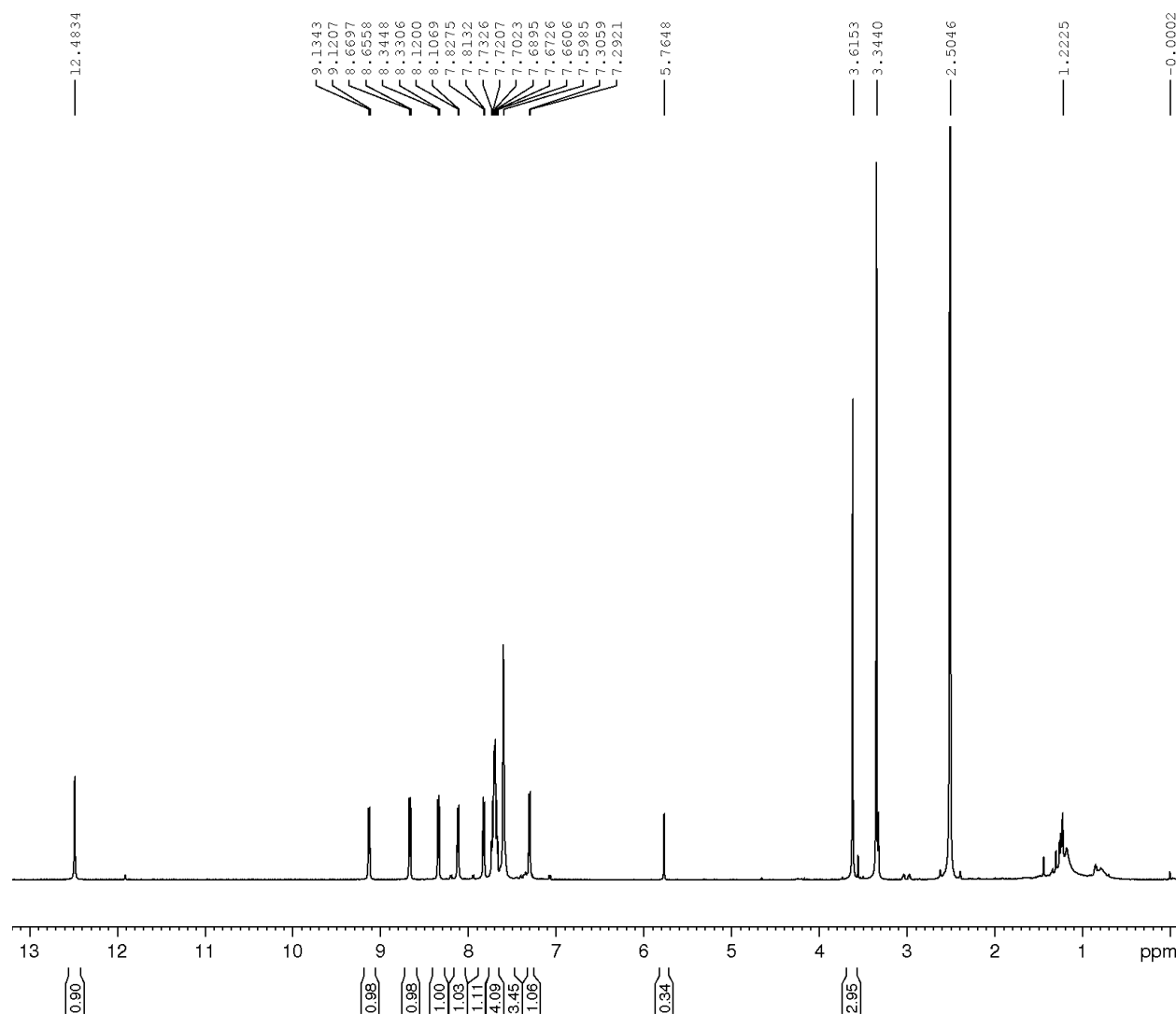
Spectrum Plot Report



Name	PGZ0835_2, Pusztai Gyongyver	Rack Pos.	Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	Plate Pos.	IRM Status	Success		
Data File	144050_qtof_dip.D	Method (Acq)	DIP_LOW_14eV.M	Comment	Acq. Time (Local)	1/7/2025 11:42:18 AM (UTC+01:00)



¹H NMR spectrum of **10b**



Standard 1H
143947
PGY0823_1A
Pusztai Gyongyver
2024.11.29. (KP)

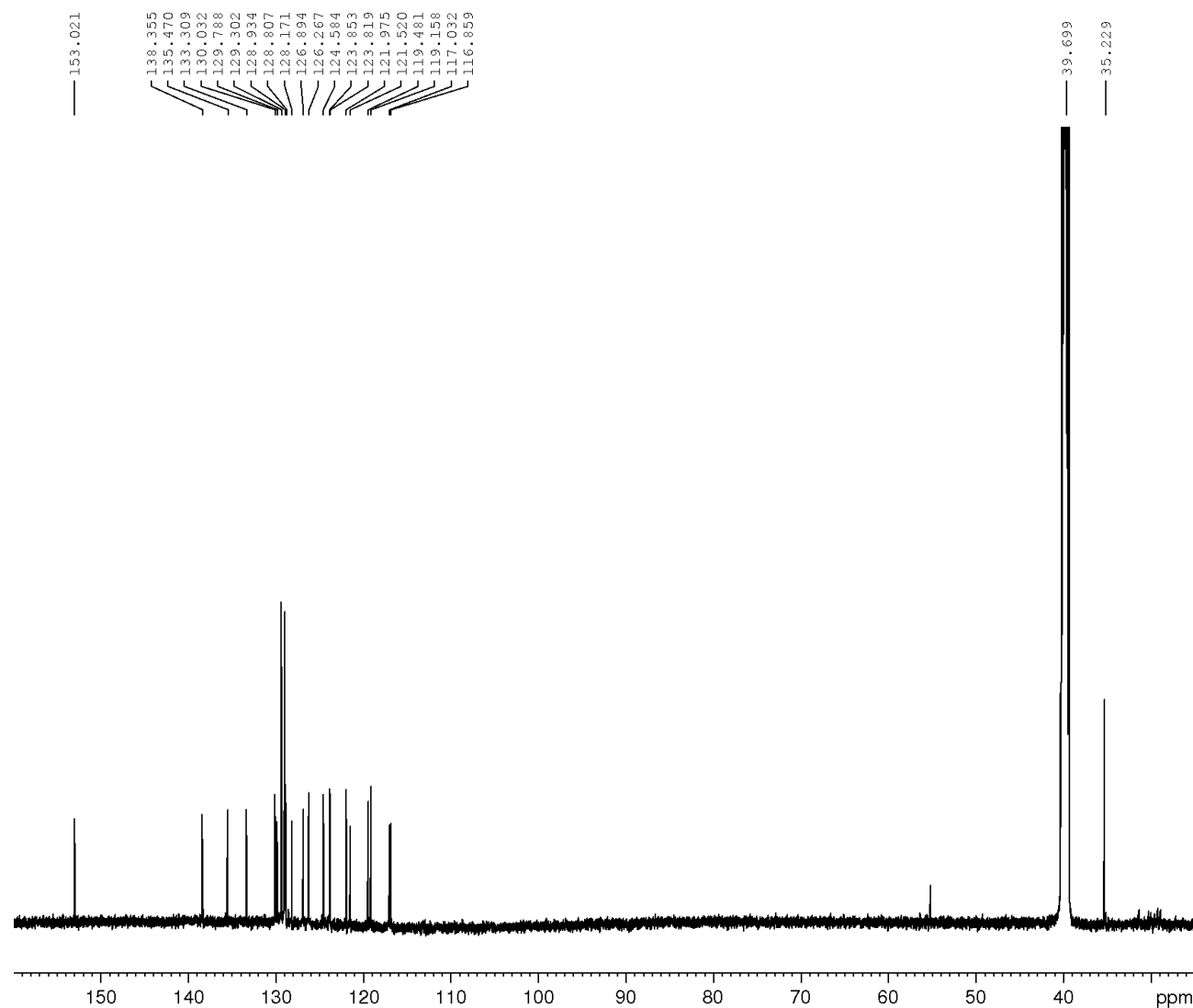
Current Data Parameters
NAME 143947
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241129
Time 15.43 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 196.07
DW 41.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.0037050 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W

F2 - Processing parameters
SI 65536
SF 600.0000020 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹³C NMR spectrum of **10b**



Standard 13C
143947
PGY0823_1A
Pusztai Gyongyver
2024.11.29. (KP)

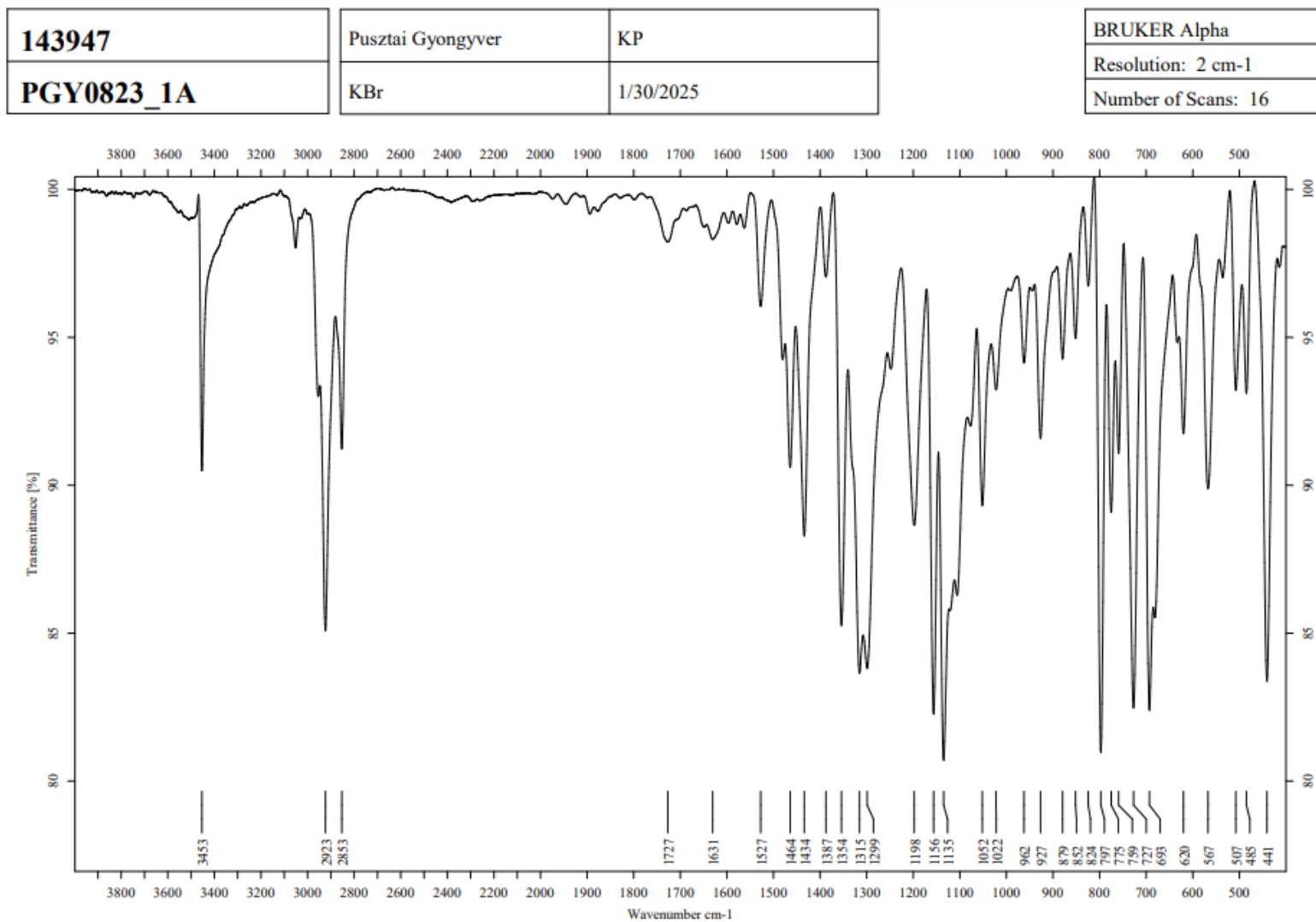
Current Data Parameters
NAME 143947
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20241129
Time 17.27 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 196.07
DW 13.800 usec
DE 18.00 usec
TE 295.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.8852070 MHz
NUC1 13C
P1 9.90 usec
PLW1 71.00000000 W
SFO2 600.0024000 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 32.90000153 W
PLW12 0.70370001 W
PLW13 0.35339001 W

F2 - Processing parameters
SI 131072
SF 150.8701607 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



IR spectrum of **10b**



HRMS spectrum of **10b**

Spectrum Plot Report



Name	PGY0823_1A, Pusztai Gyongyver	Rack Pos.	Instrument	7250A with DIP	Operator	MM
Inj. Vol. (ul)	0.5	Plate Pos.	IRM Status	Success		
Data File	143947_qtof_dip.D	Method (Acq)	DIP_70eV.M	Comment	Acq. Time (Local)	12/3/2024 9:53:56 AM (UTC+01:00)

