

Supporting Information

for

Tandem Cu-catalyzed ketenimine formation and intramolecular nucleophile capture: Synthesis of 1,2-dihydro-2-iminoquinolines from 1-(o-acetamidophenyl)propargyl alcohols

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Analytical data

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Spectroscopic data for all the compounds

***N*-(2-(1-Hydroxyprop-2-ynyl)phenyl)acetamide (2a):** 95% yield (180 mg); white solid; mp 110-112 °C; R_f = 0.20 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, DMSO-*d*₆) δ 9.29 (s, 1H), 7.60-7.56 (m, 2H), 7.31-7.27 (m, 1H), 7.18 (t, J = 7.3 Hz, 1H), 6.20 (d, J = 5.6 Hz, 1H), 5.57 (dd, J = 5.6, 2.2 Hz, 1H), 3.47 (d, J = 2.2 Hz, 1H), 2.07 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 168.7, 135.9, 134.0, 128.5, 127.6, 125.1, 84.9, 76.2, 60.1, 24.1; IR (cm⁻¹) ν 3390, 3021, 2401, 1674, 1216; HRMS (ESI-TOF) calcd for C₁₁H₁₁NO [M + H - H₂O]⁺ 172.0762, found 172.0739.

***N*-(5-Fluoro-2-(1-hydroxyprop-2-ynyl)phenyl)acetamide (2b):** 82% yield (170 mg); white solid; mp 130-132 °C; R_f = 0.20 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, DMSO-*d*₆) δ 9.34 (s, 1H), 7.61-7.55 (m, 2H), 7.03-6.96 (m, 1H), 6.33 (d, J = 5.6 Hz, 1H), 5.61 (dd, J = 5.6, 2.2 Hz, 1H), 3.52 (d, J = 2.2 Hz, 1H), 2.09 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 168.9, 163.0, 160.6, 137.7, 137.6, 129.3, 129.2, 129.1, 111.3, 111.1, 110.9, 110.7, 84.5, 76.6, 59.7, 24.3; IR (cm⁻¹) ν 3684, 3019, 2400, 1605, 1215; HRMS (ESI-TOF) calcd for C₁₁H₁₀FNO [M + H - H₂O]⁺ 190.0668, found 190.0644.

***N*-(2-(2-Hydroxybut-3-yn-2-yl)phenyl)acetamide (2c) [1]:** 79% yield (160mg); white solid; mp 133-135 °C; R_f = 0.25 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, CDCl₃) δ 9.27 (s, 1H), 8.13 (d, J = 8.0 Hz, 1H), 7.64 (dd, J = 8.0, 1.4Hz, 1H), 7.34-7.28 (m, 1H), 7.08 (t, J = 7.6 Hz, 1H), 3.35 (s, 1H), 2.76 (s, 1H), 2.15 (s, 3H), 1.88 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 168.5, 136.3, 131.4, 129.1, 126.4, 124.0, 123.6, 86.0, 74.5, 71.2, 30.5, 25.0; IR (cm⁻¹) ν 3685, 3019, 2400, 1632, 1215.

***N*-(2-(3-Hydroxypent-1-yn-3-yl)phenyl)acetamide (2d):** 75% yield (163 mg); white solid; mp 120-122 °C; R_f = 0.25 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, CDCl₃) δ 9.37 (s, 1H), 8.16 (d, J = 8.0 Hz, 1H), 7.66 (dd, J = 8.0, 1.3Hz, 1H), 7.33-7.27 (m, 1H), 7.07 (t, J = 7.5 Hz,

1H), 3.33 (s, 1H), 2.81 (s, 1H), 2.13 (s, 3H), 2.09-2.01 (m, 2H), 0.97 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.5, 136.3, 130.2, 128.9, 127.9, 123.6, 123.2, 84.7, 76.1, 75.9, 34.9, 25.1, 9.3; IR (cm^{-1}) ν 3371, 3020, 2401, 1677, 1215; HRMS (ESI-TOF) calcd for $\text{C}_{13}\text{H}_{14}\text{NO}$ [$\text{M} + \text{H} - \text{H}_2\text{O}$] $^+$ 200.1075, found 200.1067.

***N*-(2-(3-Hydroxyhex-1-yn-3-yl)phenyl)acetamide (2e):** 70% yield (162 mg); white solid; mp 148-150 °C; $R_f = 0.25$ (SiO_2 , 30% EtOAc/Hexanes); ^1H NMR (400 MHz, CDCl_3) δ 9.40 (s, 1H), 8.17 (d, $J = 8.1$ Hz, 1H), 7.66 (dd, $J = 8.1, 1.2$ Hz, 1H), 7.32-7.27 (m, 1H), 7.06 (t, $J = 7.6$ Hz, 1H), 3.32 (s, 1H), 2.82 (s, 1H), 2.13 (s, 3H), 2.06-1.92 (m, 2H), 1.60-1.51 (m, 1H), 1.33-1.27 (m, 1H), 0.89 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.6, 136.2, 130.5, 128.7, 127.7, 123.5, 122.9, 85.1, 75.6, 75.3, 44.1, 25.1, 18.2, 14.0; IR (cm^{-1}) ν 3373, 3020, 2401, 1676, 1216; HRMS (ESI-TOF) calcd for $\text{C}_{14}\text{H}_{17}\text{NO}$ [$\text{M} + \text{H} - \text{H}_2\text{O}$] $^+$ 214.1232, found 214.1223.

***N*-(2-(3-Hydroxy-4-methylpent-1-yn-3-yl)-4-methylphenyl)acetamide (2f):** 72% yield (177 mg); white solid; mp 180-182 °C; $R_f = 0.25$ (SiO_2 , 30% EtOAc/Hexanes); ^1H NMR (400 MHz, CDCl_3) δ 9.24 (s, 1H), 8.02 (d, $J = 8.2$ Hz, 1H), 7.46 (s, 1H), 7.10 (dd, $J = 8.2, 1.6$ Hz, 1H), 3.09 (s, 1H), 2.83 (s, 1H), 2.36-2.28 (m, 4H), 2.12 (s, 3H), 1.16 (d, $J = 6.5$ Hz, 3H), 0.76 (d, $J = 6.5$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 167.9, 133.4, 132.8, 129.8, 129.2, 123.2, 82.9, 80.1, 77.1, 36.5, 25.0, 21.0, 18.7, 17.1; IR (cm^{-1}) ν 3681, 3019, 2400, 1626, 1215; HRMS (ESI-TOF) calcd for $\text{C}_{15}\text{H}_{18}\text{NO}$ [$\text{M} + \text{H} - \text{H}_2\text{O}$] $^+$ 228.1388, found 228.1380.

***N*-(2-(1-Hydroxy-1-phenylprop-2-ynyl)phenyl)acetamide (2g) [1]:** 85% yield (226 mg); white solid; mp 125-127 °C; $R_f = 0.30$ (SiO_2 , 30% EtOAc/Hexanes); ^1H NMR (400 MHz, CDCl_3) δ 8.39 (s, 1H), 7.97 (d, $J = 7.9$ Hz, 1H), 7.73 (d, $J = 7.6$ Hz, 1H), 7.48-7.44 (m, 2H), 7.39-7.30 (m, 4H), 7.14 (t, $J = 7.6$ Hz, 1H), 3.61 (s, 1H), 2.96 (s, 1H), 1.79 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.3, 142.8, 136.1, 132.1, 129.4, 128.5, 128.2, 127.9, 125.6, 124.3, 123.8, 84.7, 77.4, 74.4, 24.2; IR (cm^{-1}) ν 3683, 3021, 2401, 1679, 1215.

***N*-(2-(1-Hydroxy-1-phenylprop-2-ynyl)-5-methylphenyl)acetamide (2h) [2]:** 80% yield (224 mg); white solid; mp 155-157 °C; R_f = 0.30 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, CDCl₃) δ 8.16 (s, 1H), 7.78 (d, J = 8.1 Hz, 1H), 7.58 (s, 1H), 7.46 (d, J = 6.9 Hz, 2H), 7.36-7.28 (m, 3H), 7.18 (d, J = 7.2 Hz, 1H), 3.52 (s, 1H), 2.96 (s, 1H), 2.35 (s, 3H), 1.76 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 168.2, 142.9, 133.8, 133.4, 132.4, 130.0, 128.7, 128.5, 128.4, 125.7, 124.8, 84.9, 77.5, 74.5, 24.2, 21.2; IR (cm⁻¹) ν 3403, 3021, 2401, 1638, 1215; HRMS (ESI-TOF) calcd for C₁₈H₁₇NO [M + H – H₂O]⁺ 262.1232, found 262.1232.

***N*-(2-(1-(2-Chlorophenyl)-1-hydroxyprop-2-ynyl)phenyl)acetamide (2i):** 75% yield (225 mg); white solid; mp 165-167 °C; R_f = 0.30 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, CDCl₃) δ 8.41 (s, 1H), 7.93 (d, J = 8.0 Hz, 1H), 7.69 (d, J = 7.7 Hz, 1H), 7.62-7.57 (m, 1H), 7.42-7.35 (m, 2H), 7.32-7.27 (m, 2H), 7.14 (t, J = 7.4 Hz, 1H), 4.48 (s, 1H), 2.97 (s, 1H), 1.85 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 168.6, 139.0, 135.9, 132.3, 131.8, 131.1, 129.9, 129.6, 129.1, 128.3, 127.1, 124.9, 124.5, 82.9, 77.5, 74.8, 24.4; IR (cm⁻¹) ν 3392, 3019, 2400, 1637, 1215; HRMS (ESI-TOF) calcd for C₁₇H₁₄ClNO [M + H – H₂O]⁺ 282.0685, found 282.0676.

***N*-(4-Chloro-2-(1-hydroxy-1-phenylprop-2-ynyl)phenyl)acetamide (2j) [2]:** 80% yield (240 mg); white solid; mp 160-162 °C; R_f = 0.30 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, CDCl₃) δ 8.35 (s, 1H), 7.93 (d, J = 8.7 Hz, 1H), 7.74 (s, 1H), 7.47-7.42 (m, 2H), 7.38-7.29 (m, 4H), 3.79 (s, 1H), 2.98 (s, 1H), 1.78 (s, 3H); ¹³C NMR (100 MHz, CDCl₃+DMSO-*d*₆) δ 165.8, 141.8, 133.7, 133.6, 126.8, 126.4, 126.1, 124.1, 123.4, 83.5, 76.9, 71.6, 22.8; IR (cm⁻¹) ν 3414, 3021, 1648, 1515, 1216; HRMS (ESI-TOF) calcd for C₁₇H₁₄ClNO [M + H – H₂O]⁺ 282.0685, found 282.0675.

***N*-(2-(1-(4-Fluorophenyl)-1-hydroxyprop-2-ynyl)-4-methylphenyl)acetamide (2k):** 70% yield (208 mg); white solid; mp 147-149 °C; R_f = 0.30 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, CDCl₃) δ 8.20 (s, 1H), 7.79 (d, J = 8.2 Hz, 1H), 7.55 (s, 1H), 7.46-7.40 (m, 2H), 7.18 (dd, J

= 8.2, 1.4 Hz, 1H), 7.04-6.99 (m, 2H), 3.56 (s, 1H), 2.97 (s, 1H), 2.35 (s, 3H) 1.79 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.3, 163.7, 161.3, 139.0, 133.9, 133.4, 132.2, 130.0, 128.5, 127.7, 127.6, 124.8, 115.5, 115.3, 84.9, 77.5, 74.1, 24.2, 21.2; IR (cm^{-1}) ν 3398, 3020, 2401, 1671, 1216; HRMS (ESI-TOF) calcd for $\text{C}_{18}\text{H}_{15}\text{FNO}$ $[\text{M} + \text{H} - \text{H}_2\text{O}]^+$ 280.1137, found 280.1130.

***N*-(2-(1-Hydroxy-1-(4-methoxyphenyl)prop-2-ynyl)phenyl)acetamide (2I):** 82% yield (242 mg); white solid; mp 149-151°C; R_f = 0.30 (SiO_2 , 30% EtOAc/Hexanes); ^1H NMR (400 MHz, CDCl_3) δ 8.47 (s, 1H), 8.00 (d, J = 8.0 Hz, 1H), 7.67 (d, J = 7.6 Hz, 1H), 7.40-7.35 (m, 3H), 7.12 (t, J = 7.6 Hz, 1H), 6.87-6.84 (m, 2H), 3.79 (s, 3H), 3.57 (s, 1H), 2.94 (s, 1H), 1.85 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.4, 159.6, 136.3, 134.9, 132.2, 129.4, 127.9, 127.2, 124.2, 123.9, 113.9, 85.1, 77.0, 74.3, 55.4, 24.5; IR (cm^{-1}) ν 3397, 3021, 2401, 1637, 1216; HRMS (ESI-TOF) calcd for $\text{C}_{18}\text{H}_{17}\text{NO}_2$ $[\text{M} + \text{H} - \text{H}_2\text{O}]^+$ 278.1181, found 278.1173.

1-(2-Acetamidophenyl)prop-2-ynyl acetate (3): 80% yield (185 mg); white solid; mp 118-120 °C; R_f = 0.60 (SiO_2 , 30% EtOAc/Hexanes); ^1H NMR (400 MHz, CDCl_3) δ 8.41 (s, 1H), 7.89 (d, J = 8.0 Hz, 1H), 7.63 (dd, J = 7.8, 1.3 Hz, 1H), 7.41-7.36 (m, 1H), 7.18 (t, J = 7.8 Hz, 1H), 6.52 (d, J = 2.2 Hz, 1H), 2.71 (d, J = 2.2 Hz, 1H), 2.22 (s, 3H), 2.11 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.7, 168.7, 135.6, 130.3, 129.6, 127.3, 125.3, 124.7, 79.3, 76.3, 62.9, 24.3, 20.9; IR (cm^{-1}) ν 3355, 3020, 2402, 1688, 1217; HRMS (ESI-TOF) calcd for $\text{C}_{13}\text{H}_{14}\text{NO}_3$ $[\text{M} + \text{Na}]^+$ 254.0793, found 254.0780.

(*E*)-3-(2-Acetamidophenyl)-*N*-tosylacrylamide (5): 46% yield (165 mg); white solid; mp 162-164 °C; R_f = 0.25 (SiO_2 , 30% EtOAc/Hexanes); ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 12.25 (s, 1H), 9.76 (s, 1H), 7.87 (d, J = 8.2 Hz, 2H), 7.67 (d, J = 15.7 Hz, 1H), 7.58 (d, J = 7.6 Hz, 1H), 7.46-7.37 (m, 4H), 7.23 (d, J = 7.6 Hz, 1H), 6.54 (d, J = 15.7 Hz, 1H), 2.41 (s, 3H), 2.06 (s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ 169.2, 163.8, 144.7, 140.2, 137.7, 137.0, 131.1, 130.0, 128.6,

128.2, 126.9, 126.9, 126.1, 120.1, 23.7, 21.5; IR (cm⁻¹) ν 3385, 3021, 1626, 1415, 1216; HRMS (ESI-TOF) calcd for C₁₈H₁₉N₂O₄S [M + H]⁺ 359.1066, found 359.1057.

(E)-4-Methyl-N-(quinolin-2(1H)-ylidene)benzenesulfonamide (9a): 62% yield (185 mg); white solid; mp 145-147 °C; R_f = 0.20 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, CDCl₃) δ 11.92 (s, 1H), 7.91 (d, J = 8.3 Hz, 2H), 7.87 (d, J = 9.4 Hz, 1H), 7.65-7.60 (m, 2H), 7.49 (d, J = 8.6 Hz, 1H), 7.39-7.34 (m, 1H), 7.27 (d, J = 8.3 Hz, 2H), 7.00 (d, J = 9.4 Hz, 1H), 2.40 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 154.6, 142.6, 140.9, 140.0, 136.7, 131.8, 129.4, 128.1, 126.3, 124.7, 121.4, 120.1, 117.6, 21.5; IR (cm⁻¹) ν 3411, 3020, 1636, 1415, 1216; HRMS (ESI-TOF) calcd for C₁₆H₁₅N₂O₂S [M + H]⁺ 299.0854, found 299.0845.

(E)-N-(Quinolin-2(1H)-ylidene)-4-(trifluoromethyl)benzenesulfonamide (9b): 71% yield (250 mg); white solid; mp 180-182 °C; R_f = 0.20 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, DMSO-*d*₆) δ 13.43 (s, 1H), 8.30 (d, J = 9.5 Hz, 1H), 8.10 (d, J = 7.5 Hz, 2H), 7.92 (d, J = 8.3 Hz, 2H), 7.85 (d, J = 7.5 Hz, 1H), 7.74- 7.68 (m, 1H), 7.60 (d, J = 8.3 Hz, 2H), 7.44-7.38 (m, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 156.0, 148.0, 142.8, 137.8, 132.7, 132.1, 131.8, 128.7, 128.1, 127.3, 126.6, 126.5, 126.5, 125.4, 124.8, 122.7, 121.4, 119.9, 117.4, 115.9; IR (cm⁻¹) ν 3389, 3021, 1636, 1408, 1215; HRMS (ESI-TOF) calcd for C₁₆H₁₂F₃N₂O₂S [M + H]⁺ 353.0572, found 353.0542.

(E)-N-(Quinolin-2(1H)-ylidene)-2-(trifluoromethyl)benzenesulfonamide (9c): 55% yield (194 mg); white solid; mp 178-180 °C; R_f = 0.20 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, DMSO-*d*₆) δ 13.33 (s, 1H), 8.33-8.26 (m, 2H), 7.93 (d, J = 8.2 Hz, 1H), 7.88-7.83 (m, 2H), 7.78 (t, J = 7.8 Hz, 1H), 7.71 (t, J = 7.8 Hz, 1H), 7.62 (d, J = 8.2 Hz, 1H), 7.49 (d, J = 9.5 Hz, 1H), 7.44-7.38 (m, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 155.8, 142.6, 142.5, 137.8, 133.4, 132.6, 130.4, 128.7, 128.6, 128.5, 128.4, 128.4, 126.4, 126.1, 124.9, 124.8, 122.2, 121.3, 117.4, 116.4;

IR (cm⁻¹) ν 3419, 3021, 1637, 1417, 1215; HRMS (ESI-TOF) calcd for C₁₆H₁₂F₃N₂O₂S [M + H]⁺ 353.0572, found 353.0542.

(E)-N-(Quinolin-2(1H)-ylidene)benzenesulfonamide (9d): 46% yield (131 mg); white solid; mp 170-172 °C; *R_f* = 0.20 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, CDCl₃) δ 11.91 (s, 1H), 8.03-7.99 (m, 2H), 7.87 (d, *J* = 9.4 Hz, 1H), 7.64-7.59 (m, 2H), 7.53-7.43 (m, 4H), 7.38-7.34 (m, 1H), 6.96 (d, *J* = 9.4 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 154.7, 142.9, 141.1, 136.6, 132.0, 131.9, 128.8, 128.1, 126.3, 124.8, 121.4, 120.3, 117.5; IR (cm⁻¹) ν 3411, 3021, 1636, 1393, 1215; HRMS (ESI-TOF) calcd for C₁₅H₁₃N₂O₂S [M + H]⁺ 285.0698, found 285.0689.

(E)-N-(Quinolin-2(1H)-ylidene)methanesulfonamide (9e): 36% yield (80mg); white solid; mp 200-202 °C; *R_f* = 0.15 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.89 (s, 1H), 8.23 (d, *J* = 9.3 Hz, 1H), 7.84 (d, *J* = 7.9 Hz, 1H), 7.71-7.62 (m, 2H), 7.45-7.35 (m, 2H), 3.32 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 154.9, 140.9, 131.8, 128.5, 124.4, 122.0, 119.5, 118.2, 115.9, 42.5; IR (cm⁻¹) ν 3397, 3021, 1637, 1392, 1215; HRMS (ESI-TOF) calcd for C₁₀H₁₁N₂O₂S [M + H]⁺ 223.0541, found 223.0533.

(E)-N-(7-Fluoroquinolin-2(1H)-ylidene)-4-methylbenzenesulfonamide (9f): 49% yield (155 mg); white solid; mp 190-192 °C; *R_f* = 0.15 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, DMSO-*d*₆) δ 13.21 (s, 1H), 8.23 (d, *J* = 9.4 Hz, 1H), 7.91 (dd, *J* = 6.2, 2.5 Hz, 1H), 7.86-7.76 (m, 2H), 7.44 (s, 1H), 7.37-7.24 (m, 4H), 2.34 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 163.2, 162.7, 155.6, 142.5, 141.2, 131.5, 131.4, 129.7, 126.8, 118.6, 115.1, 113.6, 103.2, 21.4; IR (cm⁻¹) ν 3411, 3021, 1637, 1412, 1216. HRMS (ESI-TOF) calcd for C₁₆H₁₄FN₂O₂S [M + H]⁺ 317.0760, found 317.0759.

(E)-N-(7-Fluoroquinolin-2(1H)-ylidene)-4-(trifluoromethyl)benzenesulfonamide (9g): 50% yield (185 mg); white solid; mp 196-198 °C; *R_f* = 0.15 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, DMSO-*d*₆) δ 13.43 (s, 1H), 8.30 (d, *J* = 9.5 Hz, 1H), 8.12 (d, *J* = 6.5 Hz, 2H), 7.99-

7.91 (m, 3H), 7.52, (s, 1H), 7.36-7.27 (m, 2H); ^{13}C NMR (100 MHz, DMSO- d_6) δ 165.3, 162.8, 156.0, 147.5, 142.1, 132.2, 131.9, 131.7, 131.6, 128.1, 127.5, 126.6, 126.6, 126.5, 125.4, 122.6, 119.9, 114.9, 113.9, 113.7; IR (cm^{-1}) ν 3414, 3022, 1637, 1404, 1216; HRMS (ESI-TOF) calcd for $\text{C}_{16}\text{H}_{11}\text{F}_4\text{N}_2\text{O}_2\text{S}$ $[\text{M} + \text{H}]^+$ 371.0477, found 371.0445.

(E)-N-(7-Fluoroquinolin-2(1H)-ylidene)-2-(trifluoromethyl)benzenesulfonamide (9h): 48% yield (178mg); white solid; mp 130-132 °C; R_f = 0.15 (SiO_2 , 30% EtOAc/Hexanes); ^1H NMR (400 MHz, DMSO- d_6) δ 13.34 (s, 1H), 8.35-8.26 (m, 2H), 7.98-7.92 (m, 2H), 7.87 (t, J = 7.3 Hz, 1H), 7.79 (t, J = 7.3 Hz, 1H), 7.45 (d, J = 8.8 Hz, 1H), 7.36-7.30 (m, 2H); ^{13}C NMR (100 MHz, DMSO- d_6) δ 165.4, 162.9, 156.1, 142.4, 142.2, 139.3, 133.5, 132.7, 131.6, 130.4, 128.5, 128.4, 126.4, 126.1, 125.8, 124.9, 122.1, 118.4, 115.7, 113.7, 113.5, 103.2, 102.9; IR (cm^{-1}) ν 3400, 3021, 1637, 1417, 1215; HRMS (ESI-TOF) calcd for $\text{C}_{16}\text{H}_{11}\text{F}_4\text{N}_2\text{O}_2\text{S}$ $[\text{M} + \text{H}]^+$ 371.0477, found 371.0445.

(E)-N-(7-Fluoroquinolin-2(1H)-ylidene)benzenesulfonamide (9i): 45% yield (136 mg); white solid; mp 180-182 °C; R_f = 0.15 (SiO_2 , 30% EtOAc/Hexanes); ^1H NMR (400 MHz, DMSO- d_6) δ 13.27 (s, 1H), 8.24 (d, J = 9.4 Hz, 1H), 7.94-7.89 (m, 3H), 7.59-7.52 (m, 4H), 7.28 (t, J = 8.5 Hz, 2H); ^{13}C NMR (100 MHz, DMSO- d_6) δ 165.6, 163.1, 154.6, 142.5, 140.4, 138.5, 138.4, 132.2, 130.3, 130.2, 128.8, 126.3, 119.2, 118.3, 113.9, 113.7, 104.3, 104.0; IR (cm^{-1}) ν 3396, 3021, 1637, 1416, 1216. HRMS (ESI-TOF) calcd for $\text{C}_{15}\text{H}_{12}\text{FN}_2\text{O}_2\text{S}$ $[\text{M} + \text{H}]^+$ 303.0604, found 303.0572.

(E)-4-Methyl-N-(4-methylquinolin-2(1H)-ylidene)benzenesulfonamide (9j): 77% yield (241 mg); white solid; mp 128-130 °C; R_f = 0.25 (SiO_2 , 30% EtOAc/Hexanes); ^1H NMR (400 MHz, CDCl_3) δ 11.79 (s, 1H), 7.87 (d, J = 8.2 Hz, 2H), 7.74 (d, J = 8.0 Hz, 1H), 7.63-7.57 (m, 1H), 7.59 (d, J = 8.0 Hz, 1H), 7.39-7.34 (m, 1H), 7.24 (d, J = 8.2 Hz, 2H), 6.82 (s, 1H), 2.52 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 154.2, 150.1, 142.5, 140.3, 136.2, 131.6, 129.3,

126.2, 124.6, 121.9, 119.6, 117.8, 21.7, 19.3; IR (cm⁻¹) ν 3423, 3043, 1633, 1515, 1218; HRMS (ESI-TOF) calcd for C₁₇H₁₇N₂O₂S [M + H]⁺ 313.1011, found 313.1005.

(E)-N-(4-Methylquinolin-2(1H)-ylidene)benzenesulfonamide (9k): 58% yield (173 mg); white solid; mp 210-212 °C; R_f = 0.25 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, DMSO-*d*₆) δ 13.05 (s, 1H), 7.93-7.86 (m, 3H), 7.70-7.65 (m, 1H), 7.58-7.51 (m, 4H), 7.44 (s, 1H), 7.42-7.37 (m, 1H), 2.58 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 155.2, 151.2, 144.3, 137.6, 132.3, 132.0, 129.3, 126.4, 125.5, 124.5, 121.5, 117.6, 115.4, 19.7; IR (cm⁻¹) ν 3391, 3021, 1636, 1408, 1215 HRMS (ESI-TOF) calcd for C₁₆H₁₅N₂O₂S [M + H]⁺ 299.0854, found 299.0846.

(E)-N-(4-methylquinolin-2(1H)-ylidene)methanesulfonamide (9l): 48% yield (114mg); white solid; mp 115-117 °C; R_f = 0.25 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, CDCl₃) δ 11.51 (s, 1H), 7.75 (d, J = 7.9 Hz, 1H), 7.59 (t, J = 7.4 Hz, 1H), 7.41-7.34 (m, 2H), 6.74 (s, 1H), 3.01 (s, 3H), 2.55 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 153.9, 149.7, 136.0, 131.4, 124.6, 124.5, 121.8, 120.2, 117.5, 42.7, 19.2; IR (cm⁻¹) ν 3404, 3021, 1638, 1410, 1215; HRMS (ESI-TOF) calcd for C₁₁H₁₃N₂O₂S [M + H]⁺ 237.0698, found 237.0673.

(E)-N-(4-Ethylquinolin-2(1H)-ylidene)-4-methylbenzenesulfonamide (9m): 58% yield (189 mg); white solid; mp 158-160 °C; R_f = 0.25 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, CDCl₃) δ 11.82 (s, 1H), 7.88 (d, J = 8.0 Hz, 2H), 7.78 (d, J = 8.1 Hz, 1H), 7.59 (t, J = 7.5 Hz, 1H), 7.43 (d, J = 8.1 Hz, 1H), 7.36 (t, J = 7.5 Hz, 1H), 7.25 (d, J = 8.0 Hz, 2H), 6.79 (s, 1H), 2.94-2.90 (m, 2H) 2.38 (s, 3H), 1.32 (t, J = 7.3 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 155.3, 154.4, 142.5, 140.3, 136.4, 131.4, 129.3, 126.3, 124.5, 124.1, 121.2, 118.0, 117.7, 25.3, 21.5, 12.8; IR (cm⁻¹) ν 3423, 3020, 1633, 1399, 1216; HRMS (ESI-TOF) calcd for C₁₈H₁₉N₂O₂S [M + H]⁺ 327.1167, found 327.1157.

(E)-4-Methyl-N-(4-propylquinolin-2(1H)-ylidene)benzenesulfonamide (9n): 61% yield (208 mg); white solid; mp 130-132 °C; R_f = 0.25 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz,

CDCl₃) δ 11.82 (s, 1H), 7.88 (d, J = 7.8 Hz, 2H), 7.78 (d, J = 8.0 Hz, 1H), 7.59 (t, J = 7.3 Hz, 1H), 7.43 (d, J = 8.0 Hz, 1H), 7.36 (t, J = 7.3 Hz, 1H), 7.25 (d, J = 7.8 Hz, 2H), 6.78 (s, 1H), 2.84 (t, J = 7.0 Hz, 2H), 2.38 (s, 3H), 1.78-1.67 (m, 2H), 1.02 (t, J = 7.2 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 154.2, 153.9, 142.5, 140.3, 136.5, 131.4, 129.4, 126.3, 124.5, 124.3, 121.3, 118.8, 118.0, 34.4, 22.1, 21.5, 13.9; IR (cm⁻¹) ν 3400, 3019, 1634, 1413, 1215; HRMS (ESI-TOF) calcd for C₁₉H₂₁N₂O₂S [M + H]⁺ 341.1324, found 341.1319.

(E)-N-(4-Isopropyl-6-methylquinolin-2(1H)-ylidene)-4-methylbenzenesulfonamide (9o):

67% yield (237 mg); white solid; mp 208-210 °C; R_f = 0.25 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, CDCl₃) δ 11.79 (s, 1H), 7.89 (d, J = 8.0 Hz, 2H), 7.61 (s, 1H), 7.42 (d, J = 8.2 Hz, 1H), 7.33 (d, J = 8.2 Hz, 1H), 7.25 (d, J = 8.0 Hz, 2H), 6.77 (s, 1H), 3.49-3.39 (m, 1H), 2.47 (s, 3H), 2.38 (s, 3H), 1.31 (d, J = 6.6 Hz, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 159.3, 153.9, 142.5, 140.4, 134.5, 134.3, 132.6, 129.3, 126.3, 123.5, 120.7, 117.9, 116.5, 28.8, 22.3, 21.5, 21.4; IR (cm⁻¹) ν 3428, 3021, 1635, 1521, 1215; HRMS (ESI-TOF) calcd for C₂₀H₂₃N₂O₂S [M + H]⁺ 355.1480, found 355.1470.

(E)-4-Methyl-N-(4-phenylquinolin-2(1H)-ylidene)benzenesulfonamide (9p):

61% yield (228 mg); white solid; mp 155-157 °C; R_f = 0.30 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, CDCl₃) δ 11.89 (s, 1H), 7.91 (d, J = 8.0 Hz, 2H), 7.64-7.60 (m, 2H), 7.55-7.46 (m, 4H), 7.43-7.41 (m, 2H), 7.31-7.27 (m, 3H), 6.86 (s, 1H), 2.39 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 153.7, 153.4, 142.7, 140.1, 137.0, 136.2, 131.6, 129.4, 129.3, 128.8, 128.8, 127.0, 126.3, 124.6, 121.0, 120.4, 117.8, 21.5; IR (cm⁻¹) ν 3423, 3021, 1631, 1524, 1215; HRMS (ESI-TOF) calcd for C₂₂H₁₉N₂O₂S [M + H]⁺ 375.1167, found 375.1162.

(E)-4-Methyl-N-(7-methyl-4-phenylquinolin-2(1H)-ylidene)benzenesulfonamide (9q):

72% yield (280 mg); white solid; mp 215-217 °C; R_f = 0.30 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, CDCl₃) δ 11.85 (s, 1H), 7.90 (d, J = 8.0 Hz, 2H), 7.59-7.47 (m, 3H), 7.46-7.34 (m,

5H), 7.28-7.24 (m, 2H), 6.84 (s, 1H), 2.38(s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 153.5, 153.2, 142.6, 140.3, 136.4, 135.2, 134.5, 133.2, 129.4, 129.3, 128.8, 128.7, 126.3, 121.0, 120.2, 117.7, 21.5, 21.2; IR (cm^{-1}) ν 3426, 3021, 1637, 1416, 1284; HRMS (ESI-TOF) calcd for $\text{C}_{23}\text{H}_{21}\text{N}_2\text{O}_2\text{S}$ $[\text{M} + \text{H}]^+$ 389.1324, found 389.1319.

(E)-N-(4-(2-Chlorophenyl)quinolin-2(1H)-ylidene)-4-methylbenzenesulfonamide (9r): 69% yield (282 mg); white solid; mp 135-137 °C; R_f = 0.30 (SiO_2 , 30% EtOAc/Hexanes); ^1H NMR (400 MHz, CDCl_3) δ 11.85 (s, 1H), 7.92 (d, J = 7.9 Hz, 2H), 7.61 (t, J = 7.2 Hz, 1H), 7.56-7.36 (m, 5H), 7.33-7.19 (m, 4H), 6.84 (s, 1H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 153.7, 150.9, 142.8, 139.9, 136.8, 135.0, 132.7, 131.7, 130.6, 130.5, 130.0, 129.5, 129.4, 127.1, 126.8, 126.4, 124.7, 121.2, 117.8, 21.5; IR (cm^{-1}) ν 3429, 3021, 1631, 1526, 1215; HRMS (ESI-TOF) calcd for $\text{C}_{22}\text{H}_{18}\text{ClN}_2\text{O}_2\text{S}$ $[\text{M} + \text{H}]^+$ 409.0778, found 409.0767.

(E)-N-(6-Chloro-4-phenylquinolin-2(1H)-ylidene)-4-methylbenzenesulfonamide (9s): 55% yield (224 mg); white solid; mp 165-167 °C; R_f = 0.30 (SiO_2 , 30% EtOAc/Hexanes); ^1H NMR (400 MHz, CDCl_3) δ 11.63 (s, 1H), 7.89 (d, J = 8.0 Hz, 2H), 7.64-7.50 (m, 5H), 7.45 (d, J = 8.5 Hz, 1H), 7.42-7.35 (m, 2H), 7.28 (d, J = 8.0 Hz, 2H), 6.91 (s, 1H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 153.2, 152.2, 143.0, 139.6, 136.2, 135.7, 131.8, 130.3, 129.6, 129.5, 129.0, 128.7, 126.4, 126.1, 122.2, 120.2, 119.8, 21.5; IR (cm^{-1}) ν 3427, 3020, 1663, 1427, 1286; HRMS (ESI-TOF) calcd for $\text{C}_{22}\text{H}_{18}\text{ClN}_2\text{O}_2\text{S}$ $[\text{M} + \text{H}]^+$ 409.0778, found 409.0769.

(E)-N-(4-(4-Fluorophenyl)-6-methylquinolin-2(1H)-ylidene)-4-methylbenzenesulfonamide (9t): 60% yield (244 mg); white solid; mp 205-207 °C; R_f = 0.30 (SiO_2 , 30% EtOAc/Hexanes); ^1H NMR (400 MHz, CDCl_3) δ 11.86 (s, 1H), 7.92 (d, J = 8.2 Hz, 2H), 7.50-7.39 (m, 4H), 7.36 (s, 1H), 7.28 (d, J = 8.2 Hz, 2H), 7.23 (t, J = 8.6 Hz, 2H), 6.85 (s, 1H), 2.41 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 164.6, 162.2, 153.4, 152.1, 142.8, 140.3, 135.3, 134.8, 133.4, 132.4, 130.8, 130.7, 129.5, 126.4, 126.2, 121.1, 120.7, 117.8, 116.2, 115.9, 21.6, 21.4; IR (cm^{-1}) ν

3423, 3021, 1630, 1409, 1216. HRMS (ESI-TOF) calcd for $C_{23}H_{20}FN_2O_2S$ $[M + H]^+$ 407.1230, found 407.1217.

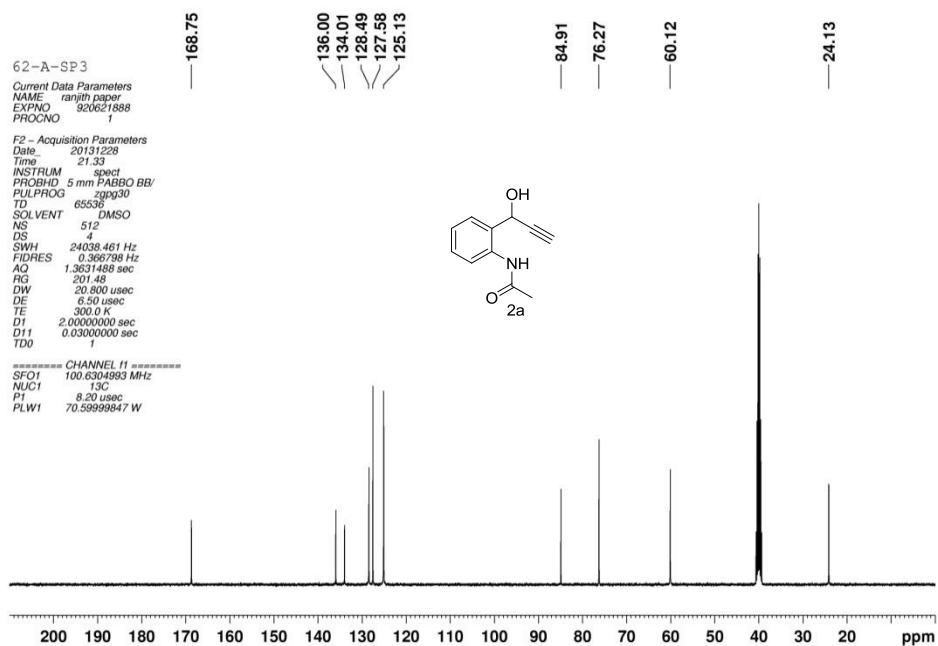
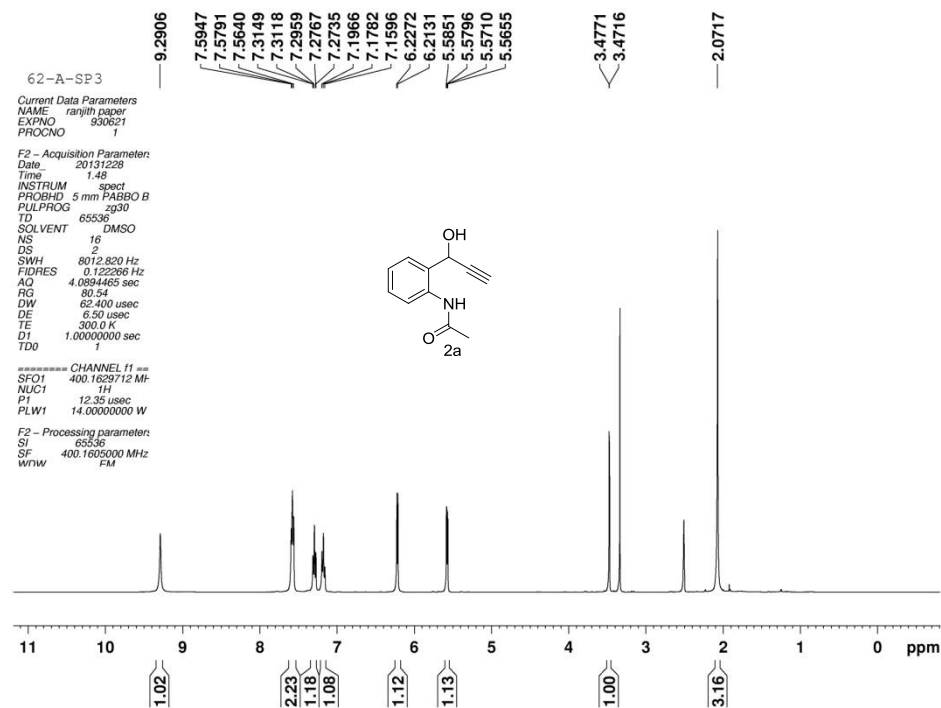
(E)-N-(4-(4-Methoxyphenyl)quinolin-2(1H)-ylidene)-4-methylbenzenesulfonamide (9u):

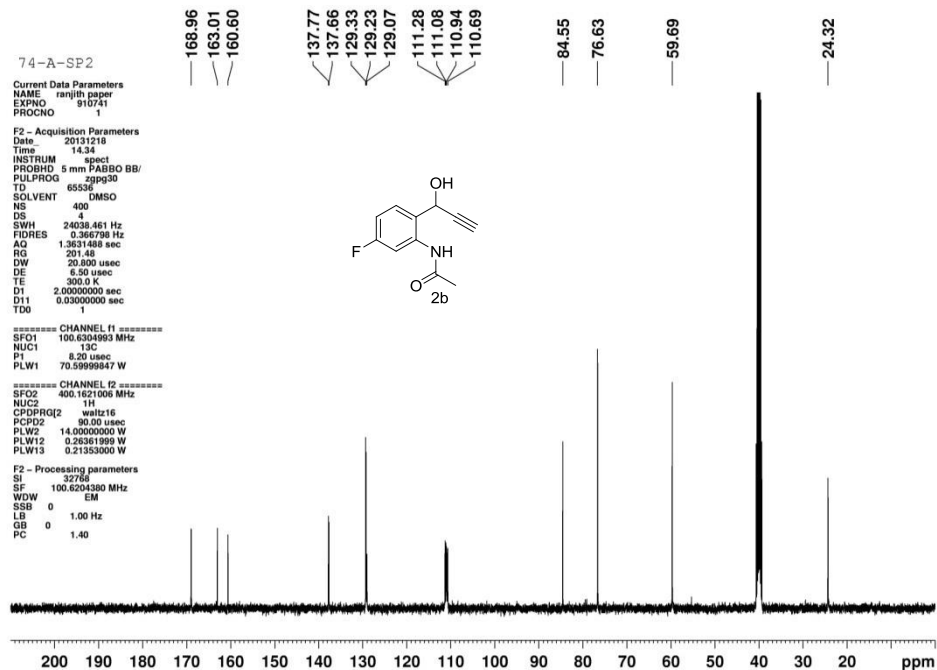
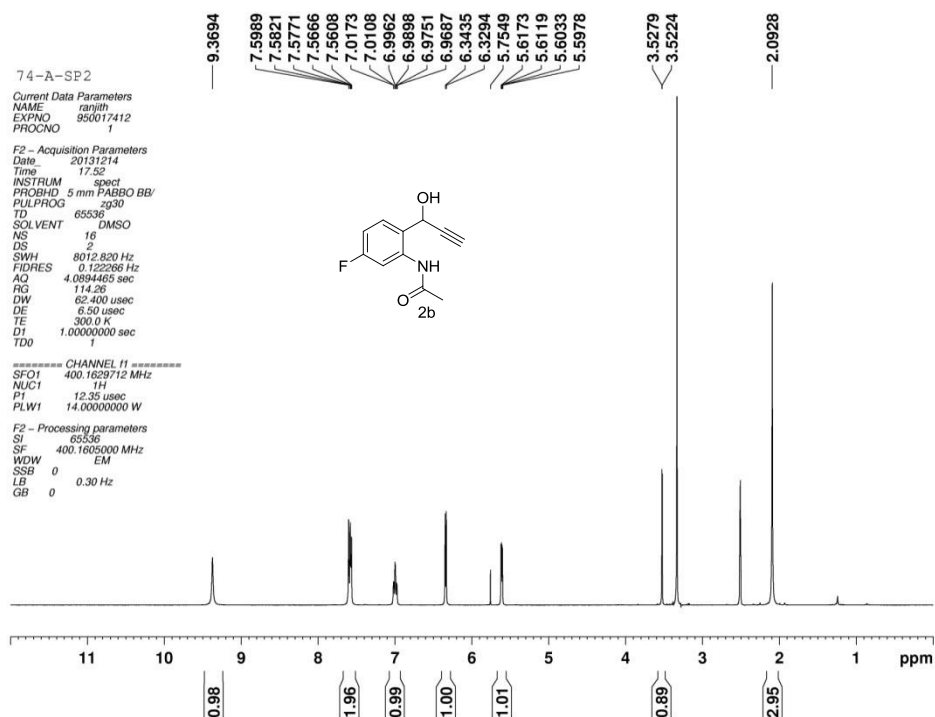
65% yield (263 mg); white solid; mp 130-132 °C; R_f = 0.30 (SiO₂, 30% EtOAc/Hexanes); ¹H NMR (400 MHz, CDCl₃) δ 11.89 (s, 1H), 7.91 (d, J = 7.6 Hz, 2H), 7.70 (d, J = 7.3 Hz, 1H), 7.62 (t, J = 6.8 Hz, 1H), 7.49 (d, J = 7.3 Hz, 1H), 7.41-7.23 (m, 5H), 7.03 (d, J = 7.6 Hz, 2H), 6.85 (s, 1H), 3.88 (s, 3H), 2.39 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 160.6, 153.8, 153.2, 142.6, 140.2, 137.0, 131.5, 130.3, 129.4, 128.5, 127.0, 126.3, 124.5, 121.1, 120.1, 117.7, 114.3, 55.4, 21.5; IR (cm⁻¹) ν 3431, 3021, 1627, 1522, 1215; HRMS (ESI-TOF) calcd for $C_{23}H_{21}N_2O_3S$ $[M + H]^+$ 405.1273, found 405.1261.

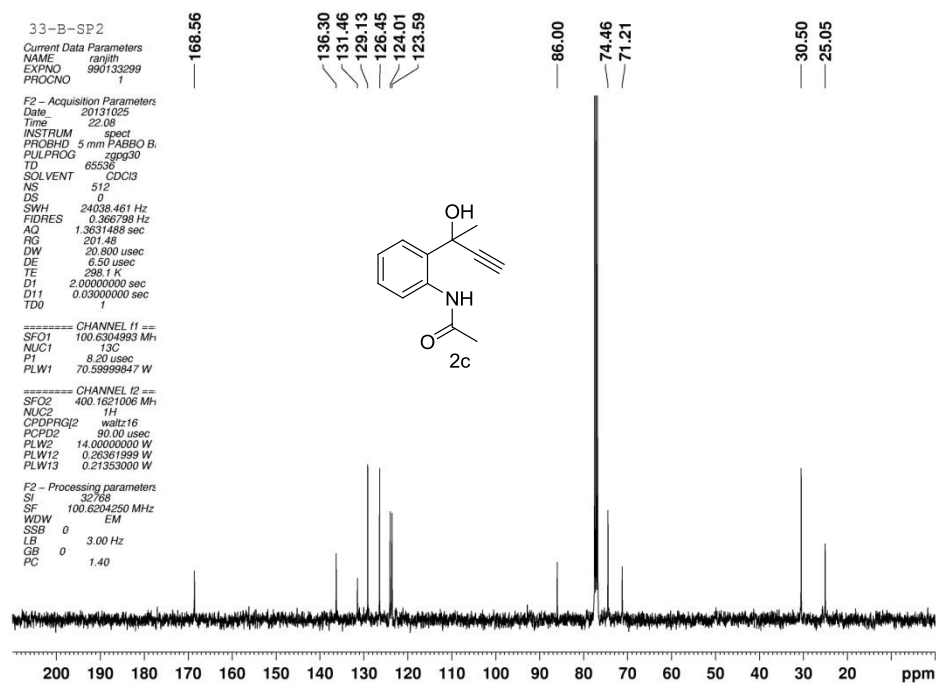
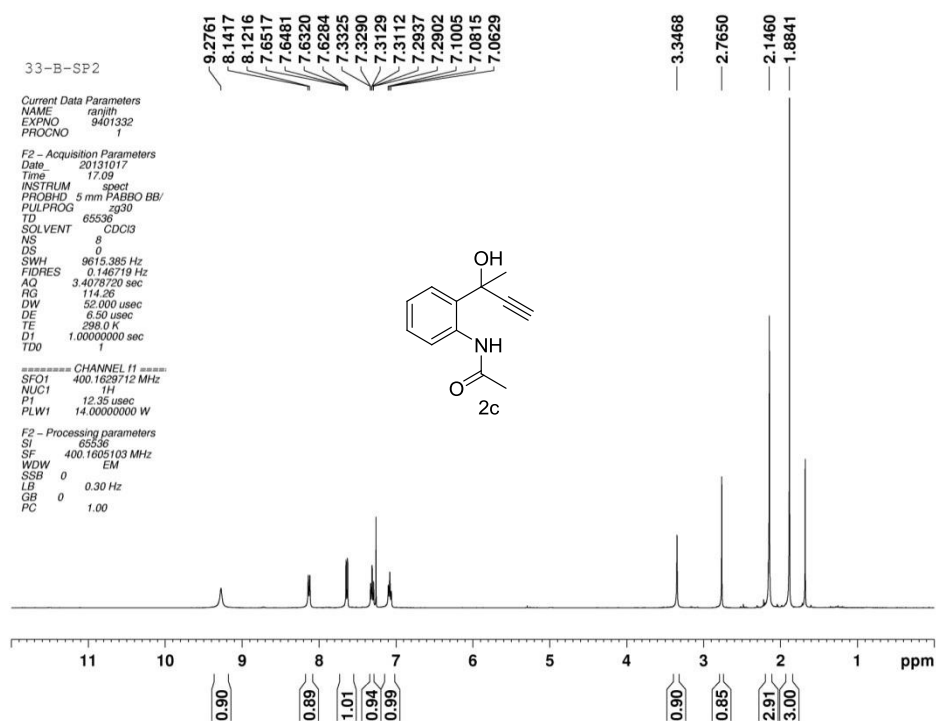
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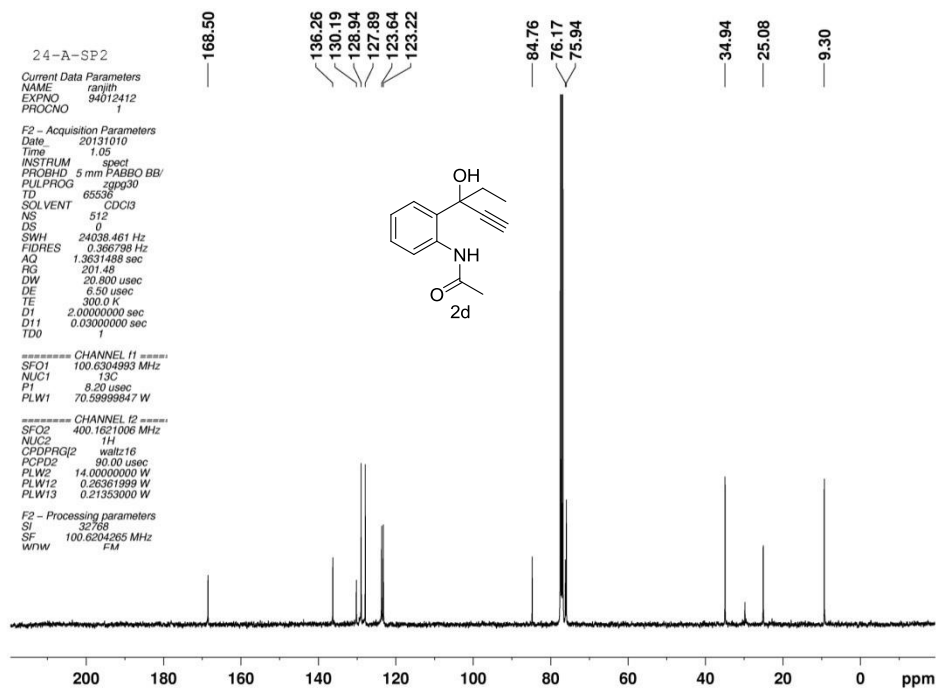
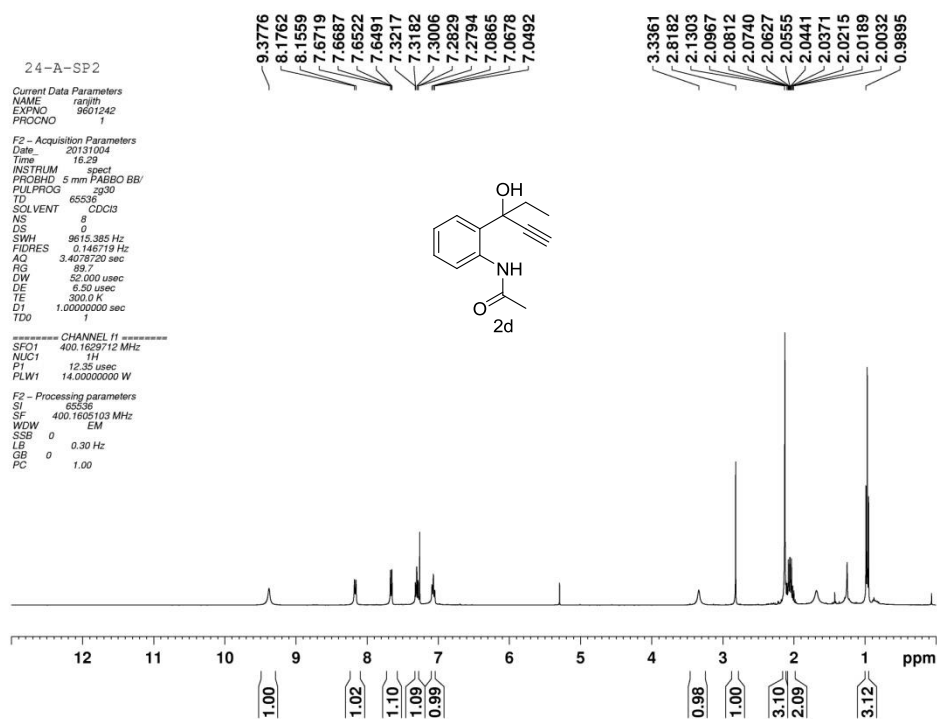
- 1, Kothandaraman, P.; Koh, B. Q.; Limpanuparb, T.; Hirao, H.; Chan, P. W. H. *Chem. Eur. J.* **2013**, *19*, 1978–1985.
2. Kothandaraman, P.; Lauw, S. J. L.; Chan, P. W. H. *Tetrahedron* **2013**, *69*, 7471–7480.

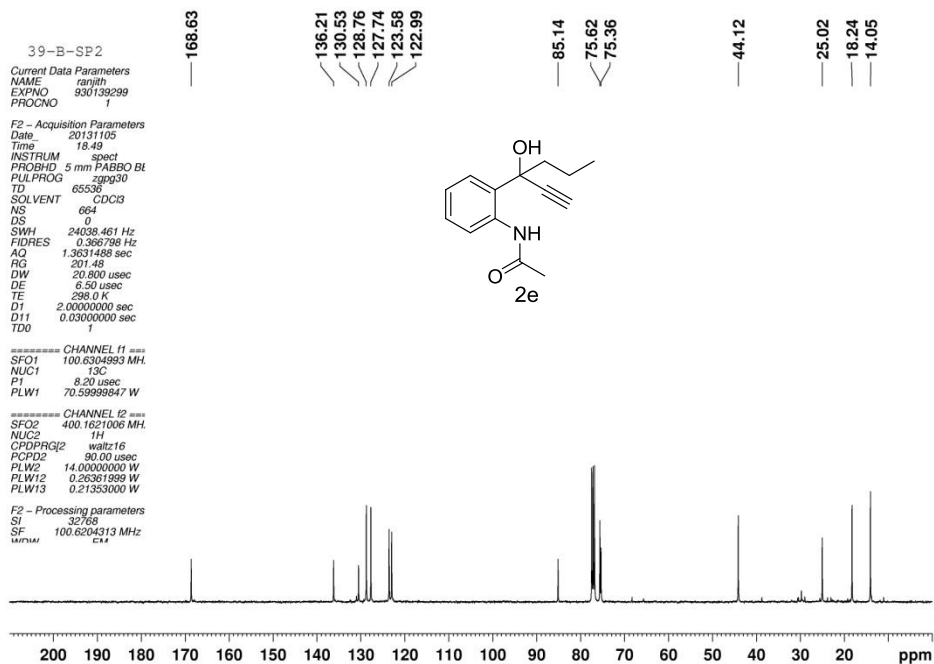
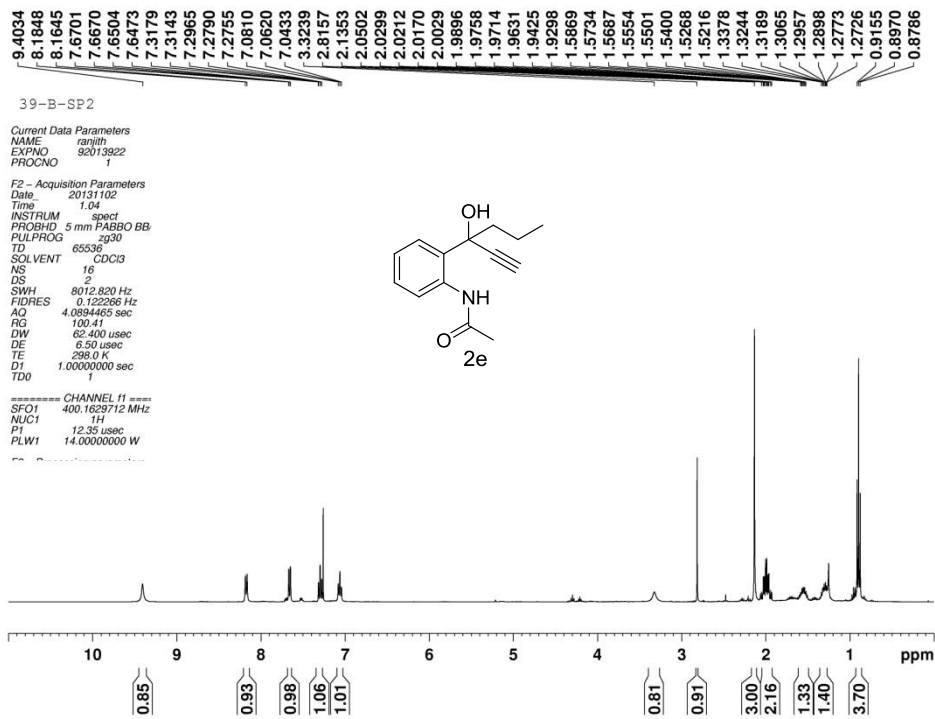
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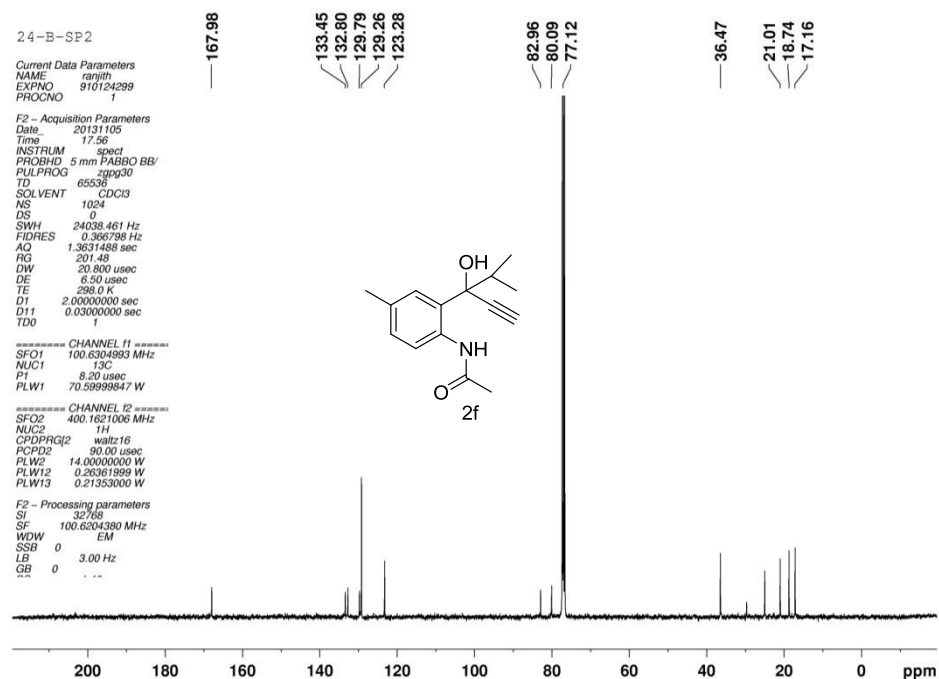
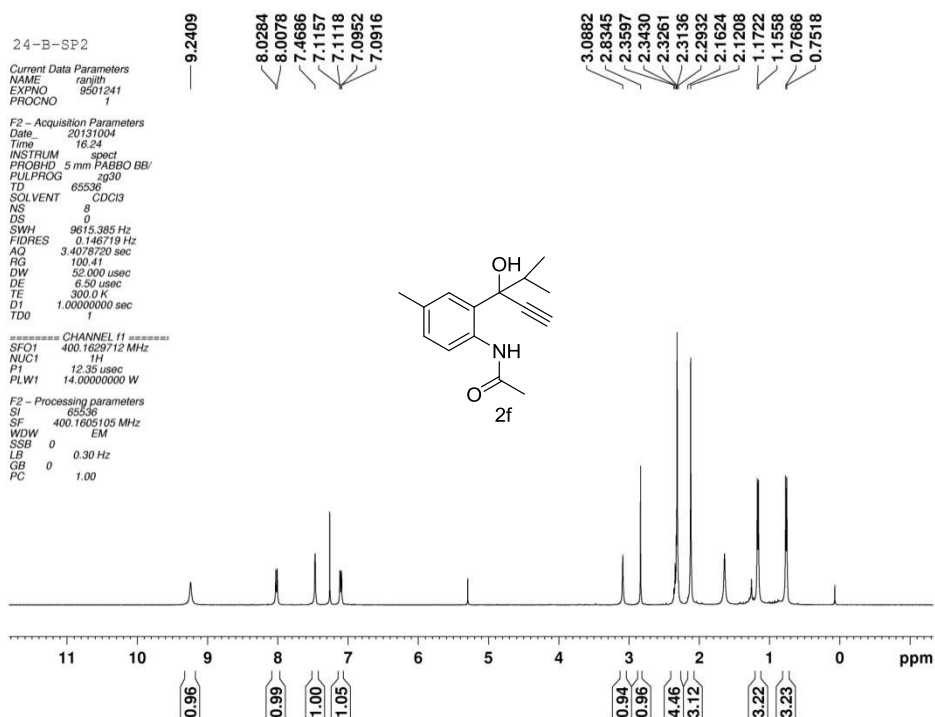


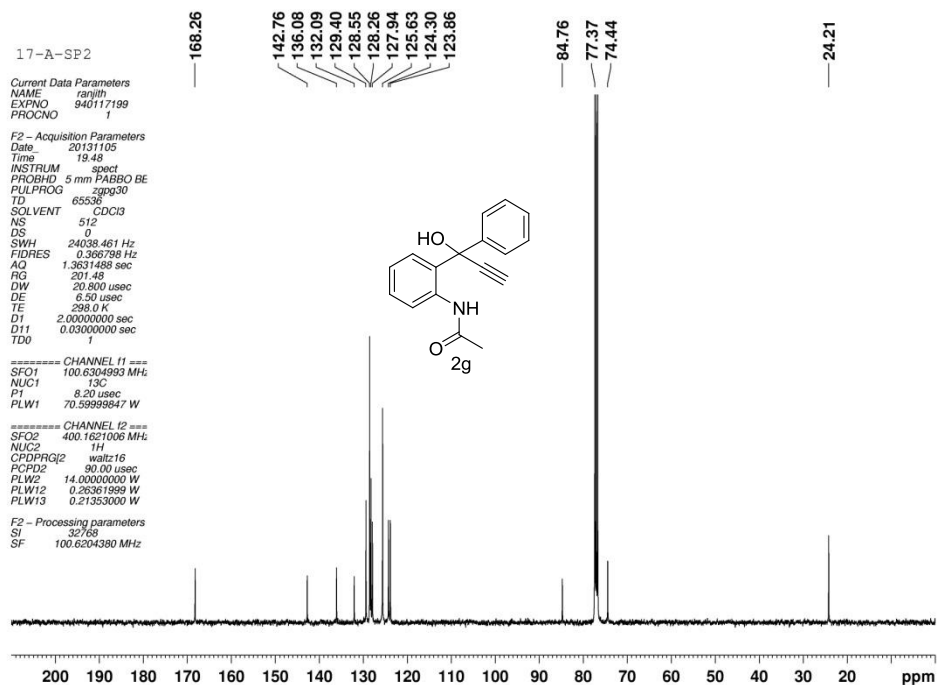
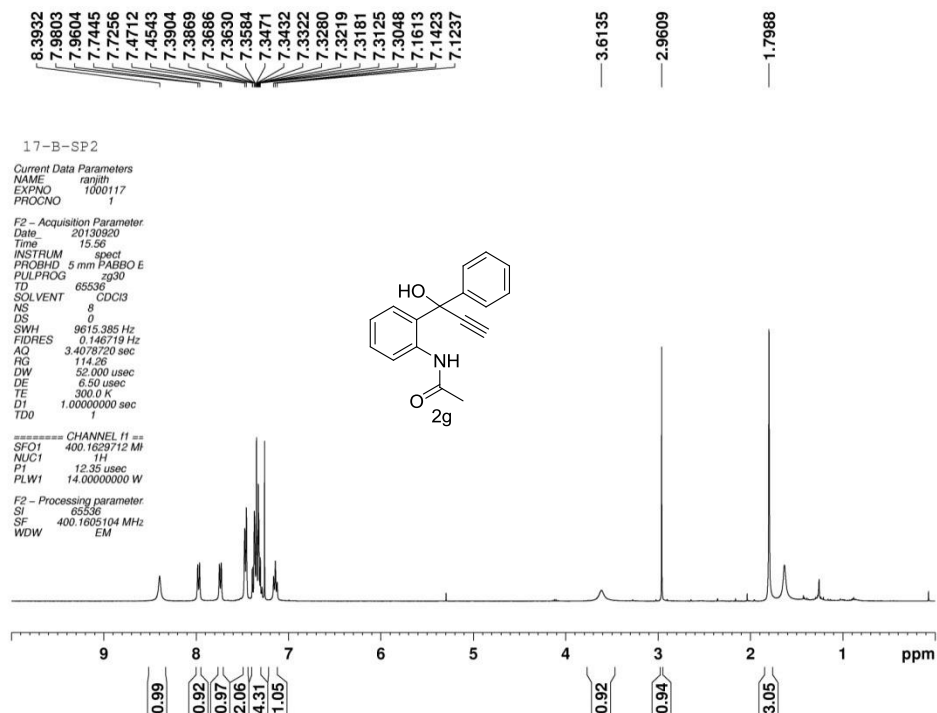


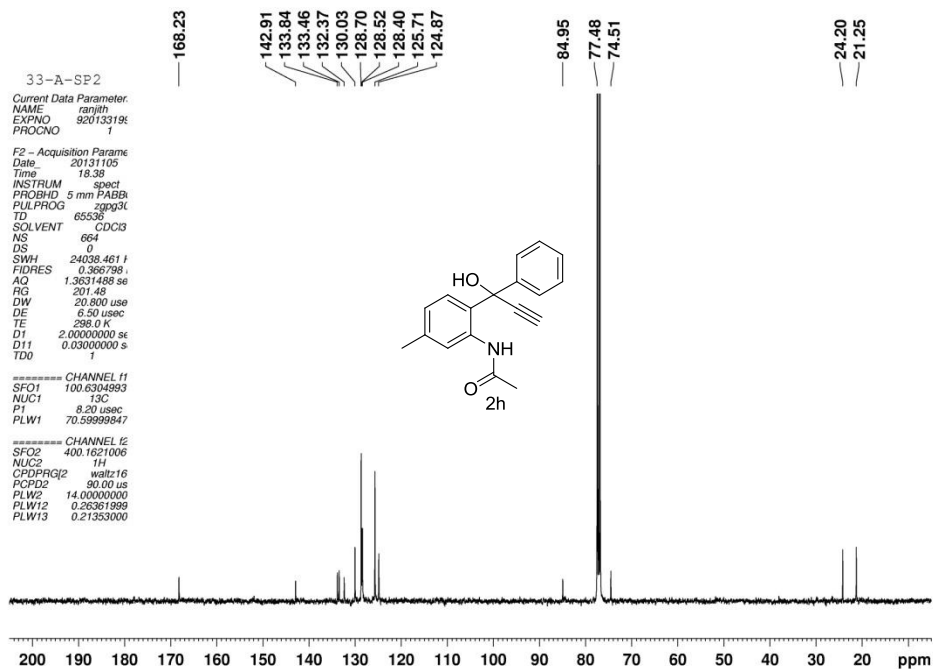
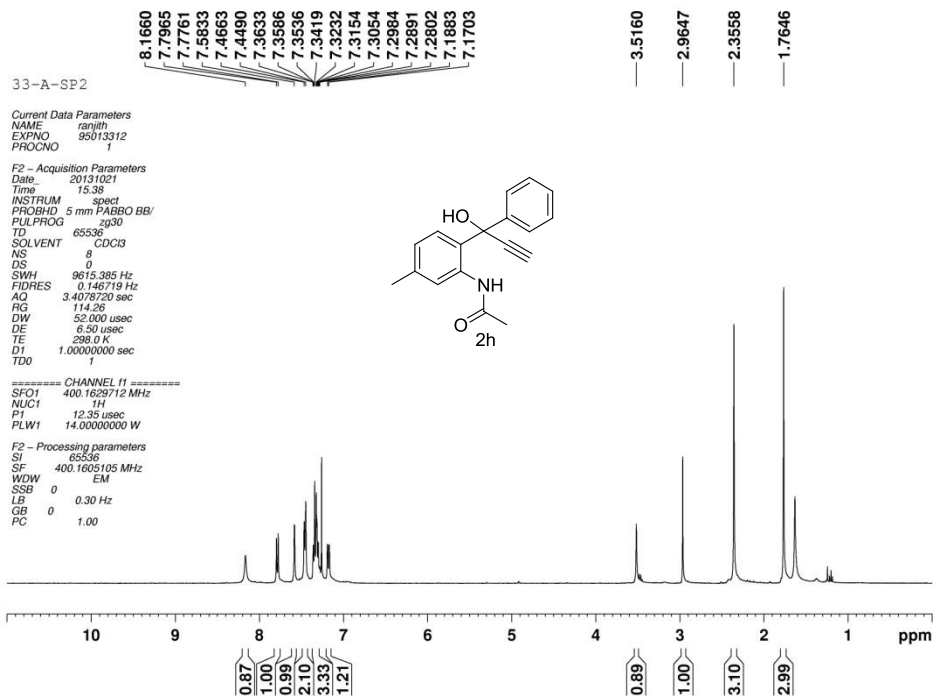


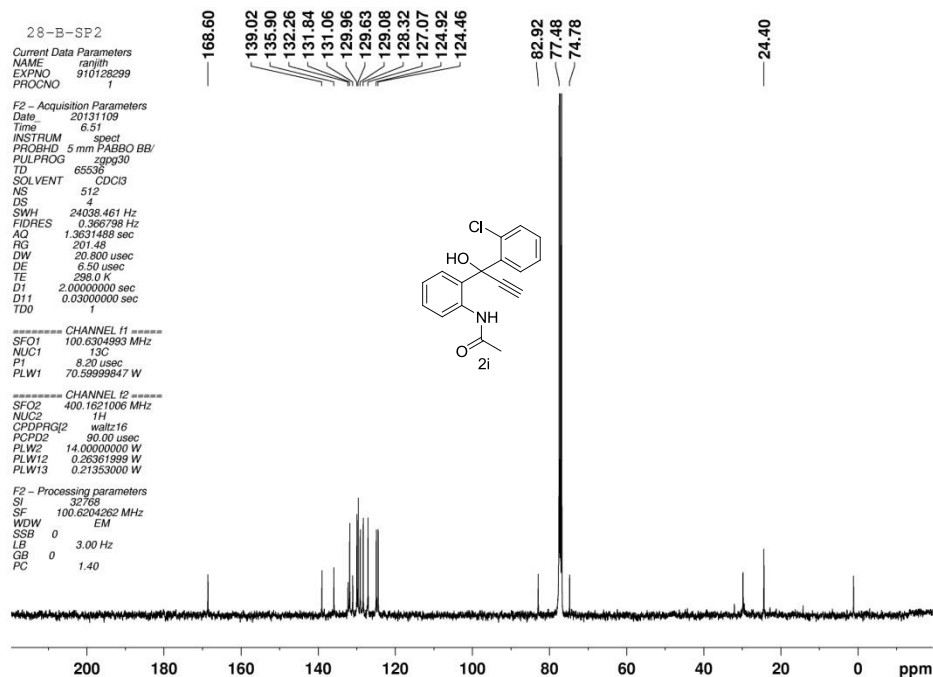
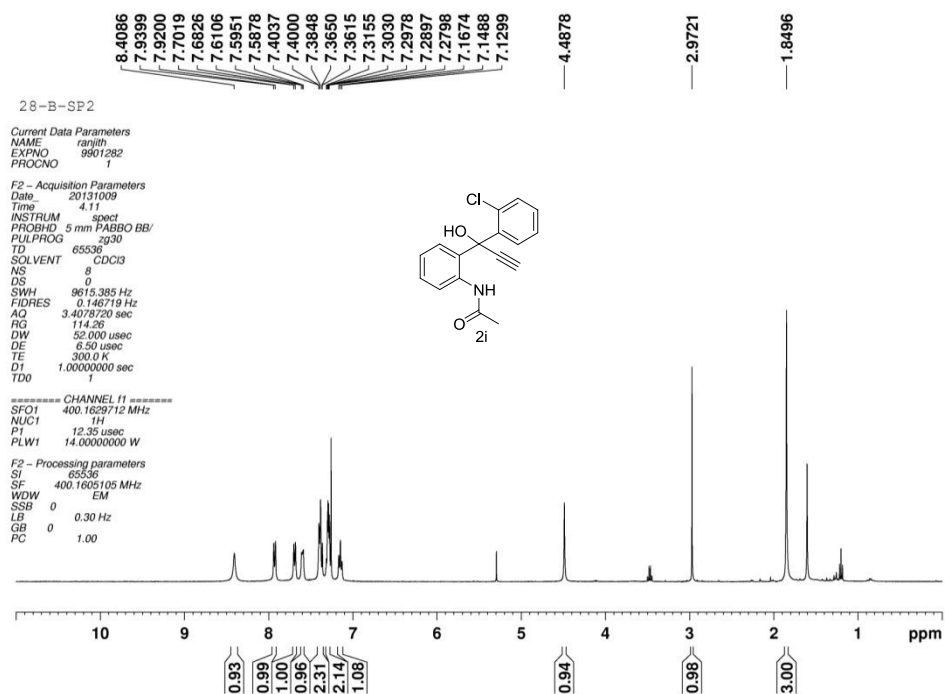


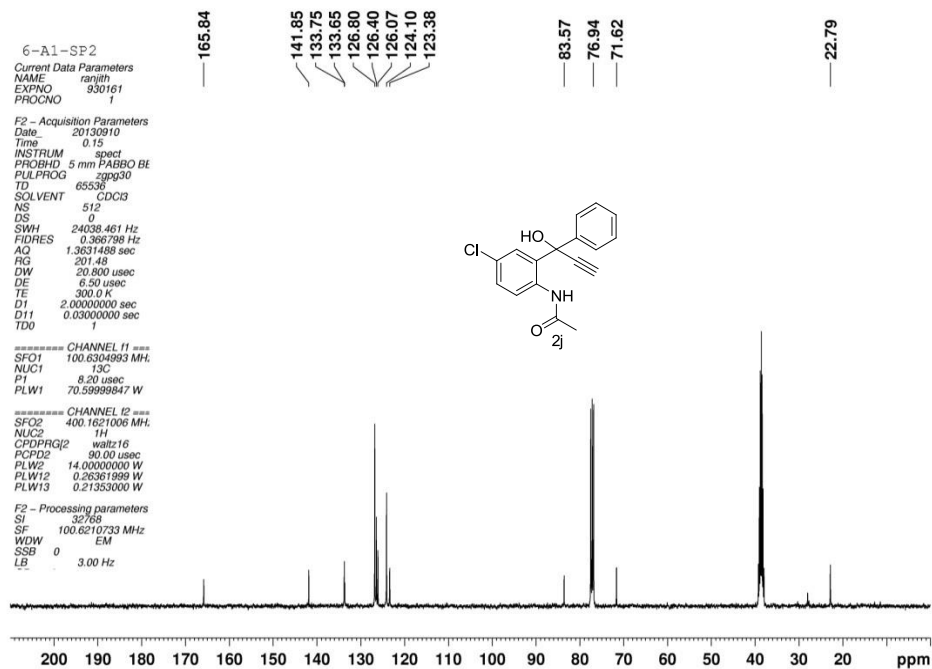
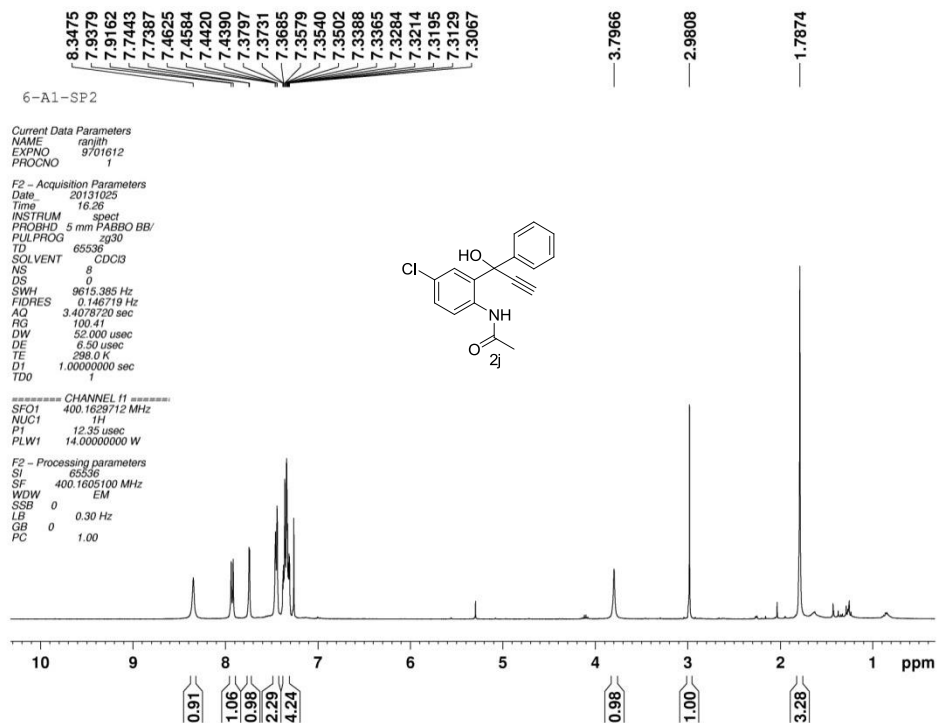


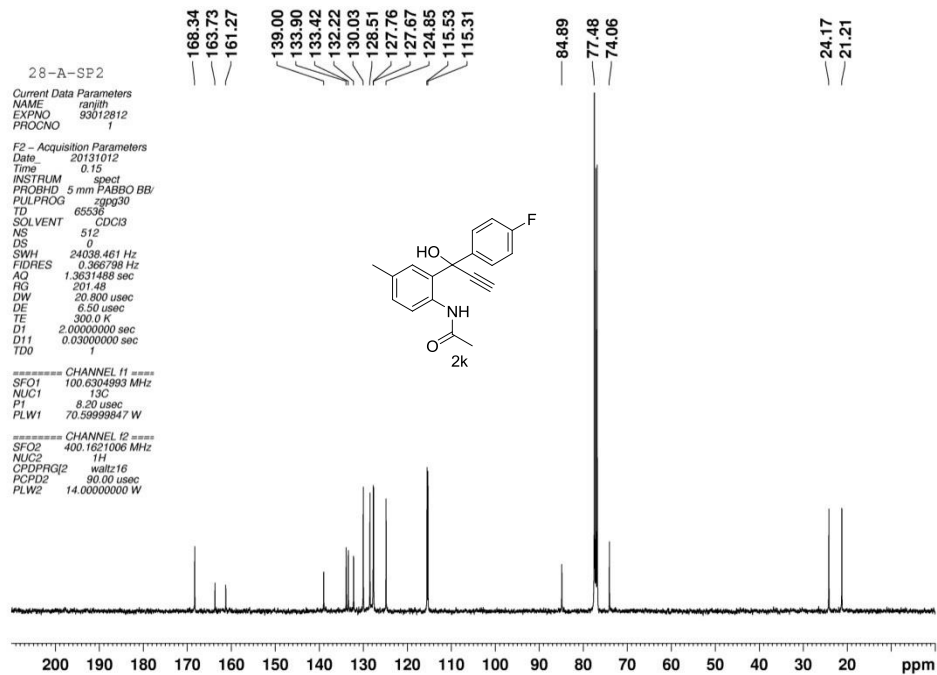
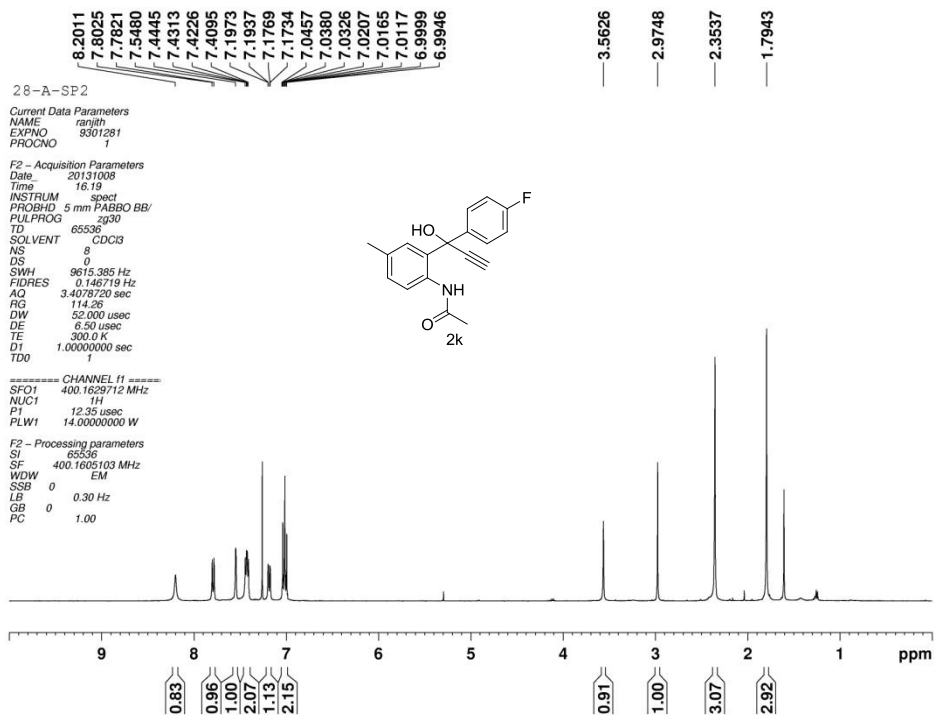


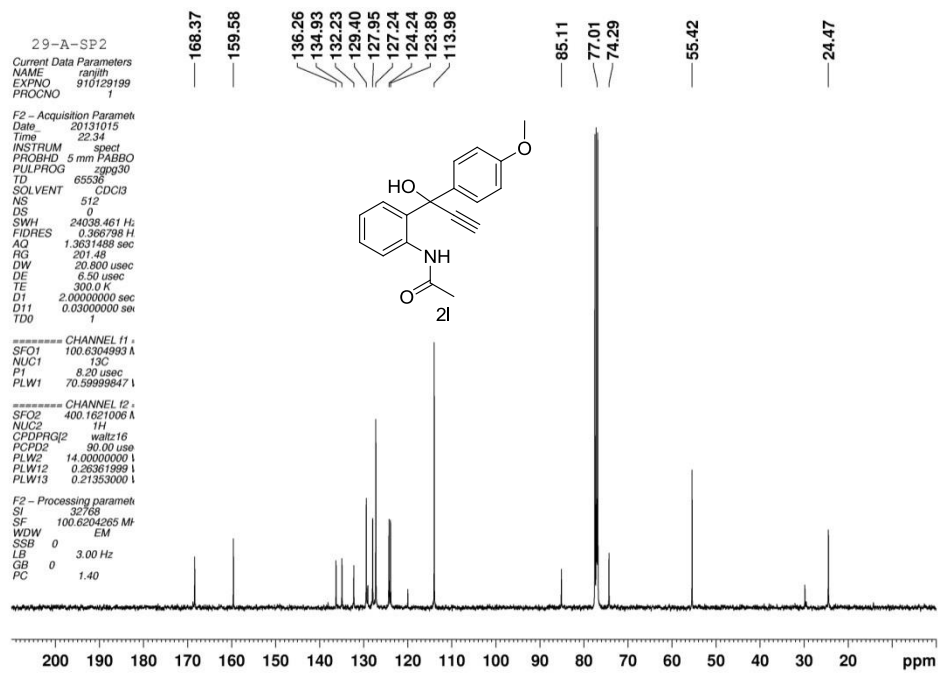
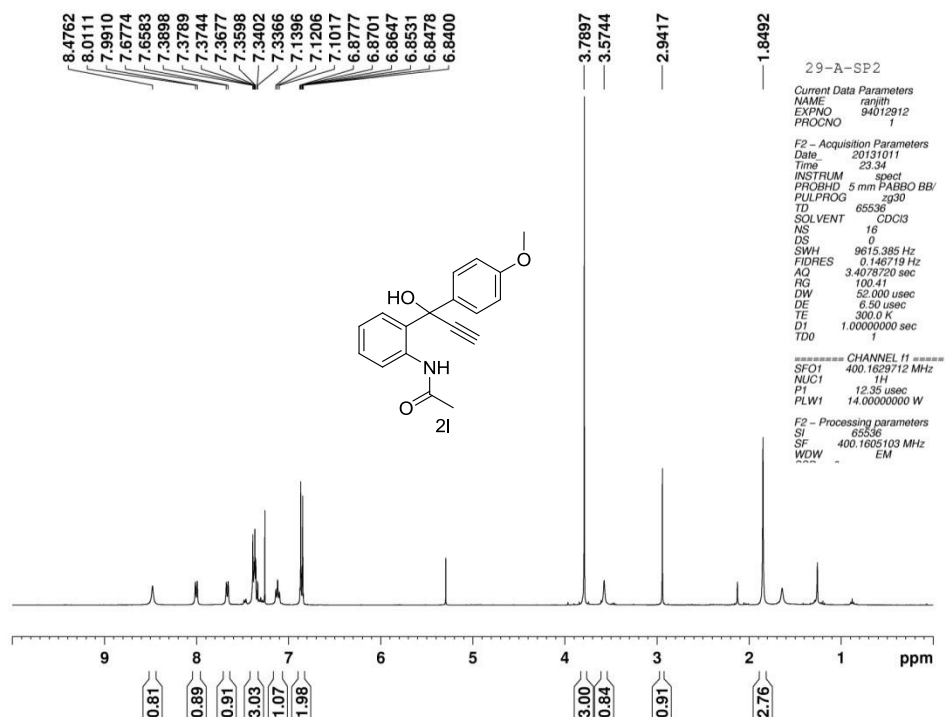


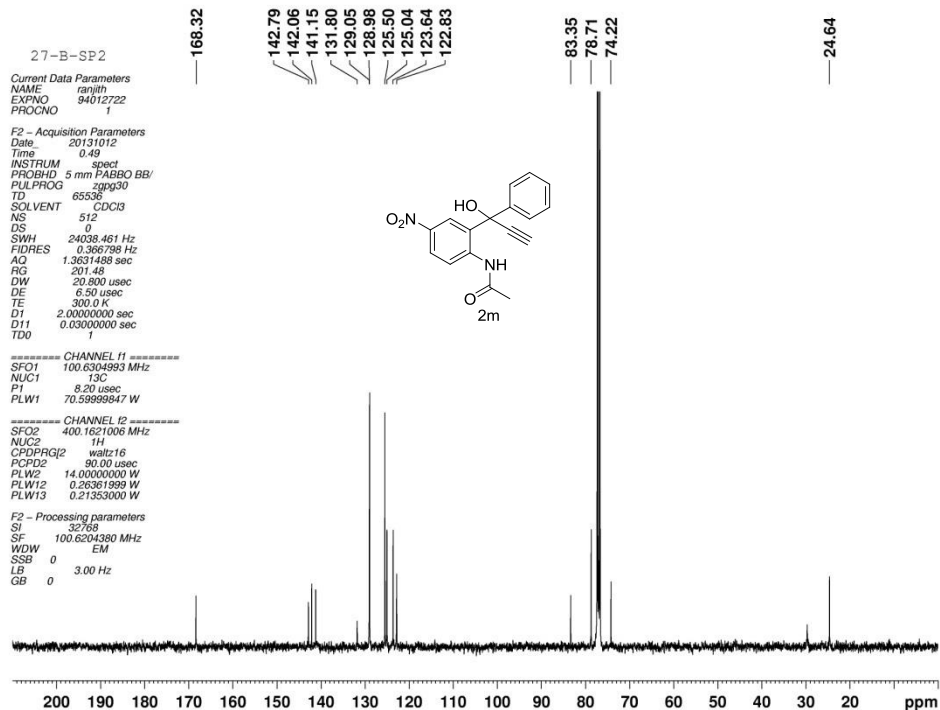
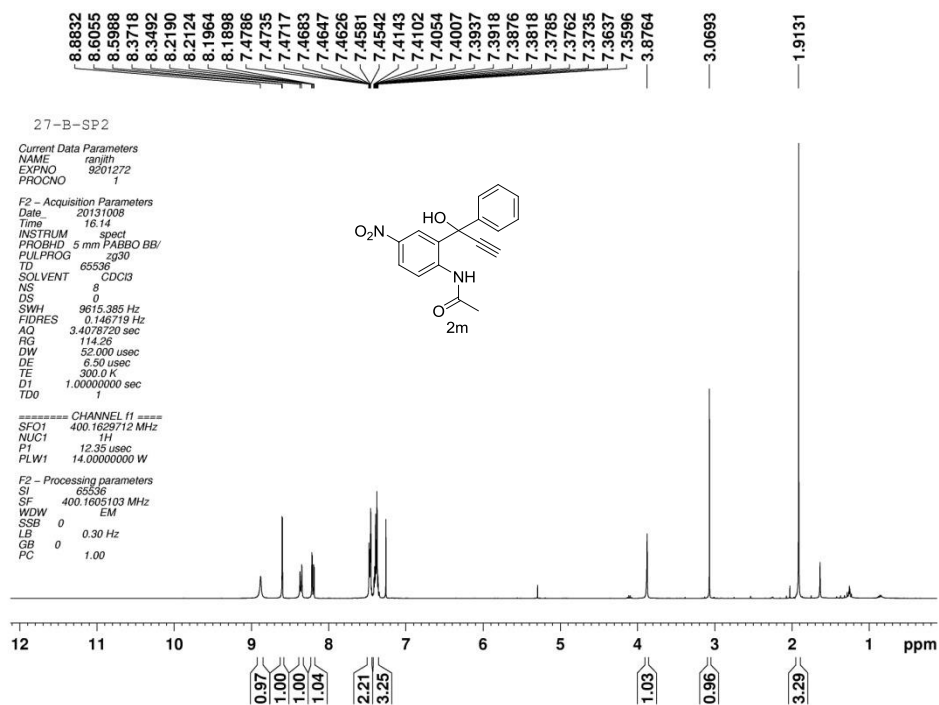


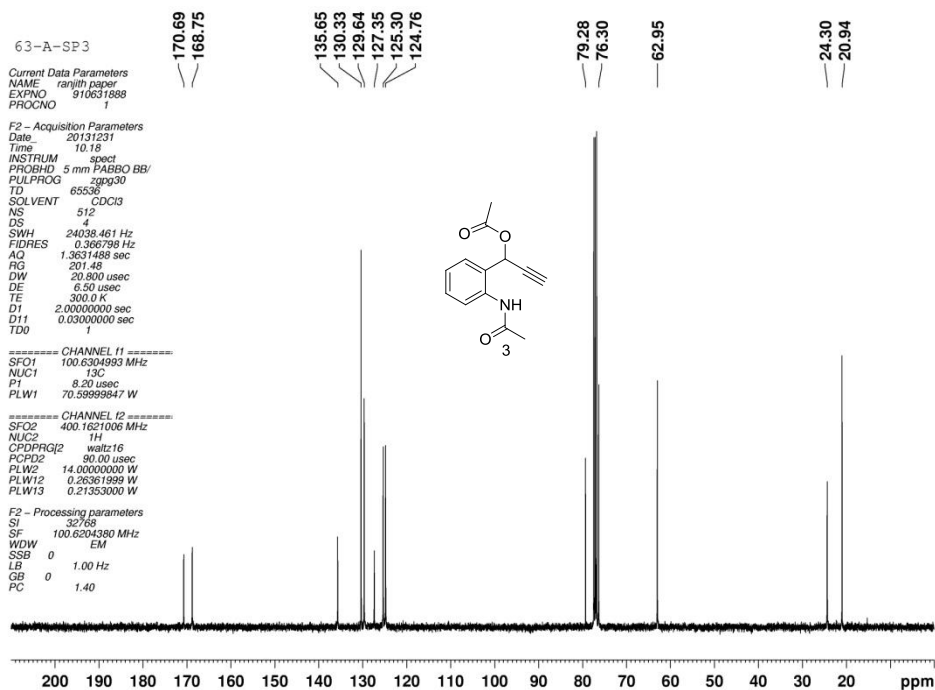
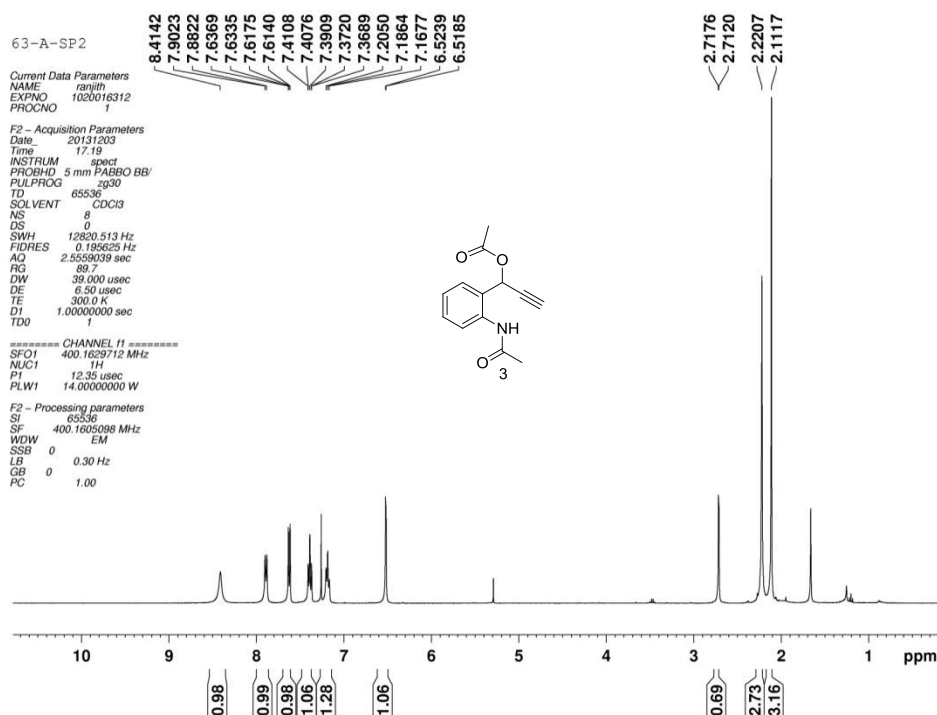


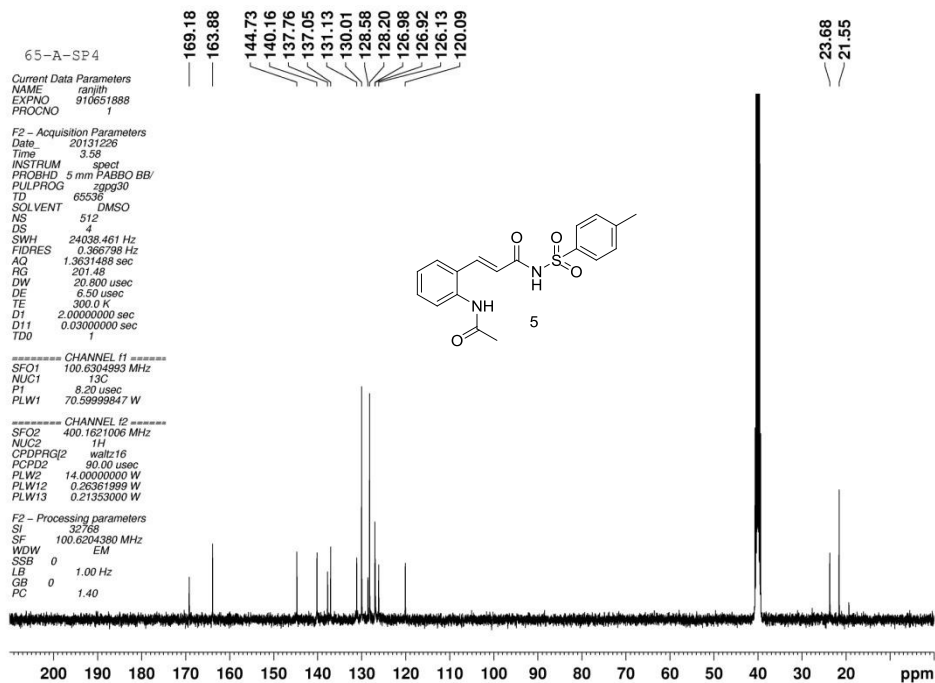
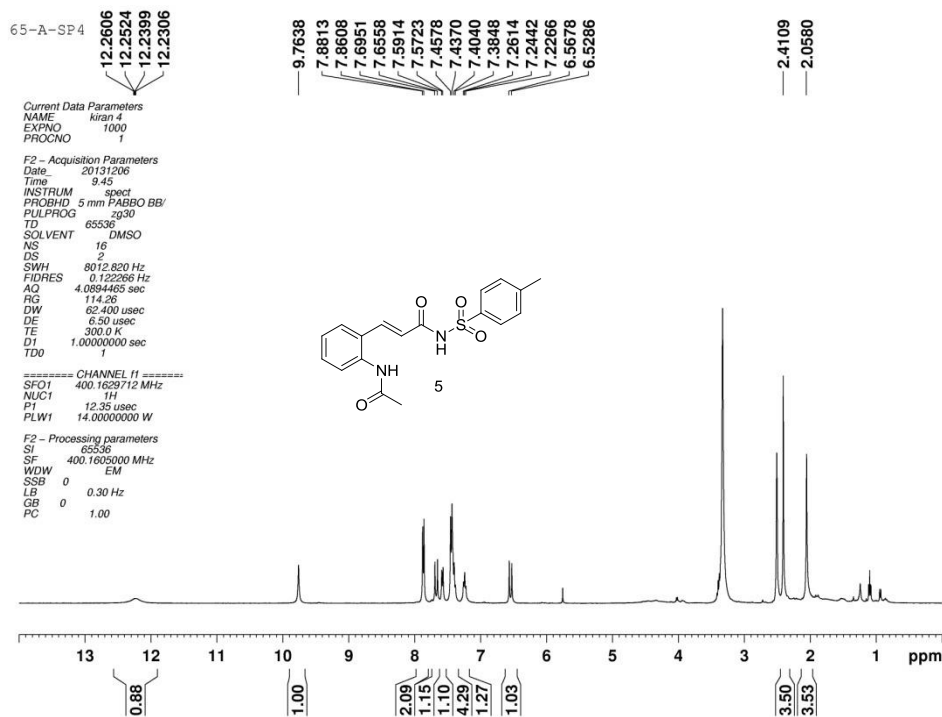


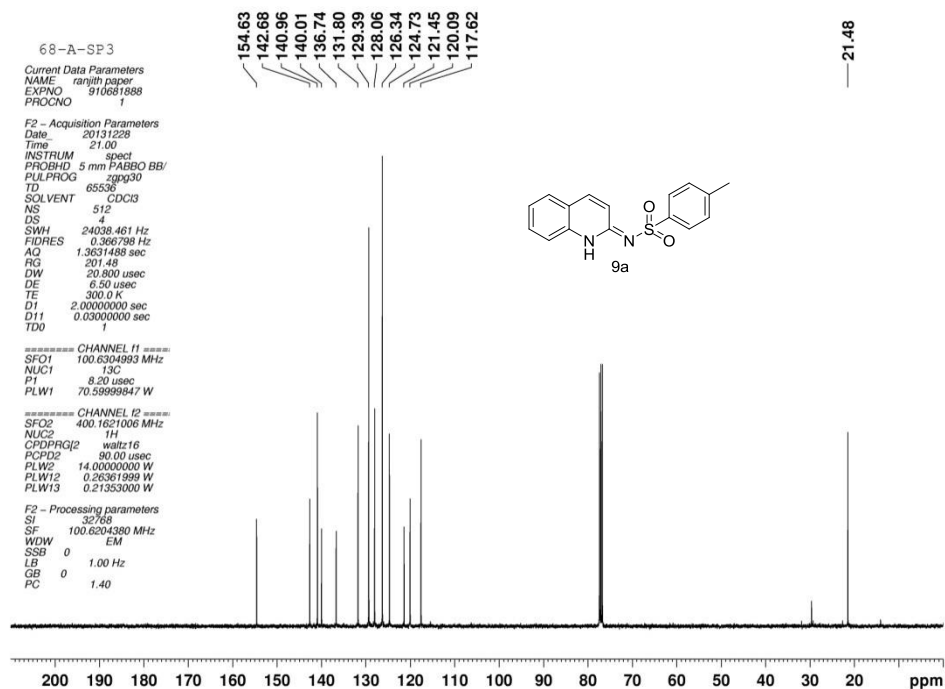
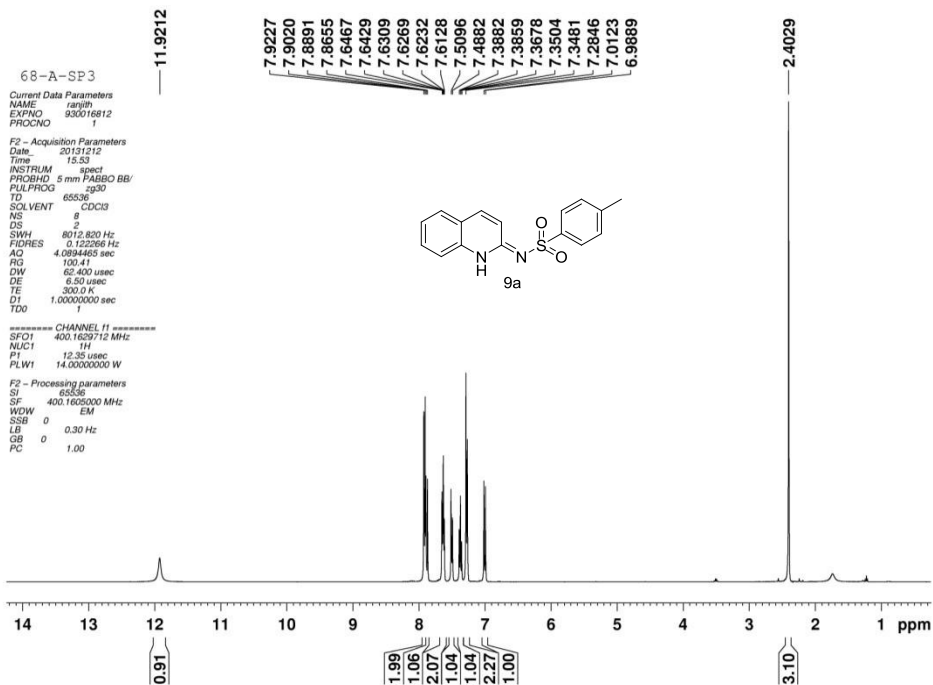


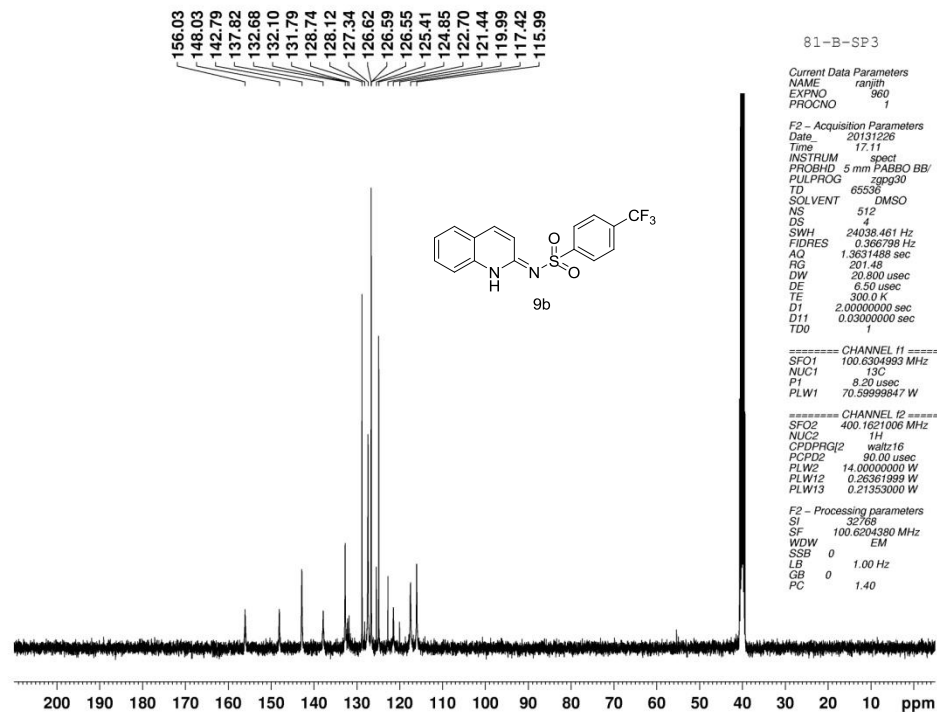
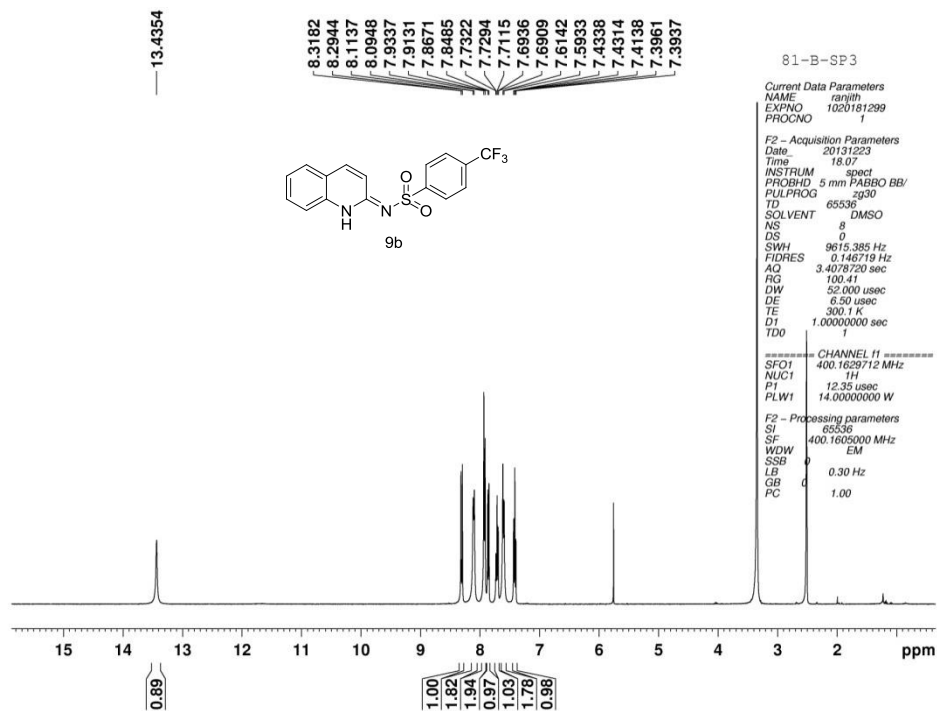


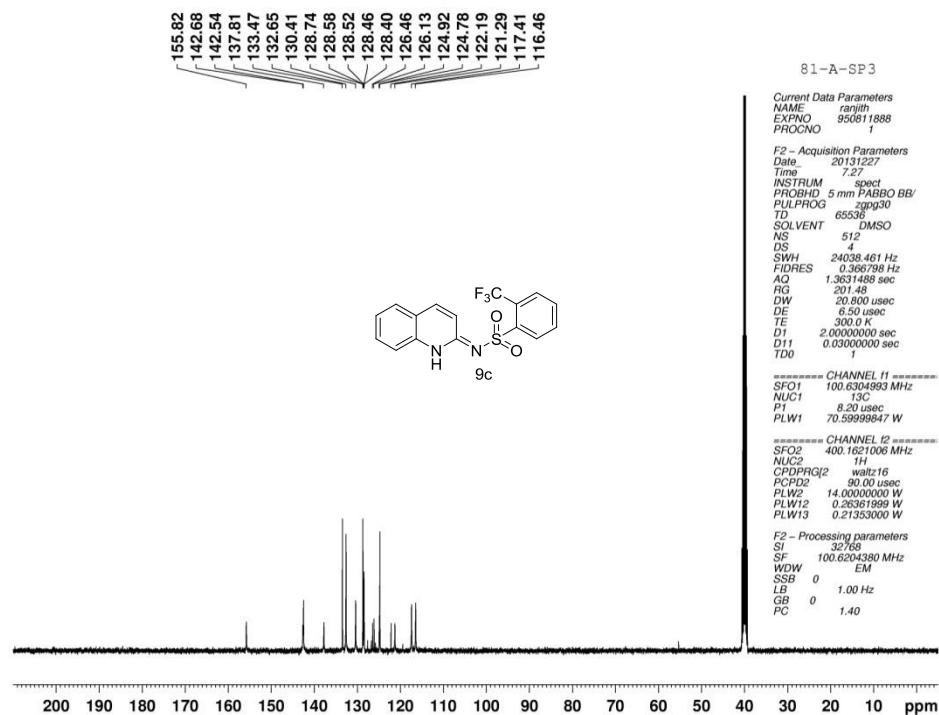
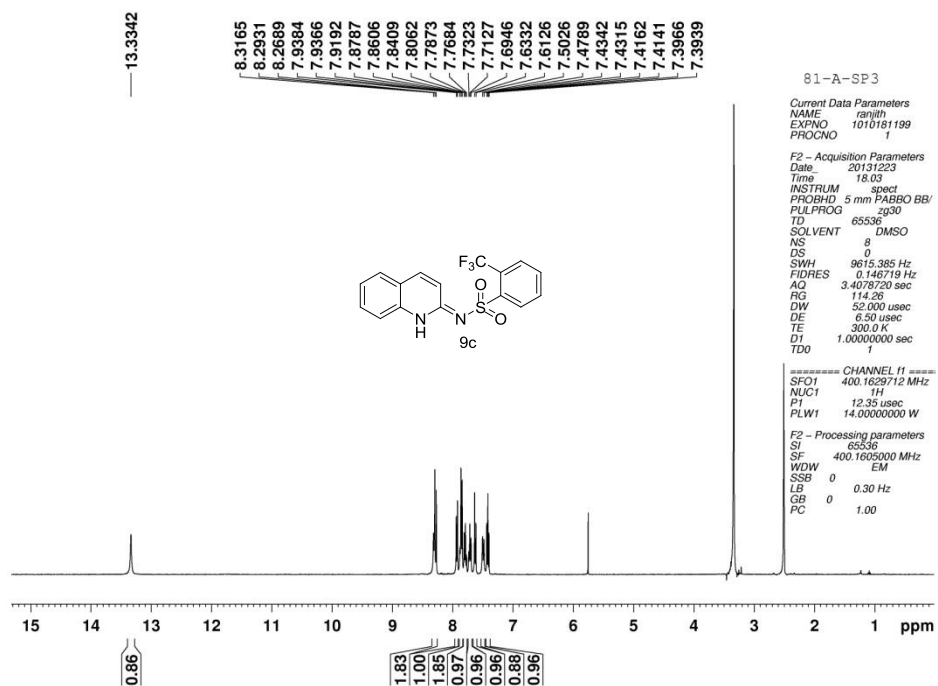


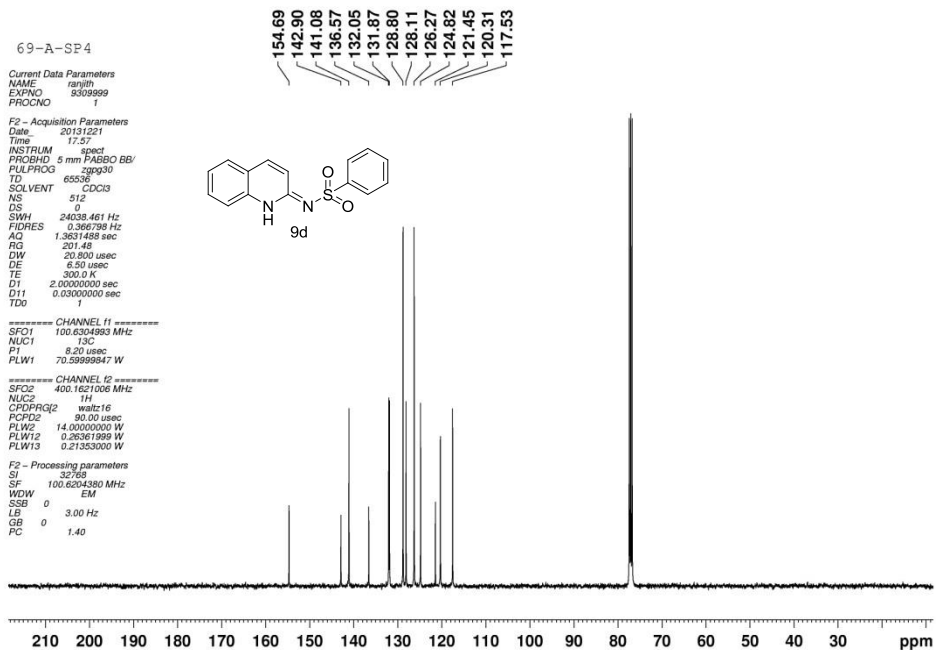
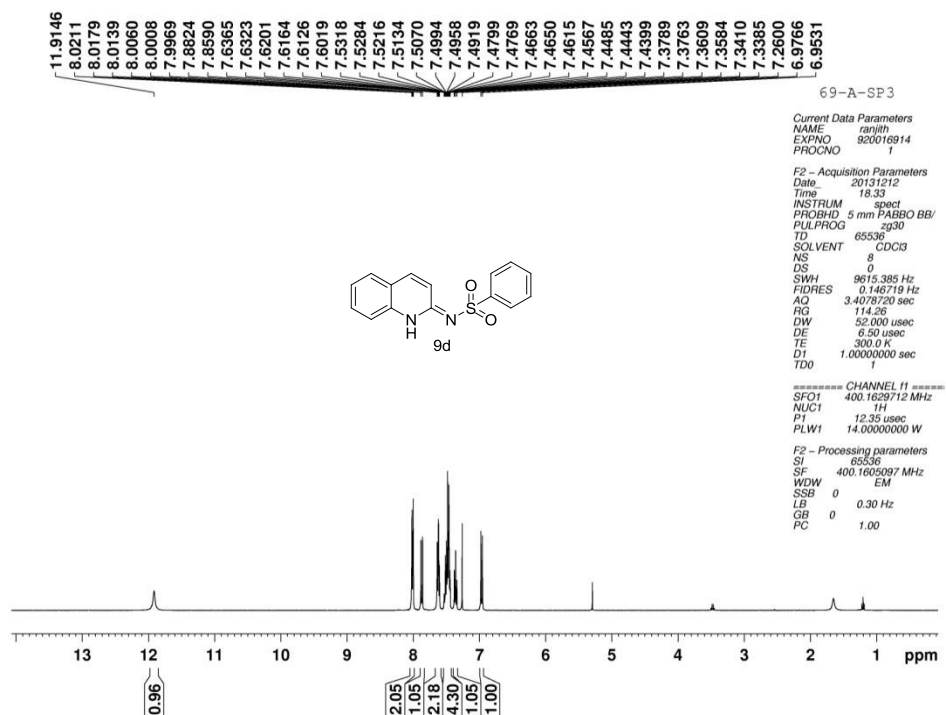


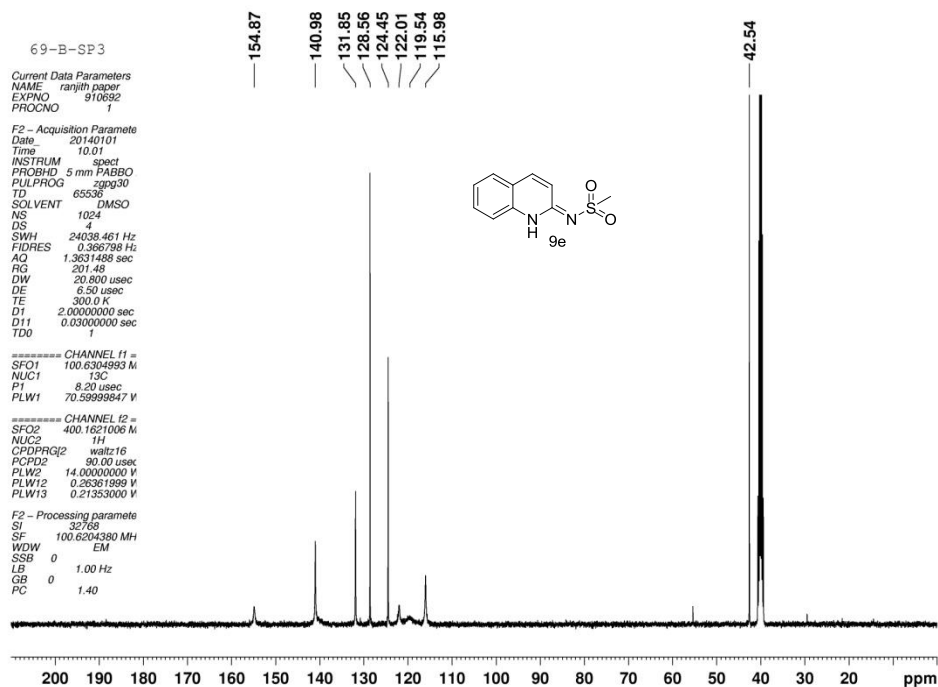
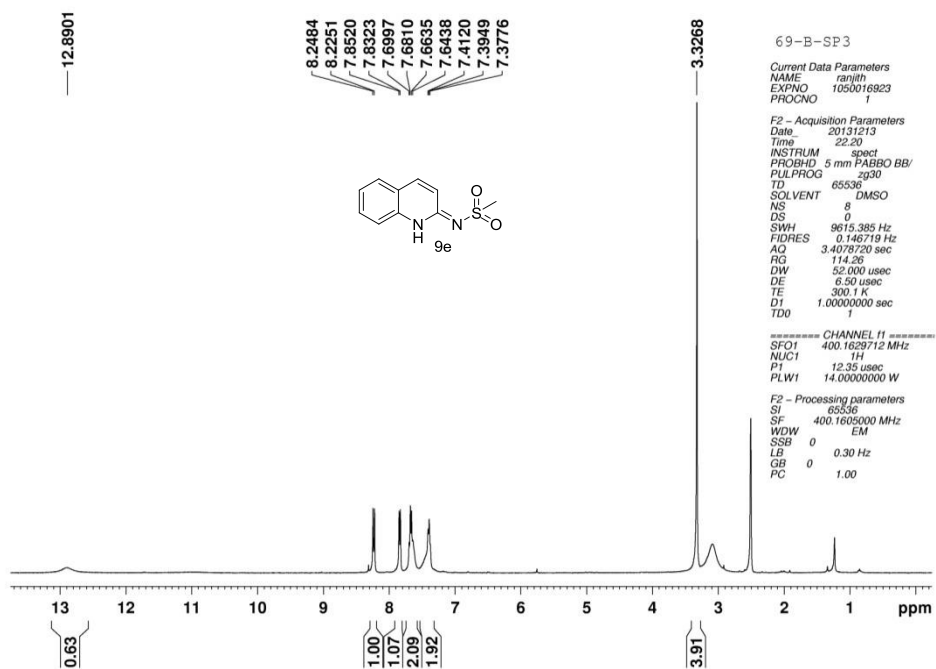


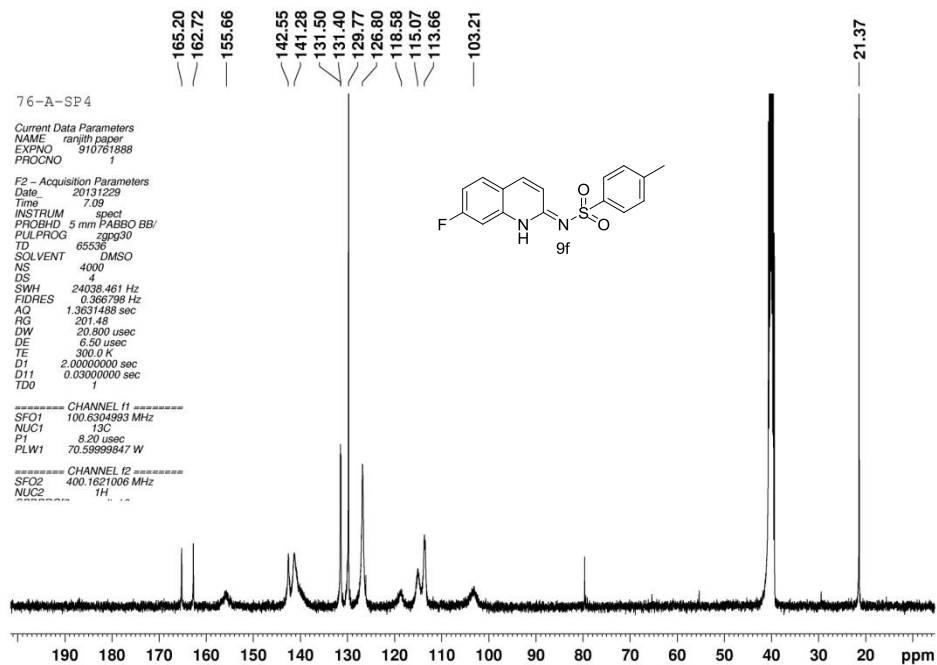
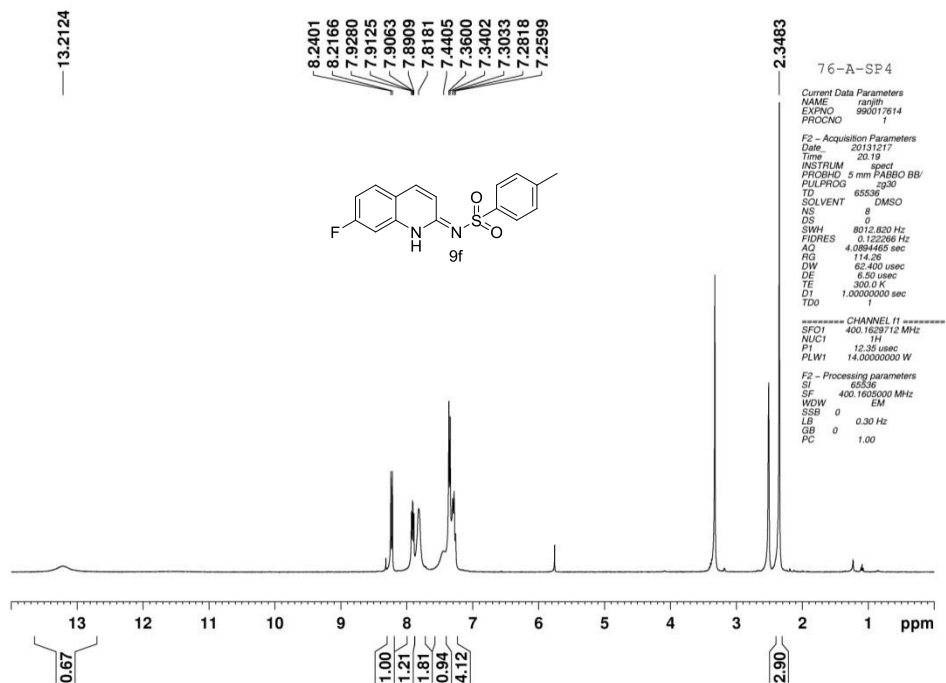


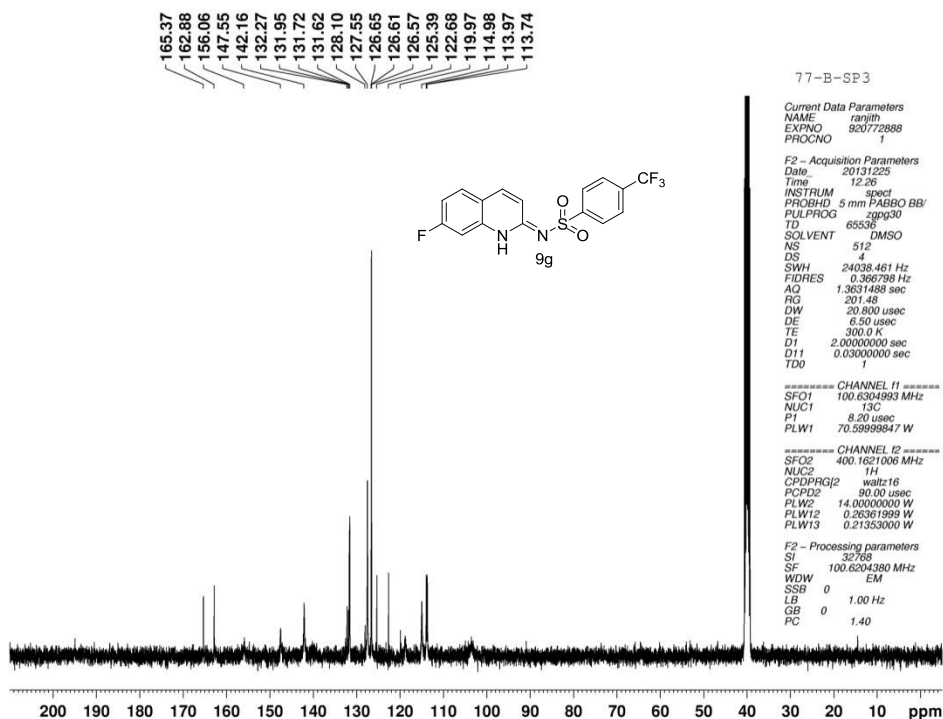
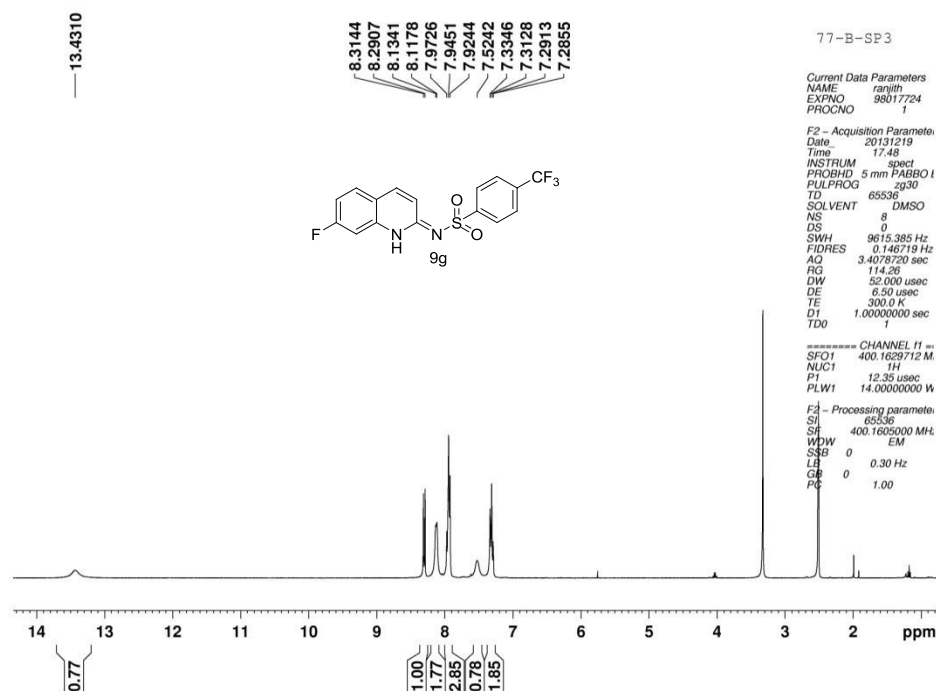


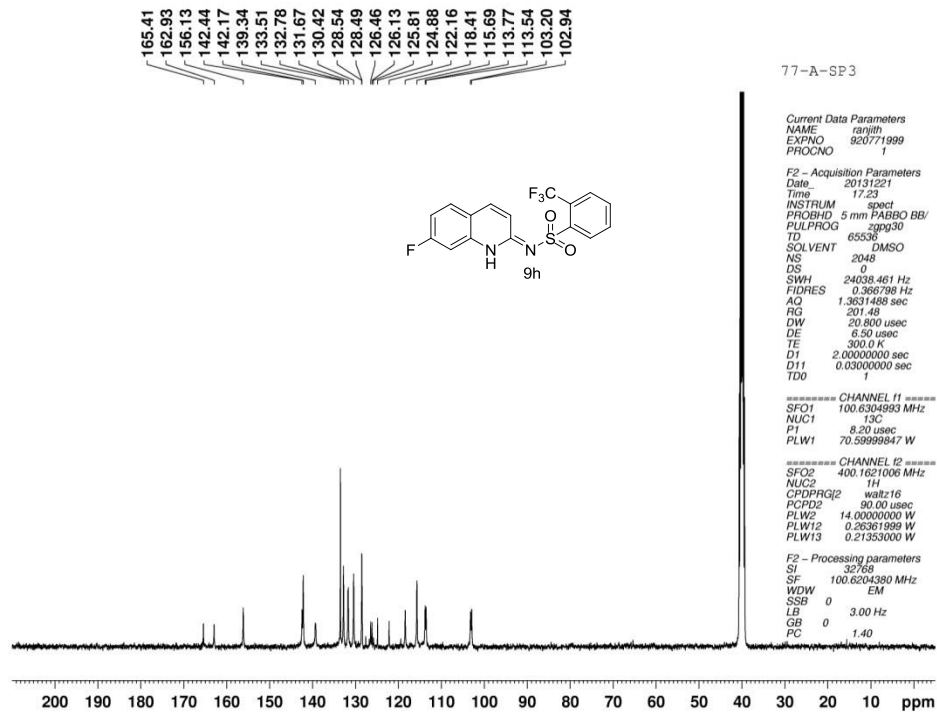
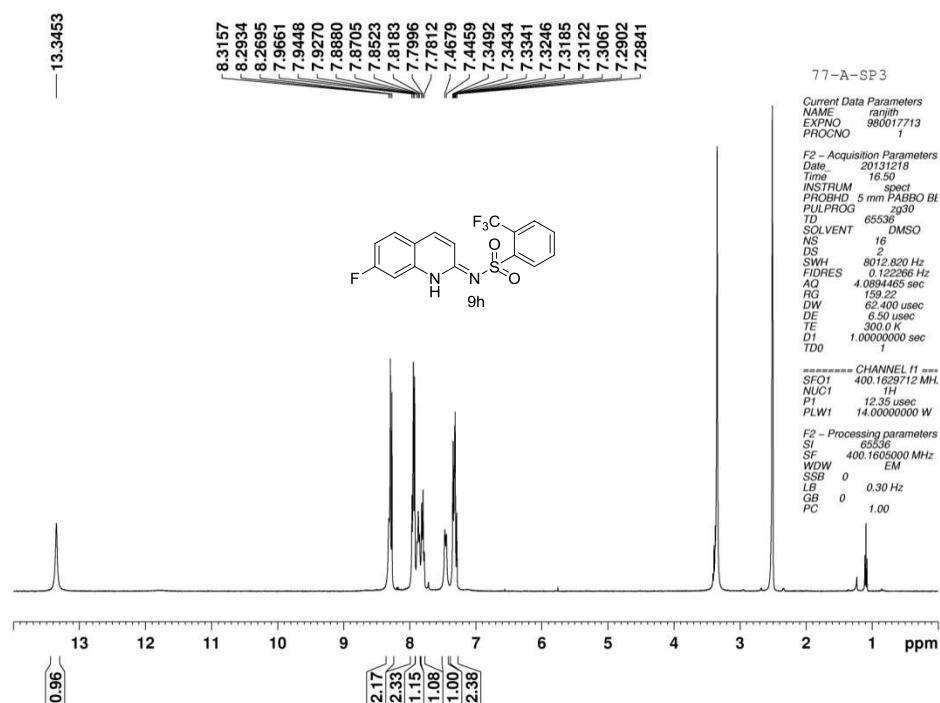


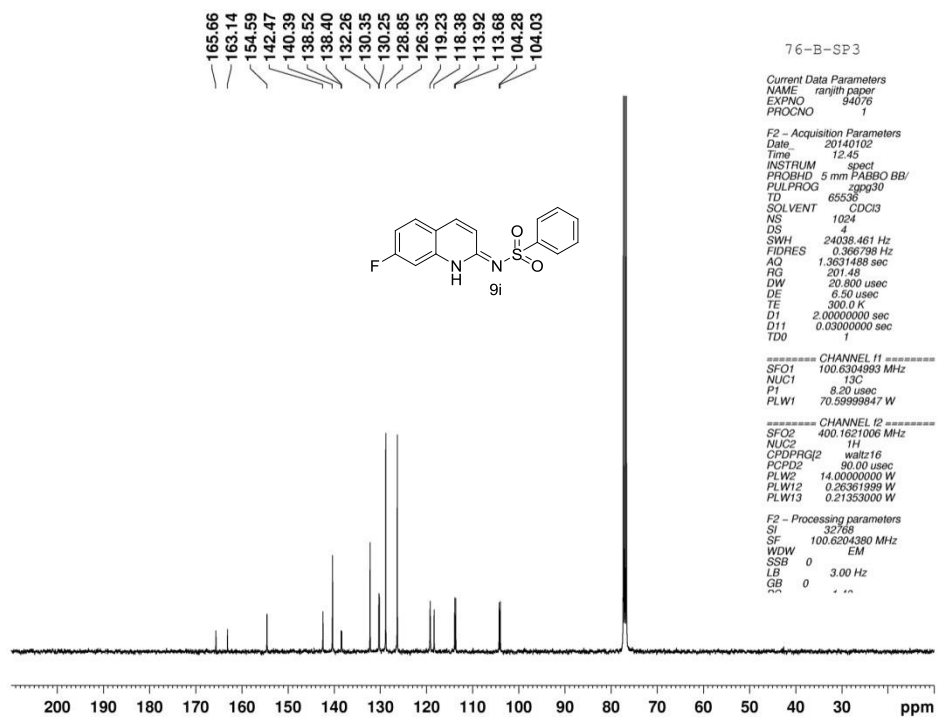
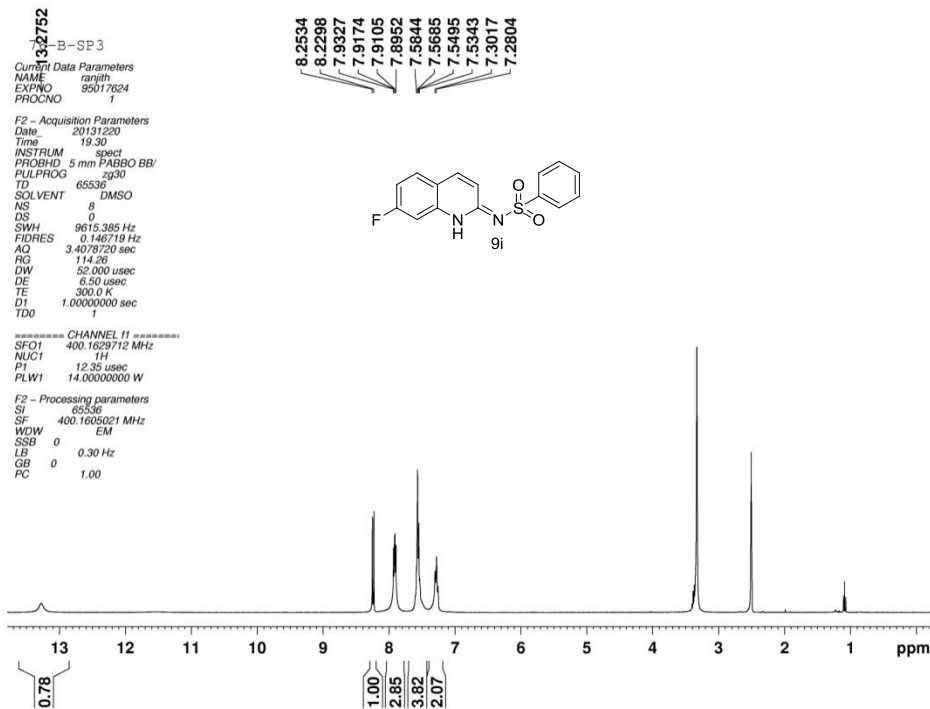


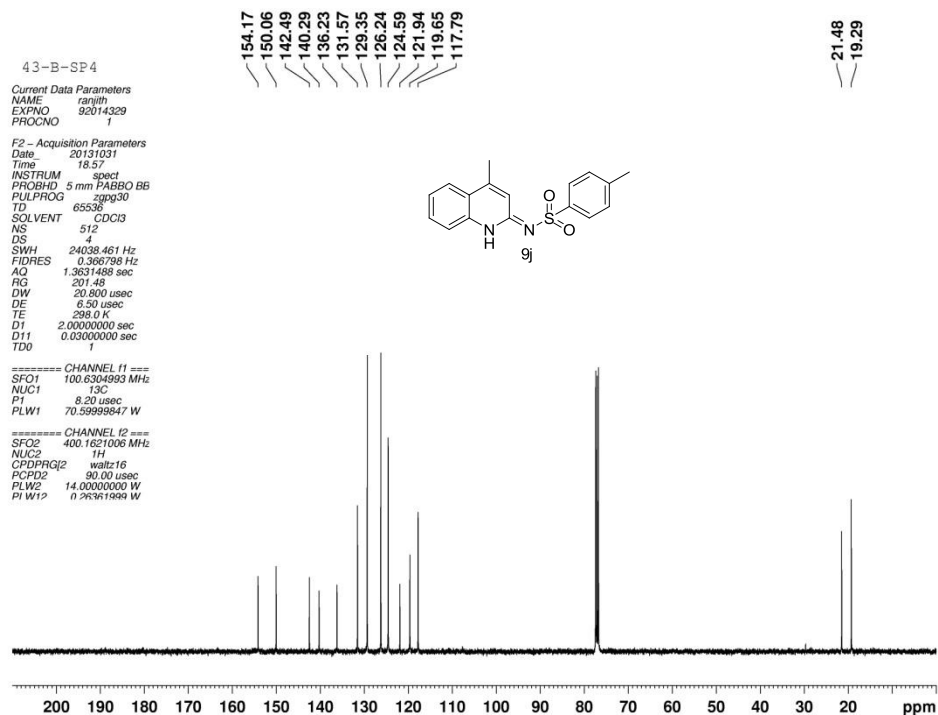
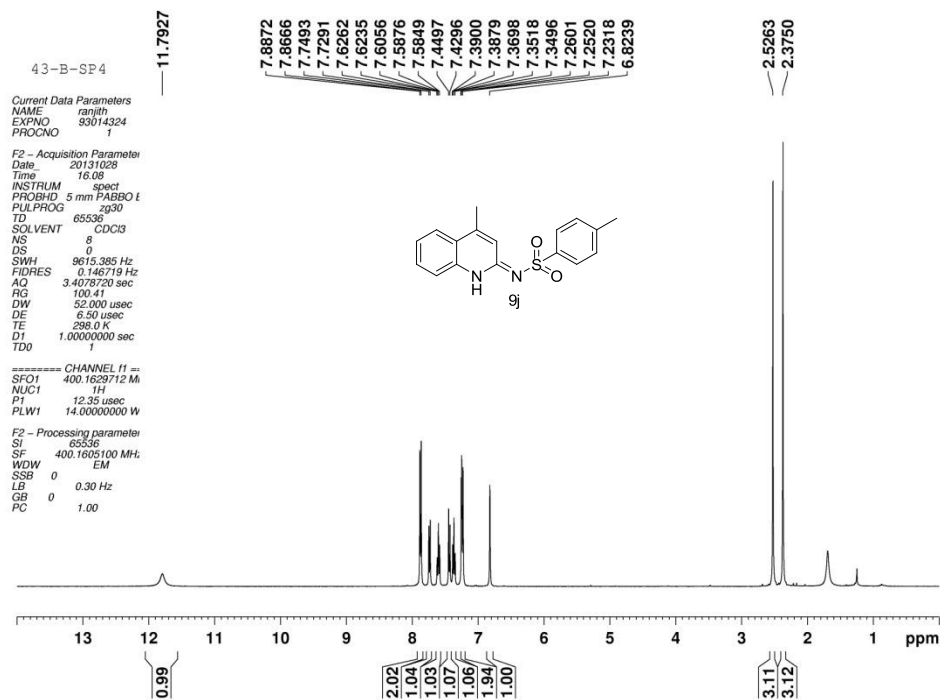


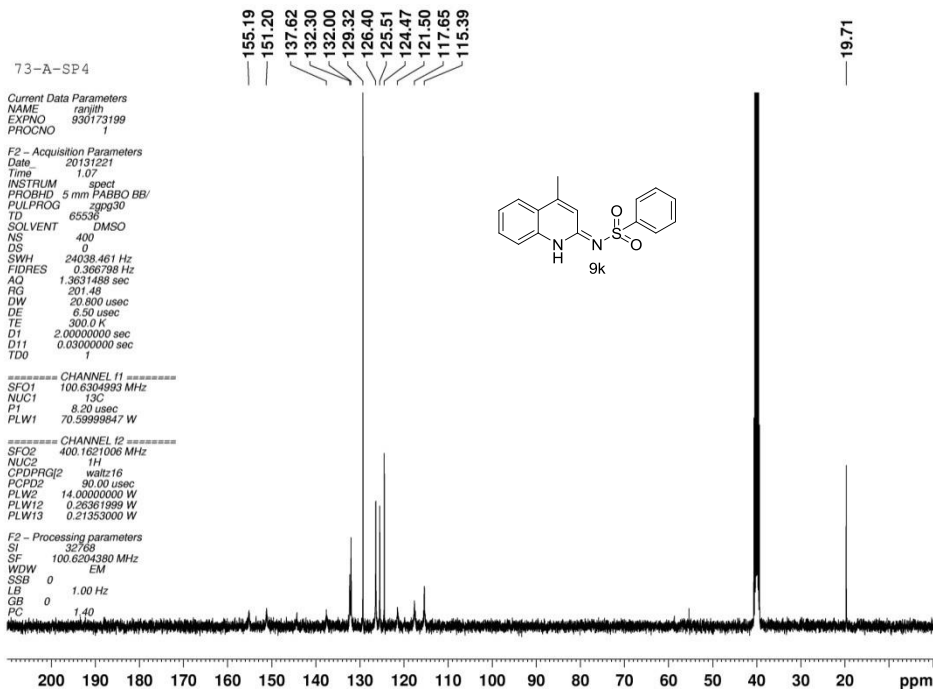
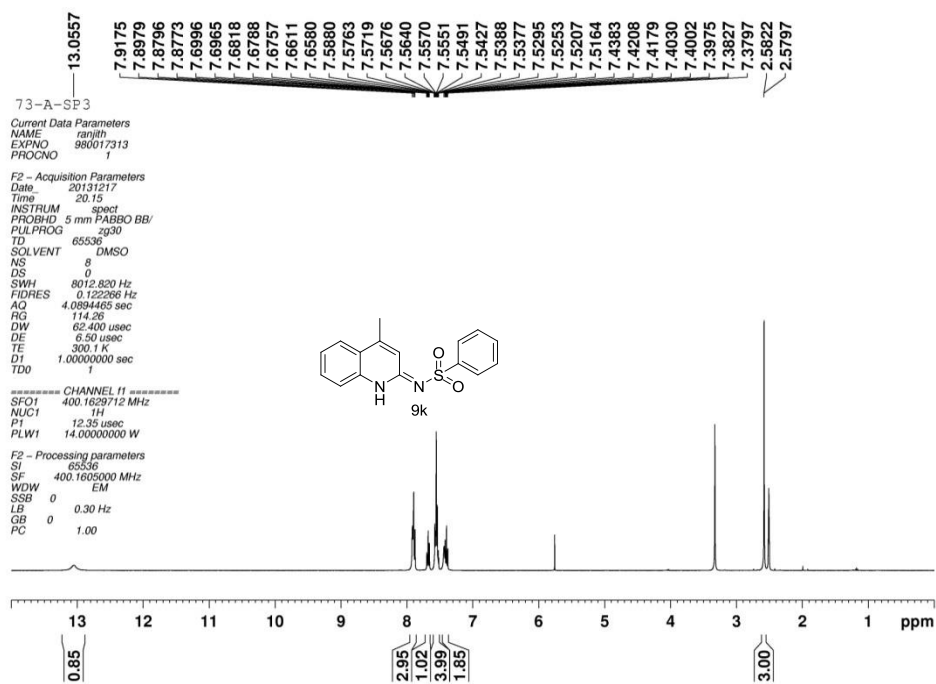


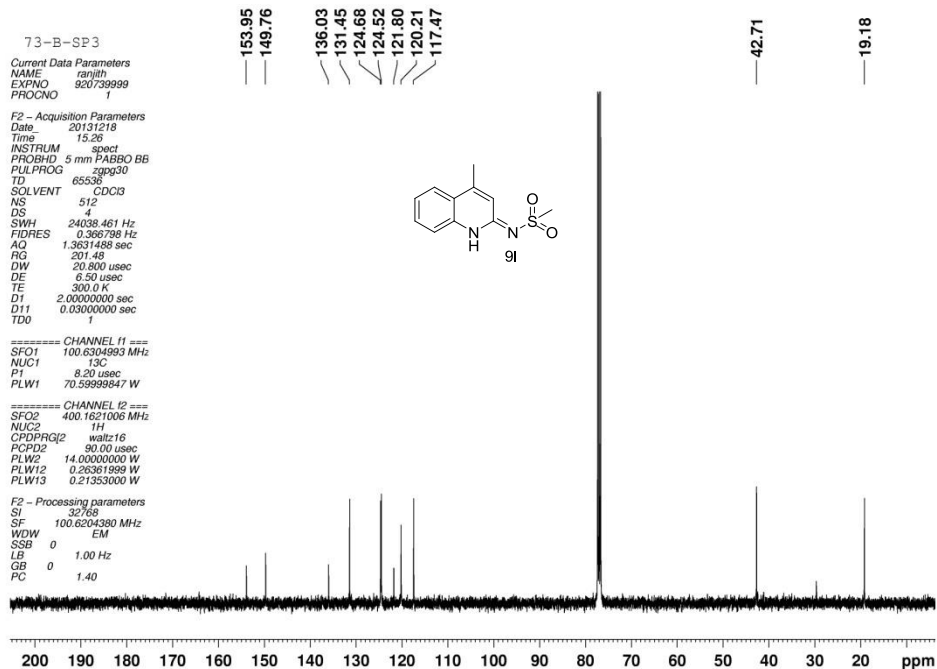
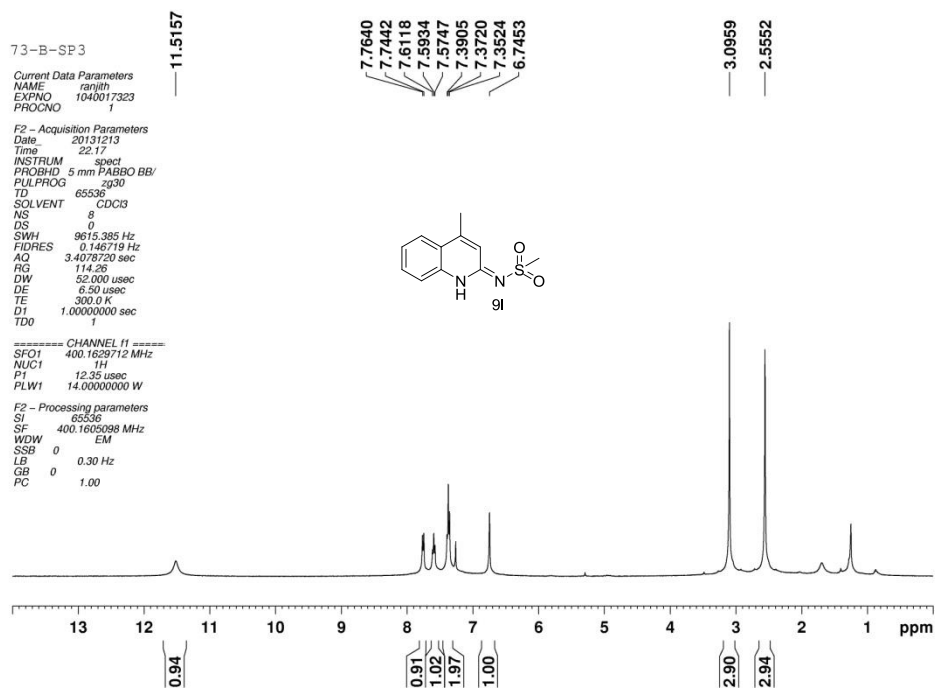


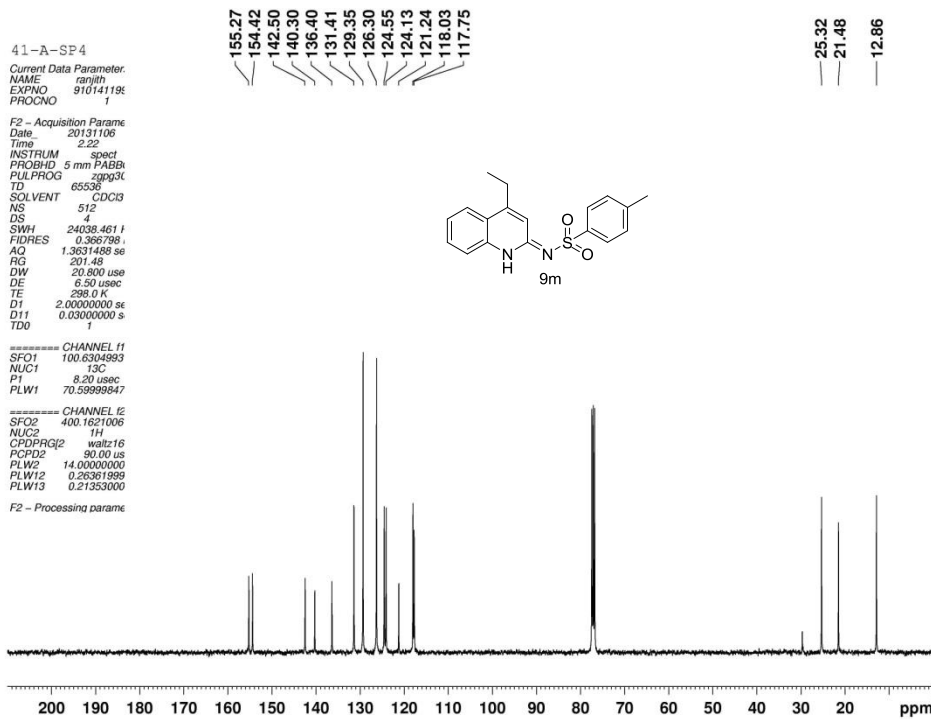
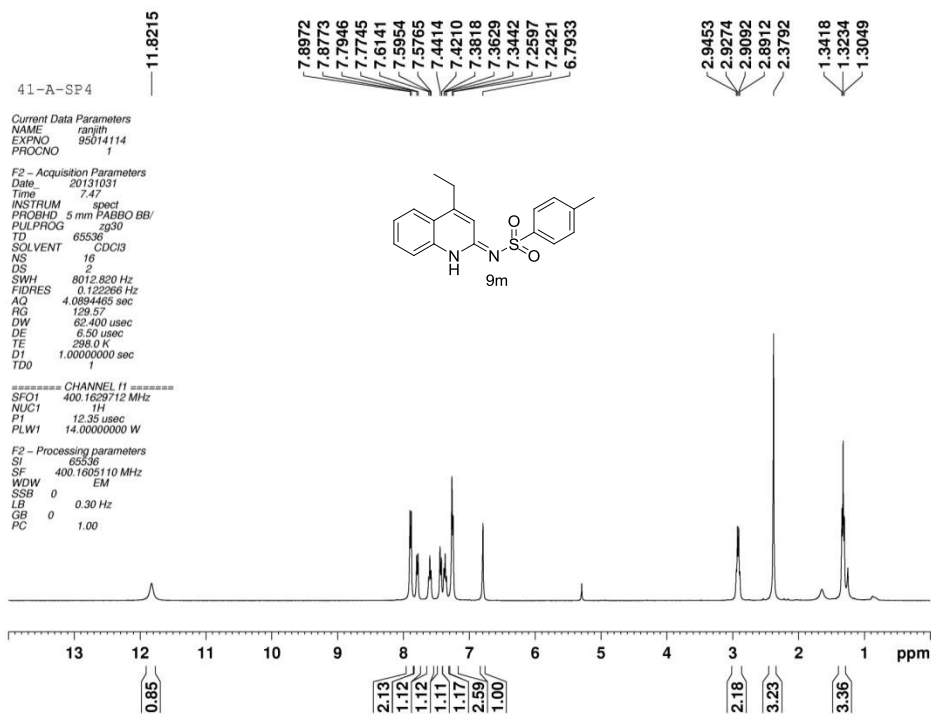


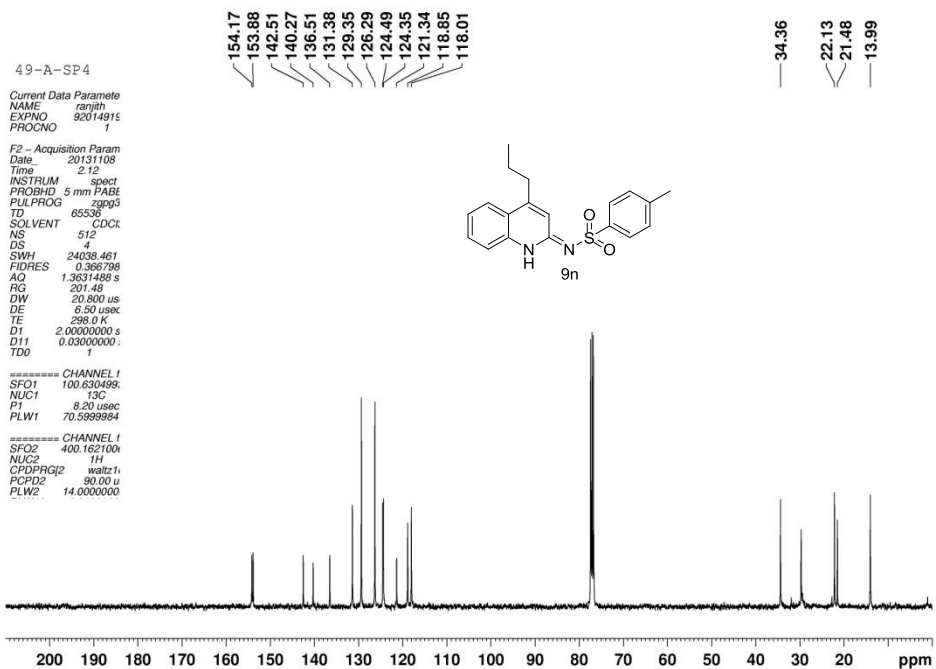
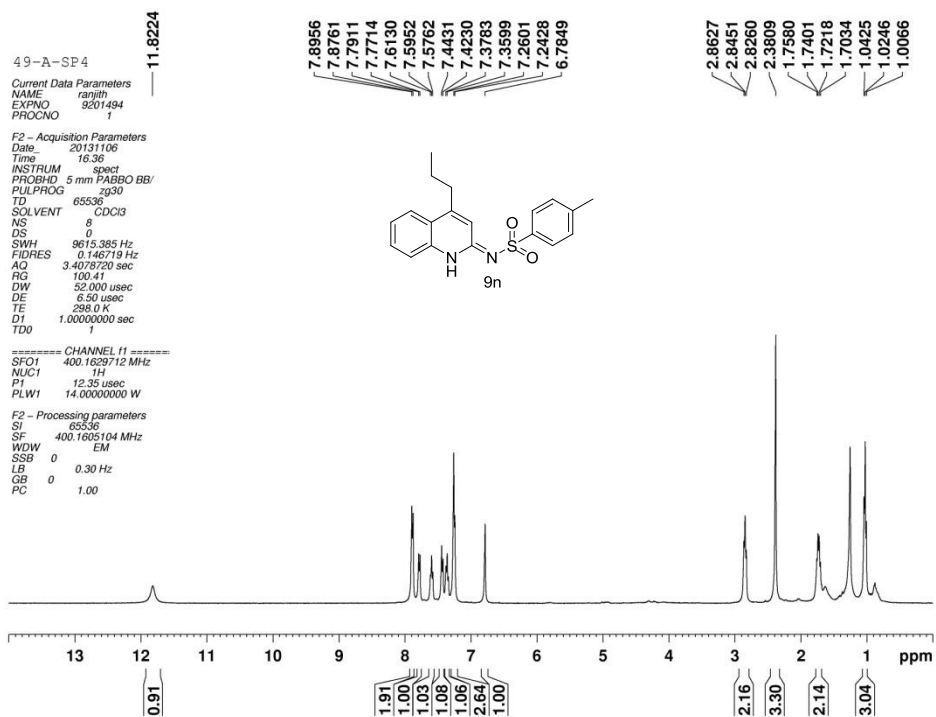


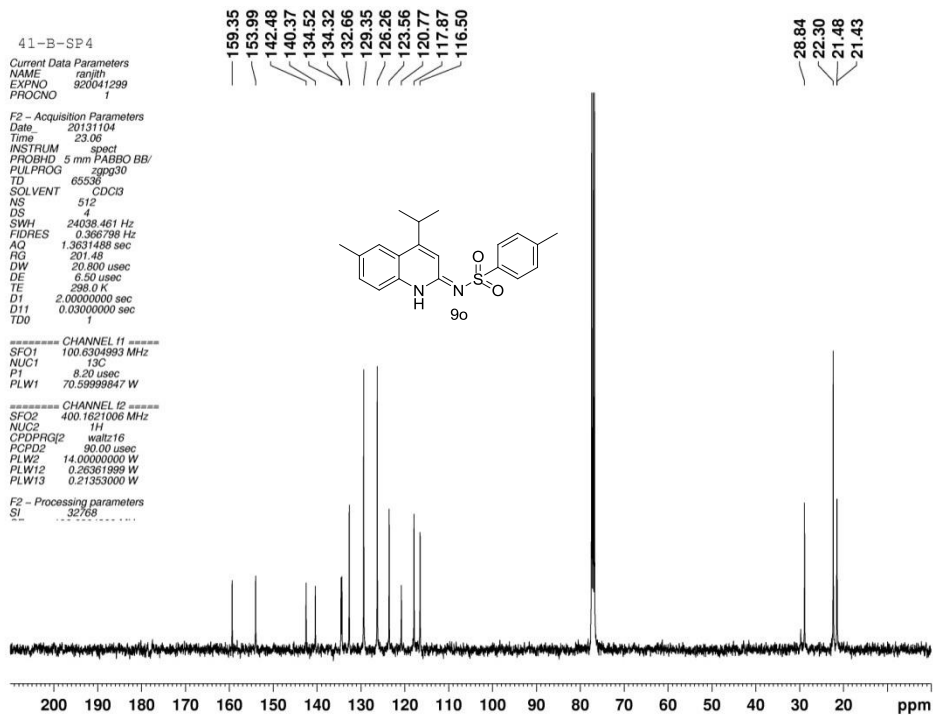
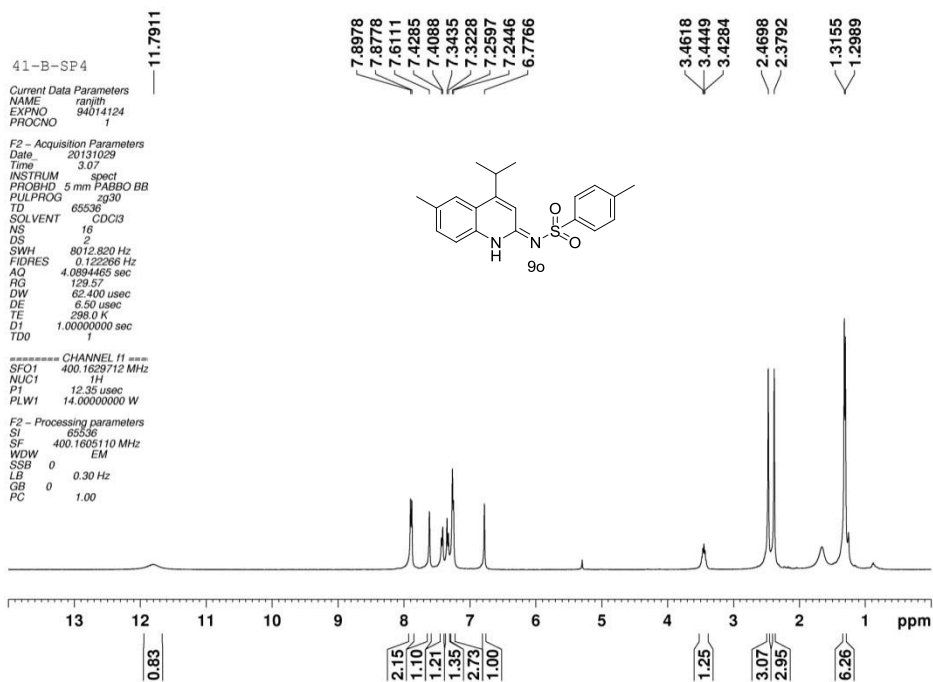


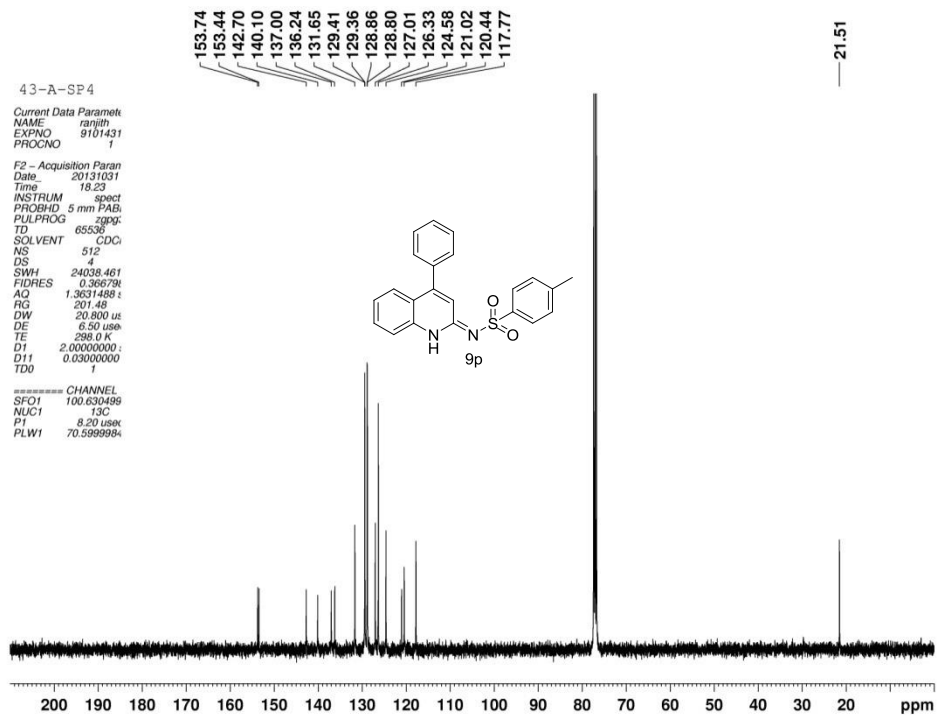
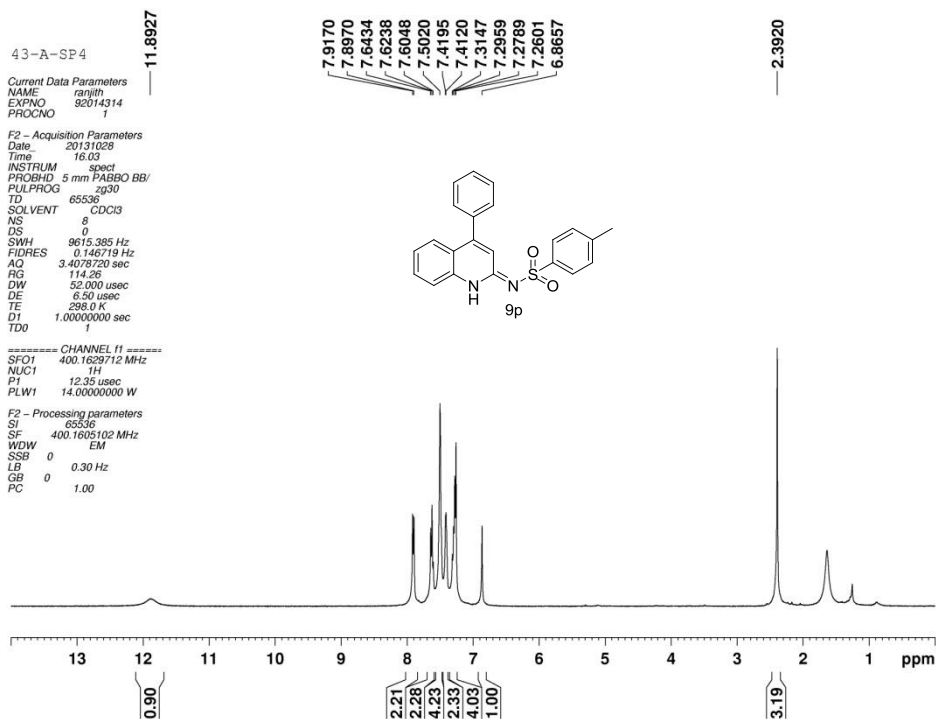


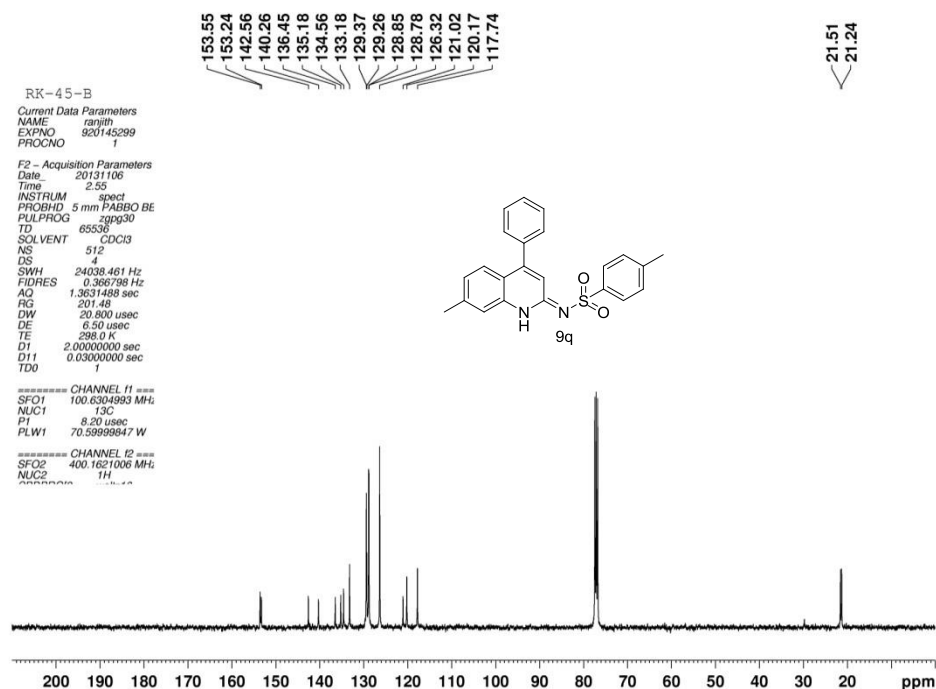
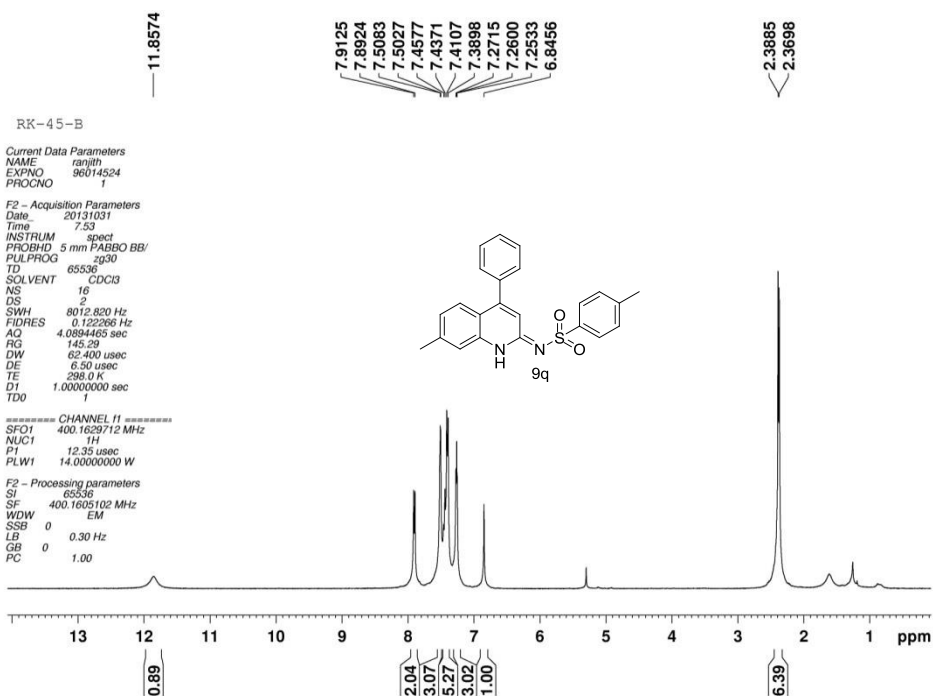


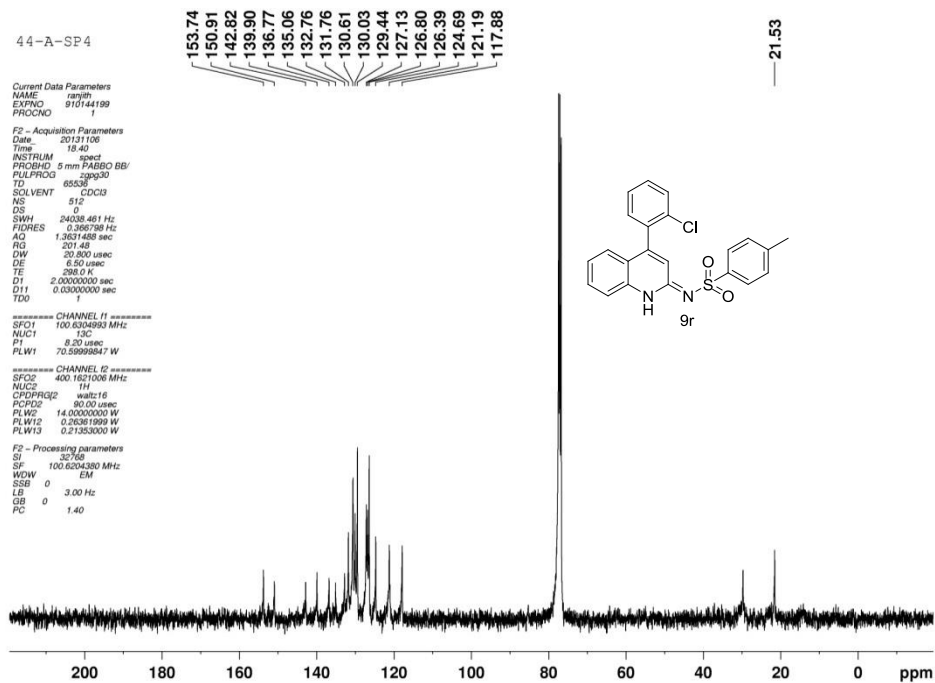
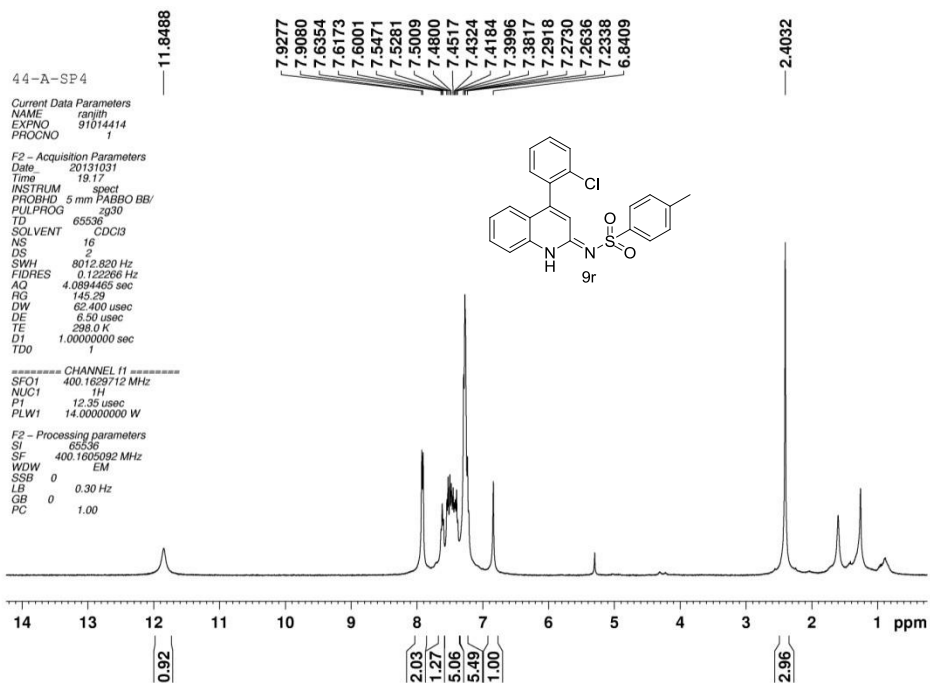


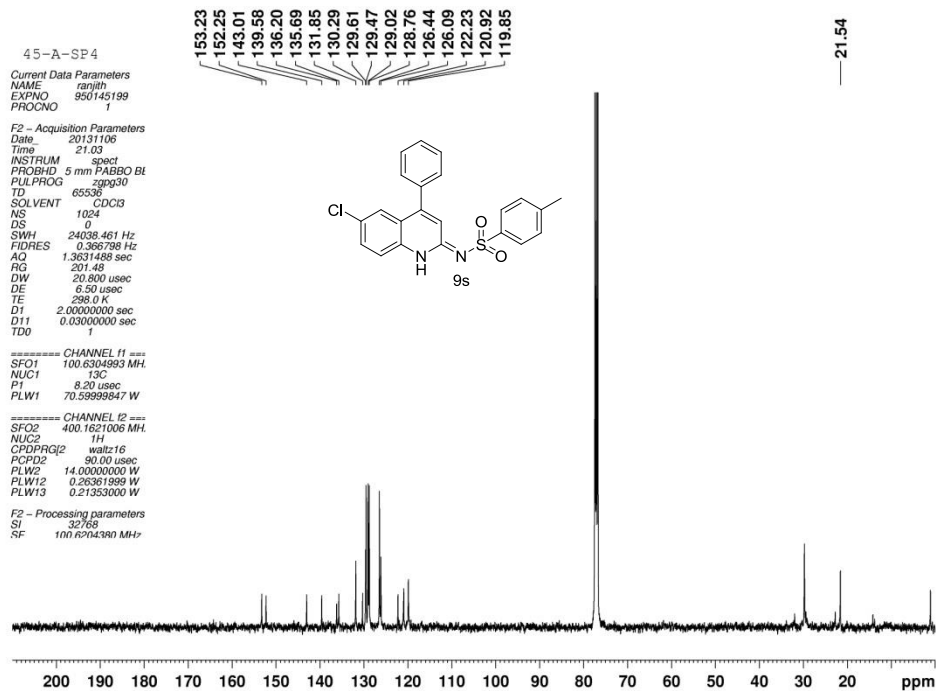
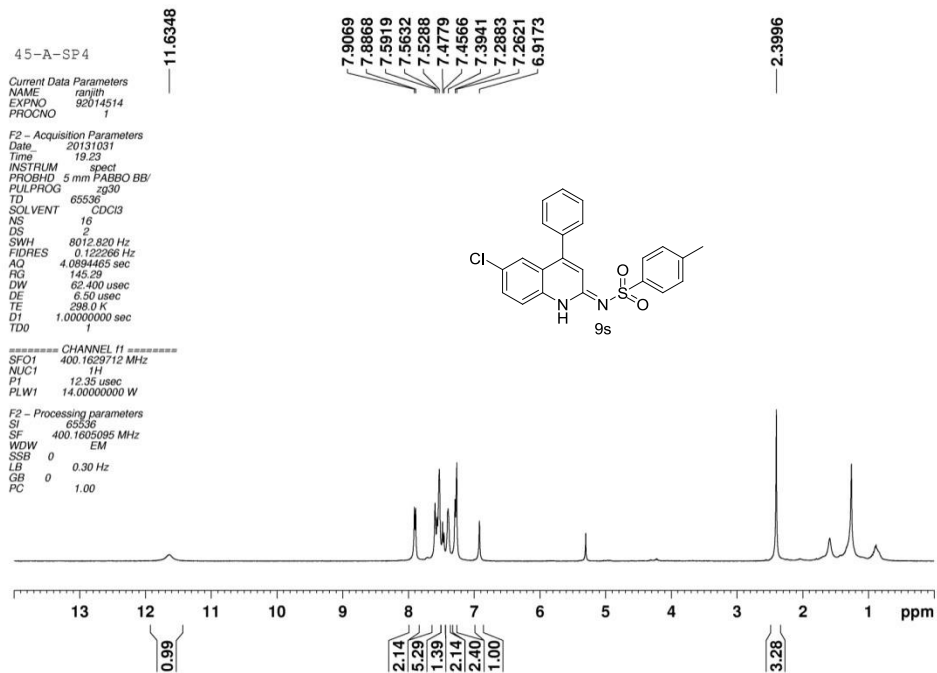


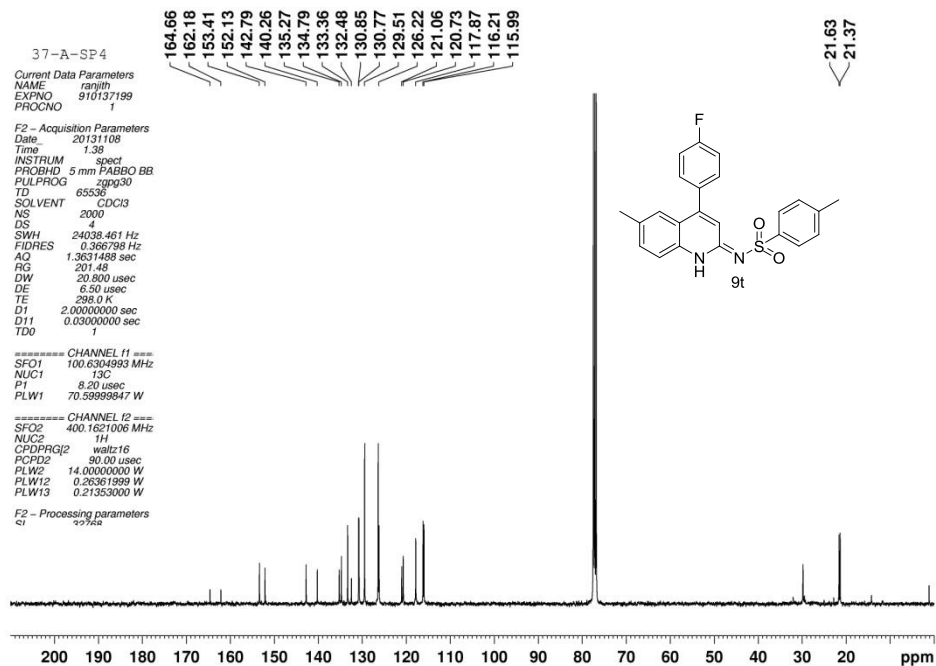
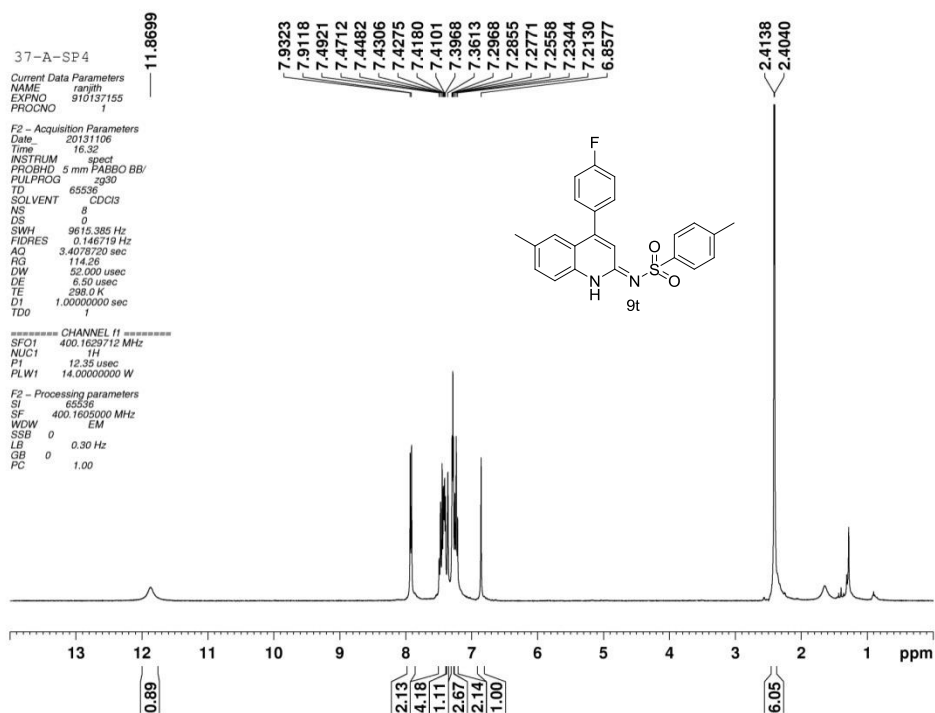


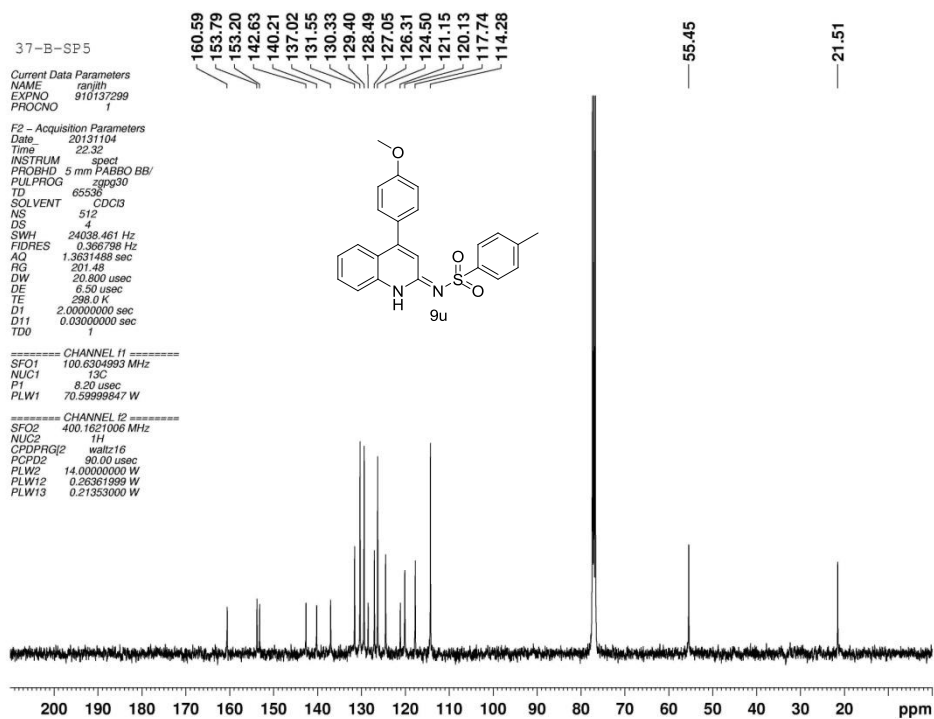
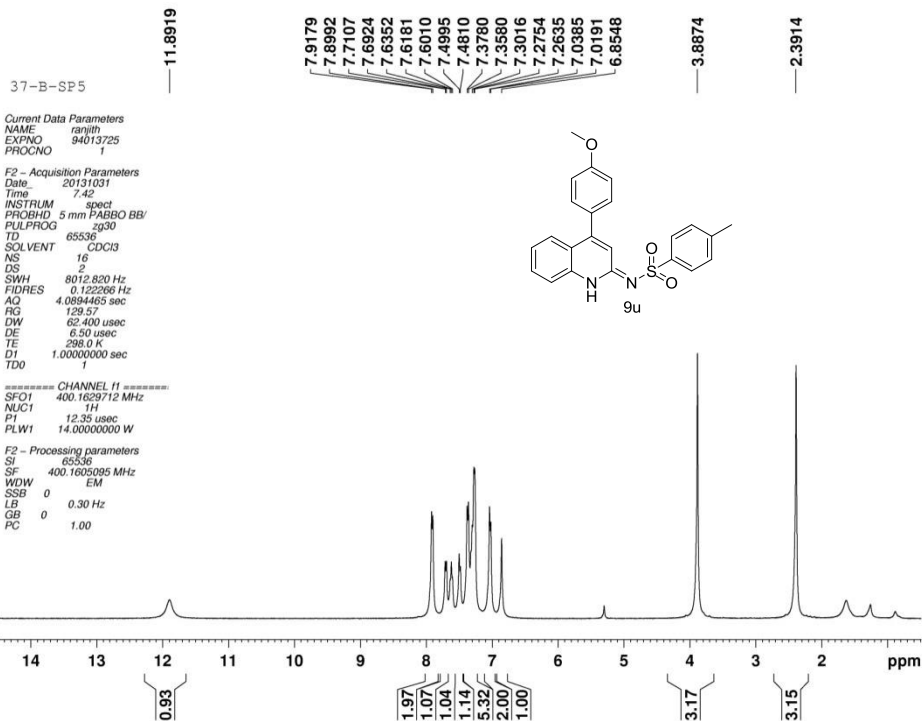












Detailed write up for the X-ray structure of 9j (CCDC number 971729)

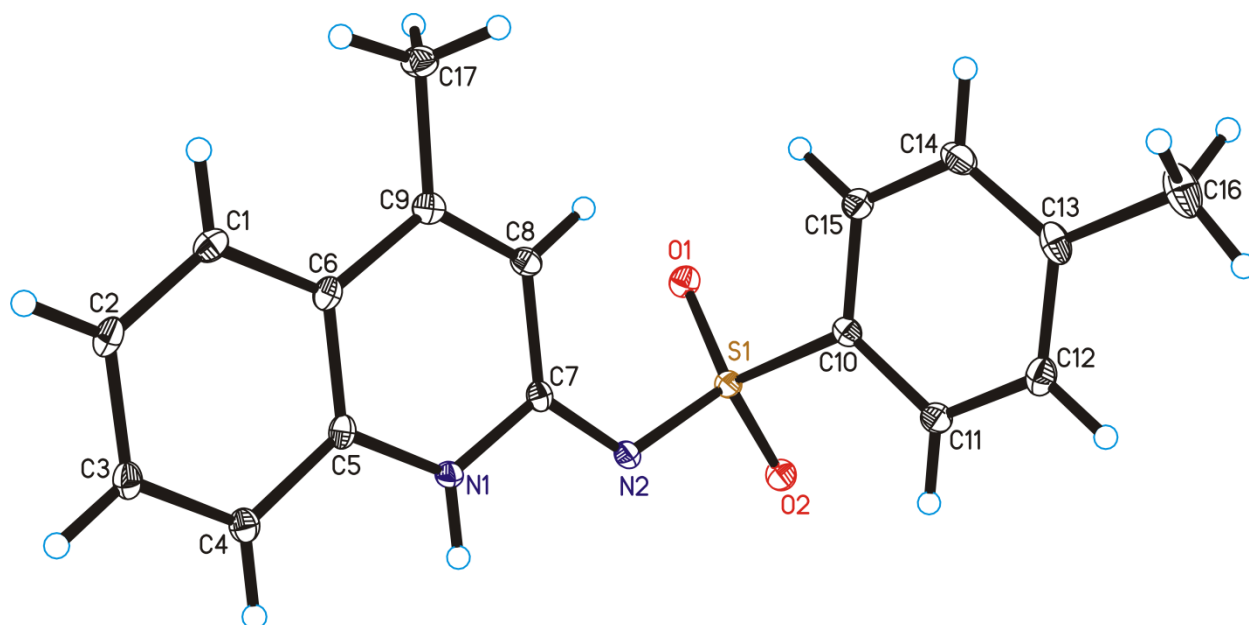


Figure S1 ORTEP diagram drawn with 30% ellipsoid probability for non-H atoms of the crystal structure of compound **9j** determined at 293 K.

Crystallization: Crystals of compound **9j** were grown from the solvent EtOAc by slow evaporation method.

X-ray data collection and structure refinement details:

A good quality yellowish color single crystal of size $0.33 \times 0.21 \times 0.06$ mm, was selected under a polarizing microscope and was mounted on a glass fiber for data collection. Single crystal X-ray data for compound **9j** were collected on the Rigaku Kappa 3 circle diffractometer equipped with the AFC12 goniometer and enhanced sensitivity (HG) Saturn724+ CCD detector in the 4×4 bin mode using the monochromated Mo-K α radiation generated from the microfocus sealed tube MicroMax-003 X-ray generator equipped with specially designed confocal multilayer optics. Data collection was performed using ω -scans of 0.5° steps at 293(2) K. Cell determination, data collection and data reduction was performed using the Rigaku CrystalClear-SM Expert 2.1 b24¹ software. Structure solution and refinement were performed by using SHELXTL-NT². Refinement of coordinates and anisotropic thermal parameters of non-hydrogen atoms were carried out by the full-matrix least-squares method. The hydrogen atoms attached to carbon atoms were generated with idealized geometries and isotropically refined using a riding model.

1. CrystalClear 2.1, Rigaku Corporation, Tokyo, Japan
2. Sheldrick, G. M. Acta Crystallogr., Sect. A 2008, 64, 112–122.

Table S1 Crystal data and structure refinement details for **9j**.

Compound	****
Empirical formula	C ₁₇ H ₁₆ N ₂ S
Formula weight	312.38
Crystal System	Triclinic
Space group	<i>P</i> -1
<i>a</i> (Å)	25.116(11)
<i>b</i> (Å)	14.416(7)
<i>c</i> (Å)	8.406(4)
α (°)	90.00
β (°)	90.00
γ (°)	90.00
<i>V</i> (Å ³)	3044(2)
<i>Z</i>	8
<i>D</i> _c (g/cm ³)	1.363
<i>F</i> ₀₀₀	1312
μ (mm ⁻¹)	0.221
θ_{max} (°)	25.38
Total reflections	21951
Unique reflections	2781
Reflections [<i>I</i> > 2σ(<i>I</i>)]	2481
Parameters	203
<i>R</i> _{int}	0.0414
Goodness-of-fit	1.097
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)]	0.0619
w <i>R</i> (<i>F</i> ² , all data)	0.1509
CCDC No.	971729

Bond lengths and angles

C1 - Distance Angles

C2 1.3759 (0.0043)

C6 1.4038 (0.0043) 120.98 (0.29)

H1 0.9300 119.51 119.51

C1 - C2 C6

C2 - Distance Angles

C1 1.3759 (0.0043)

C3 1.3991 (0.0044) 119.43 (0.29)

H2 0.9300 120.28 120.28

C2 - C1 C3

C3 - Distance Angles

C4 1.3769 (0.0044)

C2 1.3991 (0.0044) 121.37 (0.28)

H3 0.9300 119.31 119.31

C3 - C4 C2

C4 - Distance Angles

C3 1.3769 (0.0044)

C5 1.4030 (0.0040) 119.16 (0.29)

H4 0.9300 120.42 120.42

C4 - C3 C5

C5 - Distance Angles
 N1 1.3857 (0.0040)
 C4 1.4030 (0.0040) 119.95 (0.27)
 C6 1.4090 (0.0042) 119.69 (0.26) 120.36 (0.28)
 C5 - N1 C4

C6 - Distance Angles
 C1 1.4038 (0.0043)
 C5 1.4090 (0.0042) 118.69 (0.27)
 C9 1.4455 (0.0041) 123.52 (0.28) 117.80 (0.27)
 C6 - C1 C5

C7 - Distance Angles
 N2 1.3368 (0.0039)
 N1 1.3571 (0.0036) 114.94 (0.26)
 C8 1.4344 (0.0041) 128.81 (0.26) 116.24 (0.27)
 C7 - N2 N1

C8 - Distance Angles
 C9 1.3557 (0.0044)
 C7 1.4344 (0.0041) 122.81 (0.27)
 H8 0.9300 118.60 118.60
 C8 - C9 C7

C9 - Distance Angles
 C8 1.3557 (0.0044)
 C6 1.4455 (0.0041) 119.43 (0.27)

C17 1.4932 (0.0042) 120.93 (0.27) 119.64 (0.28)

C9 - C8 C6

C10 - Distance Angles

C11 1.3917 (0.0041)

C15 1.3942 (0.0042) 119.76 (0.27)

S1 1.7724 (0.0030) 119.42 (0.23) 120.82 (0.23)

C10 - C11 C15

C11 - Distance Angles

C12 1.3850 (0.0043)

C10 1.3917 (0.0041) 119.55 (0.29)

H11 0.9300 120.23 120.23

C11 - C12 C10

C12 - Distance Angles

C11 1.3850 (0.0043)

C13 1.3916 (0.0045) 121.29 (0.29)

H12 0.9300 119.35 119.35

C12 - C11 C13

C13 - Distance Angles

C14 1.3884 (0.0047)

C12 1.3916 (0.0045) 118.47 (0.28)

C16 1.5095 (0.0043) 120.89 (0.30) 120.60 (0.30)

C13 - C14 C12

C14 -	Distance	Angles	
C15	1.3839 (0.0045)		
C13	1.3884 (0.0047)	121.09 (0.29)	
H14	0.9300	119.46	119.46
	C14 -	C15	C13

C15 -	Distance	Angles	
C14	1.3839 (0.0045)		
C10	1.3942 (0.0042)	119.81 (0.29)	
H15	0.9300	120.09	120.09
	C15 -	C14	C10

C16 -	Distance	Angles		
C13	1.5095 (0.0043)			
H16A	0.9600	109.47		
H16B	0.9600	109.47	109.47	
H16C	0.9600	109.47	109.47	109.47
	C16 -	C13	H16A	H16B

C17 -	Distance	Angles		
C9	1.4932 (0.0042)			
H17A	0.9600	109.47		
H17B	0.9600	109.47	109.47	
H17C	0.9600	109.47	109.47	109.47
	C17 -	C9	H17A	H17B

N1 - Distance Angles
 C7 1.3571 (0.0036)
 C5 1.3857 (0.0040) 124.00 (0.26)
 H1A 0.8773 (0.0349) 116.49 (2.19) 119.49 (2.20)
 N1 - C7 C5

N2 - Distance Angles
 C7 1.3368 (0.0039)
 S1 1.5904 (0.0025) 123.05 (0.21)
 N2 - C7

O1 - Distance Angles
 S1 1.4472 (0.0021)
 O1 -

O2 - Distance Angles
 S1 1.4423 (0.0023)
 O2 -

S1 - Distance Angles
 O2 1.4423 (0.0023)
 O1 1.4472 (0.0022) 116.36 (0.13)
 N2 1.5904 (0.0025) 104.60 (0.13) 114.45 (0.13)
 C10 1.7724 (0.0030) 106.03 (0.14) 107.03 (0.13) 107.82 (0.14)
 S1 - O2 O1 N2

Selected torsion angles

-0.12 (0.44) C6 - C1 - C2 - C3
0.05 (0.44) C1 - C2 - C3 - C4
0.21 (0.43) C2 - C3 - C4 - C5
179.84 (0.25) C3 - C4 - C5 - N1
-0.40 (0.42) C3 - C4 - C5 - C6
-0.07 (0.42) C2 - C1 - C6 - C5
-179.42 (0.28) C2 - C1 - C6 - C9
-179.91 (0.25) N1 - C5 - C6 - C1
0.33 (0.41) C4 - C5 - C6 - C1
-0.52 (0.39) N1 - C5 - C6 - C9
179.71 (0.26) C4 - C5 - C6 - C9
-177.23 (0.28) N2 - C7 - C8 - C9
1.54 (0.41) N1 - C7 - C8 - C9
-2.22 (0.43) C7 - C8 - C9 - C6
178.08 (0.27) C7 - C8 - C9 - C17
-178.99 (0.27) C1 - C6 - C9 - C8
1.66 (0.40) C5 - C6 - C9 - C8
0.72 (0.42) C1 - C6 - C9 - C17
-178.63 (0.26) C5 - C6 - C9 - C17
-0.35 (0.45) C15 - C10 - C11 - C12
179.26 (0.23) S1 - C10 - C11 - C12
0.25 (0.47) C10 - C11 - C12 - C13
0.78 (0.47) C11 - C12 - C13 - C14
-176.94 (0.29) C11 - C12 - C13 - C16
-1.73 (0.47) C12 - C13 - C14 - C15

175.98 (0.31) C16 - C13 - C14 - C15
 1.64 (0.48) C13 - C14 - C15 - C10
 -0.58 (0.46) C11 - C10 - C15 - C14
 179.81 (0.24) S1 - C10 - C15 - C14
 178.61 (0.24) N2 - C7 - N1 - C5
 -0.33 (0.40) C8 - C7 - N1 - C5
 179.65 (0.26) C4 - C5 - N1 - C7
 -0.11 (0.41) C6 - C5 - N1 - C7
 176.92 (0.20) N1 - C7 - N2 - S1
 -4.30 (0.43) C8 - C7 - N2 - S1
 -170.78 (0.23) C7 - N2 - S1 - O2
 -42.28 (0.28) C7 - N2 - S1 - O1
 76.67 (0.26) C7 - N2 - S1 - C10
 -36.54 (0.28) C11 - C10 - S1 - O2
 143.07 (0.25) C15 - C10 - S1 - O2
 -161.37 (0.24) C11 - C10 - S1 - O1
 18.24 (0.29) C15 - C10 - S1 - O1
 75.05 (0.27) C11 - C10 - S1 - N2
 -105.34 (0.26) C15 - C10 - S1 - N2