



Supporting Information

for

Synthesis and cytotoxicity studies of novel N-arylbenzo[h]quinazolin-2-amines

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**Table S1: Cytotoxicity studies (single dose at 25 μ M)
of *N*-arylbenzo[*h*]quinazolin-2-amines 4a–s**

N°	HuH7	CaCo-2	MDA231	HCT116	PC3	MDA468	MCF7
DMSO	109	78	97	88	86	92	97
ROSCO	30	11	18	8	19	9	22
DOXO	59	59	31	14	42	24	38
TAXOL	43	36	32	7	30	18	27
4a	60	33	61	48	58	56	59
4b	69	56	86	79	72	93	70
4c	68	50	81	52	60	65	50
4d	85	63	67	54	65	72	61
4e	55	59	40	8	21	46	82
4f	59	59	77	29	54	73	78
4g	79	81	87	72	82	90	83
4h	81	48	83	82	74	94	83
4i	60	34	49	11	36	59	59
4j	92	77	91	81	78	95	81
4k	76	61	91	83	73	93	56
4l	71	38	67	56	59	78	68
4m	96	75	83	68	74	88	88
4n	79	72	91	82	82	85	97
4o	62	46	67	27	38	47	85
4p	80	54	68	17	59	72	91
4q	49	35	41	13	24	38	73
4r	80	76	101	100	89	96	85
4s	77	65	78	63	50	78	54

Effects of quinazolines **4** on seven representative tumor cell lines. The toxicity is expressed as the percentage of cell survival (from 100 % to 0 %) over DMSO control after 48 h exposure (mean of triplicates). Roscovitine (ROSCO) at 25 μ M, Doxorubicine (DOXO) and Taxol (TAXOL) both at 0.025 μ M were used as reference compounds. Effect of the solvent (DMSO) was studied at 0.25%.

Spectral and analytical data for compounds 4b–s.

Compound 4b: *N*-(*o*-tolyl)benzo[*h*]quinazolin-2-amine

65% Yield (Light brown solid) **4b**: $^1\text{H NMR}$ (400 MHz, DMSO- d_6 , δ ppm): 9.21 (br s, 1H, NH), 9.13 (s, 1H), 8.78 (d, $J = 8.4$ Hz, 1H), 7.97 (d, $J = 7.6$ Hz, 1H), 7.82-7.72 (m, 3H), 7.69-7.65 (m, 2H), 7.34-7.26 (m, 2H), 7.13-7.10 (m, 1H), 2.31 (s, 3H). $^{13}\text{C NMR}$ (75 MHz, DMSO- d_6 , δ ppm): 161.3, 159.1, 151.4, 138.5, 136.1, 132.3, 130.8, 130.3, 129.2, 128.5, 127.1, 126.4, 124.8, 124.7, 124.4 (2 x C), 123.8, 117.4, 18.7. FTIR (KBr 1%, cm^{-1}): $\tilde{\nu} = 3225, 3025, 2962, 2922, 1611, 1584, 1530, 1488, 1450, 1389, 826, 799, 763, 747, 724$. HRMS m/z (ESI): calcd for $\text{C}_{19}\text{H}_{16}\text{N}_3$ ($M + \text{H}$) $^+$ 286.1338, found 286.1342 (1 ppm). Mp: 126-128 °C.

Compound 4c: *N*-(*m*-tolyl)benzo[*h*]quinazolin-2-amine

66% Yield (White solid) **4c**: $^1\text{H NMR}$ (400 MHz, DMSO- d_6 , δ ppm): 9.96 (br s, 1H, NH), 9.29 (s, 1H), 8.99 (dd, $J = 7.6, 2.0$ Hz, 1H), 8.02 (dd, $J = 6.8, 2.0$ Hz, 1H), 7.90-7.79 (m, 5H), 7.78 (d, $J = 5.6$ Hz, 1H), 7.29 (t, $J = 7.6$ Hz, 1H), 6.85 (t, $J = 7.6$ Hz, 1H), 2.38 (s, 3H). $^{13}\text{C NMR}$ (75 MHz, DMSO- d_6 , δ ppm): 161.2, 158.1, 151.2, 141.0, 138.1, 136.1, 130.4, 129.2, 129.0, 128.6, 127.4, 124.5, 124.4, 124.3, 122.8, 119.9, 117.6, 116.5, 22.0. FTIR (KBr 1%, cm^{-1}): $\tilde{\nu} = 3281, 3212, 3139, 3111, 3052, 1609, 1585, 1544, 1506, 1452, 1395, 794, 778, 760$. HRMS m/z (ESI): calcd for $\text{C}_{19}\text{H}_{16}\text{N}_3$ ($M + \text{H}$) $^+$ 286.1338, found 286.1343 (2 ppm). Mp: 161-163 °C.

Compound 4d: *N*-(*p*-tolyl)benzo[*h*]quinazolin-2-amine

52% Yield (Off white solid) **4d**: $^1\text{H NMR}$ (400 MHz, DMSO- d_6 , δ ppm): 9.90 (br s, 1H, NH), 9.26 (s, 1H), 8.98 (dd, $J = 7.2, 1.6$ Hz, 1H), 8.00 (dd, $J = 8.8, 1.2$ Hz, 1H), 7.92 (d, $J = 8.4$ Hz, 2H), 7.83-7.75 (m, 4H), 7.22 (d, $J = 8.4$ Hz, 2H), 2.31 (s, 3H). $^{13}\text{C NMR}$ (75 MHz, DMSO- d_6 , δ ppm): 161.2, 158.2, 151.2, 138.5, 136.1, 130.9, 130.4, 129.5, 129.2, 128.6, 127.3, 124.5, 124.4, 124.1, 119.4, 117.5, 20.9. FTIR (KBr 1%, cm^{-1}): $\tilde{\nu} = 3450$ (Br), 3115, 3050, 2256, 2130, 1650, 1618, 1607, 1593, 1547, 1511, 1450, 1412, 1391, 1049, 1021, 994, 822, 801, 763. HRMS m/z (ESI): calcd for $\text{C}_{19}\text{H}_{16}\text{N}_3$ ($M + \text{H}$) $^+$ 286.1338, found 286.1339 (0 ppm). Mp: 137-139 °C.

SI Compound 4e: *N*-(2-methoxyphenyl)benzo[*h*]quinazolin-2-amine

65% Yield (Pale yellow solid) **4e**: $^1\text{H NMR}$ (400 MHz, DMSO- d_6 , δ ppm): 9.28 (br s, 1H, NH), 8.98 (dd, $J = 7.2, 0.8$ Hz, 1H), 8.60 (dd, $J = 7.6, 2.0$ Hz, 1H), 8.40 (s, 1H), 8.02 (dd, $J = 8.8, 1.2$ Hz, 1H), 7.84-7.73 (m, 4H), 7.14-7.08 (m, 3H), 3.91 (s, 3H). $^{13}\text{C NMR}$ (75 MHz, DMSO- d_6 , δ ppm): 161.3, 157.9, 151.3, 149.4, 136.1, 130.5, 129.1, 129.1, 128.6, 127.4, 124.5, 124.3, 123.2, 121.1, 120.0, 117.8, 111.4, 56.3. FTIR (KBr 1%, cm^{-1}): $\tilde{\nu} = 3430, 3400, 3048, 2972, 2944, 2841, 1584, 1531, 1482, 1453, 1427, 1383, 1245, 1020, 799, 760, 734$. HRMS m/z (ESI): calcd for $\text{C}_{19}\text{H}_{16}\text{N}_3\text{O}$ ($M + \text{H}$) $^+$ 302.1287, found 302.1291 (1 ppm). Mp: 138-140 °C.

Compound 4f: *N*-(3-methoxyphenyl)benzo[*h*]quinazolin-2-amine

60% Yield (Yellow solid) **4f**: $^1\text{H NMR}$ (400 MHz, DMSO- d_6 , δ ppm): 10.02 (br s, 1H, NH), 9.30 (s, 1H), 9.02 (d, $J = 7.6$ Hz, 1H), 8.03 (d, $J = 7.6$ Hz, 1H), 7.87 (s, 1H), 7.84-7.73 (m, 4H), 7.57 (d, $J = 8.0$ Hz, 1H), 7.30 (t, $J = 8.4$ Hz, 1H), 6.62 (dd, $J = 8.0, 2.0$ Hz, 1H), 3.85 (s, 3H). $^{13}\text{C NMR}$ (75 MHz, DMSO- d_6 , δ ppm): δ 161.2, 160.1, 158.0, 151.1, 142.3, 136.1, 130.5, 129.8, 129.2, 128.7, 127.3, 124.4, 124.4, 117.7, 111.7, 107.6, 104.9, 55.5. FTIR (KBr 1%, cm^{-1}): $\tilde{\nu} = 3267, 3122, 3097, 3046, 2991,$

2962, 2928, 2833, 1610, 1585, 1568, 1534, 1511, 1461, 1431, 1389, 1286, 1261, 1155, 861, 802, 764, 722. **HRMS m/z (ESI)**: calcd for C₁₉ H₁₆ N₃ O (M + H)⁺ 302.1287, found 302.1292 (1 ppm). **Mp**: 171-173°C.

Compound 4g: N-(4-methoxyphenyl)benzo[h]quinazolin-2-amine

58% Yield (Yellow solid) **4g**: ¹H NMR (400 MHz, DMSO-d₆, δ ppm): 9.83 (br s, 1H, NH), 9.24 (s, 1H), 8.98 (dd, J = 8.0, 1.6 Hz, 1H), 8.01 (dd, J = 8.0, 1.2 Hz, 1H), 7.94 (d, J = 8.8 Hz, 2H), 7.82-7.74 (m, 4H), 7.69 (d, J = 8.4 Hz, 1H), 7.00 (d, J = 7.2 Hz, 1H), 3.77 (s, 3H). ¹³C NMR (101 MHz, DMSO-d₆, δ ppm): 161.2, 158.3, 154.8, 151.3, 136.2, 134.2, 130.4, 129.2, 128.6, 127.2, 124.6, 124.4, 123.9, 120.9, 117.4, 114.4, 55.7. FTIR (KBr 1%, cm⁻¹): $\tilde{\nu}$ = 3426, 3248, 3046, 2964, 2920, 1610, 1588, 1544, 1504, 1452, 1414, 1389, 1256, 1231, 1099, 1026, 799, 766. **HRMS m/z (ESI)**: calcd for C₁₉ H₁₆ N₃ O (M + H)⁺ 302.1287, found 302.1290 (1 ppm). **Mp**: 186-188°C.

Compound 4h: N-(2-fluorophenyl)benzo[h]quinazolin-2-amine

66% Yield (Off white solid) **4h**: ¹H NMR (400 MHz, DMSO-d₆, δ ppm): 9.44 (br s, 1H, NH), 9.27 (s, 1H), 8.87 (d, J = 8.0 Hz, 1H), 8.11 (t, J = 6.8 Hz, 1H), 8.00 (d, J = 8.0 Hz, 1H), 7.81-7.70 (m, 4H), 7.34-7.27 (m, 2H), 7.22-7.18 (m, 1H). ¹³C NMR (101 MHz, DMSO-d₆, δ ppm): 161.3, 158.4, 155.3 (d, J_{CF} = 246.5 Hz), 151.3, 136.1, 130.5, 129.11, 128.5, 128.1 (d, J_{CF} = 11.3 Hz), 127.3, 125.1, 125.02 (d, J_{CF} = 5.6 Hz), 124.7 (d, J_{CF} = 3.8 Hz), 124.4 (d, J_{CF} = 3.1 Hz), 124.3, 117.9, 116.0 (d, J_{CF} = 19.7 Hz). ¹⁹F NMR (282 MHz, DMSO, δ ppm): -122.30 – -122.49 (m). FTIR (KBr 1%, cm⁻¹): $\tilde{\nu}$ = 3245, 3051, 3011, 1603, 1590, 1546, 1496, 1451, 1401, 1251, 1197, 804, 765, 739. **HRMS m/z (ESI)**: calcd for C₁₈ H₁₃ N₃ F (M + H)⁺ 290.1088, found 290.1087 (0 ppm). **Mp**: 161-163°C.

SI Compound 4i: N-(3-fluorophenyl)benzo[h]quinazolin-2-amine

64% Yield (Pale yellow solid) **4i**: ¹H NMR (400 MHz, DMSO-d₆, δ ppm): 10.27 (br s, 1H, NH), 9.34 (s, 1H), 8.99 (dd, J = 7.2, 3.2 Hz, 1H), 8.13-8.04 (m, 2H), 7.86-7.77 (m, 5H), 7.43 (q, J = 8.4 Hz, 1H), 6.86-6.84 (m, 1H). ¹³C NMR (75 MHz, DMSO-d₆, δ ppm): 162.9 (d, J_{CF} = 240.4 Hz), 161.3, 157.8, 151.0, 143.0 (d, J_{CF} = 11.5 Hz), 136.1, 130.7, 130.6, 129.1, 128.7, 127.5, 124.8, 124.3, 124.3, 117.9, 115.0 (d, J_{CF} = 2.5 Hz), 108.2 (d, J_{CF} = 21.3 Hz), 105.6 (d, J_{CF} = 26.7 Hz). FTIR (KBr 1%, cm⁻¹): $\tilde{\nu}$ = 3425, 3281, 1593, 1537, 1510, 1491, 1448, 1391, 1256, 1135, 1050, 1020, 1000, 853, 792, 760. ¹⁹F NMR (282 MHz, DMSO-d₆, δ ppm): -112.23 (dt, J = 12.8, 8.0 Hz). **HRMS m/z (ESI)**: calcd for C₁₈ H₁₃ N₃ F (M + H)⁺ 290.1088, found 290.1085 (1 ppm) (0 ppm). **Mp**: 187-189°C.

Compound 4j: N-(4-fluorophenyl)benzo[h]quinazolin-2-amine

65% Yield (Off white solid) **4j**: ¹H NMR (400 MHz, DMSO-d₆, δ ppm): 10.05 (br s, 1H, NH), 9.29 (s, 1H), 8.99 (dd, J = 8.0, 1.6 Hz, 1H), 8.07-8.01 (m, 3H), 7.84-7.72 (m, 4H), 7.24 (t, J = 8.8 Hz, 2H). ¹³C NMR (75 MHz, DMSO-d₆, δ ppm): 161.3, 158.7 (d, J_{CF} = 238.9 Hz), 151.2, 137.4, 137.4, 136.1, 130.5, 129.1, 128.6, 127.3, 124.6, 124.3, 124.3, 120.9 (d, J_{CF} = 7.6 Hz), 117.7, 115.6 (d, J_{CF} = 22.2 Hz). ¹⁹F NMR (282 MHz, DMSO-d₆, δ ppm): -121.55 (tt, J = 5.1, 8.7 Hz). FTIR (KBr 1%, cm⁻¹): $\tilde{\nu}$ = 3420, 3258, 3058, 1606, 1584, 1551, 1510, 1450, 1413, 1390, 1205, 1026, 995, 835, 800, 761. **HRMS m/z (ESI)**: calcd for C₁₈ H₁₃ N₃ F (M + H)⁺ 290.1088, found 290.1089 (0 ppm). **Mp**: 233-235°C.

Compound 4k: N-(2-chlorophenyl)benzo[h]quinazolin-2-amine

65% Yield (Pale yellow solid) **4k**: ¹H NMR (400 MHz, DMSO-d₆, δ ppm): 9.28 (br s, 1H, NH), 9.09 (s, 1H), 8.86 (d, J = 8.0 Hz, 1H), 8.20 (dd, J = 8.4, 1.6 Hz, 1H), 8.01 (d, J = 8.0 Hz, 1H), 7.82-7.70 (m, 4H), 7.57 (dd, J = 8.0, 1.2 Hz, 1H), 7.47 (t, J = 8.4

Hz, 1H), 7.22 (t, J = 8.0 Hz, 1H). **¹³C NMR (101 MHz, DMSO-d₆, δ ppm):** 161.4, 158.3, 151.2, 137.0, 136.1, 130.5, 130.0, 129.1, 128.5, 128.0, 127.3, 126.8, 125.5, 125.2, 124.6, 124.5, 124.3, 118.0. **FTIR (KBr 1%, cm⁻¹):** $\tilde{\nu}$ = 3420, 3103, 3063, 1582, 1523, 1443, 1385, 1296, 1049, 1028, 796, 761, 744. **HRMS m/z (ESI):** calcd for C₁₈ H₁₃ N₃ ³⁵Cl (M + H)⁺ 306.07925, found 306.0792 (0 ppm). **Mp:** 120-122°C.

Compound 4l: N-(3-chlorophenyl)benzo[h]quinazolin-2-amine

67% Yield (Pale yellow solid) **4l:** **¹H NMR (400 MHz, DMSO-d₆, δ ppm):** 10.26 (br s, 1H, NH), 9.35 (s, 1H), 8.99 (dd, J = 7.6, 1.6 Hz, 1H), 8.33 (t, J = 2.0 Hz, 1H), 8.04 (dd, J = 8.8, 1.6 Hz, 1H), 7.98 (dd, J = 8.4, 1.2 Hz, 1H), 7.85-7.75 (m, 4H), 7.44 (t, J = 8.0 Hz, 1H), 7.08 (dd, J = 7.2, 1.6 Hz, 1H). **¹³C NMR (101 MHz, DMSO-d₆, δ ppm):** 161.4, 157.8, 151.0, 142.6, 136.2, 133.5, 130.8, 130.6, 129.1, 128.7, 127.5, 124.8, 124.3, 124.3, 121.5, 118.5, 118.0, 117.5. **FTIR (KBr 1%, cm⁻¹):** $\tilde{\nu}$ = 3290, 3112, 3048, 1584, 1533, 1480, 1446, 1410, 1395, 800, 764. **HRMS m/z (ESI):** calcd for C₁₈ H₁₃ N₃ ³⁵Cl (M + H)⁺ 306.0792, found 306.0792 (0 ppm). **Mp:** 207-209°C.

Compound 4m: N-(4-chlorophenyl)benzo[h]quinazolin-2-amine

51% Yield (Off white solid) **4m:** **¹H NMR (400 MHz, DMSO-d₆, δ ppm):** 10.17 (br s, 1H, NH), 9.31 (s, 1H), 9.01 (d, J = 7.6 Hz, 1H), 8.09 (d, J = 8.8 Hz, 2H), 8.07 (d, J = 3.2 Hz, 1H), 7.85-7.72 (m, 4H), 7.48 (d, J = 3.2 Hz, 2H). **¹³C NMR (101 MHz, DMSO-d₆, δ ppm):** 161.3, 157.9, 151.1, 140.0, 136.1, 130.5, 129.1, 129.0, 128.6, 127.5, 125.5, 124.6, 124.3, 120.7, 119.3, 117.8. **FTIR (KBr 1%, cm⁻¹):** $\tilde{\nu}$ = 3426, 3256, 3099, 3046, 2924, 2851, 1605, 1582, 1544, 1490, 1452, 1400, 801, 755. **HRMS m/z (ESI):** calcd for C₁₈ H₁₃ N₃ ³⁵Cl (M + H)⁺ 306.0792, found 306.0792 (0 ppm). **Mp:** decomposition >200°C.

SI Compound 4n: N-(3,4-difluorophenyl)benzo[h]quinazolin-2-amine

67% Yield (Light brown solid) **4n:** **¹H NMR (400 MHz, DMSO-d₆, δ ppm):** 10.26 (br s, 1H, NH), 9.33 (s, 1H), 8.97 (dd, J = 7.2, 2.0 Hz, 1H), 8.29-8.23 (m, 1H), 8.05 (dd, J = 6.8, 2.0 Hz, 1H), 7.86-7.75 (m, 5H), 7.45 (q, J = 9.6 Hz, 1H). **¹³C NMR (101 MHz, DMSO-d₆, δ ppm):** 161.4, 159.6 (dd, J_{CF} = 13.2 and 242.0 Hz), 144.6 (dd, J_{CF} = 13.1 and 240 Hz), 143.6, 143.43, 138.2 (dd, J_{CF} = 2.9 and 9.6 Hz), 136.1, 130.6, 129.0, 128.7, 127.5, 124.8, 124.3, 124.3, 118.0, 117.8 (d, J_{CF} = 17.7 Hz), 115.3 (dd, J_{CF} = 2.3 and 5.2 Hz), 107.7 (d, J_{CF} = 21.8 Hz). **FTIR (KBr 1%, cm⁻¹):** $\tilde{\nu}$ = 3422, 3283, 1612, 1588, 1544, 1509, 1450, 1387, 1271, 1198, 794, 760. **HRMS m/z (ESI):** calcd for C₁₈ H₁₂ N₃ F₂ (M + H)⁺ 308.09938, found 308.0995 (0 ppm). **Mp:** 217-218°C.

Compound 4o: N-(3,5-dibromophenyl)benzo[h]quinazolin-2-amine

70% Yield (Light brown solid) **4o:** **¹H NMR (400 MHz, DMSO-d₆, δ ppm):** 10.43 (br s, 1H, NH), 9.39 (s, 1H), 8.96 (d, J = 8.0 Hz, 1H), 8.40 (d, J = 2.0 Hz, 2H), 8.07 (d, J = 7.2 Hz, 1H), 8.07 (d, J = 7.6 Hz, 1H), 7.87-7.78 (m, 4H), 7.44 (t, J = 1.6 Hz, 1H). **¹³C NMR (75 MHz, DMSO-d₆, δ ppm):** 161.5, 157.4, 150.8, 143.9, 136.2, 130.7, 129.0, 128.9, 127.5, 126.0, 125.3, 124.3, 124.1, 122.8, 120.2, 118.3. **FTIR (KBr 1%, cm⁻¹):** $\tilde{\nu}$ = 3437, 3290, 2964, 1584, 1528, 1510, 1448, 1402, 1259, 1095, 1021, 862, 796. **HRMS m/z (ESI):** calcd for C₁₈ H₁₂ N₃ ⁷⁹Br₂ (M + H)⁺ 427.9392, found 427.9393 (0 ppm). **Mp:** 234-236°C.

Compound 4p: N-(3-chloro-5-fluorophenyl)benzo[h]quinazolin-2-amine

63% Yield (Off white solid) **4p:** **¹H NMR (400 MHz, DMSO-d₆, δ ppm):** 10.47 (br s, 1H, NH), 9.38 (s, 1H), 8.95 (d, J = 7.2 Hz, 1H), 8.08-8.00 (m, 3H), 7.87-7.80 (m, 4H), 7.03 (dd, J = 6.4, 2.0 Hz, 1H). **¹³C NMR (75 MHz, DMSO-d₆, δ ppm):** 162.8 (d, J_{CF} = 243 Hz), 161.3, 157.43, 150.8, 143.7 (d, J_{CF} = 13 Hz), 136.1, 134.2 (d, J_{CF} = 13.5 Hz), 130.6, 129.0, 128.75, 127.5, 125.2, 124.2, 124.1, 118.2, 114.6 (d, J_{CF} = 2.6 Hz), 108.6 (d, J_{CF} = 25.5 Hz), 104.2 (d, J_{CF} = 26.8 Hz). **FTIR (KBr 1%, cm⁻¹):** $\tilde{\nu}$ = 3283,

3191, 3113, 1584, 1538, 1511, 1458, 1414, 1387, 1141, 801, 763. **¹⁹F NMR (282 MHz, DMSO-d₆, δ ppm):** -110.31 (dd, J_{HF} = 8.7 and 12.3 Hz). **HRMS m/z (ESI):** calcd for C₁₈ H₁₂ N₃ F ³⁵Cl (M + H)⁺ 324.0698, found 324.0696 (1 ppm). **Mp:** 233-235°C.

Compound 4q: N-(3-bromo-5-chlorophenyl)benzo[h]quinazolin-2-amine

65% Yield (Light brown solid) **4q:** **¹H NMR (400 MHz, DMSO-d₆, δ ppm):** 10.44 (br s, 1H, NH), 9.39 (s, 1H), 8.96 (d, J = 7.6 Hz, 1H), 8.37 (t, J = 1.6 Hz, 1H), 8.23 (t, J = 1.6 Hz, 1H), 8.07 (d, J = 7.6 Hz, 1H), 7.87-7.79 (m, 4H), 7.32 (t, J = 1.6 Hz, 1H). **¹³C NMR (75 MHz, DMSO-d₆, δ ppm):** 161.5, 157.4, 150.8, 143.7, 136.2, 134.6, 130.7, 129.0, 128.8, 127.6, 125.3, 124.3, 124.1, 123.4, 122.6, 119.9, 118.3, 117.4. **FTIR (KBr 1%, cm⁻¹):** $\tilde{\nu}$ = 3286, 3107, 3044, 1578, 1530, 1509, 1450, 1406, 1387, 755. **HRMS m/z (ESI):** calcd for C₁₈ H₁₂ N₃ F ³⁵Cl (M + H)⁺ 383.98976, found 383.9895 (1 ppm). **Mp:** 256-258°C.

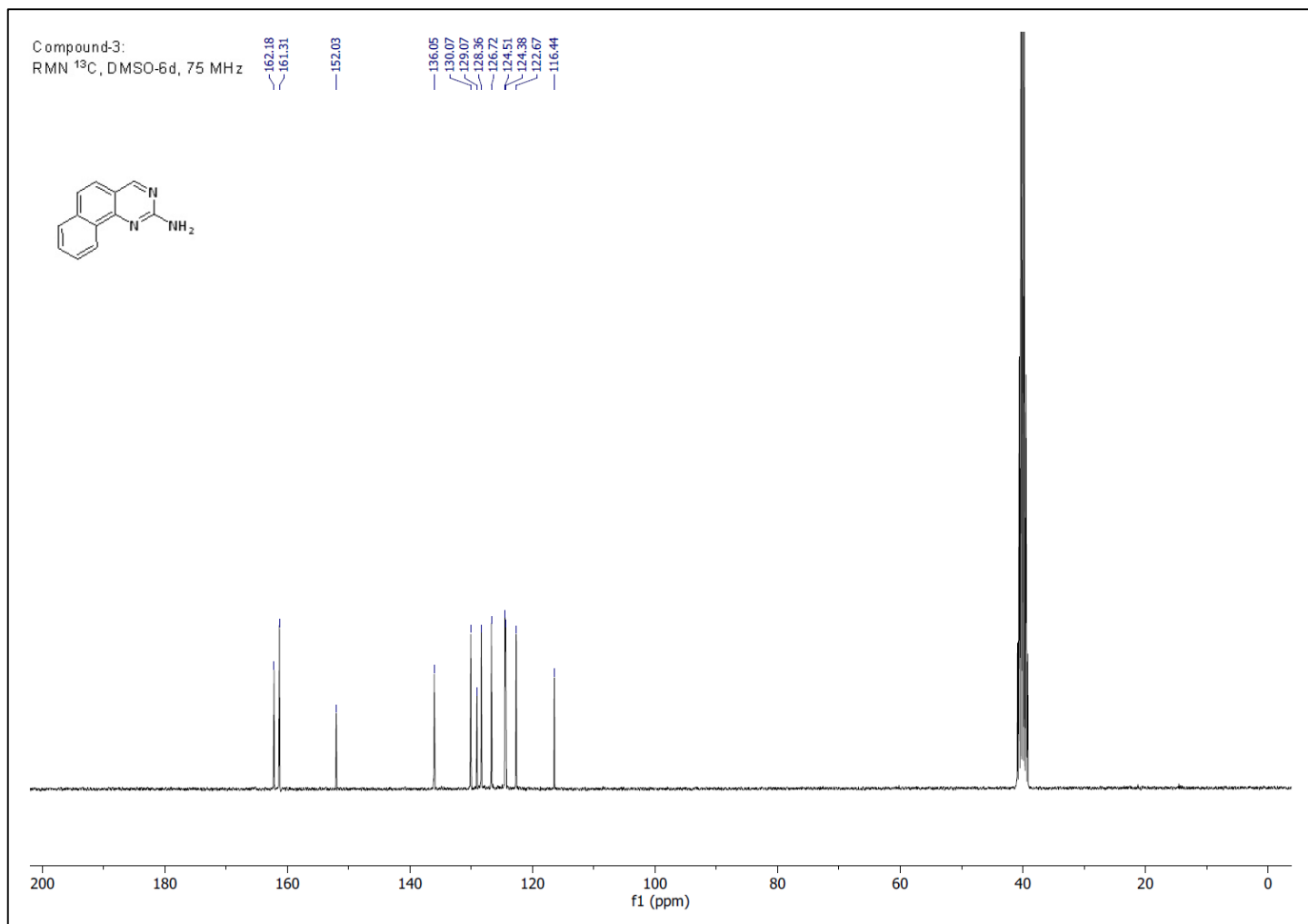
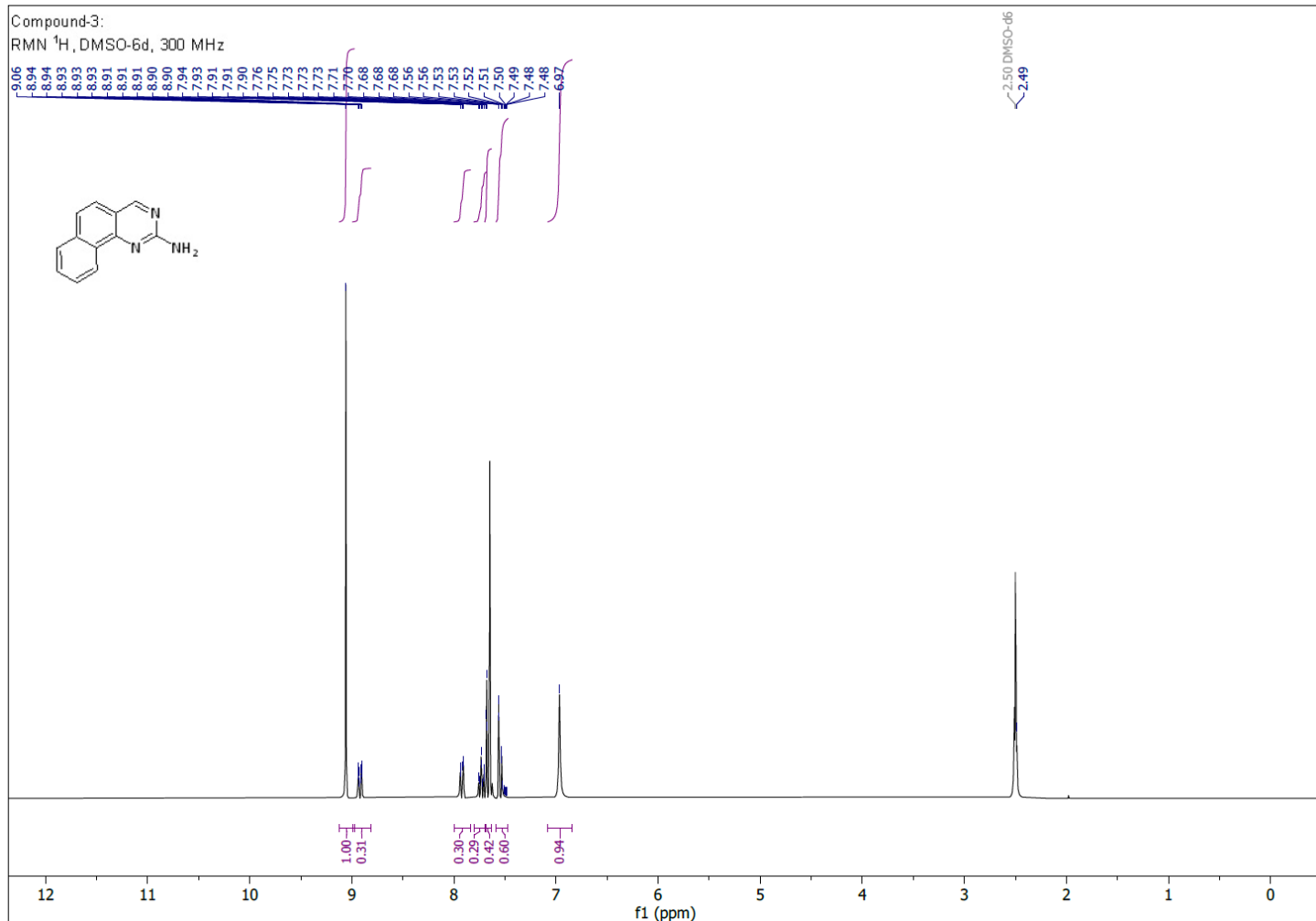
Compound 4r: N-(4-bromo-3-methylphenyl)benzo[h]quinazolin-2-amine

66% Yield (Off white solid) **4r:** **¹H NMR (400 MHz, DMSO-d₆, δ ppm):** 10.11 (br s, 1H, NH), 9.31 (s, 1H), 8.98 (dd, J = 7.2, 1.2 Hz, 1H), 8.06-8.02 (m, 2H), 7.90-7.87 (m, 1H), 7.84-7.74 (m, 4H), 7.59 (d, J = 8.4 Hz, 1H), 2.42 (s, 3H). **¹³C NMR (75 MHz, DMSO-d₆, δ ppm):** 161.2, 157.9, 151.1, 140.6, 137.5, 136.1, 132.5, 130.5, 129.1, 128.6, 124.6, 124.5, 124.3, 121.6, 118.8, 117.8, 115.9, 23.4. **FTIR (KBr 1%, cm⁻¹):** $\tilde{\nu}$ = 3428, 3273, 2254, 2126, 1609, 1584, 1542, 1450, 1510, 1023, 1000, 822, 790, 754. **HRMS m/z (ESI):** calcd for C₁₉ H₁₅ N₃ ⁷⁹Br (M + H)⁺ 364.04438, found 364.0448 (1 ppm). **Mp:** 201-202°C.

Compound 4s: N-(3,4,5-trifluorophenyl)benzo[h]quinazolin-2-amine

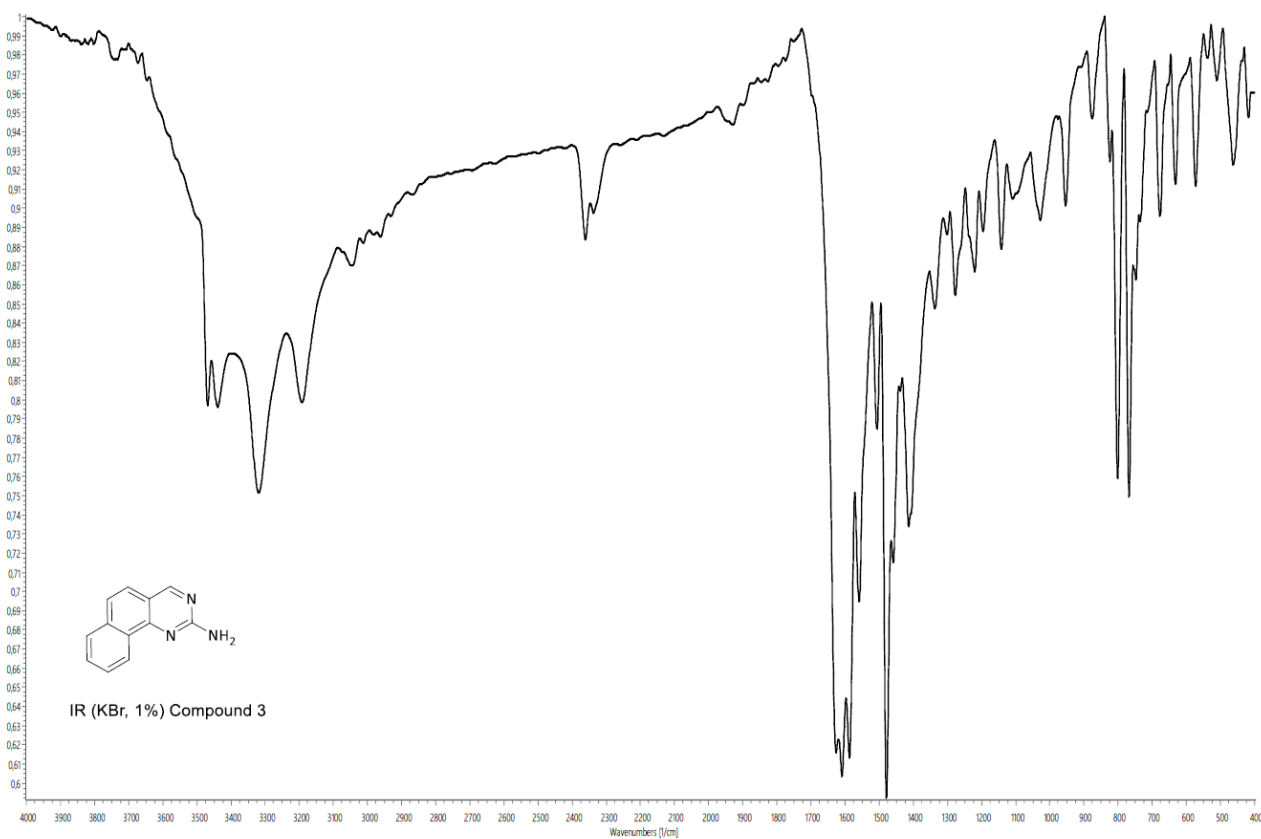
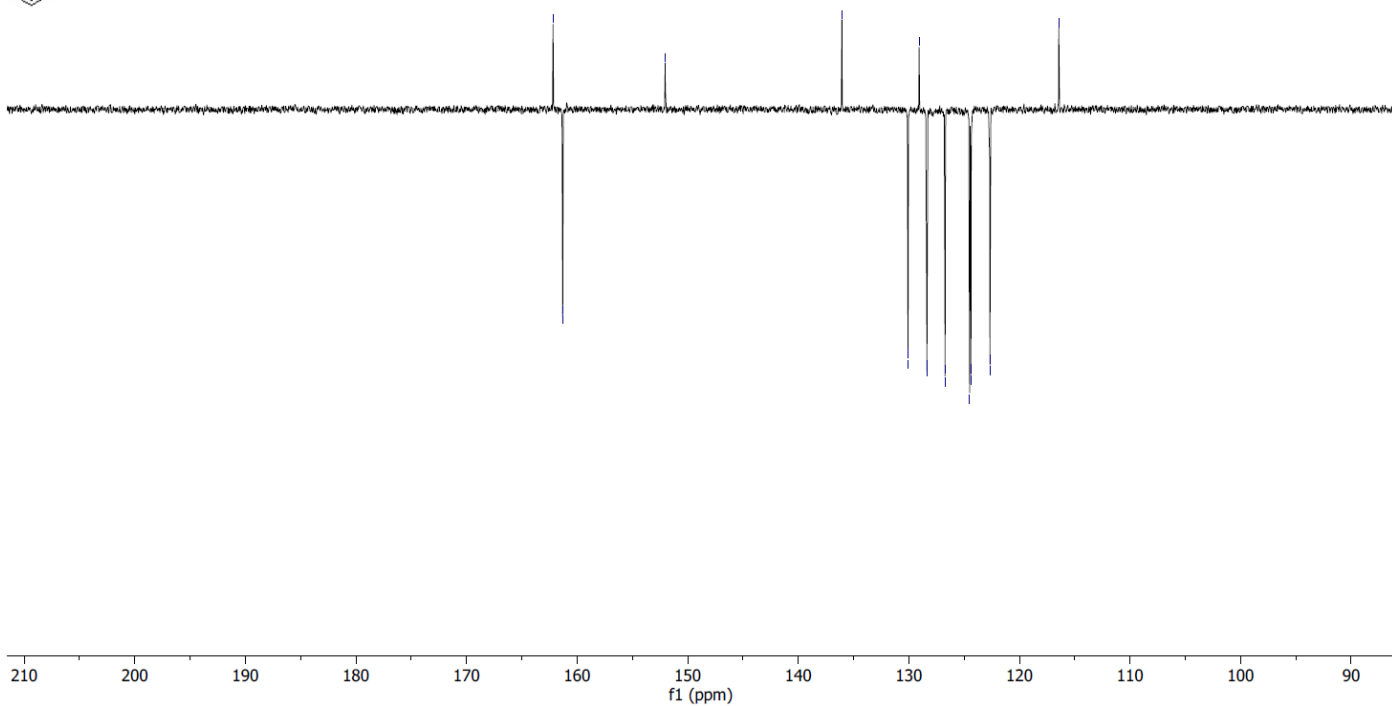
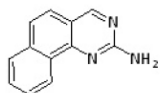
65% Yield (Light brown solid) **4s:** **¹H NMR (400 MHz, DMSO-d₆, δ ppm):** 10.42 (br s, 1H, NH), 9.37 (s, 1H), 8.95-8.93 (m, 1H), 8.07-8.05 (m, 1H), 8.01-7.97 (m, 2H), 7.87-7.80 (m, 4H). **¹³C NMR (75 MHz, DMSO-d₆, δ ppm):** 161.3, 157.3, 150.8, 150.6 (ddd, J_{CF} = 5.8, 10.7 and 242.6 Hz), 136.5 (dtd, J_{CF} = 3.3, J_{FF} = 11.8 and 149.5 Hz), 132.2 (m), 130.6, 129.0, 128.7, 127.5, 125.1, 124.2, 124.1, 118.2, 103.0, 102.6. **¹⁹F NMR (282 MHz, DMSO-d₆, δ ppm):** -130.36 and -130.46 (dd, J_{HF} = 11.0 Hz, J_{FF} = 22.1 Hz), -166.03 (tt, J_{HF} = 6.7 Hz, J_{FF} = 22.1 Hz). **HRMS m/z (ESI):** calcd for C₁₈ H₁₁ N₃ F₃ (M + H)⁺ 326.0899, found 326.0900 (0 ppm). **FTIR (KBr 1%, cm⁻¹):** $\tilde{\nu}$ = 3288, 3111, 3067, 1614, 1586, 1548, 1520, 1440, 1391, 1288, 1223, 1036, 847, 792, 761. **Mp:** 252-254°C.

Spectra: ^1H , ^{13}C , ^{13}C Jmod NMR and FT-IR data of compound 3

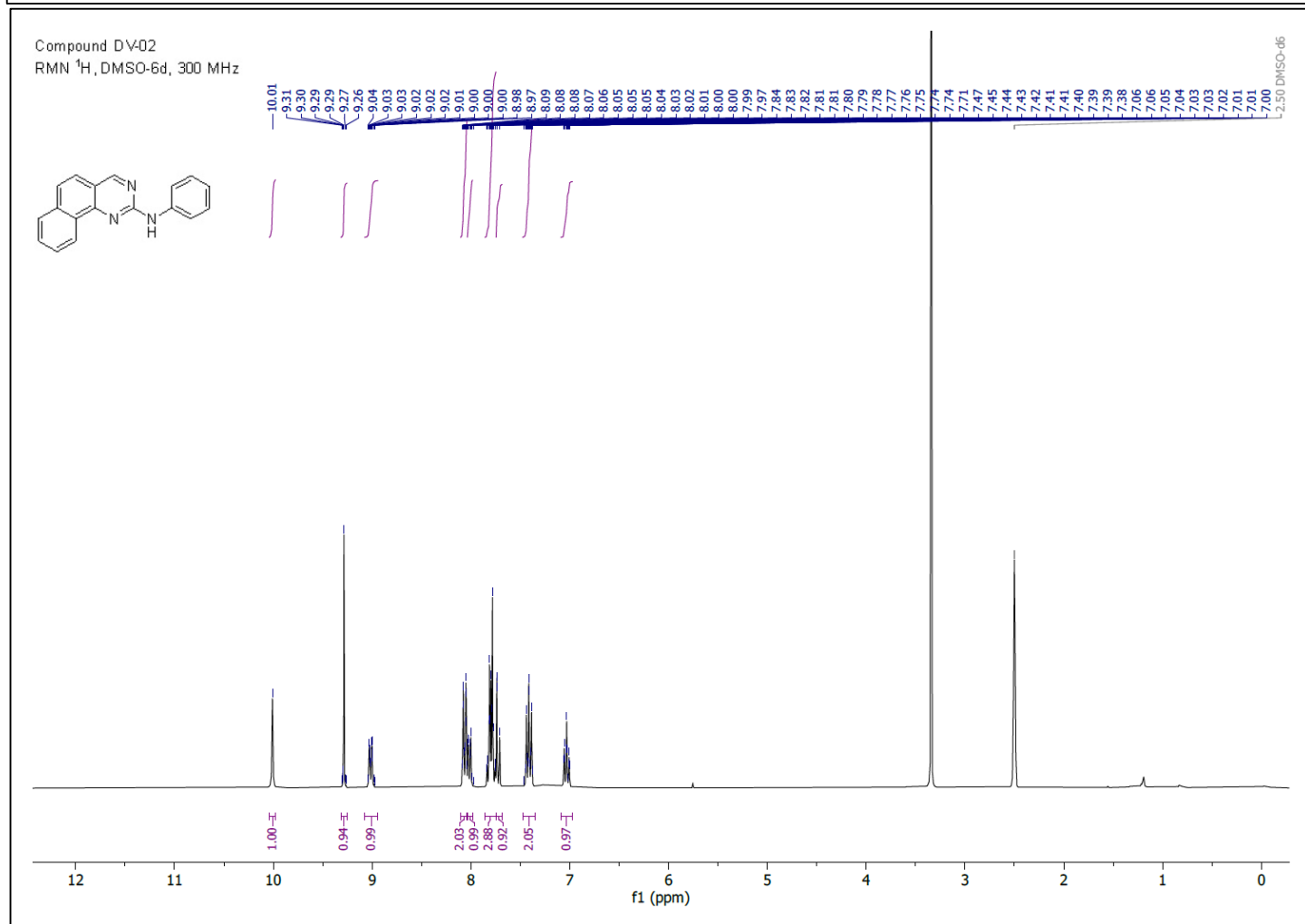
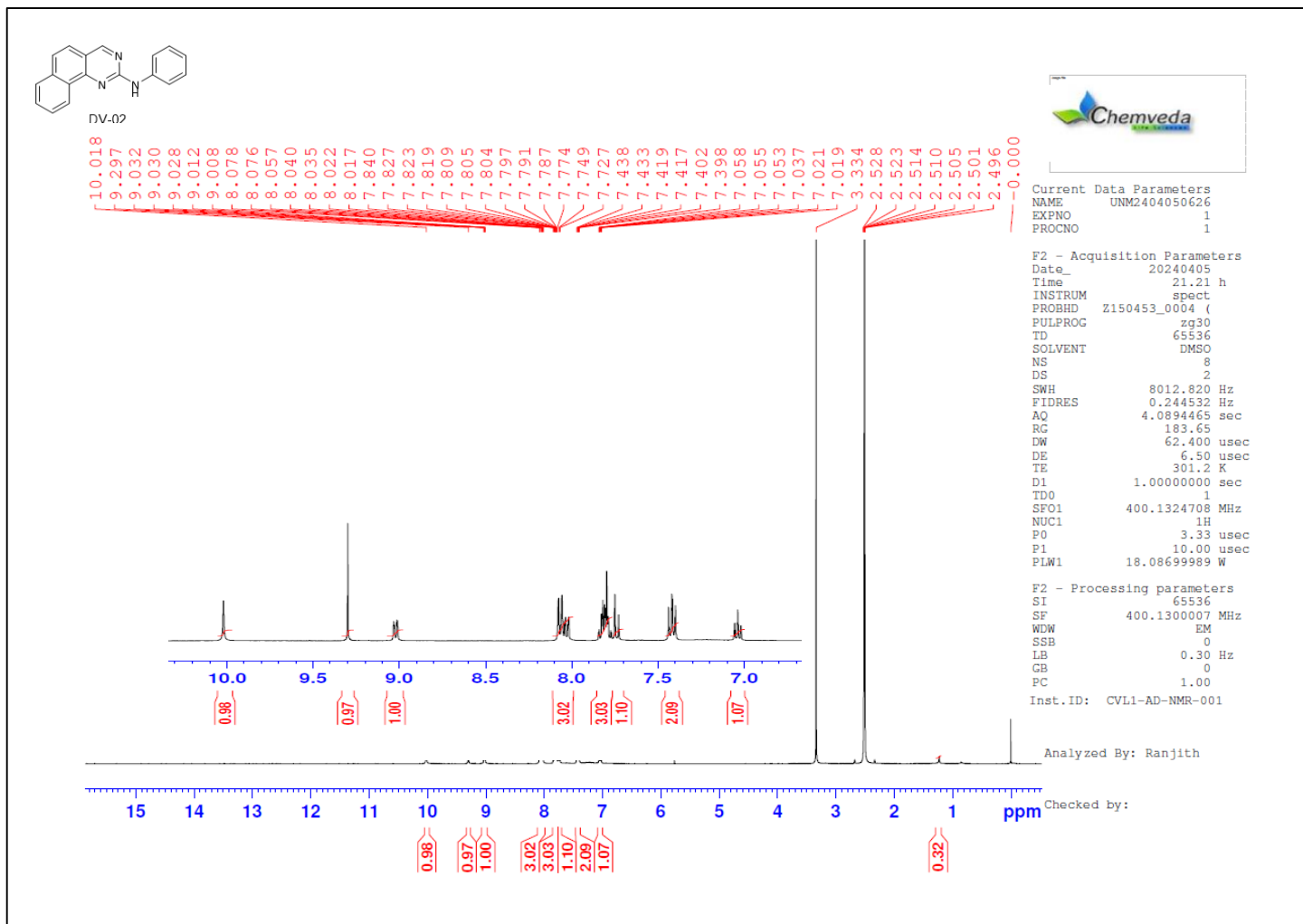


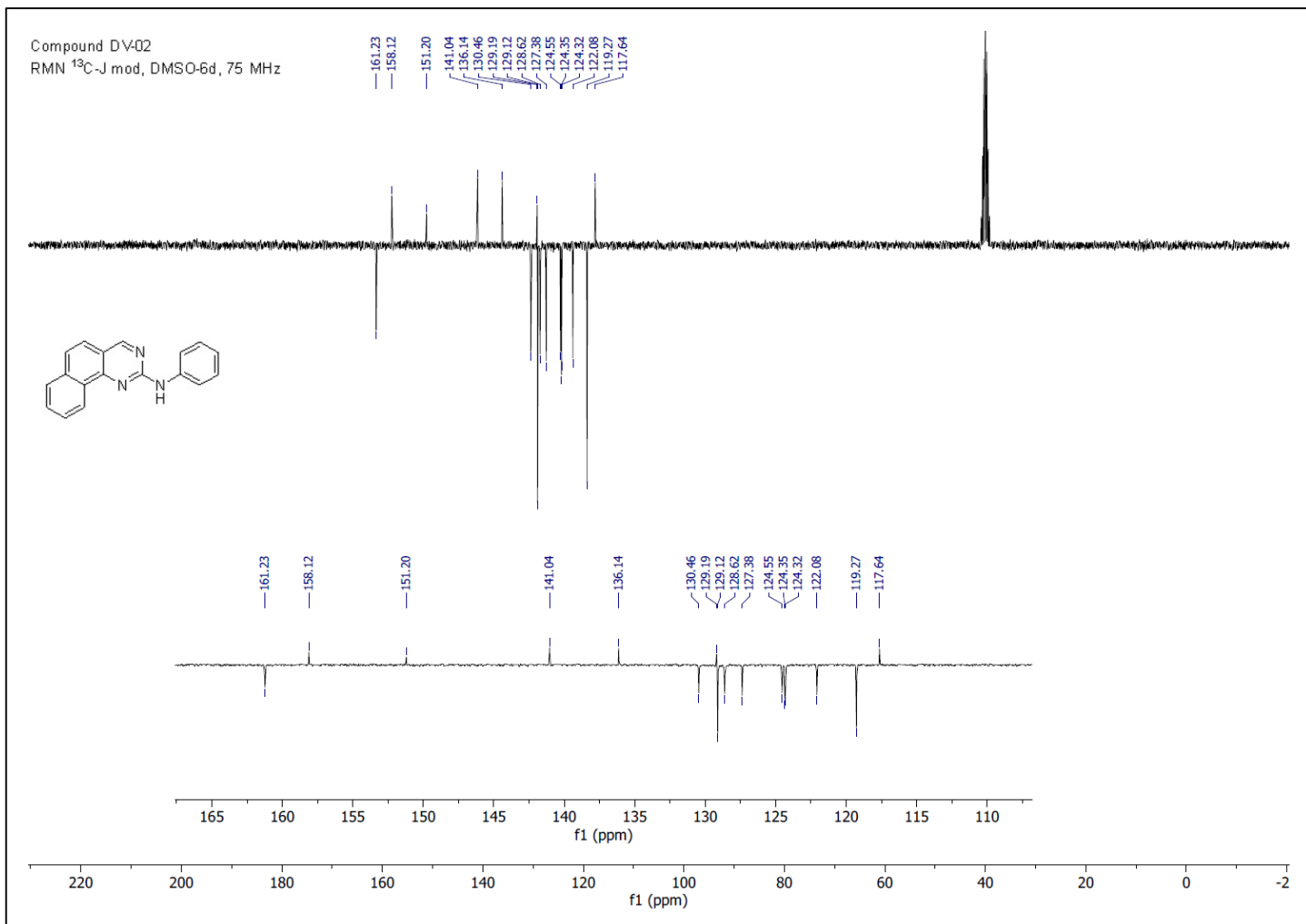
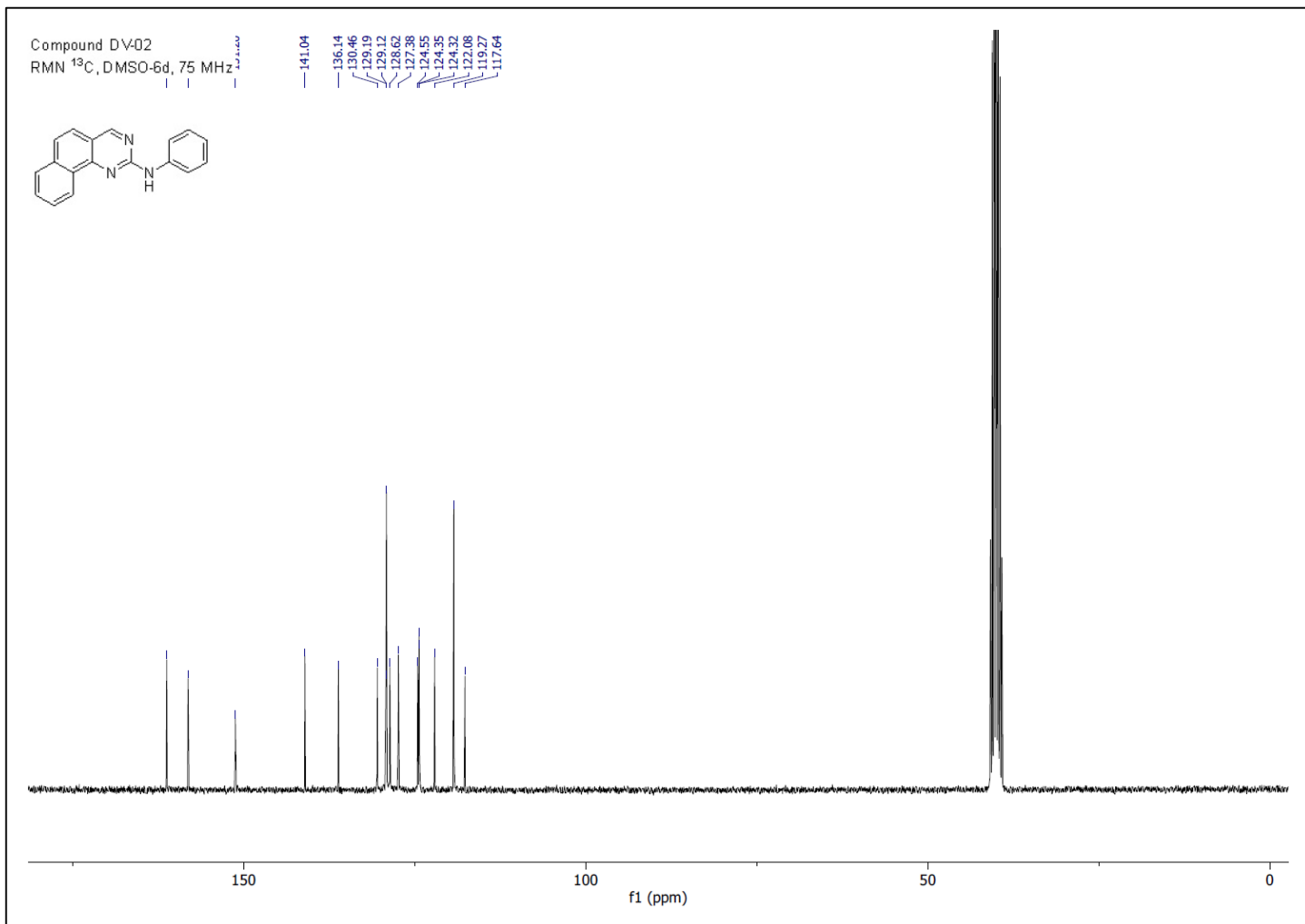
Compound-3:
RMN ^{13}C -J mod, DMSO- d_6 , 75 MHz

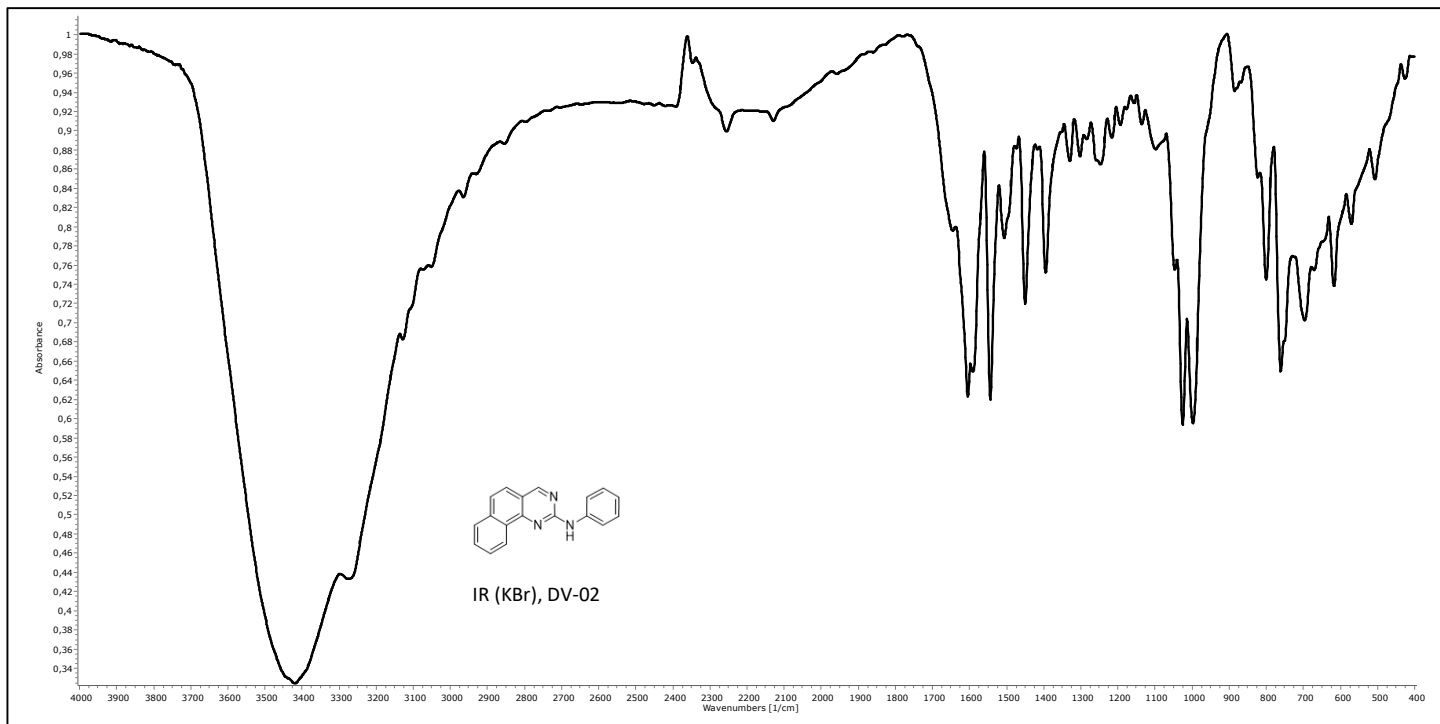
162.18
161.30
161.30
152.03
136.05
130.07
130.07
129.07
128.36
128.36
126.72
126.72
124.51
124.38
124.38
122.67
122.67
116.44



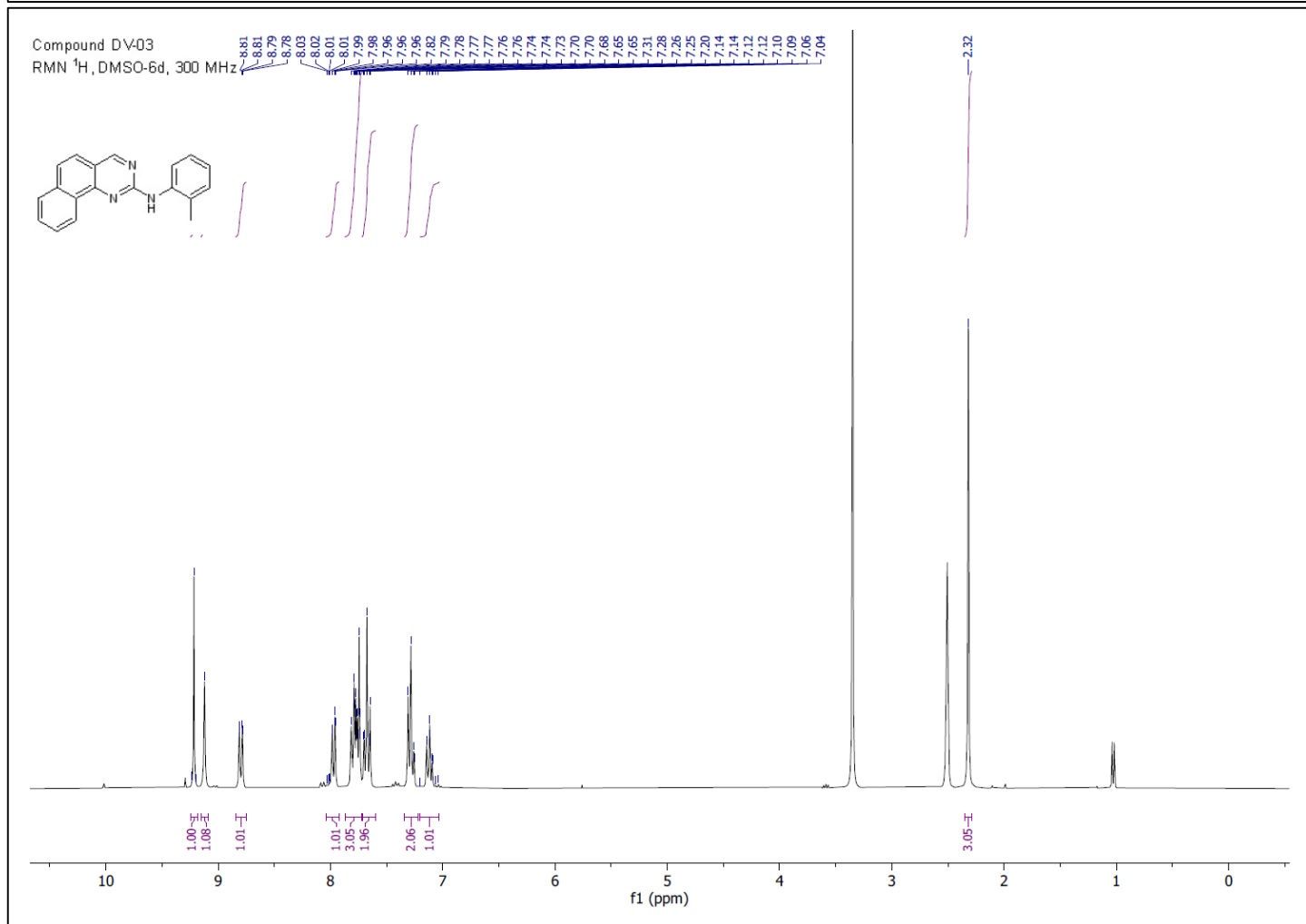
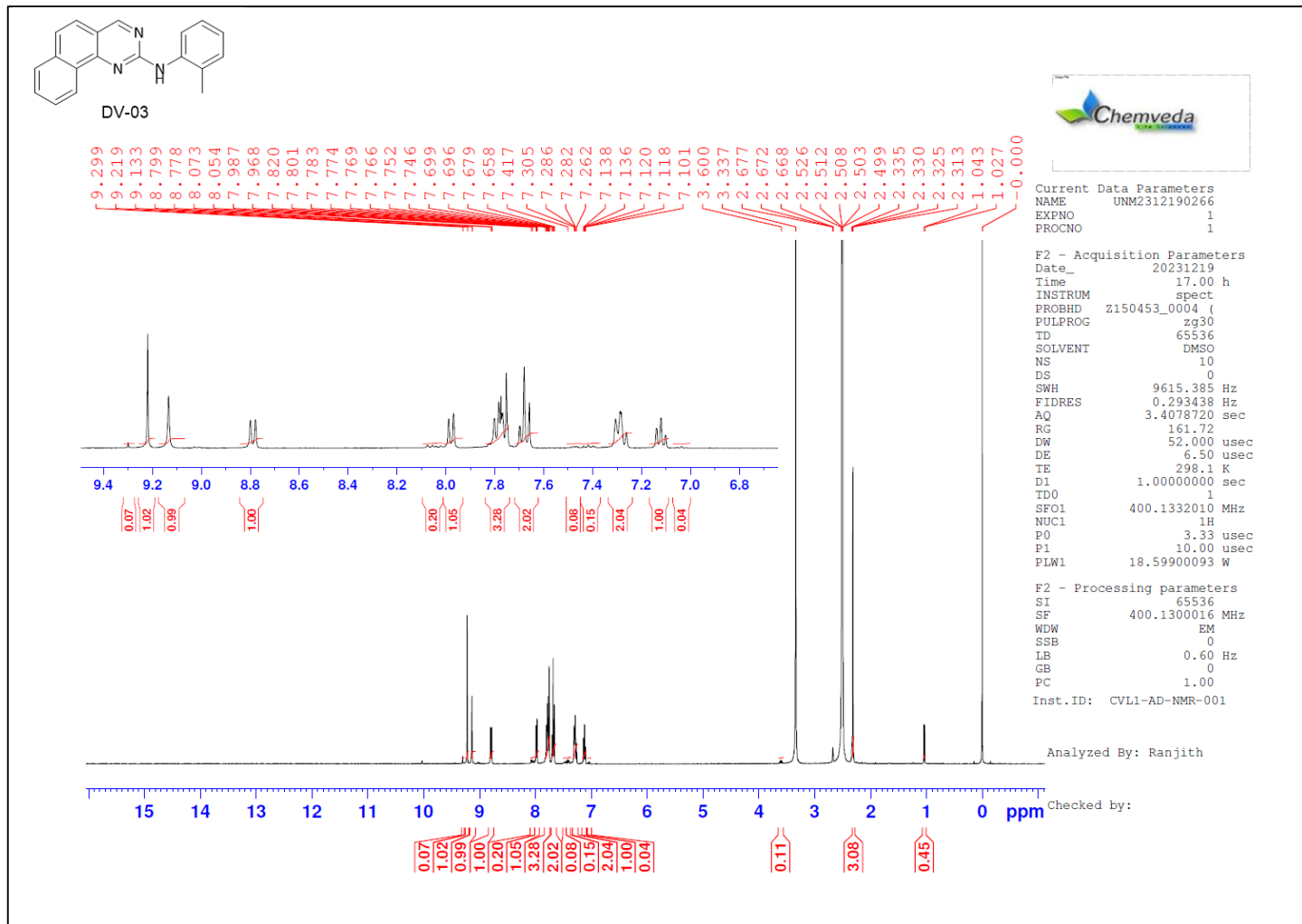
Spectra: ^1H , ^{13}C , ^{13}C Jmod NMR and FT-IR data of compound 4a (DV-02)



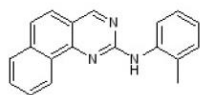




Spectra: ¹H, ¹³C, ¹³C Jmod NMR and FT-IR data of compound 4b (DV-03)

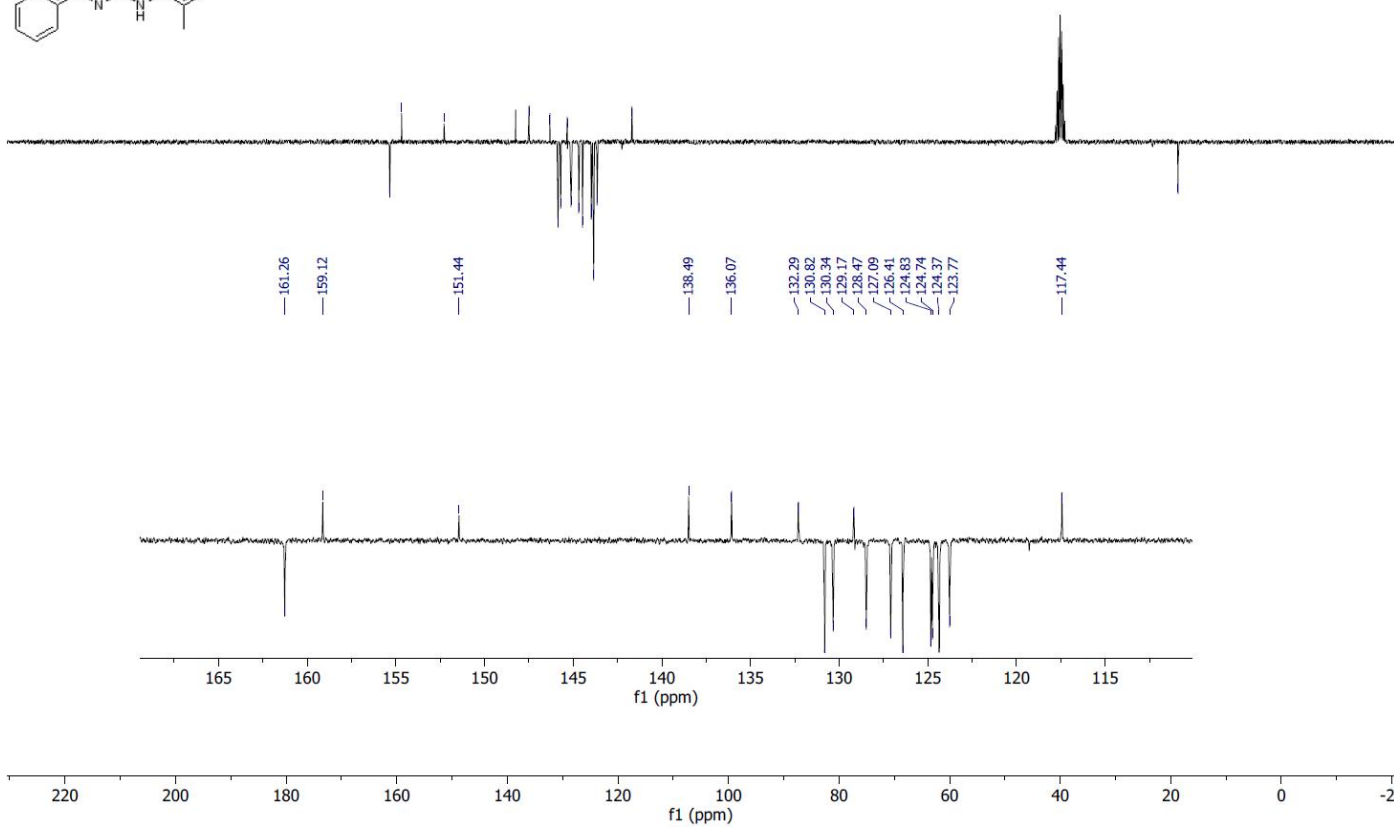


Compound DV-03
RMN ¹³C Jmod, DMSO-6d, 75 MHz

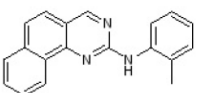


161.26
159.12
151.44
136.07
132.29
130.82
130.34
129.17
128.47
127.09
126.41
124.83
124.74
124.37
123.77
117.44

18.68

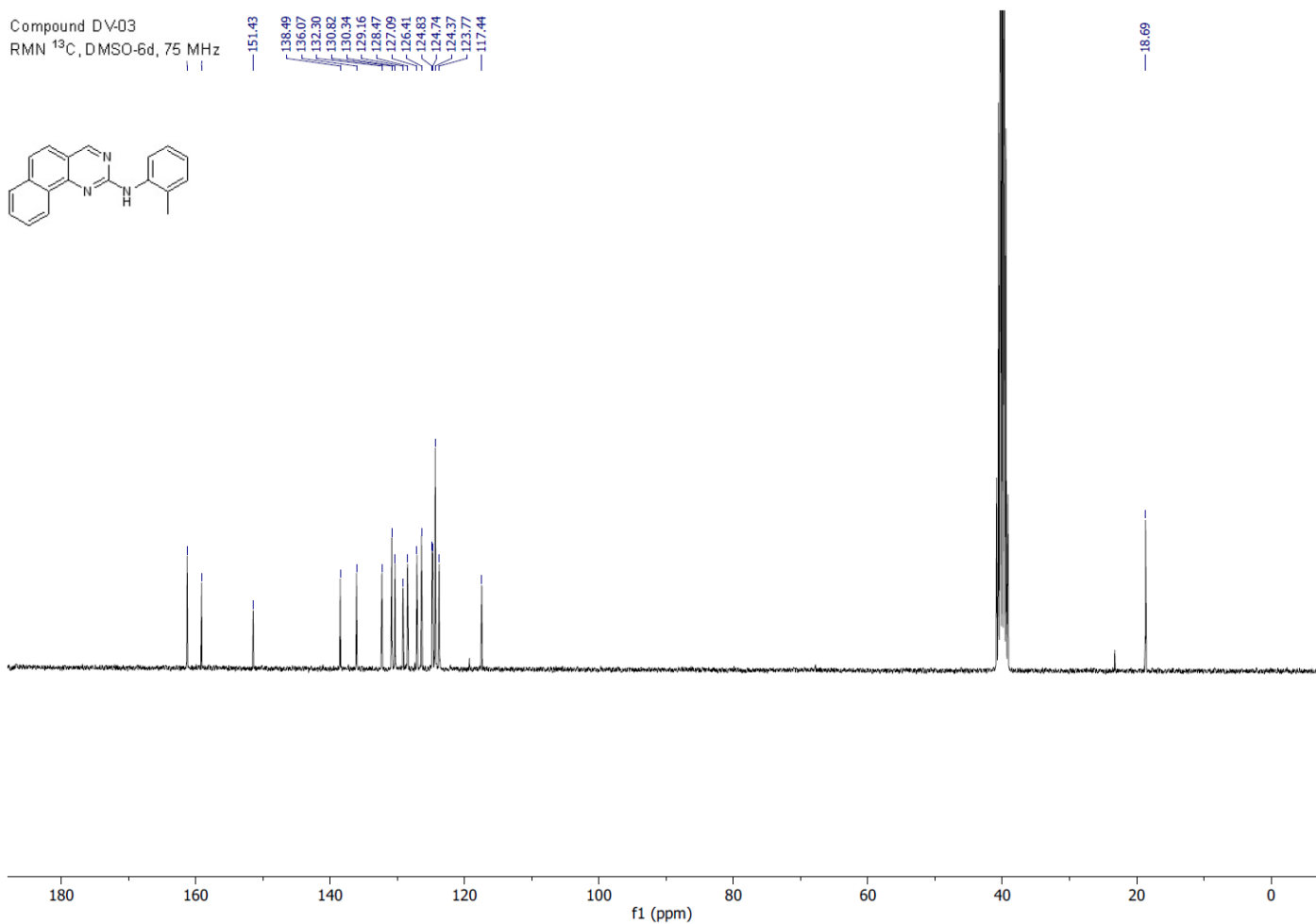


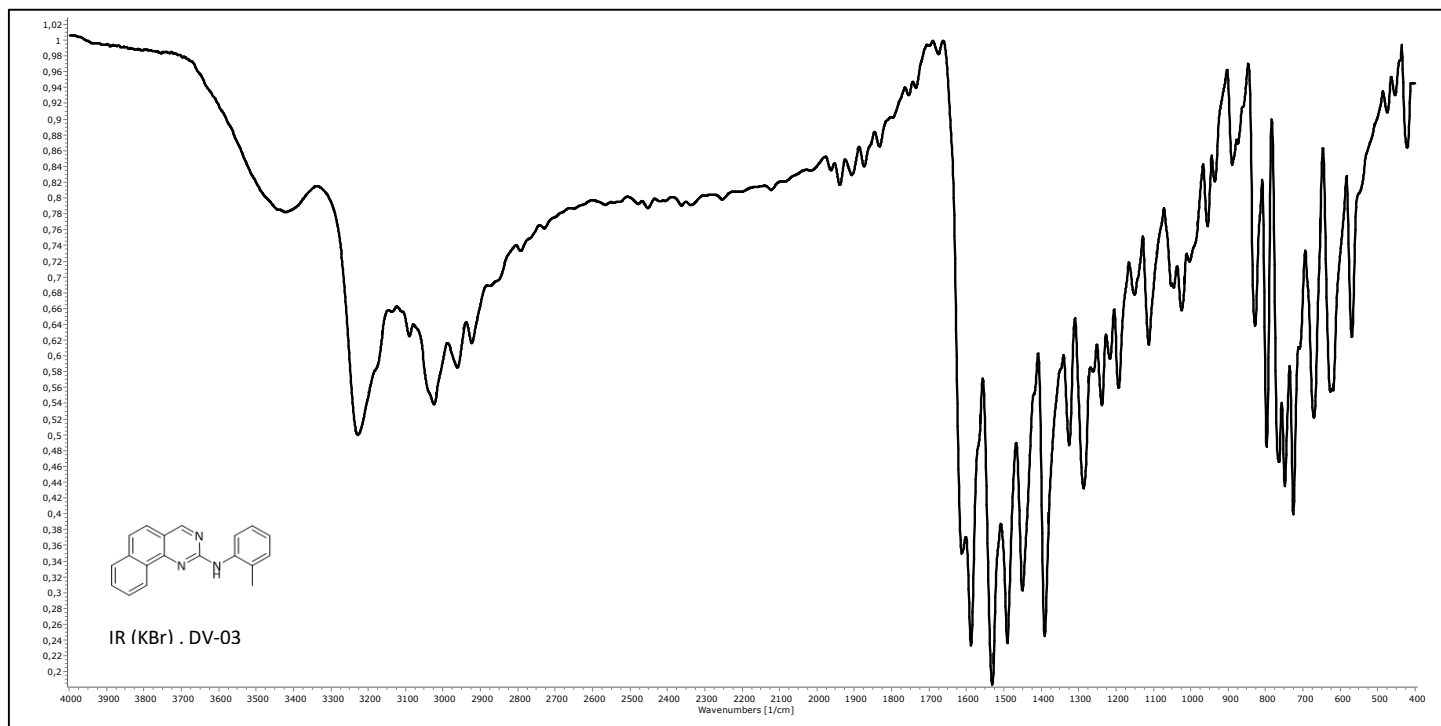
Compound DV-03
RMN ¹³C, DMSO-6d, 75 MHz



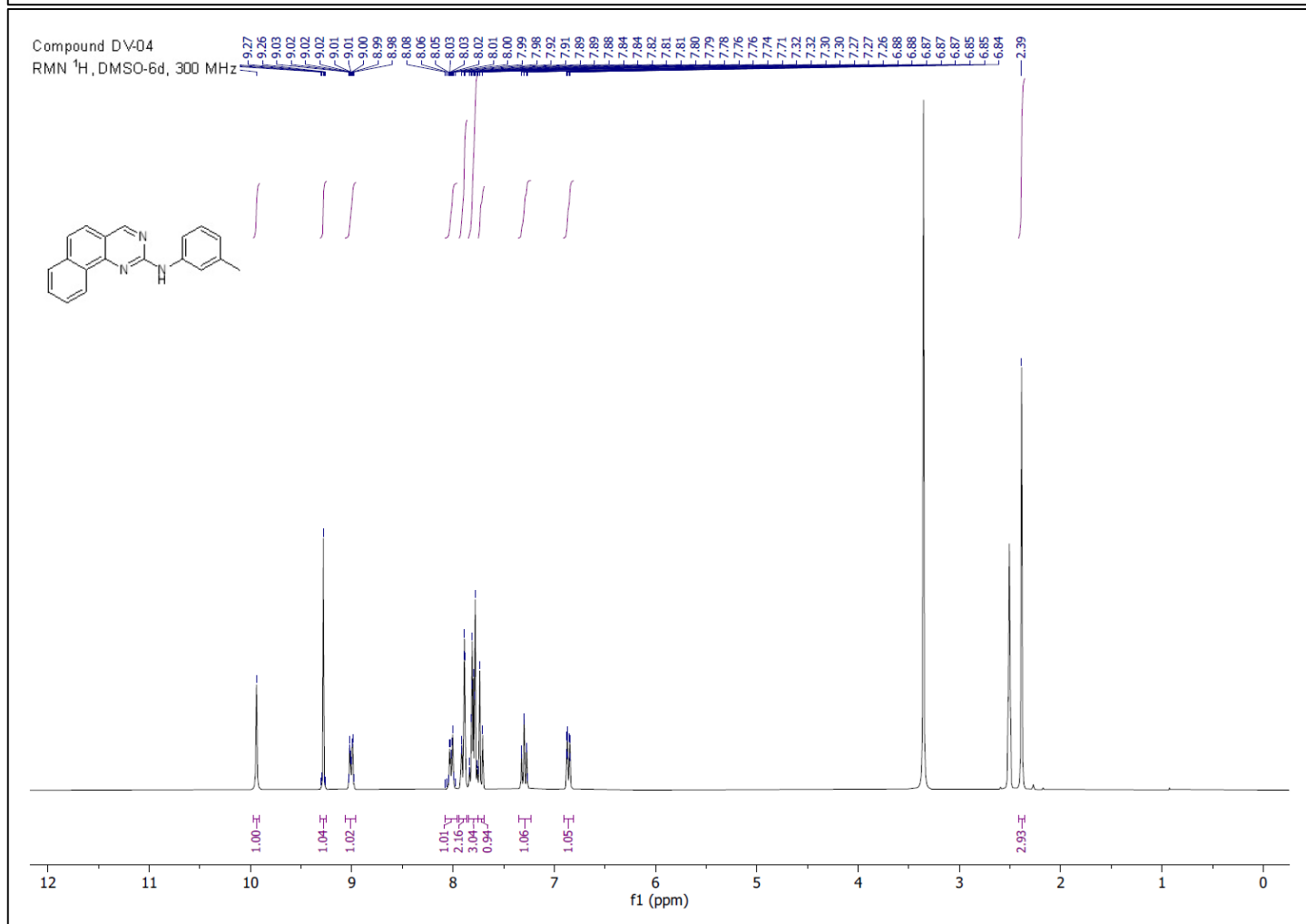
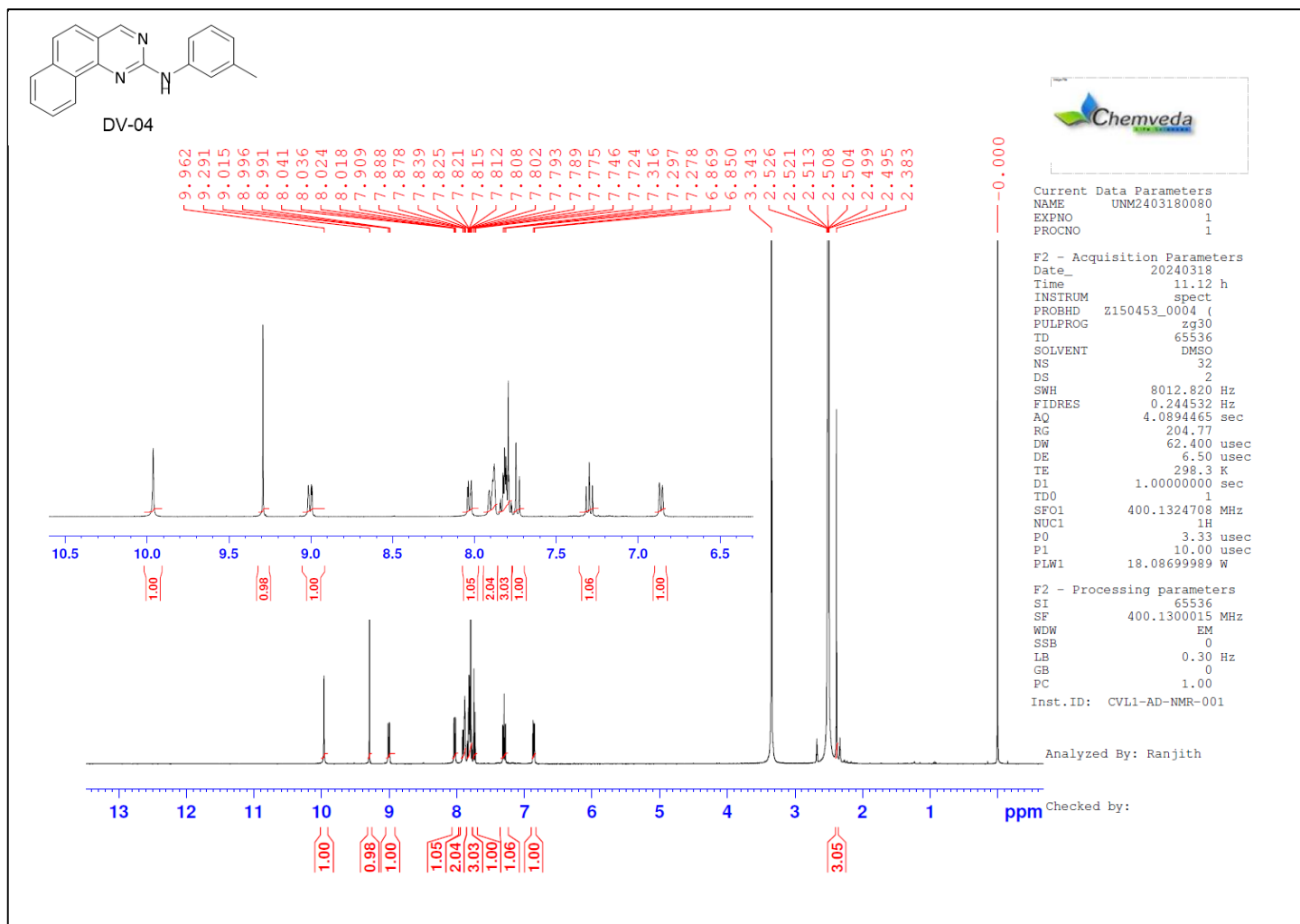
151.43
138.49
136.07
132.30
130.82
130.34
129.16
128.47
127.09
126.41
124.83
124.74
124.37
123.77
117.44

18.69

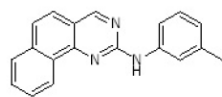




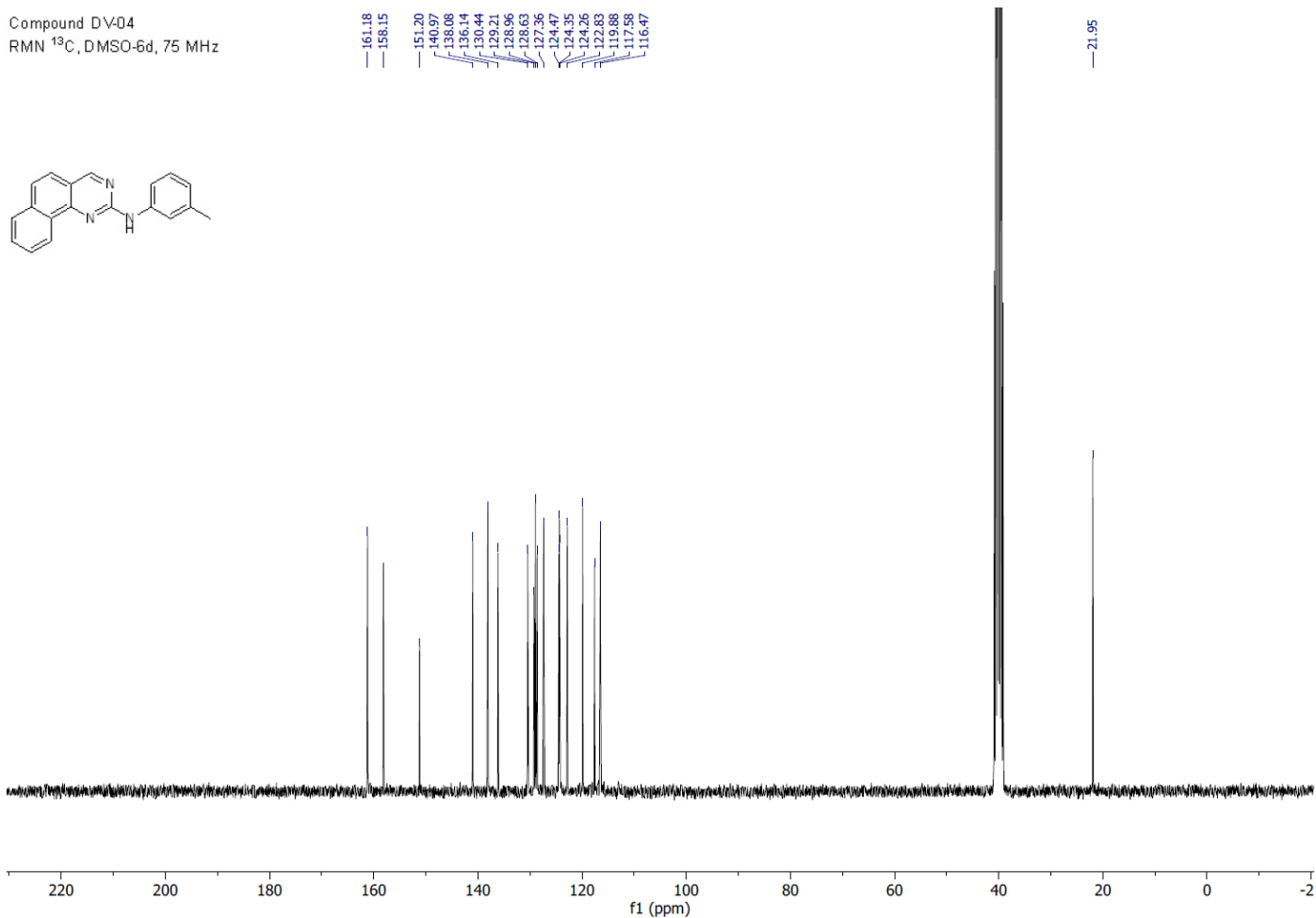
Spectra: ^1H , ^{13}C , ^{13}C Jmod NMR and FT-IR data of compound 4c (DV-04)



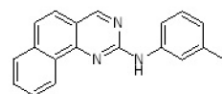
Compound DV-04
RMN ^{13}C , DMSO- d_6 , 75 MHz



161.18
158.15
151.20
140.97
138.08
136.14
130.44
129.21
128.96
128.63
127.36
124.47
124.35
124.26
122.83
119.88
117.58
116.47



Compound DV-04
RMN ^{13}C Jmod, DMSO- d_6 , 75 MHz



161.18

140.97

138.08

136.14

130.43

129.21

128.95

128.63

127.36

124.47

124.35

124.25

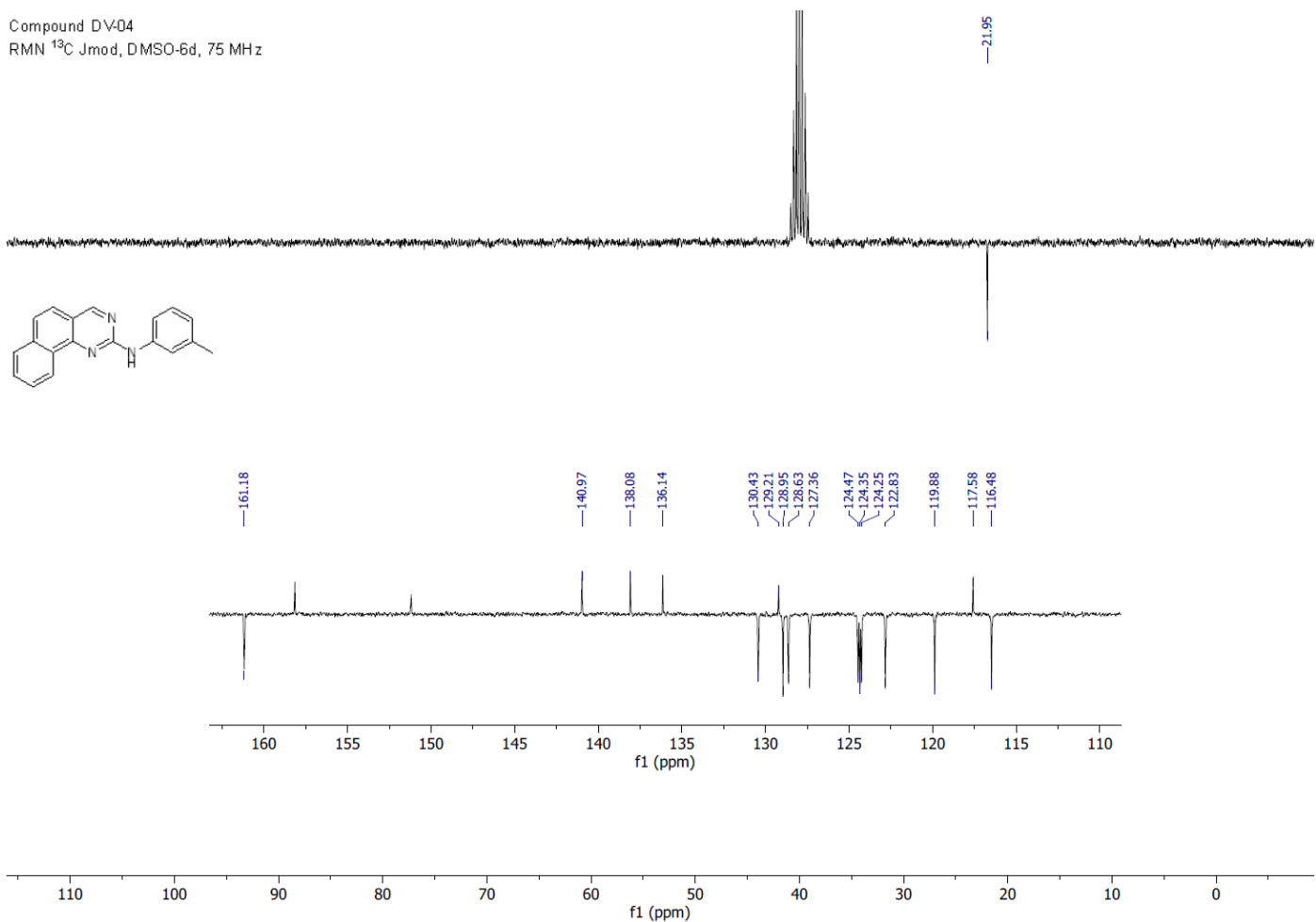
122.83

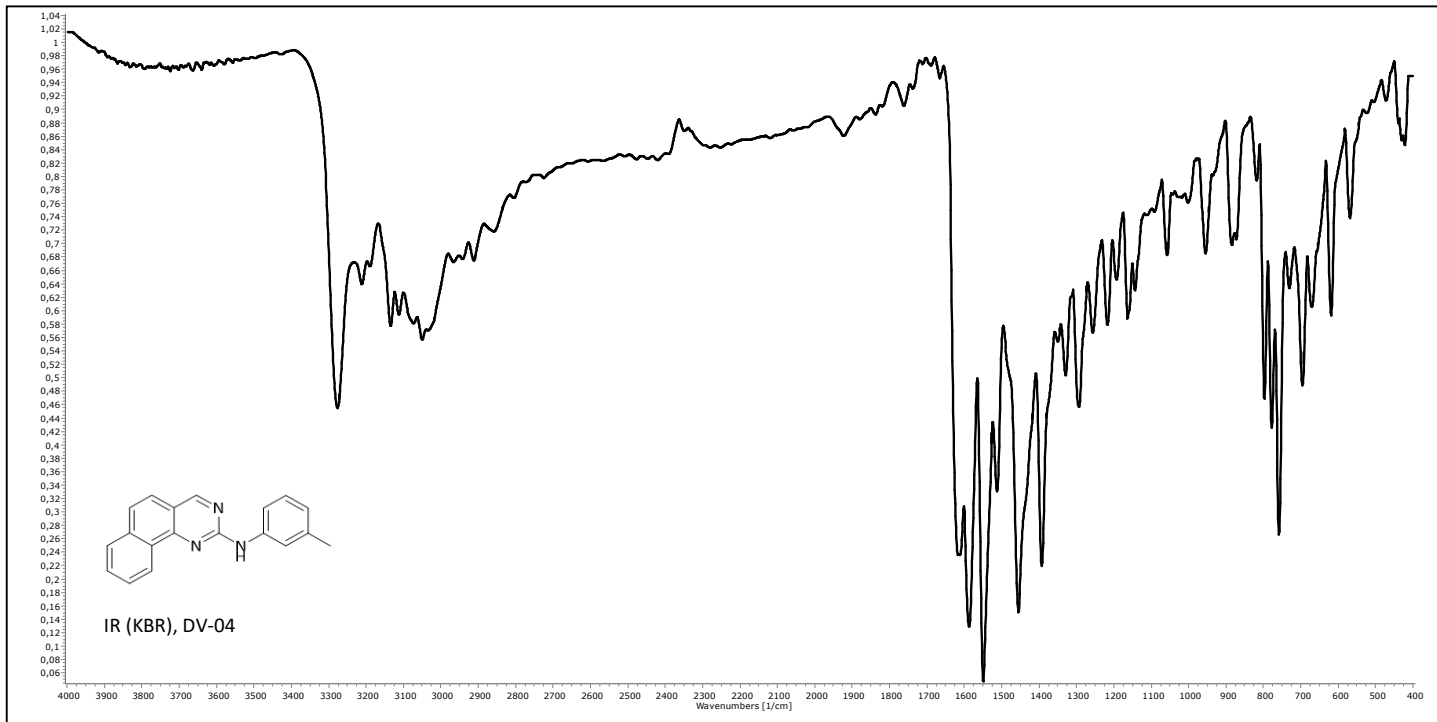
119.88

117.58

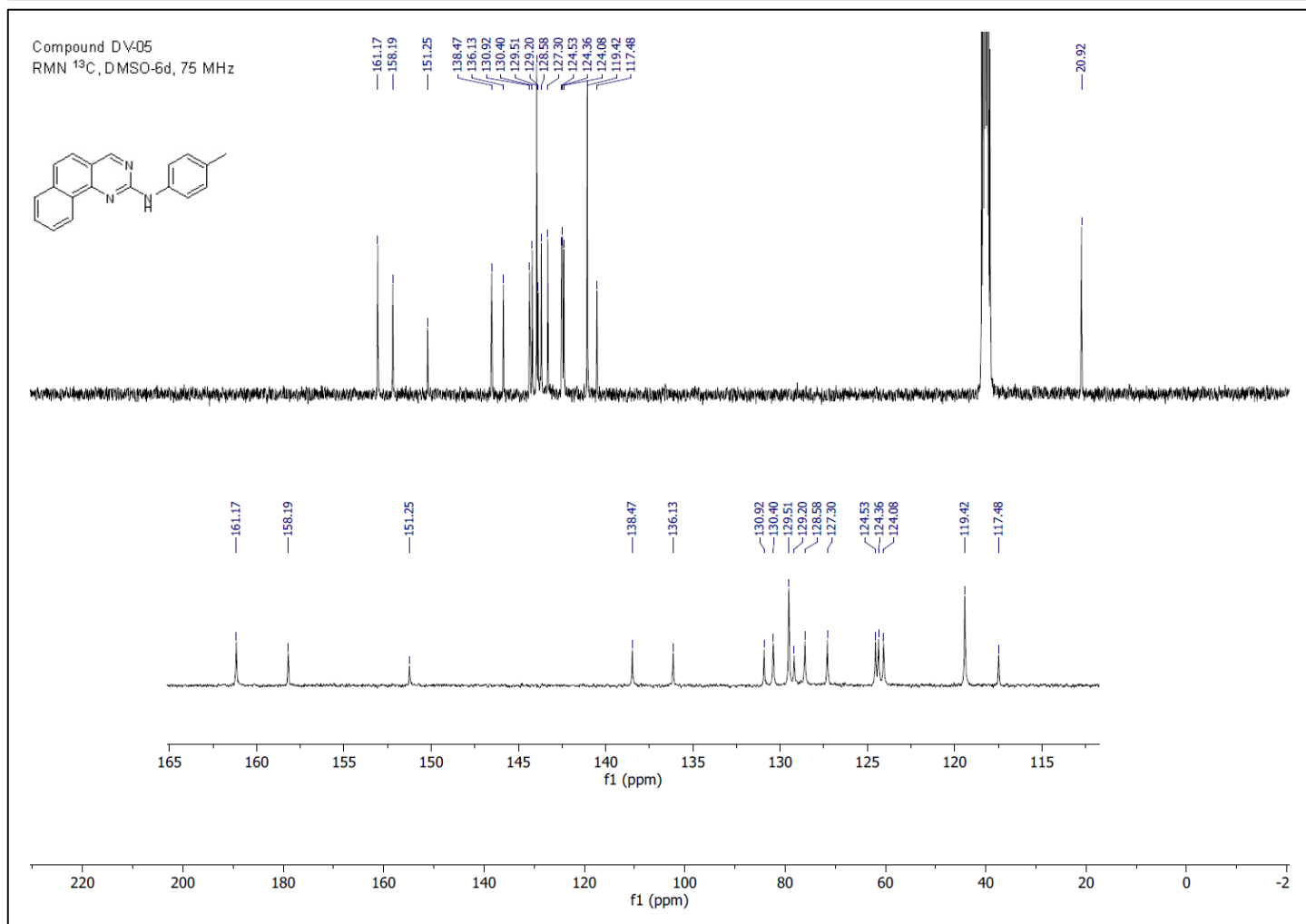
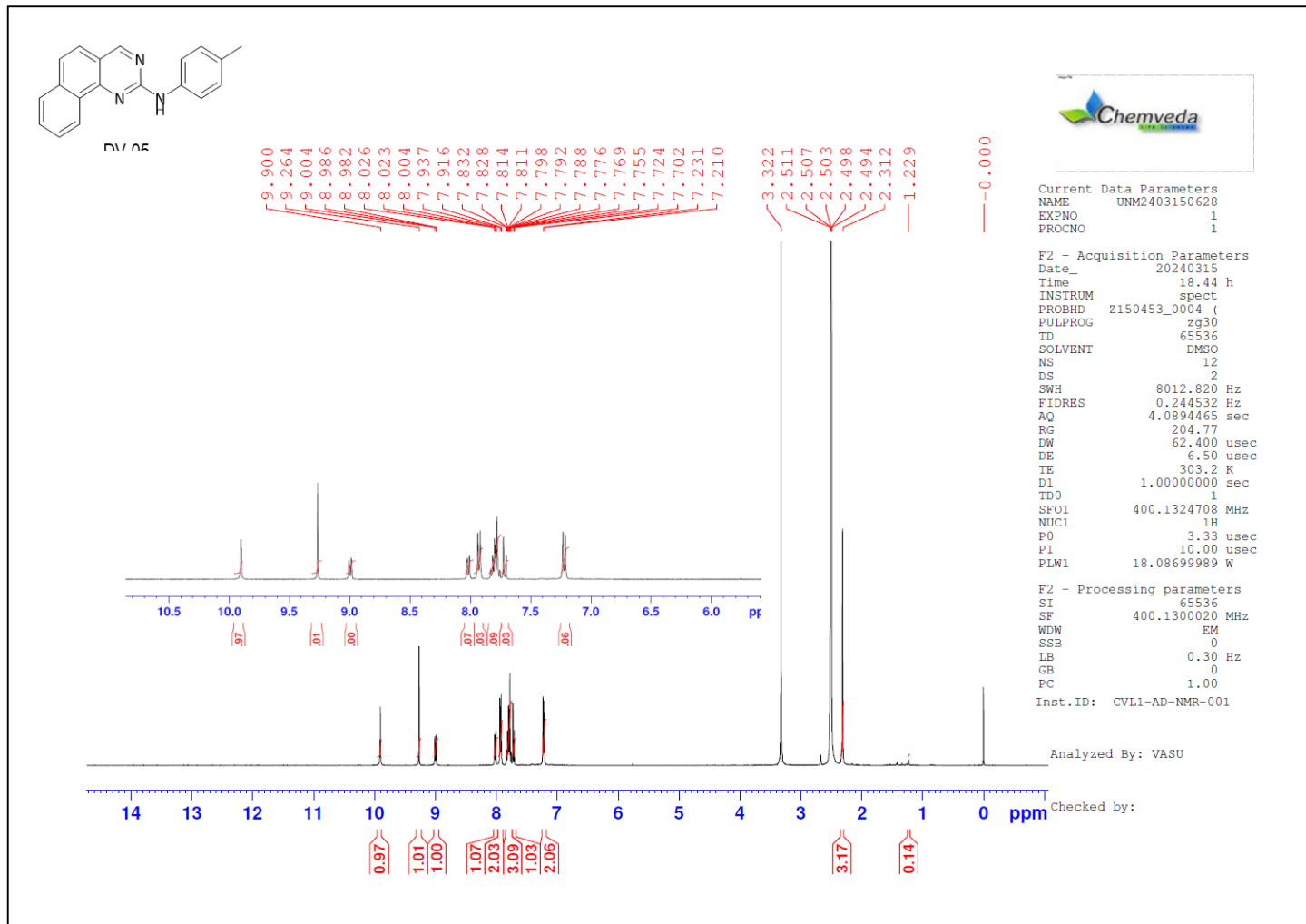
116.48

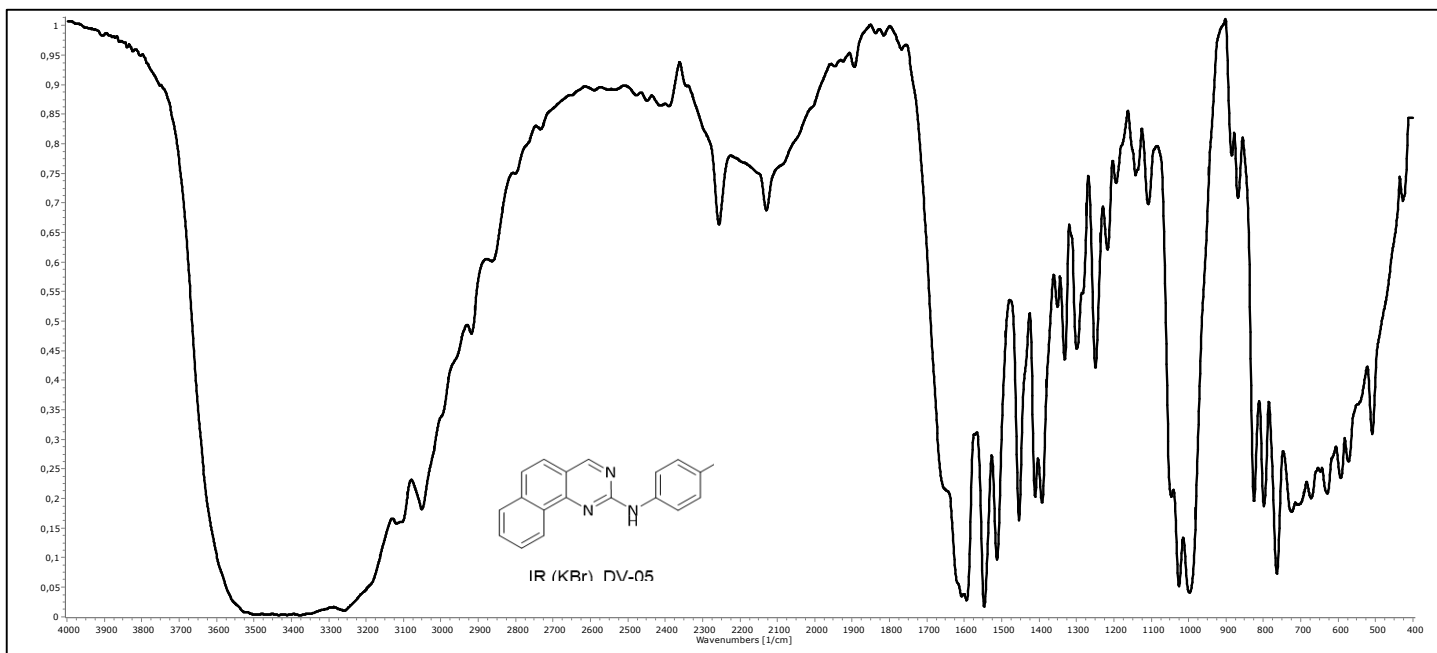
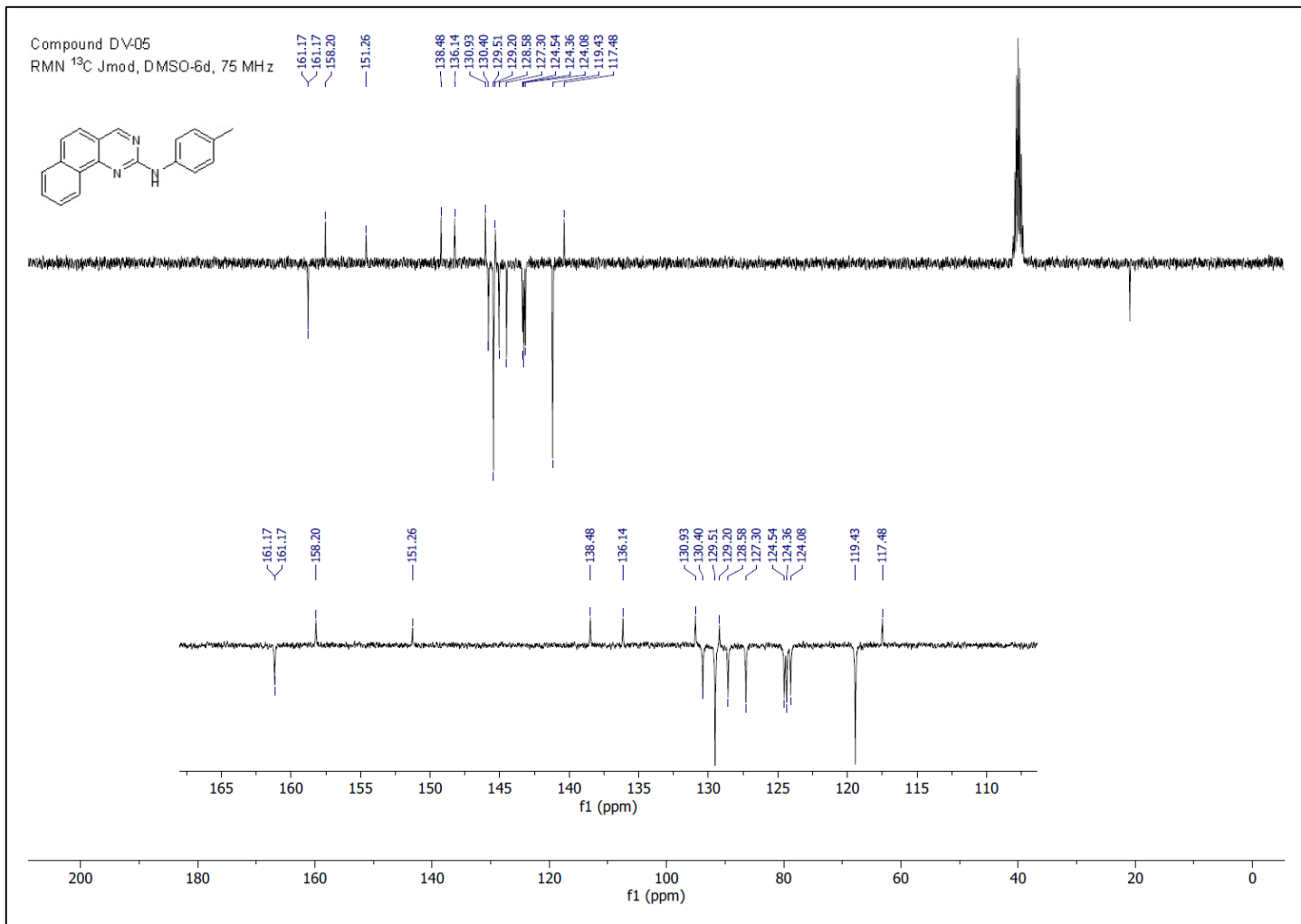
21.95



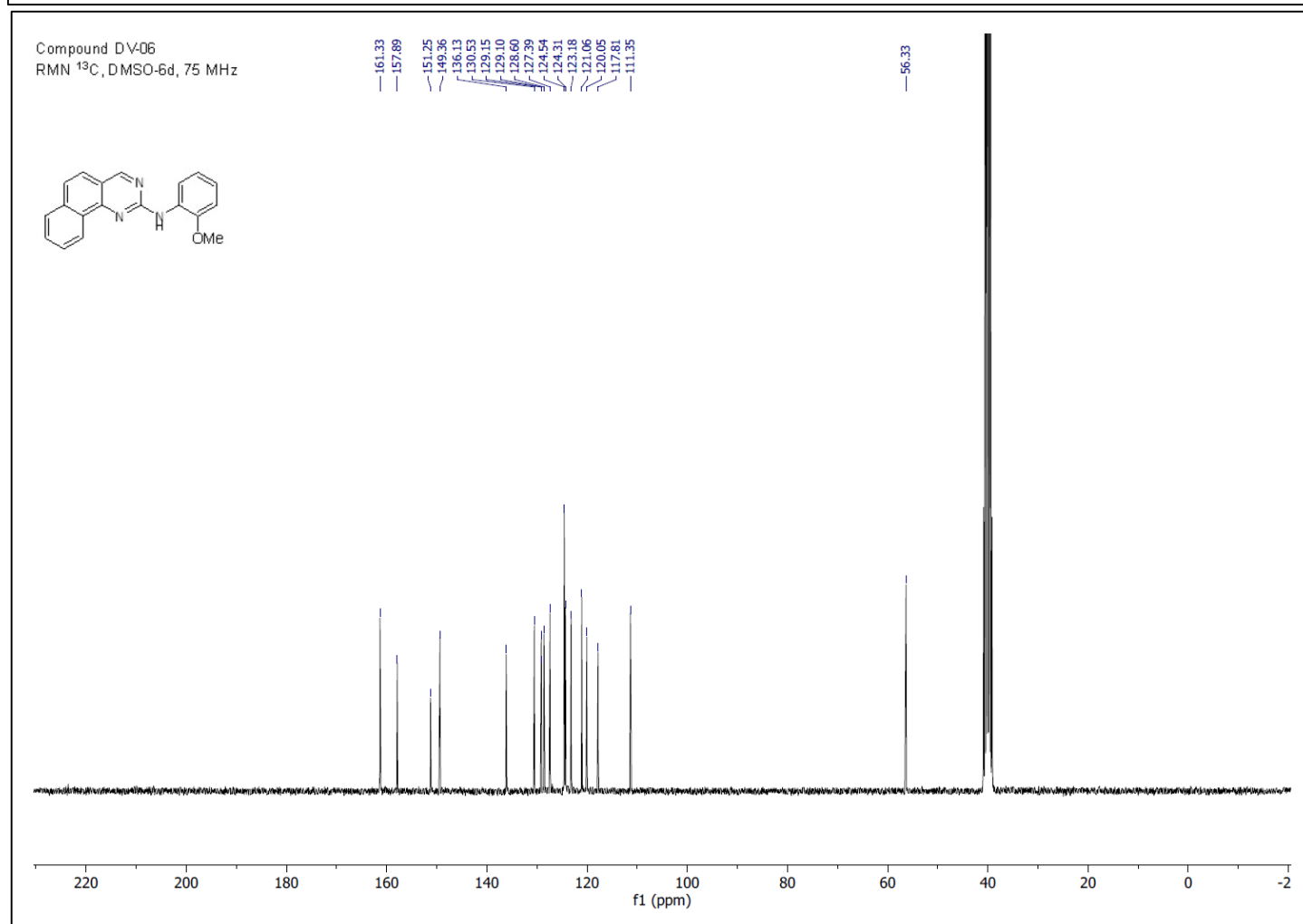
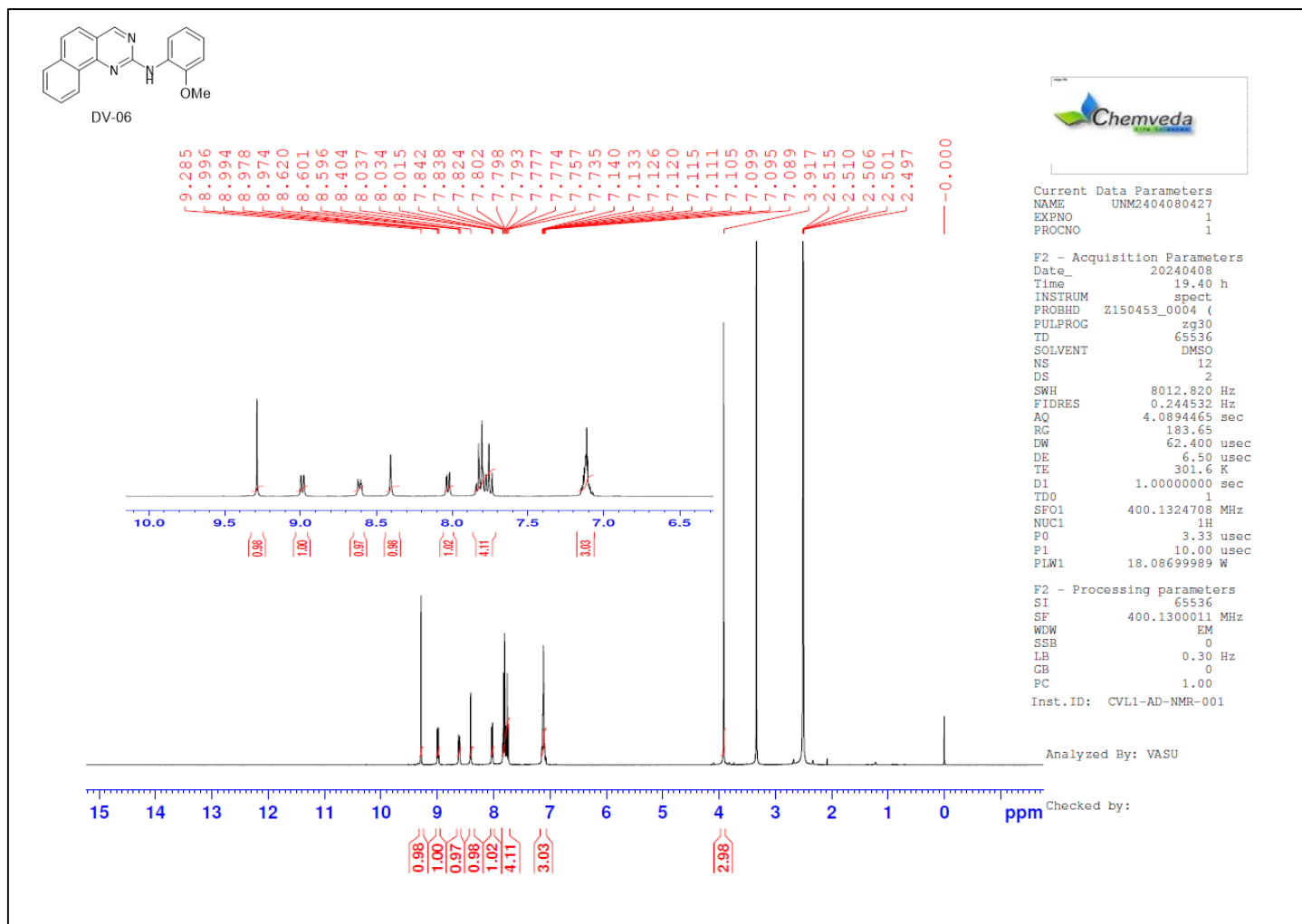


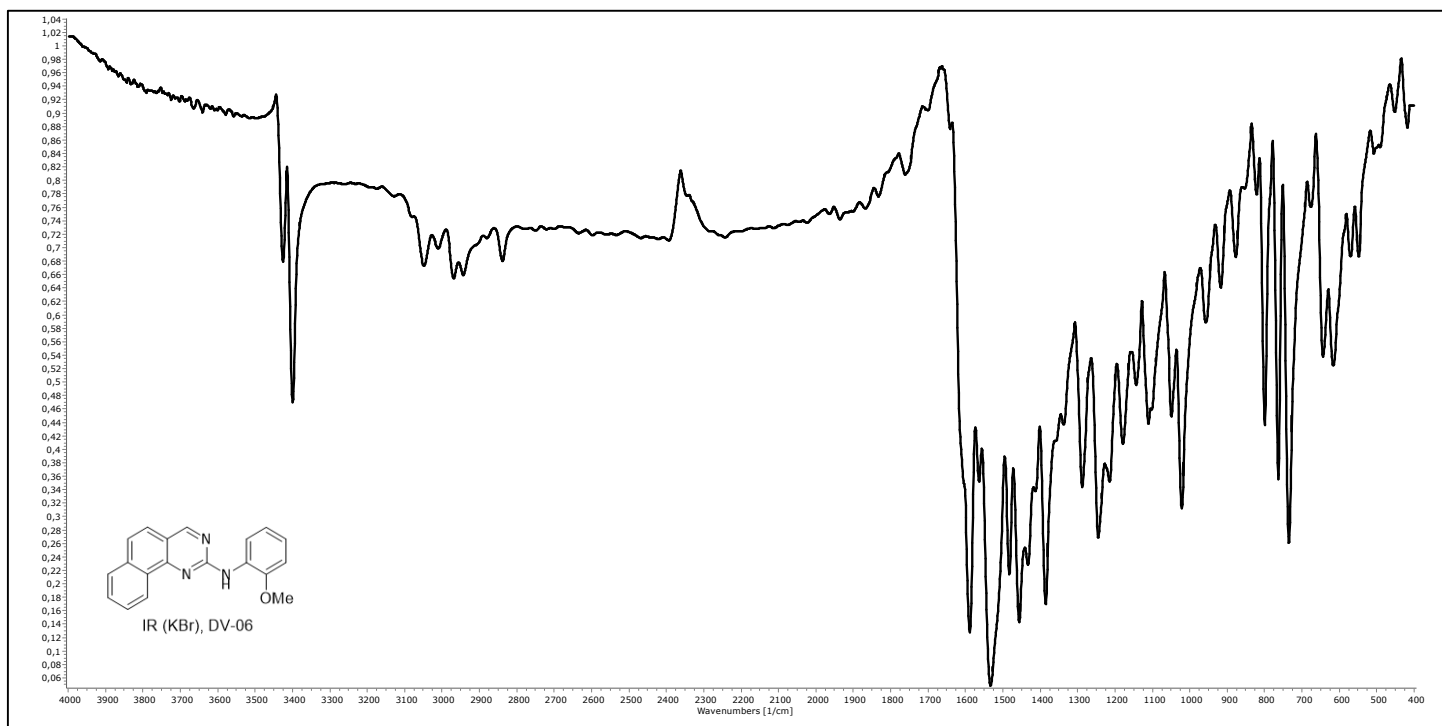
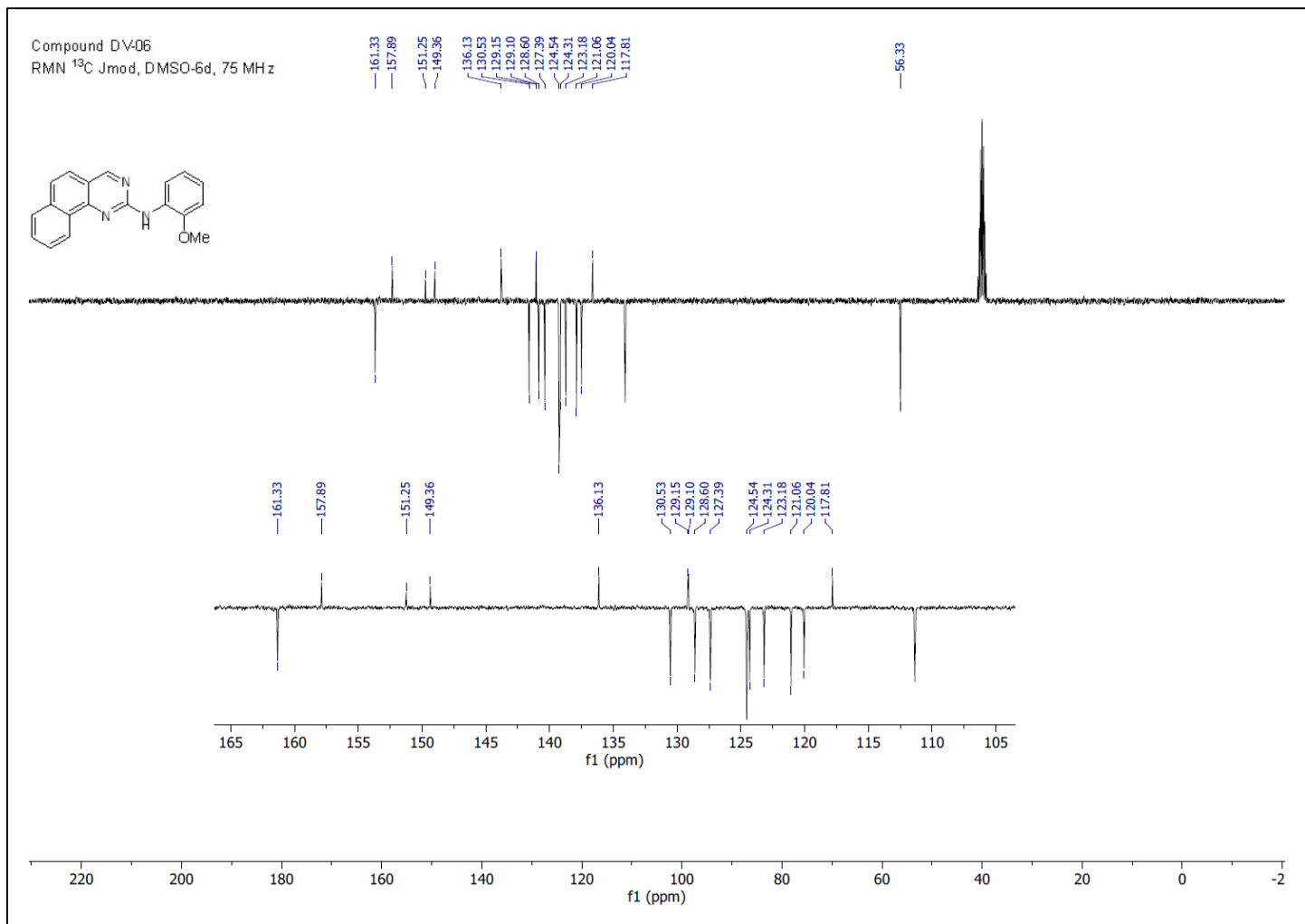
Spectra: ^1H , ^{13}C , ^{13}C Jmod NMR and FT-IR data of compound 4d (DV-05)



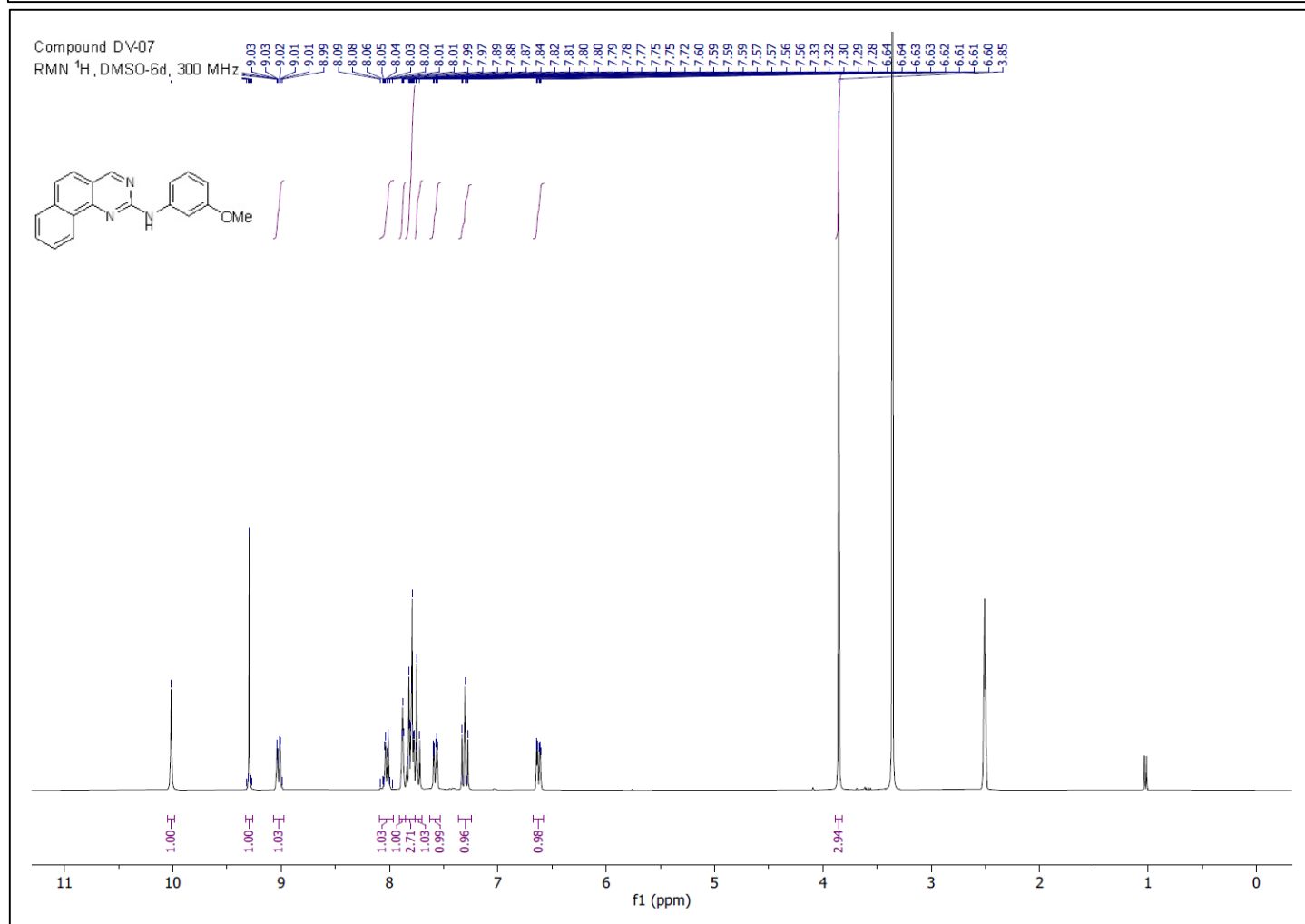
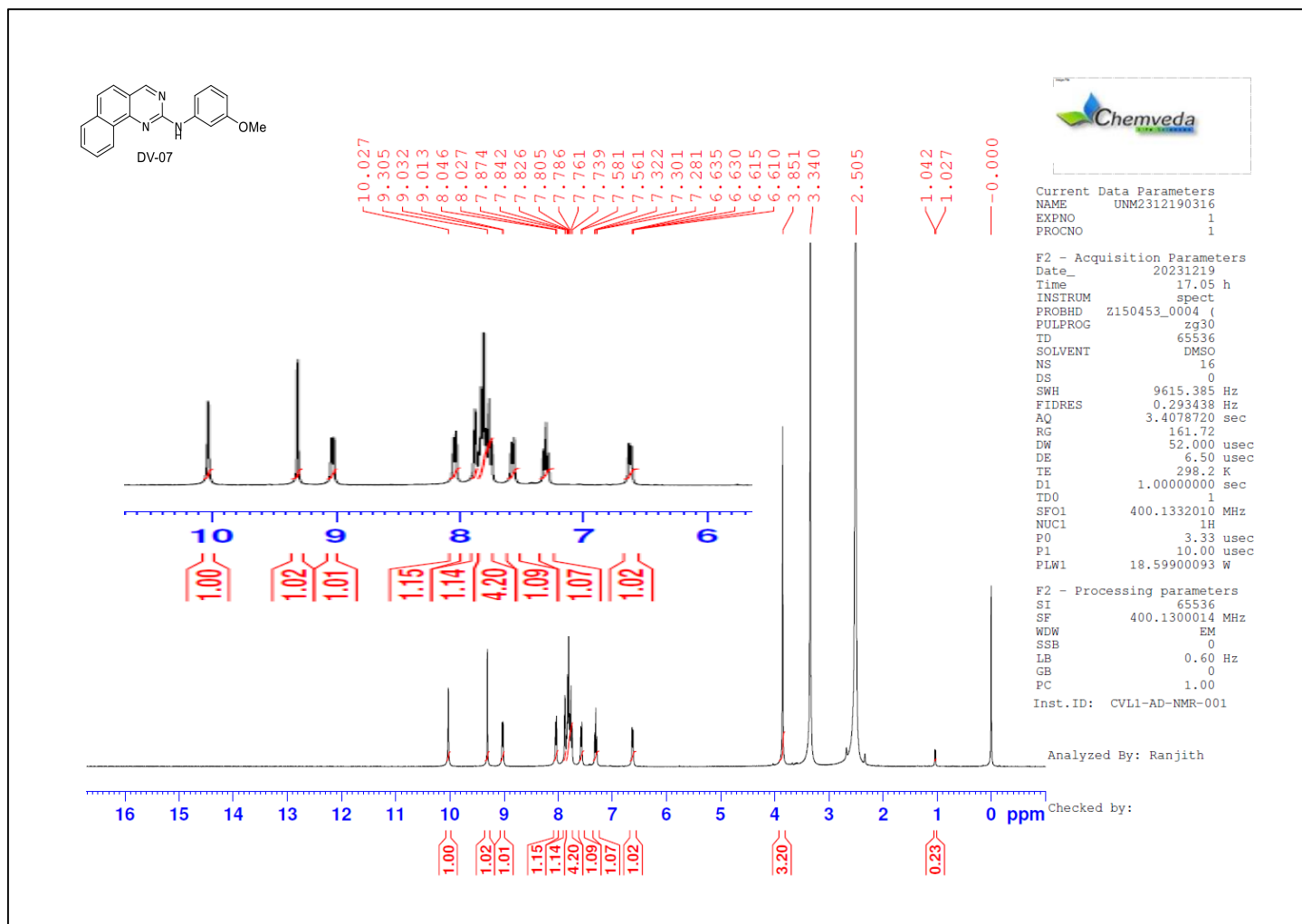


Spectra: ^1H , ^{13}C , ^{13}C Jmod NMR and FT-IR data of compound 4e (DV-06)

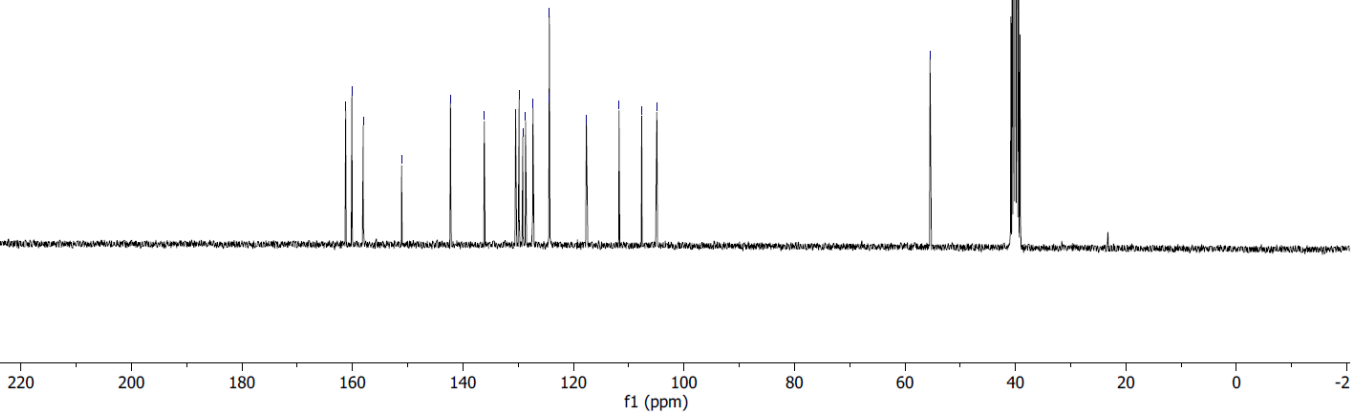
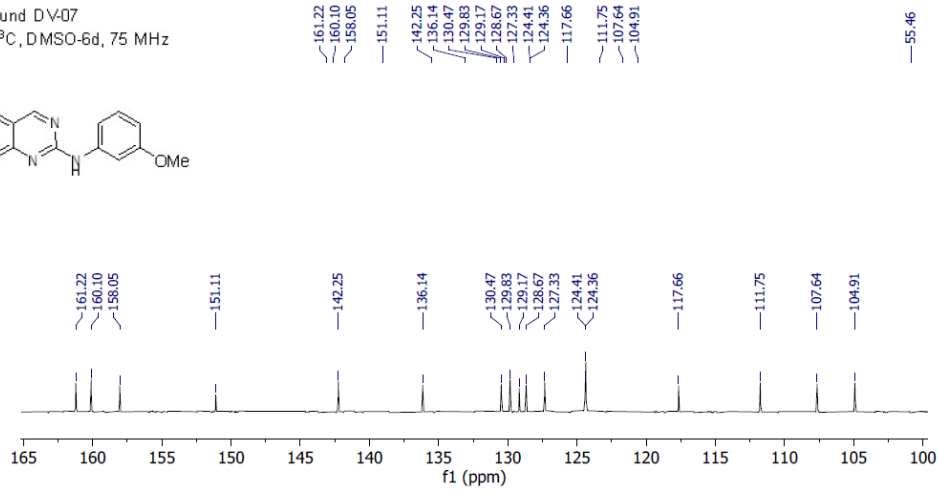
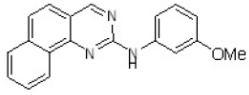




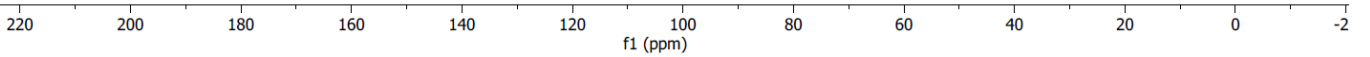
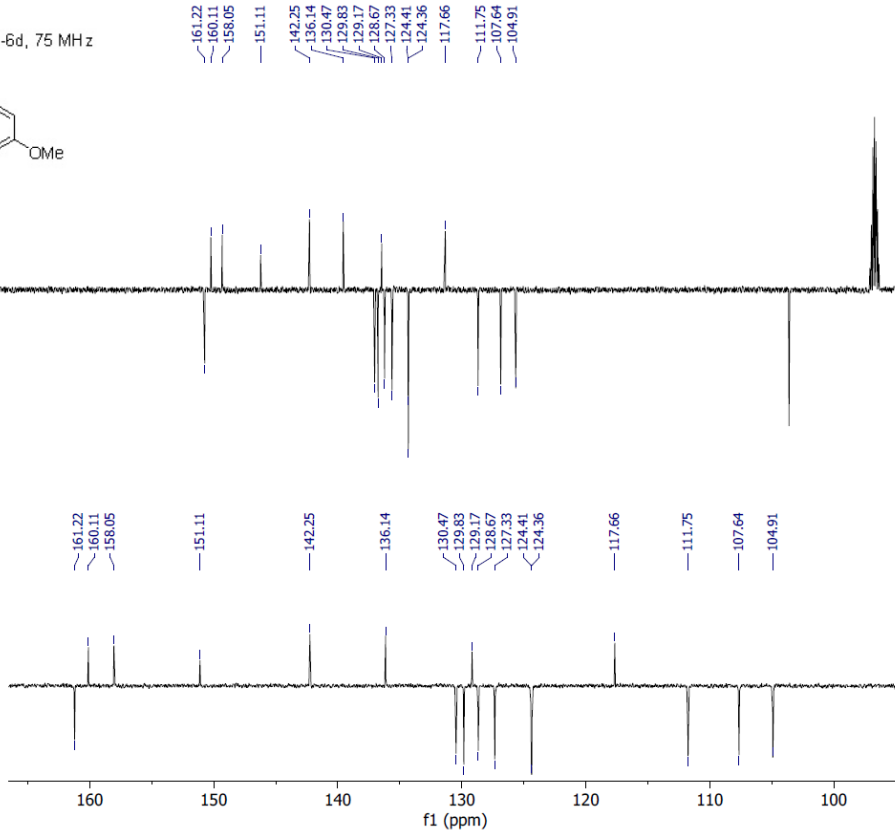
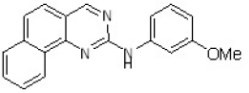
Spectra: ^1H , ^{13}C , ^{13}C Jmod NMR and FT-IR data of compound 4f (DV-07)

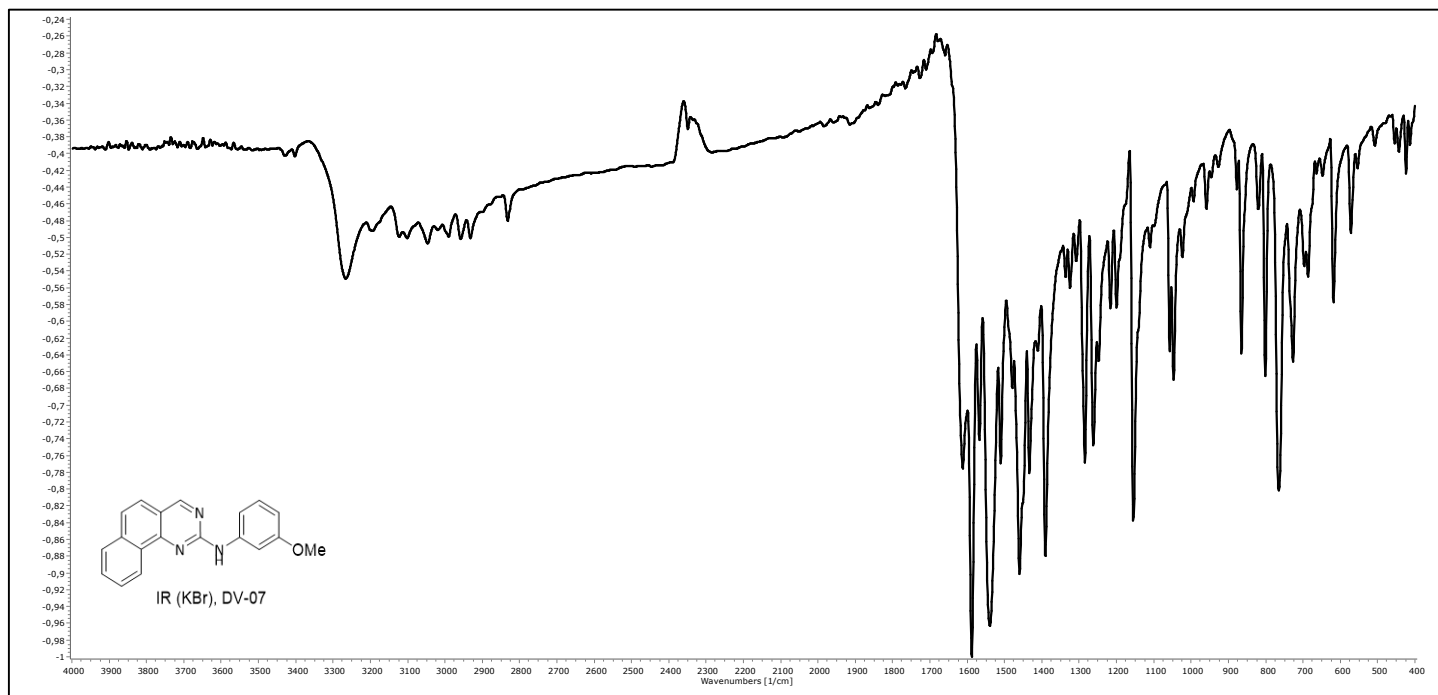


Compound DV-07
RMN ¹³C, DMSO-6d, 75 MHz

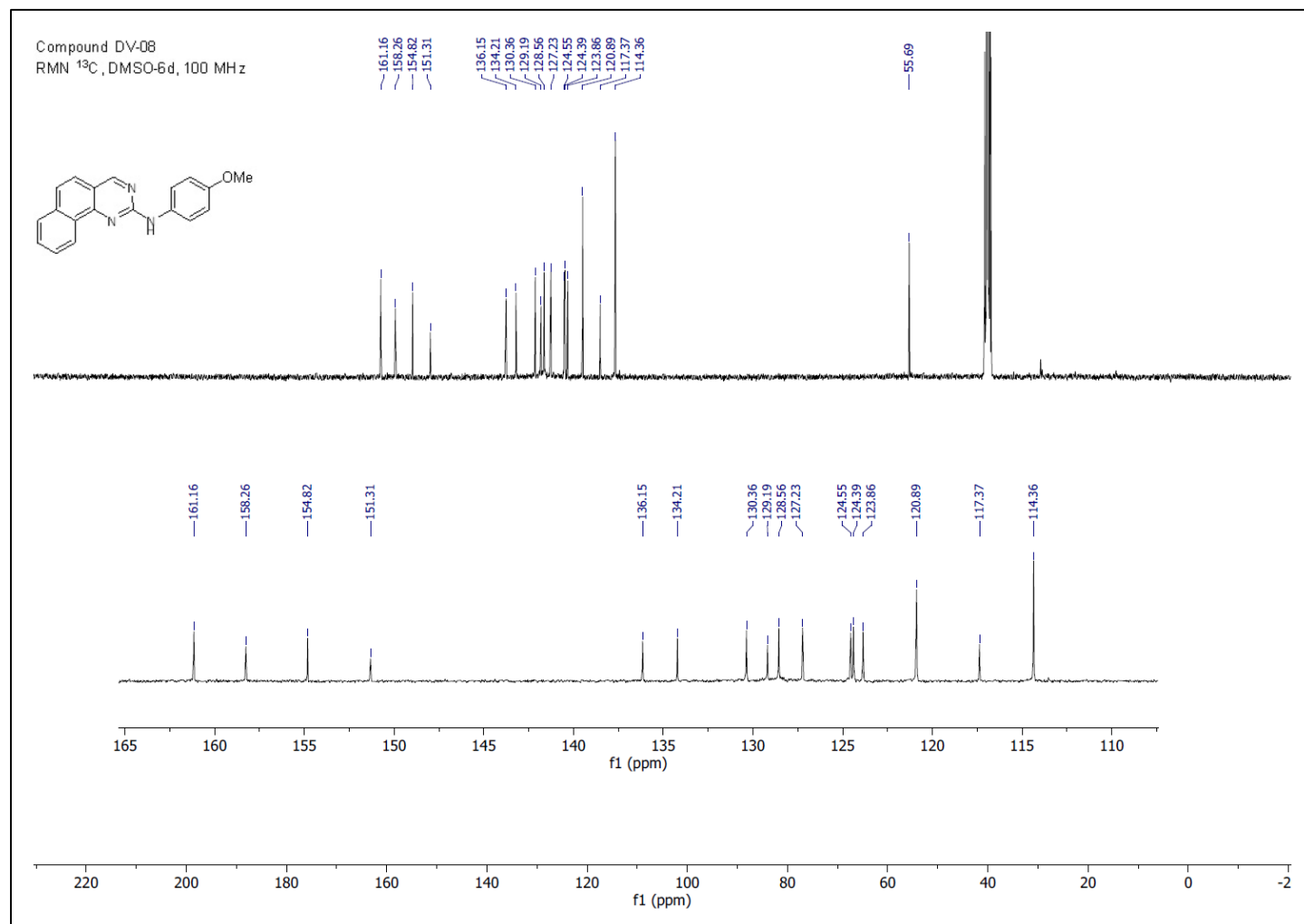
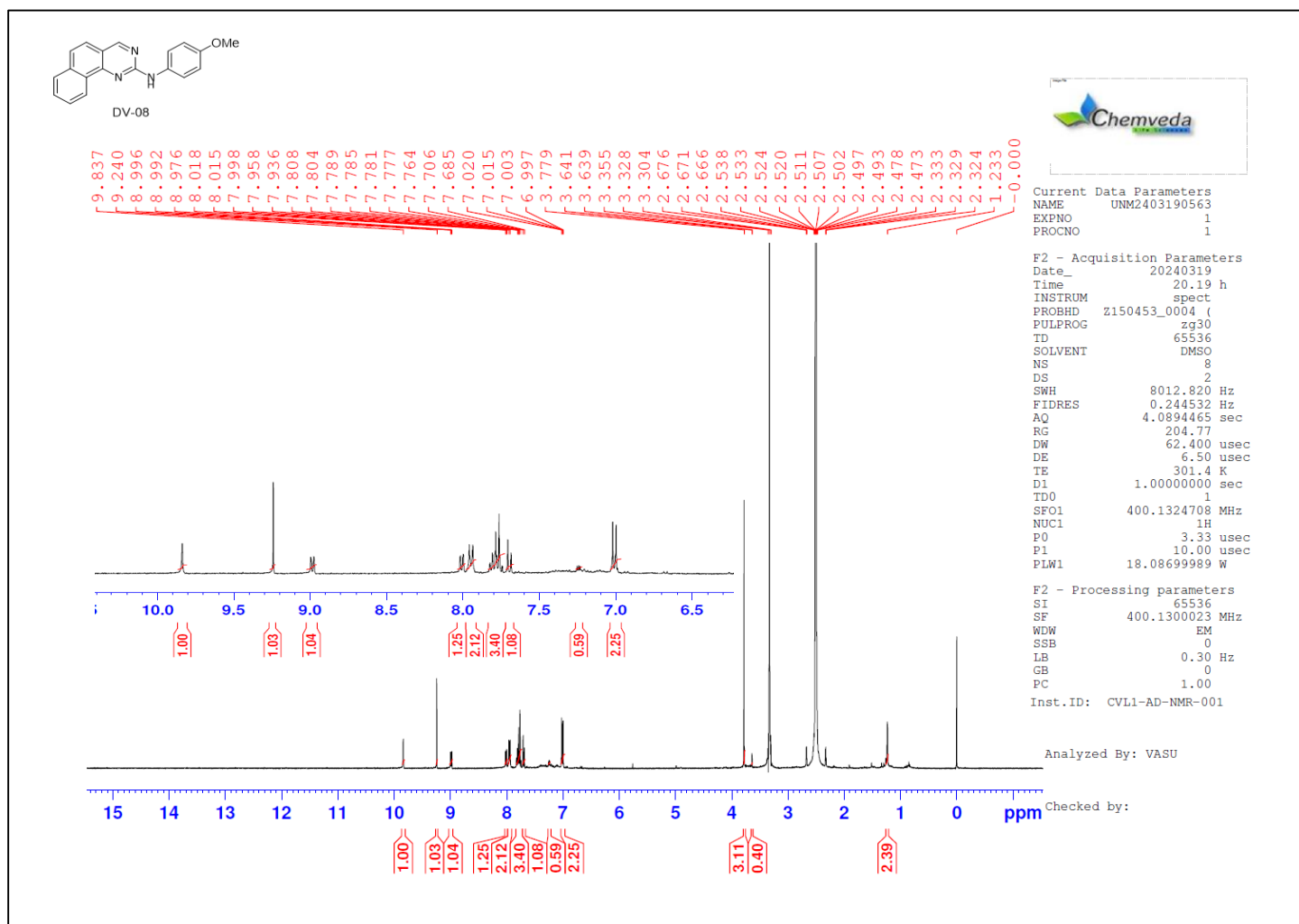


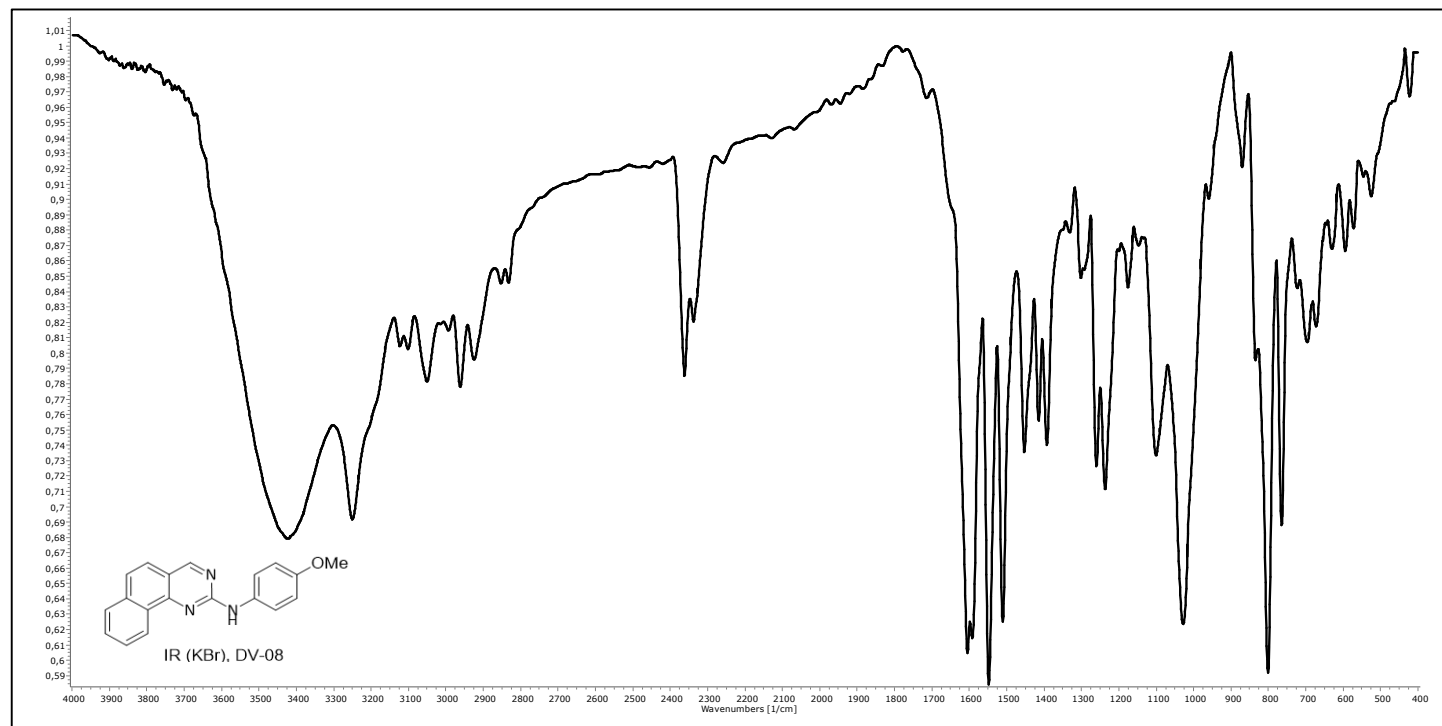
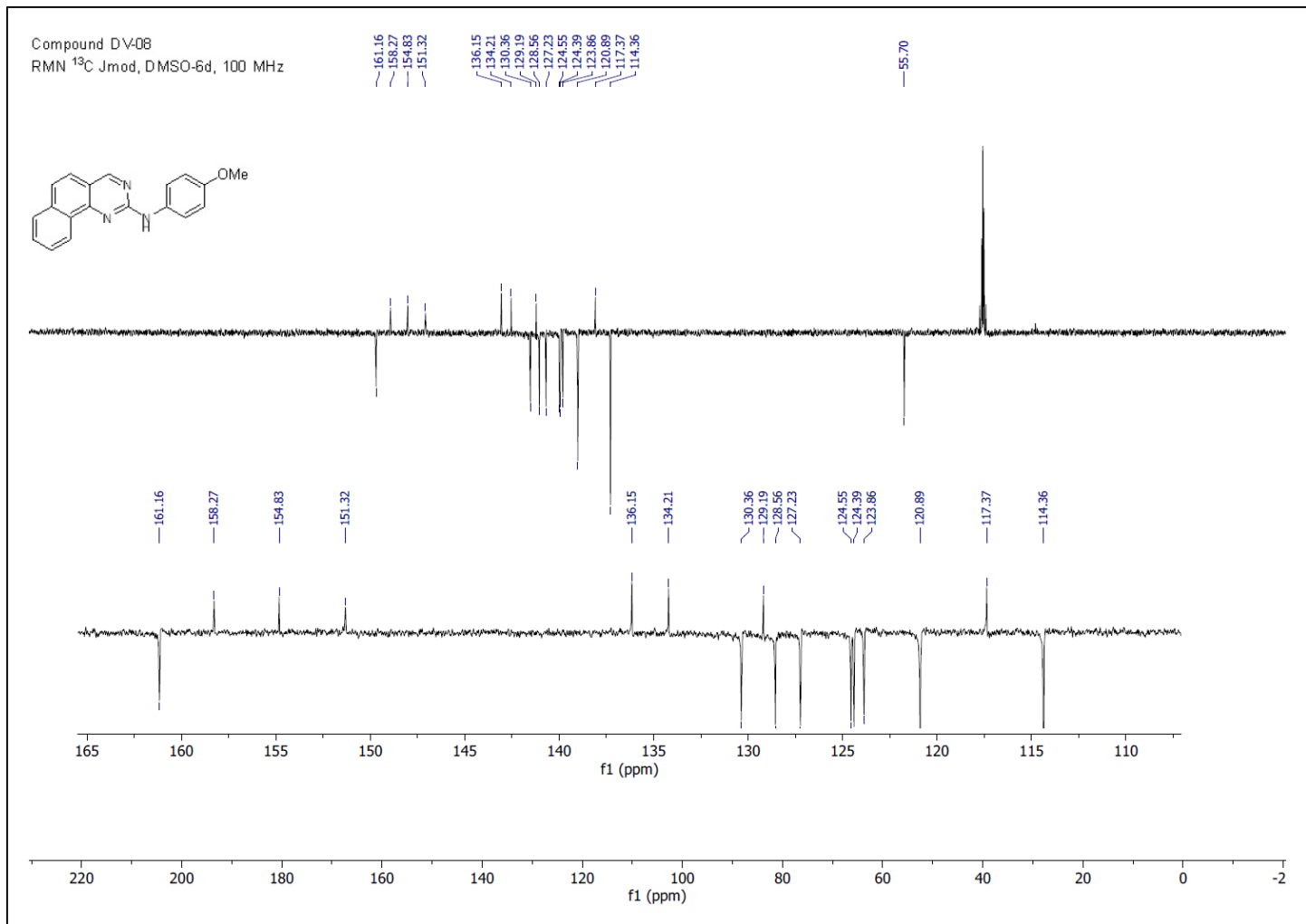
Compound DV-07
RMN ¹³C Jmod, DMSO-6d, 75 MHz



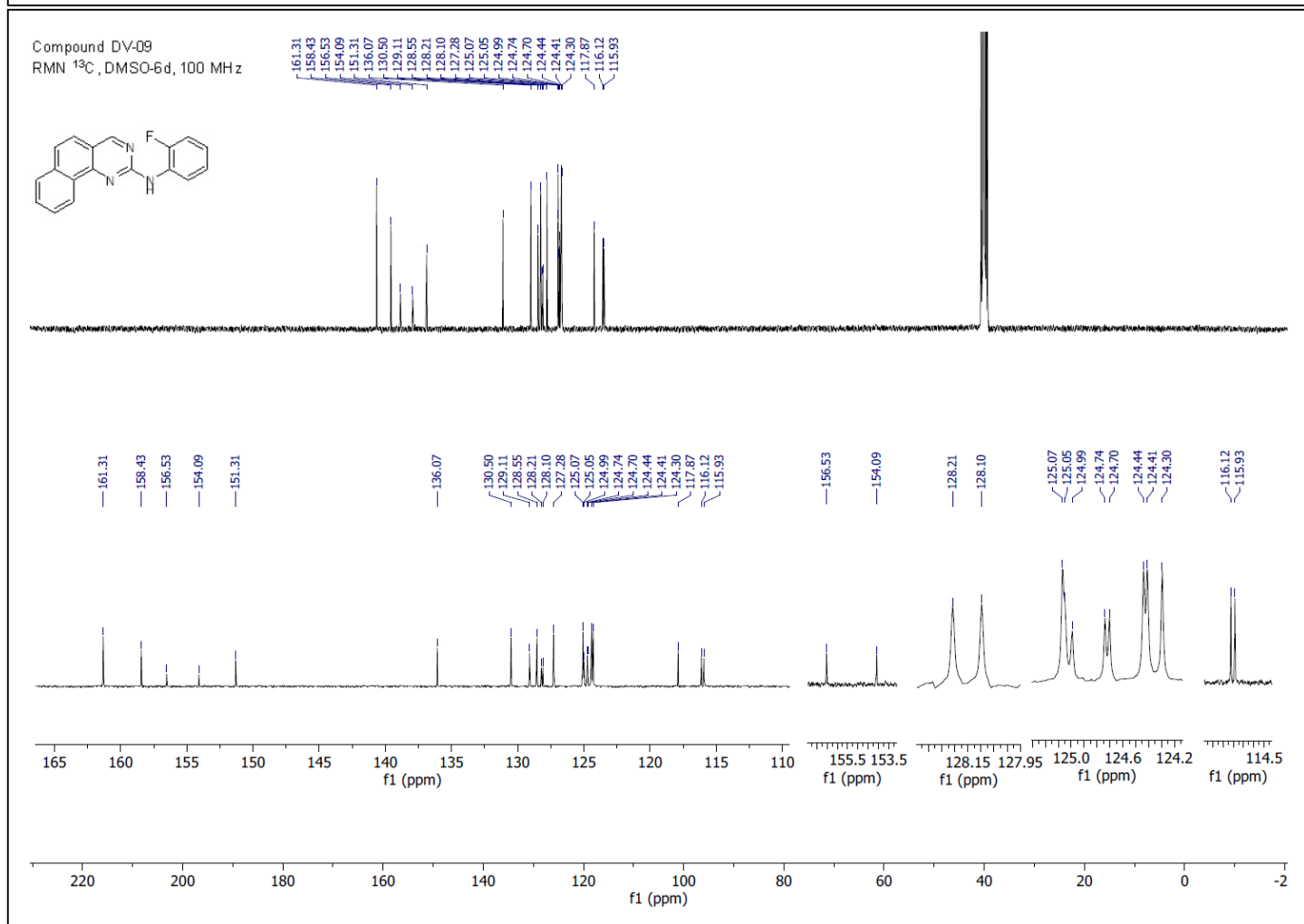
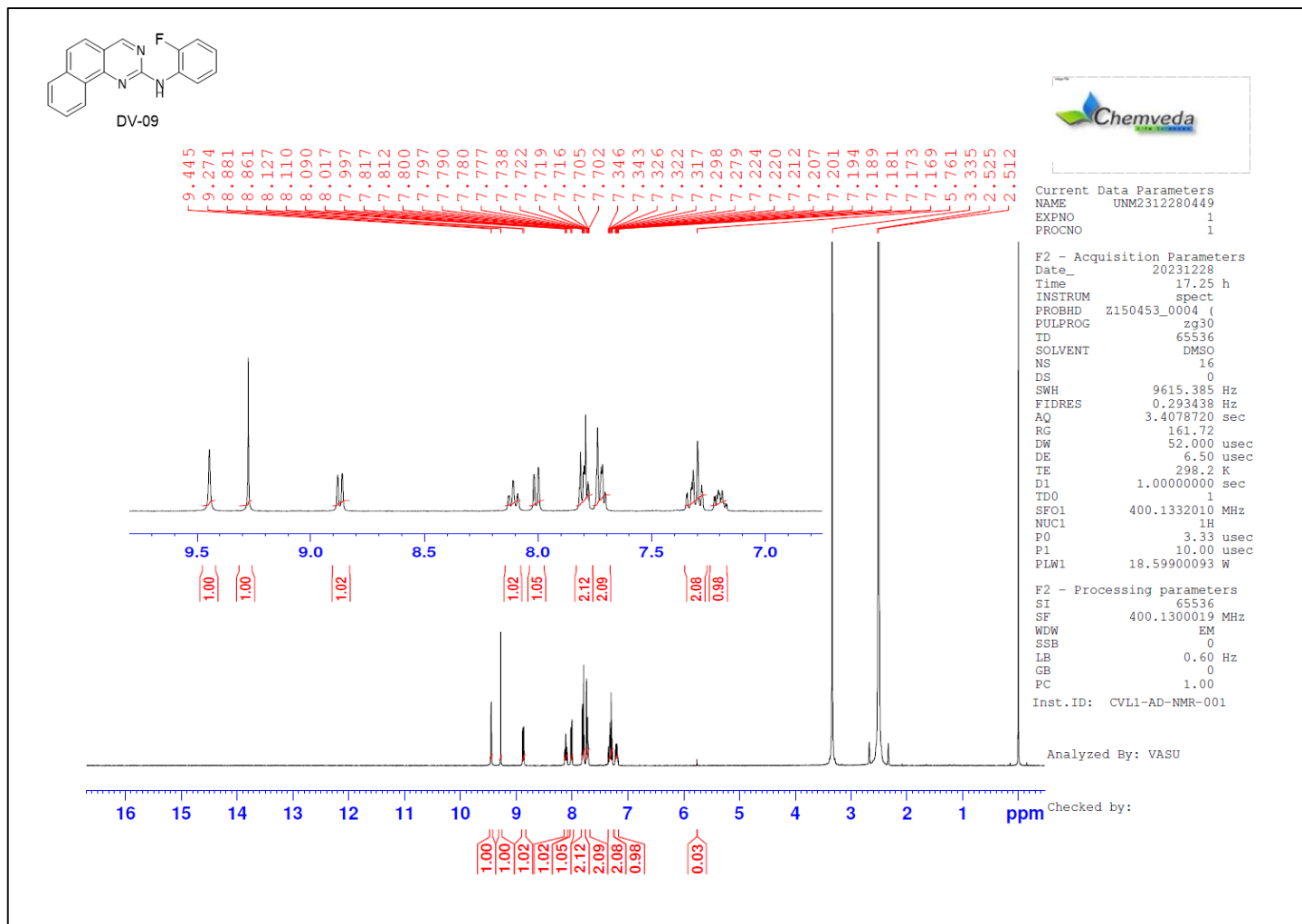


Spectra: ^1H , ^{13}C , ^{13}C Jmod NMR and FT-IR data of compound 4g (DV-08)

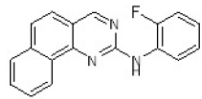




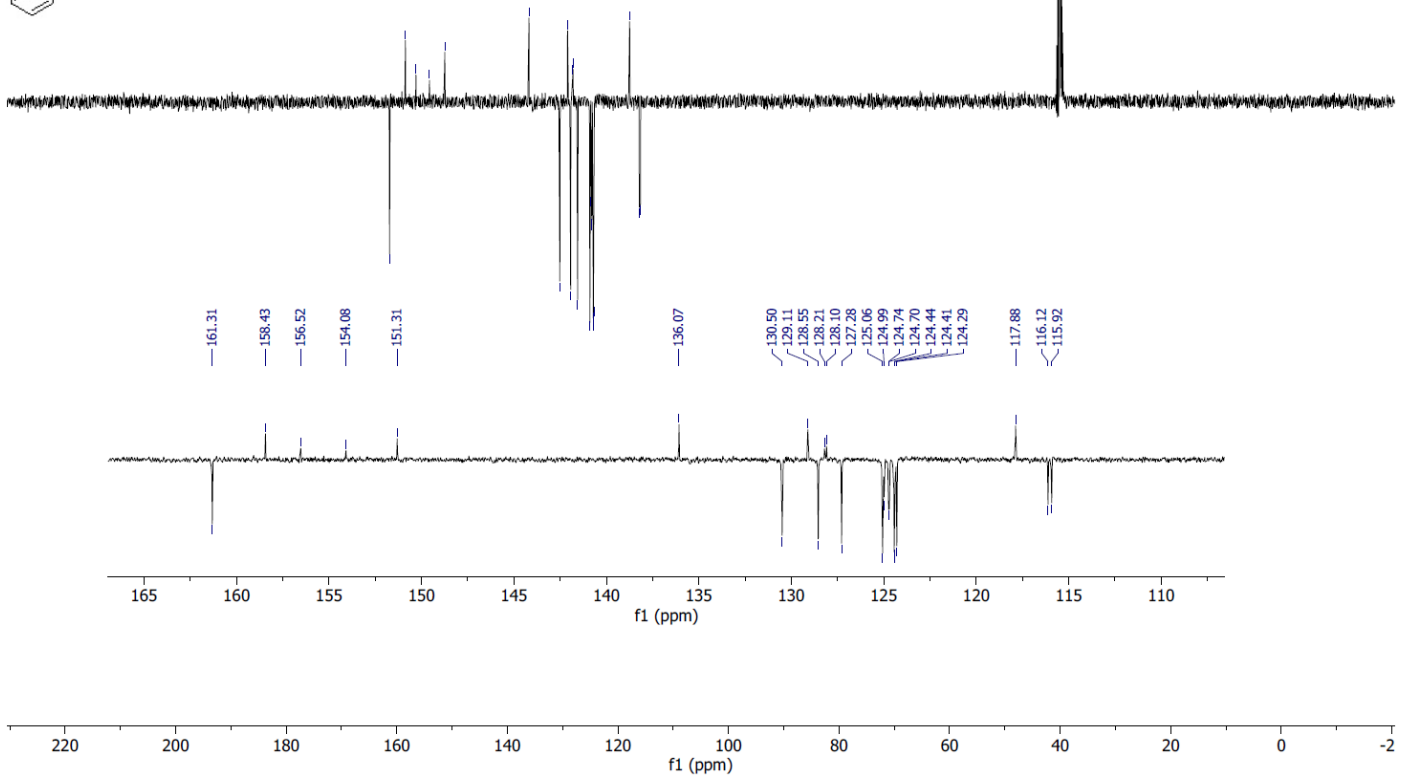
Spectra: ^1H , ^{13}C , ^{13}C Jmod NMR and FT-IR data of compound 4h (DV-09)



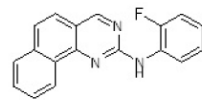
Compound DV-09
RMN ^{13}C Jmod, DMSO-6d, 100 MHz



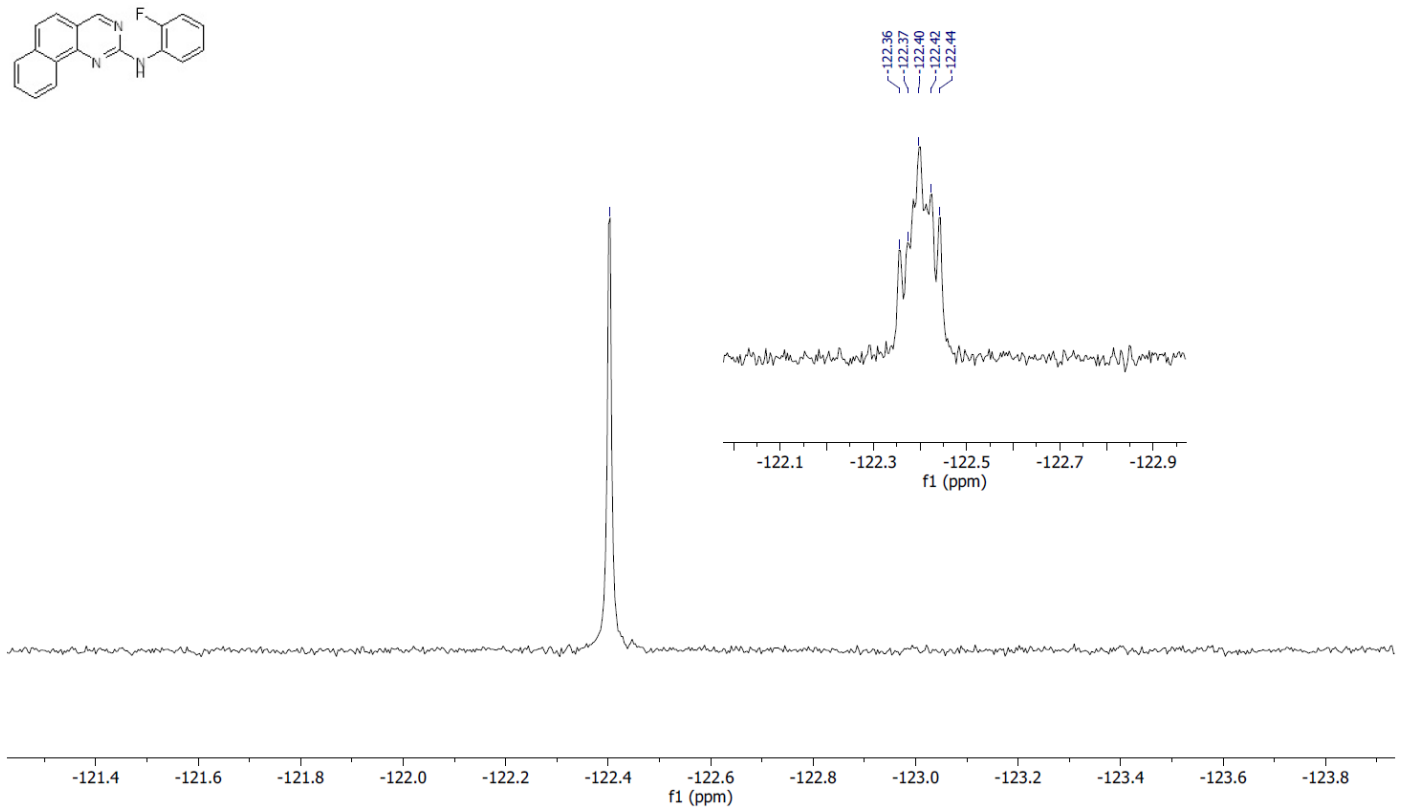
161.31
159.43
156.52
154.08
151.31
136.07
130.50
129.11
128.55
128.21
128.10
127.28
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124.70
124.44
124.41
124.29
117.88
116.12
115.92

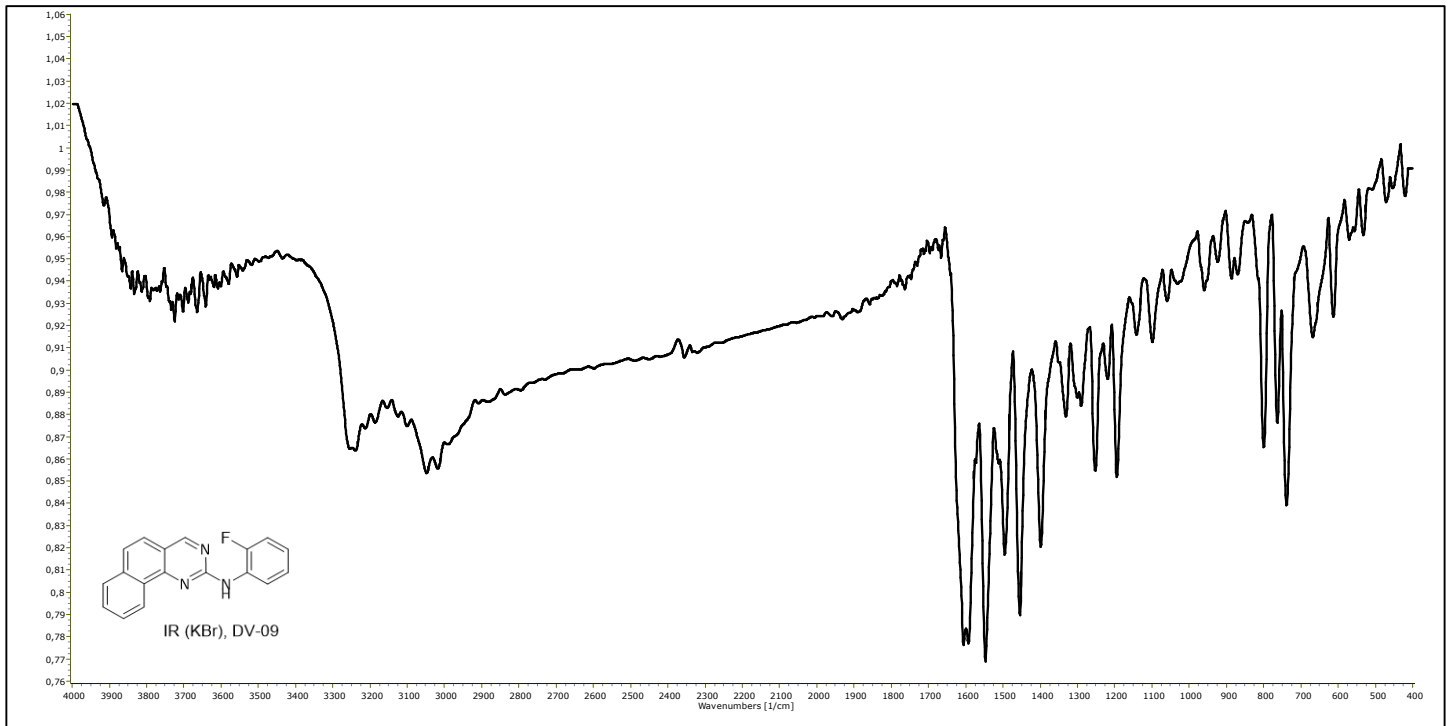


Compound DV-09
RMN ^{19}F , DMSO-6d, 282 MHz

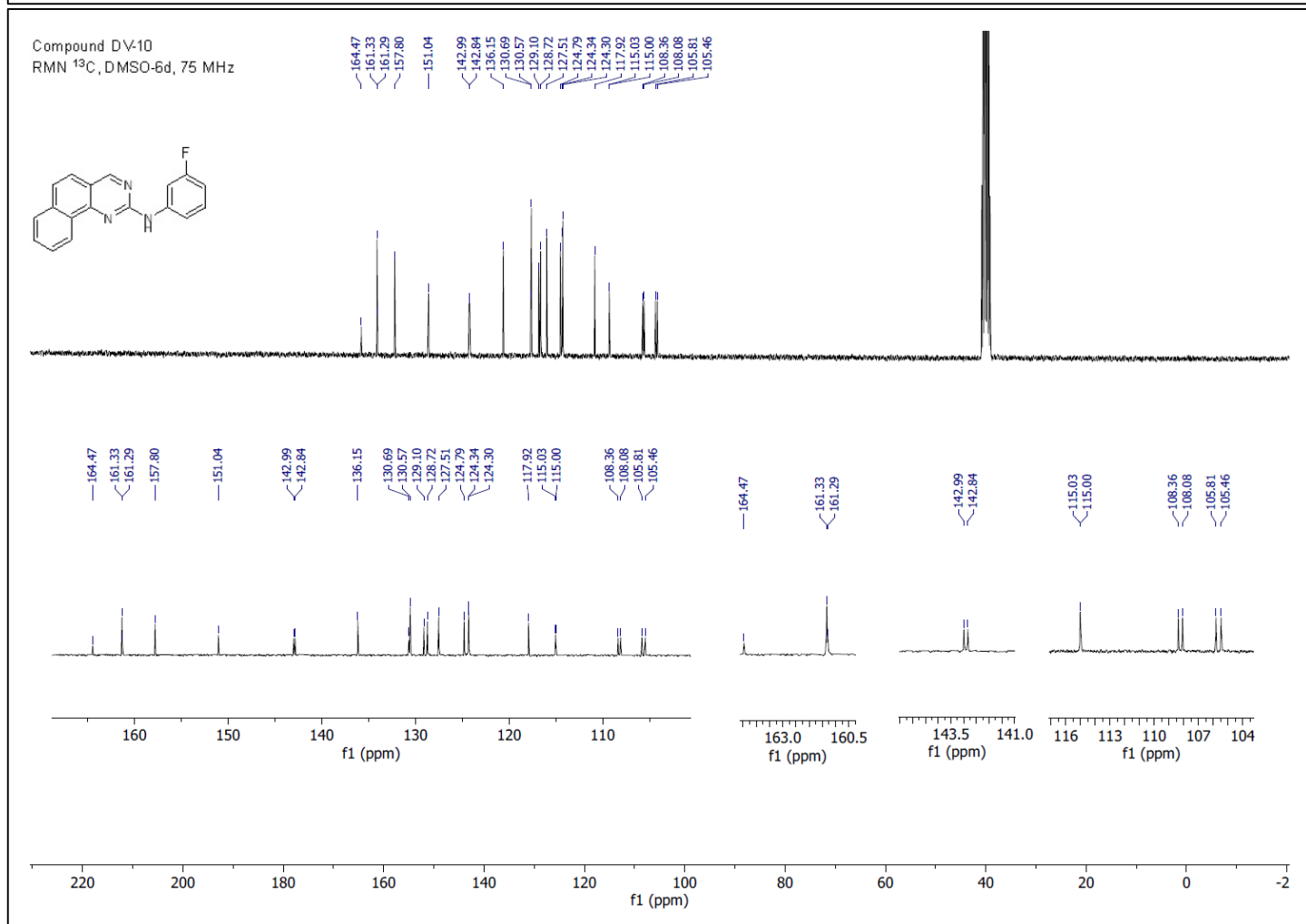
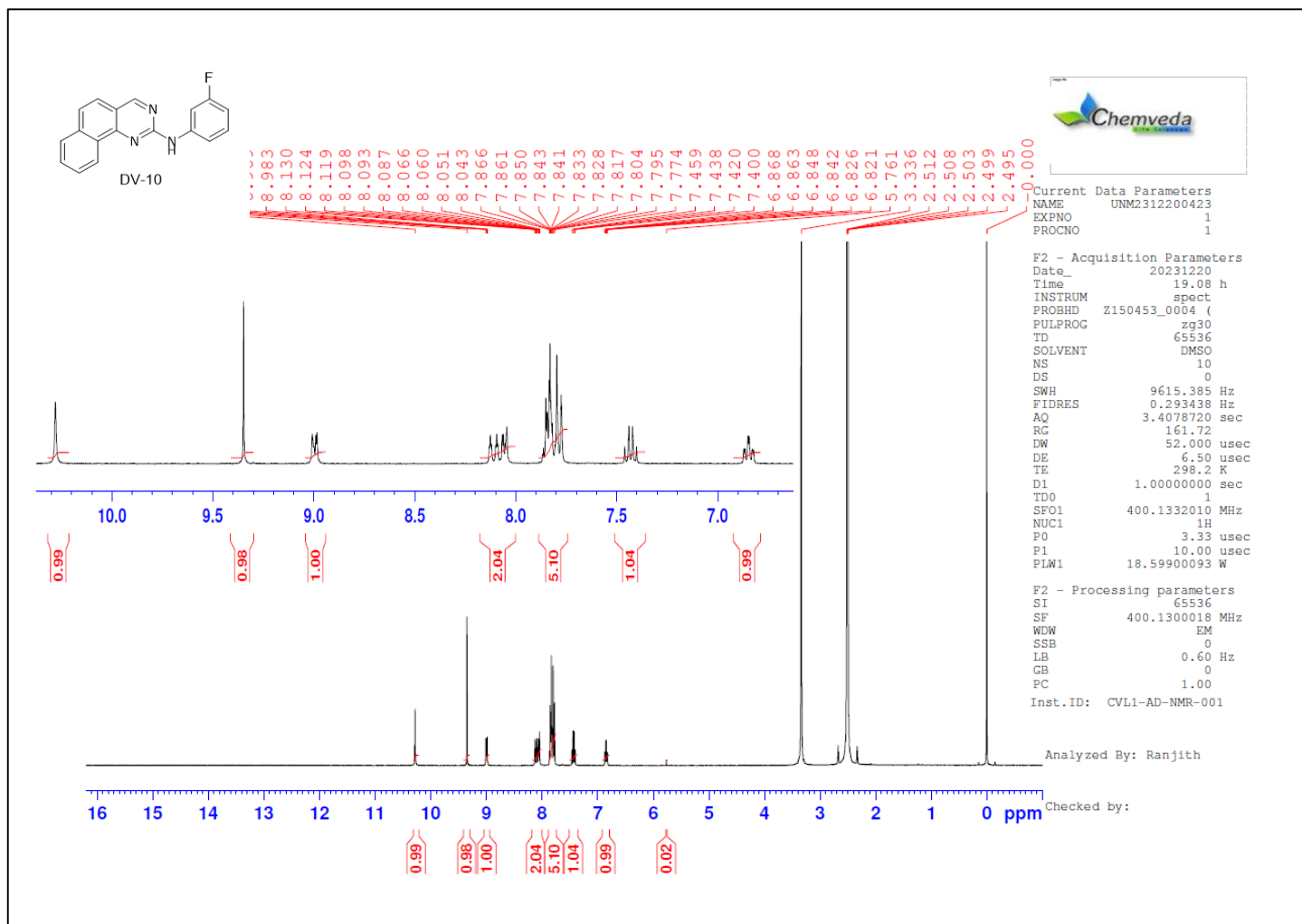


-122.40

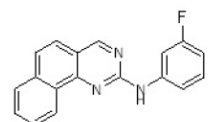




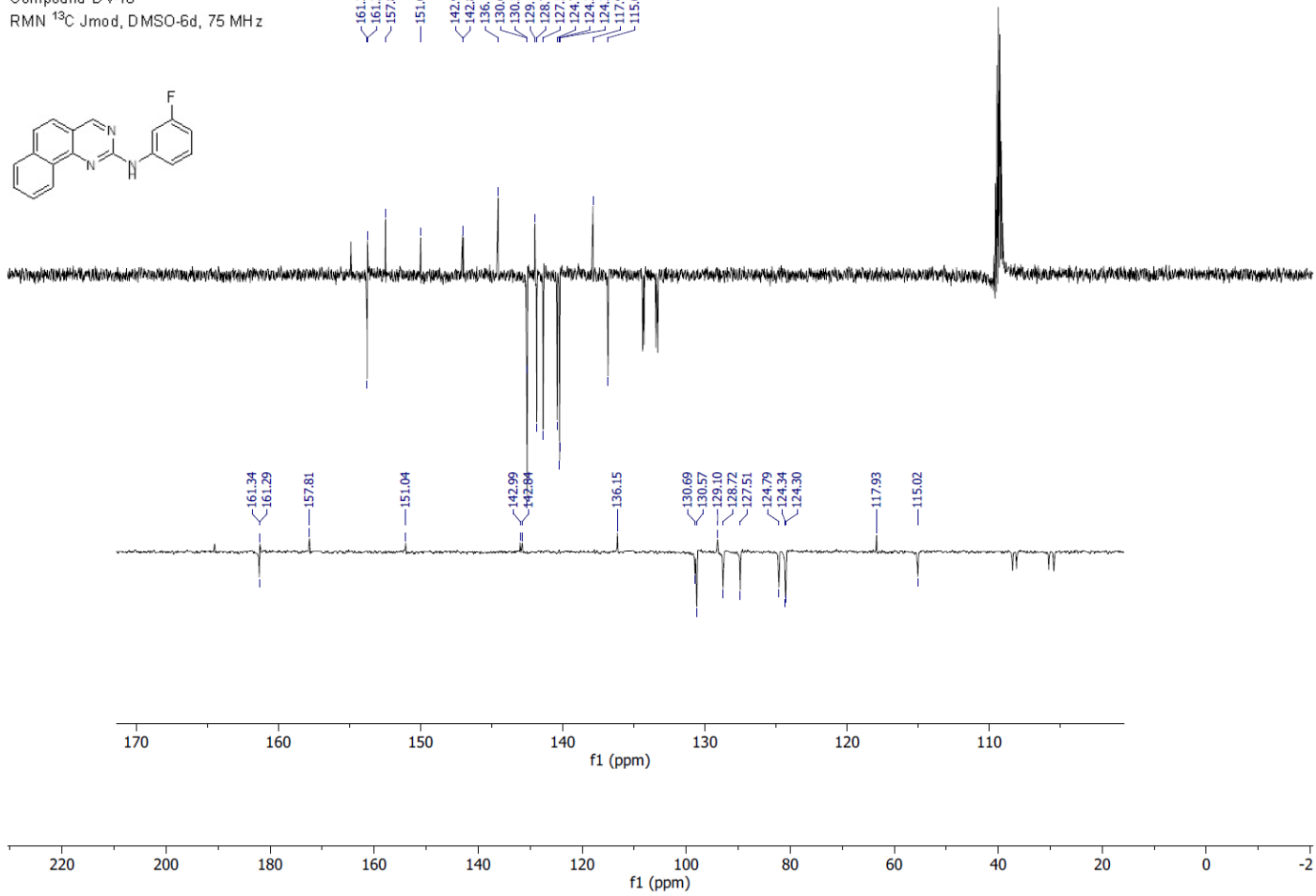
Spectra: ^1H , ^{13}C , ^{13}C Jmod NMR and FT-IR data of compound 4i (DV-10)



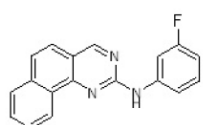
Compound DV-10
RMN ¹³C Jmod, DMSO-6d, 75 MHz



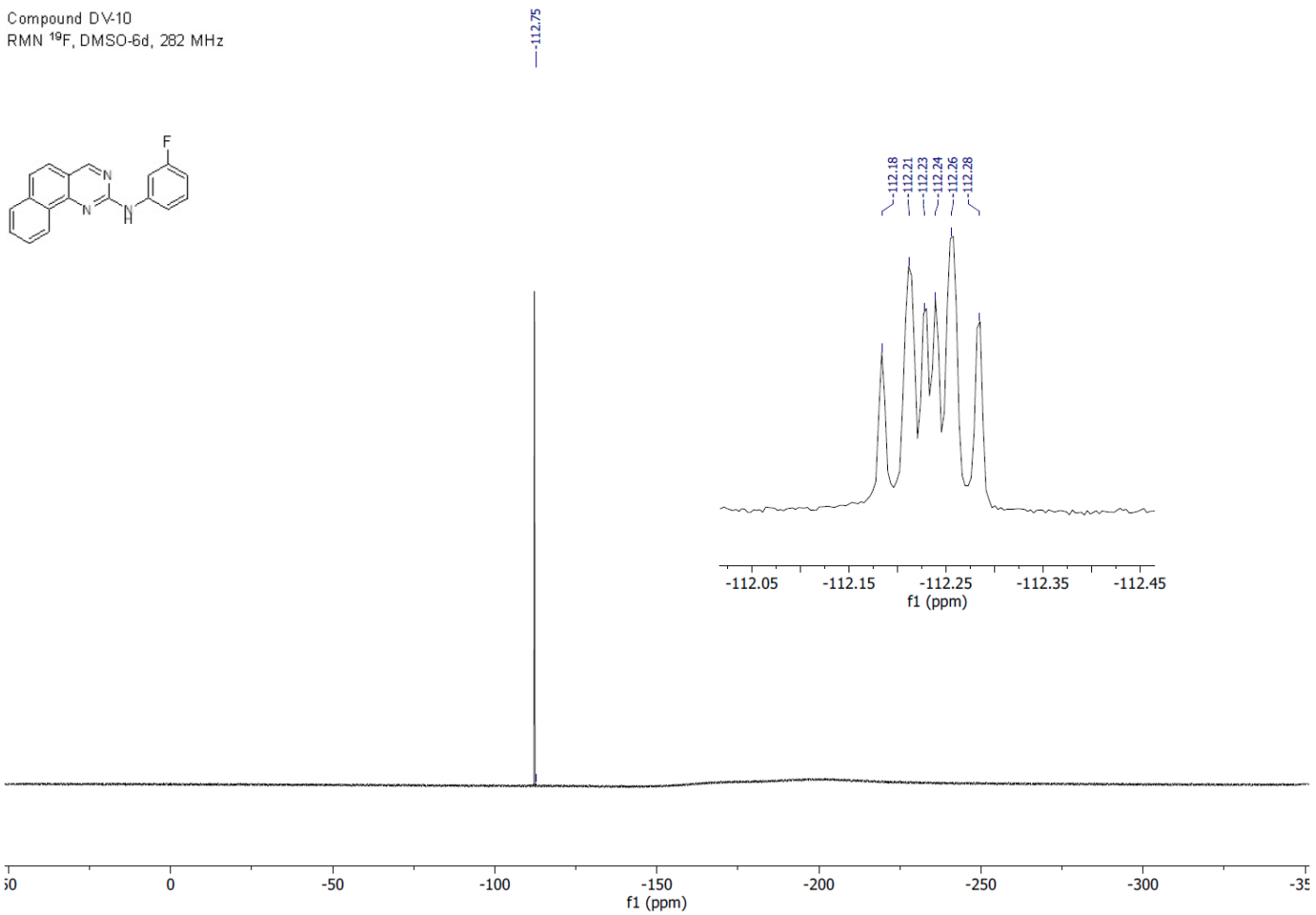
161.34
161.29
157.81
151.04
142.99
142.84
136.15
130.69
130.57
129.10
128.72
127.51
124.79
124.34
124.30
117.93
115.02

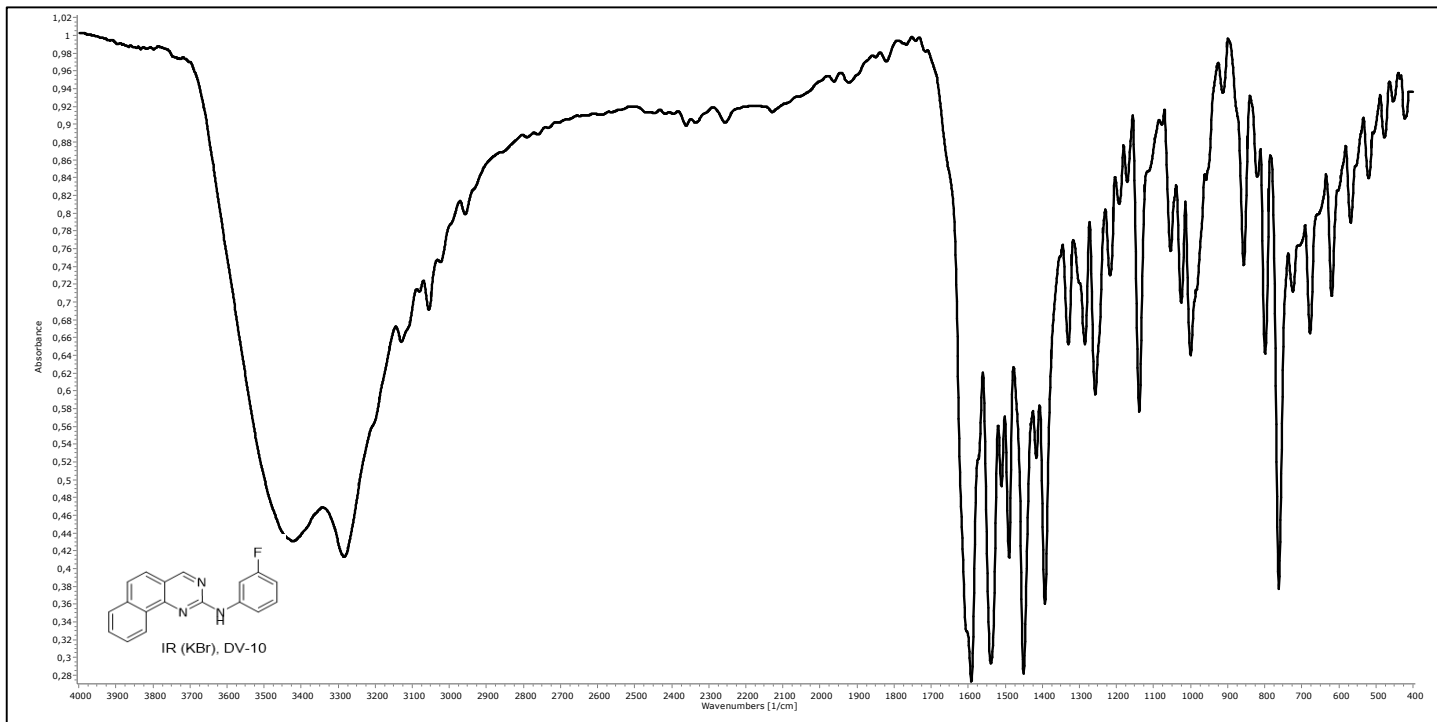


Compound DV-10
RMN ¹⁹F, DMSO-6d, 282 MHz

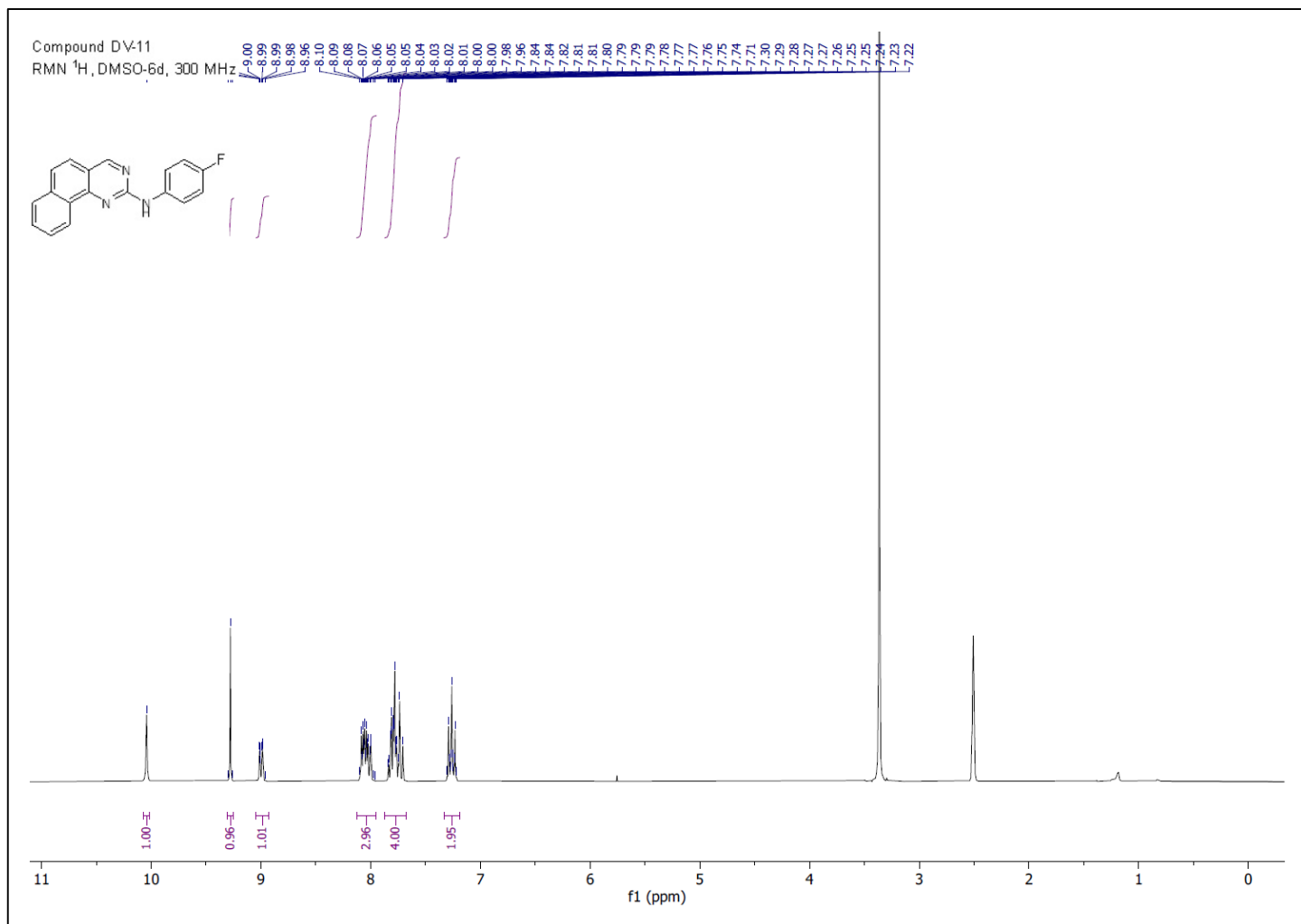
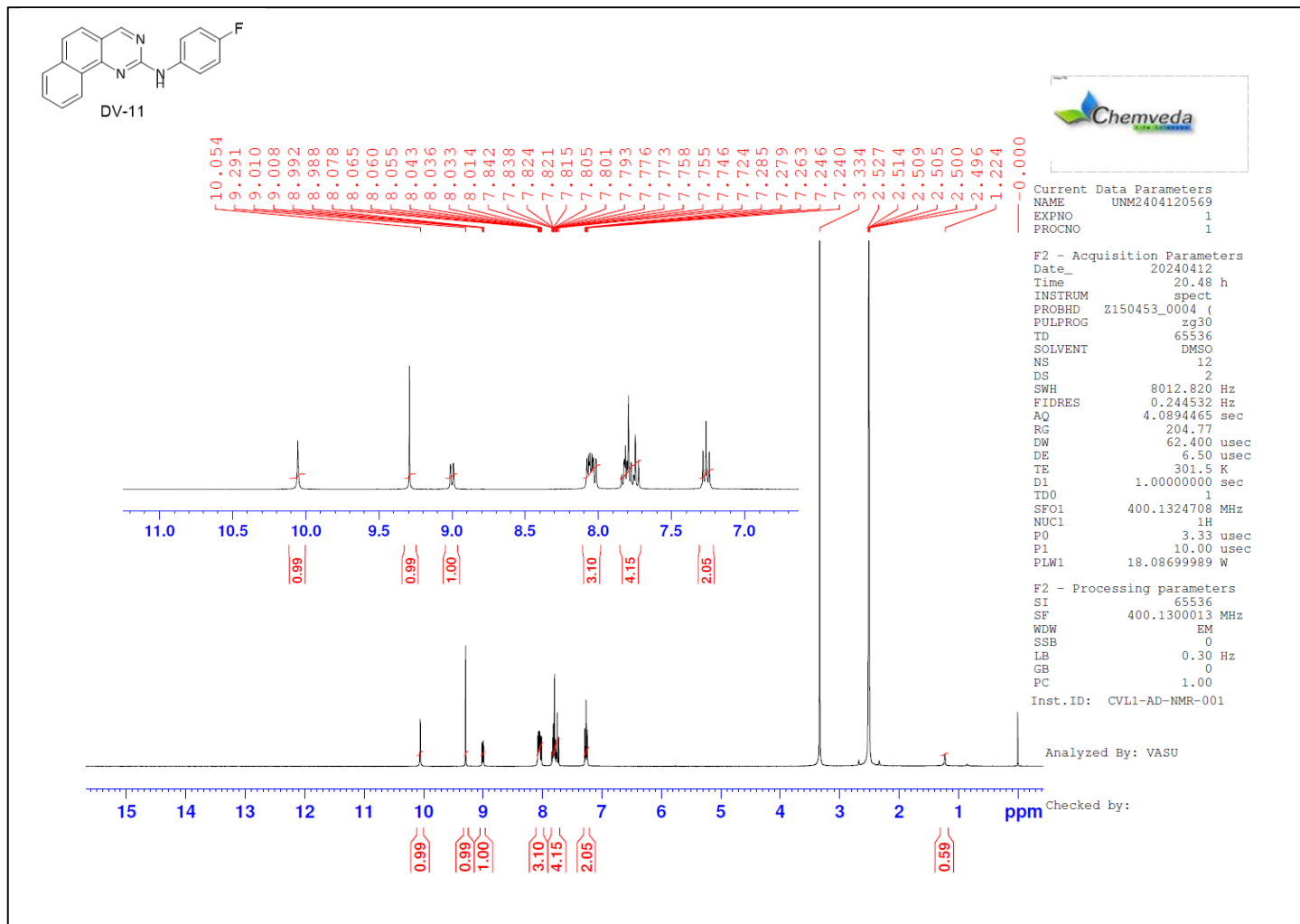


112.75

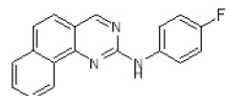




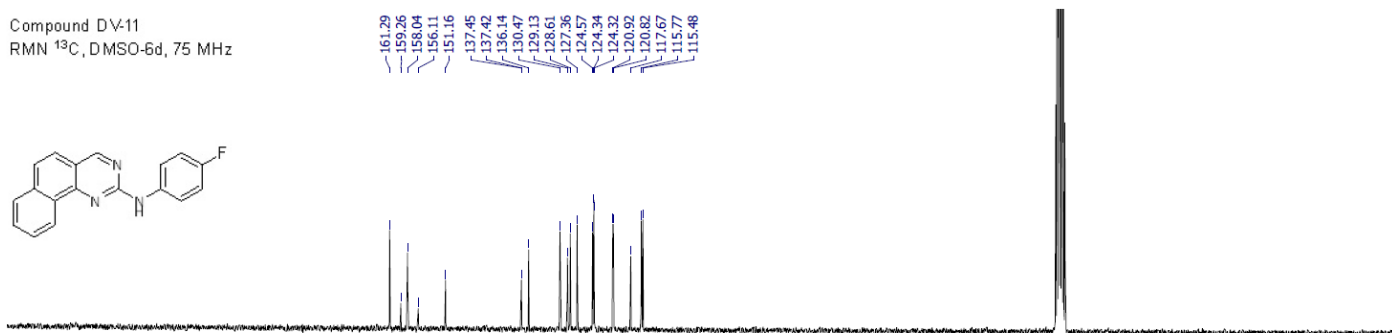
Spectra: ^1H , ^{13}C , ^{13}C Jmod NMR and FT-IR data of compound 4j (DV-11)



Compound DV-11
RMN ¹³C, DMSO-6d, 75 MHz

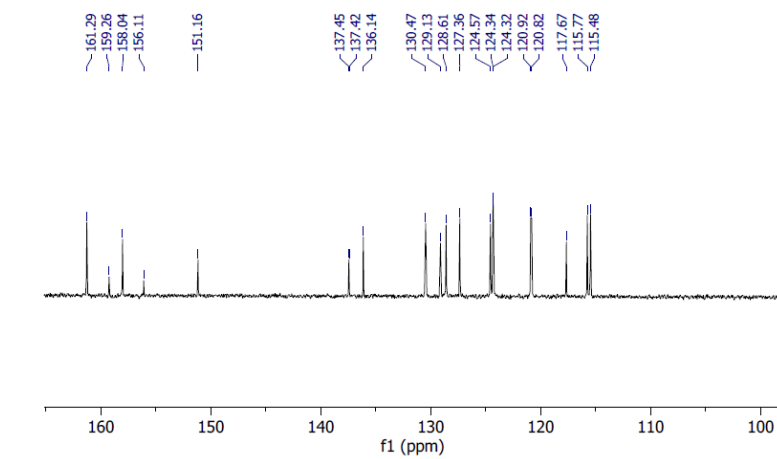


161.29
159.26
158.04
156.11
151.16
137.45
137.42
136.14
130.47
129.13
128.61
127.36
124.57
124.34
124.32
120.92
120.82
117.67
115.77
115.48



161.29
159.26
158.04
156.11
151.16

137.45
136.14
130.47
129.13
128.61
127.36
124.57
124.34
124.32
120.92
120.82
117.67
115.77
115.48



159.26
158.04
156.11
120.92
120.82
115.77
115.48

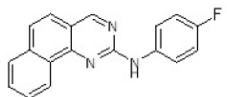
158.5
155.5

120.9
120.5

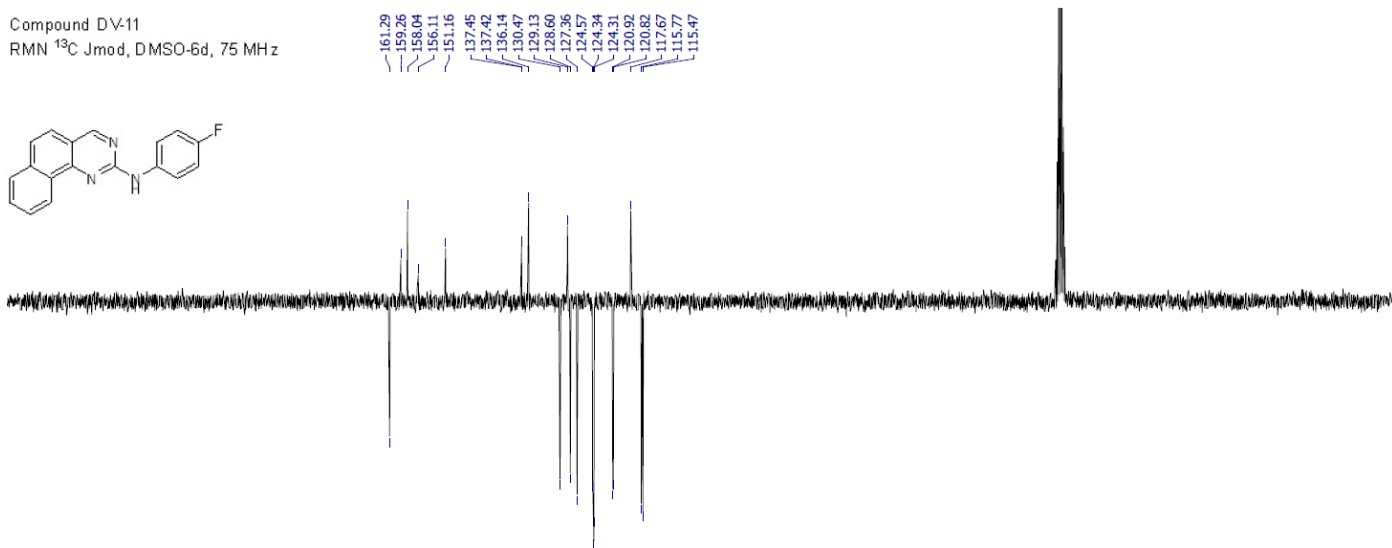
115.8
114.6

220 200 180 160 140 120 100 80 60 40 20 0 -2
f1 (ppm)

Compound DV-11
RMN ¹³C Jmod, DMSO-6d, 75 MHz



161.29
159.26
158.04
156.11
151.16
137.45
137.42
136.14
130.47
129.13
128.60
127.36
124.57
124.31
124.31
120.92
120.82
117.67
115.77
115.47



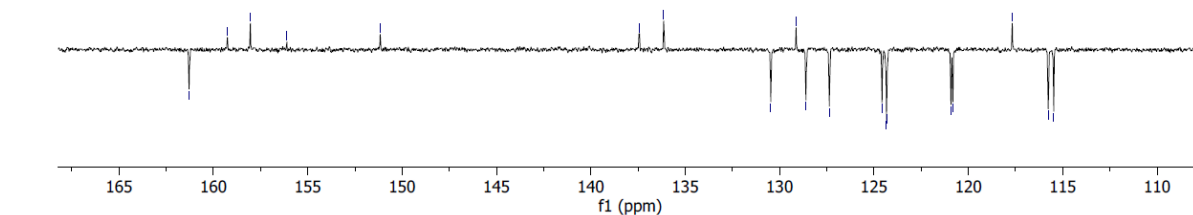
161.29
159.26
158.04
156.11

151.16
137.45
137.42
136.14

130.47
129.13
128.60
127.36

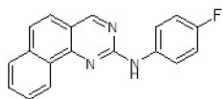
124.57
124.31
124.31
120.92
120.82

117.67
115.77
115.47

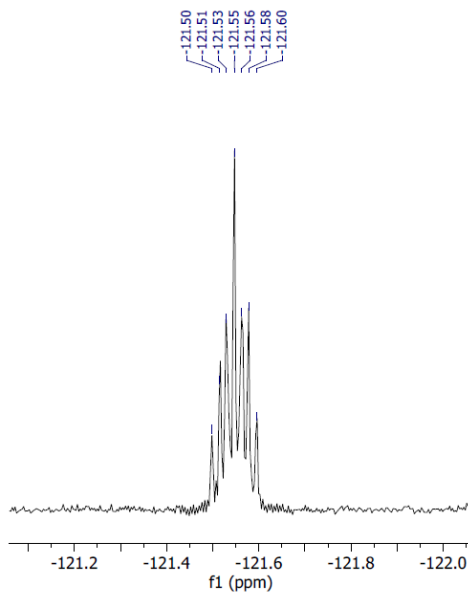


220 200 180 160 140 120 100 80 60 40 20 0 -2
f1 (ppm)

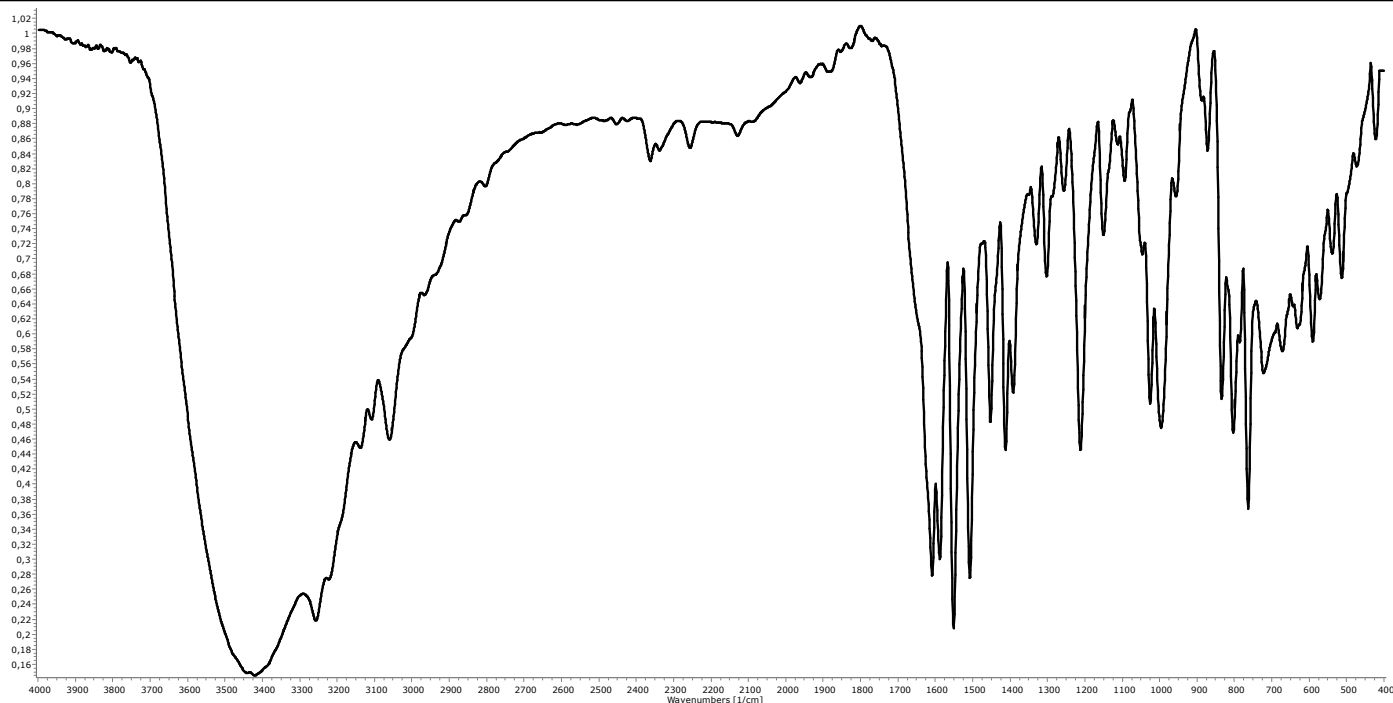
Compound DV-11
RMN ^{19}F , DMSO- d_6 , 282 MHz



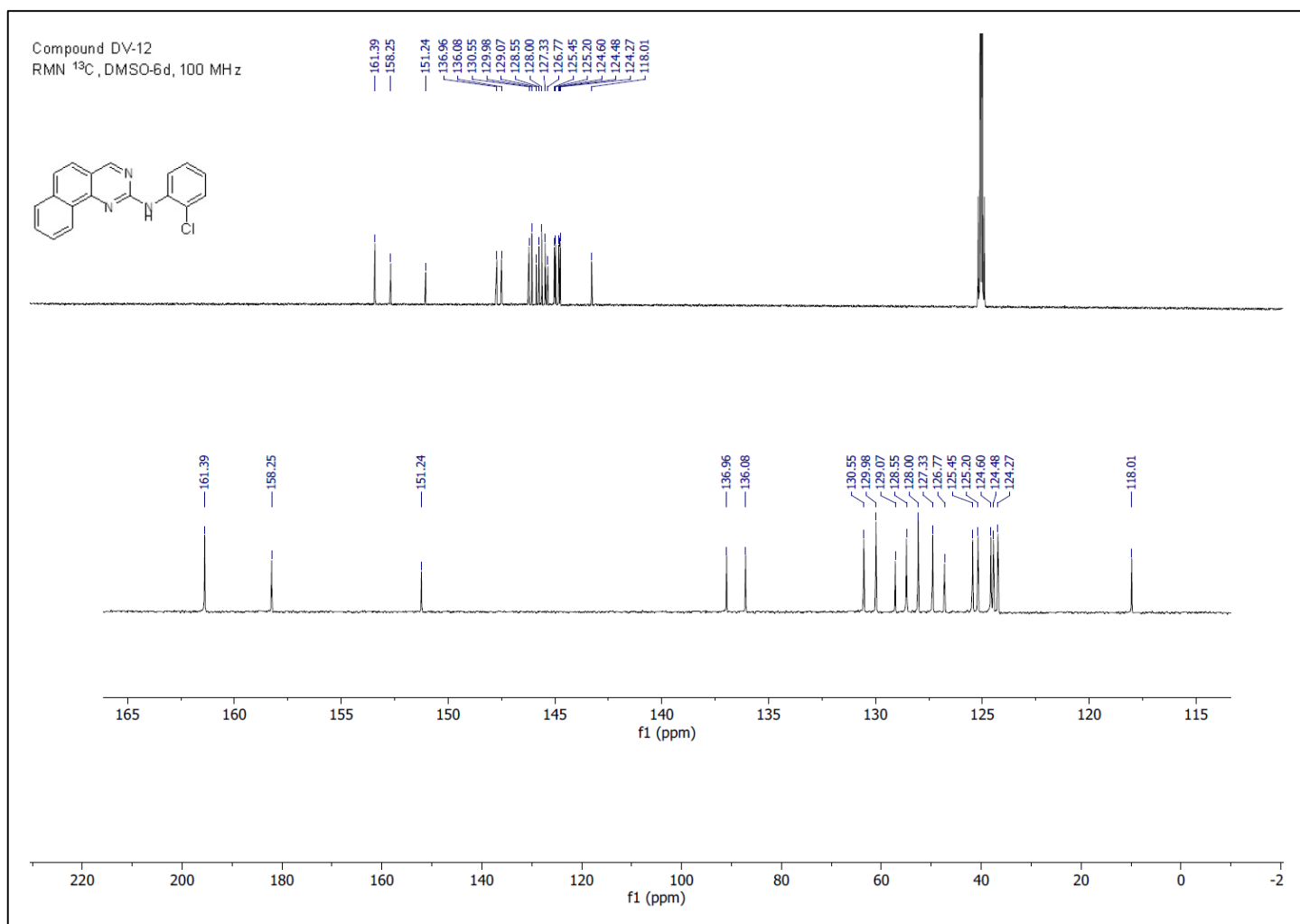
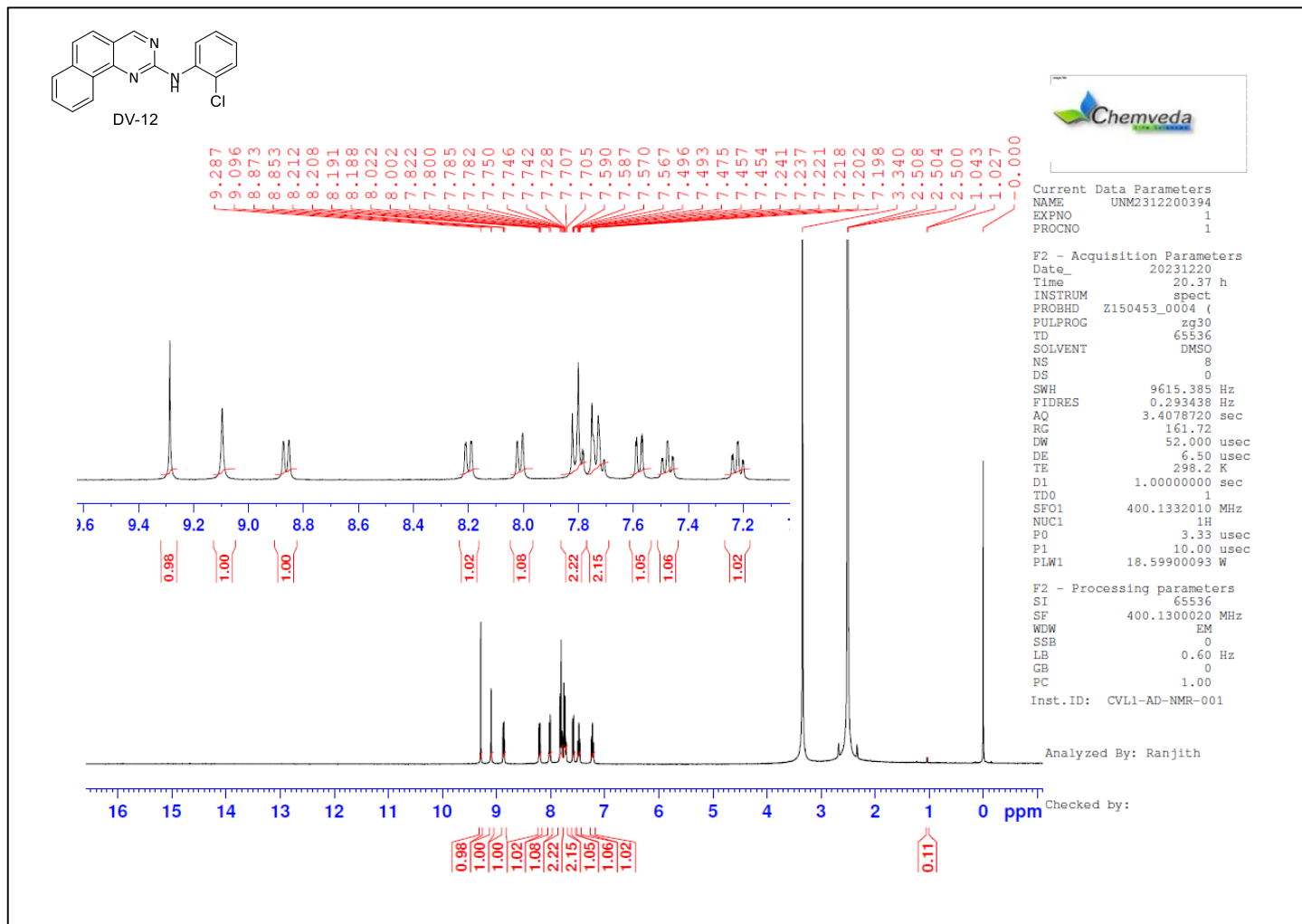
-121.54

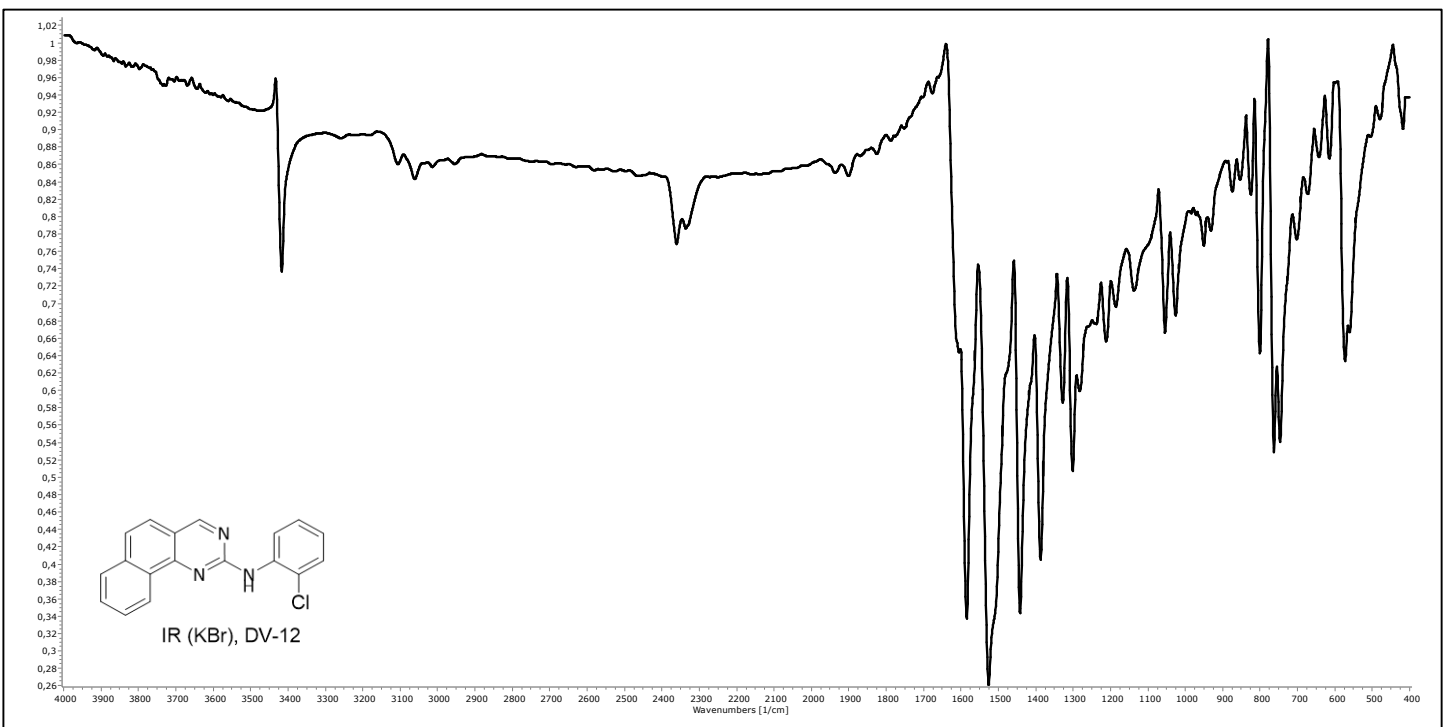
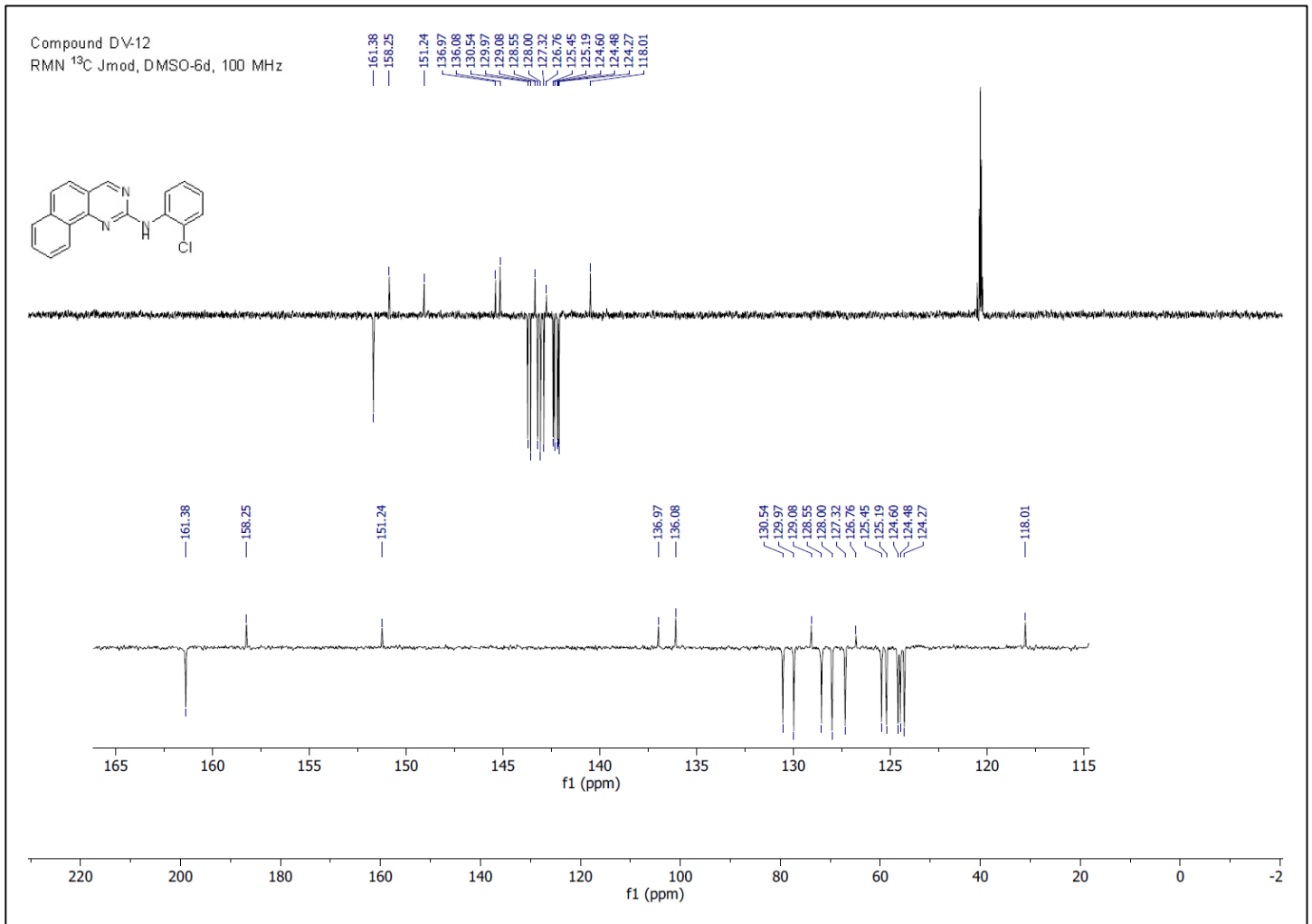


50 0 -50 -100 -150 -200 -250 -300 -350
f1 (ppm)

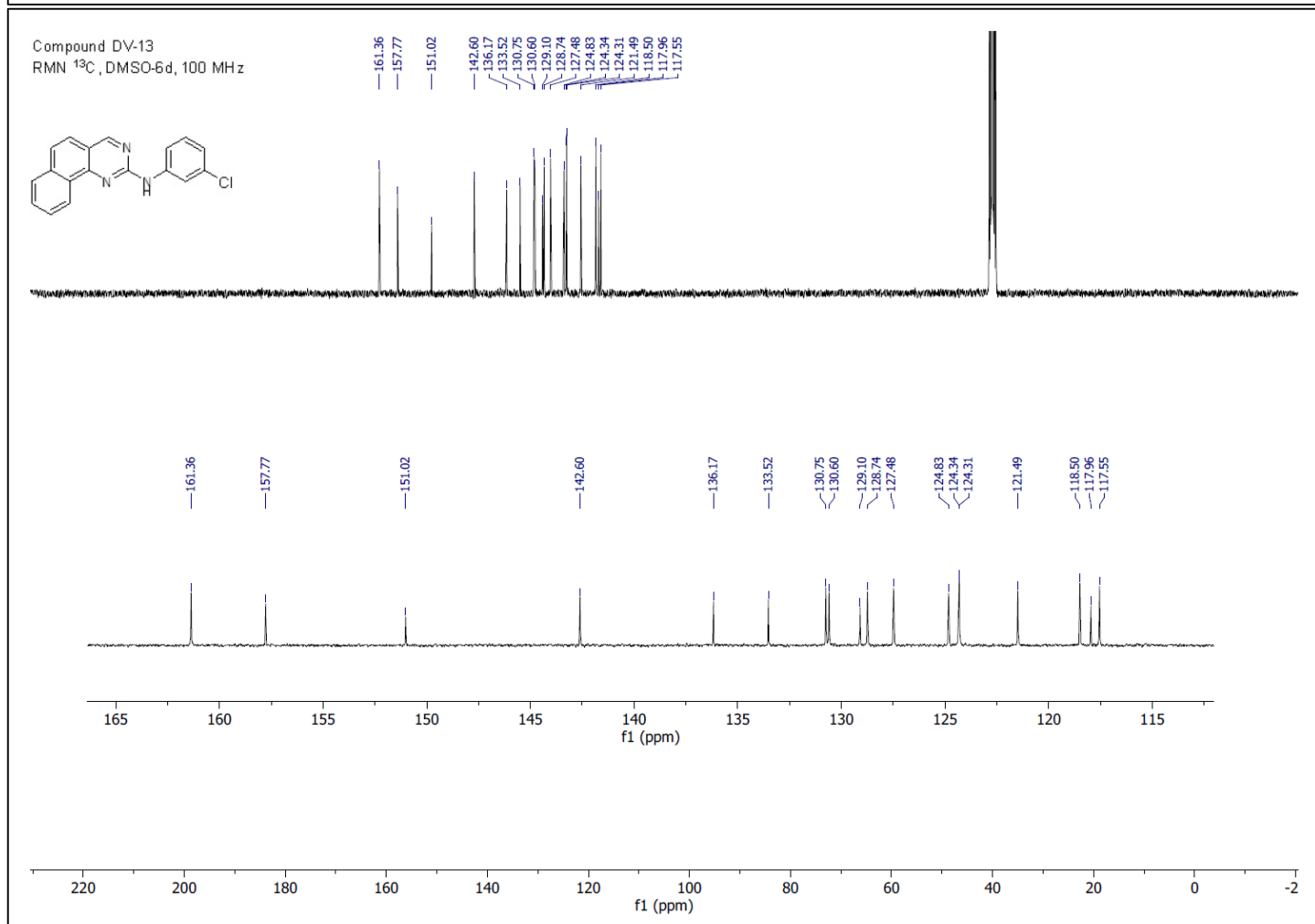
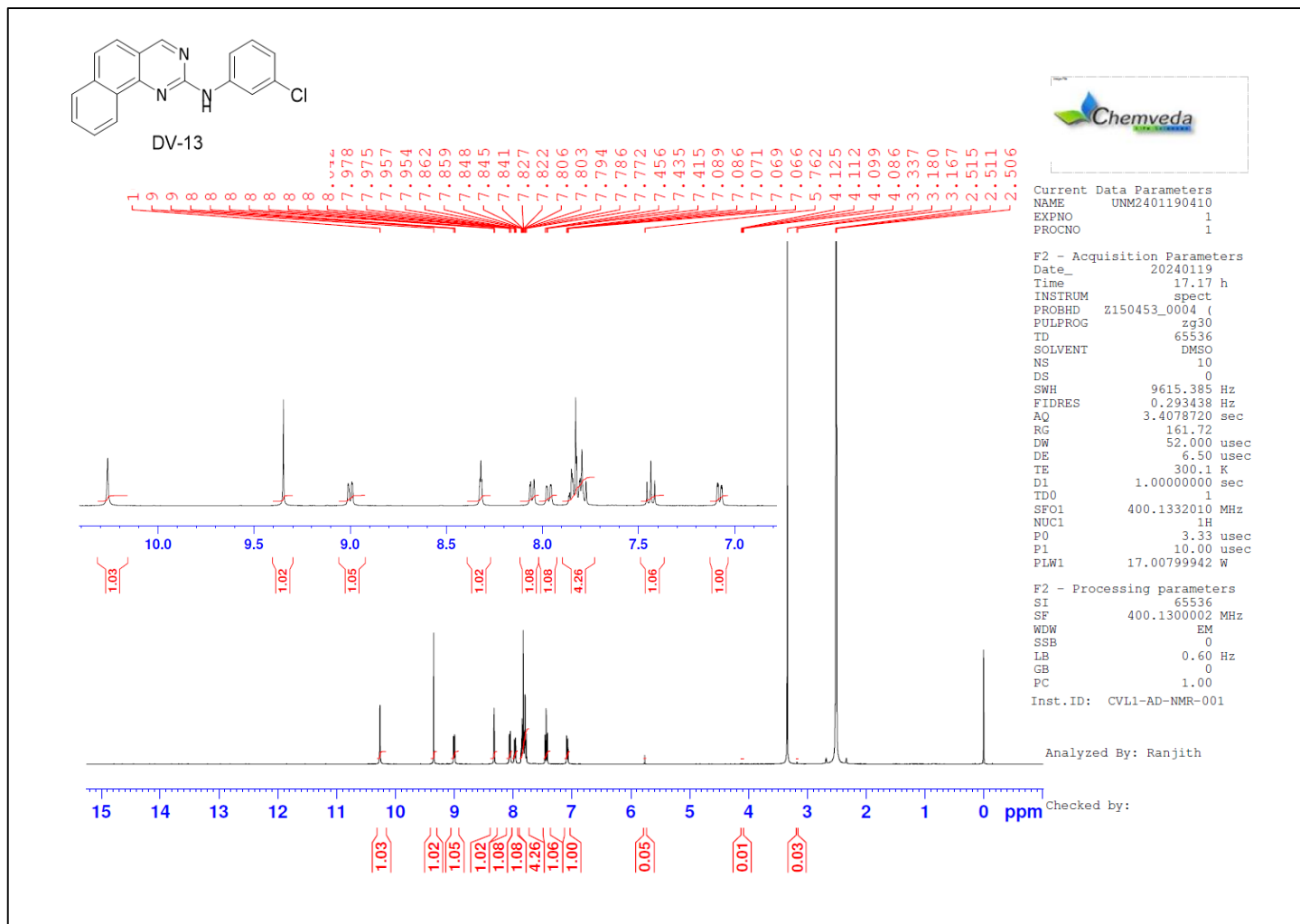


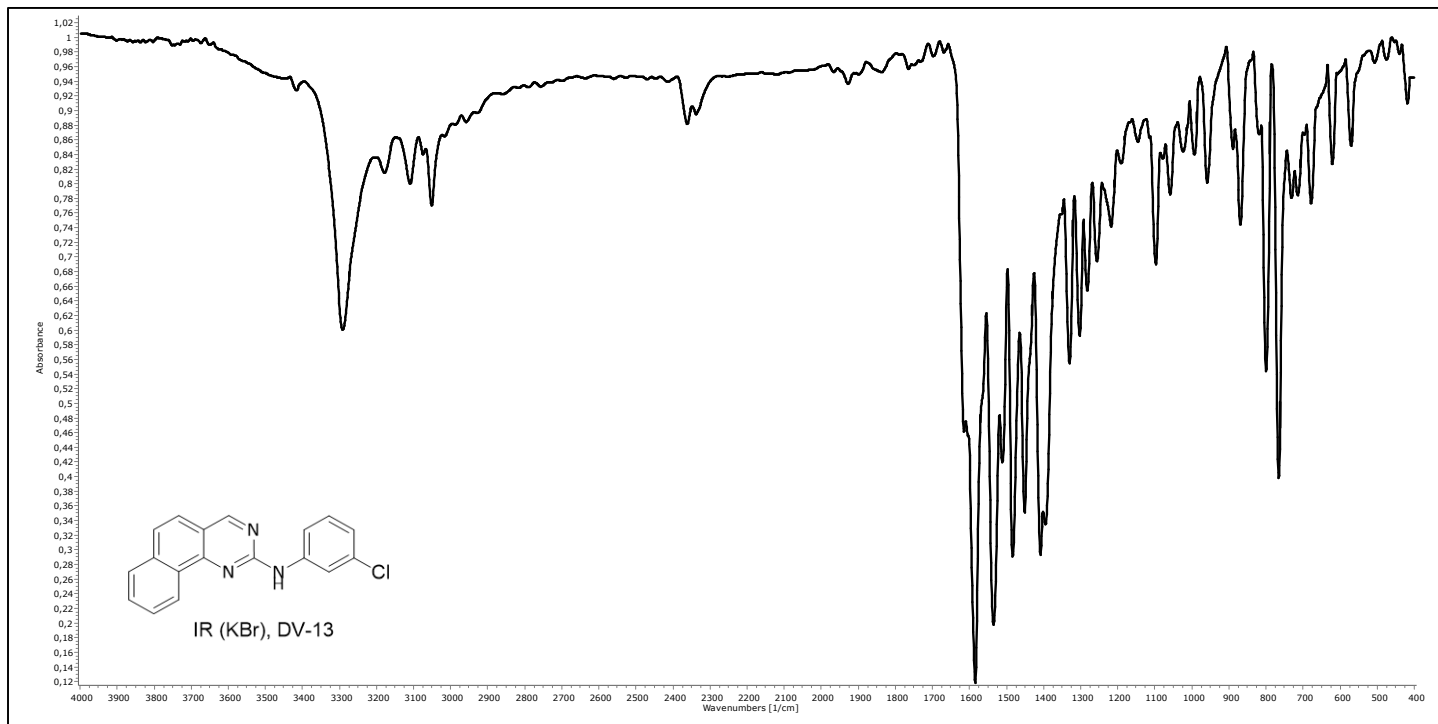
Spectra: ^1H , ^{13}C , ^{13}C Jmod NMR and FT-IR data of compound 4k (DV-12)



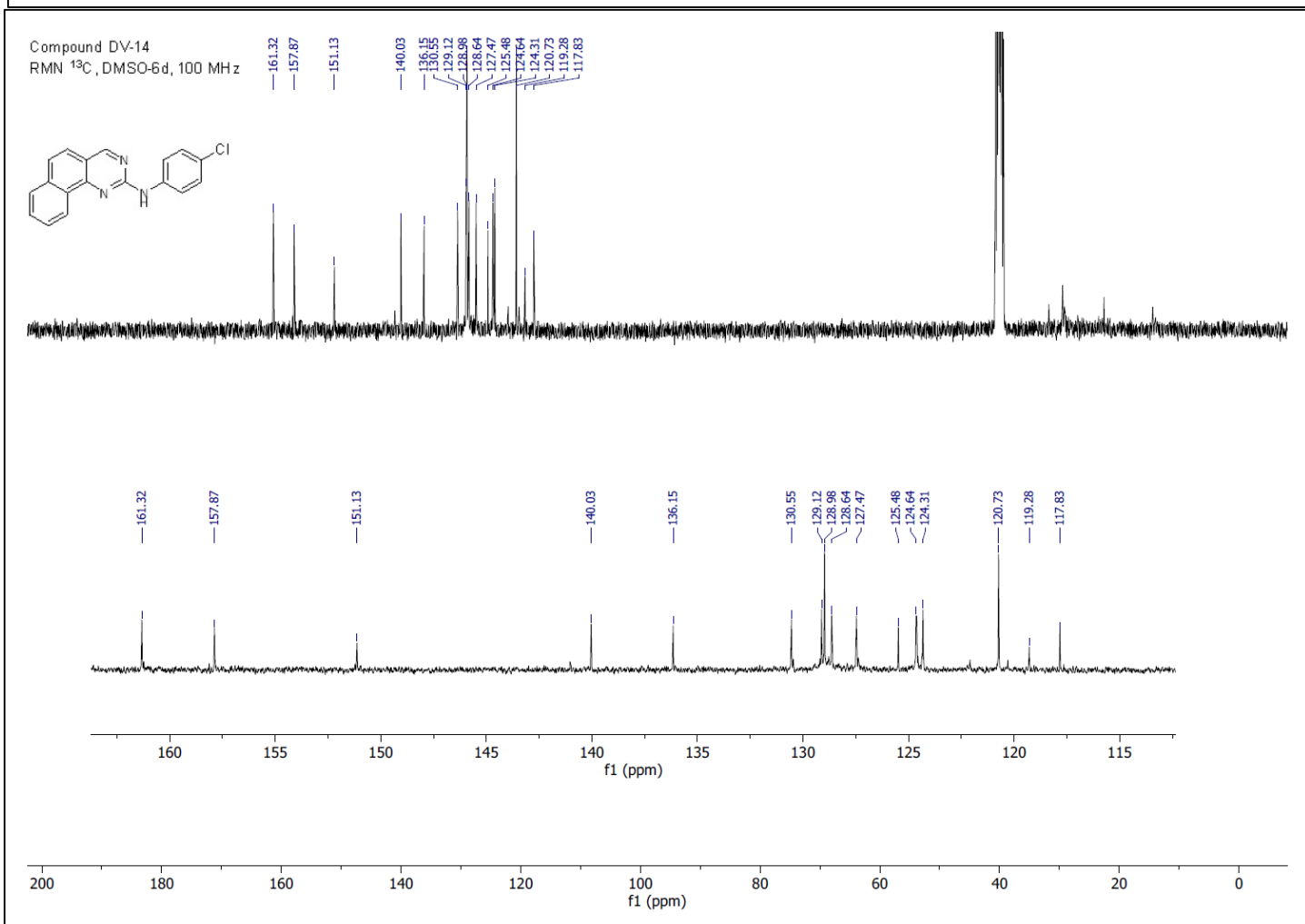
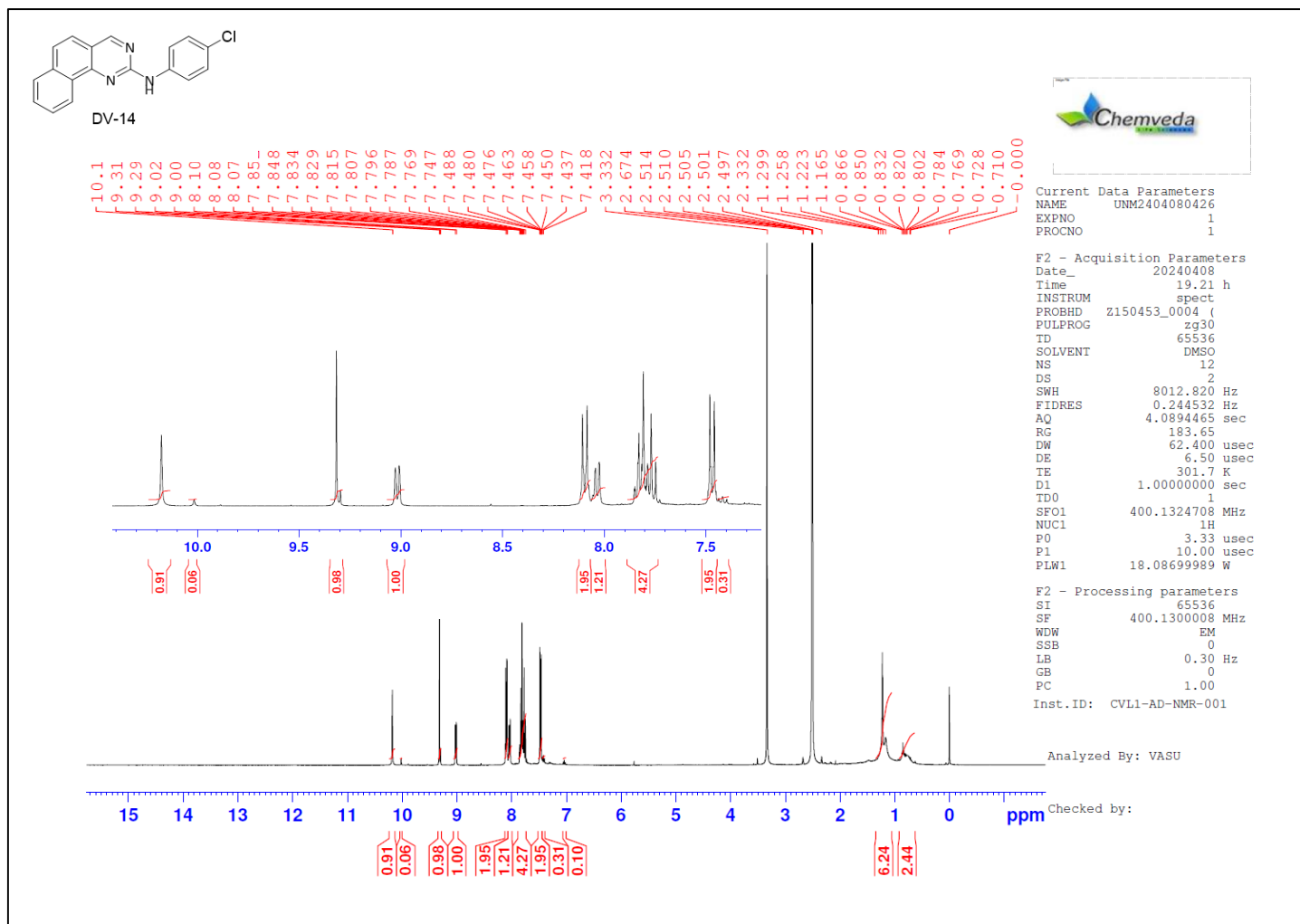


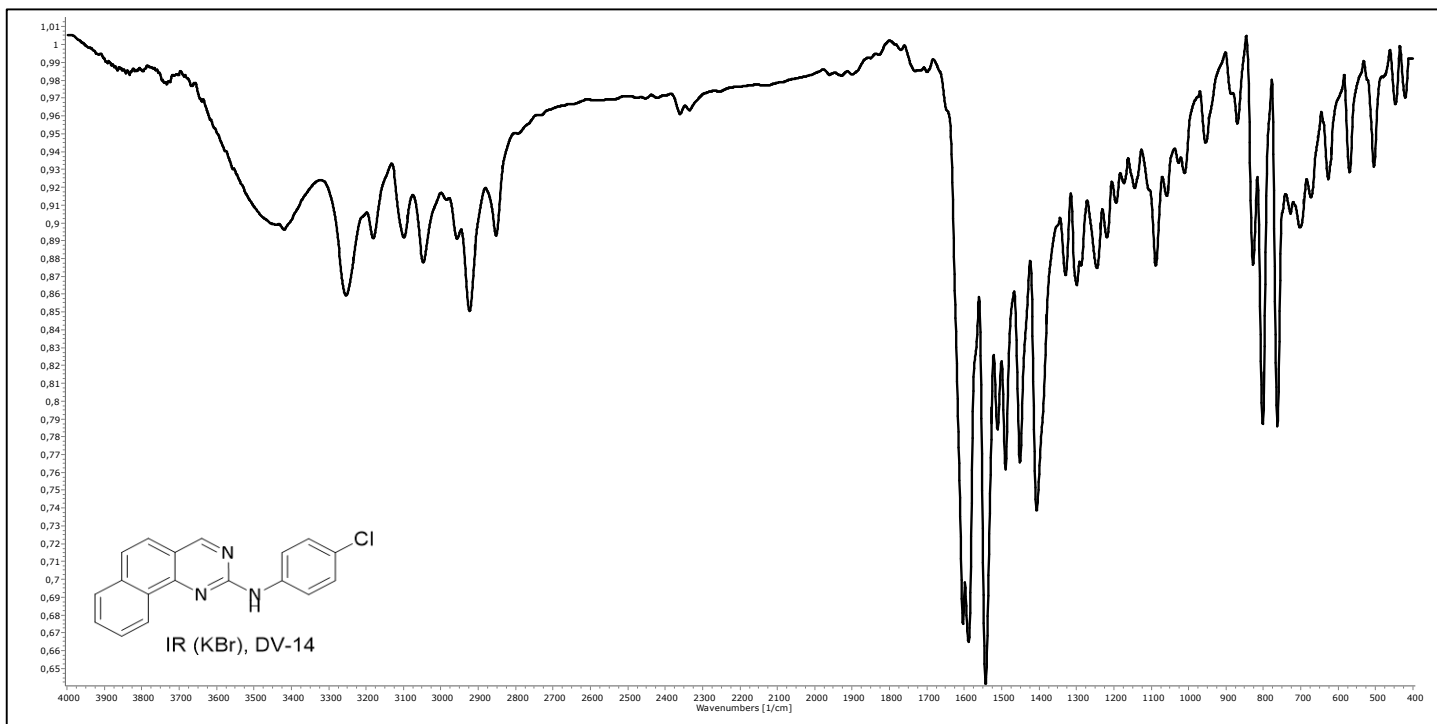
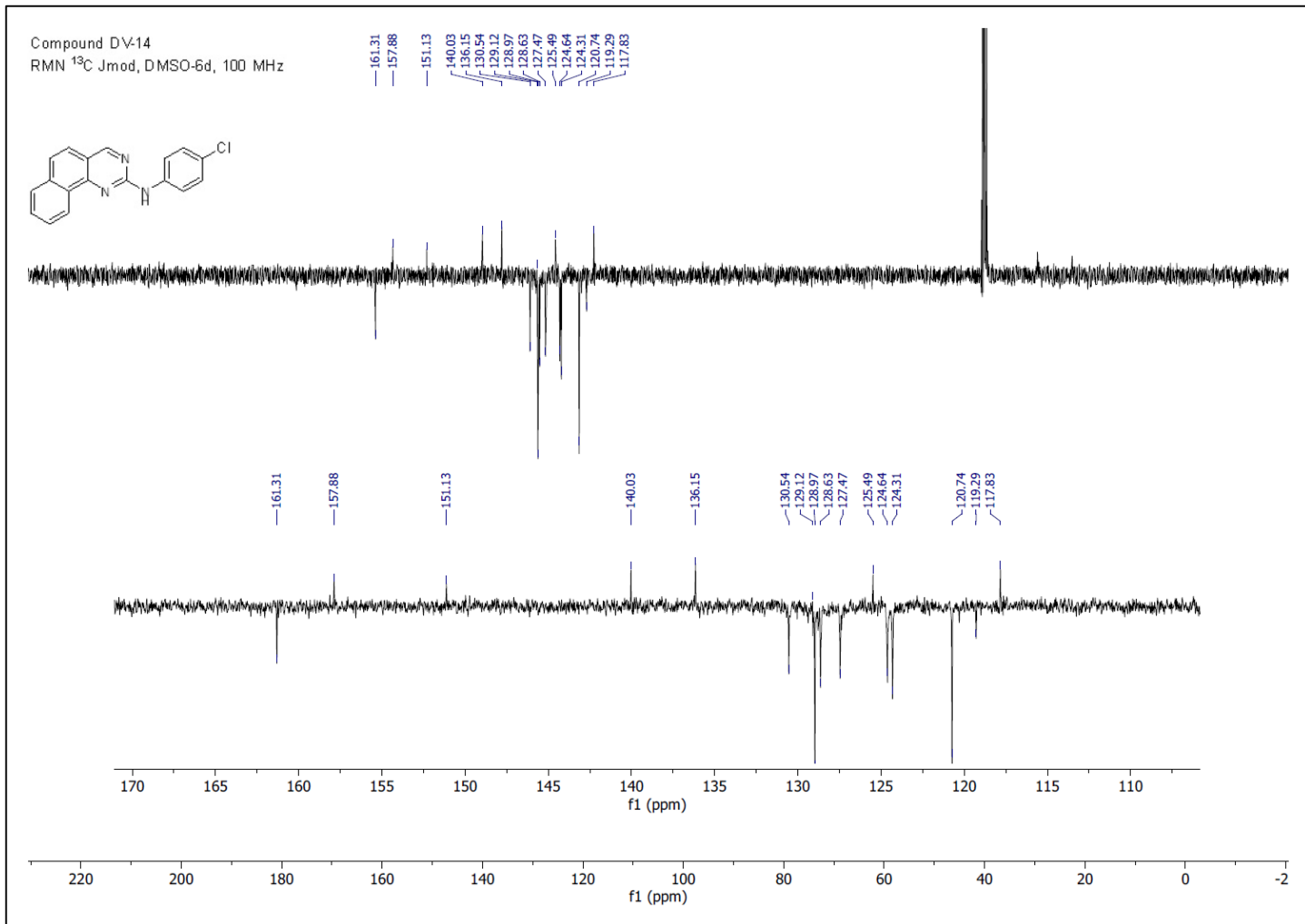
Spectra: ^1H , ^{13}C , ^{13}C Jmod NMR and FT-IR data of compound 4l (DV-13)



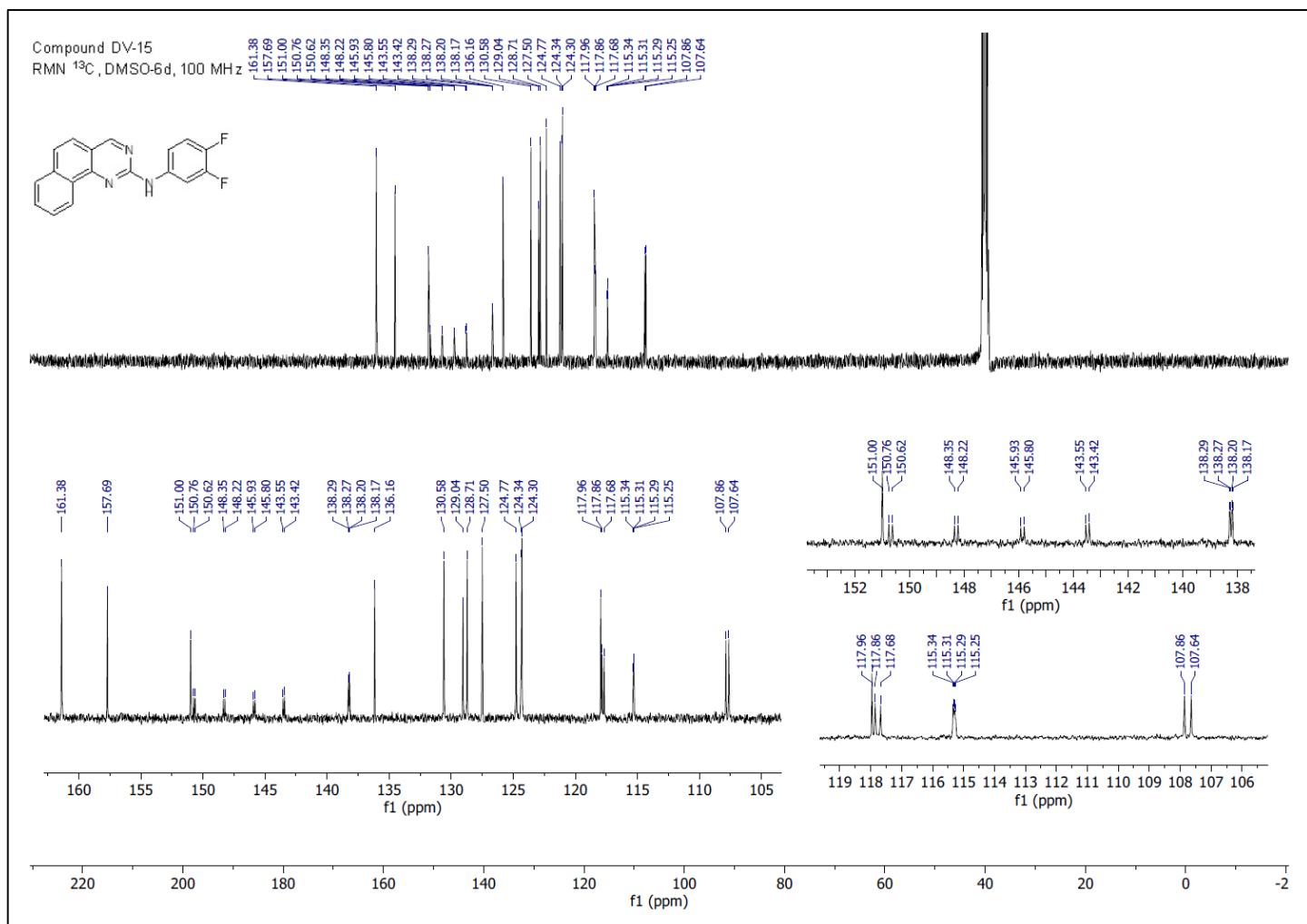
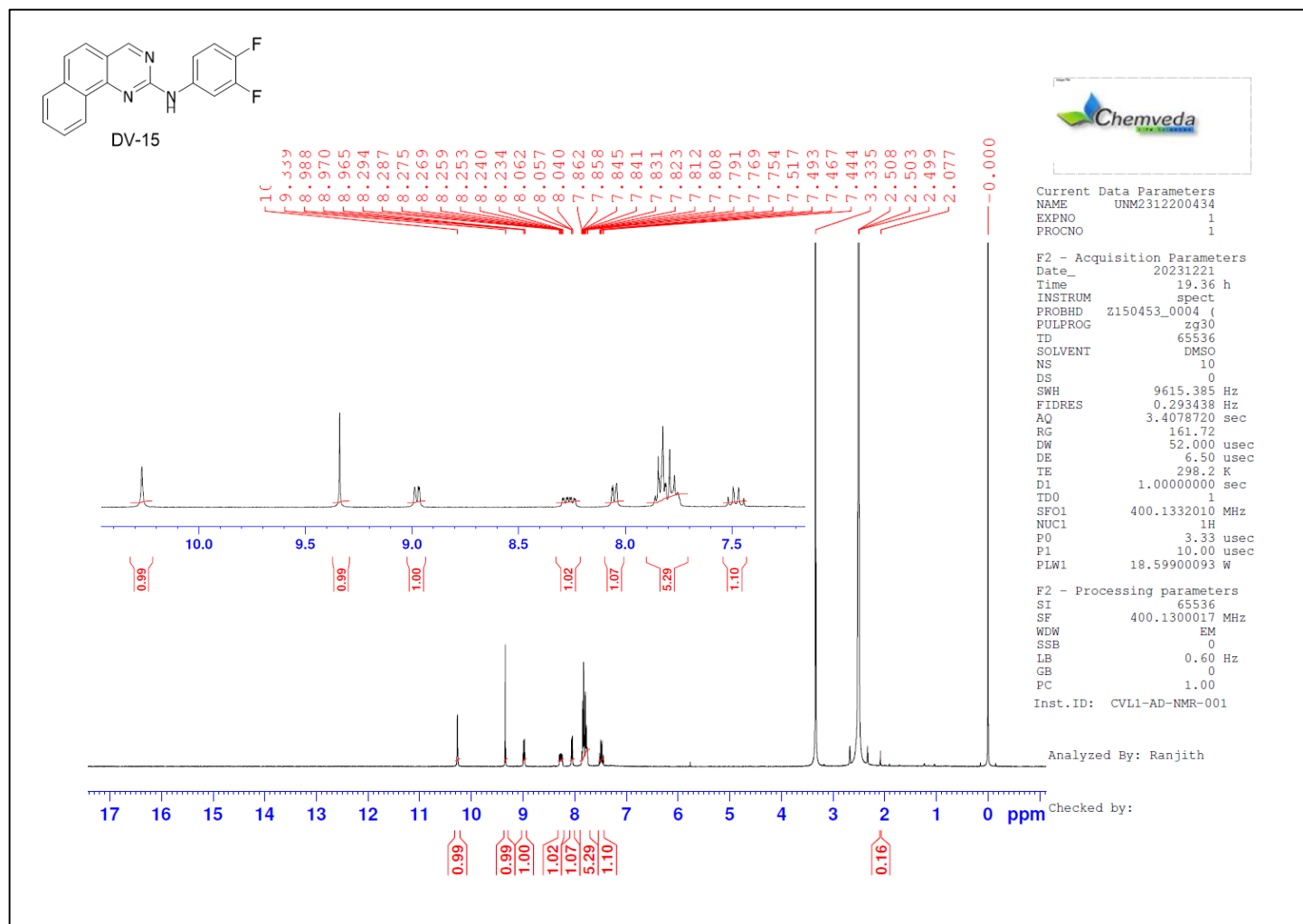


Spectra: ¹H, ¹³C, ¹³C Jmod NMR and FT-IR data of compound 4m (DV-14)



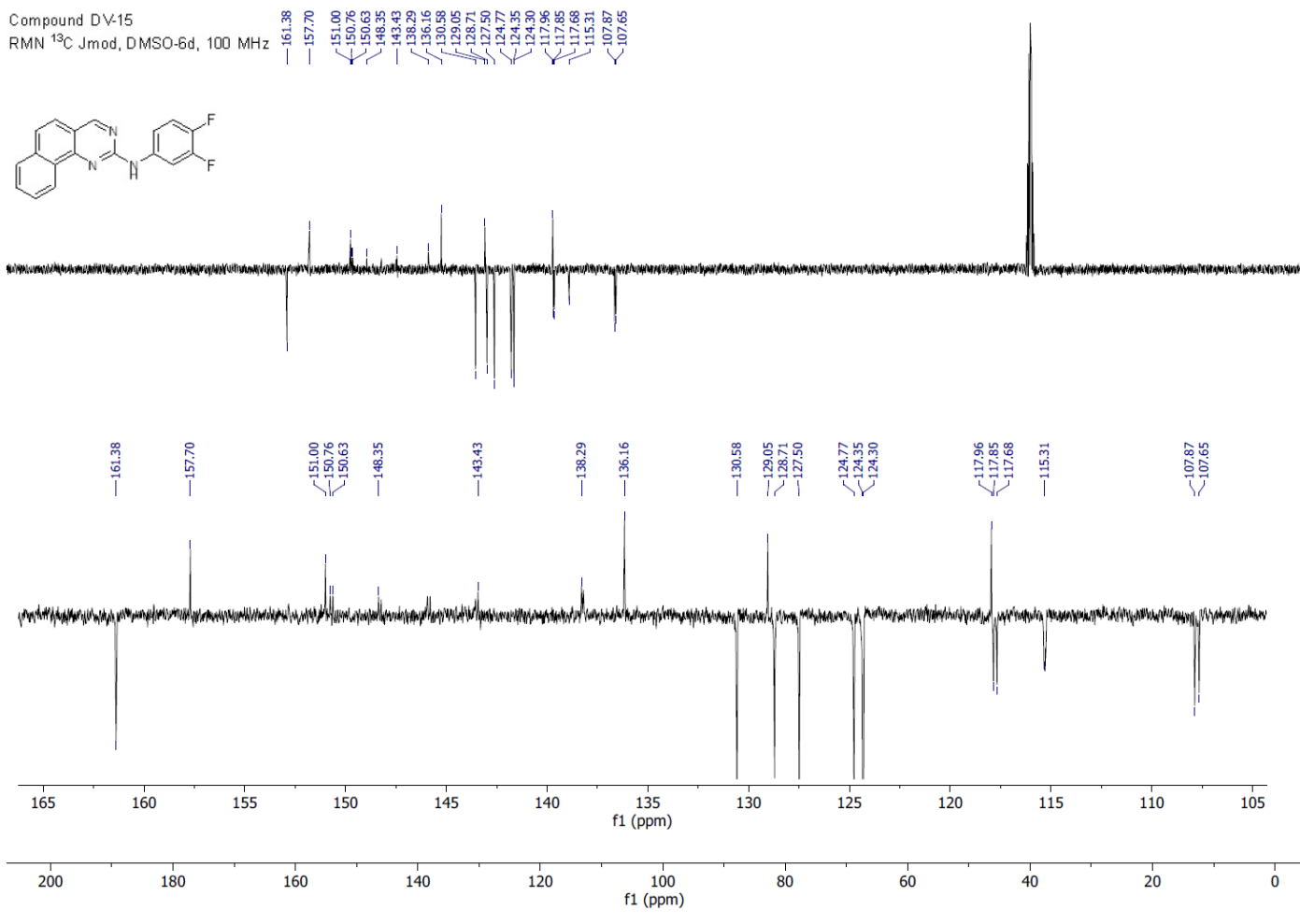
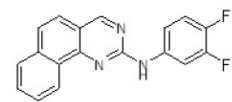


Spectra: ^1H , ^{13}C , ^{13}C Jmod NMR and FT-IR data of compound 4n (DV-15)



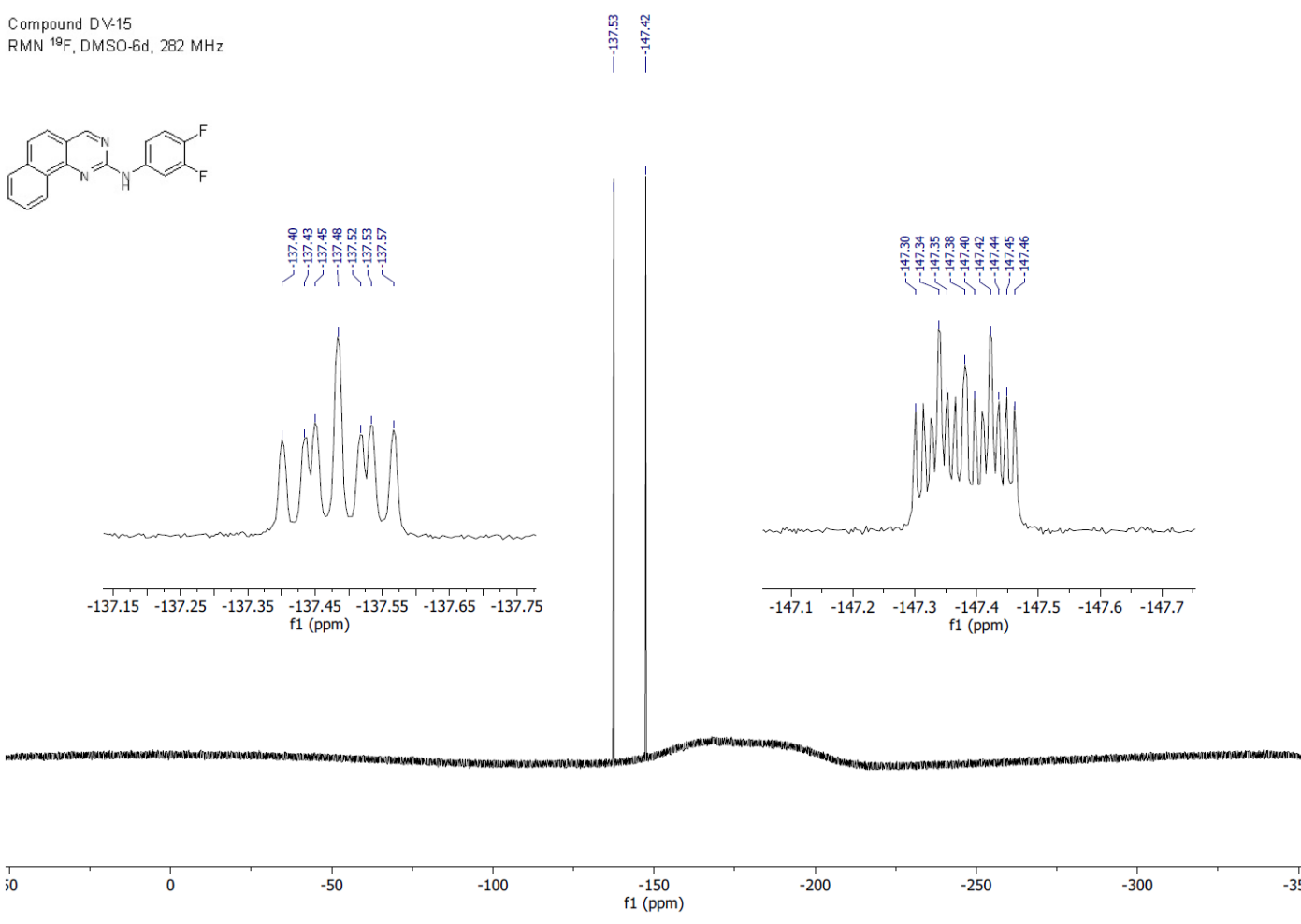
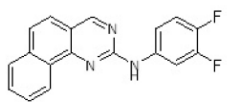
Compound DV-15

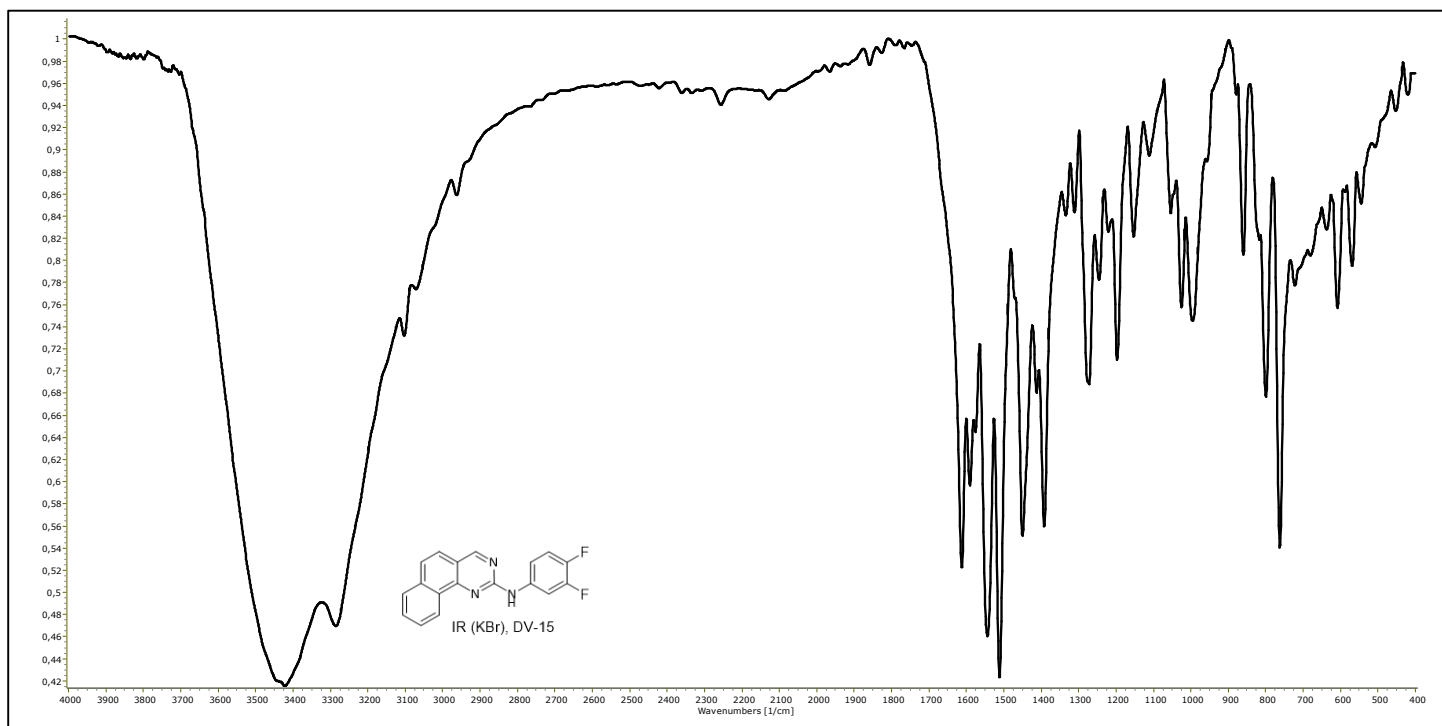
RMN ¹³C Jmod, DMSO-6d, 100 MHz



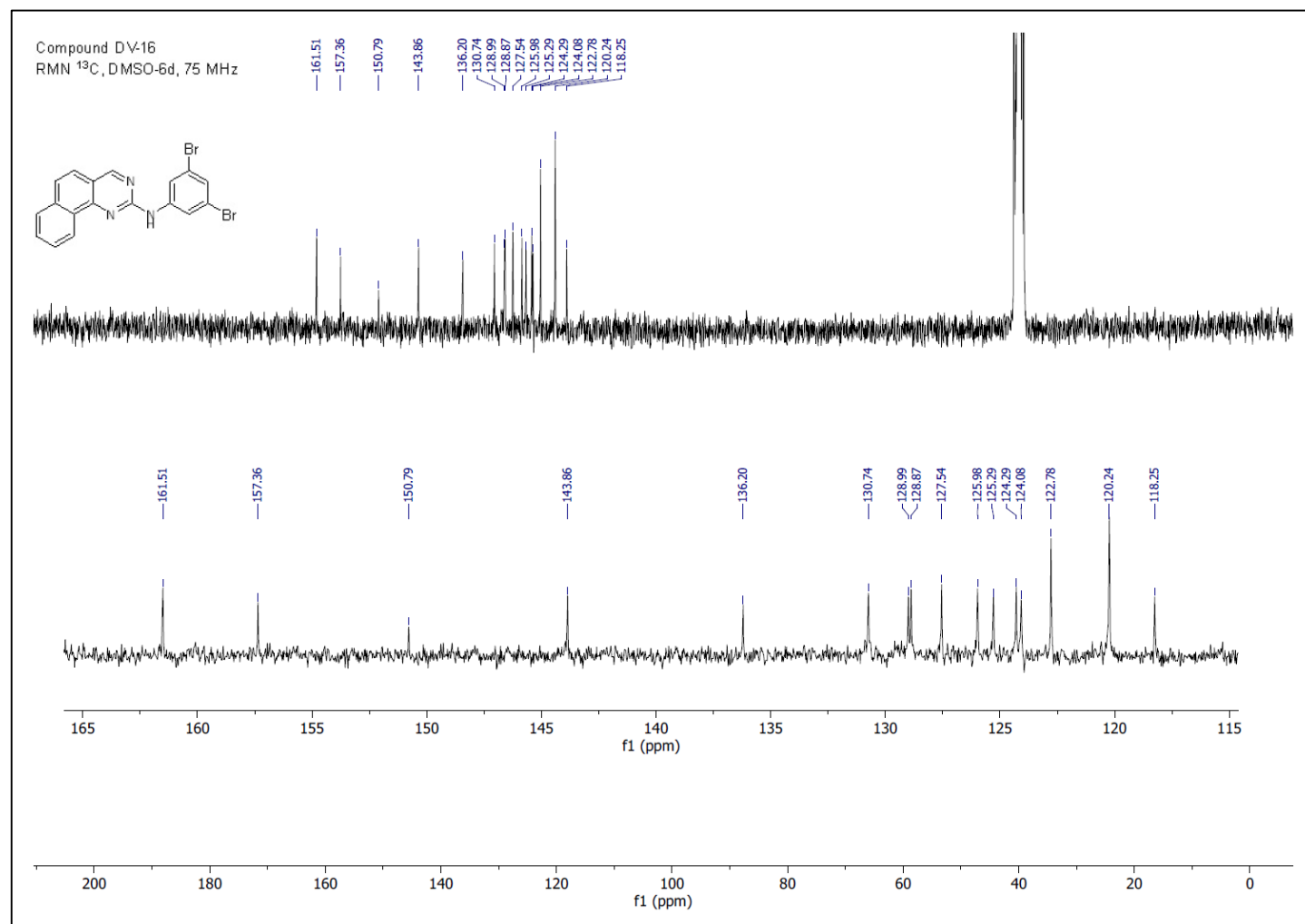
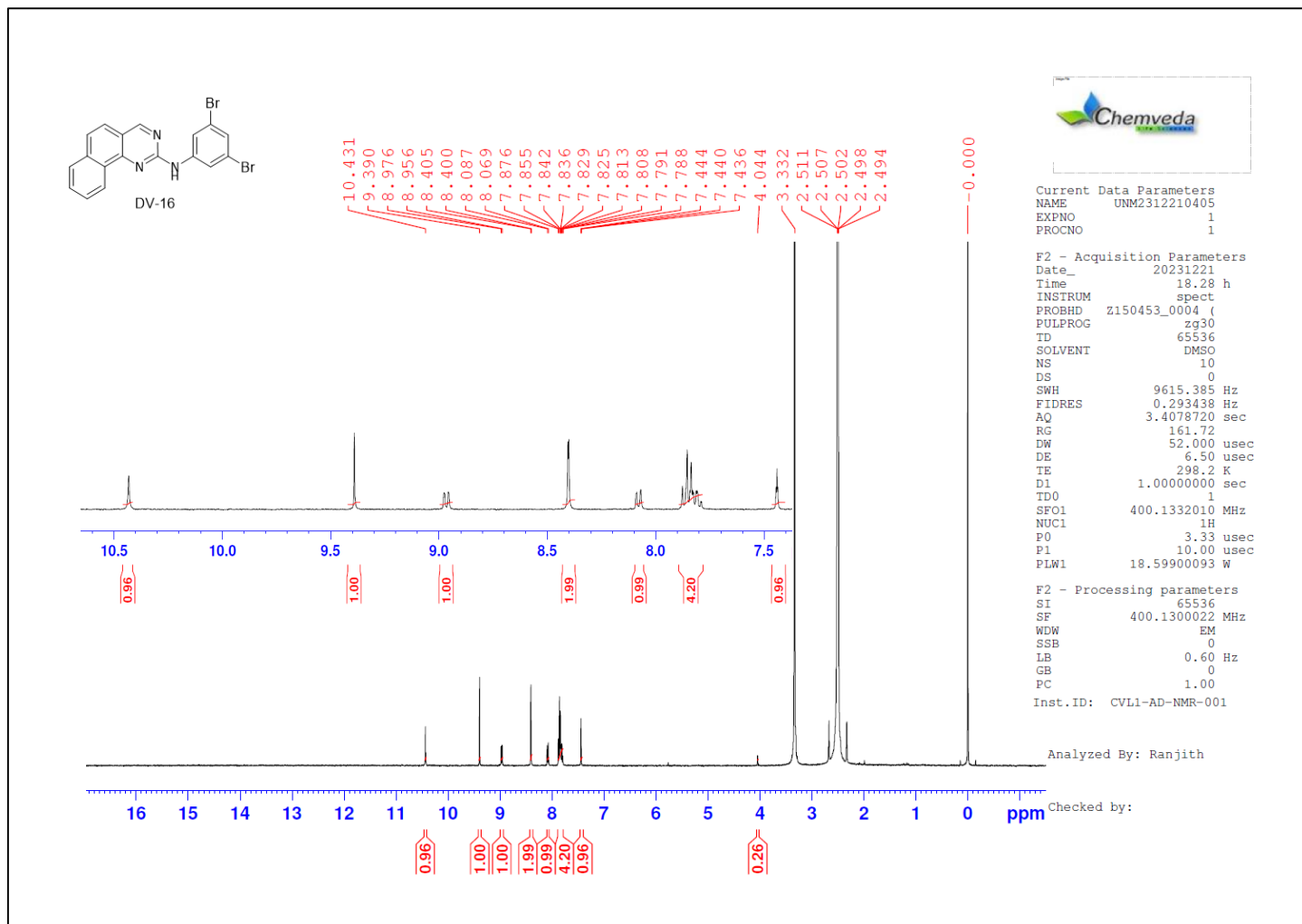
Compound DV-15

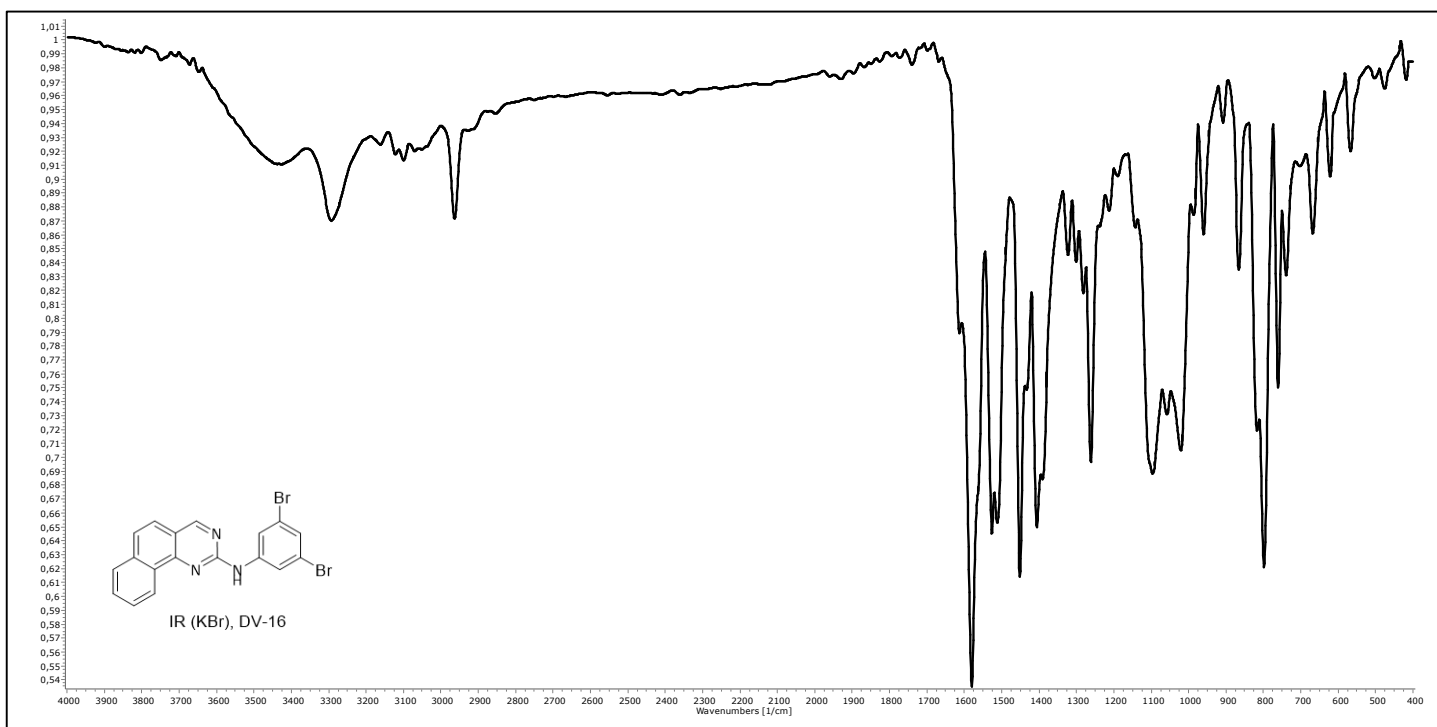
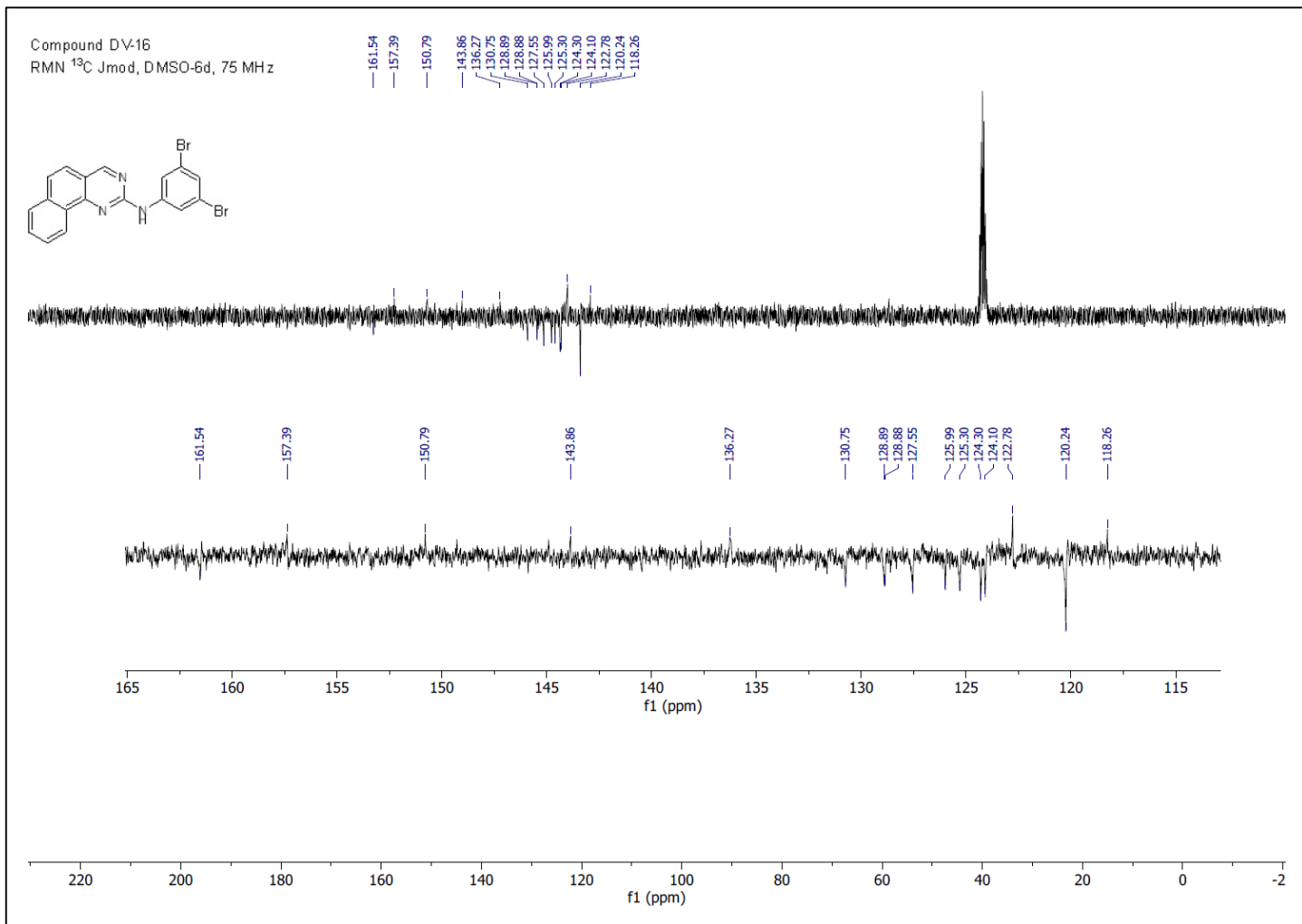
RMN ¹⁹F, DMSO-6d, 282 MHz



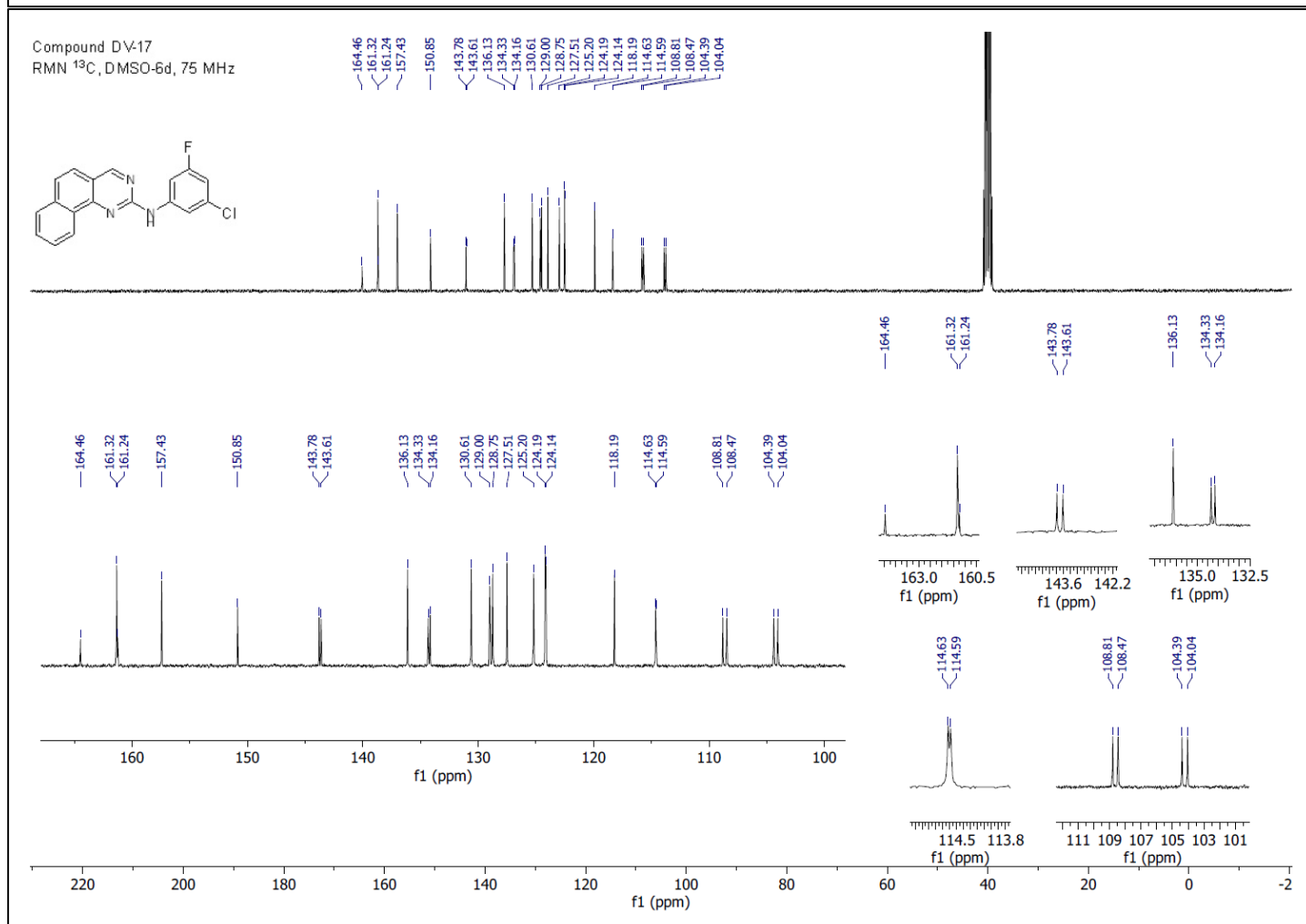
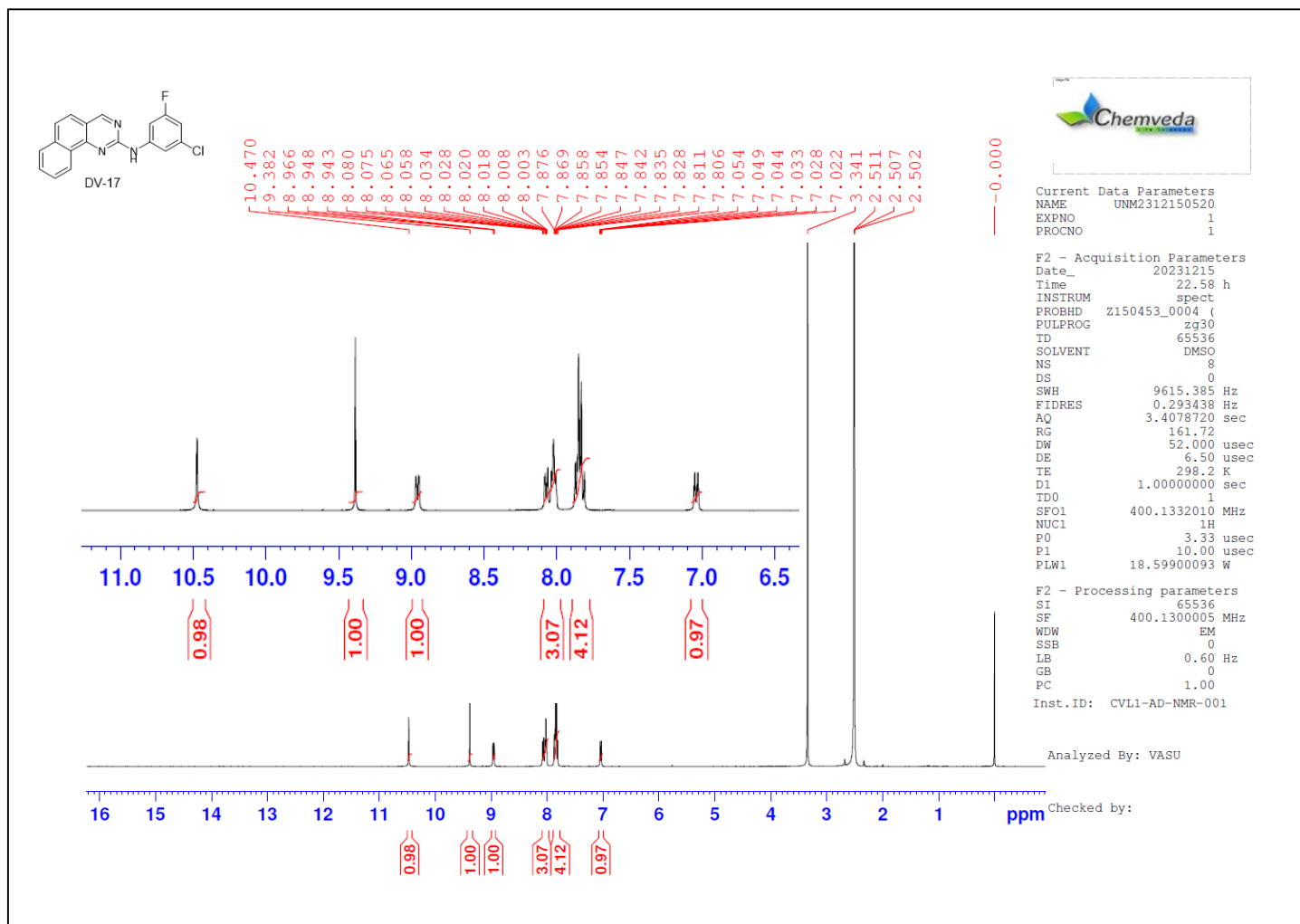


Spectra: ^1H , ^{13}C , ^{13}C Jmod NMR and FT-IR data of compound 4o (DV-16)



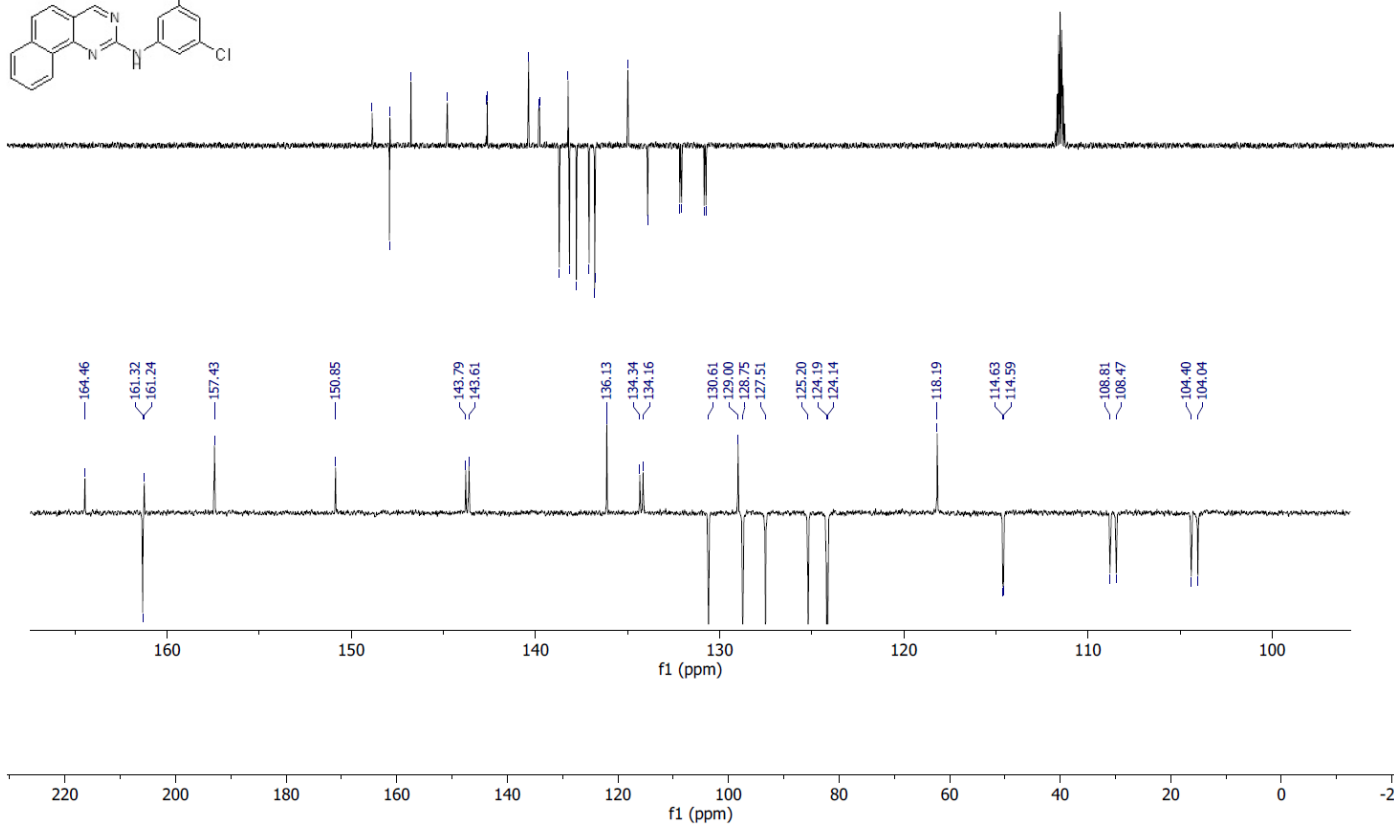
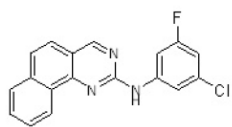


Spectra: ¹H, ¹³C, ¹³C Jmod NMR and FT-IR data of compound 4p (DV-17)

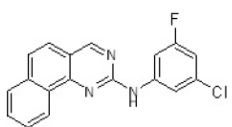


Compound DV-17
RMN ¹³C Jmod, DMSO-6d, 75 MHz

164.46
161.32
161.24
157.43
150.85
143.79
143.61
136.13
134.34
134.16
130.61
129.00
128.75
127.51
125.20
124.19
124.14
118.19
114.63
114.59
108.81
108.47
104.40
104.04



Compound DV-17
RMN ¹⁹F, DMSO-6d, 282 MHz

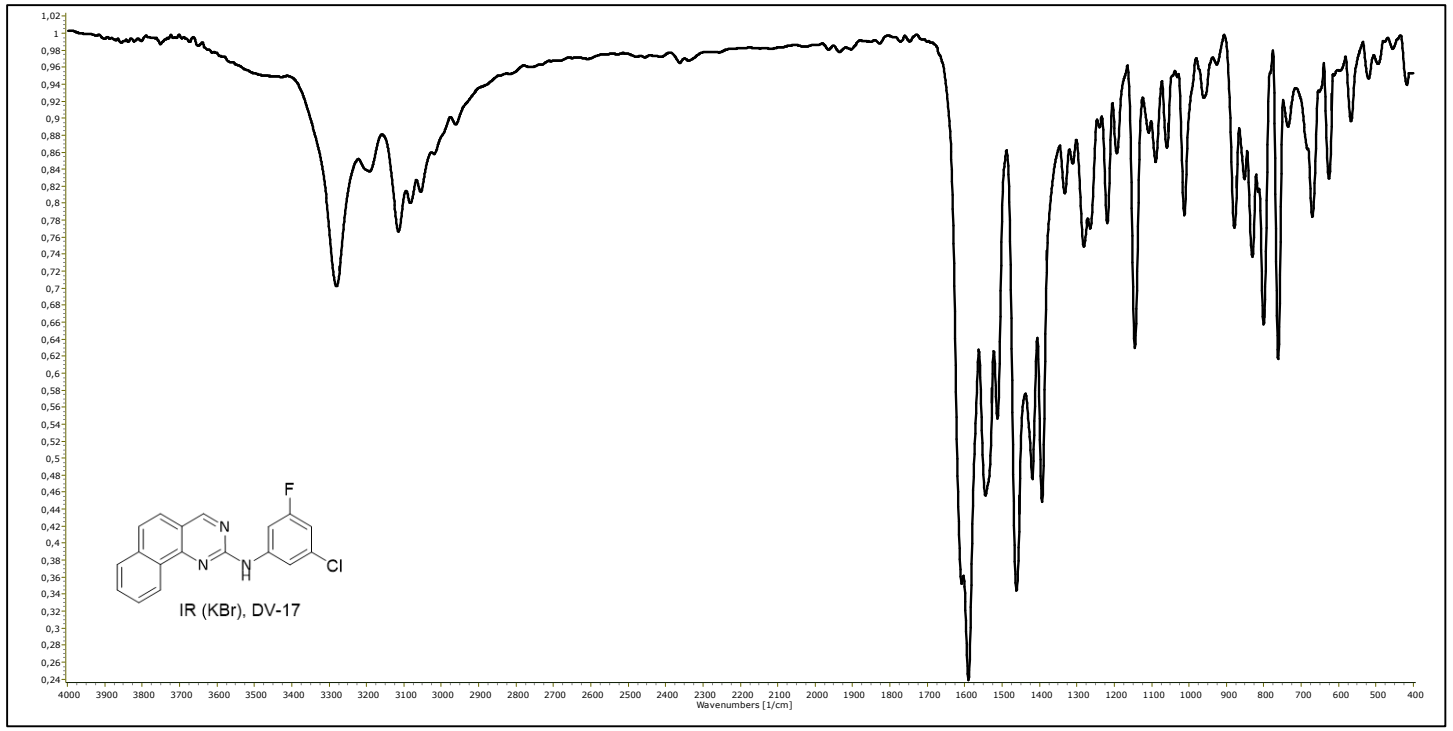


-110.38

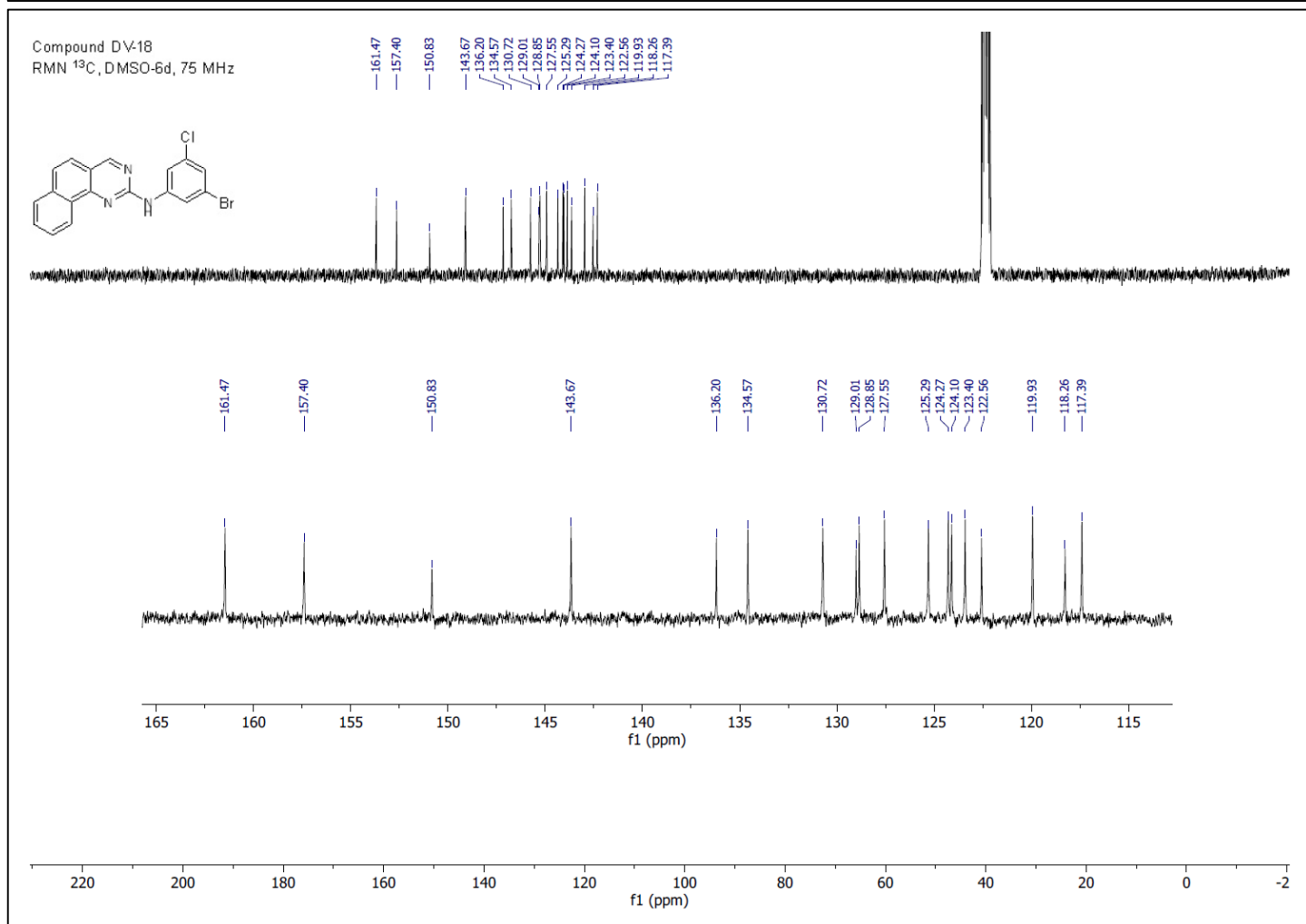
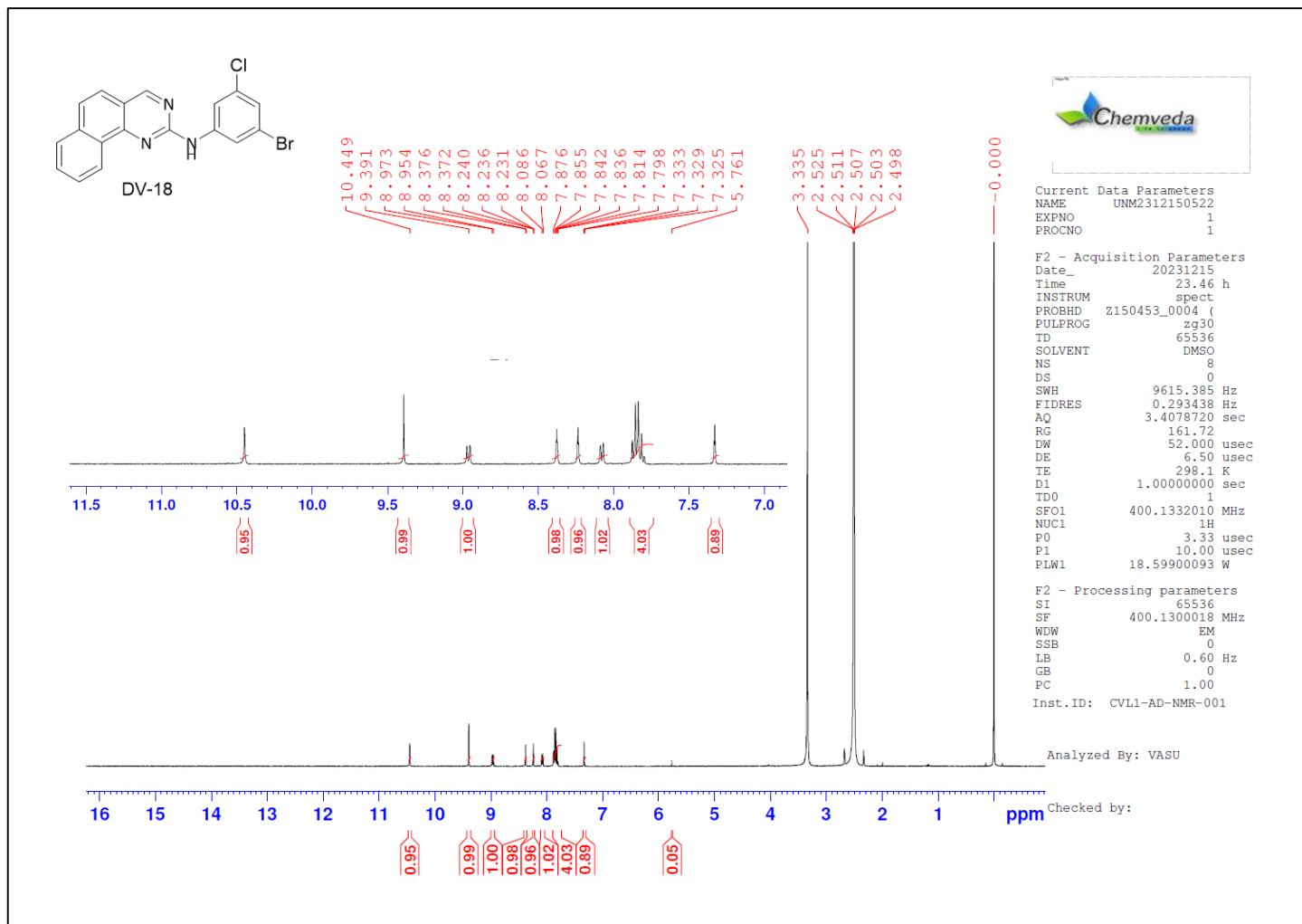
-110.24
-110.27
-110.28
-110.31

-110.0 -110.1 -110.2 -110.3 -110.4 -110.5 -110.6
f1 (ppm)

0 -100 -200 -300
f1 (ppm)

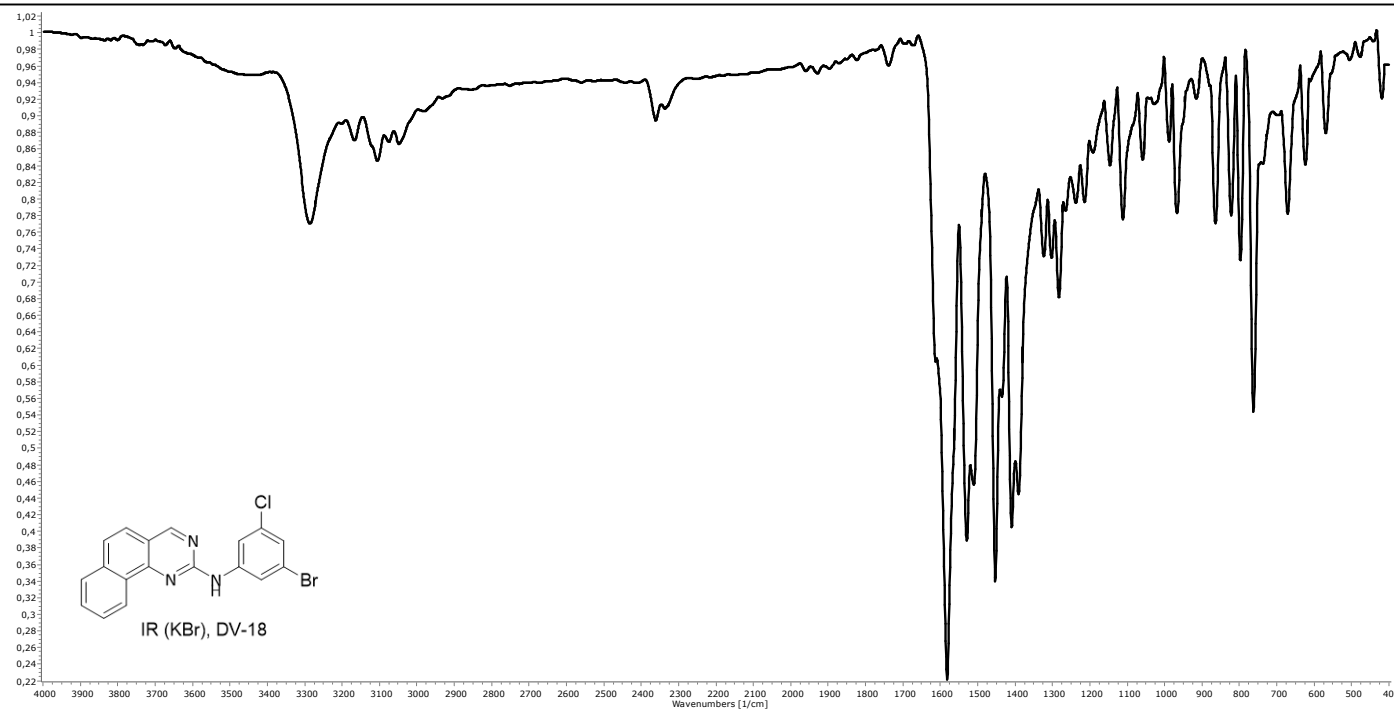
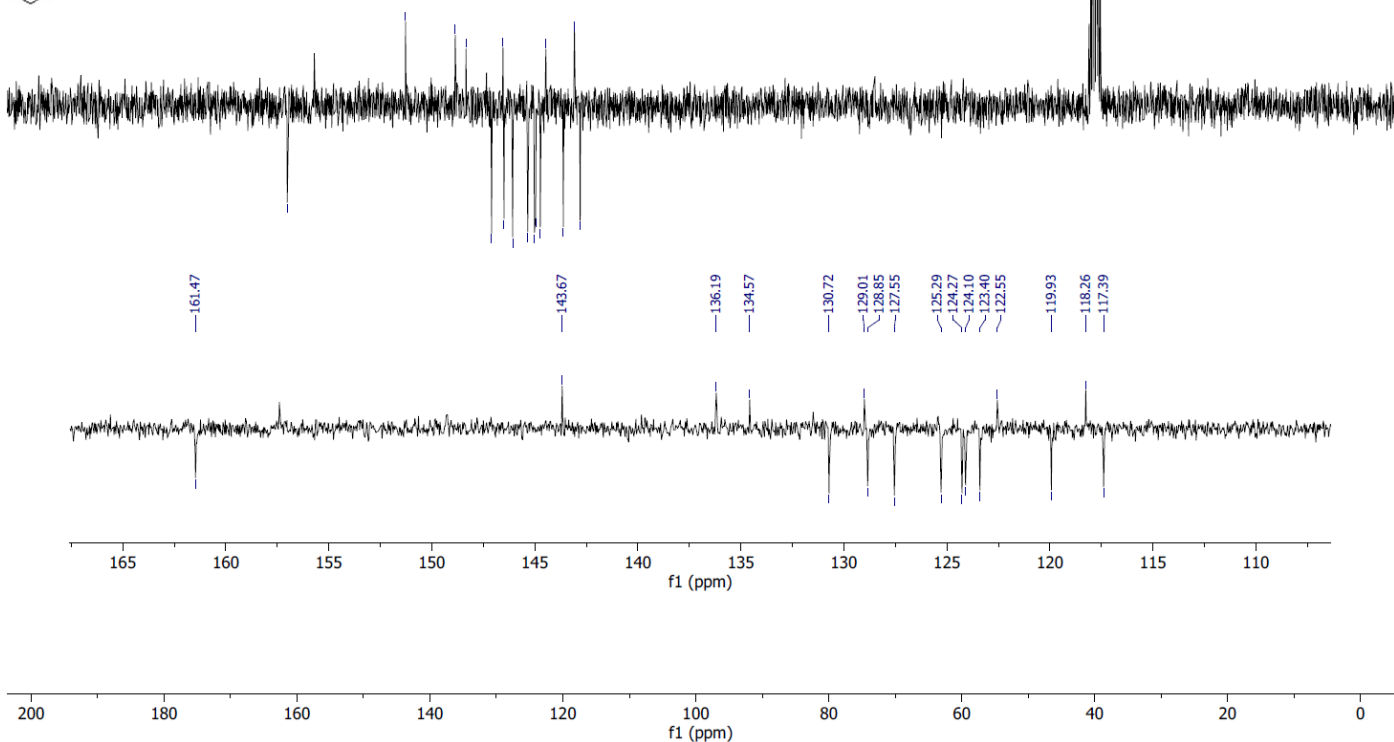
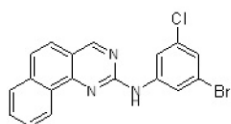


Spectra: ¹H, ¹³C, ¹³C Jmod NMR and FT-IR data of compound 4q (DV-18)

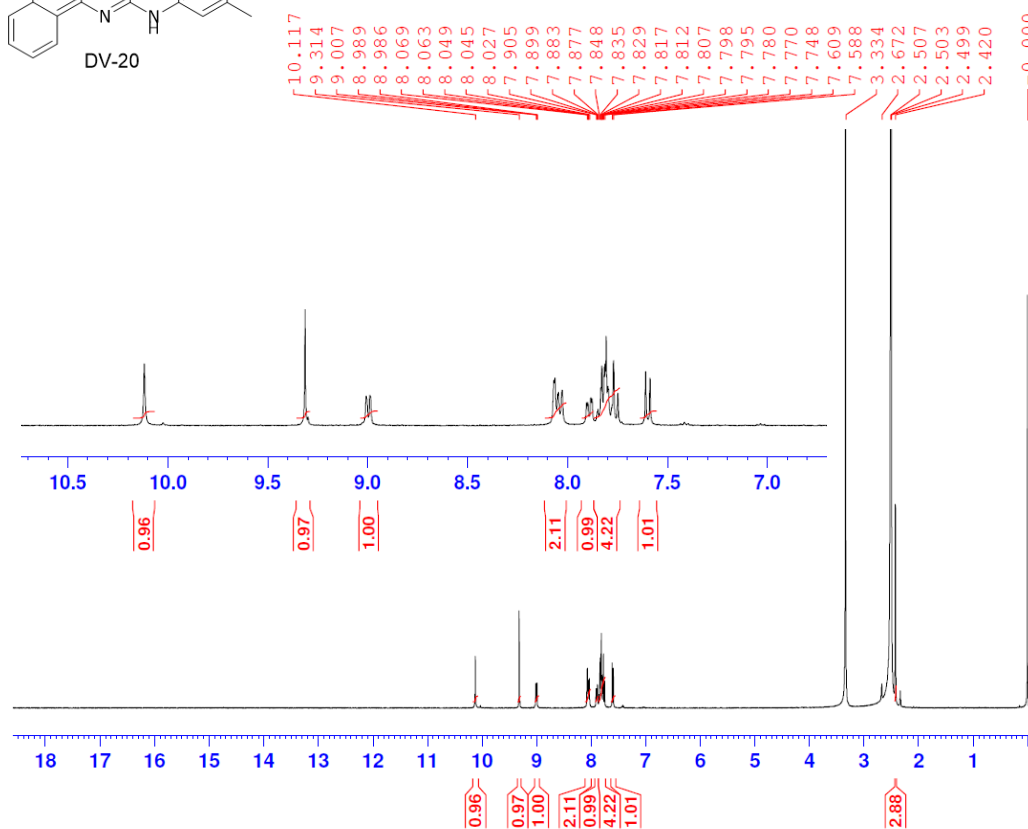
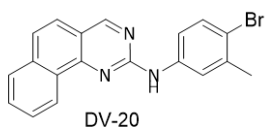


Compound DV-18

RMN ^{13}C Jmod, DMSO- d_6 , 75 MHz



Spectra: ^1H , ^{13}C , ^{13}C Jmod NMR and FT-IR data of compound 4s (DV-20)



Current Data Parameters
 NAME UNM2312150307
 EXPNO 1
 PROCNO 1

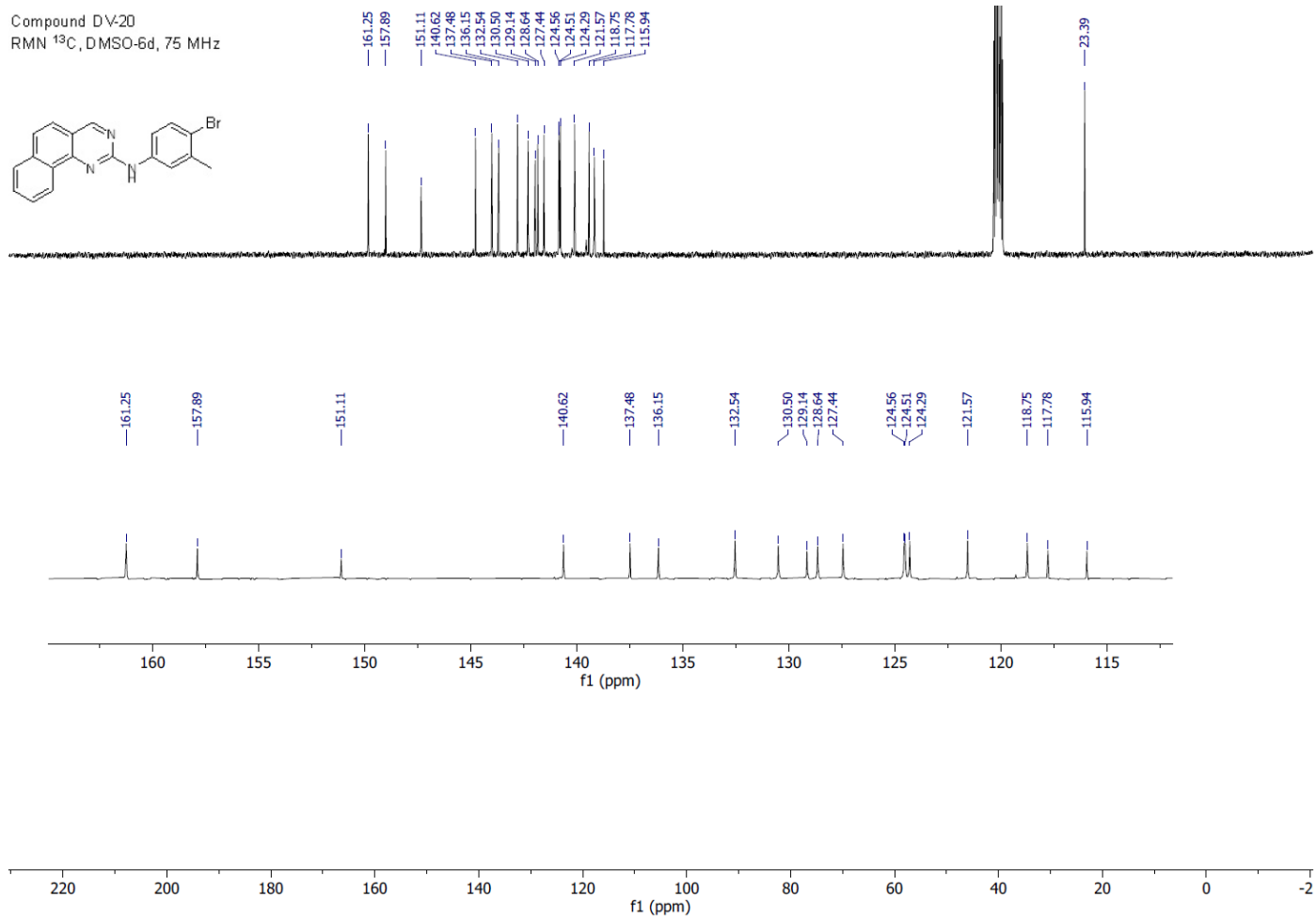
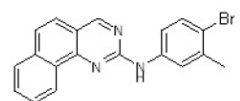
F2 - Acquisition Parameters
 Date_ 20231215
 Time_ 21.20 h
 INSTRUM spect
 PROBHD Z150453_0004 ()
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 9615.385 Hz
 FIDRES 0.293438 Hz
 AQ 3.4078720 sec
 RG 161.72
 DW 52.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1
 SFO1 400.1332010 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 18.59900093 W

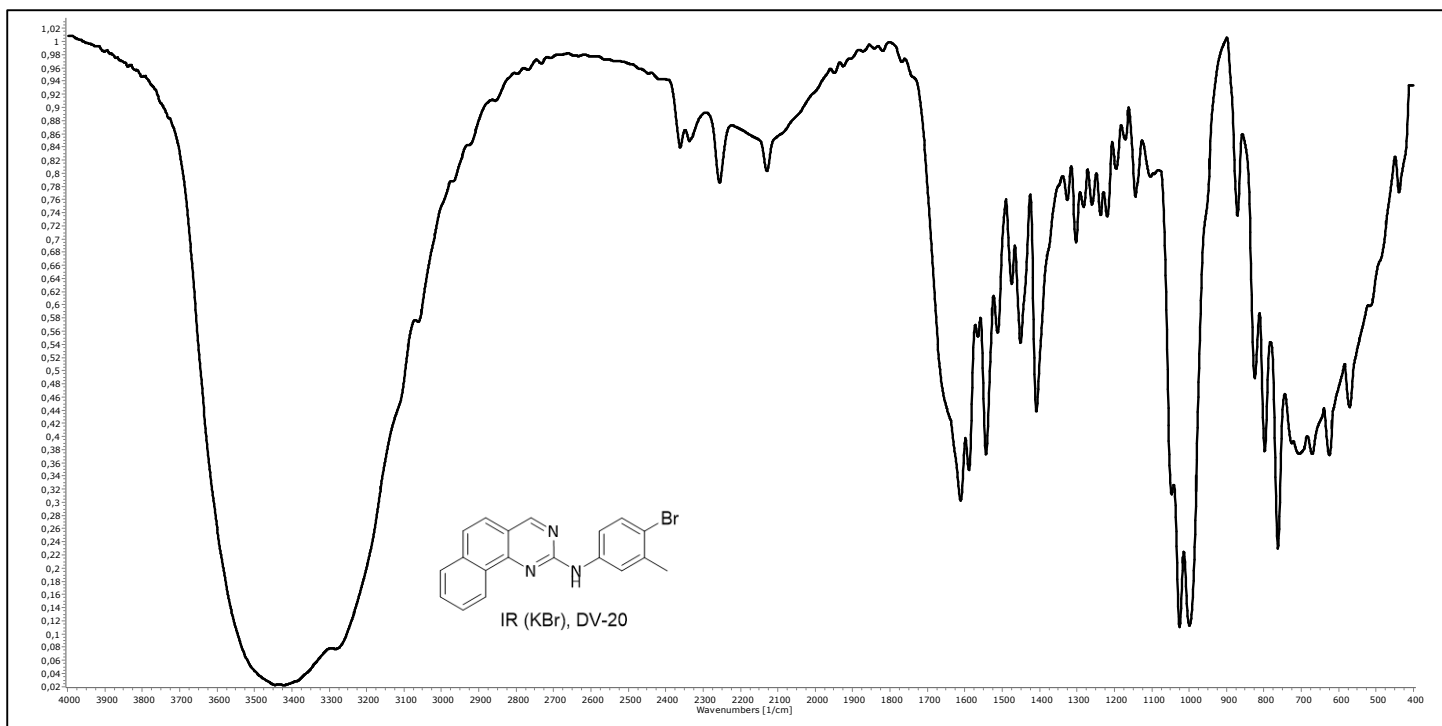
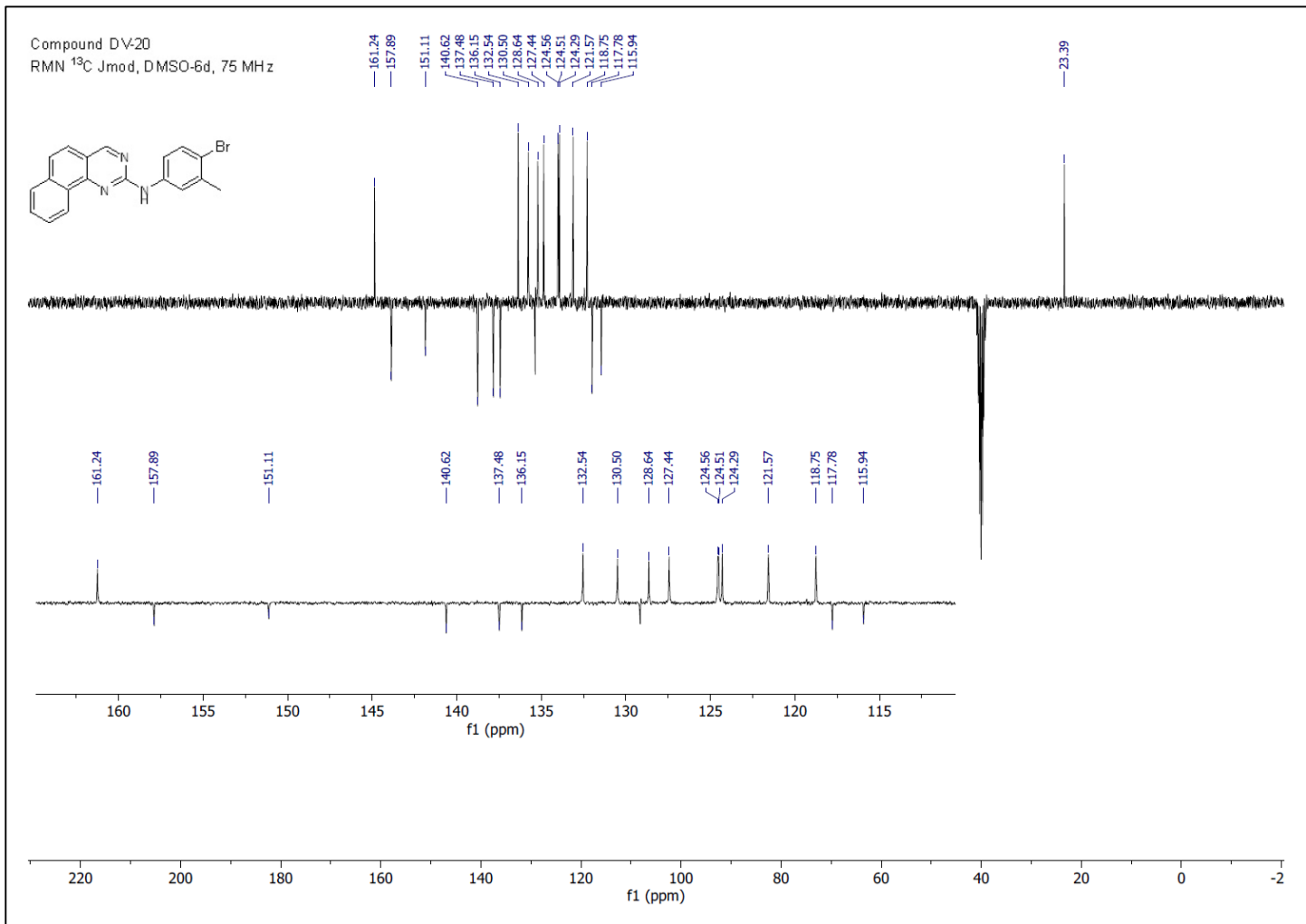
F2 - Processing parameters
 SI 65536
 SF 400.1300021 MHz
 WDW EM
 SSB 0
 LB 0.60 Hz
 GB 0
 PC 1.00
 Inst. ID: CVL1-AD-NMR-001

Analyzed By: VASU

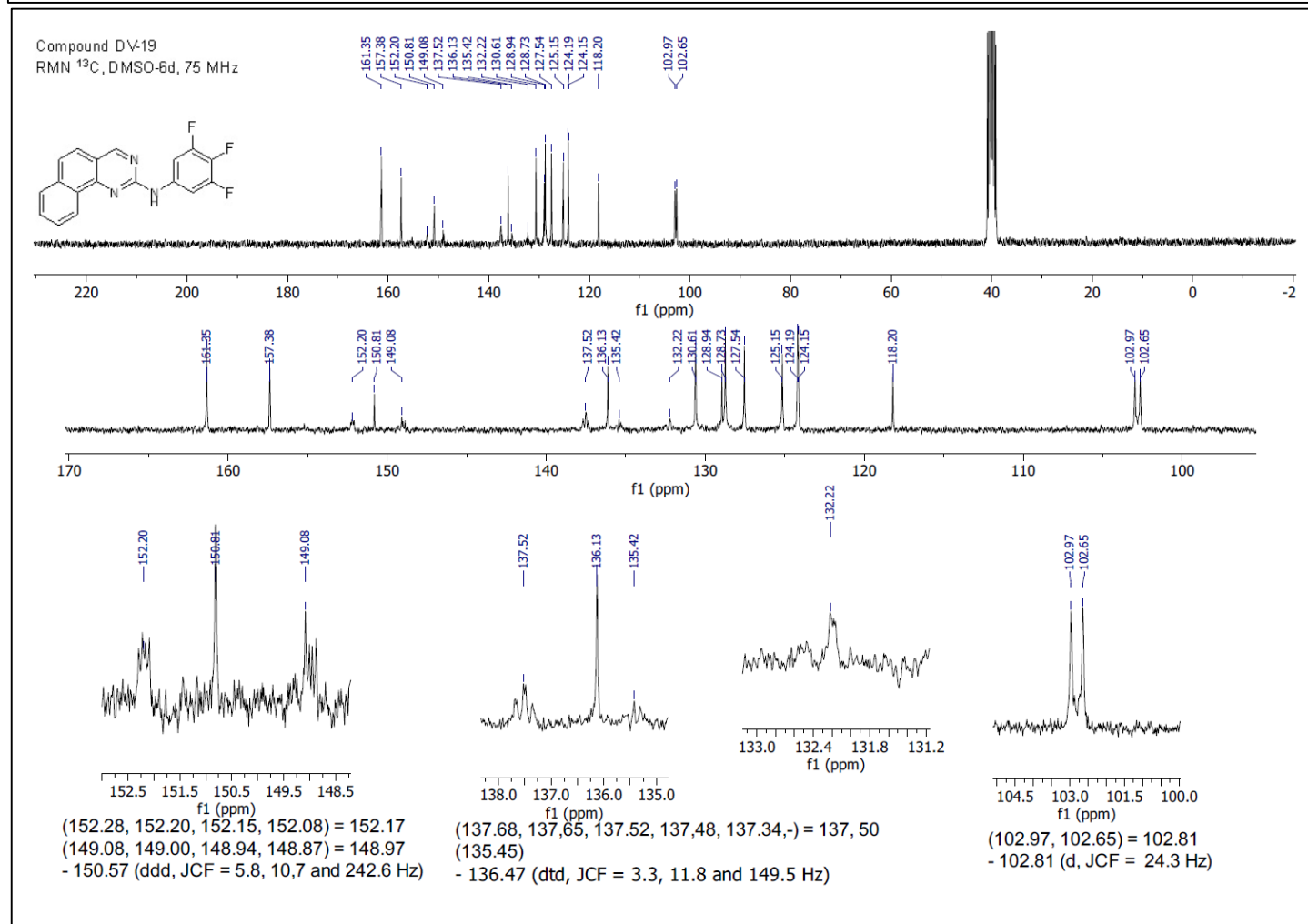
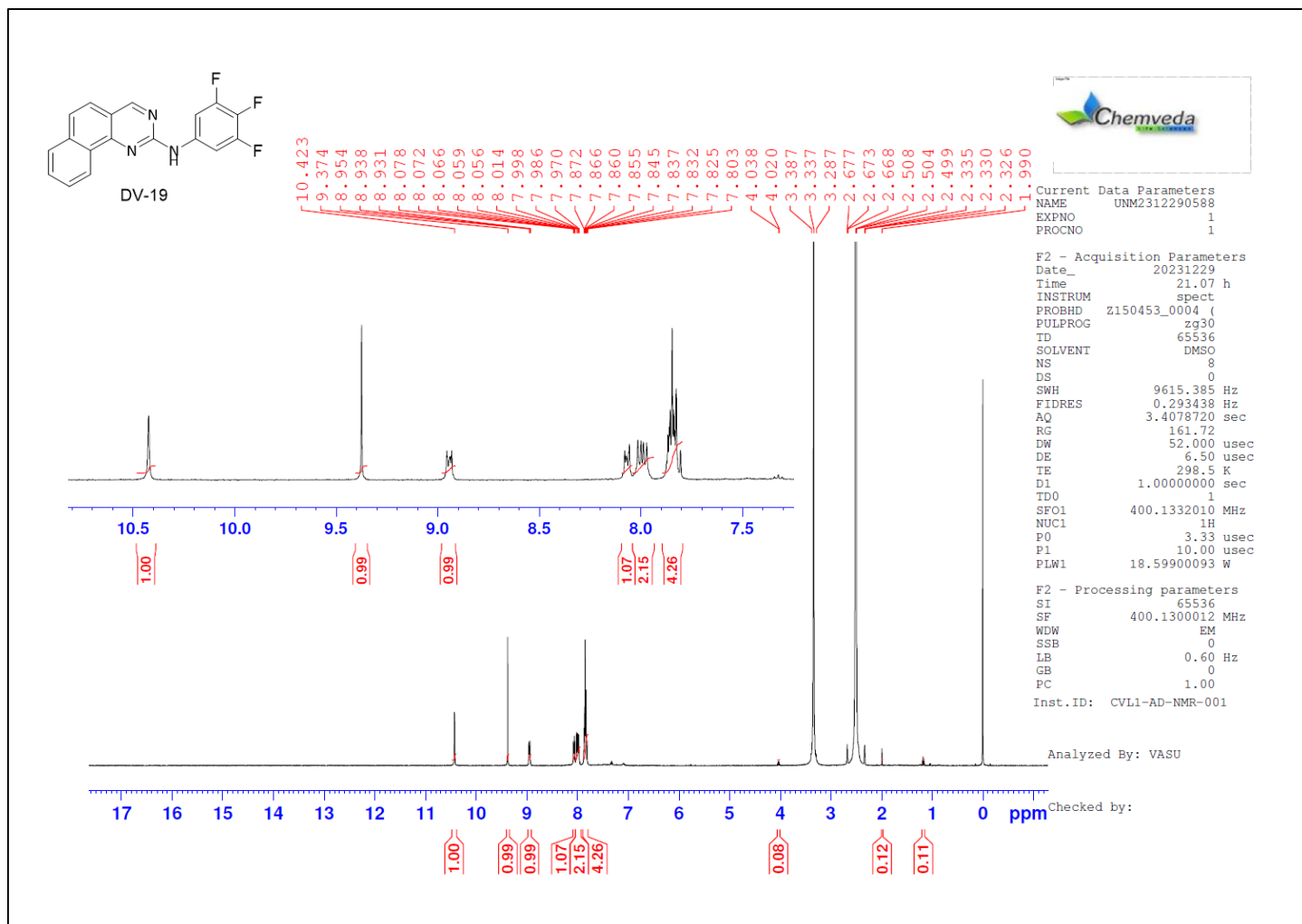
Checked by:

Compound DV-20
 RMN ^{13}C , DMSO- d_6 , 75 MHz

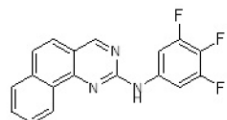




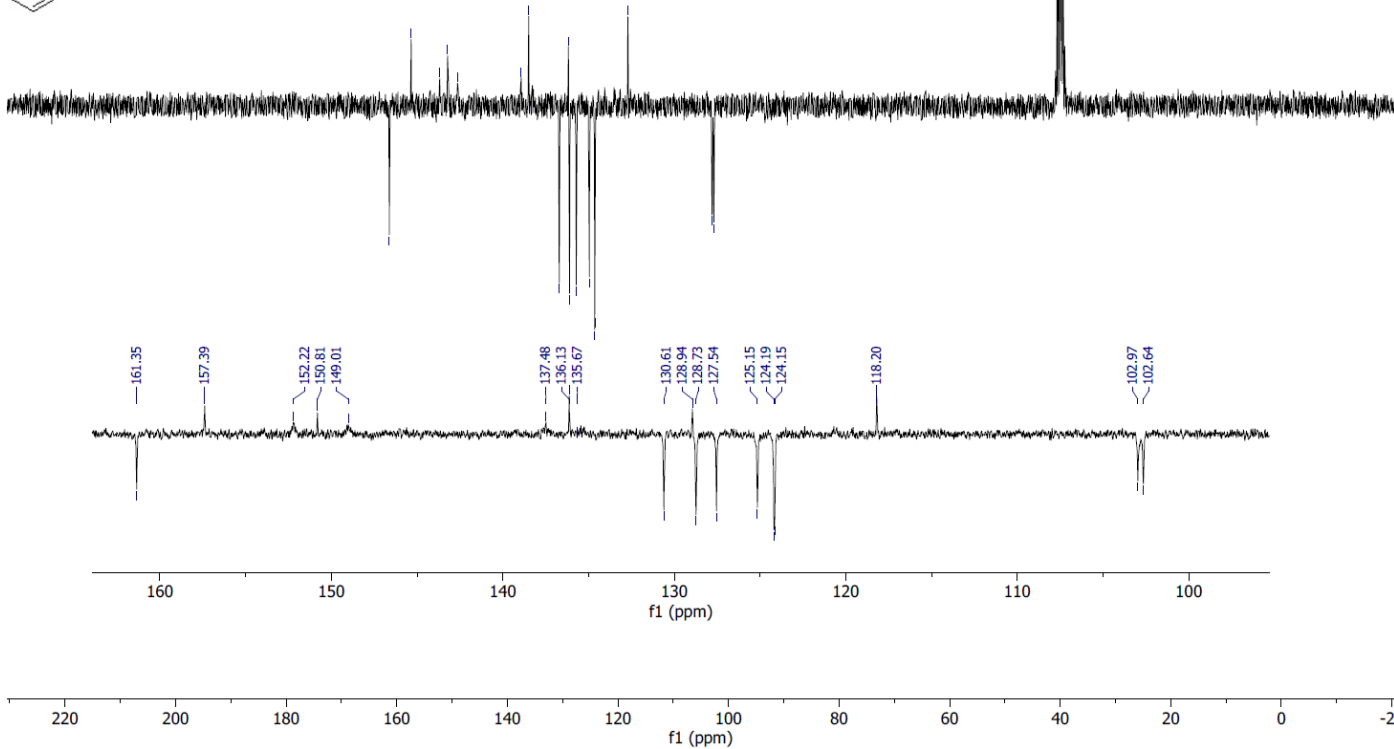
Spectra: ¹H, ¹³C, ¹³C Jmod NMR and FT-IR data of compound 4r (DV-19)



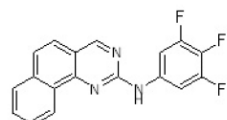
Compound DV-19
RMN ¹³C Jmod, DMSO-6d, 75 MHz



161.35
157.39
152.22
150.81
149.01
137.48
136.13
135.67
130.61
128.94
128.73
127.54
125.15
124.19
124.15
118.20
102.97
102.64



Compound DV-19
RMN ¹⁹F, DMSO-6d, 282 MHz



130.36
166.03

130.34
130.35
130.39
130.41
130.42
130.44
130.48
130.49

166.03
166.05
166.07
166.11
166.13
166.15
166.19
166.21
166.23

