Supplementary Information

Synthesis and assessment of 4-aminotetrahydroquinazoline derivatives as tick-borne encephalitis virus reproduction inhibitors

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General procedure for the synthesis of the compounds 7a–ab

3a-c, X=N→O; **5a**, X=N; R=Me — **7a-ab**

The mixture of tetrahydroquinazoline derivative **3a–c, 5a** (0.5 mmol), corresponding amine (0.5 mmol) and DIPEA (129 mg, 1.0 mmol) in ethanol (1 mL) was stirred for 24 h. The solvent was evaporated in vacuo, the product was isolated via column chromatography (SiO_2).

***N*-Butyl-2-methyl-5,6,7,8-tetrahydroquinazoline-4-amine 1-oxide (7a).**

Obtained as colorless oil (42 mg, 36%); R*f* 0.2 ($CHCl_3$); δ_H (400 MHz, $CDCl_3$): 0.96 (3H, t, $^3J_{HH}$ 7.3, CH_3, Bu), 1.32–1.46 (2H, m, CH_2, Bu), 1.53–1.63 (2H, m, CH_2, Bu), 1.75–1.87 (4H, m, $2CH_2$, cy-Hex), 2.30 (2H, br t, $^3J_{HH}$ 5.9, CH_2, cy-Hex), 2.63 (3H, s, CH_3), 2.91 (2H, br t, $^3J_{HH}$ 5.9, CH_2, cy-Hex), 3.48 (2H, dt, $^3J_{HH}$ 5.9, $^3J_{HH}$ 7.1, CH_2NH), 4.47 (1H, br s, NH); δ_C (101 MHz, $CDCl_3$): 13.8 (CH_3, Bu), 20.1 (CH_2), 20.2 (CH_3), 20.8 (CH_2), 21.0 (CH_2), 22.1 (CH_2), 24.6 (CH_2), 31.6 (CH_2), 40.9 (CH_2NH), 111.6 (C4a), 152.0 (C), 153.1 (C), 154.8 (C); HRMS (ESI^+, m/z): calc. for $C_{13}H_{21}N_3O$ [M+H] 236.1757, found 236.1760.

***N*-Benzyl-2-methyl-5,6,7,8-tetrahydroquinazoline-4-amine 1-oxide (7b).**

Obtained as yellow oil (64 mg, 50%); R*f* 0.1 (petroleum ether:ethyl acetate:MeOH 3:1:1); δ_H (400 MHz, $CDCl_3$): 1.75–1.86 (4H, m, $2CH_2$, cy-Hex), 2.32 (2H, t, $^3J_{HH}$ 5.6, CH_2, cy-Hex), 2.67 (3H, s, CH_3), 2.94 (2H, t, $^3J_{HH}$ 5.7, CH_2, cy-Hex), 4.70 (2H, d, $^3J_{HH}$ 5.4, CH_2NH), 4.98 (1H, br s, NH), 7.29–7.40 (5H, m, Ph); δ_C (101 MHz, $CDCl_3$): 20.2 (CH_3), 20.7 (CH_2, cy-Hex), 20.9 (CH_2, cy-Hex), 22.1 (CH_2, cy-Hex), 24.6 (CH_2, cy-Hex), 45.4 (CH_2NH), 111.7 (C4a), 127.7 (2CH, Ph), 127.9 (CH, Ph), 128.7 (2CH, Ph), 138.3 (C, Ph), 152.6 (C, Pyr), 154.0 (C, Pyr), 155.8 (C, Pyr); HRMS (ESI^+, m/z): calc. for $C_{16}H_{19}N_3O$ [M+H] 270.1601, found 270.1601.

***N*-Benzyl-2-*tert*-butyl-5,6,7,8-tetrahydroquinazoline-4-amine 1-oxide (7c).**

Obtained as yellowish solid (101 mg, 68%); mp 144–147°C (from $CHCl_3$, with decomposition); R*f* 0.1 (petroleum ether:ethyl acetate:MeOH 3:1:0.1); δ_H (400 MHz, $CDCl_3$): 1.51 (9H, s, $3CH_3$), 1.72–1.84 (4H, m, $2CH_2$, cy-Hex), 2.34 (2H, br t, $^3J_{HH}$ 5.6, CH_2, cy-Hex), 2.88 (2H, br t, $^3J_{HH}$ 5.6, CH_2, cy-Hex), 4.70 (2H, d, $^3J_{HH}$ 5.6, CH_2NH), 5.16 (1H, br s, NH), 7.25–7.36 (5H, m, 5CH, Ph); δ_C (101 MHz, $CDCl_3$): 20.8 (CH_2, cy-Hex), 21.2 (CH_2, cy-Hex), 22.2 (CH_2, cy-Hex), 24.6 (CH_2, cy-Hex), 26.9 ($3CH_3$), 38.7 (C, *t*-Bu), 45.2 (CH_2Ph), 111.9 (C4a, Pyr), 127.4 (CH, Ph), 127.7 (2CH, Ph), 128.6 (2CH, Ph), 139.0 (C, Ph), 150.7 (C4, Pyr), 155.1 (C8a, Pyr), 161.2 (C2, Pyr); HRMS (ESI^+, m/z): calc. for $C_{19}H_{25}N_3O$ [M+H] 312.2070, found 312.2078.

***N*-(4-Methoxybenzyl)-2-methyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7d).**

Obtained as yellowish solid (60 mg, 40%); mp 189–191°C (from $CHCl_3$, with decomposition); R*f* 0.3 (petroleum ether:ethyl acetate:MeOH 3:1:1). Found: C, 68.45; H, 7.1; N, 14.1. Calc. for $C_{17}H_{21}N_3O_2$: C, 68.2, H, 7.1, N, 14.0%. δ_H (400 MHz, $CDCl_3$): 1.68–1.81 (4H, m, $2CH_2$, cy-Hex), 2.27 (2H, t, $^3J_{HH}$ 5.8, CH_2, cy-Hex), 2.61 (3H, s, CH_3), 2.85 (2H, t, $^3J_{HH}$ 5.6, CH_2, cy-Hex), 3.76 (3H, s, CH_3O), 4.55 (2H, d, $^3J_{HH}$ 5.3, CH_2NH), 4.95 (1H, br s, NH), 6.80–6.85 (2H, m, Ar), 7.19–7.23 (2H, m, Ar); δ_C (101 MHz, $CDCl_3$): 20.2 (CH_3), 20.8 (CH_2, cy-Hex), 21.0 (CH_2, cy-Hex), 22.1 (CH_2, cy-Hex), 24.6 (CH_2, cy-Hex), 44.8 (CH_2NH), 55.3 (CH_3O), 111.8 (C4a), 114.0

(2CH, Ar), 129.2 (2CH, Ar), 130.7 (C, Ar), 151.3 (C, Pyr), 153.4 (C, Pyr), 154.7 (C, Pyr), 159.0 (C, Ar).

2-Methoxy-5-{[(2-methyl-1-oxido-5,6,7,8-tetrahydroquinazolin-4-yl)amino]methyl}phenol (7e).

Obtained as yellow oil (45 mg, 42%); R*f* 0.5 (MeOH); δ_H (400 MHz, $CDCl_3$): 1.61–1.73 (4H, m, $2CH_2$, cy-Hex), 2.40–2.48 (2H, CH_2, cy-Hex), 2.61 (3H, s, CH_3), 2.79–2.85 (2H, CH_2, cy-Hex), 3.79 (3H, s, CH_3O), 4.61 (2H, d, $^3J_{HH}$ 5.9, CH_2NH), 6.78 (1H, d, $^3J_{HH}$ 8.2, Ar), 6.83 (1H, dd, $^3J_{HH}$ 8.2, $^4J_{HH}$ 1.6, Ar), 7.01 (1H, d, $^4J_{HH}$ 1.6, 1H, Ar), 8.04 (1H, br s, NH), 9.06 (1H, br s, OH); δ_C (101 MHz, $CDCl_3$): 18.8 (CH_3), 20.3 (CH_2, cy-Hex), 20.6 (CH_2, cy-Hex), 22.6 (CH_2, cy-Hex), 24.4 (CH_2, cy-Hex), 44.8 (CH_2NH), 56.0 (CH_3O), 111.8 (CH, Ar), 113.4 (C4a), 114.3 (CH, Ar), 121.3 (CH, Ar), 129.5 (C, Ar), 145.2 (C, Pyr), 146.7 (C, Pyr), 152.5 (C, Pyr), 157.2 (C, Ar), 158.2 (C, Ar); HRMS (ESI^+, m/z): calc. for $C_{17}H_{21}N_3O_3$ [M+H] 316.1656, found 316.1667.

2-Methyl-4-morpholin-4-yl-5,6,7,8-tetrahydroquinazoline 1-oxide (7f).

Obtained as colorless oil (106 mg, 85%); R*f* 0.8 ($CHCl_3$:MeOH 10:1); δ_H (400 MHz, $CDCl_3$): 1.63–1.72 (2H, m, CH_2, cy-Hex), 1.83–1.92 (2H, m, CH_2, cy-Hex), 2.53 (2H, t, $^3J_{HH}$ 5.9, CH_2, cy-Hex), 2.64 (3H, s, CH_3), 2.94 (2H, t, $^3J_{HH}$ 5.9, CH_2, cy-Hex), 3.28–3.34 (4H, m, $2CH_2$), 3.76–3.81 (4H, m, $2CH_2$); δ_C (101 MHz, $CDCl_3$): 20.0 (CH_3), 21.2 (CH_2), 21.6 (CH_2), 25.5 (CH_2), 26.3 (CH_2), 48.9 ($2CH_2N$), 66.7 ($2CH_2O$), 118.7 (C4a), 154.6 (C), 155.2 (C), 155.7 (C); HRMS (ESI^+, m/z): calc. for $C_{13}H_{19}N_3O_2$ [M+H] 250.1550, found 250.1549.

2-Methyl-4-morpholin-4-yl-5,6,7,8-tetrahydroquinazoline (7g).

Obtained as colorless oil (76 mg, 65%); R*f* 0.3 (petroleum ether:ethyl acetate:MeOH 3:1:0.5); δ_H (400 MHz, $CDCl_3$): 1.66–1.76 (2H, m, CH_2, cy-Hex), 1.81–1.90 (2H, m, CH_2, cy-Hex), 2.50 (2H, t, $^3J_{HH}$ 6.1, CH_2, cy-Hex), 2.52 (3H, s, CH_3), 2.81 (2H, t, $^3J_{HH}$ 6.7, CH_2, cy-Hex), 3.35–3.40 (4H, m, $2CH_2$), 3.77–3.83 (4H, m, $2CH_2$); δ_C (101 MHz, $CDCl_3$): 22.3 (CH_2, cy-Hex), 22.9 (CH_2, cy-Hex), 25.3 (CH_3), 26.4 (CH_2, cy-Hex), 31.6 (CH_2, cy-Hex), 48.5 ($2CH_2$), 66.8 ($2CH_2$), 115.2 (C4a), 163.5 (C), 164.3 (C), 165.1 (C); HRMS (ESI^+, m/z): calc. for $C_{13}H_{19}N_3O$ [M+H] 234.1601, found 234.1601.

4-Morpholin-4-yl-2-*tert*-butyl-5,6,7,8-tetrahydroquinazoline 1-oxide (7h).

Obtained as yellowish solid (63 mg, 43%); mp 68–70°C (from $CHCl_3$), R*f* 0.1 (petroleum ether:ethyl acetate:MeOH 3:1:0.3); δ_H (400 MHz, $CDCl_3$): 1.47 (9H, s, $3CH_3$), 1.60–1.68 (2H, m, CH_2, cy-Hex), 1.79–1.88 (2H, m, $2CH_2$, cy-Hex), 2.50 (2H, br t, $^3J_{HH}$ 5.9, CH_2, cy-Hex), 2.87 (2H, br t, $^3J_{HH}$ 6.6, CH_2, cy-Hex), 3.24–3.28 (4H, m, $2CH_2N$), 3.74–3.78 (4H, m, $2CH_2O$); δ_C (101 MHz, $CDCl_3$): 21.51 (CH_2, cy-Hex), 21.52 (CH_2, cy-Hex), 25.4 (CH_2, cy-Hex), 26.1 (CH_2, cy-Hex), 26.6 ($3CH_3$), 38.7 (C, *t*-Bu), 48.9 ($2CH_2N$), 66.72 ($2CH_2O$), 118.8 (C4a, Pyr), 153.5 (C4, Pyr), 157.1 (C8a, Pyr), 160.3 (C2, Pyr). HRMS (ESI^+, m/z): calc. for $C_{16}H_{25}N_3O_2$ [M+H] 292.2020, found 292.2022.

2-Methyl-4-piperazin-1-yl-5,6,7,8-tetrahydroquinazoline 1-oxide (7i).

Obtained as yellowish oil (112 mg, 90%); R*f* 0.8 ($CHCl_3$:MeOH 10:1); δ_H (400 MHz, $CDCl_3$): 1.50–1.60 (2H, m, CH_2, cy-Hex), 1.71–1.80 (2H, m, CH_2, cy-Hex), 2.42 (2H, br t, $^3J_{HH}$ 5.6, CH_2, cy-Hex), 2.50 (3H, s, CH_3), 2.78 (2H, br t, $^3J_{HH}$ 5.9, CH_2, cy-Hex), 2.83–2.88 (4H, m, $2CH_2$), 3.11–3.14 (4H, m, $2CH_2$), 4.61 (1H, br s, NH); δ_C (101 MHz, $CDCl_3$): 19.8 (CH_2), 21.3 (CH_3),

21.6 (CH_2), 25.4 (CH_2), 26.1 (CH_2), 45.8 ($2CH_2$), 49.7 ($2CH_2$), 119.0 (C4a), 151.4 (C), 154.0 (C), 155.2 (2C); HRMS (ESI^+, m/z): calc. for $C_{13}H_{20}N_4O$ [M+H] 249.1710, found 249.1713.

2-Methyl-4-piperazin-1-yl-5,6,7,8-tetrahydroquinazoline (7j).

Obtained as hydrochloride, white solid (79 mg, 59%); δ_H (400 MHz, CD_3OD): 1.71–1.81 (2H, m, CH_2, cy-Hex), 1.87–1.96 (2H, m, CH_2, cy-Hex), 2.59 (3H, s, CH_3), 2.70 (2H, t, $^3J_{HH}$ 5.6, CH_2, cy-Hex), 2.88 (2H, t, $^3J_{HH}$ 6.4, CH_2, cy-Hex), 3.38–3.43 (4H, m, $2CH_2$), 4.15–4.20 (4H, m, $2CH_2$); δ_C (101 MHz, CD_3OD): 19.9 (CH_2), 20.1 (CH_3), 21.8 (CH_2), 26.3 (CH_2), 26.7 (CH_2), 43.0 ($2CH_2$), 44.4 ($2CH_2$), 114.3 (C4a), 155.4 (C), 158.1 (C), 164.1 (C); HRMS (ESI^+, m/z): calc. for $C_{13}H_{20}N_4$ [M+H] 233.1761, found: 233.1753.

4-Piperazin-1-yl-2-*tert*-butyl-5,6,7,8-tetrahydroquinazoline 1-oxide (7k).

Obtained as white solid (46 mg, 32%); mp 69–71°C (from $CHCl_3$); R*f* 0.2 (MeOH); δ_H (400 MHz, $CDCl_3/CD_3OD$): 1.42 (9H, s, $3CH_3$), 1.55–1.64 (2H, m, CH_2, cy-Hex), 1.76–1.84 (2H, m, $2CH_2$, cy-Hex), 2.46 (2H, br t, $^3J_{HH}$ 5.8, CH_2, cy-Hex), 2.80 (2H, br t, $^3J_{HH}$ 6.5, CH_2, cy-Hex), 2.86–2.92 (4H, m, $2CH_2$), 3.25–3.30 (4H, m, $2CH_2$); δ_C (101 MHz, $CDCl_3/CD_3OD$): 21.30 (CH_2, cy-Hex), 21.33 (CH_2, cy-Hex), 25.2 (CH_2, cy-Hex), 26.3 (CH_2, cy-Hex), 26.7 ($3CH_3$), 38.8 (C, *t*-Bu), 45.2 ($2CH_2$), 48.9 ($2CH_2$), 118.6 (C4a, Pyr), 155.0 (C4, Pyr), 157.2 (C8a, Pyr), 160.7 (C2, Pyr); HRMS (ESI^+, m/z): calc. for $C_{16}H_{26}N_4O$ [M+H] 291.2179, found: 291.2183.

2-Methyl-*N*-phenyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7l).

Obtained as colorless oil (61 mg, 48%); R*f* 0.9 ($CHCl_3$:MeOH 10:1); δ_H (400 MHz, $CDCl_3$): 1.77–1.84 (4H, m, $4CH_2$), 2.59 (2H, br t, $^3J_{HH}$ 5.3, CH_2), 2.62 (3H, s, CH_3), 2.86–2.91 (2H, m, CH_2), 5.01 (1H, br s, NH), 7.14 (1H, t, $^3J_{HH}$ 8.1, CH, Ph), 7.33 (2H, dd, $^3J_{HH}$ 8.1, $^3J_{HH}$ 8.1, 2CH, Ph), 7.61 (2H, d, $^3J_{HH}$ 8.1, 2CH, Ph); δ_C (101 MHz, $CDCl_3$): 20.4 (CH_3), 20.47 (CH_2), 20.52 (CH_2), 22.8 (CH_2), 24.8 (CH_2), 114.2 (C4a, Pyr), 122.2 (2CH), 125.0 (CH), 128.9 (2CH), 137.5 (C, Ph), 152.9 (C, Pyr), 154.4 (C, Pyr), 156.5 (C, Pyr); HRMS (ESI^+, m/z): calc. for $C_{15}H_{17}N_3O$ [M+H] 256.1444, found 256.1446.

***N*-Phenyl-2-*tert*-butyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7m).**

Obtained as yellowish oil (46 mg, 31%); R*f* 0.6 (MeOH); δ_H (400 MHz, $CDCl_3$): 1.53 (9H, s, $3CH_3$), 1.80–1.85 (4H, m, $2CH_2$), 2.49–2.53 (2H, m, CH_2), 2.89–2.93 (2H, m, CH_2), 6.54 (1H, s, NH), 7.06 (1H, tt, $^3J_{HH}$ 7.5, $^4J_{HH}$ 0.9, CH, Ph), 7.28–7.34 (2H, m, 2CH, Ph), 7.57–7.62 (2H, m, 2CH, Ph); δ_C (101 MHz, $CDCl_3$): 20.8 (CH_2), 21.0 (CH_2), 22.5 (CH_2), 24.9 (CH_2), 27.0 ($3CH_3$), 39.2 (C, *t*-Bu), 113.4 (C4a, Pyr), 120.3 (2CH), 123.3 (CH), 128.8 (2CH), 138.7 (C, Ph), 148.2 (C4, Pyr), 156.3 (C8a, Pyr), 161.4 (C2, Pyr); HRMS (ESI^+, m/z): calc. for $C_{18}H_{23}N_3O$ [M+H] 298.1914, found 298.1913.

2-Methyl-*N*-(4-methylphenyl)-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7n).

Obtained as yellowish oil (20 mg, 15%); R*f* 0.1 (petroleum ether:EtOAc:MeOH 3:1:1); δ_H (400 MHz, $CDCl_3$): 1.80–1.86 (4H, m, $2CH_2$), 2.31 (3H, s, CH_3, Ph), 2.45–2.51 (2H, m, CH_2), 2.62 (3H, s, CH_3, Pyr), 2.90–2.94 (2H, m, CH_2), 6.47 (1H, br s, NH), 7.12 (2H, d, $^3J_{HH}$ 8.3, 2CH, Ph), 7.41 (2H, d, $^3J_{HH}$ 8.3, 2CH, Ph); δ_C (101 MHz, $CDCl_3$): 12.0 (CH_3, Ar), 20.2 (CH_3, Pyr), 20.8 (CH_2), 20.9 (CH_2), 22.5 (CH_2), 24.8 (CH_2), 113.0 (C4a), 121.0 (2CH), 129.4 (2CH), 133.6 (C, Ar), 135.7 (C, Ar), 149.6 (C, Pyr), 154.6 (C, Pyr), 155.0 (C, Pyr); HRMS (ESI^+, m/z): calc. for $C_{16}H_{19}N_3O$ [M+H] 270.1601, found 270.1597.

2-[(2-Methyl-1-oxido-5,6,7,8-tetrahydroquinazolin-4-yl)amino]phenol (7o).
Obtained as yellowish oil (49 mg, 36%); R*f* 0.5 (MeOH); δ_H (400 MHz, $CDCl_3$): 1.63–1.71 (4H, m, $2CH_2$), 2.29–2.36 (2H, m, CH_2), 2.68 (3H, s, CH_3), 2.75–2.82 (2H, m, CH_2), 6.79–6.86 (2H, m, 2CH, Ph), 6.89 (1H, d, $^3J_{HH}$ 4.0, Ph), 8.19 (1H, d, $^3J_{HH}$ 7.8, CH, Ph); δ_C (101 MHz, $CDCl_3$): 20.3 (CH_3), 20.4 (CH_2), 20.5 (CH_2), 22.0 (CH_2), 24.6 (CH_2), 114.0 (C4a), 115.7 (CH), 119.7 (CH), 120.0 (CH), 123.9 (CH), 127.3 (CNH, Ph), 146.9 (COH, Ph), 150.8 (C, Pyr), 154.4 (C, Pyr), 155.6 (C, Pyr); HRMS (ESI^+, m/z): calc. for $C_{15}H_{17}N_3O_2$ [M+H] 272.1394, found 272.1384.

***N*-(1-Adamantylmethyl)-2-methyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7p).**
Obtained as white solid (33 mg, 20%); mp 54–56°C (from $CHCl_3$); R*f* 0.1 (petroleum ether:EtOAc:MeOH 3:1:0.1); δ_H (400 MHz, $CDCl_3$): 1.49 (6H, br s, $3CH_2$, Ad), 1.62 (3H, br d, $^2J_{HH}$ ca. 12, $3CH_2$, Ad), 1.70 (3H, br d, $^2J_{HH}$ ca. 12, $3CH_2$, Ad), 1.76–1.82 (4H, m, $2CH_2$, cy-Hex), 1.96 (3H, br s, 3CH, Ad), 2.30 (2H, br t, $^3J_{HH}$ 5.0, CH_2, cy-Hex), 2.59 (3H, s, CH_3), 2.89 (2H, br t, $^3J_{HH}$ 5.2, CH_2, cy-Hex), 3.20 (2H, d, $^3J_{HH}$ 5.9, *CH*$_2$NH), 4.54 (1H, br s, NH); δ_C (101 MHz, $CDCl_3$): 20.1 (CH_3), 20.9 (CH_2, cy-Hex), 21.0 (CH_2, cy-Hex), 22.1 (CH_2, cy-Hex), 24.5 (CH_2, cy-Hex), 28.2 (3CH, Ad), 34.0 (C, Ad), 36.9 ($3CH_2$, Ad), 40.5 ($3CH_2$, Ad), 52.3 (CH_2NH), 111.3 (C4a), 152.3 (C, Pyr), 153.1 (C, Pyr), 154.7 (C, Pyr); HRMS (ESI^+, m/z): calc. for $C_{20}H_{29}N_3O$ [M+H] 328.2383, found 328.2384.

***N*-(1-Adamantylmethyl)-2-*tert*-butyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7q).**
Obtained as white solid (48 mg, 26%); mp 160°C (with decomposition; from $CHCl_3$); R*f* 0.1 (petroleum ether:EtOAc:MeOH 3:1:0.5); δ_H (400 MHz, $CDCl_3$): 1.49 (6H, d, $^3J_{HH}$ ca. 3, $3CH_2$, Ad), 1.51 (9H, s, $3CH_3$), 1.61 (3H, br d, $^2J_{HH}$ ca. 12, $3CH_2$, Ad), 1.70 (3H, br d, $^2J_{HH}$ ca. 12, $3CH_2$, Ad), 1.75–1.84 (4H, m, $2CH_2$, cy-Hex), 1.96 (3H, br s, 3CH, Ad), 2.29 (2H, br t, $^3J_{HH}$ 5.7, CH_2, cy-Hex), 2.88 (2H, br t, $^3J_{HH}$ 5.4, CH_2, cy-Hex), 3.24 (2H, d, $^3J_{HH}$ 6.2, *CH*$_2$NH), 4.46 (1H, br s, NH); δ_C (101 MHz, $CDCl_3$): 20.9 (CH_2, cy-Hex), 21.3 (CH_2, cy-Hex), 22.1 (CH_2, cy-Hex), 24.6 (CH_2, cy-Hex), 26.9 ($3CH_3$), 28.2 (3CH, Ad), 34.2 (C, Ad), 37.0 ($3CH_2$, Ad), 38.7 (C, *t*-Bu), 40.5 ($3CH_2$, Ad), 52.2 (CH_2NH), 111.2 (C4a), 151.1 (C4, Pyr), 154.8 (C8a, Pyr), 160.7 (C2, Pyr). HRMS (ESI^+, m/z): calc. for $C_{23}H_{35}N_3O$ [M+H] 370.2853, found 370.2849.

***N*-[1-(1-Adamantyl)ethyl]-2-methyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7r).**
Obtained as yellowish oil (26 mg, 15%); R*f* 0.2 (petroleum ether:EtOAc:MeOH 3:1:1); δ_H (400 MHz, $CDCl_3$): 1.07 (3H, d, $^3J_{HH}$ 6.7, CH_3), 1.49 (3H, br d, $^3J_{HH}$ ca. 12, $3CH_2$, Ad), 1.56 (3H, br d, $^2J_{HH}$ ca. 12, $3CH_2$, Ad), 1.61 (3H, br d, $^2J_{HH}$ ca. 12, $3CH_2$, Ad), 1.71 (3H, br d, $^2J_{HH}$ ca. 12, $3CH_2$, Ad), 1.78–1.83 (4H, m, $2CH_2$, cy-Hex), 1.95–1.99 (3H, m, 3CH, Ad), 2.25–2.29 (2H, m, CH_2, cy-Hex), 2.59 (3H, s, CH_3), 2.89 (2H, t, $^3J_{HH}$ 5.8, CH_2, cy-Hex), 4.06 (1H, dq, $^3J_{HH}$ 9.3, $^3J_{HH}$ 6.7, *CH*NH), 4.41 (1H, d, $^3J_{HH}$ 9.3, NH); δ_C (101 MHz, $CDCl_3$): 14.6 (CH_3), 20.2 (CH_3, Pyr), 20.8 (CH_2, cy-Hex), 20.9 (CH_2, cy-Hex), 22.0 (CH_2, cy-Hex), 24.5 (CH_2, cy-Hex), 28.3 (3CH, Ad), 36.2 (C, Ad), 37.0 ($3CH_2$, Ad), 38.6 ($3CH_2$, Ad), 54.0 (CHNH), 111.3 (C4a), 152.4 (C, Pyr), 153.2 (C, Pyr), 155.1 (C, Pyr); HRMS (ESI^+, m/z): calc. for $C_{21}H_{31}N_3O$ [M+H] calcd 342.2540, found 342.2526.

***N*-[2-(1-Adamantyl)ethyl]-2-methyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7s).**
Obtained as white solid (61 mg, 36%); mp 227–229°C (from $CHCl_3$); R*f* 0.1 (petroleum ether:EtOAc:MeOH 3:1:0.3); δ_H (400 MHz, $CDCl_3$): 1.31–1.38 (2H, m, CH_2), 1.54 (6H, d, $^3J_{HH}$ ca. 2, $3CH_2$, Ad), 1.63 (3H, br d, $^2J_{HH}$ ca. 12, $3CH_2$, Ad), 1.71 (3H, br d, $^2J_{HH}$ ca. 12, $3CH_2$, Ad),

1.74–1.84 (4H, m, $2CH_2$, cy-Hex), 1.92–1.98 (3H, m, 3CH, Ad), 2.26 (2H, t, $^3J_{HH}$ 5.5, CH_2, cy-Hex), 2.62 (3H, s, CH_3), 2.89 (2H, t, $^3J_{HH}$ 5.5, CH_2, cy-Hex), 3.44 (2H, dt, $^3J_{HH}$ 10.7, $^3J_{HH}$ 5.4, CH_2NH), 4.38 (1H, br s, NH); δ_C (101 MHz, $CDCl_3$): 20.2 (CH_3), 20.9 (CH_2, cy-Hex), 21.0 (CH_2, cy-Hex), 22.1 (CH_2, cy-Hex), 24.5 (CH_2, cy-Hex), 28.6 (3CH, Ad), 32.1 (C, Ad), 36.3 (CH_2NH), 37.0 ($3CH_2$, Ad), 42.5 ($3CH_2$, Ad), 44.0 (CH_2Ad), 111.5 (C4a), 151.8 (C, Pyr), 153.2 (C, Pyr), 155.0 (C, Pyr); HRMS (ESI^+, m/z): calc. for $C_{21}H_{31}N_3O$ [M+H] 342.2540, found 342.2538.

***N*-[2-(1-Adamantyl)ethyl]-2-ethyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7t).**

Obtained as yellowish oil (83 mg, 47%); R*f* 0.1 (petroleum ether:EtOAc:MeOH 3:1:0.3); δ_H (400 MHz, $CDCl_3$): 1.33 (3H, t, $^3J_{HH}$ 7.5, CH_3), 1.36–1.41 (2H, m, CH_2), 1.57 (6H, d, $^3J_{HH}$ ca. 2, $3CH_2$, Ad), 1.66 (3H, br d, $^2J_{HH}$ ca. 12, $3CH_2$, Ad), 1.73 (3H, br d, $^2J_{HH}$ ca. 12, $3CH_2$, Ad), 1.77–1.87 (4H, m, $2CH_2$, cy-Hex), 1.94–2.01 (3H, m, 3CH, Ad), 2.27–2.31 (2H, m, CH_2, cy-Hex), 2.92 (2H, t, $^3J_{HH}$ 5.6, CH_2, cy-Hex), 3.07 (2H, q, $^3J_{HH}$ 7.5, CH_2, Et), 3.52 (2H, dt, $^3J_{HH}$ 10.5, $^3J_{HH}$ 5.5, CH_2NH), 4.44–4.49 (1H, m, NH); δ_C (101 MHz, $CDCl_3$): 9.7 (CH_3), 20.9 (CH_2, cy-Hex), 21.1 (CH_2, cy-Hex), 22.0 (CH_2, cy-Hex), 24.5 (CH_2, cy-Hex), 25.3 (CH_2, Et), 28.6 (3CH, Ad), 32.1 (C, Ad), 36.2 (CH_2NH), 37.0 ($3CH_2$, Ad), 42.5 ($3CH_2$, Ad), 44.1 (CH_2Ad), 111.0 (C4a), 151.7 (C, Pyr), 153.1 (C, Pyr), 158.1 (C, Pyr); HRMS (ESI^+, m/z): calc. for $C_{22}H_{33}N_3O$ [M+H] 356.2696, found 356.2690.

***N*-[2-(1-Adamantyl)ethyl]-2-*tert*-butyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7u).**

Obtained as white solid (65 mg, 34%); mp 145–147°C (from $CHCl_3$, with decomposition); R*f* 0.1 (petroleum ether:EtOAc:MeOH 3:1:0.3); δ_H (400 MHz, $CDCl_3$): 1.29–1.36 (2H, m, CH_2Ad), 1.50 (15H, br s, $3CH_2$, Ad + $3CH_3$), 1.60 (3H, br d, $^2J_{HH}$ ca. 12, $3CH_2$, Ad), 1.68 (3H, br d, $^2J_{HH}$ ca. 12, $3CH_2$, Ad), 1.72–1.79 (4H, m, $2CH_2$, cy-Hex), 1.90–1.94 (3H, m, 3CH, Ad), 2.22–2.26 (2H, m, CH_2, cy-Hex), 2.83–2.87 (2H, m, CH_2, cy-Hex), 3.46 (2H, dt, $^3J_{HH}$ 10.8, $^3J_{HH}$ 5.5, CH_2NH), 4.55 (1H, br.s, NH); δ_C (101 MHz, $CDCl_3$): 20.8 (CH_2, cy-Hex), 21.3 (CH_2, cy-Hex), 22.1 (CH_2, cy-Hex), 24.6 (CH_2, cy-Hex), 27.0 ($3CH_3$), 28.6 (3CH, Ad), 32.0 (C, Ad), 36.2 (CH_2NH), 37.0 ($3CH_2$, Ad), 38.7 (C, *t*-Bu), 42.5 ($3CH_2$, Ad), 44.1 (CH_2), 111.6 (C4a), 151.1 (C4, Pyr), 154.8 (C8a, Pyr), 161.1 (C2, Pyr). HRMS (ESI^+, m/z): calc. for $C_{24}H_{37}N_3O$ [M+H] 384.3009, found 384.3005.

***N*-[2-(2-Adamantyl)ethyl]-2-methyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7v).**

Obtained as yellowish oil (111 mg, 65%); R*f* 0.1 (petroleum ether:EtOAc:MeOH 3:1:0.1); δ_H (400 MHz, $CDCl_3$): 1.48–1.90 (21H, m, 15H, Ad + 4H, $2CH_2$, cy-Hex + 2H, CH_2), 2.30 (2H, br t, $^3J_{HH}$ 5.6, CH_2, cy-Hex), 2.59 (3H, s, CH_3), 2.85 (2H, br t, $^3J_{HH}$ 5.5, CH_2, cy-Hex), 3.39–3.51 (2H, m, CH_2NH), 4.90 (1H, br s, NH); δ_C (101 MHz, $CDCl_3$): 20.2 (CH_3), 20.8 (CH_2, cy-Hex), 20.9 (CH_2, cy-Hex), 22.1 (CH_2, cy-Hex), 24.5 (CH_2, cy-Hex), 28.0 (CH, Ad), 28.1 (CH, Ad), 31.6 ($2CH_2$, Ad), 31.9 (2CH, Ad), 32.5 (CH_2), 38.3 (CH_2), 39.1 ($2CH_2$, Ad), 39.9 (CH_2), 42.1 (CH, Ad), 111.9 (C4a), 152.8 (C, Pyr), 153.0 (C, Pyr), 155.3 (C, Pyr); HRMS (ESI^+, m/z): calc. for $C_{21}H_{31}N_3O$ [M+H] 342.2540, found 342.2537.

***N*-[2-(2-Adamantyl)ethyl]-2-*tert*-butyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7w).**

Obtained as white solid (119 mg, 62%); mp 217–219°C (from $CHCl_3$, with decomposition); R*f* 0.1 (petroleum ether:EtOAc:MeOH 3:1:0.3); δ_H (400 MHz, $CDCl_3$): 1.44–1.49 (2H, m, CH_2Ad), 1.49 (9H, s, $3CH_3$), 1.63–1.72 (9H, m, Ad), 1.73–1.77 (4H, m, $2CH_2$, cy-Hex), 1.77–1.86 (6H, m, Ad), 2.25 (2H, t, $^3J_{HH}$ 5.2 Hz, CH_2, cy-Hex), 2.85 (2H, t, $^3J_{HH}$ 5.5, CH_2, cy-Hex), 3.40–3.47

(2H, m, *CH*$_2$NH), 4.59 (1H, br s, NH); δ_C (101 MHz, $CDCl_3$): 20.9 (CH_2, cy-Hex), 21.3 (CH_2, cy-Hex), 22.1 (CH_2, cy-Hex), 24.6 (CH_2, cy-Hex), 26.8 ($3CH_3$), 27.9 (CH, Ad), 28.1 (CH, Ad), 31.7 ($2CH_2$, Ad), 31.9 (2CH, Ad), 32.8 (CH_2), 38.2 (CH_2), 38.6 (C, *t*-Bu), 39.1 ($2CH_2$, Ad), 39.9 (CH_2), 42.2 (CH, Ad), 111.6 (C4a), 150.8 (C4, Pyr), 154.8 (C8a, Pyr), 160.9 (C2, Pyr); HRMS (ESI^+, m/z): calc. for $C_{24}H_{37}N_3O$ [M+H] 384.3009, found 384.3005.

***N*-[2-(1-Adamantyloxy)ethyl]-2-methyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7x).**

Obtained as yellowish oil (41 mg, 23%); R*f* 0.1 (petroleum ether:EtOAc:MeOH 3:1:0.3); δ_H (400 MHz, $CDCl_3$): 1.57 (3H, br d, $^2J_{HH}$ ca. 12, $3CH_2$, Ad), 1.63 (3H, br d, $^2J_{HH}$ ca. 12, $3CH_2$, Ad), 1.70 (6H, d, $^3J_{HH}$ ca. 2, $3CH_2$, Ad), 1.73–1.83 (4H, m, $2CH_2$, cy-Hex), 2.12 (3H, br s, 3CH, Ad), 2.28 (2H, br t, $^3J_{HH}$ 5.6, CH_2, cy-Hex), 2.59 (3H, s, CH_3), 2.88 (2H, br t, $^3J_{HH}$ 5.8, CH_2, cy-Hex), 3.53–3.60 (4H, m, CH_2O, *CH*$_2$NH), 4.99 (1H, br s, NH); δ_C (101 MHz, $CDCl_3$): 20.1 (CH_3), 20.9 (CH_2, cy-Hex), 21.0 (CH_2, cy-Hex), 22.0 (CH_2, cy-Hex), 24.5 (CH_2, cy-Hex), 30.4 (3CH, Ad), 36.3 ($3CH_2$, Ad), 41.5 (CH_2NH), 41.6 ($3CH_2$, Ad), 58.4 (CH_2O), 72.4 (C, Ad), 111.9 (C4a), 151.6 (C, Pyr), 153.3 (C, Pyr), 154.7 (C, Pyr); HRMS (ESI^+, m/z): calc. for $C_{21}H_{31}N_3O_2$ [M+H] 358.2489, found 358.2485.

***N*-[1-Adamantyl(phenyl)methyl]-2-methyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7y).**

Obtained as yellowish oil (103 mg, 51%); R*f* 0.1 (petroleum ether:EtOAc:MeOH 3:1:0.3); δ_H (400 MHz, $CDCl_3$): 1.46 (3H, br d, $^2J_{HH}$ ca. 12, $3CH_2$, Ad), 1.53–1.60 (3H, m, $3CH_2$, Ad), 1.65–1.70 (6H, m, $3CH_2$, Ad), 1.79–1.85 (4H, m, $2CH_2$, cy-Hex), 1.95–1.99 (3H, m, 3CH, Ad), 2.36–2.44 (2H, m, CH_2, cy-Hex), 2.50 (3H, s, CH_3), 2.83–2.89 (2H, m, CH_2, cy-Hex), 4.89 (1H, d, $^3J_{HH}$ 8.5, *CH*NH), 5.10 (1H, br d, $^3J_{HH}$ 8.5, NH), 7.16–7.19 (2H, m, 2CH, Ph), 7.20–7.30 (3H, m, 3CH, Ph); δ_C (101 MHz, $CDCl_3$): 20.1 (CH_3), 20.9 (CH_2, cy-Hex), 21.0 (CH_2, cy-Hex), 22.1 (CH_2, cy-Hex), 24.5 (CH_2, cy-Hex), 28.3 (3CH, Ad), 36.5 (C, Ad), 36.8 ($3CH_2$, Ad), 38.6 (C, *t*-Bu), 39.2 ($3CH_2$, Ad), 63.5 (*CH*NH), 111.4 (C4a), 126.9 (CH, Ph), 127.6 (2CH, Ph), 128.3 (2CH, Ph), 139.5 (C, Ph), 151.0 (C, Pyr), 153.2 (C, Pyr), 154.6 (C, Pyr); HRMS (ESI^+, m/z): calc. for $C_{26}H_{33}N_3O$ [M+H] 404.2696, found 404.2696.

***N*-[1-Adamantyl(phenyl)methyl]-2-*tert*-butyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7z).**

Obtained as yellowish oil (56 mg, 25%); R*f* 0.1 (petroleum ether:EtOAc:MeOH 3:1:0.3); δ_H (400 MHz, $CDCl_3$): 1.42 (9H, s, $3CH_3$), 1.49 (3H, br d, $^2J_{HH}$ ca. 12, $3CH_2$, Ad), 1.60 (3H, br d, $^2J_{HH}$ ca. 12, $3CH_2$, Ad), 1.68–1.73 (6H, m, $3CH_2$, Ad), 1.79–1.86 (4H, m, $2CH_2$, cy-Hex), 2.00 (3H, br s, 3CH, Ad), 2.39–2.46 (2H, m, CH_2, cy-Hex), 2.84–2.90 (2H, m, CH_2, cy-Hex), 4.86 (1H, d, $^3J_{HH}$ 8.3, *CH*NH), 5.10 (1H, br d, $^3J_{HH}$ 8.3, NH), 7.16–7.19 (2H, m, 2CH, Ph), 7.21–7.31 (3H, m, 3CH, Ph); δ_C (101 MHz, $CDCl_3$): 20.9 (CH_2, cy-Hex), 21.2 (CH_2, cy-Hex), 22.1 (CH_2, cy-Hex), 24.6 (CH_2, cy-Hex), 26.8 ($3CH_3$), 28.3 (3CH, Ad), 36.3 (C, Ad), 36.8 ($3CH_2$, Ad), 39.3 ($3CH_2$, Ad), 64.1 (CH), 111.6 (C4a), 126.8 (CH, Ph), 127.5 (2CH, Ph), 128.4 (2CH, Ph), 139.7 (C, Ph), 150.1 (C, Pyr), 154.9 (C, Pyr), 160.7 (C, Pyr); HRMS (ESI^+, m/z): calc. for $C_{26}H_{39}N_3O$ [M+H] 446.3166, found 446.3162.

4-[4-(2-Adamantyl)piperazin-1-yl]-2-methyl-5,6,7,8-tetrahydroquinazoline 1-oxide (7aa).

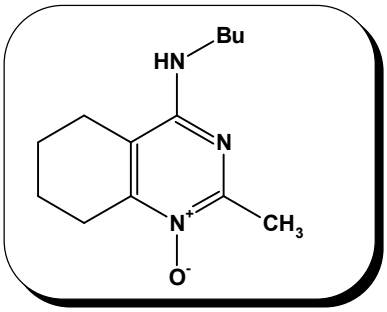
Obtained as white solid (56 mg, 29%); mp 118–120^{o}C (from $CHCl_3$); R*f* 0.1 (petroleum ether:EtOAc:MeOH 3:1:0.3); δ_H (400 MHz, $CDCl_3$): 1.37 (2H, br d, $^2J_{HH}$ ca. 12, CH_2, Ad), 1.60–1.72 (6H, m, $2CH_2$, Ad + CH_2, cy-Hex), 1.77 (1H, br.s, CH, Ad), 1.79–1.90 (5H, m, CH_2, Ad +

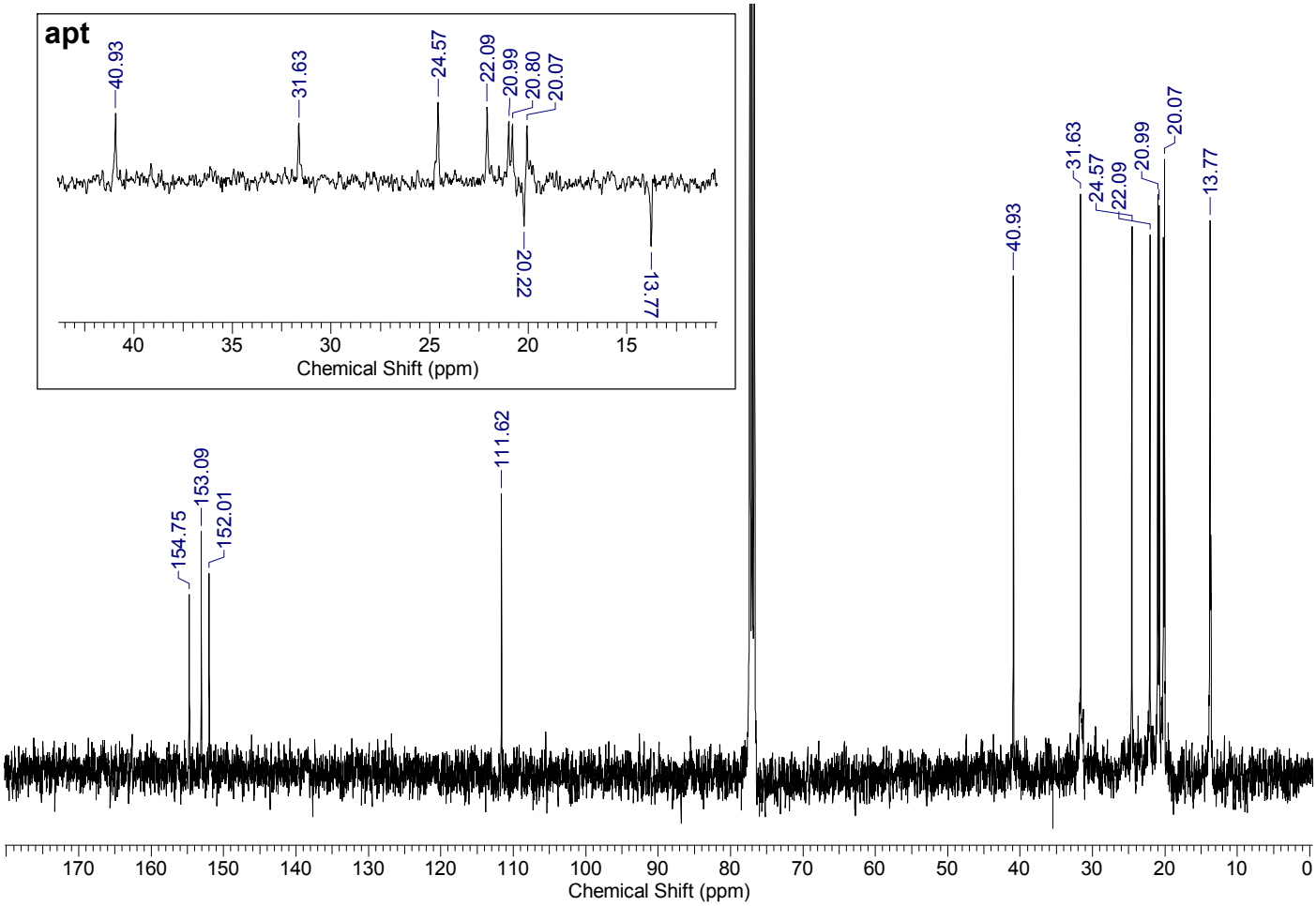
CH, Ad + CH_2, cy-Hex), 1.99–2.10 (5H, m, $2CH_2$, Ad + 3CH, Ad), 2.46–2.57 (6H, m, $2CH_2N$ + CH_2, cy-Hex), 2.61 (3H, s, CH_3), 2.91 (2H, t, $^3J_{HH}$ 6.6, CH_2, cy-Hex), 3.24–3.33 (4H, m, $2CH_2N$); δ_C (101 MHz, $CDCl_3$): 19.9 (CH_3), 21.4 (CH_2, cy-Hex), 21.7 (CH_2, cy-Hex), 25.4 (CH_2, cy-Hex), 26.2 (CH_2, cy-Hex), 27.3 (CH, Ad), 27.5 (CH, Ad), 28.9 (2CH, Ad), 31.3 ($2CH_2$, Ad), 37.2 ($2CH_2$, Ad), 37.7 (CH_2, Ad), 48.8 ($2CH_2N$), 49.4 ($2CH_2N$), 67.6 (CHN, Ad), 118.8 (C4a), 154.0 (C, Pyr), 154.97 (C, Pyr), 155.01 (C, Pyr); HRMS (ESI^+, m/z): calc. for $C_{23}H_{34}N_4O$ [M+H] 383.2805, found 383.2800.

4-[4-(2-Adamantyl)piperazin-1-yl]-2-*tert*-butyl-5,6,7,8-tetrahydroquinazoline 1-oxide (7ab). Obtained as white solid (108 mg, 51%); mp 75–78°C (from $CHCl_3$); R*f* 0.1 (petroleum ether:EtOAc:MeOH 3:1:0.3); δ_H (400 MHz, $CDCl_3$): 1.40 (2H, br d, $^2J_{HH}$ ca. 12, CH_2, Ad), 1.50 (9H, s, $3CH_3$), 1.60–1.72 (6H, m, $2CH_2$, Ad + CH_2, cy-Hex), 1.78 (1H, br s, CH, Ad), 1.80–1.89 (5H, m, CH_2, Ad + CH, Ad + CH_2, cy-Hex), 2.03–2.12 (5H, m, $2CH_2$, Ad + 3CH, Ad), 2.48–2.57 (6H, m, $2CH_2N$ + CH_2, cy-Hex), 2.90 (2H, t, $^3J_{HH}$ 6.6, CH_2, cy-Hex), 3.27–3.35 (4H, m, $2CH_2N$); δ_C (101 MHz, $CDCl_3$): 21.60 (CH_2, cy-Hex), 21.64 (CH_2, cy-Hex), 25.5 (CH_2, cy-Hex), 26.3 (CH_2, cy-Hex), 26.7 ($3CH_3$), 27.3 (CH, Ad), 27.5 (CH, Ad), 28.9 (2CH, Ad), 31.3 ($2CH_2$, Ad), 37.2 ($2CH_2$, Ad), 37.7 (CH_2, Ad), 38.7 (C, *t*-Bu), 48.8 ($2CH_2N$), 49.4 ($2CH_2N$), 67.7 (CHN, Ad), 118.5 (C4a), 154.1 (C4, Pyr), 156.7 (C8a, Pyr), 160.1 (C2, Pyr); HRMS (ESI^+, m/z): calc. for $C_{23}H_{34}N_4O$ [M+H] 425.3275, found 425.3265.

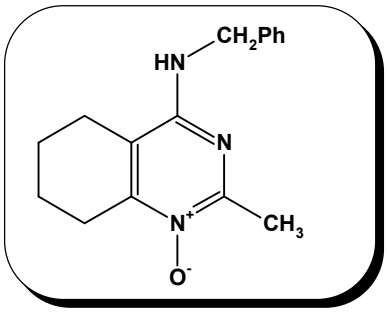
4-Ethoxy-2-methyl-5,6,7,8-tetrahydroquinazoline 1-oxide (8). Obtained as admixture in synthesis of **7g** (30% according to ^1H NMR spectra of reaction mixture), **7j** (15%), **7n** (50%), **7p** (10%), **7r** (10%). For comparison **8** was obtained in the same conditions but without addition of amine **6** into the reaction mixture and isolated via column chromatography (SiO_2) as yellowish oil (45 mg, 43%), R*f* 0.15 (petroleum ether:EtOAc:MeOH 3:1:0.1); δ_H (400 MHz, $CDCl_3$): 1.36 (3H, t, $^3J_{HH}$ 7.0, CH_3, Et), 1.65–1.75 (2H, m, $2CH_2$), 1.78–1.87 (2H, m, $2CH_2$), 2.53 2H, (br.t, $^3J_{HH}$ 6.2, CH_2), 2.63 (s, 3H, CH_3), 2.89 (2H, br.t, $^3J_{HH}$ 6.3, CH_2), 4.37 (2H, q, $^3J_{HH}$ 7.0, CH_2, Et); δ_C (101 MHz, $CDCl_3$): 14.4 (CH_3, Et), 19.8 (CH_2), 20.6 (CH_3), 21.1 (CH_2), 21.7 (CH_2), 24.8 (CH_2), 62.7 (CH_2, Et), 116.6 (C4a), 154.1 (C2), 156.1 (C8a), 156.7 (C4). HRMS (ESI^+, m/z): calc. for $C_{11}H_{16}N_2O_2$ [M+H] 209.1285, found 209.1290.

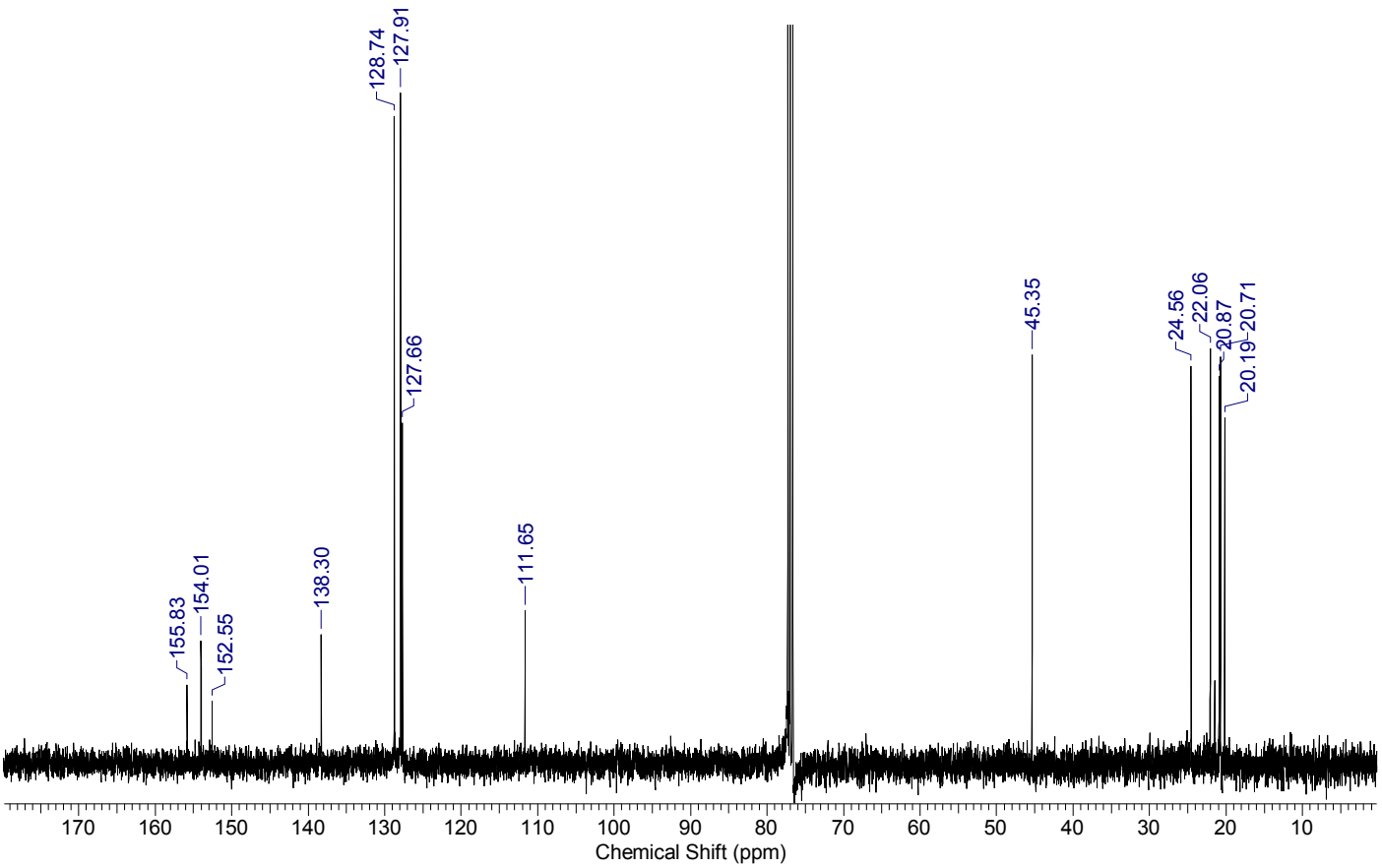
N-Butyl-2-methyl-5,6,7,8-tetrahydroquinazoline-4-amine 1-oxide (7a)



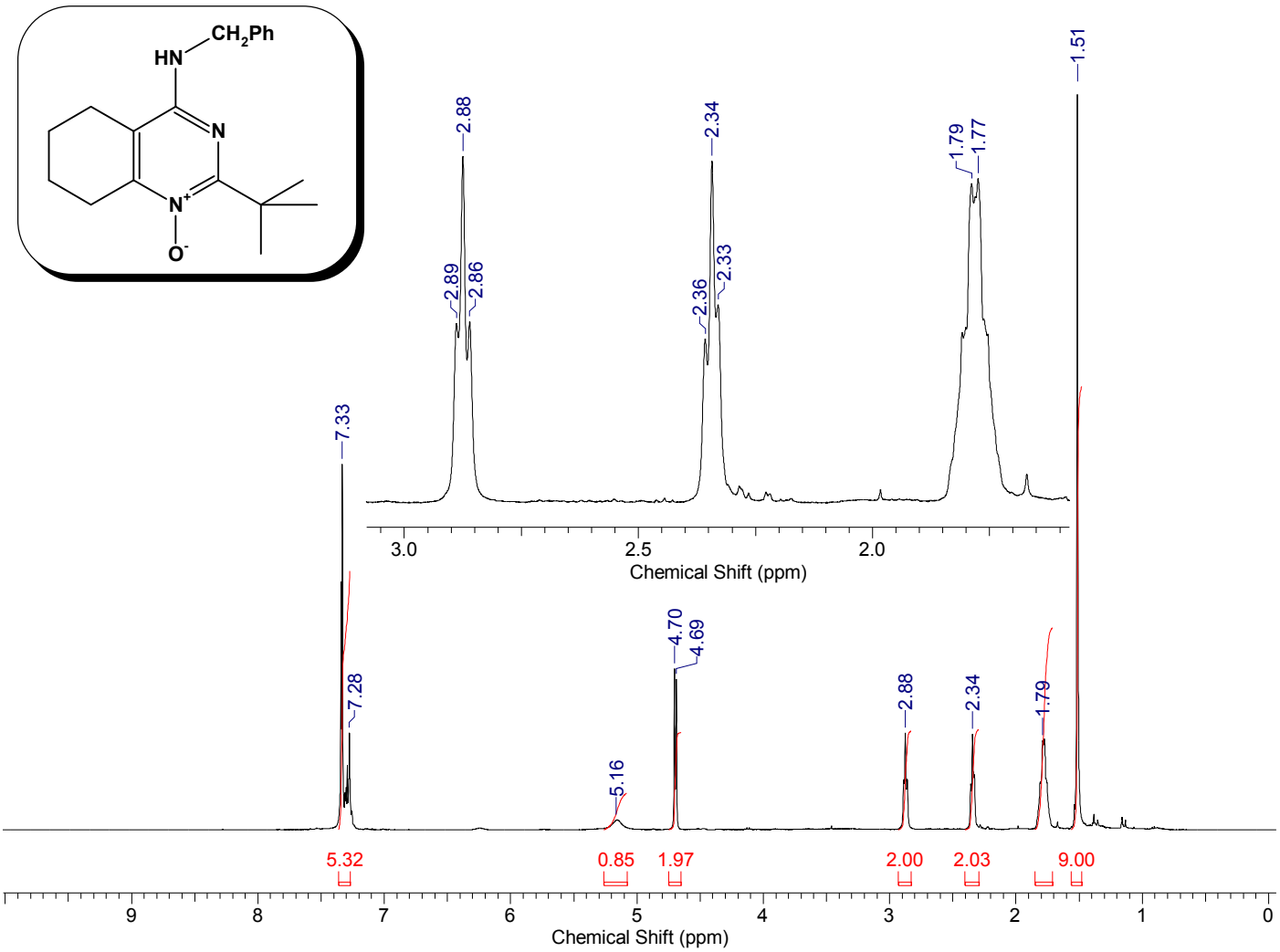


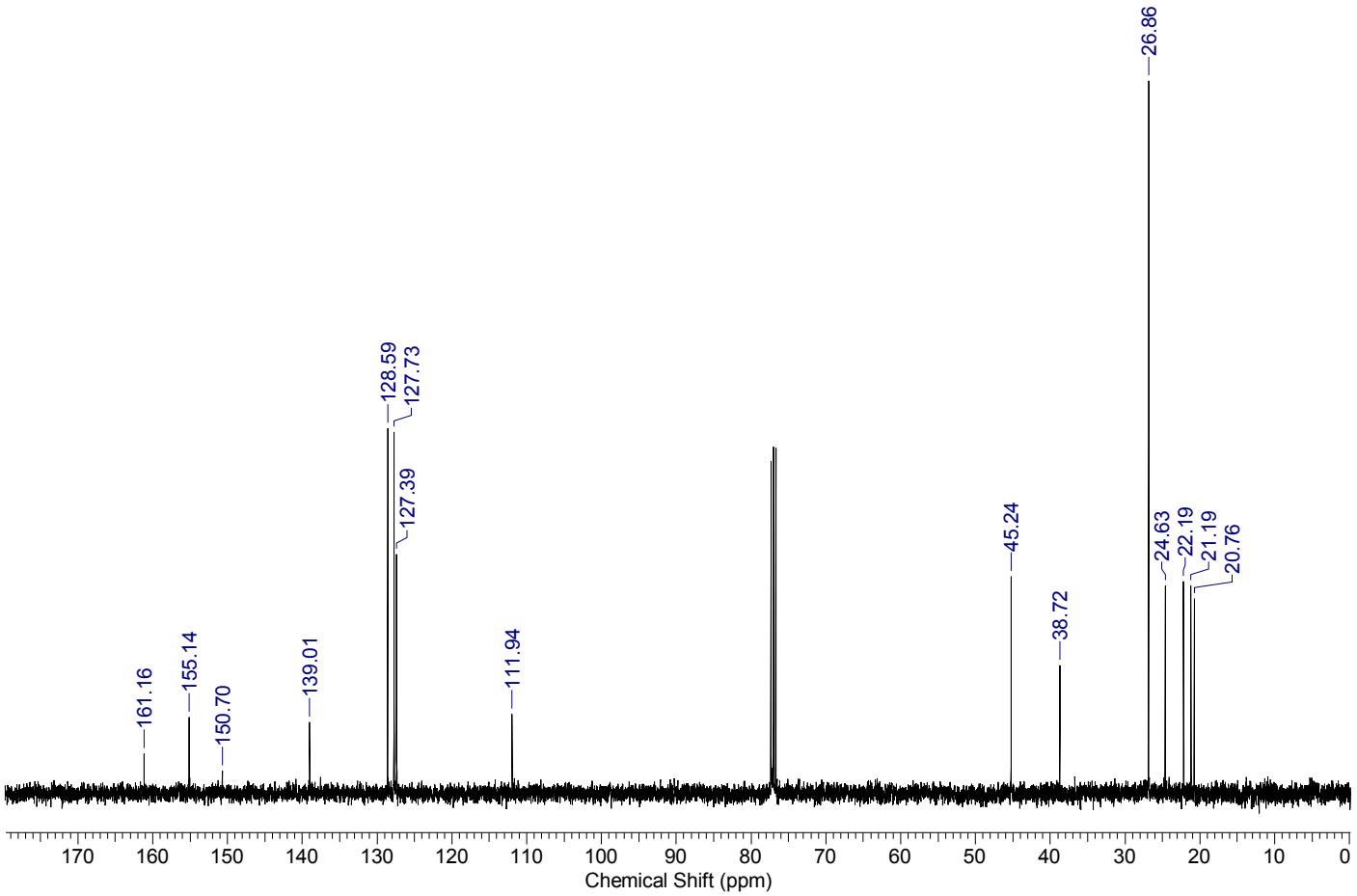
N-Benzyl-2-methyl-5,6,7,8-tetrahydroquinazoline-4-amine 1-oxide (7b)



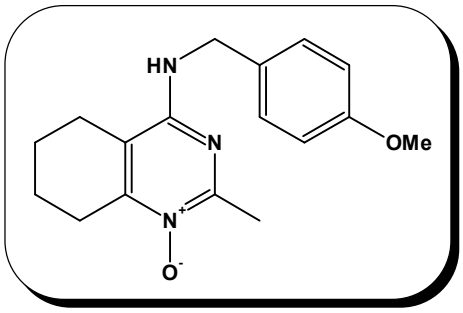


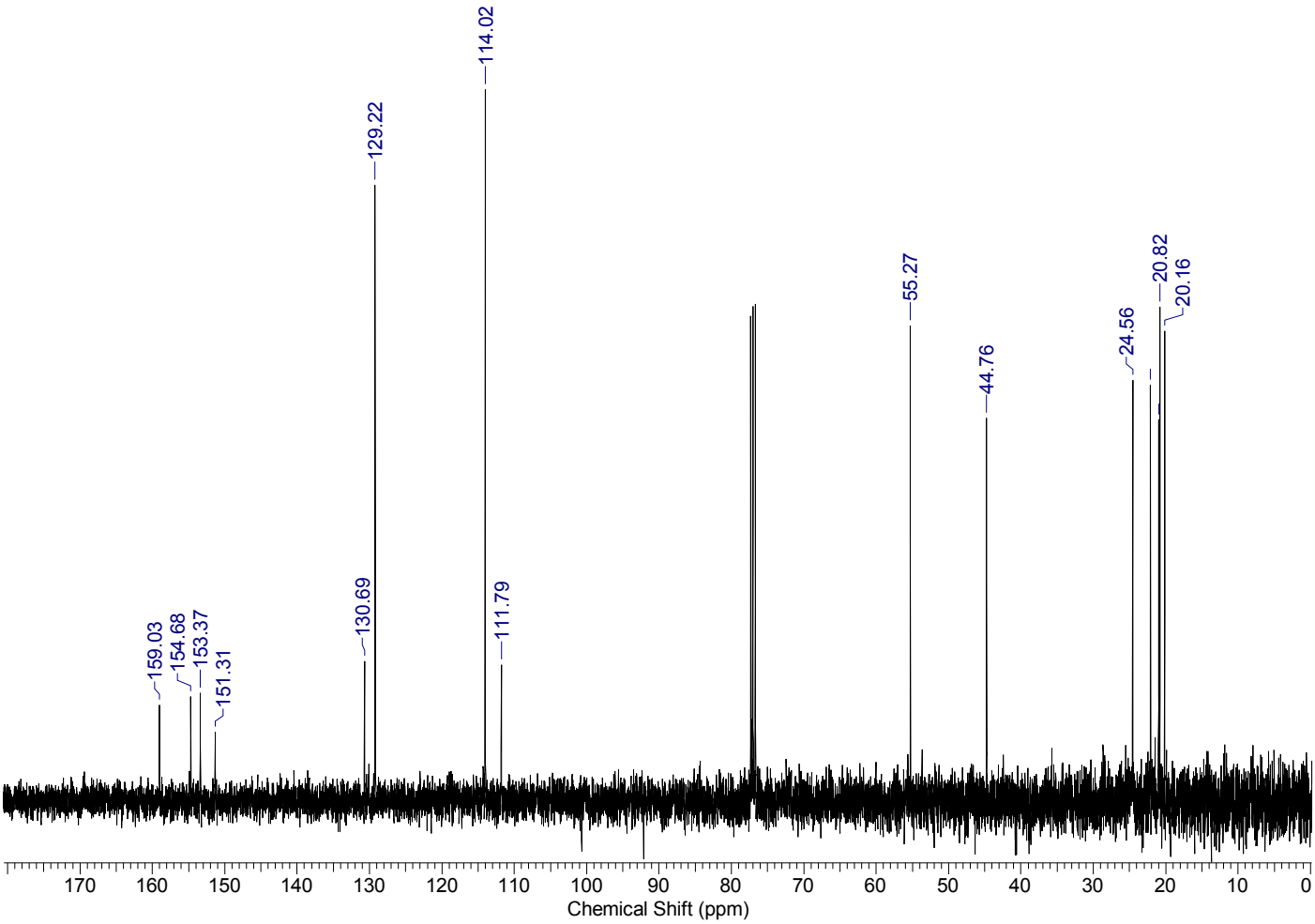
N-Benzyl-2-tert-butyl-5,6,7,8-tetrahydroquinazoline-4-amine 1-oxide (7c)



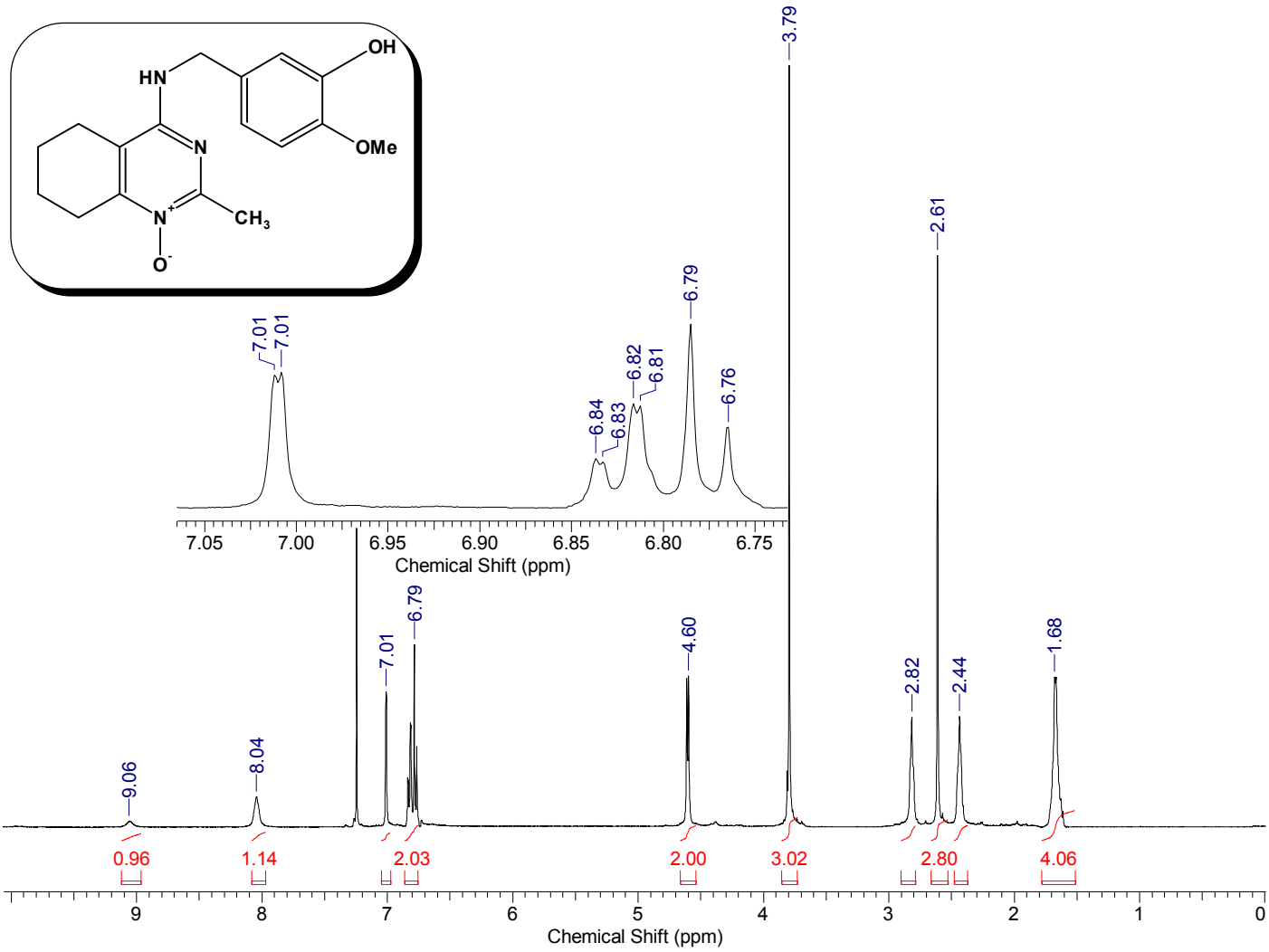


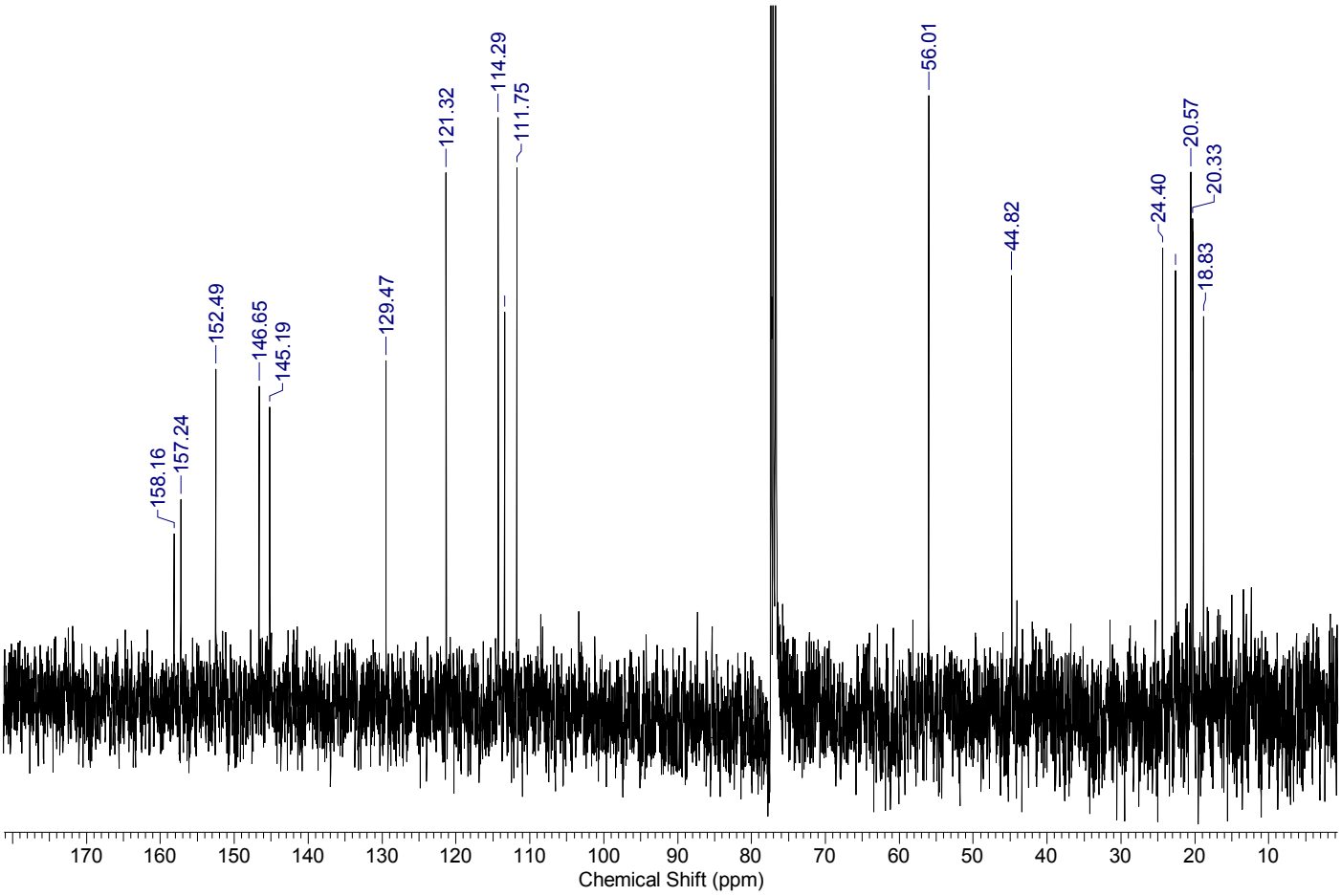
N-(4-Methoxybenzyl)-2-methyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7d)



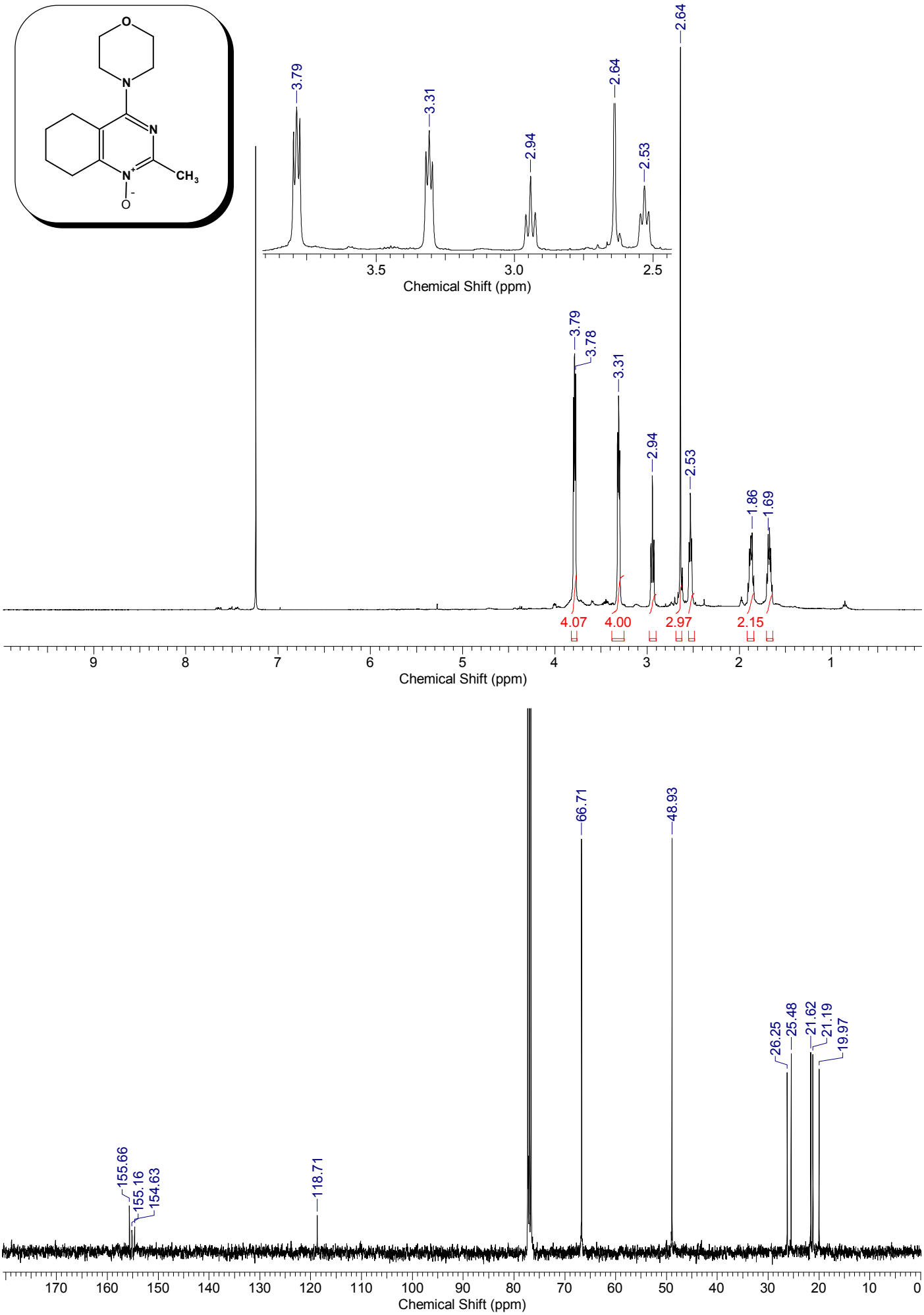


2-Methoxy-5-{[(2-methyl-1-oxido-5,6,7,8-tetrahydroquinazolin-4-yl)amino]methyl}phenol (7e)

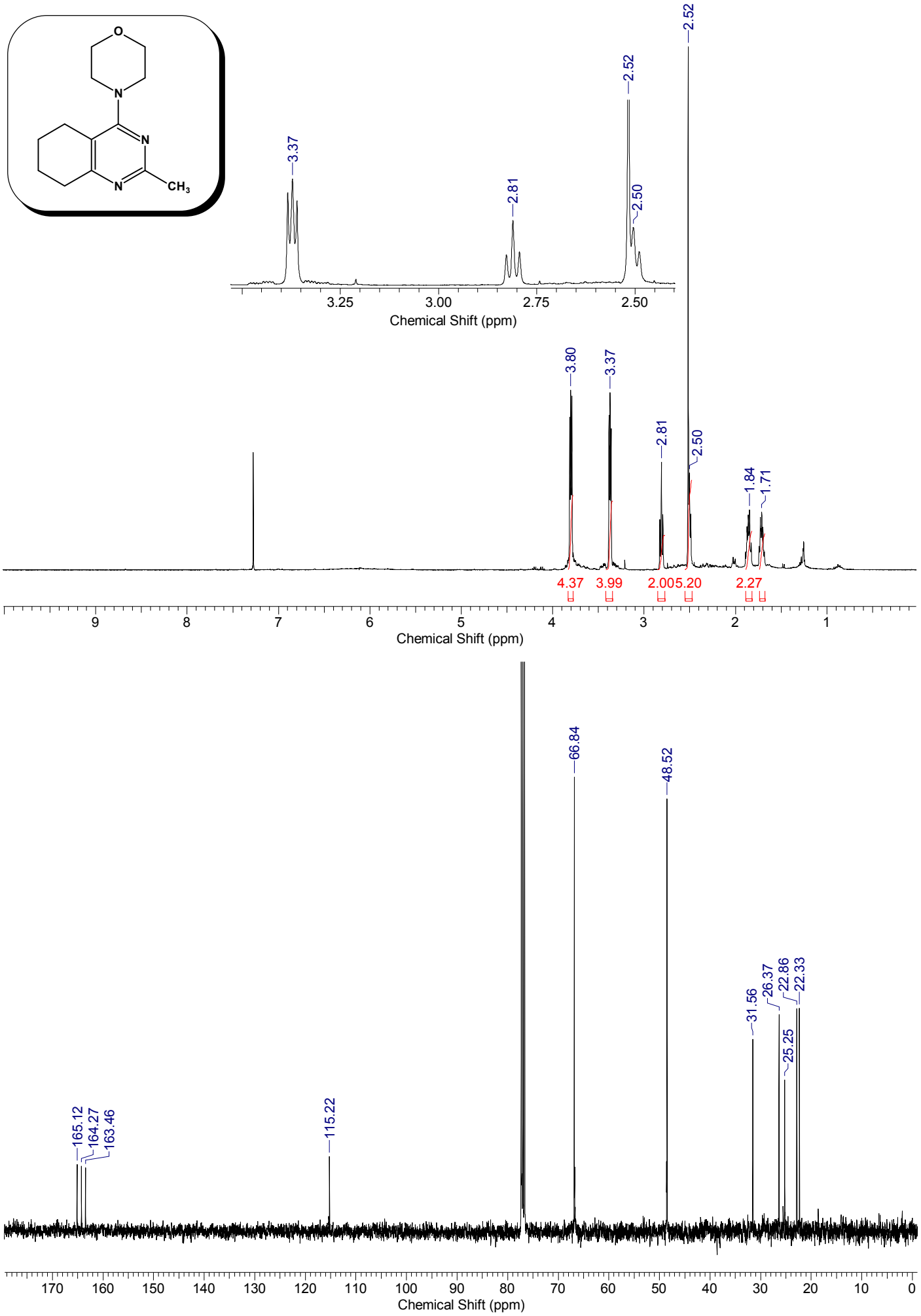




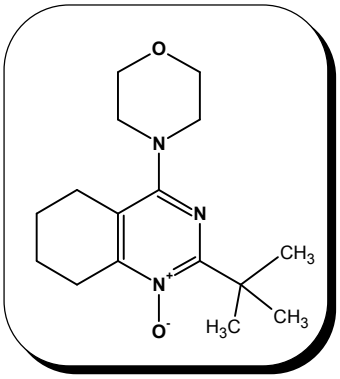
2-Methyl-4-morpholin-4-yl-5,6,7,8-tetrahydroquinazoline 1-oxide (7f)

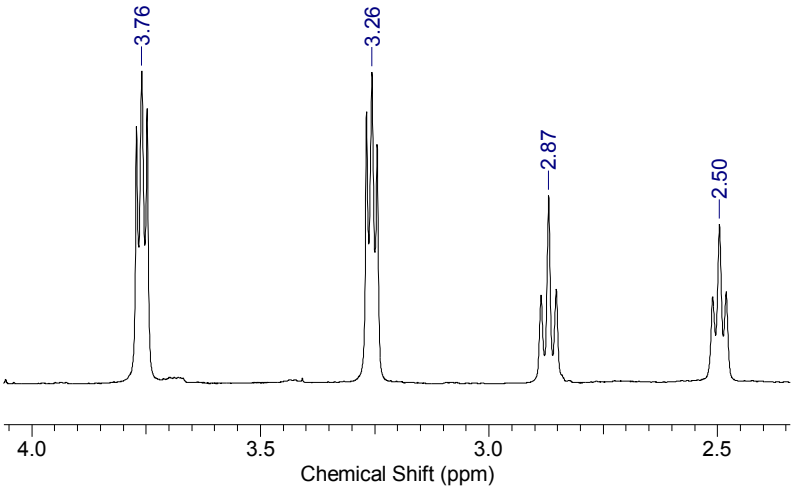


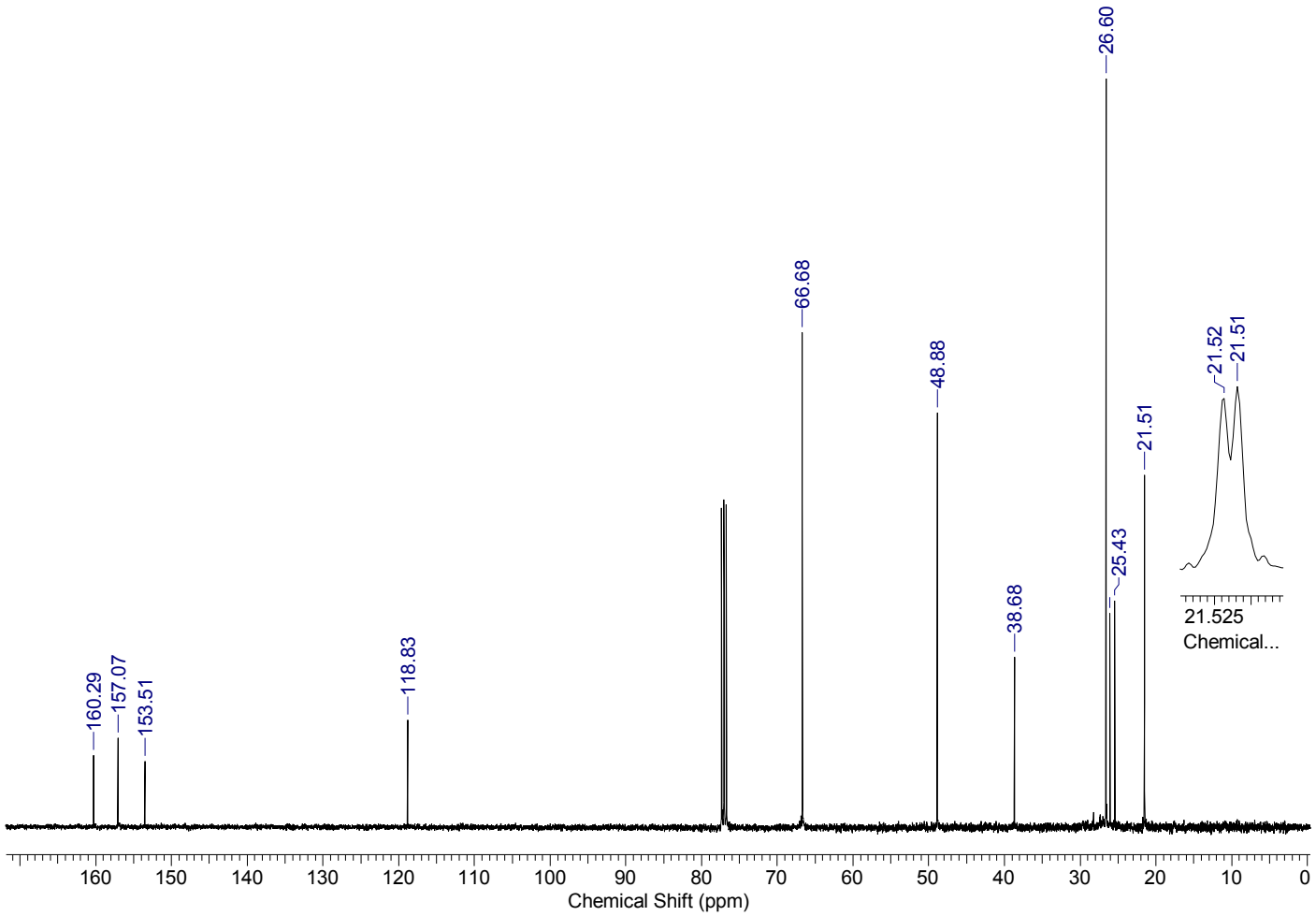
2-Methyl-4-morpholin-4-yl-5,6,7,8-tetrahydroquinazoline (7g)



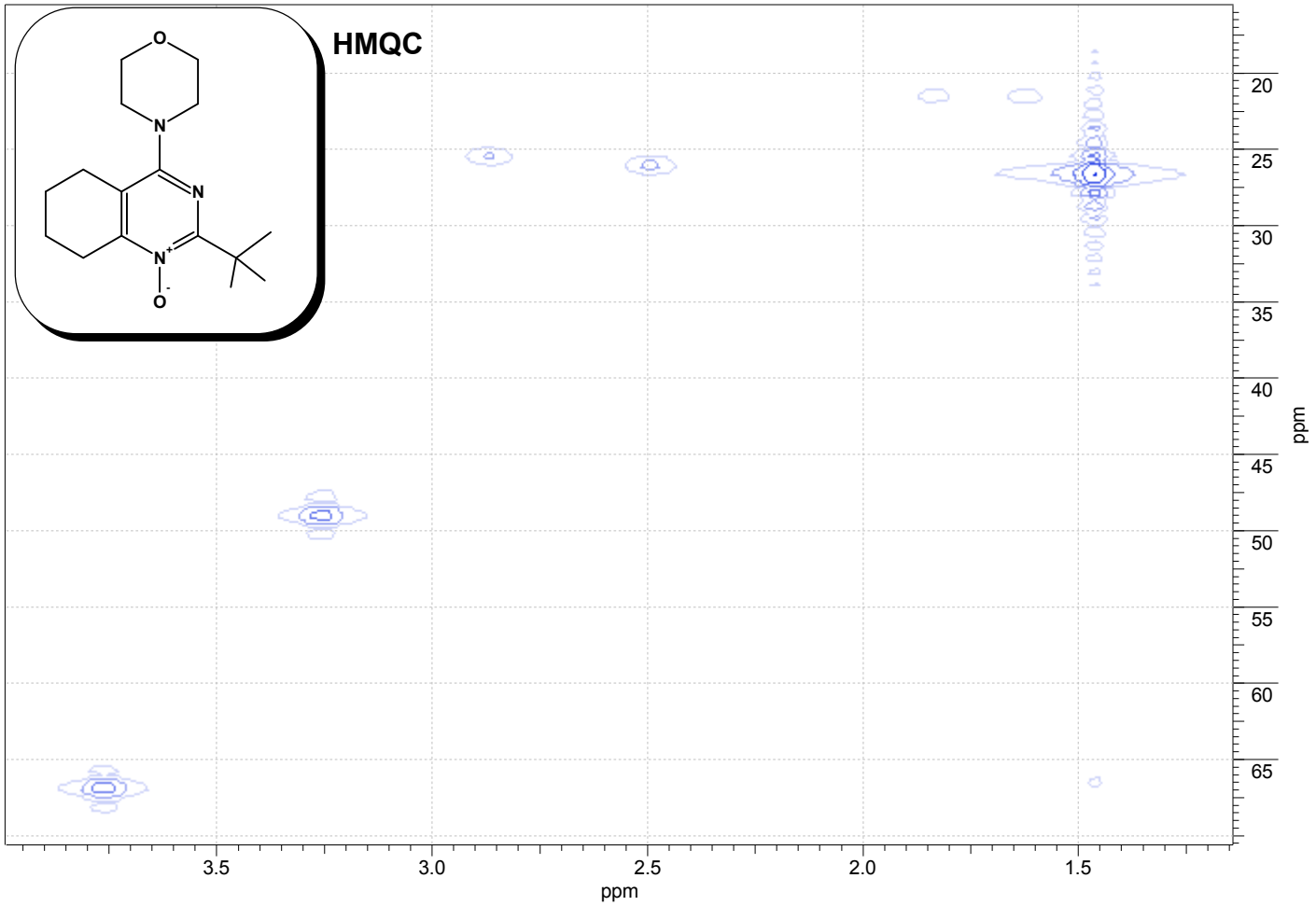
4-Morpholin-4-yl-2-tert-butyl-5,6,7,8-tetrahydroquinazoline 1-oxide (7h)

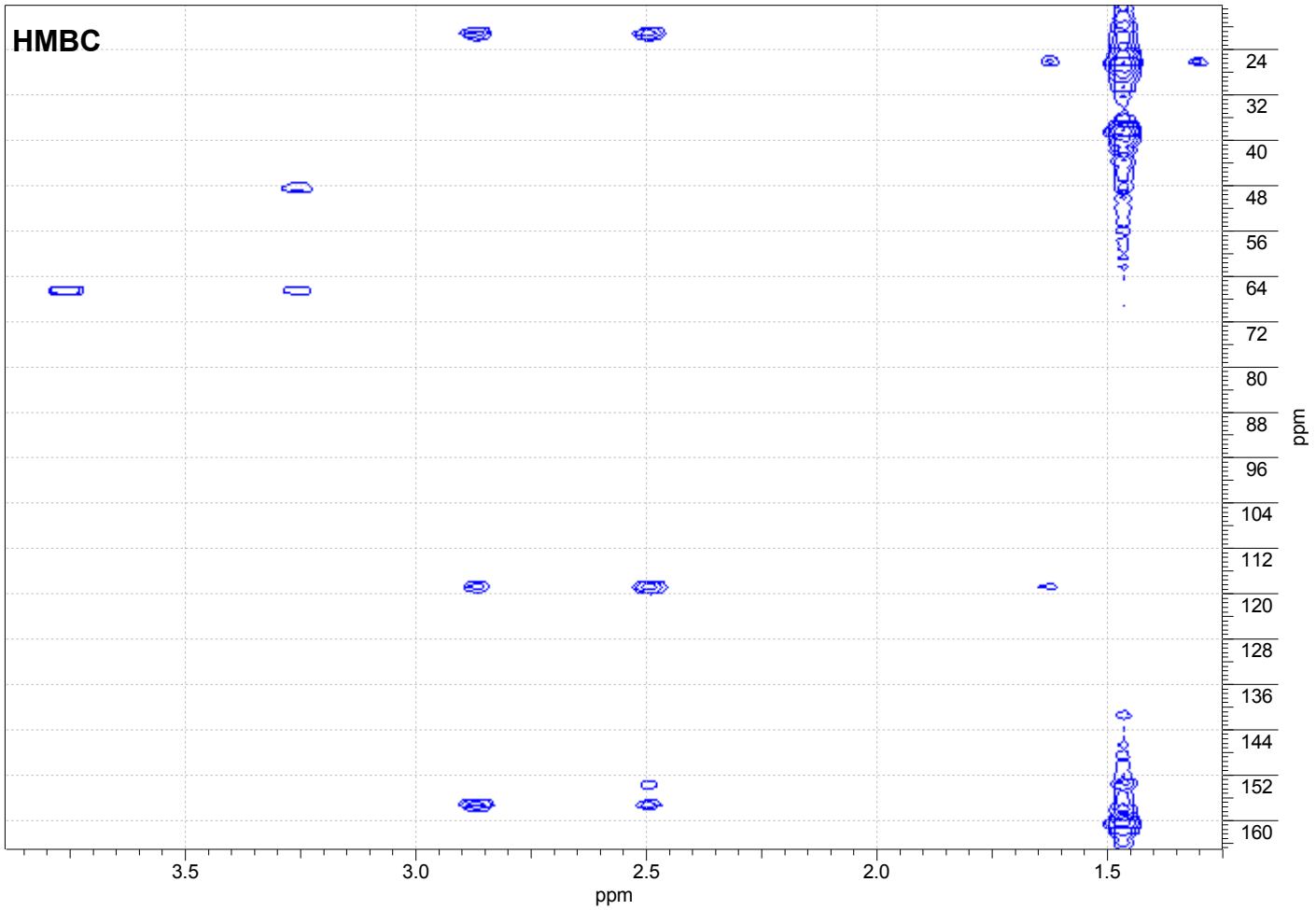




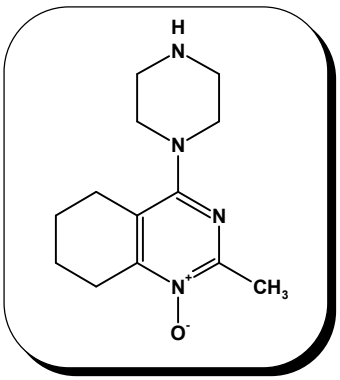


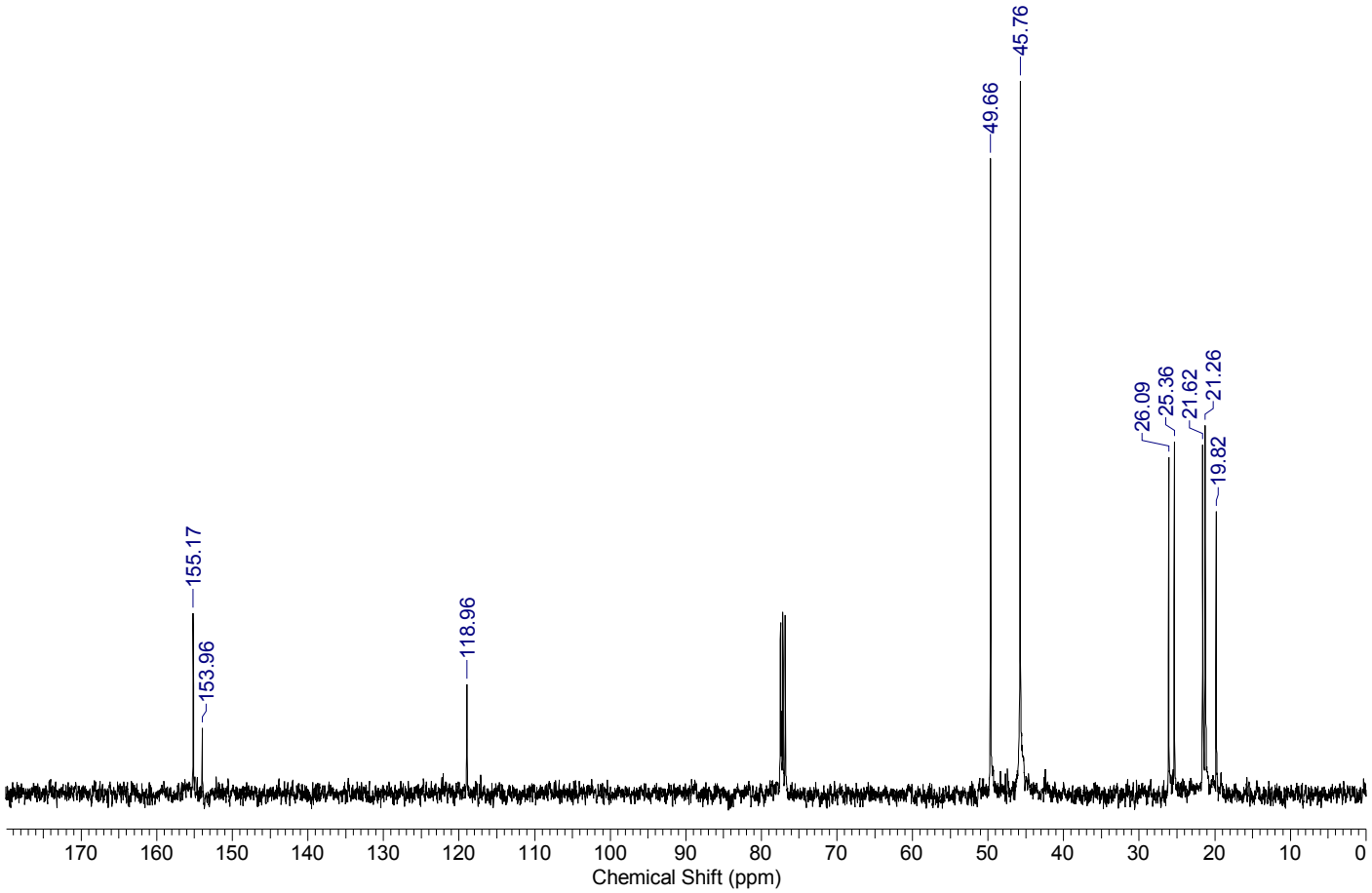
4-Morpholin-4-yl-2-tert-butyl-5,6,7,8-tetrahydroquinazoline 1-oxide (7h)



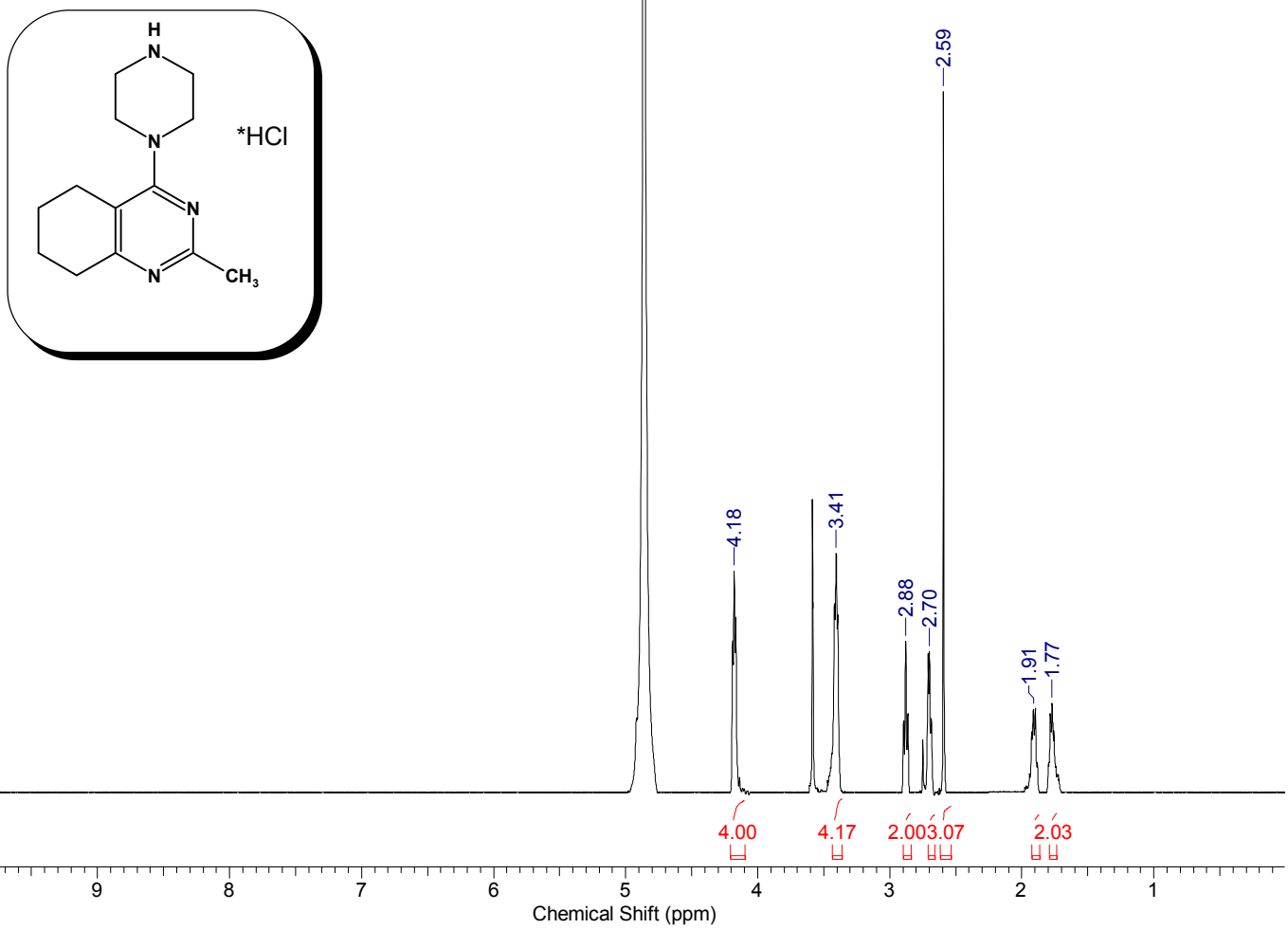


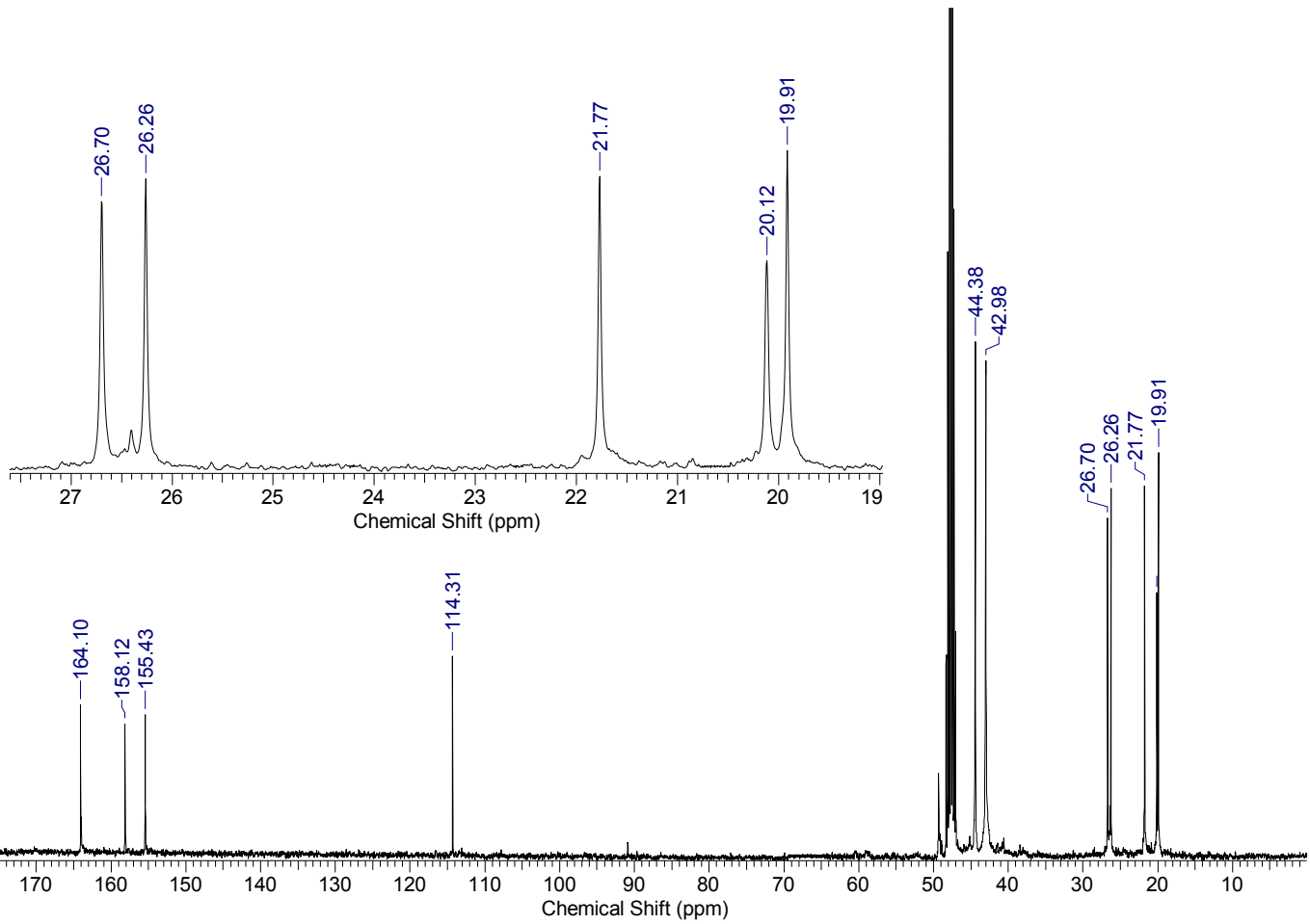
2-Methyl-4-piperazin-1-yl-5,6,7,8-tetrahydroquinazoline 1-oxide (7i)



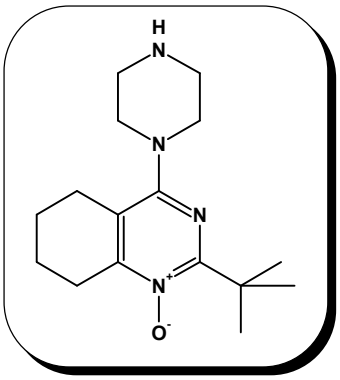


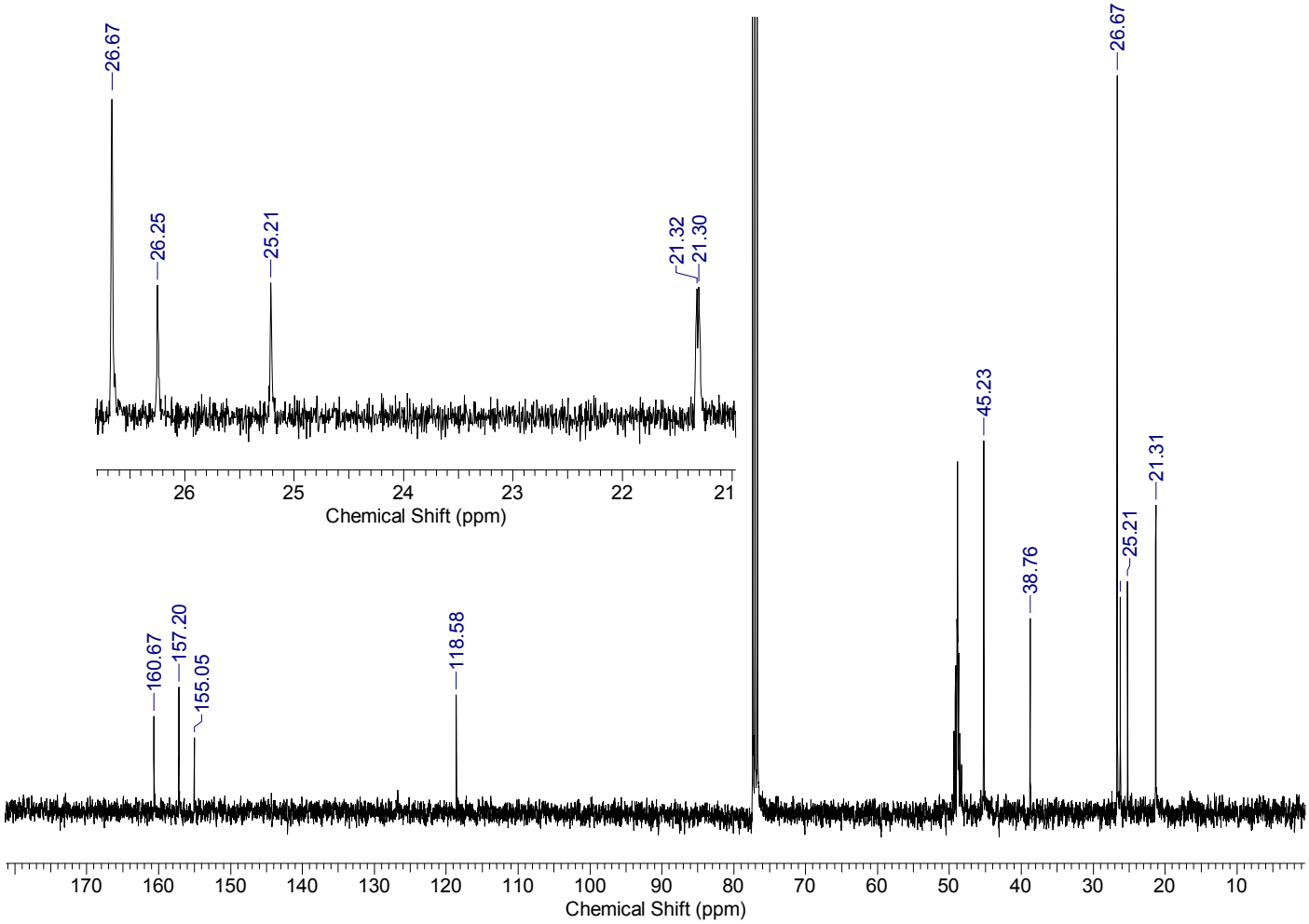
2-Methyl-4-piperazin-1-yl-5,6,7,8-tetrahydroquinazoline (7j) hydrochloride



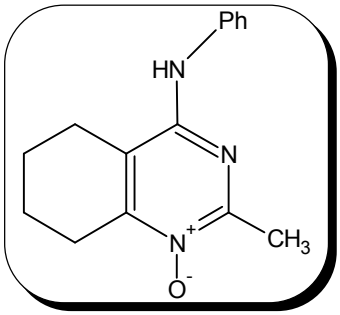


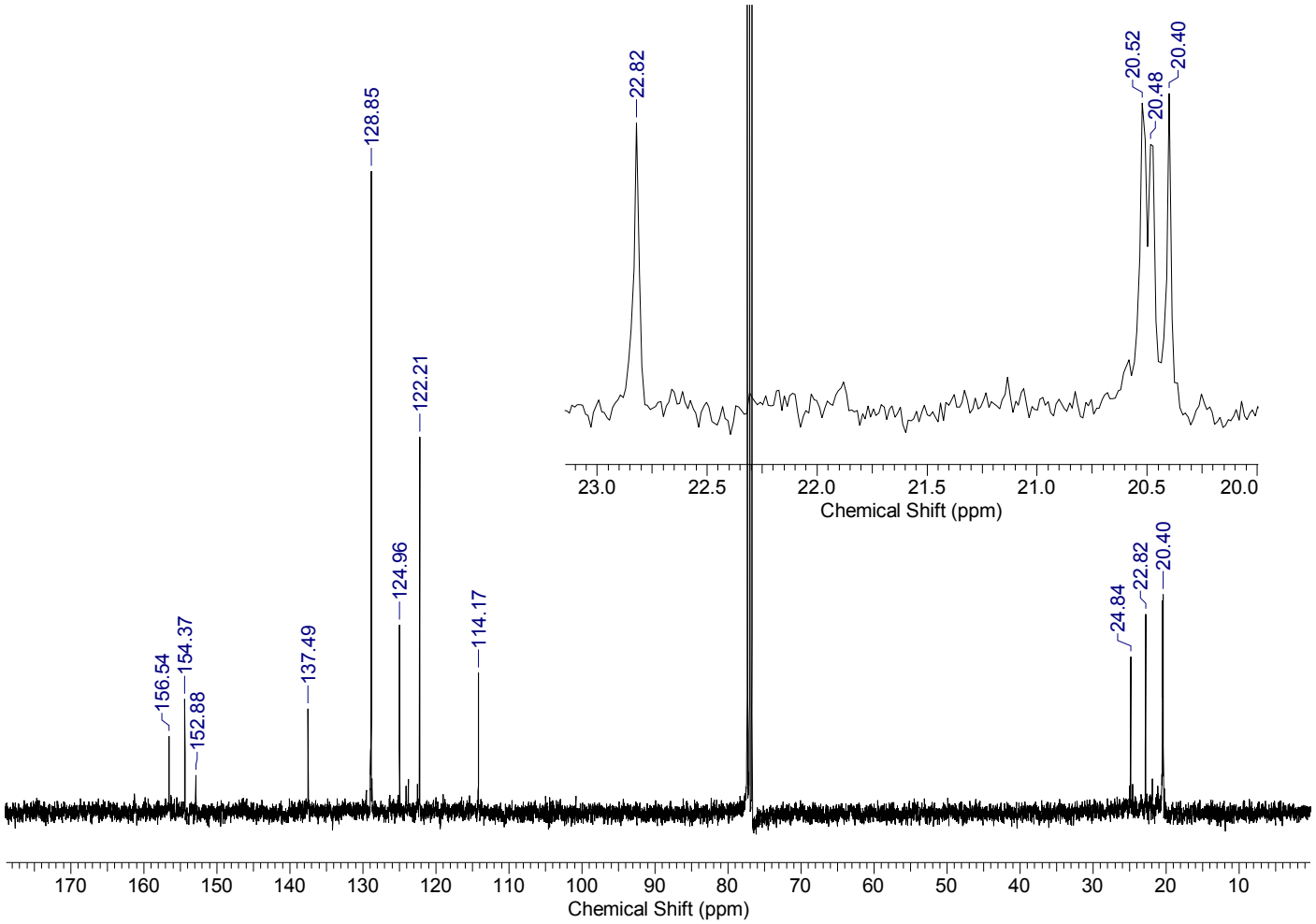
4-Piperazin-1-yl-2-tert-butyl-5,6,7,8-tetrahydroquinazoline 1-oxide (7k)



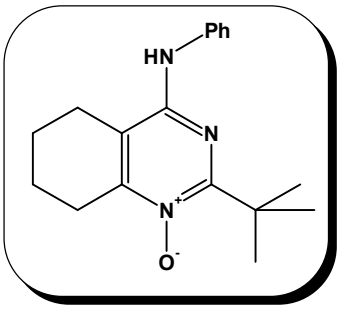


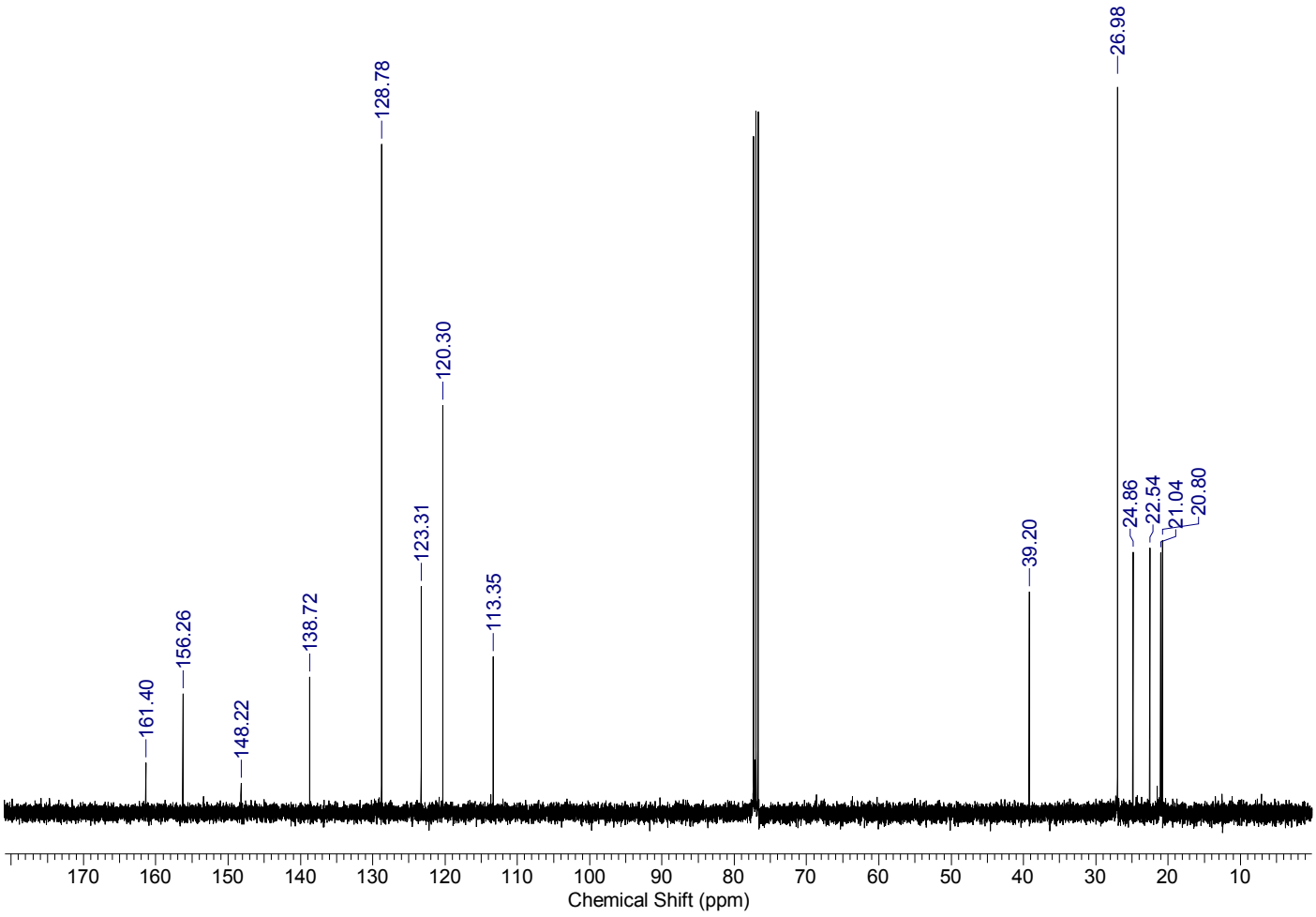
2-Methyl-N-phenyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7l)



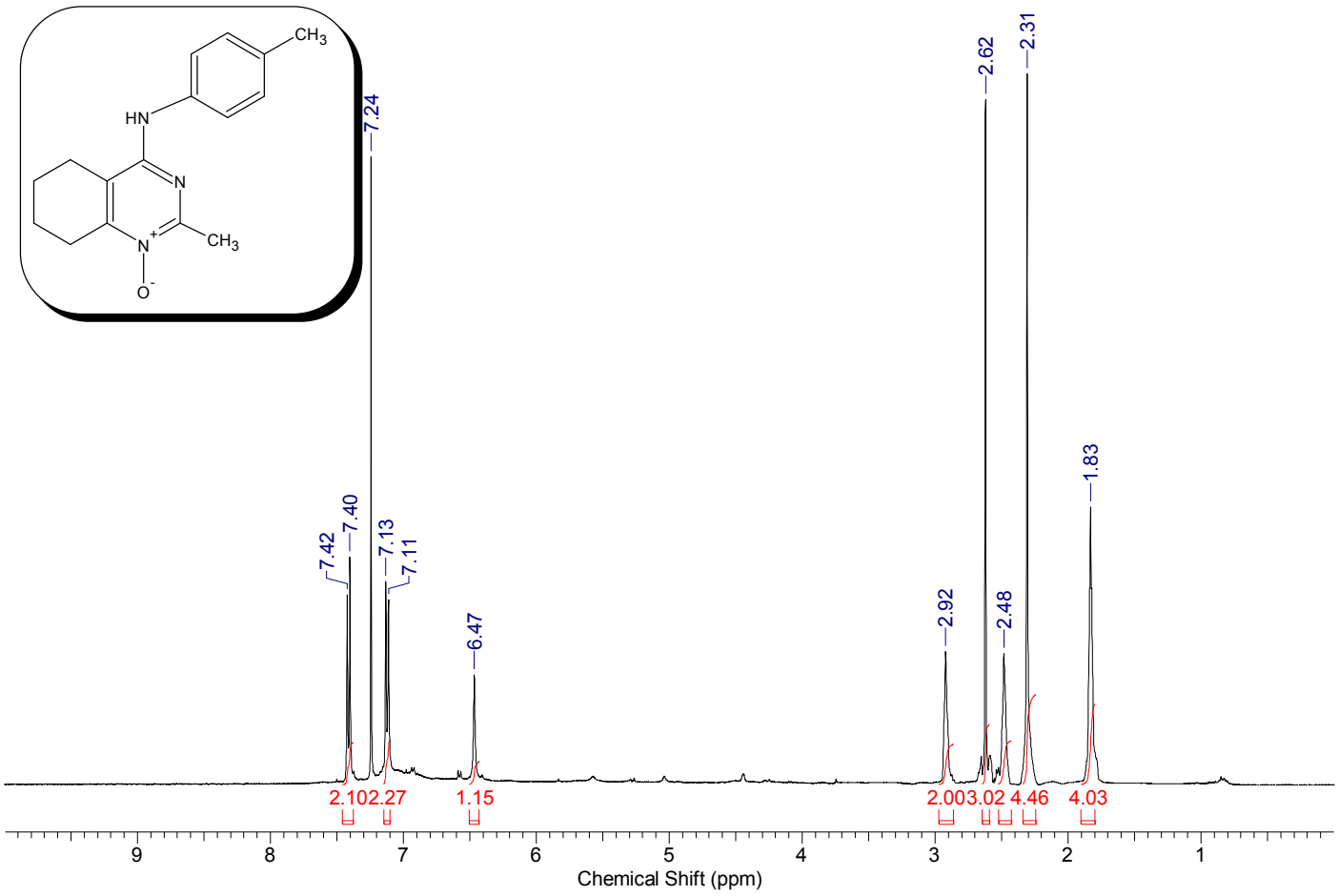


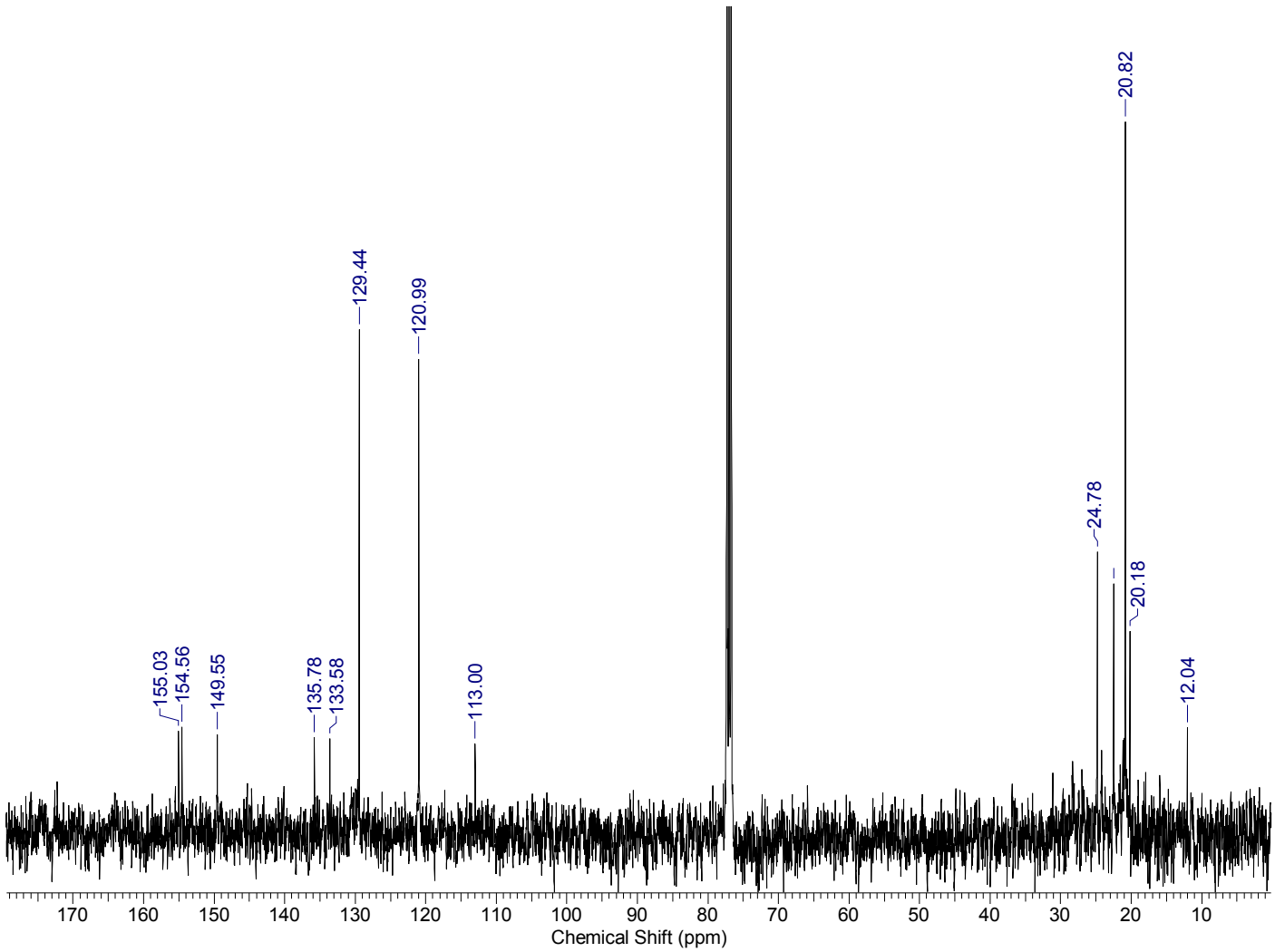
N-Phenyl-2-tert-butyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7m)



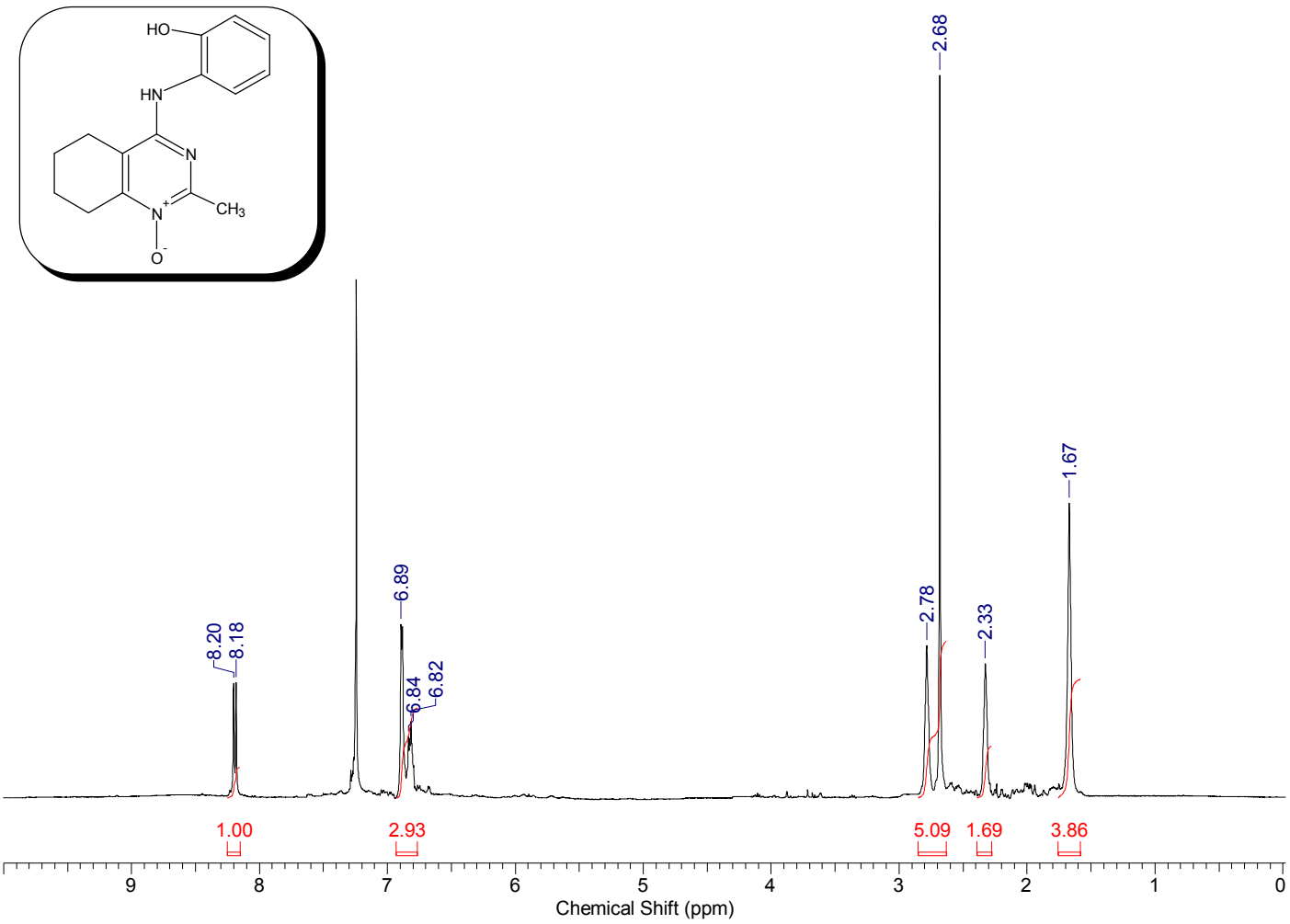


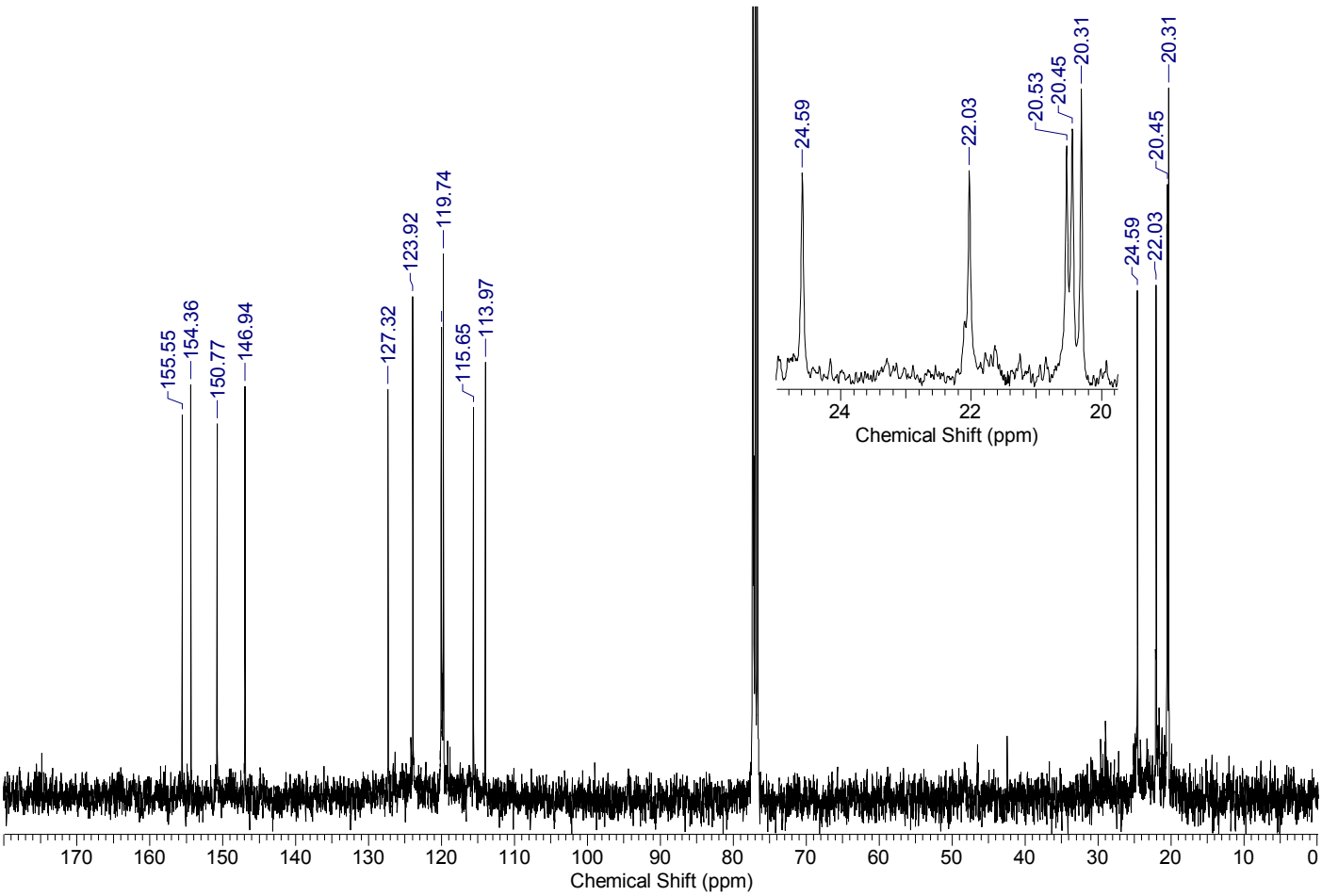
2-Methyl-N-(4-methylphenyl)-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7n)



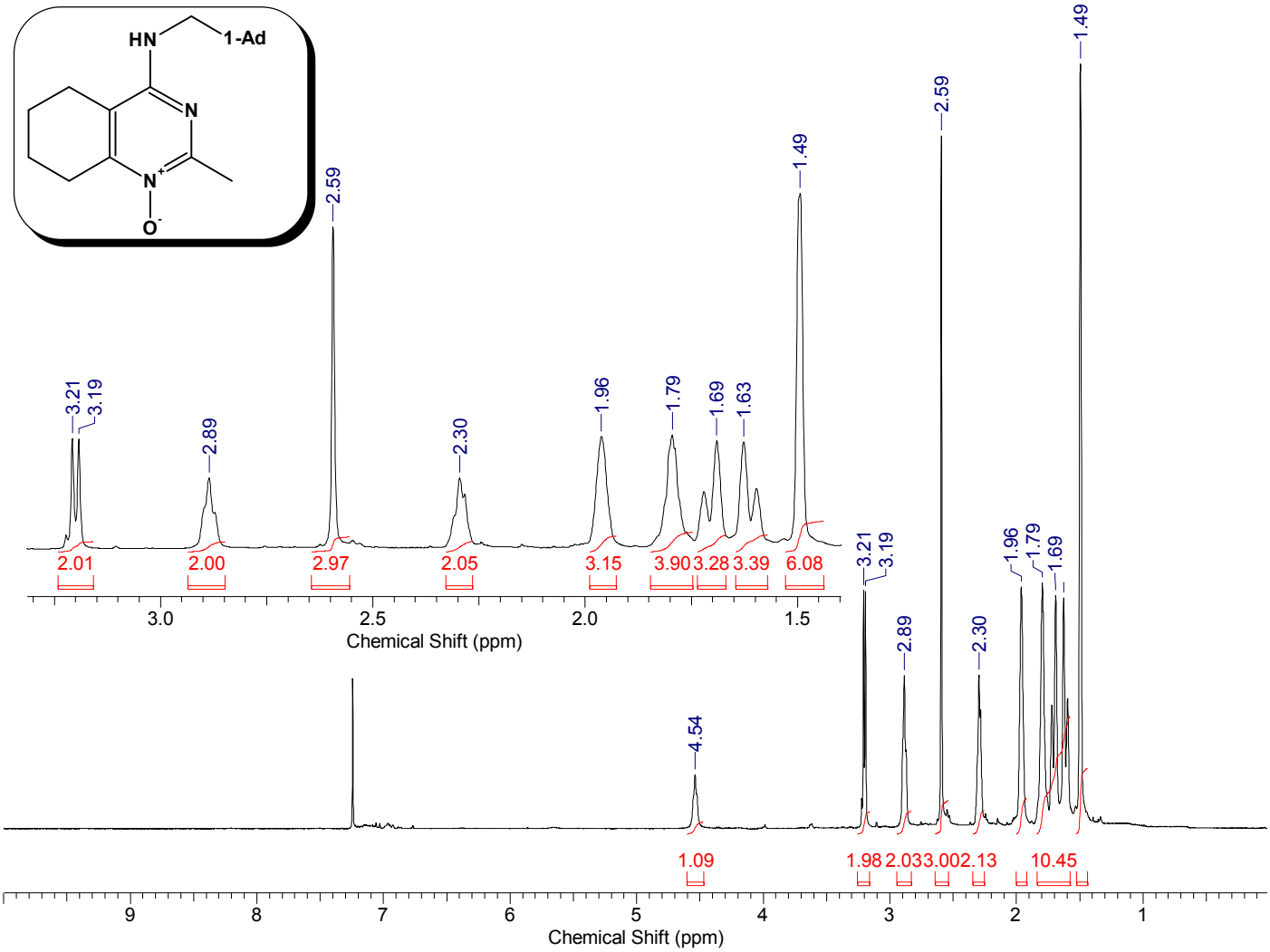


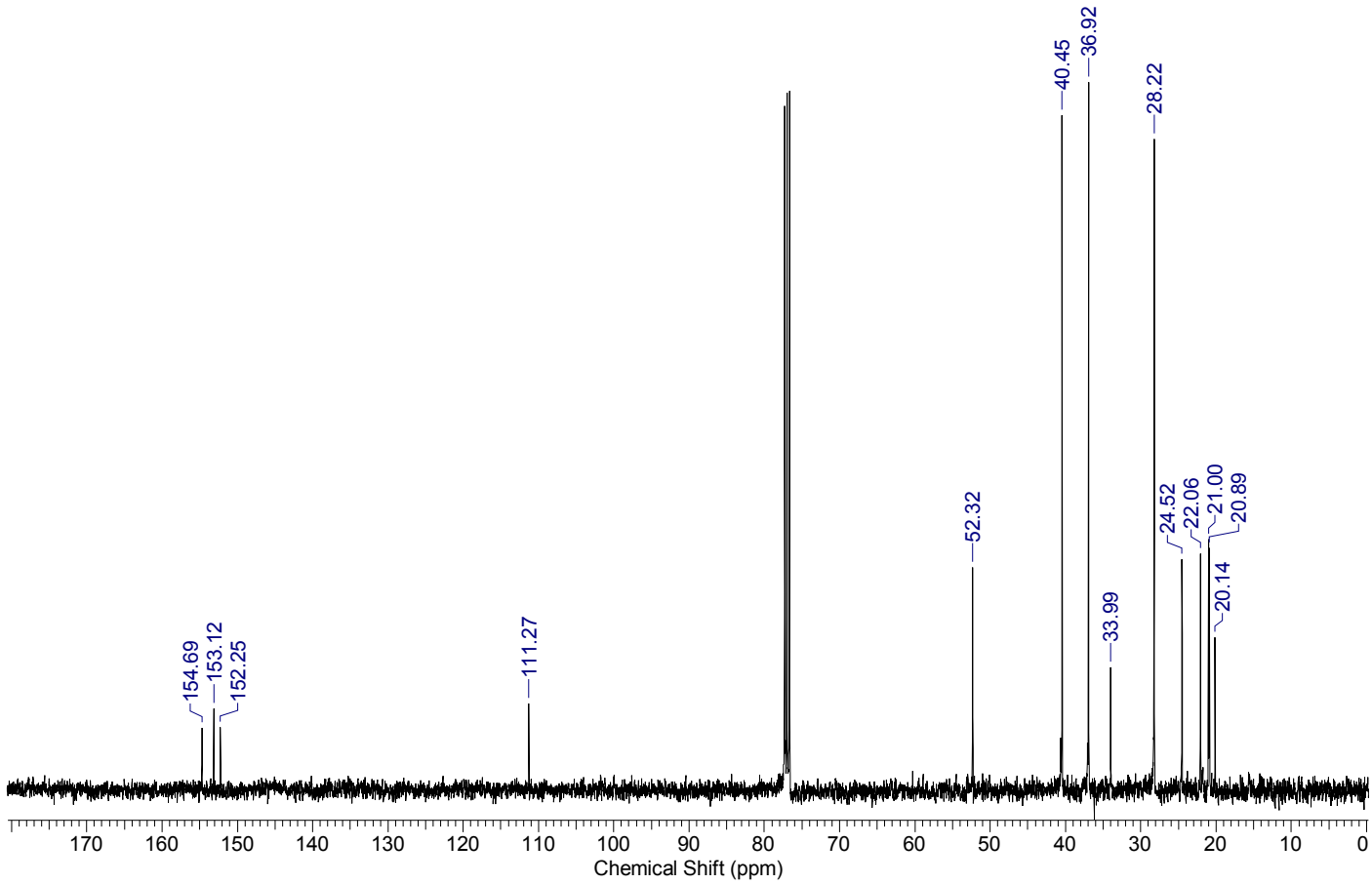
2-[(2-Methyl-1-oxido-5,6,7,8-tetrahydroquinazolin-4-yl)amino]phenol (7o)



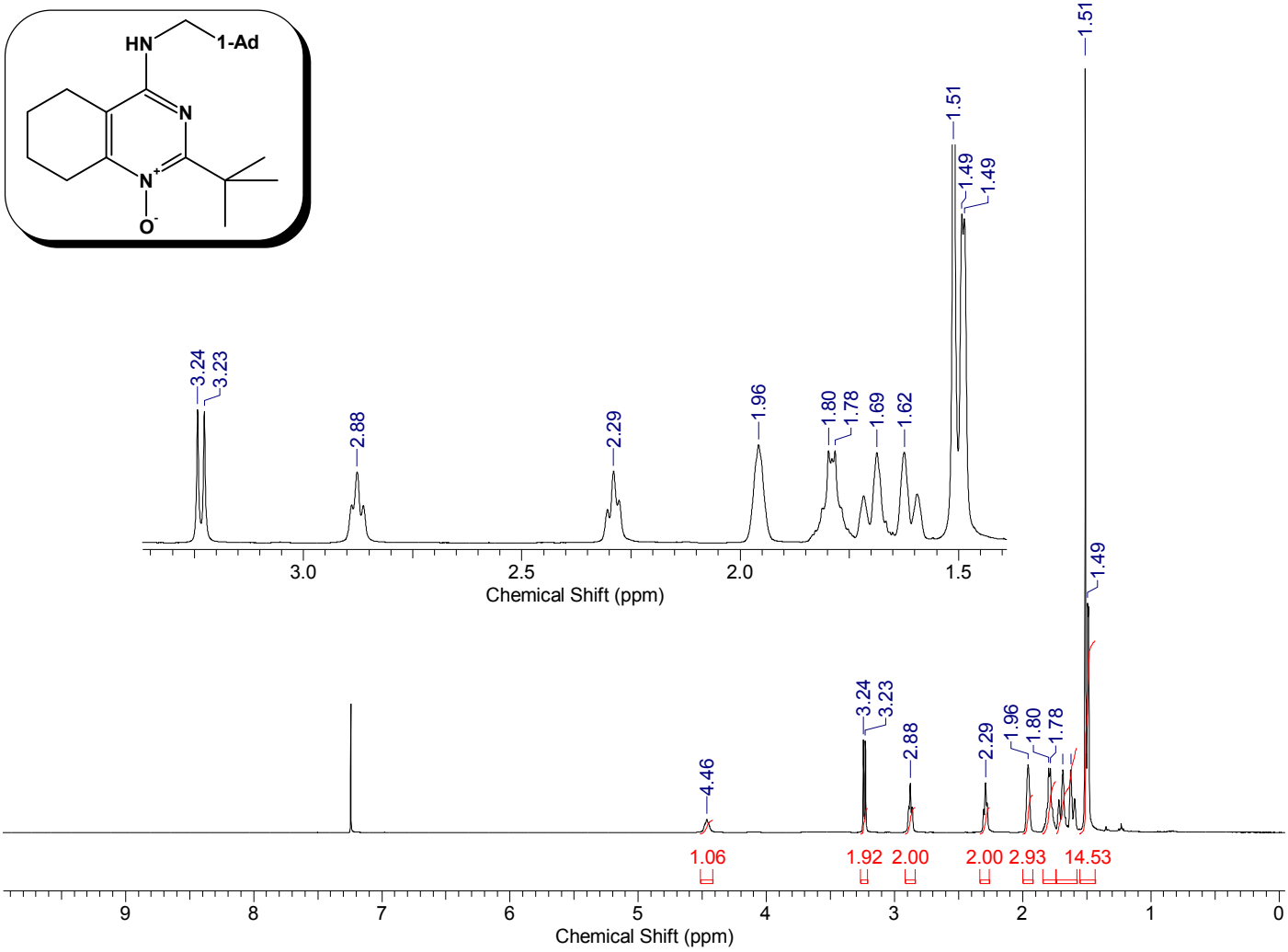


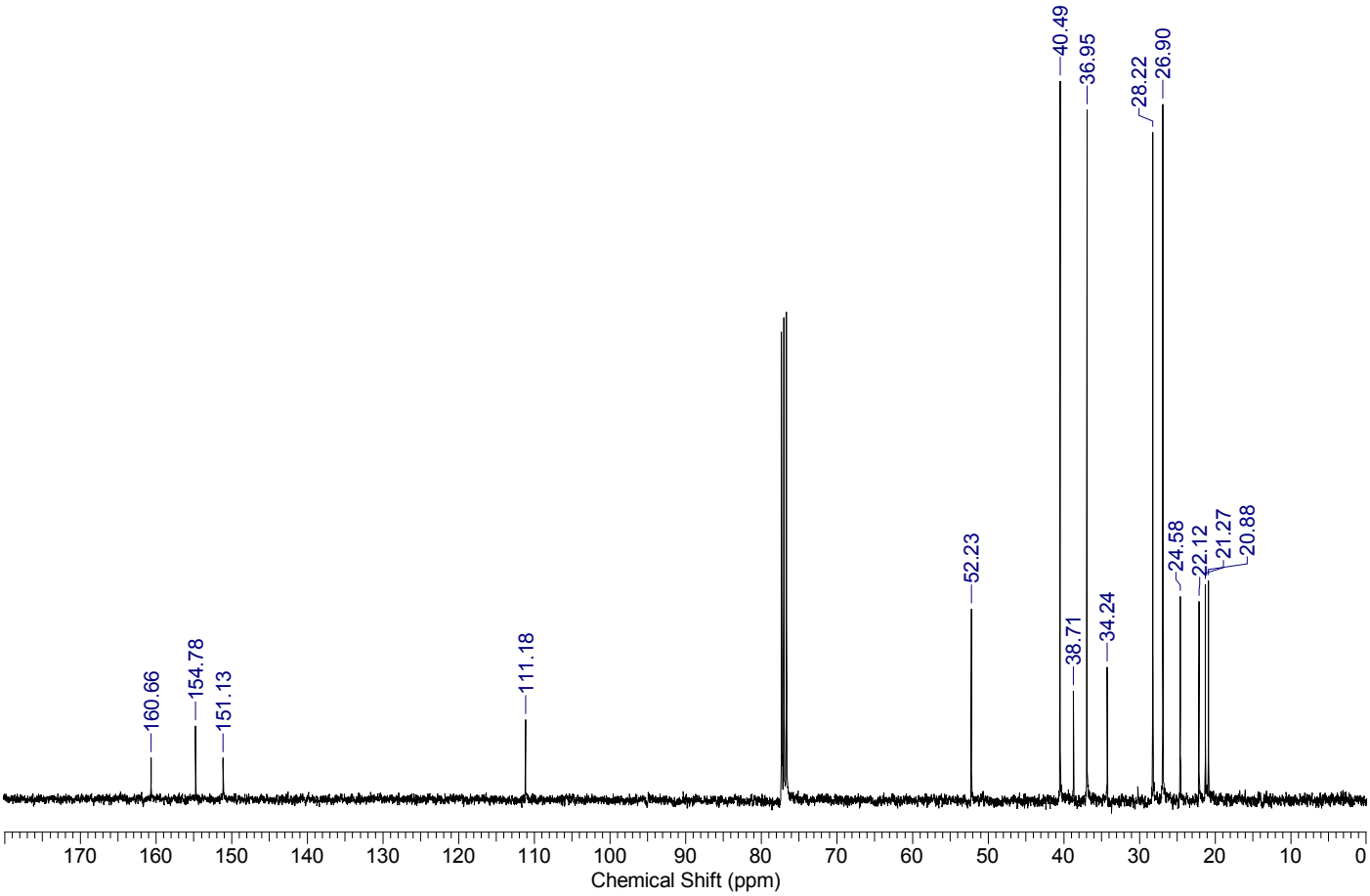
N-(1-Adamantylmethyl)-2-methyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7p)



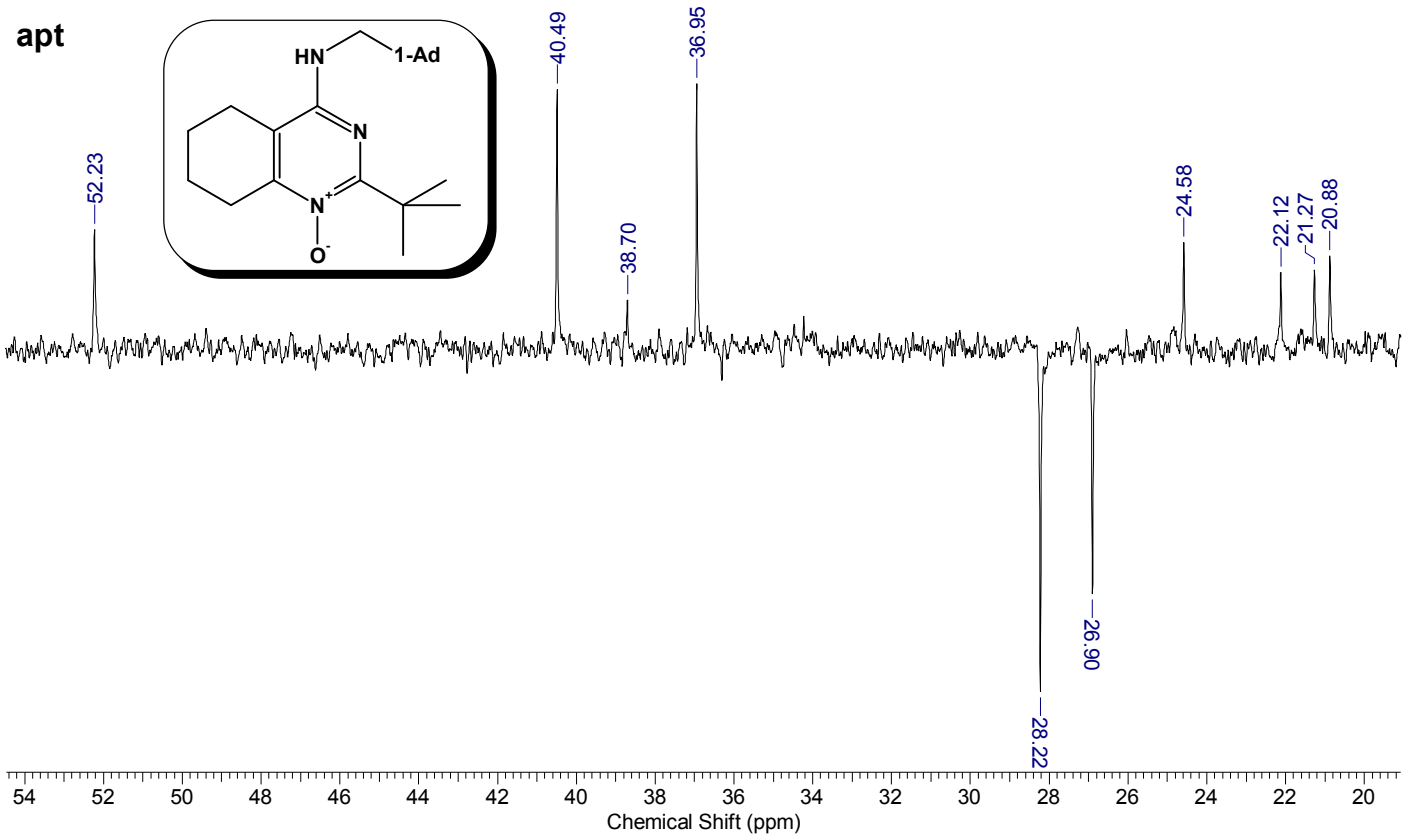


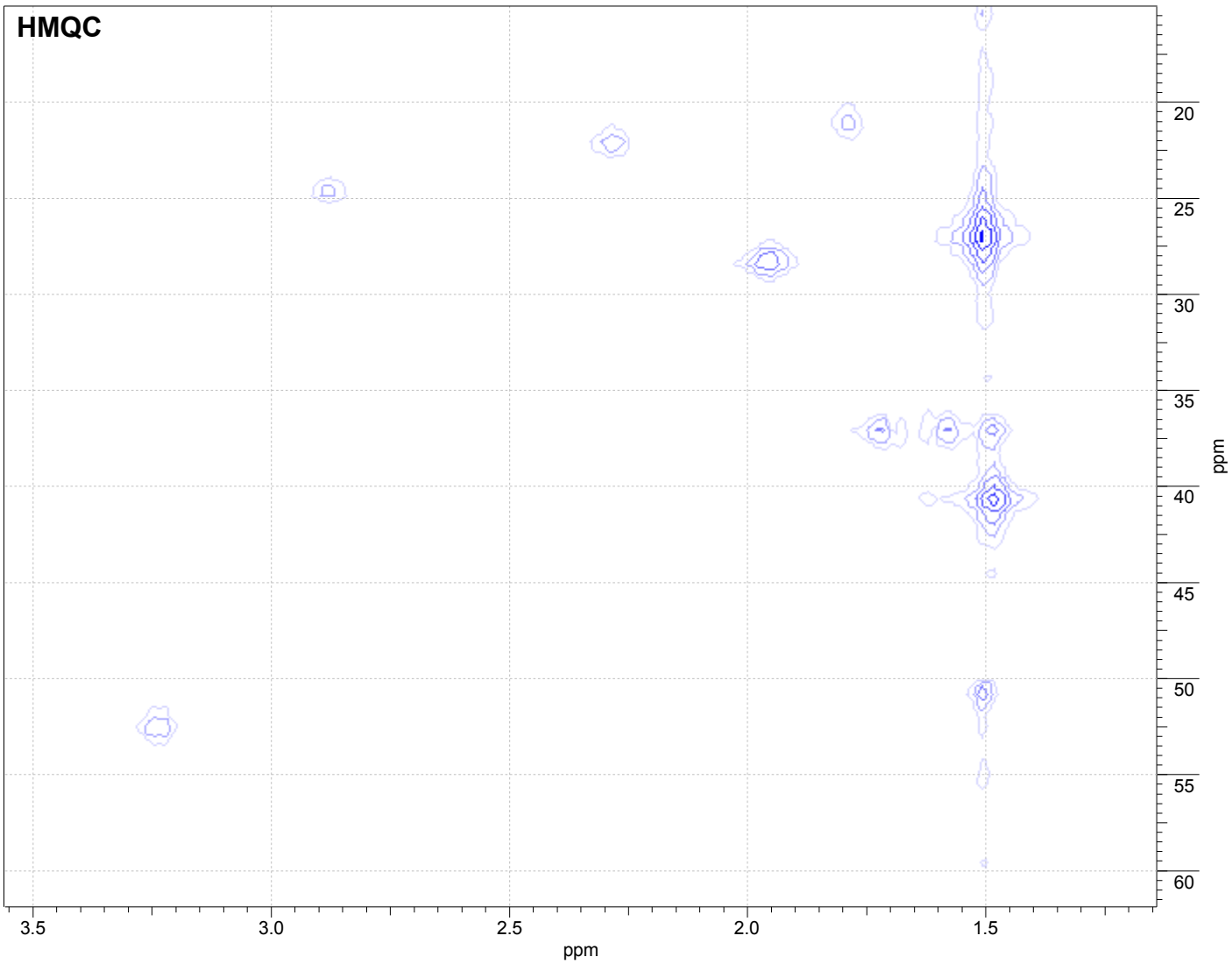
N-(1-Adamantylmethyl)-2-tert-butyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7q)



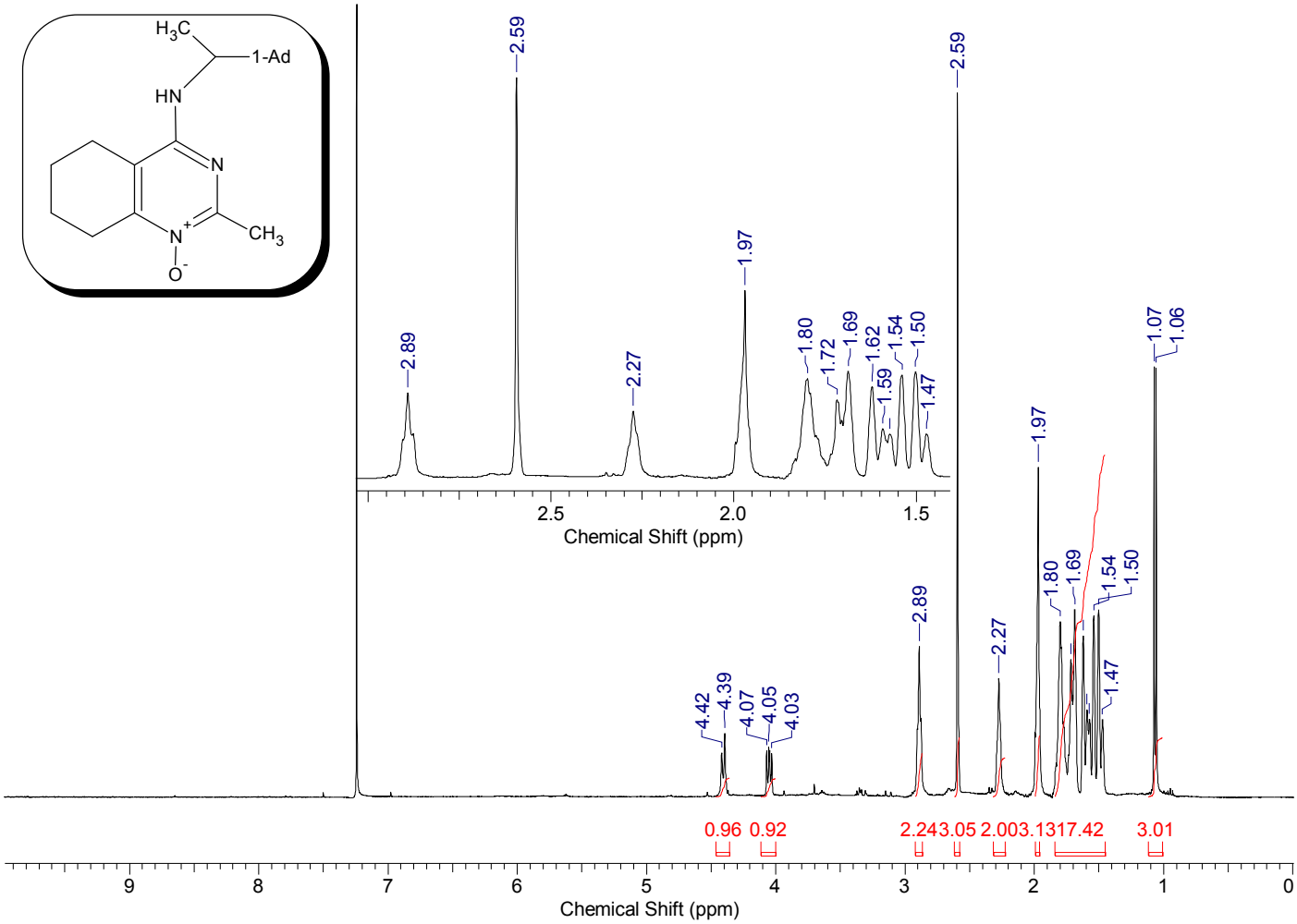


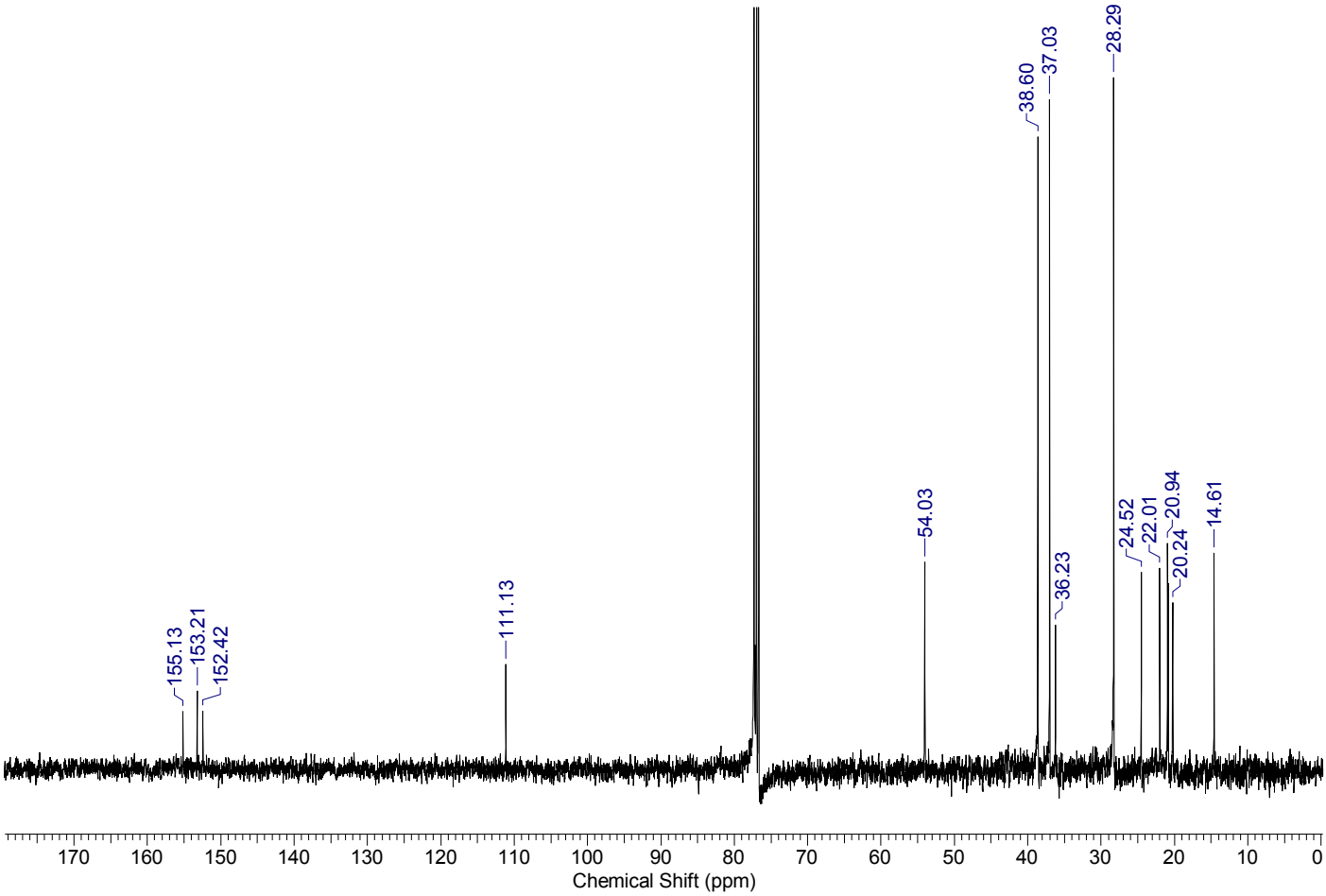
N-(1-Adamantylmethyl)-2-tert-butyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7q)





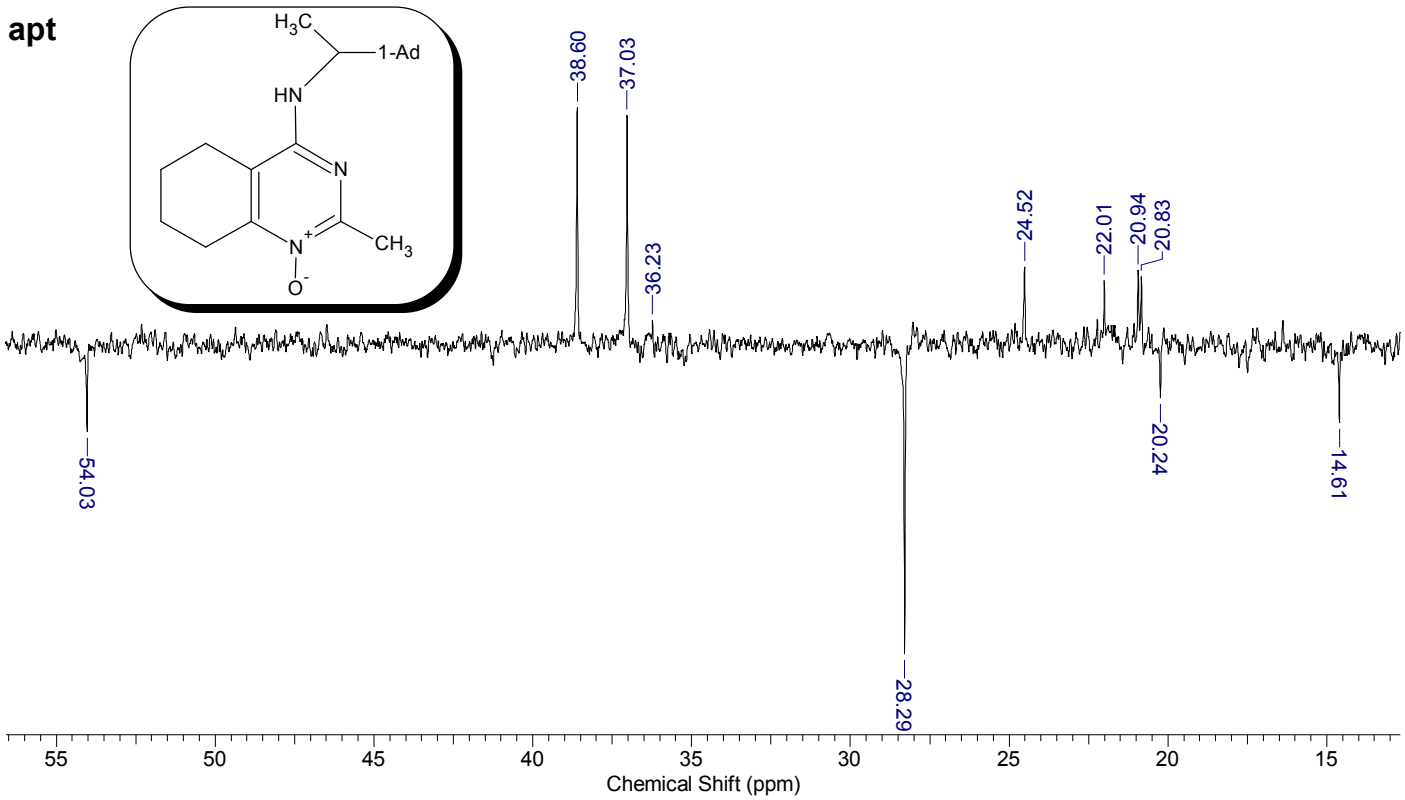
N-[1-(1-Adamantyl)ethyl]-2-methyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7r)



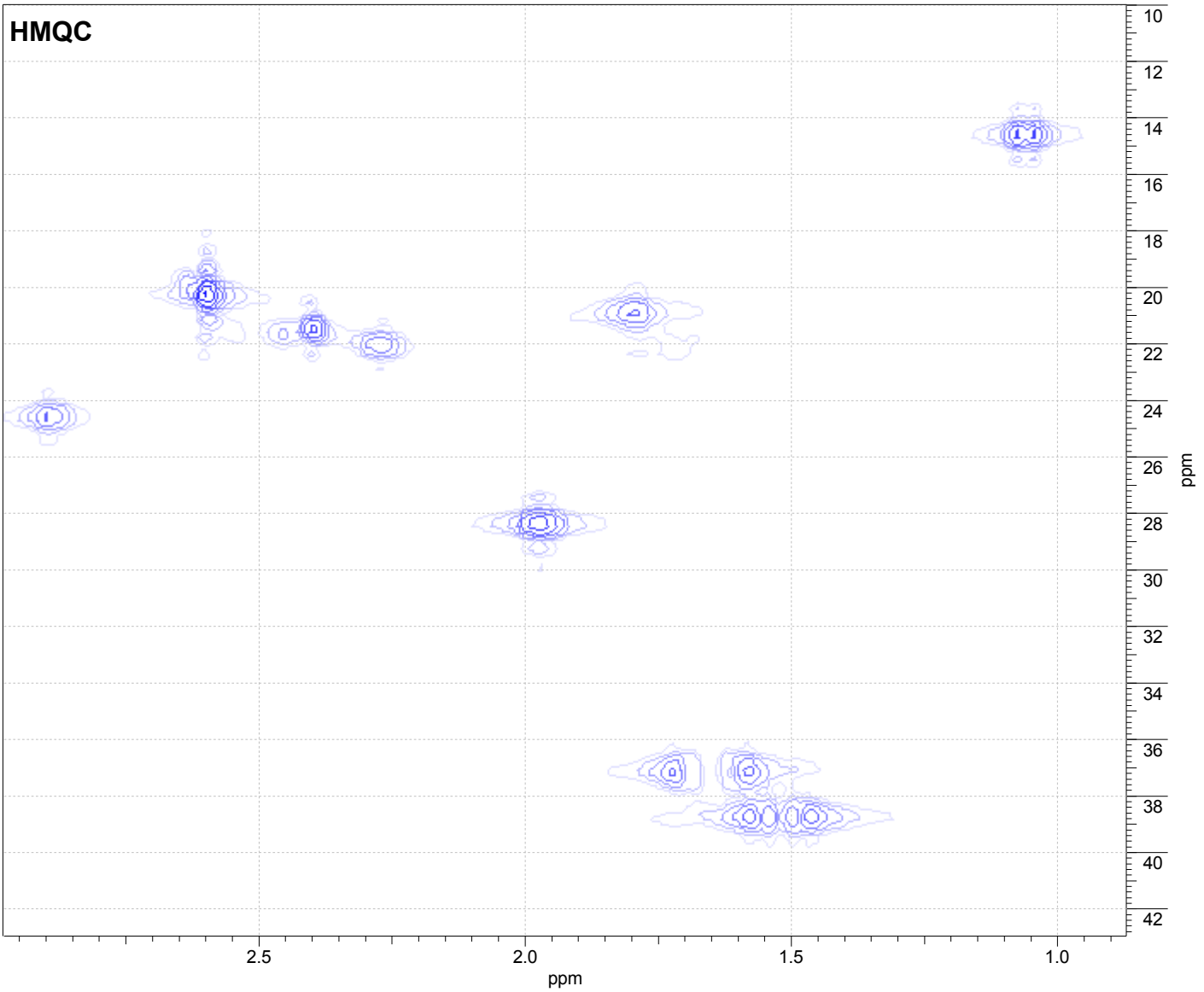


N-[1-(1-Adamantyl)ethyl]-2-methyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7r)

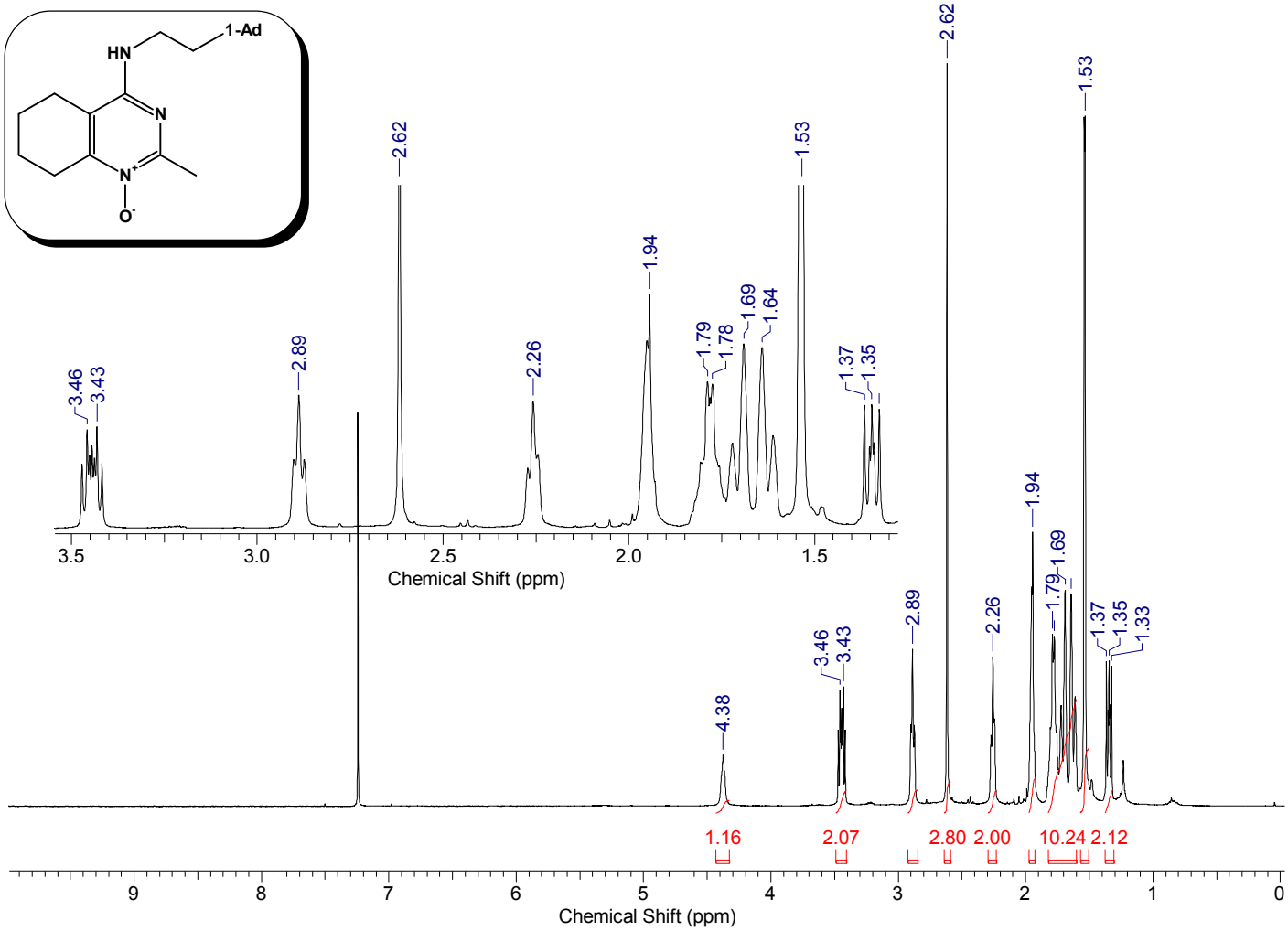
apt

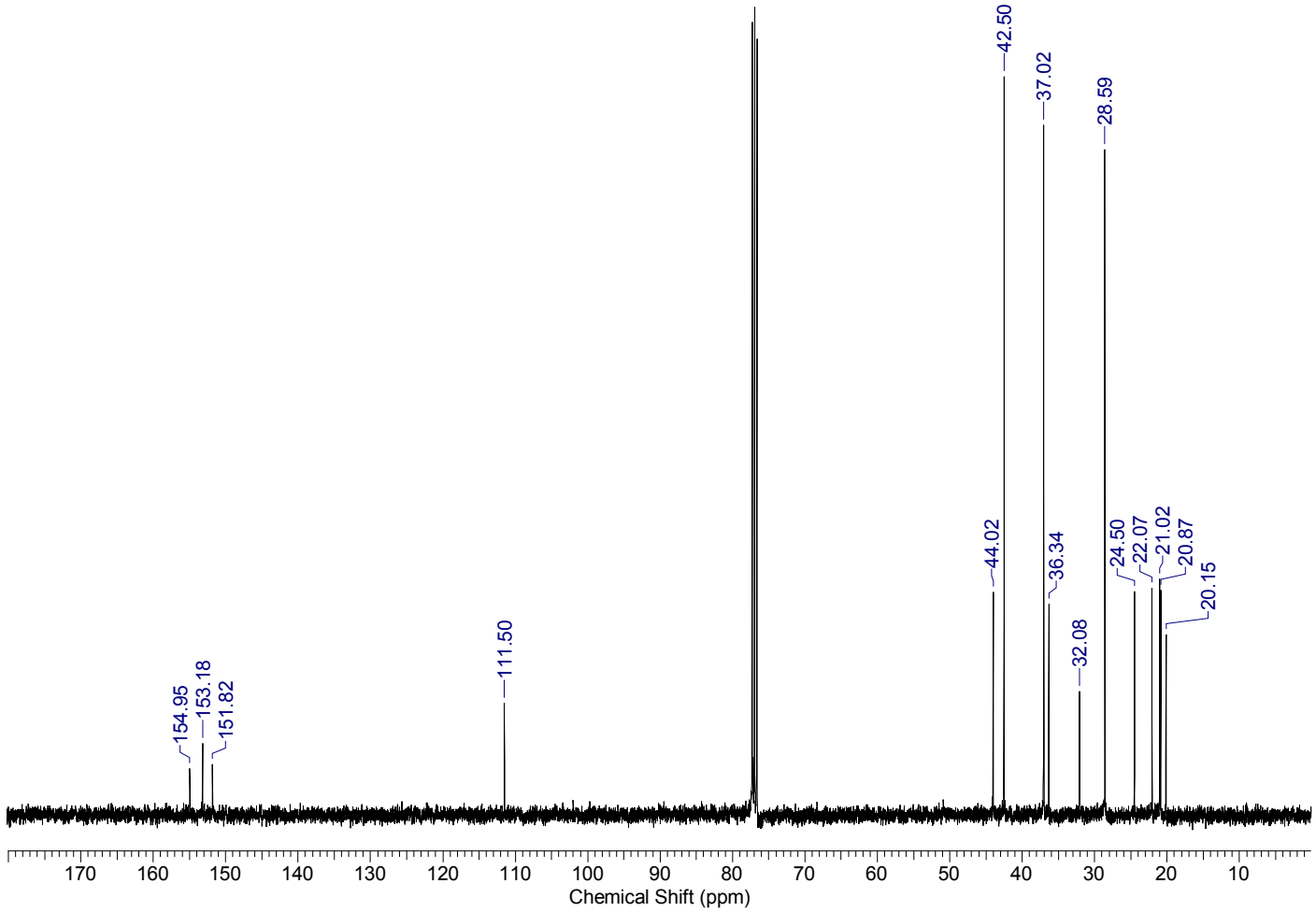


HMQC

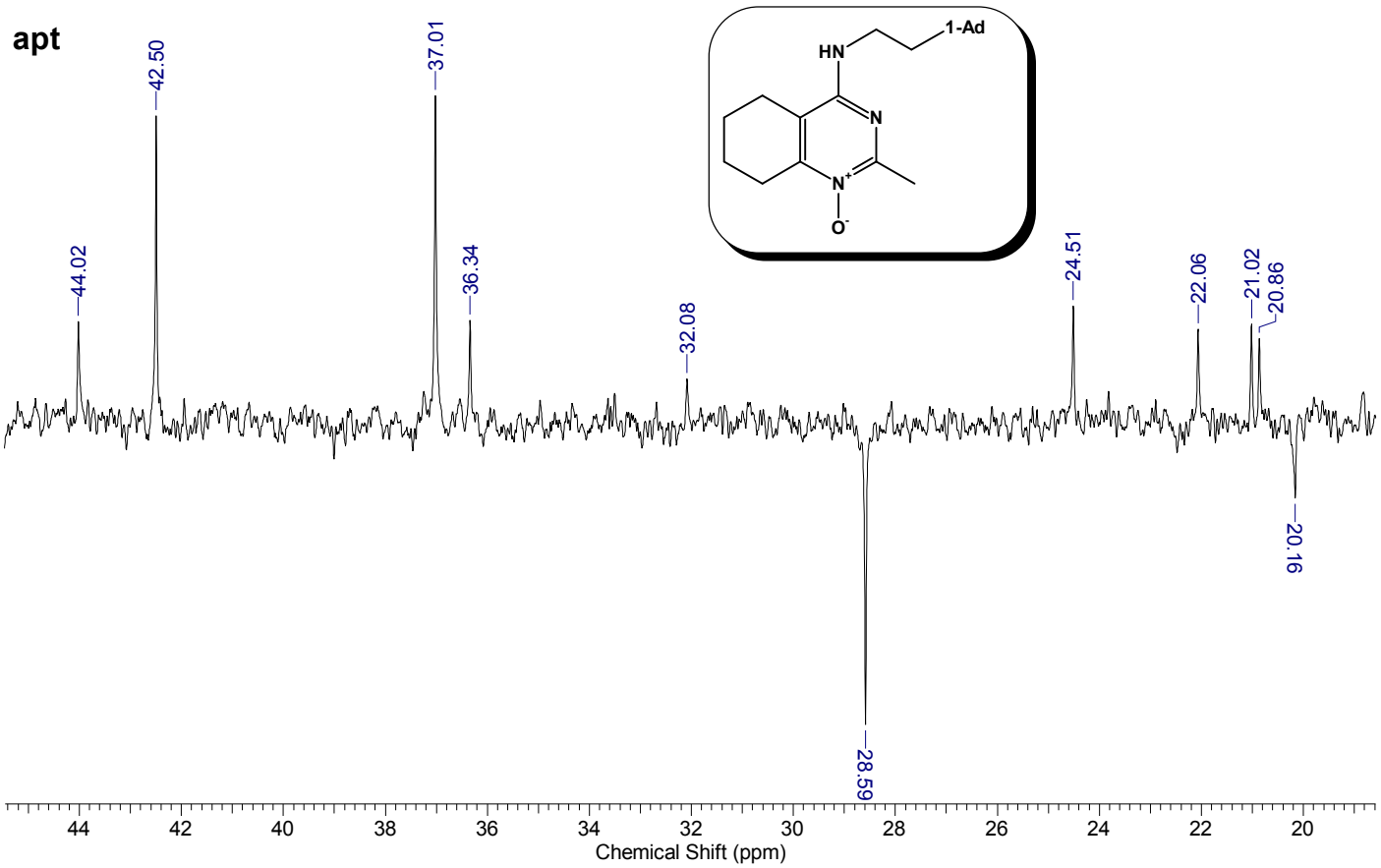


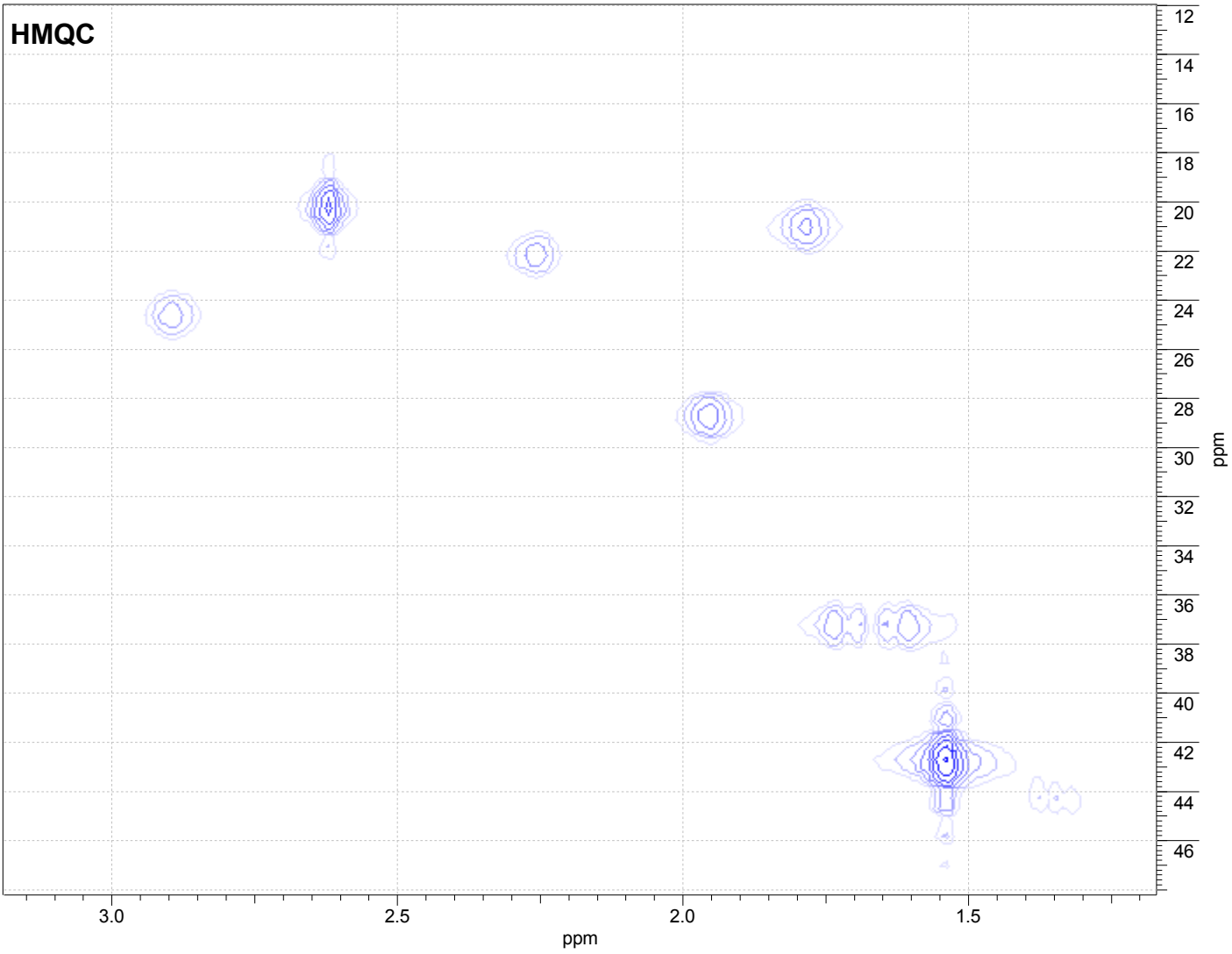
N-[2-(1-Adamantyl)ethyl]-2-methyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7s)



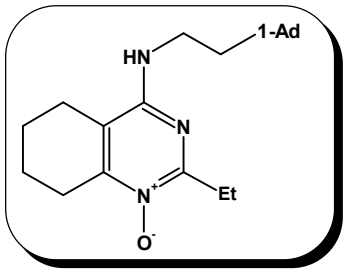


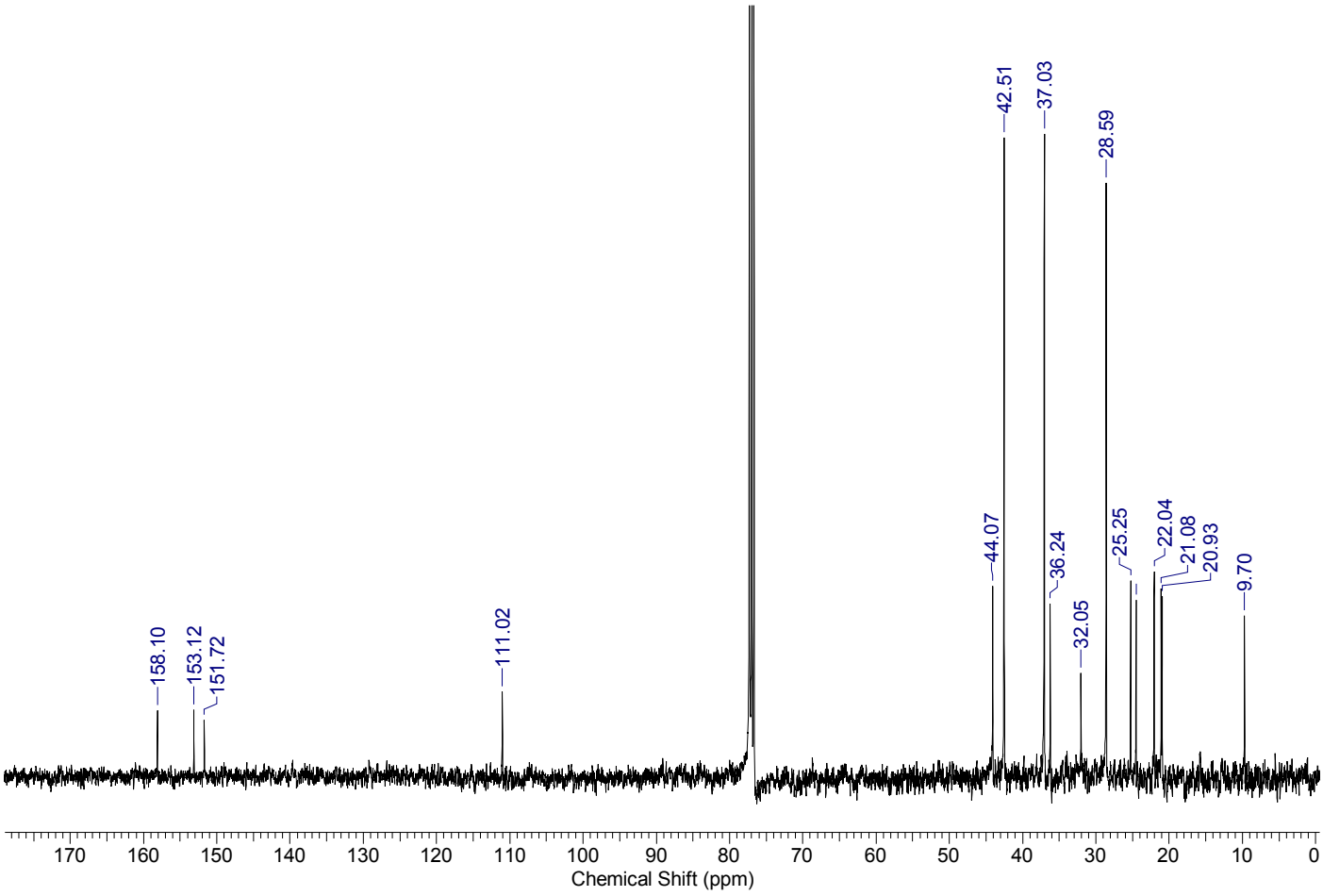
N-[2-(1-Adamantyl)ethyl]-2-methyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7s)



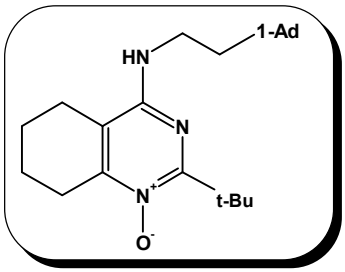


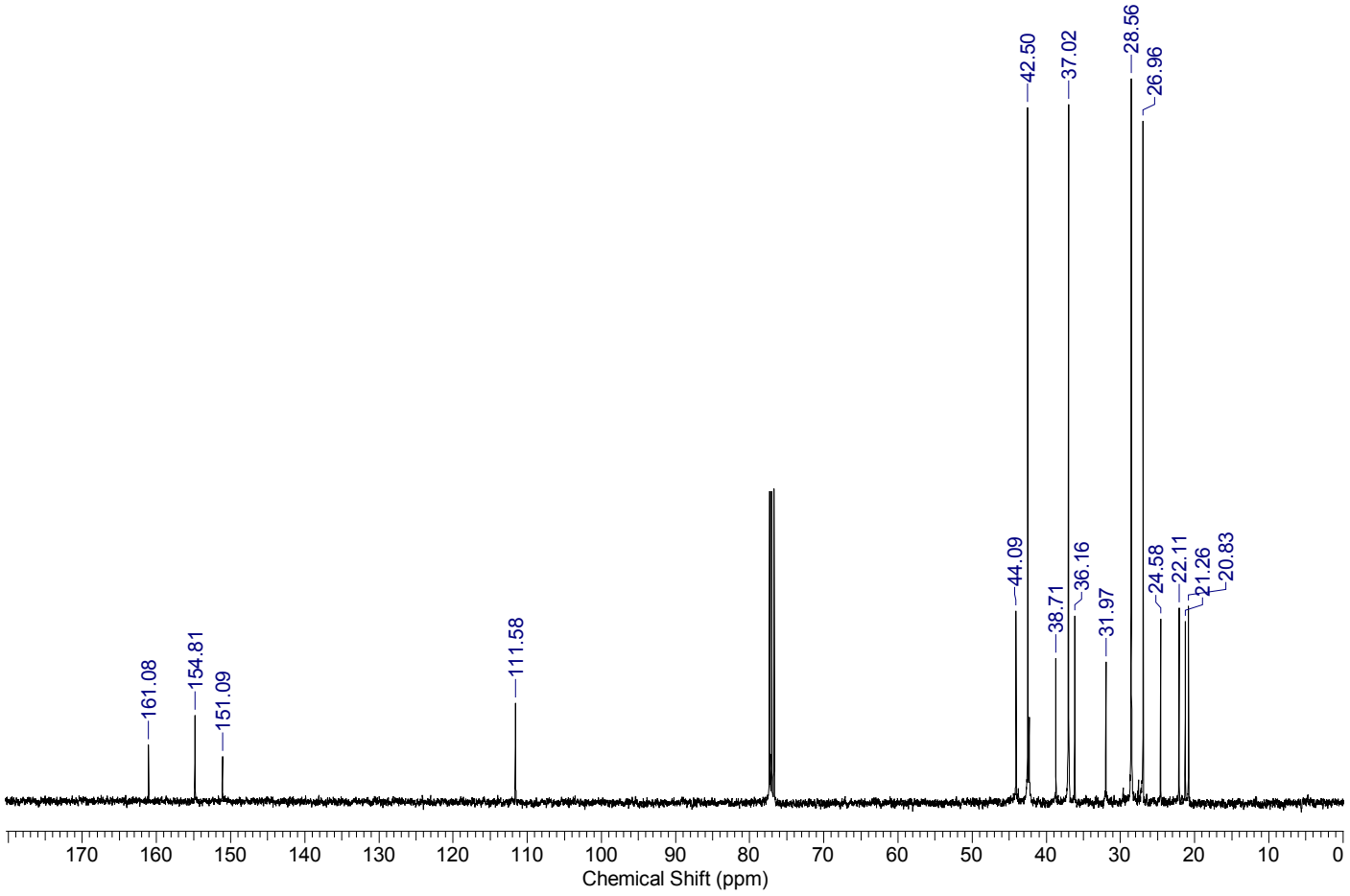
N-[2-(1-Adamantyl)ethyl]-2-ethyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7t)





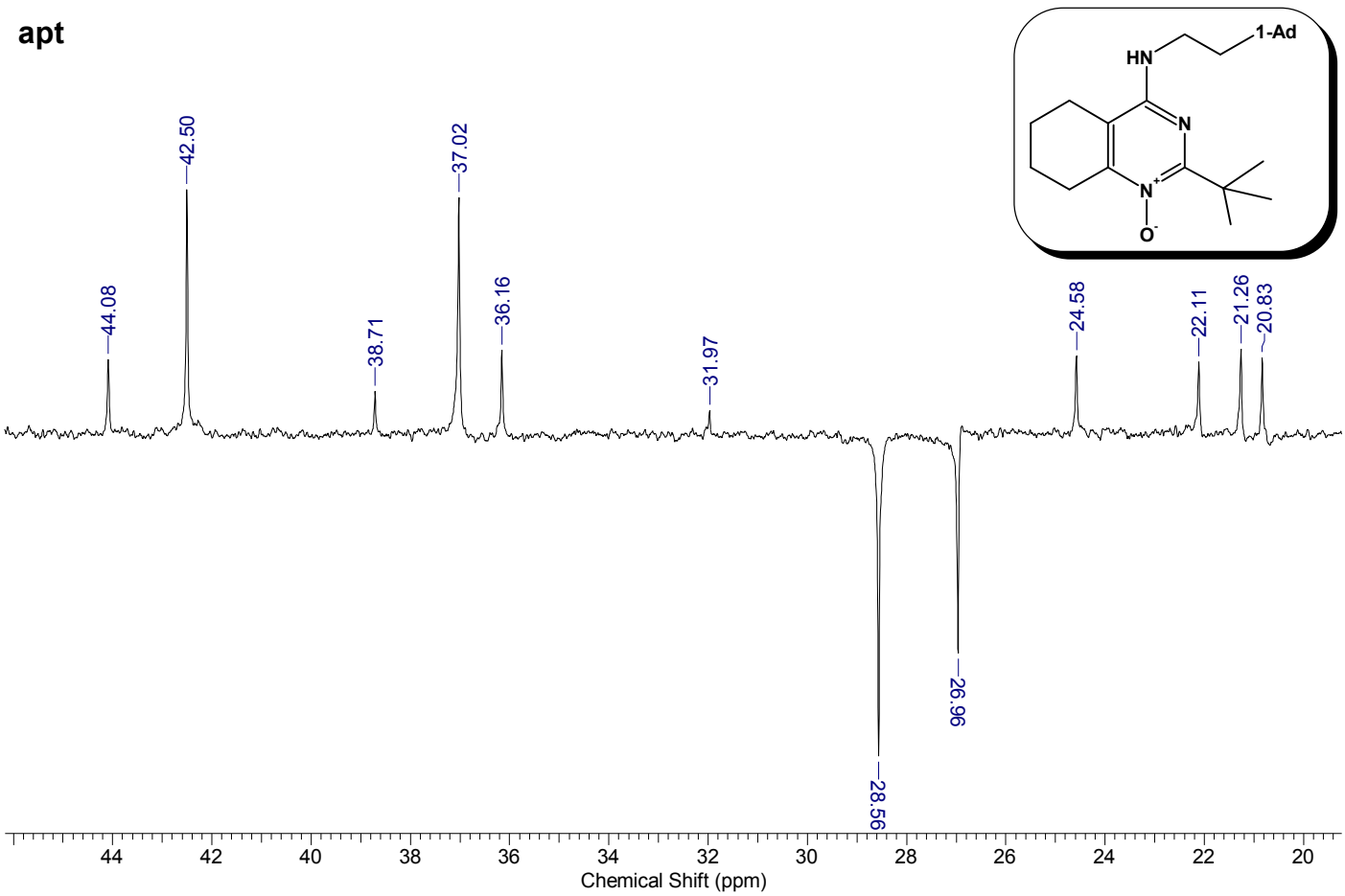
N-[2-(1-Adamantyl)ethyl]-2-tert-butyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7u)

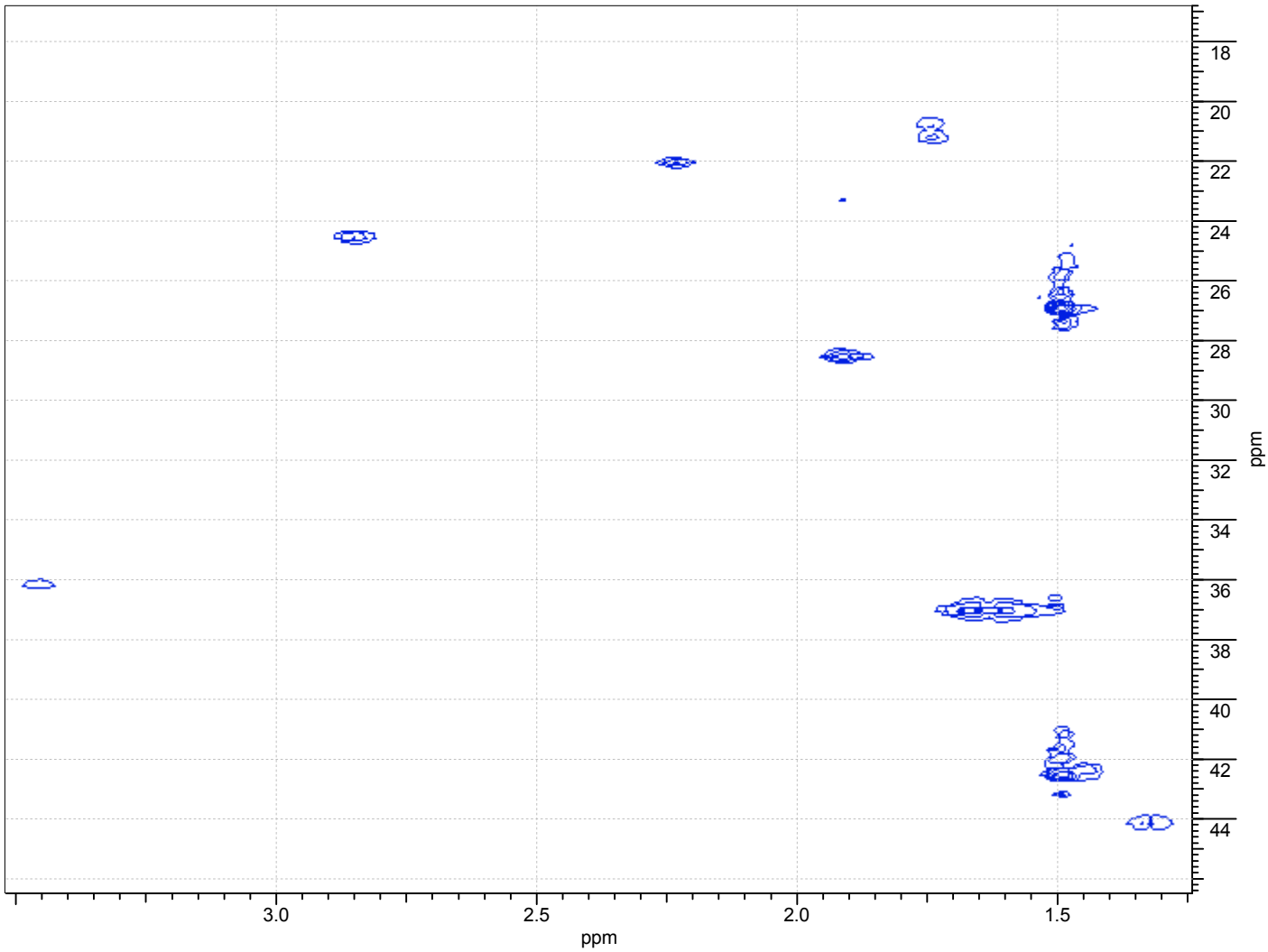




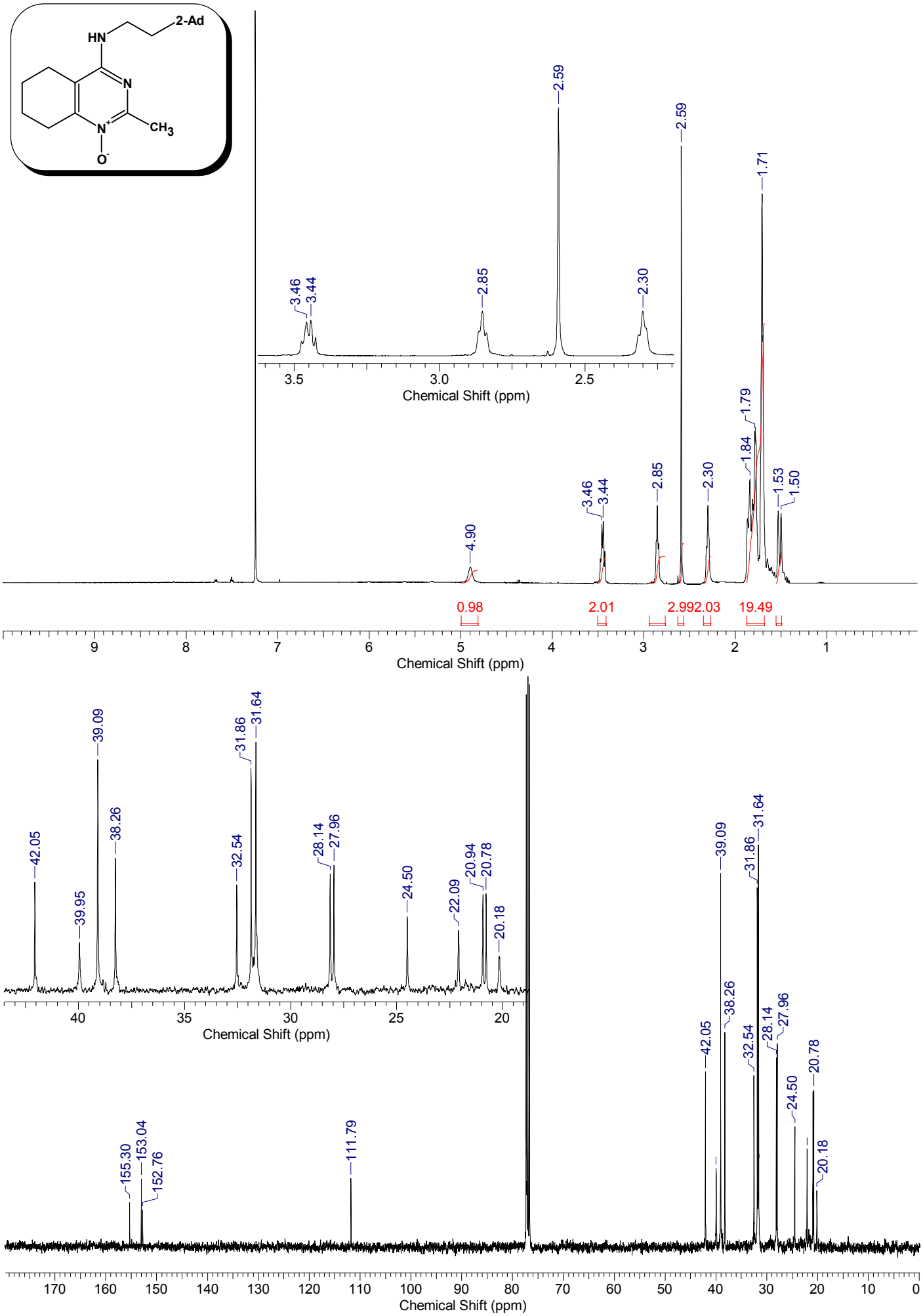
N-[2-(1-Adamantyl)ethyl]-2-tert-butyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7u)

apt

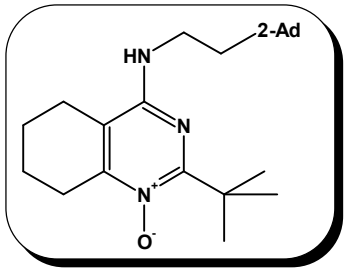


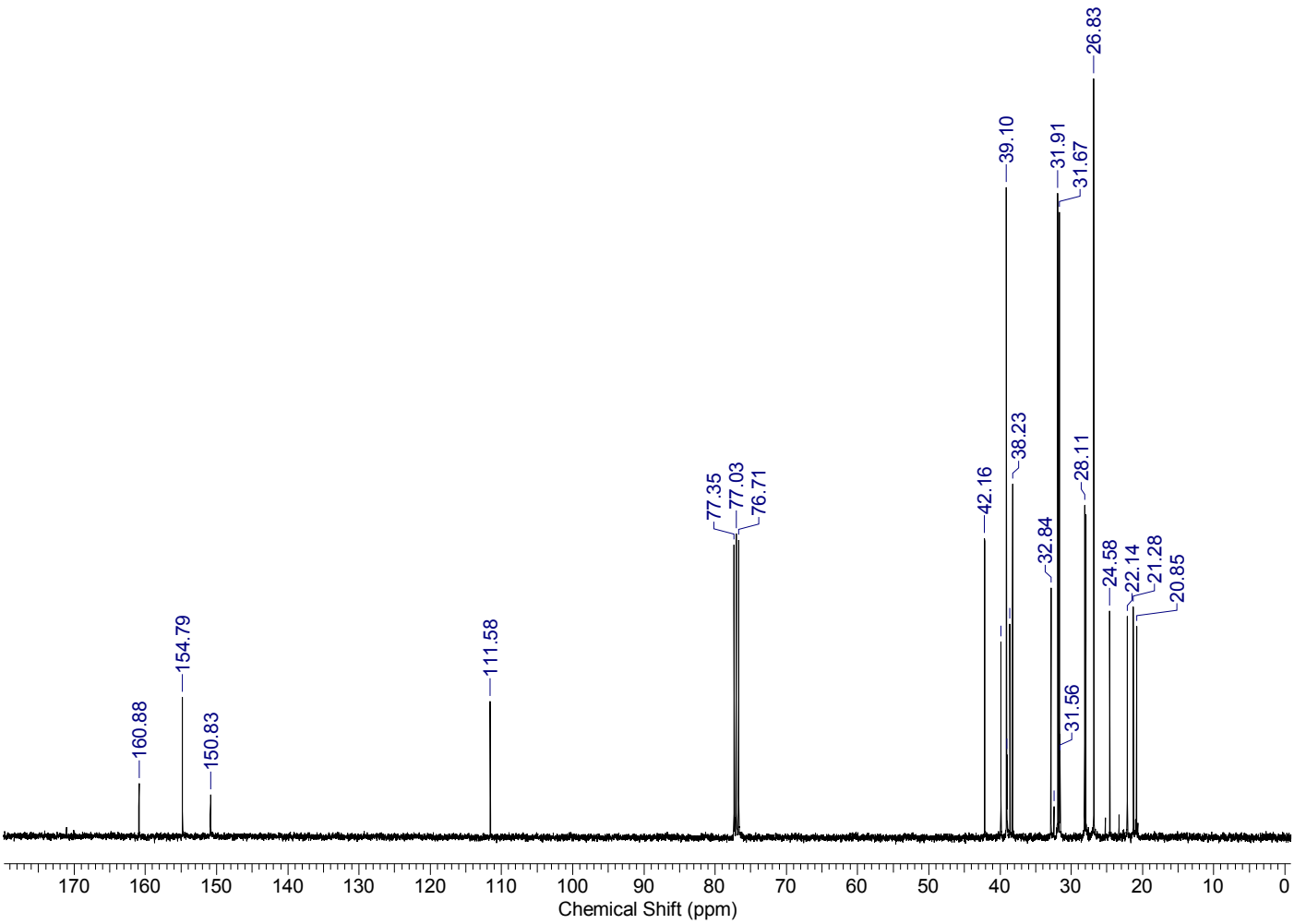


N-[2-(2-Adamantyl)ethyl]-2-methyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7v)

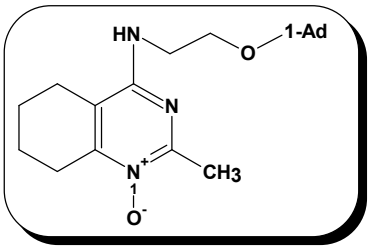


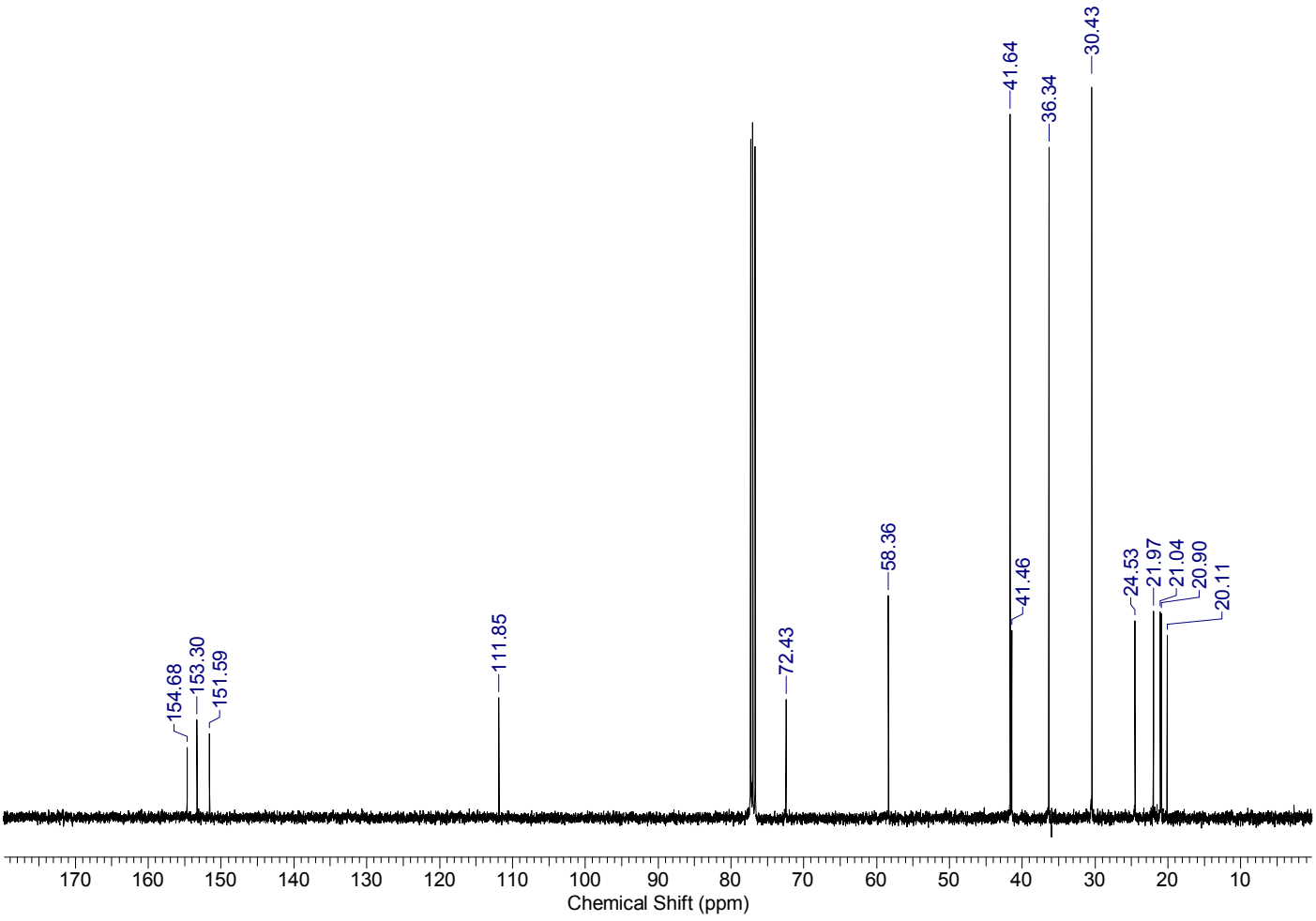
N-[2-(2-Adamantyl)ethyl]-2-tert-butyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7w)



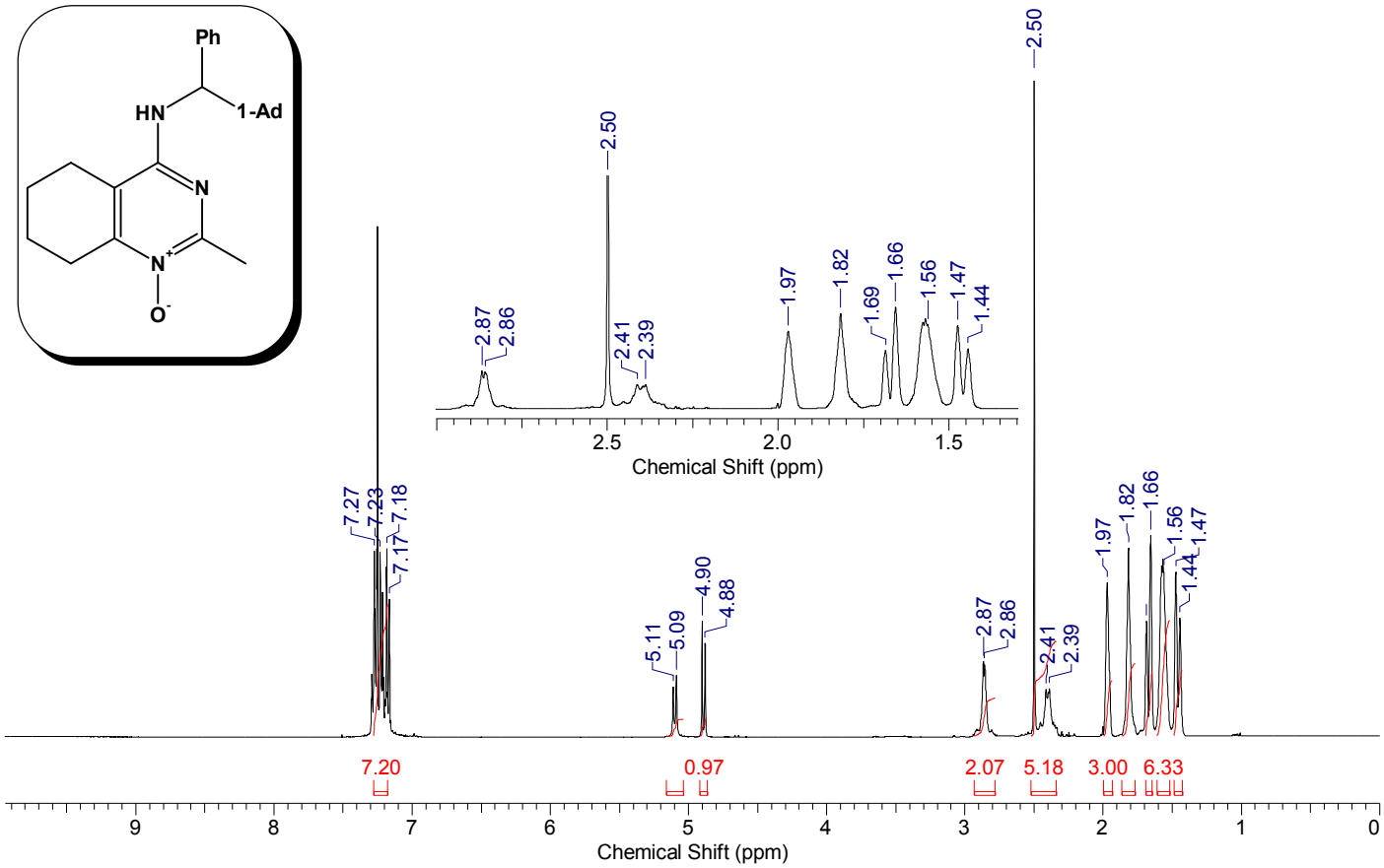


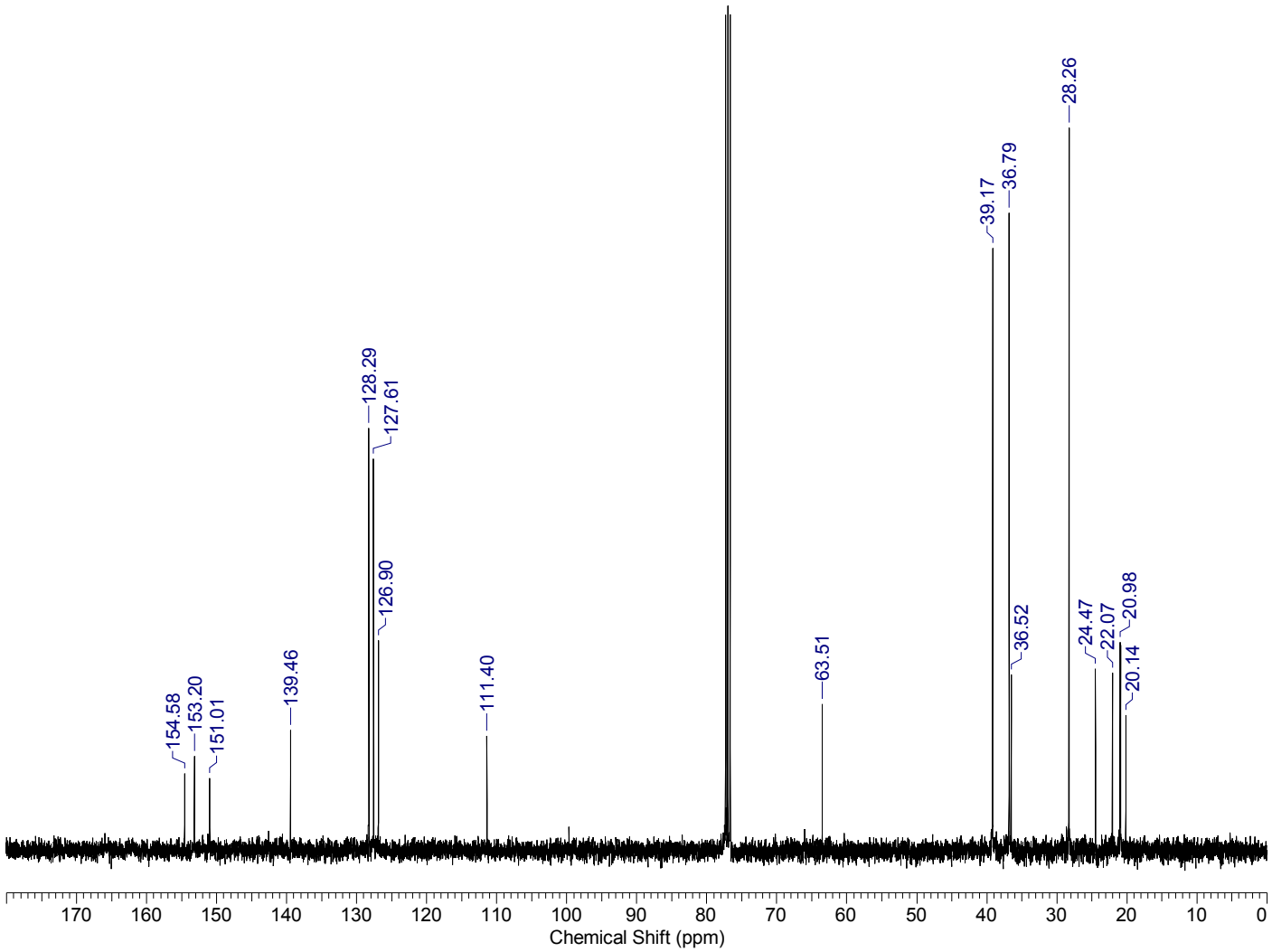
N-[2-(1-Adamantyloxy)ethyl]-2-methyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7x)



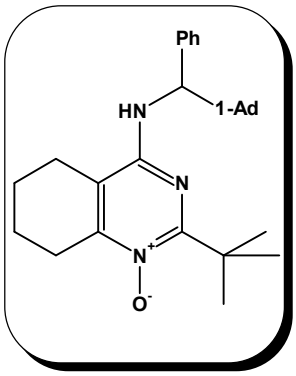


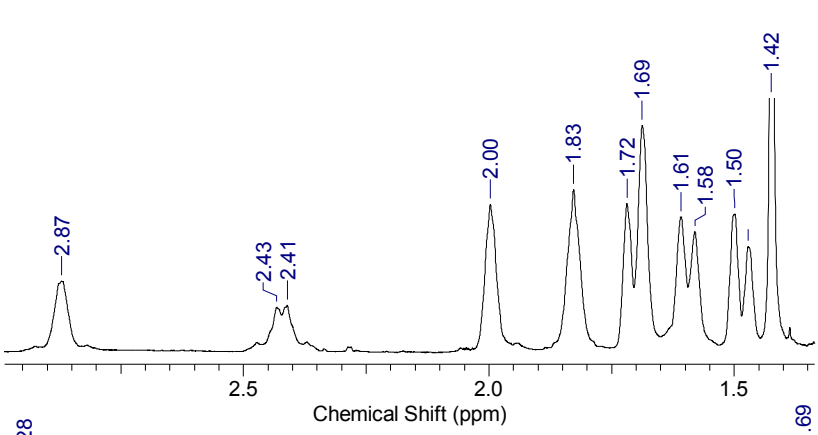
N-[1-adamantyl(phenyl)methyl]-2-methyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7y)

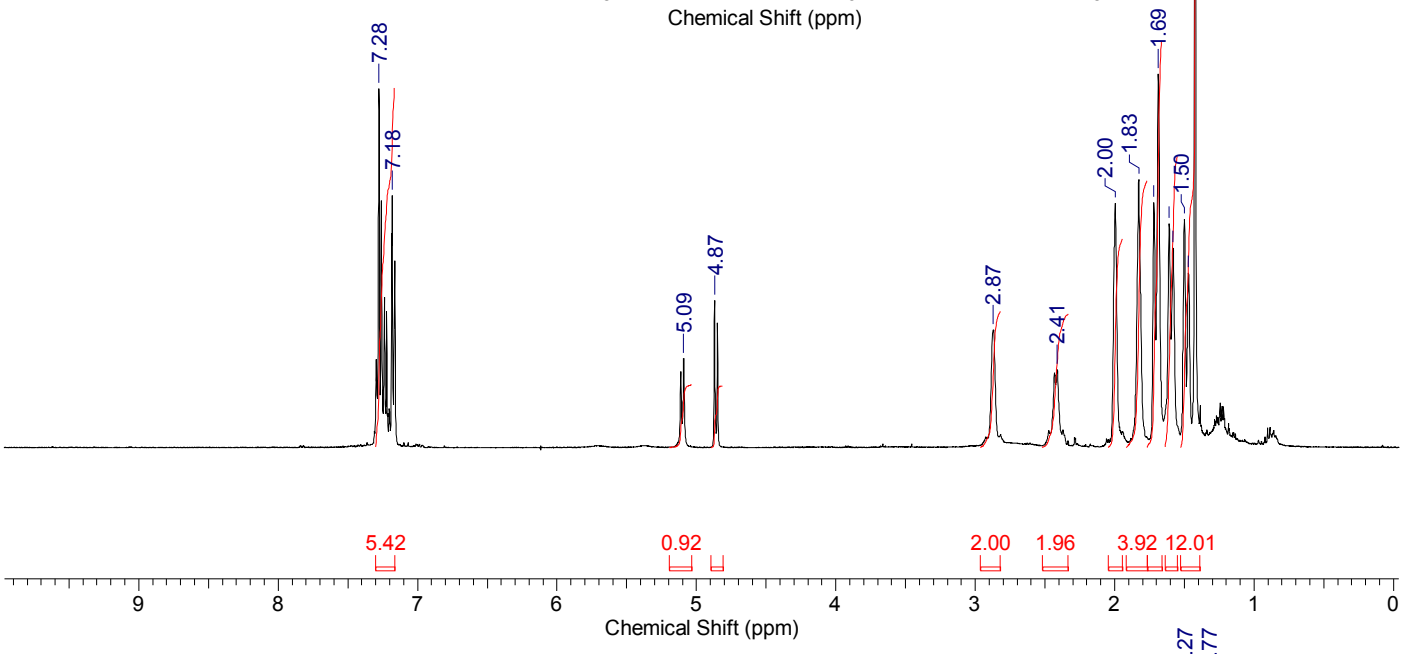


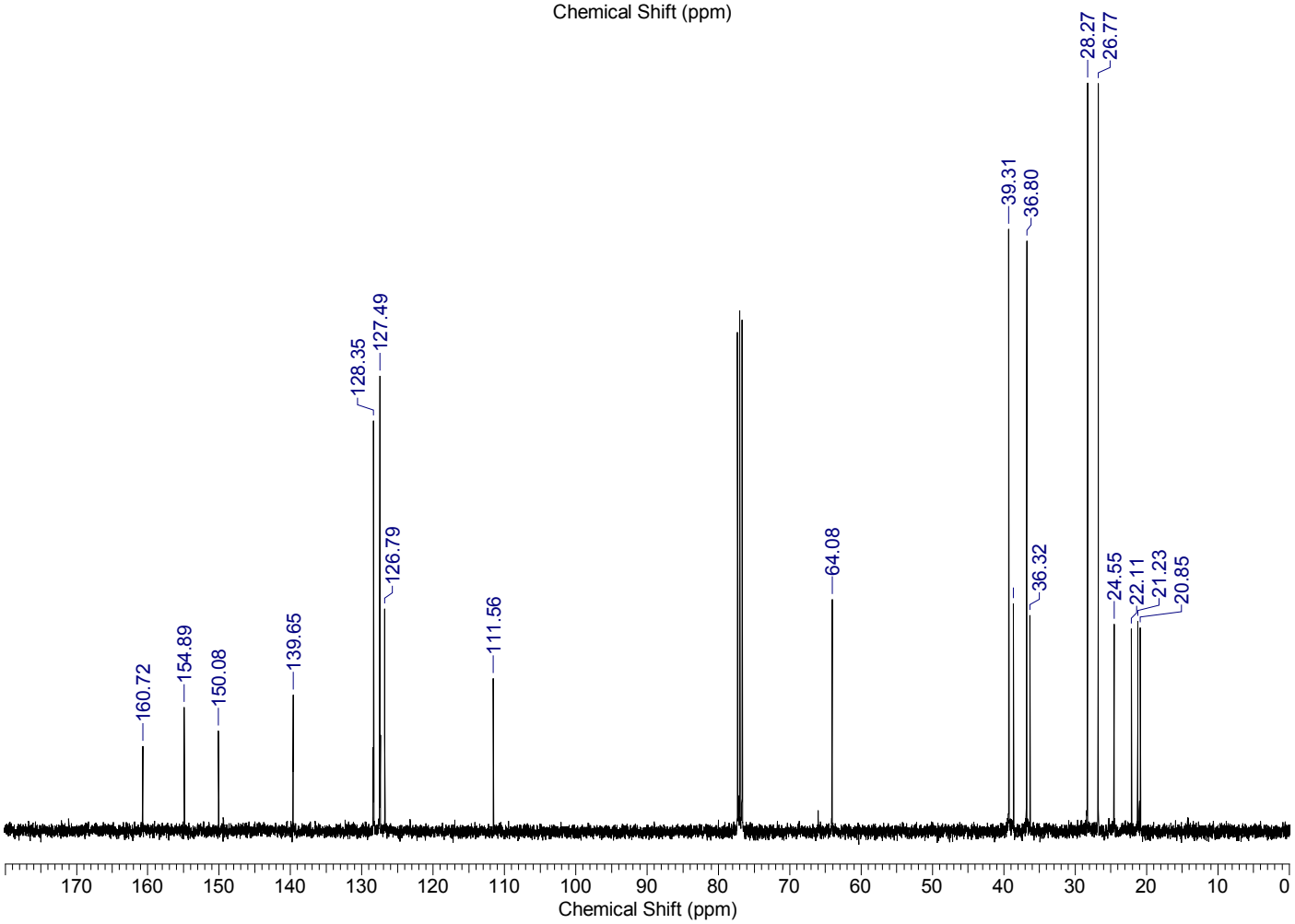


N-[1-Adamantyl(phenyl)methyl]-tert-butyl-5,6,7,8-tetrahydroquinazolin-4-amine 1-oxide (7z)









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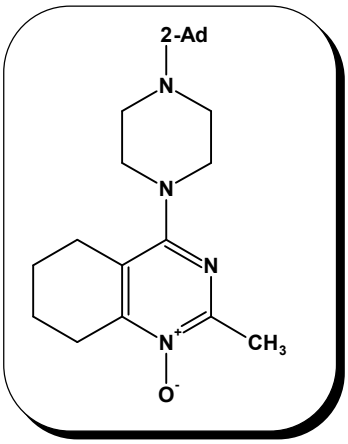

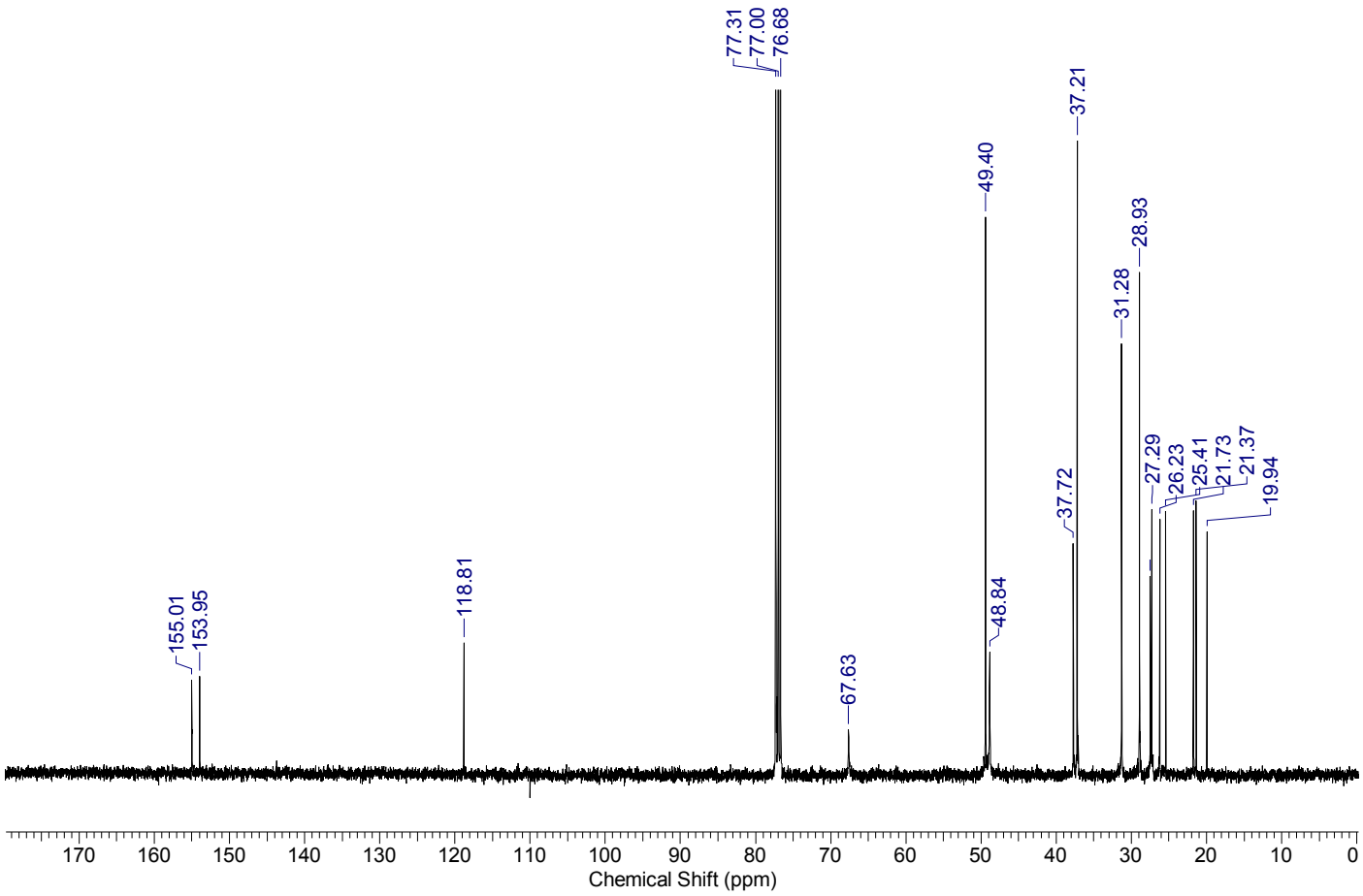

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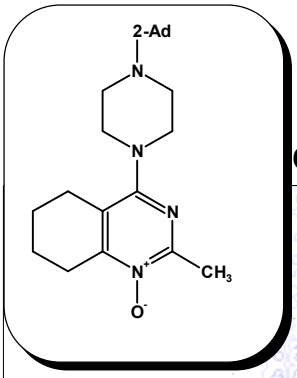
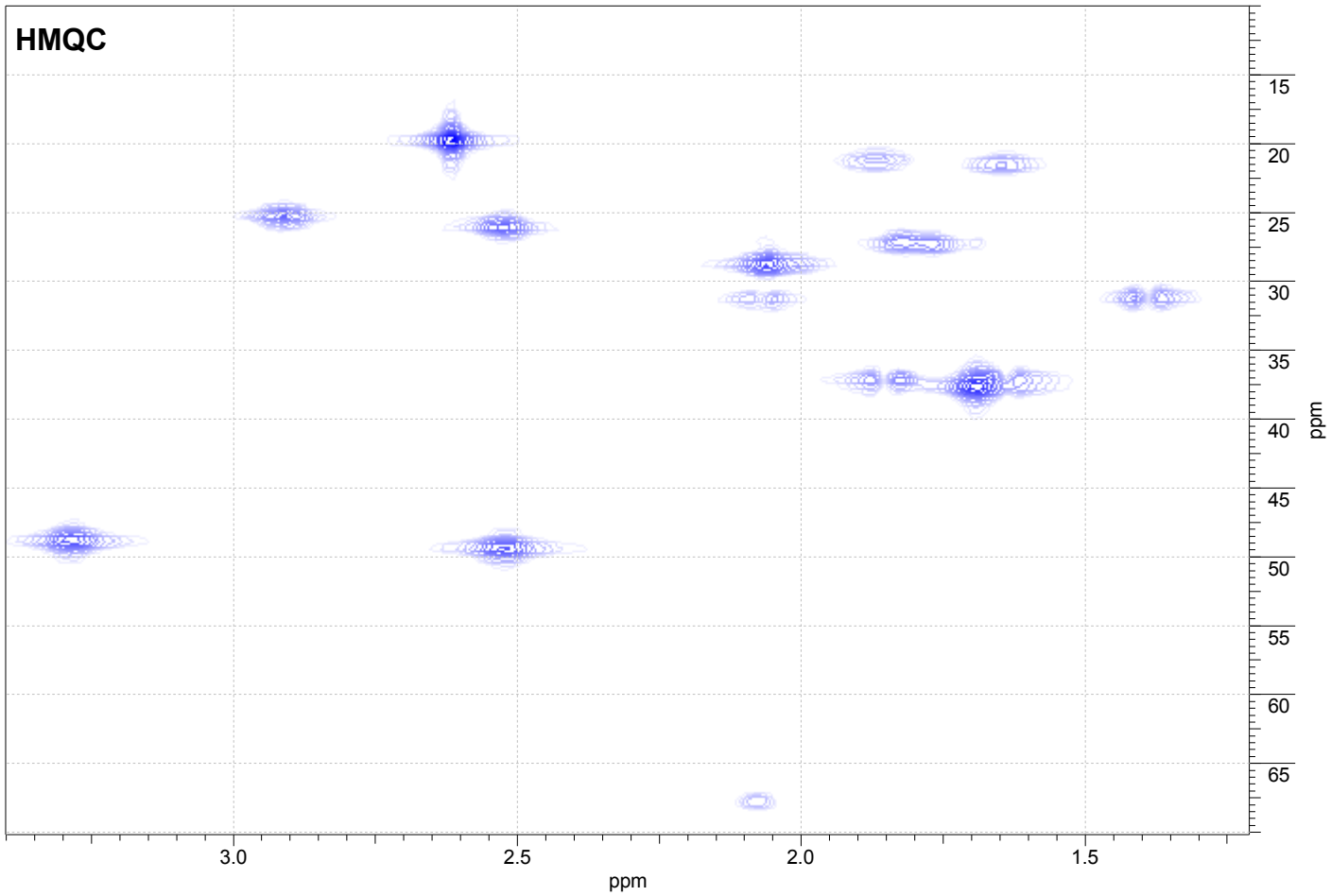
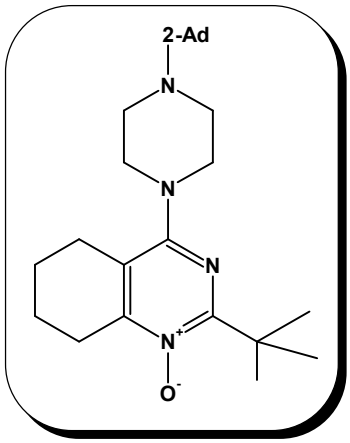


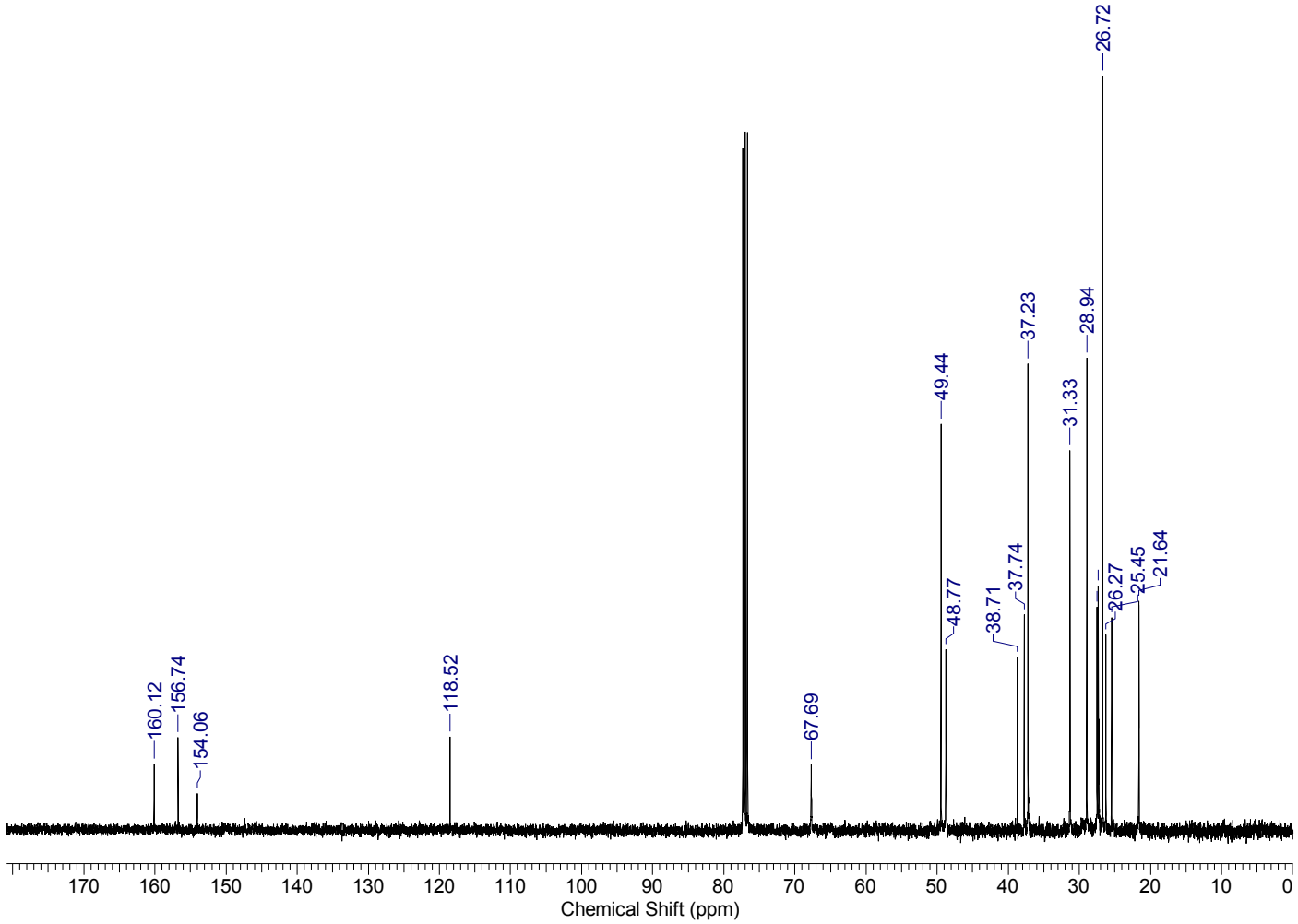
COSY H-H

HMQC



4-[4-(2-Adamantyl)piperazin-1-yl]-2-*tert*-butyl-5,6,7,8-tetrahydroquinazoline 1-oxide (5ab)





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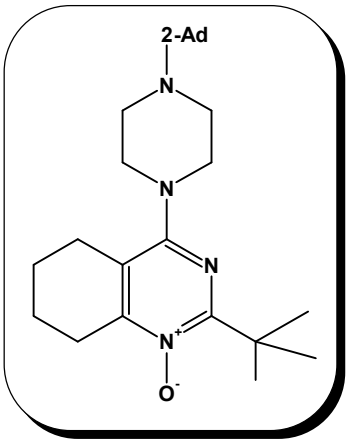

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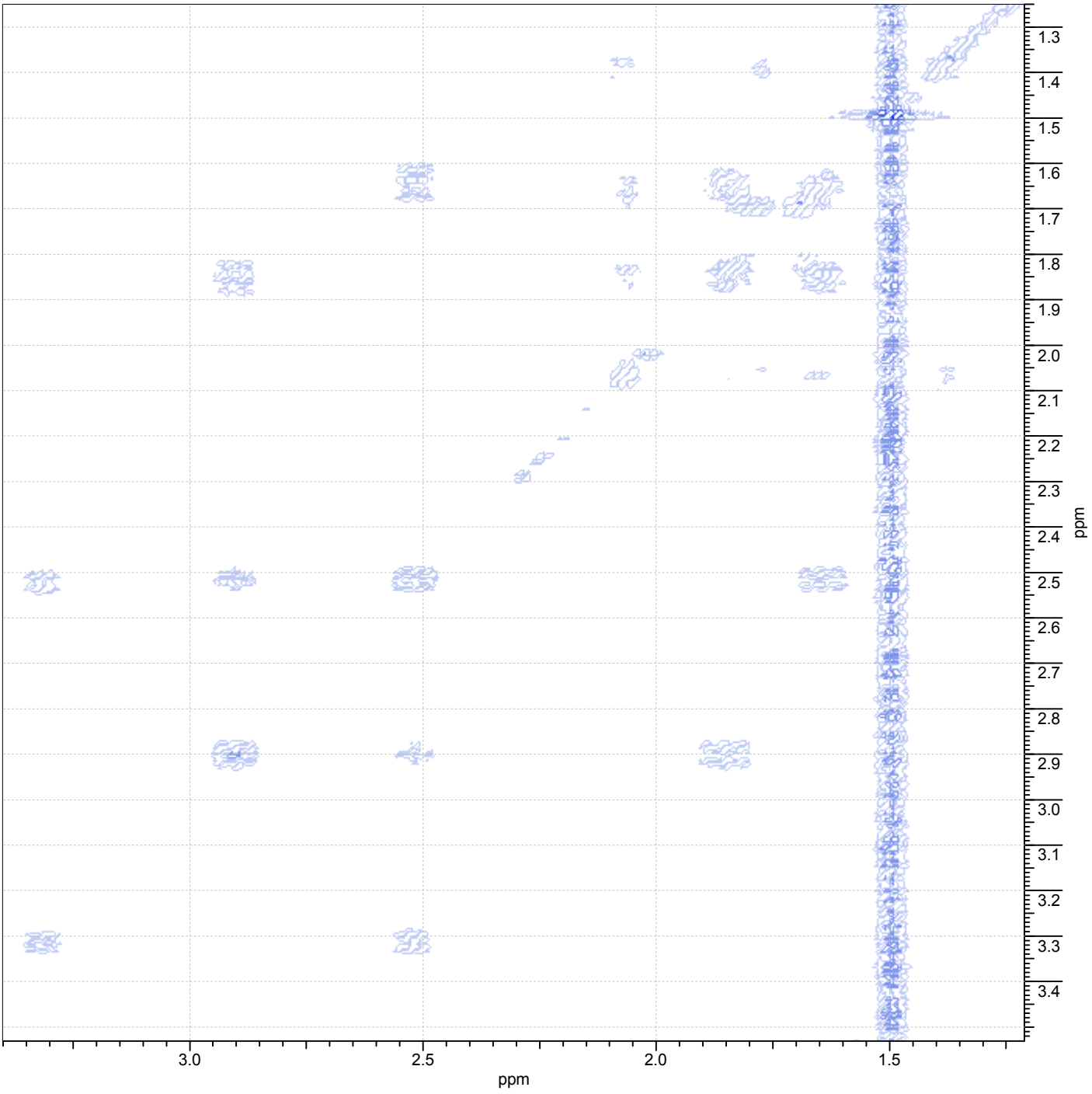

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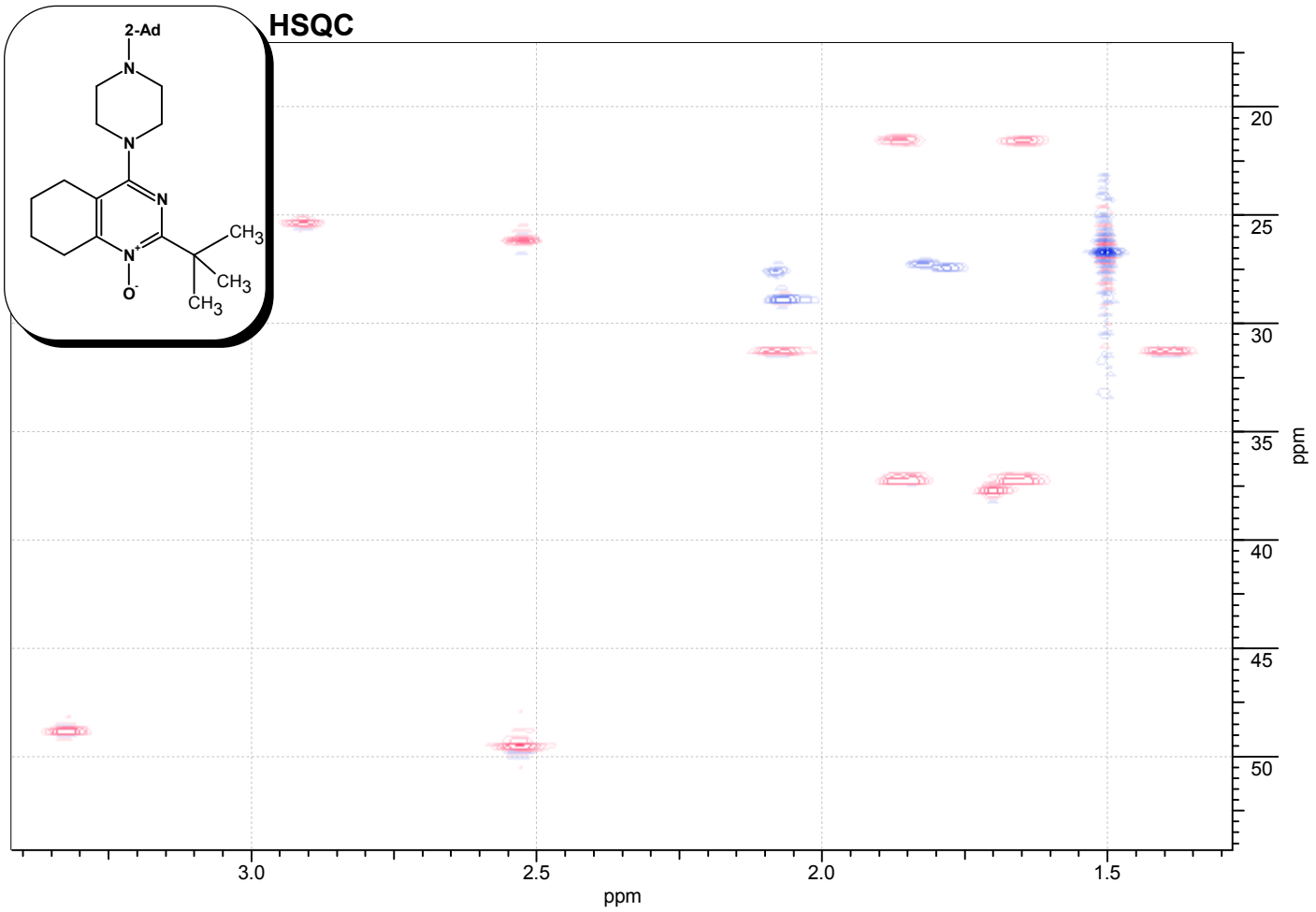
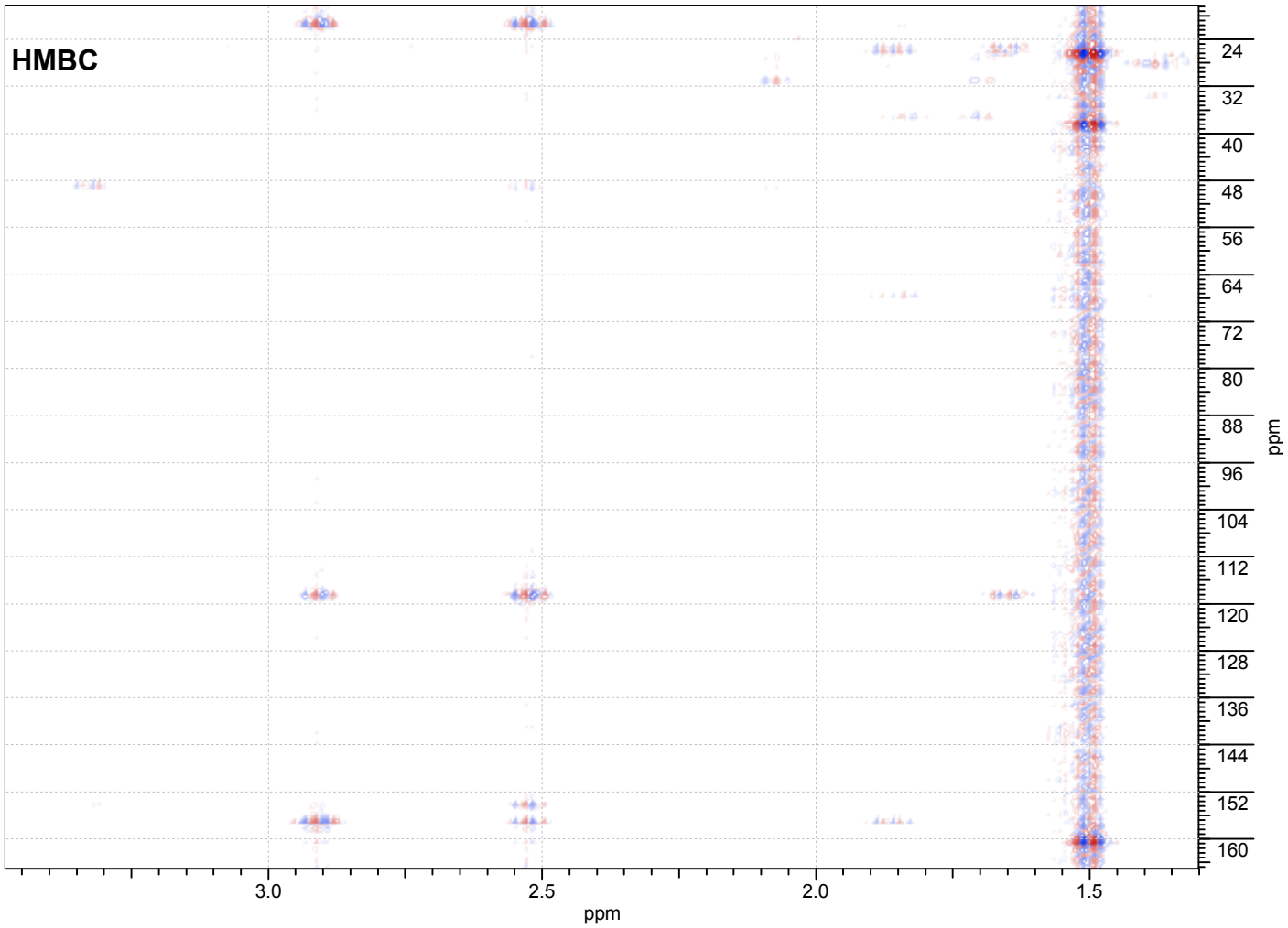
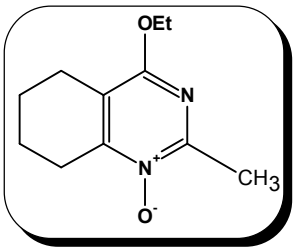
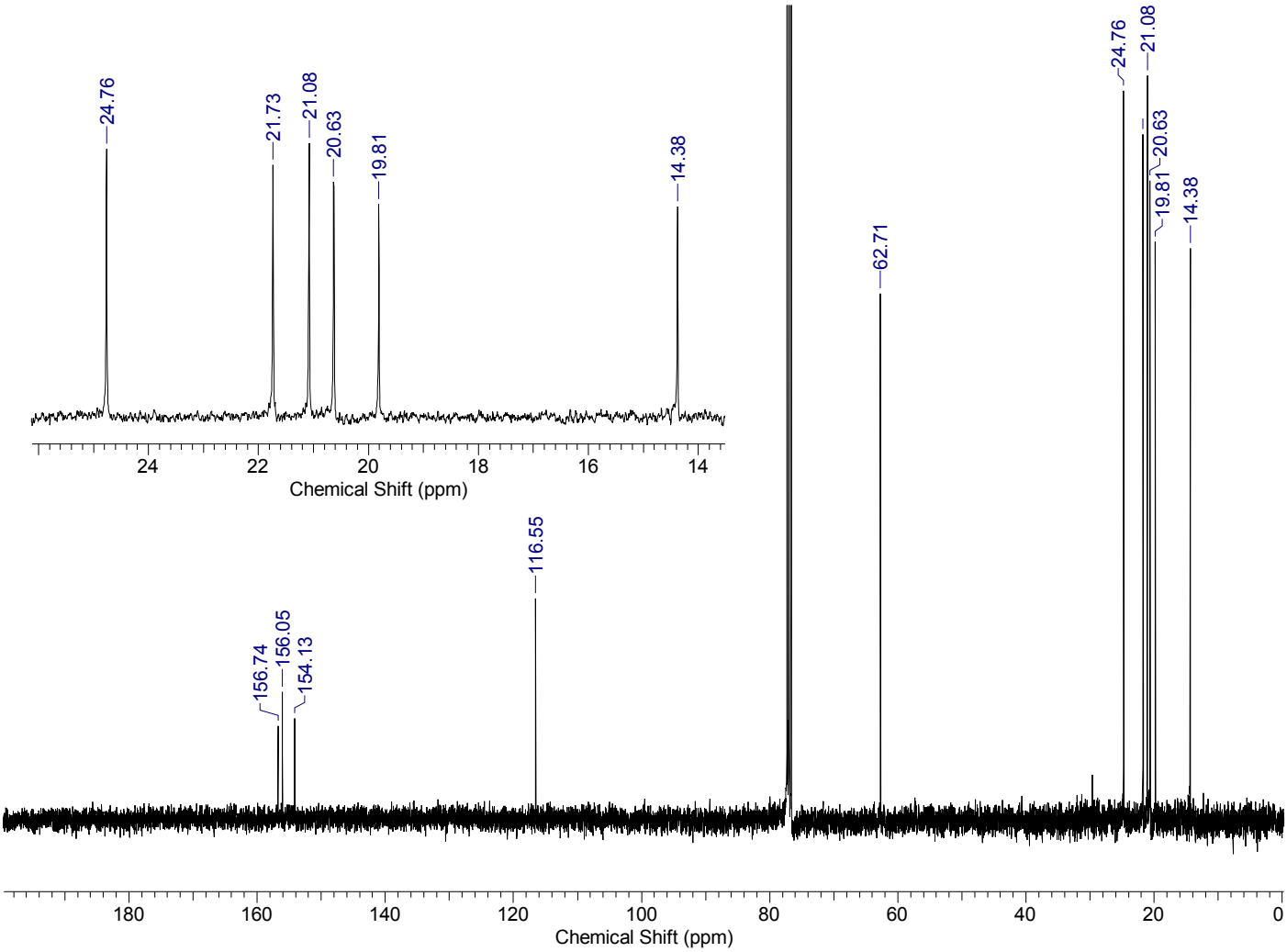


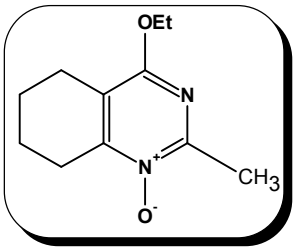


N-Etoxy-2-methyl-5,6,7,8-tetrahydroquinazoline 1-oxide (8)

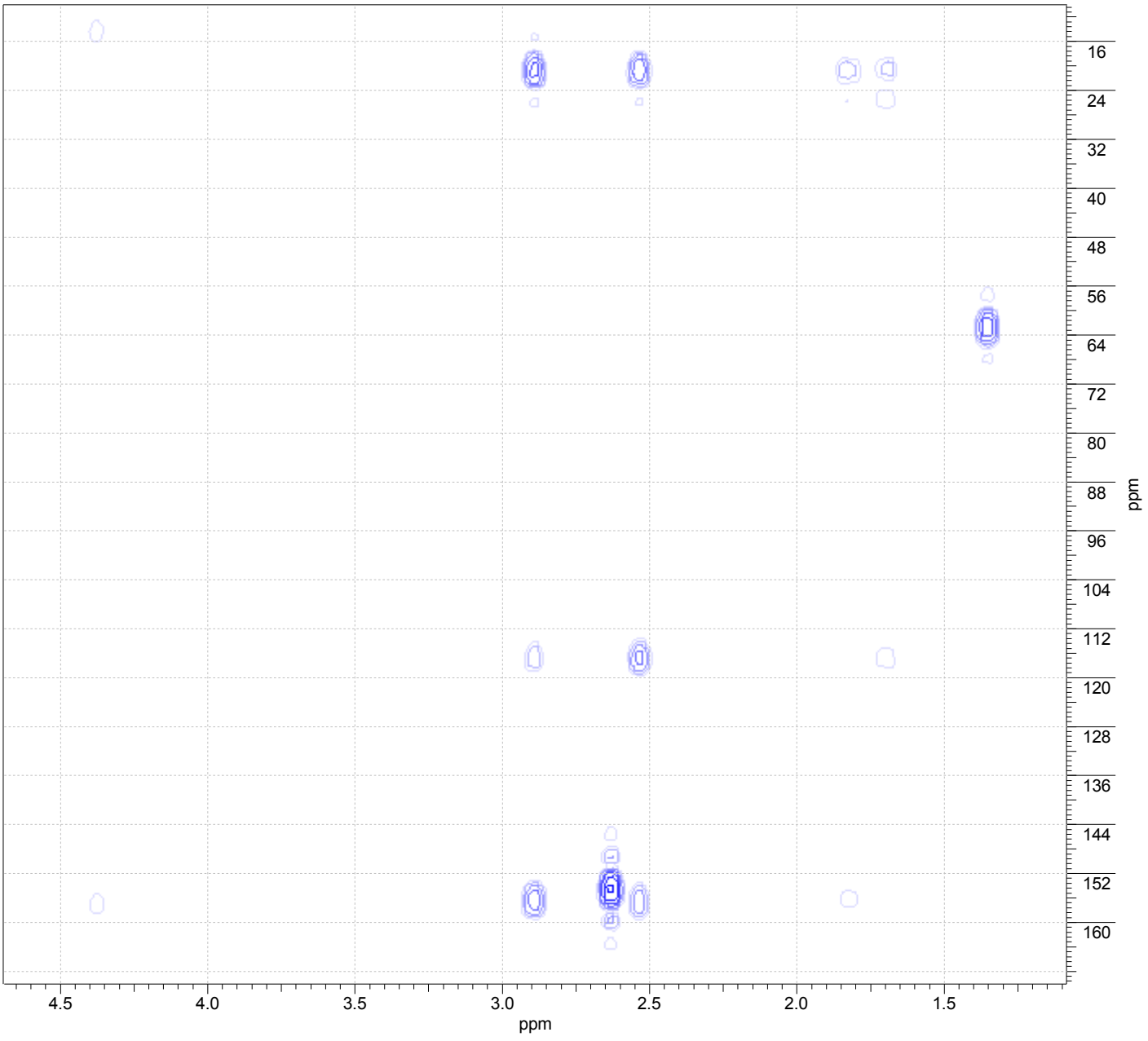




N-Etoxy-2-methyl-5,6,7,8-tetrahydroquinazoline 1-oxide (8)



HMBC



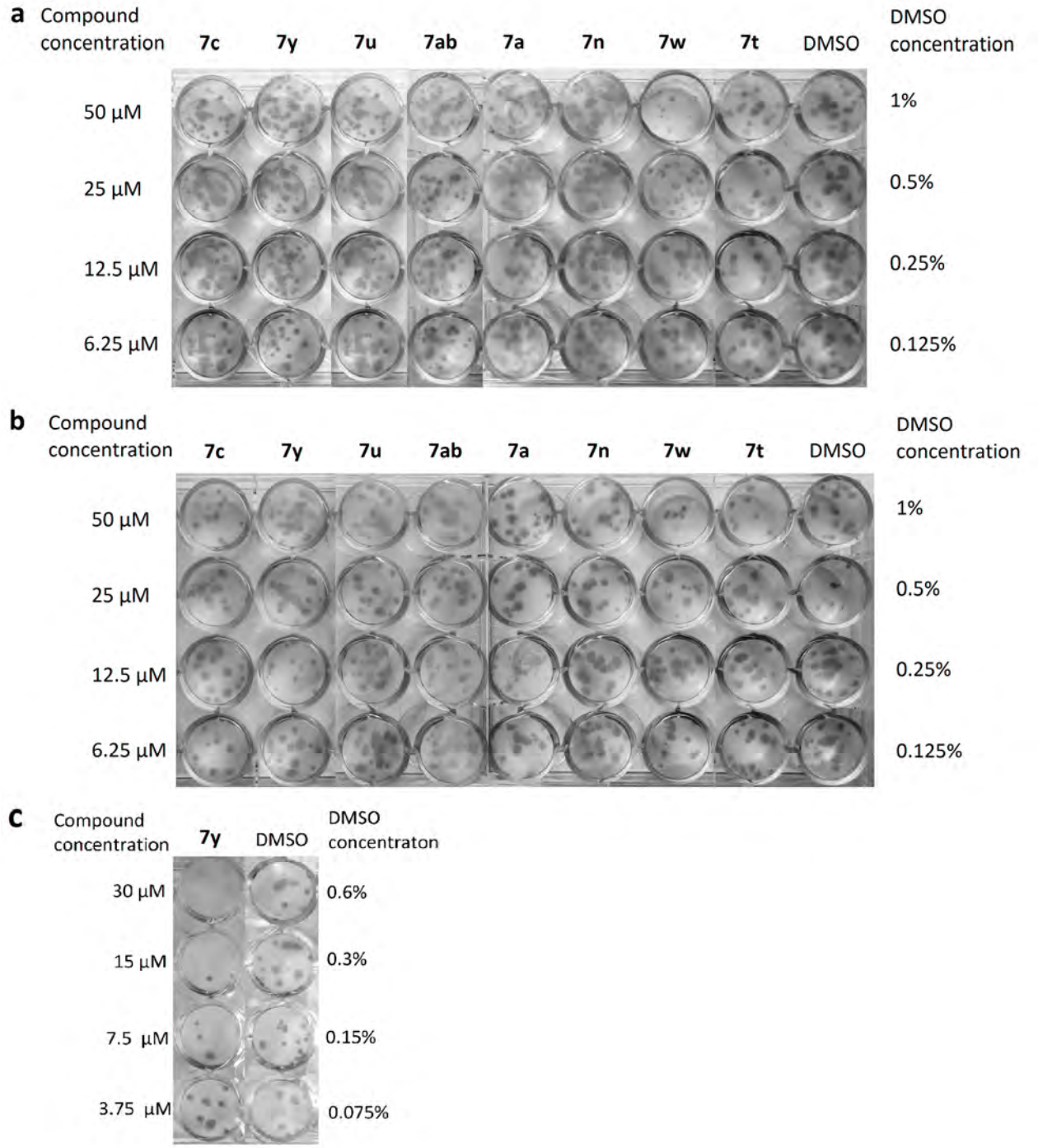


Figure S1. Time-of-addition assay results. Comparable with DMSO-control number of foci a) in second experiment (when cells were pre-incubated with the compounds for 1 h, and then virus was added to the cells) shows no impact of compound – cells interactions in inhibition of viral reproduction; b) in third experiment (when cells were pre-incubated with the virus for 1 h, then compounds were added to the cells) shows that compounds do not affect virus reproduction after virion incorporates the cell; c) results of standard PRT for compound **5y** are presented for comparison.