# Suppplementary Information

## Fused Multifunctionalized Dibenzoselenophenes from Tetraynes

Yimin Hu,*† Jie Ma,† Lidong Li, Qiong Hu, Shuang Lv, Baohua Liu and Shaowu Wang*

*School of Chemistry and Materials Science, Anhui Normal University,*

*Wuhu, Anhui 241000, China E-mail: yiminhu@ahnu.edu.cn; swwang@ahnu.edu.cn*

# Contents

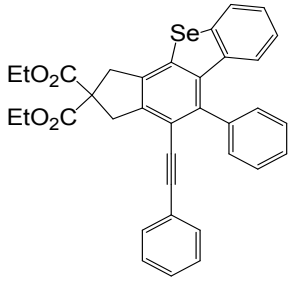
## 1. General experimental procedures

All the catalytic reactions were performed under an argon atmosphere using the oven-dried Schlenk flask. The chemicals were purchased from Alfa Aesar and Acros Chemicals. All solvents and materials were pre-dried, redistilled or recrystallized before use. $^{1}H$ NMR (300 MHz) and $^{13}C$ NMR (125 MHz) spectra were recorded on a Bruker Avance 300 spectrometerwith $CDCl_3$ as the solvent. Chemical shifts are reported in ppm by assigning TMS resonance in the $^{1}H$ NMR spectra as 0.00 ppm and $CDCl_3$ resonance in the $^{13}C$ spectra as 77.0 ppm. All coupling constants (*J* values) were reported in Hertz (Hz). Column chromatography was performed on silica gel 300–400 mesh. Melting points were determined using a Gallenkamp melting point apparatus and are uncorrected. The FT-IR spectra were recorded from KBr pellets or thin film from $CHCl_3$ on the NaCl window in the 4000-400 $cm^{-1}$ ranges on a Nicolet 5DX spectrometer. All HRMS spectra were record using EI or APCI at 70 eV. X-ray Crystallography diffraction data of **3d**, **3k**, **3s** and **3v** were collected at room temperature with a Bruker SMART Apex CCD diffractometer with Mo-Kα radiation ($\lambda$ = 0.71073 Å ) witha graphite monochromator using the ω-scan mode. Data reductions and absorption corrections were performed with SAINT and SADABS software, respectively. The structure was solved by direct methods and refined on $F^2$ by full-matrix least squares using SHELXTL. All non-hydrogen atoms were treated anisotropically. The positions of hydrogen atoms were generated geometrically.

**General procedures:**

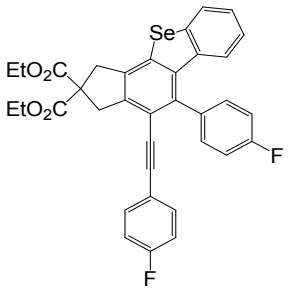
Typical experimental procedure: Tetraynes (1.2 equiv) and diphenyl diselenide (PhSeSePh) (0.5 equiv) were added to toluene (2.5 mL), the mixture was stirred at room temperature then heated at 90 °C for 8 hours in air. The reaction mixture was cooled to room temperature, and the solvent was evaporated in vacuo. The residue was purified by preparative thin-layer chromatography (TLC) on silica gel with the appropriate mixture of petroleum ether and ethyl acetate to give the fused multifunctionalized dibenzoselenophenederivatives.

## 2. Characterization Data for the New Compounds



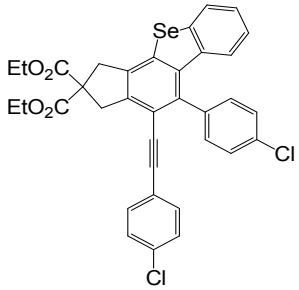

**Diethyl 5-phenyl-4-(phenylethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate（3a）**

White solid; 460 mg (78 % yield); m. p. 170-171℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.40; $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ 7.92-7.76 (d, $J$ = 7.7 Hz, 1H; Ar-H), 7.55 (s, 3H; Ar-H), 7.49-7.36 (m, 2H; Ar-H), 7.30-7.20 (m, 4H; Ar-H), 7.14-7.08 (m, 2H; Ar-H), 7.06-6.98 (t, $J$ = 7.4 Hz, 1H; Ar-H), 6.84-6.80 (d, $J$ = 8.1 Hz, 1H; Ar-H), 4.30-4.26 (dd, $J$ = 14.0, 6.9 Hz, 4H; $OCH_2CH_3$), 3.96 (s, 2H;$CH_2$), 3.81 (s, 2H;$CH_2$), 1.31 (t, $J$ = 7.0 Hz, 6H; $OCH_2CH_3$); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 171.9, 142.0, 140.5, 139.9, 138.8, 136.4, 135.9, 135.7, 131.7, 130.0, 129.2, 128.6, 128.4, 128.2, 127.1, 126.6, 126.4, 124.9, 123.8, 118.2, 97.2, 87.5, 62.5, 60.1, 42.3, 41.8, 14.5 ppm; FT-IR (KBr):$v$ 3057, 2978, 2359, 1726, 1489, 1440, 1259, 1186, 1068, 862, 748, 705, 688 cm$^{-1}$; HRMS (APCI): *m/z* calcd for $C_{35}H_{28}O_4Se$ $[M+H]^+$, 593.1226; found 593.1227.




**Diethyl 5-(4-fluorophenyl)-4-((4-fluorophenyl)ethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate（3b）**

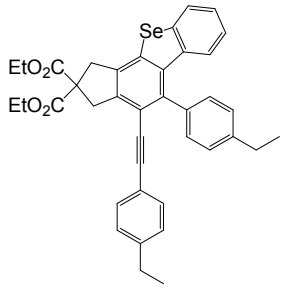
Light yellow solid; 471 mg (75 % yield); m. p. 173-174℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.38; $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ 7.87-7.83 (d, $J$ = 7.8 Hz, 1H; Ar-H), 7.40-7.36 (m, 2H; Ar-H), 7.31-7.22 (m, 3H; Ar-H), 7.19-7.02 (m, 3H;Ar-H), 6.99-6.92 (m, 2H; Ar-H), 6.85-6.79 (d, $J$ = 8.2 Hz, 1H; Ar-H), 4.32-4.27 (q, $J$ =7.1 Hz, 4H; $OCH_2CH_3$), 3.93 (s, 2H; $CH_2$), 3.80 (s, 2H; $CH_2$), 1.45-1.20 (t, $J$ = 7.1 Hz, 6H; $OCH_2CH_3$); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 171.8, 163.9, 161.9, 154.8, 140.6, 140.0, 139.9, 138.6, 136.5, 136.3, 135.8, 133.6, 133.5, 131.9, 131.8, 129.9, 126.9, 126.7, 126.5, 124.9, 118.3, 116.3, 116.1, 116.1, 115.9, 96.3, 86.9, 77.7, 77.4, 77.2, 62.5, 60.1, 42.3, 41.8, 14.5 ppm; FT-IR (KBr): $v$ 3446, 2980, 2330, 1724, 1598, 1506, 1261, 1226, 1184, 1155, 1066, 837, 810, 750, 518 cm$^{-1}$; HRMS (APCI): *m/z* calcd for $C_{35}H_{26}F_2O_4Se$ $[M+H]^+$, 629.1037; found 629.1040.




**Diethyl 5-(4-chlorophenyl)-4-((4-chlorophenyl)ethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3c)**

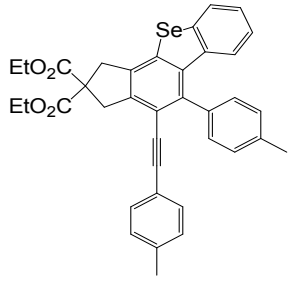
Light yellow solid; 528 mg (80 % yield); m. p. 187-188℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.46; $^1$H NMR (300 MHz, $CDCl_3$)**:** $\delta$ 7.88-7.83 (d, $J$ = 7.8 Hz, 1H; Ar-H), 7.58-7.50 (d, $J$ = 8.1 Hz, 1H; Ar-H), 7.50-7.41 (m,1H; Ar-H), 7.38-7.32 (m, 2H; Ar-H), 7.28-7,22 (m, 3H; Ar-H), 7.11-7.04 (m, 3H; Ar-H), 6.92-6.86 (d, $J$ = 8.2 Hz, 1H; Ar-H), 4.32-4.26 (q, $J$ = 7.1 Hz, 4H;O$CH_2$CH$_3$), 3.93 (s, 2H, $CH_2$), 3.80 (s, 2H, $CH_2$), 1.36-1.28 (t, $J$ = 7.1 Hz, 6H; $OCH_2CH_3$); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 171.8, 140.5, 140.0,138.9, 138.5, 136.8, 136.5, 135.6, 134.6, 134.3, 133.5, 132.9, 131.6, 130.9, 129.9, 129.5, 129.0, 128.5, 126.9, 126.8, 126.5, 125.0, 122.0, 117.9, 96.4, 88.2, 62.5, 62.4, 60.1, 42.2, 41.8, 14.5 ppm; FT-IR (KBr): $v$ 3446, 2980,

2358, 1726, 1489, 1261, 1186, 1166, 1089, 1068, 1014, 827, 750, 667, 526, 501 $cm^{-1}$; HRMS (APCI): *m/z* calcd for $C_{35}H_{26}Cl_2O_4Se$ $[M+H]^+$, 661.0046; found 661.0050.



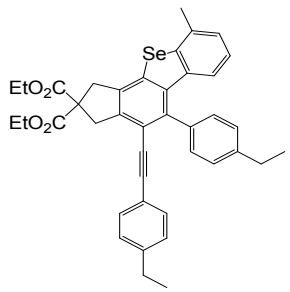

**Diethyl 5-(4-ethylphenyl)-4-((4-ethylphenyl)ethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3d)**

White solid; 480 mg (74% yield); m. p. 164-165℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.44; $^1H$ NMR (300 MHz, $CDCl_3$): $\delta$ 7.85-7.82 (d, 1H, *J* = 6.9 Hz; Ar-H), 7.42-7.36 (m, 2H; Ar-H), 7.33-7.29 (m, 2H; Ar-H), 7.25-7.22 (m, 1H; Ar-H), 7.06-6.99 (m, 5H; Ar-H), 6.93-6.91 (d, 1H, *J* = 8.1 Hz; Ar-H), 4.33-4.23 (q, 4H, *J* = 6.9 Hz; $OCH_2CH_3$), 3.95 (s, 2H; $CH_2$), 3.79 (s, 2H; $CH_2$), 2.87-2.77 (q, 4H, *J* = 7.5 Hz; $CH_2CH_3$), 2.65-2.55 (q, 4H, *J* = 7.5 Hz; $CH_2CH_3$), 1.41-1.18 (m, 12H; $CH_2CH_3$); $^{13}C$ NMR (125 MHz, $CDCl_3$): $\delta$ 171.9, 144.8, 144.2, 142.2, 139.9, 139.7, 139.0, 137.8, 136.0, 135.8, 131.8, 130.0, 128.7, 128.1, 127.2, 126.5, 126.4, 124.8, 121.1, 118.7, 97.4, 87.1, 62.4, 60.1, 42.3, 41.9, 29.4, 29.2, 16.5, 15.8, 14.5 ppm; FT-IR (KBr): *v* 3446,3047, 2962, 2927, 2358, 1724, 1508, 1458, 1261, 1186, 1068, 1018, 827, 779, 750 $cm^{-1}$; HRMS (APCI): *m/z* calcd for $C_{39}H_{36}O_4Se$ $[M + H]^+$, 649.1852; found: 649.1852.



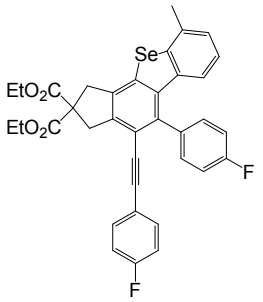

**Diethyl 5-(p-tolyl)-4-(p-tolylethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3e)**

White solid; 465mg (75 % yield); m. p. 155-156℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.41; $^1H$ NMR (300 MHz, $CDCl_3$): $\delta$ 7.88-7.80 (d, *J* = 7.7 Hz, 1H; Ar-H), 7.41-7.32 (m, 2H; Ar-H), 7.28-7.22 (m, 4H; Ar-H), 7.15-6.98 (m, 4H; Ar-H), 6.93-6.88 (d, *J* = 8.1 Hz, 1H; Ar-H), 4.32-4.24 (q, *J* = 7.1 Hz, 4H; $CH_2CH_3$), 3.94 (s, 2H; $CH_2$), 3.79 (s, 2H; $CH_2$), 2.52 (s, 3H; $CH_3$), 2.31 (s, 3H; $CH_3$), 1.36-1.27 (t, *J* = 7.1 Hz, 6H; $OCH_2CH_3$); $^{13}C$ NMR (125 MHz, $CDCl_3$):$\delta$ 171.9, 142.0, 139.9, 139.0, 138.5, 137.7, 137.5, 135.8, 131.6, 129.9, 129.8, 129.3, 127.2, 126.5, 126.3, 124.8, 120.8, 118.6, 97.3, 87.0, 62.4, 60.1, 42.3, 41.9, 21.9, 14.5 ppm; FT-IR (KBr): *v* 3446, 2980, 2922, 2358, 1728, 1647, 1508, 1458, 1261, 1184, 1068, 1018, 815, 748 $cm^{-1}$; HRMS (APCI): *m/z* calcd for $C_{37}H_{32}O_4Se$ $[M+H]^+$, 621.1539; found 621.1533.



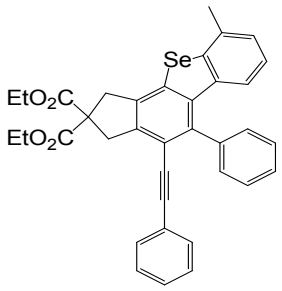
**Diethyl 5-(4-ethylphenyl)-4-((4-ethylphenyl)ethynyl)-9-methyl-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3f)**

White solid; 543 mg (82 % yield); m. p. 176-177℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.58; $^1$H NMR (300 MHz, $CDCl_3$):*δ* 7.44-7.36 (d, *J* = 7.7 Hz, 2H; Ar-H), 7.34-7.20 (m, 3H; Ar-H), 7.16-6.92 (m, 5H; Ar-H), 6.79-6.73 (d, *J* = 8.1 Hz, 1H;Ar-H), 4.34-4.22 (q, *J* = 7.0 Hz, 4H; $OCH_2CH_3$), 3.95 (s, 2H; $CH_2$), 3.82 (s, 2H; $CH_2$), 2.85-2.77 (q, *J* = 7.6 Hz, 2H; $CH_2CH_3$), 2.66-2.55 (q, *J* = 15.2, 7.6 Hz, 2H; $CH_2CH_3$), 2.53 (s, 3H;$CH_3$), 1.40-1.36 (t, *J* = 7.6 Hz, 3H; $CH_3$), 1.34-1.27 (t, *J* = 7.1 Hz, 6H; $OCH_2CH_3$), 1.22-1.16 (t, *J* = 7.5 Hz, 3H; $CH_2CH_3$); $^{13}$C NMR (125 MHz, $CDCl_3$): *δ* 171.9, 144.8, 144.1, 142.3, 141.2, 139.5, 138.9, 137.8, 136.5, 135.7, 134.7, 131.8, 130.0, 128.6, 128.1, 126.6, 125.4, 124.7, 121.1, 118.7, 97.4, 87.2, 62.4, 60.1, 42.3, 41.9, 29.3, 29.2, 23.1, 16.5, 15.8, 14.5 ppm; FT-IR (KBr): ν 3446, 2958, 2366, 1730, 1508, 1255, 1178, 1155, 1068, 1051, 1014, 831, 790, 758, 516 cm$^{-1}$; HRMS (APCI): *m/z* calcd for $C_{40}H_{38}O_4Se$ $[M+H]^+$, 663.2008; found 663.2009.




**Diethyl 5-(4-fluorophenyl)-4-((4-fluorophenyl)ethynyl)-9-methyl-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3g)**

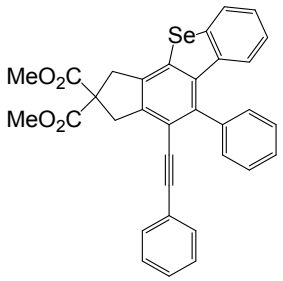
White solid; 507 mg (79 % yield); m. p. 170-171℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.53; $^1$H NMR (500 MHz, $CDCl_3$): *δ* 7.37 (m, 2H; Ar-H), 7.34-7.20 (m, 3H; Ar-H), 7.15-7.08 (m, 2H; Ar-H), 7.03-7.01 (t, *J* = 7.7 Hz, 1H, Ar-H), 6.99-6.90 (t, *J* = 8.7 Hz, 2H, Ar-H), 6.69-6.66 (d, *J* = 8.2 Hz, 1H; Ar-H), 4.36-4.19 (q, *J* = 7.0 Hz, 4H; $OCH_2CH_3$), 3.94 (s, 2H;$CH_2$), 3.83 (s, 2H;$CH_2$), 2.54 (s, 3H;$CH_3$), 1.31 (t, *J* = 7.1 Hz, 6H; $OCH_2CH_3$); $^{13}$C NMR (125 MHz, $CDCl_3$): *δ* 171.8, 163.9, 163.8, 161.9, 141.3, 140.8, 139.7, 138.5, 136.6, 136.4, 136.3, 134.9, 133.6, 133.5, 131.9, 131.9, 126.8, 125.5, 124.4, 119.8, 118.3, 116.3, 116.1, 116.1, 115.9, 105.4, 96.3, 87.0, 62.5, 60.1, 42.3, 41.8, 23.1, 14.5 ppm; FT-IR (KBr): *v* 3460, 2985, 2328, 1732, 1506, 1247, 1182, 1153, 1095, 1068, 1045, 837, 785, 684, 516 cm$^{-1}$; HRMS (APCI): *m/z* calcd for $C_{36}H_{28}F_2O_4Se$ $[M+H]^+$, 642.1194; found 642.1192.




**Diethyl 9-methyl-5-phenyl-4-(phenylethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3h)**

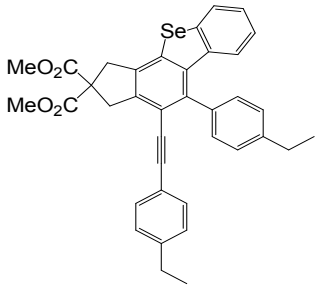
White solid; 480 mg (80 % yield); m. p. 172-173℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.56; $^1$H NMR (300 MHz, $CDCl_3$): *δ* 7.56-7.54 (m, 3H; Ar-H), 7.42-7.40 (m, 2H; Ar-H), 7.26-7.22 (d, *J* = 5.6 Hz, 3H; Ar-H), 7.11 (s, 3H; Ar-H), 6.98-6.96 (m, 1H; Ar-H), 6.70-6.66 (d, *J* = 8.1 Hz, 1H; Ar-H), 4.30-4.26 (q, *J* = 6.8 Hz, 4H; $OCH_2CH_3$), 3.96 (s, 2H; $CH_2$), 3.83 (s, 2H; $CH_2$), 2.54 (s, 3H; $CH_3$), 1.33-1.30 (t, 6H; $OCH_2CH_3$);$^{13}$C NMR (125 MHz, $CDCl_3$): *δ* 171.9, 142.1, 141.2, 140.5, 139.7, 138.7, 136.4, 135.9, 134.7, 131.7, 130.1, 129.2, 128.5, 128.4, 128.2, 126.7, 125.5, 124.6, 123.8, 118.3, 97.2, 87.6,62.5, 60.1,

42.3, 41.9, 23.1, 14.5 ppm; FT-IR (KBr): *v* 3446, 2976, 2362, 1718, 1255, 1188, 1153, 1072, 858, 790, 756, 704, 686, 418 $cm^{-1}$; HRMS (APCI): *m/z* calcd for $C_{36}H_{30}O_4Se$ $[M+H]^+$; 607.1309; found 607.1377.



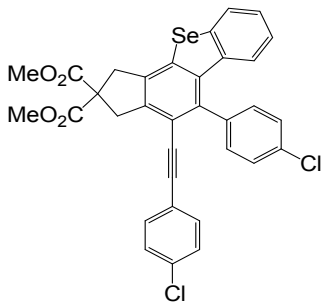

**Dimethyl 5-phenyl-4-(phenylethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3i)**

White solid; 452 mg (76% yield); m. p. 201-202℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.27; $^1H$ NMR (300 MHz, $CDCl_3$): $\delta$ 7.85-7.83 (d, *J* = 7.7 Hz, 1H; Ar-H), 7.55 (s, 3H; Ar-H), 7.42 (s, 2H; Ar-H), 7.26-7.22 (m, 4H; Ar-H), 7.13-7.10 (d, *J* = 3.3 Hz, 2H; Ar-H), 7.03-7.01 (t, *J* = 7.6 Hz, 1H; Ar-H), 6.82 (d, *J* = 8.1 Hz, 1H; Ar-H), 3.98 (s, 2H; $CH_2$), 3.82 (s, 2H; $CH_2$),3.82 (s, 6H; $OCH_3$); $^{13}C$ NMR (125 MHz, $CDCl_3$): $\delta$ 172.3, 142.1, 140.5, 139.9, 139.8, 138.8, 136.4, 135.9, 135.7, 131.8, 130.0, 129.2, 128.6, 128.5, 128.3, 127.1, 126.6, 126.4, 124.9, 123.7, 118.2, 97.3, 87.5, 59.9, 53.8, 42.4, 42.0 ppm; FT-IR (KBr): ν 3446, 3055, 2953, 2364, 1735, 1489, 1438, 1274, 1244, 1199, 1157,1072, 744, 704, 686 $cm^{-1}$; HRMS (APCI): *m/z* calcd for $C_{33}H_{24}O_4Se$ $[M+H]^+$, 595.0931; found 595.0933.



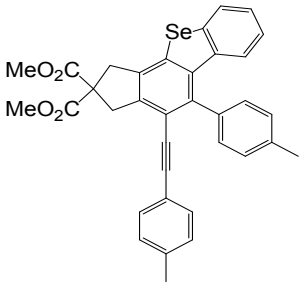

**Dimethyl 5-(4-ethylphenyl)-4-((4-ethylphenyl)ethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3j)**

White solid; 484 mg (78 % yield); m. p. 192-193℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.33; $^1H$ NMR (300 MHz, $CDCl_3$): $\delta$ 7.83 (d, *J* = 7.4 Hz, 1H; Ar-H), 7.38 (m, 2H; Ar-H), 7.29 (m, 3H; Ar-H), 7.04 (s, 4H; Ar-H), 6.92 (d, *J* = 7.9 Hz, 1H; Ar-H), 3.97 (s, 2H; $CH_2$), 3.82 (s, 2H; $CH_2$), 3.81 (s, 6H, $OCH_3$), 2.83 (d, *J* = 7.2 Hz, 2H; $CH_2CH_3$), 2.60 (d, *J* = 7.4 Hz, 2H; $CH_2CH_3$), 1.39 (t, *J* = 7.2 Hz, 3H; $CH_2CH_3$), 1.20 (t, *J* = 7.2 Hz, 3H; $CH_2CH_3$); $^{13}C$ NMR (125 MHz, $CDCl_3$): $\delta$ 172.3, 144.8, 144.2, 142.2, 139.9, 139.6, 138.9, 137.8, 136.0, 135.8, 135.6, 133.1, 131.8, 129.9, 128.7, 128.1, 127.8, 127.2, 126.5, 126.3, 124.8, 121.0, 118.7, 97.5, 87.1, 60.0, 53.7, 42.4, 41.9, 29.4, 29.2, 16.5, 15.8 ppm; FT-IR (KBr): *v* 3466, 2960, 2345, 1732, 1647, 1506, 1429,1278, 1249,1155,829,748 $cm^{-1}$; HRMS (APCI): *m/z* calcd for $C_{37}H_{32}O_4Se$ $[M+H]^+$, 621.1539; found 621.1537.



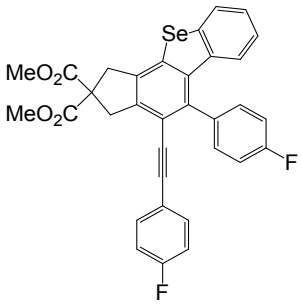
**Dimethyl5-(4-chlorophenyl)-4-((4-chlorophenyl)ethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3k)**

White solid; 524 mg (83% yield); m. p. 206-207℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.32; $^1$H NMR (500 MHz, $CDCl_3$): $\delta$ 7.88-7.83 (d, $J$ = 7.9 Hz, 1H; Ar-H), 7.58-7.53 (d, $J$ = 8.3 Hz, 2H; Ar-H), 7.39-7.34 (d, $J$ = 8.3 Hz, 2H; Ar-H), 7.30-7.22 (m, 3H; Ar-H), 7.11-7.03(m, 3H; Ar-H), 6.91-6.87 (d, $J$ = 8.2 Hz, 1H; Ar-H), 3.94 (s, 2H; $CH_2$), 3.82 (s, 2H; $CH_2$), 3.82(s, 6H; $OCH_3$); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 172.2, 140.5, 140.0, 139.8, 138.9, 138.4, 136.8, 136.3, 135.6, 134.6, 134.3, 132.8, 131.6, 129.5, 129.1, 126.9, 126.8, 126.5, 125.1, 121.9, 117.9, 96.5, 88.1, 59.9, 53.7, 42.3, 41.9 ppm; FT-IR (KBr): $v$ 3444, 2951, 2358, 1735, 1489, 1435, 1284, 1259, 1195, 1157, 1087, 1051, 1016, 825, 744, 669 cm$^{-1}$; HRMS (APCI): *m/z* calcd for$C_{33}H_{22}Cl_2O_4Se$ $[M+H]^+$, 633.0133; found 633.0135.



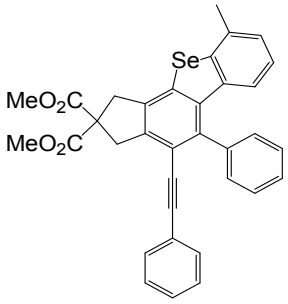

**Dimethyl 5-(p-tolyl)-4-(p-tolylethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3l)**

White solid; 468 mg (79 % yield); m. p. 167-168℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.29; $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ 7.84-7.82 (d, $J$ = 7.8 Hz, 1H; Ar-H), 7.37-7.35 (m, 3H; Ar-H), 7.27-7.24 (m, 3H; Ar-H), 7.08-7.02 (m, 5H; Ar-H), 6.92-6.88 (d, $J$ = 8.2 Hz, 1H; Ar-H), 3.96 (s, 2H; $CH_2$), 3.81 (s, 2H; $CH_2$), 3.81 (s, 6H; $OCH_3$), 2.52 (s, 3H; $CH_3$), 2.32 (s, 3H; $CH_3$); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 172.3, 142.1, 139.7, 138.9, 138.5, 137.7, 136.1, 135.6, 133.1, 131.6, 129.9, 129.8, 129.3, 129.0, 127.2, 126.5, 126.3, 124.8, 120.8, 118.6, 97.4, 87.0, 60.0, 53.6, 42.4, 42.0, 21.9 ppm; FT-IR (KBr): $v$ 3433.3, 3020.5, 2951.1, 2374.4, 1737.9, 1726.3, 1508.3, 1436.9, 1301.9, 1267.2, 1195.9, 1166.9, 1095.6, 1068.6, 815.9, 754.2, 530.4, 511.1 cm$^{-1}$; HRMS (APCI): *m/z* calcd for $C_{35}H_{28}O_4Se$ $[M+H]^+$, 593.1226; found 593.1229.



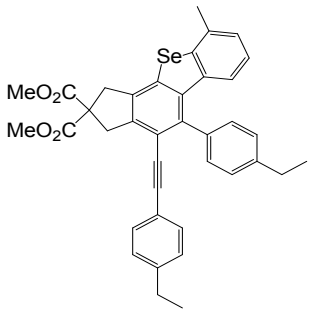

**Dimethyl 5-(4-fluorophenyl)-4-((4-fluorophenyl)ethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3m)**

White solid; 492 mg (82 % yield); m. p. 210-212℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.25; $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ 7.86-7.84 (d, $J$ = 7.7 Hz, 1H; Ar-H), 7.44-7.33 (m, 2H; Ar-H), 7.28-7.25 (m, 3H; Ar-H), 7.19-7.02 (m, 3H; Ar-H), 6.98-6.95 (m, 2H; Ar-H), 6.83 (d, $J$ = 8.2 Hz, 1H; Ar-H), 3.95 (s, 2H; $CH_2$), 3.82 (s, 2H; $CH_2$), 3.82 (s, 6H; $OCH_3$); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 172.3, 163.9, 163.8, 161.9, 161.8, 140.7, 140.0, 139.8, 138.6, 136.5, 136.4, 136.2, 135.9, 133.6, 133.5, 133.3, 131.9, 131.8, 129.9, 126.9, 126.8, 126.5, 125.0, 119.6, 118.3, 116.4, 116.2, 116.1, 115.9, 96.4, 86.9, 59.9, 53.8, 42.3, 41.9 ppm; FT-IR (KBr): $v$ 3479, 2947, 2351, 2198, 1739, 1506, 1274, 1247, 1230, 1155, 1072, 835, 748, 516 cm$^{-1}$; HRMS (APCI): *m/z* calcd for $C_{33}H_{22}F_2O_4Se$ $[M+H]^+$, 601.0724; found 601.0719.



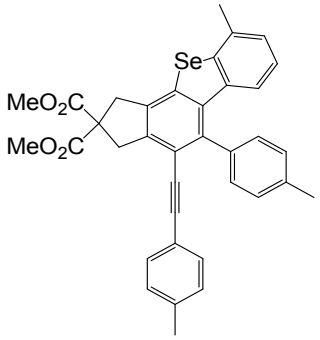

**Dimethyl 9-methyl-5-phenyl-4-(phenylethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3n)**

White solid; 490 mg (87 % yield); m. p. 188-189℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.37; $^1$H NMR (300 MHz, $CDCl_3$):$\delta$ 7.60-7.50 (m, 3H; Ar-H), 7.45-7.36 (m, 2H; Ar-H), 7.27-7.22 (dd, $J$ = 5.9, 3.3 Hz, 3H; Ar-H), 7.15-7.10 (m, 3H; Ar-H), 6.99-6.97 (t, $J$ = 7.7 Hz, 1H; Ar-H), 6.70-6.66 (d, $J$ = 8.1 Hz, 1H; Ar-H), 3.98 (s, 2H; $CH_2$), 3.85 (s, 2H; $CH_2$), 3.83 (s, 6H; $OCH_3$), 2.54 (s, 3H; $CH_3$); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 172.3, 142.2, 141.2, 140.4, 139.6, 138.7, 136.5, 136.1, 135.8, 134.8, 131.7, 130.1, 129.2, 128.6, 128.41, 128.18, 126.7, 125.5, 124.6, 123.8, 118.3, 97.3, 87.5, 60.0, 53.7, 42.4, 41.9, 23.1 ppm; FT-IR (KBr): $v$ 3454, 2953, 2372, 1743, 1635, 1431, 1296, 1244, 1165, 1051, 754, 704, 686 cm$^{-1}$; HRMS (APCI): *m/z* calcd for $C_{34}H_{26}O_4Se$ $[M+H]^+$, 579.1069; found 579.1070.



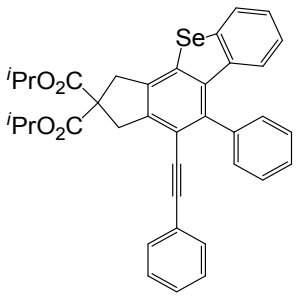

**Dimethyl 5-(4-ethylphenyl)-4-((4-ethylphenyl)ethynyl)-9-methyl-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3o)**

White solid; 469 mg (74 % yield); m. p. 179-180℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.44; $^1$H NMR (300 MHz, CDCl3): $\delta$ 7.39-7.36 (d, $J$ = 7.8 Hz, 2H; Ar-H), 7.34-7.23 (m, 2H; Ar-H), 7.16-6.93 (m, 6H; Ar-H), 6.79-6.76 (d, $J$ = 8.1 Hz, 1H; Ar-H), 3.97 (s, 2H; $CH_2$), 3.84 (s, 2H; $CH_2$), 3.83 (s, 2H; $CH_3$), 3.82 (s, 6H; $OCH_3$), 2.82 (q, $J$ = 7.5 Hz, 2H; $CH_2CH_3$), 2.60 (q, $J$ = 7.7 Hz, 2H; $CH_2CH_3$), 2.53 (s, 3H; $CH_3$), 1.41-1.37 (t, $J$ = 7.5 Hz, 3H; $CH_2CH_3$), 1.22-1.18 (t, $J$ = 7.5 Hz, 3H; $CH_2CH_3$); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 172.4, 144.8, 144.2, 141.2, 139.4, 138.8, 137.7, 136.6, 135.8, 135.6, 134.7, 131.8, 130.0, 128.7, 128.1, 126.6, 125.4, 124.7, 118.7, 97.5, 87.1, 60.1, 53.7, 42.4, 42.0, 29.4, 29.2, 23.1, 16.5, 15.8 ppm; FT-IR (KBr): $v$ 3462, 2962, 2370, 1734, 1508, 1431, 1246, 1195, 1153, 1070, 1043, 835, 792, 758cm$^{-1}$; HRMS (APCI): *m/z* calcd for $C_{38}H_{34}O_4Se$ $[M+H]^+$, 635.1695; found 635.1690.



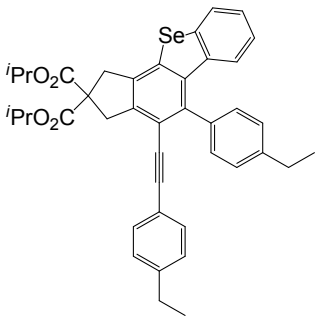

**Dimethyl 9-methyl-5-(p-tolyl)-4-(p-tolylethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3p)**

White solid; 497 mg (82 % yield); m. p. 159-160℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.38; $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ 7.41-7.24 (m, 5H; Ar-H), 7.16-6.92 (m, 6H; Ar-H), 6.78-6.74 (d, $J$ = 8.1 Hz, 1H; Ar-H), 3.96 (s, 2H; $CH_2$), 3.83 (s, 2H; $CH_2$), 3.82 (s, 6H; $OCH_3$), 2.53 (s, 3H; $CH_3$), 2.52 (s, 3H; $CH_3$), 2.31 (s, 3H; $CH_3$); $^{13}$C NMR (125 MHz, $CDCl_3$)**:** $\delta$ 172.4, 144.4, 142.2, 141.2, 139.5, 138.8, 138.5, 137.6, 136.6, 135.6, 134.7, 133.3, 133.0, 131.6, 130.9, 130.1, 129.9, 129.8, 129.3, 126.6, 125.4, 124.7, 120.8, 118.6, 97.3, 87.0, 60.0, 53.6, 42.4, 42.0, 23.1, 21.9 ppm; HRMS (APCI): *m/z* calcd for $C_{36}H_{30}O_4Se$ $[M+H]^+$, 607.1382; found 607.1388.



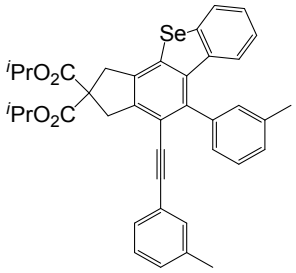

**Diisopropyl 5-phenyl-4-(phenylethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3q)**

White solid; 496 mg (80 % yield); m. p. 163-164℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.48; $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ 7.85-7.82 (d, $J$ = 7.6 Hz, 1H; Ar-H), 7.55 (s, 3H; Ar-H), 7.42 (s, 2H; Ar-H), 7.24 (m, 4H; Ar-H), 7.11 (s, 1H; Ar-H), 7.04-7.00 (t, $J$ = 7.5 Hz, 2H; Ar-H), 6.83-6.81 (d, $J$ = 8.1 Hz, 1H; Ar-H), 5.23-5.02 (m, 2H; $CH(CH_3)_2$), 3.93 (s, 2H; $CH_2$), 3.77 (s, 2H; $CH_2$), 1.29 (d, $J$ = 5.9 Hz, 12H; $CH(CH_3)_2$); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 171.4, 142.0, 140.6, 140.0, 139.9, 138.9, 136.4, 136.1, 135.6, 131.7, 130.1, 129.2, 128.6, 128.4, 128.2, 127.1, 126.6, 126.4, 124.9, 123.8, 118.3, 97.2, 87.5, 69.9, 60.1, 42.2, 41.7, 22.0 ppm; FT-IR (KBr): $\nu$ 3454, 3055, 2981, 2926, 2345, 1726, 1489, 1371, 1261, 1190, 1103, 1060, 1047, 910, 871, 786, 752, 686 cm$^{-1}$; HRMS (APCI): *m/z* calcd for $C_{37}H_{32}O_4Se$ $[M+H]^+$, 621.1539; found 621.1485.



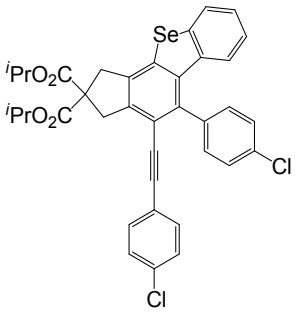

**Diisopropyl 5-(4-ethylphenyl)-4-((4-ethylphenyl)ethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3r)**

White solid; 513 mg (76 % yield); m. p. 167-168℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.53; $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ 7.85-7.83 (d, $J$ = 7.8 Hz, 1H; Ar-H), 7.39-7.38 (d, $J$ = 7.9 Hz, 2H; Ar-H), 7.31-7.29 (m, 2H; Ar-H), 7.27-7.15 (m, 1H; Ar-H), 7.15-6.96 (m, 5H; Ar-H), 6.91 (d, $J$ = 8.2 Hz, 1H; Ar-H), 5.14-5.08 (m, 2H; $CH(CH_3)_2$), 3.91 (s, 2H;$CH_2$), 3.76 (s, 2H; $CH_2$), 2.85-2.82 (q, $J$ = 7.5 Hz, 2H; $CH_2CH_3$), 2.62-2.59 (q, $J$ = 7.6 Hz, 2H; $CH_2CH_3$), 1.40-1.37 (t, $J$ = 7.6 Hz, 3H; $CH_2CH_3$), 1.30-1.28 (d, $J$ = 6.2 Hz, 12H; $CH(CH_3)_2$), 1.20-1.19 (t, $J$ = 7.6 Hz, 3H; $CH_2CH_3$); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 171.4, 144.7, 144.2, 142.2, 139.9, 139.0, 137.9, 136.0, 135.9, 135.7, 131.8, 129.9, 128.7, 128.1, 127.2, 126.4, 126.3, 124.8, 121.1, 118.7, 97.4, 87.2,69.9, 60.2, 42.2, 41.8, 29.4, 29.2, 21.9, 16.5, 15.8 ppm; FT-IR (KBr): $v$ 3454.5, 2962.7, 2927.9, 2868.2, 2351.2, 1728.2, 1508.3, 1456.3, 1371.4, 1259.5, 1188.2, 1103.3, 1060.9, 1047.4, 908.5, 871.8, 831.3, 750.3 cm$^{-1}$; HRMS (APCI): *m/z* calcd for $C_{41}H_{40}O_4Se$ $[M+H]^+$ ,677.2165; found 677.2163.




**Diisopropyl 5-(m-tolyl)-4-(m-tolylethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3s)**

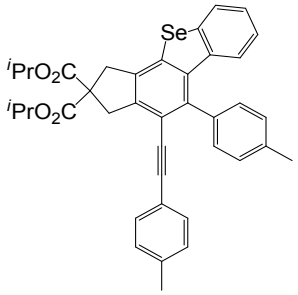
White solid; 518 mg (80 % yield); m. p. 199-200℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.58; $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ 7.85-7.83 (d, $J$ = 7.8 Hz, 1H; Ar-H), 7.45-7.44 (m, 1H; Ar-H), 7.35-7.33 (m, 2H; Ar-H), 7.30-6.99 (m, 5H; Ar-H), 6.92-6.88 (m, 3H; Ar-H), 5.13-5.08(m, 2H; $CH(CH_3)_2$), 3.92 (s, 2H;$CH_2$), 3.77 (s, 2H; $CH_2$), 2.44 (s, 3H; $CH_3$), 2.29 (s, 3H; $CH_3$), 1.32-1.27 (d, $J$ = 6.2 Hz, 12H; $CH(CH_3)_2$); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 171.4, 142.2, 140.4, 140.0, 139.9, 138.9, 138.7, 138.2, 136.3, 135.9, 135.6, 132.4, 130.6, 129.2, 129.0, 128.8, 128.7, 128.4, 127.2, 127.1, 126.5, 126.3, 124.8, 123.7, 118.3, 97.4, 87.4, 69.91, 60.2, 42.2, 41.8, 22.0, 21.6 ppm; FT-IR (KBr): $v$ 3460, 3049, 2980, 2929, 2318, 1948, 1726, 1598, 1267, 1188, 906, 875, 821, 788, 746, 688, 561, 422 cm$^{-1}$; HRMS (APCI): *m/z* calcd for $C_{39}H_{36}O_4Se$ $[M+H]^+$, 649.1852; found 649.1859.




**Diisopropyl 5-(4-chlorophenyl)-4-((4-chlorophenyl)ethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3t)**

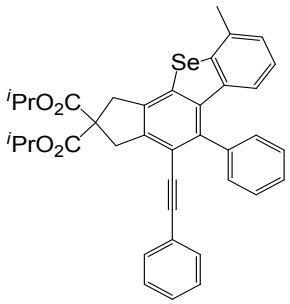
Light yellow solid; 548 mg (80 % yield); m. p. 179-180℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.54; $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ 7.87-7.83 (d, $J$ = 7.8 Hz, 1H; Ar-H), 7.56-7.54 (d, $J$ = 8.3 Hz, 2H; Ar-H), 7.37-7.34 (d, $J$ = 8.3 Hz, 2H; Ar-H), 7.28-7.23 (m, 3H; Ar-H), 7.10-7.06 (m, 3H; Ar-H), 6.90-6,87 (d, $J$ = 8.2 Hz, 1H; Ar-H), 5.13-5.08 (m, 2H; $CH(CH_3)_2$), 3.89 (s, 2H; $CH_2$), 3.76 (s, 2H; $CH_2$), 1.30-1.28 (d, $J$ = 6.2 Hz, 12H; $CH(CH_3)_2$); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 171.3, 140.5, 140.1, 140.0, 139.0, 138.5, 136.8, 136.6, 135.5, 134.5, 134.2, 132.9, 131.7, 129.5, 129.0, 126.9, 126.8, 126.5, 125.0, 122.0, 117.9,

96.3, 88.2, 70.0, 60.1, 42.2, 41.7, 22.0 ppm; FT-IR (KBr): *v* 3464, 3061, 2978, 2933, 2358, 1724, 1566, 1489, 1373, 1246, 1184, 1101, 1014, 825, 742, 721, 669 $cm^{-1}$; HRMS (APCI): *m/z* calcd for $C_{37}H_{30}Cl_2O_4Se$ $[M+H]^+$, 687.0759; found 687.0752.



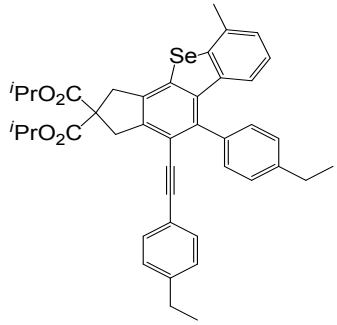

**Diisopropyl 5-(p-tolyl)-4-(p-tolylethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3u)**

White solid; 524 mg (81 % yield); m. p. 158-160℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.51; $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ 7.85-7.83 (d, *J* = 7.8 Hz, 1H; Ar-H), 7.56-7.40 (m, 1H; Ar-H), 7.38-7.34 (m, 1H; Ar-H), 7.26-7.23 (m, 4H; Ar-H), 7.15-6.97 (m, 4H; Ar-H), 6.93-6.89 (d, *J* = 7.8 Hz, 1H; Ar-H), 5.24-4.94 (m, 2H; $CH(CH_3)_2$), 3.92 (s, 2H;$CH_2$), 3.76 (s, 2H; $CH_2$), 2.53 (s, 3H; $CH_3$), 2.32 (s, 3H; $CH_3$), 1.32-1.29 (d, *J* = 4.0 Hz, 12H; $CH(CH_3)_2$); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 171.5, 142.0,139.9, 139.0, 138.8, 138.5, 137.7, 137.6, 137.3, 136.1, 135.9, 133.3, 131.7, 129.9, 129.8, 129.4, 129.3, 127.5, 127.2, 126.5, 126.3, 124.8, 120.9, 118.6, 97.3, 87.1, 69.9, 60.1, 42.24, 41.78, 21.94, 21.66 ppm; FT-IR (KBr): *v* 3454, 2976, 2918, 1903, 1726, 1562, 1508, 1458, 1388, 1371, 1265, 1190, 1107, 908, 871, 815, 750, 513, 422 $cm^{-1}$; HRMS (APCI): *m/z* calcd for $C_{39}H_{36}O_4Se$ $[M+H]^+$, 649.1852; found 649.1851.



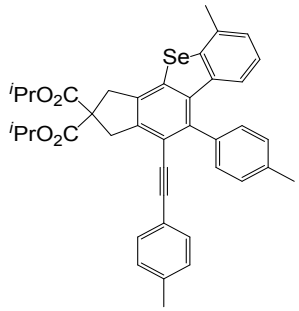

**Diisopropyl 9-methyl-5-phenyl-4-(phenylethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3v)**

White solid; 489 mg (77 % yield); m. p. 137-138℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.57; $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ 7.56-7.54 (m,3H; Ar-H), 7.44-7.35 (m, 2H; Ar-H), 7.25-7.23 (m, 2H; Ar-H), 7.14-7.04 (m, 3H; Ar-H), 7.03-6.92 (m, 1H; Ar-H), 6.69-6.67 (d, *J* = 7.9 Hz,1H; Ar-H), 5.19-5.02 (m, 2H; $CH(CH_3)_2$), 3.93 (s, 2H; $CH_2$), 3.80 (s, 2H; $CH_2$), 2.54 (s, 3H; $CH_3$), 1.33-1.29 (d, *J* = 6.2 Hz, 12H; $CH(CH_3)_2$); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 171.4, 142.1, 141.2, 140.5, 139.8, 138.7, 136.4, 136.1, 136.0, 134.7, 131.7, 130.1, 129.1, 128.5, 128.3, 128.1, 126.6, 125.4, 124.6, 123.9, 118.3, 97.2, 87.6, 69.9, 60.1, 42.3, 41.8, 23.1, 22.0 ppm; FT-IR (KBr): *v* 3462, 2972, 2933, 2345, 1728, 1456, 1271, 1242, 1190, 1103, 1031, 752., 738, 690, 524, 426 $cm^{-1}$; HRMS (APCI): *m/z* calcd for $C_{38}H_{34}O_4Se$ $[M+H]^+$, 635.1695; found 635.1691.




**Diisopropyl 5-(4-ethylphenyl)-4-((4-ethylphenyl)ethynyl)-9-methyl-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3w)**

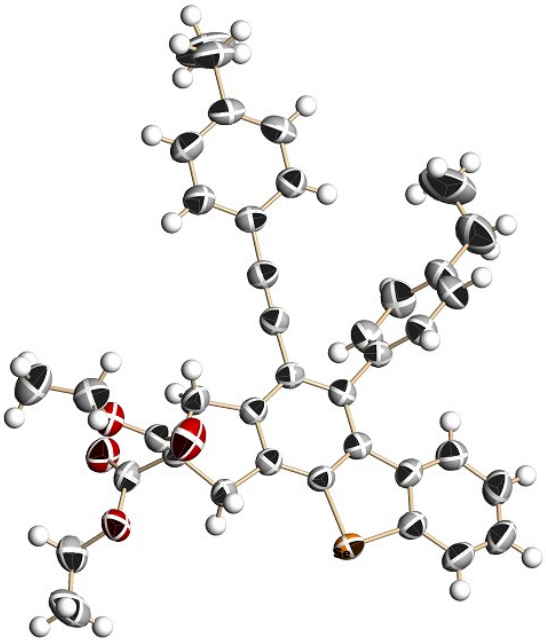
White solid; 566 mg (82 % yield); m. p. 148-150℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.64; $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ 7.39-7.38 (d, $J$ = 7.9 Hz, 2H; Ar-H), 7.34-7.23 (m, 2H; Ar-H), 7.13-6.93 (m, 6H; Ar-H), 6.77-6.75 (d, $J$ = 8.0 Hz, 1H; Ar-H), 5.14-5.08 (m, 2H; $CH(CH_3)_2$), 3.92 (s, 2H; $CH_2$), 3.78 (s, 2H; $CH_2$), 2.83-2.81 (q, $J$ = 7.5 Hz, 2H; $CH_2CH_3$), 2.60 (q, $J$ = 7.6 Hz, 2H; $CH_2CH_3$)), 2.53 (s, 3H; $CH_3$), 1.39-1.37 (t, $J$ = 7.6 Hz, 3H; $CH_2CH_3$), 1.31-1.28 (d, $J$ = 6.2 Hz, 12H; $CH(CH_3)_2$), 1.22-1.19 (t, $J$ = 7.5 Hz, 3H; $CH_2CH_3$); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 171.5, 144.7, 144.1, 142.3, 141.2, 139.6, 138.9, 137.8, 136.5, 135.8, 134.7, 131.8, 130.0, 128.6, 128.1, 126.6, 125.4, 124.7, 121.1, 118.7, 97.3, 87.2, 69.9, 60.2, 42.3, 41.8, 29.4, 29.2, 23.1, 22.0, 16.5, 15.8 ppm; FT-IR (KBr): $v$ 3462, 3049, 2956, 2929, 2868, 2358, 1732, 1575, 1508, 1465, 1454, 1373, 1273, 1246, 1193, 1157, 1103, 1064, 833, 756 cm$^{-1}$; HRMS (APCI): $m/z$ calcd for $C_{42}H_{42}O_4Se$ $[M+H]^+$, 691.2321; found 691.2328.

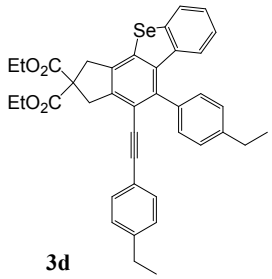



**Diisopropyl 9-methyl-5-(p-tolyl)-4-(p-tolylethynyl)-1H-benzo[b]indeno[5,4-d]selenophene-2,2(3H)-dicarboxylate (3x)**

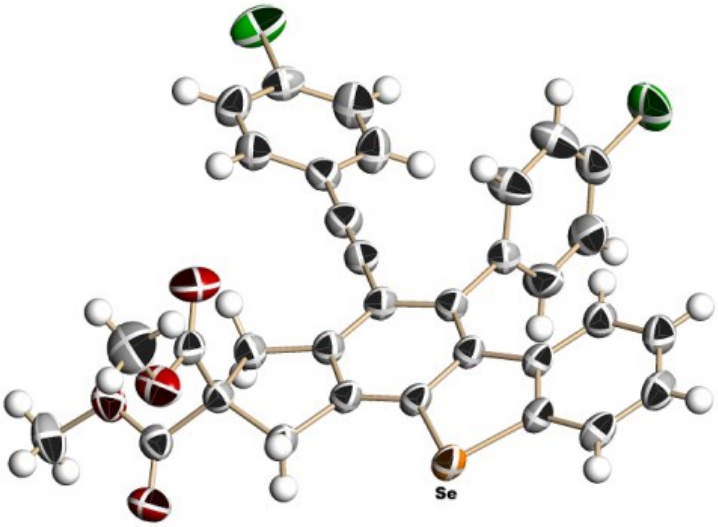
White solid; 556 mg (84 % yield); m. p. 172-173℃; TLC (petroleum ether/EtOAc = 60:1): $R_f$ = 0.59; $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ 7.38-7.33 (d, $J$ = 7.7 Hz, 2H; Ar-H), 7.29-7.24 (m, 2H; Ar-H), 7.18-6.88 (m, 6H; Ar-H), 6.78-6.74 (d, $J$ = 7.9 Hz, 1H; Ar-H), 5.14-5.08 (m, 2H; $CH(CH_3)_2$), 3.91 (s, 2H; $CH_2$), 3.78 (s, 2H; $CH_2$), 2.53 (s, 3H; $CH_3$), 2.52 (s, 3H; $CH_3$), 2.31 (s, 3H; $CH_3$), 1.32-1.28 (d, $J$ = 6.1 Hz, 12H; $CH(CH_3)_2$); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ 171.5, 142.1, 141.2, 139.8, 138.9, 138.4, 137.6, 137.5, 136.5, 135.8, 134.7, 131.6, 129.9, 129.8, 129.3, 126.6, 125.4, 124.7, 120.9, 118.7, 97.2, 87.1, 69.9, 60.2, 42.3, 41.8, 23.1, 22.0, 21.9 ppm; FT-IR (KBr): $v$ 3444, 2972, 2918, 2320, 1724, 1573, 1508, 1373, 1261, 1192, 1111, 1049, 813, 759, 511, 424 cm$^{-1}$; HRMS (APCI): $m/z$ calcd for $C_{40}H_{38}O_4Se$ $[M+H]^+$, 663.2008; found 663.2001.

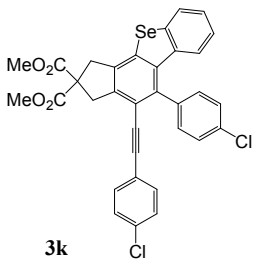
## 3. X-Ray Structure for 3d, 3k, 3s and 3v



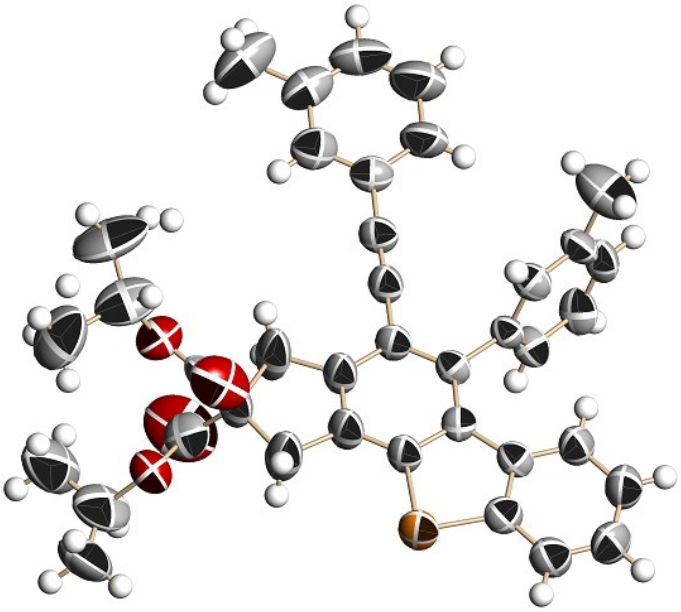


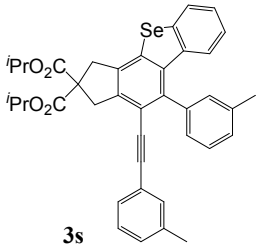

**3d**



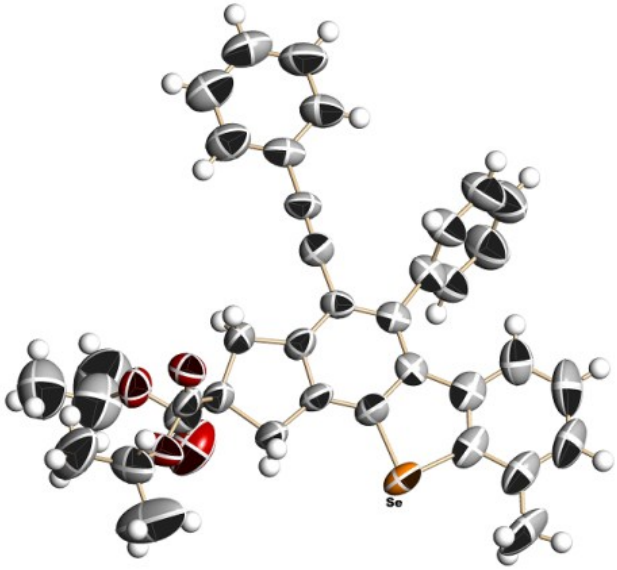



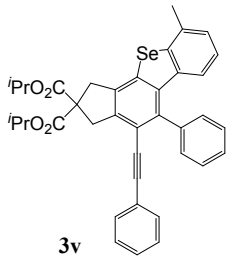

**3k**





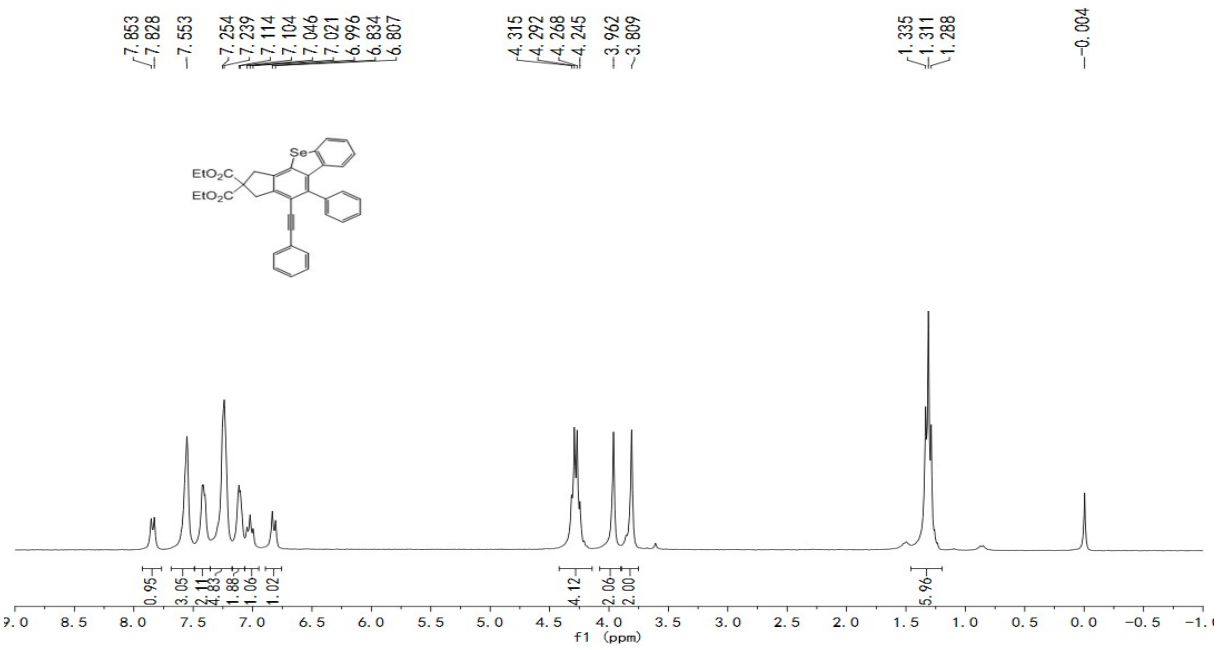

**3s**



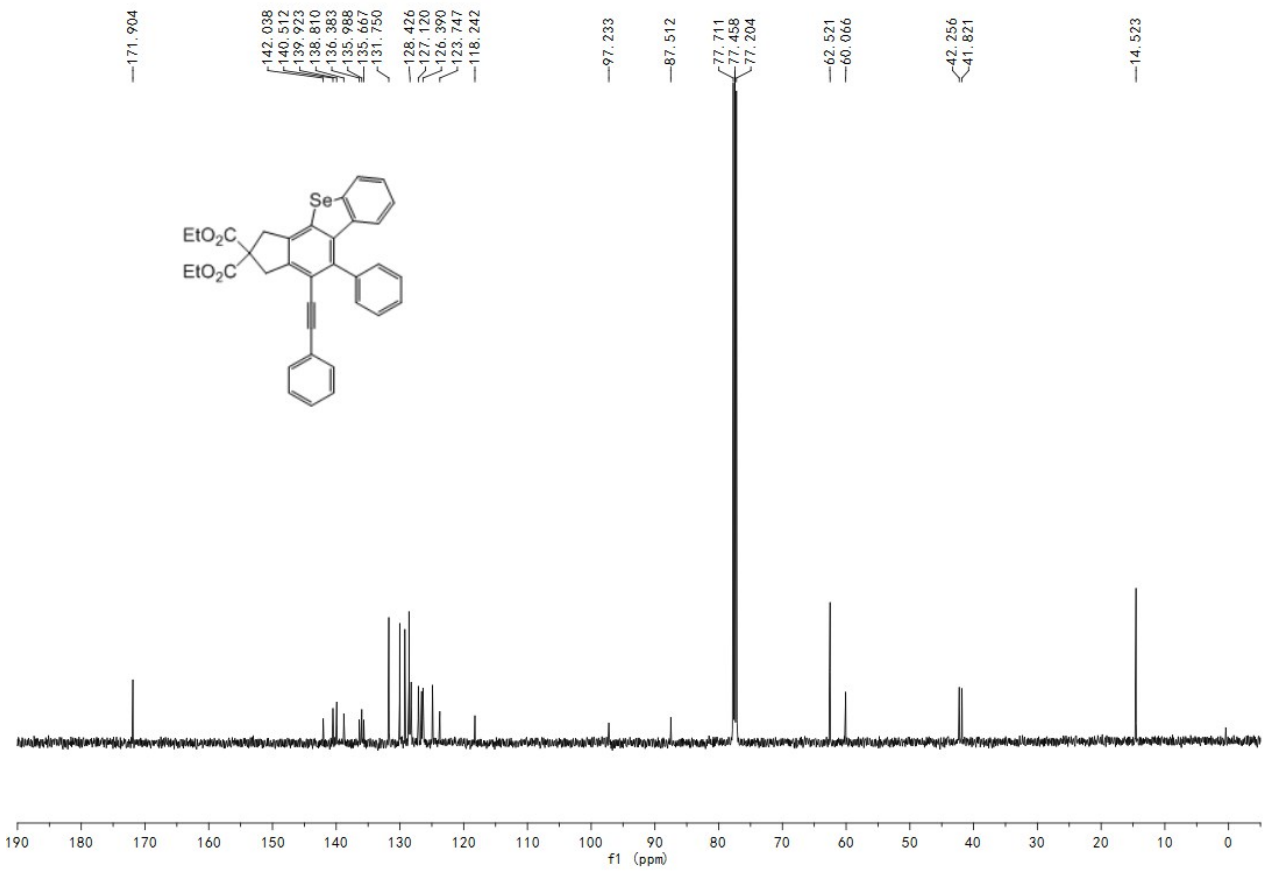



**3v**

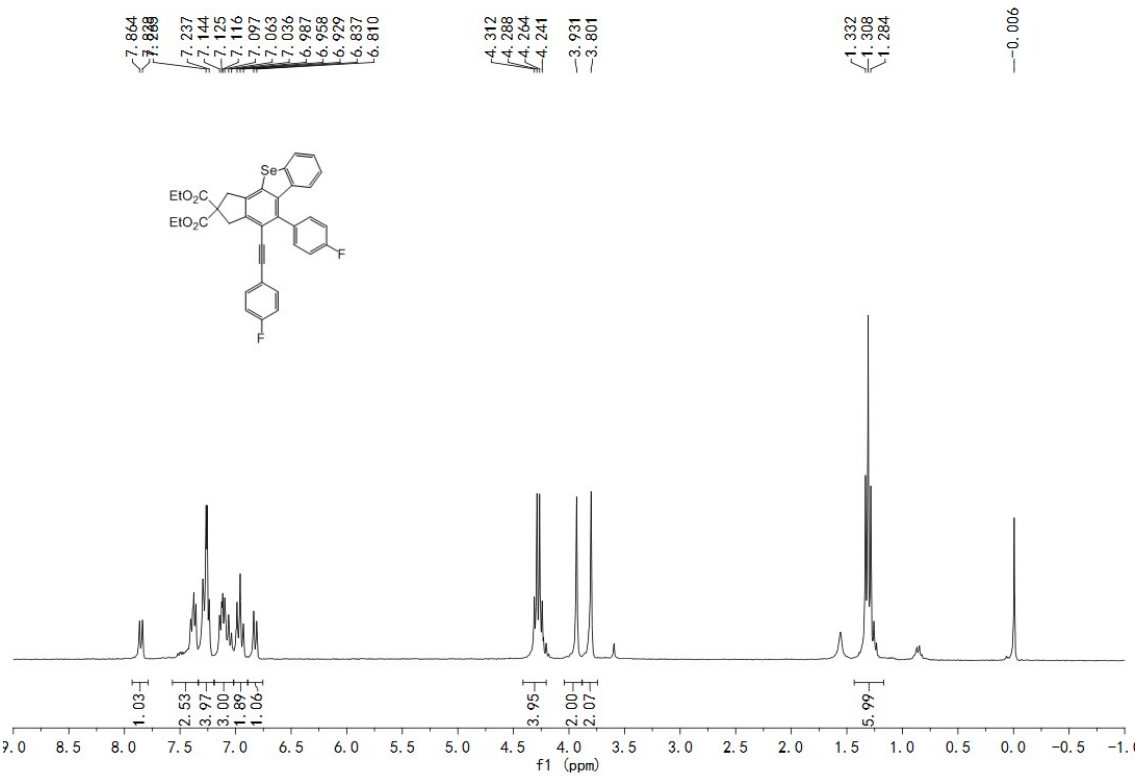
## 4. $^{1}$H NMR &$^{13}$C NMR Spectra for New Compounds


7.853
7.828
7.553
7.254
7.239
7.114
7.104
7.046
7.021
6.996
6.834
6.807
4.315
4.292
4.268
4.245
3.962
3.809
1.335
1.311
1.288
-0.004
Se
EtO2C
EtO2C
0.95
3.05
2.11
4.83
1.88
1.06
1.02
4.12
2.06
2.00
5.96
f1 (ppm)

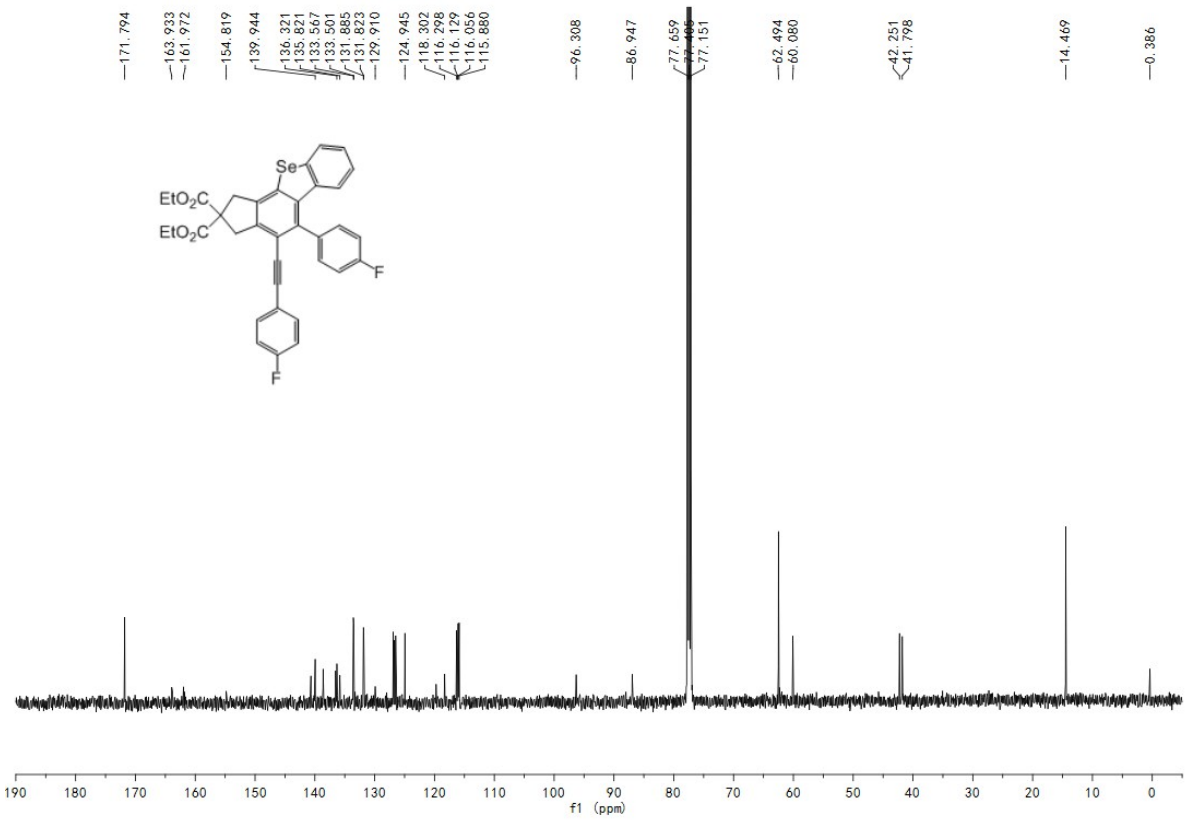
**3a**


171.904
142.038
140.512
139.923
138.810
136.383
135.988
135.667
131.750
128.426
127.120
126.390
123.747
118.242
97.233
87.512
77.711
77.458
77.204
62.521
60.066
42.256
41.821
14.523
Se
EtO2C
EtO2C
f1 (ppm)

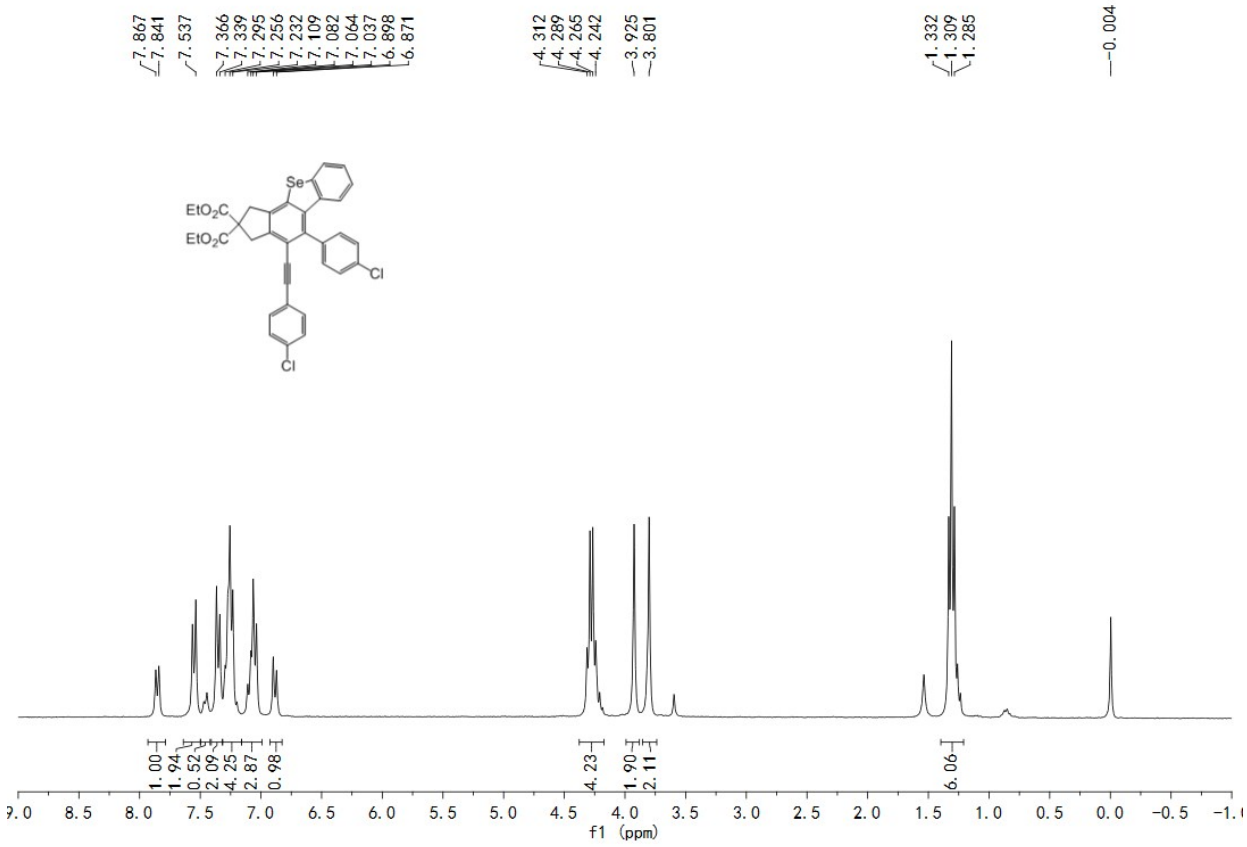
**3a**


7.864
7.237
7.144
7.125
7.116
7.097
7.063
7.036
6.987
6.958
6.929
6.837
6.810
4.312
4.288
4.264
4.241
3.931
3.801
1.332
1.308
1.284
0.006
Se
EtO2C
EtO2C
F
F
1.03
2.53
3.97
3.00
1.89
1.06
3.95
2.00
2.07
5.99
f1 (ppm)

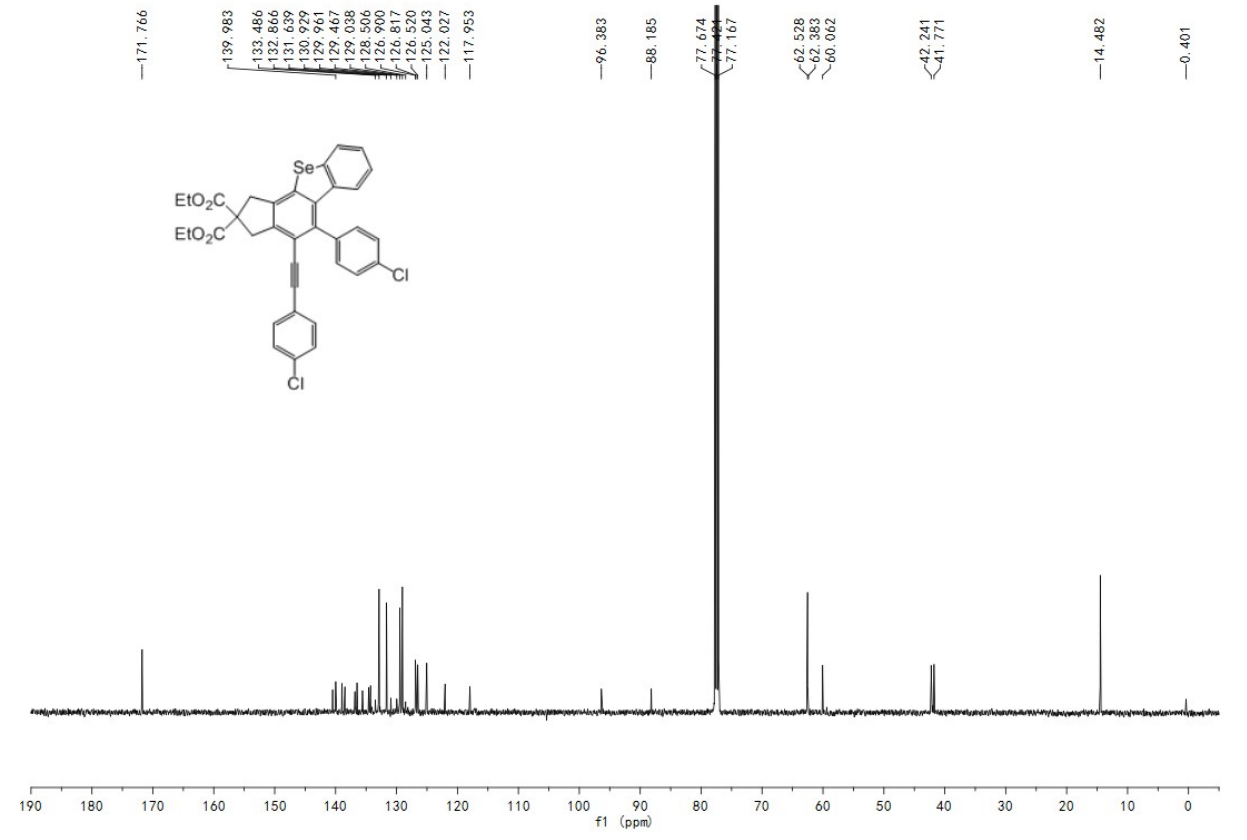
**3b**


171.794
163.933
161.972
154.819
139.944
136.321
135.821
133.567
133.501
131.885
131.823
129.910
124.945
118.302
116.298
116.129
116.056
115.880
96.308
86.947
77.659
77.151
62.494
60.080
42.251
41.798
14.469
0.386
Se
EtO2C
EtO2C
F
F
f1 (ppm)

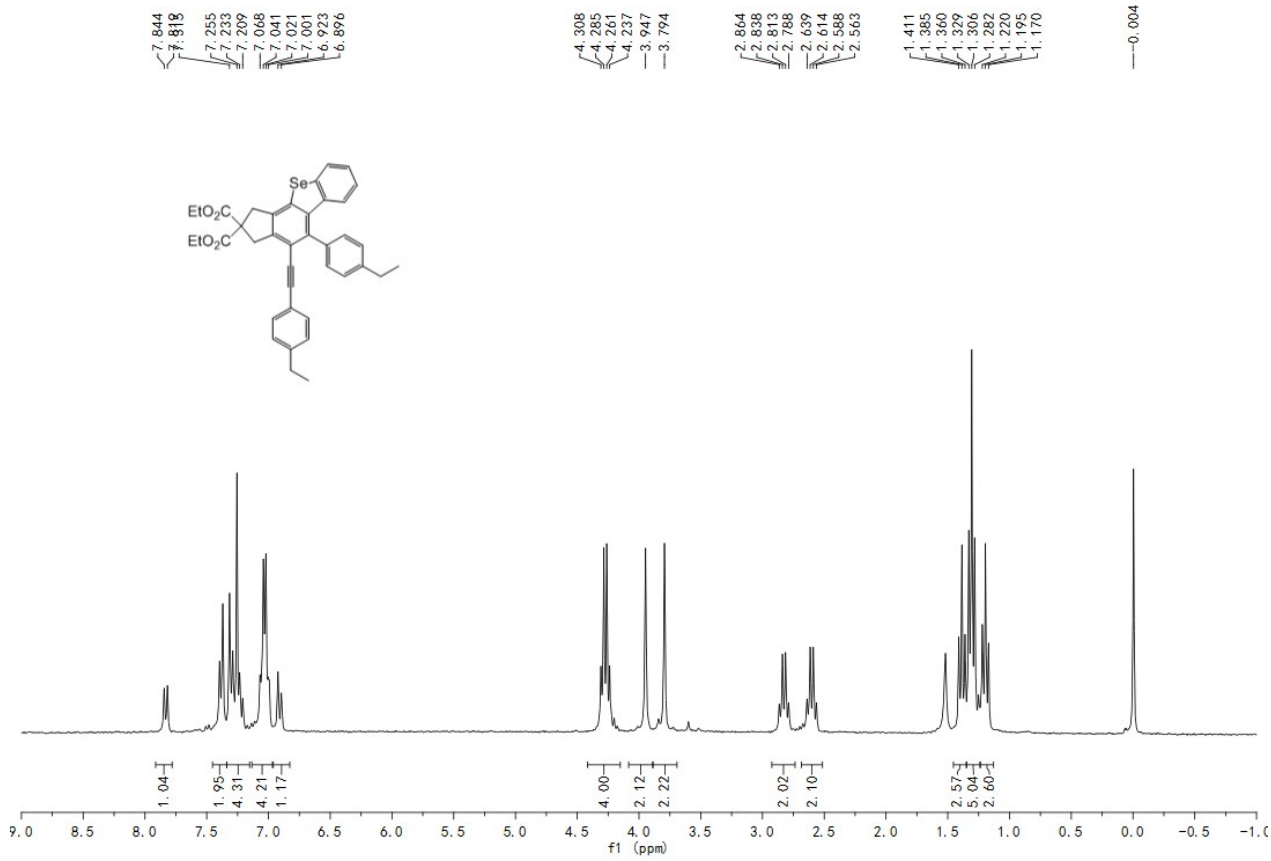
**3b**


7.867
7.841
7.537
7.366
7.339
7.295
7.256
7.232
7.109
7.082
7.064
7.037
6.898
6.871
4.312
4.289
4.265
4.242
3.925
3.801
1.332
1.309
1.285
0.004
Se
EtO2C
EtO2C
Cl
Cl
1.00
1.94
0.52
2.09
4.25
2.87
0.98
4.23
1.90
2.11
6.06
f1 (ppm)

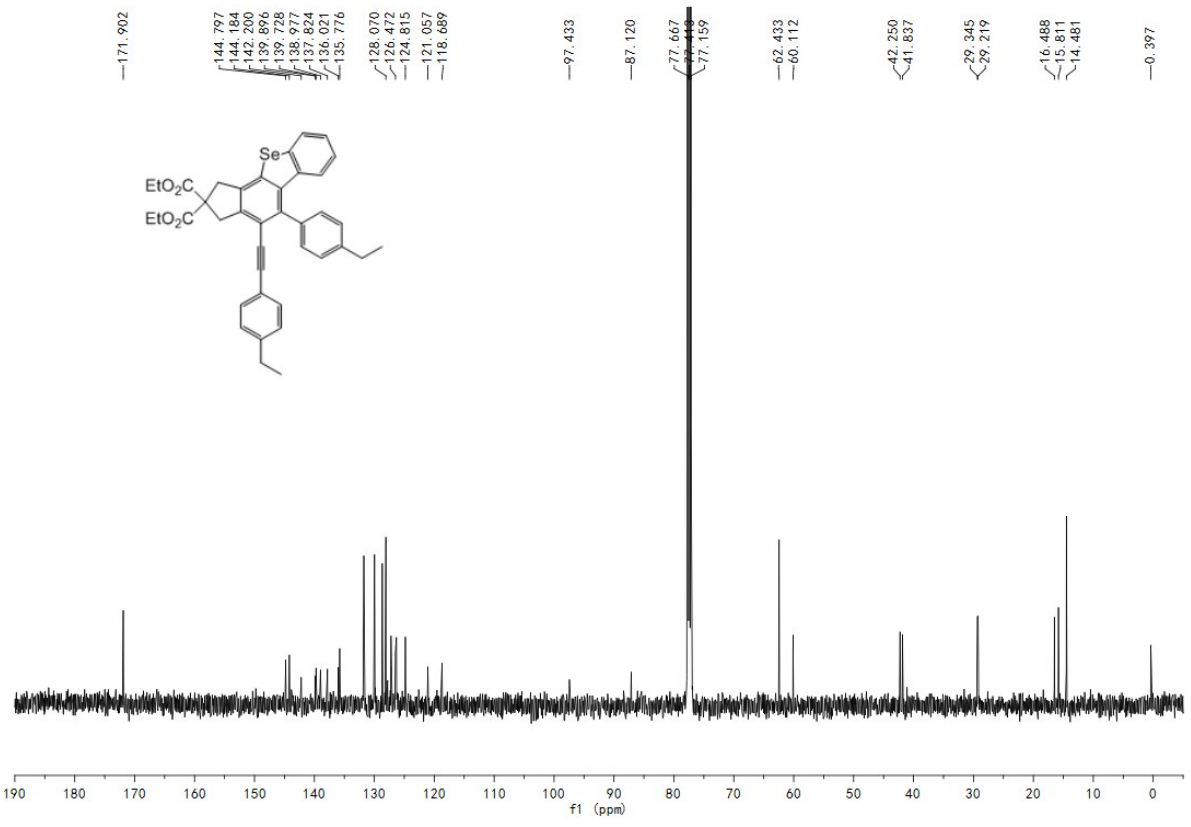
**3c**


171.766
139.983
133.486
132.866
131.639
130.929
129.961
129.467
129.038
128.506
126.900
126.817
126.520
125.043
122.027
117.953
96.383
88.185
77.674
77.421
77.167
62.528
62.383
60.062
42.241
41.771
14.482
0.401
Se
EtO2C
EtO2C
Cl
Cl
f1 (ppm)

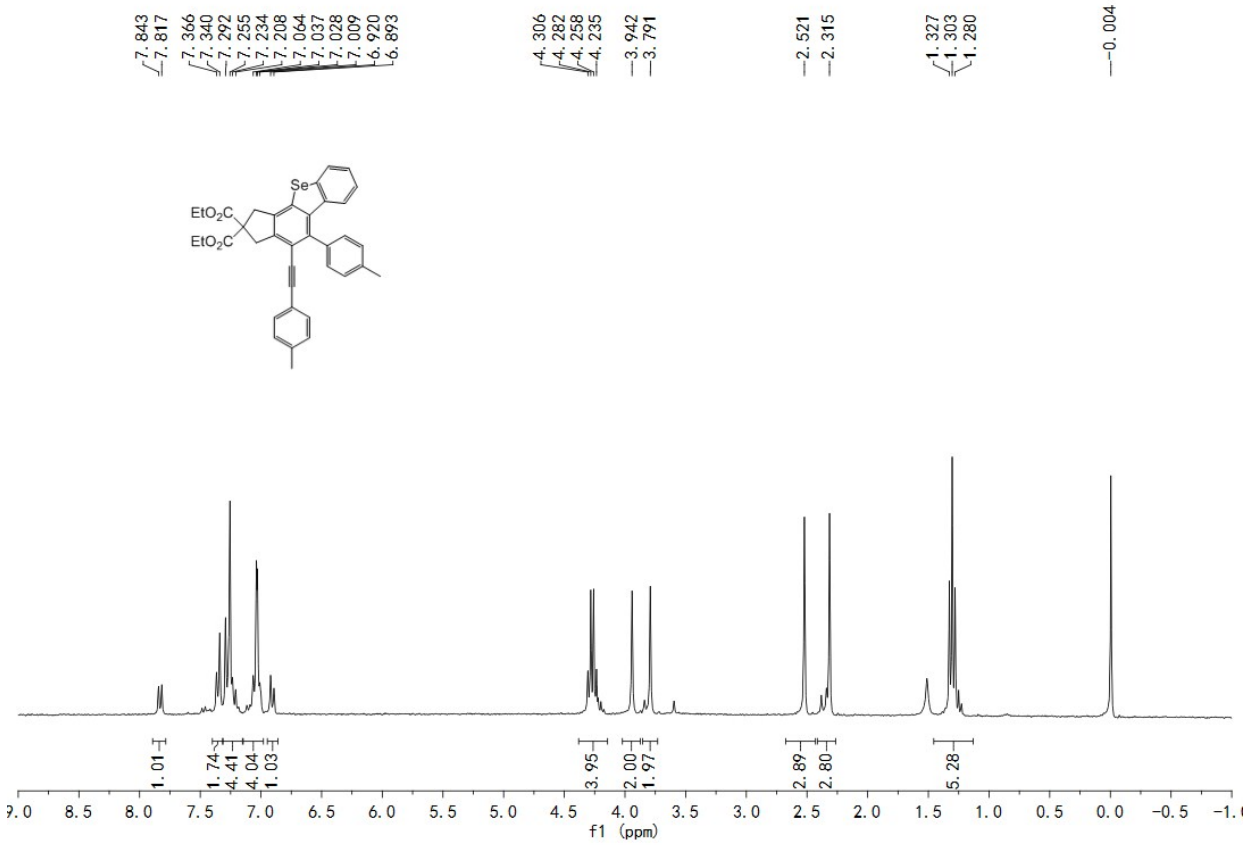
**3c**


7.844
7.818
7.255
7.233
7.209
7.068
7.041
7.021
7.001
6.923
6.896
4.308
4.285
4.261
4.237
3.947
3.794
2.864
2.838
2.813
2.788
2.639
2.614
2.588
2.563
1.411
1.385
1.360
1.329
1.306
1.282
1.220
1.195
1.170
0.004
Se
EtO2C
EtO2C
1.04
1.95
4.31
4.21
1.17
4.00
2.12
2.22
2.02
2.10
2.57
5.04
2.60
f1 (ppm)

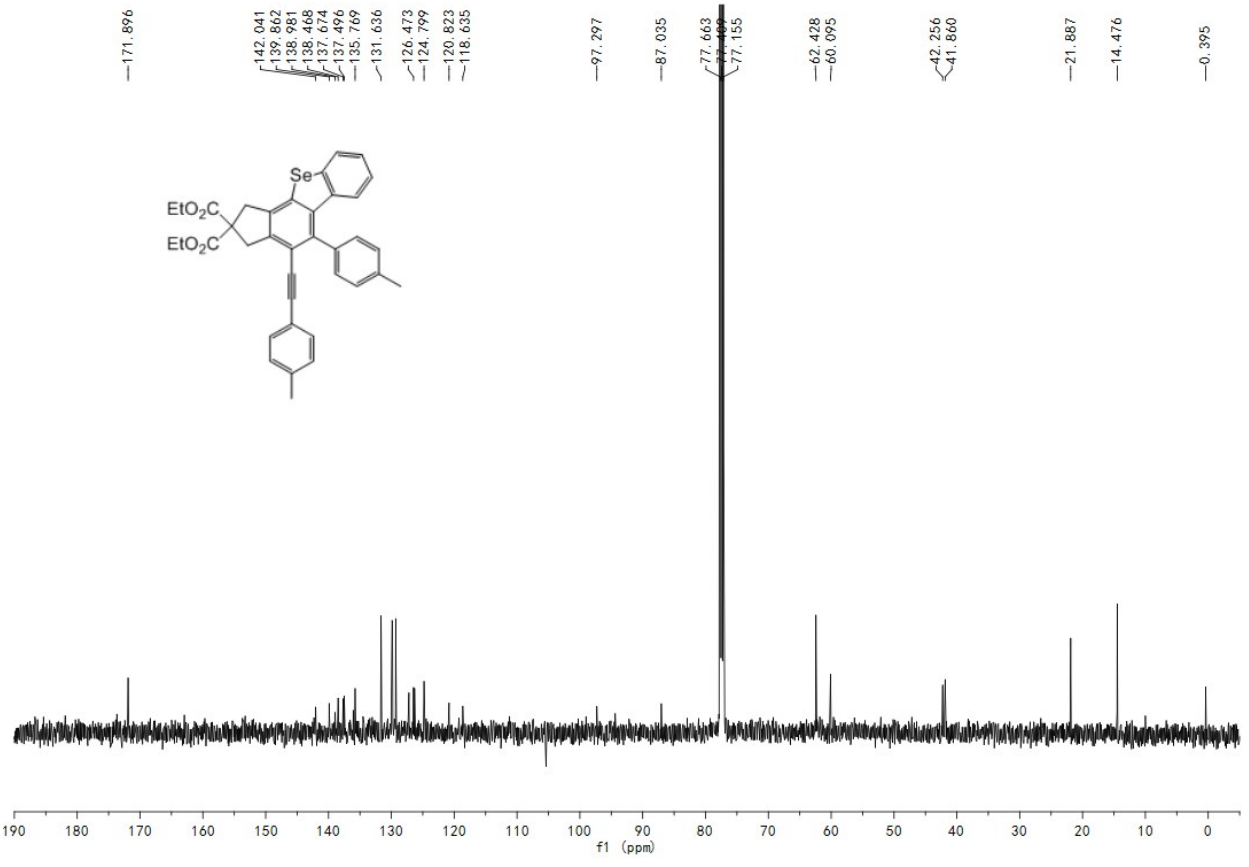
**3d**


171.902
144.797
144.184
142.200
139.896
139.728
138.977
137.824
136.021
135.776
128.070
126.472
124.815
121.057
118.689
97.433
87.120
77.667
77.416
77.159
62.433
60.112
42.250
41.837
29.345
29.219
16.488
15.811
14.481
0.397
Se
EtO2C
EtO2C
f1 (ppm)

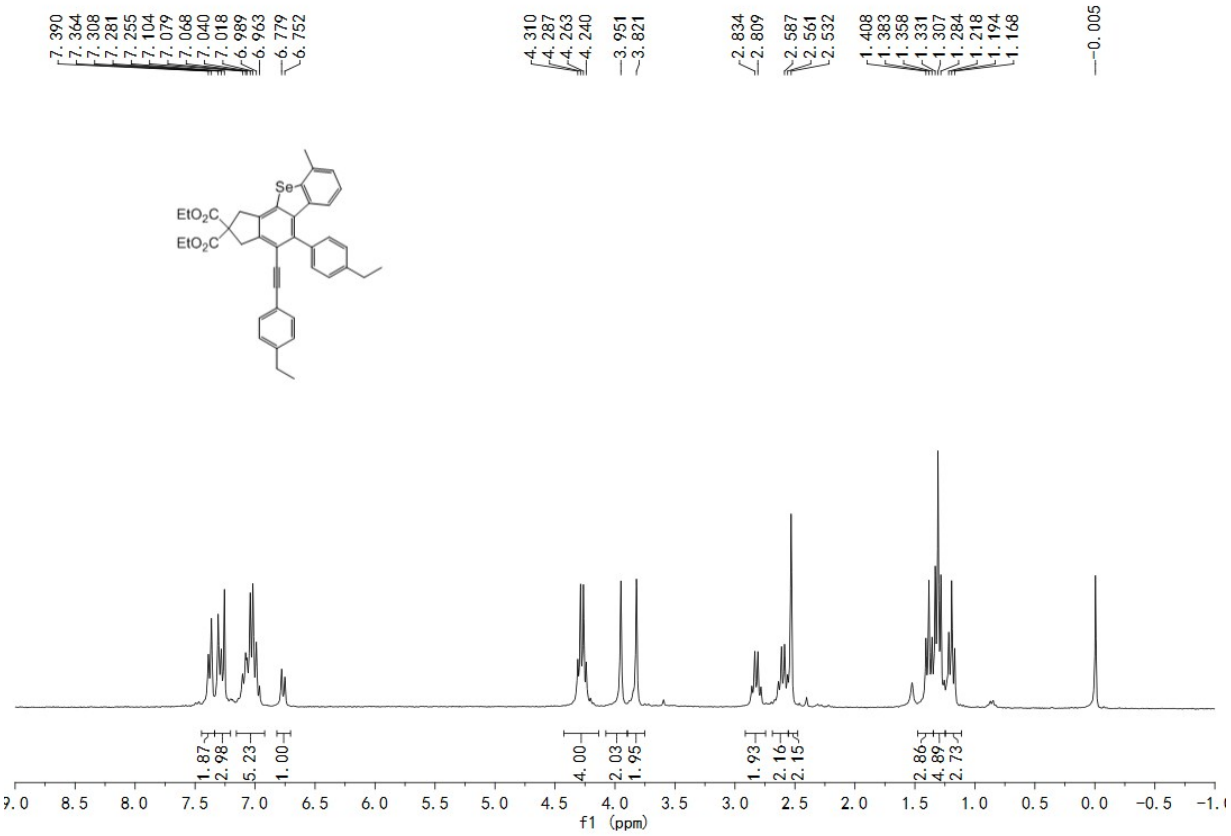
**3d**


7.843
7.817
7.366
7.340
7.292
7.255
7.234
7.208
7.064
7.037
7.028
7.009
6.920
6.893
4.306
4.282
4.258
4.235
3.942
3.791
2.521
2.315
1.327
1.303
1.280
0.004
Se
EtO2C
EtO2C
1.01
1.74
4.41
4.04
1.03
3.95
2.00
1.97
2.89
2.80
5.28
f1 (ppm)

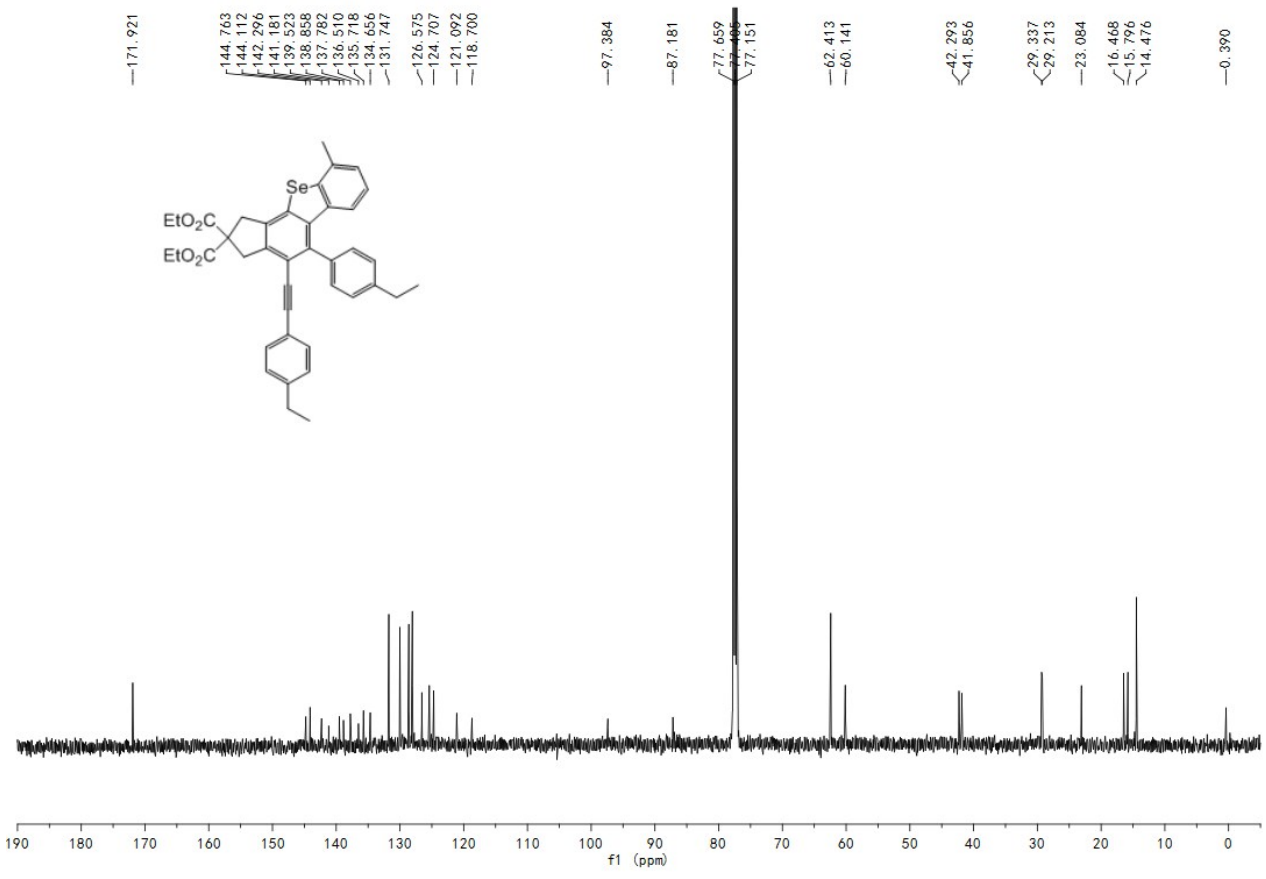
**3e**


171.896
142.041
139.862
138.981
138.468
137.674
137.496
135.769
131.636
126.473
124.799
120.823
118.635
97.297
87.035
77.663
77.155
62.428
60.095
42.256
41.860
21.887
14.476
0.395
Se
EtO2C
EtO2C
f1 (ppm)

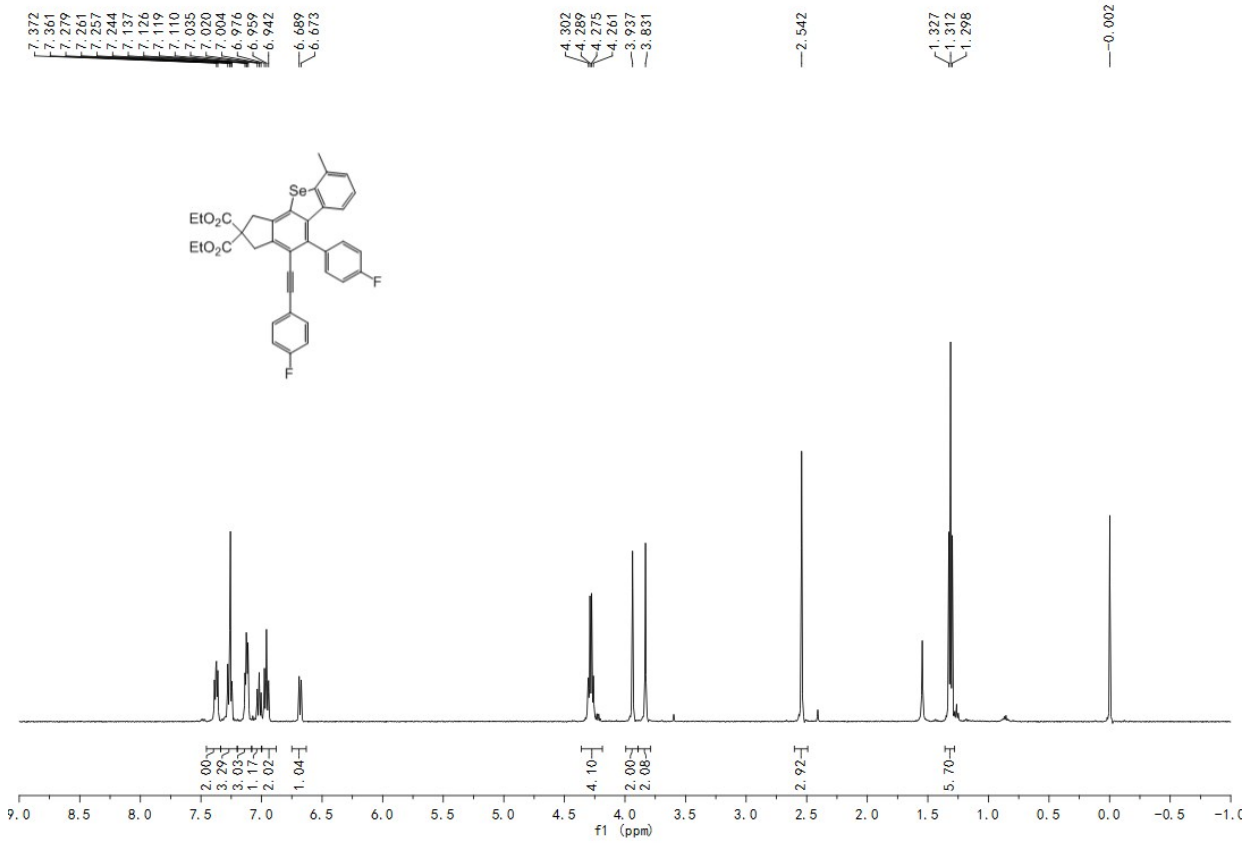
**3e**


7.390
7.364
7.308
7.281
7.255
7.104
7.079
7.068
7.040
7.018
6.989
6.963
6.779
6.752
4.310
4.287
4.263
4.240
3.951
3.821
2.834
2.809
2.587
2.561
2.532
1.408
1.383
1.358
1.331
1.307
1.284
1.218
1.194
1.168
0.005
Se
EtO2C
EtO2C
1.87
2.98
5.23
1.00
4.00
2.03
1.95
1.93
2.16
2.15
2.86
4.89
2.73
f1 (ppm)

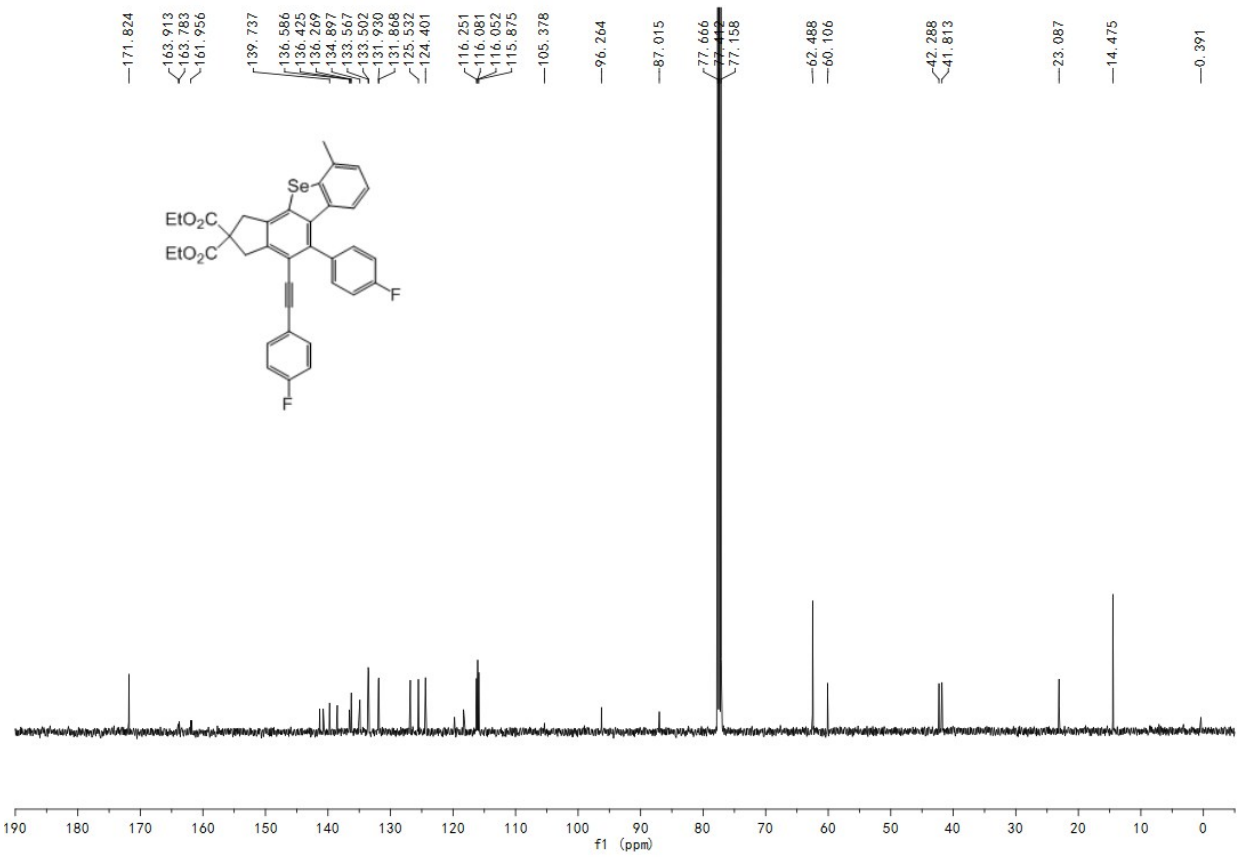
**3f**


171.921
144.763
144.112
142.296
141.181
139.523
138.858
137.782
136.510
135.718
134.656
131.747
126.575
124.707
121.092
118.700
97.384
87.181
77.659
77.485
77.151
62.413
60.141
42.293
41.856
29.337
29.213
23.084
16.468
15.796
14.476
0.390
Se
EtO2C
EtO2C
f1 (ppm)

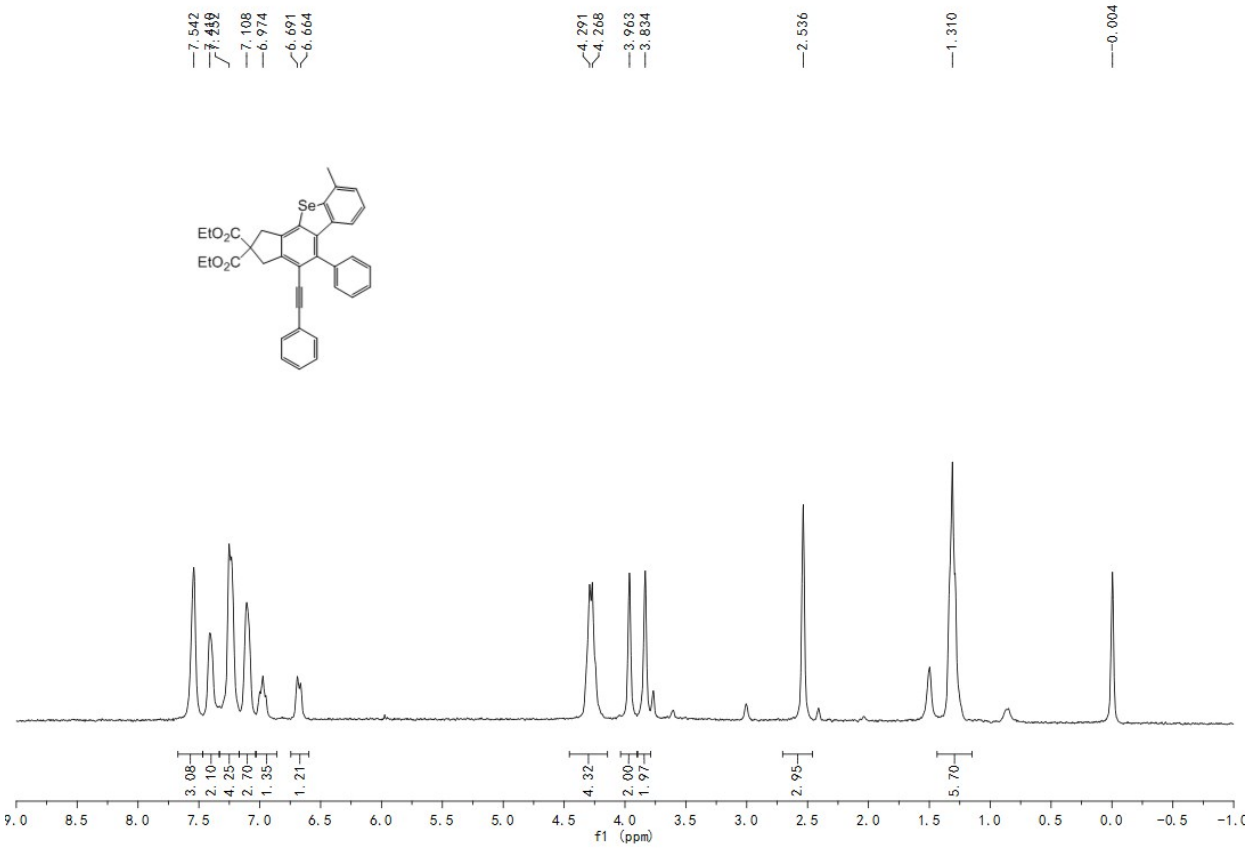
**3f**


7.372
7.361
7.279
7.261
7.257
7.244
7.137
7.126
7.119
7.110
7.035
7.020
7.004
6.976
6.959
6.942
6.689
6.673
4.302
4.289
4.275
4.261
3.937
3.831
2.542
1.327
1.312
1.298
0.002
Se
EtO2C
EtO2C
F
F
2.00
3.29
3.03
1.17
2.02
1.04
4.10
2.00
2.08
2.92
5.70
f1 (ppm)

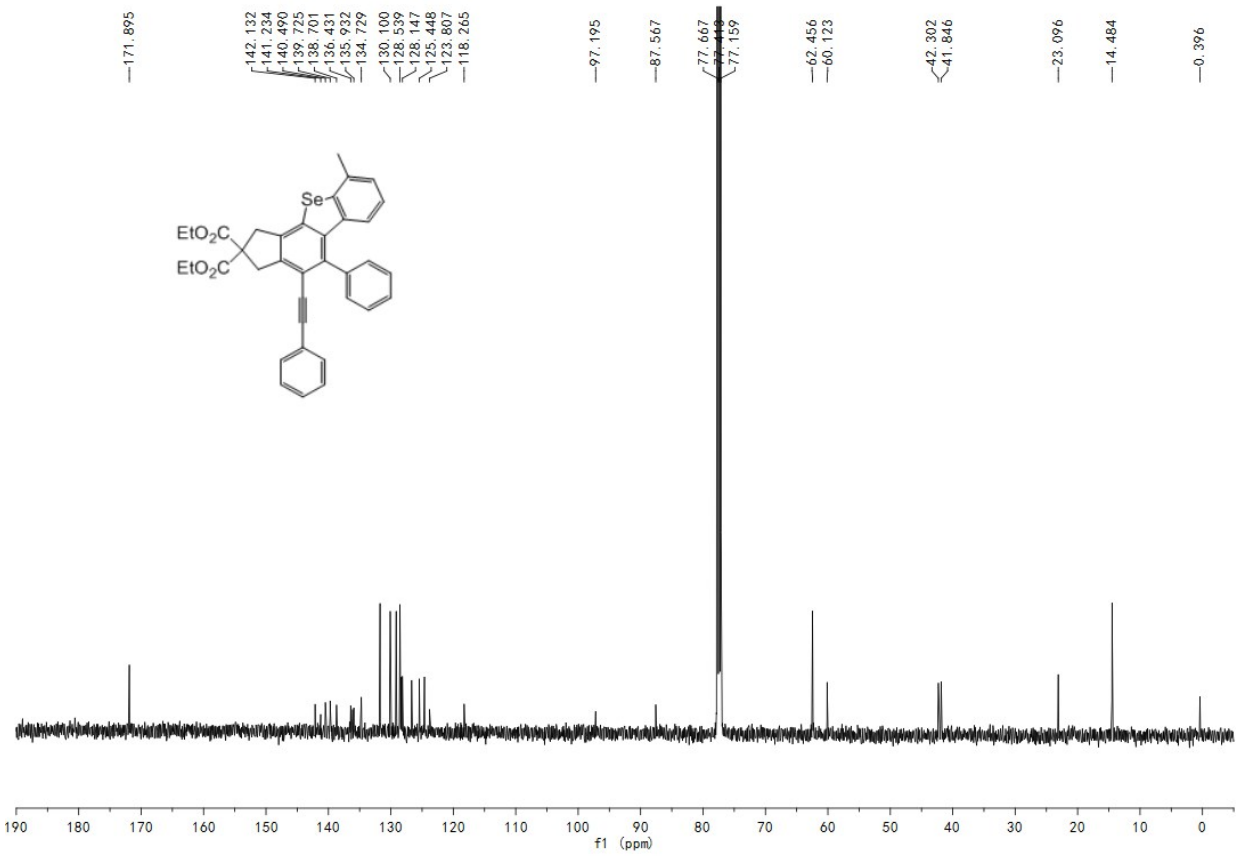
**3g**


171.824
163.913
163.783
161.956
139.737
136.586
136.425
136.269
134.897
133.567
133.502
131.930
131.868
125.532
124.401
116.251
116.081
116.052
115.875
105.378
96.264
87.015
77.666
77.448
77.158
62.488
60.106
42.288
41.813
23.087
14.475
0.391
Se
EtO2C
EtO2C
F
F
f1 (ppm)

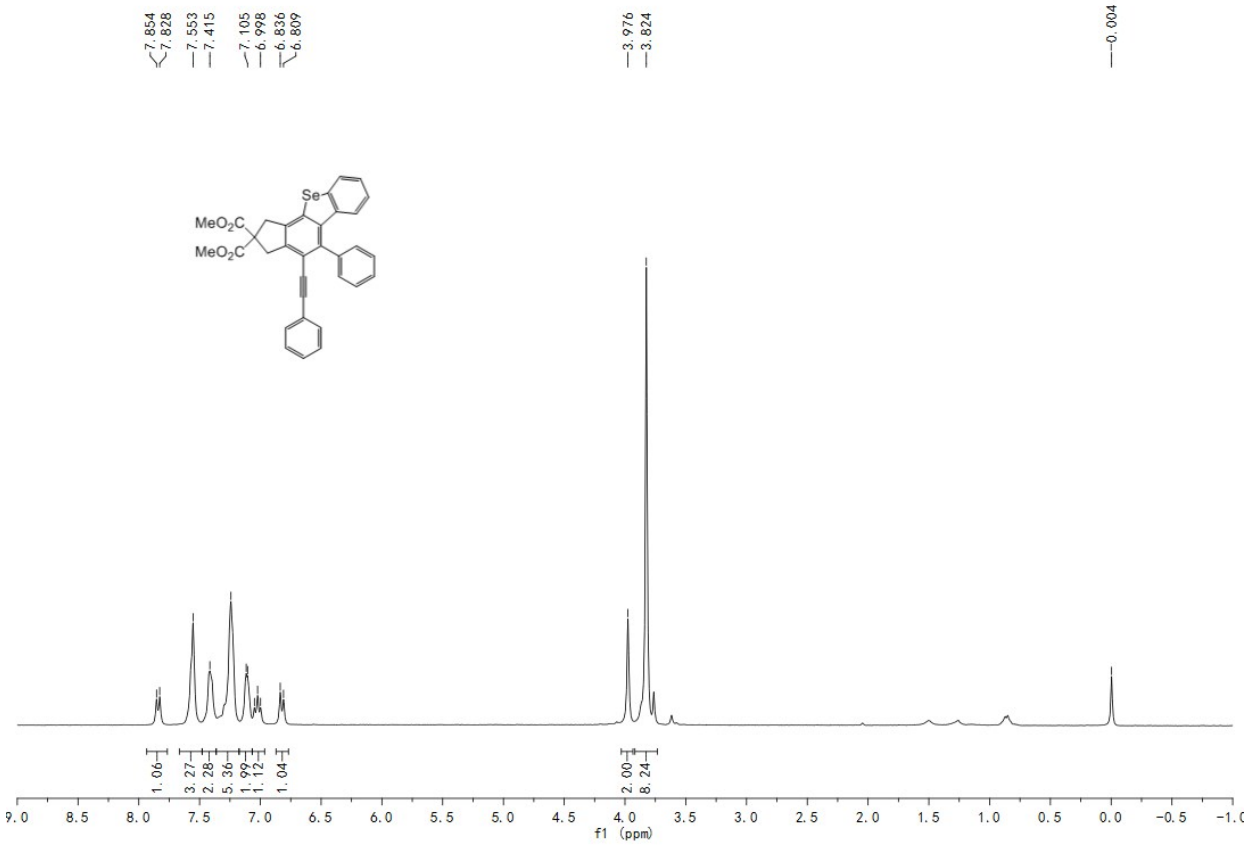
**3g**


7.542
7.459
7.108
6.974
6.691
6.664
4.291
4.268
3.963
3.834
2.536
1.310
0.004
Se
EtO2C
EtO2C
3.08
2.10
4.25
2.70
1.35
1.21
4.32
2.00
1.97
2.95
5.70
f1 (ppm)

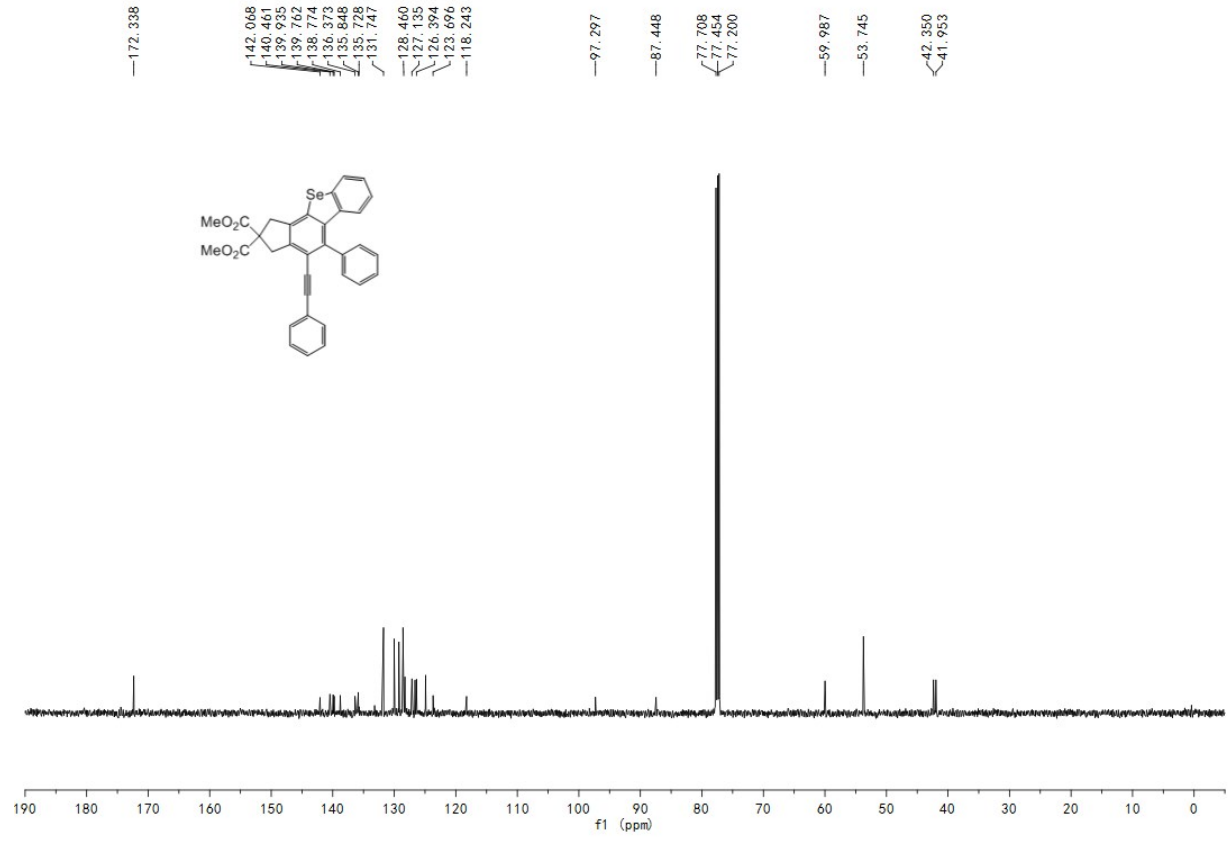
**3h**


171.895
142.132
141.234
140.490
139.725
138.701
136.431
135.932
134.729
130.100
128.539
128.147
125.448
123.807
118.265
97.195
87.567
77.667
77.159
62.456
60.123
42.302
41.846
23.096
14.484
0.396
Se
EtO2C
EtO2C
f1 (ppm)

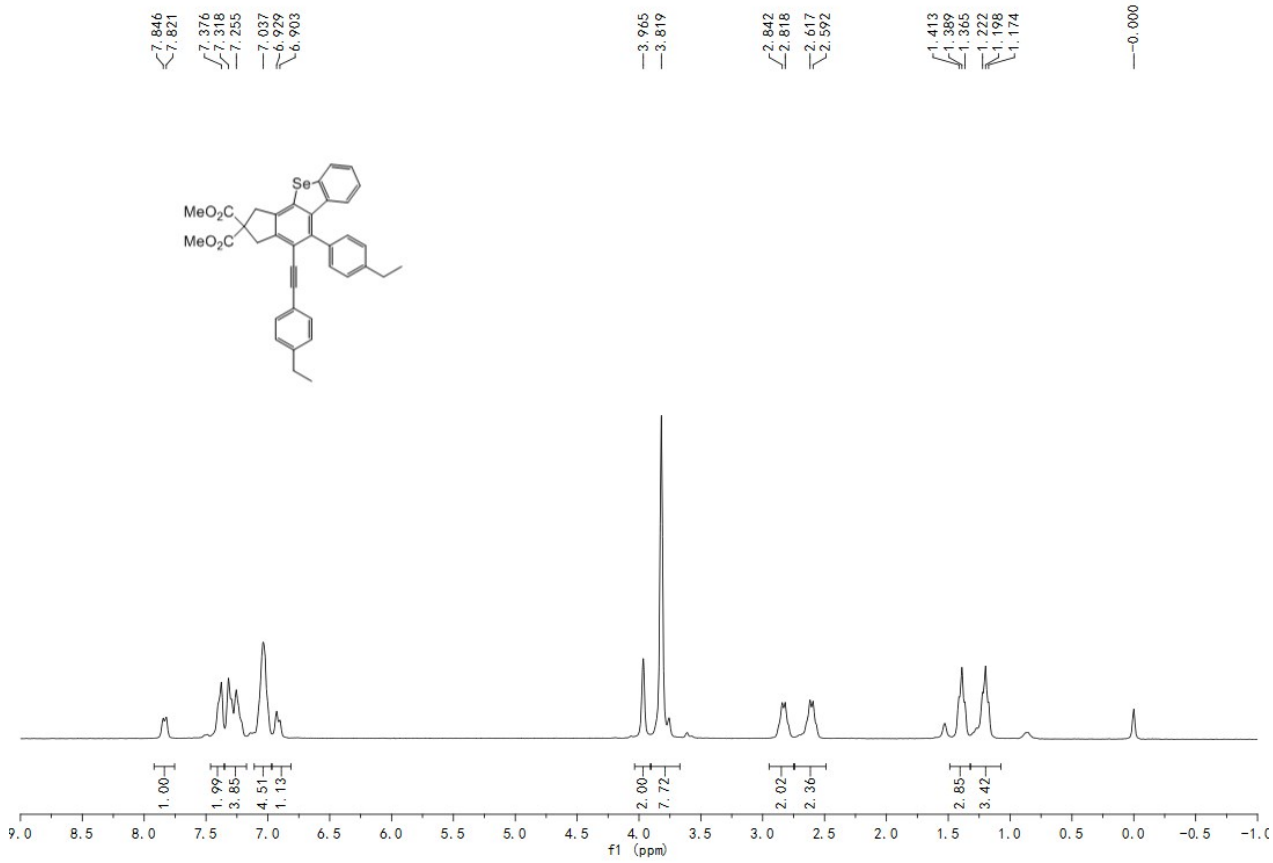
**3h**


7.854
7.828
7.553
7.415
7.105
6.998
6.836
6.809
3.976
3.824
0.004
Se
MeO2C
MeO2C
1.06
3.27
2.28
5.36
1.99
1.12
1.04
2.00
8.24
f1 (ppm)

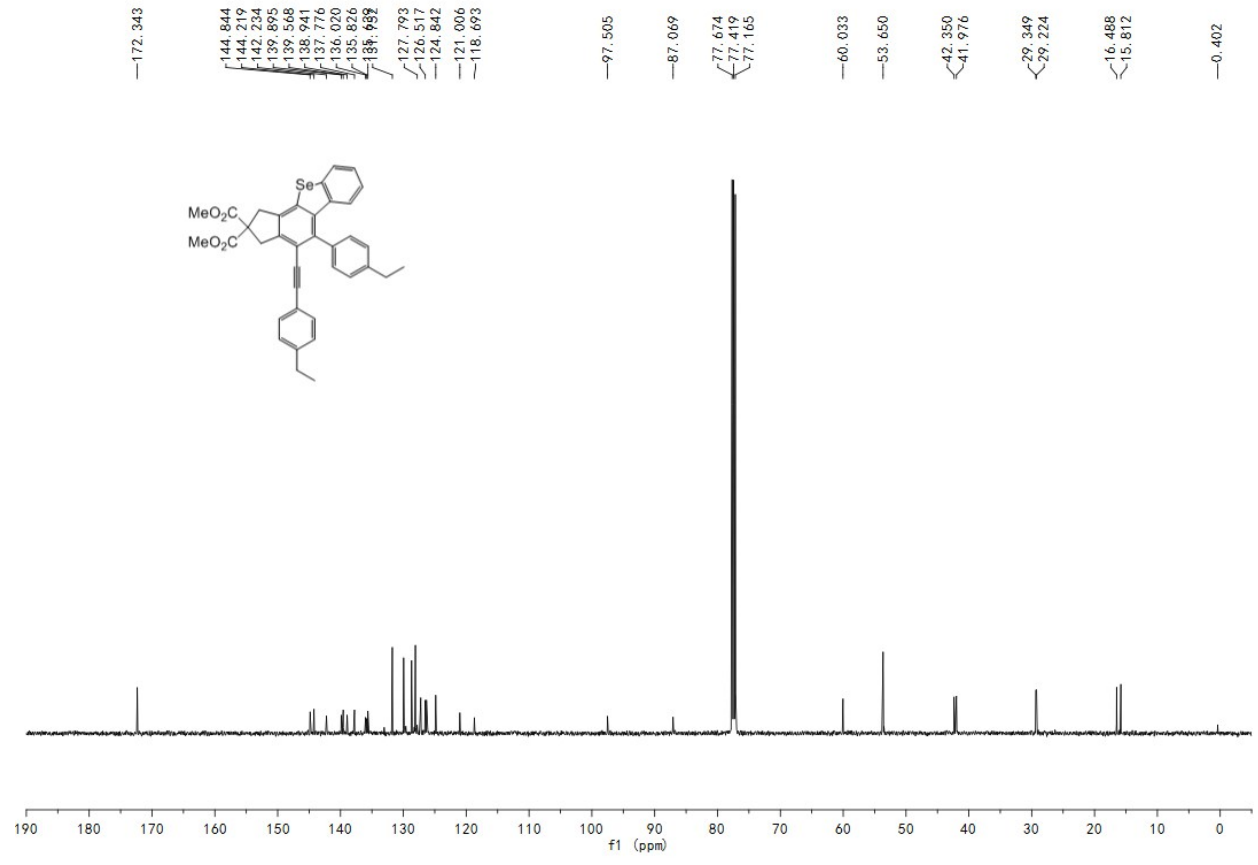
**3i**


172.338
142.068
140.461
139.935
139.762
138.774
136.373
135.848
135.728
131.747
128.460
127.135
126.394
123.696
118.243
97.297
87.448
77.708
77.454
77.200
59.987
53.745
42.350
41.953
Se
MeO2C
MeO2C
f1 (ppm)

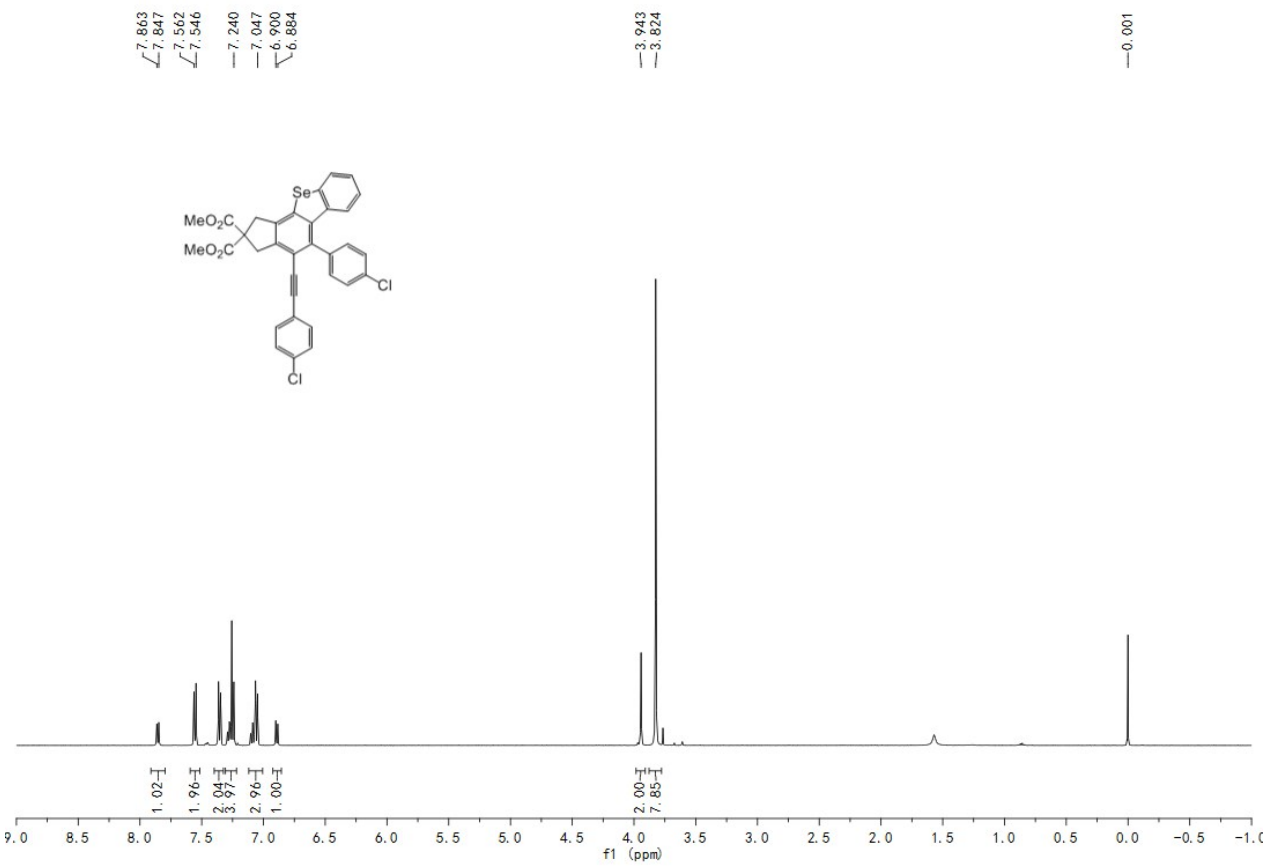
**3i**


7.846
7.821
7.376
7.318
7.255
7.037
6.929
6.903
3.965
3.819
2.842
2.818
2.617
2.592
1.413
1.389
1.365
1.222
1.198
1.174
0.000
Se
MeO2C
MeO2C
1.00
1.99
3.85
4.51
1.13
2.00
7.72
2.02
2.36
2.85
3.42
f1 (ppm)

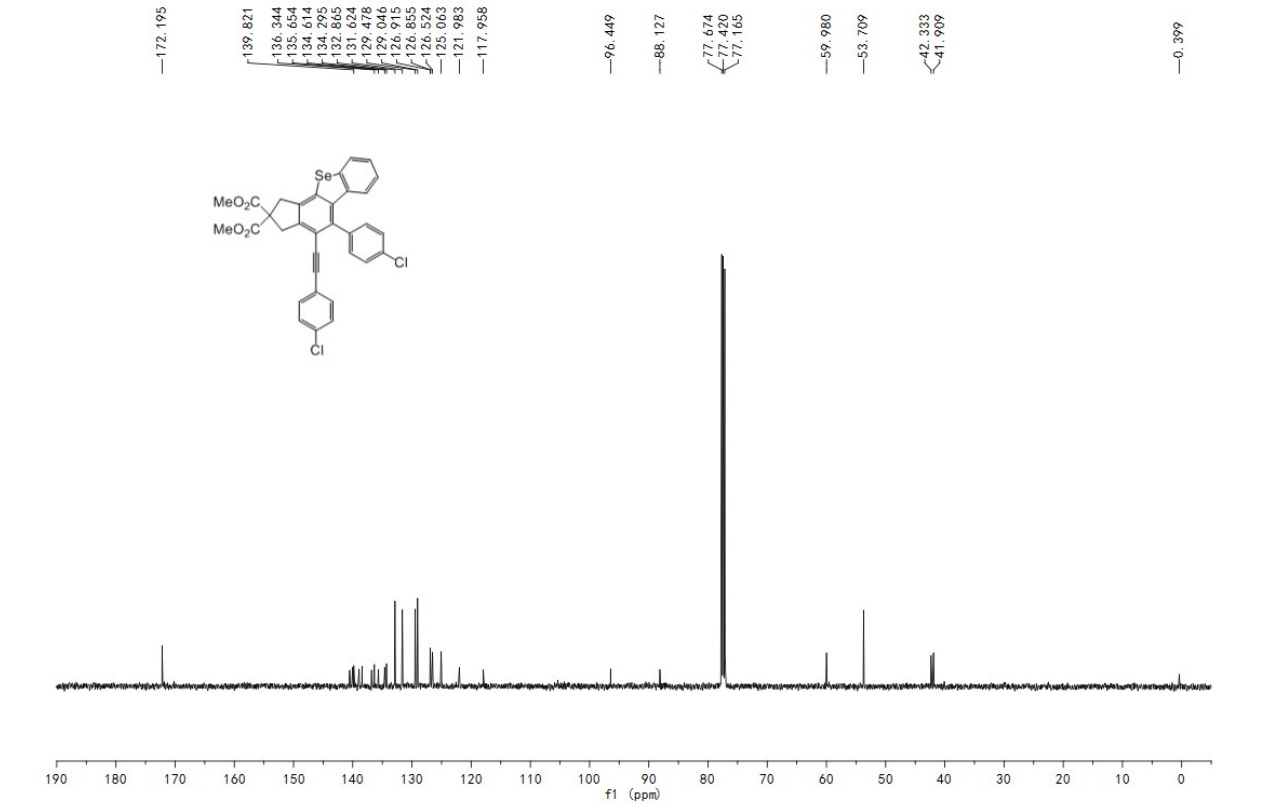
**3j**


172.343
144.844
144.219
142.234
139.895
139.568
138.941
137.776
136.020
135.826
127.793
126.517
124.842
121.006
118.693
97.505
87.069
77.674
77.419
77.165
60.033
53.650
42.350
41.976
29.349
29.224
16.488
15.812
0.402
Se
MeO2C
MeO2C
f1 (ppm)

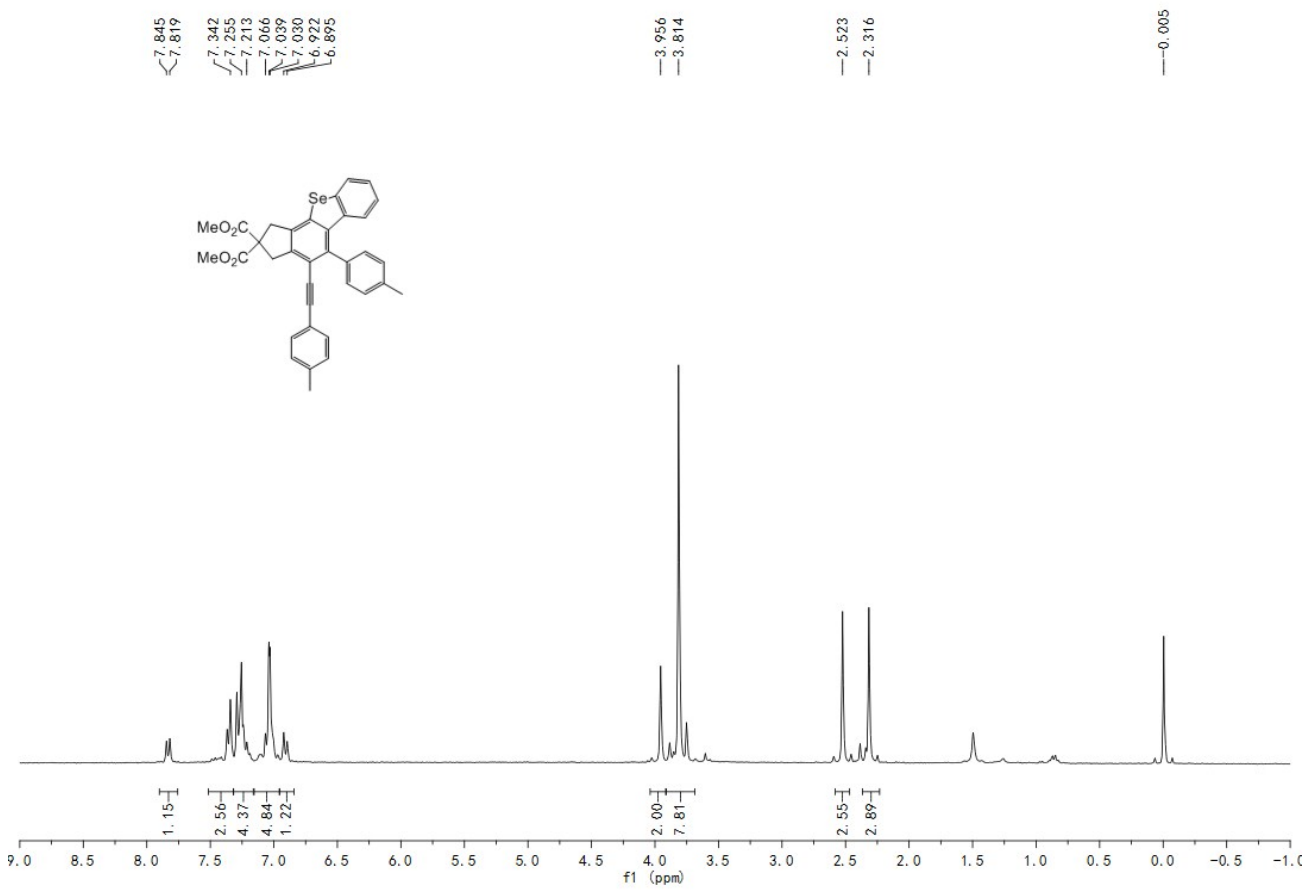
**3j**


7.863
7.847
7.562
7.546
7.240
7.047
6.900
6.884
3.943
3.824
0.001
Se
MeO2C
MeO2C
Cl
Cl
1.02
1.96
2.04
3.97
2.96
1.00
2.00
7.85
f1 (ppm)

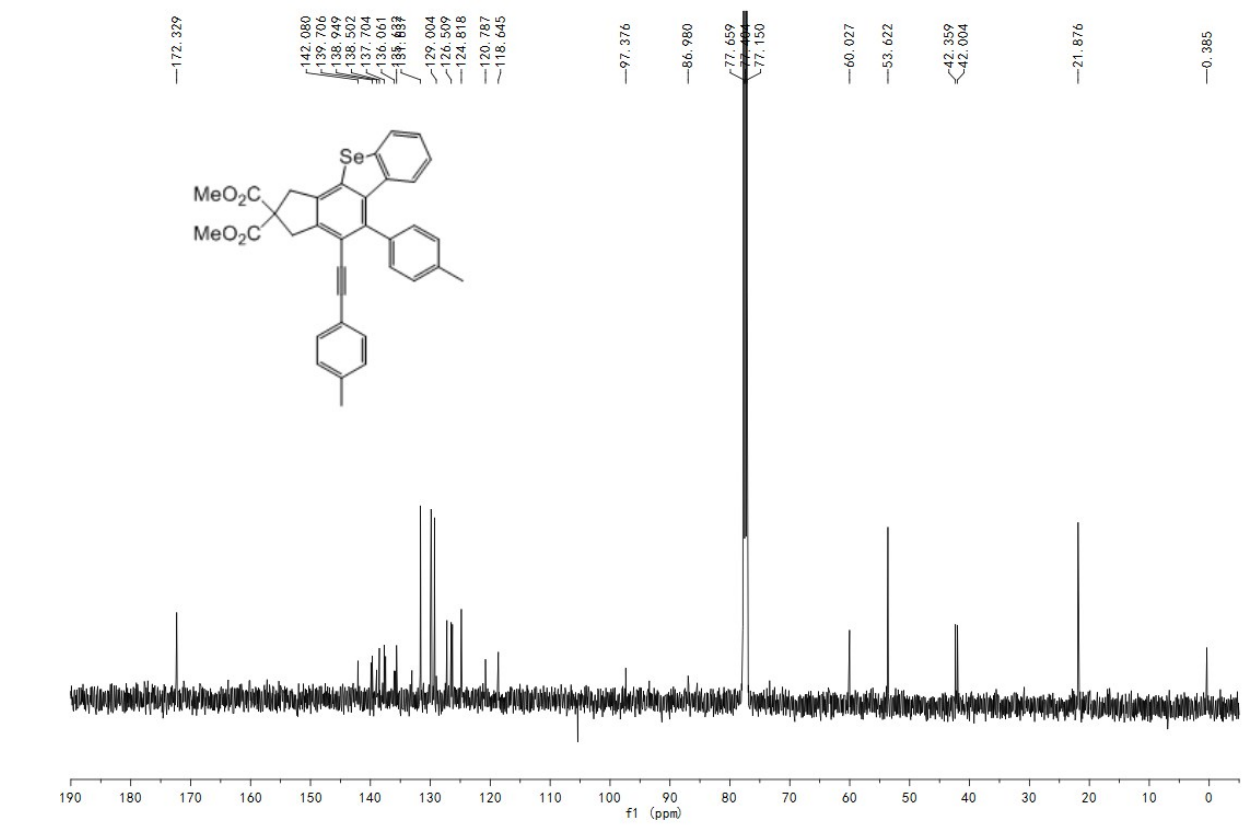
**3k**


172.195
139.821
136.344
135.654
134.614
134.295
132.865
131.624
129.478
129.046
126.915
126.855
126.524
125.063
121.983
117.958
96.449
88.127
77.674
77.420
77.165
59.980
53.709
42.333
41.909
0.399
Se
MeO2C
MeO2C
Cl
Cl
f1 (ppm)

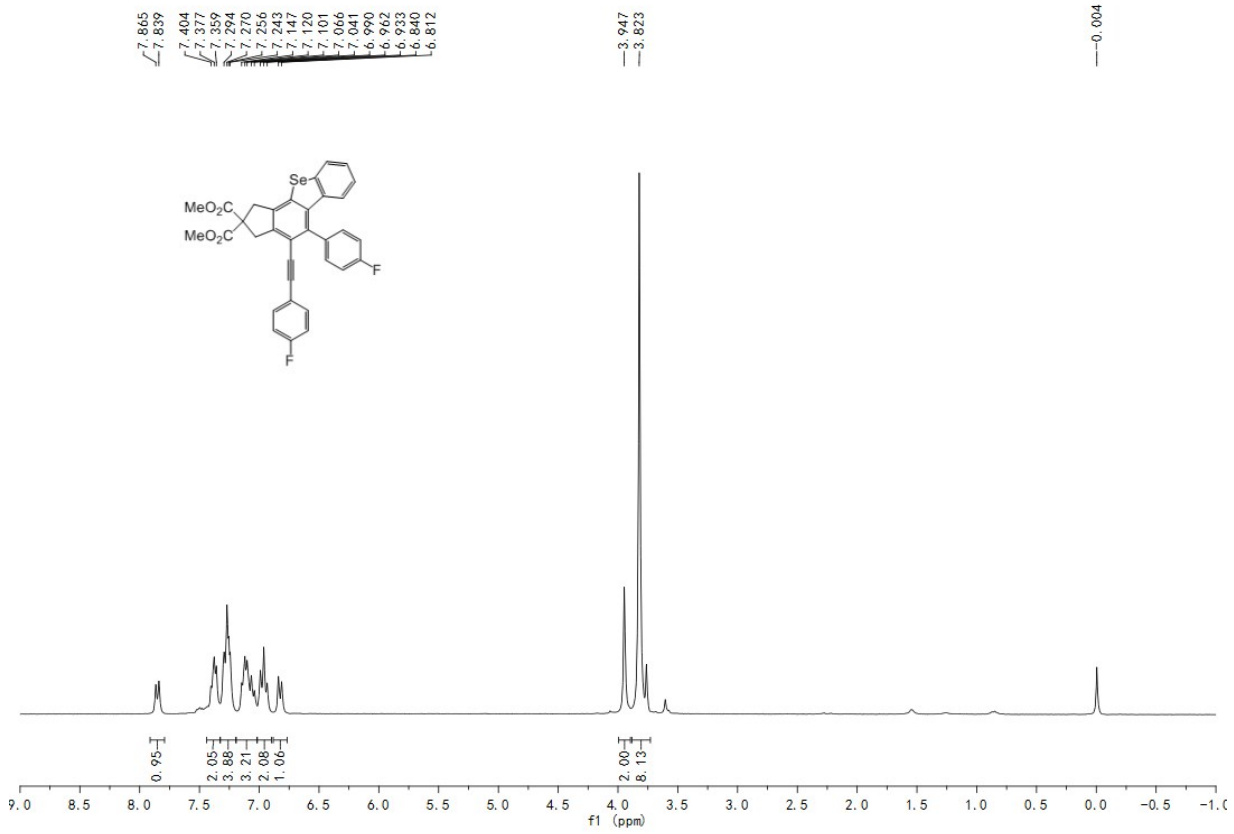
**3k**


7.845
7.819
7.342
7.255
7.213
7.066
7.039
7.030
6.922
6.895
3.956
3.814
2.523
2.316
0.005
Se
MeO2C
MeO2C
1.15
2.56
4.37
4.84
1.22
2.00
7.81
2.55
2.89
f1 (ppm)

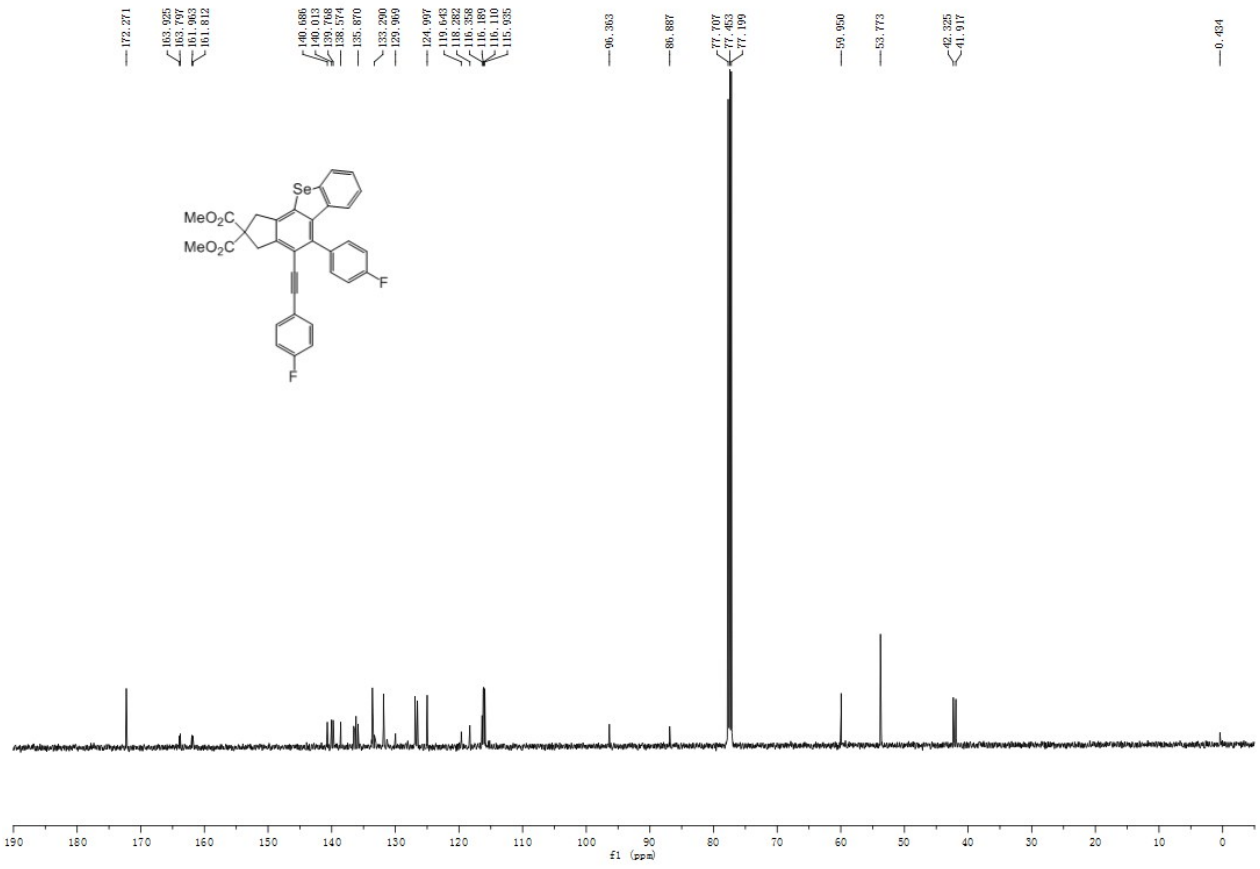
**3l**


172.329
142.080
139.706
138.949
138.502
137.704
136.061
129.004
126.509
124.818
120.787
118.645
97.376
86.980
77.659
77.150
60.027
53.622
42.359
42.004
21.876
0.385
Se
MeO2C
MeO2C
f1 (ppm)

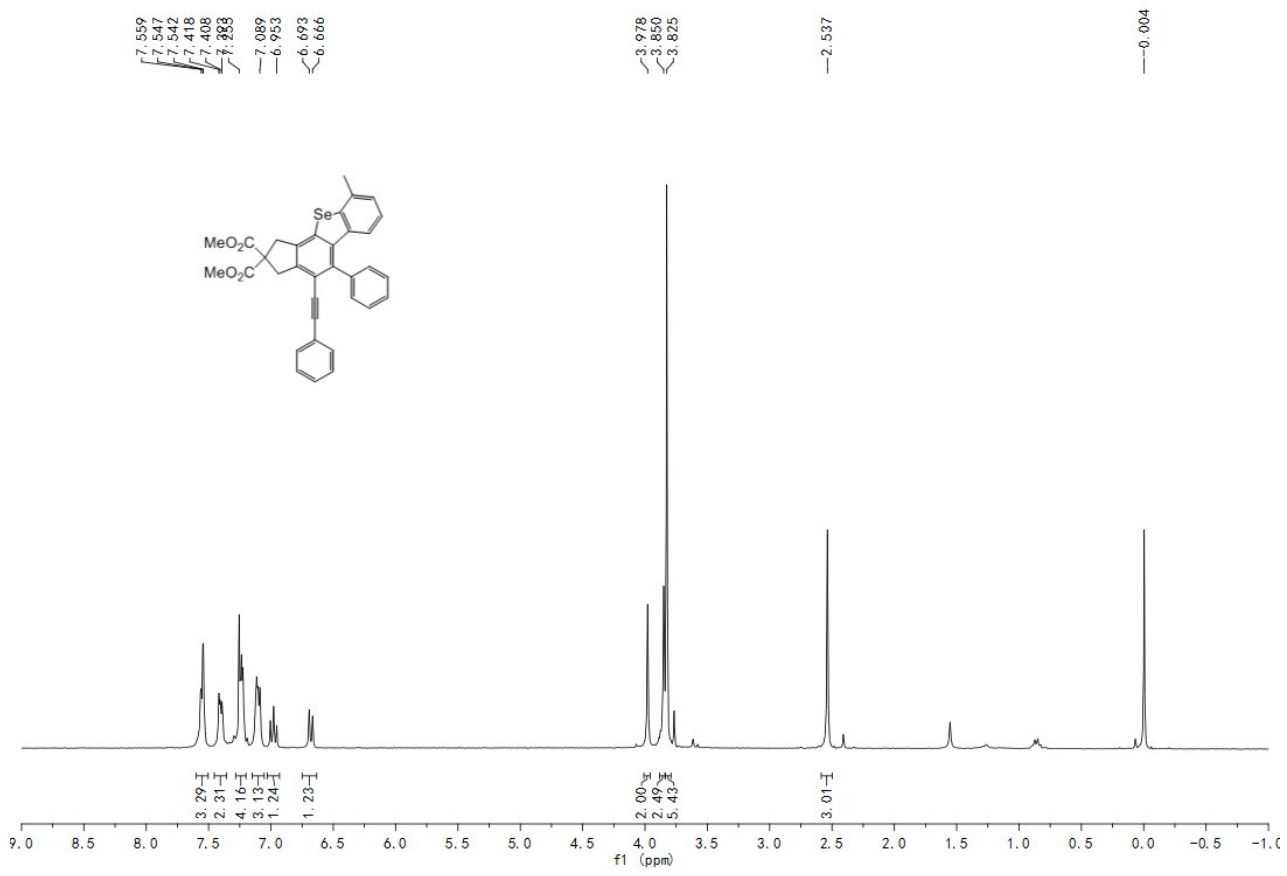
**3l**


7.865
7.839
7.404
7.377
7.359
7.294
7.270
7.256
7.243
7.147
7.120
7.101
7.066
7.041
6.990
6.962
6.933
6.840
6.812
3.947
3.823
0.004
MeO2C
MeO2C
Se
F
F
0.95
2.05
3.88
3.21
2.08
1.06
2.00
8.13
f1 (ppm)

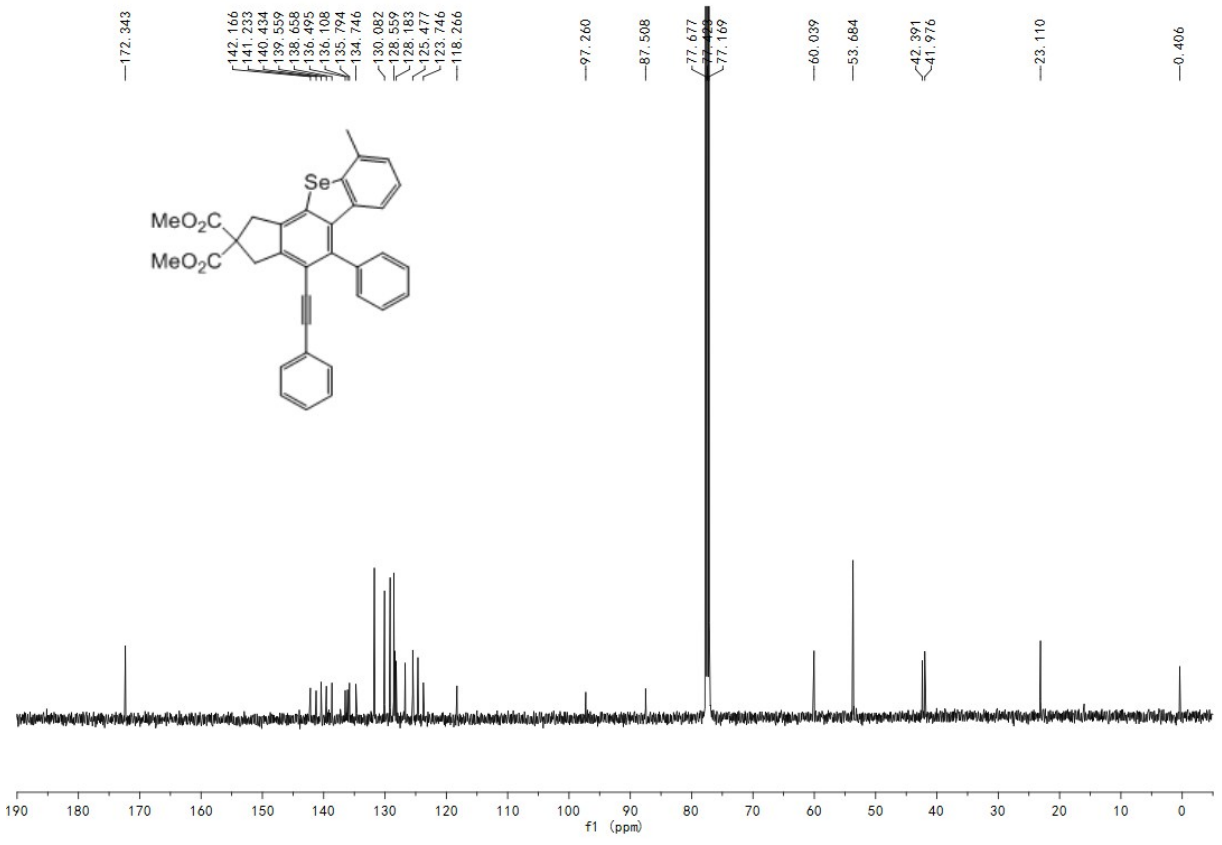
**3m**


172.271
163.925
163.797
161.963
161.812
140.686
140.013
139.768
138.574
135.870
133.290
129.969
124.997
119.643
118.282
116.358
116.189
116.110
115.935
96.363
86.887
77.707
77.453
77.199
59.950
53.773
42.325
41.917
0.434
MeO2C
MeO2C
Se
F
F
f1 (ppm)

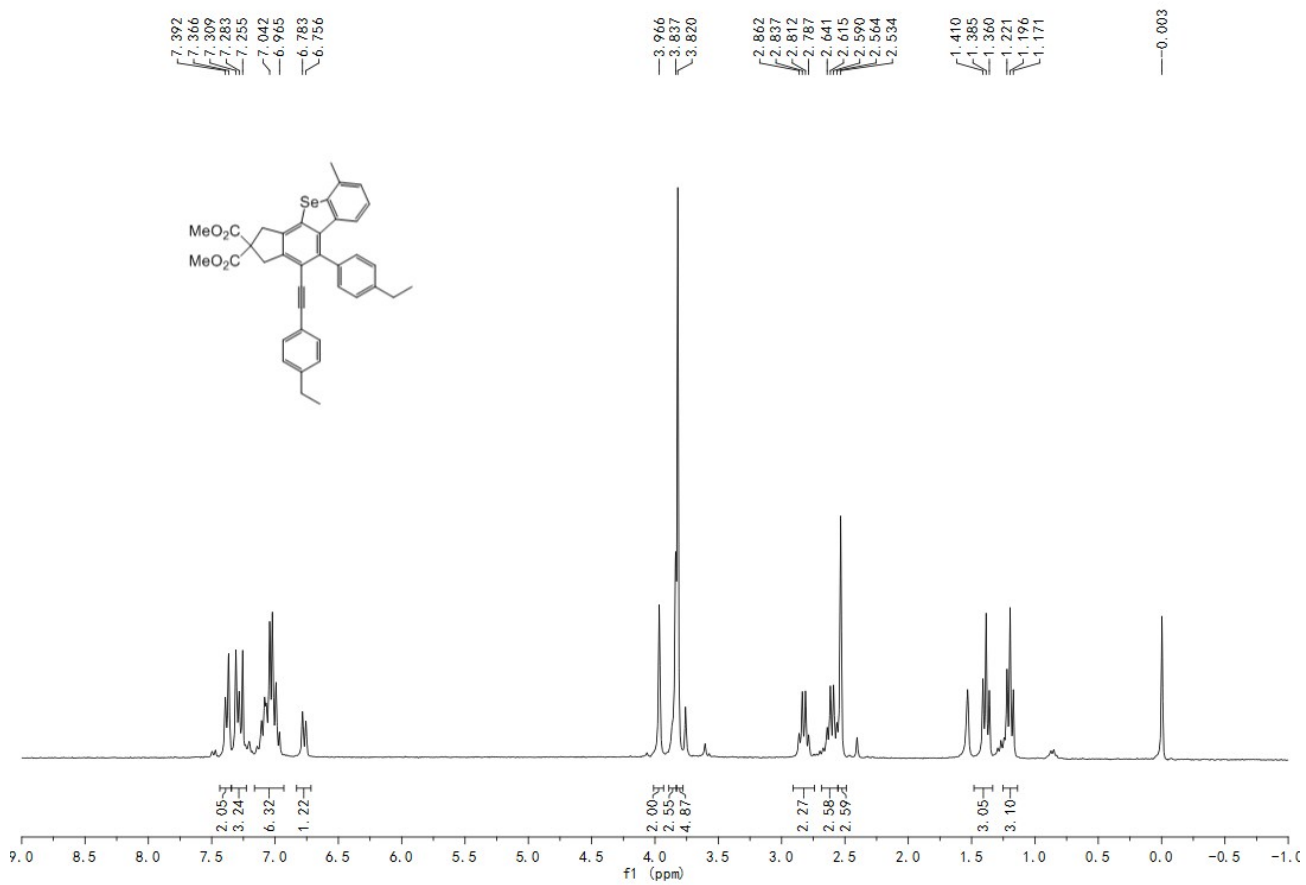
**3m**


7.559
7.547
7.542
7.418
7.408
7.089
6.953
6.693
6.666
3.978
3.850
3.825
2.537
0.004
Se
MeO2C
MeO2C
3.29
2.31
4.16
3.13
1.24
1.23
2.00
2.49
5.43
3.01
f1 (ppm)

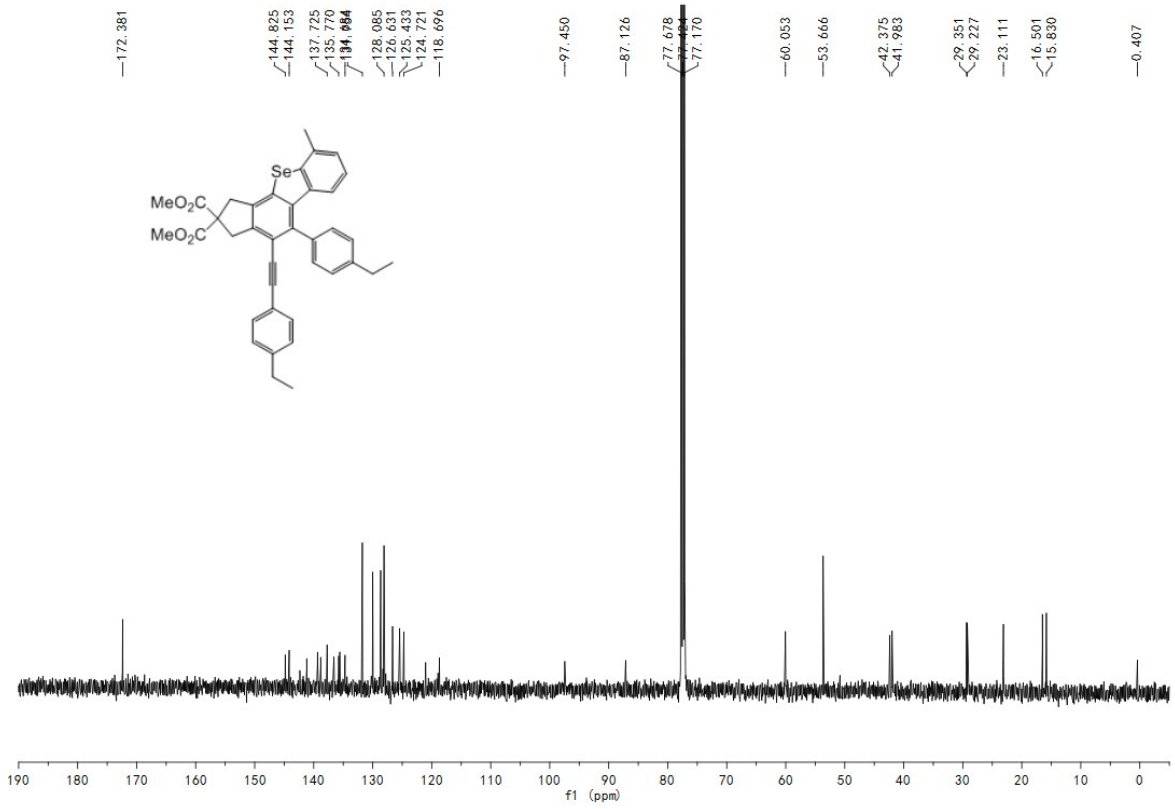
**3n**


172.343
142.166
141.233
140.434
139.559
138.658
136.495
136.108
135.794
134.746
130.082
128.559
128.183
125.477
123.746
118.266
97.260
87.508
77.677
77.169
60.039
53.684
42.391
41.976
23.110
0.406
Se
MeO2C
MeO2C
f1 (ppm)

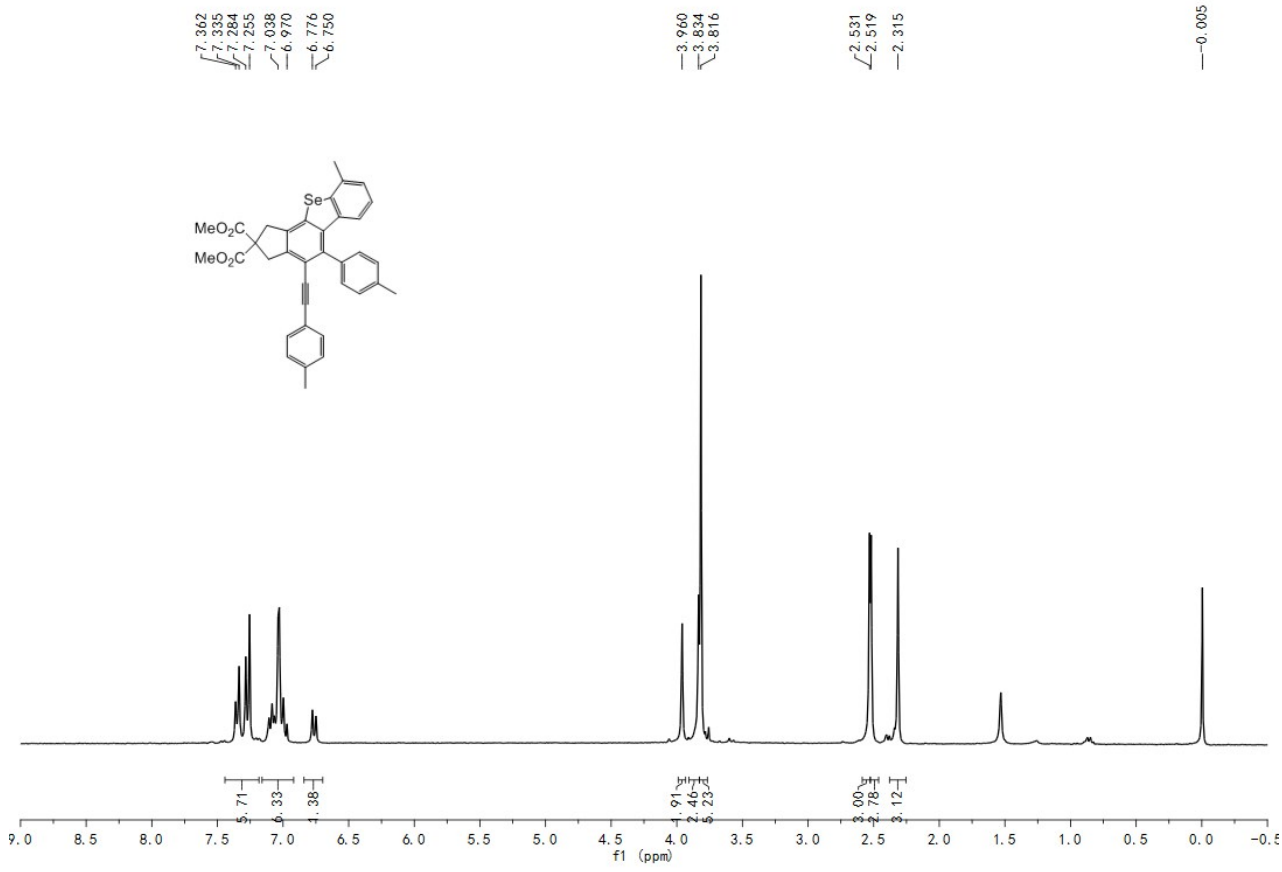
**3n**


7.392
7.366
7.309
7.283
7.255
7.042
6.965
6.783
6.756
3.966
3.837
3.820
2.862
2.837
2.812
2.787
2.641
2.615
2.590
2.564
2.534
1.410
1.385
1.360
1.221
1.196
1.171
0.003
Se
MeO2C
MeO2C
2.05
3.24
6.32
1.22
2.00
2.55
4.87
2.27
2.58
2.59
3.05
3.10
f1 (ppm)

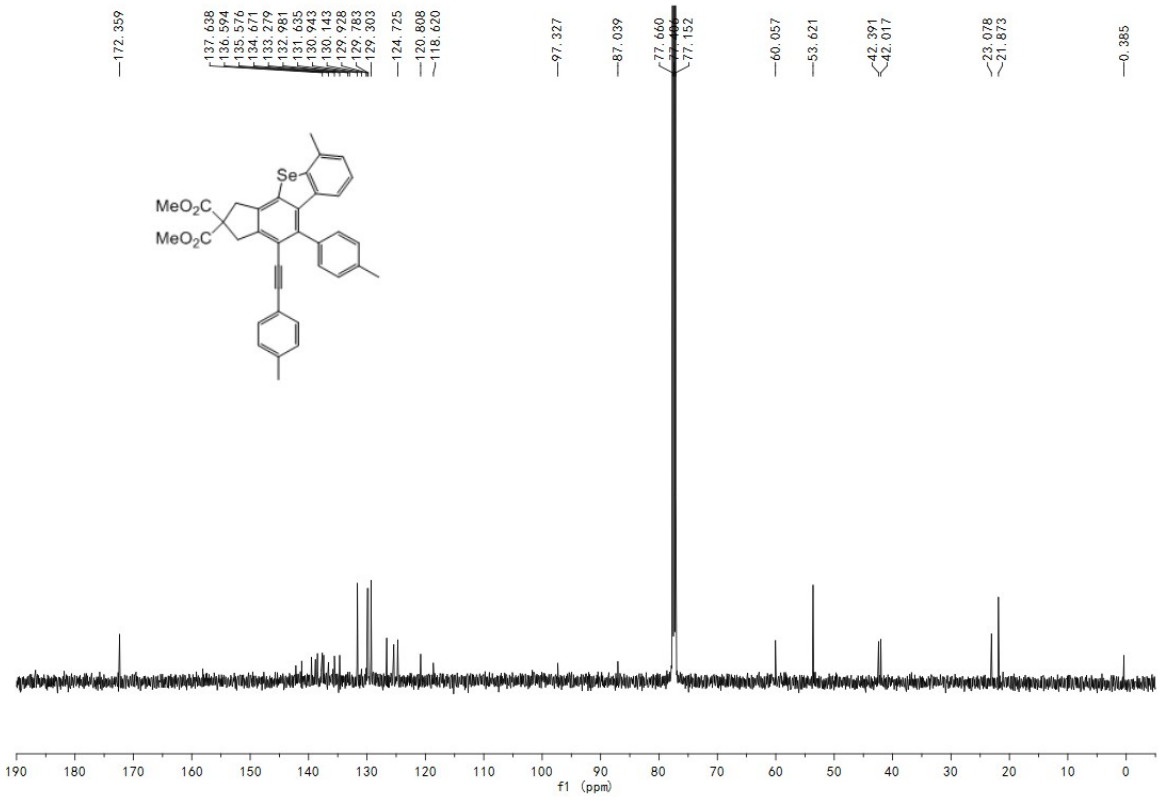
**3o**


172.381
144.825
144.153
137.725
135.770
128.085
126.631
125.433
124.721
118.696
97.450
87.126
77.678
77.170
60.053
53.666
42.375
41.983
29.351
29.227
23.111
16.501
15.830
0.407
Se
MeO2C
MeO2C
f1 (ppm)

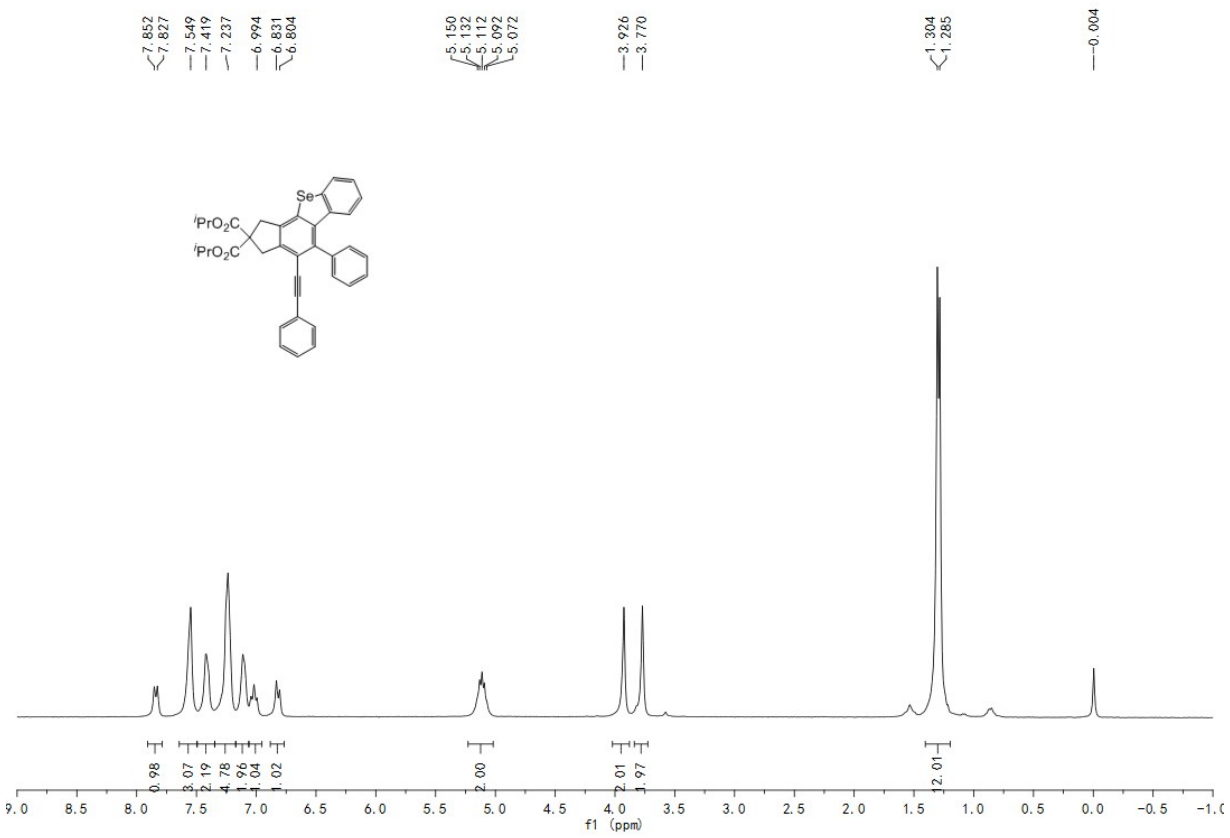
**3o**


7.362
7.335
7.284
7.255
7.038
6.970
6.776
6.750
3.960
3.834
3.816
2.531
2.519
2.315
0.005
Se
MeO2C
MeO2C
5.71
6.33
4.38
4.91
2.46
6.23
3.00
2.78
3.12
f1 (ppm)

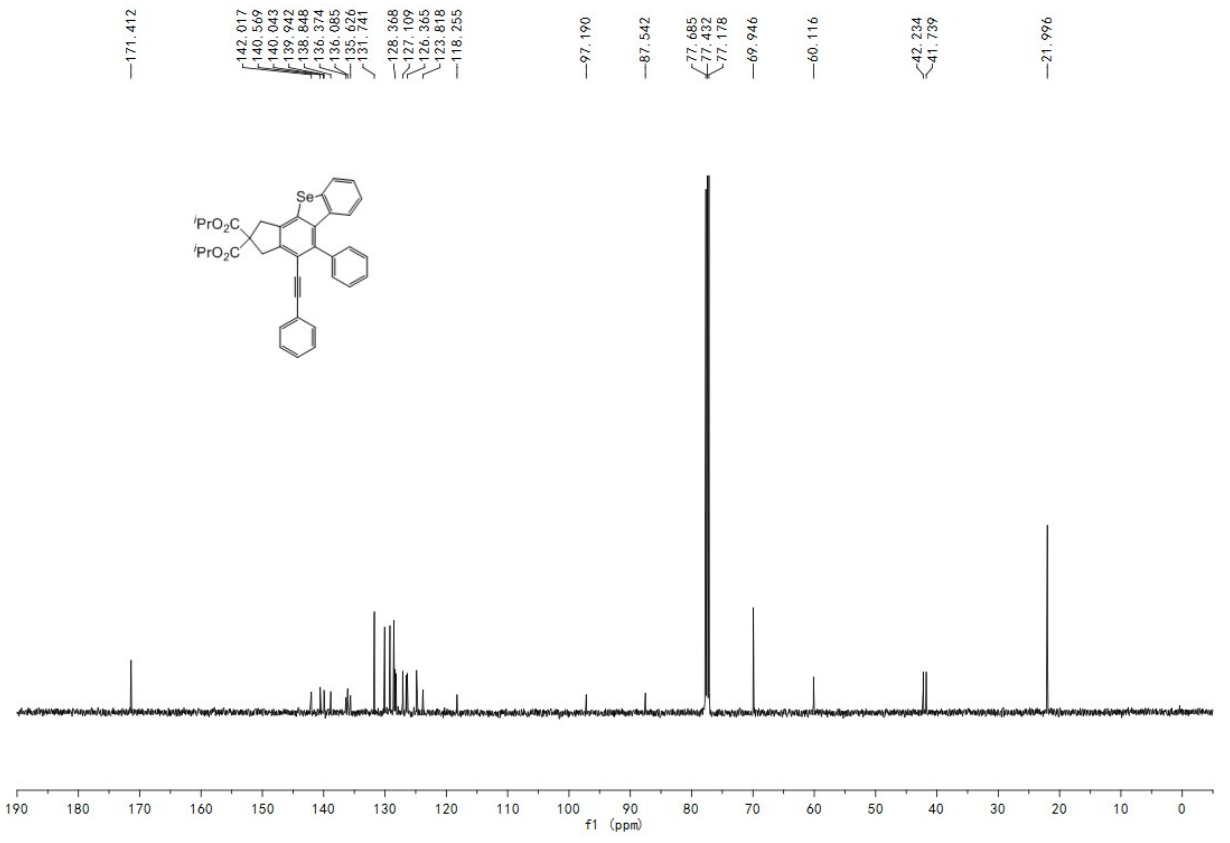
**3p**


172.359
137.638
136.594
135.576
134.671
133.279
132.981
131.635
130.943
130.143
129.928
129.783
129.303
124.725
120.808
118.620
97.327
87.039
77.660
77.402
77.152
60.057
53.621
42.391
42.017
23.078
21.873
0.385
Se
MeO2C
MeO2C
f1 (ppm)

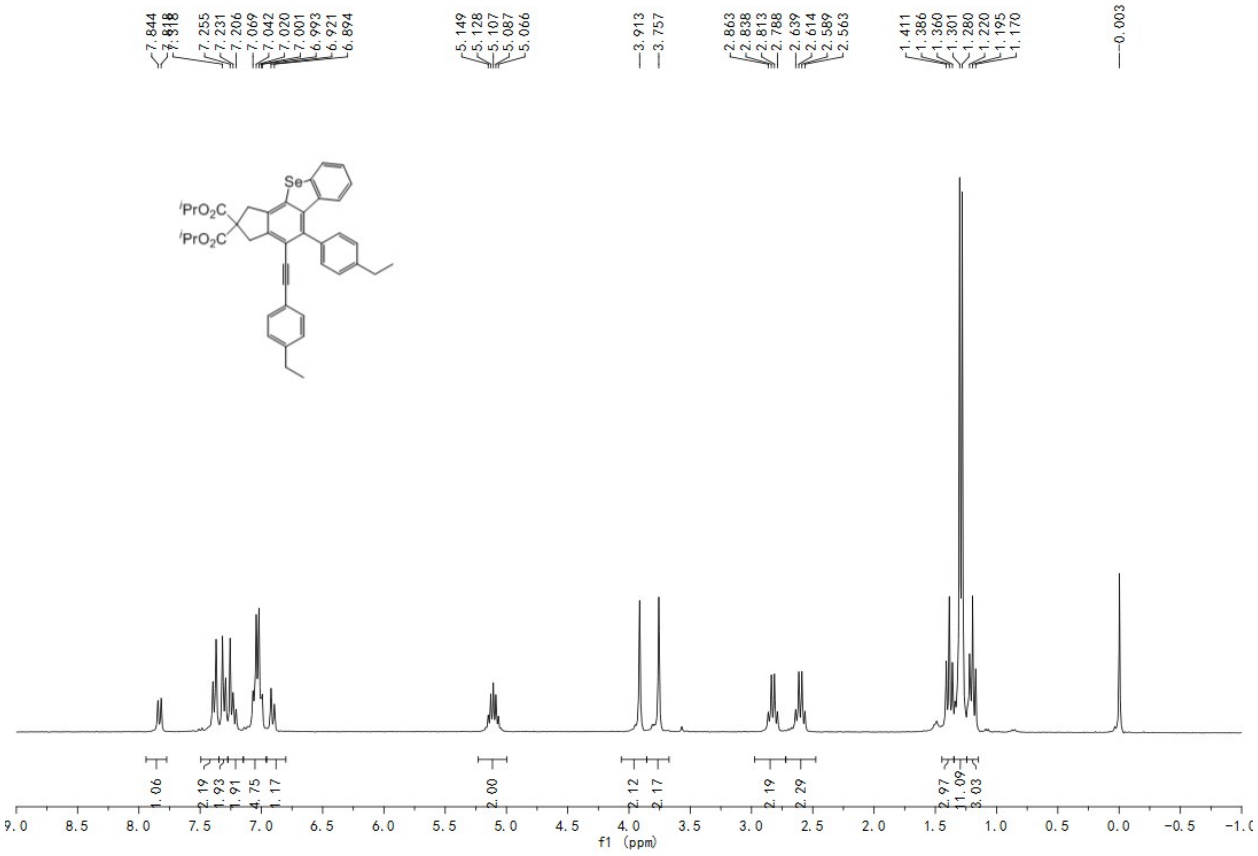
**3p**


7.852
7.827
7.549
7.419
7.237
6.994
6.831
6.804
5.150
5.132
5.112
5.092
5.072
3.926
3.770
1.304
1.285
0.004
Se
iPrO2C
iPrO2C
0.98
3.07
2.19
4.78
1.96
1.04
1.02
2.00
2.01
1.97
12.01
f1 (ppm)

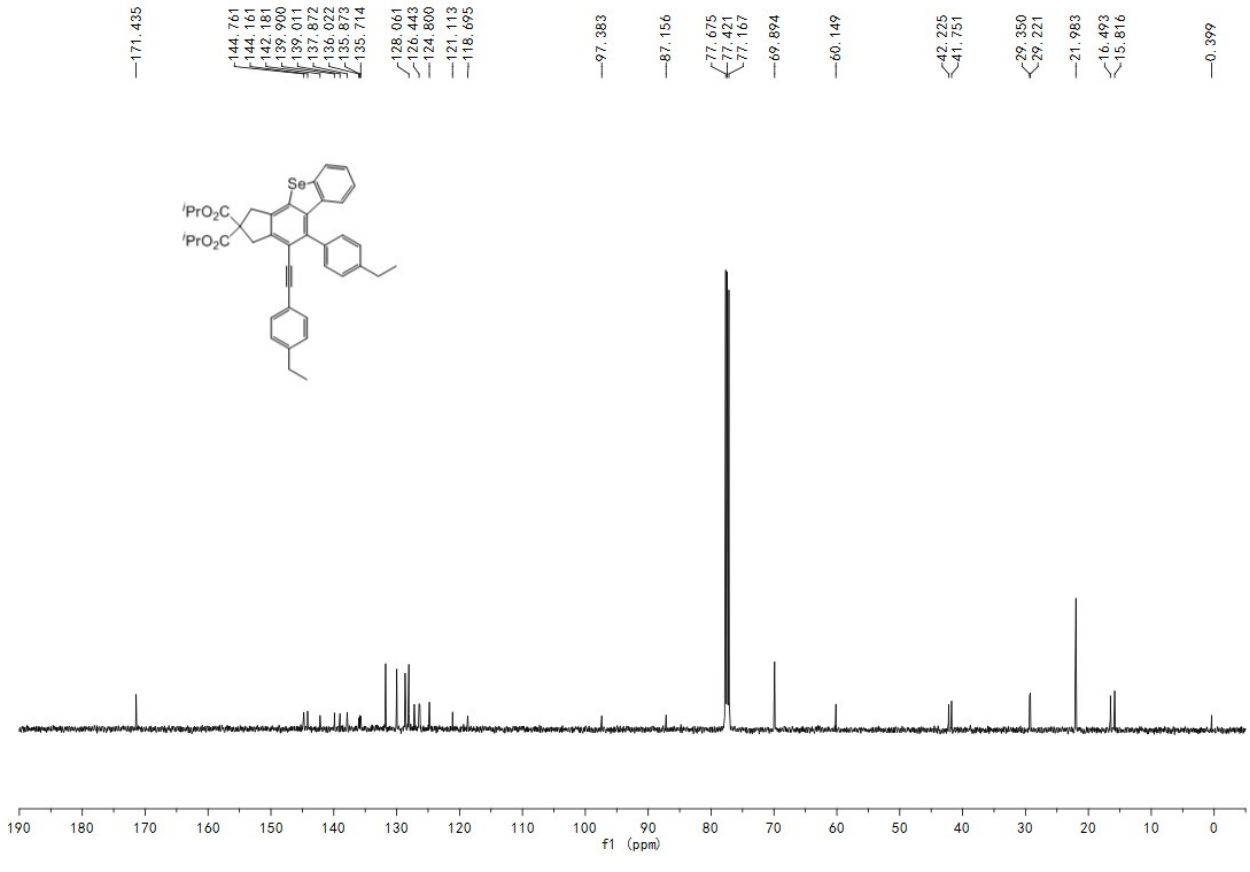
**3q**


171.412
142.017
140.569
140.043
139.942
138.848
136.374
136.085
135.626
131.741
128.368
127.109
126.365
123.818
118.255
97.190
87.542
77.685
77.432
77.178
69.946
60.116
42.234
41.739
21.996
Se
iPrO2C
iPrO2C
f1 (ppm)

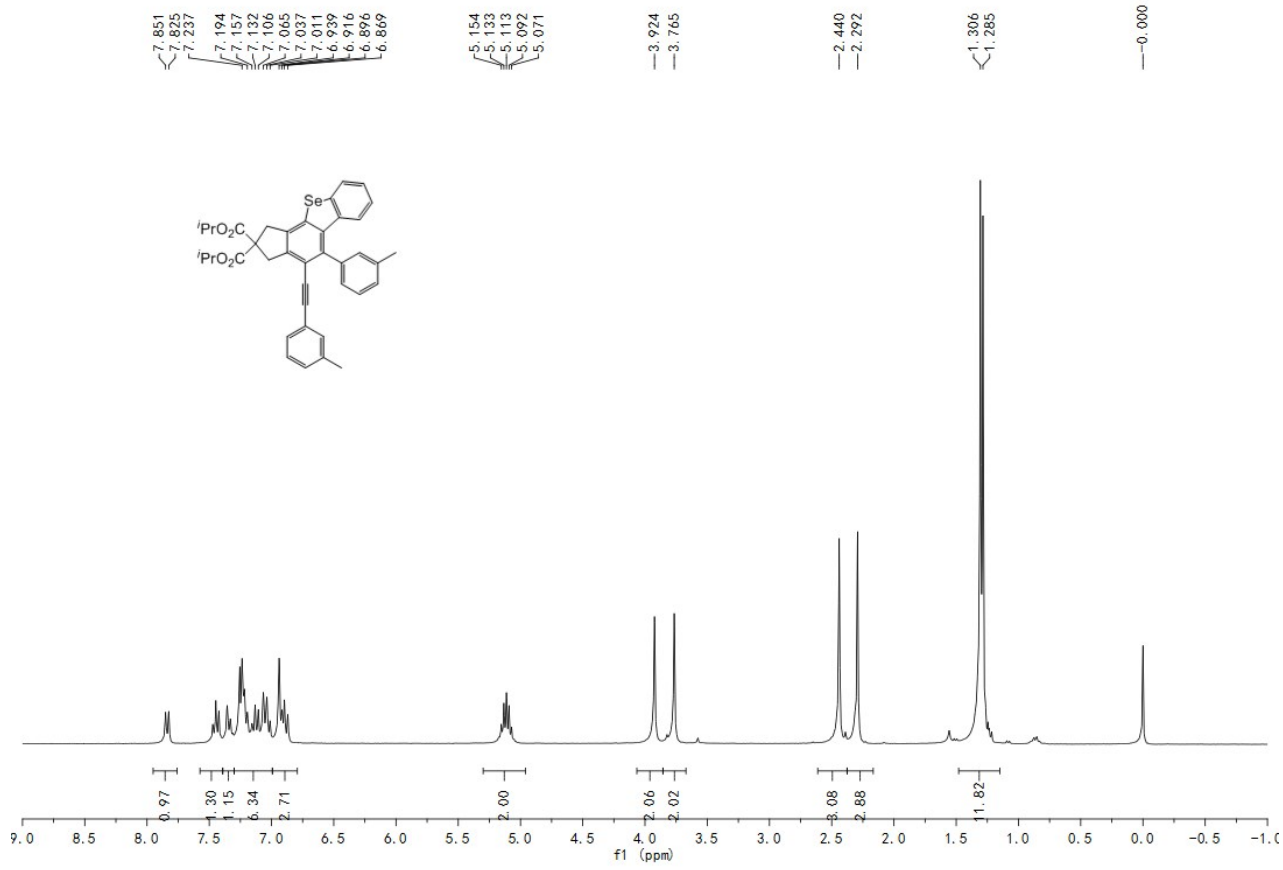
**3q**


7.844
7.818
7.255
7.231
7.206
7.069
7.042
7.020
7.001
6.993
6.921
6.894
5.149
5.128
5.107
5.087
5.066
3.913
3.757
2.863
2.838
2.813
2.788
2.639
2.614
2.589
2.563
1.411
1.386
1.360
1.301
1.280
1.220
1.195
1.170
0.003
Se
iPrO2C
iPrO2C
1.06
2.19
1.93
1.91
4.75
1.17
2.00
2.12
2.17
2.19
2.29
2.97
11.09
3.03
f1 (ppm)

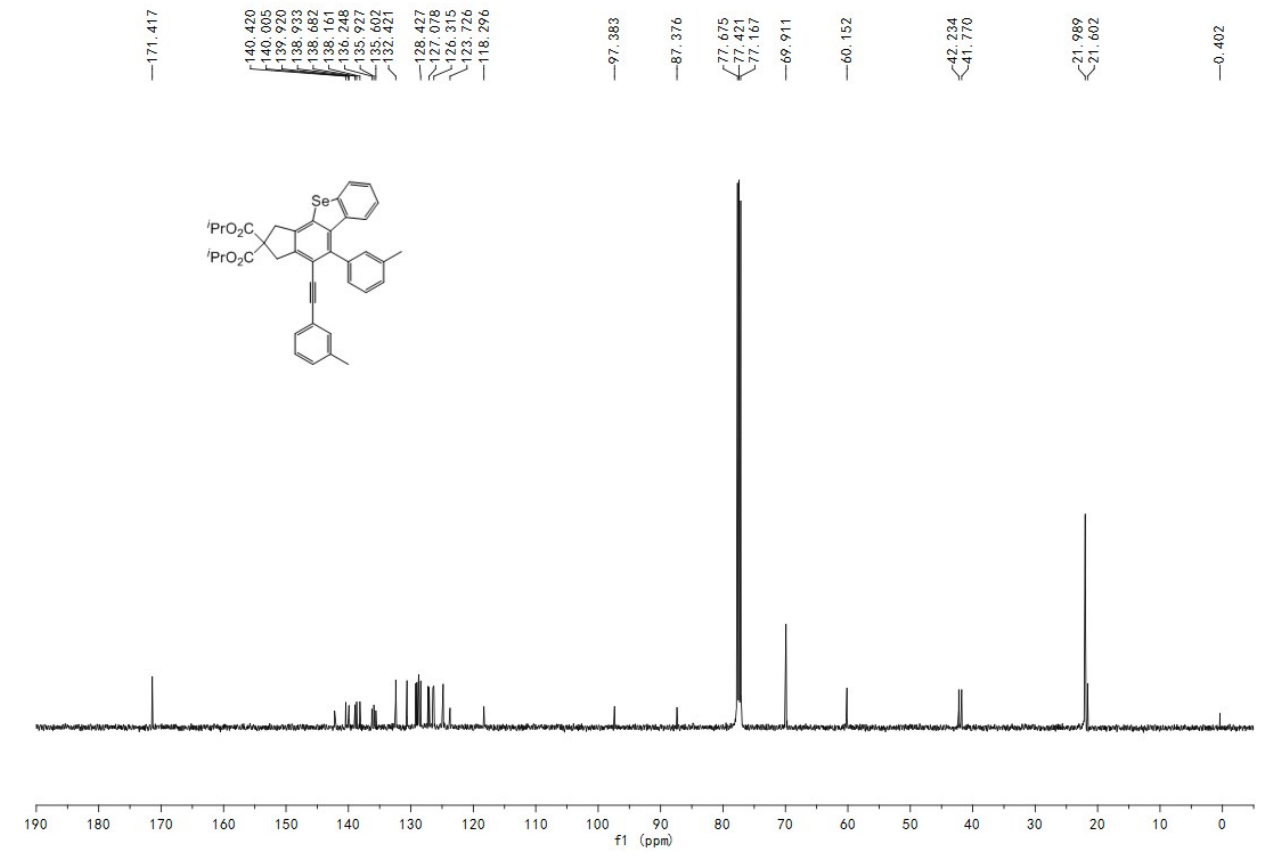
**3r**


171.435
144.761
144.161
142.181
139.900
139.011
137.872
136.022
135.873
135.714
128.061
126.443
124.800
121.113
118.695
97.383
87.156
77.675
77.421
77.167
69.894
60.149
42.225
41.751
29.350
29.221
21.983
16.493
15.816
0.399
Se
iPrO2C
iPrO2C
f1 (ppm)

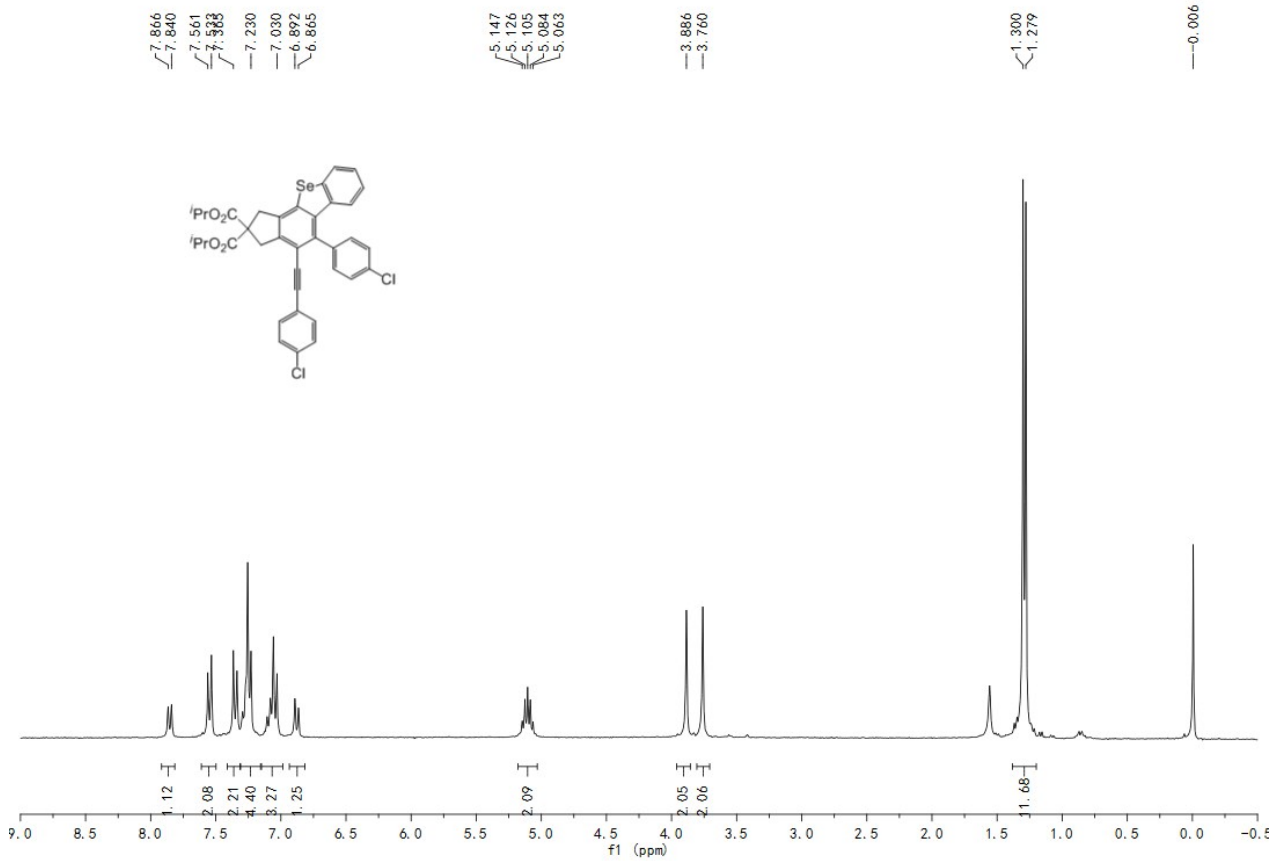
**3r**


7.851
7.825
7.237
7.194
7.157
7.132
7.106
7.065
7.037
7.011
6.939
6.916
6.896
6.869
5.154
5.133
5.113
5.092
5.071
3.924
3.765
2.440
2.292
1.306
1.285
0.000
Se
iPrO2C
iPrO2C
0.97
1.30
1.15
6.34
2.71
2.00
2.06
2.02
3.08
2.88
11.82
f1 (ppm)

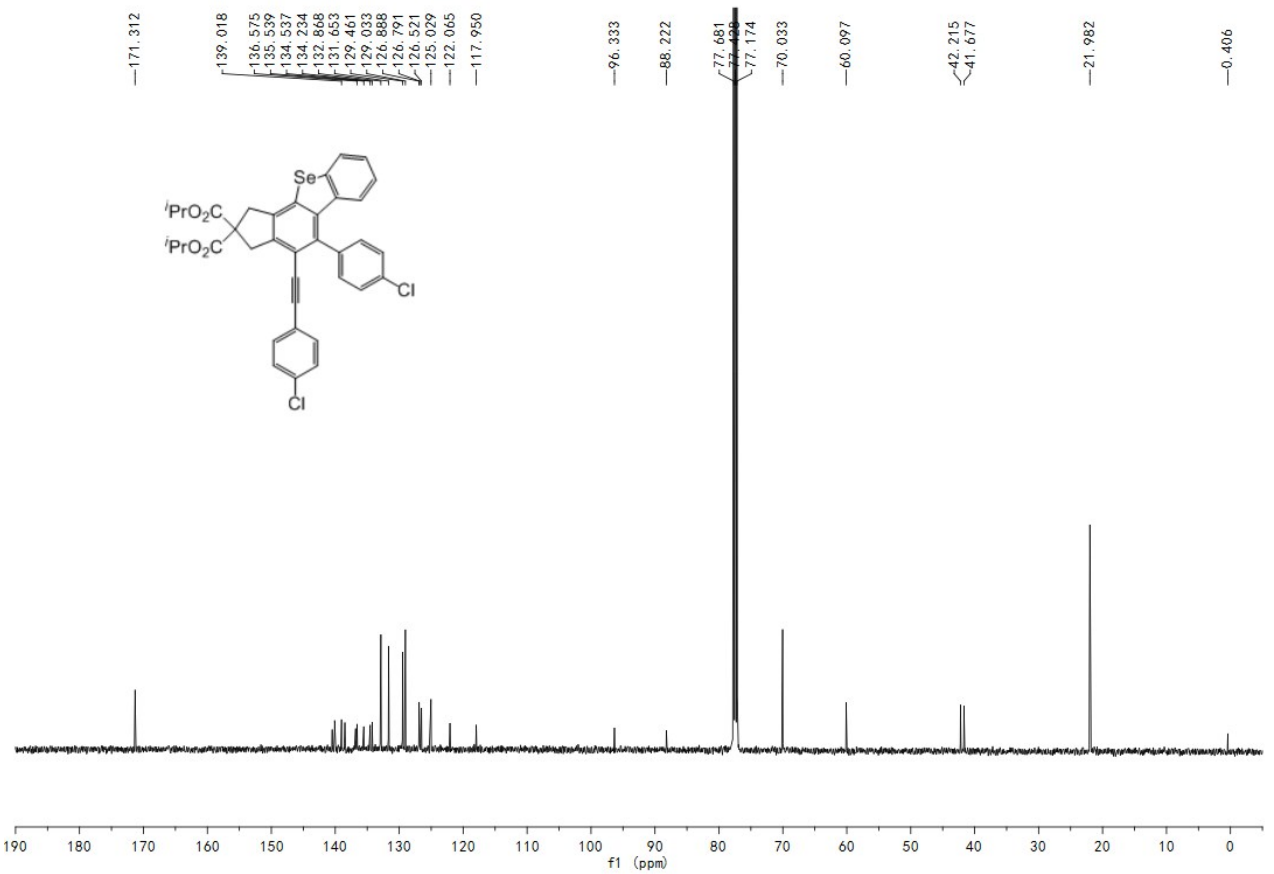
**3s**


171.417
140.420
140.005
139.920
138.933
138.682
138.161
136.248
135.927
135.602
132.421
128.427
127.078
126.315
123.726
118.296
97.383
87.376
77.675
77.421
77.167
69.911
60.152
42.234
41.770
21.989
21.602
0.402
Se
iPrO2C
iPrO2C
f1 (ppm)

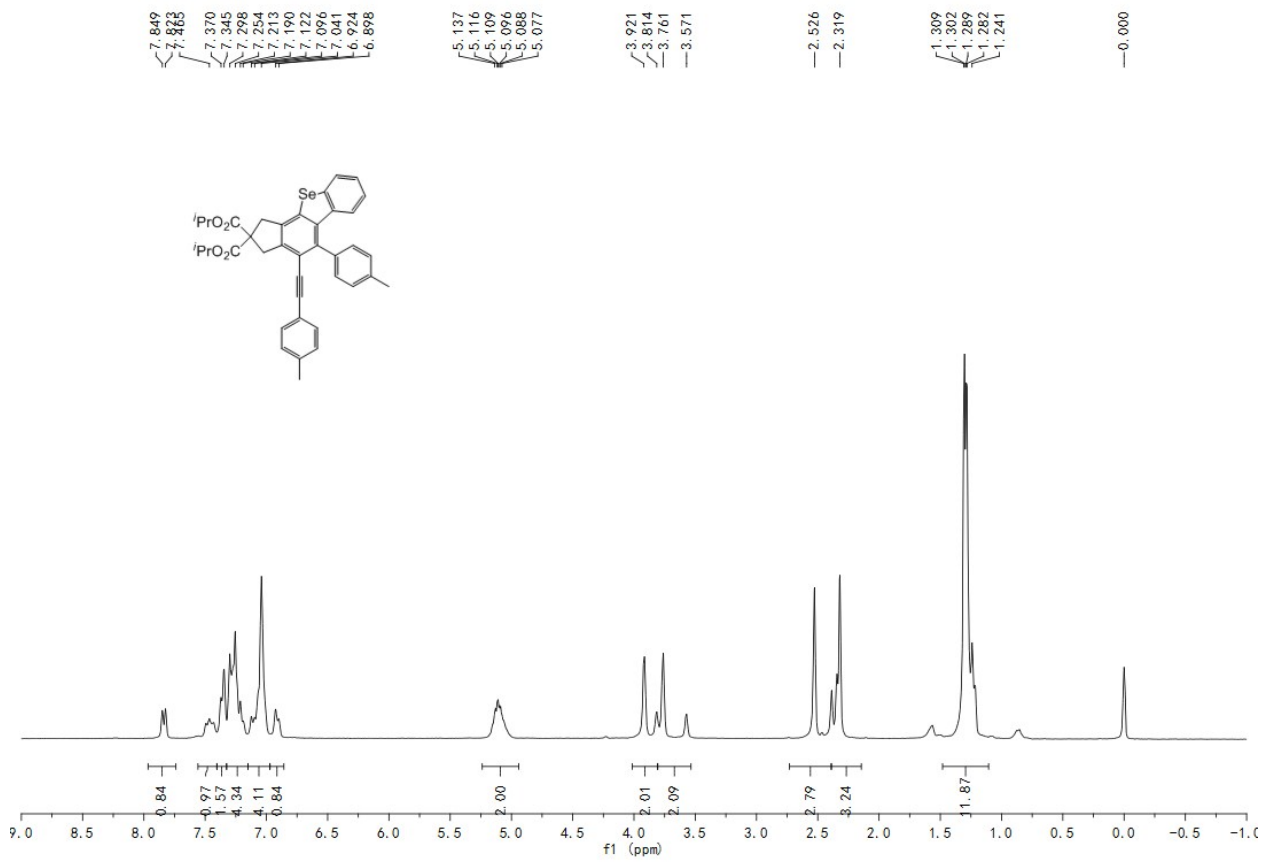
**3s**


7.866
7.840
7.561
7.230
7.030
6.892
6.865
5.147
5.126
5.105
5.084
5.063
3.886
3.760
1.300
1.279
0.006
Se
iPrO2C
iPrO2C
Cl
Cl
1.12
2.08
2.21
4.40
3.27
1.25
2.09
2.05
2.06
11.68
f1 (ppm)

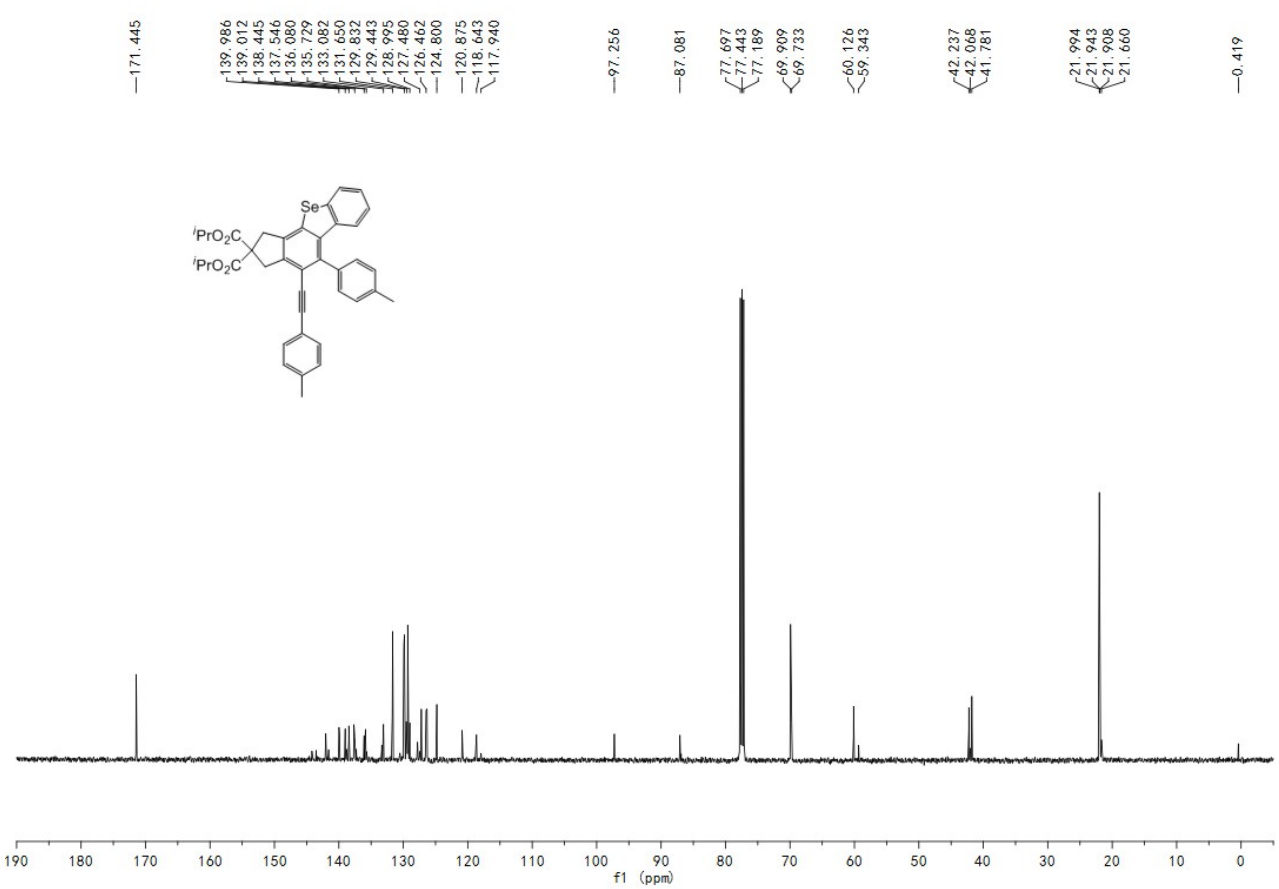
**3t**


171.312
139.018
136.575
135.539
134.537
134.234
132.868
131.653
129.461
129.033
126.888
126.791
126.521
125.029
122.065
117.950
96.333
88.222
77.681
77.438
77.174
70.033
60.097
42.215
41.677
21.982
0.406
Se
iPrO2C
iPrO2C
Cl
Cl
f1 (ppm)

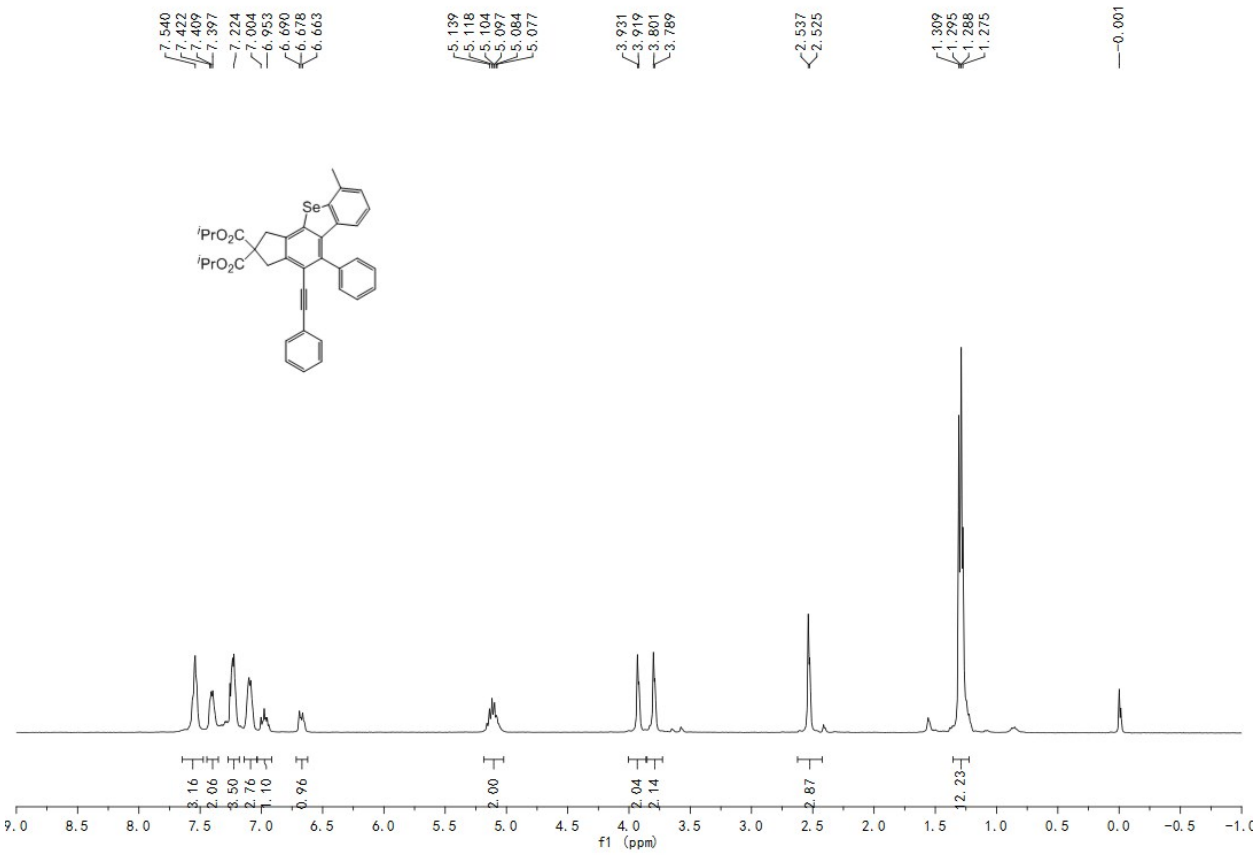
**3t**


7.849
7.823
7.463
7.370
7.345
7.298
7.254
7.213
7.190
7.122
7.096
7.041
6.924
6.898
5.137
5.116
5.109
5.096
5.088
5.077
3.921
3.814
3.761
3.571
2.526
2.319
1.309
1.302
1.289
1.282
1.241
0.000
Se
iPrO2C
iPrO2C
0.84
0.97
1.57
4.34
4.11
0.84
2.00
2.01
2.09
2.79
3.24
11.87
f1 (ppm)

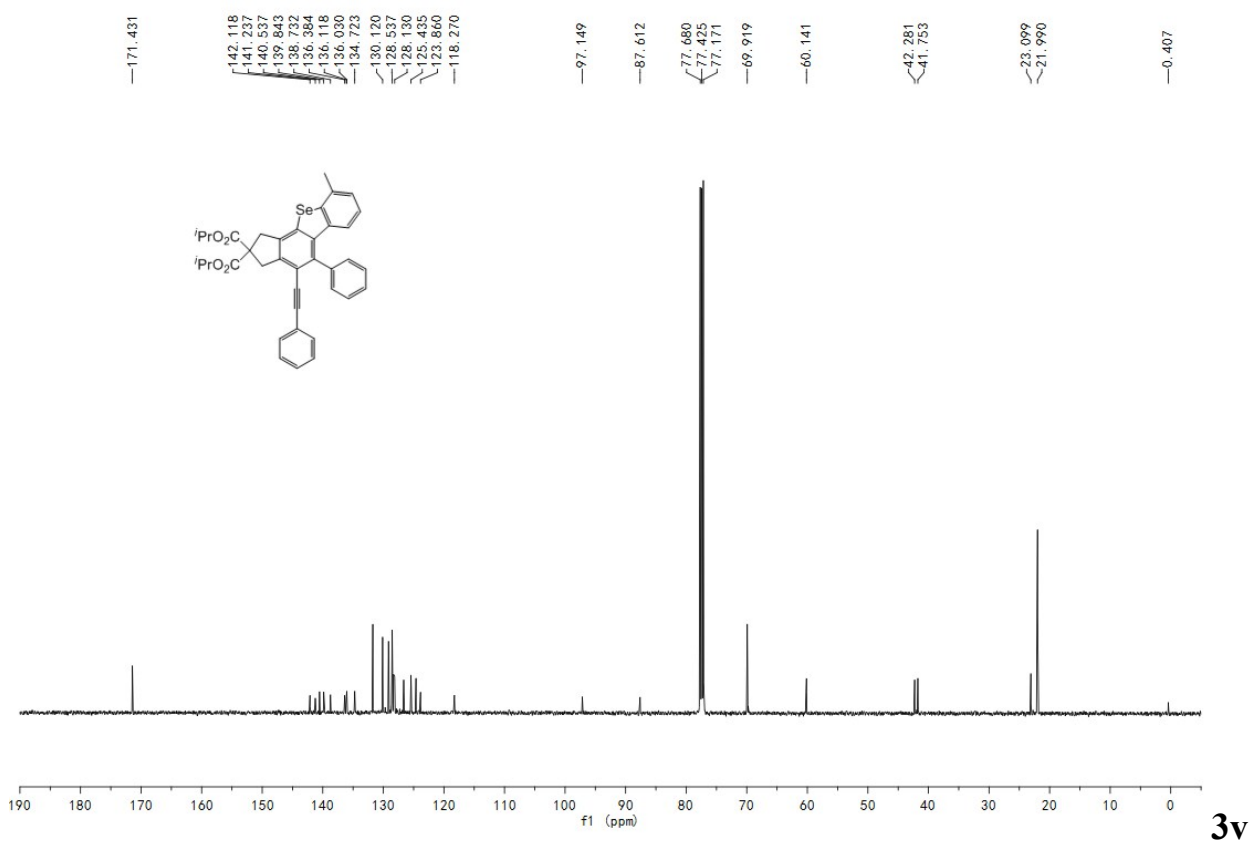
**3u**


171.445
139.986
139.012
138.445
137.546
136.080
135.729
133.082
131.650
129.832
129.443
128.995
127.480
126.462
124.800
120.875
118.643
117.940
97.256
87.081
77.697
77.443
77.189
69.909
69.733
60.126
59.343
42.237
42.068
41.781
21.994
21.943
21.908
21.660
0.419
Se
iPrO2C
iPrO2C
f1 (ppm)

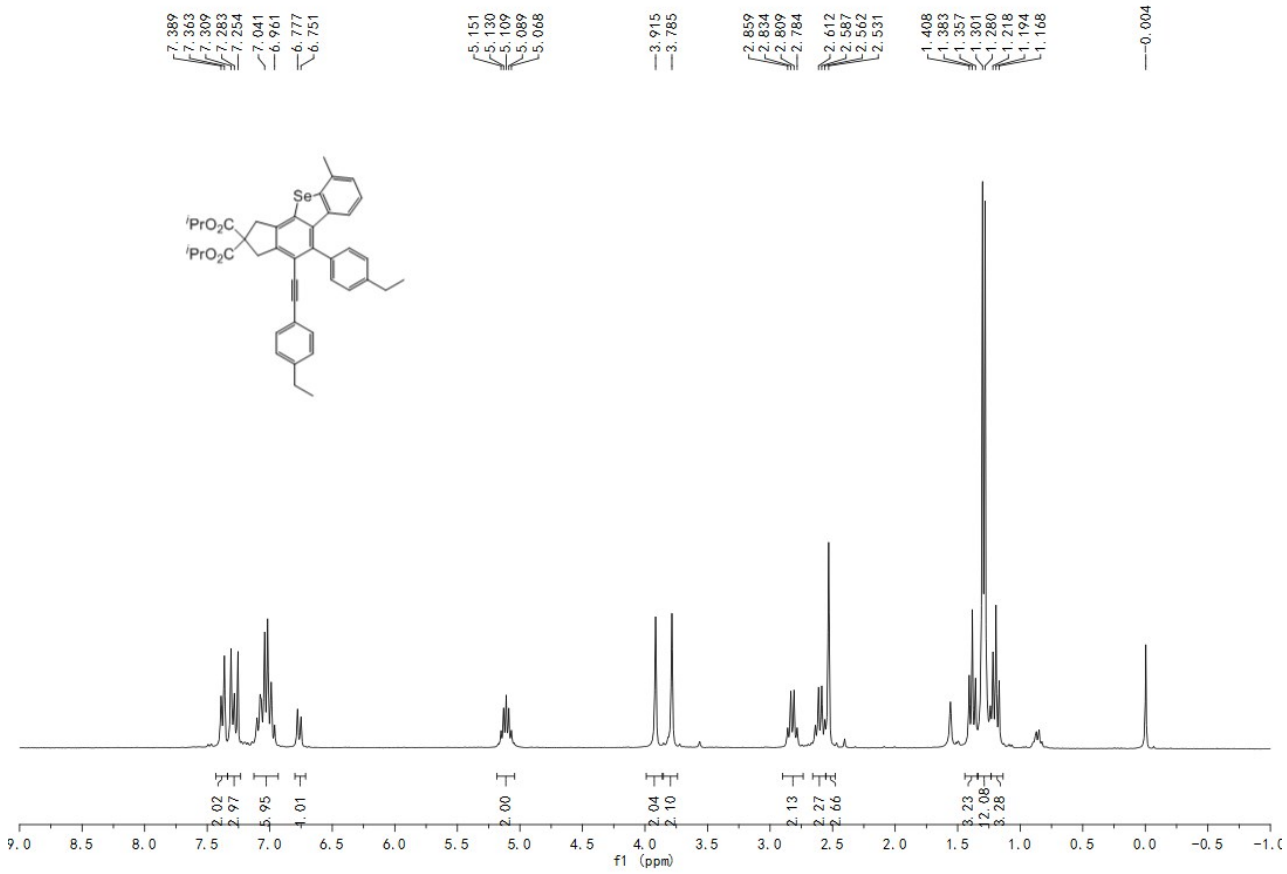
**3u**


7.540
7.422
7.409
7.397
7.224
7.004
6.953
6.690
6.678
6.663
5.139
5.118
5.104
5.097
5.084
5.077
3.931
3.919
3.801
3.789
2.537
2.525
1.309
1.295
1.288
1.275
0.001
Se
iPrO2C
iPrO2C
3.16
2.06
3.50
2.76
1.10
0.96
2.00
2.04
2.14
2.87
12.23
f1 (ppm)

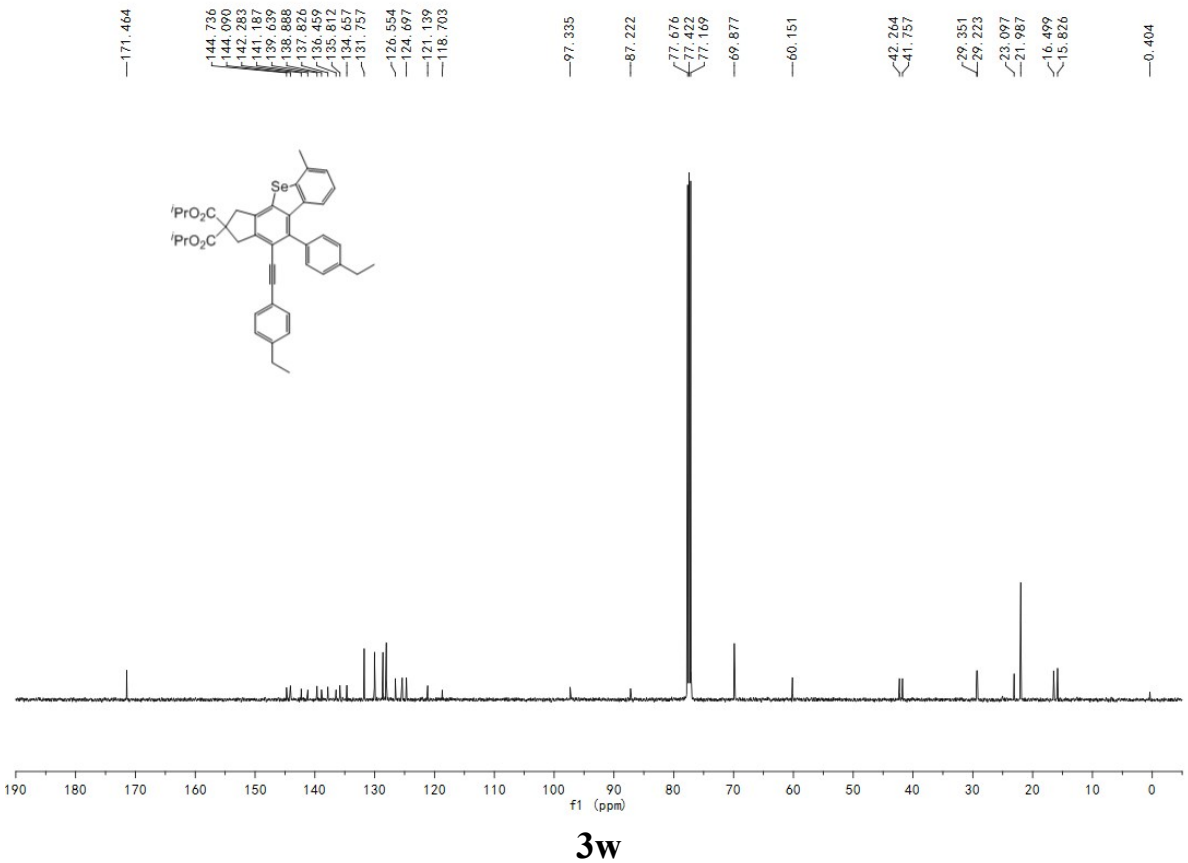
**3v**


171.431
142.118
141.237
140.537
139.843
138.732
136.384
136.118
136.030
134.723
130.120
128.537
128.130
125.435
123.860
118.270
97.149
87.612
77.680
77.425
77.171
69.919
60.141
42.281
41.753
23.099
21.990
0.407
Se
iPrO2C
iPrO2C
f1 (ppm)

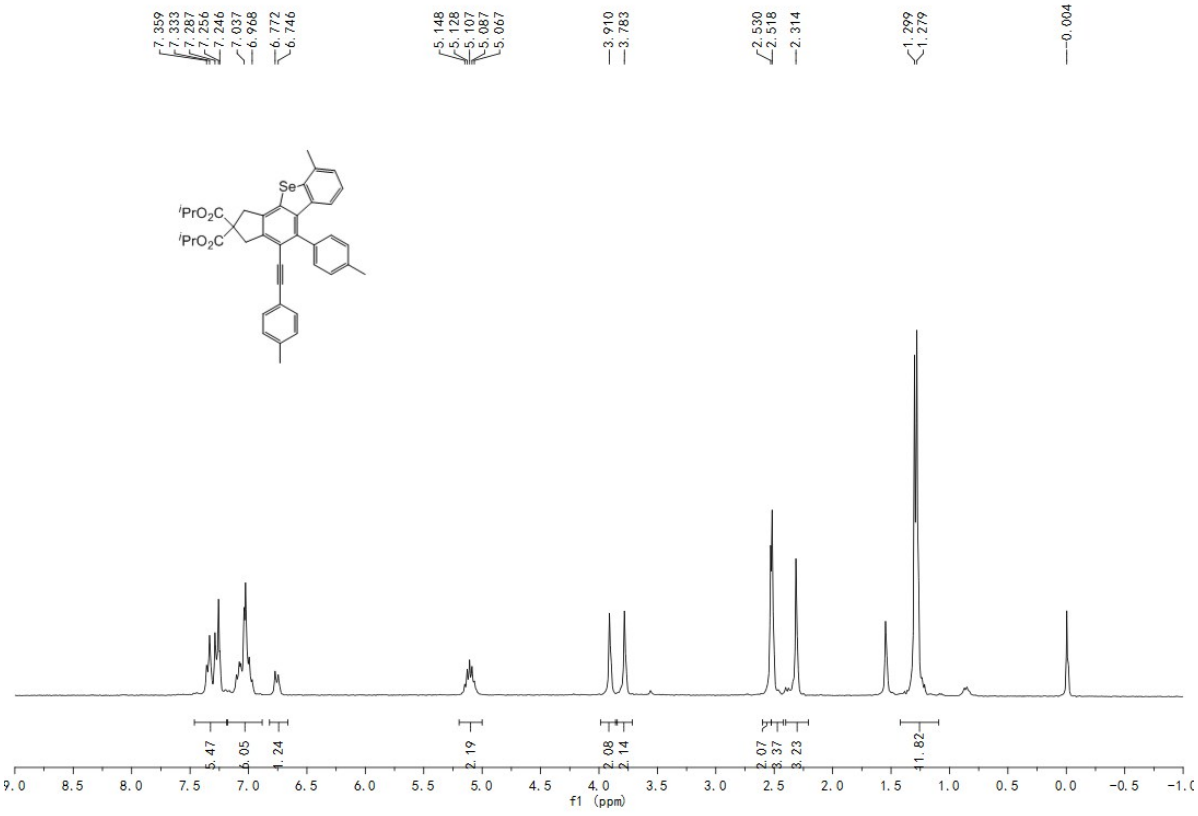
**3v**


7.389
7.363
7.309
7.283
7.254
7.041
6.961
6.777
6.751
5.151
5.130
5.109
5.089
5.068
3.915
3.785
2.859
2.834
2.809
2.784
2.612
2.587
2.562
2.531
1.408
1.383
1.357
1.301
1.280
1.218
1.194
1.168
0.004
Se
iPrO2C
iPrO2C
2.02
2.97
5.95
4.01
2.00
2.04
2.10
2.13
2.27
2.66
3.23
12.08
3.28
f1 (ppm)

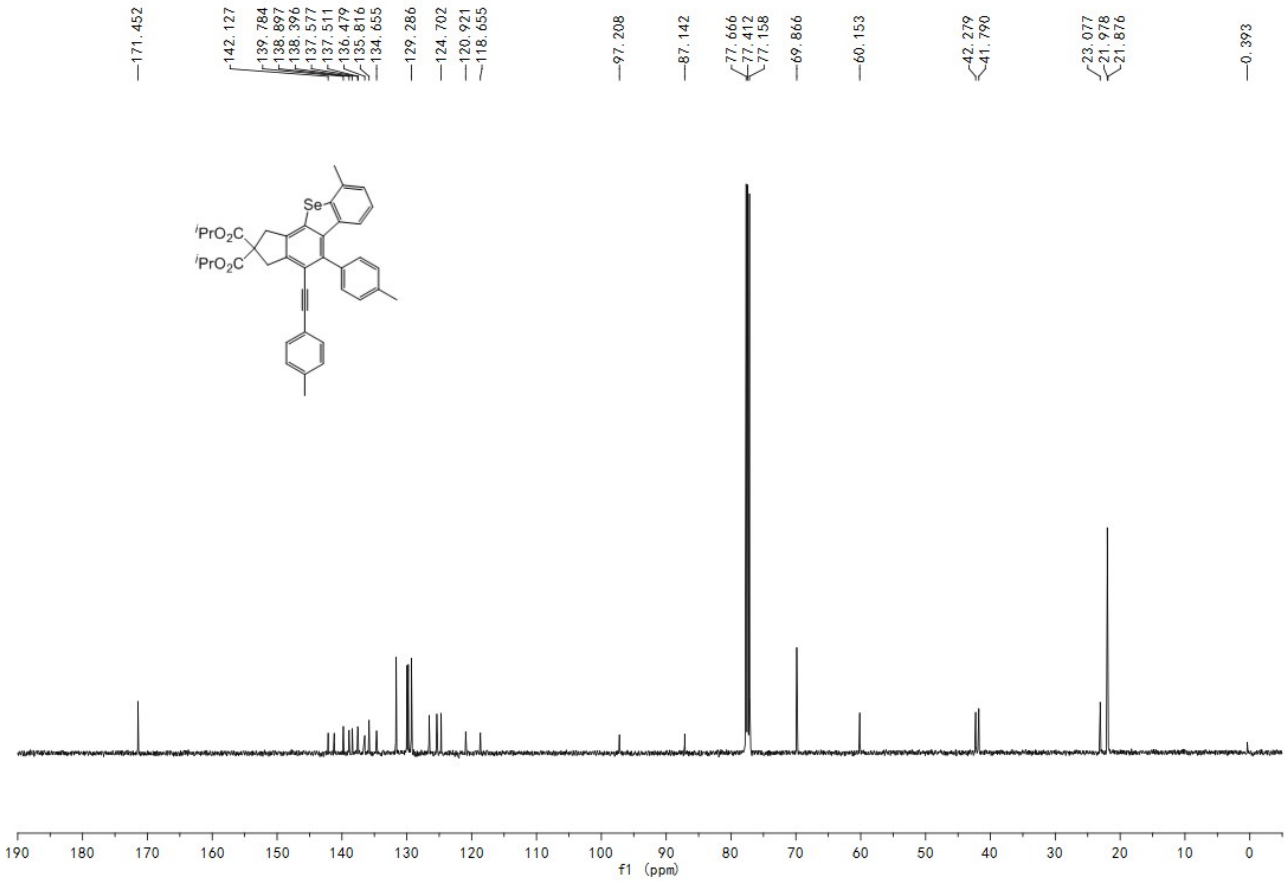
**3w**


171.464
144.736
144.090
142.283
141.187
139.639
138.888
137.826
136.459
135.812
134.657
131.757
126.554
124.697
121.139
118.703
97.335
87.222
77.676
77.422
77.169
69.877
60.151
42.264
41.757
29.351
29.223
23.097
21.987
16.499
15.826
0.404
Se
iPrO2C
iPrO2C
f1 (ppm)

**3w**


7.359
7.333
7.287
7.256
7.246
7.037
6.968
6.772
6.746
5.148
5.128
5.107
5.087
5.067
3.910
3.783
2.530
2.518
2.314
1.299
1.279
0.004
Se
iPrO2C
iPrO2C
5.47
6.05
4.24
2.19
2.08
2.14
2.07
3.37
3.23
11.82
f1 (ppm)

**3x**


171.452
142.127
139.784
138.897
138.396
137.577
137.511
136.479
135.816
134.655
129.286
124.702
120.921
118.655
97.208
87.142
77.666
77.412
77.158
69.866
60.153
42.279
41.790
23.077
21.978
21.876
0.393
Se
iPrO2C
iPrO2C
f1 (ppm)

**3x**