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Supporting Information

Scaffold-hopping and hybridization based design and building block strategic synthesis of pyridine-annulated purines: Discovery of novel apoptotic anticancer agents

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Contents

Spectral Data of Compounds

1. *N*-(4'-Methylphenmethyl)pyrido[1,2-*e*]purin-4-amine (10)

White solid; mp 145-147 ^{o}C; 254 mg, 88% yield; IR (neat) ν_{max} = 3727, 3006, 1609, 1316 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.60 (d, *J* = 6.9 Hz, 1H), 8.52 (s, 1H), 7.59 (d, *J* = 9.3 Hz, 1H), 7.43 (dd, *J* = 6.7 Hz, 9.2 Hz, 1H), 7.28-7.25 (m, 2H), 7.12 (d, *J* = 7.4 Hz, 2H), 6.92 (t, *J* = 6.7 Hz, 1H), 6.50 (s, NH), 4.85 (s, 2H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ =155.2, 151.3, 145.6, 137.3, 135.0, 129.9, 129.3, 127.8, 124.5, 121.8, 118.3, 111.7, 44.6, 21.1; HRMS (ESI-TOF) calcd for $C_{17}H_{15}N_5Na$: $[M + Na]^+$ 312.1225, found m/z 312.1221.

2. *N*-Phenylpyrido[1,2-*e*]purin-4-amine (13)

White solid; mp 151-154 ^{o}C; 224 mg, 86% yield; IR (ATR) ν_{max} = 3312, 3050, 1615, 1319 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.65 (d, *J* = 8.2 Hz, 2H), 8.12 (s, NH), 7.90 (d, *J* = 7.8 Hz, 2H), 7.66 (d, *J* = 9.3 Hz, 1H), 7.52-7.48 (m, 1H), 7.41 (dd, *J* = 7.7 Hz, 8.0 Hz, 1H), 7.14 (dd, *J* = 7.3 Hz, 7.4 Hz, 1H), 6.97 (dd, *J* = 6.8 Hz, 6.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ =152.6, 150.8, 146.1, 143.7, 138.7, 130.5, 129.1, 124.5, 123.7, 122.4, 120.2, 118.3, 111.9; HRMS (ESI-TOF) calcd for $C_{15}H_{11}N_5Na$: $[M + Na]^+$ 284.0912, found m/z 284.0910.

3. *N*-(3',4'-Dimethoxyphenyl)pyrido[1,2-*e*]purin-4-amine (15)

White solid; mp 113-115 ^{o}C; 250 mg, 78% yield; IR (ATR) ν_{max} = 3204, 2923, 1579, 1315, 1235 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.65-8.60 (m, 2H), 8.20 (s, NH), 7.64-7.58 (m, 2H), 7.50-7.46 (m, 1H), 731-7.28 (m, 1H), 6.98-6.96 (m, 1H), 6.90-6.88 (m, 1H) 3.39 (s, 3H), 3.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 152.8, 150.9, 149.2, 145.9, 145.7, 143.5, 132.1, 130.3, 124.5, 122.2, 118.2, 112.6, 111.9, 111.6, 105.6, 56.2, 55.9; HRMS (ESI-TOF) calcd for $C_{17}H_{15}N_5O_2Na$: $[M + Na]^+$ 344.1124 found m/z 344.1122.

4. *N*-(3',4',5'-Trimethoxyphenyl)pyrido[1,2-*e*]purin-4-amine (16)

Light yellow solid; mp 113-115 ^{o}C; 263 mg, 75% yield; IR (ATR) ν_{max} = 3324, 1641, 1578, 1317 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.64 (d, *J* = 6.9 Hz, 1H), 8.61 (s, 1H), 8.29 (s, NH) 7.62 (d, *J* = 9.3 Hz, 1H), 7.51-7.47 (m, 1H), 7.21 (s, 2H), 6.97 (dd, *J* = 6.7 Hz, 6.6 Hz, 1H), 3.90 (s, 6H), 3.84(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 153.3, 152.5, 150.7, 145.9, 143.5, 134.8,

134.2, 130.6, 124.5, 122.2, 118.1, 112.1, 97.9, 61.0, 56.1; HRMS (ESI-TOF) calcd for $C_{18}H_{17}N_5O_3Na$: $[M + Na]^+$ 374.1229 found m/z 374.1232.

5. *N*-(4'-Bromophenyl)pyrido[1,2-*e*]purin-4-amine (18)

Pale white solid; mp >200°C ; 305 mg, 90% yield; IR (ATR) ν_{max} = 3273, 3076, 1625, 1574, 1314 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 8.66 (d, *J* = 7.0 Hz, 1H), 8.64 (s, 1H), 8.11 (s, NH), 7.82 (d, *J* = 8.6 Hz, 2H), 7.66 (d, *J* = 9.3 Hz, 1H), 7.54-7.49 (m, 3H), 6.98 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 152.3, 150.6, 146.2, 143.8, 137.8, 132.0, 130.8, 124.6, 122.4, 121.6, 118.3, 116.1, 112.1; HRMS (ESI-TOF) calcd for $C_{15}H_{10}{}^{79}BrN_5Na$: $[M + Na]^+$ 362.0018 found m/z 362.0019.

6. *N*-Phenethylpyrido[1,2-*e*]purin-4-amine (21)

White solid; mp 122-124 °C; 260 mg, 90% yield; IR (ATR) ν_{max} = 3311, 3075, 1601, 1312 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 8.60 (d, *J* = 6.9 Hz, 1H), 8.52 (s, 1H), 7.60 (d, *J* = 9.2 Hz, 1H), 7.45-7.41 (m, 1H), 7.31-7.19 (m, 5H), 6.92 (t, *J* = 6.6 Hz, 1H), 6.28 (brs, NH), 4.00 (brs, 2H), 3.04 (t, *J* = 7.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 155.3, 151.2, 145.5, 138.8, 129.7, 128.8, 128.6, 126.5, 124.4, 121.9, 118.3, 111.7, 42.0, 35.8; HRMS (ESI-TOF) calcd for $C_{17}H_{15}N_5Na$: $[M + Na]^+$ 312.1225, found m/z 312.1223.

7. N^4-(N'-Benzylethylamino)pyrido[1,2-*e*]purin-4-amine (23)

White solid; mp 72-74 °C; 226 mg, 71% yield; IR (ATR) ν_{max} = 3280, 3028, 2816, 1617, 1309 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ = 8.70 (d, *J* = 7.2 Hz, 1H), 8.34 (s, 1H), 8.06 (brs, NH), 7.67 (d, *J* = 9.3 Hz, 1H), 7.57-7.53 (m, 1H), 7.32 (d, *J* = 7.2 Hz, 2H), 7.27 (dd, *J* = 7.2 Hz, 7.6 Hz, 2H), 7.19 (t, *J* = 7.1 Hz, 1H), 7.05 (dd, *J* = 6.6 Hz, 6.7 Hz, 1H), 3.74 (s, 2H), 3.67-3.66 (m, 2H), 2.80 (t, *J* = 6.4 Hz, 2H), 1. 89 (s, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 155.6, 151.2, 145.1, 140.9, 130.6, 128.6, 128.5, 127.1, 125.1, 118.2, 112.5, 53.0, 48.1; HRMS (ESI-TOF) Calcd for $C_{18}H_{19}N_6$ $[M+H]^+$ 319.1673 Found *m/z* 319.1671.

8. N^4-(3'-*N*,*N*-dimethylpropylamino)pyrido[1,2-*e*]purin-4-amine (24)

White solid; mp 94-96 °C; 210 mg, 78% yield; IR (ATR) ν_{max} = 3301, 2950, 1614, 1316 cm^{-1}; ^1H NMR (400 MHz, CD_3OD): δ = 8.59 (d, *J* = 6.9 Hz, 1H), 8.33 (s, 1H), 7.61 (d, *J* = 9.2 Hz, 1H),

7.58-7.54 (m, 1H), 7.05 (t, *J* = 6.5 Hz, 1H), 3.71 (brs, 2H), 2.76-2.73 (m, 2H), 2.49 (s, 6H), 2.03-1.99 (m, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ = 155.2, 150.5, 145.5, 142.2, 130.6, 124.1, 120.9, 117.4, 112.4, 56.2, 43.4, 38.2, 26.0; HRMS (ESI-TOF) Calcd for $C_{14}H_{19}N_6$ $[M+H]^+$ 271.1673 Found *m/z* 271.1665.

9. *N*-Hexylpyrido[1,2-*e*]purin-4-amine (26)

White solid; mp 65-67 °C; 229 mg, 85 % yield; IR (ATR) ν_{max} = 3321, 2927, 1611, 1312 m^{-1}; ^{1}H NMR (400 MHz, CD_3OD): δ = 8.56 (d, *J* = 6.9 Hz, 1H), 8.29 (s, 1H), 7.61-7.56 (m, 2H), 7.07-7.04 (m, 1H), 3.58 (s, 2H), 1.73-1.69 (m, 2H), 1.46-1.42 (m, 2H), 1.35-1.32 (m, 4H) 0.91-0.87 (m, 3H); ^{13}C NMR (100 MHz, CD_3OD): δ = 155.0, 150.5, 145.4, 141.8, 130.8, 124.1, 120.7, 117.2, 112.6, 40.6, 31.3, 28.9, 26.3, 22.2, 13.0; HRMS (ESI-TOF) calcd for $C_{15}H_{19}N_5Na$: $[M + Na]^+$ 292.1538 found m/z 292.1539.

10. 4-(3',4',5'-Trimethoxyphenoxy)pyrido[1,2-*e*]purine (30)

White solid; mp >200°C; 229 mg, 65% yield; IR (ATR) ν_{max} = 3062, 2986, 1639,1573,1306, 1119 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.73 (d, *J* = 6.9 Hz, 1H), 8.65 (s, 1H), 7.79 (d, *J* = 9.4 Hz, 1H), 7.61-7.56 (m, 1H), 7.03 (t, *J* = 6.8 Hz, 1H), 6.60 (s, 2H), 3.89 (s, 3H), 3.85 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 160.7, 153.7, 149.6, 148.4, 147.9, 147.3, 135.7, 131.7, 124.7, 123.6, 119.1, 112.4, 99.3, 60.9, 56.2; HRMS (ESI-TOF) calcd for $C_{18}H_{16}N_4O_4Na$: $[M + Na]^+$ 375.1070 found m/z 375.1070.

11. 3-Benzylpyrido[1,2-*e*]purine-2,4(1*H*,3*H*)-dione (33)

White solid; mp >200 °C; 175 mg, 62% yield; IR (ATR) ν_{max} = 3034, 1665, 1568, cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.28 (d, *J* = 6.9 Hz, 1H), 7.38 (d, *J* = 9.3 Hz, 1H), 7.28-7.23 (m, 4H), 7.19-7.13 (m, 2H), 6.78 (t, *J* = 6.7 Hz, 1H) 5.12 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 160.1, 155.7, 142.5, 141.0, 139.5, 127.9, 127.3, 126.3, 125.3, 123.9, 117.9, 116.7, 110.7, 43.1; HRMS (ESI-TOF) calcd for $C_{16}H_{12}N_4O_2Na$: $[M + Na]^+$ 315.0858 found m/z 315.0858.

12. 3-Phenylpyrido[1,2-*e*]purine-2,4(1*H*,3*H*)-dione (34)

White solid; mp >200 °C; 161 mg, 58% yield; IR (ATR) ν_{max} = 3396, 1662, 1553, cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.38 (d, *J* = 6.9 Hz, 1H), 7.51 (d, *J* = 9.3 Hz, 1H), 7.47-7.43 (m, 2H),

7.36 (t, *J* = 7.4 Hz, 1H) 7.27-7.21 (m, 3H), 6.93 (dd *J* = 6.8 Hz, 6.7 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 159.8, 152.9, 141.9, 137.9, 129.8, 129.1, 127.9, 126.5, 124.4, 118.7, 118.1, 112.7; HRMS (ESI-TOF) calcd for $C_{15}H_{10}N_4O_2Na$: $[M + Na]^+$ 301.0702 found m/z 301.0702.

13. 3-(4'-Tolyl)pyrido[1,2-*e*]purine-2,4(1*H*,3*H*)-dione (35)

White solid; mp >200 °C; 175 mg, 60% yield; IR (ATR) ν_{max} = 3630, 3116, 1673, 1511 cm^{-1}; ^{1}H NMR (400 MHz, CD_3OD): δ = 8.33 (d, *J* = 7.0 Hz, 1H), 7.44 (d, *J* = 9.4 Hz, 1H), 7.31-7.26 (m, 3H), 7.12 (d, *J* = 8.2 Hz, 2H), 6.85 (dd *J* = 6.8 Hz, 6.9 Hz, 1H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, CD_3OD): δ = 161.7, 158.6, 145.0, 142.9, 137.1, 135.6, 129.2, 128.5, 127.0, 123.7, 117.3, 116.9, 111.3, 19.8; HRMS (ESI-TOF) calcd for $C_{16}H_{12}N_4O_2Na$: $[M + Na]^+$ 315.0858 found m/z 315.0860.

14. 3-(4'-Chlorophenyl)pyrido[1,2-*e*]purine-2,4(1*H*,3*H*)-dione (36)

Light yellow solid; mp >200 °C; 178 mg, 57% yield; IR (ATR) ν_{max} = 3394, 1661, 1553, 1244 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.45 (d, *J* = 6.4 Hz, 1H), 7.56-7.52 (m, 3H), 7.33-7.27 (m, 3H), 6.99 (t, *J* = 6.5 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 159.3, 151.7, 142.1, 136.2, 132.8, 131.7, 129.3, 126.9, 124.5, 118.8, 118.2, 113.3; HRMS (ESI-TOF) calcd for $C_{15}H_9ClN_4O_2Na$: $[M + Na]^+$ 335.0312 found m/z 335.0311.

15. 3-(4'-Methoxyphenyl)pyrido[1,2-*e*]purine-2,4(1*H*,3*H*)-dione (37)

Pale yellow solid; mp >200 °C; 197 mg, 64% yield; IR (ATR) ν_{max} = 3411, 1657, 1551, 1244 cm^{-1}; ^{1}H NMR (400 MHz, CD_3OD): δ = 8.33 (d, *J* = 6.9 Hz, 1H), 7.44 (d, *J* = 9.4 Hz, 1H), 7.31-7.27 (m, 1H), 7.15 (d, *J* = 8.8 Hz, 2H), 7.03 (d, *J* = 8.8 Hz, 2H), 6.86 (dd *J* = 6.6 Hz, 6.7 Hz, 1H) 3.85 (s, 3H); ^{13}C NMR (100 MHz, CD_3OD): δ = 161.8, 159.1, 144.9, 130.8, 129.6, 127.0, 123.7, 117.3, 116.9, 113.9, 111.3, 54.5; HRMS (ESI-TOF) calcd for $C_{16}H_{12}N_4O_3Na$: $[M + Na]^+$ 331.0807 found m/z 331.0801.

16. 3-(3'-Chlorophenyl)pyrido[1,2-*e*]purine-2,4(1*H*,3*H*)-dione (38)

Greenish yellow solid; mp >200 °C; 178 mg, 57% yield; IR (ATR) ν_{max} = 3006, 1666, 1563, 750 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.21 (d, *J* = 7.7 Hz, 1H), 7.43 (t, *J* = 7.7 Hz, 1H),

7.38-7.32 (m, 2H), 7.18 (dd, *J* = 1.6 Hz, 1.8 Hz, 1H), 7.13-7.09 (m, 2H), 6.73 (dd, *J* = 6.8 Hz, 7.3 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 160.4, 156.6, 145.9, 141.4, 140.8, 132.1, 129.5, 129.4, 128.3, 126.1, 124.9, 123.6, 117.8, 116.5, 110.1; HRMS (ESI-TOF) calcd for $C_{15}H_{10}ClN_4O_2$: $[M + H]^+$ 313.0494 found m/z 313.0484.

17. 3-(4'-Fluorophenyl)pyrido[1,2-*e*]purine-2,4(1*H*,3*H*)-dione (39)

Pale yellow solid; mp >200 ˚C; 178 mg, 60% yield; IR (ATR) ν_{max} = 3344,1666, 1567, 1505 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.24 (dt, *J* = 6.9 Hz, 1.2 Hz, 1H), 7.34 (dt, *J* = 9.4 Hz, 1.0 Hz, 1H), 7.24-7.19 (m, 2H), 7.15-7.09 (m, 3H), 6.74 (ddd, *J* = 6.9 Hz, 6.5 Hz, 1.0 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 160.4 ($^1J_{C\text{-}F}$ = 240 Hz), 160.6, 157.1, 145.7, 140.8, 135.8 ($^4J_{C\text{-}F}$ = 3 Hz), 131.0 ($^3J_{C\text{-}F}$ = 8 Hz), 124.9, 123.7, 117.8, 116.6, 114.7 ($^2J_{C\text{-}F}$ = 23 Hz), 110.1; HRMS (ESI-TOF) calcd for $C_{15}H_{10}FN_4O_2$: $[M + H]^+$ 297.0790 found m/z 297.0782.

18. 3-(4'-Isopropylphenyl)pyrido[1,2-*e*]purine-2,4(1*H*,3*H*)-dione (40)

Pale yellow solid; mp >200 ˚C; 185 mg, 58% yield; IR (ATR) ν_{max} = 3356, 2959, 1664, 1557 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.21 (d, *J* = 6.7 Hz, 1H), 7.33 (d, *J* = 9.3 Hz, 1H), 7.25 (d, *J* = 8.3 Hz, 2H), 7.11 (ddd, *J* = 6.5 Hz, 6.4 Hz, 1.2 Hz, 1H), 6.99 (d, *J* = 8.3 Hz, 1H), 6.73 (dd, *J* = 7.0 Hz, 0.8 Hz, 1H), 2.92 (m, 1H), 1.26 (s, 3H), 1.24 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 161.4, 157.8, 146.6, 146.3, 141.4, 137.9, 129.6, 126.5, 125.6, 124.3, 118.5, 117.2, 110.7, 33.6, 24.5; HRMS (ESI-TOF) calcd for $C_{18}H_{17}N_4O_2$: $[M + H]^+$ 321.1353 found m/z 321.1341.

19. 3-(3',4',5'-Trimethoxyphenyl)pyrido[1,2-*e*]purine-2,4(1*H*,3*H*)-dione (41)

Light yellow solid; mp >200 ˚C; 224 mg, 61% yield; IR (ATR) ν_{max} = 3355, 2989, 1663, 1597, 1275 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.44 (d, *J* = 6.7 Hz, 1H), 7.46 (d, *J* = 9.2 Hz, 1H), 7.27 (dd, *J* = 8.7 Hz, 6.7 Hz, 1H), 6.87 (dd, *J* = 6.7 Hz, 6.6 Hz, 1H), 6.34 (s, 2H), 3.17 (m, 9H); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 176.1, 160.2, 153.2, 143.3, 142.7, 139.1, 136.5, 127.3, 124.7, 121.5, 118.5, 111.8, 107.7, 60.4, 56.3; HRMS (ESI-TOF) calcd for $C_{18}H_{17}N_4O_5$: $[M + H]^+$ 369.1201 found m/z 369.1208.

20. 3-Benzylpyrido[1,2-*e*]purin-2(1*H*)-thione-4(3*H*)-one (42)

Pale yellow solid; mp >200 ºC; 197 mg, 65% yield; IR (ATR) ν_{max} = 3333, 2925, 1677, 1541 cm^{-}

[1]; ^{1}H NMR (400 MHz, CD_3OD): δ = 8.55 (d, *J* = 7.0 Hz, 1H), 7.48 (d, *J* = 9.4 Hz, 1H), 7.38-7.34 (m, 3H), 7.25-7.22 (m, 2H), 7.16 (t, *J* = 7.3 Hz, 1H), 6.93-6.89 (m, 1H) 6.00 (s, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ = 175.0, 160.2, 143.9, 141.9, 138.2, 128.4, 127.6, 127.0, 126.1, 124.2, 120.6, 117.2, 111.9, 50.2; HRMS (ESI-TOF) calcd for $C_{16}H_{12}N_4OSNa$: $[M + Na]^+$ 331.0630 found m/z 331.0625.

21. Pyrido[1,2-*e*]purine-2,4(1*H*,3*H*)-dione (V)

White solid; mp >200 °C; 101 mg, 50% yield; IR (ATR) ν_{max} = 3394, 1661, 1553 cm^{-1}; ^{1}H NMR (400 MHz, CD_3OD): δ = 7.98 (d, *J* = 7.0 Hz, 1H), 7.38 (d, *J* = 9.2 Hz, 1H), 7.10-7.06 (m, 1H), 6.80 (dd *J* = 6.7 Hz, 6.8 Hz, 1H); ^{13}C NMR (100 MHz, CD_3OD): δ = 172.8, 161.3, 139.3, 135.6, 124.1, 123.4, 122.8, 118.3, 112.6; HRMS (ESI-TOF) calcd for $C_9H_7N_4O_2$ $[M + H]^+$ 203.0571 found m/z 203.0564.

22. 2,4-Dichloropyrido[1,2-*e*]purine (VI)

White solid; mp >200 °C; 127 mg, 53% yield; IR (ATR) ν_{max} = 3104, 1550, 1147, 906 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.70 (d, *J* = 6.8 Hz, 1H), 7.79 (d, *J* = 9.3 Hz, 1H), 7.69-7.65 (m, 1H), 7.09 (t, *J* = 6.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 151.9, 149.7, 149.6, 147.3, 133.6, 131.7, 125.1, 119.2, 113.3; HRMS (ESI-TOF) Calcd for $C_9H_4Cl_2N_4Na$: $[M + Na]^+$ 260.9711 found m/z 260.9712.

23. 2-Chloro-*N*-phenethylpyrido[1,2-*e*]purin-4-amine (VII)

White solid; mp 170-172 °C; 290 mg, 90% yield; IR (ATR) ν_{max} = 3260, 2927, 1613, 1345, 1310 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.57 (d, *J* = 6.8 Hz, 1H), 7.59 (d, *J* = 9.2 Hz, 1H), 7.47-7.42 (m, 1H), 7.34-7.30 (m, 2H), 7.28-7.22 (m, 3H) 6.94 (t, *J* = 6.8 Hz, 1H) 6.39 (s, 1H) 3.99 (d, *J* = 5.9 Hz, 2H), 3.04 (t, *J* = 7.0 Hz, 2H) ; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 155.8, 145.8, 138.4, 129.9, 128.8, 128.7, 126.6, 124.4, 118.4, 112.1, 42.2, 35.5; HRMS (ESI-TOF) Calcd for $C_{17}H_{14}ClN_5Na$: $[M + Na]^+$ 324.1018 found m/z 324.1021.

24. 2-Morpholino-N^4-(2'-phenethyl)pyrido[1,2-*e*]purin-4-amine (43)

White solid; mp 154-156 °C; 197 mg, 82% yield; IR (ATR) ν_{max} = 3375, 2922, 2851, 1593, 1432, 1112 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.36 (d, *J* = 6.9, Hz, 1H), 7.49-7.47 (m, 2H),

7.31-7.25 (m, 5H), 7.23-7.19 (m, 1H), 6.79 (t, *J* = 6.6 Hz, 1H), 3.87-3.79 (m, 10H), 3.03 (t, J = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 175.6, 158.6, 154.9, 143.4, 139.5, 128.8, 128.5, 128.3, 126.2, 123.9, 117.3, 114.7, 111.2, 67.0, 45.1 ($2CH_2$), 42.2, 35.7, ; HRMS (ESI-TOF) Calcd for $C_{21}H_{23}N_6O$ $[M+H]^+$ 375.1935 Found *m/z* 375.1940.

25. *N*^{4}-(4'-Methoxyphenmethyl)-2-morpholinopyrido[1,2-*e*]purin-4-amine (44)

Light yellow solid; mp 84-86 ^{o}C; 304 mg, 78% yield; IR (ATR) ν_{max} = 3479, 3104, 1602, 1485, 1111 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.35 (d, *J* = 6.9, Hz, 1H), 7.43 (d, *J* = 9.2 Hz, 1H), 7.27-7.22 (m, 3H), 6.82 (d, *J* = 8.0 Hz, 2H), 6.74 (dd *J* = 6.8 Hz, 6.7 Hz, 1H), 6.56 (brs, NH), 4.74 (s, 2H), 3.88-3.85, (m, 4H), 3.82-3.79 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 158.8, 158.2, 155.0, 143.9, 130.8, 129.9, 129.3, 129.0, 127.6, 123.9, 118.1, 113.8, 110.7, 67.0, 55.3, 45.1, 44.1; HRMS (ESI-TOF) Calcd for $C_{21}H_{22}N_6O_2$ $[M+H]^+$ 391.1884 Found *m/z* 391.1895.

26. *N*^{4}-(4'-Chlorophenmethyl)-2-morpholinopyrido[1,2-*e*]purin-4-amine (45)

Yellow solid; mp 175-177 ^{o}C; 300 mg, 76% yield; IR (ATR) ν_{max} = 3385, 3243, 2922, 2850, 1638, 1607, 1104 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.35 (d, *J* = 6.9, Hz, 1H), 7.44 (d, *J* = 9.3 Hz, 1H), 7.25-7.21 (m, 5H), 6.76 (t, *J* = 6.7 Hz, 1H), 6.68 (brs, NH), 4.76 (s, 2H), 3.85-3.83, (m, 4H), 3.80-3.78 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 158.2, 154.9, 143.9, 137.4, 132.9, 128.9, 128.5, 127.8, 123.9, 118.1, 115.8, 110.8, 66.9, 45.1, 43.9; HRMS (ESI-TOF) Calcd for $C_{20}H_{19}ClN_6O$ $[M+H]^+$ 395.1389 Found *m/z* 395.1388.

27. 2-Morpholino-*N*^{4}-(3'-morpholinopropyl)pyrido[1,2-*e*]purin-4-amine (46)

Greenish yellow solid; mp 84-86 ^{o}C; 298 mg, 75% yield; IR (ATR) ν_{max} = 3333, 2921, 2852, 1601, 1113 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.34 (d, *J* = 6.8, Hz, 1H), 7.47 (d, *J* = 9.3 Hz, 1H), 7.25-7.21 (m, 1H), 6.85 (brs, NH), 6.74 (t, *J* = 6.7 Hz, 1H), 3.84-3.71, (m, 14H), 2.59-2.49 (m, 6H) 1.92-1.85 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 158.3, 155.3, 144.9, 143.8, 127.5, 123.9, 118.1, 116.0, 110.7, 67.0, 66.8, 57.2, 53.7, 45.1, 29.7, 25.7; HRMS (ESI-TOF) Calcd for $C_{20}H_{28}N_7O_2$ $[M+H]^+$ 398.2306 Found *m/z* 398.2327.

28. 3-Benzyl-2-(methylthio)pyrido[1,2-*e*]purin-4(3*H*)-one (VIII)

White solid; mp 194-196 ^{o}C; 209 mg, 65% yield; IR (ATR) ν_{max} = 3386, 1685, 1311 cm^{-1}; ^{1}H

NMR (400 MHz, CD_3OD:$CDCl_3$ (3:1)): δ = 8.48 (d, *J* = 6.8 Hz, 1H), 7.60 (d, *J* = 9.4 Hz, 1H), 7.48 (t, *J* = 8.0 Hz, 1H), 7.30-7.24 (m, 5H), 7.02 (t, *J* = 6.8 Hz, 1H), 5.46 (s, 2H), 2.67 (s, 3H); ^{13}C NMR (100 MHz, CD_3OD:$CDCl_3$ (3:1)): δ = 158.4, 158.2, 145.0, 140.7, 135.2, 129.7, 128.3, 127.4, 127.0, 123.8, 122.1, 117.6, 113.2, 14.8; HRMS (ESI-TOF) Calcd for $C_{17}H_{14}N_4OS$ $[M+H]^+$ 323.0968 Found *m/z* 323.0968.

29. 3-Benzyl-2-(hexylamino)pyrido[1,2-*e*]purin-4(3*H*)-one (47)

Greenish yellow solid; mp 148-150 °C; 199 mg, 53% yield; IR (ATR) ν_{max} = 3360, 2922, 2852, 1677, 1588, 1337 cm^{-1}; ^1H NMR (400 MHz, CD_3OD): δ = 8.32 (d, *J* = 6.9, Hz, 1H), 7.50 (d, *J* = 9.4 Hz, 1H), 7.39-7.35 (m, 1H), 7.33-7.30 (m, 2H), 7.26 (d, *J* = 7.2 Hz, 1H), 7.21 (d, *J* = 7.1 Hz, 2H), 6.94-6.91, (m, 1H), 5.42 (s, 2H), 3.44 (t, *J* = 6.8 Hz, 2H) 1.55-1.48 (m, 2H), 1.24-1.18 (m, 4H), 1.12-1.10 (m,, 2H), 0.84 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, CD_3OD): δ = 158.7, 151.4, 144.0, 142.9, 135.4, 128.4, 128.2, 127.2, 126.1, 123.5, 117.5, 117.3, 112.0, 43.2, 41.7, 31.2, 28.4, 26.0, 22.2, 12.9; HRMS (ESI-TOF) Calcd for $C_{22}H_{26}N_5O$ $[M+H]^+$ 376.2139 Found *m/z* 376.2145.

30. 3-Benzyl-2-((4'-methoxyphenmethyl)amino)pyrido[1,2-*e*]purin-4(3*H*)-one (48)

Yellow solid; mp 193-195 °C; 201 mg, 49% yield; IR (ATR) ν_{max} = 3452, 3285, 3143, 1703, 1621, 1603, 1186 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 8.26 (d, *J* = 7.0, Hz, 1H), 7.57 (d, *J* = 9.4 Hz, 1H), 7.31-7.25 (m, 3H), 7.23-7.20 (m, 2H), 7.15 (d, *J* = 8.6 Hz, 1H), 7.08-7.06 (m, 1H), 6.96 (d, *J* = 8.5 Hz, 1H), 6.83-6.75, (m, 3H), 5.41 (s, 1H), 5.36 (s, 1H), 4.59 (d, *J* = 4.8 Hz, 1H) 5.50 (d, *J* = 4.7 Hz, 1H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.5, 158.9, 150.8, 135.1, 129.3, 128.8, 128.6, 128.15, 128.11, 127.4, 127.1, 126.7, 123.5, 118.9, 114.7, 113.9, 111.8, 55.3, 45.9, 44.4,; HRMS (ESI-TOF) Calcd for $C_{24}H_{22}N_5O_2$ $[M+H]^+$ 412.1775 Found *m/z* 412.1779.

31. 3-Benzyl-2-((3',4'-dimethoxyphenethyl)amino)pyrido[1,2-*e*]purin-4(3*H*)-one (49)

Light yellow solid; mp 181-183 °C; 218 mg, 48% yield; IR (ATR) ν_{max} = 3308, 1655, 1601, 1322 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 8.29 (dt, *J* = 5.9 Hz, 1.0 Hz, 1H), 7.63 (d, *J* = 9.4 Hz, 1H), 7.28-7.19 (m, 5H), 7.05-7.03 (m, 2H), 6.82 (dd *J* = 6.8 Hz, 6.7 Hz, 1H), 6.75 (d, *J* = 7.8 Hz, 1H), 6.61-6.58, (m, 2H), 5.25 (s, 2H), ,3.90,(s, 3H), 3.82 (s, 3H), 3.73-3.69 (m, 2H), 2.81 (t, *J* =

6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 158.5, 151.1, 149.2, 147.9, 144.0, 134.7, 129.1, 128.7, 128.0, 127.9, 127.2, 126.5, 123.4, 120.5, 119.4, 118.9, 111.8, 111.4, 111.3, 55.9, 55.8, 44.6, 43.1, 34.3; HRMS (ESI-TOF) Calcd for $C_{26}H_{26}N_5O_3$ $[M+H]^+$ 456.2037 Found *m/z* 456.2039.

NMR Spectra of Compounds

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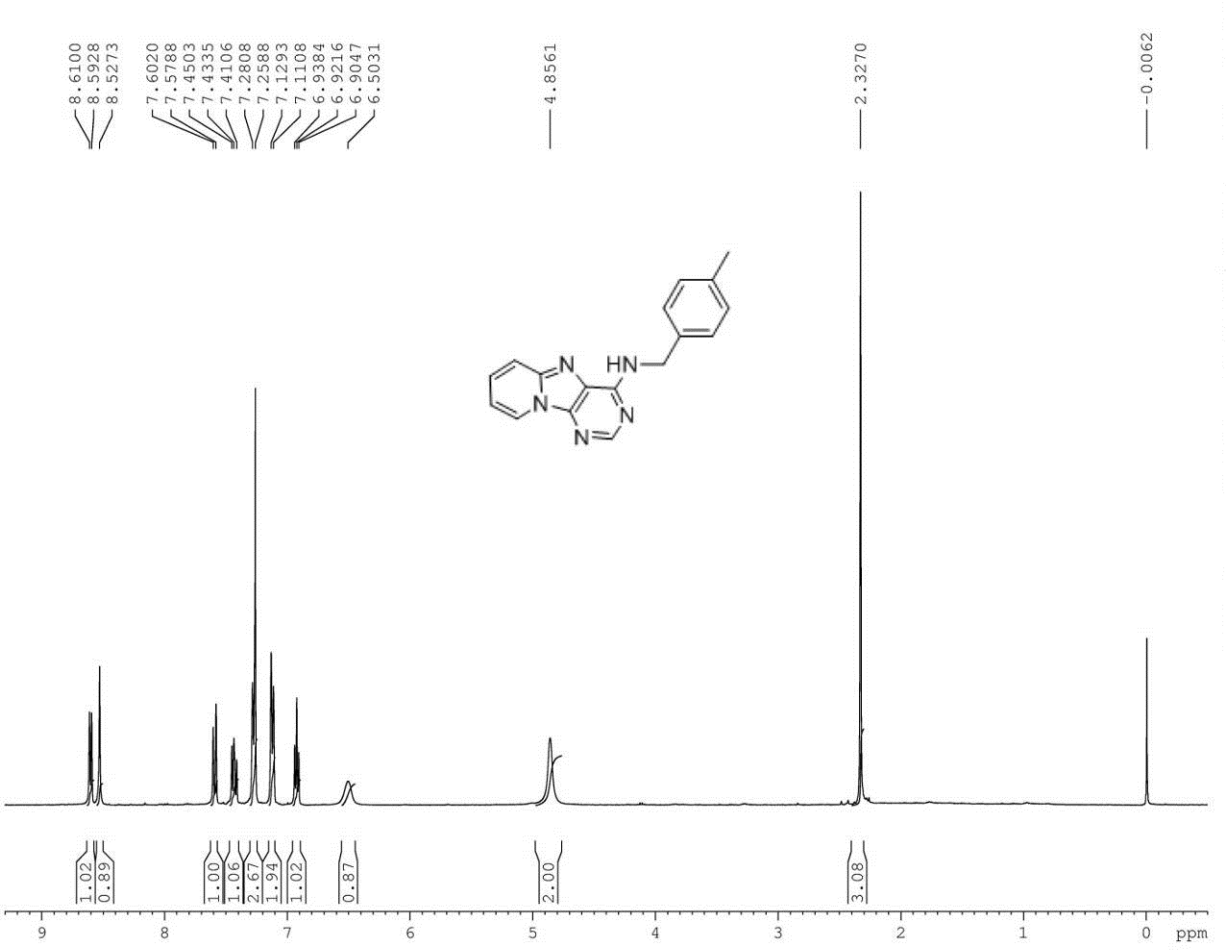

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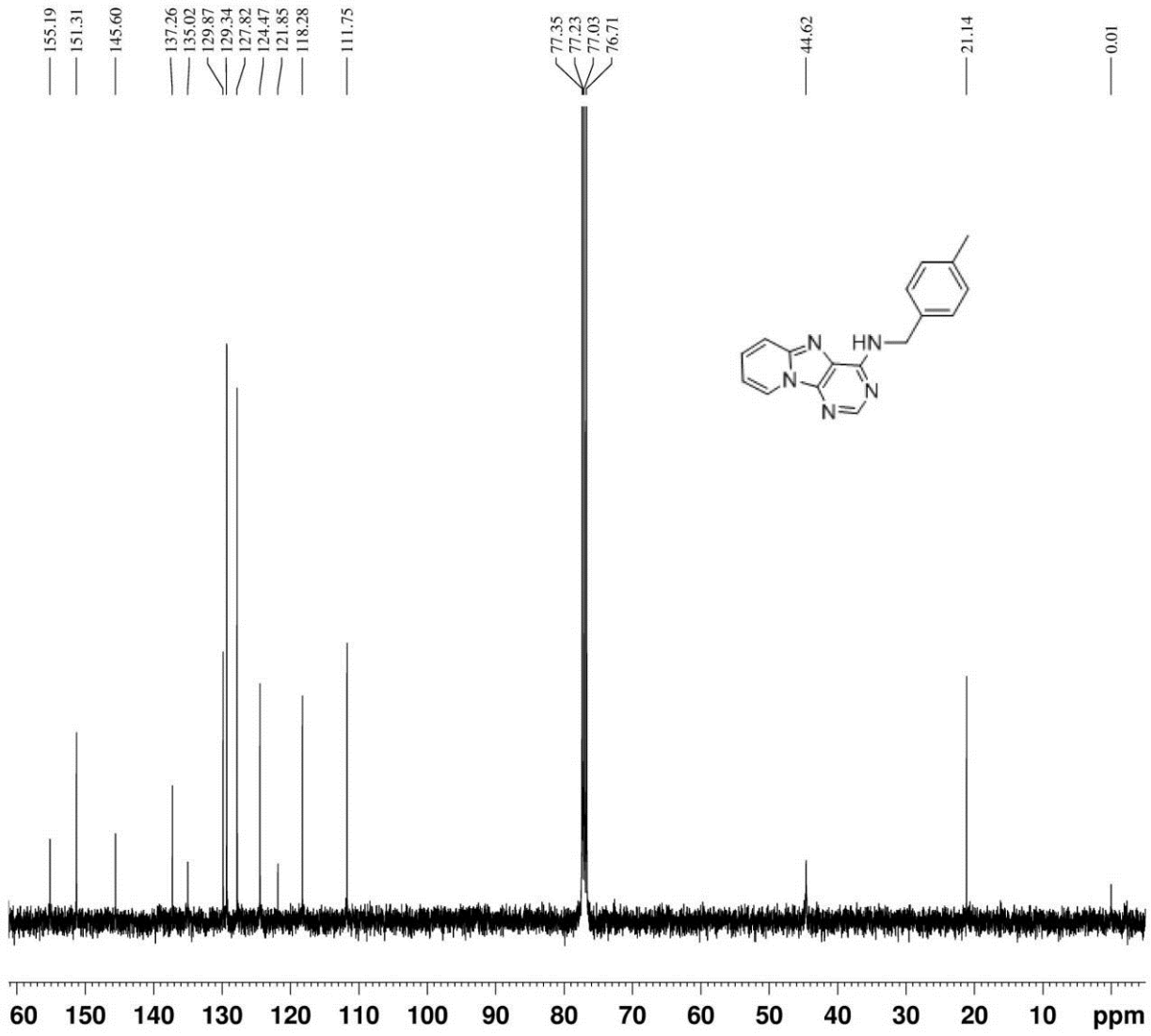
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77.23
77.03
76.71
44.62
21.14
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HN
N
N
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40
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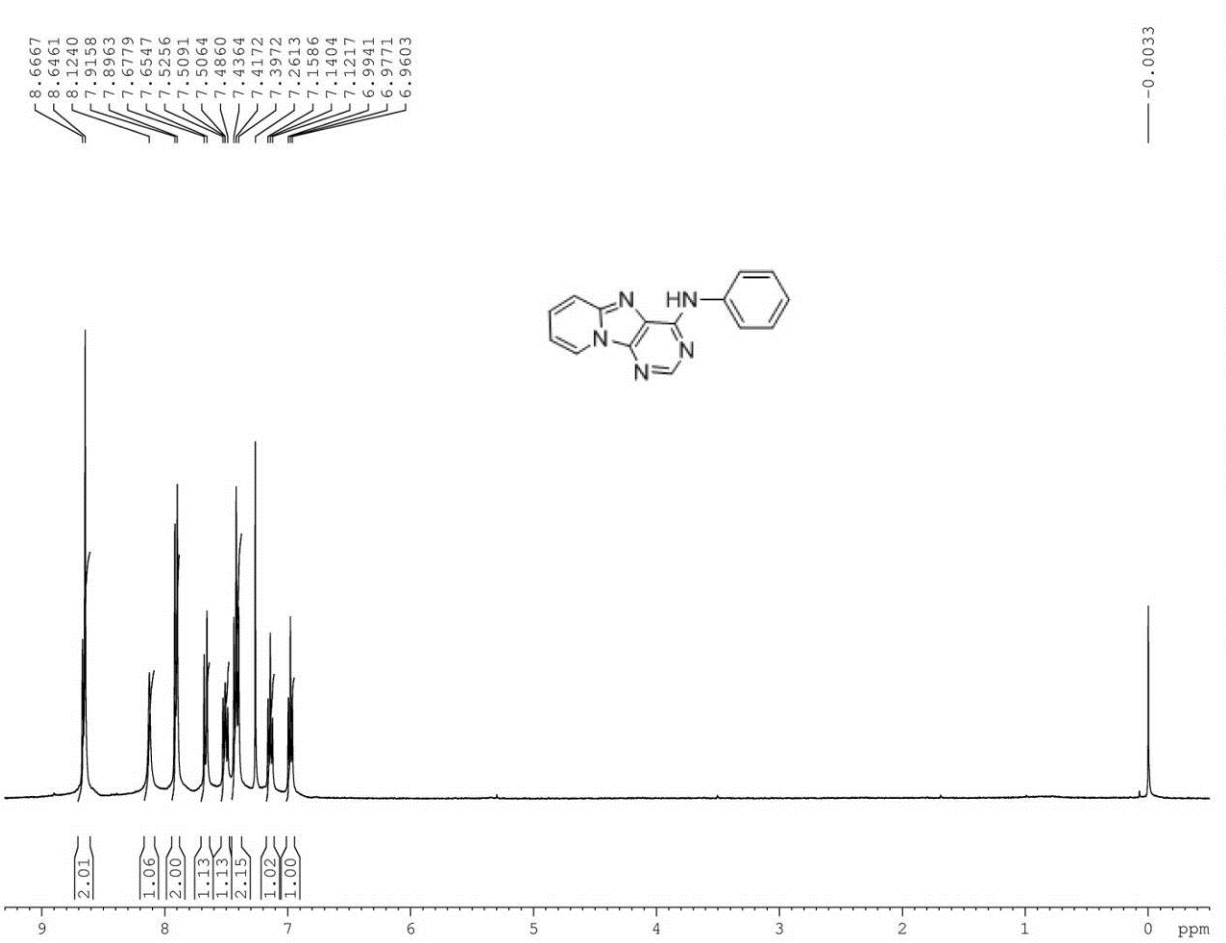
10
ppm

13: ^{1}H NMR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7.2613
7.1586
7.1404
7.1217
6.9941
6.9771
6.9603
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HN
N
N
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2.01
1.06
2.00
1.13
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7
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5
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3
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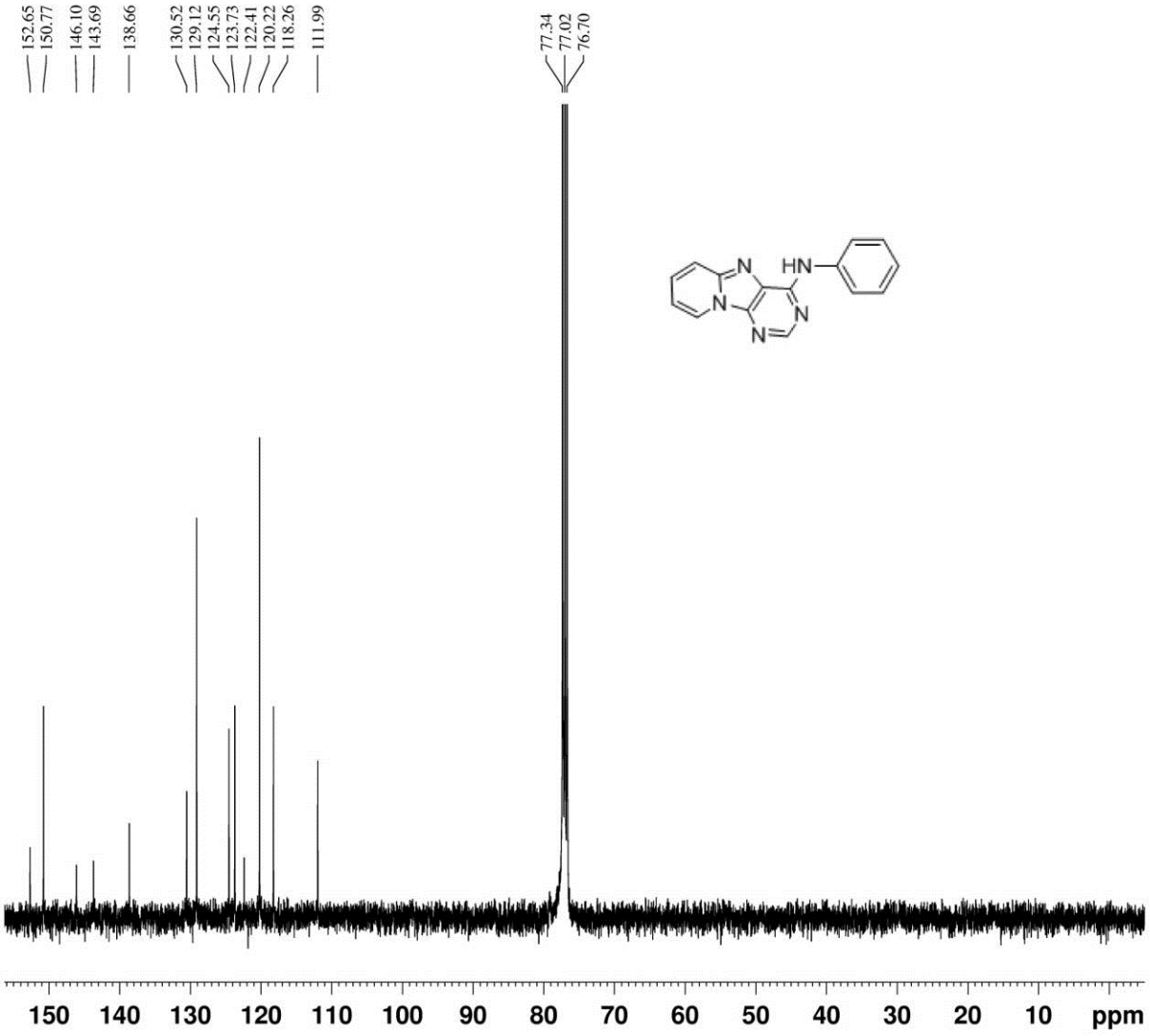
ppm

13: ^{13}C NMR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76.70
HN
N
N
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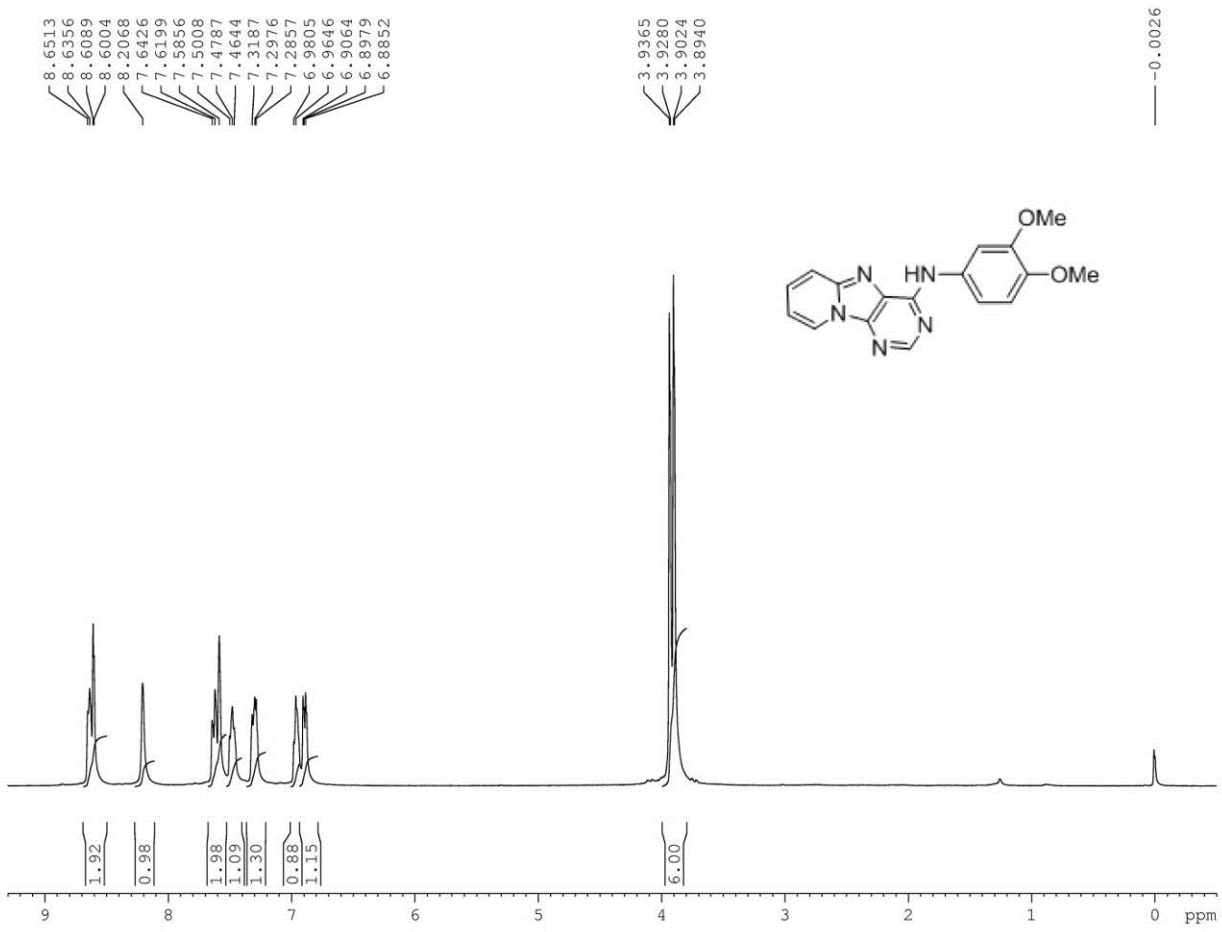
ppm

15: ^{1}H NMR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7.3187
7.2976
7.2857
6.9805
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N
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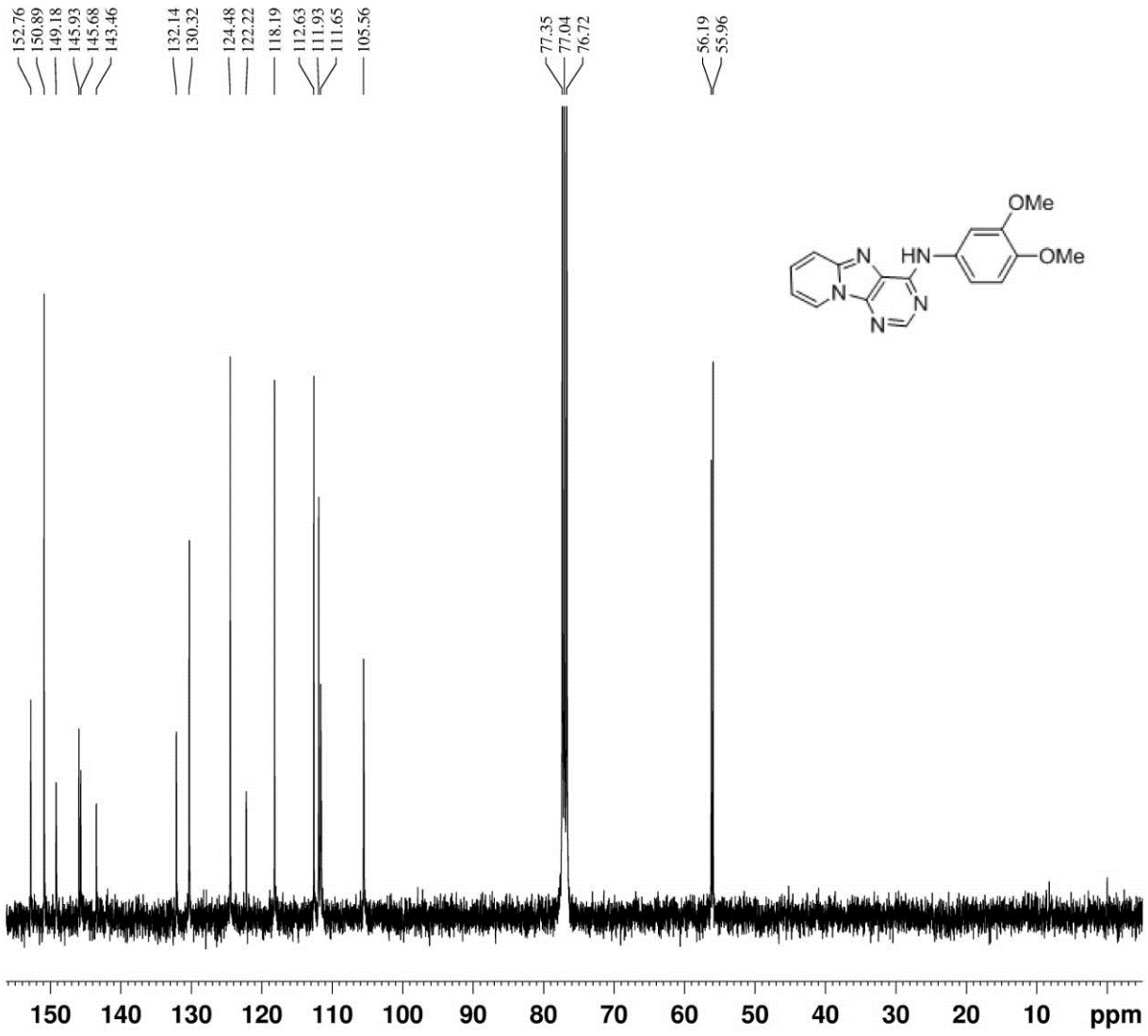
15: ^{13}C NMR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111.93
111.65
105.56
77.35
77.04
76.72
56.19
55.96
OMe
HN
OMe
N
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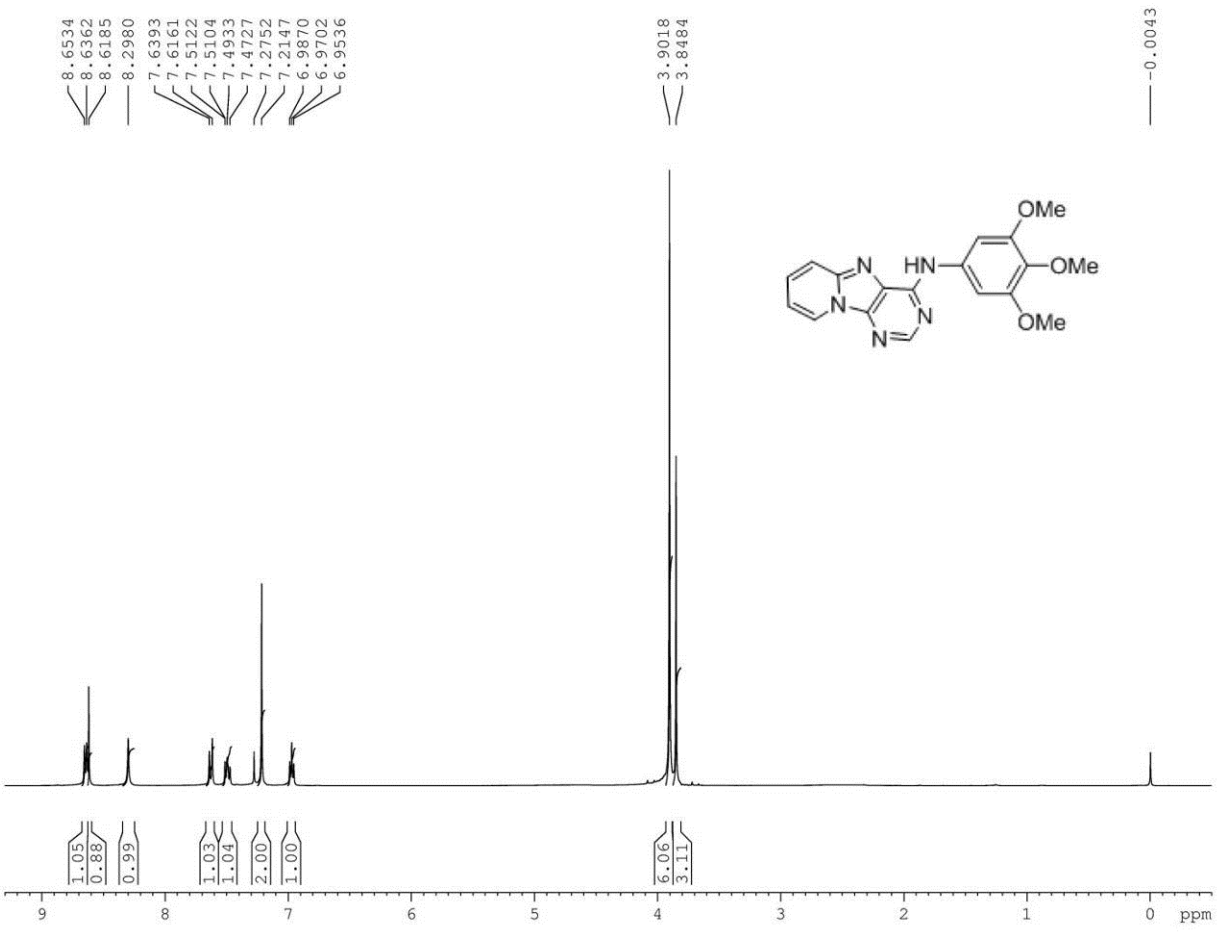
ppm

16: ^{1}H NMR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6.9702
6.9536
3.9018
3.8484
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OMe
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OMe
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N
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1.03
1.04
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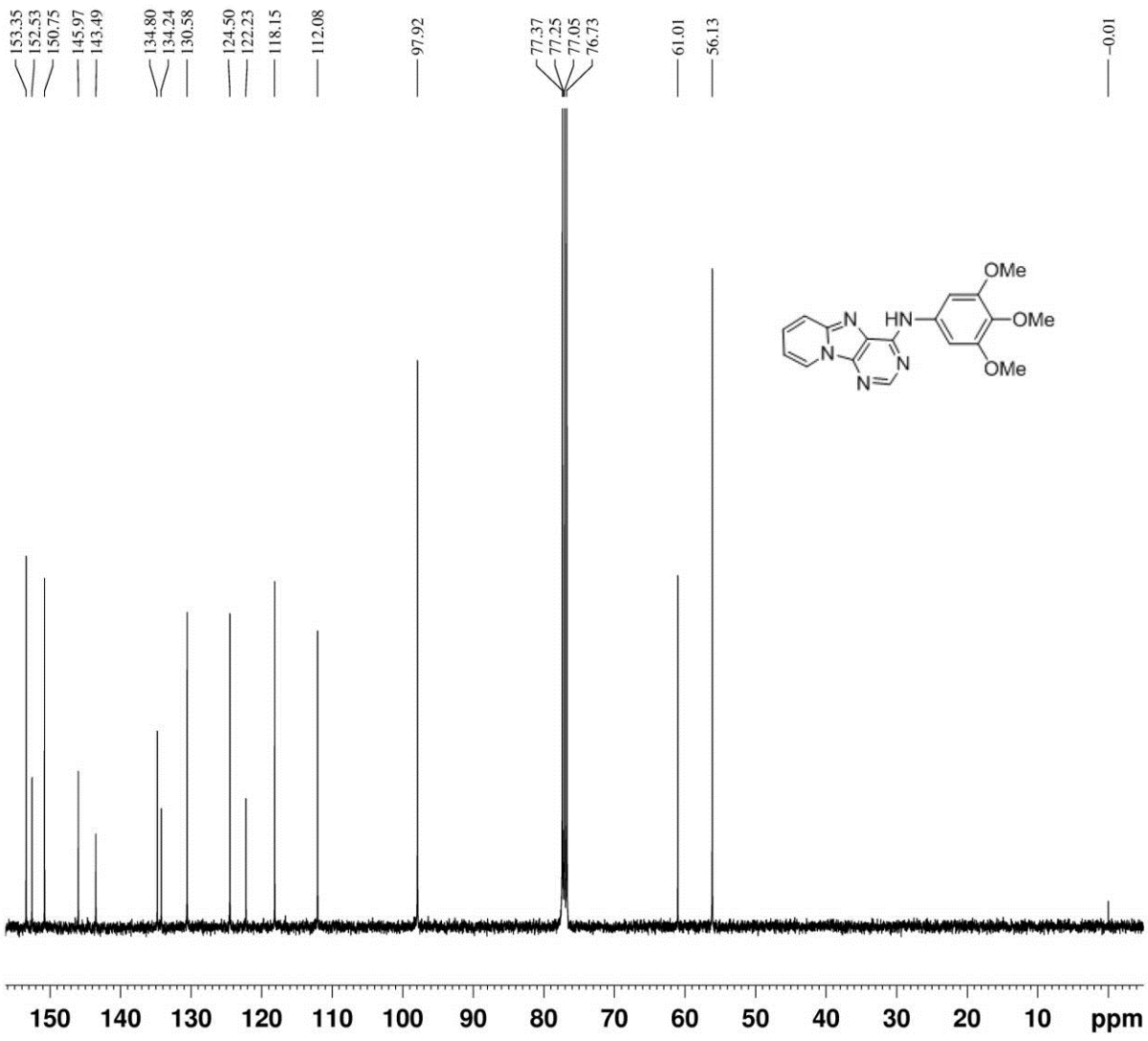
ppm

16: ^{13}C NMR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77.25
77.05
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HN
OMe
OMe
N
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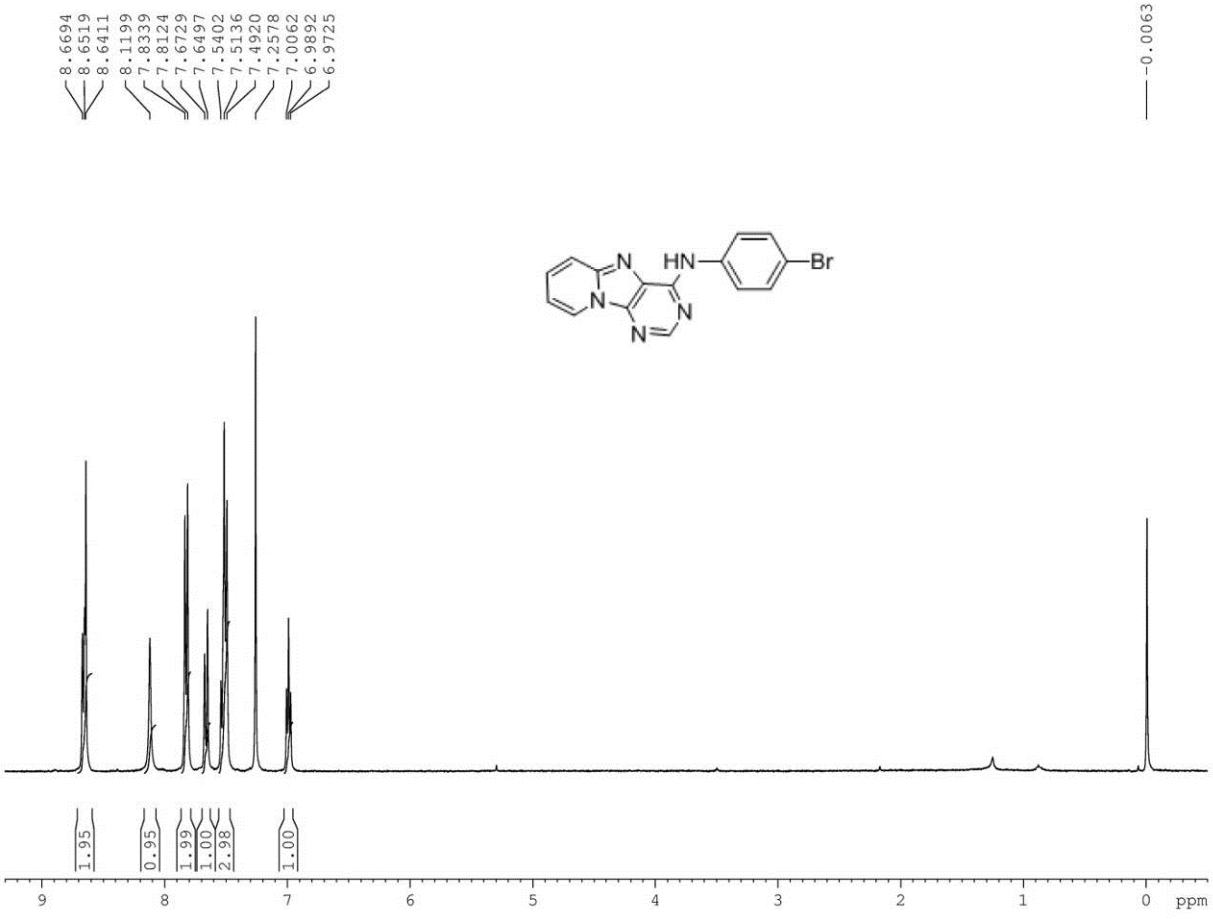
ppm

18: ^{1}H NMR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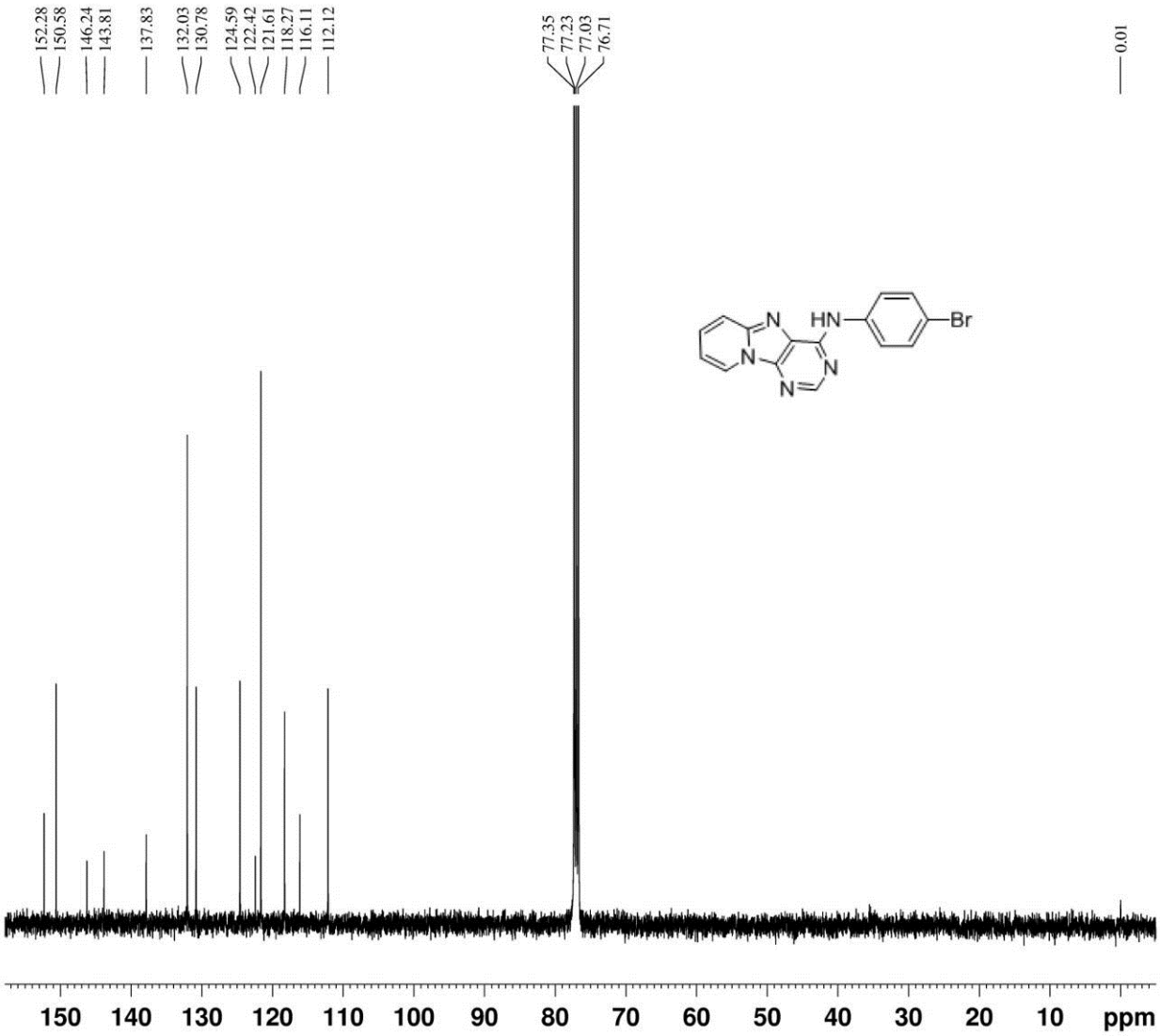
ppm

18: ^{13}C NMR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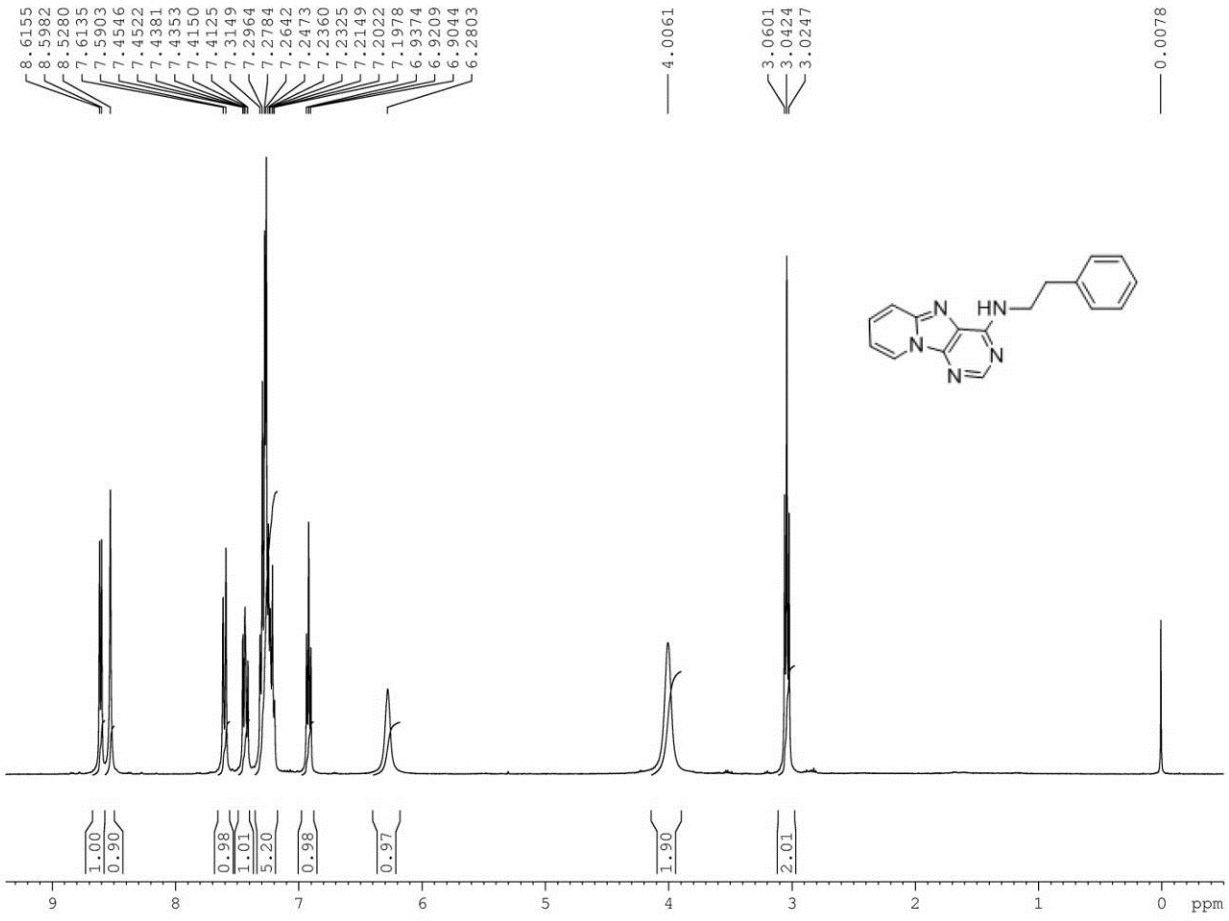
21: ^{1}H NMR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7.4125
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7.2964
7.2784
7.2642
7.2473
7.2360
7.2325
7.2149
7.2022
7.1978
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6.9209
6.9044
6.2803
4.0061
3.0601
3.0424
3.0247
0.0078
HN
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1.01
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3
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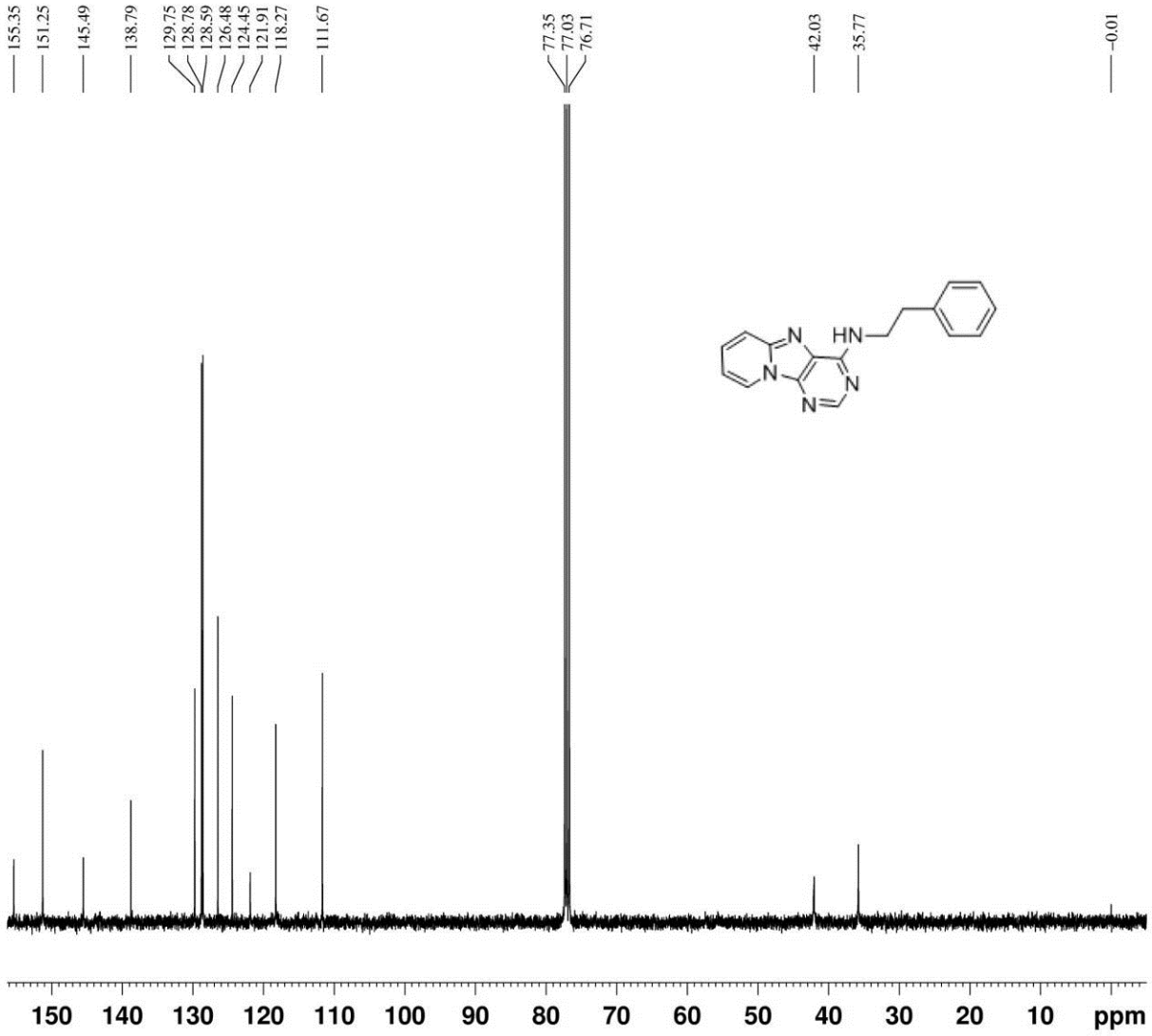
ppm

21: ^{13}C NMR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77.03
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40
30
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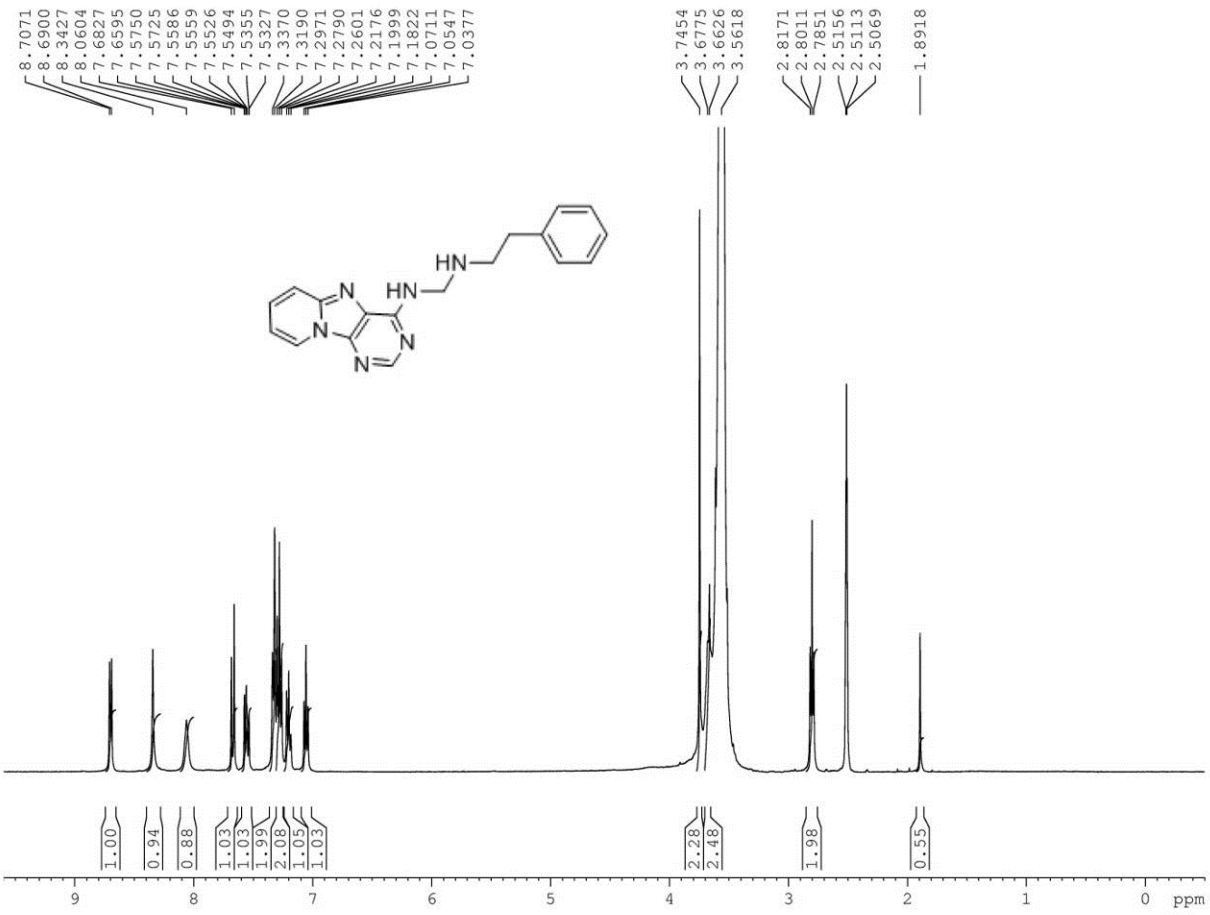
ppm

23: ^{1}H NMR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7.5355
7.5327
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7.2601
7.2176
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7.1822
7.0711
7.0547
7.0377
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3.6775
3.6626
3.5618
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2.8011
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1.03
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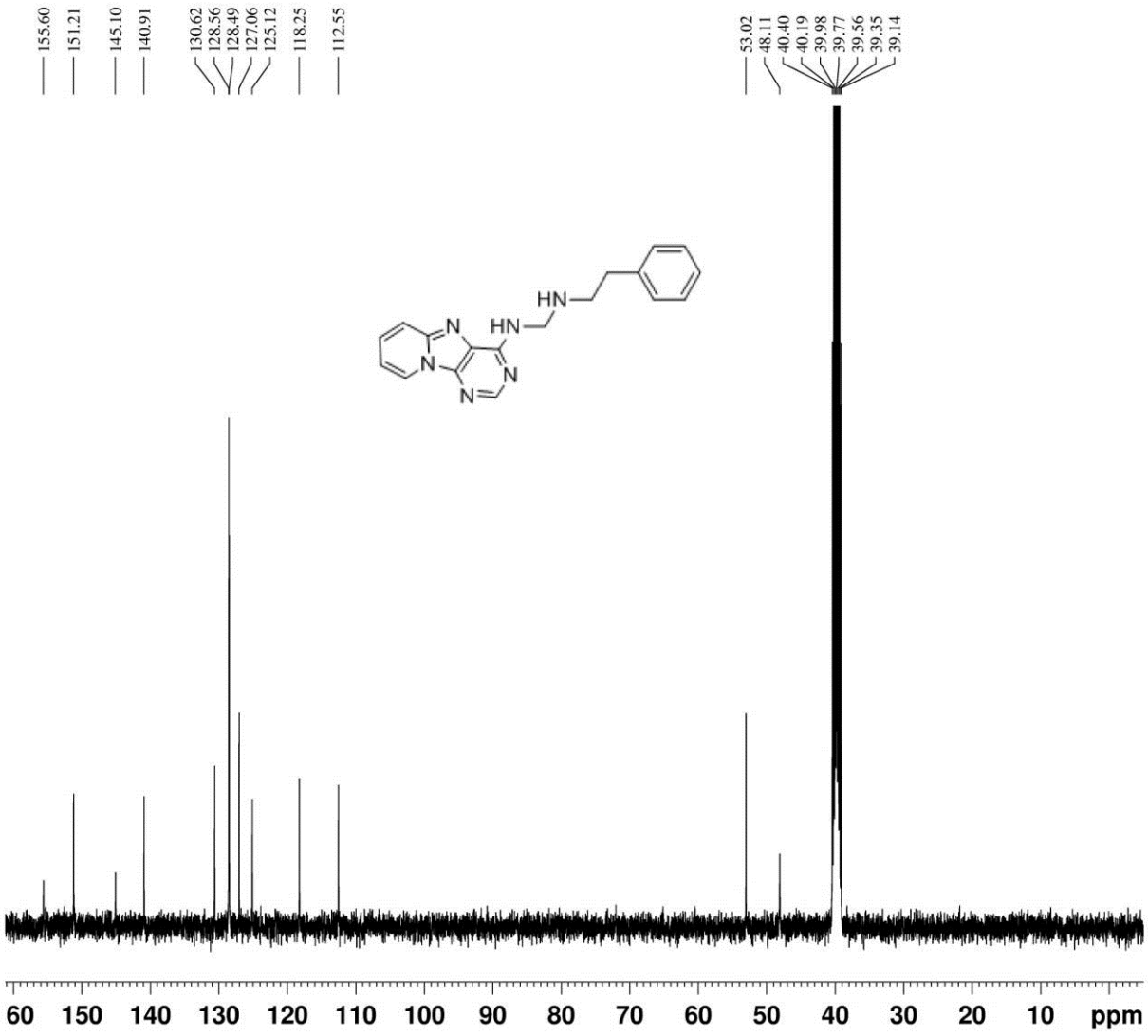
ppm

23: ^{13}C NMR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HN
N
N
N
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60
150
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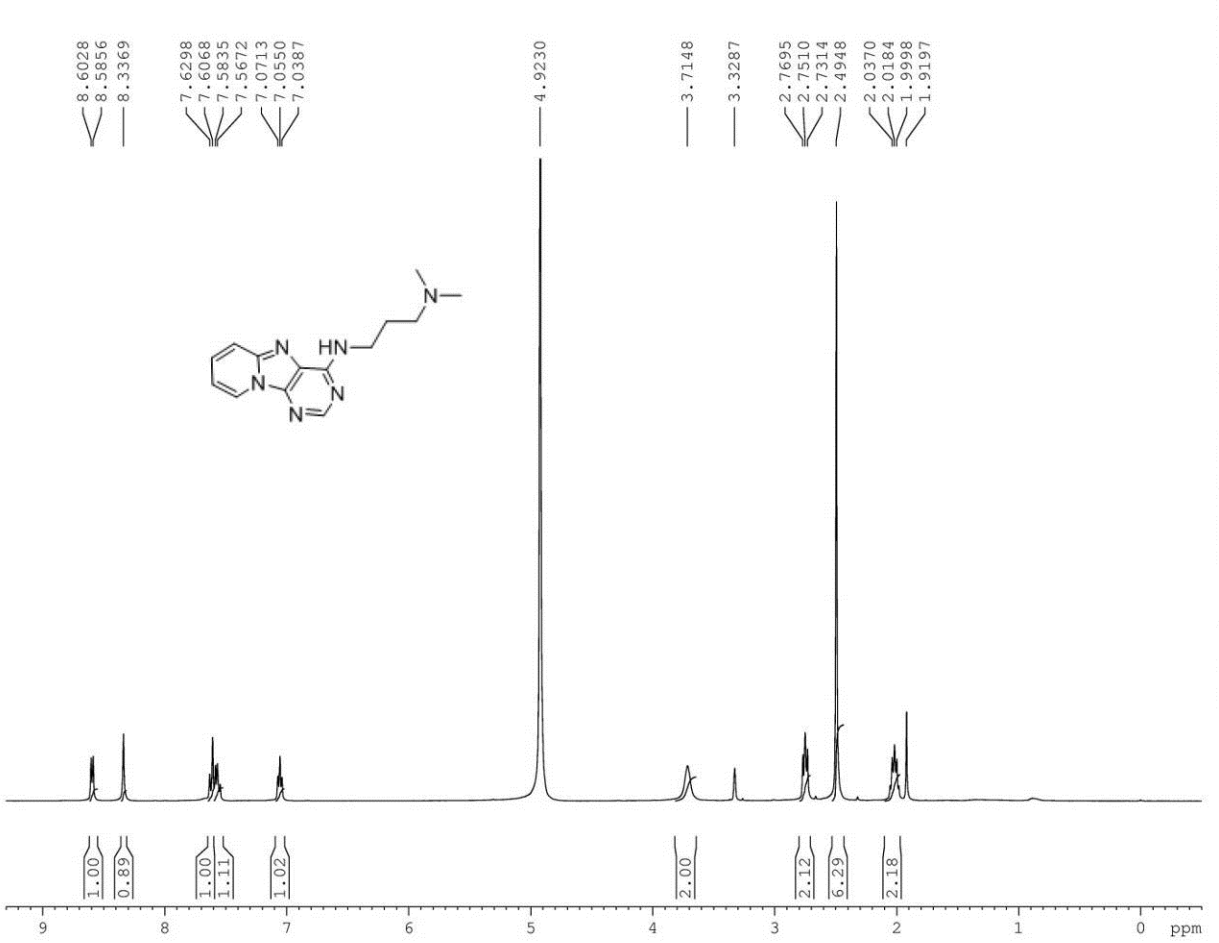
10
ppm

24: ^{1}H NMR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2.7695
2.7510
2.7314
2.4948
2.0370
2.0184
1.9998
1.9197
HN
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0.89
1.00
1.11
1.02
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8
7
6
5
4
3
2
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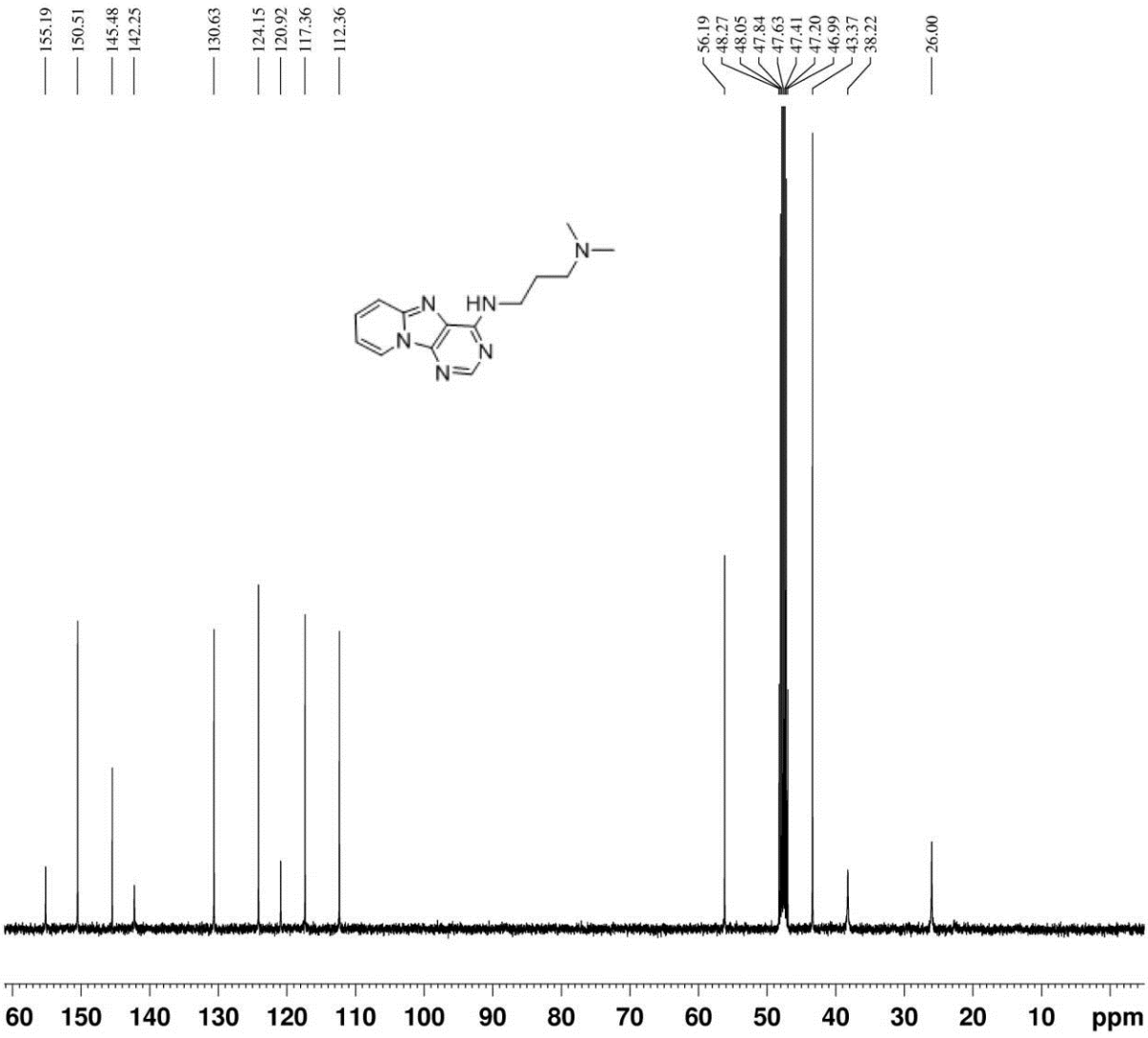
0
ppm

24: ^{13}C NMR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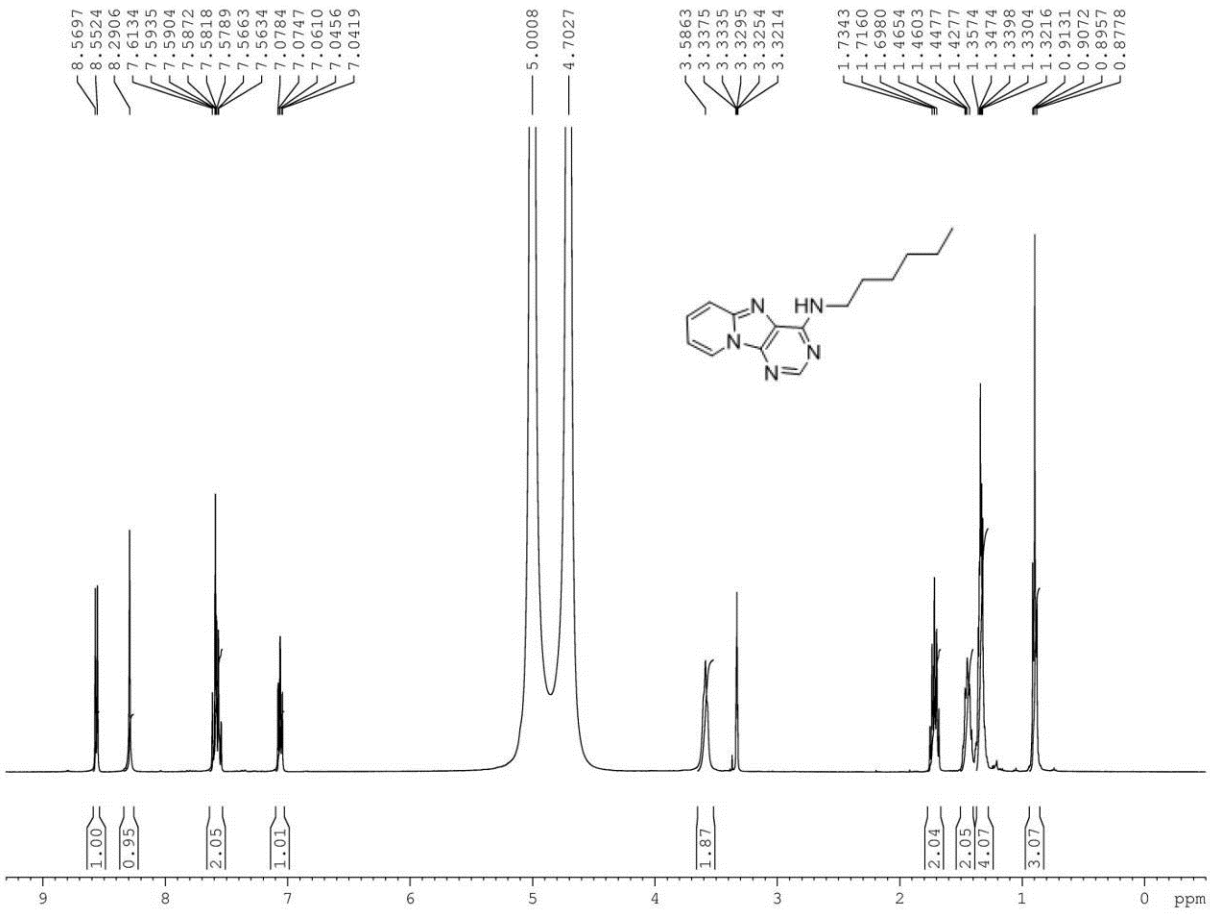
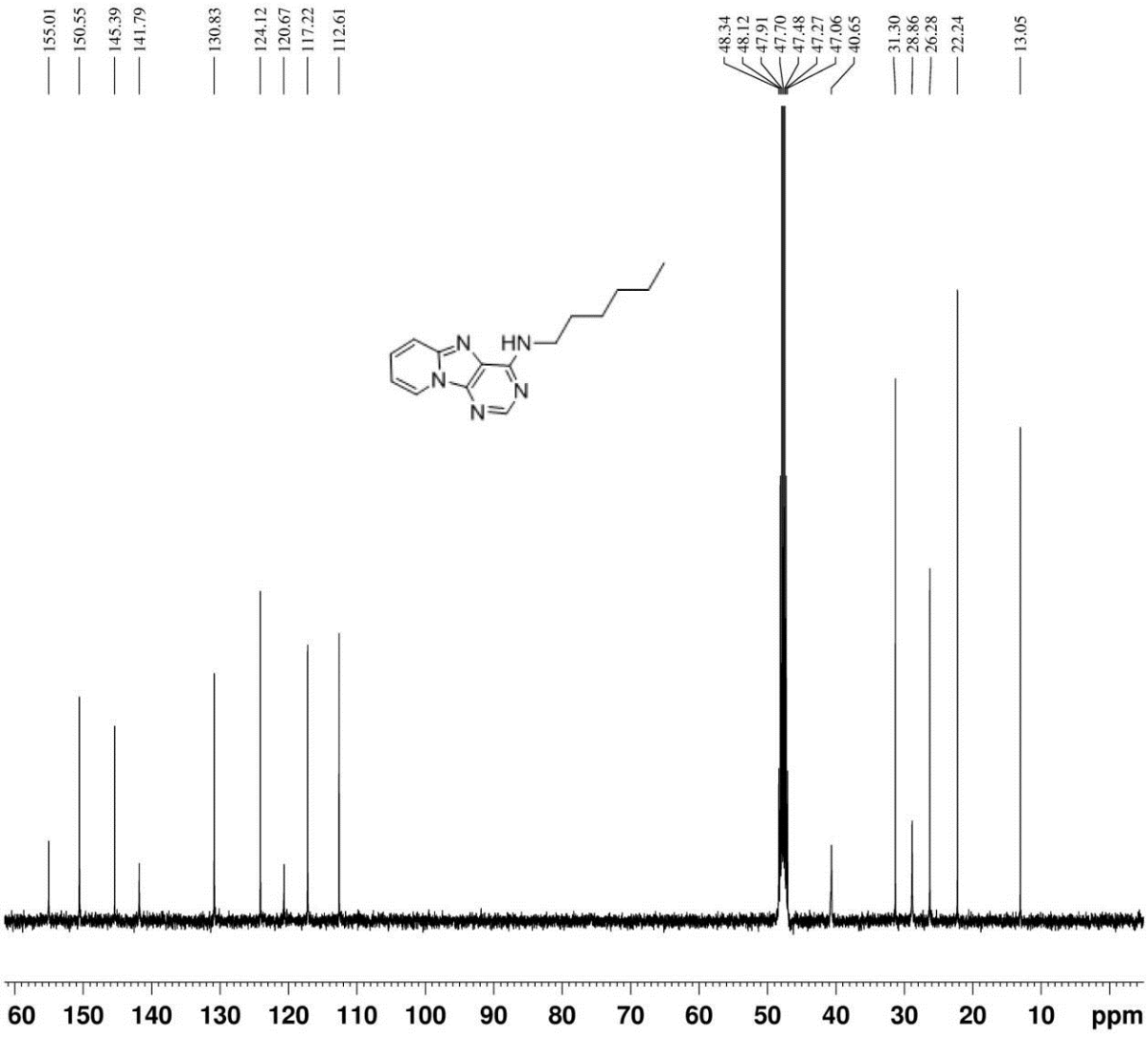
47.41
47.20
46.99
43.37
38.22
26.00
HN
N
60 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

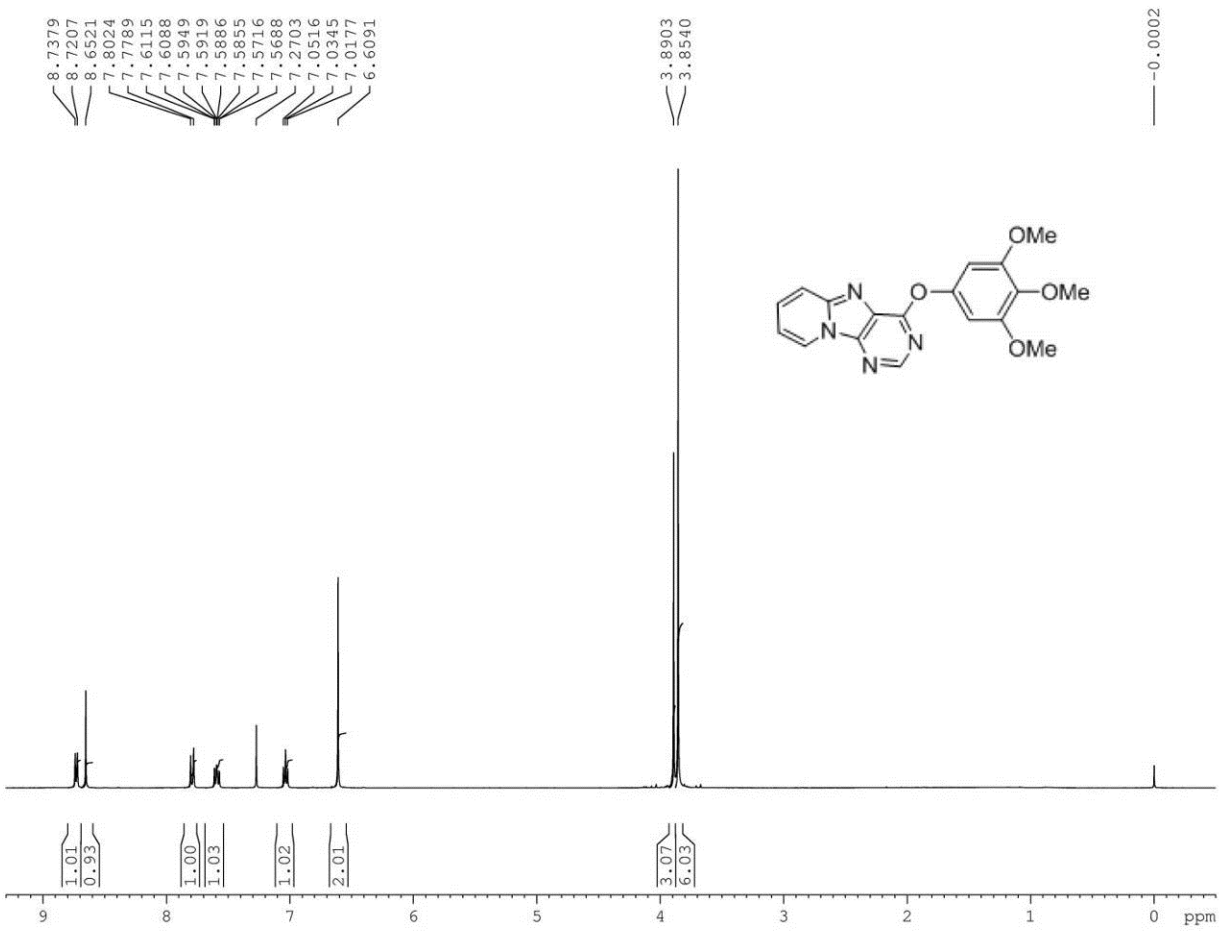
26: ^{1}H NMR


8.5697
8.5524
8.2906
7.6134
7.5935
7.5904
7.5872
7.5818
7.5789
7.5663
7.5634
7.0784
7.0747
7.0610
7.0456
7.0419
5.0008
4.7027
3.5863
3.3375
3.3335
3.3295
3.3254
3.3214
1.7343
1.7160
1.6980
1.4654
1.4603
1.4477
1.4277
1.3574
1.3474
1.3398
1.3304
1.3216
0.9131
0.9072
0.8957
0.8778
HN
N
N
N
1.00
0.95
2.05
1.01
1.87
2.04
2.05
4.07
3.07
9
8
7
6
5
4
3
2
1
0
ppm

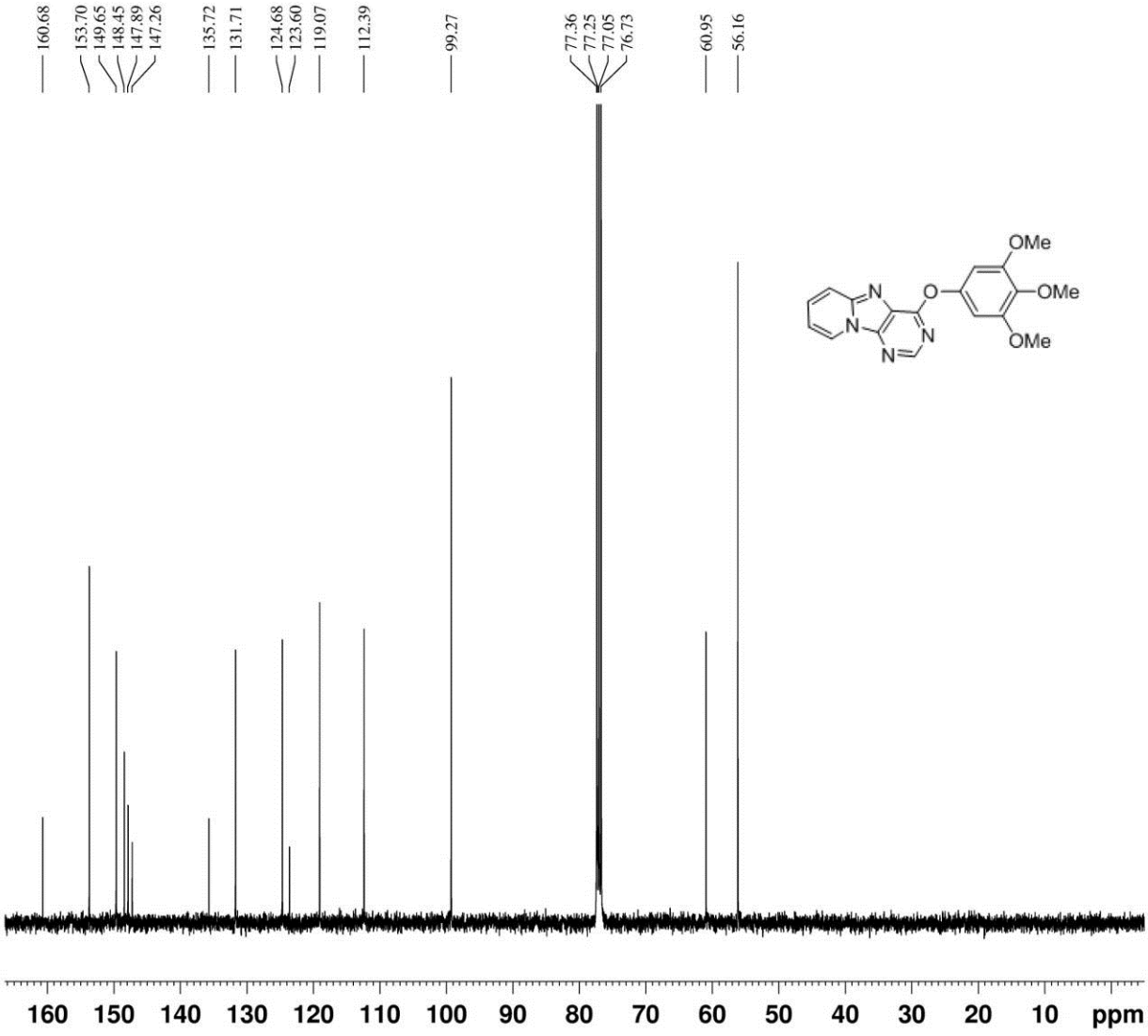
26: ^{13}C NMR


155.01
150.55
145.39
141.79
130.83
124.12
120.67
117.22
112.61
48.34
48.12
47.91
47.70
47.48
47.27
47.06
40.65
31.30
28.86
26.28
22.24
13.05
HN
N
N
N
N
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

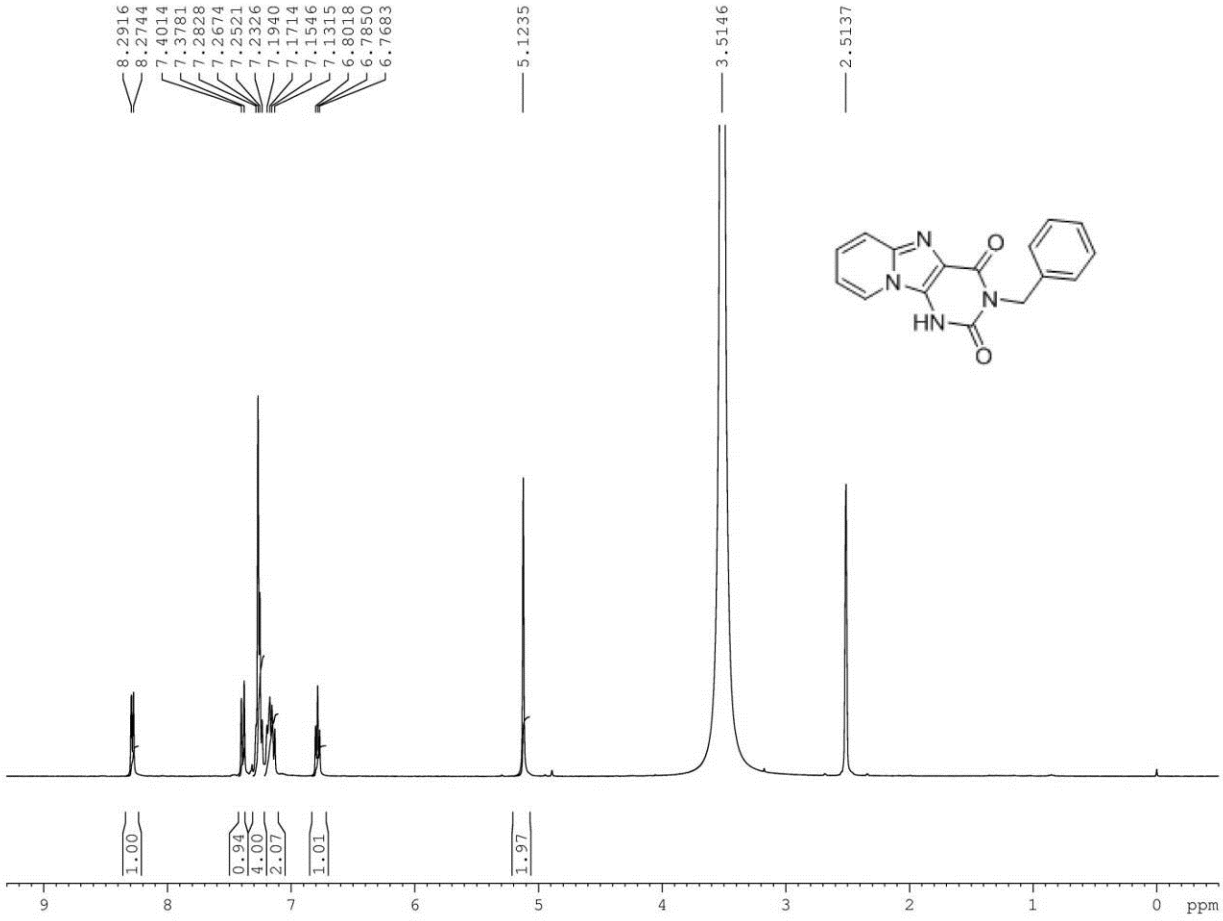
30: ^{1}H NMR


8.7379
8.7207
8.6521
7.8024
7.7789
7.6115
7.6088
7.5949
7.5919
7.5886
7.5855
7.5716
7.5688
7.2703
7.0516
7.0345
7.0177
6.6091
3.8903
3.8540
-0.0002
OMe
OMe
OMe
N
O
N
N
N
1.01
0.93
1.00
1.03
1.02
2.01
3.07
6.03
9
8
7
6
5
4
3
2
1
0
ppm

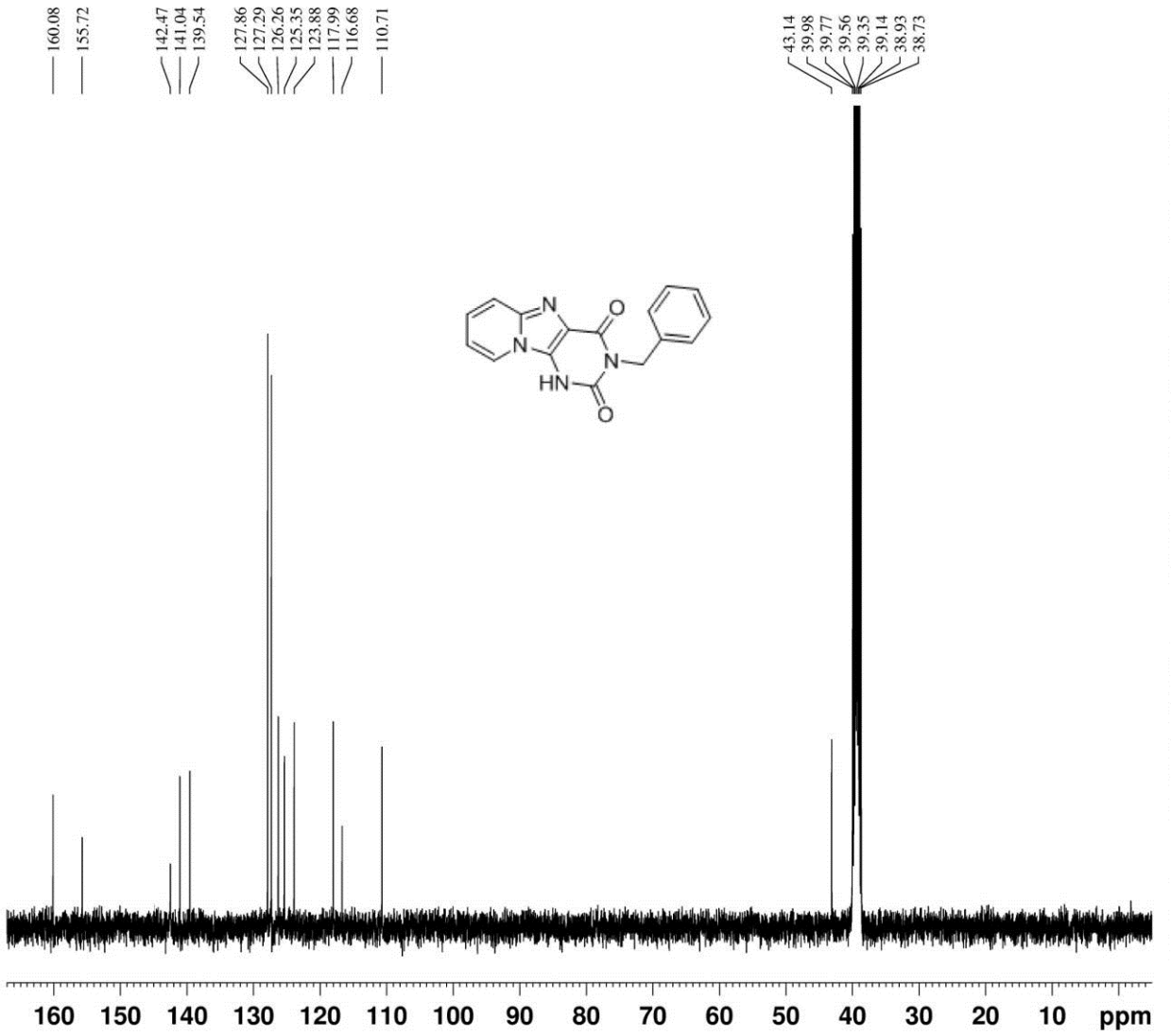
30: ^{13}C NMR


160.68
153.70
149.65
148.45
147.89
147.26
135.72
131.71
124.68
123.60
119.07
112.39
99.27
77.36
77.25
77.05
76.73
60.95
56.16
OMe
OMe
OMe
N
O
N
N
N
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

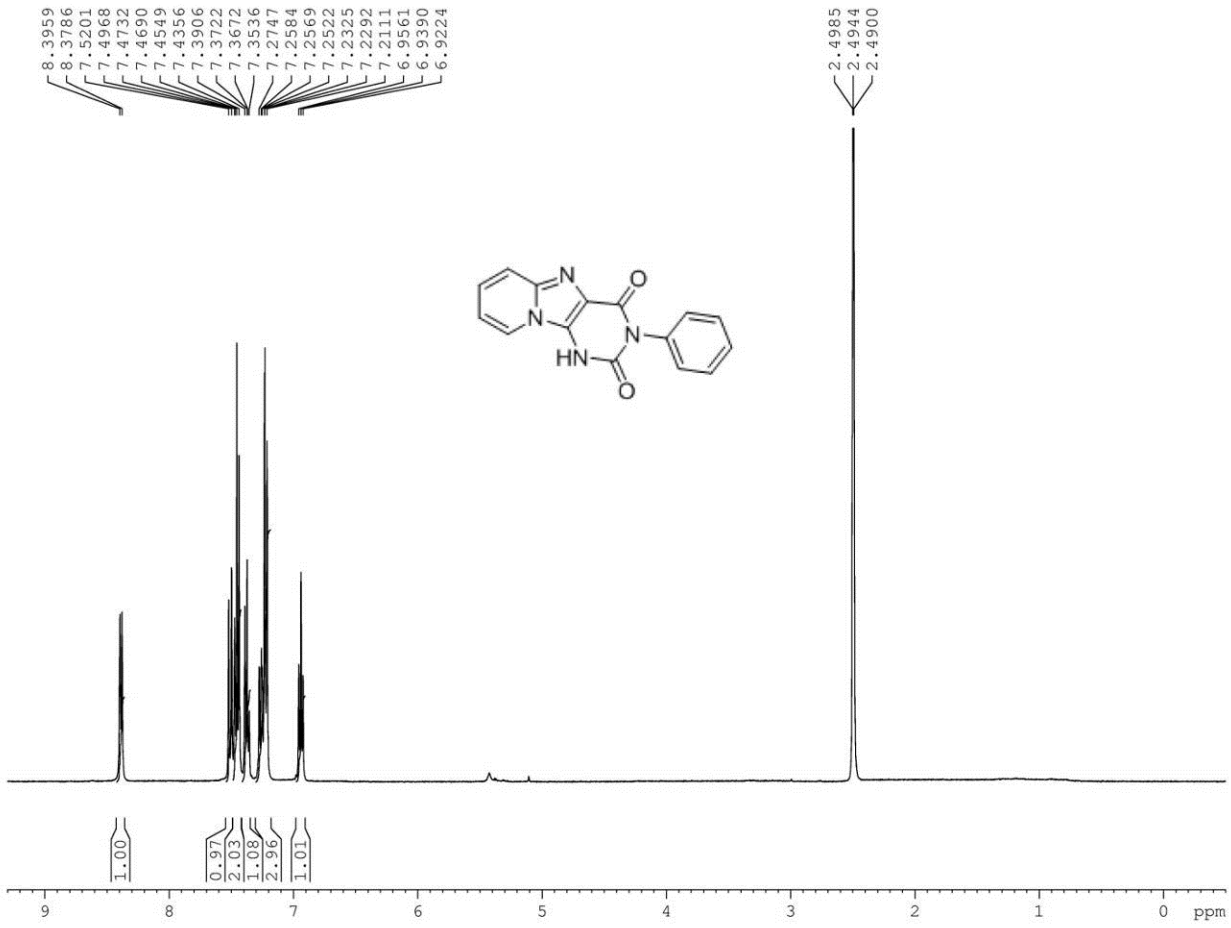
33: ^{1}H NMR


8.2916
8.2744
7.4014
7.3781
7.2828
7.2674
7.2521
7.2326
7.1940
7.1714
7.1546
7.1315
6.8018
6.7850
6.7683
5.1235
3.5146
2.5137
N
O
N
N
HN
O
1.00
0.94
4.00
2.07
1.01
1.97
9
8
7
6
5
4
3
2
1
0
ppm

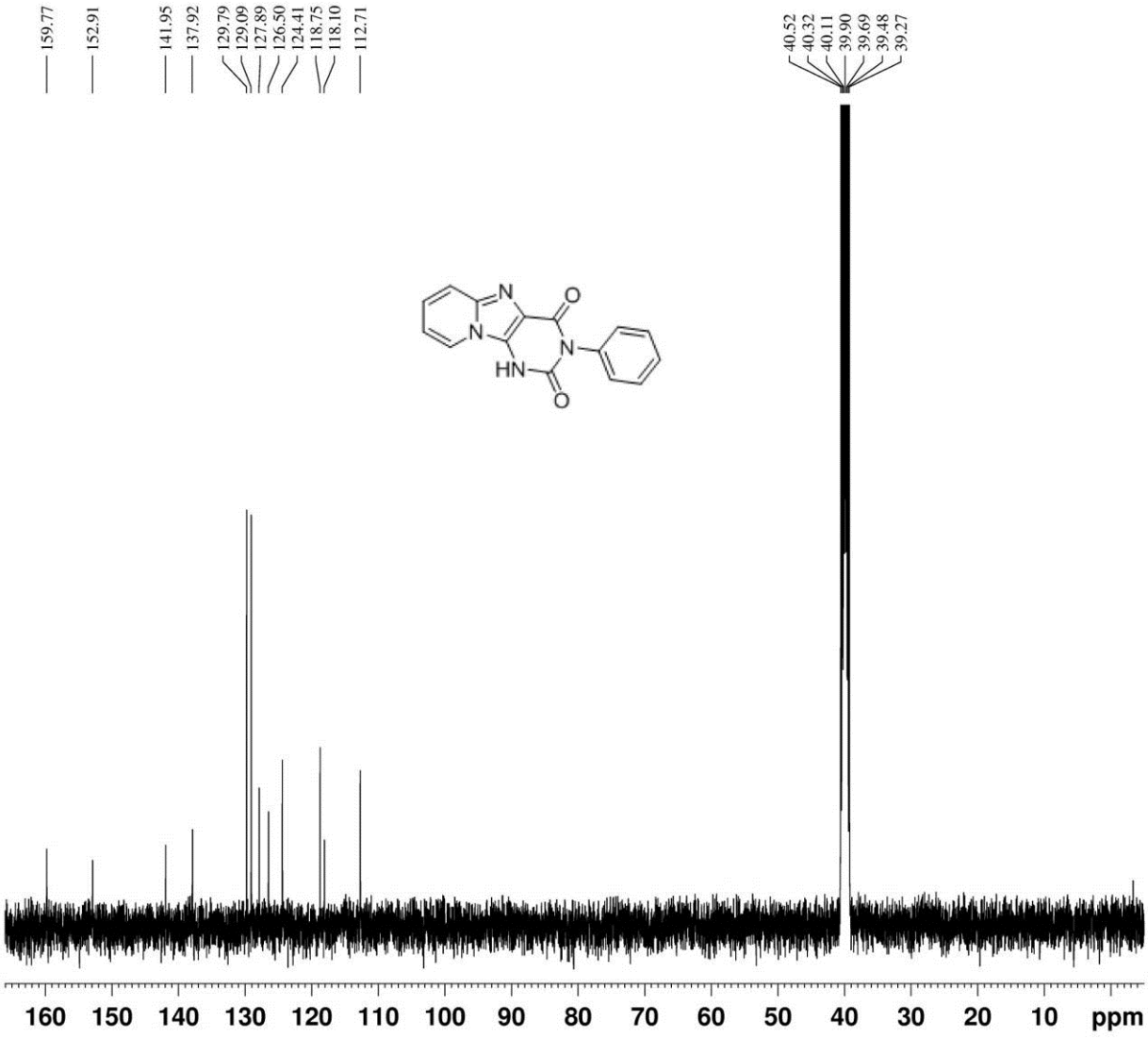
33: ^{1}H NMR


160.08
155.72
142.47
141.04
139.54
127.86
127.29
126.26
125.35
123.88
117.99
116.68
110.71
43.14
39.98
39.77
39.56
39.35
39.14
38.93
38.73
N
O
N
N
HN
O
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

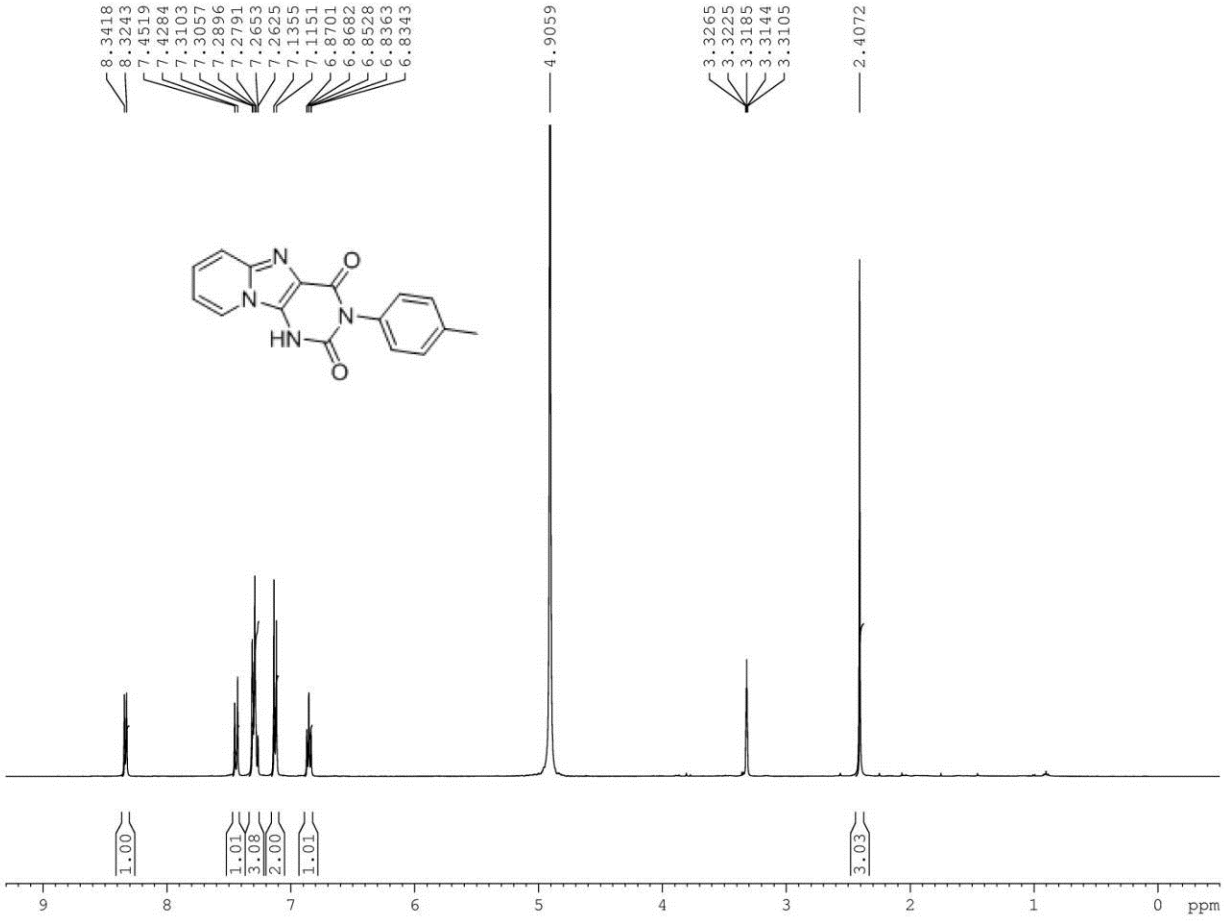
34: ^{1}H NMR


8.3959
8.3786
7.5201
7.4968
7.4732
7.4690
7.4549
7.4356
7.3906
7.3722
7.3672
7.3536
7.2747
7.2584
7.2569
7.2522
7.2325
7.2292
7.2111
6.9561
6.9390
6.9224
2.4985
2.4944
2.4900
N
O
N
HN
O
1.00
0.97
2.03
1.08
2.96
1.01
9
8
7
6
5
4
3
2
1
0
ppm

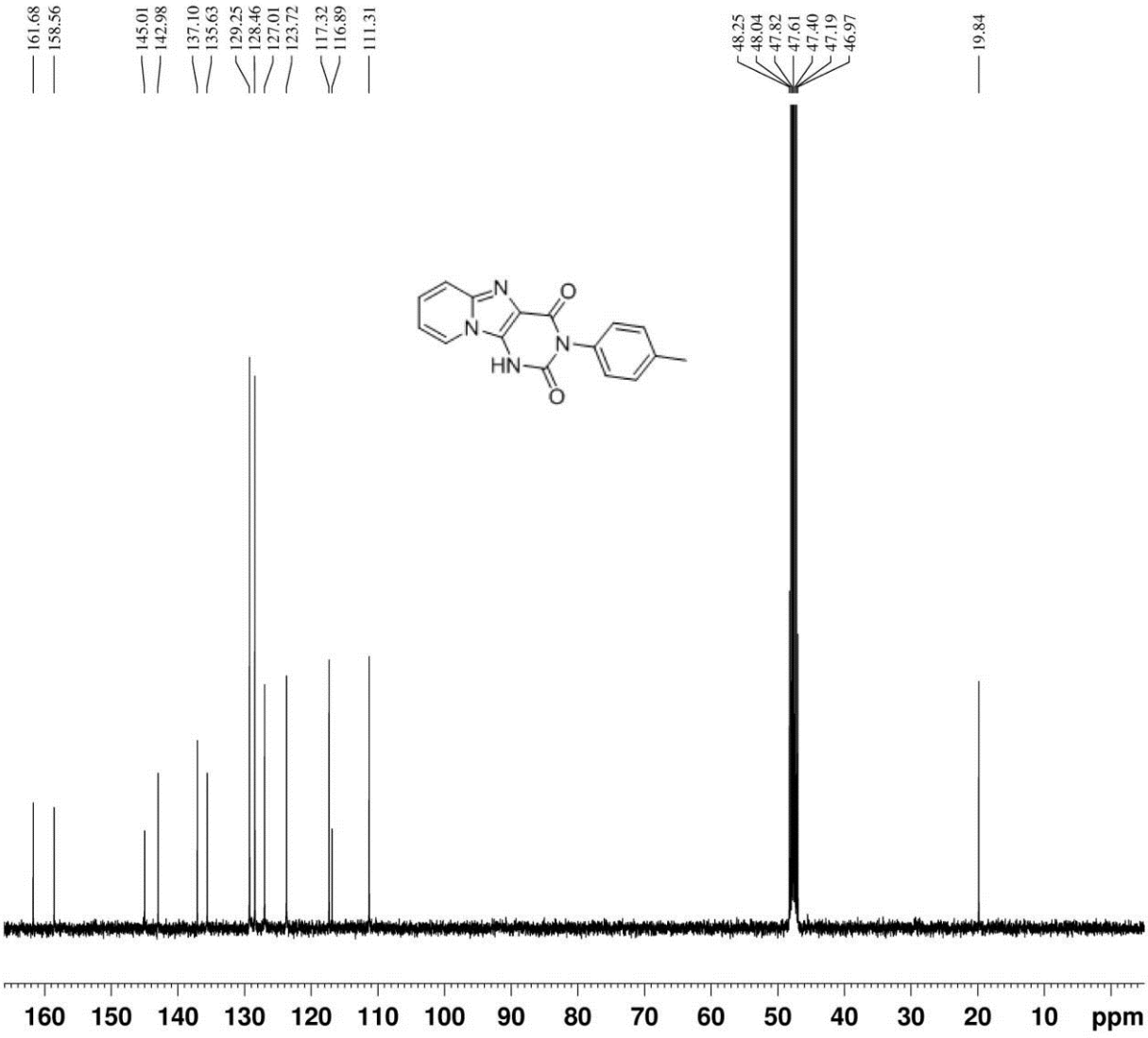
34: ^{13}C NMR


159.77
152.91
141.95
137.92
129.79
129.09
127.89
126.50
124.41
118.75
118.10
112.71
40.52
40.32
40.11
39.90
39.69
39.48
39.27
N
O
N
N
HN
O
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

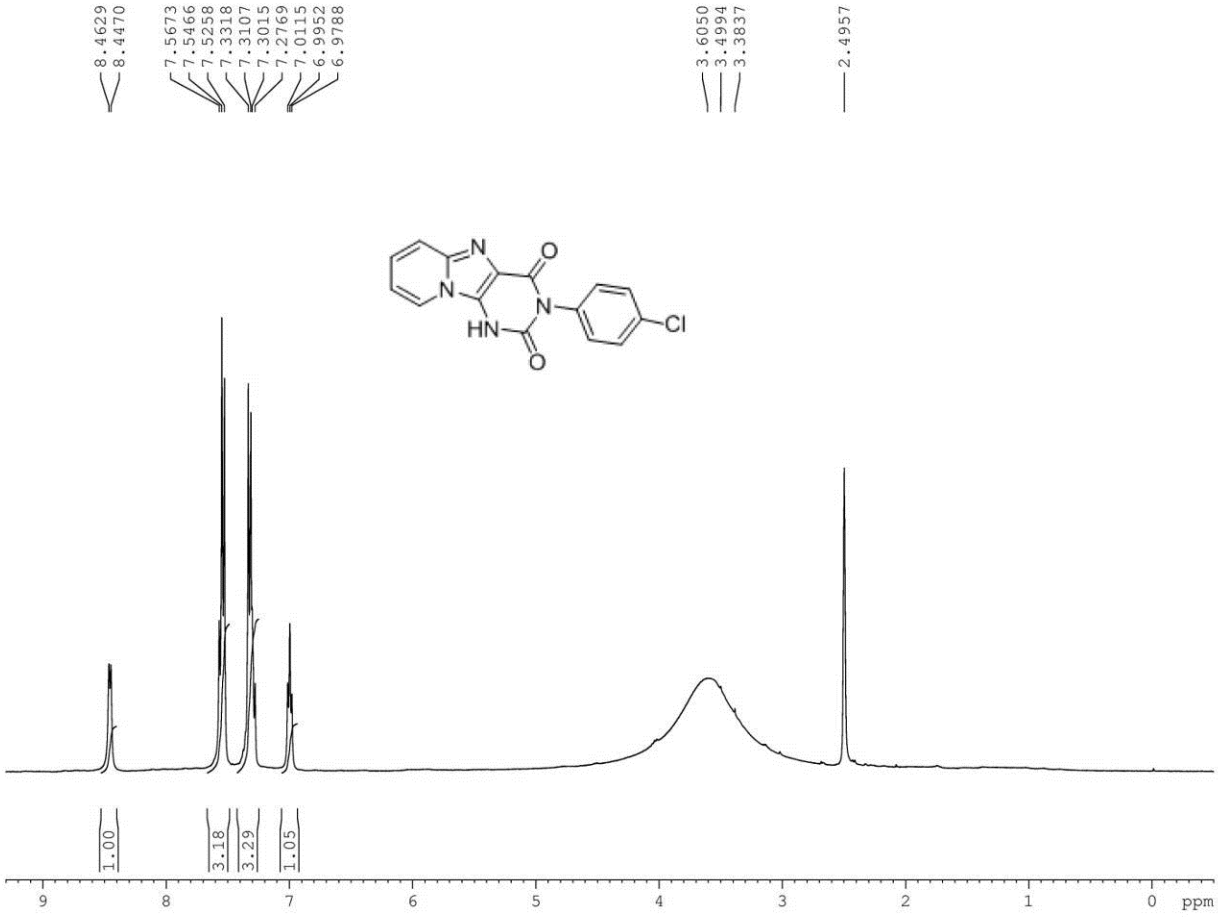
35: ^{1}H NMR


8.3418
8.3243
7.4519
7.4284
7.3103
7.3057
7.2896
7.2791
7.2653
7.2625
7.1355
7.1151
6.8701
6.8682
6.8528
6.8363
6.8343
4.9059
3.3265
3.3225
3.3185
3.3144
3.3105
2.4072
N
O
N
HN
O
1.00
1.01
3.08
2.00
1.01
3.03
9
8
7
6
5
4
3
2
1
0
ppm

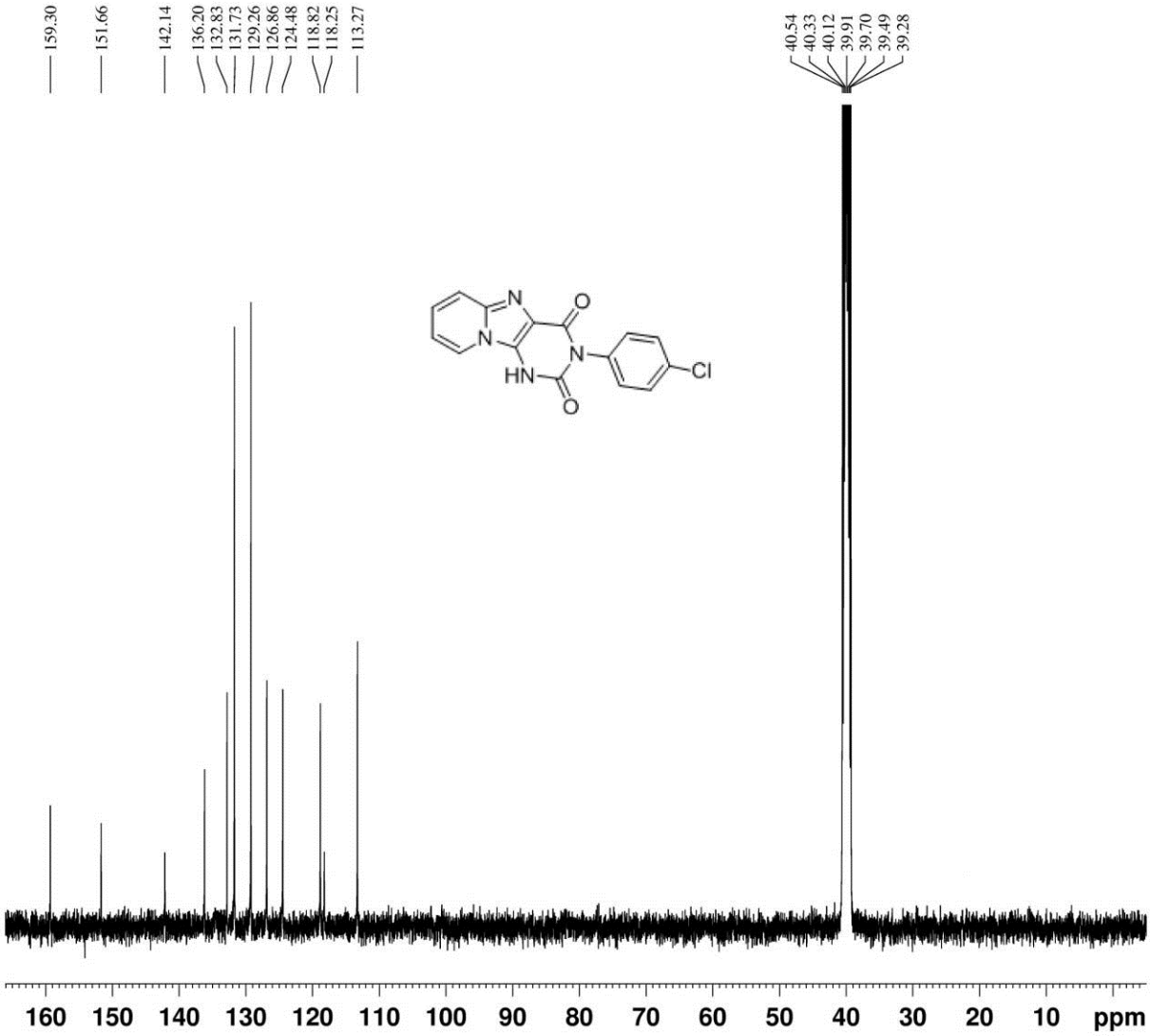
35: ^{13}C NMR


161.68
158.56
145.01
142.98
137.10
135.63
129.25
128.46
127.01
123.72
117.32
116.89
111.31
48.25
48.04
47.82
47.61
47.40
47.19
46.97
19.84
N
O
N
N
HN
O
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

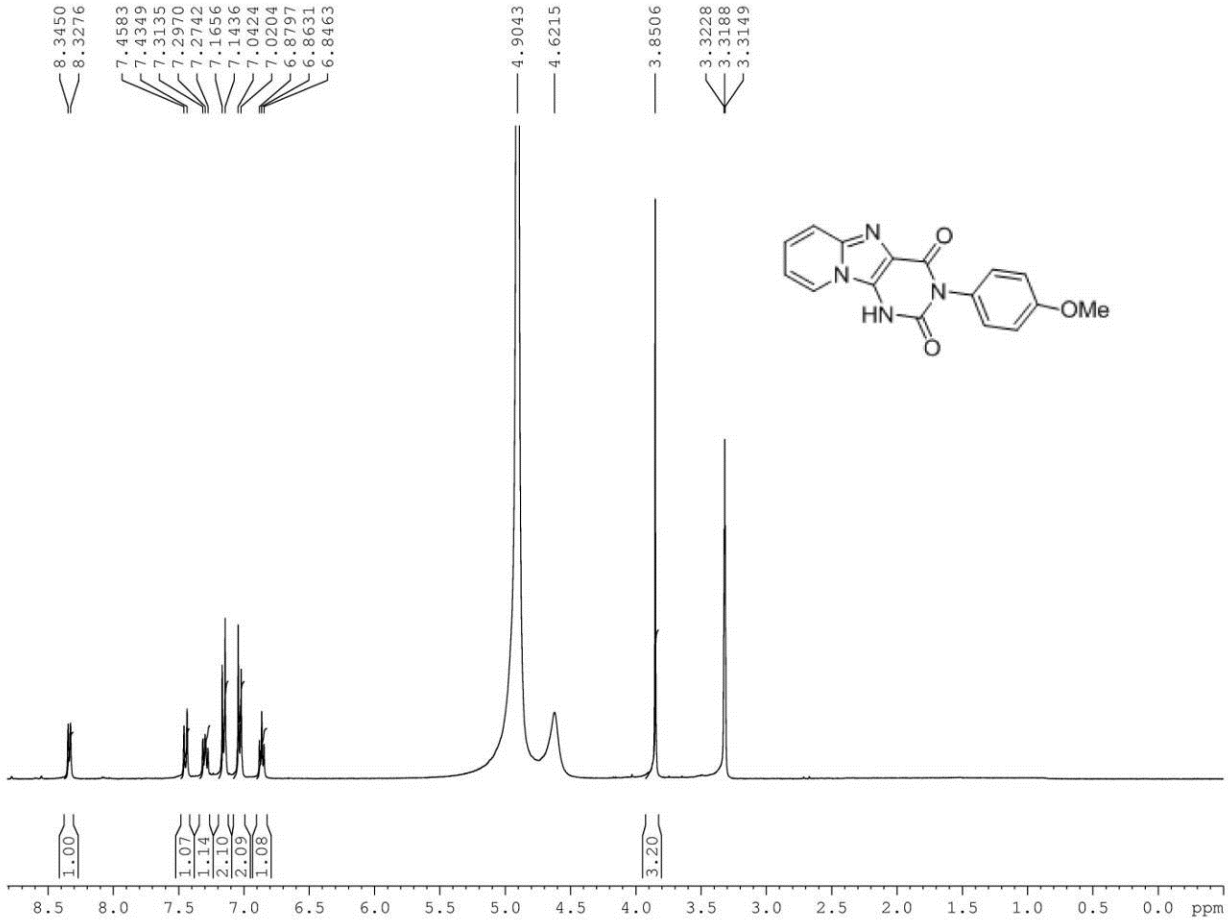
36: ^{1}H NMR


8.4629
8.4470
7.5673
7.5466
7.5258
7.3318
7.3107
7.3015
7.2769
7.0115
6.9952
6.9788
3.6050
3.4994
3.3837
2.4957
N
O
N
N
HN
O
Cl
1.00
3.18
3.29
1.05
9
8
7
6
5
4
3
2
1
0
ppm

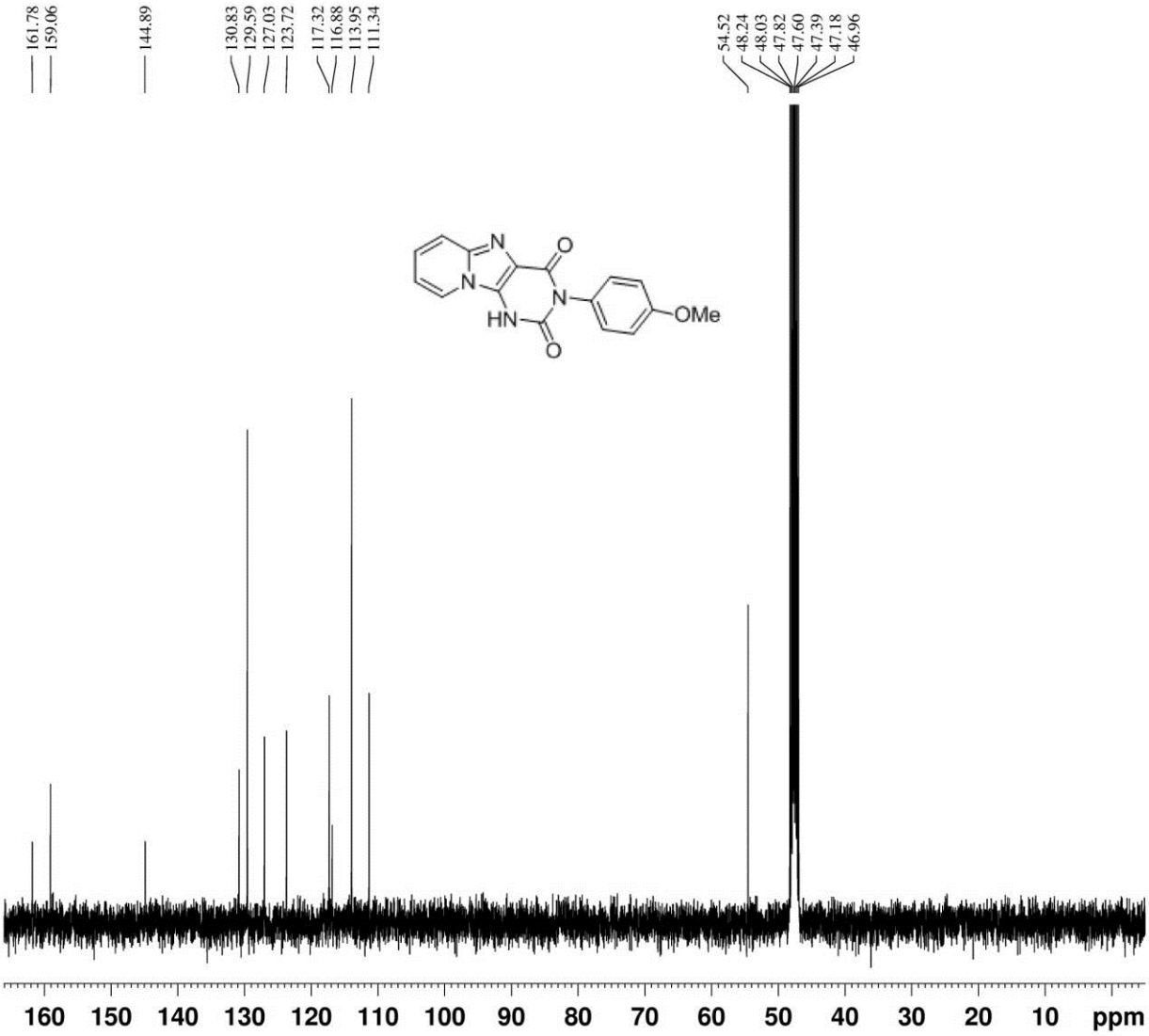
36: ^{13}C NMR


159.30
151.66
142.14
136.20
132.83
131.73
129.26
126.86
124.48
118.82
118.25
113.27
40.54
40.33
40.12
39.91
39.70
39.49
39.28
N
O
N
N
HN
O
Cl
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

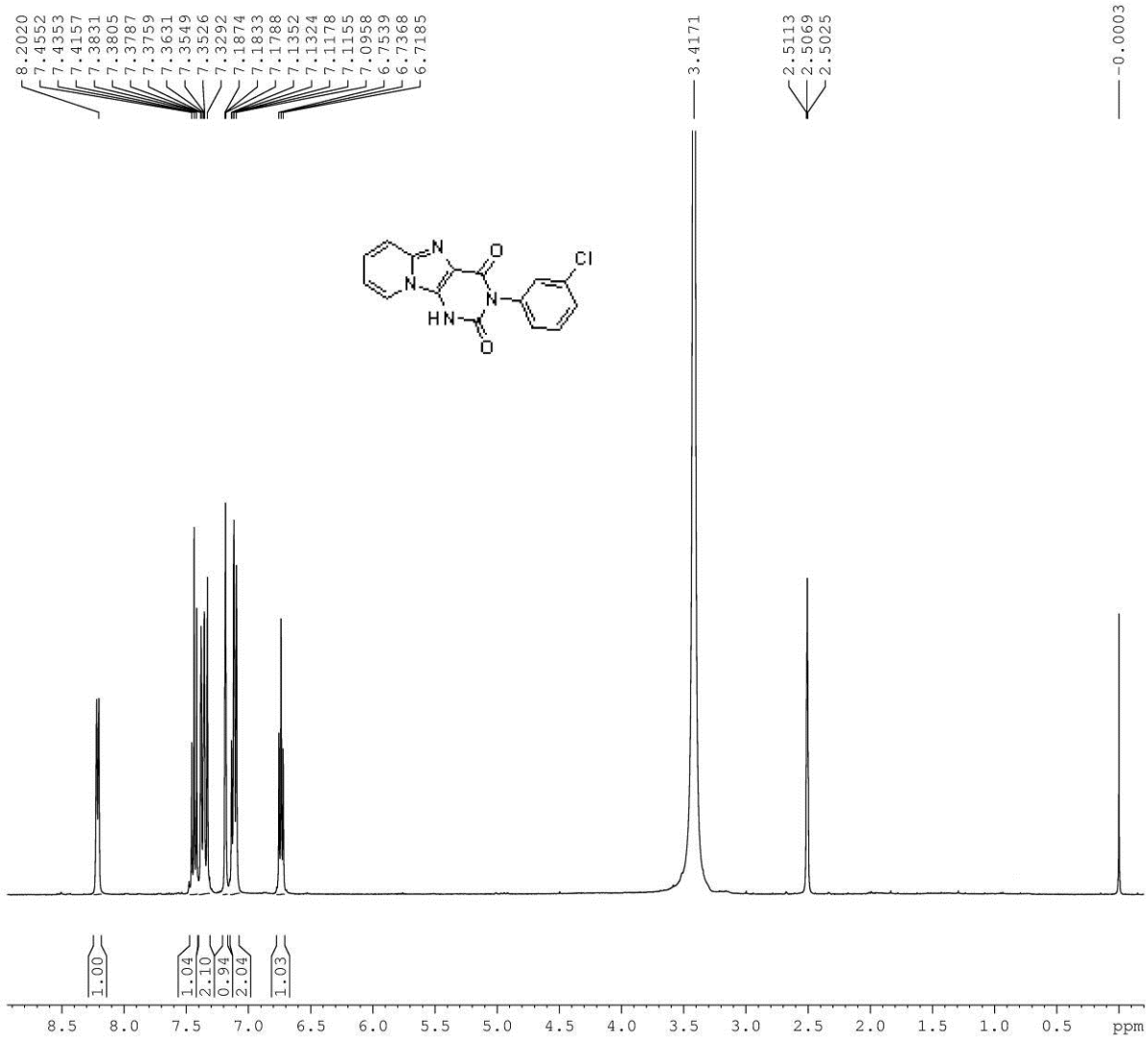
37: ^{1}H NMR


8.3450
8.3276
7.4583
7.4349
7.3135
7.2970
7.2742
7.1656
7.1436
7.0424
7.0204
6.8797
6.8631
6.8463
4.9043
4.6215
3.8506
3.3228
3.3188
3.3149
N
O
N
N
HN
O
OMe
1.00
1.07
1.14
2.10
2.09
1.08
3.20
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

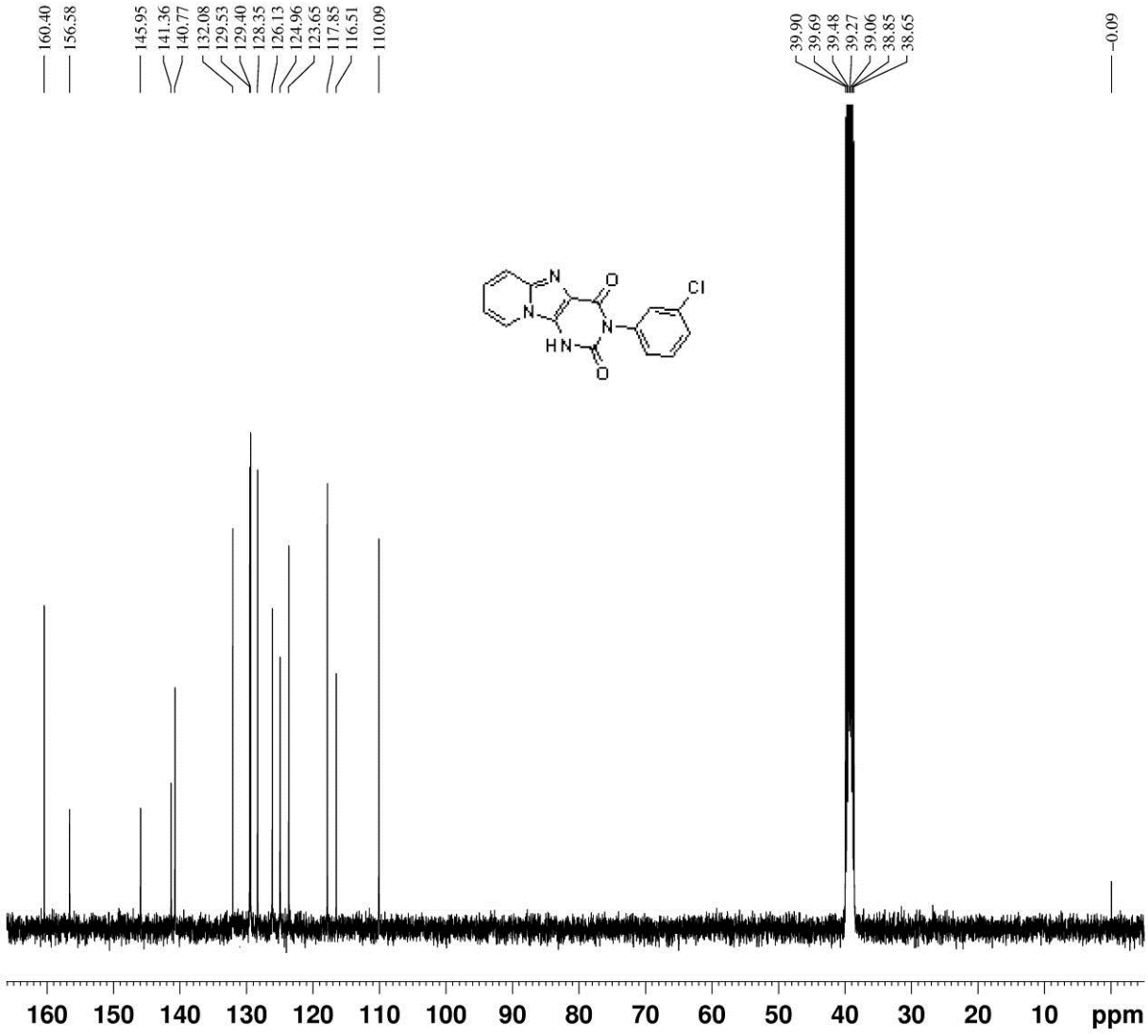
37: ^{13}C NMR


161.78
159.06
144.89
130.83
129.59
127.03
123.72
117.32
116.88
113.95
111.34
54.52
48.24
48.03
47.82
47.60
47.39
47.18
46.96
N
O
N
N
HN
O
OMe
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

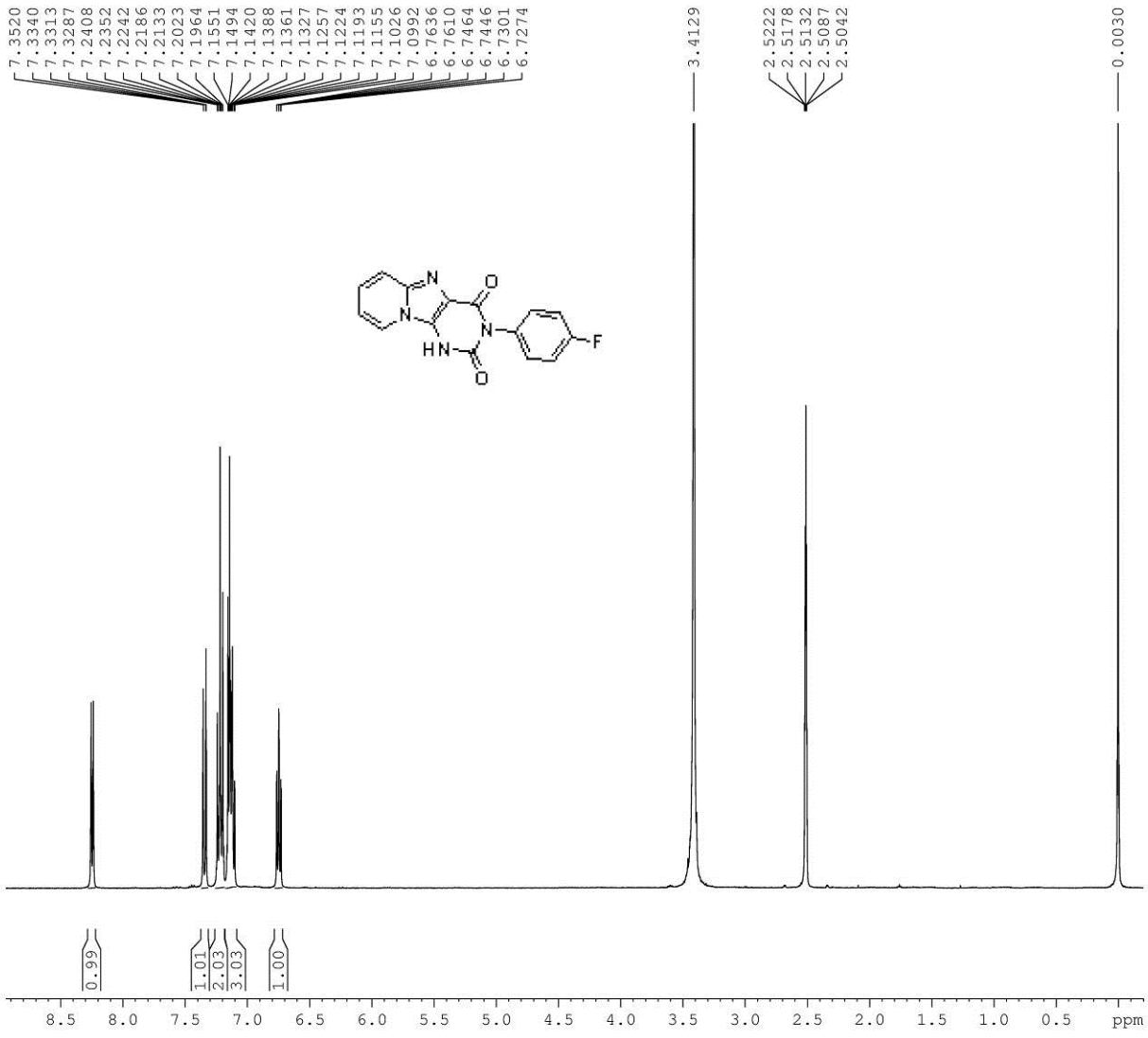
38: ^{1}H NMR


8.2020
7.4552
7.4353
7.4157
7.3831
7.3805
7.3787
7.3759
7.3631
7.3549
7.3526
7.3292
7.1874
7.1833
7.1788
7.1352
7.1324
7.1178
7.1155
7.0958
6.7539
6.7368
6.7185
3.4171
2.5113
2.5069
2.5025
0.0003
N
O
Cl
N
HN
O
1.00
1.04
2.10
0.94
2.04
1.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

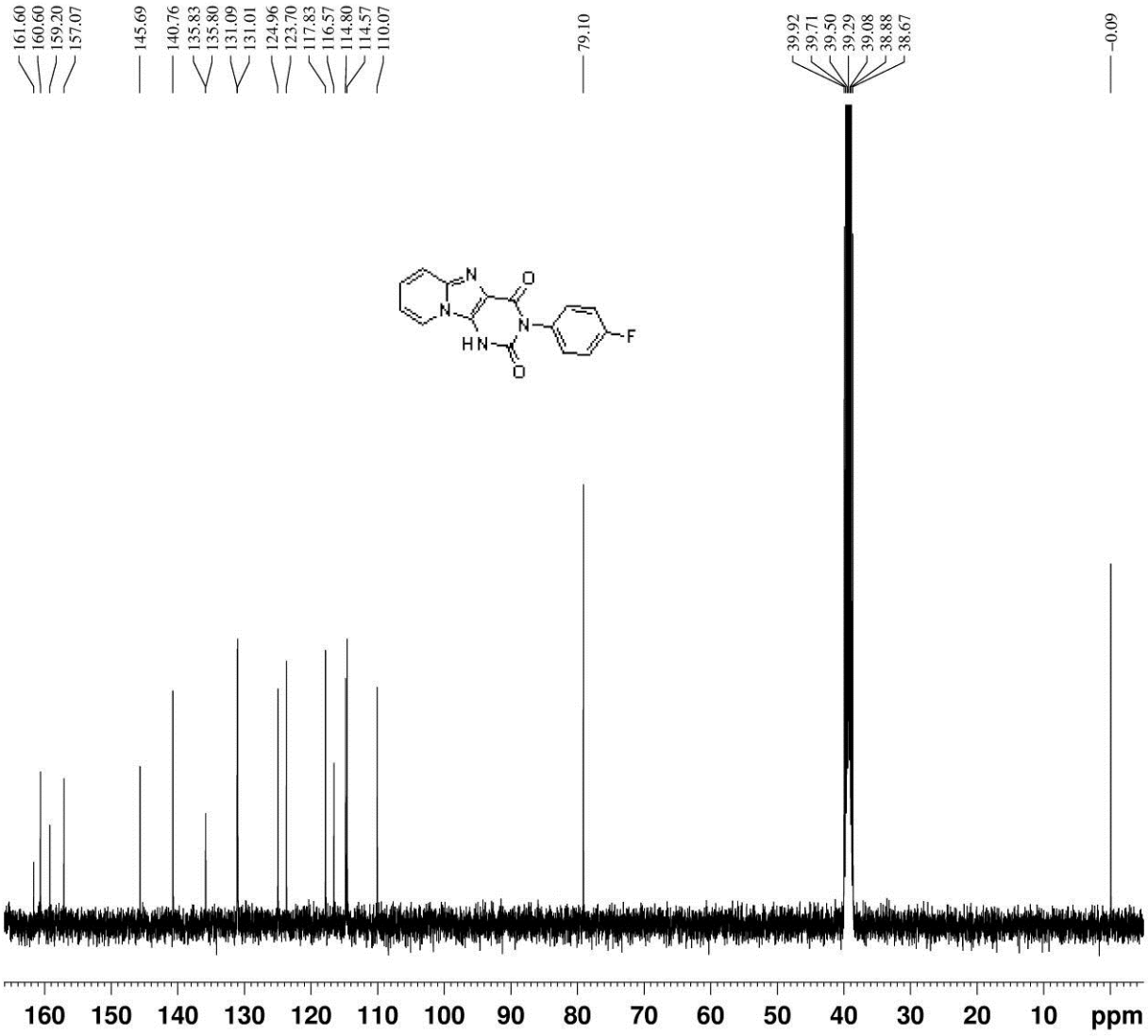
38: ^{13}C NMR


160.40
156.58
145.95
141.36
140.77
132.08
129.53
129.40
128.35
126.13
124.96
123.65
117.85
116.51
110.09
39.90
39.69
39.48
39.27
39.06
38.85
38.65
-0.09
N
O
Cl
N
HN
O
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

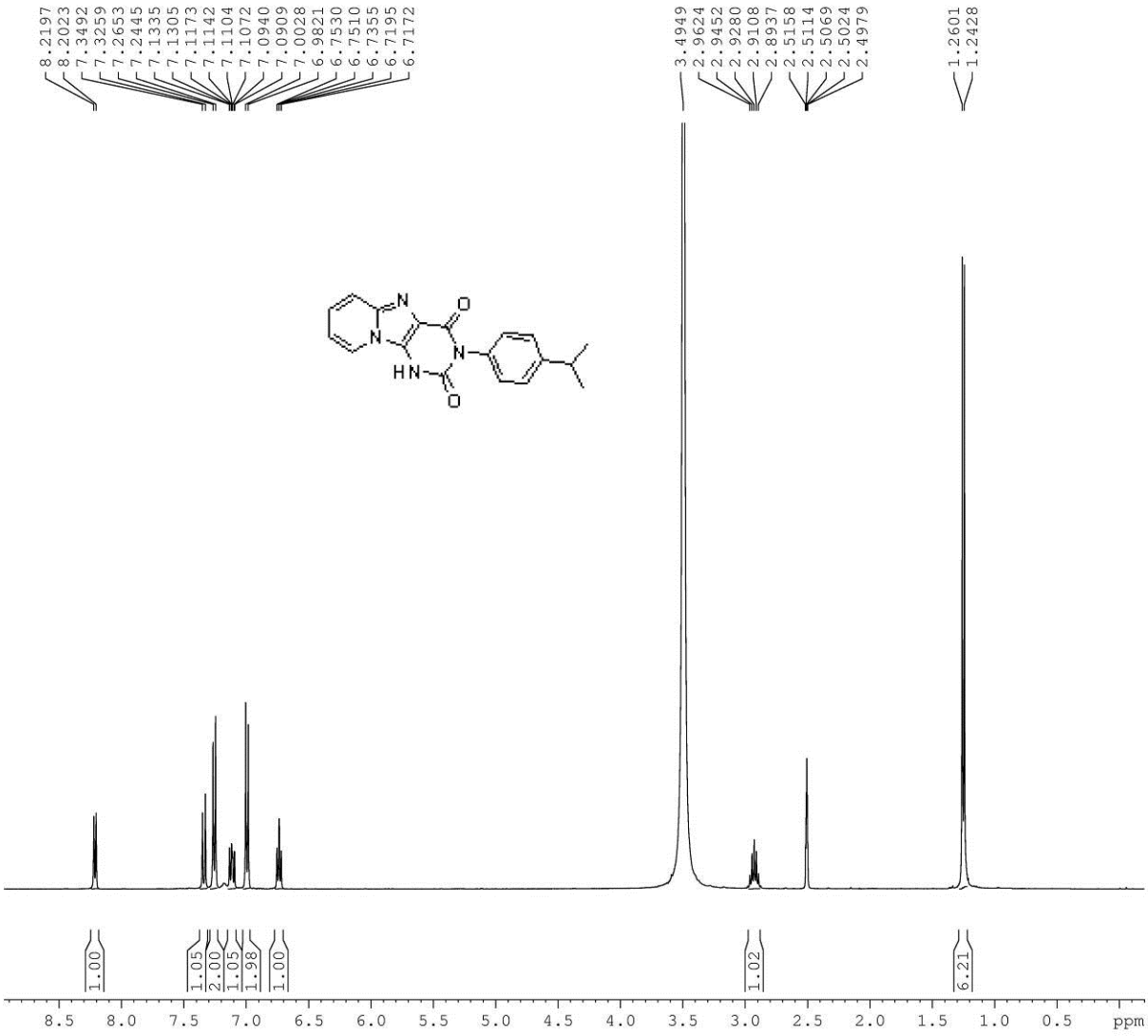
39: ^{1}H NMR


7.3520
7.3340
7.3313
7.3287
7.2408
7.2352
7.2242
7.2186
7.2133
7.2023
7.1964
7.1551
7.1494
7.1420
7.1388
7.1361
7.1327
7.1257
7.1224
7.1193
7.1155
7.1026
7.0992
6.7636
6.7610
6.7464
6.7446
6.7301
6.7274
3.4129
2.5222
2.5178
2.5132
2.5087
2.5042
0.0030
N
O
N
N
HN
O
F
0.99
1.01
2.03
3.03
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

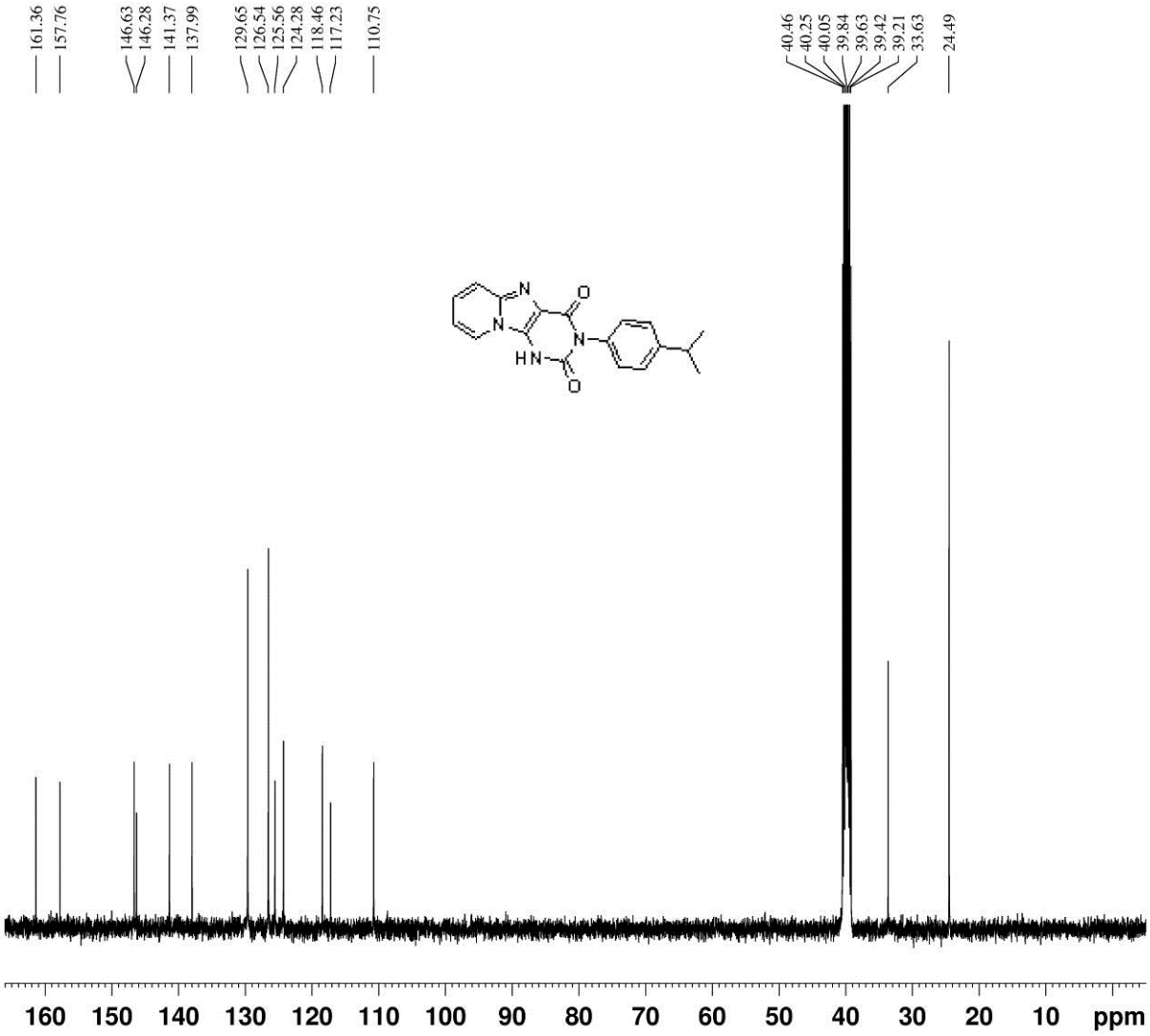
39: ^{13}C NMR


161.60
160.60
159.20
157.07
145.69
140.76
135.83
135.80
131.09
131.01
124.96
123.70
117.83
116.57
114.80
114.57
110.07
79.10
39.92
39.71
39.50
39.29
39.08
38.88
38.67
-0.09
N
O
N
N
HN
O
F
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

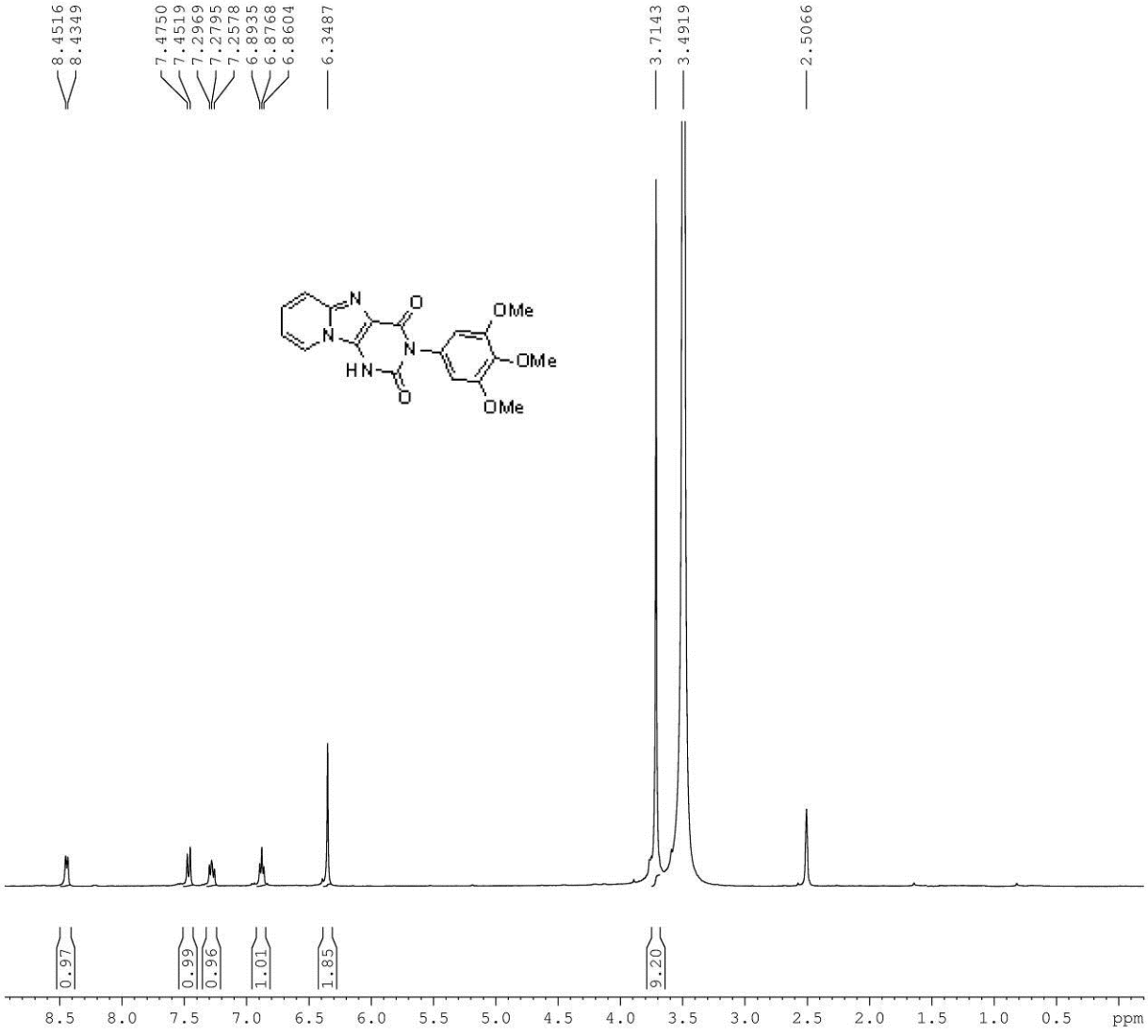
40: ^{1}H NMR


8.2197
8.2023
7.3492
7.3259
7.2653
7.2445
7.1335
7.1305
7.1173
7.1142
7.1104
7.1072
7.0940
7.0909
7.0028
6.9821
6.7530
6.7510
6.7355
6.7195
6.7172
3.4949
2.9624
2.9452
2.9280
2.9108
2.8937
2.5158
2.5114
2.5069
2.5024
2.4979
1.2601
1.2428
1.00
1.05
2.00
1.05
1.98
1.00
1.02
6.21
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

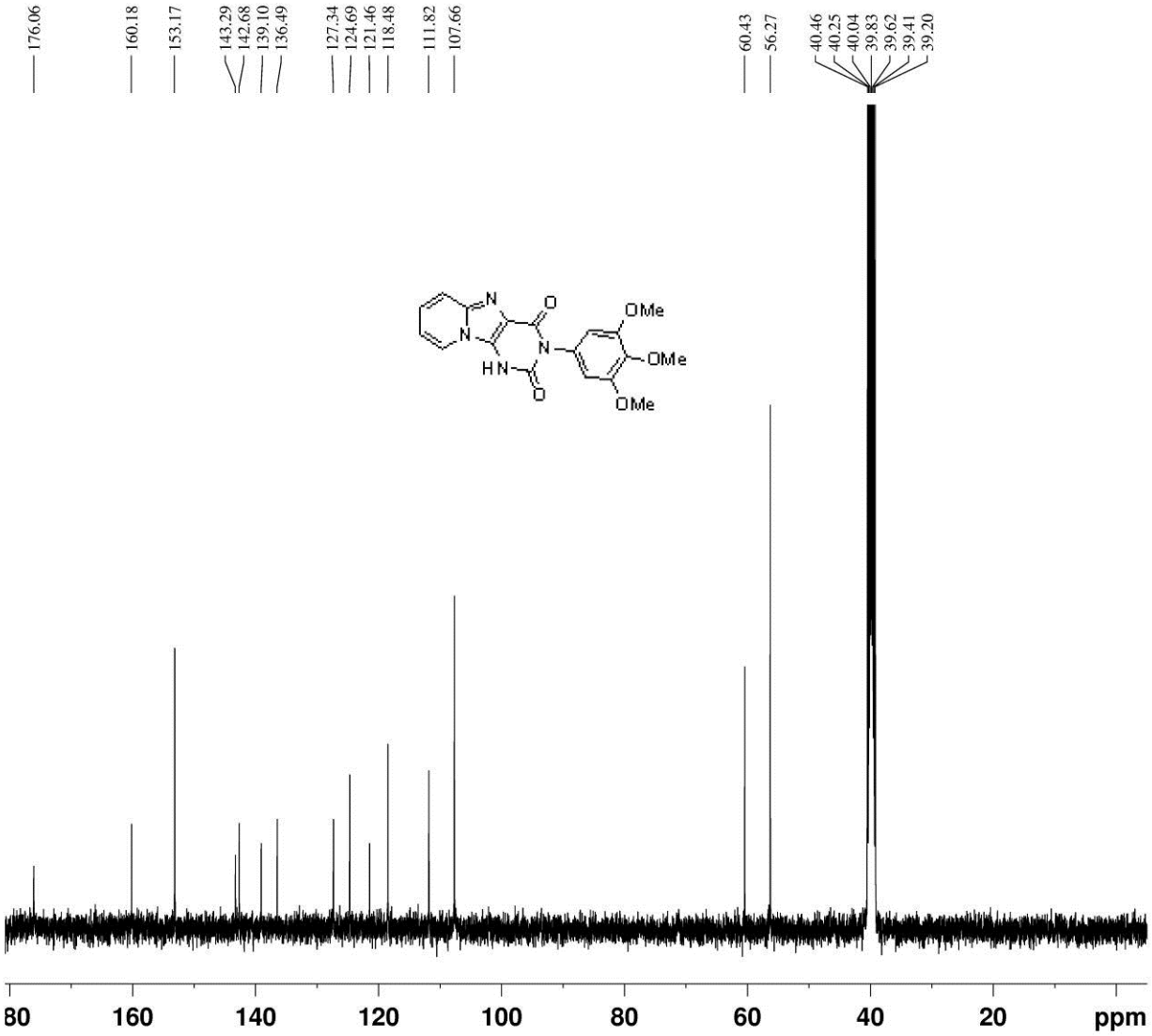
40: ^{13}C NMR


161.36
157.76
146.63
146.28
141.37
137.99
129.65
126.54
125.56
124.28
118.46
117.23
110.75
40.46
40.25
40.05
39.84
39.63
39.42
39.21
33.63
24.49
N
O
N
HN
O
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

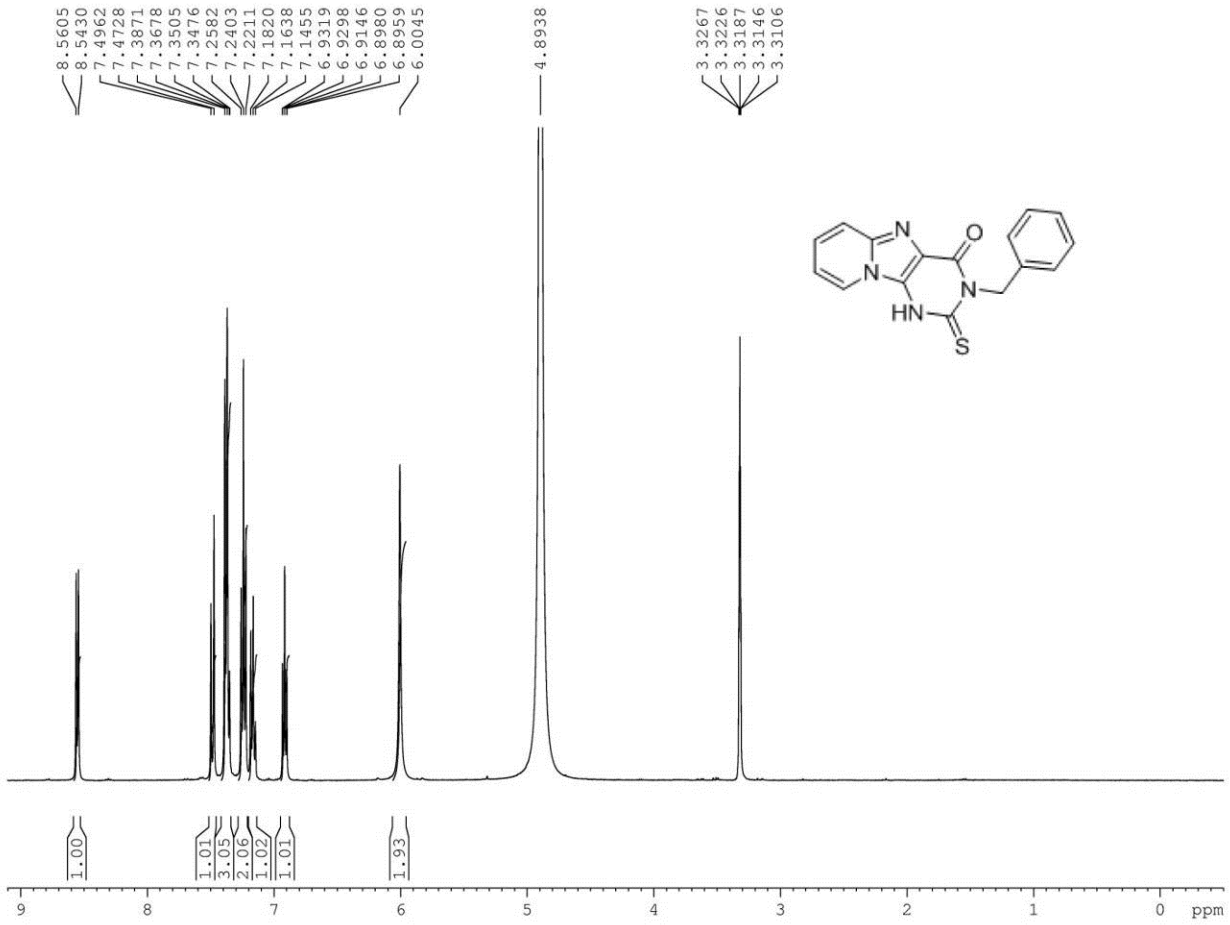
41: ^{1}H NMR


8.4516
8.4349
7.4750
7.4519
7.2969
7.2795
7.2578
6.8935
6.8768
6.8604
6.3487
3.7143
3.4919
2.5066
OMe
OMe
OMe
HN
0.97
0.99
0.96
1.01
1.85
9.20
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

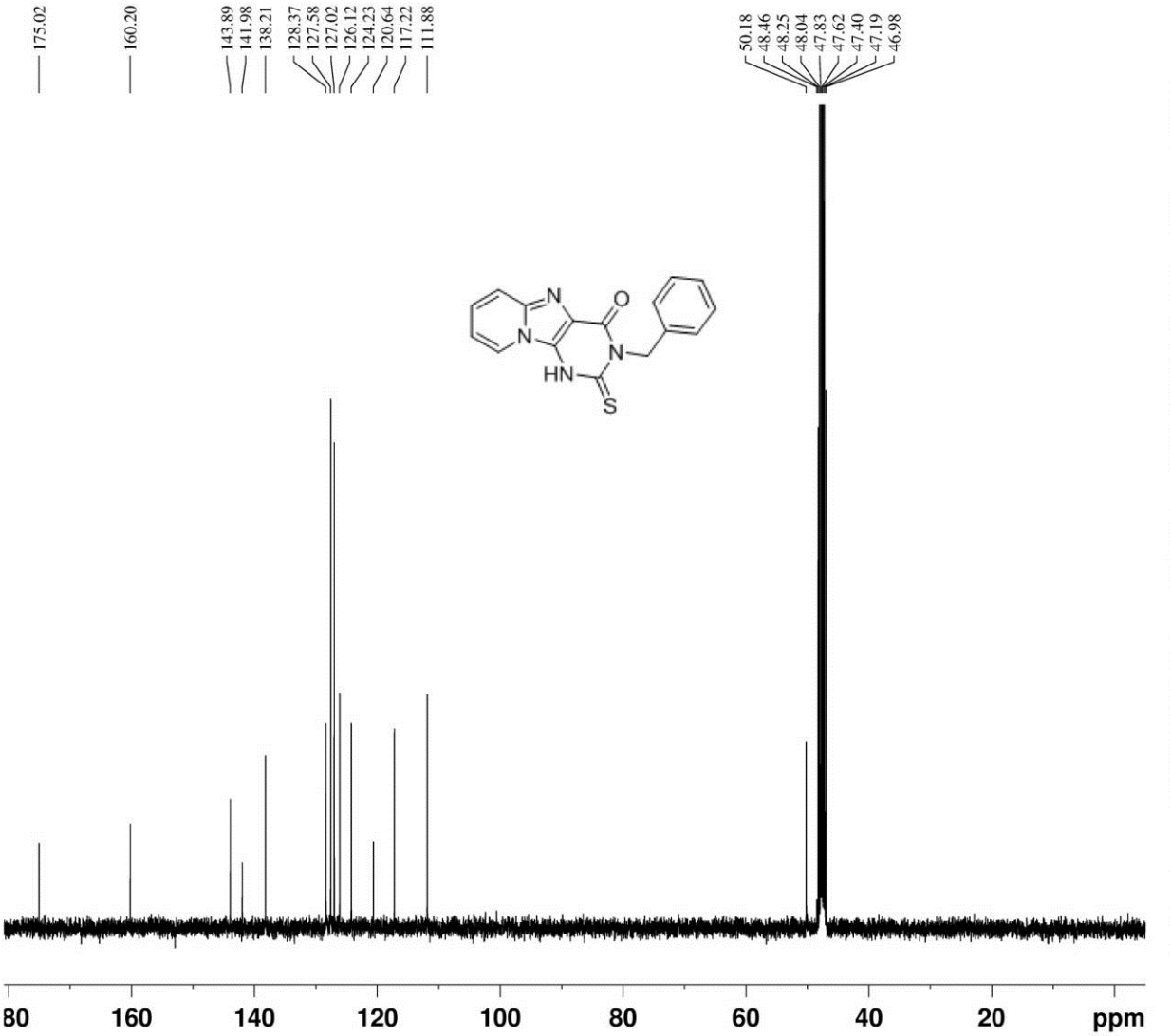
41: ^{13}C NMR


176.06
160.18
153.17
143.29
142.68
139.10
136.49
127.34
124.69
121.46
118.48
111.82
107.66
60.43
56.27
40.46
40.25
40.04
39.83
39.62
39.41
39.20
N
O
N
N
HN
O
OMe
OMe
OMe
80
160
140
120
100
80
60
40
20
ppm

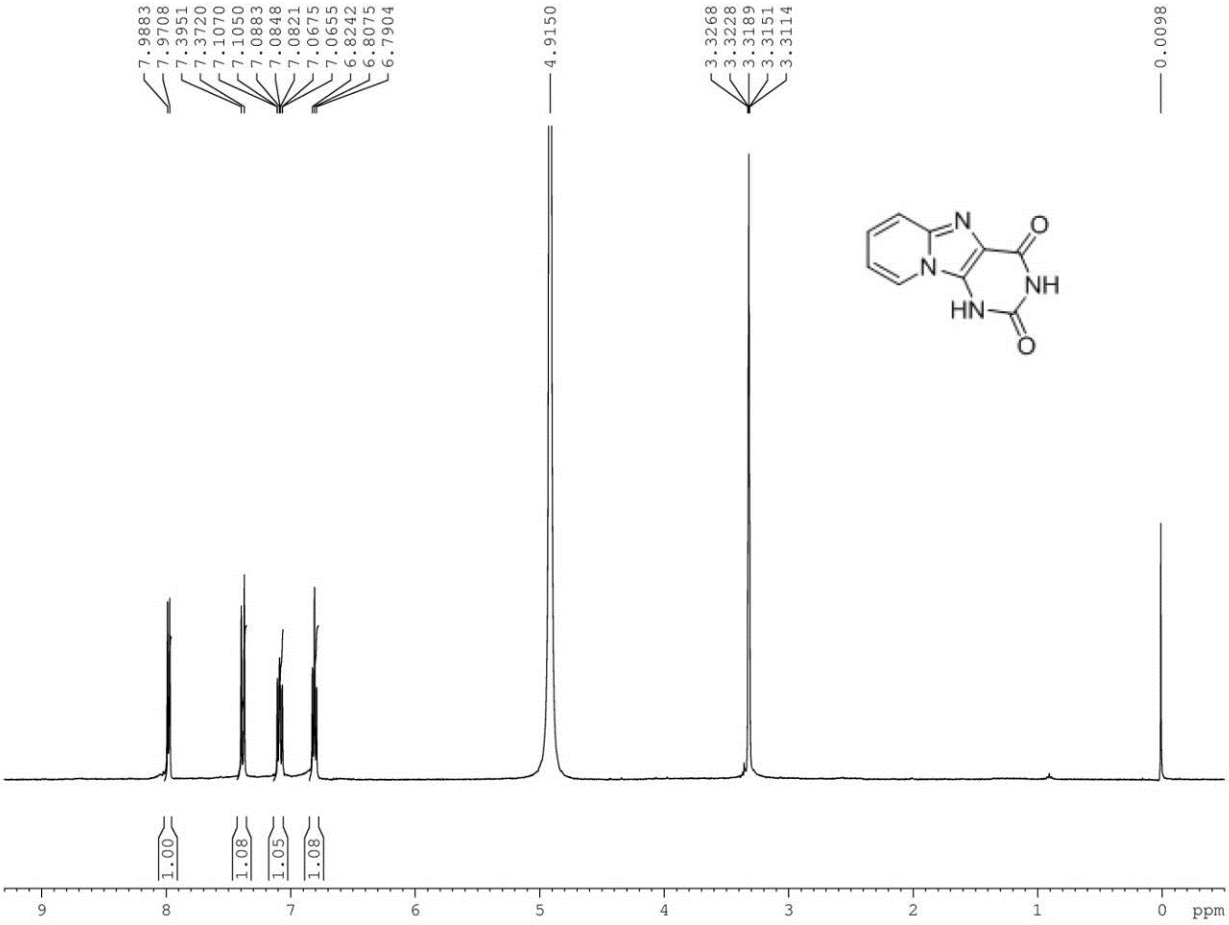
42: ^{1}H NMR


8.5605
8.5430
7.4962
7.4728
7.3871
7.3678
7.3505
7.3476
7.2582
7.2403
7.2211
7.1820
7.1638
7.1455
6.9319
6.9298
6.9146
6.8980
6.8959
6.0045
4.8938
3.3267
3.3226
3.3187
3.3146
3.3106
N
O
N
N
HN
S
1.00
1.01
3.05
2.06
1.02
1.01
1.93
9
8
7
6
5
4
3
2
1
0
ppm

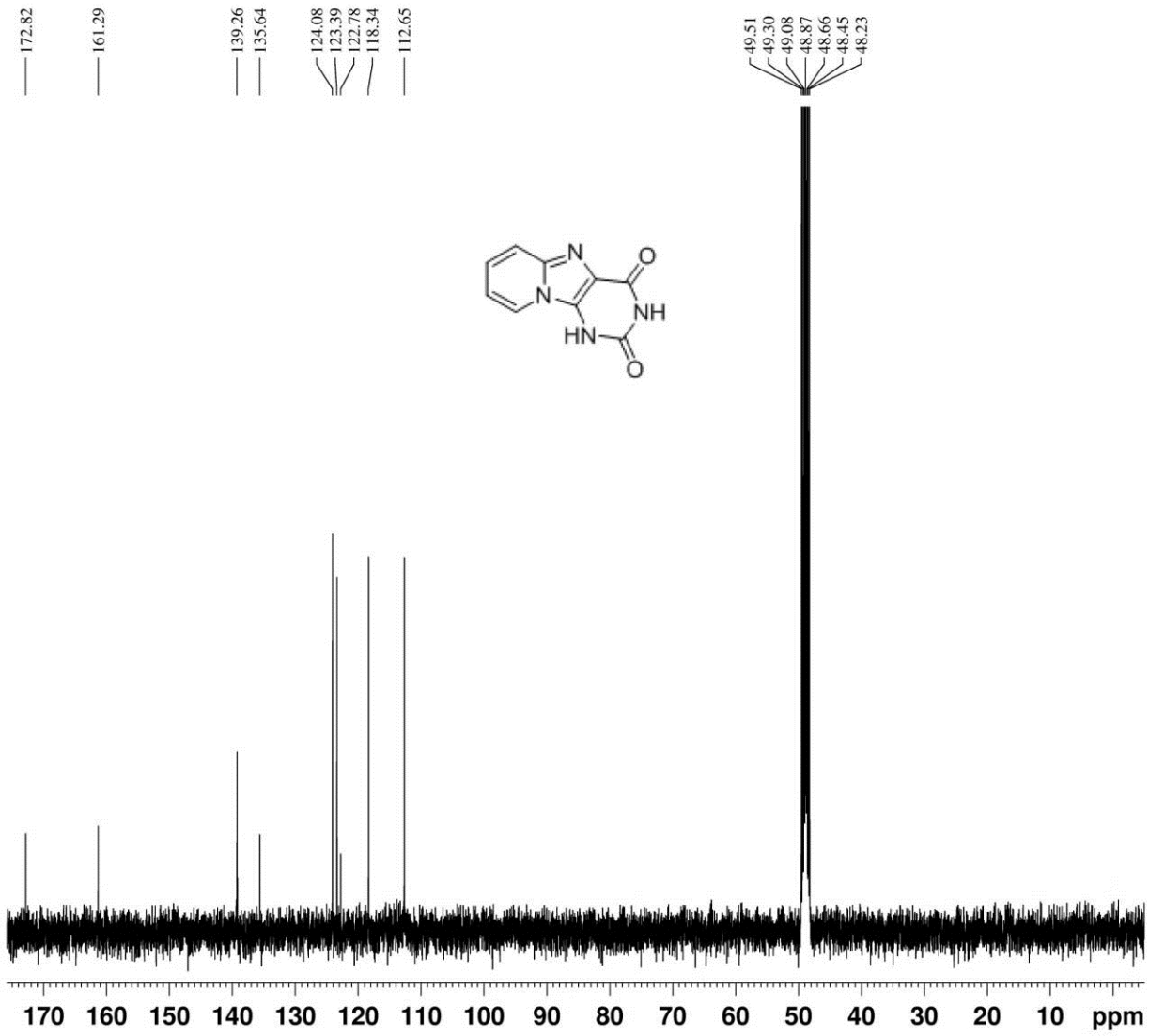
42: ^{13}C NMR


175.02
160.20
143.89
141.98
138.21
128.37
127.58
127.02
126.12
124.23
120.64
117.22
111.88
50.18
48.46
48.25
48.04
47.83
47.62
47.40
47.19
46.98
N
O
N
N
HN
S
80
160
140
120
100
80
60
40
20
ppm

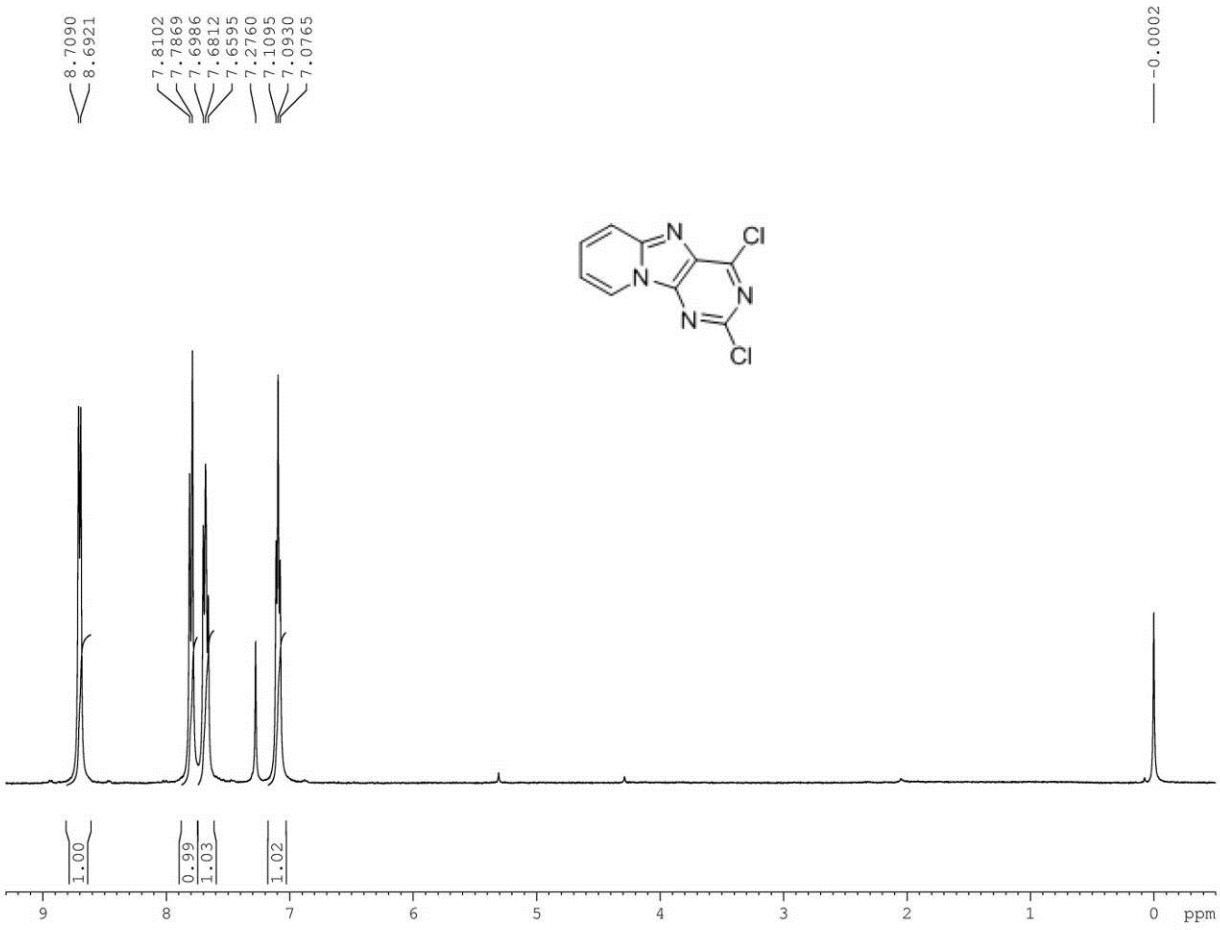
V: ^{1}H NMR


7.9883
7.9708
7.3951
7.3720
7.1070
7.1050
7.0883
7.0848
7.0821
7.0675
7.0655
6.8242
6.8075
6.7904
4.9150
3.3268
3.3228
3.3189
3.3151
3.3114
0.0098
N
O
N
NH
HN
O
1.00
1.08
1.05
1.08
9
8
7
6
5
4
3
2
1
0
ppm

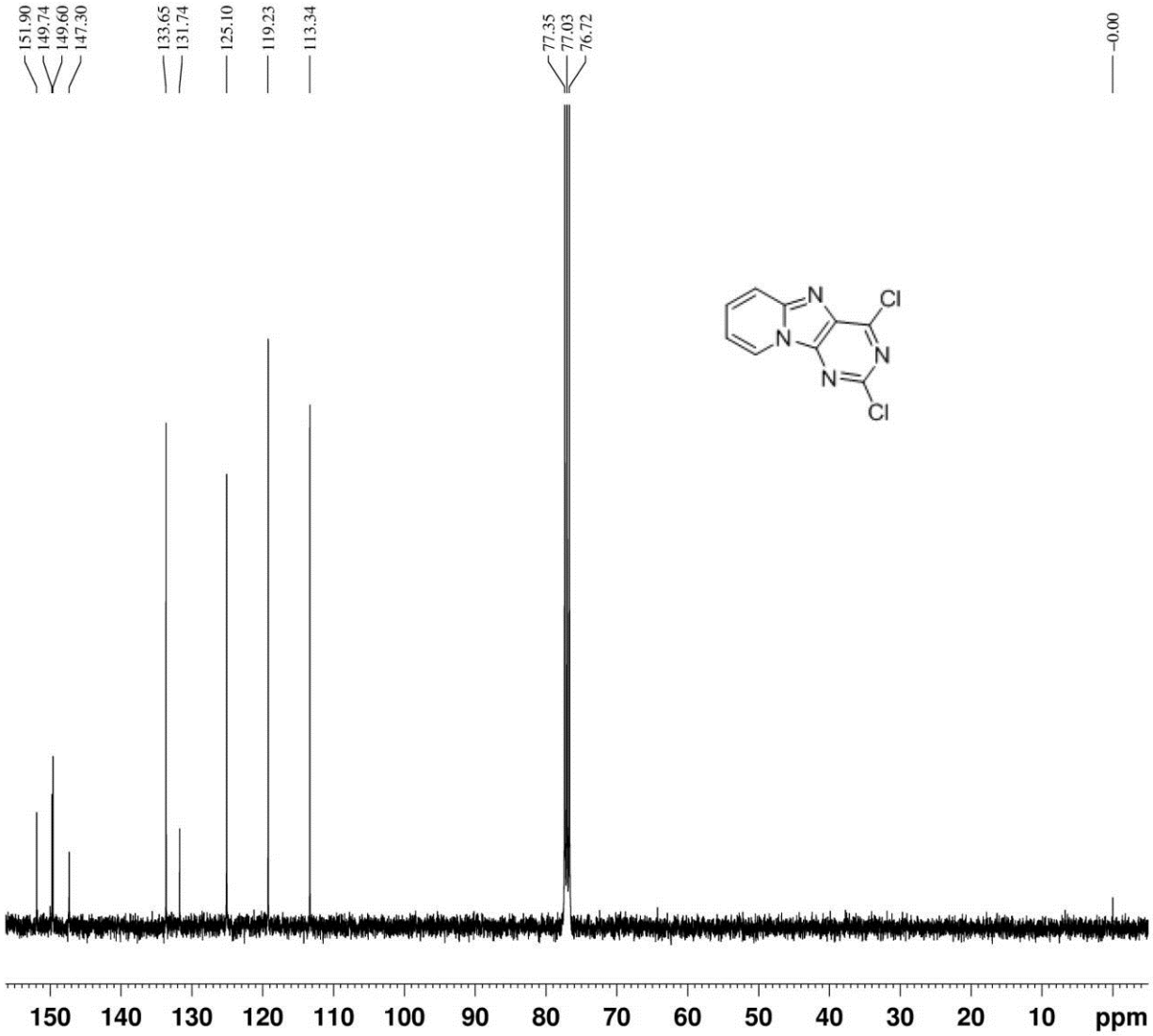
V: ^{13}C NMR


172.82
161.29
139.26
135.64
124.08
123.39
122.78
118.34
112.65
49.51
49.30
49.08
48.87
48.66
48.45
48.23
N
O
N
NH
HN
O
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

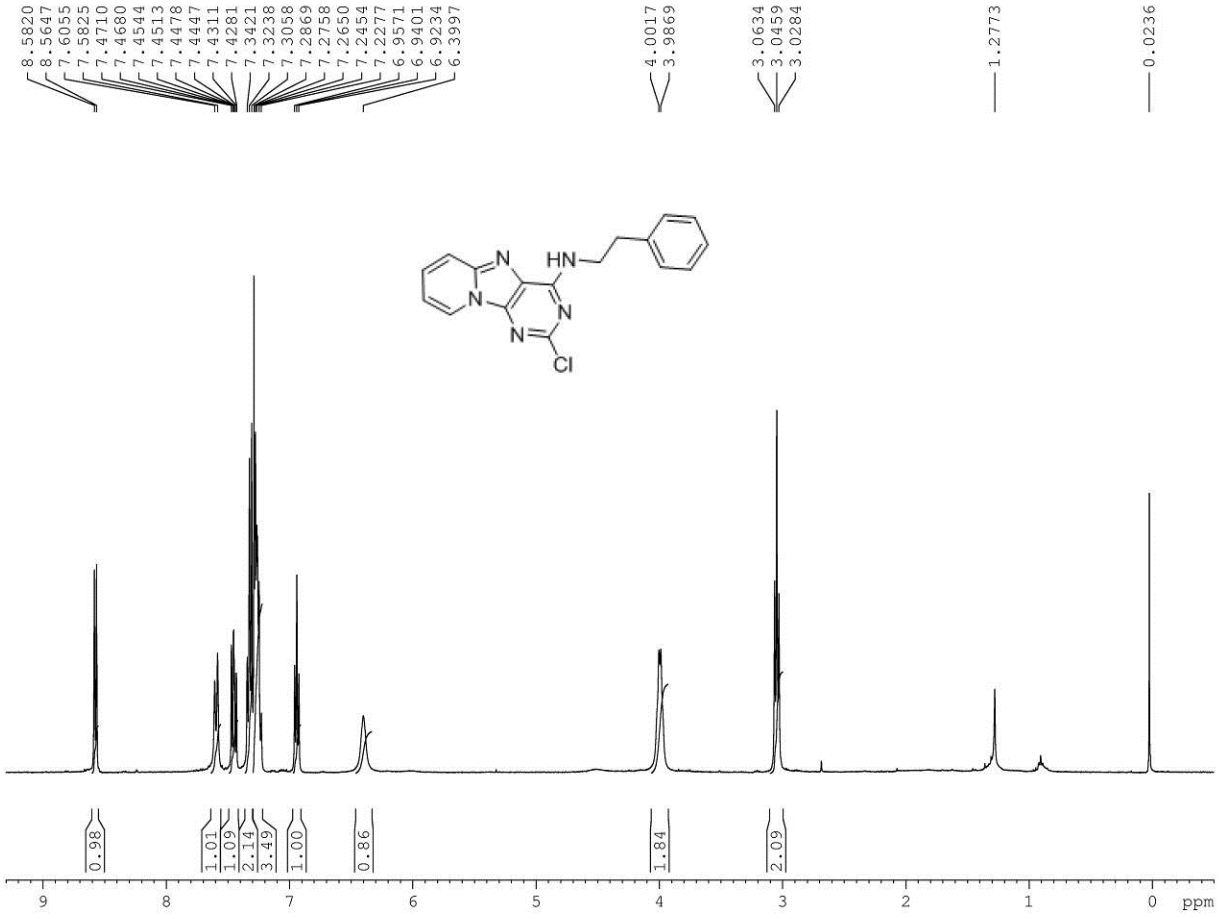
VI: ^{1}H NMR


8.7090
8.6921
7.8102
7.7869
7.6986
7.6812
7.6595
7.2760
7.1095
7.0930
7.0765
-0.0002
N
Cl
N
N
N
Cl
1.00
0.99
1.03
1.02
9
8
7
6
5
4
3
2
1
0
ppm

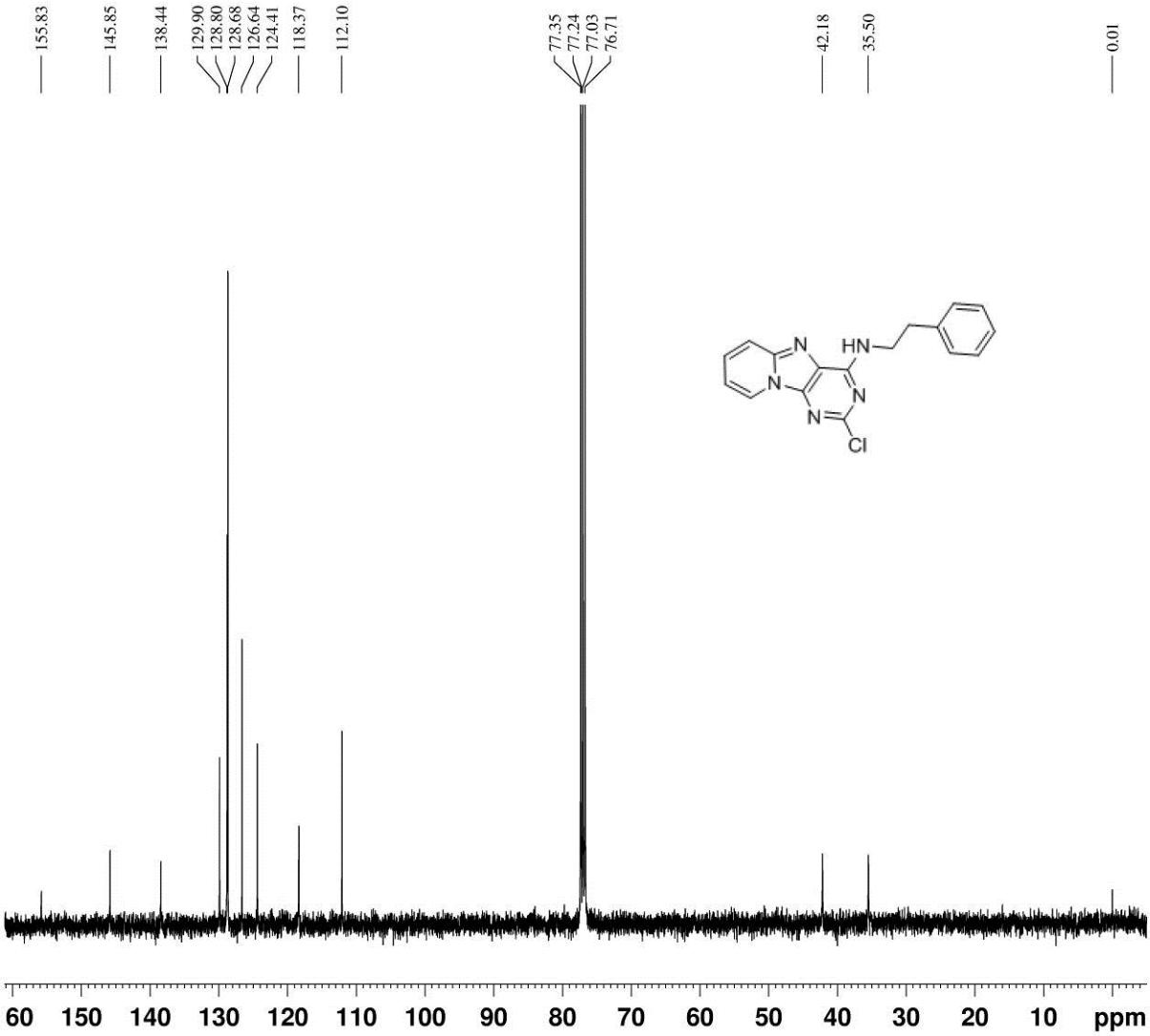
VI: ^{13}C NMR


151.90
149.74
149.60
147.30
133.65
131.74
125.10
119.23
113.34
77.35
77.03
76.72
0.00
N
Cl
N
N
N
Cl
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

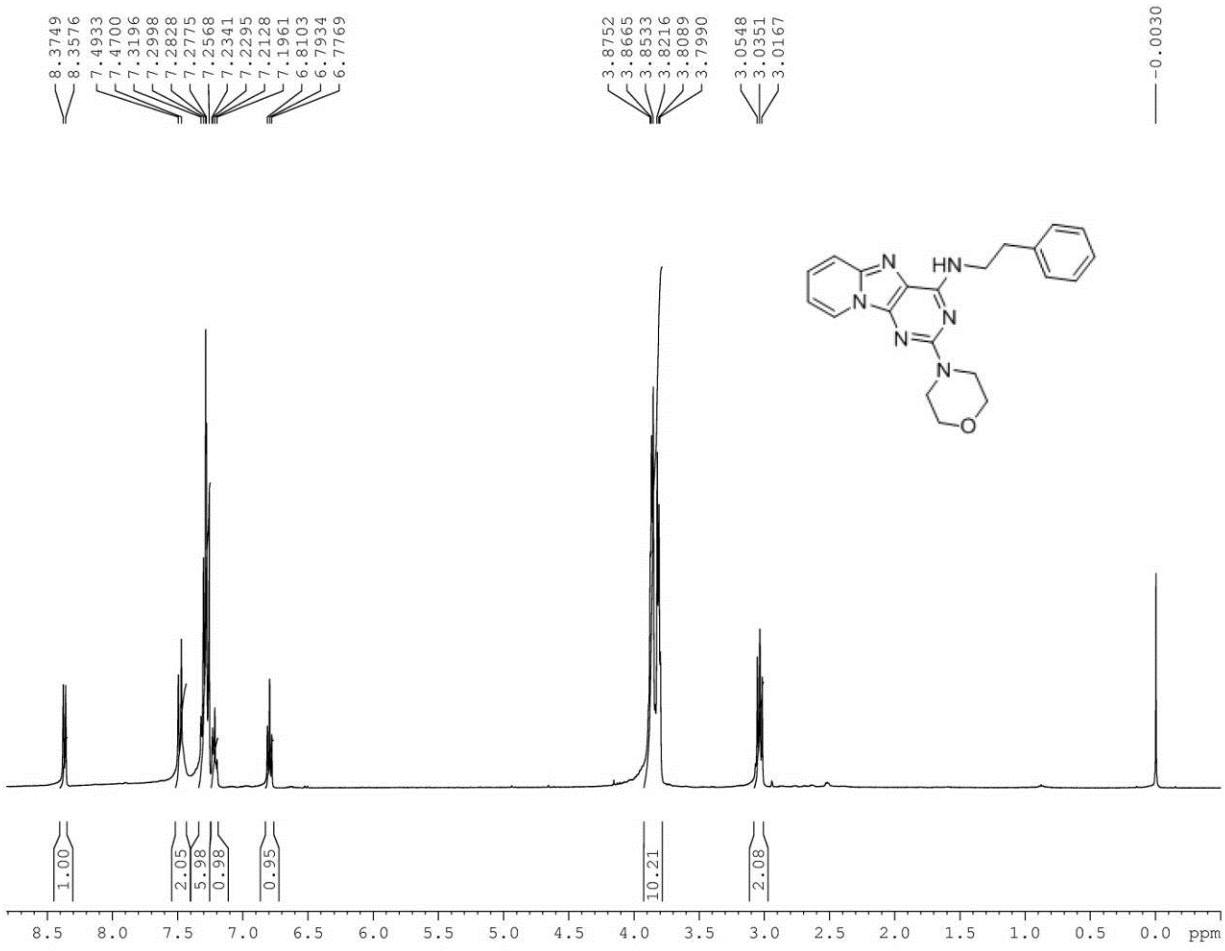
VII: ^{1}H NMR


8.5820
8.5647
7.6055
7.5825
7.4710
7.4680
7.4544
7.4513
7.4478
7.4447
7.4311
7.4281
7.3421
7.3238
7.3058
7.2869
7.2758
7.2650
7.2454
7.2277
6.9571
6.9401
6.9234
6.3997
4.0017
3.9869
3.0634
3.0459
3.0284
1.2773
0.0236
HN
N
N
N
N
Cl
0.98
1.01
1.09
2.14
3.49
1.00
0.86
1.84
2.09
9
8
7
6
5
4
3
2
1
0
ppm

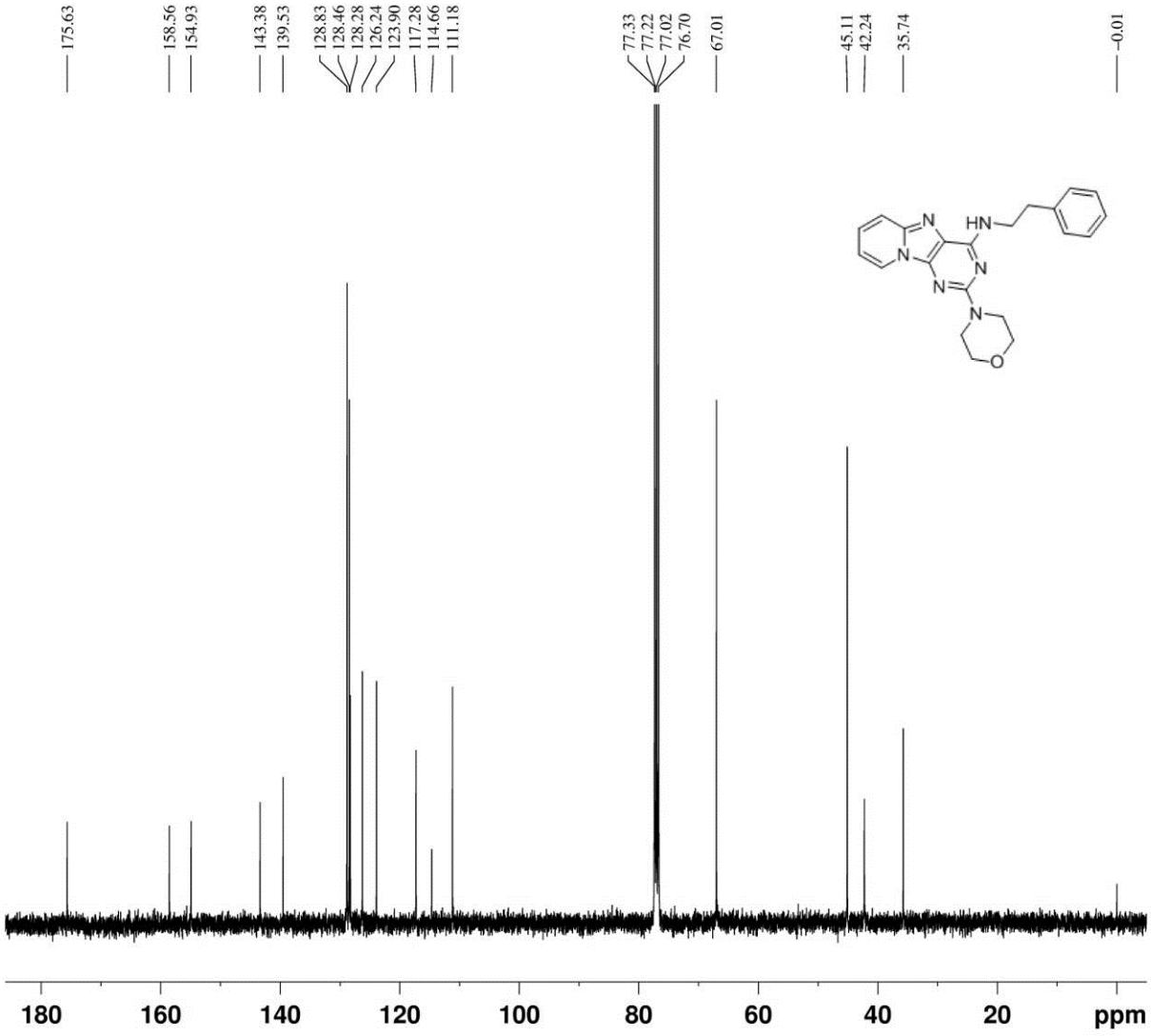
VII: ^{13}C NMR


155.83
145.85
138.44
129.90
128.80
128.68
126.64
124.41
118.37
112.10
77.35
77.24
77.03
76.71
42.18
35.50
0.01
HN
N
N
N
N
Cl
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

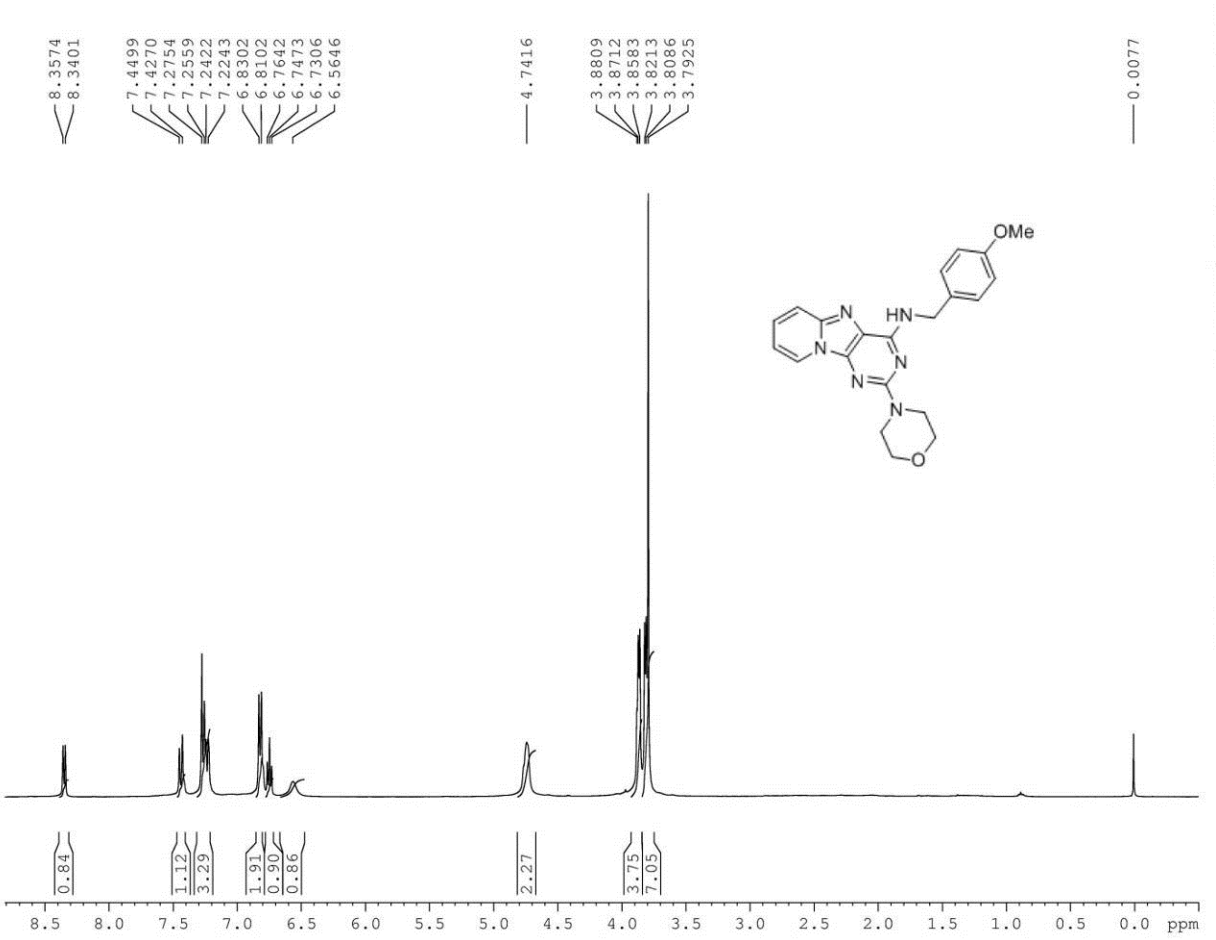
43: ^{1}H NMR


8.3749
8.3576
7.4933
7.4700
7.3196
7.2998
7.2828
7.2775
7.2568
7.2341
7.2295
7.2128
7.1961
6.8103
6.7934
6.7769
3.8752
3.8665
3.8533
3.8216
3.8089
3.7990
3.0548
3.0351
3.0167
0.0030
HN
N
N
N
N
O
1.00
2.05
5.98
0.98
0.95
10.21
2.08
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

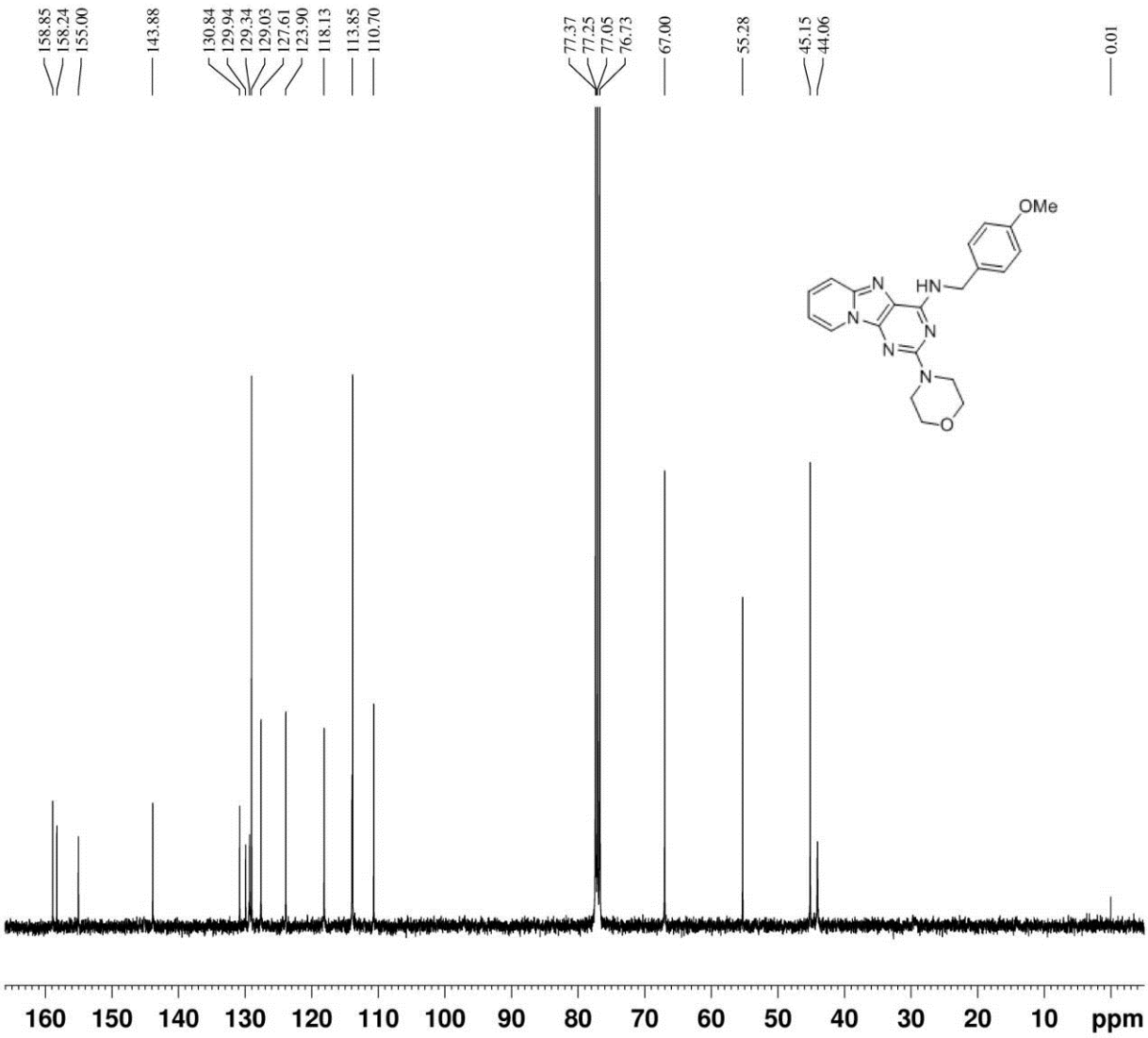
43: ^{13}C NMR


175.63
158.56
154.93
143.38
139.53
128.83
128.46
128.28
126.24
123.90
117.28
114.66
111.18
77.33
77.22
77.02
76.70
67.01
45.11
42.24
35.74
-0.01
HN
N
N
N
N
O
180
160
140
120
100
80
60
40
20
ppm

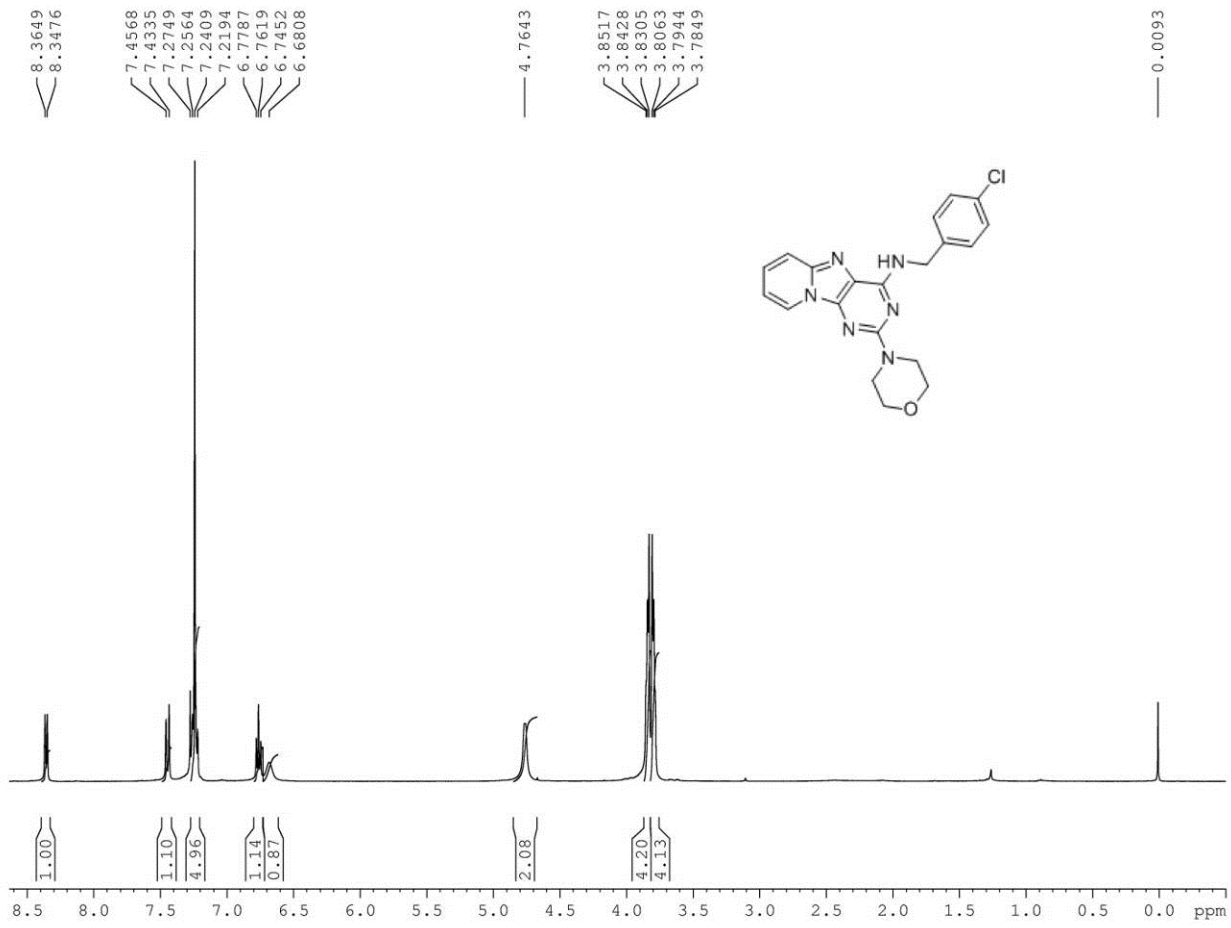
44: ^{1}H NMR


8.3574
8.3401
7.4499
7.4270
7.2754
7.2559
7.2422
7.2243
6.8302
6.8102
6.7642
6.7473
6.7306
6.5646
4.7416
3.8809
3.8712
3.8583
3.8213
3.8086
3.7925
0.0077
OMe
HN
N
N
N
N
O
0.84
1.12
3.29
1.91
0.90
0.86
2.27
3.75
7.05
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

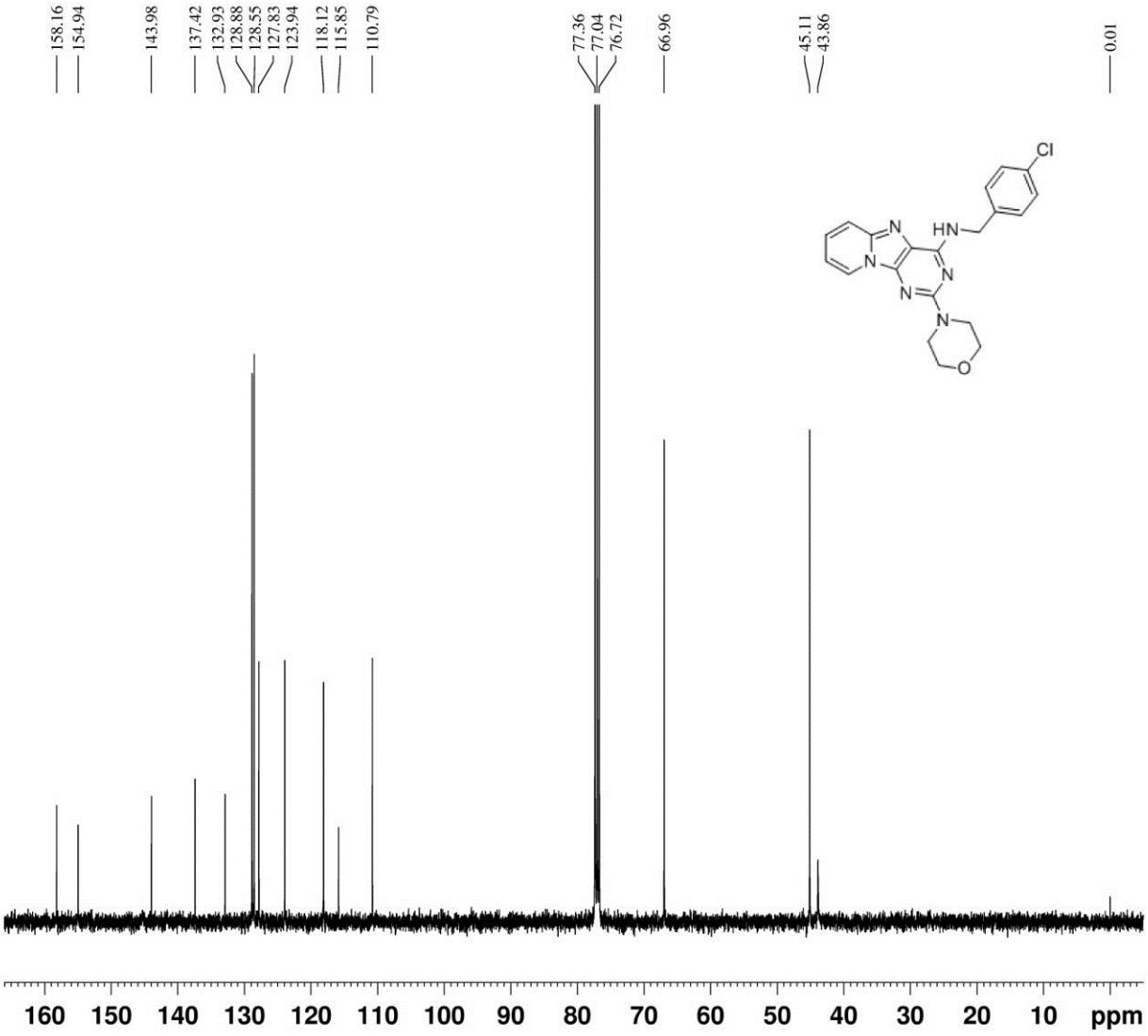
44: ^{13}C NMR


158.85
158.24
155.00
143.88
130.84
129.94
129.34
129.03
127.61
123.90
118.13
113.85
110.70
77.37
77.25
77.05
76.73
67.00
55.28
45.15
44.06
0.01
OMe
HN
N
N
N
N
O
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

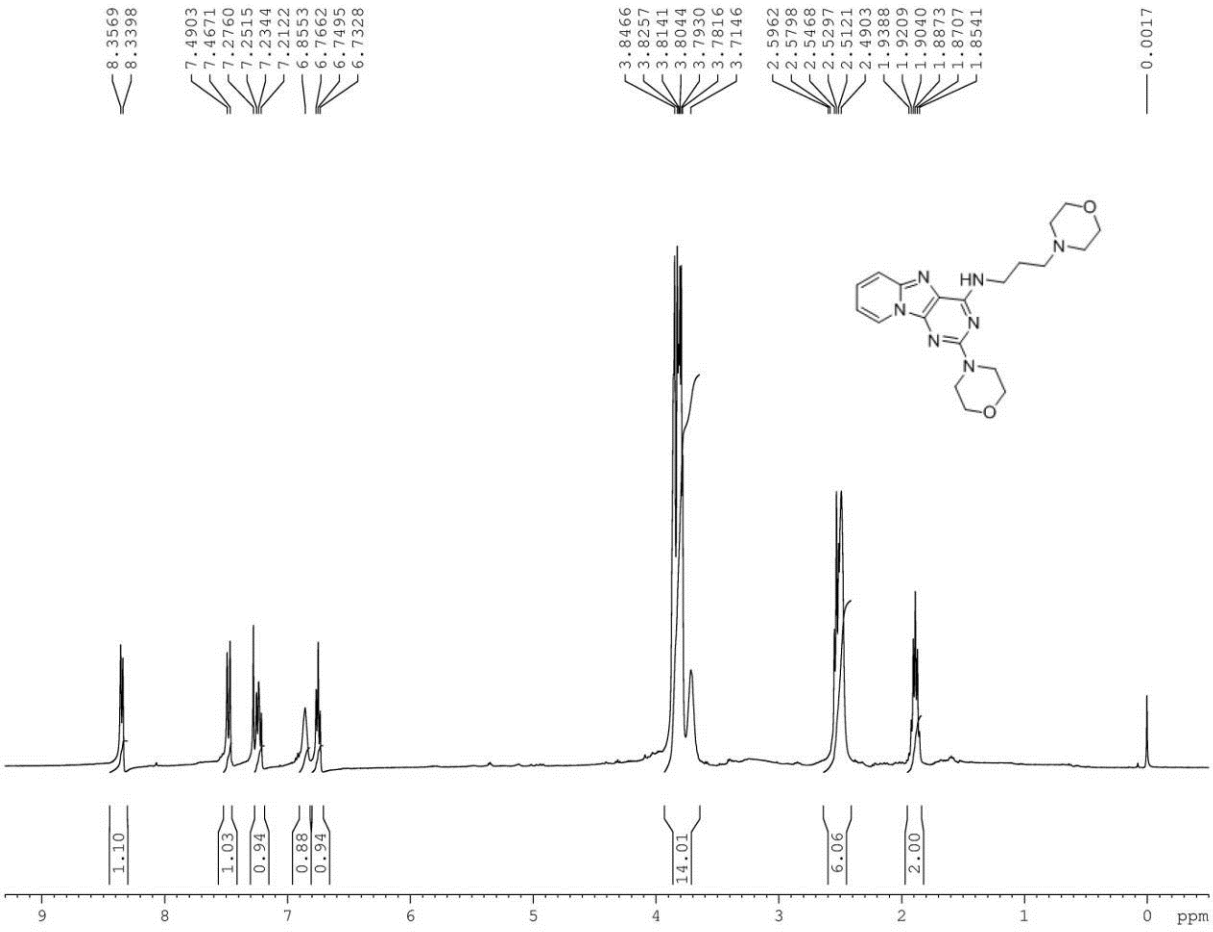
45: ^{1}H NMR


8.3649
8.3476
7.4568
7.4335
7.2749
7.2564
7.2409
7.2194
6.7787
6.7619
6.7452
6.6808
4.7643
3.8517
3.8428
3.8305
3.8063
3.7944
3.7849
0.0093
Cl
HN
N
N
N
N
O
1.00
1.10
4.96
1.14
0.87
2.08
4.20
4.13
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

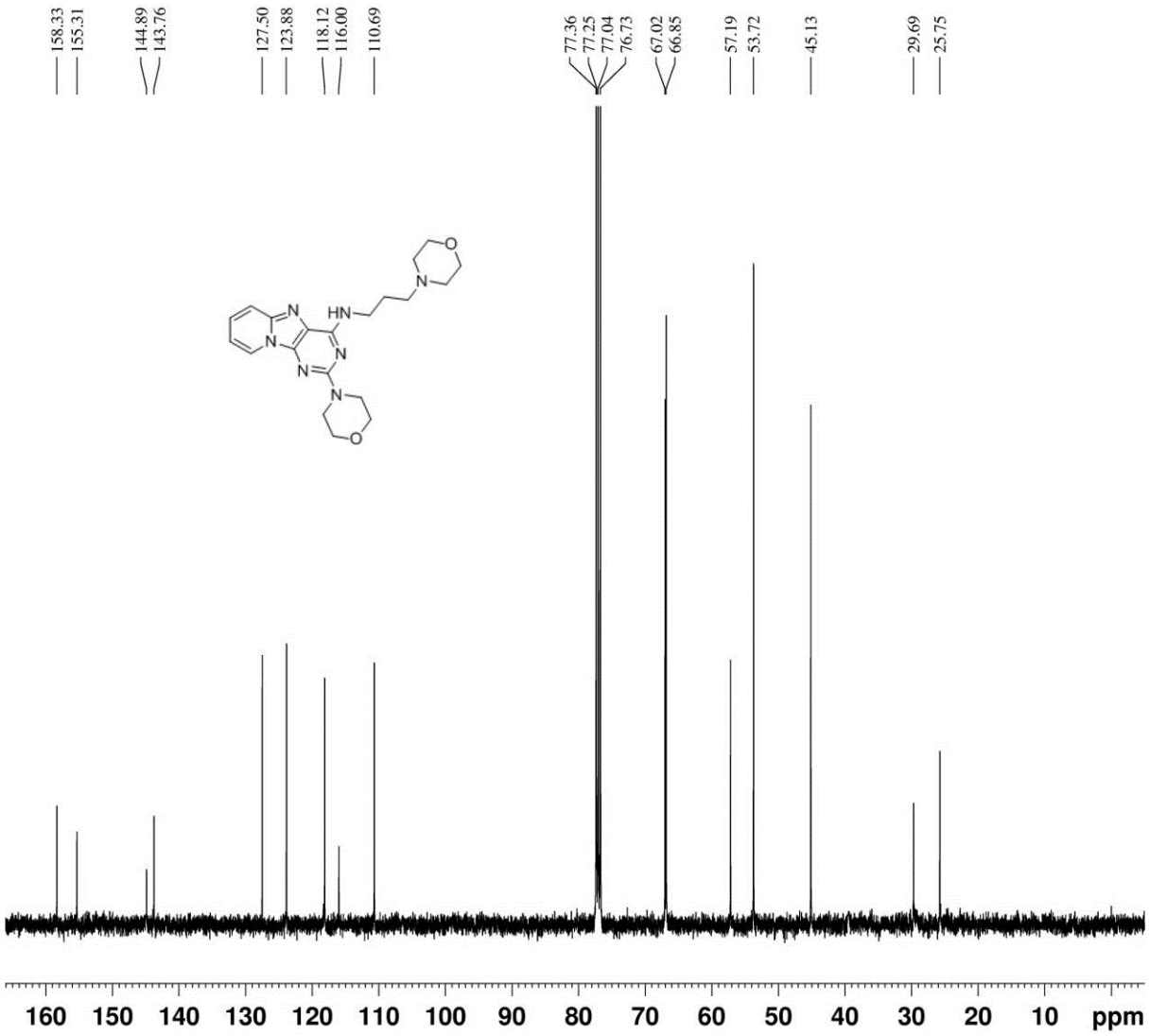
45: ^{13}C NMR


158.16
154.94
143.98
137.42
132.93
128.88
128.55
127.83
123.94
118.12
115.85
110.79
77.36
77.04
76.72
66.96
45.11
43.86
0.01
Cl
HN
N
N
N
N
O
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

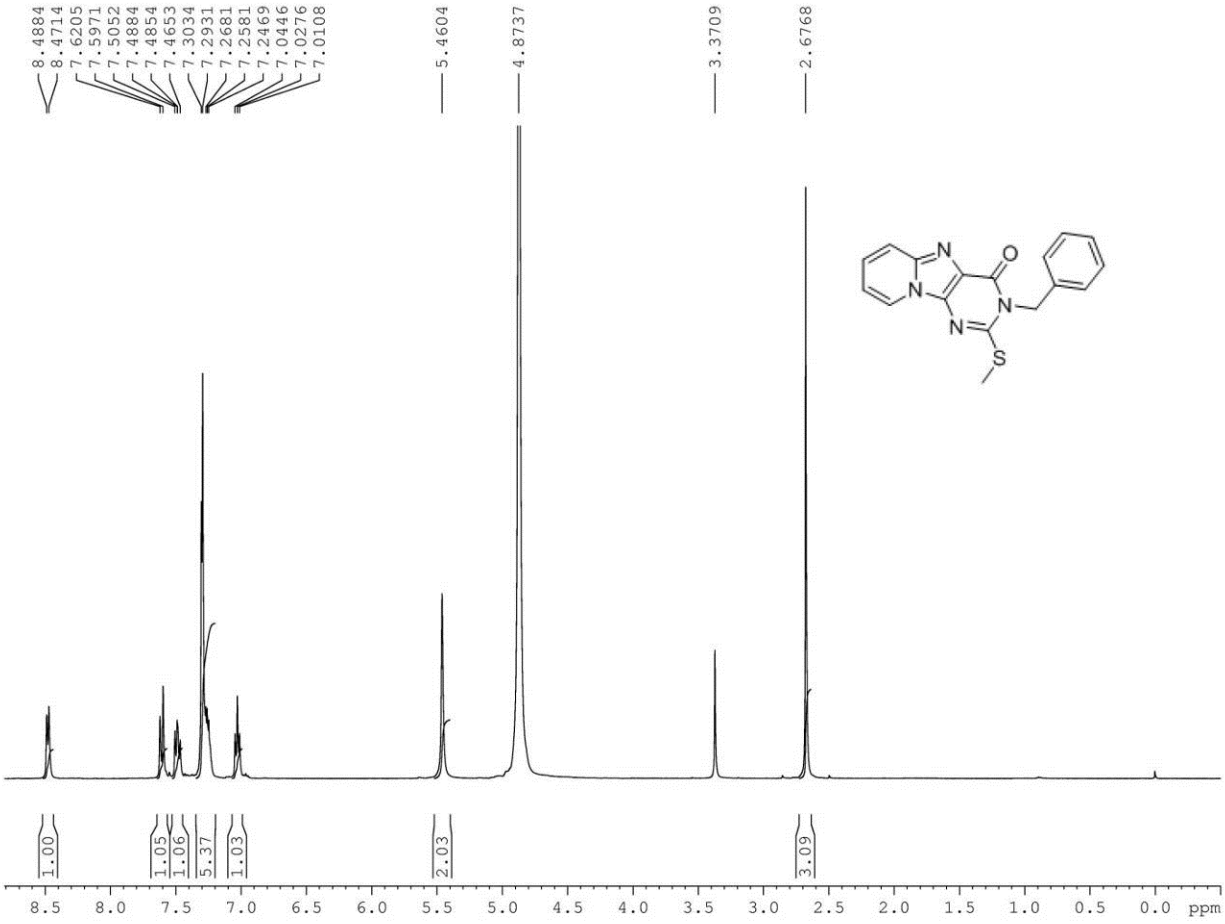
46: ^{1}H NMR


8.3569
8.3398
7.4903
7.4671
7.2760
7.2515
7.2344
7.2122
6.8553
6.7662
6.7495
6.7328
3.8466
3.8257
3.8141
3.8044
3.7930
3.7816
3.7146
2.5962
2.5798
2.5468
2.5297
2.5121
2.4903
1.9388
1.9209
1.9040
1.8873
1.8707
1.8541
0.0017
HN
1.10
1.03
0.94
0.88
0.94
14.01
6.06
2.00
9
8
7
6
5
4
3
2
1
0
ppm

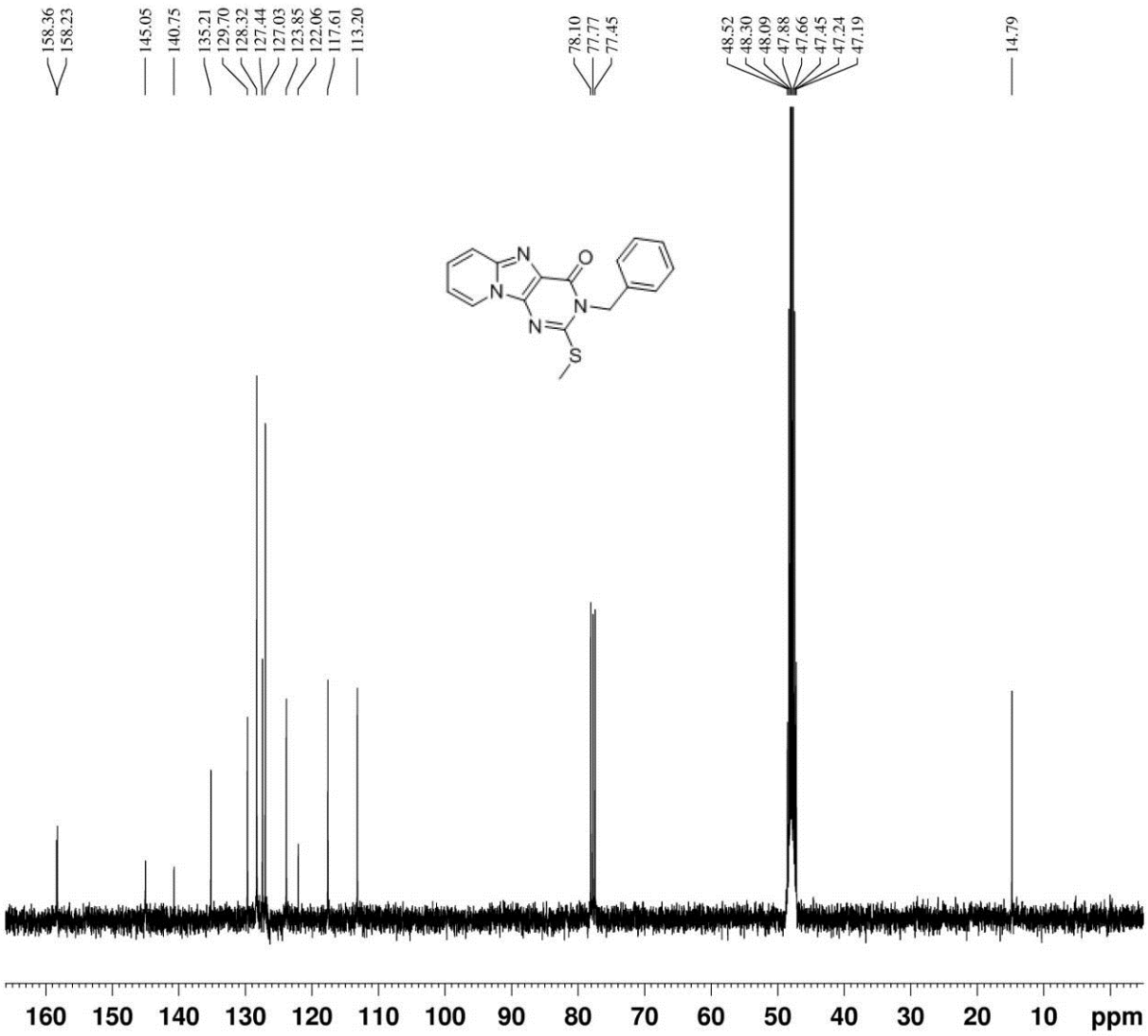
46: ^{13}C NMR


158.33
155.31
144.89
143.76
127.50
123.88
118.12
116.00
110.69
77.36
77.25
77.04
76.73
67.02
66.85
57.19
53.72
45.13
29.69
25.75
HN
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

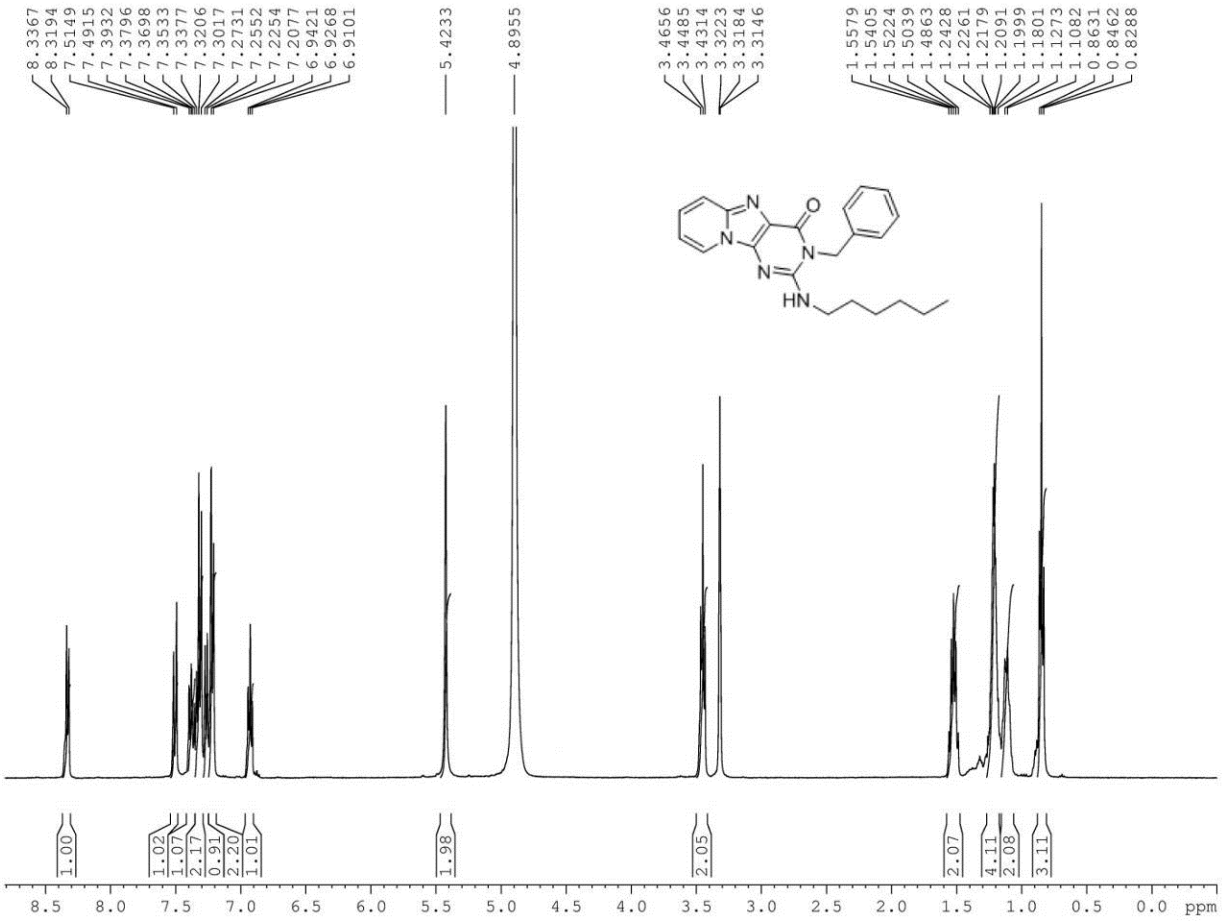
VIII: ^{1}H NMR


8.4884
8.4714
7.6205
7.5971
7.5052
7.4884
7.4854
7.4653
7.3034
7.2931
7.2681
7.2581
7.2469
7.0446
7.0276
7.0108
5.4604
4.8737
3.3709
2.6768
1.00
1.05
1.06
5.37
1.03
2.03
3.09
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

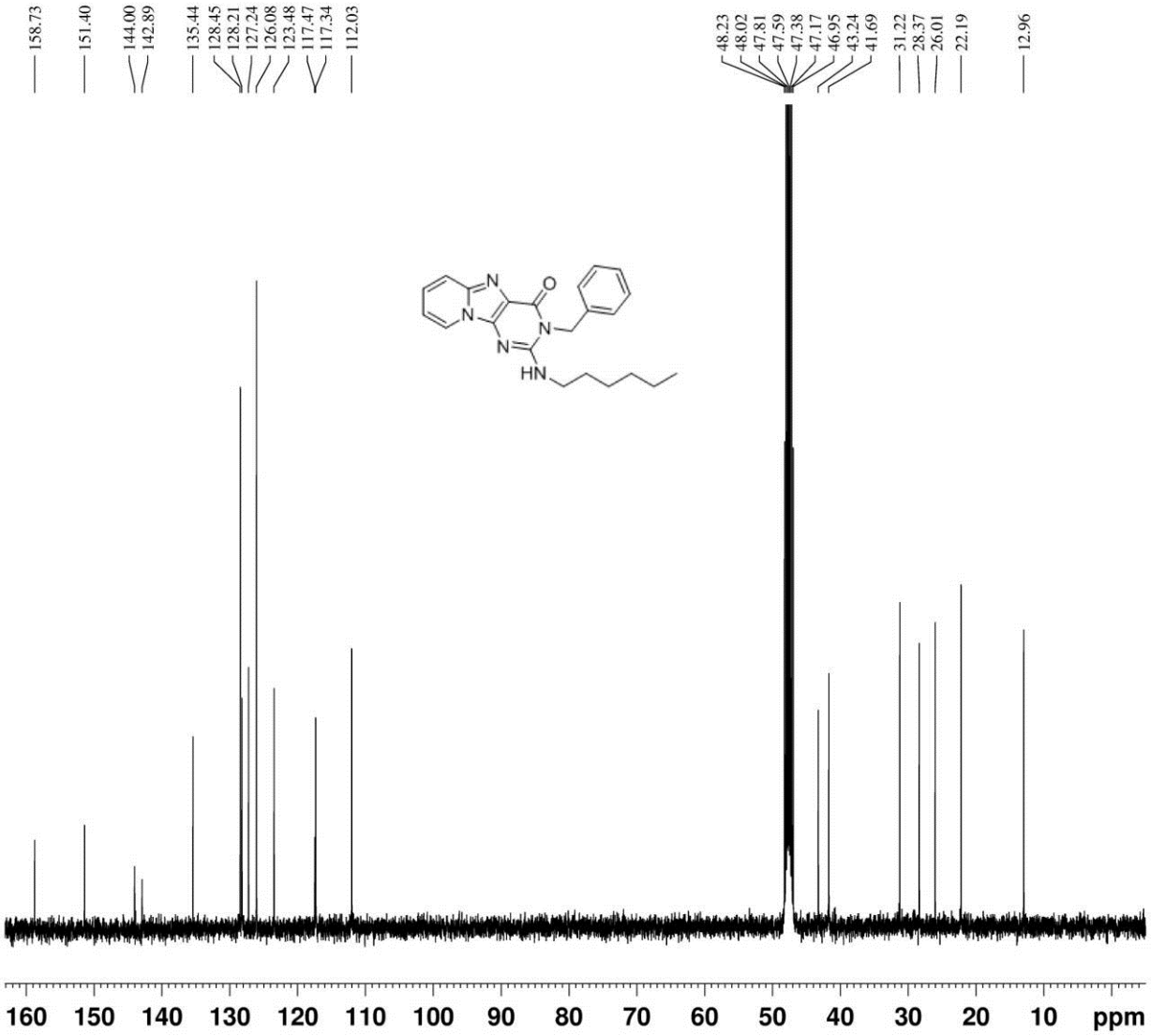
VIII: ^{13}C NMR


158.36
158.23
145.05
140.75
135.21
129.70
128.32
127.44
127.03
123.85
122.06
117.61
113.20
78.10
77.77
77.45
48.52
48.30
48.09
47.88
47.66
47.45
47.24
47.19
14.79
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

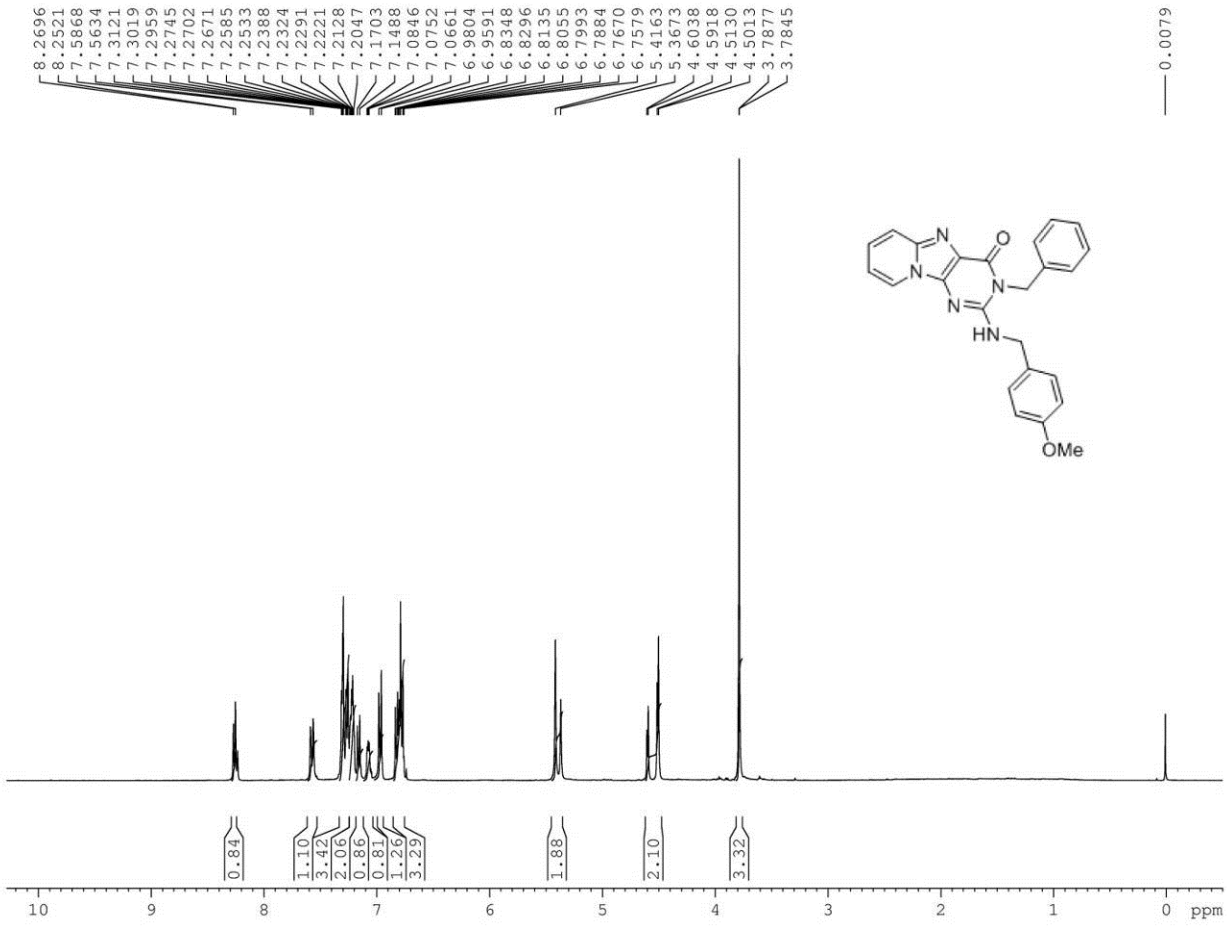
47: ^{1}H NMR


8.3367
8.3194
7.5149
7.4915
7.3932
7.3796
7.3698
7.3533
7.3377
7.3206
7.3017
7.2731
7.2552
7.2254
7.2077
6.9421
6.9268
6.9101
5.4233
4.8955
3.4656
3.4485
3.4314
3.3223
3.3184
3.3146
1.5579
1.5405
1.5224
1.5039
1.4863
1.2428
1.2261
1.2179
1.2091
1.1999
1.1801
1.1273
1.1082
0.8631
0.8462
0.8288
1.00
1.02
1.07
2.17
0.91
2.20
1.01
1.98
2.05
2.07
4.11
2.08
3.11
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

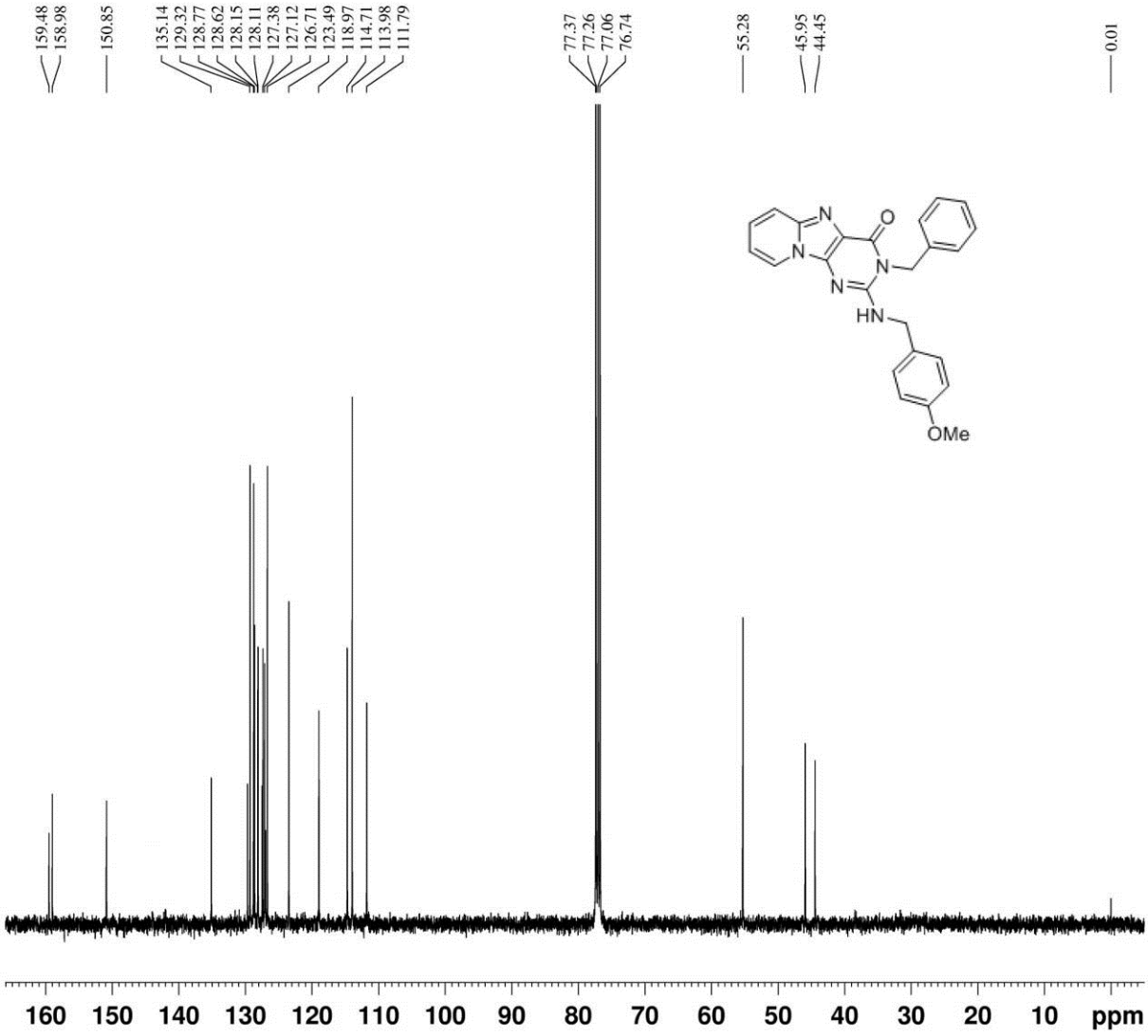
47: ^{13}C NMR


158.73
151.40
144.00
142.89
135.44
128.45
128.21
127.24
126.08
123.48
117.47
117.34
112.03
48.23
48.02
47.81
47.59
47.38
47.17
46.95
43.24
41.69
31.22
28.37
26.01
22.19
12.96
N
O
N
N
N
HN
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

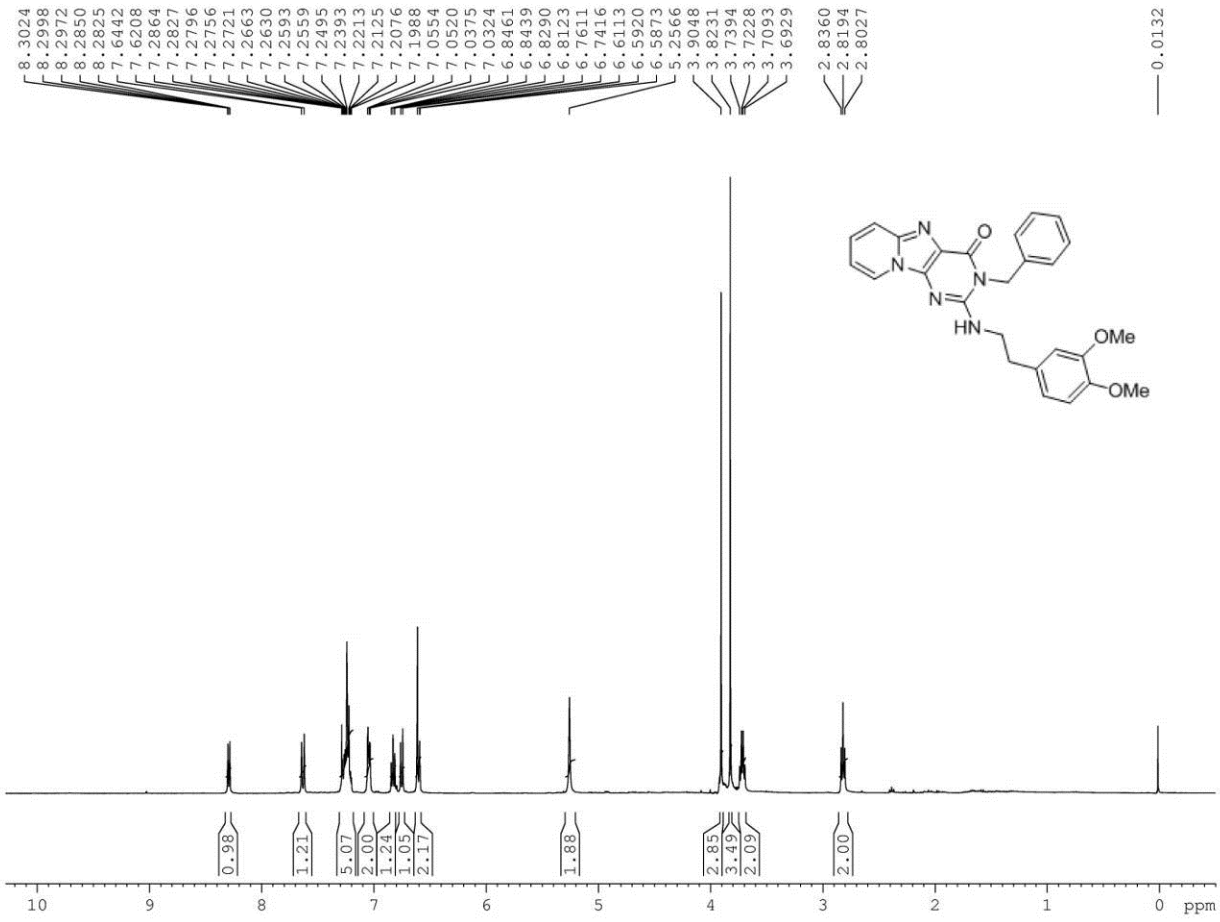
48: ^{1}H NMR


8.2696
8.2521
7.5868
7.5634
7.3121
7.3019
7.2959
7.2745
7.2702
7.2671
7.2585
7.2533
7.2388
7.2324
7.2291
7.2221
7.2128
7.2047
7.1703
7.1488
7.0846
7.0752
7.0661
6.9804
6.9591
6.8348
6.8296
6.8135
6.8055
6.7993
6.7884
6.7670
6.7579
5.4163
5.3673
4.6038
4.5918
4.5130
4.5013
3.7877
3.7845
0.0079
N
O
N
N
HN
OMe
0.84
1.10
3.42
2.06
0.86
0.81
1.26
3.29
1.88
2.10
3.32
10
9
8
7
6
5
4
3
2
1
0
ppm

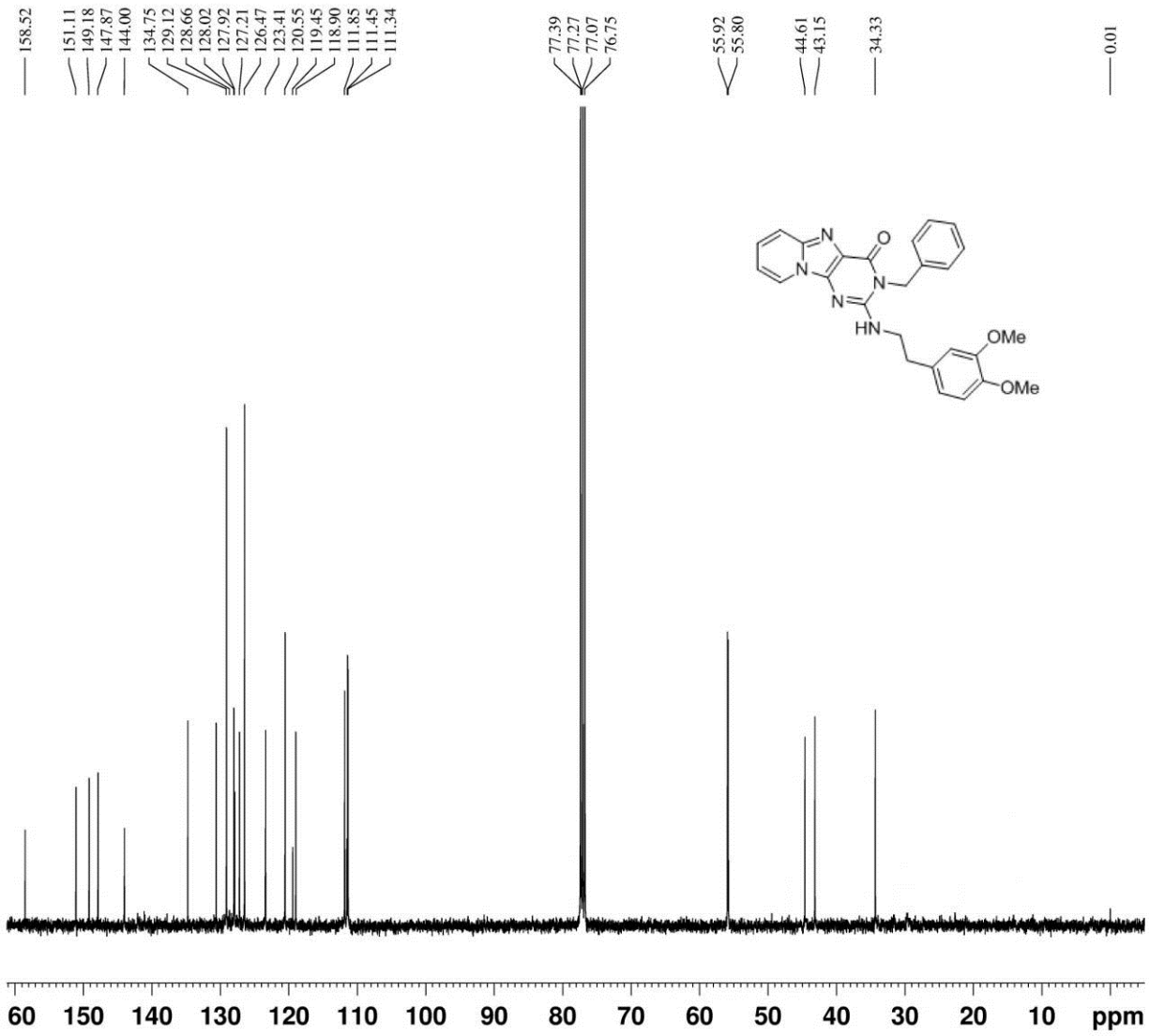
48: ^{13}C NMR


159.48
158.98
150.85
135.14
129.32
128.77
128.62
128.15
128.11
127.38
127.12
126.71
123.49
118.97
114.71
113.98
111.79
77.37
77.26
77.06
76.74
55.28
45.95
44.45
0.01
N
O
N
N
N
HN
OMe
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

49: ^{1}H NMR


8.3024
8.2998
8.2972
8.2850
8.2825
7.6442
7.6208
7.2864
7.2827
7.2796
7.2756
7.2721
7.2663
7.2630
7.2593
7.2559
7.2495
7.2393
7.2213
7.2125
7.2076
7.1988
7.0554
7.0520
7.0375
7.0324
6.8461
6.8439
6.8290
6.8123
6.7611
6.7416
6.6113
6.5920
6.5873
5.2566
3.9048
3.8231
3.7394
3.7228
3.7093
3.6929
2.8360
2.8194
2.8027
0.0132
N
O
N
N
HN
OMe
OMe
0.98
1.21
5.07
2.00
1.24
1.05
2.17
1.88
2.85
3.49
2.09
2.00
10
9
8
7
6
5
4
3
2
1
0
ppm

49: ^{13}C NMR


158.52
151.11
149.18
147.87
144.00
134.75
129.12
128.66
128.02
127.92
127.21
126.47
123.41
120.55
119.45
118.90
111.85
111.45
111.34
77.39
77.27
77.07
76.75
55.92
55.80
44.61
43.15
34.33
0.01
N
O
N
N
N
HN
OMe
OMe
60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm