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Supporting Information for

New domino heteroannelation of enaminones: Diversity synthesis of fused naphthyridines

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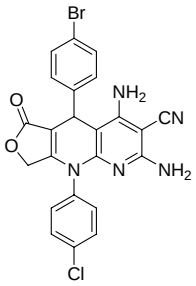
2,4-Diamino-5-(4-bromophenyl)-9-(4-chlorophenyl)-5,6,8,9-tetrahydro-6-oxofuro[3,4-b][1,8] naphthyridine-3-carbonitrile (4a)



Pale yellow solid, mp: 286-287 ^{o}C

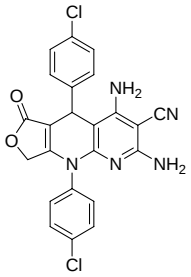
IR (KBr, ν, cm^{-1}): 3470, 3385 (νNH$_2$), 3329, 3220 (νNH$_2$), 2202 (νCN), 1738 (νC=O);

^{1}H NMR (400 MHz, DMSO-d_6) (δ,ppm): 7.56 (d, J = 8.0 Hz, 2H, ArH), 7.48 (t, J = 8.8 Hz, 4H, ArH), 7.37 (d, J = 7.6 Hz, 2H, ArH), 6.24 (s, 2H, NH$_2$), 6.19 (s, 2H, NH$_2$), 5.11 (s, 1H, CH), 4.58 (d, J = 16.0 Hz, 1H, CH$_2$), 4.50 (d, J = 16.4 Hz, 1H, CH$_2$);

^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 176.5, 164.1, 163.6, 161.4, 161.3, 156.7, 148.5, 141.4, 138.2, 136.2, 136.0, 135.2, 134.5, 125.0, 121.7, 105.1, 96.6, 70.5, 38.5;

HRMS (ESI) m/z: calc. for $C_{23}H_{15}BrClN_5O_2$: 507.9994; [M-H$^-$] found: 507.9999.

2,4-Diamino-5,9-bis(4-chlorophenyl)-5,6,8,9-tetrahydro-6-oxofuro[3,4-b][1,8]naphthyridine-3-carbonitrile(4b)



Pale yellow solid, mp: 282-283 ^{o}C

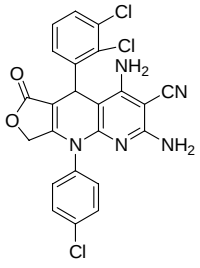
IR (KBr, ν, cm^{-1}): 3470, 3383 (νNH$_2$), 3327, 3203 (νNH$_2$), 2205 (νCN), 1733 (νC=O);

^{1}H NMR (400 MHz, DMSO-d_6) (δ,ppm): 7.56 (d, J = 8.4 Hz, 2H, ArH), 7.46 (d, J = 8.4 Hz, 2H, ArH), 7.42 (d, J = 8.4 Hz, 2H, ArH), 7.35 (d, J = 8.4 Hz, 2H, ArH), 6.25 (s, 2H, NH$_2$), 6.20 (s, 2H, NH$_2$), 5.12 (s, 1H, CH), 4.58 (d, J = 16.0 Hz, 1H, CH$_2$), 4.50 (d, J = 16.4 Hz, 1H, CH$_2$);

^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 171.2, 158.9, 158.4, 156.2, 151.4, 142.8, 136.2, 132.9, 131.2, 130.8, 129.5, 129.3, 128.1, 116.4, 99.9, 91.4, 79.1, 70.7, 65.3, 33.2;

HRMS (ESI) *m/z*: calc. For 462.0525; [M-H$^-$] found: 462.0550.

2,4-Diamino-5-(2,3-dichlorophenyl)-9-(4-chlorophenyl)-5,6,8,9-tetrahydro-6-oxofuro[3,4-b][1,8]naphthyridine-3-carbonitrile(4c)



Pale yellow solid, mp: 284-285 ^{o}C

IR (KBr, ν, cm^{-1}): 3475, 3385 (νNH$_2$), 3330, 3204 (νNH$_2$), 2208 (νCN), 1730 (νC=O);

^{1}H NMR (400 MHz, DMSO-d_6) (δ,ppm): 7.68 (d, J = 7.6 Hz, 1H, ArH), 7.57 (t, J = 7.6 Hz, 3H, ArH), 7.48 (d, J = 8.0 Hz, 2H, ArH), 7.37 (t, J = 7.6 Hz, 1H, ArH), 6.27 (s, 2H , NH$_2$) 5.79 (s, 2H, NH$_2$), 5.43 (s, 1H, CH), 4.63 (d, J = 16.0 Hz, 1H, CH$_2$), 4.55 (d, J = 16.4 Hz, 1H, CH$_2$);

HRMS (ESI) m/z: calc. for $C_{23}H_{14}Cl_3N_5O_2$: 496.0135; [M-H$^-$] found: 496.0107.

2,4-diamino-9-(4-chlorophenyl)-5,6,8,9-tetrahydro-6-oxo-5-phenylfuro[3,4-b][1,8]naphthyridine-3-carbonitrile(4d)

Pale yellow solid, mp: 243-244 ^{o}C

IR (KBr, ν, cm^{-1}): 3468, 3357 (νNH$_2$), 3244 (νNH$_2$), 2206 (νCN), 1748 (νC=O);

^{1}H NMR (400 MHz, DMSO-d_6) (δ,ppm): 7.56 (d, J = 8.8 Hz, 2H, ArH), 7.46

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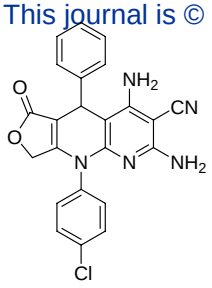
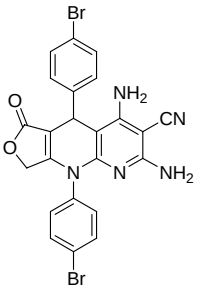


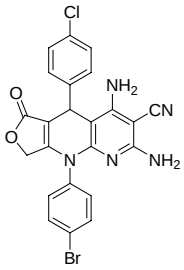
(d, J = 8.8 Hz, 2H, ArH), 7.41 (d, J = 7.2 Hz, 2H, ArH), 7.29 (t, J = 7.6 Hz, 2H, ArH), 7.19 (t, J = 7.2 Hz, 1H, ArH), 6.20 (s, 2H, NH_2), 6.17 (s, 2H, NH_2), 5.08 (s, 1H,CH), 4.58 (d, J = 16.0 Hz, 1H, CH_2), 4.50 (d, J = 16.4 Hz, 1H, CH_2);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 171.4, 163.0, 158.9, 158.7, 156.0, 151.7, 144.2, 137.7, 132.1, 129.9, 129.8, 128.4, 128.2, 127.5, 118.6, 99.9, 70.6, 67.9, 65.2, 33.7, 20.7, 20.3;
HRMS (ESI) m/z: calc. for $C_{23}H_{16}ClN_5O_2$: 428.0914; [M-H$^-$] found: 428.0947.

2,4-diamino-5,9-bis(4-bromophenyl)-5,6,8,9-tetrahydro-6-oxofuro[3,4-b][1,8]naphthyridine-3-carbonitrile(4e)



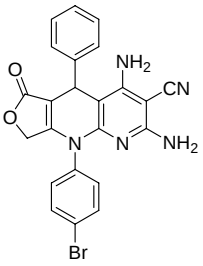
Pale yellow solid, mp: 292-293 °C;
IR (KBr, ν, cm^{-1}):3478, 3396 (νNH$_2$), 3337, 3202 (νNH$_2$), 2208 (νCN), 1754 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ,ppm): 7.69 (d, J = 8.4 Hz, 2H, ArH), 7.48 (d, J = 8.0 Hz, 2H, ArH), 7.38 (q, J = 15.2, 8.2 Hz, 4H, ArH), 6.24 (s, 2H, NH_2), 6.20 (s, 2H, NH_2), 5.10 (s, 1H, CH), 4.59 (d, J = 16.0 Hz, 2H, CH_2), 4.50 (d, J = 16.4 Hz, 2H, CH_2);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 171.3, 158.8, 157.9, 156.1, 151.3, 141.1, 136.7, 135.7, 132.3, 131.1, 128.8, 127.5, 121.5, 116.5, 100.5, 92.1, 70.7, 65.2, 33.4, 20.6;
HRMS (ESI) m/z: calc. for $C_{23}H_{15}Br_2N_5O_2$: 551.9490; [M-H$^-$] found: 551.9493.

2,4-Diamino-9-(4-bromophenyl)-5-(4-chlorophenyl)-5,6,8,9-tetrahydro-6-oxofuro[3,4-b][1,8] naphthyridine-3-carbonitrile (4f)



Pale yellow solid, mp: 277-278 °C;
IR (KBr, ν, cm^{-1}): 3479, 3367 (νNH$_2$), 3239 (νNH$_2$), 2205 (νCN), 1749 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ,ppm):7.68 (d, J = 8.0 Hz, 2H, ArH), 7.44–7.30 (m, 6H, ArH), 6.21 (s, 2H, NH_2), 6.17 (s, 2H, NH_2), 5.11 (s, 1H, CH), 4.57 (d, J = 16.0 Hz, 1H, CH_2), 4.50 (d, J = 16.4 Hz, 1H, CH_2);
HRMS (ESI) m/z: calc. for $C_{23}H_{15}BrClN_5O_2$: 507.9994; [M-H$^-$] found:507.9994.

2,4-Diamino-9-(4-bromophenyl)-5,6,8,9-tetrahydro-6-oxo-5-phenylfuro[3,4-b][1,8]naphthyridine-3-carbonitrile(4g)



Pale yellow solid, mp: 233-234 °C;
IR (KBr, ν, cm^{-1}): 3477 (νNH$_2$), 3364 (νNH$_2$), 3244 (νNH$_2$), 2207 (νCN), 1744 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ,ppm): 7.69 (d, J = 8.0 Hz, 2H, ArH), 7.41 (d, J = 5.2 Hz, 4H, ArH), 7.30 (t, J = 7.2 Hz, 2H, ArH), 7.20 (d, J = 7.2 Hz, 1H, ArH), 6.17 (d, J = 7.2 Hz, 4H, 2NH$_2$), 5.08 (s, 1H, CH), 4.59 (d, J = 16.4 Hz, 1H CH_2), 4.51 (d, J = 16.0 Hz, 1H CH_2);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 171.2, 158.8, 158.1, 156.1, 151.4, 143.9, 136.7, 132.2, 131.1, 128.2, 127.6, 126.6, 121.5, 116.4, 100.5, 92.0, 70.8, 65.2, 33.8;
HRMS (ESI) m/z: calc. for $C_{23}H_{16}BrN_5O_2$: 474.0386; [M-H$^-$] found: 474.0386.

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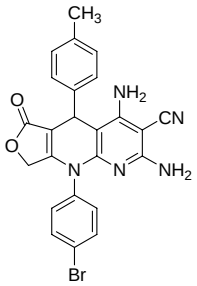
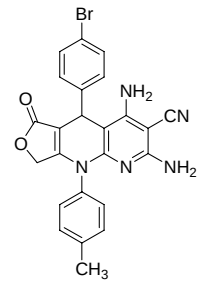
2,4-Diamino-9-(4-bromophenyl)-5,6,8,9-tetrahydro-6-oxo-5-p-tolylfuro[3,4-b][1,8]naphthyridine-3-carbonitrile(4h)



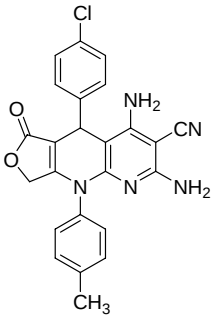
Pale yellow solid, mp: 244-245 °C;
IR (KBr, ν, cm^{-1}): 3467, 3392 (νNH$_2$), 3338, 3241 (νNH$_2$), 2205 (νCN), 1757 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ,ppm): 7.68 (d, J = 8.4 Hz, 2H, ArH), 7.38 (d, J = 8.4 Hz, 2H, ArH), 7.27 (d, J =8.0 Hz, 2H, ArH), 7.08 (d, J = 7.6 Hz, 2H, ArH), 6.14 (s, 4H, 2NH$_2$), 5.02 (s, 1H, CH), 4.57 (d, J = 16.0 Hz, 1H, CH$_2$), 4.48 (d, J = 16.0 Hz, 1H, CH$_2$), 2.24 (s, 3H, CH$_3$);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 171.3, 158.8, 157.9, 156.1, 151.3, 141.0, 136.7, 135.7, 132.3, 131.1, 128.8, 127.5, 121.5, 116.5, 100.5, 92.1, 70.7, 65.2, 33.4, 20.6
HRMS (ESI) m/z: calc. for $C_{24}H_{18}BrN_5O_2$: 488.0542; [M-H$^-$] found: 488.0568.

2,4-Diamino-5-(4-bromophenyl)-5,6,8,9-tetrahydro-6-oxo-9-p-tolylfuro[3,4-b][1,8]naphthyridine-3-carbonitrile(4i)



Pale yellow solid, mp: 267-268 °C;
IR (KBr, ν, cm^{-1}): 3482, 3382 (νNH$_2$), 3325, 3203 (νNH$_2$), 2199 (νCN), 1739 (νC=O)
^{1}H NMR (400 MHz, DMSO-d_6) (δ,ppm): 7.49 (d, J = 8.4 Hz, 2H, ArH), 7.35 (d, J = 8.4 Hz, 2H, ArH), 7.28 (s, 4H, ArH), 6.18 (s, 2H, NH$_2$), 6.11 (s, 2H, NH$_2$), 5.10 (s, 1H, CH), 4.52 (d, J = 16.0 Hz, 1H, CH$_2$), 4.41 (d, J = 16.0 Hz, 1H, CH$_2$), 2.36 (s, 3H, CH$_3$) ;
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 171.3, 159.0, 158.9, 156.1, 151.7, 143.4, 137.8, 134.7, 131.0, 129.8, 128.5, 119.7, 116.5, 99.4, 91.4, 70.6, 65.3, 33.3, 20.7;
HRMS (ESI) m/z: calc. for $C_{24}H_{18}BrN_5O_2$: 488.0542; [M-H$^-$] found:488.0562.

2,4-Diamino-5-(4-chlorophenyl)-5,6,8,9-tetrahydro-6-oxo-9-p-tolylfuro[3,4-b][1,8]naphthyridine-3-carbonitrile(4j)



Pale yellow solid, mp: 255-256 °C;
IR (KBr, ν, cm^{-1}): 3481, 3394 (νNH$_2$), 3360, 3248 (νNH$_2$), 2200 (νCN), 1738 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ,ppm): 7.41 (d, J = 6.8 Hz, 2H, ArH), 7.35 (d, J = 8.0 Hz, 2H, ArH), 7.28 (s, 4H, ArH), 6.19 (s, 2H, NH$_2$), 6.10 (s, 2H, NH$_2$), 5.12 (s, 1H, CH), 4.52 (d, J = 16.0 Hz, 1H, CH$_2$), 4.41 (d, J = 16.0 Hz, 1H, CH$_2$), 2.36 (s, 3H, CH$_3$);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 171.3, 158.9, 156.1, 151.8, 143.0, 137.8, 134.7, 131.1, 129.8, 129.4, 128.5, 128.1, 116.4, 99.5, 70.7, 65.3, 33.2, 30.7, 20.7;
HRMS (ESI) m/z: calc. for $C_{24}H_{18}Cl_2N_5O_2$: 442.1071; [M-H$^-$] found: 442.1072.

2,4-Diamino-5,6,8,9-tetrahydro-6-oxo-5-phenyl-9-p-tolylfuro[3,4-b][1,8]naphthyridine-3-carbonitrile (4k)

Pale yellow solid, mp: 231-232 °C;

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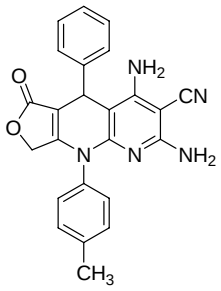
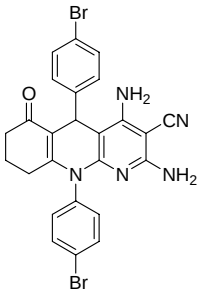


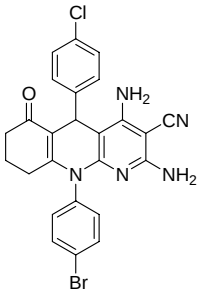
IR (KBr, ν, cm^{-1}): 3453, 3359 (νNH_2), 3244 (νNH_2), 2203 (νCN), 1748 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ,ppm): 7.40 (d, J = 7.6 Hz, 2H, ArH), 7.33 – 7.25 (m, 6H, ArH), 7.20 (d, J = 7.2 Hz, 1H, ArH), 6.09 (d, J = 21.6 Hz, 4H, 2NH_2), 5.07 (s, 1H, CH), 4.52 (d, J = 16.0 Hz, 1H, CH_2), 4.41 (d, J = 16.4 Hz, 1H, CH_2), 2.36 (s, 3H, CH_3);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 171.4, 158.9, 156.0, 151.7, 144.2, 137.7, 134.8, 132.1, 129.9, 129.8, 128.5, 128.2, 127.5, 118.6, 99.9, 91.9, 82.7, 70.6, 68.0, 33.8, 20.7, 20.3;
HRMS (ESI) m/z: calc. for $C_{24}H_{19}N_5O_2$: 408.1460; [M-H$^-$] found: 408.1460.

2,4-Diamino-5,10-bis(4-bromophenyl)-5,6,7,8,9,10-hexahydro-6-oxobenzo[b][1,8]naphthyridine-3-carbonitrile (5a)



Pale yellow solid, mp: >300 ^{o}C;
IR (KBr, ν, cm^{-1}): 3473, 3441 (νNH_2), 3362, 3241 (νNH_2), 2200 (νCN), 1607 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.68 (d, J = 7.6 Hz, 2H, ArH), 7.41 (d, J = 7.2 Hz, 2H, ArH), 7.35 (d, J = 7.6 Hz, 2H, ArH), 7.27 (d, J = 7.2 Hz, 2H, ArH), 6.29 (s, 2H, NH_2), 5.93 (s, 2H, NH_2), 5.26 (s, 1H, CH), 2.18 (s, 3H, CH_2), 1.94 (d, J = 17.2 Hz, 1H, CH_2), 1.79 (s, 1H, CH_2), 1.57 (s, 1H, CH_2);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 194.3, 158.4, 155.3, 153.5, 151.6, 145.3, 138.5, 131.9, 130.8, 129.8, 121.1, 119.0, 112.5, 92.5, 70.3, 36.1, 32.1, 20.7, 18.5;
HRMS (ESI) m/z: calc. for $C_{25}H_{19}Br_2N_5O$: 563.9854; [M-H$^-$] found: 563.9844.

2,4-Diamino-10-(4-bromophenyl)-5-(4-chlorophenyl)-5,6,7,8,9,10-hexahydro-6-oxobenzo[b][1,8]naphthyridine-3-carbonitrile(5b)



Pale yellow solid, mp: >300 ^{o}C;
IR (KBr, ν, cm^{-1}): 3479, 3366 (νNH_2), 3357, 3240 (νNH_2), 2202 (νCN), 1607 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.69 (d, J = 7.2 Hz, 2H, ArH), 7.41 (d, J = 7.2 Hz, 2H, ArH), 7.28 (s, 4H, ArH), 6.30 (s, 2H, NH_2), 5.94 (s, 2H, NH_2), 5.27 (s, 1H, CH), 2.19 (s, 3H, CH_2), 1.94 (d, J = 17.6 Hz, 1H, CH_2), 1.79 (s, 1H, CH_2), 1.58 (s, 1H, CH_2);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 194.3, 158.4, 155.3, 153.5, 151.6, 144.9, 138.5, 131.9, 130.5, 129.4, 127.9, 121.1, 116.7, 112.6, 92.5, 70.3, 32.0, 28.3, 20.7;
HRMS (ESI) m/z: calc. for $C_{25}H_{19}BrClN_5O$: 520.0357; [M-H$^-$] found: 520.0375.

2,4-Diamino-10-(4-bromophenyl)-5,6,7,8,9,10-hexahydro-6-oxo-5-p-tolylbenzo[b][1,8]naphthyridine-3-carbonitrile(5c)

Pale yellow solid, mp: 295-296 ^{o}C;
IR (KBr, ν, cm^{-1}): 3481, 3394 (νNH_2), 3360 (νNH_2), 2200 (νCN), 1608 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.68 (d, J = 7.2 Hz, 2H, ArH), 7.25

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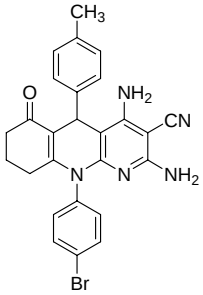
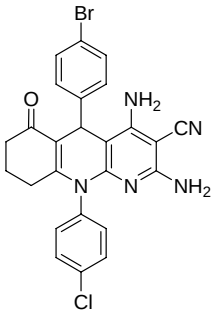


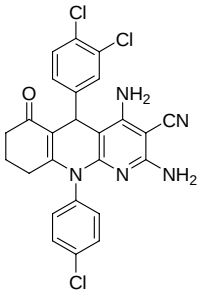
(s, 4H, ArH), 7.02 (d, J = 6.8 Hz, 2H, ArH), 6.17 (s, 2H, NH_2), 5.88 (s, 2H, NH_2), 5.18 (s, 1H, CH), 2.22 (s, 3H, CH_3), 2.18(s, 3H, CH_2) 1.94 (d, J = 16.4 Hz, 1H, CH_2), 1.78 (s, 1H, CH_2), 1.56 (s, 1H, CH_2);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 194.3, 158.2, 153.0, 151.6, 143.0, 138.6, 134.9, 132.5, 132.4, 131.9, 131.8, 128.6, 127.4, 121.0, 116.7, 113.2, 93.3, 70.4, 36.1, 32.2, 28.2, 20.8, 20.6;
HRMS (ESI) m/z: calc. for $C_{26}H_{22}BrN_5O$: 500.0907; [M-H$^-$] found: 500.0896.

2,4-Diamino-5-(4-bromophenyl)-10-(4-chlorophenyl)-5,6,7,8,9,10-hexahydro-6-oxobenzo[b][1,8]naphthyridine-3-carbonitrile (5d)



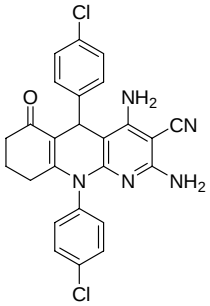
Pale yellow solid, mp: >300 ^{o}C;
IR (KBr, ν, cm^{-1}): 3450, 3389 (νNH$_2$), 3346 (νNH$_2$), 2193 (νCN), 1604 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.55 (d, J = 8.4 Hz, 2H, ArH), 7.42 (d, J = 8.4 Hz, 2H, ArH), 7.39 – 7.30 (m, 4H, ArH), 6.31 (s, 2H, NH_2), 5.94 (s, 2H, NH_2), 5.26 (s, 1H, CH), 2.30 – 2.12 (m, 3H, CH_2), 1.94 (d, J = 17.6 Hz, 1H, CH_2), 1.79 (d, J = 8.4, 1H, CH_2), 1.58 (s, 1H, CH_2);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 194.3, 158.4, 155.3, 153.6, 151.7, 145.3, 138.1, 132.5, 130.8, 129.8, 129.0, 119.0, 116.7, 112.5, 92.5, 79.2, 70.4, 56.0, 36.1, 32.1, 28.3, 20.7, 18.5;
HRMS (ESI) m/z: calc. for $C_{25}H_{19}BrClN_5O$: 520.0357; [M-H$^-$] found:520.0360.

2,4-Diamino-5-(3,4-dichlorophenyl)-10-(4-chlorophenyl)-5,6,7,8,9,10-hexahydro-6-oxobenzo[b][1,8]naphthyridine-3-carbonitrile (5e)



Pale yellow solid, mp: >300 ^{o}C;
IR (KBr, ν, cm^{-1}): 3441, 3389 (νNH$_2$), 3362 (νNH$_2$), 2194 (νCN), 1617 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.75 (s, 1H, ArH), 7.56 (d, J = 8.4 Hz, 2H, ArH), 7.49 (d, J = 8.4 Hz, 1H, ArH), 7.33 (d, J = 8.0 Hz, 2H, ArH), 7.26 (d, J = 8.0 Hz, 1H, ArH), 6.40 (s, 2H, NH_2), 5.98 (s, 2H, NH_2), 5.29 (s, 1H, CH), 2.19 (s, 3H, CH_2), 1.95 (d, J = 17.6 Hz, 1H, CH_2), 1.79 (s, 1H, CH_2), 1.59 (s, 1H, CH_2);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 194.4, 158.5, 155.4, 153.9, 151.7, 146.8, 138.0, 132.6, 130.5, 130.0, 129.9, 129.0, 128.4, 127.6, 116.6, 112.0, 91.9, 70.4, 36.0, 32.1, 28.3, 20.7;
HRMS (ESI) m/z: calc. for $C_{25}H_{18}Cl_3N_5O$: 508.0499; [M-H$^-$] found: 508.0513.

2,4-diamino-5,10-bis(4-chlorophenyl)-5,6,7,8,9,10-hexahydro-6-oxobenzo[b][1,8]naphthyridine-3-carbonitrile(5f)



Pale yellow solid, mp: >300 ^{o}C;
IR (KBr, ν, cm^{-1}): 3442, 3392 (νNH$_2$), 3369 (νNH$_2$), 2201 (νCN), 1614 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.55 (d, J = 8.8 Hz, 2H, ArH), 7.45 – 7.37 (m, 2H, ArH), 7.33 (d, J = 8.4 Hz, 2H, ArH), 7.31 – 7.24 (m, 2H, ArH), 6.31 (s, 2H, NH_2), 5.94 (s, 2H, NH_2), 5.26 (s, 1H, CH), 2.23 – 2.15 (m, 3H,

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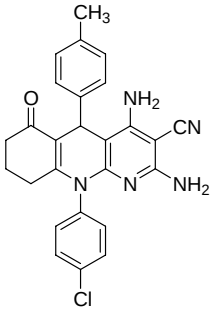
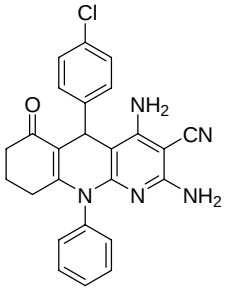
CH_2), 2.00–1.89 (m, 1H, CH_2), 1.79 (s, 1H, CH_2), 1.57 (s, 1H, CH_2);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 194.3, 158.4, 155.3, 153.5, 151.7, 144.9, 138.1, 132.5, 130.5, 129.4, 129.0, 127.9, 116.7, 112.6, 92.6, 78.9, 78.6, 70.4, 36.1, 32.0, 28.3, 20.7;
HRMS (ESI) m/z: calc. for $C_{25}H_{19}Cl_2N_5O$: 474.0888; [M-H$^-$] found: 474.0886.

2,4-Diamino-10-(4-chlorophenyl)-5,6,7,8,9,10-hexahydro-6-oxo-5-p-tolylbenzo[b][1,8]naphthyridine-3-carbonitrile(5g)



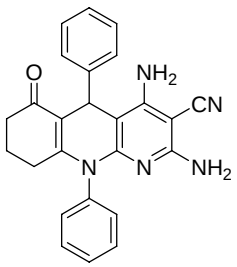
Pale yellow solid, mp: >300 °C;
IR (KBr, ν, cm^{-1}): 3447, 3385 (νNH$_2$), 3357 (νNH$_2$), 2200 (νCN), 1614 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.56 (d, J = 8.4 Hz, 2H, ArH), 7.41 – 7.16 (m, 4H, ArH), 7.03 (d, J = 7.2 Hz, 2H, ArH), 6.19 (s, 2H, NH$_2$), 5.90 (s, 2H, NH$_2$), 5.19 (s, 1H, CH), 2.22 (s, 3H, CH_3), 2.18 (s, 3H, CH_2), 1.94 (d, J = 17.6 Hz, 1H), 1.79 (s, 1H, CH_2), 1.57 (s, 1H, CH_2);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 194.3, 158.3, 155.2, 153.1, 151.7, 143.0, 138.2, 134.9, 132.4, 129.0, 128.6, 127.4, 116.7, 113.2, 93.2, 70.3, 36.1, 32.2, 28.2, 20.8, 20.6;
HRMS (ESI) m/z: calc. for $C_{26}H_{22}ClN_5O$: 454.1435; [M-H$^-$] found: 454.1435.

2,4-Diamino-5-(4-chlorophenyl)-5,6,7,8,9,10-hexahydro-6-oxo-10-phenylbenzo[b][1,8]naphthyridine-3-carbonitrile(5h)



Pale yellow solid, mp: 290-291 °C;
IR (KBr, ν, cm^{-1}): 3442, 3358 (νNH$_2$), 3246 (νNH$_2$), 2193 (νCN), 1607 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.50 (t, J = 7.2 Hz, 2H, ArH), 7.46 – 7.38 (m, 3H, ArH), 7.32 – 7.24 (m, 4H, ArH), 6.27 (s, 2H, NH$_2$), 5.84 (s, 2H, NH$_2$), 5.27 (s, 1H, CH), 2.19 (s, 3H, CH_2), 1.92 (s, 1H, CH_2), 1.76 (s, 1H, CH_2), 1.56 (s, 1H, CH_2);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 194.3, 158.4, 155.2, 153.9, 151.9, 145.0, 139.2, 130.4, 129.3, 129.0, 128.0, 127.9, 116.7, 112.4, 92.7, 70.3, 36.1, 32.0, 28.3, 20.7;
HRMS (ESI) m/z: calc. for $C_{25}H_{20}ClN_5O$: 440.1278; [M-H$^-$] found: 440.1694.

2,4-Diamino-5,6,7,8,9,10-hexahydro-6-oxo-5,10-diphenylbenzo[b][1,8]naphthyridine-3-carbonitrile(5i)



Pale yellow solid, mp: 288-289 °C;
IR (KBr, ν, cm^{-1}): 3441, 3355 (νNH$_2$), 3239 (νNH$_2$), 2197 (νCN), 1617 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.50 (t, J = 7.4 Hz, 2H, ArH), 7.46 – 7.38 (m, 3H, ArH), 7.31 – 7.26 (m, 2H, ArH), 7.23 (d, J = 7.6 Hz, 2H, ArH), 7.12 (t, J = 7.2 Hz, 1H, ArH), 6.21 (s, 2H, NH$_2$), 5.82 (s, 2H, NH$_2$), 5.24 (s, 1H, CH), 2.18 (d, J = 4.4 Hz, 3H, CH_2), 1.91 (d, J = 17.6 Hz, 1H, CH_2), 1.77 (d, J = 4.8 Hz, 1H, CH_2), 1.61 – 1.48 (m, 1H, CH_2);

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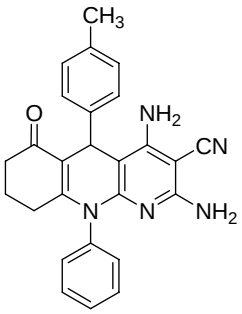
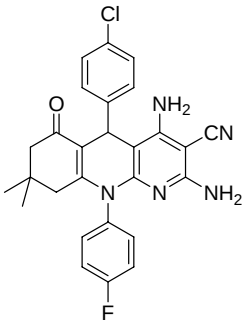
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 194.3, 158.3, 155.2, 153.7, 151.9, 146.1, 139.3, 129.0, 128.0, 127.5, 125.9, 116.8, 112.9, 112.7, 93.2, 70.3, 36.1, 32.6, 28.2, 20.8;
HRMS (ESI) m/z: calc. for$C_{25}H_{21}N_5O$: 406.1668; [M-H$^-$] found: 406.1694.

2,4-Diamino-5,6,7,8,9,10-hexahydro-6-oxo-10-phenyl-5-p-tolylbenzo[b][1,8]naphthyridine-3-carbonitrile (5j)



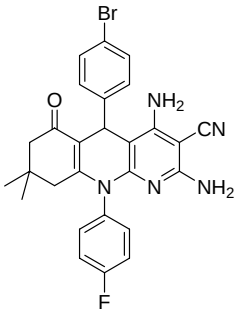
Pale yellow solid, mp: 293-294 ^{o}C;
IR (KBr, ν, cm^{-1}): 3440, 3386 (νNH$_2$), 3358, 3254 (νNH$_2$), 2194 (νCN), 1614 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.51 (t, J = 7.2 Hz, 2H, ArH), 7.43 (t, J = 7.2 Hz, 1H, ArH), 7.28 (t, J = 6.4 Hz, 4H, ArH), 7.04 (d, J = 7.6 Hz, 2H, ArH), 6.18 (s, 2H, NH$_2$), 5.82 (s, 2H, NH$_2$), 5.19 (s, 1H, CH), 2.23 (s, 3H, CH$_3$), 2.18 (d, J = 4.4 Hz, 3H, CH$_2$), 1.90 (d, J = 17.6 Hz, 1H, CH$_2$), 1.84 – 1.72 (m, 1H, CH$_2$), 1.56 (s, 1H, CH$_2$);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 194.3, 158.2, 155.1, 153.5, 151.8, 143.1, 139.3, 134.9, 129.0, 128.6, 127.9, 127.3, 116.8, 113.0, 93.3, 70.3, 36.1, 32.1, 28.2, 20.6.
HRMS (ESI) m/z: calc. for $C_{26}H_{23}N_5O$: 420.1824; [M-H$^-$] found: 420.1827.

2,4-Diamino-5-(4-chlorophenyl)-10-(4-fluorophenyl)-5,5a,6,7,8,9,9a,10-octahydro-8,8-dimethyl-6-oxobenzo[*b*][1,8]naphthyridine-3-carbonitrile(5k)



Pale yellow solid, mp: >300 ^{o}C;
IR (KBr, ν, cm^{-1}): 3445, 3394 (νNH$_2$), 3340, 3230 (νNH$_2$), 2220 (νCN), 1607 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.42 (d, J = 7.6 Hz, 2H, ArH), 7.38 – 7.24 (m, 6H, ArH), 6.28 (s, 2H, NH$_2$), 5.89 (s, 2H, NH$_2$), 5.24 (s, 1H, CH), 2.19 (d, J = 15.2 Hz, 2H, CH$_2$), 1.98 (d, J = 16.4 Hz, 1H, CH$_2$), 1.76 (d, J = 17.6 Hz, 1H, CH$_2$), 0.87 (s, 3H, CH$_3$), 0.66 (s, 3H, CH$_3$);
HRMS (ESI) m/z: calc. for $C_{27}H_{24}ClFN_5O$: 488.1647; [M-H$^-$] found: 488.1622.

2,4-Diamino-5-(4-bromophenyl)-10-(4-fluorophenyl)-5,6,7,8,9,10-hexahydro-8,8-dimethyl-6-oxobenzo[b][1,8]naphthyridine-3-carbonitrile (5l)



Pale yellow solid, mp: >300 ^{o}C;
IR (KBr, ν, cm^{-1}): 3446, 3390 (νNH$_2$), 3342, 3235 (νNH$_2$), 2199 (νCN), 1609 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.42 (d, J = 7.6 Hz, 2H, ArH), 7.39–7.28 (m, 6H, ArH), 6.28 (s, 2H, NH$_2$), 5.89 (s, 2H, NH$_2$), 5.23 (s, 1H, CH), 2.19 (d, J = 15.2 Hz, 2H, CH$_2$), 1.98 (d, J = 16.0 Hz, 1H, CH$_2$), 1.76 (d, J = 17.6 Hz, 1H, CH$_2$), 0.87 (s, 3H, CH$_3$), 0.67 (s, 3H, CH$_3$);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 199.2, 165.5 (J_{CF} = 243.0 Hz), 163.6, 160.5, 157.2, 157.0, 150.2, 140.5 (J_{CF} = 3.0 Hz), 136.0, 135.0, 124.2, 121.8 (J_{CF} = 7.3 Hz), 121.1 (J_{CF} = 22.7 Hz), 116.6, 97.8, 75.6, 54.7, 46.7, 37.4, 37.2, 34.4, 31.3;
HRMS (ESI) m/z: calc. for $C_{27}H_{22}BrFN_5O$: 532.0969; [M-H$^-$] found: 532.0936.

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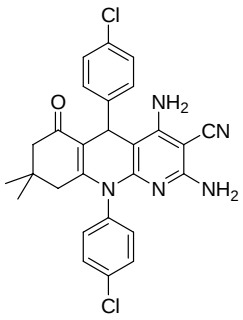
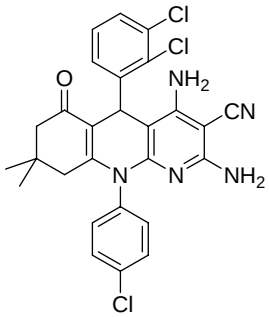
2,4-Diamino-5,10-bis(4-chlorophenyl)-5,6,7,8,9,10-hexahydro-8,8-dimethyl-6-oxobenzo[b][1,8]naphthyridine-3-carbonitrile(5m)



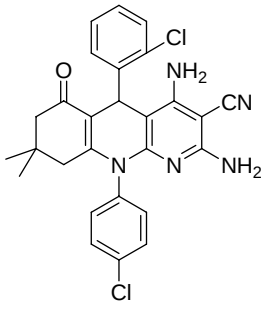
Pale yellow solid, mp: >300 ^{o}C;
IR (KBr, ν, cm^{-1}): 3446, 3397 (νNH$_2$), 3343, 3237 (νNH$_2$), 2198 (νCN), 1609 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.57 (d, J = 8.4 Hz, 2H, ArH), 7.43 (d, J = 8.4 Hz, 2H, ArH), 7.30 (q, 4H, ArH), 6.30 (s, 2H, NH$_2$), 5.93 (s, 2H, NH$_2$), 5.25 (s, 1H, CH), 2.20 (q, 2H, CH$_2$), 1.99 (d, J = 16.0 Hz, 1H, CH$_2$), 1.77 (d, J = 17.2 Hz, 1H, CH$_2$), 0.87 (s, 3H, CH$_3$), 0.67 (s, 3H, CH$_3$);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm):194.0, 158.3, 155.3, 152.2, 151.8, 144.8, 138.0, 132.6, 131.7, 129.5, 129.2, 128.6, 128.1, 116.3, 91.8, 70.5, 49.3, 41.6, 34.3, 31.9, 29.1, 26.0;
HRMS (ESI) m/z: calc. for $C_{27}H_{22}Cl_2N_5O$: 502.1201; [M-H$^-$] found: 502.1193.

2,4-Diamino-5-(2,3-dichlorophenyl)-10-(4-chlorophenyl)-5,6,7,8,9,10-hexahydro-8,8-dimethyl-6-oxobenzo[b][1,8]naphthyridine-3-carbonitrile(5n)



Pale yellow solid, mp: >300 ^{o}C;
IR (KBr, ν, cm^{-1}): 3441, 3397 (νNH$_2$), 3343, 3237 (νNH$_2$), 2197 (νCN), 1609 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.66 (d, J = 7.6 Hz, 1H, ArH), 7.58 (d, J = 8.4 Hz, 2H, ArH), 7.46 (d, J = 7.6 Hz, 1H, ArH), 7.41 – 7.27 (m, 3H, ArH), 6.01 (s, 2H, NH$_2$), 5.86 (s, 2H, NH$_2$), 5.40 (s, 1H, CH), 2.18 (q, 2H, CH$_2$), 1.94 (d, J = 16.0 Hz, 1H, CH$_2$), 1.83 (d, J = 17.2 Hz, 1H, CH$_2$), 0.88 (s, 3H, CH$_3$), 0.73 (s, 3H, CH$_3$);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm):194.0, 158.3, 155.2, 151.8, 151.3, 145.6, 138.1, 132.5, 129.1, 127.9, 127.4, 126.0, 111.9, 93.2, 70.3, 49.5, 41.4, 32.7, 31.9, 29.2, 25.9;
HRMS (ESI) m/z: calc. for $C_{27}H_{21}Cl_3N_5O$: 536.0812; [M-H$^-$] found: 536.0798.

2,4-Diamino-5-(2-chlorophenyl)-10-(4-chlorophenyl)-5,6,7,8,9,10-hexahydro-8,8-dimethyl-6-oxobenzo[b][1,8]naphthyridine-3-carbonitrile(5o)



Pale yellow solid, mp: >300 ^{o}C;
IR (KBr, ν, cm^{-1}): 3451, 3394 (νNH$_2$), 3338, 3231 (νNH$_2$), 2200 (νCN), 1604(νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.64 (d, J = 7.6 Hz, 1H, ArH), 7.59 (d, J = 7.6 Hz, 2H, ArH), 7.40 – 7.26 (m, 4H, ArH), 7.18 (t, J = 7.2 Hz, 1H, ArH), 5.96 (s, 2H, NH$_2$), 5.86 (s, 2H, NH$_2$), 5.30 (s, 1H, CH), 2.25 – 2.12 (m, 2H, CH$_2$), 1.93 (d, J = 16.4 Hz, 1H, CH$_2$), 1.82 (d, J = 17.6 Hz, 1H, CH$_2$), 0.88 (s, 3H, CH$_3$), 0.73 (s, 3H, CH$_3$);
HRMS (ESI) m/z: calc. for $C_{27}H_{22}Cl_2N_5O$: 502.1201; [M-H$^-$] found: 502.1189.

2,4-Diamino-10-(4-chlorophenyl)-5,6,7,8,9,10-hexahydro-8,8-dimethyl-6-oxo-5-phenylbenzo[b][1,8]naphthyridine-3-carbonitrile(5p)

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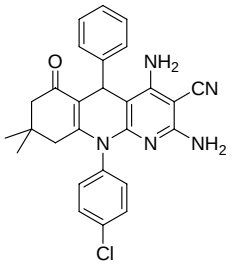
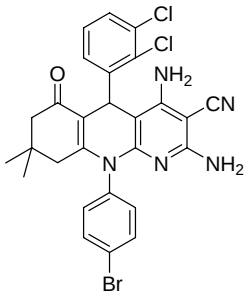


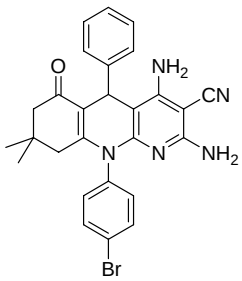
Pale yellow solid, mp: 287-288 °C;
IR (KBr, ν, cm^{-1}): 3452, 3381 (νNH$_2$), 3356, 3253 (νNH$_2$), 2195 (νCN), 1609 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.57 (d, J = 8.4 Hz, 2H, ArH), 7.41 (d, J = 7.2 Hz, 2H, ArH), 7.30 (d, J = 8.4 Hz, 2H, ArH), 7.23 (t, J = 7.6 Hz, 2H, ArH), 7.11 (t, J = 7.2 Hz, 1H, ArH), 6.23 (s, 2H, NH$_2$), 5.90 (s, 2H, NH$_2$), 5.21 (s, 1H, CH), 2.19 (d, J = 16.4 Hz, 2H, CH$_2$), 1.98 (d, J = 16.0 Hz, 1H, CH$_2$), 1.78 (d, J = 17.2 Hz, 1H, CH$_2$), 0.87 (s, 3H, CH$_3$), 0.67 (s, 3H, CH$_3$);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 194.1, 158.3, 155.2, 151.8, 151.3, 145.6, 138.1, 132.5, 129.2, 127.9, 127.4, 126.0, 116.7, 111.9, 93.2, 70.4, 49.5, 41.4, 32.7, 32.0, 30.7, 29.2, 25.9, 25.4;
HRMS (ESI) m/z: calc. for $C_{27}H_{23}ClN_5O$: 468.1591; [M-H$^-$] found: 468.1589.

2,4-Diamino-10-(4-bromophenyl)-5-(2,3-dichlorophenyl)-5,6,7,8,9,10-hexahydro-8,8-dimethyl-6-oxobenzo[b][1,8]naphthyridine-3-carbonitrile(5q)



Pale yellow solid, mp: >300 °C;
IR (KBr, ν, cm^{-1}): 3467, 3379 (νNH$_2$), 3347, 3252 (νNH$_2$), 2192 (νCN), 1603 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.71 (d, J = 8.4 Hz, 2H, ArH), 7.66 (d, J = 7.6 Hz, 1H, ArH), 7.46 (d, J = 8.0 Hz, 1H, ArH), 7.31 (t, J = 7.8 Hz, 3H, ArH), 6.04 (s, 2H, NH$_2$), 5.87 (s, 2H, NH$_2$), 5.39 (s, 1H, CH), 2.17 (q, J = 16.8, 6.5 Hz, 2H, CH$_2$), 1.94 (d, J = 16.0 Hz, 1H, CH$_2$), 1.82 (d, J = 17.2 Hz, 1H, CH$_2$), 0.87 (s, 3H, CH$_3$), 0.72 (s, 3H, CH$_3$);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 199.2, 163.4, 160.5, 157.3, 156.9, 150.0, 143.7, 137.4, 137.0, 135.9, 134.8, 133.8, 133.3, 126.5, 121.5, 115.0, 93.4, 70.4, 54.6, 46.9, 39.5, 37.2, 34.4, 31.4;
HRMS (ESI) m/z: calc. for $C_{27}H_{21}BrCl_2N_5O$: 582.0279; [M-H$^-$] found: 582.0267.

2,4-Diamino-10-(4-bromophenyl)-5,6,7,8,9,10-hexahydro-8,8-dimethyl-6-oxo-5-phenylbenzo[b][1,8]naphthyridine-3-carbonitrile(5r)



Pale yellow solid, mp: 292-293 °C;
IR (KBr, ν, cm-1): 3475, 3379 (νNH$_2$), 3355, 3248 (νNH$_2$), 2203 (νCN), 1609 (νC=O);
^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.70 (d, J = 8.4 Hz, 2H, ArH), 7.40 (d, J = 7.6 Hz, 2H, ArH), 7.23 (t, J = 7.2 Hz, 4H, ArH), 7.11 (t, J = 7.2 Hz, 1H, ArH), 6.21 (s, 2H, NH$_2$), 5.89 (s, 2H, NH$_2$), 5.20 (s, 1H, CH), 2.18 (d, J = 16.0 Hz, 2H, CH$_2$), 1.98 (d, J = 16.0 Hz, 1H, CH$_2$), 1.78 (d, J = 17.2 Hz, 1H, CH$_2$), 0.87 (s, 3H, CH$_3$), 0.67 (s, 3H, CH$_3$);
^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 194.0, 158.3, 155.2, 151.7, 151.2, 145.6, 138.6, 132.1, 127.9, 127.5, 126.0, 121.1, 116.7, 111.9, 93.1, 70.4, 49.5, 41.4, 32.7, 32.0, 29.2, 26.0;
HRMS (ESI) m/z: calc. for $C_{27}H_{23}BrN_5O$: 514.1063; [M-H$^-$] found: 514.1087.

2,4-Diamino-10-(4-bromophenyl)-5,6,7,8,9,10-hexahydro-8,8-dimethyl-6-oxo-5-p-tolylbenzo[b][1,8]naphthyridine-3-carbonitrile(5s)

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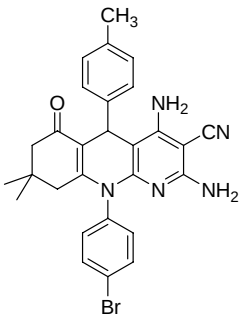


Pale yellow solid, mp: 293-295 ^{o}C;

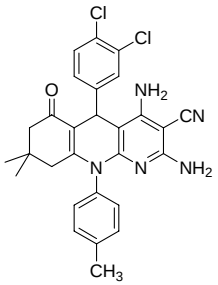
IR (KBr, ν, cm-1): 3463, 3375 (νNH_2), 3351, 3264 (νNH_2), 2198 (νCN), 1603 (νC=O);

^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.69 (d, J = 8.4 Hz, 2H, ArH), 7.27 (d, J = 7.6 Hz, 2H, ArH), 7.22 (d, J = 8.4 Hz, 2H, ArH), 7.02 (d, J = 7.6 Hz, 2H, ArH), 6.17 (s, 2H, NH_2), 5.87 (s, 2H, NH_2), 5.15 (s, 1H, CH), 2.21 (s, 3H, CH_3), 2.15 (q, 2H, CH_2), 1.97 (d, J = 16.4 Hz, 1H, CH_2), 1.77 (d, J = 17.6 Hz, 1H, CH_2), 0.87 (s, 3H, CH_3), 0.68 (s, 3H, CH_3);

^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 194.0, 158.2, 155.2, 151.7, 151.0, 142.7, 138.6, 134.9, 132.1, 128.5, 127.3, 121.1, 116.7, 112.0, 93.3, 70.4, 49.5, 41.4, 32.3, 31.9, 29.2, 26.0, 20.6.

HRMS (ESI) m/z: calc. for $C_{28}H_{25}BrN_5O$: 528.1221; [M-H$^-$] found: 528.1204.

2,4-Diamino-5-(3,4-dichlorophenyl)-5,6,7,8,9,10-hexahydro-8,8-dimethyl-6-oxo-10-p-tolylbenzo[b][1,8]naphthyridine-3-carbonitrile(5t)



Pale yellow solid, mp: >300 ^{o}C;

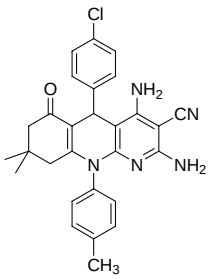
IR (KBr, ν, cm-1): 3471, 3421, 3365, 3215, 2199 (νCN), 1601 (νC=O);

^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.76 (s, 1H, ArH), 7.52 (d, J = 8.0 Hz, 1H, ArH), 7.30 (t, J = 8.8 Hz, 3H, ArH), 7.13 (d, J = 6.4 Hz, 2H, ArH), 6.38 (s, 2H, NH_2), 5.90 (s, 2H, NH_2), 5.27 (s, 1H, CH), 2.39 (s, 3H, CH_3), 2.18 (t, J = 16.0 Hz, 2H, CH_2), 2.00 (d, J = 16.0 Hz, 1H, CH_2), 1.78 (d, J = 17.2 Hz, 1H, CH_2), 0.86 (s, 3H, CH_3), 0.66 (s, 3H, CH_3);

^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 194.0, 158.5, 155.3, 152.5, 152.1, 146.6, 137.3, 136.4, 130.4, 130.0, 129.8, 129.7, 128.3, 127.5, 116.6, 110.7, 92.1, 70.4, 49.3, 41.4, 31.9, 29.1, 26.0, 20.8;

HRMS (ESI) m/z: calc. for $C_{28}H_{24}Cl_2N_5O$: 516.1358; [M-H$^-$] found: 516.1360.

2,4-Diamino-5-(4-chlorophenyl)-5,6,7,8,9,10-hexahydro-8,8-dimethyl-6-oxo-10-p-tolylbenzo[b][1,8]naphthyridine-3-carbonitrile(5u)



Pale yellow solid, mp: 299-300 ^{o}C;

IR (KBr, ν, cm-1): 3446, 3397, 3341, 3235, 2195 (νCN), 1600 (νC=O);

^{1}H NMR (400 MHz, DMSO-d_6) (δ, ppm): 7.42 (d, J = 7.6 Hz, 2H, ArH), 7.31 (s, 4H, ArH), 7.13 (d, J = 6.4 Hz, 2H, ArH), 6.26 (s, 2H, NH_2), 5.85 (s, 2H, NH_2), 5.24 (s, 1H, CH), 2.39 (s, 3H, CH_3), 2.18 (t, J = 15.2 Hz, 2H, CH_2), 1.98 (d, J = 15.6 Hz, 1H, CH_2), 1.76 (d, J = 16.8 Hz, 1H, CH_2), 0.86 (s, 3H, CH_3), 0.66 (s, 3H, CH_3);

^{13}C NMR (100 MHz, DMSO-d_6) (δ, ppm): 193.9, 158.4, 155.2, 152.1, 144.6, 137.2, 136.5, 130.4, 129.6, 129.3, 127.8, 116.7, 111.2, 92.7, 70.3, 49.4, 41.4, 32.1, 31.9, 29.2, 26.0, 20.8;

HRMS (ESI) m/z: calc. for $C_{28}H_{25}ClN_5O$: 482.1748; [M-H$^-$] found: 482.1748.

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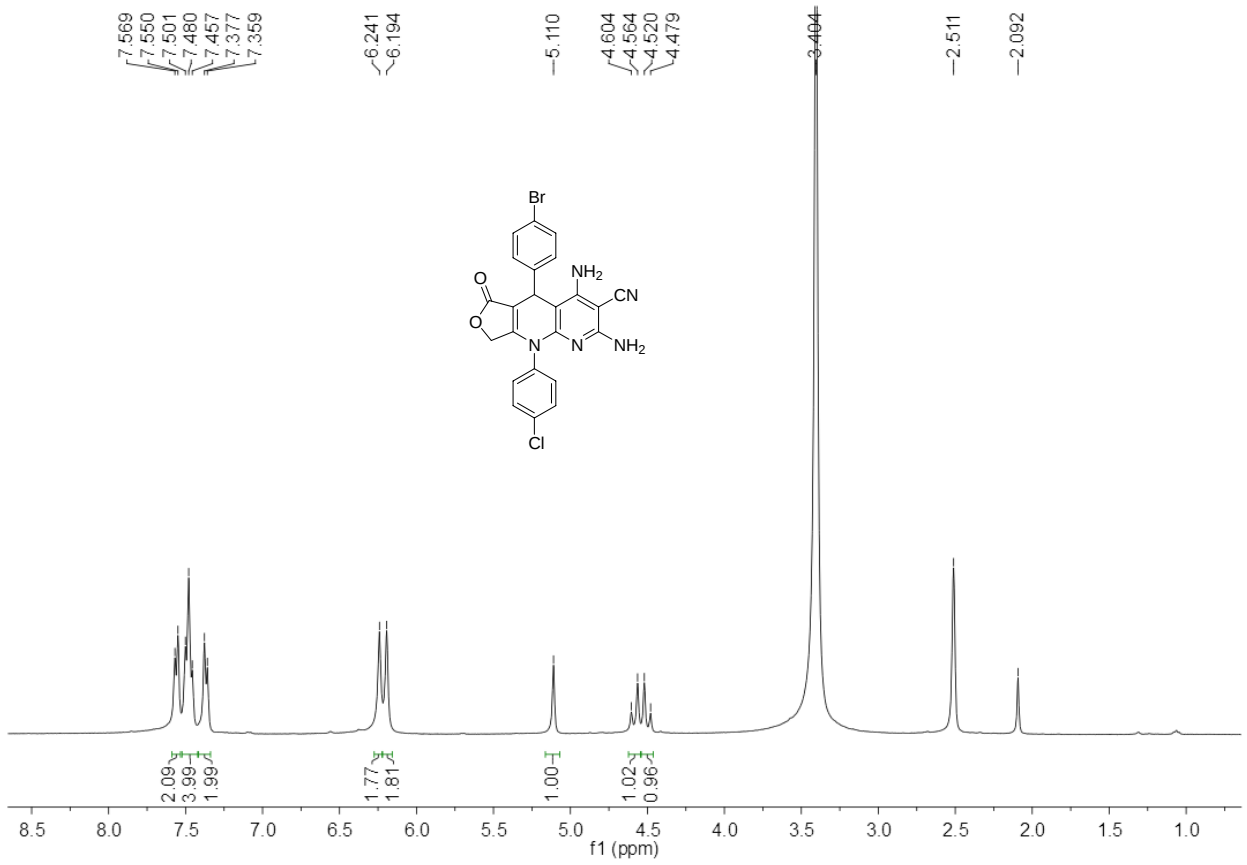
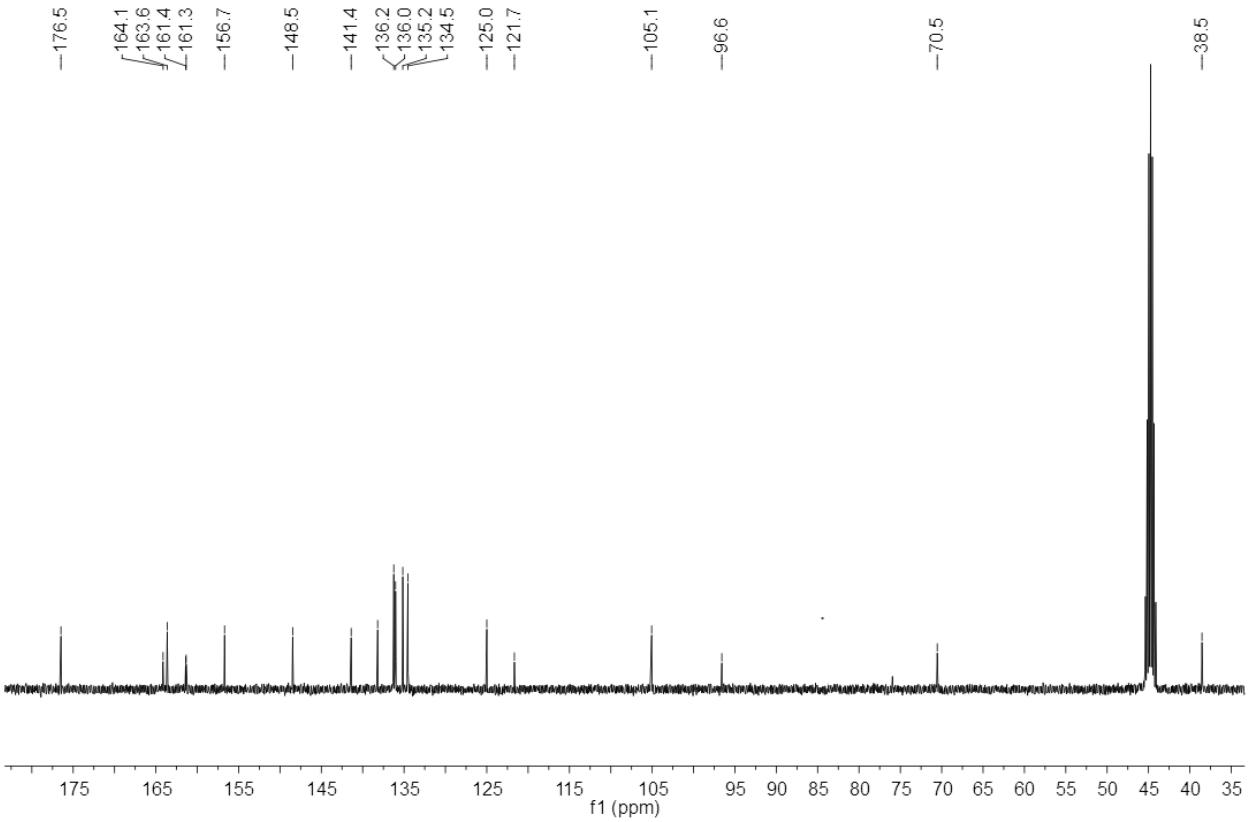


^{1}H NMR Spectrum of Compound 4a



^{13}C NMR Spectrum of Compound 4a

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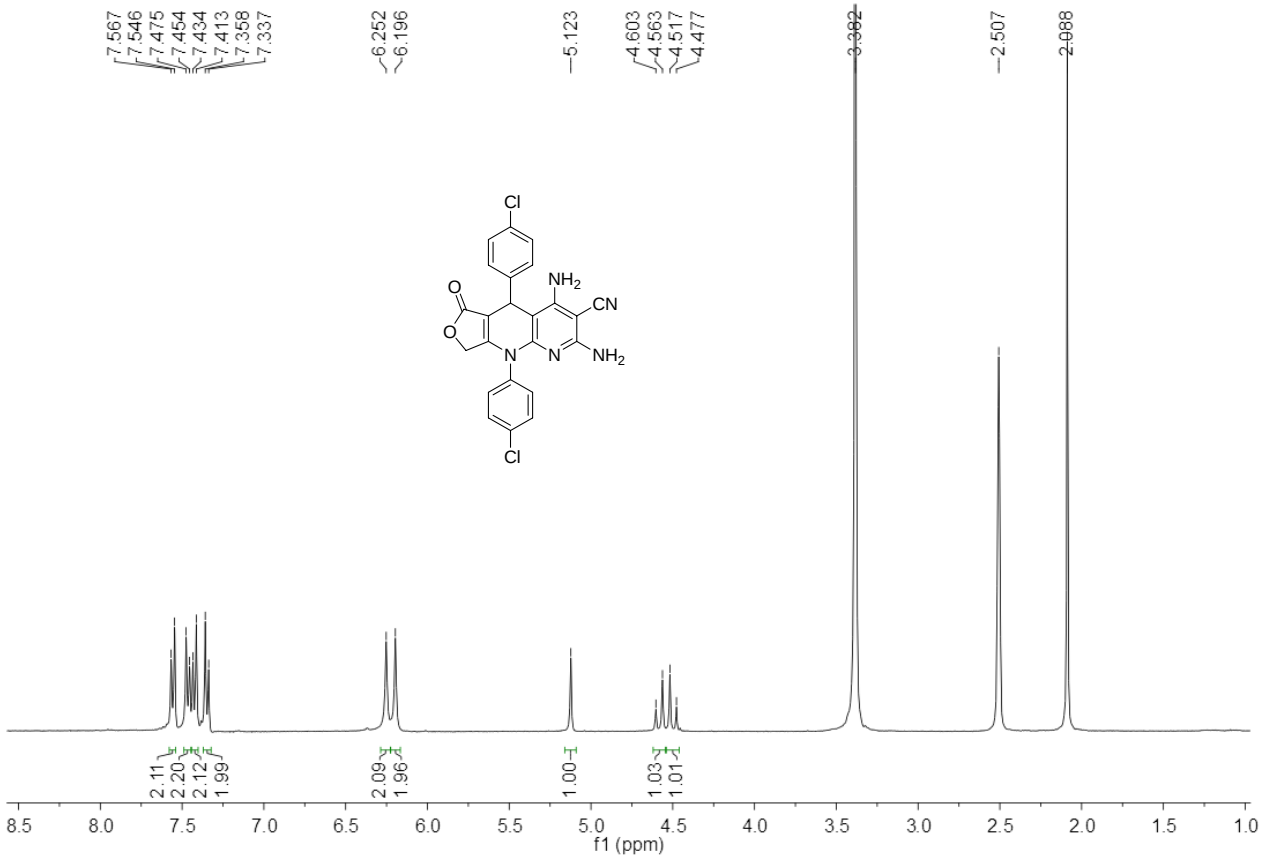
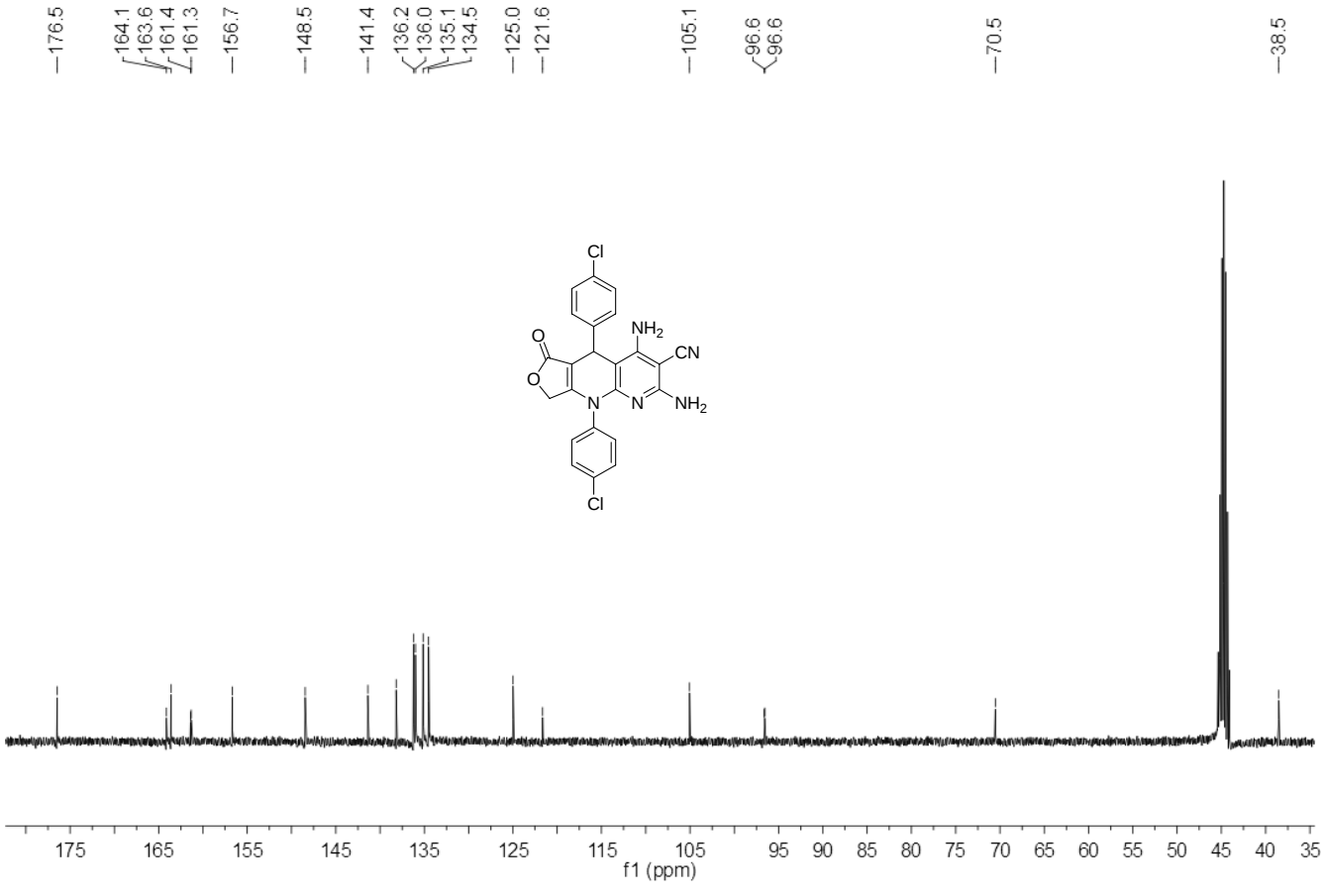


^{1}H NMR Spectrum of Compound 4b



^{13}C NMR Spectrum of Compound 4b

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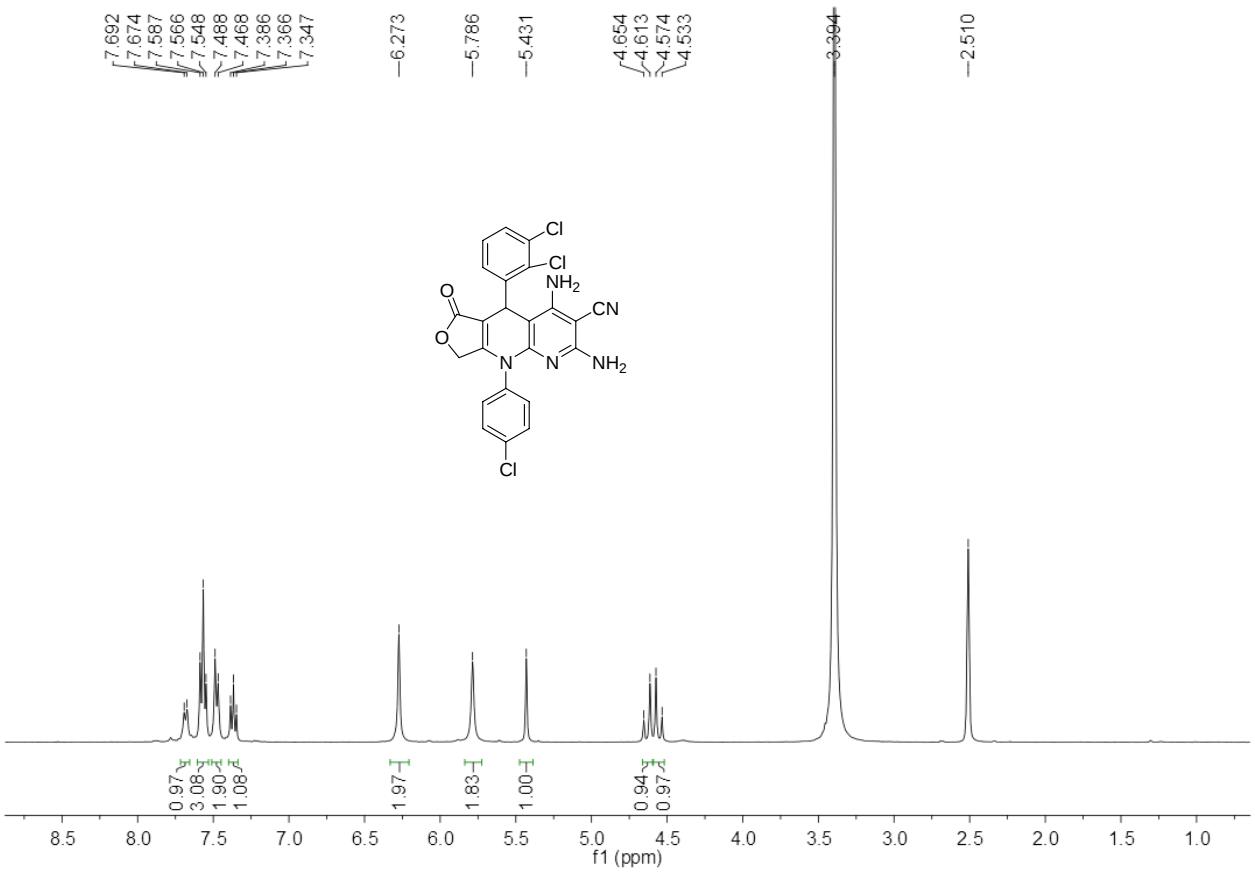
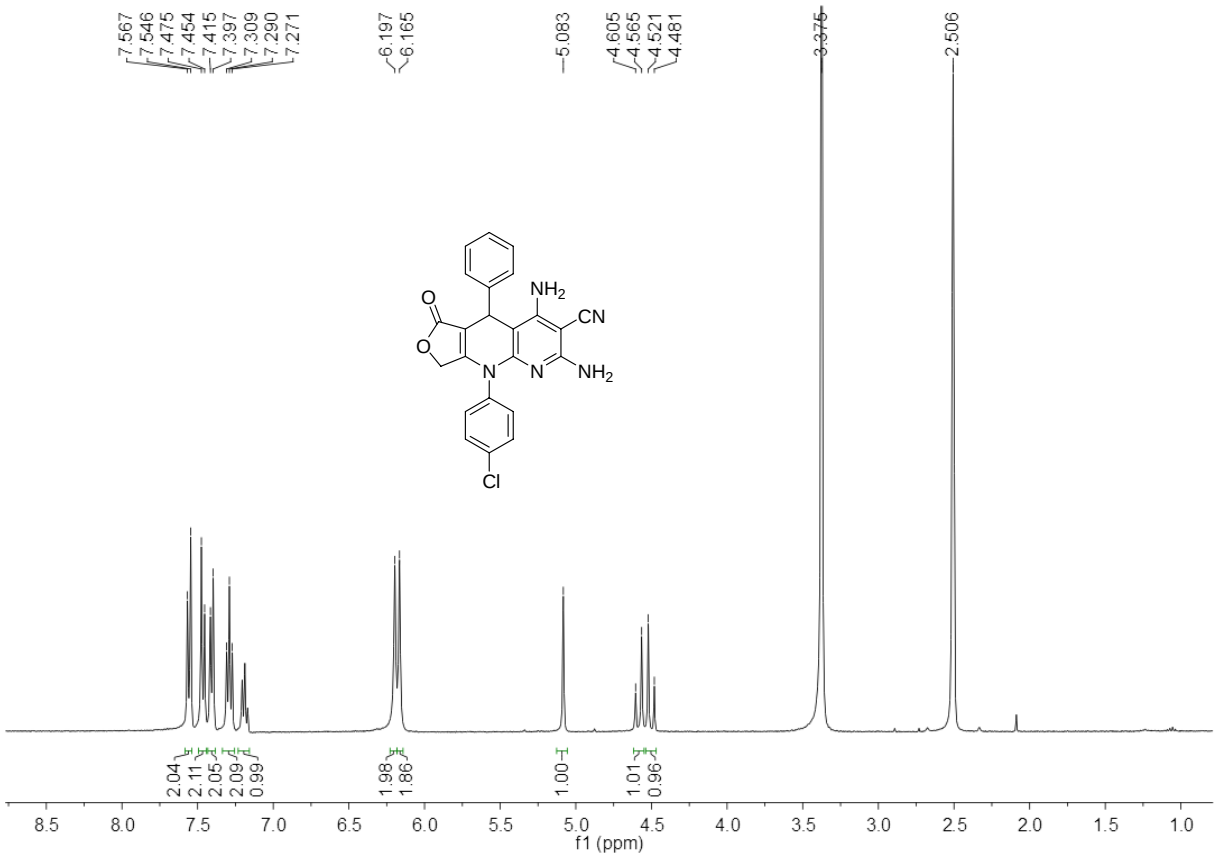


^{1}H NMR Spectrum of Compound 4c



^{1}H NMR Spectrum of Compound 4d

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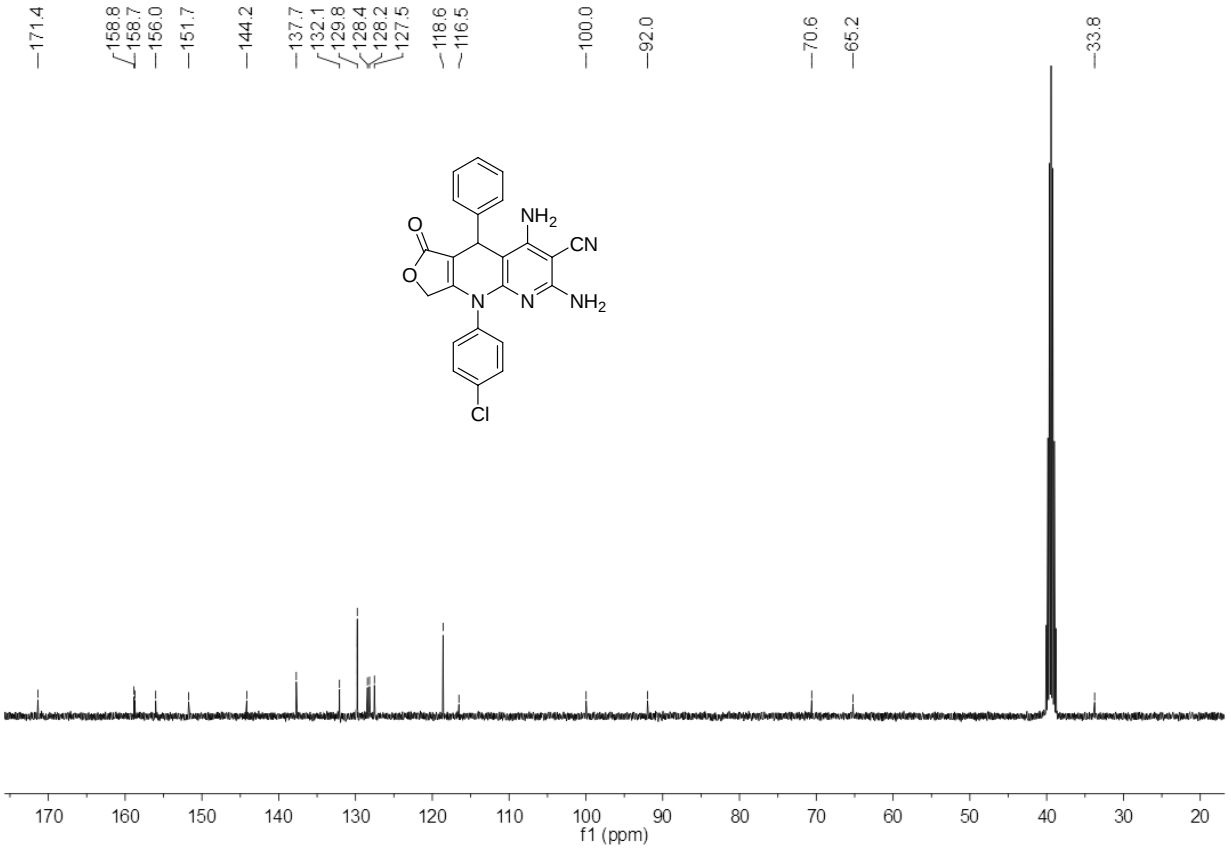
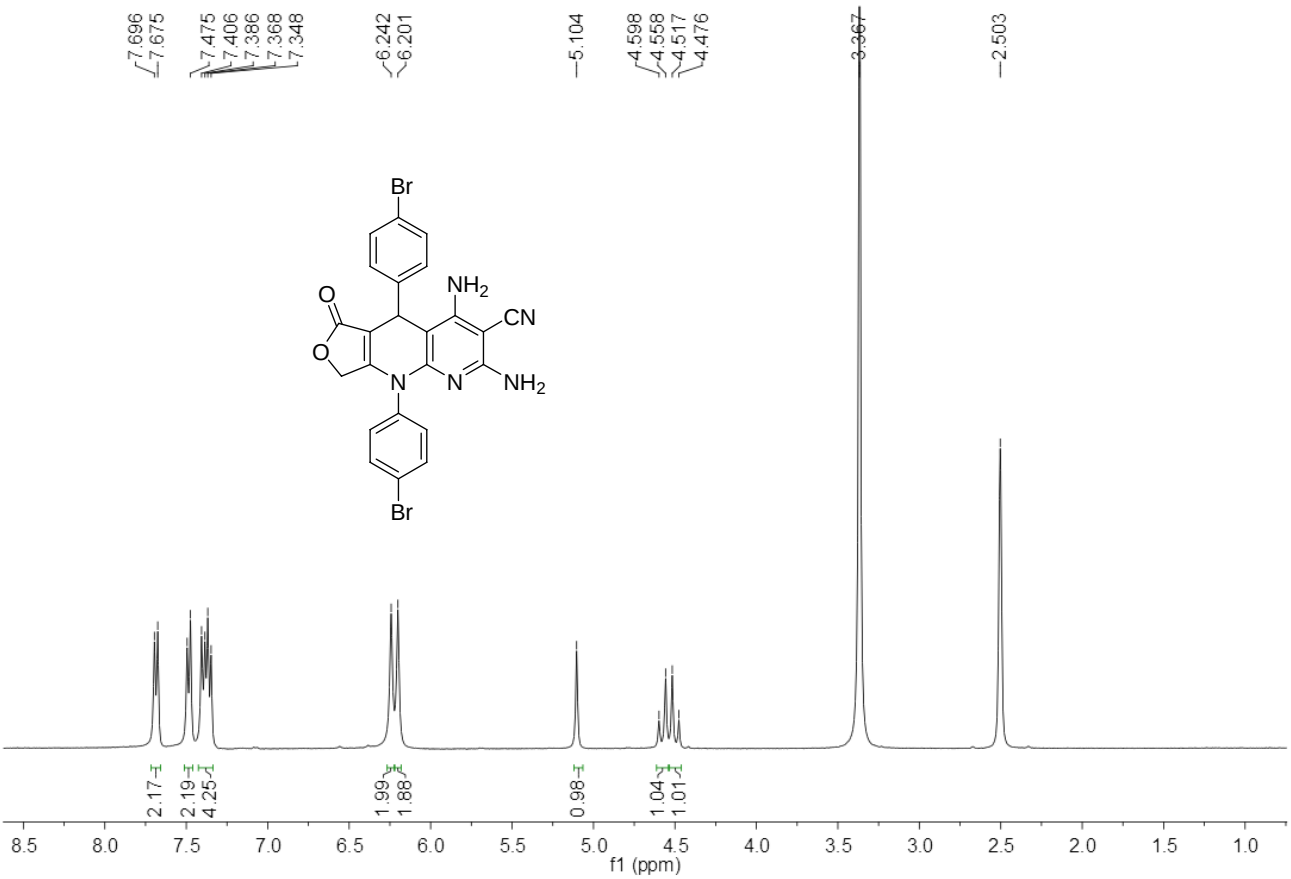


^{13}C NMR Spectrum of Compound 4d



^{1}H NMR Spectrum of Compound 4e

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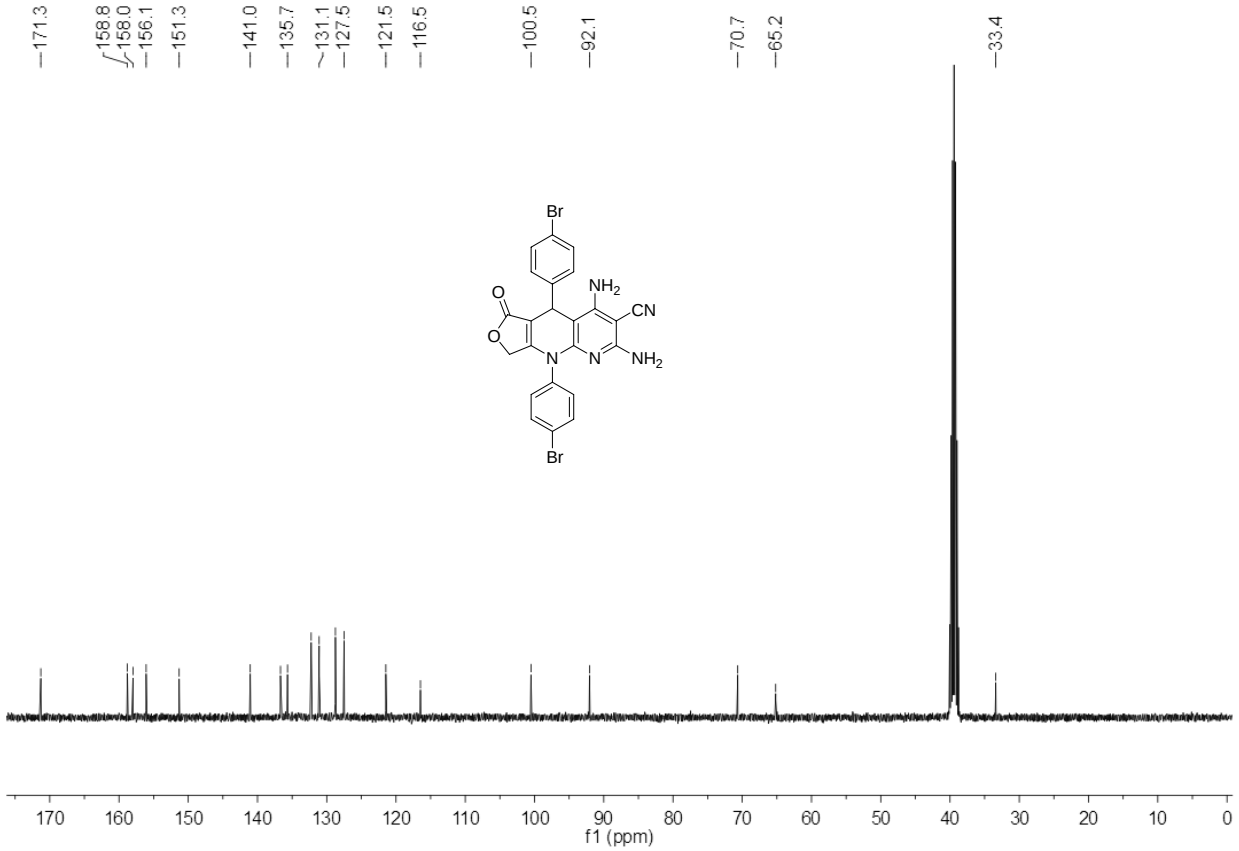
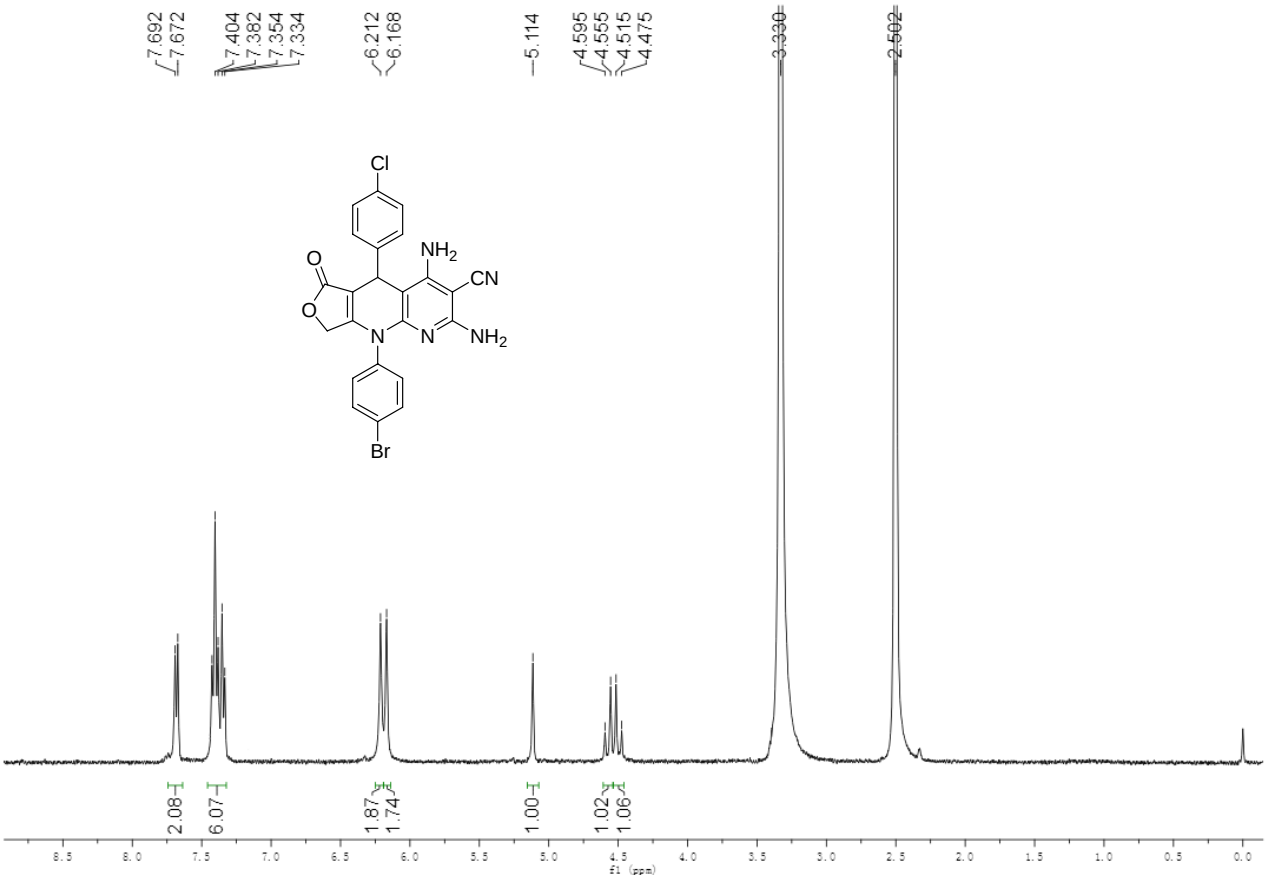


^{13}C NMR Spectrum of Compound 4e



^{1}H NMR Spectrum of Compound 4f

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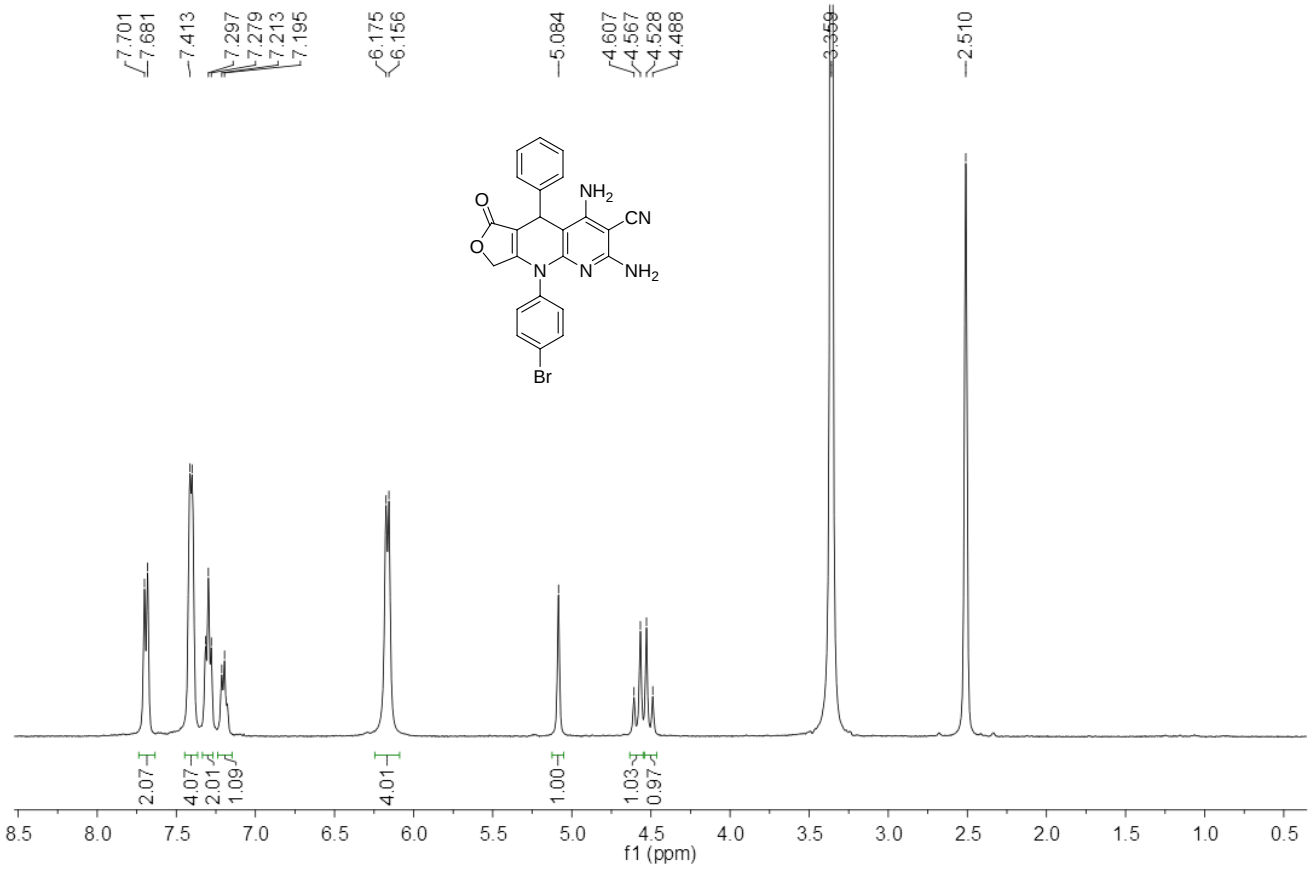
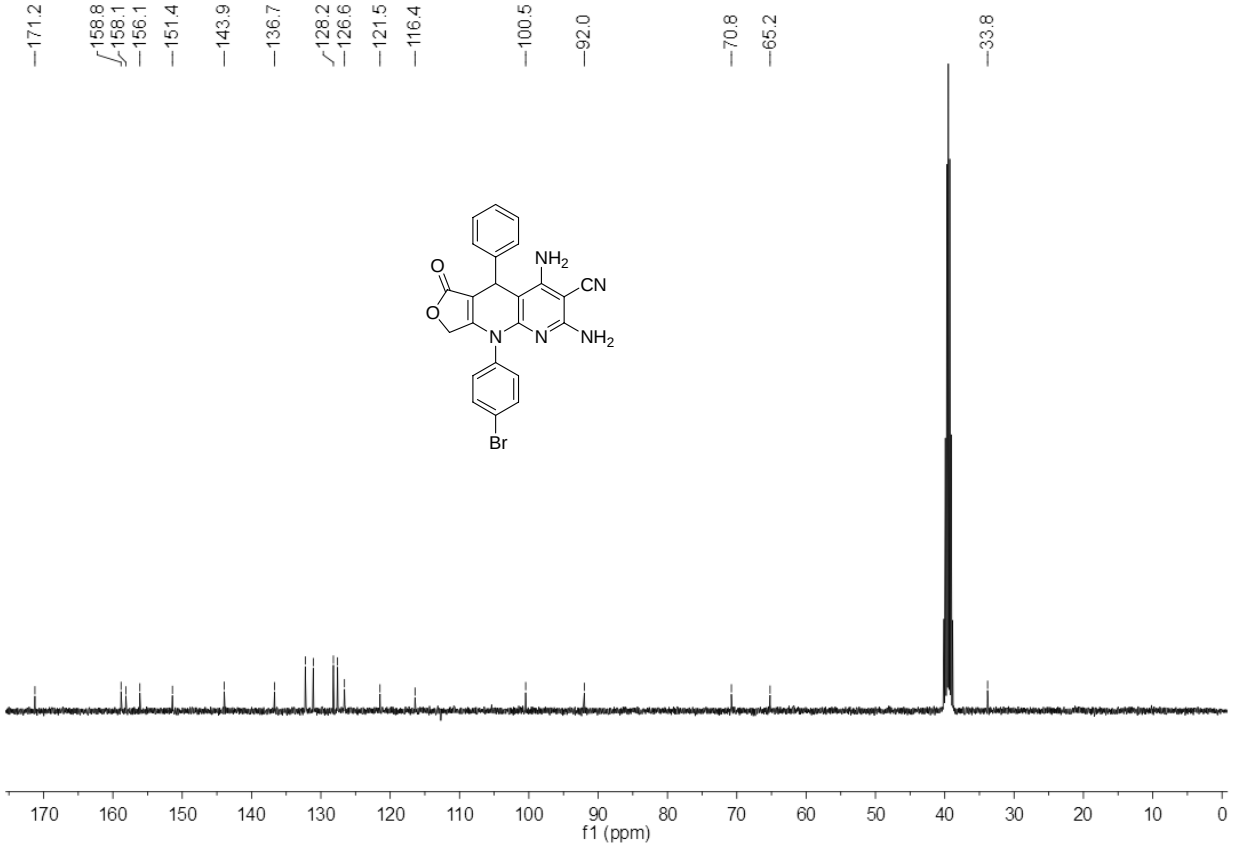


^{1}H NMR Spectrum of Compound 4g



^{13}C NMR Spectrum of Compound 4g

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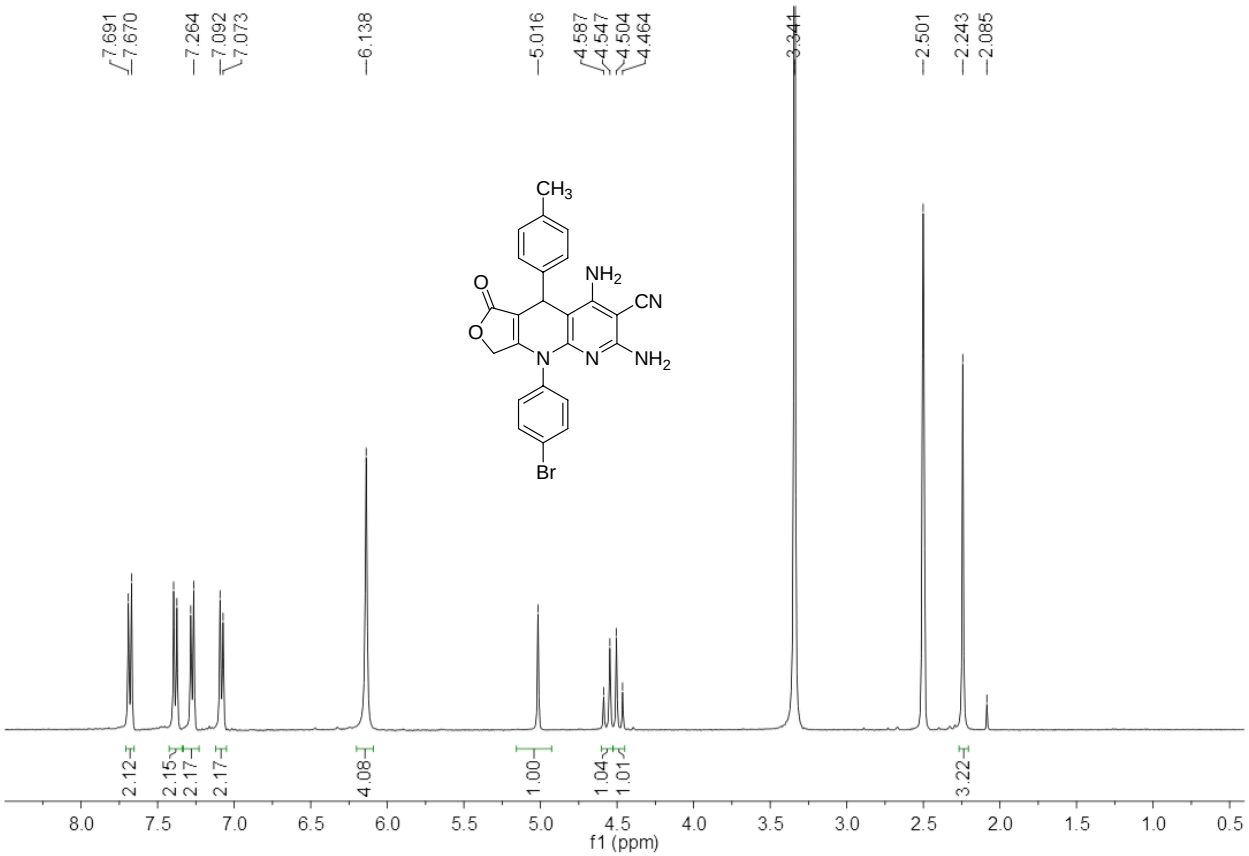
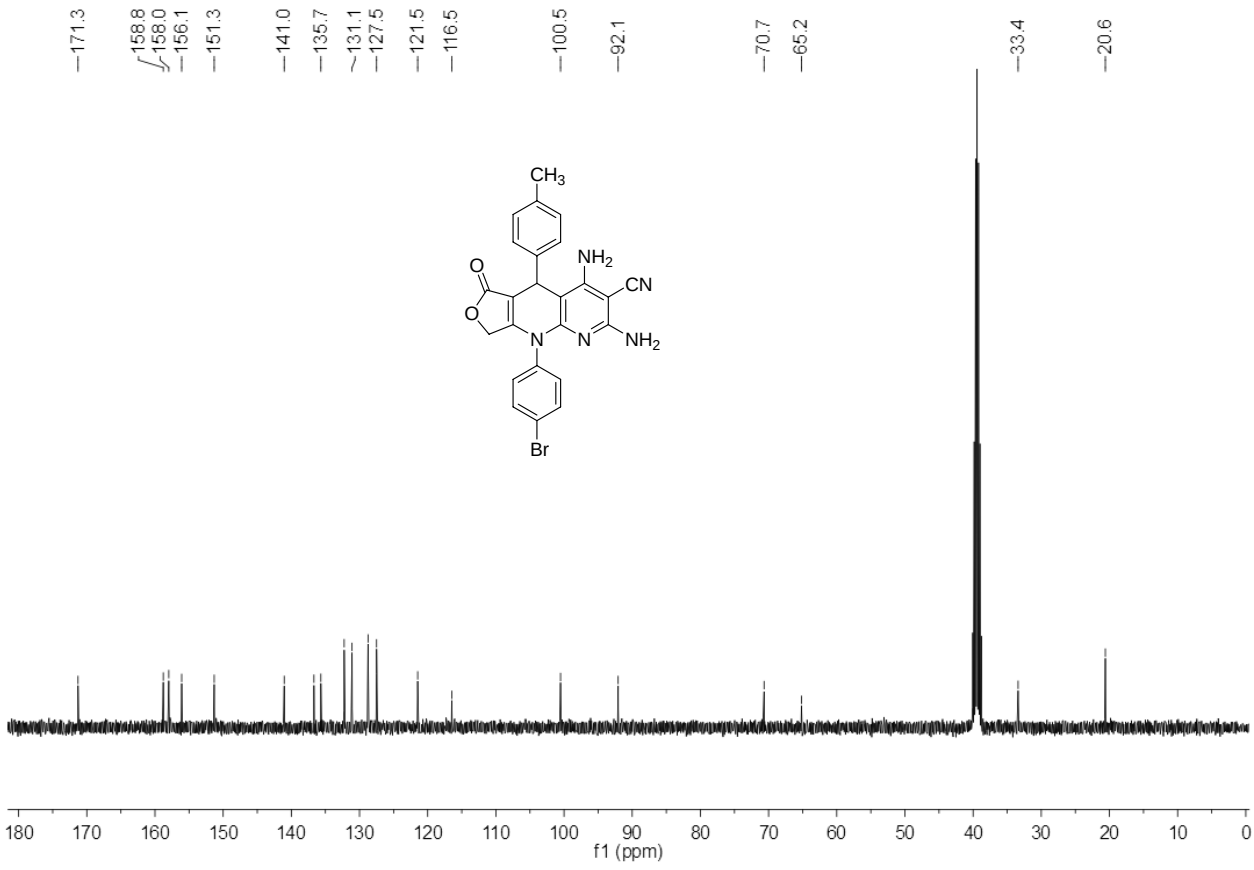


^{1}H NMR Spectrum of Compound 4h



^{13}C NMR Spectrum of Compound 4h

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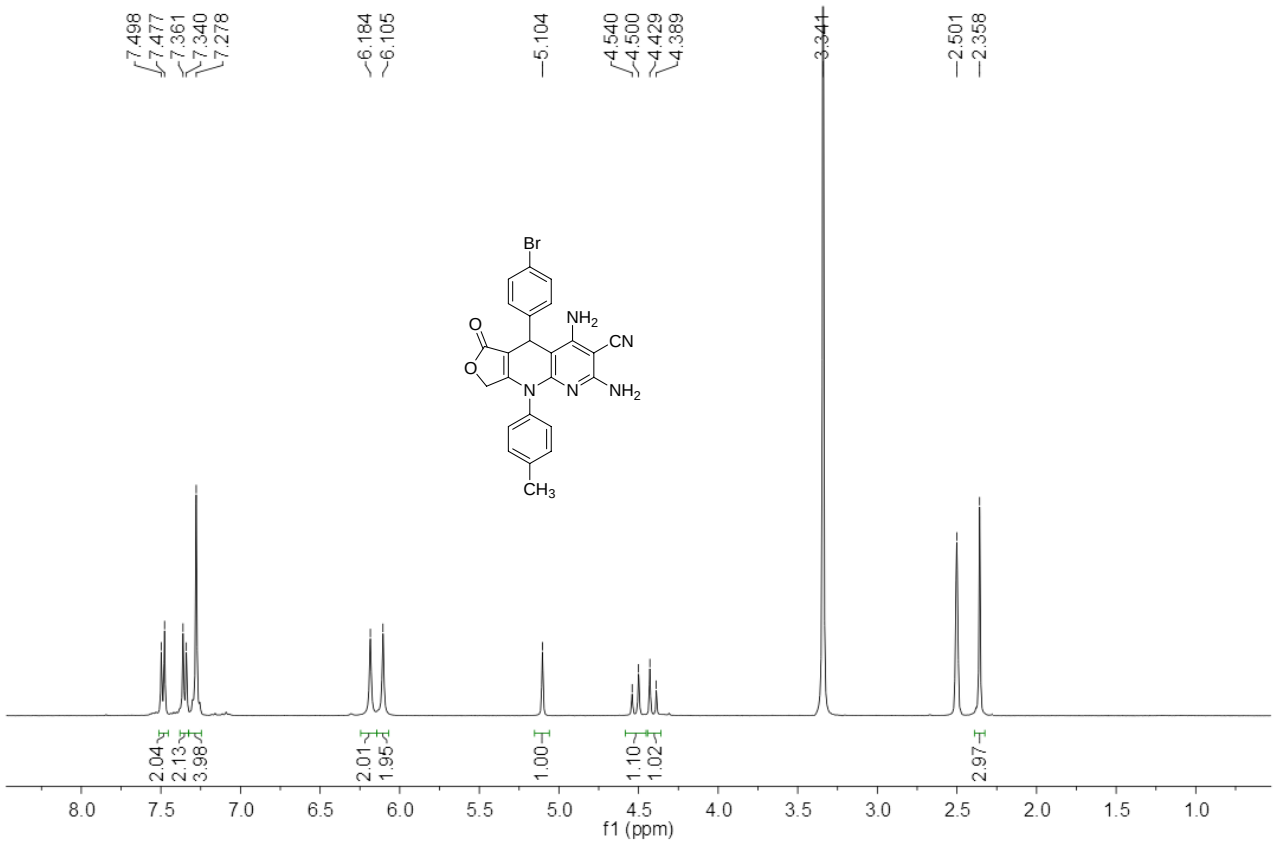
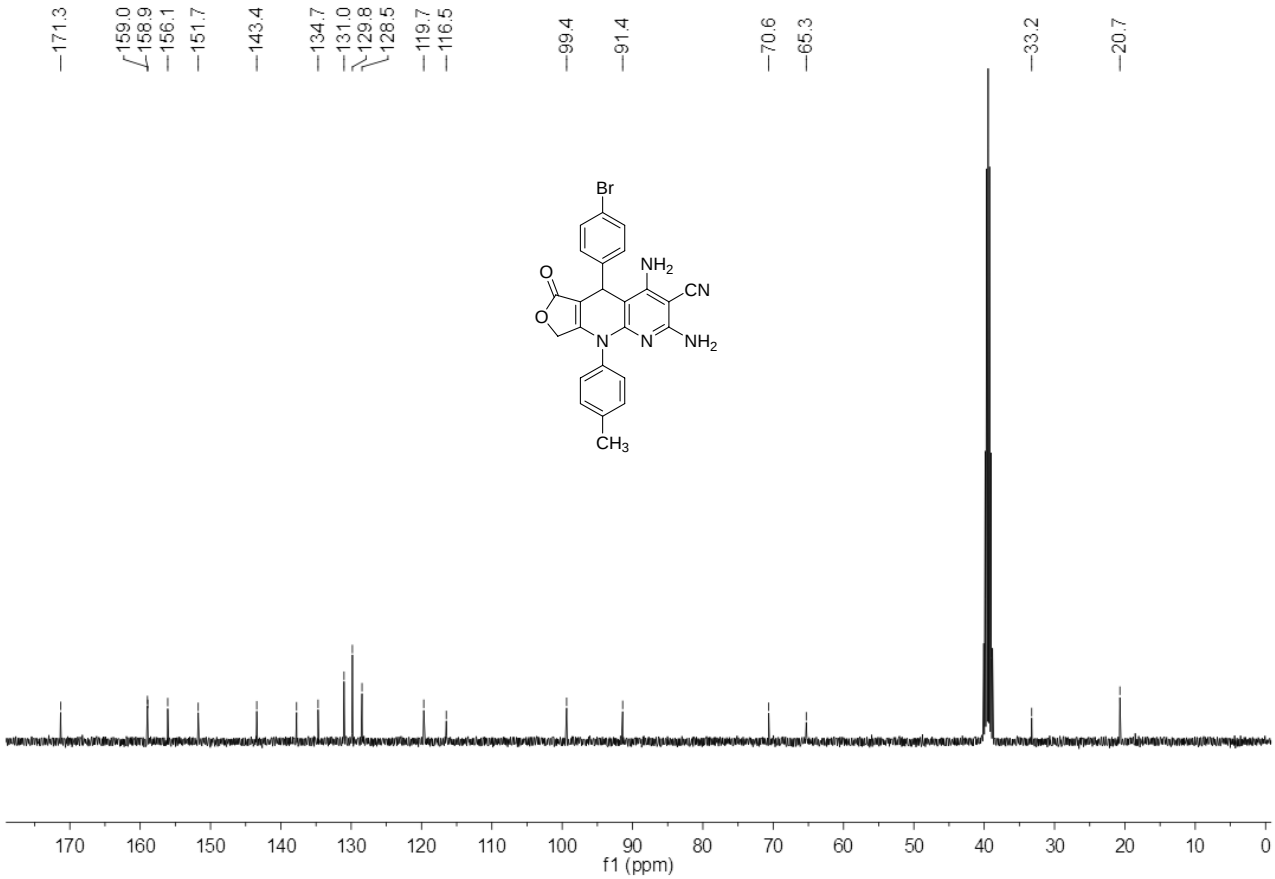


^{1}H NMR Spectrum of Compound 4i



^{13}C NMR Spectrum of Compound 4i

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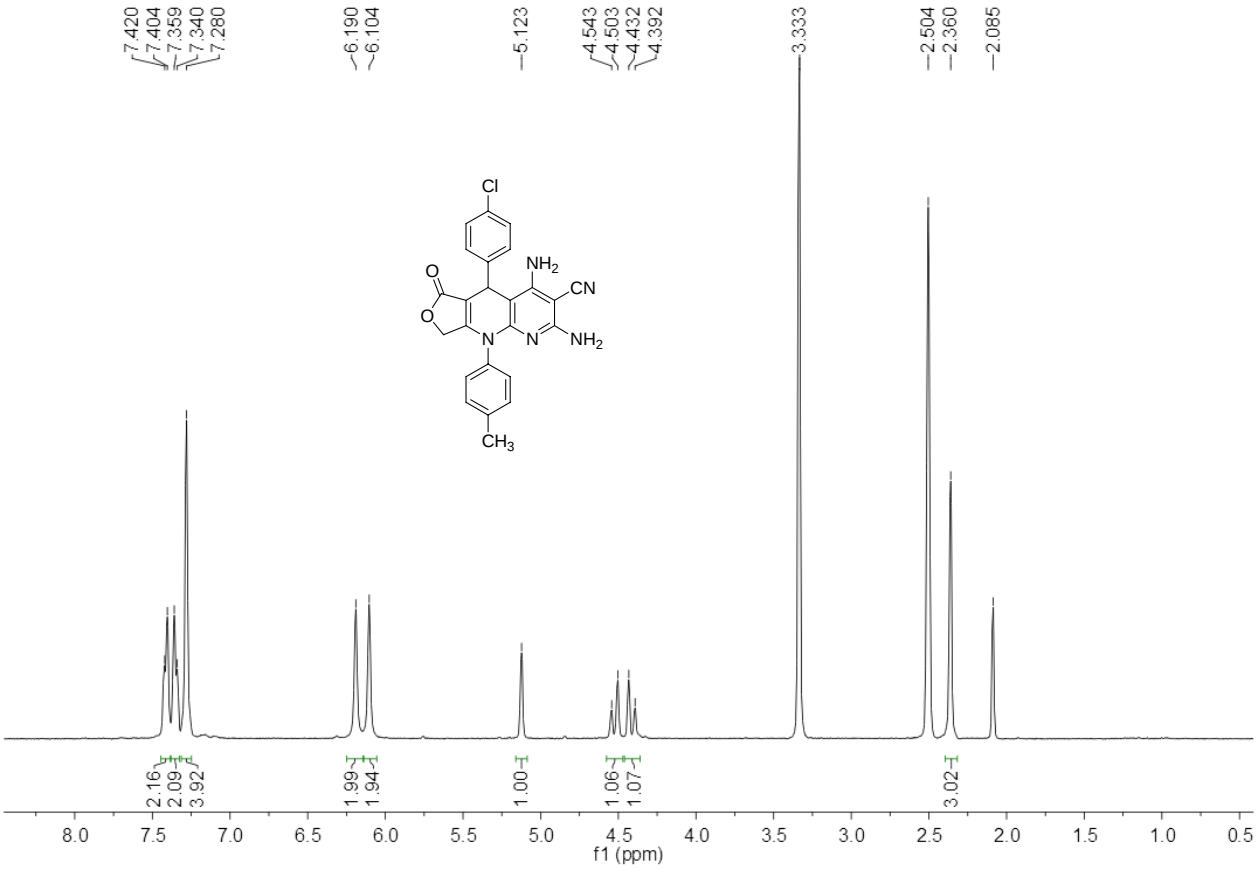
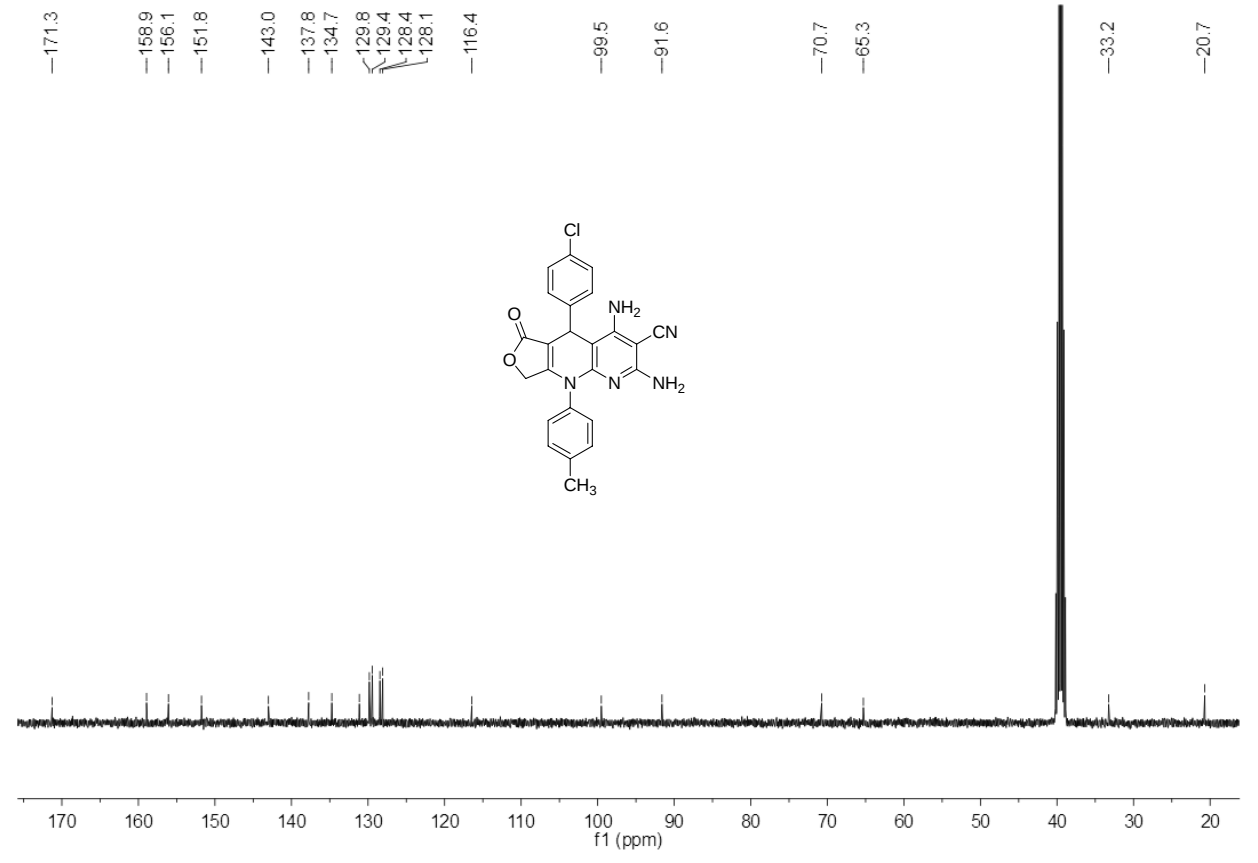


^{1}H NMR Spectrum of Compound 4j



^{13}C NMR Spectrum of Compound 4j

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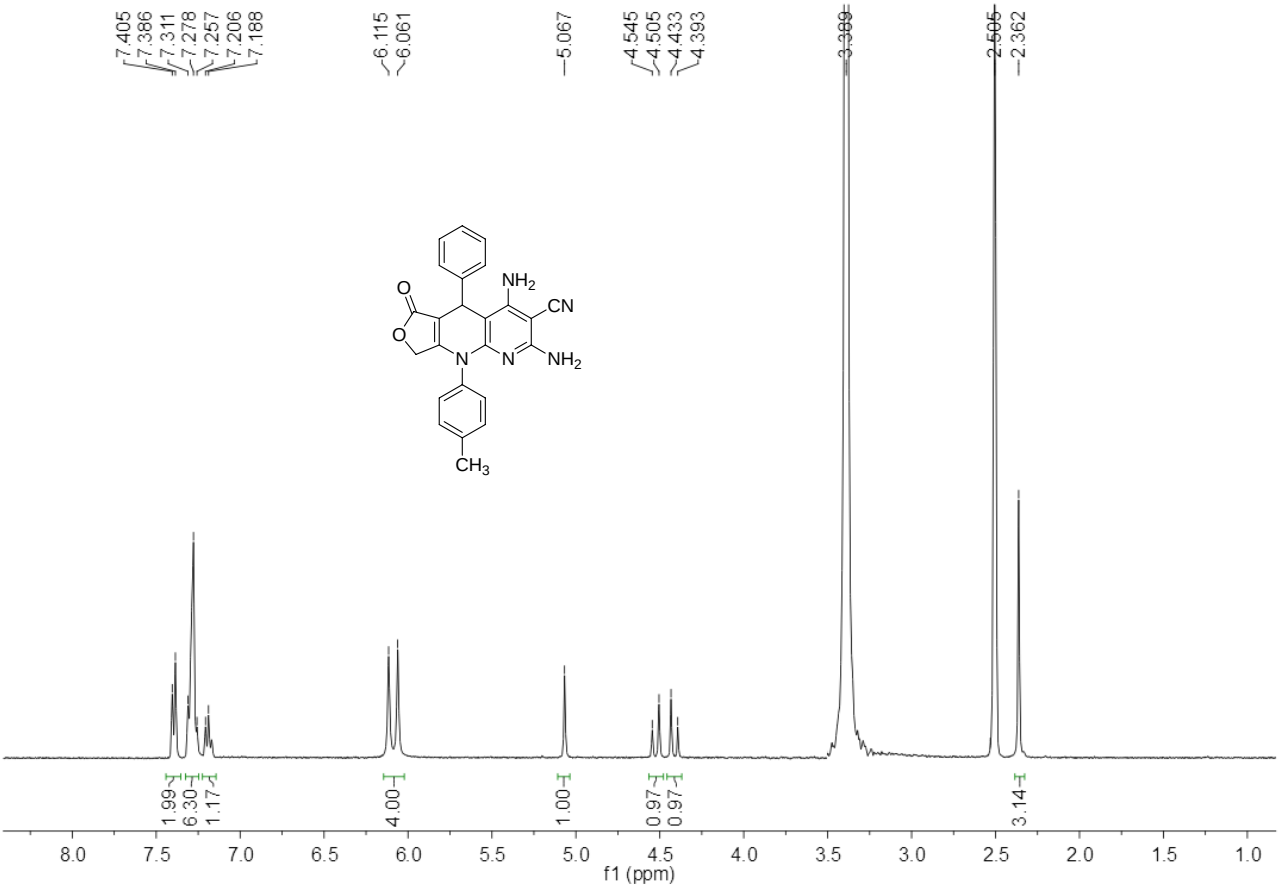
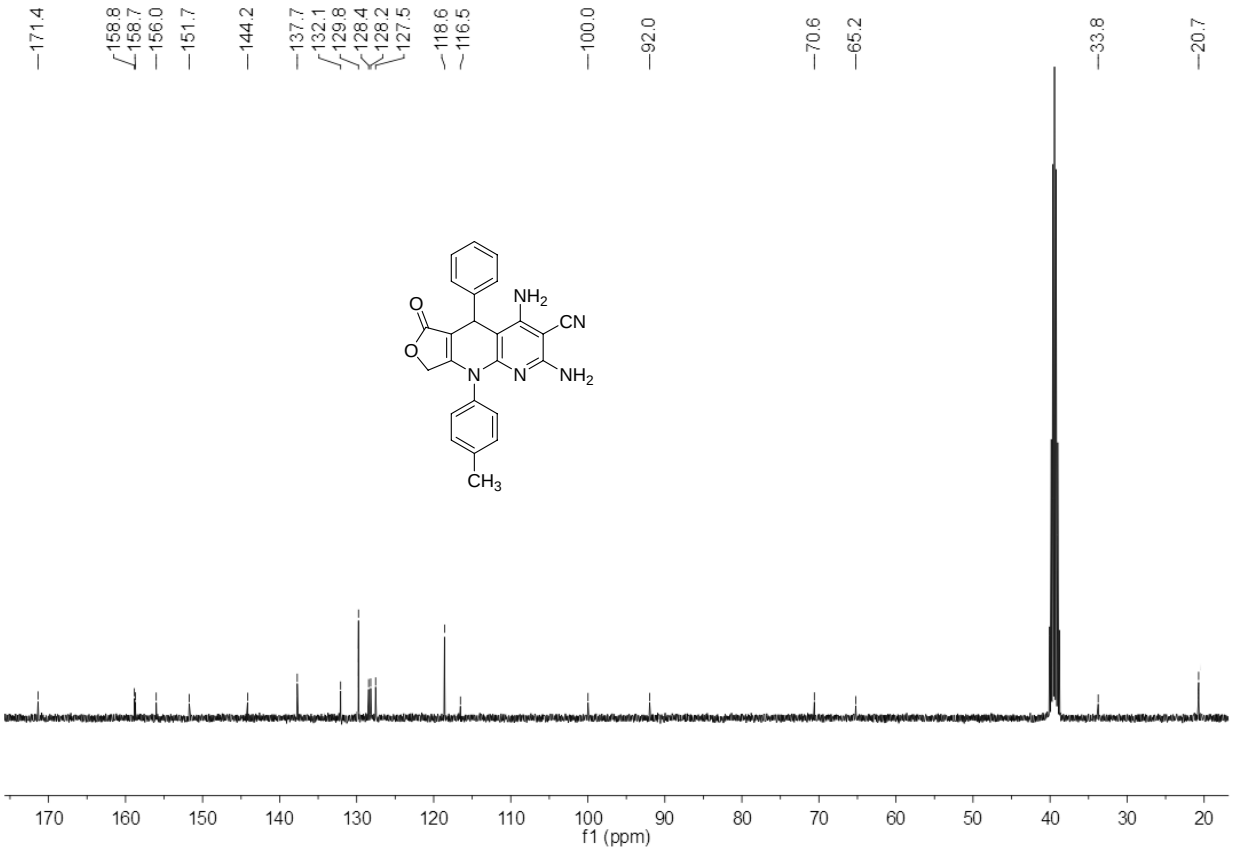


^{1}H NMR Spectrum of Compound 4k



^{13}C NMR Spectrum of Compound 4k

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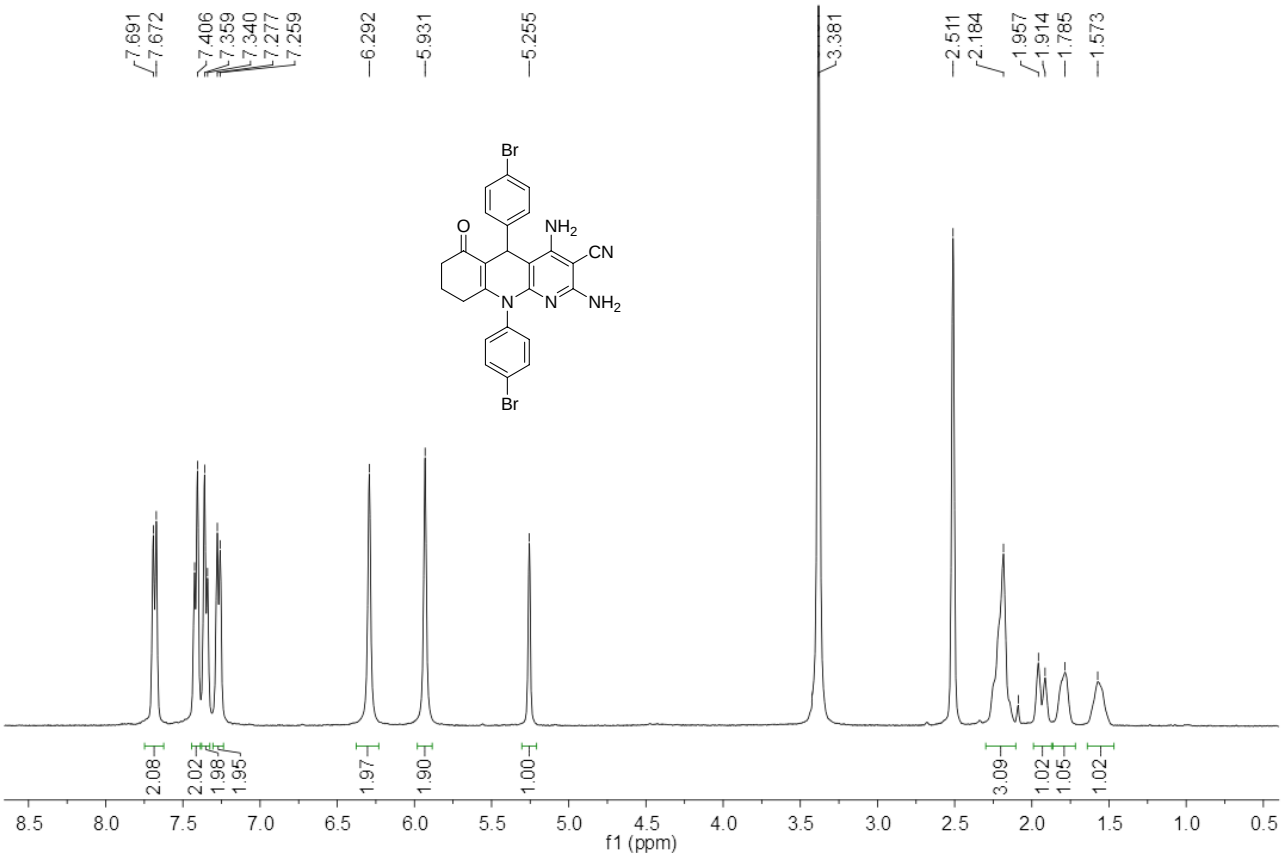
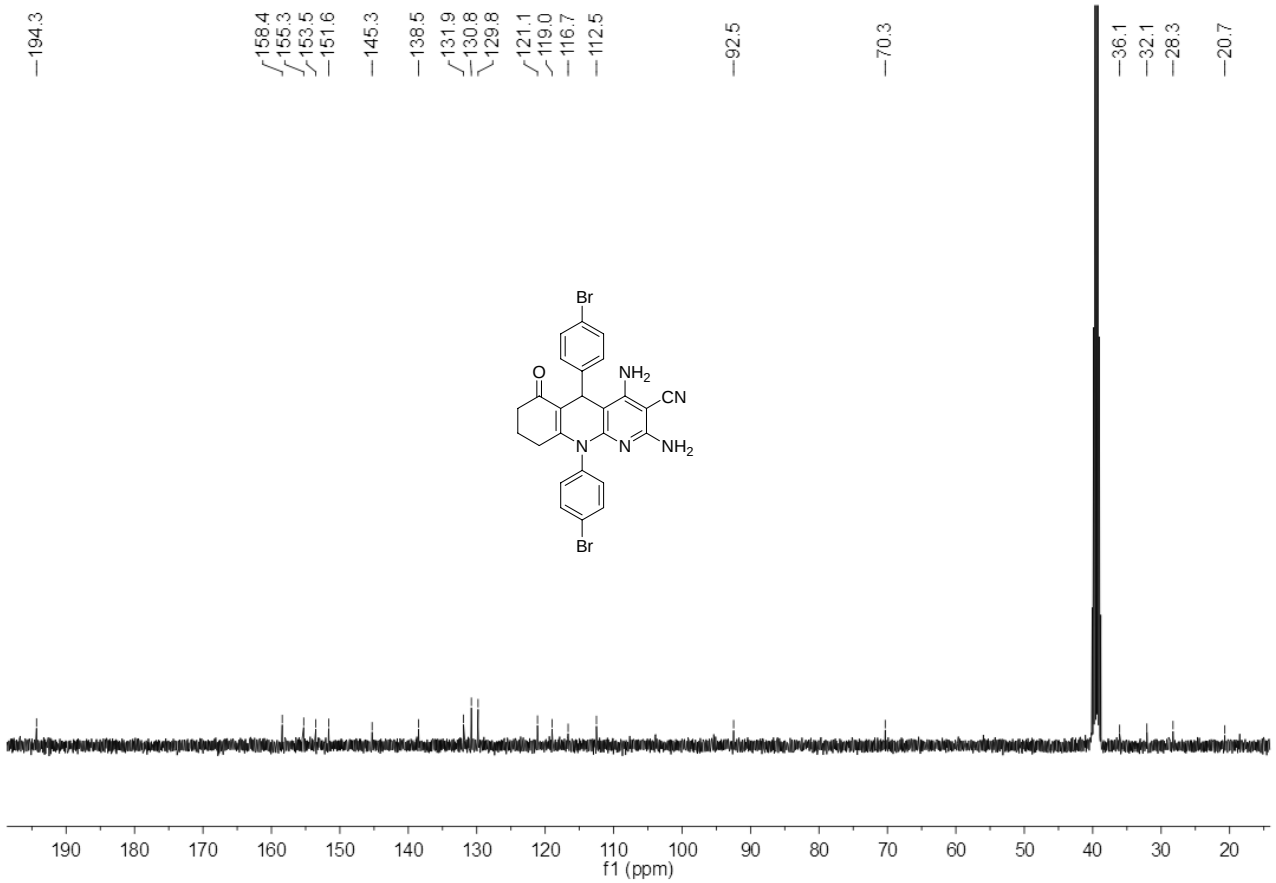


^{1}H NMR Spectrum of Compound 5a



^{13}C NMR Spectrum of Compound 5a

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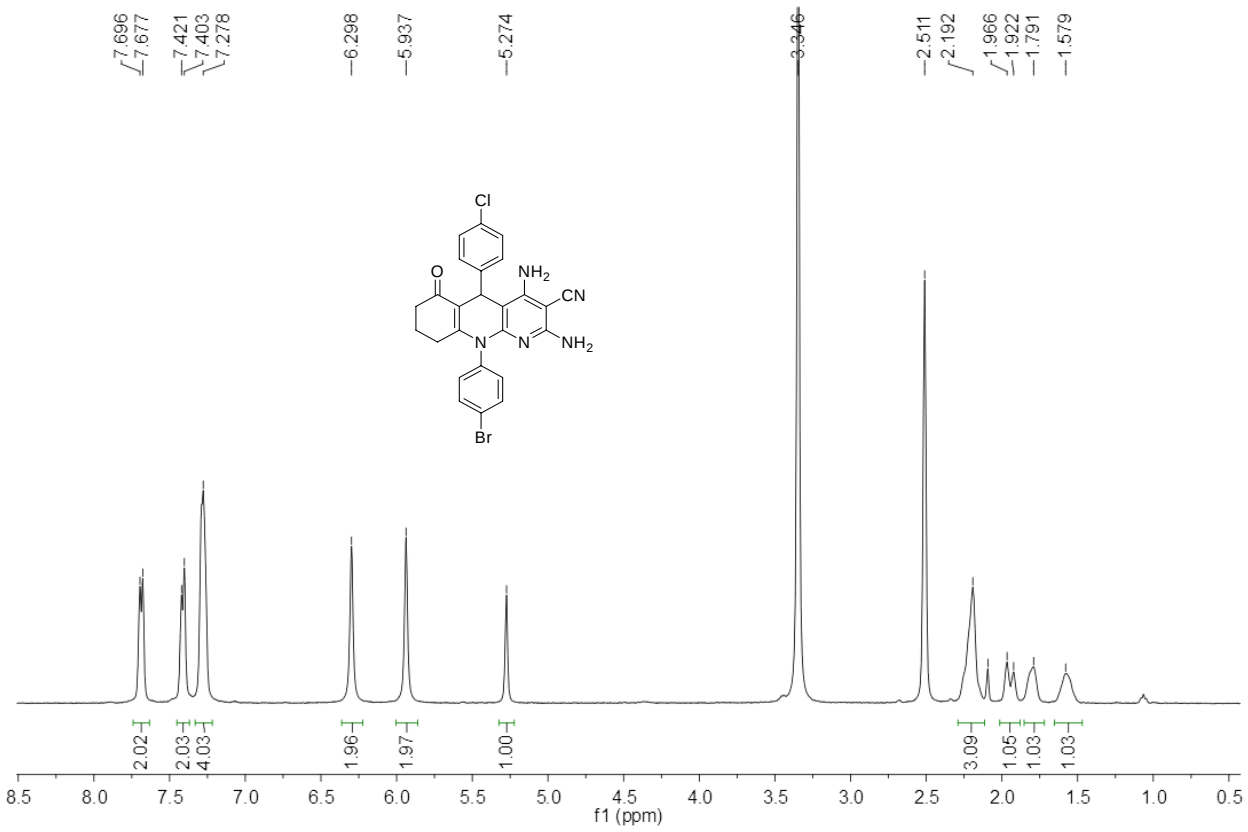
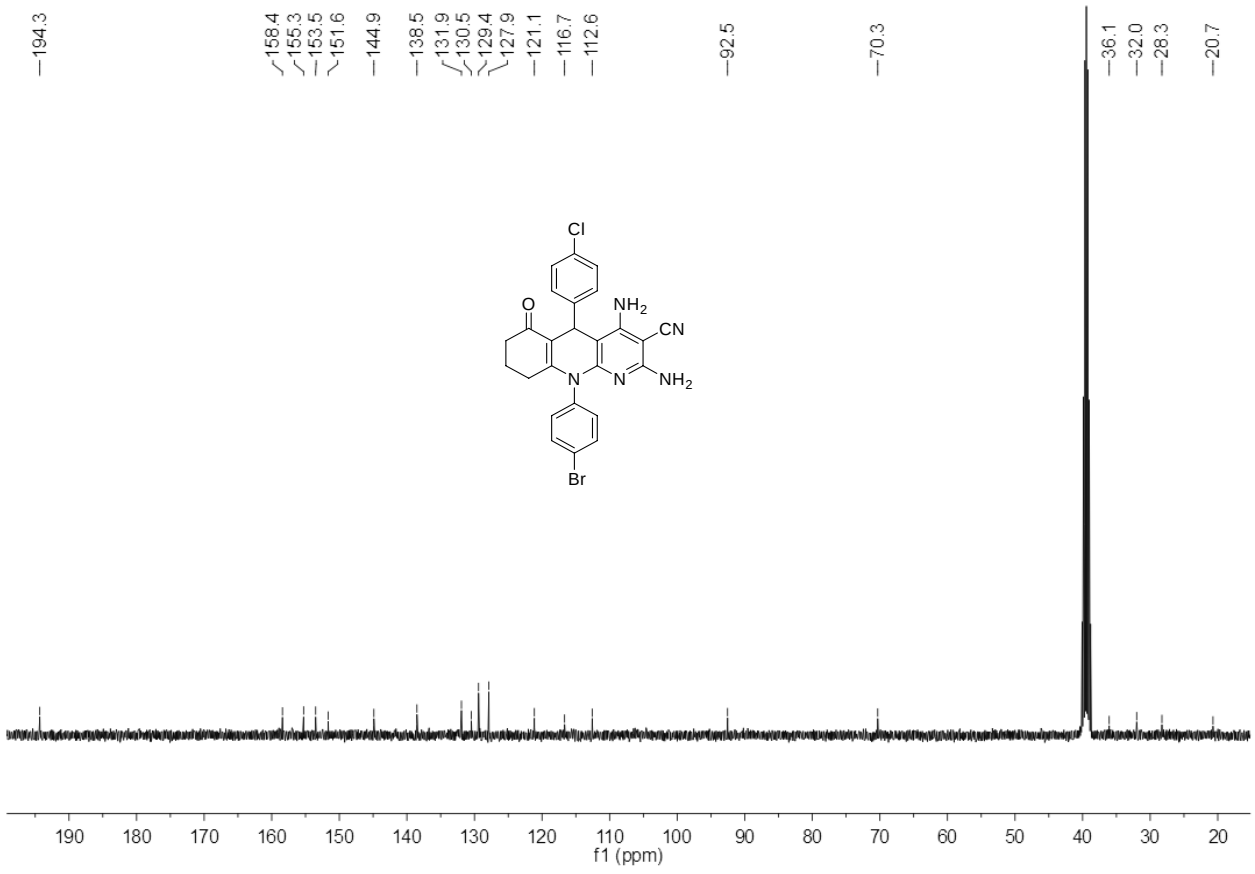


^{1}H NMR Spectrum of Compound 5b



^{13}C NMR Spectrum of Compound 5b

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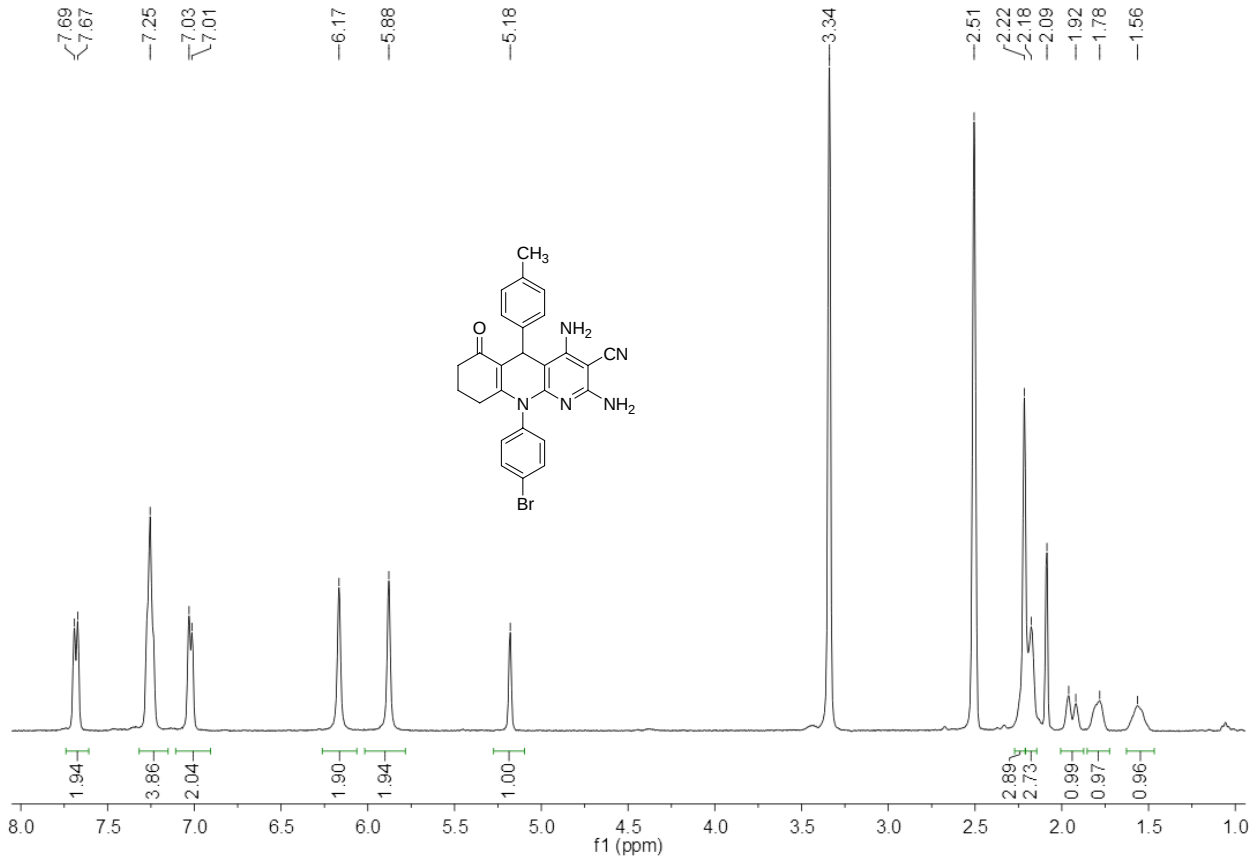
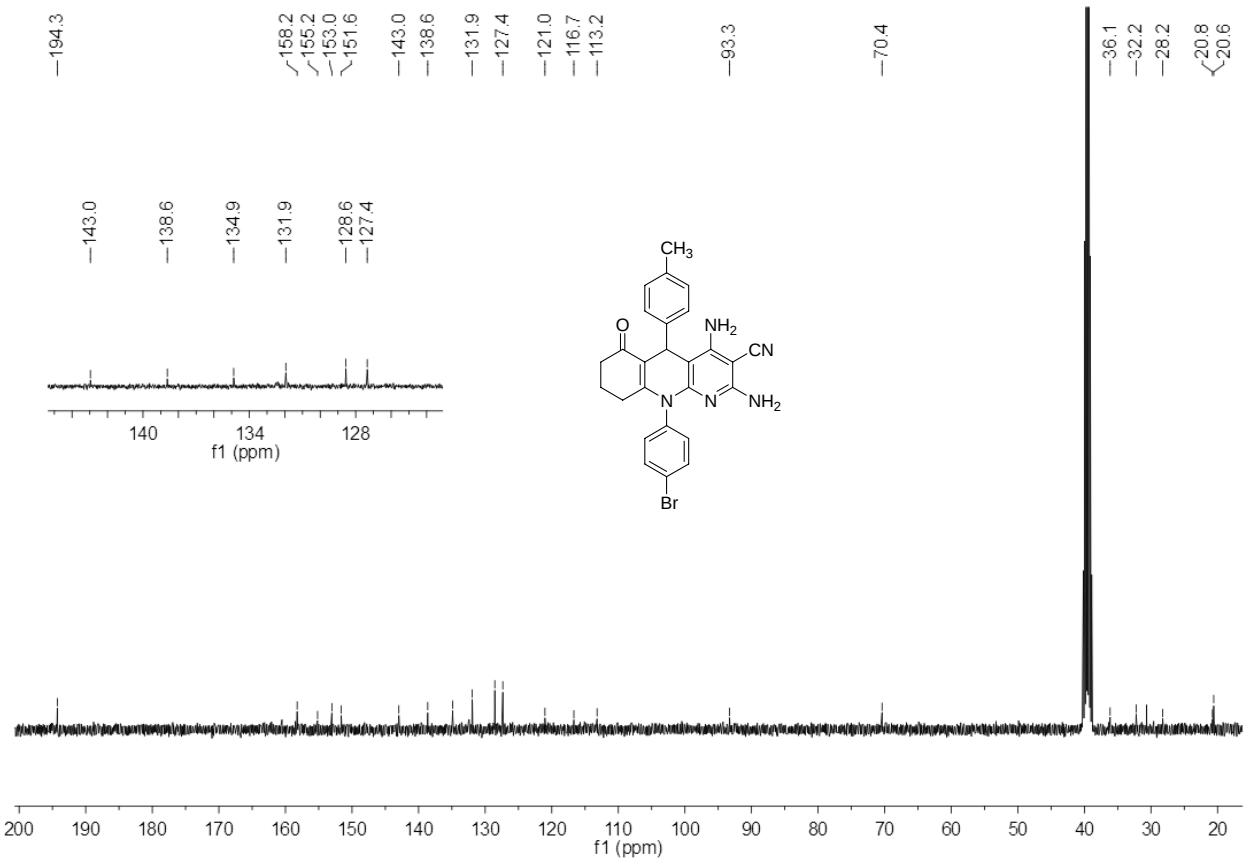


^{1}H NMR Spectrum of Compound 5c



^{13}C NMR Spectrum of Compound 5c

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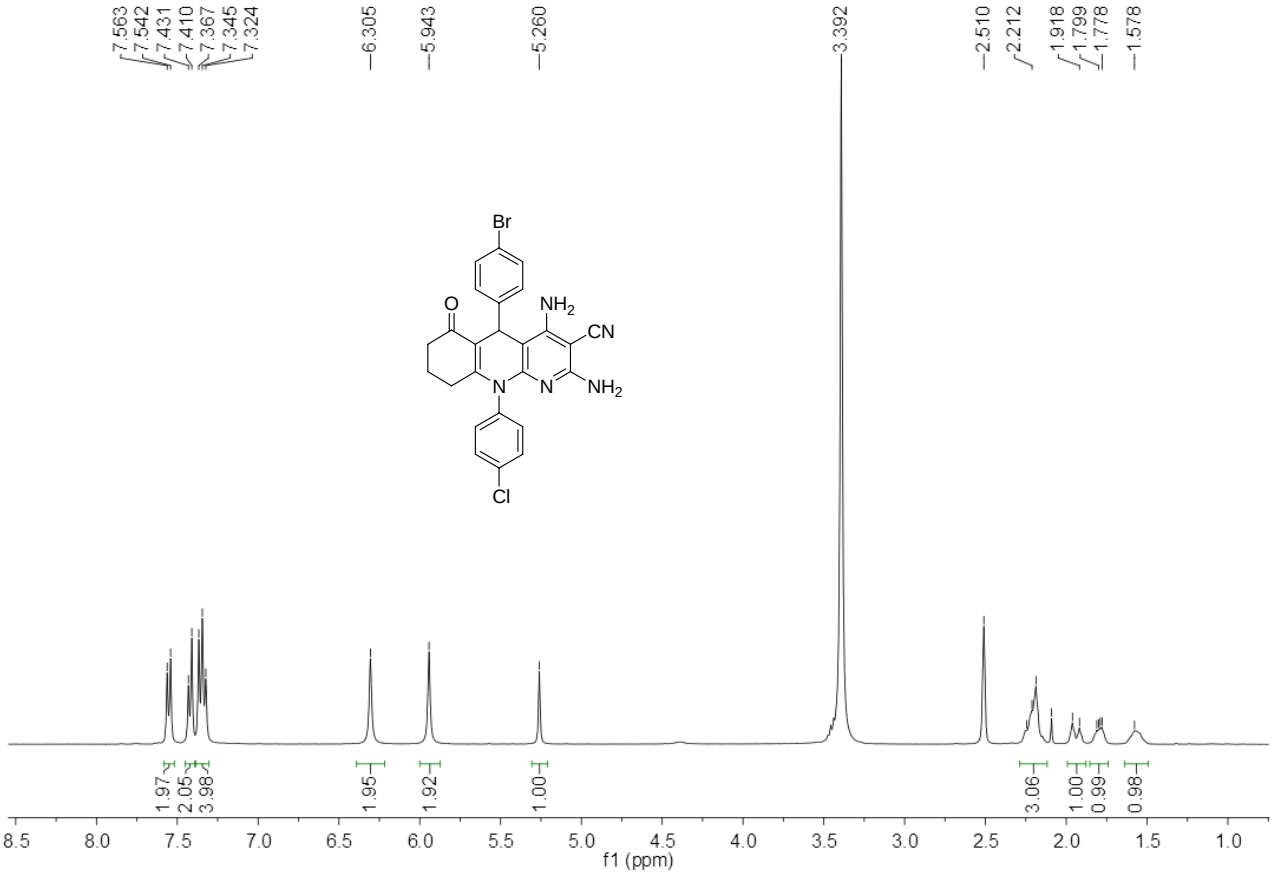
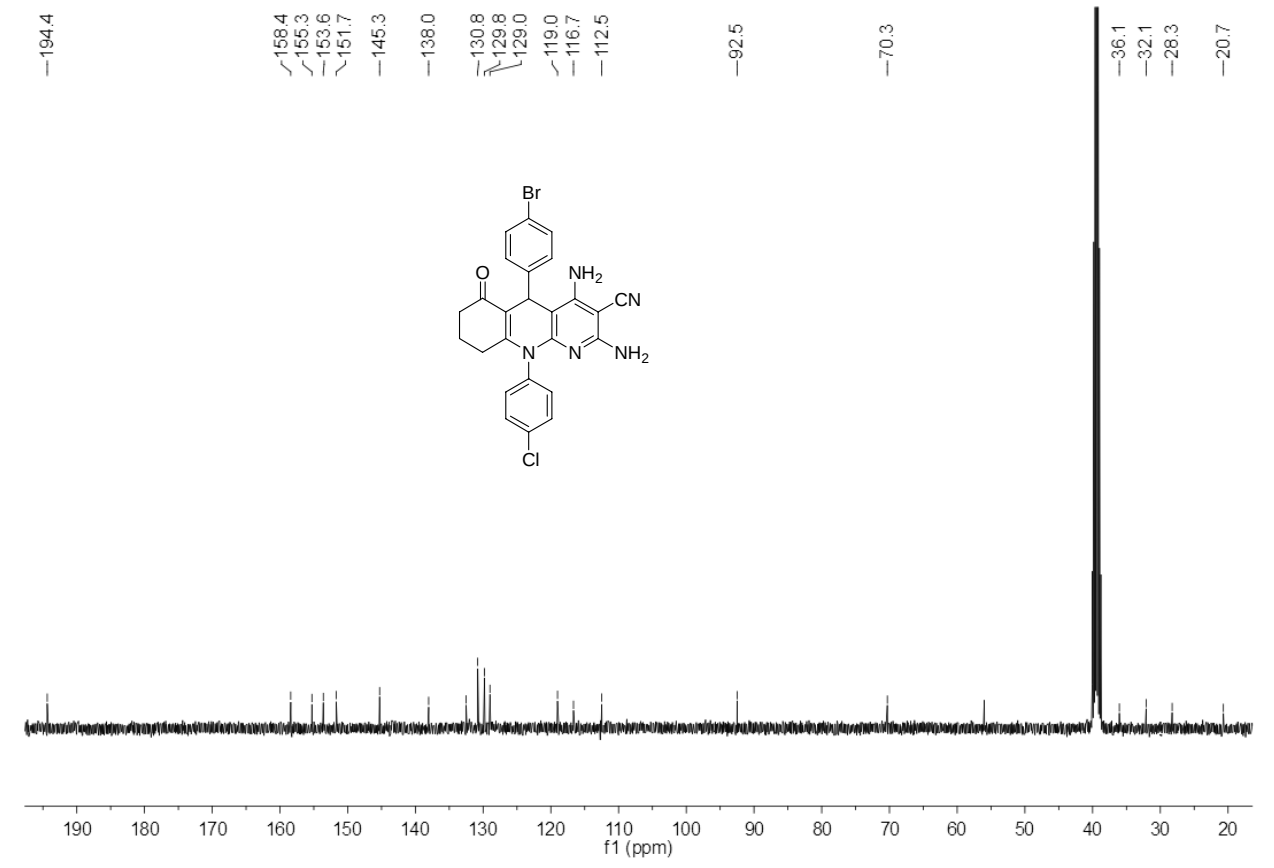


^{1}H NMR Spectrum of Compound 5d



^{13}C NMR Spectrum of Compound 5d

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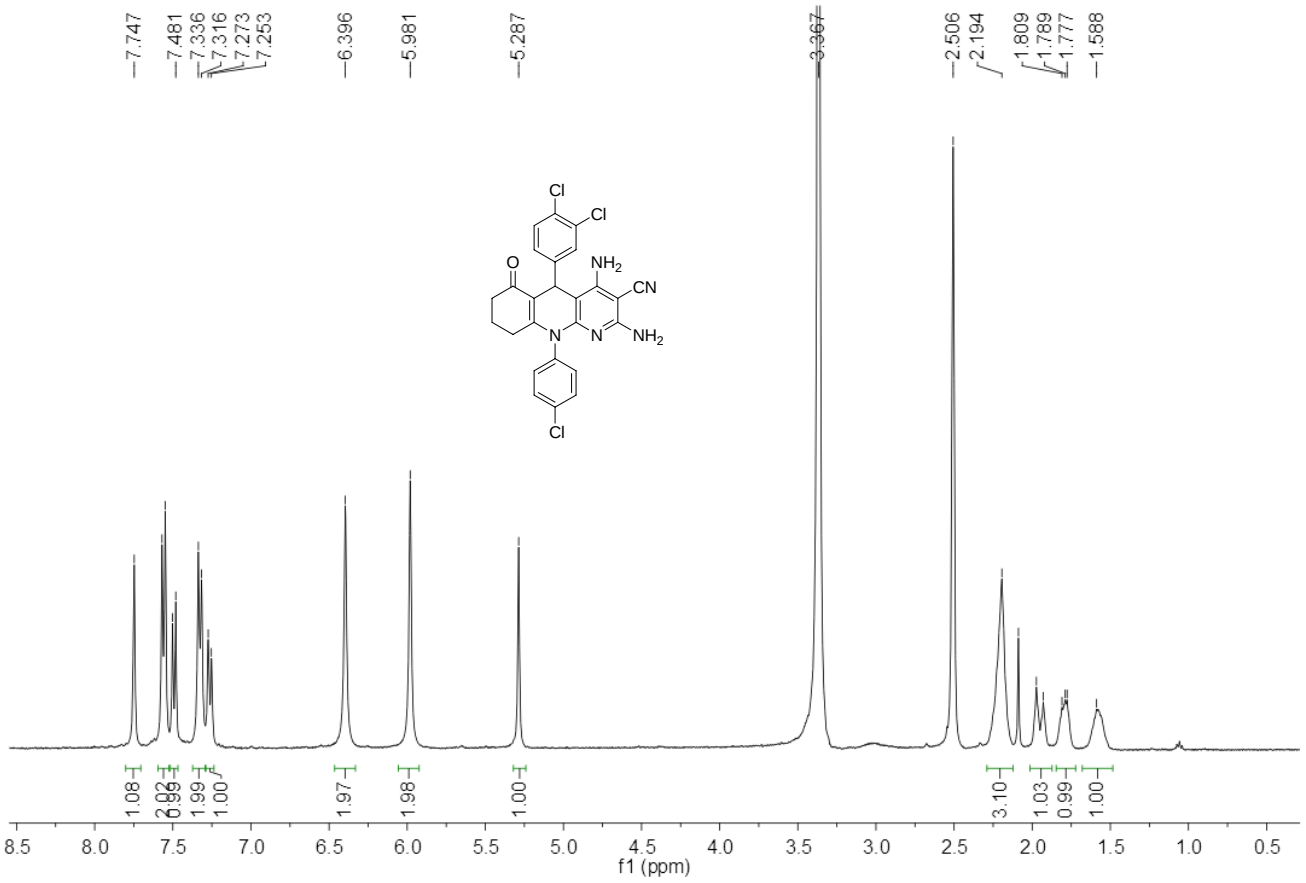
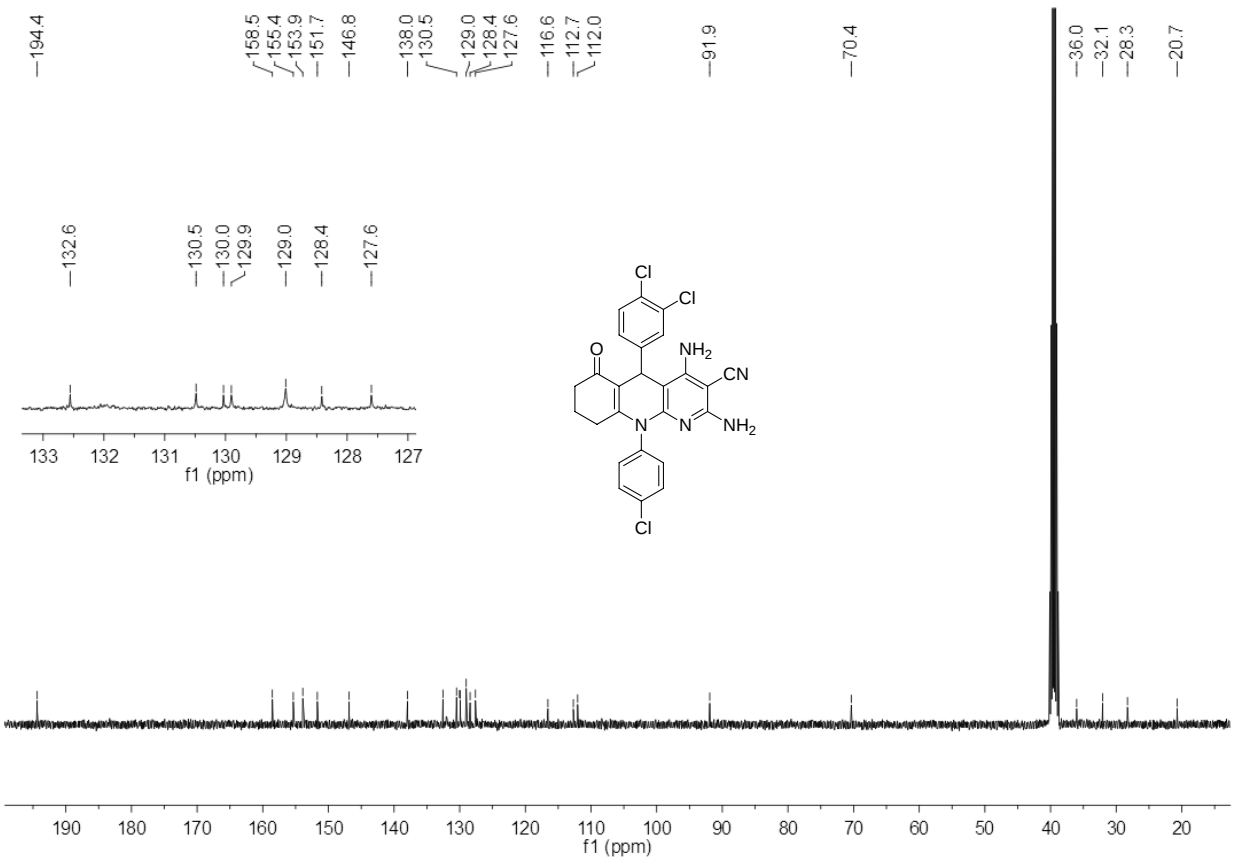


^{1}H NMR Spectrum of Compound 5e



^{13}C NMR Spectrum of Compound 5e

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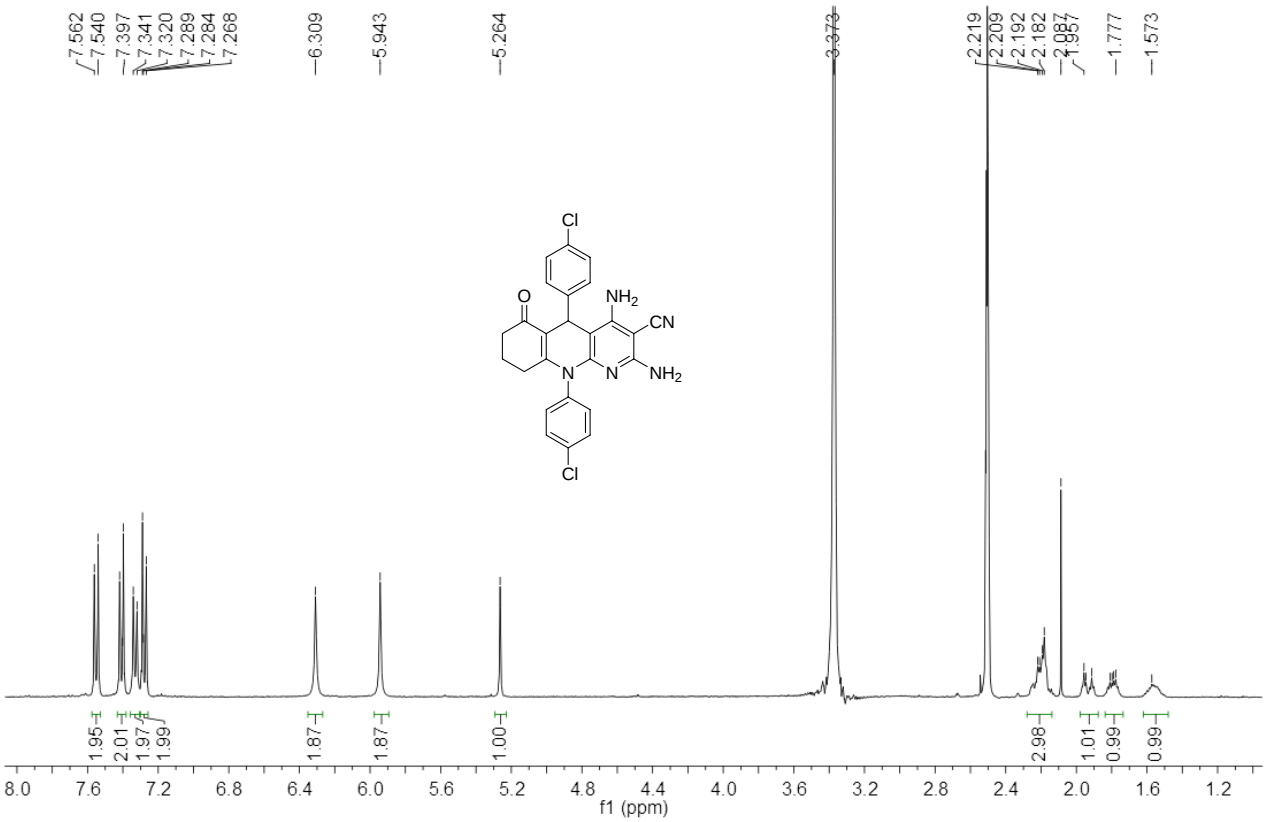
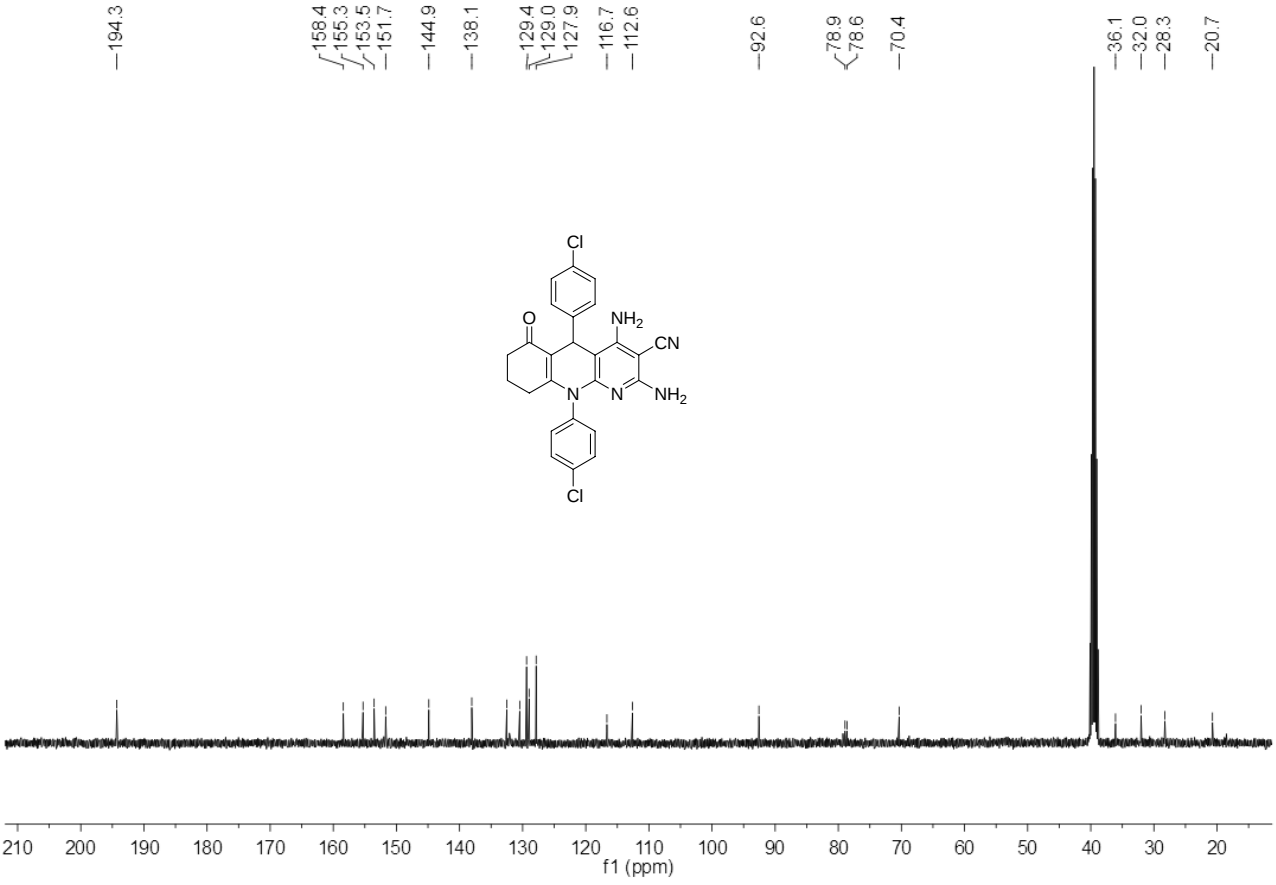


^{1}H NMR Spectrum of Compound 5f



^{13}C NMR Spectrum of Compound 5f

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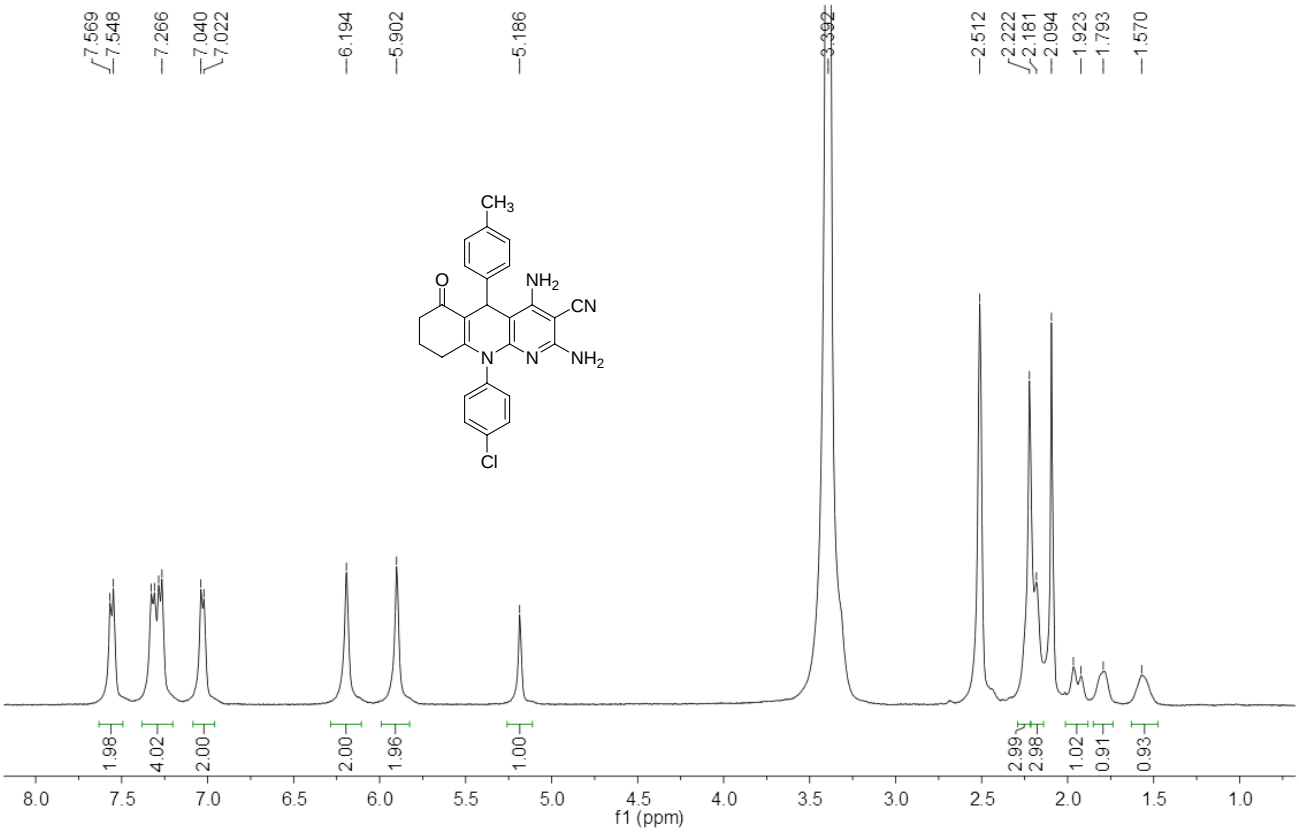
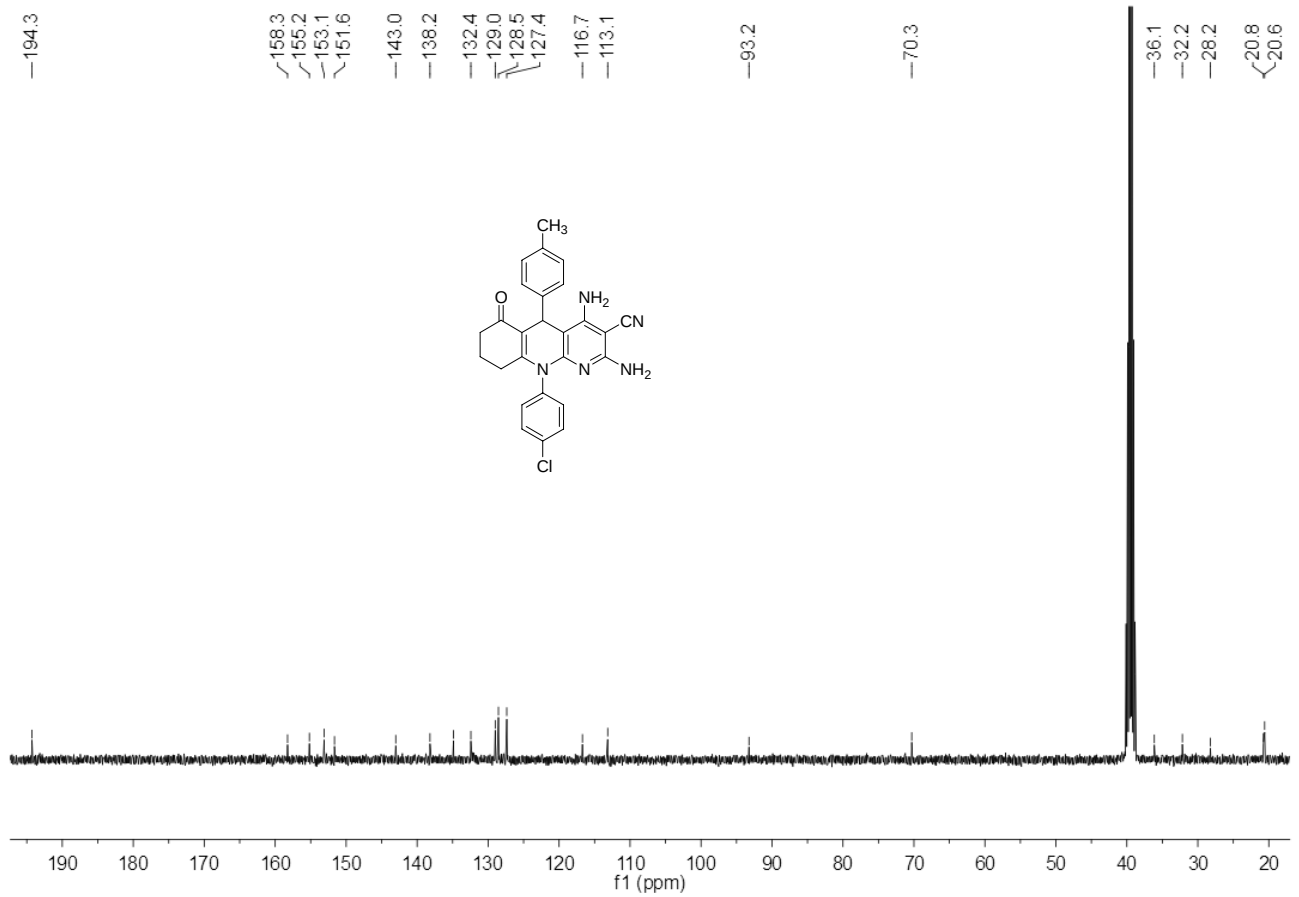


^{1}H NMR Spectrum of Compound 5g



^{13}C NMR Spectrum of Compound 5g

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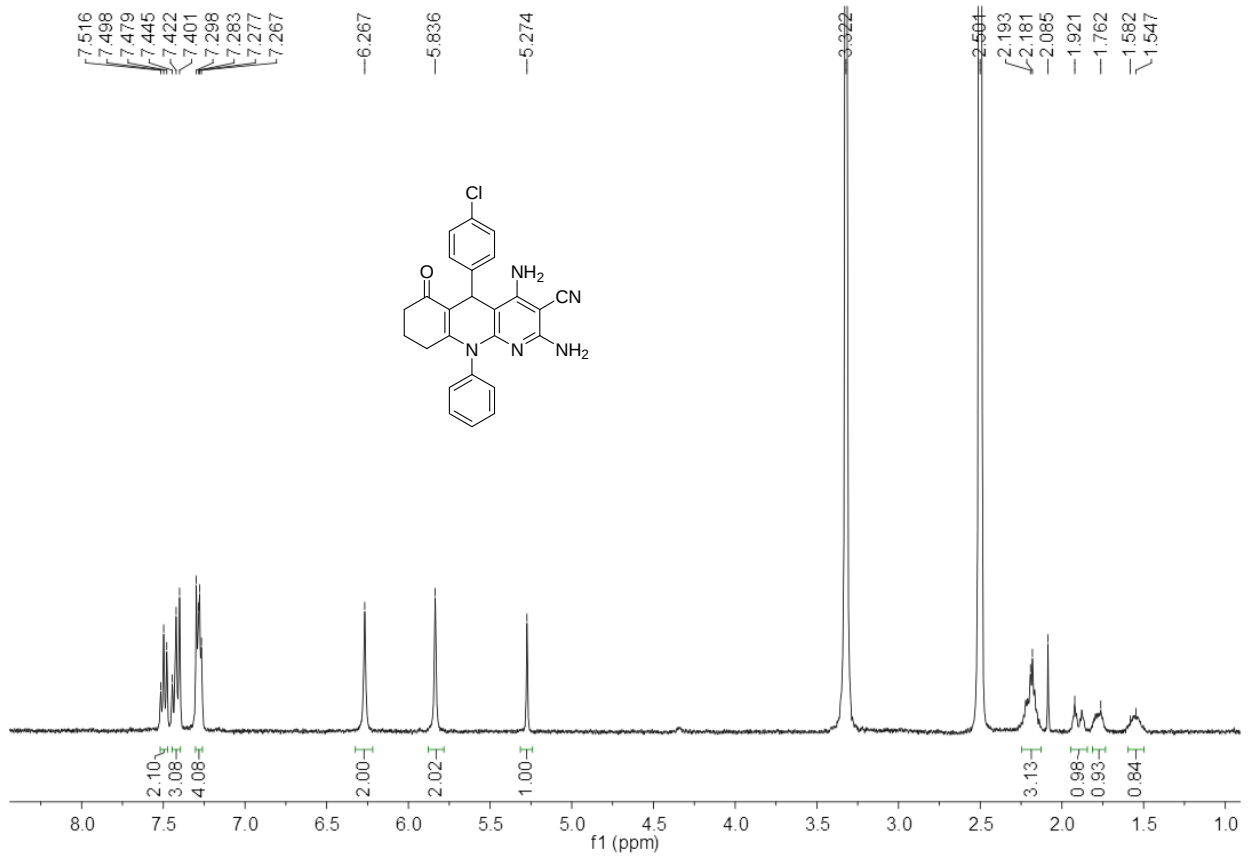
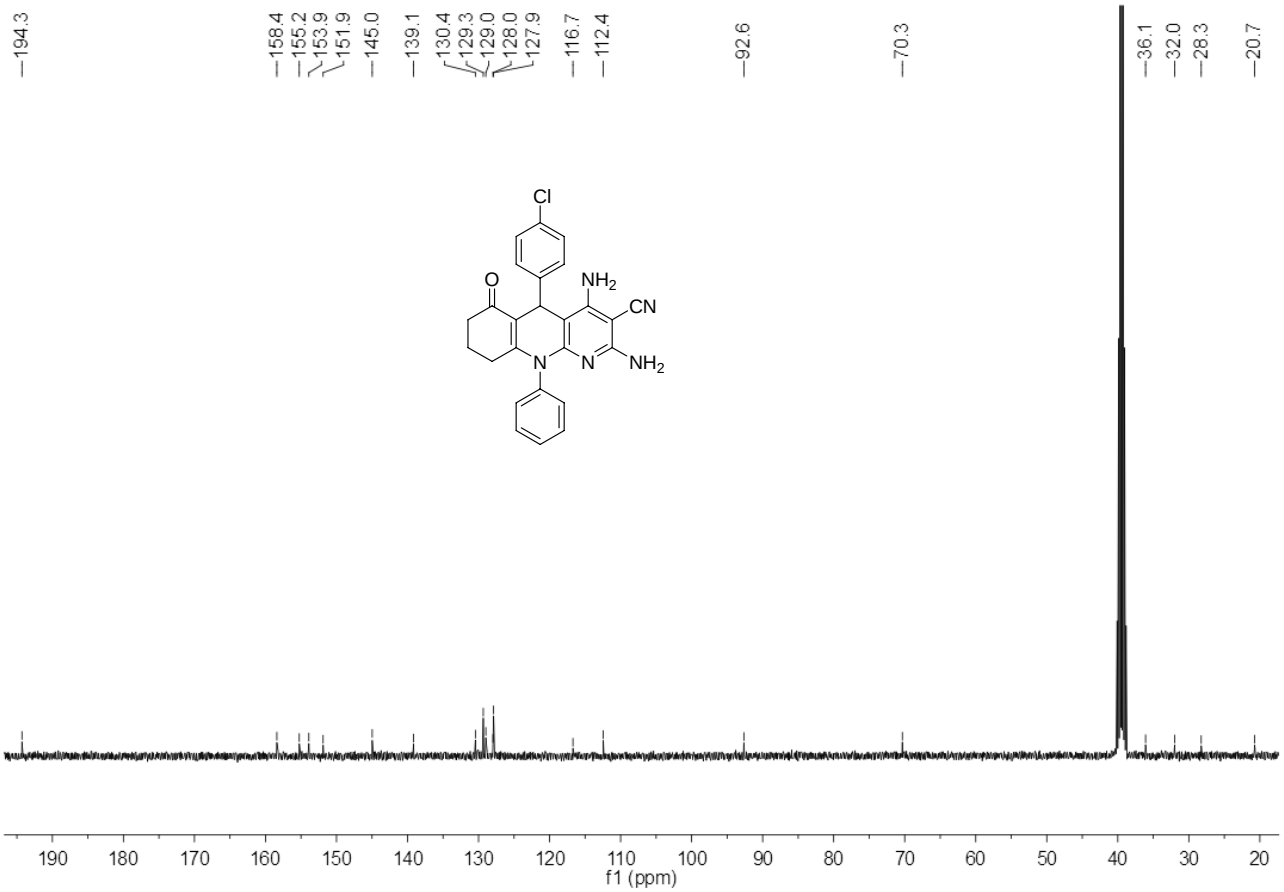


^{1}H NMR Spectrum of Compound 5h



^{13}C NMR Spectrum of Compound 5h

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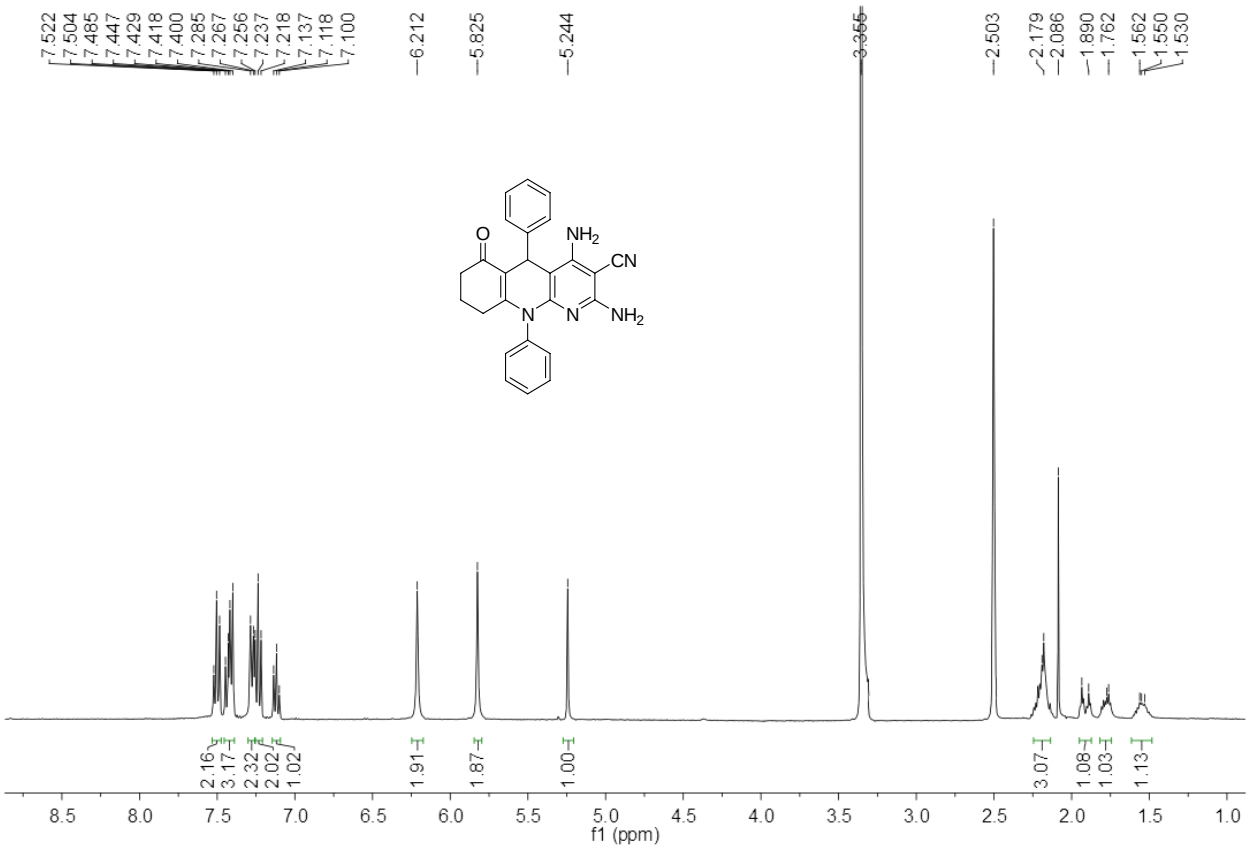
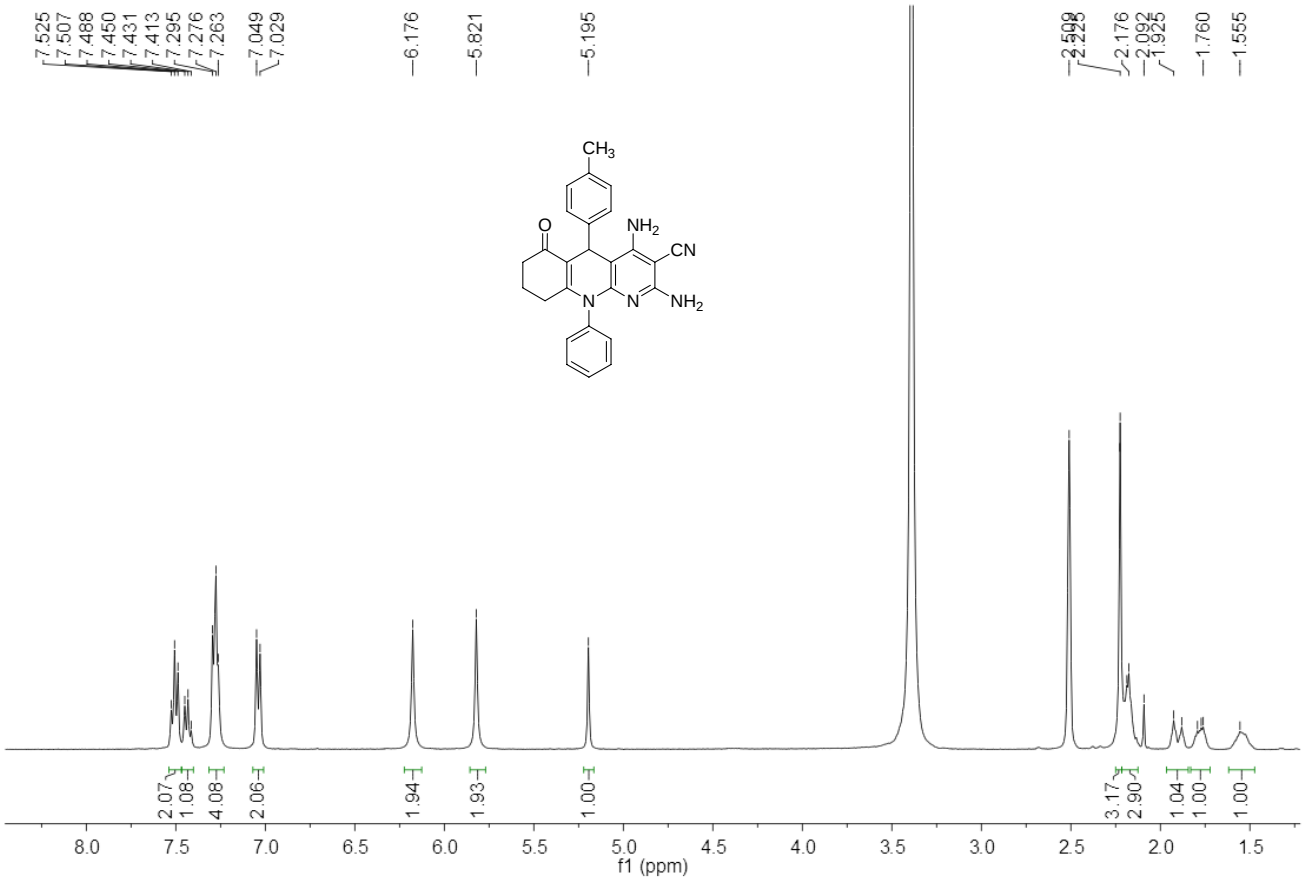


^{1}H NMR Spectrum of Compound 5i



^{1}H NMR Spectrum of Compound 5j

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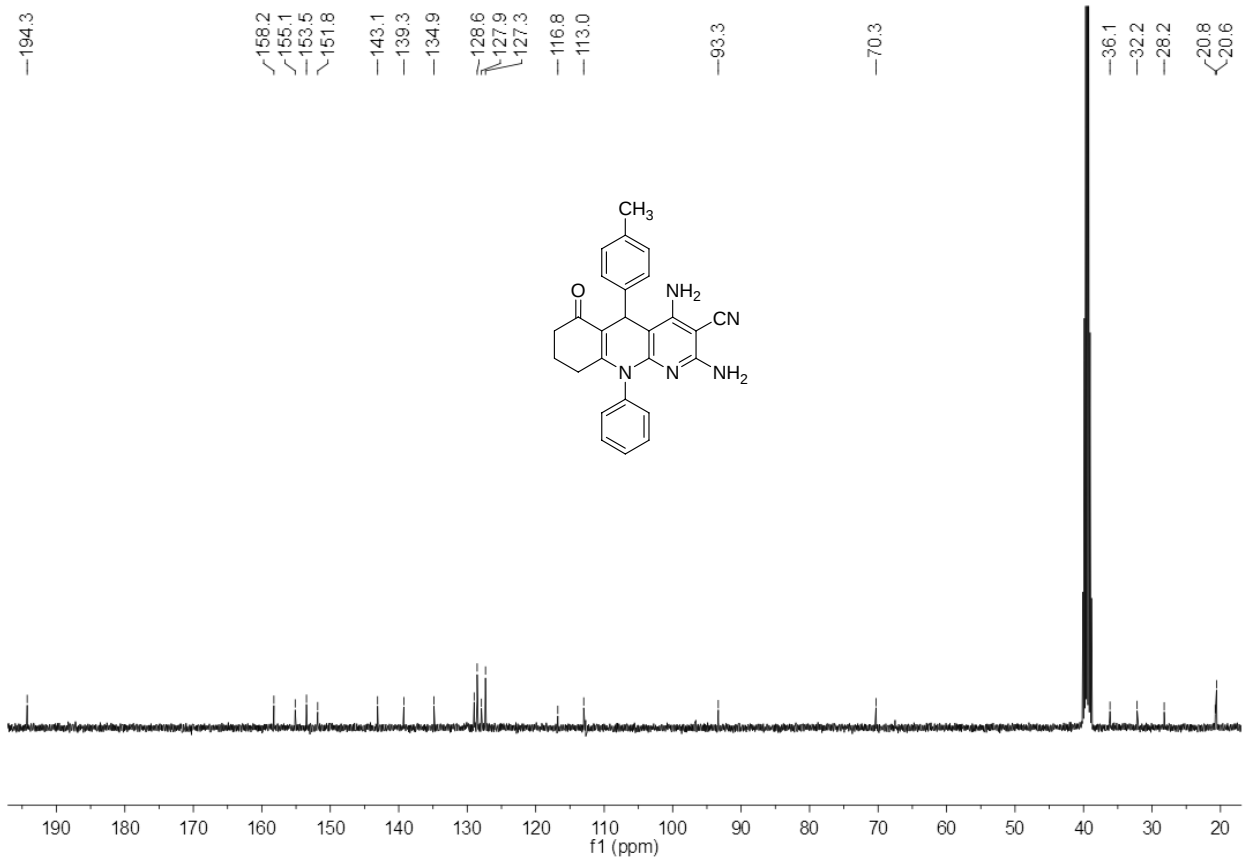
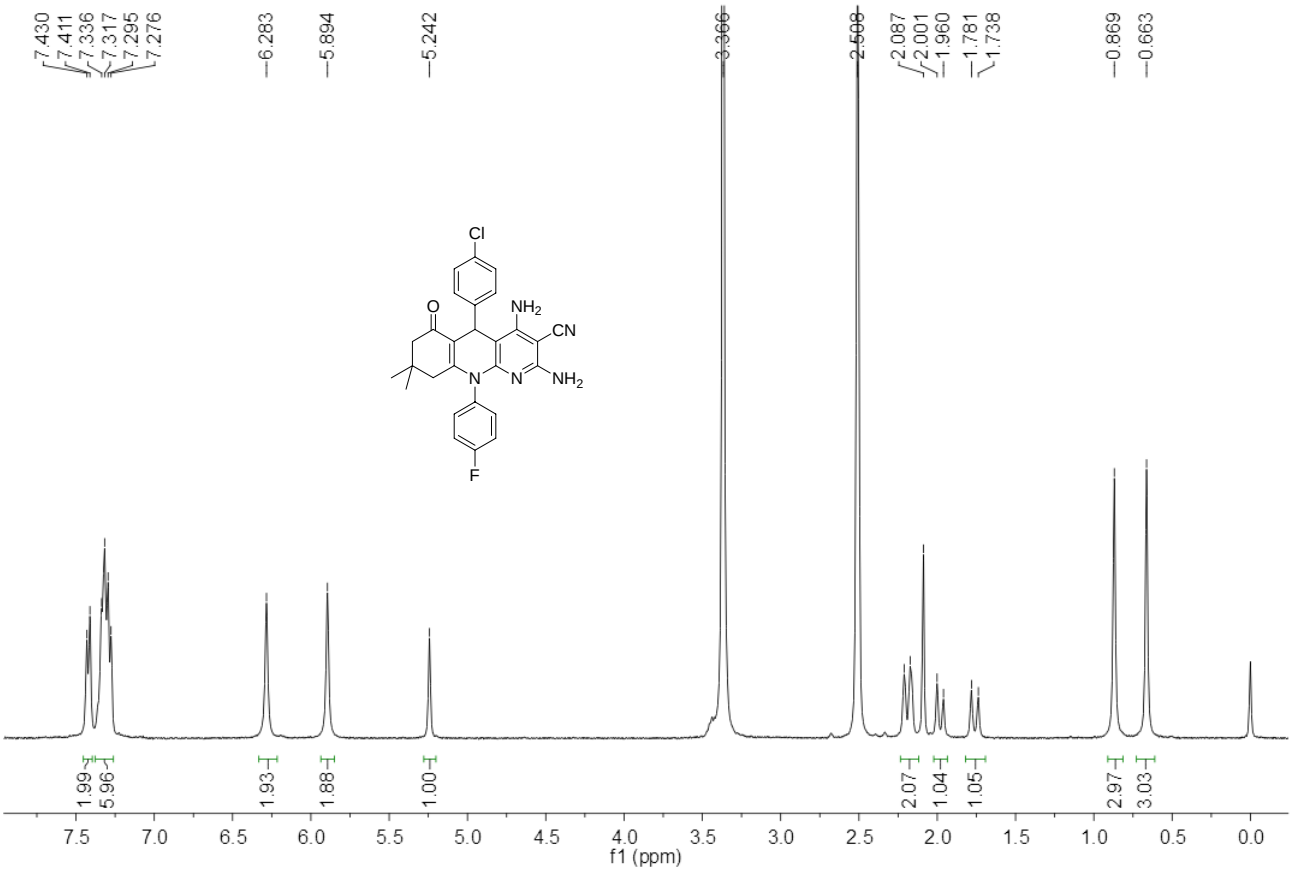


^{13}C NMR Spectrum of Compound 5j



^{1}H NMR Spectrum of Compound 5k

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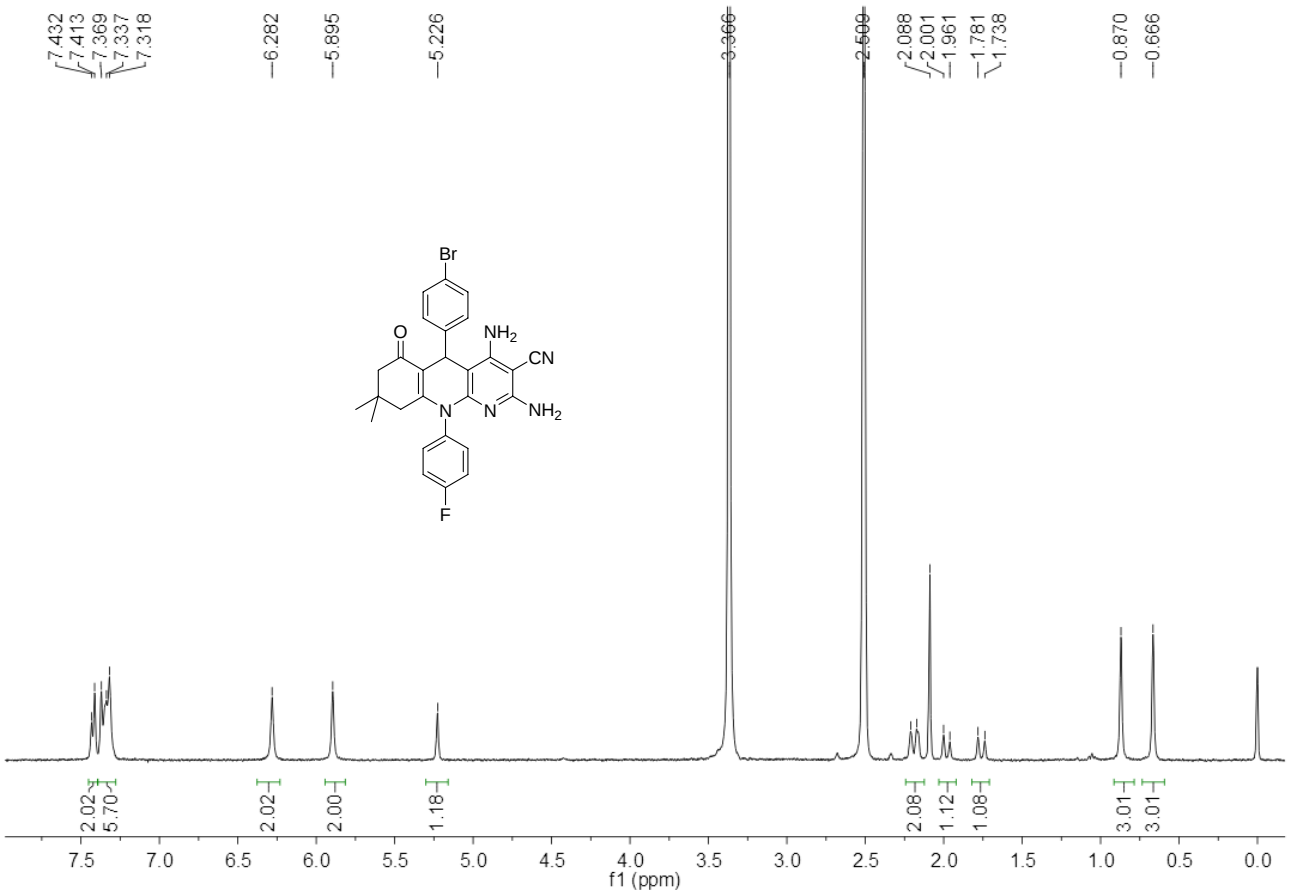
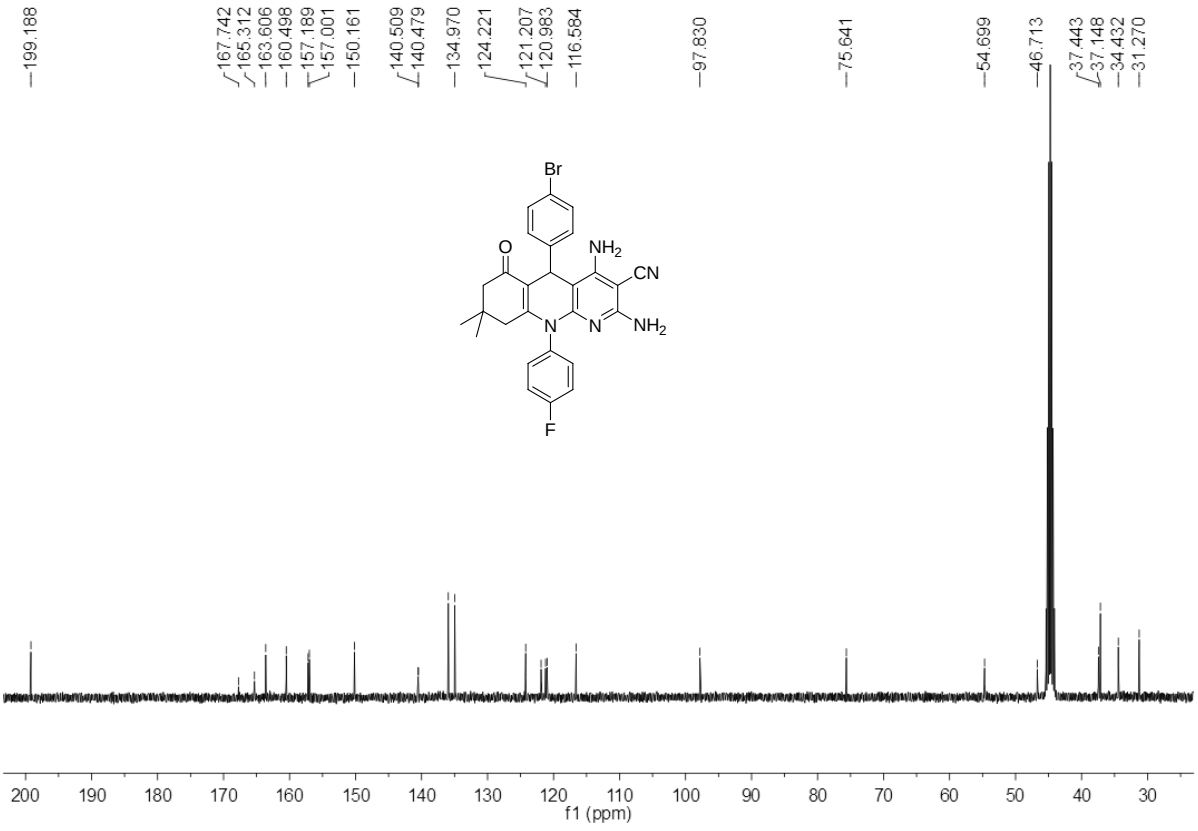


^{1}H NMR Spectrum of Compound 5l



^{13}C NMR Spectrum of Compound 5l

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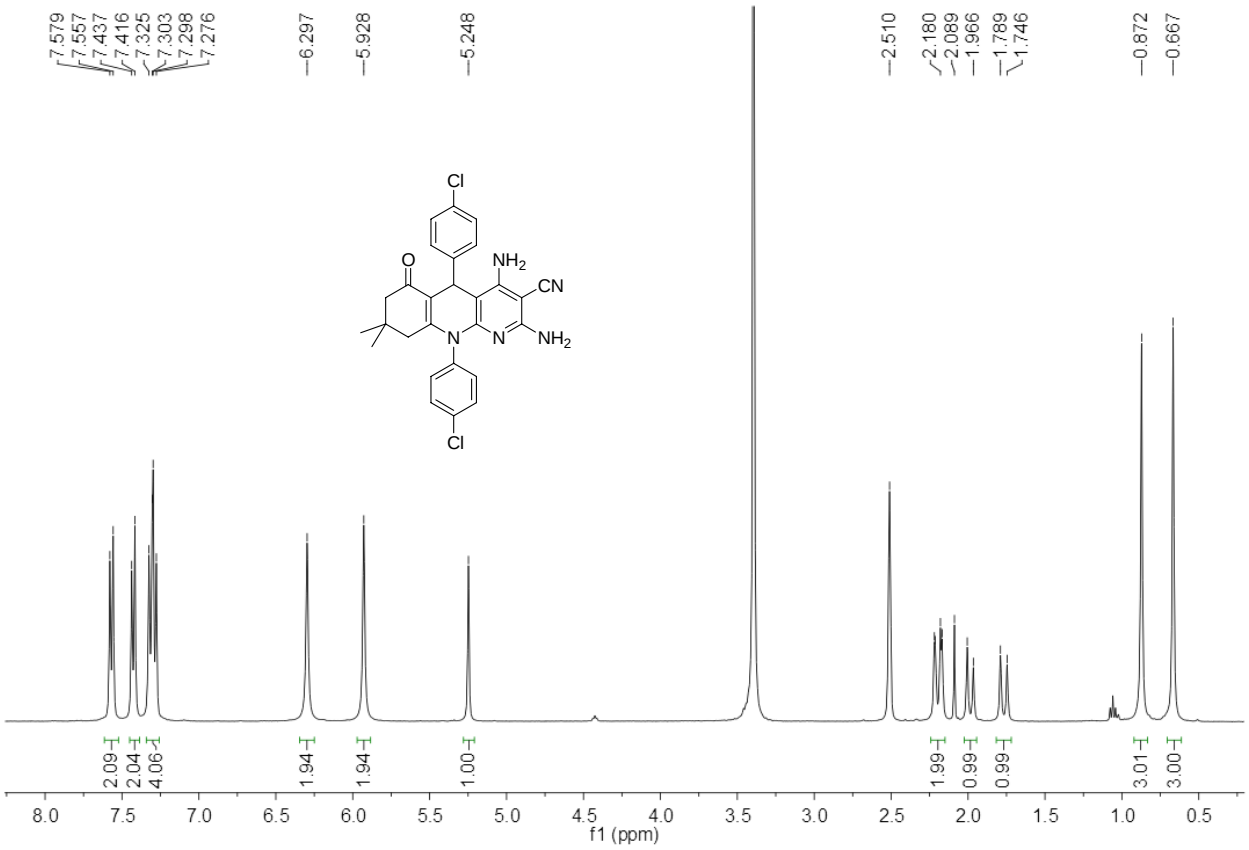
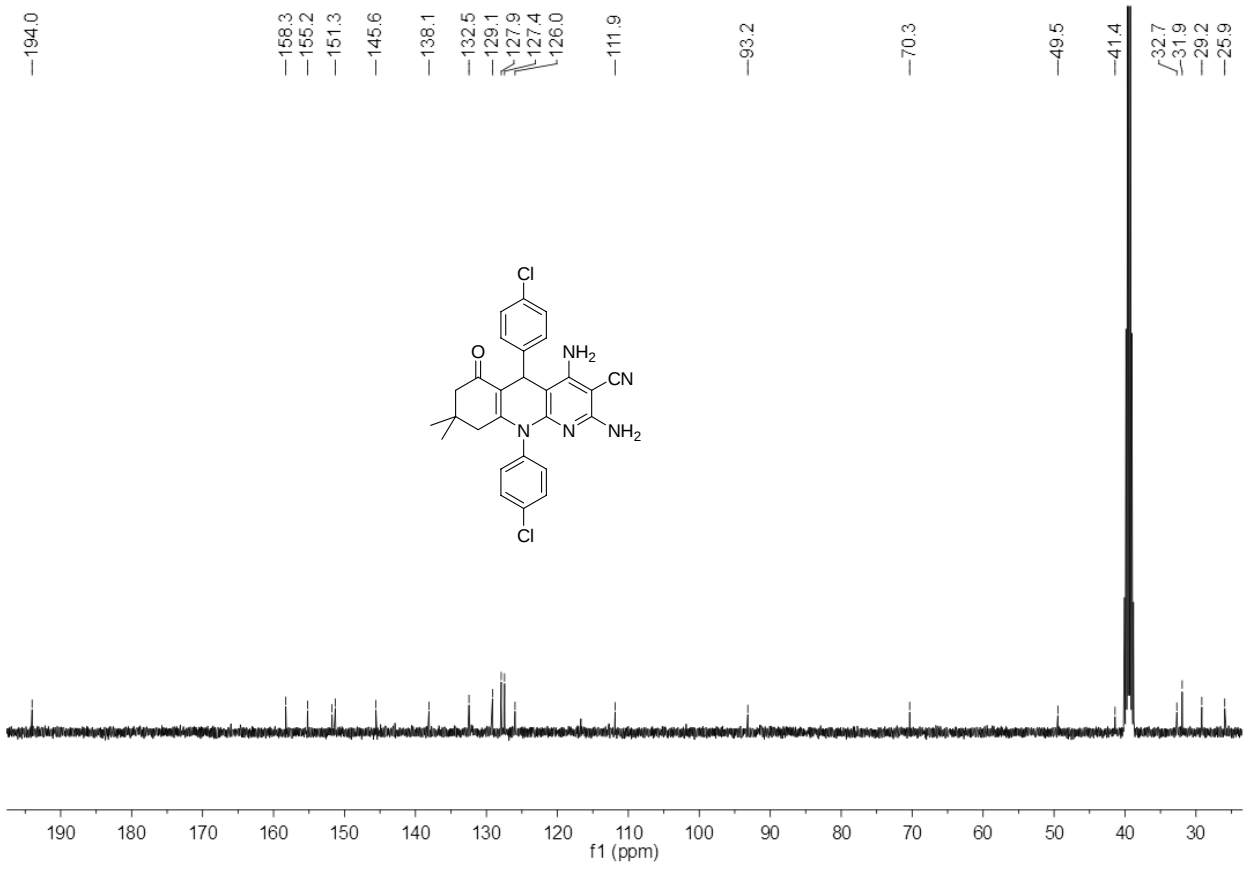


^{1}H NMR Spectrum of Compound 5m



^{13}C NMR Spectrum of Compound 5m

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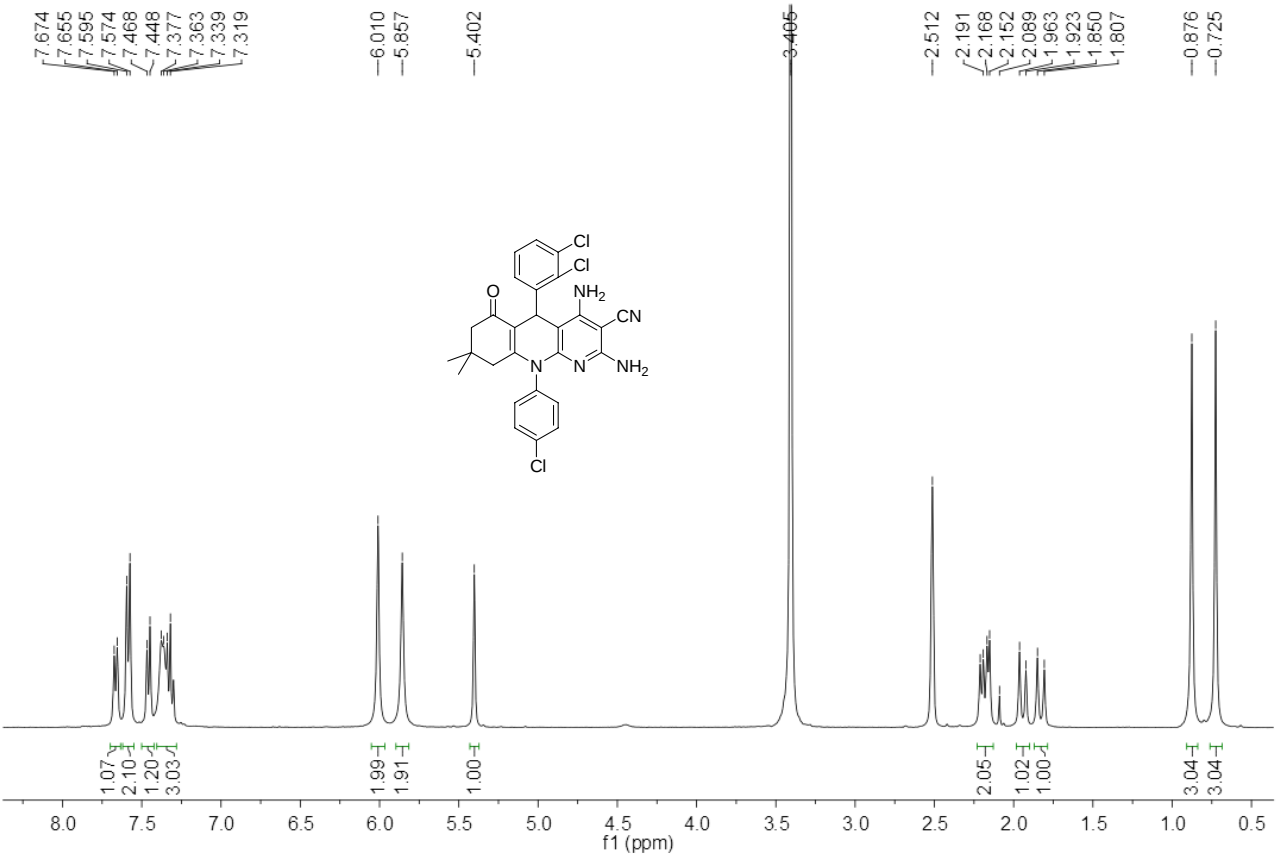
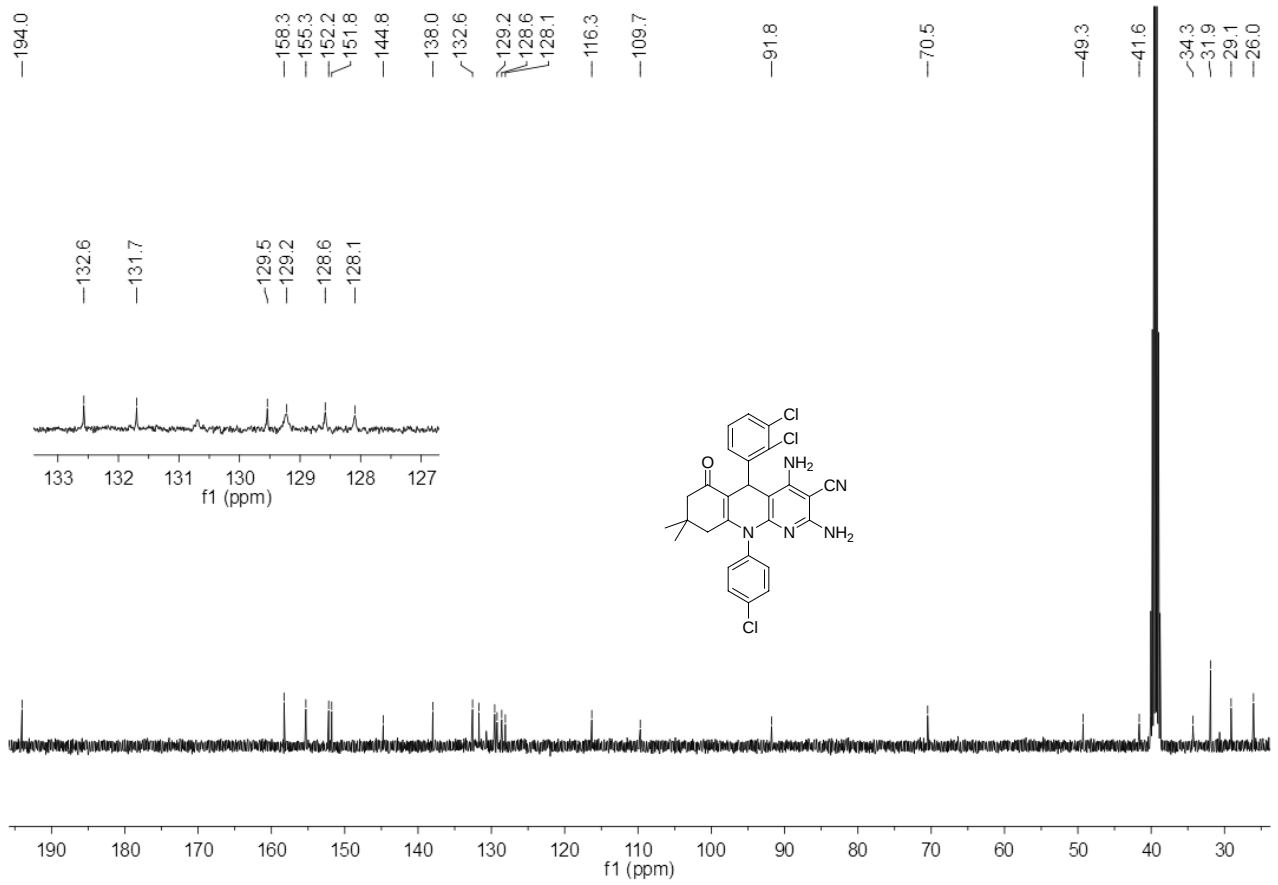


^{1}H NMR Spectrum of Compound 5n



^{13}C NMR Spectrum of Compound 5n

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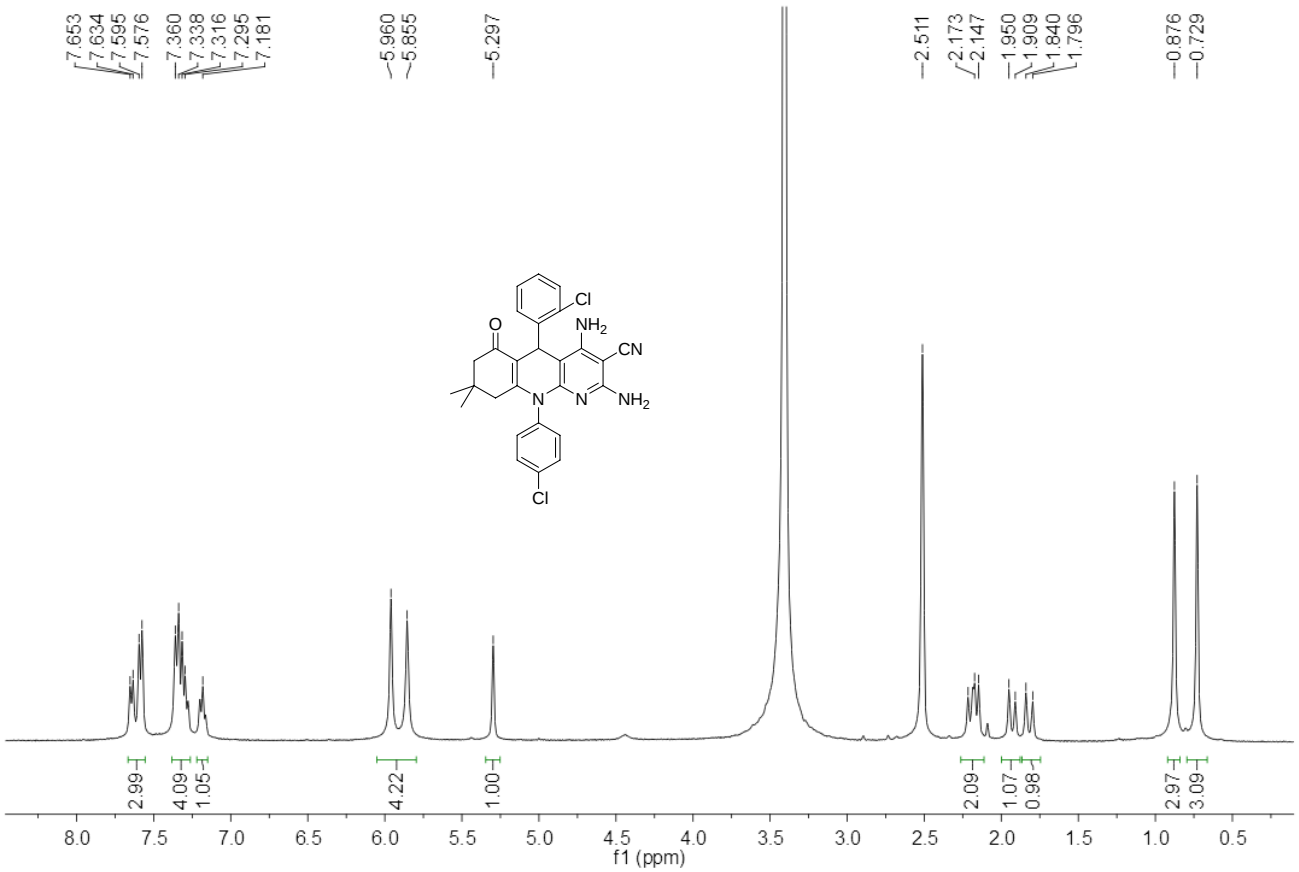
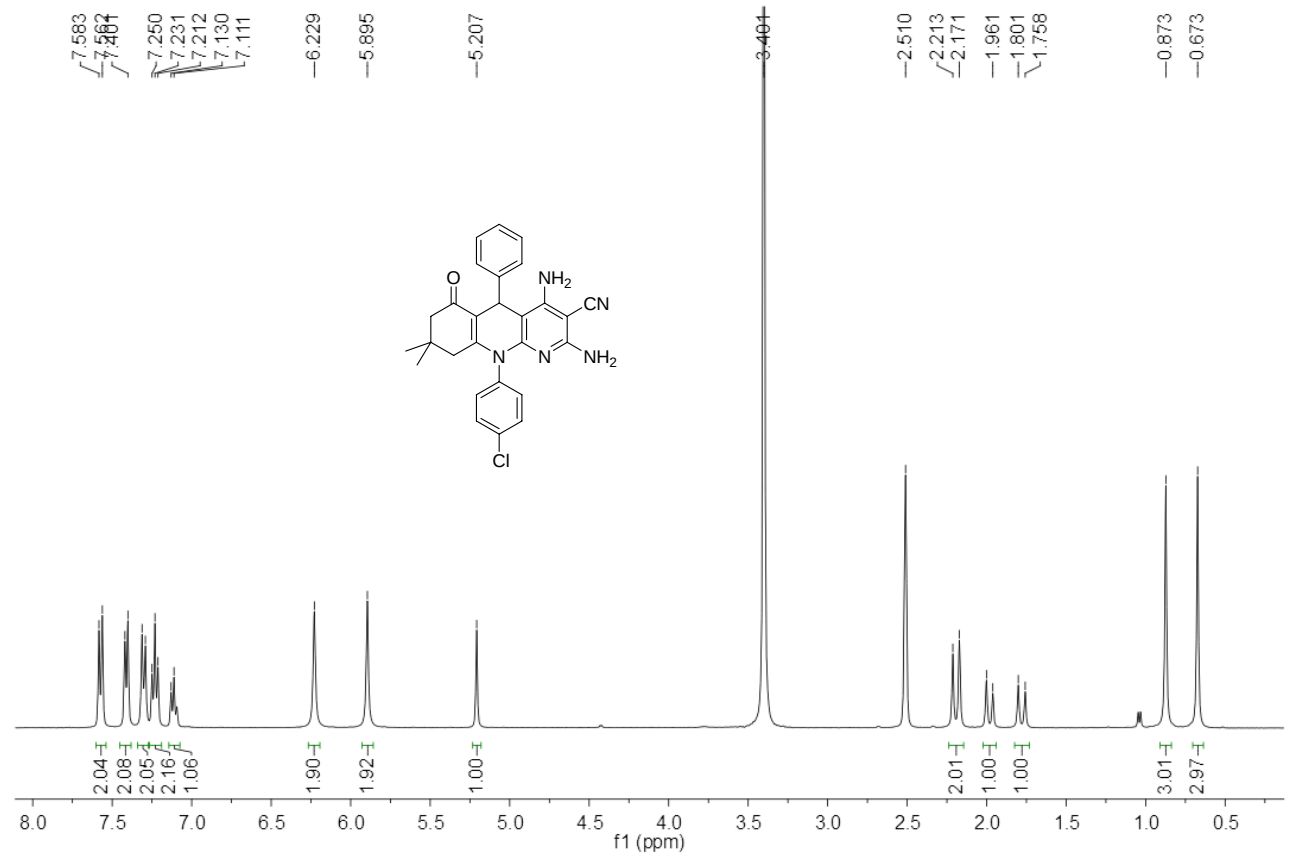


^{1}H NMR Spectrum of Compound 5o



^{1}H NMR Spectrum of Compound 5p

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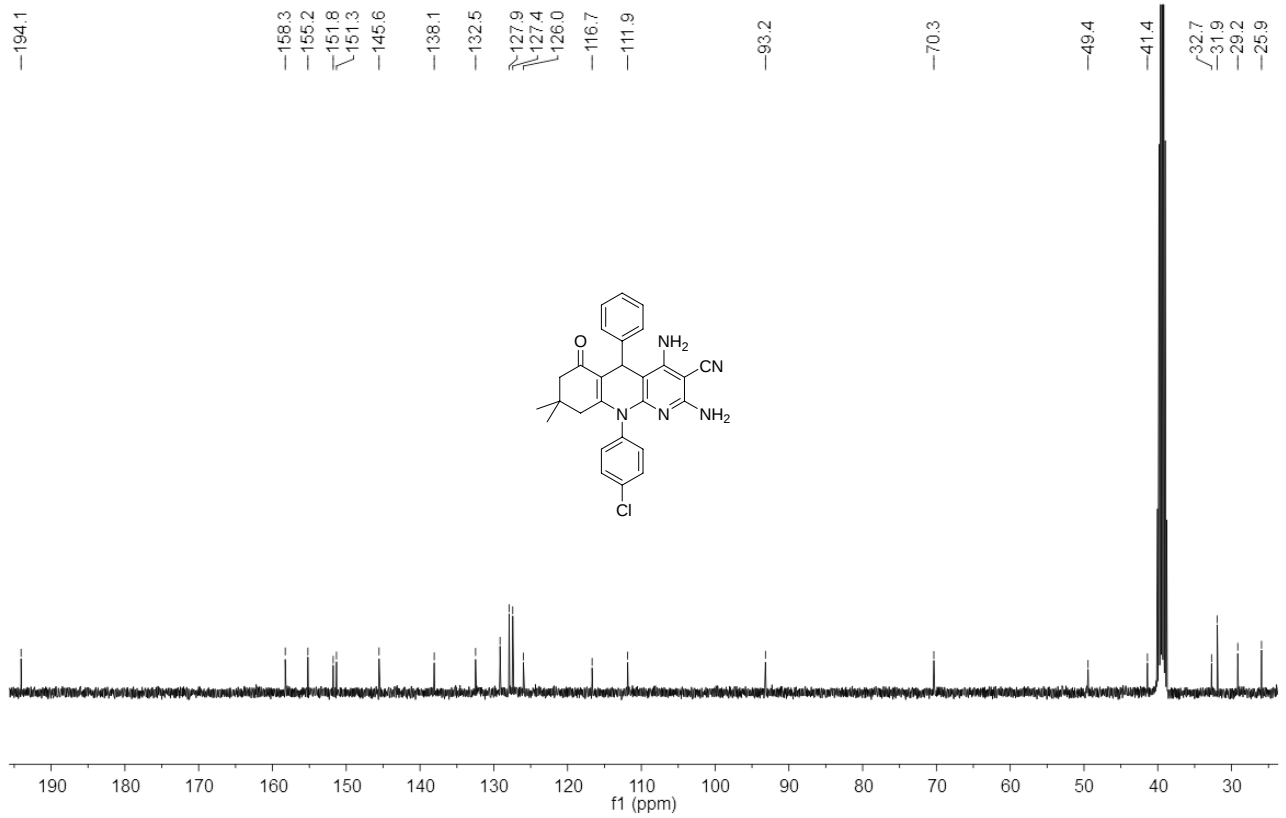
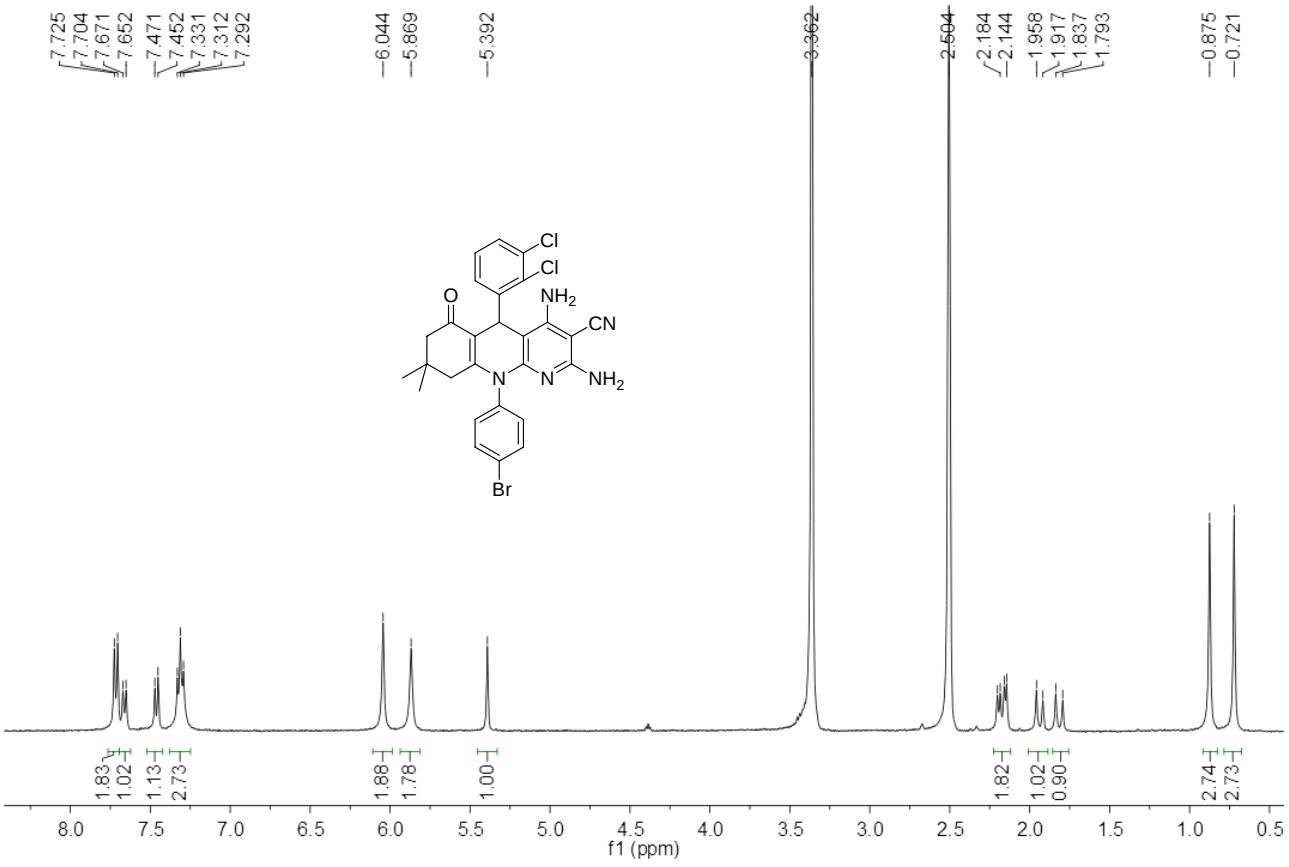


^{13}C NMR Spectrum of Compound 5p



^{1}H NMR Spectrum of Compound 5q

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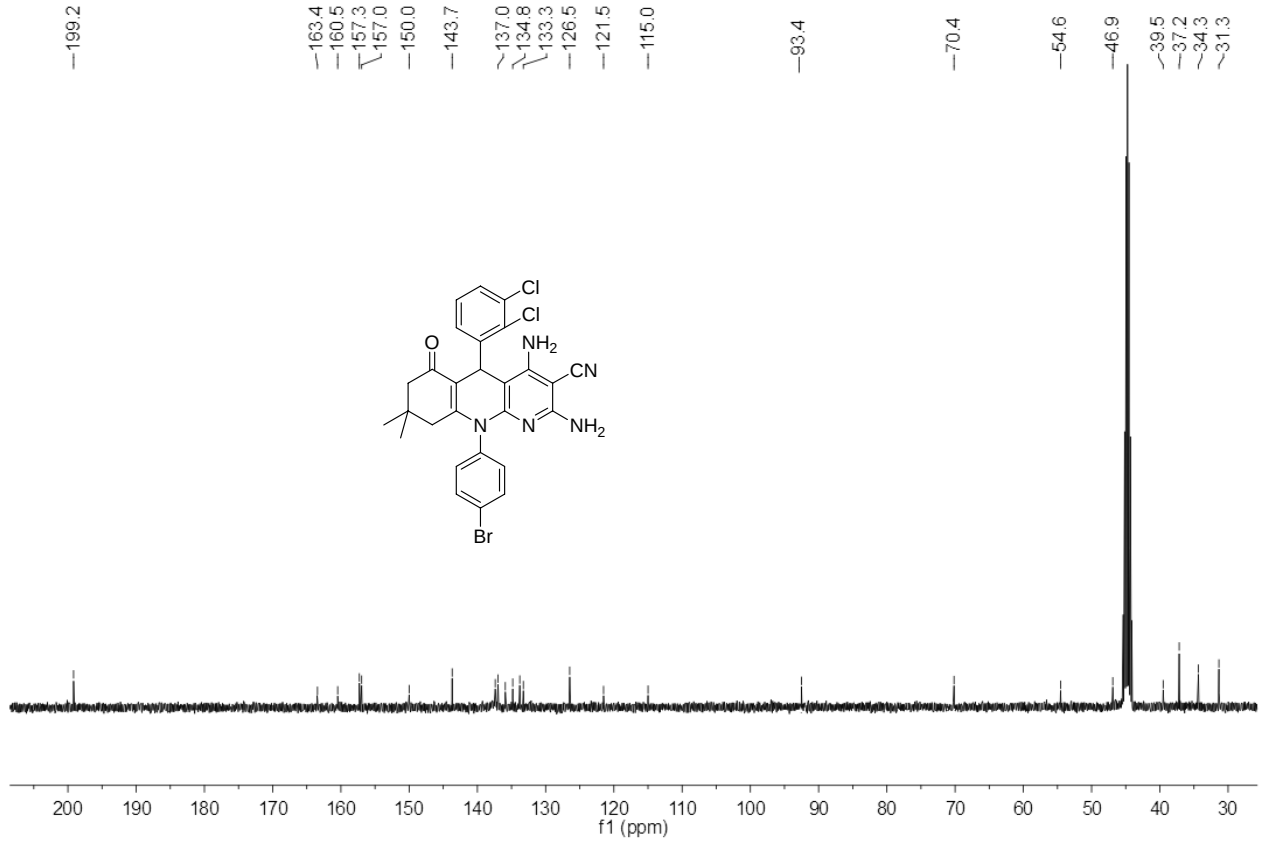
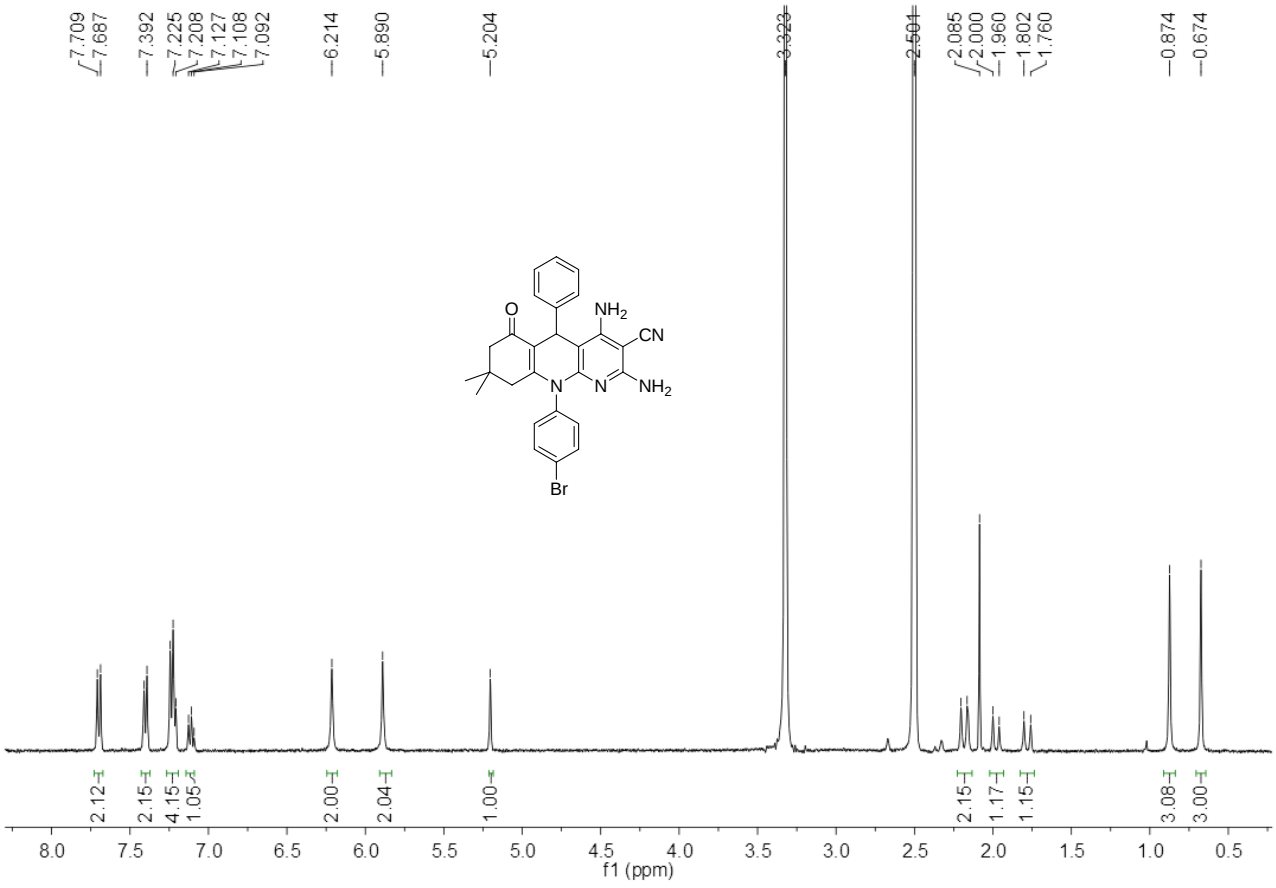


^{13}C NMR Spectrum of Compound 5q



^{1}H NMR Spectrum of Compound 5r

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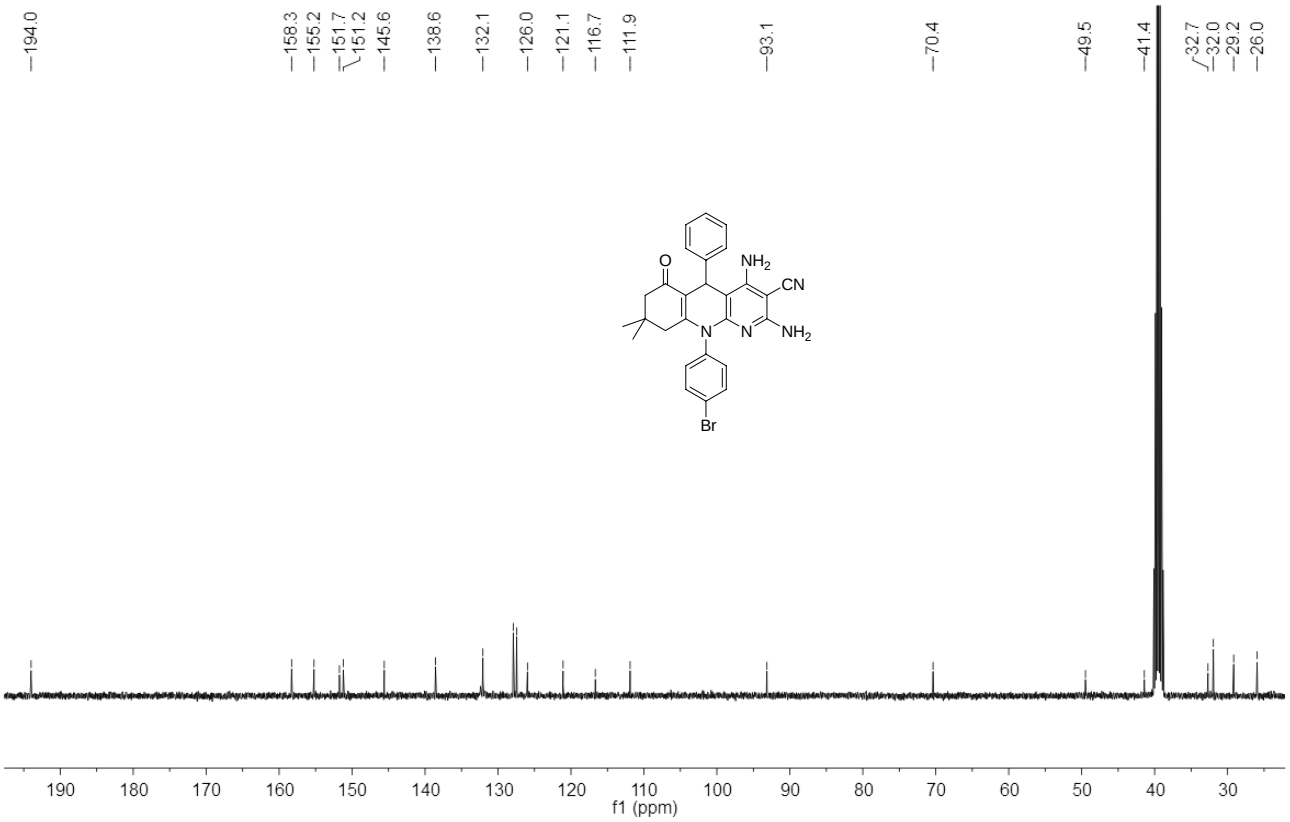
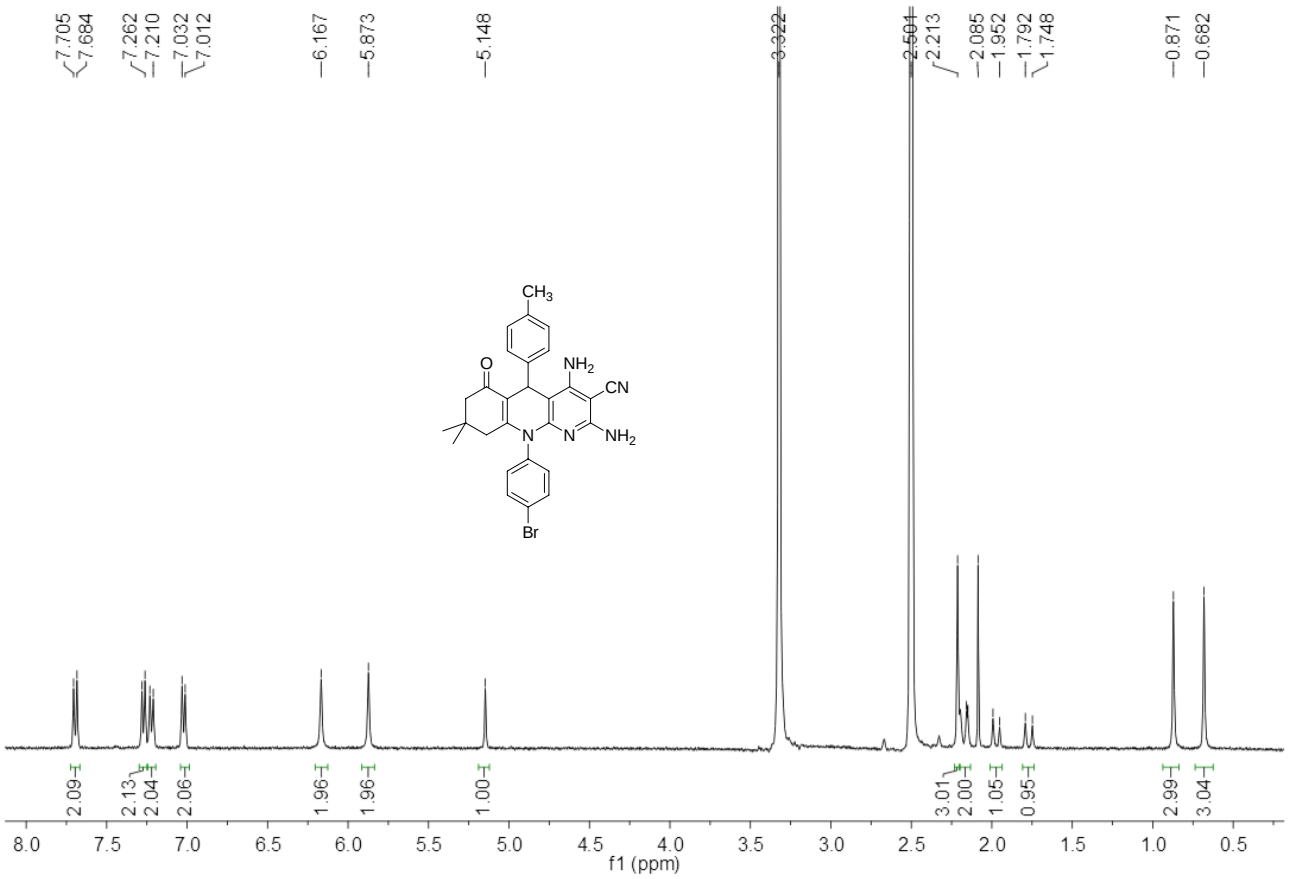


^{13}C NMR Spectrum of Compound 5r



^{1}H NMR Spectrum of Compound 5s

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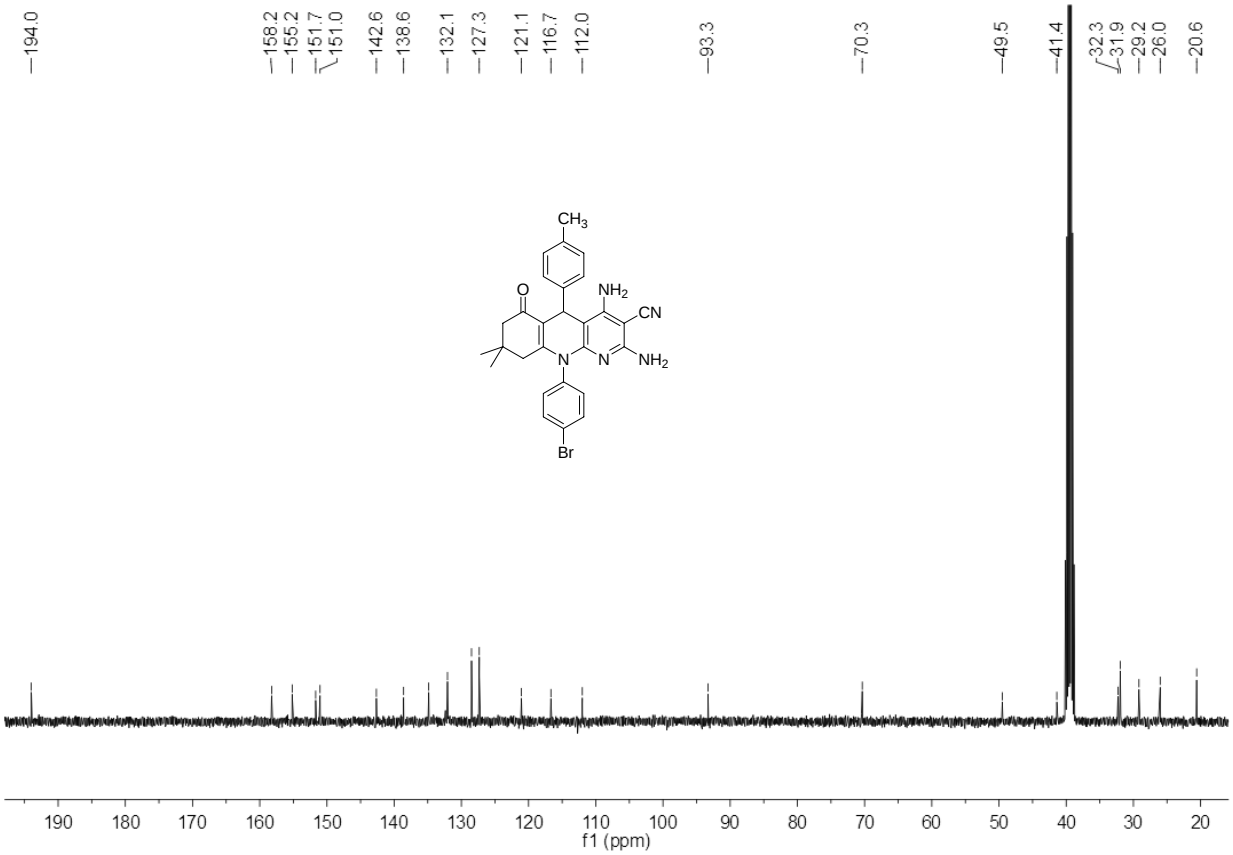
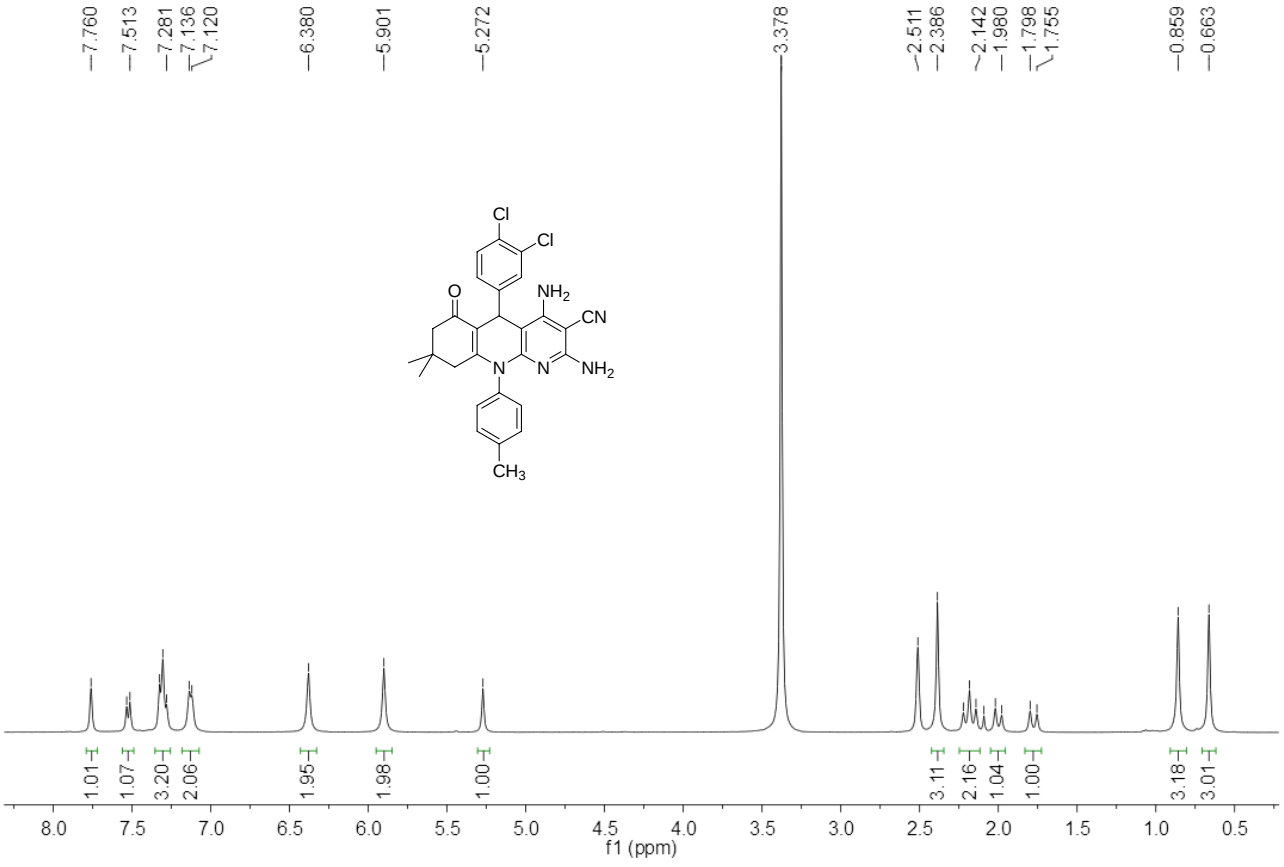


^{13}C NMR Spectrum of Compound 5s



^{1}H NMR Spectrum of Compound 5t

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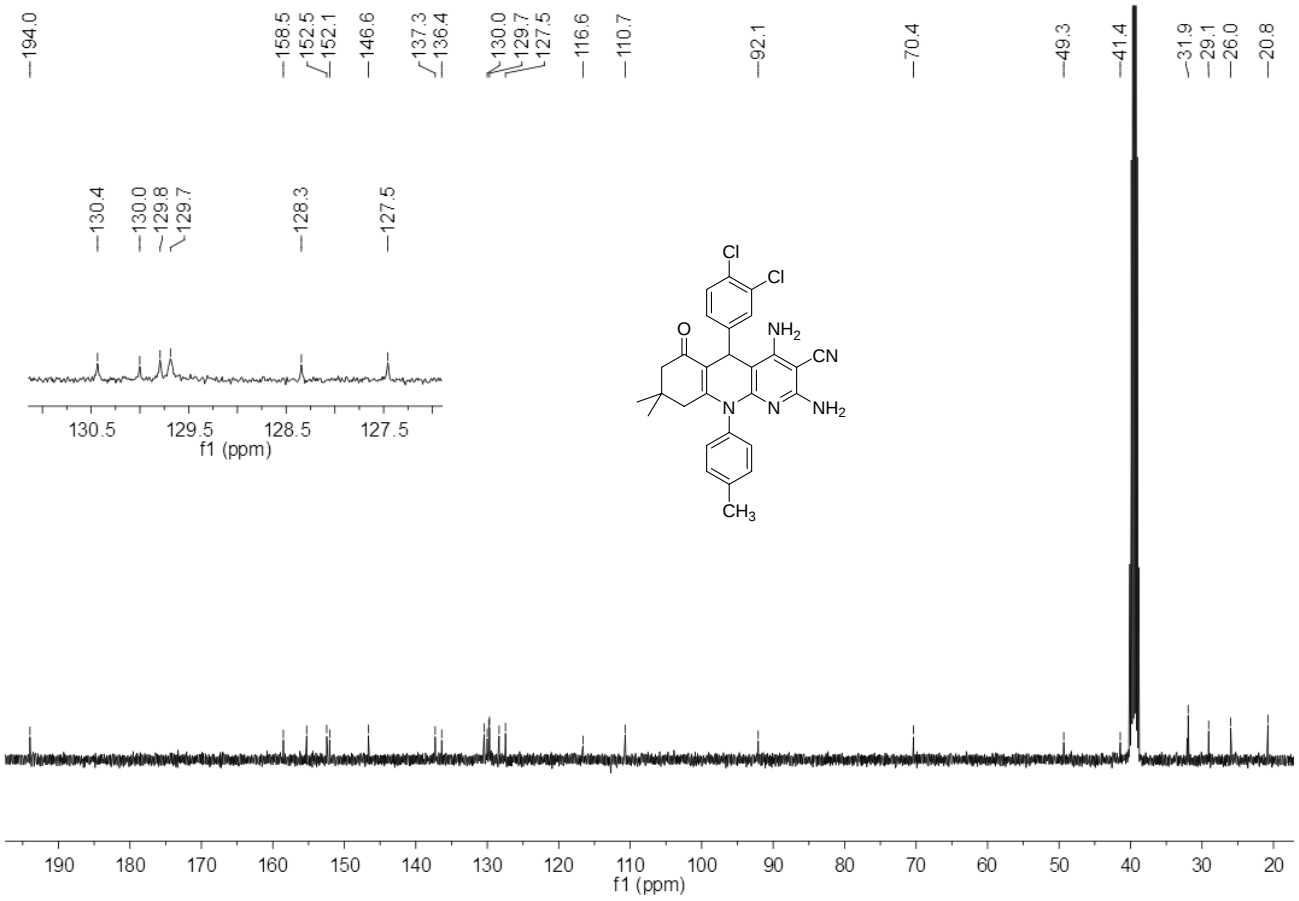
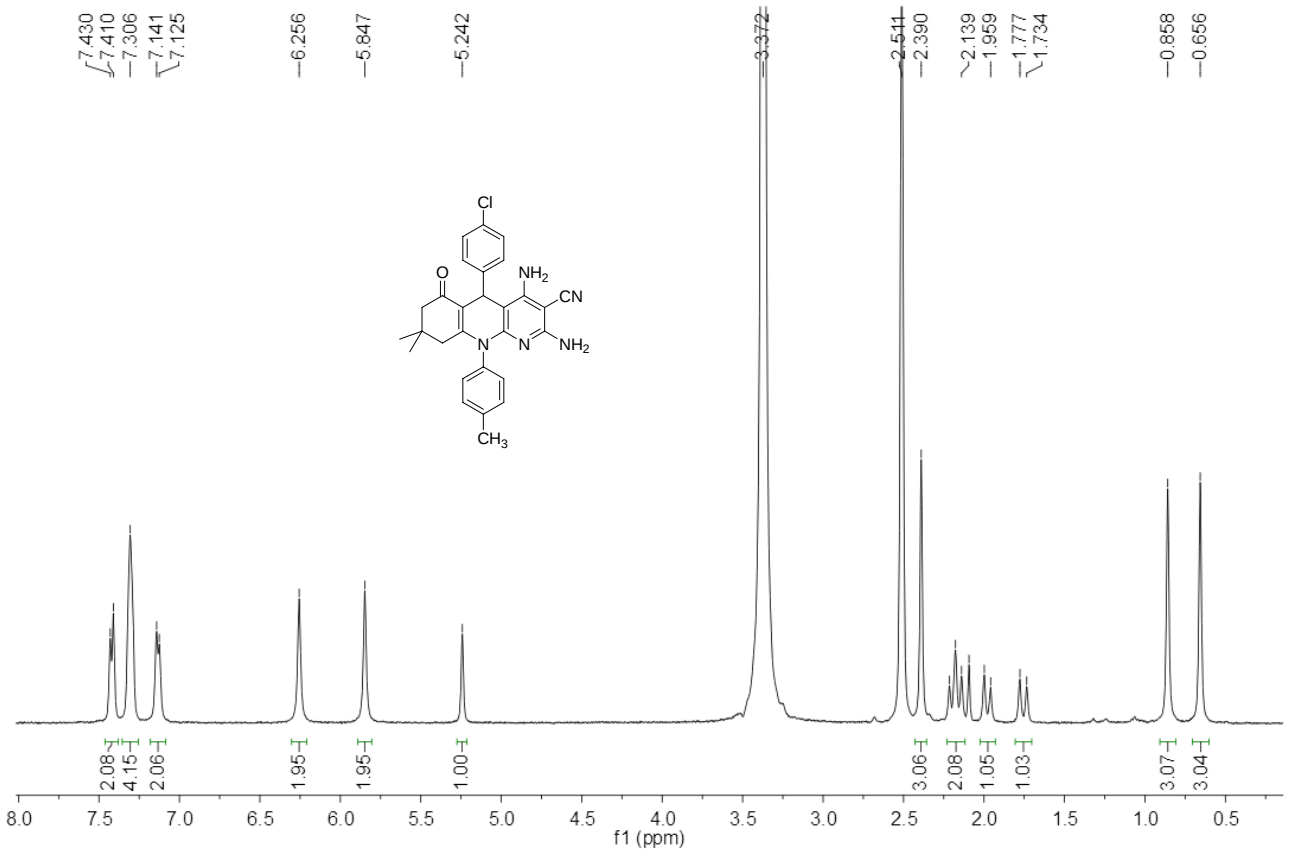


^{13}C NMR Spectrum of Compound 5t



^{1}H NMR Spectrum of Compound 5u

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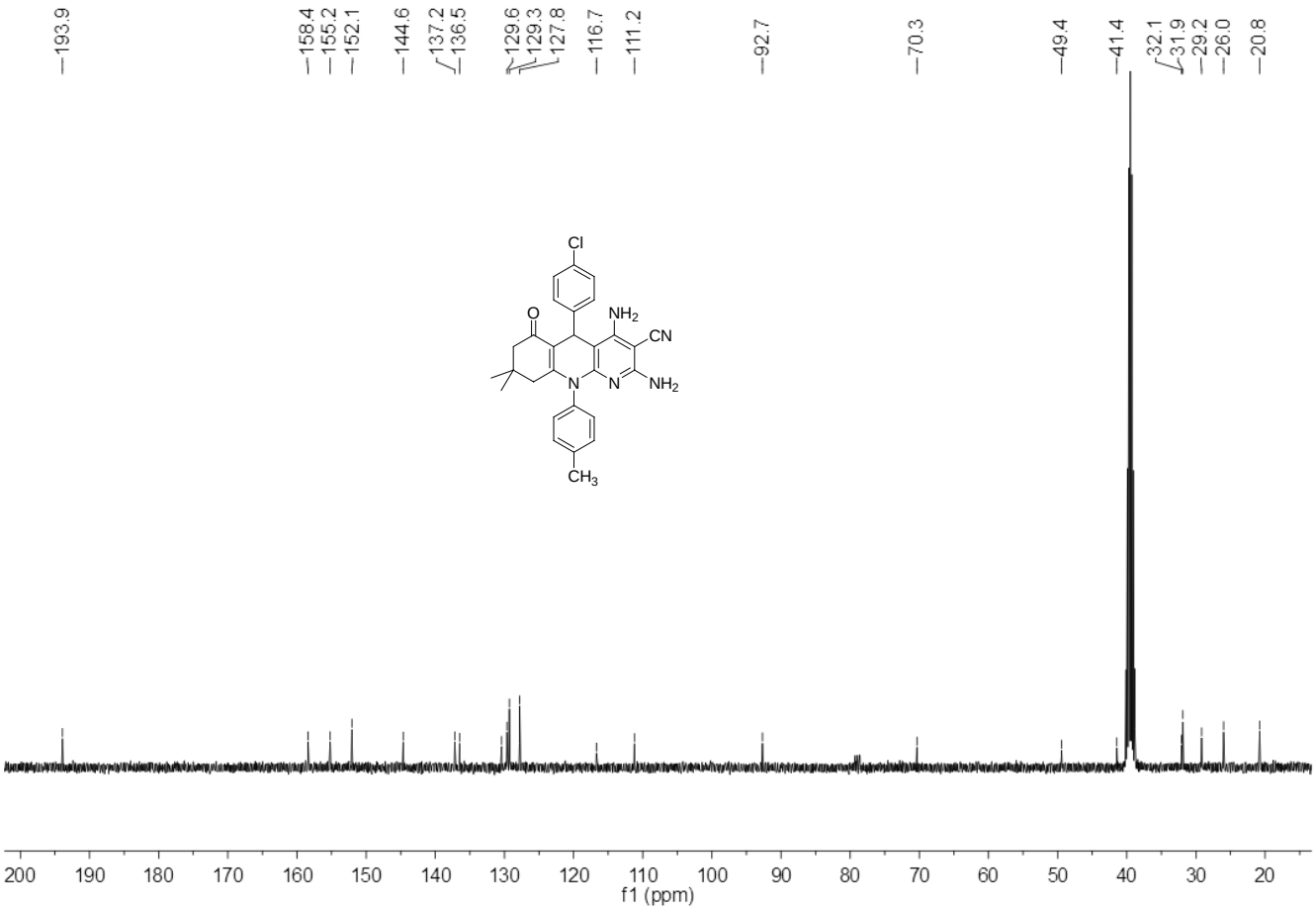

^{13}C NMR Spectrum of Compound 5u