Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

An Efficient Approach to 4-Chloro Quinolines *via* TMSCl-mediated Cascade Cyclization of *Ortho*-Propynol Phenyl Azides

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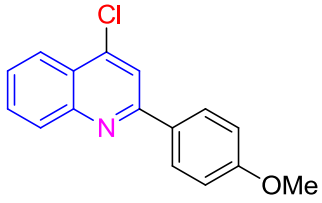
General Remarks:
Column chromatography was carried out on silica gel. ^{1}H NMR spectra were recorded on 400 MHz in $CDCl_3$, ^{13}C NMR spectra were recorded on 100 MHz in $CDCl_3$ using TMS as internal standard. IR spectra were recorded on an FT-IR spectrometer and only major peaks are reported in cm^{-1}. Melting points were determined on a microscopic apparatus and were uncorrected. All products were further characterized by HRMS (high resolution mass spectra); copies of their ^{1}H NMR and ^{13}C NMR spectra are provided. Solvents were dried under standard method. Compounds **2a**[1a], **2d**[1b], **2e**[1a], **2f**[1c], **2g**[1a], **2h**[1b], **2i**[1a], **2l**[1b], **2o**[1d], **2p**[1e], **3a**[1f], **6a**[1g] are known compounds.

General procedure for the preparation of product 4-chloro quinolines 2: The reaction of *ortho*-propynol phenyl azides (**1**) (0.2 mmol), TMSCl (0.7 mmol), in CH_3NO_2 (2.0 mL) at 60 ℃ under air atmosphere. After 1.0 hours, as monitored by TLC, the mixture was concentrated and purified by flash chromatography on silica gel to afford **2**.

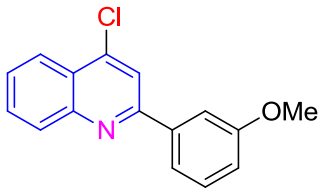
Characterization data of 2a-2v, 2ab, 2ac, 3a-6a

4-chloro-2-(4-methoxyphenyl)quinoline: 2a



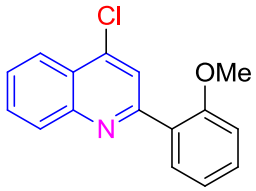
was obtained according to the above method. White solid, mp: 77-79 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.89 (s, 3 H), 7.04 (dd, *J* = 3.2, 8.0 Hz, 2 H), 7.57 – 7.61 (m, 1 H), 7.74 – 7.78 (m, 1 H), 7.93 (s, 1 H), 8.10 – 8.15 (m, 3 H), 8.20 (d, *J* = 8.4 Hz, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.4, 114.3, 118.6, 123.9, 125.0, 126.8, 128.9, 129.8, 130.5, 131.1, 143.0, 149.1, 156.8, 161.2.

4-chloro-2-(3-methoxyphenyl)quinoline: 2b



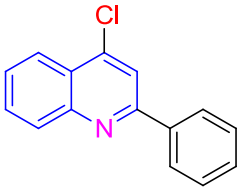
was obtained according to the above method. Colorless liquid, ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.93 (s, 3 H), 7.03 (dd, *J* = 2.4, 8.0 Hz, 1 H), 7.44 (t, *J* = 8.0 Hz, 1 H), 7.60 – 7.68 (m, 2 H), 7.72 – 7.80 (m, 2 H), 7.96 (s, 1 H), 8.21 (dd, *J* = 8.4, 22.5 Hz, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.5, 112.6, 115.9, 119.2, 119.9, 123.9, 125.4, 127.3, 129.9, 130.1, 130.6, 140.0, 143.1, 149.0, 157.1, 160.2. HRMS (ESI, m/z): calcd for $C_{16}H_{12}ClNO$: M+H = 270.0680; found: 270.0683.

4-chloro-2-(2-methoxyphenyl)quinoline: 2c



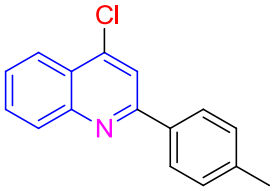
was obtained according to the above method. White solid, mp: 89-91 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.89 (s, 3 H), 7.04 (d, *J* = 8.0 Hz, 1 H), 7.13 (t, *J* = 7.6 Hz, 1 H), 7.42 – 7.46 (m, 1 H), 7.60 – 7.64 (m, 1 H), 7.74 – 7.78 (m, 1 H), 7.86 (dd, *J* = 1.6, 7.6 Hz, 1 H), 8.03 (s, 1 H), 8.17 – 8.24 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.7, 111.4, 121.3, 123.4, 123.9, 125.2, 127.1, 128.5, 119.9, 130.1, 130.8, 131.1, 141.5, 148.9, 156.8, 157.2. HRMS (ESI, m/z): calcd for $C_{16}H_{12}ClNO$: M+H = 270.0680; found: 270.0684.

4-chloro-2-phenylquinoline: 2d



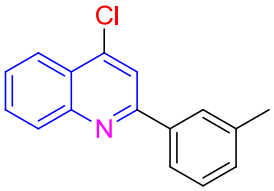
was obtained according to the above method. White solid, mp: 82-84 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49 – 7.56 (m, 3 H), 7.63 (t, *J* = 8.0 Hz, 1 H), 7.77 – 7.81 (m, 1 H), 7.98 (s, 1 H), 8.14 (d, *J* = 6.8 Hz, 2 H), 8.17 (d, *J* = 6.8 Hz, 1 H), 8.20 – 8.25 (m, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 119.1, 124.0, 125.3, 127.2, 127.5, 128.9, 129.8, 130.0, 130.6, 138.6, 143.2, 149.1, 157.3.

4-chloro-2-(*p*-tolyl)quinoline: 2e



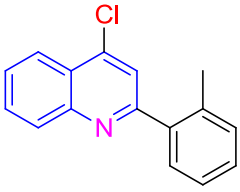
was obtained according to the above method. White solid, mp: 78-80 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.43 (s, 3 H), 7.33 (d, *J* = 7.6 Hz, 2 H), 7.58 – 7.62 (m, 1 H), 7.74 – 7.79 (m, 1 H), 7.95 (s, 1 H), 8.05 (d, *J* = 8.4 Hz, 2 H), 8.15 – 8.22 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.4, 118.9, 123.9, 125.2, 127.0, 127.4, 129.7, 130.0, 130.5, 135.8, 140.0, 143.0, 149.1, 157.2.

4-chloro-2-(*m*-tolyl)quinoline: 2f



was obtained according to the above method. Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.49 (s, 3 H), 7.30 (d, *J* = 7.2 Hz, 1 H), 7.42 (t, *J* = 7.6 Hz, 1 H), 7.60 – 7.64 (m, 1 H), 7.76 – 7.80 (m, 1 H), 7.91 (d, *J* = 7.6 Hz, 1 H), 7.97 (d, *J* = 4.4 Hz, 2 H), 8.21 (dd, *J* = 8.4, 17.6 Hz, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 119.2, 123.9, 124.6, 125.3, 127.2, 128.2, 128.8, 130.0, 130.5, 130.6, 138.6, 138.7, 143.1, 149.1, 157.5.

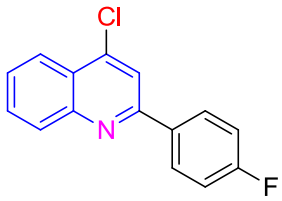
4-chloro-2-(*o*-tolyl)quinoline: 2g



was obtained according to the above method. White solid, mp: 67-69 ^{o}C. ^{1}H NMR

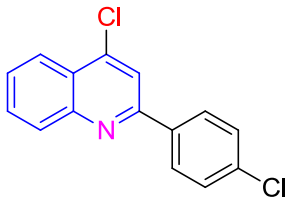
(400 MHz, $CDCl_3$): δ 2.43 (s, 3 H), 7.33 – 7.36 (m, 3 H), 7.49 (d, *J* = 6.4 Hz, 1 H), 7.65 – 7.69 (m, 2 H), 7.78 – 7.82 (m, 1 H), 8.17 (d, *J* = 8.4 Hz, 1 H), 8.28 (d, *J* = 8.4 Hz, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.3, 122.4, 123.9, 125.0, 126.1, 127.4, 128.9, 129.6, 129.9, 130.5, 131.0, 136.1, 139.6, 142.4, 148.7, 160.1.

4-chloro-2-(4-fluorophenyl)quinoline: 2h



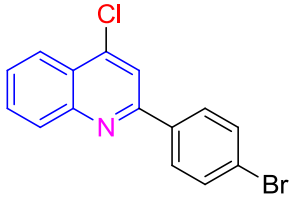
was obtained according to the above method. White solid, mp: 88-90 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.22 (t, *J* = 8.8 Hz, 2 H), 7.60 – 7.65 (m, 1 H), 7.77 – 7.81 (m, 1 H), 7.93 (s, 1 H), 8.13 – 8.17 (m, 3 H), 8.23 (d, *J* = 8.4 Hz, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 115.8, 116.0, 118.7, 124.0, 125.2, 127.3, 129.4, 129.4, 130.0, 130.7, 134.7, 143.3, 149.0, 156.1, 162.8, 165.3.

4-chloro-2-(4-chlorophenyl)quinoline: 2i



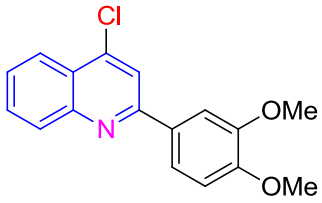
was obtained according to the above method. White solid, mp: 100-102 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51 (dd, *J* = 2.0, 6.8 Hz, 2 H), 7.62 – 7.66 (m, 1 H), 7.77 – 7.81 (m, 1 H), 7.94 (s, 1 H), 8.10 (dd, *J* = 2.0, 6.8 Hz, 2 H), 8.17 (d, *J* = 8.4 Hz, 1 H), 8.23 (d, *J* = 8.4 Hz, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 118.7, 124.0, 125.4, 127.5, 128.8, 129.1, 130.0, 130.7, 136.1, 137.0, 143.4, 149.0, 155.9.

2-(4-bromophenyl)-4-chloroquinoline: 2j



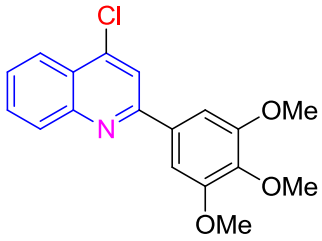
was obtained according to the above method. White solid, mp: 114-116 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 – 7.68 (m, 3 H), 7.77 – 7.81 (m, 1 H), 7.94 (s, 1 H), 8.04 (d, *J* = 8.4 Hz, 2 H), 8.17 (d, *J* = 8.8 Hz, 1 H), 8.23 (d, *J* = 8.4 Hz, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 118.6, 124.0, 124.5, 125.4, 127.5, 129.0, 130.0, 130.7, 132.1, 137.4, 143.4, 149.0, 156.0. HRMS (ESI, m/z): calcd for $C_{15}H_9BrClN$: M+H = 317.9680; found: 317.9687.

4-chloro-2-(3,4-dimethoxyphenyl)quinoline: 2l



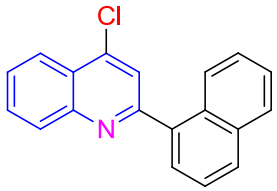
was obtained according to the above method. White solid, mp: 107-109 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.96 (s, 3 H), 4.05 (s, 3 H), 6.98 (d, *J* = 8.4 Hz, 1 H), 7.57 – 7.64 (m, 2 H), 7.74 – 7.78 (m, 1 H), 7.84 (d, *J* = 2.4 Hz, 1 H), 7.93 (s, 1 H), 8.15 – 8.21 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.9, 56.0, 110.2, 111.0, 118.6, 120.3, 123.9, 125.0, 126.9, 129.8, 130.5, 131.3, 142.9, 149.0, 149.4, 150.7, 156.7.

4-chloro-2-(3,4,5-trimethoxyphenyl)quinoline: 2m



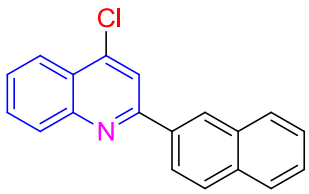
was obtained according to the above method. White solid, mp: 109-111 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.93 (s, 3 H), 4.01 (s, 6 H), 7.37 (s, 2 H), 7.60 – 7.64 (m, 1 H), 7.76 – 7.80 (m, 1 H), 7.92 (s, 1 H), 8.20 (dd, *J* = 8.4, 18.0 Hz, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 56.3, 61.0, 104.8, 118.9, 123.9, 125.2, 127.2, 129.9, 130.6, 124.1, 139.8, 143.1, 148.9, 153.6, 156.8. HRMS (ESI, m/z): calcd for $C_{18}H_{16}ClNO_3$: M+H = 330.0891; found: 330.0890.

4-chloro-2-(naphthalen-1-yl)quinoline: 2n



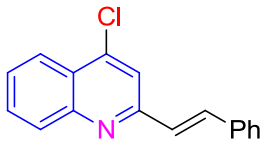
was obtained according to the above method. White solid, mp: 112-114 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49 – 7.55 (m, 2 H), 7.60 (t, *J* = 8.0 Hz, 1 H), 7.70 (dd, *J* = 7.2, 8.0 Hz, 2 H), 7.82 – 7.86 (m, 2 H), 7.93 – 7.98 (m, 2 H), 8.13 (d, *J* = 8.4 Hz, 1 H), 8.24 (d, *J* = 8.8 Hz, 1 H), 8.33 (d, *J* = 8.4 Hz, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 123.2, 124.0, 125.2, 125.3, 125.4, 126.1, 126.8, 127.6, 127.8, 128.5, 129.6, 130.1, 130.7, 131.0, 134.0, 137.6, 142.7, 148.9, 159.3. HRMS (ESI, m/z): calcd for $C_{19}H_{12}ClN$: M+H = 290.0731; found: 290.0731.

4-chloro-2-(naphthalen-2-yl)quinoline: 2o



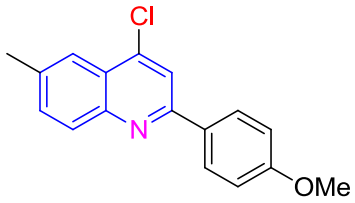
was obtained according to the above method. White solid, mp: 107-109 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53 – 7.57 (m, 2 H), 7.64 (t, *J* = 7.2 Hz, 1 H), 7.78 – 7.82 (m, 1 H), 7.90 (dd, *J* = 3.2, 6.0 Hz, 1 H), 8.00 (dd, *J* = 3.2, 6.0 Hz, 2 H), 8.14 (s, 1 H), 8.24 (t, J = 8.0 Hz, 2 H), 8.34 (dd, *J* = 1.2, 8.4 Hz, 1 H), 8.59 (s, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 119.2, 124.0, 124.7, 125.4, 126.5, 127.0, 127.3, 127.7, 128.7, 128.9, 130.1, 130.6, 133.4, 134.0, 135.9, 143.2, 149.1, 157.1.

(*E*)-4-chloro-2-styrylquinoline: 2p



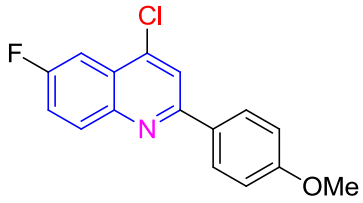
was obtained according to the above method. Yellow solid, mp: 108-110 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31 – 7.36 (m, 2 H), 7.41 (t, *J* = 7.2 Hz, 2 H), 7.58 (t, *J* = 7.2 Hz, 1 H), 7.62 – 7.69 (m, 3 H), 7.73 – 7.77 (m, 2 H), 8.08 (d, *J* = 8.4 Hz, 1 H), 8.17 (d, *J* = 8.4 Hz, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 119.3, 124.0, 125.4, 127.1, 127.3, 127.9, 128.8, 128.9, 129.5, 130.6, 135.3, 136.1, 142.7, 149.0, 155.9.

4-chloro-2-(4-methoxyphenyl)-6-methylquinoline: 2q



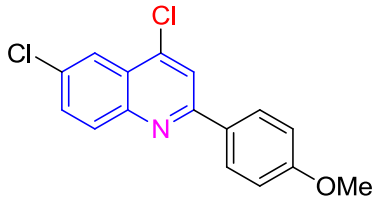
was obtained according to the above method. White solid, mp: 104-106 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.48 (s, 3 H), 3.79 (s, 3 H), 6.94 (d, *J* = 8.8 Hz, 2 H), 7.48 (dd, *J* = 1.6, 8.4 Hz, 1 H), 7.79 (s, 1 H), 7.86 (s, 1 H), 7.94 (d, *J* = 8.4 Hz, 1 H), 7.99 – 8.01 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.8, 55.4, 114.2, 118.5, 122.7, 124.9, 128.7, 129.5, 131.2, 132.7, 136.9, 142.2, 147.6, 155.9, 161.0. HRMS (ESI, m/z): calcd for $C_{17}H_{14}ClNO$: M+H = 284.0837; found: 284.0839.

4-chloro-6-fluoro-2-(4-methoxyphenyl)quinoline: 2r



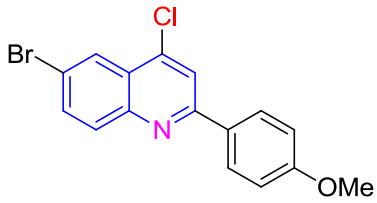
was obtained according to the above method. White solid, mp: 99-101 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.88 (s, 3 H), 7.03 (d, *J* = 8.8 Hz, 2 H), 7.47 – 7.52 (m, 1 H), 7.79 (dd, *J* = 2.8, 9.2 Hz, 1 H), 7.92 (s, 1 H), 8.06 – 8.13 (m, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.4, 107.6, 107.9, 114.3, 119.1, 120.5, 120.7, 125.7, 125.8, 128.7, 130.8, 132.3, 132.4, 142.1, 142.1, 146.1, 156.2, 156.2, 159.5, 161.2, 162.0. HRMS (ESI, m/z): calcd for $C_{16}H_{11}ClFNO$: M+H = 288.0586; found: 288.0589.

4,6-dichloro-2-(4-methoxyphenyl)quinoline: 2s



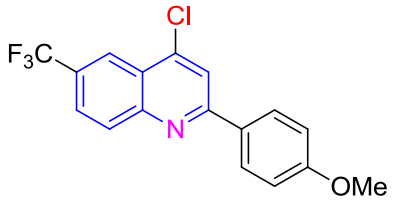
was obtained according to the above method. White solid, mp: 144-146 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.88 (s, 3 H), 7.02 (d, *J* = 8.8 Hz, 2 H), 7.66 (dd, *J* = 2.0, 8.4 Hz, 1 H), 7.91 (s, 1 H), 8.03 – 8.09 (m, 3 H), 8.15 (d, *J* = 2.0 Hz, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.4, 114.4, 119.3, 123.0, 125.7, 128.9, 130.6, 131.4, 131.4, 132.8, 141.9, 147.4, 157.0, 161.4. HRMS (ESI, m/z): calcd for $C_{16}H_{11}Cl_2NO$: M+H = 304.0290; found: 304.0286.

6-bromo-4-chloro-2-(4-methoxyphenyl)quinoline: 2t



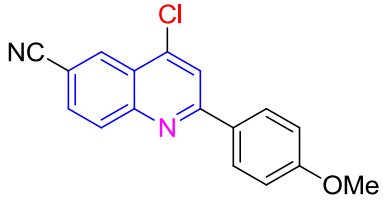
was obtained according to the above method. White solid, mp: 150-152 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.89 (s, 3 H), 7.03 (d, *J* = 8.2 Hz, 2 H), 7.79 (dd, *J* = 2.0, 8.8 Hz, 1 H), 7.91 (s, 1 H), 7.98 (d, *J* = 8.8 Hz, 1 H), 8.08 – 8.10 (m, 2 H), 8.33 (d, *J* = 2.0 Hz, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.4, 114.3, 119.2, 120.8, 126.1, 126.2, 128.8, 130.6, 131.4, 133.9, 141.7, 147.6, 157.1, 161.3. HRMS (ESI, m/z): calcd for $C_{16}H_{11}BrClNO$: M+H = 347.9785; found: 347.9780.

4-chloro-2-(4-methoxyphenyl)-6-(trifluoromethyl)quinoline: 2u



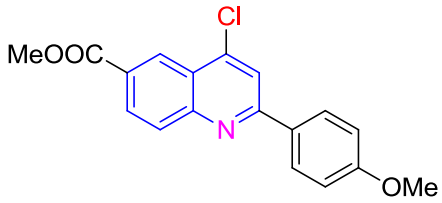
was obtained according to the above method. White solid, mp: 122 - 124 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.90 (s, 3 H), 7.05 (d, *J* = 8.8 Hz, 2 H), 7.90 (dd, *J* = 1.6, 8.8 Hz, 1 H), 7.99 (s, 1 H), 8.13 (d, *J* = 8.8 Hz, 2 H), 8.22 (d, *J* = 8.8 Hz, 1 H), 8.49 (s, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.4, 114.4, 119.5, 122.1, 122.2, 124.2, 126.2, 126.2, 128.3, 128.6, 128.8, 129.1, 130.3, 131.0, 143.7, 150.0, 158.8, 161.7. HRMS (ESI, m/z): calcd for $C_{17}H_{11}ClF_3NO$: M+H = 338.0554; found: 338.0553.

4-chloro-2-(4-methoxyphenyl)quinoline-6-carbonitrile: 2v



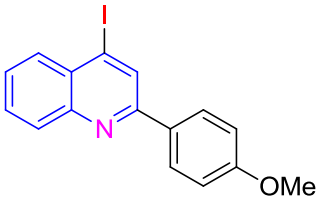
was obtained according to the above method. White solid, mp: 188-190 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.91 (s, 3 H), 7.06 (d, *J* = 8.8 Hz, 2 H), 7.87 (dd, *J* = 1.6, 8.8 Hz, 1 H), 8.03 (s, 1 H), 8.14 – 8.20 (m, 3 H), 8.57 (d, *J* = 1.6 Hz, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.5, 110.2, 114.5, 118.6, 119.9, 124.7, 129.2, 130.0, 130.4, 131.5, 131.2, 143.2, 150.1, 159.5, 162.0. HRMS (ESI, m/z): calcd for $C_{17}H_{11}ClN_2O$: M+H = 295.0633; found: 295.0633.

methyl 4-chloro-2-(4-methoxyphenyl)quinoline-6-carboxylate: 2w



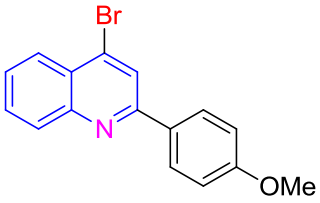
was obtained according to the above method. White solid, mp: 201-203 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.90 (s, 3 H), 4.02 (s, 3 H), 7.06 (d, *J* = 8.8 Hz, 2 H), 7.99 (s, 1 H), 8.15 (dd, *J* = 3.2, 8.8 Hz, 3 H), 8.33 (dd, *J* = 1.2, 8.8 Hz, 1 H), 8.93 (d, *J* = 1.2 Hz, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 52.5, 55.4, 114.4, 119.2, 124.4, 127.1, 128.1, 129.1, 130.1, 130.1, 130.5, 144.2, 151.0, 158.8, 161.6, 166.5. HRMS (ESI, m/z): calcd for $C_{18}H_{14}ClNO_3$: M+H = 328.0735; found: 328.0739.

4-iodo-2-(4-methoxyphenyl)quinoline: 2ab



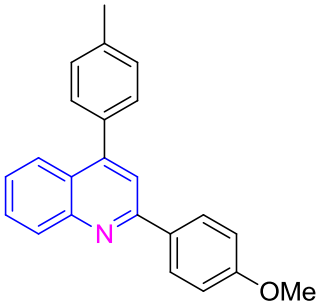
was obtained according to the above method. White solid, mp: 128-130 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.89 (s, 3 H), 7.03 – 7.05 (m, 2 H), 7.54 – 7.58 (m, 1 H), 7.70 – 7.74 (m, 1 H), 7.98 (d, *J* = 8.4 Hz, 1 H), 8.05 (d, *J* = 8.4 Hz, 1 H), 8.09 – 8.12 (m, 2 H), 8.42 (s, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 66.4, 112.5, 114.3, 127.4, 128.9, 128.9, 130.1, 130.1, 130.5, 130.6, 131.4, 147.8, 156.7, 161.1. HRMS (ESI, m/z): calcd for $C_{16}H_{12}INO$: M+H = 362.0036; found: 362.0032.

4-bromo-2-(4-methoxyphenyl)quinoline: 2ac



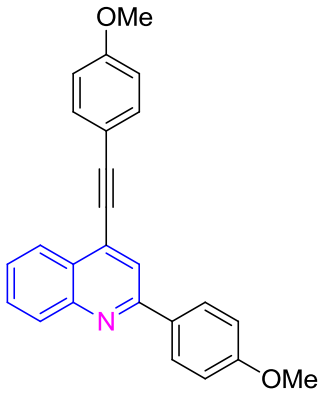
was obtained according to the above method. White solid, mp: 121-123 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.88 (s, 3 H), 7.03 (dd, *J* = 2.0, 6.8 Hz, 2 H), 7.55 – 7.59 (m, 1 H), 7.71 – 7.76 (m, 1 H), 8.09 – 8.15 (m, 5 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.4, 114.3, 122.4, 126.3, 126.5, 127.0, 128.9, 129.8, 130.5, 130.8, 134.5, 148.5, 156.7, 161.1. HRMS (ESI, m/z): calcd for $C_{16}H_{12}BrNO$: M+H = 314.0175; found: 314.0179.

2-(4-methoxyphenyl)-4-(*p*-tolyl)quinoline: 3a



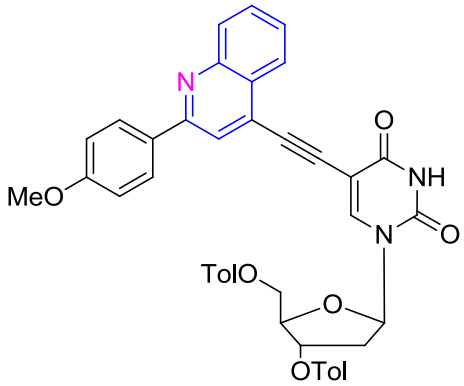
White solid, mp: 122 - 124 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.47 (s, 3 H), 3.87 (s, 3 H), 7.03 (d, *J* = 8.8 Hz, 2 H), 7.34 (d, *J* = 8.0 Hz, 2 H), 7.43 – 7.46 (m, 3 H), 7.67 – 7.71 (m, 1 H), 7.75 (s, 1 H), 7.89 – 7.91 (m, 1 H), 8.14 – 8.21 (m, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.3, 55.3, 114.2, 118.8, 125.6, 125.6, 125.8, 128.9, 129.2, 129.3, 129.4, 129.9, 132.3, 135.5, 138.2, 148.8, 149.0, 156.4, 160.8.

2-(4-methoxyphenyl)-4-((4-methoxyphenyl)ethynyl)quinoline: 4a



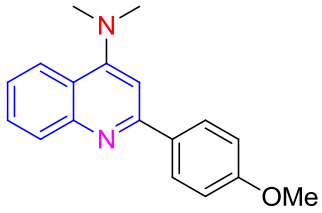
White solid, mp: 191 - 193 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.86 (s, 3 H), 3.89 (s, 3 H), 6.95 (d, *J* = 8.8 Hz, 2 H), 7.05 (d, *J* = 8.8 Hz, 2 H), 7.55 – 7.59 (m, 1 H), 7.63 (d, *J* = 8.8 Hz, 2 H), 7.71 – 7.75 (m, 1 H), 8.00 (s, 1 H), 8.13 – 8.16 (m, 3 H), 8.33 (d, *J* = 7.6 Hz, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.4, 84.5, 98.2, 114.2, 114.2, 114.4, 120.9, 125.7, 126.3, 126.3, 128.8, 129.8, 129.9, 130.5, 131.8, 133.5, 148.2, 156.4, 160.4, 160.9. HRMS (ESI, m/z): calcd for $C_{25}H_{19}NO_2$: M+H = 366.1489; found: 366.1490.

5-(5-((2-(4-methoxyphenyl)quinolin-4-yl)ethynyl)-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2-(((4-methylbenzoyl)oxy)methyl)tetrahydrofuran-3-yl 4-methylbenzoate: 5a



White solid, mp: 198 - 200 ^{o}C. ^{1}H NMR (400 MHz, d^{6}-DMSO): δ 2.04 (s, 3 H), 2.39 (s, 3 H), 2.63 – 2.67 (m, 1 H), 2.72 – 2.79 (m, 1 H), 3.85 (s, 3 H), 4.58 – 4.61 (m, 1 H), 4.66 (d, *J* = 4.8 Hz, 2 H), 5.62 – 5.64 (m, 1 H), 6.32 (t, *J* = 7.2 Hz, 1 H), 7.10 – 7.12 (m, 4 H), 7.35 (d, *J* = 7.6 Hz, 2 H), 7.63 (t, *J* = 7.2 Hz, 1 H), 7.80 – 7.94 (m, 6 H), 8.07 (d, *J* = 8.4 Hz, 1 H), 8.21 (d, *J* = 7.2 Hz, 2 H), 8.29 (d, *J* = 8.0 Hz, 1 H), 8.36 (s, 1 H), 11.98 (s, 1 H). ^{13}C NMR (100 MHz, d^{6}-DMSO): δ 21.3, 21.7, 37.4, 55.8, 64.7, 74.9, 82.3, 86.3, 88.9, 91.8, 98.6, 114.8, 120.2, 125.9, 126.0, 126.9, 126.9, 127.4, 129.1, 129.3, 129.7, 129.8, 130.0, 130.9, 131.0, 132.0, 144.2, 144.6, 145.1, 147.9, 149.8, 155.8, 161.3, 161.8, 165.7, 166.1. HRMS (ESI, m/z): calcd for $C_{43}H_{35}N_3O_8$: M+H = 722.2497; found: 722.2495.

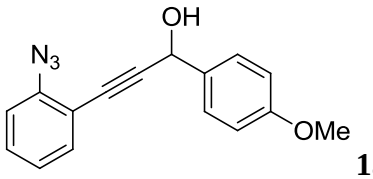
2-(4-methoxyphenyl)-*N*,*N*-dimethylquinolin-4-amine: 6a



^{1}H NMR (400 MHz, $CDCl_3$): δ 3.07 (s, 3 H), 3.88 (s, 3 H), 7.03 (d, *J* = 8.8 Hz, 2 H), 7.18 (s, 1 H), 7.40 – 7.44 (m, 1 H), 7.61 – 7.65 (m, 1 H), 8.04 – 8.09 (m, 4 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 44.0, 55.4, 105.1, 114.0, 121.9, 124.2, 128.8, 128.9, 130.0, 133.1, 149.8, 157.4, 158.1, 160.5.

Reference

1. a) S. Akila, S. Selvi, K. Balasubramanian, *Tetrahedron*, **2001**, *57*, 3465-3469. b) K. H. Kumar, P. T. Perumal, *J. Heterocyclic Chem.*, **2008**, *45*, 597; c) L. Strekowski, M. Say, M. Henary, P. Ruiz, L. Manzel, D. E. Macfarlane, A. J. Bojarski, *J. Med. Chem.* **2003,** *46*, 1242-1249. d) L. Strekowski, M. Say, O. Zegrocka, F. A. Tanious, W. D. Wilson, L. Manzelb, D. E. Macfarlane, *Bioorg. Med. Chem.* **2003**,*11*, 1079 – 1085. e) Z. Jamal, Y.-C. Teo, G. S. Lim, Tetrahedron **2016**, *72* 2132-2138. f) S. Rotzoll, B. Willy, J. Schönhaber, F. Rominger, T. J. J. Müller, *Eur. J. Org. Chem.* **2010**, 3516–3524. g) J.-Y. Tsai, C.-S. Chang, Y.-F. Huang, H.-S. Che, S.-K. Lin, F. F. Wong, L.-J. Huang, S.-C. Kuo, *Tetrahedron*, **2008**, *64*, 11751 – 11755.



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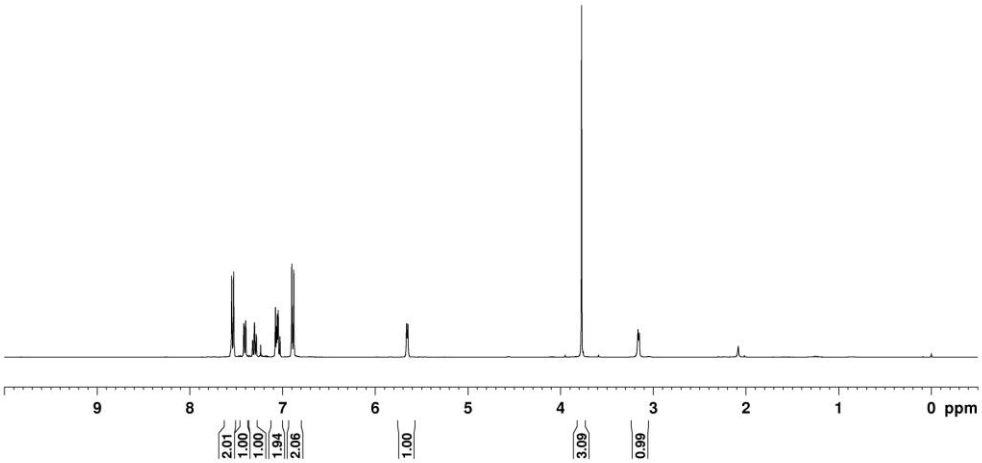

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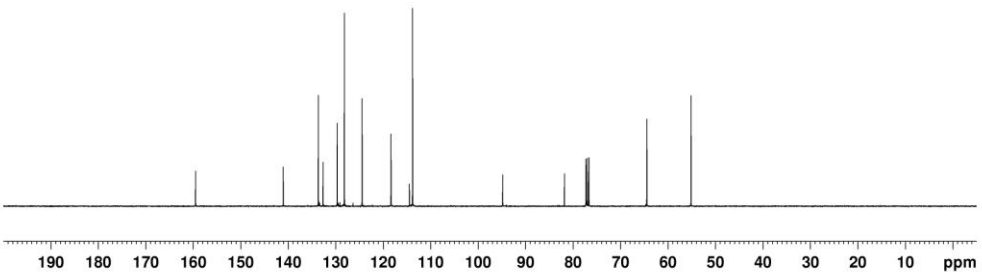

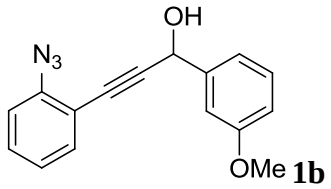

1b

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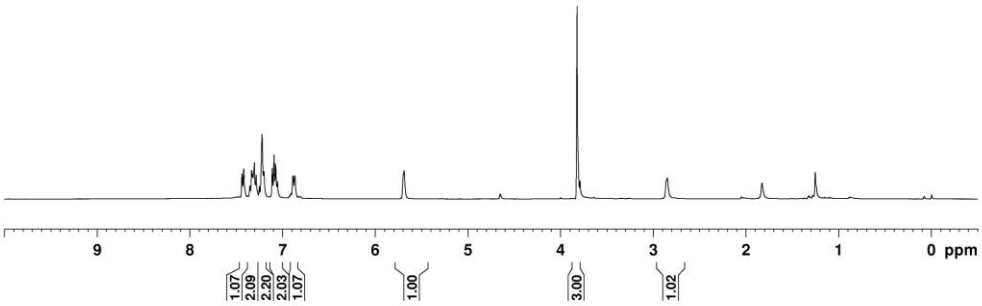

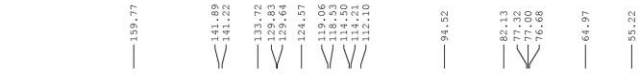

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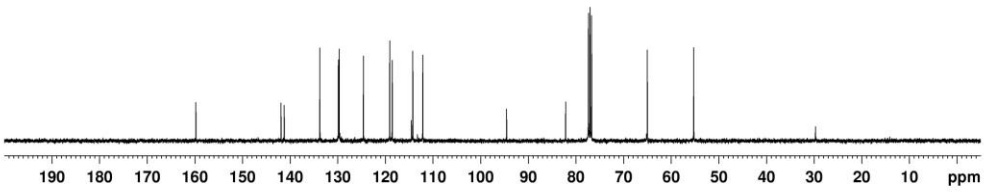

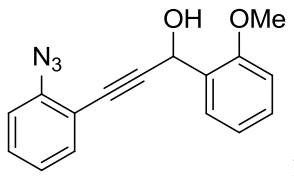

1c

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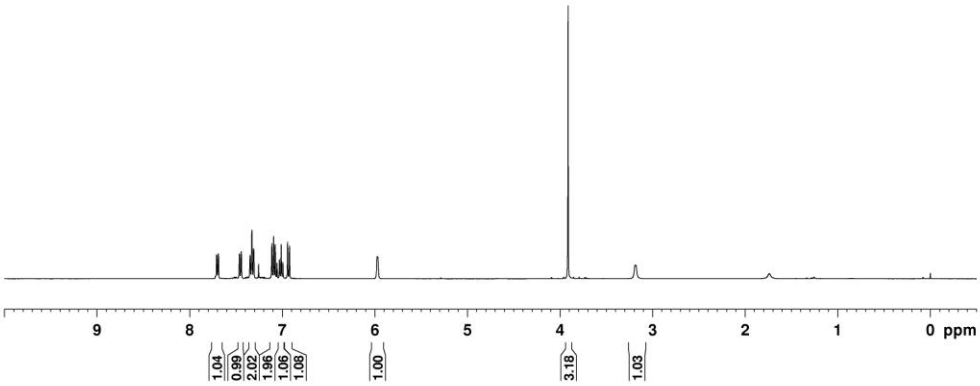
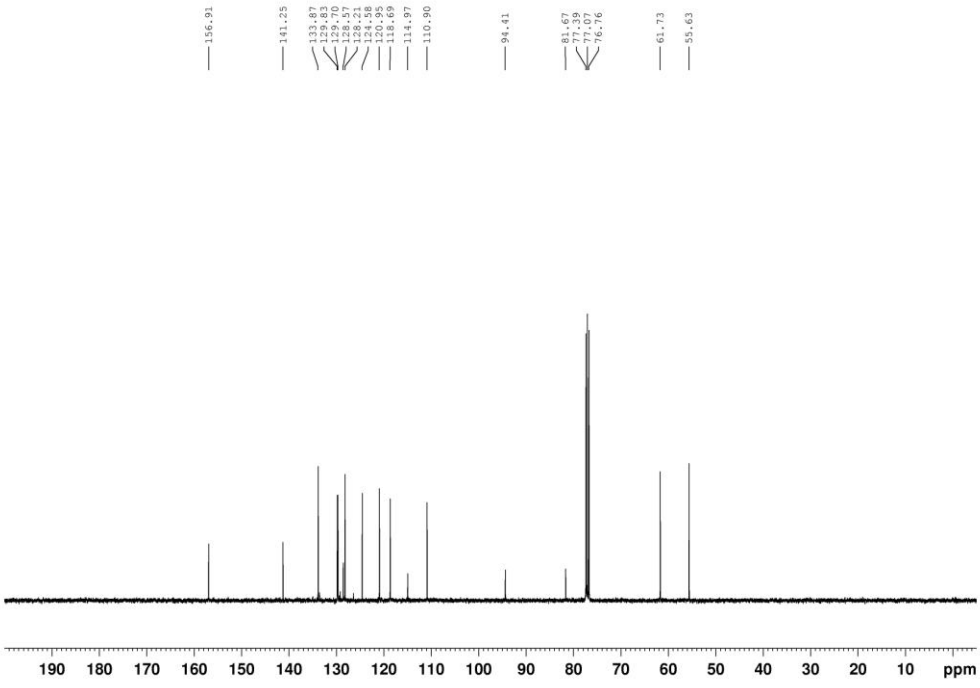
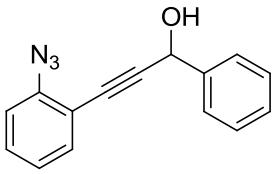
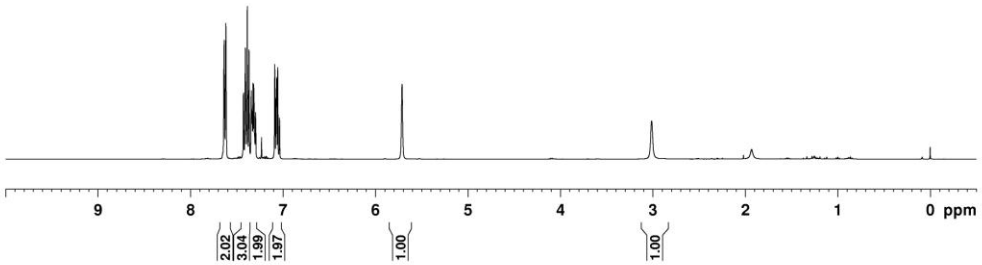






1d

sxr1707011-1-Ph-yl



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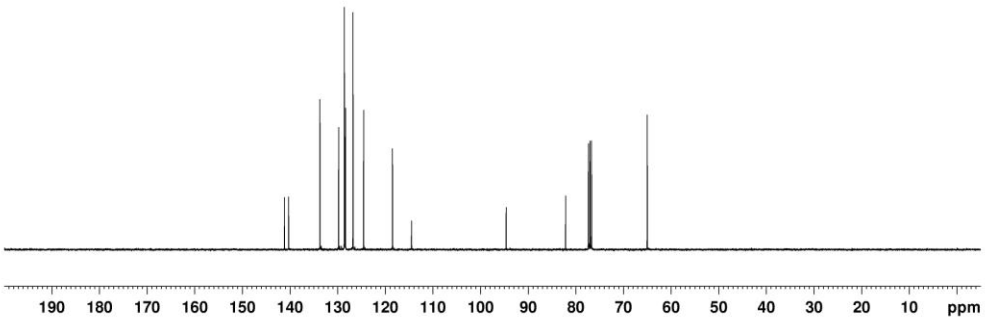

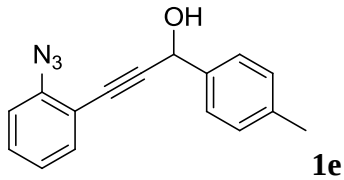

1e

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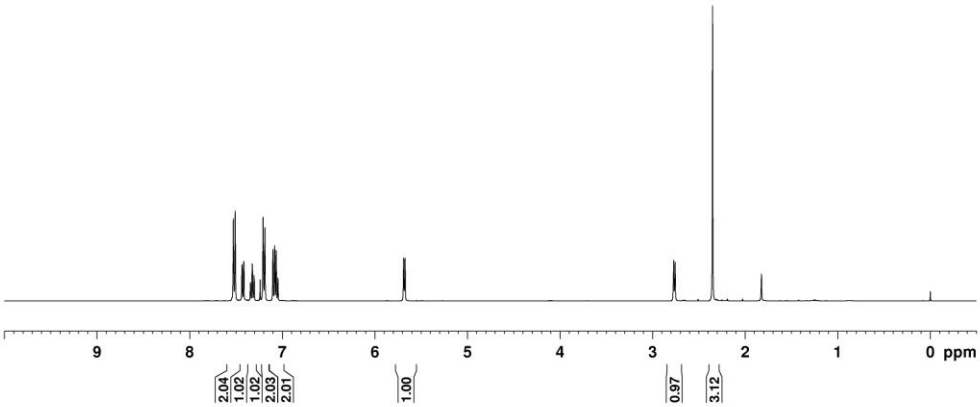

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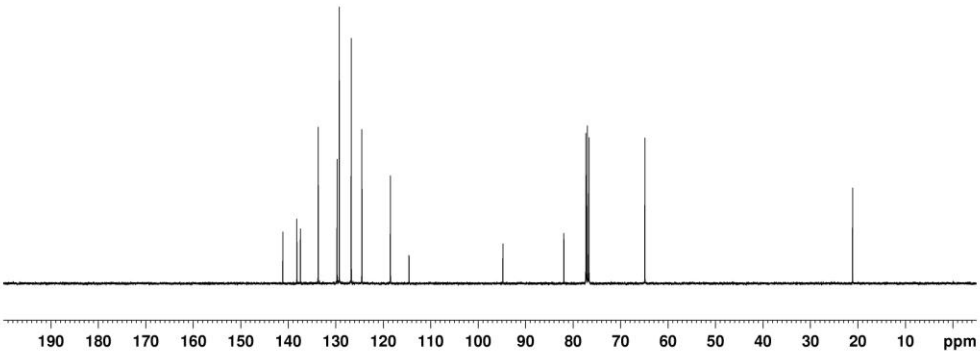

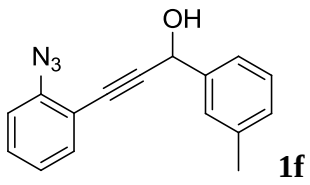

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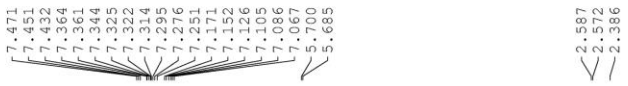

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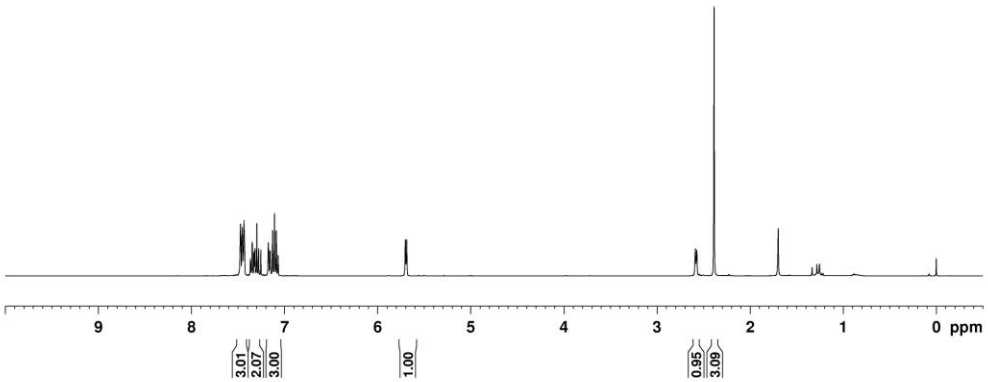

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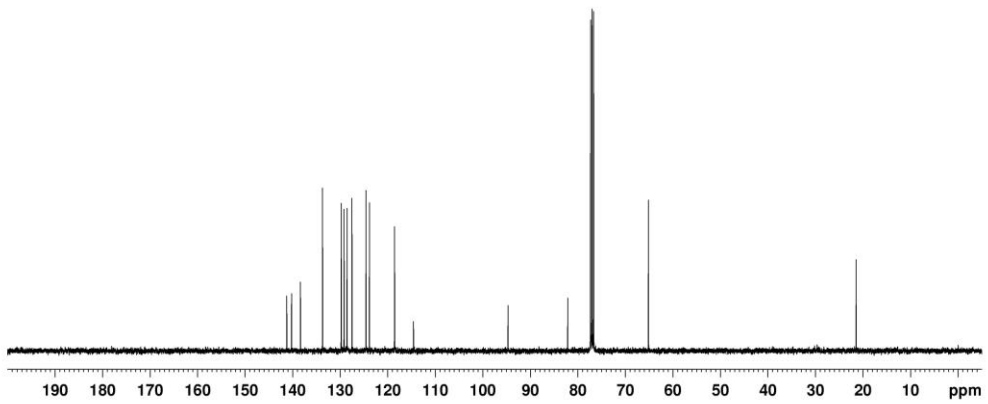

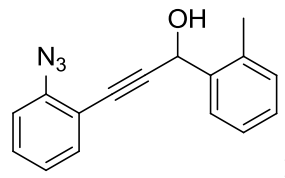

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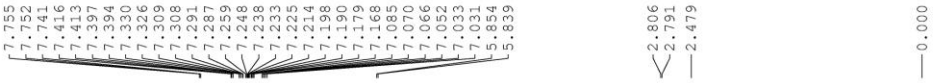

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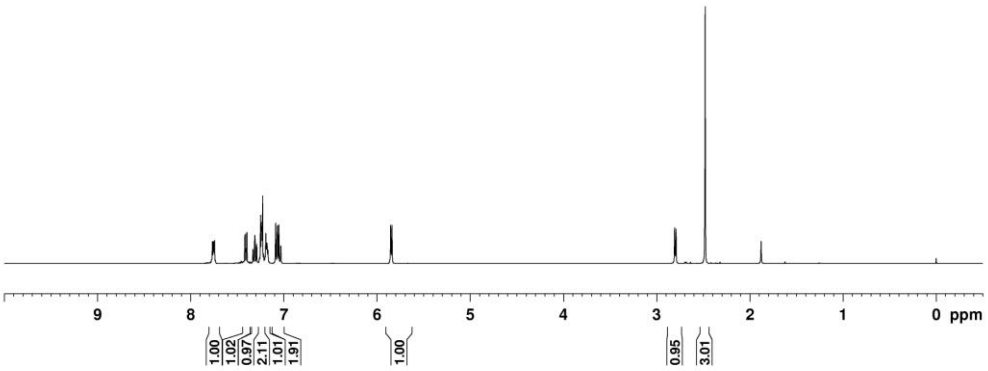

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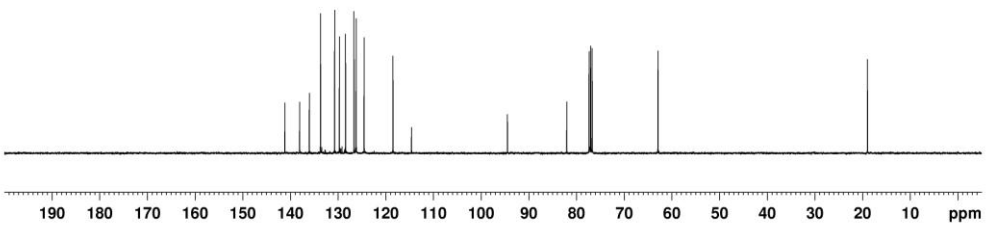

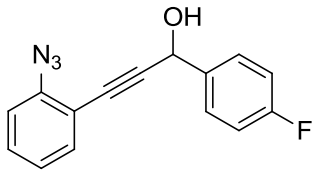
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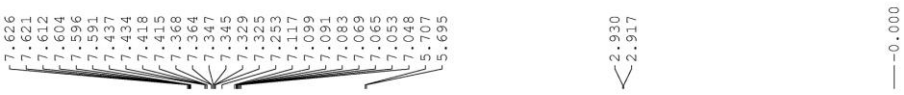
N3
F

1h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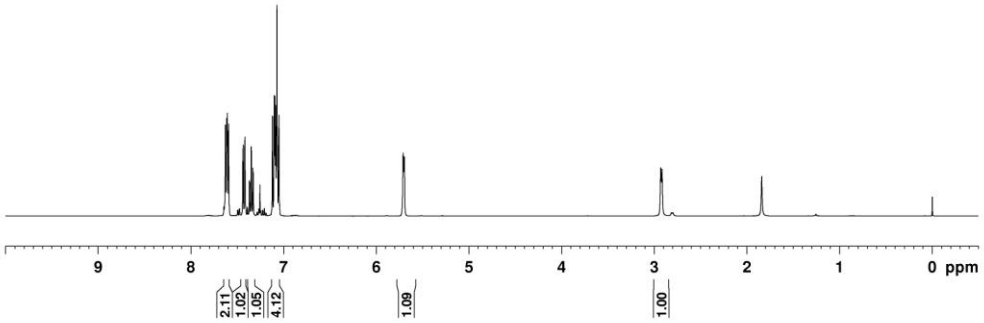
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1.02
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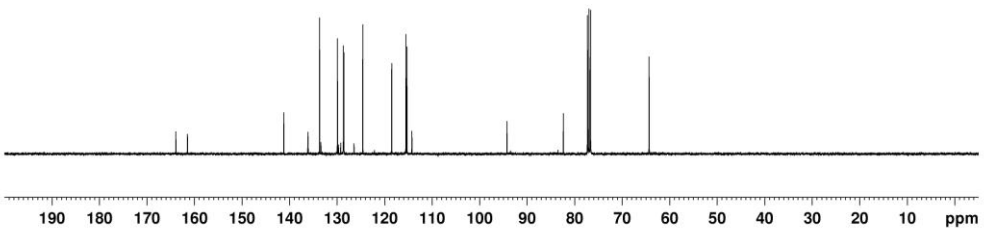
4.12
1.09
1.00


163.90
161.45
141.24
136.18
136.15
133.70
129.96
128.68
128.60
124.61
118.52
115.55
115.33
114.29
94.29
82.39
77.32
77.00
76.68
64.36
sxr1707013-1-p-F-yl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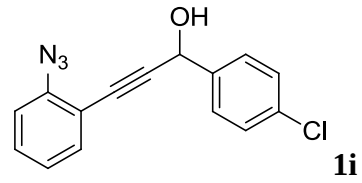
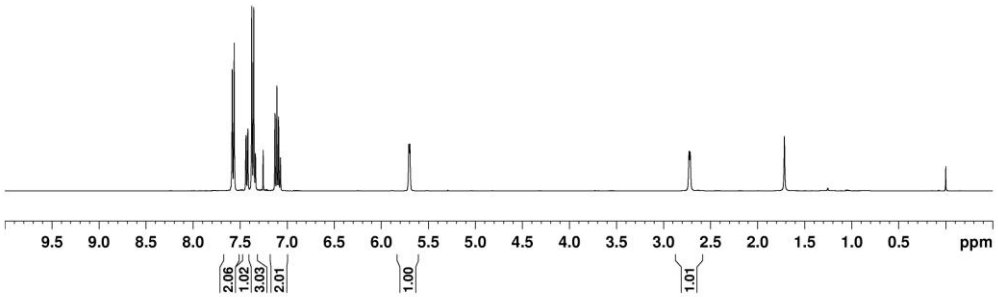
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

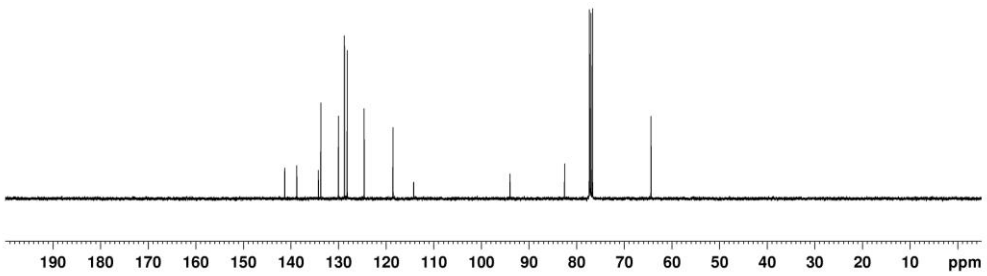


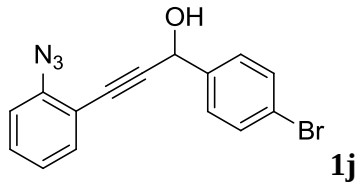
1i

sxr1707014-1-p-Cl-yl

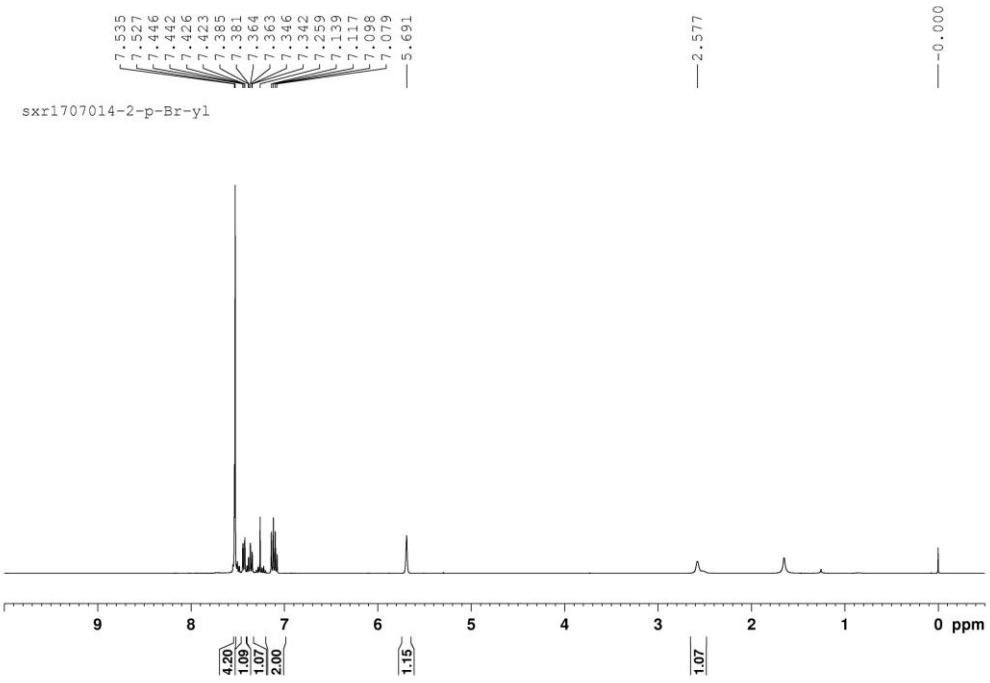


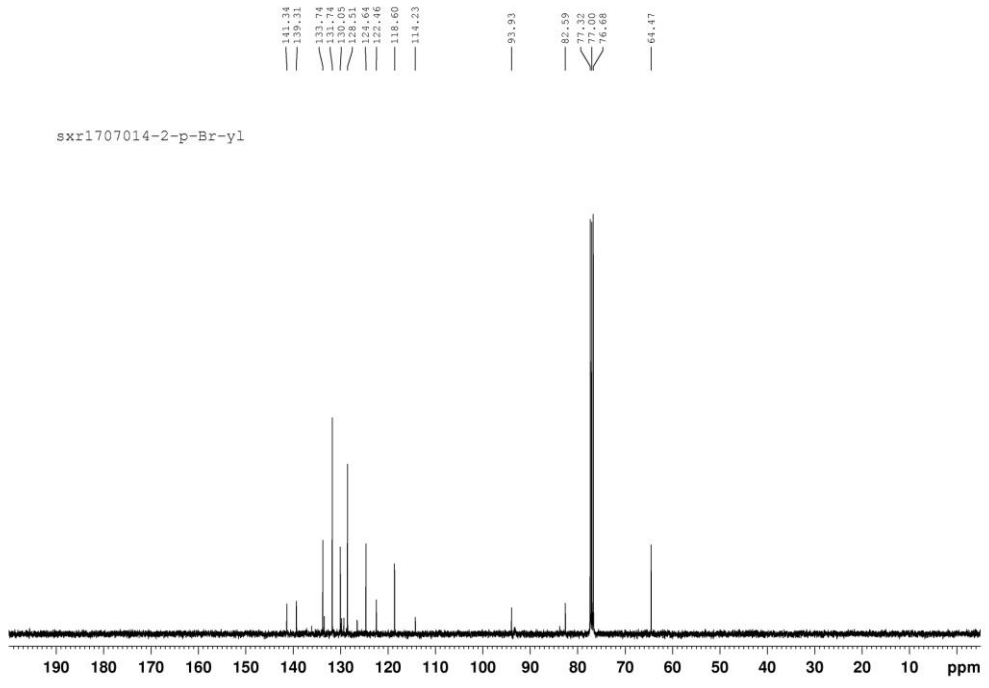
sxr1707014-1-p-Cl-yl

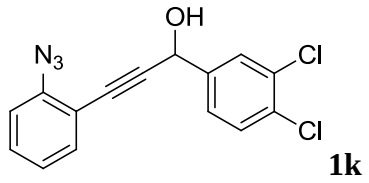



OH
N3
Br

1j

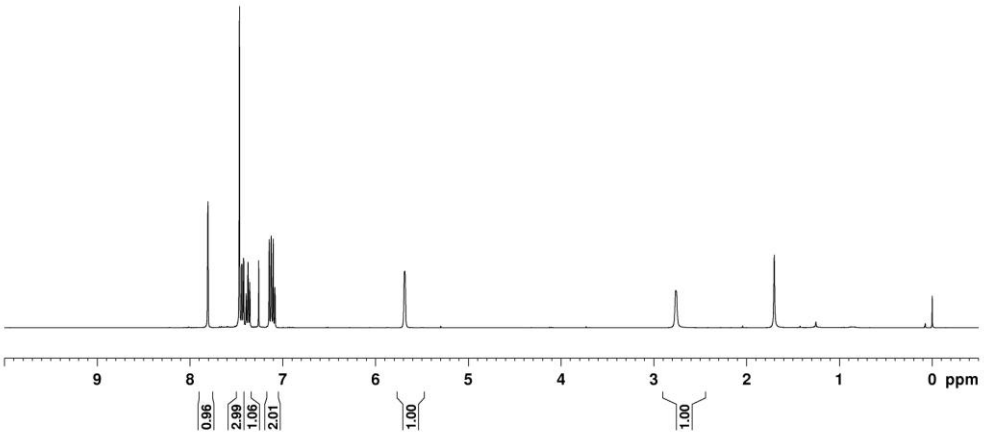

7.535
7.527
7.446
7.442
7.426
7.423
7.385
7.381
7.364
7.363
7.346
7.342
7.259
7.139
7.117
7.098
7.079
5.691
2.577
0.000
sxr1707014-2-p-Br-yl
9
8
7
6
5
4
3
2
1
0 ppm
4.20
1.09
1.07
2.00
1.15
1.07


141.34
139.31
133.74
131.74
130.55
128.51
124.64
122.46
118.60
114.23
93.93
82.59
77.32
77.00
76.68
64.47
sxr1707014-2-p-Br-yl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

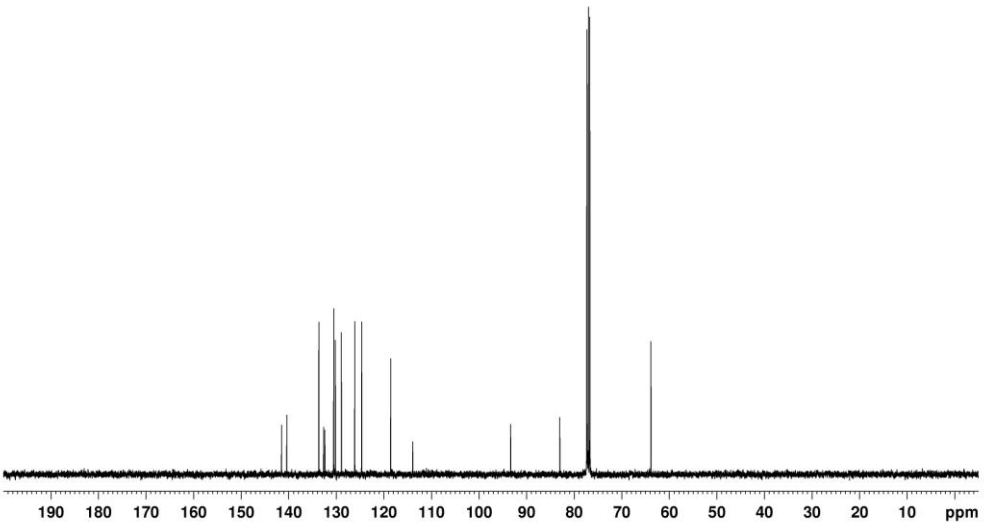


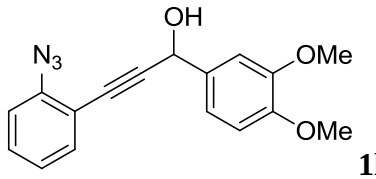
1k

sxr1707019-3,4-er-Cl-yl

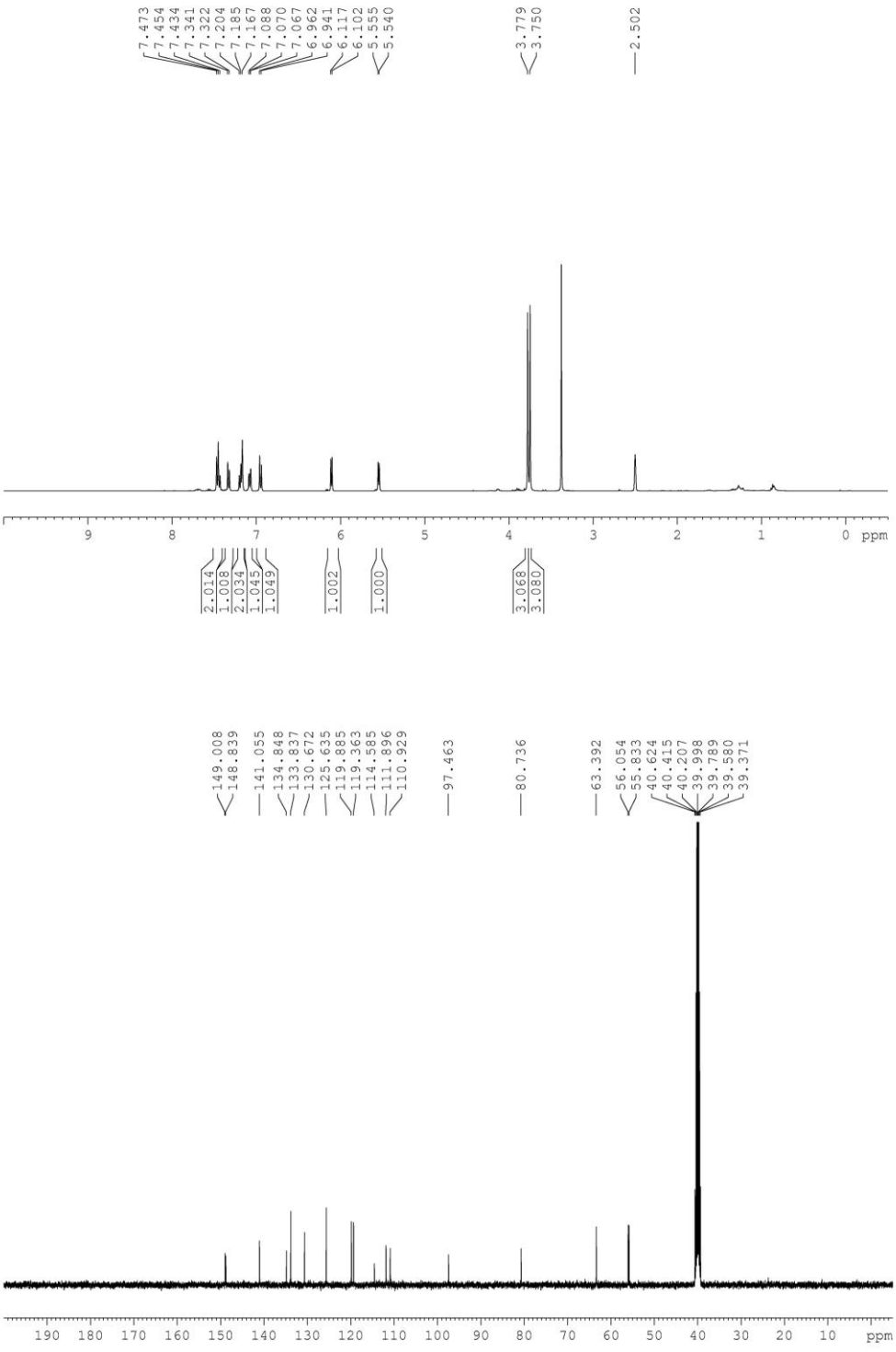


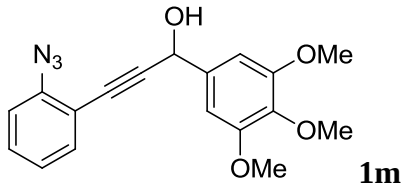
sxr1707019-3,4-er-Cl-yl



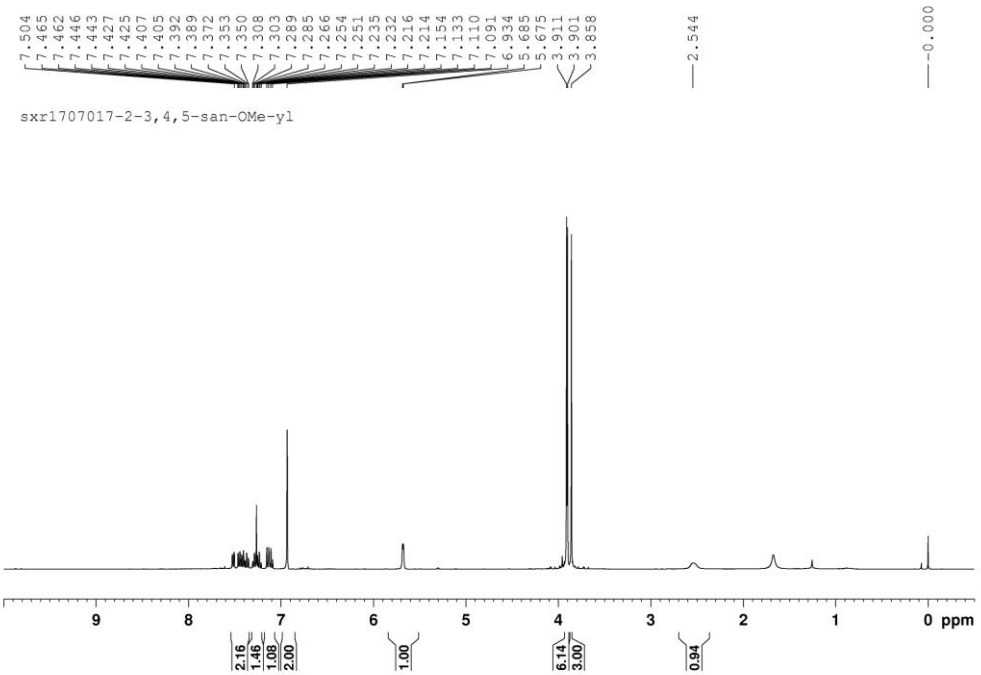

OH
N3
OMe
OMe

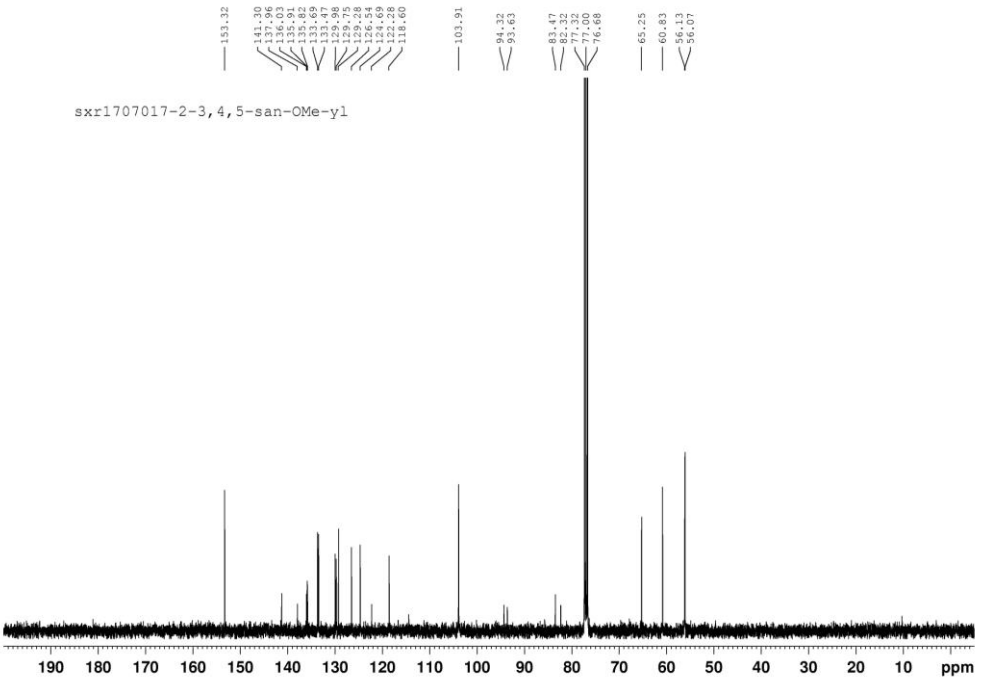
1l

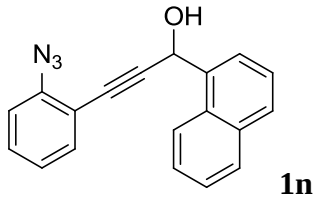

7.473
7.454
7.434
7.341
7.322
7.204
7.185
7.167
7.088
7.070
7.067
6.962
6.941
6.117
6.102
5.555
5.540
3.779
3.750
2.502
9 8 7 6 5 4 3 2 1 0 ppm
2.014
1.008
2.034
1.045
1.049
1.002
1.000
3.068
3.080
149.008
148.839
141.055
134.848
133.837
130.672
125.635
119.885
119.363
114.585
111.896
110.929
97.463
80.736
63.392
56.054
55.833
40.624
40.415
40.207
39.998
39.789
39.580
39.371
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


OH
N3
OMe
OMe
OMe

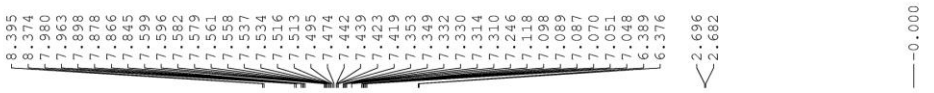
1m


7.504
7.465
7.462
7.446
7.443
7.427
7.425
7.407
7.405
7.392
7.389
7.372
7.353
7.350
7.308
7.303
7.289
7.285
7.266
7.254
7.251
7.235
7.232
7.216
7.214
7.154
7.133
7.110
7.091
6.934
5.685
5.675
3.911
3.901
3.858
2.544
0.000
sxr1707017-2-3,4,5-san-OMe-yl
9
8
7
6
5
4
3
2
1
0 ppm
2.16
1.46
1.08
2.00
1.00
6.14
3.00
0.94

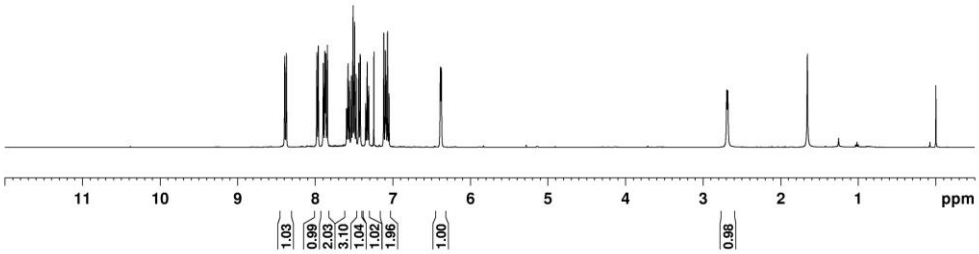

153.32
141.30
137.66
136.03
135.91
135.82
133.69
133.17
129.98
129.75
129.28
126.54
124.69
122.28
118.60
103.91
94.32
93.63
83.47
77.32
77.00
76.68
65.25
60.83
56.13
56.07
sxr1707017-2-3,4,5-san-OMe-yl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



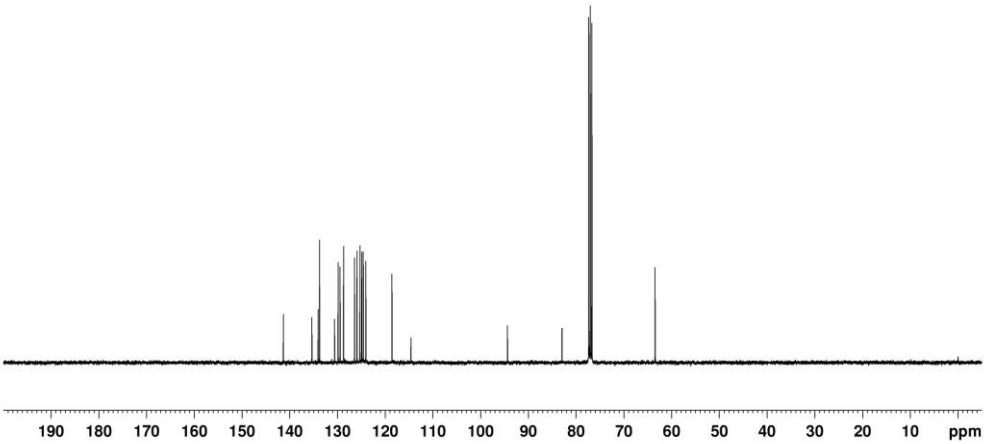
1n

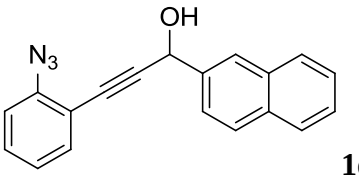


sxr170718-1-nai-1-yl

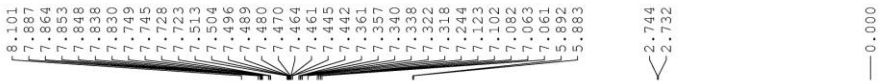


sxr170718-1-nai-1-yl

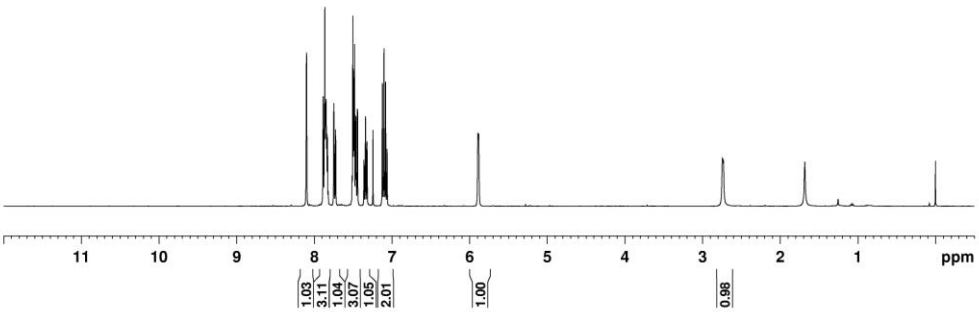




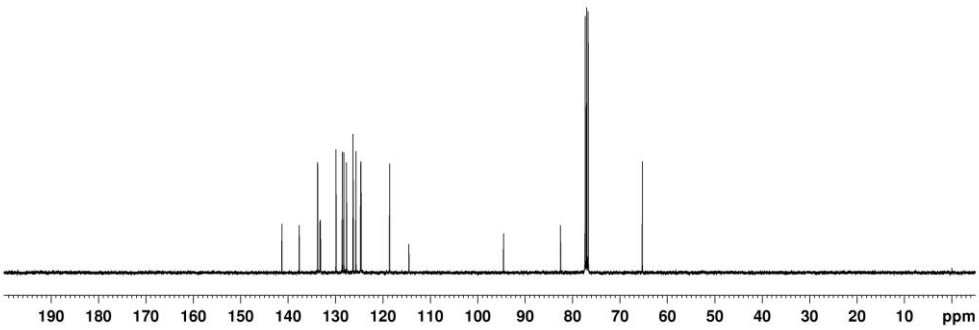
1o

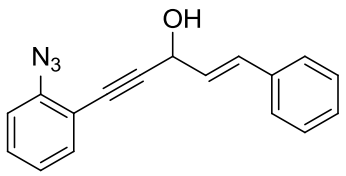


sxr170718-2-nai-2-yl

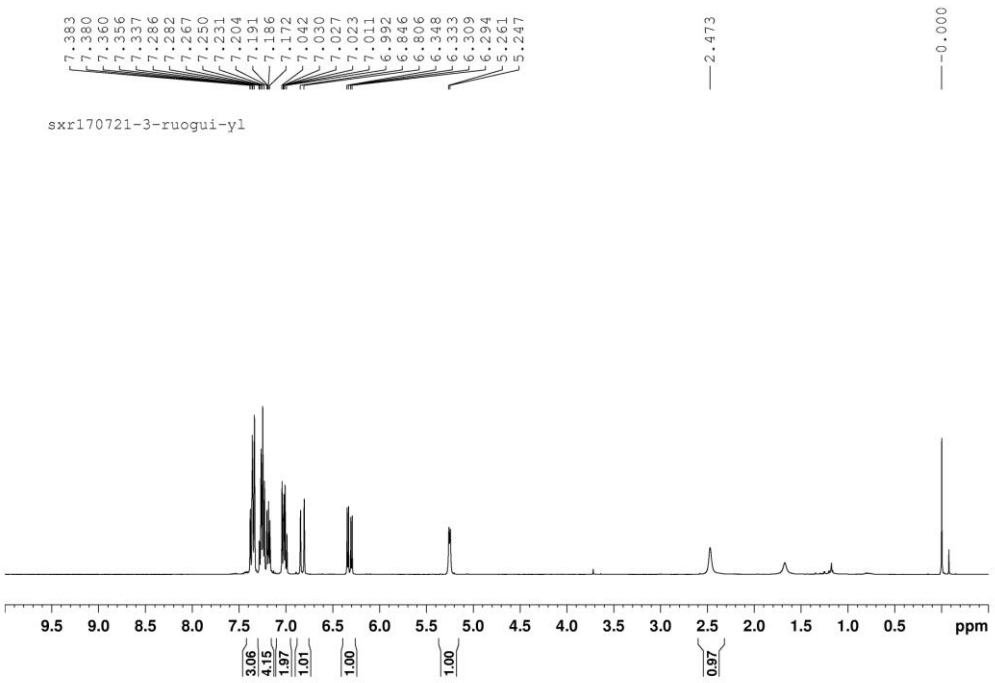


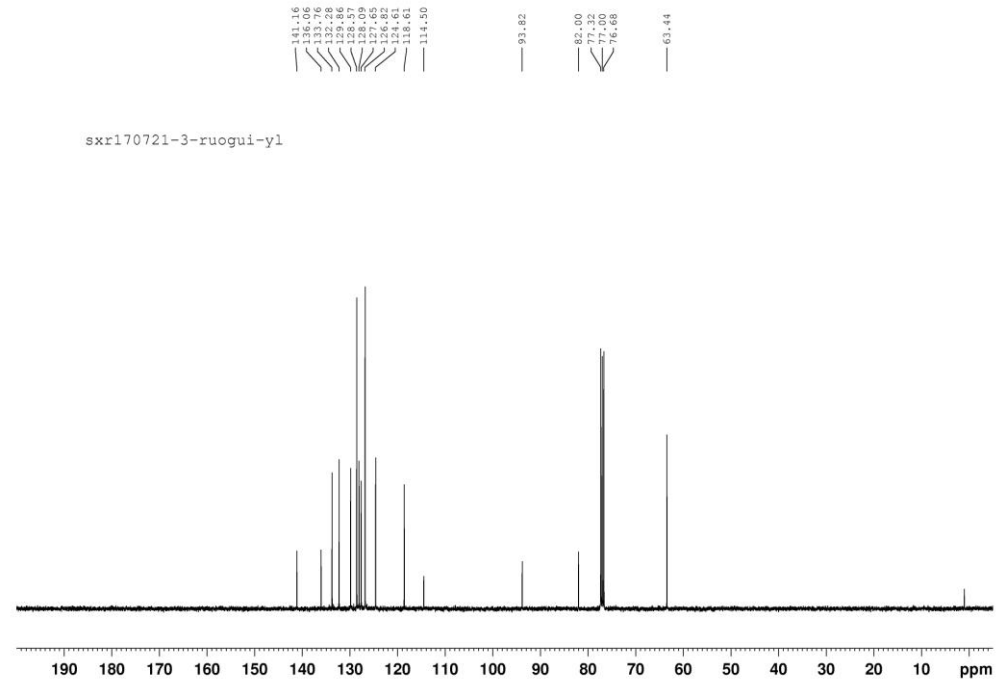
sxr170718-2-nai-2-yl

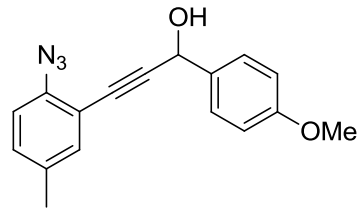



OH
N3

1p

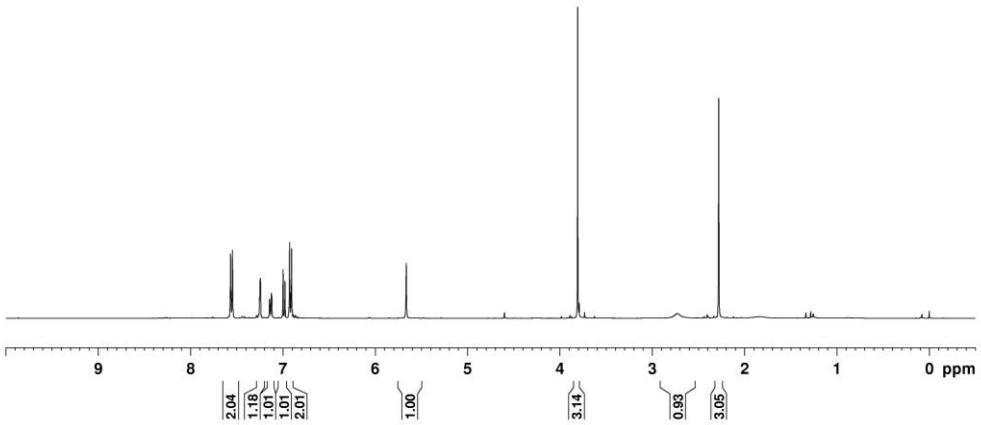

7.383
7.380
7.360
7.356
7.337
7.286
7.282
7.267
7.250
7.231
7.204
7.191
7.186
7.172
7.042
7.030
7.027
7.023
7.011
6.992
6.846
6.806
6.348
6.333
6.309
6.294
5.261
5.247
2.473
0.000
sxr170721-3-ruogui-yl
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
3.06
4.15
1.97
1.01
1.00
1.00
0.97


141.16
136.06
133.76
132.28
129.86
128.37
128.09
127.65
126.82
124.61
118.61
114.50
93.82
82.00
77.32
77.00
76.68
63.44
sxr170721-3-ruogui-yl
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

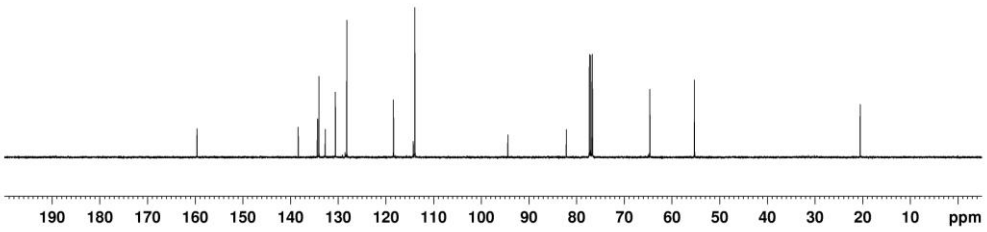


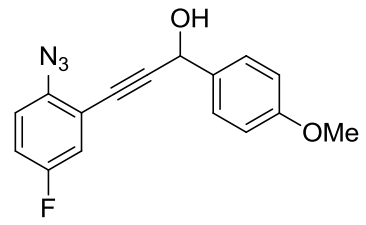
1q

sxr170722-2-p'-Me-yl



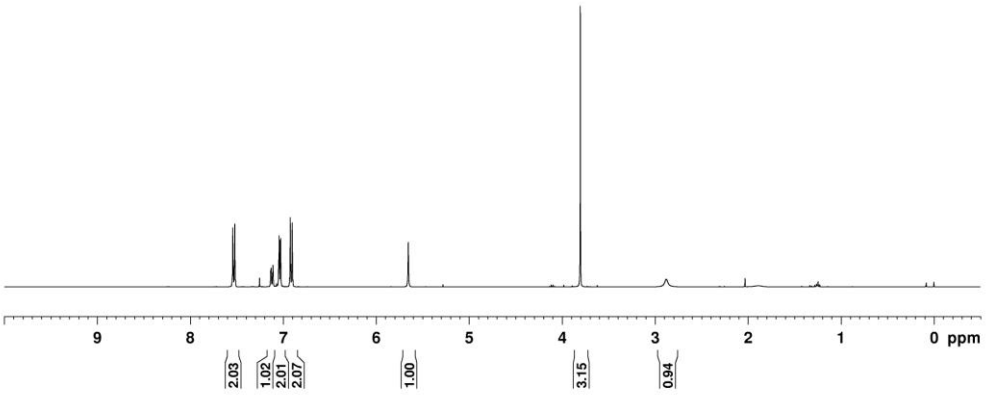
sxr170722-2-p'-Me-yl



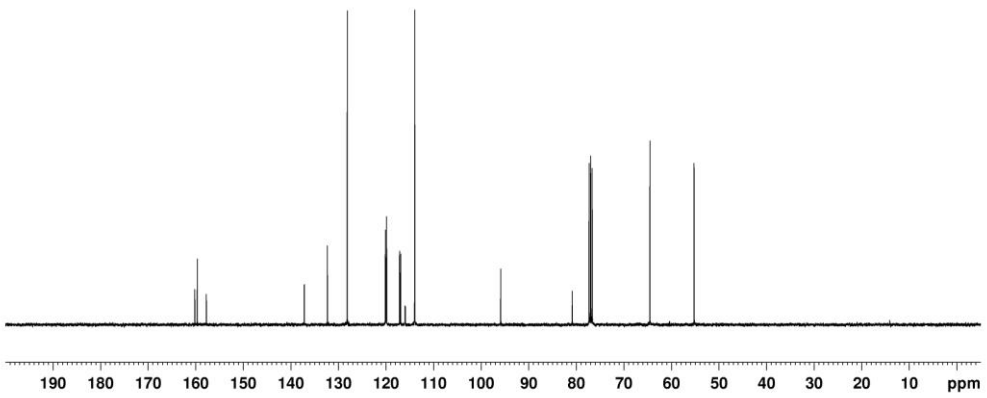


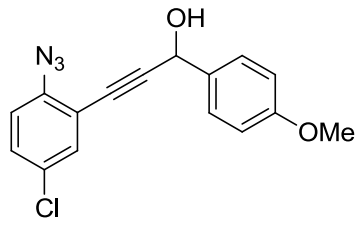
1r

sxr170721-2-p'-F-yl



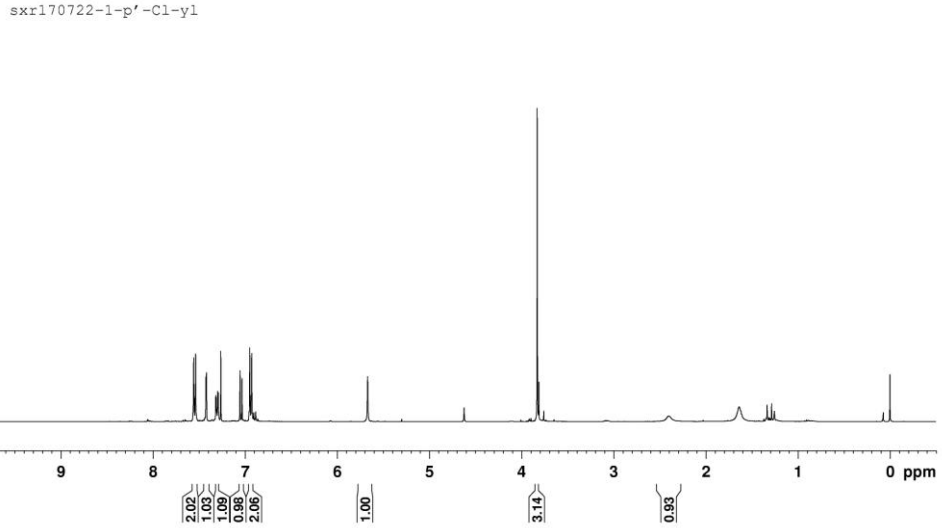
sxr170721-2-p'-F-yl

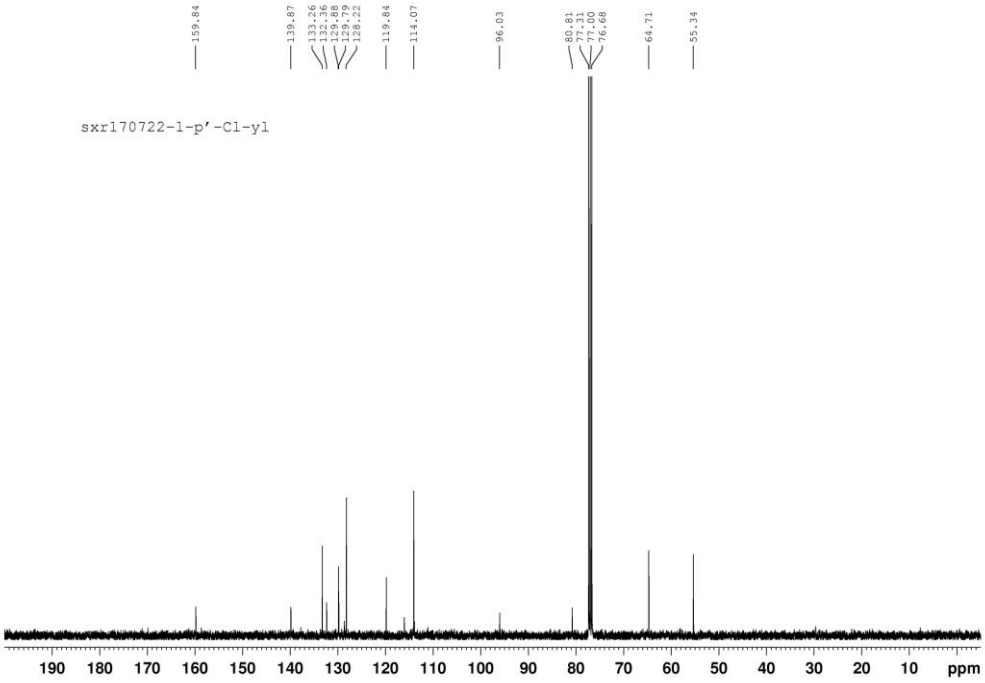


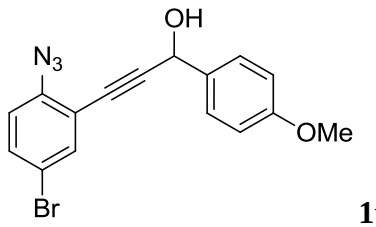

OH
N3
OMe
Cl

1s


7.557
7.535
7.423
7.417
7.317
7.311
7.296
7.290
7.261
7.053
7.032
6.948
6.926
5.668
3.828
2.403
0.000

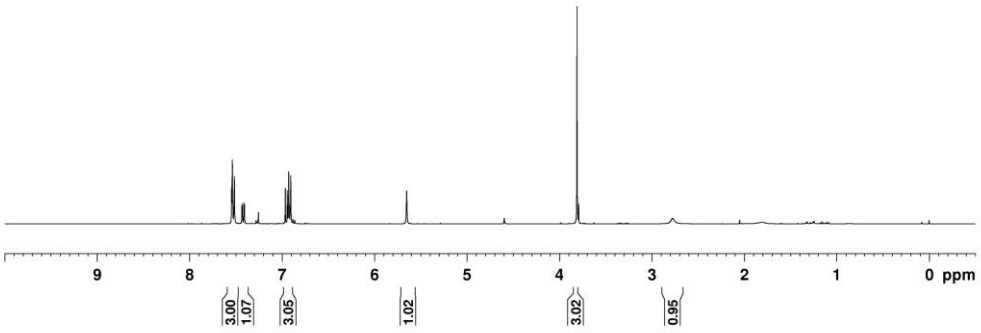

sxr170722-1-p'-Cl-yl
9
8
7
6
5
4
3
2
1
0 ppm
2.02
1.03
1.09
0.98
2.06
1.00
3.14
0.93


159.84
139.87
133.26
132.36
129.88
129.79
128.22
119.84
114.07
96.03
80.81
77.31
77.00
76.68
64.71
55.34
sxr170722-1-p'-Cl-yl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

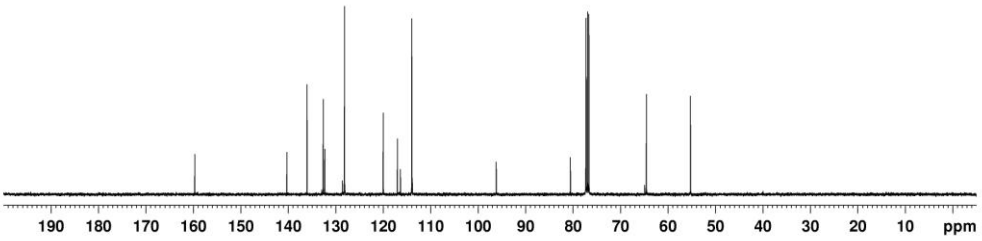


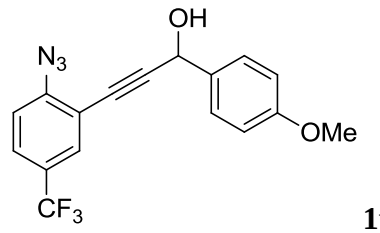
1t

sxr170807-2-p'-Br-yl

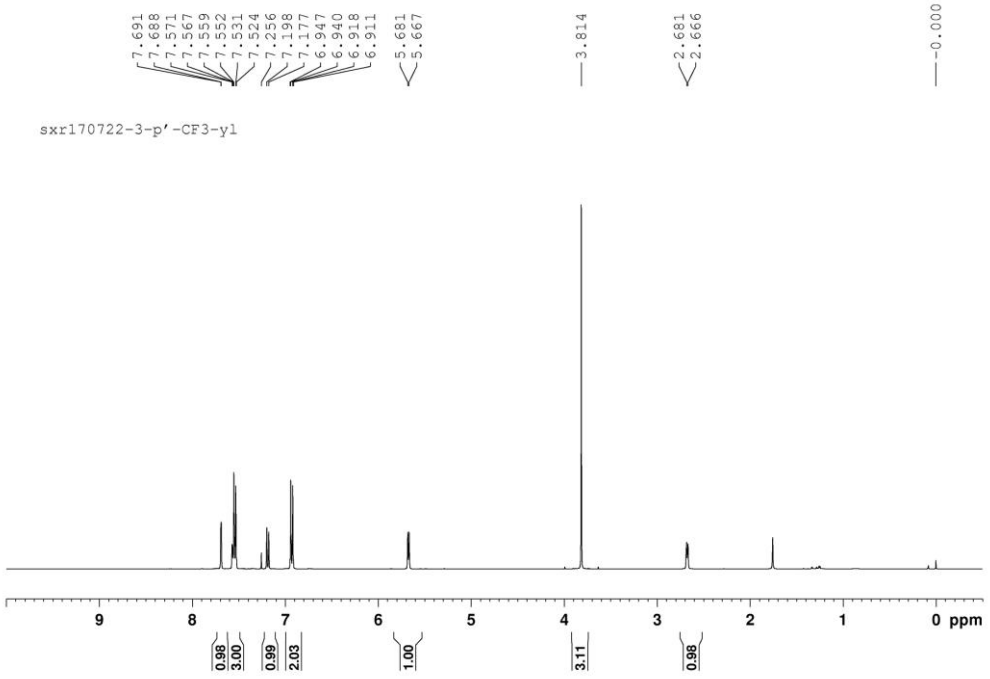


sxr170807-2-p'-Br-yl




OH
N3
OMe
CF3

1u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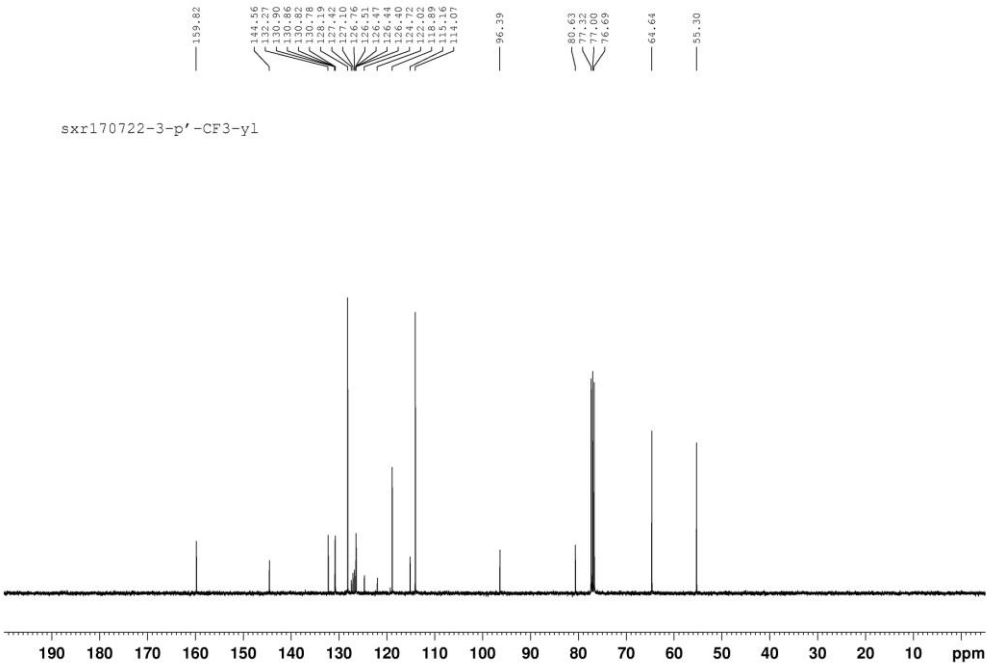
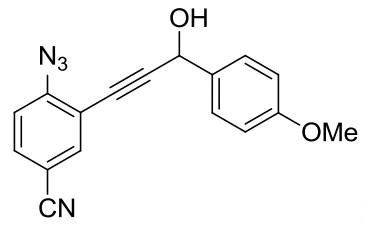
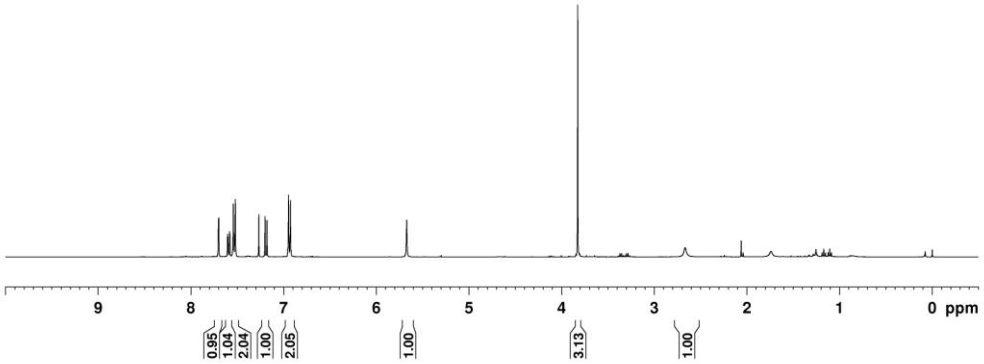
7.688
7.571
7.567
7.559
7.552
7.531
7.524
7.256
7.198
7.177
6.947
6.940
6.918
6.911
5.681
5.667
3.814
2.681
2.666
0.000
sxr170722-3-p'-CF3-yl
9
8
7
6
5
4
3
2
1
0 ppm
0.98
3.00
0.99
2.03
1.00
3.11
0.98


159.82
144.56
133.27
130.90
130.86
130.82
130.78
130.19
127.42
127.10
126.76
126.51
126.47
126.44
126.40
124.72
124.22
118.89
115.16
114.07
96.39
80.63
77.32
77.00
76.69
64.64
55.30
sxr170722-3-p'-CF3-yl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

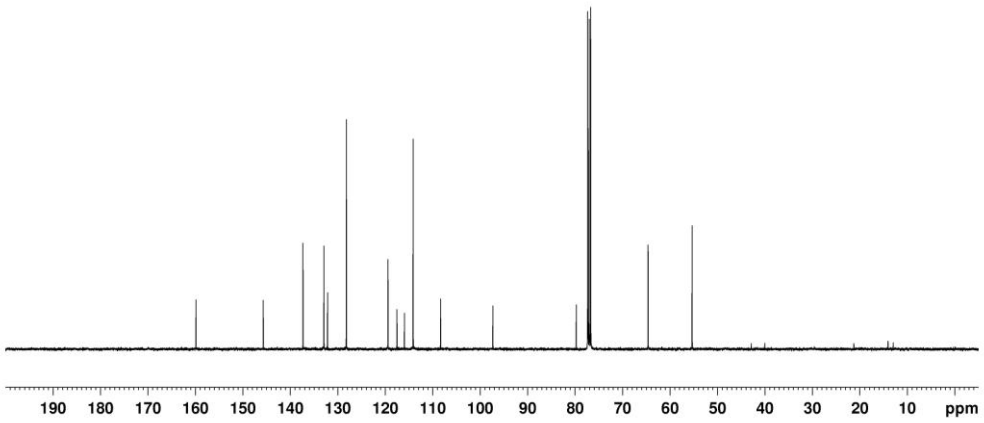


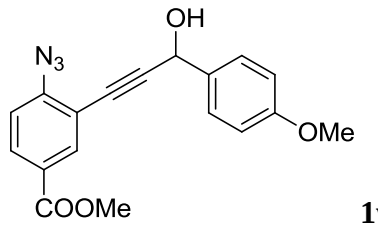
1v

sxr170808-2-p'-CN-yl



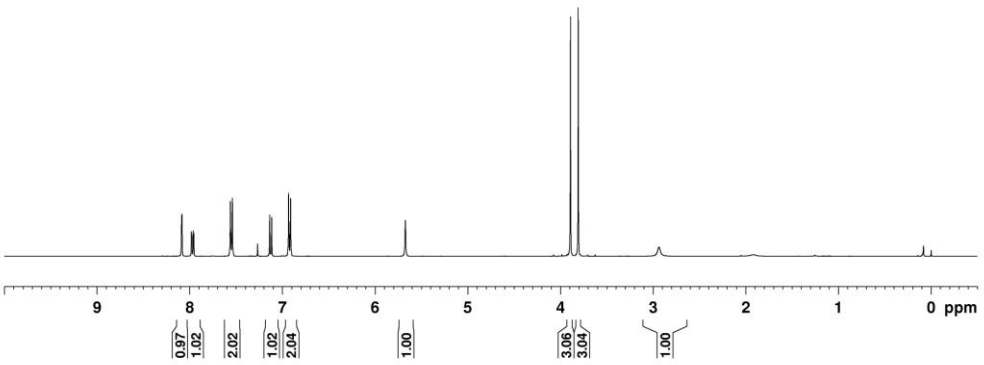
sxr170808-2-p'-CN-yl



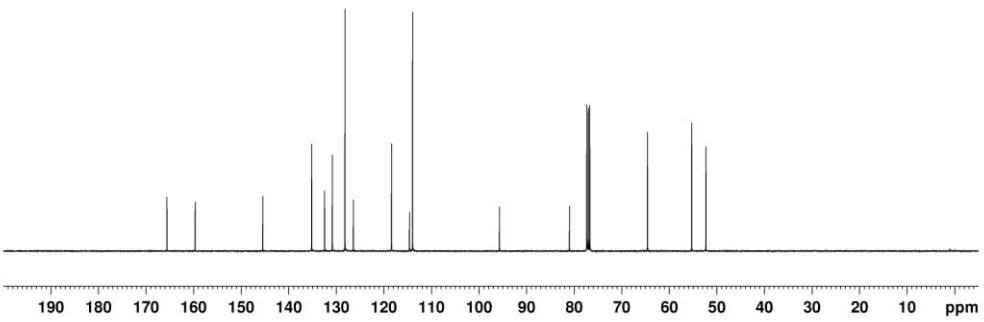


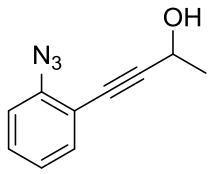
1w

sxr170915-1-p'-COOMe-yl



sxr170915-1-p'-COOMe-yl





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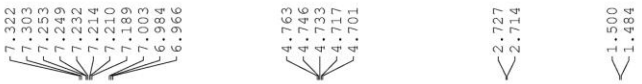
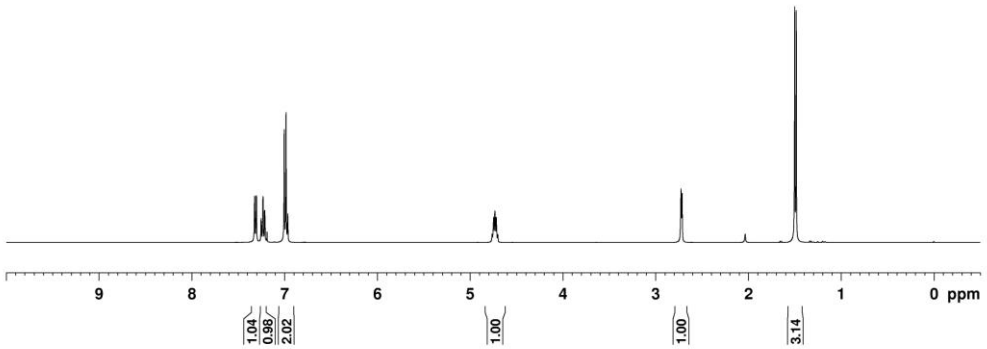
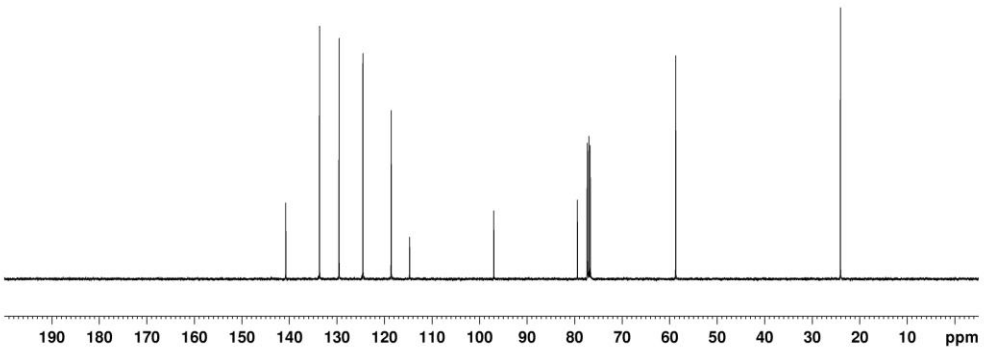
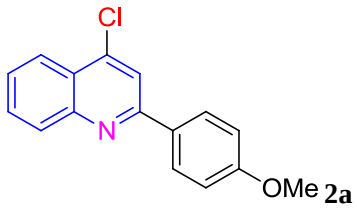


sxr180311-1-jiaji-yl

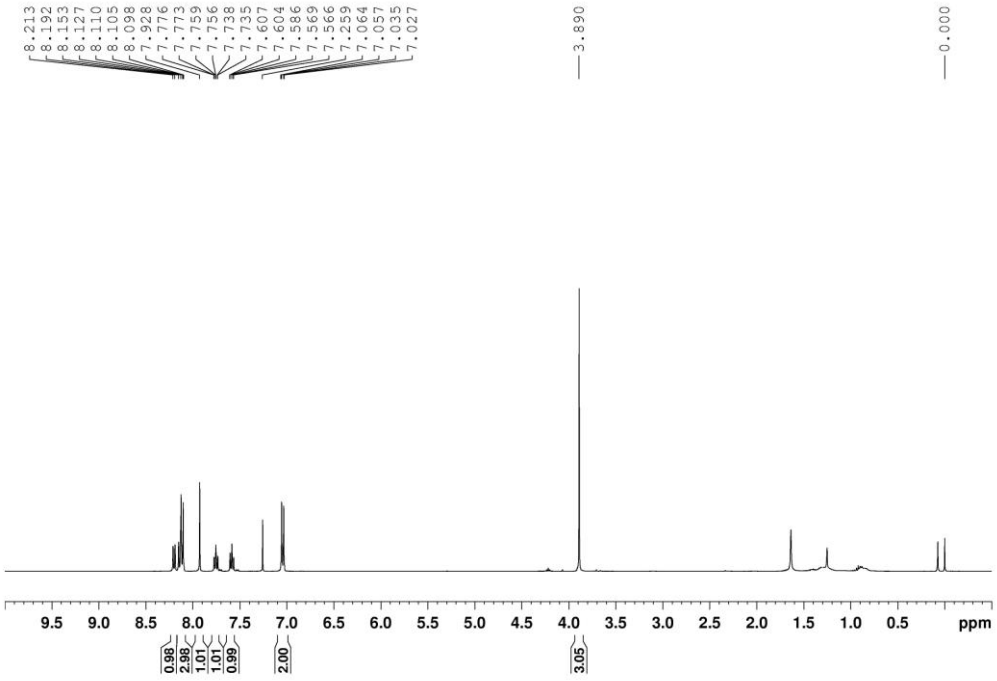


sxr180311-1-jiaji-yl




Cl
N
OMe

2a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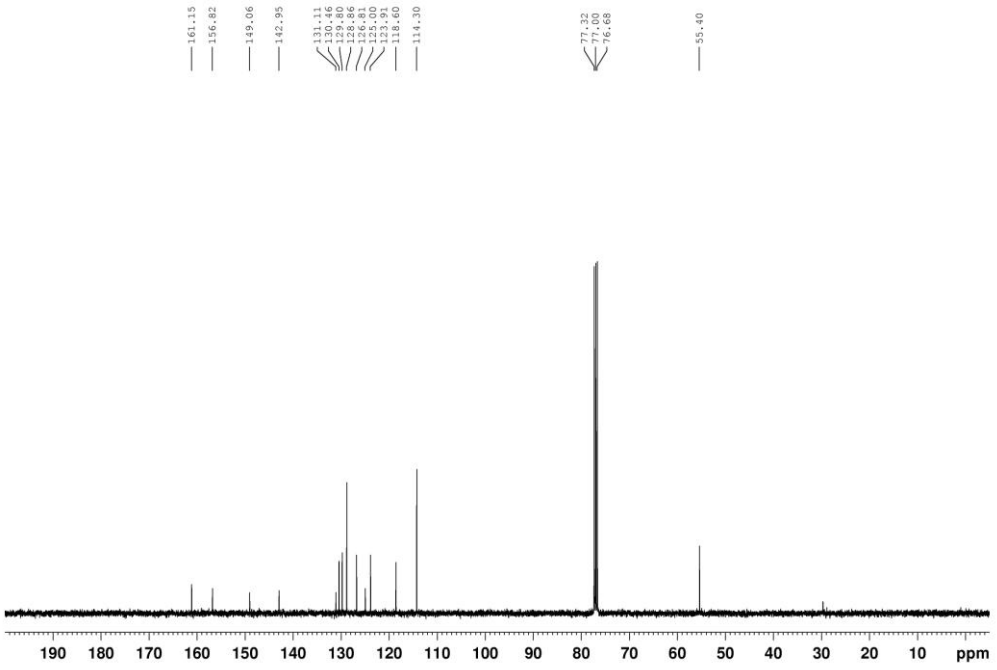
8.192
8.153
8.127
8.110
8.105
8.098
7.928
7.776
7.773
7.759
7.756
7.738
7.735
7.607
7.604
7.586
7.569
7.566
7.259
7.064
7.057
7.035
7.027
3.890
0.000
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.98
2.98
1.01
1.01
0.99
2.00
3.05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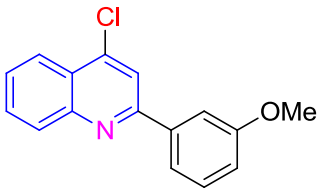
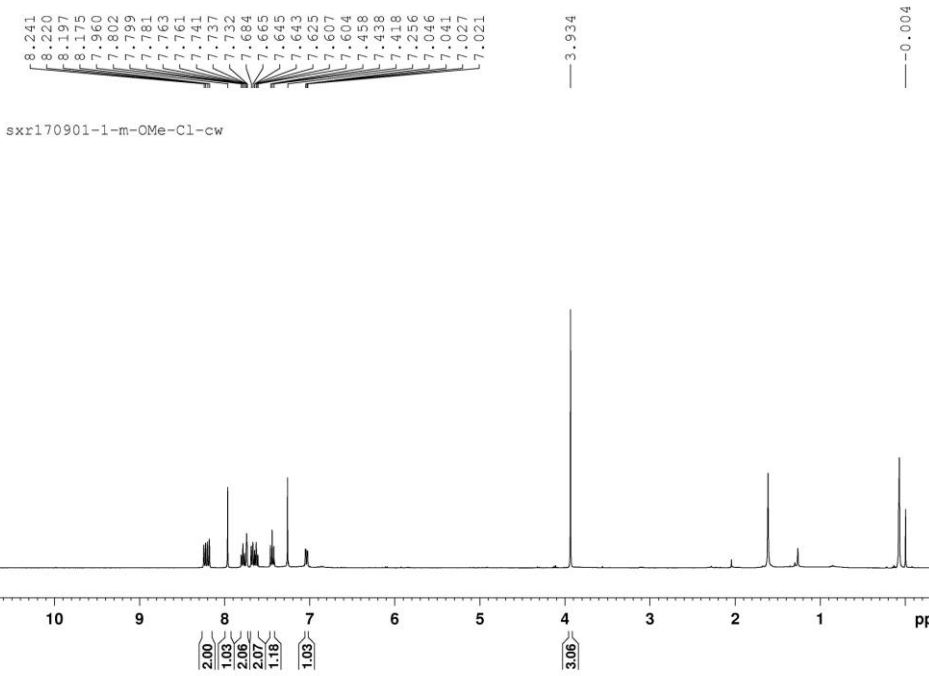
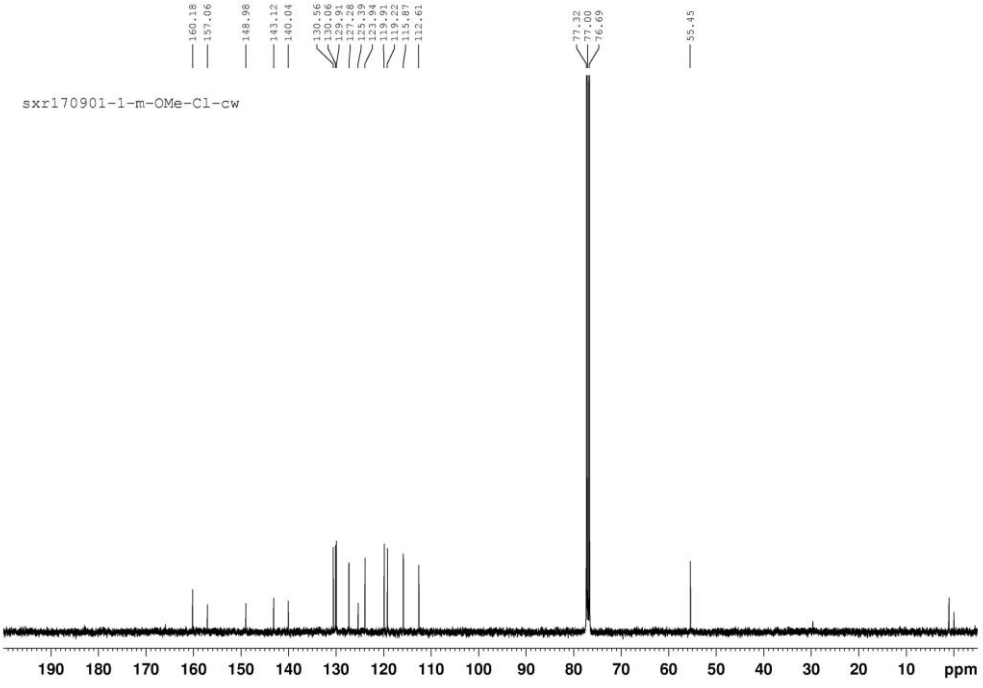
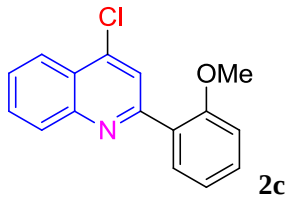
156.82
149.06
142.95
131.11
130.46
129.80
128.86
126.81
125.00
123.91
118.80
114.30
77.32
77.00
76.68
55.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


Cl
N
OMe

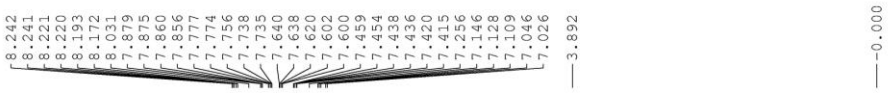
2b


8.241
8.220
8.197
8.175
7.960
7.802
7.799
7.781
7.763
7.761
7.741
7.737
7.732
7.684
7.665
7.645
7.643
7.625
7.607
7.604
7.458
7.438
7.418
7.256
7.046
7.041
7.027
7.021
3.934
-0.004
sxr170901-1-m-OMe-Cl-cw
10
9
8
7
6
5
4
3
2
1
ppm
2.00
1.03
2.06
2.07
1.18
1.03
3.06

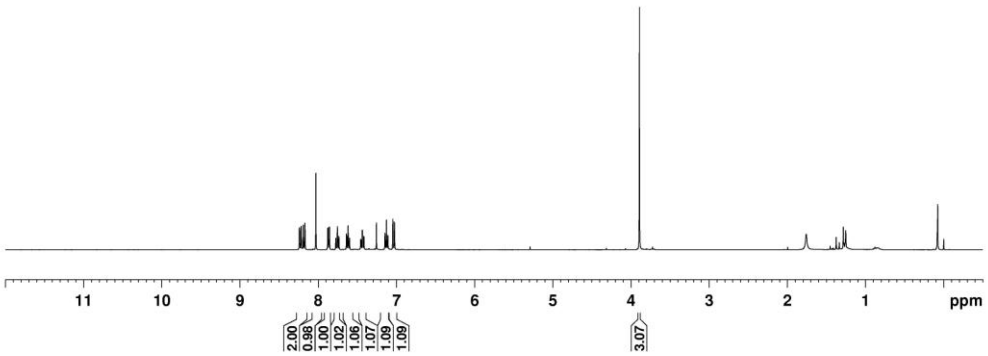

160.18
157.06
148.98
143.12
140.04
130.56
130.06
129.91
127.28
125.39
123.94
119.91
119.22
115.87
112.61
77.32
77.00
76.69
55.45
sxr170901-1-m-OMe-Cl-cw
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



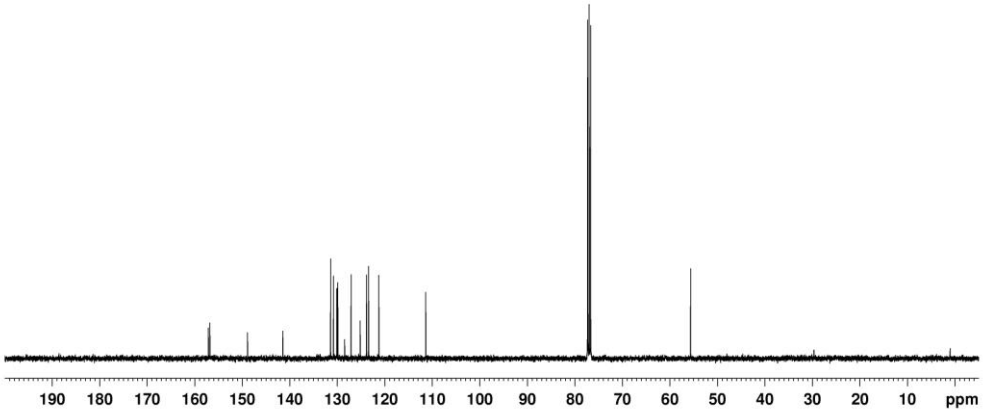
2c

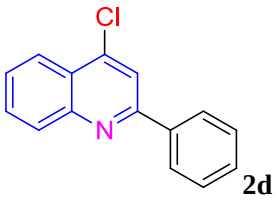


sxr170830-1-o-OMe-Cl-cw

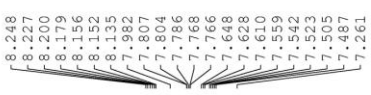


sxr170830-1-o-OMe-Cl-cw

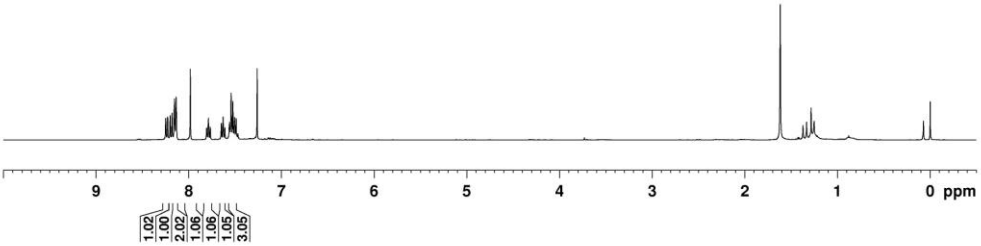


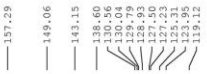


2d

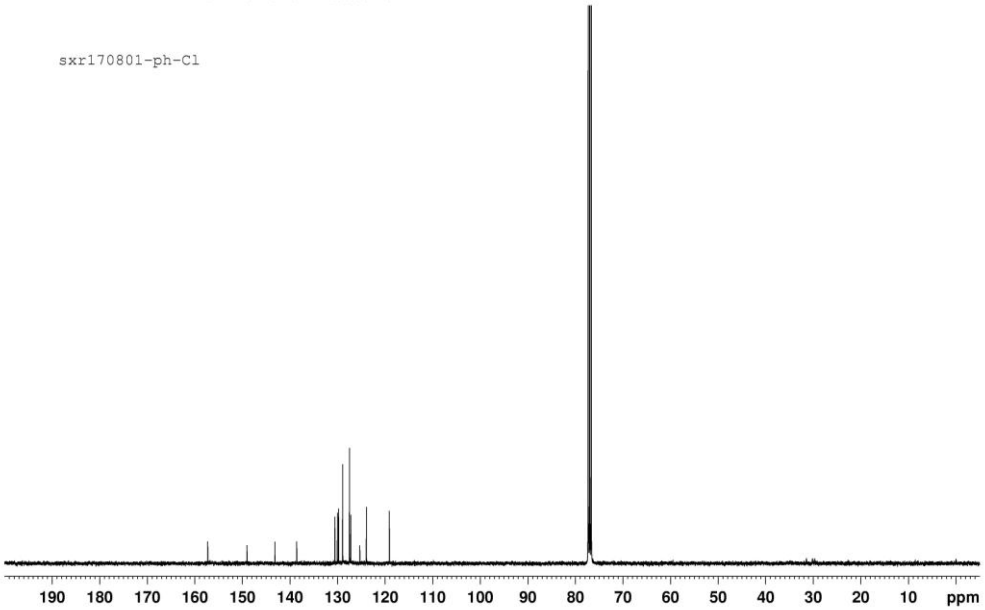


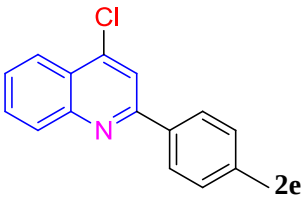
sxr170801-ph-Cl



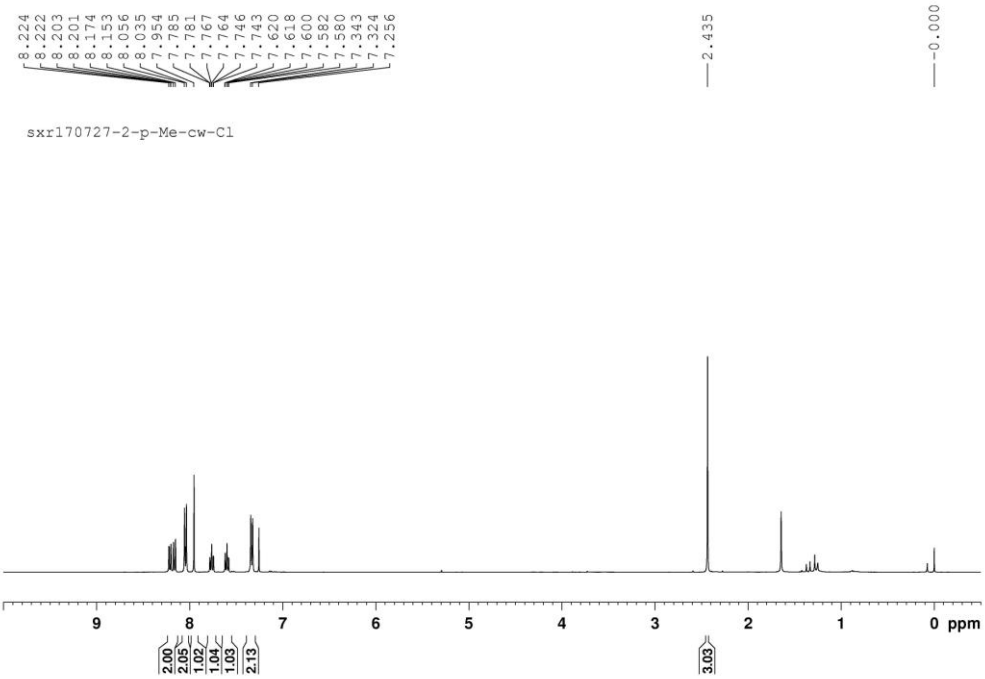


sxr170801-ph-Cl




Cl
N

2e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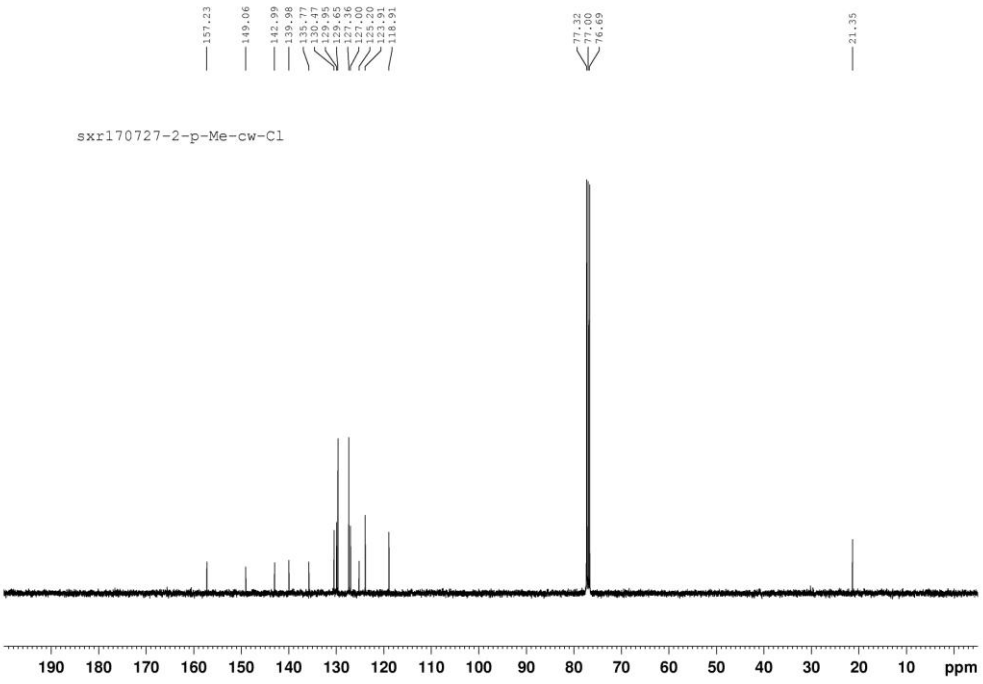
8.153
8.056
8.035
7.954
7.785
7.781
7.767
7.764
7.746
7.743
7.620
7.618
7.600
7.582
7.580
7.343
7.324
7.256
2.435
0.000
sxr170727-2-p-Me-cw-Cl
9
8
7
6
5
4
3
2
1
0 ppm
2.00
2.05
1.02
1.04
1.03
2.13
3.03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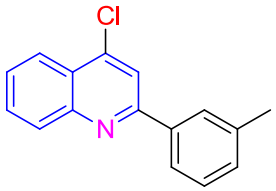
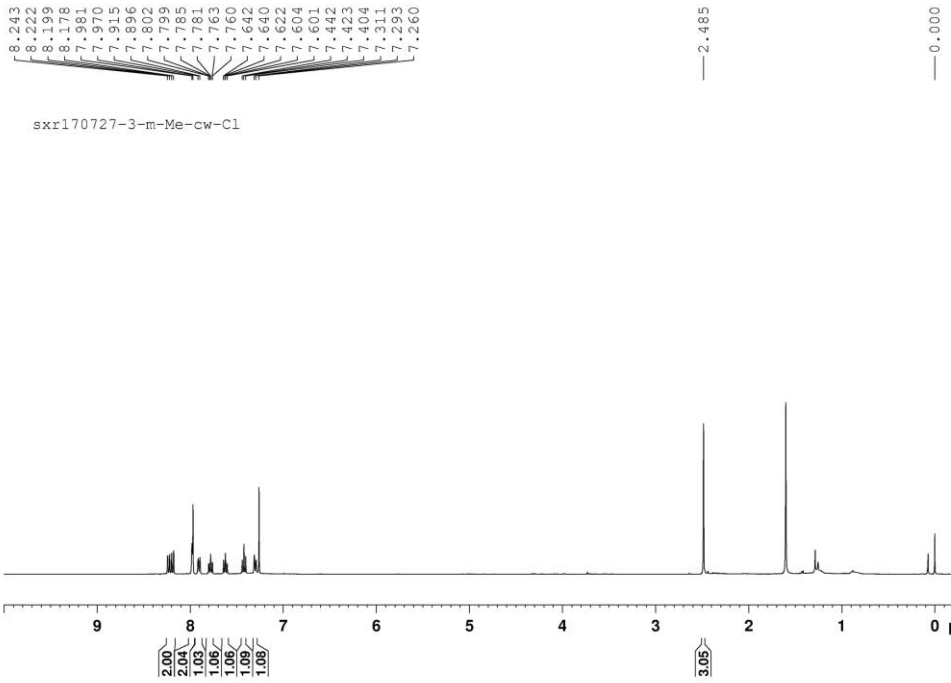
135.77
130.47
129.85
129.65
127.36
127.00
125.20
123.31
118.91
77.32
77.00
76.69
21.35
sxr170727-2-p-Me-cw-Cl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Cl
N

2f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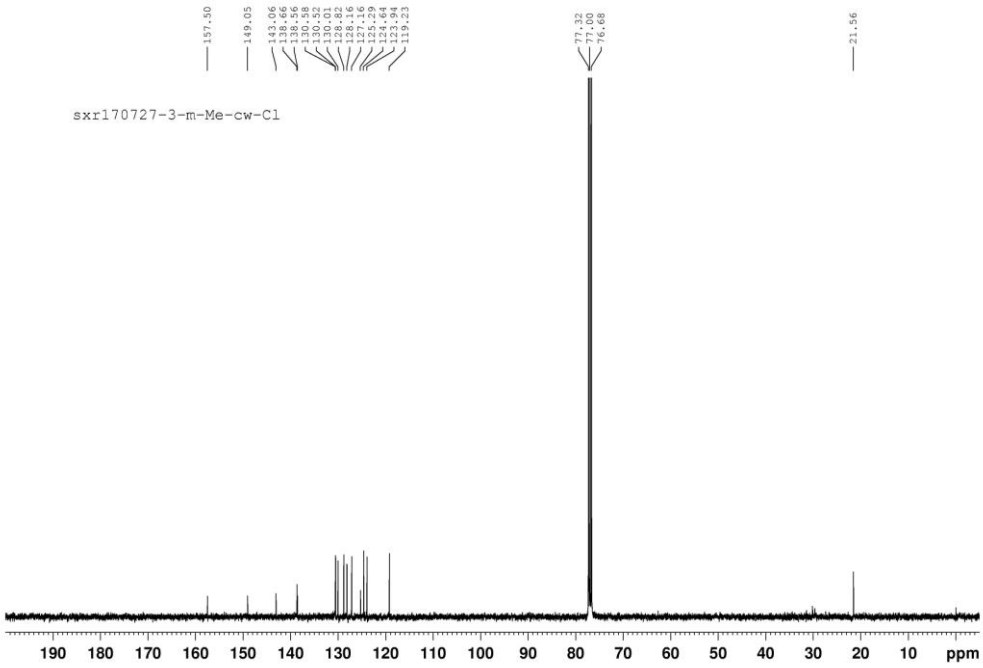
8.222
8.199
8.178
7.981
7.970
7.915
7.896
7.802
7.799
7.785
7.781
7.763
7.760
7.642
7.640
7.622
7.604
7.601
7.442
7.423
7.404
7.311
7.293
7.260
2.485
0.000
sxr170727-3-m-Me-cw-Cl
9
8
7
6
5
4
3
2
1
0 ppm
2.00
2.04
1.03
1.06
1.06
1.09
1.08
3.05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143.06
138.66
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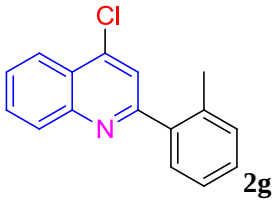
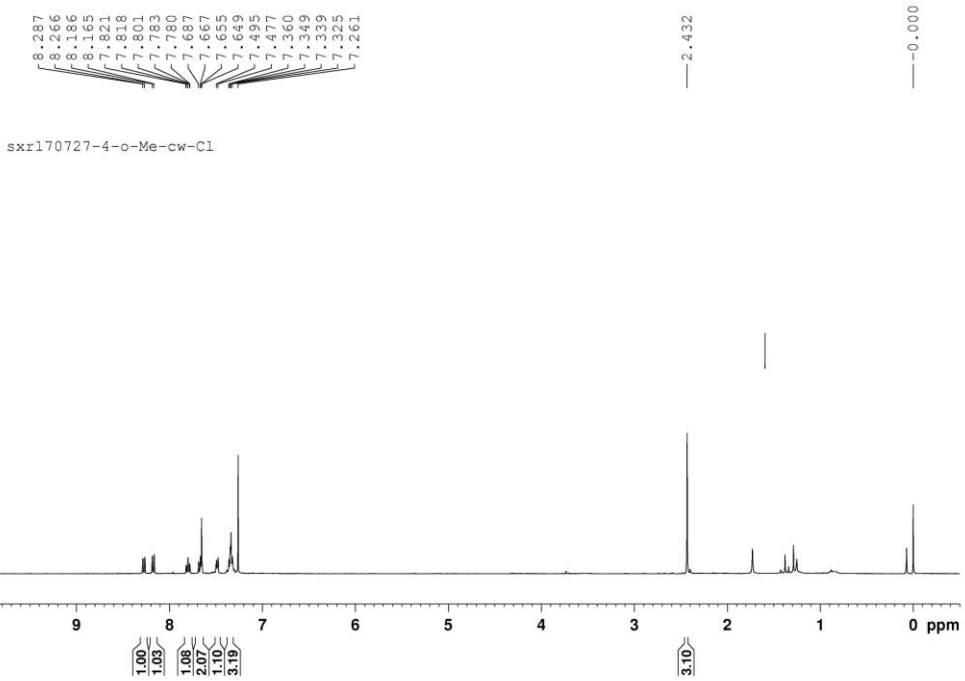
130.58
130.53
130.01
128.82
128.16
127.16
125.09
124.64
123.94
119.23
77.32
77.00
76.68
21.56
sxr170727-3-m-Me-cw-Cl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Cl
N

2g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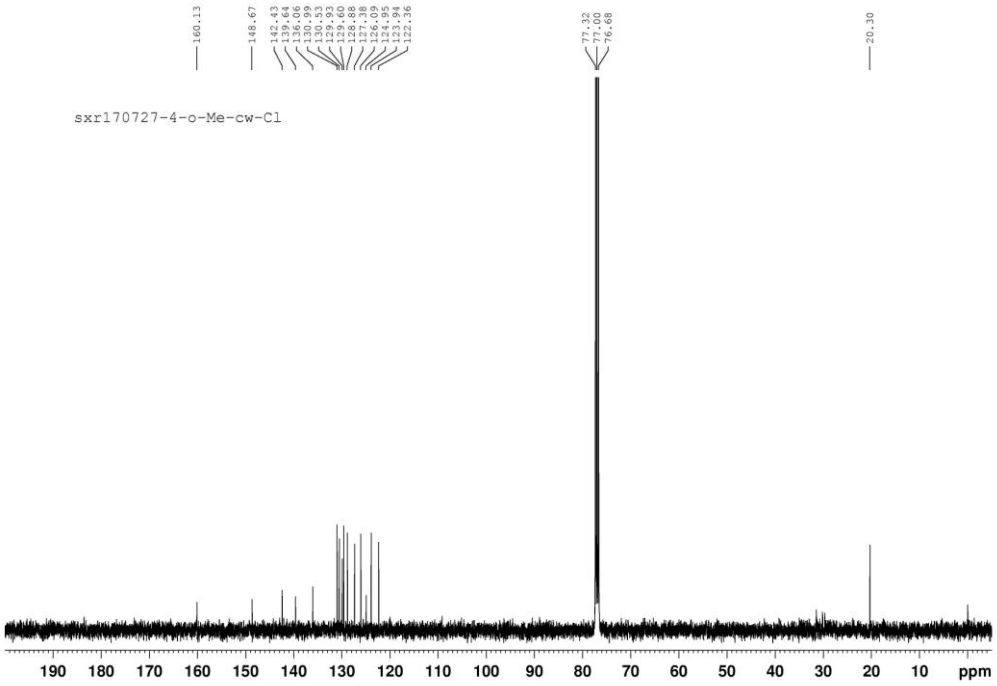
8.266
8.186
8.165
7.821
7.818
7.801
7.783
7.780
7.687
7.667
7.655
7.649
7.495
7.477
7.360
7.349
7.339
7.325
7.261
2.432
0.000
sxr170727-4-o-Me-cw-Cl
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.03
1.08
2.07
1.10
3.19
3.10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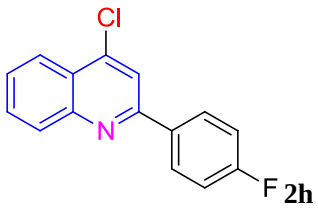
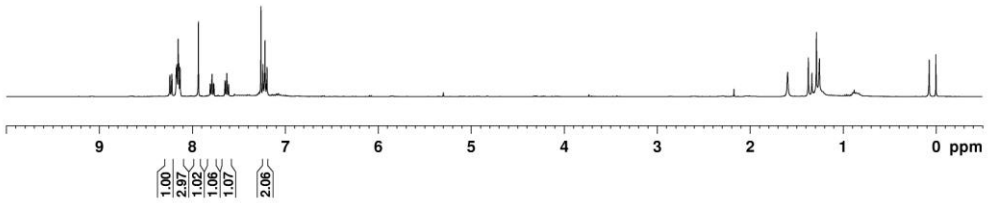
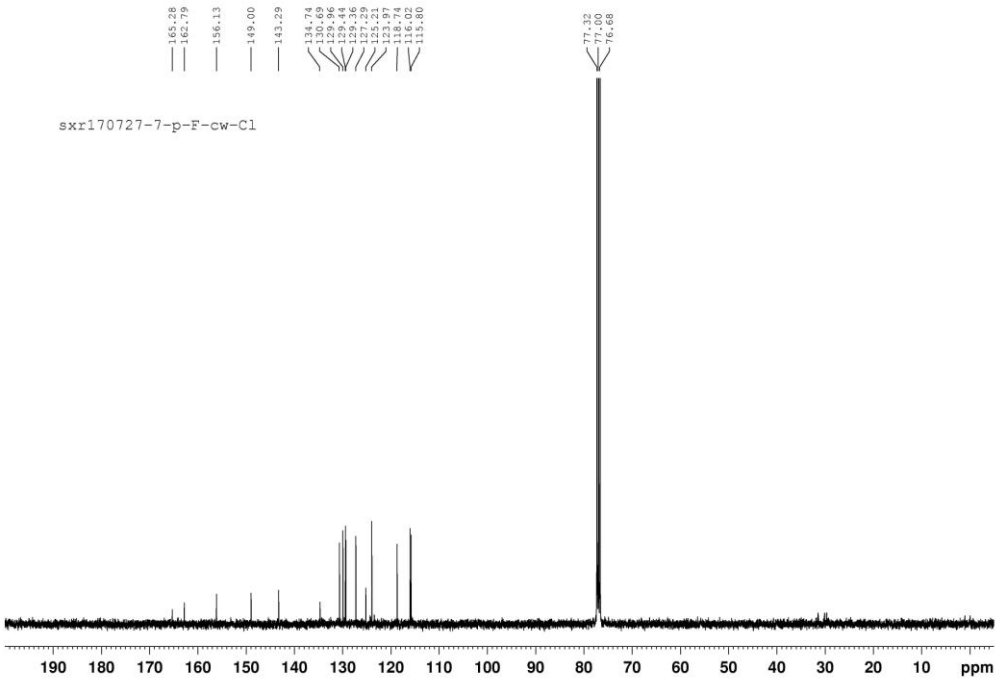
127.38
126.09
124.95
123.94
122.36
77.32
77.00
76.68
20.30
sxr170727-4-o-Me-cw-Cl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Cl
N
F

2h


8.220
8.172
8.165
8.160
8.151
8.143
8.135
8.130
7.933
7.807
7.804
7.789
7.786
7.768
7.765
7.648
7.646
7.628
7.610
7.607
7.260
7.239
7.217
7.195
0.000
sxr170727-7-p-F-cw-Cl


9
8
7
6
5
4
3
2
1
0 ppm
1.00
2.97
1.02
1.06
1.07
2.06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128.56
127.29
125.21
123.97
118.74
116.02
115.80
77.32
77.00
76.68
sxr170727-7-p-F-cw-Cl
190
180
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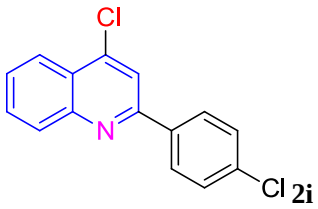
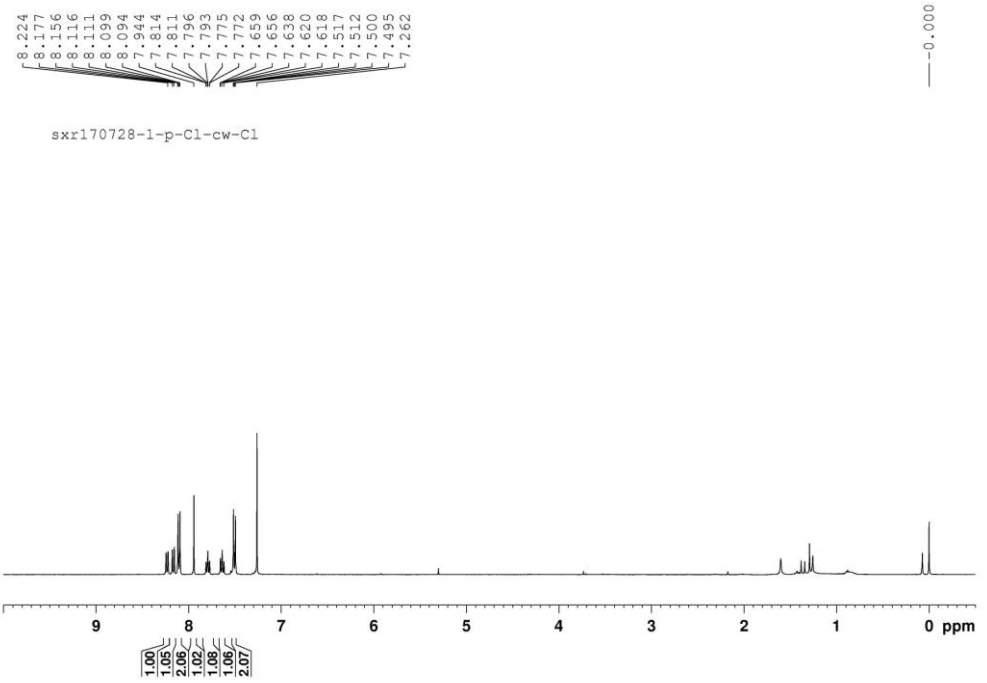
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Cl
N
Cl

2i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8.177
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8.111
8.099
8.094
7.944
7.814
7.811
7.796
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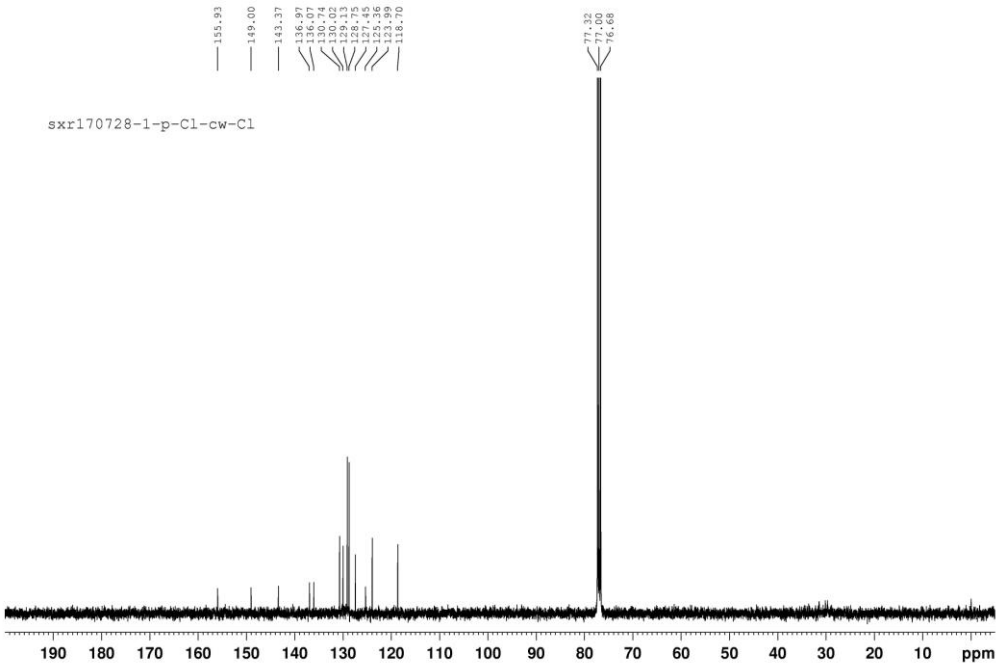
7.775
7.772
7.659
7.656
7.638
7.620
7.618
7.517
7.512
7.500
7.495
7.262
-0.000
sxr170728-1-p-Cl-cw-Cl
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.05
2.06
1.02
1.08
1.06
2.07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136.07
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130.02
129.13
129.05
125.36
123.99
118.70
77.32
77.00
76.68
sxr170728-1-p-Cl-cw-Cl
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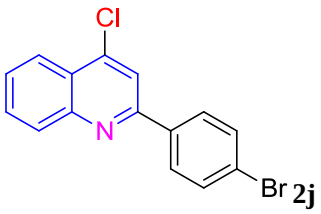
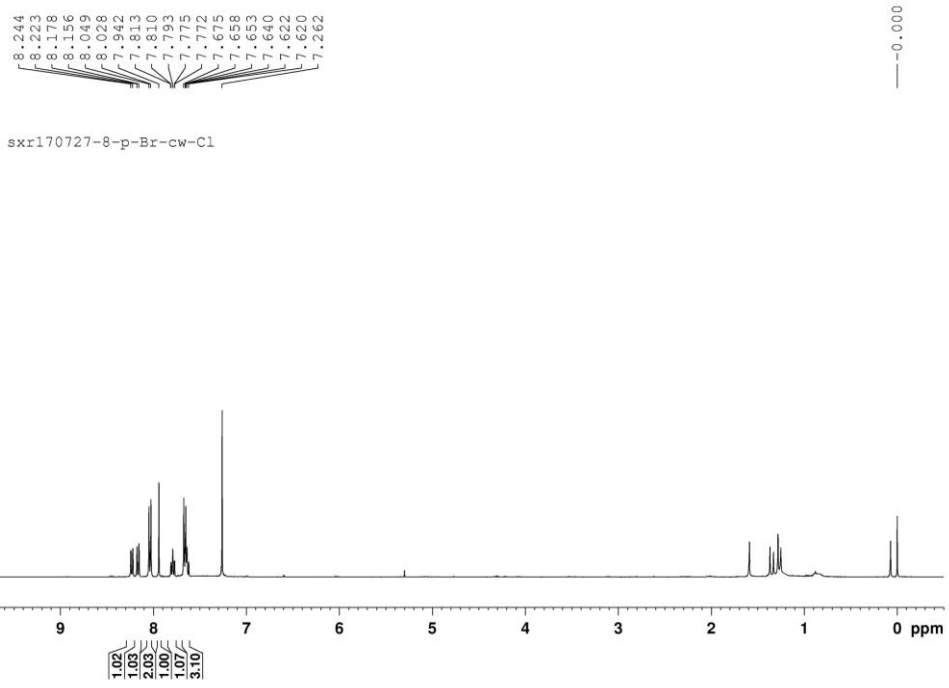
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Cl
N
Br

2j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8.028
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7.813
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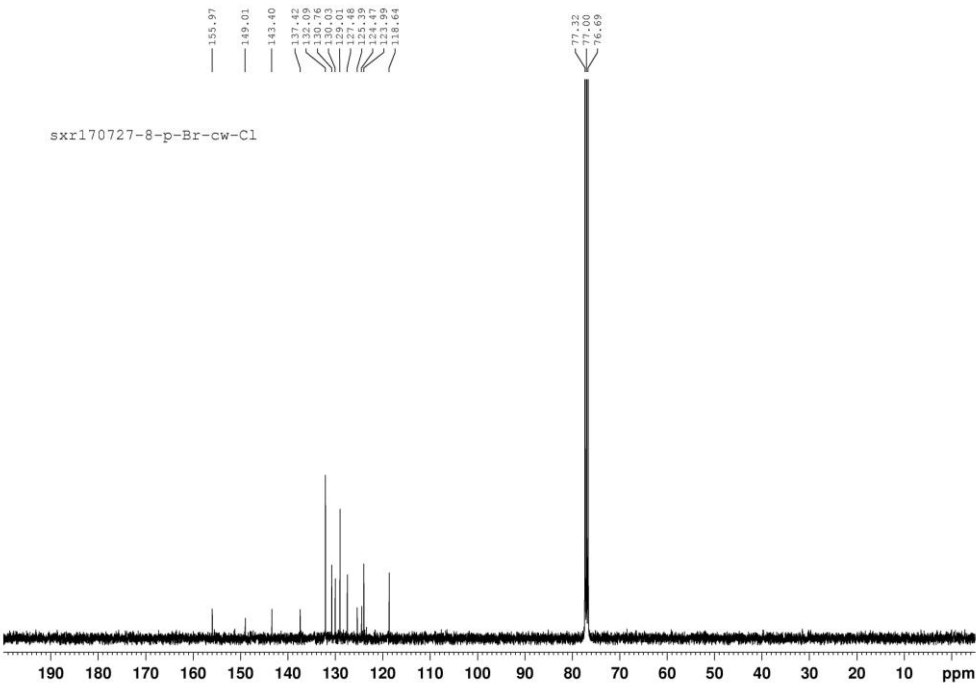
7.793
7.775
7.772
7.675
7.658
7.653
7.640
7.622
7.620
7.262
0.000
sxr170727-8-p-Br-cw-Cl
9
8
7
6
5
4
3
2
1
0 ppm
1.02
1.03
2.03
1.00
1.07
3.10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149.01
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137.42
132.09
130.76
130.03
129.01
127.48
125.39
124.47
123.89
118.64
77.32
77.00
76.69
sxr170727-8-p-Br-cw-Cl
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180
170
160
150
140
130
120
110
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90
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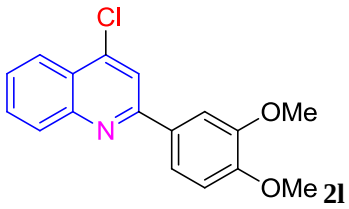
70
60
50
40
30
20
10
ppm



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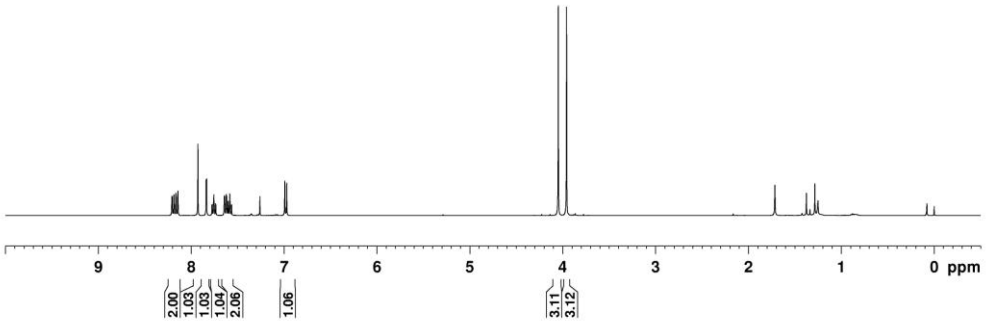
sxr170727-5-3,4-erOMe-cw-Cl



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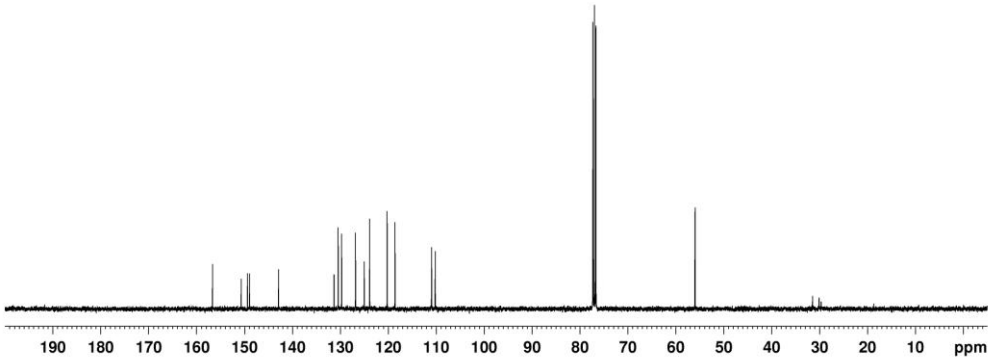

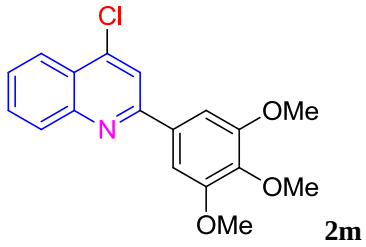

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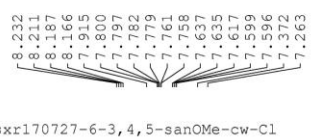

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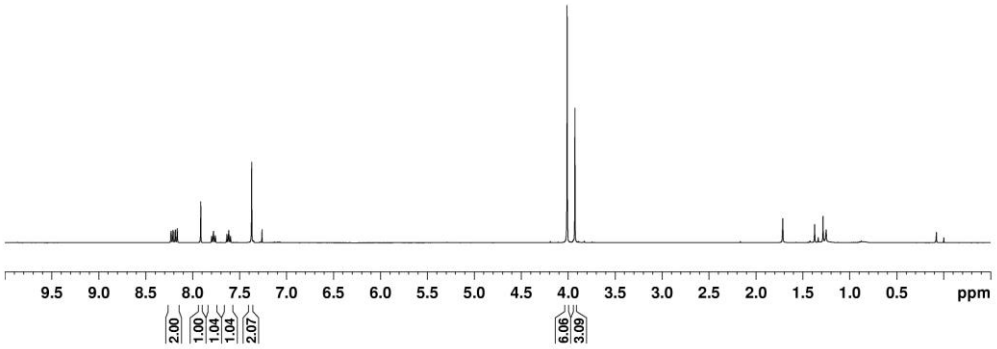

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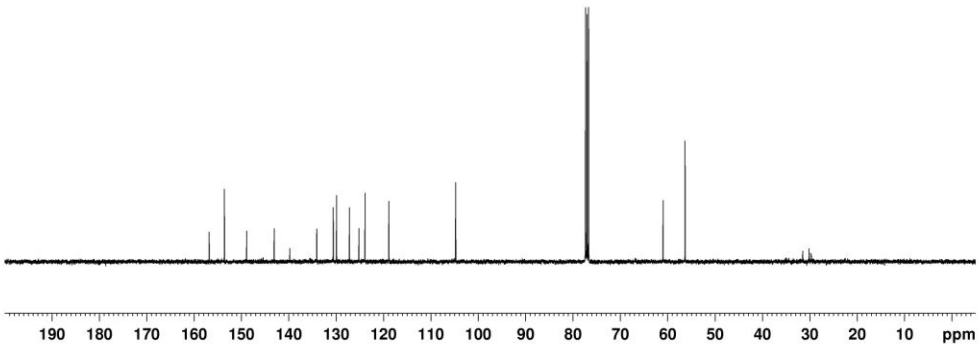
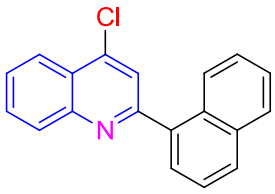
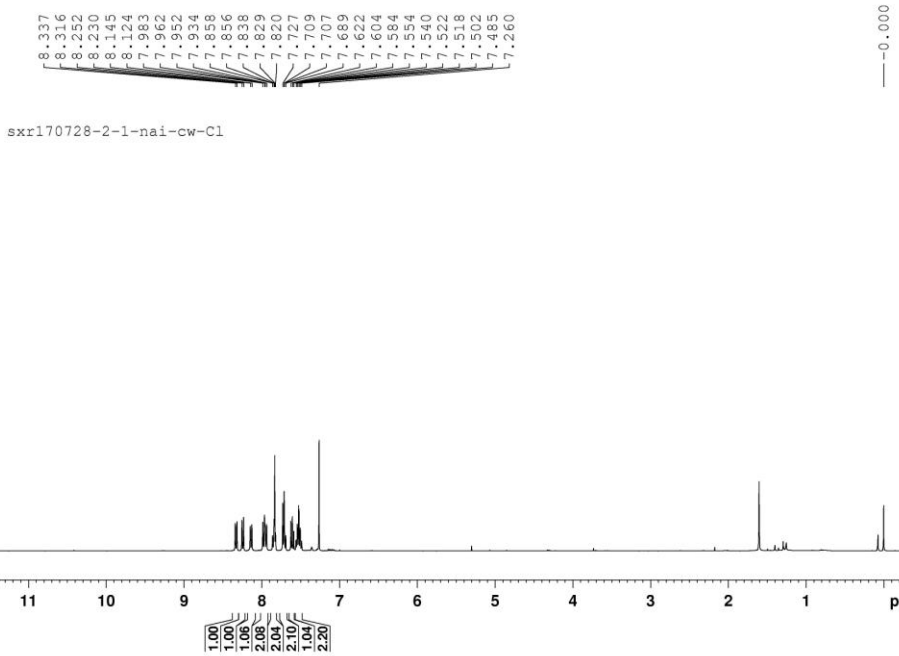



Cl
N

2n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8.124
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7.962
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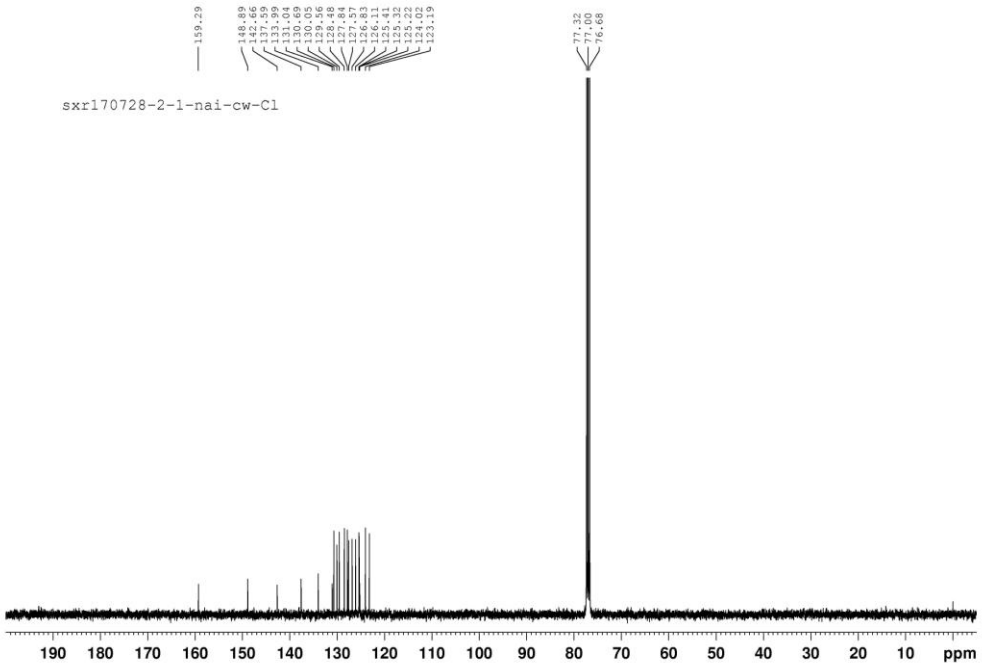
7.934
7.858
7.856
7.838
7.829
7.820
7.727
7.709
7.707
7.689
7.622
7.604
7.584
7.554
7.540
7.522
7.518
7.502
7.485
7.260
0.000
sxr170728-2-1-nai-cw-Cl
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.00
1.06
2.08
2.04
2.10
1.04
2.20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148.89
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131.04
130.69
130.05
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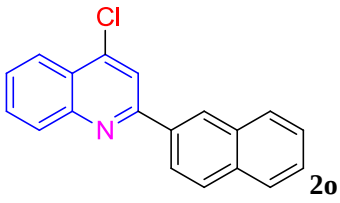
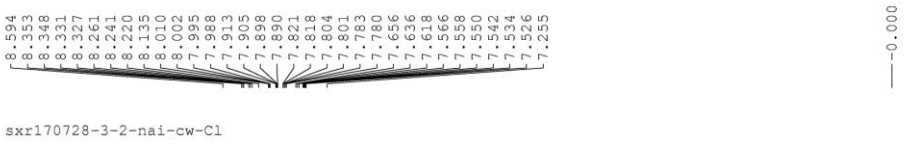
128.48
128.04
127.57
126.83
126.11
125.41
125.22
125.22
124.02
123.19
77.32
77.00
76.68
sxr170728-2-1-nai-cw-Cl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Cl
N

2o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8.353
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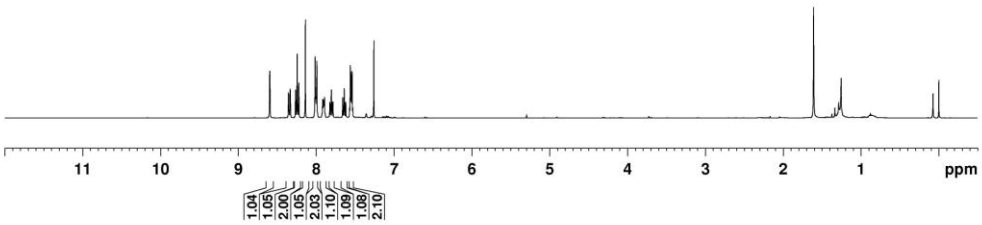
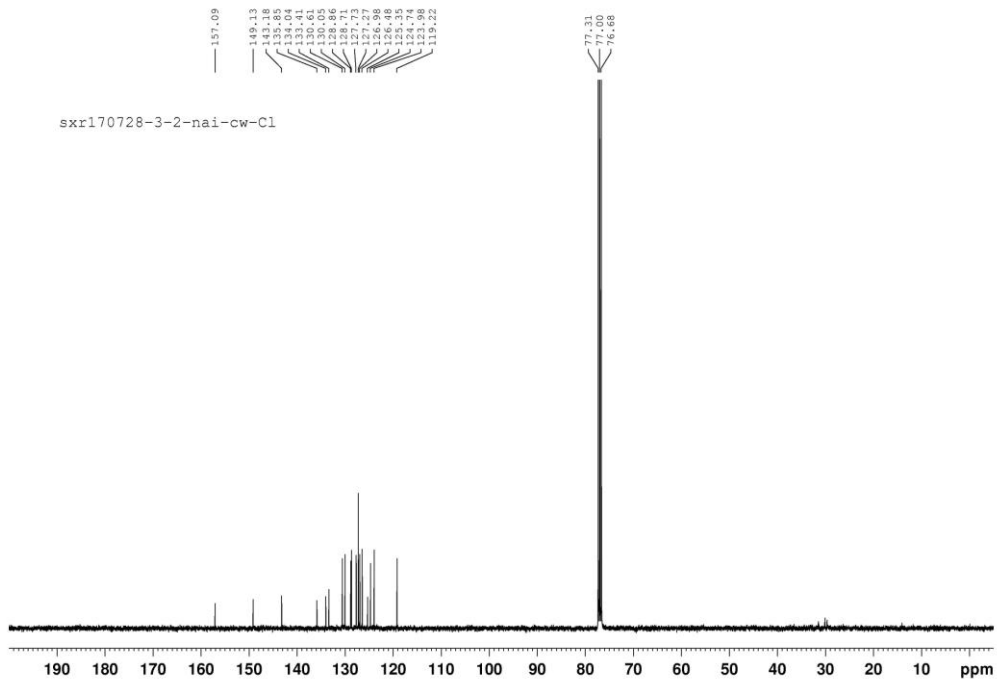
8.331
8.327
8.261
8.241
8.220
8.135
8.010
8.002
7.995
7.988
7.913
7.905
7.898
7.890
7.821
7.818
7.804
7.801
7.783
7.780
7.656
7.636
7.618
7.566
7.558
7.550
7.542
7.534
7.526
7.255
-0.000
sxr170728-3-2-nai-cw-Cl


11
10
9
8
7
6
5
4
3
2
1
ppm
1.04
1.05
2.00
1.05
2.03
1.10
1.09
1.08
2.10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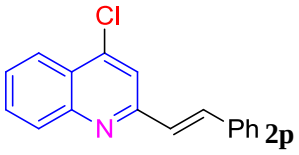
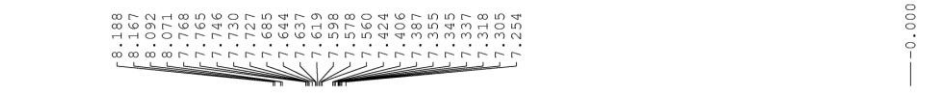
149.13
143.18
135.85
134.84
133.41
130.61
130.05
128.86
128.71
127.73
127.27
126.98
126.48
125.35
124.74
123.98
119.22
77.31
77.00
76.68
sxr170728-3-2-nai-cw-Cl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Cl
N
Ph

2p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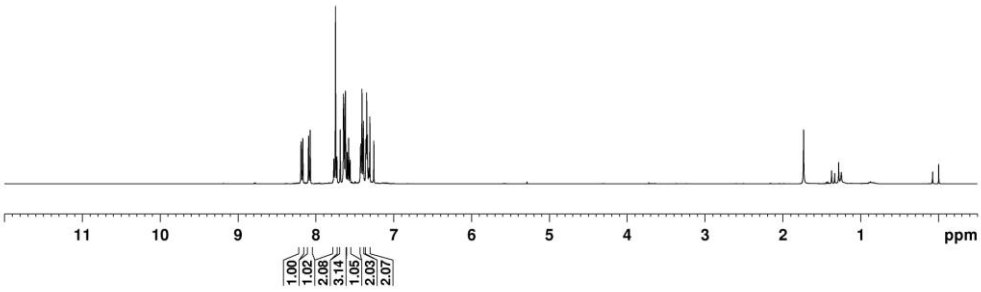
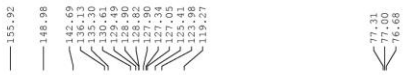
7.730
7.727
7.685
7.644
7.637
7.619
7.598
7.578
7.560
7.424
7.406
7.387
7.355
7.345
7.337
7.318
7.305
7.254
-0.000
sxr170728-4-ruoguii-cw-Cl


11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.02
2.08
3.14
1.05
2.05
2.07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130.61
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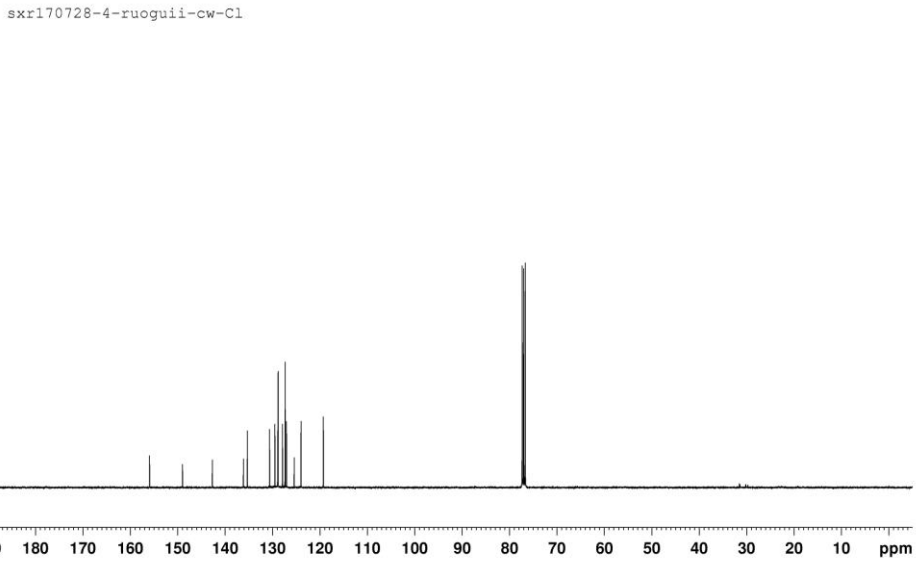
128.62
127.90
127.34
127.05
125.11
123.98
119.27
77.31
77.00
76.68


sxr170728-4-ruoguii-cw-Cl
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180
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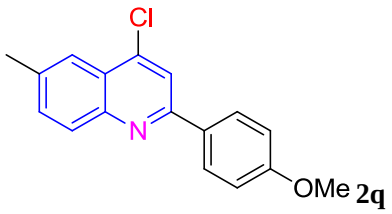
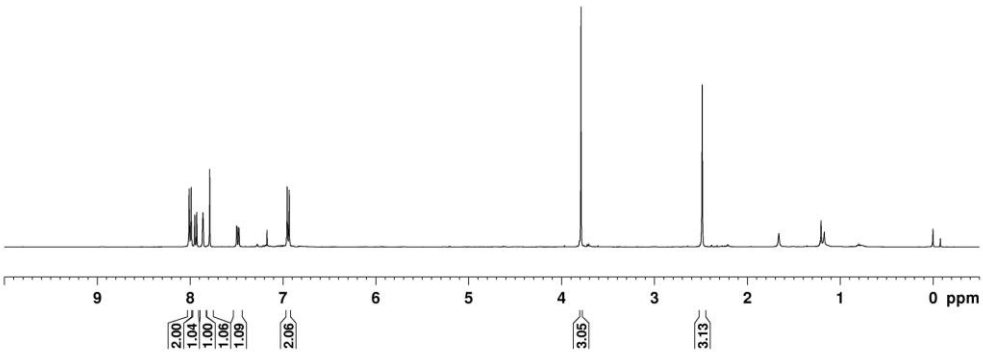
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

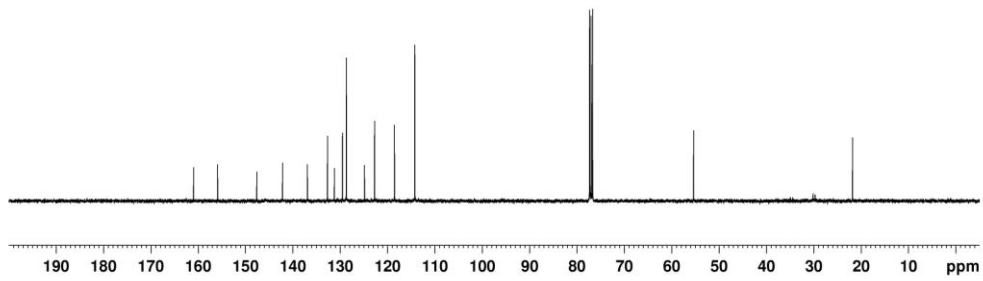


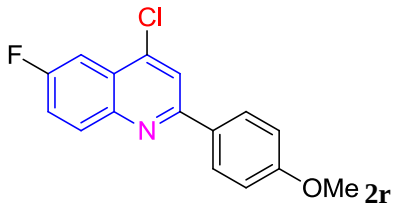
2q

sxr170726-3-p'-Me-cw-Cl



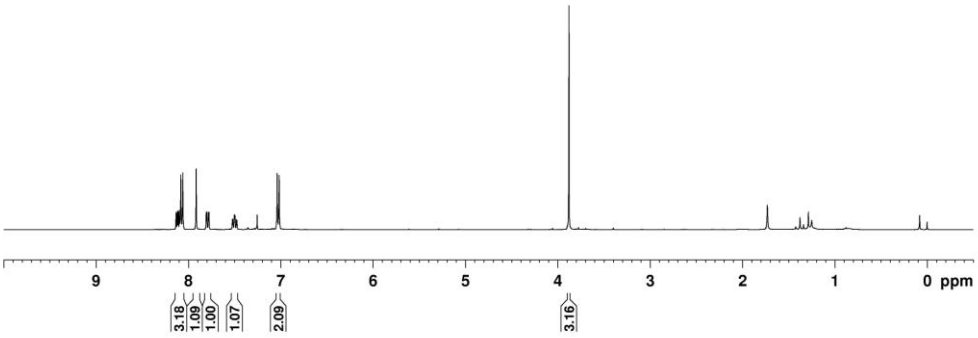
sxr170726-3-p'-Me-cw-Cl



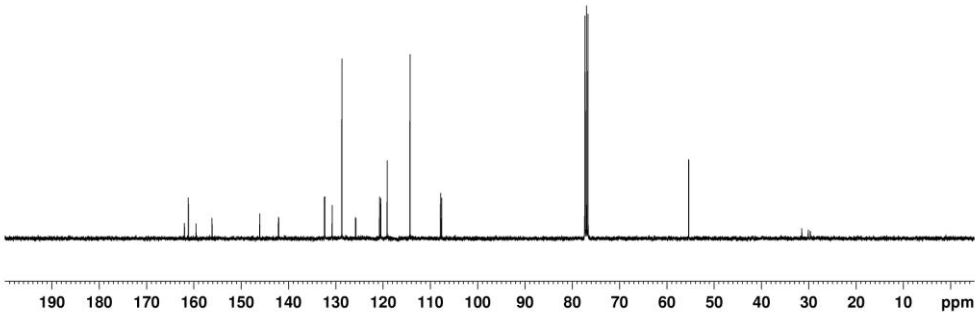


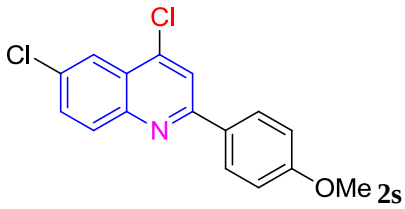
2r

sxr170726-4-p'-F-cw-Cl

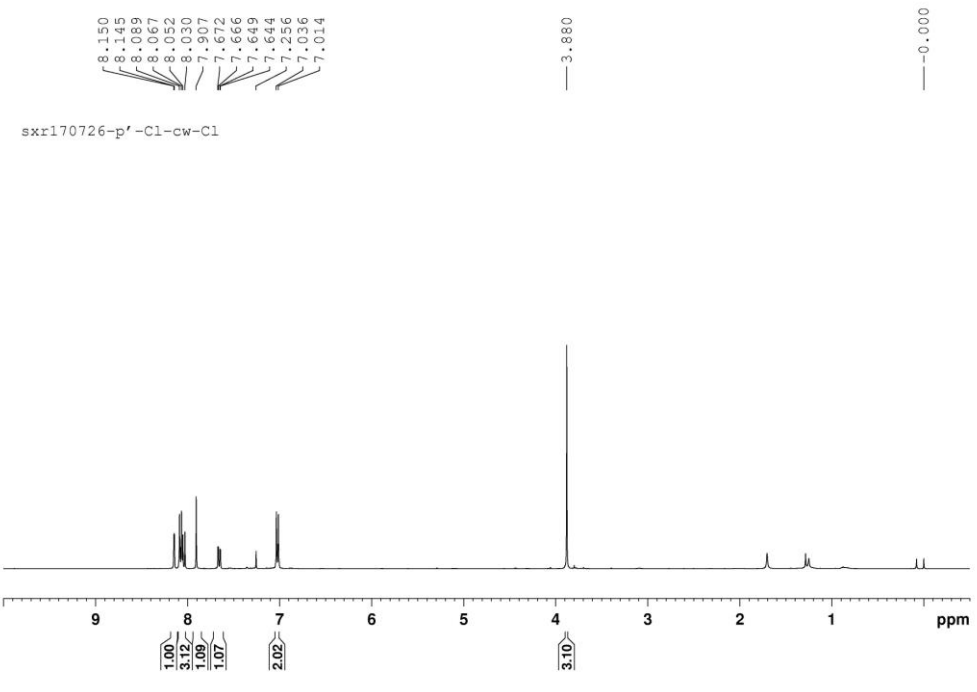


sxr170726-4-p'-F-cw-Cl




Cl
Cl
N
OMe

2s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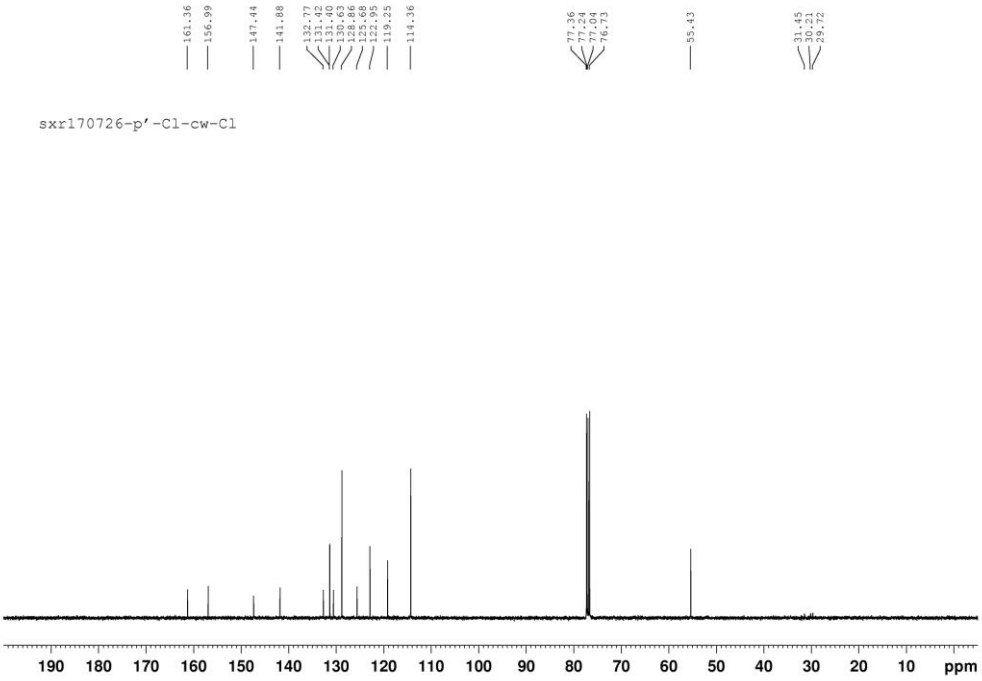
8.030
7.907
7.672
7.666
7.649
7.644
7.256
7.036
7.014
3.880
0.000
sxr170726-p'-Cl-cw-Cl
9
8
7
6
5
4
3
2
1
ppm
1.00
3.12
1.09
1.07
2.02
3.10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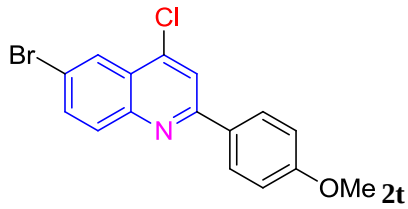
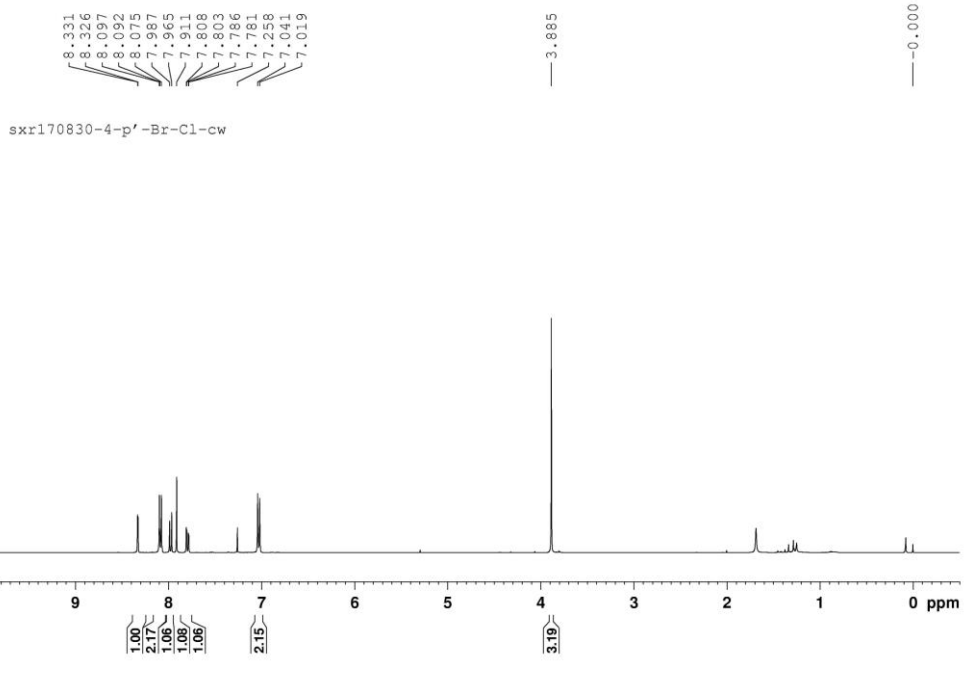
147.44
141.88
132.77
131.42
131.40
130.63
128.86
125.68
122.95
119.25
114.36
77.36
77.24
77.04
76.73
55.43
31.45
30.21
29.72
sxr170726-p'-Cl-cw-Cl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


Cl
Br
N
OMe

2t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8.092
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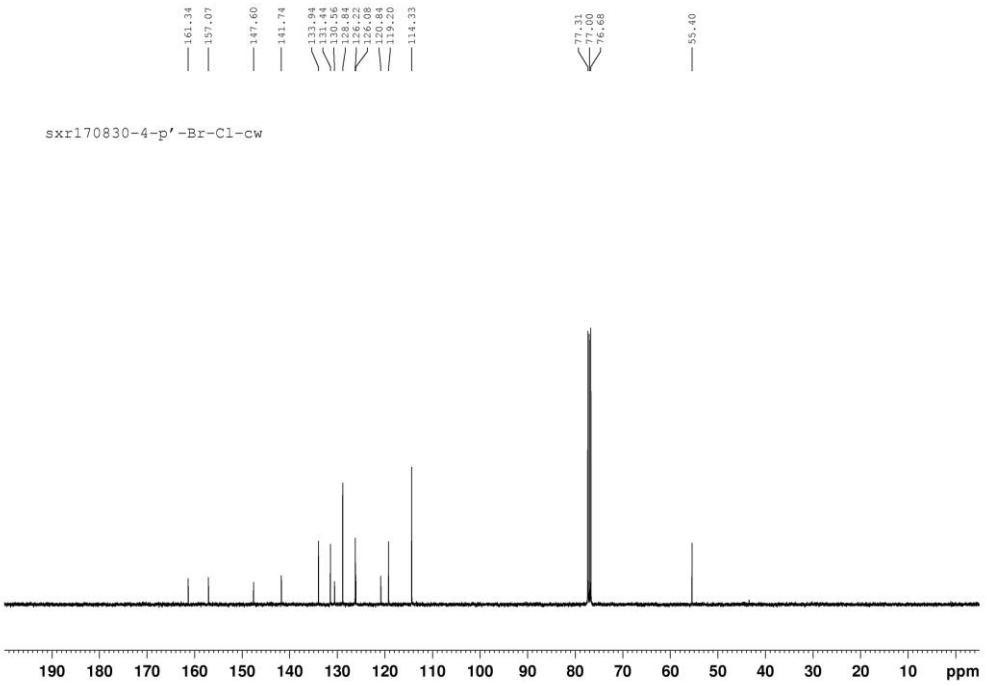
7.987
7.965
7.911
7.808
7.803
7.786
7.781
7.258
7.041
7.019
3.885
0.000
sxr170830-4-p'-Br-Cl-cw
9
8
7
6
5
4
3
2
1
0 ppm
1.00
2.17
1.06
1.08
1.06
2.15
3.19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141.74
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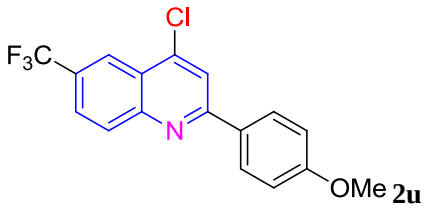
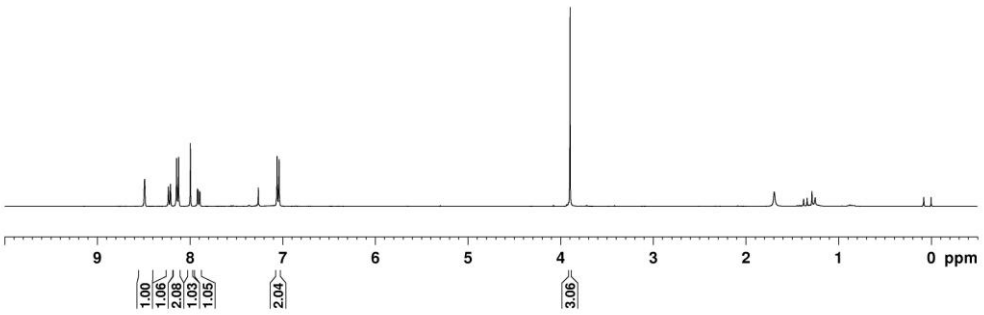
130.56
128.84
126.72
126.08
120.84
119.20
114.33
77.31
77.00
76.68
55.40
sxr170830-4-p'-Br-Cl-cw
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

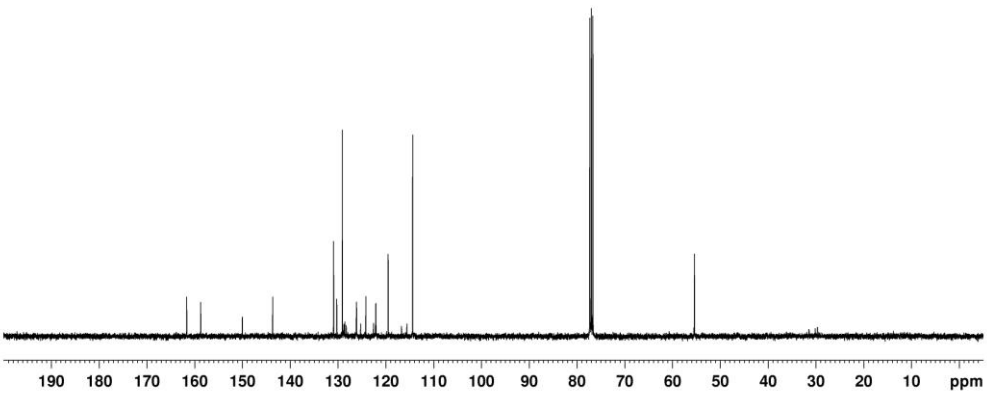


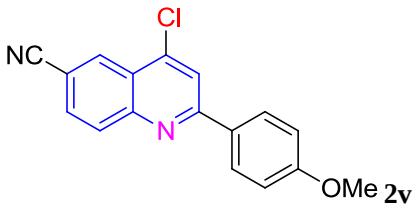
2u

sxr170726-5-p'-CF3-cw-Cl

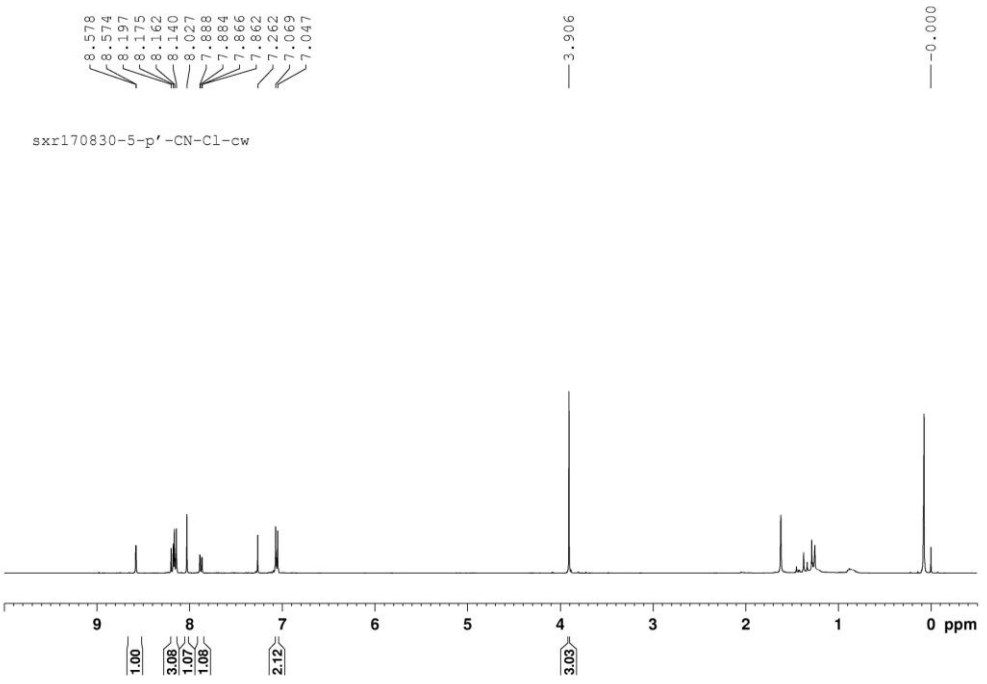


sxr170726-5-p'-CF3-cw-Cl




Cl
NC
N
OMe

2v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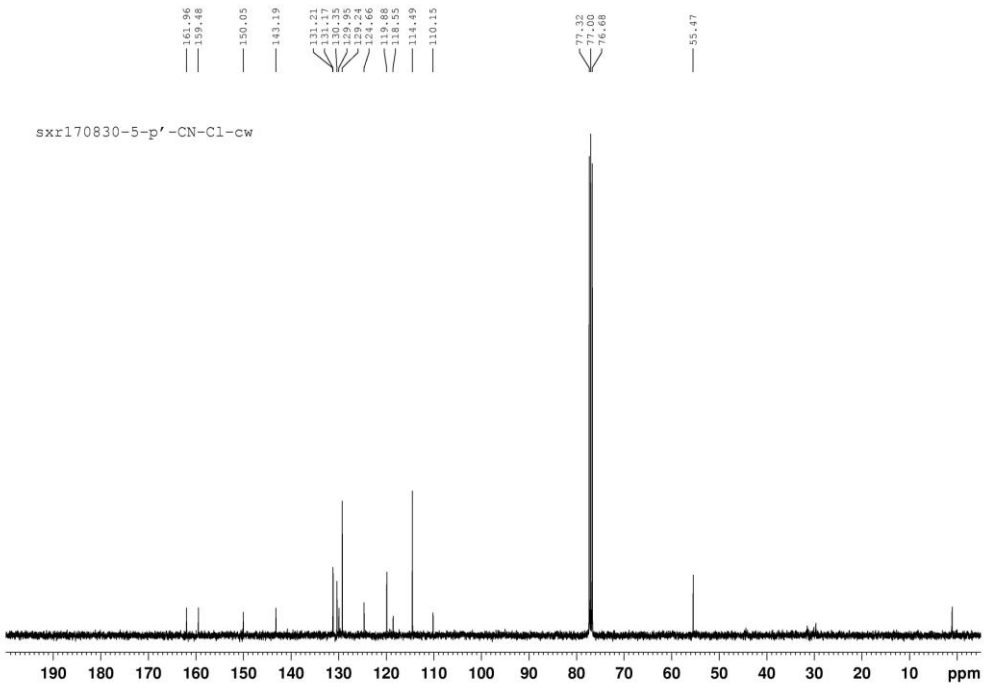
8.027
7.888
7.884
7.866
7.862
7.262
7.069
7.047
3.906
-0.000
sxr170830-5-p'-CN-Cl-cw
9
8
7
6
5
4
3
2
1
0 ppm
1.00
3.08
1.07
1.08
2.12
3.03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143.19
131.21
131.17
130.35
129.95
129.24
124.66
119.88
118.55
114.49
110.15
77.32
77.00
76.68
55.47
sxr170830-5-p'-CN-Cl-cw
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150
140
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120
110
100
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70
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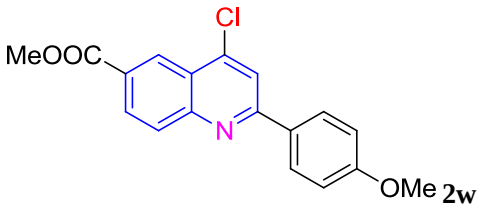
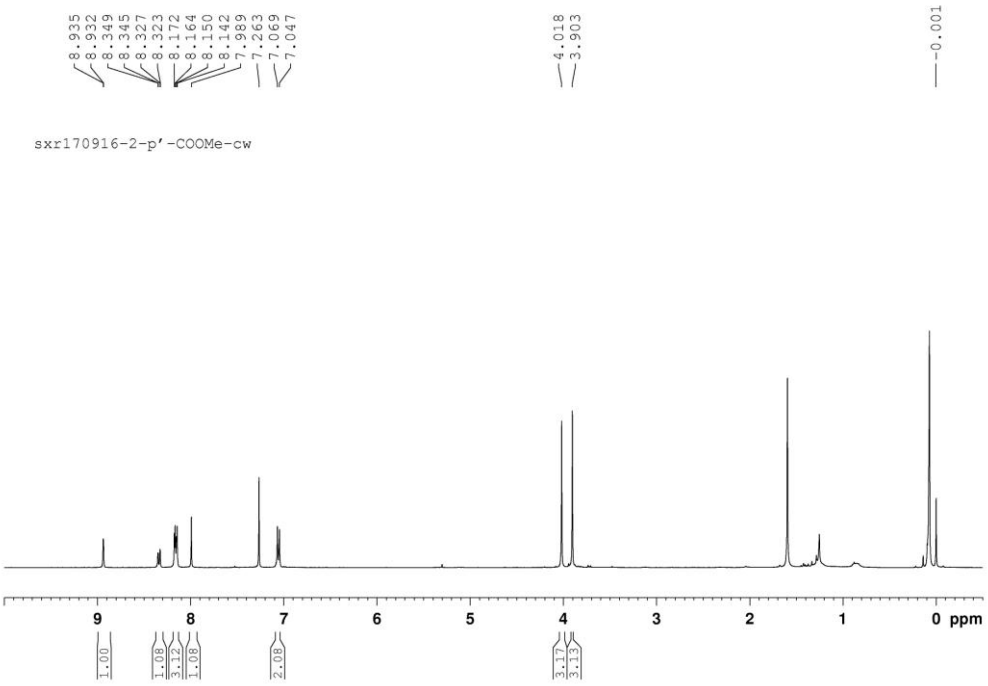
40
30
20
10
ppm


Cl
MeOOC
N
OMe

2w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8.349
8.345
8.327
8.323
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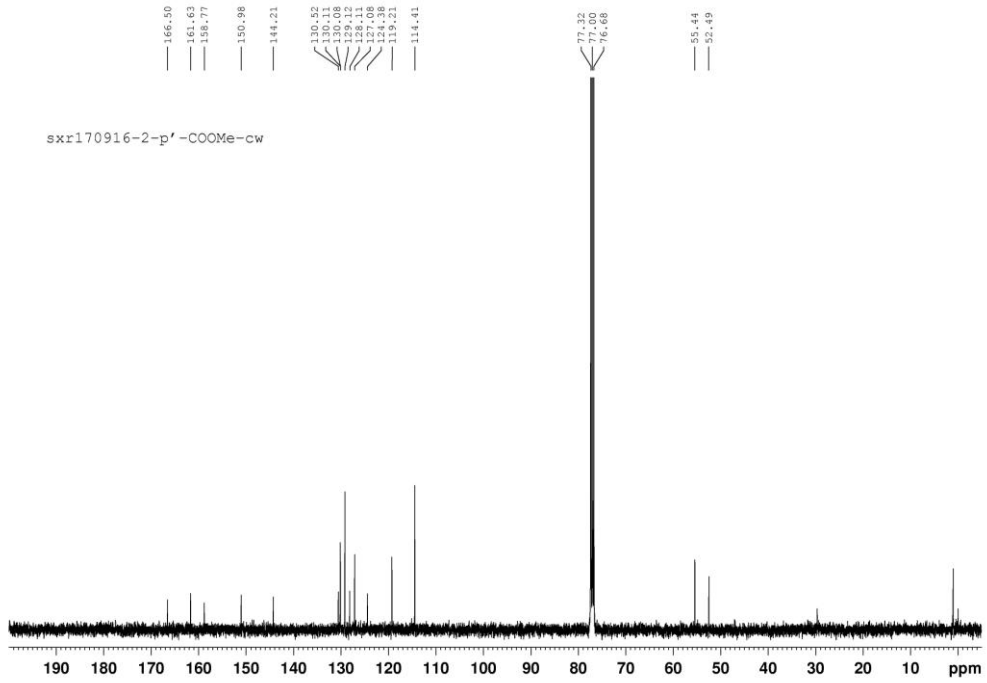
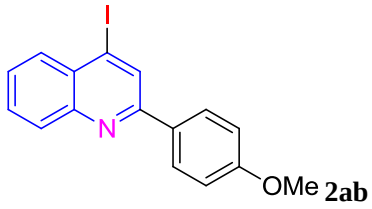
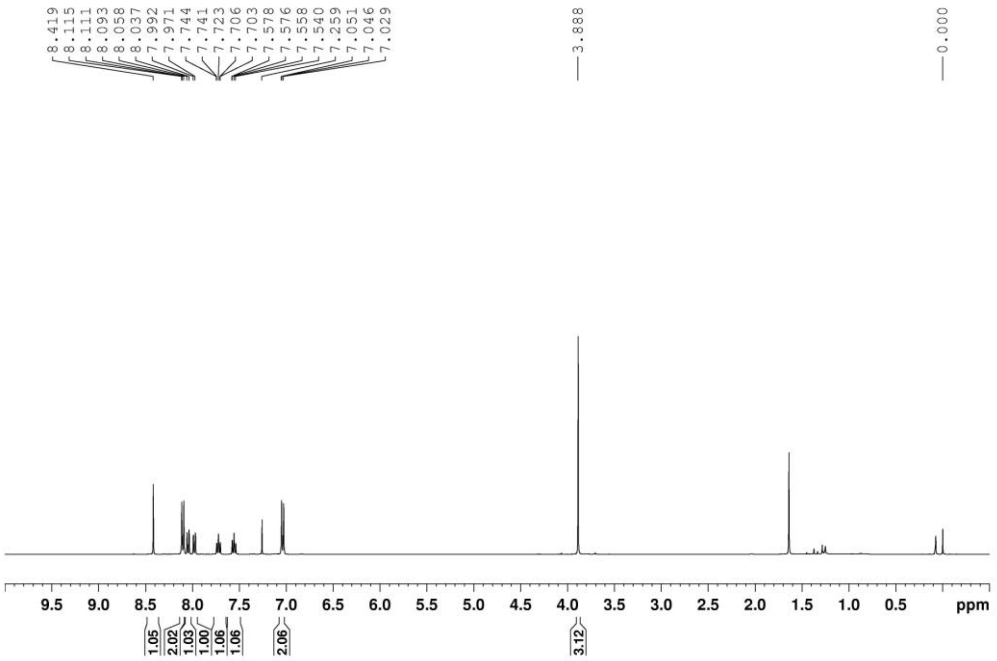
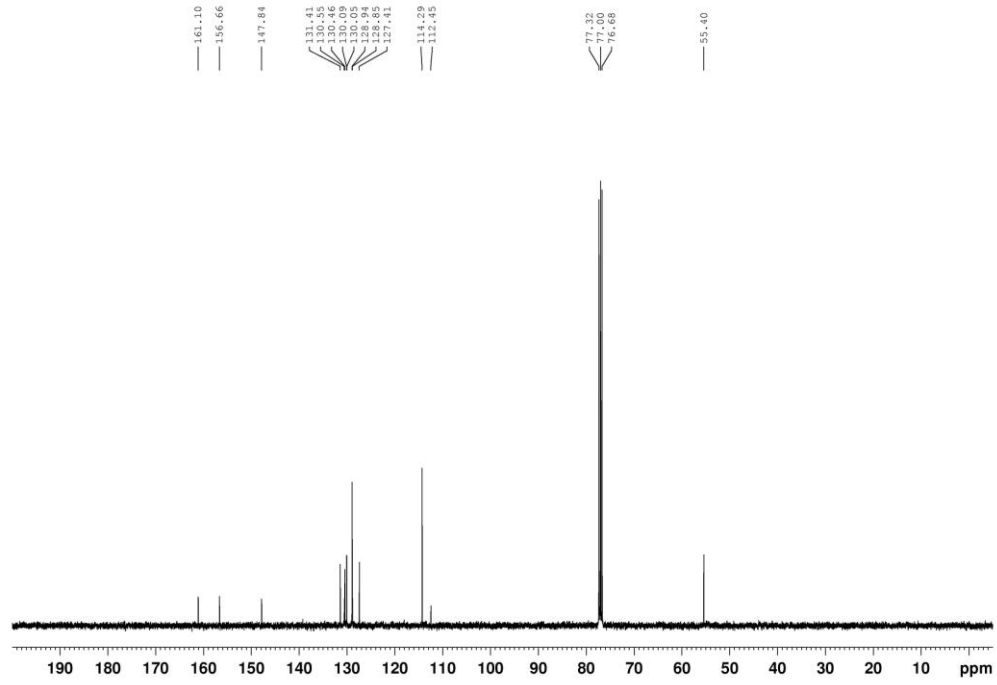
8.164
8.150
8.142
7.989
7.263
7.069
7.047
4.018
3.903
0.001
sxr170916-2-p'-COOMe-cw
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.08
3.12
1.08
2.08
3.17
3.13

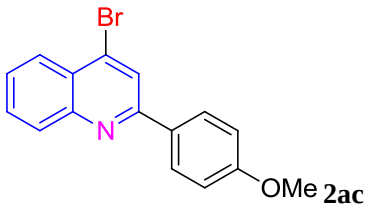

166.50
161.63
158.77
150.98
144.21
130.52
130.11
130.08
129.12
128.11
127.80
124.38
119.21
114.41
77.32
77.00
76.68
55.44
52.49
sxr170916-2-p'-COOMe-cw
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


I
N
OMe

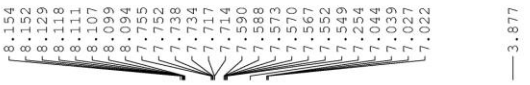
2ab

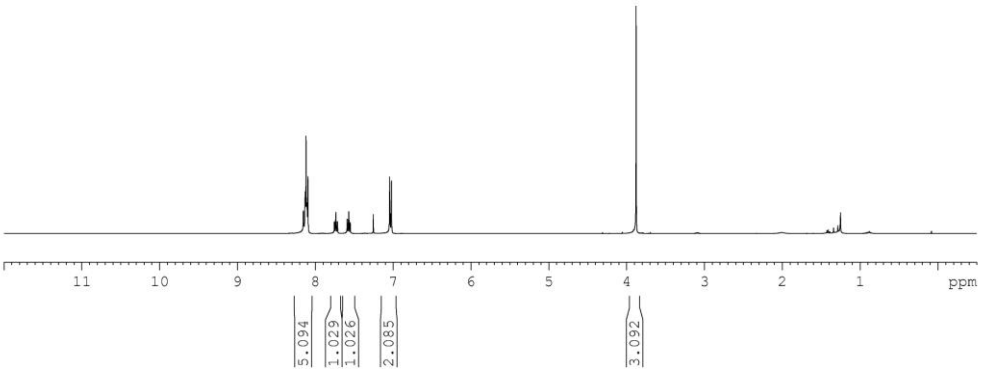

8.419
8.115
8.111
8.093
8.058
8.037
7.992
7.971
7.744
7.741
7.723
7.706
7.703
7.578
7.576
7.558
7.540
7.259
7.051
7.046
7.029
3.888
0.000
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.05
2.02
1.03
1.00
1.06
1.06
2.06
3.12

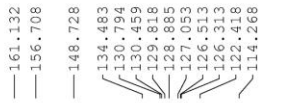

161.10
156.66
147.84
131.41
130.55
130.46
130.09
130.05
128.94
128.85
127.41
114.29
112.45
77.32
77.00
76.68
55.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

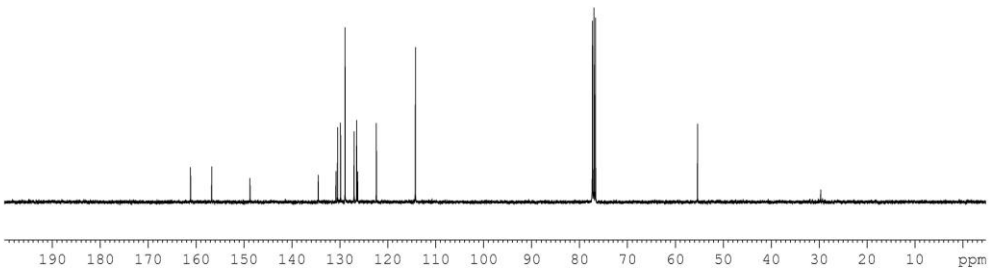

Br
N
OMe

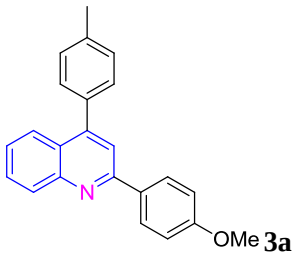
2ac


8.154
8.152
8.129
8.118
8.111
8.107
8.099
8.094
7.755
7.752
7.738
7.734
7.717
7.714
7.590
7.588
7.573
7.570
7.567
7.552
7.549
7.254
7.044
7.039
7.027
7.022
3.877


11
10
9
8
7
6
5
4
3
2
1
ppm
5.094
1.029
1.026
2.085
3.092

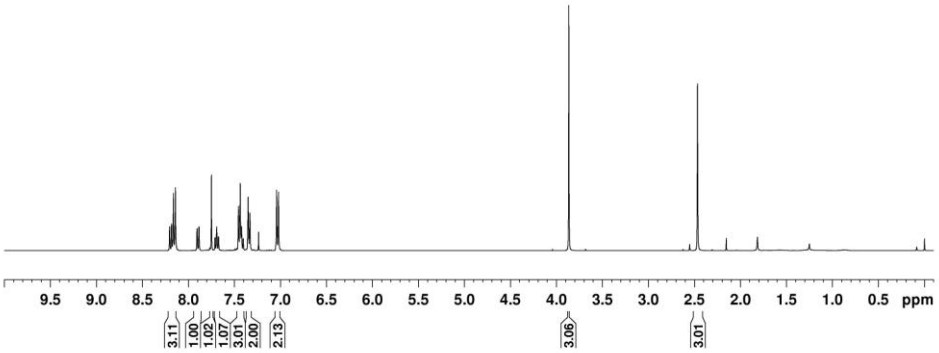

161.132
156.708
148.728
134.483
130.794
130.459
129.818
128.885
127.053
126.513
126.313
122.418
114.268
77.317
76.999
76.681
55.376


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

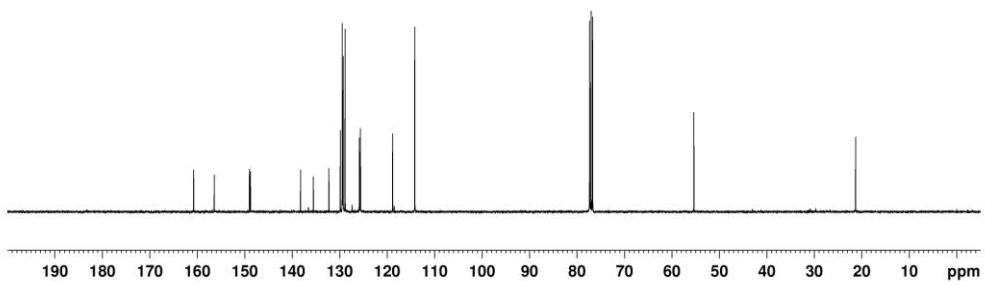


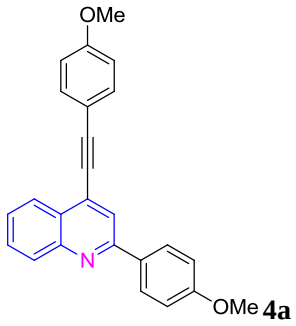
3a

sxr171114-p-Me-bps-cw



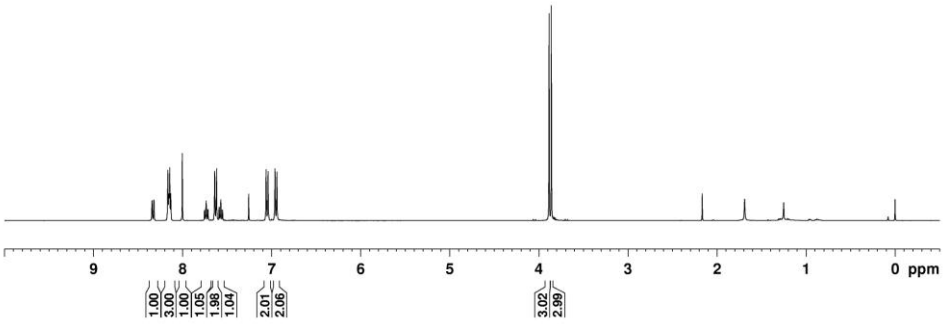
sxr171114-p-Me-bps-cw



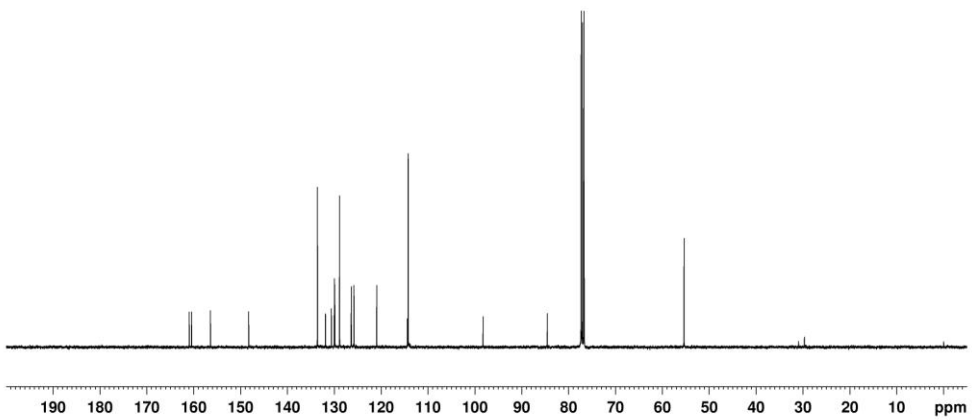

OMe
N
OMe

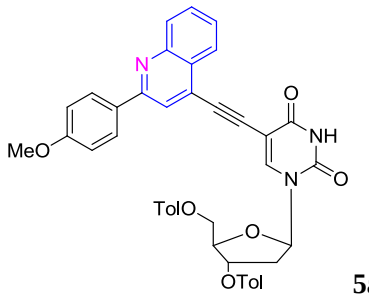
4a


8.338
8.319
8.163
8.150
8.146
8.141
8.130
8.000
7.751
7.748
7.731
7.713
7.710
7.637
7.615
7.587
7.585
7.567
7.549
7.547
7.254
7.059
7.037
6.960
6.938
3.885
3.859
0.000
sxr171114-p-OMe-bps-cw

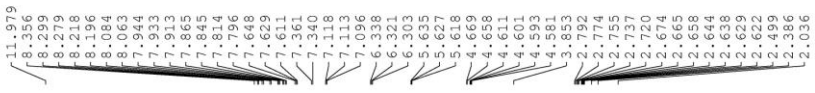

9
8
7
6
5
4
3
2
1
0 ppm
1.00
3.00
1.00
1.05
1.98
1.04
2.01
2.06
3.02
2.99


160.88
160.39
156.36
148.20
133.53
131.79
130.53
129.90
129.83
128.80
126.33
126.29
125.73
120.87
119.40
114.22
114.21
98.24
84.52
77.32
77.00
76.68
55.37
sxr171114-p-OMe-bps-cw


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


N
O
NH
MeO
N
O
TolO
O
OTol

5a


11.979
8.356
8.299
8.279
8.218
8.196
8.084
8.063
7.944
7.933
7.913
7.865
7.845
7.814
7.796
7.648
7.629
7.611
7.361
7.340
7.118
7.113
7.096
6.338
6.321
6.303
5.635
5.627
5.618
4.669
4.658
4.611
4.601
4.593
4.581
3.853
2.792
2.774
2.755
2.737
2.720
2.674
2.665
2.658
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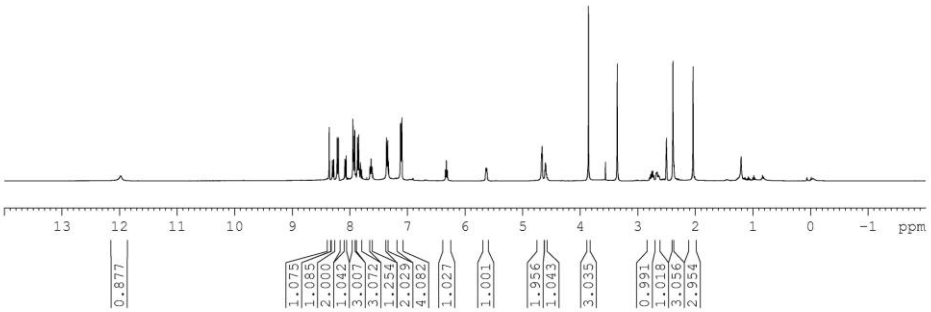
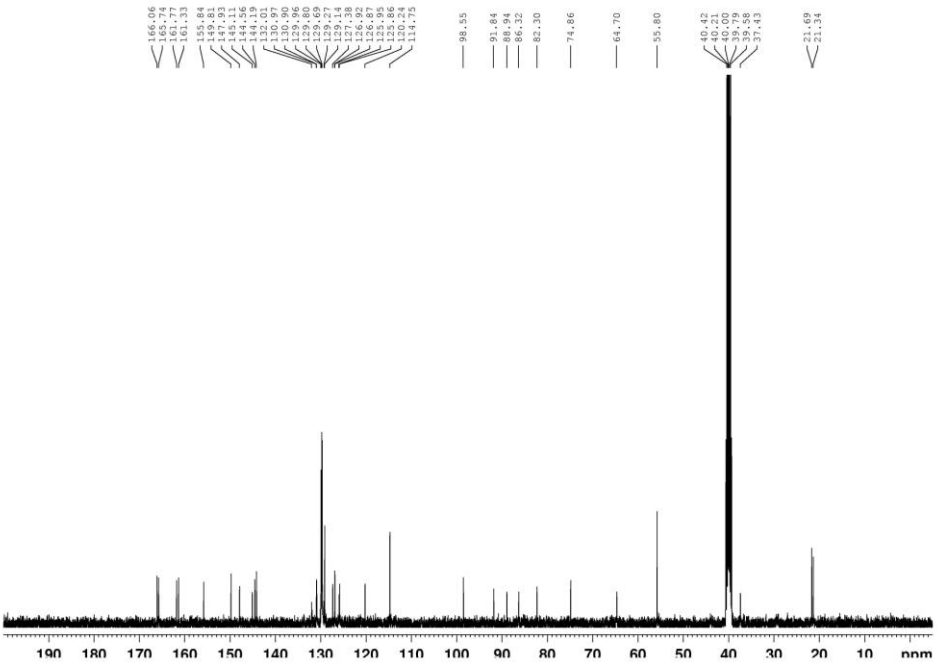
2.629
2.622
2.499
2.386
2.036


13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm
0.877
1.075
1.085
2.000
1.042
3.007
3.072
1.254
2.029
4.082
1.027
1.001
1.956
1.043
3.035
0.991
1.018
3.056
2.954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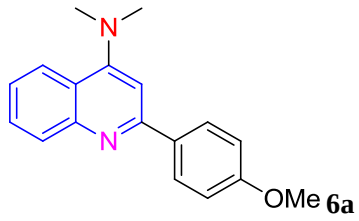
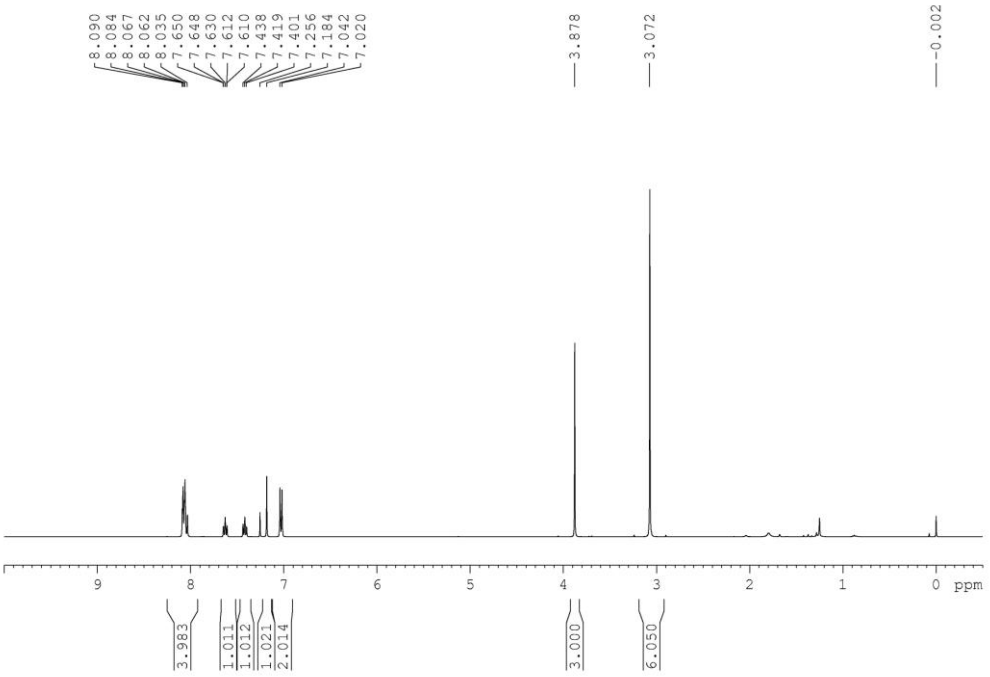
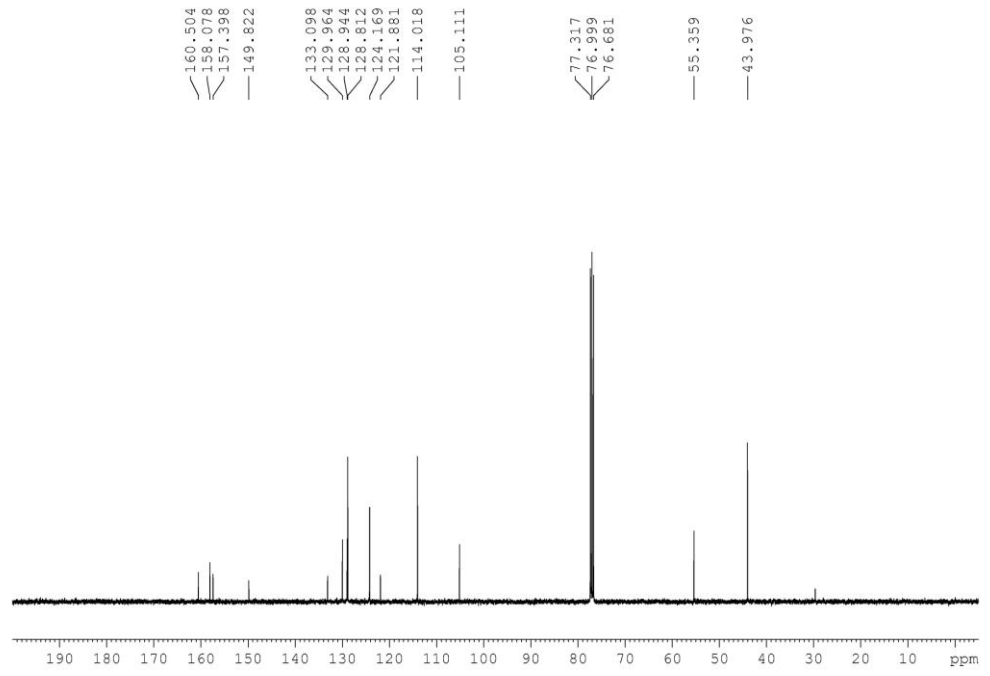
161.33
155.84
149.81
147.93
147.11
144.56
144.19
132.01
130.87
130.90
129.96
129.80
129.69
129.27
129.14
127.38
127.09
126.87
125.95
125.86
125.74
114.75
98.55
91.84
88.94
86.32
82.30
74.86
64.70
55.80
40.42
40.21
40.00
39.79
39.58
37.43
21.69
21.34
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


N
N
OMe

6a


8.090
8.084
8.067
8.062
8.035
7.650
7.648
7.630
7.612
7.610
7.438
7.419
7.401
7.256
7.184
7.042
7.020
3.878
3.072
0.002
9
8
7
6
5
4
3
2
1
0
ppm
3.983
1.011
1.012
1.021
2.014
3.000
6.050


160.504
158.078
157.398
149.822
133.098
129.964
128.944
128.812
124.169
121.881
114.018
105.111
77.317
76.999
76.681
55.359
43.976
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm