

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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Supporting Information for

A domino synthetic strategy leading to two-carbon-tethered fused acridine/indole pairs and fused acridine derivatives

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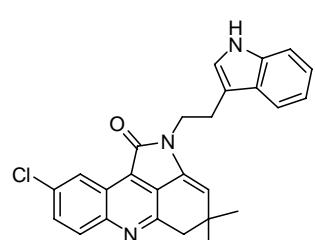
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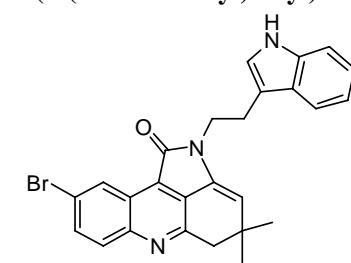
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2-(2-(1H-Indol-3-yl)ethyl)-9-chloro-4,4-dimethyl-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3a)



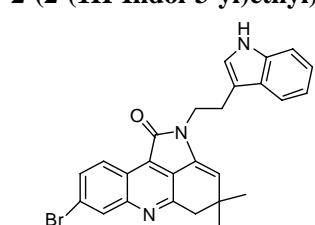
Yellow solid; mp: 244.6–244.9 °C;
IR (KBr, v, cm⁻¹): 3189, 2941, 2892, 1687, 1650, 1625, 1444, 1335, 1090, 966, 837.
¹H NMR (400 MHz, DMSO-*d*₆) (δ ppm): 10.80 (s, 1H, NH), 8.39 (s, 1H, ArH), 8.05 (d, *J* = 9.2 Hz, 1H, ArH), 7.75 (d, *J* = 9.2 Hz, 1H, ArH), 7.52 (d, *J* = 7.6 Hz, 1H, ArH), 7.32 (d, *J* = 8.0 Hz, 1H, ArH), 7.09 (s, 1H, ArH), 7.04 (t, *J* = 7.6 Hz, 1H, ArH), 6.90 (t, *J* = 7.2 Hz, 1H), 5.48 (s, 1H), 4.01 (t, *J* = 6.4 Hz, 2H, CH₂), 3.08 (t, *J* = 6.4 Hz, 2H, CH₂), 2.95 (s, 2H, CH₂), 1.06 (s, 6H, CH₃).
HRMS (ESI) *m/z*: calcd for C₂₆H₂₃ClN₃O: 428.1530 [M+H]⁺, found: 428.1524.

2-(2-(1H-Indol-3-yl)ethyl)-8-bromo-4,4-dimethyl-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3b)



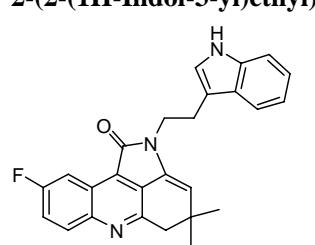
Yellow solid; mp: 223.7–223.9 °C;
IR (KBr, v, cm⁻¹): 3345, 2954, 1693, 1660, 1601, 1337, 1102, 738.
¹H NMR (400 MHz, DMSO-*d*₆) δ: 10.81 (s, 1H, NH), 8.40 (d, *J* = 8.8 Hz, 1H, ArH), 8.27 (d, *J* = 2.0 Hz, 1H, ArH), 7.85 (dd, *J* = 8.8, 2.0 Hz, 1H, ArH), 7.51 (d, *J* = 8.0 Hz, 1H, ArH), 7.32 (d, *J* = 8.0 Hz, 1H, ArH), 7.13 (d, *J* = 2.0 Hz, 1H, ArH), 7.04 (t, *J* = 7.6 Hz, 1H, ArH), 6.89 (t, *J* = 7.4 Hz, 1H, ArH), 5.48 (s, 1H, CH), 4.03 (t, *J* = 6.8 Hz, 2H, CH₂), 3.08 (t, *J* = 6.8 Hz, 2H, CH₂), 2.97 (s, 2H, CH₂), 1.06 (s, 6H, CH₃).
HRMS (ESI) *m/z*: calcd for C₂₆H₂₃BrN₃O: 428.1024 [M+H]⁺, found: 428.1047.

2-(2-(1H-Indol-3-yl)ethyl)-9-bromo-4,4-dimethyl-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3c)



Yellow solid; mp: 228.4–228.9 °C;
IR (KBr, v, cm⁻¹): 3212, 2941, 2892, 1687, 1650, 1442, 1334, 1285, 834, 734.
¹H NMR (400 MHz, DMSO-*d*₆) (δ ppm): 10.81 (s, 1H, NH), 8.54 (d, *J* = 2.0 Hz, 1H, ArH), 7.97 (d, *J* = 8.8 Hz, 1H, ArH), 7.86 (dd, *J* = 8.8, 2.4 Hz, 1H, ArH), 7.51 (d, *J* = 8.0 Hz, 1H, ArH), 7.32 (d, *J* = 8.0 Hz, 1H), 7.12 (d, *J* = 2.0 Hz, 1H, ArH), 7.03 (d, *J* = 8.0 Hz, 1H, ArH), 6.90 (t, *J* = 7.2 Hz, 1H, ArH), 5.47 (s, 1H, CH), 4.00 (t, *J* = 6.8 Hz, 2H, CH₂), 3.08 (t, *J* = 6.8 Hz, 2H, CH₂), 2.93 (s, 2H, CH₂), 1.06 (s, 6H, CH₃).
HRMS (ESI) *m/z*: calcd for C₂₆H₂₃BrN₃O: 472.1024 [M+H]⁺, found: 472.1031.

2-(2-(1H-Indol-3-yl)ethyl)-9-fluoro-4,4-dimethyl-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3d)



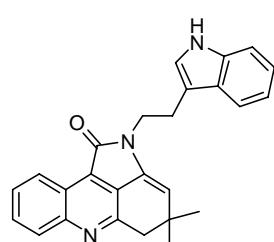
Yellow solid; mp: 222.6–223.9 °C;
IR (KBr, v, cm⁻¹): 3694, 3189, 2940, 2892, 1688, 1651, 1530, 1338, 841, 736.
¹H NMR (400 MHz, DMSO-*d*₆) (δ ppm): 10.81 (s, 1H, NH), 8.16–8.07 (m, 2H, ArH), 7.70–7.65 (m, 1H, rH), 7.52 (d, *J* = 8.0 Hz, 1H, ArH), 7.32 (d, *J* = 8.8 Hz, 1H, ArH), 7.13 (d, *J* = 2.0 Hz, 1H, ArH), 7.04 (t, *J* = 7.6 Hz, 1H, ArH), 6.90 (t, *J* = 7.6 Hz, 1H, ArH), 5.49 (s, 1H, CH), 4.03 (t, *J* = 6.8 Hz, 2H, CH₂), 3.09 (t, *J* = 6.8 Hz, 2H, CH₂), 2.96 (s, 2H, CH₂), 1.07 (s, 6H, CH₃).
HRMS (ESI) *m/z*: calcd for C₂₆H₂₃FN₃O: 412.1825 [M+H]⁺, found: 412.1824.

2-(2-(1H-Indol-3-yl)ethyl)-4,4-dimethyl-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3e)

Yellow solid; mp: 230.7–230.9 °C;

IR (KBr, v, cm⁻¹): 3693, 3172, 1688, 1651, 1584, 1338, 1031, 733.

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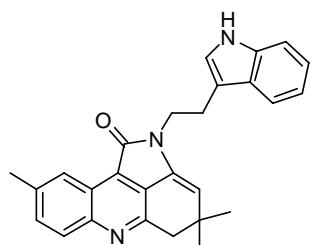


¹H NMR (400 MHz, DMSO-*d*₆) (δ ppm) : 10.80 (s, 1H, NH), 8.53 (d, *J* = 8.0 Hz, 1H, ArH), 8.09 (d, *J* = 8.4 Hz, 1H, ArH), 7.78 (t, *J* = 7.6 Hz, 1H, ArH), 7.70 (t, *J* = 7.6 Hz, 1H, ArH), 7.53 (d, *J* = 7.6 Hz, 1H, ArH), 7.32 (d, *J* = 8.0 Hz, 1H, ArH), 7.13 (s, 1H, ArH), 7.04 (t, *J* = 7.6 Hz, 1H, ArH), 6.91 (t, *J* = 7.6 Hz, 1H, CH), 5.45 (s, 1H, CH), 4.04 (t, *J* = 6.4 Hz, 2H, CH₂), 3.09 (t, *J* = 6.4 Hz, 2H, CH₂), 2.98 (s, 2H, CH₂), 1.08 (s, 6H, CH₃).

¹³C NMR (100 MHz, DMSO-*d*₆) (δ ppm) : 166.4, 154.5, 148.8, 136.2, 132.1, 129.3, 129.2, 127.6, 127.3, 126.0, 124.3, 123.2, 123.2, 121.8, 120.9, 118.2, 118.1, 118.0, 112.7, 111.4, 110.9, 43.2, 40.7, 36.4, 30.1, 24.3.

HRMS (ESI) *m/z*: calcd for C₂₆H₂₄N₃O: 394.1919 [M+H]⁺, found: 394.1942.

2-(2-(1H-Indol-3-yl)ethyl)-4,4,9-trimethyl-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3f)

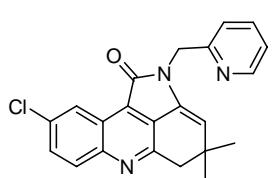


Yellow solid; mp: 225.7–225.9 °C;
IR (KBr, v, cm⁻¹): 3856, 3652, 2939, 1687, 1655, 1432, 1336, 1031, 731.
¹H NMR (400 MHz, DMSO-*d*₆) (δ ppm) : 10.79 (s, 1H, NH), 8.30 (s, 1H, ArH), 7.97 (d, *J* = 8.4 Hz, 1H, ArH), 7.60 (d, *J* = 8.4 Hz, 1H, ArH), 7.53 (d, *J* = 8.0 Hz, 1H, ArH), 7.32 (d, *J* = 8.0 Hz, 1H, ArH), 7.12 (s, 1H, ArH), 7.04 (t, *J* = 7.6 Hz, 1H, ArH), 6.91 (d, *J* = 7.6 Hz, 1H), 5.43 (s, 1H), 4.03 (t, *J* = 6.8 Hz, 2H, CH₂), 3.09 (t, *J* = 6.8 Hz, 2H, CH₂), 2.95 (s, 2H, CH₂), 2.54 (s, 3H, CH₃), 1.07 (s, 6H, CH₃).

¹³C NMR (100 MHz, DMSO-*d*₆) (δ ppm): 166.5, 153.4, 147.4, 137.3, 136.2, 132.1, 131.1, 129.0, 127.3, 126.0, 123.7, 123.1, 122.2, 121.8, 120.8, 118.2, 118.0, 117.8, 111.4, 110.9, 43.1, 40.6, 36.3, 30.2, 24.3, 21.2.

HRMS (ESI) *m/z*: calcd for C₂₇H₂₆N₃O: 408.2076 [M+H]⁺, found: 408.2072.

9-Chloro-4,4-dimethyl-2-(pyridin-2-ylmethyl)-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3g)



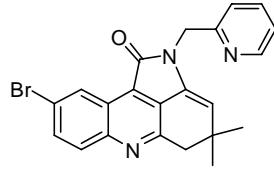
Yellow solid; mp: 173.4–174.0 °C;
IR (KBr, v, cm⁻¹): 3061, 2958, 2869, 1693, 1660, 1589, 1531, 1477, 1458, 1436, 1341, 1277, 1216, 1177, 1085, 980, 838, 776, 621, 500.

¹H NMR (400 MHz, CDCl₃) (δ ppm) : 8.58 (s, 1H, ArH), 8.31 (s, 1H, ArH), 8.14 (s, 1H, ArH), 7.65 (s, 1H, ArH), 7.49 (s, 1H, ArH), 7.35 – 7.15 (m, 2H, ArH), 5.61 (s, 1H, CH), 5.15 (s, 2H, CH₂), 3.13 (s, 2H, CH₂), 1.27 (s, 6H, CH₃).

¹³C NMR (100 MHz, CDCl₃) (δ ppm) : 167.1, 162.6, 160.1, 156.4, 153.6, 149.3, 146.6, 137.1, 132.5, 131.7, 131.6, 127.2, 125.1, 125.1, 123.4, 123.3, 122.7, 121.8, 119.3, 119.0, 118.9, 108.4, 108.1, 45.9, 43.9, 37.1, 30.8.

HRMS (ESI) *m/z*: calcd for C₂₂H₁₉ClN₃ONa: 398.1036 [M+H]⁺, found: 398.1021.

9-Bromo-4,4-dimethyl-2-(pyridin-2-ylmethyl)-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3h)



Yellow solid; mp: 173.6–173.9 °C;
IR (KBr, v, cm⁻¹): 3698, 2953, 1696, 1655, 1568, 1444, 1331, 831, 754.

¹H NMR (400 MHz, DMSO-*d*₆) (δ ppm) : 8.61–8.51 (m, 2H, ArH), 8.07 (d, *J* = 8.8 Hz, 1H, ArH), 7.93 (d, *J* = 8.8 Hz, 1H, ArH), 7.77 (t, *J* = 7.6 Hz, 1H, ArH), 7.29–7.27 (m, 2H, ArH), 5.87 (s, 1H, CH), 5.10 (s, 1H, CH₂), 3.12 (s, 1H, CH₂), 1.22 (s, 6H, CH₃).

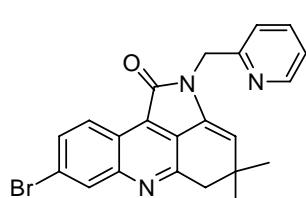
HRMS (ESI) *m/z*: calcd for C₂₂H₁₉BrN₃O: 420.0711 [M+H]⁺, found: 420.0731.

8-Bromo-4,4-dimethyl-2-(pyridin-2-ylmethyl)-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3i)

Yellow solid; mp: 168.9–167.2 °C;

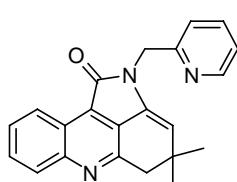
IR (KBr, v, cm⁻¹): 3059, 2958, 2864, 1699, 1659, 1630, 1437, 1291, 839, 752.

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¹H NMR (400 MHz, DMSO-*d*₆) (δ ppm) : 8.51 (d, *J* = 4.4 Hz, 1H, ArH), 8.42 (d, *J* = 8.8 Hz, 1H, ArH), 8.32 (d, *J* = 2.0 Hz, 1H, ArH), 7.88 (dd, *J* = 8.8, 2.0 Hz, 1H, ArH), 7.77 (m, 1H, , ArH), 7.29 (m, 2H, ArH), 5.84 (s, 1H, CH), 5.10 (s, 2H, CH₂), 3.13 (s, 2H, CH₂), 1.22 (s, 6H, CH₃).
HRMS (ESI) *m/z*: calcd for C₂₂H₁₉BrN₃O: 420.0711 [M+H]⁺, found: 420.0724.

4,4-Dimethyl-2-(pyridin-2-ylmethyl)-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3j)



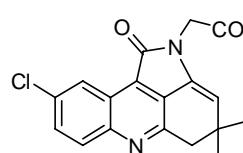
Yellow solid; mp: 167.8–167.9 °C;
IR (KBr, v, cm⁻¹): 2960, 1694, 1660, 1591, 1568, 1524, 1475, 1465, 1341, 1297, 1145, 1087, 993, 839, 770, 621.

¹H NMR (400 MHz, CDCl₃) (δ ppm) : 8.70 (d, *J* = 6.4 Hz, 1H, ArH), 8.58 (s, 1H, ArH), 8.16 (d, *J* = 6.8 Hz, 1H, ArH), 7.74 (s, 1H, ArH), 7.65 (s, 2H, ArH), 7.40 – 6.96 (m, 2H, ArH), 5.56 (s, 1H, CH), 5.15 (s, 2H, CH₂), 3.15 (s, 2H, CH₂), 1.26 (s, 6H, CH₃).

¹³C NMR (100 MHz, CDCl₃) (δ ppm): 167.5, 156.5, 154.4, 149.5, 149.3, 137.0, 132.7, 129.4, 129.4, 127.7, 126.7, 125.4, 124.2, 122.6, 121.7, 118.2, 45.9, 44.1, 37.1, 30.8.

HRMS (ESI) *m/z*: calcd for C₂₂H₂₀N₃O: 342.1606 [M+H]⁺, found: 342.1614.

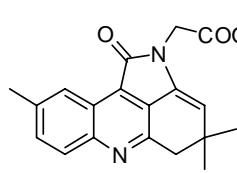
2-(9-Chloro-4,4-dimethyl-1-oxo-4,5-dihydropyrrolo[2,3,4-kl]acridin-2(1H)-yl)acetic acid (3k)



Yellow solid; mp: 169.3–169.7°C;
IR (KBr, v, cm⁻¹): 3655, 2958, 1709, 1664, 1651, 1510, 1440, 708, 621.
¹H NMR (400 MHz, DMSO-*d*₆) (δ ppm): 8.50 – 8.13 (m, 1H, ArH), 8.08 (d, *J* = 8.8 Hz, 1H, ArH), 7.71 (t, *J* = 8.8 Hz, 1H, ArH), 5.99 (s, 1H, CH), 4.55 (s, 2H, CH₂), 3.14 (s, 2H, CH₂), 1.28 (s, 6H, CH₃).

HRMS (ESI) *m/z*: calcd for C₁₈H₁₆ClN₂O₃: 343.0849 [M+H]⁺, found: 343.0821.

2-(4,4,9-Trimethyl-1-oxo-4,5-dihydropyrrolo[2,3,4-kl]acridin-2(1H)-yl)acetic acid (3l)

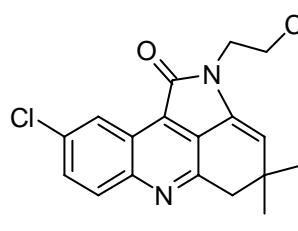


Yellow solid; mp: 179.1–179.3°C;
IR (KBr, v, cm⁻¹): 2958, 1707, 1664, 1651, 1510, 1440, 708, 621.
¹H NMR (400 MHz, CDCl₃) (δ ppm) : 8.43 (s, 1H, ArH), 8.12 (d, *J* = 7.2 Hz, 1H, ArH), 7.57 (d, *J* = 8.0 Hz, 1H, ArH), 5.51 (s, 1H, CH), 4.61 (s, 2H, CH₂), 3.22 (s, 2H, CH₂), 2.57 (s, 3H, CH₃), 1.31 (s, 6H, CH₃).

¹³C NMR (100 MHz, CDCl₃) (δ ppm): 175.2, 167.3, 154.3, 148.9, 132.5, 129.7, 128.7, 127.9, 126.6, 125.8, 124.2, 122.5, 117.6, 43.5, 37.0, 36.1, 33.3, 30.9.

HRMS (ESI) *m/z*: calcd for C₁₉H₁₉N₂O₃: 323.1396 [M+H]⁺, found: 323.1382.

3-(9-Chloro-4,4-dimethyl-1-oxo-4,5-dihydropyrrolo[2,3,4-kl]acridin-2(1H)-yl)propanoic acid (3m)

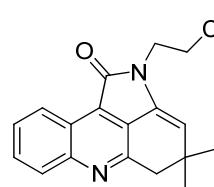


Yellow solid; mp: 178.1–178.5°C;
IR (KBr, v, cm⁻¹): 3664, 2960, 2558, 1704, 1650, 1510, 1281, 1086, 831.
¹H NMR (400 MHz, CDCl₃) (δ ppm): 8.63 (s, 1H, ArH), 8.13 (d, *J* = 8.8 Hz, 1H, ArH), 7.67 (d, *J* = 8.8 Hz, 1H, ArH), 5.70 (s, 1H, CH), 4.12 (t, *J* = 6.8 Hz, 2H, CH₂), 3.17 (s, 2H, CH₂), 2.86 (t, *J* = 6.8 Hz, 2H, CH₂), 1.32 (s, 6H, CH₃).

HRMS (ESI) *m/z*: calcd for C₁₉H₁₈ClN₂O₃: 357.1006 [M+H]⁺, found: 375.1025.

3-(4,4-Dimethyl-1-oxo-4,5-dihydropyrrolo[2,3,4-kl]acridin-2(1H)-yl)propanoic acid (3n)

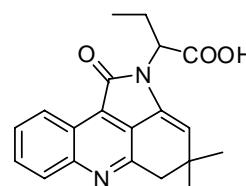
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Yellow solid; mp: 205.1–205.5°C;
IR (KBr, v, cm⁻¹): 2958, 1963, 1700, 1651, 1632, 1440, 1199, 771.
¹H NMR (400 MHz, CDCl₃) (δ ppm) : 8.65 (d, J = 8.0 Hz, 1H, ArH), 8.20 (d, J = 8.4 Hz, 1H, ArH), 7.73 (t, J = 7.6 Hz, 1H, ArH), 7.64 (t, J = 7.2 Hz, 1H, ArH), 5.67 (s, 1H, CH), 4.14 (t, J = 6.8 Hz, 2H, CH₂), 3.16 (s, 2H, CH₂), 2.93 – 2.77 (m, 2H, CH₂), 1.30 (s, 6H, CH₃).

HRMS (ESI) m/z : calcd for C₁₉H₁₉N₂O₃: 323.1396 [M+H]⁺, found: 323.1380.

2-(4,4-Dimethyl-1-oxo-4,5-dihydropyrrolo[2,3,4-kl]acridin-2(1H)-yl)butanoic acid (3o)



Yellow solid; mp: 222.3–222.4°C;
IR (KBr, v, cm⁻¹): 3694, 2961, 1694, 1655, 1524, 1463, 1414, 1339, 1299, 1254, 1223, 1152, 1045, 913, 871, 772, 644, 604.
¹H NMR (400 MHz, CDCl₃) (δ ppm) : 8.66 (d, J = 8.0 Hz, 1H, ArH), 8.18 (d, J = 8.4 Hz, 1H, ArH), 7.72 (t, J = 7.6 Hz, 1H, ArH), 7.64 (t, J = 7.4 Hz, 1H, ArH), 5.63 (s, 1H, CH), 5.32 – 4.93 (m, 1H, CH), 3.20 (s, 2H, CH₂), 2.46 – 2.27 (m, 1H, CH₂), 2.26 – 2.11 (m, 1H, CH₂), 1.32 (s, 3H, CH₃), 1.26 (s, 3H, CH₃), 0.96 (t, J = 7.2 Hz, 3H, CH₃).

¹³C NMR (100 MHz, CDCl₃) (δ ppm) : 173.1, 167.5, 154.4, 131.5, 129.8, 128.5, 128.0, 126.8, 125.2, 124.2, 122.5, 119.2, 55.4, 43.2, 37.2, 30.9, 30.8, 22.9, 10.8.

HRMS (ESI) m/z : calcd for C₂₀H₂₁N₂O₃: 337.1552 [M+H]⁺, found: 337.1522.

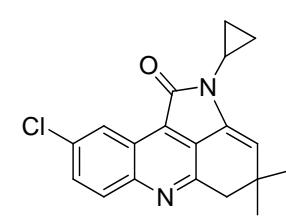
2-(4,4,9-Trimethyl-1-oxo-4,5-dihydropyrrolo[2,3,4-kl]acridin-2(1H)-yl)butanoic acid (3p)



Yellow solid; mp: 210.3–210.5°C;
IR (KBr, v, cm⁻¹): 3694, 2961, 1694, 1657, 1223, 1045, 913, 771.
¹H NMR (400 MHz, CDCl₃) (δ ppm) : 8.42 (s, 1H, ArH), 8.07 (d, J = 8.4 Hz, 1H, ArH), 7.54 (d, J = 8.8 Hz, 1H, ArH), 5.60 (s, 1H, CH), 5.25 – 4.82 (m, 1H, CH), 3.18 (s, 2H, CH₂), 2.55 (s, 3H, CH₃), 2.51 – 2.21 (m, 1H, CH₂), 2.25 – 1.94 (m, 1H, CH₂), 1.32 (s, 3H, CH₃), 1.26 (s, 3H, CH₃), 0.95 (t, J = 7.2 Hz, 3H, CH₃).

HRMS (ESI) m/z : calcd for C₂₁H₂₃N₂O₃: 351.1709 [M+H]⁺, found: 373.1515.

9-Chloro-2-cyclopropyl-4,4-dimethyl-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3q)

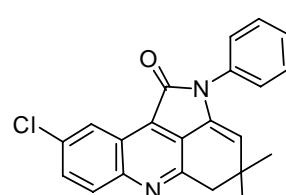


Yellow solid; mp: 166.8–167.3°C;
IR (KBr, v, cm⁻¹): 3809, 3632, 3040, 2953, 2932, 1707, 1653, 1507, 1444, 1338, 1293, 1159, 1128, 1032, 890, 840, 719, 633.
¹H NMR (400 MHz, CDCl₃) (δ ppm): 8.62 (s, 1H, ArH), 8.04 (d, J = 5.6 Hz, 1H, ArH), 7.64 (d, J = 6.8 Hz, 1H, ArH), 5.76 (s, 1H, CH), 3.13 (s, 2H, CH₂), 2.82 (s, 1H, CH), 1.35 (s, 6H, CH₃), 1.09 (s, 2H, CH₂), 1.00 (s, 2H, CH₂).

¹³C NMR (100 MHz, CDCl₃) (δ ppm): 167.6, 154.6, 147.7, 133.7, 133.6, 130.6, 130.1, 126.77, 124.4, 123.2, 123.1, 118.4, 43.9, 37.1, 31.0, 22.2, 5.8.

HRMS (ESI) m/z : calcd for C₁₉H₁₈ClN₂O: 325.1108 [M+H]⁺, found: 325.1129.

9-chloro-2-(4-chlorophenyl)-4,4-dimethyl-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3r)

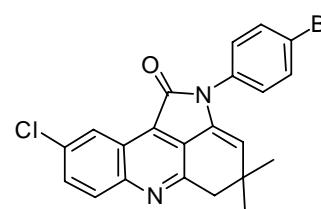


Yellow solid, mp: 179–181 °C;
IR (KBr, v, cm⁻¹): 2961, 1707, 1646, 1508, 1494, 1439, 1366, 1342, 1291, 1151, 1140, 1092, 1078, 899, 825, 792, 748, 719, 632, 512.
¹H NMR (400 MHz, DMSO-*d*₆) (δ ppm): 8.44 (s, 1H, ArH), 8.14 (d, J = 8.8 Hz, 1H, ArH), 7.83 (d, J = 9.2 Hz, 1H, ArH), 7.67–7.56 (m, 4H, ArH), 5.86 (s, 1H, CH), 3.16 (s, 2H, CH₂), 1.28 (s, 6H, CH₃).

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HRMS (ESI): m/z calcd for: C₂₂H₁₇Cl₂N₂O, 395.0718 [M+H]⁺, found: 395.0714.

2-(4-Bromophenyl)-9-chloro-4,4-dimethyl-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3s)

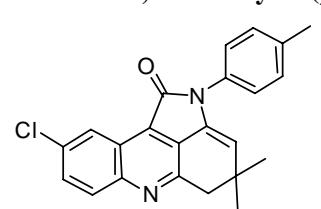


Yellow solid, mp: 177-178 °C;
IR (KBr, v, cm⁻¹): 2957, 1703, 1646, 1602, 1508, 1492, 1441, 1365, 1341, 1209, 1152, 1139, 1086, 1077, 889, 847, 827, 793, 748, 717, 630, 600, 513;
¹H NMR (400 MHz, DMSO-d₆) (δ , ppm): 8.46 (s, 1H, ArH), 8.15 (d, J = 8.8Hz, 1H, ArH), 7.85-7.78 (m, 3H, ArH), 7.51 (d, J = 8.0Hz, 2H, ArH), 5.87 (s, 1H, CH), 3.17 (s, 2H, CH₂), 1.28 (s, 6H, CH₃);

¹³C NMR (100 MHz, DMSO-d₆) (δ , ppm): 167.6, 165.3, 155.5, 147.4, 133.6, 132.3, 131.8, 131.4, 130.9, 129.9, 128.4, 122.4, 121.9, 120.4, 120.3, 117.1, 43.2, 37.0, 30.7, 30.2;

HRMS (ESI): m/z calcd for: C₂₂H₁₇BrClN₂O, 439.0213 [M+H]⁺, found: 439.0190.

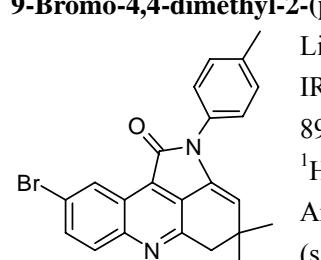
9-Chloro-4,4-dimethyl-2-(p-tolyl)-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3t)



Yellow solid, mp: 183-185 °C;
IR (KBr, v, cm⁻¹): 2958, 1701, 1645, 1515, 1506, 1439, 1365, 1340, 1293, 1152, 1139, 1091, 892, 829, 818, 742, 703, 621, 517.
¹H NMR (400 MHz, DMSO-d₆) (δ , ppm): 8.47 (s, 1H, ArH), 8.17-8.14 (m, 1H, ArH), 7.83 (d, J = 8.8Hz, 1H, ArH), 7.40 (s, 4H, ArH), 5.77 (s, 1H, CH), 3.17 (s, 2H, CH₂), 2.40 (s, 3H, CH₃), 1.28 (s, 6H, CH₃).

HRMS (ESI): m/z calcd for: C₂₃H₁₉ClN₂NaO, 397.1084 [M+H]⁺, found: 397.1080.

9-Bromo-4,4-dimethyl-2-(p-tolyl)-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3u)

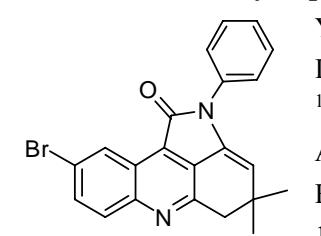


Light yellow solid; mp: 202.3-203.1°C;
IR (KBr, v, cm⁻¹): 2959, 1701, 1645, 1515, 1439, 1365, 1340, 1293, 1140, 1091, 1024, 892, 818, 760, 704, 621, 517.
¹H NMR (400 MHz, CDCl₃) (δ ppm): 8.88 (s, 1H, ArH), 8.03 (d, J = 8.8 Hz, 1H, ArH), 7.82 (d, J = 8.8 Hz, 1H, ArH), 7.52 – 7.31 (m, 4H, ArH), 5.63 (s, 1H, CH), 3.20 (s, 2H, CH₂), 2.44 (s, 3H, CH₃), 1.32 (s, 6H, CH₃).

¹³C NMR (100 MHz, CDCl₃) (δ ppm): 166.2, 155.0, 137.6, 133.3, 133.0, 131.9, 130.8, 130.0, 126.9, 126.6, 126.2, 123.7, 122.2, 119.1, 59.0, 44.0, 37.1, 30.9, 21.2.

HRMS (ESI) m/z: calcd for C₂₃H₂₀BrN₂O: 419.0759 [M+H]⁺, found: 419.0726.

9-Bromo-4,4-dimethyl-2-phenyl-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3v)



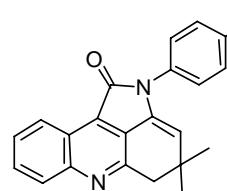
Yellow solid; mp: 178.1-178.5°C;
IR (KBr, v, cm⁻¹): 3664, 2959, 2932, 1695, 1646, 1596, 1338, 1139, 839, 732.
¹H NMR (400 MHz, CDCl₃) (δ ppm) : 8.87 (s, 1H, ArH), 8.03 (d, J = 8.8 Hz, 1H, ArH), 7.82 (d, J = 8.8 Hz, 1H, ArH), 7.55 (t, J = 7.6 Hz, 2H, ArH), 7.50 (d, J = 7.6 Hz, 2H, ArH), 7.42 (t, J = 7.2 Hz, 1H, ArH), 5.67 (s, 1H, CH), 3.20 (s, 2H, CH₂), 1.33 (s, 6H, CH₃).

¹³C NMR (100 MHz, CDCl₃) (δ ppm): 166.1, 155.0, 148.1, 134.6, 133.1, 133.0, 130.8, 129.4, 127.6, 127.0, 126.6, 126.3, 124.1, 123.6, 122.2, 119.2, 44.0, 37.2, 30.9

HRMS (ESI) m/z: calcd for C₂₂H₁₈BrN₂O: 405.0603 [M+H]⁺, found: 406.0633.

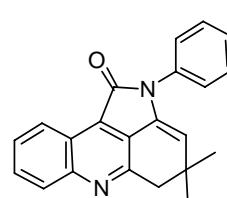
2-(4-Chlorophenyl)-4,4-dimethyl-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3w)

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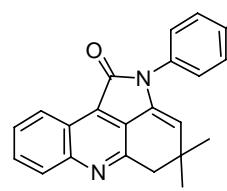
Yellow solid, mp: 182-183 °C;
IR (KBr, v, cm⁻¹): 2958, 1699, 1651, 1496, 1467, 1411, 1404, 1377, 1346, 1298, 1147, 1117, 1093, 1018, 831, 825, 775, 741, 643, 590, 512.
¹H NMR (400 MHz, DMSO-*d*₆) (δ , ppm): 8.53 (d, *J* = 6.8 Hz, 1H, ArH), 8.14 (d, *J* = 7.6 Hz, 1H, ArH), 7.81-7.59 (m, 6H, ArH), 5.80 (s, 1H, CH), 3.16 (s, 2H, CH₂), 1.28 (s, 6H, CH₃).
HRMS (ESI): m/z calcd for: C₂₂H₁₈ClN₂O, 361.1108 [M+H]⁺, found: 361.1093.

2-(4-Bromophenyl)-4,4-dimethyl-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3x)



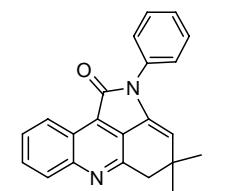
Yellow solid, mp: 188-189 °C;
IR (KBr, v, cm⁻¹): 2958, 1698, 1649, 1515, 1466, 1399, 1346, 1299, 1136, 1120, 1088, 820, 776, 751, 742, 644, 580, 515;
¹H NMR (400 MHz, DMSO-*d*₆) (δ , ppm): 8.56 (d, *J* = 8.0 Hz, 1H, ArH), 8.16 (d, *J* = 8.0 Hz, 1H, ArH), 7.86-7.74 (m, 4H, ArH), 7.54-7.51 (m, 2H, ArH), 5.82 (s, 1H, CH), 3.18 (s, 2H, CH₂), 1.28 (s, 6H, CH₃);
HRMS (ESI): m/z calcd for: C₂₂H₁₇BrN₂NaO, 427.0422, found: 427.0423.

4,4-Dimethyl-2-(p-tolyl)-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3y)



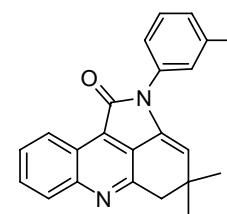
Yellow solid, mp: 182-183 °C;
IR (KBr, v, cm⁻¹): 2958, 1698, 1649, 1515, 1466, 1399, 1346, 1299, 1136, 1120, 1088, 820, 776, 751, 742, 644, 580, 515;
¹H NMR (400 MHz, DMSO-*d*₆) (δ , ppm): 8.57 (d, *J* = 8.0 Hz, 1H, ArH), 8.16 (d, *J* = 8.0 Hz, 1H, ArH), 7.83 (t, *J* = 8.0 Hz, 1H, ArH), 7.75 (t, *J* = 7.6 Hz, 1H, ArH), 7.42-7.38 (m, 4H, ArH), 5.72 (s, 1H, CH), 3.18 (s, 2H, CH₂), 2.40 (s, 3H, CH₃), 1.28 (s, 6H, CH₃);
HRMS (ESI): m/z calcd for: C₂₃H₂₀N₂NaO, 363.1473 [M+H]⁺, found: 363.1160.

4,4-Dimethyl-2-phenyl-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3z)



Yellow solid; mp: 176.0-176.3 °C;
IR (KBr, v, cm⁻¹): 3809, 3632, 3059, 2956, 2934, 1679, 1648, 1596, 1494, 1468, 1402, 1345, 1298, 1115, 1065, 833, 777, 735, 696, 585.
¹H NMR (400 MHz, CDCl₃) (δ ppm): 8.74 (d, *J* = 8.0 Hz, 1H, ArH), 8.21 (d, *J* = 8.4 Hz, 1H, ArH), 7.77 (t, *J* = 7.6 Hz, 1H, ArH), 7.68 (t, *J* = 7.6 Hz, 1H, ArH), 7.59 - 7.47 (m, 4H, ArH), 7.42 (t, *J* = 7.2 Hz, 1H, ArH), 5.64 (s, 1H, CH), 3.24 (s, 2H, CH₂), 1.34 (s, 6H, CH₃).
¹³C NMR (100 MHz, CDCl₃) (δ ppm): 166.6, 154.5, 135.5, 134.7, 133.3, 129.7, 129.4, 129.3, 127.9, 127.5, 126.5, 126.4, 124.3, 122.7, 118.4, 44.0, 37.1, 30.9.
HRMS (ESI) m/z: calcd for C₂₂H₁₉N₂O, 327.1497, found: 327.1458.

2-(3-Chlorophenyl)-4,4-dimethyl-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3aa)



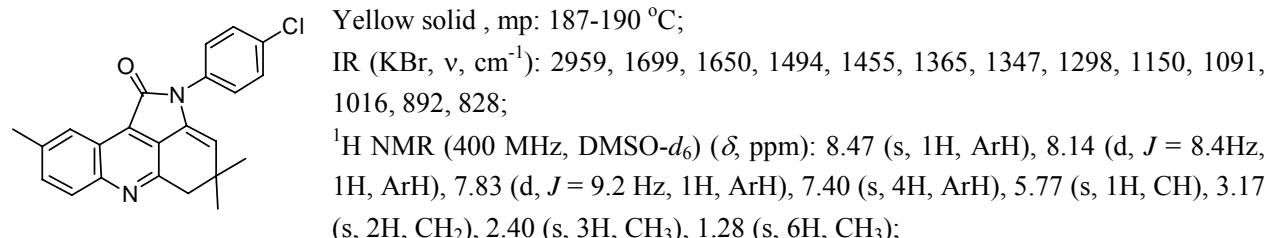
Yellow solid; mp: 175.1-175.5 °C;
IR (KBr, v, cm⁻¹): 3033, 2956, 2932, 1720, 1646, 1592, 1483, 1088, 970, 775;
¹H NMR (400 MHz, CDCl₃) (δ ppm): 8.72 (d, *J* = 8.0 Hz, 1H, ArH), 8.20 (d, *J* = 8.4 Hz, 1H, ArH), 7.77 (d, *J* = 8.0 Hz, 1H, ArH), 7.69 (d, *J* = 7.6 Hz, 1H, ArH), 7.55 (s, 1H, ArH), 7.47 (d, *J* = 7.8 Hz, 1H, ArH), 7.44 - 7.34 (m, 2H, ArH), 5.65 (s, 1H, CH), 3.24 (s, 2H, CH₂), 1.34 (s, 6H, CH₃).

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^{13}C NMR (100 MHz, CDCl_3) (δ ppm) 166.5, 154.5, 135.9, 135.0, 132.9, 130.3, 129.8, 129.4, 128.0, 127.7, 126.6, 126.4, 124.8, 124.5, 124.2, 122.5, 118.6, 44.0, 37.1, 30.8.

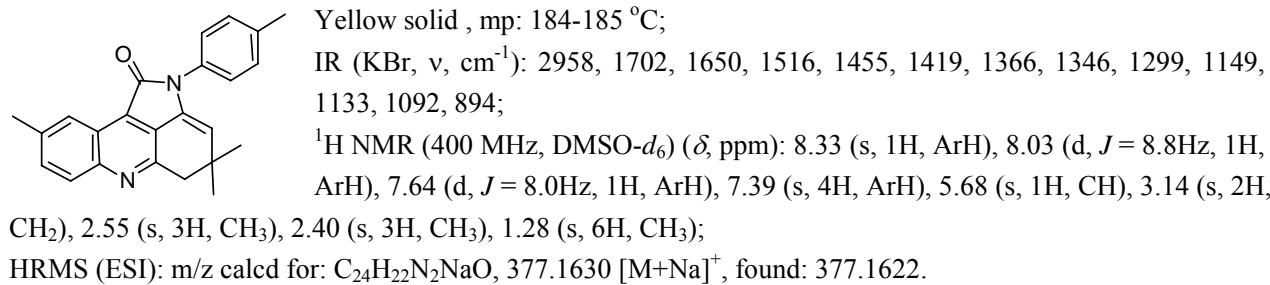
HRMS (ESI) m/z : calcd for $\text{C}_{22}\text{H}_{18}\text{ClN}_2\text{O}$: 361.1108 [$\text{M}+\text{H}]^+$, found: 361.1090.

2-(4-Chlorophenyl)-4,4,9-trimethyl-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3bb)

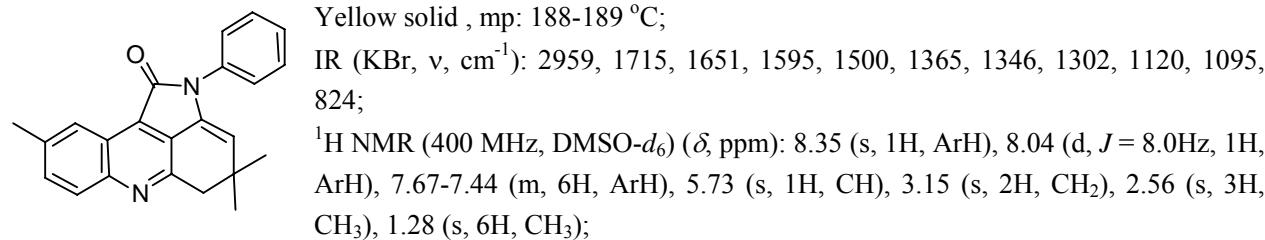


HRMS (ESI): m/z calcd for: $\text{C}_{23}\text{H}_{19}\text{ClN}_2\text{NaO}$, 397.1084 [$\text{M}+\text{Na}]^+$, found: 397.1045.

4,4,9-Trimethyl-2-(p-tolyl)-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3cc)

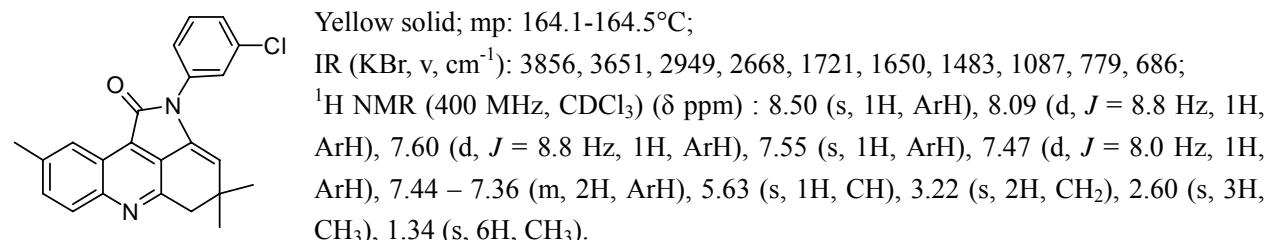


4,4,9-Trimethyl-2-phenyl-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3dd)



HRMS (ESI): m/z calcd for: $\text{C}_{23}\text{H}_{20}\text{N}_2\text{NaO}$, 363.1473 [$\text{M}+\text{Na}]^+$, found: 363.1160.

2-(3-chlorophenyl)-4,4,9-trimethyl-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3ee)

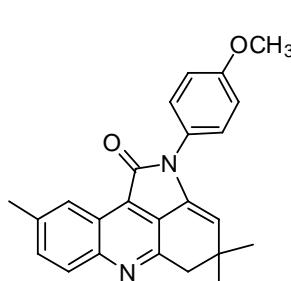


HRMS (ESI): m/z calcd for: $\text{C}_{23}\text{H}_{19}\text{ClN}_2\text{NaO}$, 397.1084 [$\text{M}+\text{Na}]^+$, found: 397.1069.

2-(4-Methoxyphenyl)-4,4,9-trimethyl-4,5-dihydropyrrolo[2,3,4-kl]acridin-1(2H)-one (3ff)

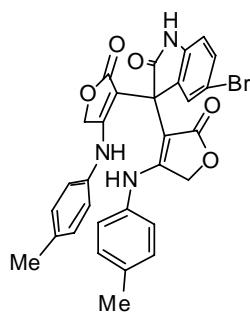
Yellow solid; mp: 207.1-207.3°C;

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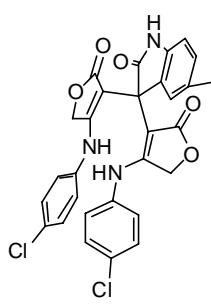
IR (KBr, v, cm⁻¹): 3033, 2956, 2932, 1720, 1646, 1592, 1483, 1088, 970, 775;
¹H NMR (400 MHz, CDCl₃) (δ ppm) : 8.51 (s, 1H, ArH), 8.09 (s, 1H, ArH), 7.59 (s, 1H, ArH), 7.41 (s, 2H, ArH), 7.06 (s, 2H, ArH), 5.54 (s, 1H, CH), 3.88 (s, 3H, OCH₃), 3.21 (s, 2H, CH₂), 2.59 (s, 3H, CH₃), 1.32 (s, 6H, CH₃).
¹³C NMR (100 MHz, CDCl₃) (δ ppm) : 166.3, 158.8, 153.3, 138.2, 133.8, 131.8, 127.8, 127.4, 126.4, 123.3, 122.6, 117.9, 114.7, 55.6, 43.9, 37.0, 30.9, 21.7.
HRMS (ESI) *m/z*: calcd for C₂₃H₂₀ClN₂O: 375.1264 [M+H]⁺, found: 375.1225.

3,3'-(5-Bromo-2-oxoindoline-3,3-diyl)bis(4-(p-tolylamino)furan-2(5H)-one (4a)



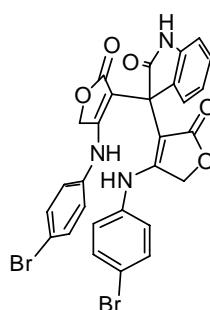
White solid; mp 267.7-279.4 °C;
IR (KBr, v, cm⁻¹): 3337, 3036, 2861, 1750, 1716, 1604, 1475, 1056, 818, 759.
¹H NMR (400 MHz, DMSO-*d*₆) (δ , ppm) : 10.52 (s, 1H, NH), 8.97 (s, 2H, NH), 7.42 (d, J = 2.0 Hz, 1H, ArH), 7.33 (s, 1H, ArH), 7.14 (d, J = 8.0 Hz, 4H, ArH), 7.00 (d, J = 8.0 Hz, 4H, ArH), 6.71 (d, J = 8.0 Hz, 1H, ArH), 4.67 (s, 4H, CH₂), 2.28 (s, 6H, CH₃).
¹³C NMR (100 MHz, DMSO-*d*₆) (δ ppm): 177.8, 171.5, 163.3, 141.6, 136.1, 134.8, 134.1, 130.1, 129.6, 127.8, 123.8, 112.6, 110.7, 65.5, 48.9, 20.4.
HRMS (ESI) *m/z*: calcd for C₃₀H₂₅BrN₃O₅: 586.09778 [M+H]⁺, found: 586.09789.

3,3'-(5-Methyl-2-oxoindoline-3,3-diyl)bis(4-((4-chlorophenyl)amino)furan-2(5H)-one (4b)



White solid; mp 235.0-237.3°C;
IR (KBr, v, cm⁻¹): 3450, 3346, 3321, 2937, 1736, 1644, 1514, 1247, 1031, 832.
¹H NMR (400 MHz, DMSO-*d*₆) (δ , ppm) : 10.34 (s, 1H, NH), 8.99 (s, 2H, NH), 7.36 (d, J = 8.8 Hz, 4H, ArH), 7.08 (d, J = 8.4 Hz, 5H, 4H, ArH), 6.93 (s, 1H, 4H, ArH), 6.65 (d, J = 7.6 Hz, 1H, 4H, ArH), 4.73 (s, 4H, CH₂), 2.24 (s, 3H, CH₃).
¹³C NMR (100 MHz, DMSO-*d*₆) (δ ppm): 178.0, 171.2, 162.2, 139.9, 137.8, 131.2, 129.4, 129.1, 127.9, 125.9, 124.9, 112.7, 108.6, 65.4, 49.0, 20.9;
HRMS (ESI) *m/z*: calcd for C₂₉H₂₂Cl₂N₃O₅: 562.0931 [M+H]⁺, found: 562.0952.

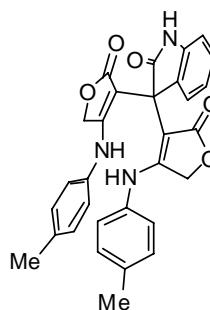
3,3'-(2-Oxoindoline-3,3-diyl)bis(4-((4-bromophenyl)amino)furan-2(5H)-one (4c)



White solid; mp 276.5-279.4 °C;
IR (KBr, v, cm⁻¹): 3409, 3001, 1750, 1737, 1617, 1411, 1179, 757.
¹H NMR (400 MHz, DMSO-*d*₆) (δ , ppm) : 10.44 (s, 1H, NH), 9.00 (s, 2H, NH), 7.50 (d, J = 8.8 Hz, 4H, ArH), 7.27 (d, J = 7.6 Hz, 1H, ArH), 7.12 (m, 1H, ArH), 7.03 (d, J = 8.8 Hz, 4H, ArH), 6.89 (t, J = 7.4 Hz, 1H, ArH), 6.75 (d, J = 7.8 Hz, 1H, ArH), 4.73 (s, 4H, CH₂).
¹³C NMR (100 MHz, DMSO-*d*₆) (δ ppm): 178.0, 171.3, 162.3, 142.2, 138.2, 131.9, 131.2, 127.5, 125.4, 125.3, 120.9, 117.3, 108.9, 65.5, 48.9;

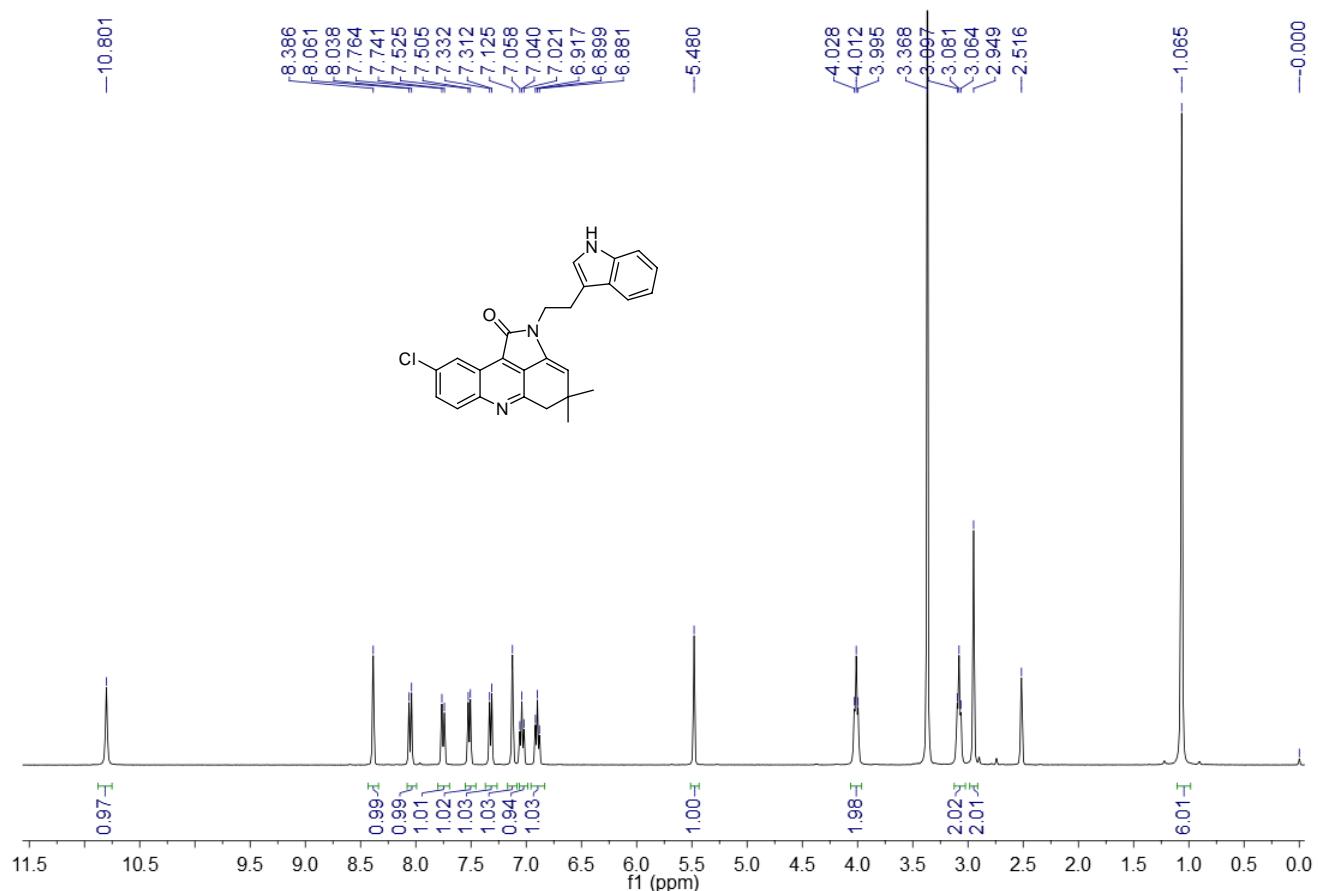
HRMS (ESI) *m/z*: calcd for C₂₈H₂₀Br₂N₃O₅: 637.9743 [M+H]⁺, found: 637.9759.

3,3'-(2-Oxoindoline-3,3-diyl)bis(4-(p-tolylamino)furan-2(5H)-one (4d)

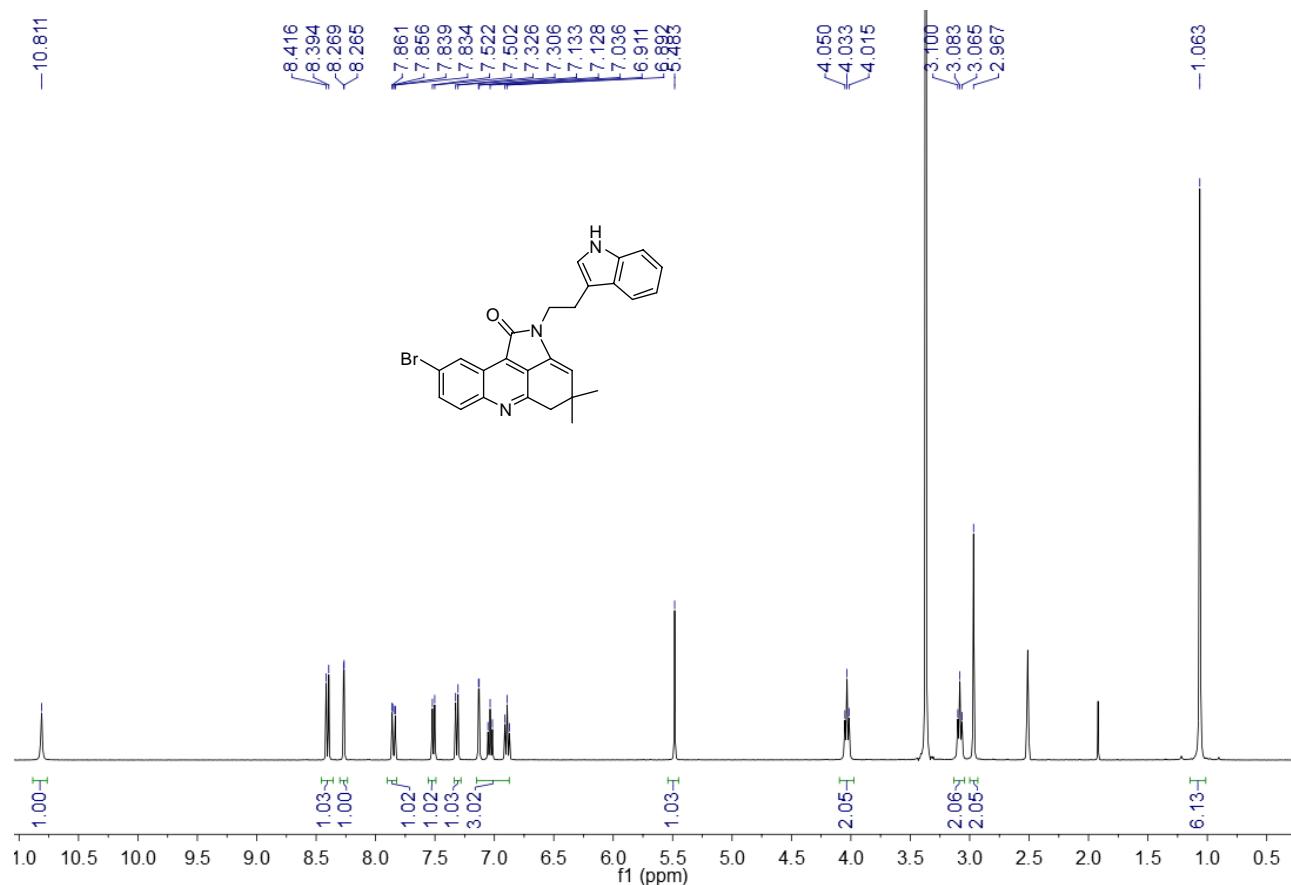


White solid; mp 289.1-289.4°C;
IR (KBr, v, cm⁻¹): 3448, 3343, 3324, 1736, 1617, 1515, 1417, 1096, 831.
¹H NMR (400 MHz, DMSO-*d*₆) (δ , ppm) : 10.40 (s, 1H, NH), 8.86 (s, 2H, NH), 7.29 (d, J = 7.2 Hz, 1H, ArH), 7.14 (d, J = 7.6 Hz, 5H, ArH), 7.00 (d, J = 7.6 Hz, 4H, ArH), 6.89 (t, J = 7.6 Hz, 1H, ArH), 6.75 (d, J = 7.6 Hz, 1H, ArH), 4.67 (s, 4H, CH₂), 2.28 (s, 6H, CH₃).
¹³C NMR (100 MHz, DMSO-*d*₆) (δ ppm): 178.2, 171.4, 163.2, 142.1, 136.1, 134.7, 131.6, 129.6, 127.4, 125.2, 123.7, 120.9, 114.3, 108.9, 65.3, 48.8, 20.4;
HRMS (ESI) *m/z*: calcd for C₃₀H₂₆N₃O₅: 508.1866 [M+H]⁺, found: 508.1872.

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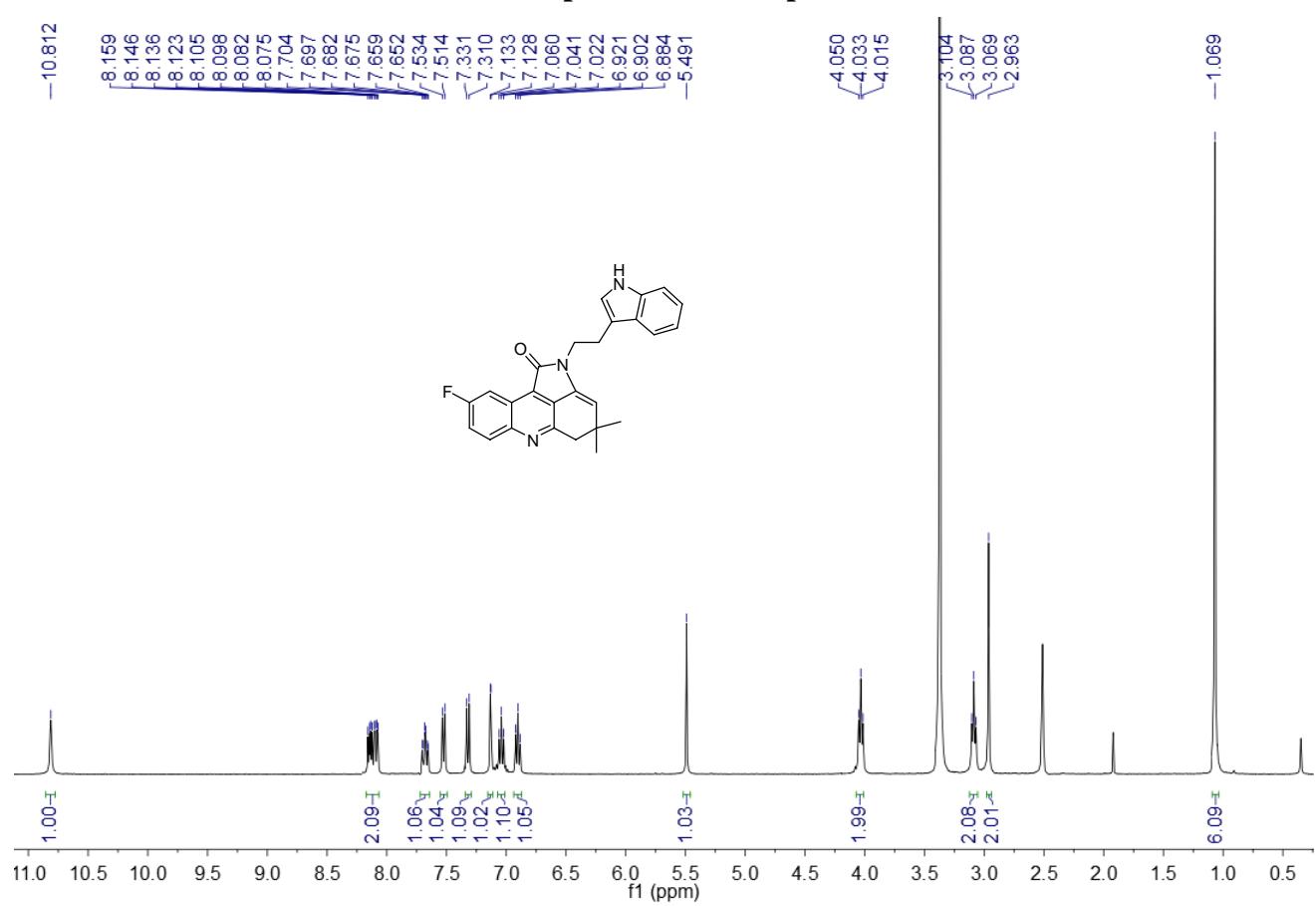
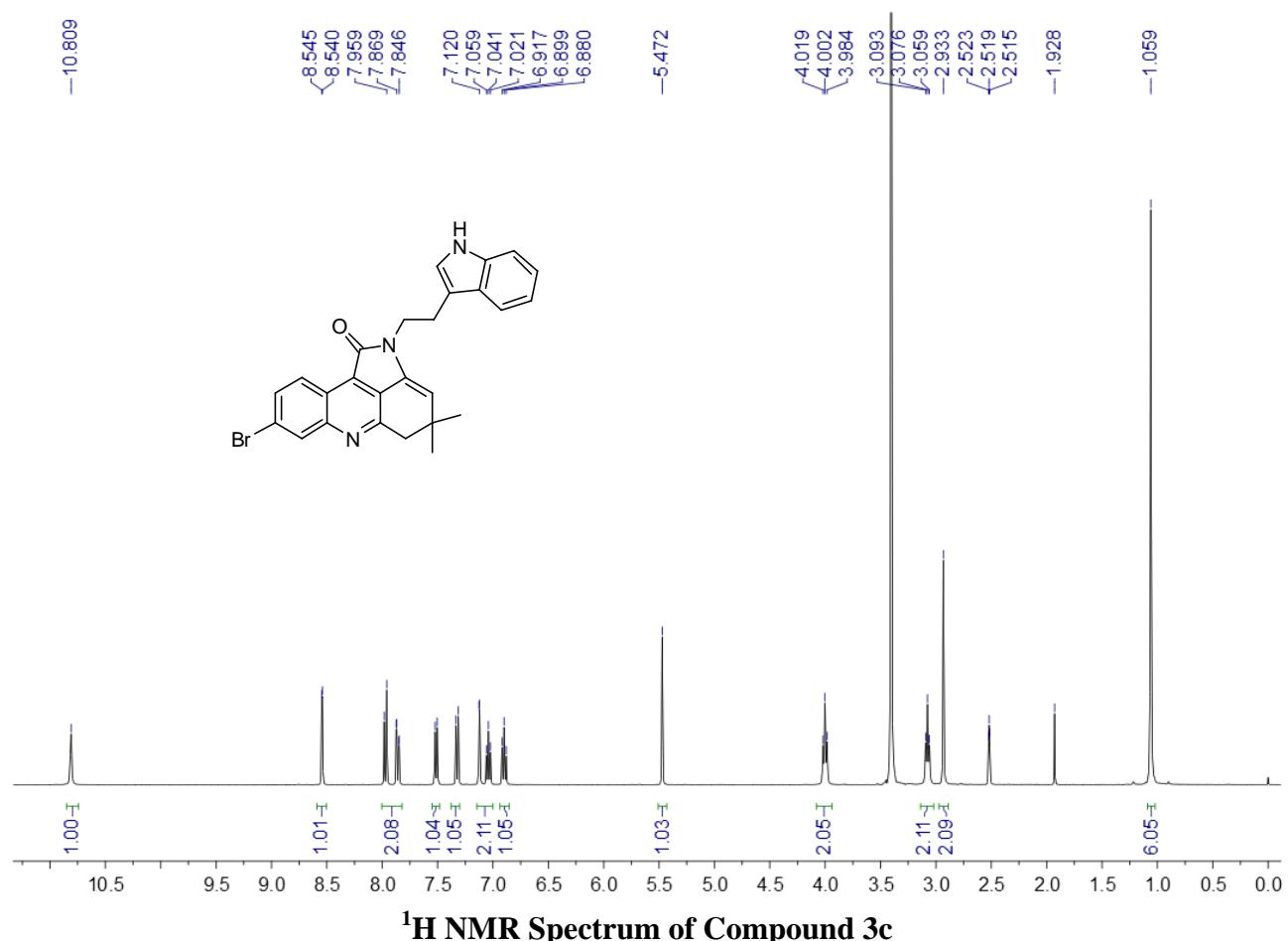


¹H NMR Spectrum of Compound 3a



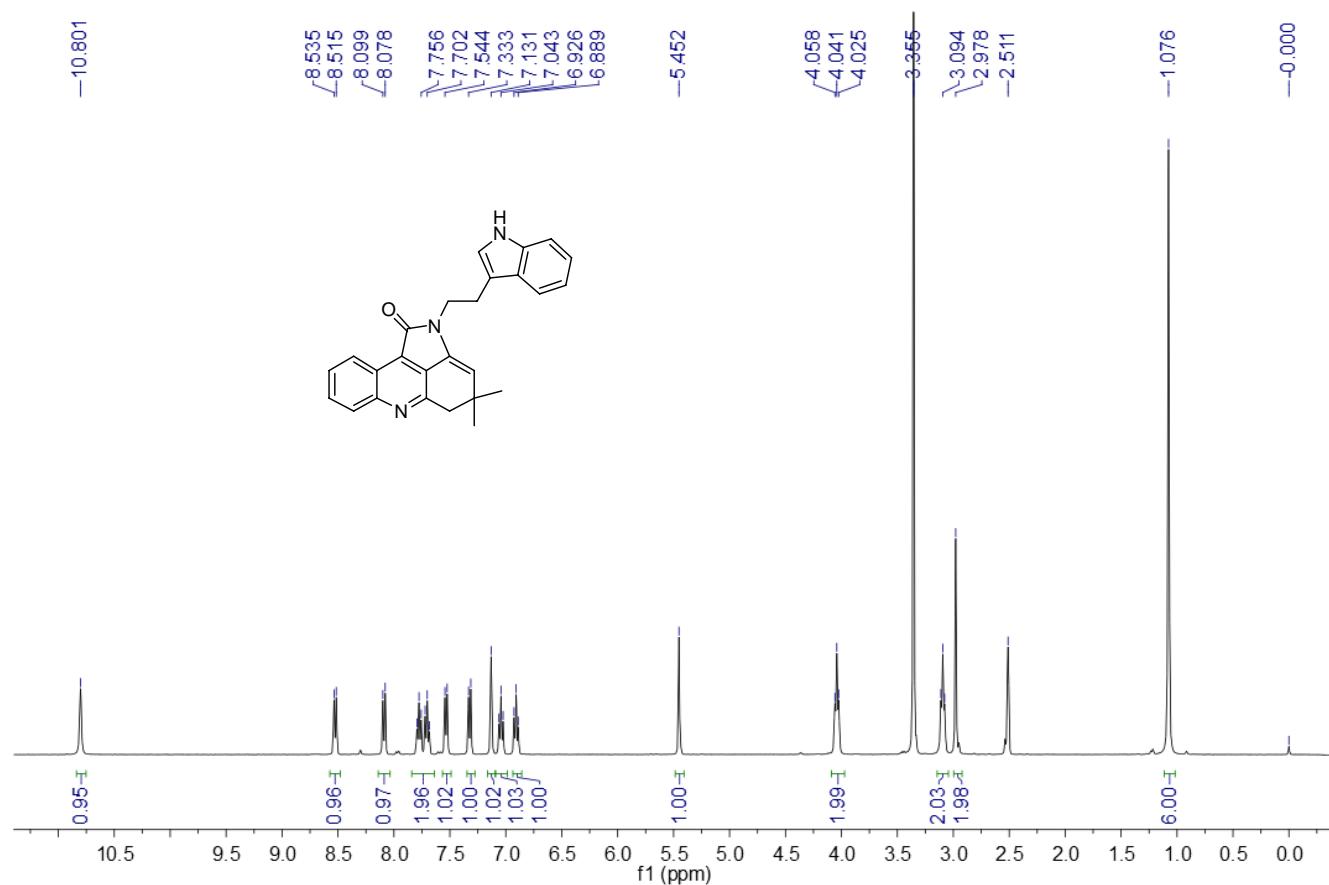
¹H NMR Spectrum of Compound 3b

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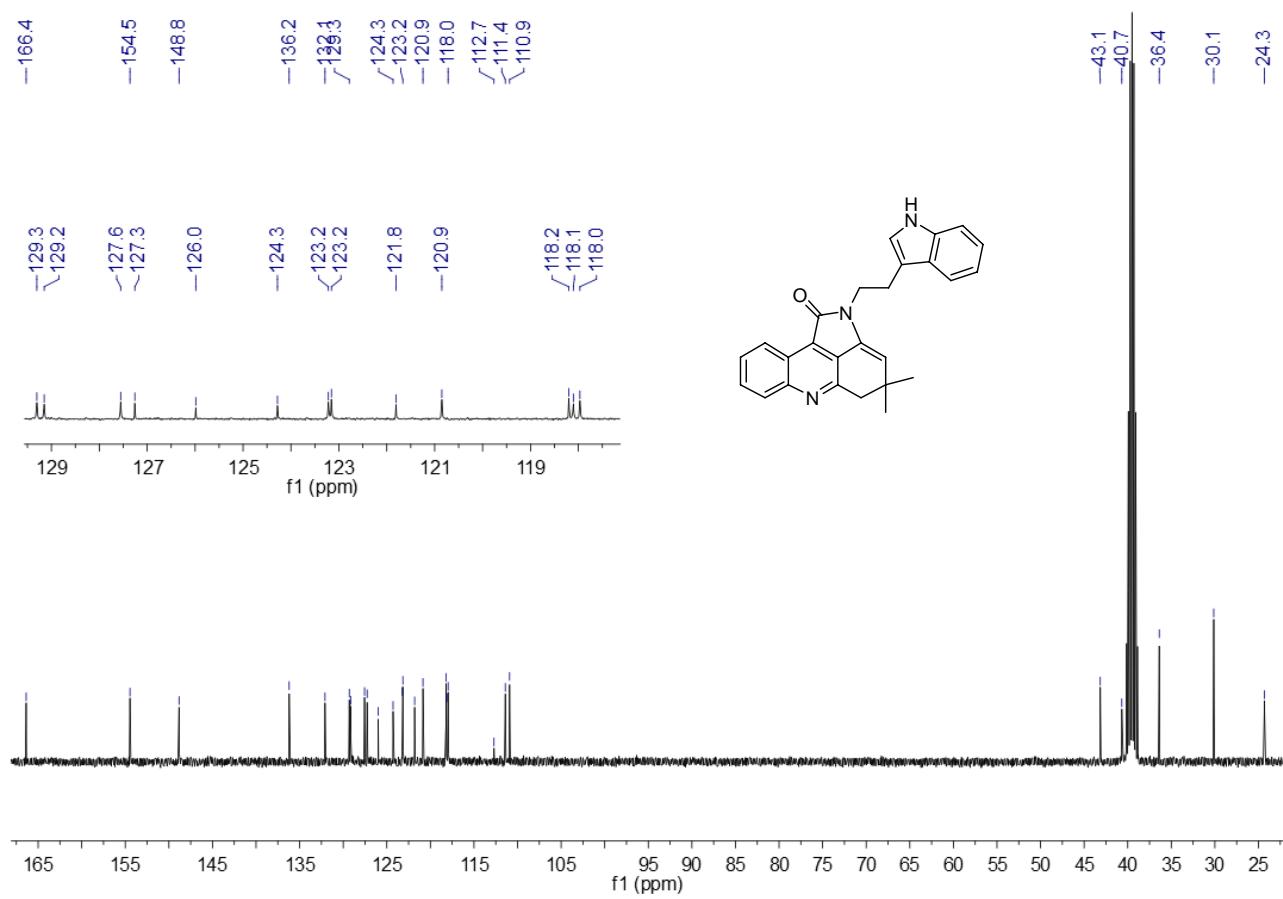


¹H NMR Spectrum of Compound 3d

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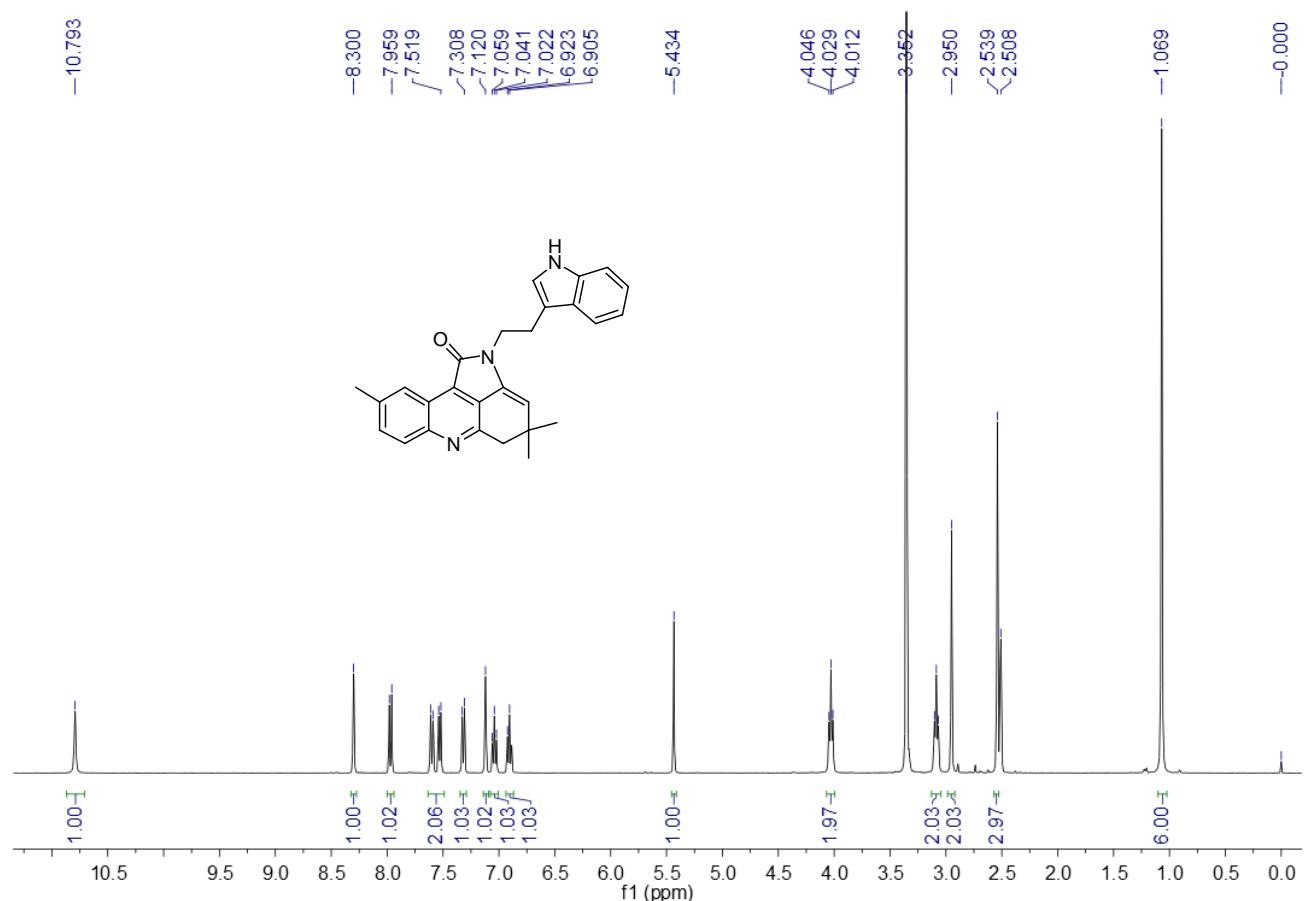


¹H NMR Spectrum of Compound 3e

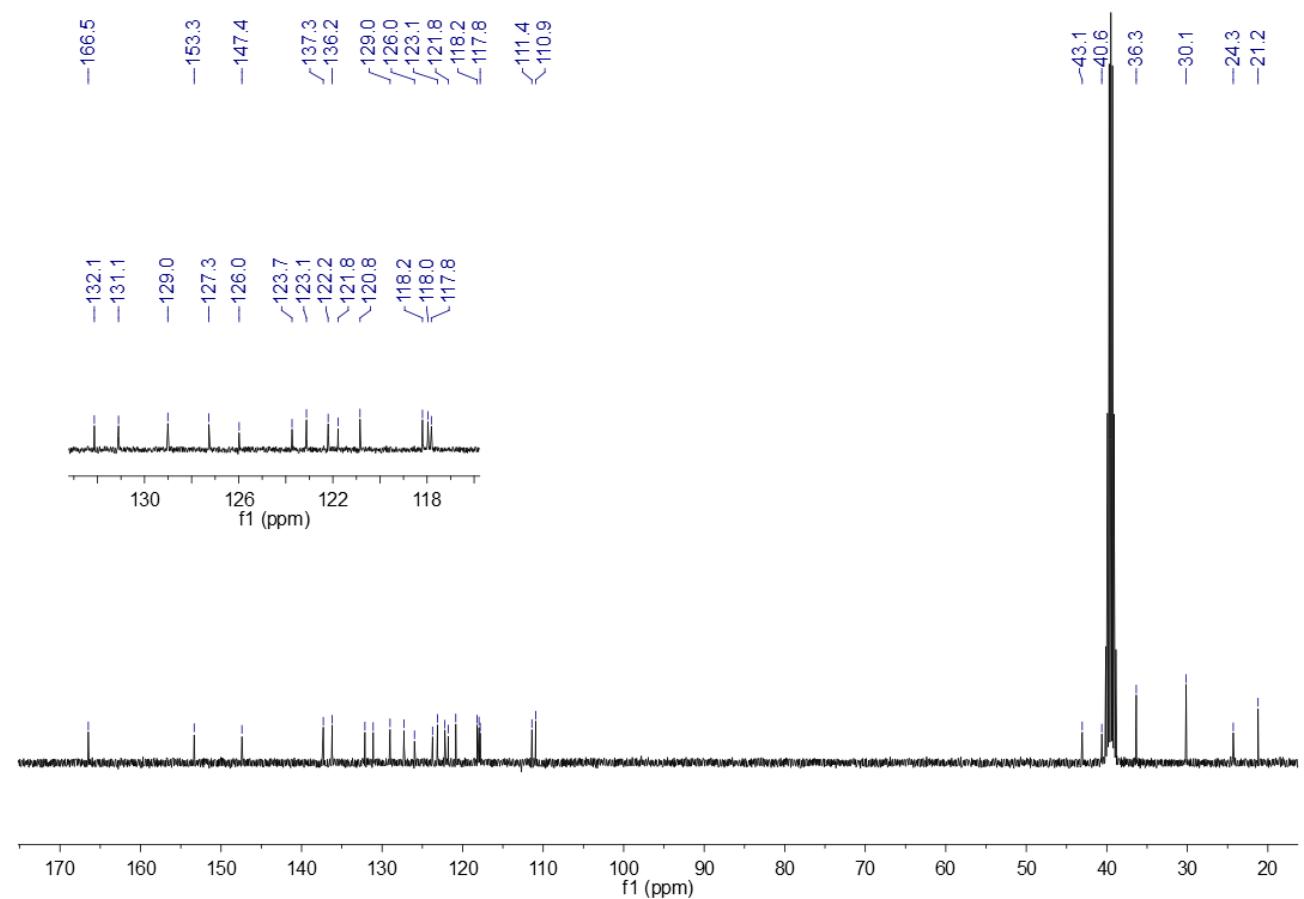


¹³C NMR Spectrum of Compound 3e

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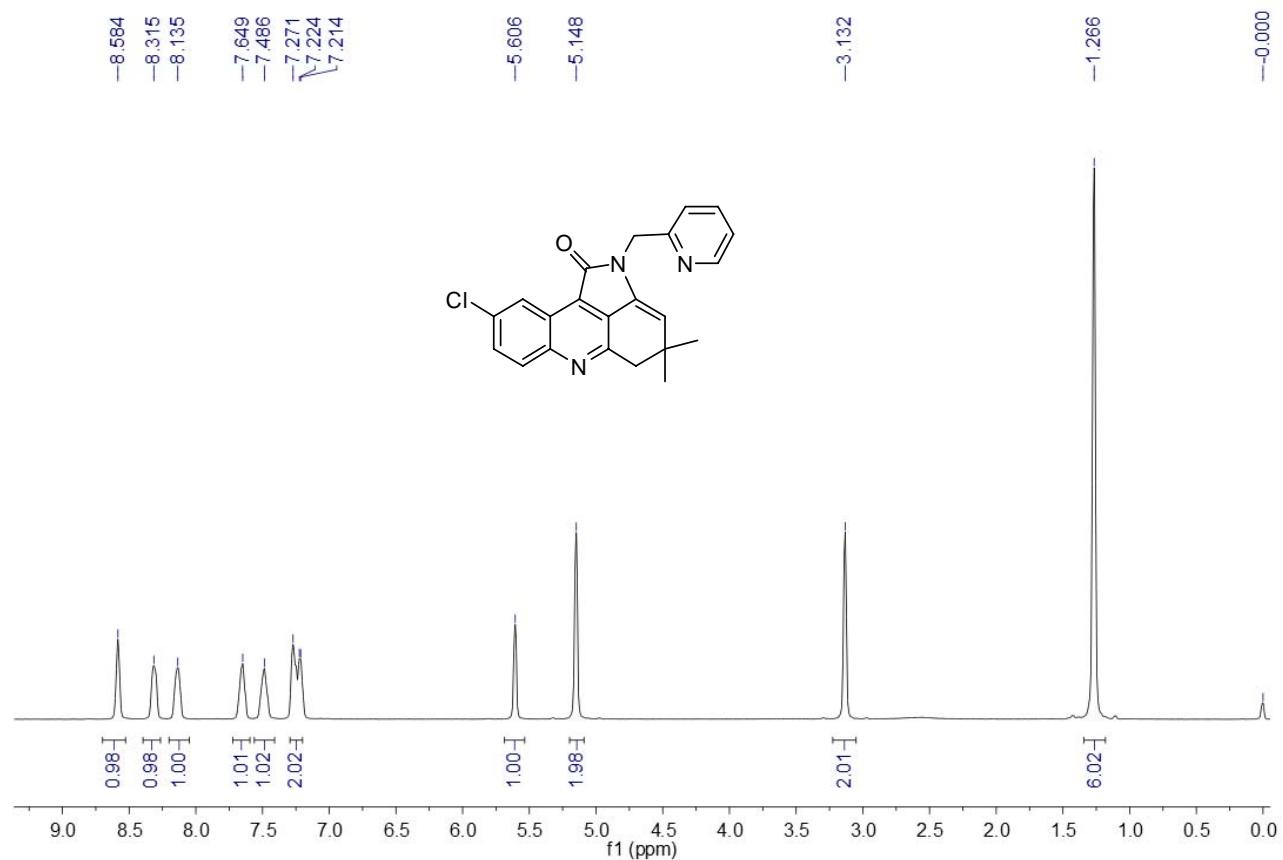


¹H NMR Spectrum of Compound 3f

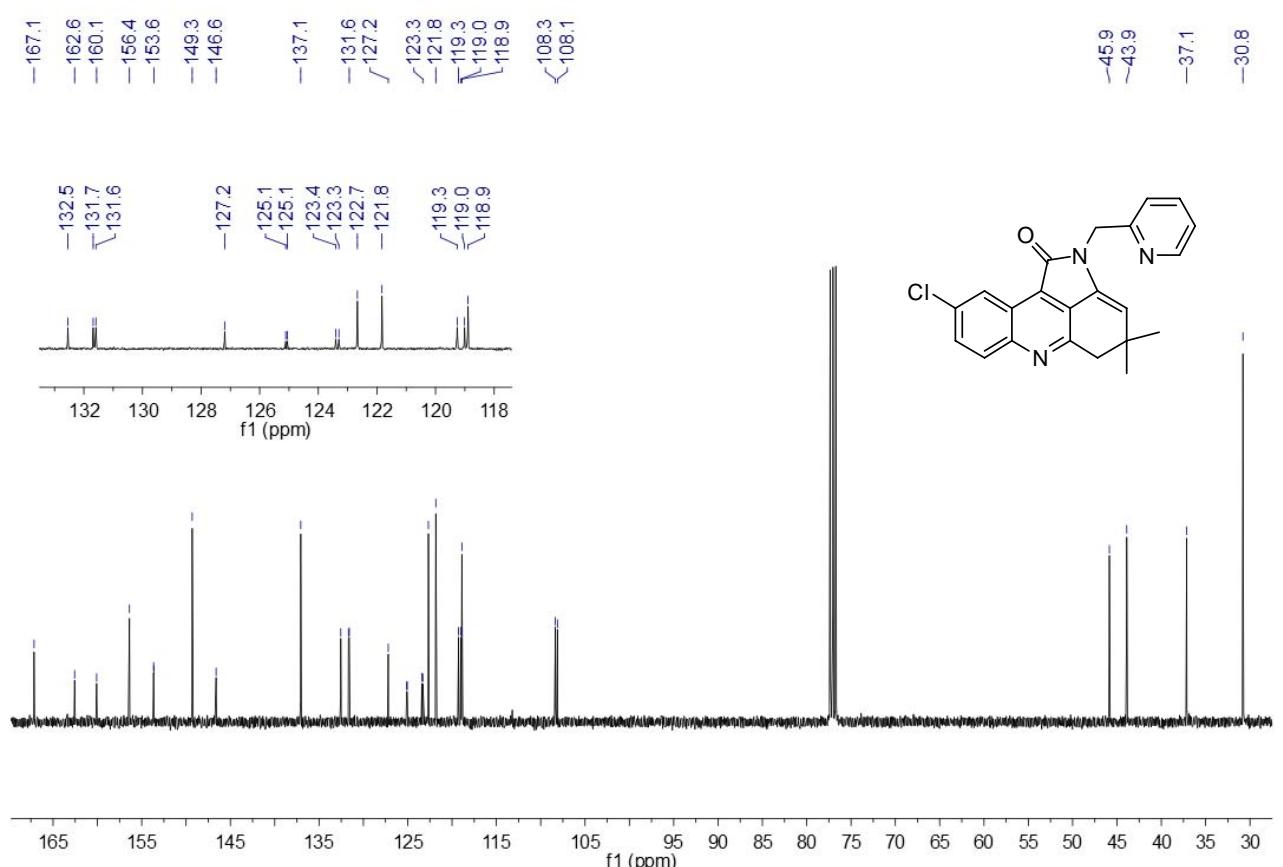


¹³C NMR Spectrum of Compound 3f

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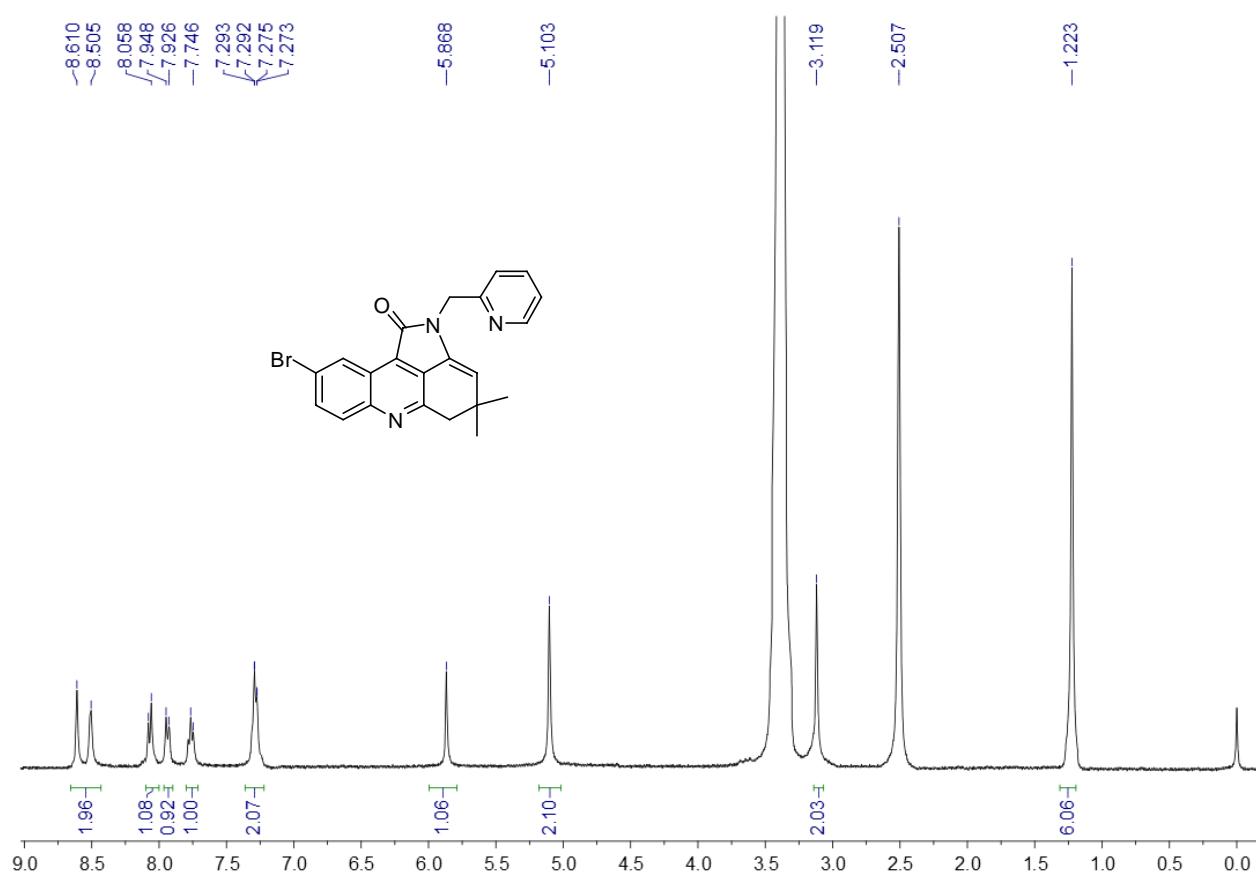


¹H NMR Spectrum of Compound 3g

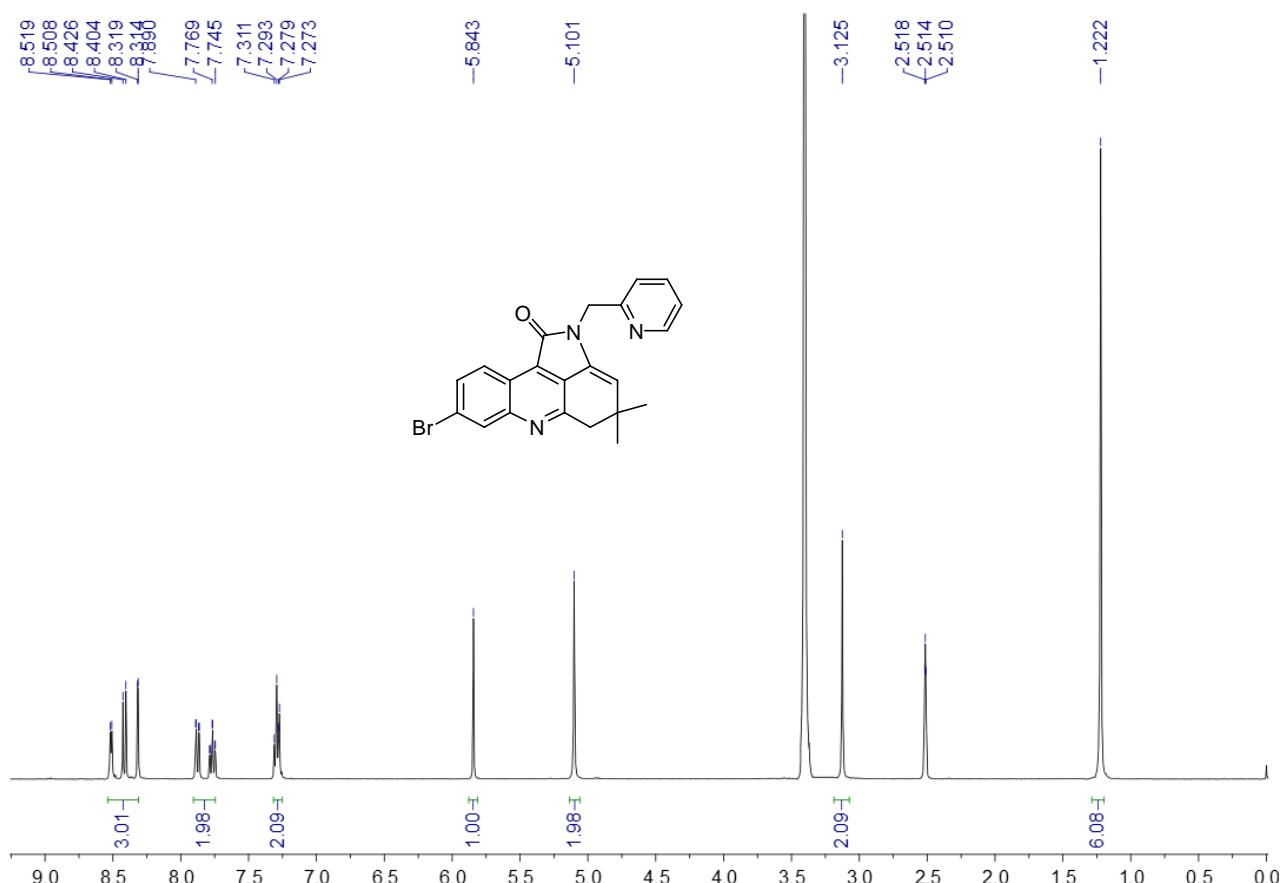


¹³C NMR Spectrum of Compound 3g

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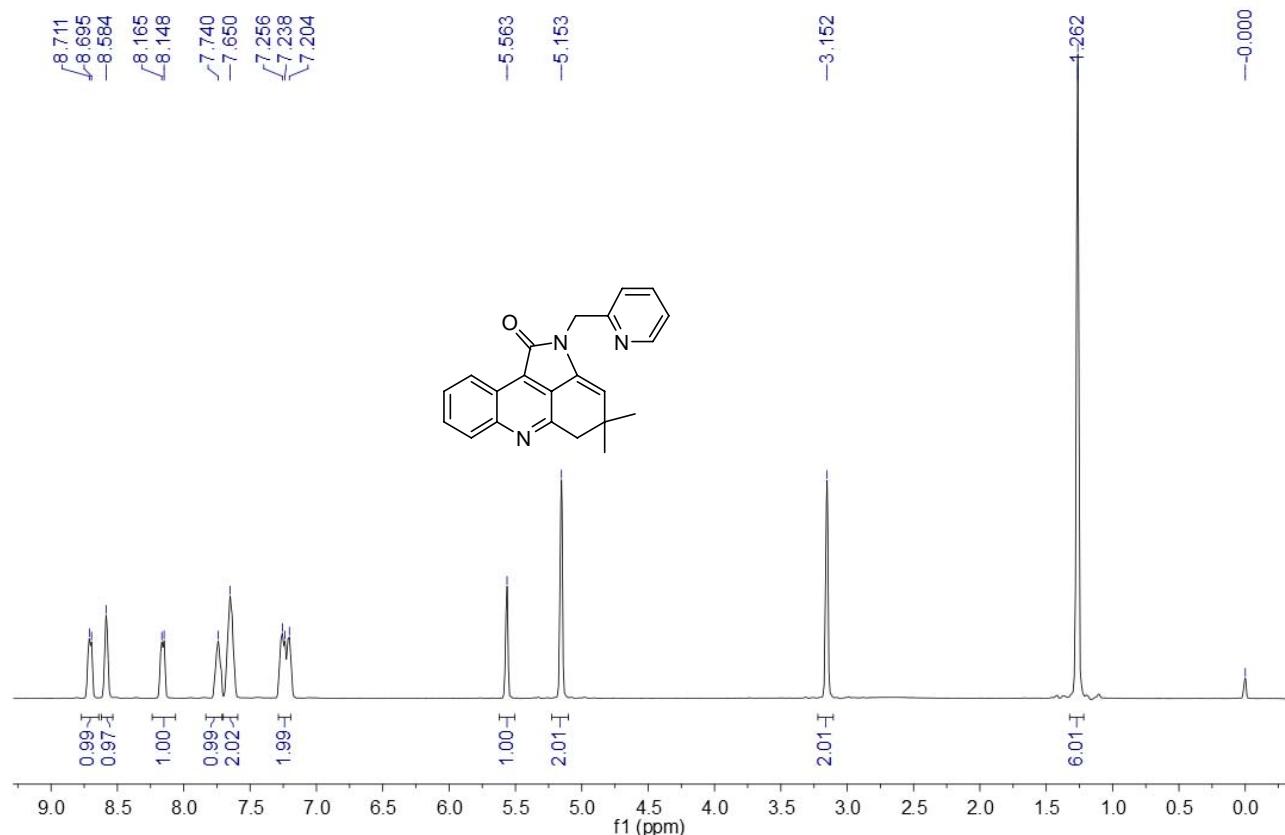


¹H NMR Spectrum of Compound 3h

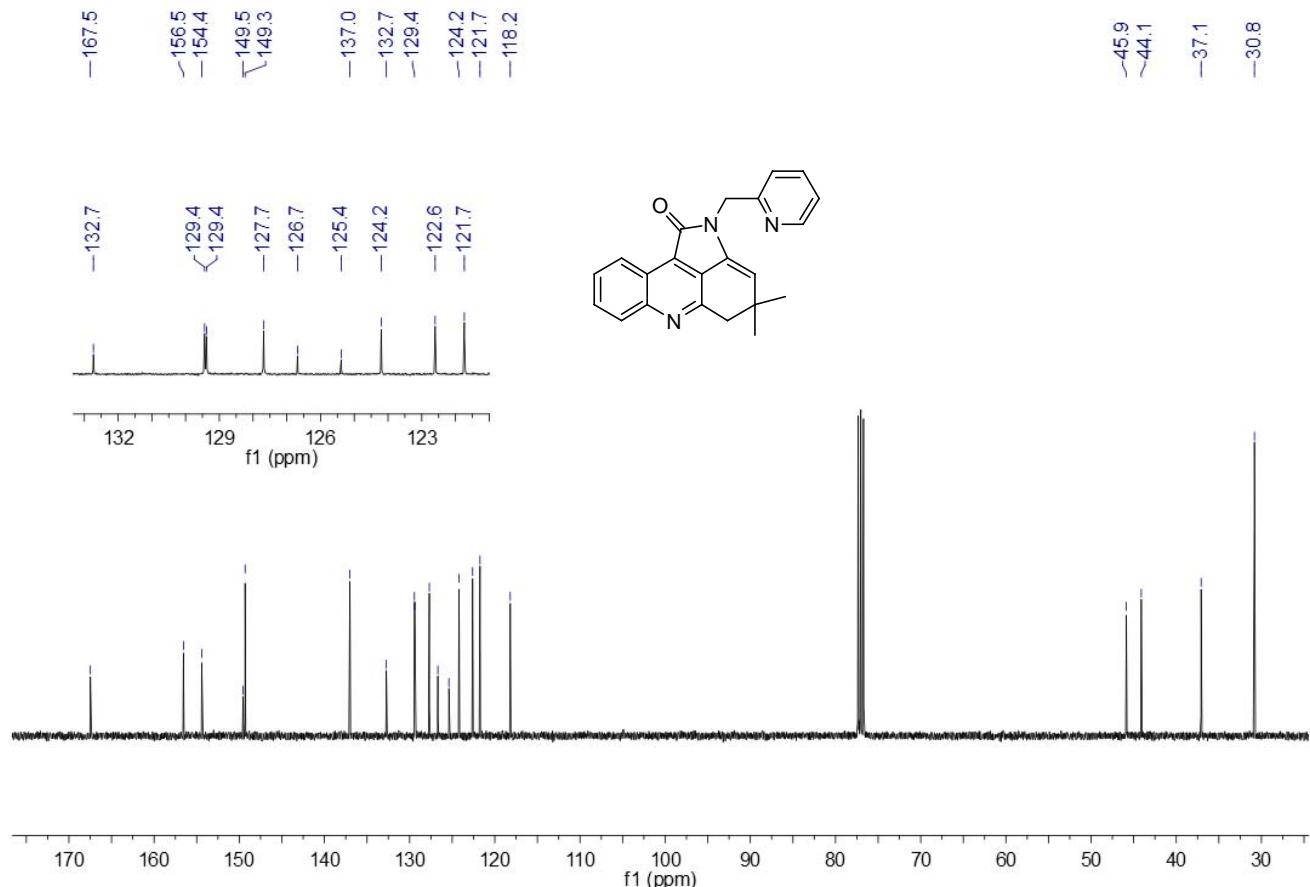


¹H NMR Spectrum of Compound 3i

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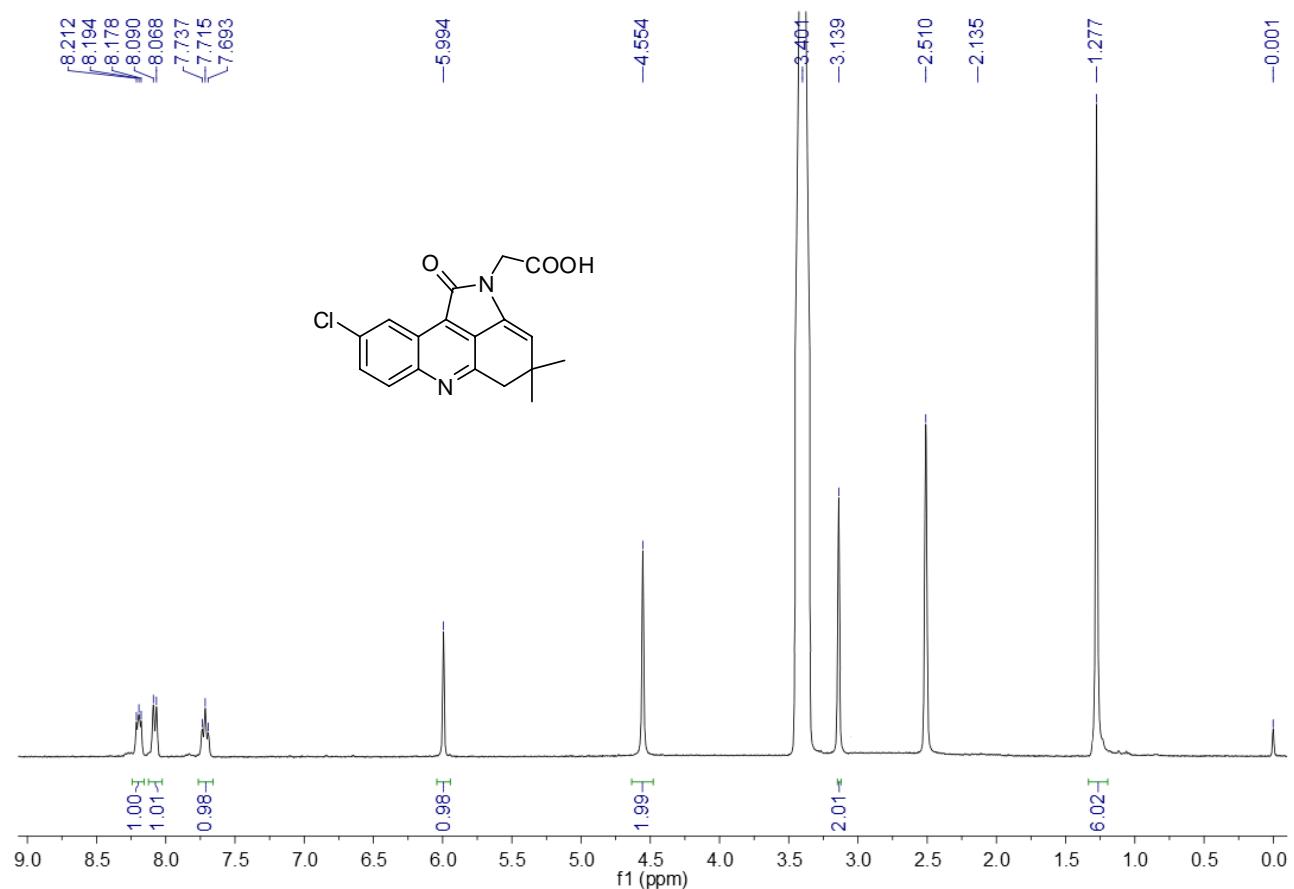


¹H NMR Spectrum of Compound 3j

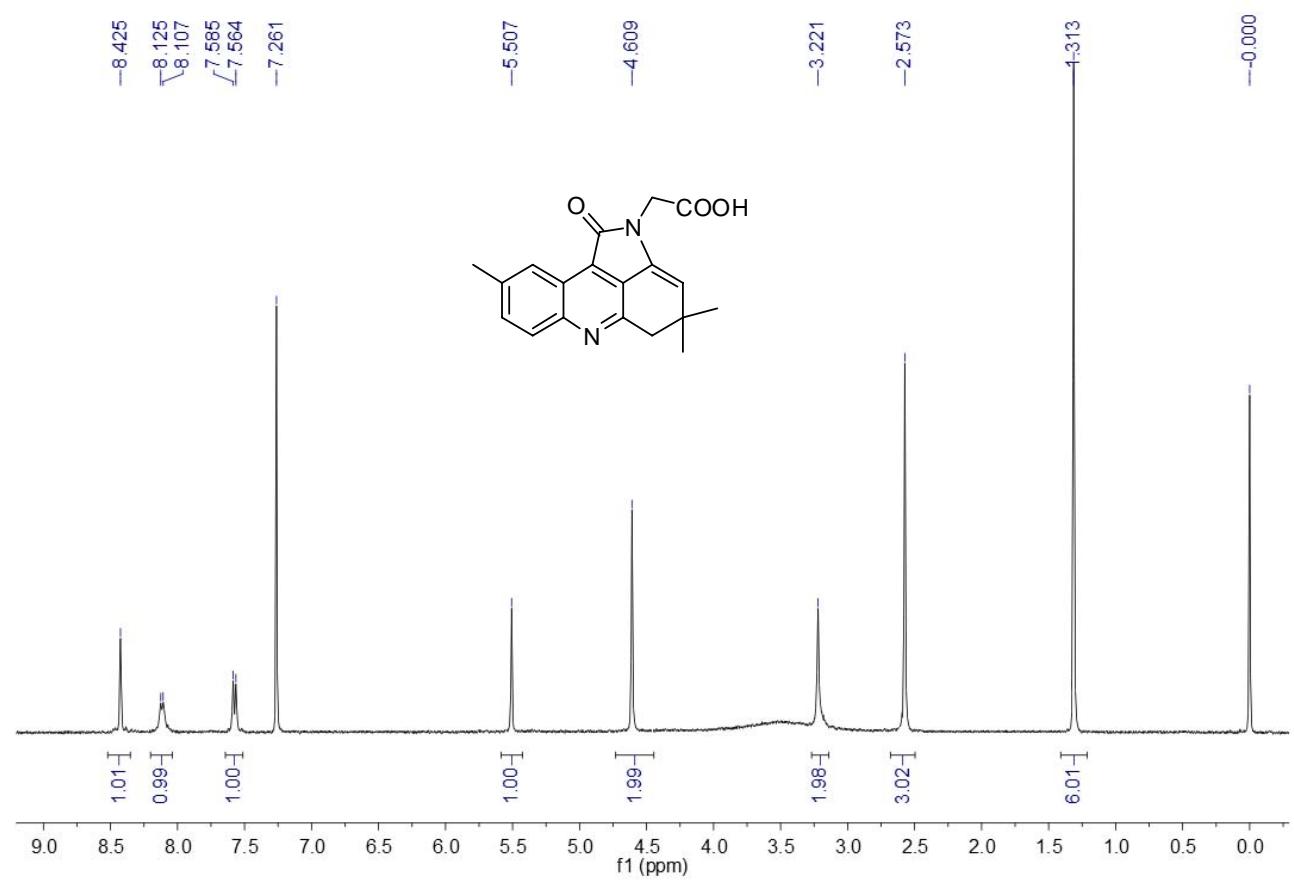


¹³C NMR Spectrum of Compound 3j

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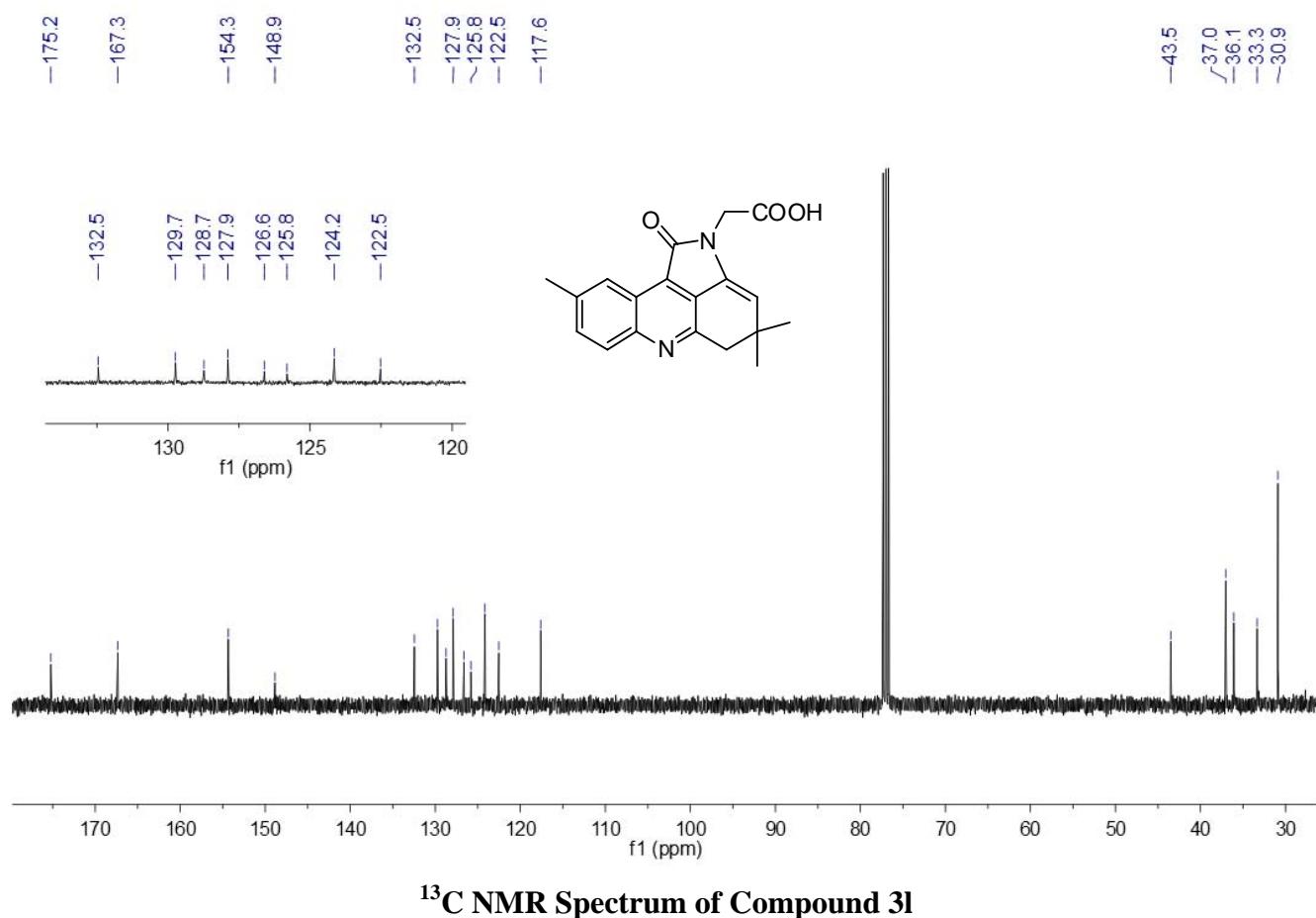


¹H NMR Spectrum of Compound 3k

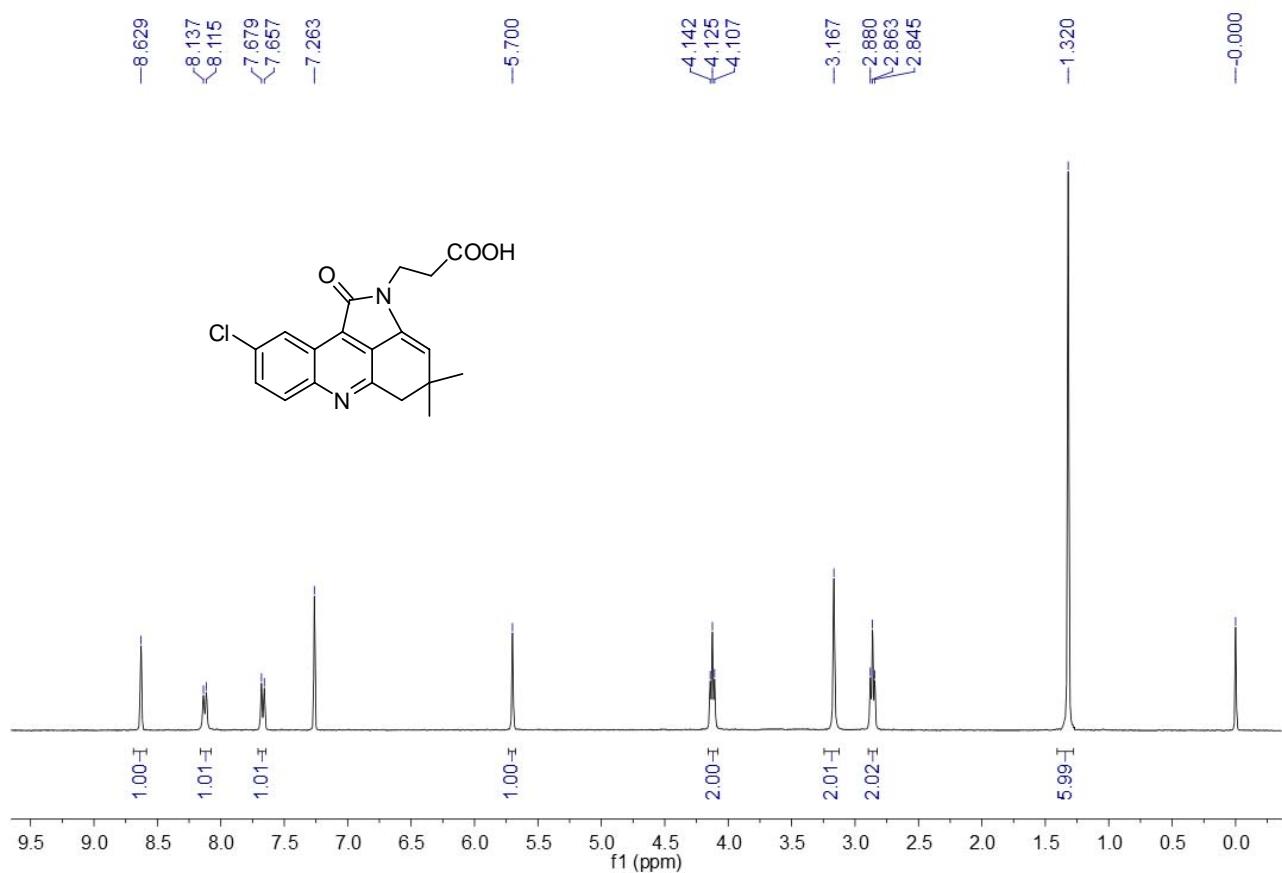


¹H NMR Spectrum of Compound 3l

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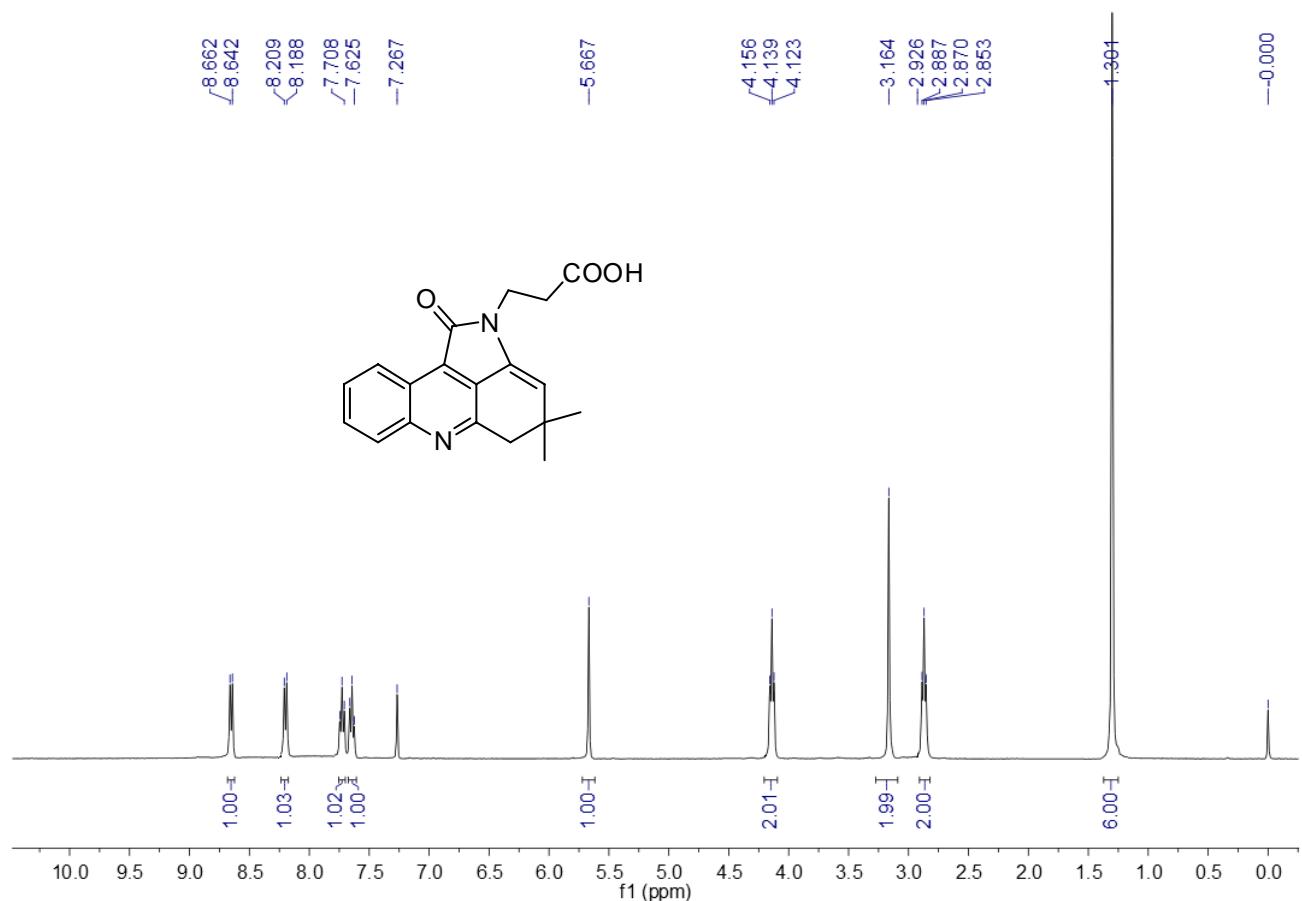


¹³C NMR Spectrum of Compound 3l

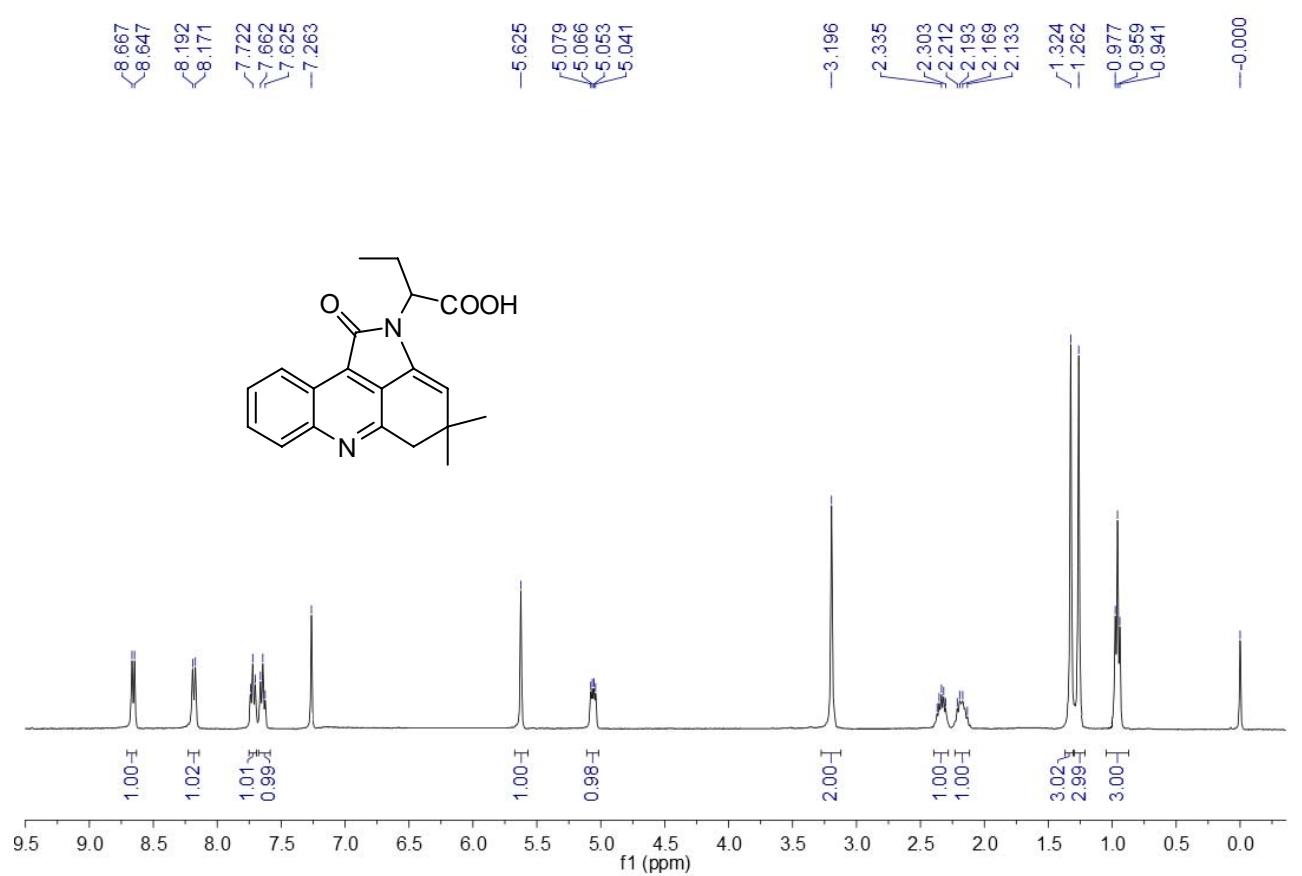


¹H NMR Spectrum of Compound 3m

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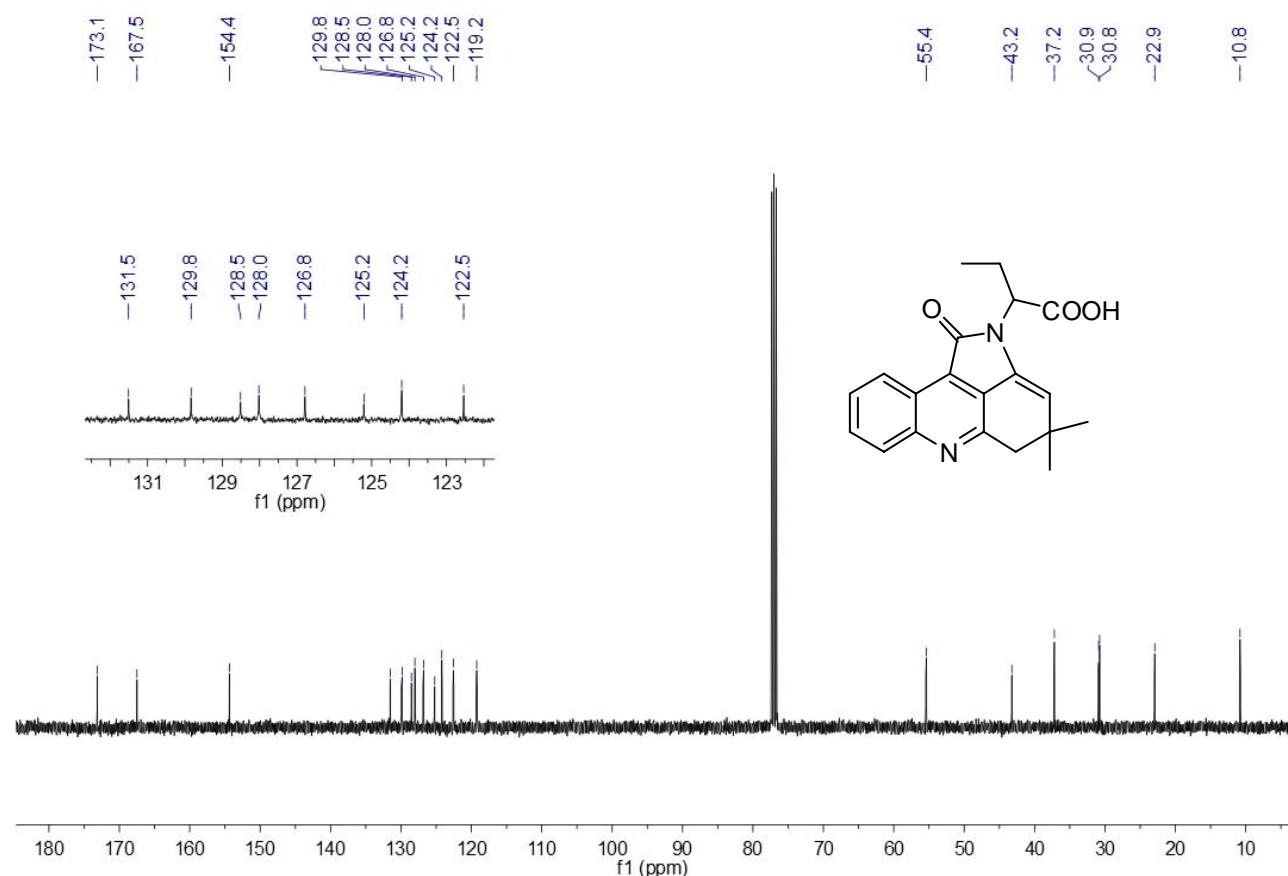


¹H NMR Spectrum of Compound 3n

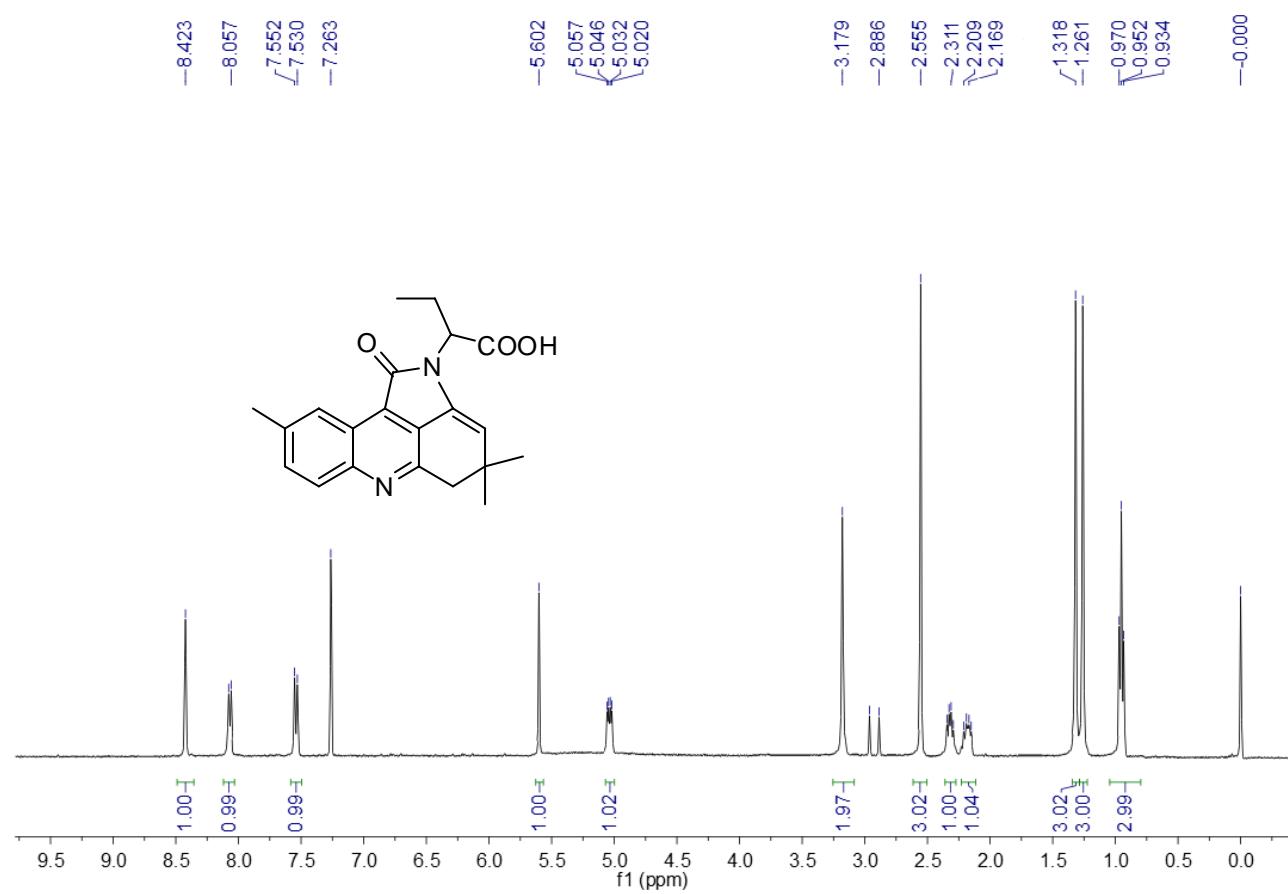


¹H NMR Spectrum of Compound 3o

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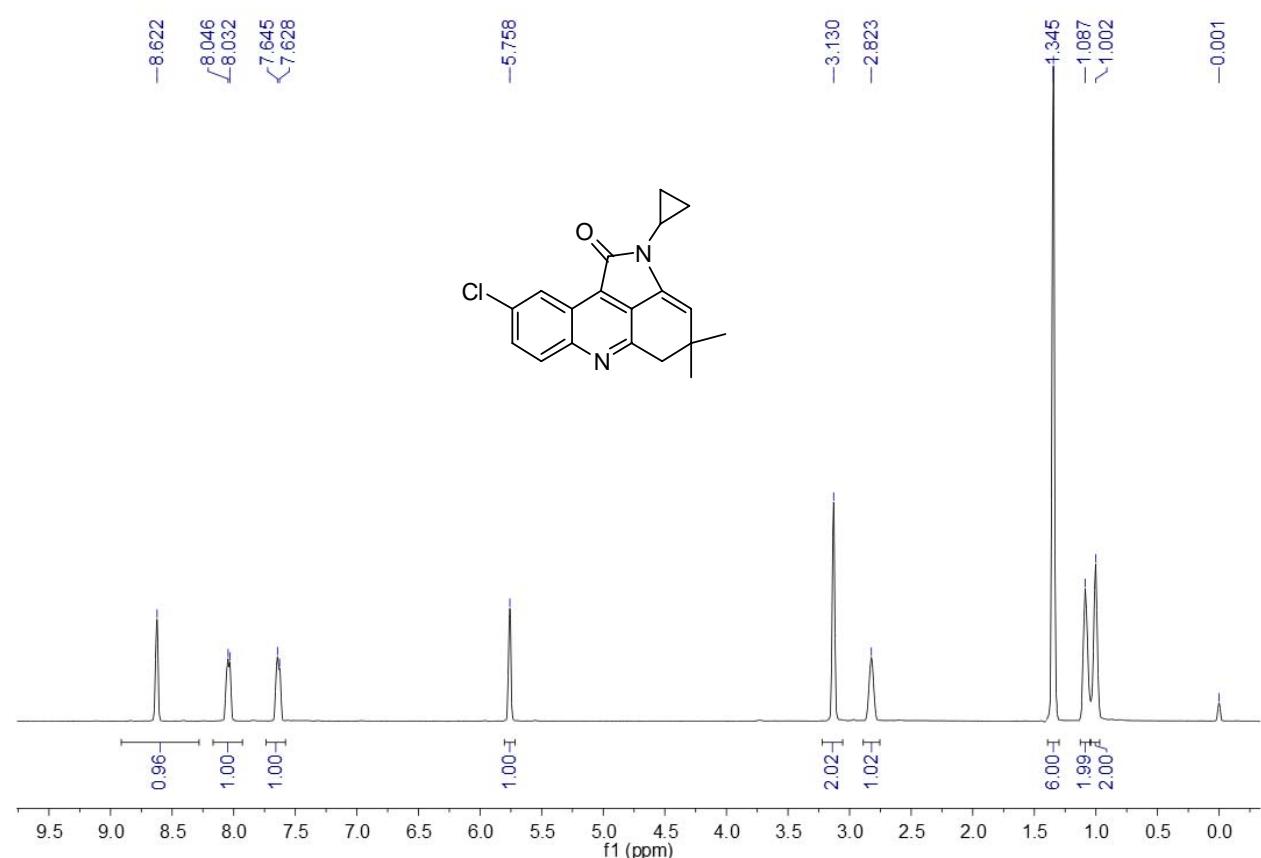


¹³C NMR Spectrum of Compound 3o

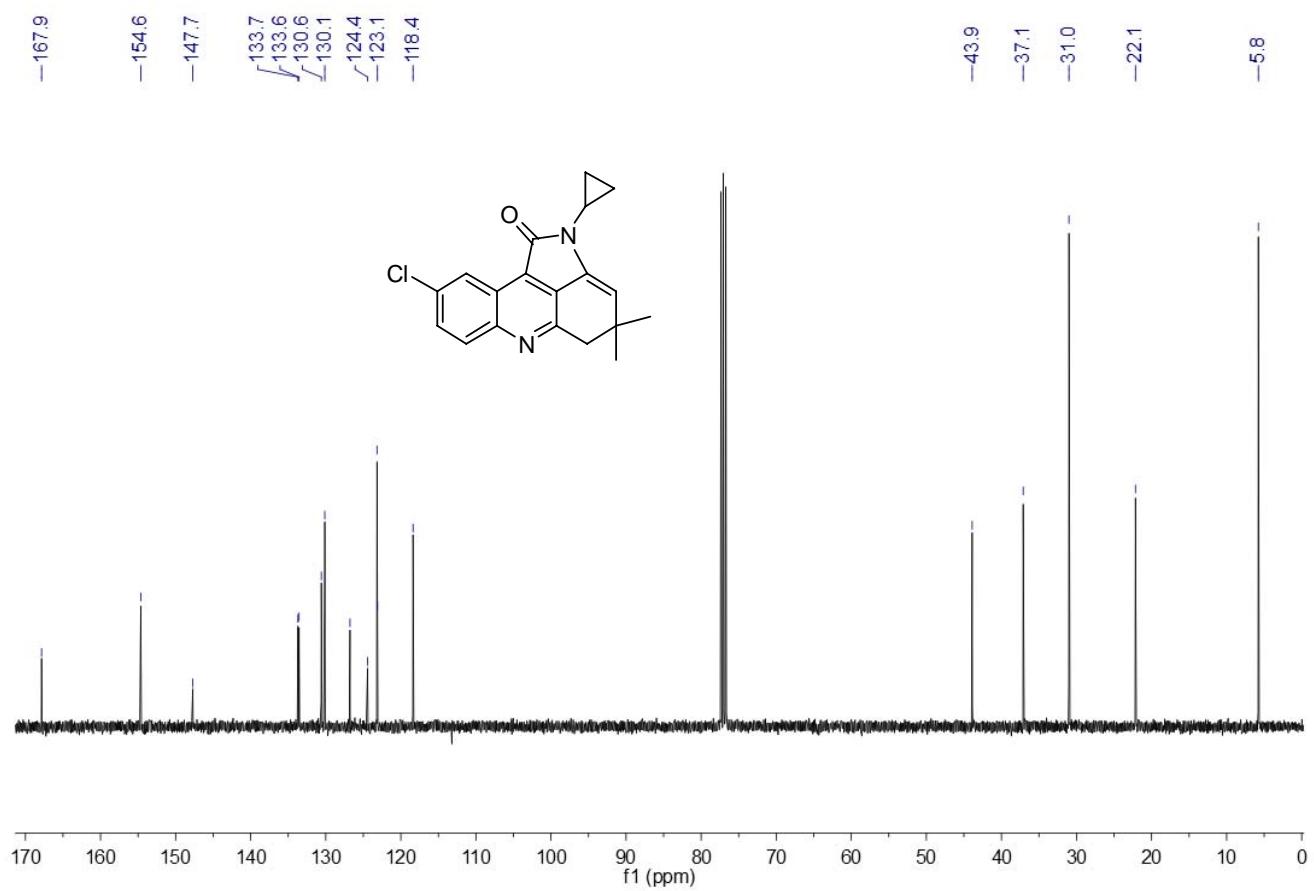


¹H NMR Spectrum of Compound 3p

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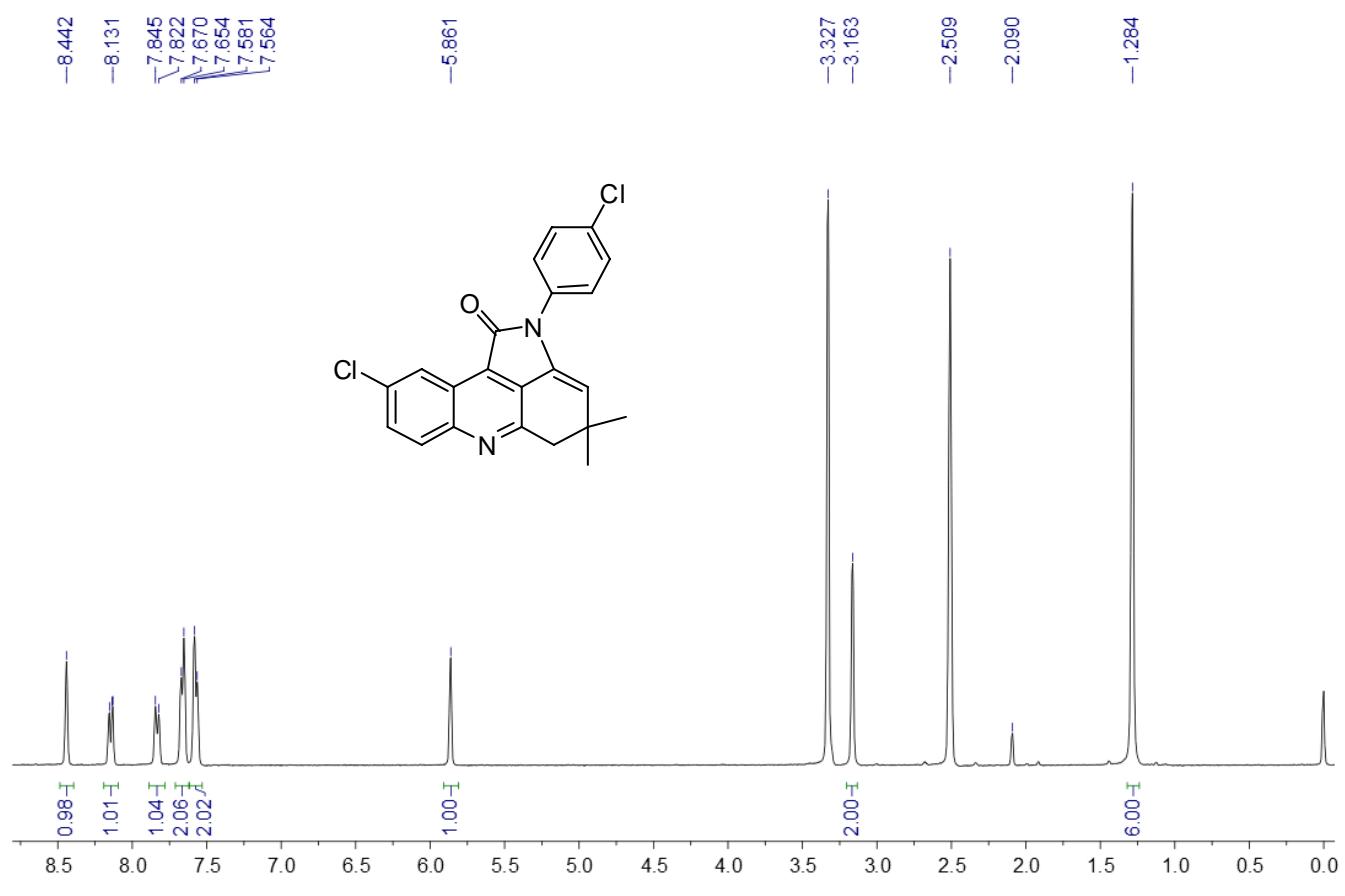


¹H NMR Spectrum of Compound 3q

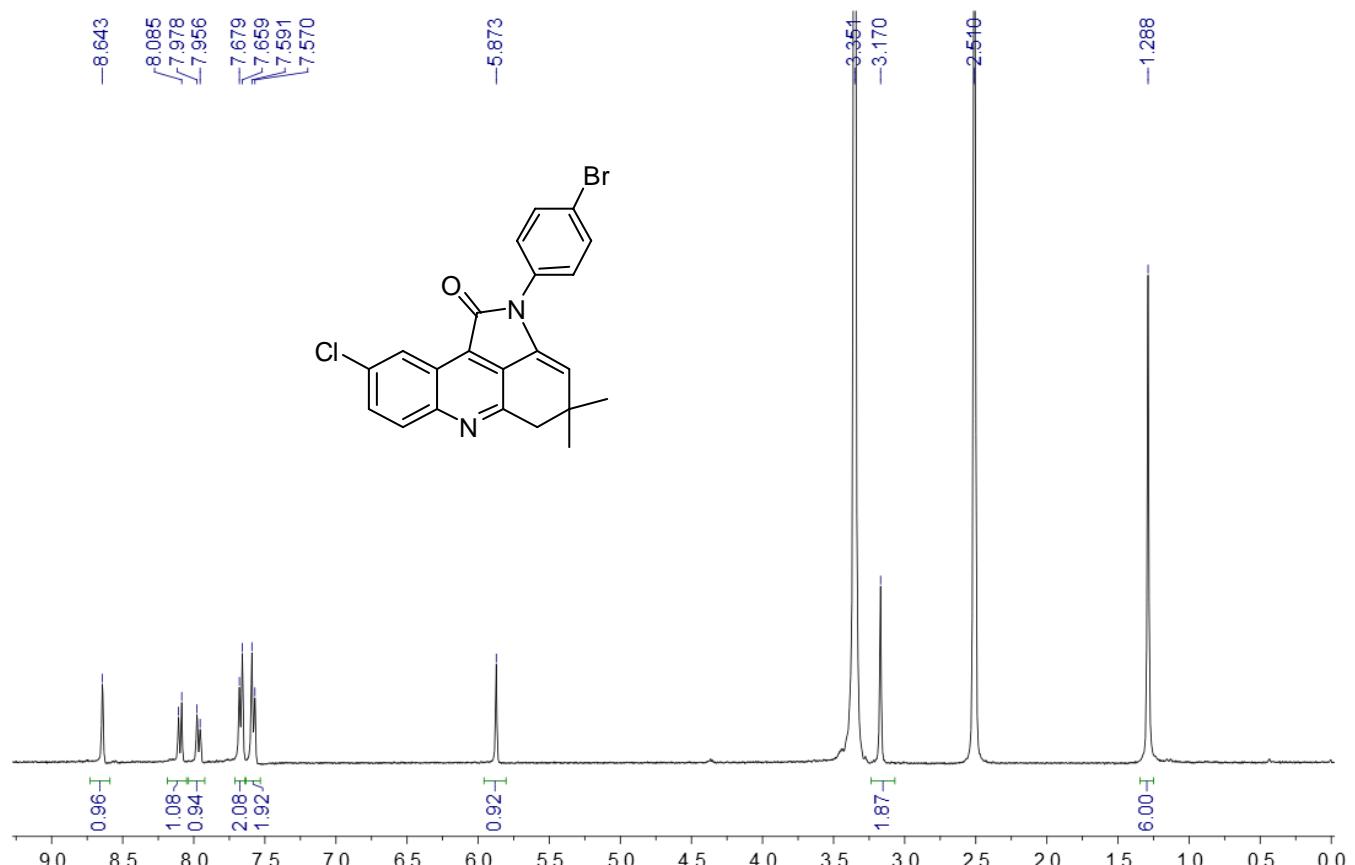


¹³C NMR Spectrum of Compound 3q

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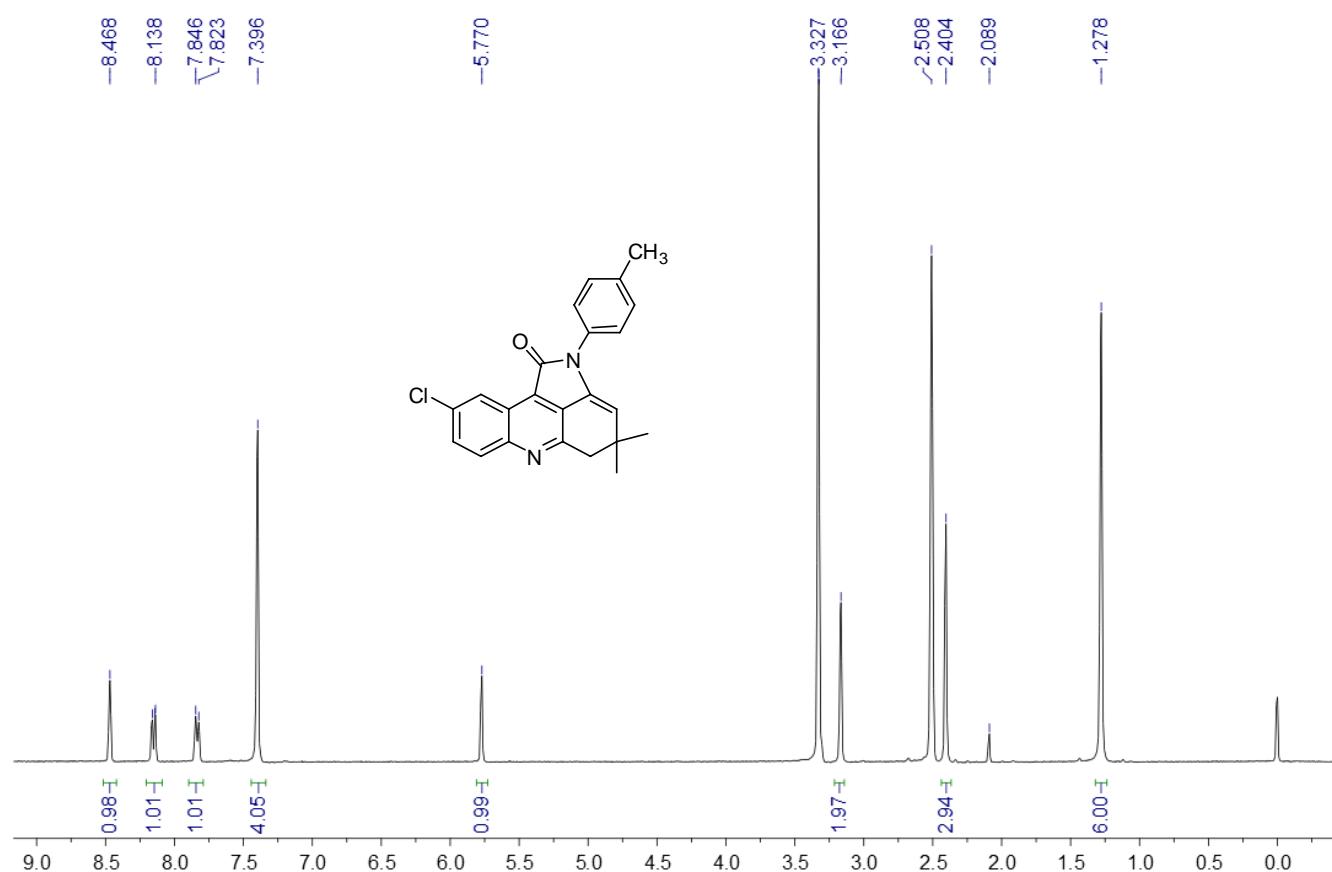


¹H NMR Spectrum of Compound 3r

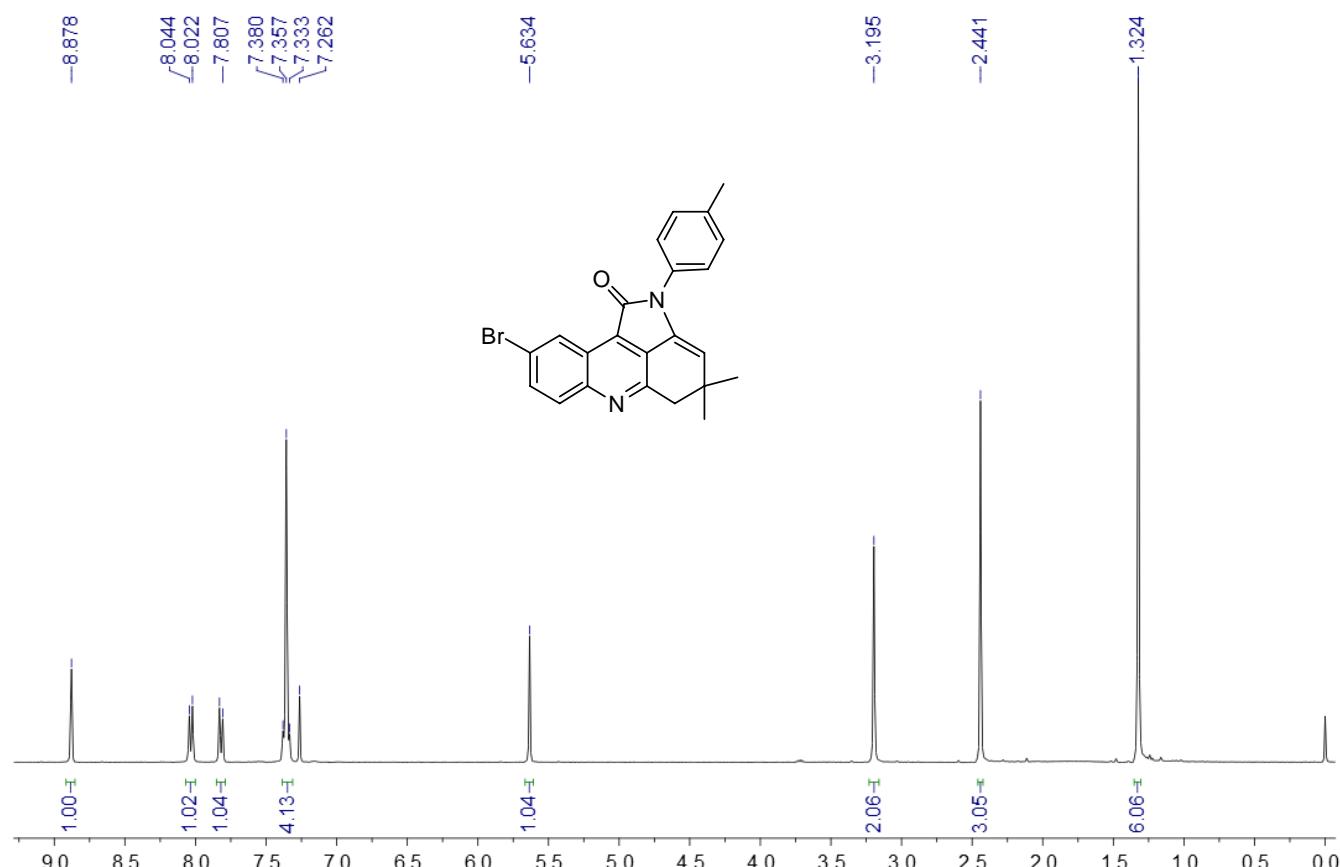


¹H NMR Spectrum of Compound 3s

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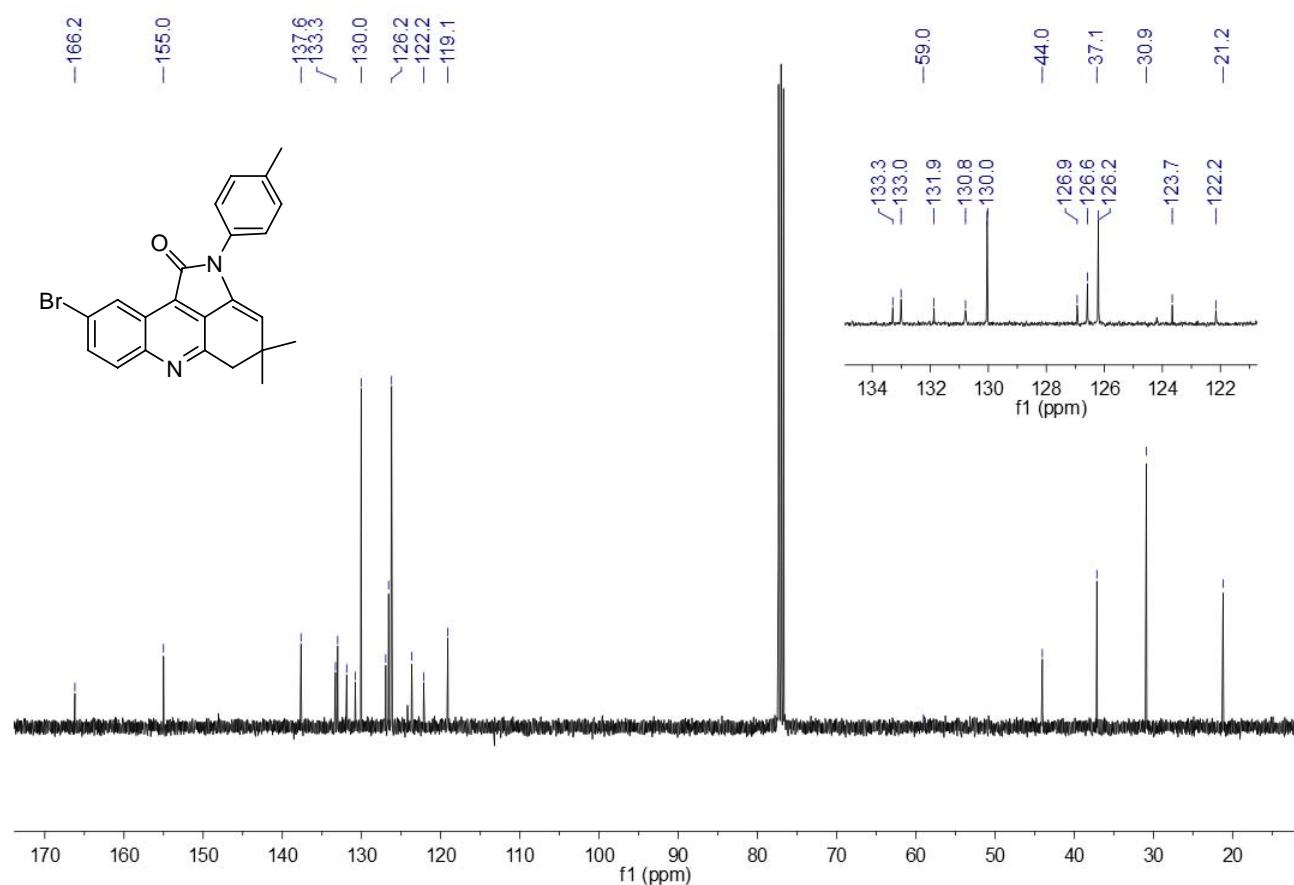


¹H NMR Spectrum of Compound 3t

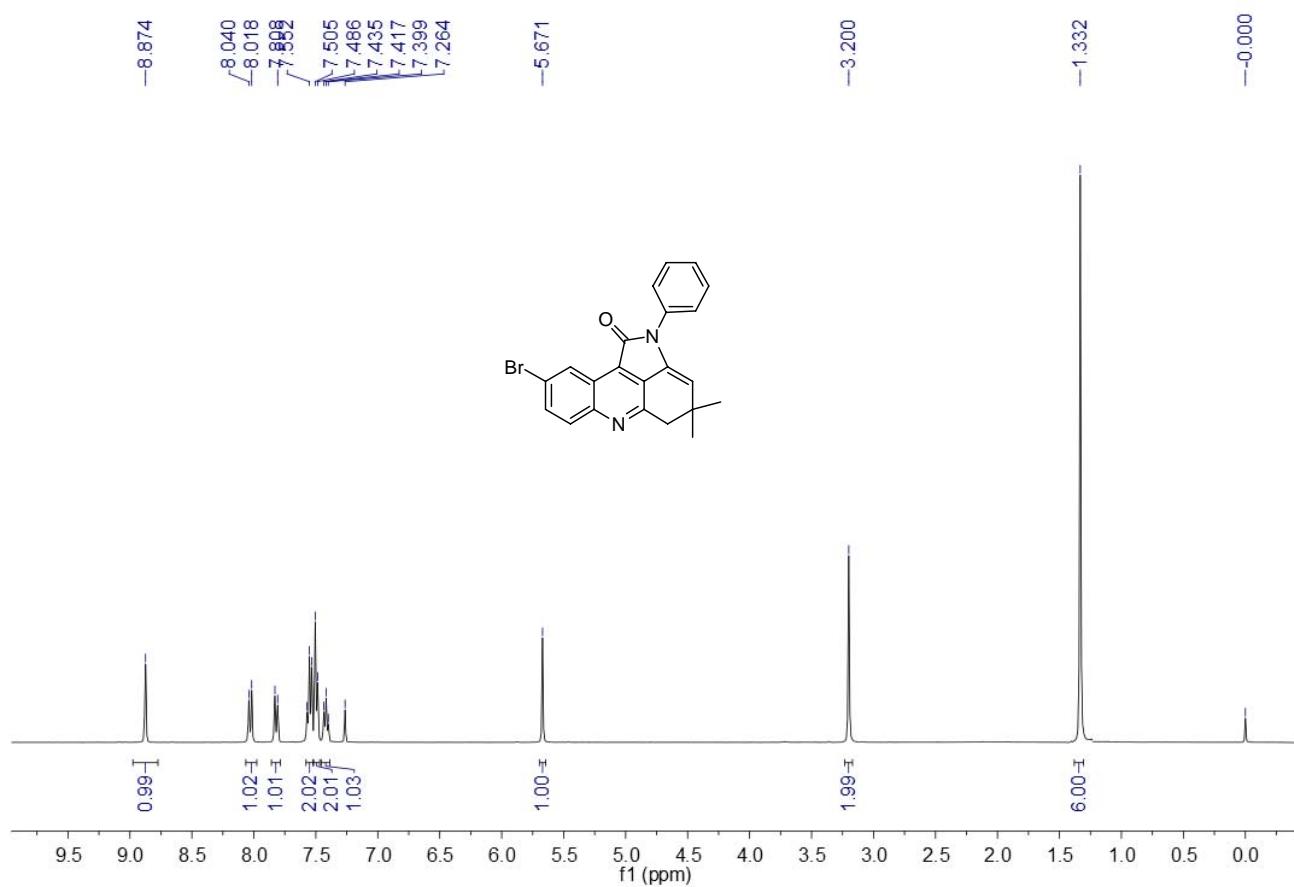


¹H NMR Spectrum of Compound 3u

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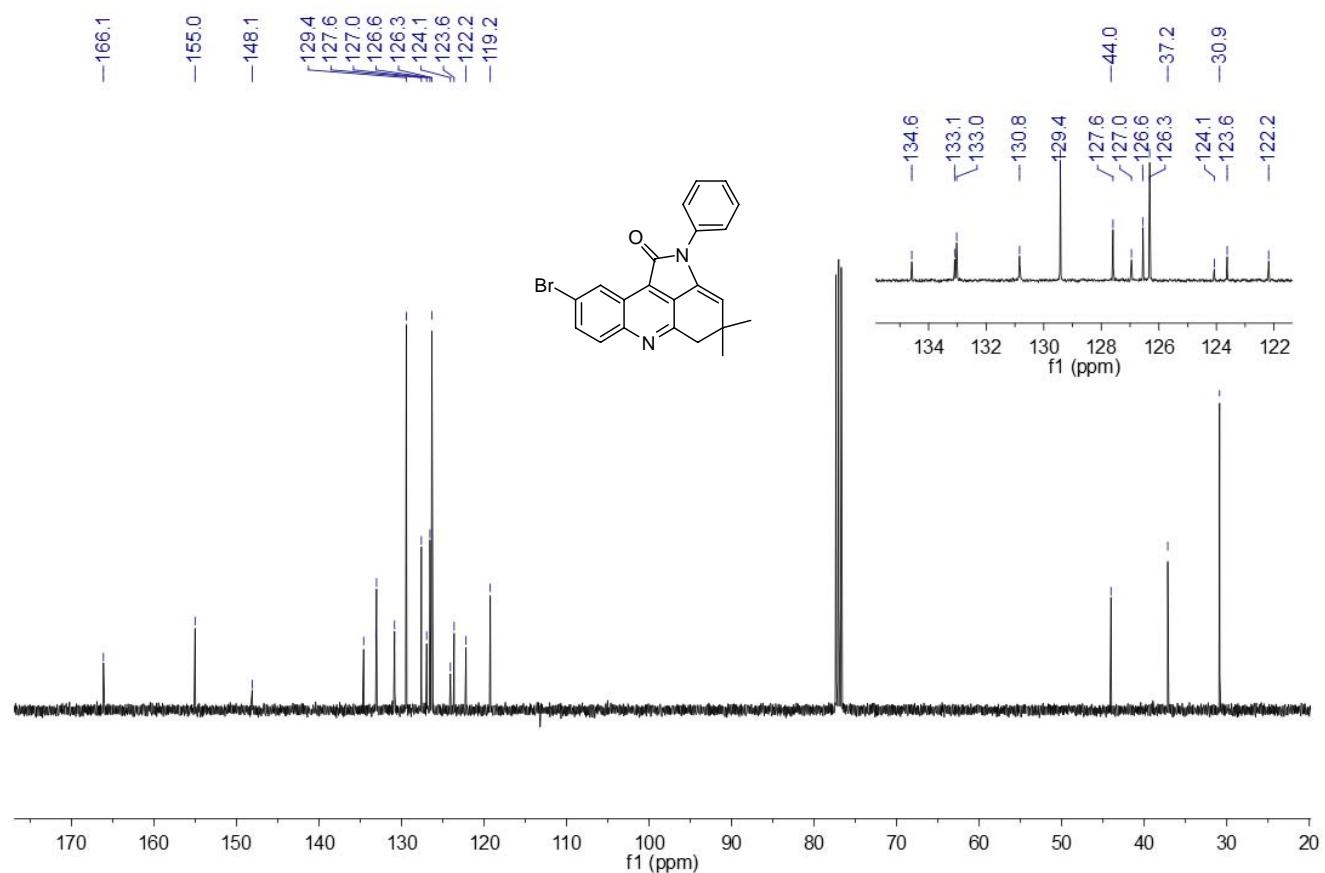


¹³C NMR Spectrum of Compound 3u

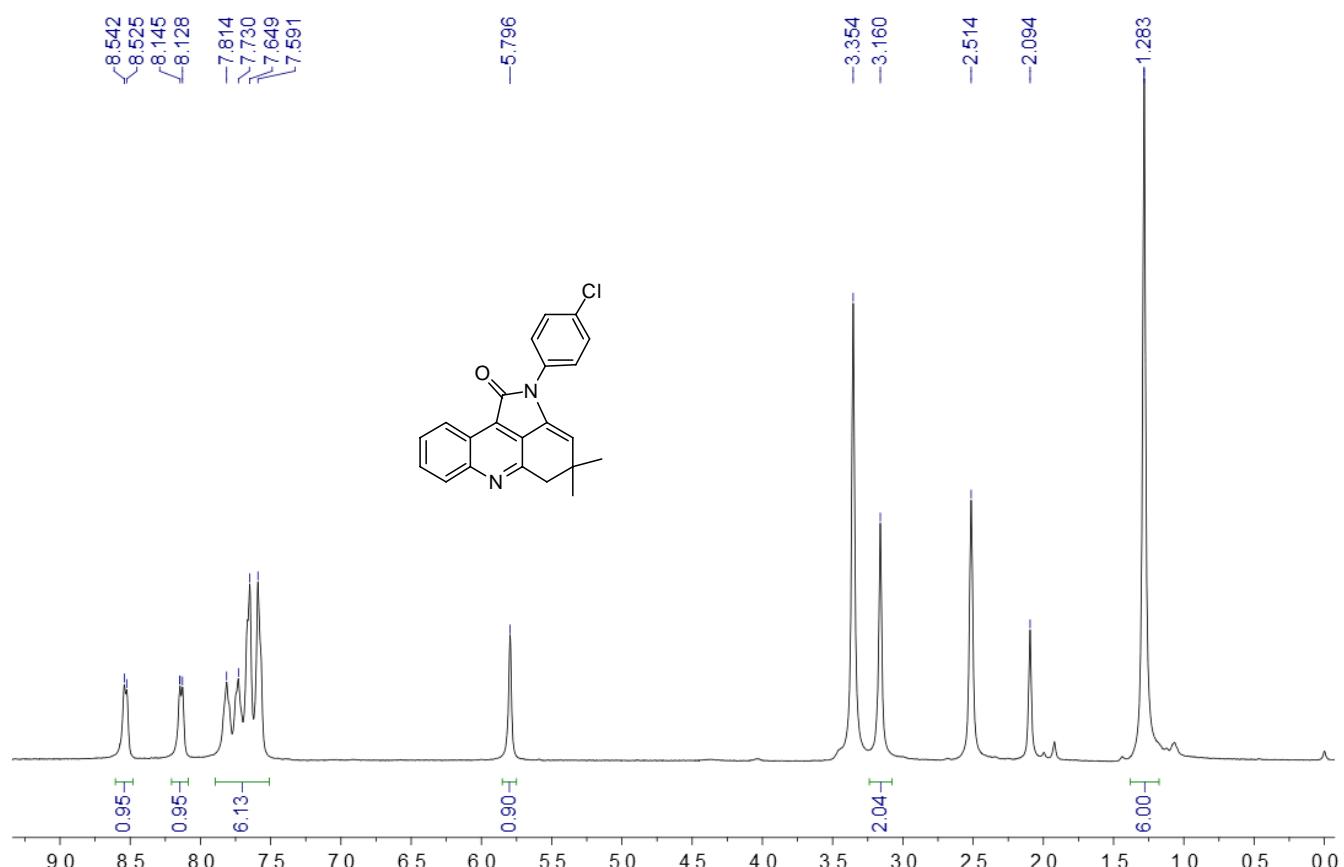


¹H NMR Spectrum of Compound 3v

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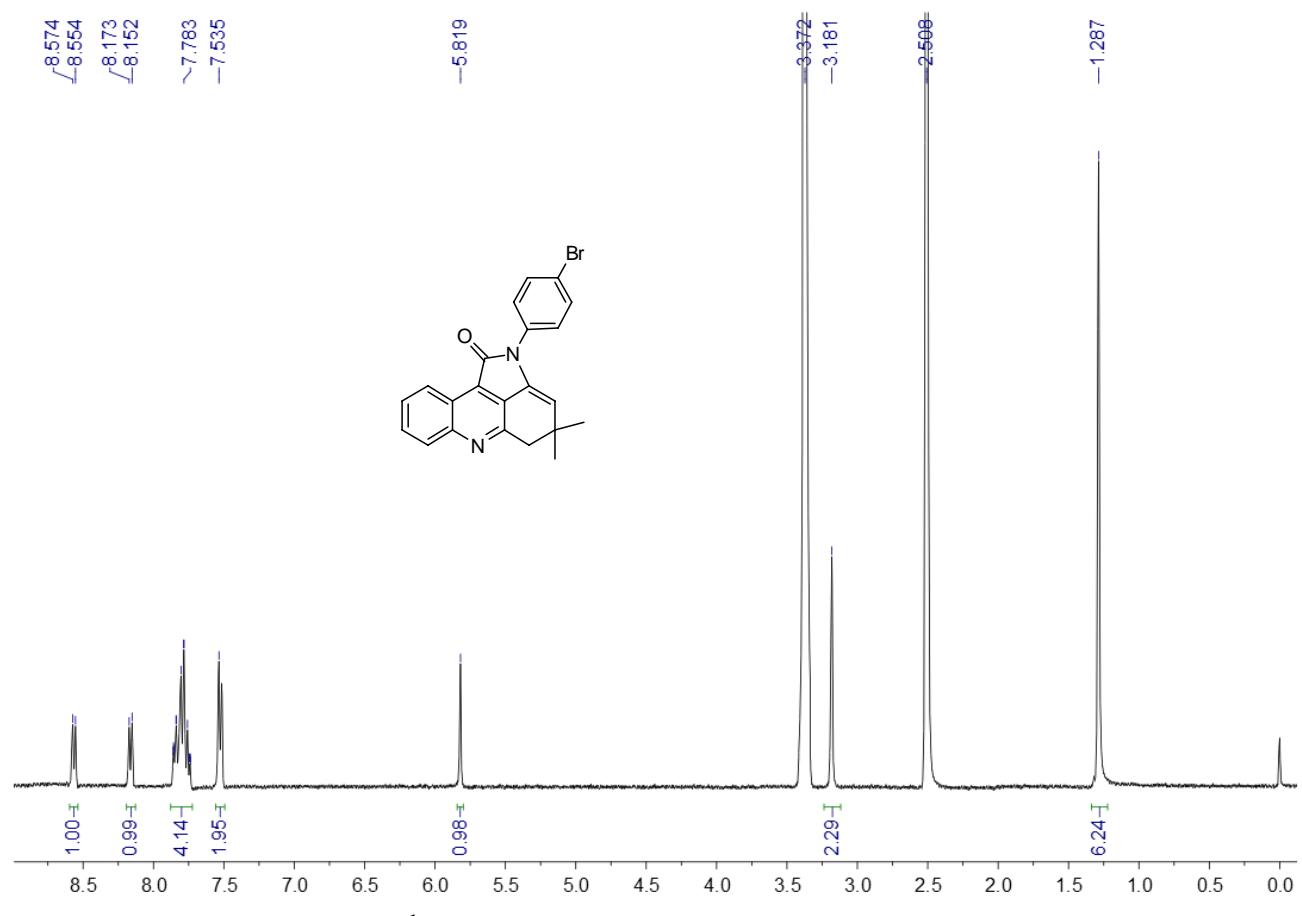


¹³C NMR Spectrum of Compound 3v

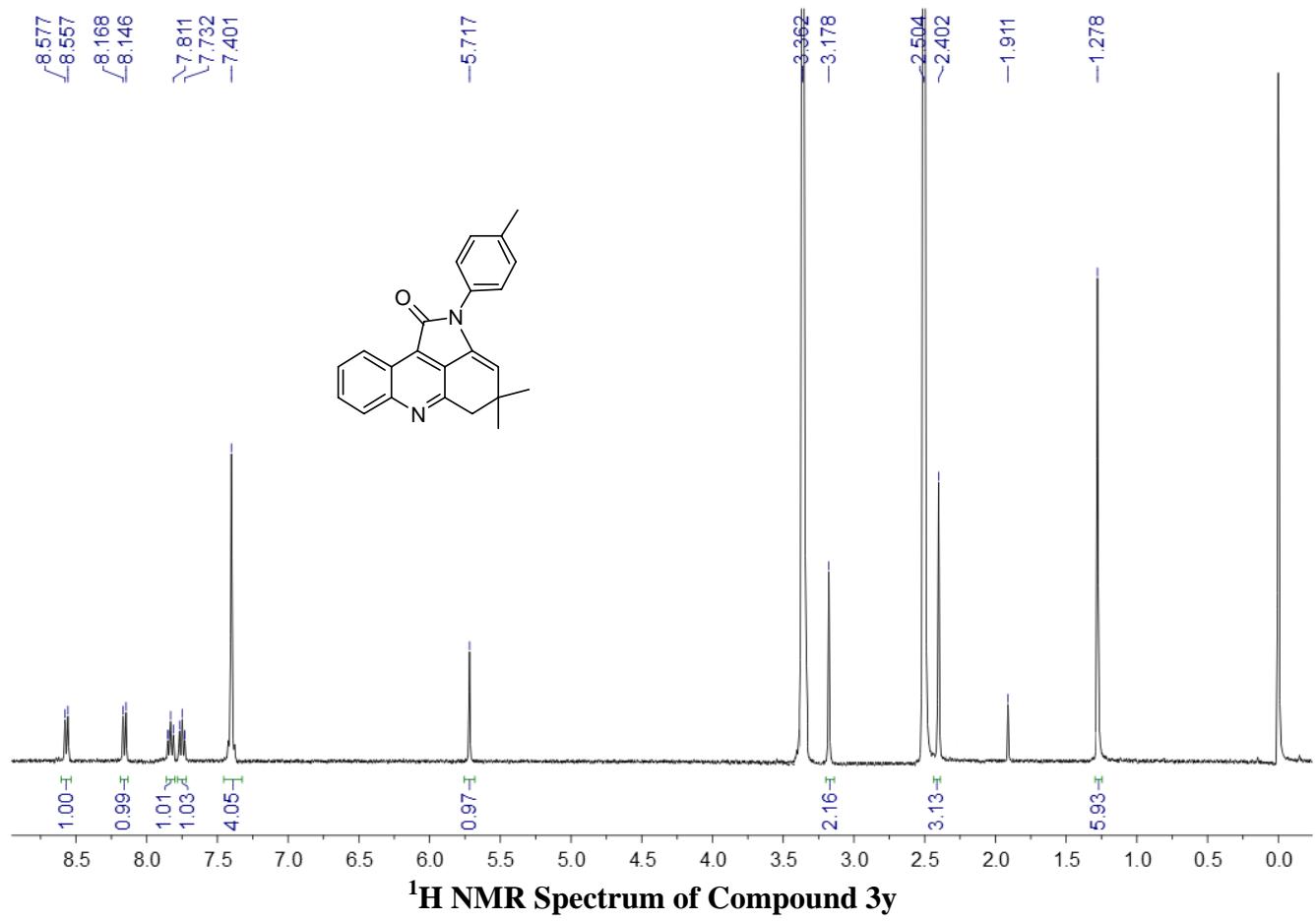


¹H NMR Spectrum of Compound 3w

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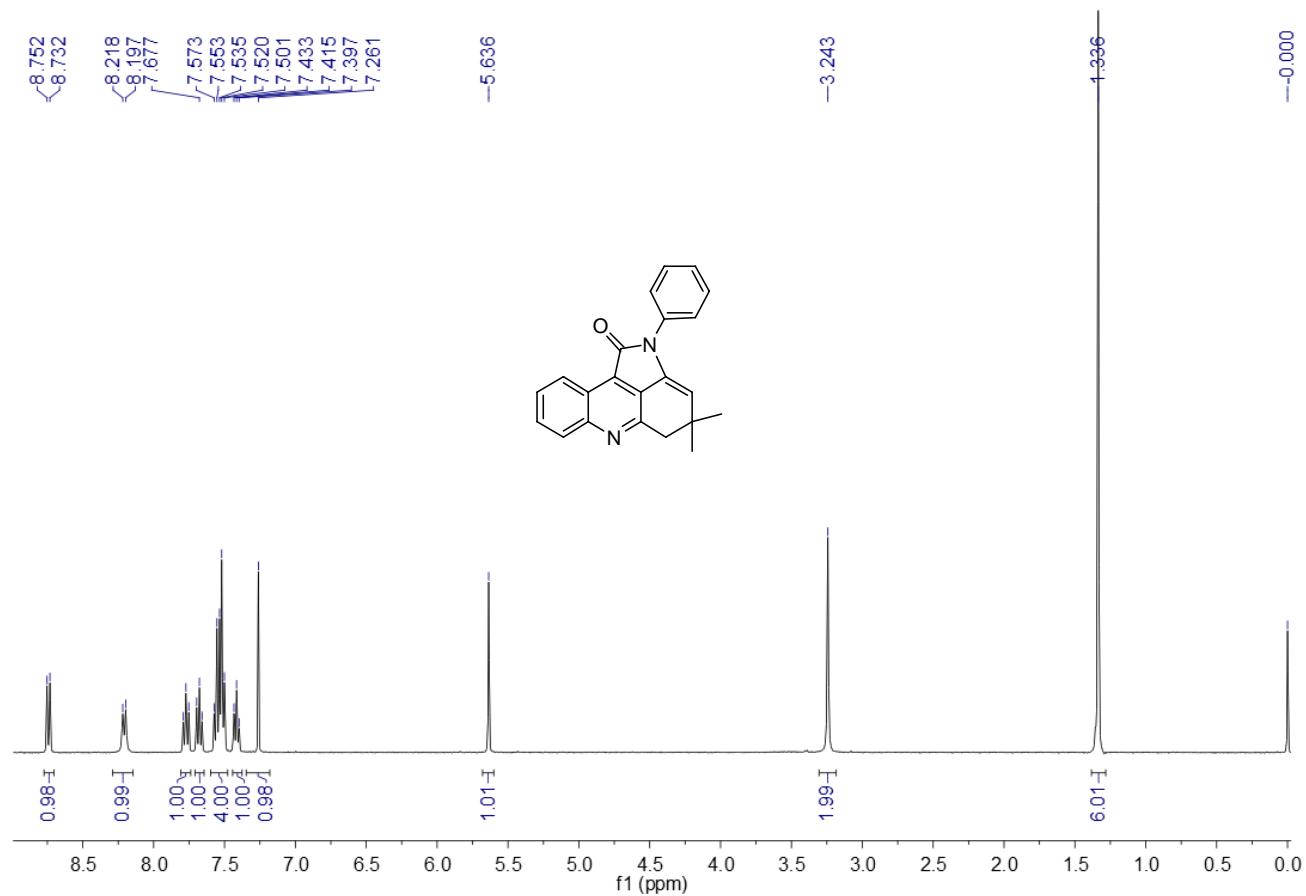


¹H NMR Spectrum of Compound 3x

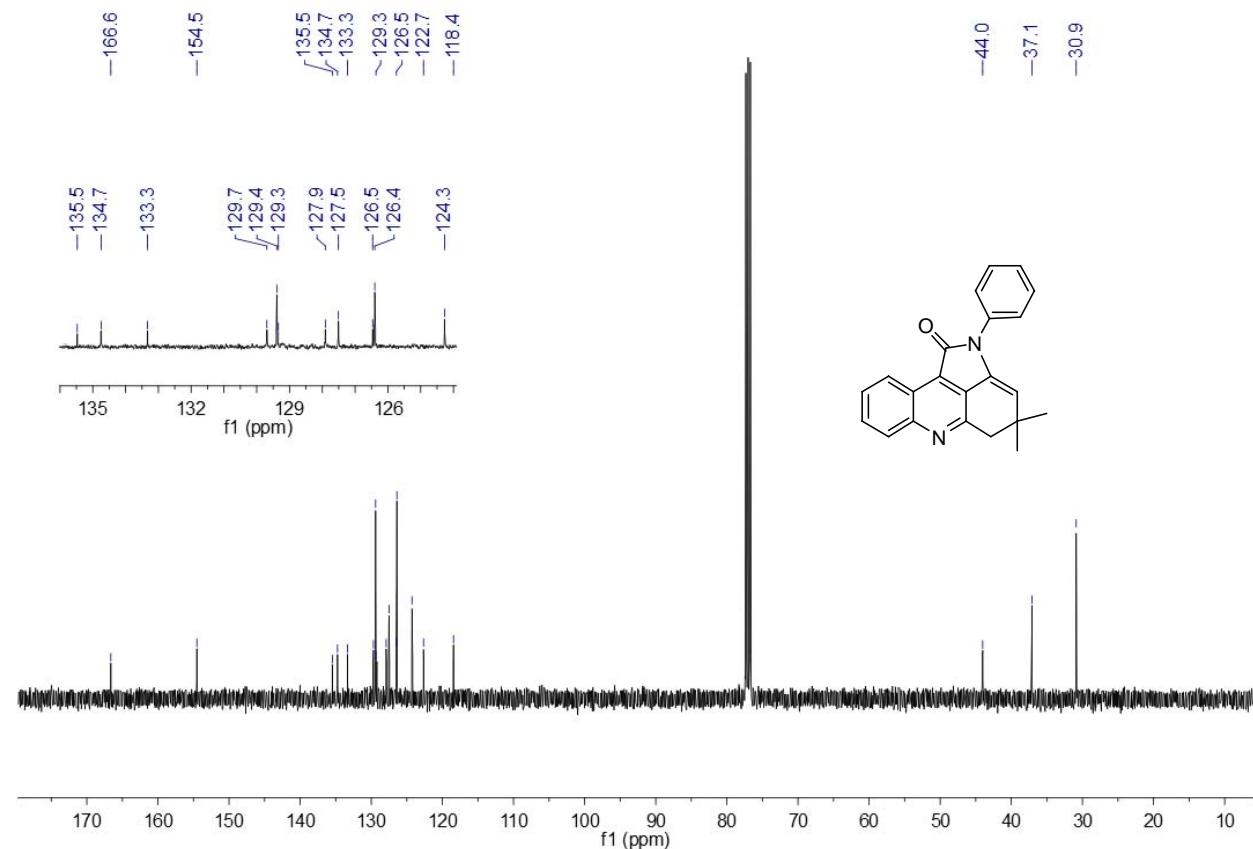


¹H NMR Spectrum of Compound 3y

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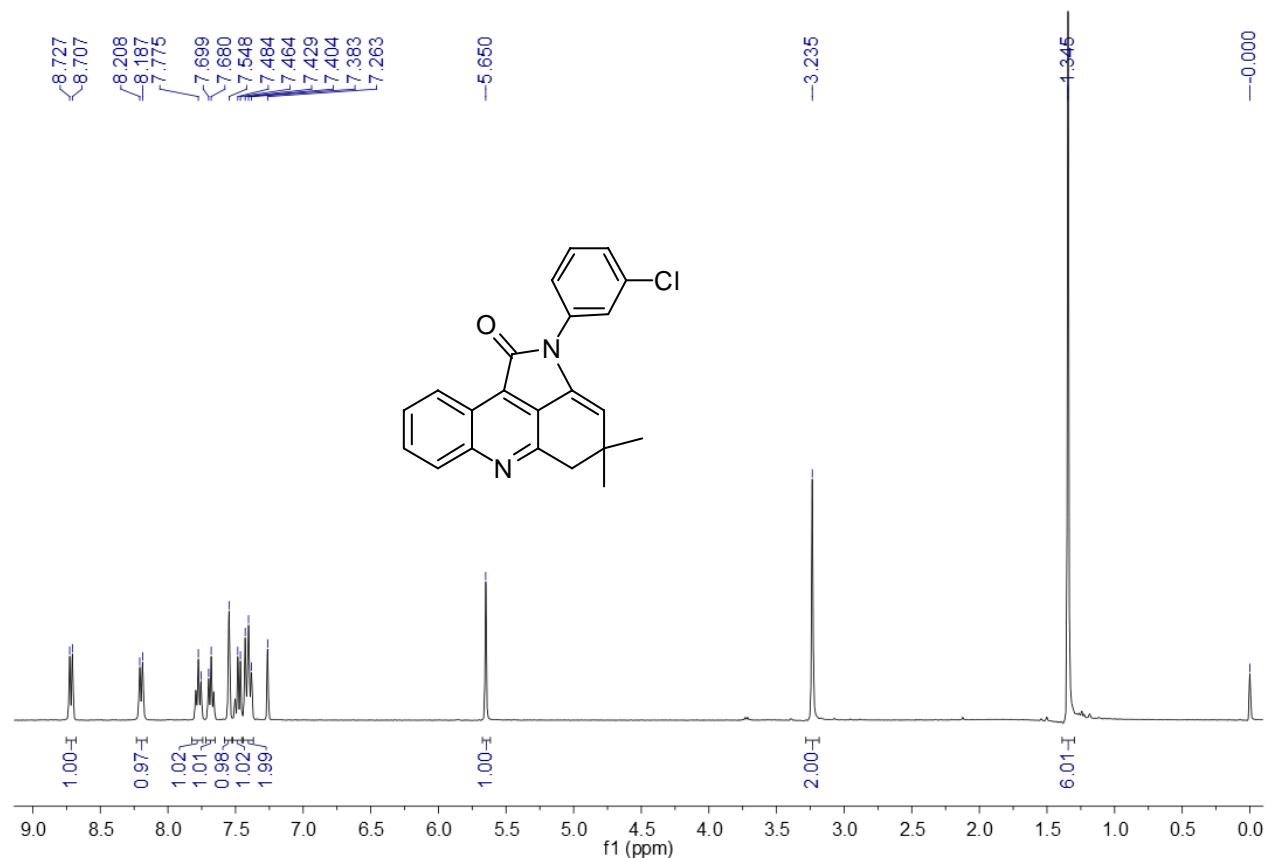


¹H NMR Spectrum of Compound 3z

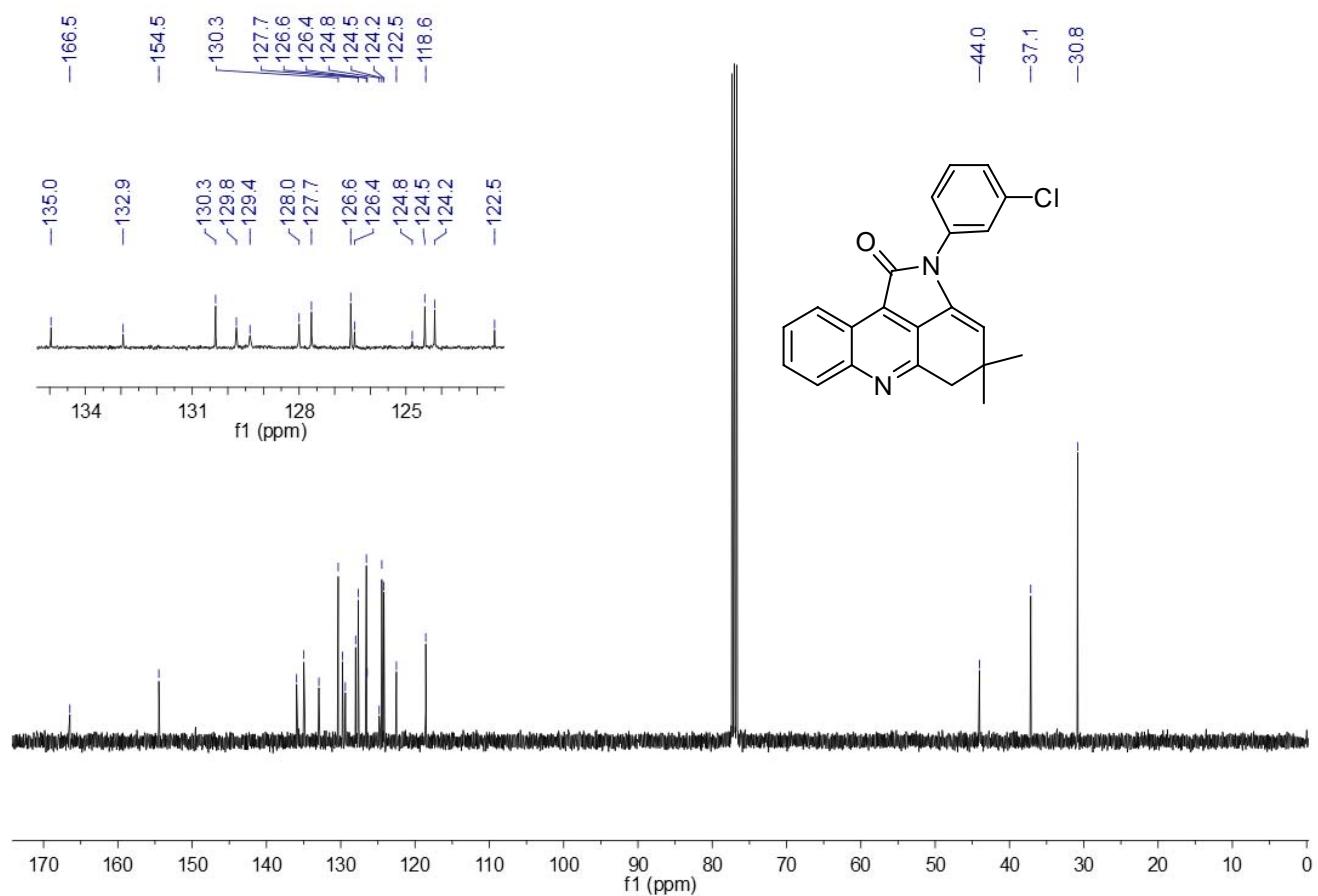


¹³C NMR Spectrum of Compound 3z

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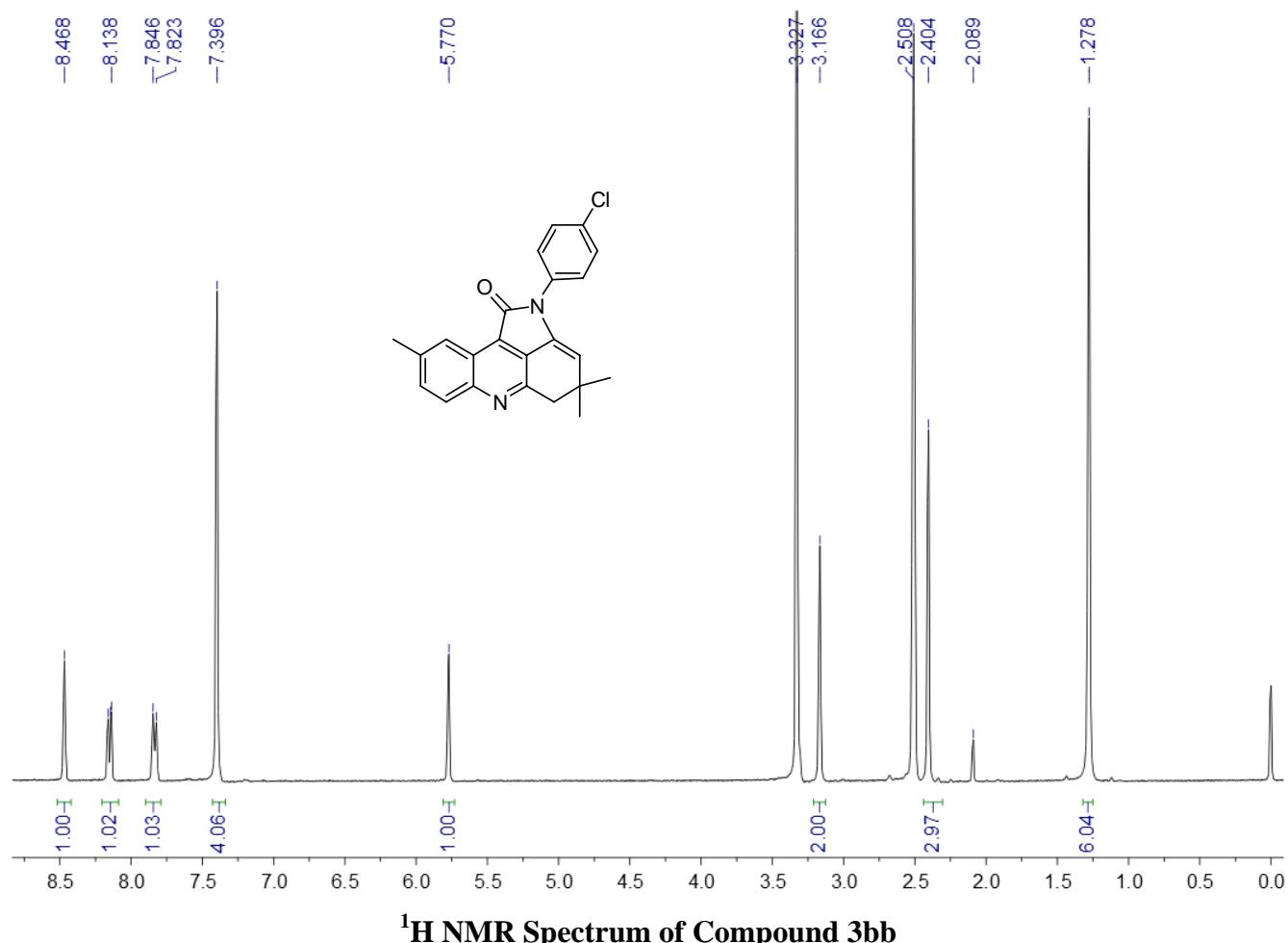


¹H NMR Spectrum of Compound 3aa

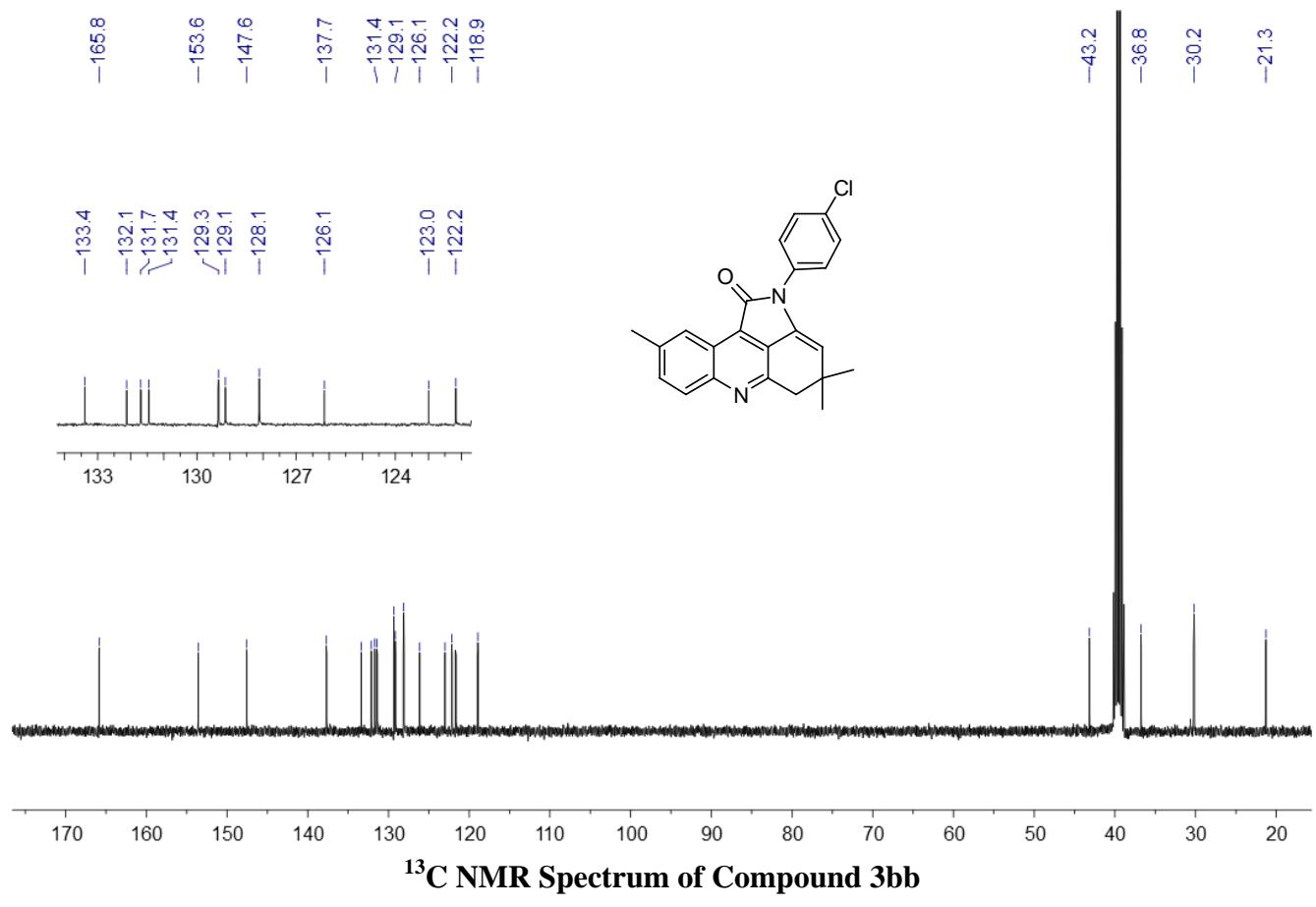


¹³C NMR Spectrum of Compound 3aa

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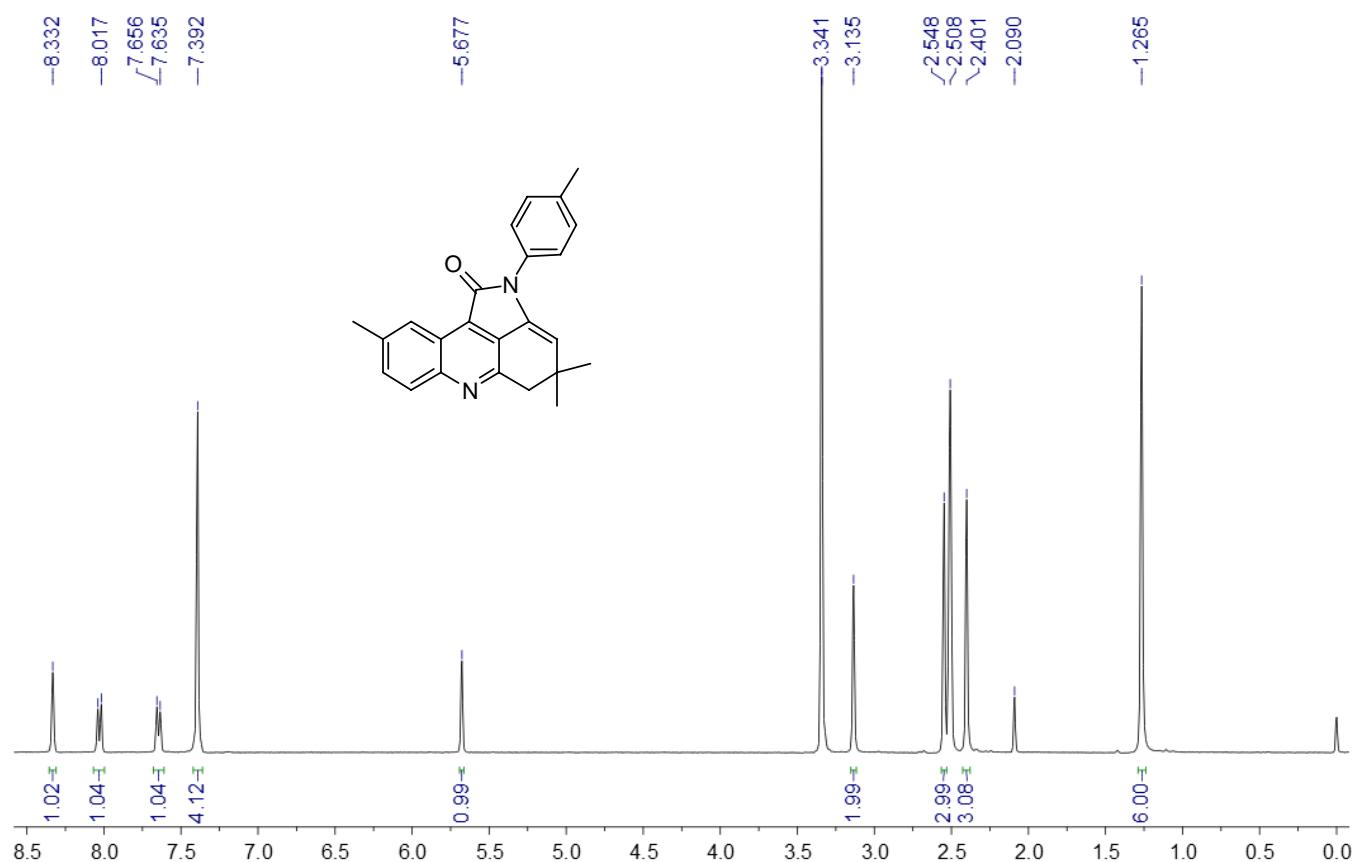


¹H NMR Spectrum of Compound 3bb

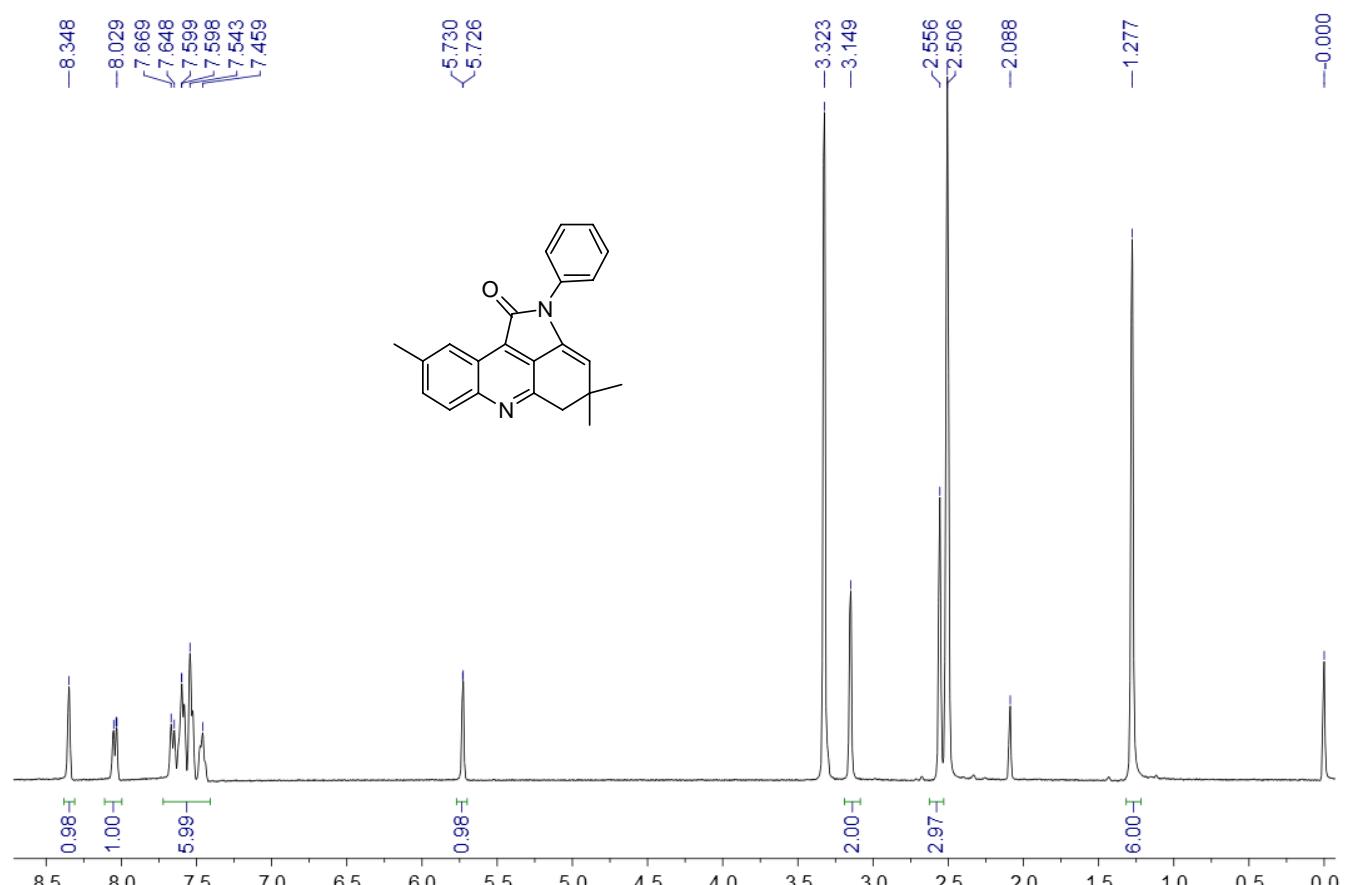


¹³C NMR Spectrum of Compound 3bb

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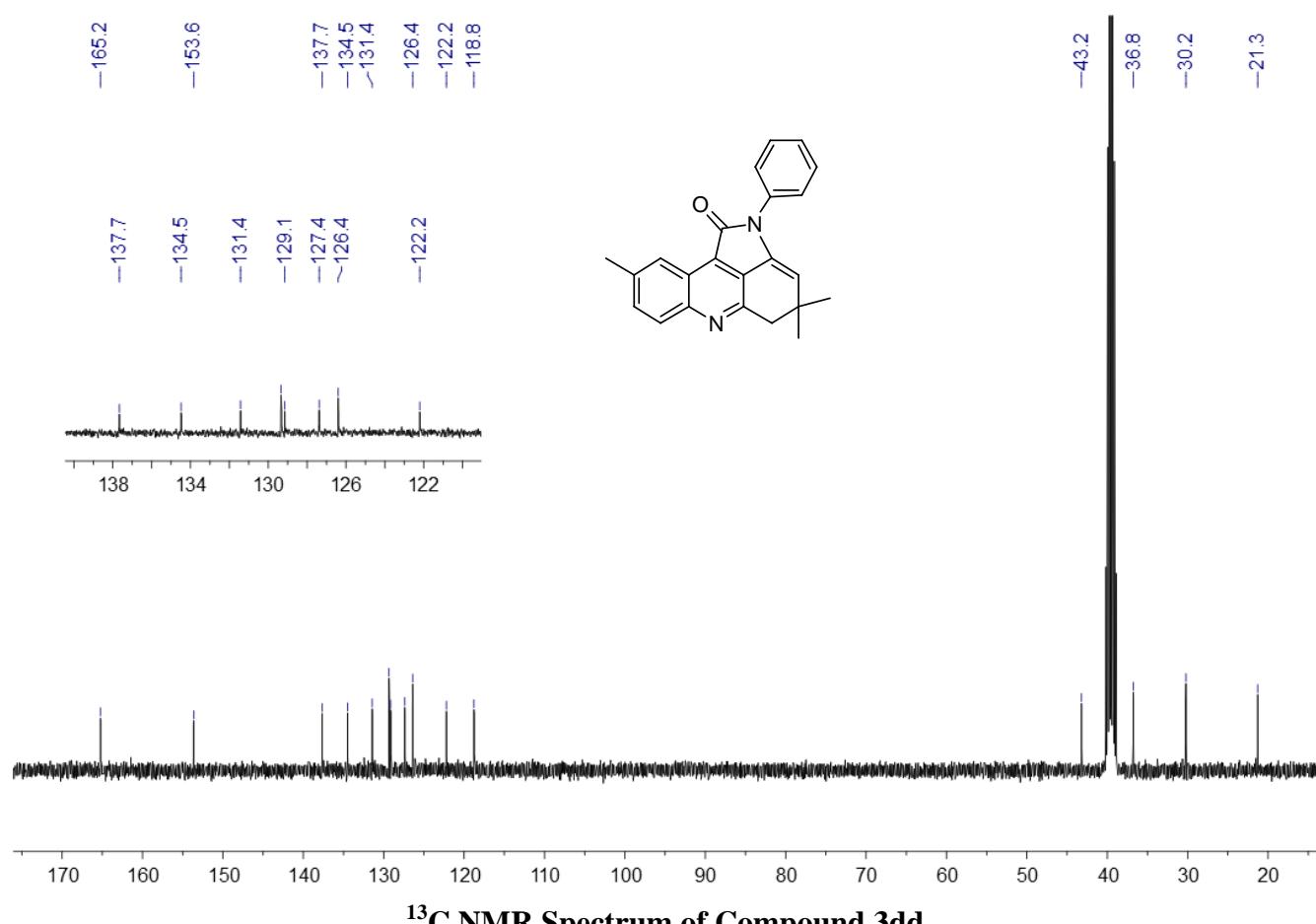


¹H NMR Spectrum of Compound 3cc

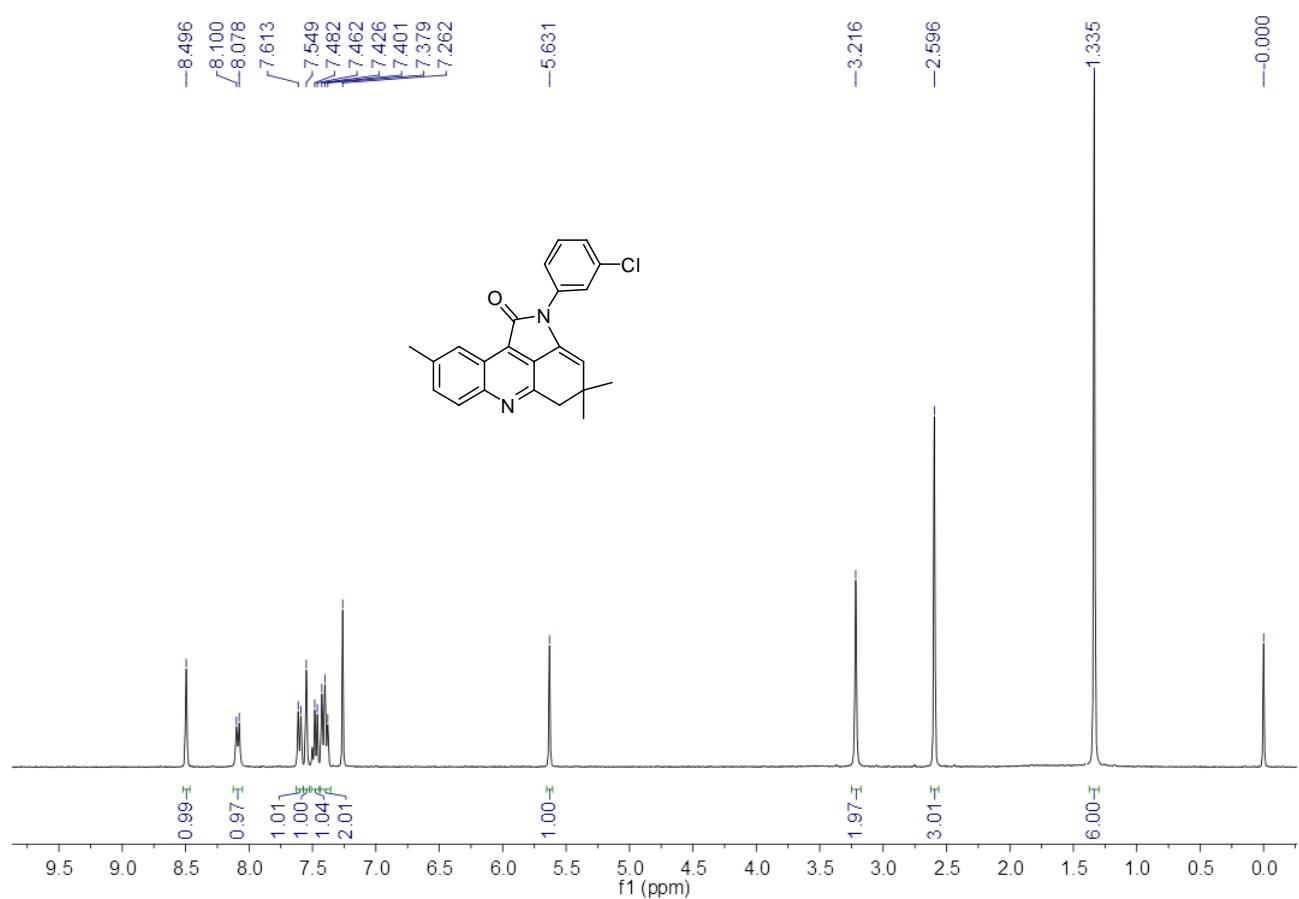


¹H NMR Spectrum of Compound 3dd

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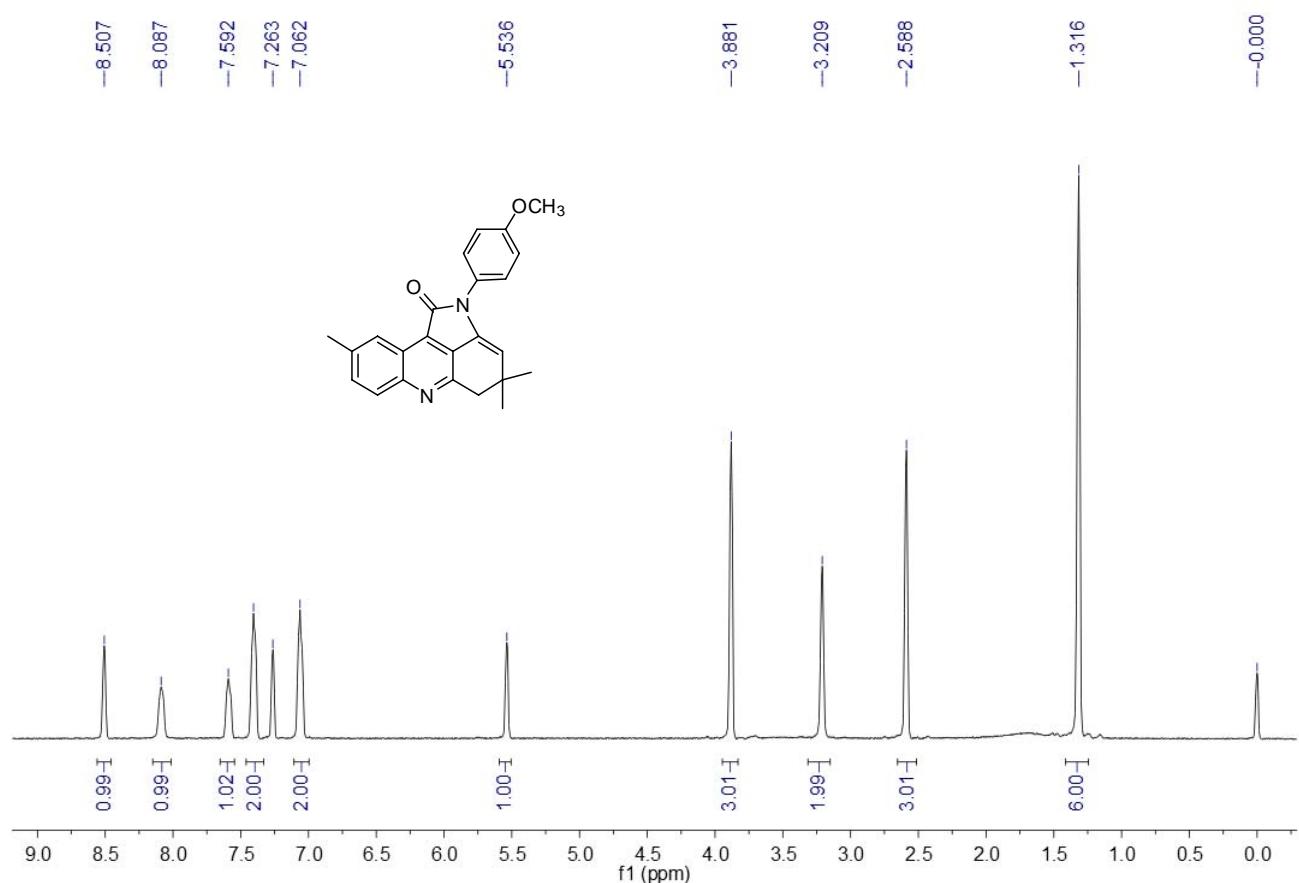


¹³C NMR Spectrum of Compound 3dd

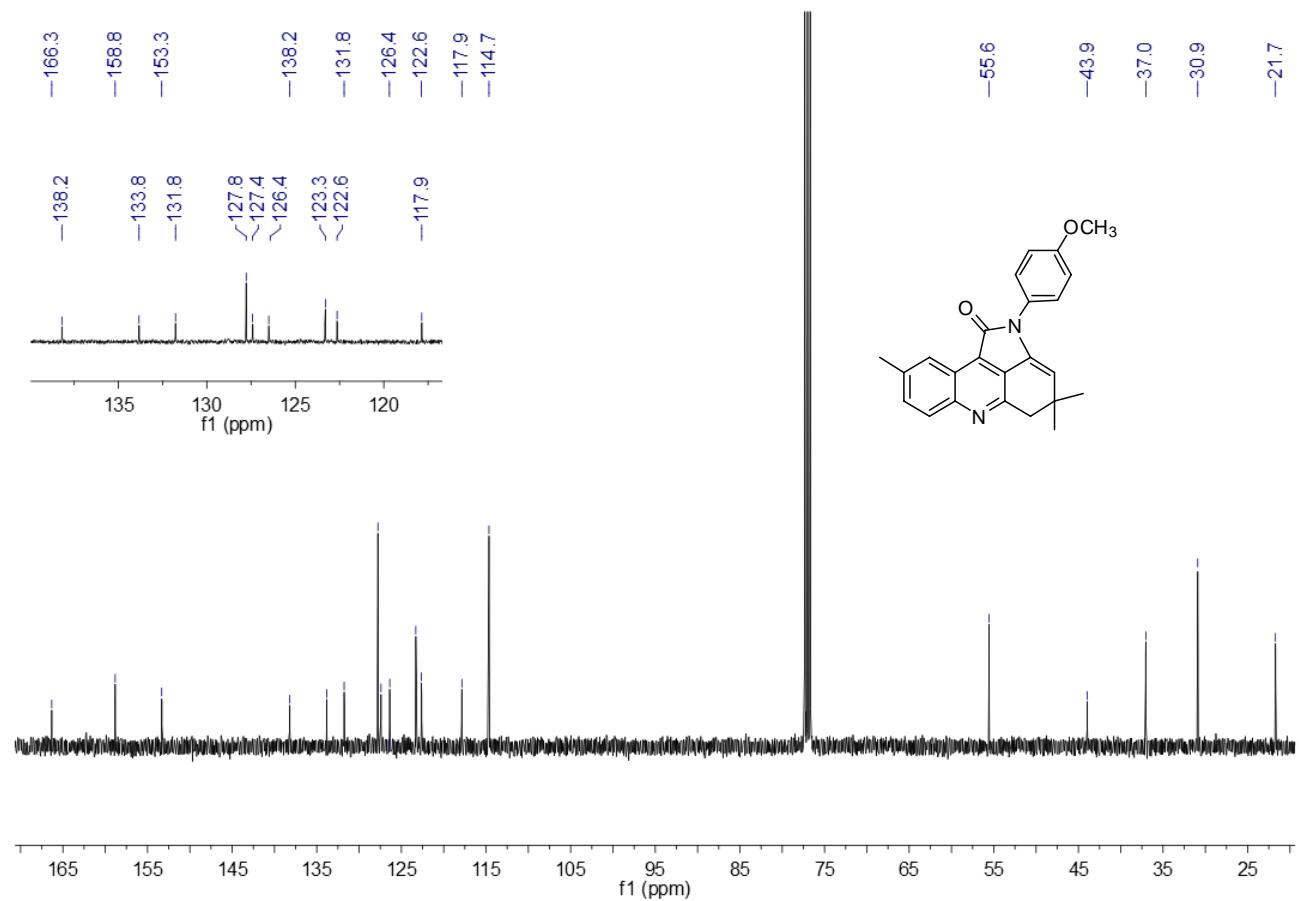


¹H NMR Spectrum of Compound 3bb

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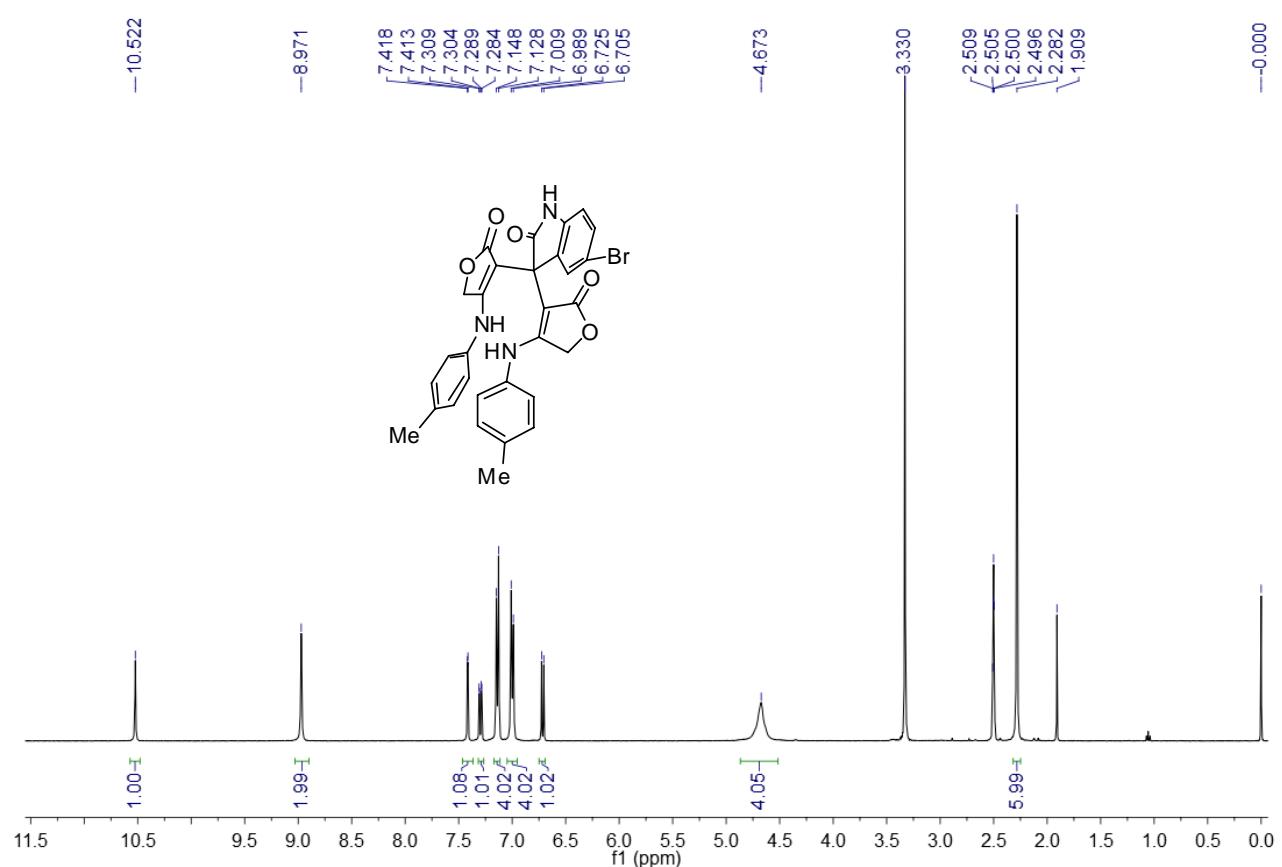


¹H NMR Spectrum of Compound 3ff

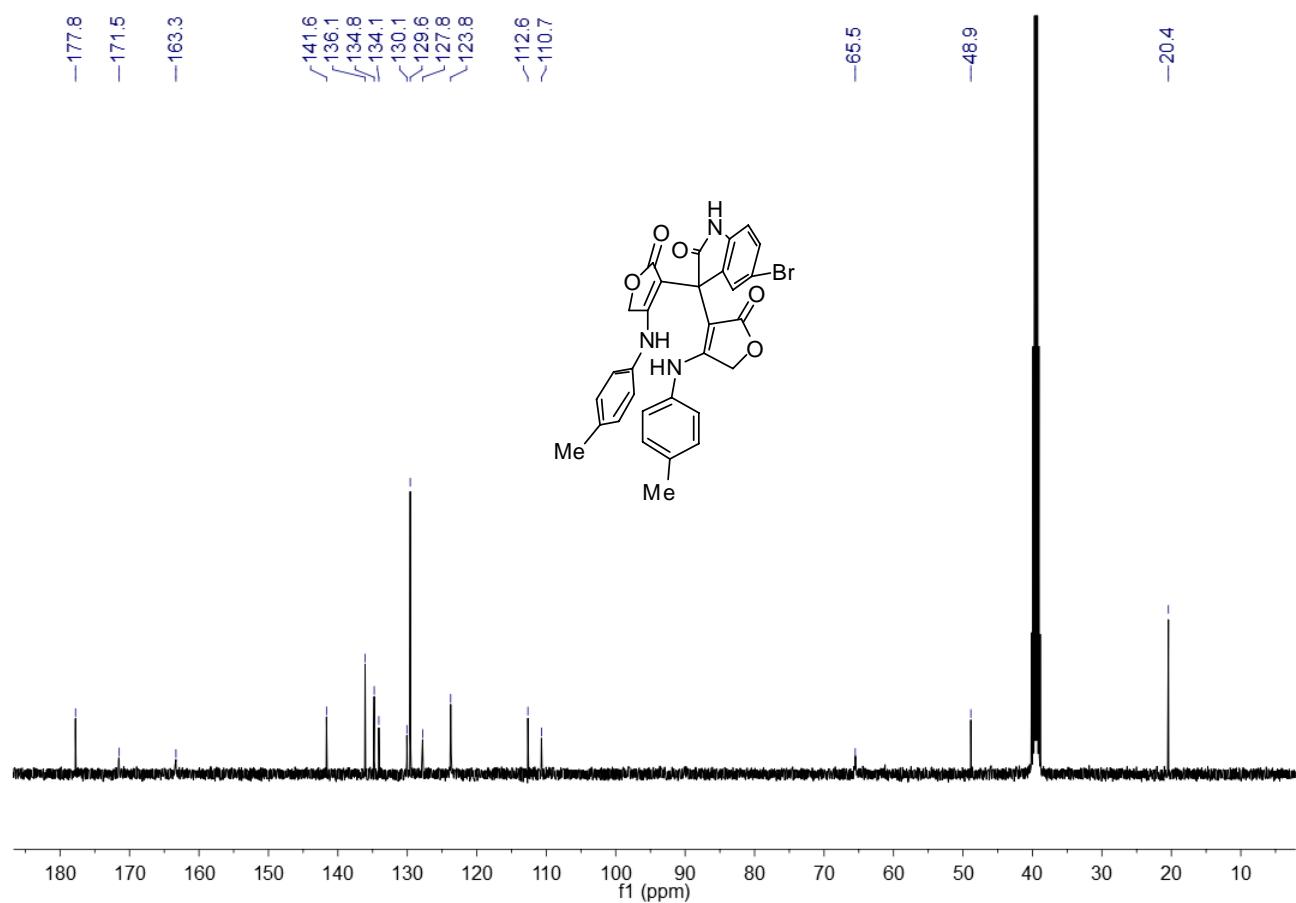


¹³C NMR Spectrum of Compound 3ff

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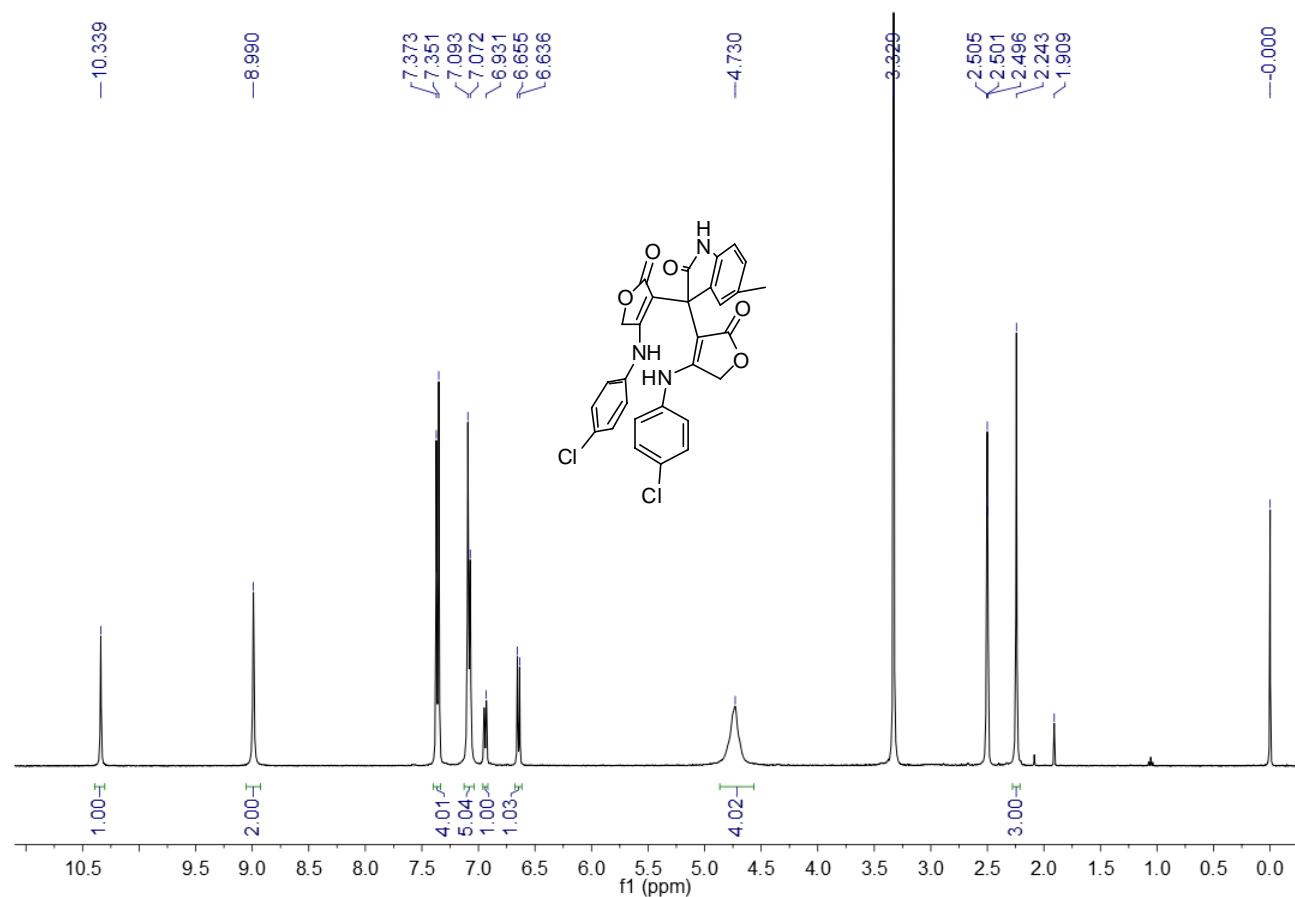


¹H NMR Spectrum of Compound 4a

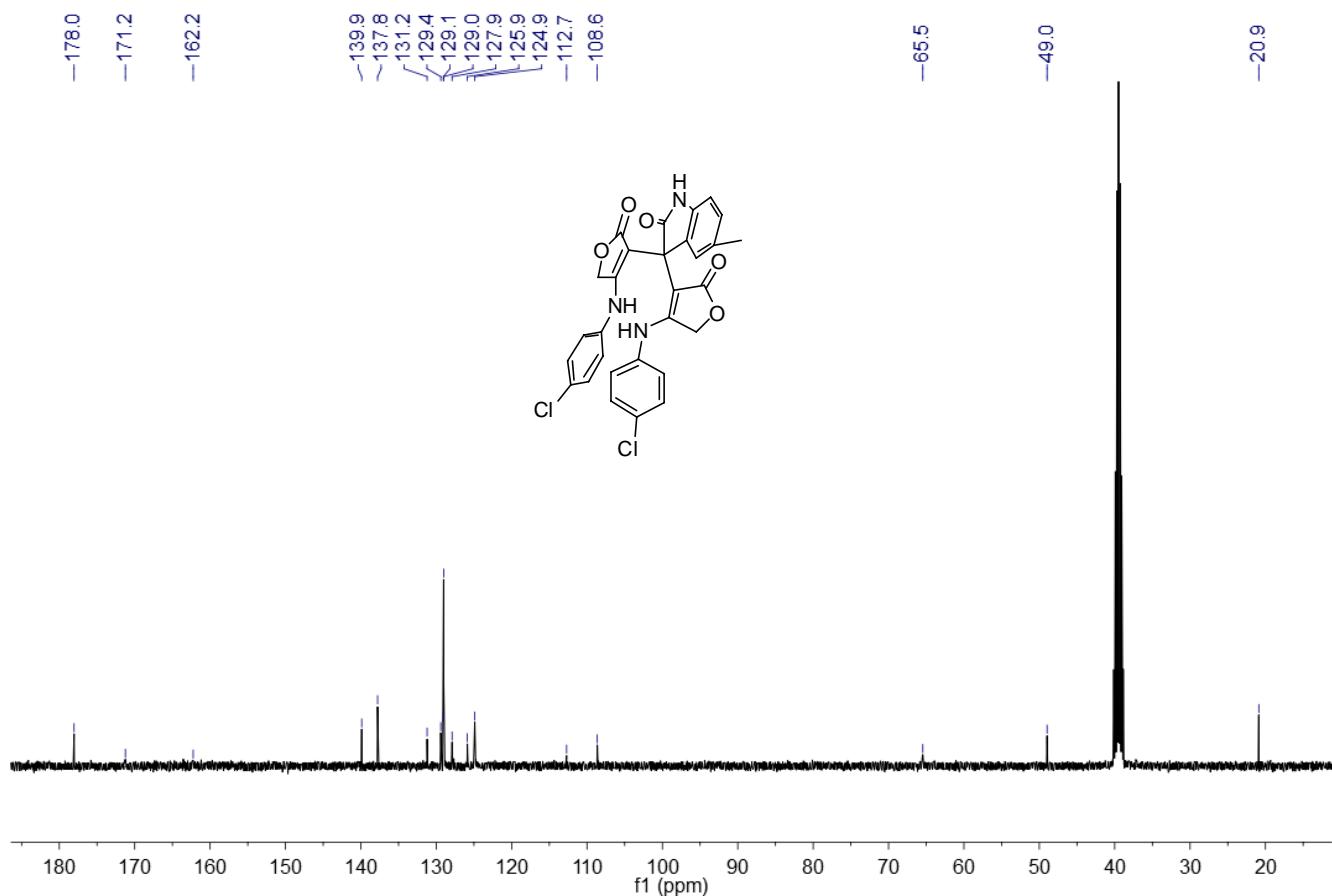


¹³C NMR Spectrum of Compound 4a

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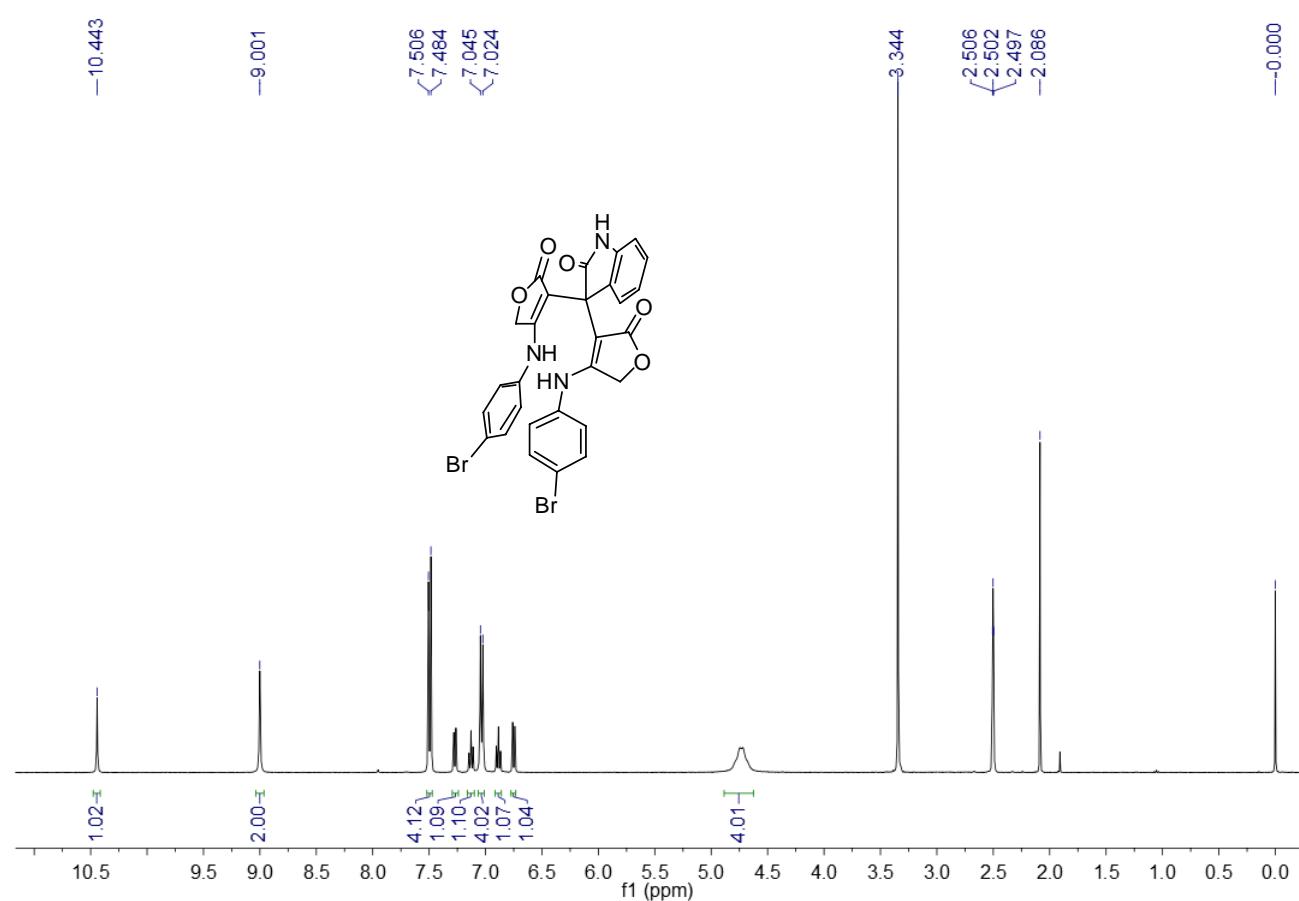


¹H NMR Spectrum of Compound 4b

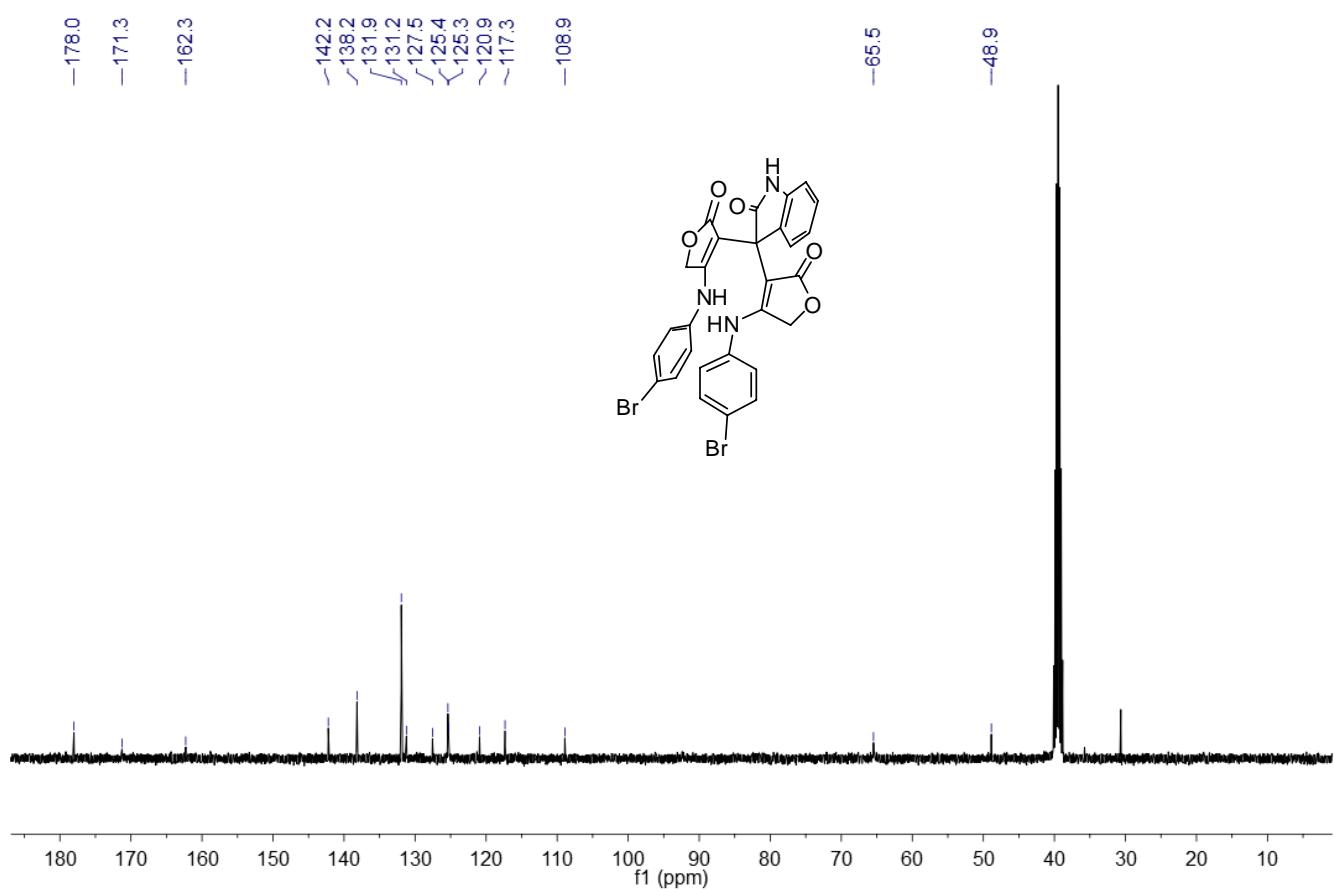


¹³C NMR Spectrum of Compound 4b

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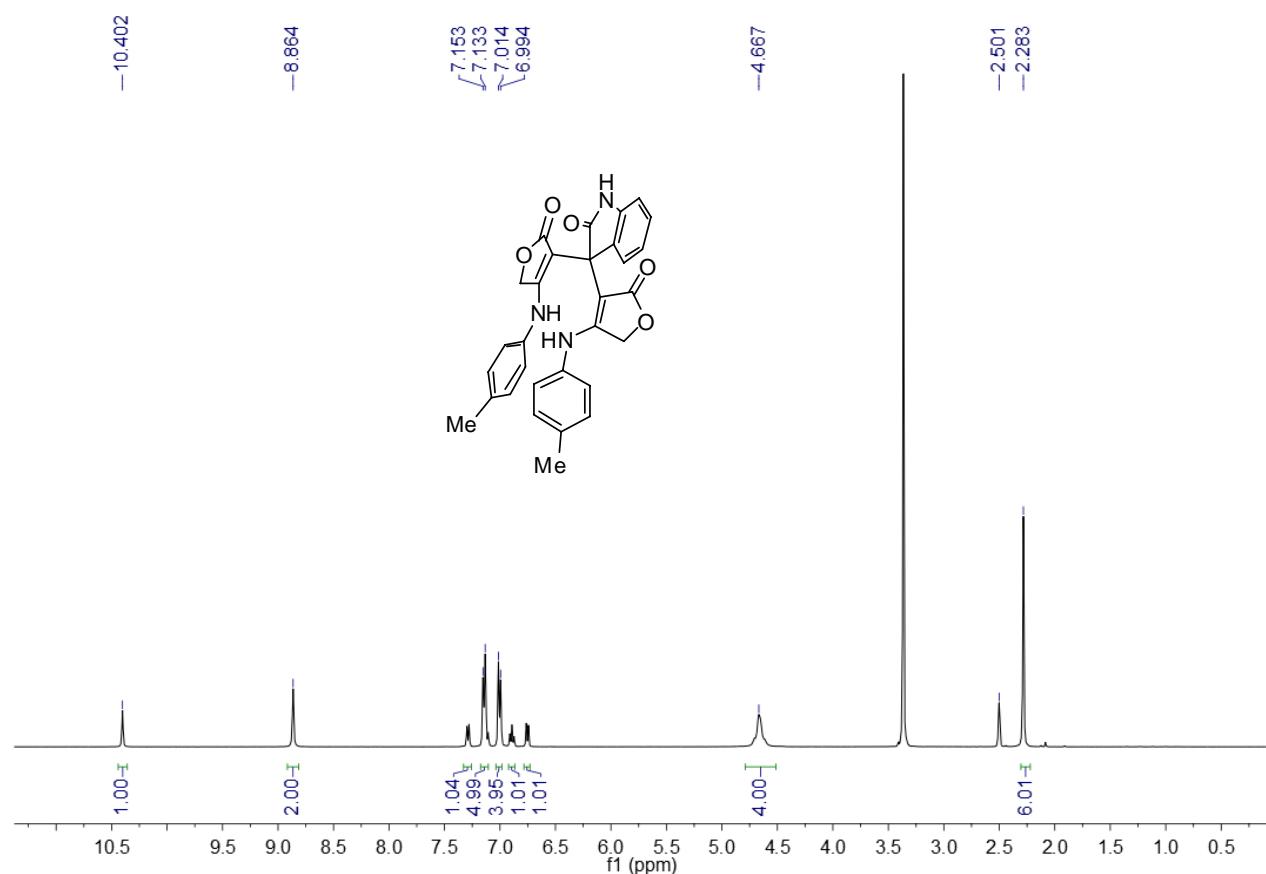


¹H NMR Spectrum of Compound 4c

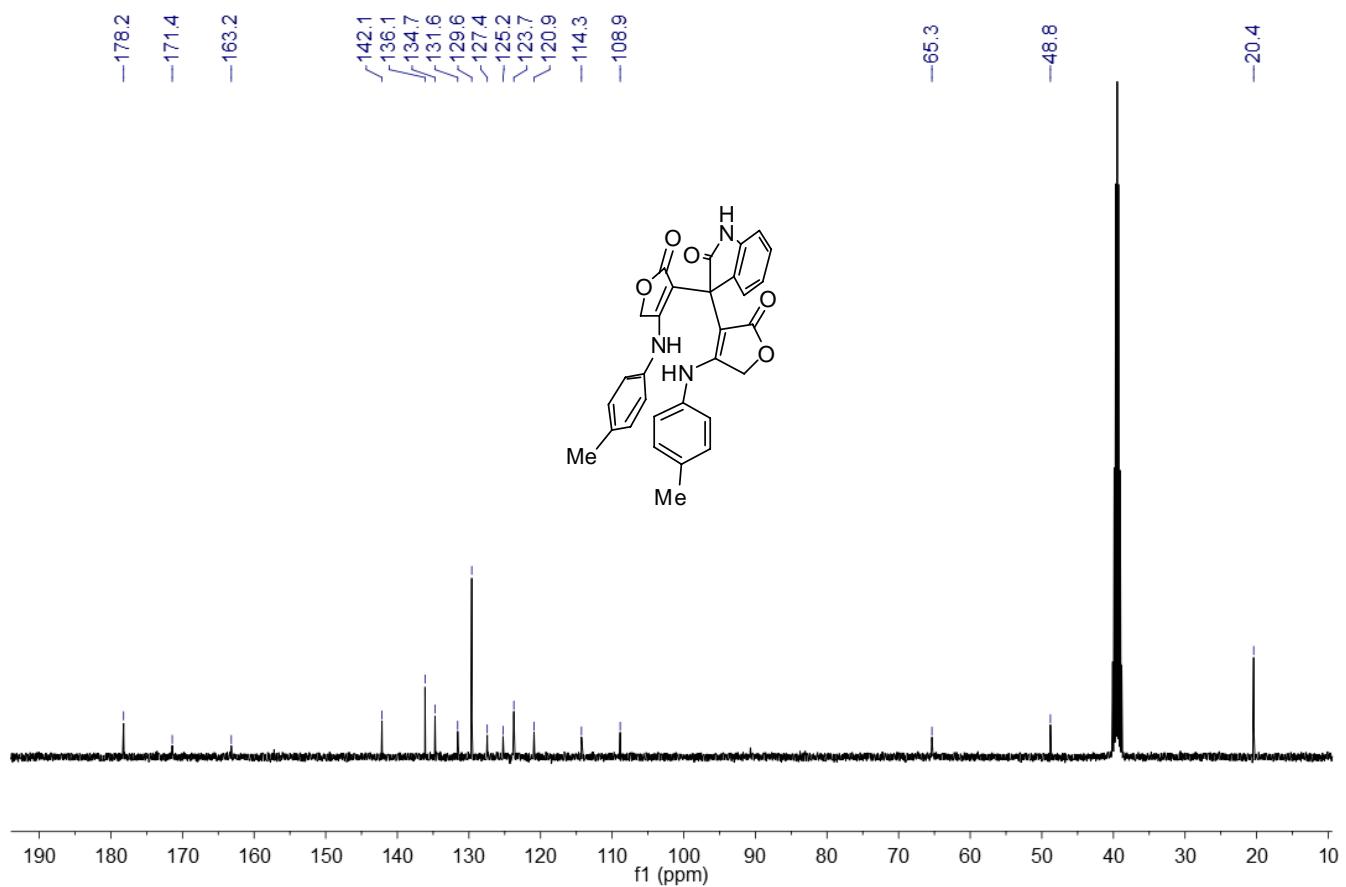


¹³C NMR Spectrum of Compound 4c

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¹H NMR Spectrum of Compound 4d



¹³C NMR Spectrum of Compound 4d