Supporting Information

Synthesis of thiocyanato-containing phenanthrenes and dihydronaphthalenes via Lewis acid-activated tandem electrophilic thiocyanation/carbocyclization of alkynes

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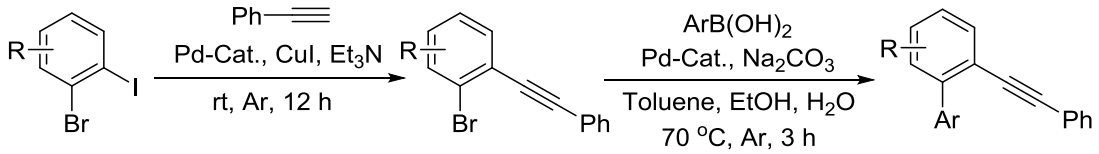
1. General Information

All chemicals were bought from commercial companies and used directly unless noted. The solvents were dried by standard methods when necessary. All reactions monitored by TLC. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were recorded on a Bruker 400 or 700 instrument in $CDCl_3$. All the NMR spectra were referenced to residual $CHCl_3$ (7.26 ppm, ^{1}H; 77.16 ppm, $^{13}C\{^{1}H\}$). Data for ^{1}H NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, q = quartet, septet; coupling constant(s) are in Hz, integration). Data for $^{13}C\{^{1}H\}$ NMR are reported in terms of chemical shift (δ, ppm). The high resolution mass spectrum (HRMS) were recorded on an Agilent (Q-TOF6520) unit with an ESI source. IR spectra were measured on a Shimadzu IRAffinnity-1s spectrometer. Melting points were measured on a binocular microscope XT4A melting point apparatus (uncorrected).

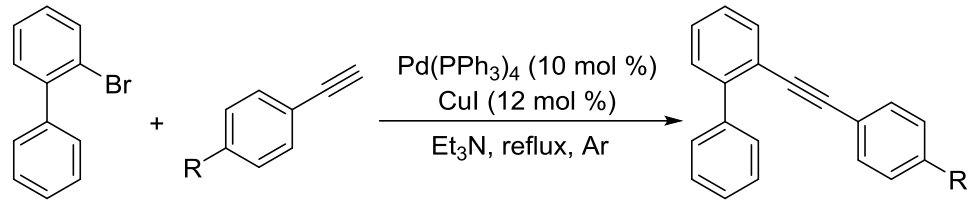
2. Preparation of the Starting Materials

Reagents **2a–d** were synthesized according to our previous works.[1–4] arene–alkynes **1a**,[5–6] **1b–d**,[7] **1e–k**,[5,8] **1l**,[9] **1m**,[10–11] **1n–r**,[5–6] **1s–v**,[5,8] **1w**[7] were synthesized according to the previously reported procedures. The unconjugated arene–alkynes **4a–g**,[12] **4h**,[13] **4i**,[14] **4j**[15] were synthesized following the known literature procedures. Other substrates **6**,[16] **8**,[9] and **10**[8] were prepared according to literature procedures. The slightly modified procedures of **1a–d**, **1n–r**, **1e–k**, **1s–v** and **4a–g** as follows.

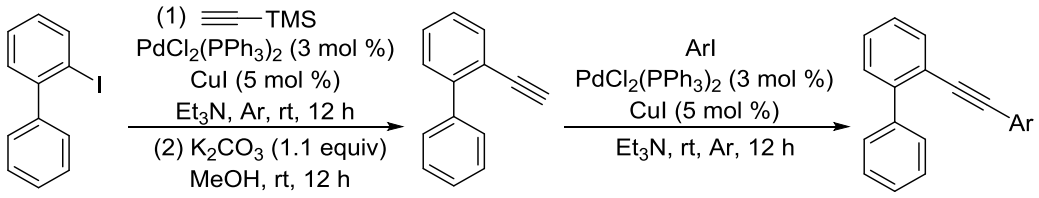


Procedure for the Synthesis of 1a and 1n–r. An oven-dried flask was charged with *o*-bromoiodobenzene (987 mg, 3.5 mmol), $PdCl_2(PPh_3)_2$ (123 mg, 0.175 mmol) and CuI (67 mg, 0.35 mmol). The flask was degassed and filled with argon, then Et_3N (30.0 ml) was added. The mixture was stirred for 15 min before being treated with phenylacetylene (393 mg, 3.85 mmol) dropwise. The resulting solution was stirred at room temperature for 12 h. After the completion of the reaction, the reaction was quenched with sat. NH_4Cl and extracted with ethyl acetate. The combined organic extracts were dried over Na_2SO_4, filtered, and concentrated in vacuo. The crude mixture was purified by flash chromatography using petroleum ether as an eluent. Under an argon atmosphere, to a solution of Na_2CO_3 (424 mg, 4.0 mmol) in toluene (10.0 mL),

ethanol (5.0 mL), and water (5.0 mL) was added the above products (512 mg, 2.0 mmol) at room temperature. Then, to this mixture was added aryl boronic acid (2.6 mmol, 1.3 equiv) and $PdCl_2(PPh_3)_2$ (70 mg, 0.1 mmol), and the resulting solution was heated to 70 ^oC for 3 h. After the completion of the reaction, the solution was cooled to room temperature and extracted with ethyl acetate, the combined organic phased were washed with brine and dried over Na_2SO_4, filtered, and concentrated in vacuo. The residue was purified by flash chromatography (petroleum ether/EtOAc = 100:1, v/v).

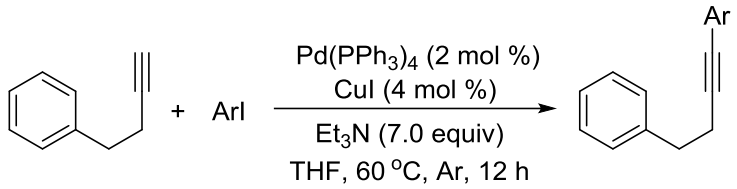


Procedure for the Synthesis of 1b–d. Under an argon atmosphere, 2-bromo-1,1'-biphenyl (466 mg, 2.0 mmol), 4-substituted phenylacetylene (2.2 mmol, 1.1 equiv), $Pd(PPh_3)_4$ (231 mg, 0.2 mmol), CuI (46 mg, 0.24 mmol), and Et_3N (8.0 mL) were added continuously into an oven-dried flask and the resulting mixture was refluxed for 10 h. After the completion of the reaction, it was cooled to room temperature and extracted with ethyl acetate, the combined organic phased were washed with brine and dried over Na_2SO_4, filtered, and concentrated in vacuo. The residue was purified by flash chromatography (petroleum ether/EtOAc = 100:1, v/v).

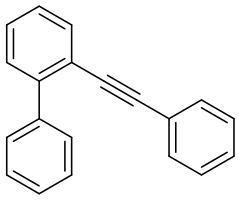


Procedure for the Synthesis of 1e–k and 1s–v. Under an argon atmosphere, 2-iodo-1,1'-biphenyl (1.12 g, 4.0 mmol), $PdCl_2(PPh_3)_2$ (84 mg, 0.12 mmol), and CuI (38 mg, 0.2 mmol) were charged into an oven-dried flask. Then, Et_3N (15.0 mL) was added and the mixture was stirred for 15 min. Subsequently, trimethylsilylacetylene (392 mg, 4.0 mmol) was added dropwise to the mixture and stirred at room temperature for 12 h. The resulting solution was passed through a layer of Celite, then extracted with ethyl acetate, the combined organic phased were washed with brine and dried over Na_2SO_4, filtered, and concentrated in vacuo. The residue was dissolved in MeOH (40.0 mL). K_2CO_3 (607 mg, 4.4 mmol) was added to the mixture and stirred at room temperature for 12 h. After

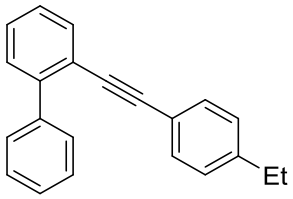
the completion of the reaction, the solid material was removed by filtration. The filtrate was concentrated in vacuo. The crude mixture was purified by flash chromatography using petroleum ether as an eluent. To a solution of aryl iodide (1.0 mmol, 1.0 equiv) and the above products (187 mg, 1.05 mmol) in Et_3N (10.0 mL) were added $PdCl_2(PPh_3)_2$ (21 mg, 0.03 mmol) and CuI (9.5 mg, 0.05 mmol). The mixture was then stirred under an argon atmosphere at room temperature for 12 h. After the completion of the reaction, the reaction was quenched with sat. NH_4Cl and extracted with ethyl acetate. The combined organic extracts were washed with brine and dried over Na_2SO_4, filtered, and concentrated in vacuo. The residue was purified by flash chromatography (petroleum ether/EtOAc = 100:1 to 50:1, v/v).



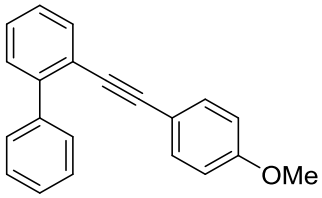
Procedure for the Synthesis of 4a–g. An oven-dried flask was charged with $Pd(PPh_3)_4$ (23 mg, 0.02 mmol), CuI (7.6 mg, 0.04 mmol) and THF (3.0 mL) under an argon atmosphere, and the mixture was stirred for 5 min. Then aryl iodide (1.0 mmol, 1.0 equiv) and Et_3N (707 mg, 7.0 mmol) were added and stirred for 5 min. Subsequently, 4-phenyl-1-butyne (143 mg, 1.1 mmol) was added dropwise and the solution was heated to 60 °C for 12 h. After the completion of the reaction, the solution was cooled to room temperature and extracted with ethyl acetate, the combined organic phased were washed with brine and dried over Na_2SO_4, filtered, and concentrated in vacuo. The residue was purified by flash chromatography using petroleum ether as an eluent.



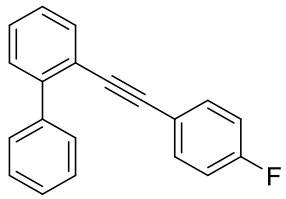
2-(Phenylethynyl)-1,1'-biphenyl (1a).[5] Yellow oil; 396 mg, 78% yield; ^1H NMR (400 MHz, $CDCl_3$) δ 7.70–7.66 (m, 3H), 7.49–7.39 (m, 5H), 7.37–7.29 (m, 6H).



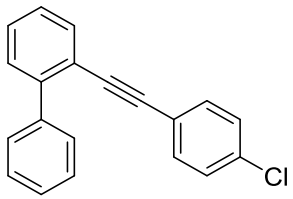
2-((4-Ethylphenyl)ethynyl)-1,1'-biphenyl (1b).[7] Yellow oil; 180 mg, 32% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69–7.64 (m, 3H), 7.48–7.37 (m, 5H), 7.33 (td, J = 7.2, 1.6 Hz, 1H), 7.26 (d, J = 8.0 Hz, 2H), 7.13 (d, J = 8.0 Hz, 2H), 2.64 (q, J = 7.6 Hz, 2H), 1.22 (t, J = 7.6 Hz, 3H).



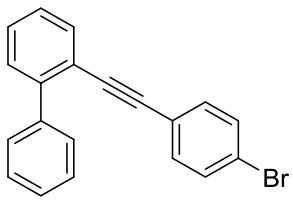
2-((4-Methoxyphenyl)ethynyl)-1,1'-biphenyl (1c).[7] Yellow oil; 310 mg, 55% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 7.2 Hz, 2H), 7.63 (d, J = 7.6 Hz, 1H), 7.46 (t, J = 7.2 Hz, 2H), 7.42–7.36 (m, 3H), 7.33 (td, J = 7.2, 1.6 Hz, 1H), 7.27 (d, J = 9.2 Hz, 2H), 6.82 (d, J = 8.8 Hz, 2H), 3.80 (s, 3H).



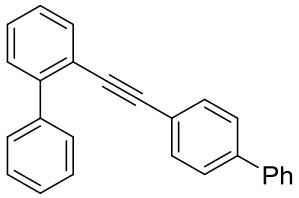
2-((4-Fluorophenyl)ethynyl)-1,1'-biphenyl (1d).[8] Yellow oil; 228 mg, 42% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (t, J = 7.2 Hz, 3H), 7.49–7.39 (m, 5H), 7.36–7.29 (m, 3H), 6.99 (t, J = 8.8 Hz, 2H).



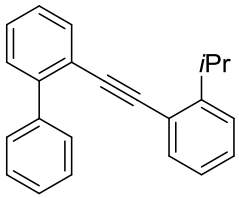
2-((4-Chlorophenyl)ethynyl)-1,1'-biphenyl (1e).[7] Yellow oil; 247 mg, 86% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65–7.62 (m, 3H), 7.46–7.37 (m, 5H), 7.32 (td, J = 7.2, 2.0 Hz, 1H), 7.23 (dd, J = 11.6, 8.8 Hz, 4H).



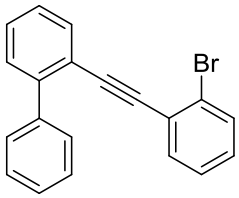
2-((4-Bromophenyl)ethynyl)-1,1'-biphenyl (1f).[7] Colorless oil; 265 mg, 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, J = 7.2 Hz, 3H), 7.48–7.39 (m, 7H), 7.34 (td, J = 7.6, 2.0 Hz, 1H), 7.18 (d, J = 8.4 Hz, 2H).



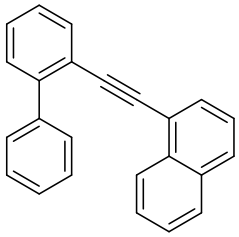
2-([1,1'-Biphenyl]-4-ylethynyl)-1,1'-biphenyl (1g).[7] White solid; 214 mg, 65% yield; mp: 64–66 °C (lit. 94.1–95.3 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (t, J = 7.2 Hz, 3H), 7.60–7.34 (m, 15H).



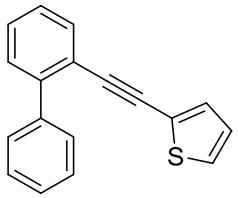
2-((2-Isopropylphenyl)ethynyl)-1,1'-biphenyl (1h). Colorless oil; 257 mg, 87% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69–7.63 (m, 3H), 7.47–7.34 (m, 7H), 7.27–7.22 (m, 2H), 7.11 (td, J = 7.2, 1.6 Hz, 1H), 3.21 (septet, J = 6.9 Hz, 1H), 1.15 (d, J = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.5, 143.8, 140.8, 133.0, 132.3, 129.6, 129.4, 128.5, 128.3, 128.0, 127.4, 127.1, 125.4, 124.8, 122.2, 122.2, 92.7, 91.1, 31.4, 23.1; IR (KBr, cm^{-1}) 3059, 2961, 2866, 2212, 1952, 1595, 1474, 1362, 1078; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{23}H_{21}$ 297.1638, found 297.1641.



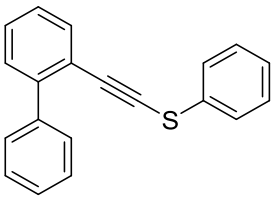
2-((2-Bromophenyl)ethynyl)-1,1'-biphenyl (1i).[17] Colorless oil; 268 mg, 81% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 7.6 Hz, 1H), 7.69 (d, J = 7.2 Hz, 2H), 7.56 (d, J = 8.0 Hz, 1H), 7.48–7.32 (m, 7H), 7.22 (t, J = 7.0 Hz, 1H), 7.13 (td, J = 8.0, 1.6 Hz, 1H).



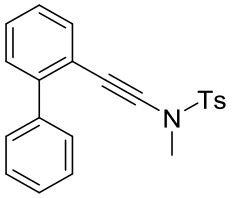
1-([1,1'-Biphenyl]-2-ylethynyl)naphthalene (1j).[8] Colorless oil; 257 mg, 85% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, J = 8.4 Hz, 1H), 7.81 (t, J = 8.4 Hz, 3H), 7.72 (d, J = 6.8 Hz, 2H), 7.62 (d, J = 7.2 Hz, 1H), 7.53–7.38 (m, 9H).



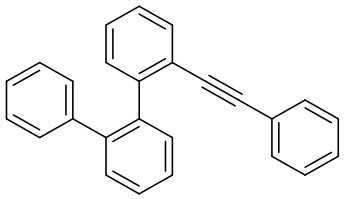
2-([1,1'-Biphenyl]-2-ylethynyl)thiophene (1k).[8] Colorless oil; 187 mg, 72% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67–7.62 (m, 3H), 7.48–7.39 (m, 5H), 7.33 (td, J = 7.2, 1.6 Hz, 1H), 7.24 (dd, J = 5.2, 1.2 Hz, 1H), 7.11 (d, J = 3.6 Hz, 1H), 6.96 (dd, J = 5.2, 3.6 Hz, 1H).



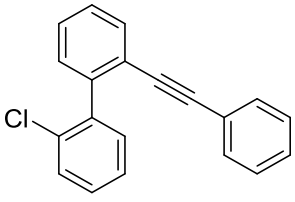
([1,1'-Biphenyl]-2-ylethynyl)(phenyl)sulfane (1l).[9] Yellow oil; 285 mg, 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, J = 8.0 Hz, 3H), 7.46–7.38 (m, 5H), 7.36–7.32 (m, 1H), 7.25–7.17 (m, 5H).



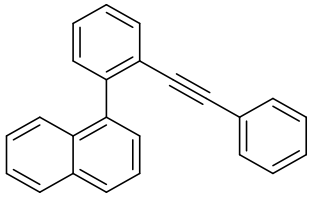
***N*-([1,1'-Biphenyl]-2-ylethynyl)-*N*,4-dimethylbenzenesulfonamide (1m).**[11] Yellow oil; 368 mg, 68% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, J = 7.2 Hz, 2H), 7.51 (d, J = 8.4 Hz, 2H), 7.46 (d, J = 8.4 Hz, 1H), 7.41 (t, J = 7.2 Hz, 2H), 7.36–7.26 (m, 4H), 7.21 (d, J = 8.0 Hz, 2H), 2.98 (s, 3H), 2.40 (s, 3H).



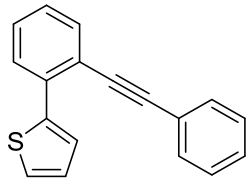
2-(Phenylethynyl)-1,1':2',1''-terphenyl (1n).[7] Yellow solid; 459 mg, 70% yield; mp: 75–76 °C (lit. 77.7–78.0 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51–7.40 (m, 5H), 7.25–7.14 (m, 12H), 7.08 (d, J = 8.0 Hz, 1H).



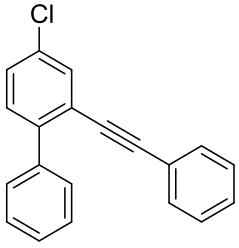
2-Chloro-2'-(phenylethynyl)-1,1'-biphenyl (1o). Yellow oil; 430 mg, 75% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (dd, J = 6.2, 2.7 Hz, 1H), 7.51–7.49 (ddd, J = 8.1, 6.7, 3.8 Hz, 1H), 7.42–7.37 (m, 3H), 7.35–7.32 (m, 3H), 7.24–7.21 (m, 3H), 7.18–7.16 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.1, 139.7, 133.5, 131.8, 131.7, 131.4, 129.8, 129.4, 128.9, 128.2, 128.1, 128.0, 127.8, 126.3, 123.3, 123.1, 92.7, 88.5; IR (KBr, cm^{-1}) 3059, 2924, 2853, 2218, 1923, 1809, 1697, 1597, 1497, 1437, 1070, 1036; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{20}H_{14}Cl$ 289.0779, found 289.0779.



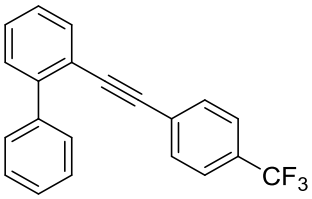
1-(2-(Phenylethynyl)phenyl)naphthalene (1p).[20] Brown oil; 490 mg, 81% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (t, J = 8.2 Hz, 2H), 7.73 (t, J = 8.0 Hz, 2H), 7.58 (t, J = 7.4 Hz, 1H), 7.54–7.41 (m, 6H), 7.19–7.10 (m, 3H), 6.81 (d, J = 8.0 Hz, 2H).



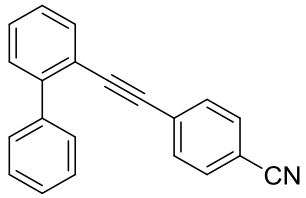
2-(2-(Phenylethynyl)phenyl)thiophene (1q).[20] Yellow oil; 379 mg, 73% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66–7.60 (m, 3H), 7.53–7.51 (m, 2H), 7.40–7.35 (m, 5H), 7.29 (td, J = 7.2, 1.2 Hz, 1H), 7.14 (dd, J = 4.8, 3.6 Hz, 1H).



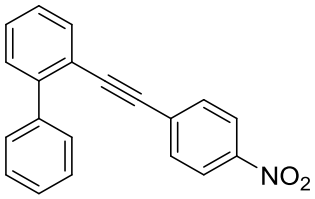
4-Chloro-2-(phenylethynyl)-1,1'-biphenyl (1r).[7] Yellow oil; 402 mg, 70% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, J = 6.0 Hz, 3H), 7.50–7.40 (m, 3H), 7.37 (s, 2H), 7.36–7.32 (m, 5H).



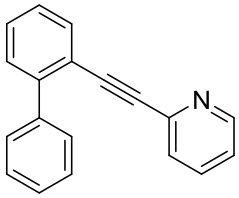
2-((4-(Trifluoromethyl)phenyl)ethynyl)-1,1'-biphenyl (1s).[8] Colorless oil; 270 mg, 84% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (t, J = 6.4 Hz, 3H), 7.56 (d, J = 8.4 Hz, 2H), 7.51–7.41 (m, 7H), 7.39–7.35 (m, 1H).



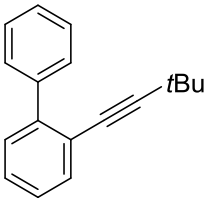
4-([1,1'-Biphenyl]-2-ylethynyl)benzonitrile (1t).[8] White solid; 220 mg, 79% yield; mp: 79–80 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, J = 7.6 Hz, 1H), 7.62 (d, J = 6.8 Hz, 2H), 7.56 (d, J = 8.8 Hz, 2H), 7.49–7.36 (m, 8H).



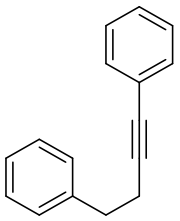
2-((4-Nitrophenyl)ethynyl)-1,1'-biphenyl (1u).[7] Yellow solid; 248 mg, 83% yield; mp: 99–100 °C (lit. 100–101 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, J = 8.8 Hz, 2H), 7.67 (d, J = 7.6 Hz, 1H), 7.63 (d, J = 6.8 Hz, 2H), 7.50–7.36 (m, 8H).



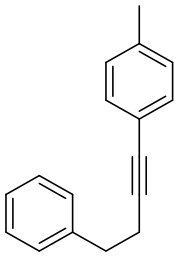
2-([1,1'-Biphenyl]-2-ylethynyl)pyridine (1v).[18] Yellow oil; 158 mg, 62% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, J = 4.4 Hz, 1H), 7.75 (d, J = 7.6 Hz, 1H), 7.67 (d, J = 6.8 Hz, 2H), 7.58 (t, J = 7.8 Hz, 1H), 7.48–7.33 (m, 6H), 7.18 (d, J = 8.0 Hz, 2H).



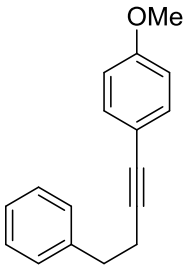
2-(3,3-Dimethylbut-1-yn-1-yl)-1,1'-biphenyl (1w).[7] Colorless oil; 252 mg, 60% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, J = 6.2 Hz, 2H), 7.48 (d, J = 6.1 Hz, 1H), 7.40–7.23 (m, 6H), 1.17 (s, 9H).



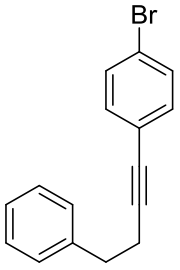
But-1-yne-1,4-diyldibenzene (4a).[12] Colorless oil; 195 mg, 95% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38–7.36 (m, 2H), 7.33–7.22 (m, 8H), 2.92 (t, J = 7.6 Hz, 2H), 2.69 (t, J = 7.6 Hz, 2H).



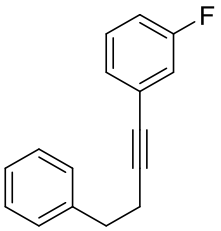
1-Methyl-4-(4-phenylbut-1-yn-1-yl)benzene (4b).[19] Colorless oil; 202 mg, 92% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37–7.28 (m, 7H), 7.12 (d, J = 8.0 Hz, 2H), 2.96 (t, J = 7.6 Hz, 2H), 2.72 (t, J = 7.6 Hz, 2H), 2.36 (s, 3H).



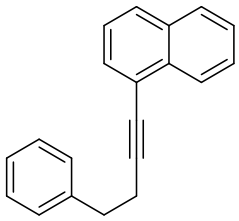
1-Methoxy-4-(4-phenylbut-1-yn-1-yl)benzene (4c).[12] Yellow oil; 219 mg, 93% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34–7.23 (m, 7H), 6.82 (d, J = 9.2 Hz, 2H), 3.80 (s, 3H), 2.93 (t, J = 7.6 Hz, 2H), 2.69 (t, J = 7.6 Hz, 2H).



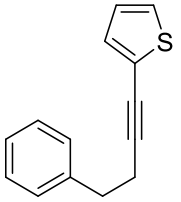
1-Bromo-4-(4-phenylbut-1-yn-1-yl)benzene (4d).[19] Colorless oil; 235 mg, 83% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, J = 8.4 Hz, 2H), 7.33–7.20 (m, 7H), 2.91 (t, J = 7.6 Hz, 2H), 2.68 (t, J = 7.6 Hz, 2H).



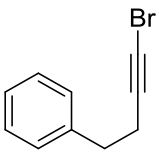
1-Fluoro-3-(4-phenylbut-1-yn-1-yl)benzene (4e).[19] Colorless oil; 179 mg, 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31–7.15 (m, 6H), 7.12 (d, J = 6.8 Hz, 1H), 7.04 (d, J = 8.8 Hz, 1H), 6.95–6.92 (m, 1H), 2.89 (t, J = 7.6 Hz, 2H), 2.66 (t, J = 7.6 Hz, 2H).



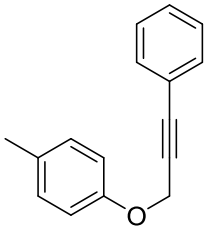
1-(4-Phenylbut-1-yn-1-yl)naphthalene (4f).[12] White solid; 220 mg, 86% yield; mp: 45–46 °C (lit. 49–51 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18–8.16 (m, 1H), 7.84–7.81 (m, 1H), 7.78 (d, J = 8.0 Hz, 1H), 7.60 (d, J = 7.2 Hz, 1H), 7.51–7.49 (m, 2H), 7.39 (t, J = 7.6 Hz, 1H), 7.36 (d, J = 4.4 Hz, 4H), 7.28 (t, J = 4.2 Hz, 1H), 3.04 (t, J = 7.2 Hz, 2H), 2.89 (t, J = 7.2 Hz, 2H).



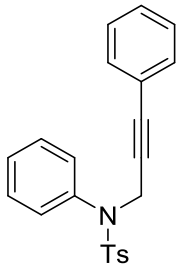
2-(4-Phenylbut-1-yn-1-yl)thiophene (4g).[12] Yellow oil; 169 mg, 80% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32–7.20 (m, 5H), 7.15 (dd, J = 5.2, 0.8 Hz, 1H), 7.10 (d, J = 3.2 Hz, 1H), 6.92 (dd, J = 5.2, 3.8 Hz, 1H), 2.91 (t, J = 7.6 Hz, 2H), 2.70 (t, J = 7.6 Hz, 2H).



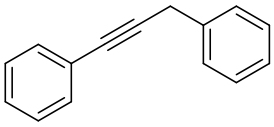
(4-Bromobut-3-yn-1-yl)benzene (4h).[13] Colorless oil; 197 mg, 95% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (t, J = 7.2 Hz, 2H), 7.23–7.18 (m, 3H), 2.82 (t, J = 7.6 Hz, 2H), 2.48 (t, J = 7.6 Hz, 2H).



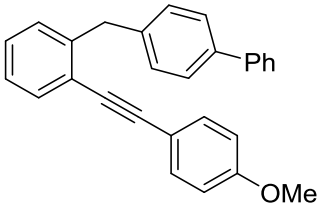
1-Methyl-4-((3-phenylprop-2-yn-1-yl)oxy)benzene (4i).[14] White solid; 362 mg, 82% yield; mp: 59–60 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46–7.44 (m, 2H), 7.32–7.31 (m, 3H), 7.13 (d, J = 8.4 Hz, 2H), 6.95 (d, J = 8.8 Hz, 2H), 4.90 (s, 2H), 2.32 (s, 3H).



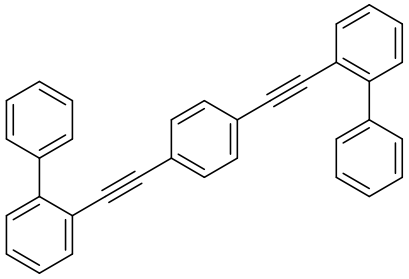
4-Methyl-*N*-phenyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (4j).[13] White solid; 524 mg, 73% yield; mp: 90–91 °C (lit. 90–92 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, J = 8.4 Hz, 2H), 7.32 (s, 5H), 7.30–7.23 (m, 3H), 7.19–7.16 (m, 4H), 4.66 (s, 2H), 2.36 (s, 3H).



Prop-1-yne-1,3-diyldibenzene (6).[16] Colorless oil; 326 mg, 85% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46–7.41 (m, 4H), 7.35–7.23 (m, 6H), 3.83 (s, 2H).

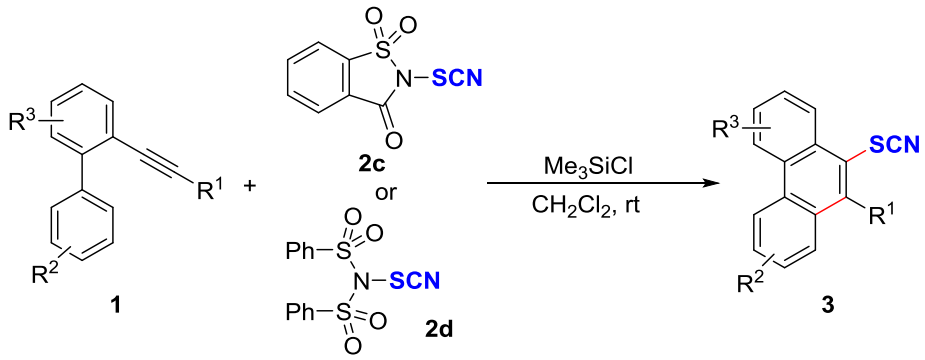


4-(2-((4-Methoxyphenyl)ethynyl)benzyl)-1,1'-biphenyl (8).[9] White solid; 386 mg, 74% yield; mp: 94–95 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57–7.50 (m, 5H), 7.43–7.39 (m, 4H), 7.35–7.29 (m, 3H), 7.25–7.18 (m, 3H). 6.86 (d, J = 8.9 Hz, 2H), 4.27 (s, 2H), 3.81 (s, 3H).

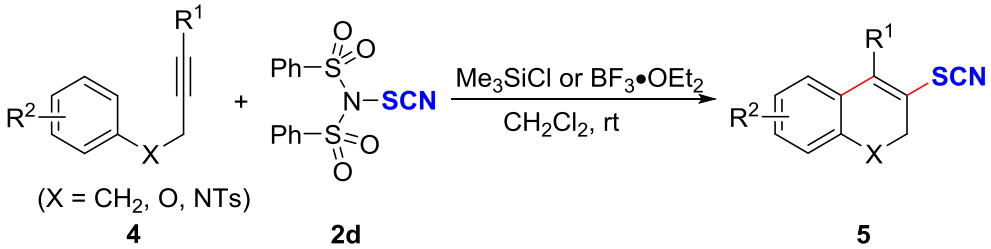


1,4-Bis([1,1'-biphenyl]-2-ylethynyl)benzene (10).[8] Yellow solid; 165 mg, 77% yield; mp: 159–160 °C (lit. 163–164 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66–7.62 (m, 6H), 7.47–7.39 (m, 10H), 7.35–7.31 (m, 2H), 7.22 (s, 4H).

3. General procedure for the synthesis of the desired products

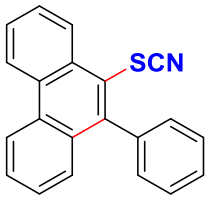


General Procedure for the Synthesis of 3. To a 25 mL Schlenk tube containing **1** (0.1 mmol, 1.0 equiv) was added CH_2Cl_2 (1.0 mL) under an argon atmosphere. Then, **2c** (0.2 mmol, 2.0 equiv) or **2d** (0.3 mmol, 3.0 equiv) was added. Subsequently, the mixture was added acid and stirred at room temperature for an appropriate time. When the reaction was completed, the product was purified by column chromatography on silica gel with petroleum ether/ethyl acetate to afford the product **3**.

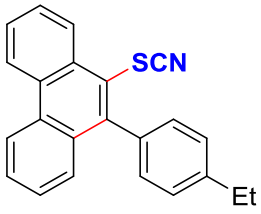


General Procedure for the Synthesis of 5 and 9. To a 25 mL Schlenk tube containing **4** and **8** (0.1 mmol, 1.0 equiv) was added dichloromethane (1.0 mL) under an argon atmosphere. Then **2d** (0.3 mmol, 3.0 equiv) was added. Subsequently, the mixture was added acid (0.12 mmol, 1.2 equiv) and stirred at room temperature for an appropriate time. When the reaction was completed, the product was purified by column chromatography on silica gel with petroleum ether/ethyl acetate to afford the

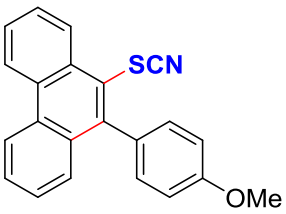
products **5** and **9**.



9-Phenyl-10-thiocyanatophenanthrene (3a). White solid; 28.3 mg, 91% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.40; mp: 211–212 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 (d, J = 7.6 Hz, 1H), 8.77 (d, J = 8.4 Hz, 1H), 8.64 (d, J = 7.6 Hz, 1H), 7.85–7.73 (m, 3H), 7.61–7.48 (m, 5H), 7.38 (d, J = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.6, 139.0, 131.8, 131.5, 131.2, 130.4, 129.7, 129.1, 128.8, 128.6, 128.4, 128.3, 127.9, 127.3, 126.8, 123.2, 122.8, 119.4, 111.3 (SCN); IR (KBr, cm^{-1}) 2995, 2151 (SCN), 1647, 1508, 1456; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{14}NS$ 312.0841, found 312.0847.

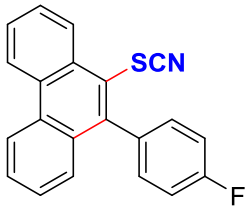


9-(4-Ethylphenyl)-10-thiocyanatophenanthrene (3b). White solid; 32.2 mg, 95% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.40; mp: 126–127 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, J = 8.4 Hz, 1H), 8.67 (d, J = 8.4 Hz, 1H), 8.55 (d, J = 7.6 Hz, 1H), 7.75–7.63 (m, 3H), 7.45–7.40 (m, 2H), 7.33 (d, J = 8.0 Hz, 2H), 7.19 (d, J = 8.0 Hz, 2H), 2.74 (q, J = 7.6 Hz, 2H), 1.30 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.8, 144.4, 136.2, 132.0, 131.5, 131.2, 130.5, 129.7, 129.2, 128.8, 128.2, 128.1, 127.8, 127.2, 126.8, 123.2, 122.7, 119.5, 111.4 (SCN), 28.8, 15.4; IR (KBr, cm^{-1}) 2961, 2924, 2149 (SCN), 1645, 1531, 1456; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{23}H_{18}NS$ 340.1154, found 340.1151.

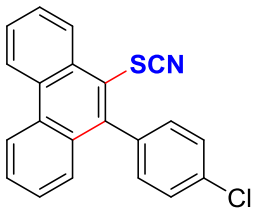


9-(4-Methoxyphenyl)-10-thiocyanatophenanthrene (3c). White solid; 33.0 mg, 97% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.20; mp: 182–183 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, J = 7.6 Hz, 1H), 8.76 (d, J = 8.4 Hz, 1H), 8.63 (d, J = 7.6 Hz, 1H), 7.83–7.71 (m, 3H), 7.56–7.49 (m, 2H), 7.29 (d, J = 8.8 Hz, 2H), 7.11 (d, J = 8.8

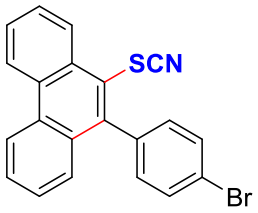
Hz, 2H), 3.94 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 159.6, 147.4, 132.2, 131.5, 131.2, 131.2, 131.0, 130.5, 129.2, 128.8, 128.3, 127.8, 127.3, 126.9, 123.2, 122.8, 119.9, 114.0, 111.4 (SCN), 55.4; IR (KBr, cm^{-1}) 3061, 2928, 2837, 2154 (SCN), 1605, 1508, 1460, 1252, 1175, 1030; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{22}H_{16}NOS$ 342.0947, found 342.0943.



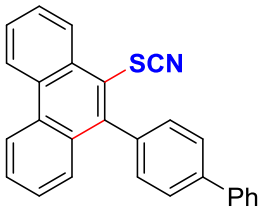
9-(4-Fluorophenyl)-10-thiocyanatophenanthrene (3d). Yellow solid; 26.9 mg, 82% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.38; mp: 212–213 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82–8.77 (m, 2H), 8.65–8.63 (m, 1H), 7.85–7.74 (m, 3H), 7.54 (t, J = 7.4 Hz, 1H), 7.47 (d, J = 8.0 Hz, 1H), 7.37–7.34 (m, 2H), 7.29 (t, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.7 (d, J = 248.1 Hz), 146.6, 134.8 (d, J = 3.6 Hz), 131.8, 131.6, 131.5 (d, J = 8.1 Hz), 131.2, 130.3, 129.0, 128.9, 128.4, 128.1, 127.4, 126.9, 123.2, 122.9, 119.9, 115.8 (d, J = 21.7 Hz), 111.1 (SCN); IR (KBr, cm^{-1}) 3065, 2154 (SCN), 1697, 1506, 1456, 1339; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{13}FNS$ 330.0747, found 330.0748.



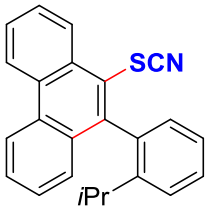
9-(4-Chlorophenyl)-10-thiocyanatophenanthrene (3e). Yellow solid; 19.0 mg, 55% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.38; mp: 185–186 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82–8.77 (m, 2H), 8.66–8.63 (m, 1H), 7.85–7.75 (m, 3H), 7.59–7.52 (m, 3H), 7.46 (dd, J = 8.0, 0.8 Hz, 1H), 7.33 (d, J = 8.4 Hz, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 146.4, 137.3, 134.6, 131.6, 131.5, 131.3, 131.1, 130.3, 129.0, 129.0, 128.8, 128.4, 128.1, 127.5, 126.9, 123.3, 122.9, 119.7, 111.0 (SCN); IR (KBr, cm^{-1}) 2922, 2153 (SCN), 1682, 1487, 1393; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{13}ClNS$ 346.0452, found 346.0456.



9-(4-Bromophenyl)-10-thiocyanatophenanthrene (3f). Yellow solid; 29.2 mg, 75% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.38; mp: 177–178 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81–8.76 (m, 2H), 8.65–8.63 (m, 1H), 7.84–7.72 (m, 5H), 7.53 (t, J = 7.2 Hz, 1H), 7.46 (d, J = 7.2 Hz, 1H), 7.26 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.5, 136.7, 132.4, 132.1, 132.0, 130.7, 130.1, 129.4, 129.3, 129.3, 128.9, 128.3,128.2, 127.9, 127.2, 126.2, 123.4, 123.1, 110.7 (SCN); IR (KBr, cm^{-1}) 2922, 2153 (SCN), 1645, 1487, 1261; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{13}BrNS$ 389.9947, found 389.9942.

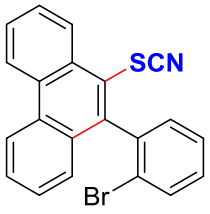


9-([1,1'-Biphenyl]-4-yl)-10-thiocyanatophenanthrene (3g). Yellow solid; 34.8 mg, 90% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.30; mp: 216–218 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83–8.78 (m, 2H), 8.66 (d, J = 7.6 Hz, 1H), 7.86–7.74 (m, 7H), 7.59–7.39 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.4, 141.2, 140.4, 137.9, 131.8, 131.6, 131.2, 130.4, 130.2, 129.1, 128.9, 128.9, 128.3, 127.9, 127.7, 127.3, 127.3, 127.2, 126.9, 123.2, 122.8, 119.5, 111.3 (SCN); IR (KBr, cm^{-1}) 2916, 2149 (SCN), 1697, 1485, 1445; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{27}H_{18}NS$ 388.1154, found 388.1161.

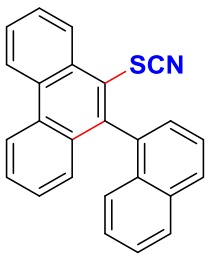


9-(2-Isopropylphenyl)-10-thiocyanatophenanthrene (3h). White solid; 27.8 mg, 79% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.40; mp: 105–107 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (d, J = 8.0 Hz, 1H), 8.78 (d, J = 8.4 Hz, 1H), 8.63 (d, J = 8.0 Hz, 1H), 7.86–7.80 (m, 2H), 7.75 (t, J = 7.6 Hz, 1H), 7.56 (d, J = 4.4 Hz, 2H), 7.51 (t, J = 7.6 Hz, 1H), 7.40–7.35 (m, 2H), 7.17 (d, J = 7.6 Hz, 1H), 2.44 (septet, J = 6.7 Hz, 1H),

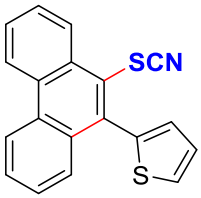
1.17 (d, J = 6.8 Hz, 3H), 0.99 (d, J = 5.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.1, 146.9, 137.1, 131.9, 131.5, 131.3, 130.2, 129.8, 129.2, 129.0, 128.9, 128.3, 127.9, 127.3, 126.8, 126.1, 126.1, 123.3, 122.8, 119.7, 110.9 (SCN), 30.7, 24.1; IR (KBr, cm^{-1}) 3067, 2963, 2153 (SCN), 1487, 1447, 1364, 1265, 1157; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{24}H_{20}NS$ 354.1311, found 354.1312.



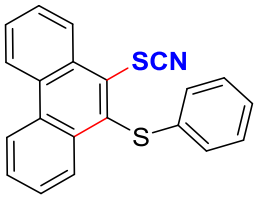
9-(2-Bromophenyl)-10-thiocyanatophenanthrene (3i). Yellow oil; 20.6 mg, 53% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.30; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.87–8.82 (m, 2H), 8.69 (d, J = 8.8 Hz, 1H), 7.88–7.85 (m, 3H), 7.80 (t, J = 7.6 Hz, 1H), 7.58 (dd, J = 12.8, 6.8 Hz, 2H), 7.50–7.38 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.2, 139.7, 133.0, 131.7, 131.4, 130.8, 130.3, 130.2, 129.0, 128.3, 128.2, 127.8, 127.6, 126.9, 124.2, 123.3, 123.0, 119.8, 110.6 (SCN); IR (KBr, cm^{-1}) 3063, 2922, 2156 (SCN), 1472, 1447, 1263, 1188; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{13}BrNS$ 389.9947, found 389.9951.



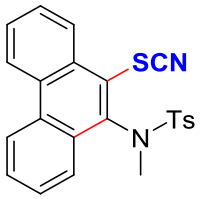
9-(Naphthalen-1-yl)-10-thiocyanatophenanthrene (3j). White solid; 28.1 mg, 78% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.30; mp: 206–207 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92–8.89 (m, 1H), 8.85 (d, J = 8.4 Hz, 1H), 8.71–8.69 (m, 1H), 8.10 (d, J = 8.4 Hz, 1H), 8.04 (d, J = 8.4 Hz, 1H), 7.90–7.88 (m, 2H), 7.79–7.70 (m, 2H), 7.57–7.52 (m, 2H), 7.44 (t, J = 7.6 Hz, 1H), 7.37–7.32 (m, 2H), 7.25 (d, J = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.8, 136.4, 133.6, 132.2, 132.0, 131.6, 131.5, 130.4, 129.1, 129.0, 128.5, 128.4, 128.1, 128.0, 127.5, 127.0, 126.8, 126.4, 125.5, 125.5, 123.3, 122.8, 120.7, 111.1 (SCN); IR (KBr, cm^{-1}) 3055, 2924, 2153 (SCN), 1717, 1506, 1456, 1339, 1263; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{25}H_{16}NS$ 362.0998, found 362.0991.



2-(10-Thiocyanatophenanthren-9-yl)thiophene (3k). White solid; 25.6 mg, 81% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.35; mp: 190–192 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80–8.77 (m, 1H), 8.75 (d, J = 8.0 Hz, 1H), 8.65–8.62 (m, 1H), 7.84–7.79 (m, 2H), 7.78–7.73 (m, 1H), 7.70 (d, J = 8.4 Hz, 1H), 7.61 (dd, J = 5.0, 1.0 Hz, 1H), 7.59–7.55 (m, 1H), 7.28 (dd, J = 5.0, 3.4 Hz, 1H), 7.19 (dd, J = 3.6, 1.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.1, 139.1, 134.6, 132.8, 131.5, 131.2, 130.4, 129.7, 129.1, 128.8, 128.7, 128.6, 128.5, 127.9, 126.9, 126.6, 126.5, 121.2, 110.8 (SCN); IR (KBr, cm^{-1}) 2920, 2149 (SCN), 1647, 1541, 1506, 1456, 1339; HRMS (ESI) *m/z*: [M + H]$^+$ calcd for $C_{19}H_{12}NS_2$ 318.0406, found 318.0398.

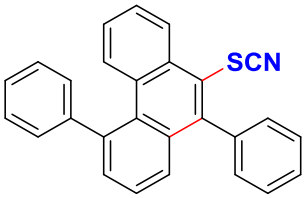


Phenyl(10-thiocyanatophenanthren-9-yl)sulfane (3l). White solid; 33.8 mg, 99% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.20; mp: 169–170 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76–8.74 (m, 1H), 8.71 (d, J = 8.4 Hz, 2H), 8.63–8.61 (m, 1H), 7.81–7.79 (m, 2H), 7.74 (t, J = 7.6 Hz, 1H), 7.61 (t, J = 7.8 Hz, 1H), 7.18 (t, J = 7.4 Hz, 2H), 7.13–7.05 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.3, 137.8, 131.9, 131.6, 131.5, 131.4, 131.3, 130.3, 129.0, 128.8, 128.4, 128.1, 127.4, 126.8, 123.2, 122.9, 122.7, 119.6, 110.9 (SCN); IR (KBr, cm^{-1}) 2922, 2153 (SCN), 1647, 1558, 1456, 1339; HRMS (ESI) *m/z*: [M + H]$^+$ calcd for $C_{21}H_{14}NS_2$ 344.0562, found 344.0562.

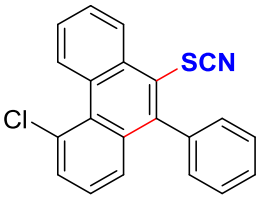


***N*,4-Dimethyl-*N*-(10-thiocyanatophenanthren-9-yl)benzenesulfonamide (3m).** White solid; 16.6 mg, 40% yield; Eluent PE/EtOAc (10:1, v/v), TLC R_f = 0.30; mp: 204–205 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (t, J = 9.6 Hz, 2H), 8.51–8.49 (m, 1H), 7.77–7.74 (m, 2H), 7.66 (t, J = 7.0 Hz, 1H), 7.57 (d, J = 8.0 Hz, 2H), 7.50 (d, J = 8.0 Hz, 1H), 7.40 (t, J = 7.6 Hz, 1H), 7.23 (d, J = 8.0 Hz, 2H), 3.46 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.1, 141.4, 136.6, 132.9, 131.3, 130.1, 129.9, 129.6,

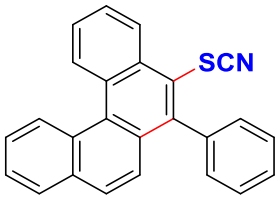
129.2, 128.8, 128.5, 127.7, 127.6, 127.5, 125.9, 124.7, 123.3, 123.3, 111.0 (SCN), 38.3, 21.6; IR (KBr, cm^{-1}) 2924, 2154 (SCN), 1697, 1541, 1456, 1339, 1159; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{23}H_{19}N_2O_2S_2$ 419.0882, found 419.0891.



4,10-Diphenyl-9-thiocyanatophenanthrene (3n). Yellow solid; 21.5 mg, 56% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.38; mp: 59–60 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, J = 8.4 Hz, 1H), 7.81 (d, J = 8.4 Hz, 1H), 7.58–7.50 (m, 5H), 7.44–7.32 (m, 9H), 7.14 (t, J = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.4, 144.7, 140.5, 139.4, 133.3, 133.0, 131.3, 130.1, 129.8, 129.3, 129.2, 129.0, 128.7, 128.6, 128.4, 127.7, 127.4, 126.2, 125.8, 120.0, 111.3 (SCN); IR (KBr, cm^{-1}) 3055, 2922, 2153 (SCN), 1653, 1491, 1441, 1265; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{27}H_{18}NS$ 388.1154, found 388.1156.

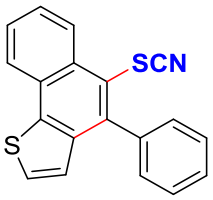


4-Chloro-10-phenyl-9-thiocyanatophenanthrene (3o). White solid; 25.2 mg, 73% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.40; mp: 225–226 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 9.85 (d, J = 8.0 Hz, 1H), 8.61 (dd, J = 8.2, 1.0 Hz, 1H), 7.81–7.69 (m, 3H), 7.54–7.49 (m, 3H), 7.36 (dd, J = 8.4, 1.6 Hz, 1H), 7.31 (d, J = 7.6 Hz, 1H), 7.28–7.25 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.1, 138.7, 132.5, 131.6, 131.3, 130.2, 129.5, 129.0, 128.8, 128.4, 128.4, 127.5, 127.3, 127.2, 127.1, 123.3, 122.7, 122.6, 111.1 (SCN); IR (KBr, cm^{-1}) 2918, 2153 (SCN), 1647, 1522, 1508, 1458, 1339, 1260; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{13}ClNS$ 346.0452, found 346.0451.

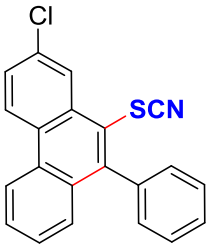


6-Phenyl-5-thiocyanatobenzo[c]phenanthrene (3p). White solid; 26.3 mg, 73% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.40; mp: 201–203 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 9.11 (d, J = 8.4 Hz, 1H), 9.04 (d, J = 8.0 Hz, 1H), 8.75 (d, J = 8.0 Hz, 1H),

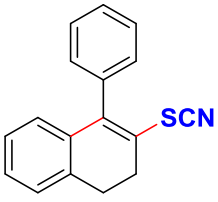
8.00 (d, J = 7.6 Hz, 1H), 7.86 (t, J = 7.0 Hz, 1H), 7.82–7.67 (m, 4H), 7.61–7.58 (m, 3H), 7.41–7.37 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.6, 139.1, 134.0, 131.6, 130.9, 130.3, 130.2, 130.0, 129.3, 129.0, 129.0, 128.7, 128.5, 128.3, 127.9, 127.8, 127.4, 127.0, 126.7, 126.2, 126.2, 119.1, 111.2 (SCN); IR (KBr, cm^{-1}) 2920, 2151 (SCN), 1651, 1506, 1420, 1375, 1263; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{25}H_{16}NS$ 362.0998, found 362.0997.



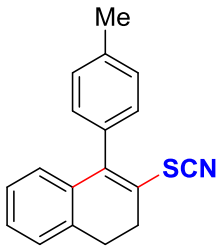
4-Phenyl-5-thiocyanatonaphtho[1,2-b]thiophene (3q). Brown oil; 28.5 mg, 90% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.35; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58–7.56 (m, 1H), 7.47–7.42 (m, 4H), 7.34 (d, J = 3.6 Hz, 1H), 7.31–7.26 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.5, 137.5, 134.3, 133.8, 131.5, 128.8, 128.8, 128.7, 128.6, 128.4, 127.6, 122.9, 121.0, 117.9, 110.4 (SCN), 94.9, 88.6; IR (KBr, cm^{-1}) 3059, 2963, 2156 (SCN), 1597, 1491, 1422, 1261; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{12}NS_2$ 318.0406, found 318.0410.



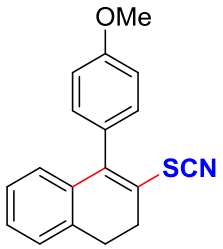
2-Chloro-9-phenyl-10-thiocyanatophenanthrene (3r). White solid; 17.2 mg, 50% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.38; mp: 201–202 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66–8.62 (m, 2H), 8.55 (d, J = 2.0 Hz, 1H), 7.70–7.66 (m, 2H), 7.52–7.40 (m, 5H), 7.29 (dd, J = 7.6, 2.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.1, 138.6, 134.6, 131.8, 131.8, 131.1, 129.6, 129.5, 129.3, 128.7, 128.6, 128.4, 127.6, 126.1, 124.9, 122.7, 118.4, 110.8 (SCN); IR (KBr, cm^{-1}) 2922, 2151 (SCN), 1715, 1557, 1504, 1479, 1339, 1217; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{13}ClNS$ 346.0452, found 346.0452.



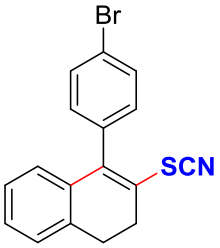
4-Phenyl-3-thiocyanato-1,2-dihydronaphthalene (5a). White solid; 21.3 mg, 81% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.50; mp: 67–68 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49–7.44 (m, 3H), 7.20–7.16 (m, 4H), 7.08–7.04 (m, 1H), 6.62 (d, J = 7.6 Hz, 1H), 3.09 (t, J = 8.0 Hz, 2H), 2.94 (t, J = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.4, 136.7, 134.8, 134.5, 129.5, 129.0, 128.7, 128.3, 127.6, 126.7, 126.2, 122.1, 110.5 (SCN), 29.3, 28.6; IR (KBr, cm^{-1}) 3061, 2926, 2153 (SCN), 1684, 1541, 1489, 1456, 1339, 1279; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{14}NS$ 264.0841, found 264.0843.



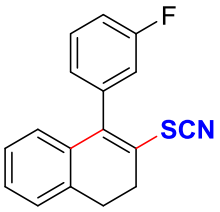
3-Thiocyanato-4-(p-tolyl)-1,2-dihydronaphthalene (5b). Colorless oil; 21.6 mg, 78% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.50; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (t, J = 7.4 Hz, 2H), 7.11 (d, J = 4.8 Hz, 2H), 6.98 (d, J = 8.0 Hz, 3H), 6.57 (d, J = 7.6 Hz, 1H), 3.00 (t, J = 7.8 Hz, 2H), 2.85 (t, J = 8.2 Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.3, 138.6, 135.0, 134.5, 133.6, 129.7, 129.4, 128.2, 127.5, 126.7, 126.2, 121.9, 110.5 (SCN), 29.3, 28.6, 21.4; IR (KBr, cm^{-1}) 3022, 2922, 2153 (SCN), 1684, 1616, 1508, 1483, 1456, 1279; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{18}H_{16}NS$ 278.0998, found 278.0995.



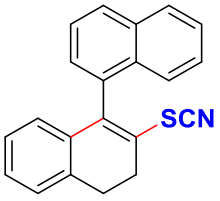
4-(4-Methoxyphenyl)-3-thiocyanato-1,2-dihydronaphthalene (5c). White solid; 19.6 mg, 67% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.35; mp: 93–94 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (d, J = 4.0 Hz, 2H), 7.13–7.09 (m, 3H), 7.02 (d, J = 8.8 Hz, 2H), 6.69 (d, J = 8.0 Hz, 1H), 3.90 (s, 3H) , 3.11 (t, J = 8.0 Hz, 2H), 2.96 (t. J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 140.8, 135.1, 134.5, 130.8, 128.7, 128.2, 127.5, 126.7, 126.2, 122.2, 114.4, 110.6 (SCN), 55.3, 29.3, 28.6; IR (KBr, cm^{-1}) 3028, 2932, 2153 (SCN), 1605, 1508, 1454, 1288, 1248, 1175; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{18}H_{16}NOS$ 294.0947, found 294.0954.



4-(4-Bromophenyl)-3-thiocyanato-1,2-dihydronaphthalene (5d). Colorless oil; 27.8 mg, 82% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.40; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, J = 8.4 Hz, 2H), 7.13 (d, J = 4.4 Hz, 2H), 7.02–6.98 (m, 3H), 6.52 (d, J = 8.0 Hz, 1H), 3.01 (t, J = 7.8 Hz, 2H), 2.86 (t, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.4, 135.5, 134.4, 134.4, 132.3, 131.2, 128.6, 127.7, 126.8, 126.0, 123.0, 122.5, 110.0 (SCN), 29.4, 28.5; IR (KBr, cm^{-1}) 3063, 2926, 2154 (SCN), 1609, 1587, 1483, 1450, 1393, 1279, 1069, 1013; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{13}BrNS$ 341.9947, found 341.9950.

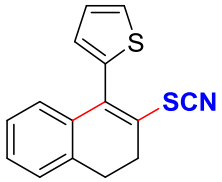


4-(3-Fluorophenyl)-3-thiocyanato-1,2-dihydronaphthalene (5e). Colorless oil; 22.4 mg, 80% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.40; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48–7.42 (m, 1H), 7.21 (d, J = 4.3 Hz, 2H), 7.16–7.12 (m, 1H), 7.10–7.06 (m, 1H), 6.97 (d, J = 7.6 Hz, 1H), 6.91 (d, J = 9.1 Hz, 1H), 6.61 (d, J = 7.7 Hz, 1H), 3.09 (t, J = 7.9 Hz, 2H), 2.94 (t, J = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.0 (d, J = 248.4 Hz), 140.3 (d, J = 1.9 Hz), 138.7, 138.6, 134.4 (d, J = 4.0 Hz), 130.7 (d, J = 8.4 Hz), 128.5, 127.6, 126.8, 126.0, 125.3 (d, J = 3.0 Hz), 122.6, 116.6 (d, J = 21.7 Hz), 115.8 (d, J = 20.9 Hz), 110.0 (SCN), 29.4, 28.5; IR (KBr, cm^{-1}) 2926, 2154 (SCN), 1653, 1581, 1487, 1456, 1339, 1265, 1213, 1148; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{13}FNS$ 282.0747, found 282.0743.

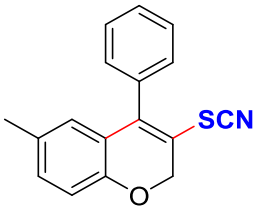


2-Thiocyanato-3,4-dihydro-1,1'-binaphthalene (5f). White solid; 26.6 mg, 85% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.38; mp: 102–104 °C; ^{1}H NMR (400 MHz,

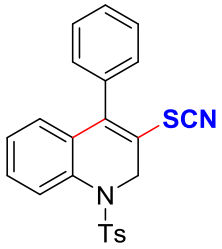
$CDCl_3$) δ 7.95 (t, J = 8.9 Hz, 2H), 7.58–7.51 (m, 3H), 7.43 (t, J = 7.6 Hz, 1H), 7.32 (d, J = 7.0 Hz, 1H), 7.26 (d, J = 7.2 Hz, 1H), 7.18 (t, J = 7.9 Hz, 1H), 6.96 (t, J = 7.6 Hz, 1H), 6.44 (d, J = 7.7 Hz, 1H), 3.26–3.00 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.3, 133.6, 133.0, 132.9, 132.8, 130.2, 128.3, 127.6, 127.3, 126.8, 126.5, 125.9, 125.8, 125.5, 125.0, 124.5, 123.9, 123.0, 109.3 (SCN), 28.2, 27.7; IR (KBr, cm^{-1}) 3055, 2955, 2153 (SCN), 1715, 1651, 1539, 1506, 1456, 1339, 1260; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{16}NS$ 314.0998, found 314.1001.



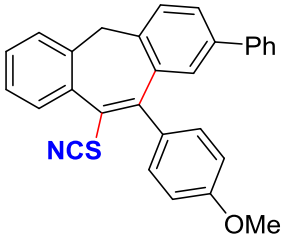
2-(2-Thiocyanato-3,4-dihydronaphthalen-1-yl)thiophene (5g). Yellow oil; 19.4 mg, 72% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.40; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, J = 5.2 Hz, 1H), 7.24–7.21 (m, 2H), 7.18–7.13 (m, 2H), 7.01 (d, J = 3.2 Hz, 1H), 6.85 (d, J = 7.6 Hz, 1H), 3.10 (t, J = 7.8 Hz, 2H), 2.98 (t, J = 8.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.3, 134.8, 134.1, 133.5, 129.4, 128.5, 127.7, 127.4, 127.3, 126.9, 126.7, 125.8, 110.2 (SCN); 29.4, 28.3; IR (KBr, cm^{-1}) 3065, 2932, 2153 (SCN), 1717, 1684, 1603, 1541, 1481, 1456, 1435, 1275, 1215; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{15}H_{12}NS_2$ 270.0406, found 270.0403.



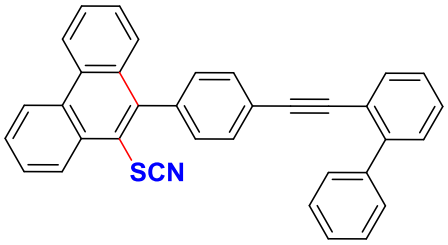
6-Methyl-4-phenyl-3-thiocyanato-2*H*-chromene (5i). Yellow oil; 21.7 mg, 78% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.40; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44–7.40 (m, 3H), 7.15–7.12 (m, 2H), 6.94 (dd, J = 8.4, 1.6 Hz, 1H), 6.77 (d, J = 8.4 Hz, 1H), 6.39 (d, J = 1.6 Hz, 1H), 4.99 (s, 2H), 2.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.4, 141.4, 134.4, 131.4, 131.3, 129.2, 129.1, 129.0, 126.9, 123.5, 116.1, 111.9, 108.6 (SCN), 67.6, 20.6; IR (KBr, cm^{-1}) 3057, 2924, 2154 (SCN), 1670, 1489, 1456, 1277, 1233, 1026; HRMS (ESI) *m/z*: $[M - H]^-$ calcd for $C_{17}H_{12}NOS$ 278.0634, found 278.0633.



4-Phenyl-3-thiocyanato-1-tosyl-1,2-dihydroquinoline (5j). White solid; 27.0 mg, 65% yield; Eluent PE/EtOAc (10:1, v/v), TLC R_f = 0.32; mp: 177–179 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, J = 8.0 Hz, 1H), 7.36–7.23 (m, 6H), 7.12 (d, J = 8.4 Hz, 2H), 7.07 (t, J = 7.6 Hz, 1H), 6.50 (d, J = 8.8 Hz, 1H), 6.40 (d, J = 6.8 Hz, 2H), 4.79 (s, 2H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.2, 140.8, 135.5, 134.4, 134.2, 130.6, 129.5, 129.1, 129.0, 128.8, 127.6, 127.4, 127.2, 126.6, 115.2, 108.4 (SCN), 48.8, 21.5; IR (KBr, cm^{-1}) 2920, 2851, 2154 (SCN), 1647, 1541, 1508, 1456, 1362, 1167, 1084; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{23}H_{19}N_2O_2S_2$ 419.0882, found 419.0890.



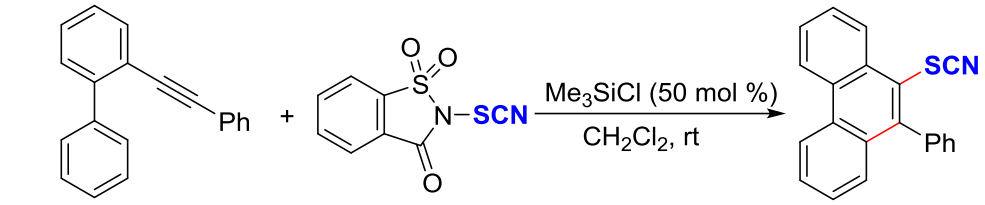
11-(4-Methoxyphenyl)-2-phenyl-10-thiocyanato-5*H*-dibenzo[a,d][7]annulene (9). White solid; 38.0 mg, 88% yield; Eluent PE/EtOAc (20:1, v/v), TLC R_f = 0.35; mp: 185–186 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86–7.84 (m, 1H), 7.48 (dd, J = 7.9, 1.9 Hz, 1H), 7.39–7.25 (m, 9H), 7.17 (d, J = 8.4 Hz, 2H), 7.00–6.97 (m, 3H), 3.90 (d, J = 2.1 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1, 147.0, 141.5, 140.5, 140.5, 139.1, 136.6, 133.4, 133.4, 131.3, 130.1, 129.5, 129.3, 128.7, 128.5, 127.3, 127.0, 126.7, 126.6, 125.9, 114.2, 111.3 (SCN), 55.4, 40.6; IR (KBr, cm^{-1}) 3028, 2930, 2839, 2153 (SCN), 1605, 1508, 1479, 1294, 1252, 1177, 1028; HRMS (ESI) *m/z*: $[M - H]^-$ calcd for $C_{29}H_{20}NOS$ 430.1260, found 430.1264.



9-(4-([1,1'-biphenyl]-2-ylethynyl)phenyl)-10-thiocyanatophenanthrene (12). Yellow solid; 41.0 mg, 84% yield; Eluent PE/EtOAc (10:1, v/v), TLC R_f = 0.50; mp: 177–179 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85–8.80 (m, 2H), 8.68–8.66 (m, 1H),

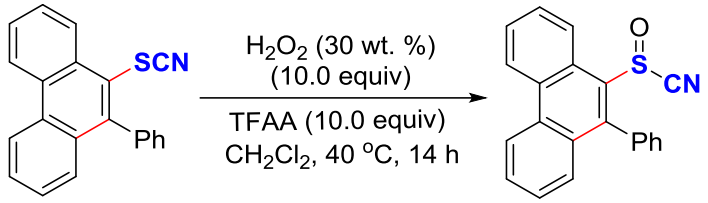
7.89–7.84 (m, 2H), 7.81–7.75 (m, 4H), 7.59–7.39 (m, 10H), 7.34 (d, J = 8.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.0, 144.2, 140.6, 138.7, 133.0, 131.6, 131.6, 131.5, 131.2, 130.3, 129.8, 129.6, 129.4, 129.0, 128.9, 128.8, 128.4, 128.0, 128.0, 127.6, 127.4, 127.1, 126.8, 123.7, 123.2, 122.8, 121.5, 119.4, 111.1 (SCN), 91.7, 90.6; IR (KBr, cm^{-1}) 3063, 2924, 2853, 2214, 2153 (SCN), 1717, 1653, 1508, 1449, 1396, 1265, 1157; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{35}H_{22}NS$ 488.1467, found 488.1464.

4. Gram scale reaction and derivatization of products



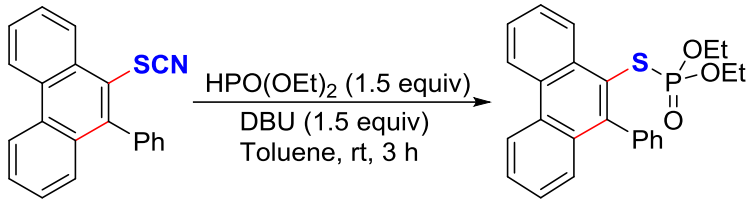
1a, 4.0 mmol, 1.016 g **2c** **3a**, 86%

Gram scale reaction. To a 100 mL oven-dried flask containing **1a** (1.016 g, 4.0 mmol) was added dichloromethane (40.0 mL) under an argon atmosphere. Then **2c** (1.92 g, 8.0 mmol) was added. Subsequently, the mixture was added trimethylchlorosilane (216 mg, 2.0 mmol) and stirred at room temperature for 24 h. When the reaction was completed, the mixture was concentrated in vacuo and the product was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1, v/v) to afford the product **3a** (1.065 g, 86% yield).



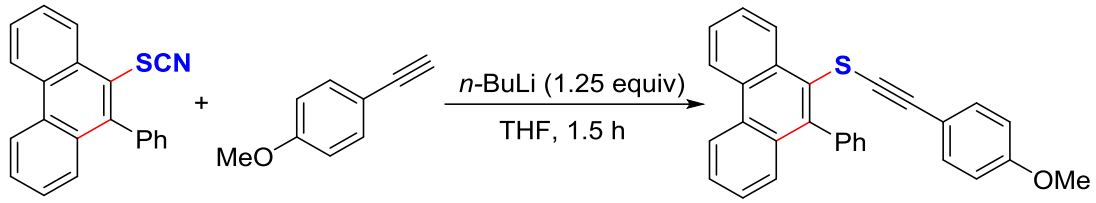
3a **13**, 41%

Procedure for the synthesis of 13. Hydrogen peroxide (30 wt. % in water, 10.0 equiv) was added dropwise at 0 °C to a solution of trifluoroacetic anhydride (10.0 equiv) in dichloromethane (10.0 mL). After being stirred for 40 min, **3a** (155.5 mg, 0.5 mmol) was added slowly and the mixture was stirred at 40 °C for 14 h. When the reaction was completed, the reaction was quenched with water, extracted with dichloromethane, the combined organic phased were washed with brine and dried over anhydrous Na_2SO_4, filtered, and concentrated in vacuo. The residue was purified by flash chromatography on silica gel with petroleum ether/ethyl acetate.



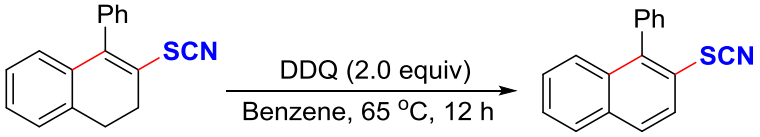
3a **14**, 78%

Procedure for the synthesis of 14. To a solution of **3a** (31.1 mg, 0.1 mmol) and diethyl phosphite (20.7 mg, 0.15 mmol) in dry toluene (1.0 mL) was added DBU (23.0 mg, 0.15 mmol) dropwise and the solution was stirred for 3 h. When the reaction was completed, the mixture was concentrated in vacuo and the product was purified by column chromatography on silica gel with petroleum ether/ethyl acetate.



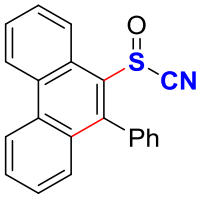
3a **15**, 73%

Procedure for the synthesis of 15. Under an argon atmosphere, a solution of 4-methoxyphenylacetylene (26.4 mg, 0.2 mmol) in dry THF (2.0 mL) was cooled to –78 °C. Then *n*-BuLi (0.1 mL, 0.25 mmol, 2.5 M in *n*-hexane) was added dropwise. Subsequently, **3a** (74.6 mg, 0.24 mmol) was added slowly and the mixture was gradually warmed to room temperature for 1.5 h. When the reaction was completed, the solution was quenched with water (2 drops), concentrated in vacuo and the product was purified by column chromatography on silica gel with petroleum ether/ethyl acetate.

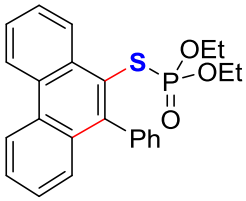


5a **16**, 96%

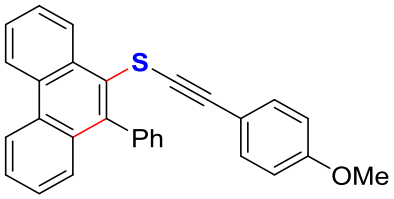
Procedure for the synthesis of 16. To a solution of **5a** (26.3 mg, 0.1 mmol) in benzene (1.0 mL) was added DDQ (45.4 mg, 0.2 mmol) and the solution was stirred at 65 °C for 12 h. When the reaction was completed, the mixture was cooled to room temperature and concentrated in vacuo, the residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate.



10-Phenylphenanthrene-9-sulfinyl cyanide (13). Yellow solid; 67.0 mg, 41% yield; Eluent PE/EtOAc (10:1, v/v), TLC R_f = 0.50; mp: 165–167 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97–8.95 (m, 1H), 8.86–8.83 (m, 1H), 8.80 (d, J = 8.4 Hz, 1H), 7.88–7.81 (m, 3H), 7.62–7.58 (m, 5H), 7.50–7.48 (m, 1H), 7.32 (d, J = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.3, 135.1, 132.8, 131.2, 130.4, 130.3, 130.0, 129.7, 129.5, 129.1, 128.8, 128.8, 128.6, 127.8, 126.3, 125.3, 123.5, 123.1, 116.2; IR (KBr, cm^{-1}) 2924, 2853, 2153 (CN), 1738, 1661, 1449, 1375, 1167, 1101; HRMS (ESI) *m/z*: [M + H]$^+$ calcd for $C_{21}H_{14}NOS$ 328.0791, found 328.0792.

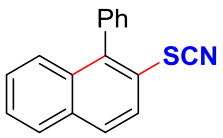


***O,O*-Diethyl *S*-(10-phenylphenanthren-9-yl) phosphorothioate (14).** White solid; 33.0 mg, 78% yield; Eluent PE/EtOAc (5:1, v/v), TLC R_f = 0.40; mp: 112–114 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.87–8.84 (m, 1H), 8.76–8.73 (m, 2H), 7.73–7.64 (m, 3H), 7.53–7.44 (m, 7H), 3.91–3.74 (m, 4H), 1.14 (t, J = 7.1 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.4 (d, J = 7.9 Hz), 140.3 (d, J = 2.0 Hz), 132.8 (d, J = 2.1 Hz), 132.4 (d, J = 3.5 Hz), 131.1 (d, J = 2.2 Hz), 130.9 (d, J = 1.7 Hz), 130.8 (d, J = 1.5 Hz), 128.7 (d, J = 1.4 Hz), 128.4, 127.9, 127.7 (d, J = 1.5 Hz), 127.3, 127.1 (d, J = 2.6 Hz), 126.7, 122.7, 122.6 (d, J = 1.4 Hz), 122.4 (d, J = 8.9 Hz), 63.9 (d, J = 7.0 Hz), 16.0 (d, J = 7.2 Hz); ^{31}P NMR (162 MHz, $CDCl_3$) δ 21.9; IR (KBr, cm^{-1}) 3067, 2982, 2926, 1485, 1447, 1393, 1256, 1157, 1016; HRMS (ESI) *m/z*: [M + H]$^+$ calcd for $C_{24}H_{24}O_3PS$ 423.1178, found 423.1184.



((4-Methoxyphenyl)ethynyl)(10-phenylphenanthren-9-yl)sulfane (15). Yellow oil; 60.7 mg, 73% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.40; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (d, J = 7.7 Hz, 1H), 8.77–8.72 (m, 2H), 7.79–7.71 (m, 2H), 7.68–7.64 (m, 1H), 7.58–7.41 (m, 7H), 7.22 (d, J = 9.3 Hz, 2H), 6.73 (d, J = 8.6 Hz, 2H), 3.73 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 144.5, 139.8, 133.3, 132.1, 131.1, 131.0, 131.0, 130.2, 128.6, 128.2, 128.1, 127.7, 127.7, 127.5, 127.2, 126.8, 126.8, 122.9, 122.6, 115.5, 113.8, 91.5, 77.8, 55.3; IR (KBr, cm^{-1}) 3069, 2928, 2837, 2164, 1603, 1568,

1504, 1447, 1290, 1250, 1171, 1032; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{29}H_{21}OS$ 417.1308, found 417.1316.



1-Phenyl-2-thiocyanatonaphthalene (16). Colorless oil; 25.0 mg, 96% yield; Eluent PE/EtOAc (50:1, v/v), TLC R_f = 0.60; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 8.8 Hz, 1H), 7.90 (d, J = 8.2 Hz, 1H), 7.83 (d, J = 8.8 Hz, 1H), 7.56–7.51 (m, 4H), 7.43–7.42 (m, 2H), 7.30–7.28 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.7, 136.4, 133.0, 132.9, 130.0, 129.8, 129.0, 128.9, 128.1, 127.4, 127.0, 126.2, 124.8, 122.2, 110.9 (SCN); IR (KBr, cm^{-1}) 3057, 2924, 2851, 2154 (SCN), 1684, 1584, 1504, 1491, 1443, 1385, 1321, 1267; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{12}NS$ 262.0685, found 262.0678.

5. X-Ray Structure of 3d (CCDC 2210343)

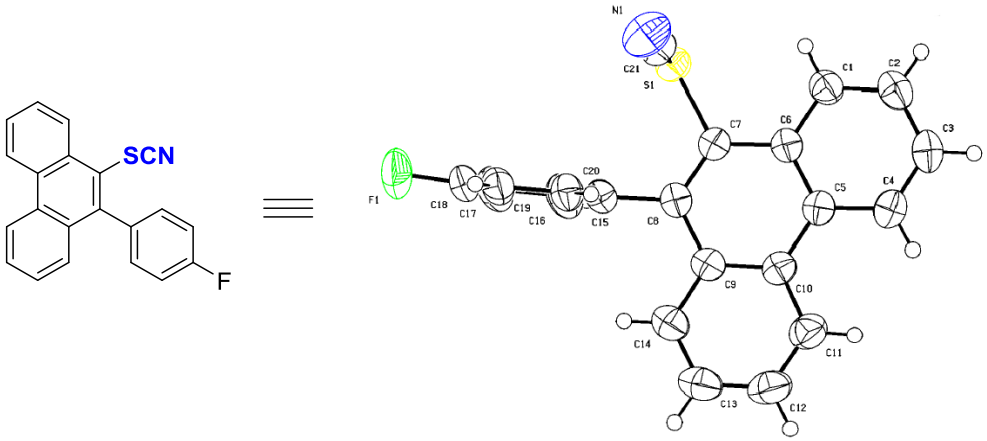


Table 1. Crystal data and structure refinement for the product **3d** (CCDC 2210343).

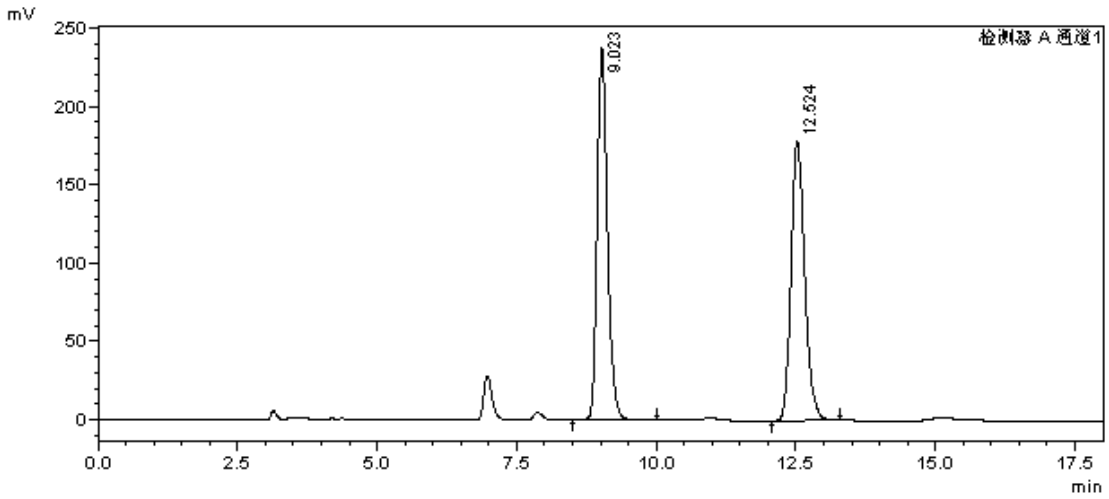
Identification code	**3d**
Empirical formula	$C_{21}H_{12}FNS$
Formula weight	329.38
Temperature/K	293
Space group	P 1 21/c 1
Hall group	–P 2ybc
a/Å	11.3845(1)
b/Å	16.8992(1)
c/Å	8.1309(1)
α/°	90

β/°	92.673(1)
γ/°	90
Volume/Å^3	1562.59(3)
Z	4
ρcalcg/cm^3	1.400
μ/mm^{-1}	1.929
F(000)	680.0
Bond precision	C–C = 0.0021 A
Wavelength	1.54184
Data completeness	0.995
Theta (max)	68.207
h, k, lmax	13, 20, 9
R, wR_2	0.0346(2651), 0.0945(2849)
S	1.052
Npar	218

6. HPLC Chromatograms

Compound **13** chiral separation

HPLC: on AD-H column (*n*-hexane/*iso*-propanol, 90:10, v/v, 1.0 mL/min, 254 nm).



Peak	**Time**	Area	**Area/%**
1	**9.023**	3037052	**50.018**
2	**12.524**	3034845	**49.982**
total		6071897	**100.000**

7. References

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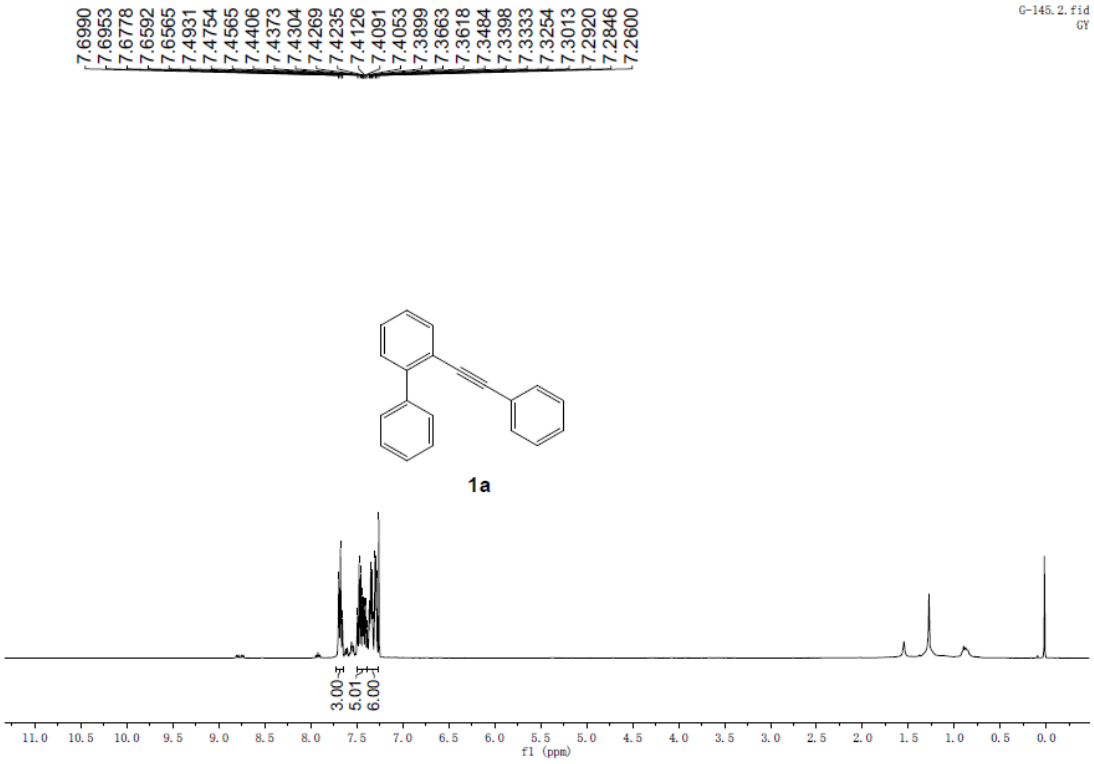
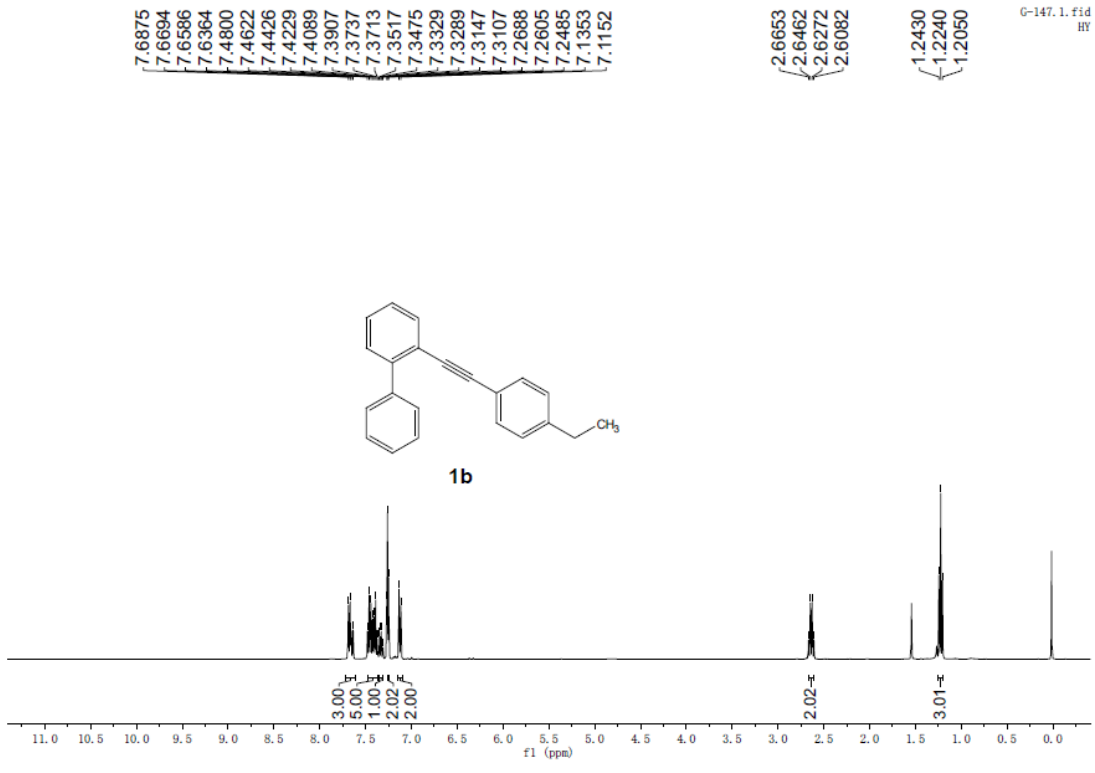
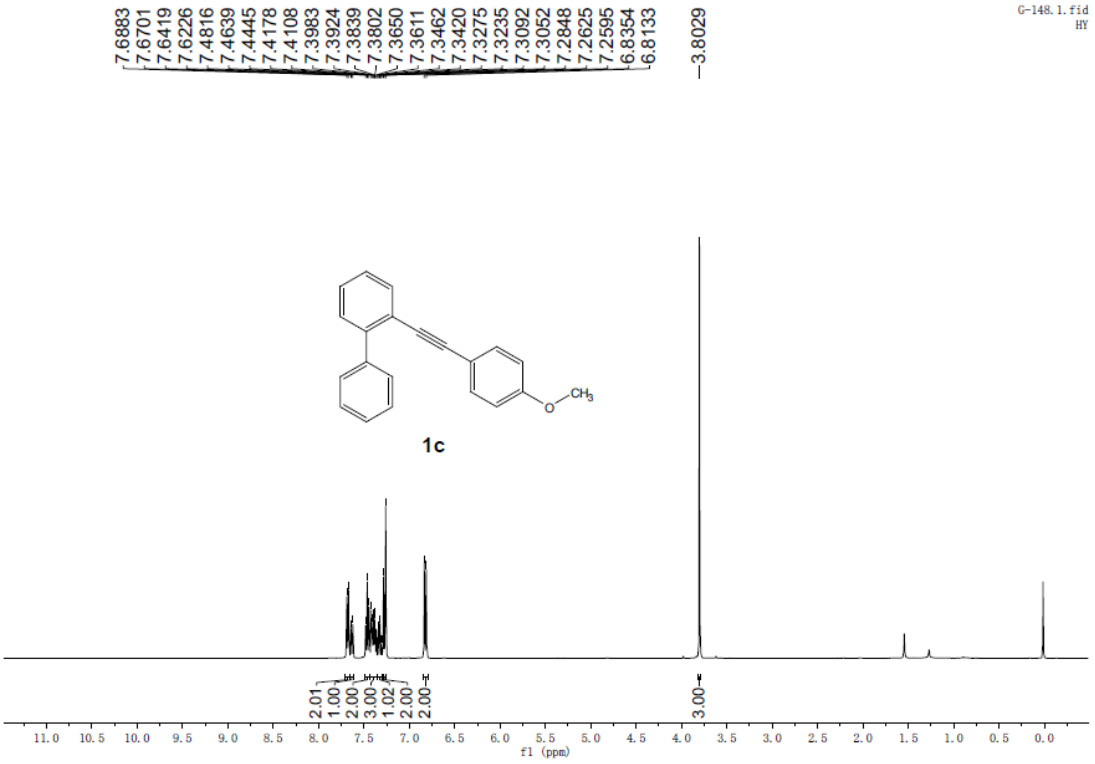
8. Copies of ^{1}H, ^{13}C and ^{31}P NMR spectra



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7.3839
7.3802
7.3650
7.3611
7.3462
7.3420
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7.3235
7.3092
7.3052
7.2848
7.2625
7.2595
6.8354
6.8133
3.8029
G-148.1.fid
HY
O
CH3
1c
2.01
1.00
2.00
3.00
1.02
2.00
2.00
3.00
11.0 10.5 10.0 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 0.0
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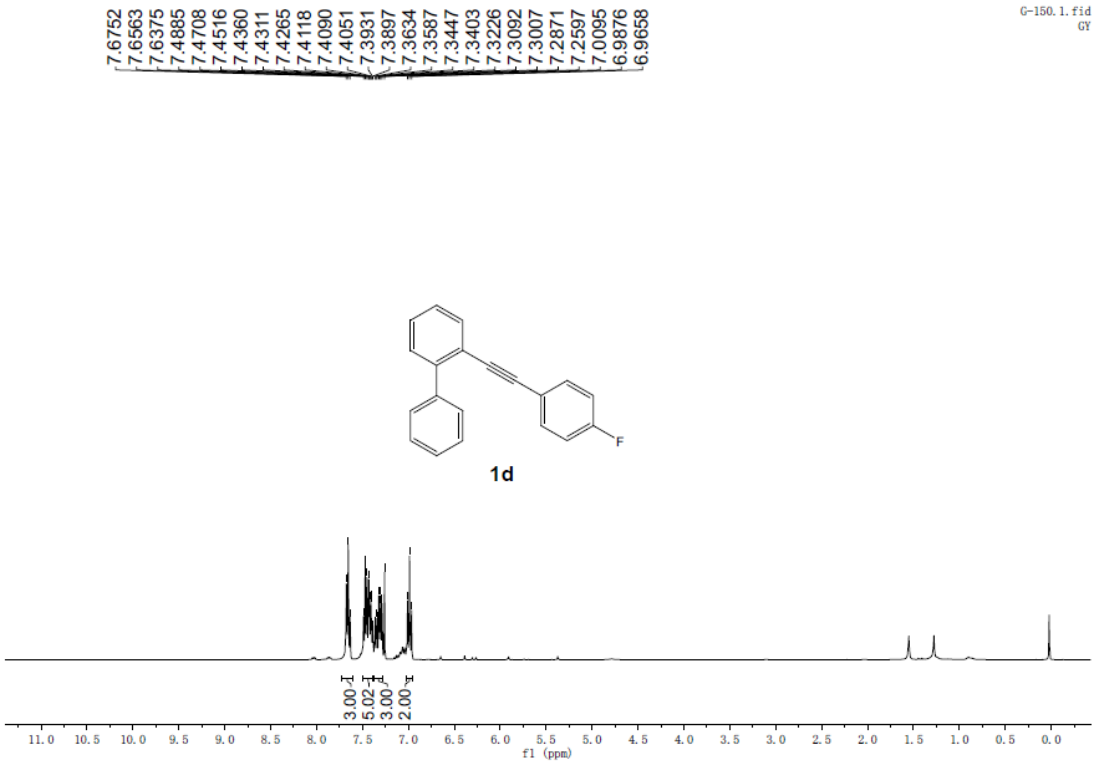
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GY
F
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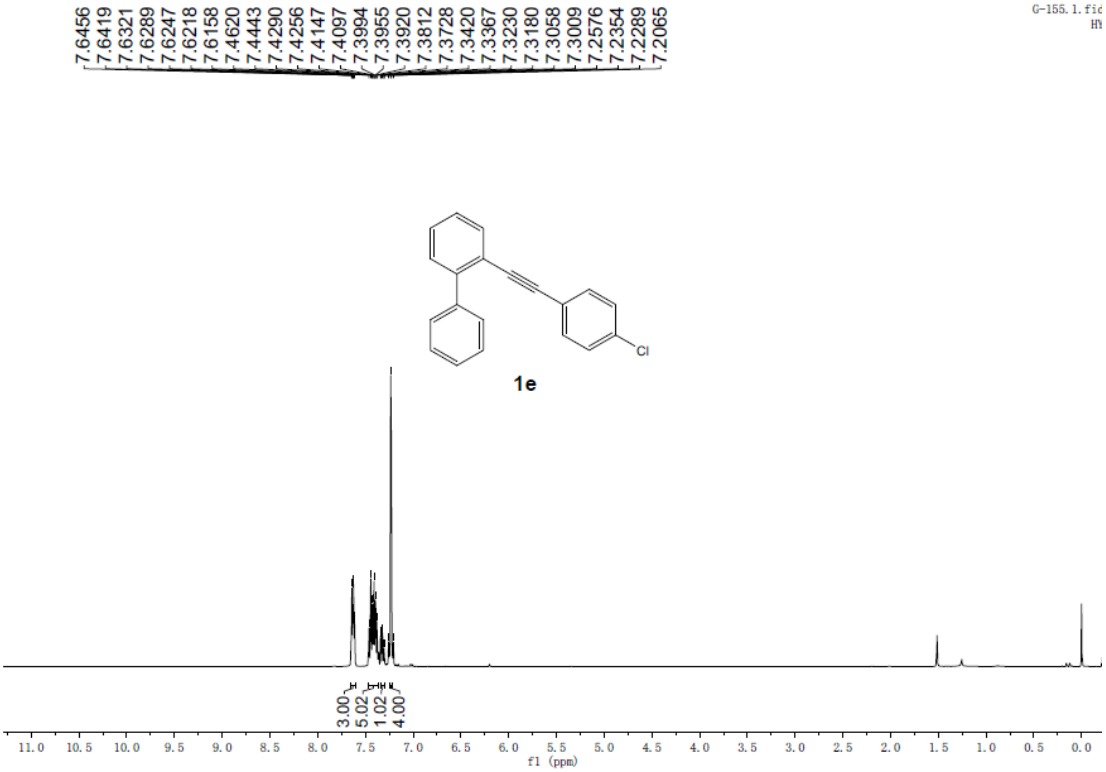
3.00
5.02
3.00
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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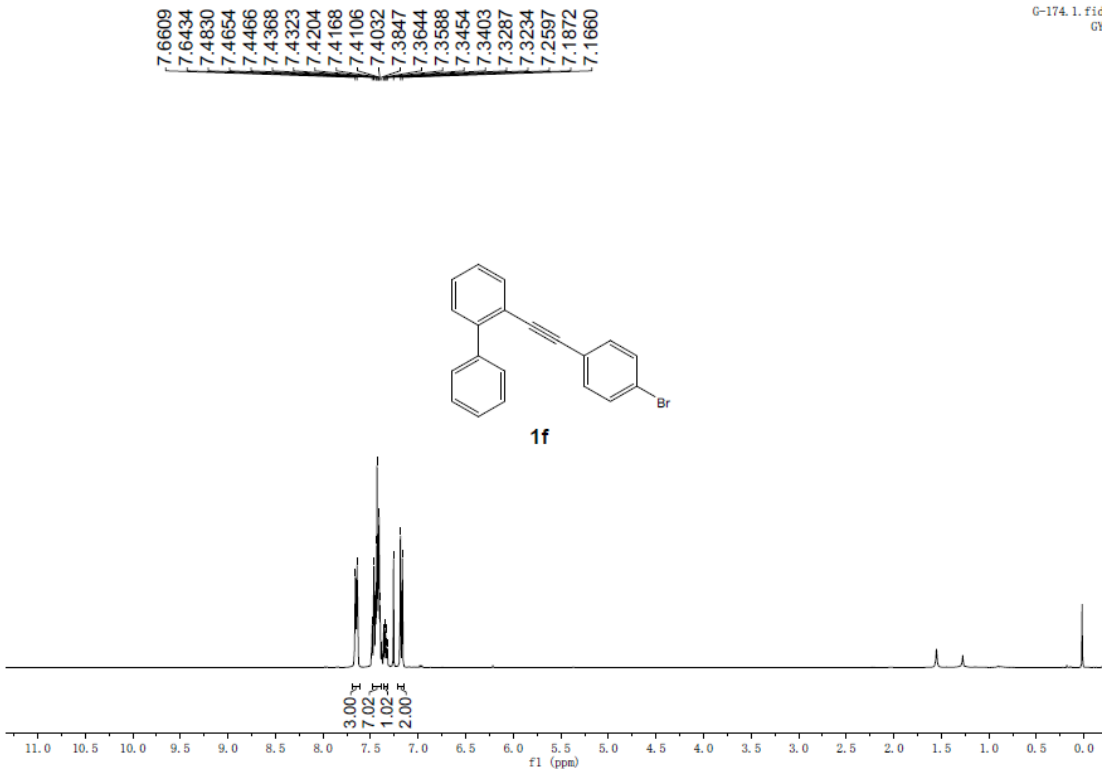
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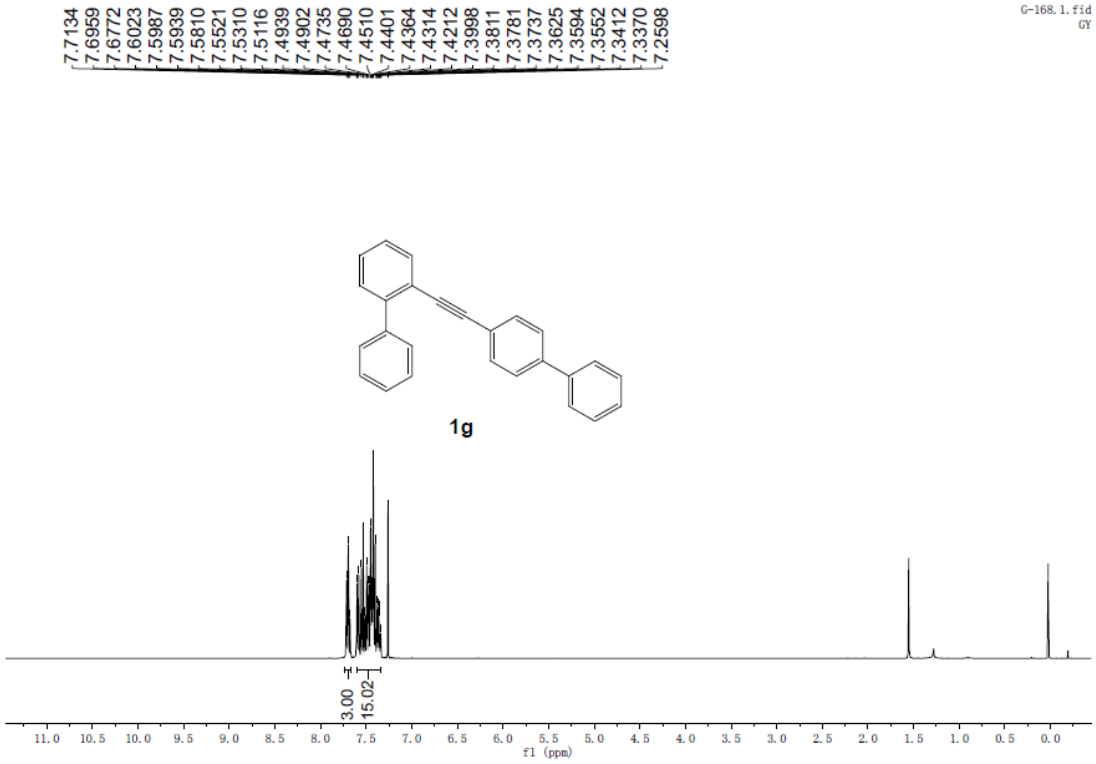
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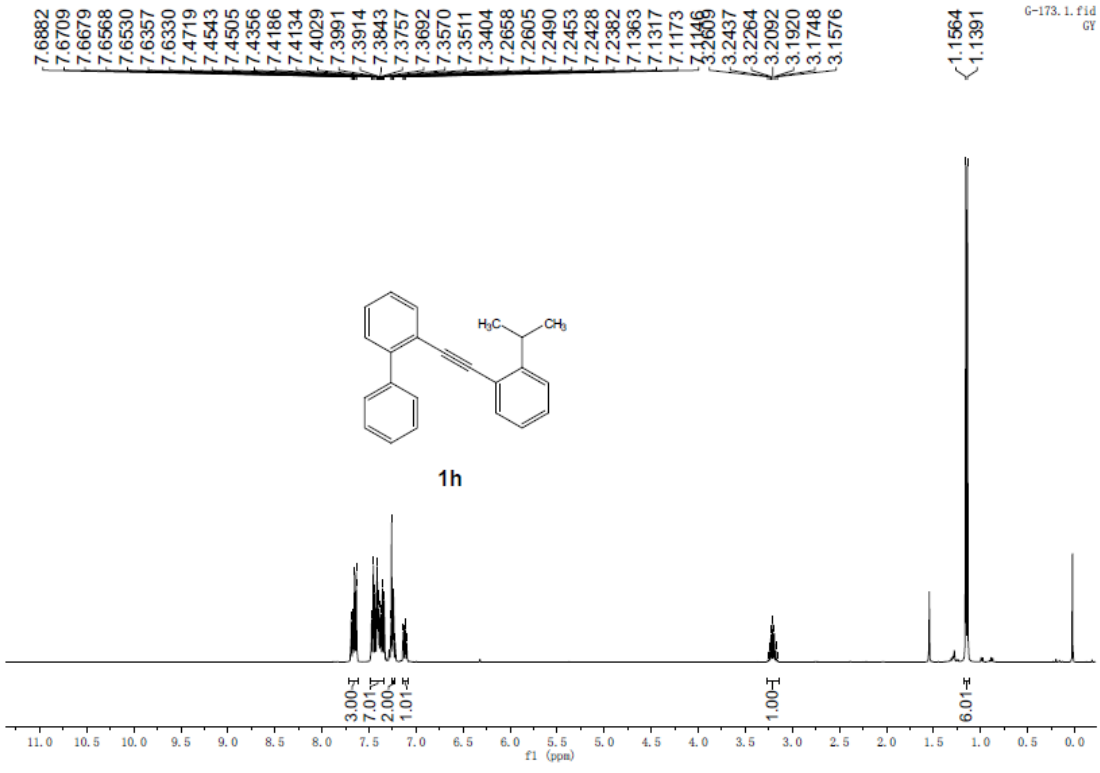
1g
3.00
15.02
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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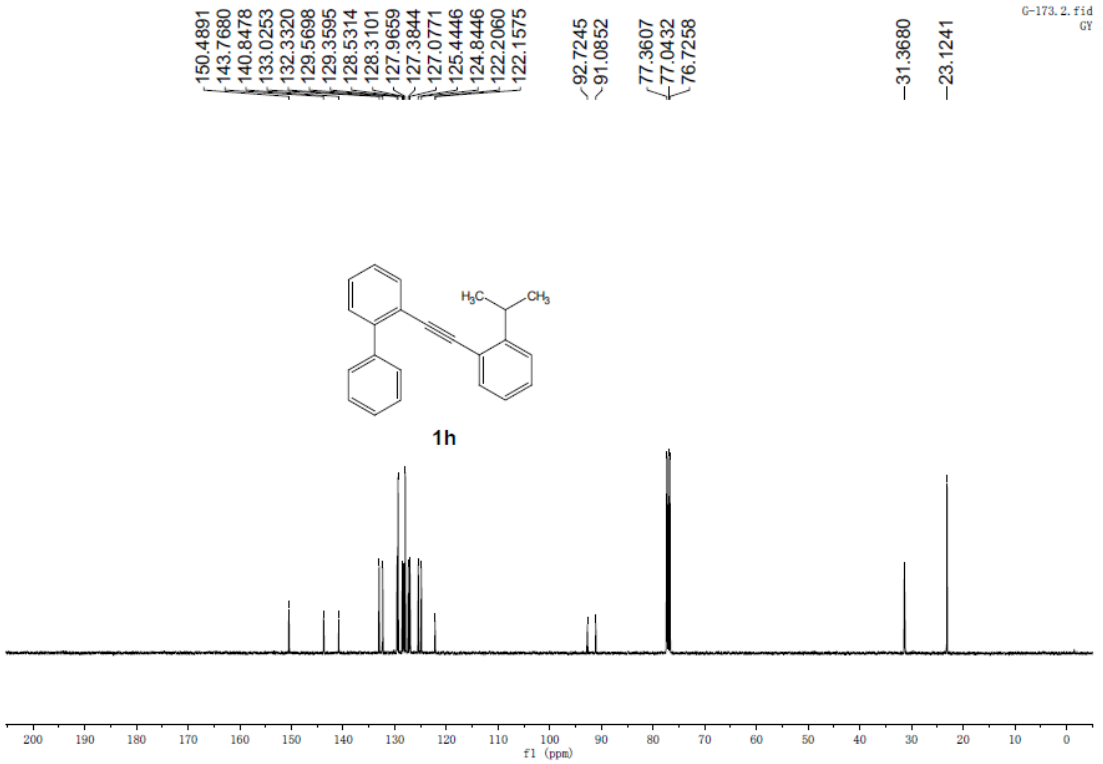
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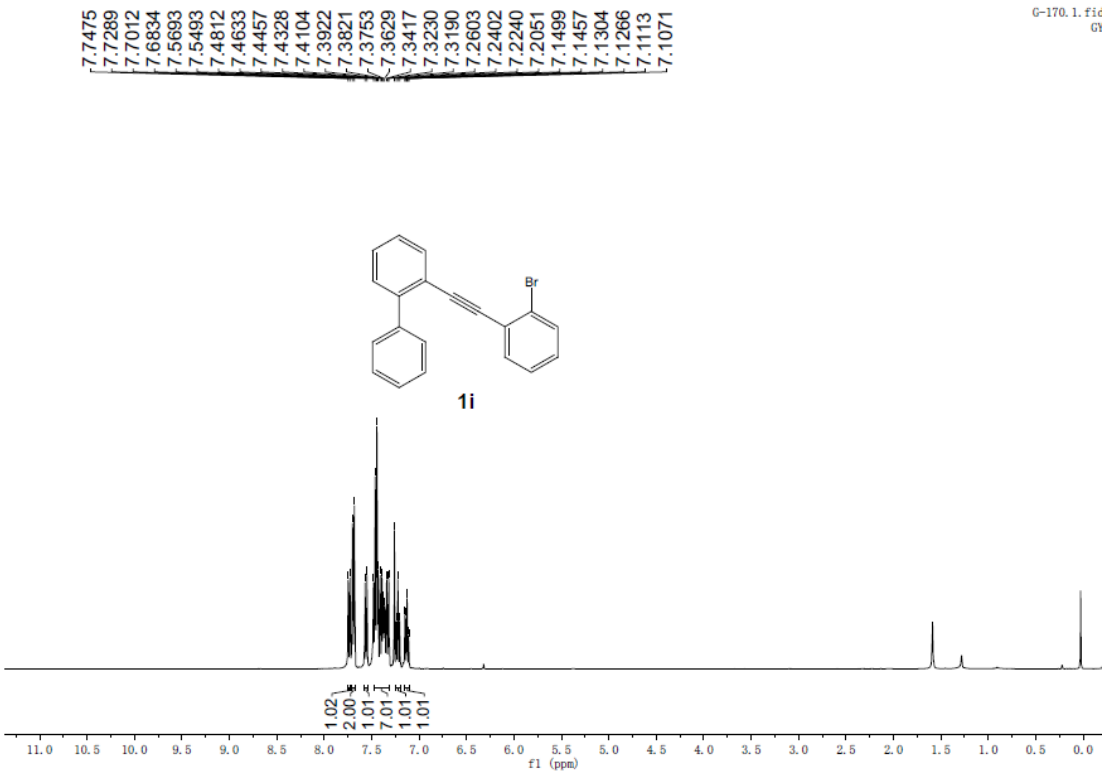
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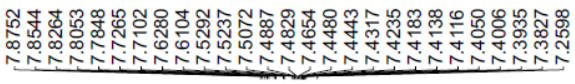

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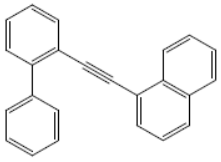

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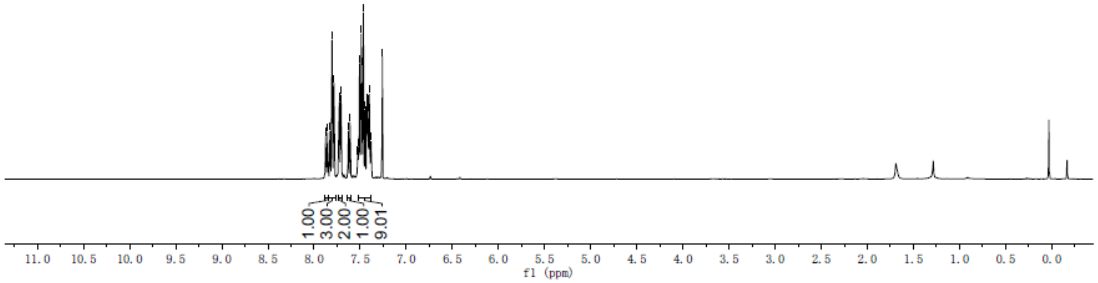

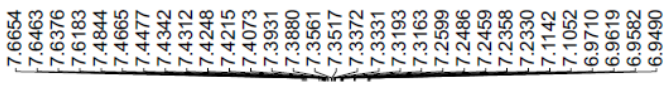

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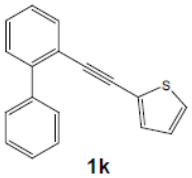

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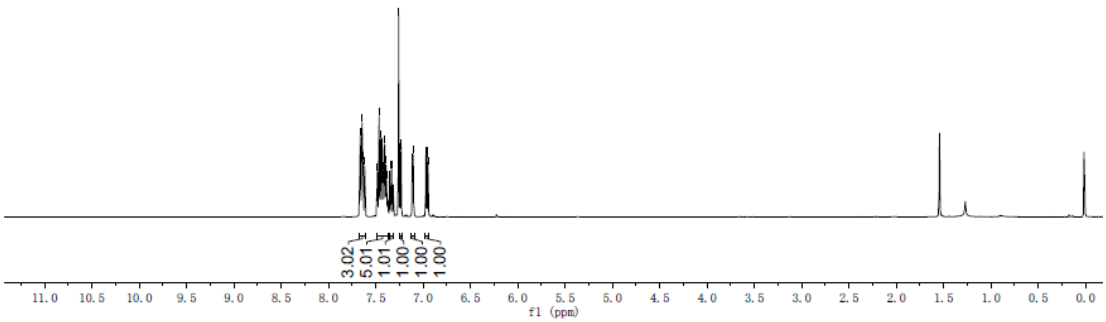

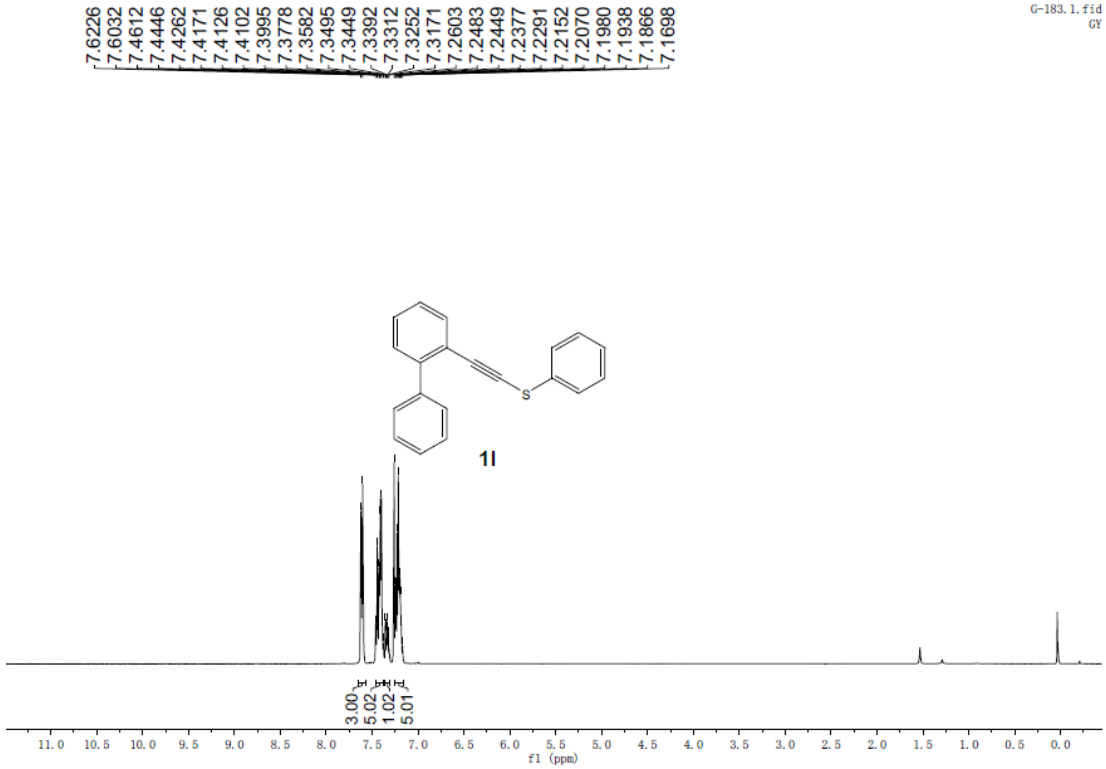
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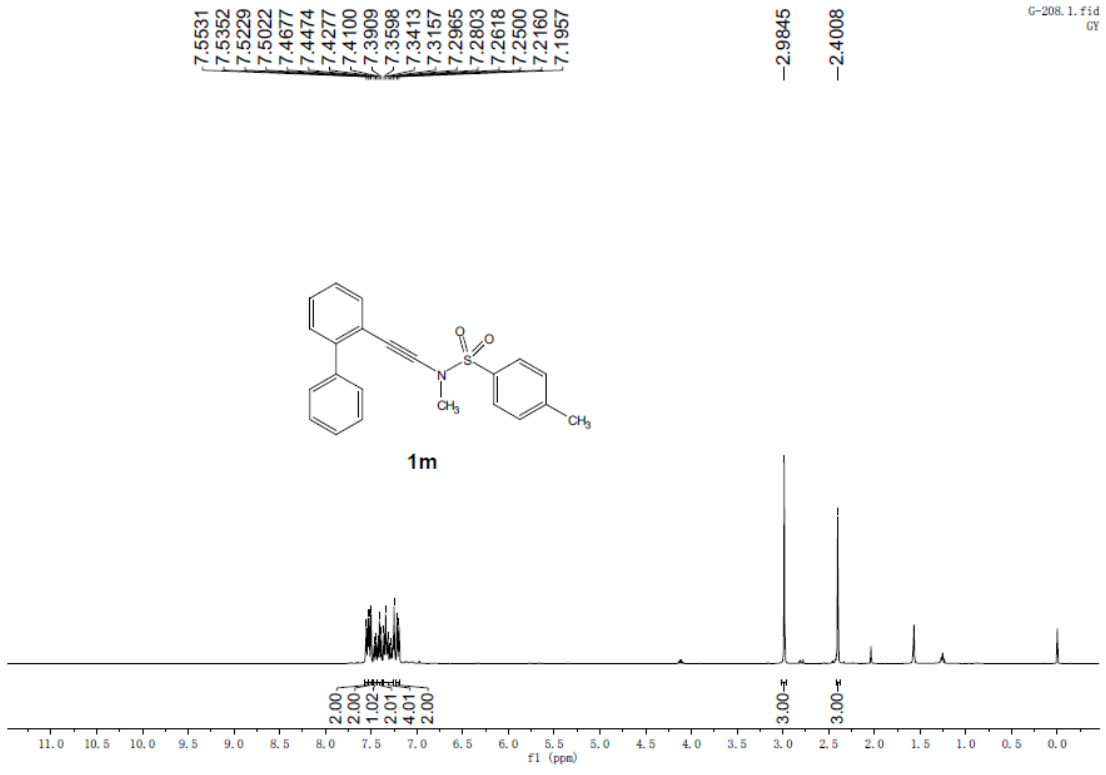
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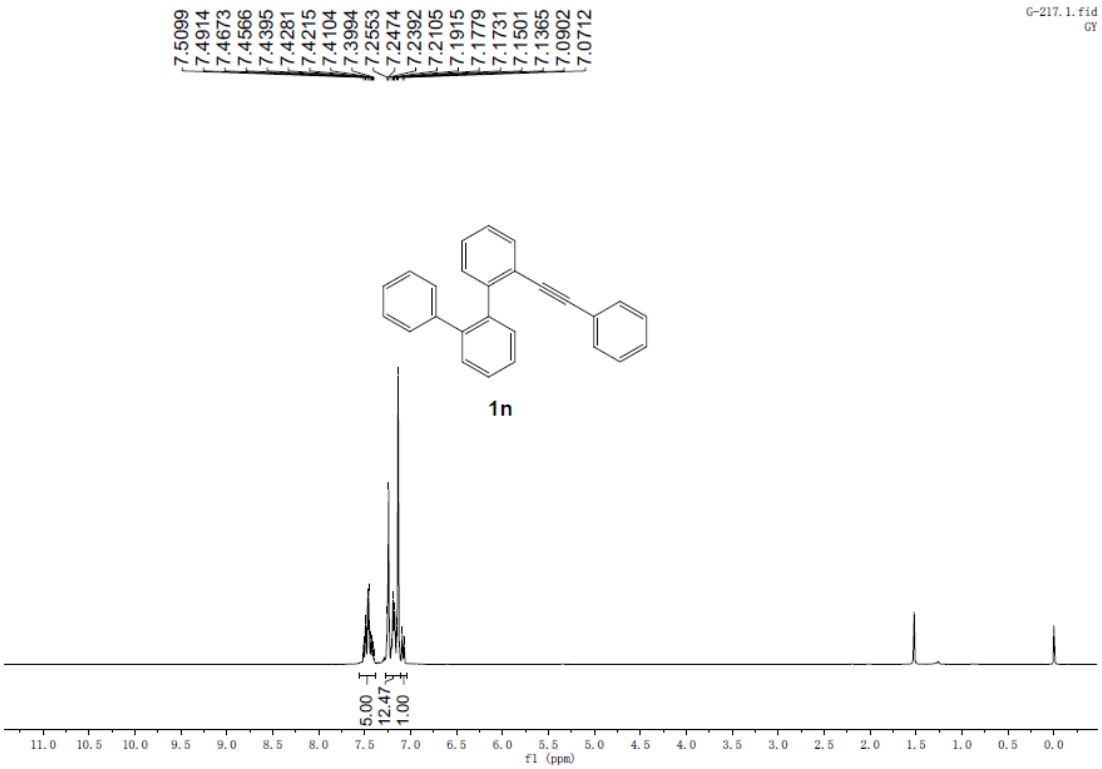
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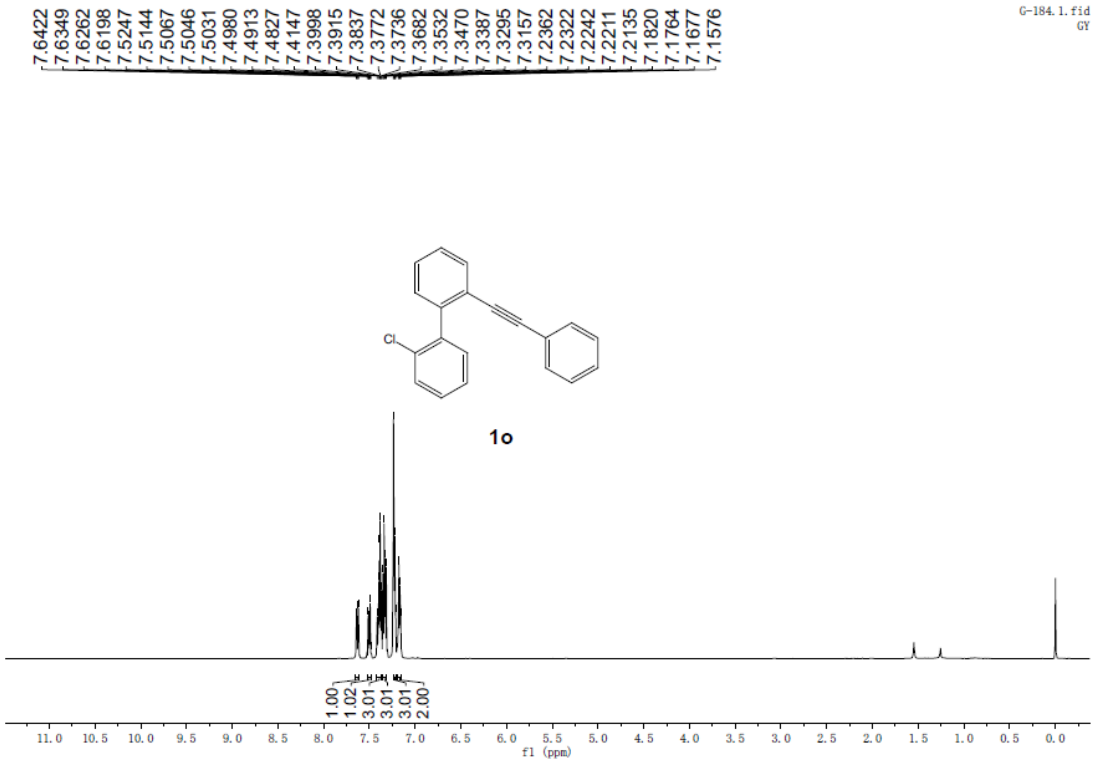
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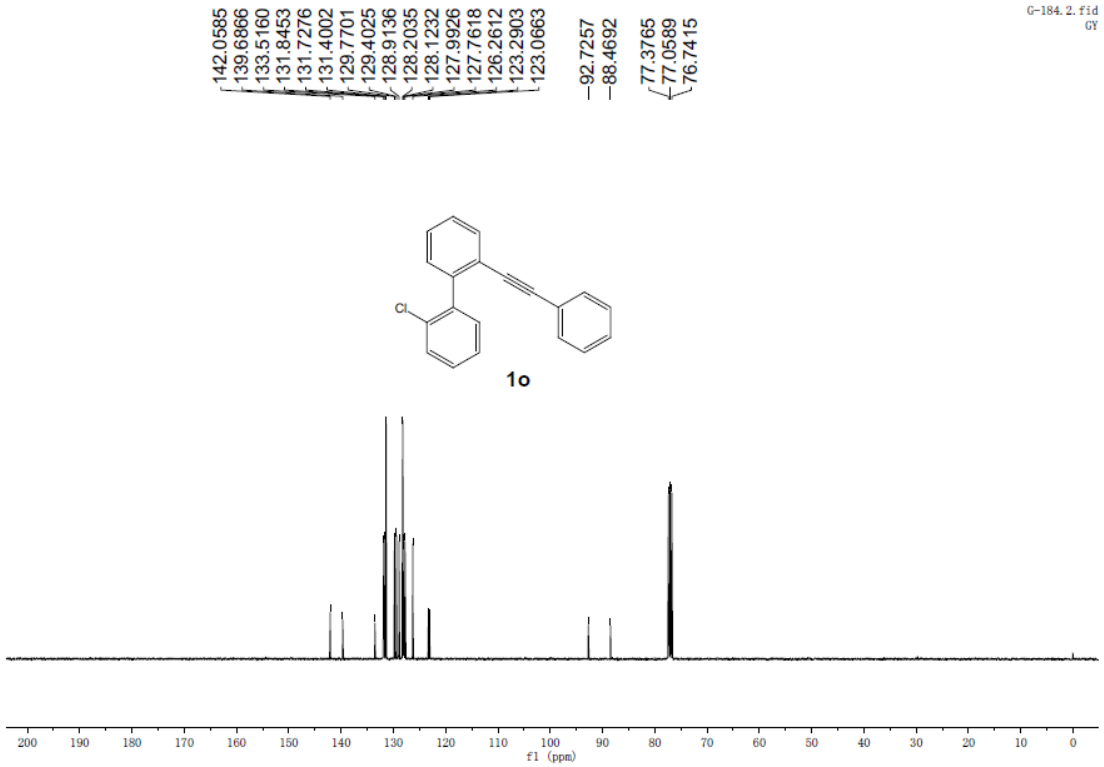
f1 (ppm)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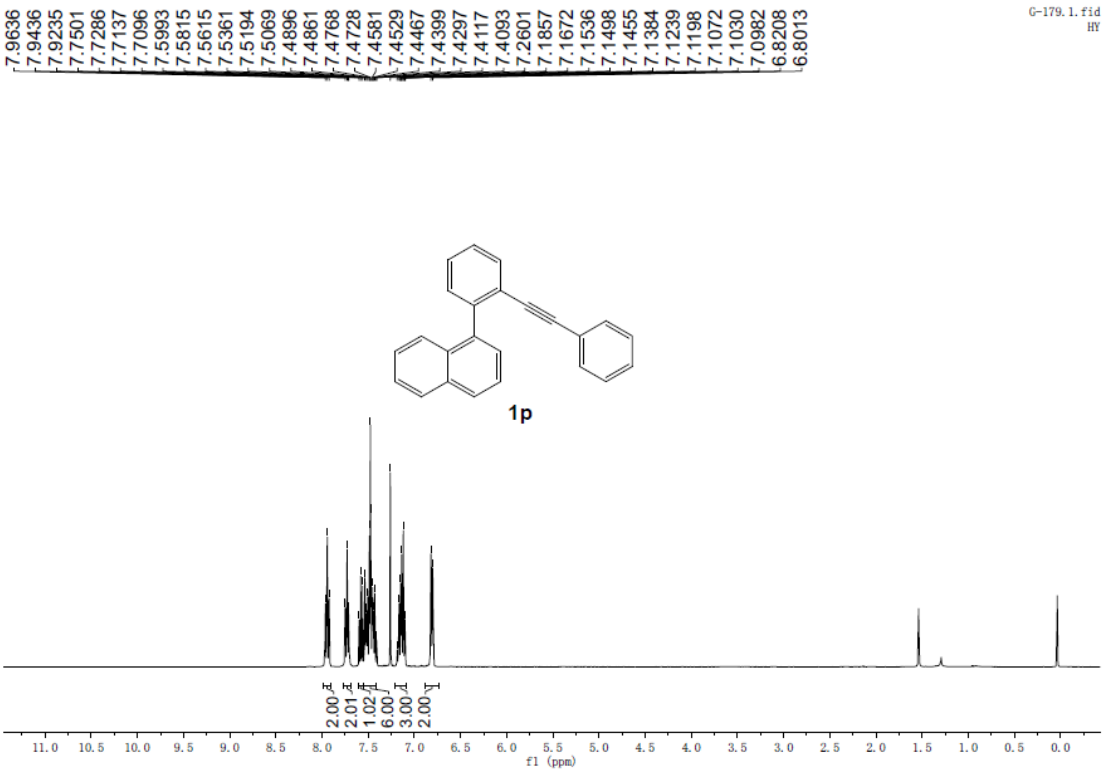
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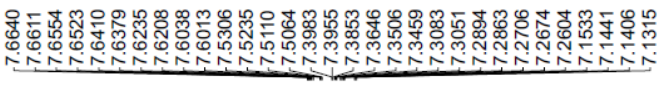
3.00
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)



G-178.1.fid
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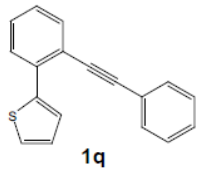

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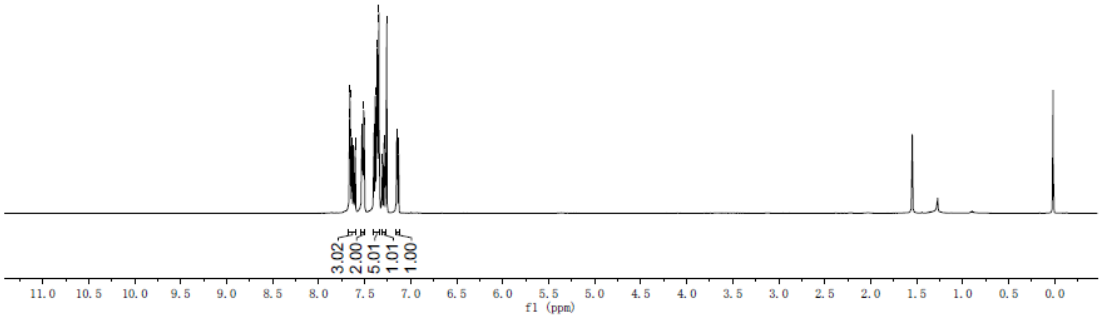
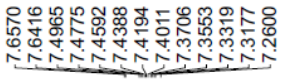
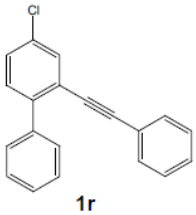




G-164.1.fid
GY



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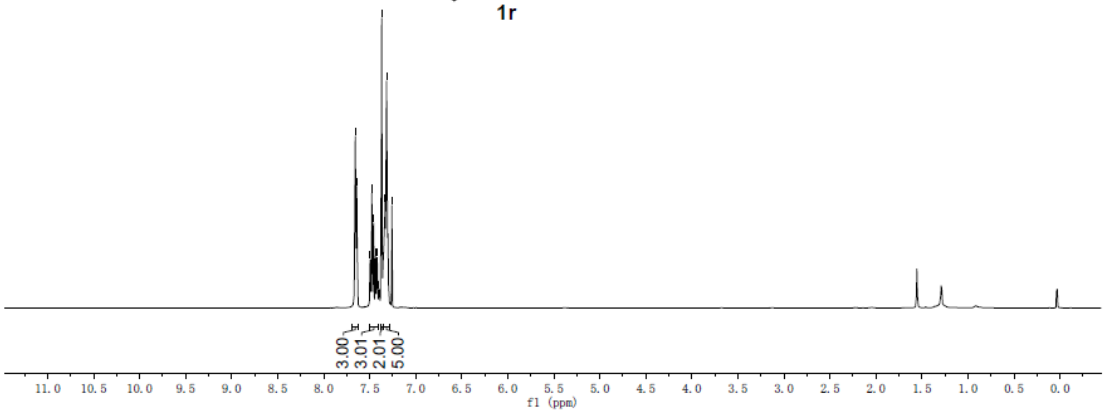

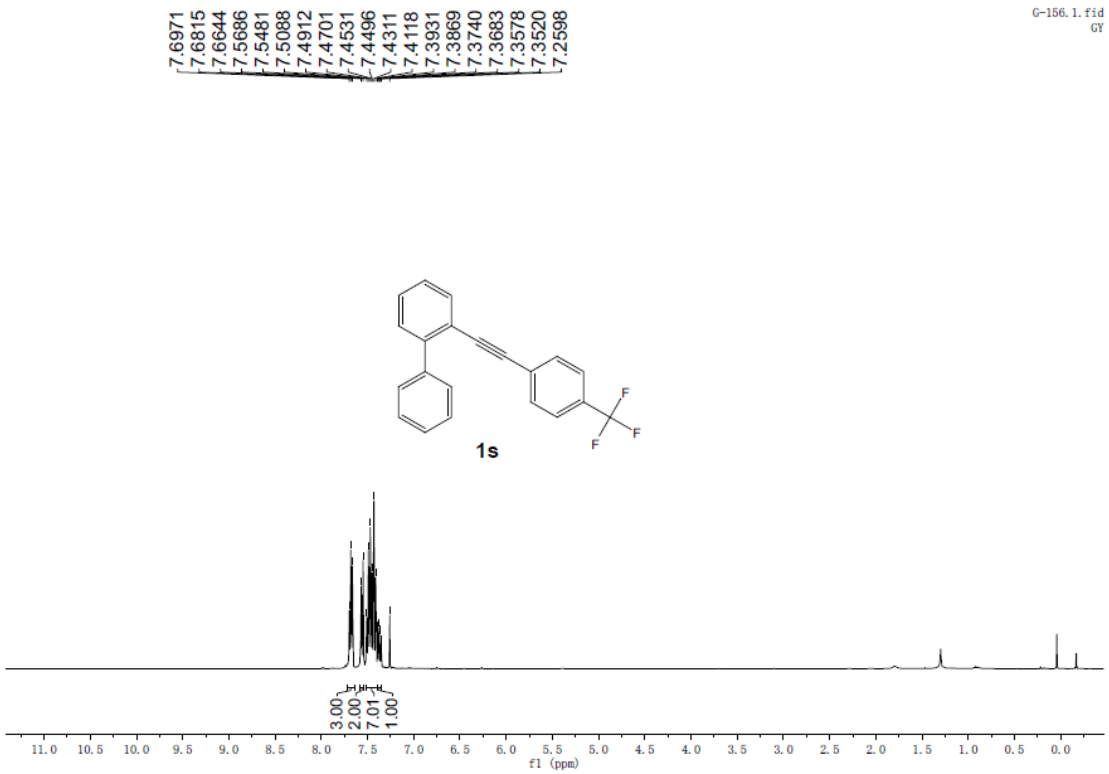
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7.5481
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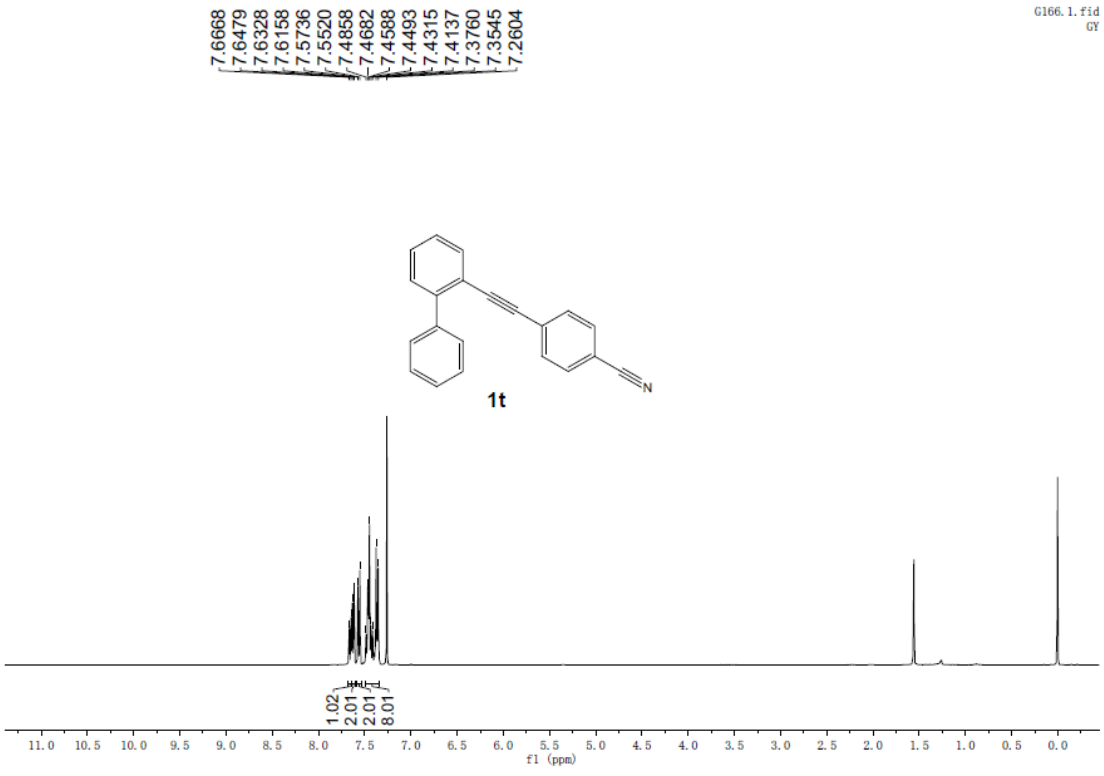
7.4912
7.4701
7.4531
7.4496
7.4311
7.4118
7.3931
7.3869
7.3740
7.3683
7.3578
7.3520
7.2598
G-156.1.fid
GY
F
F
F
1s
3.00
2.00
7.01
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


7.6668
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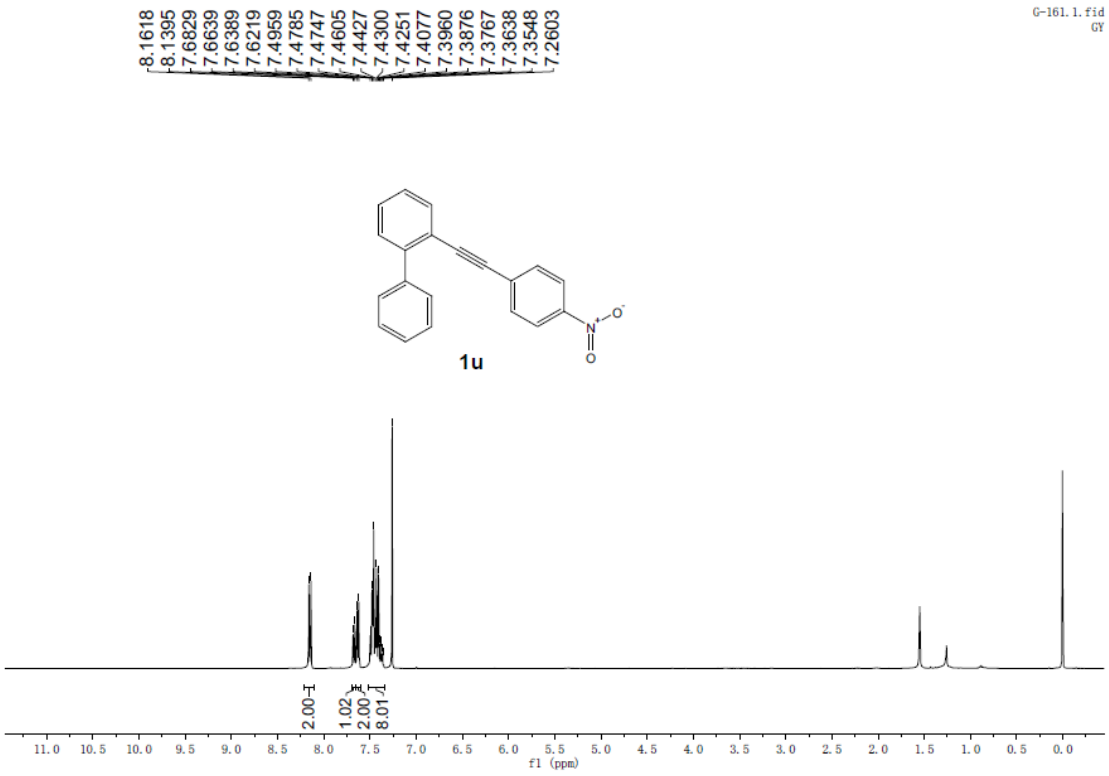
7.6158
7.5736
7.5520
7.4858
7.4682
7.4588
7.4493
7.4315
7.4137
7.3760
7.3545
7.2604
G166.1.fid
GY
N
1t
1.02
2.01
2.01
8.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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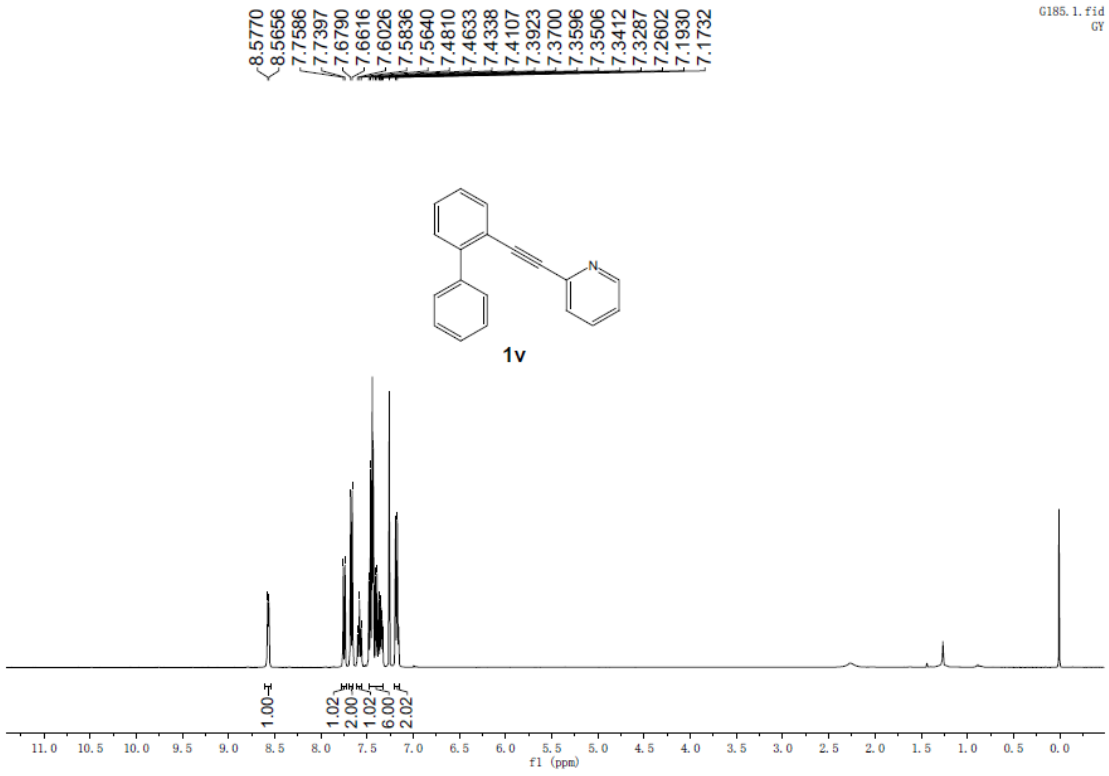
7.6829
7.6639
7.6389
7.6219
7.4959
7.4785
7.4747
7.4605
7.4427
7.4300
7.4251
7.4077
7.3960
7.3876
7.3767
7.3638
7.3548
7.2603
G-161.1.fid
GY
1u
2.00
1.02
2.00
8.01
f1 (ppm)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8.5656
7.7586
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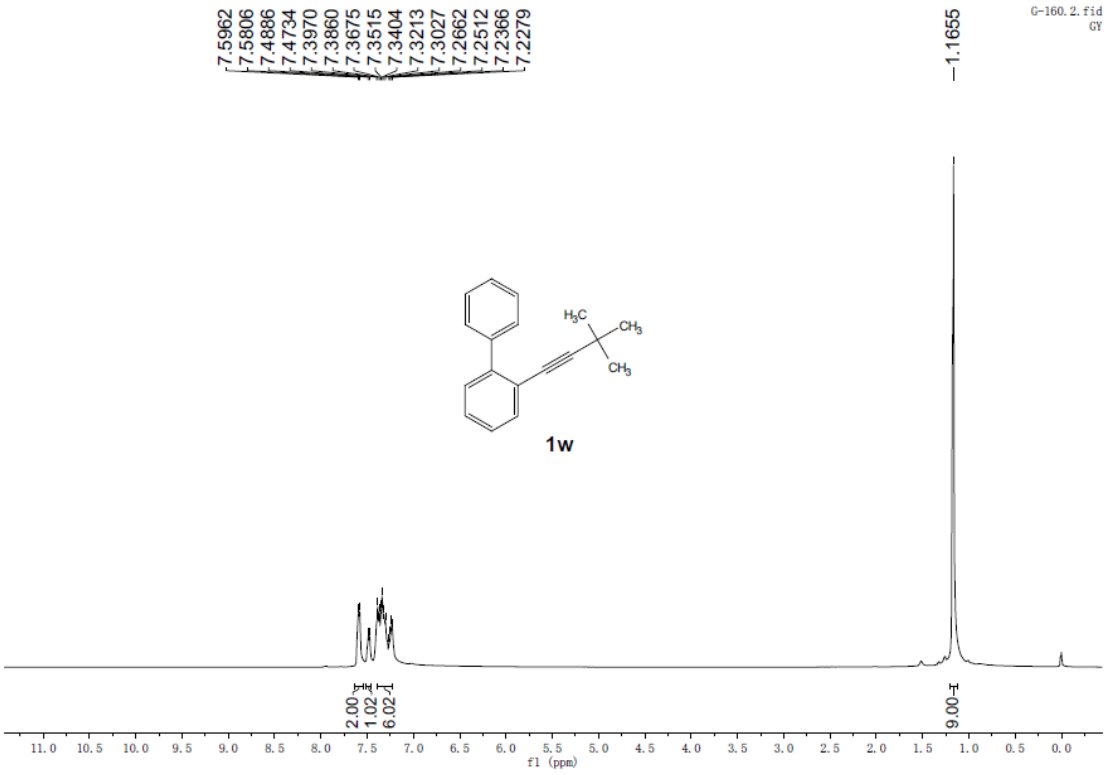
7.6790
7.6616
7.6026
7.5836
7.5640
7.4810
7.4633
7.4338
7.4107
7.3923
7.3700
7.3596
7.3506
7.3412
7.3287
7.2602
7.1930
7.1732
G185.1.fid
GY
1v
1.00
1.02
2.00
1.02
6.00
2.02
f1 (ppm)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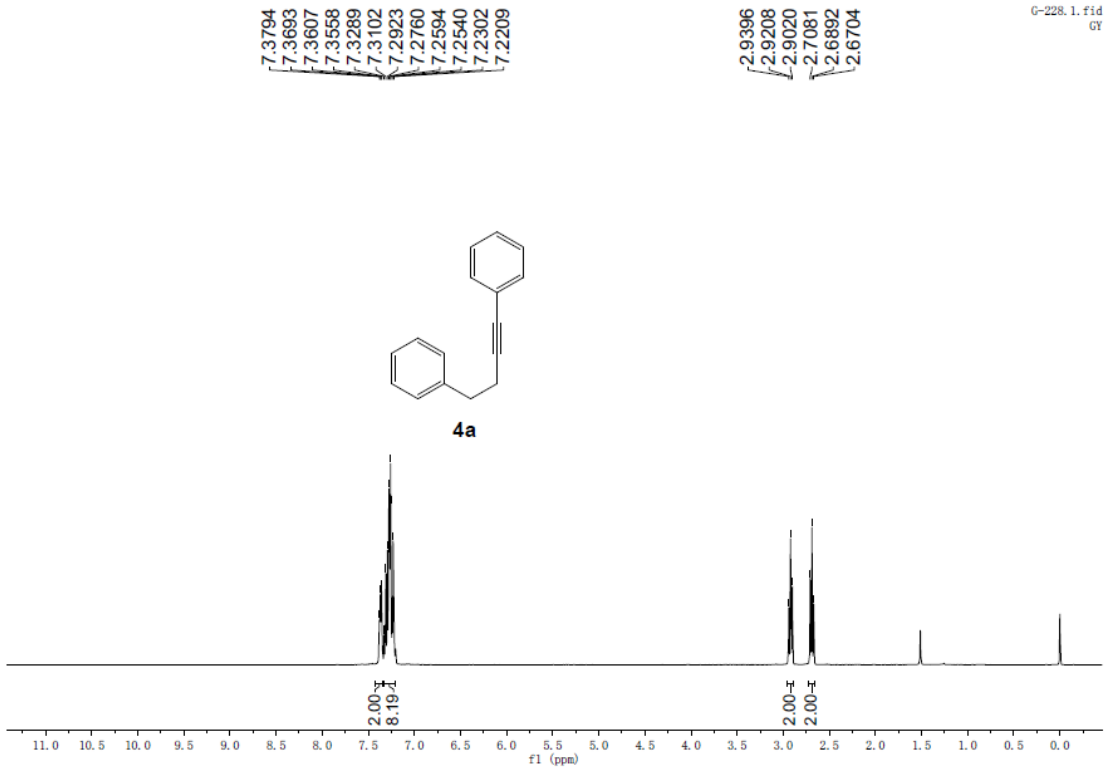
7.5806
7.4886
7.4734
7.3970
7.3860
7.3675
7.3515
7.3404
7.3213
7.3027
7.2662
7.2512
7.2366
7.2279
1.1655
G-160.2.fid
GY
H3C
CH3
CH3
1w
2.00
1.02
6.02
9.00
f1 (ppm)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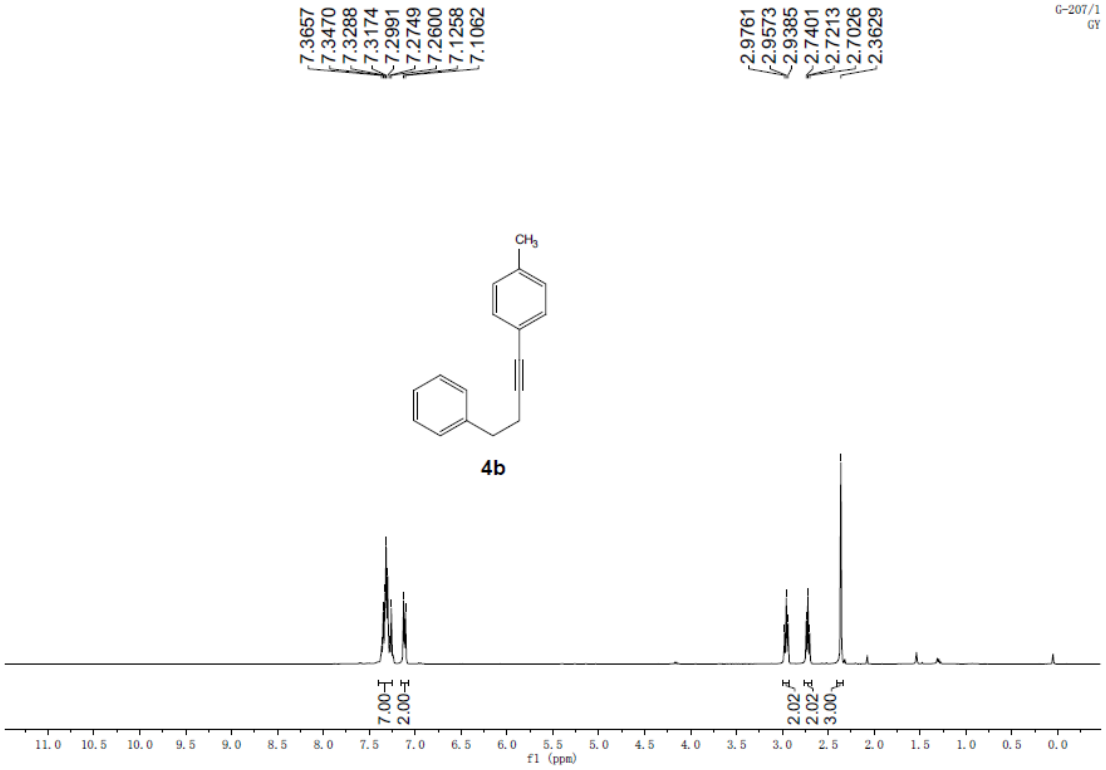
7.3693
7.3607
7.3558
7.3289
7.3102
7.2923
7.2760
7.2594
7.2540
7.2302
7.2209
2.9396
2.9208
2.9020
2.7081
2.6892
2.6704
G-228.1.fid
GY
4a
2.00
8.19
2.00
2.00
f1 (ppm)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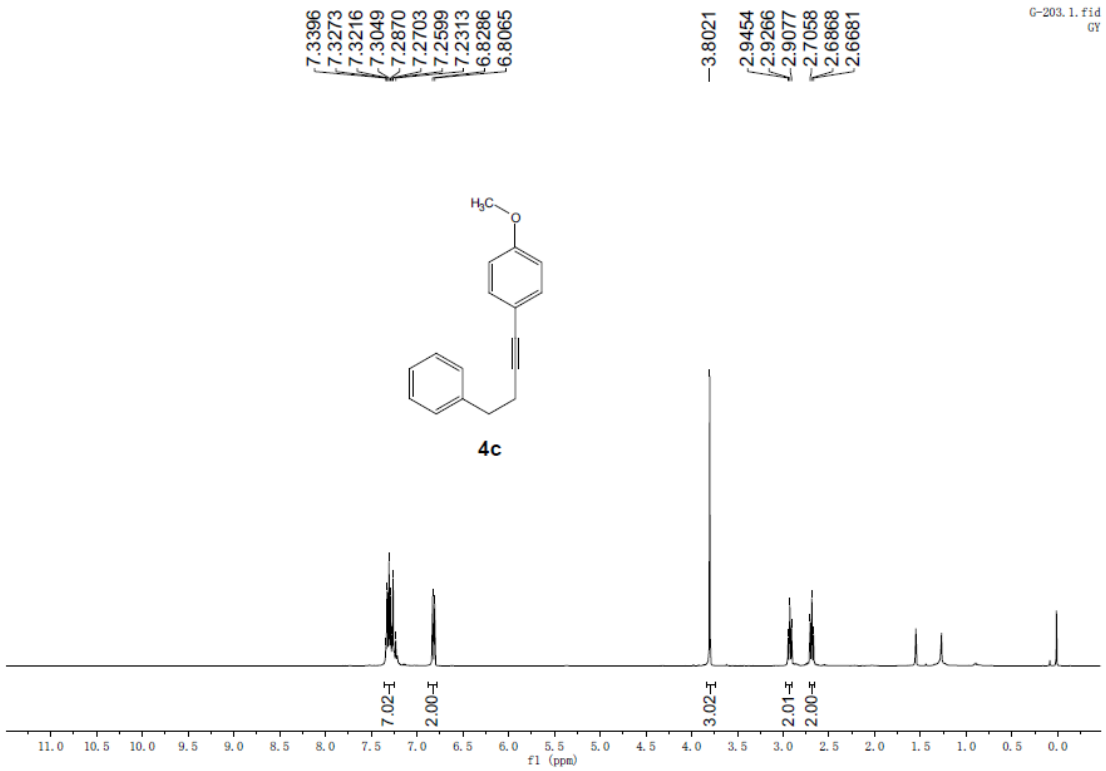
7.3288
7.3174
7.2991
7.2749
7.2600
7.1258
7.1062
2.9761
2.9573
2.9385
2.7401
2.7213
2.7026
2.3629
G-207/1
GY
CH3
4b
7.00
2.00
2.02
2.02
3.00
f1 (ppm)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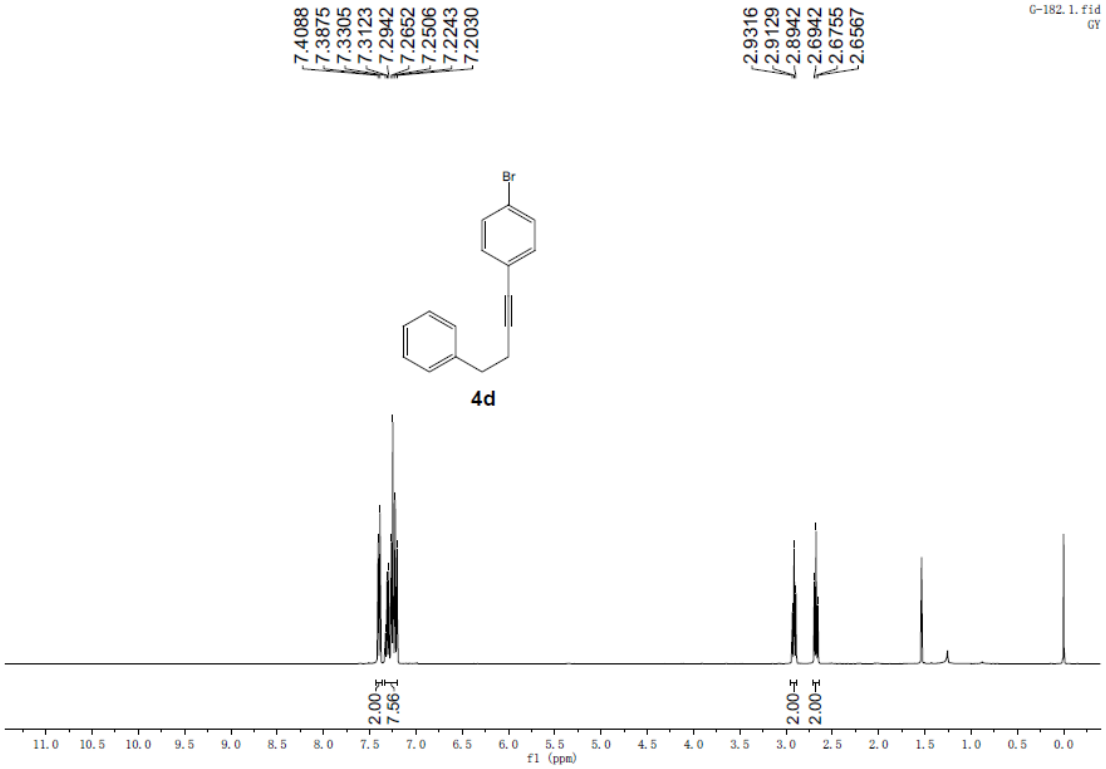
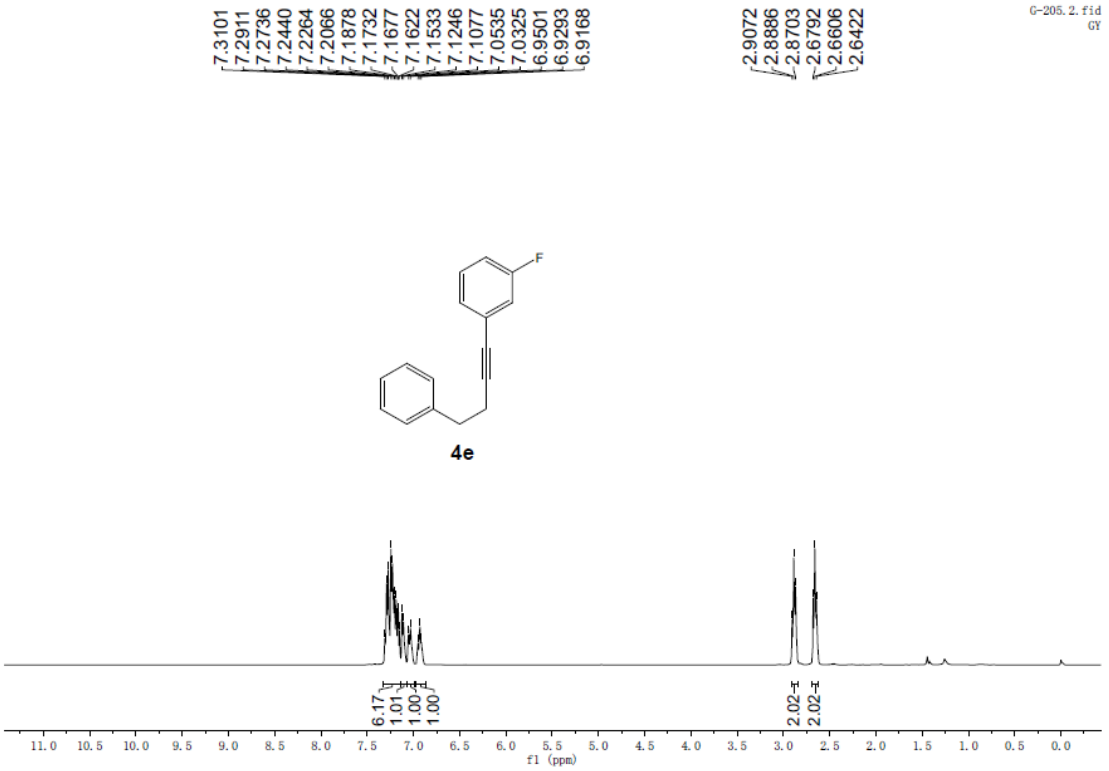
7.3216
7.3049
7.2870
7.2703
7.2599
7.2313
6.8286
6.8065
3.8021
2.9454
2.9266
2.9077
2.7058
2.6868
2.6681
G-203.1.fid
GY
H3C
O
4c
7.02
2.00
3.02
2.01
2.00
f1 (ppm)


7.4088
7.3875
7.3305
7.3123
7.2942
7.2652
7.2506
7.2243
7.2030
2.9316
2.9129
2.8942
2.6942
2.6755
2.6567
G-182.1.fid
GY
Br
4d
2.00
7.56
2.00
2.00
f1 (ppm)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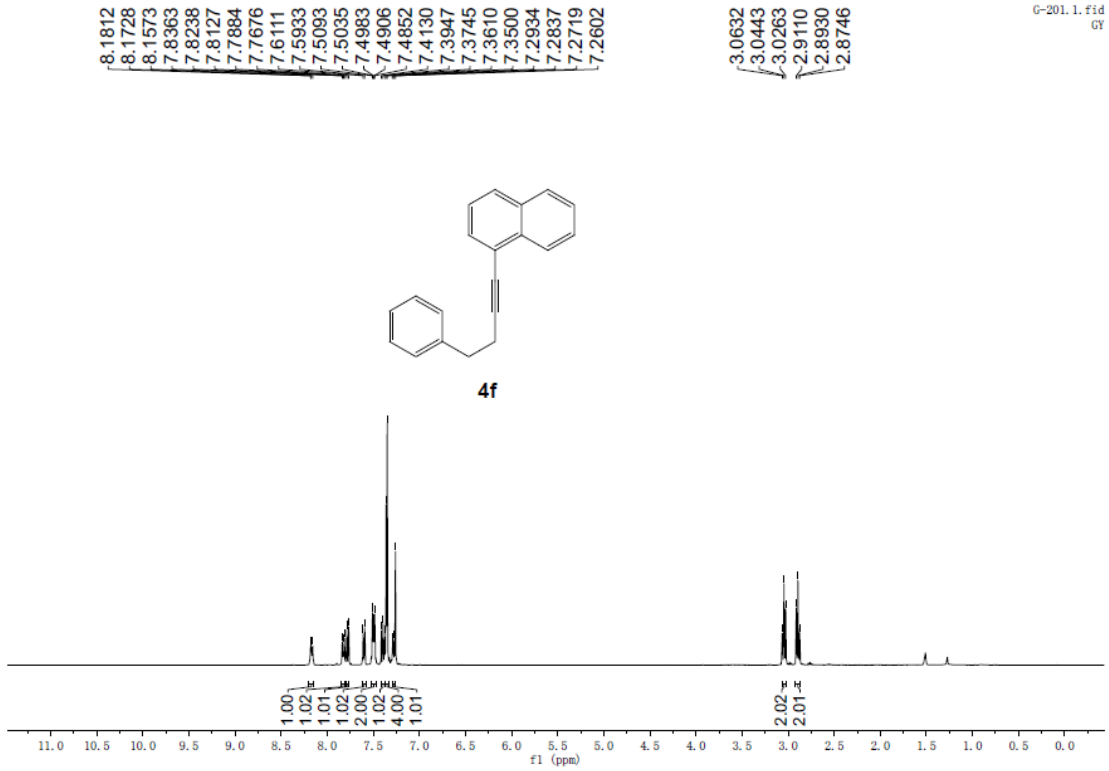
7.2911
7.2736
7.2440
7.2264
7.2066
7.1878
7.1732
7.1677
7.1622
7.1533
7.1246
7.1077
7.0535
7.0325
6.9501
6.9293
6.9168
2.9072
2.8886
2.8703
2.6792
2.6606
2.6422
G-205.2.fid
GY
F
4e
6.17
1.01
1.00
1.00
2.02
2.02
f1 (ppm)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7.8127
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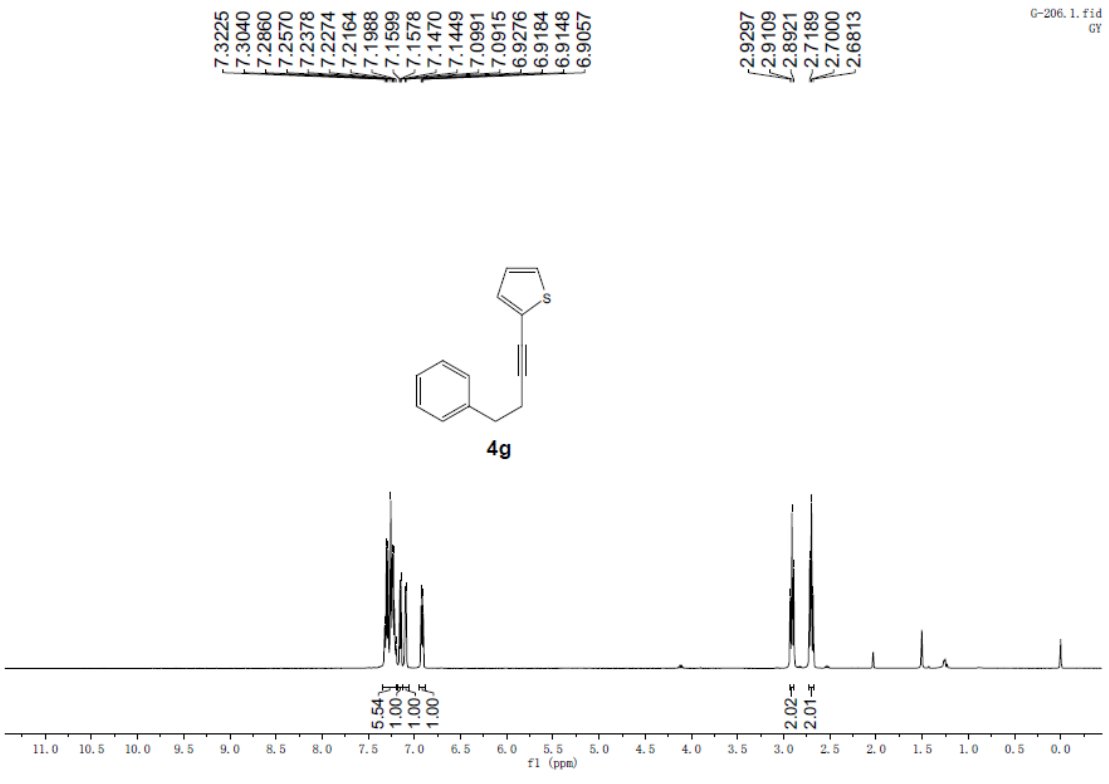
7.7676
7.6111
7.5933
7.5093
7.5035
7.4983
7.4906
7.4852
7.4130
7.3947
7.3745
7.3610
7.3500
7.2934
7.2837
7.2719
7.2602
3.0632
3.0443
3.0263
2.9110
2.8930
2.8746
G-201.1.fid
GY
4f
1.00
1.02
1.01
1.02
2.00
1.02
4.00
1.01
2.02
2.01
f1 (ppm)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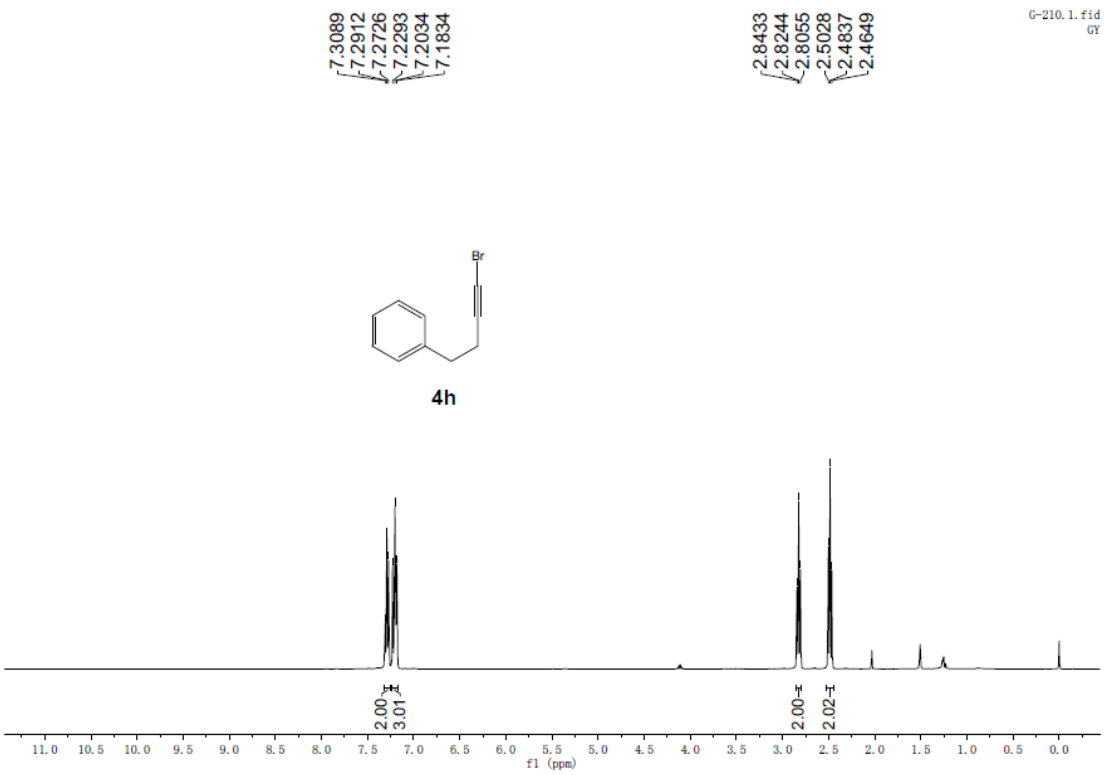
7.2860
7.2570
7.2378
7.2274
7.2164
7.1988
7.1599
7.1578
7.1470
7.1449
7.0991
7.0915
6.9276
6.9184
6.9148
6.9057
2.9297
2.9109
2.8921
2.7189
2.7000
2.6813
G-206.1.fid
GY
S
4g
5.54
1.00
1.00
1.00
2.02
2.01
f1 (ppm)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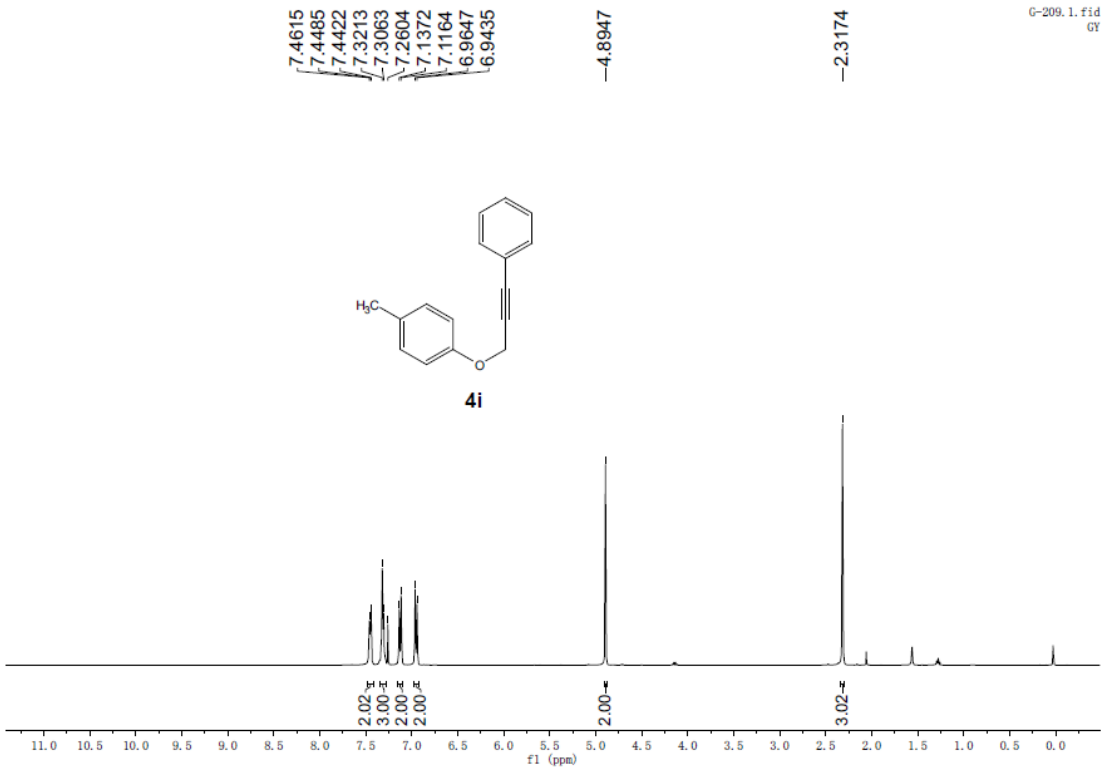
7.2726
7.2293
7.2034
7.1834
2.8433
2.8244
2.8055
2.5028
2.4837
2.4649
G-210.1.fid
GY
Br
4h
2.00
3.01
2.00
2.02
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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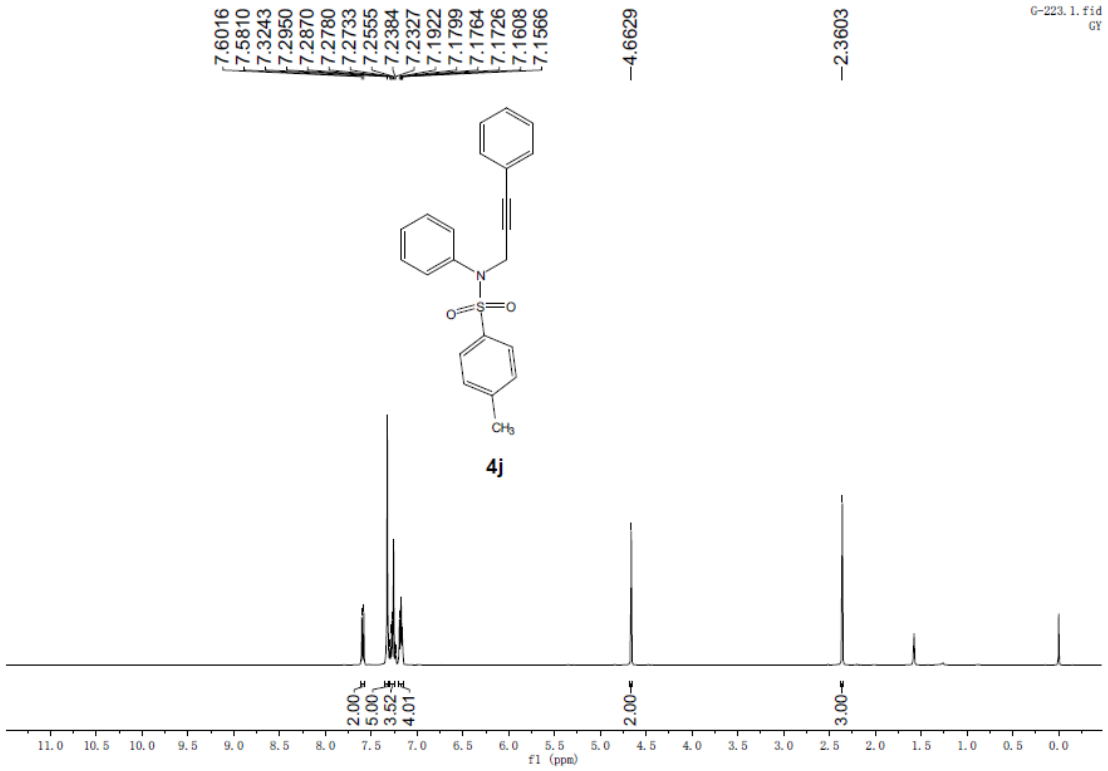
7.4422
7.3213
7.3063
7.2604
7.1372
7.1164
6.9647
6.9435
4.8947
2.3174
G-209.1.fid
GY
H3C
O
4i
2.02
3.00
2.00
2.00
2.00
3.02
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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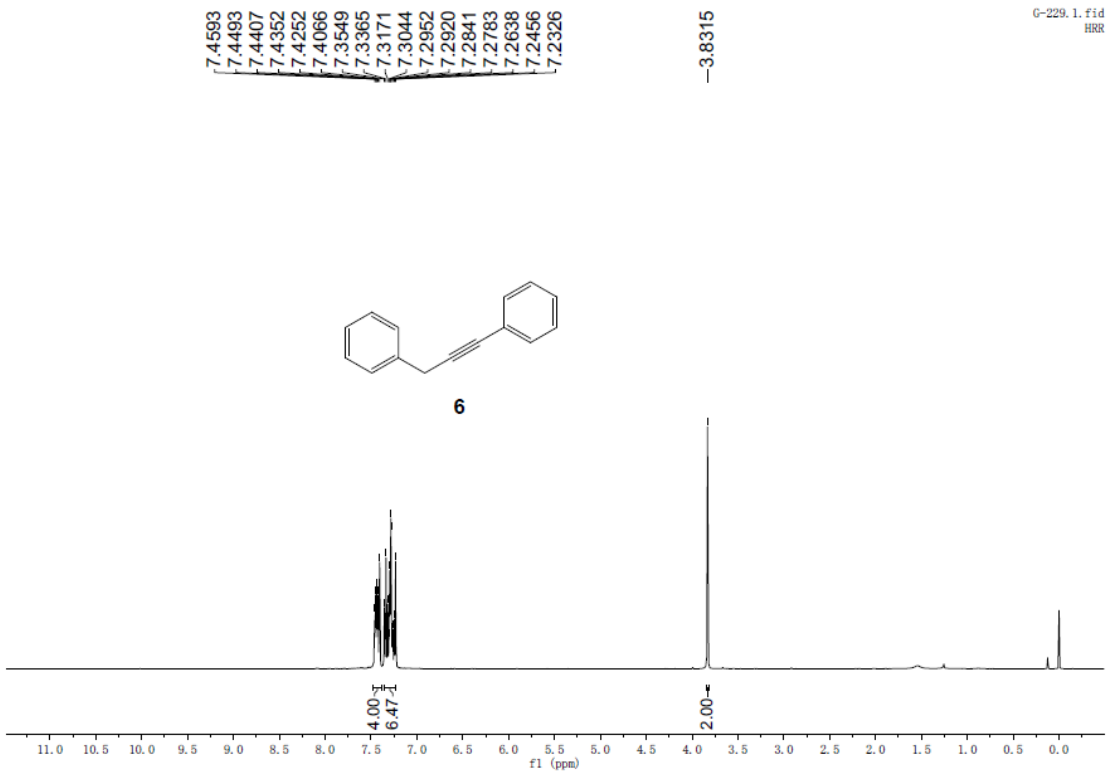
7.2780
7.2733
7.2555
7.2384
7.2327
7.1922
7.1799
7.1764
7.1726
7.1608
7.1566
4.6629
2.3603
G-223.1.fid
GY
4j
2.00
5.00
3.52
4.01
2.00
3.00
f1 (ppm)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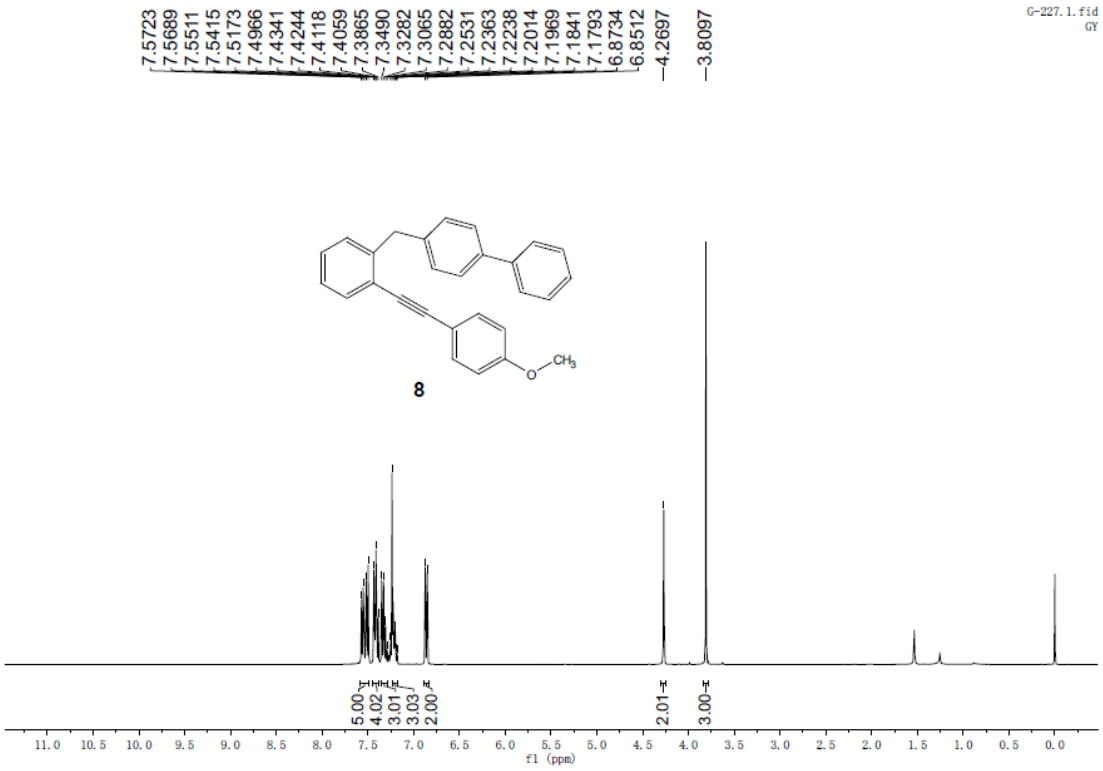
7.4407
7.4352
7.4252
7.4066
7.3549
7.3365
7.3171
7.3044
7.2952
7.2920
7.2841
7.2783
7.2638
7.2456
7.2326
3.8315
G-229.1.fid
HRR
6
4.00
6.47
2.00
f1 (ppm)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7.4118
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7.3865
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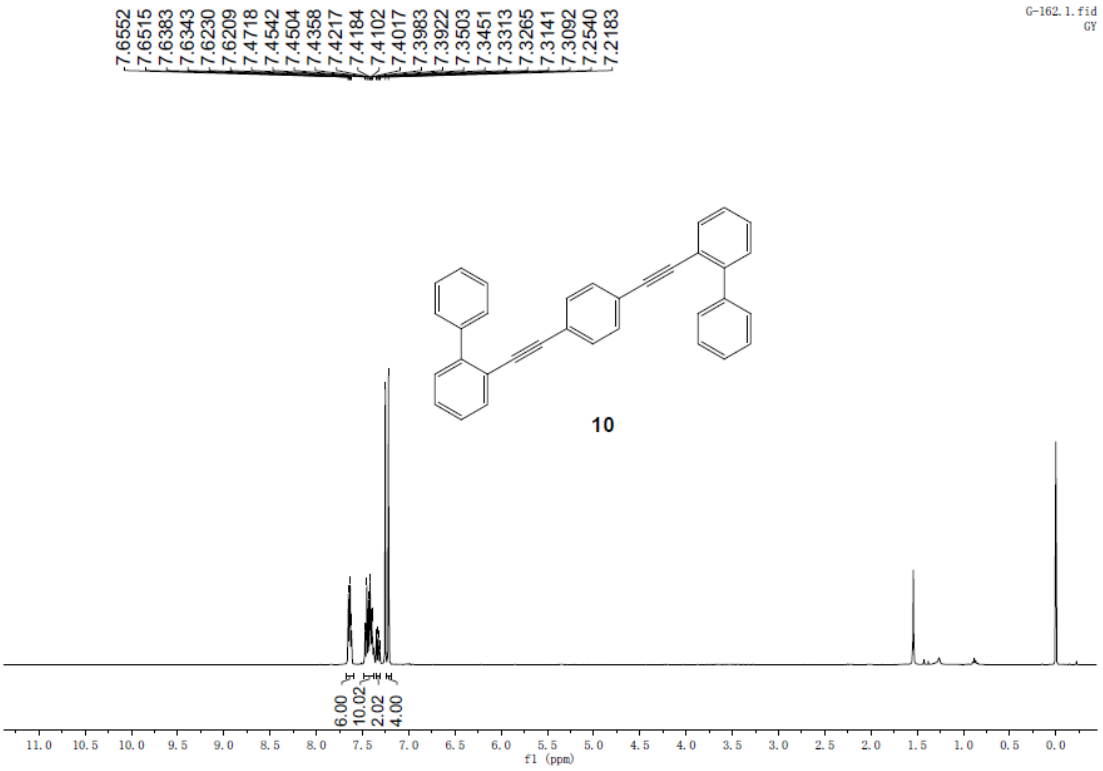
7.3282
7.3065
7.2882
7.2531
7.2363
7.2238
7.2014
7.1969
7.1841
7.1793
6.8734
6.8512
4.2697
3.8097
O
CH3
8
5.00
4.02
3.01
3.03
2.00
2.01
3.00
f1 (ppm)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7.4358
7.4217
7.4184
7.4102
7.4017
7.3983
7.3922
7.3503
7.3451
7.3313
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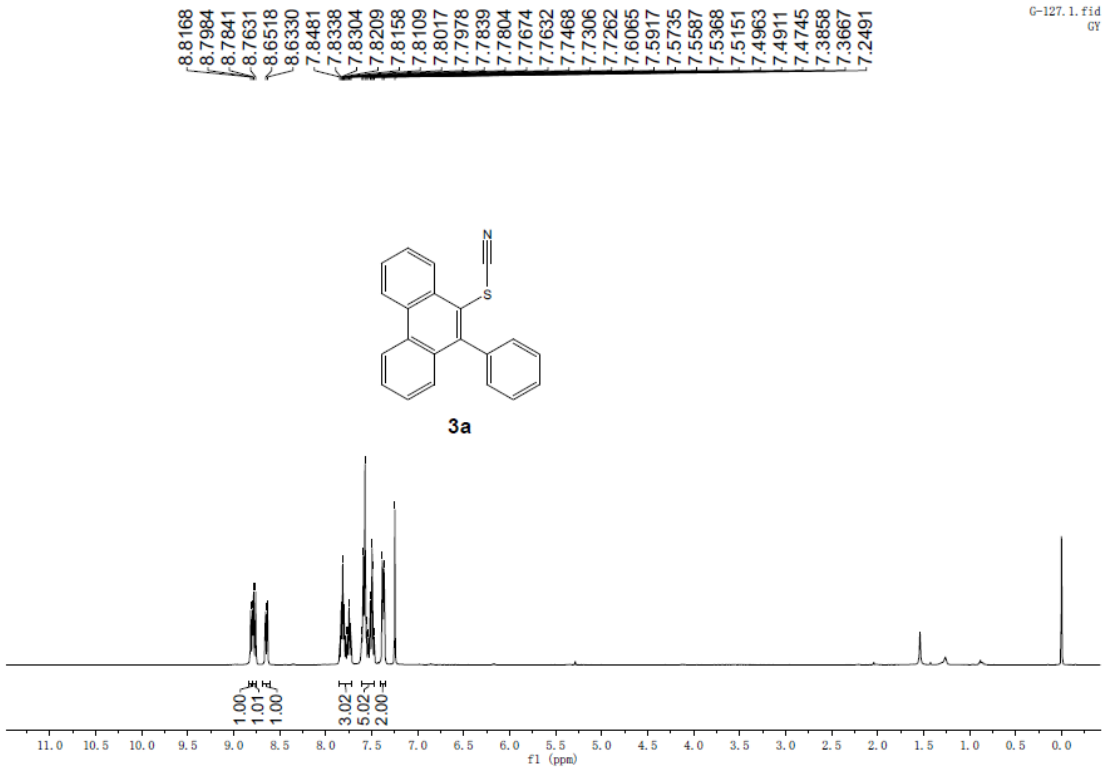
7.2183
10
6.00
10.02
2.02
4.00
f1 (ppm)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7.8017
7.7978
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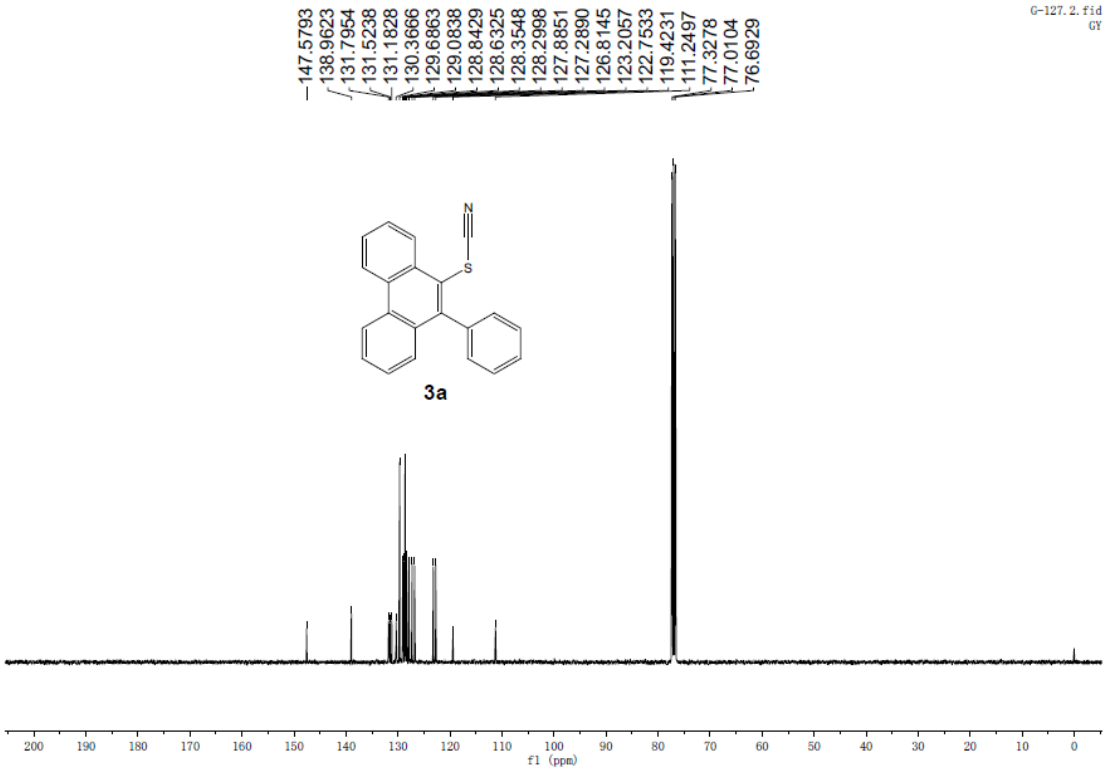
7.7674
7.7632
7.7468
7.7306
7.7262
7.6065
7.5917
7.5735
7.5587
7.5368
7.5151
7.4963
7.4911
7.4745
7.3858
7.3667
7.2491
G-127.1.fid
GY
N
S
3a
1.00
1.01
1.00
3.02
5.02
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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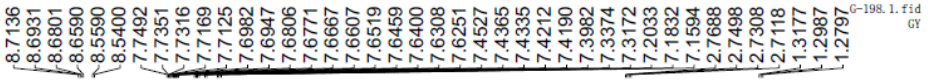
131.1828
130.3666
129.6863
129.0838
128.8429
128.6325
128.3548
128.2998
127.8851
127.2890
126.8145
123.2057
122.7533
119.4231
111.2497
77.3278
77.0104
76.6929
G-127.2.fid
GY
N
S
3a
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.5590
8.5400
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7.6607
7.6519
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7.6400
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7.6251
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7.3982
7.3374
7.3172
7.2033
7.1832
7.1594
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2.7498
2.7308
2.7118
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1.2987
1.2797
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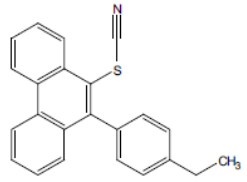
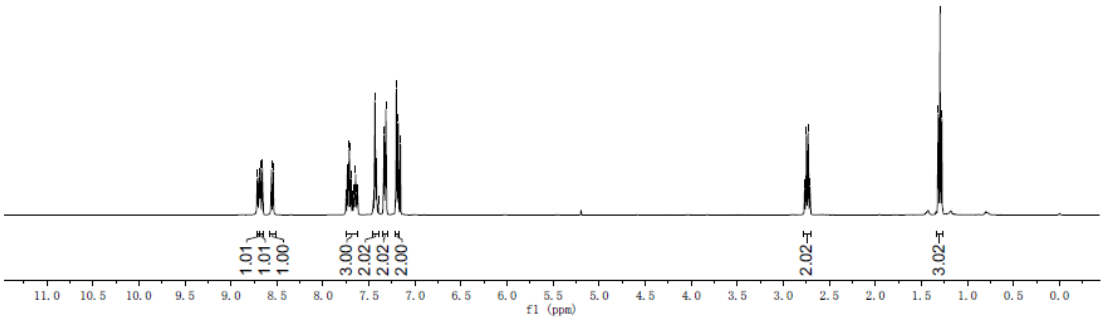
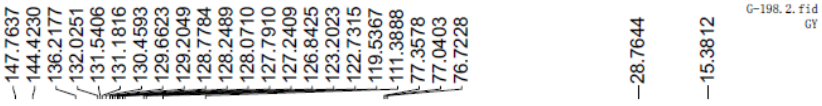
GY


N
S
CH3

3b


1.01
1.01
1.00
3.00
2.02
2.02
2.00
2.02
3.02
11.0 10.5 10.0 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 0.0
f1 (ppm)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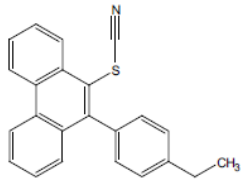
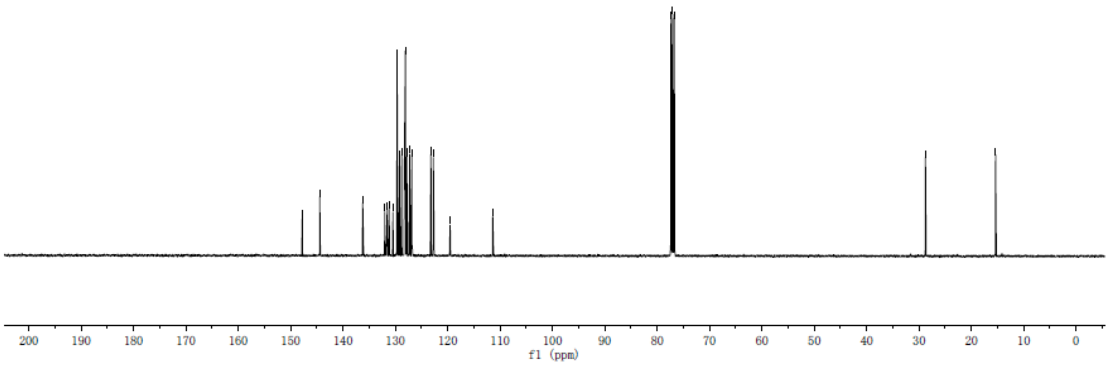
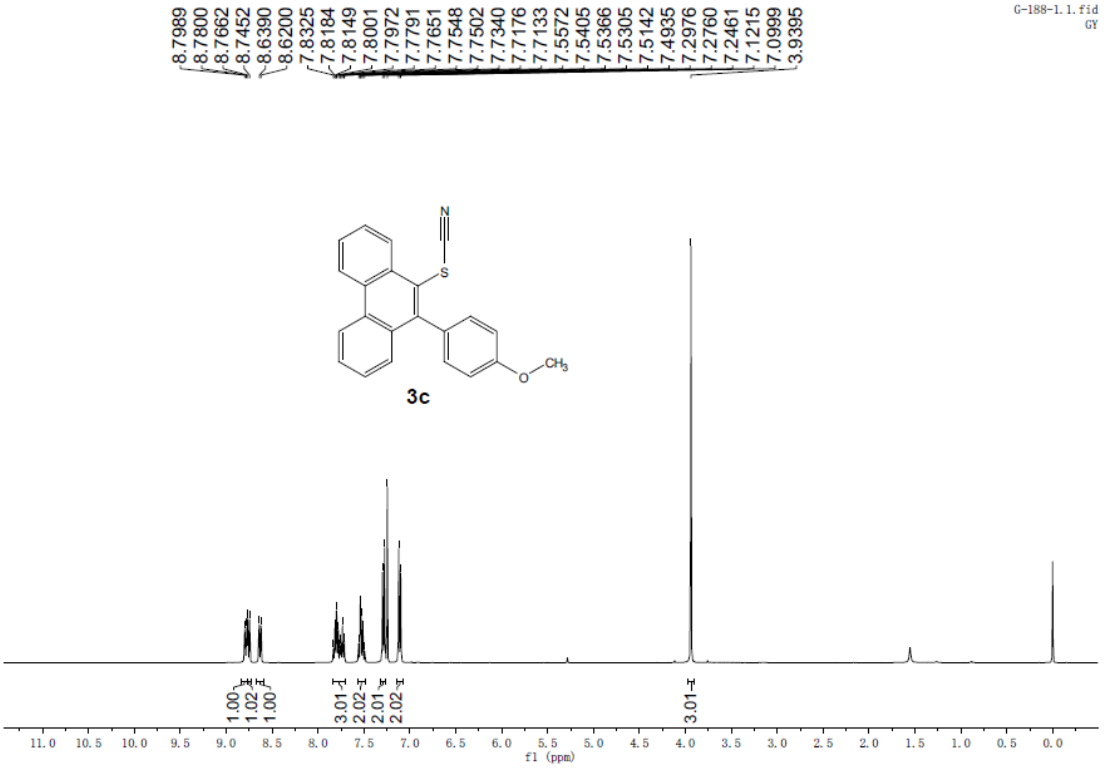
136.2177
132.0251
131.5406
131.1816
130.4593
129.6623
129.2049
128.7784
128.2489
128.0710
127.7910
127.2409
126.8425
123.2023
122.7315
119.5367
111.3888
77.3578
77.0403
76.7228
28.7644
15.3812
G-198.2.fid
GY


N
S
CH3

3b


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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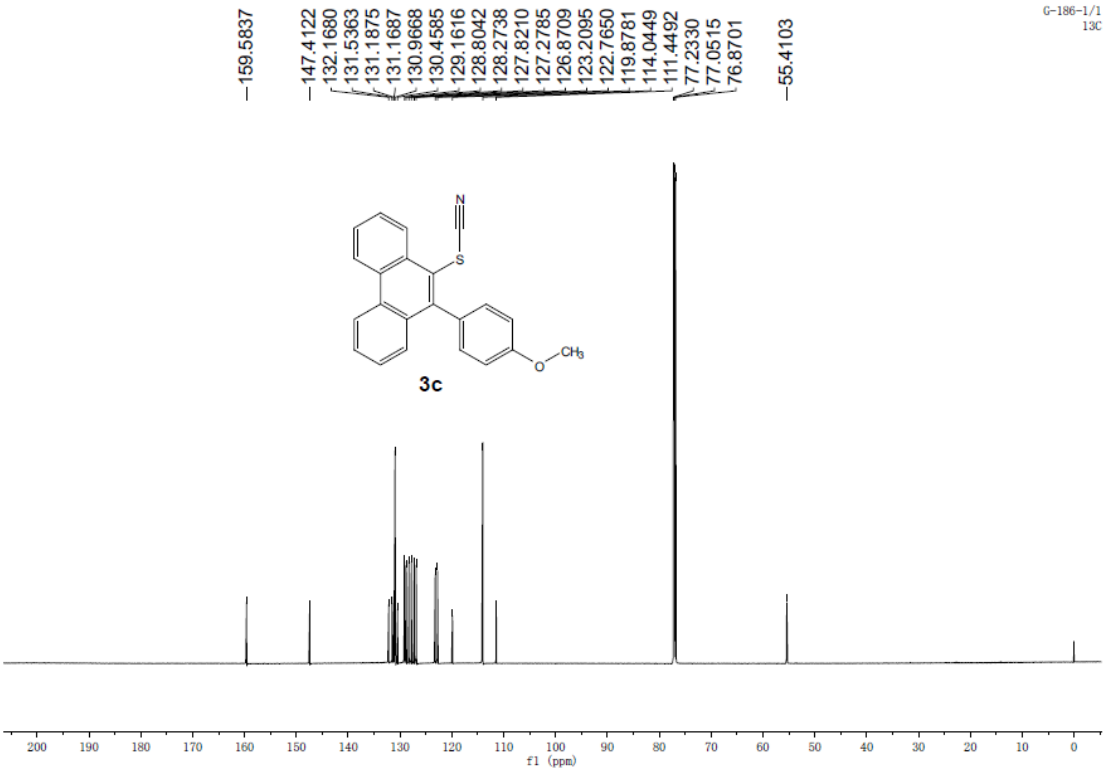
8.7800
8.7662
8.7452
8.6390
8.6200
7.8325
7.8184
7.8149
7.8001
7.7972
7.7791
7.7651
7.7548
7.7502
7.7340
7.7176
7.7133
7.5572
7.5405
7.5366
7.5305
7.5142
7.4935
7.2976
7.2760
7.2461
7.1215
7.0999
3.9395
G-188-1.1.fid
GY
N
S
O
CH3
3c
1.00
1.02
1.00
3.01
2.02
2.01
2.02
3.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 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 0.0
f1 (ppm)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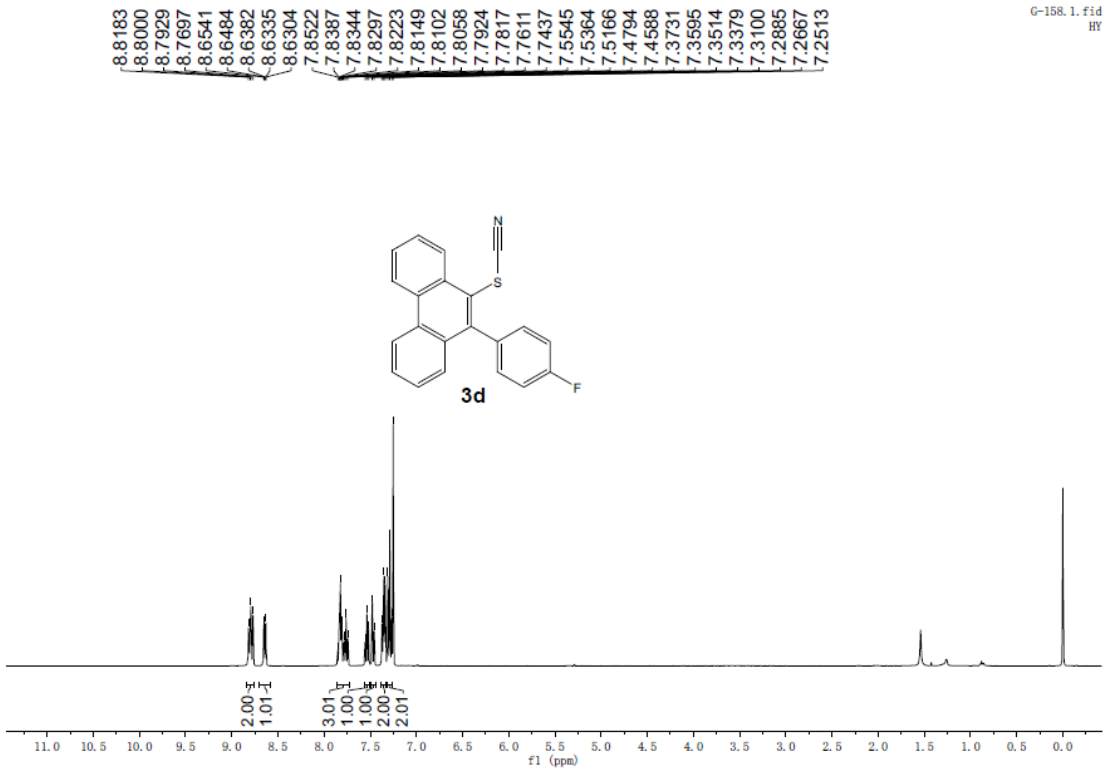
131.1875
131.1687
130.9668
130.4585
129.1616
128.8042
128.2738
127.8210
127.2785
126.8709
123.2095
122.7650
119.8781
114.0449
111.4492
77.2330
77.0515
76.8701
55.4103
G-186-1/1
13C
N
S
O
CH3
3c
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.8000
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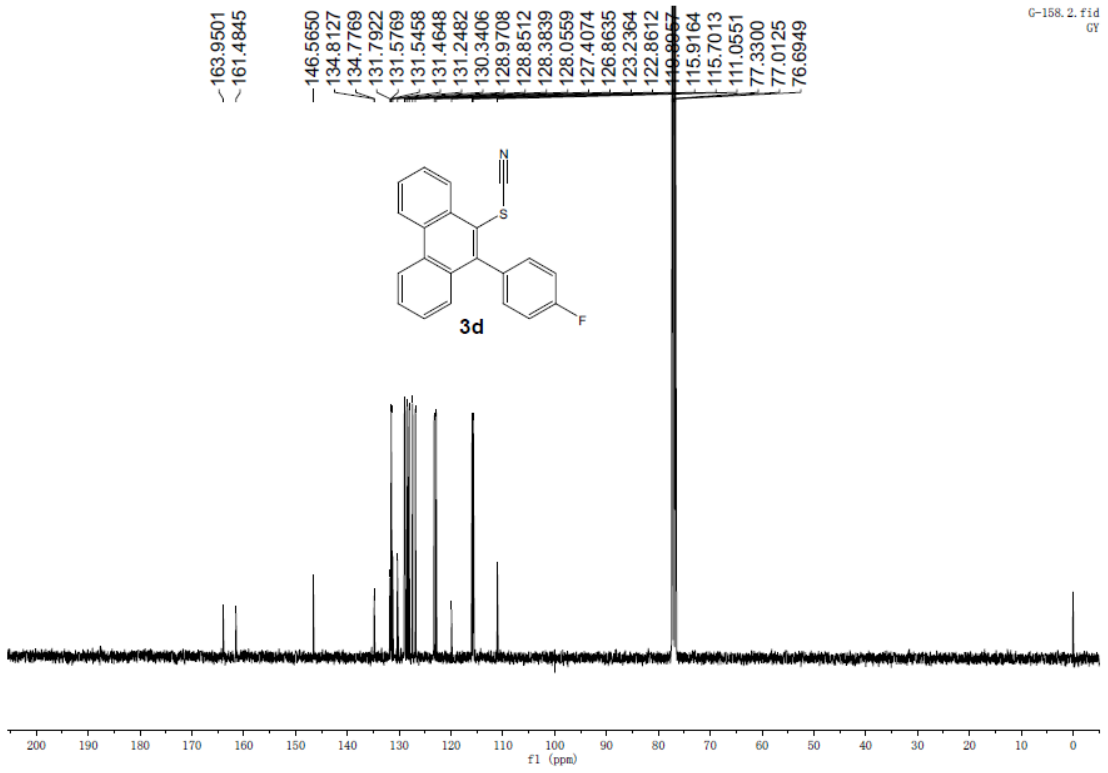
8.7697
8.6541
8.6484
8.6382
8.6335
8.6304
7.8522
7.8387
7.8344
7.8297
7.8223
7.8149
7.8102
7.8058
7.7924
7.7817
7.7611
7.7437
7.5545
7.5364
7.5166
7.4794
7.4588
7.3731
7.3595
7.3514
7.3379
7.3100
7.2885
7.2667
7.2513
G-158.1.fid
HY
N
S
F
3d
2.00
1.01
3.01
1.00
1.00
2.00
2.01
11.0 10.5 10.0 9.5 9.0 8.5 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 0.0
f1 (ppm)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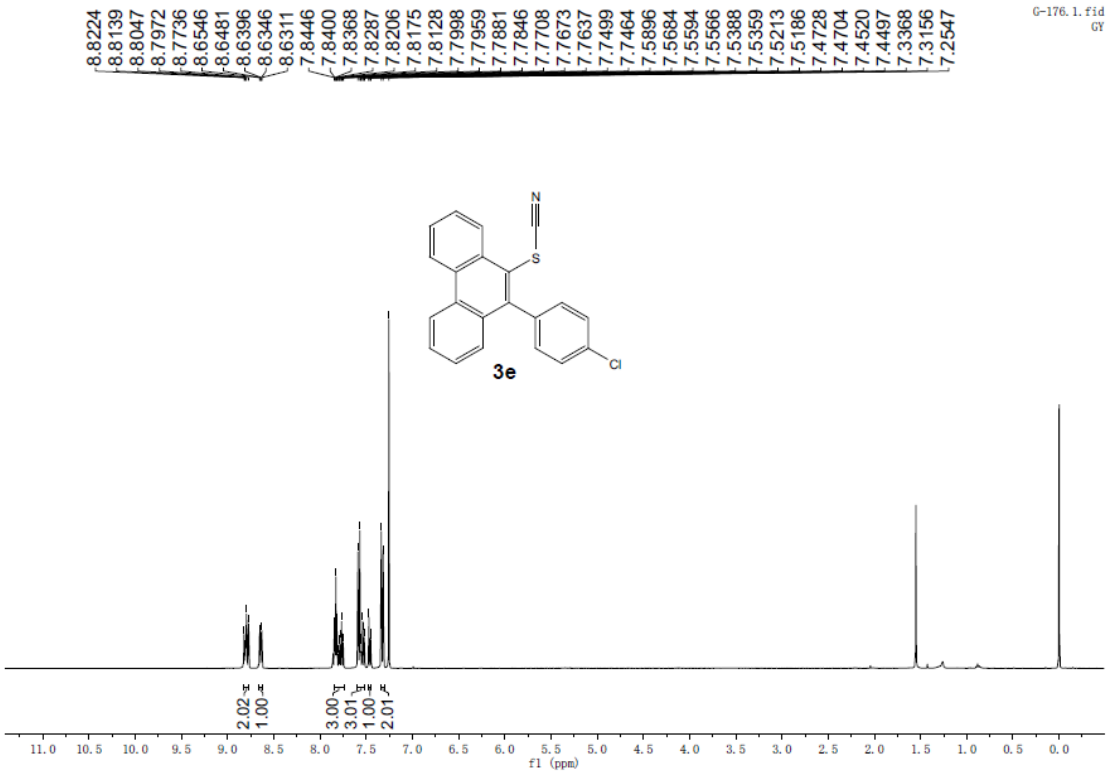
161.4845
146.5650
134.8127
134.7769
131.7922
131.5769
131.5458
131.4648
131.2482
130.3406
128.9708
128.8512
128.3839
128.0559
127.4074
126.8635
123.2364
122.8612
115.9164
115.7013
111.0551
77.3300
77.0125
76.6949
G-158.2.fid
GY
N
S
F
3d
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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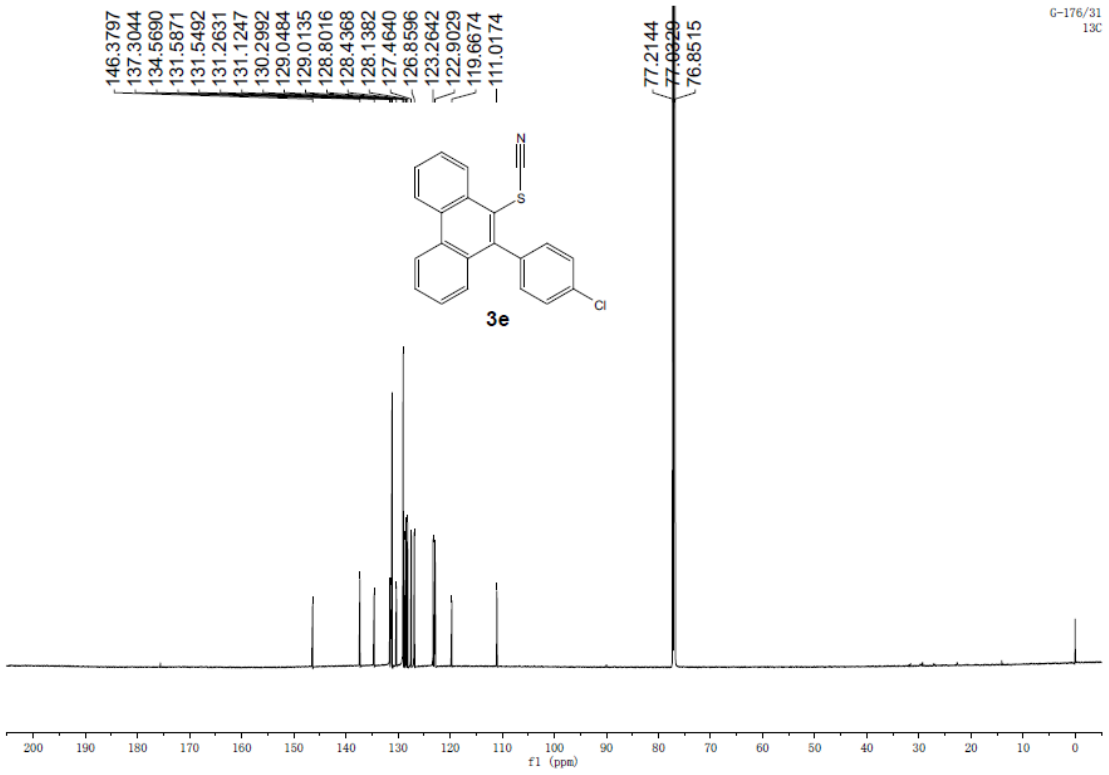
8.8139
8.8047
8.7972
8.7736
8.6546
8.6481
8.6396
8.6346
8.6311
7.8446
7.8400
7.8368
7.8287
7.8206
7.8175
7.8128
7.7998
7.7959
7.7881
7.7846
7.7708
7.7673
7.7637
7.7499
7.7464
7.5896
7.5684
7.5594
7.5566
7.5388
7.5359
7.5213
7.5186
7.4728
7.4704
7.4520
7.4497
7.3368
7.3156
7.2547
G-176.1.fid
GY
N
S
Cl
3e
2.02
1.00
3.00
3.01
1.00
2.01
f1 (ppm)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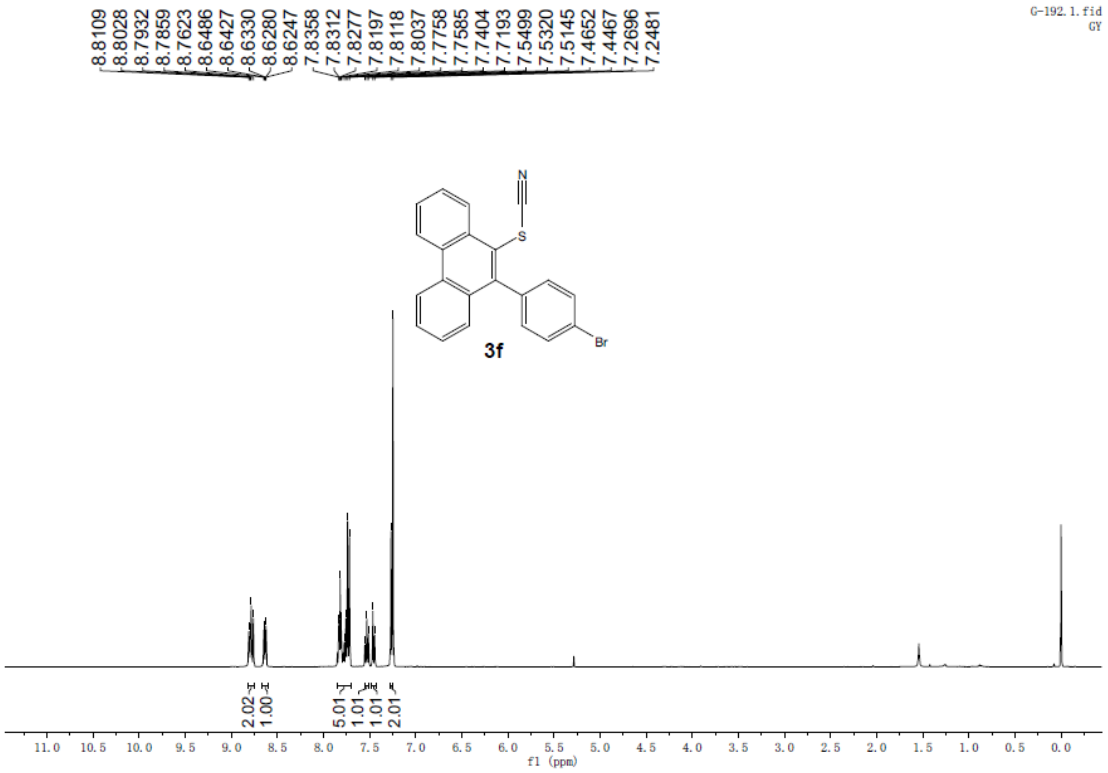
137.3044
134.5690
131.5871
131.5492
131.2631
131.1247
130.2992
129.0484
129.0135
128.8016
128.4368
128.1382
127.4640
126.8596
123.2642
122.9029
119.6674
111.0174
77.2144
77.0829
76.8515
G-176/31
13C
N
S
Cl
3e
f1 (ppm)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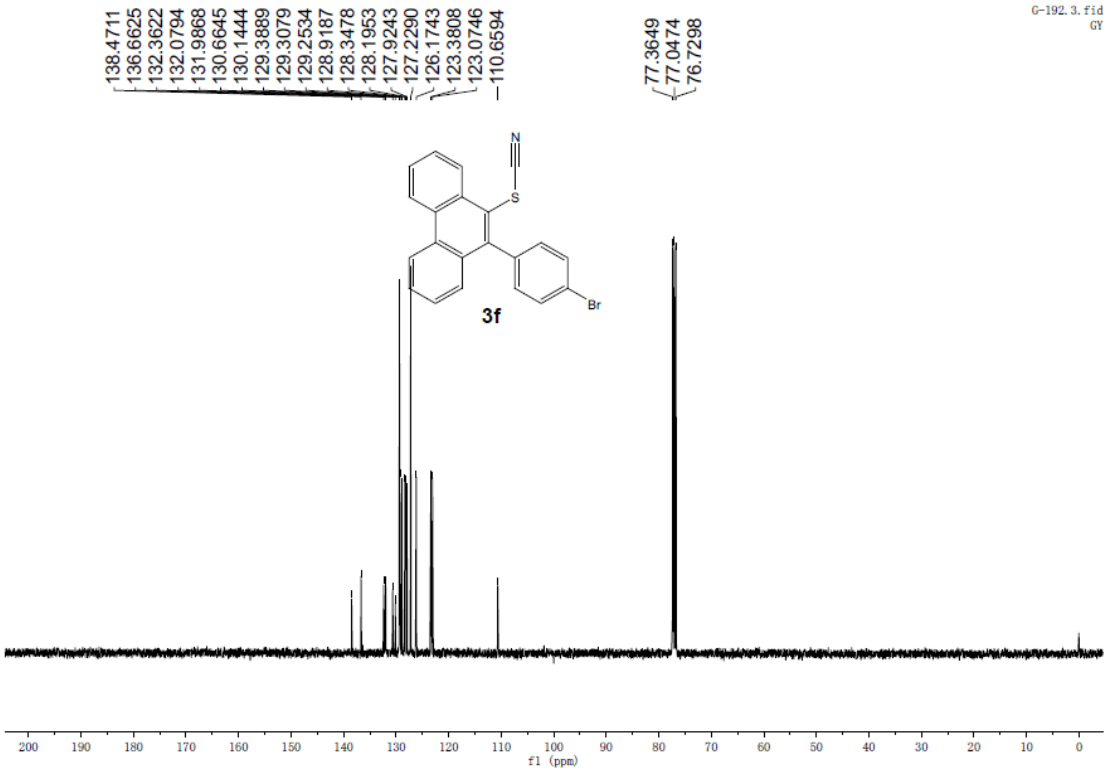
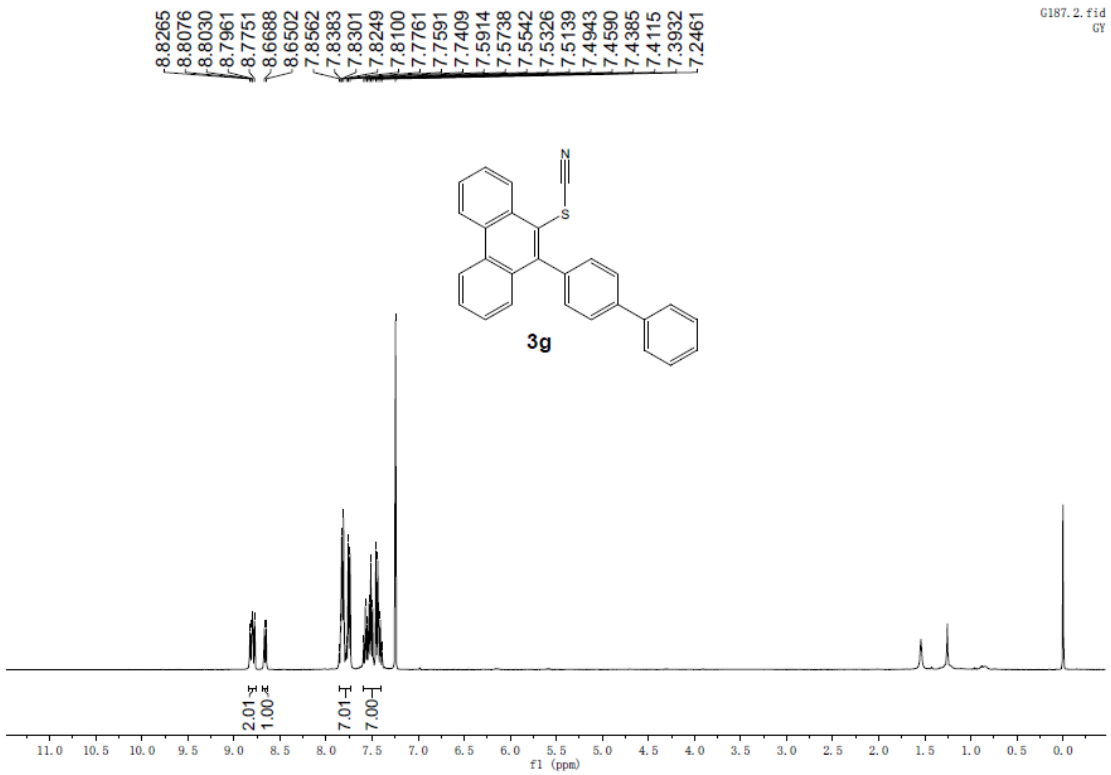
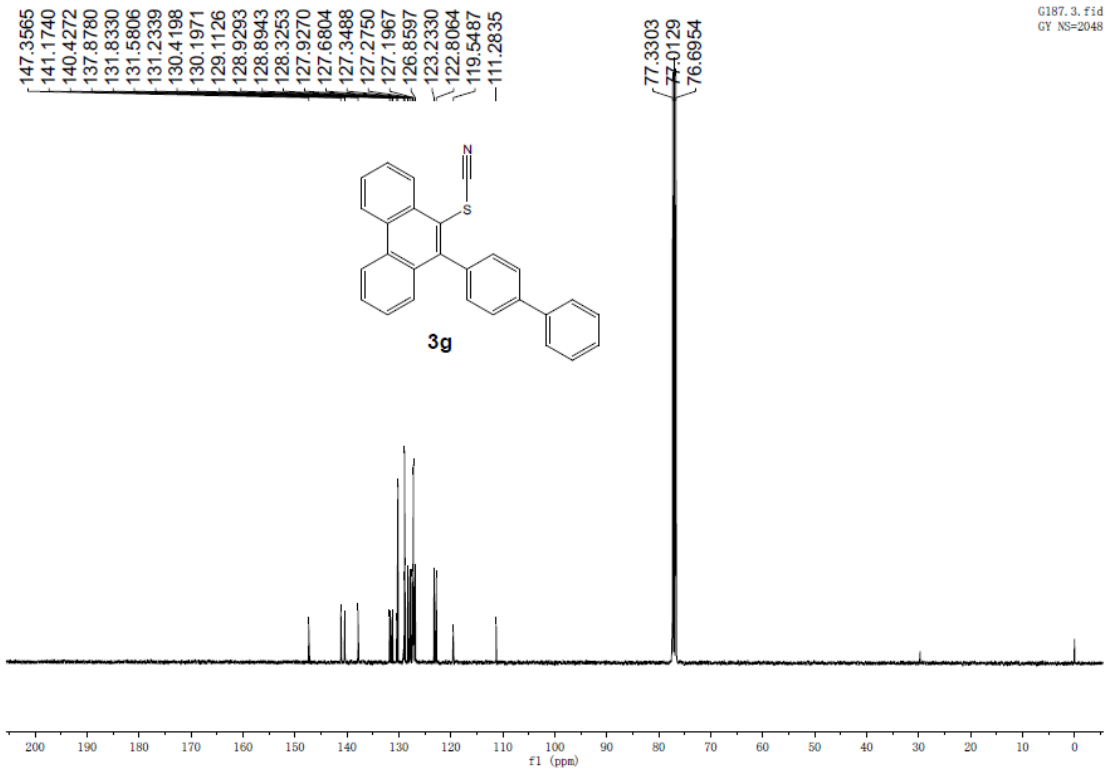
8.8028
8.7932
8.7859
8.7623
8.6486
8.6427
8.6330
8.6280
8.6247
7.8358
7.8312
7.8277
7.8197
7.8118
7.8037
7.7758
7.7585
7.7404
7.7193
7.5499
7.5320
7.5145
7.4652
7.4467
7.2696
7.2481
G-192.1.fid
GY
N
S
Br
3f
2.02
1.00
5.01
1.01
1.01
2.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


138.4711
136.6625
132.3622
132.0794
131.9868
130.6645
130.1444
129.3889
129.3079
129.2534
128.9187
128.3478
128.1953
127.9243
127.2290
126.1743
123.3808
123.0746
110.6594
77.3649
77.0474
76.7298
G-192.3.fid
GY
N
S
Br
3f
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


G187.2.fid
GY
8.8265
8.8076
8.8030
8.7961
8.7751
8.6688
8.6502
7.8562
7.8383
7.8301
7.8249
7.8100
7.7761
7.7591
7.7409
7.5914
7.5738
7.5542
7.5326
7.5139
7.4943
7.4590
7.4385
7.4115
7.3932
7.2461
3g
2.01
1.00
7.01
7.00
f1 (ppm)


G187.3.fid
GY NS=2048
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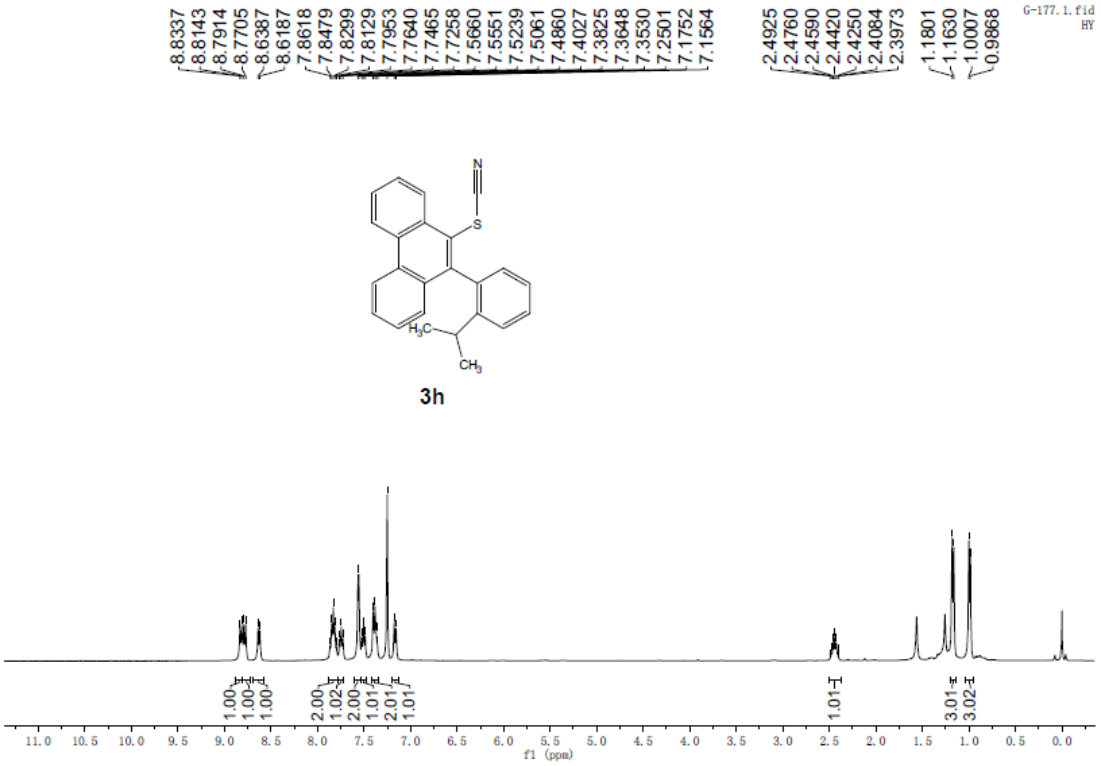
141.1740
140.4272
137.8780
131.8330
131.5806
131.2339
130.4198
130.1971
129.1126
128.9293
128.8943
128.3253
127.9270
127.6804
127.3488
127.2750
127.1967
126.8597
123.2330
122.8064
119.5487
111.2835
77.3303
77.0129
76.6954
3g
f1 (ppm)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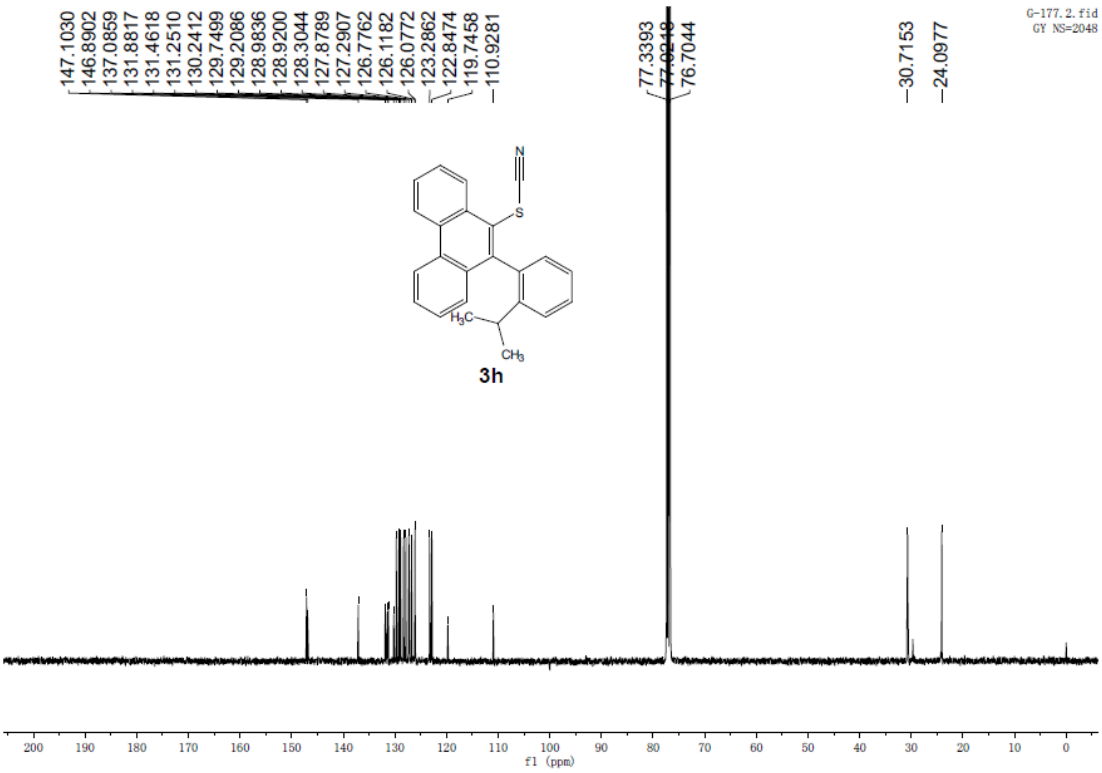
8.8143
8.7914
8.7705
8.6387
8.6187
7.8618
7.8479
7.8299
7.8129
7.7953
7.7640
7.7465
7.7258
7.5660
7.5551
7.5239
7.5061
7.4860
7.4027
7.3825
7.3648
7.3530
7.2501
7.1752
7.1564
2.4925
2.4760
2.4590
2.4420
2.4250
2.4084
2.3973
1.1801
1.1630
1.0007
0.9868
G-177.1.fid
HY
N
S
H3C
CH3
3h
1.00
1.00
1.00
2.00
1.02
2.00
1.01
2.01
1.01
1.01
3.01
3.02
11.0 10.5 10.0 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 0.0
f1 (ppm)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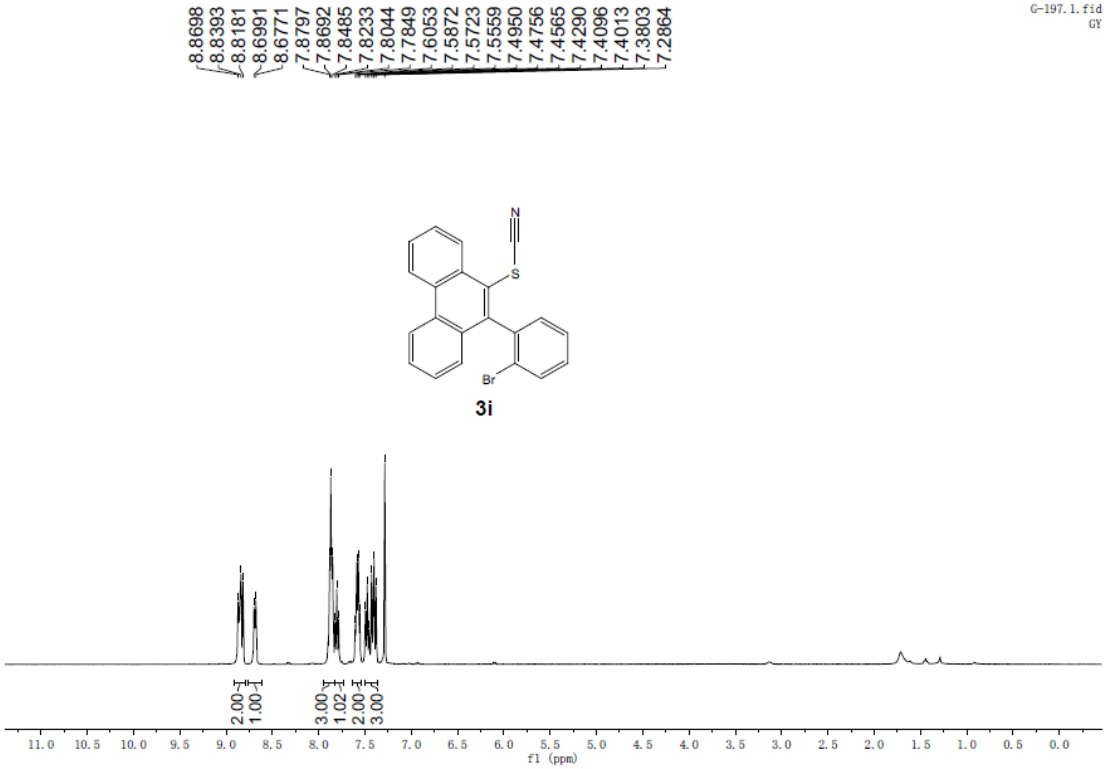
137.0859
131.8817
131.4618
131.2510
130.2412
129.7499
129.2086
128.9836
128.9200
128.3044
127.8789
127.2907
126.7762
126.1182
126.0772
123.2862
122.8474
119.7458
110.9281
77.3393
77.0218
76.7044
30.7153
24.0977
G-177.2.fid
GY NS=2048
N
S
H3C
CH3
3h
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


G-197.1.fid
GY
8.8698
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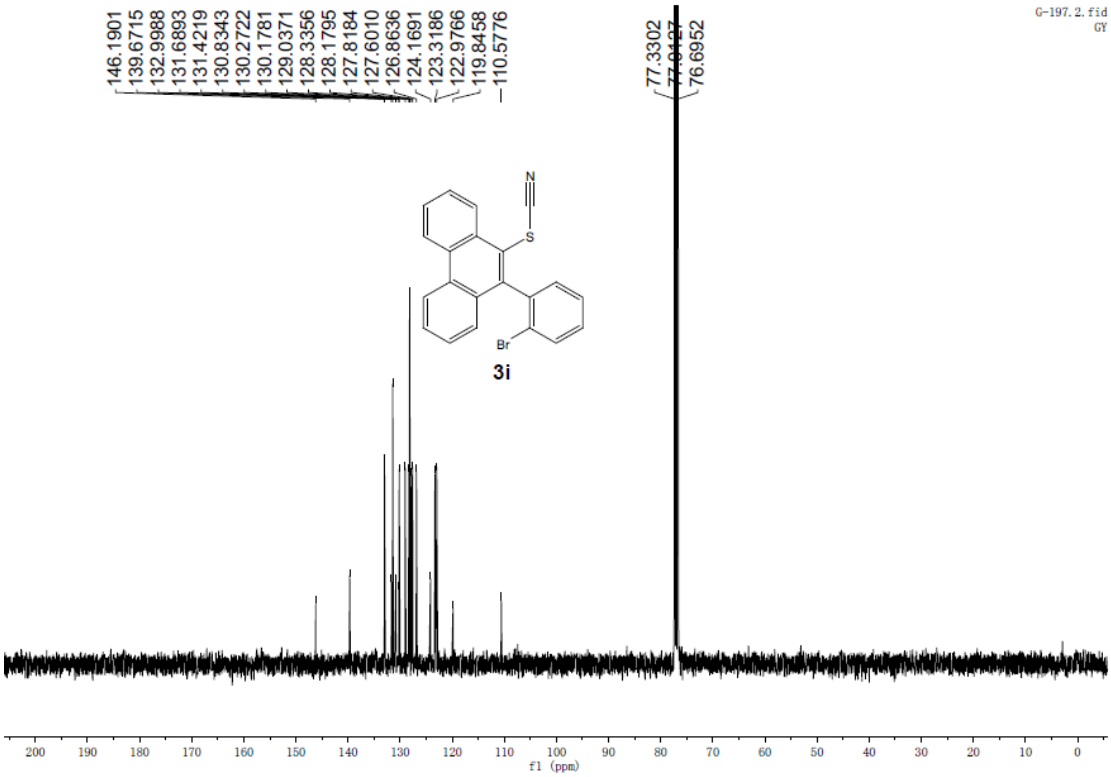
8.8181
8.6991
8.6771
7.8797
7.8692
7.8485
7.8233
7.8044
7.7849
7.6053
7.5872
7.5723
7.5559
7.4950
7.4756
7.4565
7.4290
7.4096
7.4013
7.3803
7.2864
N
S
Br
3i
2.00
1.00
3.00
1.02
2.00
3.00
f1 (ppm)


G-197.2.fid
GY
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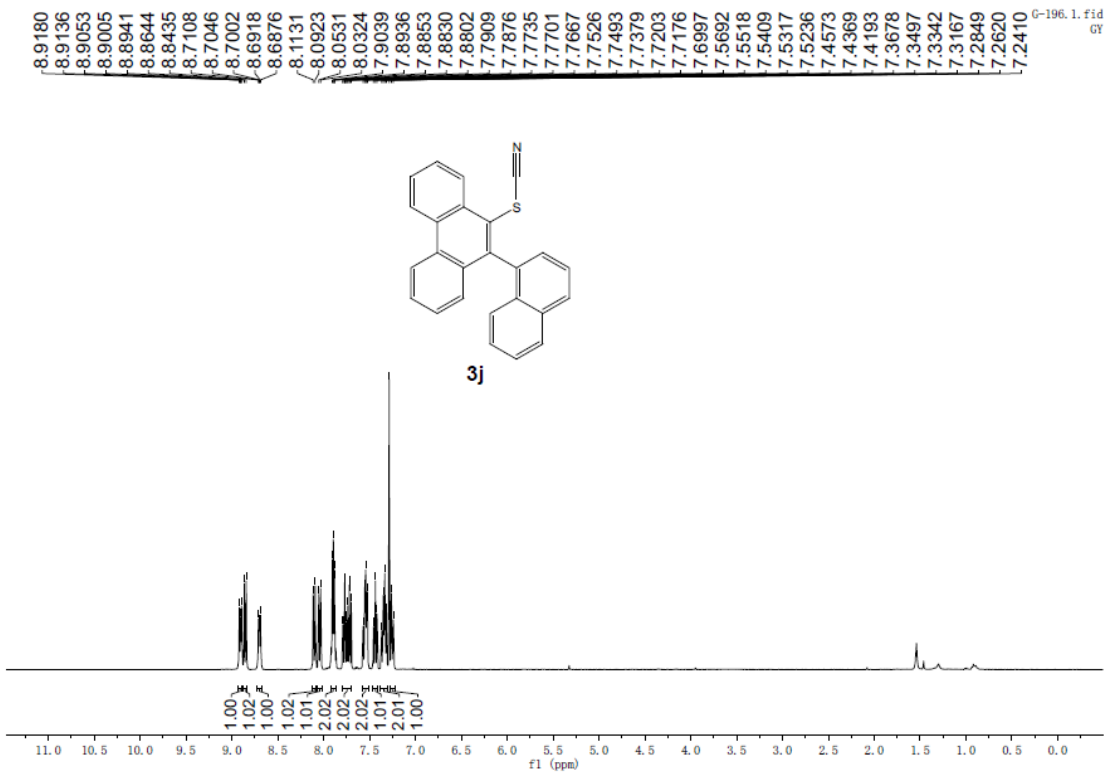
132.9988
131.6893
131.4219
130.8343
130.2722
130.1781
129.0371
128.3356
128.1795
127.8184
127.6010
126.8636
124.1691
123.3186
122.9766
119.8458
110.5776
77.3302
77.0427
76.6952
N
S
Br
3i
f1 (ppm)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8.9053
8.9005
8.8941
8.8644
8.8435
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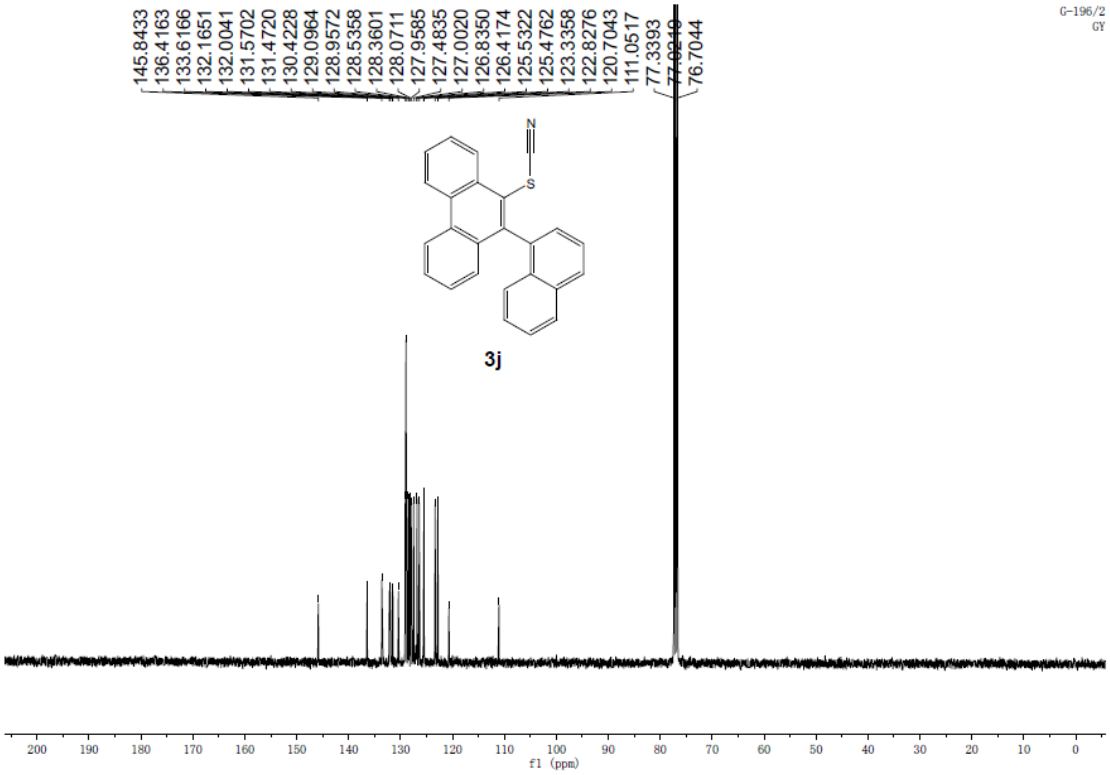
8.7046
8.7002
8.6918
8.6876
8.1131
8.0923
8.0531
8.0324
7.9039
7.8936
7.8853
7.8830
7.8802
7.7909
7.7876
7.7735
7.7701
7.7667
7.7526
7.7493
7.7379
7.7203
7.7176
7.6997
7.5692
7.5518
7.5409
7.5317
7.5236
7.4573
7.4369
7.4193
7.3678
7.3497
7.3342
7.3167
7.2849
7.2620
7.2410
G-196.1.fid
GY
N
S
3j
1.00
1.02
1.00
1.02
1.01
2.02
2.02
2.02
1.01
2.01
1.00
11.0 10.5 10.0 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 0.0
f1 (ppm)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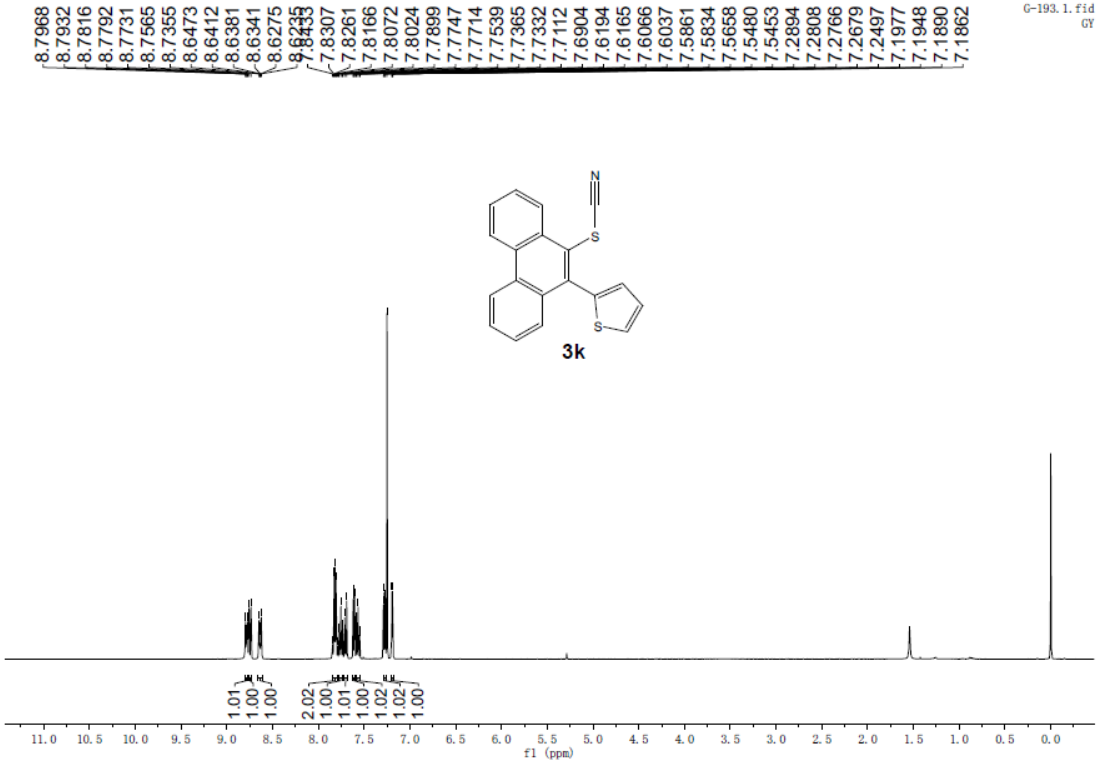
128.9572
128.5358
128.3601
128.0711
127.9585
127.4835
127.0020
126.8350
126.4174
125.5322
125.4762
123.3358
122.8276
120.7043
111.0517
77.3393
76.7044
G-196/2
GY
N
S
3j
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.7731
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8.7355
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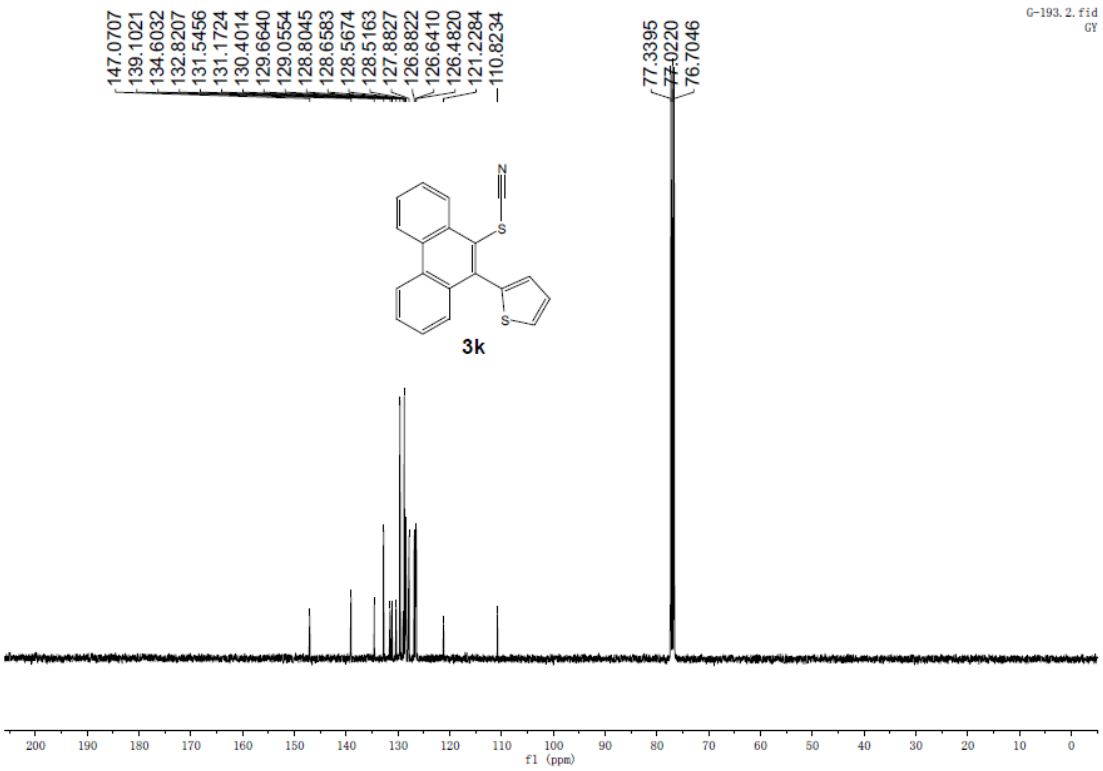
8.6412
8.6381
8.6341
8.6275
8.6235
8.8433
7.8307
7.8261
7.8166
7.8072
7.8024
7.7899
7.7747
7.7714
7.7539
7.7365
7.7332
7.7112
7.6904
7.6194
7.6165
7.6066
7.6037
7.5861
7.5834
7.5658
7.5480
7.5453
7.2894
7.2808
7.2766
7.2679
7.2497
7.1977
7.1948
7.1890
7.1862
G-193.1.fid
GY
N
S
S
3k
1.01
1.00
1.00
2.02
1.00
1.01
1.00
1.02
1.02
1.00
11.0 10.5 10.0 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 0.0
f1 (ppm)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132.8207
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131.1724
130.4014
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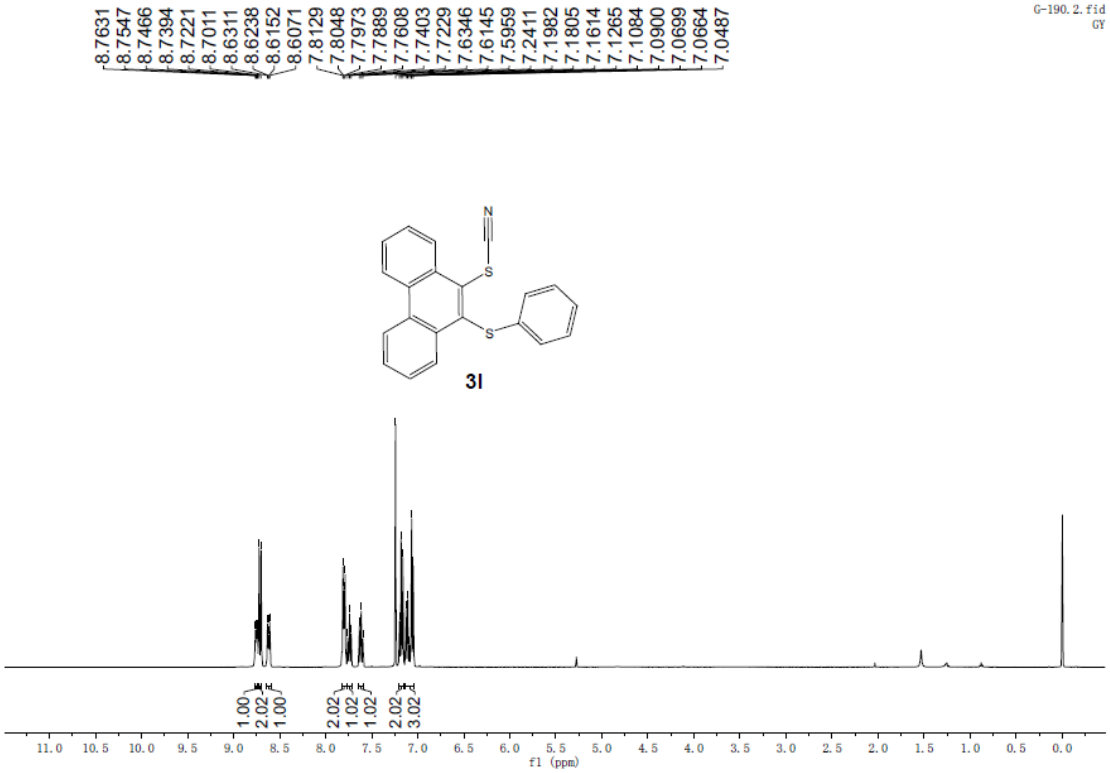
129.0554
128.8045
128.6583
128.5674
128.5163
127.8827
126.8822
126.6410
126.4820
121.2284
110.8234
77.3395
77.0220
76.7046
G-193.2.fid
GY
N
S
S
3k
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.7394
8.7221
8.7011
8.6311
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8.6152
8.6071
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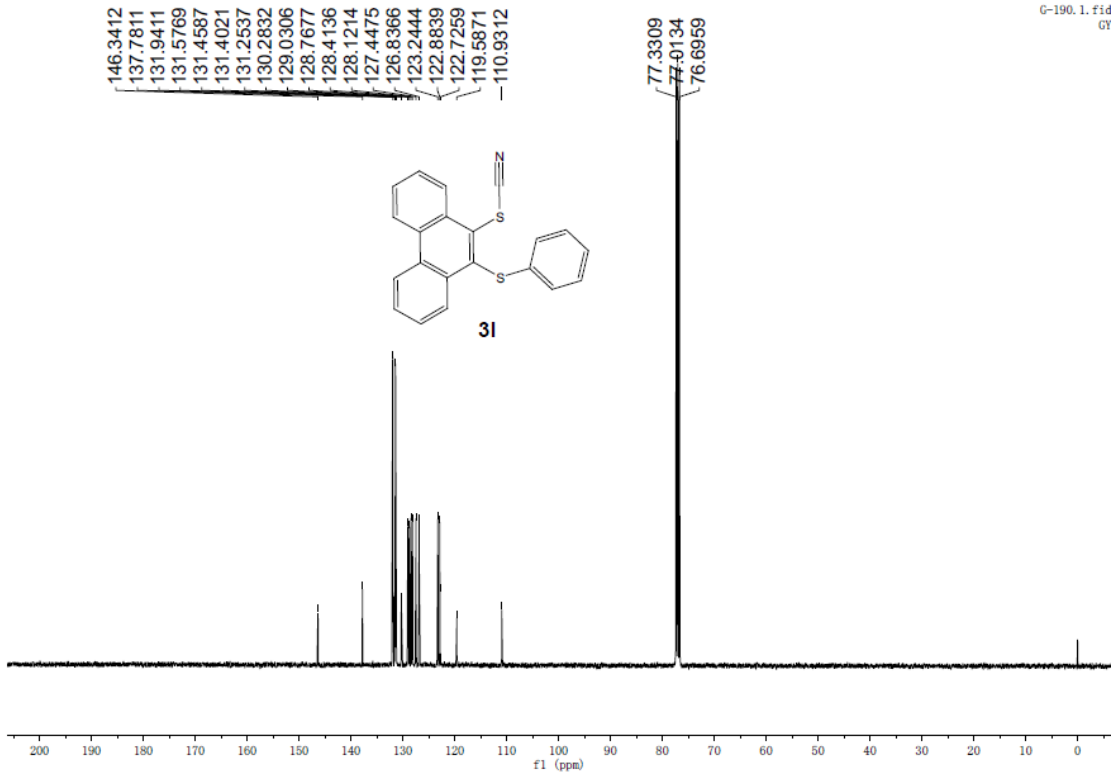
7.7608
7.7403
7.7229
7.6346
7.6145
7.5959
7.2411
7.1982
7.1805
7.1614
7.1265
7.1084
7.0900
7.0699
7.0664
7.0487
G-190.2.fid
GY
N
S
S
3l
1.00
2.02
1.00
2.02
1.02
1.02
2.02
3.02
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.4021
131.2537
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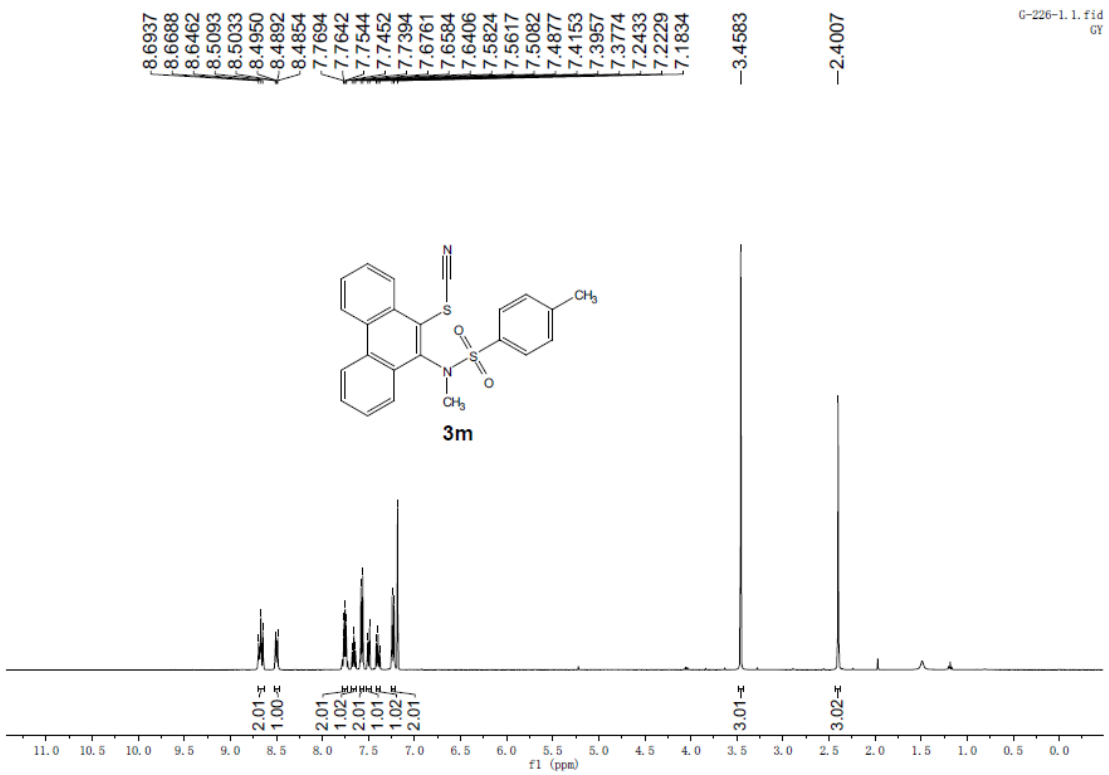
129.0306
128.7677
128.4136
128.1214
127.4475
126.8366
123.2444
122.8839
122.7259
119.5871
110.9312
77.3309
77.0134
76.6959
G-190.1.fid
GY
N
S
S
3l
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.4892
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7.7694
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7.7544
7.7452
7.7394
7.6761
7.6584
7.6406
7.5824
7.5617
7.5082
7.4877
7.4153
7.3957
7.3774
7.2433
7.2229
7.1834
3.4583
2.4007
G-226-1.1.fid
GY
3m
2.01
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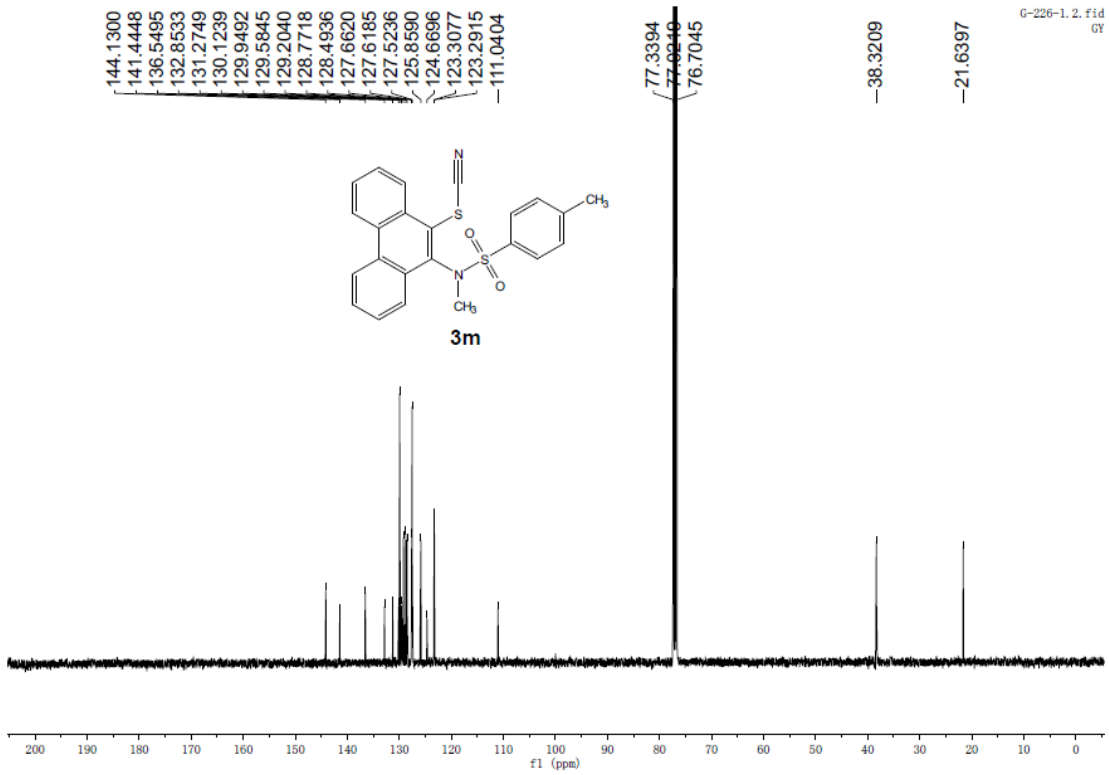
2.01
1.02
2.01
1.01
1.02
2.01
3.01
3.02
f1 (ppm)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129.9492
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128.4936
127.6620
127.6185
127.5236
125.8590
124.6696
123.3077
123.2915
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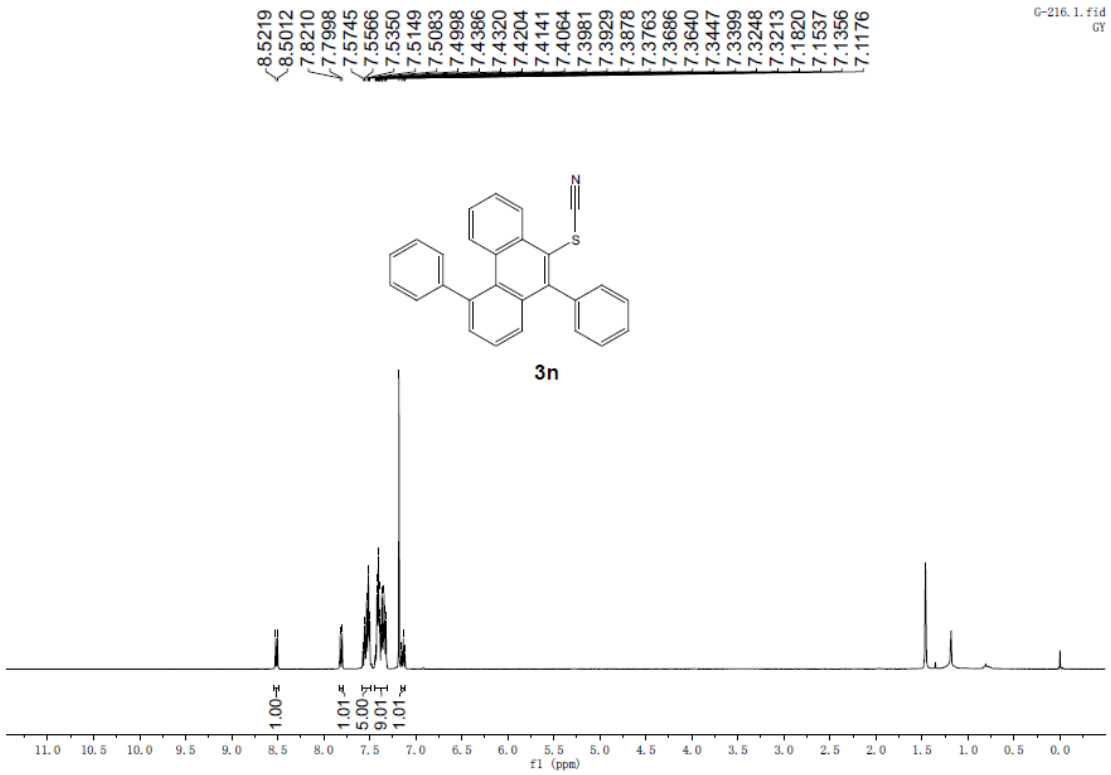
77.3394
77.0210
76.7045
38.3209
21.6397
G-226-1.2.fid
GY
3m
f1 (ppm)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7.5350
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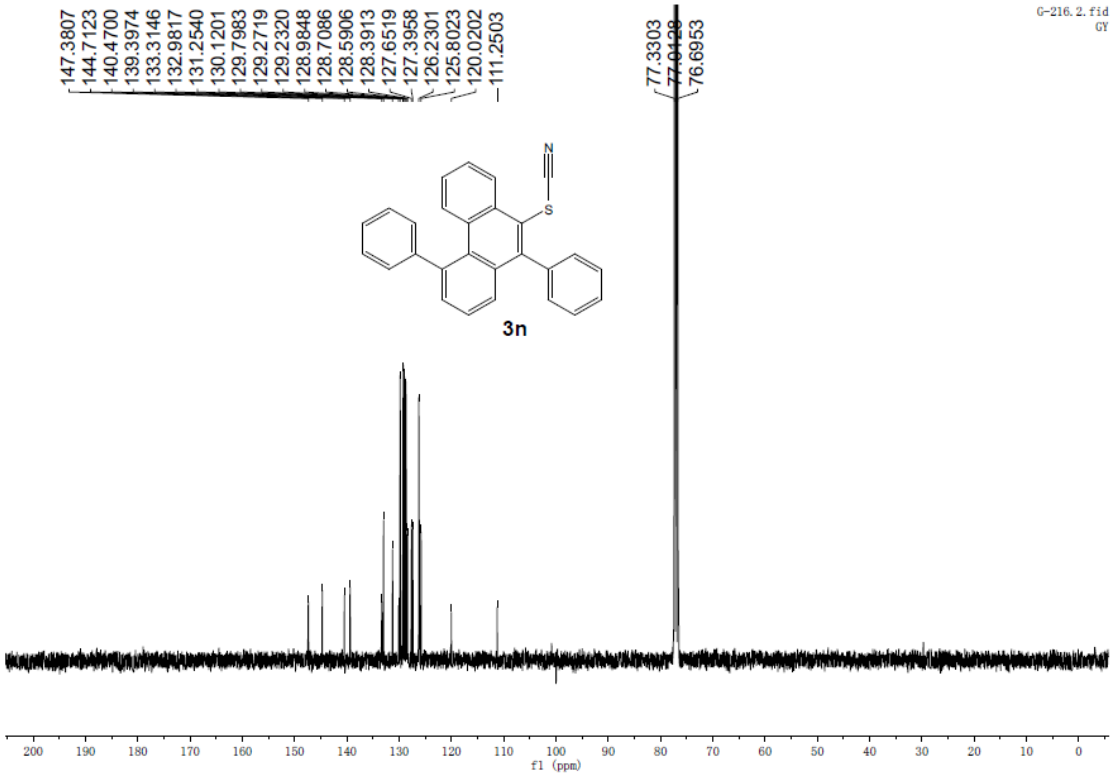
7.5083
7.4998
7.4386
7.4320
7.4204
7.4141
7.4064
7.3981
7.3929
7.3878
7.3763
7.3686
7.3640
7.3447
7.3399
7.3248
7.3213
7.1820
7.1537
7.1356
7.1176
G-216.1.fid
GY
N
S
3n
1.00
1.01
5.00
9.01
1.01
f1 (ppm)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128.9848
128.7086
128.5906
128.3913
127.6519
127.3958
126.2301
125.8023
120.0202
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77.3303
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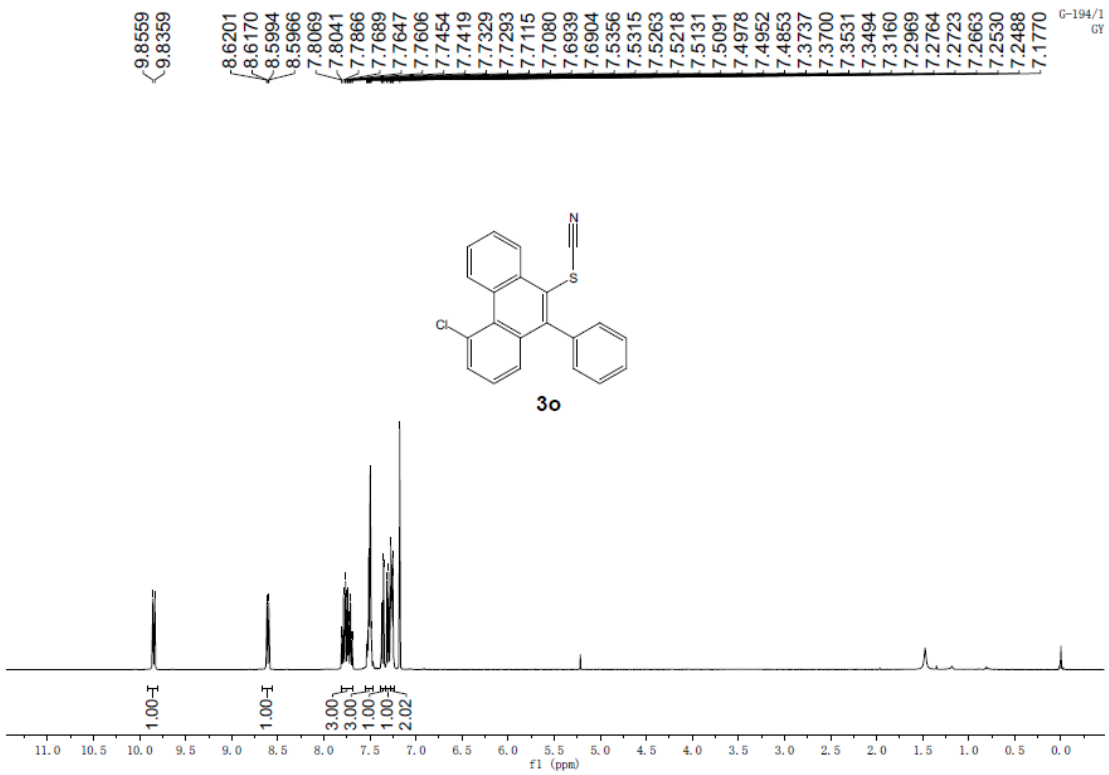
76.6953
G-216.2.fid
GY
N
S
3n
f1 (ppm)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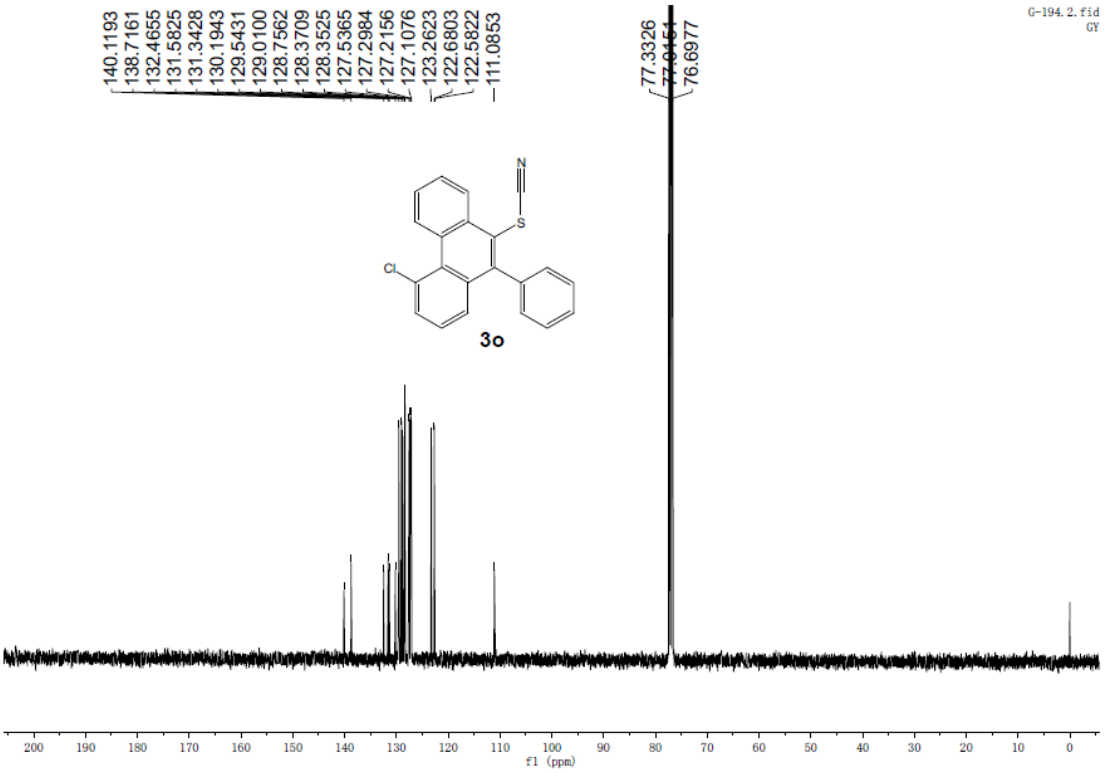
7.7647
7.7606
7.7454
7.7419
7.7329
7.7293
7.7115
7.7080
7.6939
7.6904
7.5356
7.5315
7.5263
7.5218
7.5131
7.5091
7.4978
7.4952
7.4853
7.3737
7.3700
7.3531
7.3494
7.3160
7.2969
7.2764
7.2723
7.2663
7.2530
7.2488
7.1770
G-194/1
GY
N
S
Cl
3o
1.00
1.00
3.00
3.00
1.00
1.00
2.02
f1 (ppm)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131.3428
130.1943
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128.3525
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127.2984
127.2156
127.1076
123.2623
122.6803
122.5822
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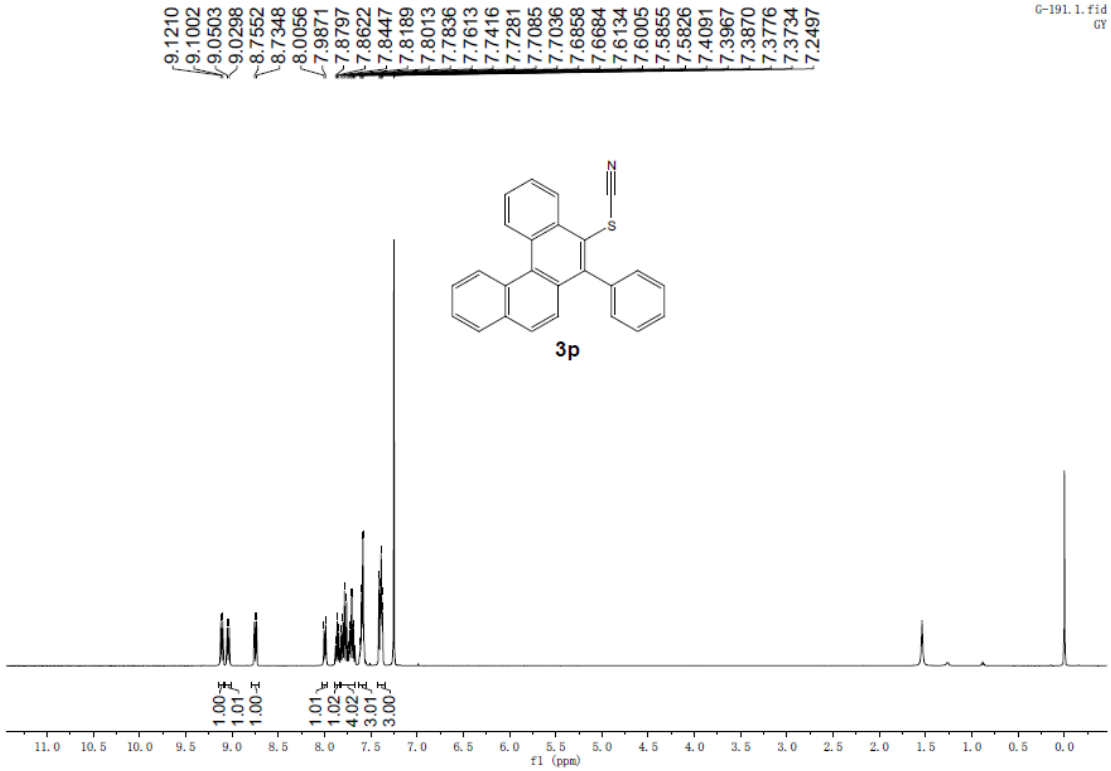
77.3326
77.0451
76.6977
G-194.2.fid
GY
N
S
Cl
3o
f1 (ppm)


G-191.1.fid
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9.0503
9.0298
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8.0056
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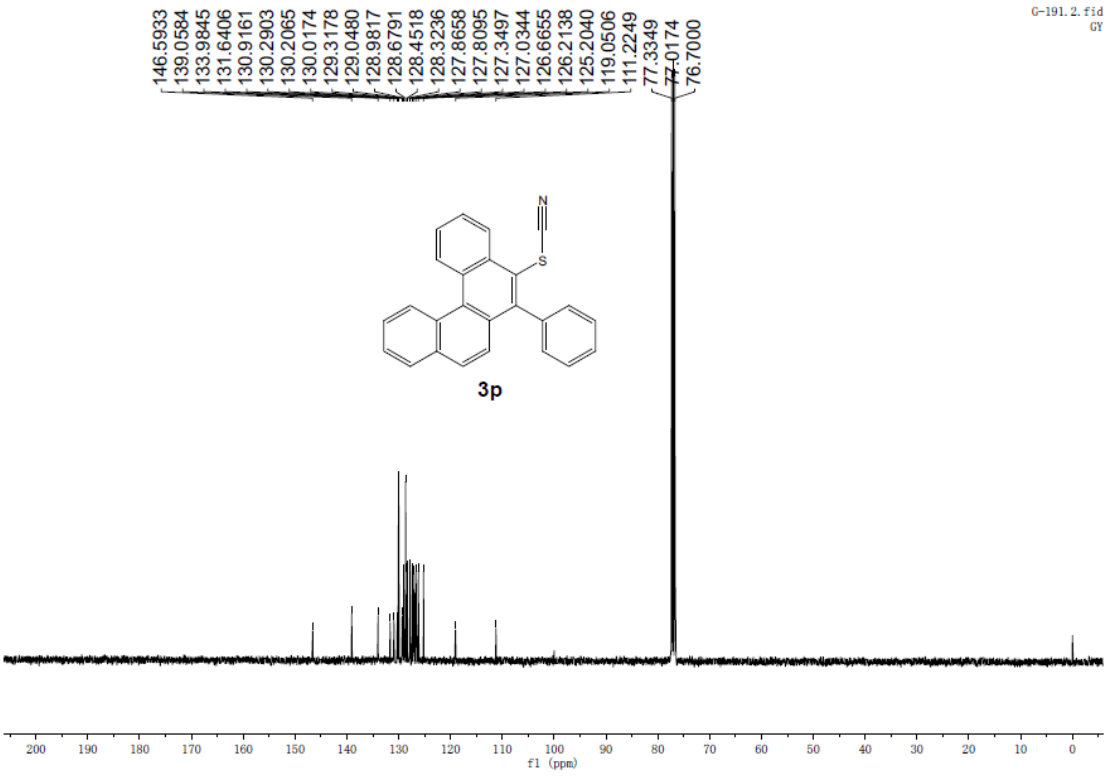
7.8797
7.8622
7.8447
7.8189
7.8013
7.7836
7.7613
7.7416
7.7281
7.7085
7.7036
7.6858
7.6684
7.6134
7.6005
7.5855
7.5826
7.4091
7.3967
7.3870
7.3776
7.3734
7.2497
N
S
3p
1.00
1.01
1.00
1.01
1.02
4.02
3.01
3.00
f1 (ppm)


G-191.2.fid
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127.3497
127.0344
126.6655
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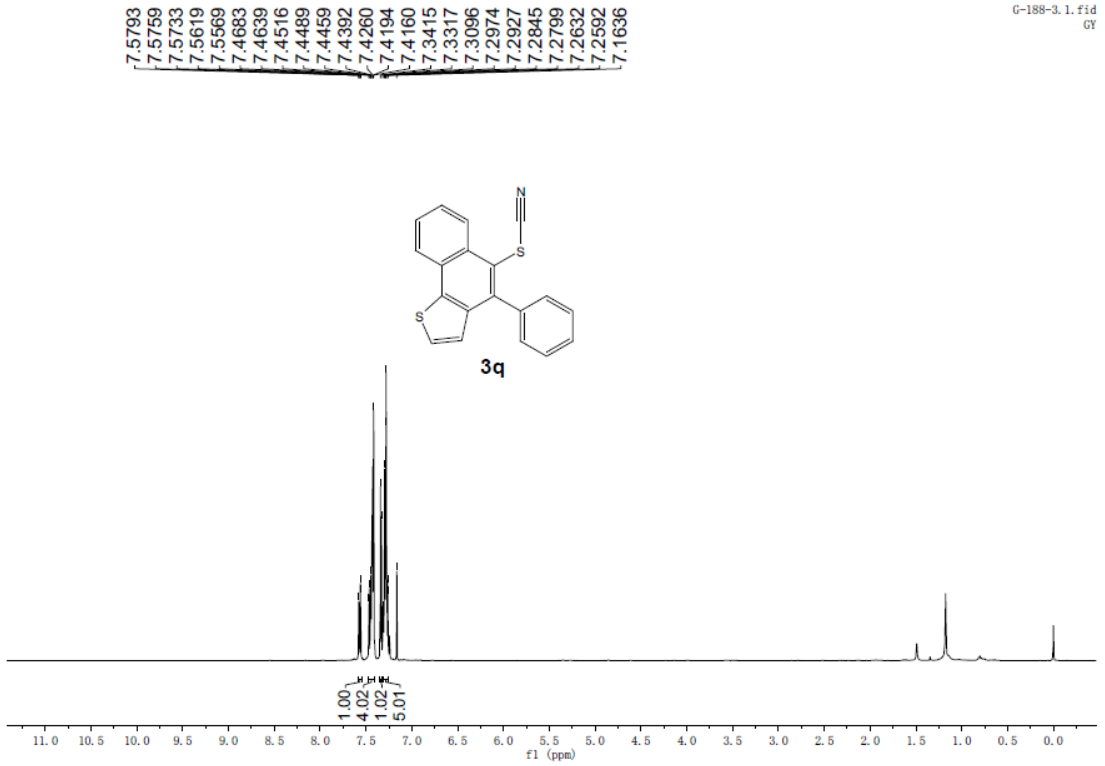
77.0174
76.7000
N
S
3p
f1 (ppm)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7.4639
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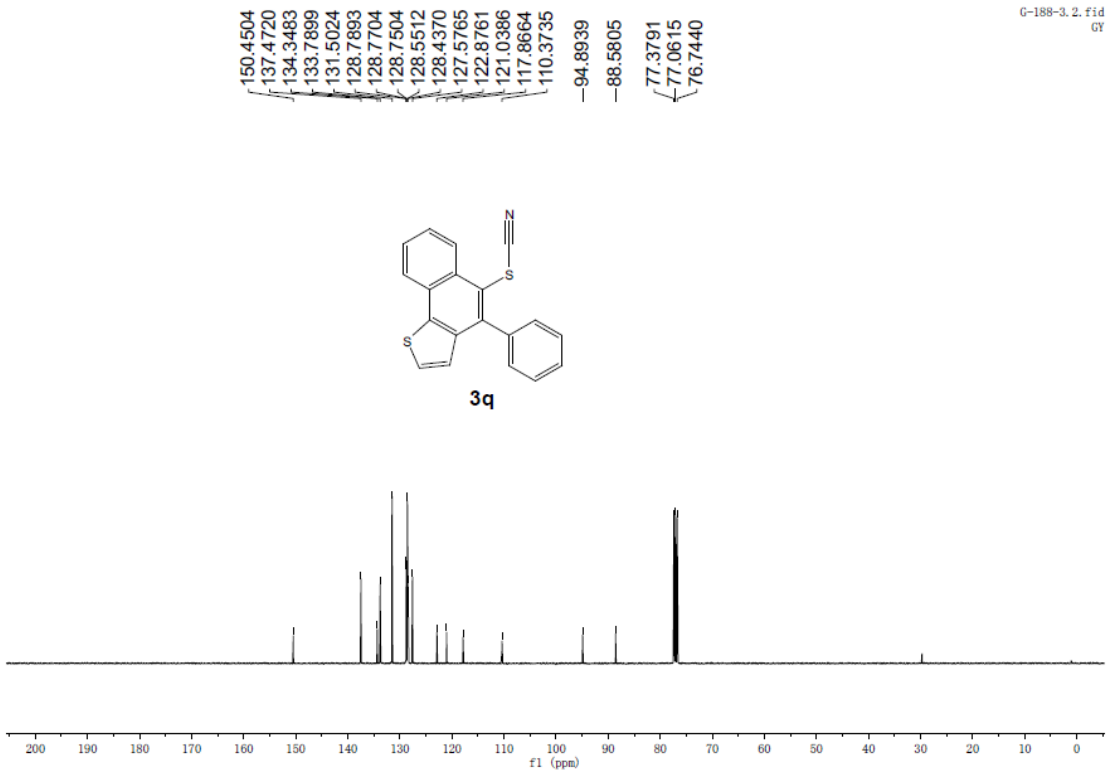
7.4392
7.4260
7.4194
7.4160
7.3415
7.3317
7.3096
7.2974
7.2927
7.2845
7.2799
7.2632
7.2592
7.1636
G-188-3.1.fid
GY
N
S
S
3q
1.00
4.02
1.02
5.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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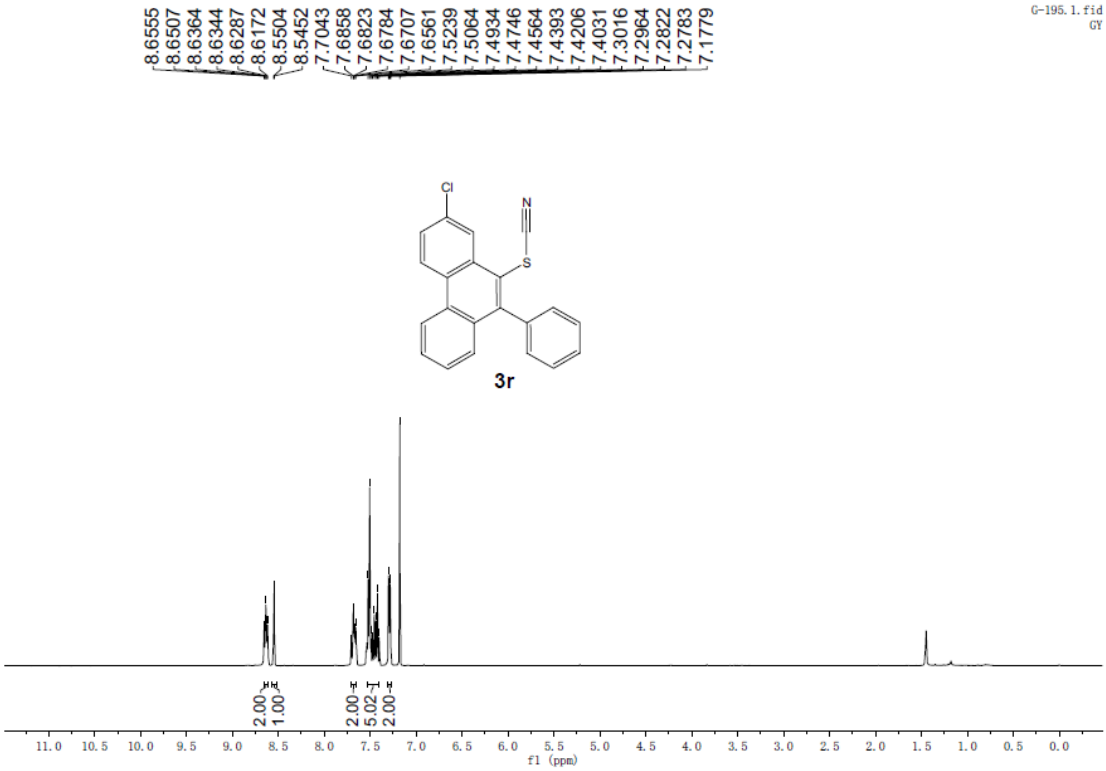
122.8761
121.0386
117.8664
110.3735
94.8939
88.5805
77.3791
77.0615
76.7440
G-188-3.2.fid
GY
N
S
S
3q
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.6287
8.6172
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7.6823
7.6784
7.6707
7.6561
7.5239
7.5064
7.4934
7.4746
7.4564
7.4393
7.4206
7.4031
7.3016
7.2964
7.2822
7.2783
7.1779
G-195.1.fid
GY
Cl
N
S
3r
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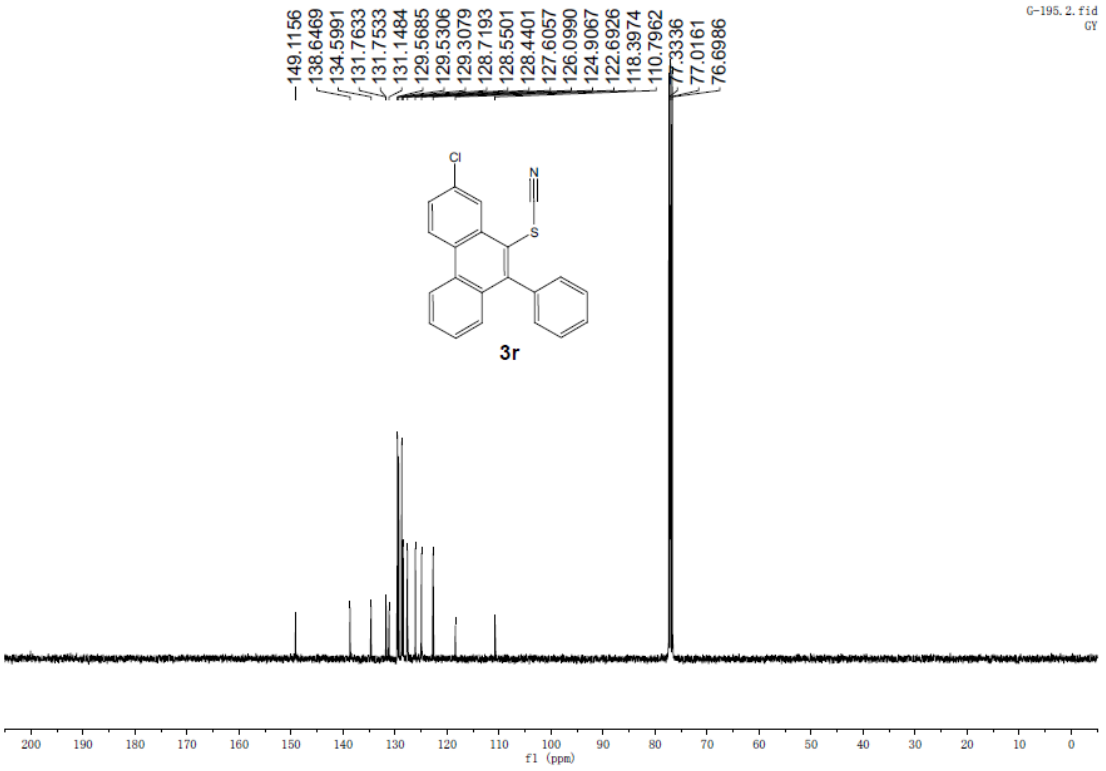
1.00
2.00
5.02
2.00
f1 (ppm)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127.6057
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124.9067
122.6926
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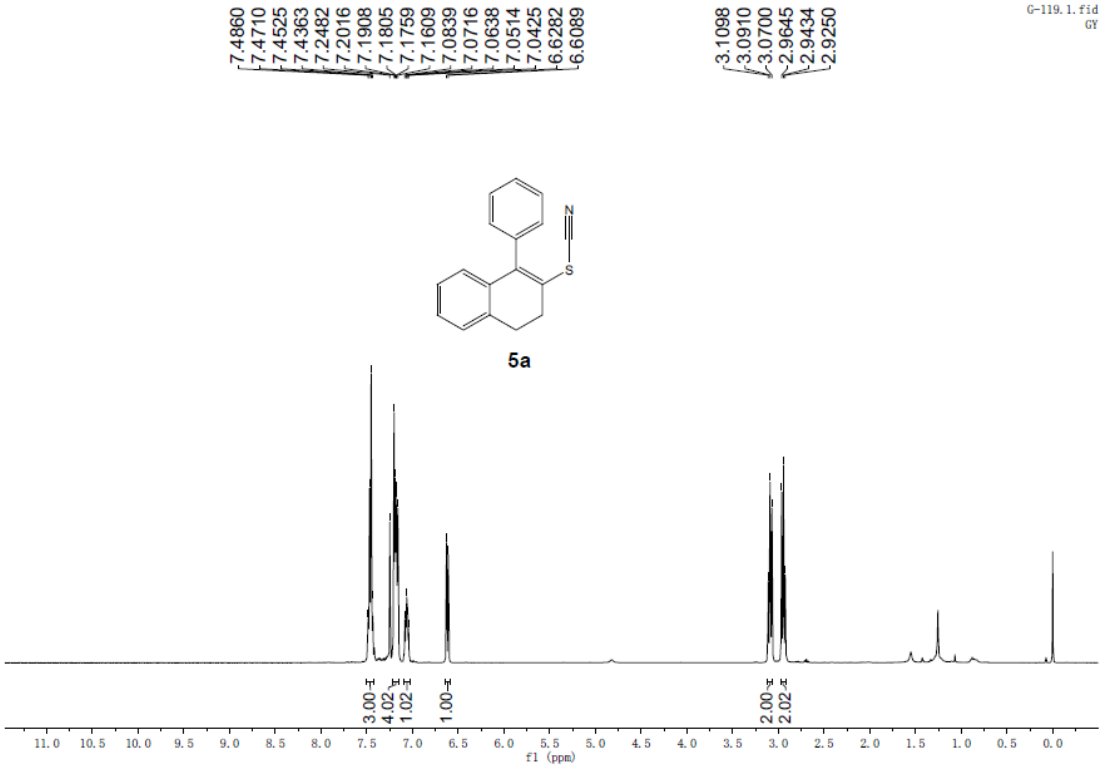
G-195.2.fid
GY
Cl
N
S
3r
f1 (ppm)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7.2482
7.2016
7.1908
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7.1759
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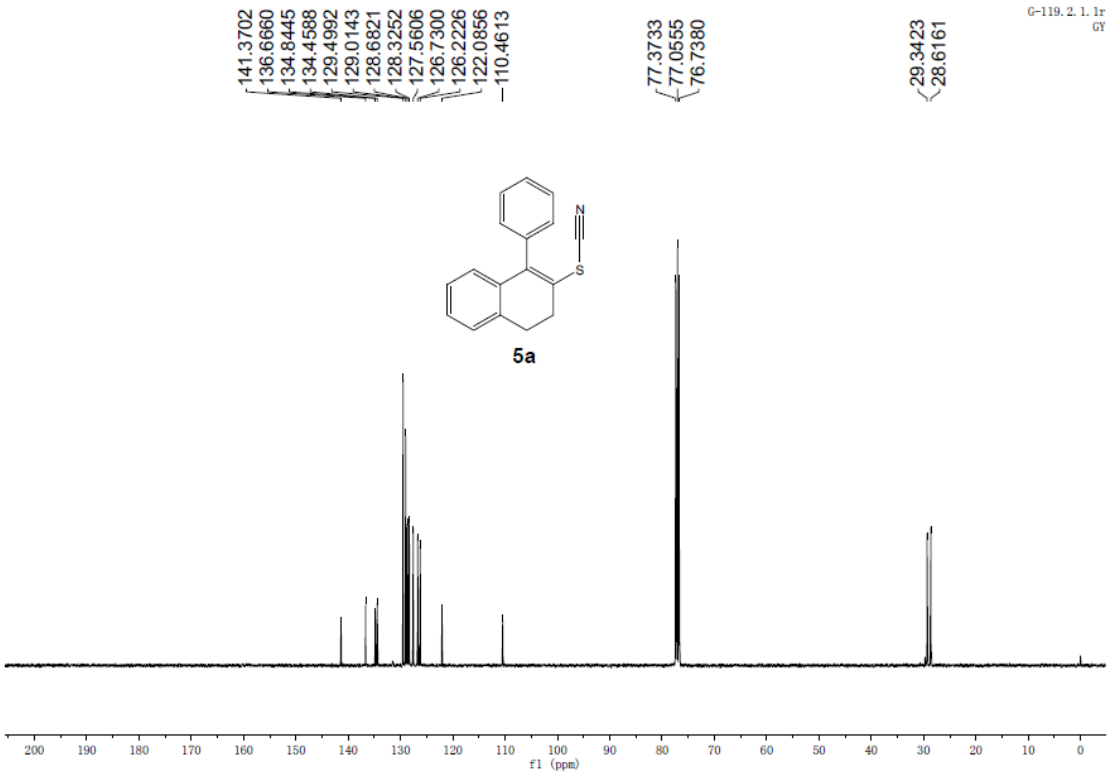
7.0839
7.0716
7.0638
7.0514
7.0425
6.6282
6.6089
3.1098
3.0910
3.0700
2.9645
2.9434
2.9250
G-119.1.fid
GY
N
S
5a
3.00
4.02
1.02
1.00
2.00
2.02
f1 (ppm)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122.0856
110.4613
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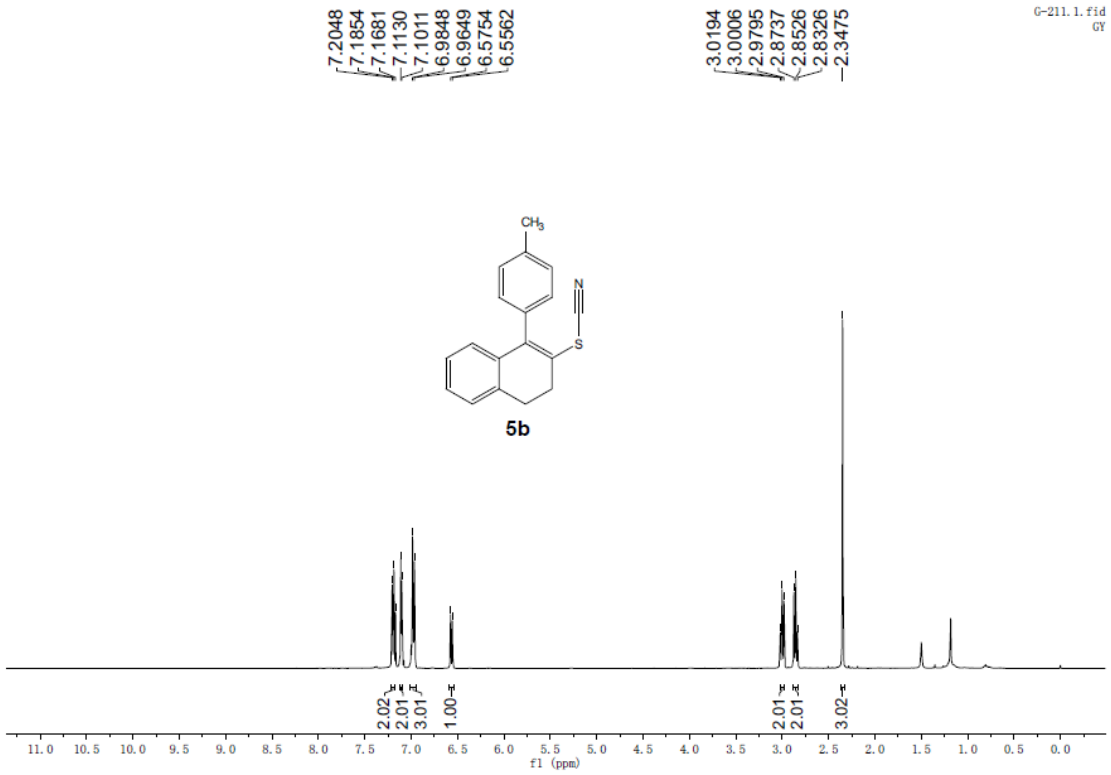
77.0555
76.7380
29.3423
28.6161
G-119.2.1.1r
GY
N
S
5a
f1 (ppm)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7.1130
7.1011
6.9848
6.9649
6.5754
6.5562
3.0194
3.0006
2.9795
2.8737
2.8526
2.8326
2.3475
G-211.1.fid
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CH3
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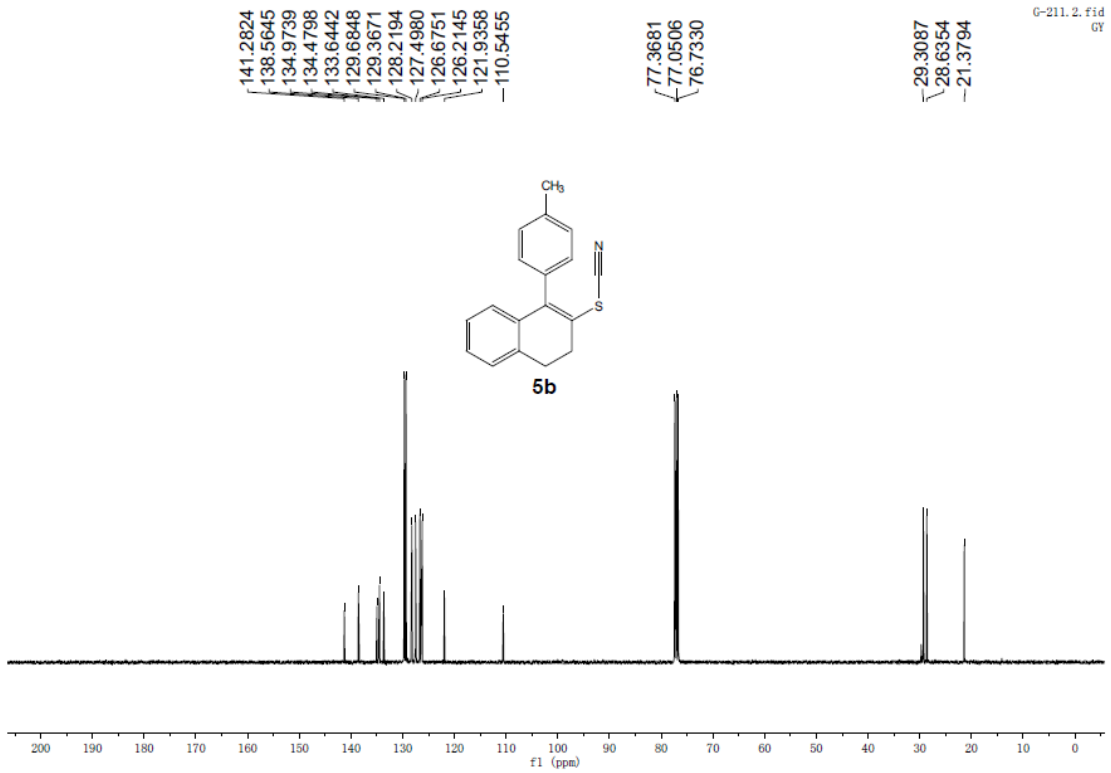
S
5b
2.02
2.01
3.01
1.00
2.01
2.01
3.02
f1 (ppm)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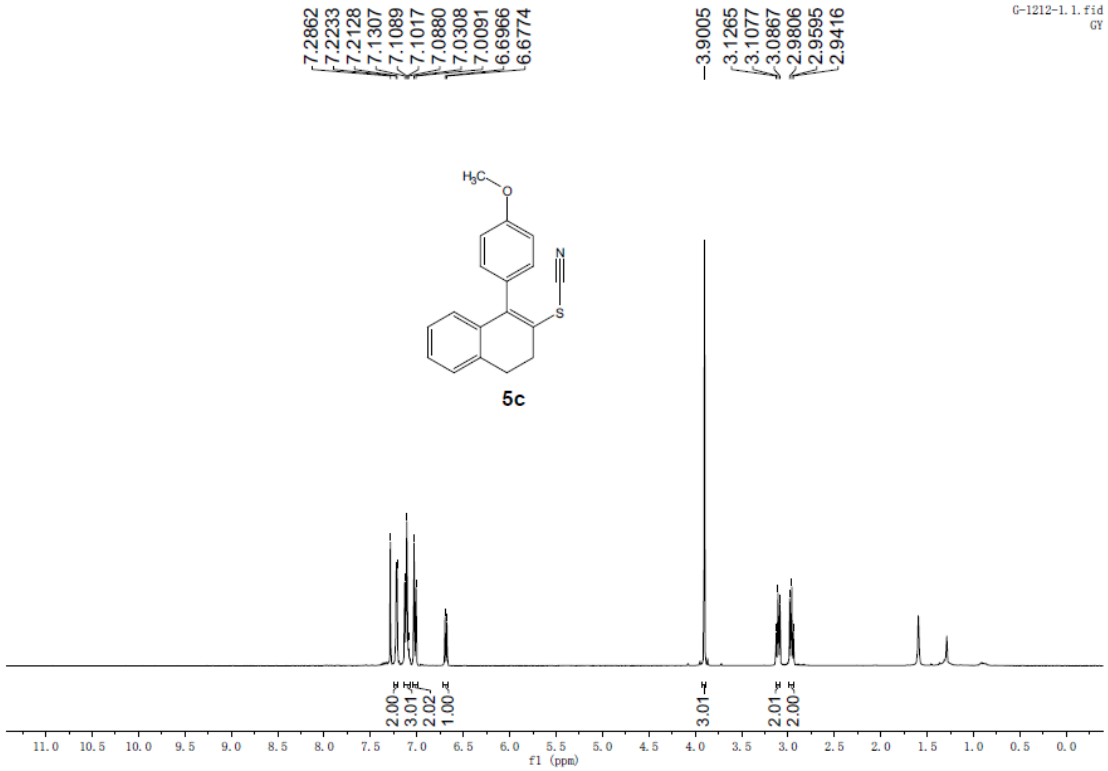
CH3
N
S
5b
f1 (ppm)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7.1017
7.0880
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7.0091
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6.6774
3.9005
3.1265
3.1077
3.0867
2.9806
2.9595
2.9416
G-1212-1.1.fid
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O
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S
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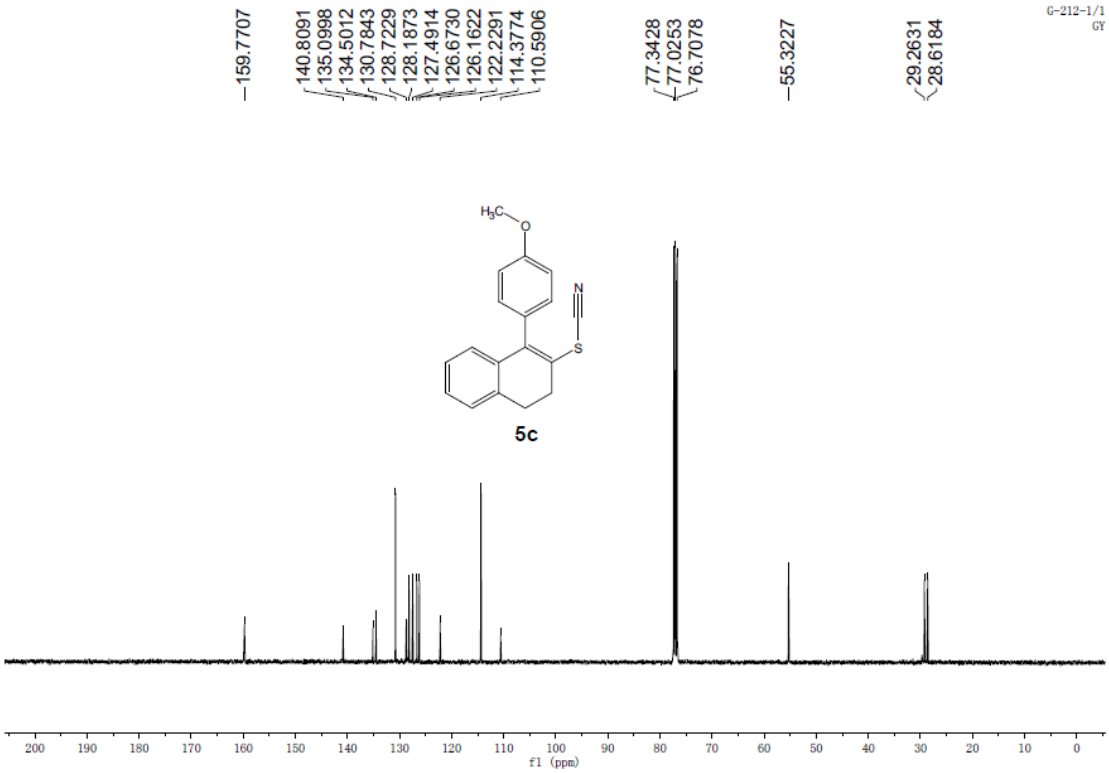
3.01
2.01
2.00
f1 (ppm)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77.0253
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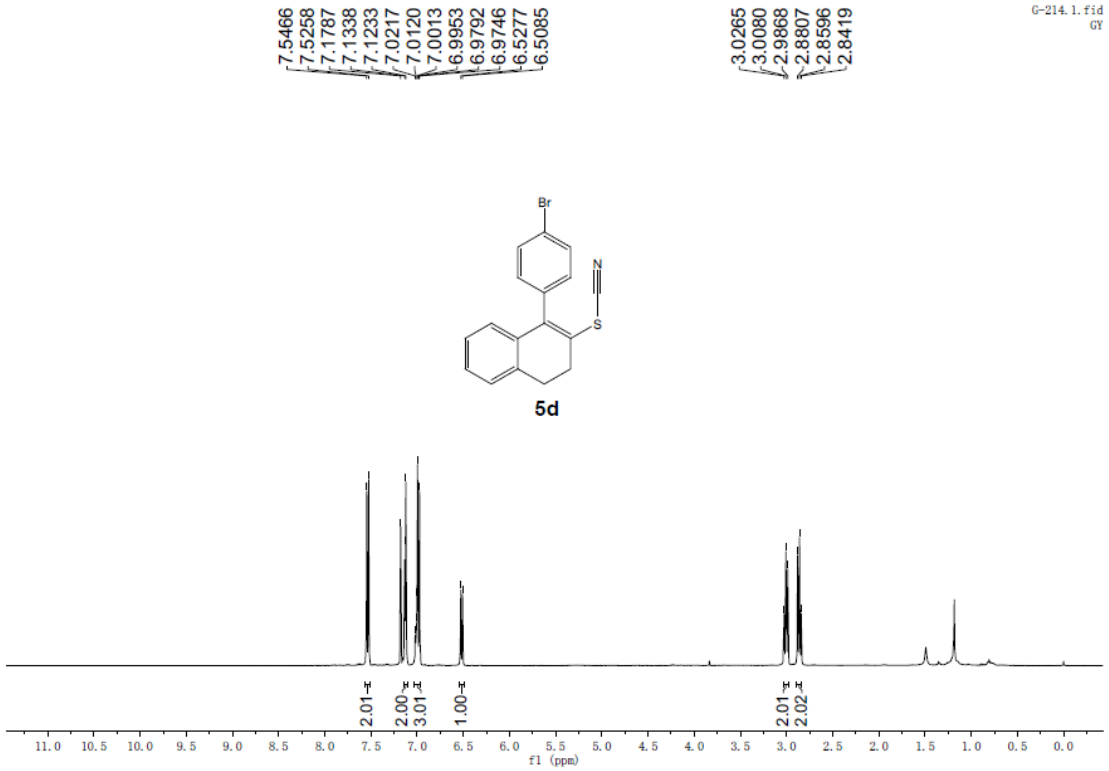
H3C
O
N
S
5c
f1 (ppm)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6.5277
6.5085
3.0265
3.0080
2.9868
2.8807
2.8596
2.8419
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Br
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S
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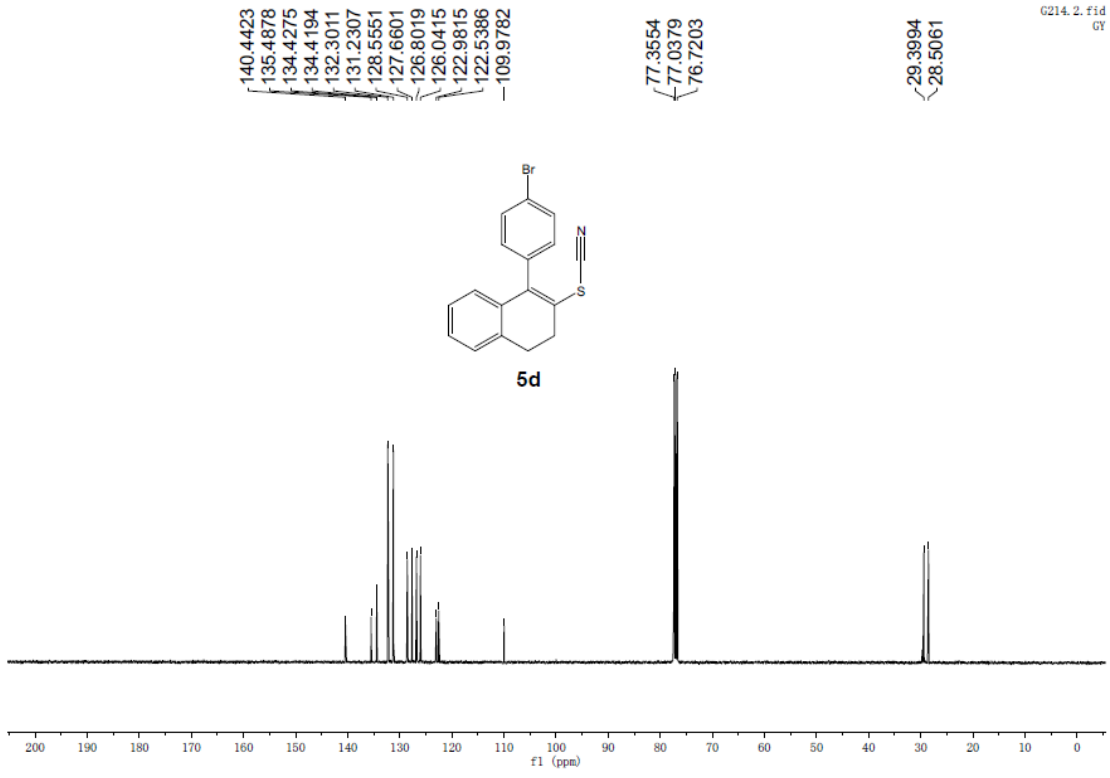
2.00
3.01
1.00
2.01
2.02
f1 (ppm)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GY
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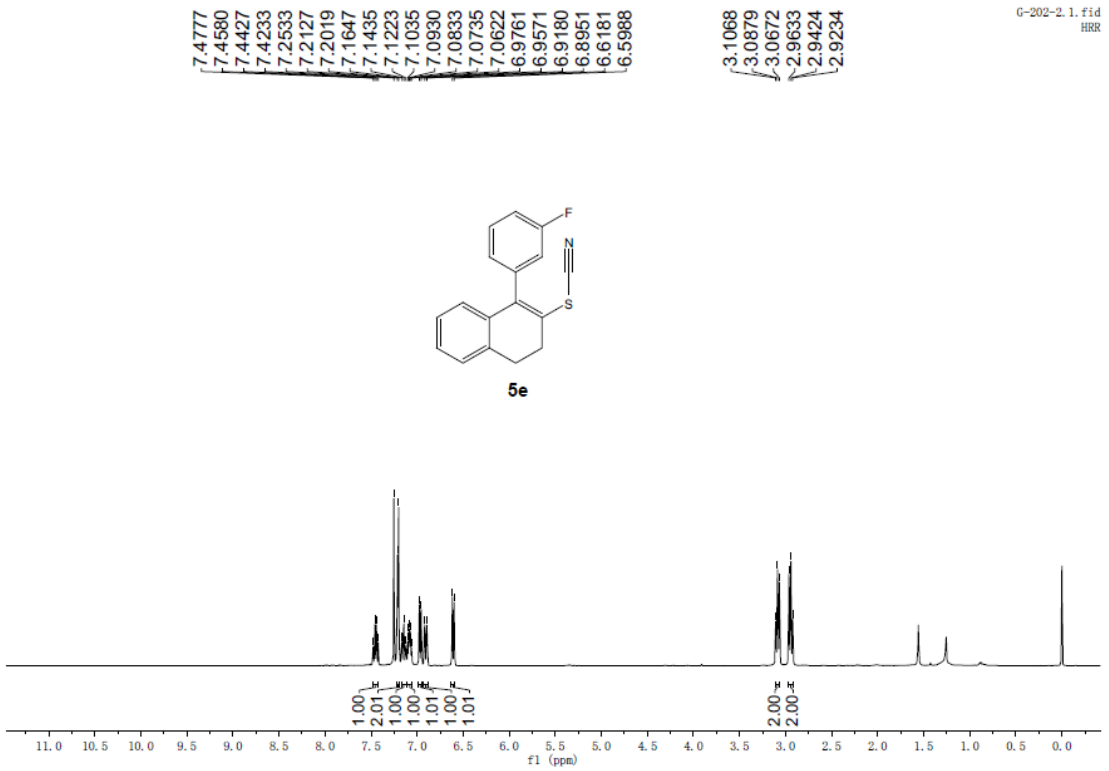
S
5d
f1 (ppm)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6.6181
6.5988
3.1068
3.0879
3.0672
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2.9424
2.9234
G-202-2.1.fid
HRR
F
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1.00
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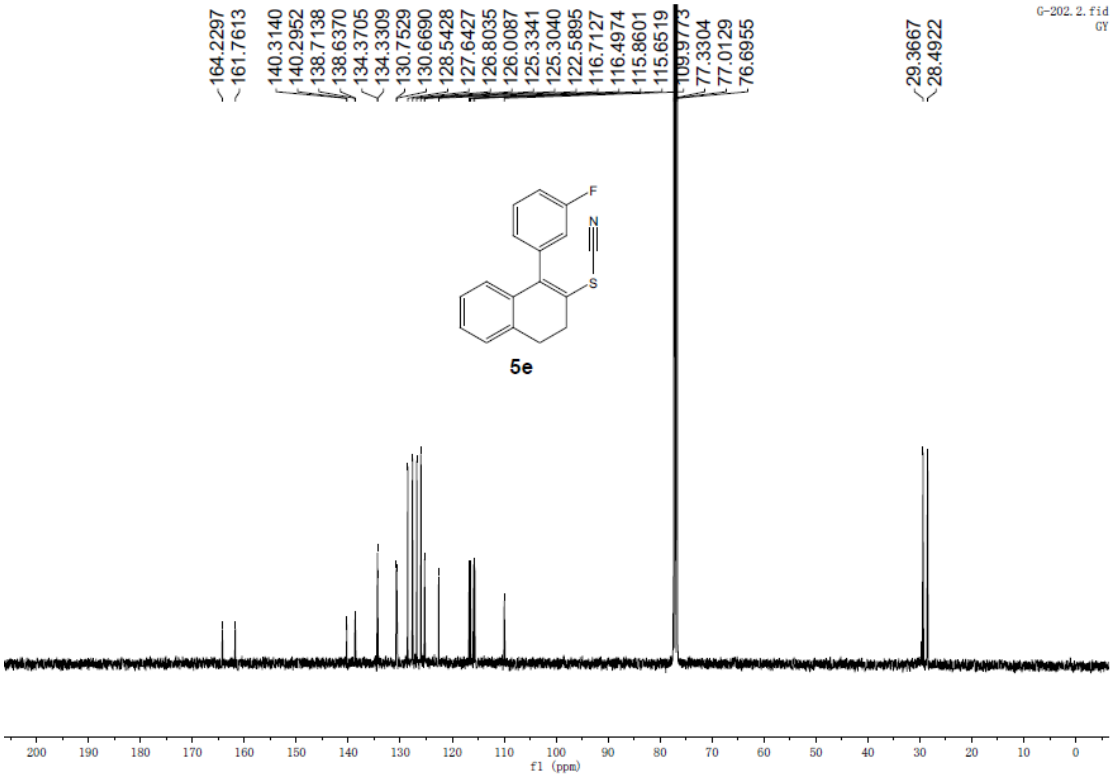
1.01
2.00
2.00
f1 (ppm)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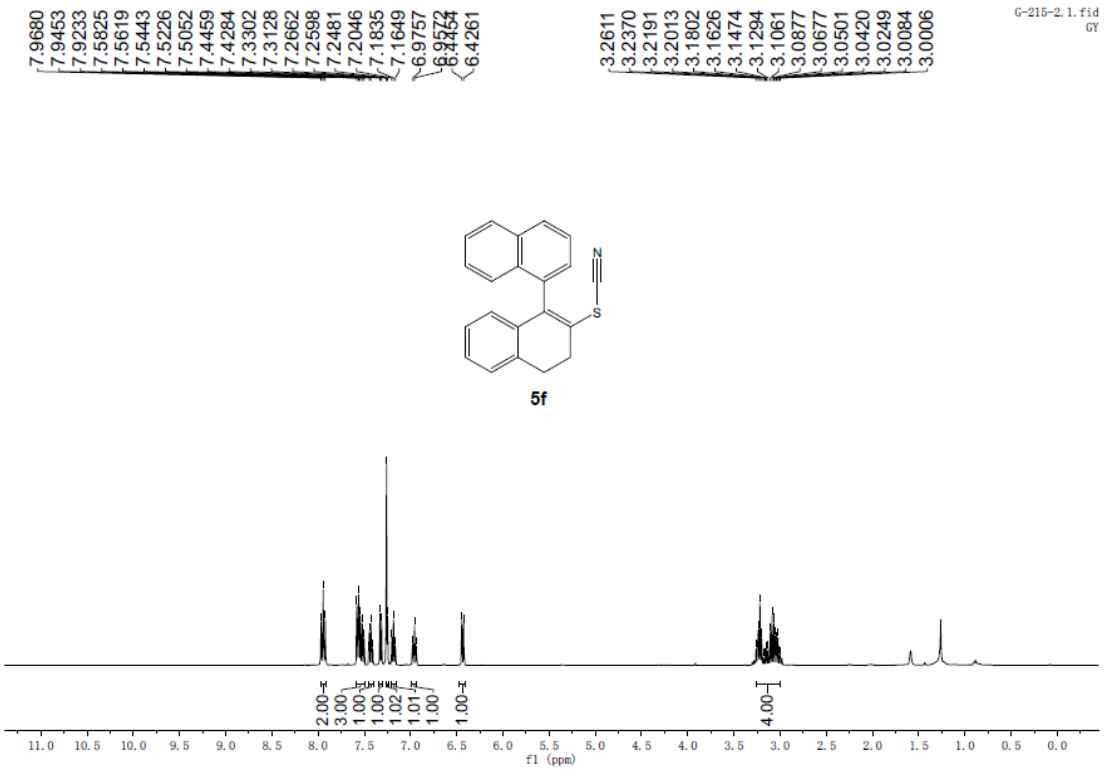
GY
F
N
S
5e
f1 (ppm)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G-215-2.1.fid
GY
N
S
5f
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3.00
1.00
1.00
1.02
1.01
1.00
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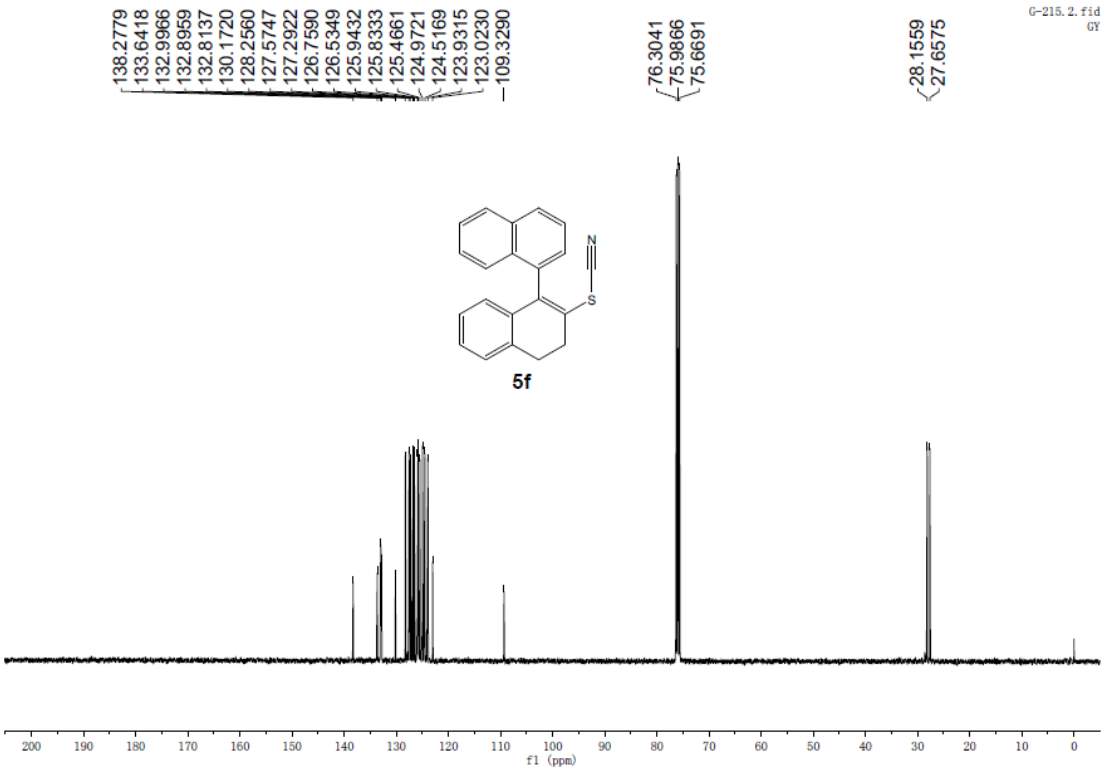
f1 (ppm)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130.1720
128.2560
127.5747
127.2922
126.7590
126.5349
125.9432
125.8333
125.4661
124.9721
124.5169
123.9315
123.0230
109.3290
76.3041
75.9866
75.6691
28.1559
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GY
N
S
5f
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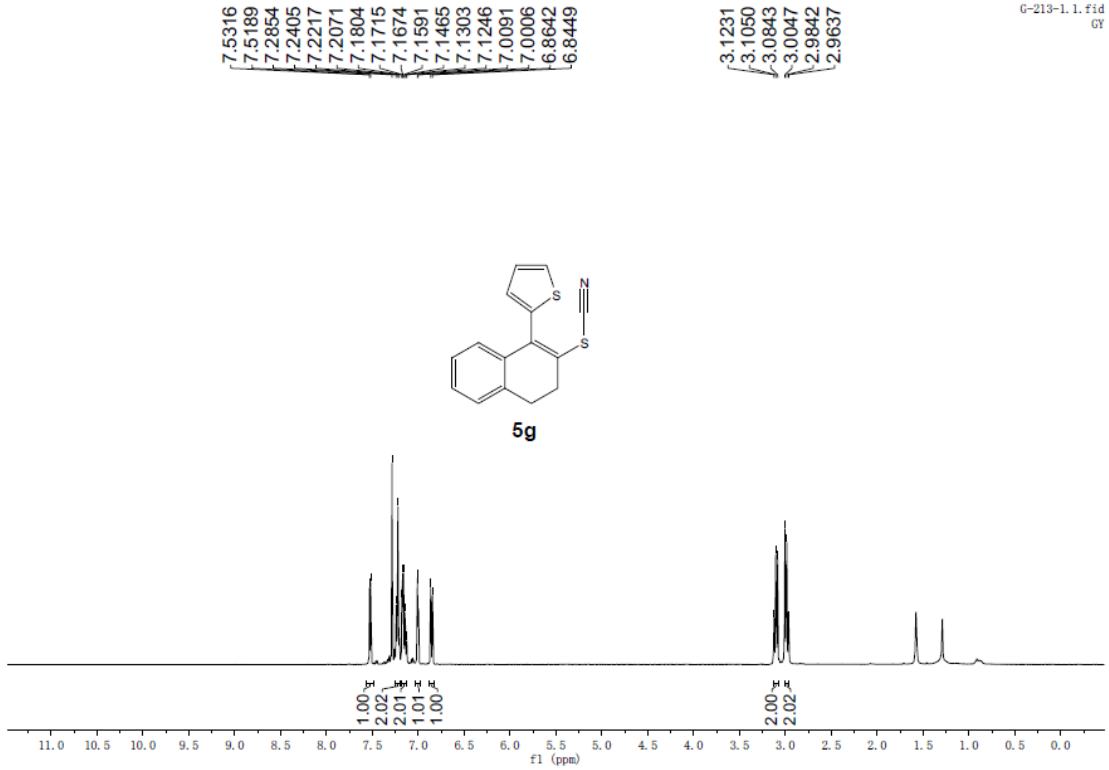
f1 (ppm)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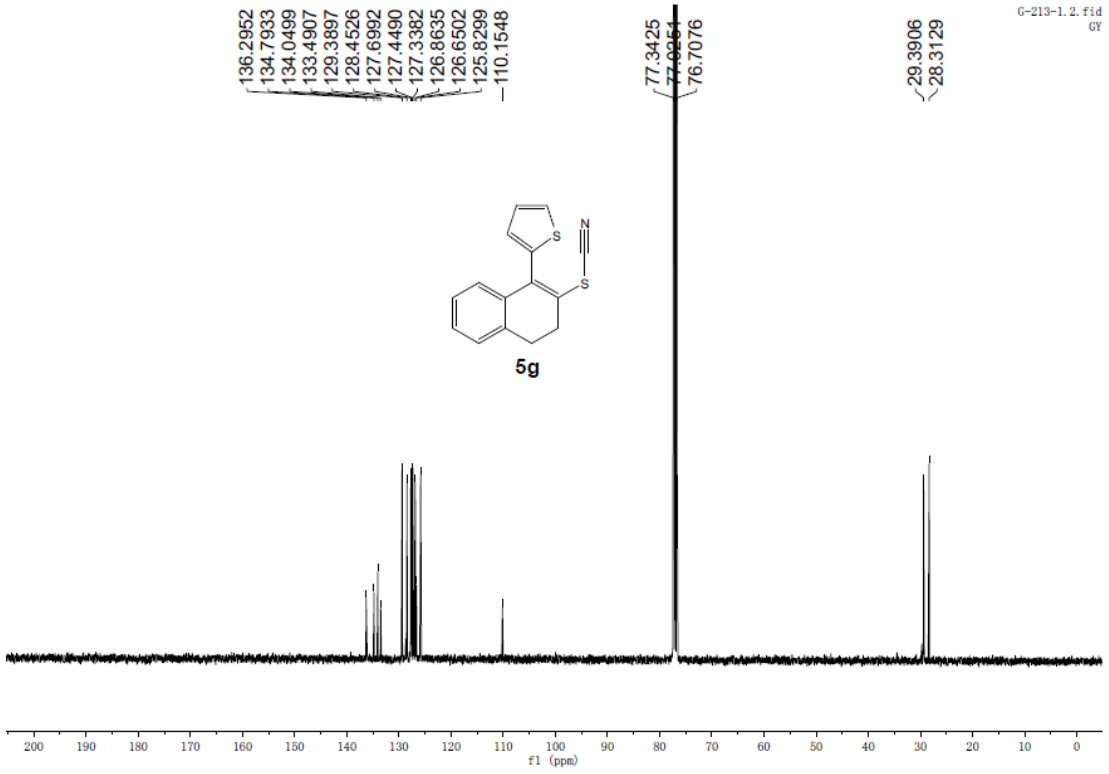
7.2217
7.2071
7.1804
7.1715
7.1674
7.1591
7.1465
7.1303
7.1246
7.0091
7.0006
6.8642
6.8449
3.1231
3.1050
3.0843
3.0047
2.9842
2.9637
G-213-1.1.fid
GY
N
S
S
5g
1.00
2.02
2.01
1.01
1.00
2.00
2.02
f1 (ppm)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134.0499
133.4907
129.3897
128.4526
127.6992
127.4490
127.3382
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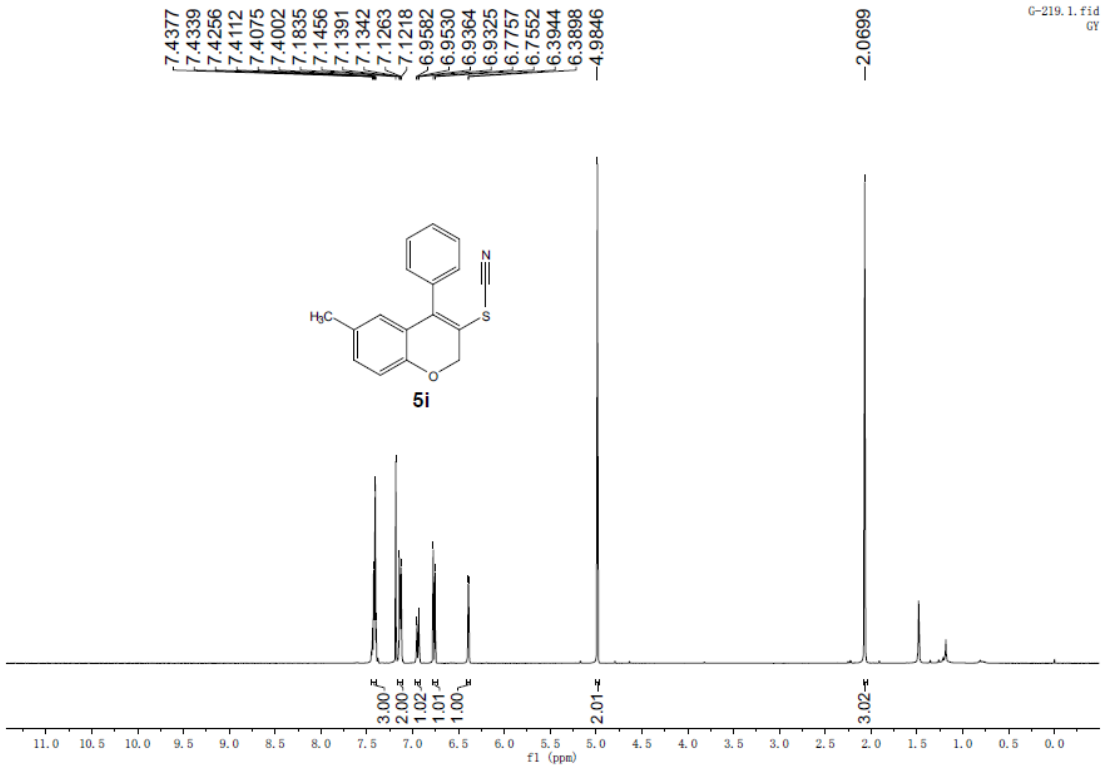
126.6502
125.8299
110.1548
77.3425
77.0854
76.7076
29.3906
28.3129
G-213-1.2.fid
GY
N
S
S
5g
f1 (ppm)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7.4339
7.4256
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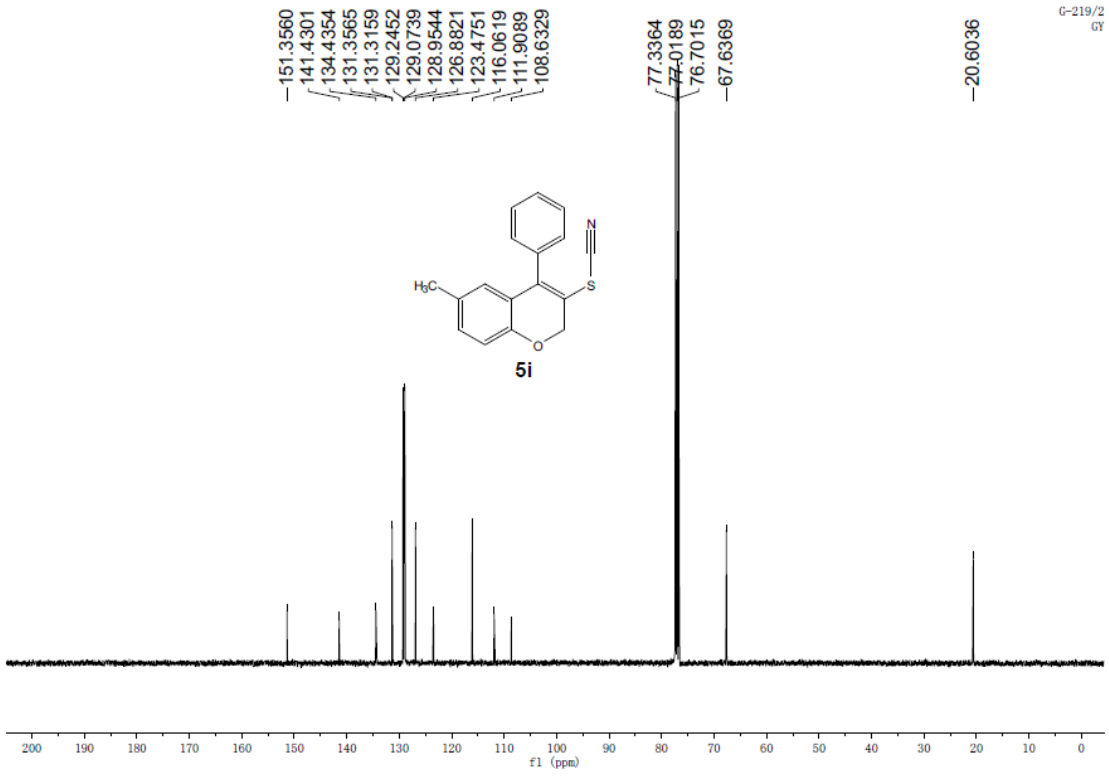
7.4002
7.1835
7.1456
7.1391
7.1342
7.1263
7.1218
6.9582
6.9530
6.9364
6.9325
6.7757
6.7552
6.3944
6.3898
4.9846
2.0699
G-219.1.fid
GY
N
S
H3C
O
5i
3.00
2.00
1.02
1.01
1.00
2.01
3.02
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.3159
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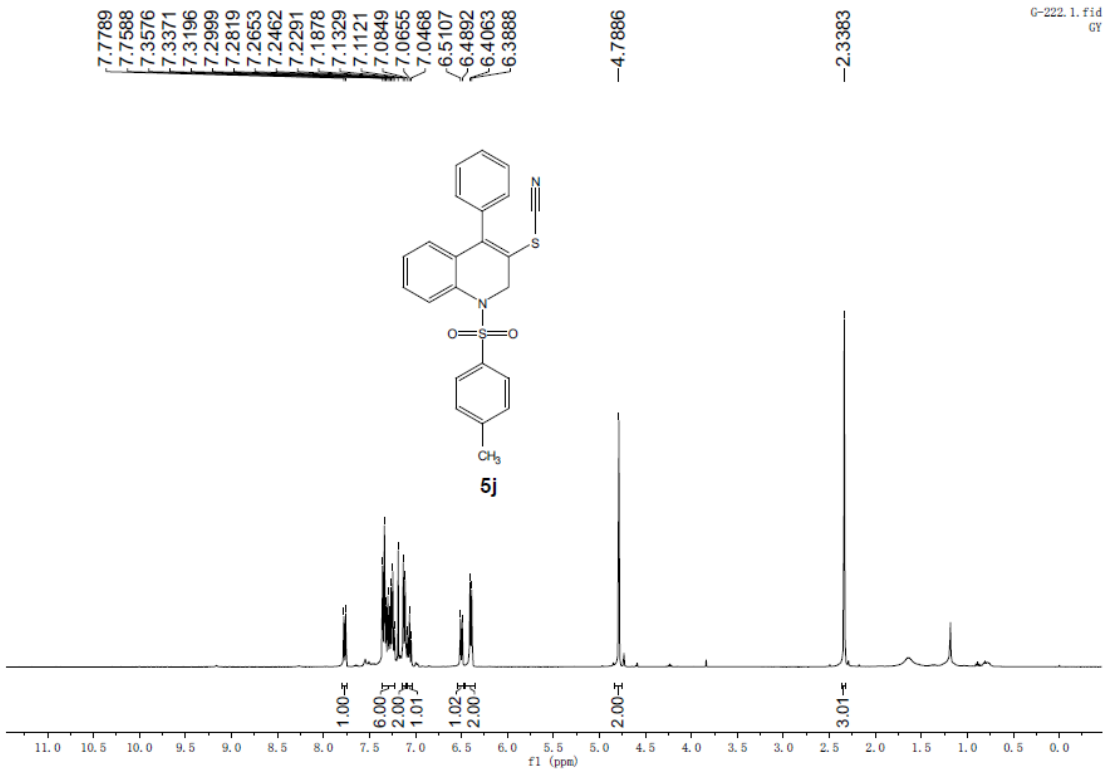
129.0739
128.9544
126.8821
123.4751
116.0619
111.9089
108.6329
77.3364
77.0189
76.7015
67.6369
20.6036
G-219/2
GY
N
S
H3C
O
5i
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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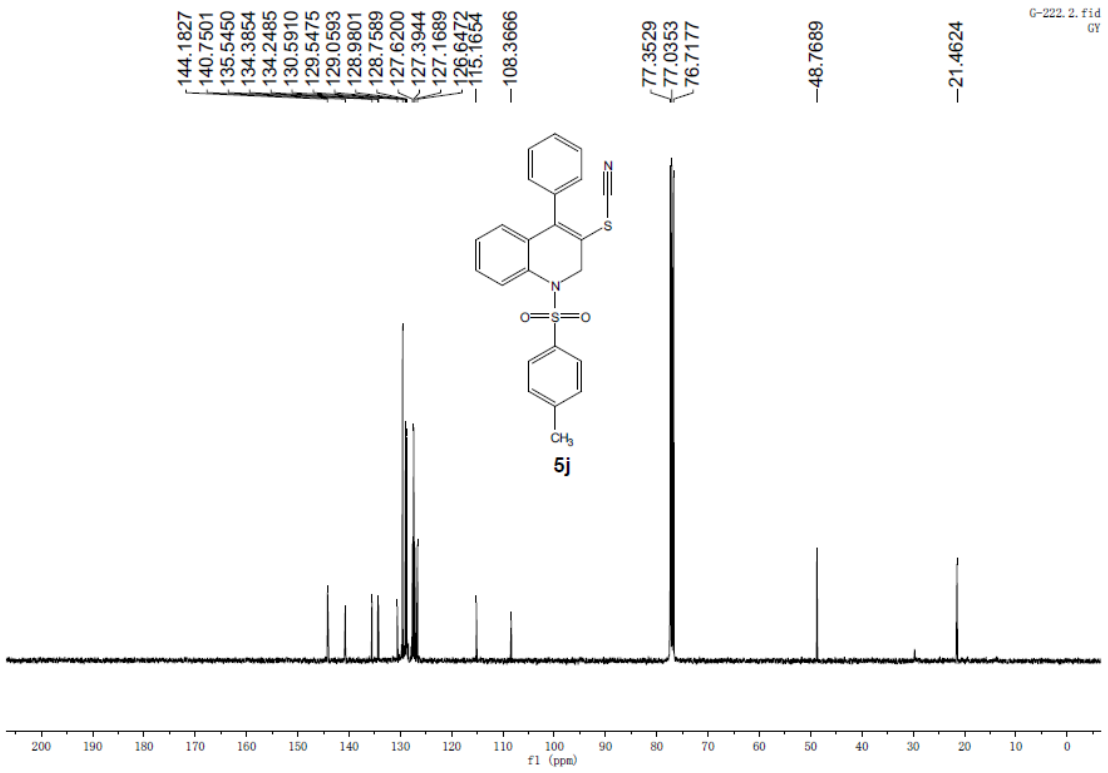
7.7588
7.3576
7.3371
7.3196
7.2999
7.2819
7.2653
7.2462
7.2291
7.1878
7.1329
7.1121
7.0849
7.0655
7.0468
6.5107
6.4892
6.4063
6.3888
4.7886
2.3383
G-222.1.fid
GY
5j
1.00
6.00
2.00
1.01
1.02
2.00
2.00
3.01
f1 (ppm)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135.5450
134.3854
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128.9801
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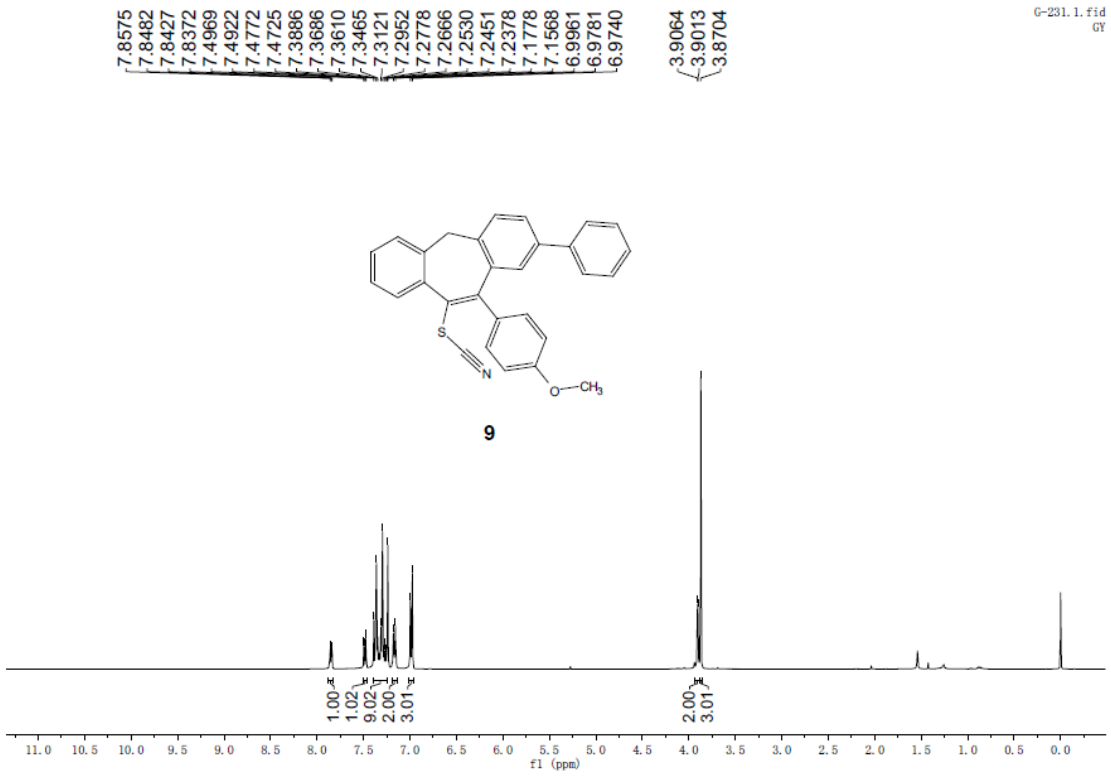
127.6200
127.3944
127.1689
126.6472
115.1654
108.3666
77.3529
77.0353
76.7177
48.7689
21.4624
G-222.2.fid
GY
5j
f1 (ppm)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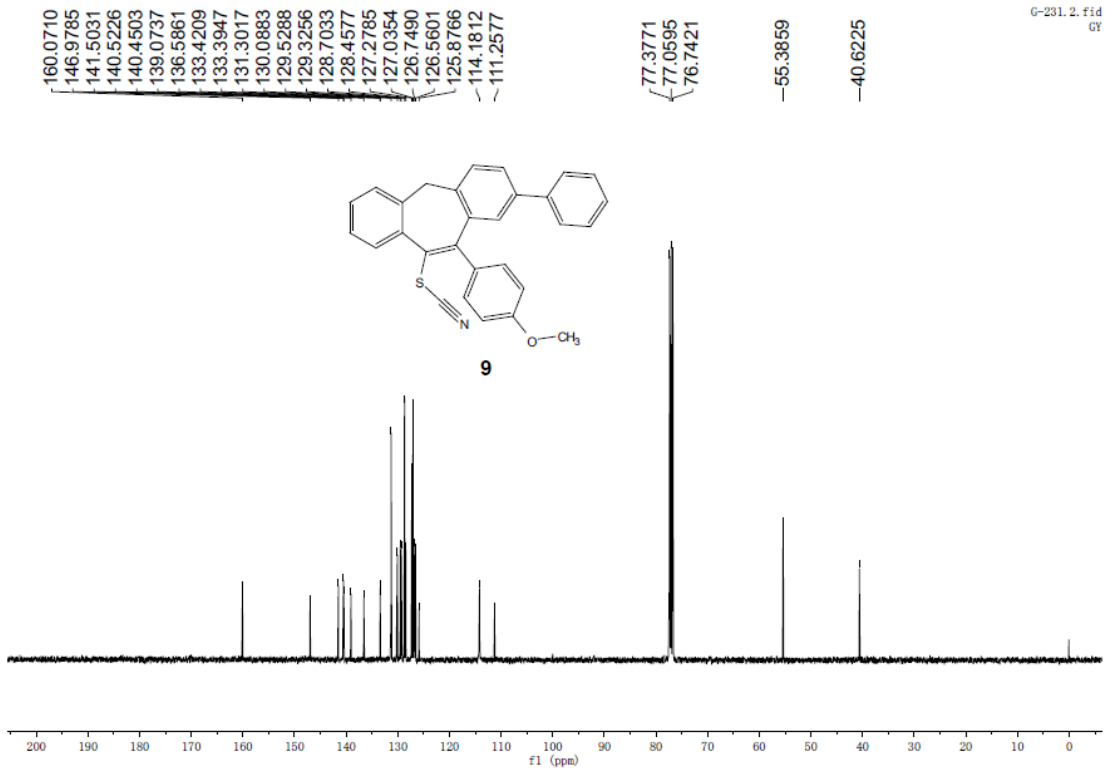
7.8482
7.8427
7.8372
7.4969
7.4922
7.4772
7.4725
7.3886
7.3686
7.3610
7.3465
7.3121
7.2952
7.2778
7.2666
7.2530
7.2451
7.2378
7.1778
7.1568
6.9961
6.9781
6.9740
3.9064
3.9013
3.8704
G-231.1.fid
GY
S
N
O
CH3
9
1.00
1.02
9.02
2.00
3.01
2.00
3.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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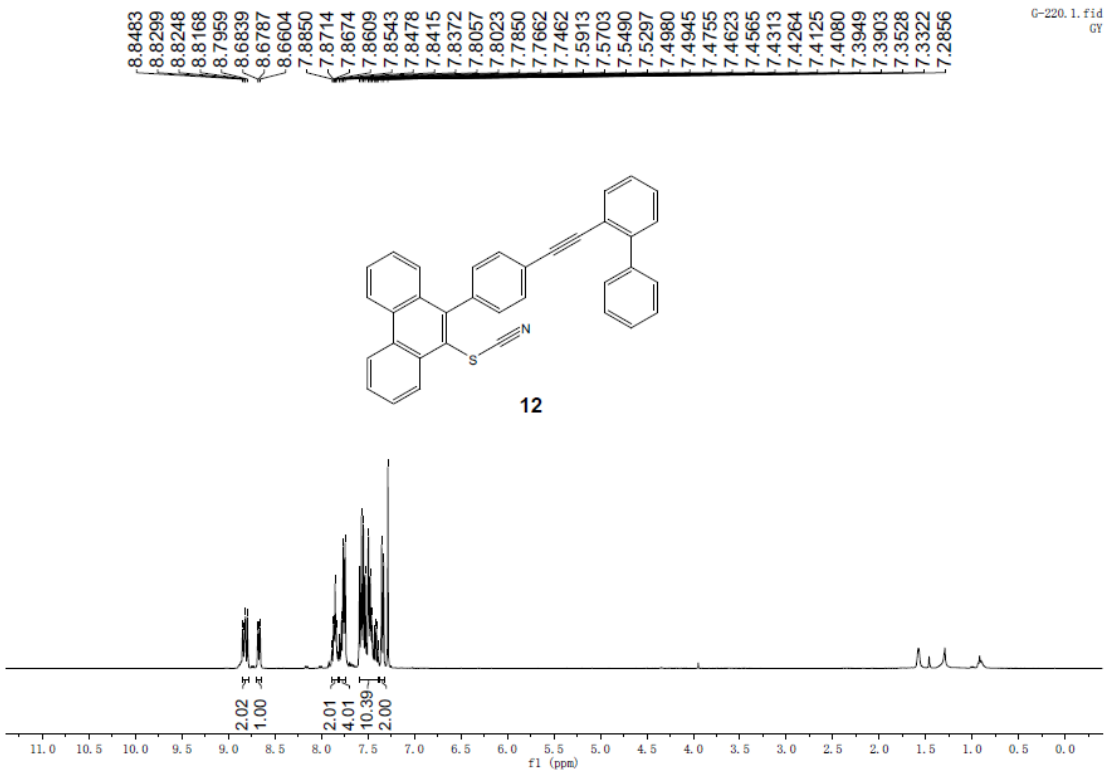
146.9785
141.5031
140.5226
140.4503
139.0737
136.5861
133.4209
133.3947
131.3017
130.0883
129.5288
129.3256
128.7033
128.4577
127.2785
127.0354
126.7490
126.5601
125.8766
114.1812
111.2577
77.3771
77.0595
76.7421
55.3859
40.6225
G-231.2.fid
GY
S
N
O
CH3
9
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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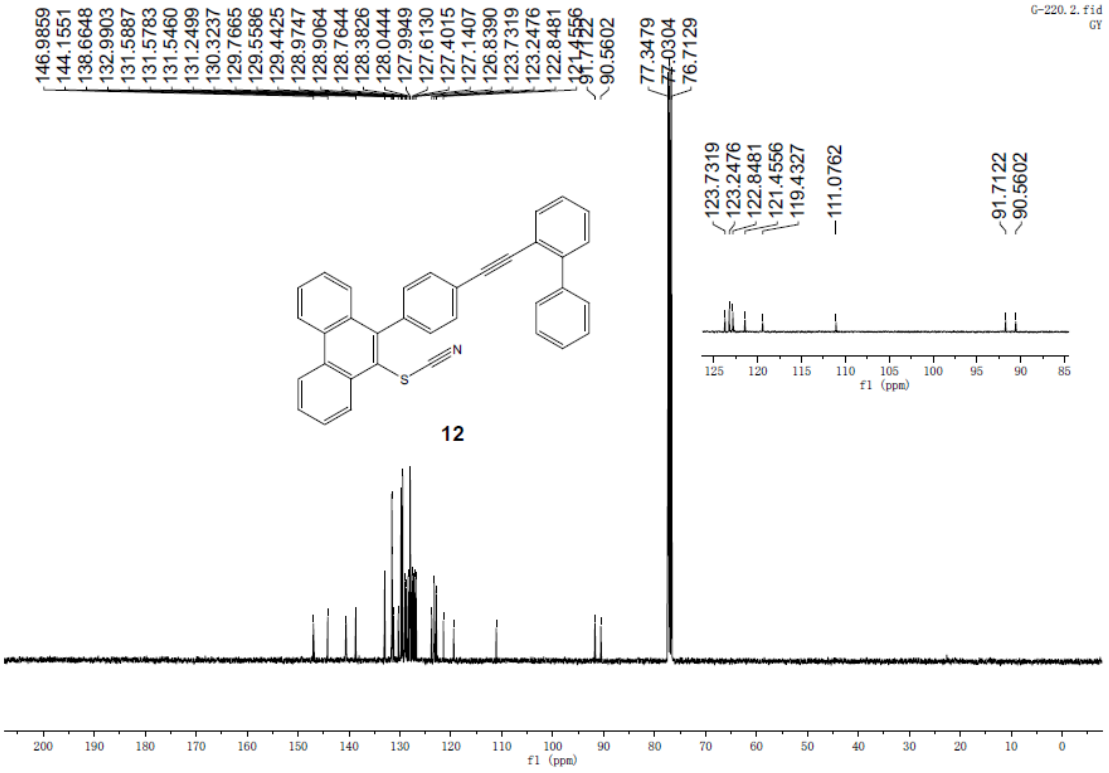
8.8248
8.8168
8.7959
8.6839
8.6787
8.6604
7.8850
7.8714
7.8674
7.8609
7.8543
7.8478
7.8415
7.8372
7.8057
7.8023
7.7850
7.7662
7.7462
7.5913
7.5703
7.5490
7.5297
7.4980
7.4945
7.4755
7.4623
7.4565
7.4313
7.4264
7.4125
7.4080
7.3949
7.3903
7.3528
7.3322
7.2856
G-220.1.fid
GY
N
S
12
2.02
1.00
2.01
4.01
10.39
2.00
f1 (ppm)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131.5783
131.5460
131.2499
130.3237
129.7665
129.5586
129.4425
128.9747
128.9064
128.7644
128.3826
128.0444
127.9949
127.6130
127.4015
127.1407
126.8390
123.7319
123.2476
122.8481
121.4556
91.7122
90.5602
77.3479
77.0304
76.7129
G-220.2.fid
GY
123.7319
123.2476
122.8481
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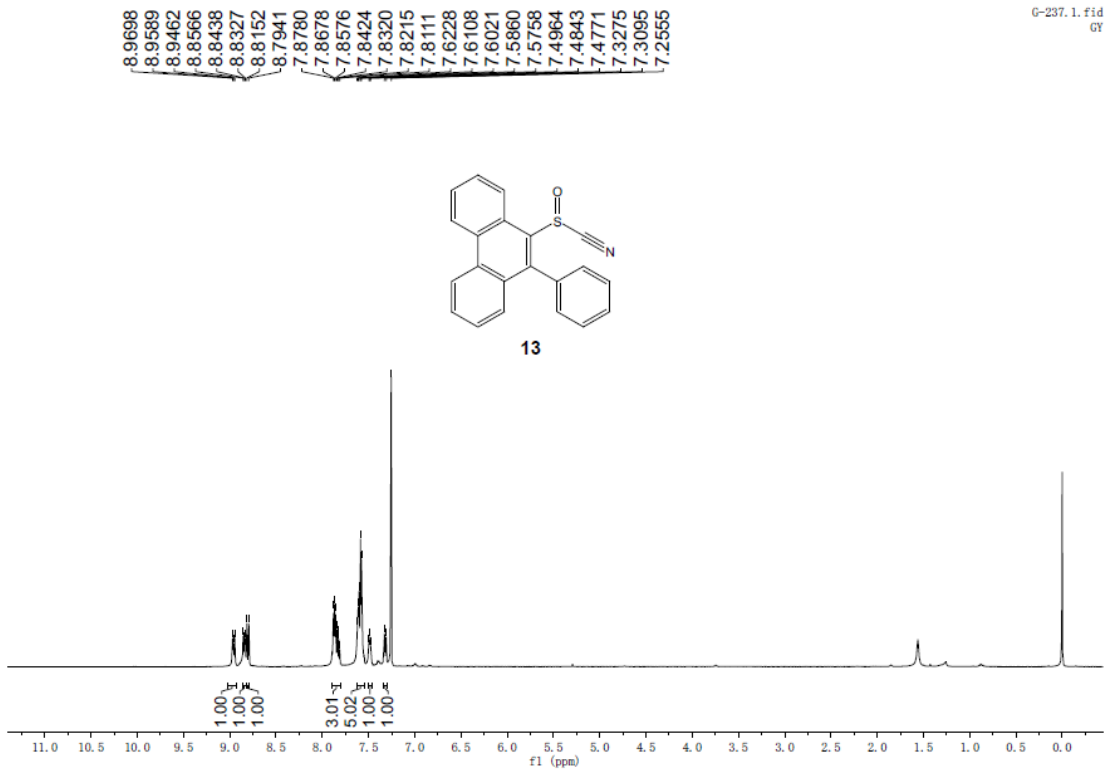
119.4327
111.0762
91.7122
90.5602
N
S
12
f1 (ppm)
f1 (ppm)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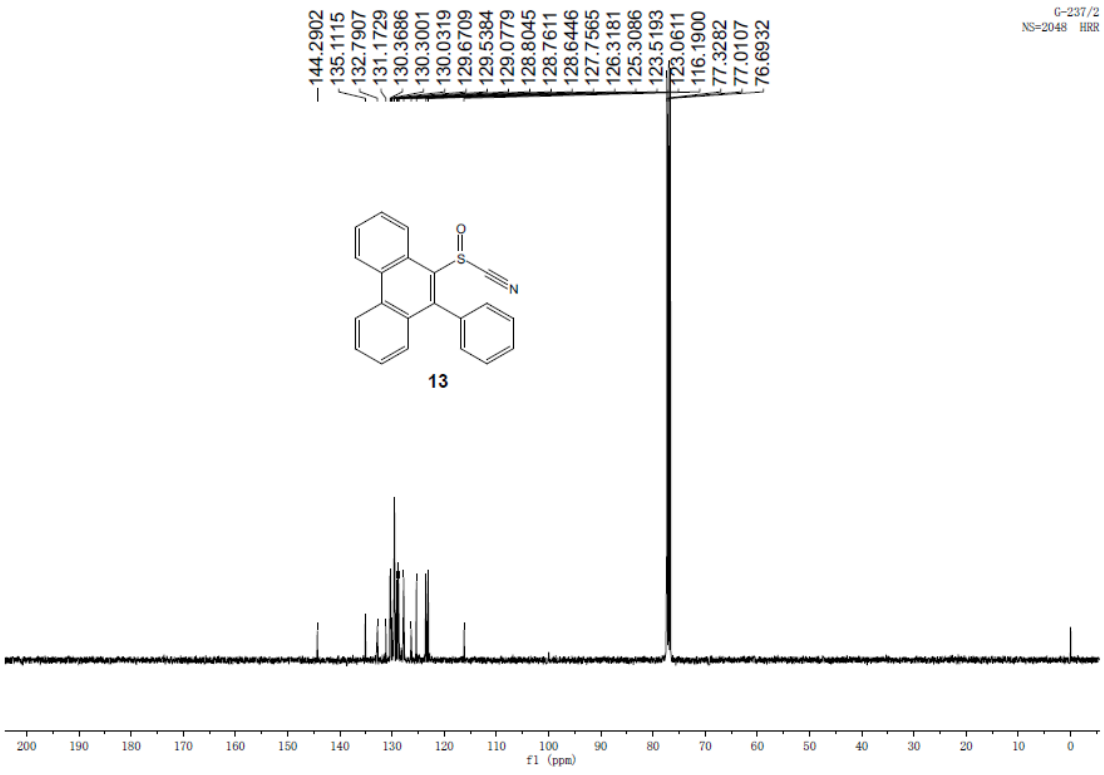
8.9589
8.9462
8.8566
8.8438
8.8327
8.8152
8.7941
7.8780
7.8678
7.8576
7.8424
7.8320
7.8215
7.8111
7.6228
7.6108
7.6021
7.5860
7.5758
7.4964
7.4843
7.4771
7.3275
7.3095
7.2555
G-237.1.fid
GY
O
S
N
13
1.00
1.00
1.00
3.01
5.02
1.00
1.00
f1 (ppm)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131.1729
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130.0319
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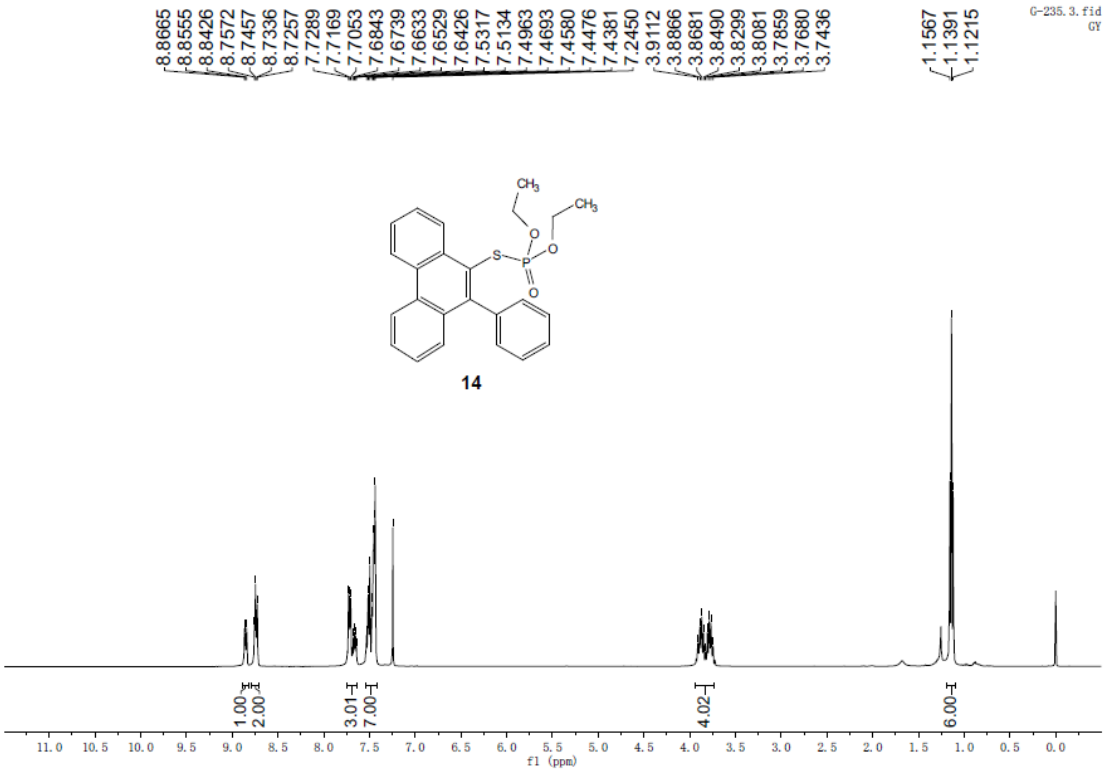
129.0779
128.8045
128.7611
128.6446
127.7565
126.3181
125.3086
123.5193
123.0611
116.1900
77.3282
77.0107
76.6932
G-237/2
NS=2048 HRR
O
S
N
13
f1 (ppm)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8.8555
8.8426
8.7572
8.7457
8.7336
8.7257
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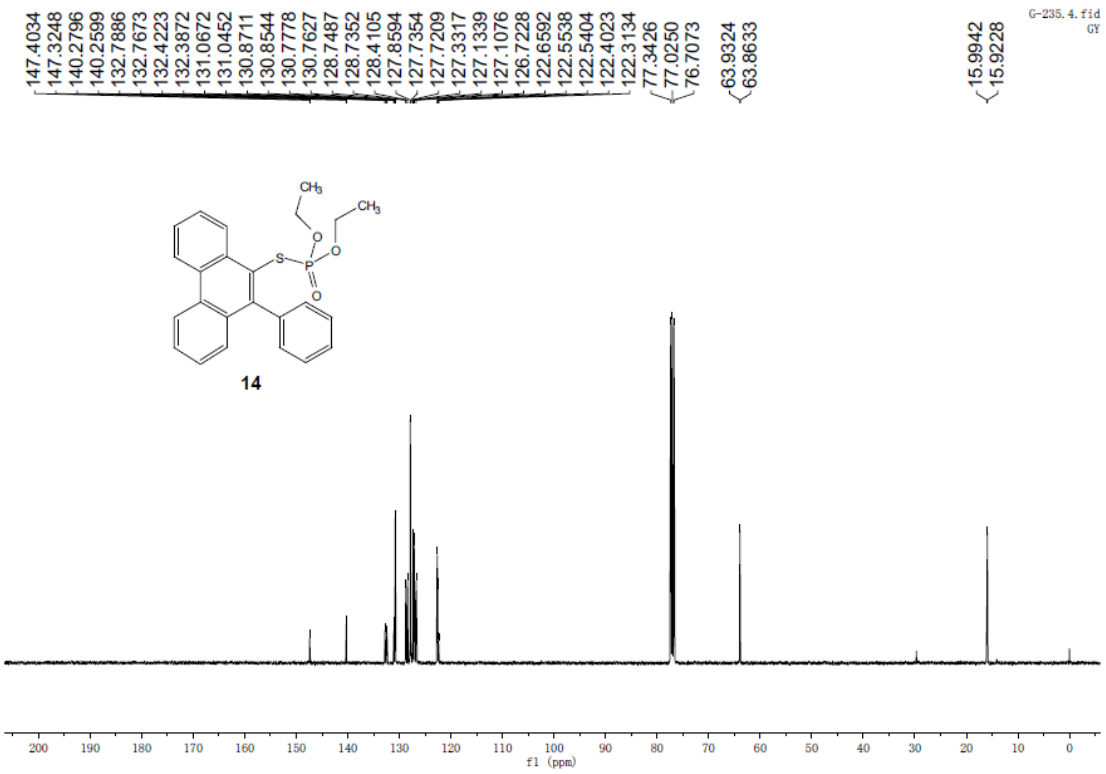
7.7169
7.7053
7.6843
7.6739
7.6633
7.6529
7.6426
7.5317
7.5134
7.4963
7.4693
7.4580
7.4476
7.4381
7.2450
3.9112
3.8866
3.8681
3.8490
3.8299
3.8081
3.7859
3.7680
3.7436
1.1567
1.1391
1.1215
G-235.3.fid
GY
14
1.00
2.00
3.01
7.00
4.02
6.00
f1 (ppm)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140.2599
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132.4223
132.3872
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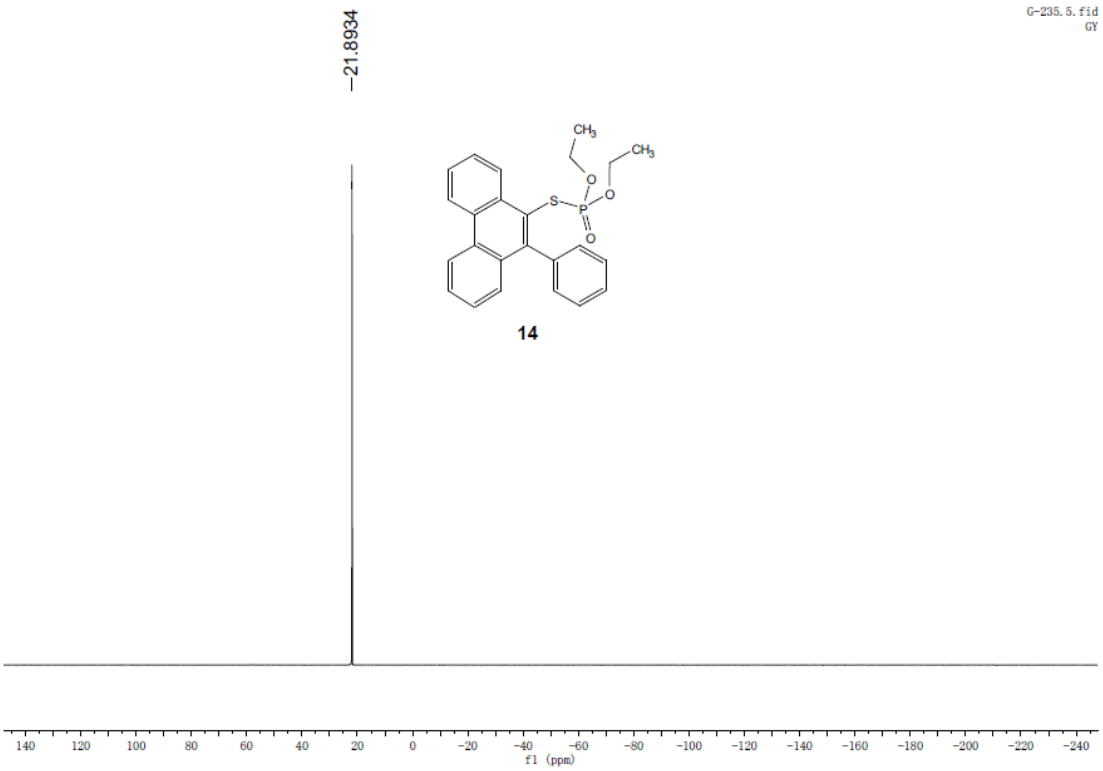
131.0452
130.8711
130.8544
130.7778
130.7627
128.7487
128.7352
128.4105
127.8594
127.7354
127.7209
127.3317
127.1339
127.1076
126.7228
122.6592
122.5538
122.5404
122.4023
122.3134
77.3426
77.0250
76.7073
63.9324
63.8633
15.9942
15.9228
G-235.4.fid
GY
14
f1 (ppm)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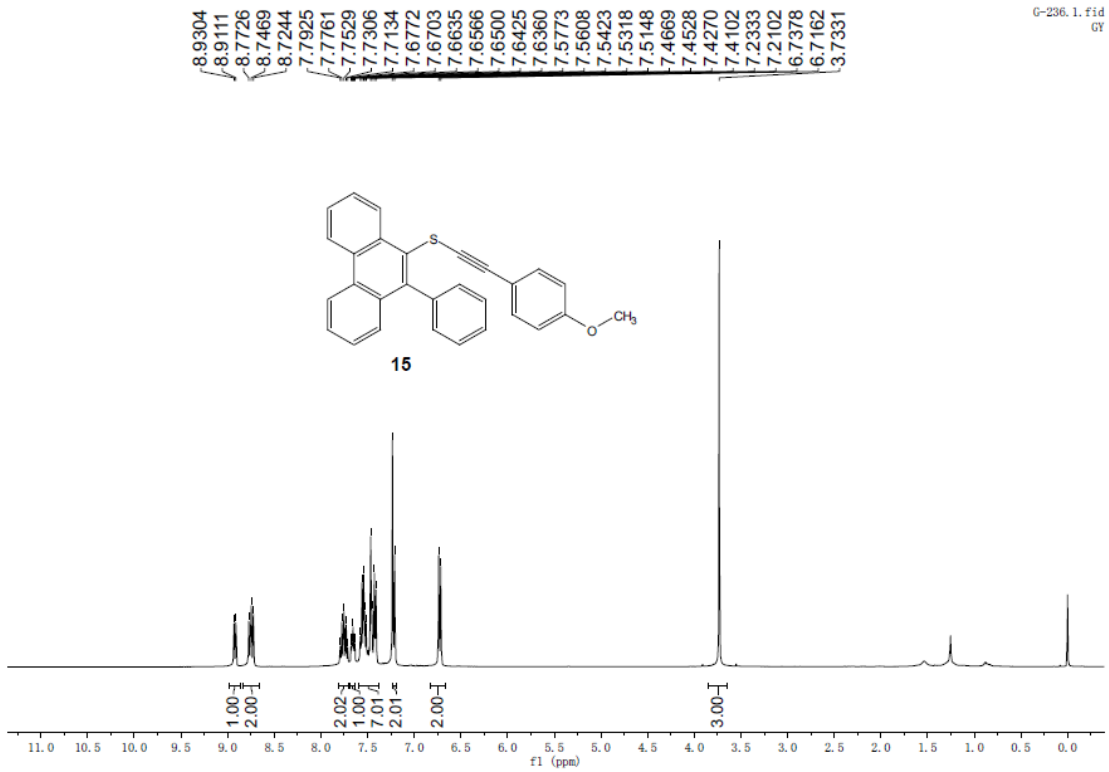
CH3
CH3
O
O
S
P
O
140
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
f1 (ppm)

14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7.7761
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7.7306
7.7134
7.6772
7.6703
7.6635
7.6566
7.6500
7.6425
7.6360
7.5773
7.5608
7.5423
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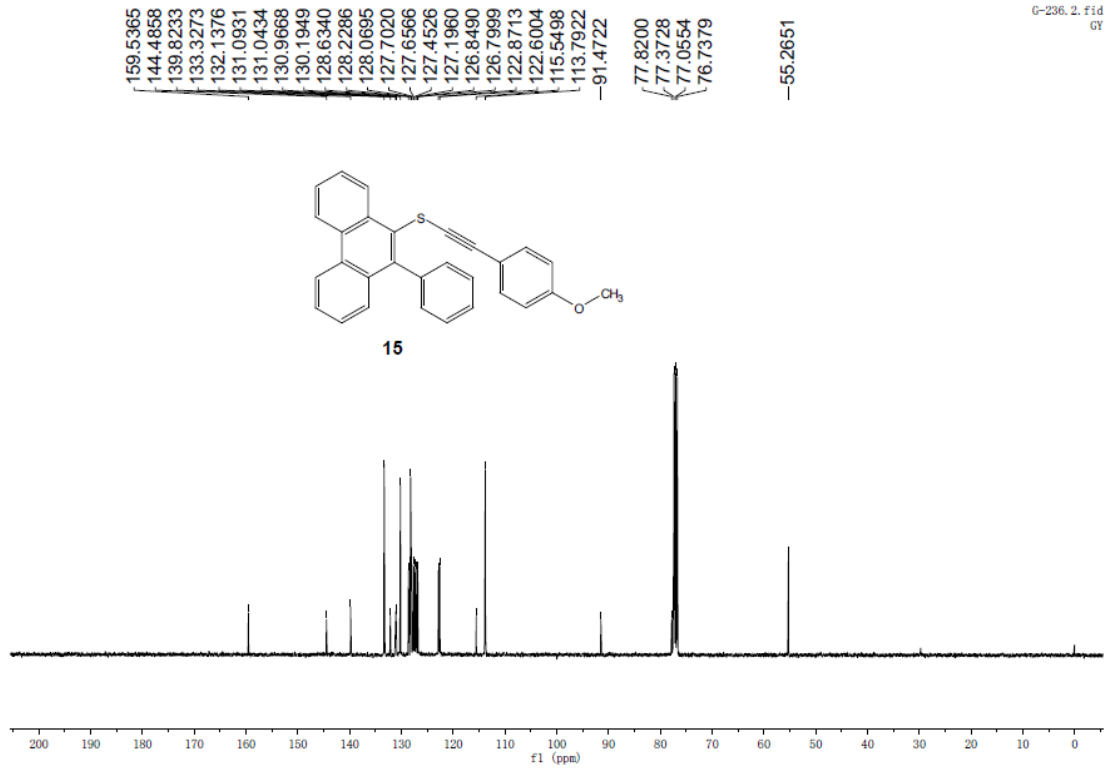
7.5148
7.4669
7.4528
7.4270
7.4102
7.2333
7.2102
6.7378
6.7162
3.7331
G-236.1.fid
GY
S
CH3
O
15
1.00
2.00
2.02
1.00
7.01
2.01
2.00
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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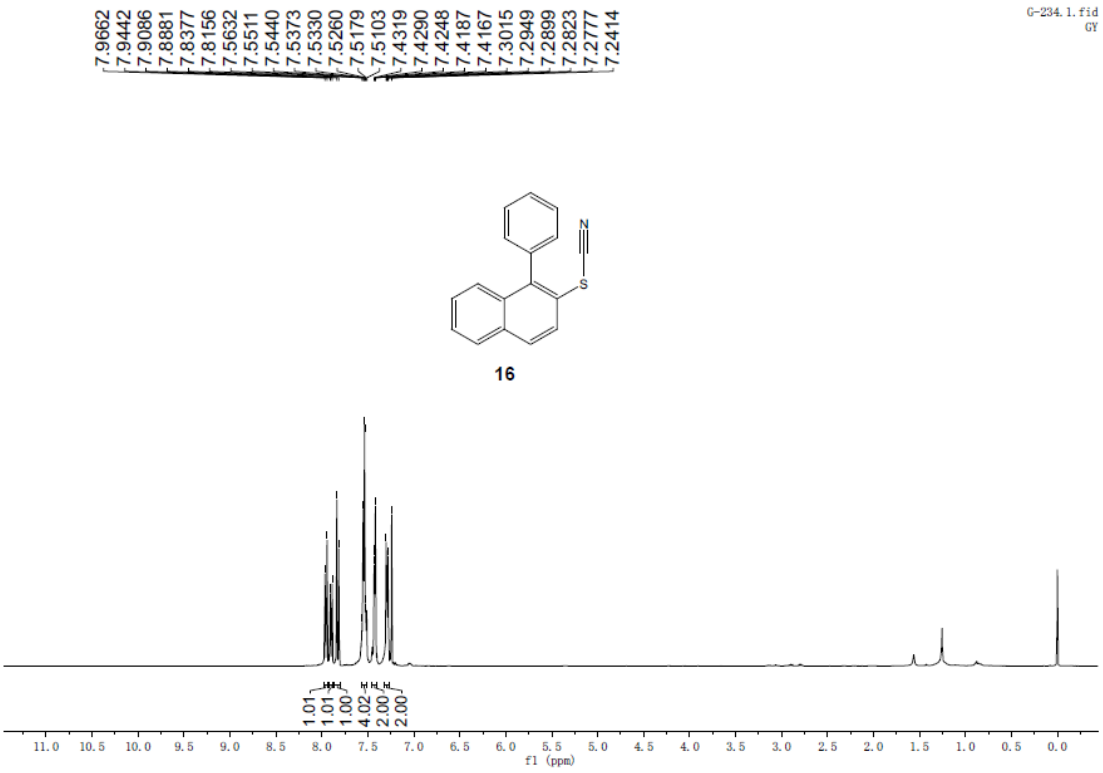
127.1960
126.8490
126.7999
122.8713
122.6004
115.5498
113.7922
91.4722
77.8200
77.3728
77.0554
76.7379
55.2651
G-236.2.fid
GY
S
CH3
O
15
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.5373
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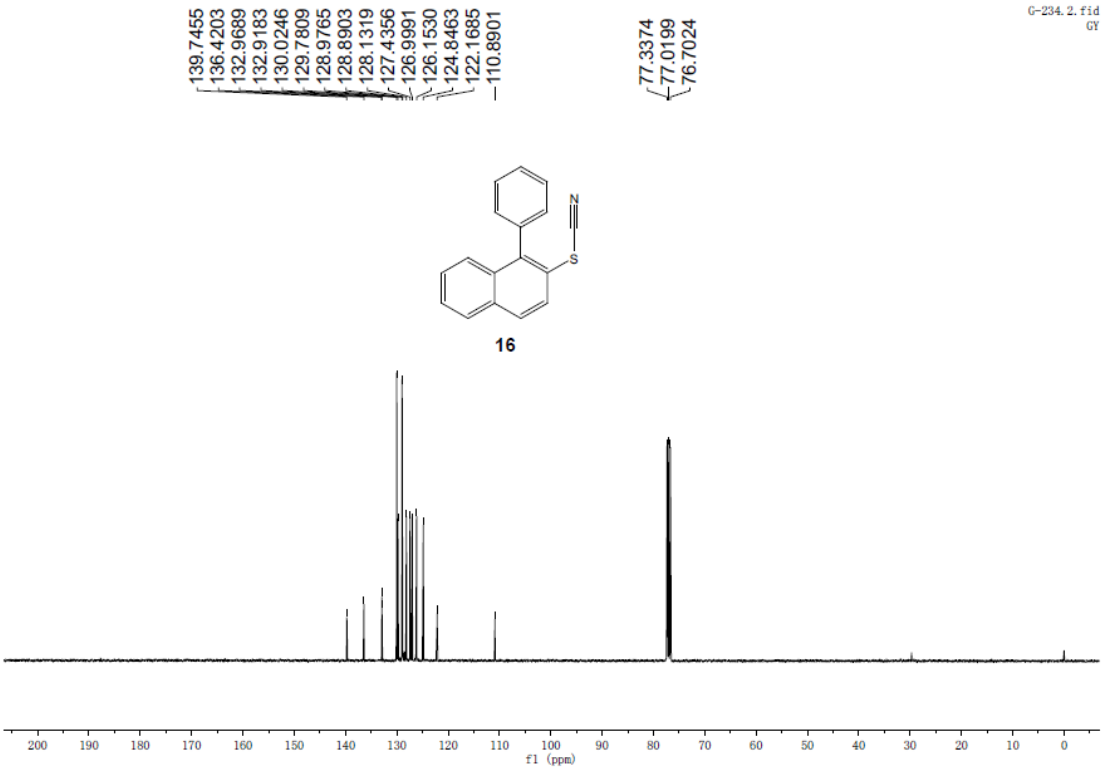
7.5260
7.5179
7.5103
7.4319
7.4290
7.4248
7.4187
7.4167
7.3015
7.2949
7.2899
7.2823
7.2777
7.2414
G-234.1.fid
GY
N
S
1.01
1.01
1.00
4.02
2.00
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

16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127.4356
126.9991
126.1530
124.8463
122.1685
110.8901
77.3374
77.0199
76.7024
G-234.2.fid
GY
N
S
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

16