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Supplementary Material

A TELESCOPIC METHOD FOR THE SYNTHESIS OF 3-INDOLYL AZO DERIVATIVES

Rongfei Liu[a,#], Yiwen Huo[a,#], Qinjiang Zhou[a], Yue Liu[b,*] and Jinxing Hu[a,*]
[a]School of Pharmacy, Shandong Second Medical University, 261053 Weifang, Shandong, PR China
[b]School of Basic Medical Sciences, Shandong Second Medical University, 261053 Weifang, Shandong, PR China

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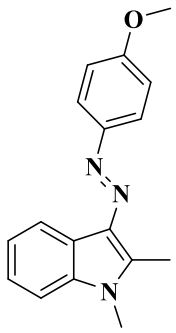
*e-mail: liuyue@sdsmu.edu.cn; jinxinghu2013@sdsmu.edu.cn

ORCID:
Hu Jinxing: https://orcid.org/0000-0002-1533-7146

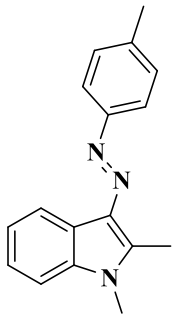
Spectral data of products



4a

*3-((4-Methoxyphenyl)diazenyl)-1,2-dimethyl-1H-indole (**4a**)*

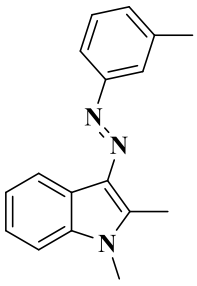
Yield: 77%; yellow solid; m.p. 124.7-126.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60-8.49 (m, 1H), 7.87 (d, *J* 8.8 Hz, 2H), 7.29 (d, *J* 8.5 Hz, 3H), 6.99 (d, *J* 8.8 Hz, 2H), 3.88 (s, 3H), 3.75 (s, 3H), 2.81 (s, 3H); ^{13C} NMR (101 MHz, $CDCl_3$) δ 160.11, 136.15, 132.04, 129.36, 124.80, 123.82, 122.80, 122.21, 118.76, 114.35, 113.98, 113.89, 111.83, 55.60, 55.16, 11.79; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{17}H_{18}N_3O$ $[M + H]^+$: 280.1450, found: 280.1455.



4b

*1,2-Dimethyl-3-(p-tolyldiazenyl)-1H-indole (**4b**)*

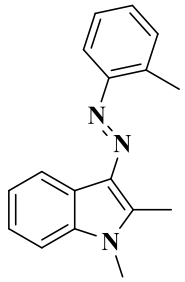
Yield: 71%; yellow solid; m.p. 152.9-154.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (dd, *J* 5.4, 3.2 Hz, 1H), 7.79 (d, *J* 8.1 Hz, 2H), 7.28 (dd, *J* 6.2, 4.5 Hz, 4H), 7.25-7.21 (m, 1H), 3.75 (s, 3H), 2.81 (s, 3H), 2.41 (s, 3H); ^{13C} NMR (101 MHz, $CDCl_3$) δ 152.30, 144.55, 138.33, 136.86, 132.24, 129.54, 123.07, 122.70, 122.53, 121.52, 119.06, 108.80, 29.82, 21.39, 10.14; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{17}H_{18}N_3$ $[M + H]^+$: 264.1501, found: 264.1506.



4c

*1,2-Dimethyl-3-(m-tolyldiazenyl)-1H-indole (**4c**)*

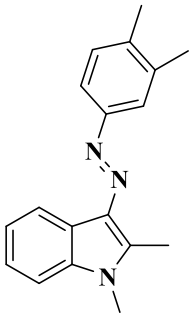
Yield: 68%; yellow solid; m.p. 139.3-140.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61-8.52 (m, 1H), 7.69 (d, *J* 7.8 Hz, 2H), 7.39-7.26 (m, 4H), 7.15 (d, *J* 7.2 Hz, 1H), 3.77 (s, 3H), 2.84 (s, 3H), 2.45 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.36, 144.87, 138.61, 136.88, 132.42, 129.09, 128.70, 123.14, 122.80, 122.57, 122.18, 119.04, 118.84, 108.82, 29.85, 21.55, 10.19; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{17}H_{18}N_3$ $[M + H]^+$: 264.1501, found: 264.1505.



4d

*1,2-Dimethyl-3-(o-tolyldiazenyl)-1H-indole (**4d**)*

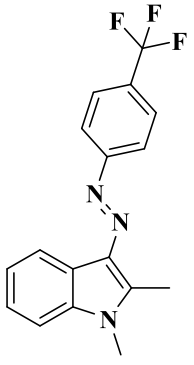
Yield: 64%; yellow solid; m.p. 132.5-133.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53-8.45 (m, 1H), 7.71 (d, *J* 6.9 Hz, 1H), 7.35-7.28 (m, 4H), 7.24 (s, 2H), 3.78 (s, 3H), 2.85 (s, 3H), 2.76 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.35, 144.83, 136.88, 136.00, 133.22, 130.93, 128.23, 126.29, 123.14, 122.90, 122.39, 118.95, 114.89, 108.85, 29.84, 18.24, 10.18; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{17}H_{18}N_3$ $[M + H]^+$: 264.1501, found: 264.1505.



4e

*3-((3,4-Dimethylphenyl)diazenyl)-1,2-dimethyl-1H-indole (**4e**)*

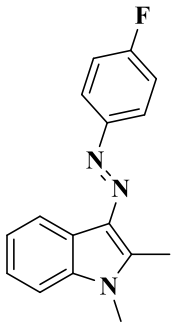
Yield: 46%; yellow solid; m.p. 160.5-161.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (dd, *J* 5.5, 3.2 Hz, 1H), 7.74-7.57 (m, 2H), 7.33-7.26 (m, 3H), 7.22 (d, *J* 8.0 Hz, 1H), 3.75 (s, 3H), 2.82 (s, 3H), 2.34 (d, *J* 16.1 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.09, 137.05, 136.92, 132.17, 130.09, 123.16, 122.78, 122.65, 119.02, 108.86, 29.87, 20.03, 19.74, 10.20; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{18}H_{20}N_3$ $[M + H]^+$: 278.1657, found: 278.1661.



4f

*1,2-Dimethyl-3-((4-(trifluoromethyl)phenyl)diazenyl)-1H-indole (**4f**)*

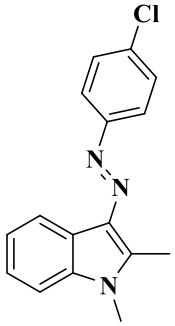
Yield: 88%; yellow solid; m.p. 157.5-158.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63-8.44 (m, 1H), 7.94 (d, *J* 8.2 Hz, 2H), 7.71 (d, *J* 8.3 Hz, 2H), 7.36-7.28 (m, 3H), 3.79 (s, 3H), 2.84 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.49, 146.56, 137.06, 132.92, 129.81, 129.50, 129.18, 128.85, 126.07, 126.04, 126.00, 125.96, 125.78, 123.58, 123.31, 123.08, 122.58, 121.68, 118.84, 109.00, 29.96, 10.20; ^{19}F NMR (377 MHz, $CDCl_3$) δ –114.59, –115.27, –116.06; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{17}H_{15}N_3F_3$ $[M + H]^+$: 318.1218, found: 318.1223.



4g

*3-((4-Fluorophenyl)diazenyl)-1,2-dimethyl-1H-indole (**4g**)*

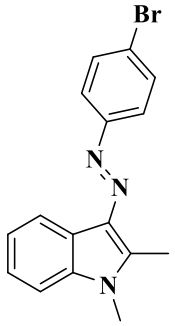
Yield: 56%; yellow solid; m.p. 140.7-141.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63-8.46 (m, 1H), 7.87 (dd, *J* 8.7, 5.4 Hz, 2H), 7.31 (d, *J* 7.1 Hz, 3H), 7.15 (t, *J* 8.6 Hz, 2H), 3.77 (s, 3H), 2.82 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.97, 161.51, 150.78, 145.02, 136.89, 132.22, 123.23, 123.17, 123.08, 122.86, 122.47, 118.96, 115.75, 115.52, 108.88, 29.85, 10.13; ^{19}F NMR (377 MHz, $CDCl_3$) δ –114.05; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{16}H_{15}N_3F$ $[M + H]^+$: 268.1250, found: 268.1255.



4h

*3-((4-Chlorophenyl)diazenyl)-1,2-dimethyl-1H-indole (**4h**)*

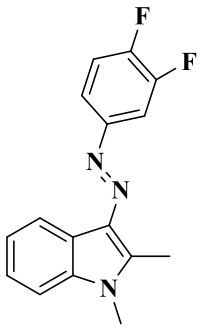
Yield: 29%; yellow solid; m.p. 132.4-134.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59-8.44 (m, 1H), 7.82 (d, *J* 8.6 Hz, 2H), 7.42 (d, *J* 8.6 Hz, 2H), 7.35-7.27 (m, 3H), 3.77 (s, 3H), 2.82 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.74, 145.60, 136.97, 133.57, 132.43, 129.01, 123.36, 123.02, 122.80, 122.52, 118.92, 108.94, 29.90, 10.17; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{16}H_{15}N_3Cl$ $[M + H]^+$: 284.0955, found: 284.0958.



4i

*3-((4-Bromophenyl)diazenyl)-1,2-dimethyl-1H-indole (**4i**)*

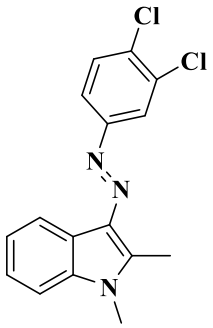
Yield: 28%; yellow solid; m.p. 159.4-161.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65-8.36 (m, 1H), 7.75 (d, *J* 8.6 Hz, 2H), 7.58 (d, *J* 8.6 Hz, 2H), 7.35-7.27 (m, 3H), 3.76 (s, 3H), 2.81 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.19, 145.55, 136.96, 132.50, 131.95, 123.35, 123.15, 123.02, 122.51, 121.82, 118.94, 108.92, 29.90, 10.18; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{16}H_{15}N_3Br$ $[M + H]^+$: 328.0449, found: 328.0454.



4j

*3-((3,4-Difluorophenyl)diazenyl)-1,2-dimethyl-1H-indole (**4j**)*

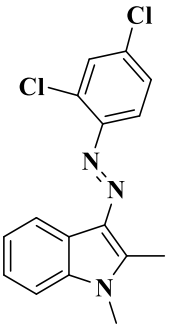
Yield: 63%; yellow solid; m.p. 157.9-158.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53-8.47 (m, 1H), 7.75-7.62 (m, 2H), 7.30 (dd, *J* 10.9, 4.1 Hz, 3H), 7.23 (d, *J* 9.0 Hz, 1H), 3.78 (s, 3H), 2.83 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.23, 152.09, 151.53, 151.40, 151.18, 149.76, 149.62, 149.05, 148.92, 145.77, 136.98, 132.26, 123.43, 123.09, 122.45, 119.73, 119.70, 119.67, 119.64, 118.88, 117.10, 116.91, 108.96, 108.22, 108.04, 29.91, 10.15; ^{19}F NMR (377 MHz, $CDCl_3$) δ –137.00, –138.34; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{16}H_{14}N_3F_2$ $[M + H]^+$: 286.1156, found: 286.1160.



4k

*3-((3,4-Dichlorophenyl)diazenyl)-1,2-dimethyl-1H-indole (**4k**)*

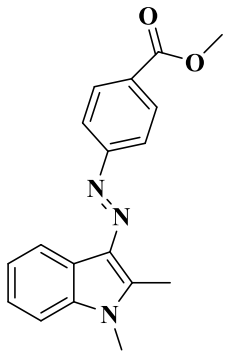
Yield: 50%; yellow solid; m.p. 132.1-132.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59-8.44 (m, 1H), 7.96 (d, *J* 1.6 Hz, 1H), 7.73 (d, *J* 8.4 Hz, 1H), 7.53 (d, *J* 8.5 Hz, 1H), 7.31 (dd, *J* 9.8, 3.6 Hz, 3H), 3.78 (s, 3H), 2.83 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.56, 146.28, 137.05, 132.94, 132.62, 131.27, 130.52, 123.56, 123.26, 122.55, 122.33, 121.82, 118.86, 109.00, 29.98, 10.24; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{16}H_{14}N_3Cl_2$ $[M + H]^+$: 318.0565, found: 318.0570.



4l

*3-((2,4-Dichlorophenyl)diazenyl)-1,2-dimethyl-1H-indole (**4l**)*

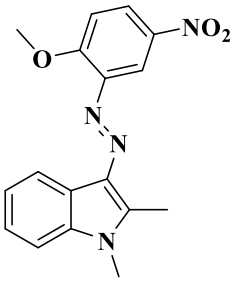
Yield: 34%; yellow solid; m.p. 179.7-180.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* 5.9 Hz, 1H), 7.81 (d, *J* 8.7 Hz, 1H), 7.58 (d, *J* 1.8 Hz, 1H), 7.43-7.31 (m, 4H), 3.81 (s, 3H), 2.86 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.77, 146.37, 137.07, 134.01, 133.82, 133.53, 129.94, 127.40, 123.67, 122.85, 118.86, 117.62, 108.88, 29.99, 10.21; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{16}H_{14}N_3Cl_2$ $[M + H]^+$: 318.0565, found: 318.0567.



4m

*Methyl-4-((1,2-dimethyl-1H-indol-3-yl)diazenyl)benzoate (**4m**)*

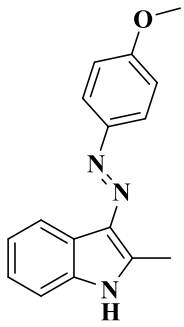
Yield: 37%; yellow solid; m.p. 189.6-190.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65-8.57 (m, 1H), 7.73 (d, *J* 7.8 Hz, 2H), 7.43-7.31 (m, 4H), 7.19 (d, *J* 7.2 Hz, 1H), 3.81 (s, 3H), 2.88 (s, 3H), 2.50 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.09, 157.33, 146.58, 137.08, 133.15, 130.53, 129.01, 123.57, 123.32, 122.66, 121.39, 118.86, 108.97, 52.12, 30.00, 10.25; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{18}H_{18}N_3O_2$ $[M + H]^+$: 308.1399, found: 308.1403.



4n

*3-((2-Methoxy-5-nitrophenyl)diazenyl)-1,2-dimethyl-1H-indole (**4n**)*

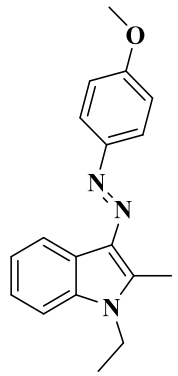
Yield: 30%; yellow solid; m.p. 229.6-230.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (d, *J* 2.7 Hz, 1H), 8.56-8.50 (m, 1H), 8.21 (dd, *J* 9.1, 2.7 Hz, 1H), 7.33 (d, *J* 5.0 Hz, 2H), 7.12 (d, *J* 9.1 Hz, 1H), 6.80 (d, *J* 8.8 Hz, 1H), 4.15 (s, 3H), 3.96 (s, 3H), 2.89 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.40, 146.86, 143.32, 141.91, 137.11, 133.94, 124.14, 123.71, 123.63, 122.58, 118.94, 111.75, 111.68, 108.97, 56.84, 30.08, 10.43; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{17}H_{17}N_4O_3$ $[M + H]^+$: 325.1301, found: 325.1304.



4o

*3-((4-Methoxyphenyl)diazenyl)-2-methyl-1H-indole(**4o**)*

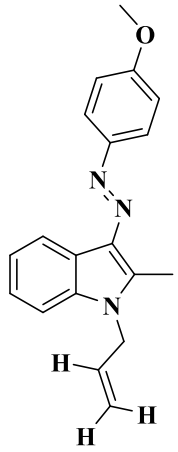
Yield: 47%; yellow solid; m.p. 138.6-138.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, *J* 6.1 Hz, 1H), 8.21 (s, 1H), 7.88 (d, *J* 8.2 Hz, 2H), 7.29 (s, 1H), 7.24-7.18 (m, 1H), 7.00 (d, *J* 8.2 Hz, 2H), 3.88 (s, 3H), 2.82 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.11, 136.15, 132.04, 129.36, 124.80, 123.82, 122.80, 122.21, 118.76, 114.35, 113.89, 111.83, 55.60, 11.79; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{16}H_{16}N_3O$ $[M + H]^+$: 266.1293, found: 266.1298.



4p

*1-Ethyl-3-((4-methoxyphenyl)diazenyl)-2-methyl-1H-indole (**4p**)*

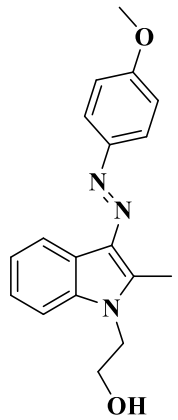
Yield: 81%; yellow solid; m.p. 109.5-110.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65-8.49 (m, 1H), 7.87 (d, *J* 8.8 Hz, 2H), 7.35-7.29 (m, 1H), 7.27 (s, 1H), 7.26-7.22 (m, 1H), 6.99 (d, *J* 8.8 Hz, 2H), 4.22 (q, *J* 7.2 Hz, 2H), 3.90-3.84 (m, 3H), 2.86-2.78 (m, 3H), 1.43 (t, *J* 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.97, 135.96, 132.02, 129.36, 123.37, 122.89, 122.85, 119.17, 114.09, 109.03, 55.55, 38.47, 14.88, 10.01; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{18}H_{20}N_3O$ $[M + H]^+$: 294.1606, found: 294.1609.



4q

*1-Allyl-3-((4-methoxyphenyl)diazenyl)-2-methyl-1H-indole (**4q**)*

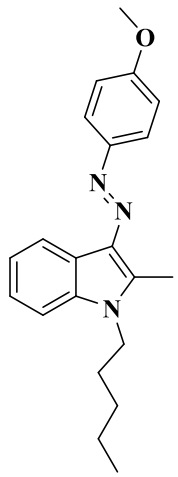
Yield: 60%; yellow solid; m.p. 111.0-111.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63-8.48 (m, 1H), 7.88 (d, *J* 8.8 Hz, 2H), 7.27 (s, 2H), 7.26-7.20 (m, 1H), 7.00 (d, *J* 8.8 Hz, 2H), 5.99 (ddd, *J* 14.8, 9.6, 4.4 Hz, 1H), 5.19 (d, *J* 10.4 Hz, 1H), 4.93 (d, *J* 17.1 Hz, 1H), 4.78 (d, *J* 2.4 Hz, 2H), 3.88 (s, 3H), 2.79 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.06, 148.36, 143.84, 136.31, 132.24, 132.03, 123.18, 123.02, 122.69, 122.62, 119.26, 116.93, 114.07, 109.15, 55.54, 45.58, 9.91; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{19}H_{20}N_3O$ $[M + H]^+$: 306.1606, found: 306.1610.



4r

*2-(3-((4-Methoxyphenyl)diazenyl)-2-methyl-1H-indol-1-yl)ethan-1-ol (**4r**)*

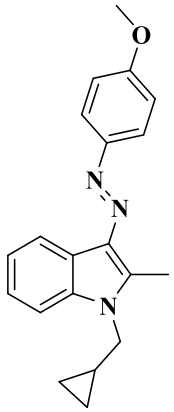
Yield: 39%; yellow solid; m.p. 104.7-105.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59-8.53 (m, 1H), 7.86 (d, *J* 8.9 Hz, 2H), 7.33 (d, *J* 8.7 Hz, 1H), 7.27 (d, *J* 7.0 Hz, 1H), 7.25 (s, 1H), 6.99 (d, *J* 8.9 Hz, 2H), 4.32 (t, *J* 5.3 Hz, 2H), 4.00 (t, *J* 5.3 Hz, 2H), 3.88 (s, 3H), 2.84 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.02, 136.44, 131.99, 123.39, 122.92, 122.79, 122.56, 119.15, 114.10, 109.35, 60.93, 55.55, 45.83, 10.39; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{18}H_{20}N_3O_2$ $[M + H]^+$: 310.1556 , found: 310.1560.



4s

*3-((4-Methoxyphenyl)diazenyl)-2-methyl-1-pentyl-1H-indole (**4s**)*

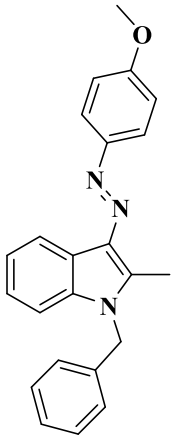
Yield: 62%; yellow solid; m.p. 99.8-99.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (dd, *J* 5.5, 3.2 Hz, 1H), 7.87 (d, *J* 8.8 Hz, 2H), 7.30 (dd, *J* 13.6, 10.6 Hz, 2H), 7.24 (s, 1H), 6.99 (d, *J* 8.8 Hz, 2H), 4.14 (t, *J* 7.4 Hz, 2H), 3.88 (s, 3H), 2.82 (s, 3H), 1.82 (d, *J* 6.6 Hz, 2H), 1.38 (d, *J* 3.1 Hz, 4H), 0.92 (d, *J* 6.7 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.95, 148.23, 144.10, 136.24, 132.07, 123.07, 122.92, 122.68, 122.61, 119.23, 114.06, 109.18, 55.54, 43.72, 29.51, 29.14, 22.45, 13.99, 10.18; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{21}H_{26}N_3O$ $[M + H]^+$: 336.2076, found: 336.2080.



4t

*1-(Cyclopropylmethyl)-3-((4-methoxyphenyl)diazenyl)-2-methyl-1H-indole (**4t**)*

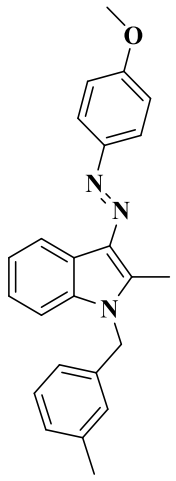
Yield: 88%; yellow solid; m.p. 145.2-147.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60-8.54 (m, 1H), 7.87 (d, *J* 8.7 Hz, 2H), 7.39-7.32 (m, 1H), 7.27 (s, 1H), 7.25-7.23 (m, 1H), 7.00 (d, *J* 8.8 Hz, 2H), 4.09 (d, *J* 6.4 Hz, 2H), 3.88 (s, 3H), 2.84 (s, 3H), 1.27 (s, 1H), 0.60 (d, *J* 7.6 Hz, 2H), 0.41 (d, *J* 5.0 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.96, 148.72, 143.21, 136.47, 132.24, 122.98, 122.92, 122.52, 122.44, 119.29, 114.03, 109.26, 55.53, 47.47, 11.28, 10.35, 4.10; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{20}H_{22}N_3O$ $[M + H]^+$: 320.1763, found: 320.1768.



4u

*1-Benzyl-3-((4-methoxyphenyl)diazenyl)-2-methyl-1H-indole (**4u**)*

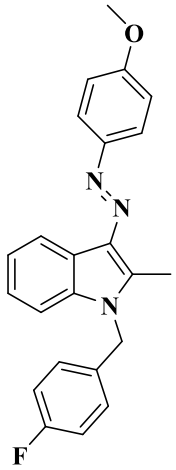
Yield: 42%; yellow solid; m.p. 142.2-143.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (d, *J* 7.5 Hz, 1H), 7.89 (d, *J* 8.8 Hz, 2H), 7.29 (dd, *J* 12.1, 4.3 Hz, 3H), 7.22 (dd, *J* 13.2, 6.3 Hz, 3H), 7.06 (d, *J* 7.0 Hz, 2H), 7.00 (d, *J* 8.7 Hz, 2H), 5.41 (s, 2H), 3.88 (s, 3H), 2.78 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.12, 148.62, 143.52, 136.62, 136.53, 132.46, 128.98, 128.28, 127.69, 126.03, 123.26, 123.08, 122.71, 122.60, 119.42, 114.06, 109.30, 55.54, 46.85, 10.17; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{23}H_{22}N_3O$ $[M + H]^+$: 356.1763, found: 356.1767.



4v

*3-((4-Methoxyphenyl)diazenyl)-2-methyl-1-(3-methylbenzyl)-1H-indole (**4v**)*

Yield: 33%; yellow solid; m.p. 126.5-128.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (d, *J* 7.5 Hz, 1H), 7.89 (d, *J* 8.8 Hz, 2H), 7.29 (s, 1H), 7.24-7.15 (m, 3H), 7.07 (d, *J* 7.5 Hz, 1H), 7.00 (d, *J* 8.8 Hz, 2H), 6.89-6.84 (m, 2H), 5.37 (s, 2H), 3.88 (s, 3H), 2.79 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.11, 148.65, 143.63, 138.78, 136.66, 136.50, 132.43, 128.88, 128.47, 126.61, 123.24, 123.13, 123.08, 122.69, 122.56, 119.41, 114.07, 109.36, 55.54, 46.85, 21.47, 10.20; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{24}H_{24}N_3O$ $[M + H]^+$: 370.1919, found: 370.1924.



4w

*1-(4-Fluorobenzyl)-3-((4-methoxyphenyl)diazenyl)-2-methyl-1H-indole (**4w**)*

Yield: 45%; yellow solid; m.p. 135.9-136.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (d, *J* 7.6 Hz, 1H), 7.89 (d, *J* 8.8 Hz, 2H), 7.30-7.25 (m, 2H), 7.22 (s, 1H), 7.05-6.95 (m, 6H), 5.37 (s, 2H), 3.88 (s, 3H), 2.77 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.45, 161.00, 160.20, 151.90, 148.43, 143.42, 136.47, 132.48, 132.23, 132.19, 127.74, 127.66, 123.38, 123.10, 122.84, 122.71, 119.44, 116.04, 115.82, 114.08, 109.20, 55.54, 46.22, 10.15; ^{19}F NMR (377 MHz, $CDCl_3$) δ –62.02; HRMS (ESI-Q-TOF, *m/z*) calcd. for $C_{23}H_{21}N_3OF$ $[M + H]^+$: 374.1669, found: 374.1673.

AttachedChart

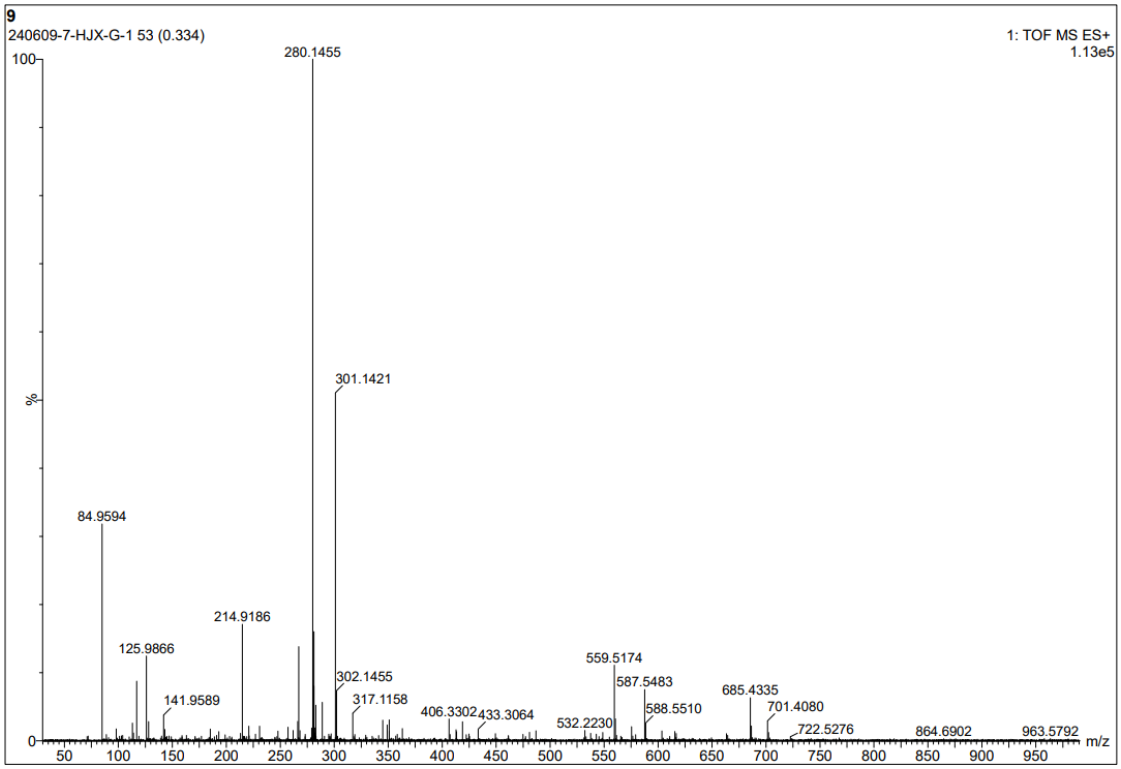
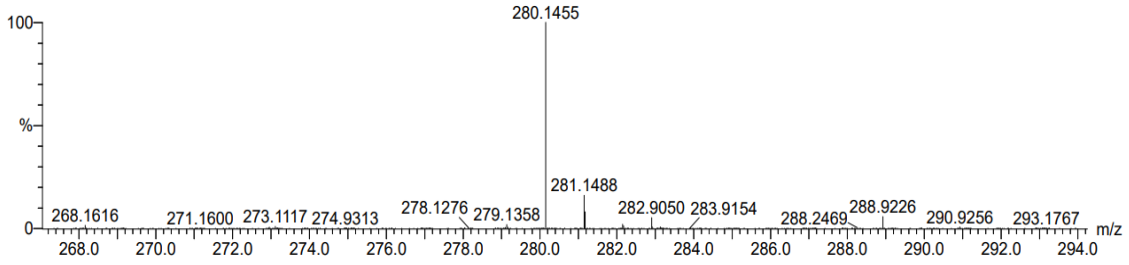


Figure 1S. *HR mass spectrum (ESI) of compound* ***4a***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
578 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 17-17 H: 18-18 N: 0-100 O: 0-100 Na: 0-3
9
240609-7-HJX-G-1 53 (0.334)



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
280.1455	280.1450	0.5	1.8	10.5	442.4	n/a	n/a	C17 H18 N3 O

Figure 2S. *HR mass spectrum (ESI) of compound* ***4a***

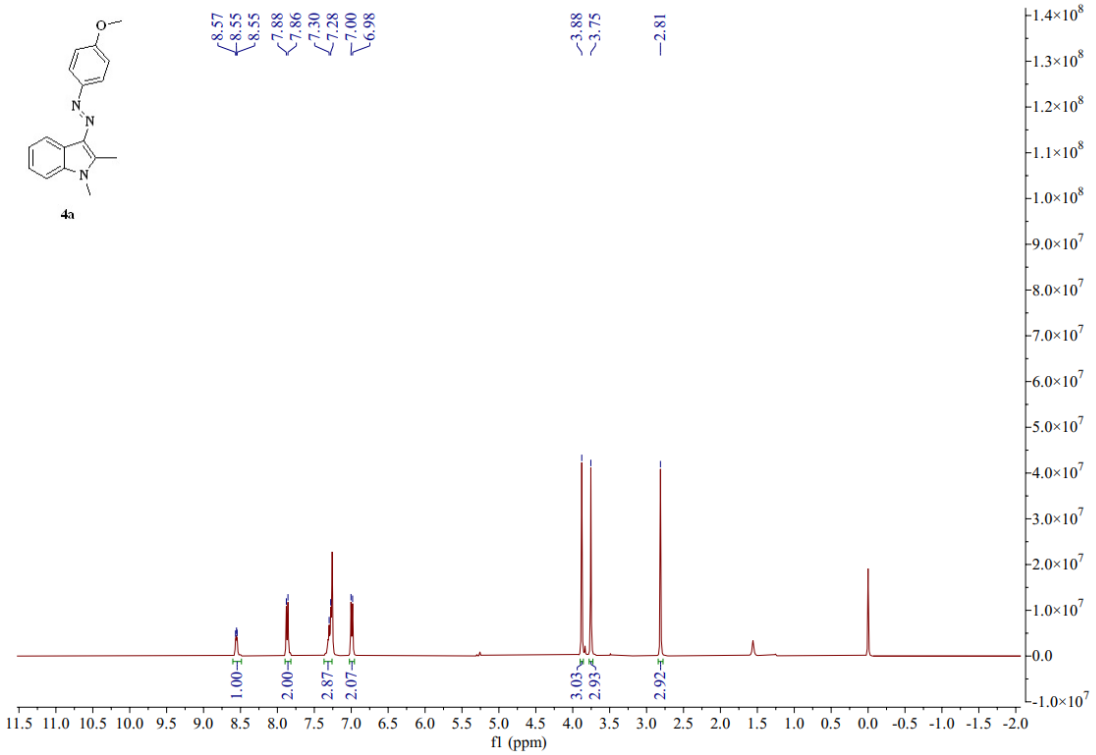


Figure 3S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4a***

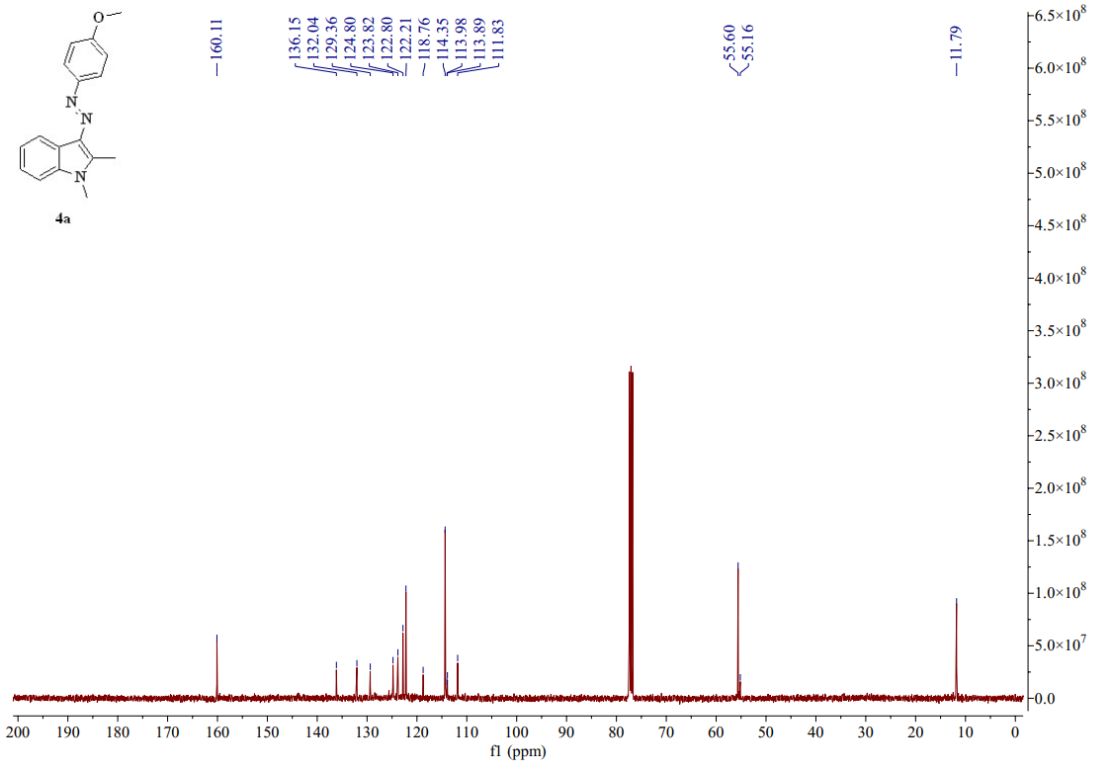


Figure 4S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4a***

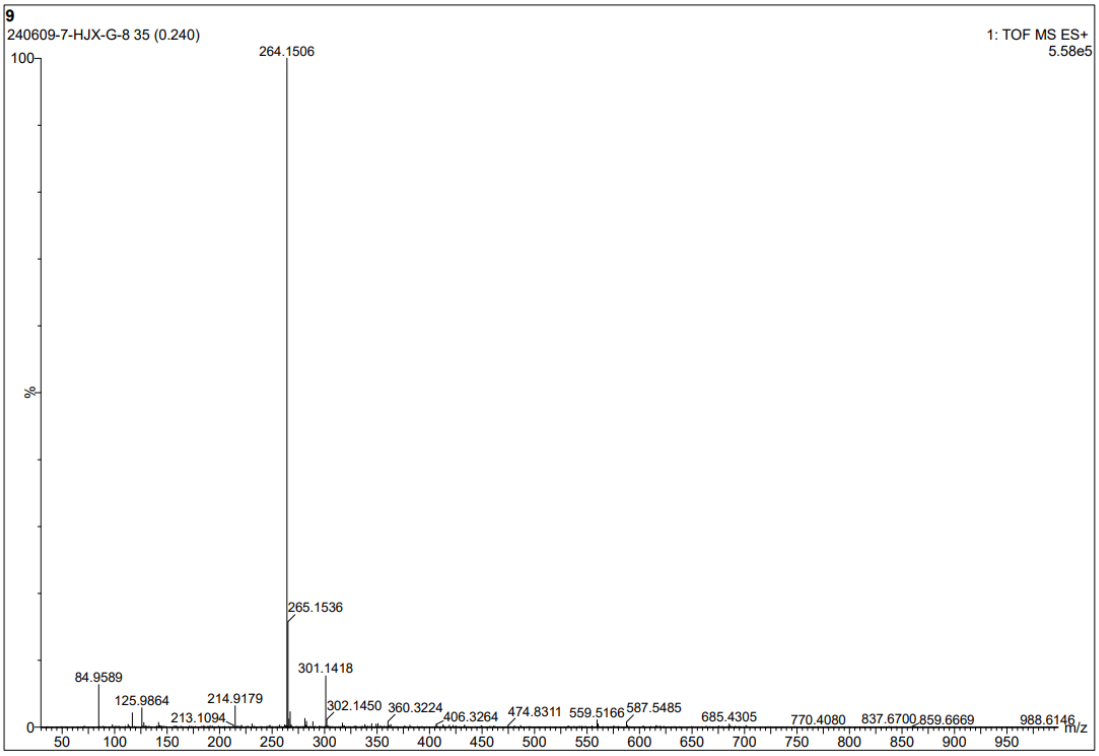
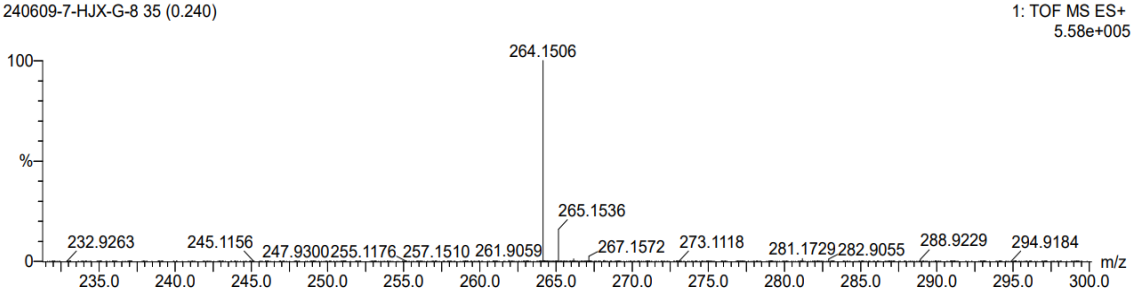


Figure 5S. *HR mass spectrum (ESI) of compound* ***4b***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
518 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 17-17 H: 18-18 N: 0-100 O: 0-100 Na: 0-3
9
240609-7-HJX-G-8 35 (0.240)



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
264.1506	264.1501	0.5	1.9	10.5	704.9	n/a	n/a	C17 H18 N3

Figure 6S. *HR mass spectrum (ESI) of compound* ***4b***

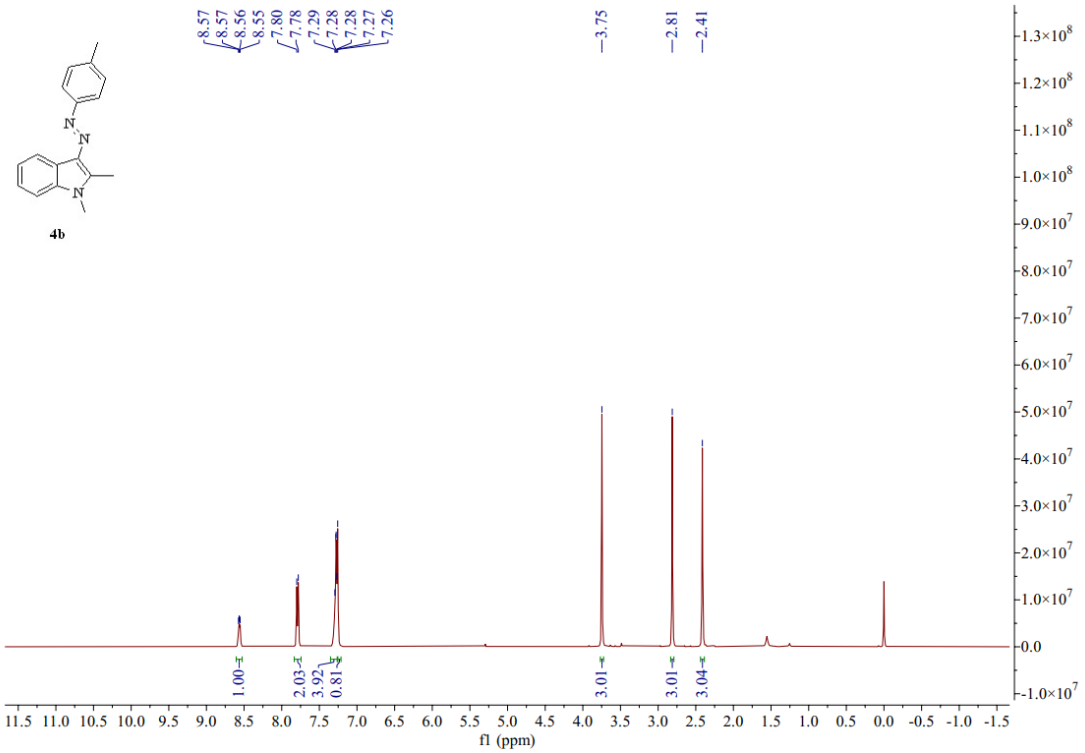


Figure 7S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4b***

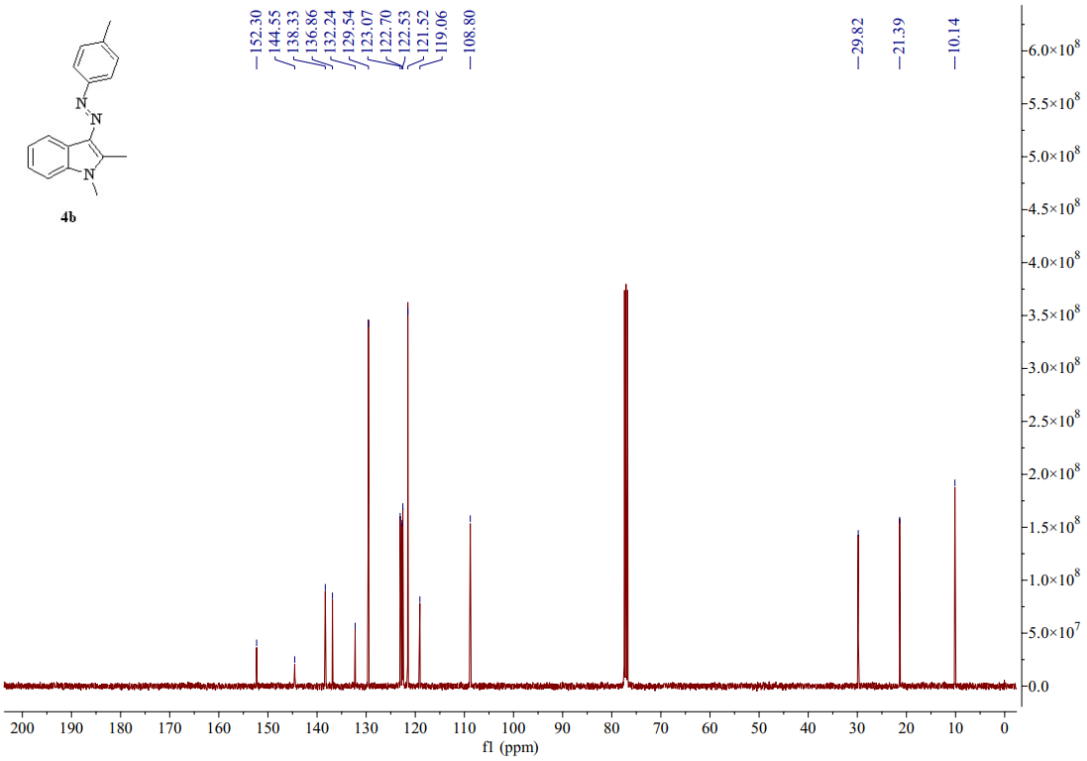


Figure 8S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4b***

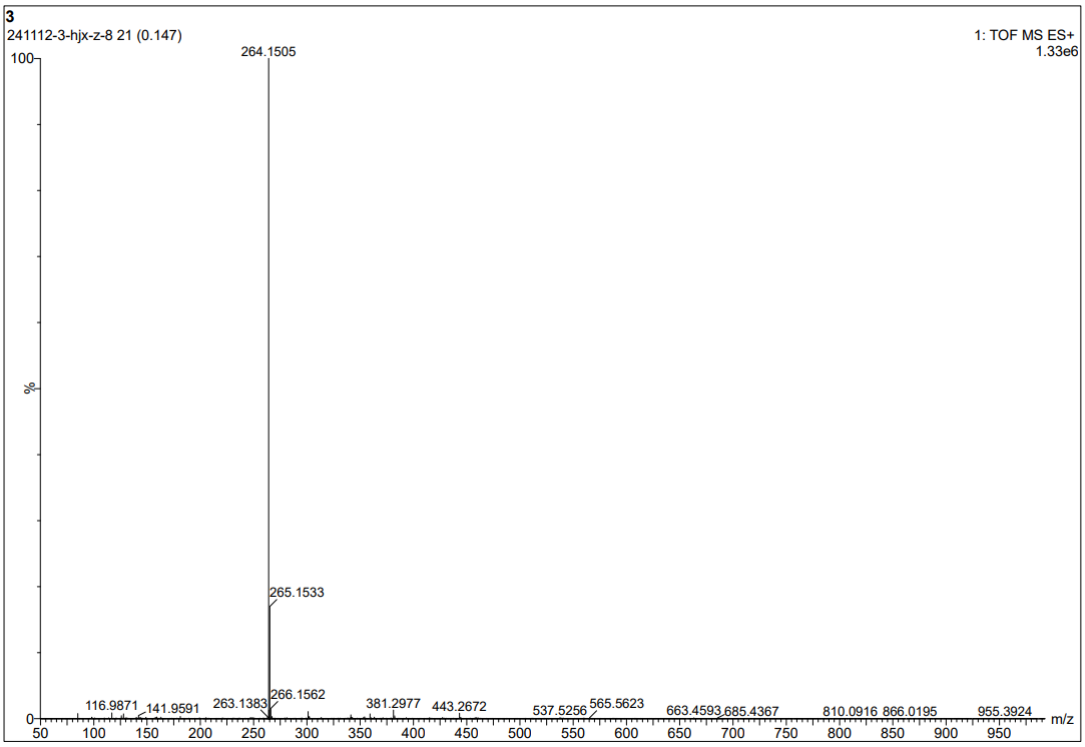
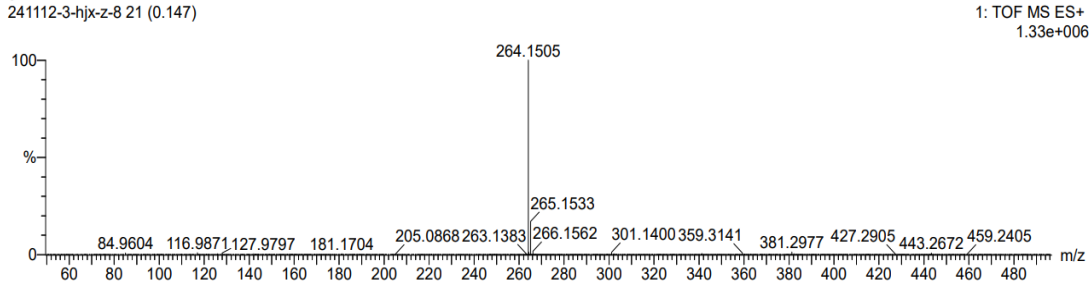


Figure 9S. *HR mass spectrum (ESI) of compound* ***4c***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
161 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 17-17 H: 18-18 N: 0-100 O: 0-100



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
264.1505	264.1501	0.4	1.5	10.5	992.1	n/a	n/a	C17 H18 N3

Figure 10S. *HR mass spectrum (ESI) of compo und* ***4c***

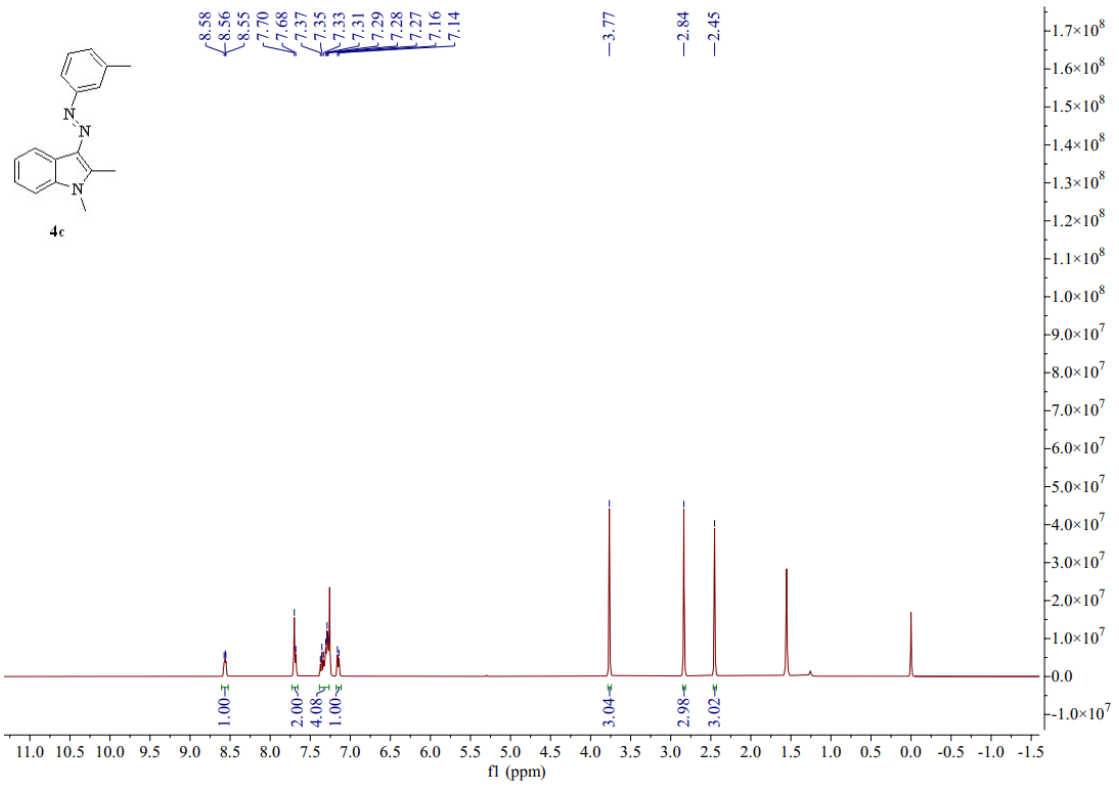


Figure 11S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4c***

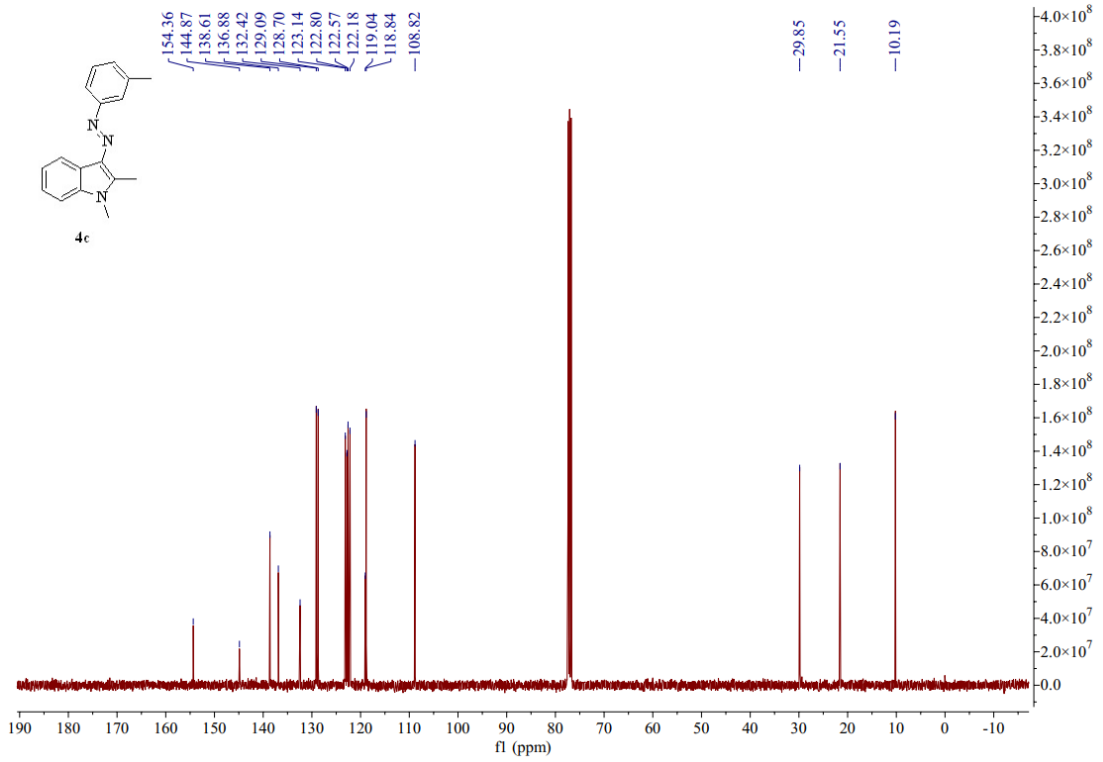


Figure 12S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4c***

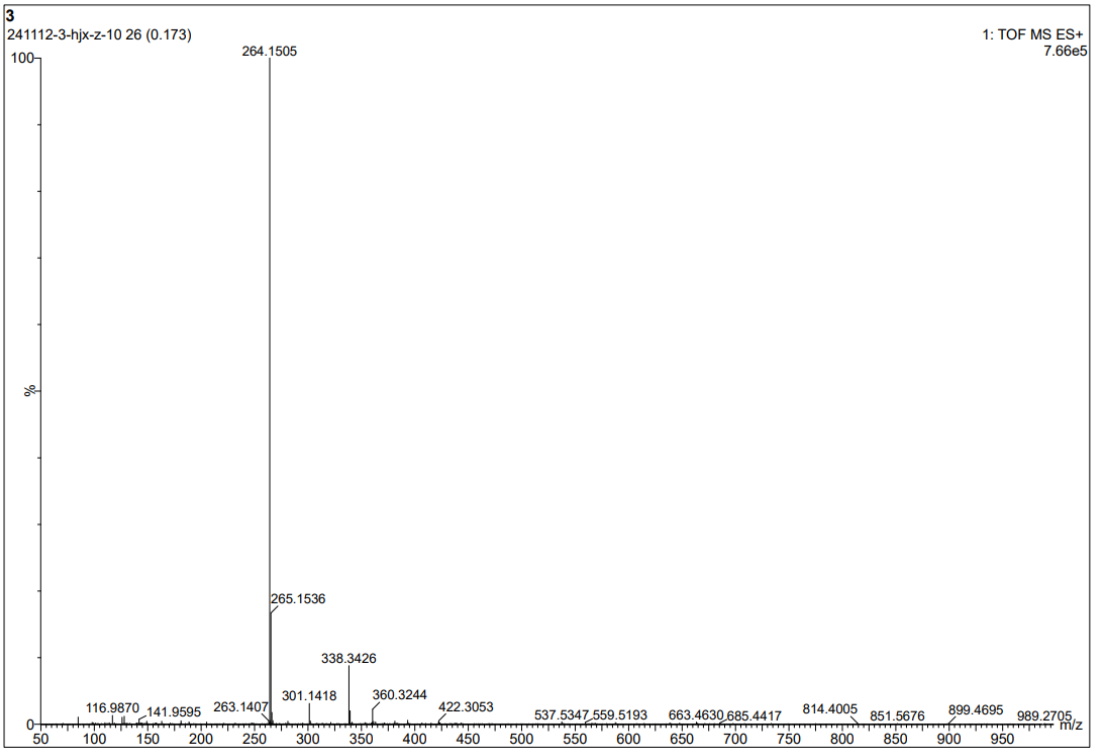
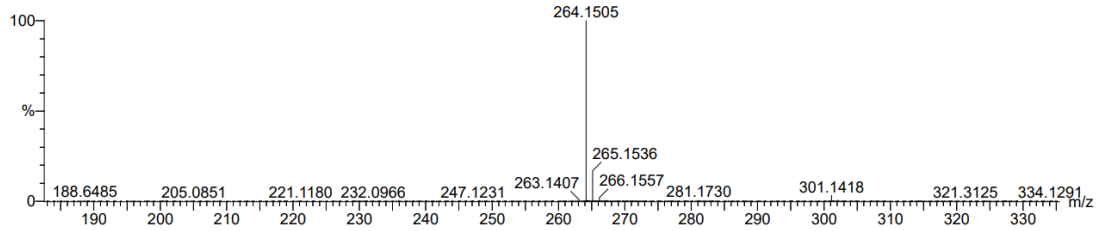


Figure 13S. *HR mass spectrum (ESI) of compound* ***4d***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
161 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 17-17 H: 18-18 N: 0-100 O: 0-100
3
241112-3-hjx-z-10 26 (0.173)
1: TOF MS ES+
7.66e+005



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
264.1505	264.1501	0.4	1.5	10.5	873.1	n/a	n/a	C17 H18 N3

Figure 14S. *HR mass spectrum (ESI) of compound* ***4d***

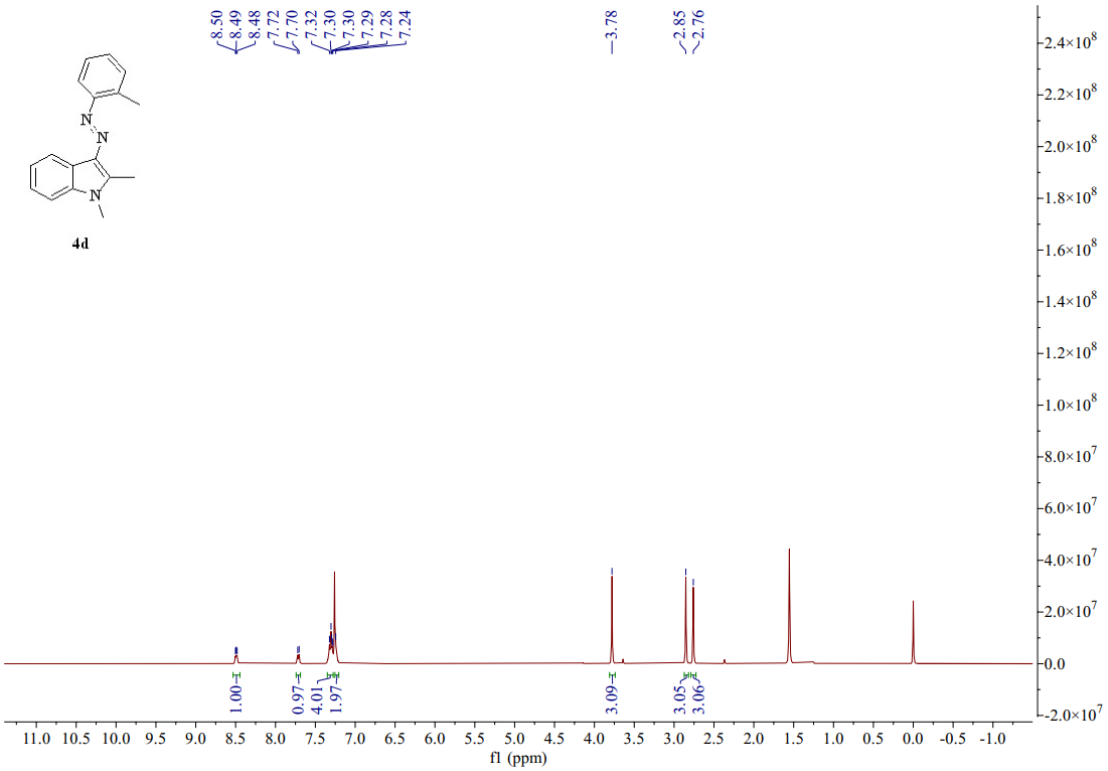


Figure 15S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4d***

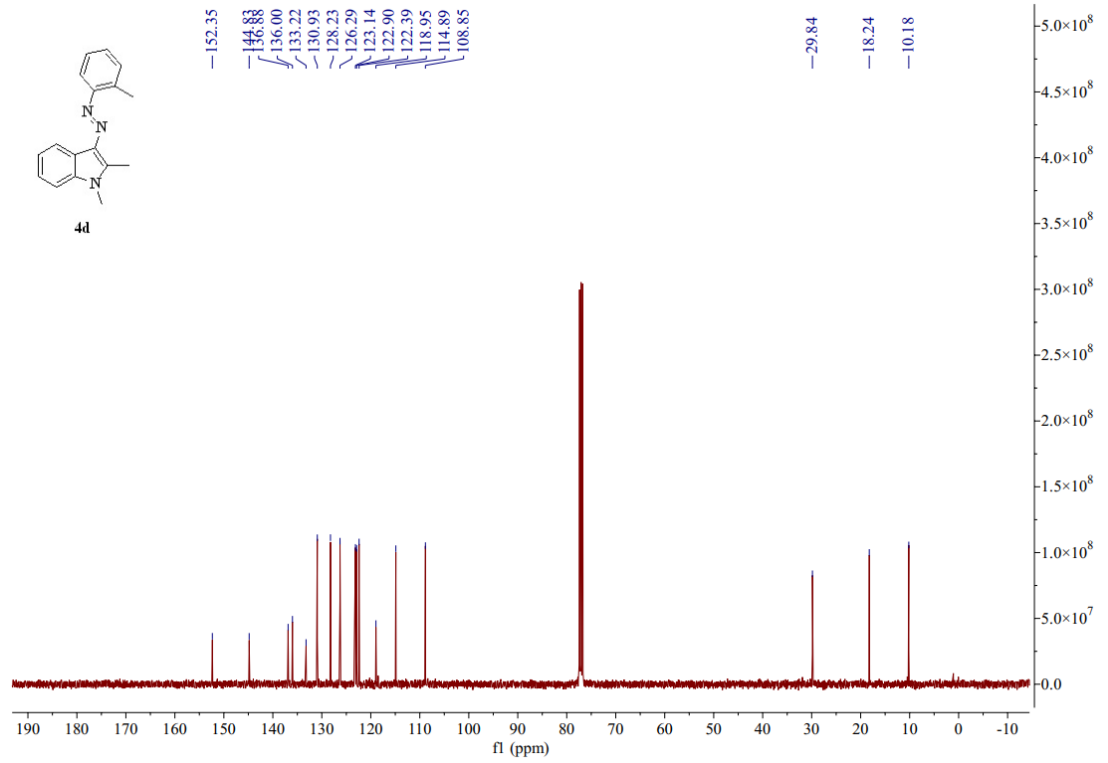


Figure 16S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4d***

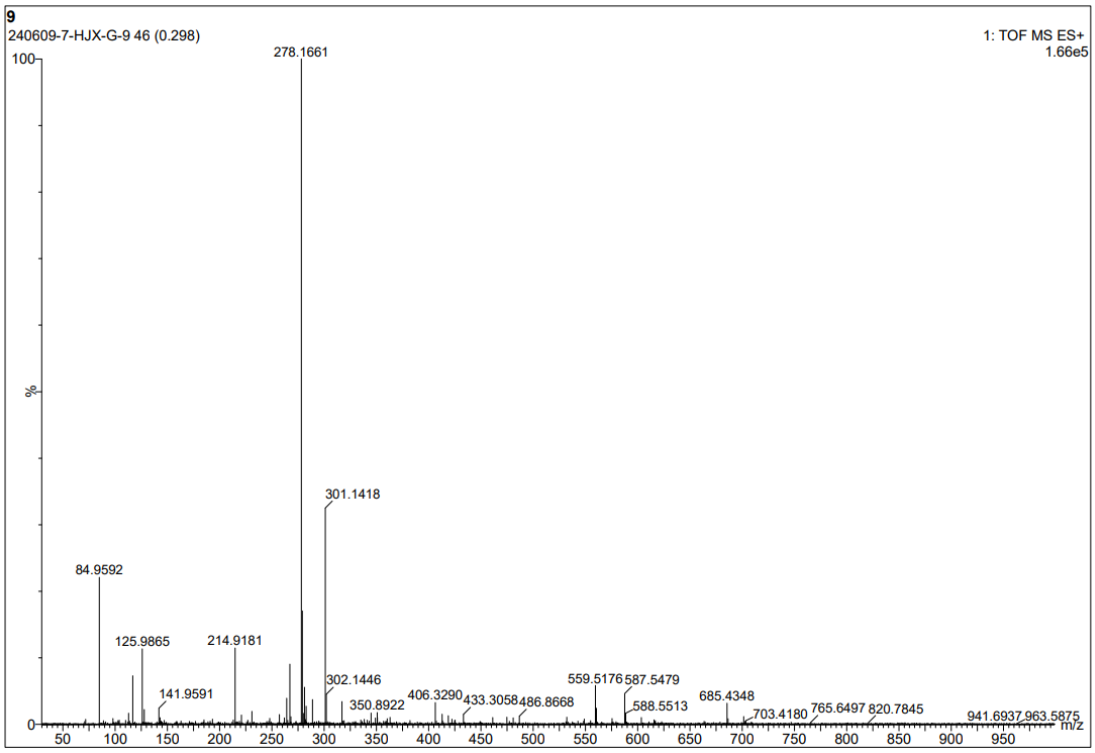
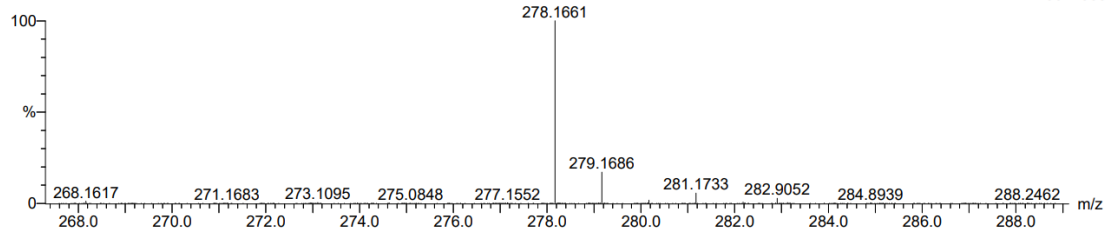


Figure 17S. *HR mass spectrum (ESI) of compound* ***4e***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
579 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 18-18 H: 20-20 N: 0-100 O: 0-100 Na: 0-3
9
240609-7-HJX-G-9 46 (0.298)
1: TOF MS ES+
1.66e+005



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
278.1661	278.1657	0.4	1.4	10.5	527.0	n/a	n/a	C18 H20 N3

Figure 18S. *HR mass spectrum (ESI) of compound* ***4e***

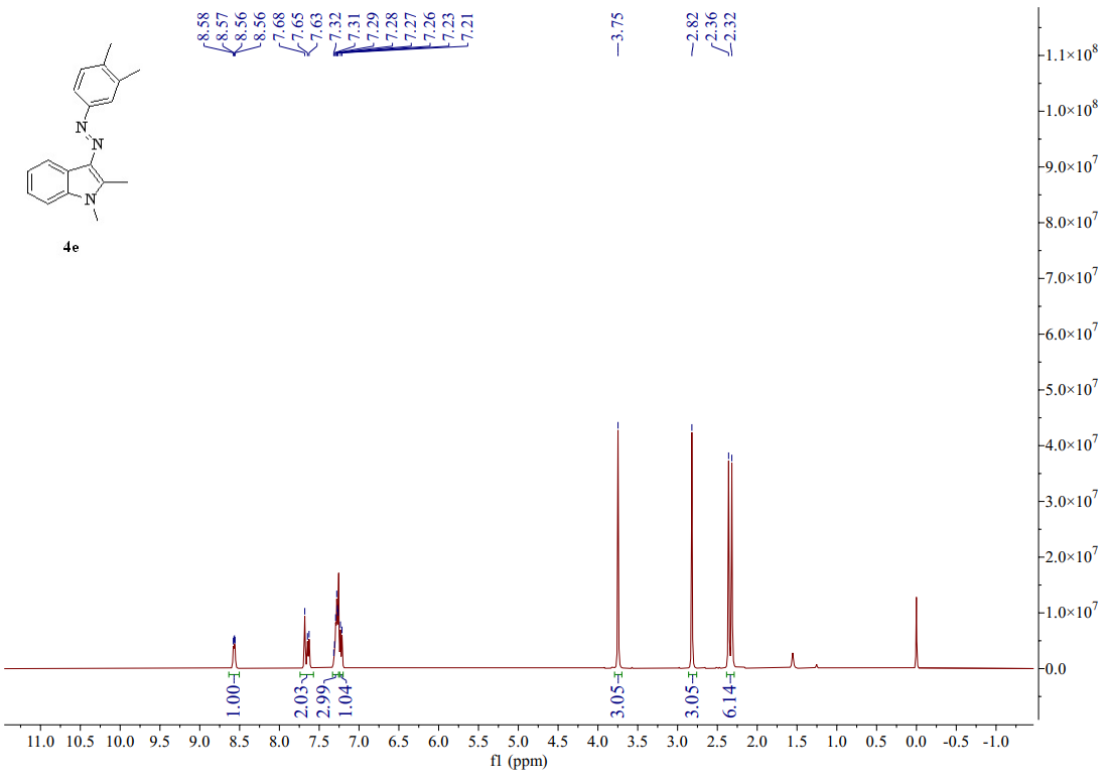


Figure 19S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4e***

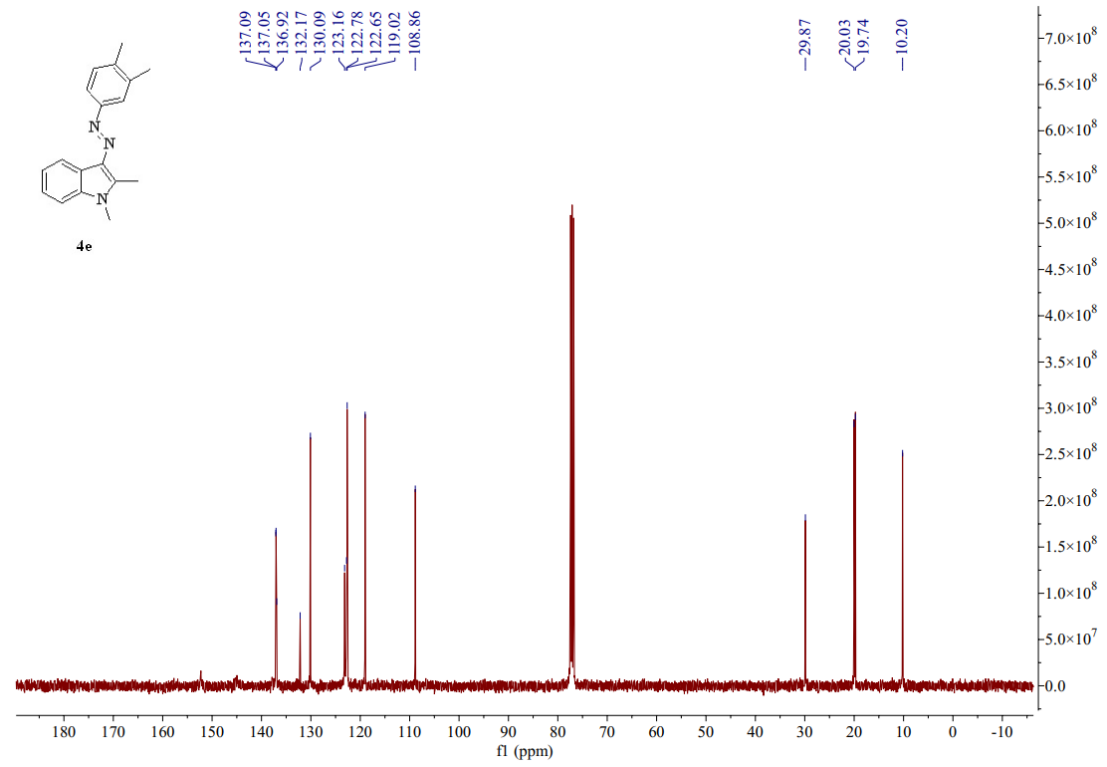


Figure 20S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4e***

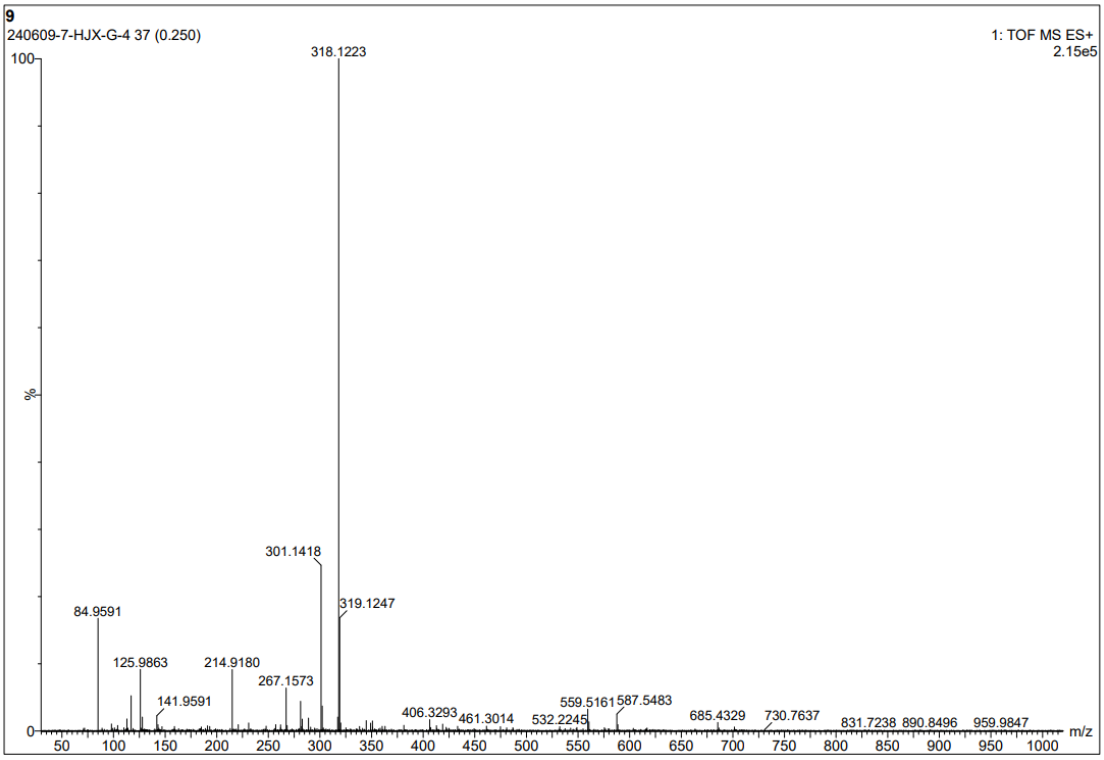
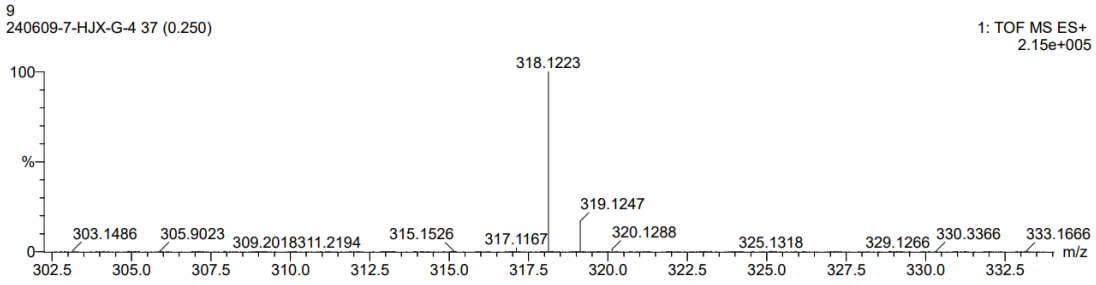


Figure 21S. *HR mass spectrum (ESI) of compound* ***4f***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1733 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 17-17 H: 15-15 N: 0-100 O: 0-100 Na: 0-3 F: 1-3



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
318.1223	318.1218	0.5	1.6	10.5	499.6	n/a	n/a	C17 H15 N3 F3

Figure 22S. *HR mass spectrum (ESI) of compound* ***4f***

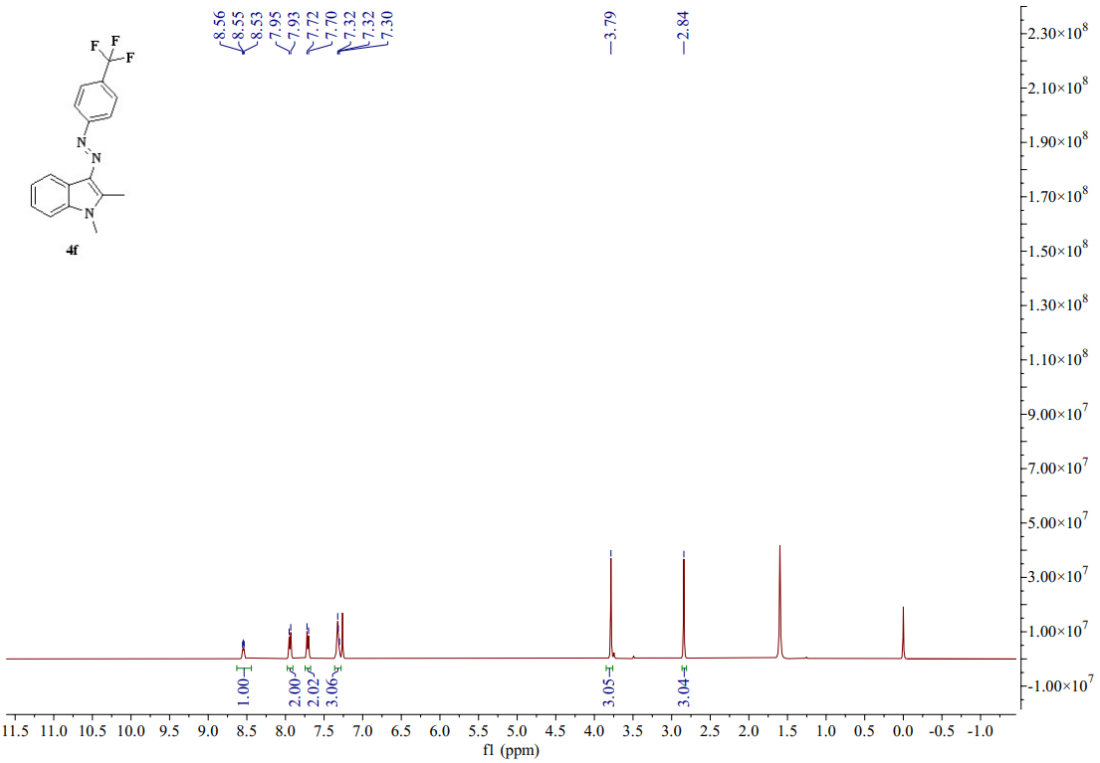


Figure 23S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4f***

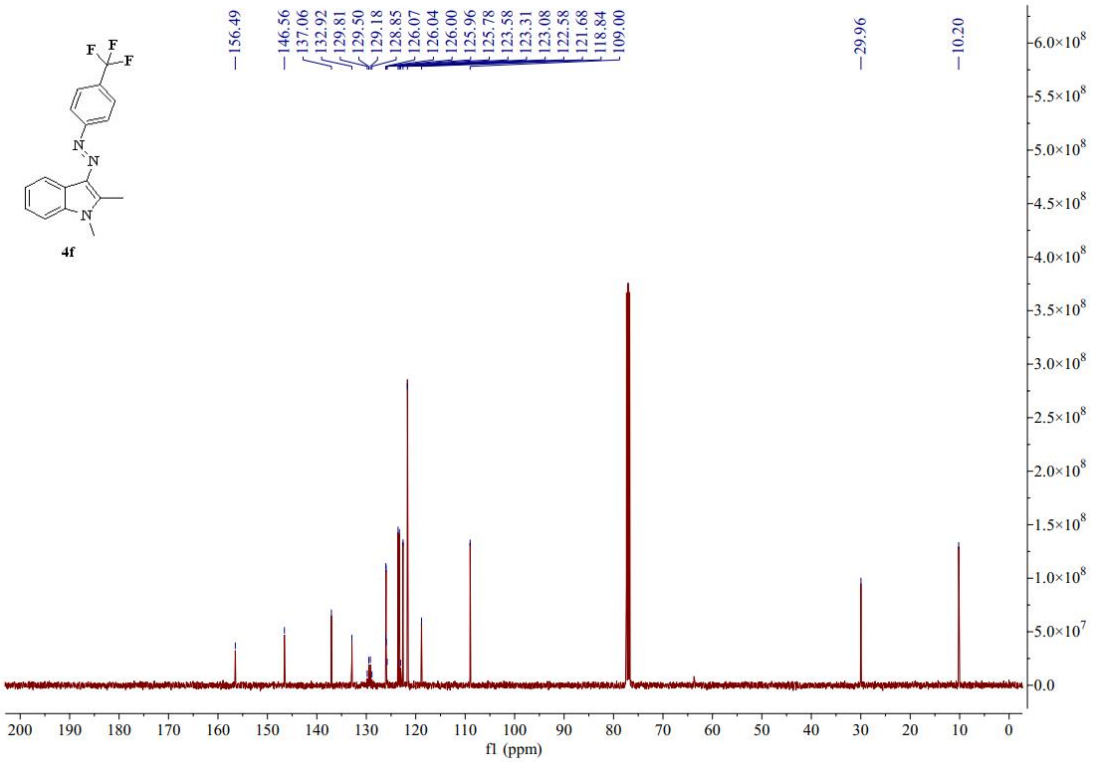


Figure 24S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4f***

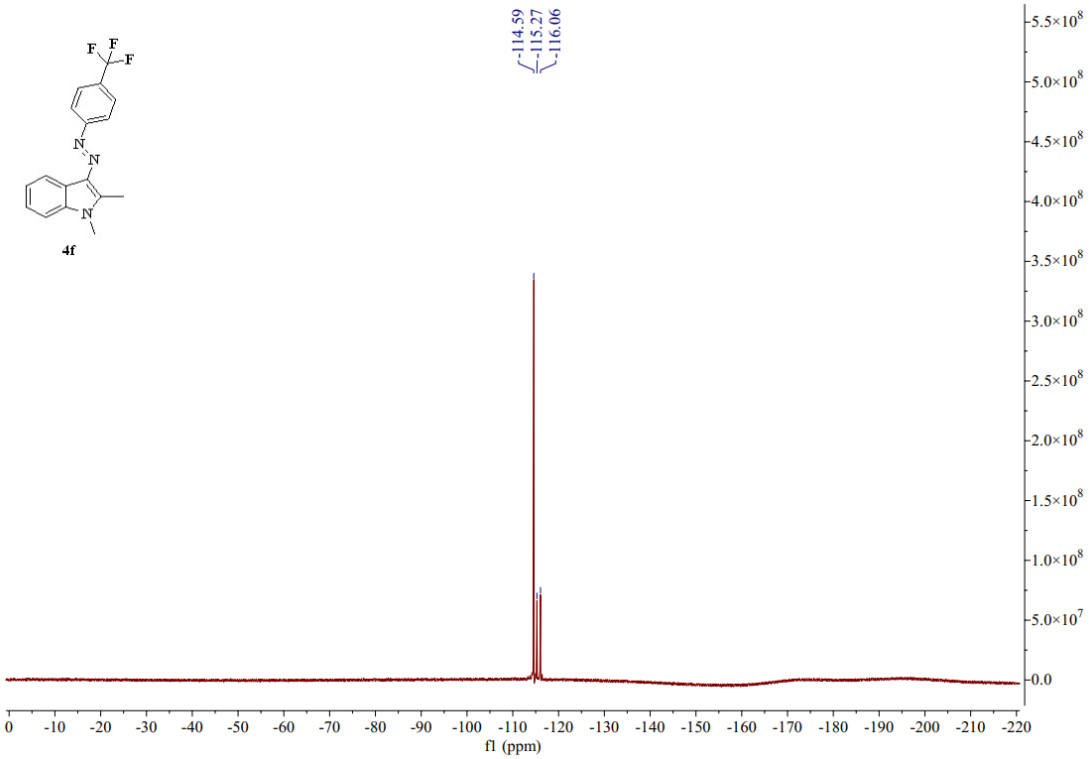


Figure 25S. *^{19}F NMR spectrum ($CDCl_3$, 377 MHz) of compound* ***4f***

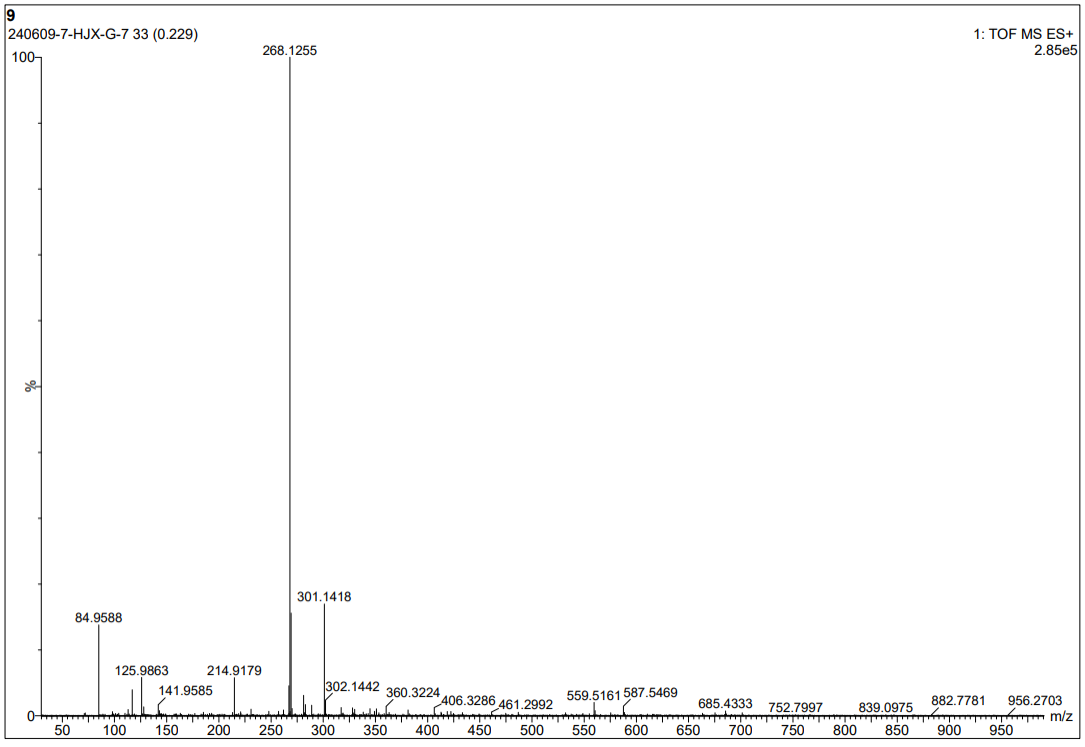


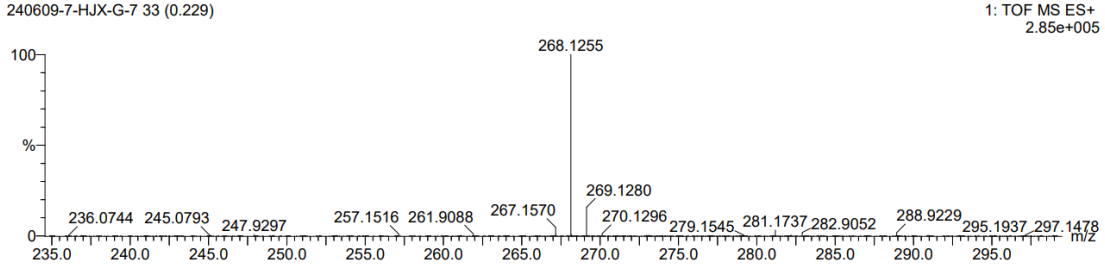
Figure 26S. *HR mass spectrum (ESI) of compound* ***4g***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1181 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 16-16 H: 15-15 N: 0-100 O: 0-100 Na: 0-3 F: 1-3

9
240609-7-HJX-G-7 33 (0.229)



Minimum:				-1.5			
Maximum:		5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
268.1255	268.1250	0.5	1.9	10.5	518.8	n/a	n/a	C16 H15 N3 F

Figure 27S. *HR mass spectrum (ESI) of compound* ***4g***

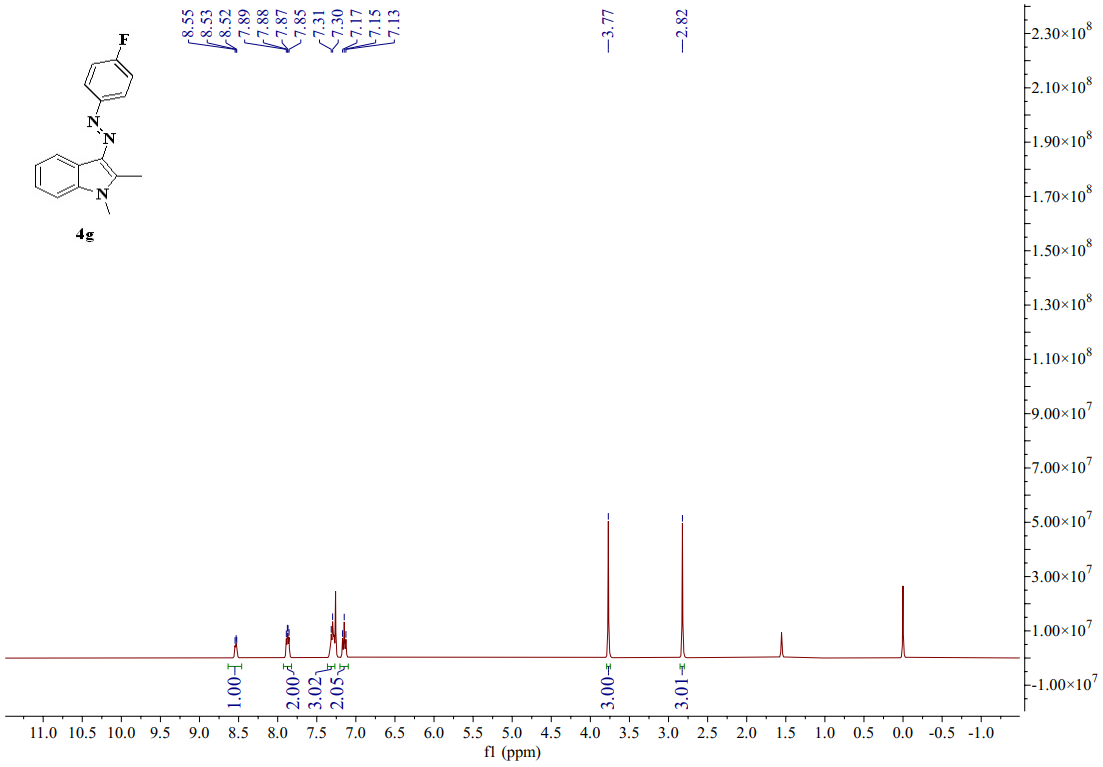


Figure 28S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4g***

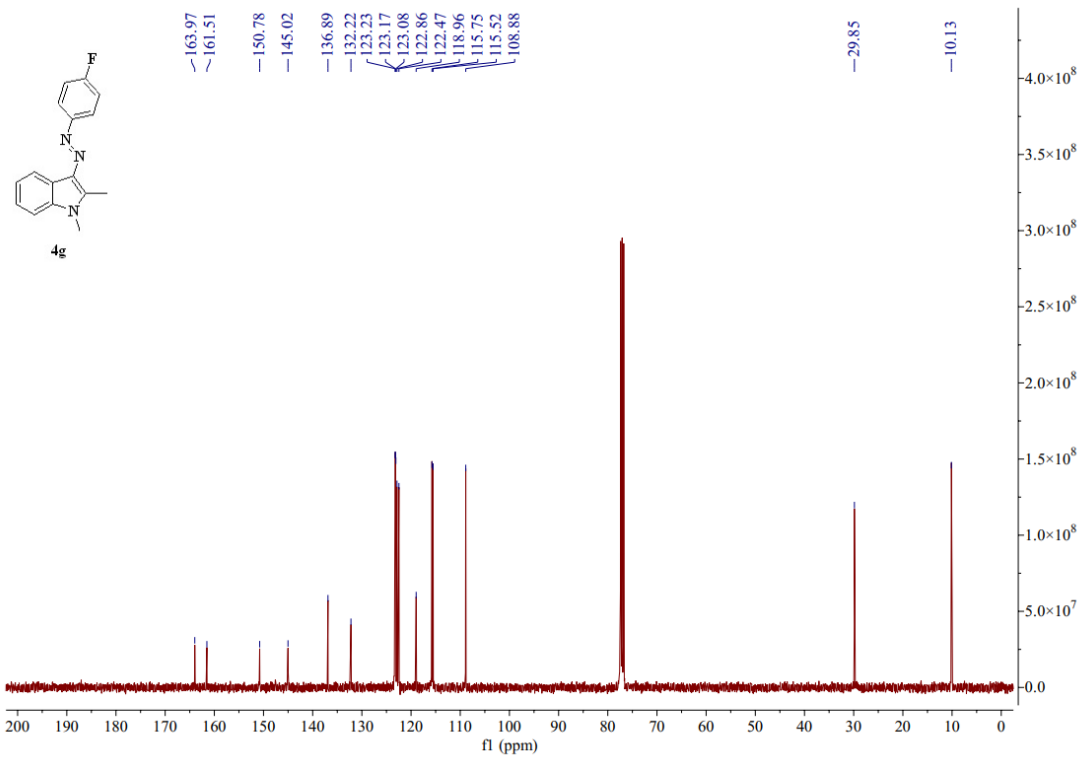


Figure 29S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4g***

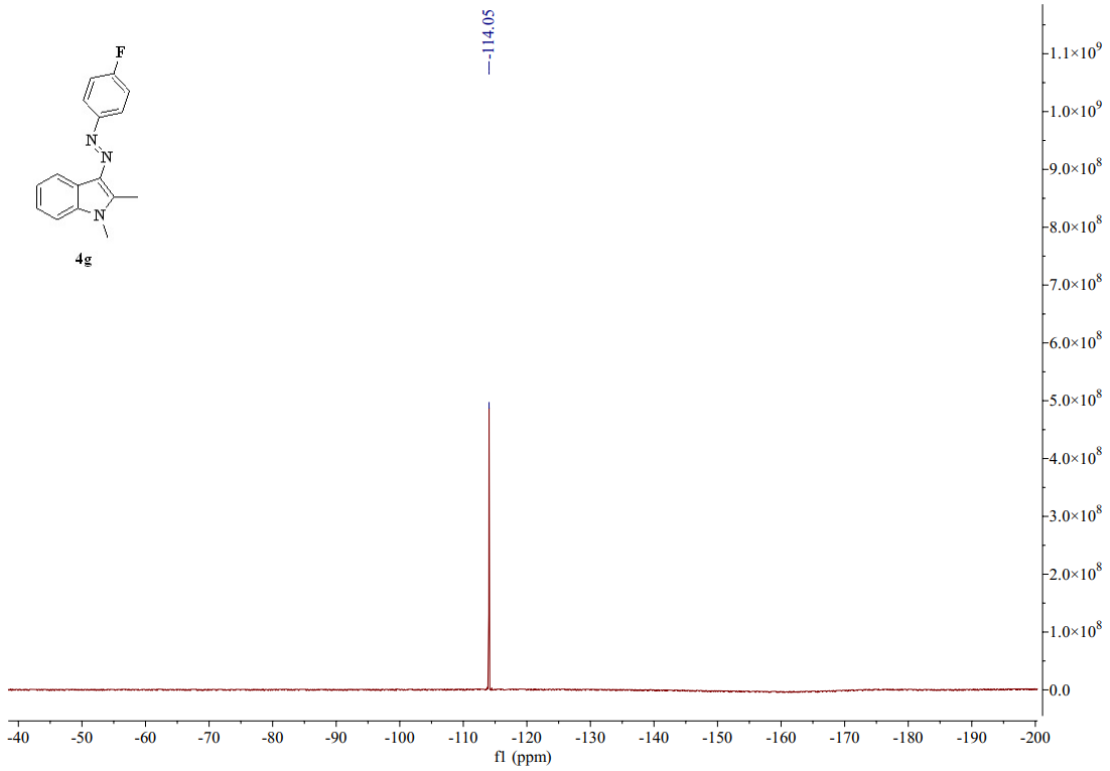


Figure 30S. *^{19}F NMR spectrum ($CDCl_3$, 377 MHz) of compound* ***4g***

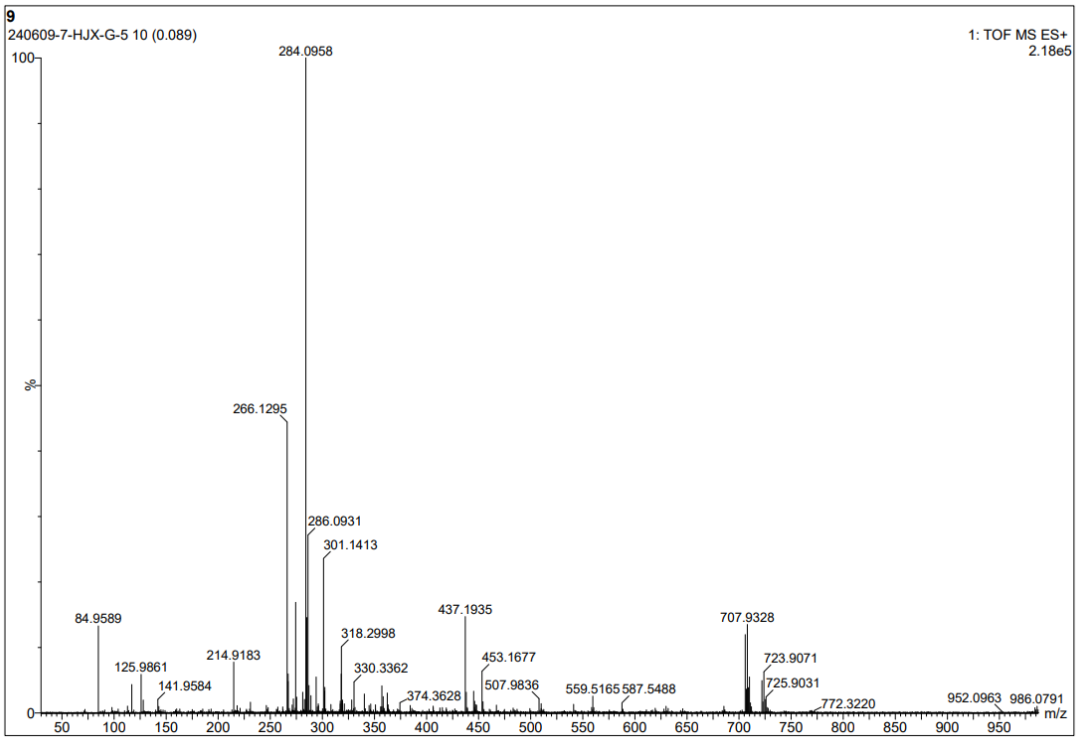
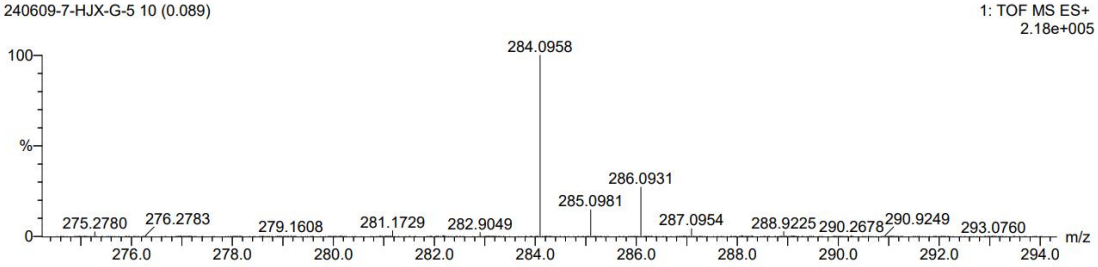


Figure 31S. *HR mass spectrum (ESI) of compound* ***4h***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
797 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 16-16 H: 15-15 N: 0-100 O: 0-100 Na: 0-3 Cl: 1-2
9
240609-7-HJX-G-5 10 (0.089)



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
284.0958	284.0955	0.3	1.1	10.5	547.5	n/a	n/a	C16 H15 N3 Cl

Figure 32S. *HR mass spectrum (ESI) of compound* ***4h***

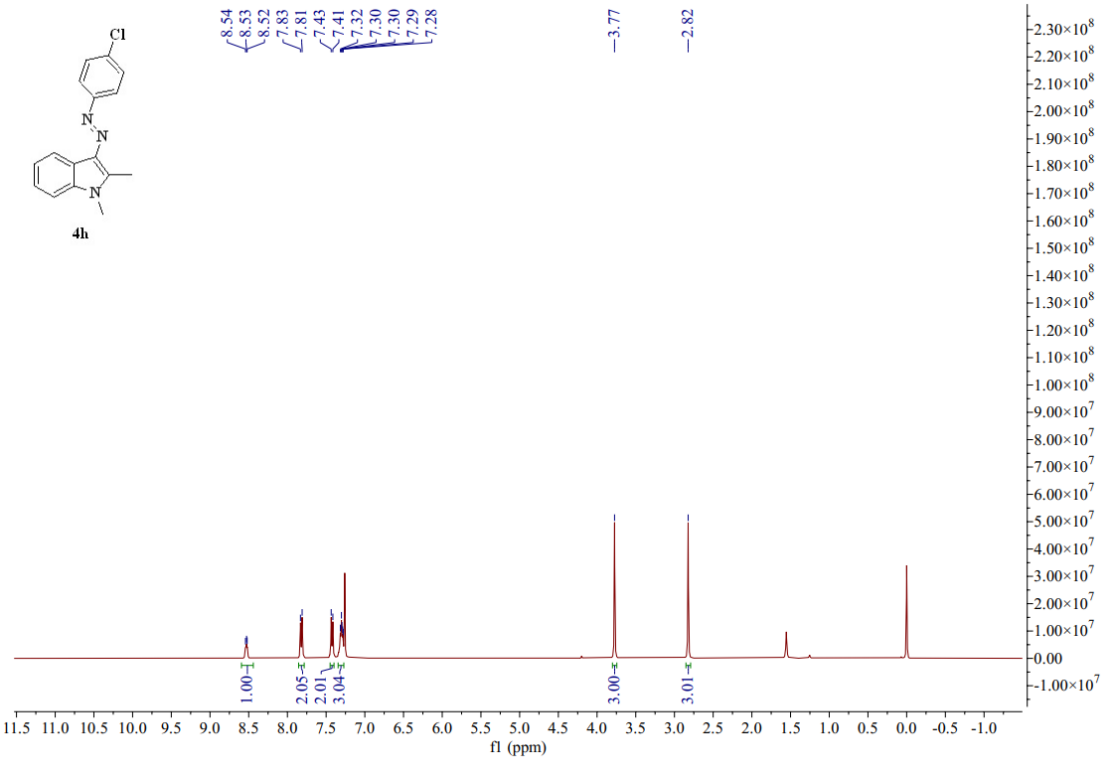


Figure 33S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4h***

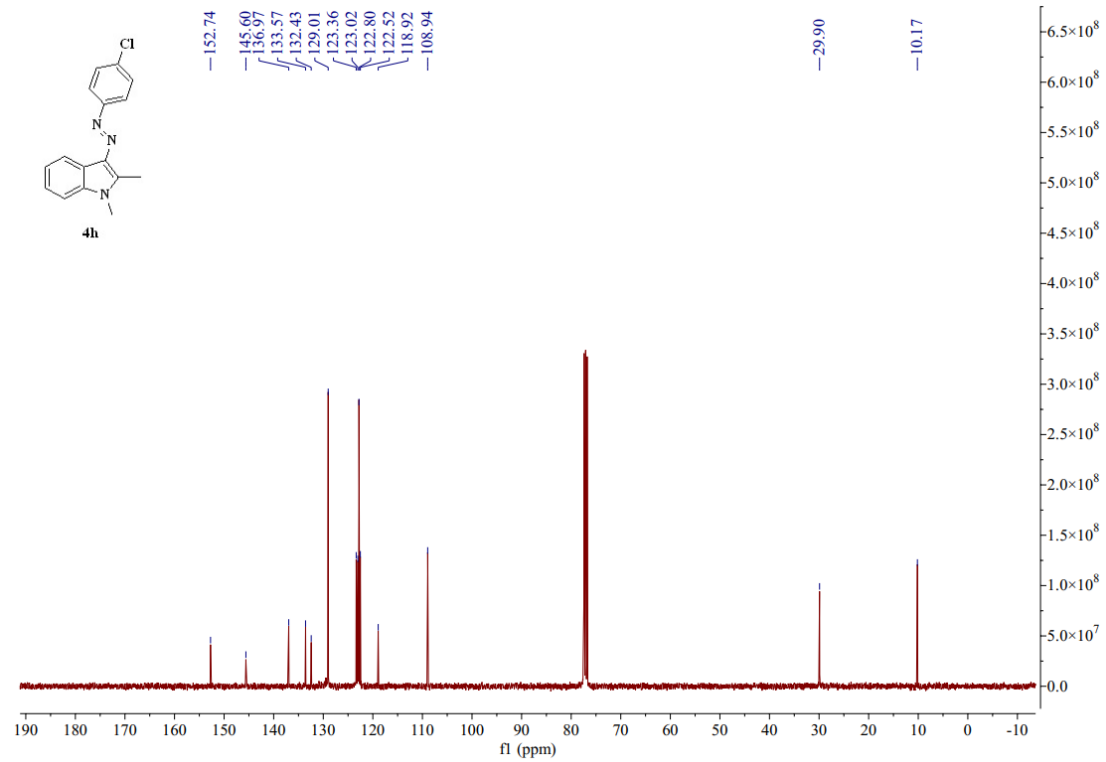


Figure 34S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4h***

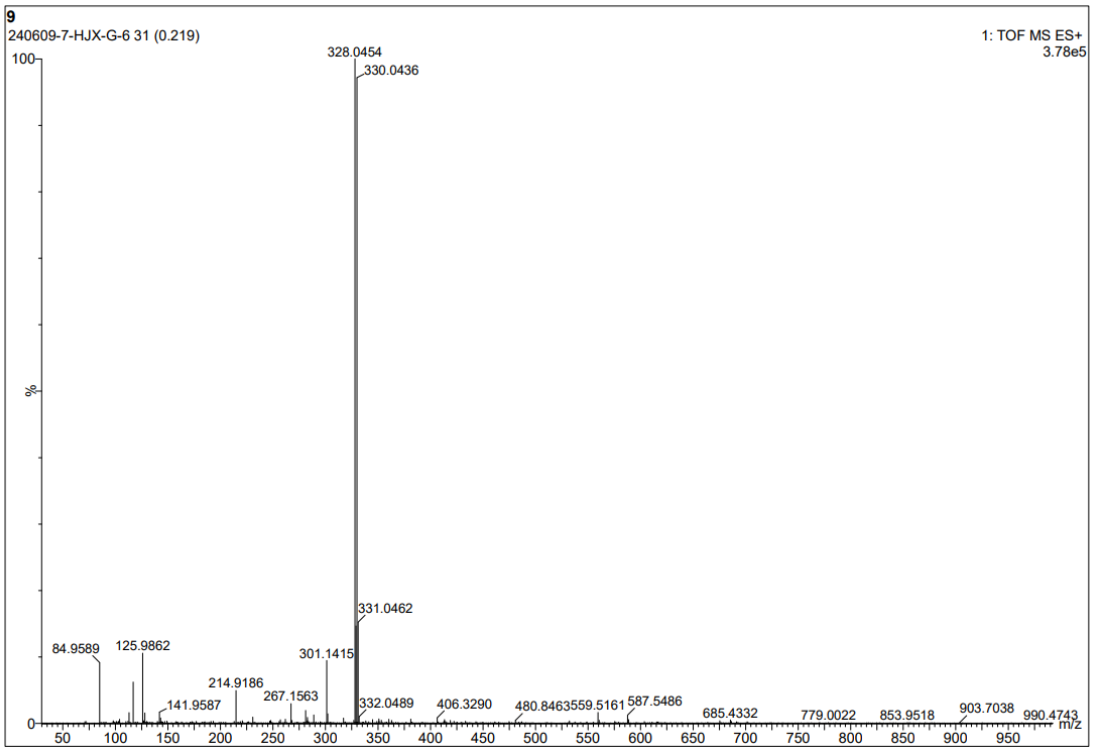
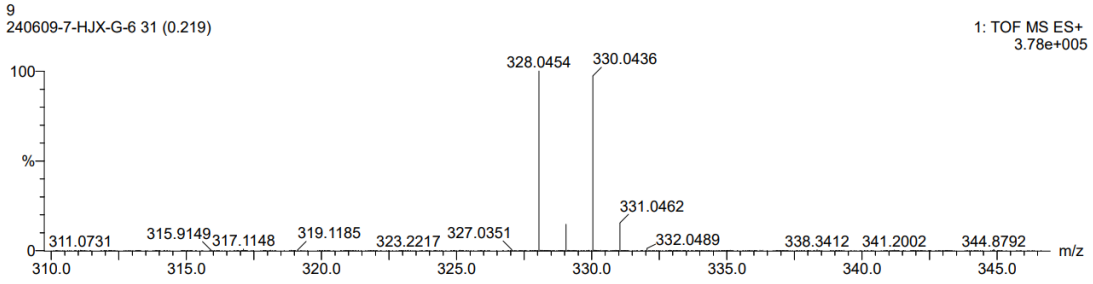


Figure 35S. *HR mass spectrum (ESI) of compound* ***4i***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
665 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 16-16 H: 15-15 N: 0-100 O: 0-100 Na: 0-3 Br: 1-2



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
328.0454	328.0449	0.5	1.5	10.5	737.2	n/a	n/a	C16 H15 N3 Br

Figure 36S. *HR mass spectrum (ESI) of compound* ***4i***

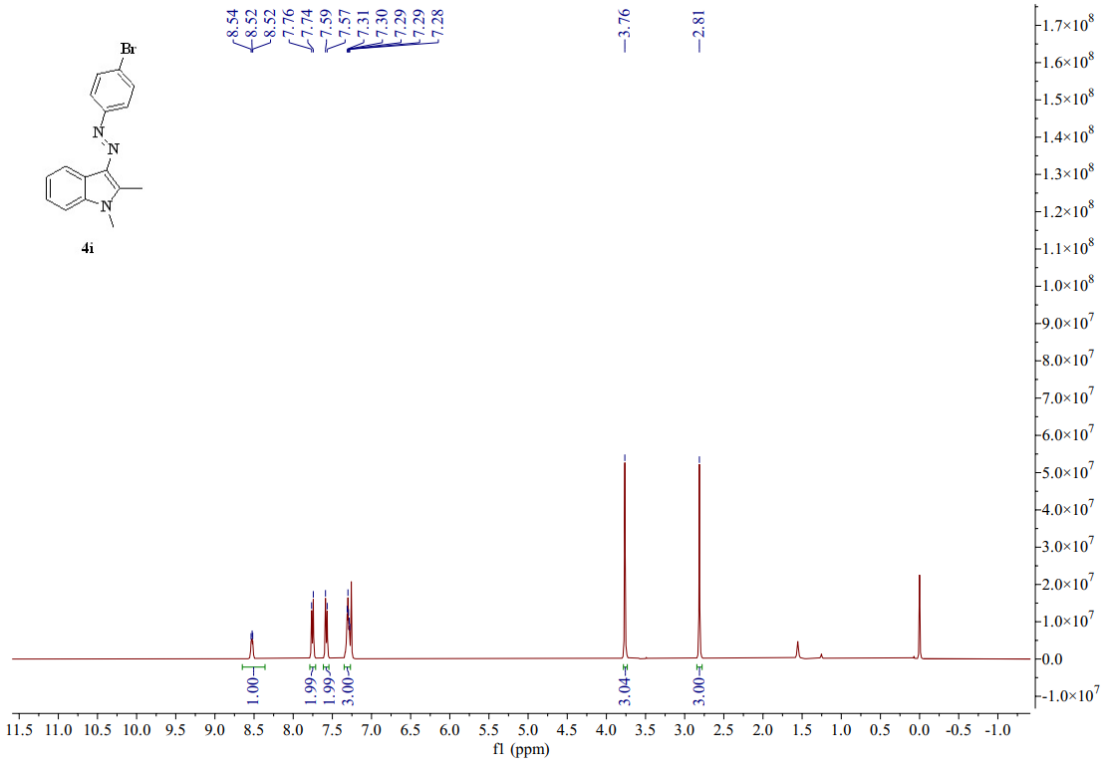


Figure 37S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4i***

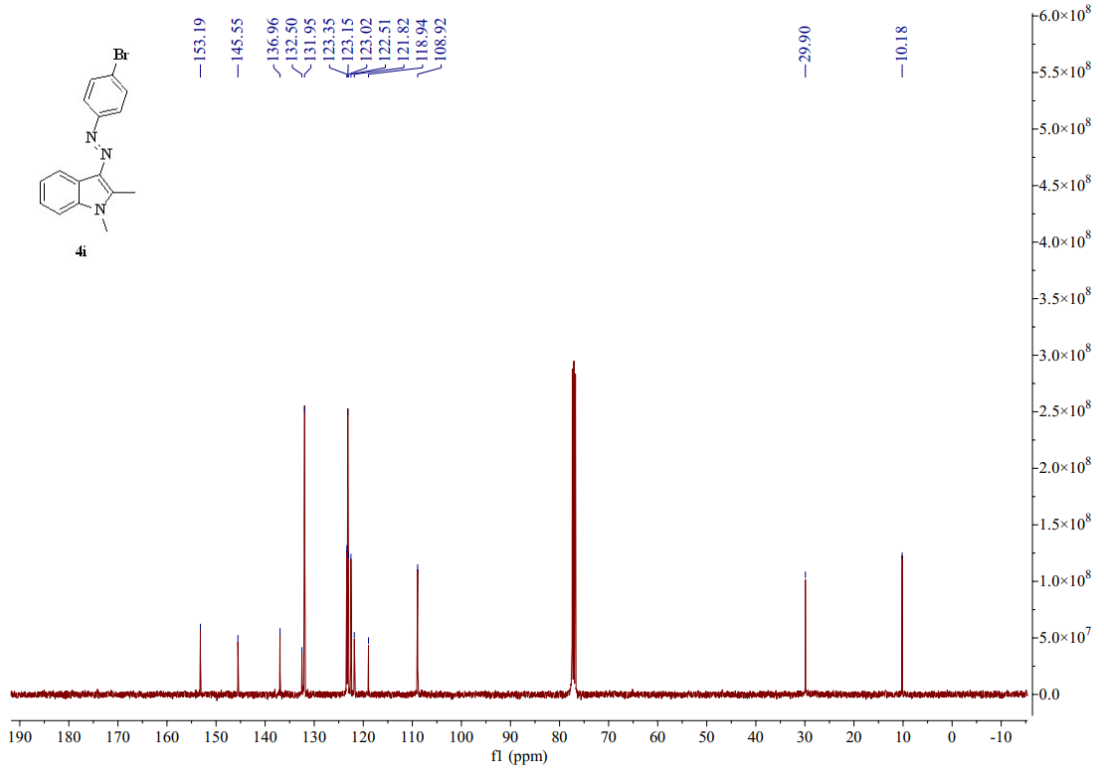


Figure 38S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4i***

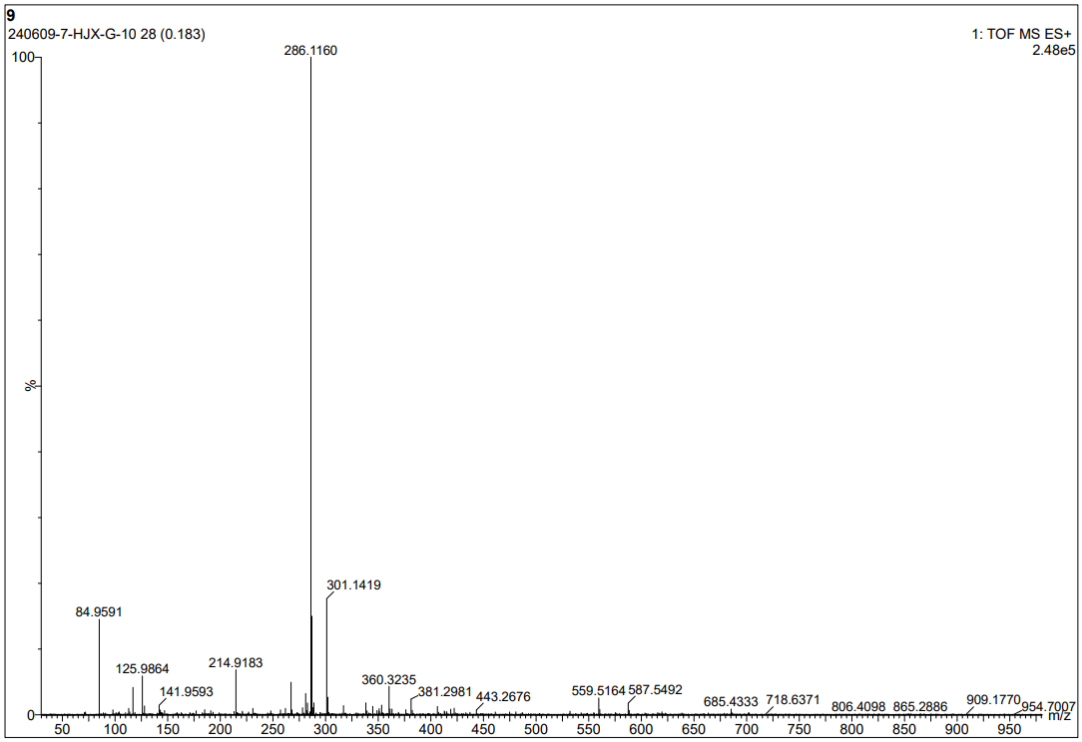
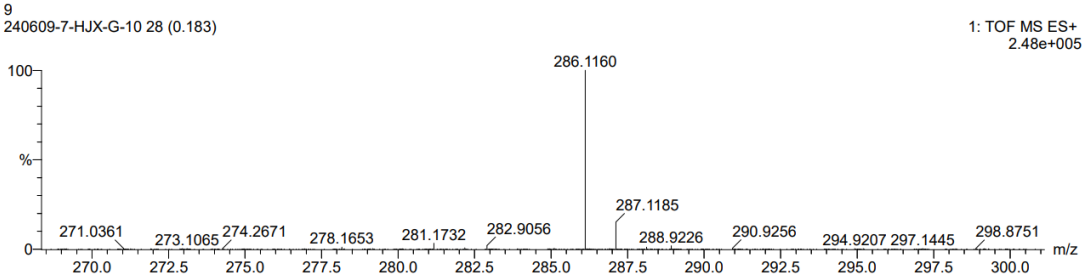


Figure 39S. *HR mass spectrum (ESI) of compound* ***4j***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1361 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 16-16 H: 14-14 N: 0-100 O: 0-100 Na: 0-3 F: 1-3



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
286.1160	286.1156	0.4	1.4	10.5	614.2	n/a	n/a	C16 H14 N3 F2

Figure 40S. *HR mass spectrum (ESI) of compound* ***4j***

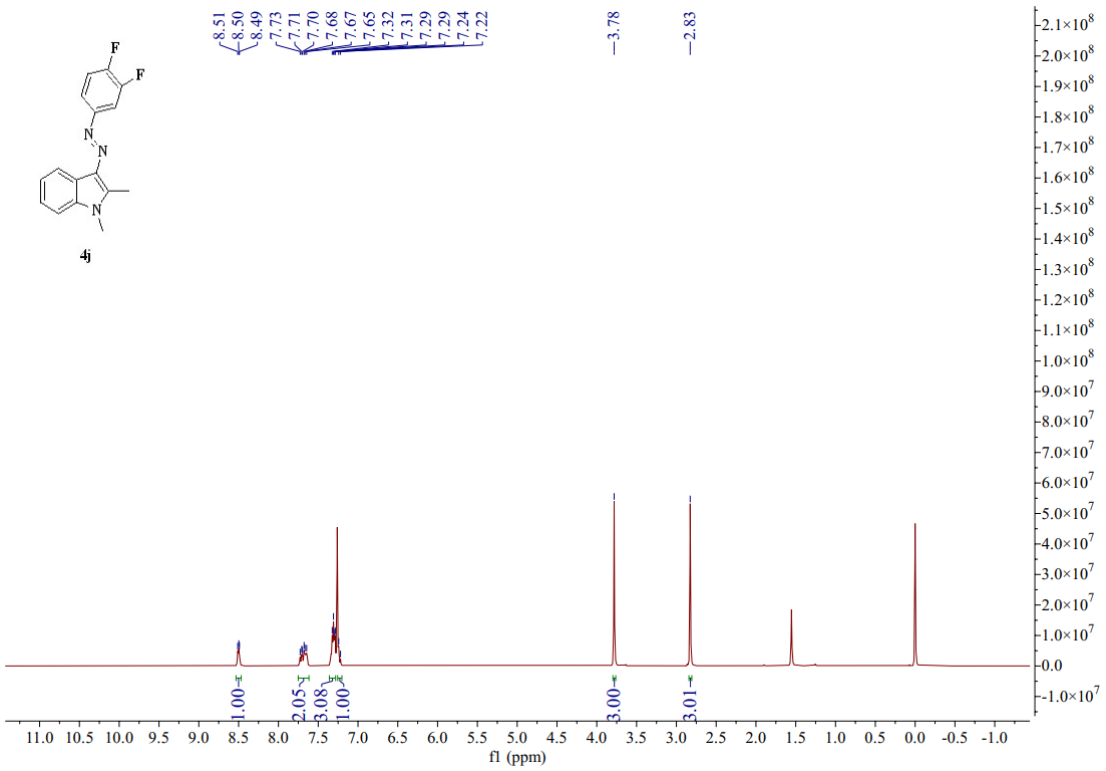


Figure 41S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4j***

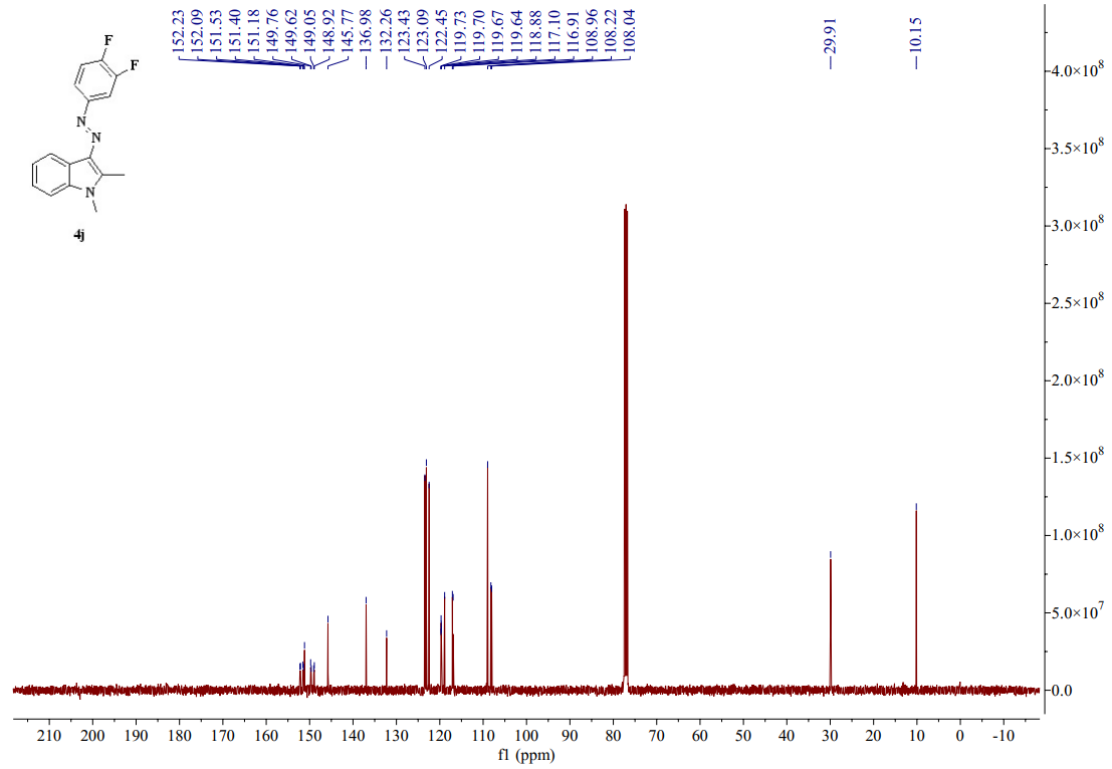


Figure 42S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4j***

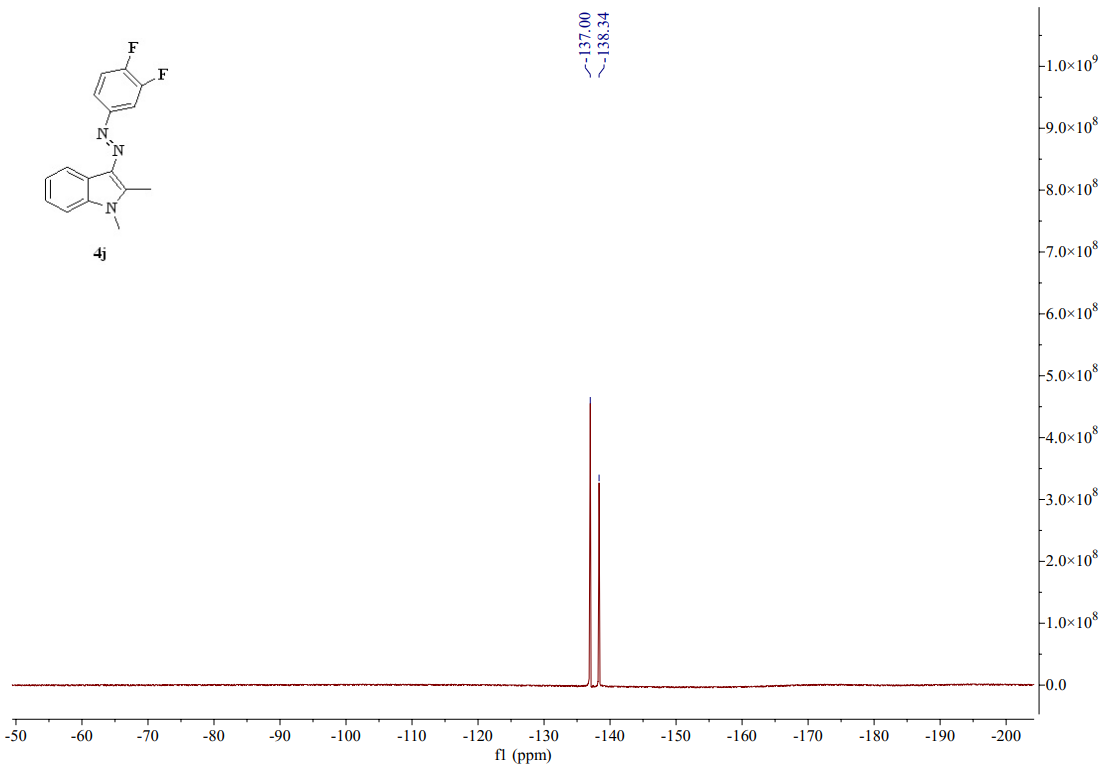


Figure 43S. *^{19}F NMR spectrum ($CDCl_3$, 377 MHz) of compound* ***4j***

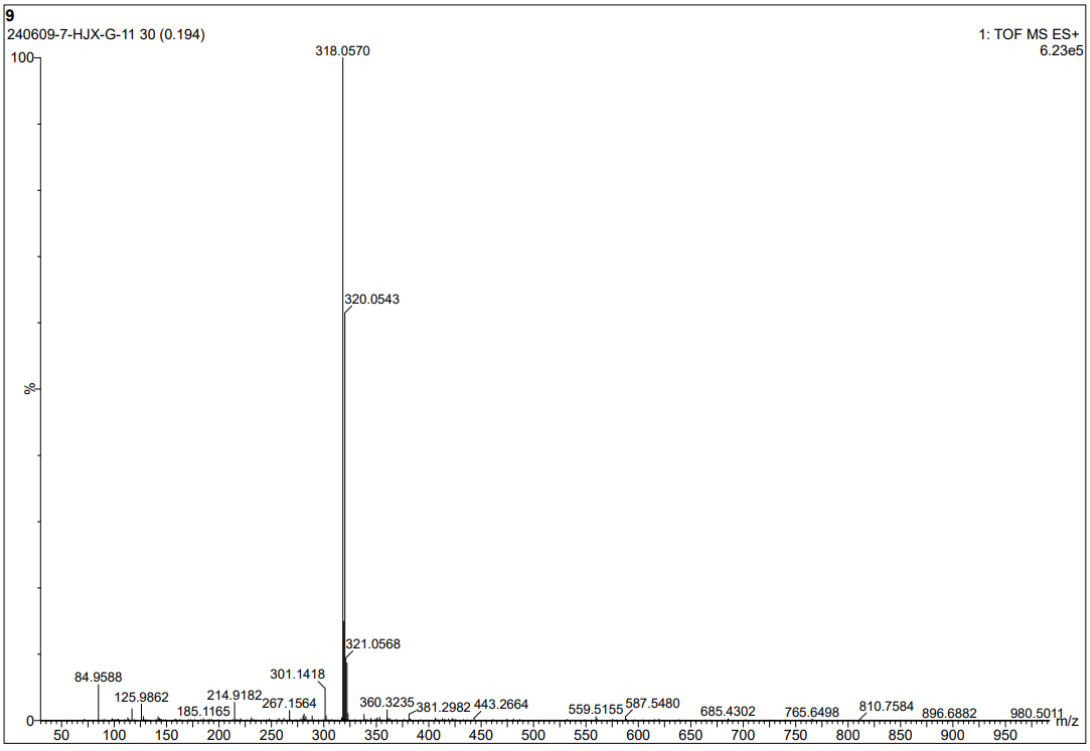
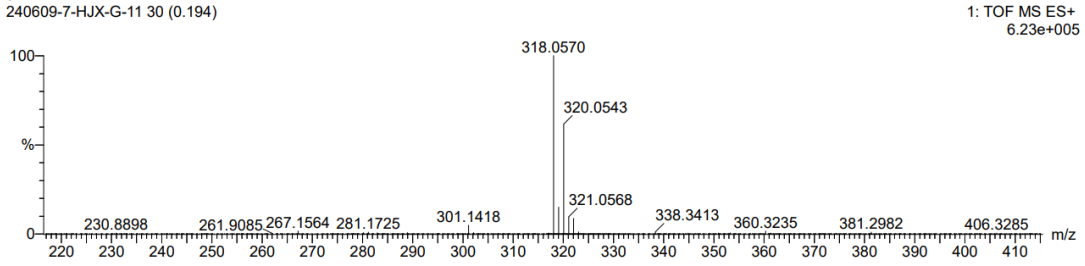


Figure 44S. *HR mass spectrum (ESI) of compound* ***4k***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1028 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 16-16 H: 14-14 N: 0-100 O: 0-100 Na: 0-3 Cl: 1-2
9
240609-7-HJX-G-11 30 (0.194)



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
318.0570	318.0565	0.5	1.6	10.5	886.0	n/a	n/a	C16 H14 N3 Cl2

Figure 45S. *HR mass spectrum (ESI) of compound* ***4k***

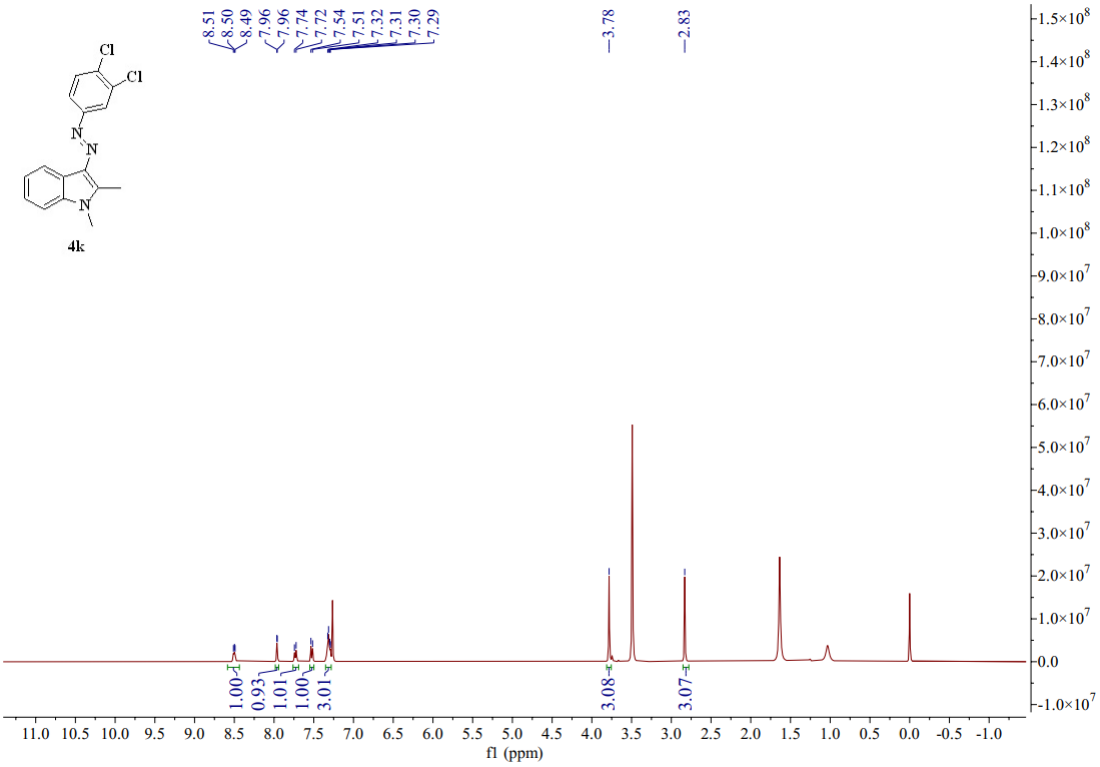


Figure 46S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4k***

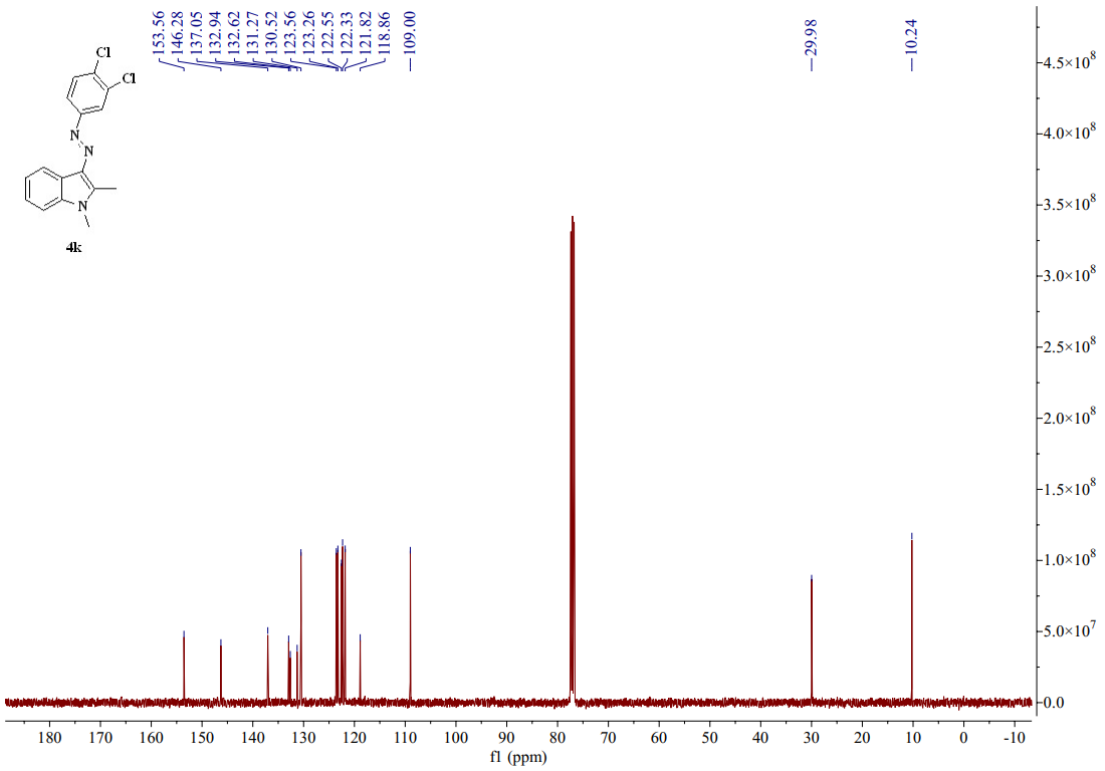


Figure 47S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4k***

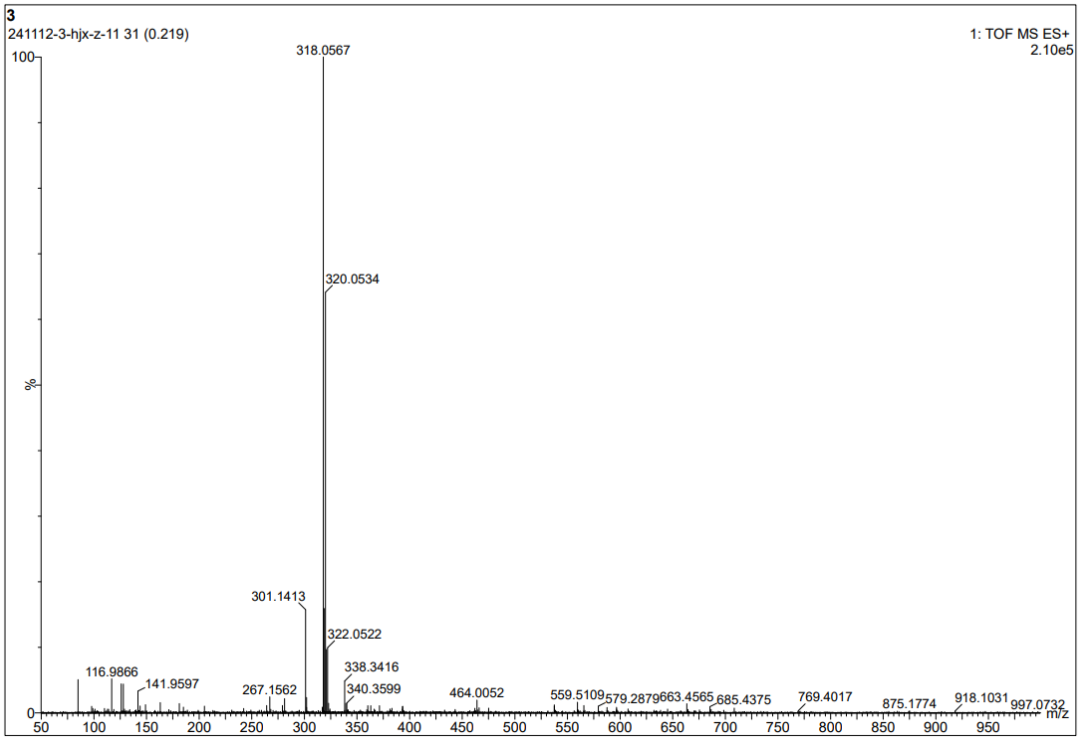
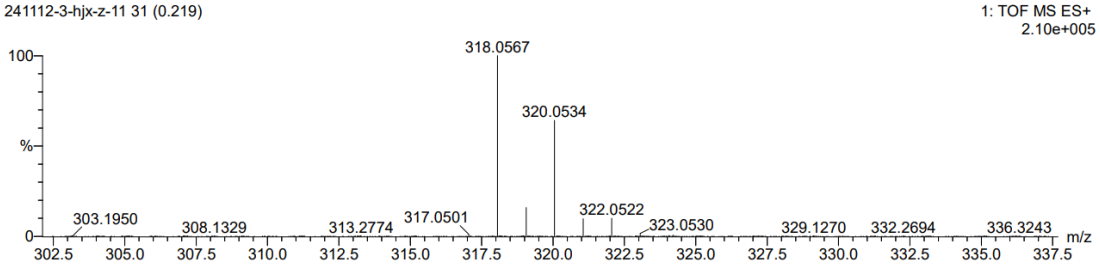


Figure 48S. *HR mass spectrum (ESI) of compound* ***4l***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
516 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 16-16 H: 14-14 N: 0-100 O: 0-100 Cl: 1-4
3
241112-3-hjx-z-11 31 (0.219)



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
318.0567	318.0565	0.2	0.6	10.5	615.8	n/a	n/a	C16 H14 N3 Cl2

Figure 49S. *HR mass spectrum (ESI) of compound* ***4l***

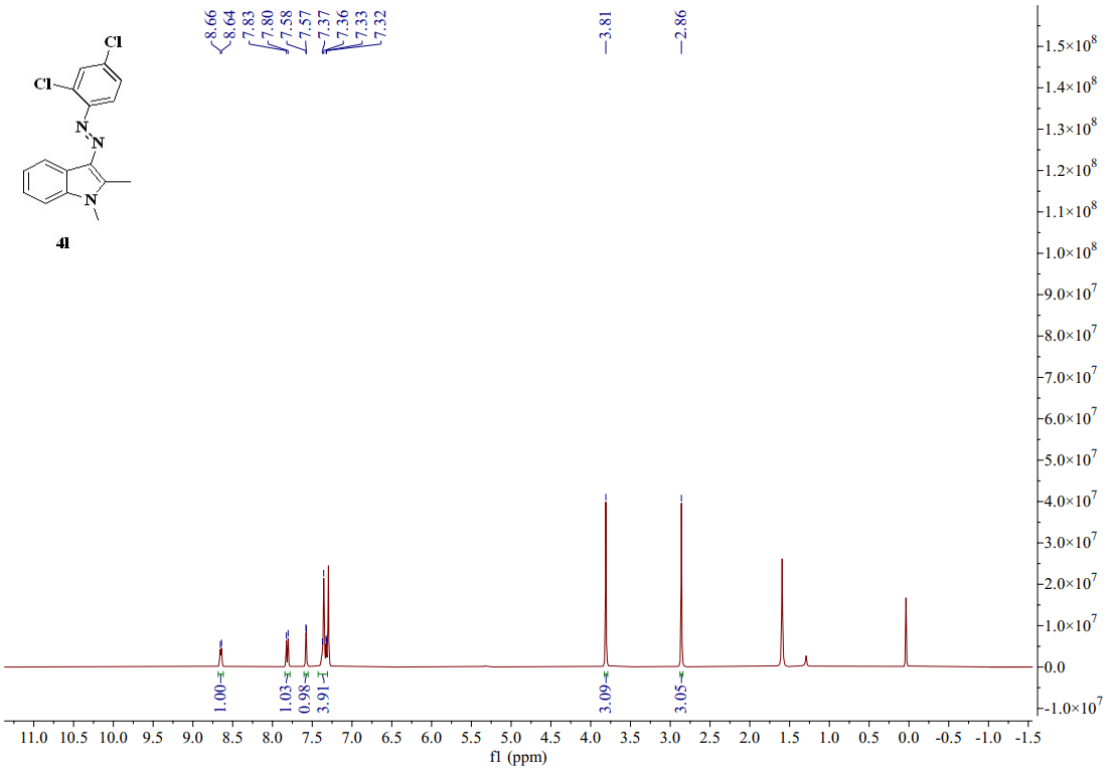


Figure 50S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4l***

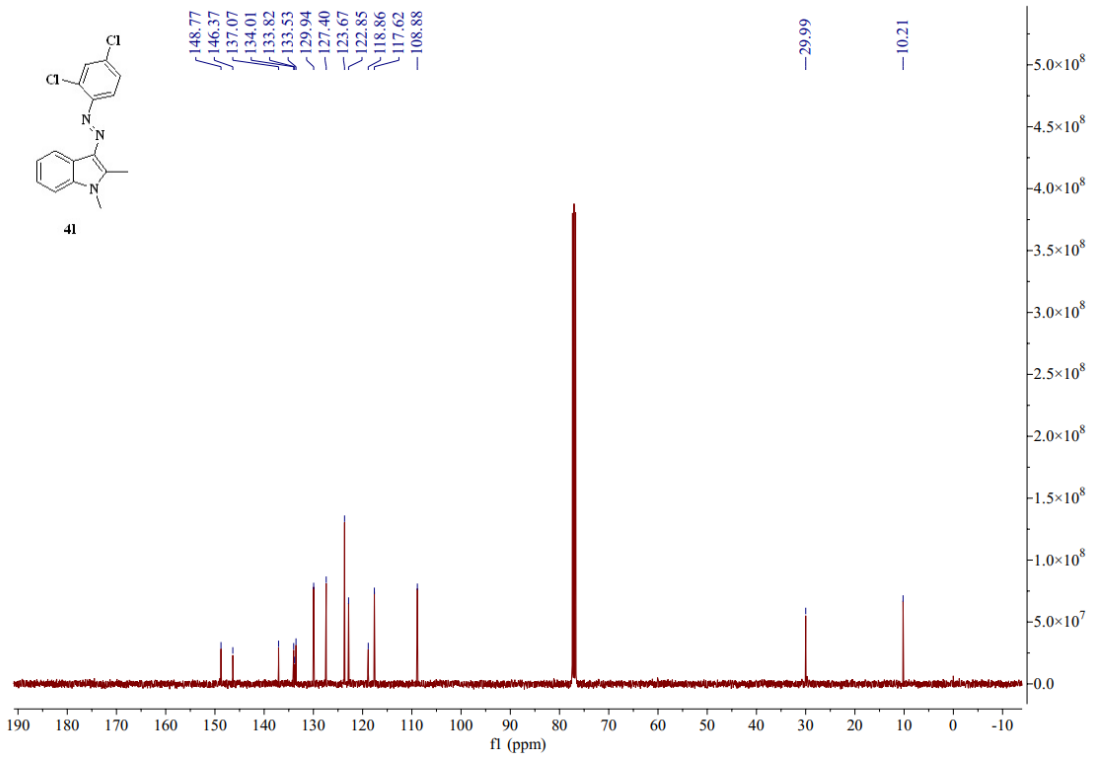


Figure 51S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4l***

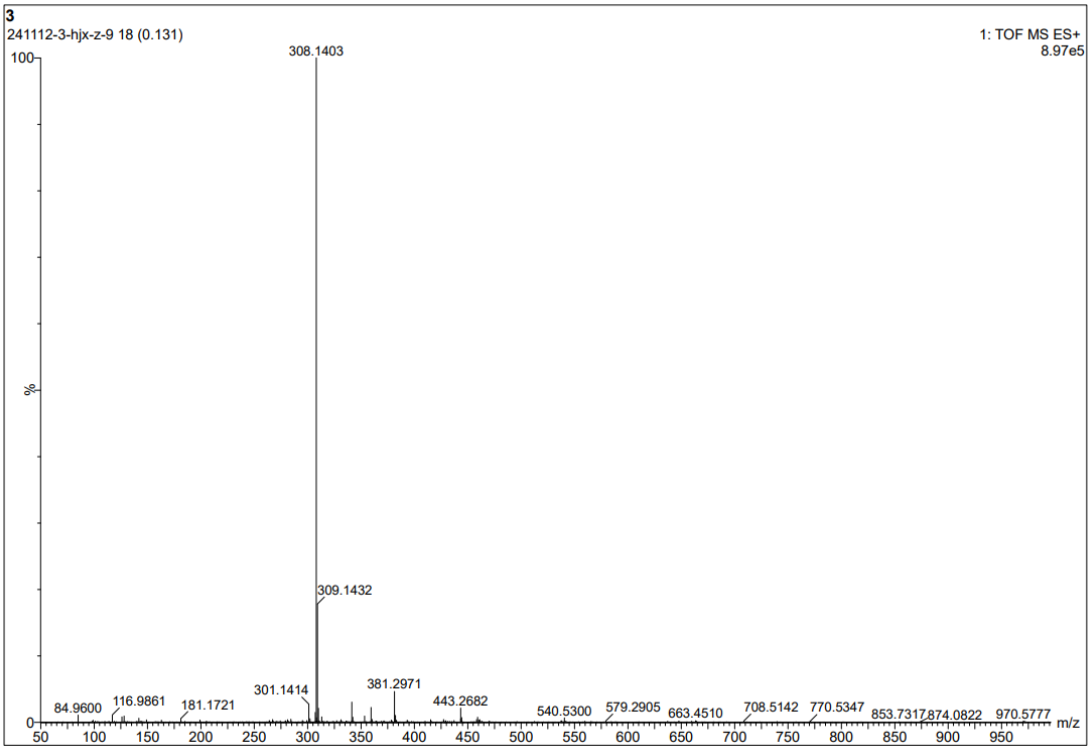
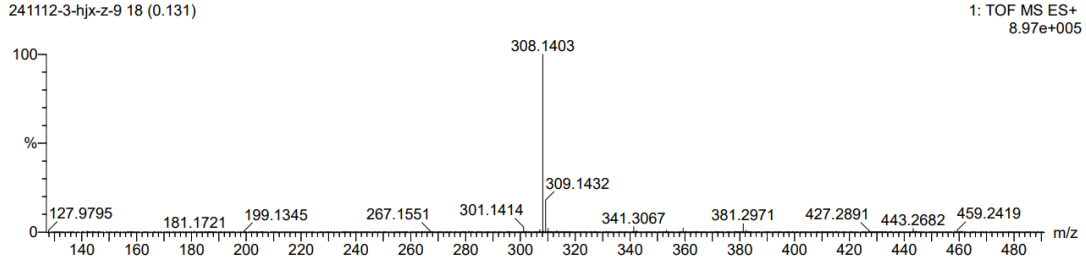


Figure 52S. *HR mass spectrum (ESI) of compound* ***4m***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
211 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 18-18 H: 18-18 N: 0-100 O: 0-100
3
241112-3-hjx-z-9 18 (0.131)



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
308.1403	308.1399	0.4	1.3	11.5	896.7	n/a	n/a	C18 H18 N3 O2

Figure 53S. *HR mass spectrum (ESI) of compound* ***4m***

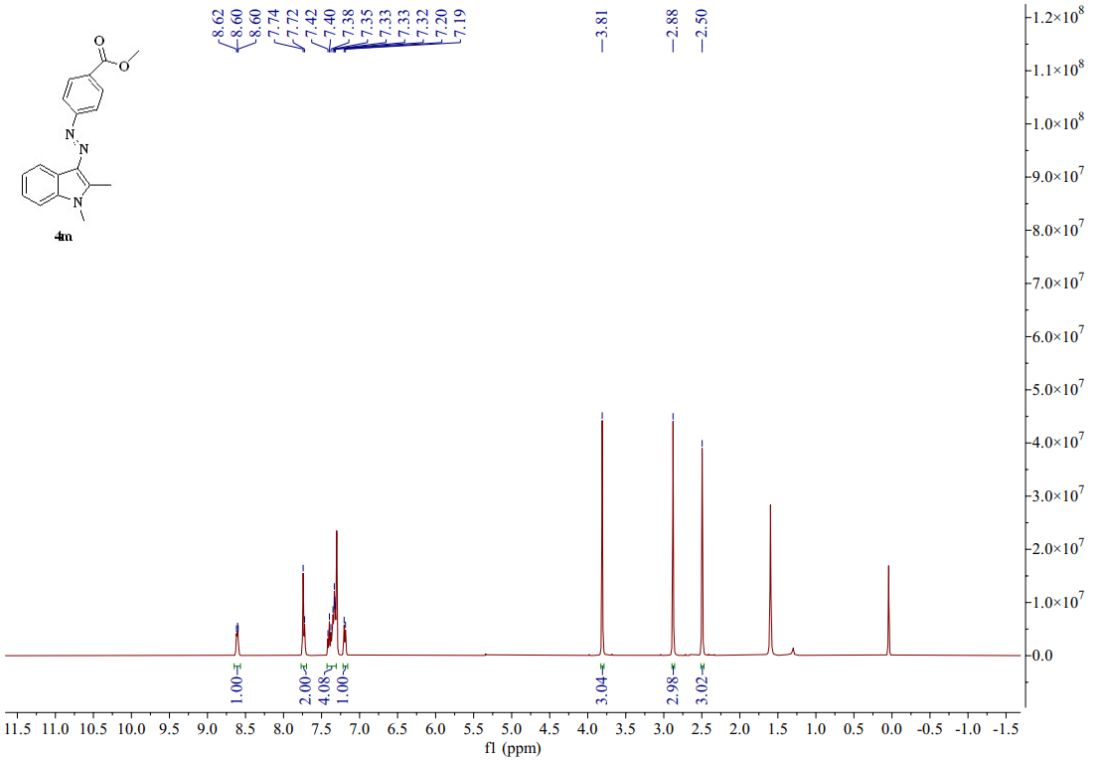


Figure 54S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4m***

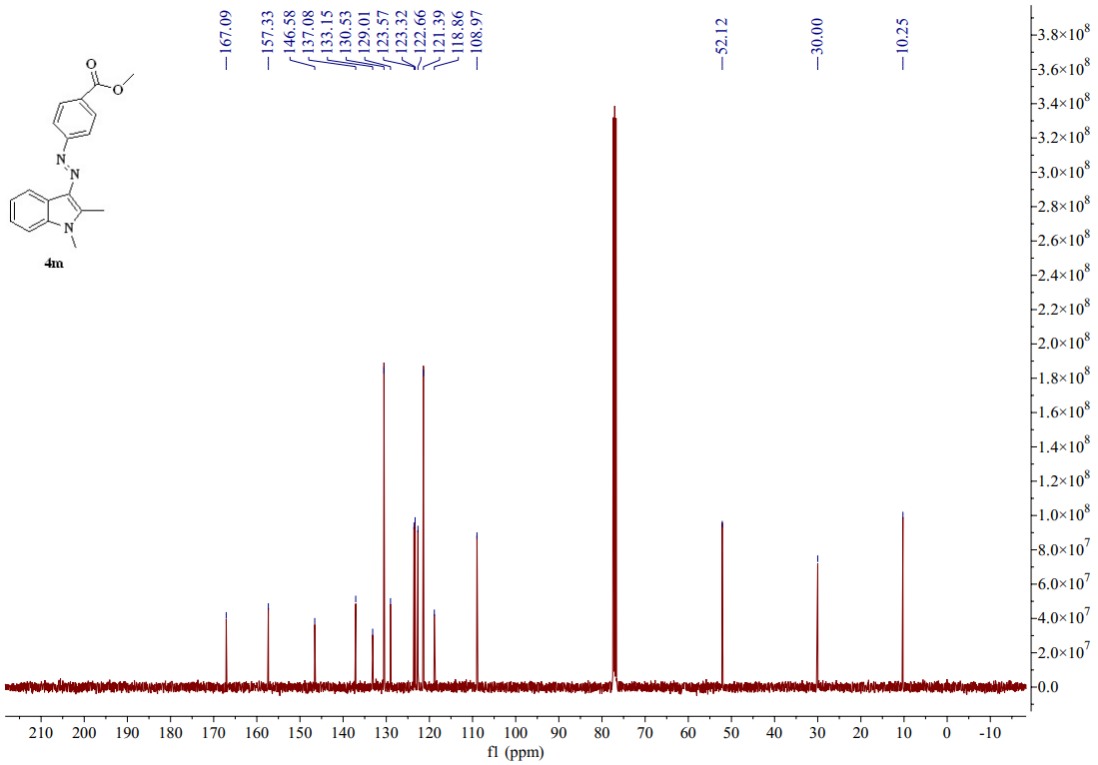


Figure 55S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4m***

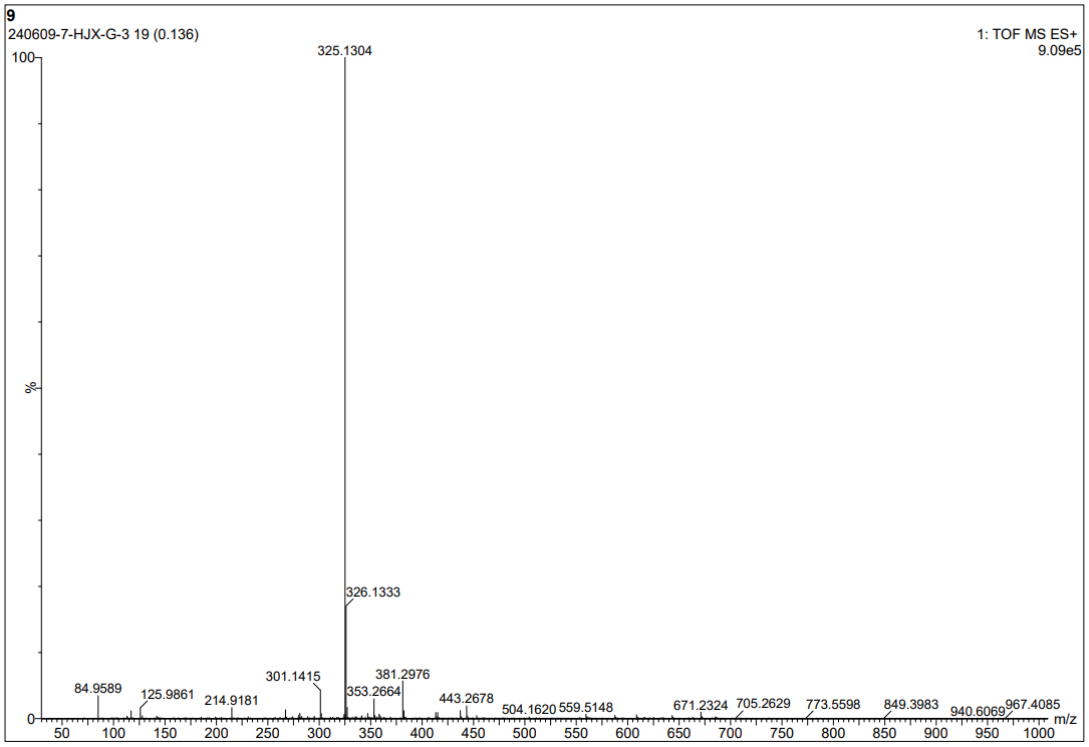
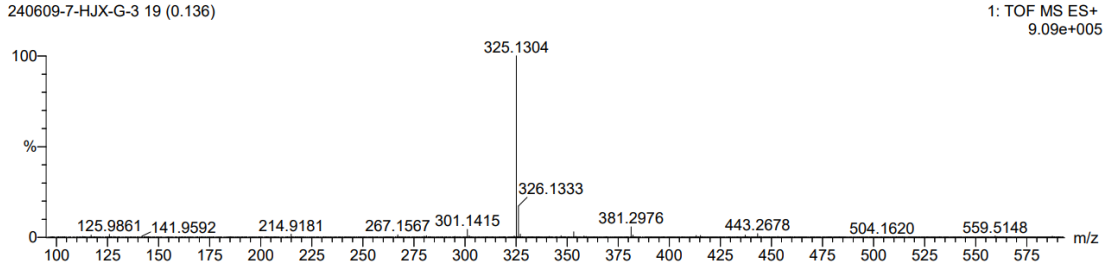


Figure 56S. *HR mass spectrum (ESI) of compound* ***4n***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
757 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 17-17 H: 17-17 N: 0-100 O: 0-100 Na: 0-3
9
240609-7-HJX-G-3 19 (0.136)



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
325.1304	325.1301	0.3	0.9	11.5	799.3	n/a	n/a	C17 H17 N4 O3

Figure 57S. *HR mass spectrum (ESI) of compound* ***4n***

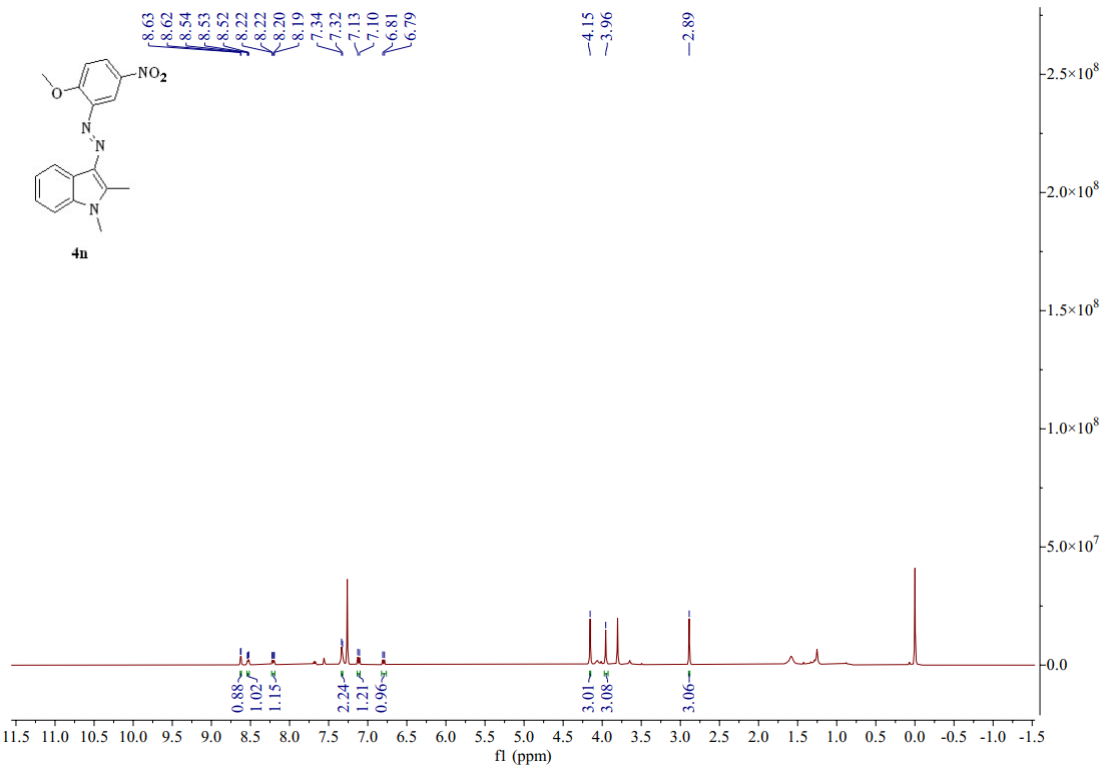


Figure 58S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4n***

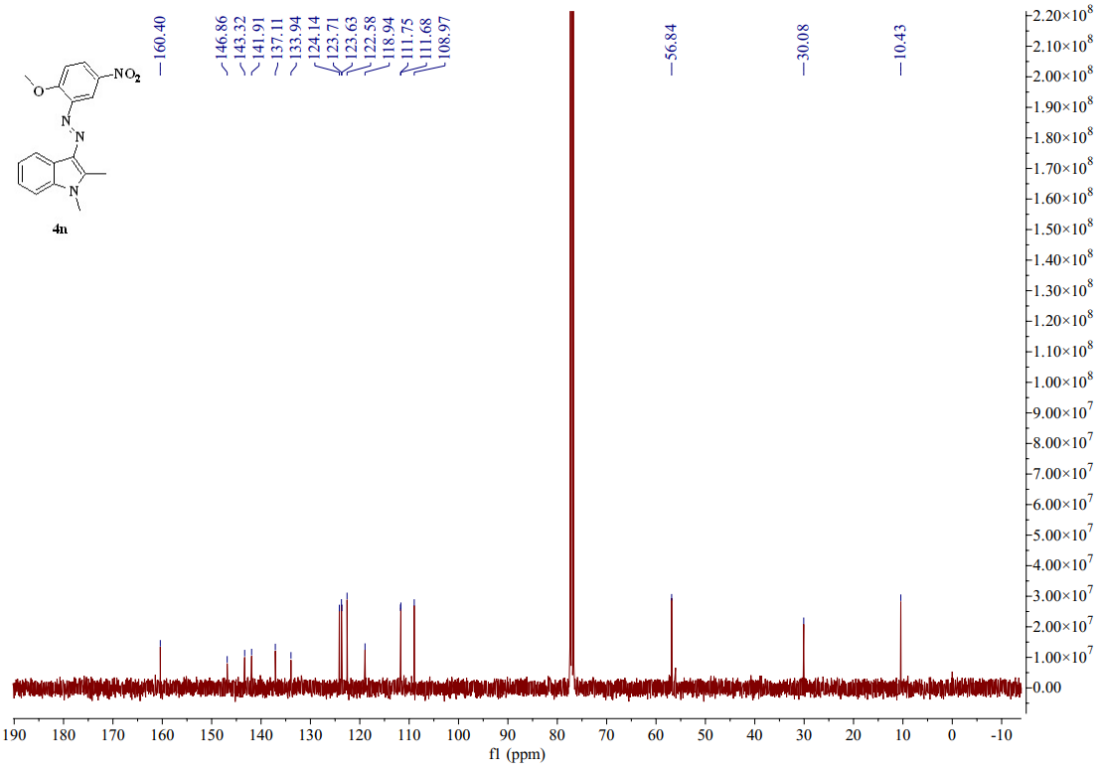


Figure 59S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4n***

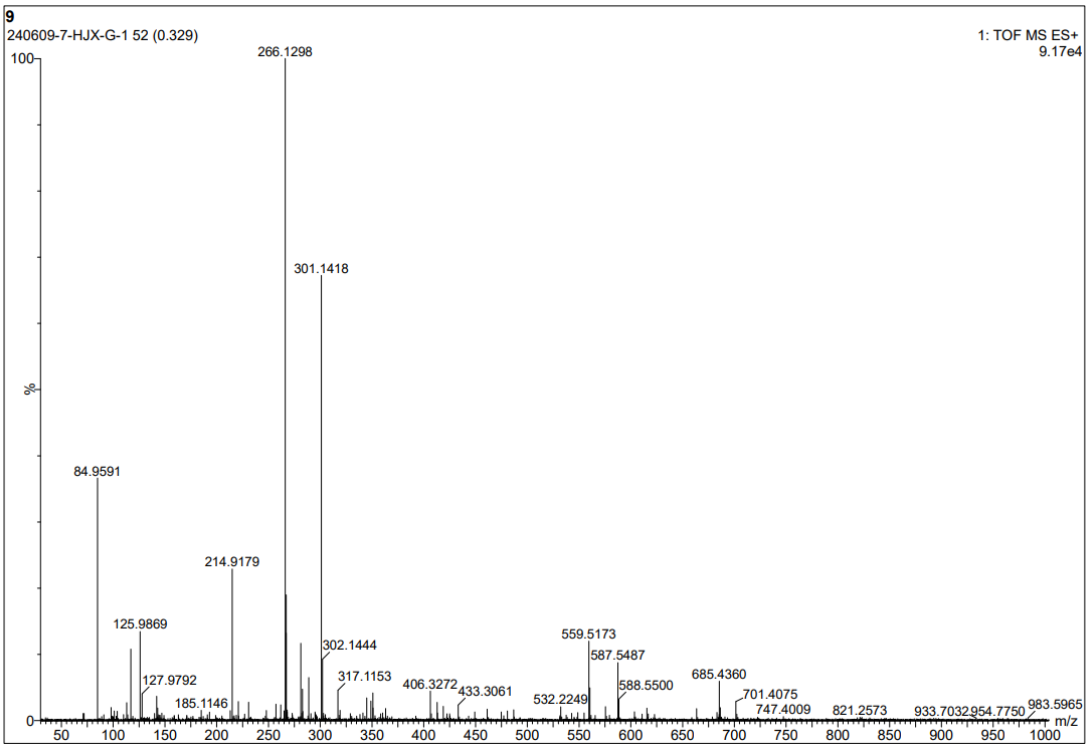
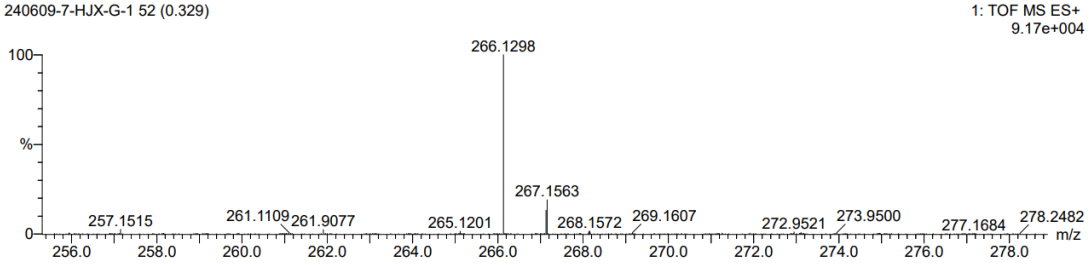


Figure 60S. *HR mass spectrum (ESI) of compound* ***4o***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
515 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 16-16 H: 16-16 N: 0-100 O: 0-100 Na: 0-3
9
240609-7-HJX-G-1 52 (0.329)



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
266.1298	266.1293	0.5	1.9	10.5	397.5	n/a	n/a	C16 H16 N3 O

Figure 61S. *HR mass spectrum (ESI) of compound* ***4o***

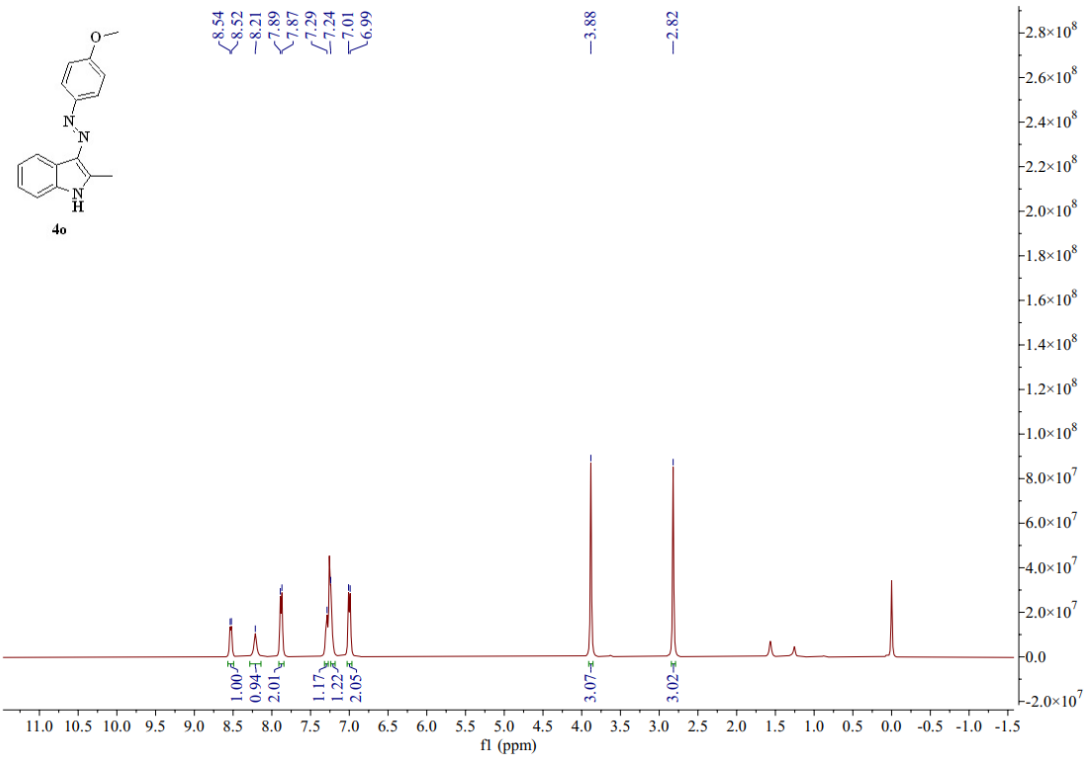


Figure 62S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4o***

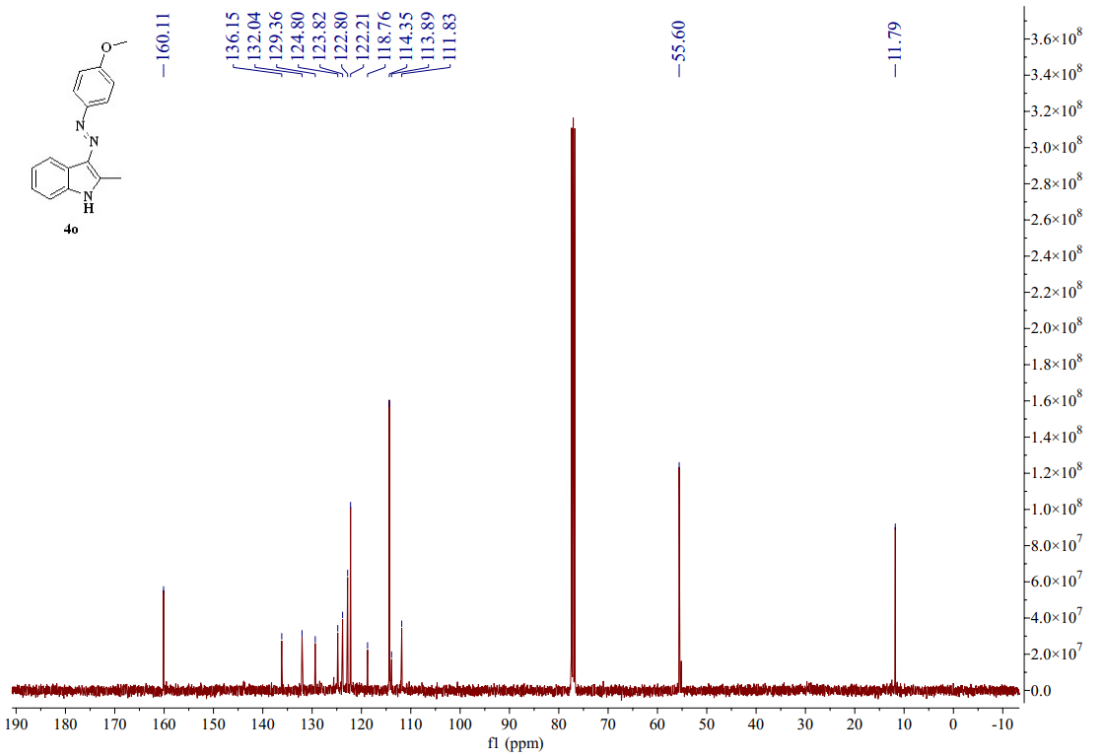


Figure 63S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4o***

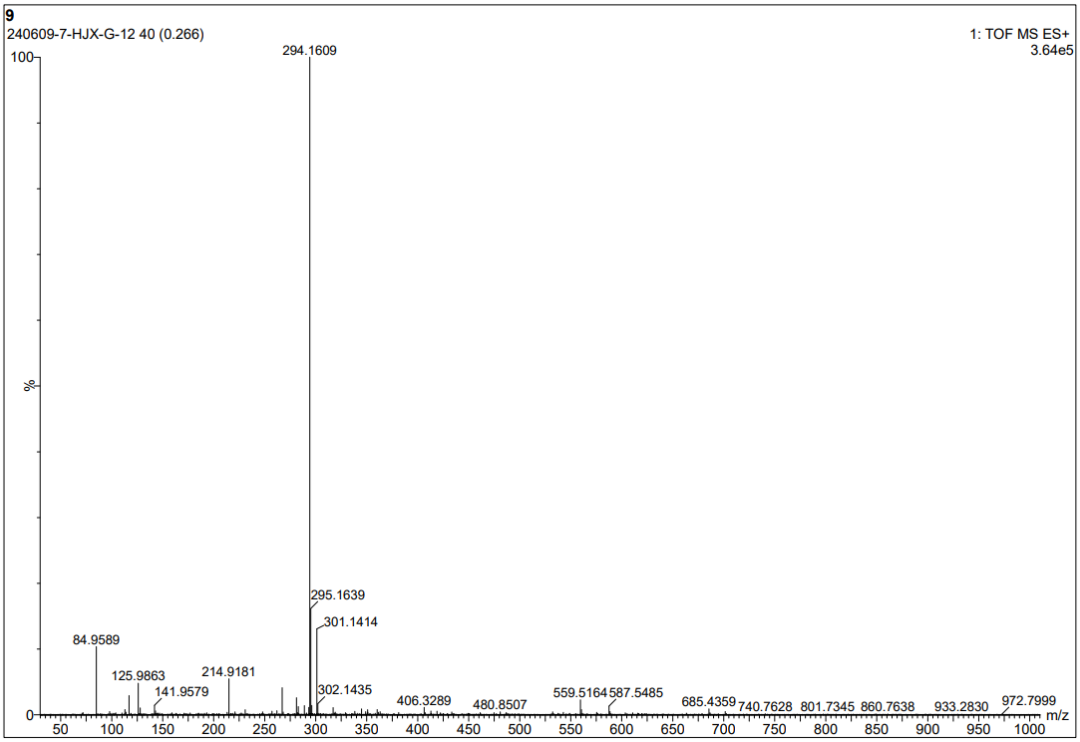
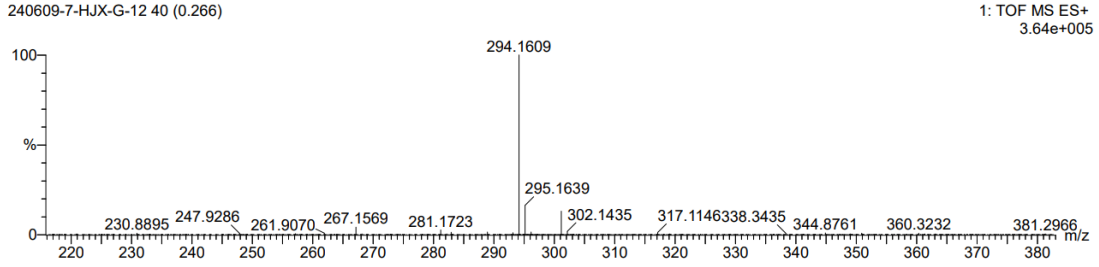


Figure 64S. *HR mass spectrum (ESI) of compound* ***4p***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
641 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 18-18 H: 20-20 N: 0-100 O: 0-100 Na: 0-3
9
240609-7-HJX-G-12 40 (0.266)



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
294.1609	294.1606	0.3	1.0	10.5	601.0	n/a	n/a	C18 H20 N3 O

Figure 65S. *HR mass spectrum (ESI) of compound* ***4p***

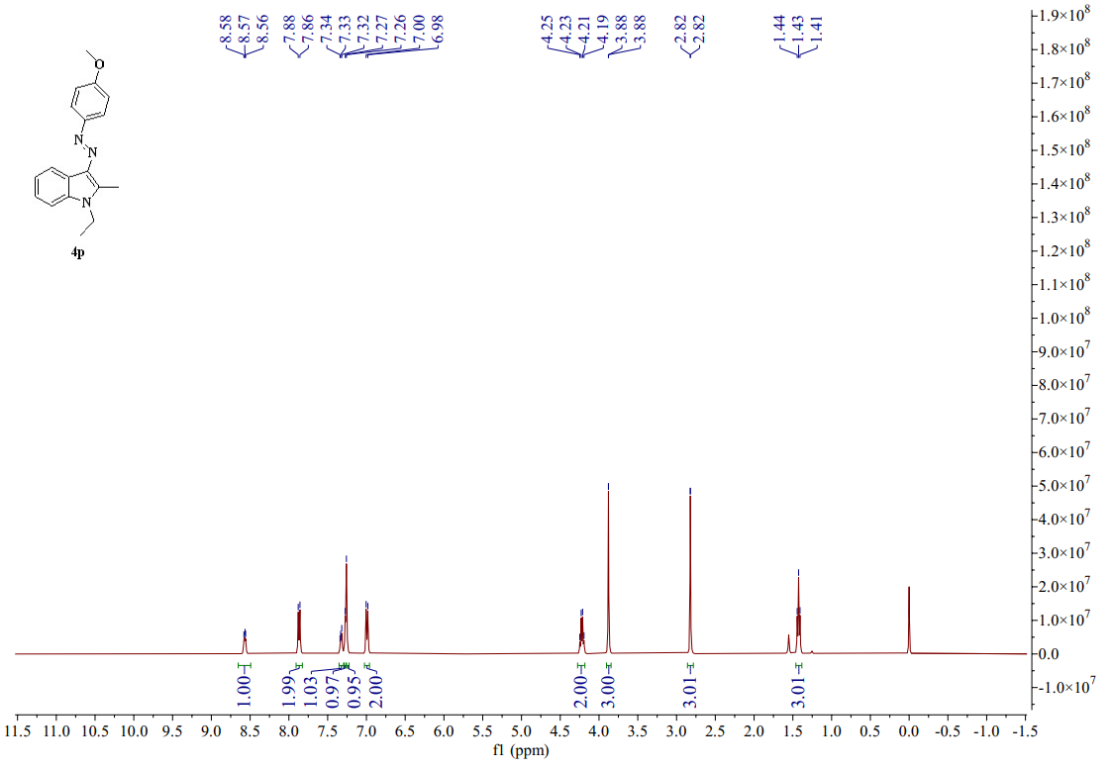


Figure 66S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4p***

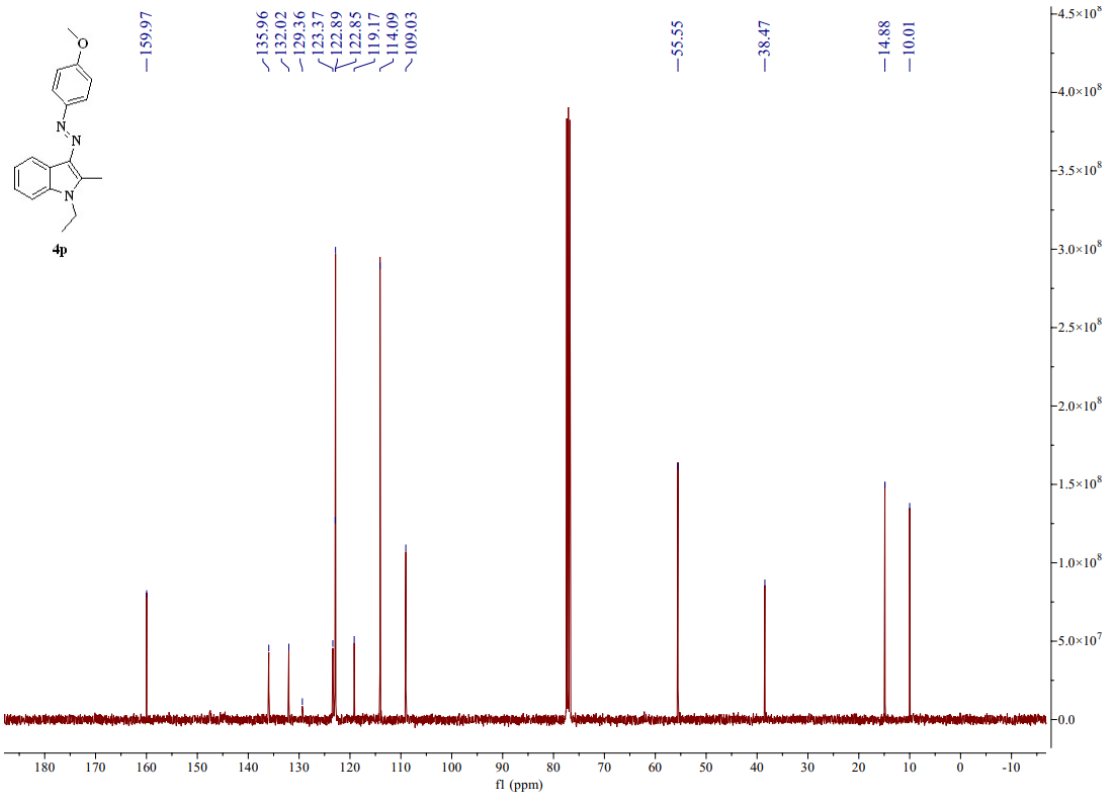


Figure 67S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4p***

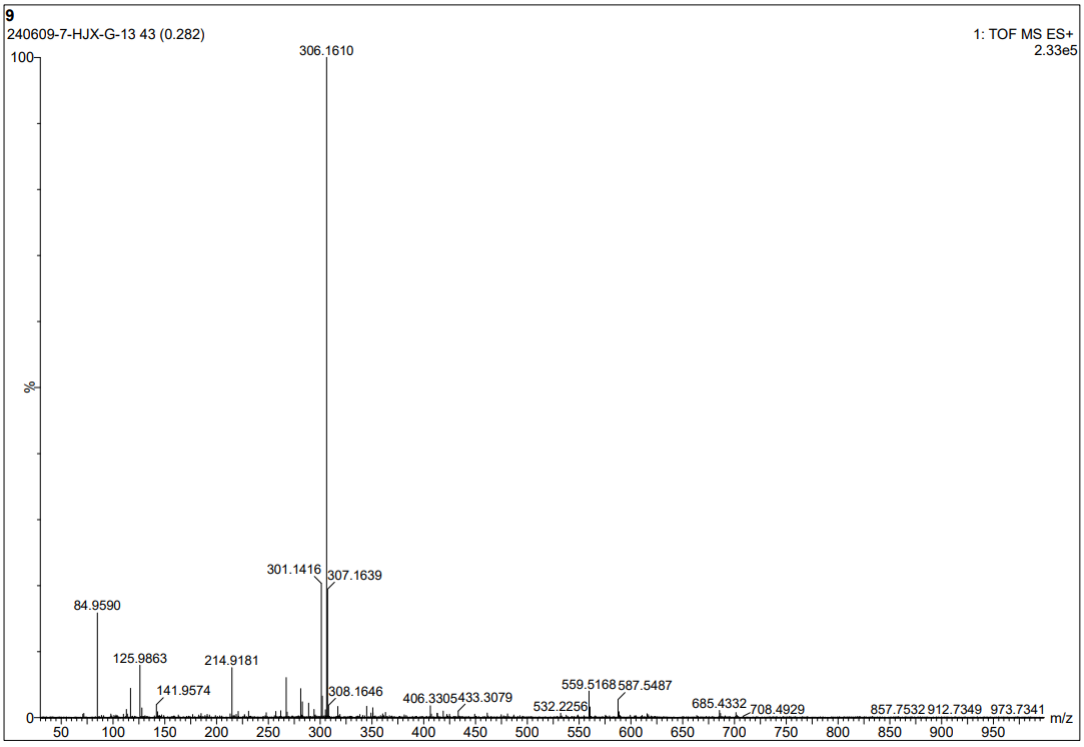
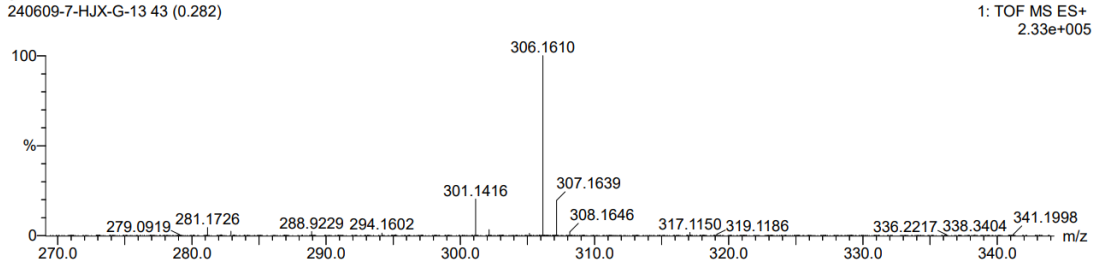


Figure 68S. *HR mass spectrum (ESI) of compound* ***4q***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
699 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 19-19 H: 20-20 N: 0-100 O: 0-100 Na: 0-3
9
240609-7-HJX-G-13 43 (0.282)



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
306.1610	306.1606	0.4	1.3	11.5	607.4	n/a	n/a	C19 H20 N3 O

Figure 69S. *HR mass spectrum (ESI) of compound* ***4q***

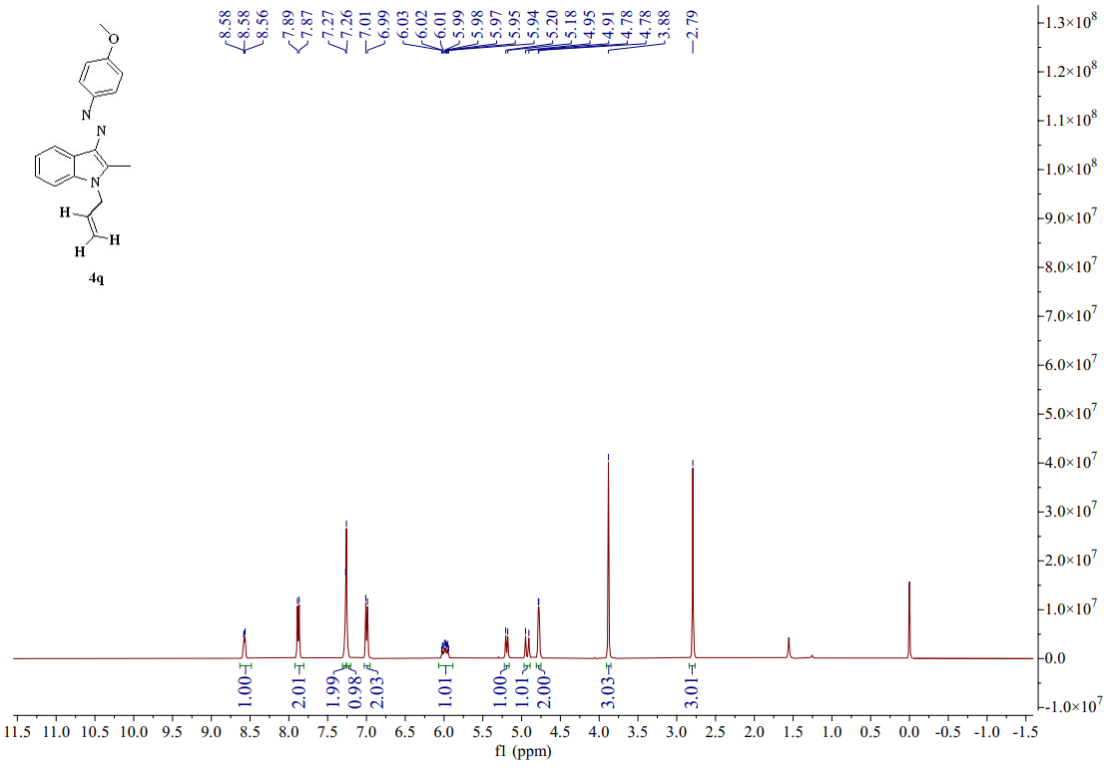


Figure 70S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4q***

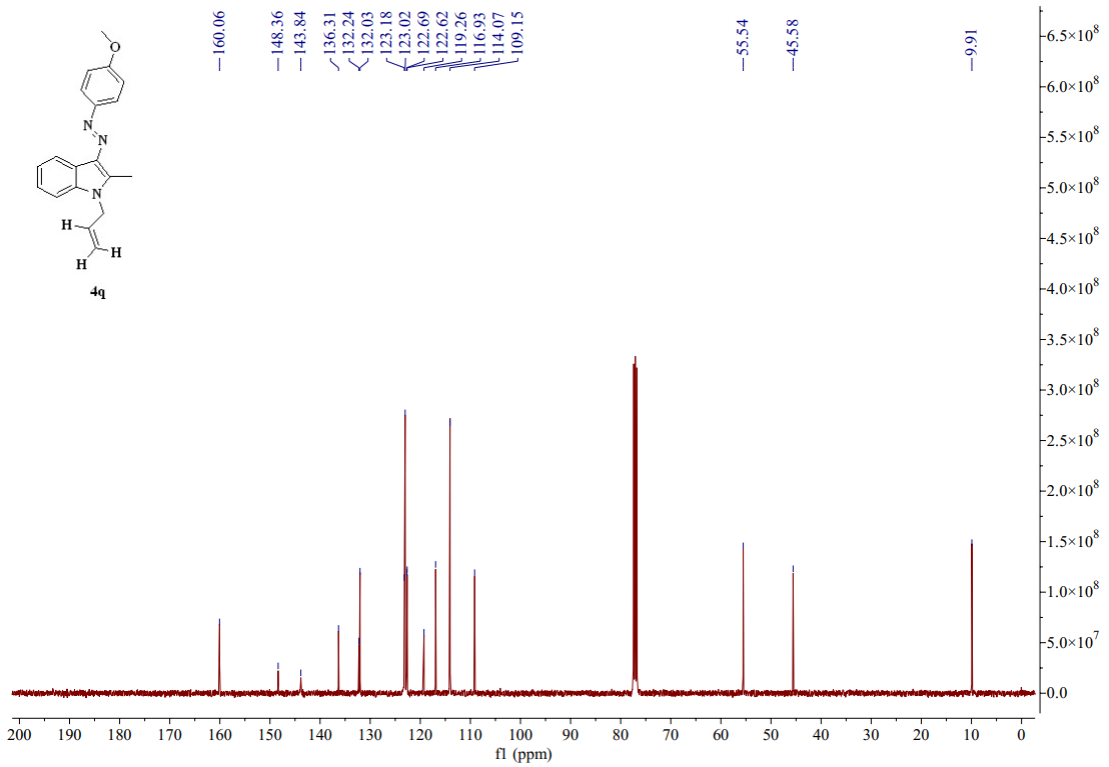


Figure 71S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4q***

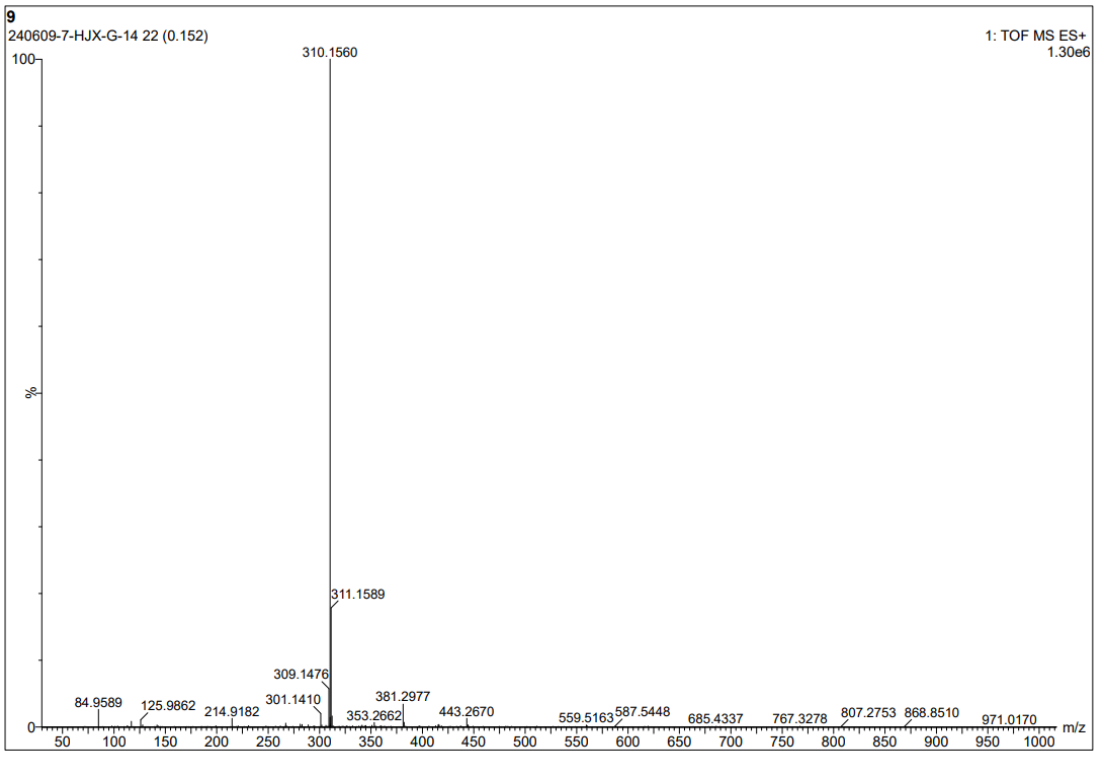
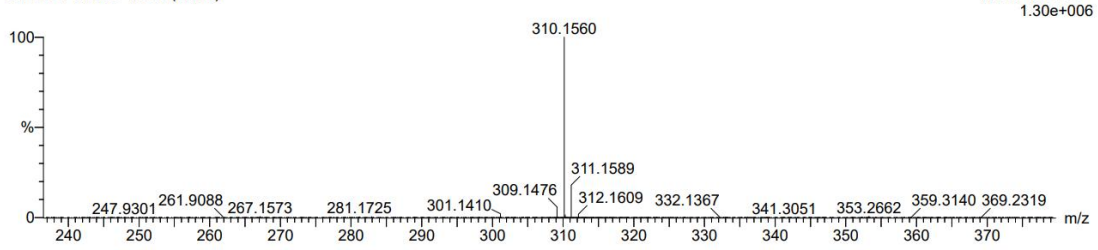


Figure 72S. *HR mass spectrum (ESI) of compound* ***4r***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
706 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 18-18 H: 20-20 N: 0-100 O: 0-100 Na: 0-3
9
240609-7-HJX-G-14 22 (0.152) 1: TOF MS ES+ 1.30e+006



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
310.1560	310.1556	0.4	1.3	10.5	856.9	n/a	n/a	C18 H20 N3 O2

Figure 73S. *HR mass spectrum (ESI) of compound* ***4r***

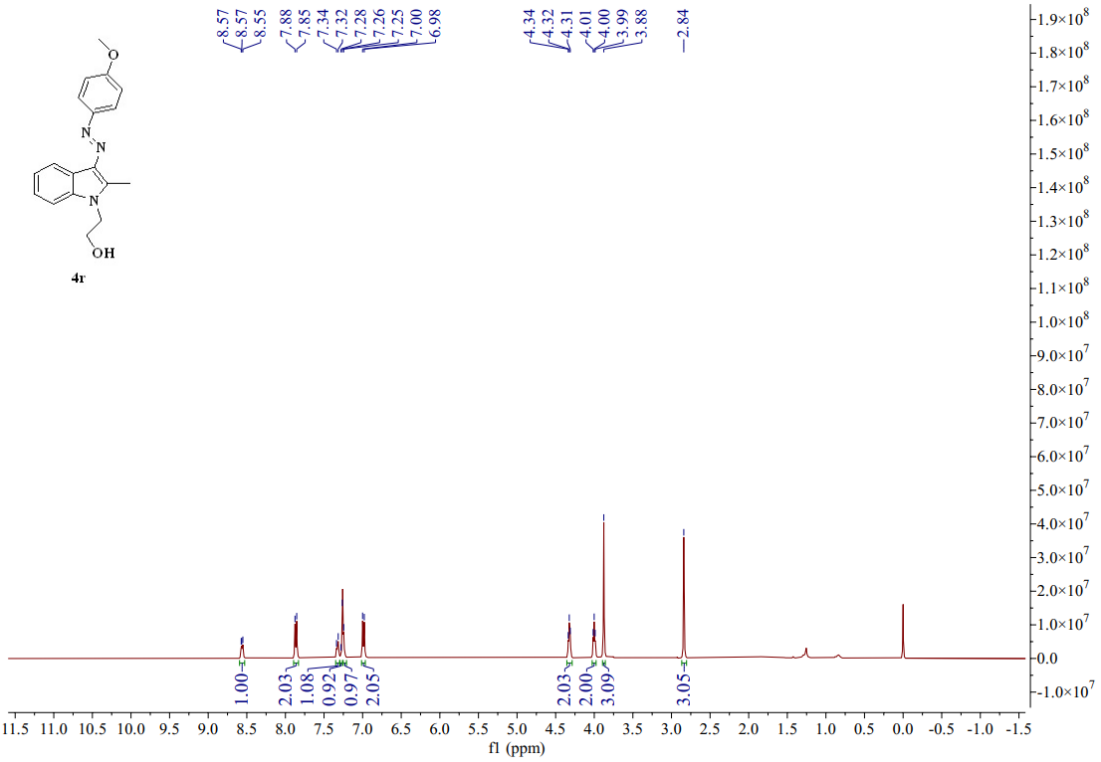


Figure 74S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4r***

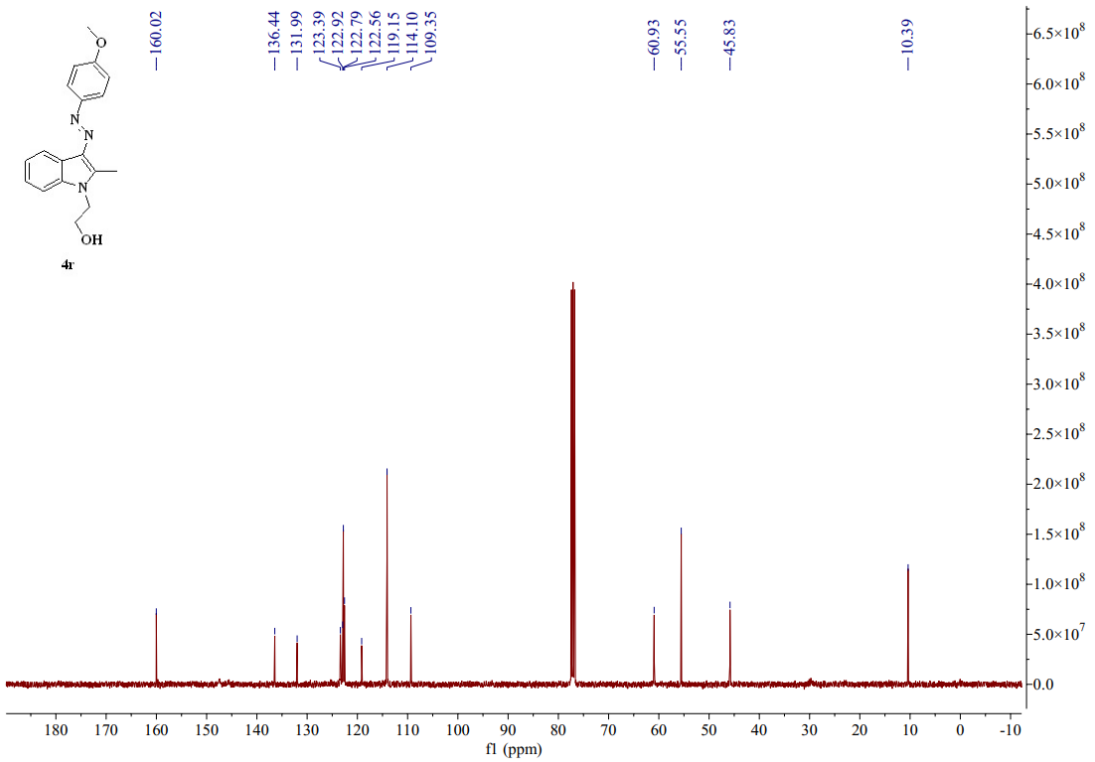


Figure 75S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4r***

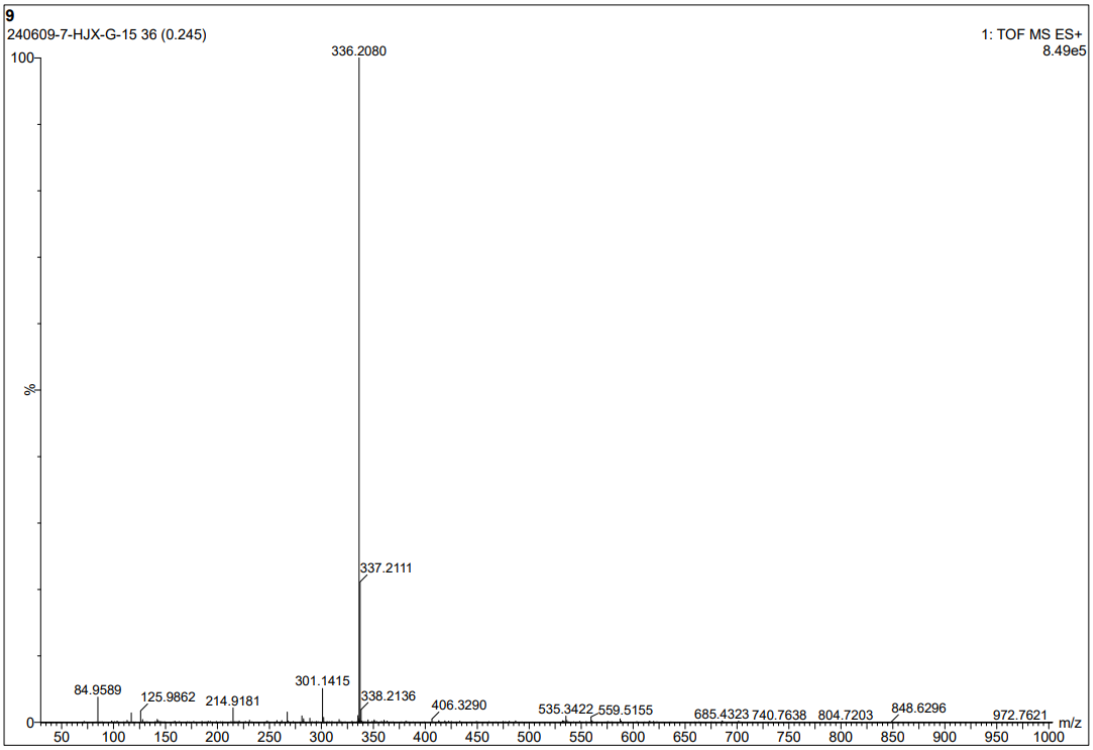
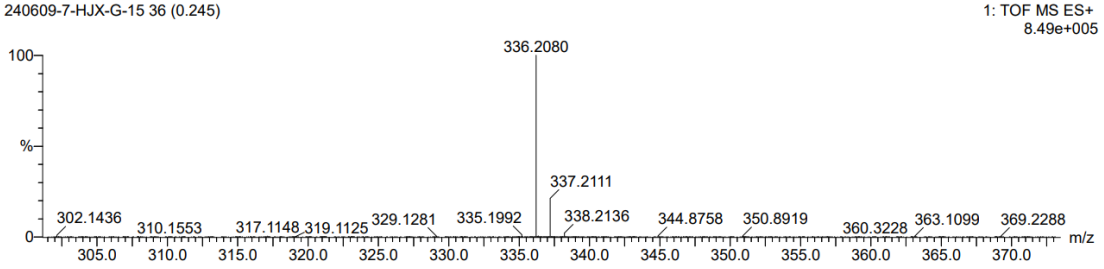


Figure 76S. *HR mass spectrum (ESI) of compound* ***4s***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
854 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 21-21 H: 26-26 N: 0-100 O: 0-100 Na: 0-3
9
240609-7-HJX-G-15 36 (0.245)



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
336.2080	336.2076	0.4	1.2	10.5	790.7	n/a	n/a	C21 H26 N3 O

Figure 77S. *HR mass spectrum (ESI) of compound* ***4s***

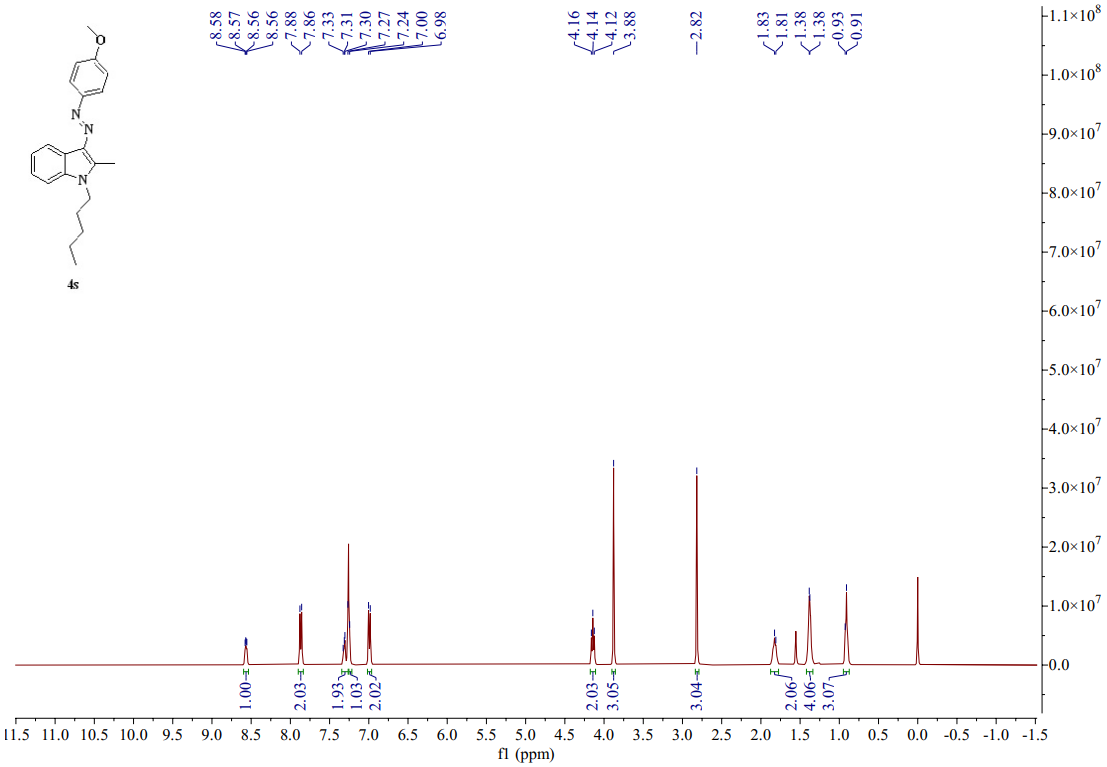


Figure 78S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4s***

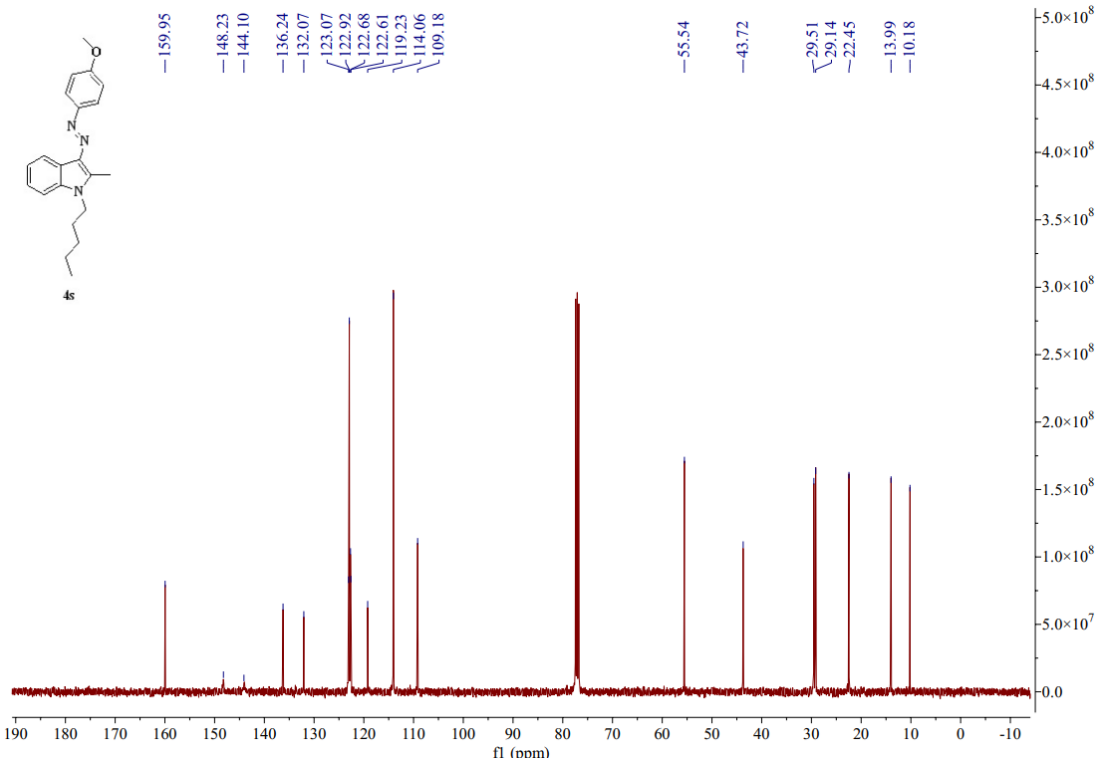


Figure 79S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4s***

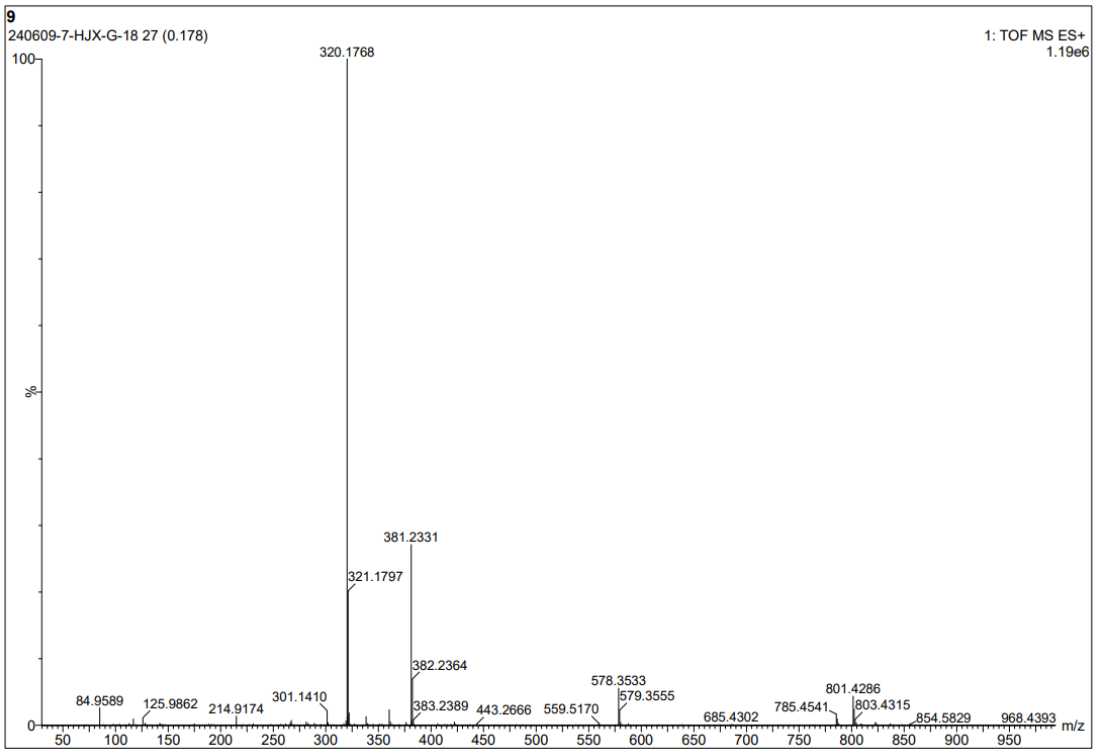
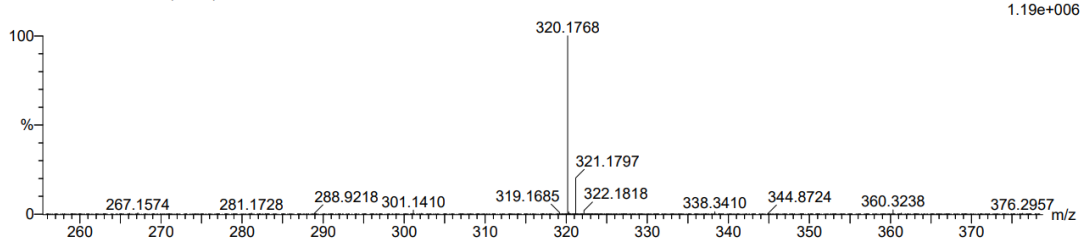


Figure 80S. *HR mass spectrum (ESI) of compound* ***4t***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
770 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 20-20 H: 22-22 N: 0-100 O: 0-100 Na: 0-3
9
240609-7-HJX-G-18 27 (0.178)



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
320.1768	320.1763	0.5	1.6	11.5	854.3	n/a	n/a	C20 H22 N3 O

Figure 81S. *HR mass spectrum (ESI) of compound* ***4t***

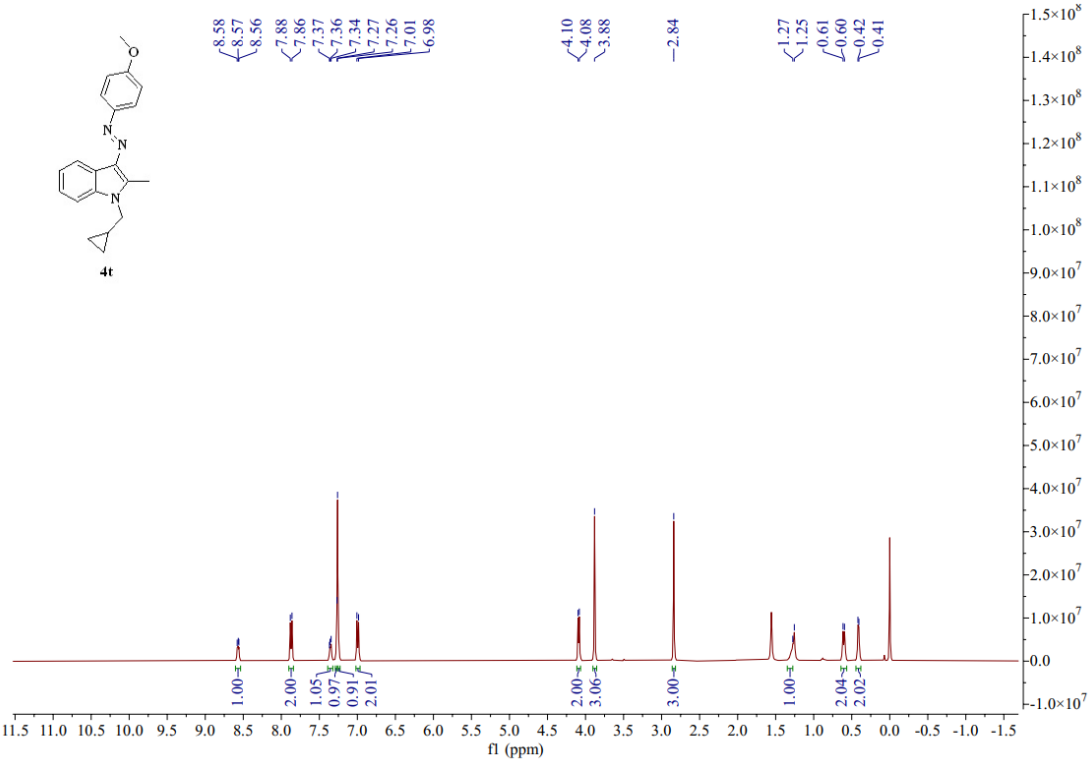


Figure 82S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4t***

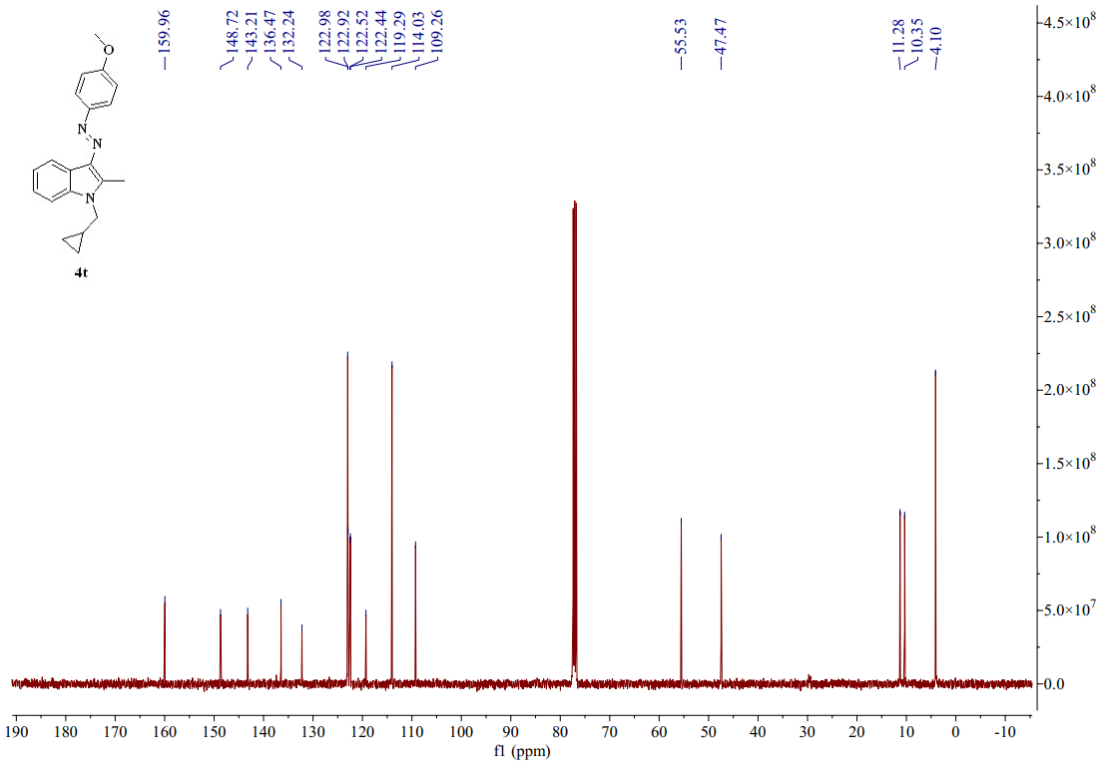


Figure 83S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4t***

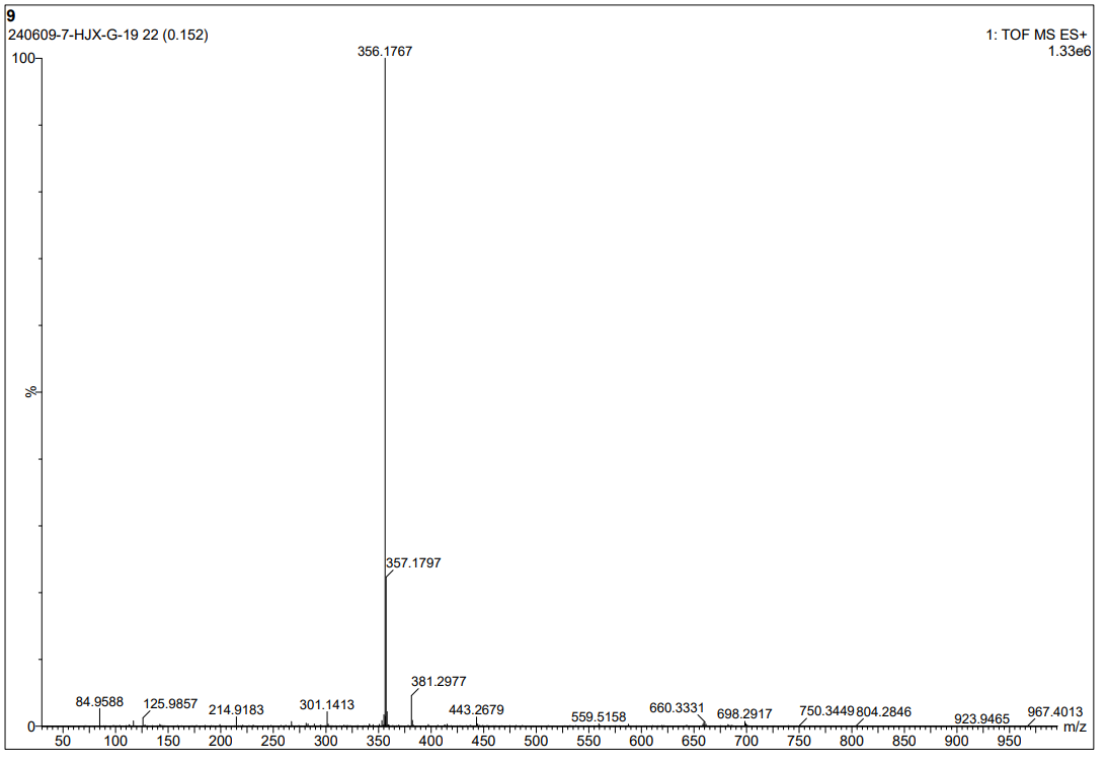
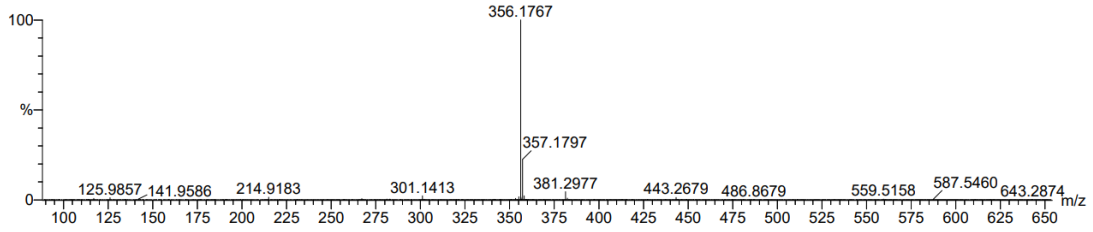


Figure 84S. *HR mass spectrum (ESI) of compound* ***4u***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
976 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 23-23 H: 22-22 N: 0-100 O: 0-100 Na: 0-3
9
240609-7-HJX-G-19 22 (0.152) 1: TOF MS ES+ 1.33e+006



Minimum:			-1.5					
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
356.1767	356.1763	0.4	1.1	14.5	871.5	n/a	n/a	C23 H22 N3 O

Figure 85S. *HR mass spectrum (ESI) of compound* ***4u***

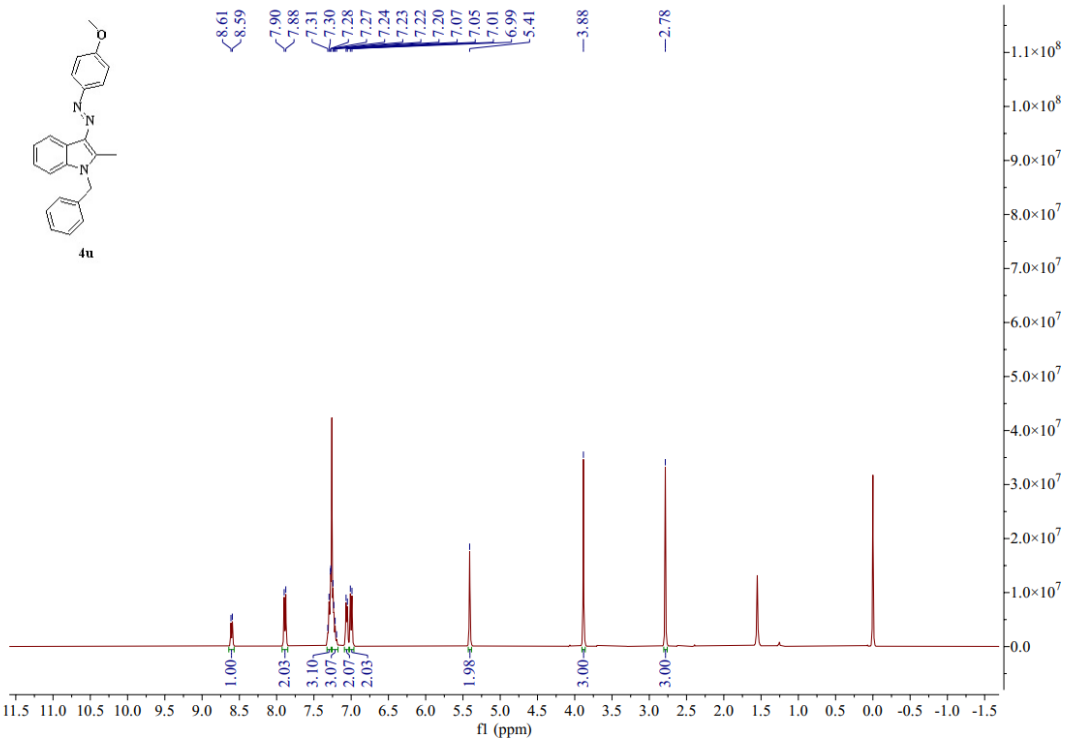


Figure 86S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4u***

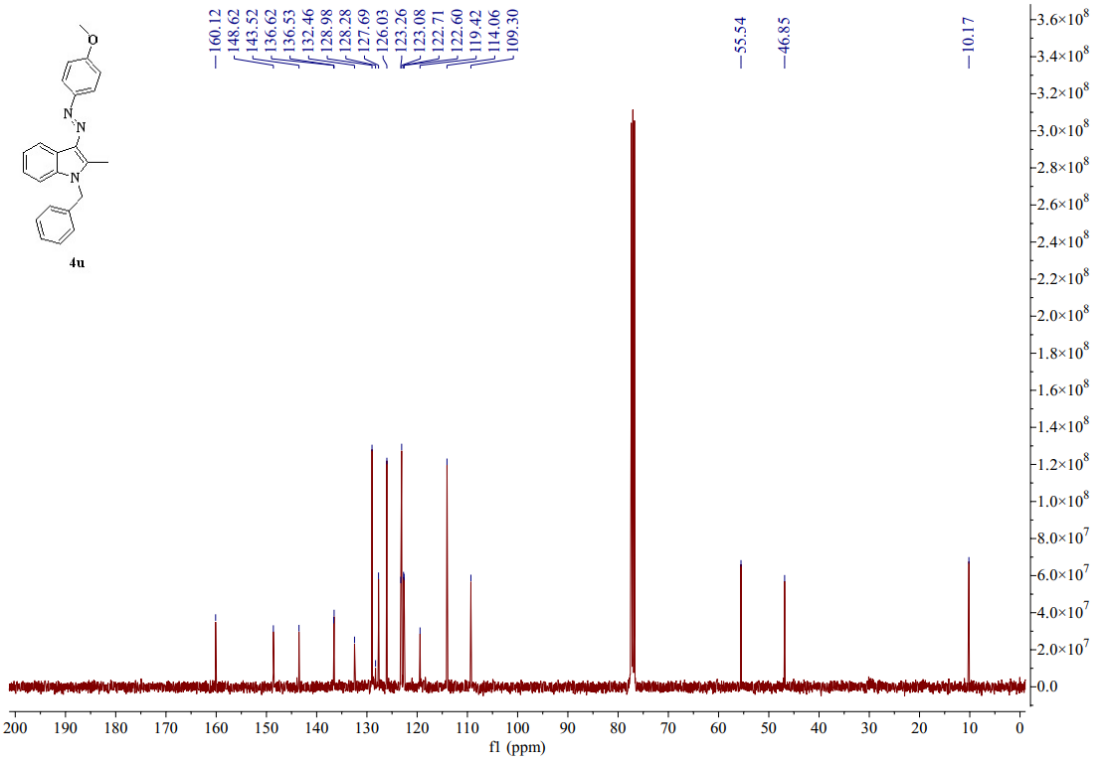


Figure 87S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4u***

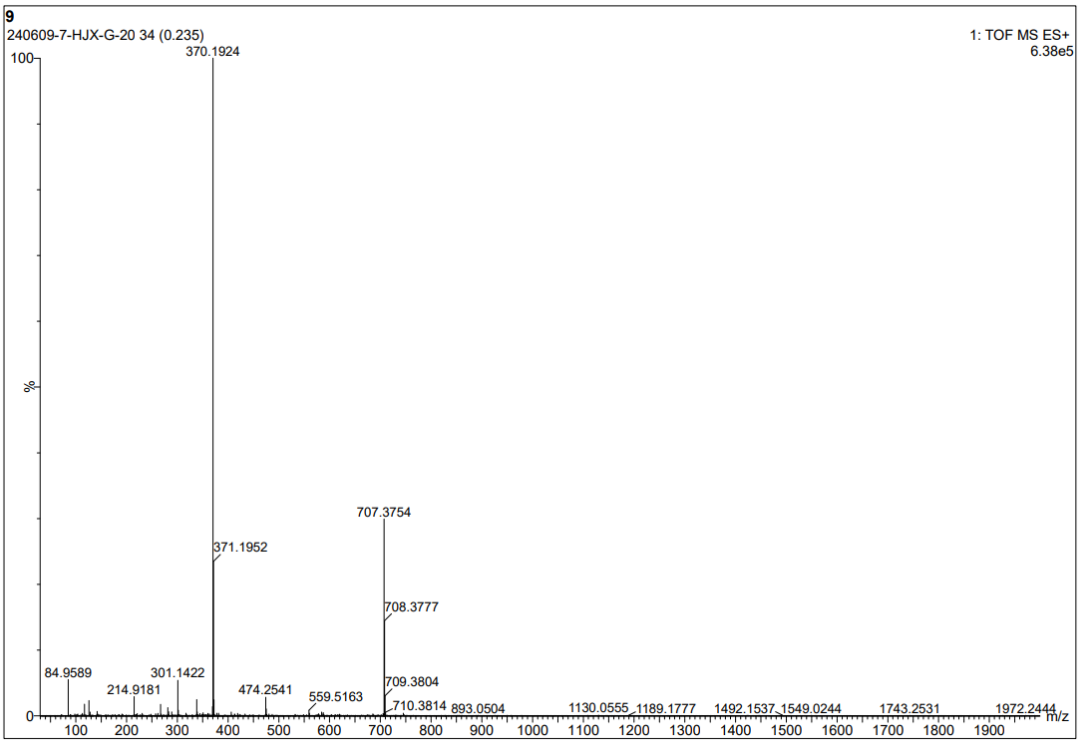
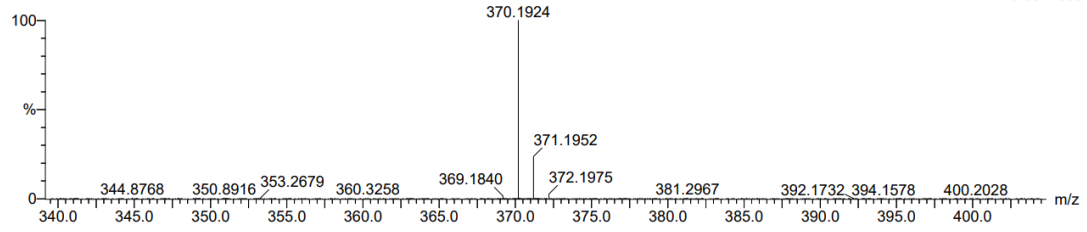


Figure 88S. *HR mass spectrum (ESI) of compound* ***4v***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1059 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 24-24 H: 24-24 N: 0-100 O: 0-100 Na: 0-3
9
240609-7-HJX-G-20 34 (0.235) 1: TOF MS ES+ 6.39e+005



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
370.1924	370.1919	0.5	1.4	14.5	668.2	n/a	n/a	C24 H24 N3 O

Figure 89S. *HR mass spectrum (ESI) of compound* ***4v***

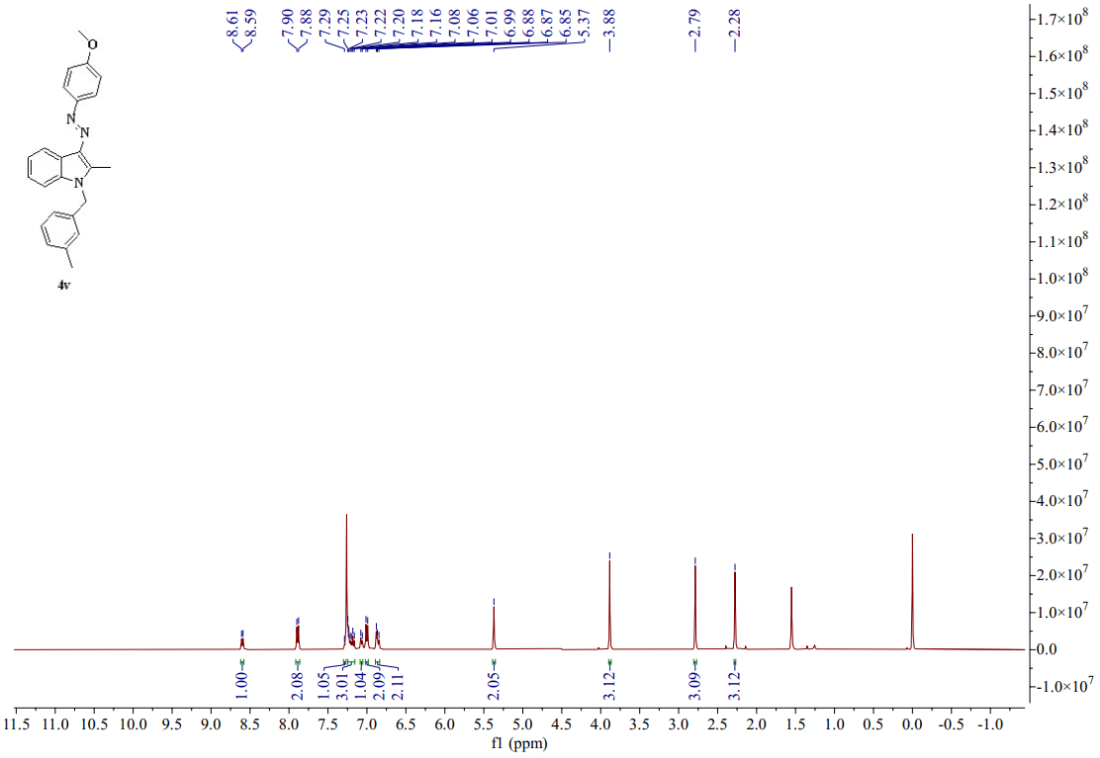


Figure 90S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4v***

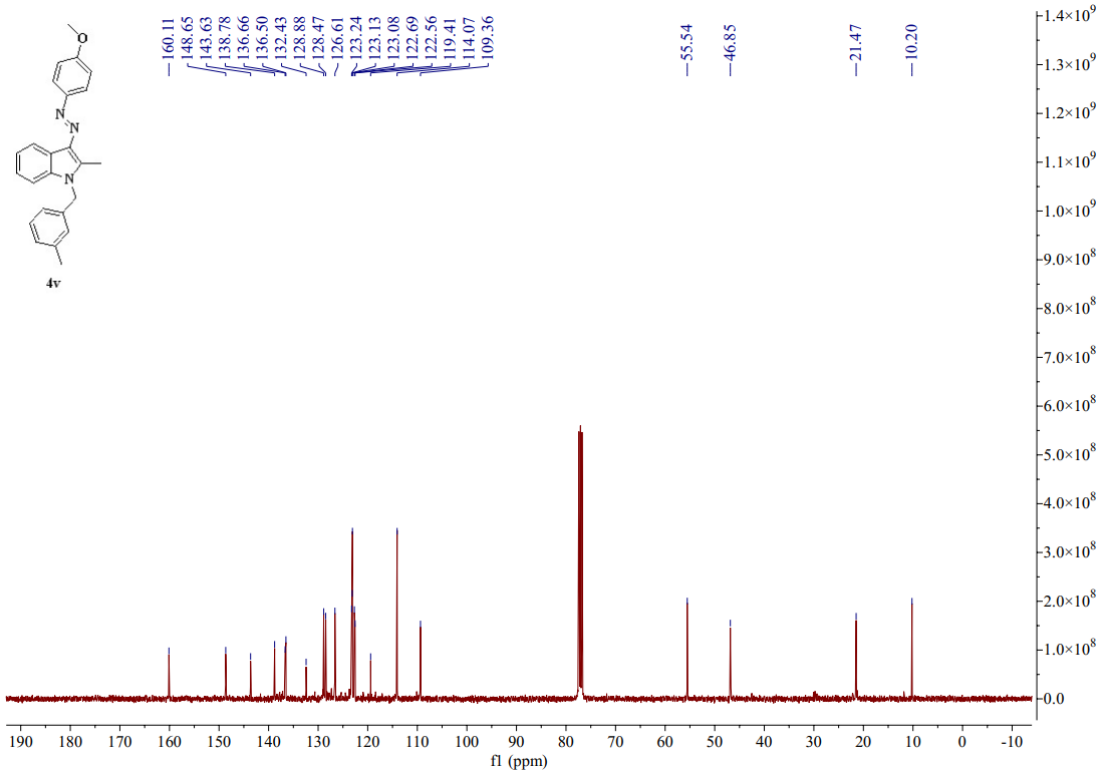


Figure 91S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4v***

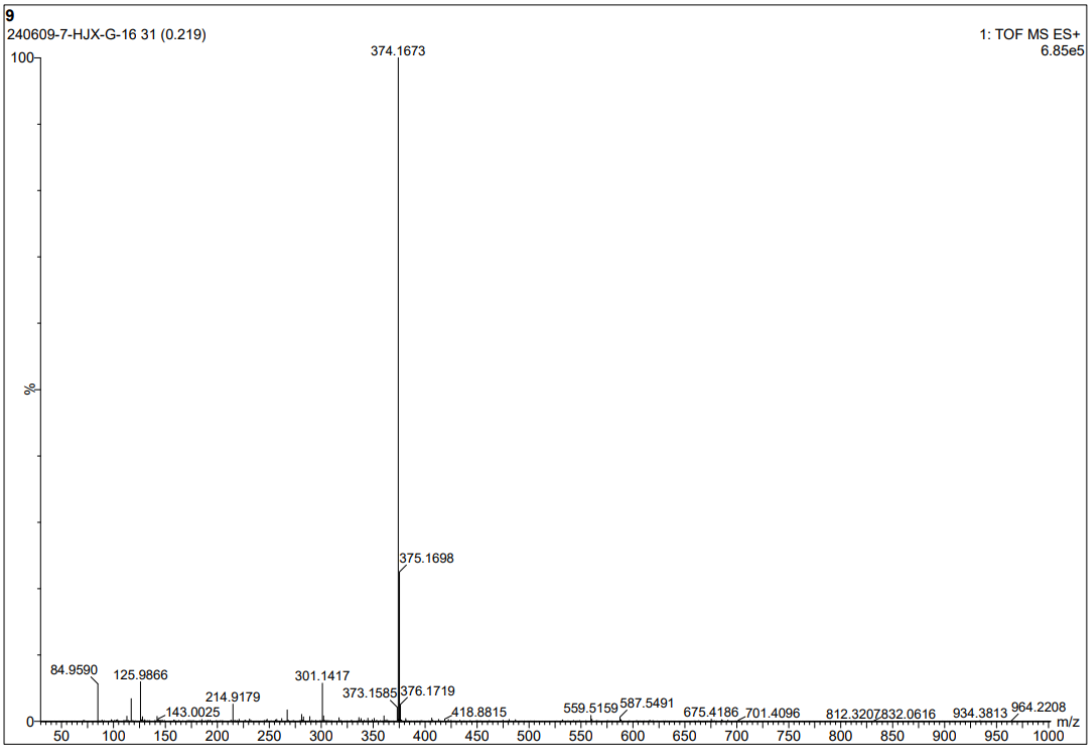


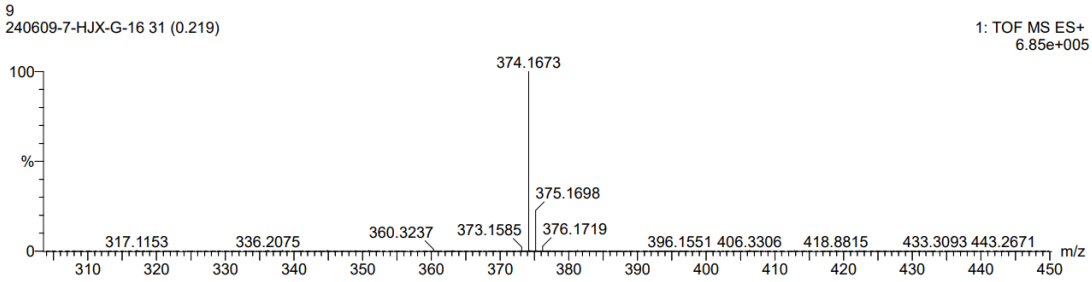
Figure 92S. *HR mass spectrum (ESI) of compound* ***4w***

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
2635 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 23-23 H: 21-21 N: 0-100 O: 0-100 Na: 0-3 F: 1-3

9
240609-7-HJX-G-16 31 (0.219)



Minimum:			-1.5				
Maximum:		5.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
374.1673	374.1669	0.4	1.1	14.5	717.4	n/a	n/a	C23 H21 N3 O F

Figure 93S. *HR mass spectrum (ESI) of compound* ***4w***

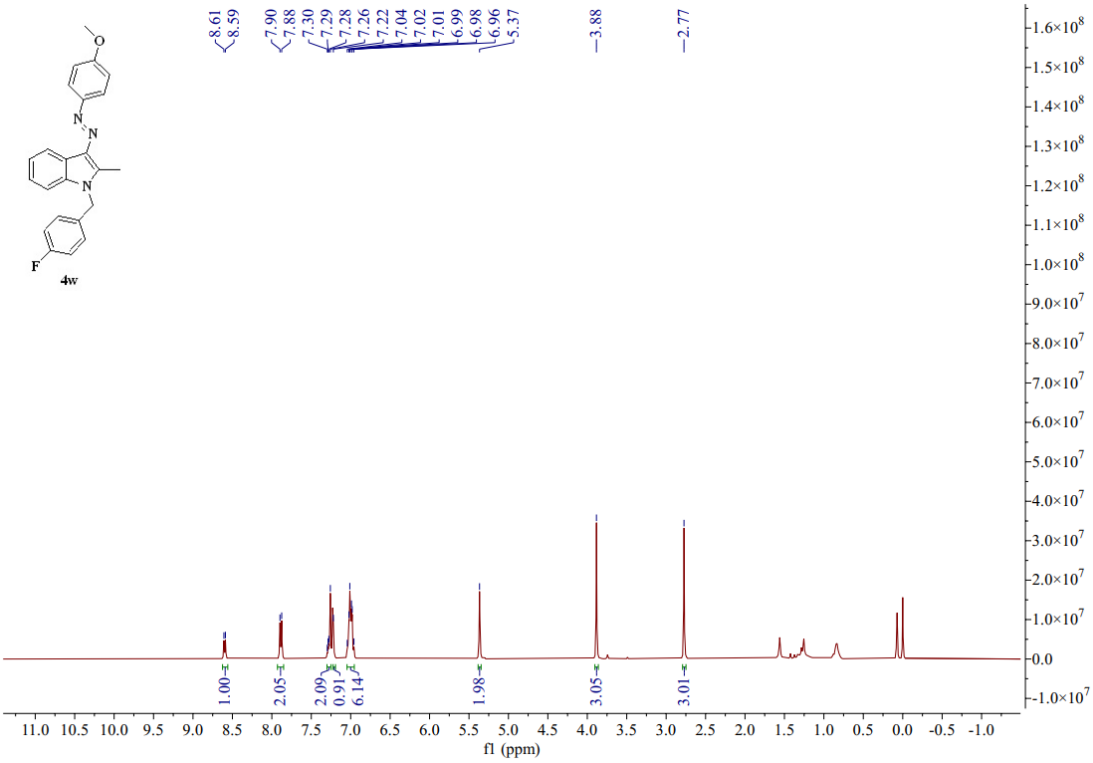


Figure 94S. *^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound* ***4w***

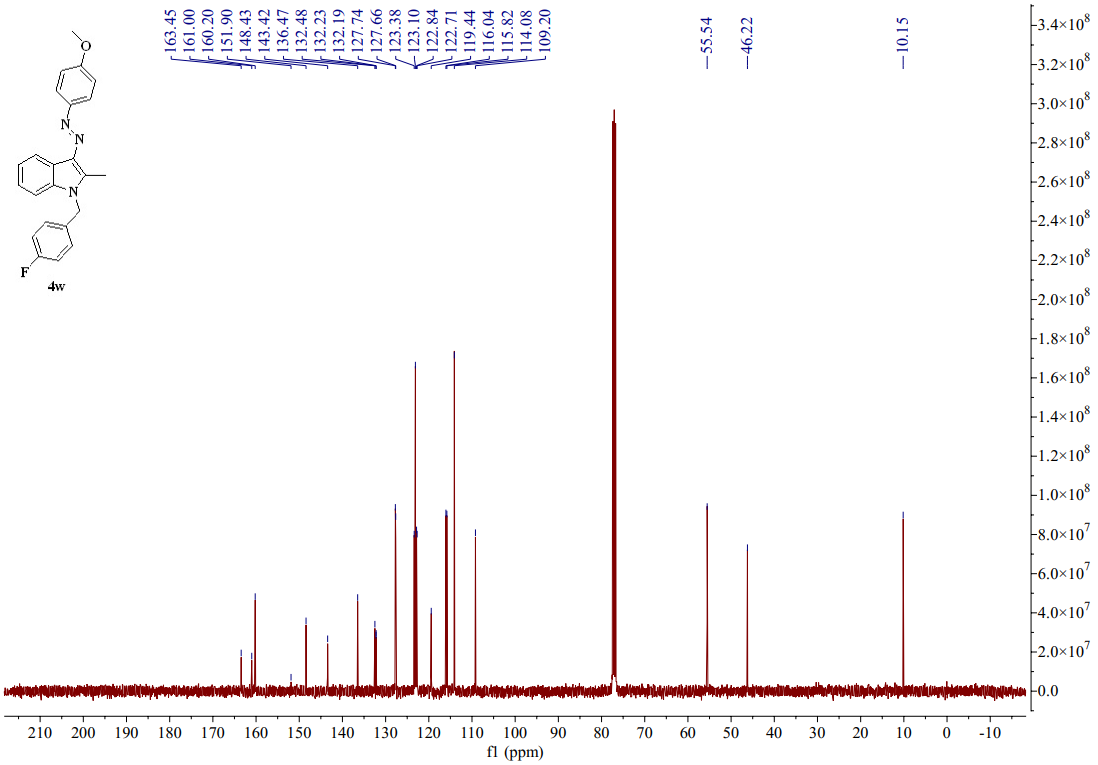


Figure 95S. *^{13}C NMR spectrum ($CDCl_3$, 101 MHz) of compound* ***4w***

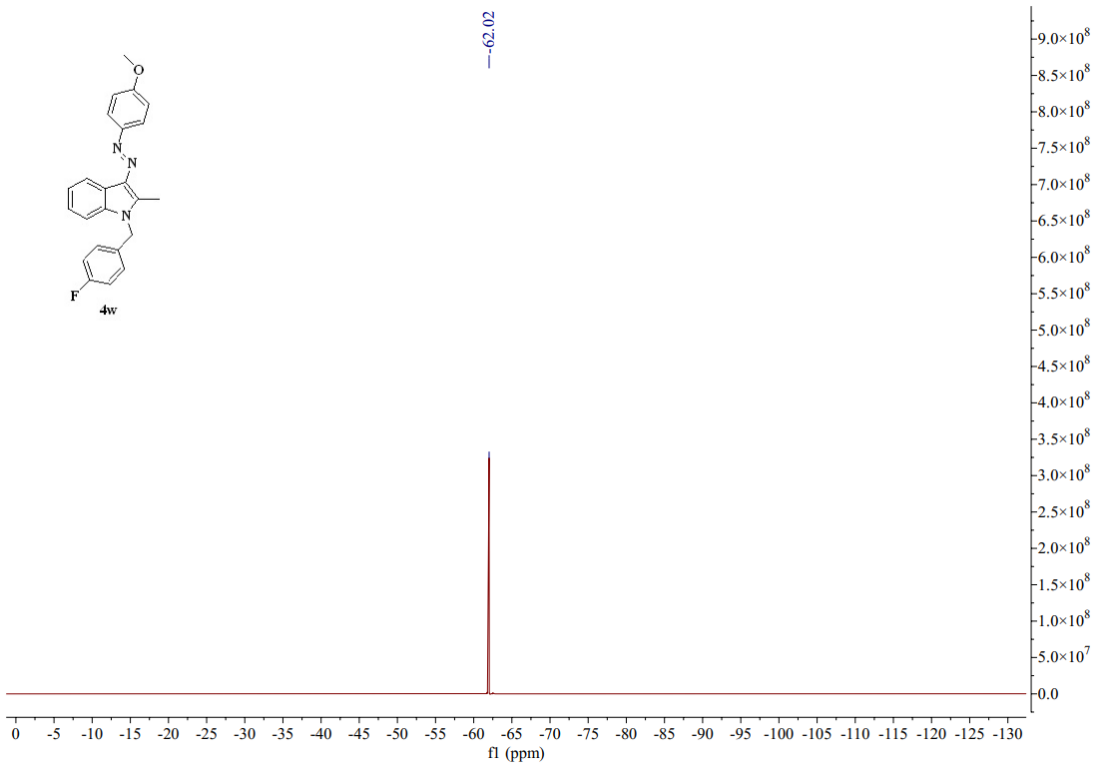


Figure 96S. *^{19}F NMR spectrum (CDCl3,377 MHz) of compound* ***4w***