Supporting Information

A Palladium-Catalyzed Multi-Component Annulation Approach towards Synthesis of Phenanthrenes

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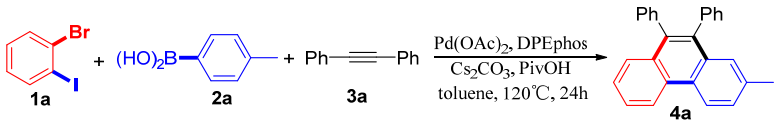
I. General Information

All reactions were carried out using pre-dried sealed tube. All solvents were dried and distilled before use according to the standard methods. Alkynes were prepared according to the literature procedures [1-5]. The 1H and 13C NMR spectra of the known compounds showed good agreement with the literature data. Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. High Resolution mass spectrometry (HRMS) data report were performed on Waters Micromass GCT Premier, ionization mode: EI+ and IonSpec 4.7 Tesla FTMS. Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum (bp. 60-90 ℃). 1H and 13C NMR data were recorded with Bruker Advance 400 MHz spectrometers with tetramethylsilane as an internal standard. All chemical shifts (δ) are reported in ppm and coupling constants (J) in Hz. The chemical shifts (δ) were given in part per million relatives to internal tetramethylsilane (0 ppm for 1H) and CDCl3 (77.0 ppm for 13C).

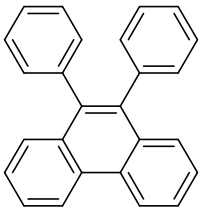
II. Experimental Procedures

Typical Procedure for the Synthesis of Phenanthrenes by Palladium-Catalyzed Cascade Reaction of o-Bromoaryl iodides with Boronic acids and Alkynes



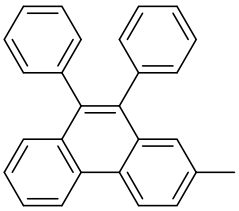
General procedure: To an oven dried sealed tube containing 4-methylphenylboronic acid (0.30 mmol, 40.8 mg) and biphenylacetylene (0.75 mmol, 133.5 mg) and $Pd(OAc)_2$ (0.015 mmol, 3.4 mg), DPEphos (0.030 mmol, 16.2 mg), PivOH (0.3 mmol, 30.6 mg), Cs_2CO_3 (0.6 mmol, 195.6 mg) was added under air atmosphere. 1-bromo-2-iodobenzene (0.30 mmol, 84.9 mg) and toluene (2.0 mL) were injected into the reaction tube via syringe. The mixture was allowed to stir at room temperature for 5 minutes and then heated to 120℃ with vigorous stirring for 24 hours. After quenched by saturated NH_4Cl solution, the reaction mixture was extracted with ethyl acetate (3 * 15 mL). The organic layers were combined, dried (Na_2SO_4) and filtered, and the solvent was removed under reduced pressure. Column chromatography on silica gel (petroleum ether) afforded the desired product 95.1 mg (92 % yield).

III. Characterization Data



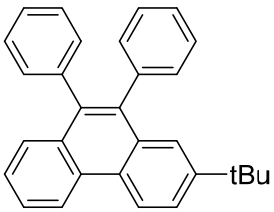
9, 10-diphenylphenanthrene (4b)[6]

White solid, 91% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.88 – 8.74 (m, 2H), 7.65 (ddd, *J* = 8.3, 6.8, 1.4 Hz, 2H), 7.60 – 7.53 (m, 2H), 7.48 (ddd, *J* = 8.2, 6.8, 1.2 Hz, 2H), 7.31 – 7.10 (m, 10H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.5, 137.2, 131.9, 131.0, 130.0, 127.8, 127.5, 126.6, 126.5, 126.4, 122.5 ppm.



2-methyl-9, 10-diphenylphenanthrene (4a)

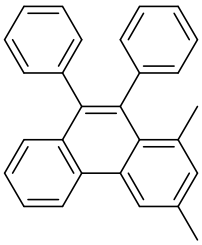
White solid, 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (d, *J* = 8.3 Hz, 1H), 8.69 (d, *J* = 8.5 Hz, 1H), 7.63 (ddd, *J* = 8.3, 6.8, 1.4 Hz, 1H), 7.57 – 7.40 (m, 3H), 7.33 (s, 1H), 7.28 – 7.07 (m, 10H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.7, 139.6, 137.2, 136.9, 136.4, 131.9, 131.5, 131.0, 130.0, 128.2, 127.8, 127.8, 127.5, 127.5, 127.3, 126.4, 126.3, 126.1, 122.4, 122.3, 21.7 ppm. HRMS: (APCI) Calcd for $C_{27}H_{21}$ $[M+H]^+$: 345.1638, found: 345.1638.



2-(tert-butyl)-9, 10-diphenylphenanthrene (4c)

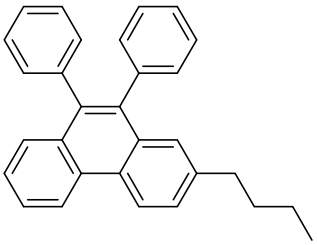
White solid, 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (d, *J* = 8.3 Hz, 1H), 8.78 (d, *J* = 8.8 Hz, 1H), 7.78 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.72 – 7.64 (m, 1H), 7.61 – 7.56 (m, 2H), 7.53 – 7.46 (m, 1H), 7.23 (dddd, *J* = 8.1, 6.4, 5.5, 1.2 Hz, 10H), 1.32 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.3, 139.7, 139.6, 137.4, 137.1, 131.6, 131.1, 131.0, 129.9, 127.7,

127.5, 127.5, 126.4, 126.3, 126.2, 124.6, 123.6, 122.3, 122.3, 34.8, 31.2 ppm. HRMS: (APCI) Calcd for $C_{30}H_{27}$ $[M+H]^+$: 387.2107, found: 387.2104.



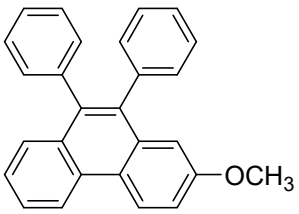
1, 3-dimethyl-9, 10-diphenylphenanthrene (4d)[7]

White solid, 88% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (d, *J* = 8.5 Hz, 1H), 8.54 (s, 1H), 7.59 (ddd, *J* = 8.4, 6.5, 1.8 Hz, 1H), 7.47 – 7.33 (m, 2H), 7.21 – 7.13 (m, 4H), 7.11 – 7.01 (m, 7H), 2.57 (s, 3H), 1.87 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.2, 140.1, 137.9, 136.7, 136.6, 135.5, 133.2, 131.6, 131.5, 131.3, 131.2, 130.1, 128.2, 127.6, 127.3, 126.9, 126.4, 126.1, 126.0, 122.9, 121.1, 25.2, 21.6 ppm.



2-butyl-9, 10-diphenylphenanthrene (4e)

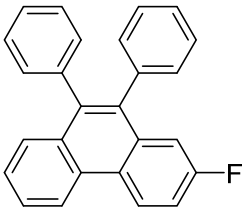
White solid, 93% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (d, *J* = 8.3 Hz, 1H), 8.71 (d, *J* = 8.5 Hz, 1H), 7.63 (ddd, *J* = 8.3, 6.8, 1.4 Hz, 1H), 7.56 – 7.48 (m, 2H), 7.47 – 7.40 (m, 1H), 7.33 (s, 1H), 7.27 – 7.10 (m, 10H), 2.71 – 2.62 (m, 2H), 1.63 – 1.55 (m, 2H), 1.32 (dd, *J* = 14.9, 7.4 Hz, 2H), 0.88 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.4, 139.7, 139.7, 137.2, 137.0, 131.9, 131.5, 131.1, 130.0, 128.0, 127.8, 127.5, 127.4, 126.8, 126.4, 126.3, 126.1, 122.4, 122.3, 35.7, 33.6, 22.3, 13.9 ppm. HRMS: (APCI) Calcd for $C_{30}H_{27}$ $[M+H]^+$: 387.2107, found: 387.2108.



2-methoxy-9, 10-diphenylphenanthrene (4f)[8]

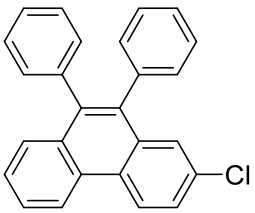
White solid, 83% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (dd, *J* = 8.7, 6.0 Hz, 2H), 7.63 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H), 7.52 (dd, *J* = 8.3, 0.9 Hz, 1H), 7.42 (ddd, *J* = 8.2, 6.9, 1.2

Hz, 1H), 7.30 (dd, *J* = 9.1, 2.7 Hz, 1H), 7.23 (ddd, *J* = 6.5, 4.3, 1.5 Hz, 4H), 7.21 – 7.17 (m, 2H), 7.17 – 7.13 (m, 4H), 6.94 (d, *J* = 2.7 Hz, 1H), 3.71 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.2, 139.6, 139.6, 137.8, 136.7, 133.3, 131.0, 130.9, 130.8, 130.1, 127.8, 127.6, 127.5, 126.5, 126.5, 126.4, 125.6, 124.4, 124.1, 122.0, 116.2, 108.8, 55.1 ppm.



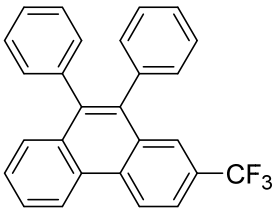
2-fluoro-9, 10-diphenylphenanthrene (4g)[8]

White solid, 81% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (dd, *J* = 9.2, 5.6 Hz, 1H), 8.72 (d, *J* = 8.3 Hz, 1H), 7.66 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H), 7.59 – 7.53 (m, 1H), 7.51 – 7.44 (m, 1H), 7.39 (ddd, *J* = 9.1, 7.9, 2.7 Hz, 1H), 7.29 – 7.09 (m, 11H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.6, 160.2, 139.2, 138.96, 138.4, 136.6, 136.6, 133.6, 133.5, 131.4, 130.8, 129.7, 128.0, 127.8, 127.6, 126.7, 126.6, 126.4, 124.8, 124.8, 122.3, 115.4, 115.1, 112.3, 112.1 ppm.



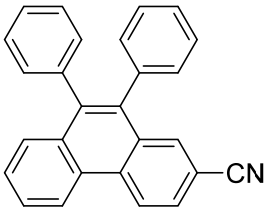
2-chloro-9, 10-diphenylphenanthrene (4h)[9]

White solid, 80% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72 (dd, *J* = 8.6, 5.7 Hz, 2H), 7.70 – 7.63 (m, 1H), 7.60 (dd, *J* = 8.9, 2.2 Hz, 1H), 7.55 (d, *J* = 7.2 Hz, 1H), 7.52 (d, *J* = 2.2 Hz, 1H), 7.51 – 7.46 (m, 1H), 7.29 – 7.16 (m, 6H), 7.15 – 7.09 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.2, 138.8, 138.5, 136.4, 133.1, 132.7, 131.8, 130.9, 130.9, 129.6, 128.4, 128.0, 127.8, 127.6, 126.9, 126.9, 126.8, 126.6, 124.2, 122.4 ppm.



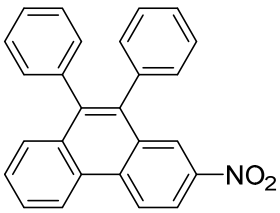
9, 10-diphenyl-2-(trifluoromethyl) phenanthrene (4i)[10]

White solid, 78% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (d, *J* = 9.0 Hz, 1H), 8.81 (d, *J* = 8.3 Hz, 1H), 7.85 (d, *J* = 7.7 Hz, 2H), 7.71 (ddd, *J* = 8.3, 6.7, 1.6 Hz, 1H), 7.64 – 7.51 (m, 2H), 7.31 – 7.18 (m, 6H), 7.17 – 7.11 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.0, 138.7, 138.4, 137.1, 132.6, 132.0, 131.4, 130.9, 130.8, 129.3, 128.5, 128.2, 128.1, 127.8, 127.7, 125.7, 125.1, 125.0, 123.4, 123.0, 122.9, 122.2, 122.2 ppm.



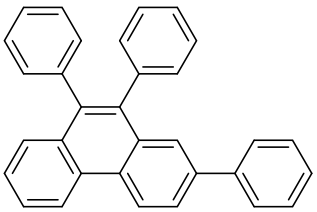
9, 10-diphenylphenanthrene-2-carbonitrile (4j)

White solid, 71% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.87 (d, *J* = 8.6 Hz, 1H), 8.79 (d, *J* = 8.4 Hz, 1H), 7.92 (d, *J* = 1.6 Hz, 1H), 7.84 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.73 (ddd, *J* = 8.3, 6.1, 2.1 Hz, 1H), 7.60 (q, *J* = 6.1 Hz, 2H), 7.33 – 7.19 (m, 6H), 7.17 – 7.08 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.2, 138.6, 138.0, 136.5, 133.10, 132.9, 132.5, 131.6, 130.8, 130.7, 129.0, 128.3, 128.2, 128.0, 127.8, 127.7, 127.2, 126.9, 123.6, 123.0, 119.4, 109.9 ppm. HRMS: (APCI) Calcd for $C_{27}H_{18}N$ $[M+H]^+$: 356.1434, found: 356.1434.



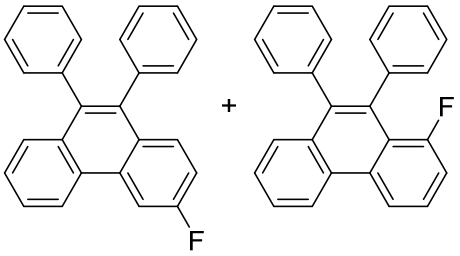
2-nitro-9, 10-diphenylphenanthrene (4k)

White solid, 82% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72 (dd, *J* = 8.6, 5.6 Hz, 2H), 7.66 (dd, *J* = 11.1, 4.1 Hz, 1H), 7.60 (dd, *J* = 8.9, 2.2 Hz, 1H), 7.55 (d, *J* = 7.4 Hz, 1H), 7.52 (d, *J* = 2.2 Hz, 1H), 7.51 – 7.46 (m, 1H), 7.30 – 7.17 (m, 6H), 7.16 – 7.08 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.2, 138.8, 138.5, 136.4, 133.1, 132.7, 131.79, 130.9, 130.9, 129.6, 128.4, 128.0, 127.8, 127.6, 126.9, 126.9, 126.8, 126.6, 124.2, 122.4 ppm.



2, 9, 10-triphenylphenanthrene (4l)

White solid, 87% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.87 (d, *J* = 8.6 Hz, 1H), 8.82 (d, *J* = 8.3 Hz, 1H), 7.92 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.80 (s, 1H), 7.72 – 7.64 (m, 1H), 7.57 (t, *J* = 7.1 Hz, 3H), 7.50 (t, *J* = 7.2 Hz, 1H), 7.41 (t, *J* = 7.2 Hz, 2H), 7.32 (t, *J* = 7.3 Hz, 1H), 7.29 – 7.13 (m, 10H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.0, 139.5, 139.3, 139.2, 137.6, 137.4, 132.2, 131.9, 131.0, 131.0, 129.8, 129.1, 128.8, 127.9, 127.6, 127.6, 127.3, 127.3, 126.6, 126.6, 126.5, 126.5, 125.9, 125.6, 123.1, 122.5 ppm. HRMS: (APCI) Calcd for $C_{32}H_{23}$ $[M+H]^+$: 407.1794, found: 407.1794.

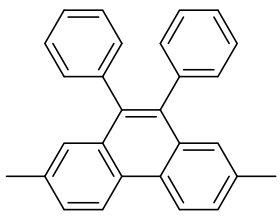


3-fluoro-9,10-diphenylphenanthrene(4na)[9]

White solid, 56% (1.6: 1) yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 8.1 Hz, 1H), 8.43 (dd, *J* = 11.1, 2.5 Hz, 1H), 7.75 – 7.66 (m, 1H), 7.63 – 7.50 (m, 3H), 7.32 – 7.21 (m, 7H), 7.20 – 7.14 (m, 4H).

1-fluoro-9,10-diphenylphenanthrene (4nb)

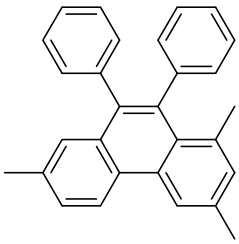
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 (d, *J* = 8.4 Hz, 1H), 8.67 (d, *J* = 8.4 Hz, 1H), 7.71 (ddd, *J* = 8.3, 5.9, 2.4 Hz, 1H), 7.64 (td, *J* = 8.1, 5.0 Hz, 1H), 7.57 – 7.49 (m, 2H), 7.32 – 7.10 (m, 11H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.3, 158.9, 141.8, 141.8, 139.2, 138.9, 133.0, 132.5, 132.0, 131.0, 129.7, 129.7, 129.3, 128.0, 127.5, 127.2, 126.8, 126.7, 126.4, 125.9, 122.9, 120.9, 120.9, 118.6, 118.6, 113.4, 113.2 ppm. HRMS: (APCI) Calcd for $C_{26}H_{18}F$ $[M+H]^+$: 349.1387, found: 349.1385.



2, 7-dimethyl-9, 10-diphenylphenanthrene (4q)

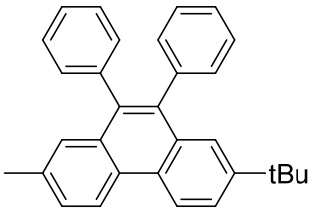
White solid, 86% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 8.4 Hz, 2H), 7.46 (dd, *J* = 8.5, 1.5 Hz, 2H), 7.30 (s, 2H), 7.26 – 7.17 (m, 6H), 7.15 – 7.10 (m, 4H), 2.40 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.8, 137.0, 135.9, 131.6, 131.1, 128.1, 127.9, 127.5,

127.2, 126.3, 122.2, 77.3, 21.7 ppm. HRMS: (APCI) Calcd for $C_{28}H_{23}$ $[M+H]^+$: 359.1794, found: 359.1794.



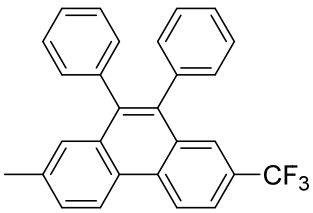
1, 3, 7-trimethyl-9, 10-diphenylphenanthrene (4r)

White solid, 89% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 8.6 Hz, 1H), 8.50 (s, 1H), 7.43 (dd, *J* = 8.5, 1.4 Hz, 1H), 7.22 – 7.11 (m, 5H), 7.11 – 7.00 (m, 7H), 2.56 (s, 3H), 2.37 (s, 3H), 1.86 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.3, 140.1, 137.7, 136.8, 136.5, 136.1, 135.4, 132.8, 131.6, 131.5, 131.3, 131.2, 128.0, 128.0, 127.8, 127.3, 127.04, 126.9, 125.9, 122.8, 120.9, 25.2, 21.6 ppm. HRMS: (APCI) Calcd for $C_{29}H_{25}$ $[M+H]^+$: 373.1591, found: 373.1590.



2-(tert-butyl)-7-methyl-9, 10-diphenylphenanthrene (4s)

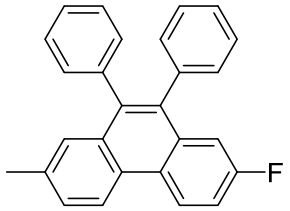
White solid, 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (dd, *J* = 12.9, 8.7 Hz, 2H), 7.71 (dd, *J* = 8.7, 2.0 Hz, 1H), 7.51 (s, 1H), 7.46 (dd, *J* = 8.5, 1.3 Hz, 1H), 7.30 (s, 1H), 7.27 – 7.10 (m, 10H), 2.41 (s, 2H), 1.27 (s, 5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.8, 139.8, 139.7, 137.5, 136.8, 135.9, 131.7, 131.2, 131.1, 131.0, 128.0, 127.8, 127.8, 127.5, 127.4, 127.2, 126.3, 124.5, 123.6, 122.3, 122.0, 34.8, 31.2, 21.7 ppm. HRMS: (APCI) Calcd for $C_{31}H_{29}$ $[M+H]^+$: 401.2264, found: 401.2265.



2-methyl-9, 10-diphenyl-7-(trifluoromethyl) phenanthrene (4t)

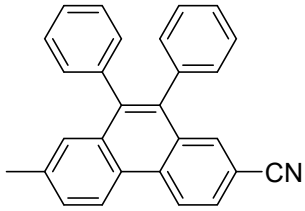
White solid, 86% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (d, *J* = 9.0 Hz, 1H), 8.69 (d, *J* = 8.5 Hz, 1H), 7.81 (d, *J* = 7.6 Hz, 2H), 7.53 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.36 (s, 1H), 7.30 –

7.18 (m, 6H), 7.17 – 7.08 (m, 4H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.1, 138.6, 138.4, 137.7, 137.2, 132.7, 132.1, 131.0, 130.9, 130.9, 128.7, 128.0, 127.8, 127.7, 127.5, 127.2, 126.9, 126.7, 125.8, 125.0, 125.0, 123.2, 122.9, 122.1, 122.1, 21.8 ppm. HRMS: (APCI) Calcd for $C_{28}H_{20}F_3$ $[M+H]^+$: 413.1512, found: 413.1506.



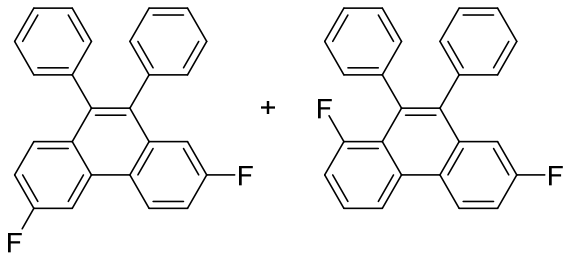
2-fluoro-7-methyl-9, 10-diphenylphenanthrene (4u)

White solid, 83% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (dd, *J* = 9.2, 5.6 Hz, 1H), 8.61 (d, *J* = 8.5 Hz, 1H), 7.50 (d, *J* = 8.5 Hz, 1H), 7.36 (ddd, *J* = 18.1, 9.8, 5.8 Hz, 2H), 7.28 – 7.07 (m, 11H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.4, 159.9, 139.3, 139.1, 138.2, 136.7, 136.2, 133.2, 133.1, 131.5, 130.9, 128.5, 127.7, 127.6, 127.4, 126.7, 126.5, 124.6, 124.5, 122.2, 115.3, 115.1, 112.3, 112.0, 21.7 ppm. HRMS: (APCI) Calcd for $C_{27}H_{20}F$ $[M+H]^+$: 363.1544, found: 363.1540.



7-methyl-9, 10-diphenylphenanthrene-2-carbonitrile (4v)

White solid, 80% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (d, *J* = 8.6 Hz, 1H), 8.66 (d, *J* = 8.5 Hz, 1H), 7.88 (d, *J* = 1.3 Hz, 1H), 7.79 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.55 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.36 (s, 1H), 7.31 – 7.18 (m, 6H), 7.16 – 7.06 (m, 4H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.9, 138.7, 138.4, 138.2, 136.6, 133.1, 133.0, 132.5, 131.2, 130.8, 130.7, 128.9, 127.9, 127.7, 127.6, 127.6, 127.1, 126.9, 126.8, 123.4, 123.0, 119.5, 109.4, 21.8 ppm. HRMS: (APCI) Calcd for $C_{28}H_{20}N$ $[M+H]^+$: 370.1590, found: 70.1588.

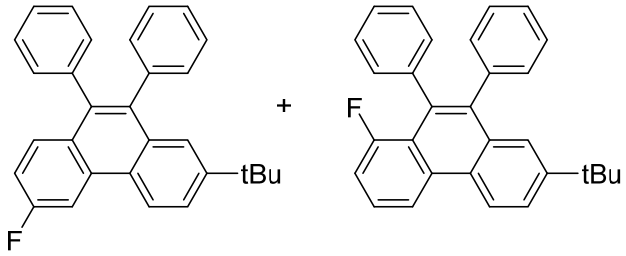


2, 6-difluoro-9, 10-diphenylphenanthrene (4wa)

White solid, 80% (1:2.1) yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (dd, *J* = 9.1, 5.5 Hz, 1H), 8.31 (dd, *J* = 11.0, 2.6 Hz, 1H), 7.54 (dd, *J* = 9.1, 6.0 Hz, 1H), 7.40 (ddd, *J* = 9.1, 7.9, 2.7 Hz, 1H), 7.30 – 7.16 (m, 8H), 7.15 – 7.09 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0, 162.9, 160.5, 160.4, 139.0, 138.7, 138.0, 135.9, 134.1, 134.0, 131.5, 131.4, 130.9, 130.8, 130.5, 130.4, 128.2, 127.8, 127.7, 126.8, 126.8, 126.0, 125.1, 125.0, 115.5, 115.4, 115.3, 115.2, 112.5, 112.3, 107.5, 107.3 ppm. HRMS: (APCI) Calcd for $C_{26}H_{17}F_2$ $[M+H]^+$: 367.1293, found: 367.1290.

1,7-difluoro-9,10-diphenylphenanthrene (4wb)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (dd, *J* = 9.2, 5.5 Hz, 1H), 8.53 (d, *J* = 8.4 Hz, 1H), 7.60 (td, *J* = 8.1, 5.1 Hz, 1H), 7.44 – 7.35 (m, 1H), 7.28 – 7.02 (m, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.9, 161.5, 160.5, 158.9, 141.5, 141.5, 138.6, 138.4, 134.3, 133.8, 132.3, 130.8, 129.6, 129.5, 127.7, 127.3, 127.1, 126.9, 126.7, 126.0, 125.4, 125.3, 120.5, 118.5, 118.4, 115.9, 115.7, 113.3, 113.0, 112.5, 112.3 ppm. HRMS: (APCI) Calcd for $C_{26}H_{17}F_2$ $[M+H]^+$: 367.1293, found: 367.1290.



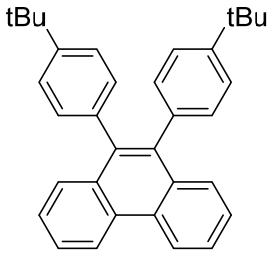
2-(tert-butyl)-6-fluoro-9, 10-diphenylphenanthrene (4xa)

White solid, 84% (1:1.3) yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (d, *J* = 8.7 Hz, 1H), 8.36 (dd, *J* = 11.0, 2.6 Hz, 1H), 7.73 (dd, *J* = 8.7, 2.0 Hz, 1H), 7.57 – 7.47 (m, 2H), 7.31 – 7.09 (m, 11H), 1.27 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.7, 160.2, 150.1, 139.5, 139.3, 136.7, 132.1, 131.6, 131.5, 131.0, 130.1, 130.1, 128.4, 127.6, 127.5, 127.2, 127.2, 126.5, 126.5, 124.7, 123.7, 122.5, 115.1, 114.9, 107.4, 107.2, 34.9, 31.2 ppm. HRMS: (APCI) Calcd for $C_{30}H_{26}F$ $[M+H]^+$: 405.2013, found: 405.2011.

7-(tert-butyl)-1-fluoro-9,10-diphenylphenanthrene (4xb)

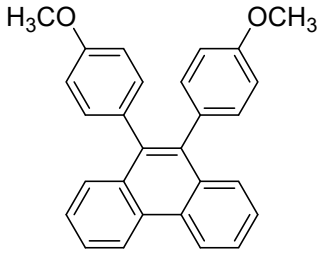
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 8.8 Hz, 1H), 8.58 (d, *J* = 8.3 Hz, 1H), 7.73 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.56 (td, *J* = 8.1, 5.0 Hz, 1H), 7.44 (d, *J* = 1.9 Hz, 1H), 7.15 (dddd, *J* = 15.3, 11.3, 10.3, 6.9 Hz, 1H), 1.25 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.4, 158.9,

150.1, 142.0, 1412.0, 139.4, 139.0, 132.9, 132.5, 132.4, 131.9, 130.9, 129.8, 129.7, 127.4, 127.1, 126.8, 126.7, 126.6, 126.4, 125.8, 125.1, 123.8, 122.7, 120.7, 120.6, 118.5, 118.5, 113.0, 1128, 34.8, 31.1 ppm. HRMS: (APCI) Calcd for $C_{30}H_{26}F$ $[M+H]^+$: 405.2013, found: 405.2013.



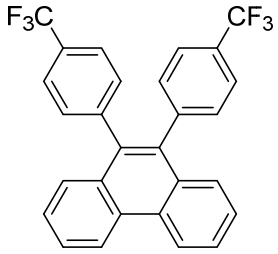
9, 10-bis (4-(tert-butyl) phenyl) phenanthrene (6a)[6]

White solid, 88% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (d, *J* = 8.3 Hz, 2H), 7.71 (d, *J* = 8.2 Hz, 2H), 7.68 – 7.60 (m, 2H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.18 (d, *J* = 8.3 Hz, 4H), 7.01 (d, *J* = 8.3 Hz, 4H), 1.26 (s, 18H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.9, 137.6, 136.5, 131.9, 130.7, 129.9, 127.9, 126.5, 126.2, 124.1, 122.4, 34.4, 31.3 ppm.



9, 10-bis (4-methoxyphenyl) phenanthrene (6b)[8]

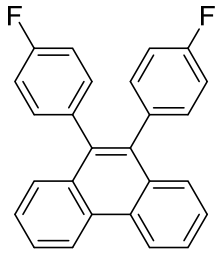
White solid, 86% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, *J* = 8.3 Hz, 2H), 7.64 (t, *J* = 7.6 Hz, 2H), 7.59 (d, *J* = 7.8 Hz, 2H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.05 (d, *J* = 8.6 Hz, 4H), 6.79 (d, *J* = 8.6 Hz, 4H), 3.79 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.9, 137.1, 132.3, 132.0, 131.9, 129.9, 127.8, 126.5, 126.2, 122.4, 113.1, 55.1 ppm.



9, 10-bis (4-(trifluoromethyl) phenyl) phenanthrene (6c)[8]

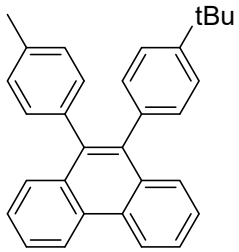
White solid, 80% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 (d, *J* = 8.4 Hz, 2H), 7.71 (t, *J* = 7.6 Hz, 2H), 7.52 (t, *J* = 6.7 Hz, 6H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.32 – 7.23 (m, 4H). ^{13}C

NMR (101 MHz, $CDCl_3$) δ 1423.0, 135.9, 131.3, 131.0, 130.2, 129.3, 129.0, 127.5, 127.1, 124.9, 124.8, 122.7 ppm.



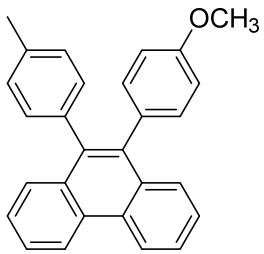
9, 10-bis (4-fluorophenyl) phenanthrene (6d)[8]

White solid, 83% yield. ^1H NMR (400 MHz, $CDCl_3$) δ 8.80 (d, J = 8.4 Hz, 2H), 7.67 (ddd, J = 8.3, 6.0, 2.2 Hz, 2H), 7.58 – 7.43 (m, 4H), 7.15 – 7.03 (m, 4H), 6.95 (t, J = 8.6 Hz, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.8, 160.3, 136.5, 135.3, 135.3, 132.5, 132.4, 131.7, 130.1, 127.6, 126.8, 126.6, 122.6, 114.9, 114.7 ppm.



9-(4-(tert-butyl) phenyl)-10-(p-tolyl) phenanthrene (6e)

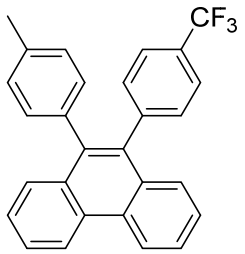
White solid, 88% yield. ^1H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, J = 8.3 Hz, 2H), 7.62 (dd, J = 16.3, 8.2 Hz, 4H), 7.53 – 7.41 (m, 2H), 7.28 – 7.19 (m, 2H), 7.10 – 6.99 (m, 6H), 2.30 (s, 3H), 1.29 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.1, 137.3, 137.2, 136.6, 136.5, 135.6, 132.1, 130.9, 130.7, 129.9, 128.2, 128.0, 127.9, 126.5, 126.2, 124.3, 122.4, 122.4, 34.43, 31.4, 21.2 ppm. HRMS: (APCI) Calcd for $C_{31}H_{29}$ $[M+H]^+$: 401.2264, found: 401.2261.



9-(4-methoxyphenyl)-10-(p-tolyl) phenanthrene (6f)

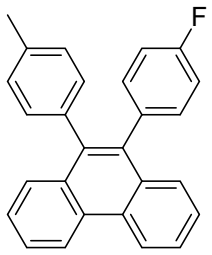
White solid, 87% yield. ^1H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, J = 8.2 Hz, 2H), 7.64 (t, J = 7.5 Hz, 2H), 7.60 – 7.53 (m, 2H), 7.47 (dd, J = 11.3, 7.0 Hz, 2H), 7.11 – 6.99 (m, 4H),

6.79 (d, J = 8.5 Hz, 2H), 3.79 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.9, 137.5, 136.8, 136.6, 135.8, 132.3, 132.1, 132.0, 132.0, 130.8, 129.9, 128.4, 127.9, 127.8, 126.5, 126.2, 122.4, 113.0, 55.1, 21.2 ppm. HRMS: (APCI) Calcd for $C_{28}H_{23}O$ $[M+H]^+$: 375.1743, found: 375.1741.



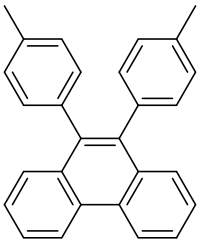
9-(p-tolyl)-10-(4-(trifluoromethyl) phenyl) phenanthrene (6g)

White solid, 81% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (dd, J = 8.2, 3.2 Hz, 2H), 7.66 (t, J = 7.6 Hz, 2H), 7.58 (d, J = 8.3 Hz, 1H), 7.53 – 7.45 (m, 4H), 7.41 (d, J = 8.2 Hz, 1H), 7.27 (d, J = 7.9 Hz, 2H), 7.02 (dd, J = 18.9, 7.9 Hz, 4H), 2.31 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.7, 137.5, 136.3, 135.8, 135.7, 131.9, 131.4, 131.3, 130.7, 130.1, 130.0, 128.8, 128.5, 128.0, 127.3, 126.8, 126.7, 126.7, 126.5, 124.6, 124.6, 122.6, 122.5, 21.2 ppm. HRMS: (APCI) Calcd for $C_{28}H_{20}F_3$ $[M+H]^+$: 413.1512, found: 413.1512.



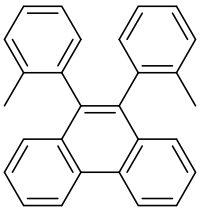
9-(4-fluorophenyl)-10-(p-tolyl) phenanthrene (6h)

White solid, 85% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (d, J = 8.3 Hz, 2H), 7.66 (t, J = 7.3 Hz, 2H), 7.57 (d, J = 8.2 Hz, 1H), 7.50 (dd, J = 12.8, 5.9 Hz, 3H), 7.11 (dd, J = 8.3, 5.6 Hz, 2H), 7.06 (d, J = 7.9 Hz, 2H), 7.00 (d, J = 8.0 Hz, 2H), 6.94 (t, J = 8.8 Hz, 2H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.7, 160.2, 137.6, 136.3, 136.1, 136.0, 135.6, 135.5, 132.5, 132.5, 131.9, 131.9, 130.7, 130.0, 129.9, 128.4, 127.9, 127.5, 126.6, 126.6, 126.5, 126.4, 122.5, 122.4, 114.7, 114.5, 21.2 ppm. HRMS: (APCI) Calcd for $C_{27}H_{20}F$ $[M+H]^+$: 363.1544, found: 363.1544.



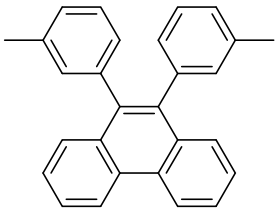
9, 10-di-p-tolylphenanthrene (6i)[8]

White solid, 83% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 (dd, *J* = 8.3, 0.5 Hz, 2H), 7.68 (ddd, *J* = 8.3, 6.8, 1.4 Hz, 2H), 7.60 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.50 (ddd, *J* = 8.2, 6.8, 1.2 Hz, 2H), 7.13 – 7.03 (m, 8H), 2.36 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.2, 136.6, 135.8, 132.2, 130.8, 129.9, 128.3, 127.8, 126.5, 126.2, 122.4, 21.25 ppm.



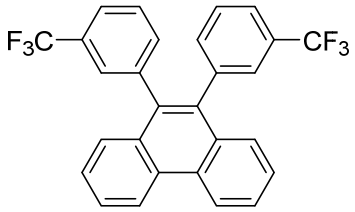
9, 10-di-o-tolylphenanthrene (6j)[11]

White solid, 64% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (d, *J* = 8.3 Hz, 2H), 7.76 – 7.66 (m, 2H), 7.57 – 7.47 (m, 2H), 7.40 (dd, *J* = 8.3, 1.1 Hz, 2H), 7.25 – 7.07 (m, 8H), 1.97 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.2, 136.7, 136.6, 132.3, 131.7, 129.9, 129.6, 127.4, 127.0, 126.8, 126.4, 124.7, 122.6, 20.0 ppm.



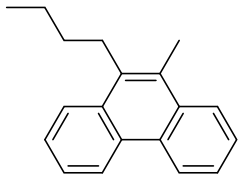
9, 10-di-m-tolylphenanthrene (6k)[12]

White solid, 78% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (d, *J* = 8.3 Hz, 2H), 7.69 (ddd, *J* = 8.3, 6.9, 1.3 Hz, 2H), 7.62 (d, *J* = 8.3 Hz, 2H), 7.57 – 7.47 (m, 2H), 7.17 (td, *J* = 7.5, 3.2 Hz, 2H), 7.08 – 6.96 (m, 6H), 2.30 (d, *J* = 3.2 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.4, 137.2, 136.9, 136.8, 131.9, 131.8, 131.7, 129.9, 128.1, 128.0, 127.9, 127.3, 127.3, 127.1, 127.1, 126.5, 126.2, 122.4, 21.4, 21.3 ppm.



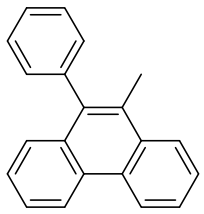
9, 10-bis (3-(trifluoromethyl) phenyl) phenanthrene (6l)

White solid, 62% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.87 (d, *J* = 8.3 Hz, 2H), 7.76 (t, *J* = 6.7 Hz, 2H), 7.57 (dd, *J* = 12.8, 5.5 Hz, 4H), 7.54 – 7.31 (m, 8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.9, 136.3, 134.3, 134.0, 131.0, 130.2, 128.3, 128.0, 127.7, 127.4, 127.1, 123.6, 122.7 ppm. HRMS: (APCI) Calcd for $C_{28}H_{16}F_6$ $[M+H]^+$: 467.1229, found: 467.1230.



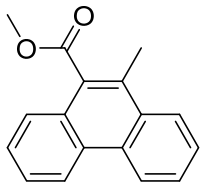
9-butyl-10-methylphenanthrene (6m)[13]

White solid, 76% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (dd, *J* = 7.5, 5.3 Hz, 2H), 8.23 – 8.06 (m, 2H), 7.77 – 7.57 (m, 4H), 3.33 – 3.10 (m, 2H), 2.77 (d, *J* = 1.8 Hz, 3H), 1.78 – 1.67 (m, 2H), 1.61 (dd, *J* = 14.5, 7.6 Hz, 2H), 1.06 (td, *J* = 7.2, 1.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 134.2, 132.2, 131.4, 129.7, 129.4, 129.0, 126.6, 126.5, 125.4, 125.3, 124.6, 124.5, 122.9, 122.7, 32.4, 29.3, 23.3, 15.6, 14.1 ppm.



9-methyl-10-phenylphenanthrene (6n)[14]

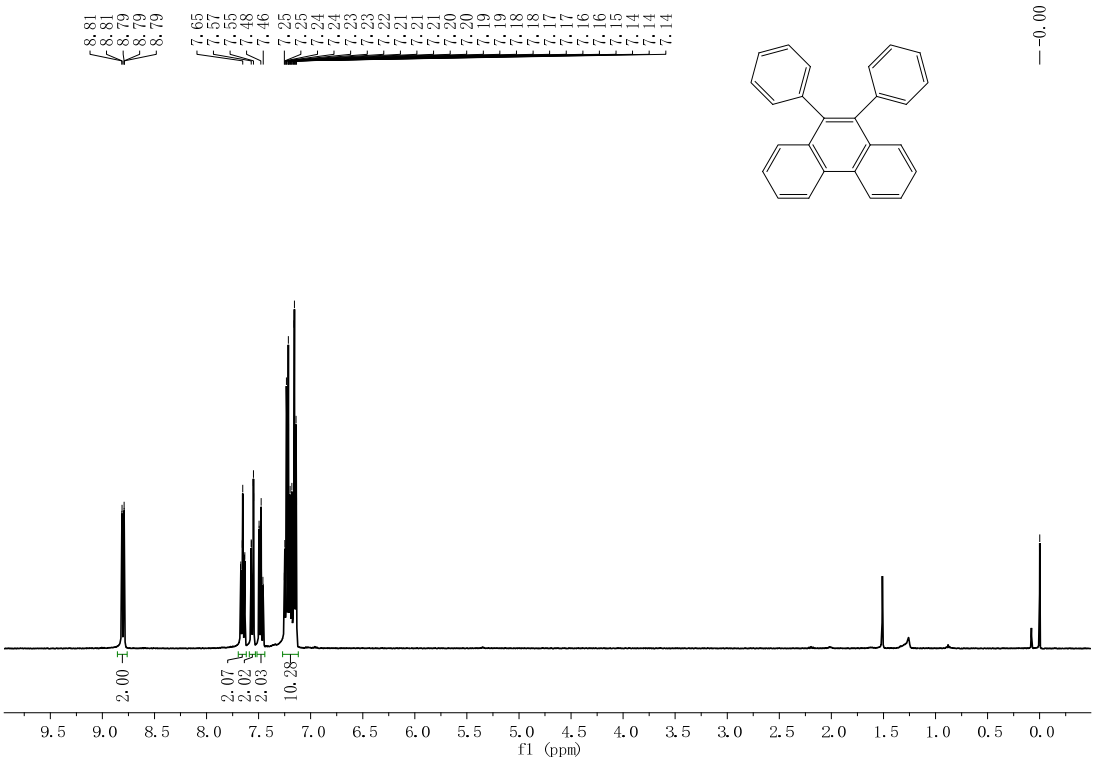
White solid, 57% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.88 – 8.74 (m, 2H), 8.29 – 8.15 (m, 1H), 7.87 – 7.69 (m, 2H), 7.68 – 7.55 (m, 3H), 7.48 (ddd, *J* = 22.1, 14.4, 7.6 Hz, 4H), 7.36 (d, *J* = 7.6 Hz, 2H), 7.31 – 7.16 (m, 2H), 2.52 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.5, 140.7, 137.0, 132.3, 131.9, 130.6, 130.3, 129.9, 129.9, 129.8, 129.3, 128.4, 127.8, 127.4, 127.0, 126.8, 126.4, 126.33, 126.2, 125.6, 125.1, 122.8, 122.3, 17.3 ppm.

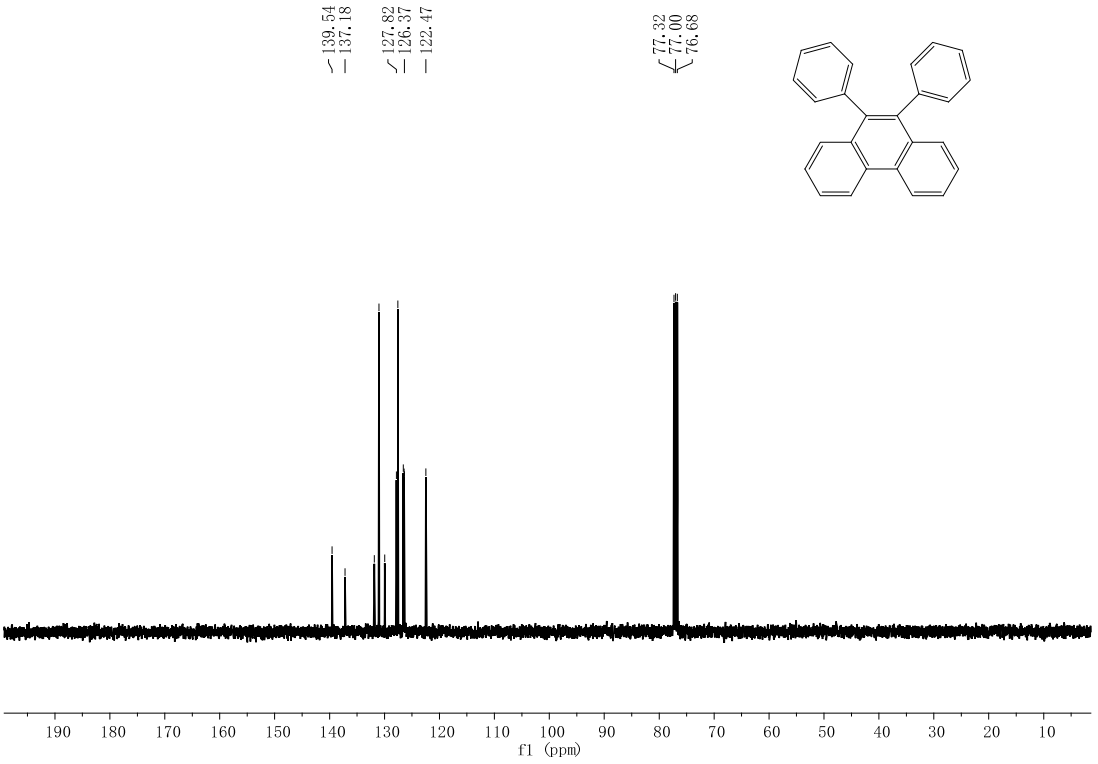


Methyl 10-methylphenanthrene-9-carboxylate (6o)[15]

White solid, 30% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (dd, *J* = 12.8, 7.9 Hz, 2H), 8.16 (d, *J* = 7.6 Hz, 1H), 7.69 (ddd, *J* = 21.9, 15.4, 7.5 Hz, 5H), 4.12 (s, 3H), 2.73 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.8, 130.9, 130.4, 130.1, 129.8, 129.4, 128.1, 127.3, 127.1, 127.0, 126.4, 125.2, 125.1, 122.95, 122.7, 52.4, 17.2 ppm.

Ⅳ. Copies of Product 1H NMR and 13C NMR

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77.00
76.68
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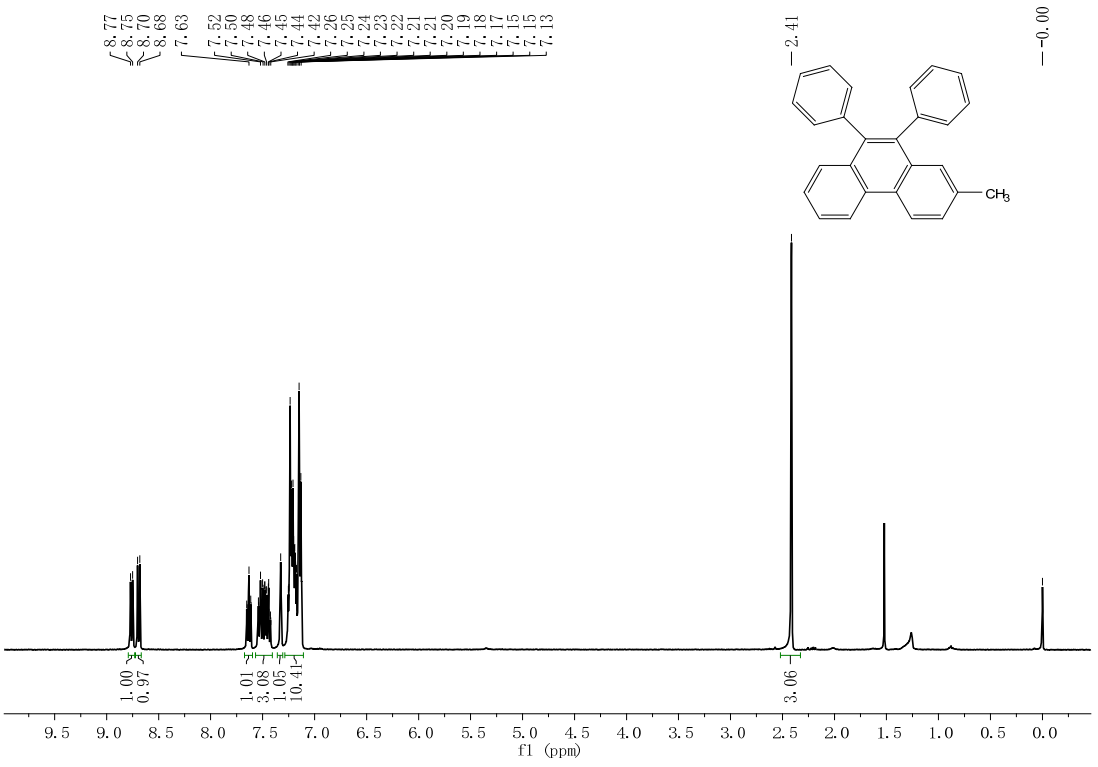
f1 (ppm)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7.48
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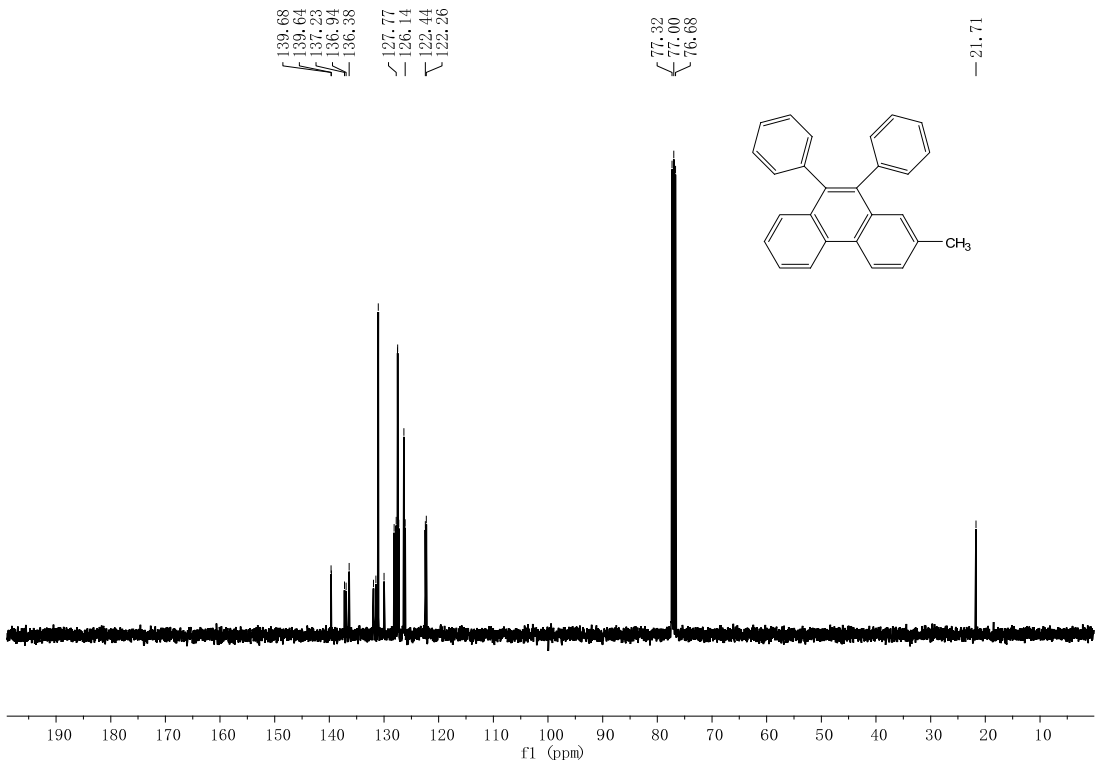
7.25
7.24
7.23
7.22
7.21
7.21
7.20
7.19
7.18
7.17
7.15
7.15
7.13
2.41
-0.00
CH3
1.00
0.97
1.01
3.08
1.05
10.41
3.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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21.71
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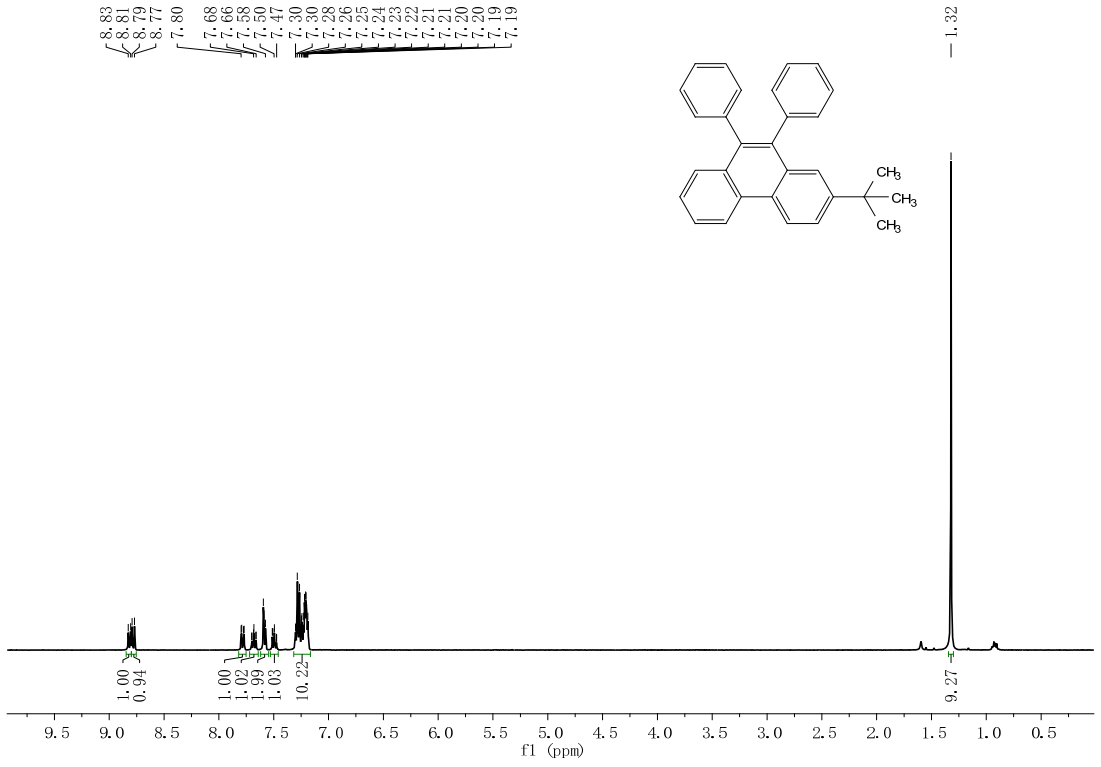
f1 (ppm)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7.25
7.24
7.23
7.22
7.21
7.21
7.20
7.20
7.19
7.19
1.32
CH3
CH3
CH3
1.00
0.94
1.00
1.02
1.99
1.03
10.22
9.27
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
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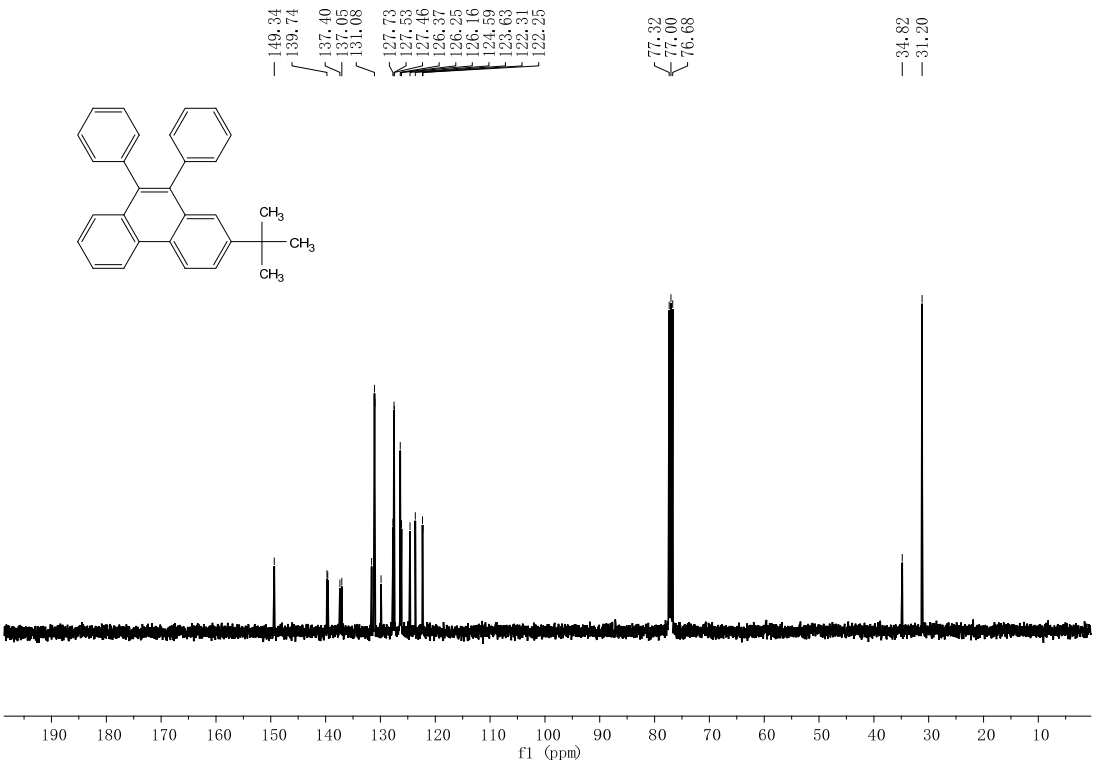
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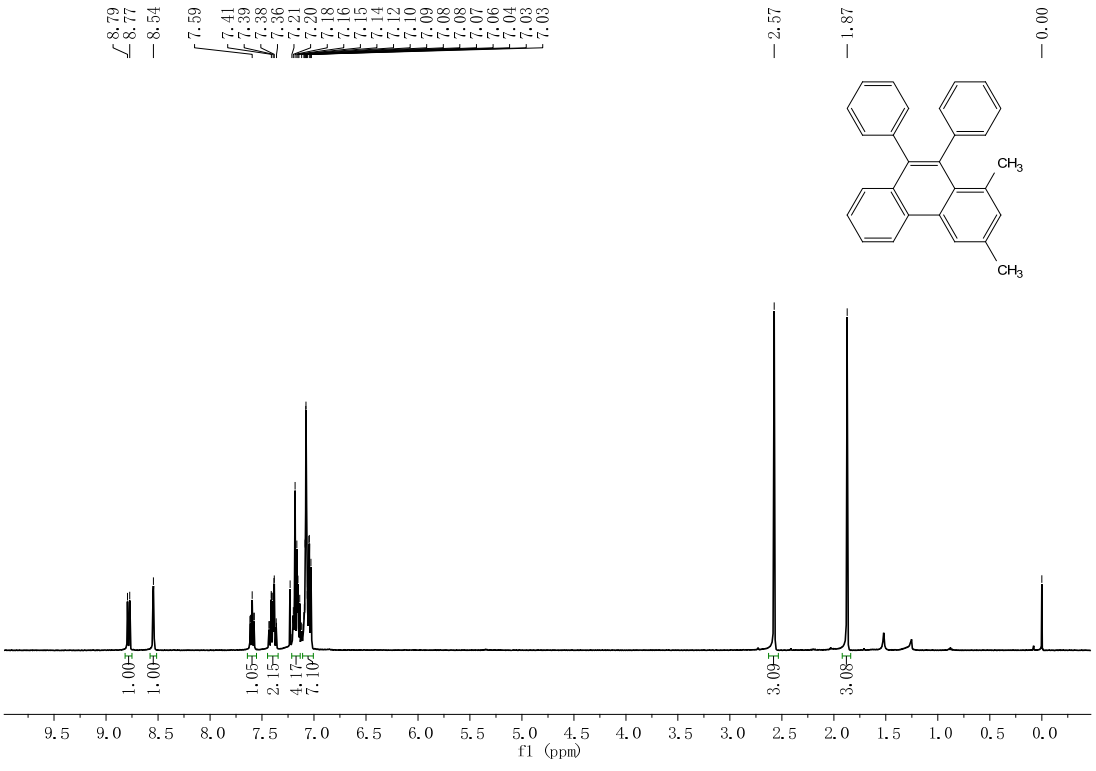
122.25
77.32
77.00
76.68
34.82
31.20
CH3
CH3
CH3
f1 (ppm)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7.36
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7.15
7.14
7.12
7.10
7.09
7.08
7.08
7.07
7.06
7.04
7.03
7.03
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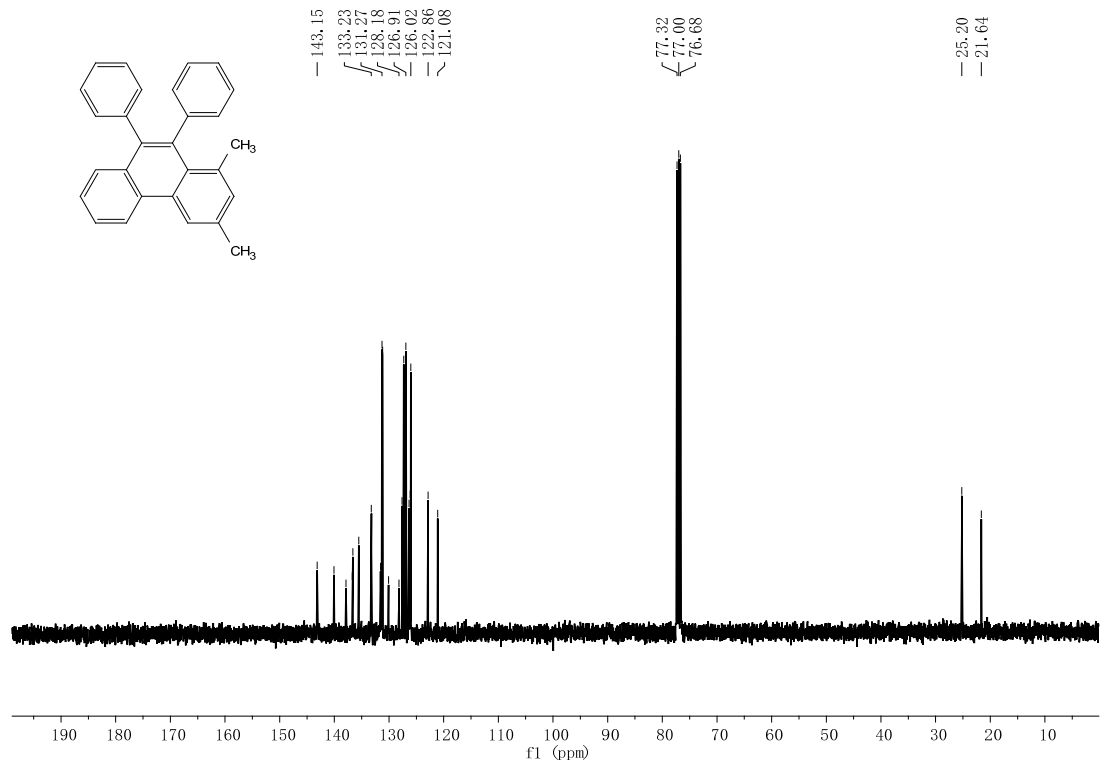
7.10
3.09
3.08
f1 (ppm)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121.08
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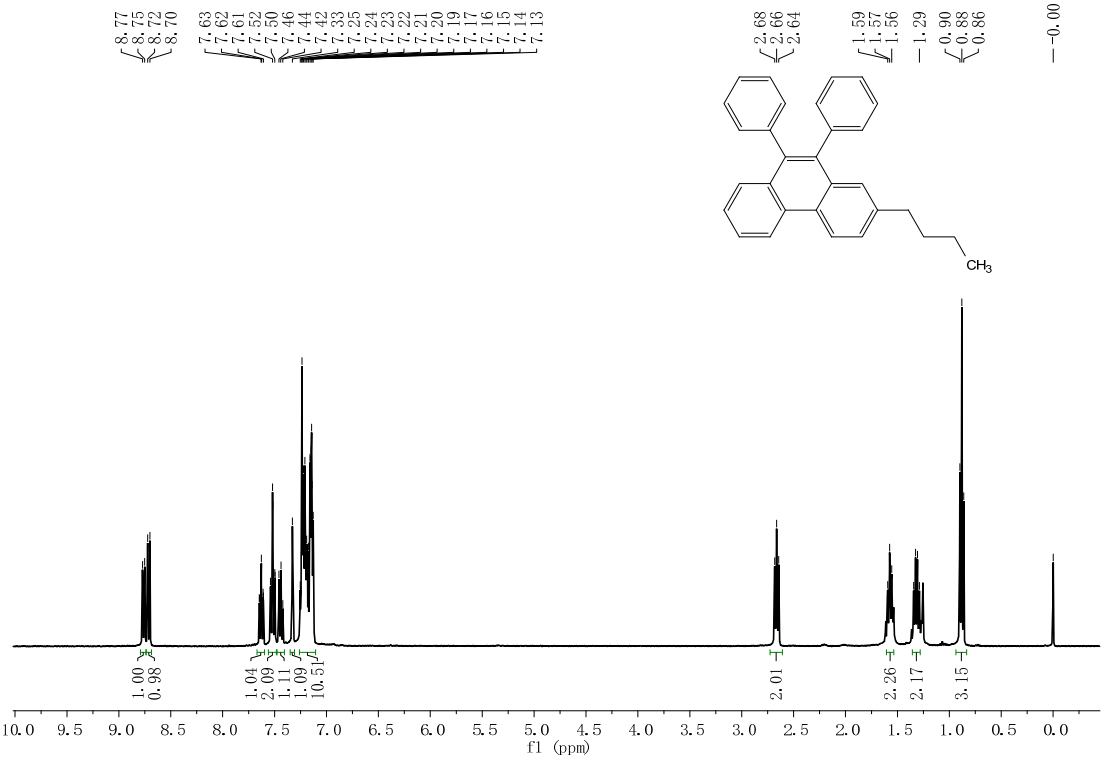
25.20
21.64
CH3
CH3
f1 (ppm)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7.33
7.25
7.24
7.23
7.22
7.21
7.20
7.19
7.17
7.16
7.15
7.14
7.13
2.68
2.66
2.64
1.59
1.57
1.56
1.29
0.90
0.88
0.86
0.00
CH3
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1.09
10.51
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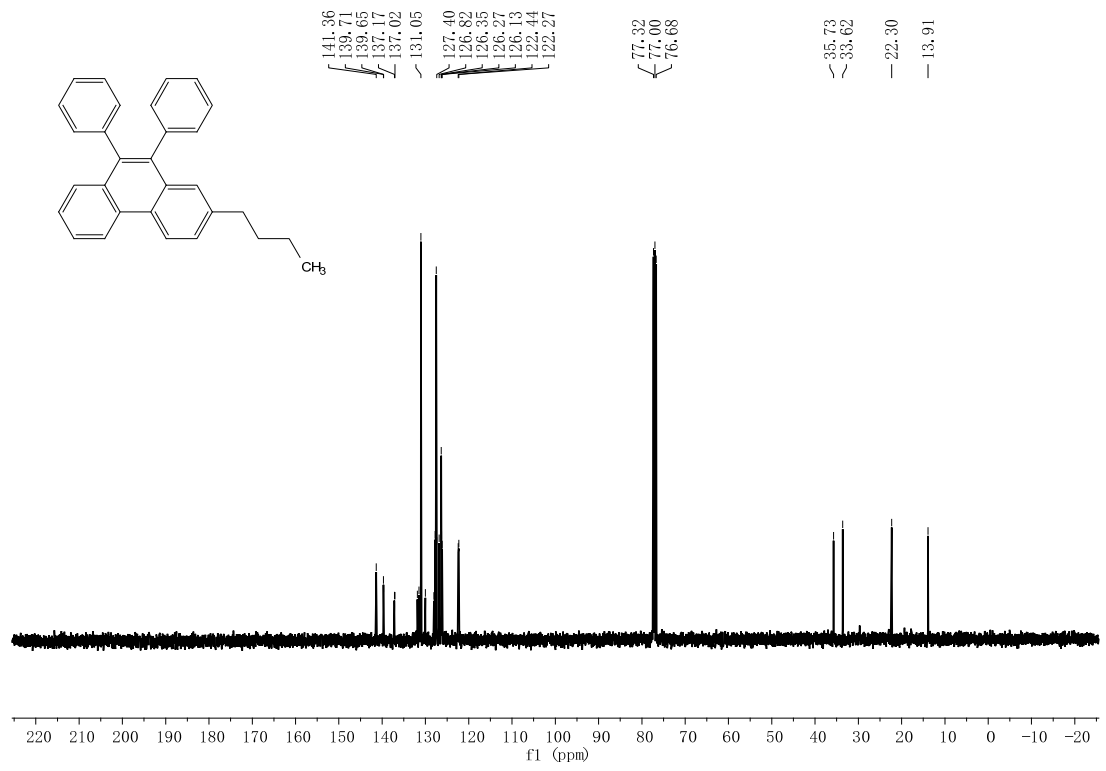
2.26
2.17
3.15
f1 (ppm)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77.32
77.00
76.68
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33.62
22.30
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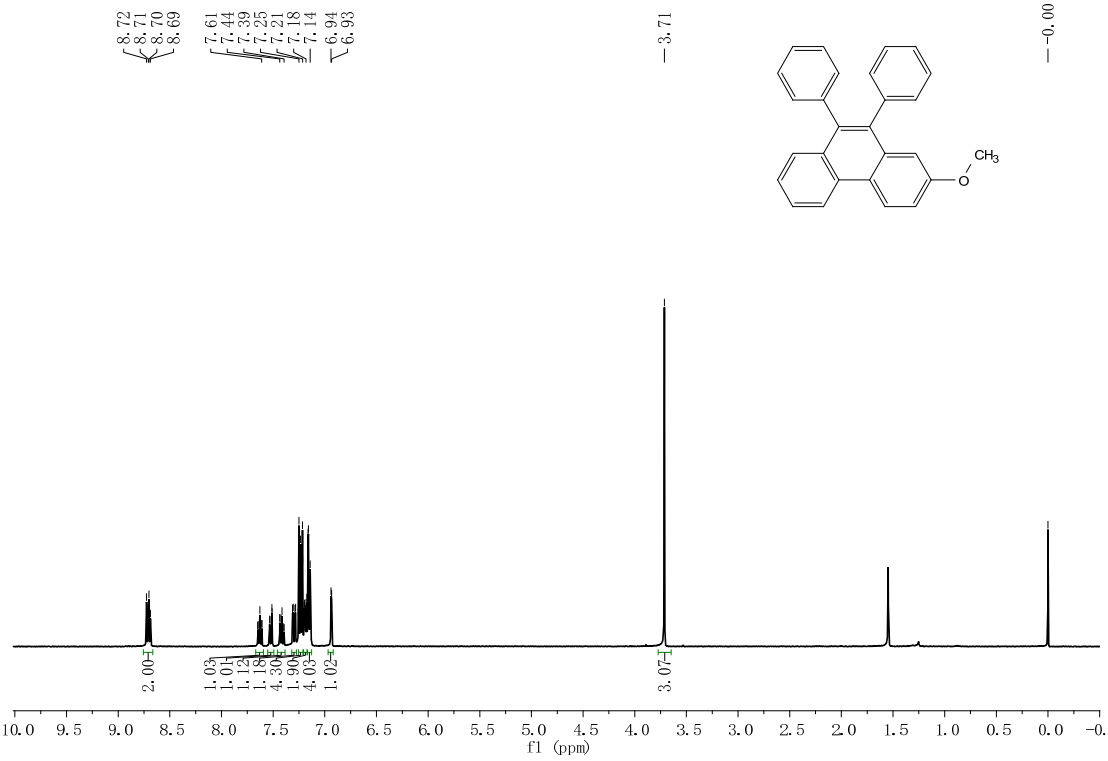
CH3
f1 (ppm)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7.14
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6.93
3.71
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1.18
4.30
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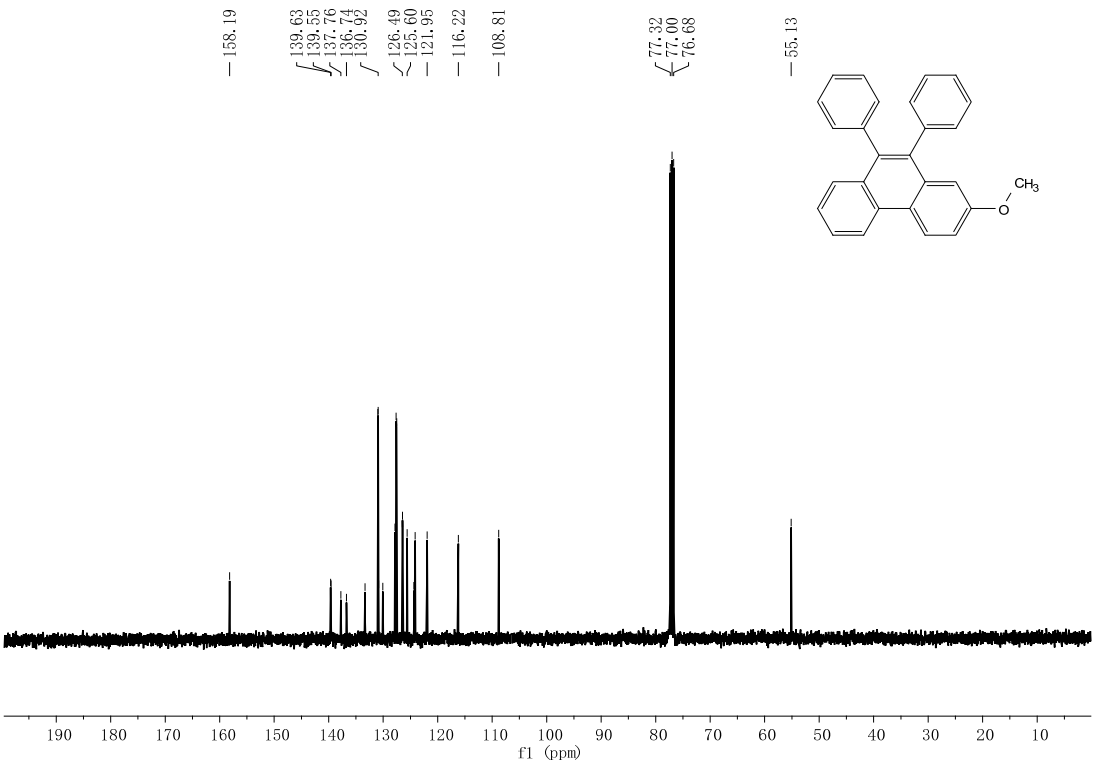
4.05
1.02
3.07
f1 (ppm)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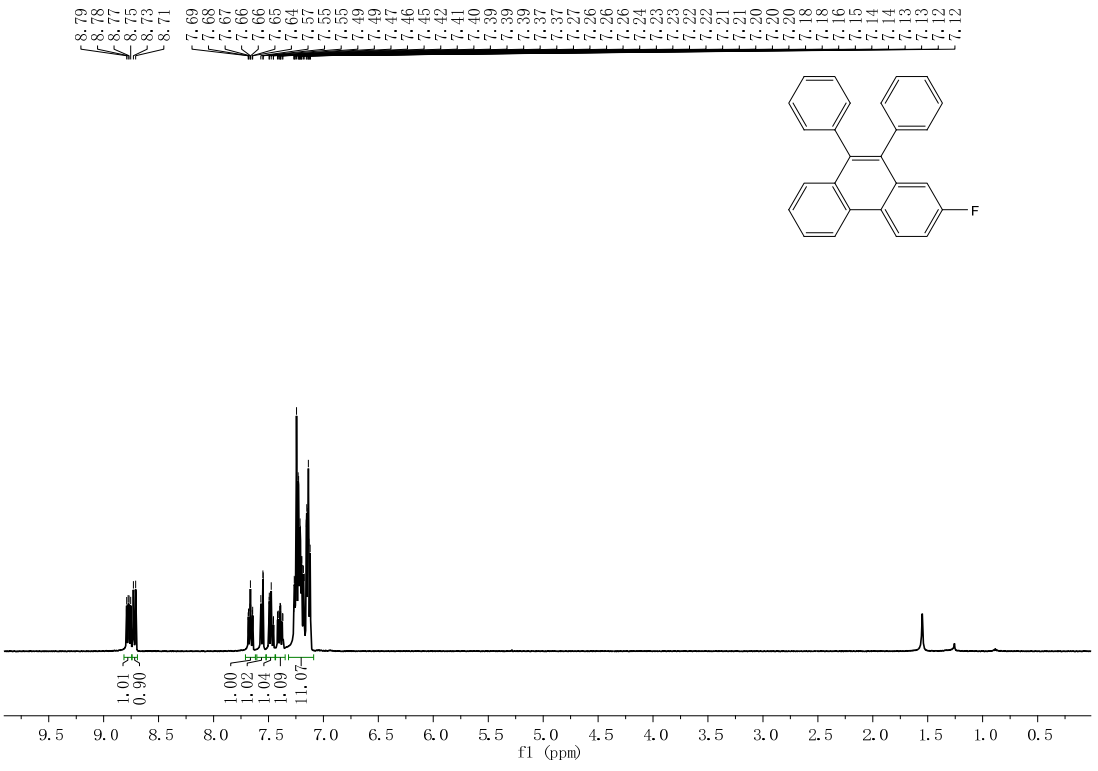
55.13
CH3
O
f1 (ppm)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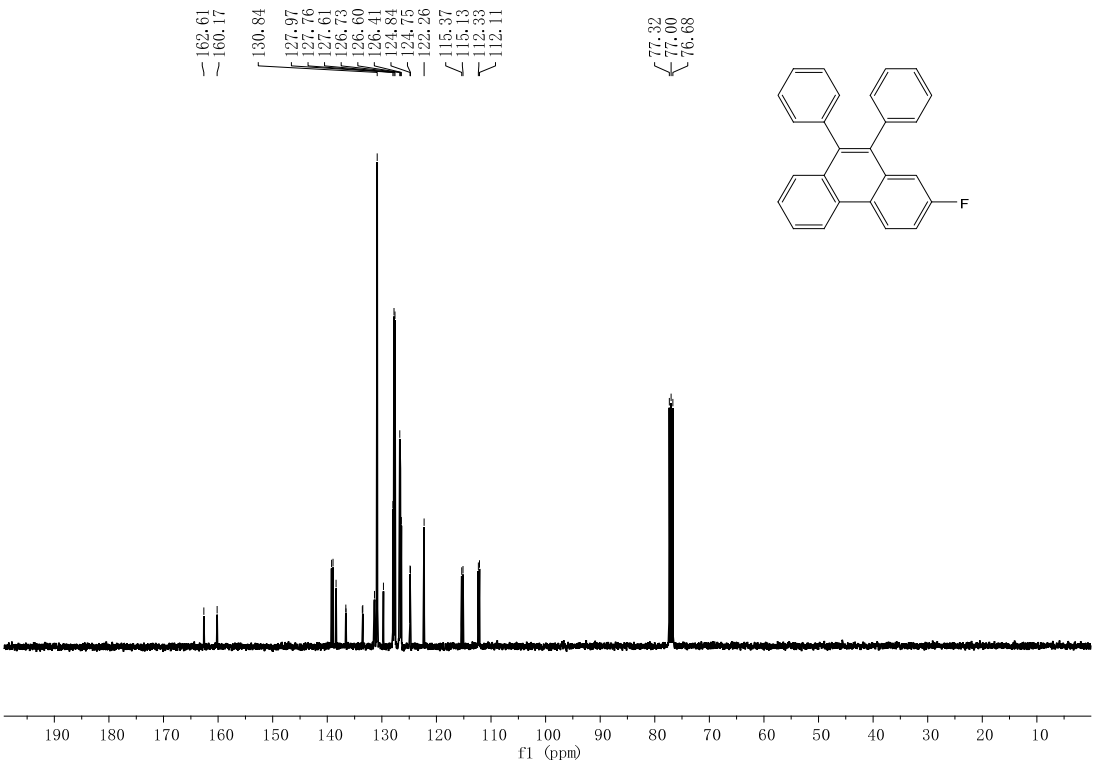
f1 (ppm)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124.75
122.26
115.37
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77.32
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76.68
F
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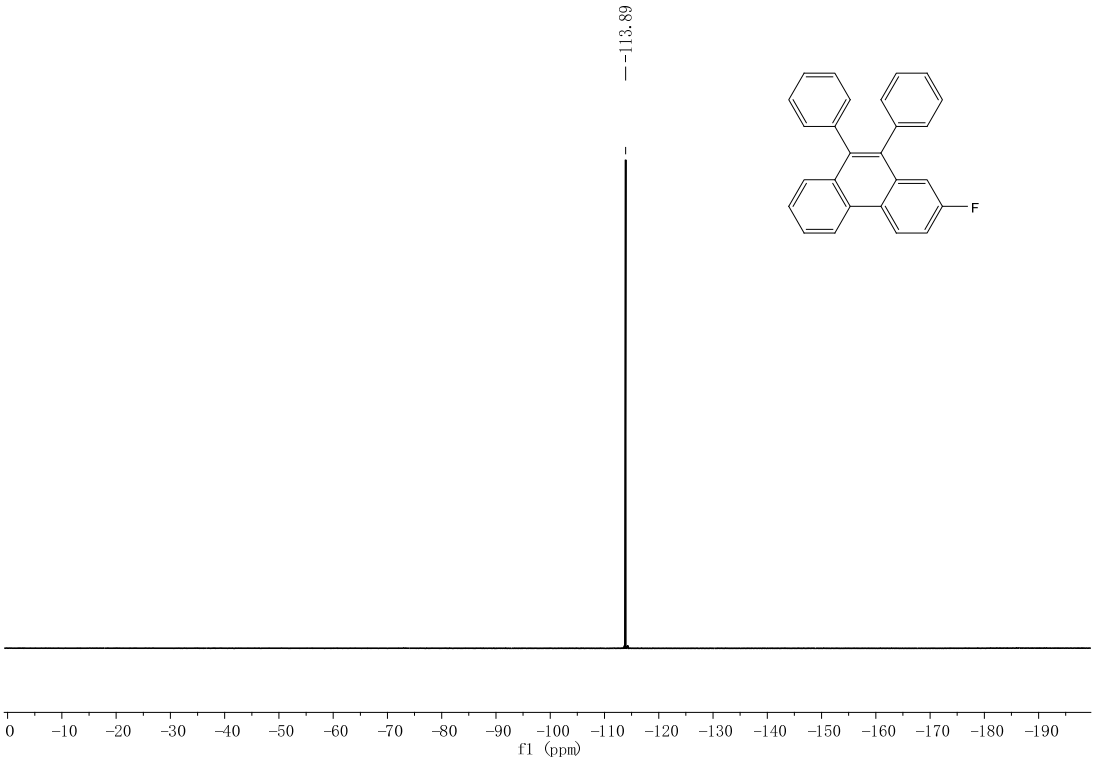
f1 (ppm)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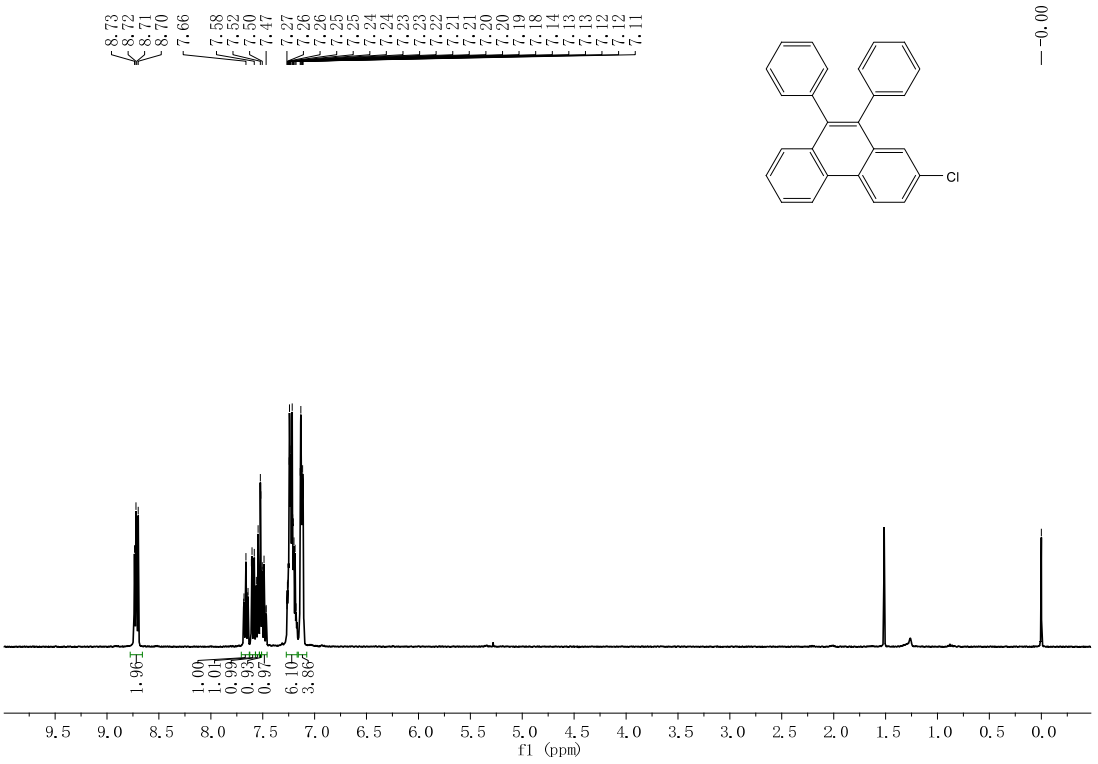
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7.20
7.19
7.18
7.14
7.13
7.13
7.12
7.12
7.11
-0.00
Cl
1.96
1.00
1.01
0.99
0.93
0.97
6.10
3.86
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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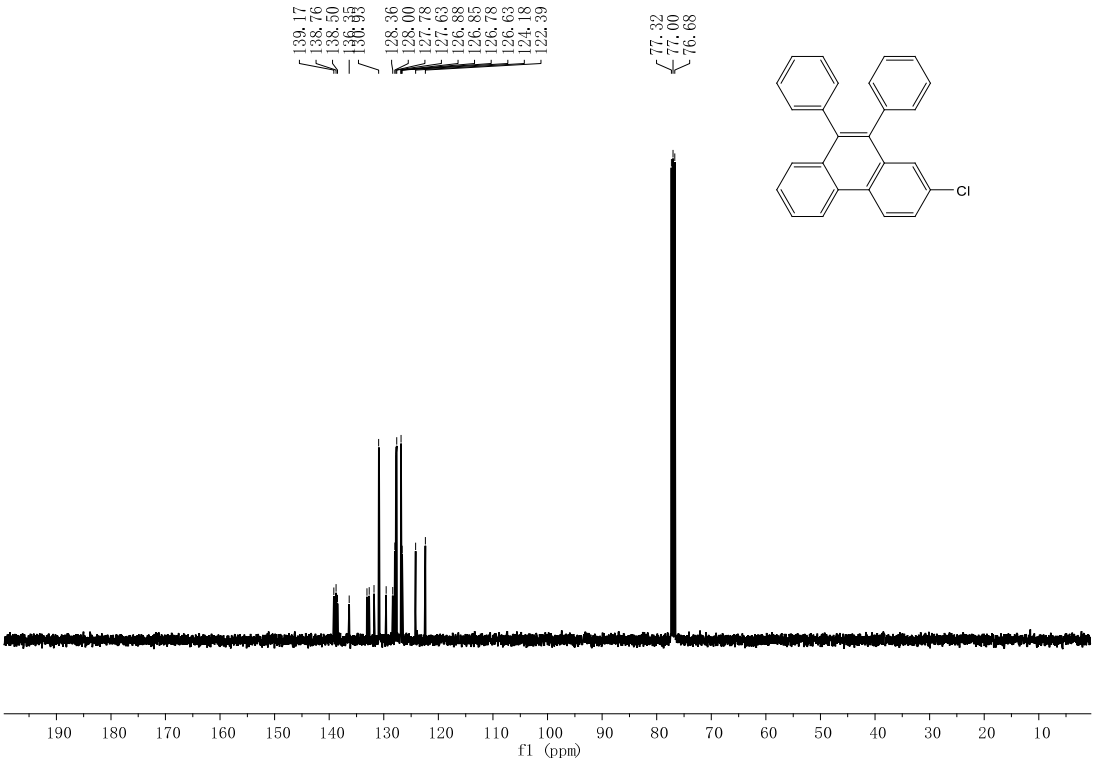
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77.00
76.68
Cl
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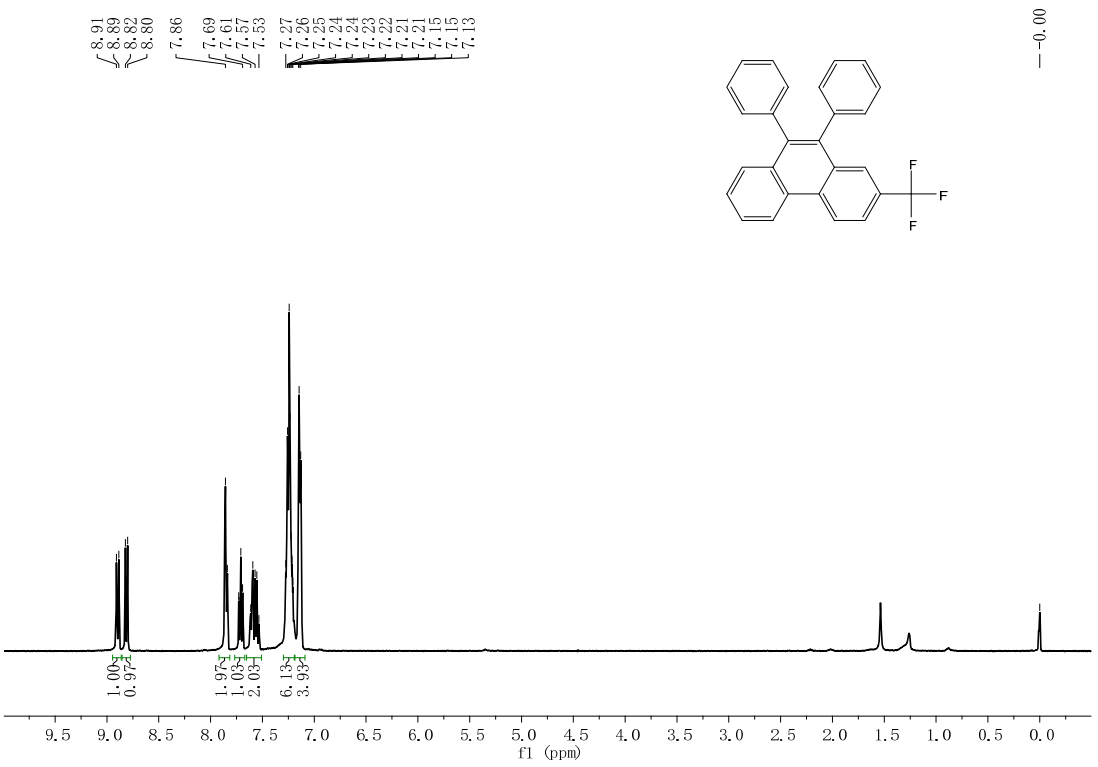
f1 (ppm)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-0.00
F
F
F
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1.97
1.03
2.03
6.13
3.93
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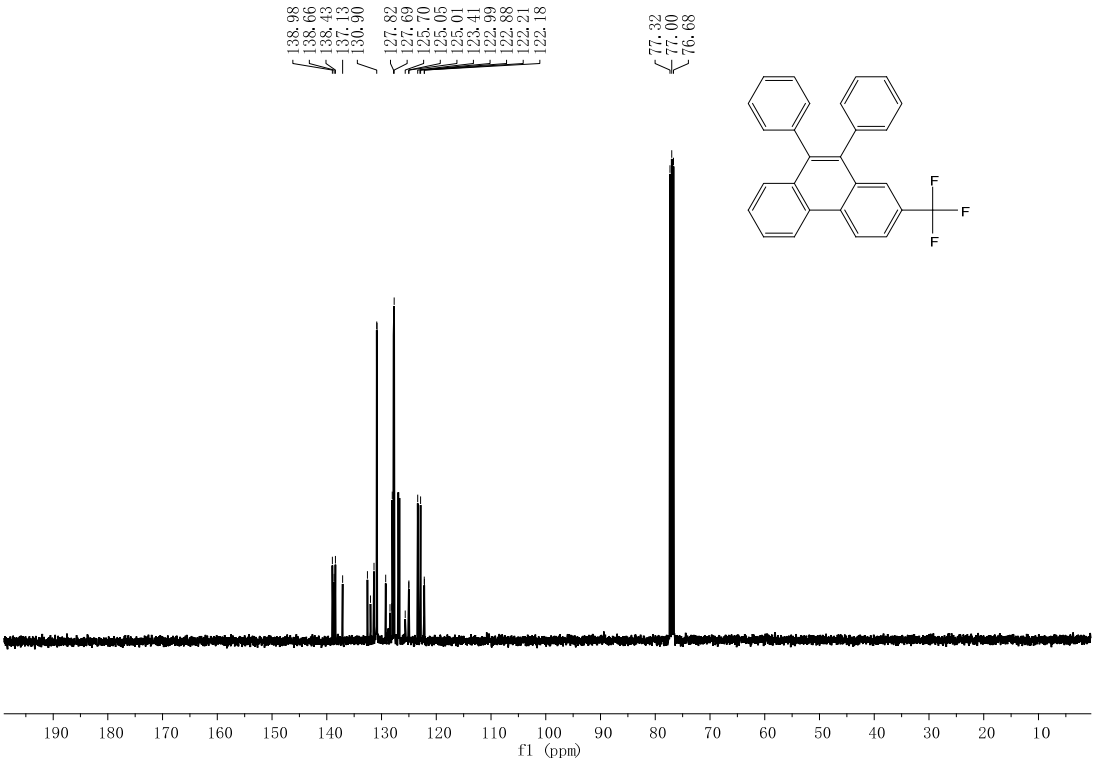
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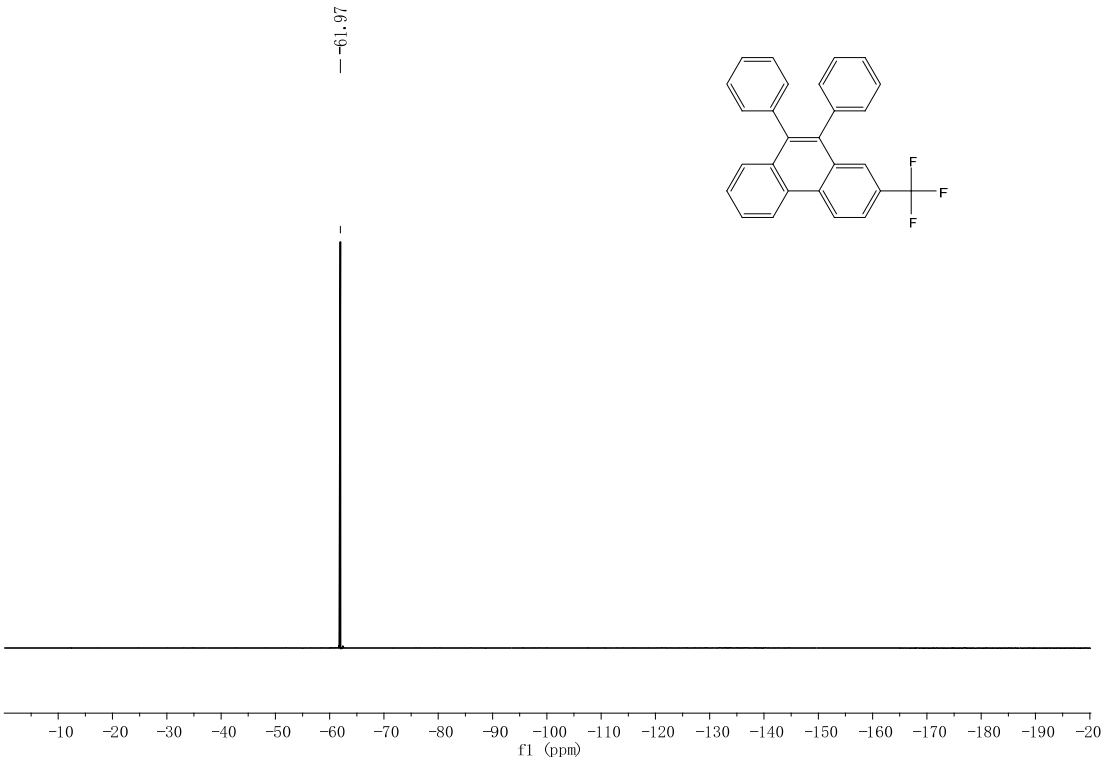
f1 (ppm)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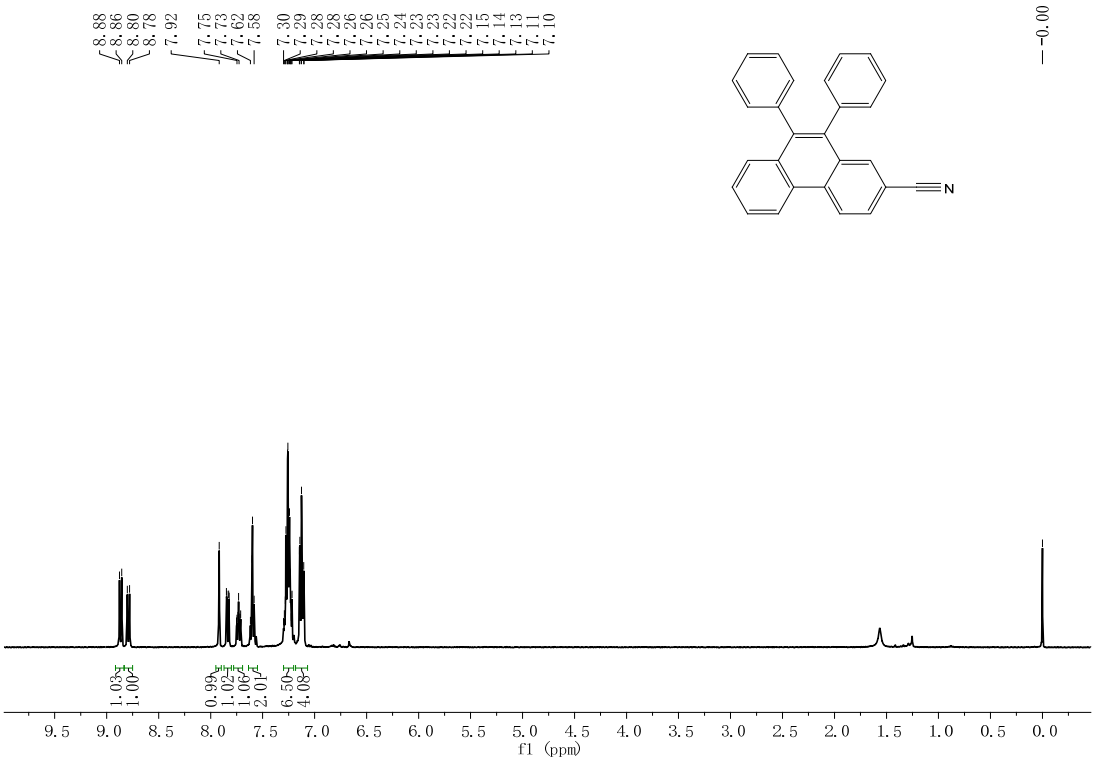
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7.10
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1.00
0.99
1.02
1.06
2.01
6.50
4.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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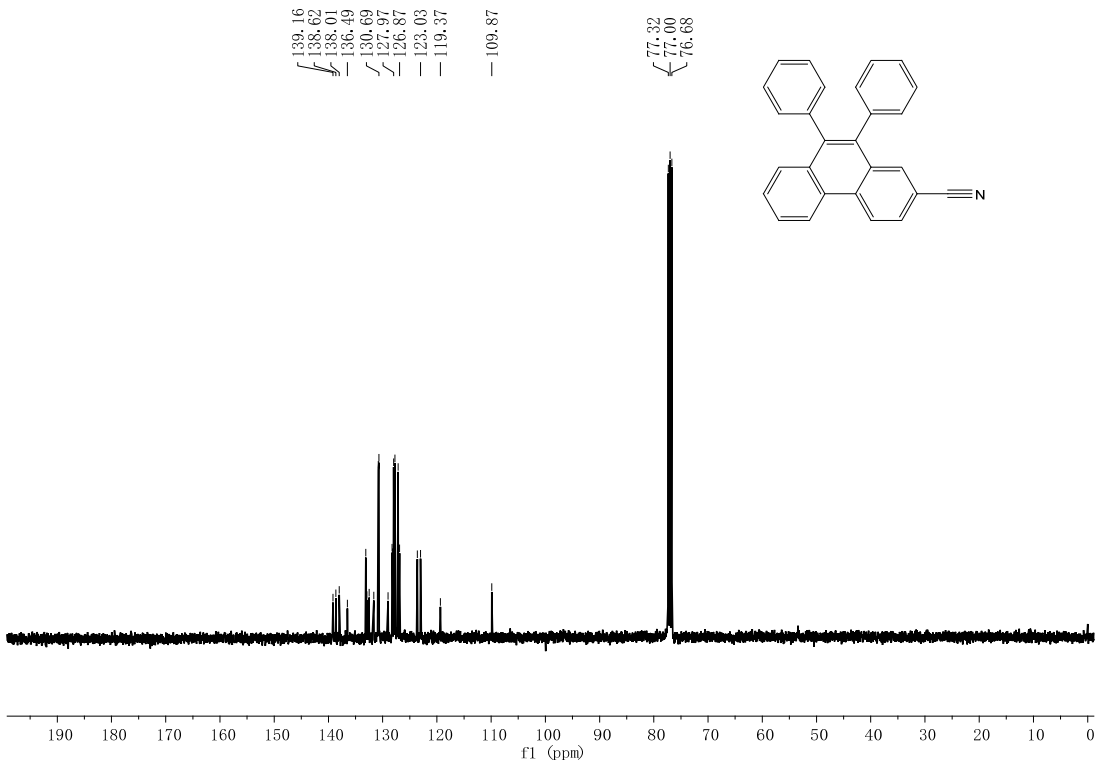
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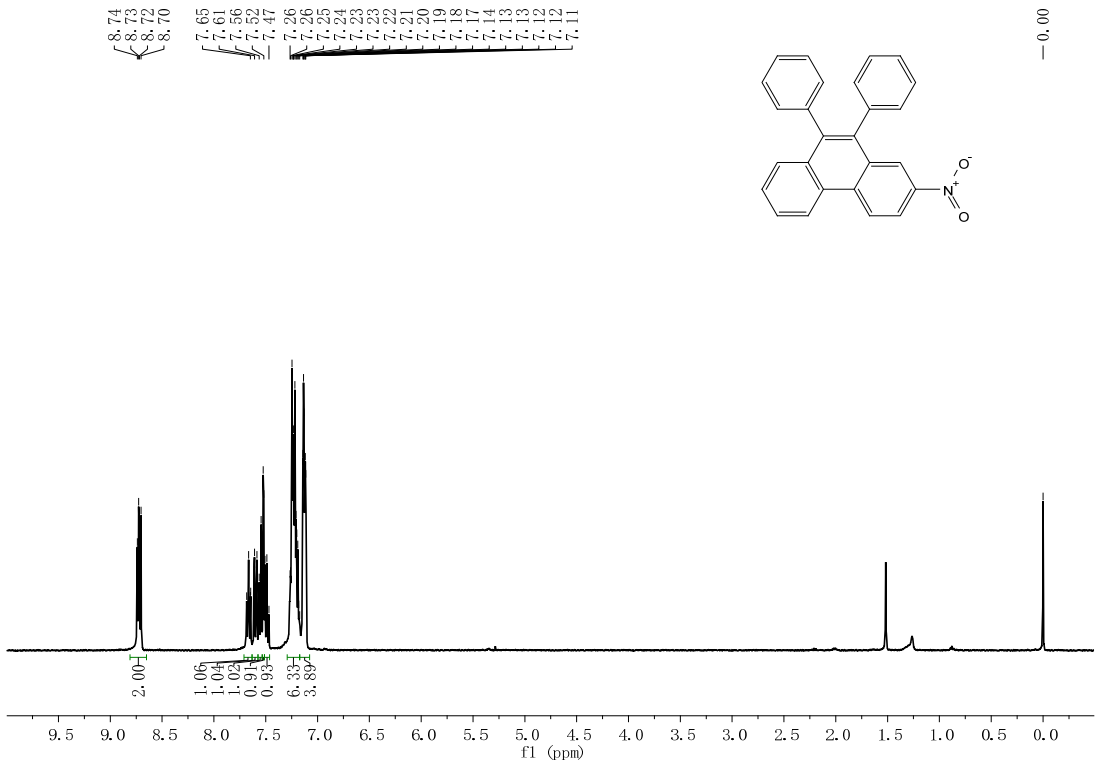
f1 (ppm)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7.12
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O-
O
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1.02
0.91
0.93
6.33
3.89
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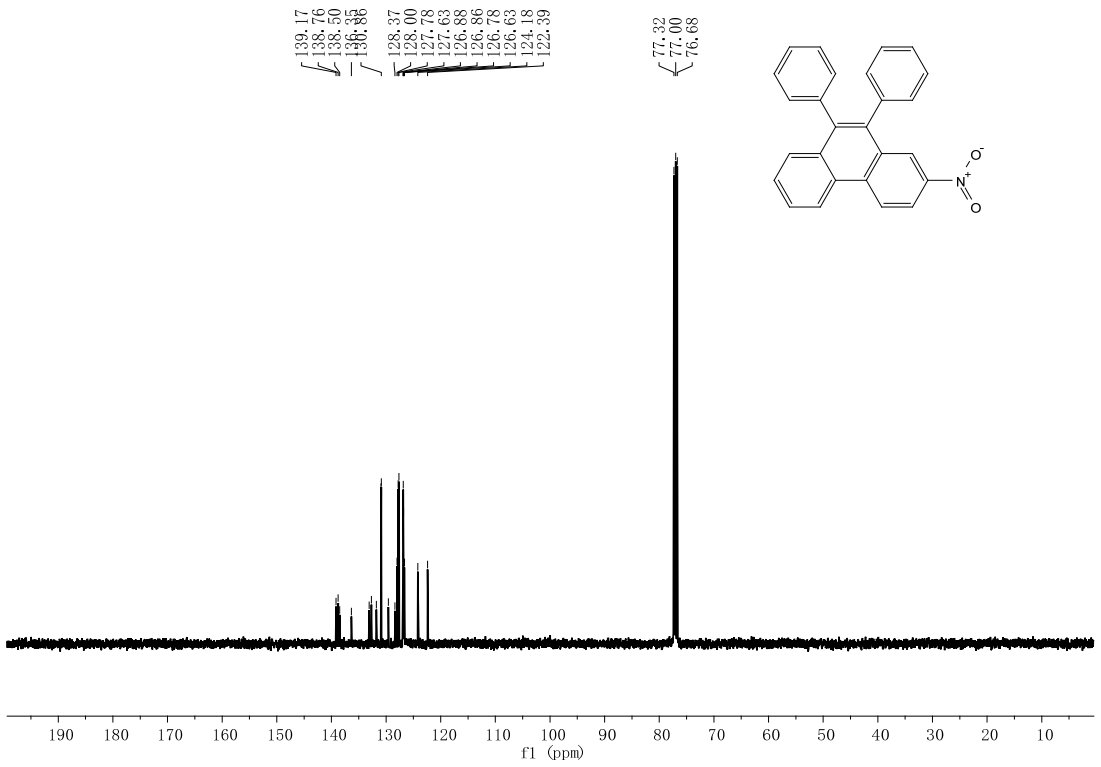
f1 (ppm)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77.00
76.68
O
N+
O-
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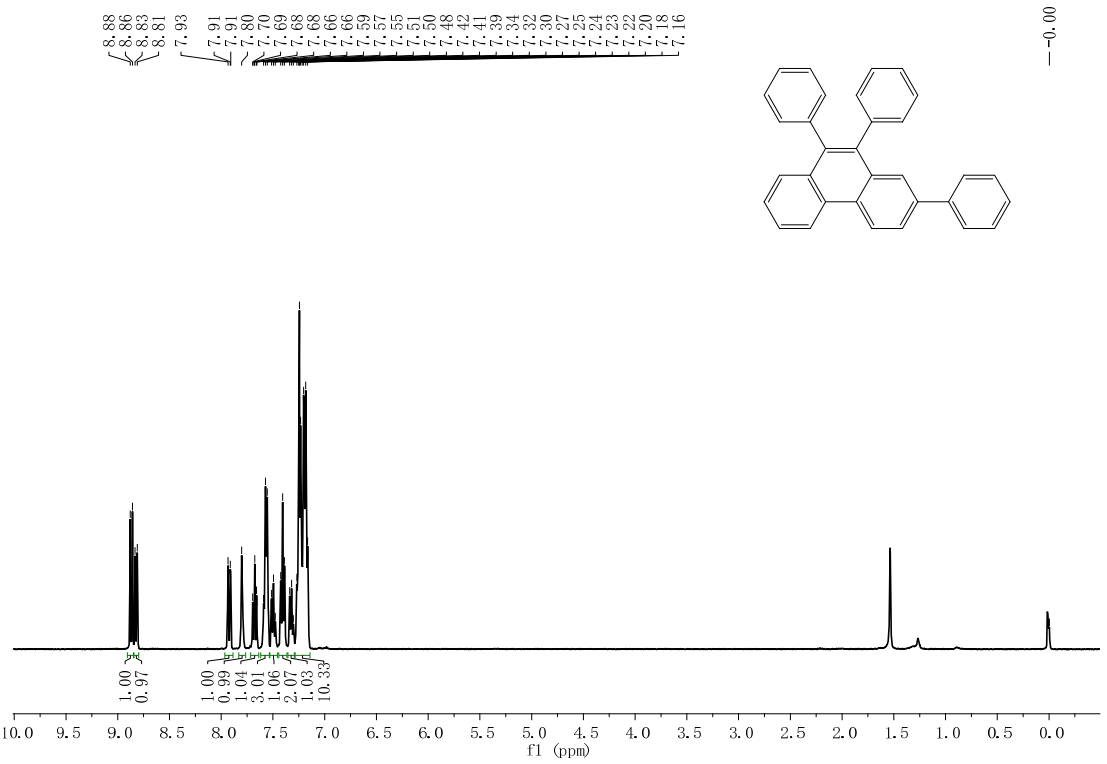
f1 (ppm)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0.99
1.04
3.01
1.06
2.07
1.03
10.33
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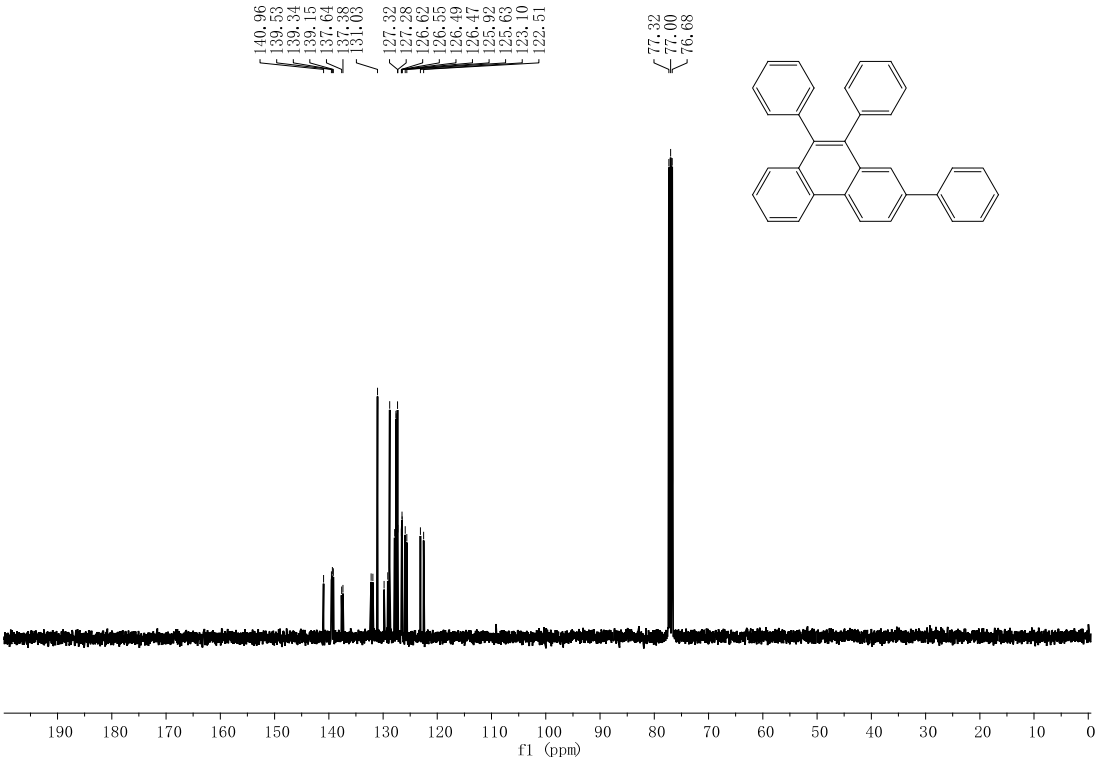
f1 (ppm)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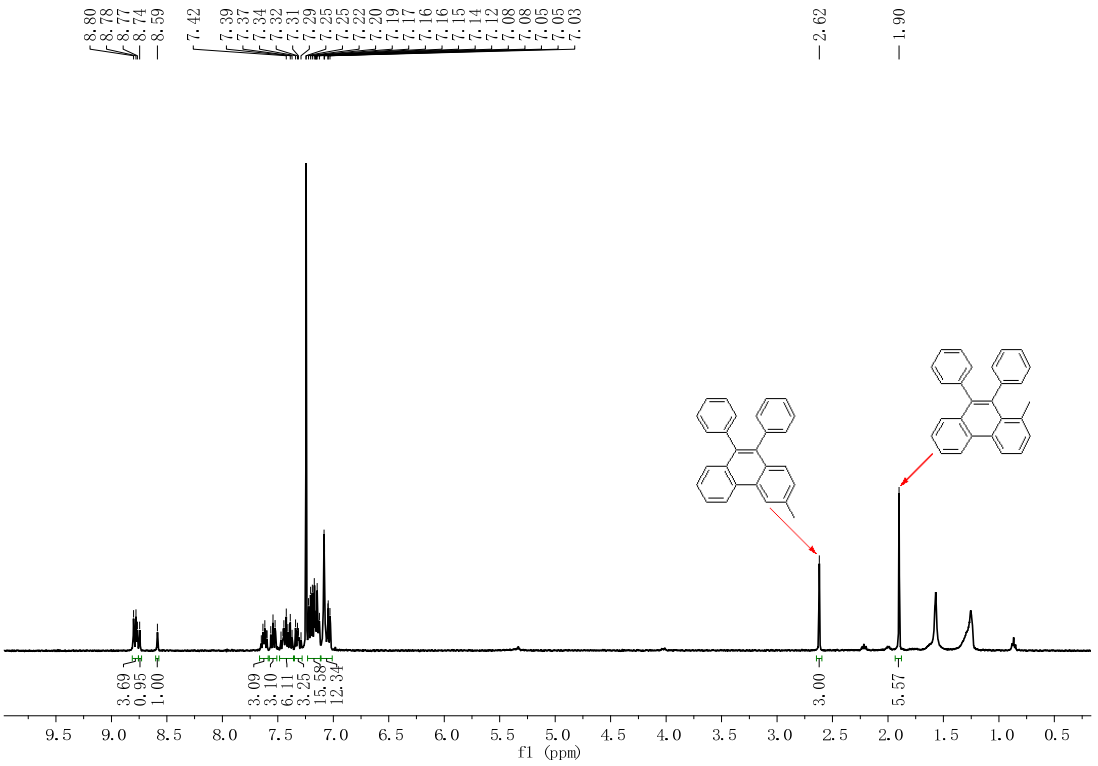
f1 (ppm)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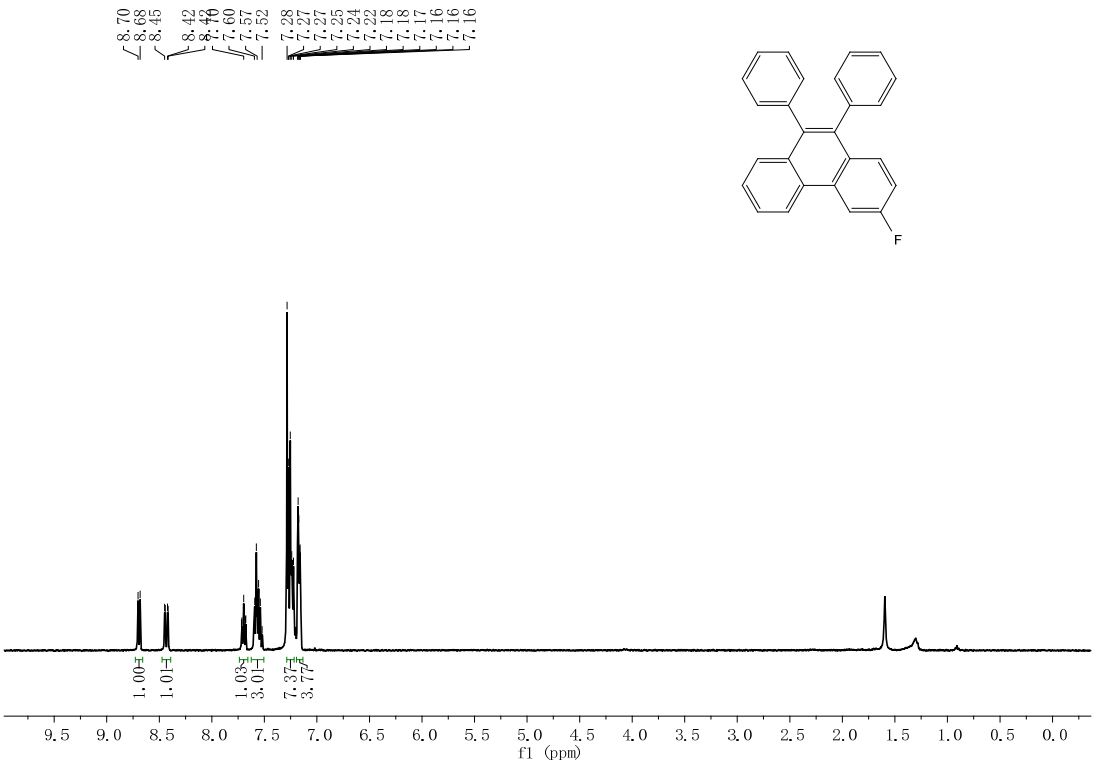
7.25
7.22
7.20
7.19
7.17
7.16
7.16
7.15
7.14
7.12
7.08
7.08
7.05
7.05
7.03
2.62
1.90
3.69
0.95
1.00
3.09
3.10
6.11
3.25
15.58
12.34
3.00
5.57
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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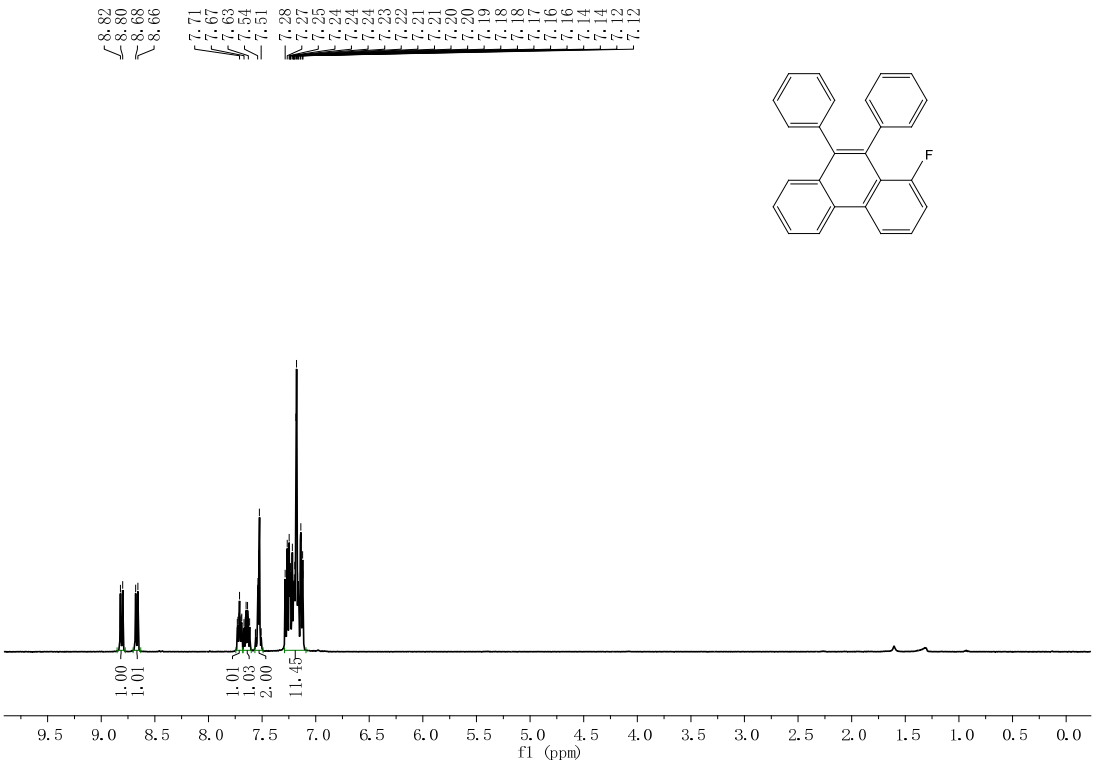
7.27
7.25
7.24
7.22
7.18
7.17
7.16
7.16
7.16
F
1.00
1.01
1.03
3.01
7.37
3.77
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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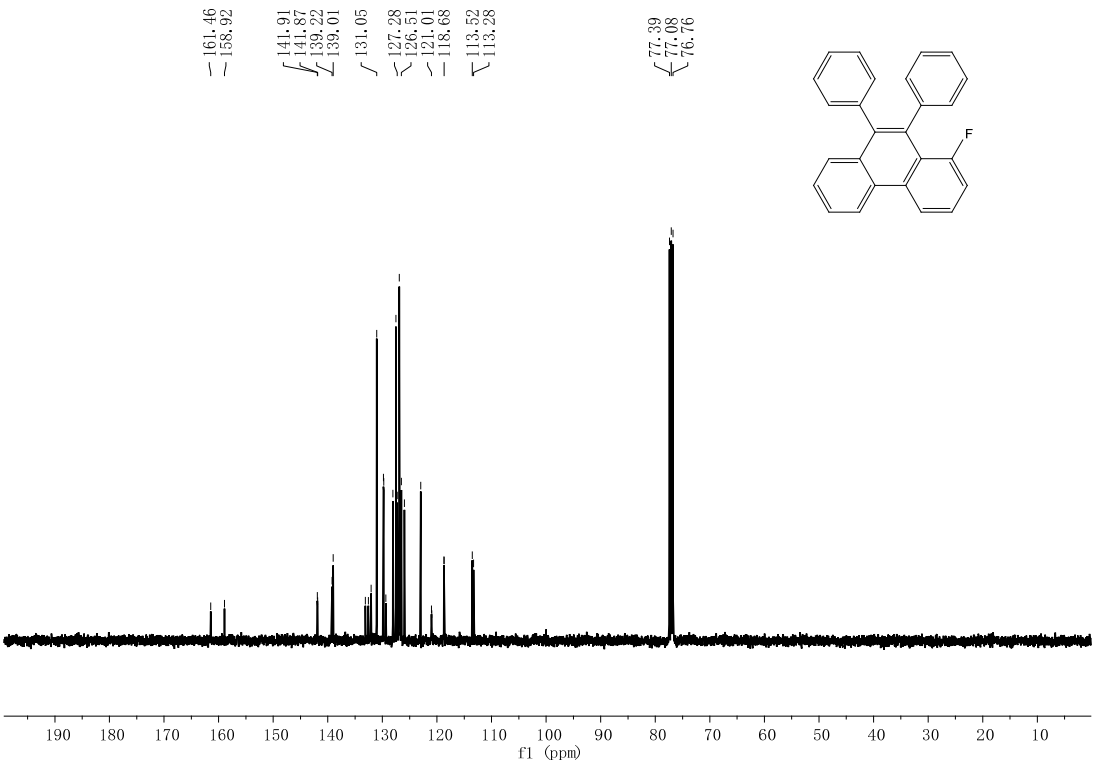
7.24
7.24
7.24
7.23
7.22
7.21
7.21
7.20
7.20
7.19
7.18
7.18
7.17
7.16
7.16
7.14
7.14
7.12
7.12
F
1.00
1.01
1.01
1.03
2.00
11.45
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.05
127.28
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121.01
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113.52
113.28
77.39
77.08
76.76
F
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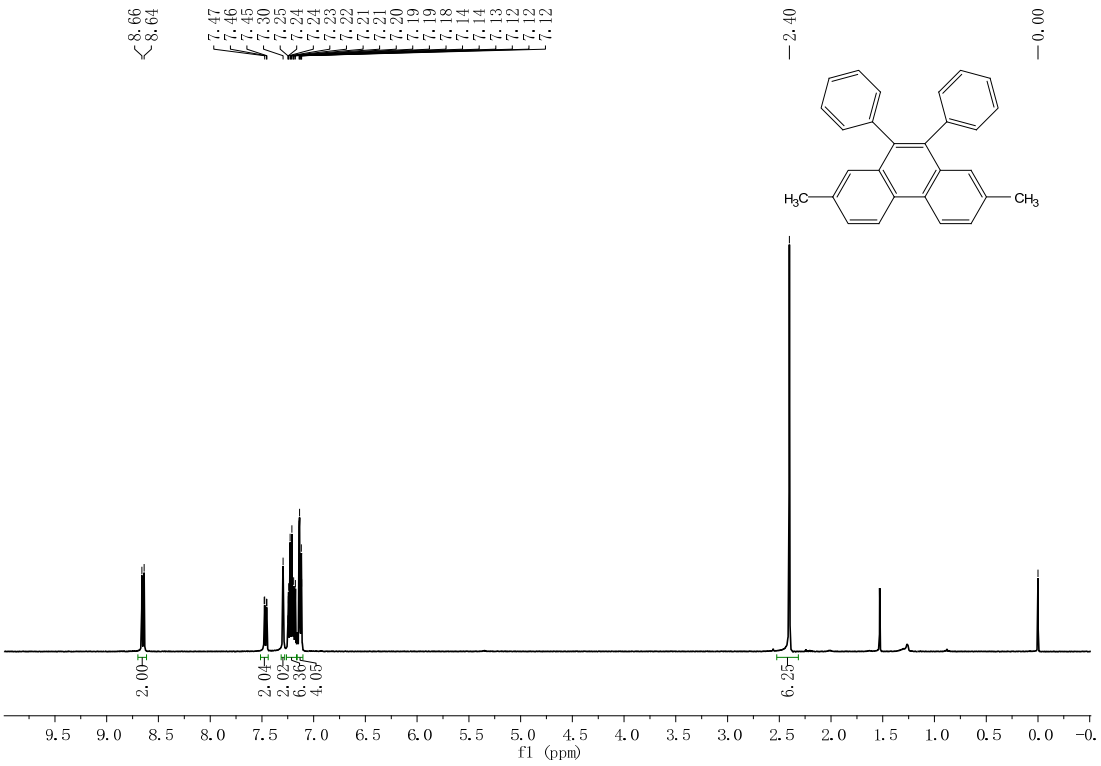
f1 (ppm)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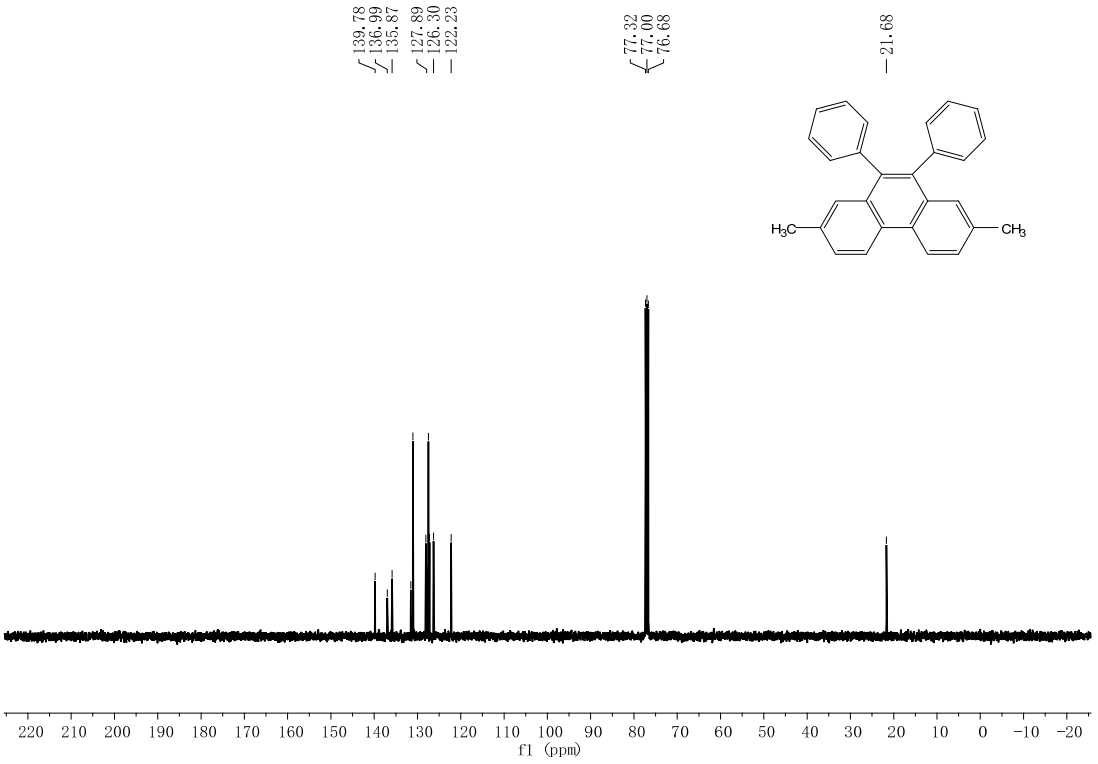
7.25
7.24
7.24
7.23
7.22
7.21
7.21
7.20
7.19
7.19
7.18
7.14
7.14
7.13
7.12
7.12
7.12
2.40
0.00
H3C
CH3
2.00
2.04
2.02
6.38
4.05
6.25
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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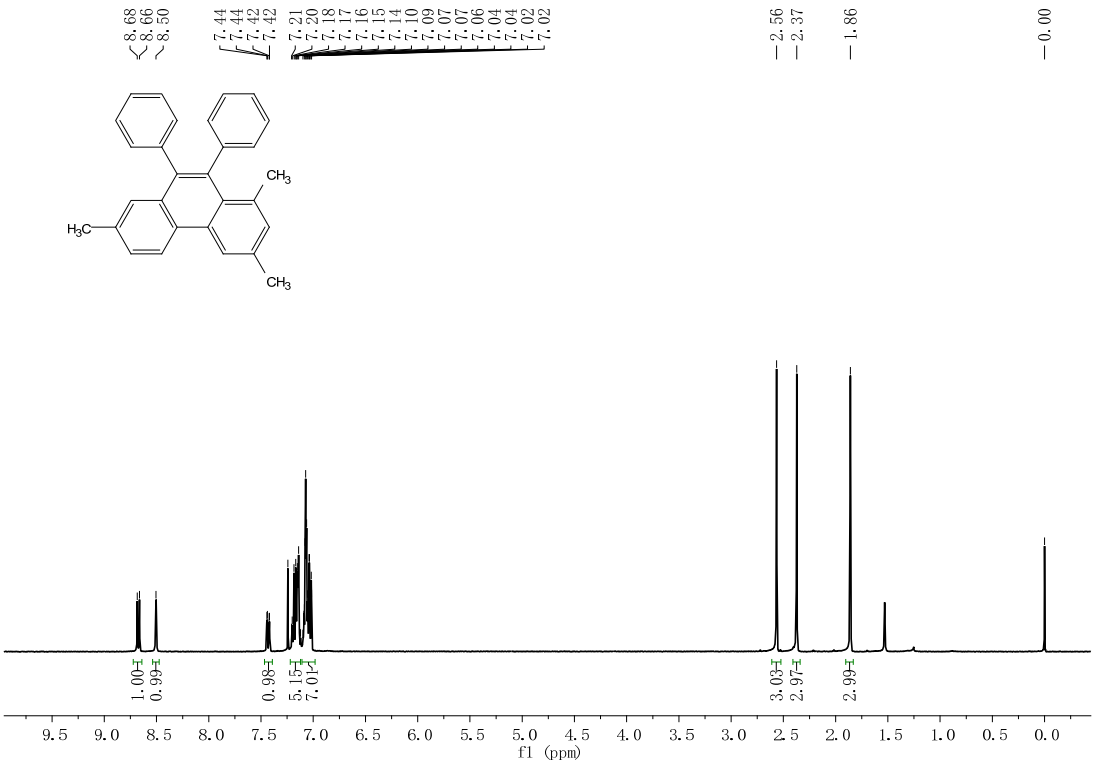
77.32
77.00
76.68
21.68
H3C
CH3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.17
7.16
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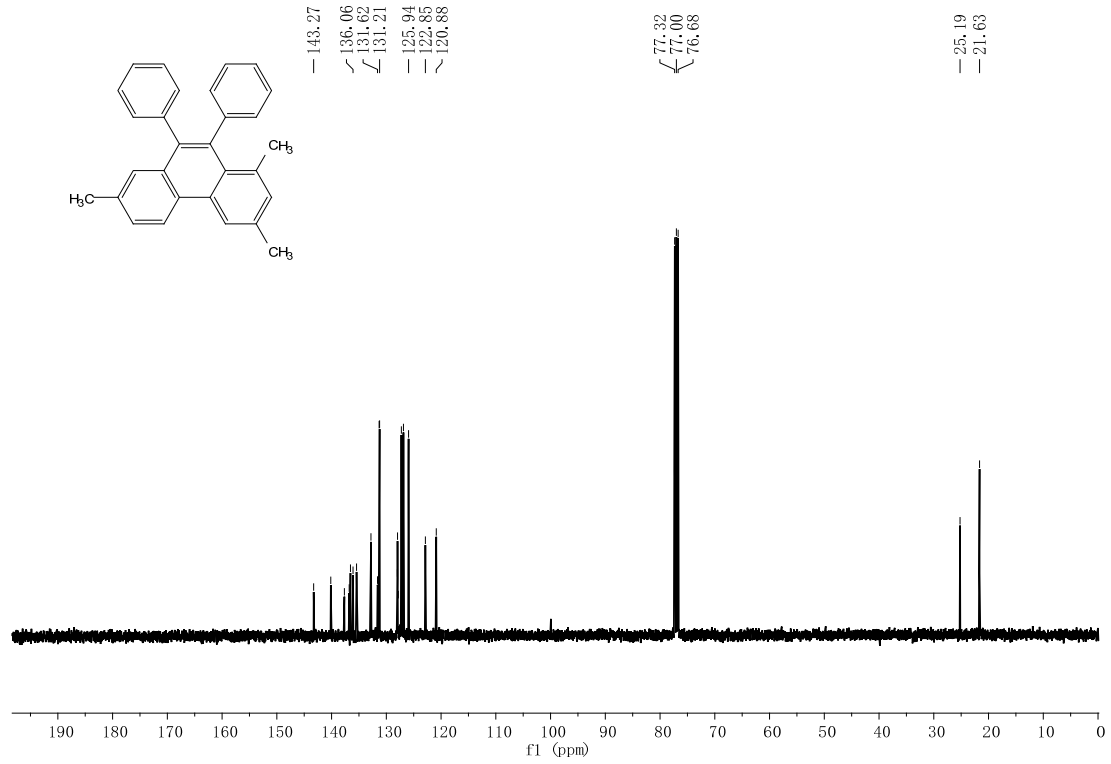
7.14
7.10
7.09
7.07
7.07
7.06
7.04
7.04
7.02
7.02
2.56
2.37
1.86
0.00
CH3
H3C
CH3
1.00
0.99
0.98
5.15
7.01
3.03
2.97
2.99
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.62
131.21
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77.32
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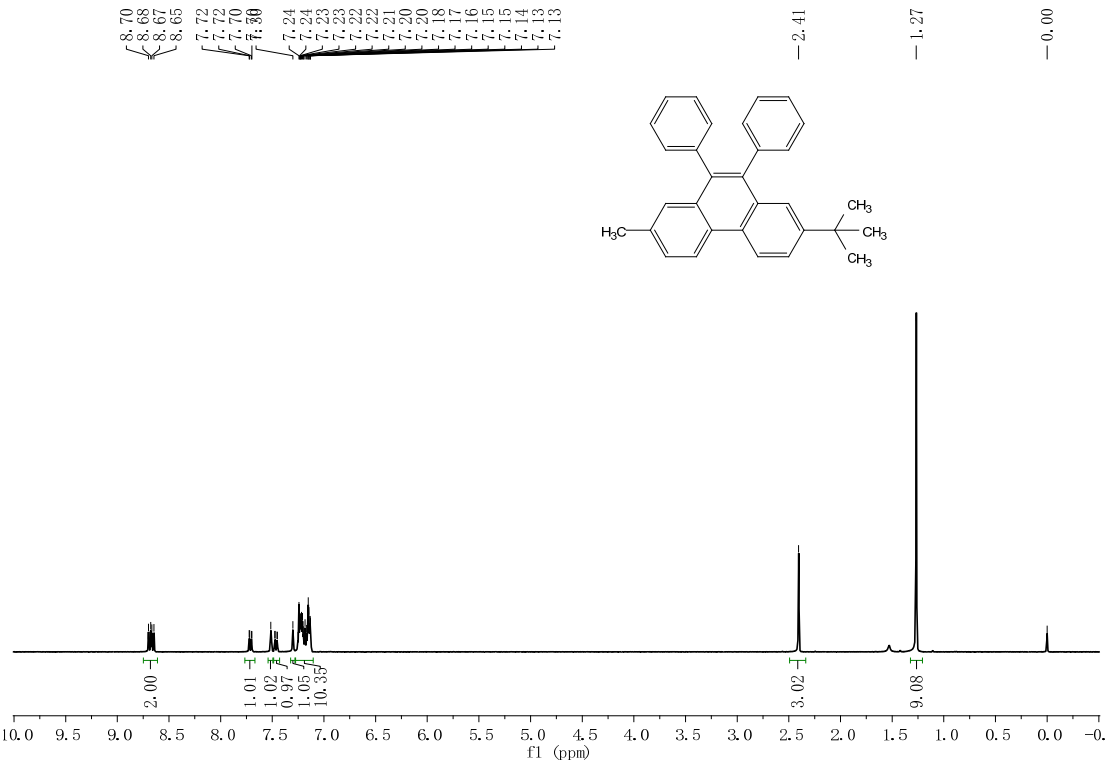
76.68
25.19
21.63
CH3
H3C
CH3
f1 (ppm)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7.72
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7.30
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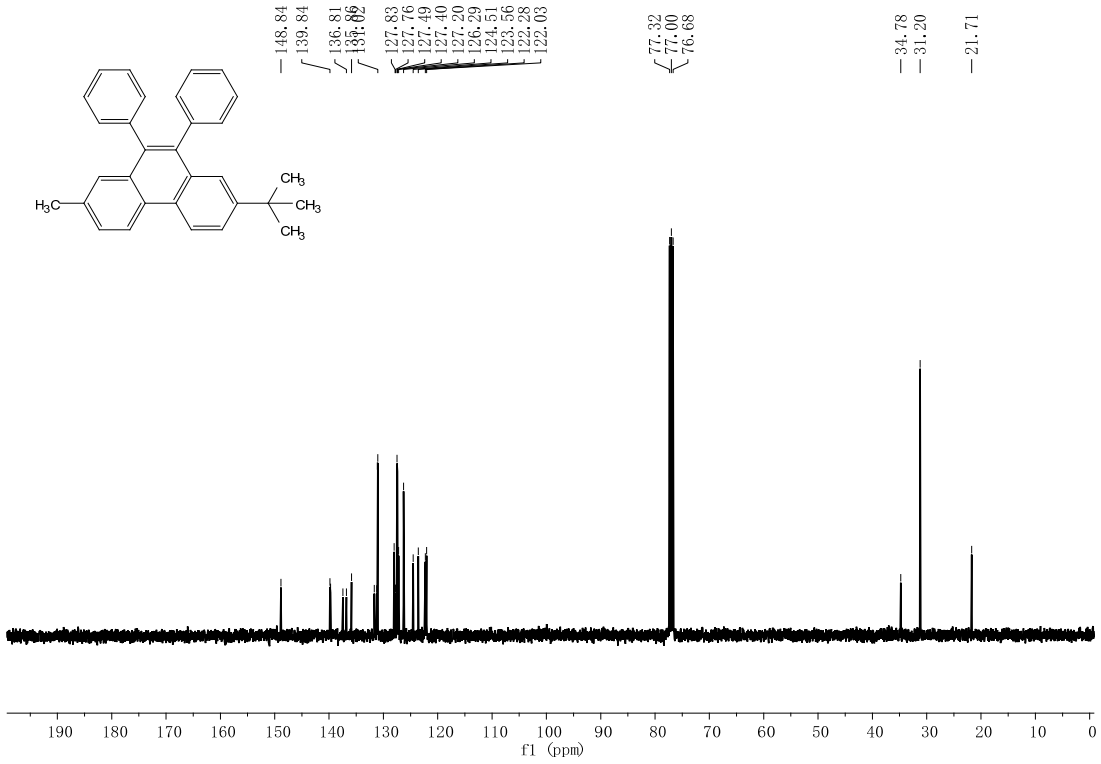
7.24
7.23
7.23
7.22
7.22
7.21
7.20
7.20
7.18
7.17
7.16
7.15
7.15
7.14
7.13
7.13
2.41
1.27
0.00
CH3
H3C
CH3
CH3
2.00
1.01
1.02
0.97
1.05
10.33
3.02
9.08
f1 (ppm)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124.51
123.56
122.28
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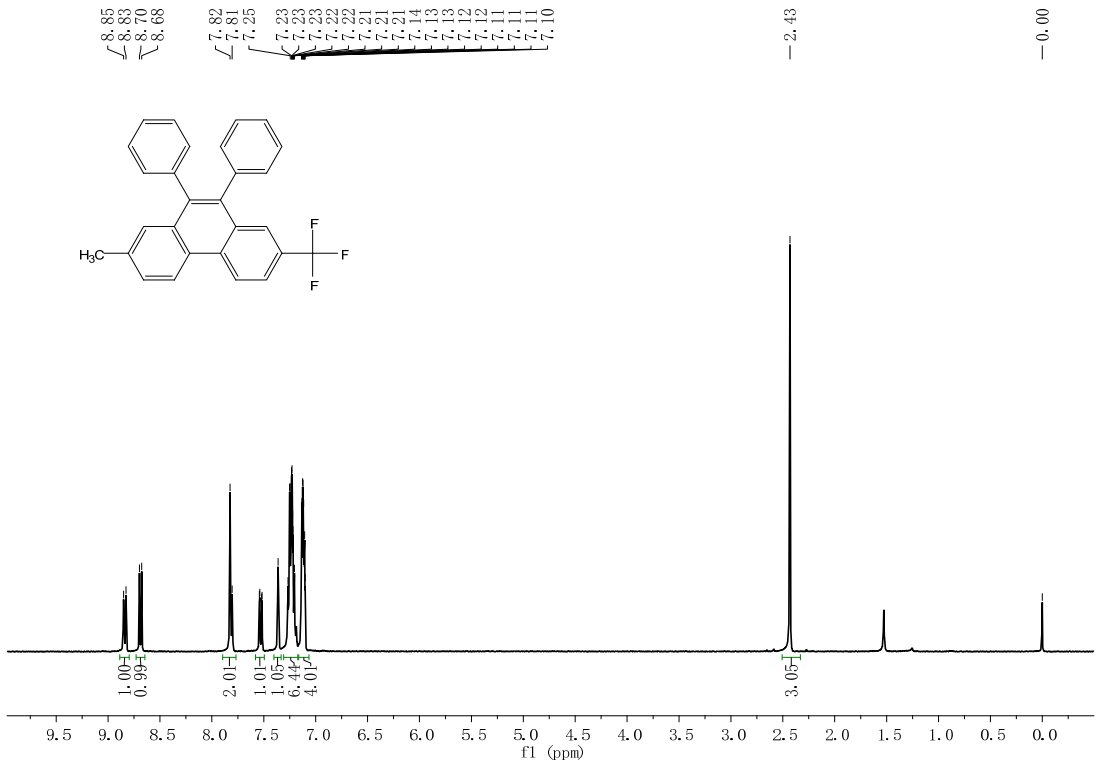
77.00
76.68
34.78
31.20
21.71
H3C
CH3
CH3
CH3
f1 (ppm)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7.23
7.22
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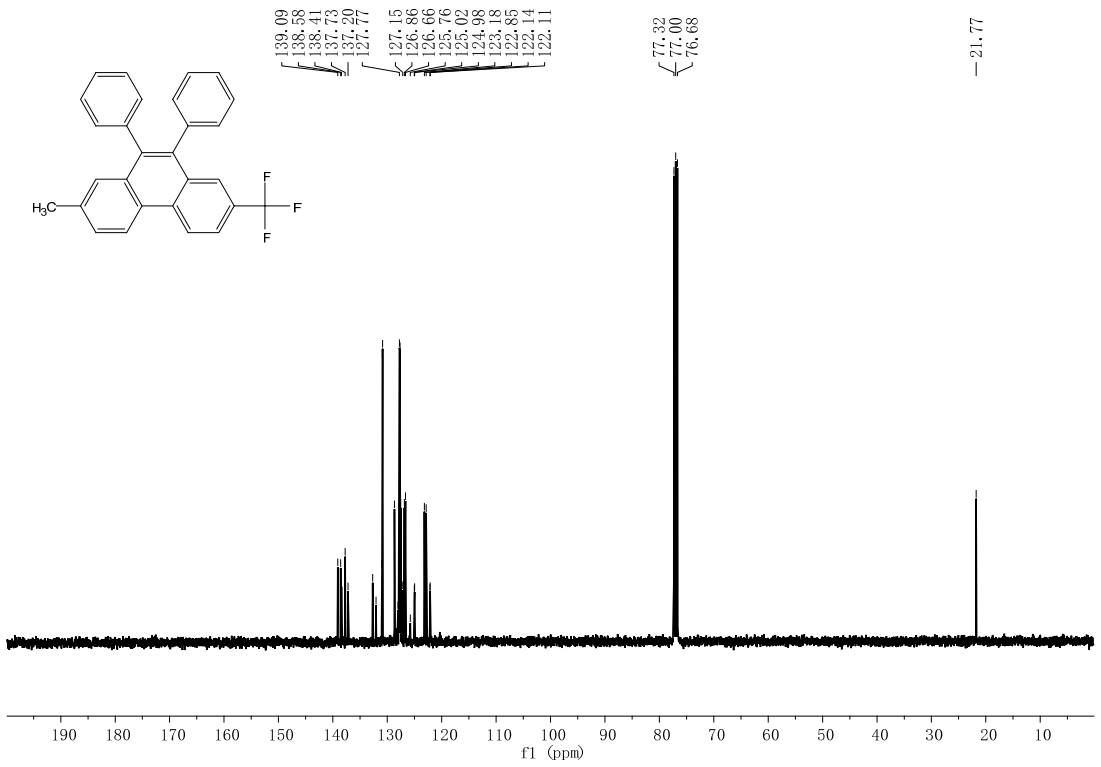
7.21
7.14
7.13
7.13
7.12
7.12
7.11
7.11
7.11
7.10
2.43
0.00
H3C
F
F
F
1.00
0.99
2.01
1.01
1.05
6.44
4.01
3.05
f1 (ppm)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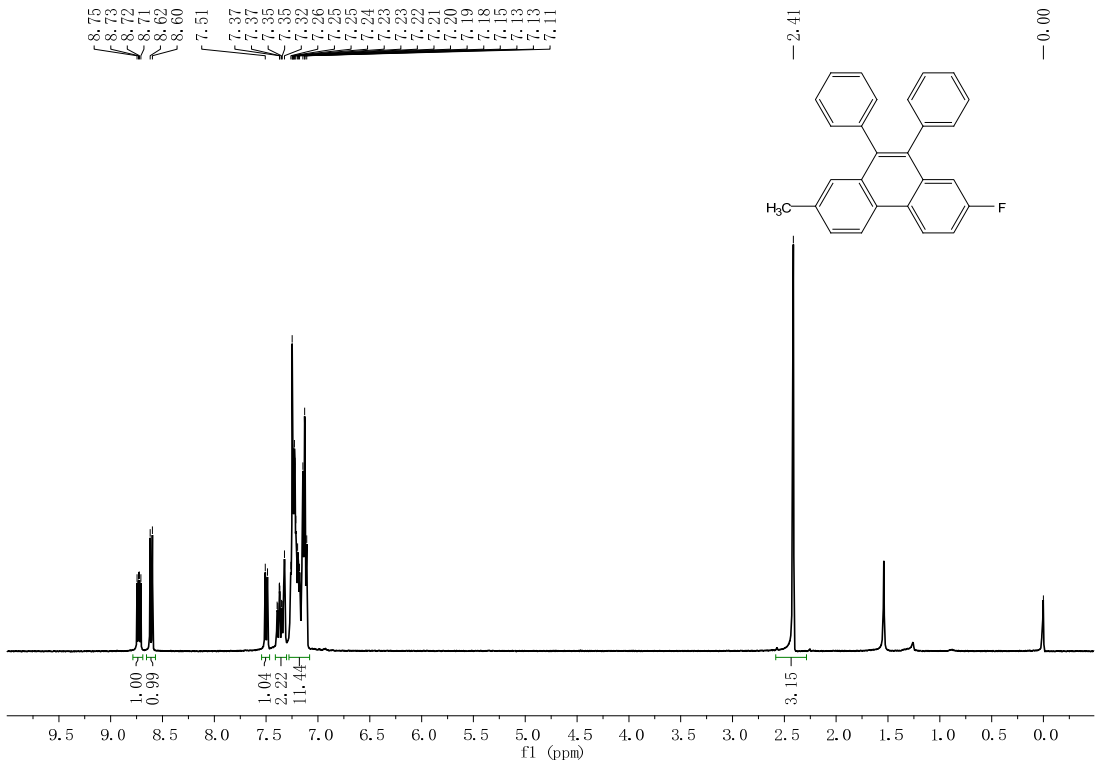
126.66
125.76
125.02
124.98
123.18
122.85
122.14
122.11
77.32
77.00
76.68
21.77
F
F
F
H3C
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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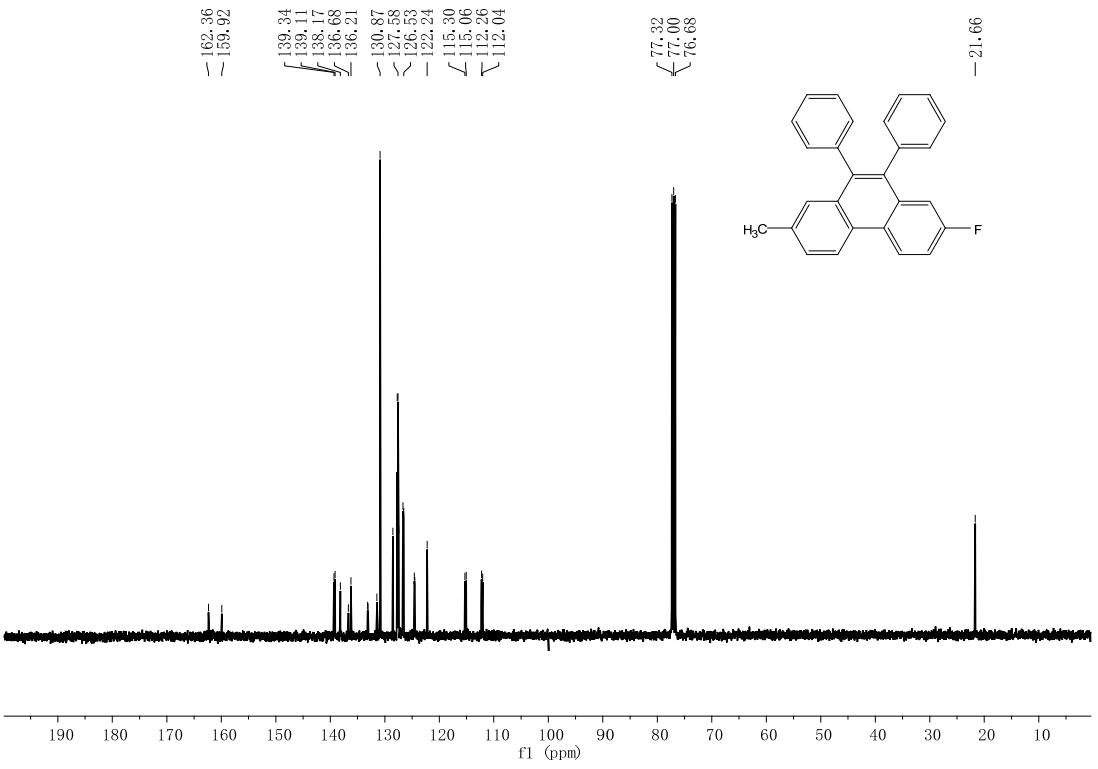
7.24
7.23
7.23
7.22
7.21
7.20
7.19
7.18
7.15
7.13
7.13
7.11
2.41
0.00
H3C
F
1.00
0.99
1.04
2.22
11.44
3.15
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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136.21
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126.53
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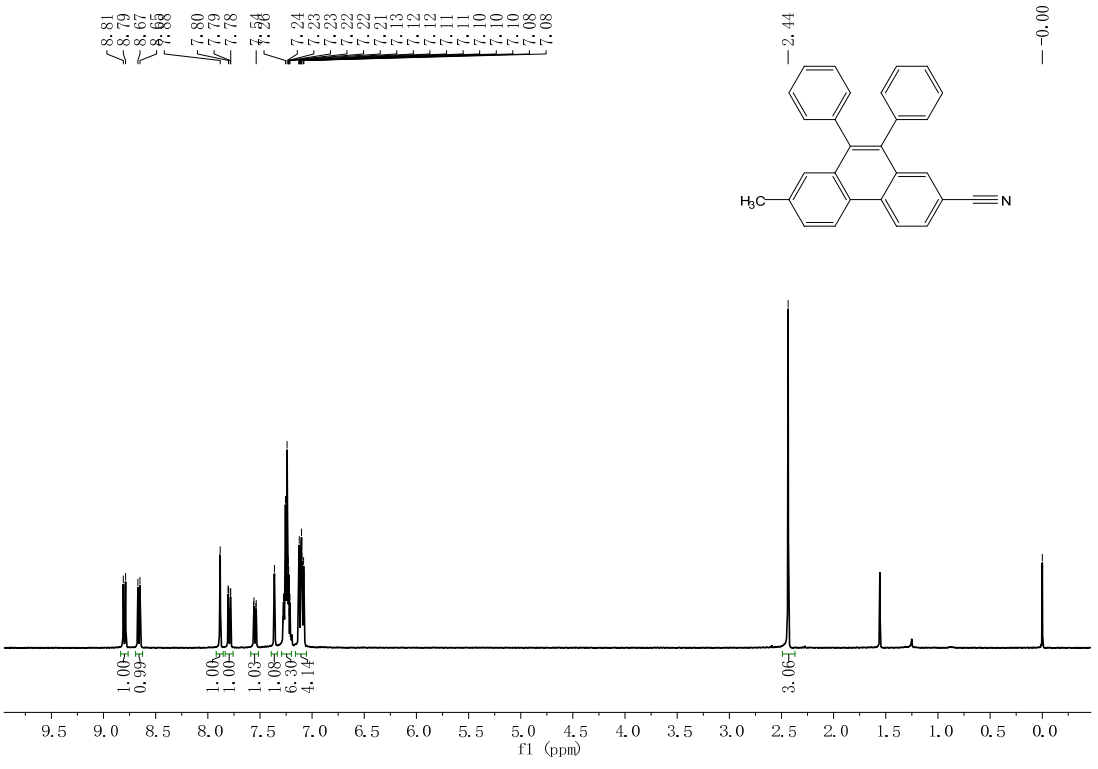
115.06
112.26
112.04
77.32
77.00
76.68
21.66
H3C
F
f1 (ppm)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7.79
7.78
7.54
7.24
7.23
7.23
7.22
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7.21
7.13
7.12
7.12
7.11
7.11
7.10
7.10
7.10
7.08
7.08
2.44
0.00
H3C
N
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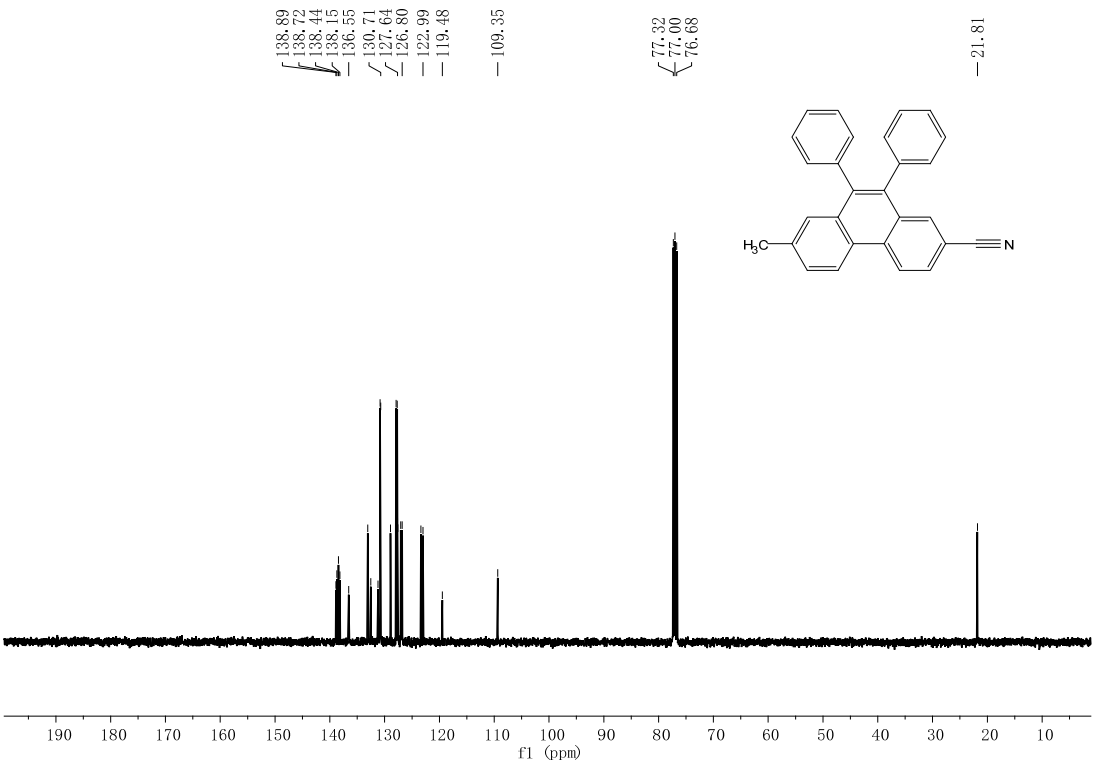
0.99
1.00
1.00
1.03
1.08
6.30
4.14
3.06
f1 (ppm)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H3C
N
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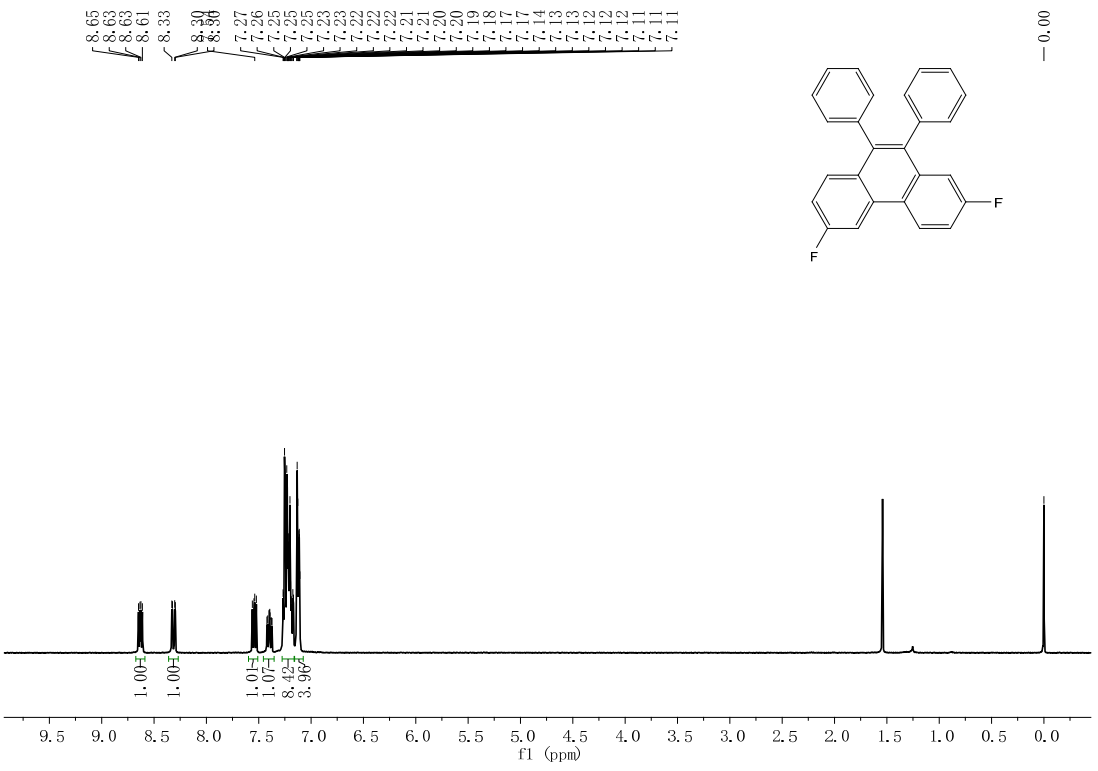
f1 (ppm)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7.23
7.23
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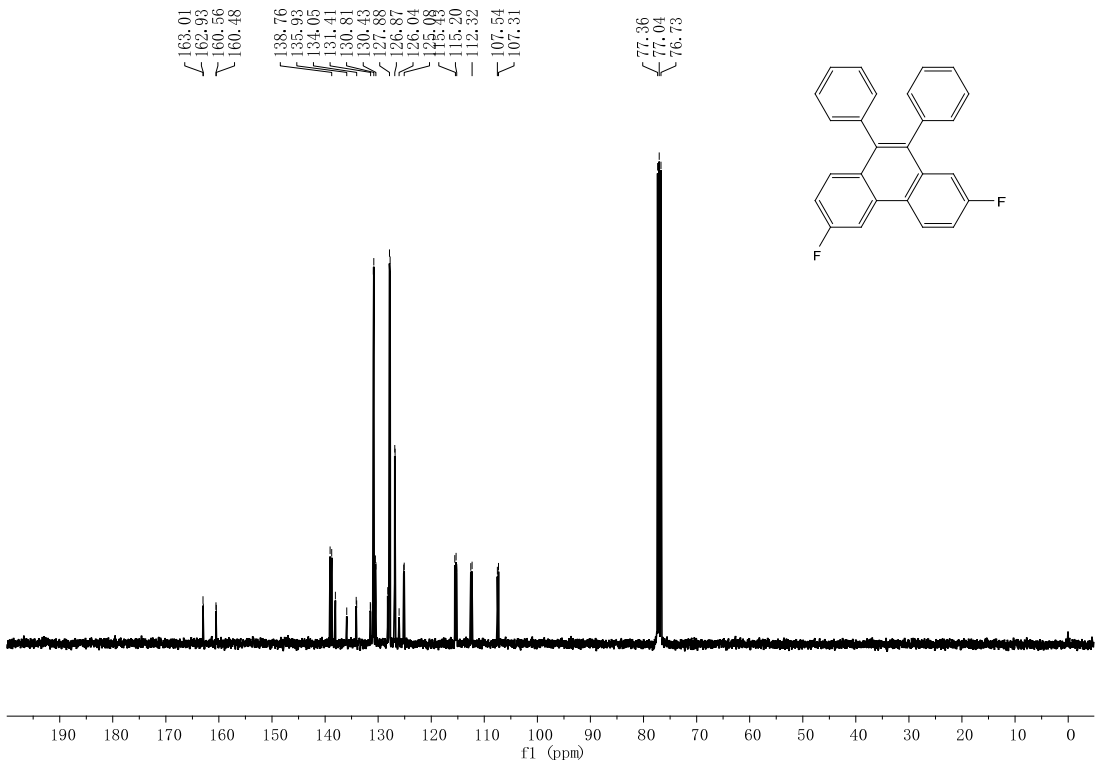
7.22
7.22
7.21
7.21
7.20
7.20
7.19
7.18
7.17
7.17
7.14
7.13
7.13
7.12
7.12
7.12
7.11
7.11
7.11
0.00
F
F
1.00
1.00
1.01
1.07
8.42
3.96
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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126.04
125.98
125.43
116.20
112.32
107.54
107.31
77.36
77.04
76.73
F
F
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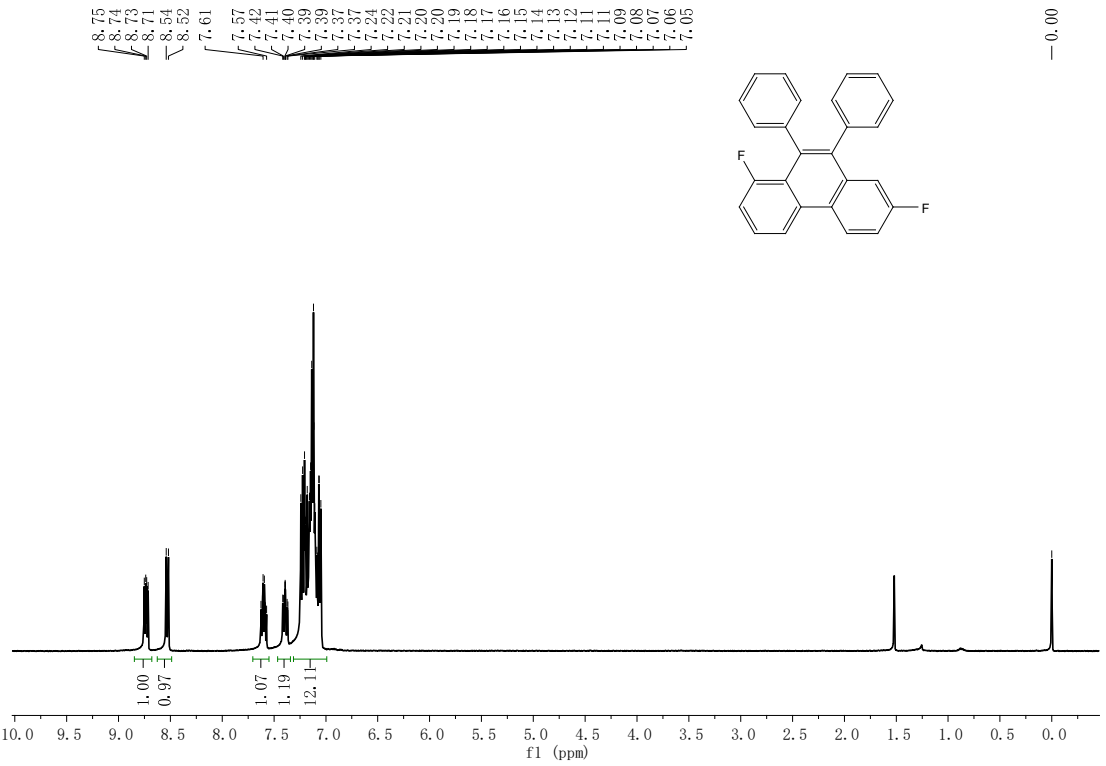
f1 (ppm)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7.57
7.42
7.41
7.40
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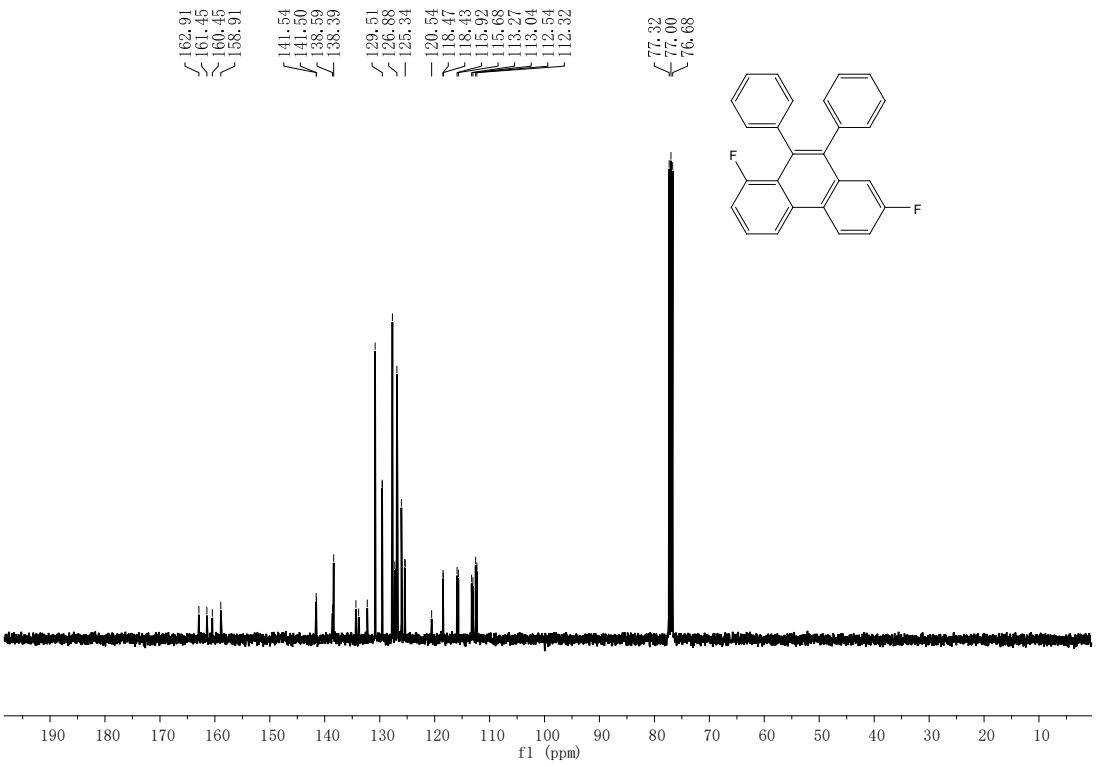
7.39
7.37
7.37
7.24
7.22
7.21
7.20
7.20
7.19
7.18
7.17
7.16
7.15
7.14
7.13
7.12
7.11
7.11
7.09
7.08
7.07
7.06
7.05
0.00
F
F
1.00
0.97
1.07
1.19
12.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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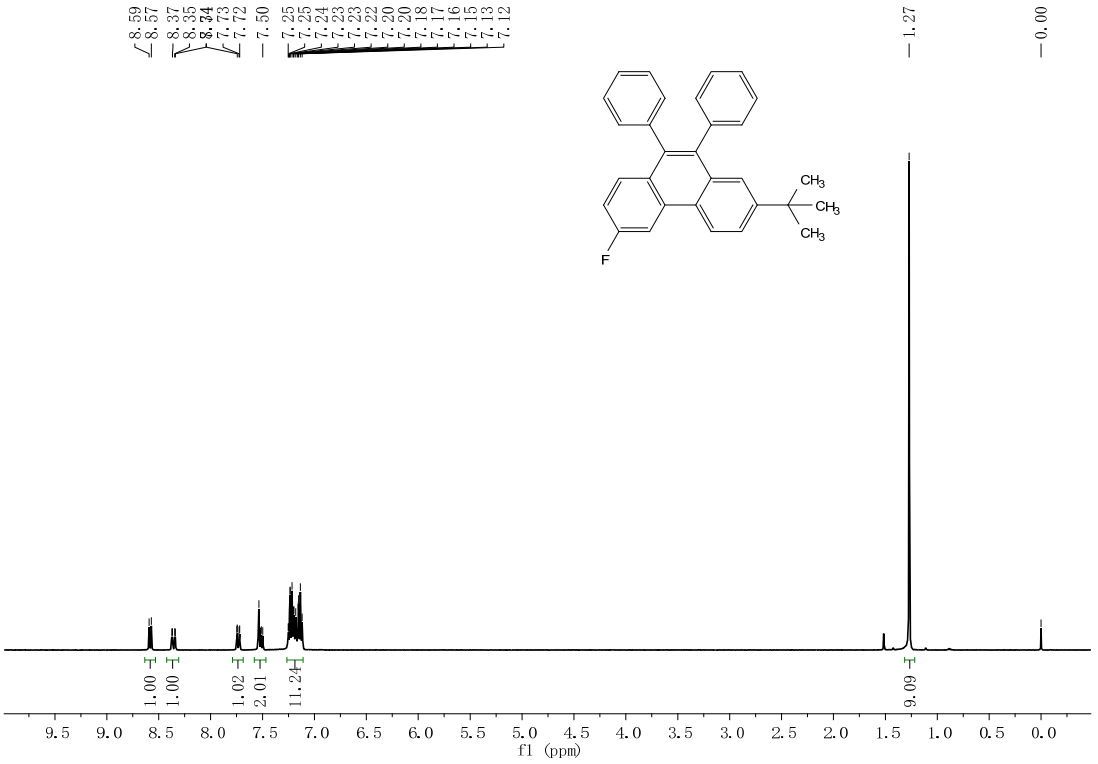
113.27
113.04
112.54
112.32
77.32
77.00
76.68
F
F
f1 (ppm)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7.23
7.22
7.20
7.18
7.17
7.16
7.15
7.13
7.12
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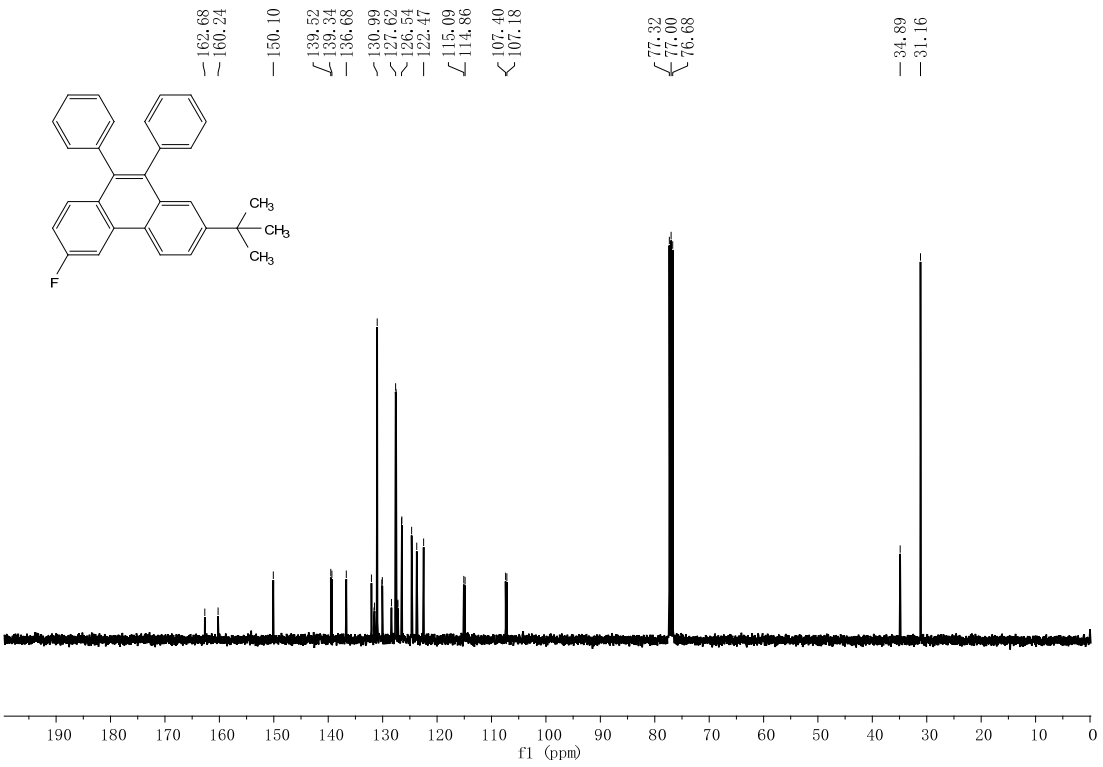
CH3
CH3
CH3
F
1.00
1.00
1.02
2.01
11.24
9.09
f1 (ppm)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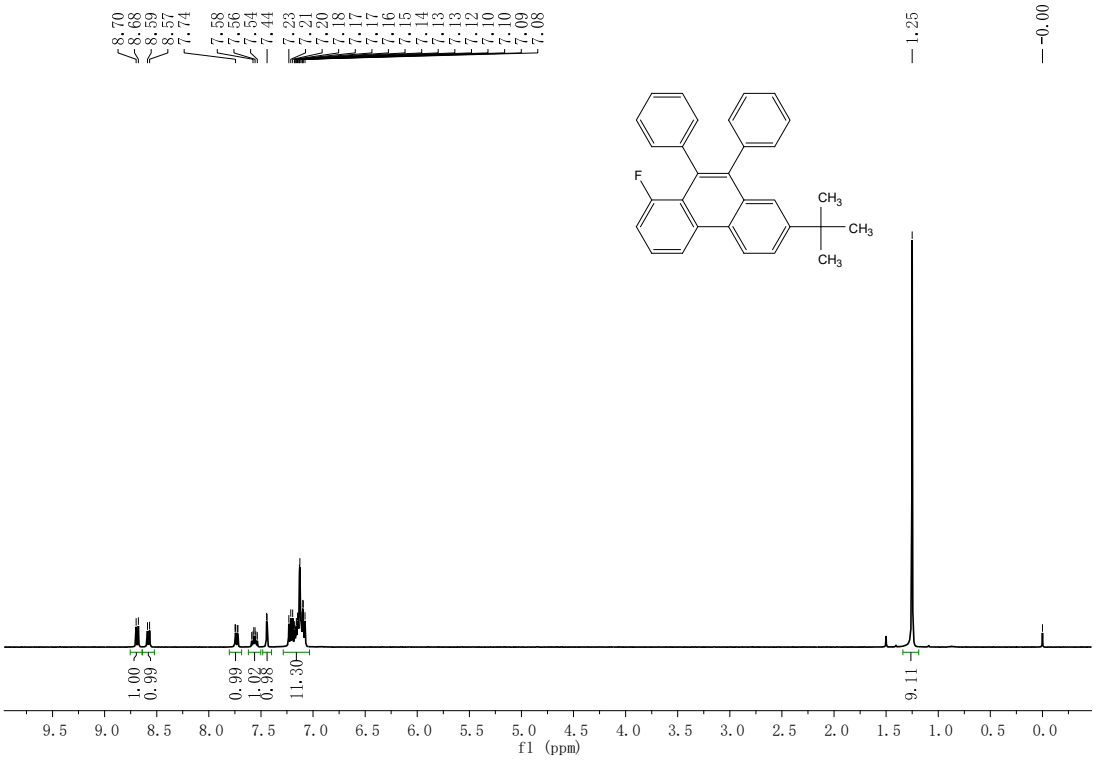
77.00
76.68
34.89
31.16
CH3
CH3
CH3
F
f1 (ppm)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7.56
7.54
7.44
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7.20
7.18
7.17
7.17
7.16
7.15
7.14
7.13
7.13
7.12
7.10
7.10
7.09
7.08
1.25
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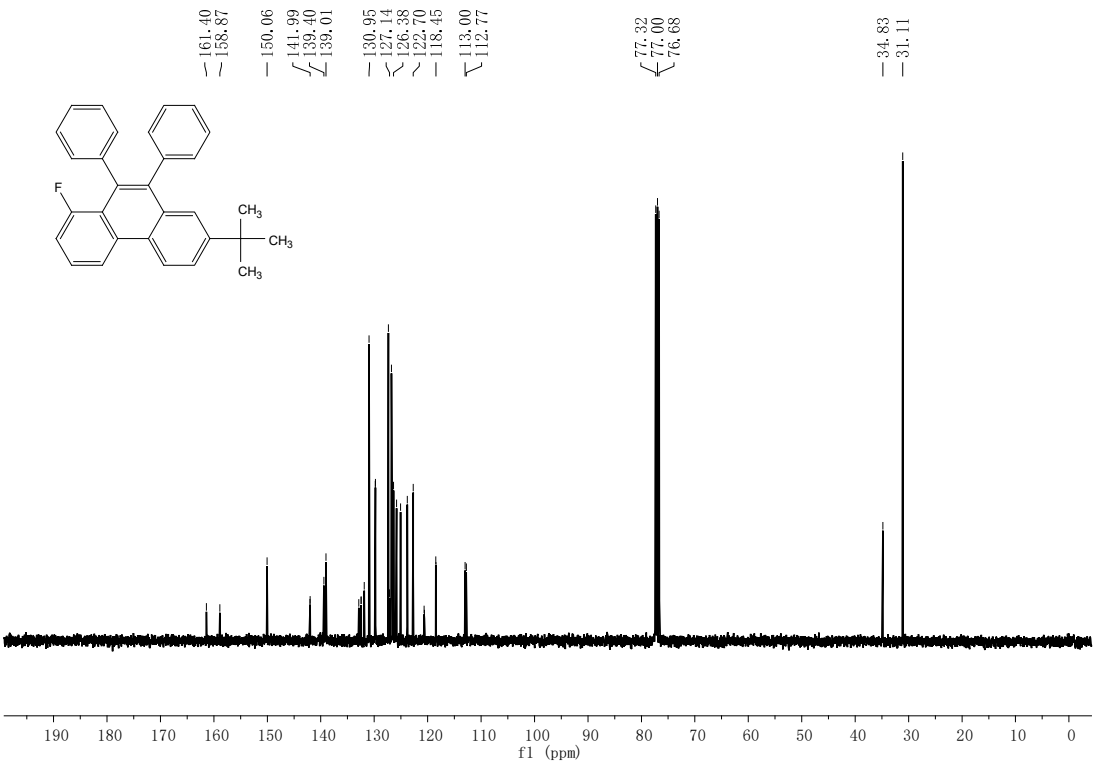
F
CH3
CH3
CH3
1.00
0.99
0.99
1.02
0.98
11.30
9.11
f1 (ppm)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139.01
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122.70
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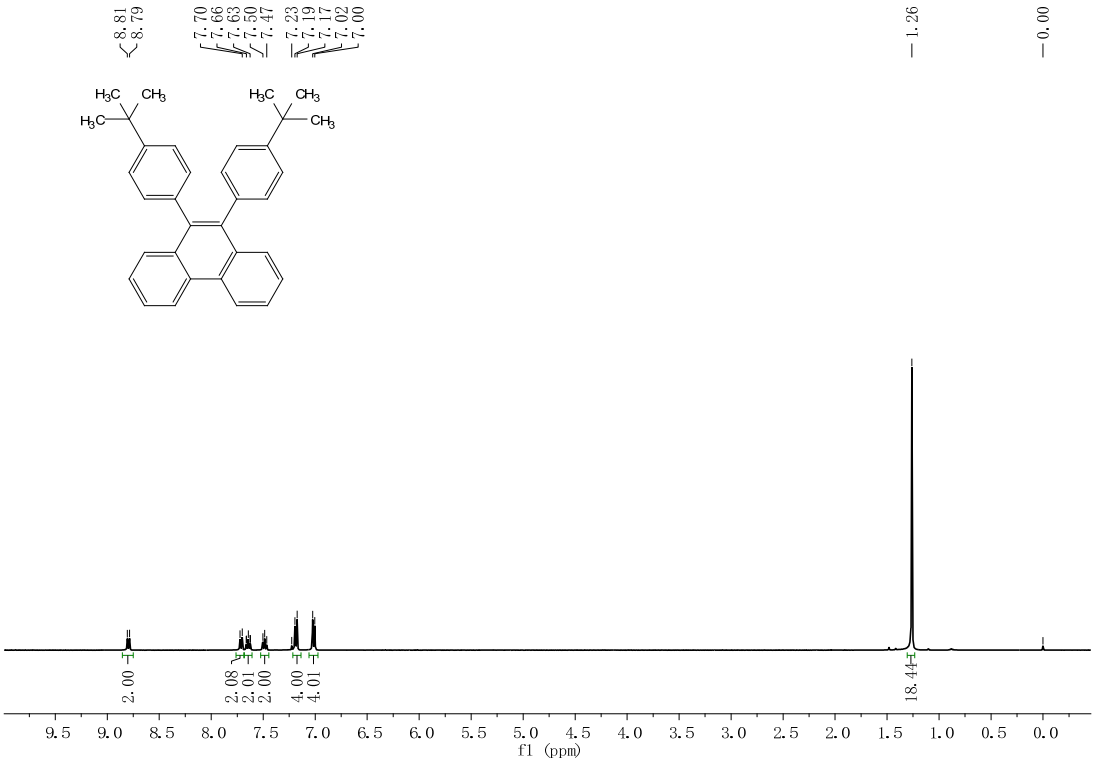
77.32
77.00
76.68
34.83
31.11
F
CH3
CH3
CH3
f1 (ppm)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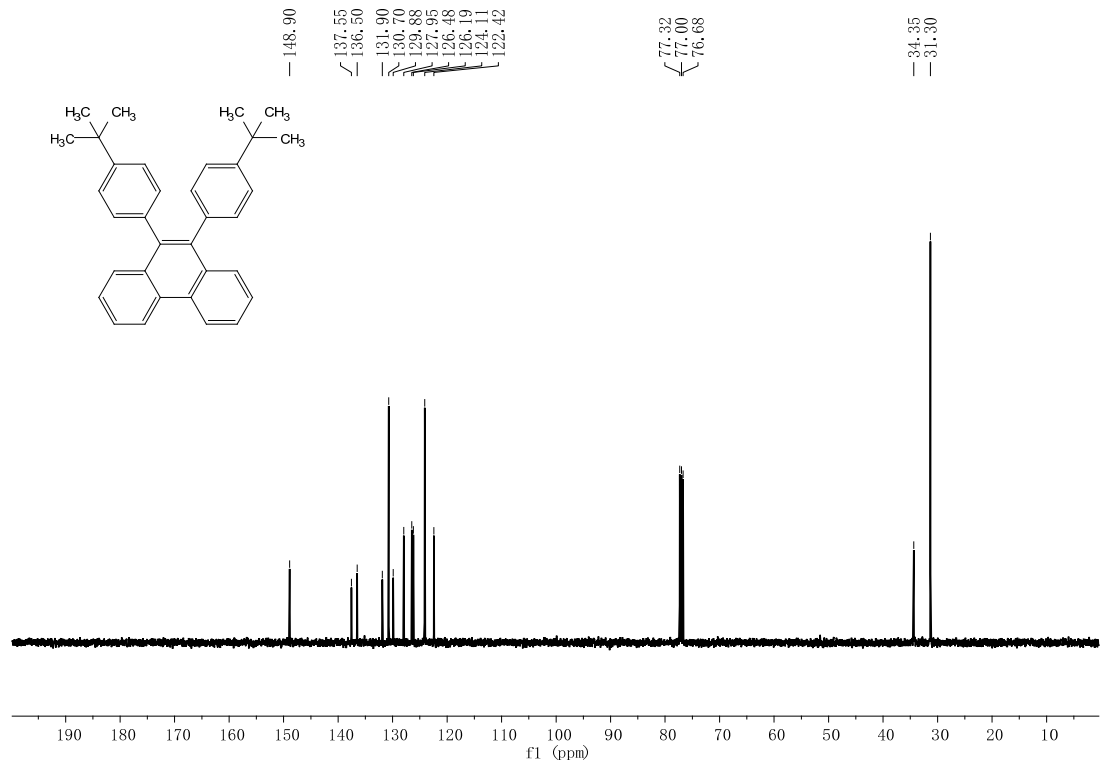
7.50
7.47
7.23
7.19
7.17
7.02
7.00
1.26
0.00
H3C
CH3
H3C
CH3
H3C
CH3
H3C
CH3
2.00
2.08
2.01
2.00
4.00
4.01
18.44
f1 (ppm)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131.90
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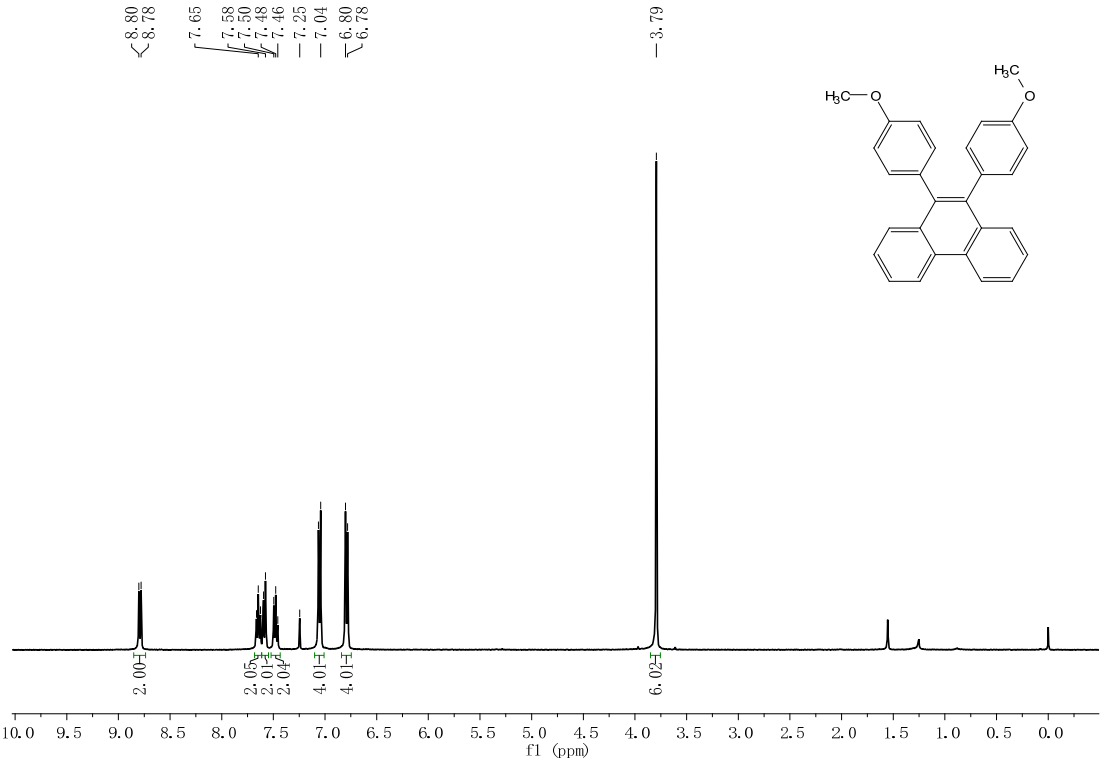
129.88
127.95
126.48
126.19
124.11
122.42
77.32
77.00
76.68
34.35
31.30
H3C CH3
H3C
H3C CH3
CH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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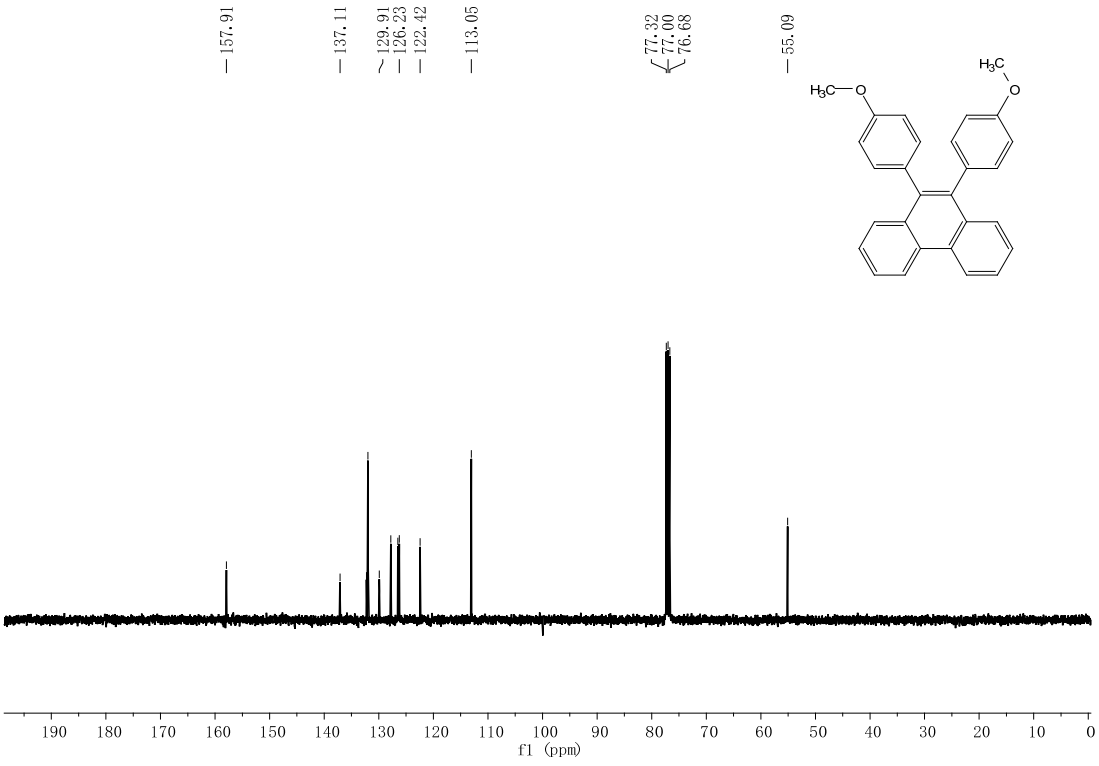
7.50
7.48
7.46
7.25
7.04
6.80
6.78
3.79
H3C
H3C—O
O
2.00
2.05
2.01
2.04
4.01
4.01
6.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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137.11
129.91
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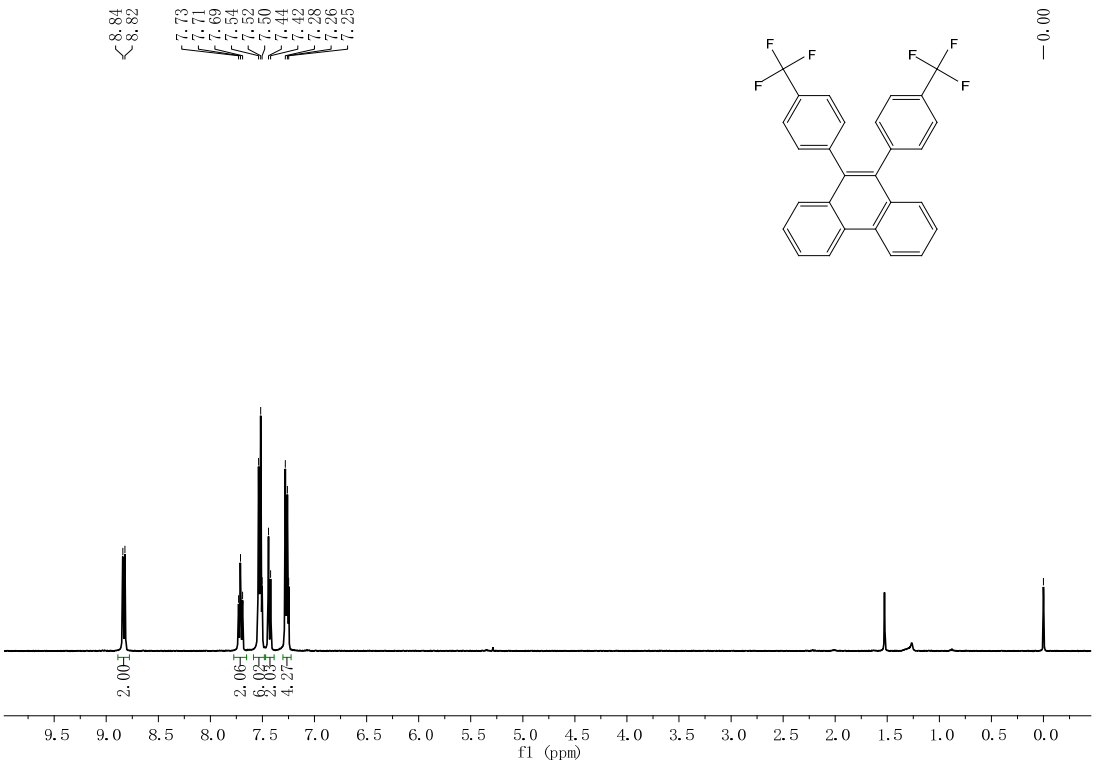
113.05
77.32
77.00
76.68
55.09
H3C
O
H3C
O
f1 (ppm)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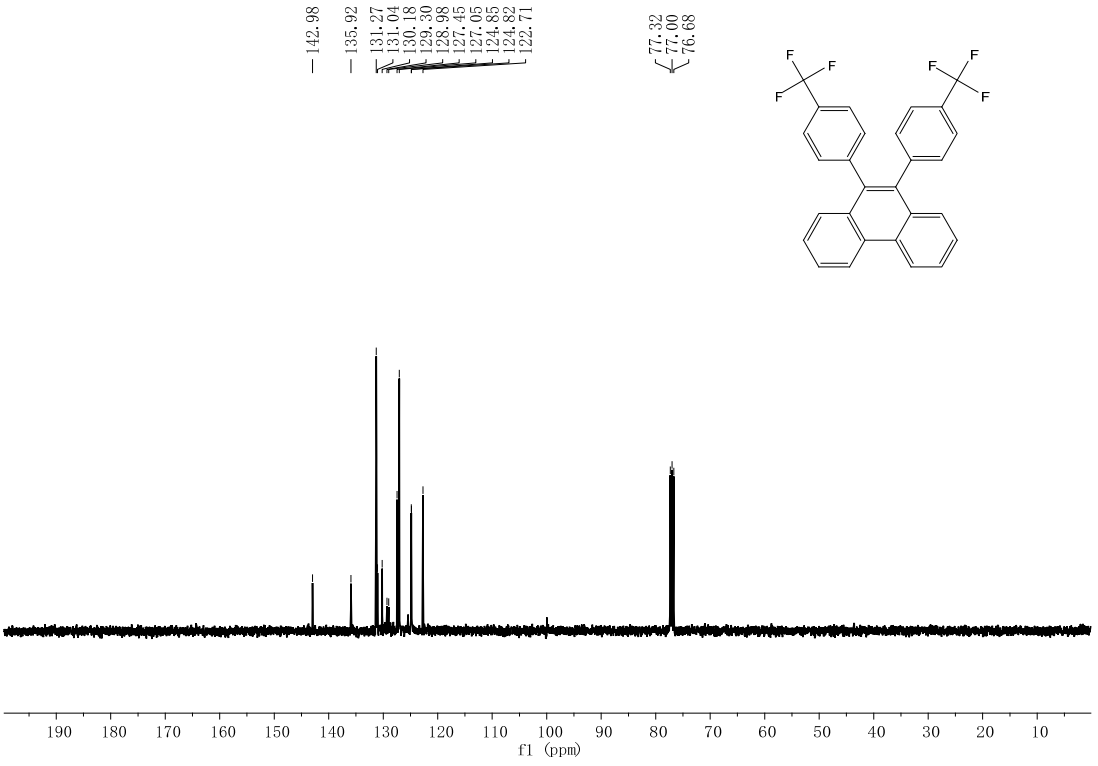
8.82
7.73
7.71
7.69
7.54
7.52
7.50
7.44
7.42
7.28
7.26
7.25
0.00
F
F
F
F
F
F
2.00
2.06
6.08
2.04
4.27
f1 (ppm)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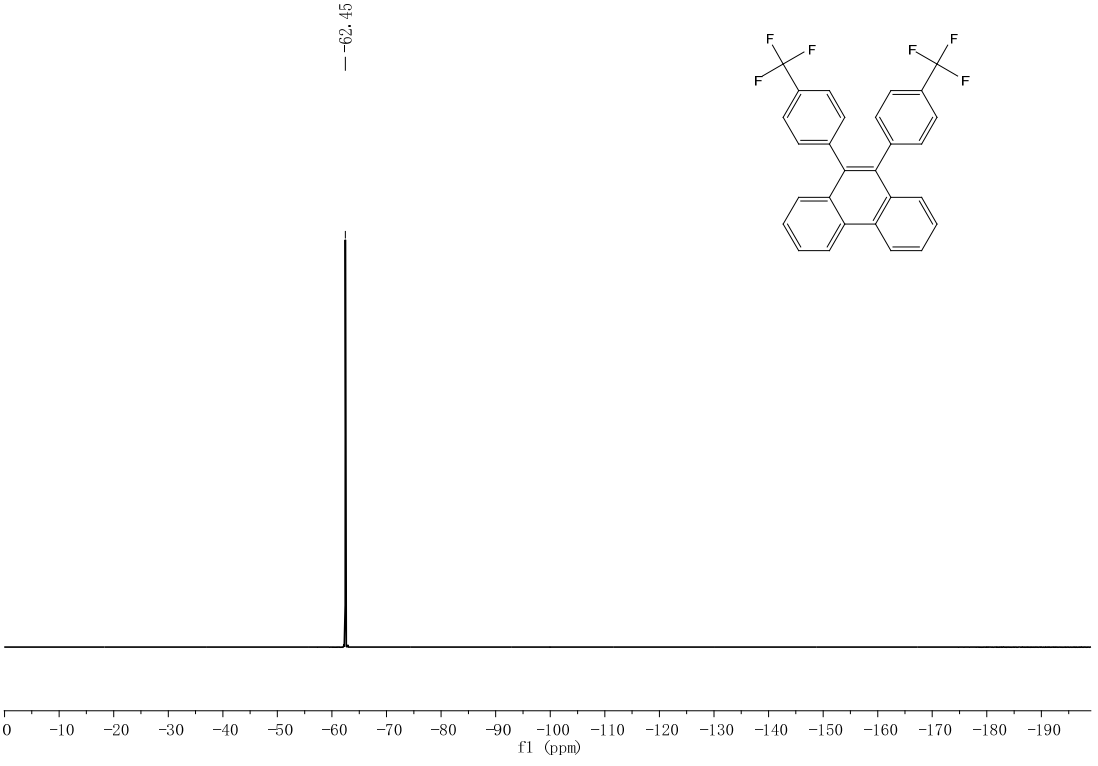
135.92
131.27
131.04
130.18
129.30
128.98
127.45
127.05
124.85
124.82
122.71
77.32
77.00
76.68
F
F
F
F
F
F
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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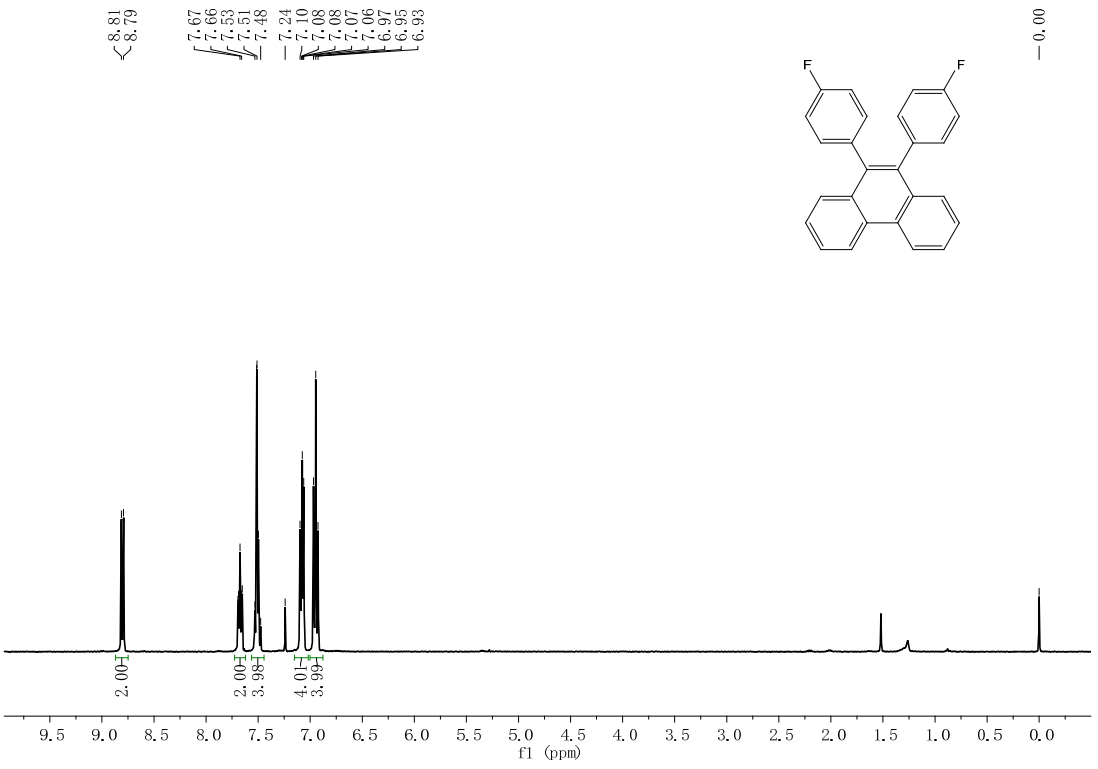
F
F
F
F
F
F
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)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8.79
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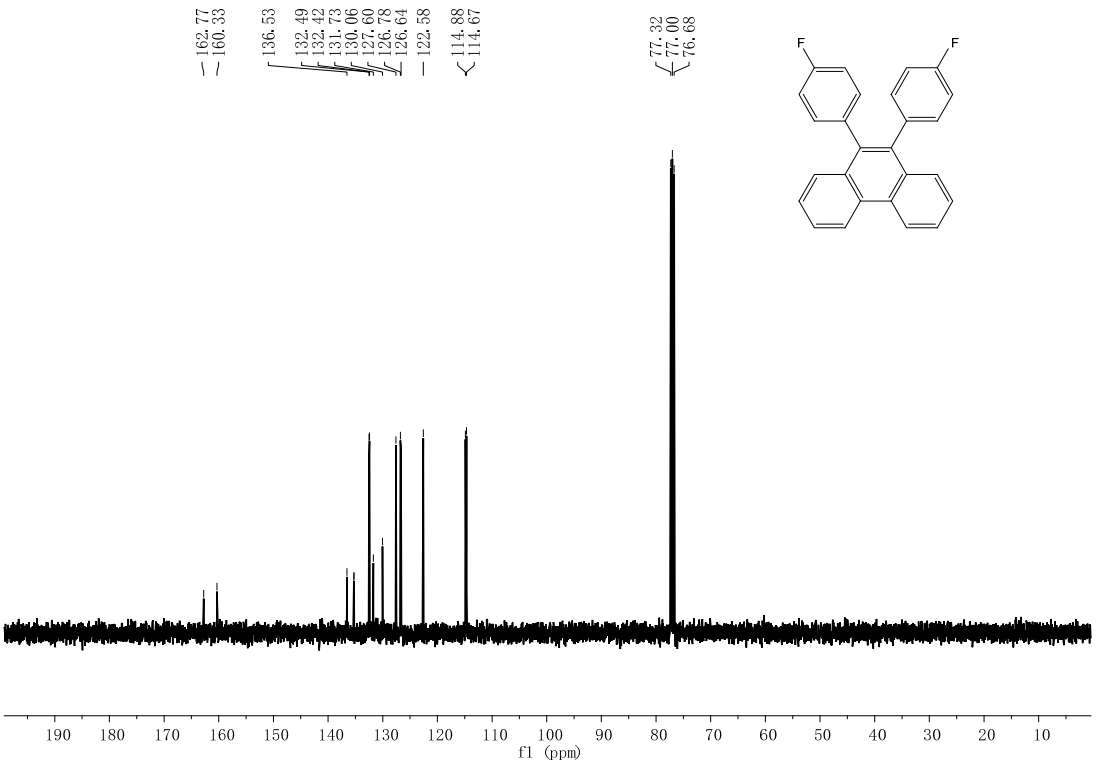
7.53
7.51
7.48
7.24
7.10
7.08
7.08
7.07
7.06
6.97
6.95
6.93
0.00
F
F
2.00
2.00
3.98
4.01
3.99
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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160.33
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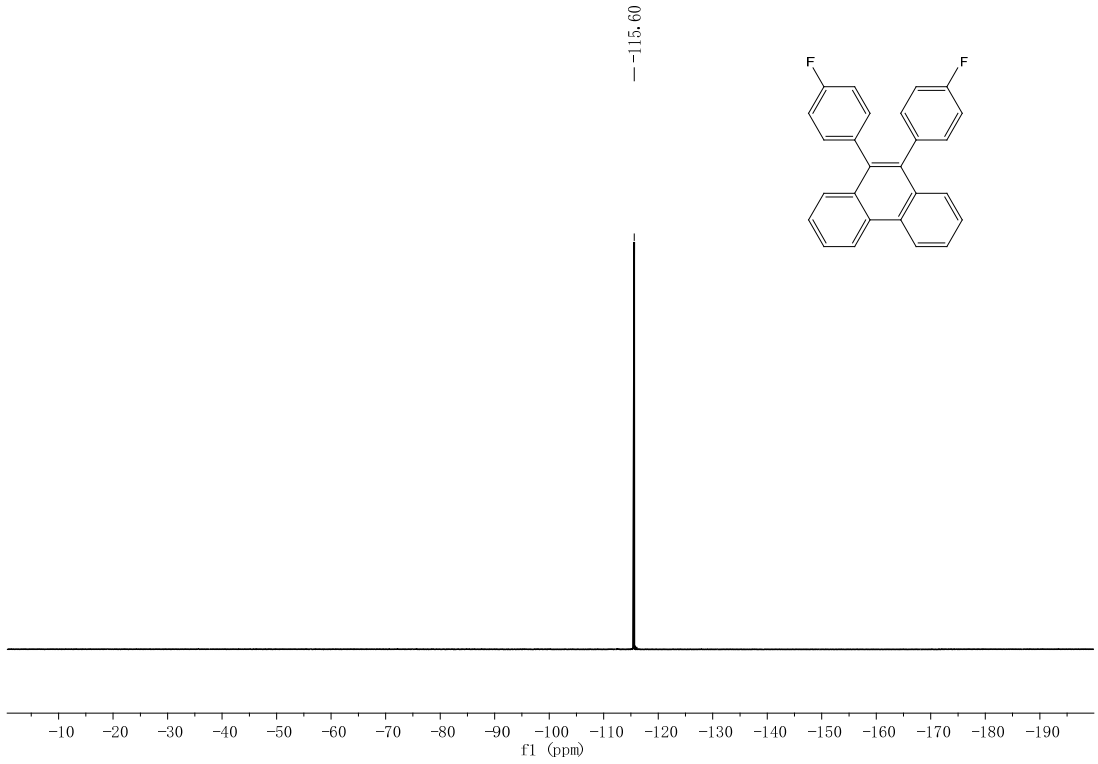
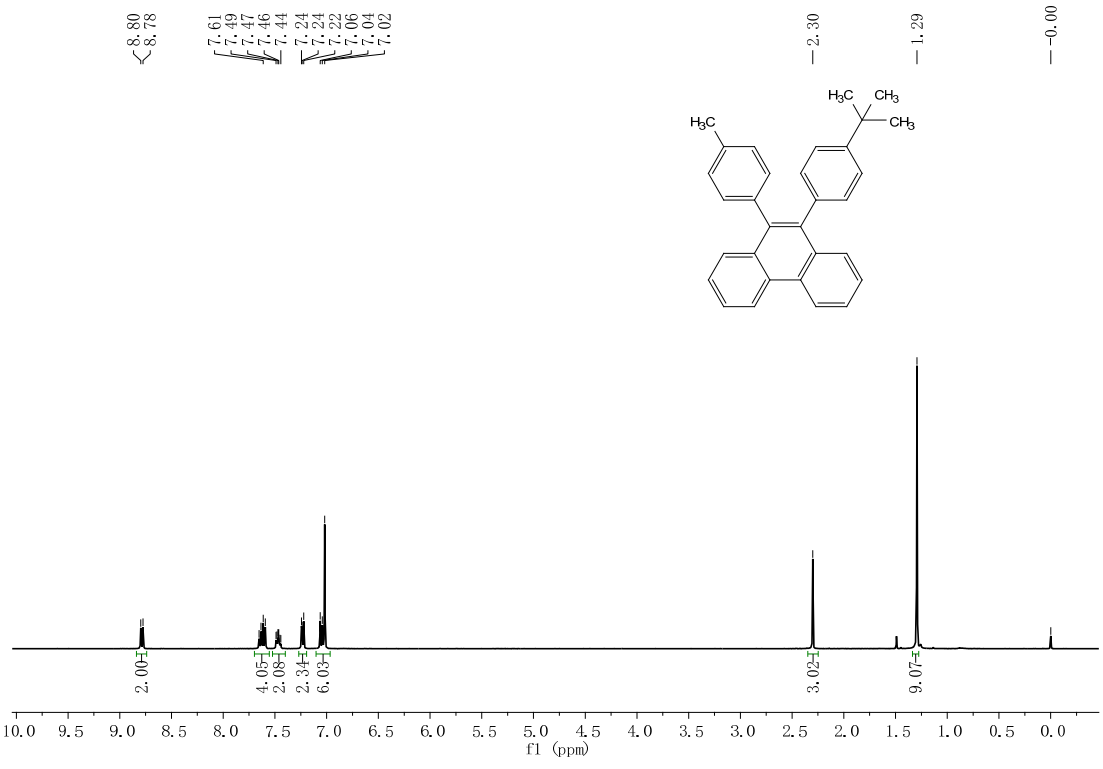
131.73
130.06
127.60
126.78
126.64
122.58
114.88
114.67
77.32
77.00
76.68
F
F
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


-115.60
F
F
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)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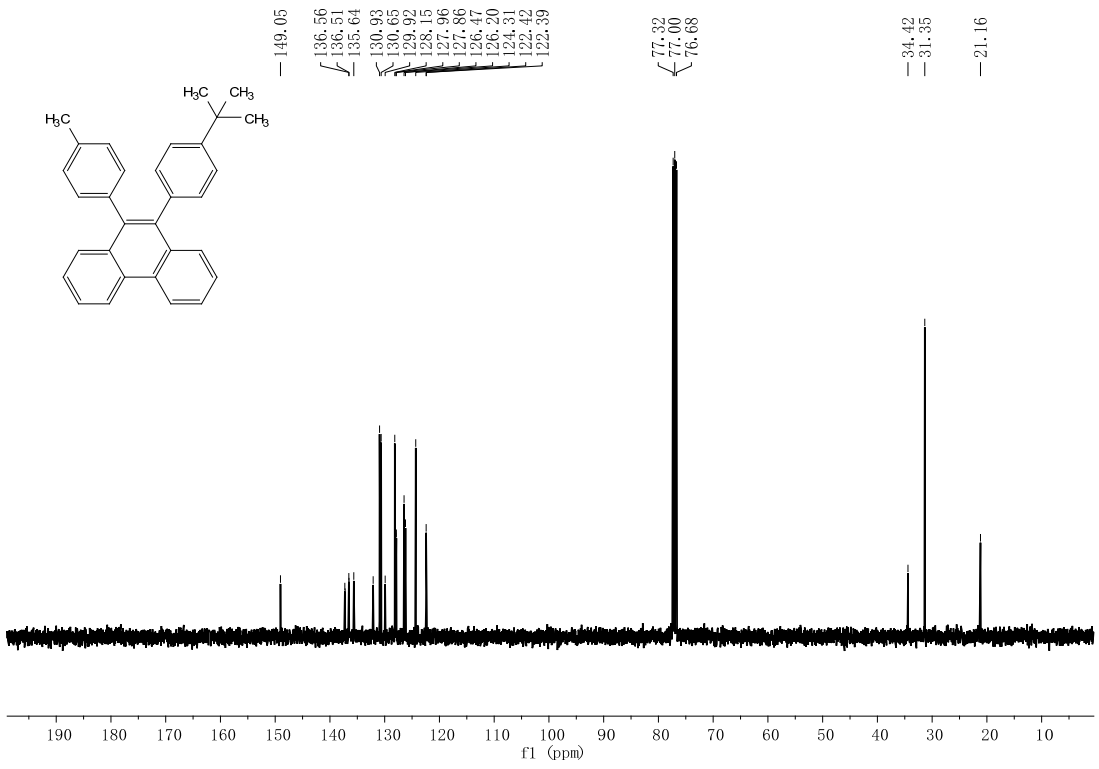
8.78
7.61
7.49
7.47
7.46
7.44
7.24
7.24
7.22
7.06
7.04
7.02
2.30
1.29
0.00
H3C
CH3
H3C
CH3
2.00
4.05
2.08
2.34
6.03
3.02
9.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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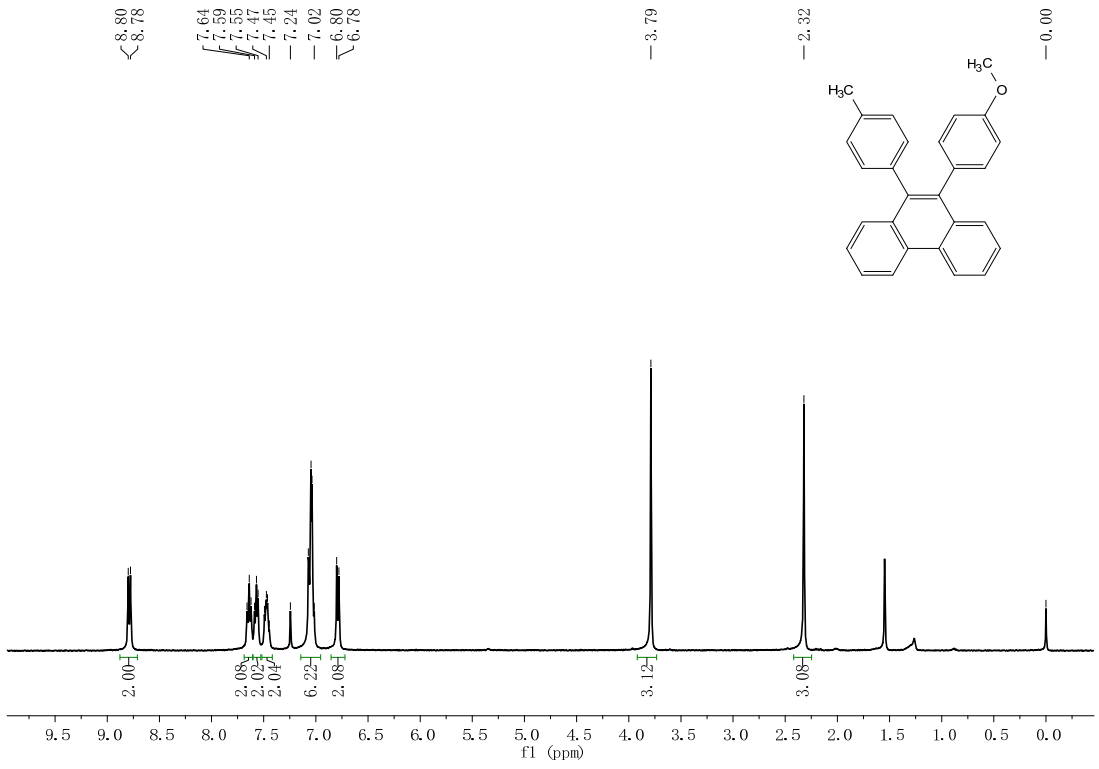
128.15
127.96
127.86
126.47
126.20
124.31
122.42
122.39
77.32
77.00
76.68
34.42
31.35
21.16
H3C
CH3
CH3
H3C
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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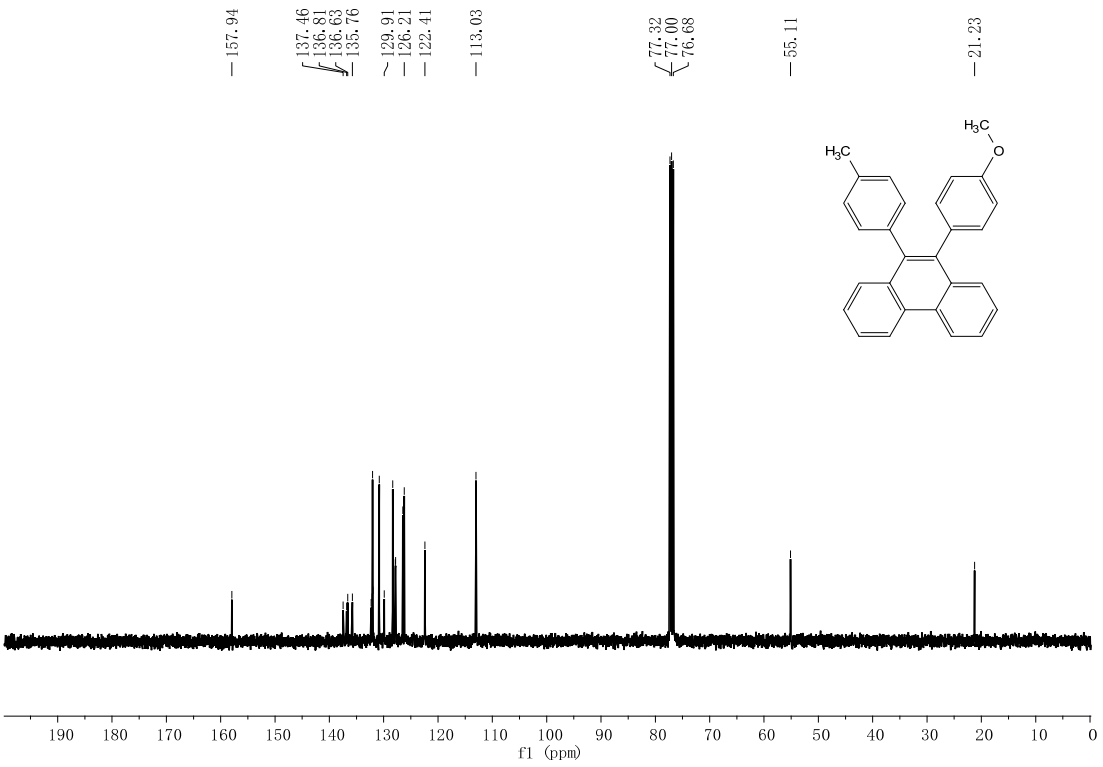
8.78
7.64
7.59
7.55
7.47
7.45
7.24
7.02
6.80
6.78
3.79
2.32
0.00
H3C
H3C
O
2.00
2.08
2.02
2.04
6.22
2.08
3.12
3.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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136.63
135.76
129.91
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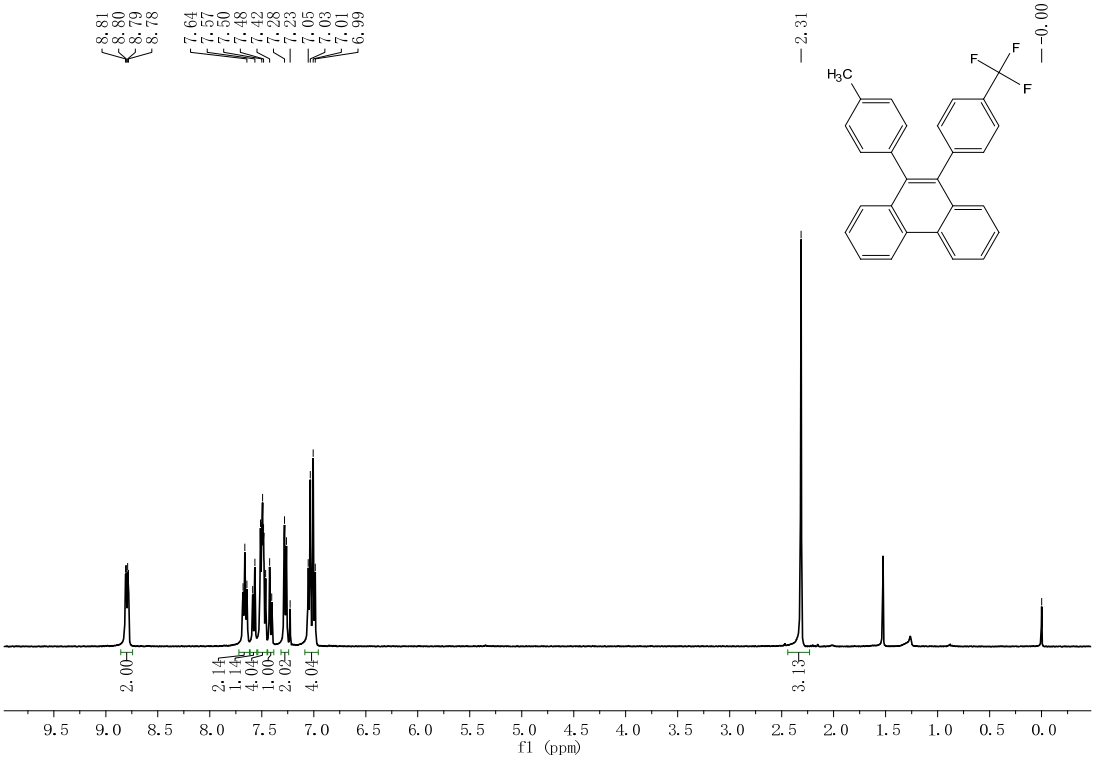
122.41
113.03
77.32
77.00
76.68
55.11
21.23
H3C
O
H3C
f1 (ppm)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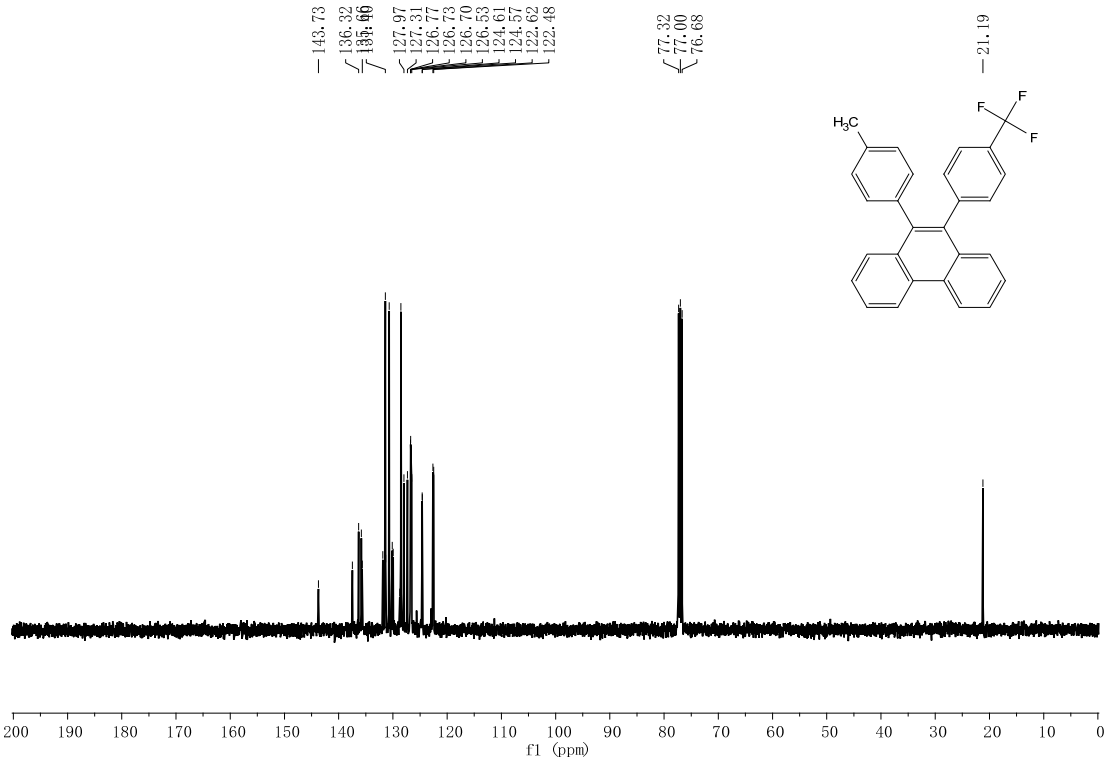
8.80
8.79
8.78
7.64
7.57
7.50
7.48
7.42
7.28
7.23
7.05
7.03
7.01
6.99
2.31
0.00
H3C
F
F
F
2.00
2.14
1.14
4.04
1.00
2.02
4.04
3.13
f1 (ppm)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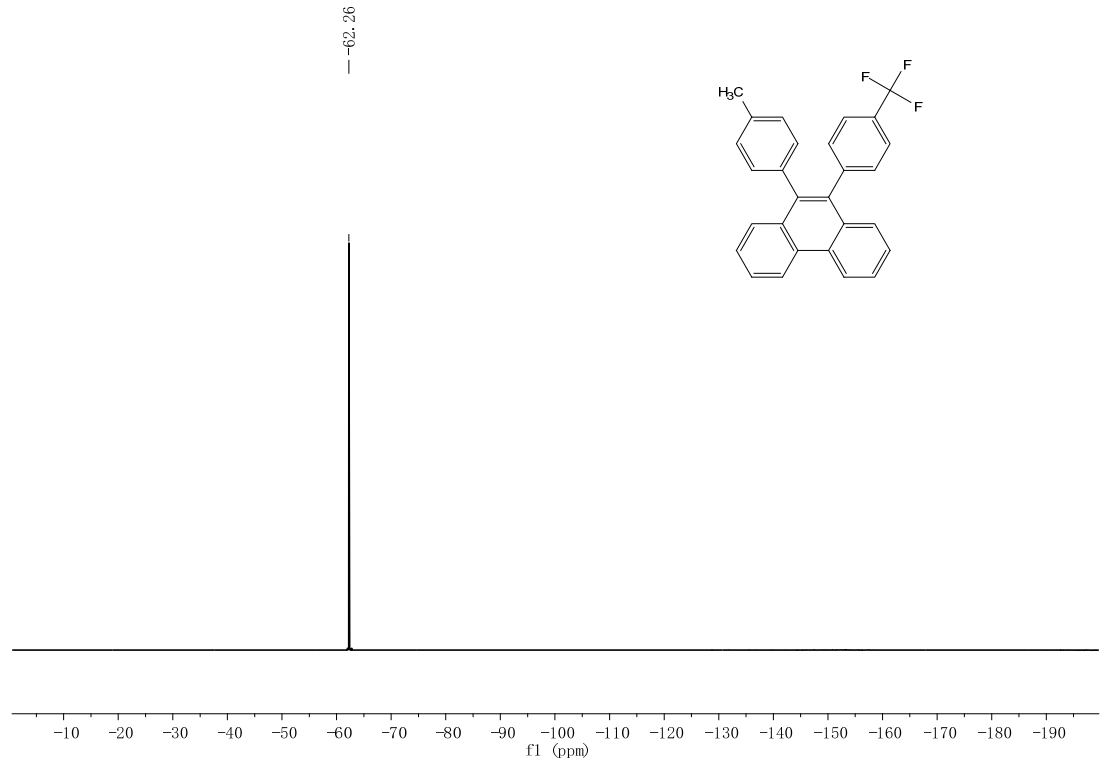
126.73
126.70
126.53
124.61
124.57
122.62
122.48
77.32
77.00
76.68
21.19
H3C
F
F
F
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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F
F
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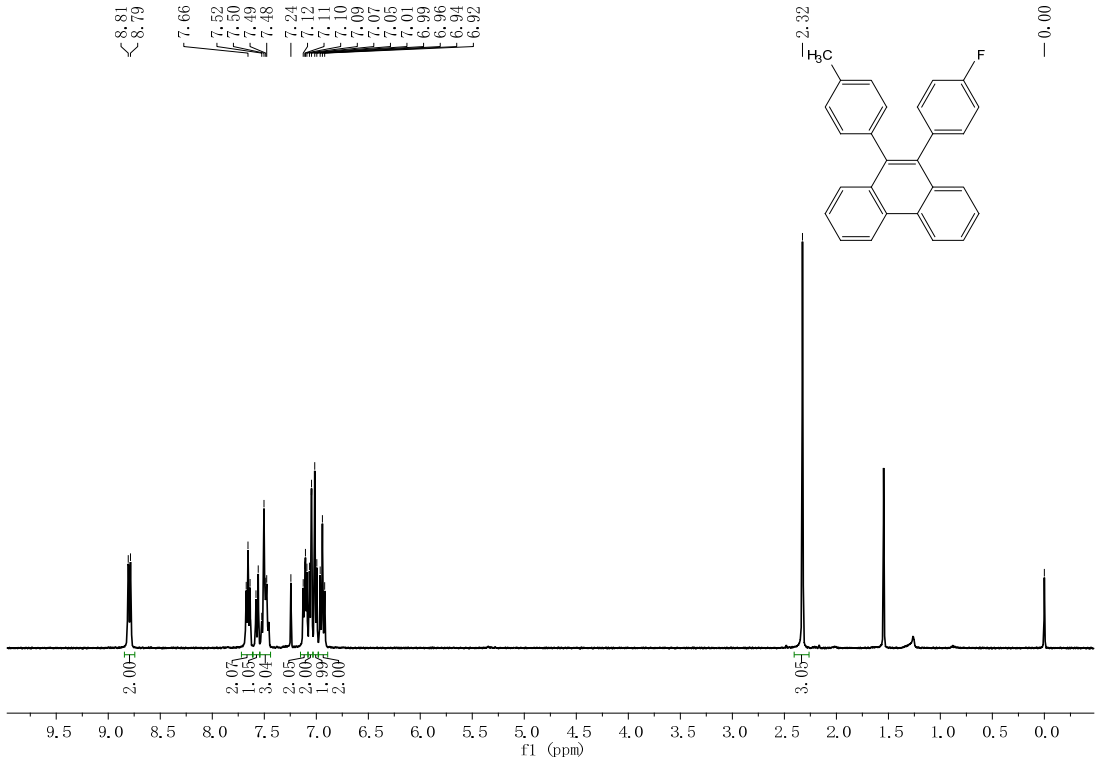
f1 (ppm)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8.79
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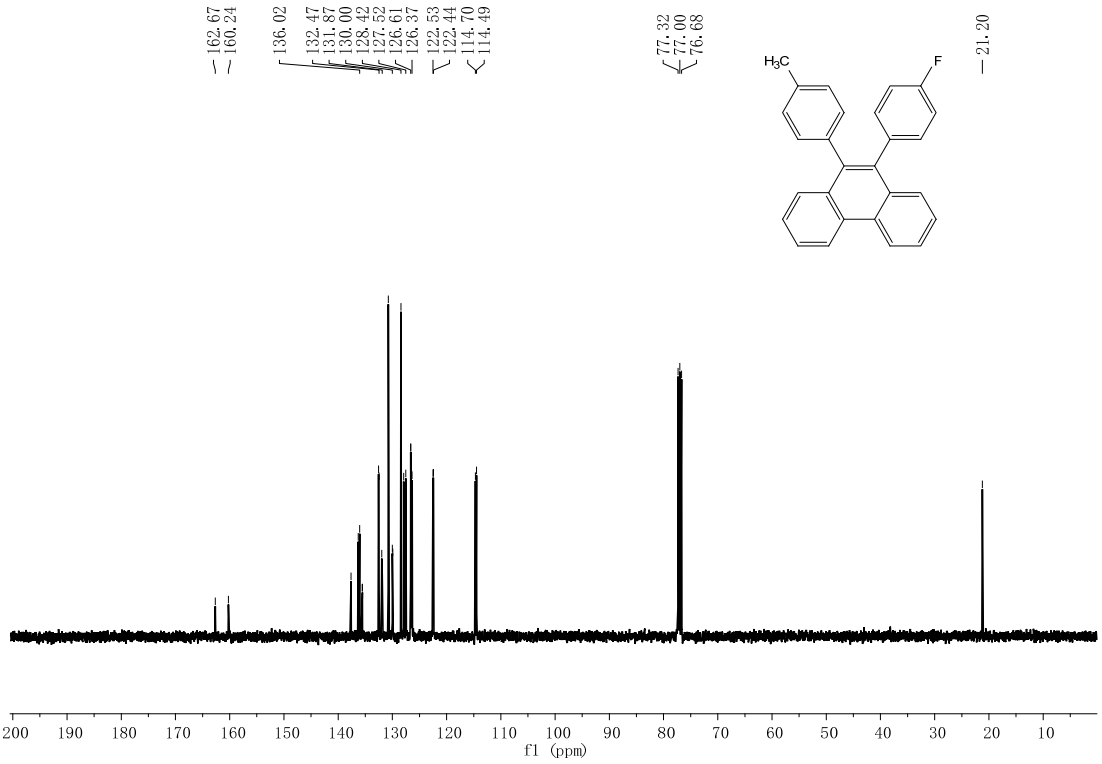
7.52
7.50
7.49
7.48
7.24
7.12
7.11
7.10
7.09
7.07
7.05
7.01
6.99
6.96
6.94
6.92
2.32
0.00
H3C
F
2.00
2.07
1.05
3.04
2.05
2.00
1.99
2.00
3.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.52
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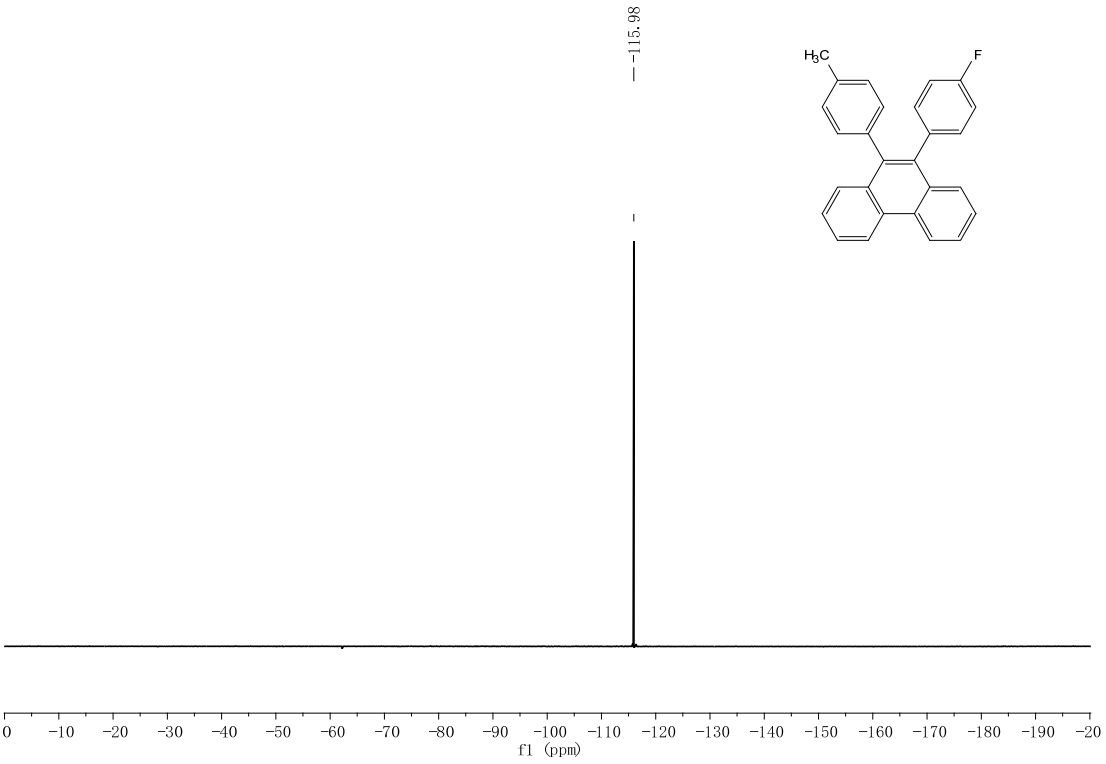
126.37
122.53
122.44
114.70
114.49
77.32
77.00
76.68
21.20
H3C
F
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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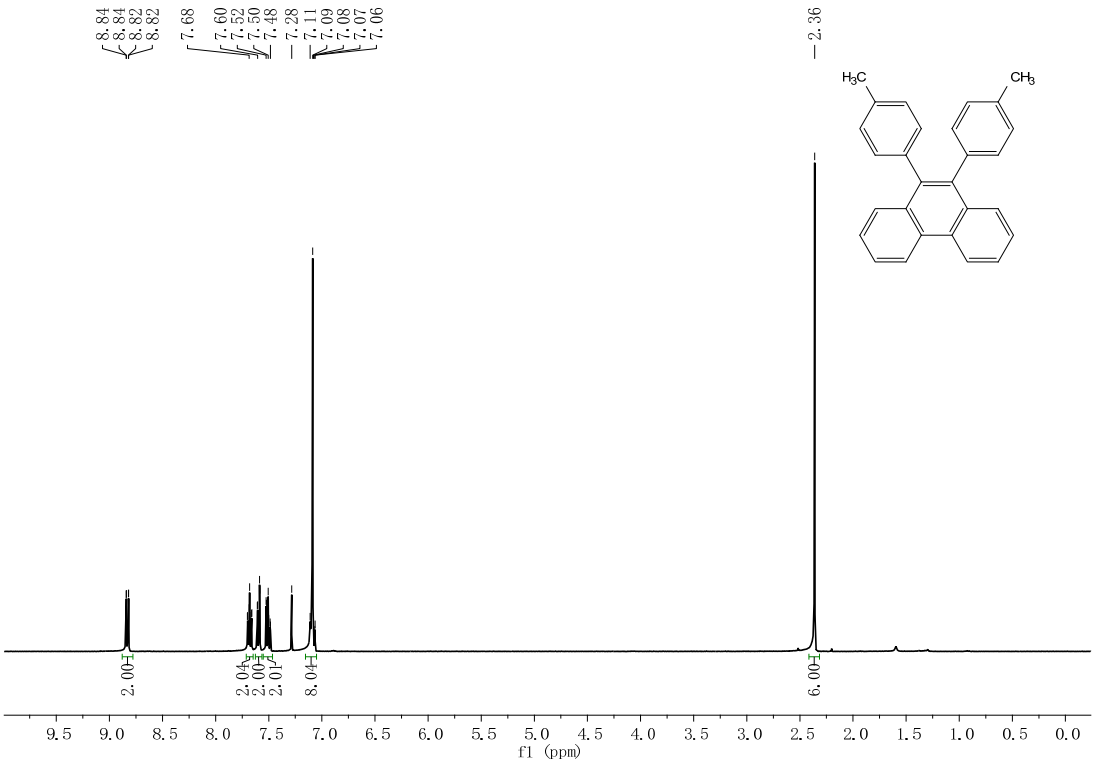
f1 (ppm)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8.82
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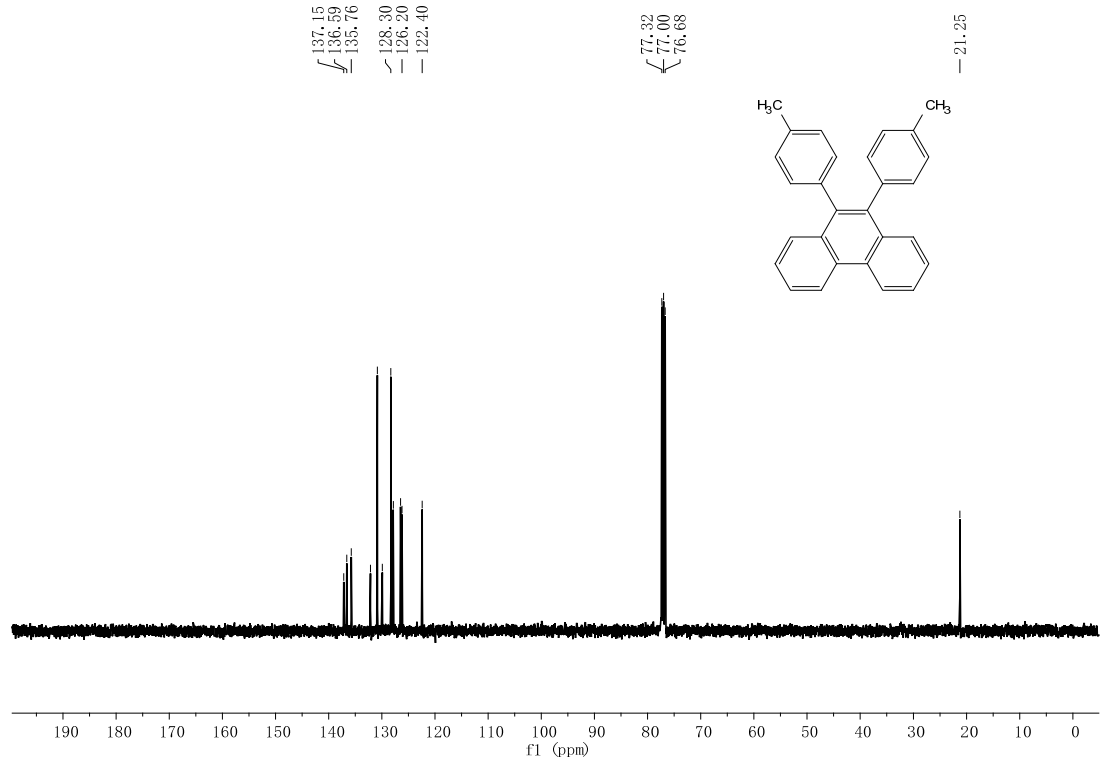
7.50
7.48
7.28
7.11
7.09
7.08
7.07
7.06
2.36
H3C
CH3
2.00
2.04
2.00
2.01
8.04
6.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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76.68
21.25
H3C
CH3
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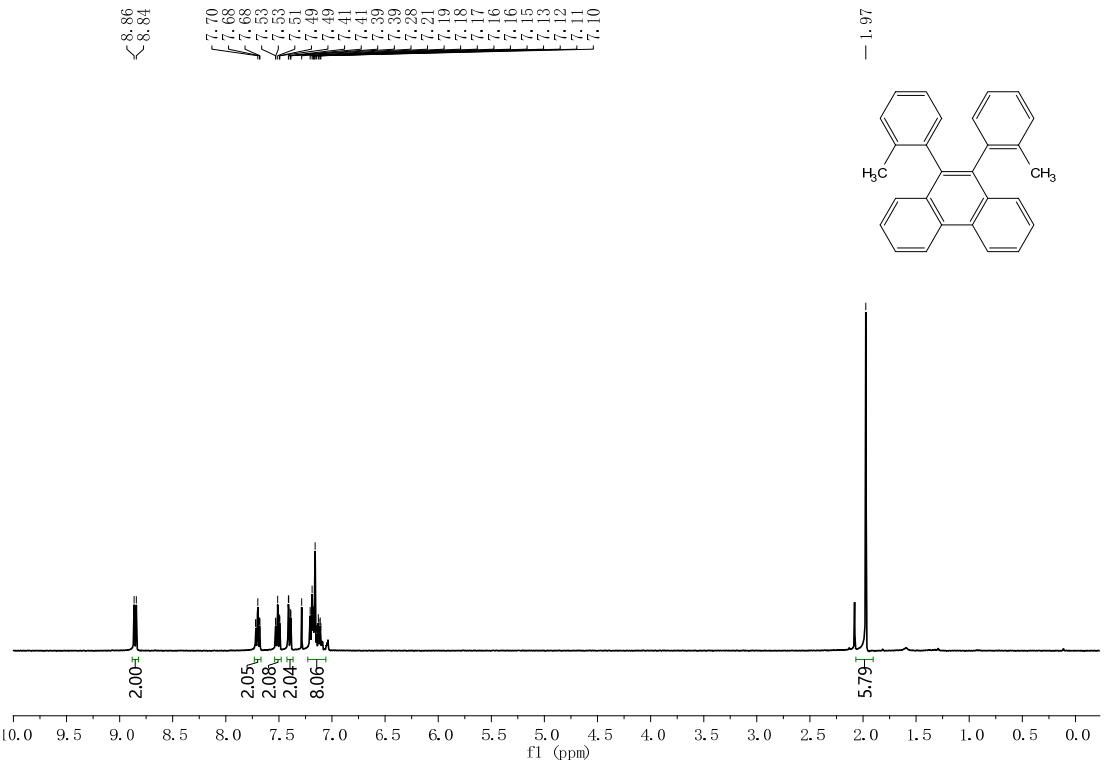
f1 (ppm)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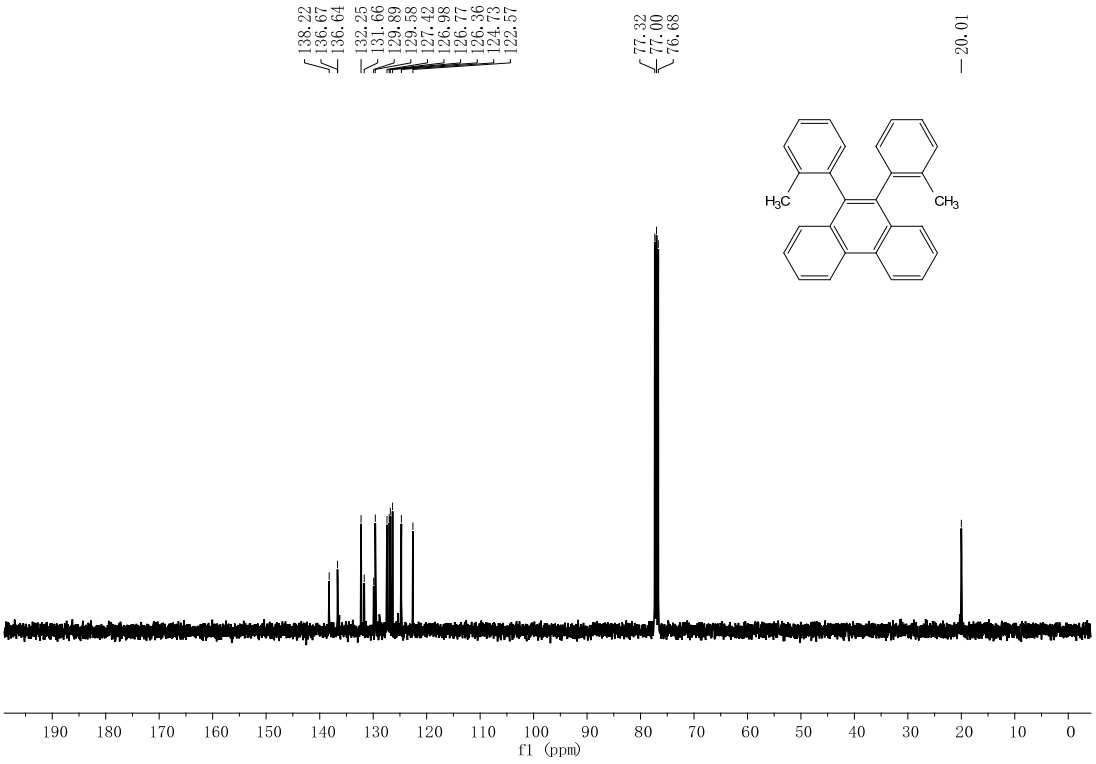
7.39
7.28
7.21
7.19
7.18
7.17
7.16
7.16
7.15
7.13
7.12
7.11
7.10
1.97
H3C
CH3
2.00
2.05
2.08
2.04
8.06
5.79
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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76.68
20.01
H3C
CH3
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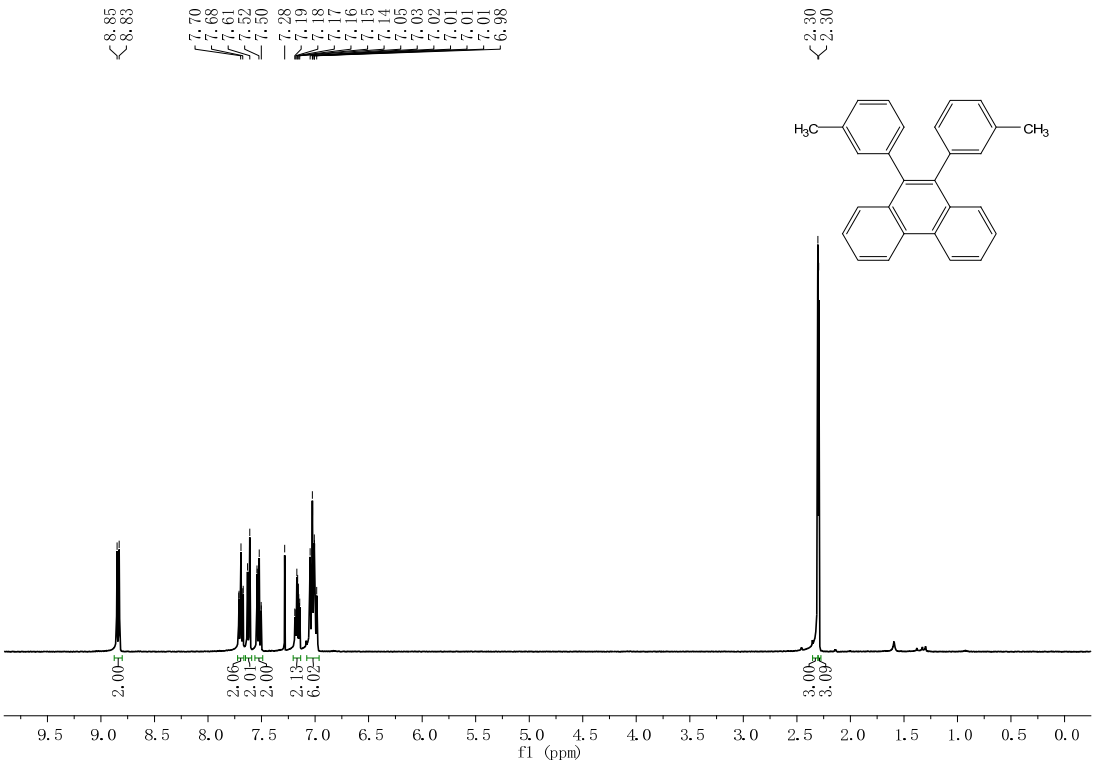
f1 (ppm)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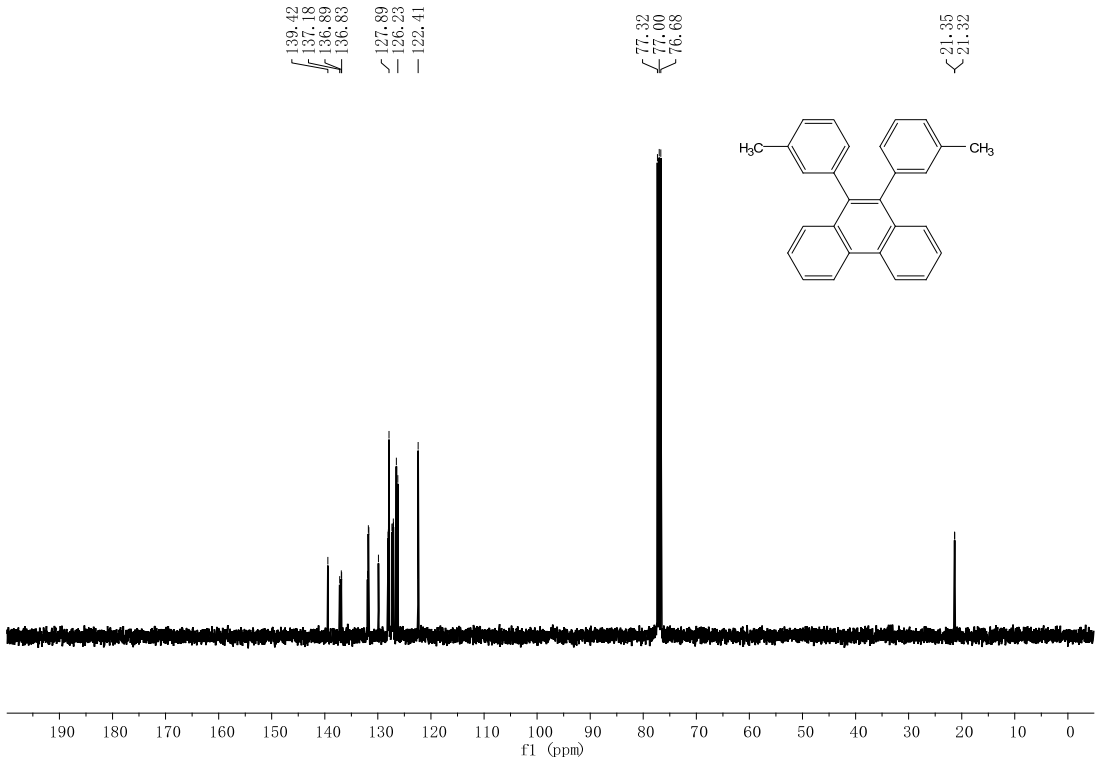
7.16
7.15
7.14
7.05
7.03
7.02
7.01
7.01
7.01
6.98
2.30
2.30
H3C
CH3
2.00
2.06
2.01
2.00
2.13
6.02
3.00
3.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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122.41
77.32
77.00
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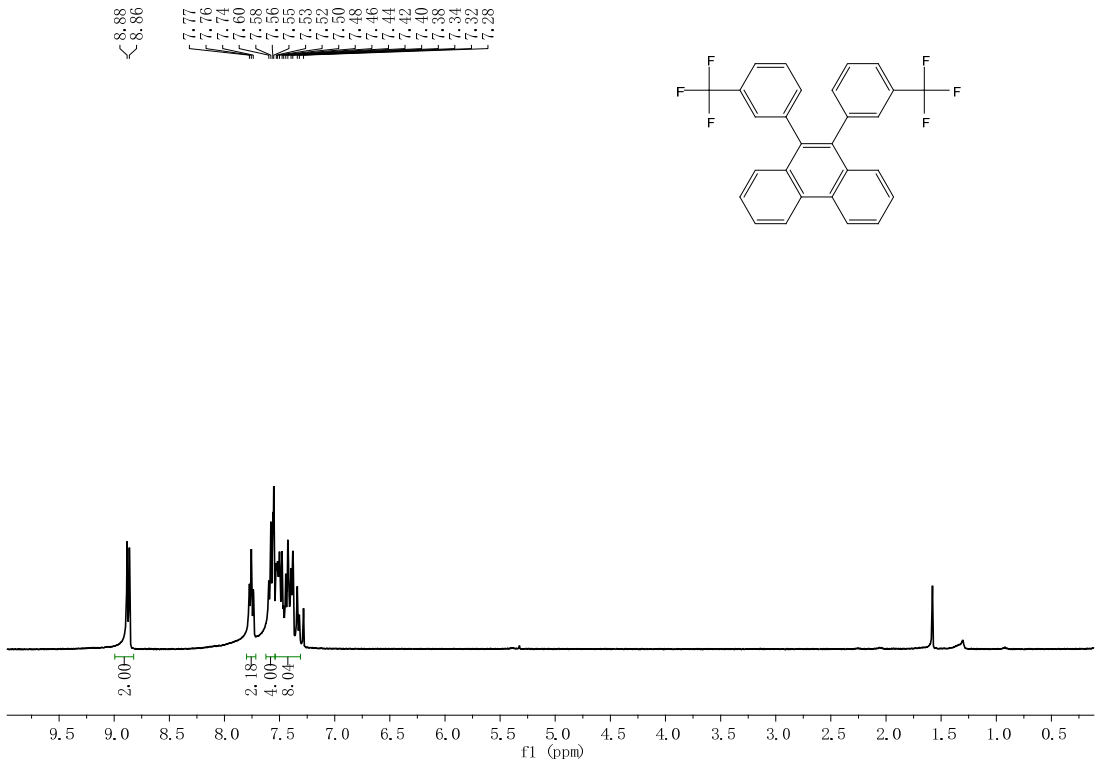
21.35
21.32
H3C
CH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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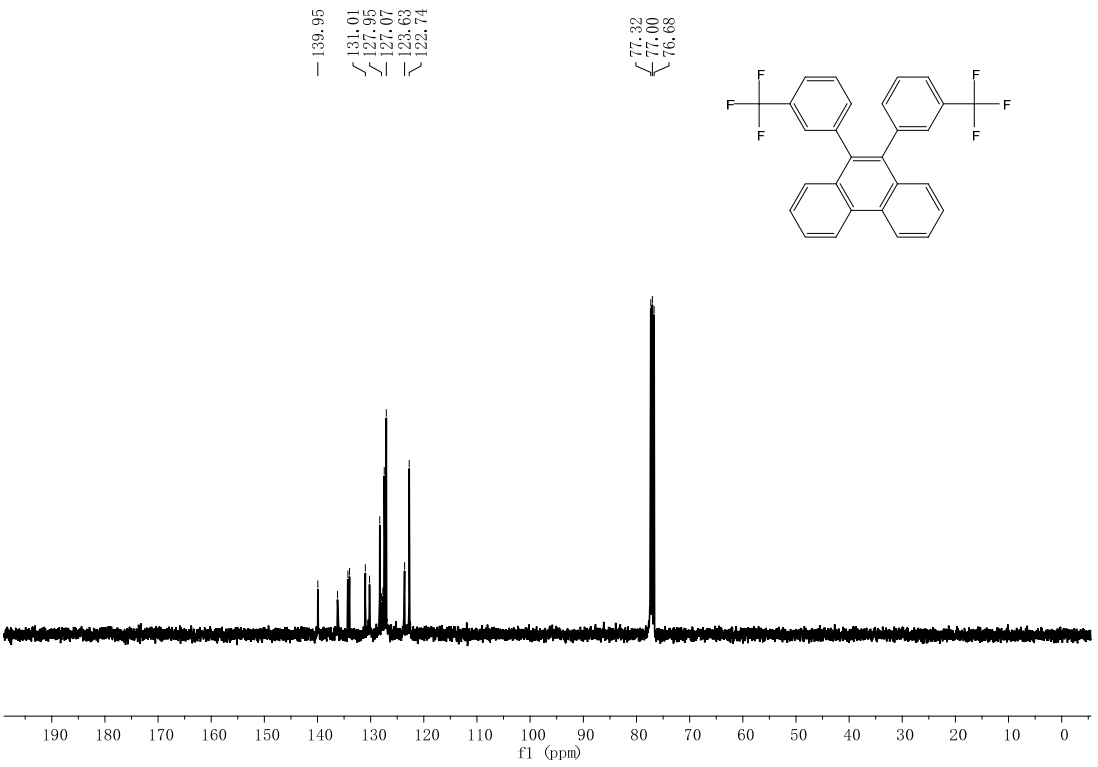
7.52
7.50
7.48
7.46
7.44
7.42
7.40
7.38
7.34
7.32
7.28
F
F
F
F
F
F
2.00
2.18
4.00
8.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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122.74
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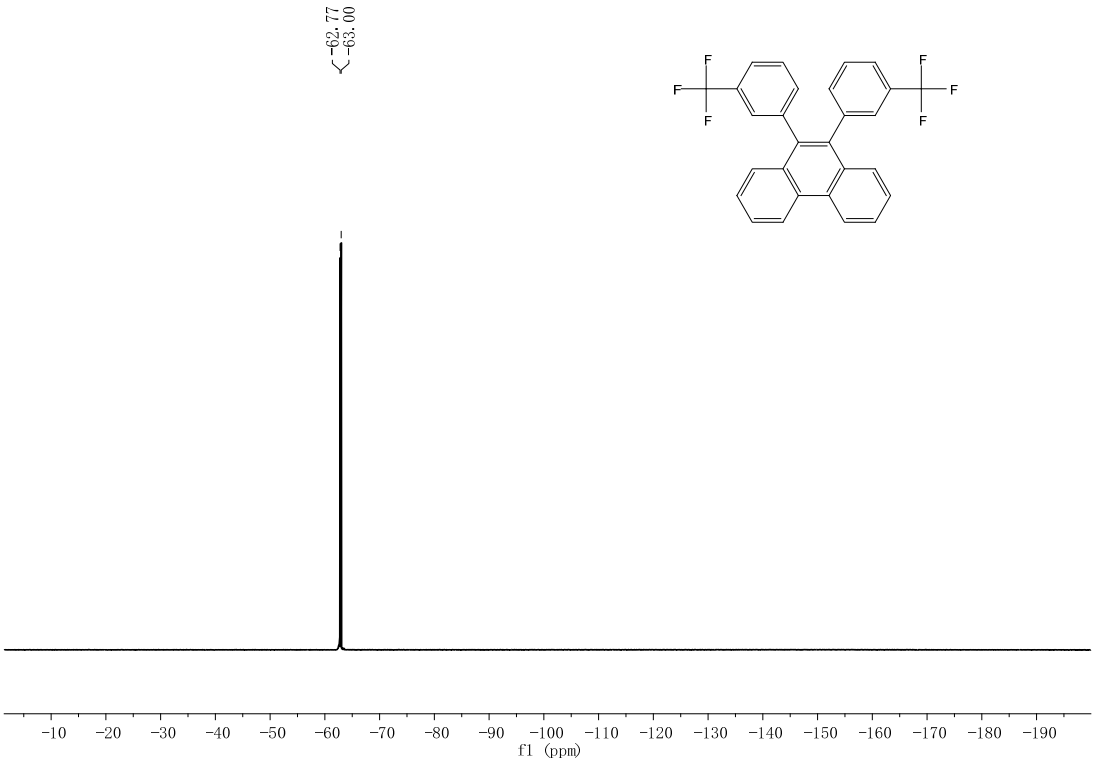
77.00
76.68
F
F
F
F
F
F
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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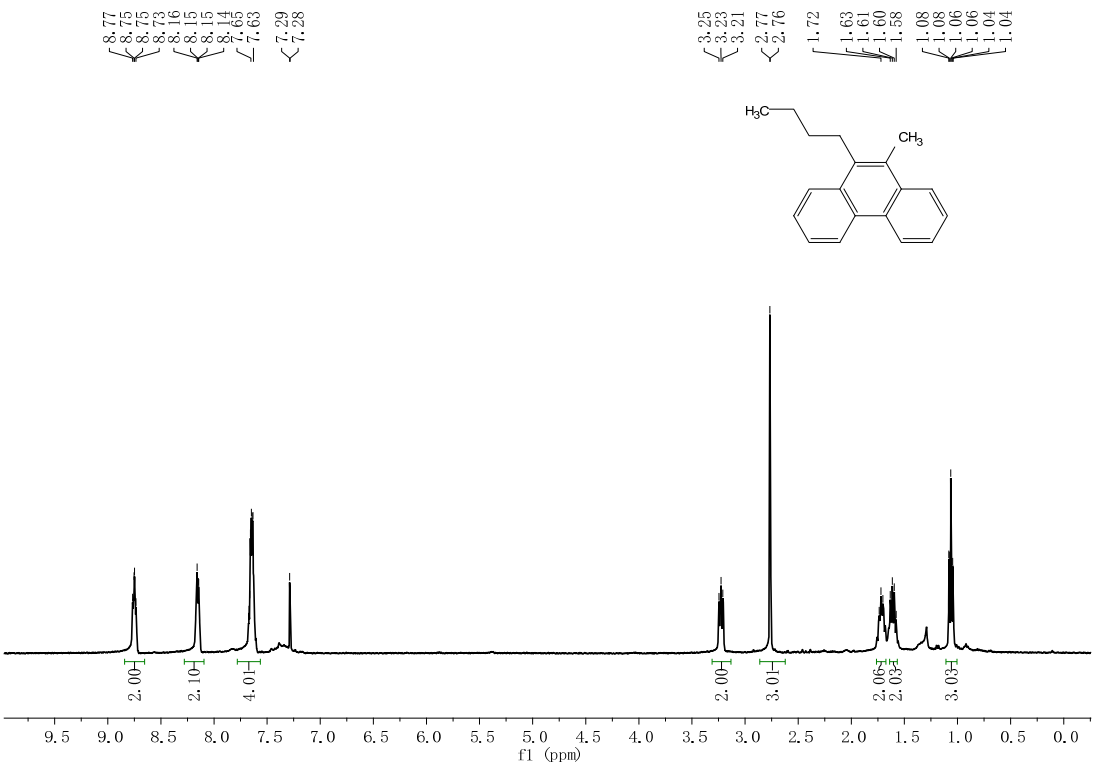
F
F
F
F
F
F
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)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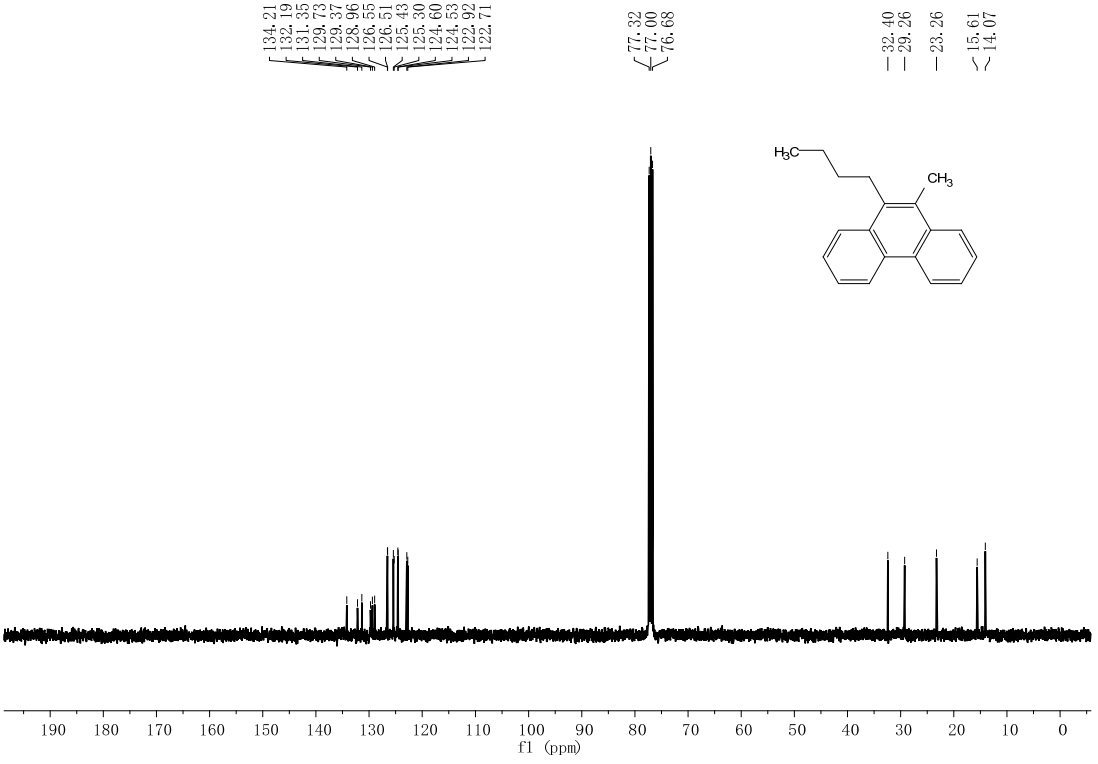
3.23
3.21
2.77
2.76
1.72
1.63
1.61
1.60
1.58
1.08
1.08
1.06
1.06
1.04
1.04
H3C
CH3
2.00
2.10
4.01
2.00
3.01
2.06
2.03
3.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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124.60
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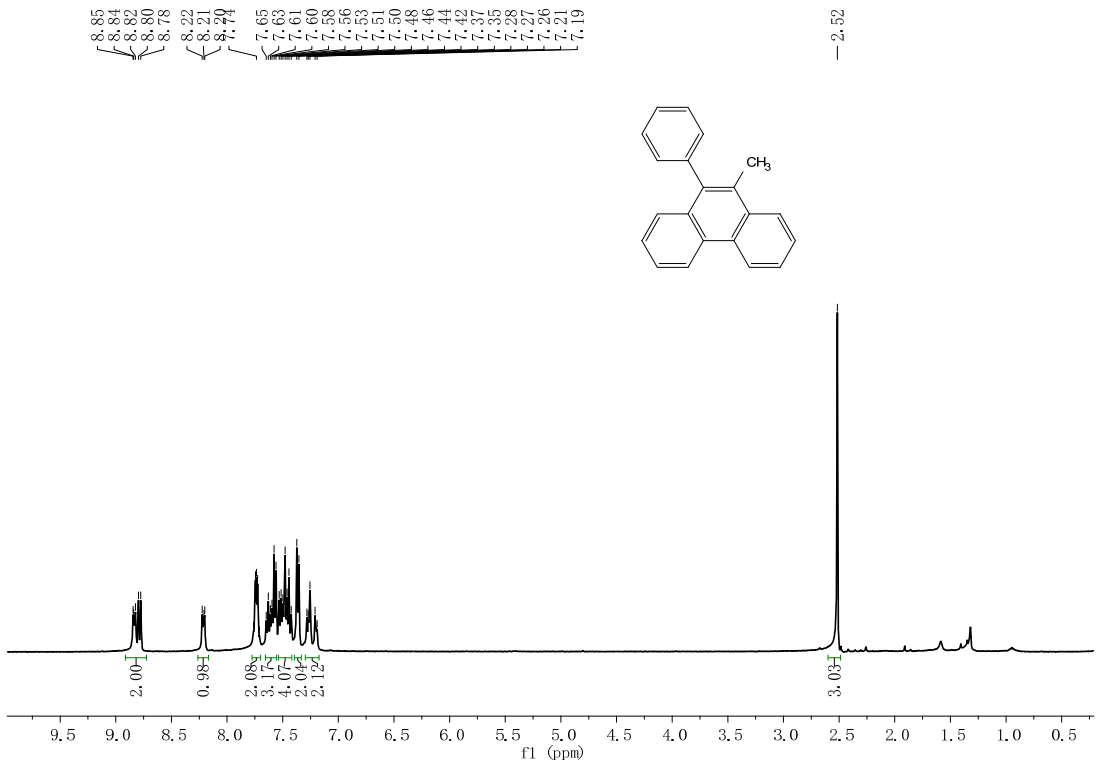
122.92
122.71
77.32
77.00
76.68
32.40
29.26
23.26
15.61
14.07
H3C
CH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.60
7.58
7.56
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7.51
7.50
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7.46
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7.42
7.37
7.35
7.28
7.27
7.26
7.21
7.19
2.52
CH3
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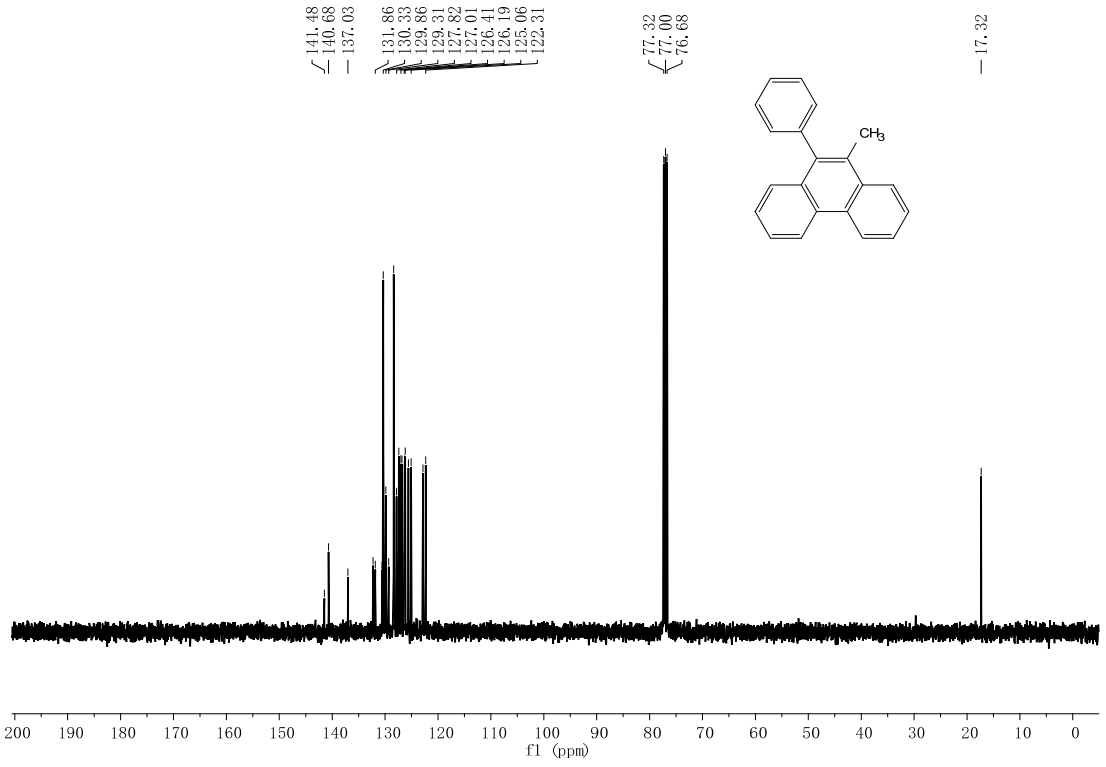
0.98
2.08
3.17
4.07
2.04
2.12
3.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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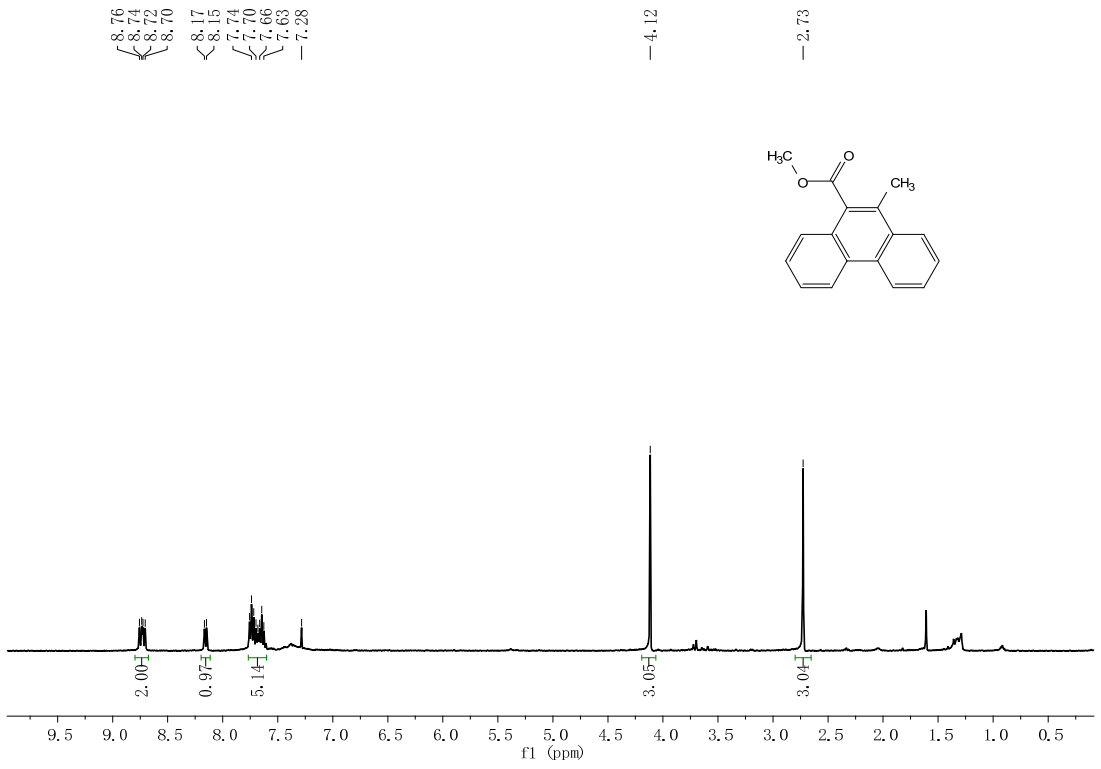
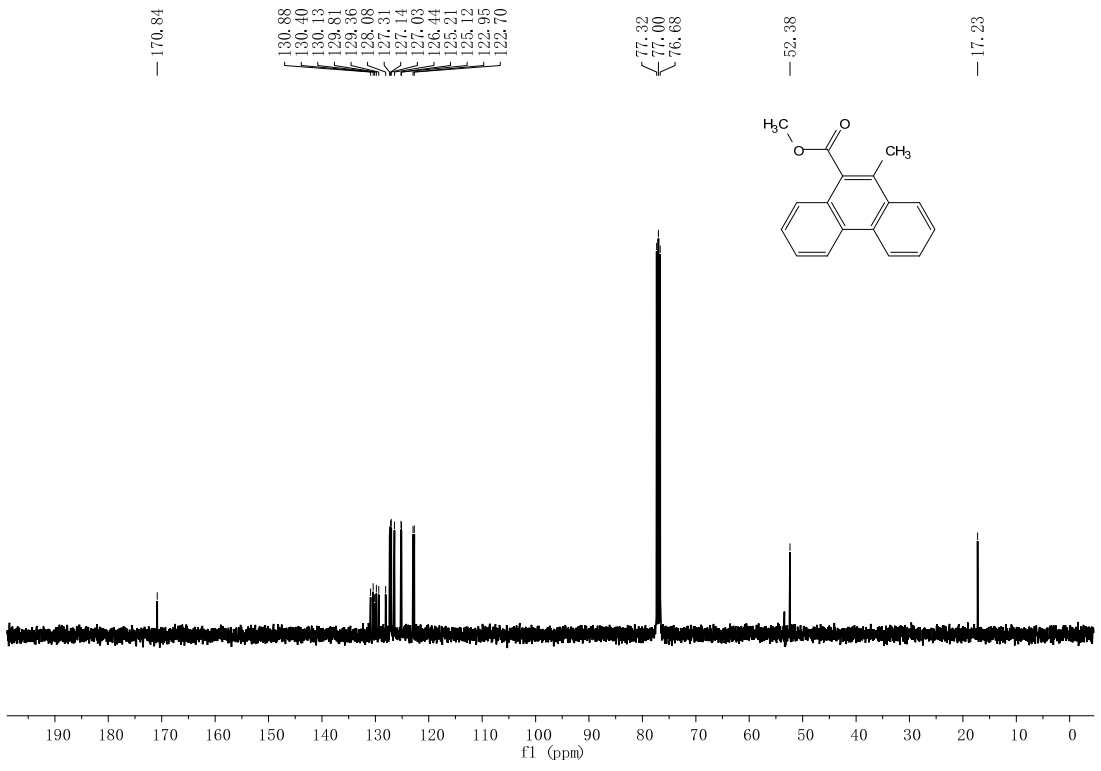
129.86
129.31
127.82
127.01
126.41
126.19
125.06
122.31
77.32
77.00
76.68
17.32
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.76
8.74
8.72
8.70
8.17
8.15
7.74
7.70
7.66
7.63
7.28
4.12
2.73
H3C
O
O
CH3
2.00
0.97
5.14
3.05
3.04
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
f1 (ppm)


170.84
130.88
130.40
130.13
129.81
129.36
128.08
127.31
127.14
127.03
126.44
125.21
125.12
122.95
122.70
77.32
77.00
76.68
52.38
17.23
H3C
O
O
CH3
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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