Supporting Information

Development of Photochromic Fused *2H*-Naphthopyrans with Promising Thermal Fading Rates

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CONTENTS

1. General Information

Transient Absorption Spectroscopy. UV−vis absorption spectra were measured with a UV-3600 Plus UV-vis-NIR spectrophotometer equipped with a temperature-controlled cell holder (Shimadzu Corp.). Light irradiation was carried out using a solar simulator with a xenon 300W lamp, 200−2000nm (EOS Technologies Inc.) or a UV-LED (UV-400, Keyence), equipped with a UV-L6 lens unit (365 nm, 260 mW). The transient absorption spectra and the time variation were recorded on a USB 4000 multichannel detector (Ocean Optics, Inc.).

Computational Details. All DFT calculations were conducted by using Gaussian 09.[1] Geometry optimizations were carried out at the M06-2X level of theory with the SDD basis set for copper and the 6-31+G(d,p) basis set for the other atoms. Vibrational frequencies were computed to check whether each optimized structure is an energy minimum or a transition state. To obtain more accurate electronic energies, single-point energy calculations were performed at the SMD[2]-M06-2X/ 6-311++g(d,p) level with the M06-2X/6-31+G(d,p) optimized structures. TDDFT calculations were performed at the MPW1PW91/6-31+G(d,p) level of the theory for the optimized structures. The HOMO orbital coefficient was calculated by using the NBO[3,4] module of Gaussian 09, NCIPLOT[5,6] and Multiwfn.[7,8] The structures of molecules were generated using CYLView[9] and VMD.[10]

Synthesis and Characterization. All air- and moisture-sensitive manipulations were carried out under nitrogen atmosphere with standard Schlenk technique. All glassware was washed with distilled water and dried. Column chromatography was performed using 200-300 mesh silica gels. The NMR spectra were recorded on a Bruker-400 instrument and chemical shifts are reported in ppm relative to the residual deuterated solvents. High-resolution mass spectra (HRMS) were performed with electrospray spectrometer Waters Micromass Q-TOF Premier Mass Spectrometer. The intensity data were collected on an a Rigaku 002 Saturn 944 diffractometer using graphite-monochromated Cu Kα (λ = 1.54184 Å) radiation. Unless otherwise noted, all reagents and reaction solvents were purchased from commercial sources, and used without further purification.

1,1-Diphenylprop-2-yn-1-ol (**5a**)[11], 1-([1,1'-Biphenyl]-4-yl)-1-phenylprop-2-yn-1-ol (**5b**)[12], 1,1-Bis(4-methoxyphenyl)prop-2-yn-1-ol (**5c**)[13], methyl 2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoate(**1a**)[15] were prepared according to the procedures in literatures.

2. Synthesis

B_2Pin_2 (2.2 g, 8.6 mmol), methyl 2-bromobenzoate (5.4 mmol), sodium carbonate (3.5 g, 25.7 mmol) and $Pd(PPh_3)_2Cl_2$ (360 mg, 0.44 mmol) were added to a 100 mL round-bottom flask, placed under nitrogen, dissolved in 1,4-dioxane (40 mL), and stirred for 12 h at 80 °C. After completion as determined by TLC analysis, the reaction mixture was extracted with EA (3×20 mL) and the combined organic layers were washed with brine (30 mL). The solution was then dried ($MgSO_4$), filtered, and concentrated. The crude product was purified by flash column chromatography (PE : EA = 20 : 1) to give methyl 2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl) benzoate derivatives (**1b-1d**).

Methyl 4-fluoro-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoate (1b)

Colorless oil, 1.4 g, 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.96-7.94 (m, 1H), 7.15-7.13 (m, 1H), 7.07 (d, *J* = 8.0 Hz, 1H), 3.90 (s, 3H), 1.41 (s, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 167.50, 165.16 (d, *J* = 254.9 Hz), 131.55 (d, *J* = 8.9 Hz), 129.44 (d, *J* = 2.8 Hz), 119.06 (d, *J* = 20.9 Hz), 115.98 (d, *J* = 21.9 Hz), 84.32, 52.41, 24.83.

Methyl 4-methyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoate (1c) [14]

Colorless oil, 462 mg, 31% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.75 (d, *J* = 7.1 Hz, 1H), 7.27 (s, 1H), 7.25-7.23 (m, 1H), 3.87 (s, 3H), 2.42 (s, 3H), 1.43 (s, 12H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 168.76, 141.34, 133.50, 133.22, 128.55, 125.98, 83.87, 52.23, 25.37, 21.53.

Methyl 5-methoxy-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoate (1d) [15]

Colorless oil, 426 mg, 27% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.45-7.41 (m, 2H), 7.05-7.02 (m, 1H), 3.88 (s, 3H), 3.81 (s, 3H), 1.38 (s, 12H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 168.35, 160.34, 135.60, 133.89, 117.94, 113.71, 83.83, 55.31, 52.29, 24.84.

4-Bromo-L-Naphthol (1.8 g, 7.8 mmol), methyl 2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoate derivatives (**1a-1d**) (8.6 mmol), potassium carbonate (6.6 g, 48 mmol) and $Pd(PPh_3)_4$ (1.1 g, 1mmol) were added to a 250 mL round-bottom flask, placed under nitrogen, dissolved in THF/H_2O (20 mL/10 mL), and stirred for 12 h at 80 °C. After completion as determined by TLC analysis, the reaction mixture was extracted with EA (3×20 mL) and the combined organic layers were washed with brine (30 mL). The solution was then dried ($MgSO_4$), filtered, and concentrated. The crude product was purified by flash column chromatography (PE : EA = 100 : 1) to give **methyl 2-(4-hydroxy naphthalen-1-yl) benzoate derivatives** (**2a-2d**).

methyl 2-(4-hydroxynaphthalen-1-yl)benzoate (2a)

Light pink solid, 430 mg, 19%. m.p. 58.5-60.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ

8.11 (d, *J* = 8.0 Hz, 1H), 7.89 (d, *J* = 9.2 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.38-7.22 (m, 5H), 7.00 (d, *J* = 7.6 Hz, 1H), 6.66 (s, 1H), 6.47 (d, *J* = 7.6 Hz, 1H), 3.36 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 168.99, 151.47, 141.51, 132.88, 132.34, 131.63, 131.21, 129.77, 127.19, 126.29, 126.20, 125.10, 124.65, 124.32, 122.09, 108.03, 52.09. HRMS-ESI calcd for $C_{18}H_{14}O_3$ $[M+H]^+$ 279.10212; found 279.10145

Methyl 4-fluoro-2-(4-hydroxynaphthalen-1-yl)benzoate (2b)

Light pink solid, 383 mg, 15% yield. m.p. 141.0-142.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.21 (d, *J*= 8.0 Hz, 1H), 8.06-8.04 (m, 1H), 7.48-7.36 (m, 3H), 7.22-7.15 (m, 1H), 7.12 (d, *J* = 8.0 Hz, 2H), 6.64 (d, *J* = 8.0 Hz, 1H), 5.99 (s, 1H), 3.48 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 167.57, 164.51 (d, *J* = 254.2 Hz), 151.57, 144.91 (d, *J* = 8.8 Hz), 132.70 (d, *J* = 8.8 Hz), 130.65, 127.90 (d, *J* = 3.0 Hz), 126.67, 126.00, 125.10, 125.06, 124.24, 122.11, 119.38 (d, *J* = 21.4 Hz), 114.55 (d, *J* = 21.3 Hz), HRMS-ESI calcd for $C_{18}H_{13}FO_3$ $[M+H]^+$ 297.0927; found 297.0922.

Methyl 2-(4-hydroxynaphthalen-1-yl)-4-methylbenzoate (2c)

White solid, 366 mg, 16% yield. m.p. 162.5-163.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.20 (d, *J* = 8.0 Hz, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.50-7.34 (m, 3H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.22 (s, 1H), 7.12 (d, *J* = 7.6 Hz, 1H), 6.59 (d, *J* = 7.6 Hz, 1H), 6.25 (s, 1H), 3.51 (s, 3H), 2.45 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 168.69, 151.27, 142.38, 141.85, 133.21, 133.04, 131.79, 130.17, 128.65, 128.05, 126.31, 126.01, 125.29, 124.71, 124.30, 122.08, 108.17, 52.02, 21.52. HRMS-ESI calcd for $C_{19}H_{16}O_3$ $[M+H]^+$ 293.1178; found 293.1172.

Methyl 2-(4-hydroxynaphthalen-1-yl)-5-methoxybenzoate (2d)

Yellow solid, 531 mg, 20% yield. m.p. 173.5-174.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.21 (d, *J* = 8.0 Hz, 1H), 7.52 (m, 1H), 7.49-7.41 (m, 2H), 7.40- 7.35 (m, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.17-7.09 (m, 2H), 6.71 (d, *J* = 8.0 Hz, 1H), 3.92 (s, 3H), 3.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 168.35, 158.63, 150.93, 133.72, 133.45, 133.39, 132.59, 131.72, 126.37, 126.23, 125.46, 124.83, 124.21, 121.88, 117.91, 114.49, 108.05, 55.61, 52.03. HRMS-ESI calcd for $C_{19}H_{16}O_4$ $[M+H]^+$ 309.1127; found 309.1126.

Methyl 2-(4-hydroxynaphthalen-1-yl)benzoate derivatives (**2a-2d**) (3.4 mmol) was added to a 250 mL round-bottom flask, placed under nitrogen, dissolved in anhydrous THF (50 ml). To this solution methylmagnesium bromide (20.3 mmol, 3M, THF) was added dropwise over ~10 min and the mixture was heated at 40 °C for 3 h. After completion as determined by TLC analysis, the reaction mixture was cooled to 0 °C and brine (20 mL) were cautiously added. Then the reaction mixture was extracted with EA (3×20 mL) and the combined organic layers were washed with brine (30 mL). The solution was then dried ($MgSO_4$), filtered, and concentrated. The crude product was purified by flash column chromatography (PE : EA = 100 : 1) to give 4-(2-(2-hydroxypropan-2-yl)phenyl)naphthalen-1-ol derivatives (**3a-3d**).

4-(2-(2-hydroxypropan-2-yl)phenyl)naphthalen-1-ol (3a)

Pink solid, 230 mg, 76%. m.p. 173.7-175.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, *J* = 8.4 Hz, 1H), 7.62 (d, *J* = 8.0 Hz, 1H), 7.41-7.19 (m, 6H), 7.15 (d, *J* = 7.6 Hz, 1H), 6.62 (d, *J* = 7.6 Hz, 1H), 6.09 (s, 1H), 1.36 (s, 3H), 1.34 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 151.46, 147.27, 137.36, 134.09, 133.37, 132.84, 127.65, 127.12, 126.87, 126.59, 126.27, 126.18, 125.21, 124.53, 121.89, 107.57, 74.64, 32.34, 32.09. HRMS-ESI calcd for $C_{19}H_{18}O_2$ $[M-H]^-$ 277.12285; found 277.12320.

4-(5-Fluoro-2-(2-hydroxypropan-2-yl)phenyl)naphthalen-1-ol (3b)

White solid, 772 mg, 77% yield. m.p. 135.6-137.1 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.23 (d, *J* = 8.0 Hz, 1H), 7.68-7.66 (m, 1H), 7.45-7.43 (m, 2H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.19 (d, *J* = 8.0 Hz, 1H), 7.14-7.08 (m, 1H), 6.83-6.82 (m, 1H), 6.62 (d, *J* = 8.0 Hz, 1H), 6.54 (s, 1H), 1.44-1.41 (m, 3H), 1.39-1.36 (m, 3H).^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 160.84 (d, *J* = 247.2 Hz), 151.90, 143.30 (d, *J* = 8.4 Hz), 139.86, 139.79, 133.74, 131.39, 128.15 (d, *J* = 8.0 Hz), 127.22, 126.96, 126.65, 125.32, 124.57, 122.09, 119.89 (d, *J* = 20.3 Hz), 114.48 (d, *J* = 20.1 Hz), 107.46, 74.49, 32.42, 32.04. HRMS-ESI calcd for $C_{19}H_{17}FO_2$ $[M+H]^+$ 295.1134; found 295.1144.

4-(2-(2-Hydroxypropan-2-yl)-5-methylphenyl)naphthalen-1-ol (3c)

White solid, 638 mg, 64% yield. m.p. 117.8-118.9 °C. ^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ (ppm) 10.16 (s, 1H), 8.18 (d, *J* = 8.0 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.38-7.36 (m, 2H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 7.5 Hz, 1H), 6.90 (d, *J* = 7.5 Hz, 1H), 6.77 (s, 1H), 4.78 (s, 1H), 2.26 (s, 3H), 1.23 (s, 3H), 1.19 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d*$_6$): δ (ppm) 152.83, 146.55, 137.52, 134.87, 134.33, 133.41, 132.00, 128.16, 127.95, 126.99, 126.23, 124.72, 124.63, 122.45, 107.30, 71.96, 33.41, 31.35, 20.68. HRMS-ESI calcd for $C_{20}H_{20}O_2$ $[M+H]^+$ 293.1542; found 293.1538.

4-(2-(2-Hydroxypropan-2-yl)-4-methoxyphenyl)naphthalen-1-ol (3d)

White solid, 838 mg, 80% yield. m.p. 173.5-174.9 °C. ^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ (ppm) 10.16 (s, 1H), 8.17 (d, *J* = 8.0 Hz, 1H), 7.54 (s, 1H), 7.38-7.36 (m, 2H), 7.16-7.14 (m, 2H), 6.95-6.76 (m, 3H), 4.90 (s, 1H), 3.82 (s, 3H), 1.26 (s, 3H), 1.21 (s, 3H). ^{13}C NMR (101 MHz, DMSO-*d*$_6$): δ (ppm) 158.70, 152.86, 151.08, 134.76, 134.05, 131.55, 129.86, 128.53, 126.96, 126.19, 124.79, 124.62, 122.46, 112.69, 111.19, 107.33, 72.01, 55.36, 33.15, 30.94.

4-(2-(2-hydroxypropan-2-yl)phenyl)naphthalen-1-ol derivatives (**3a-3d**) (3.4 mmol) was added to a 250 mL round-bottom flask, dissolved in xylene (100ml). To this solution *p*-toluenesulfonic acid (70 mg, 0. 4 mmol) was added and the mixture was heated to reflux at 150 °C for 3 h. After completion as determined by TLC analysis, the reaction mixture was extracted with EA (3×20 mL) and the combined organic layers were washed with brine (30 mL). The solution was then dried ($MgSO_4$), filtered, and concentrated. The crude product was purified by flash column chromatography (PE : EA = 100 : 1) to give 7,7-dimethyl-7H-benzo[c]fluoren-5-ol derivatives (**4a-4d**).

7,7-Dimethyl-7*H*-benzo[c]fluoren-5-ol (4a)

White solid, 752 mg, 96% yield. m.p. 174.6-176.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.71 (d, *J* =10.0 Hz, 1H), 8.29 (d, *J* =10.0 Hz, 1H), 8.23 (d, *J* =10.0 Hz, 1H), 7.69-7.65 (m, 1H), 7.54-7.51 (m, 2H), 7.44-7.40 (m, 1H), 7.31 (d, *J* =10.0 Hz, 1H), 6.97 (s, 1H), 5.32 (s, 1H), 1.51 (s, 6H). ^{13}C NMR (101 MHz, DMSO-d6) δ (ppm) 154.32, 154.04, 153.87, 140.43, 130.38, 127.79, 127.59, 125.32, 124.90, 124.39, 123.96, 123.94, 123.79, 122.77, 121.80, 103.90, 46.76, 27.12. HRMS-ESI calcd for C41H32O2 $[M + H]^+$ 261.1274; found 261.1277.

10-Fluoro-7,7-dimethyl-7*H*-benzo[c]fluoren-5-ol (4b)

White solid, 572 mg, 61% yield. m.p. 125.3-126.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.49 (d, *J* = 8.0 Hz, 1H), 8.26 (d, *J* = 8.0 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.59 (t, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 8.0 Hz, 1H), 7.30-7.28 (m, 1H), 6.90 (t, *J* = 8.0 Hz, 1H), 6.81 (s, 1H), 5.94 (s, 1H), 1.35 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 162.60 (d, *J* = 241.0 Hz), 154.48, 152.32, 149.28, 142.11 (d, *J* = 8.6 Hz), 130.42, 127.67, 125.42 (d, *J* = 2.9 Hz), 124.70, 124.27, 123.50, 123.08, 122.86 (d, *J* = 9.4 Hz), 111.55 (d, *J* = 22.3 Hz), 109.23 (d, *J* = 24.6 Hz), 104.20, 46.40, 26.80.

7,7,10-Trimethyl-7*H*-benzo[c]fluoren-5-ol (4c)

White solid, 559 mg, 60% yield. m.p. 168.8-170.1 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.74 (d, *J* = 8.0 Hz, 1H), 8.30 (d, *J* = 8.0 Hz, 1H), 8.07 (s, 1H), 7.68 (t, *J* = 8.0 Hz, 1H), 7.54 (s, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.14 (s, 1H), 6.94 (s, 1H), 5.30 (s, 1H), 2.54 (s, 3H), 1.49 (s, 6H). ^{13}C NMR (101 MHz, DMSO-d_6) δ (ppm) 154.33, 154.16, 151.05, 140.60, 136.57, 130.36, 127.71, 125.99, 124.82, 124.34, 124.04, 123.98, 123.73, 122.53, 122.40, 103.92, 46.38, 27.22, 21.87. HRMS-ESI calcd for $C_{20}H_{18}O$ $[M+H]^+$ 274.1358; found 274.1360.

9-Methoxy-7,7-dimethyl-7*H*-benzo[c]fluoren-5-ol (4d)

White solid, 473 mg, 48% yield. m.p. 173.5-174.9 °C .^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 10.29 (s, 1H), 8.59 (d, *J* = 8.0 Hz, 1H), 8.26 (d, *J* = 8.0 Hz, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.63 (t, *J* = 8.0 Hz, 1H), 7.48 (t, *J* = 8.0 Hz, 1H), 7.19 (s, 1H), 7.04 (s, 1H), 6.92 (d, *J* = 8.0 Hz, 1H), 3.82 (s, 3H), 1.44 (s, 6H). ^{13}C NMR (101 MHz, DMSO-d_6) δ (ppm) 157.48, 155.47, 152.80, 152.51, 132.68, 129.25, 126.99, 124.25, 123.75, 123.61, 123.41, 123.18, 121.85, 112.05, 108.97, 103.52, 55.22, 46.28, 26.75. HRMS-ESI calcd for $C_{20}H_{18}O_2$ $[M+H]^+$ 290.1307; found 290.1309.

7,7-Dimethyl-7H-benzo[c]fluoren-5-ol derivatives (**4a-4d**) (0.72 mmol), alkynol (**5a-5c**) (0.9 mmol) were added to a 100 mL round-bottom flask, dissolved in toluene (20 mL), followed by dodecylbenzenesulphonic acid (1~2 drop) and the resulting mixture was stirred for 3 h at 40 °C. After completion as determined by TLC analysis, the reaction mixture was extracted with EA (3×20 mL) and the combined organic layers were washed with brine (30 mL). The solution was then dried ($MgSO_4$), filtered, and concentrated. The crude product was purified by flash column chromatography (PE: EA=100:1) to give **5NP**, respectively.

13,13-Dimethyl-3,3-diphenyl-3,13-dihydrobenzo-indeno[*2,1-f*]chromene (5NP-a)

Brown solid, 1.18 g, 77% yield. m.p. 214.3-216.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.63 (d, *J* = 10.0 Hz, 1H), 8.47 (d, *J* = 10.0 Hz, 1H), 8.18 (d, *J* = 10.0 Hz, 1H), 7.60-7.25 (m, 15H), 7.22-7.19 (m, 1H), 6.27 (d, *J* = 10.0 Hz, 1H), 1.63 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 154.94, 148.33, 147.50, 144.94, 139.89, 130.13, 128.18, 127.89, 127.53, 127.13, 127.00, 126.96, 126.94, 126.89, 125.42, 124.84, 123.72, 123.20, 122.04, 121.85, 121.01, 113.08, 82.48, 47.68, 26.14. HRMS-ESI calcd for $C_{41}H_{32}O_2$ $[M+H]^+$ 451.2056; found 451.2062.

3,3-Bis(4-methoxyphenyl)-13,13-dimethyl-3,13-di-hydrobenzo[h]indeno[*2,1-f*]chromene (5NP-b)

Light brown solid, 1.41 g, 81% yield. m.p. 221.5- 223.4 °C. ^{1}H NMR(400 MHz, $CDCl_3$): δ (ppm) 8.64 (d, *J* =10.0 Hz, 1H), 8.45 (d, *J* = 8.4 Hz, 1H), 8.19 (d, *J* =10.0 Hz, 1H), 7.62-7.54 (m, 1H), 7.51-7.42 (m, 6H), 7.39-7.36 (m, 1H), 7.31-7.27 (m, 2H), 6.83 (d, *J* = 10.0 Hz, 4H), 6.21 (d, *J* = 10.0 Hz, 1H), 3.76 (s, 6H), 1.65 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 158.90, 154.95, 148.41, 147.53, 139.96, 137.29, 130.10, 128.33, 128.24, 127.08, 127.01, 126.82, 125.39, 124.90, 124.78, 123.72, 123.24, 122.04, 121.86, 120.63, 113.48, 113.12, 82.15, 55.22, 47.69, 26.15. HRMS-ESI calcd for $C_{41}H_{32}O_2$ $[M+H]^+$ 511.2268; found 511.2270.

3-([1,1'-Biphenyl]-4-yl)-13,13-dimethyl-3-phenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene (5NP-c)

Purple solid, 1.13 g, 63% yield. m.p. 195.3-196.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.66 (d, *J* = 10.0 Hz, 1H), 8.52 (d, *J* = 10.0 Hz, 1H), 8.21 (d, *J* = 10.0 Hz, 1H), 7.65-7.28 (m, 20H), 6.32 (d, *J* = 10.0 Hz, 1H), 1.67 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 154.98, 148.38, 147.56, 144.93, 144.00, 140.67, 140.42, 139.93, 130.20, 128.77, 128.29, 127.87, 127.64, 127.39, 127.36, 127.23, 127.14, 127.07, 126.99, 126.93, 125.51, 124.95, 124.90, 123.81, 123.26, 122.12, 121.91, 121.13, 113.16, 82.45, 47.74, 26.20. HRMS-ESI calcd for $C_{41}H_{32}O_2$ $[M+H]^+$ 527.2369; found 527.2378.

10-Fluoro-13,13-dimethyl-3,3-diphenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene (5NP-F-a)

Light pink solid, 213 mg, 63% yield. m.p. 141.0-142.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.49-8.40 (m, 2H), 7.79 (d, *J* = 10.0 Hz, 1H), 7.56-7.54 (m, 1H), 7.51-7.43 (m, 5H), 7.33 -7.29 (m, 1H), 7.28-7.26 (m, 3H), 7.25-7.16 (m, 4H), 6.92-6.90 (m, 1H), 6.23 (d, *J* = 10.0 Hz, 1H), 1.58 (s, 6H).^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 162.55 (d, *J* = 240.5 Hz), 150.23, 148.83, 148.58, 144.82, 141.58 (d, *J* = 8.8 Hz), 129.98, 128.20, 128.00, 127.59, 127.44, 126.12 (d, *J* = 3.2 Hz), 125.04, 124.83, 123.29, 122.56 (d, *J* = 9.2 Hz), 120.73, 112.98, 111.88 (d, *J* = 22.7 Hz), 109.33 (d, *J* = 24.6 Hz), 99.88, 82.60, 47.30, 26.14. HRMS-ESI calcd for $C_{34}H_{26}FO$ $[M+H]^+$ 469.1968; found 469.1960.

10-Fluoro-3,3-bis(4-methoxyphenyl)-13,13-dimethyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene(5NP-F-b)

Light yellow solid, 248 mg, 65% yield. m.p. 216.9- 218.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.33-8.31 (m, 2H), 7.69 (d, *J* = 10.0 Hz, 1H), 7.43-1.41 (m, 1H), 7.36-7.30 (m, 1H), 7.29- 7.24 (m, 4H), 7.19-7.17 (m, 1H), 7.11-7.07 (m, 1H), 6.84-6.75 (m, 1H), 6.68-6.67 (m, 4H), 6.05 (d, *J* = 10.0 Hz, 1H), 3.58 (s, 6H), 1.47 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 162.52 (d, *J* = 240.9 Hz), 158.95, 150.25, 148.93, 148.62, 141.61 (d, *J* = 8.8 Hz), 137.16, 129.96, 128.56, 128.34, 127.40, 125.94 (d, *J*= 3.0 Hz), 125.09, 124.99, 123.44, 123.39, 122.54 (d, *J* = 9.4 Hz), 120.35, 113.51, 113.04, 111.81 (d, *J* = 22.6 Hz), 109.28 (d, *J* = 24.4 Hz), 82.28, 55.22, 47.31, 26.15. HRMS-ESI calcd for $C_{36}H_{29}FO_3$ $[M+H]^+$ 529.2179; found 529.2174.

3-([1,1'-Biphenyl]-4-yl)-10-fluoro-13,13-dimethyl-3-phenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene (5NP-F-c)

Light pink solid, 102 mg, 26% yield. m.p. 216.9-218.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.46-8.44 (m, 2H), 7.79-7.77 (m, 1H), 7.50-7.46 (m, 10H), 7.28-7.24 (m, 8H), 6.90-6.88 (m, 1H), 6.24 (d, *J* = 10.0 Hz, 1H), 1.56 (s, 6H).^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 162.55 (d, *J* = 245.1 Hz), 150.28, 148.87, 148.62, 144.80, 143.85, 141.55 (d, *J* = 8.8 Hz), 140.71, 140.57, 130.02, 128.76, 128.30, 127.97, 127.68, 127.51, 127.36, 127.11, 126.99, 126.89, 126.17 (d, *J* = 3.1 Hz), 125.12, 124.87, 123.34, 122.57 (d, *J* = 9.4 Hz), 120.84, 113.05, 111.90 (d, *J* = 22.8 Hz), 109.34 (d, *J* = 24.6 Hz), 82.55, 47.34, 26.18. HRMS-ESI calcd for $C_{40}H_{29}FO$ $[M+H]^+$ 545.2281; found 545.2273.

10,13,13-Trimethyl-3,3-diphenyl-3,13-dihydrobenzo[h]indeno[2,1-f]chromene (5NP-Me-a)

Yellow oil, 161 mg, 48% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) δ 8.66 (d, *J* = 8.4 Hz, 1H), 8.48 (d, *J* = 8.0 Hz, 1H), 8.01 (s, 1H), 7.61-7.46 (m, 6H), 7.34-7.31 (m, 6H), 7.23 (t, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 1H), 6.27 (d, *J* = 8.0 Hz, 1H), 2.49 (s, 3H), 1.63 (s, 6H).^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 152.20, 148.20, 147.85, 144.98, 140.04, 136.44, 130.14, 128.18, 127.80, 127.52, 127.05, 126.95, 126.89, 126.19, 124.78, 123.78, 123.17, 122.87, 121.50, 121.02, 113.09, 82.43, 47.33, 26.25, 21.89. HRMS-ESI calcd for $C_{35}H_{28}O$ $[M+H]^+$ 465.2218; found 465.2219.

3,3-Bis(4-methoxyphenyl)-10,13,13-trimethyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene (5NP-Me-b)

Yellow solid, 170 mg, 45% yield. m.p. 134.8-135.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.65 (d, *J* = 8.0 Hz, 1H), 8.44 (d, *J* = 8.0 Hz, 1H), 8.01 (s, 1H), 7.61-7.54 (m, 1H), 7.51-7.39 (m, 5H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.27 (d, *J* = 10.0 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 6.85-6.80 (m, 4H), 6.20 (d, *J* = 8.0 Hz, 1H), 3.75 (s, 6H), 2.49 (s, 3H), 1.63 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 158.86, 152.21, 148.32, 147.87, 140.13, 137.32, 136.42, 130.10, 128.24, 128.21, 126.98, 126.78, 126.13, 124.83, 124.70, 123.76, 123.20, 122.85, 121.49, 120.62, 113.45, 113.12, 82.10, 55.22, 47.33, 26.25, 21.89. HRMS-ESI calcd for $C_{37}H_{32}O_3$ $[M+H]^+$ 525.2430; found 525.2431.

3-([1,1'-Biphenyl]-4-yl)-10,13,13-trimethyl-3-phenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene (5NP-Me-c)

Yellow solid, 222 mg, 57% yield. m.p. 207.3-209.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.70 (d, *J* = 8.4 Hz, 1H), 8.54 (d, *J* = 8.4 Hz, 1H), 8.05 (s, 1H), 7.62 (m, 5H), 7.54 (m, 5H), 7.45-7.32 (m, 7H), 7.31-7.27 (m, 1H), 7.15-7.13 (m, 1H), 6.33 (d, *J* = 8.4 Hz, 1H), 2.52 (s, 3H), 1.66 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 152.24, 148.23, 147.89, 144.95, 144.02, 140.66, 140.38, 140.09, 136.47, 130.19, 128.74, 128.26, 127.76, 127.60, 127.37, 127.33, 127.12, 127.04, 126.96, 126.91, 126.24, 124.86, 124.82, 123.84, 123.21, 122.91, 121.53, 121.11, 113.14, 82.40, 47.37, 26.29, 21.91. HRMS-ESI calcd for $C_{41}H_{32}O$ $[M+H]^+$ 541.2531; found 541.2532.

11-Methoxy-13,13-dimethyl-3,3-diphenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene (5NP-OMe-a)

Yellow oil, 169 mg, 49% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.53 (d, *J*= 8.4 Hz, 1H), 8.45-8.43 (m, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.54-7.48 (m, 5H), 7.45-7.43 (m, 1H), 7.29-7.26 (m, 2H), 7.24 (s, 1H), 7.21-7.16 (m, 2H), 6.97 (d, *J* = 10.0 Hz, 1H), 6.88-6.86 (m, 1H), 6.23 (d, *J* = 10.0 Hz, 1H), 3.84 (s, 3H), 1.59 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 158.14, 157.03, 147.51, 146.57, 145.02, 132.91, 129.58, 128.18, 127.99, 127.52, 127.03, 126.92, 126.90, 126.85, 124.79, 123.70, 123.18, 122.65, 121.07, 113.21, 111.91, 108.47, 82.36, 55.52, 47.67, 26.37. HRMS-ESI calcd for $C_{35}H_{28}O_2$ $[M+H]^+$ 480.2168; found 480.2175.

11-Methoxy-3,3-bis(4-methoxyphenyl)-13,13-dimethyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene (5NP-OMe-b)

Pink solid, 183 mg, 47% yield. m.p. 217.0-218.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.58 (d, *J* = 8.4 Hz, 1H), 8.44 (d, *J* = 8.4 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.59-7.53 (m, 1H), 7.51-7.41 (m, 5H), 7.27 (d, *J* = 10.0 Hz, 1H), 7.03-7.01 (m, 1H), 6.93-6.91 (m, 1H), 6.87-6.80 (m, 4H), 6.22 (d, *J* = 10.0 Hz, 1H), 3.90 (s, 3H), 3.76 (s, 6H), 1.64 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 158.86, 158.10, 157.02, 147.51, 146.57, 137.34, 132.96, 129.53, 128.37, 128.22, 126.85, 126.82, 124.81, 124.68, 123.65, 123.18, 122.59, 120.65, 113.45, 113.20, 111.88, 108.44, 82.00, 55.51, 55.21, 47.65, 26.35. HRMS-ESI calcd for $C_{37}H_{32}O_4$ $[M+H]^+$ 541.2379; found 541.2436.

3-([1,1'-Biphenyl]-4-yl)-11-methoxy-13,13-dimethyl-3-phenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene (5NP-OMe-c)

Brown solid, 144 mg, 36% yield. m.p. 149.0-150.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.59 (d, *J* = 8.0 Hz, 1H), 8.50 (d, *J* = 8.0 Hz, 1H), 8.09 (d, *J* = 8.0 Hz, 1H), 7.55 (m, 11H), 7.40 (t, *J* = 8.0 Hz, 2H), 7.35-7.33 (m, 4H), 7.02-7.00 (m, 1H), 6.93-6.91 (m, 1H), 6.32 (d, *J* = 8.0 Hz, 1H), 3.90 (s, 3H), 1.65 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 158.12, 157.02, 147.48, 146.56, 144.94, 144.01, 140.66, 140.34, 132.88, 129.57, 128.72, 128.23, 127.89, 127.56, 127.34, 127.30, 127.10, 127.06, 126.93, 126.88, 124.81, 124.77, 123.70, 123.17, 122.64, 121.13, 113.20, 111.90, 108.44, 82.26, 55.52, 47.67, 26.37. HRMS-ESI calcd for $C_{41}H_{32}O_2$ $[M+H]^+$ 557.2481; found 557.2472.

3-Bromo-7,7-dimethyl-7H-benzo[de]anthracene (**6**) [16] (6.0 g, 18.6 mmol), Cs_2CO_3 (12.2 g, 37.2 mmol) and $Pd_2(dba)_3$ (1.5 g, 1.86 mmol), ^{t}BuXPhos (791 mg, 1.86 mmol)

were added to a 250 mL round-bottom flask, placed under nitrogen, dissolved in MeOH/toluene(70 mL/70 mL), and stirred for 12 h at 80 °C. After completion as determined by TLC analysis, the reaction mixture was extracted with EA (3×20 mL) and the combined organic layers were washed with brine (30 mL). The solution was then dried ($MgSO_4$), filtered, and concentrated. The crude product was purified by flash column chromatography (PE : EA = 100 : 1) to give 3-methoxy-7,7-dimethyl-7*H*-benzo[*de*]anthracene (**7**). White solid, 3.6 g, 71% yield. m.p. 137.5-139.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.21-8.18 (m, 1H), 8.08-8.05 (m, 2H), 7.71 (d, *J* =10.0 Hz, 1H), 7.68-7.65 (m, 1H), 7.58-7.55 (m, 1H), 7.35-7.29 (m, 2H), 6.92 (d, *J* =10.0 Hz, 1H), 4.07 (s, 3H), 1.75 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 155.24, 143.15, 142.81, 130.91, 127.67, 126.99, 126.91, 126.40, 125.67, 125.36, 123.87, 122.45, 122.27, 119.72, 119.06, 104.00, 55.59, 38.77, 34.91. HRMS-ESI calcd for $C_{20}H_{18}O$ $[M+H]^+$ 275.1430; found 275.1431.

3-Methoxy-7,7-dimethyl-7*H*-benzo[*de*]anthracene (**7**) (3.0 mmol) was added to a 50 mL round-bottom flask, placed under nitrogen, dissolved in DCM (10ml). To this solution BBr_3 (1M, 3.2 mmol) was added and the mixture was cooled at 0 °C for 4 h. After completion as determined by TLC analysis, the reaction mixture was extracted with EA (3×20 mL) and the combined organic layers were washed with brine (30 mL). The solution was then dried ($MgSO_4$), filtered, and concentrated. The crude product was purified by flash column chromatography (PE : EA = 10 : 1) to give 7,7-dimethyl-7*H*-benzo[*de*] anthracen-3-ol (**8**). White solid, 634mg, 81% yield. m.p. 155.7-157.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.99 (d, *J* =10.0 Hz, 1H), 7.95-7.91 (m, 1H), 7.85 (d, *J* =10.0 Hz, 1H), 7.59 (d, *J* =10.0 Hz, 1H), 7.55-7.53 (m, 1H), 7.48-7.46 (m, 1H), 7.23-7.20 (m, 2H), 6.77 (d, *J* =10.0 Hz, 1H), 1.62 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 151.35, 143.13, 130.92, 127.95, 127.05, 126.93, 126.44, 125.69, 124.22, 123.86, 122.90, 122.27, 119.38, 119.10, 108.91, 38.80, 34.94. HRMS-ESI calcd for $C_{19}H_{16}O$ $[M+H]^+$ 261.1274; found 261.1268.

7,7-Dimethyl-7*H*-benzo[*de*]anthracen-3-ol (**8**) (1.0 g, 3.4 mmol), alkynol (**5a-5c**) (3.8 mmol) were added to a 50 mL round-bottom flask, dissolved in toluene (20 ml), followed by dodecylbenzenesulphonic acid (1~2 drop) and the resulting mixture was stirred for 3 h at 40 °C. After completion as determined by TLC analysis, the reaction mixture was extracted with EA (3×20 mL) and the combined organic layers were washed with brine (30 mL). The solution was then dried ($MgSO_4$), filtered, and concentrated. The crude product was purified by flash column chromatography (PE : EA = 100 : 1) to give **6NP-a**, **6NP-b**, and **6NP-c**, respectively.

8,8-Dimethyl-3,3-diphenyl-3,8-dihydroanthra[*9,1-gh*]chromene (6NP-a)

White solid, 343 mg, 76% yield. m.p. 174.9-176.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.36 (d, *J* =10.0 Hz, 1H), 8.11-8.00 (m, 1H), 7.87 (s, 1H), 7.75-7.55 (m, 7H), 7.37-7.35 (m, 8H), 6.89 (d, *J* = 10.0 Hz, 1H), 6.32 (d, *J* =10.0 Hz, 1H), 1.77 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 147.70, 145.26, 143.31, 143.14, 130.67, 128.25, 127.97, 127.74, 127.59, 127.18, 126.96, 126.47, 126.15, 124.56, 123.99, 123.94, 122.88, 122.36, 119.85, 117.71, 115.36, 83.48, 38.73, 35.00. HRMS-ESI calcd for $C_{34}H_{26}O$ $[M+H]^+$ 451.2056; found 451.2060.

3,3-Bis(4-methoxyphenyl)-8,8-dimethyl-3,8-dihydroanthra[*9,1-gh*]chromene (6NP-b)

White solid, 1.42 g, 82% yield. m.p. 206.3-208.1 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.26 (d, *J* =10.0 Hz, 1H), 8.09-7.98 (m, 1H), 7.82 (s, 1H), 7.65 (d, *J* =10.0 Hz, 2H), 7.57-7.54 (m, 1H), 7.47 (d, *J* =10.0 Hz, 4H), 7.35-7.29 (m, 2H), 6.88 (d, *J* =10.0 Hz, 4H), 6.82 (d, *J* =10.0 Hz, 1H), 6.21 (d, *J* = 10.0 Hz, 1H), 3.79 (s, 6H), 1.73 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 158.92, 147.70, 143.25, 143.05, 137.59, 130.69, 128.24, 128.10, 127.88, 127.06, 126.90, 126.39, 126.00, 124.53, 123.80, 123.54, 122.65, 122.29, 119.81, 117.66, 115.30, 113.50, 83.09, 55.23, 38.68, 34.93. HRMS-ESI calcd for $C_{36}H_{30}O$ $[M+H]^+$ 511.2268; found 511.2275.

3-([1,1'-Biphenyl]-4-yl)-8,8-dimethyl-3-phenyl-3,8-dihydroanthra[*9,1-gh*]chromene (6NP-c)

White solid, 1.49 g, 83% yield. m.p. 144.5-146.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.39-8.29 (m, 1H), 8.05 (s, 1H), 7.85-7.82 (m, 1H), 7.65-7.58 (m, 11H), 7.47-7.30 (m, 8H), 6.90-6.87 (m, 1H), 6.33-6.29 (m, 1H), 1.75 (s, 3H), 1.71 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 147.67, 145.17, 144.24, 143.30, 143.15, 140.69, 140.42, 130.64, 128.75, 128.28, 127.97, 127.64, 127.62, 127.37, 127.33, 127.16, 127.12, 126.97, 126.94, 126.44, 126.16, 124.55, 124.05, 123.94, 122.91, 122.35, 119.83, 117.69, 115.35, 83.37, 38.72, 34.99, 34.95. HRMS-ESI calcd for $C_{40}H_{30}O$ $[M+H]^+$ 527.2369; found 527.2367.

Dimethyl 2-bromoisophthalate (7.8 mmol), 2-(4-methoxynaphthalen-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (8.6 mmol), potassium carbonate (5.1g, 37.4mmol) and $Pd(PPh_3)_4$ (1.1g, 1mmol) were added to a 250 mL round-bottom flask, placed under nitrogen, dissolved in THF/H_2O (20 mL/10 mL), and stirred for 12 h at 80 °C. After completion as determined by TLC analysis, the reaction mixture was extracted with EA (3×20 mL) and the combined organic layers were washed with brine (30 mL). The solution was then dried ($MgSO_4$), filtered, and concentrated. The crude product was purified by flash column chromatography (PE : EA = 20 : 1) to give dimethyl 2-(4-methoxynaphthalen-1-yl)isophthalate (**9**). White solid, 2.02 g, 67% yield. m.p. 217.0-218.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.30 (d, *J* =10.0 Hz, 1H), 8.01 (d, *J* =10.0 Hz, 2H), 7.58-7.55 (m, 1H), 7.47-7.31 (m, 3H), 7.14 (d, *J* =10.0 Hz, 1H), 6.82 (d, *J* =10.0 Hz, 1H), 4.04 (s, 3H), 3.33 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 167.96, 155.01, 140.28, 134.21, 133.30, 132.18, 129.21, 127.44, 126.46, 125.75, 125.09, 124.85, 122.07, 102.81, 55.39, 51.98. HRMS-ESI calcd for $C_{21}H_{18}O_5$ $[M+ H]^+$ 351.1226; found 351.1232.

Dimethyl 2-(4-methoxynaphthalen-1-yl)isophthalate (**9**) (1.0g, 3.3mmol) was added

to a 100 mL round-bottom flask, placed under nitrogen, dissolved in anhydrous THF (50ml). To this solution methylmagnesium bromide (13mmol, 3M, THF) was added dropwise over ~5 min and the mixture was heated at 40 °C for 3 h. After completion as determined by TLC analysis, the reaction mixture was cooled to 0 °C and brine (20 mL) were cautiously added. Then the reaction mixture was extracted with EA (3×20 mL) and the combined organic layers were washed with brine (30 mL). The solution was then dried ($MgSO_4$), filtered, and concentrated. The crude product was purified by flash column chromatography (PE : EA = 15 : 1) to give 2,2'-(2-(4-methoxynaphthalen-1-yl)-1,3-phenylene)bis(propan-2-ol) (**10**). Pink oil, 822 mg, 71% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.21 (d, *J* =10.0 Hz, 1H), 7.61 (d, *J* =10.0 Hz, 2H), 7.40-7.26 (m, 4H), 7.25-7.17 (m, 1H), 6.79 (d, *J* =10.0 Hz, 1H), 3.98 (s, 3H), 1.22 (s, 6H), 1.11 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 155.63, 148.54, 135.64, 134.36, 130.48, 128.62, 127.69, 127.43, 126.70, 125.76, 125.55, 125.23, 122.19, 102.44, 74.98, 55.53, 32.88.

2,2'-(2-(4-Methoxynaphthalen-1-yl)-1,3-phenylene)bis(propan-2-ol) (**10**) (3.4 mmol) was added to a 50 mL round-bottom flask, dissolved in xylene (20ml). To this solution polyphosphoric acid (96 mg, 0.4 mmol) was added and the mixture was heated to reflux at 150 °C for 3 h. After completion as determined by TLC analysis, the reaction mixture was extracted with EA (3×20 mL) and the combined organic layers were washed with brine (30 mL). The solution was then dried ($MgSO_4$), filtered, and concentrated. The crude product was purified by flash column chromatography (PE : EA = 100 : 1) to give 9-methoxy-1,1,5,5-tetramethyl-1,5-dihydrobenzo[*mno*]aceanthrylene (**11**). White solid, 536 mg, 50% yield. m.p. 173.3-174.7 °C. ^{1}H NMR(400 MHz, $CDCl_3$): δ (ppm) 8.00 (d, *J* =10.0 Hz, 1H), 7.58 (d, *J* =10.0 Hz, 1H), 7.52-7.49 (m, 1H), 7.35 (d, *J* = 10.0 Hz, 1H), 7.23 (d, *J* =10.0 Hz, 2H), 6.92 (s, 1H), 4.05 (s, 3H), 1.73 (s, 6H), 1.58 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 155.88, 151.19, 145.18, 144.75, 138.80, 135.07, 126.46, 126.29, 125.59, 124.33, 124.21, 123.88, 123.45, 119.95, 119.93, 100.31, 56.03, 51.83, 40.47, 33.90, 25.99. HRMS-ESI calcd for $C_{23}H_{22}O$ $[M+H]^+$ 315.1749; found 315.1737.

9-Methoxy-1,1,5,5-tetramethyl-1,5-dihydrobenzo[*mno*]aceanthrylene (**11**) (3.0 mmol) was added to a 50 mL round-bottom flask, placed under nitrogen, dissolved in DCM (10ml). To this solution BBr_3 (1M, 3.2 mmol) was added and the mixture was cooled at 0 °C for 4 h. After completion as determined by TLC analysis, the reaction mixture was extracted with EA (3×20 mL) and the combined organic layers were washed with brine (30 mL). The solution was then dried ($MgSO_4$), filtered, and concentrated. The crude product was purified by flash column chromatography (PE : EA = 100 : 1) to give 1,1,5,5-tetramethyl-1,5-dihydrobenzo[mno]aceanthrylen-9-ol (**12**).White solid, 1.27 g, 86% yield. m.p. 221.2-222.3 °C. ^{1}H NMR (400 MHz, DMSO-d6) δ (ppm) 10.06 (s, 1H), 7.95 (d, *J* =10.0 Hz, 1H), 7.62 (d, *J* =10.0 Hz, 1H), 7.48-7.46 (m, 1H), 7.36 (d, *J* = 10.0 Hz, 1H), 7.26 (d, *J* =10.0 Hz, 1H), 7.16-7.13 (m, 1H), 7.04 (s, 1H), 1.65 (s, 6H), 1.51 (s, 6H). ^{13}C NMR (101 MHz, DMSO-d6) δ (ppm)

153.87, 150.84, 146.11, 144.77, 138.32, 134.92, 126.69, 126.28, 124.25, 124.16, 123.96, 123.86, 123.58, 120.53, 120.42, 104.76, 51.55, 40.43, 34.20, 26.24. HRMS-ESI calcd for $C_{37}H_{30}O$ $[M+H]^+$ 491.2369; found 491.2367.

1,1,5,5-Tetramethyl-1,5-dihydrobenzo[*mno*]aceanthrylen-9-ol (**12**) (0.68 mmol), alkynol (0.76 mmol) were added to a 50 mL round-bottom flask, dissolved in toluene (20 mL), followed by dodecylbenzenesulphonic acid (1~2 drop) and the resulting mixture was stirred for 3 h at 40 °C. After completion as determined by TLC analysis, the reaction mixture was extracted with EA (3×20 mL) and the combined organic layers were washed with brine (30 mL). The solution was then dried ($MgSO_4$), filtered, and concentrated. The crude product was purified by flash column chromatography (PE : EA = 50 : 1) to give **5/6NP-a**, **5/6NP-b**, and **5/6NP-c**, respectively.

8,8,12,12-Tetramethyl-3,3-diphen-yl-8,12-dihydro-*3H*-aceanthryleno[1,10-fgh]chromene (5/6NP-a)

Light purple solid, 244 mg, 73% yield. m.p. 232.8- 233.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.10 (d, *J* =10.0 Hz, 1H), 7.59-7.47 (m, 6H), 7.32 (m, 6H), 7.23 (d, *J* = 10.0 Hz, 3H), 7.14 (d, *J* =10.0 Hz, 1H), 6.25 (d, *J* = 10.0 Hz, 1H), 1.65 (s, 6H), 1.71 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 151.54, 147.55, 145.31, 144.80, 140.18, 138.94, 134.63, 128.15, 127.81, 127.44, 126.92, 126.70, 126.66, 126.32, 124.17, 123.70, 123.66, 123.45, 120.73, 119.95, 119.55, 114.22, 82.45, 52.36, 40.16, 33.91, 25.81. HRMS-ESI calcd for $C_{37}H_{30}O$ $[M+H]^+$ 491.2369; found 491.2370.

3,3-Bis(4-methoxyphenyl)-8,8,12,12-te-tramethyl-8,12-dihydro-*3H*-aceanthryleno[1,10-fgh]chromene (5/6NP-b)

Purple solid, 214 mg, 57% yield. m.p. 221.2-222.3 °C. ^{1}H NMR(400 MHz, $CDCl_3$) δ (ppm) 8.05 (d, *J* = 10.0 Hz, 1H), 7.51-7.38 (m, 7H), 7.29 (d, *J* = 10.0 Hz, 1H), 7.20 (s, 1H), 7.08 (d, *J* = 10.0 Hz, 1H), 6.81 (d, *J* = 10.0 Hz, 4H), 6.16 (d, *J* = 10.0 Hz, 1H), 3.71 (s, 6H), 1.64 (s, 6H), 1.68 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 158.86, 151.56, 144.82, 140.23, 138.94, 137.69, 134.75, 128.27, 126.70, 126.63, 126.21, 124.17, 123.74, 123.67, 123.48, 120.35, 120.00, 119.59, 114.28, 113.52, 113.47, 82.09, 55.23, 52.39, 40.19, 33.95, 25.85. HRMS-ESI calcd for $C_{39}H_{34}O_3$ $[M+H]^+$ 551.2581; found 551.2589.

3-([1,1'-Biphenyl]-4-yl)-8,8,12,12-te-tramethyl-3-phenyl-8,12-dihydro-*3H*-aceanthryleno[1,10-fgh]chromene (5/6NP-c)

Blue solid, 239 mg, 62% yield. m.p. 227.1-228.5 °C ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.19-8.11 (m, 1H), 7.62 (t, *J* =10.0 Hz, 4H), 7.59-7.50 (m, 6H), 7.45-7.31 (m, 6H), 7.28 (d, *J* =10.0 Hz, 1H), 7.24 (s, 2H), 7.18 (d, *J* =10.0 Hz, 1H), 6.30 (d, *J* = 10.0 Hz, 1H), 1.73 (s, 6H), 1.67 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 151.59, 147.62, 145.30, 144.89, 144.39, 140.71, 140.31, 140.24, 139.00, 134.70, 128.78, 128.27, 127.80, 127.56, 127.41, 127.35, 127.14, 126.96, 126.80, 126.78, 126.44, 124.24, 123.81, 123.73, 123.52, 120.84, 120.02, 119.63, 114.30, 82.39, 52.43, 40.22, 34.01, 33.95, 25.89. HRMS-ESI calcd for $C_{43}H_{34}O$ $[M+H]^+$ 567.2681; found 567.2690.

4-Bromo-naphthalen-L-ol (2.2 g, 10 mmol), phenylboronic acid (12 mmol), sodium carbonate (5.1 g, 48 mmol) and $Pd(PPh_3)_4$ (1.1 g, 1 mmol) were added to a 250 mL round-bottom flask, and dissolved in THF/H_2O (40 mL/16 mL), and stirred for 12 h at 80°C. After completion as determined by TLC analysis, the reaction mixture was extracted with EA (3×20 mL) and the combined organic layers were washed with brine (30 mL). The solution was then dried ($MgSO_4$), filtered, and concentrated. The crude product was purified by flash column chromatography (PE: EA=100:1) to give 4-phenylnaphthalen-1-ol (**13**). White solid, 1.5 g, 68% yield. m.p. 131.7-133.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.27 (d, *J*= 8.0 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.55-7.36 (m, 7H), 7.27 (d, *J* = 8.0 Hz, 1H), 6.88 (d, *J* = 8.0 Hz, 1H), 5.25 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) 150.33, 140.22, 132.73, 132.14, 129.70, 127.68, 126.37, 126.26, 126.00, 125.43, 124.61, 123.87, 121.26, 107.60. HRMS-ESI calcd for $C_{16}H_{11}FO$ $[M+H]^+$ 221.0961; found 221.0962.

4-Phenylnaphthalen-1-ol (**13**) (1.28 mmol), alkynol (1.6 mmol), and toluene (40 mL) were added to a 100 mL round-bottom flask, followed by dodecylbenzenesulphonic acid (1~2 drop) and the resulting mixture was stirred for 3 h at 40°C. After completion as determined by TLC analysis, the reaction mixture was extracted with EA (3×20 mL) and the combined organic layers were washed with brine (30 mL). The solution was then dried ($MgSO_4$), filtered, and concentrated. The crude product was purified by flash column chromatography (PE: EA=100:1) to give **NP-a**, **NP-b**, and **NP-c**, respectively.

2,2,6-Triphenyl-*2H*-benzo[h]chromene (NP-a)

White solid, 410 mg, 78% yield. m.p. 140.1-141.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.44 (d, *J* = 8.0 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.58-7.30 (m, 15H), 7.30-7.23 (m, 2H), 7.12 (m, 1H), 6.75 (m, 1H), 6.22 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 147.24, 145.24, 140.61, 133.03, 132.70, 130.19, 128.20, 127.59, 127.54, 127.12, 127.01, 126.96, 126.92, 126.87, 126.85, 126.83, 126.41, 125.99, 125.55, 125.48, 124.79, 123.71, 122.23, 114.88, 83.36. HRMS-ESI calcd for $C_{16}H_{11}FO$ $[M+H]^+$ 411.1743; found 411.1740.

2,2-Bis(4-methoxyphenyl)-6-phenyl-*2H*-benzo[h]chromene (NP-b)

Light pink solid, 537 mg, 89% yield. m.p. 115.6-117.4 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.46-8.44 (m, 1H), 7.84-7.80 (m, 1H), 7.48-7.44 (m, 11H), 7.22-7.10 (m, 1H), 6.93-6.84 (m, 4H), 6.80-6.70 (m, 1H), 6.26-6.14 (m, 1H), 3.81 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ(ppm) 158.94, 147.30, 140.67, 137.62, 132.85, 132.68, 130.23, 128.25, 128.06, 126.93, 126.34, 125.99, 125.59, 125.40, 124.86, 123.35, 122.26, 115.02, 113.51, 100.06, 82.87, 55.24. HRMS-ESI calcd for $C_{16}H_{11}FO$ $[M+H]^+$ 471.1955; found 471.1961.

2-([1,1'-Biphenyl]-4-yl)-2,6-diphenyl-*2H*-benzo[h]chromene (NP-c)

Light purple solid, 455 mg, 73% yield. m.p. 156.3-158.1 °C. ^{1}H NMR (400 MHz,

$CDCl_3$): δ (ppm) 8.48 (d, *J* = 8.4 Hz, 1H), 7.80 (d, *J* = 8.4 Hz, 1H), 7.65-7.54 (m, 8H), 7.54-7.48 (m, 1H), 7.48-7.27 (m, 12H), 7.15 (s, 1H), 6.78 (d, *J* = 10.0 Hz, 1H), 6.27 (d, J = 10.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 147.27, 145.19, 144.26, 140.67, 140.60, 140.41, 133.10, 132.74, 130.22, 128.77, 128.28, 128.25, 127.63, 127.54, 127.38, 127.35, 127.13, 126.98, 126.94, 126.47, 126.04, 125.59, 125.55, 124.82, 123.81, 122.26, 114.92, 83.29. HRMS-ESI calcd for $C_{16}H_{11}FO$ $[M+H]^+$ 487.2056; found 487.2063.

Preparation of composite photochromic polymer film

The polymethyl methacrylate (PMMA) and the photochromic compound **5NP-F-b** were dissolved in THF. The solution was placed on a glass slide in horizontal in dark and the solvent was allowed to evaporate overnight at room temperature. Then the film was removed from the glass slide and the film thickness was measured with a micrometer. The thickness of the film was kept about 1 mm by controlling the solution used, and the concentration of the photochromic compounds in the PMMA film were maintained in 1% w/w.

3. Crystal data of 5NP-F-b

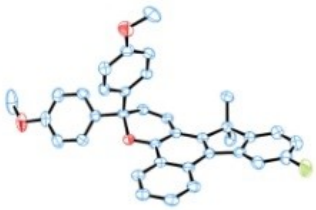

Table S1. Crystal data and structure refinement for **5NP-F-b**

Identification code	**5NP-F-b**
Empirical formula	$C_{36}H_{29}FO_3$
Formula weight	1099.64
Temperature	113(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 17.961(4) A alpha = 90 deg. b = 12.157(2) A beta = 104.70(3) deg. c = 26.684(5) A gamma = 90 deg.
Volume	5636(2) $Å^3$
Z, Calculated density	4, 1.296 g/cm^3
Absorption coefficient	0.131 mm^{-1}
F(000)	2308
Crystal size	0.200 x 0.180 x 0.120 mm
Theta range for data collection	1.236 to 25.017 deg.
Reflections collected / unique	53341 / 9946 [R(int) = 0.0986]
Completeness to theta = 25.017	99.9 %
Absorption correction	Semi-empirical from equivalents

Max. and min. transmission	1 and 0.8653
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9946 / 32 / 756
Goodness-of-fit on F^2	1.121
Final R indices [I>2sigma(I)]	$R_1 = 0.0892$, $wR_2 = 0.2341$
R indices (all data)	$R_1 = 0.1226$, $wR_2 = 0.2618$
CCDC no.	2049253

4. NMR Spectra

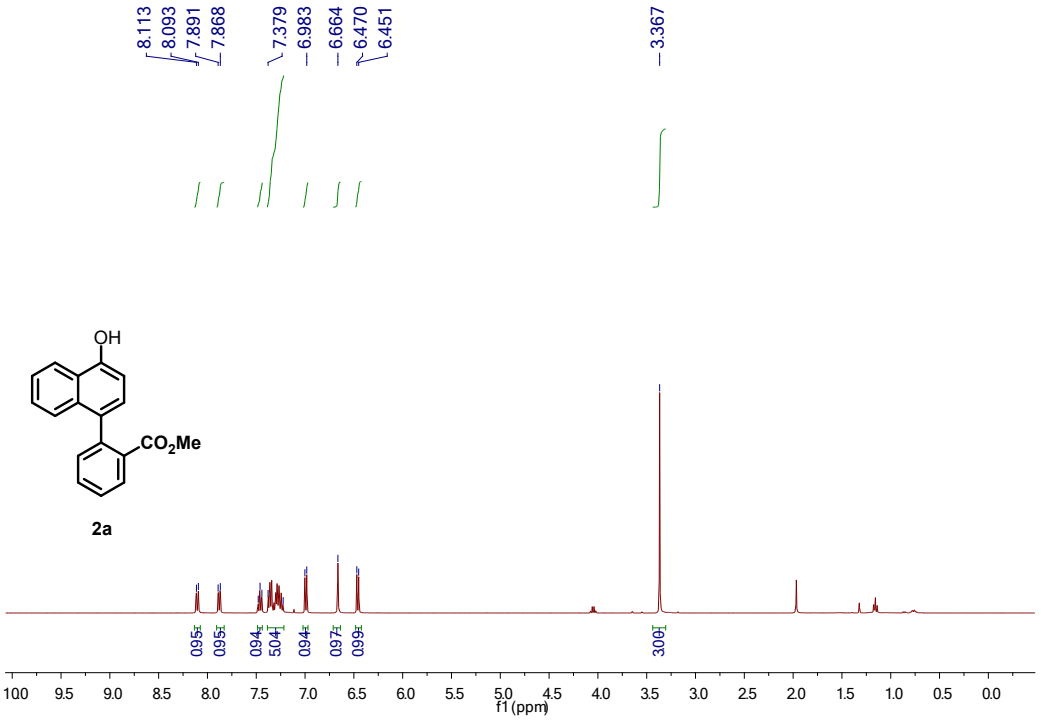

Fig. S1. ^{1}H NMR spectrum of **methyl 2-(4-hydroxynaphthalen-1-yl)benzoate (2a)** in $CDCl_3$.

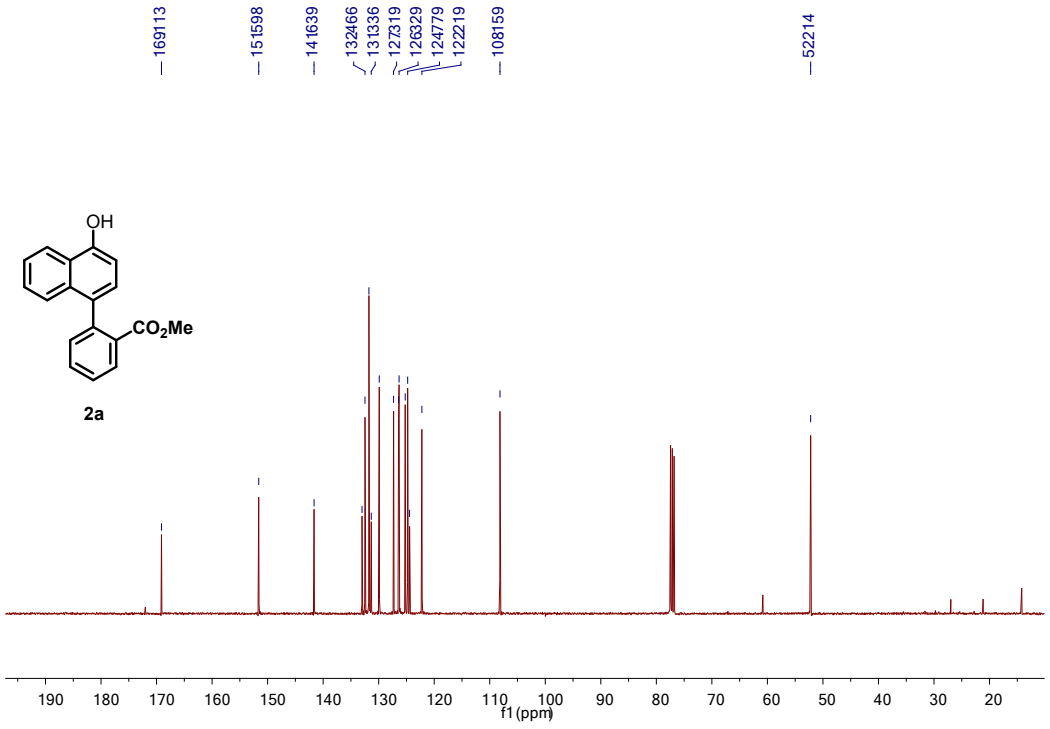

Fig. S2. ^{13}C NMR spectrum of **methyl 2-(4-hydroxynaphthalen-1-yl)benzoate (2a)** in $CDCl_3$.

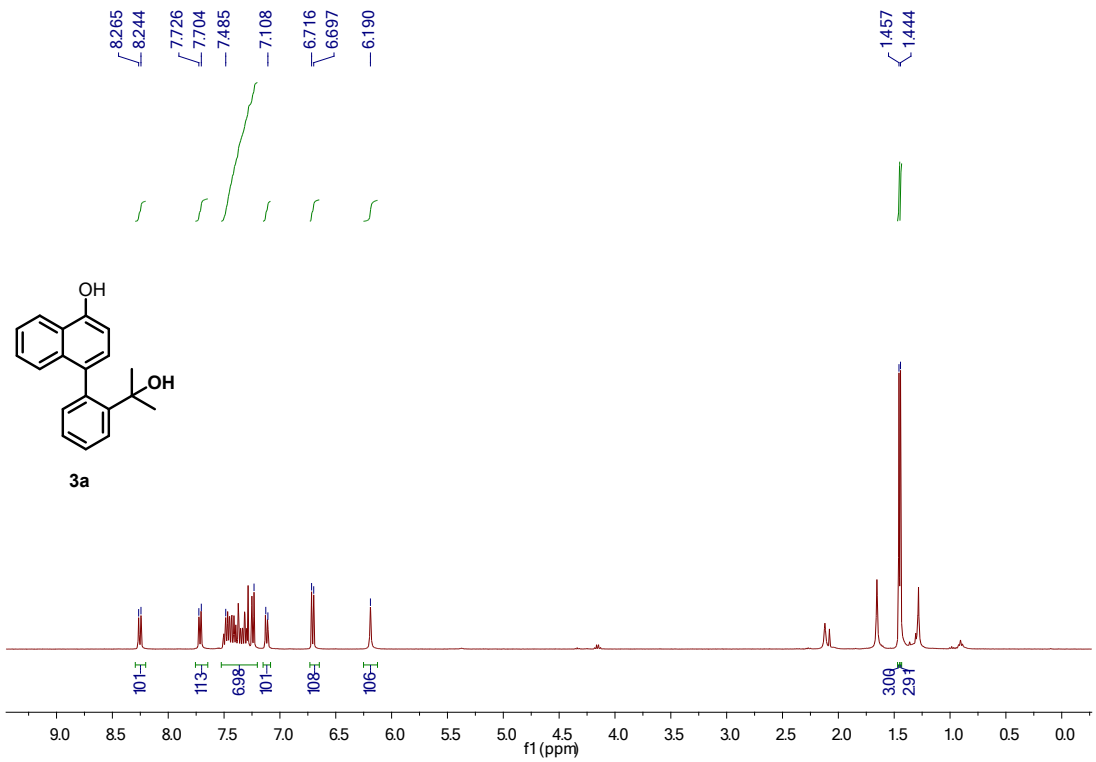

Fig. S3. ^{1}H NMR spectrum of **4-(2-(2-hydroxypropan-2-yl)phenyl)naphthalen -1-ol (3a)** in $CDCl_3$.

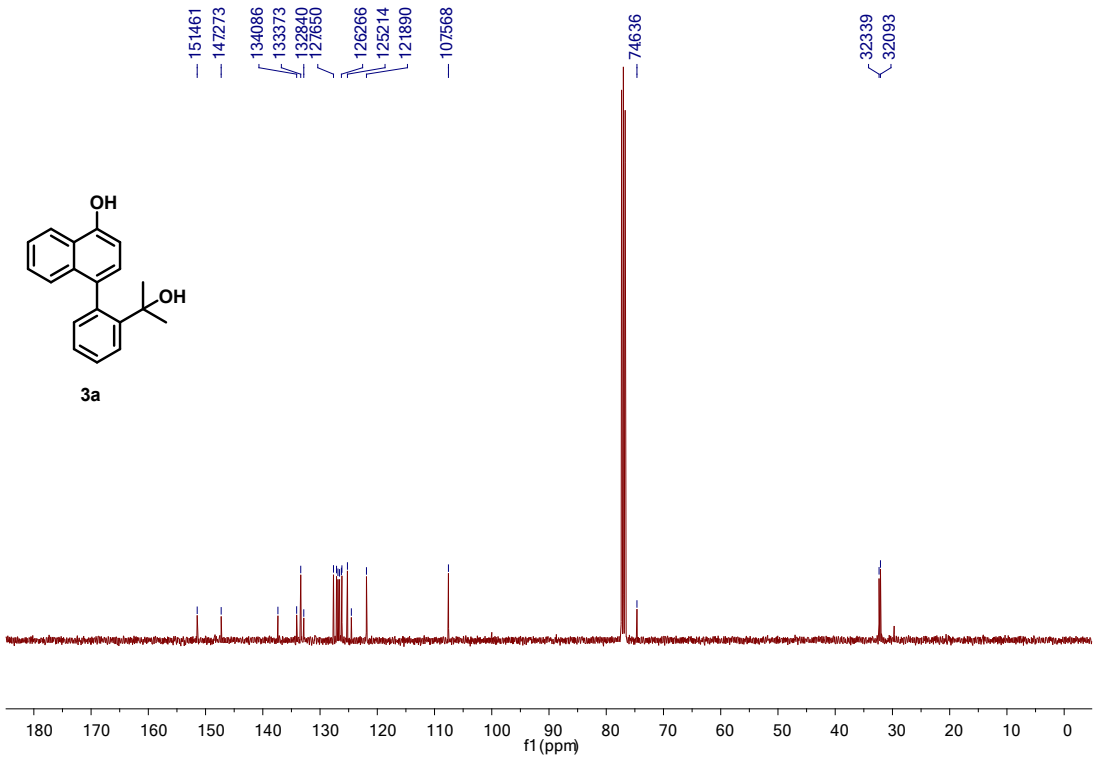

Fig. S4. ^{13}C NMR spectrum of **4-(2-(2-hydroxypropan-2-yl)phenyl)naphthalen -1-ol (3a)** in $CDCl_3$.

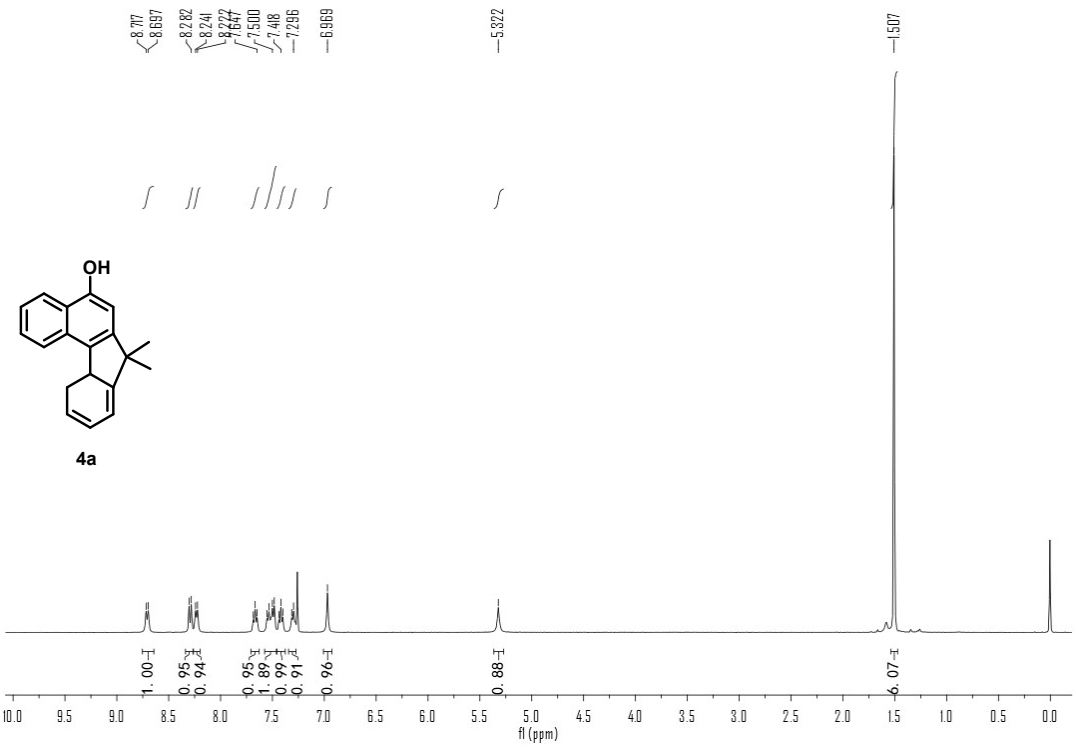

Fig. S5. ^{1}H NMR spectrum of **7,7-Dimethyl-7H-benzo[c]fluoren-5-ol (4a)** in $CDCl_3$.

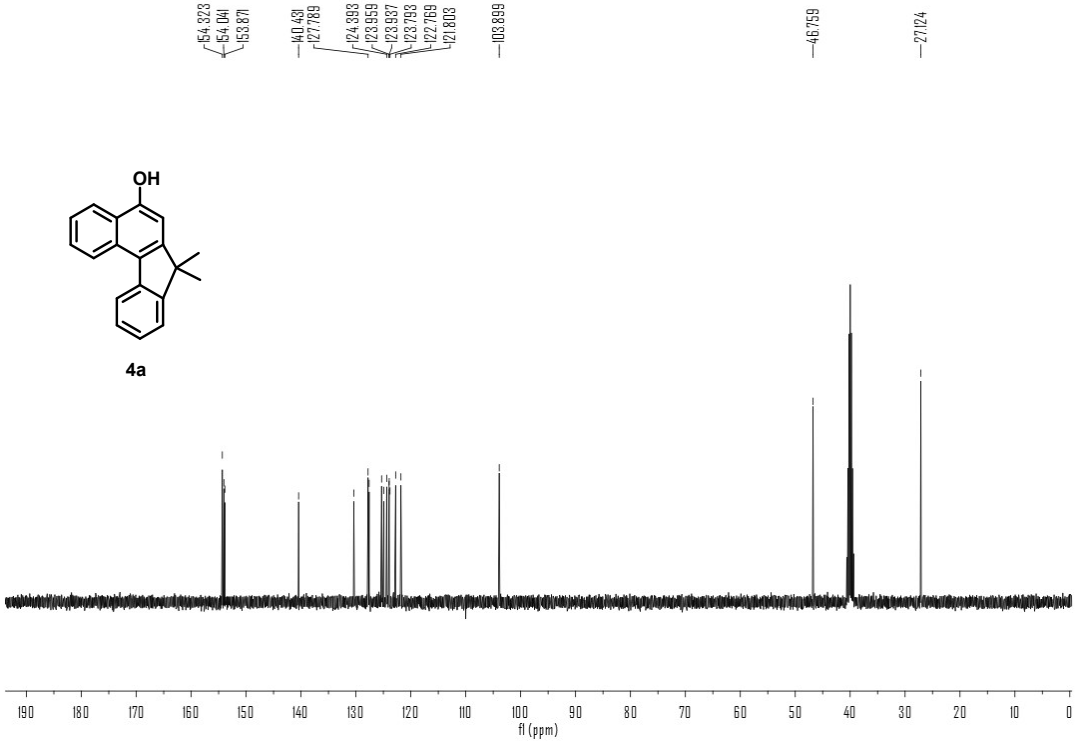

Fig. S6. ^{13}C NMR spectrum of **7,7-Dimethyl-7H-benzo[c]fluoren-5-ol (4a)** in $CDCl_3$.

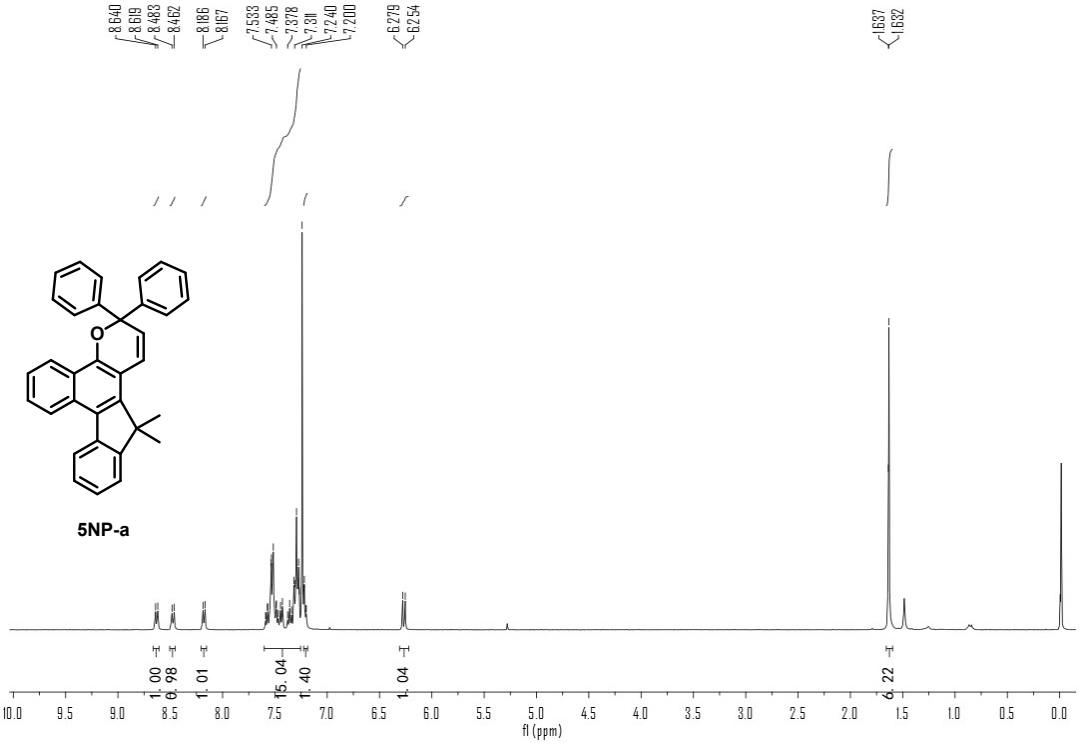

Fig. S7. ^{1}H NMR spectrum of **13,13-dimethyl-3,3-diphenyl-3,13-dihydrobenzo [*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

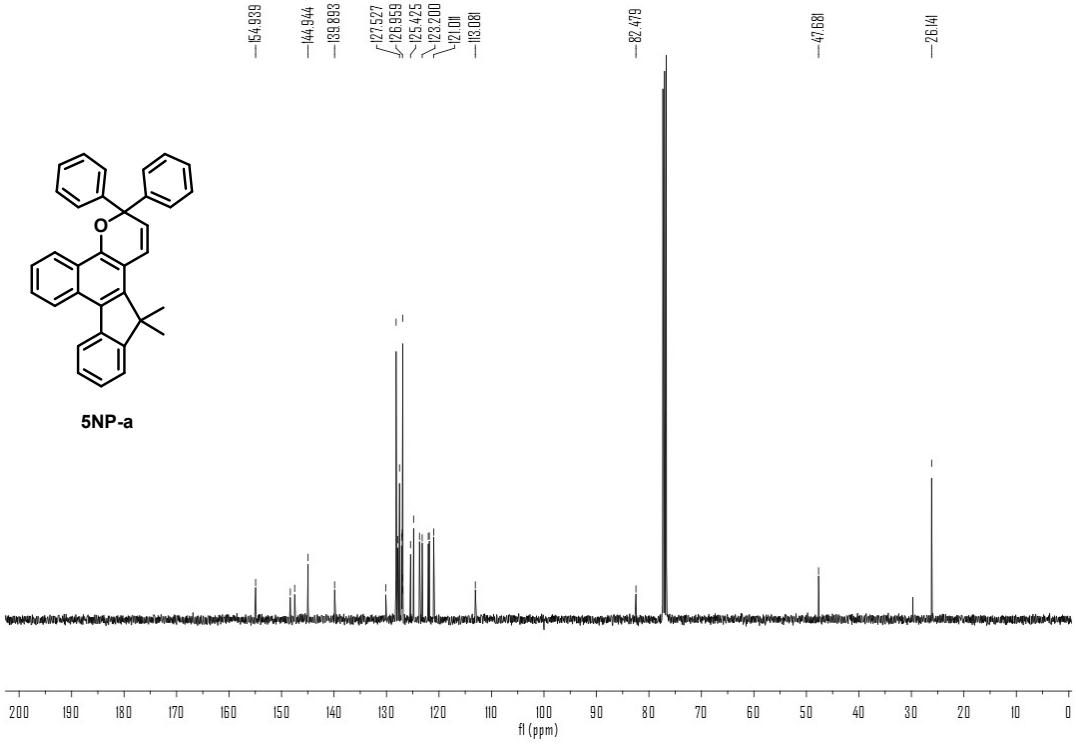

Fig. S8. ^{13}C NMR spectrum of **13,13-dimethyl-3,3-diphenyl-3,13-dihydrobenzo [*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

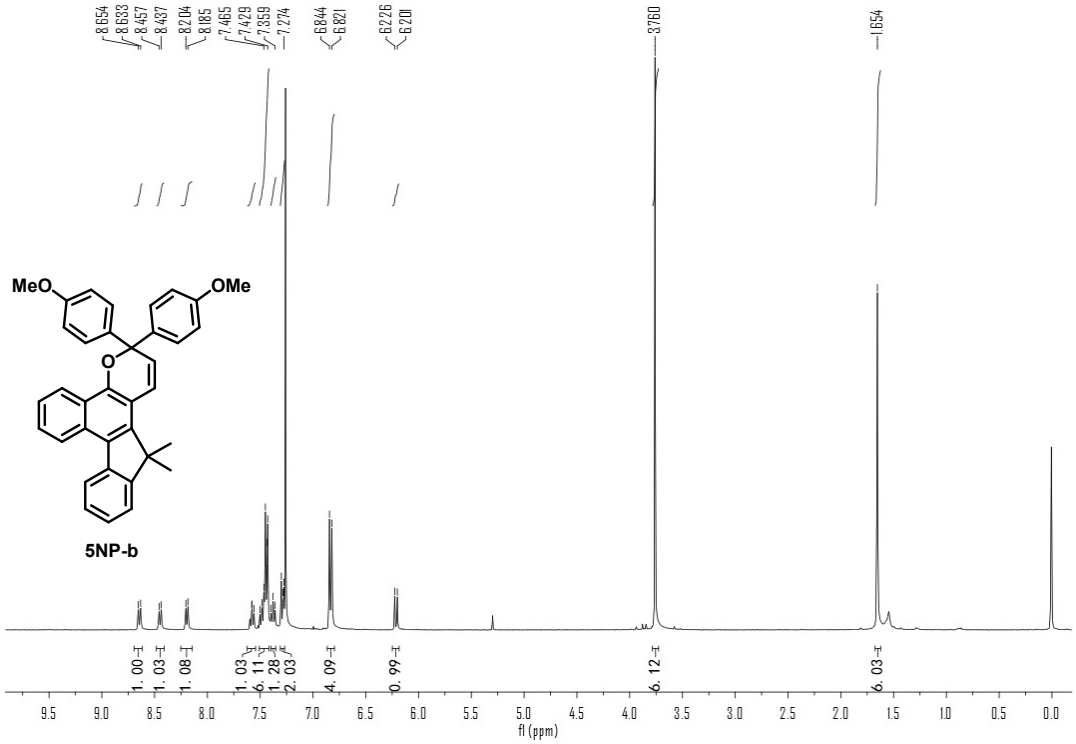

Fig. S9. ^{1}H NMR spectrum of **3,3-bis(4-methoxyphenyl)-13,13-dimethyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

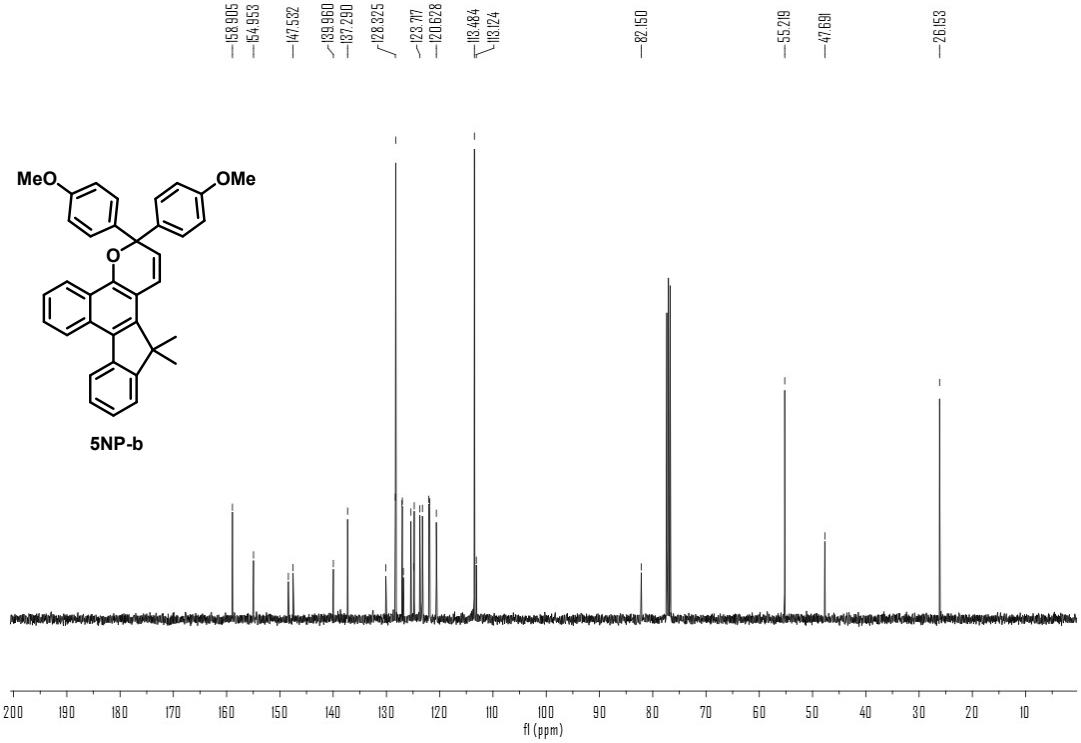

Fig. S10. ^{13}C NMR spectrum of **3,3-bis(4-methoxyphenyl)-13,13-dimethyl-3,13-di-hydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

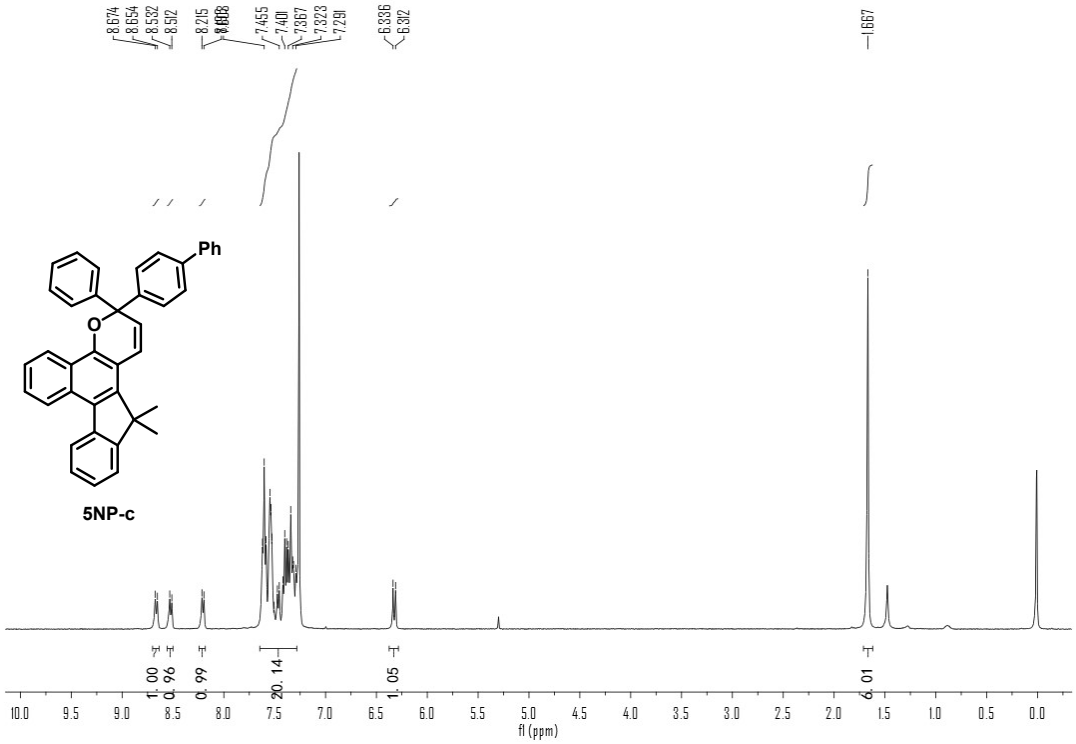

Fig. S11. ^{1}H NMR spectrum of **3-([1,1'-biphenyl]-4-yl)-13,13-dimethyl-3-phenyl -3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

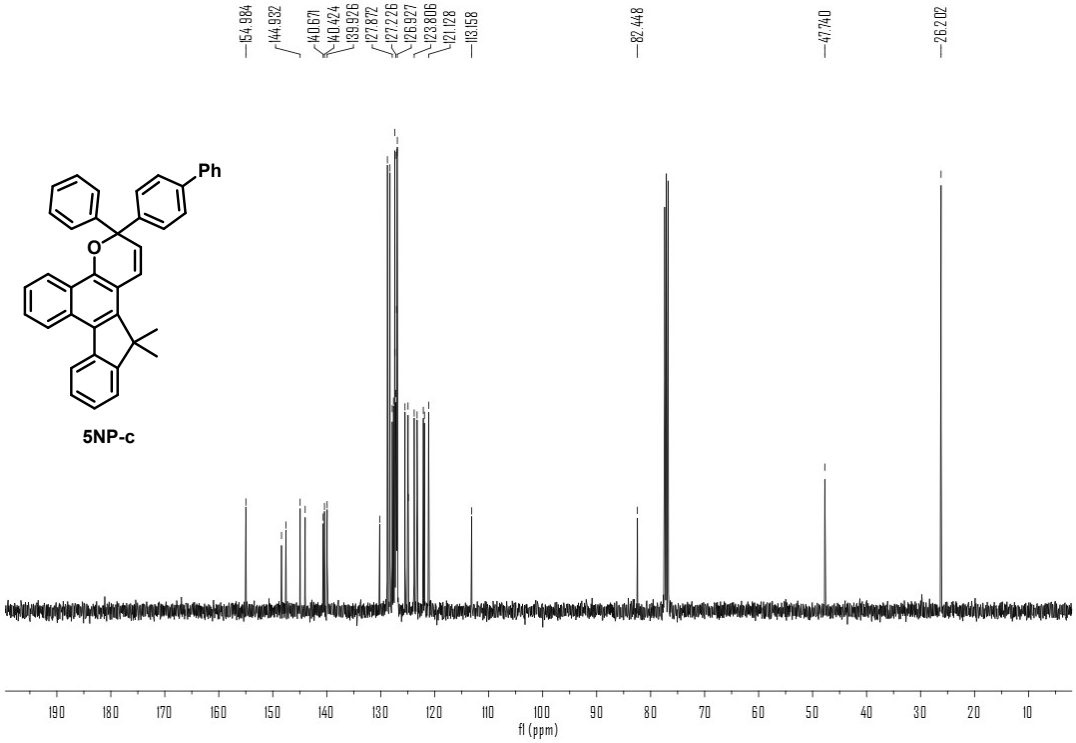

Fig. S12. ^{13}C NMR spectrum of **3-([1,1'-biphenyl]-4-yl)-13,13-dimethyl-3- phenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

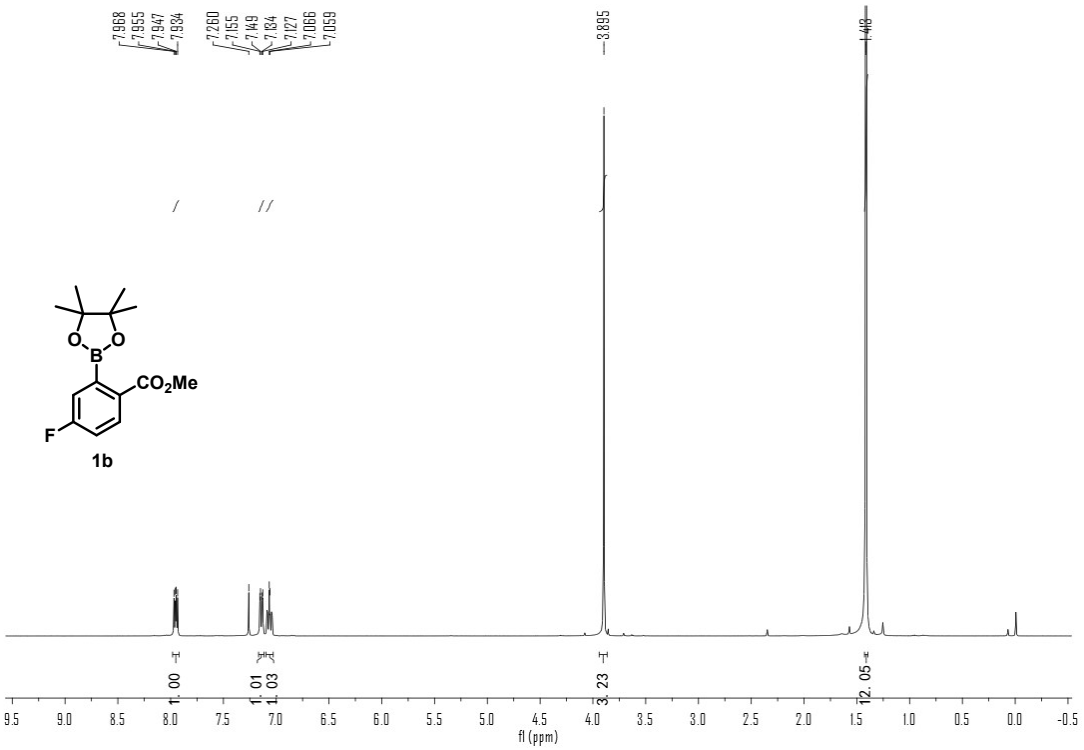

Fig. S13. ^{1}H NMR spectrum of **methyl 4-fluoro-2-(4,4,5,5-tetramethyl-1,3,2-di oxaborolan-2-yl)benzoate (1b)** in $CDCl_3$.

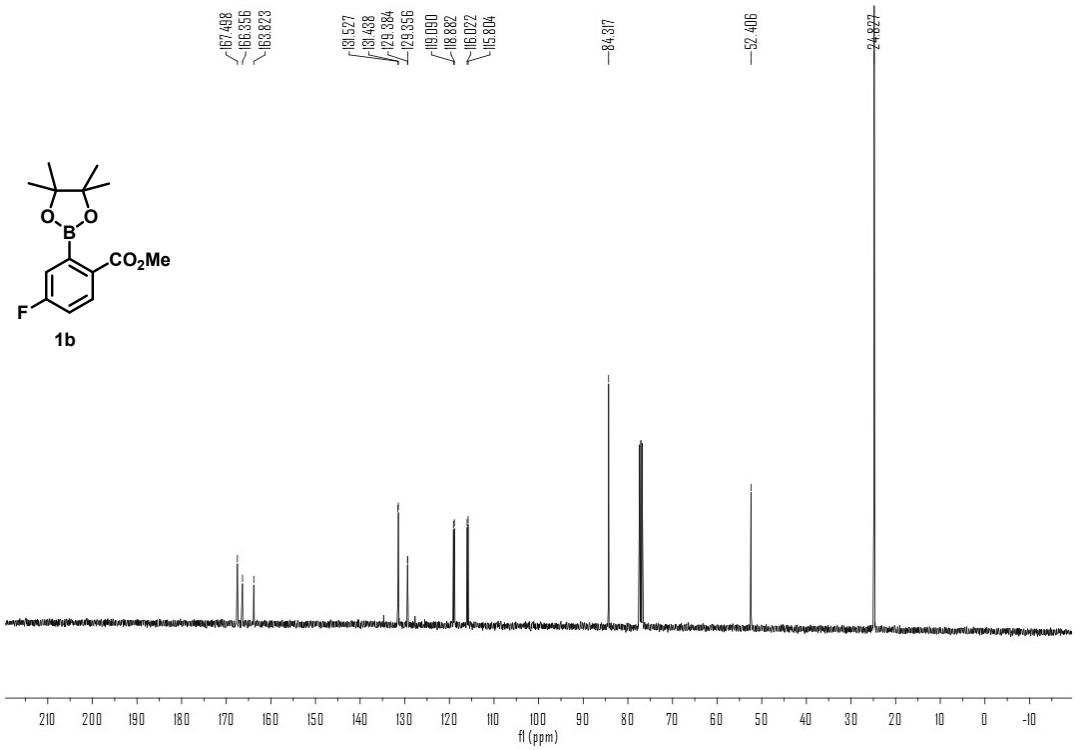

Fig. S14. ^{13}C NMR spectrum of **methyl 4-fluoro-2-(4,4,5,5-tetramethyl-1,3,2-di oxaborolan-2-yl)benzoate (1b)** in $CDCl_3$.

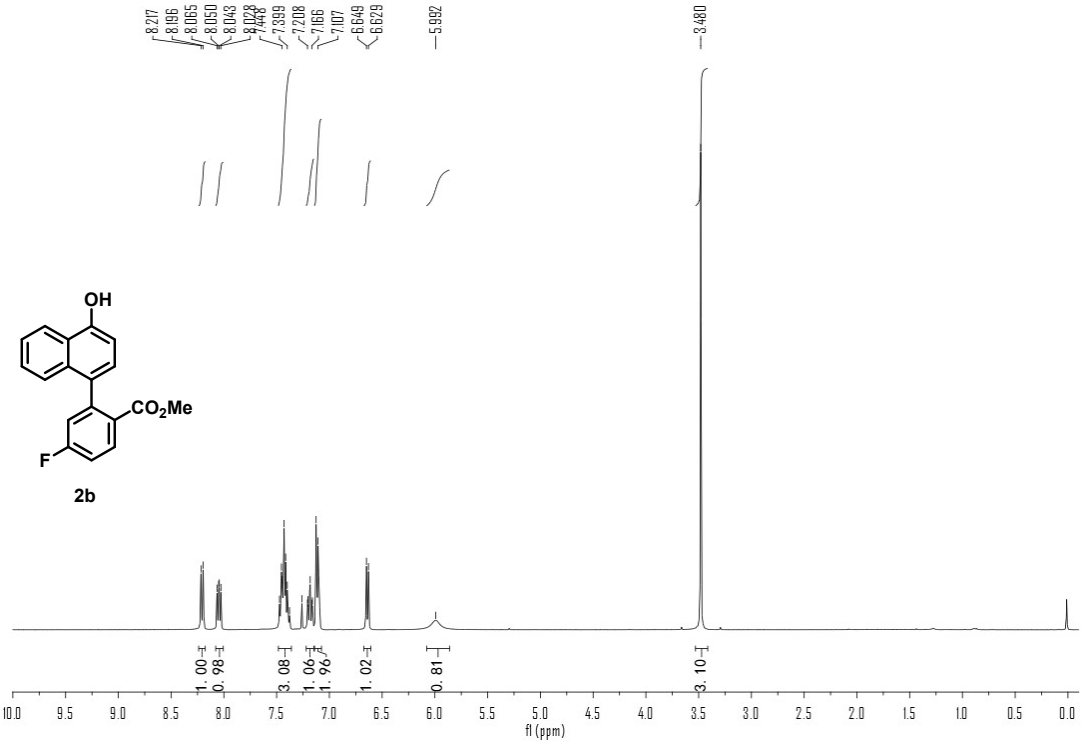

Fig. S15. ^{1}H NMR spectrum of **methyl 4-fluoro-2-(4-hydroxynaphthalen-1-yl) benzoate (2b)** in $CDCl_3$.

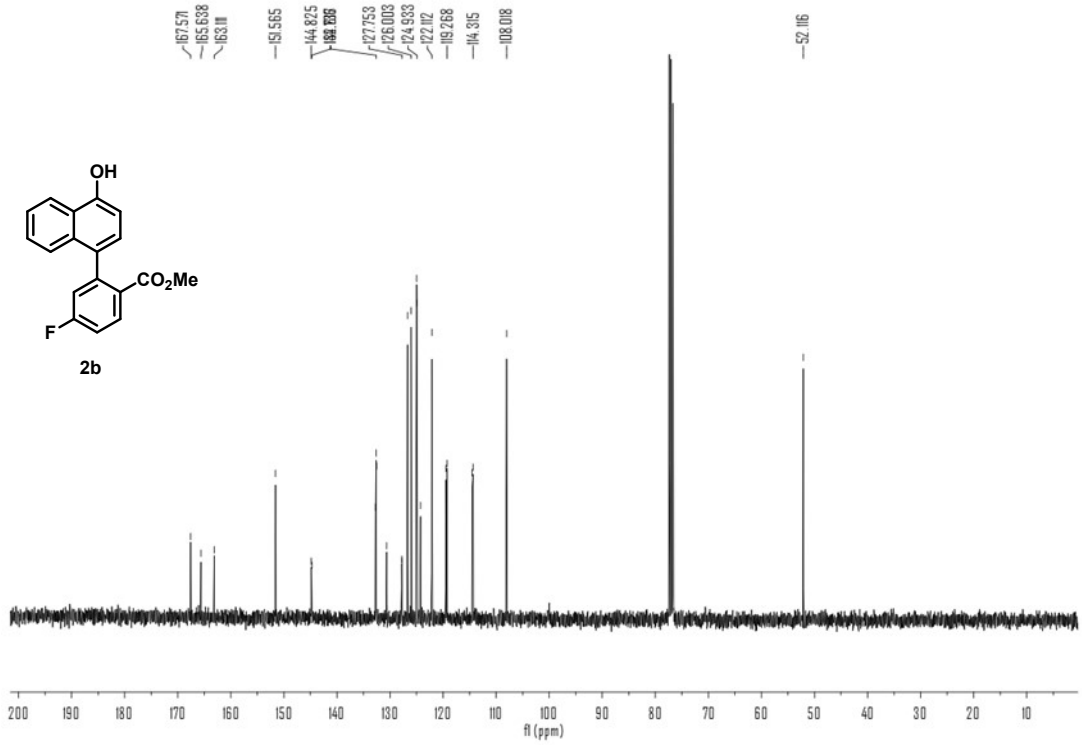

Fig. S16. ^{13}C NMR spectrum of **methyl 4-fluoro-2-(4-hydroxynaphthalen-1-yl) benzoate (2b)** in $CDCl_3$.

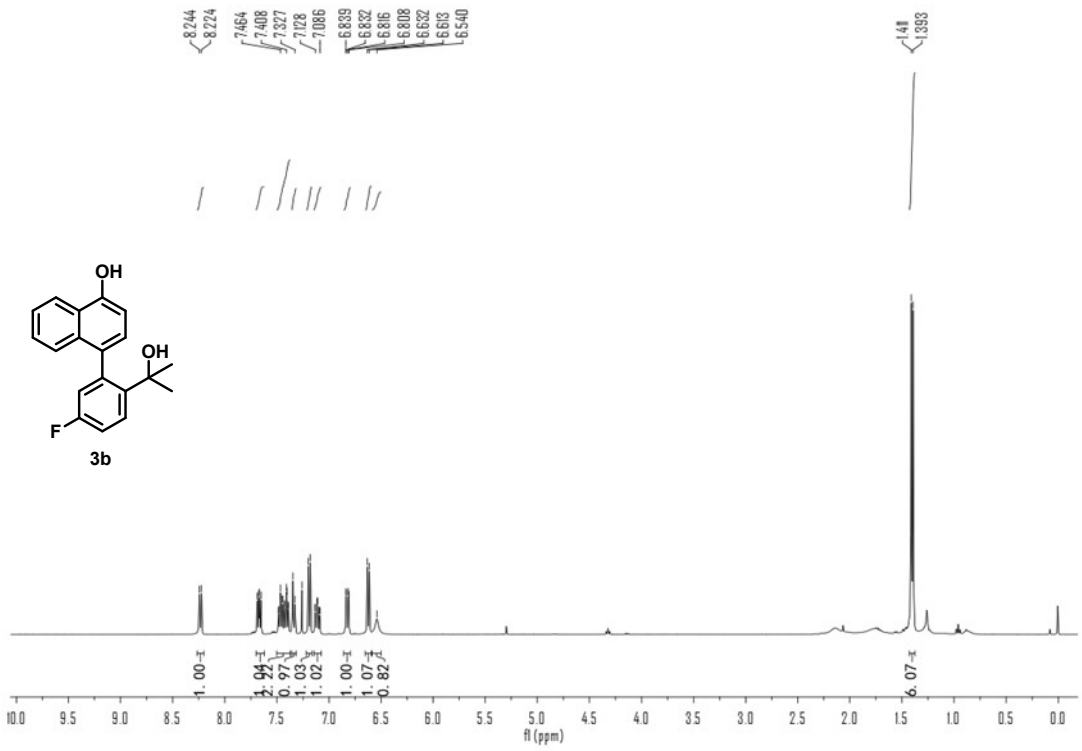

Fig. S17. ^{1}H NMR spectrum of **4-(5-fluoro-2-(2-hydroxypropan-2-yl)phenyl)naphthalen-1-ol (3b)** in $CDCl_3$.

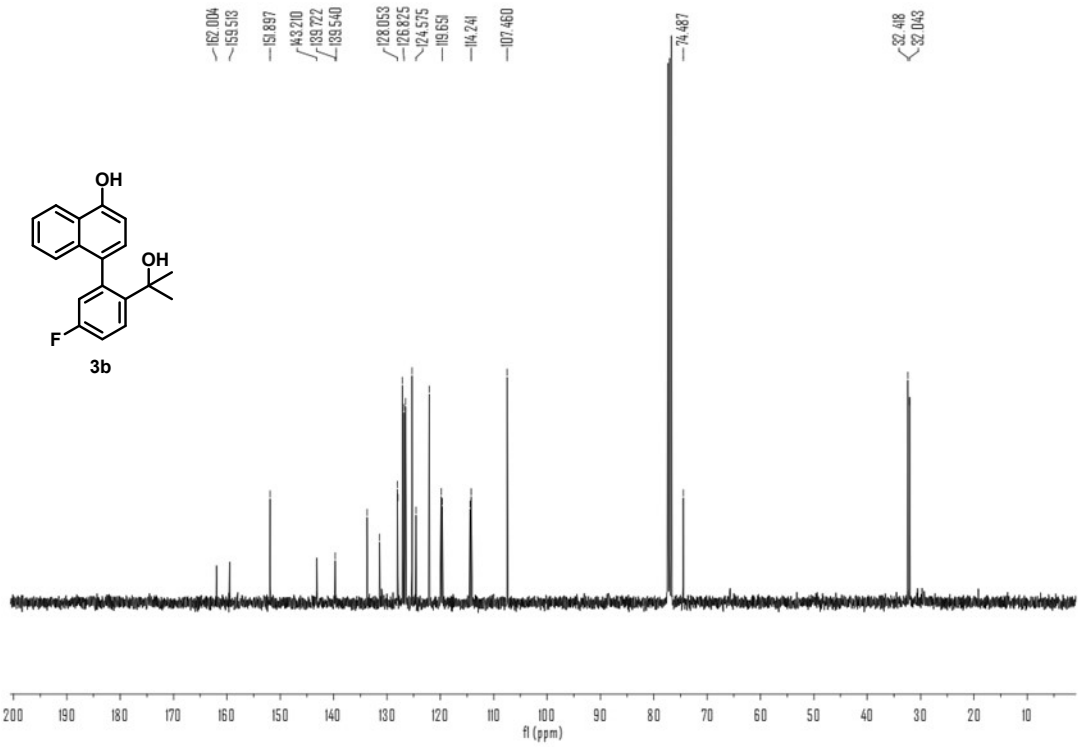

Fig. S18. ^{13}C NMR spectrum of **4-(5-fluoro-2-(2-hydroxypropan-2-yl) phenyl)naphthalen-1-ol (3b)** in $CDCl_3$.

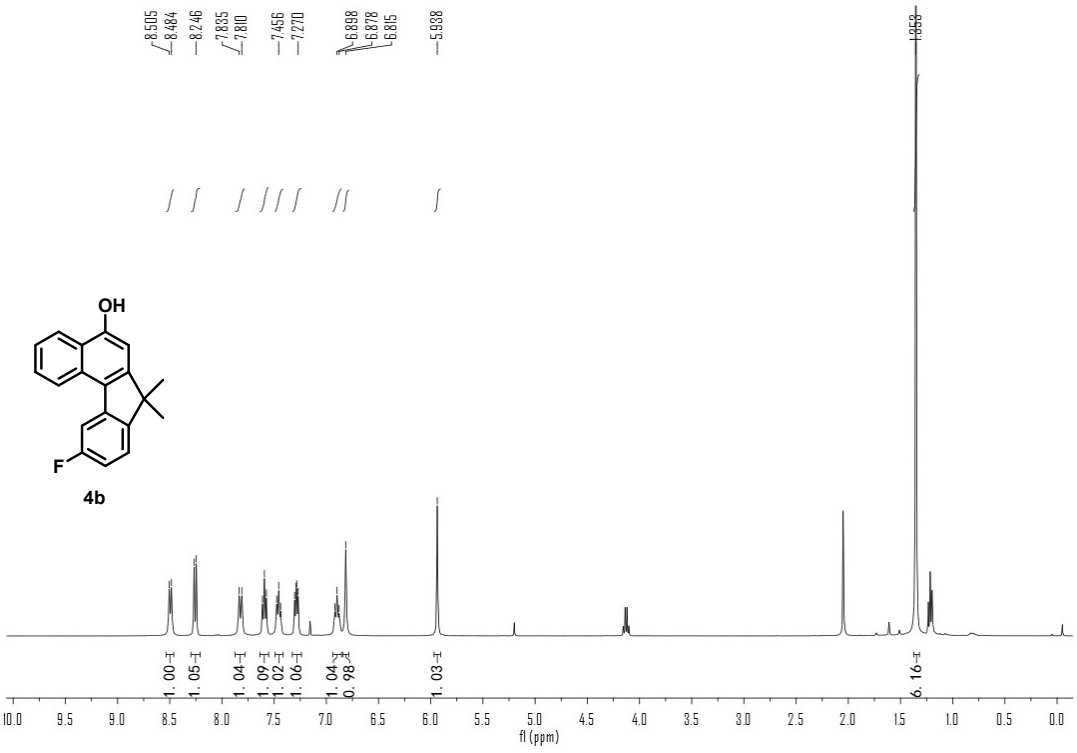

Fig. S19. ^{1}H NMR spectrum of **10-fluoro-7,7-dimethyl-*7H*-benzo[*c*]fluoren-5-ol (4b)** in $CDCl_3$.

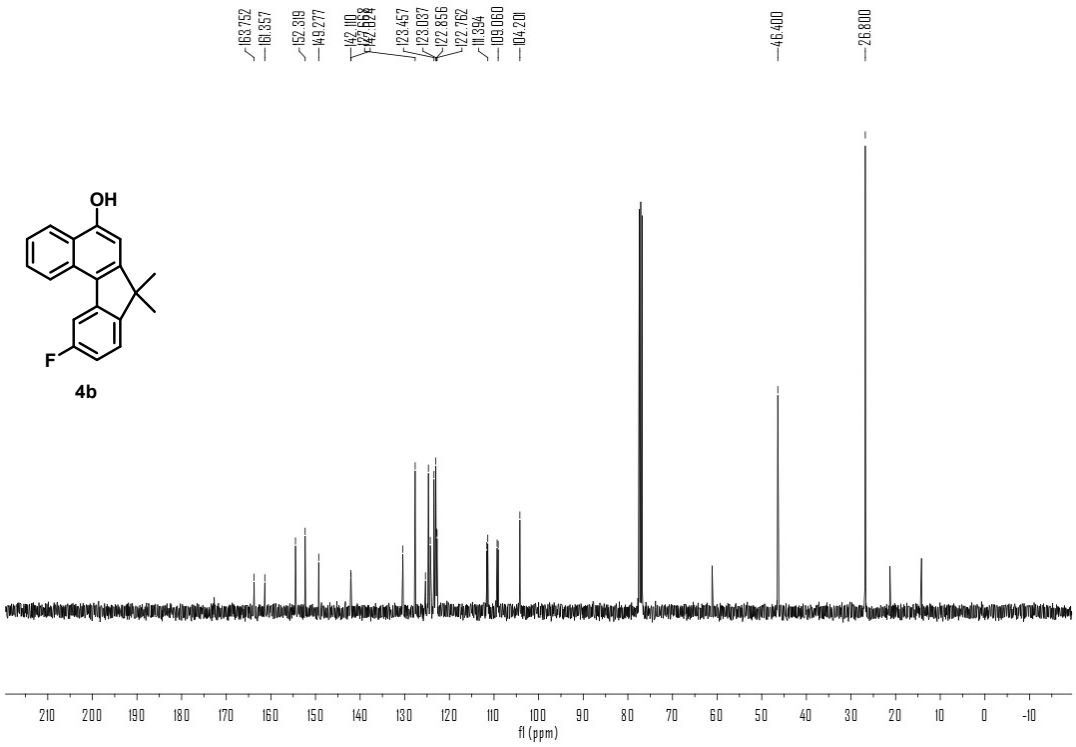

Fig. S20. ^{13}C NMR spectrum of **10-fluoro-7,7-dimethyl-*7H*-benzo[*c*]fluoren-5-ol (4b)** in $CDCl_3$.

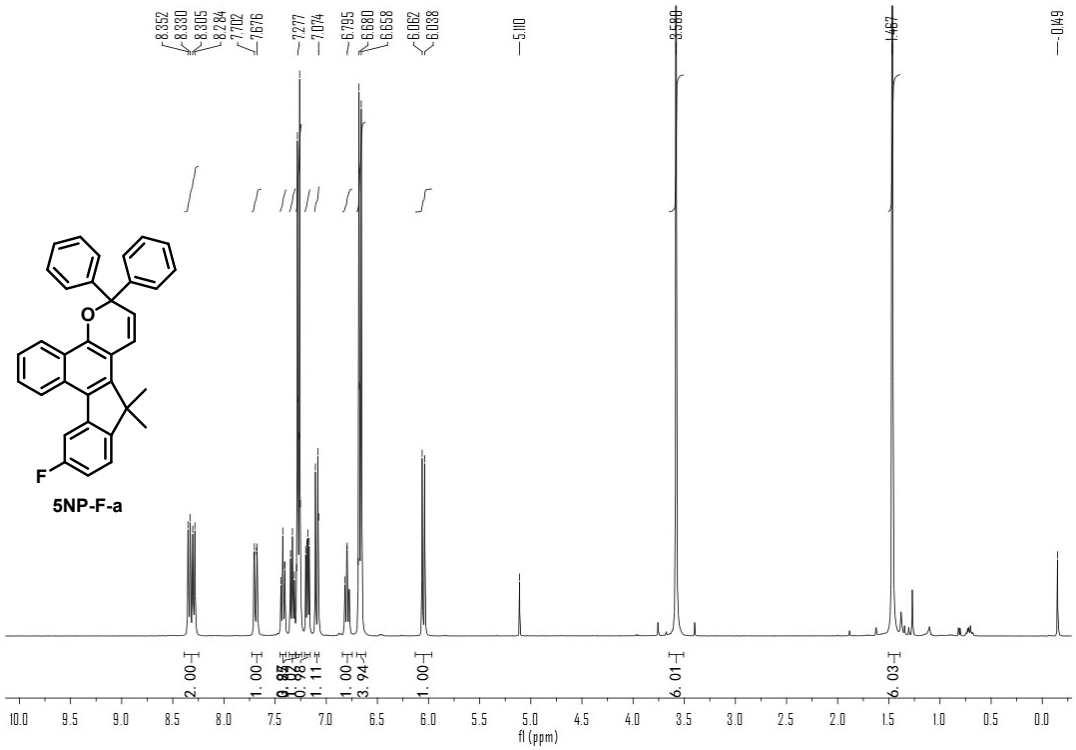

Figure S21. ^{1}H NMR spectrum of **10-fluoro-13,13-dimethyl-3,3-di-phenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

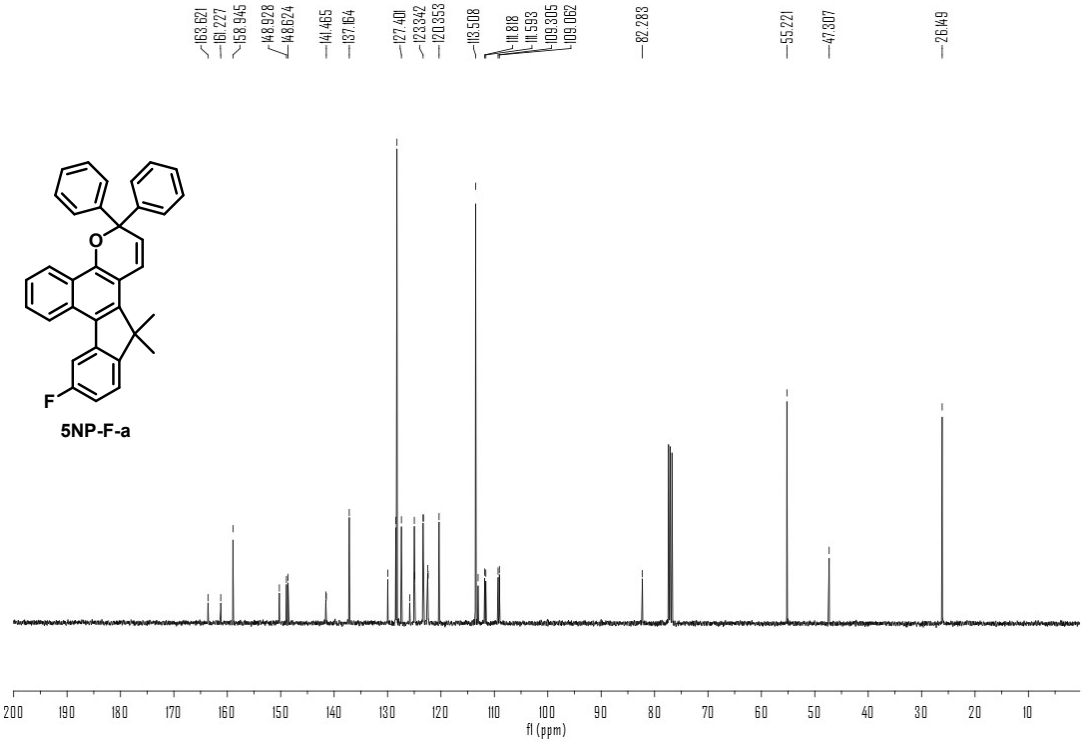

Figure S22. ^{13}C NMR spectrum of **10-fluoro-13,13-dimethyl-3,3-diphenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

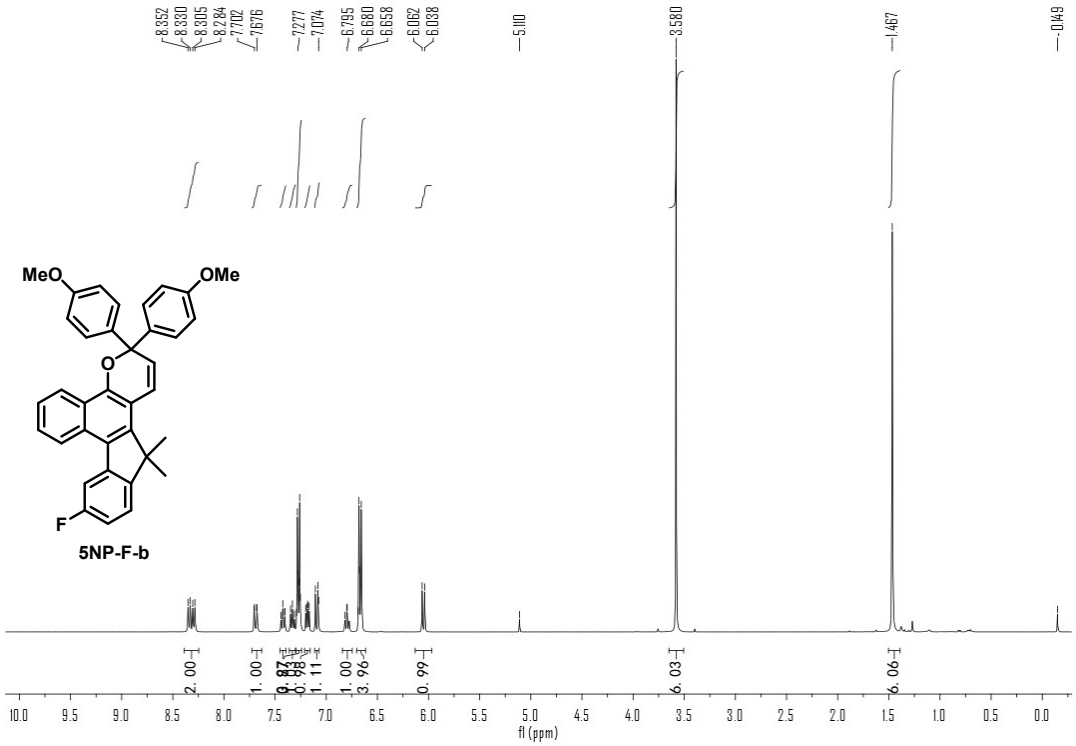

Fig. S23. ^{1}H NMR spectrum of **10-fluoro-3,3-bis(4-methoxyphenyl)-13,13-dimethyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

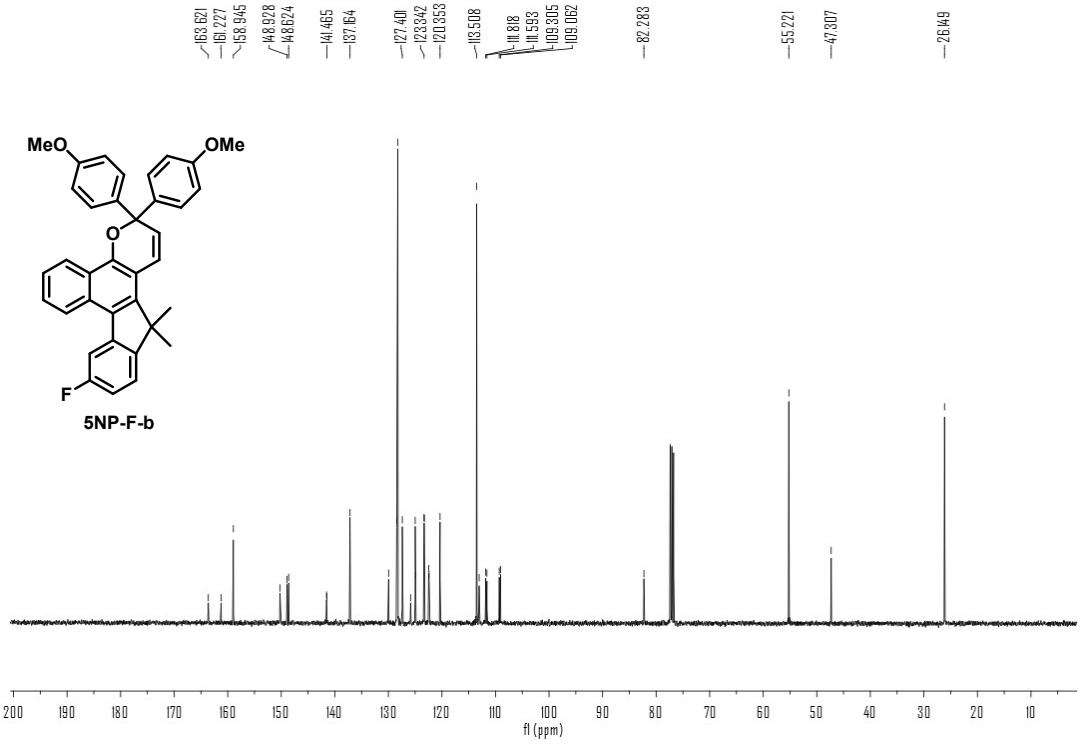

Fig. S24. ^{13}C NMR spectrum of **10-fluoro-3,3-bis(4-methoxyphenyl)-13,13-dimethyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

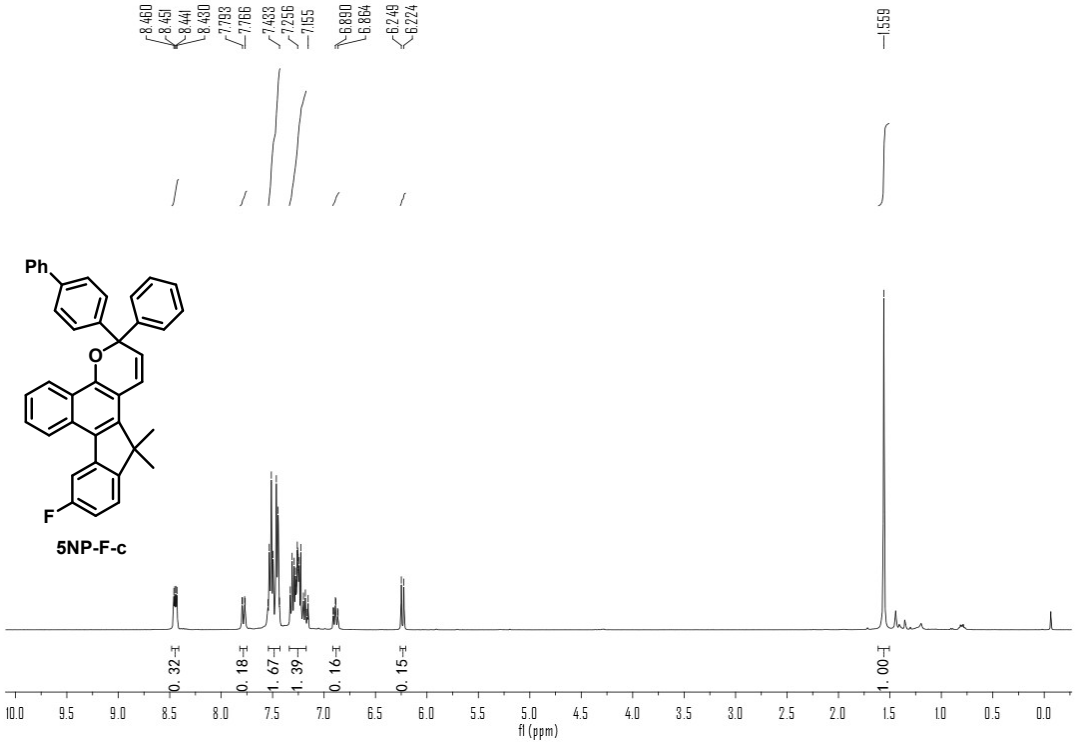

Figure S25. ^{1}H NMR spectrum of **3-([1,1'-biphenyl]-4-yl)-10-fluoro-13,13 -dimethyl-3-phenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

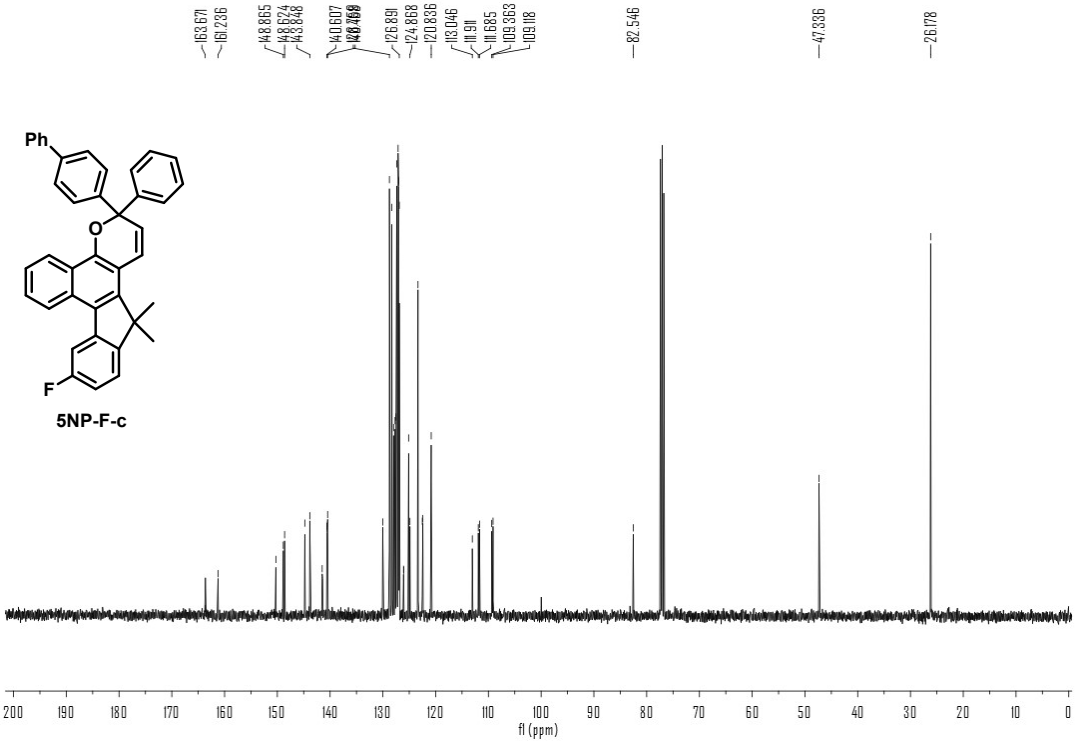

Figure S26. ^{13}C NMR spectrum of **3-([1,1'-biphenyl]-4-yl)-10-fluoro-13,13-dimethyl-3-phenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

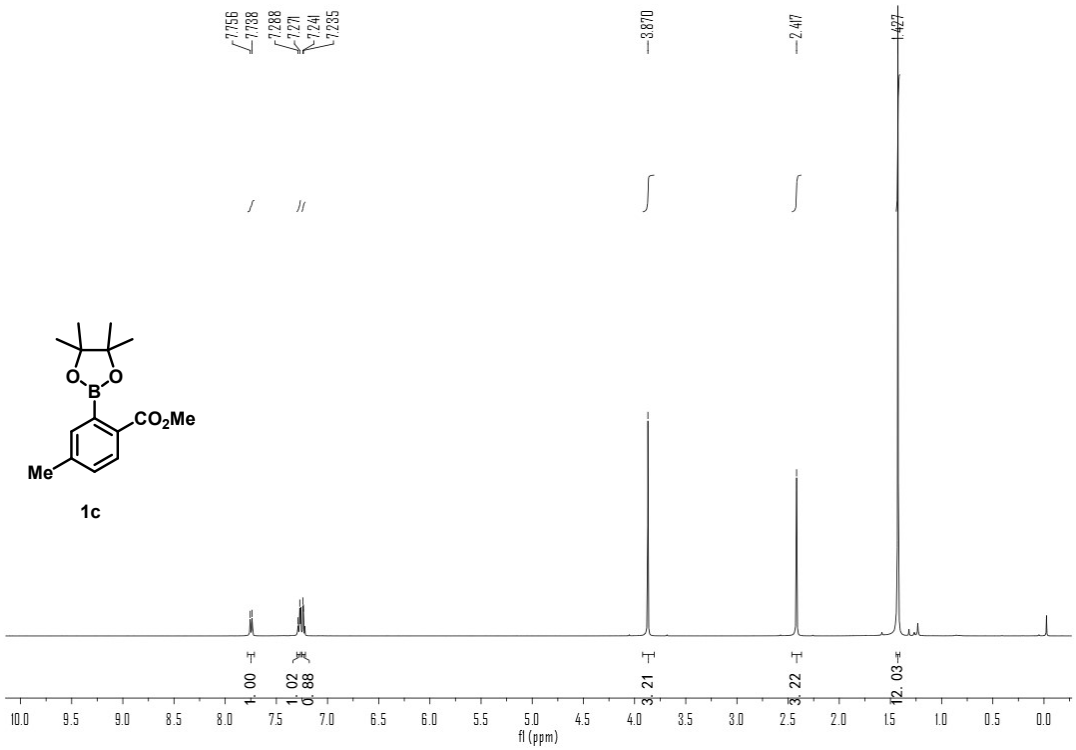

Fig. S27. ^{1}H NMR spectrum of **methyl 4-methyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoate (1c)** in $CDCl_3$.

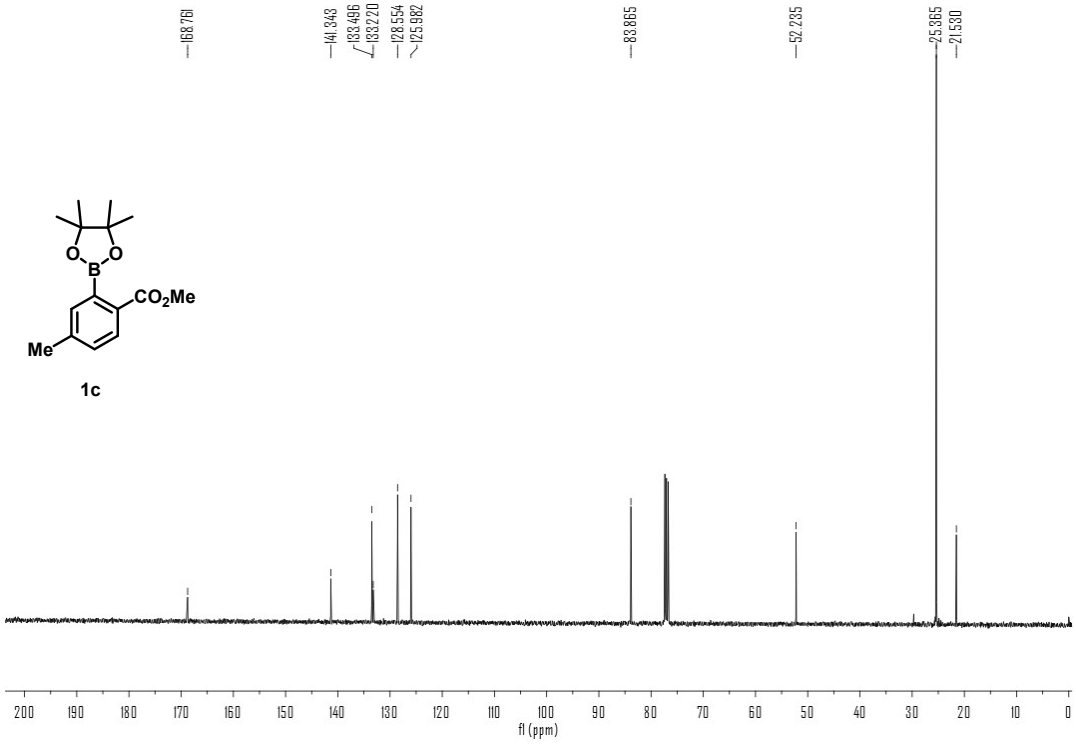

Fig. S28. ^{13}C NMR spectrum of **methyl 4-methyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoate (1c)** in $CDCl_3$.

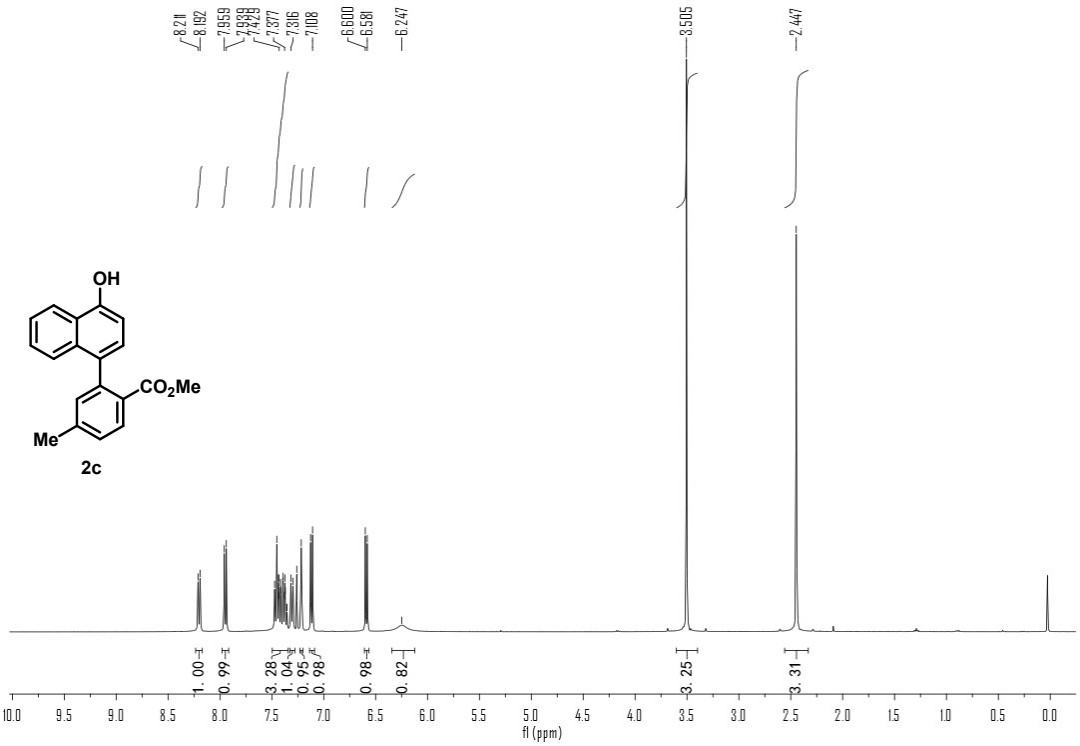

Fig. S29. ^{1}H NMR spectrum of **methyl 2-(4-hydroxynaphthalen-1-yl)-4-methylbenzoate (2c)** in $CDCl_3$.

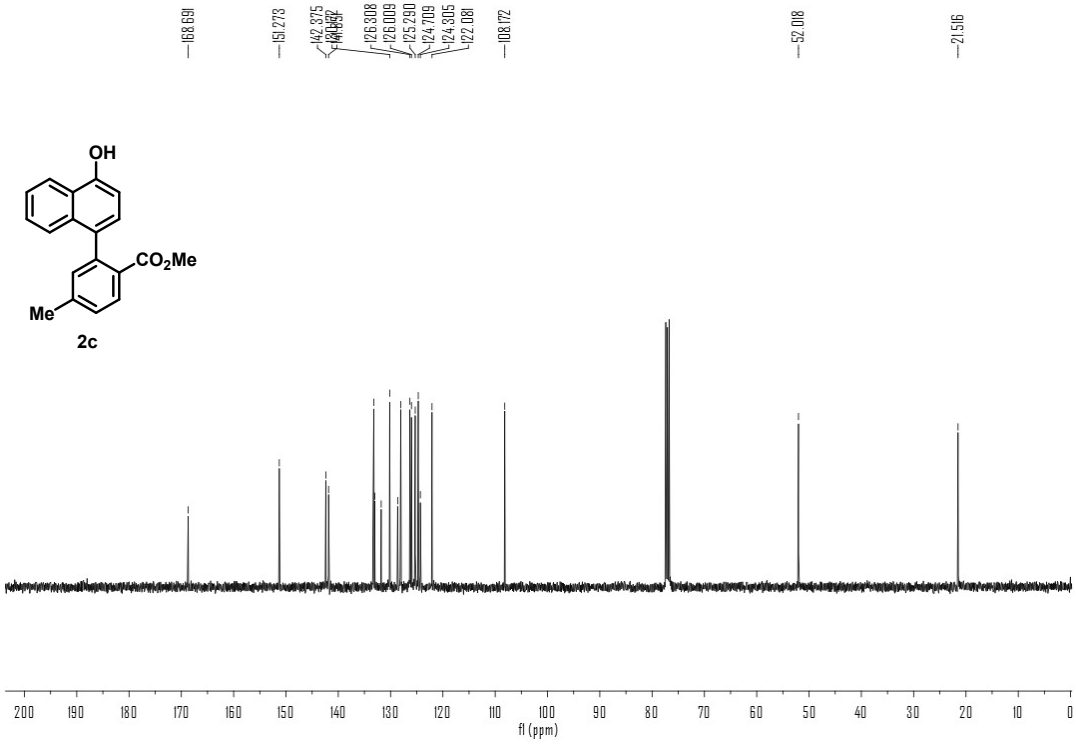

Fig. S30. ^{13}C NMR spectrum of **methyl 2-(4-hydroxynaphthalen-1-yl)-4-methyl benzoate (2c)** in $CDCl_3$.

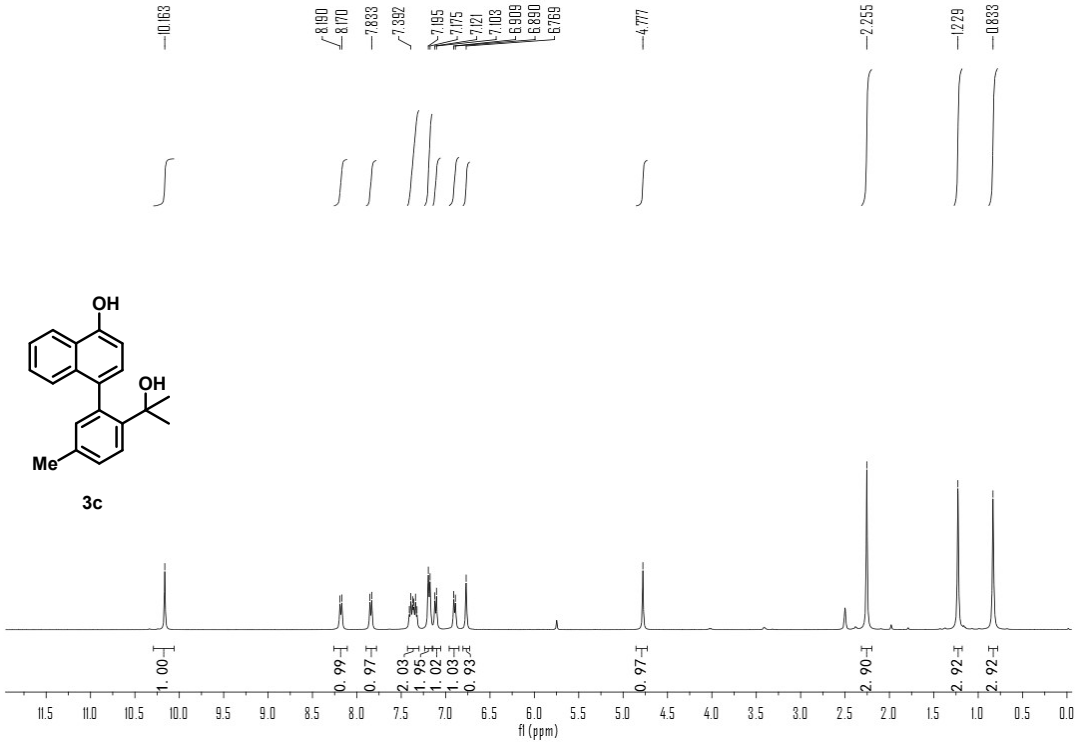

Fig. S31. ^{1}H NMR spectrum of **4-(2-(2-hydroxypropan-2-yl)-5-methylphenyl) naphthalen-1-ol (3c)** in $CDCl_3$.

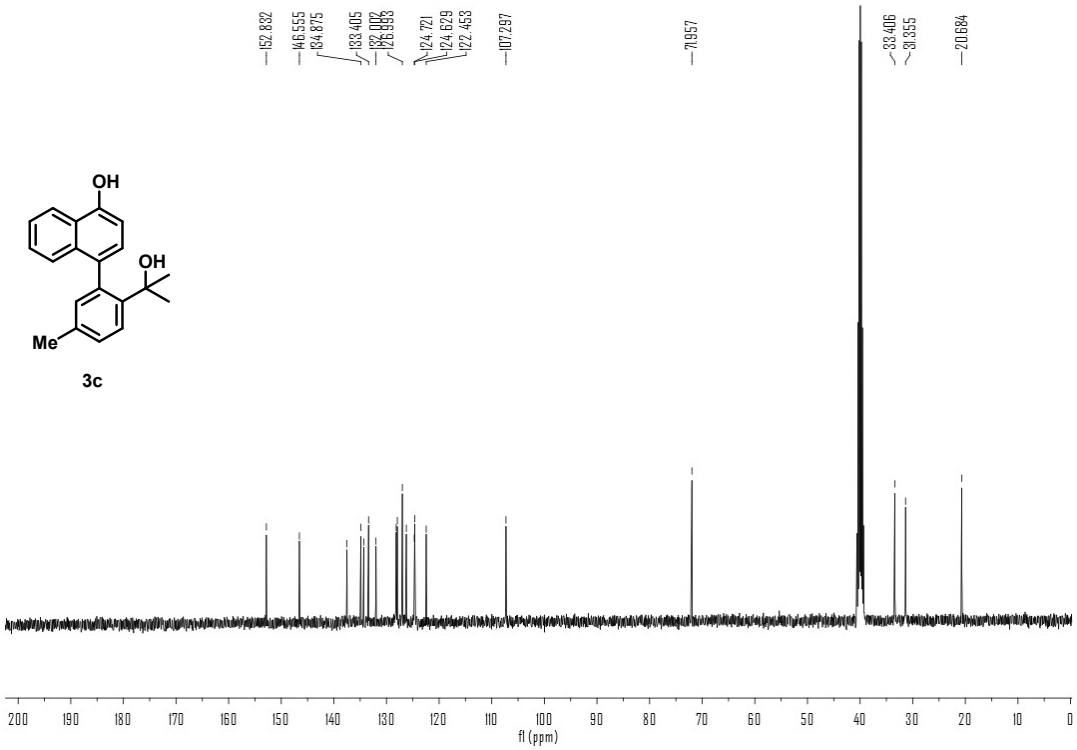

Fig. S32. ^{13}C NMR spectrum of **4-(2-(2-hydroxypropan-2-yl)-5-methylphenyl) naphthalen-1-ol (3c)** in $CDCl_3$.

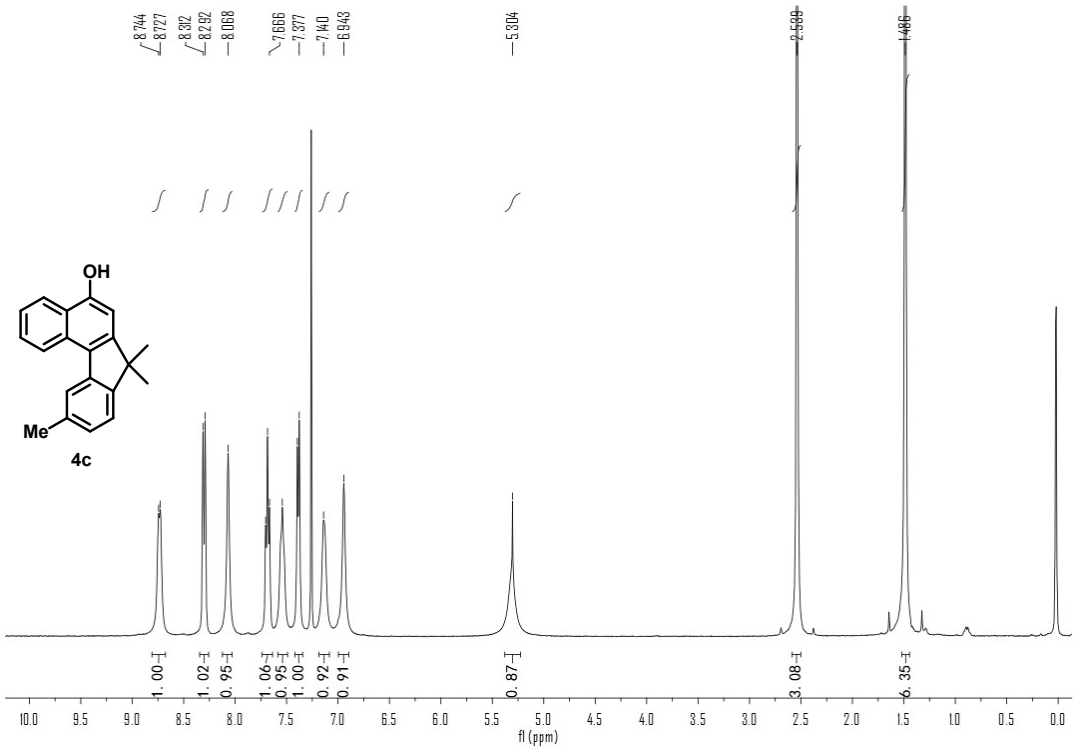

Fig. S33. ^{1}H NMR spectrum of **7,7,10-trimethyl-*7H*-benzo[*c*]fluoren-5-ol (4c)** in $CDCl_3$.

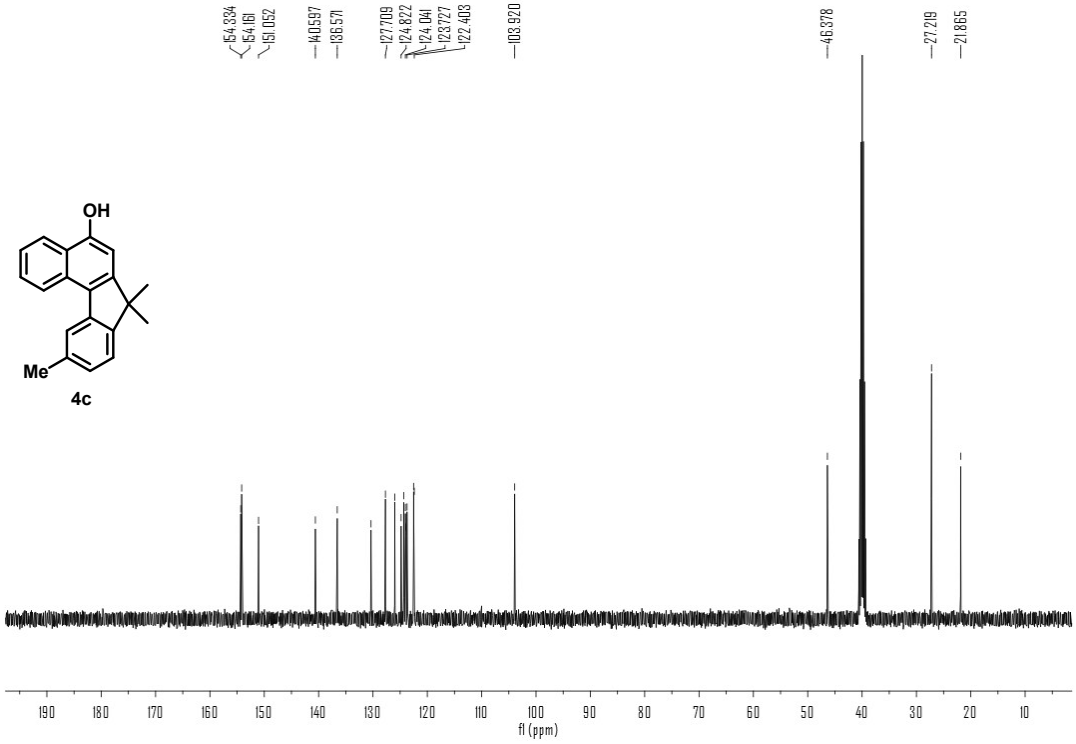

Fig. S34. ^{13}C NMR spectrum of **7,7,10-trimethyl-*7H*-benzo[*c*]fluoren-5-ol (4c)** in $CDCl_3$.

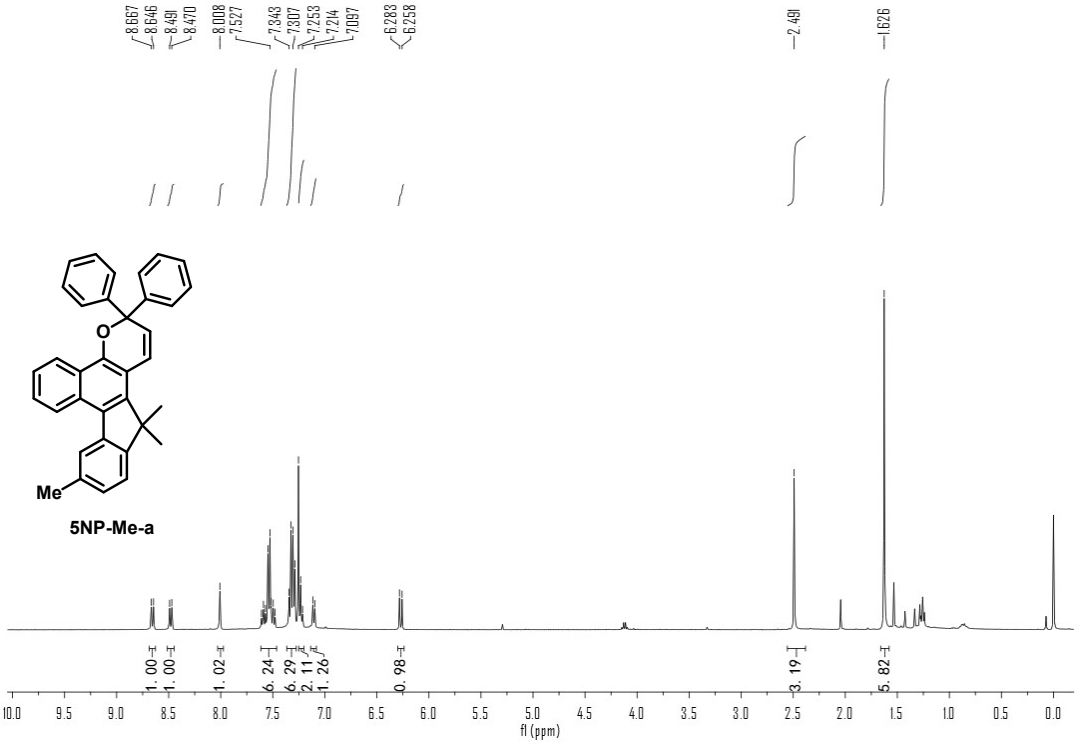

Figure S35. ^{1}H NMR spectrum of **10,13,13-trimethyl-3,3-diphenyl-3,13-dihydro benzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

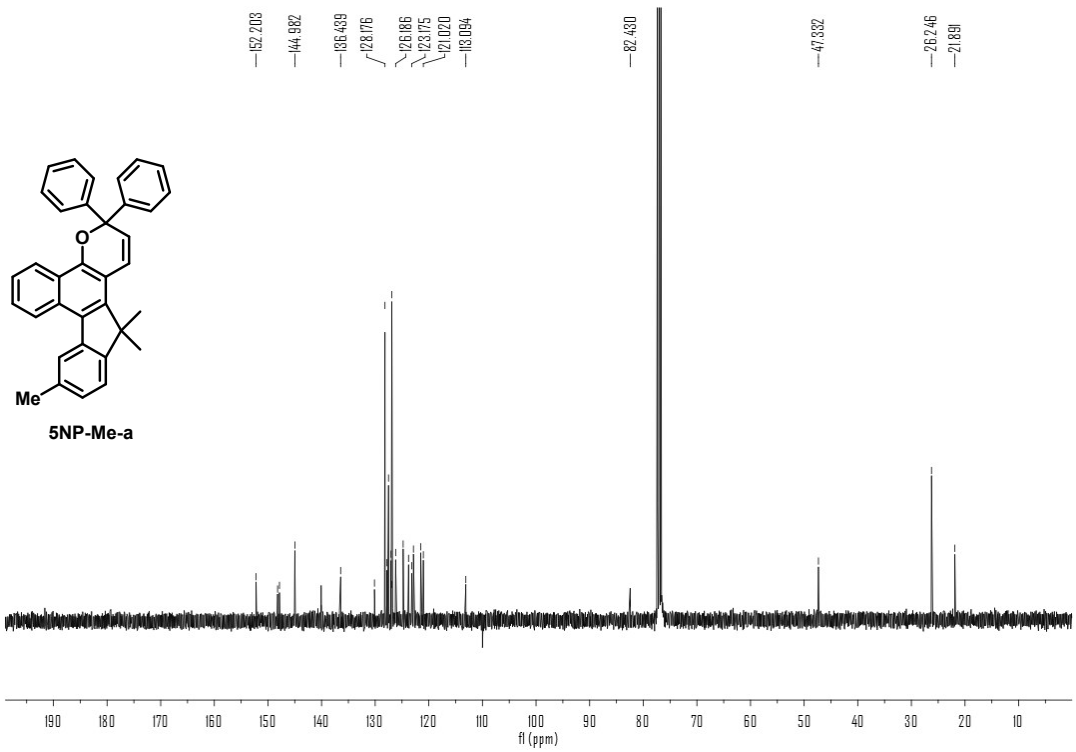

Figure S36. ^{13}C NMR spectrum of **10,13,13-trimethyl-3,3-diphenyl-3,13-dihydro benzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

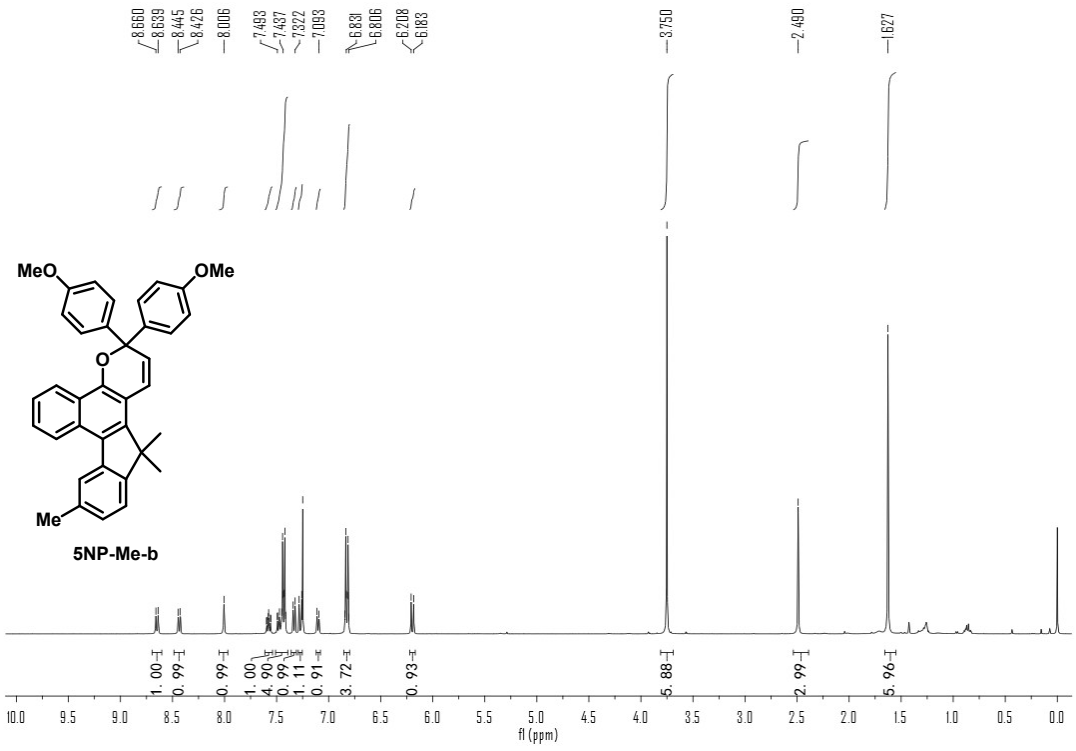

Fig. S37. ^{1}H NMR spectrum of **3,3-bis(4-methoxyphenyl)-10,13,13-trimethyl- 3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

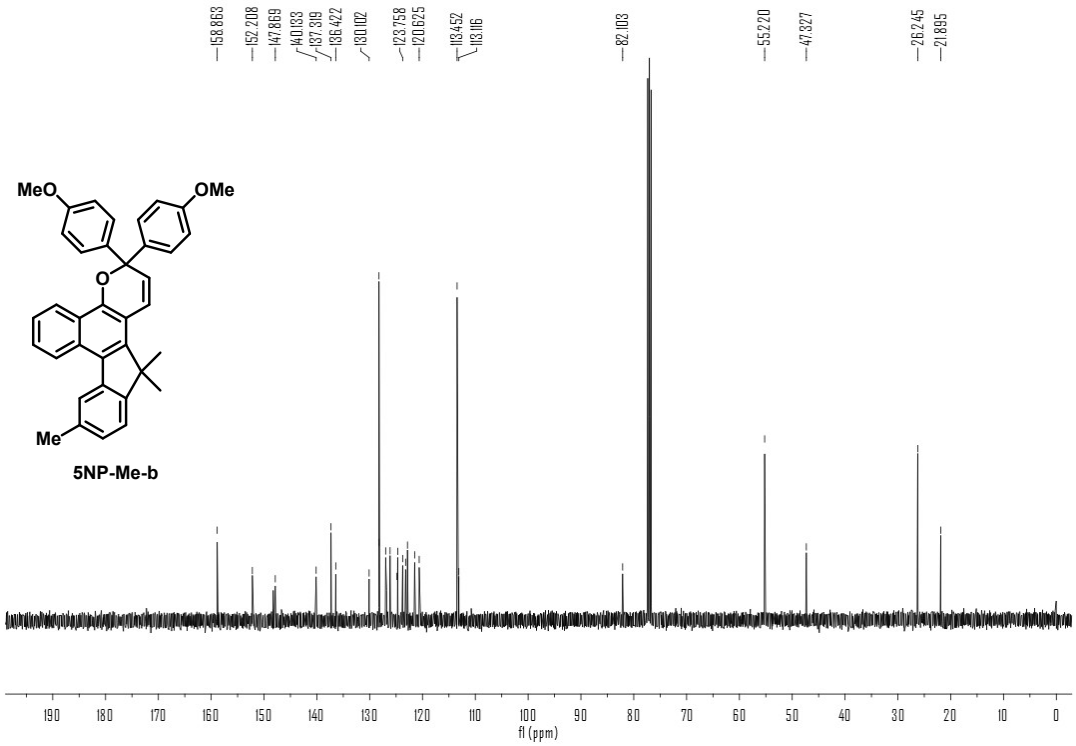

Fig. S38. ^{13}C NMR spectrum of**3,3-bis(4-methoxyphenyl)-10,13,13-trimethyl -3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

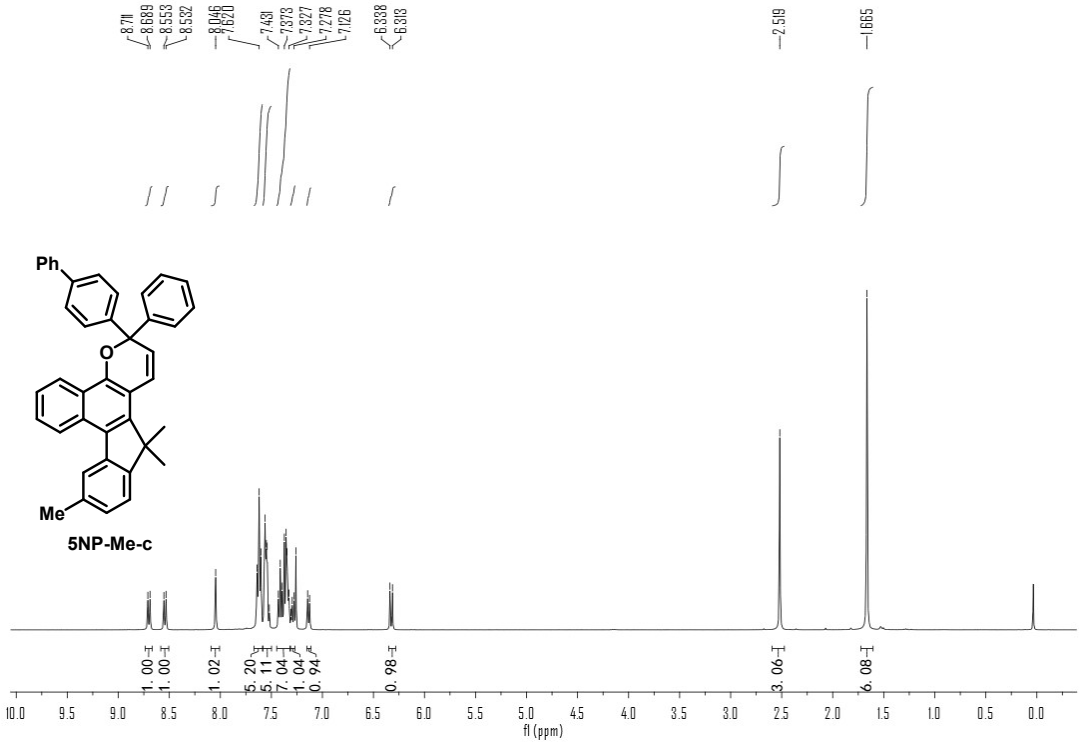

Figure S39. ^{1}H NMR spectrum of **3-([1,1'-biphenyl]-4-yl)-10,13,13-trimethyl-3-phenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

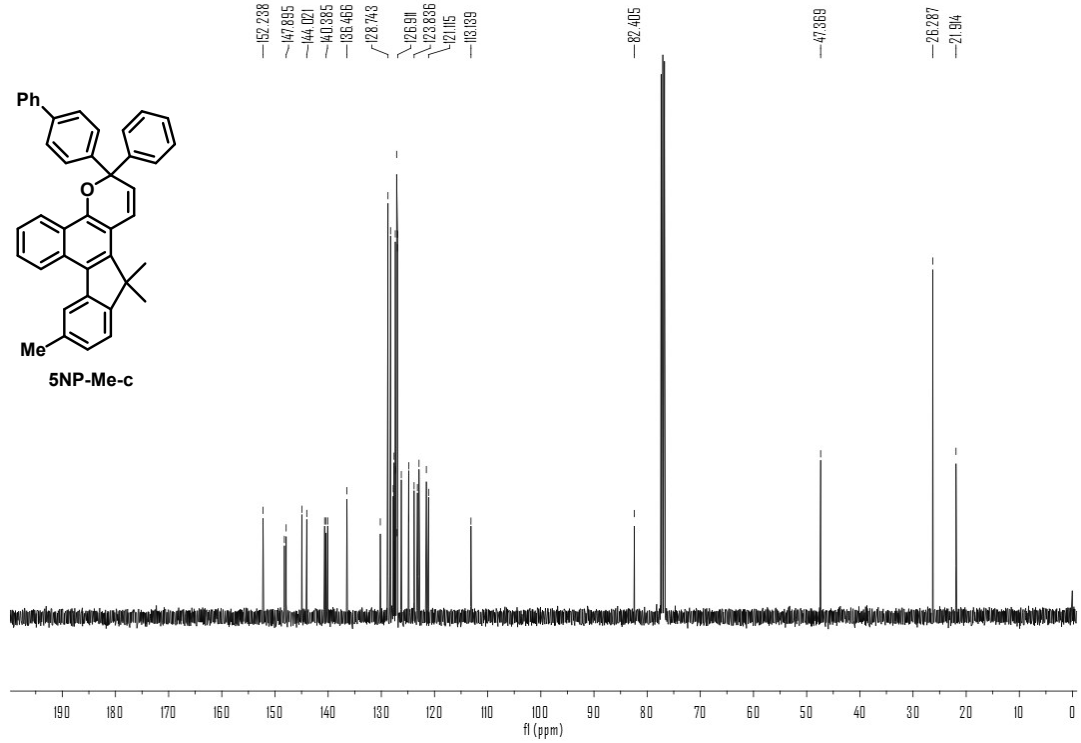

Figure S40. ^{13}C NMR spectrum of **3-([1,1'-biphenyl]-4-yl)-10,13,13-trimethyl-3 -phenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

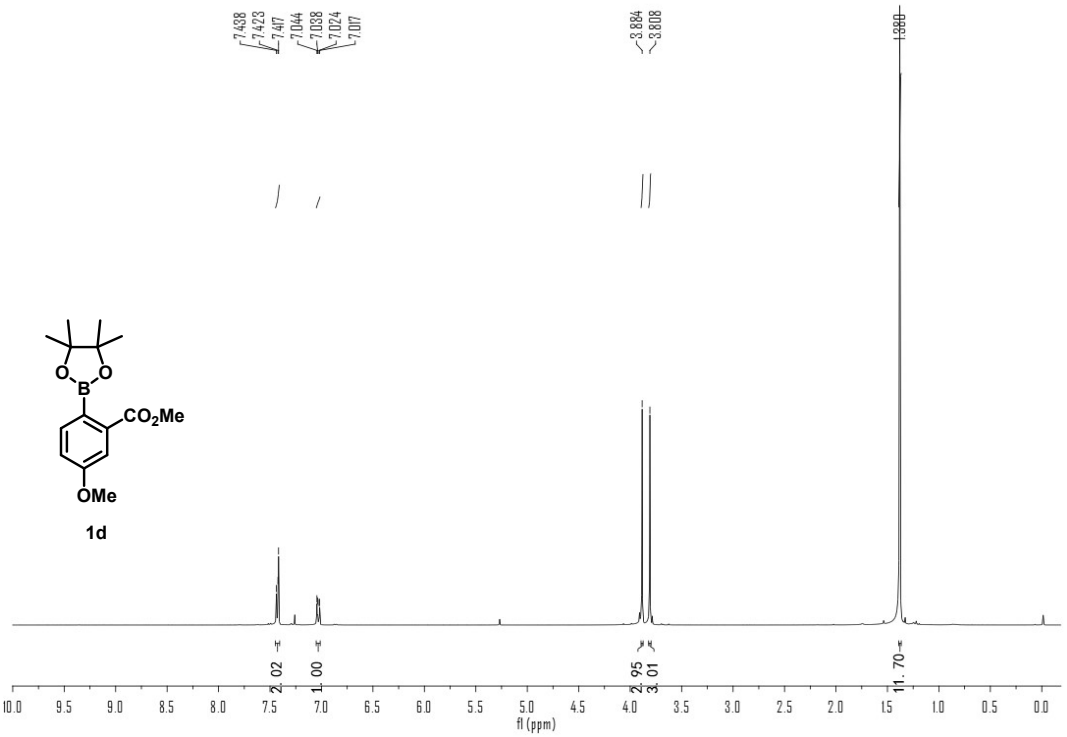

Fig. S41. ^{1}H NMR spectrum of **methyl 5-methoxy-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoate (1d)** in $CDCl_3$.

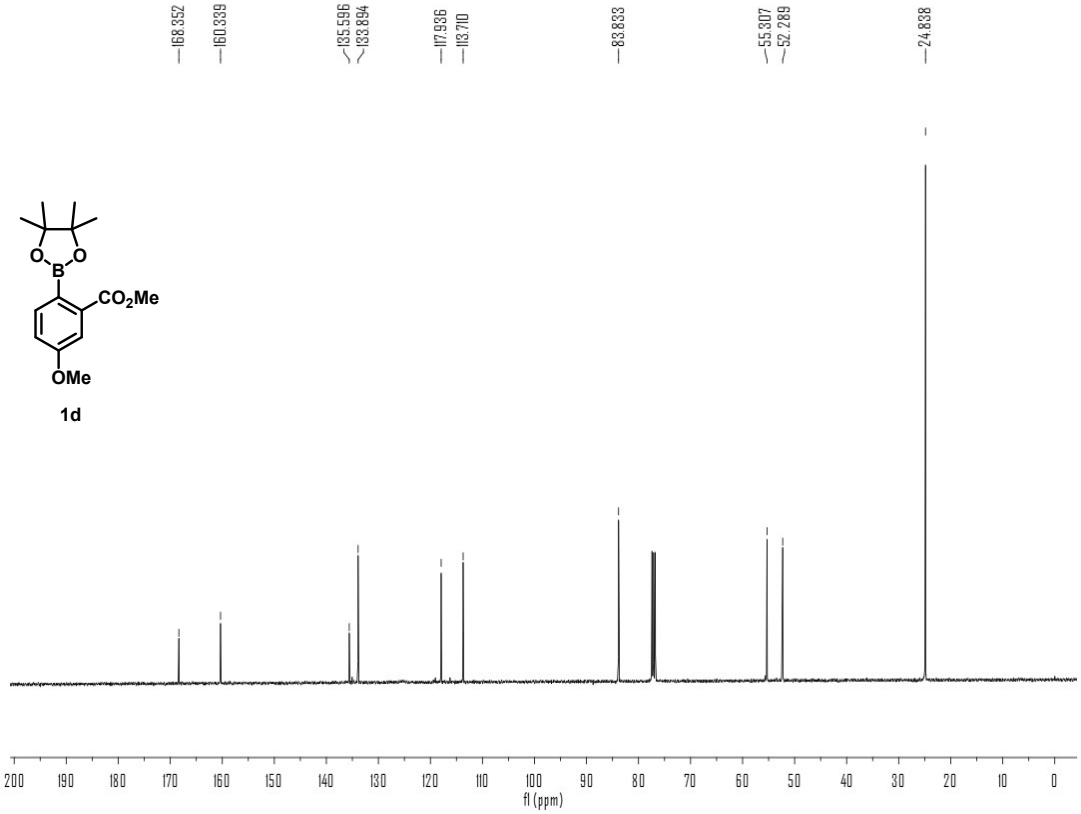

Fig. S42. ^{13}C NMR spectrum of **methyl 5-methoxy-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoate (1d)** in $CDCl_3$.

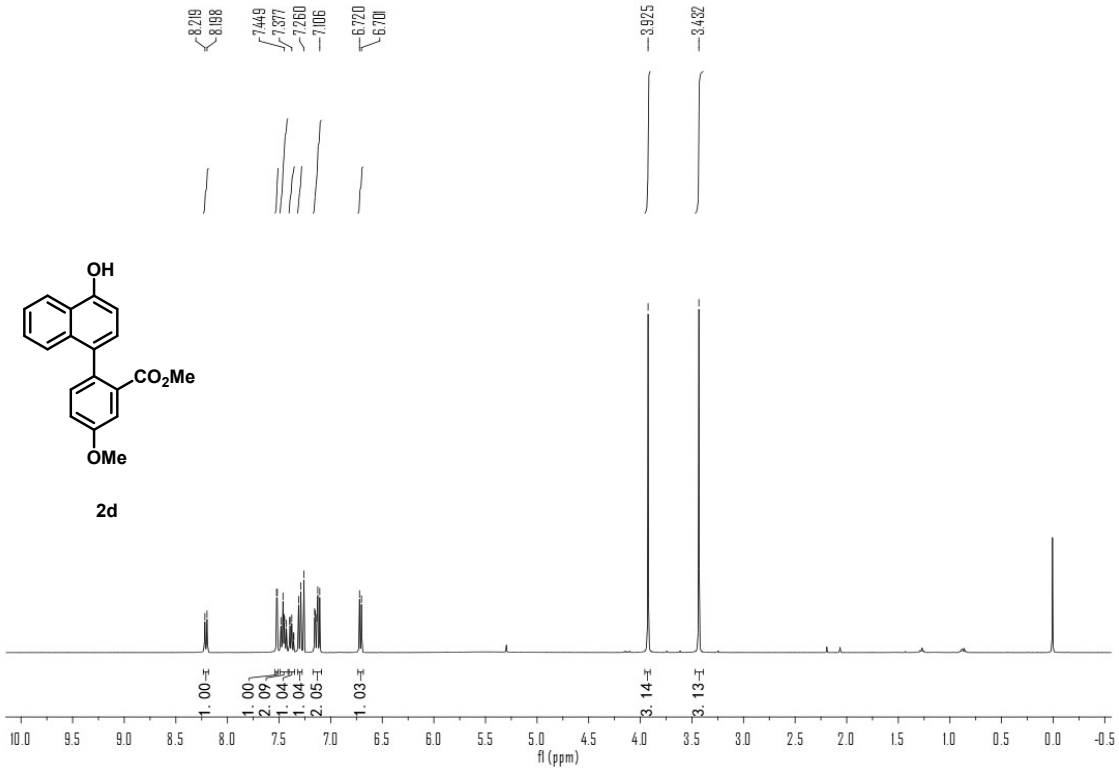

Fig. S43. ^{1}H NMR spectrum of **4-(2-(2-hydroxypropan-2-yl)-4-methoxyphenyl) naphthalen-1-ol (2d)** in $CDCl_3$.

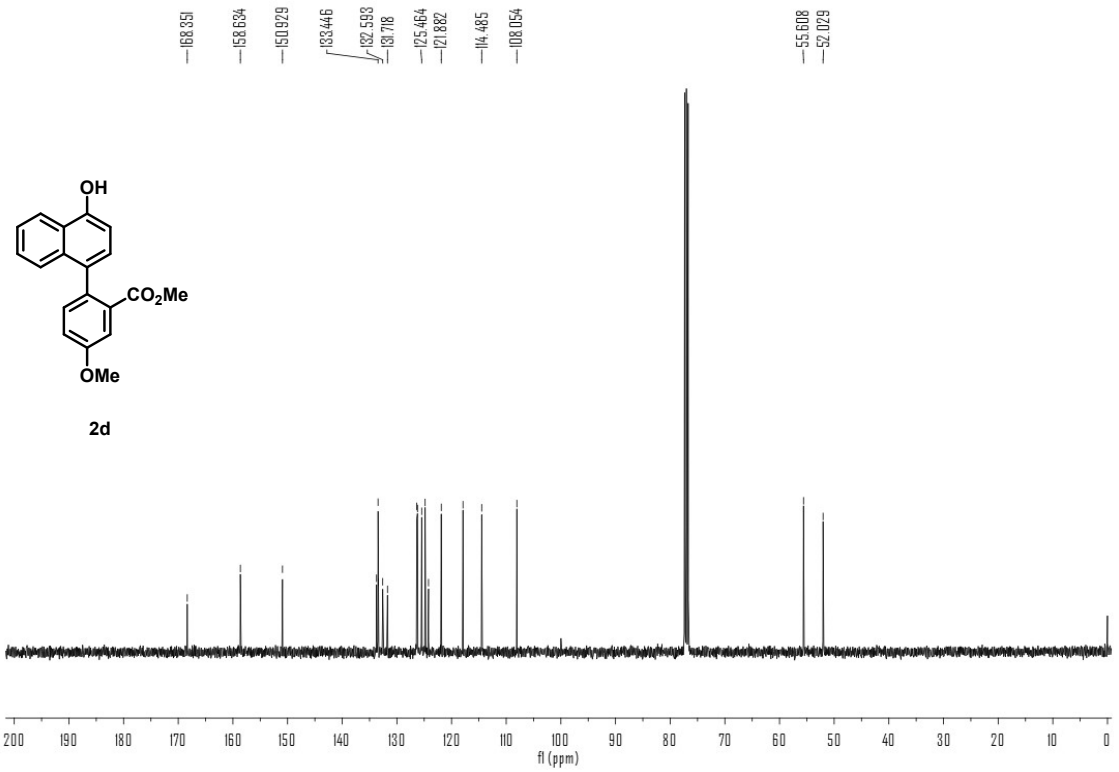

Fig. S44. ^{13}C NMR spectrum of **4-(2-(2-hydroxypropan-2-yl)-4-methoxyphenyl) naphthalen-1-ol (2d)** in $CDCl_3$.

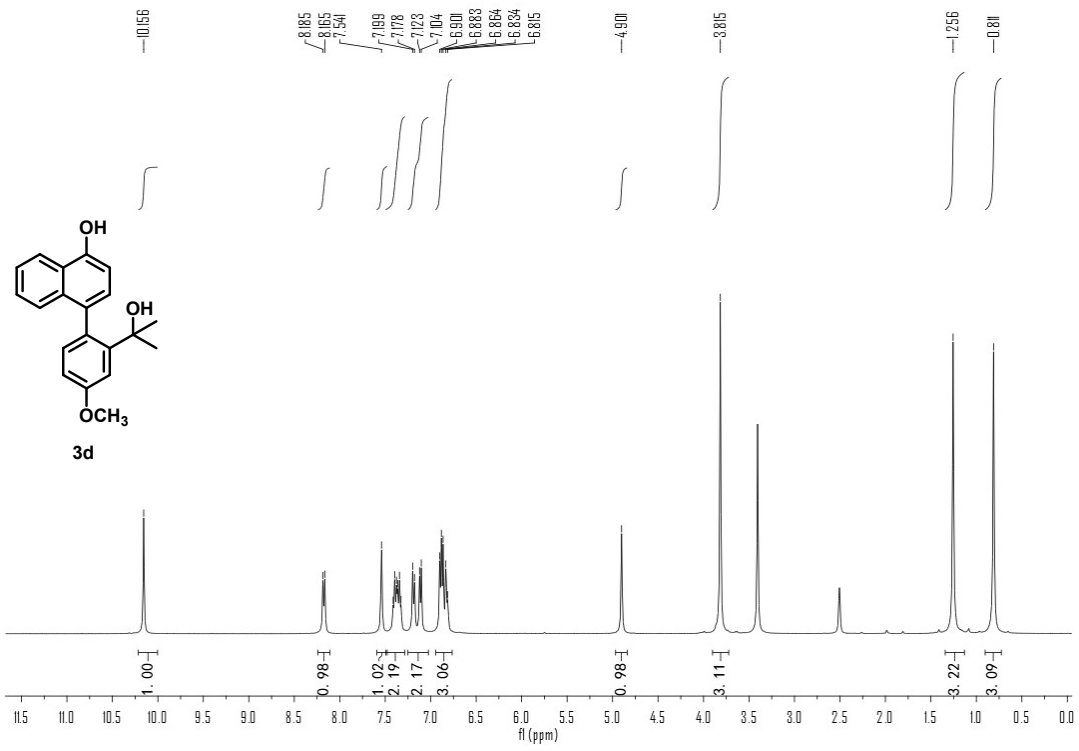

Fig. S45. ^{1}H NMR spectrum of **4-(2-(2-hydroxypropan-2-yl)-4-methoxyphenyl) naphthalen-1-ol (3d)** in DMSO-d_6.

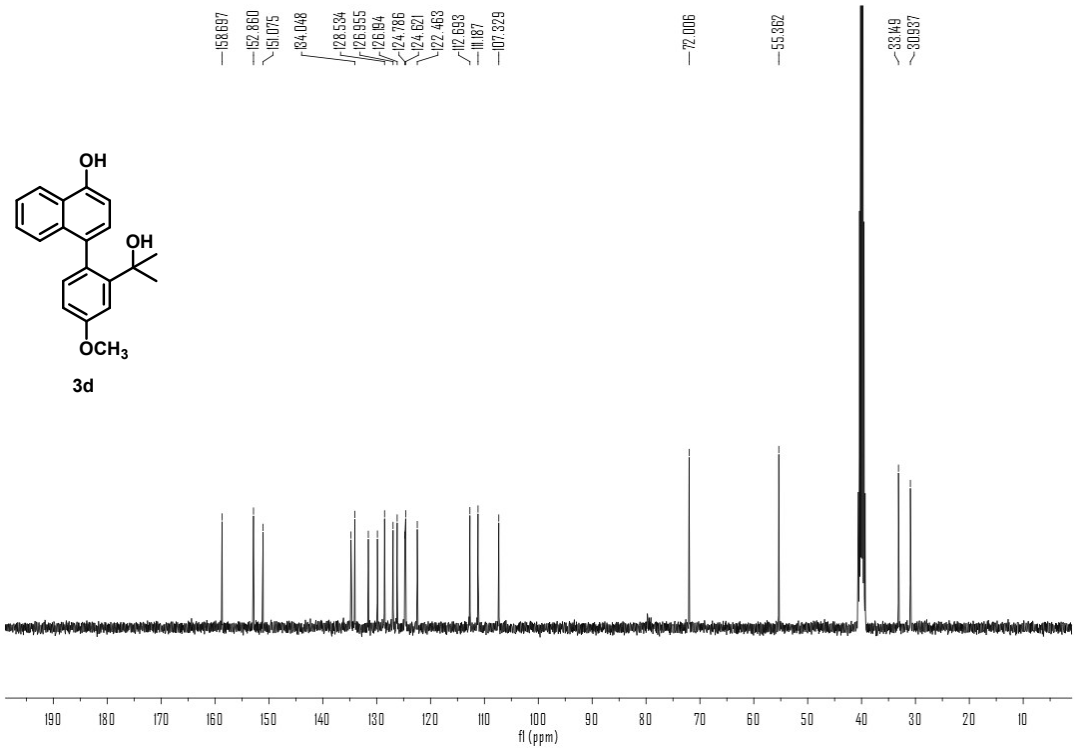

Fig. S46. ^{13}C NMR spectrum of **4-(2-(2-hydroxypropan-2-yl)-4-methoxyphenyl) naphthalen-1-ol (3d)** in DMSO-d_6.

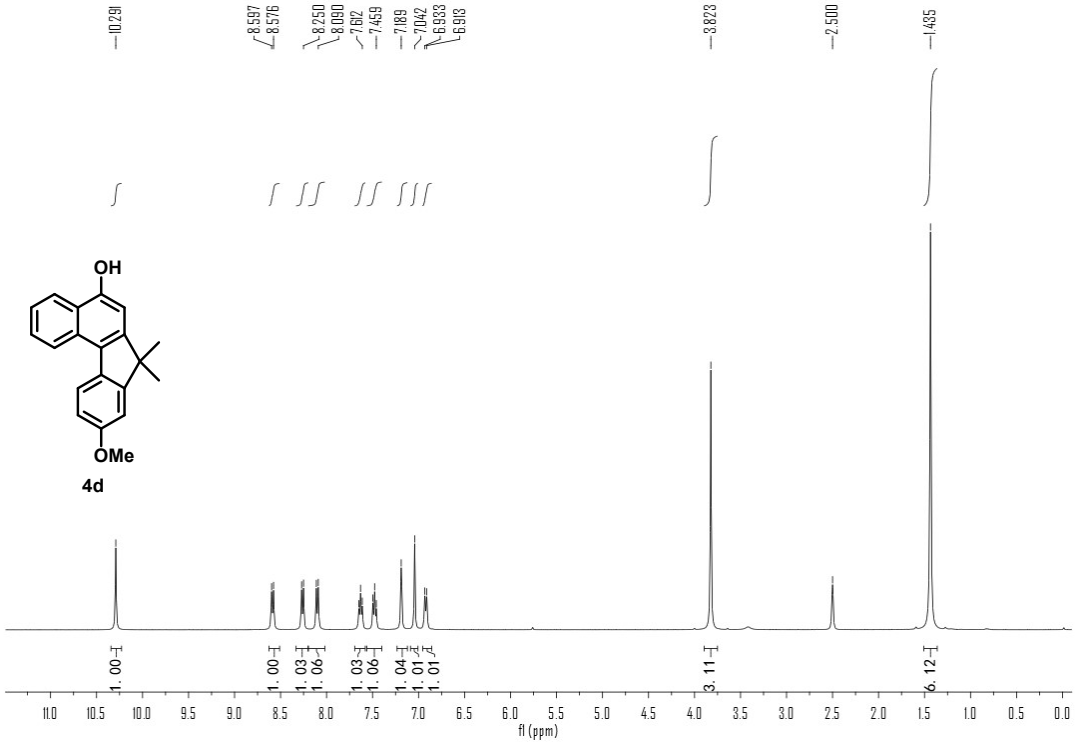

Fig. S47. ^{1}H NMR spectrum of **9-methoxy-7,7-dimethyl-*7H*-benzo[*c*]fluoren-5-ol (4d)** in DMSO-d_6.

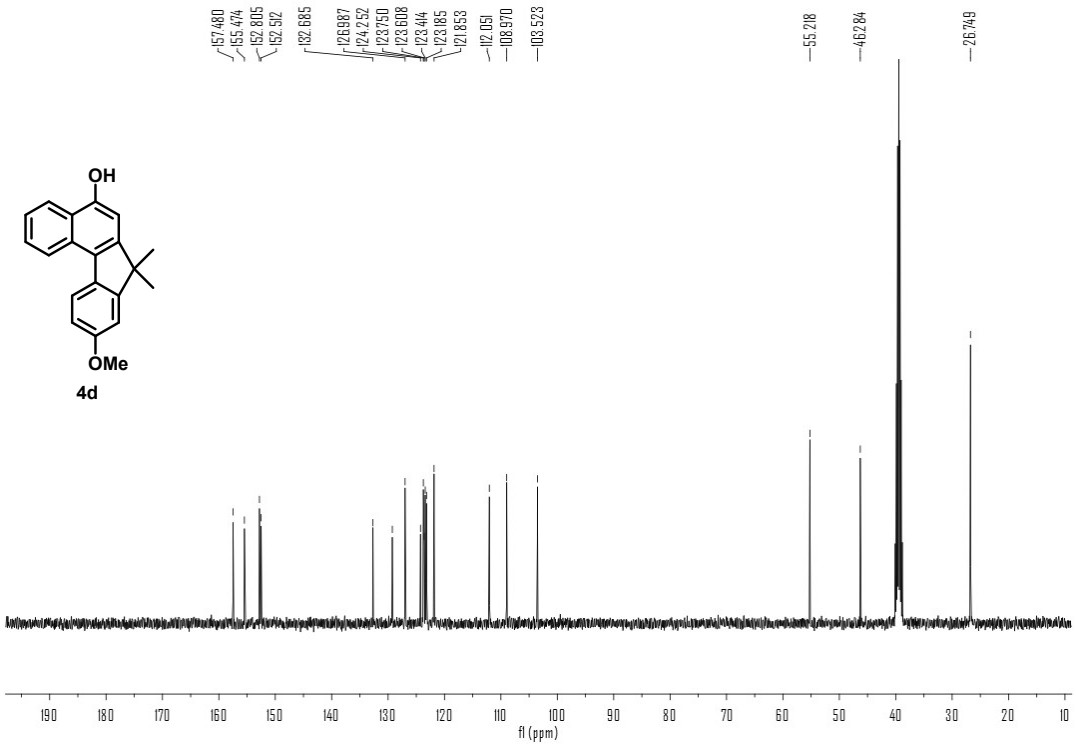

Fig. S48. ^{13}C NMR spectrum of **9-methoxy-7,7-dimethyl-*7H*-benzo[*c*]fluoren-5-ol (4d)** in DMSO-d_6.

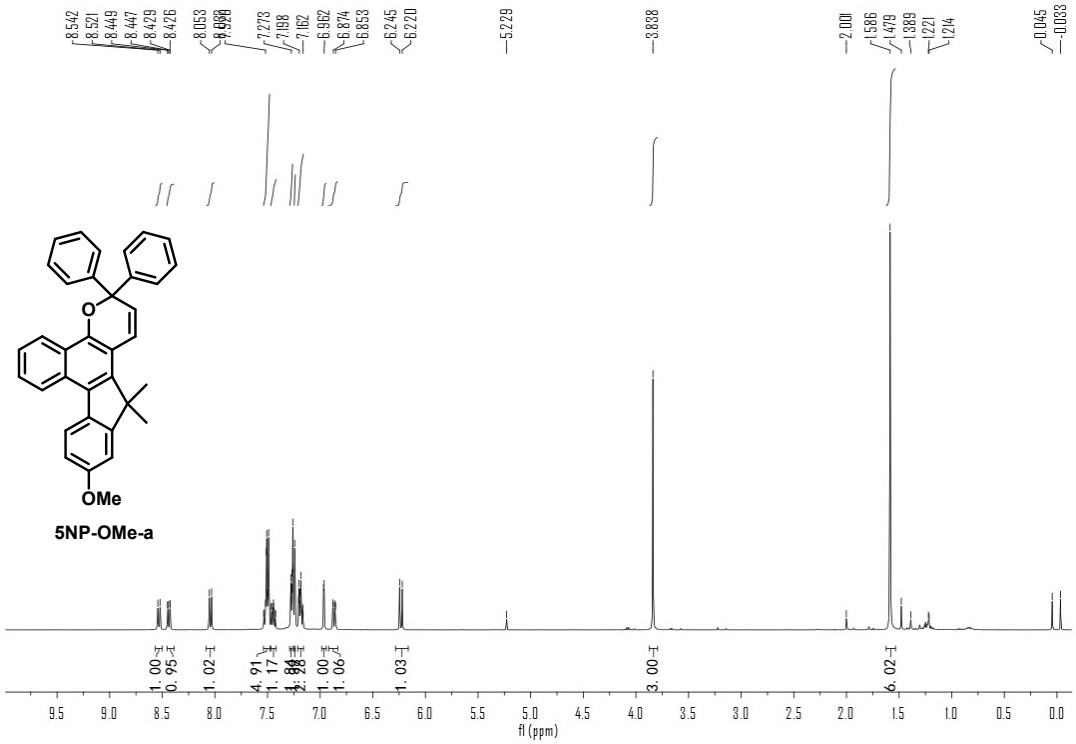

Figure S49. ^{1}H NMR spectrum of **11-methoxy-13,13-dimethyl-3,3-diphenyl-3, 13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

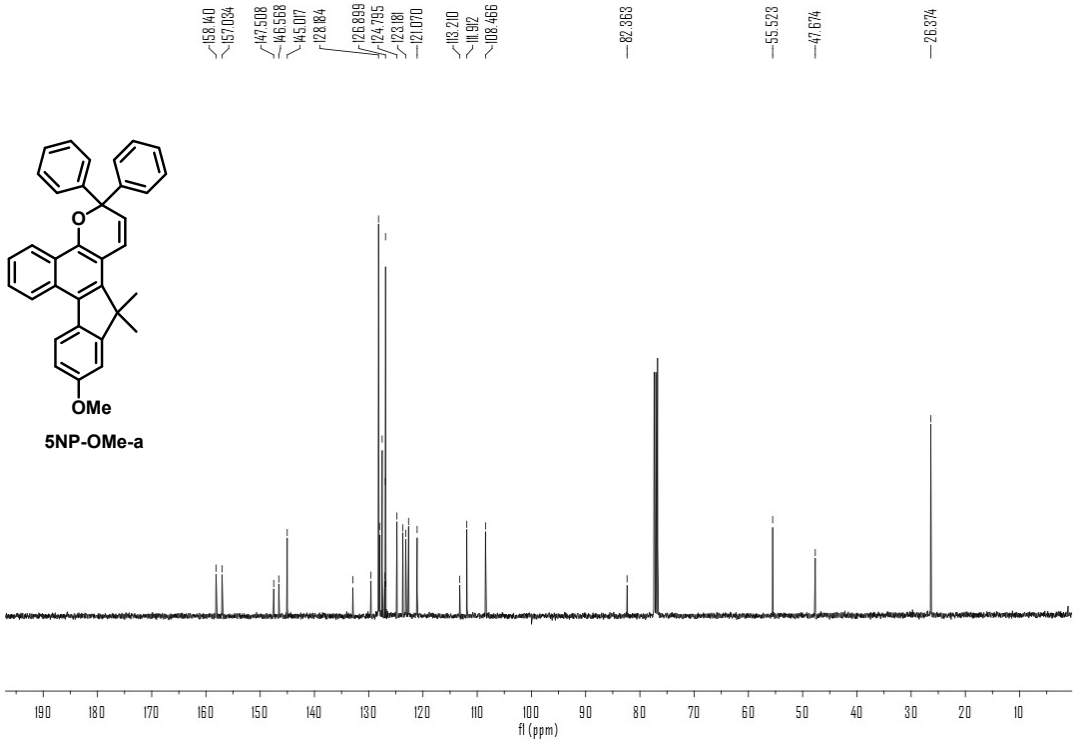

Figure S50. ^{13}C NMR spectrum of **11-methoxy-13,13-dimethyl-3,3-diphenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

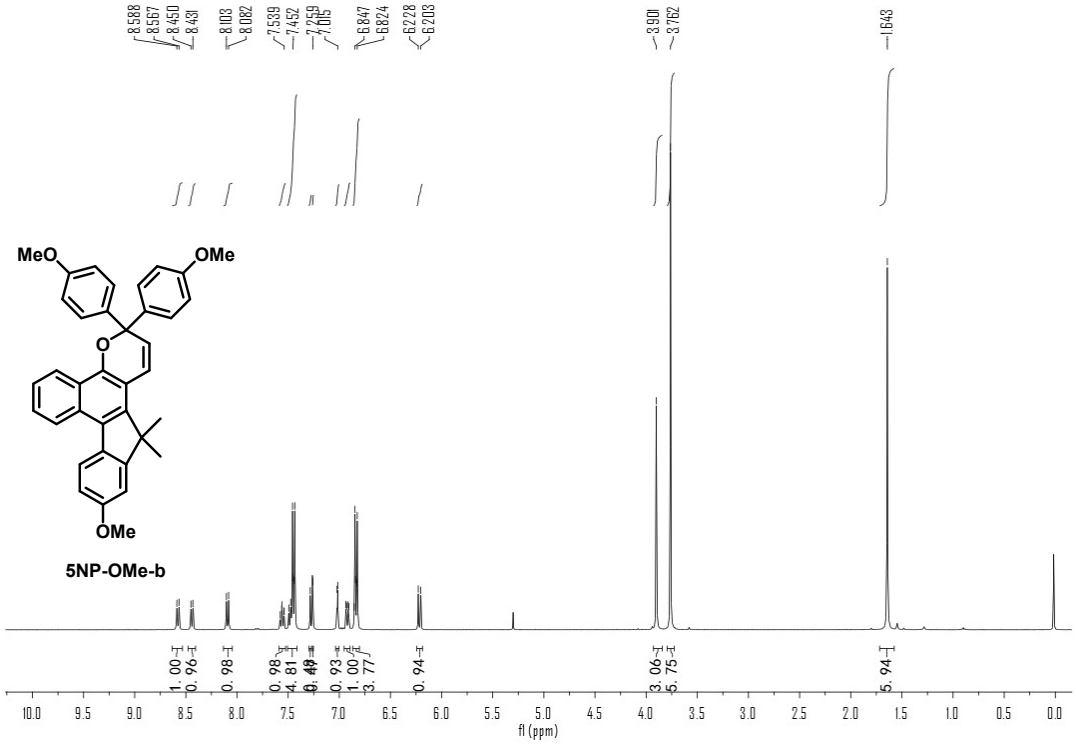

Fig. S51. ^{1}H NMR spectrum of **11-methoxy-3,3-bis(4-methoxyphenyl)-13,13-dimethyl-3,13-dihydrobenzo[h]indeno[*2,1-f*]chromene** in $CDCl_3$.

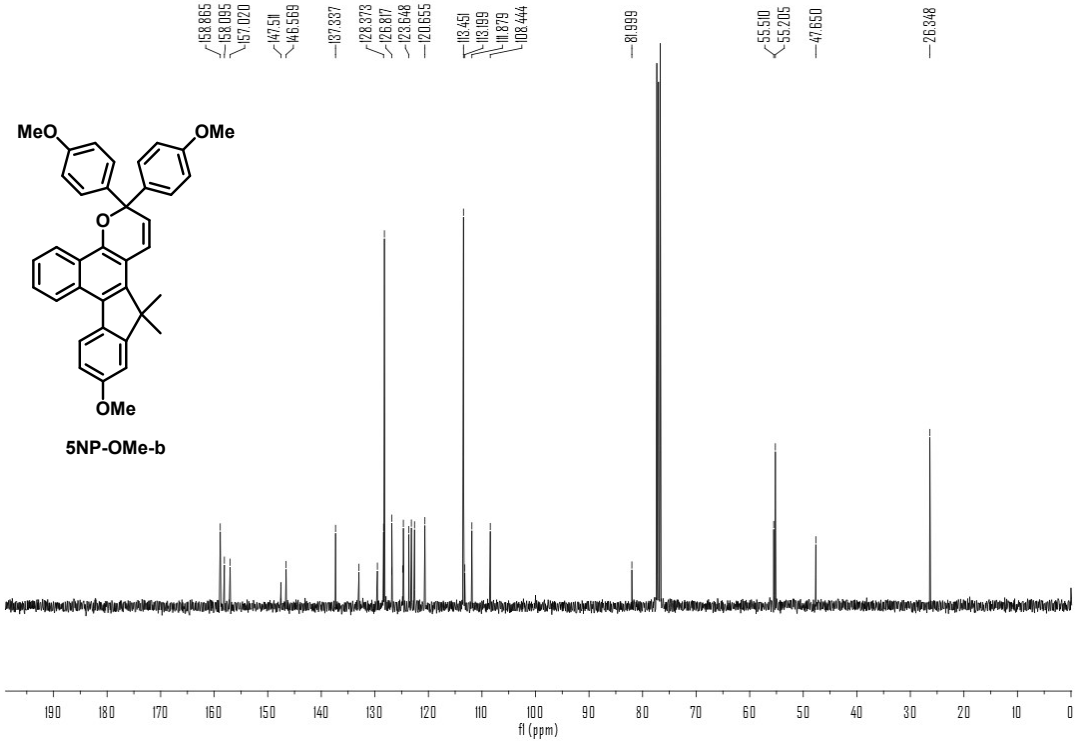

Fig. S52. ^{13}C NMR spectrum of **11-methoxy-3,3-bis(4-methoxyphenyl)-13,13-dimethyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

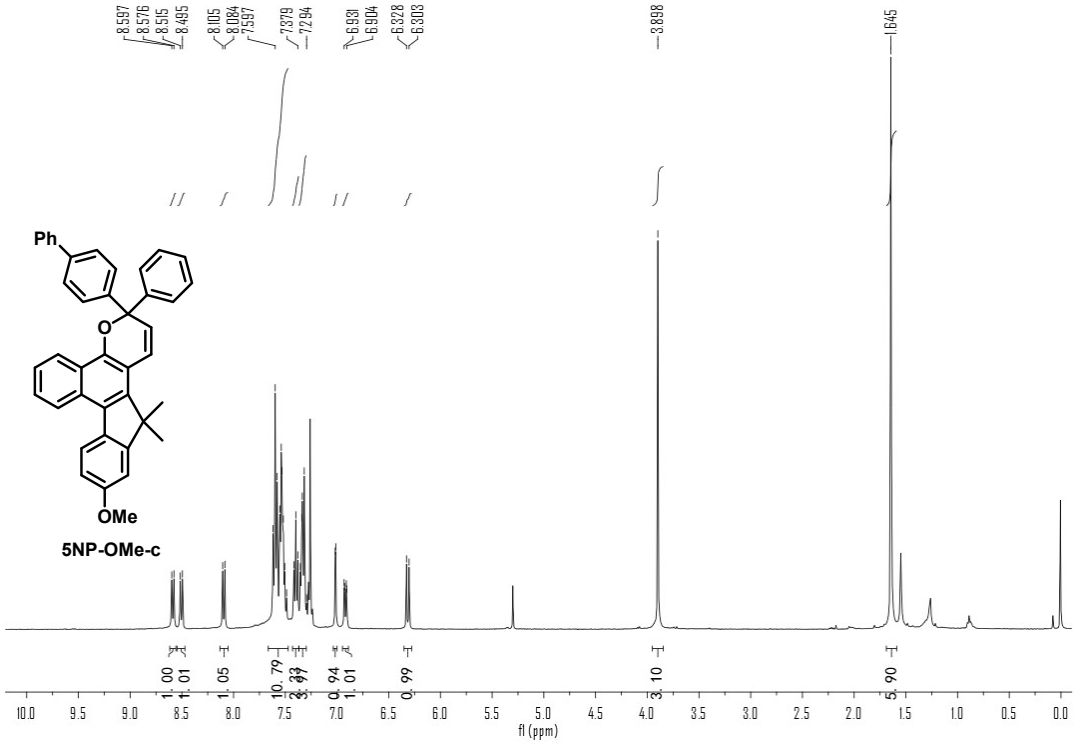

Figure S53. ^{1}H NMR spectrum of **3-([1,1'-biphenyl]-4-yl)-11-methoxy-13,13-dimethyl-3-phenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

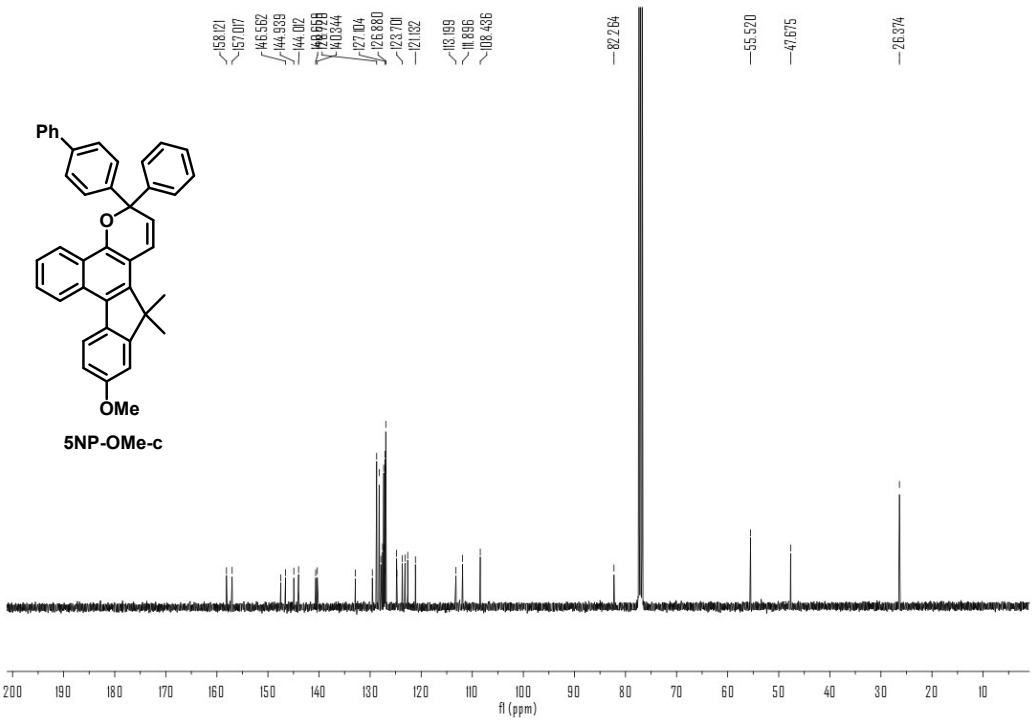

Figure S54. ^{13}C NMR spectrum of **3-([1,1'-biphenyl]-4-yl)-11-methoxy-13,13-dimethyl-3-phenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene** in $CDCl_3$.

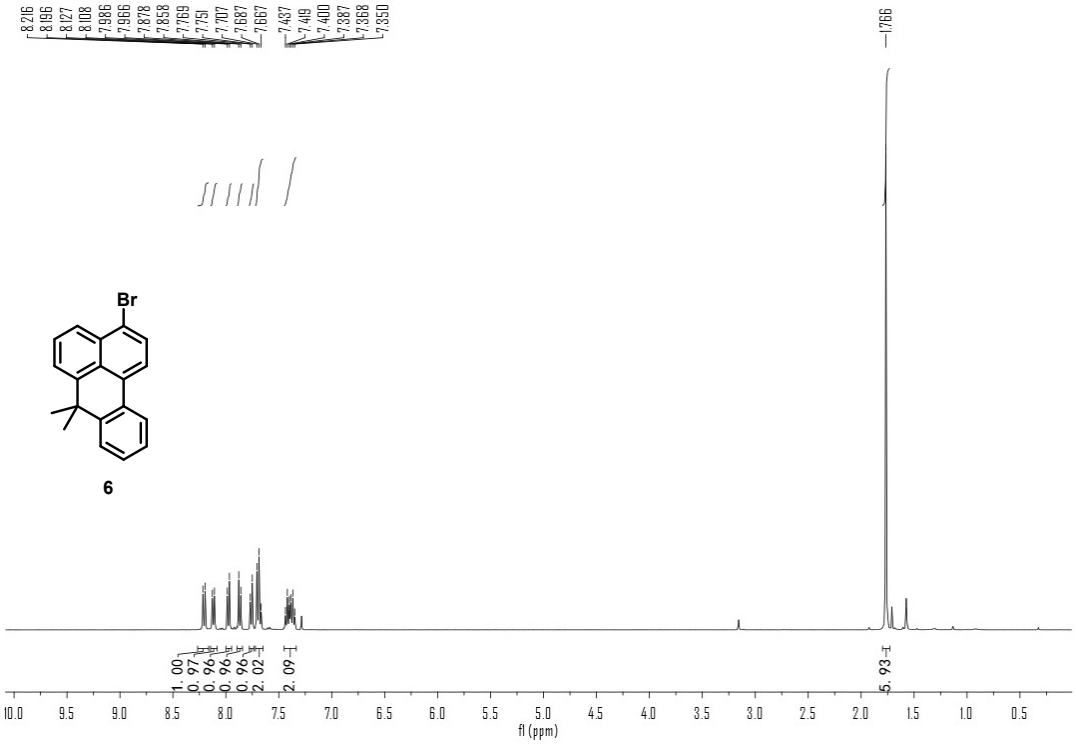

Fig. S55. ^{1}H NMR spectrum of **3-bromo-7,7-dimethyl-*7H*-benzo[*de*]anthracene (6)** in $CDCl_3$.

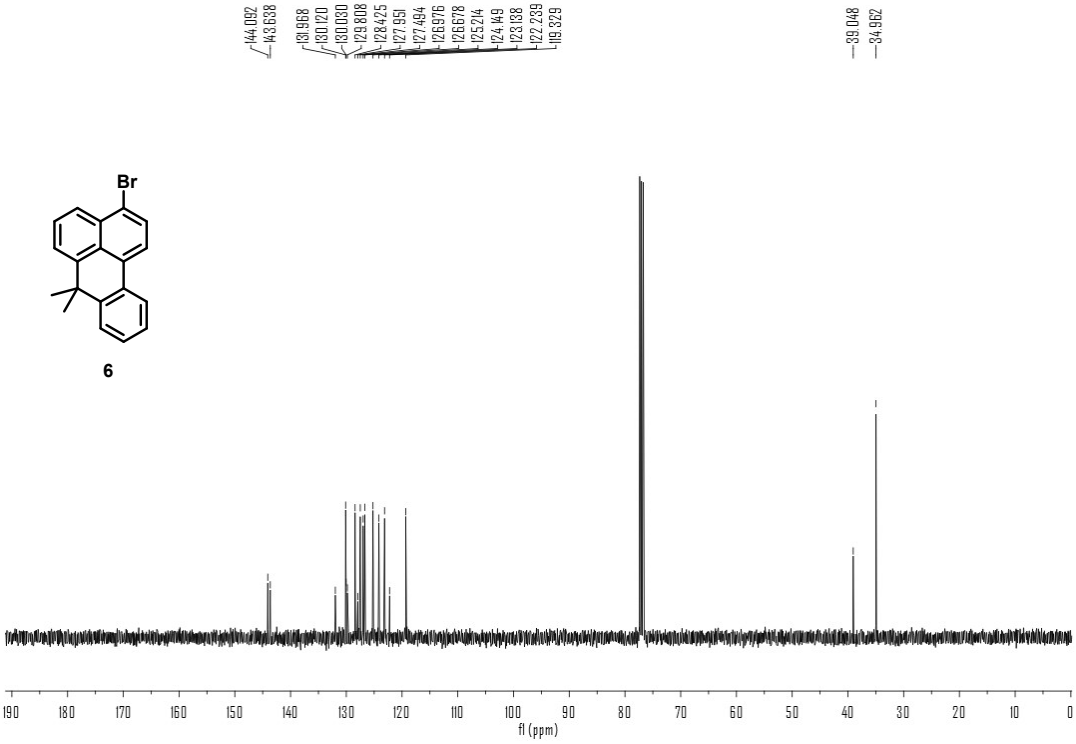

Fig. S56. ^{13}C NMR spectrum of **3-bromo-7,7-dimethyl-*7H*-benzo[*de*]anthracene (6)** in $CDCl_3$.

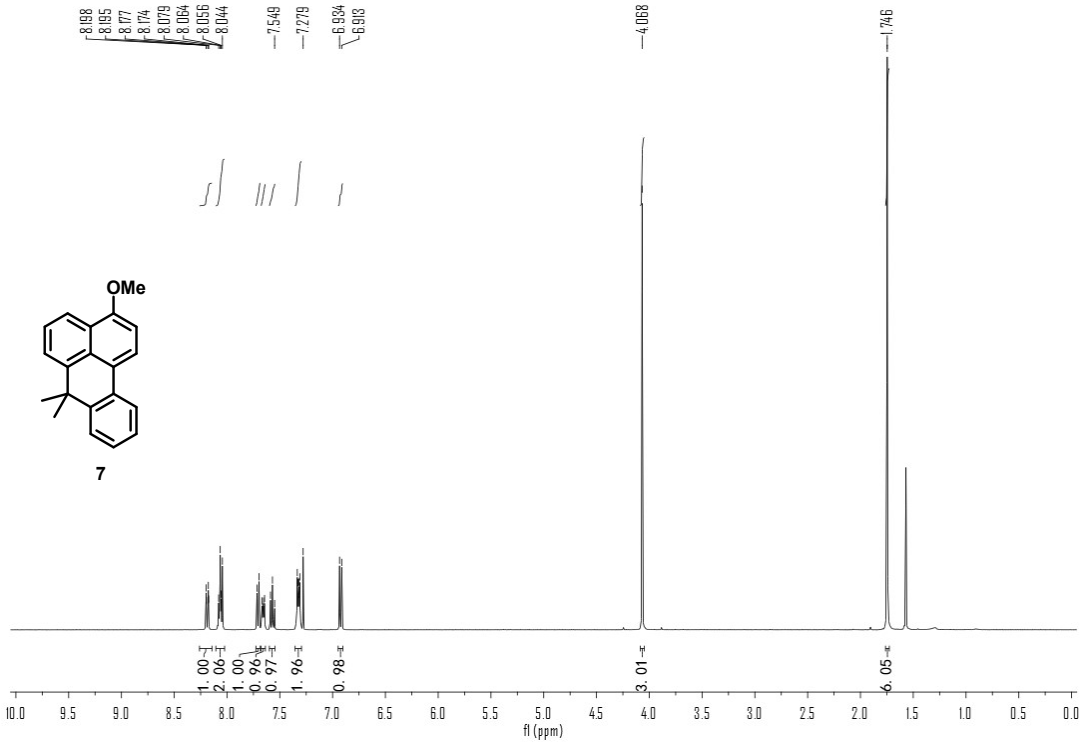

Fig. S57. ^{1}H NMR spectrum of **3-methoxy-7,7-dimethyl-*7H*-benzo[*de*] anthracene (7)** in $CDCl_3$.

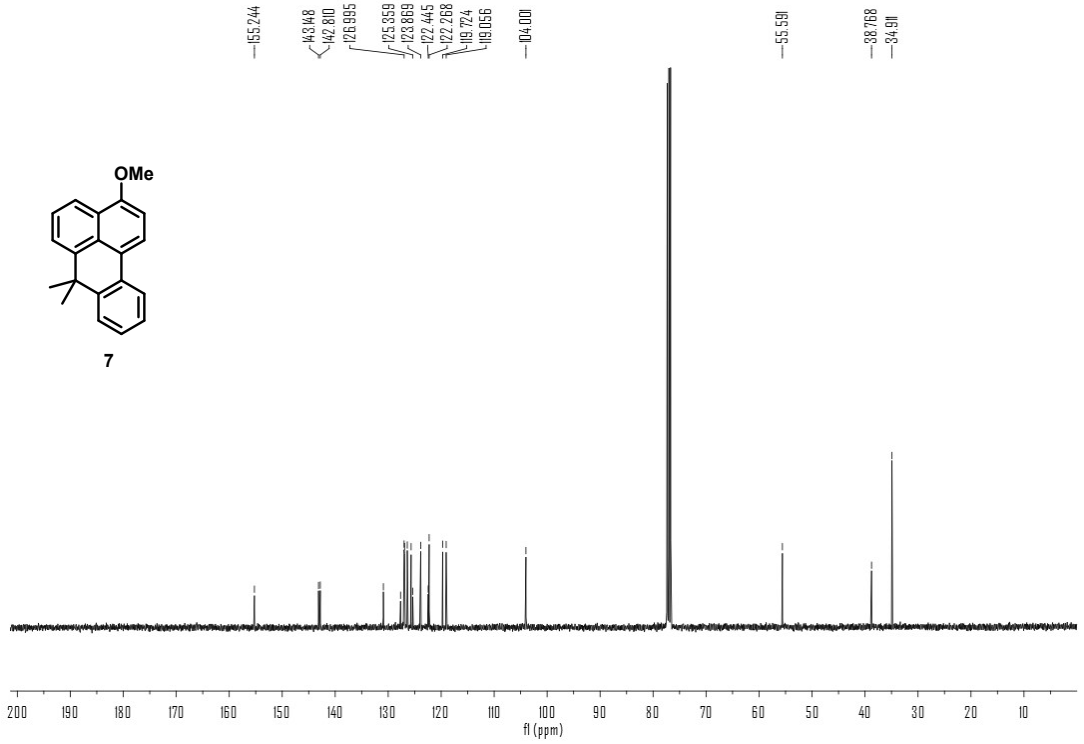

Fig. S58. ^{13}C NMR spectrum of **3-methoxy-7,7-dimethyl-*7H*-benzo[*de*] anthracene (7)** in $CDCl_3$.

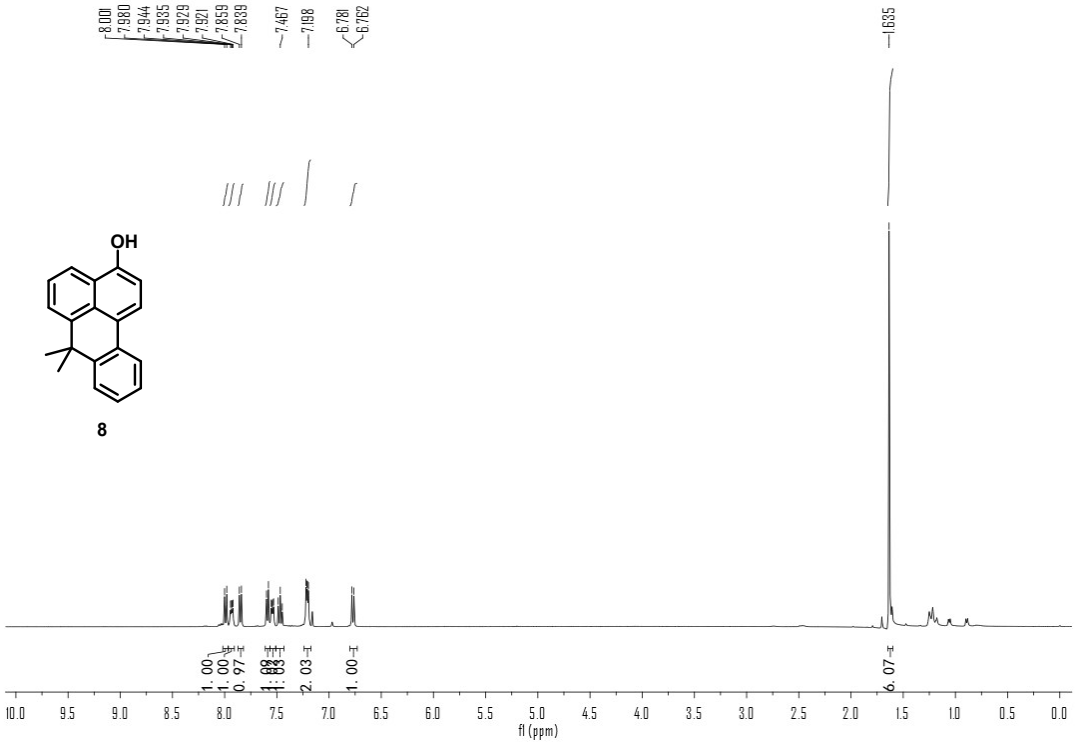

Fig. S59. ^{1}H NMR spectrum of **7,7-dimethyl-*7H*-benzo[*de*]anthracen-3-ol (8)** in $CDCl_3$.

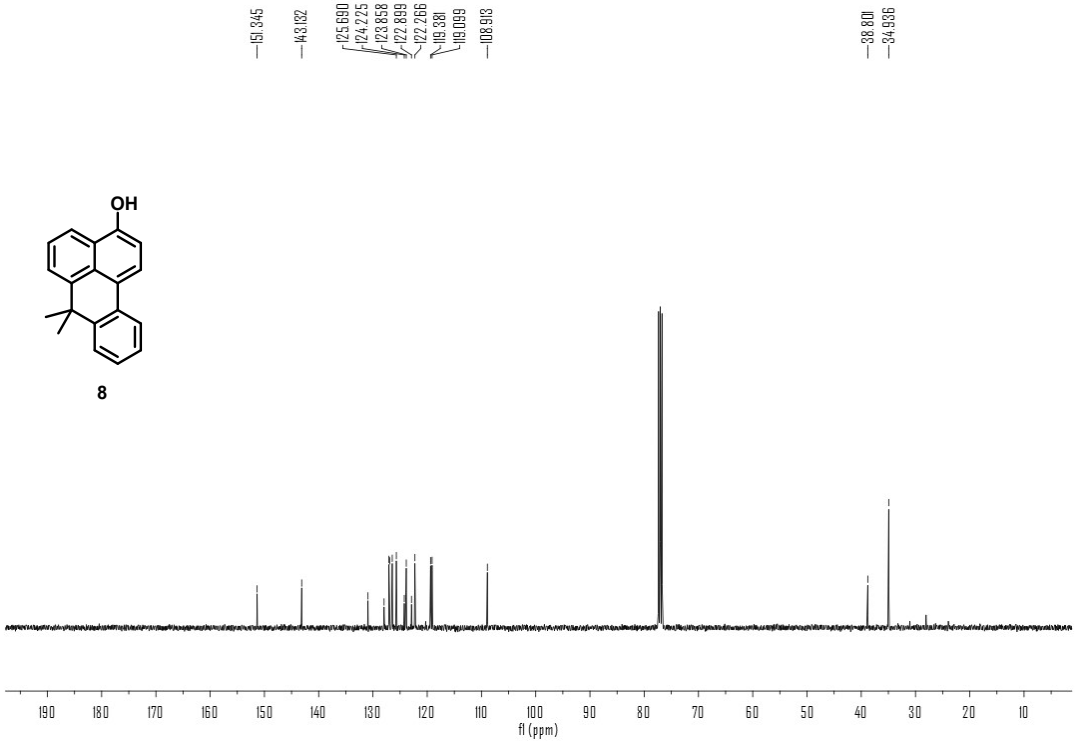

Fig. S60. ^{13}C NMR spectrum of **7,7-dimethyl-*7H*-benzo[*de*]anthracen-3-ol (8)** in $CDCl_3$.

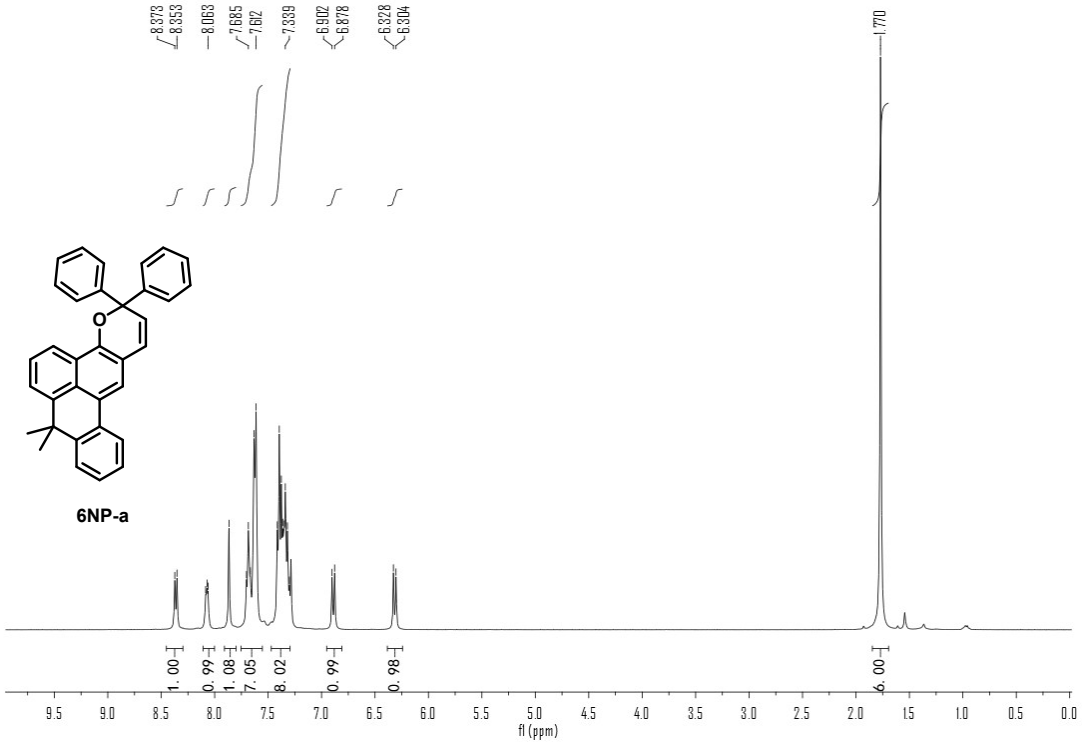

Fig. S61. ^{1}H NMR spectrum of **8,8-dimethyl-3,3-diphenyl-3,8-dihydroanthra [*9,1-gh*]chromene** in $CDCl_3$.

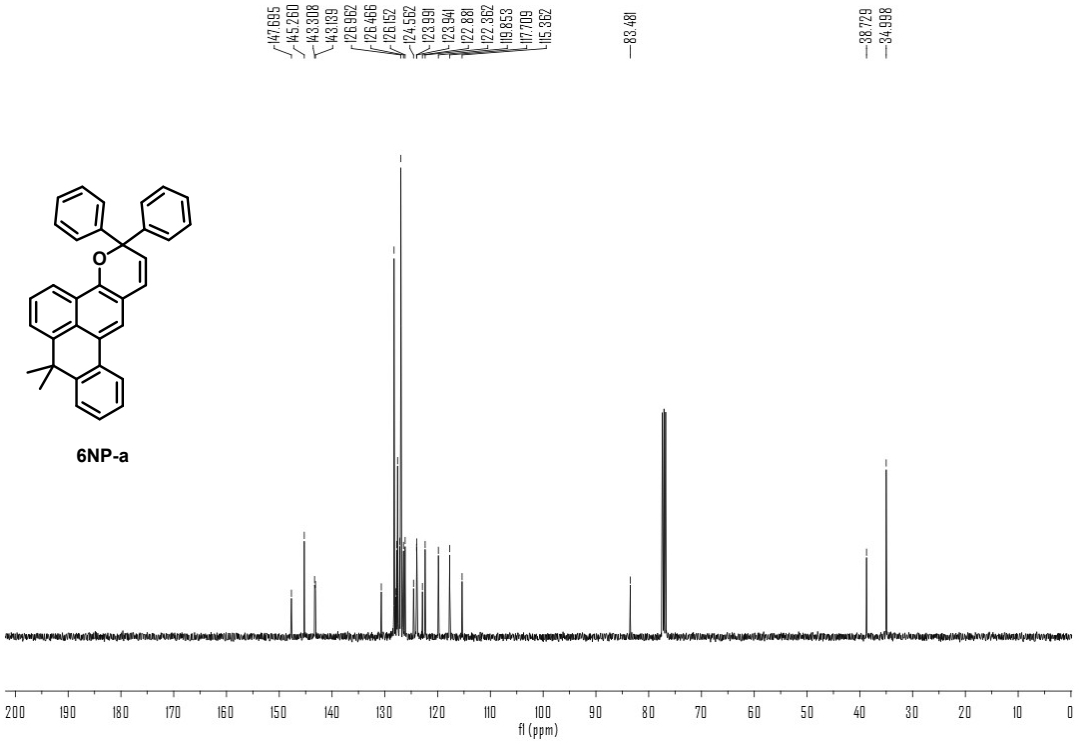

Fig. S62. ^{13}C NMR spectrum of **8,8-dimethyl-3,3-diphenyl-3,8-dihydroanthra [*9,1-gh*] chromene** in $CDCl_3$.

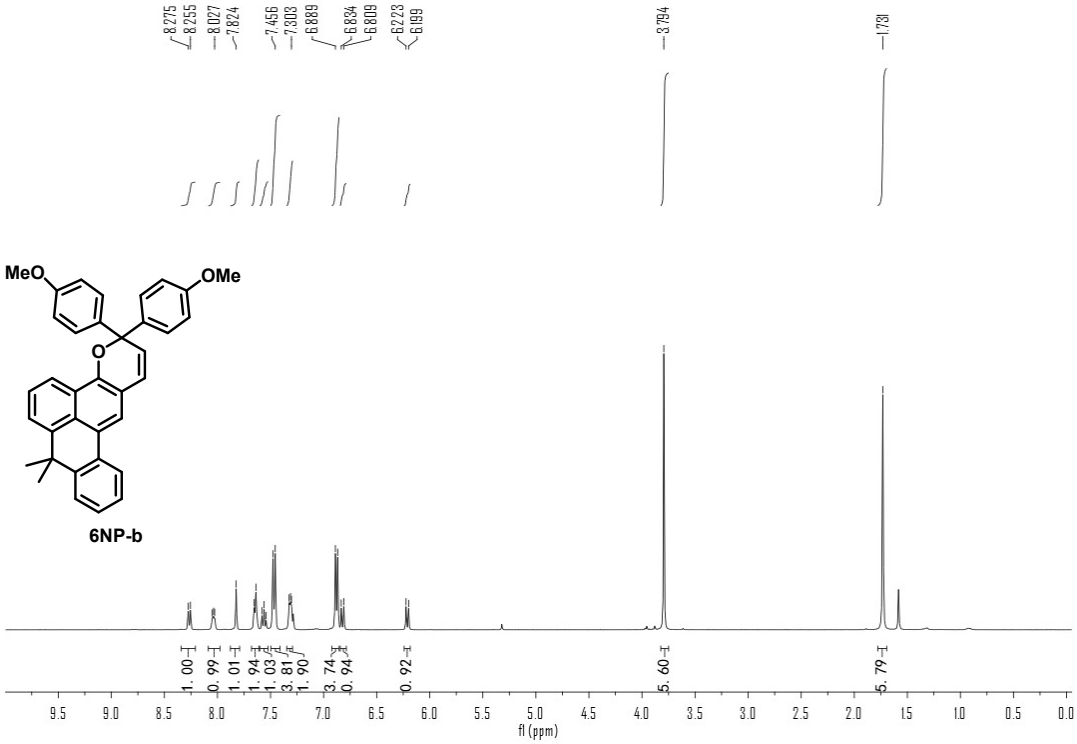

Fig. S63. ^{1}H NMR spectrum of **3,3-bis(4-methoxyphenyl)-8,8-dimethyl-3,8-dihydroanthra[*9,1-gh*]chromene** in $CDCl_3$

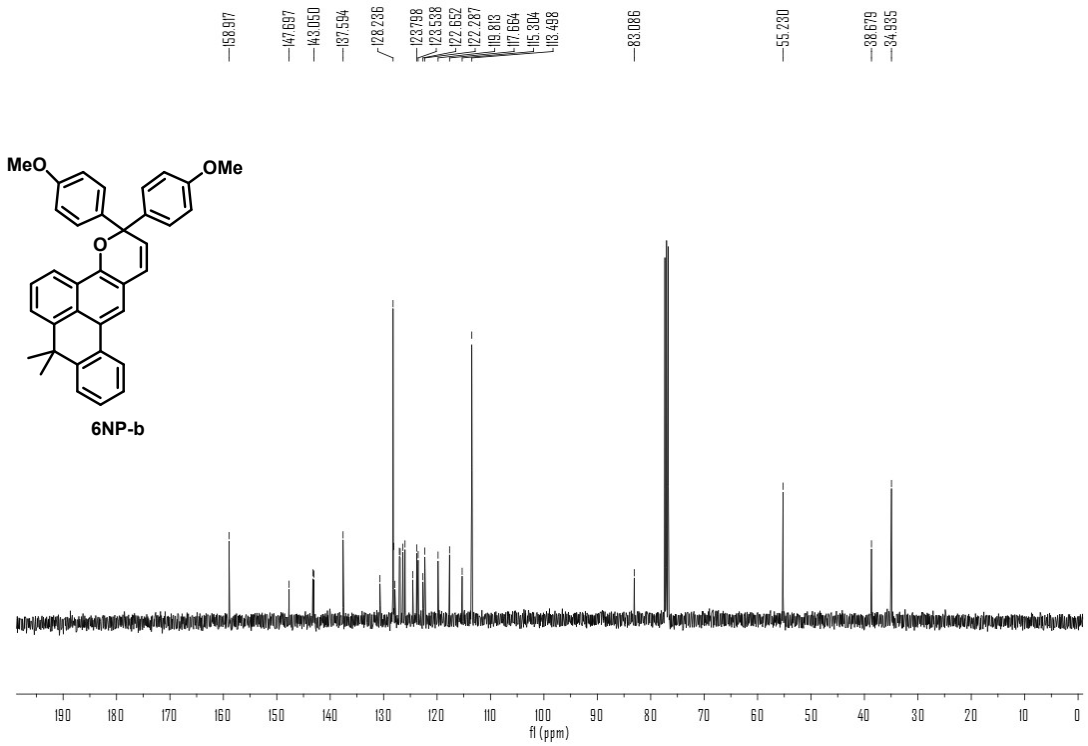

Fig. S64. ^{13}C NMR spectrum of **3,3-bis(4-methoxyphenyl)-8,8-dimethyl-3,8-dih ydroa-nthra[*9,1-gh*]chromene** in $CDCl_3$.

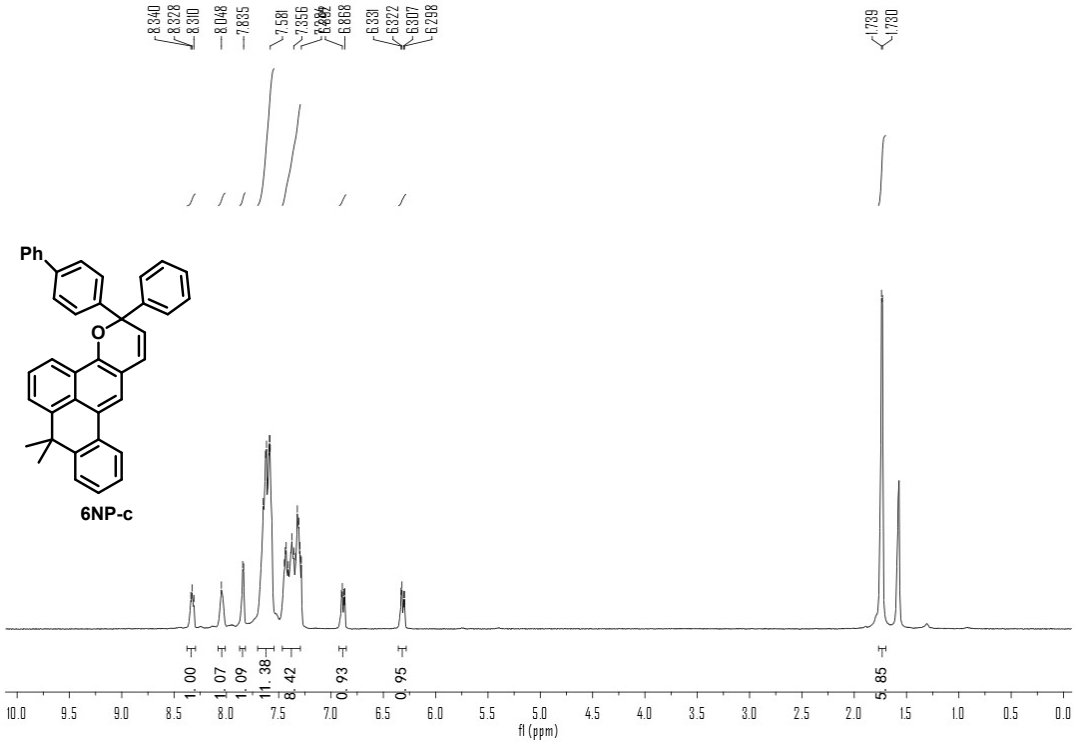

Fig. S65. ^{1}H NMR spectrum of **3-([1,1'-biphenyl]-4-yl)-8,8-dimethyl-3-phenyl- 3,8-dihydroanthra[*9,1-gh*]chromene** in $CDCl_3$.

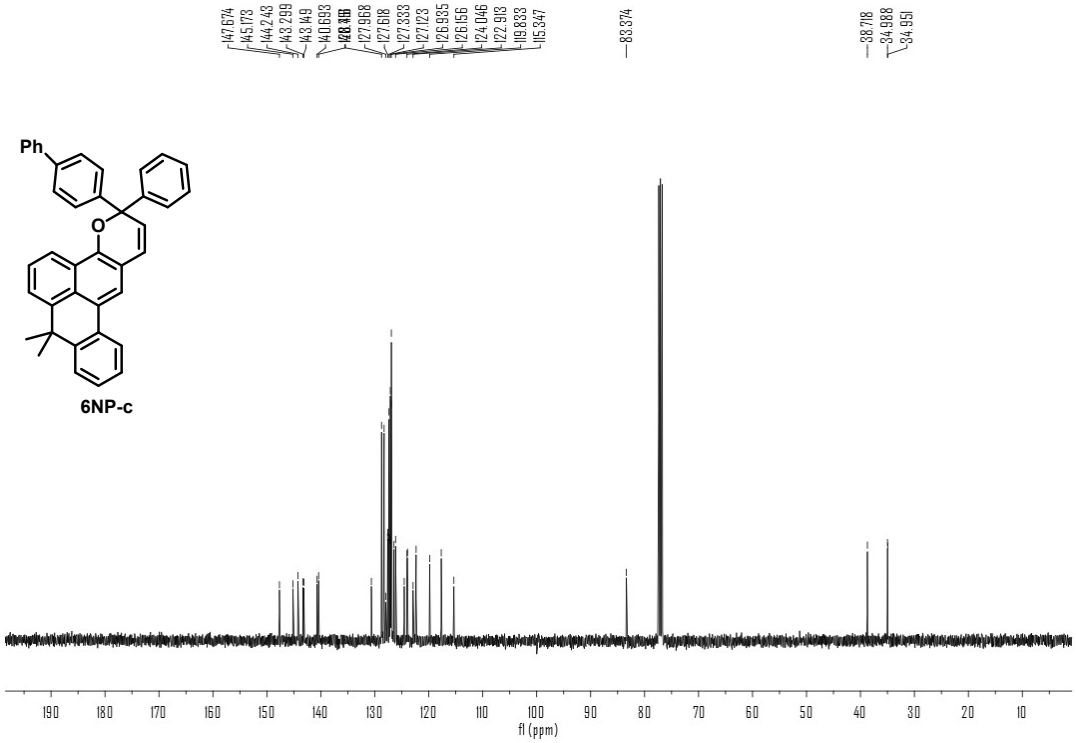

Fig. S66. ^{13}C NMR spectrum of **3-([1,1'-biphenyl]-4-yl)-8,8-dimethyl-3-phenyl- 3,8-dihydroanthra[*9,1-gh*]chromene** in $CDCl_3$.

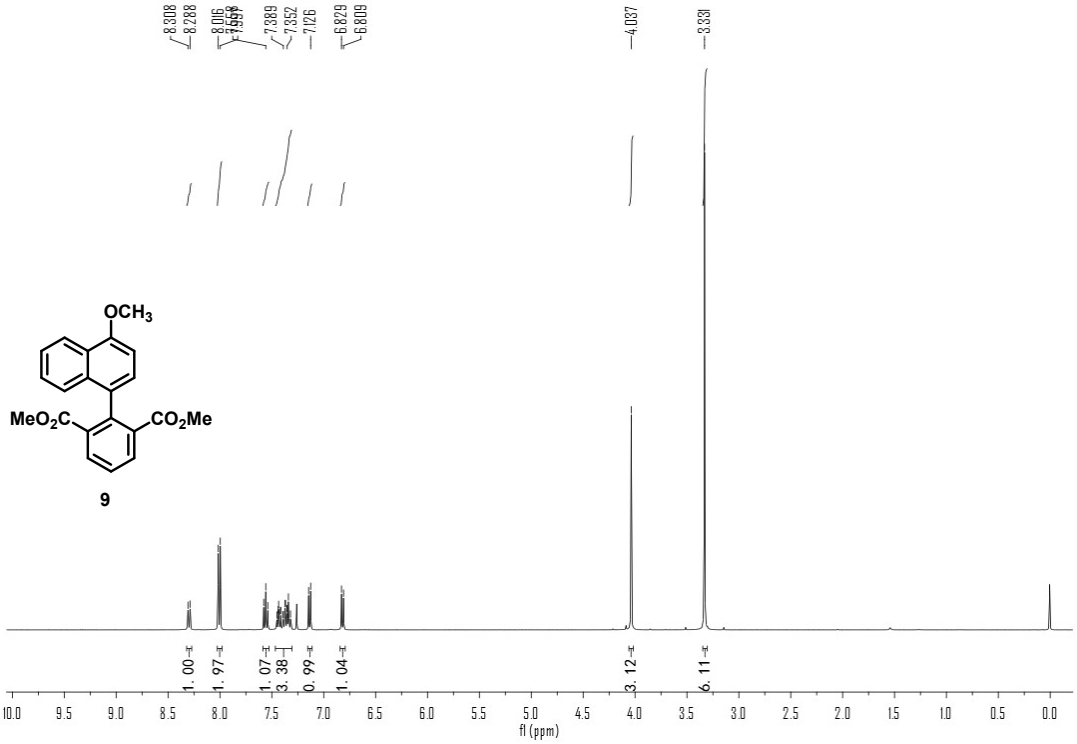

Fig. S67. ^{1}H NMR spectrum of **dimethyl 2-(4-methoxynaphthalen-1-yl) (9) isophthalate** in $CDCl_3$.

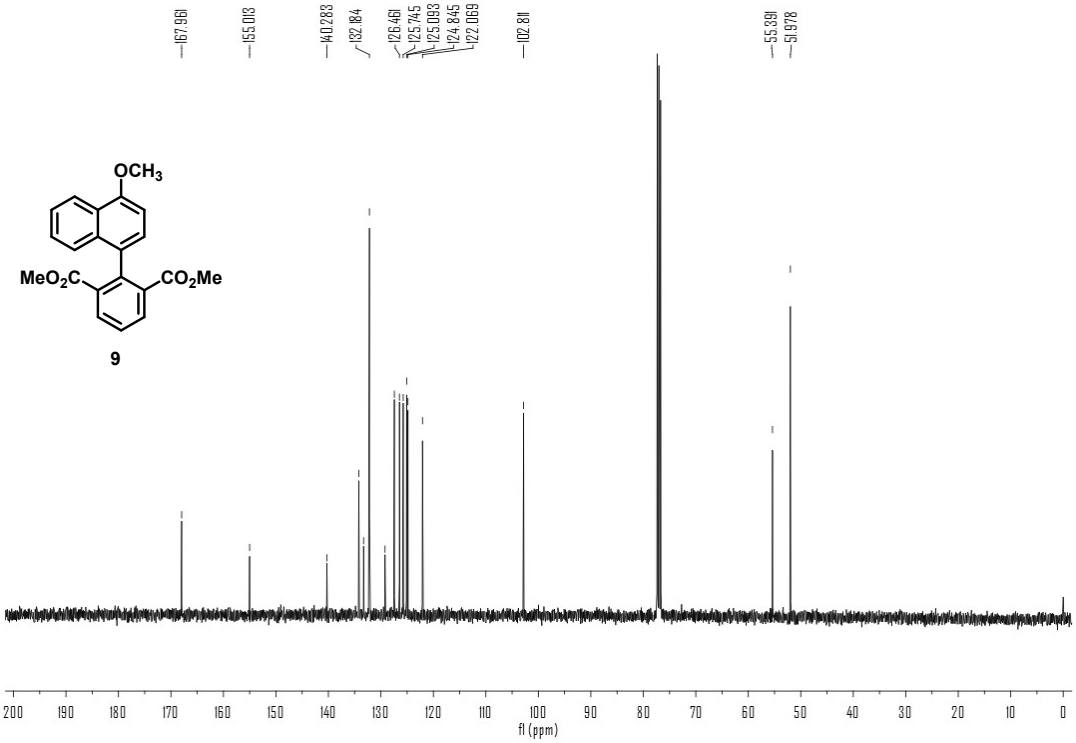

Fig. S68. ^{13}C NMR spectrum of **dimethyl 2-(4-methoxynaphthalen-1-yl) isophthalate (9)** in $CDCl_3$.

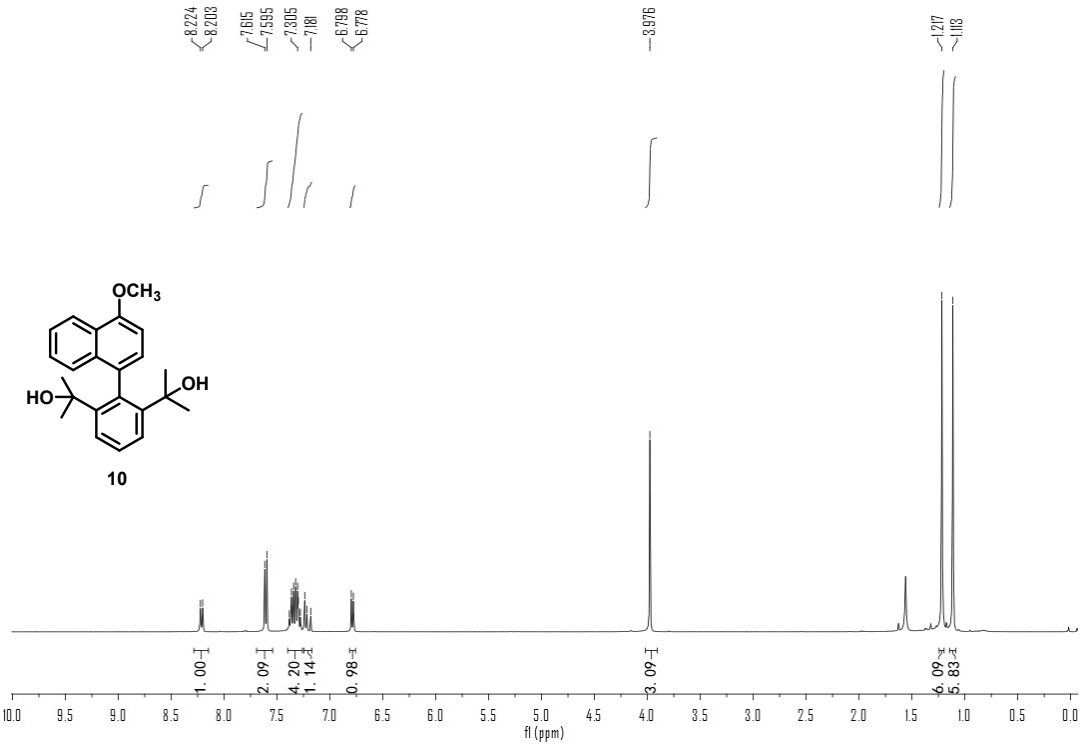

Fig. S69. ^{1}H NMR spectrum of **dimethyl 2-(4-methoxynaphthalen-1-yl) isophthalate (10)** in $CDCl_3$.

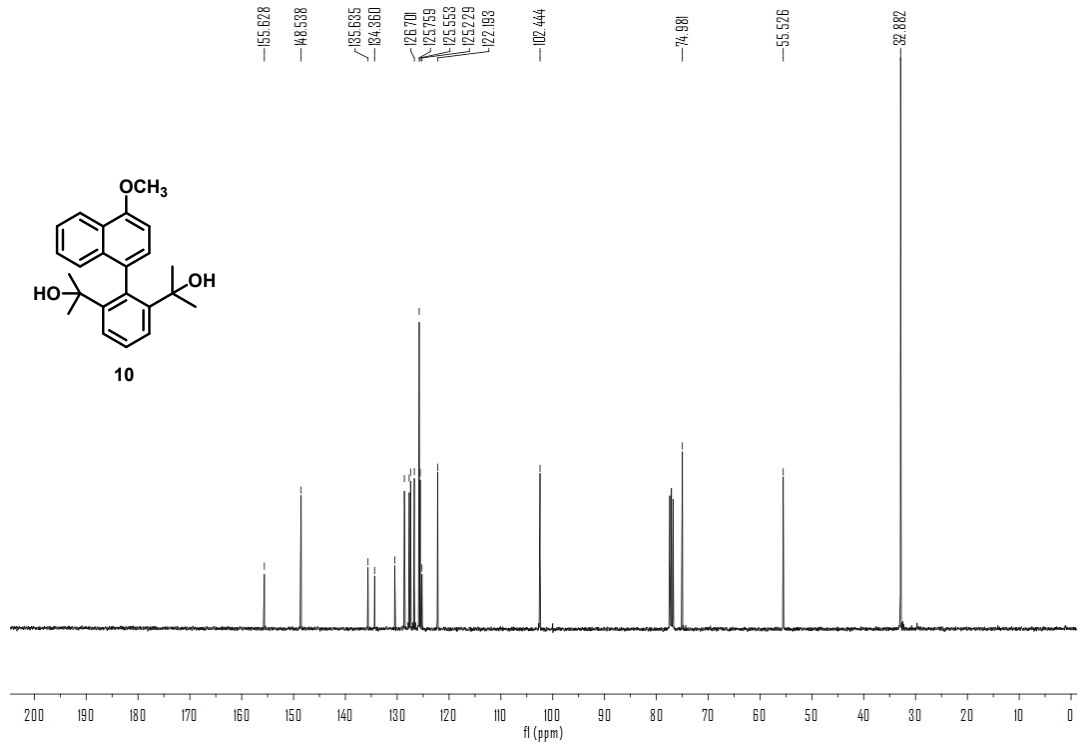

Fig. S70. ^{13}C NMR spectrum of **dimethyl 2-(4-methoxynaphthalen-1-yl) isophthalate (10)** in $CDCl_3$.

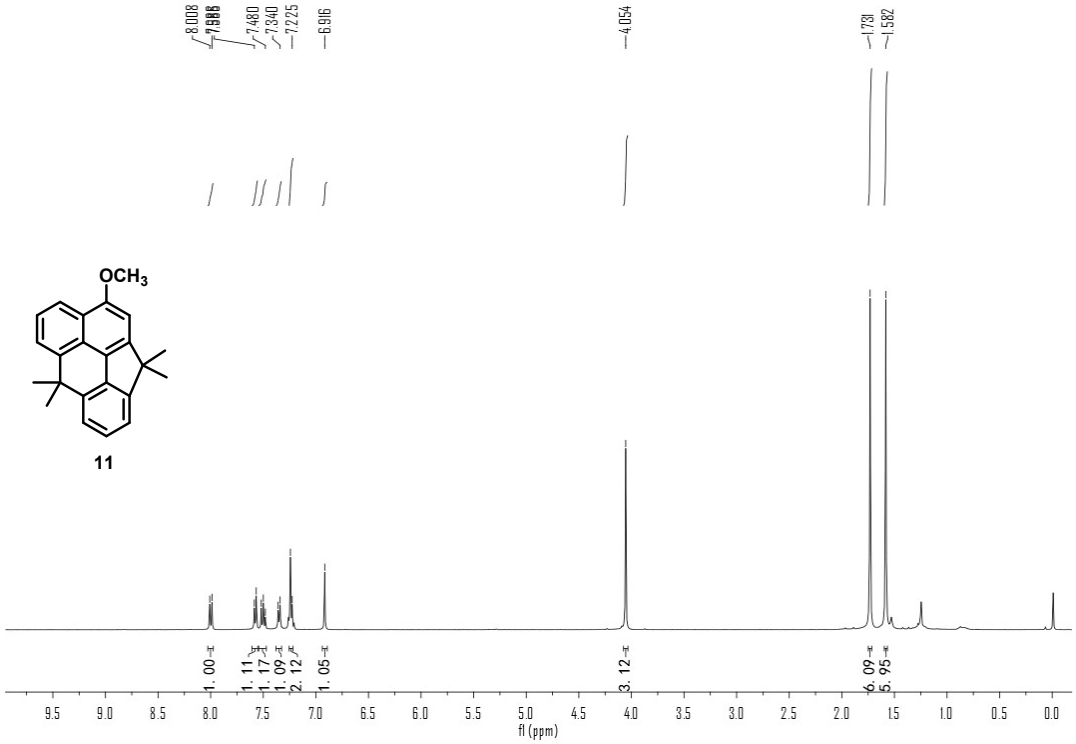

Fig. S71. ^{1}H NMR spectrum of **9-methoxy-1,1,5,5-tetramethyl-1,5-dihydro benzo[*mno*]aceanthrylene (11)** in $CDCl_3$.

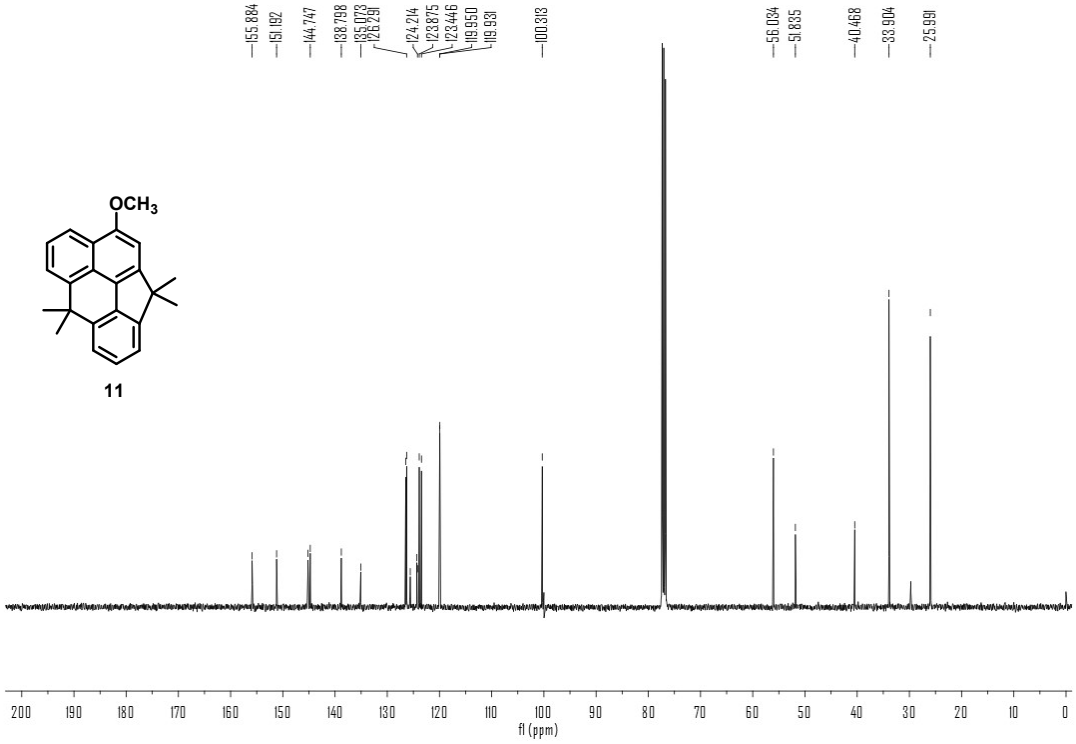

Fig. S72. ^{13}C NMR spectrum of **9-methoxy-1,1,5,5-tetramethyl-1,5-dihydro benzo[*mno*]aceanthrylene (11)** in $CDCl_3$.

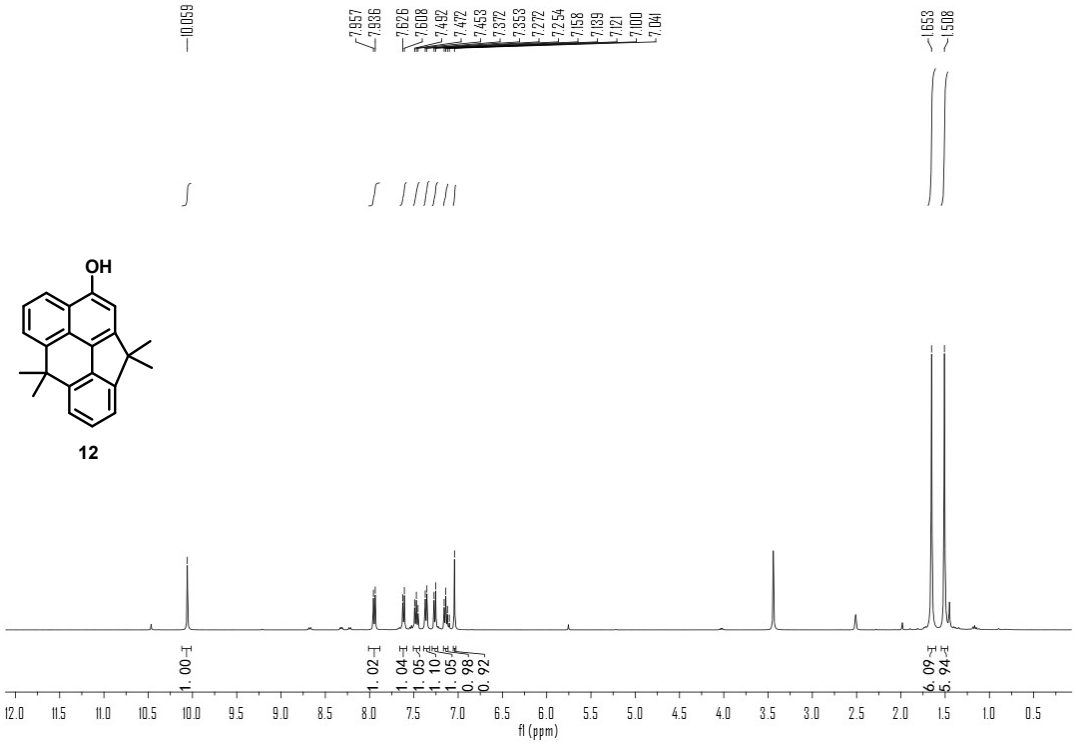

Fig. S73. ^{1}H NMR spectrum of **9-methoxy-1,1,5,5-tetramethyl-1,5-dihydro benzo[*mno*]aceanthrylene (12)** in $CDCl_3$.

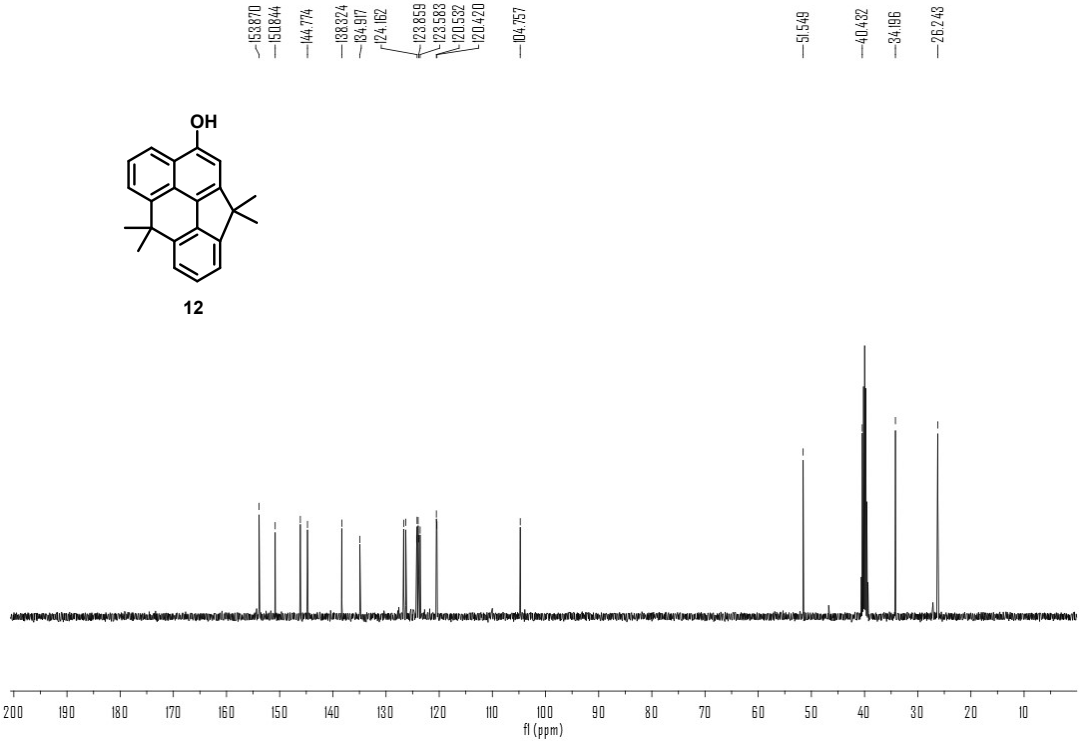

Fig. S74. ^{13}C NMR spectrum of **9-methoxy-1,1,5,5-tetramethyl-1,5-dihydro benzo[*mno*]aceanthrylene (12)** in $CDCl_3$.

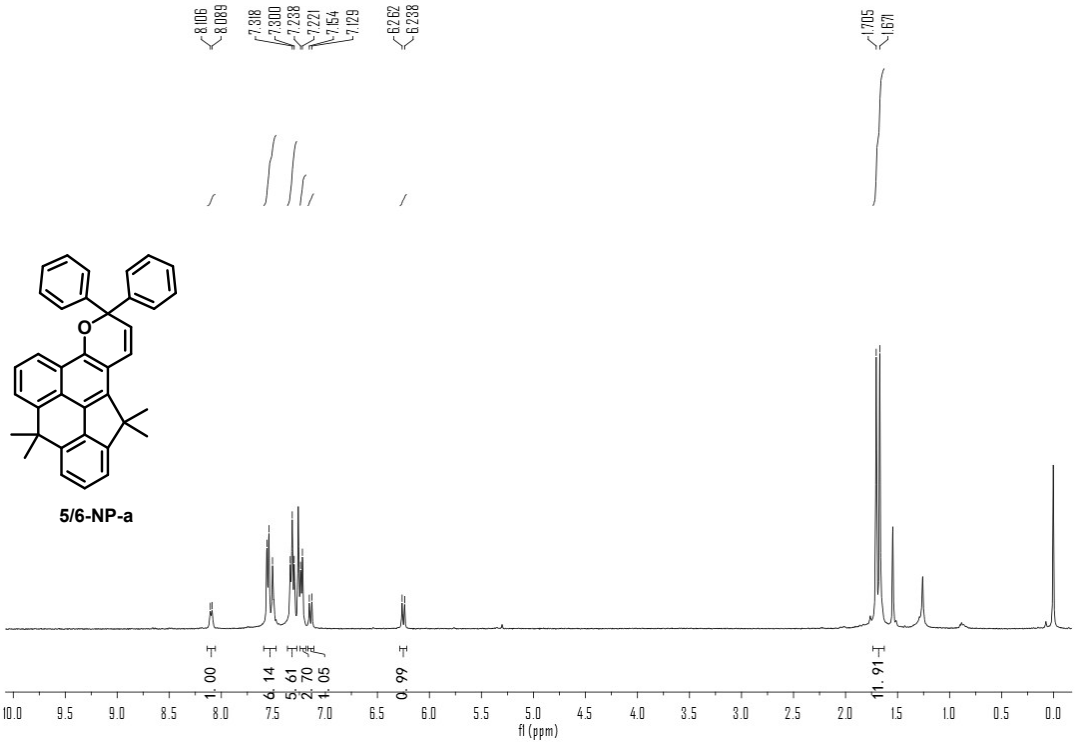

Fig. S75. ^{1}H NMR spectrum of **8,8,12,12-tetramethyl-3,3-diphen-yl- 8,12-dihydro-*3H*-aceanthryleno[*1,10-fgh*]chromene** in $CDCl_3$.

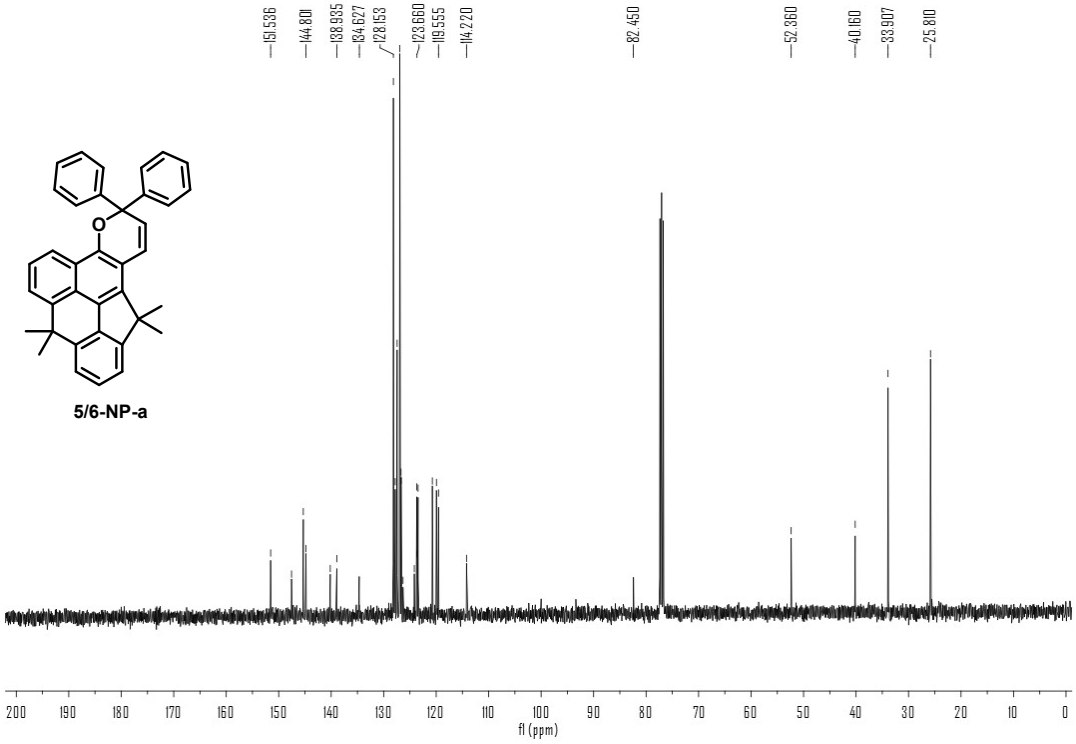

Fig. S76. ^{13}C NMR spectrum of **8,8,12,12-tetramethyl-3,3-diphen-yl- 8,12-dihydro-*3H*-aceanthryleno[*1,10-fgh*]chromene** in $CDCl_3$.

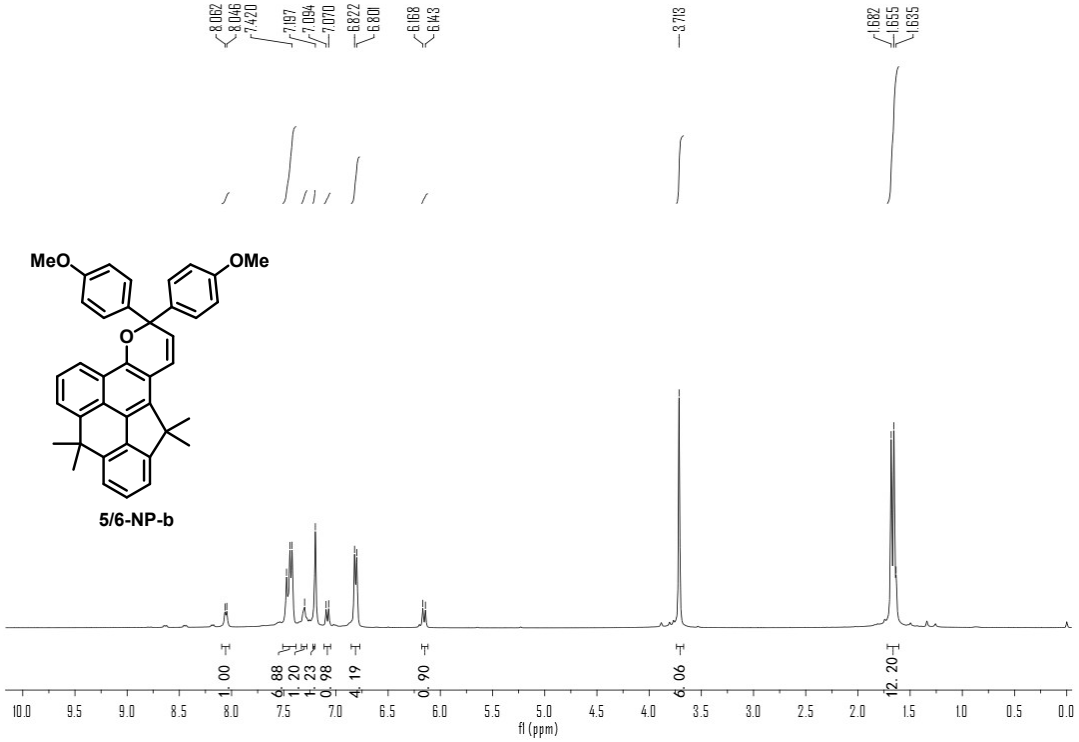

Fig. S77. ^{1}H NMR spectrum of **3,3-bis(4-methoxyphenyl)-8,8,12,12-tetramethyl-8,12-dihydro-*3H*-aceanthryleno[*1,10-fgh*]chromene** in $CDCl_3$.

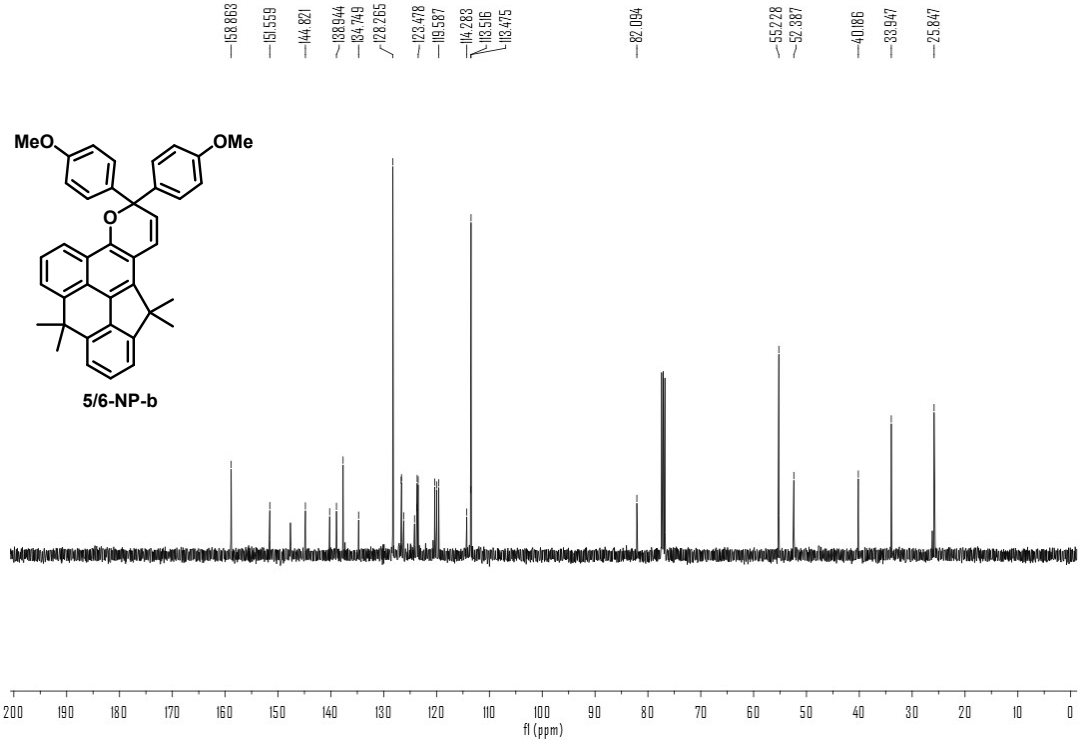

Fig. S78. ^{13}C NMR spectrum of **3,3-bis(4-methoxyphenyl)-8,8,12,12-tetramethyl -8,12-dihydro-*3H*-aceanthryleno[*1,10-fgh*]chromene** in $CDCl_3$.

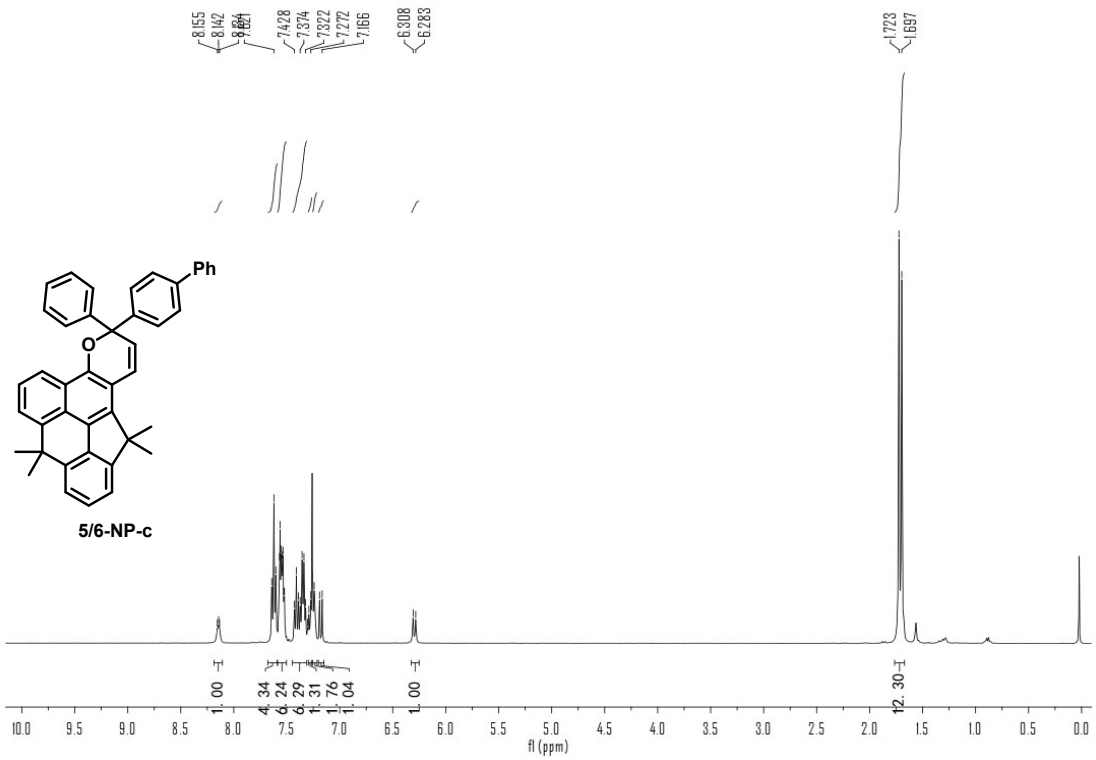

Fig. S79. ^{1}H NMR spectrum of **3-([1,1'-biphenyl]-4-yl)-8,8,12,12-tetramethyl -3-phenyl-8,12-dihydro-*3H*-aceanthryleno[*1,10-fgh*]chromene** in $CDCl_3$.

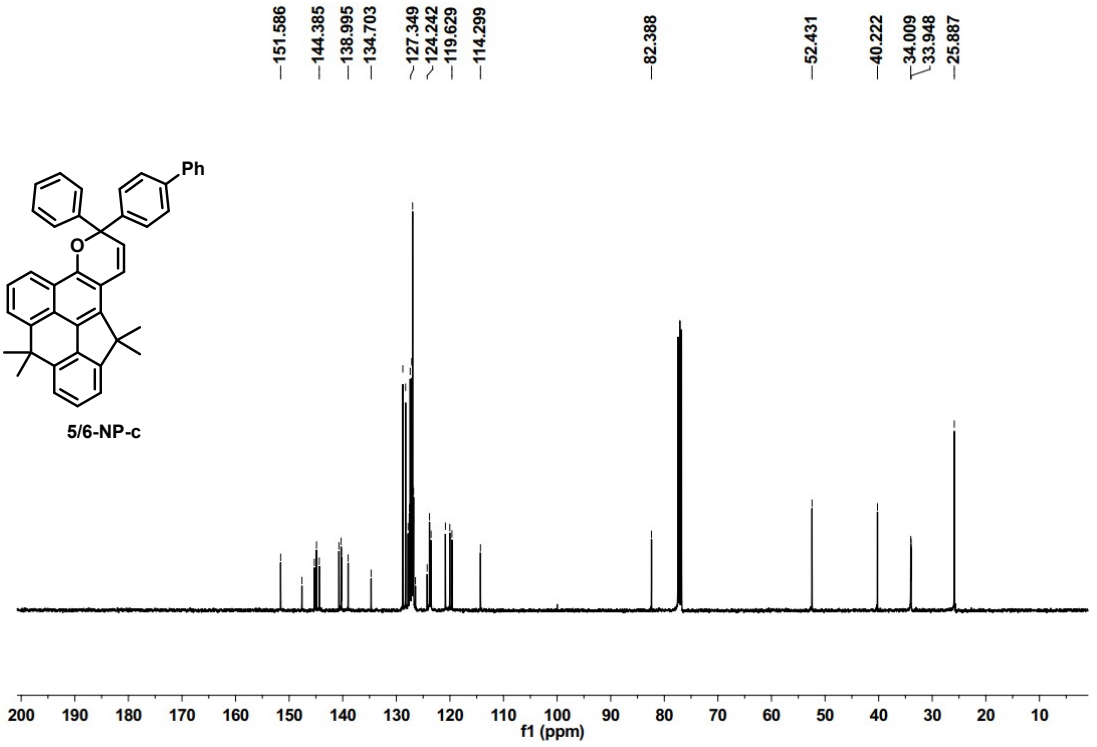

Fig. S80. ^{13}C NMR spectrum of **3-([1,1'-biphenyl]-4-yl)-8,8,12,12-tetramethyl -3-phenyl-8,12-dihydro-*3H*-aceanthryleno[*1,10-fgh*]chromene** in $CDCl_3$.

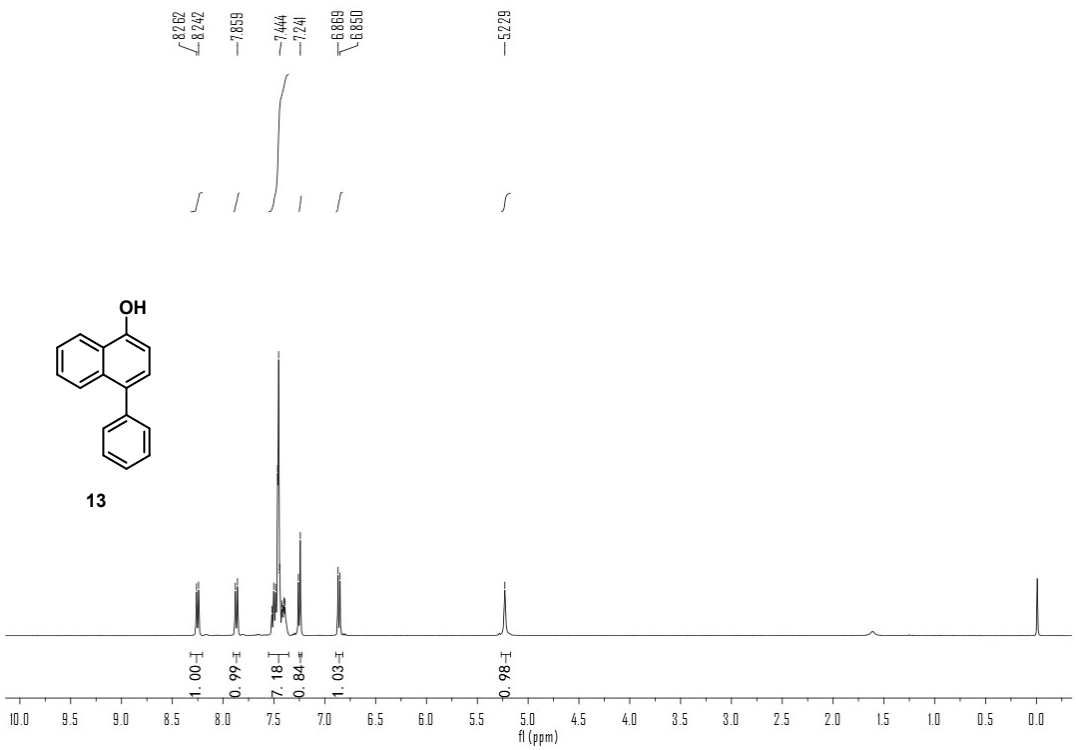

Fig. S81. ^{1}H NMR spectrum of **4-phenylnaphthalen-1-ol (13)** in $CDCl_3$.

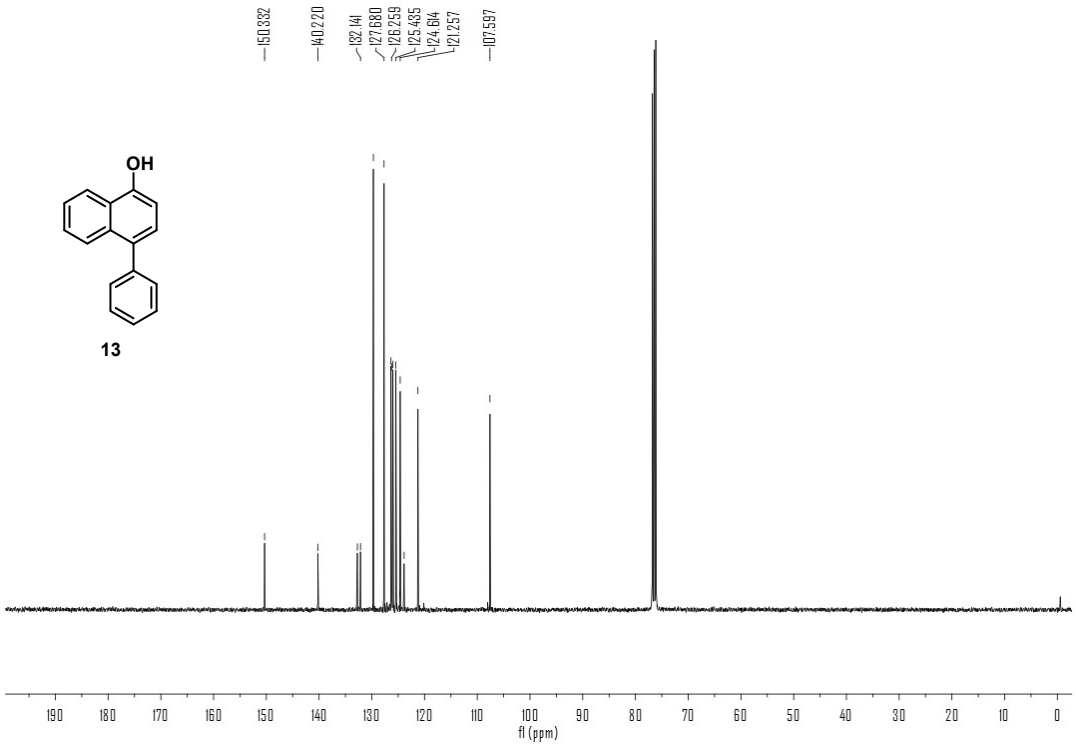

Fig. S82. ^{13}C NMR spectrum of **4-phenylnaphthalen-1-ol (13)** in $CDCl_3$.

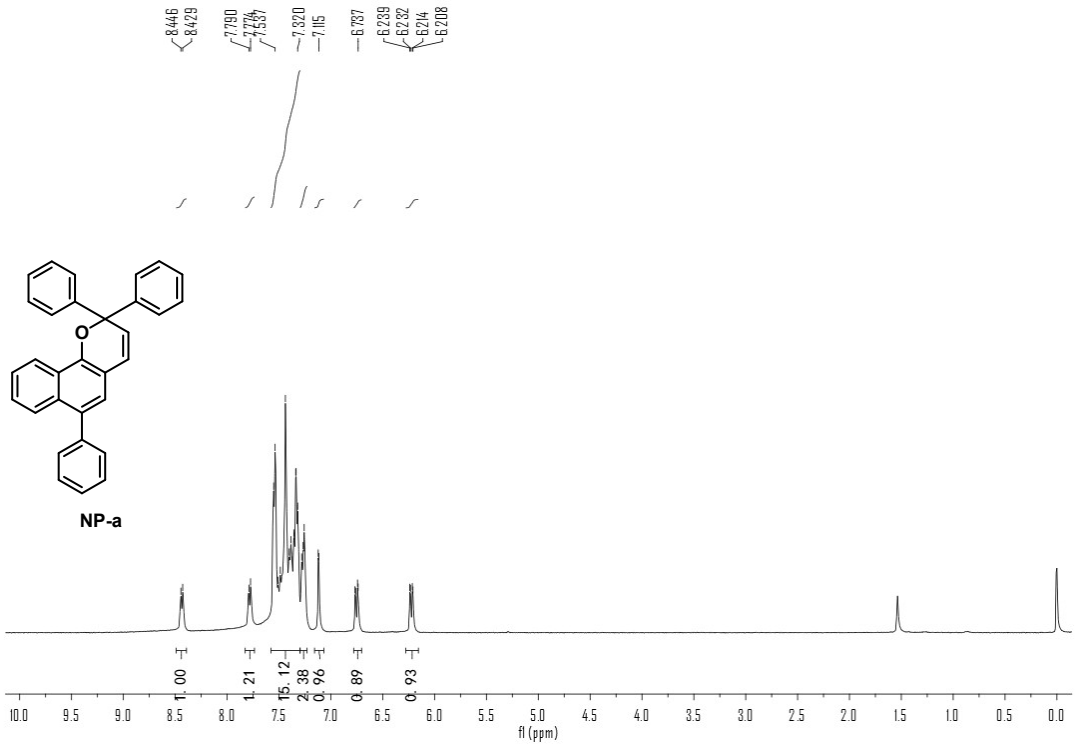

Fig. S83. ^{1}H NMR spectrum of **2,2,6-triphenyl-*2H*-benzo[*h*]chromene** in $CDCl_3$.

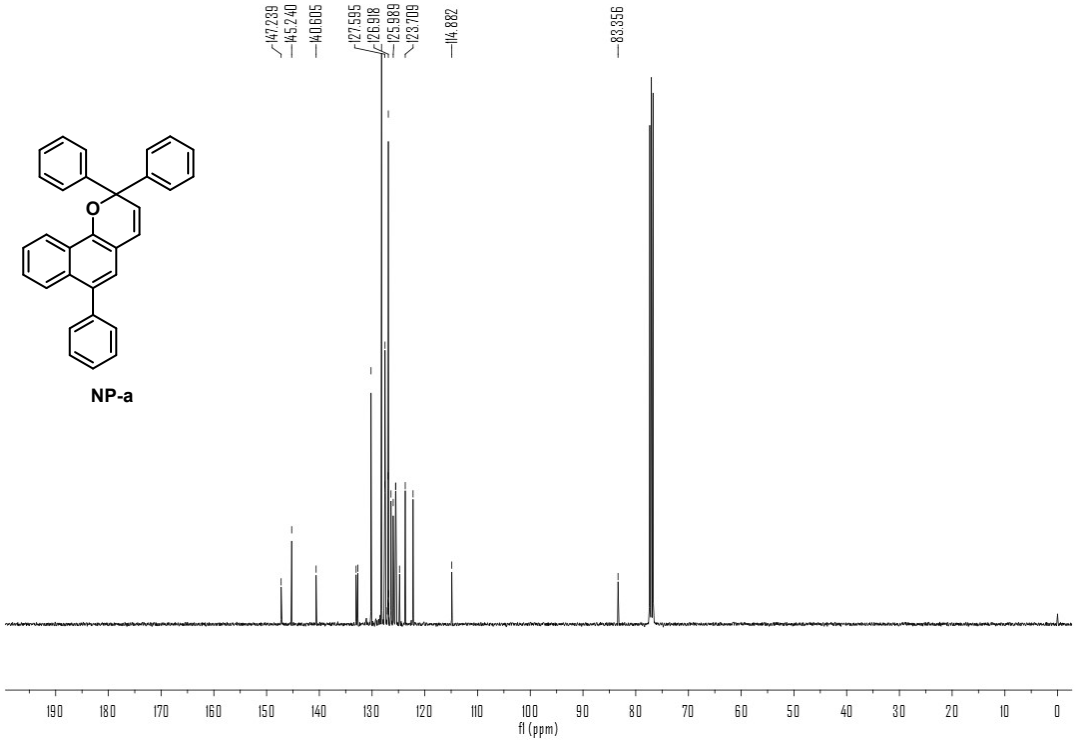

Fig. S84. ^{13}C NMR spectrum of **2,2,6-triphenyl-*2H*-benzo[*h*]chromene** in $CDCl_3$.

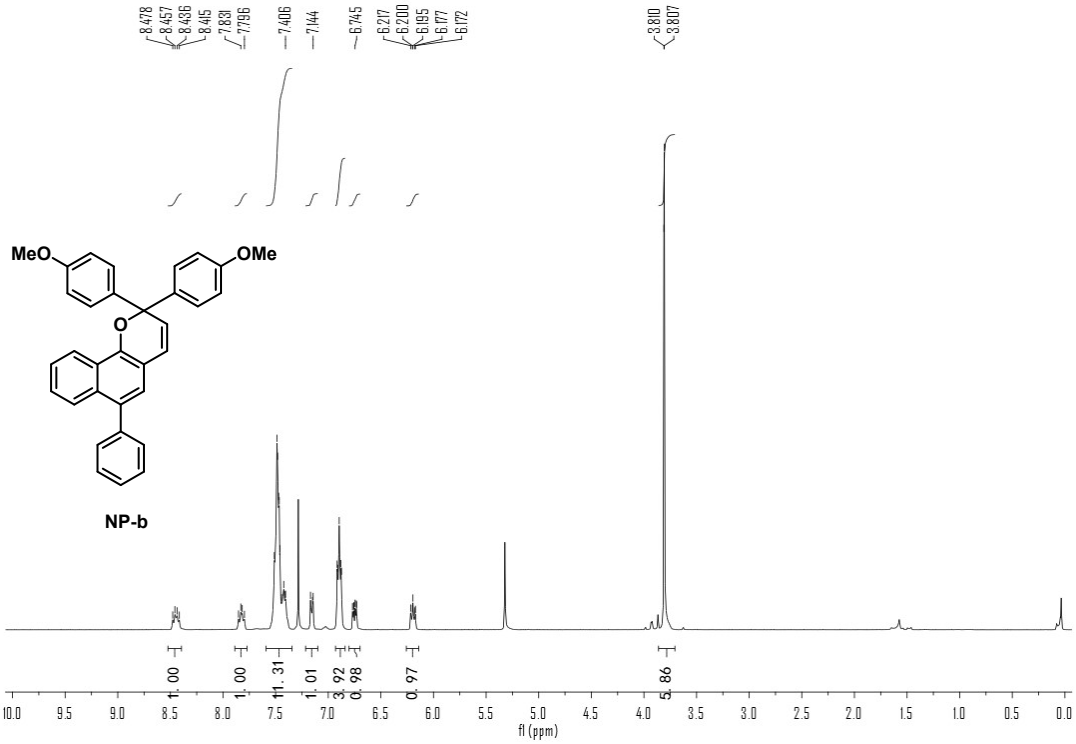

Fig. S85. ^{1}H NMR spectrum of **2,2-bis(4-methoxyphenyl)-6-phenyl-*2H*-benzo[*h*]chromene** in $CDCl_3$.

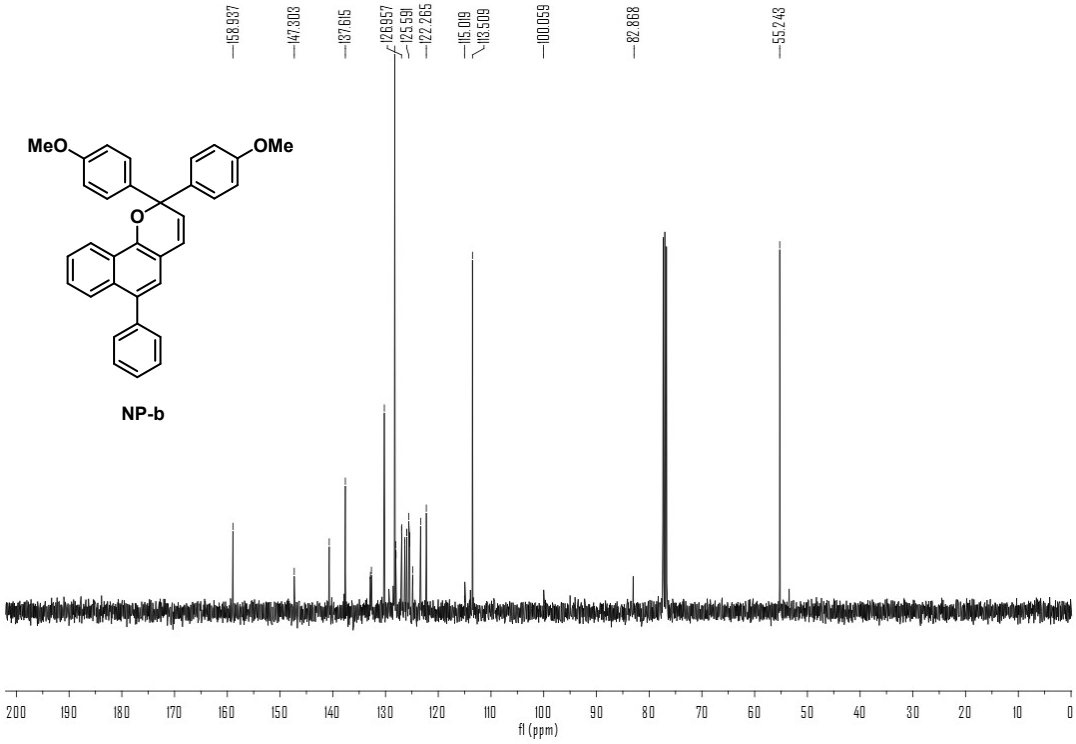

Fig. S86. ^{13}C NMR spectrum of **2,2-bis(4-methoxyphenyl)-6-phenyl-*2H*-benzo[*h*]chromene** in $CDCl_3$.

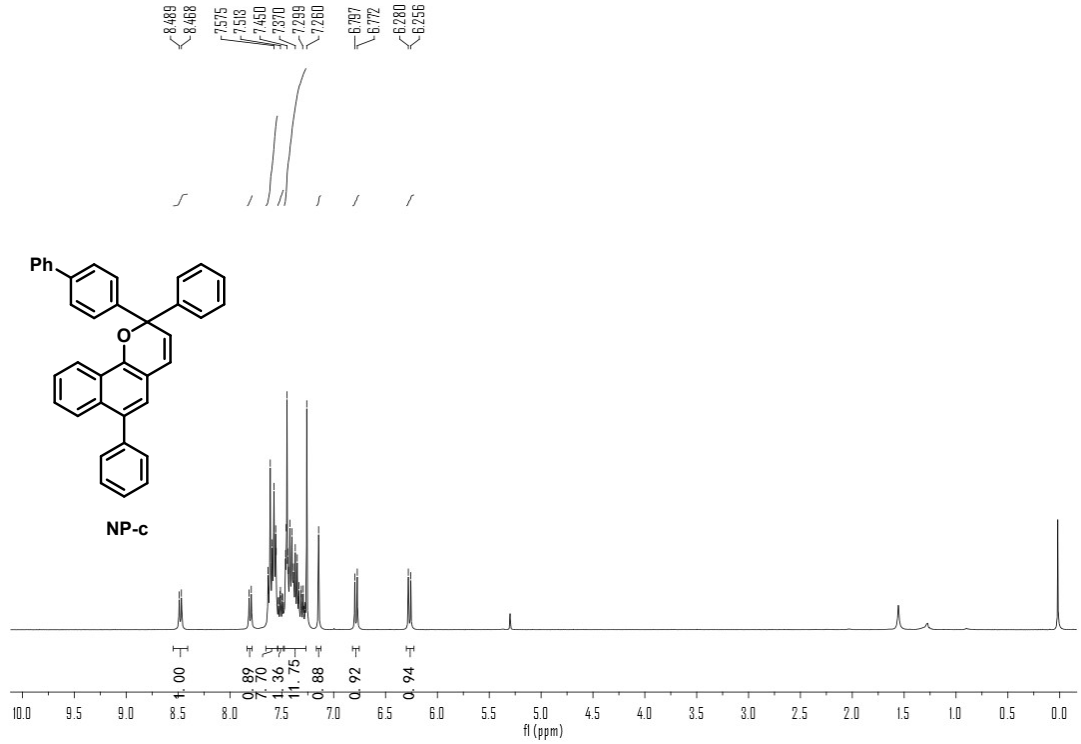

Fig. S87. ^{1}H NMR spectrum of **2-([1,1'-biphenyl]-4-yl)-2,6-diphenyl-*2H*-benzo [*h*]chromene** in $CDCl_3$.

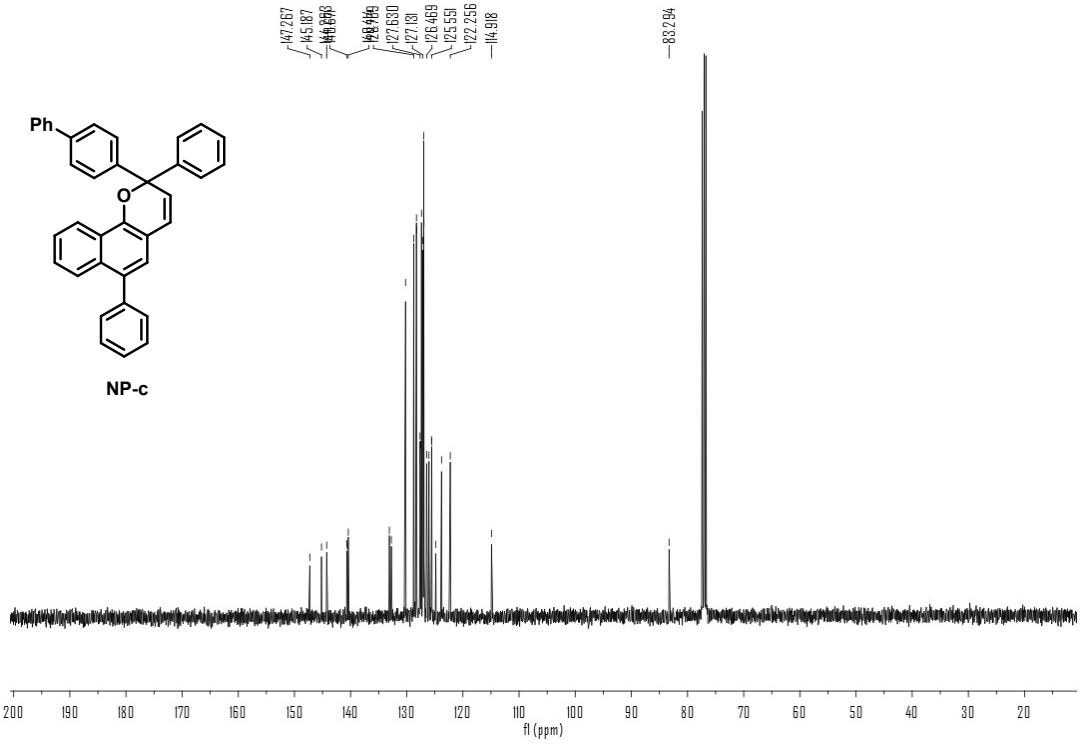

Fig. S88. ^{13}C NMR spectrum of **2-([1,1'-biphenyl]-4-yl)-2,6-diphenyl-*2H*-benzo [*h*]chromene** in $CDCl_3$.

5. HR-ESI-TOF-MS Spectra

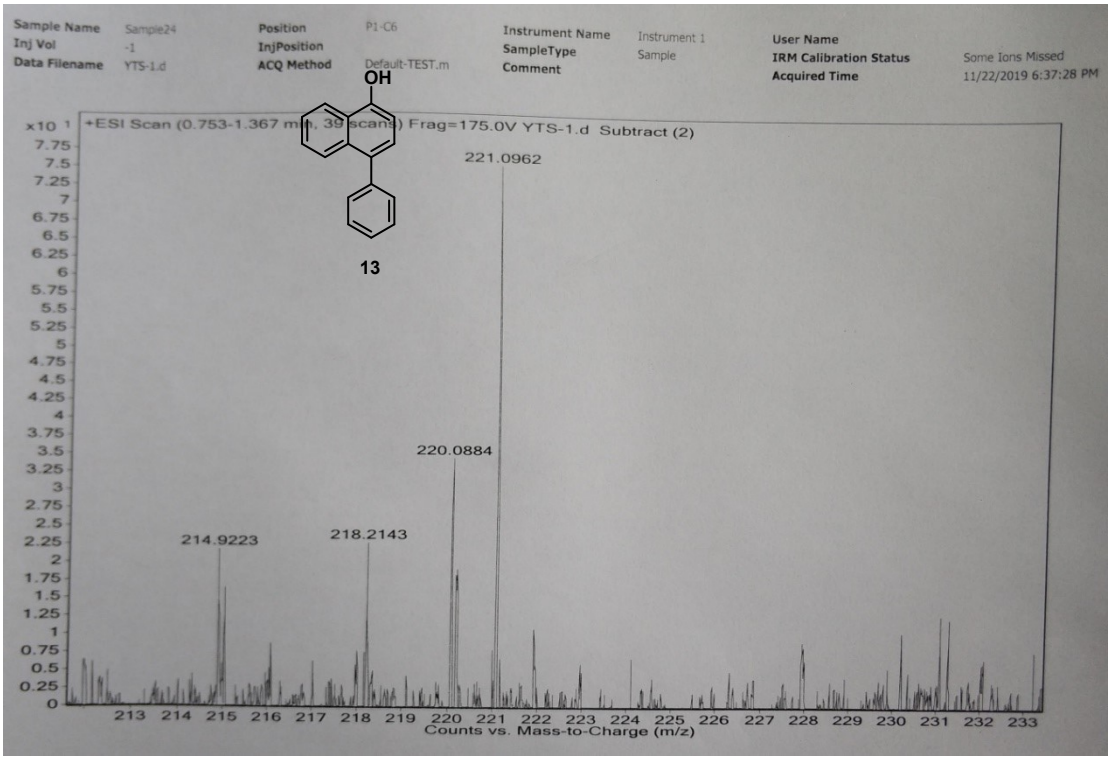

Fig. S89. HR-ESI-TOF-MS of **4-phenylnaphthalen-1-ol**.

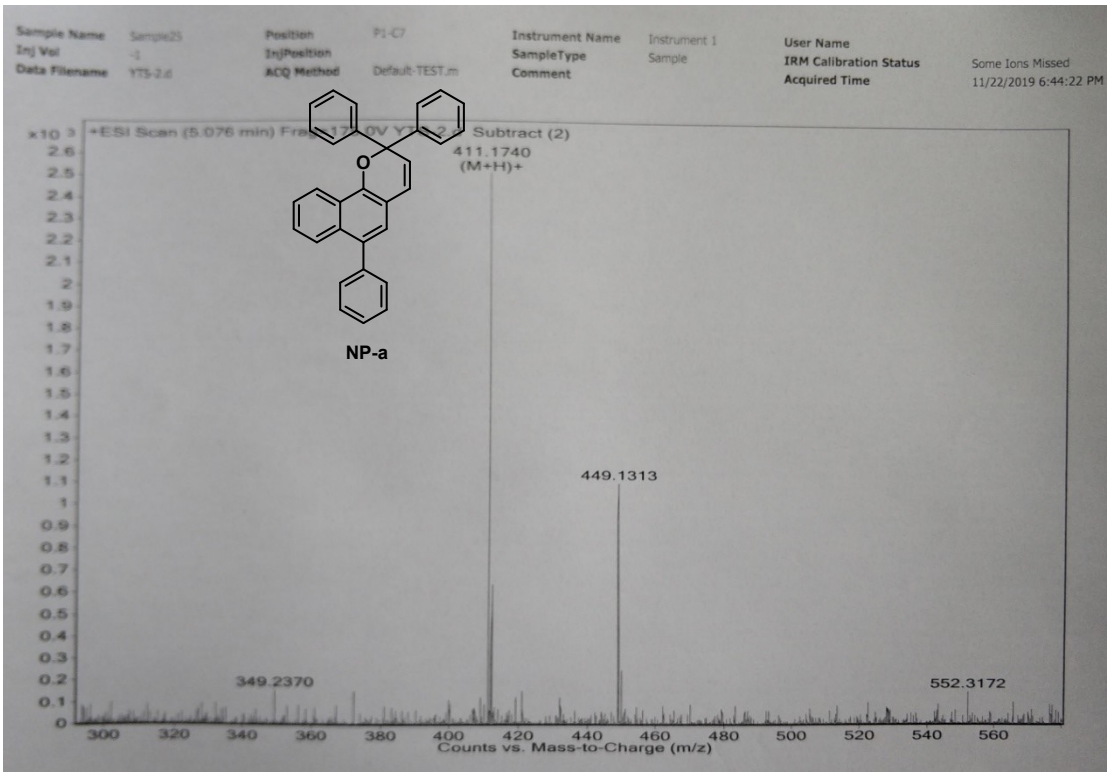

Fig. S90. HR-ESI-TOF-MS of **2,2,6-triphenyl-*2H*-benzo[*h*]chromene**.

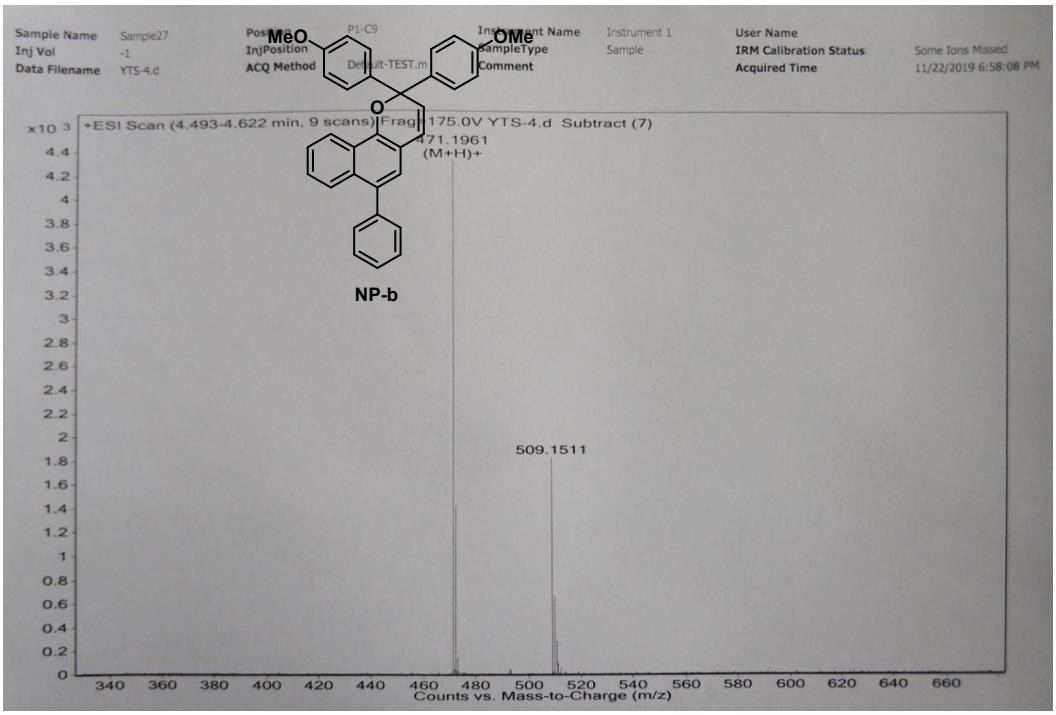

Fig. S91. HR-ESI-TOF-MS of **2-([1,1'-biphenyl]-4-yl)-2,6-diphenyl-*2H*-benzo[*h*]chromene**.

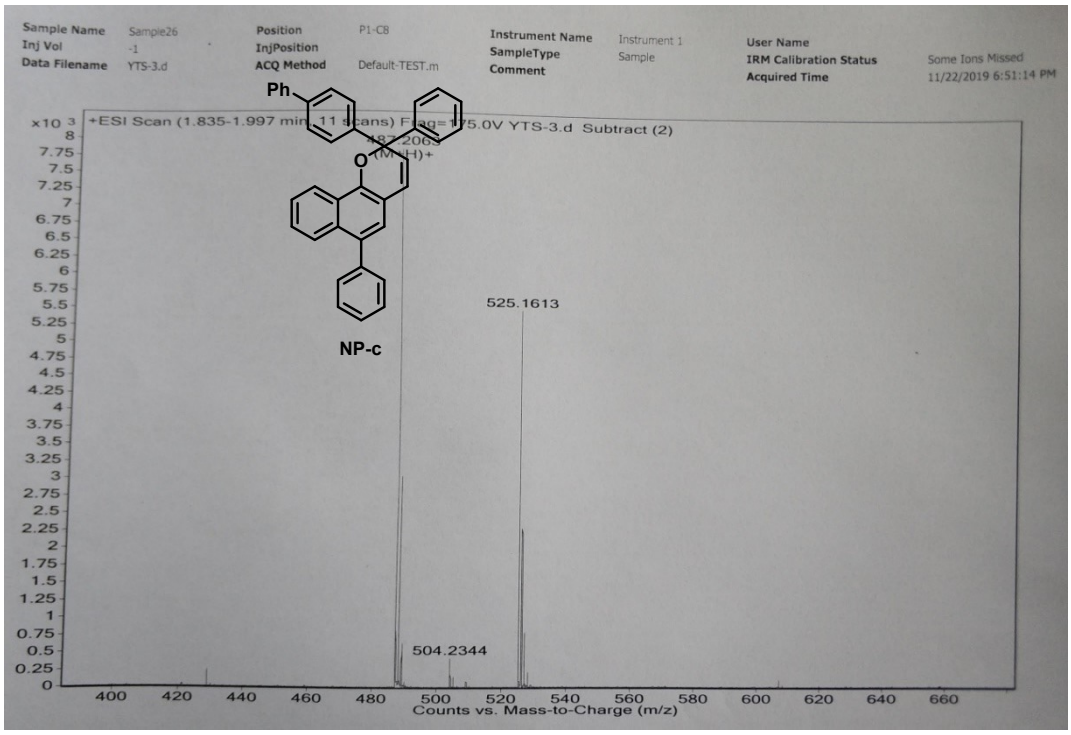

Fig. S92. HR-ESI-TOF-MS of **2,2-bis(4-methoxyphenyl)-6-phenyl-*2H*-benzo[*h*]chromene**.

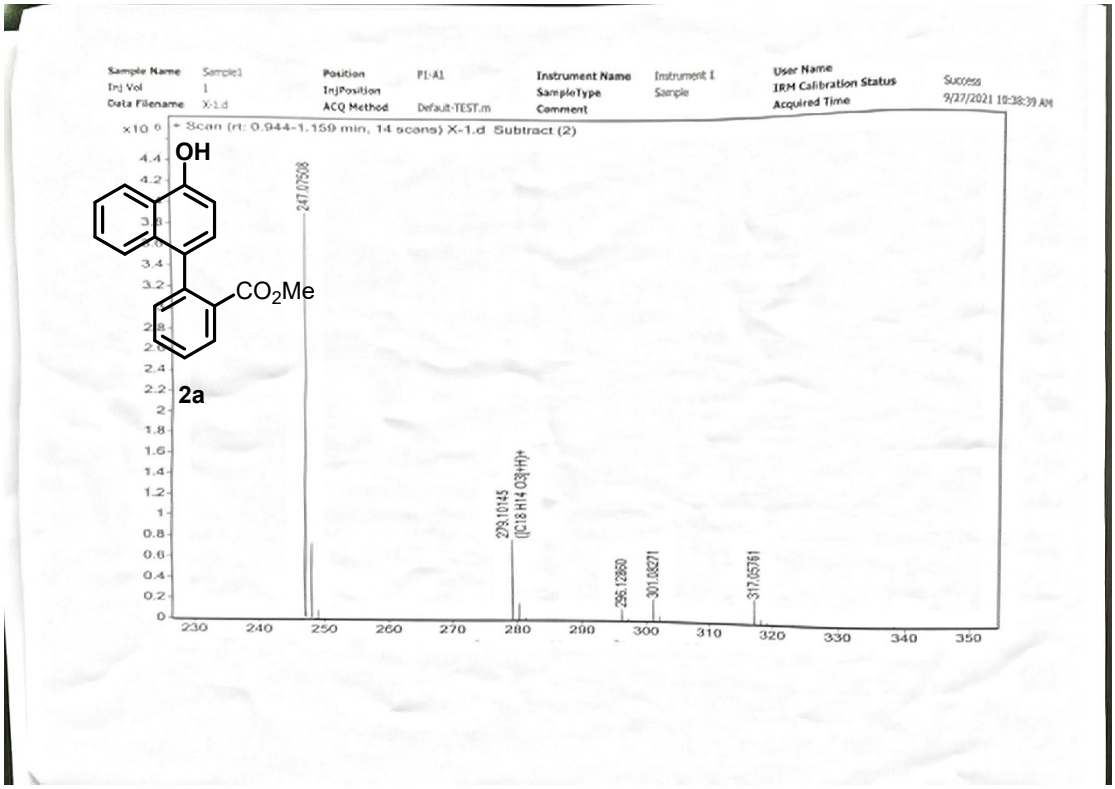

Fig. S93. HR-ESI-TOF-MS of **methyl 2-(4-hydroxynaphthalen-1-yl)benzoate (6a)**.

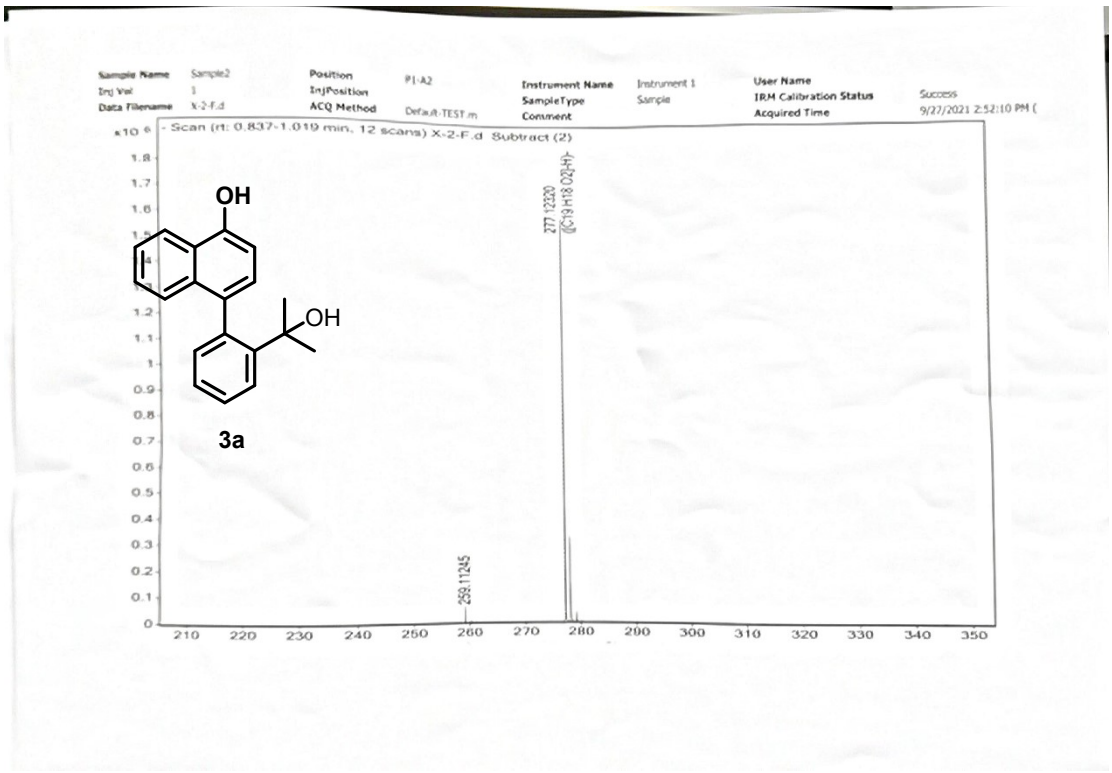

Fig. S94. 4-(2-(2-hydroxypropan-2-yl)phenyl)naphthalen-1-ol (7a).

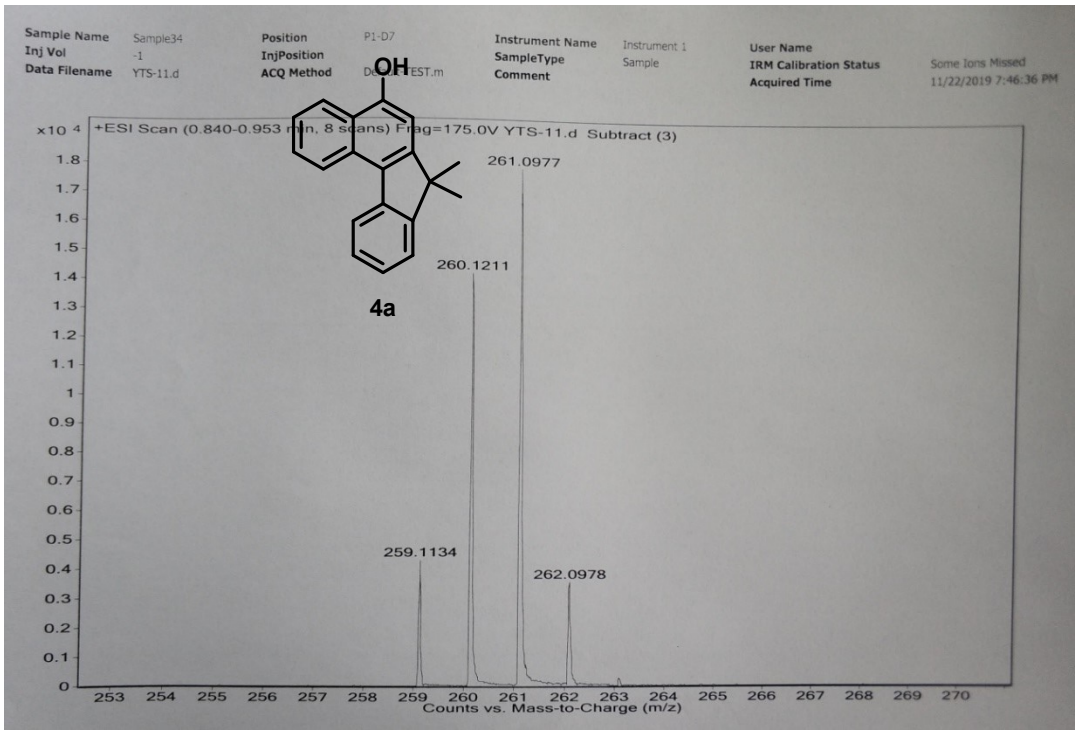

Fig. S95. HR-ESI-TOF-MS of **7,7-dimethyl-*7H*-benzo[*c*]fluoren-5-ol**.

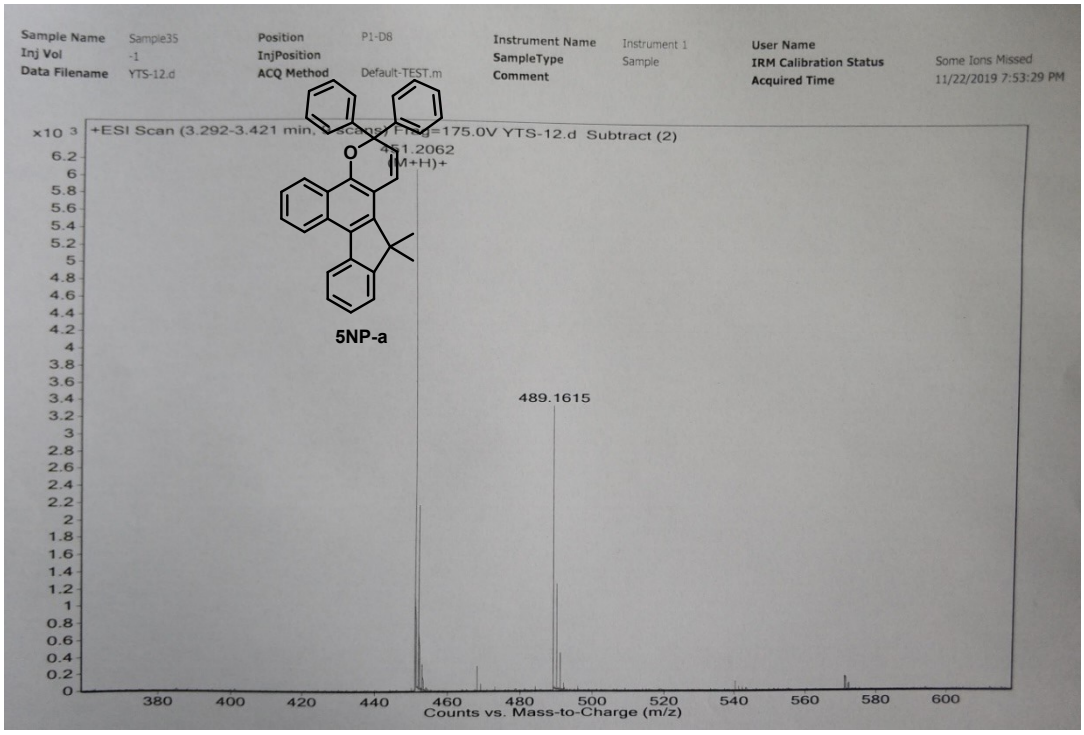

Fig. S96. HR-ESI-TOF-MS of **13,13-dimethyl-3,3-diphenyl-3,13-dihydrobenzo [h]indeno[*2,1-f*]chromene**.

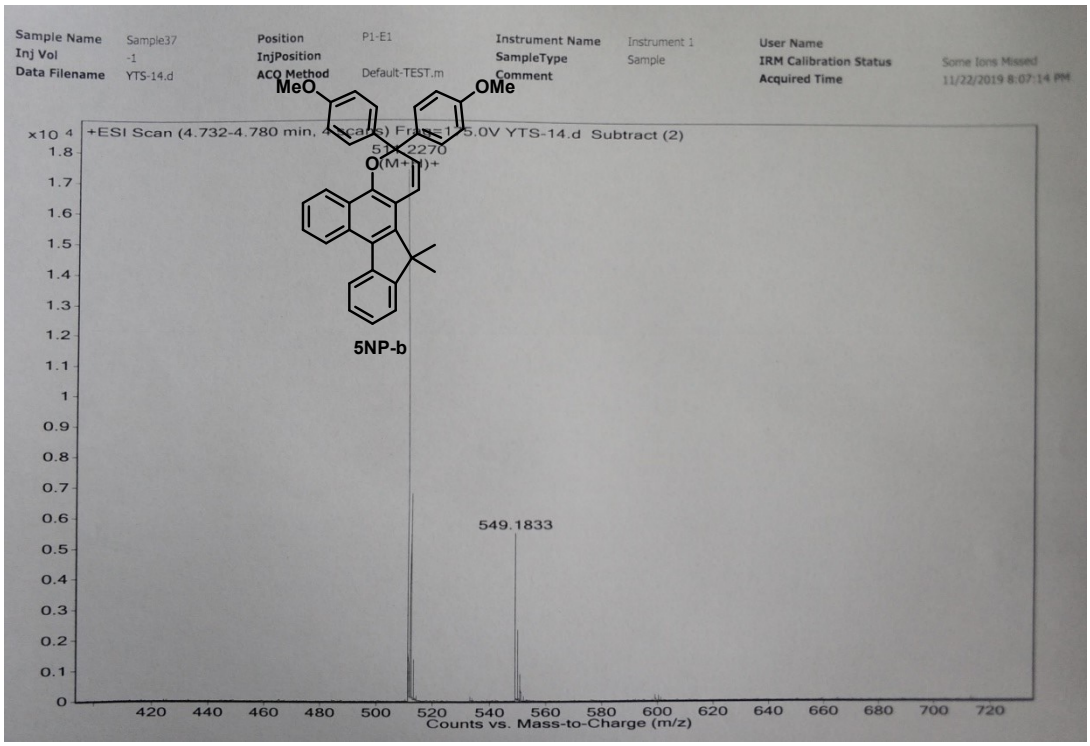

Fig. S97. HR-ESI-TOF-MS of **3,3-bis(4-methoxyphenyl)-13,13-dimethyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene**.

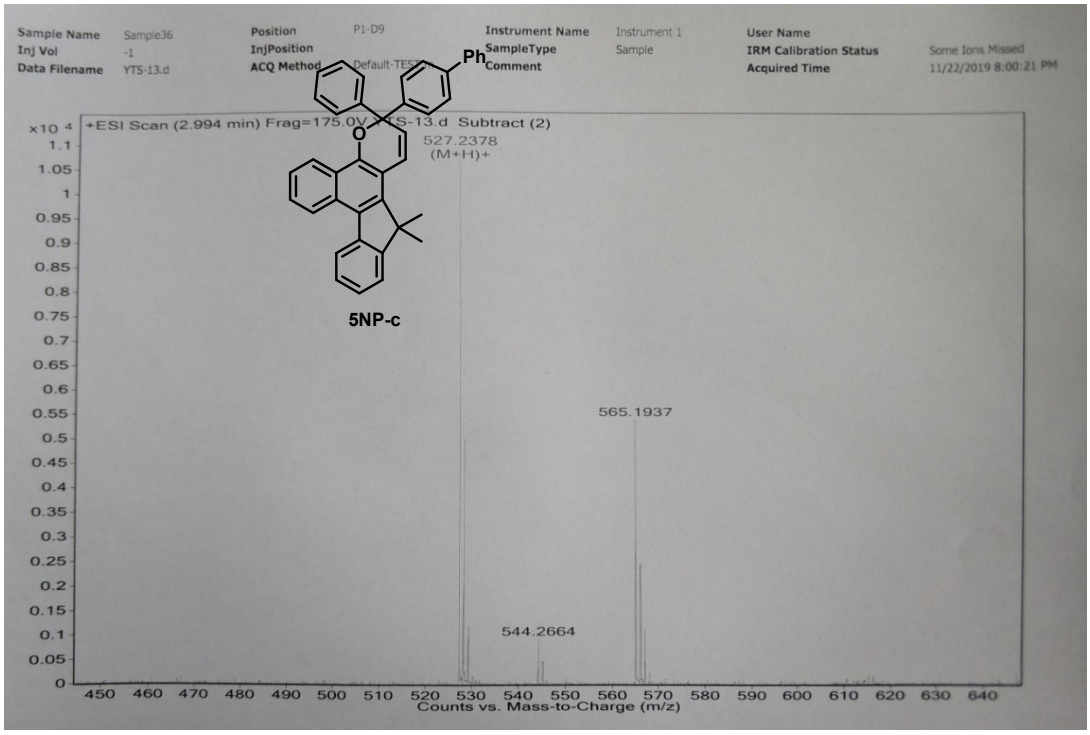

Fig. S98. HR-ESI-TOF-MS of **3-([1,1'-biphenyl]-4-yl)-13,13-dimethyl -3-phenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene.**

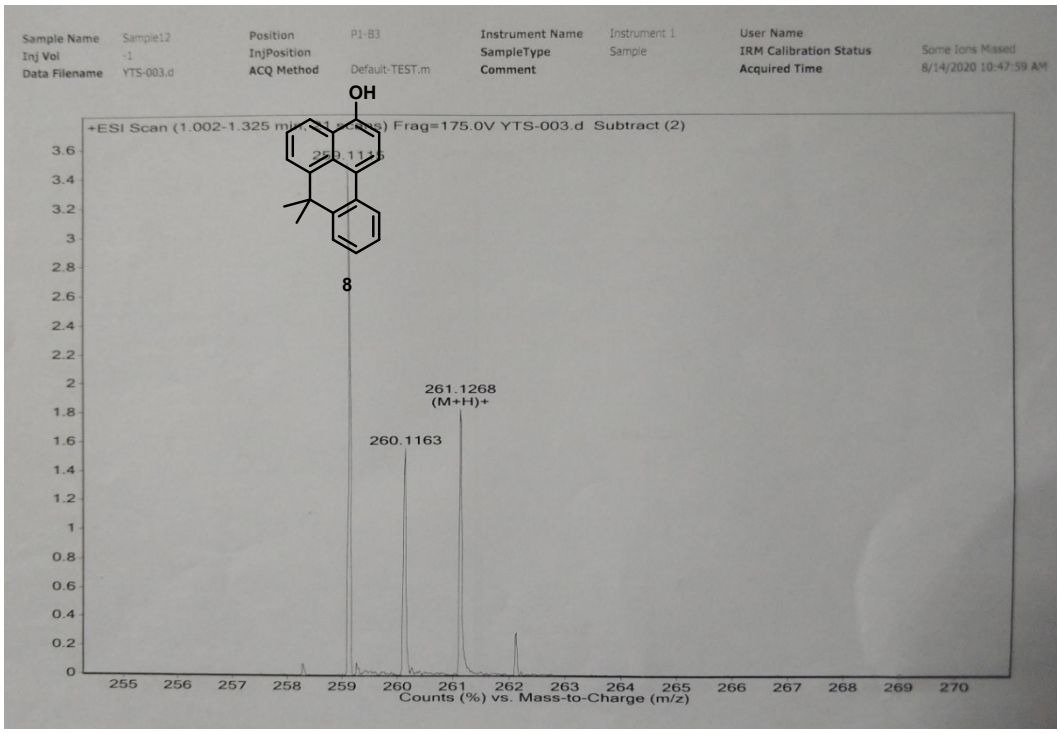

Fig. S99. HR-ESI-TOF-MS of **7,7-dimethyl-*7H*-benzo[*de*]anthracen-3-ol**.

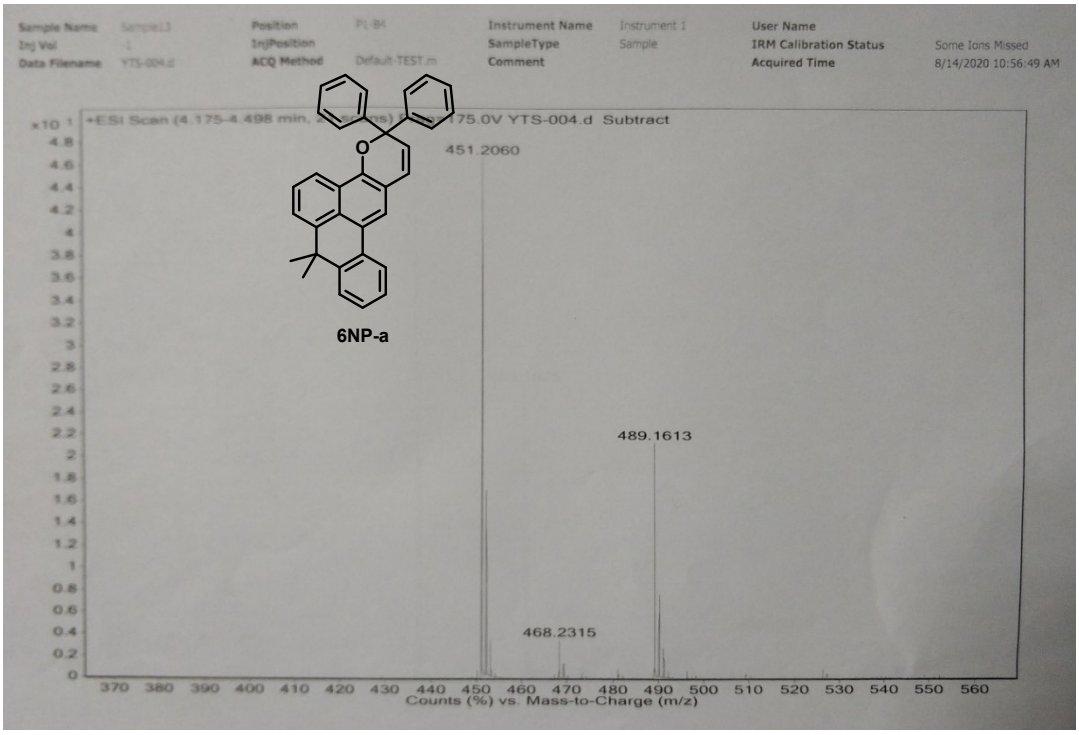

Fig. S100. HR-ESI-TOF-MS of **8,8-dimethyl-3,3-diphenyl-3,8-dihydroanthra [*9,1-gh*]chromene**.

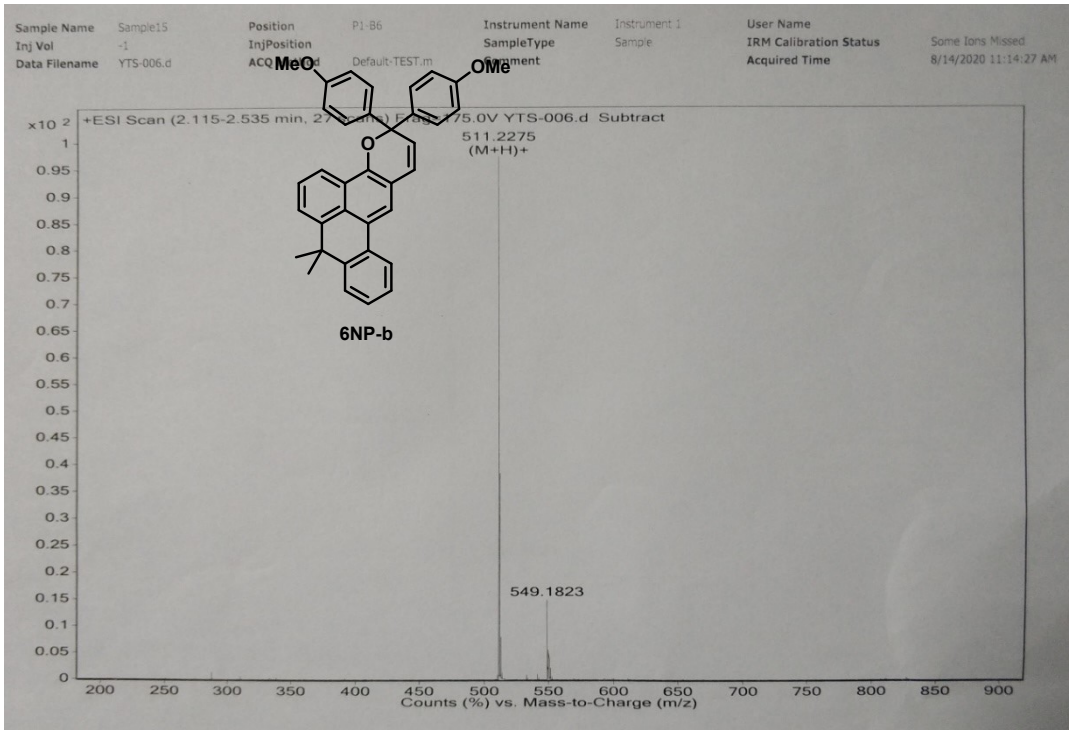

Fig. S101. HR-ESI-TOF-MS of **3,3-bis(4-methoxyphenyl)-8,8-dimethyl-3,8-dihydroanthra[*9,1-gh*]chromene**.

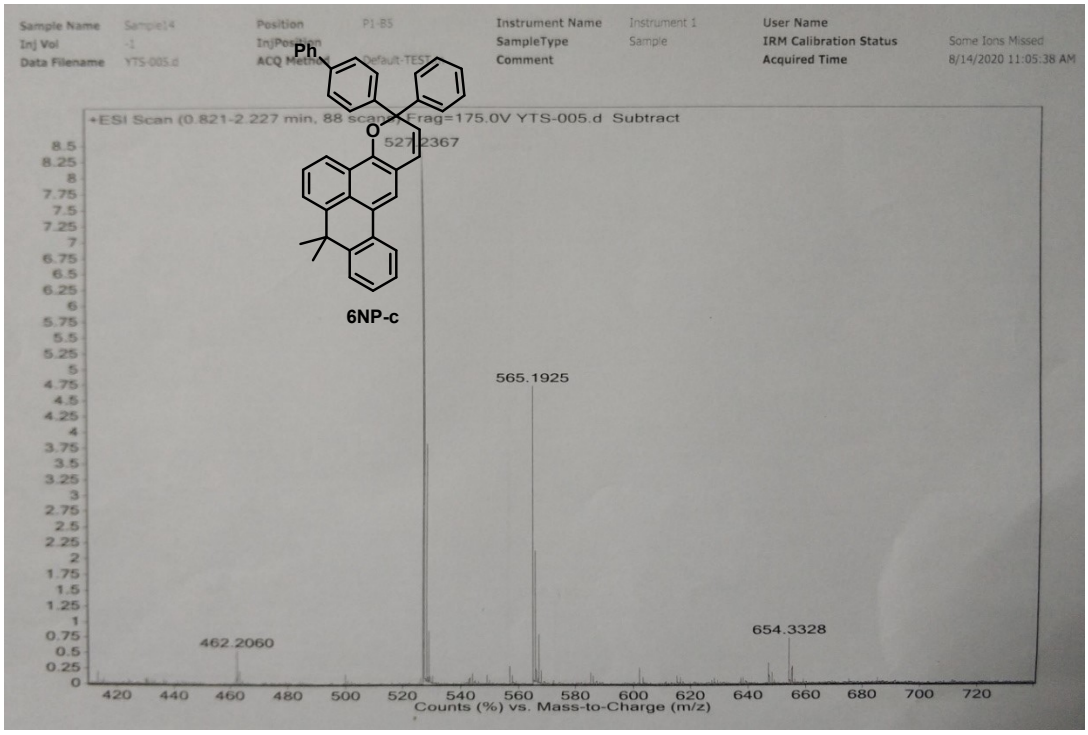

Fig. S102. HR-ESI-TOF-MS of **3-([1,1'-biphenyl]-4-yl)-8,8-dimethyl-3-phenyl- 3,8-dihydroanthra[9,*1-gh*]chromene**.

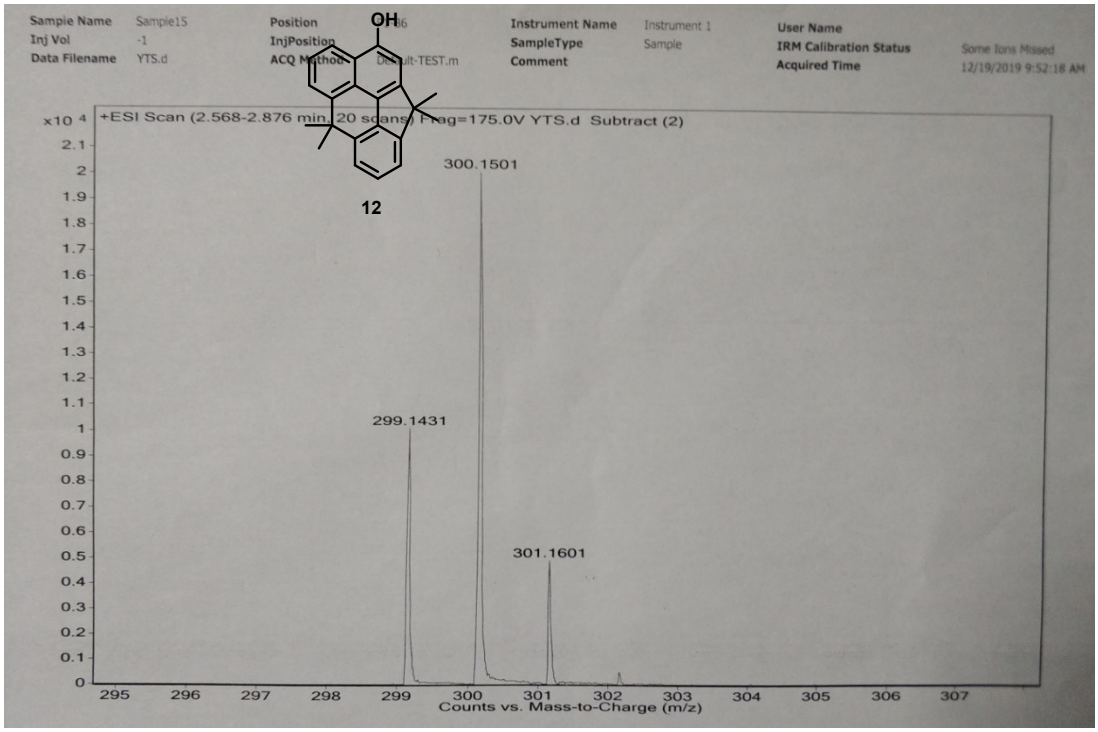

Fig. S103. HR-ESI-TOF-MS of **9-methoxy-1,1,5,5-tetramethyl-1,5-dihydrobenzo[*mno*]aceanthrylene**.

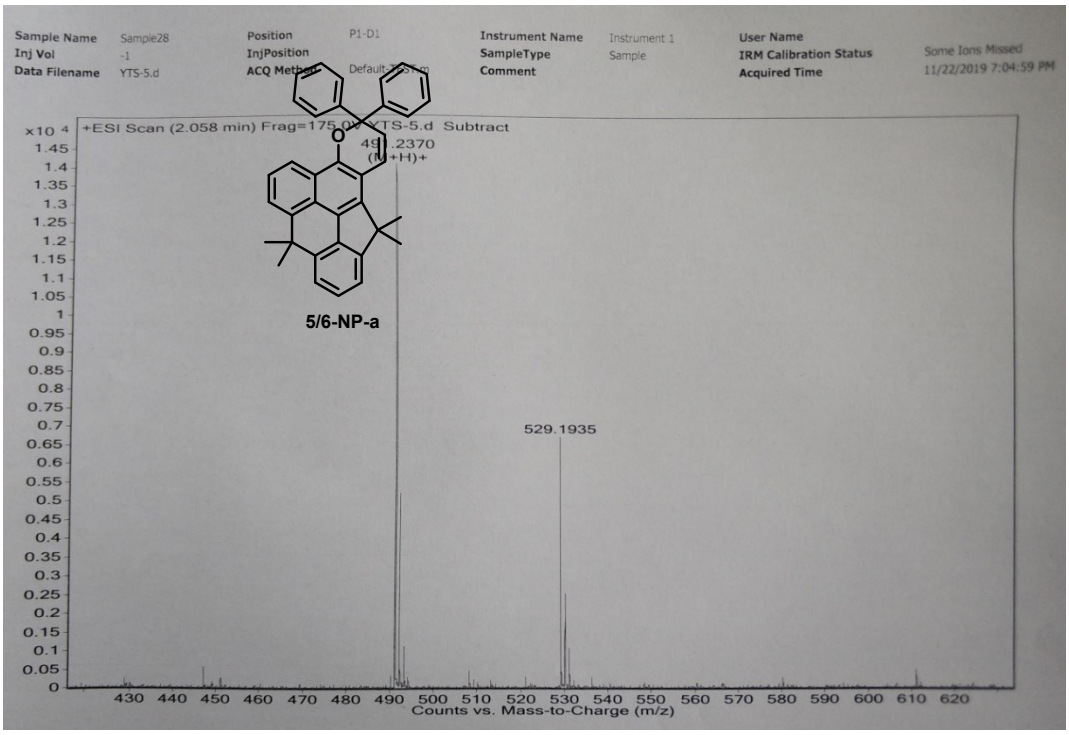

Fig. S104. HR-ESI-TOF-MS of **8,8,12,12-tetramethyl-3,3-diphenyl-8,12- dihydro-*3H*-aceanthryleno[*1,10-fgh*]chromene**.

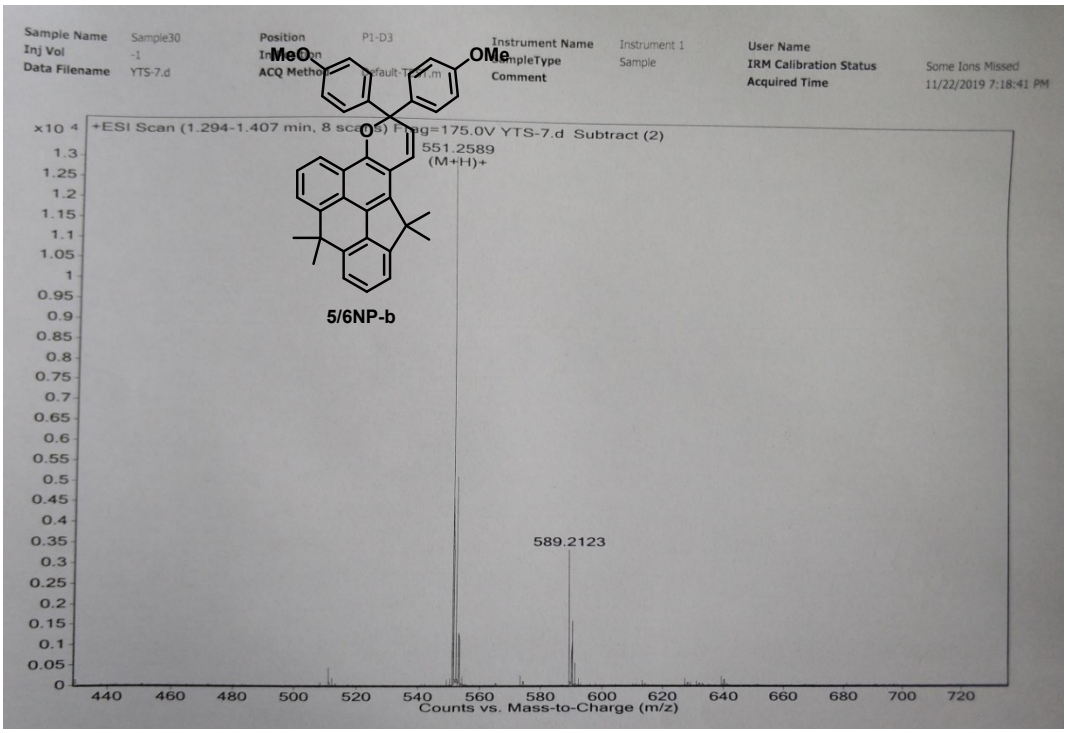

Fig. S105. HR-ESI-TOF-MS of **3,3-bis(4-methoxyphenyl)-8,8,12,12-tetra-methyl-8,12-dihydro-*3H*-aceanthryleno[*1,10-fgh*]chromene**.

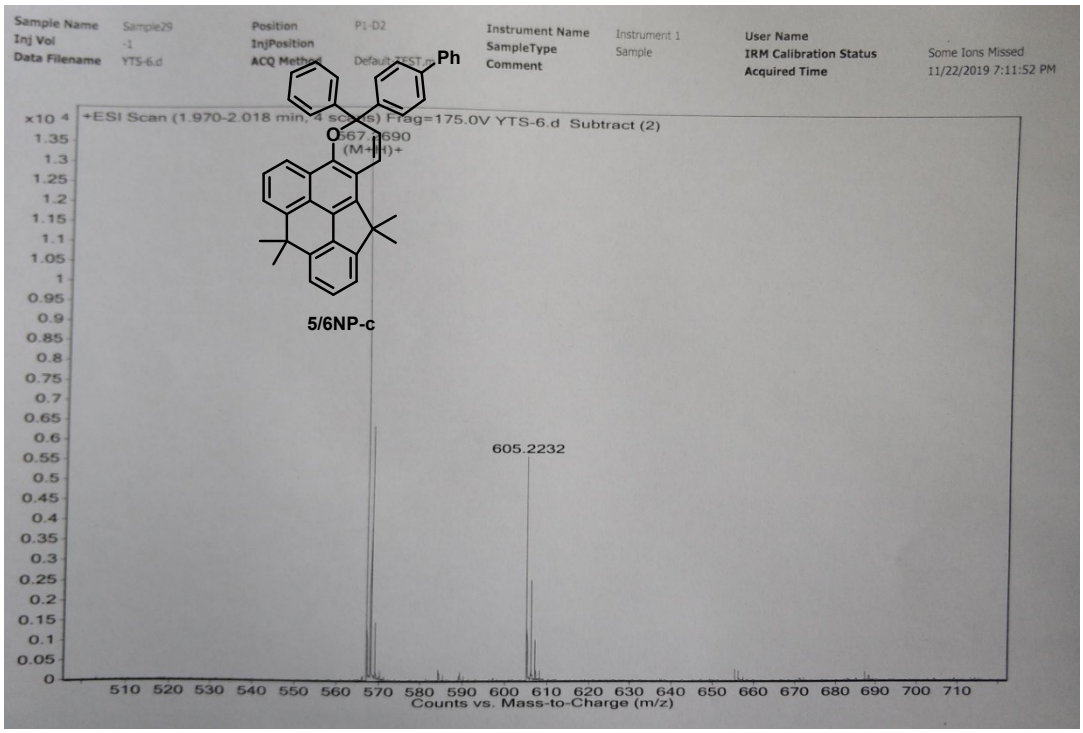

Fig. S106. HR-ESI-TOF-MS of **3-([1,1'-biphenyl]-4-yl)-8,8,12,12-te-tramethyl-3-phenyl-8,12-dihydro-3H-aceanthryleno[*1,10-fgh*]chromene**

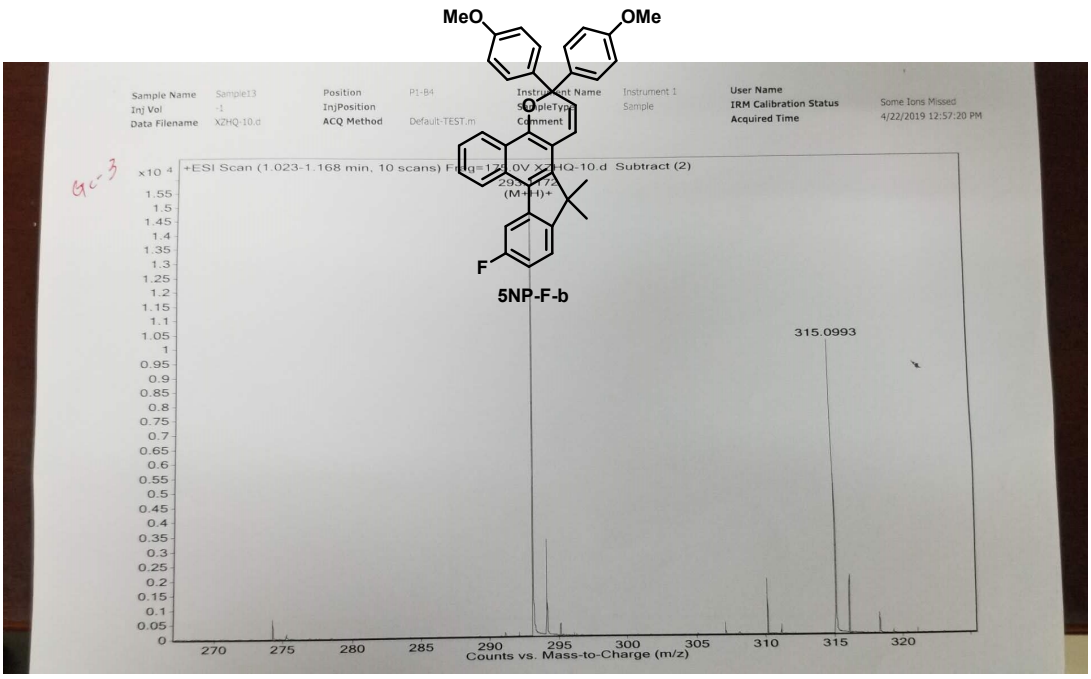

Fig. S107. HR-ESI-TOF-MS of **10-fluoro-3,3-bis(4-methoxyphenyl)-13,13-dimethyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene**.

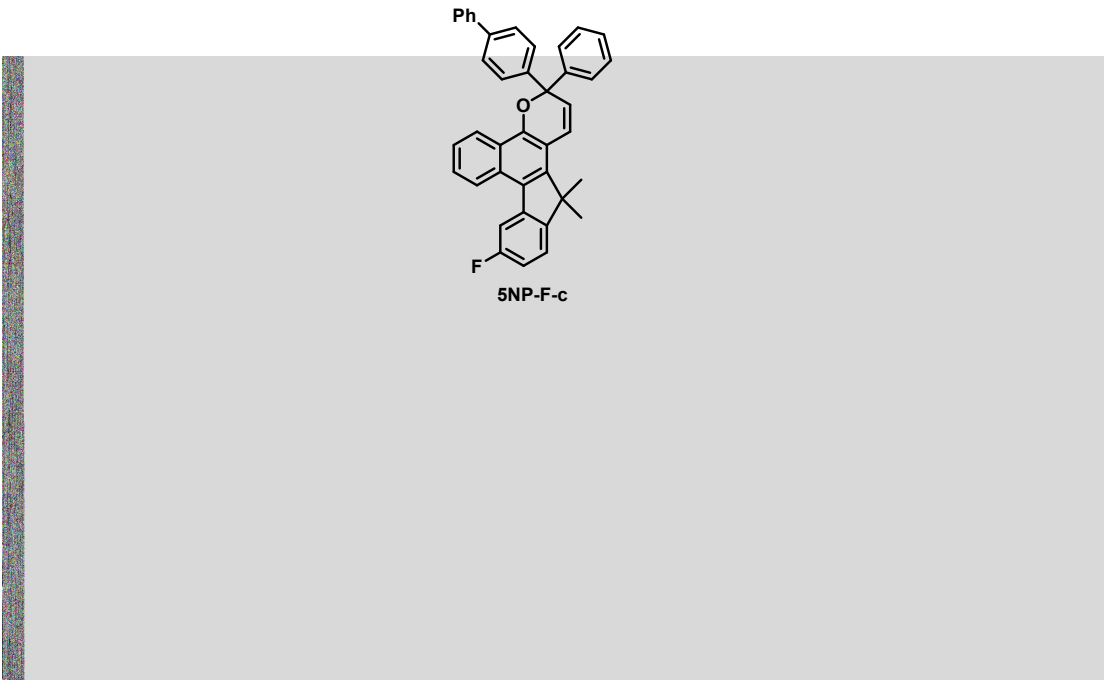

Fig. S108. HR-ESI-TOF-MS of **3-([1,1'-biphenyl]-4-yl)-10-fluoro-13,13- dimethyl-3-phenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene**.

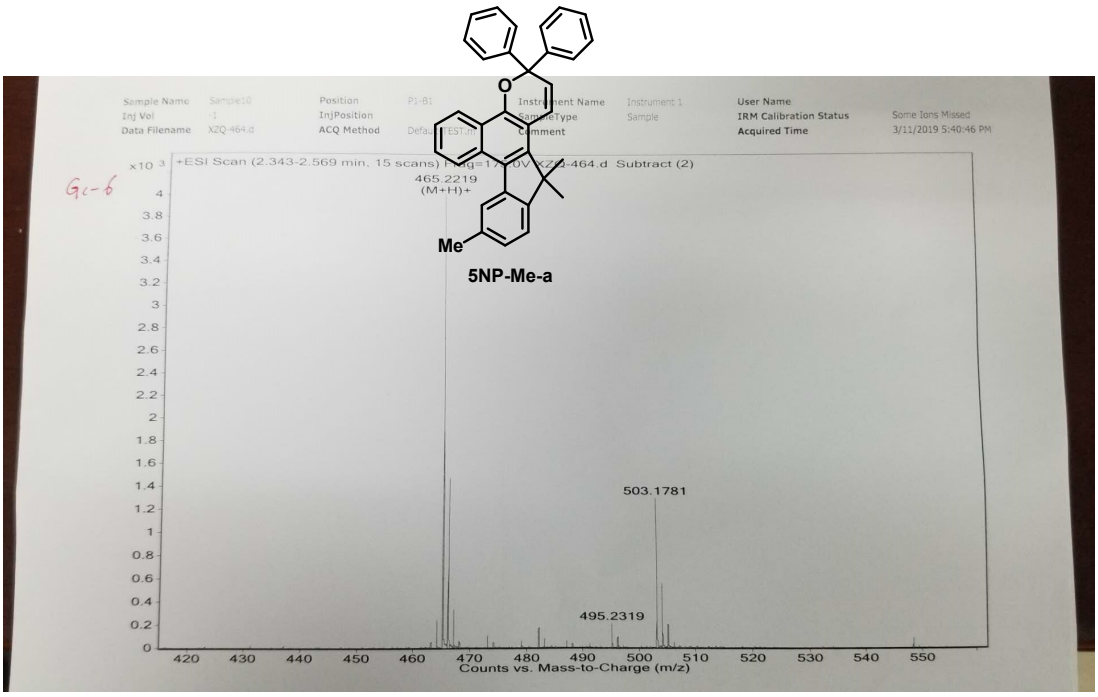

Fig. S109. HR-ESI-TOF-MS of **10,13,13-trimethyl-3,3-diphenyl-3,13-dihydro benzo[*h*]indeno[*2,1-f*]chromene**.

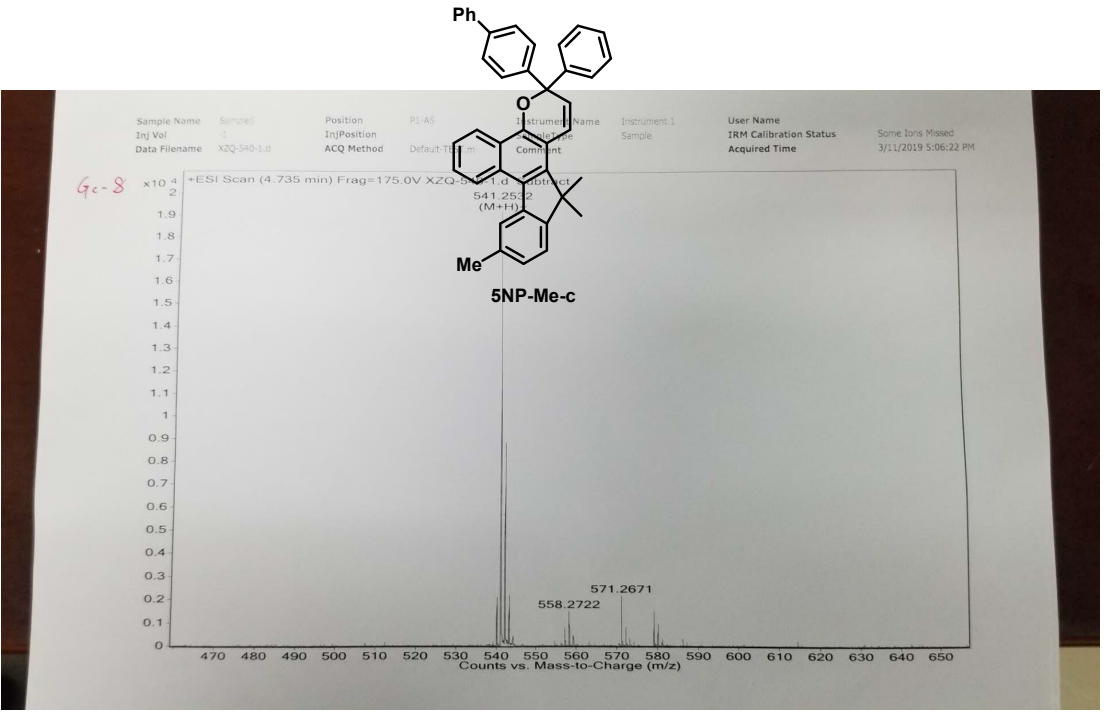

Fig. S110. HR-ESI-TOF-MS of **3-([1,1'-biphenyl]-4-yl)-10,13,13-trimethyl -3-phenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene**.

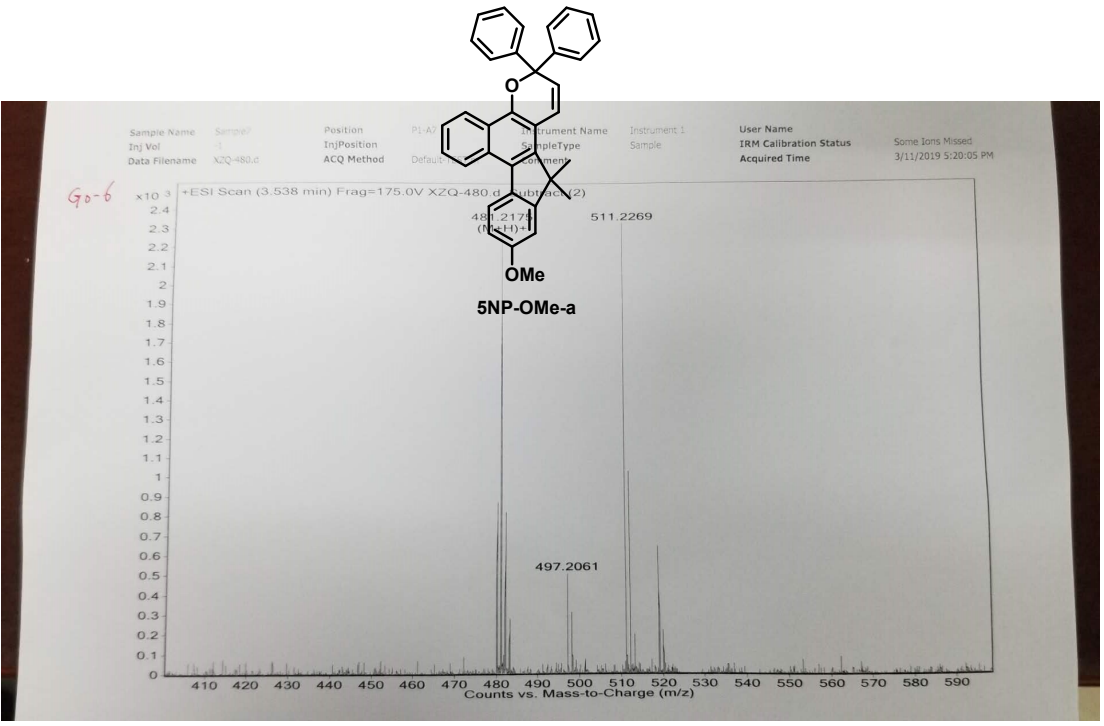

Fig. S111. HR-ESI-TOF-MS of **11-methoxy-13,13-dimethyl-3,3-diphenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene**.

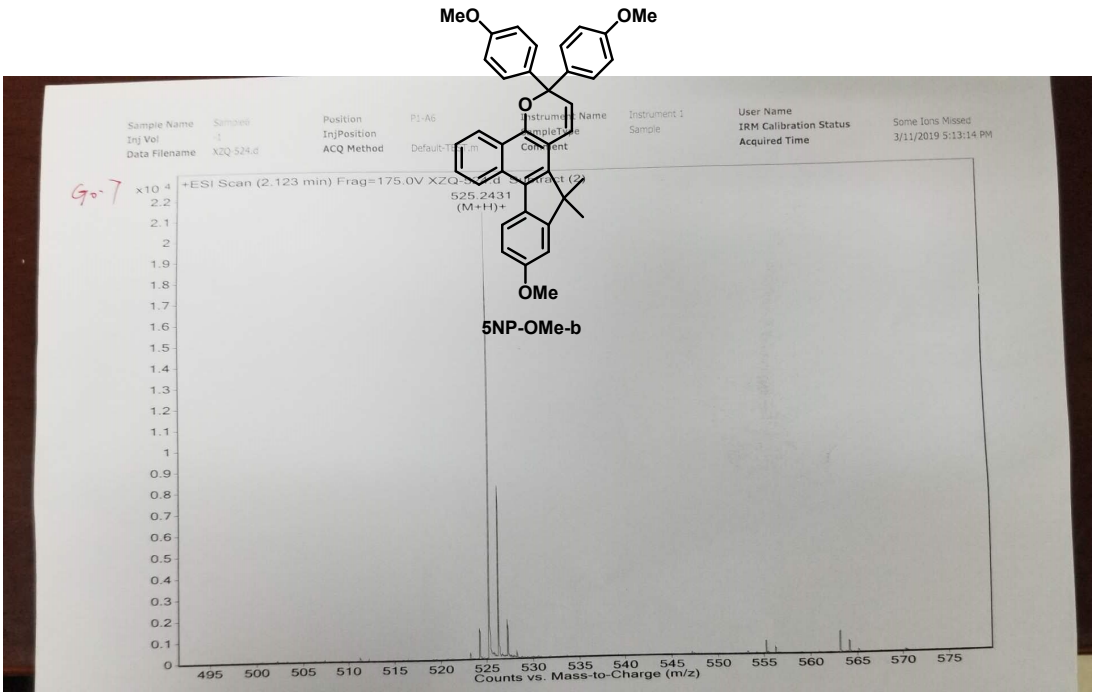

Fig. S112. HR-ESI-TOF-MS of **11-methoxy-3,3-bis(4-methoxyphenyl)-13,13-dimethyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene**.

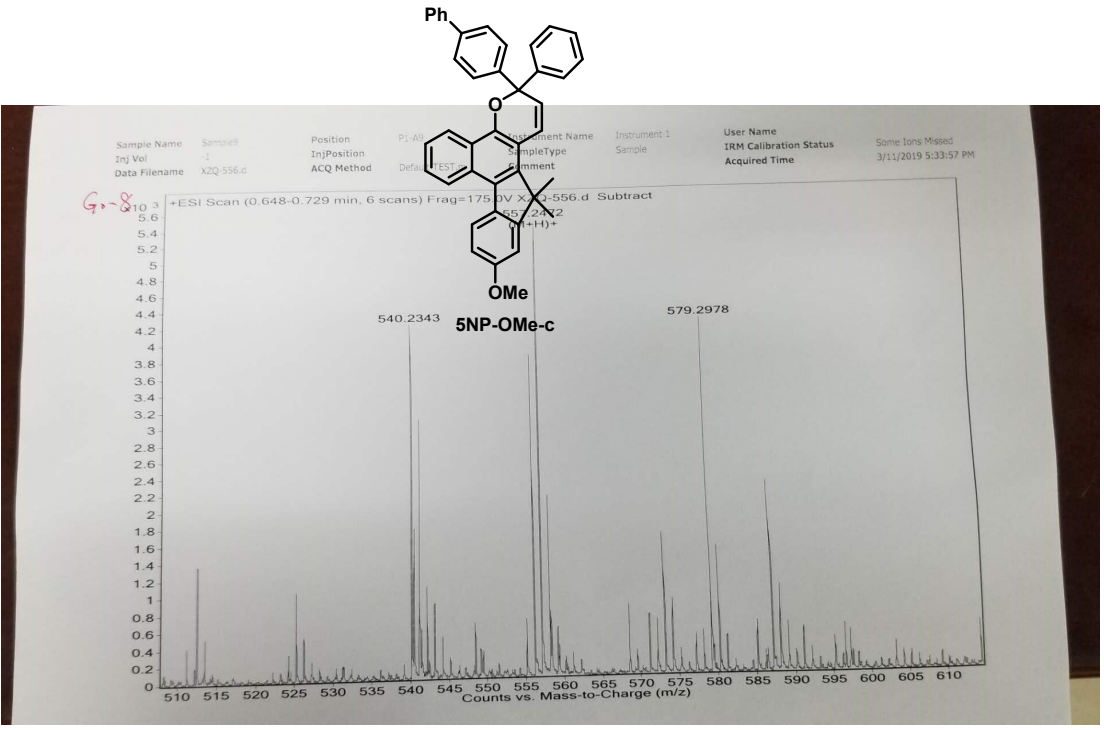

Fig. S113. HR-ESI-TOF-MS of **3-([1,1'-biphenyl]-4-yl)-11-methoxy-13,13-dimethyl-3-phenyl-3,13-dihydrobenzo[*h*]indeno[*2,1-f*]chromene**.

6. Transient UV−Vis Absorption Spectroscopy

Table S2. Reaction Kinetics Parameters for the Thermal Back Reaction of the Colored Species of **NPs** in ethyl acetate (8.0×10^{-5} M) at 298 K.

compounds	A_1	k_1	A_2	k_2
NP-a	0.42	0.14	0.42	0.0014
NP-b	0.99	0.188	0.02	0.00002
NP-c	0.63	0.128	0.35	0.0031
5NP-a	0.31	0.036	0.02	0.0004
5NP-b	6.93	0.315	0.07	0.0068
5NP-c	0.98	0.050	0.02	0.0009
6NP-a	2.07	0.036	0.93	0.0001
6NP-b	1.25	0.184	0.08	0.0001
6NP-c	1.24	0.036	0.44	0.00012
5/6NP-a	0.90	0.063	0.20	0.0002
5/6NP-b	2.73	0.612	0.27	0.00012
5/6NP-c	1.72	0.092	0.33	0.00002
5NP-F-a	0.06	0.074	0.02	0.00015
5NP-F-b	5.17	0.717	0.16	0.00003
5NP-F-c	0.96	0.109	0.21	0.00009
5NP-Me-a	0.56	0.317	0.46	0.00908
5NP-Me-b	5.50	0.229	0.05	0.00035
5NP-Me-c	0.58	0.239	0.11	0.00004
5NP-OMe-a	0.05	0.136	0.02	0.00016
5NP-OMe-b	0.32	0.142	0.04	0.00016
5NP-OMe-c	1.05	0.196	0.20	0.00061
PMMA film	0.93	0.145	0.03	0.00426

The half-lives (τ1/2 at 298 K) of the TC form were determined from the fitting curves of the time variation of the absorbance using the following biexponential equation, where $k1$ is the rate constant for the thermal back reaction of the TC form and $k2$ is that of the TT form.

$$f_{(t)} = A_1 e^{-k_1 t} + A_2 e^{-k_2 t} + A_0$$

The generation ratio of the TT form was defined as $A_2/(A_1+A_2)$ by assuming the molar extinction coefficients of the TC and TT forms are same.

7. DFT Calculations

All calculations were carried out using the Gaussian 09 program (Revision D.01). The molecular structure was fully optimized at the M06-2X/6-31+G(d,p) level of the theory, and analytical second derivative was computed using vibrational analysis to confirm each stationary point to be a minimum. TDDFT calculations were performed at the MPW1PW91/6-31+G(d,p) level of the theory for the optimized structures. TDDFT calculations were performed at the MPW1PW91/6-31+G(d,p) level of the theory for the optimized structures.

7.1 The Calculated UV-vis Absorption Spectra

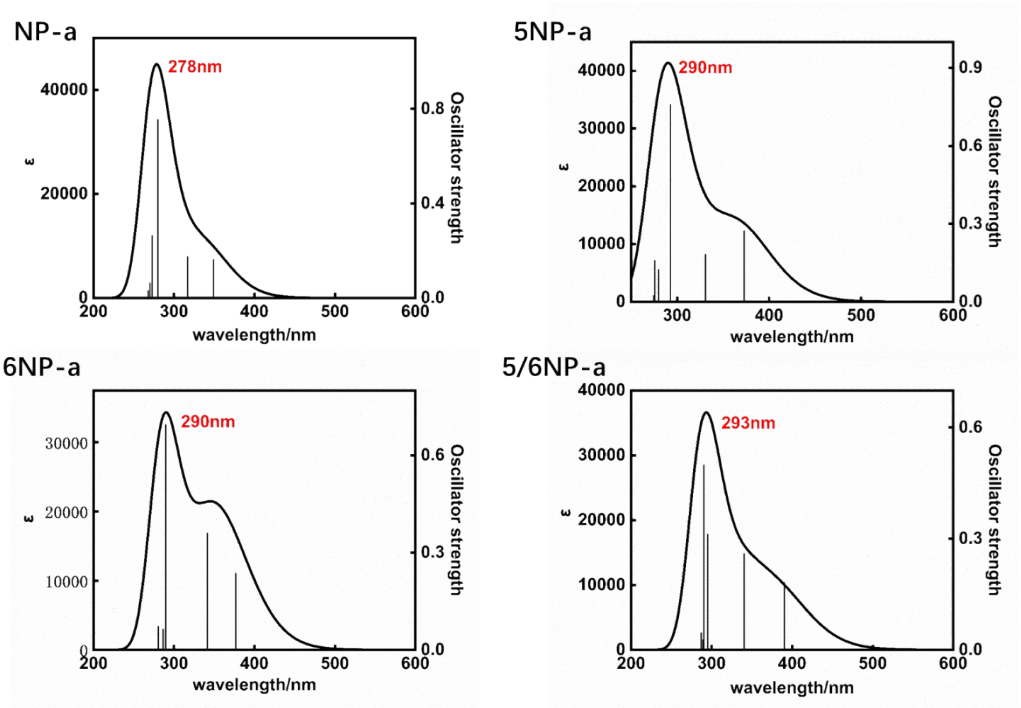

Fig. S114. UV-vis absorption spectra of the CFs for (a) **NP-a**, (b) **5NP-a**, (c) **6NP-a** and (d) **5/6NP-a** in ethyl acetate solutions. The calculated spectra (MPW1PW91/6-

31+G(d)// M06-2X/6-31+G(d,p) level of the theory) are shown.

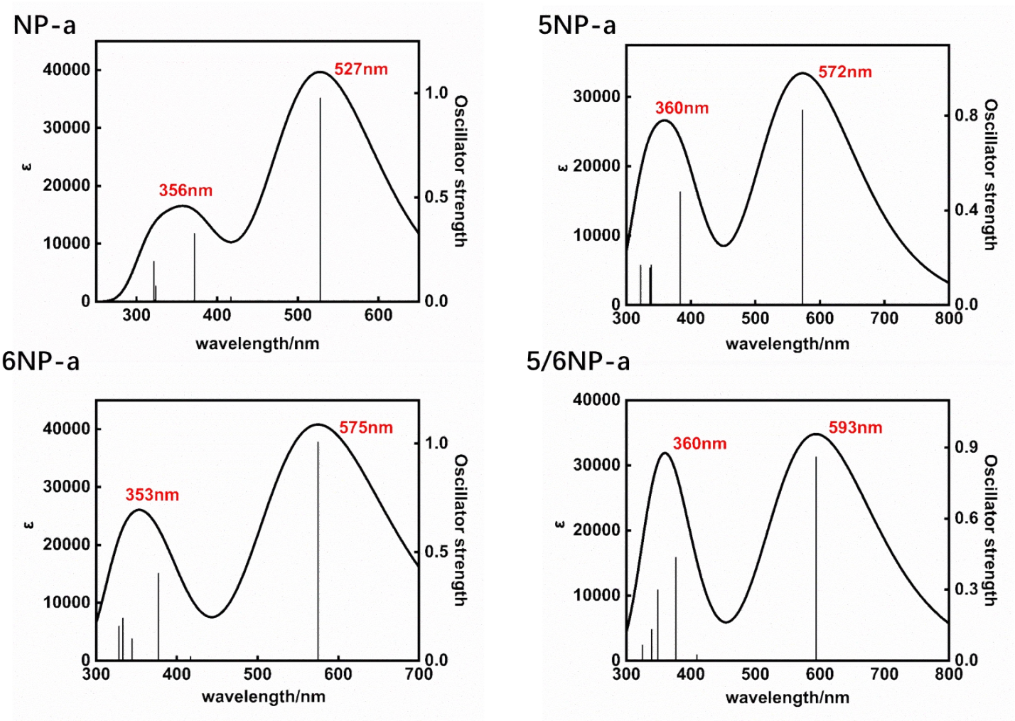

Fig. S115. UV-vis absorption spectra of the TCs for (a) **NP-a**, (b) **5NP-a**, (c) **6NP-a** and (d) **5/6NP-a** in ethyl acetate solutions. The calculated spectra (MPW1PW91/6-31+G(d)// M06-2X/6-31+G(d,p) level of the theory) are shown.

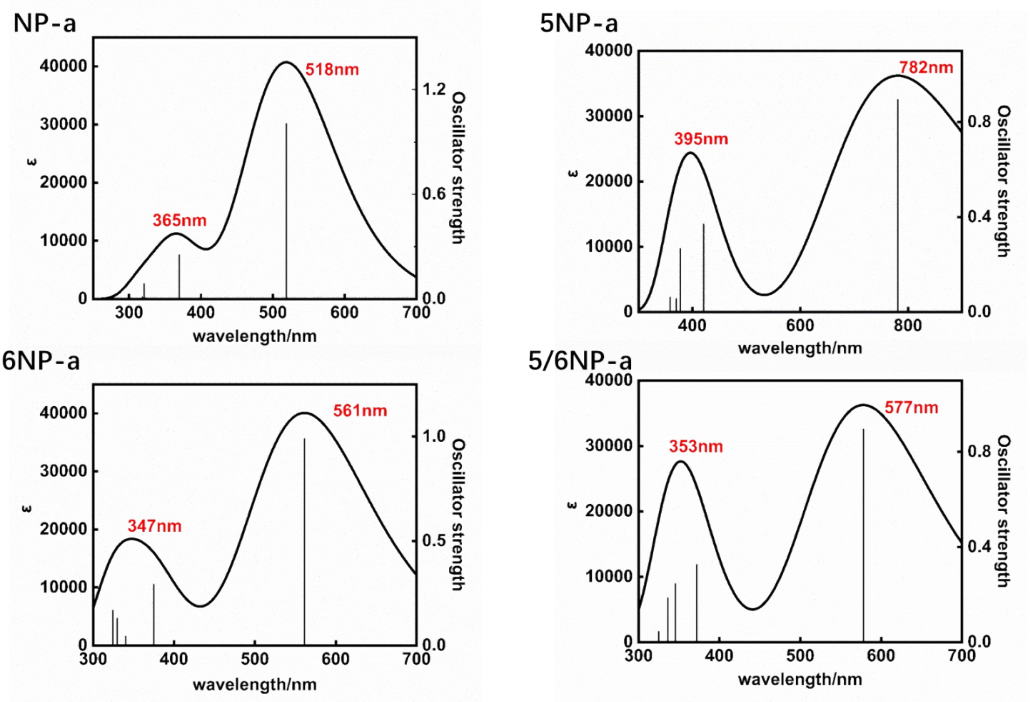

Fig. S116. UV-vis absorption spectra of the TTs for (a) **NP-a**, (b) **5NP-a**, (c) **6NP-a** and (d) **5/6NP-a** in ethyl acetate solutions. The calculated spectra (MPW1PW91/6-

31+G(d)// M06-2X/6-31+G(d,p) level of the theory) are shown.

7.2 Calculated Structures

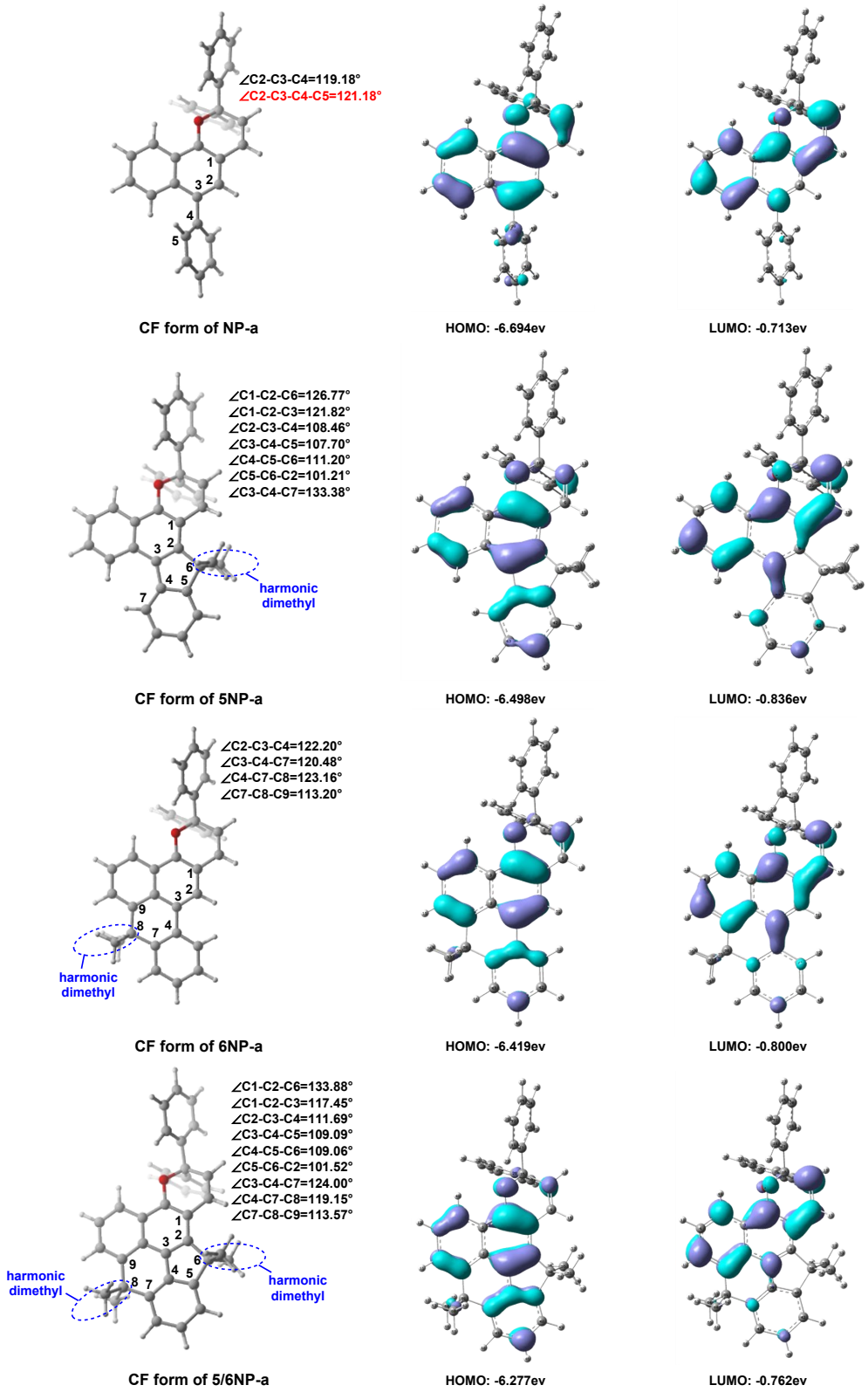

Fig. S117. Calculated structure and orbit of **NP-a**, **5NP-a**, **6NP**-a and **5/6NP-a** at the

M06-2X/6-31+G(d,p) level of theory. All energies are in kcal/mol, and bond lengths are in Å.

7.3 Calculated Potential Energy Surface

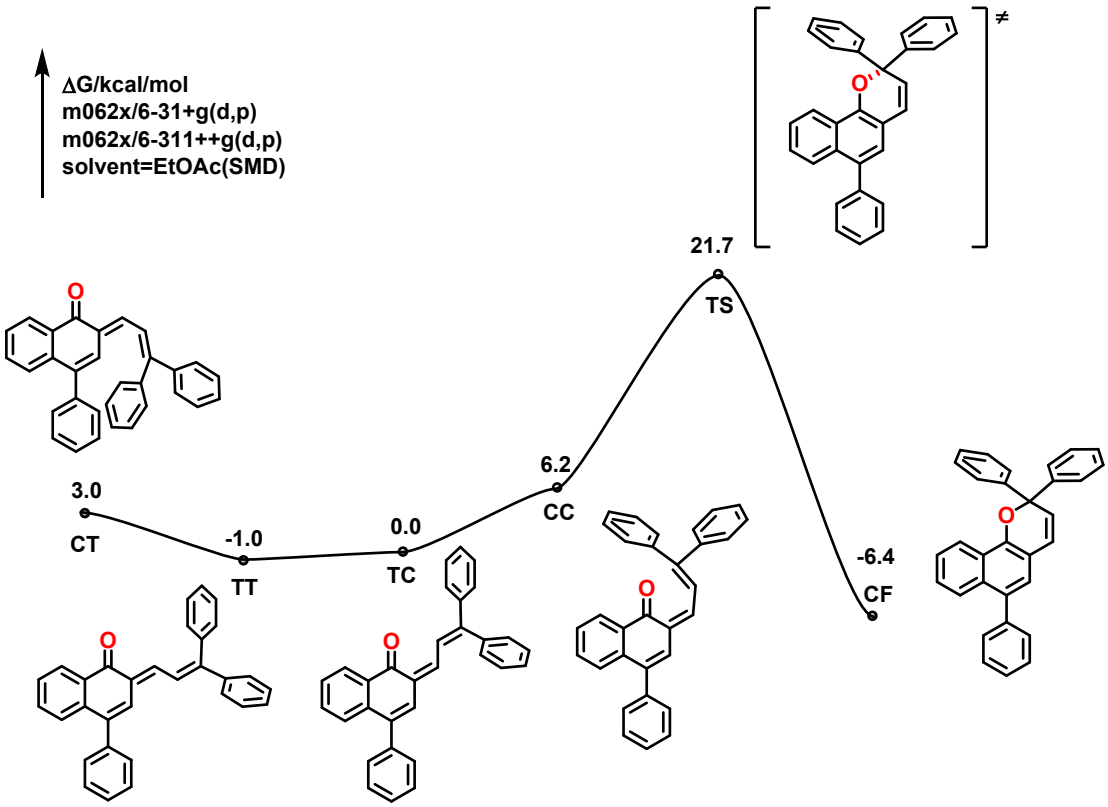

Fig. S118. Calculated potential energy surface for decolorization reaction of **NP-a** at the (SMD)M06-2X/6-311++G(d,p)//M06-2X/6-31+G(d,p) level of theory.

7.4 Calculated Intrinsic Reaction Coordinate (IRC) of NP-a-TS

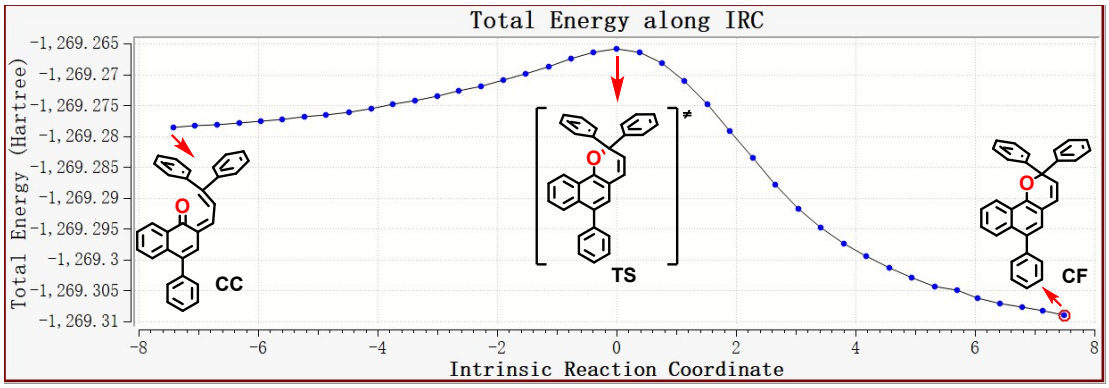

Fig. S119. Calculated Intrinsic Reaction Coordinate (IRC) of **NP-a-TS** at the M06-2X/6-31+G(d,p) level of theory.

7.5 Calculated TC, TT and TS form structures

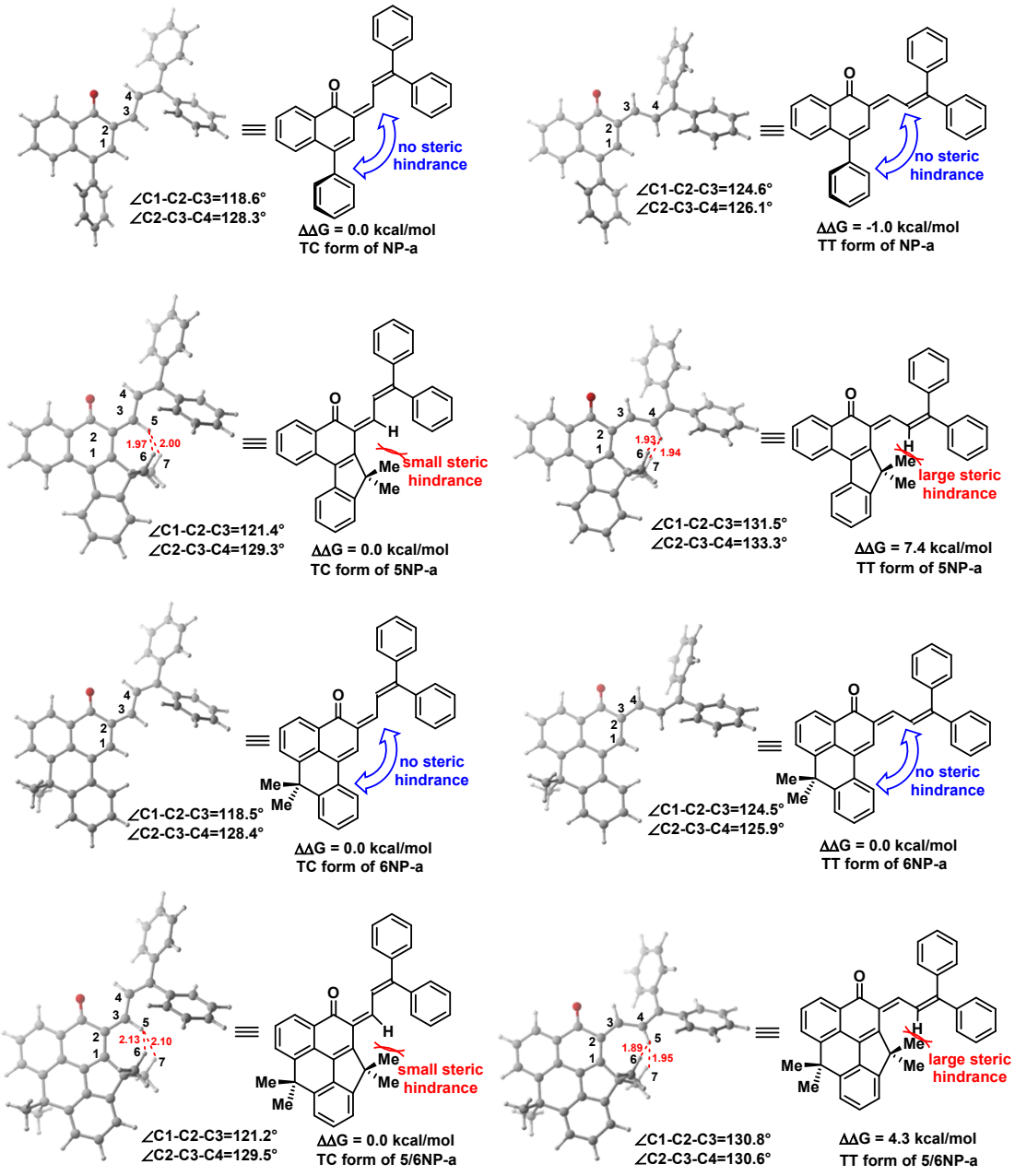

Fig. S120. Calculated TC and TT form structures of **NP-a, 5NP-a, 6NP-a and 5/6NP-a** at the (SMD)m06-2x/6-311++g(d,p)//m06-2x/6-31+g(d,p) level of theory. All energies are in kcal/mol, and bond lengths are in Å.

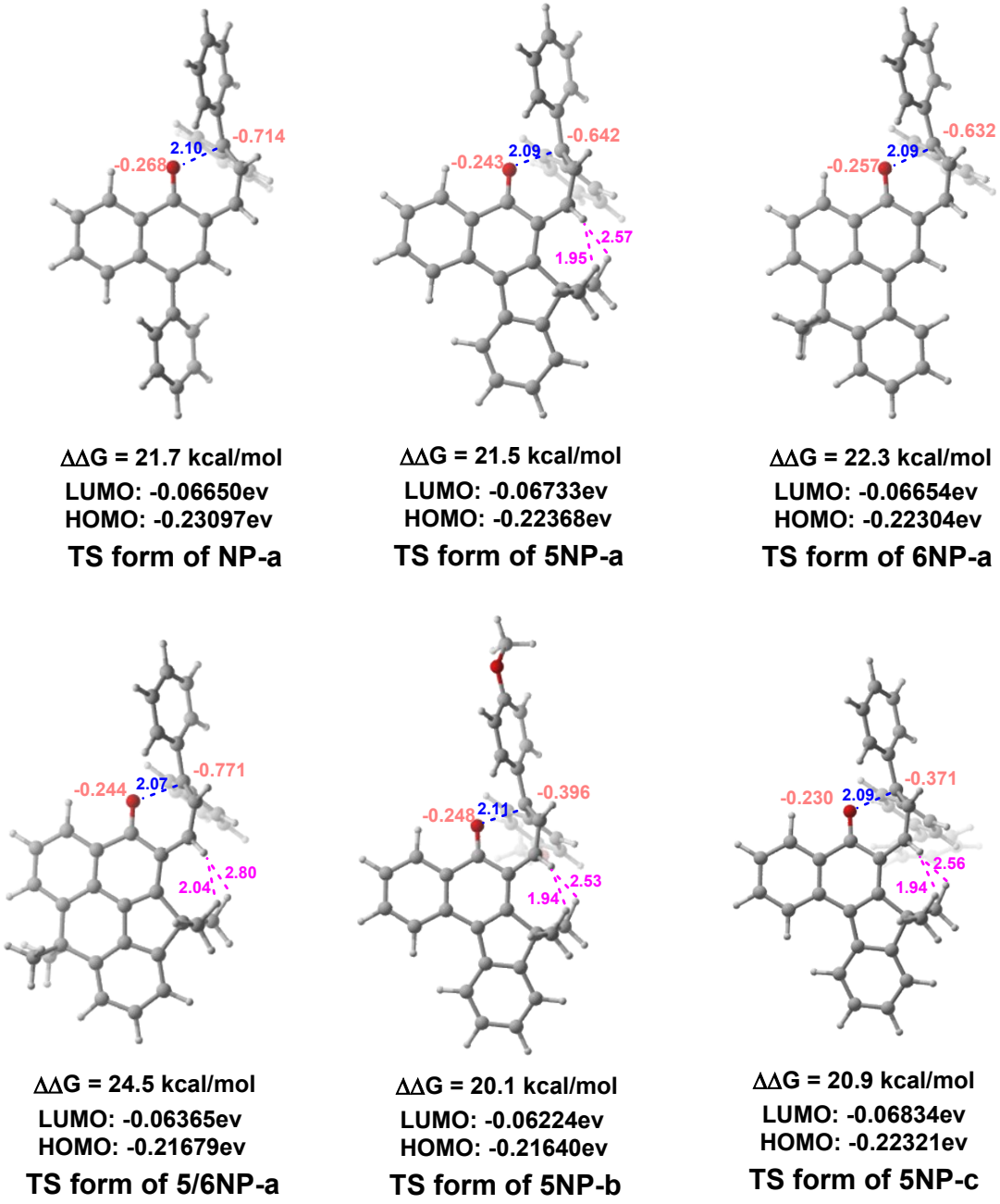

Fig. S121. Calculated structure, orbit and the Gibbs free energy for transient state of decolorization reaction of several naphthopyran derivatives. All energies are in kcal/mol, and bond lengths are in Å.

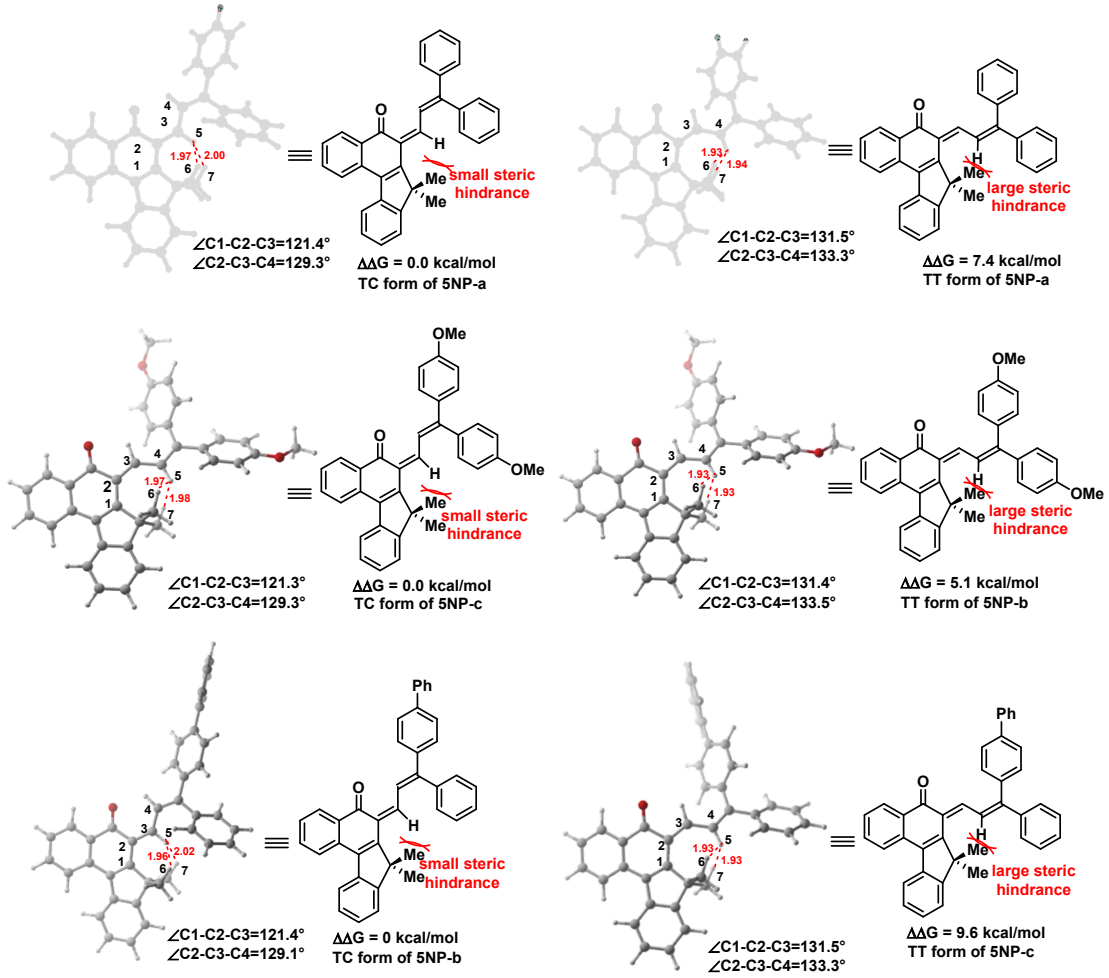

Fig. S122. Calculated TC and TT form structures of **5NP-a, 5NP-b and 5NP-c** at the (SMD)m06-2x/6-311++g(d,p)//m06-2x/6-31+g(d,p) level of theory. All energies are in kcal/mol, and bond lengths are in Å.

7.6 Calculated Cartesian Coordinates and Thermodynamic Energy

NP-a-CF

C,0,2.4030973849,2.917111605,0.754580483
C,0,1.872038136,0.7013250748,-0.1043310485
C,0,0.4952110625,1.0714794014,-0.1261140731
C,0,1.0377561654,3.282739823,0.700613487
C,0,2.2561648635,-0.6195312371,-0.5185069293
C,0,-0.4652117527,0.1079861216,-0.535748695
C,0,-0.0938327736,-1.166801882,-0.9128425459
C,0,1.2803206069,-1.5114994909,-0.8973816411
C,0,-1.1464579117,-2.0572673969,-1.3926017858
C,0,-2.4278817774,-1.7469342258,-1.1686444647
H,0,3.1369717957,3.6312980539,1.1148643028
H,0,0.7319803886,4.2770773,1.0100047624
H,0,-3.2491950029,-2.3630479475,-1.5210371594

O,0,-1.7632391748,0.511498339,-0.6146218844
H,0,-0.8675937063,-2.951097424,-1.9445873805
C,0,-2.7667970355,-0.4962224591,-0.3779096293
C,0,-4.0775936072,0.0898700322,-0.899344716
C,0,-5.2969917453,-0.3909102267,-0.4153002928
C,0,-4.0744325189,1.0496464142,-1.9127471246
C,0,-6.4983997537,0.0823843867,-0.9379240609
H,0,-5.3072993326,-1.1288708914,0.3826378258
C,0,-5.2782447341,1.5297067334,-2.4272790691
H,0,-3.1280734628,1.4200749048,-2.2906774524
C,0,-6.4925985997,1.0471249489,-1.9442894692
H,0,-7.4390780952,-0.2970456541,-0.5511781031
H,0,-5.264344665,2.2818578634,-3.2100373625
H,0,-7.4285206483,1.4214505593,-2.3469903999
C,0,-2.8291808796,-0.7396756319,1.1355764295
C,0,-3.0159254695,0.3698725946,1.9681724421
C,0,-2.7096996728,-2.0048256612,1.7050557578
C,0,-3.0803258791,0.2147357856,3.3474711969
H,0,-3.1102934099,1.3562266046,1.5211140501
C,0,-2.7835240847,-2.1636490364,3.0915910616
H,0,-2.5511522805,-2.8708043897,1.0702440315
C,0,-2.9671116344,-1.0573357725,3.9139281254
H,0,-3.2208233414,1.0833924332,3.9831662285
H,0,-2.6895249993,-3.1548578508,3.52424029
H,0,-3.0198180406,-1.1804497327,4.991144398
C,0,3.6822985216,-1.0420738171,-0.563350154
C,0,4.1068907627,-2.1731401672,0.1428974898
C,0,5.4313222533,-2.6024268187,0.0711127244
C,0,5.9386852956,-0.7779038624,-1.4193397563
C,0,6.3514510311,-1.9051478252,-0.7086500079
H,0,5.7443671451,-3.4792123428,0.6296438698
H,0,7.3832213705,-2.237587254,-0.7643883684
C,0,0.1005839863,2.3739858319,0.2761513116
H,0,-0.9538062951,2.6261992111,0.246979487
H,0,1.5696992477,-2.5064500977,-1.2285202529
H,0,3.3916493364,-2.7085661216,0.7612677441
H,0,6.6472067775,-0.234157816,-2.0366633109
C,0,4.6156910541,-0.3505008603,-1.3471242337
H,0,4.292158226,0.5190244535,-1.9132265122
C,0,2.8078682187,1.6620788023,0.3668460939
H,0,3.8555457445,1.3890001853,0.4316749907

Zero-point correction= 0.438287 (Hartree/Particle)
Thermal correction to Energy= 0.462276
Thermal correction to Enthalpy= 0.463220

Thermal correction to Gibbs Free Energy= 0.382150
Sum of electronic and zero-point Energies= -1268.875894
Sum of electronic and thermal Energies= -1268.851905
Sum of electronic and thermal Enthalpies= -1268.850961
Sum of electronic and thermal Free Energies= -1268.932030

5NP-a-CF

C,0,1.6202620372,4.1653971444,-0.1711470015
C,0,1.6427653051,1.7342071307,-0.3371352008
C,0,0.2202877097,1.7634614609,-0.4427765018
C,0,0.209688176,4.1786978524,-0.2470947885
C,0,2.296448055,0.4624789083,-0.3711318019
C,0,-0.4870477118,0.541491024,-0.6082926857
C,0,0.1547690405,-0.6815485691,-0.7123293615
C,0,1.5675585888,-0.6984452614,-0.583656508
C,0,-0.6978162791,-1.8418699274,-0.9822223973
C,0,-2.0163405052,-1.7616223385,-0.771543985
H,0,2.1633275491,5.1011169536,-0.0804731897
H,0,-0.3270088714,5.1209640608,-0.2028788274
H,0,-2.6902499437,-2.5871060023,-0.9785751072
O,0,-1.8399678519,0.6326622148,-0.7390211518
H,0,-0.26364416,-2.753020196,-1.3771035619
C,0,-2.601143132,-0.4762958161,-0.2226264174
C,0,-4.0203370467,-0.2967838576,-0.7547928563
C,0,-5.0916401724,-0.9048476069,-0.0951237302
C,0,-4.254556019,0.4021462416,-1.9399768021
C,0,-6.3811960213,-0.8148194461,-0.6135643866
H,0,-4.9178550325,-1.4400068013,0.8349284441
C,0,-5.5478326151,0.4995809514,-2.4519500765
H,0,-3.4225553007,0.8704699269,-2.4542103149
C,0,-6.6138778566,-0.1091128391,-1.7930659119
H,0,-7.2053203274,-1.2892959063,-0.0898622017
H,0,-5.7206908244,1.0515557459,-3.3708220256
H,0,-7.6196595657,-0.0319208657,-2.1941546857
C,0,-2.561779352,-0.3958679182,1.3087673591
C,0,-2.9932142665,0.7914490237,1.9109856273
C,0,-2.1085019422,-1.4396185409,2.1115672663
C,0,-2.9711399353,0.9310024593,3.2932822913
H,0,-3.3460758034,1.6055449113,1.282619473
C,0,-2.0939212036,-1.3040831407,3.5022847256
H,0,-1.7571456558,-2.360080922,1.6557364116
C,0,-2.5229237292,-0.1214743028,4.0948566513
H,0,-3.3048910006,1.8587235026,3.7477730913
H,0,-1.7394413846,-2.1249005137,4.1181733827

H,0,-2.5073567609,-0.0148931659,5.1750660895
C,0,3.7195167726,0.095999015,-0.1908149644
C,0,3.8226279812,-1.2994147962,-0.3306009295
C,0,4.8710413903,0.8324842907,0.1043295499
C,0,5.0387033109,-1.9537339228,-0.2076236287
C,0,6.0942559971,0.1720050263,0.2319552679
H,0,4.8485554197,1.9032938551,0.2555104838
C,0,6.1863787163,-1.209509357,0.0736965467
H,0,5.101693731,-3.033720459,-0.3209076429
H,0,7.1461753343,-1.7056454872,0.1773283638
C,0,-0.4765590508,2.9973990405,-0.38268138
H,0,-1.5588700396,2.9822585311,-0.4494736943
C,0,2.3140722766,2.9785499688,-0.2122639297
H,0,3.3934397286,3.0033118766,-0.1704794154
C,0,2.4704469275,-1.9232846726,-0.6134413877
C,0,2.5027314716,-2.5979027894,-1.9981340887
H,0,3.2648050999,-3.3839565643,-2.0074644687
H,0,1.5460867369,-3.0591610792,-2.2549712919
H,0,2.7528731594,-1.8678740051,-2.7731245598
C,0,2.1026672693,-2.9331806901,0.4866516738
H,0,2.114176394,-2.4497319426,1.4678760802
H,0,1.1068227794,-3.3553708627,0.3238676902
H,0,2.8231631019,-3.7575795338,0.4987233832
H,0,6.9852176315,0.7475832032,0.463400188
Zero-point correction= 0.500998 (Hartree/Particle)
Thermal correction to Energy= 0.528206
Thermal correction to Enthalpy= 0.529150
Thermal correction to Gibbs Free Energy= 0.442468
Sum of electronic and zero-point Energies= -1385.511318
Sum of electronic and thermal Energies= -1385.484110
Sum of electronic and thermal Enthalpies= -1385.483166
Sum of electronic and thermal Free Energies= -1385.569848

6NP-a-CF

C,0,2.2103358854,2.8456311076,0.5961686808
C,0,1.639701847,0.6329834956,-0.1870995369
C,0,0.266925975,1.0276233696,-0.1885128328
C,0,0.8543756814,3.2275695546,0.5935667768
C,0,1.9991615398,-0.6962101632,-0.5911572343
C,0,-0.7153855261,0.0848024401,-0.5893520006
C,0,-0.3663473086,-1.1890260994,-0.9848318271
C,0,0.9976649768,-1.5594401925,-0.9789422504
C,0,-1.4395804303,-2.0666120609,-1.4435040731
C,0,-2.7113932958,-1.7449856724,-1.1845230856

H,0,2.9479927181,3.5784851158,0.9099441097
H,0,0.5802970141,4.2315210866,0.9020688762
H,0,-3.5475987811,-2.3538293413,-1.5141117141
O,0,-2.0091940247,0.5057619814,-0.6430776797
H,0,-1.1841551415,-2.9621952316,-2.0041729252
C,0,-3.019692884,-0.4909304305,-0.3870882534
C,0,-4.3337791582,0.1085056934,-0.8834876205
C,0,-5.5476913641,-0.3764108217,-0.3892495753
C,0,-4.3420597591,1.0847186431,-1.8803347536
C,0,-6.7549940054,0.1091735577,-0.8858203742
H,0,-5.5477879471,-1.1268185475,0.3976384519
C,0,-5.5520143233,1.5771076185,-2.3687838986
H,0,-3.4001345519,1.4582943399,-2.2663119803
C,0,-6.7606890472,1.0905148796,-1.8759573336
H,0,-7.6912444421,-0.2735269793,-0.4913659319
H,0,-5.5470970664,2.3423962696,-3.1391710067
H,0,-7.701139612,1.4746622607,-2.2586005288
C,0,-3.0529146074,-0.7294301279,1.1280326605
C,0,-3.260775017,0.3801823593,1.9552979614
C,0,-2.8717372452,-1.9837873746,1.7048924774
C,0,-3.2856798696,0.2363672261,3.33670006
H,0,-3.4024515348,1.3580701765,1.5017136182
C,0,-2.9049925392,-2.1315270662,3.094184544
H,0,-2.6943307302,-2.8488257658,1.0735818692
C,0,-3.1101901391,-1.0252375066,3.9109969712
H,0,-3.4444030187,1.1050846007,3.9683092129
H,0,-2.7623693881,-3.1140766605,3.5334360055
H,0,-3.1317798177,-1.1402844196,4.990265624
C,0,3.4255182339,-1.0953349799,-0.5823191418
C,0,3.8176556912,-2.3898333617,-0.9694044566
C,0,4.4176788676,-0.1843164211,-0.1850516015
C,0,5.1457399023,-2.7832306477,-0.9704865802
C,0,5.7571995577,-0.5995358687,-0.191235683
C,0,6.1307983657,-1.8783279895,-0.5771967053
H,0,5.4112191405,-3.7906152698,-1.2752240207
H,0,7.1772896942,-2.1663260237,-0.5701617523
C,0,-0.110610924,2.3315223782,0.2090277443
H,0,-1.1623141303,2.5946280833,0.2045474837
C,0,2.6207971106,1.5795267478,0.2207692843
C,0,4.1103009026,1.2444122636,0.2600824969
H,0,1.2280296645,-2.5687072416,-1.3021303608
H,0,3.0725447167,-3.1132868129,-1.2780520271
C,0,4.8581139338,2.2225397821,-0.6738445698
H,0,5.9362792496,2.0432209426,-0.649397467

H,0,4.5123512299,2.1032569618,-1.7047395772
H,0,4.6835829473,3.2584297636,-0.3706498998
C,0,4.6133916112,1.4241663465,1.7104970604
H,0,4.0852203315,0.742293027,2.3833486768
H,0,5.6846970456,1.2180128713,1.7827045178
H,0,4.4438208822,2.4476569883,2.0559375678
H,0,6.5322661739,0.0964712956,0.1156075881
Zero-point correction= 0.501747 (Hartree/Particle)
Thermal correction to Energy= 0.528661
Thermal correction to Enthalpy= 0.529605
Thermal correction to Gibbs Free Energy= 0.442763
Sum of electronic and zero-point Energies= -1385.514499
Sum of electronic and thermal Energies= -1385.487585
Sum of electronic and thermal Enthalpies= -1385.486641
Sum of electronic and thermal Free Energies= -1385.573483

5/6NP-a-CF
C,0,-1.9861915944,-3.4173025651,-0.2116688312
C,0,-1.4526586302,-1.1043594707,-0.3525544433
C,0,-0.069927434,-1.3753385494,-0.4808307548
C,0,-0.6055078885,-3.7158513162,-0.3460090413
C,0,-1.842512901,0.23709562,-0.3533907599
C,0,0.8073410339,-0.2510753875,-0.5959020424
C,0,0.3743551642,1.0774902779,-0.6111139451
C,0,-1.0202260708,1.3229880057,-0.4778747695
C,0,1.3996241539,2.098804195,-0.8192220134
C,0,2.692124104,1.7930706294,-0.6593973481
H,0,-2.682105891,-4.2458683521,-0.1081869986
H,0,-0.2969300082,-4.7569238373,-0.3406012913
H,0,3.4866053473,2.5148204508,-0.8216575292
O,0,2.129072544,-0.5453246613,-0.7707612972
H,0,1.0988954718,3.0964169418,-1.1244914323
C,0,3.0741267863,0.3924083321,-0.2225960018
C,0,4.4274534027,0.0262099853,-0.8280747787
C,0,5.6056795447,0.4194829159,-0.1883712156
C,0,4.5024630586,-0.6312560923,-2.056722124
C,0,6.8440079023,0.1595981748,-0.7708454172
H,0,5.5540740221,0.9198405395,0.7754112276
C,0,5.7433807732,-0.8995499156,-2.6332110235
H,0,3.5871925205,-0.9333605458,-2.5534177964
C,0,6.9164785251,-0.5035222312,-1.9949999485
H,0,7.7524826012,0.4679376682,-0.2625689817
H,0,5.7909732088,-1.4179751644,-3.5860505844
H,0,7.8816124792,-0.7108289204,-2.4467731307

C,0,3.0800275289,0.2173209063,1.3016190527
C,0,3.3112196913,-1.065400824,1.8111448888
C,0,2.8679012944,1.2723845643,2.1856148461
C,0,3.328935496,-1.2873434631,3.1827644895
H,0,3.4772790418,-1.8863379184,1.1179066652
C,0,2.8933461763,1.0523776116,3.5652007915
H,0,2.6750075477,2.2692863275,1.8014063618
C,0,3.1226818945,-0.2246426753,4.0656271685
H,0,3.5047042231,-2.2874880795,3.5668920299
H,0,2.7263661199,1.882225976,4.2451326986
H,0,3.1387451952,-0.396344333,5.137442099
C,0,-3.2062308966,0.6242399185,-0.1898849487
C,0,-3.2893828895,2.0154932534,-0.1988442994
C,0,-4.2503639814,-0.2685936599,-0.0397241244
C,0,-4.5459471852,2.5831528019,-0.0468433785
C,0,-5.5117293405,0.3234793767,0.112651689
C,0,-5.6446446562,1.7182319277,0.1084608266
H,0,-4.6998855342,3.6595160268,-0.0429862852
H,0,-6.6350198429,2.1464929893,0.2304937863
C,0,0.3464910652,-2.7285731317,-0.4748676328
H,0,1.3999593106,-2.9694339723,-0.5692083526
C,0,-2.4439252543,-2.1140819635,-0.2065997527
C,0,-1.8778767514,2.6028489726,-0.3969454643
C,0,-1.8314834665,3.4228439533,-1.6965417482
H,0,-2.54496613,4.2517295879,-1.6404693627
H,0,-0.83709609,3.8473104668,-1.8642766866
H,0,-2.0931671235,2.8002827981,-2.556540579
C,0,-1.4689572142,3.4683393147,0.8046218895
H,0,-1.5211402069,2.890765037,1.7317954342
H,0,-0.4447608993,3.837487748,0.684887879
H,0,-2.1358239615,4.3324679429,0.89443615
C,0,-3.9535880411,-1.7790219524,-0.0555901623
C,0,-4.7158105914,-2.4107362985,-1.2387297958
H,0,-5.7882985033,-2.2089908515,-1.1525824317
H,0,-4.362086607,-1.9991724932,-2.1883068257
H,0,-4.5727691707,-3.4956169134,-1.2573344497
C,0,-4.4640611657,-2.3900119105,1.2650320848
H,0,-3.9357816394,-1.9567812737,2.1190228744
H,0,-5.5345017543,-2.1970581797,1.3867373073
H,0,-4.3118382658,-3.4734148283,1.2775408854
H,0,-6.4042922379,-0.2856242666,0.2361574648
Zero-point correction= 0.563645 (Hartree/Particle)
Thermal correction to Energy= 0.592885
Thermal correction to Enthalpy= 0.593829

Thermal correction to Gibbs Free Energy= 0.504759
Sum of electronic and zero-point Energies= -1502.144012
Sum of electronic and thermal Energies= -1502.114772
Sum of electronic and thermal Enthalpies= -1502.113828
Sum of electronic and thermal Free Energies= -1502.202898

5NP-b-CF

C,0,-2.3763484845,-0.1755776332,4.2555556947
C,0,-2.4566266458,-0.4668933802,1.8372160551
C,0,-1.0329757123,-0.5580435299,1.8353741935
C,0,-0.9655821236,-0.2461944632,4.2381130625
C,0,-3.1420902063,-0.5820708673,0.5874123992
C,0,-0.3535980544,-0.778021675,0.6051637605
C,0,-1.0268650835,-0.9709602282,-0.5901858499
C,0,-2.4414103265,-0.8623264932,-0.5766605115
C,0,-0.2013904684,-1.3195606707,-1.7492438242
C,0,1.1177588569,-1.1009917401,-1.7180582613
H,0,-2.8970622318,-0.0418314818,5.1987932885
H,0,-0.4067556717,-0.1591505112,5.164490246
H,0,1.771677483,-1.3805579219,-2.5381763018
O,0,1.0029069883,-0.8733893628,0.6695309368
H,0,-0.6559768619,-1.7884572231,-2.6141729057
C,0,1.7309434468,-0.4369745053,-0.49949443
C,0,3.1541281293,-0.9439183098,-0.2874022108
C,0,4.2730790323,-0.1651066778,-0.5555036227
C,0,3.3455469423,-2.268276697,0.1349666955
C,0,5.566707269,-0.6787779174,-0.4099861115
H,0,4.1531467991,0.8641493857,-0.8797988725
C,0,4.6181880598,-2.7888169917,0.2899983911
H,0,2.4794694872,-2.8857256053,0.3533572562
C,0,5.7395633143,-1.993990289,0.0165908077
H,0,6.4150291716,-0.0406396704,-0.6265848771
H,0,4.7763111868,-3.8088657238,0.6244053839
C,0,1.657389021,1.0884142734,-0.5738400825
C,0,1.7554022921,1.8331577267,0.5992174778
C,0,1.5408865123,1.7708583715,-1.7879582267
C,0,1.7347027084,3.2272808197,0.5796822514
H,0,1.8421257823,1.3150100835,1.5502550719
C,0,1.5302940809,3.1586013131,-1.8282635055
H,0,1.4510856172,1.2139601725,-2.7160651287
C,0,1.6242474303,3.894410986,-0.6432120168
H,0,1.8007776755,3.7722332094,1.5137467758
H,0,1.4394796126,3.6963123851,-2.766217422
C,0,-4.5763752649,-0.4415119239,0.2495992418

C,0,-4.7160532639,-0.6791835791,-1.1291973698
C,0,-5.7103931329,-0.1067065599,0.9961784358
C,0,-5.9515957818,-0.6169537036,-1.7549768963
C,0,-6.9532447606,-0.0399737505,0.3641986354
H,0,-5.6593547028,0.1221158797,2.0522370021
C,0,-7.0818071543,-0.2973290048,-0.9994670141
H,0,-6.0429791853,-0.8064347179,-2.8221671788
H,0,-8.0563854091,-0.2396298301,-1.473925338
C,0,-0.3073679526,-0.4368192981,3.0482508971
H,0,0.7741487119,-0.512176383,3.0130538312
C,0,-3.0983162043,-0.2820486426,3.0898024189
H,0,-4.1771804656,-0.2487204904,3.1388938368
C,0,-3.3776729968,-0.9882015487,-1.7703357334
C,0,-3.4086094519,-2.4179691867,-2.3435638664
H,0,-4.1938043755,-2.4942516772,-3.1026450987
H,0,-2.4624110744,-2.6933676458,-2.8154687314
H,0,-3.6238943678,-3.1425515205,-1.5531716535
C,0,-3.0546584925,0.0410077246,-2.8664018979
H,0,-3.0666587299,1.0541891498,-2.4545562109
H,0,-2.0689630372,-0.1385811354,-3.3048598358
H,0,-3.7990578803,-0.0163217311,-3.6673383408
O,0,1.5953411596,5.2469654086,-0.7796318498
O,0,6.9470351481,-2.5920824507,0.1989897333
C,0,1.6980010794,6.0287699885,0.3926467951
H,0,1.6609115556,7.0674491809,0.0661438271
H,0,0.8633262544,5.8303517923,1.0753041462
H,0,2.6463141407,5.8425685022,0.9110333383
C,0,8.1046235892,-1.8181586932,-0.0364147161
H,0,8.137551975,-0.9444172579,0.6254173953
H,0,8.9515043927,-2.4689342716,0.1786613025
H,0,8.1547867897,-1.4866855455,-1.0805315826
H,0,-7.8305851402,0.2222967639,0.9474258906
Zero-point correction= 0.566996 (Hartree/Particle)
Thermal correction to Energy= 0.599197
Thermal correction to Enthalpy= 0.600142
Thermal correction to Gibbs Free Energy= 0.502433
Sum of electronic and zero-point Energies= -1614.411271
Sum of electronic and thermal Energies= -1614.379069
Sum of electronic and thermal Enthalpies= -1614.378125
Sum of electronic and thermal Free Energies= -1614.475834

5NP-c-CF

C,0,-2.1992534036,-0.1109452233,4.1707738146
C,0,-2.3267708686,-0.4137921908,1.756076095

C,0,-1.03526054,-1.0179064163,1.7991680449
C,0,-0.9088569955,-0.6851291588,4.1960643109
C,0,-2.9732726452,-0.2901934187,0.4860330059
C,0,-0.4562067129,-1.5010062244,0.5939714346
C,0,-1.1119304831,-1.436952498,-0.6243556346
C,0,-2.3857827482,-0.8129735259,-0.6567983905
C,0,-0.4292616001,-2.0564117911,-1.7629092774
C,0,0.8771424666,-2.3332814147,-1.6862082238
H,0,-2.6558809909,0.2289122613,5.0952665407
H,0,-0.3739612156,-0.7754332613,5.1360579158
H,0,1.4193346258,-2.8082083668,-2.4977835412
O,0,0.7585511713,-2.1065001994,0.7024128954
H,0,-0.9877624005,-2.3109428933,-2.6560556173
C,0,1.6399044378,-1.9749011825,-0.4282535891
C,0,2.7673847253,-2.9795570736,-0.2089654204
C,0,3.924046456,-2.8833337464,-0.9885986701
C,0,2.6495724762,-4.0172712496,0.7147709665
C,0,4.9489595135,-3.8139872743,-0.8474021416
H,0,4.0280628294,-2.066478407,-1.6992368979
C,0,3.6830842516,-4.9434339399,0.8623777642
H,0,1.7514358059,-4.0965979967,1.3165977246
C,0,4.832283927,-4.8471925362,0.0826161908
H,0,5.8430728179,-3.7268138296,-1.4568218678
H,0,3.5847450285,-5.7433634509,1.5898521165
H,0,5.6342509979,-5.5693745293,0.199092135
C,0,2.1774007022,-0.5382481456,-0.4293849931
C,0,2.9037515801,-0.109162674,0.6872217195
C,0,1.9480599738,0.3617736381,-1.4668361159
C,0,3.3927520276,1.1870164547,0.7597063091
H,0,3.0937686766,-0.8086748424,1.4977624142
C,0,2.4443419322,1.6641670713,-1.3965091614
H,0,1.3657323856,0.0550619808,-2.3303082229
C,0,3.1730037002,2.0967543557,-0.2860904095
H,0,3.976205464,1.4952527298,1.6226660305
H,0,2.2338593807,2.3611191042,-2.2028342846
C,0,-4.2469785671,0.3601645889,0.1030050021
C,0,-4.4127000416,0.1926304068,-1.2831720331
C,0,-5.2122883084,1.0771125025,0.8167582285
C,0,-5.517092632,0.7014254505,-1.949209051
C,0,-6.322324759,1.5919165018,0.1446017443
H,0,-5.1256069186,1.263486221,1.8786888486
C,0,-6.4826185381,1.4061428265,-1.2272869604
H,0,-5.6303012939,0.5609791983,-3.0217886185
H,0,-7.3516991628,1.8135714078,-1.7340175217

C,0,-0.3390483223,-1.1320659626,3.02965992
H,0,0.6480752274,-1.5812486865,3.023875641
C,0,-2.8847574949,0.0226555725,2.9859926546
H,0,-3.8755961319,0.4527111953,3.0025461808
C,0,-3.2566537165,-0.5819445479,-1.8841450738
C,0,-3.7852833672,-1.8956682539,-2.4905624806
H,0,-4.5121895713,-1.6727156781,-3.2784252224
H,0,-2.9870063913,-2.4948354113,-2.9350840011
H,0,-4.2830185534,-2.4969579314,-1.7246368714
C,0,-2.5340895395,0.2659236619,-2.9448700105
H,0,-2.1774703695,1.2028427259,-2.5071034316
H,0,-1.6754484919,-0.2674090583,-3.3633393171
H,0,-3.2176090982,0.5059839723,-3.7658411607
C,0,3.7029980583,3.4814514823,-0.2101780145
C,0,4.2545615541,4.0993733645,-1.3395262479
C,0,3.66556781,4.1967384199,0.993435382
C,0,4.7556405619,5.3964772998,-1.2680315029
H,0,4.3128427424,3.5475647415,-2.273677562
C,0,4.1674881604,5.493363239,1.0661760957
H,0,3.2177018581,3.740248845,1.8717640662
C,0,4.714742596,6.0981248873,-0.0643145732
H,0,5.186830266,5.8565414068,-2.1518933585
H,0,4.1233323959,6.0356852374,2.0057487482
H,0,5.1056170985,7.109194295,-0.0073121912
H,0,-7.0677436792,2.1488020147,0.7039723625
Zero-point correction= 0.582655 (Hartree/Particle)
Thermal correction to Energy= 0.614567
Thermal correction to Enthalpy= 0.615511
Thermal correction to Gibbs Free Energy= 0.516789
Sum of electronic and zero-point Energies= -1616.402603
Sum of electronic and thermal Energies= -1616.370691
Sum of electronic and thermal Enthalpies= -1616.369747
Sum of electronic and thermal Free Energies= -1616.468468

NP-a -TC

C,0,4.4861783627,-2.9000608064,0.2793724026
C,0,2.8258238664,-1.1312298756,0.1395314183
C,0,1.8204322937,-2.1000627311,0.3442728799
C,0,3.4851742622,-3.8481571631,0.5074095827
C,0,2.4503950994,0.2772244635,-0.0561057108
C,0,0.3750360069,-1.7383500559,0.3414868441
C,0,0.0459198743,-0.3180120598,0.0455145831
C,0,1.1426643019,0.6195203384,-0.1121694637
C,0,-1.2362149736,0.1467152344,-0.0716470965

C,0,-2.4637259004,-0.6025544239,-0.0215180395
H,0,5.5266522809,-3.2078670436,0.2392687709
H,0,3.7424492242,-4.8922832963,0.6525408895
H,0,-2.3836888103,-1.682208425,0.0059301244
O,0,-0.4798968546,-2.5878635942,0.5649762016
H,0,-1.3348407054,1.2134698075,-0.2719644774
C,0,-3.7003676329,-0.0294454394,-0.0375798916
C,0,-4.9103970017,-0.8744069774,-0.1728473737
C,0,-6.1135872438,-0.5043994355,0.4482030282
C,0,-4.8790974264,-2.0650868716,-0.9152697973
C,0,-7.2423292728,-1.3124229915,0.3500453813
H,0,-6.1554778992,0.4149334795,1.0248117998
C,0,-6.0100331922,-2.8684126487,-1.0182567795
H,0,-3.9672467153,-2.3485916927,-1.4316066915
C,0,-7.1950372032,-2.4971023145,-0.3834150213
H,0,-8.1601427215,-1.0167004361,0.8484684454
H,0,-5.9684762663,-3.7818843583,-1.6030519077
H,0,-8.0773340147,-3.1240258921,-0.4651234909
C,0,-3.9042715641,1.4352636763,0.1020589196
C,0,-4.7306011214,2.1230870573,-0.7987420686
C,0,-3.2962939101,2.1519562284,1.1411836893
C,0,-4.9161951833,3.49683882,-0.6817303293
H,0,-5.2191776446,1.5716482659,-1.5973753739
C,0,-3.4935247595,3.5259362607,1.2663243698
H,0,-2.6830860513,1.6191684553,1.8626835723
C,0,-4.298515382,4.2022312455,0.3521167658
H,0,-5.5466811886,4.0181111396,-1.3951706182
H,0,-3.021872847,4.0653679092,2.0816380809
H,0,-4.4510238875,5.2726243858,0.4478243556
C,0,3.4899374914,1.3316175172,-0.1960470172
C,0,3.4966963049,2.1714662683,-1.3153264176
C,0,4.4359555807,3.1950217462,-1.4323957301
C,0,5.3863140143,2.5607859009,0.6897792561
C,0,5.3838674948,3.3920540452,-0.430944005
H,0,4.4291952938,3.8343602026,-2.3097838585
H,0,6.1167479016,4.1875658156,-0.5213548521
C,0,2.157845351,-3.4436631013,0.5332025852
H,0,1.3512368493,-4.1520103759,0.6923939593
H,0,0.8795085317,1.6652884055,-0.2598435425
H,0,2.765251889,2.0082188011,-2.1018769346
H,0,6.1164844893,2.7131030916,1.478652988
C,0,4.4489963315,1.5382533868,0.8052584379
H,0,4.444822449,0.9005764187,1.6853914982
C,0,4.1625017072,-1.5613066535,0.096813423

H,0,4.9507456813,-0.8409008232,-0.0928167442
Zero-point correction= 0.437192 (Hartree/Particle)
Thermal correction to Energy= 0.462132
Thermal correction to Enthalpy= 0.463076
Thermal correction to Gibbs Free Energy= 0.379356
Sum of electronic and zero-point Energies= -1268.859807
Sum of electronic and thermal Energies= -1268.834868
Sum of electronic and thermal Enthalpies= -1268.833923
Sum of electronic and thermal Free Energies= -1268.917643

5NP-a- TC

C,0,-4.35643006,3.918968479,0.7532647621
C,0,-3.0000312299,1.9666272547,0.24802938
C,0,-1.8712354032,2.808407107,0.1933949125
C,0,-3.2383446586,4.7490521425,0.6535097616
C,0,-2.8096123339,0.533944009,0.021443345
C,0,-0.5024258348,2.2610824443,-0.0220057608
C,0,-0.3442379472,0.7739989124,-0.0219367389
C,0,-1.561972642,-0.0232051044,-0.0476460661
C,0,0.8939593607,0.1866667491,-0.0216076964
C,0,2.1955472593,0.8024475697,-0.0662280312
H,0,-5.327229073,4.3416905916,0.9942464728
H,0,-3.3346426867,5.8194014799,0.8038956083
H,0,2.2439687749,1.875998808,-0.1861865542
O,0,0.444215468,3.0254567293,-0.1628782377
H,0,0.9097510037,-0.8957058298,-0.007268838
C,0,3.3543312219,0.0863875913,-0.0062762918
C,0,4.6605335092,0.7514637425,-0.2220649625
C,0,5.817479415,0.2725531213,0.4121214579
C,0,4.7714118929,1.8763220118,-1.0549344205
C,0,7.0403793117,0.9140230063,0.2404351228
H,0,5.7516410337,-0.5993819347,1.0561579526
C,0,5.9953649237,2.5129221037,-1.2297433696
H,0,3.895783524,2.238621532,-1.5846980602
C,0,7.1341604844,2.0368261473,-0.580259007
H,0,7.9216866453,0.5366205383,0.7497825849
H,0,6.0615075448,3.3777887432,-1.882348559
H,0,8.0896415245,2.5330518527,-0.7186890924
C,0,3.3761628574,-1.3724519467,0.2852969076
C,0,4.0218303278,-2.2577848451,-0.5886464854
C,0,2.7698014318,-1.8849134393,1.438663264
C,0,4.0310258765,-3.6252514229,-0.3311079074
H,0,4.5087353244,-1.8643835549,-1.4770066691
C,0,2.7905840675,-3.2532914789,1.7037411522

H,0,2.29152804,-1.1987957093,2.1334576267
C,0,3.4150647975,-4.1269190361,0.8162222816
H,0,4.5225379185,-4.3009318422,-1.0242271059
H,0,2.3203833268,-3.634503403,2.6051874643
H,0,3.4288914721,-5.1930418393,1.0198427408
C,0,-3.8275581091,-0.5205649736,-0.151601996
C,0,-3.1496914919,-1.7461155252,-0.2576839434
C,0,-5.22095947,-0.4993027234,-0.2757472645
C,0,-3.8341363076,-2.9395821727,-0.4282602949
C,0,-5.90814438,-1.7006336406,-0.4544647427
H,0,-5.7857767918,0.4236823647,-0.2694360436
C,0,-5.2274891569,-2.9160023449,-0.5185152145
H,0,-3.2972495919,-3.8825001735,-0.5018383707
H,0,-5.7790665301,-3.8408717244,-0.6543542663
C,0,-1.9984567265,4.1867885077,0.3823545994
H,0,-1.1005254922,4.7932702591,0.3236264632
C,0,-4.239728209,2.5480314566,0.5548975654
H,0,-5.1156694269,1.9261193371,0.6744001638
C,0,-1.6498760503,-1.5437312499,-0.1867719208
C,0,-1.104713293,-2.2822581994,1.0525106296
H,0,-1.3390260476,-3.3490055226,0.9746319205
H,0,-0.0205323894,-2.1897109823,1.151928531
H,0,-1.5724591983,-1.8937795378,1.9619959822
C,0,-1.0071227118,-2.0743457503,-1.48212971
H,0,-1.410262494,-1.5461749772,-2.3510684943
H,0,0.0798105052,-1.9605744464,-1.4834232515
H,0,-1.2302276776,-3.1399196109,-1.5950723479
H,0,-6.9893102481,-1.6838202605,-0.5516719376
Zero-point correction= 0.500287 (Hartree/Particle)
Thermal correction to Energy= 0.528397
Thermal correction to Enthalpy= 0.529341
Thermal correction to Gibbs Free Energy= 0.439646
Sum of electronic and zero-point Energies= -1385.494317
Sum of electronic and thermal Energies= -1385.466207
Sum of electronic and thermal Enthalpies= -1385.465262
Sum of electronic and thermal Free Energies= -1385.554958

6NP-a -TC

C,0,4.1724495712,-2.9775348196,0.2929050649
C,0,2.5548743972,-1.1945631635,0.1540094096
C,0,1.5330618546,-2.1627109275,0.2929399965
C,0,3.1638018329,-3.9257171955,0.4340398355
C,0,2.1995559939,0.2215291951,0.0025648112
C,0,0.0910393857,-1.7889357276,0.2898140761

C,0,-0.2169061891,-0.3535449388,0.0702618285
C,0,0.8900923827,0.5705884494,-0.0470938831
C,0,-1.492599403,0.136238081,-0.0337887953
C,0,-2.7333729273,-0.5892452412,0.0009908728
H,0,5.2043358191,-3.3164661291,0.2897913646
H,0,3.4159214529,-4.9759575517,0.539966971
H,0,-2.6737218896,-1.6701260432,0.0286112727
O,0,-0.7739802131,-2.6416560496,0.4535391591
H,0,-1.5716222237,1.2105202925,-0.1990949645
C,0,-3.9588561268,0.0086664451,-0.0224536863
C,0,-5.1876718227,-0.8100358173,-0.1478625739
C,0,-6.3854872767,-0.3922575388,0.4528780687
C,0,-5.1820546073,-2.0228001937,-0.8548636572
C,0,-7.5339486636,-1.1732893455,0.369953594
H,0,-6.4082061159,0.5437350146,1.003118762
C,0,-6.332468276,-2.7996145252,-0.9420295228
H,0,-4.2749537748,-2.3457078971,-1.3564806764
C,0,-7.5119428745,-2.380283378,-0.3271503307
H,0,-8.4470947466,-0.8392015104,0.8527750425
H,0,-6.3104401653,-3.7307688149,-1.4995184923
H,0,-8.4093120455,-2.987270221,-0.3955214807
C,0,-4.1329473461,1.4797751771,0.0995512913
C,0,-4.9177122583,2.1766821566,-0.8301025687
C,0,-3.5389903154,2.1925970661,1.1489887481
C,0,-5.0767722339,3.5551667837,-0.7304505344
H,0,-5.3964069917,1.6286272775,-1.6371942012
C,0,-3.7095930387,3.571553546,1.2566104983
H,0,-2.9572694132,1.6529156781,1.8913894371
C,0,-4.4733915788,4.2567563348,0.3141457008
H,0,-5.6750729746,4.0832142849,-1.4664426788
H,0,-3.248760339,4.1078116365,2.0804169321
H,0,-4.6052402336,5.3311491626,0.3962513709
C,0,3.2898468696,1.2163217391,-0.1041243354
C,0,3.0050049753,2.5929638229,-0.1900385139
C,0,4.6339082788,0.8084097258,-0.1197129447
C,0,4.0049521853,3.5421384519,-0.3088514069
C,0,5.6346458022,1.7844497895,-0.246114138
C,0,5.3389678527,3.1349660634,-0.3437637988
H,0,3.7468797024,4.5945067337,-0.3722910338
H,0,6.1379883343,3.8630304852,-0.4410007093
C,0,1.8388599253,-3.5143290413,0.4362050236
H,0,1.0200344587,-4.2176546991,0.5444513181
C,0,3.8969126358,-1.6134201948,0.1550055538
C,0,5.069962623,-0.6491610366,0.0033613449

H,0,0.6064925081,1.6081472165,-0.1880593842
H,0,1.9785388009,2.9378617599,-0.1578243235
C,0,5.9798462194,-0.7836950393,1.2463511085
H,0,6.8563330313,-0.1359697793,1.1626664071
H,0,5.431539095,-0.5050467842,2.1508004285
H,0,6.335887609,-1.8107529063,1.3621770584
C,0,5.8639583301,-1.0394553241,-1.2644475026
H,0,5.2318973821,-0.9512671443,-2.1528221711
H,0,6.7343592191,-0.3911297572,-1.3952917397
H,0,6.2219131678,-2.0704718418,-1.1979062905
H,0,6.6764056686,1.4789722879,-0.2663615125
Zero-point correction= 0.500971 (Hartree/Particle)
Thermal correction to Energy= 0.528719
Thermal correction to Enthalpy= 0.529663
Thermal correction to Gibbs Free Energy= 0.440613
Sum of electronic and zero-point Energies= -1385.498725
Sum of electronic and thermal Energies= -1385.470977
Sum of electronic and thermal Enthalpies= -1385.470033
Sum of electronic and thermal Free Energies= -1385.559083

5/6NP-a -TC
C,0,4.2325264772,-3.2393553741,0.2869574807
C,0,2.5758811633,-1.541678686,0.1271296413
C,0,1.5477547831,-2.4862937855,0.2321088071
C,0,3.2191303438,-4.1995425799,0.3920135032
C,0,2.196392157,-0.1714503925,-0.0150835779
C,0,0.1160426114,-2.0334245056,0.2053287021
C,0,-0.1907522455,-0.5596205709,0.028249968
C,0,0.9466120935,0.3413366051,-0.0688380821
C,0,-1.4751554581,-0.0907798121,-0.0441167242
C,0,-2.7179352785,-0.8194281708,-0.0290144132
H,0,5.2665563495,-3.5743011452,0.3125885286
H,0,3.4906184161,-5.2454848395,0.4951760484
H,0,-2.6676810193,-1.9000090897,-0.056629187
O,0,-0.7718877637,-2.8658020957,0.3296751917
H,0,-1.5747011495,0.9840030338,-0.1639487574
C,0,-3.9387564209,-0.2136434348,-0.0086912917
C,0,-5.1769964761,-1.0149889419,-0.1544507418
C,0,-6.3618299575,-0.6156177428,0.4832001177
C,0,-5.1939038384,-2.1937922706,-0.9166887723
C,0,-7.5185619023,-1.3822975771,0.382930825
H,0,-6.3673983038,0.2944932898,1.0757167737
C,0,-6.3522235179,-2.9567709611,-1.0202222431
H,0,-4.2977835353,-2.5002602771,-1.4474425503

C,0,-7.518333039,-2.5567823532,-0.3680355862
H,0,-8.4209593162,-1.0630765961,0.8951217104
H,0,-6.3472448807,-3.8617108316,-1.6197748742
H,0,-8.4218773524,-3.1529493055,-0.4493296215
C,0,-4.0962093176,1.2526318157,0.1823978051
C,0,-4.8747647099,2.003413375,-0.7097308052
C,0,-3.4850330194,1.9083252934,1.2588252135
C,0,-5.0098027561,3.378782634,-0.5473230261
H,0,-5.3673846975,1.4994759815,-1.5369471706
C,0,-3.6290208474,3.2841987061,1.4280865886
H,0,-2.9063759127,1.3259858347,1.9714949648
C,0,-4.3866143562,4.0234652666,0.5222044842
H,0,-5.6042424484,3.9493974835,-1.2541332249
H,0,-3.1510553361,3.7758238983,2.2700815096
H,0,-4.4984223447,5.0954636426,0.6518719092
C,0,3.1955683643,0.8419111466,-0.127944827
C,0,2.5694141129,2.0811501898,-0.2589157121
C,0,4.5587281639,0.6071911367,-0.110127537
C,0,3.3742739928,3.2026059243,-0.3845005161
C,0,5.356463864,1.7524102933,-0.2368383638
C,0,4.7683405644,3.0162340105,-0.3702128108
H,0,2.9616611029,4.2027247446,-0.4924872
H,0,5.4147751323,3.8835919948,-0.4658135886
C,0,1.8752662285,-3.8337371417,0.3682390189
H,0,1.0822130799,-4.5695646881,0.4537796706
C,0,3.9412403284,-1.8796180886,0.1523138574
C,0,1.046680567,1.8755913346,-0.2318517307
C,0,0.4397868285,2.6253868257,0.9664689148
H,0,0.6443521659,3.6976519722,0.8777105786
H,0,-0.645700421,2.4944404462,1.0118805226
H,0,0.873944349,2.2668098777,1.9043239718
C,0,0.4332026765,2.3714317455,-1.552581873
H,0,0.8563504345,1.8275657651,-2.401922831
H,0,-0.6533132375,2.2445553121,-1.5660069636
H,0,0.6478160223,3.4371728932,-1.6838582766
C,0,5.0767758885,-0.8306845557,0.0417854371
C,0,5.9441093624,-0.9042433399,1.3158041512
H,0,6.7718648846,-0.1910846263,1.2525193512
H,0,5.3490877475,-0.6637941069,2.2013420356
H,0,6.3679655654,-1.9047431929,1.4437384679
C,0,5.9457872098,-1.1706842162,-1.186748361
H,0,5.3500481649,-1.1308336707,-2.1030171375
H,0,6.7698227017,-0.4565086405,-1.2795120302
H,0,6.3761524712,-2.1725505365,-1.0962485381

H,0,6.4414044109,1.6797303205,-0.2341826936
Zero-point correction= 0.563187 (Hartree/Particle)
Thermal correction to Energy= 0.594317
Thermal correction to Enthalpy= 0.595261
Thermal correction to Gibbs Free Energy= 0.499601
Sum of electronic and zero-point Energies= -1502.131257
Sum of electronic and thermal Energies= -1502.100128
Sum of electronic and thermal Enthalpies= -1502.099184
Sum of electronic and thermal Free Energies= -1502.194844

5NP-b -TC

C,0,5.5317046455,-3.8665885501,0.6174883419
C,0,4.0932389166,-1.9560056793,0.1795855924
C,0,2.9899544406,-2.833720329,0.1684345122
C,0,4.4371496693,-4.732126668,0.5591466437
C,0,3.8494020855,-0.5309515382,-0.0360598768
C,0,1.5957056168,-2.3303516799,0.0179269404
C,0,1.3929874322,-0.8517594329,0.0055324452
C,0,2.5818584909,-0.0159590973,-0.0640856763
C,0,0.1344577435,-0.3046748962,0.0410271506
C,0,-1.1456736413,-0.9576129927,0.0163849222
H,0,6.5247276244,-4.2586514232,0.815476206
H,0,4.5735642762,-5.7995710842,0.6982368964
H,0,-1.1666040285,-2.0236308367,-0.1625010733
O,0,0.6659021441,-3.1258204874,-0.0577610614
H,0,0.0842486261,0.7769544674,0.0629814567
C,0,-2.3251243874,-0.2822346524,0.1630200051
C,0,-3.6128194345,-0.9651360966,-0.0765716452
C,0,-4.7732337414,-0.5748436297,0.6018958447
C,0,-3.7154133615,-2.0380683305,-0.9838730018
C,0,-5.9892539942,-1.2295414532,0.4133055772
H,0,-4.7257325548,0.248006824,1.3089932701
C,0,-4.9152717562,-2.6936305041,-1.1869357104
H,0,-2.8424460638,-2.3435877832,-1.5520470882
C,0,-6.0622460984,-2.2963105777,-0.4854153118
H,0,-6.8594662648,-0.902612105,0.9693991144
H,0,-4.9991850249,-3.5130254592,-1.8927596129
C,0,-2.3762674542,1.1397803041,0.5828096172
C,0,-3.1312761557,2.0783707151,-0.1442807245
C,0,-1.6902673858,1.5862805626,1.713987658
C,0,-3.1648983252,3.4106689708,0.2272491985
H,0,-3.6845965598,1.7501467676,-1.0198636152
C,0,-1.7254919193,2.9242765985,2.1121700152
H,0,-1.1264699474,0.8704003758,2.3067006874

C,0,-2.4594223594,3.8429271945,1.3598656943
H,0,-1.1844871405,3.2275979879,3.0005339533
C,0,4.8255484118,0.5552307884,-0.2481864671
C,0,4.1049172989,1.7577220969,-0.3392859723
C,0,6.2141693496,0.579910058,-0.417137123
C,0,4.7432720835,2.9716275212,-0.5410502875
C,0,6.8551316686,1.8019840772,-0.6264847445
H,0,6.8097936275,-0.3232522197,-0.4221338988
C,0,6.1332363813,2.9937348973,-0.6771985479
H,0,4.1729180885,3.8953489465,-0.6052846813
H,0,6.64933126,3.934865013,-0.8382034138
C,0,3.169928938,-4.2084534616,0.3442794041
H,0,2.2898077512,-4.8426507235,0.3196377591
C,0,5.3629493174,-2.4997197815,0.4322102285
H,0,6.2233983447,-1.8515699032,0.5196326626
C,0,2.6153412263,1.5057817116,-0.2198880844
C,0,2.0820652665,2.2424688078,1.0256966058
H,0,2.284614603,3.3144155755,0.9302631491
H,0,1.0039766757,2.1214116813,1.1551770229
H,0,2.5848922198,1.8773476231,1.926101014
C,0,1.9178068893,1.9974429651,-1.5024664036
H,0,2.3181473384,1.4756456084,-2.3763552615
H,0,0.8369586128,1.8400028932,-1.4730322419
H,0,2.0961158661,3.0695859201,-1.631997556
O,0,-7.1914606969,-2.9981421739,-0.7524375192
C,0,-8.3741900827,-2.6318561429,-0.0703990951
H,0,-9.14817426,-3.3110829904,-0.4250405072
H,0,-8.2560312993,-2.745433066,1.0134355551
H,0,-8.659444667,-1.5989557179,-0.3016442899
H,0,7.9325160791,1.8197122793,-0.7585328984
H,0,-3.729756645,4.1431967261,-0.3394516788
O,0,-2.5567796724,5.1652975837,1.6470810235
C,0,-1.8489463434,5.6500414326,2.7709138628
H,0,-2.0482497265,6.7198992409,2.8131563765
H,0,-2.2009189505,5.175805207,3.6943974644
H,0,-0.771191007,5.481916695,2.6608149685

Zero-point correction=	0.566526 (Hartree/Particle)
Thermal correction to Energy=	0.599703
Thermal correction to Enthalpy=	0.600647
Thermal correction to Gibbs Free Energy=	0.499323
Sum of electronic and zero-point Energies=	-1614.395585
Sum of electronic and thermal Energies=	-1614.362408
Sum of electronic and thermal Enthalpies=	-1614.361463
Sum of electronic and thermal Free Energies=	-1614.462788

5NP-c- TC

C,0,4.9266738817,4.4775899621,-0.920142229
C,0,3.982271233,2.3196107596,-0.3229452835
C,0,2.7040430473,2.9118432513,-0.3436185901
C,0,3.6600156406,5.0641148213,-0.8918994993
C,0,4.0822389935,0.8946122844,-0.0092803194
C,0,1.4708392682,2.1052056197,-0.1250036475
C,0,1.6217376697,0.6192874181,-0.0478238359
C,0,2.9751880362,0.0947028112,0.0627794873
C,0,0.5320245593,-0.2121626414,-0.0621786828
C,0,-0.8674507574,0.1246140422,-0.0998795183
H,0,5.7974901836,5.0764755023,-1.1692726733
H,0,3.5398103826,6.1214727702,-1.1041131294
H,0,-1.1370730865,1.1687311159,-0.0211814041
O,0,0.3835333468,2.6636036806,-0.0444487175
H,0,0.7406850325,-1.2739224658,-0.0213792529
C,0,-1.8566112136,-0.8102757504,-0.1897405968
C,0,-3.2755505387,-0.4118363807,-0.0527813276
C,0,-4.2887024654,-1.1174852798,-0.7205617481
C,0,-3.6495376303,0.6846764808,0.7400781784
C,0,-5.6181729159,-0.7269789278,-0.6188149625
H,0,-4.0280771651,-1.9775676427,-1.3303201311
C,0,-4.9792483442,1.0690983282,0.8446113244
H,0,-2.8902299722,1.2323018199,1.2896739966
C,0,-5.9884395763,0.3733605084,0.1648696387
H,0,-6.3845748576,-1.2981356857,-1.1350028494
H,0,-5.2394230872,1.9328492095,1.4495738264
C,0,-1.5772985551,-2.2497464208,-0.4385953725
C,0,-2.1122988091,-3.2298906269,0.4093436298
C,0,-0.7965042512,-2.6547784582,-1.5284459713
C,0,-1.846203027,-4.5779151722,0.1898860336
H,0,-2.7319525316,-2.9244277896,1.2481643182
C,0,-0.5403297918,-4.0060305047,-1.7558081565
H,0,-0.4033368747,-1.9014234054,-2.2065576971
C,0,-1.0596308877,-4.9700921447,-0.8942653482
H,0,0.06207459,-4.3029713682,-2.6089860534
H,0,-0.8593160989,-6.0224041171,-1.0697536302
C,0,5.2876135377,0.0899880315,0.2650306985
C,0,4.8760531402,-1.2417238194,0.4355104894
C,0,6.6378659996,0.4146636452,0.4316806248
C,0,5.7870323711,-2.2497029466,0.7125563976
C,0,7.5523530331,-0.5995893818,0.7176406447
H,0,6.9956996929,1.4345137532,0.3782020682

C,0,7.1389700063,-1.9249551335,0.8458349432
H,0,5.4565603338,-3.2783386364,0.8370177056
H,0,7.8656048731,-2.7012299127,1.0641284883
C,0,2.5529287911,4.2744052378,-0.6126769468
H,0,1.5484188452,4.6852258477,-0.6079359609
C,0,5.0862924072,3.1252357914,-0.6413228321
H,0,6.0739138421,2.6907833757,-0.7088649952
C,0,3.3705192674,-1.363054762,0.3059334249
C,0,3.0446898457,-2.2739496504,-0.8955115699
H,0,3.5046759189,-3.2559675145,-0.7444802162
H,0,1.9708515453,-2.4305596834,-1.0240070306
H,0,3.4473281688,-1.8453810411,-1.8180031994
C,0,2.7946650533,-1.937690492,1.6136410794
H,0,3.0461728193,-1.2897156815,2.4581318986
H,0,1.7079233555,-2.0476324543,1.5743640015
H,0,3.2233284402,-2.927284137,1.8009795611
H,0,-2.2555012846,-5.3241801405,0.8636514346
C,0,-7.4081343893,0.7876598939,0.2799283525
C,0,-7.9289632514,1.2237589937,1.5051243853
C,0,-8.2560365015,0.7565735165,-0.8348949104
C,0,-9.2593332079,1.619014714,1.6128167717
H,0,-7.2915700004,1.2295892535,2.3847836566
C,0,-9.5865887241,1.1518205096,-0.727888646
H,0,-7.8609797942,0.4454958777,-1.7979852142
C,0,-10.0934481117,1.5849985382,0.4963442767
H,0,-9.6469191484,1.947783363,2.5721772688
H,0,-10.2258728687,1.1314270604,-1.6051006974
H,0,-11.1304277972,1.8947066756,0.5794203962
H,0,8.6003079141,-0.3482132654,0.8490411453
Zero-point correction= 0.582254 (Hartree/Particle)
Thermal correction to Energy= 0.615004
Thermal correction to Enthalpy= 0.615949
Thermal correction to Gibbs Free Energy= 0.515102
Sum of electronic and zero-point Energies= -1616.385282
Sum of electronic and thermal Energies= -1616.352531
Sum of electronic and thermal Enthalpies= -1616.351587
Sum of electronic and thermal Free Energies= -1616.452434

NP-a -TT

C,0,4.992911933,-2.4039666368,0.0236529259
C,0,2.9576666402,-1.0767439291,0.0428704217
C,0,2.2246084148,-2.2616121458,0.2646289633
C,0,4.2600164891,-3.567511657,0.2689350805
C,0,2.2501194345,0.2092605202,-0.0797324875

C,0,0.7381798536,-2.2448559529,0.3489249825
C,0,0.0698006218,-0.9232557763,0.1644289782
C,0,0.8975242672,0.2486091406,-0.0399367932
C,0,-1.2936329453,-0.9081539077,0.217064808
C,0,-2.1334371046,0.2570058323,0.1181903732
H,0,6.0720792393,-2.4545531956,-0.0845720326
H,0,4.7647906635,-4.5237493664,0.3601006559
H,0,-1.6532215979,1.2315717985,0.1326105332
O,0,0.1040637822,-3.2721711968,0.5463817091
H,0,-1.7709767841,-1.8721949327,0.379076761
C,0,-3.4922752811,0.2381257394,0.0426662175
C,0,-4.2551709194,1.5088373947,0.1090556787
C,0,-5.4213770806,1.6802685664,-0.6522733099
C,0,-3.8255298946,2.5670148508,0.9236249256
C,0,-6.1192017315,2.8837317171,-0.6211507958
H,0,-5.7707623766,0.8664496182,-1.2809727867
C,0,-4.5280492368,3.7678816099,0.9595934942
H,0,-2.9514034647,2.4340080862,1.5541191416
C,0,-5.6748711339,3.9322098411,0.1838757534
H,0,-7.0121918969,3.0030140429,-1.2265953958
H,0,-4.1861604894,4.5718864034,1.6037357507
H,0,-6.2239727474,4.8679879756,0.2134725373
C,0,-4.269270538,-1.0151398685,-0.1257190676
C,0,-5.3955440581,-1.254657902,0.6756729791
C,0,-3.9131828075,-1.9666253449,-1.0904771423
C,0,-6.1258394098,-2.4300129235,0.5368343752
H,0,-5.6872703894,-0.5153340201,1.4164851311
C,0,-4.6523647093,-3.1384931738,-1.23705825
H,0,-3.0618624747,-1.7749906031,-1.7372481944
C,0,-5.756151525,-3.3754277474,-0.4208435957
H,0,-6.9855418244,-2.6088684917,1.1748695532
H,0,-4.3643972049,-3.8646917499,-1.9903443983
H,0,-6.3296665156,-4.2901272687,-0.5324738884
C,0,3.0100745378,1.4775168814,-0.2450490677
C,0,2.7610168823,2.3134347163,-1.339101389
C,0,3.432981852,3.5275642197,-1.4746776893
C,0,4.619223321,3.0968465014,0.5788716696
C,0,4.3642862386,3.922145442,-0.5170196154
H,0,3.2311662117,4.1617131323,-2.3324007224
H,0,4.8888997321,4.8665266053,-0.6220290536
C,0,2.8781093015,-3.4909291622,0.3811943862
H,0,2.2712902003,-4.3740350826,0.5538761724
H,0,0.4118894405,1.215191466,-0.1385588663
H,0,2.0434666343,1.9985143143,-2.0916318452

H,0,5.3372523681,3.4013453551,1.3340701107
C,0,3.9498629064,1.8838740756,0.712379801
H,0,4.141004424,1.2484593398,1.5731767309
C,0,4.3520037996,-1.1756501643,-0.0903727002
H,0,4.9357211322,-0.2851391766,-0.2962835236
Zero-point correction= 0.437159 (Hartree/Particle)
Thermal correction to Energy= 0.462136
Thermal correction to Enthalpy= 0.463080
Thermal correction to Gibbs Free Energy= 0.379274
Sum of electronic and zero-point Energies= -1268.860148
Sum of electronic and thermal Energies= -1268.835171
Sum of electronic and thermal Enthalpies= -1268.834227
Sum of electronic and thermal Free Energies= -1268.918033

5NP-a- TT

C,0,6.112709459,2.8352069404,0.5068996341
C,0,4.3485839201,1.2239467143,0.0710311905
C,0,3.5120280588,2.291702251,-0.3021848655
C,0,5.2900930811,3.8813107891,0.0841876775
C,0,3.8011518612,-0.1318909637,0.0234981717
C,0,2.084241764,2.0585870519,-0.6491460982
C,0,1.5031893552,0.6886514169,-0.3849703539
C,0,2.4618673187,-0.3801882548,-0.1259856451
C,0,0.1340732075,0.688496239,-0.4282055114
C,0,-0.8597463434,-0.3411763944,-0.2571968259
H,0,7.121730363,3.0426028056,0.8500030975
H,0,5.6583241741,4.9019664094,0.0832121228
H,0,-0.5634742069,-1.3799166091,-0.2609203155
O,0,1.4039974485,2.9738261269,-1.0887206954
H,0,-0.2743528787,1.6721240062,-0.6508483228
C,0,-2.1940656639,-0.0975898275,-0.1235746921
C,0,-3.145452324,-1.2365549599,-0.1198834319
C,0,-4.2880511336,-1.21058466,0.6942674987
C,0,-2.9184433421,-2.368040586,-0.918155486
C,0,-5.1607767181,-2.2940282771,0.7286685995
H,0,-4.4807246798,-0.3389224205,1.3128521065
C,0,-3.7954644887,-3.4481368021,-0.8885836977
H,0,-2.0634103882,-2.3862395023,-1.5880947751
C,0,-4.9177879892,-3.4168952382,-0.0616865743
H,0,-6.0327596938,-2.2613141676,1.3742788744
H,0,-3.6090545629,-4.3099604148,-1.5216932244
C,0,-2.7576309826,1.2634828178,0.0500756261
C,0,-3.880969103,1.6585636004,-0.692023179
C,0,-2.2012610919,2.1685411275,0.9639534935

C,0,-4.4121596791,2.9354202671,-0.546262298
H,0,-4.3272998262,0.958970754,-1.3933437483
C,0,-2.7414227441,3.4432012345,1.1181798631
H,0,-1.3507350945,1.8611719176,1.5655297362
C,0,-3.8437530439,3.8314479794,0.3602350862
H,0,-5.2713601001,3.2324026311,-1.1393087545
H,0,-2.2992594181,4.1314883928,1.8312318856
C,0,4.5334410224,-1.4087166309,0.1215885999
C,0,3.58363145,-2.4414090685,0.1019546288
C,0,5.8940782842,-1.7331681673,0.1547511619
C,0,3.9580227175,-3.7744045545,0.1717161468
C,0,6.2717458158,-3.075067185,0.2175452648
H,0,6.6666860794,-0.9773786676,0.0982514323
C,0,5.3165544282,-4.0914690043,0.2394945555
H,0,3.2099160651,-4.5633583093,0.1608718059
H,0,5.6306232414,-5.1290730596,0.2919135939
C,0,3.9877170948,3.6047327756,-0.3107191596
H,0,3.3067747275,4.3914234923,-0.6189475049
C,0,5.6499183814,1.5239902662,0.5013375471
H,0,6.2950560665,0.7385222478,0.8703078285
C,0,2.1850069767,-1.8781376314,-0.0345687055
C,0,1.5663937728,-2.4316581952,-1.3345456468
H,0,1.3056941835,-3.4882393095,-1.2117836661
H,0,0.6750330821,-1.8871366703,-1.647613794
H,0,2.2963223949,-2.3533567031,-2.1453563173
C,0,1.4089085305,-2.2397583577,1.2515429125
H,0,2.018322713,-1.9843338034,2.1231764569
H,0,0.4585523003,-1.7158542596,1.3484460181
H,0,1.2141688812,-3.3170751993,1.2774911674
H,0,7.3269277356,-3.3287175654,0.2416528481
H,0,-4.2619376872,4.8261926183,0.4769860511
H,0,-5.6030933119,-4.258278883,-0.0399748739
Zero-point correction= 0.500702 (Hartree/Particle)
Thermal correction to Energy= 0.528712
Thermal correction to Enthalpy= 0.529656
Thermal correction to Gibbs Free Energy= 0.440538
Sum of electronic and zero-point Energies= -1385.485199
Sum of electronic and thermal Energies= -1385.457189
Sum of electronic and thermal Enthalpies= -1385.456245
Sum of electronic and thermal Free Energies= -1385.545363

6NP-a- TT

C,0,-4.6367003027,-2.5600469328,-0.5600772931
C,0,-2.6694363327,-1.2373149294,-0.1248391931

C,0,-1.8934392905,-2.4069030809,-0.2932196687
C,0,-3.8696096289,-3.7107868081,-0.7091685561
C,0,-2.0061657919,0.041509687,0.1658944686
C,0,-0.4072092593,-2.3677916484,-0.2104361662
C,0,0.2127304134,-1.0205757847,-0.0849630568
C,0,-0.6513275784,0.1161653509,0.1351812689
C,0,1.5738307631,-0.9524957627,-0.1730872383
C,0,2.3585706631,0.2540478896,-0.1939655248
H,0,-5.7124846121,-2.6357064933,-0.6872630561
H,0,-4.349157145,-4.6568999299,-0.938641726
H,0,1.8310841807,1.1964583356,-0.3167621743
O,0,0.2593685579,-3.3912265953,-0.2727235158
H,0,2.0909678086,-1.9031922805,-0.2860976578
C,0,3.717783211,0.3093125119,-0.1340639161
C,0,4.4138396353,1.5977343881,-0.3710421731
C,0,5.5767601712,1.9292842848,0.340648052
C,0,3.9178461522,2.5163938493,-1.3081574327
C,0,6.2060034508,3.1542896333,0.1403833154
H,0,5.9781058651,1.2245470398,1.0633788541
C,0,4.5506116367,3.7385990767,-1.5118126496
H,0,3.0466868886,2.2540121552,-1.9011264254
C,0,5.6949548694,4.0640097341,-0.7850086125
H,0,7.0976290791,3.4002885877,0.708680738
H,0,4.1563584982,4.4322802624,-2.2479179564
H,0,6.190063055,5.0166358547,-0.9450417927
C,0,4.5489887989,-0.878092165,0.1804440703
C,0,5.6980872775,-1.1594207179,-0.5741339916
C,0,4.2147609443,-1.7295587017,1.2419281926
C,0,6.471882813,-2.2803649488,-0.2927687366
H,0,5.9728846722,-0.4986493052,-1.3917461796
C,0,4.9963564324,-2.8458974171,1.5298995109
H,0,3.3459781027,-1.5020776928,1.8528645591
C,0,6.1232080594,-3.1267489996,0.7605228425
H,0,7.3491038249,-2.4947326603,-0.895117352
H,0,4.724191707,-3.493715892,2.3569749157
H,0,6.7307832037,-3.9983253948,0.9827362745
C,0,-2.8521935651,1.2177072601,0.4622899306
C,0,-2.2786248551,2.4158128845,0.9303137728
C,0,-4.2447389854,1.1614083336,0.2881025911
C,0,-3.0405438374,3.5463771082,1.1677164578
C,0,-4.9992979428,2.3217124325,0.5185152199
C,0,-4.417412627,3.5056715862,0.9447883569
H,0,-2.5662816375,4.4530169896,1.5299512455
H,0,-5.031421093,4.3840230269,1.1169963001

C,0,-2.4903217524,-3.6331913831,-0.5711980168
H,0,-1.8502927594,-4.5019683675,-0.6856282332
C,0,-4.0657047055,-1.3181359966,-0.2603351071
C,0,-4.9843196966,-0.1058091449,-0.1344594196
H,0,-0.166840197,1.0704124614,0.3009786712
H,0,-1.2146997706,2.4632812186,1.130789941
C,0,-5.6553697996,0.1423386565,-1.5045206061
H,0,-6.3441369265,0.9903426859,-1.4512486027
H,0,-4.9003173885,0.3584791159,-2.2659314533
H,0,-6.2238070726,-0.736464938,-1.8226686756
C,0,-6.0686804474,-0.4136580939,0.9242384017
H,0,-5.6089599766,-0.5816856453,1.9023554861
H,0,-6.7763965892,0.413744857,1.0144889221
H,0,-6.6403177267,-1.3049142194,0.6545964942
H,0,-6.073660632,2.2984505321,0.3637880762
Zero-point correction= 0.501473 (Hartree/Particle)
Thermal correction to Energy= 0.529126
Thermal correction to Enthalpy= 0.530070
Thermal correction to Gibbs Free Energy= 0.441933
Sum of electronic and zero-point Energies= -1385.498399
Sum of electronic and thermal Energies= -1385.470747
Sum of electronic and thermal Enthalpies= -1385.469802
Sum of electronic and thermal Free Energies= -1385.557940

5/6NP-a -TT

C,0,-4.6838730665,2.8092142634,0.2216344432
C,0,-2.7654005779,1.4003777807,0.1760274789
C,0,-1.921440531,2.5027469007,0.3401930675
C,0,-3.8528518563,3.9219234144,0.3876537787
C,0,-2.1530788269,0.1077365363,0.0776697258
C,0,-0.4412159775,2.2895705596,0.3976248668
C,0,0.1311507472,0.8758616266,0.2686152096
C,0,-0.8340675327,-0.2109899558,0.1175874264
C,0,1.4977093298,0.860626373,0.2869230027
C,0,2.4233445994,-0.2380972958,0.2035429213
H,0,-5.75837587,2.9681452204,0.1791487068
H,0,-4.2976513554,4.9086444555,0.4707264856
H,0,2.0431933343,-1.2472601365,0.2754940709
O,0,0.2916756595,3.2561509929,0.5400025391
H,0,1.9448220926,1.8457830628,0.396928549
C,0,3.771556458,-0.1064254538,0.0640991966
C,0,4.6367727013,-1.3106867868,0.1307556641
C,0,5.7792687613,-1.4117138158,-0.6777434569
C,0,4.331460923,-2.3755852151,0.9913542747

C,0,6.5749305599,-2.5527953202,-0.6452684101
H,0,6.0340437918,-0.591638913,-1.3428964251
C,0,5.1317228921,-3.5137451262,1.0288500709
H,0,3.477364697,-2.295611363,1.6578602327
C,0,6.2541646146,-3.6085763376,0.2072997582
H,0,7.4483876955,-2.6169581838,-1.2866540003
H,0,4.8853519121,-4.3222874196,1.710140349
H,0,6.87925871,-4.4954014741,0.23770757
C,0,4.440250283,1.1967718116,-0.1777734425
C,0,5.5750779637,1.5475156757,0.5688935319
C,0,3.9771361538,2.085387954,-1.1566460653
C,0,6.2111392185,2.7665842529,0.3611958997
H,0,5.9494886817,0.8586244873,1.3211599002
C,0,4.6219770021,3.3014793089,-1.3726145728
H,0,3.1149831975,1.8119171337,-1.7581859292
C,0,5.736592914,3.6470218019,-0.6118228211
H,0,7.079532227,3.0297314811,0.957009562
H,0,4.2507227532,3.978705178,-2.1351049896
H,0,6.236086253,4.5964631204,-0.7773241723
C,0,-2.9835169318,-1.0462520718,-0.0807309859
C,0,-2.1751117008,-2.1780584887,-0.1446401046
C,0,-4.3657372795,-1.0289303172,-0.1562952512
C,0,-2.7859391098,-3.4128659732,-0.2968936647
C,0,-4.9685969676,-2.2842596451,-0.3120800327
C,0,-4.1887427945,-3.4446158239,-0.3797055491
H,0,-2.216934918,-4.3376326329,-0.3518873566
H,0,-4.6871937628,-4.4017178671,-0.500655773
C,0,-2.4691999134,3.7787845368,0.4482840484
H,0,-1.809790675,4.6309623077,0.5776089249
C,0,-4.1664099605,1.5154896443,0.1117195464
C,0,-0.7077143477,-1.7515109277,-0.0129999138
C,0,-0.1433794735,-2.3964940512,1.2676124031
H,0,-0.1050030946,-3.4847738915,1.1506531807
H,0,0.858983082,-2.043502016,1.5148030202
H,0,-0.7943694201,-2.1655781864,2.1158405399
C,0,0.0375598218,-2.1868100267,-1.2879016647
H,0,-0.4657523776,-1.77788616,-2.1689366995
H,0,1.0762217967,-1.8541046178,-1.3095493032
H,0,0.02835159,-3.2790826518,-1.3664981144
C,0,-5.1131317486,0.3065717257,-0.0730934735
C,0,-6.0887603032,0.25065393,1.1208174963
H,0,-6.7849130101,-0.5857713407,1.0054739463
H,0,-5.543069755,0.1178700525,2.0592605235
H,0,-6.6768131195,1.1706508299,1.1892273217

C,0,-5.914026056,0.5010877662,-1.3777537272
H,0,-5.2416041098,0.5457669356,-2.2391810125
H,0,-6.6089819282,-0.331355991,-1.5257065853
H,0,-6.496785318,1.4265150822,-1.3450129624
H,0,-6.049585948,-2.3773681651,-0.3830154842
Zero-point correction= 0.563461 (Hartree/Particle)
Thermal correction to Energy= 0.594559
Thermal correction to Enthalpy= 0.595503
Thermal correction to Gibbs Free Energy= 0.501010
Sum of electronic and zero-point Energies= -1502.125075
Sum of electronic and thermal Energies= -1502.093977
Sum of electronic and thermal Enthalpies= -1502.093033
Sum of electronic and thermal Free Energies= -1502.187526

5NP-b- TT

C,0,-5.7274299583,3.2978075556,-0.4270060574
C,0,-4.0514470282,1.5834782387,-0.0378827478
C,0,-3.1380609889,2.5995918267,0.29794324
C,0,-4.8276122355,4.2936938737,-0.041472147
C,0,-3.5870180073,0.197385784,-0.0005018396
C,0,-1.7147601002,2.2828074152,0.596341591
C,0,-1.2308837495,0.8771900994,0.3377811559
C,0,-2.2607560278,-0.1303316797,0.1111791767
C,0,0.1380213863,0.7855827514,0.3593348034
C,0,1.0598802613,-0.3045272935,0.1884792923
H,0,-6.7333518189,3.5649859666,-0.7368625492
H,0,-5.1319270424,5.3352990147,-0.0363040985
H,0,0.6948133968,-1.3208848407,0.1734374902
O,0,-0.9642853518,3.1634350873,0.9929479568
H,0,0.6109543689,1.7431693197,0.5691209534
C,0,2.4134616763,-0.150830629,0.0834063488
C,0,3.2833305469,-1.3487936156,0.1091081656
C,0,4.4631021115,-1.4032644956,-0.6410723919
C,0,2.9438602621,-2.4798525947,0.8752556763
C,0,5.268841378,-2.5405053477,-0.6581859103
H,0,4.7525086177,-0.5443961623,-1.2396711167
C,0,3.736075425,-3.6137966333,0.8756008884
H,0,2.0585040506,-2.4530220306,1.5040785774
C,0,4.9037228433,-3.6545379054,0.1019973422
H,0,6.1660904196,-2.5444915532,-1.2652119637
H,0,3.4827532787,-4.4805449654,1.4768426727
C,0,3.0687669445,1.1666393967,-0.0805231389
C,0,4.2005594595,1.4935379357,0.6735269897
C,0,2.5923367045,2.1179115403,-0.9996169169

C,0,4.8270096111,2.7316416899,0.5512298848
H,0,4.591799193,0.7705167531,1.3840379625
C,0,3.2131841243,3.3469493811,-1.1453228012
H,0,1.7312670687,1.8766574053,-1.6162663041
C,0,4.3303881405,3.6649522153,-0.3640209813
H,0,5.690269022,2.953418955,1.1668922912
H,0,2.8512700639,4.0821737789,-1.8557991888
C,0,-4.3970402764,-1.0339083002,-0.0742692888
C,0,-3.5099837392,-2.1210040495,-0.082079157
C,0,-5.774782966,-1.2784060251,-0.0648528267
C,0,-3.9633770736,-3.429606829,-0.1391866313
C,0,-6.2319565846,-2.5960116302,-0.1138455863
H,0,-6.4999980951,-0.4788750953,0.0156441283
C,0,-5.3395833376,-3.6666699128,-0.1643033161
H,0,-3.2625009157,-4.2611492021,-0.1506206065
H,0,-5.7156295252,-4.6841390809,-0.2050999275
C,0,-3.5323028121,3.9395077856,0.3112261006
H,0,-2.79379392,4.6847357933,0.5890440422
C,0,-5.3460247056,1.9609732341,-0.4261099417
H,0,-6.0505517158,1.2144509646,-0.7662203599
C,0,-2.077525751,-1.6417938335,0.0171511754
C,0,-1.4640584926,-2.2288262462,1.3052046549
H,0,-1.2663868911,-3.2988798545,1.1794022614
H,0,-0.5378746595,-1.7339417302,1.5987272131
H,0,-2.1723268996,-2.1084689933,2.1301111514
C,0,-1.3543694792,-2.0488047472,-1.2858361054
H,0,-1.9704141031,-1.7624120956,-2.1431235252
H,0,-0.3800753777,-1.5763970727,-1.4071571168
H,0,-1.2183356529,-3.135200609,-1.3129851087
O,0,4.8661352212,4.8936197617,-0.5702993533
O,0,5.6150411663,-4.8077818386,0.1639723132
C,0,5.9768599255,5.2727648376,0.2176120701
H,0,6.2294917878,6.2873542765,-0.08790628
H,0,5.7253122772,5.2641053017,1.2844916133
H,0,6.8340195258,4.6131751762,0.0369824468
C,0,6.8108110896,-4.8881600244,-0.5861481235
H,0,7.2177989798,-5.8807131173,-0.3974668177
H,0,6.6134784215,-4.7720708115,-1.6582988472
H,0,7.5318063301,-4.1284960736,-0.2619795997
H,0,-7.3006207874,-2.787210676,-0.1042720576
Zero-point correction= 0.566920 (Hartree/Particle)
Thermal correction to Energy= 0.600030
Thermal correction to Enthalpy= 0.600974
Thermal correction to Gibbs Free Energy= 0.500330

Sum of electronic and zero-point Energies= -1614.386514
Sum of electronic and thermal Energies= -1614.353404
Sum of electronic and thermal Enthalpies= -1614.352460
Sum of electronic and thermal Free Energies= -1614.453104

5NP-c- TT

C,0,6.1581924251,2.7877074644,0.5809049762
C,0,4.3801469239,1.1994076888,0.1180334076
C,0,3.5525710722,2.2806068247,-0.2362857455
C,0,5.344161646,3.8480331751,0.1773920883
C,0,3.8209660264,-0.1506125081,0.0473142385
C,0,2.1230262619,2.0657432657,-0.5879050082
C,0,1.5301885008,0.6965828745,-0.3475877039
C,0,2.4794717325,-0.3844172593,-0.1061193283
C,0,0.1610541081,0.7084167122,-0.3940629693
C,0,-0.8414590205,-0.3153210462,-0.2428797642
H,0,7.169165129,2.9805266797,0.9267863854
H,0,5.720846377,4.8654552924,0.1943076527
H,0,-0.5531640824,-1.356229278,-0.2557956745
O,0,1.451038728,2.9941040609,-1.0123606753
H,0,-0.2382298038,1.6987916137,-0.6029799814
C,0,-2.1755478941,-0.0633480746,-0.1190389004
C,0,-3.1345708167,-1.1960365931,-0.1388378173
C,0,-4.2821245117,-1.1743873308,0.6683720744
C,0,-2.910070157,-2.317004618,-0.9523694433
C,0,-5.1622828069,-2.2522153729,0.6813563354
H,0,-4.4729330557,-0.3106249412,1.2985385952
C,0,-3.7945312683,-3.3914853846,-0.9442344298
H,0,-2.0505382581,-2.3311628021,-1.6166137603
C,0,-4.9217615635,-3.3648966611,-0.1240031921
H,0,-6.0381810008,-2.2229806481,1.3218034291
H,0,-3.6098002922,-4.2450858188,-1.5888664183
C,0,-2.7326195279,1.2974546369,0.0652524094
C,0,-3.8506657217,1.7086532618,-0.6757975822
C,0,-2.1821051719,2.1950157591,0.9897325652
C,0,-4.3776288125,2.9835068841,-0.5194415516
H,0,-4.3047632321,1.0184377879,-1.3813921397
C,0,-2.7197452145,3.4670970621,1.1545080558
H,0,-1.3305273246,1.8867283151,1.5893707915
C,0,-3.8217172629,3.8848699321,0.39967688
H,0,-5.2488153092,3.2787887733,-1.0969863247
H,0,-2.2628366505,4.1536018756,1.8611375352
C,0,4.5417775901,-1.4354993787,0.1229660482
C,0,3.5827540784,-2.4592231541,0.0851940076

C,0,5.899374841,-1.7726747536,0.1506946398
C,0,3.9451574922,-3.7965775797,0.1318066513
C,0,6.265018689,-3.1188547503,0.190091021
H,0,6.678707068,-1.0229130186,0.1078070918
C,0,5.300746921,-4.1269337558,0.1941358508
H,0,3.1898562924,-4.578368923,0.1072074697
H,0,5.6055061403,-5.1680737687,0.2283773247
C,0,4.0392818572,3.5895030176,-0.2217363798
H,0,3.3650147493,4.3873665971,-0.5155950979
C,0,5.6842974178,1.4807504388,0.5526058611
H,0,6.323005011,0.6834875815,0.9072237091
C,0,2.1892749511,-1.8811402076,-0.0412849379
C,0,1.5659354212,-2.4054140167,-1.3511590632
H,0,1.2936998644,-3.4611217694,-1.2471816267
H,0,0.6809592445,-1.8455978339,-1.655154777
H,0,2.2974439925,-2.3207988048,-2.1599195857
C,0,1.4098837475,-2.2584173284,1.2384022111
H,0,2.0227063574,-2.0262123474,2.1141323618
H,0,0.4655975063,-1.7257318524,1.3460304273
H,0,1.2031636178,-3.3337895295,1.2443411203
H,0,7.3178860684,-3.3822763293,0.2099382824
C,0,-4.3928996699,5.2433535488,0.571094919
C,0,-4.8253126762,5.9810227156,-0.5383910714
C,0,-4.5105783746,5.8153705938,1.8442662669
C,0,-5.3611102329,7.2561739168,-0.379208107
H,0,-4.7147205374,5.5613673951,-1.5342775989
C,0,-5.0467051477,7.0903634545,2.0040797896
H,0,-4.2013227579,5.2457445288,2.7161178747
C,0,-5.474135453,7.8153734158,0.8927717128
H,0,-5.6817219023,7.8177442733,-1.2511551612
H,0,-5.1381617403,7.514896109,2.9990196604
H,0,-5.8915597592,8.8095005593,1.0169621549
H,0,-5.6126752784,-4.2019527572,-0.1189490991
Zero-point correction= 0.582190 (Hartree/Particle)
Thermal correction to Energy= 0.614895
Thermal correction to Enthalpy= 0.615839
Thermal correction to Gibbs Free Energy= 0.515353
Sum of electronic and zero-point Energies= -1616.376383
Sum of electronic and thermal Energies= -1616.343678
Sum of electronic and thermal Enthalpies= -1616.342734
Sum of electronic and thermal Free Energies= -1616.443220

NP-a -TS

C,0,-2.4709982818,-2.7594797773,1.4288371471

C,0,-1.7397234308,-0.7945356352,0.1925282624
C,0,-0.4026977783,-1.2426027552,0.3256005386
C,0,-1.1459209054,-3.2161135996,1.5201328854
C,0,-2.0180687898,0.4408867246,-0.5223544905
C,0,0.7251732816,-0.4166150868,-0.1314832879
C,0,0.402282134,0.7646040843,-0.8983990555
C,0,-0.9756259307,1.1442884724,-1.0421319548
C,0,1.35351727,1.2634810321,-1.8120030439
C,0,2.7012000399,0.9419678474,-1.795421025
H,0,-3.2752537025,-3.3375999223,1.8738265167
H,0,-0.9244714854,-4.1528437908,2.0213809324
H,0,3.2553757027,0.9180170801,-2.7295397776
O,0,1.8991852089,-0.8023096234,0.1219209771
H,0,0.9587042093,1.7777313896,-2.6889372567
C,0,3.3532614185,0.5180373815,-0.6167612432
C,0,4.5469297729,-0.3509417402,-0.7732031424
C,0,5.7572671058,-0.0659684372,-0.1277925314
C,0,4.4749519127,-1.4584602671,-1.6293573743
C,0,6.8768214723,-0.864718277,-0.3496007969
H,0,5.8259448647,0.7937747199,0.5312658809
C,0,5.5897423409,-2.2622456209,-1.8390233288
H,0,3.5244009296,-1.6956112712,-2.0977150718
C,0,6.7951317107,-1.9641944601,-1.2017663251
H,0,7.8132643725,-0.6269232064,0.14483121
H,0,5.5180413318,-3.1257092466,-2.4926431645
H,0,7.6664478219,-2.5905382167,-1.3660966269
C,0,3.2335354864,1.3011823835,0.6439390309
C,0,3.464855603,0.6845591626,1.8835722544
C,0,2.9445556271,2.6693793944,0.6105937284
C,0,3.3891729675,1.419040964,3.060163143
H,0,3.6729444796,-0.3801793824,1.9114366928
C,0,2.8738649292,3.4060717792,1.7917070743
H,0,2.7865423101,3.1552524095,-0.3464193952
C,0,3.0928162919,2.7833327972,3.0175510768
H,0,3.5562094106,0.9278846395,4.013524479
H,0,2.6512901861,4.4675602249,1.7506643498
H,0,3.0366237155,3.3567594119,3.9376556701
C,0,-3.4083051013,0.9228193276,-0.7378332507
C,0,-3.7784860709,2.2103192986,-0.3323338375
C,0,-5.0639834235,2.6933919222,-0.5734769205
C,0,-5.6443468124,0.6084264321,-1.6325044625
C,0,-6.0016348019,1.8932847827,-1.2222744647
H,0,-5.3334964435,3.6935189708,-0.2479424748
H,0,-7.0035958764,2.2668137652,-1.408813373

C,0,-0.1250053809,-2.4505067199,0.9918555686
H,0,0.9124230355,-2.7540575351,1.0829223749
H,0,-1.1871105608,2.0342957666,-1.6319742554
H,0,-3.0504072396,2.8281052683,0.1860543927
H,0,-6.3659825754,-0.0184199712,-2.1474744949
C,0,-4.3600856028,0.1280859501,-1.3923201199
H,0,-4.0797171119,-0.8669463301,-1.7277690236
C,0,-2.7606468069,-1.5712188987,0.7850049324
H,0,-3.7861449308,-1.2208704515,0.7398906611
Zero-point correction= 0.435534 (Hartree/Particle)
Thermal correction to Energy= 0.459516
Thermal correction to Enthalpy= 0.460460
Thermal correction to Gibbs Free Energy= 0.380377
Sum of electronic and zero-point Energies= -1268.830132
Sum of electronic and thermal Energies= -1268.806150
Sum of electronic and thermal Enthalpies= -1268.805206
Sum of electronic and thermal Free Energies= -1268.885289

5NP-a -TS

C,0,1.968727666,4.2849282554,0.8251950383
C,0,1.7571140108,1.9535832137,0.1625488765
C,0,0.3503529776,2.1065653548,0.1820993563
C,0,0.5723543478,4.4189319958,0.8669367384
C,0,2.3014055689,0.6710496588,-0.2258610921
C,0,-0.5403760943,0.9751610716,-0.1288266623
C,0,0.0538592936,-0.1771915595,-0.7840172223
C,0,1.4864533386,-0.2937630217,-0.7643672632
C,0,-0.7648314262,-0.9180192672,-1.6627595478
C,0,-2.1513706272,-0.9047829629,-1.6385886509
H,0,2.6019682978,5.1363722549,1.0555192376
H,0,0.1225279108,5.3690642948,1.1361436444
H,0,-2.7042260768,-1.0521636248,-2.5620014805
O,0,-1.7697209631,1.1040207915,0.1107622777
H,0,-0.2832507494,-1.3751721792,-2.5227377862
C,0,-2.8676204228,-0.583337567,-0.4673602668
C,0,-4.2413356702,-0.0441362313,-0.626181193
C,0,-5.3257112335,-0.5706613181,0.0875448962
C,0,-4.468179187,0.9860264605,-1.5493230888
C,0,-6.613405281,-0.0872352761,-0.1328648322
H,0,-5.1618098459,-1.3727728187,0.8002738805
C,0,-5.7521954744,1.4763161718,-1.7581875332
H,0,-3.6187483798,1.4162635226,-2.0714103473
C,0,-6.8288873159,0.9372793666,-1.0524085201
H,0,-7.4482113281,-0.5116910794,0.4156062967

H,0,-5.9136688737,2.2841617298,-2.4647661928
H,0,-7.831874248,1.3190889961,-1.2158897302
C,0,-2.5284967934,-1.2294199811,0.8321543498
C,0,-2.8522852308,-0.5984988942,2.0427076091
C,0,-1.9318234824,-2.4941621465,0.8650489226
C,0,-2.5609928198,-1.2110547186,3.2553765204
H,0,-3.3032525979,0.388387982,2.0184159138
C,0,-1.6429523419,-3.1090018042,2.0817429438
H,0,-1.7041154196,-2.9974875797,-0.068827692
C,0,-1.9529135582,-2.4681184819,3.2785602077
H,0,-2.8023924483,-0.7060964957,4.1853036411
H,0,-1.1788050828,-4.0902499841,2.0913820738
H,0,-1.7263045407,-2.945442645,4.2268621808
C,0,3.678127204,0.1500174798,-0.13828754
C,0,3.6785158593,-1.1432642916,-0.6909394833
C,0,4.8583417875,0.6557144576,0.4141473785
C,0,4.8320907922,-1.9093016913,-0.7361168631
C,0,6.0179028696,-0.1216252582,0.3759737257
H,0,4.8954533102,1.6232511746,0.8984571816
C,0,6.0142783619,-1.3912060241,-0.1992895565
H,0,4.8203669817,-2.9059434311,-1.17169121
H,0,6.9251111463,-1.9810499589,-0.2196281403
C,0,-0.2245264151,3.3334332621,0.5562911875
H,0,-1.3068030427,3.4022017522,0.583611311
C,0,2.5486507736,3.0762345996,0.4850872364
H,0,3.6266931831,3.0059255104,0.4298075268
C,0,2.2960144257,-1.5167759683,-1.1925264495
C,0,2.3689643626,-1.6955212621,-2.724267078
H,0,3.1387338751,-2.4353135314,-2.9656911106
H,0,1.4293026941,-2.0584256591,-3.1465957725
H,0,2.6355974409,-0.7532320203,-3.2110274877
C,0,1.7839403924,-2.8014826667,-0.5251744198
H,0,1.755428887,-2.6870893736,0.5623249427
H,0,0.7723167114,-3.0377412017,-0.8720722267
H,0,2.4355880492,-3.6459174431,-0.7723238334
H,0,6.9334901114,0.2701081211,0.8080982469

Zero-point correction=	0.498497 (Hartree/Particle)
Thermal correction to Energy=	0.525592
Thermal correction to Enthalpy=	0.526536
Thermal correction to Gibbs Free Energy=	0.441198
Sum of electronic and zero-point Energies=	-1385.465199
Sum of electronic and thermal Energies=	-1385.438104
Sum of electronic and thermal Enthalpies=	-1385.437160
Sum of electronic and thermal Free Energies=	-1385.522498

6NP-a-TS

C,0,-2.4896084307,-2.7890402837,1.2457753126
C,0,-1.7358331958,-0.7846095919,0.1325237368
C,0,-0.4007169857,-1.2297449434,0.3082619149
C,0,-1.1707312128,-3.2212828048,1.4224971502
C,0,-1.9944078294,0.4573958392,-0.5730008866
C,0,0.737448134,-0.4158069064,-0.14280788
C,0,0.428764787,0.7122878401,-0.9870422032
C,0,-0.9399996303,1.1060815024,-1.144159198
C,0,1.39335401,1.1429848265,-1.9220829759
C,0,2.7385493556,0.8182961004,-1.8624078242
H,0,-3.293361383,-3.4211920693,1.6118153671
H,0,-0.9733732299,-4.1666817016,1.9176318819
H,0,3.3077012699,0.7261184607,-2.783230435
O,0,1.9052765955,-0.7826696762,0.1608470025
H,0,1.0120570041,1.5952369001,-2.8383108516
C,0,3.369868062,0.4775688377,-0.6452838725
C,0,4.5639418964,-0.4020642701,-0.7202676385
C,0,5.7658821615,-0.0693387659,-0.0821087917
C,0,4.5024048835,-1.5707539706,-1.4916669035
C,0,6.8874196356,-0.8824770711,-0.2276788465
H,0,5.8267008439,0.8375234552,0.5112534164
C,0,5.619048032,-2.3881924586,-1.6247785082
H,0,3.5581353273,-1.8422619182,-1.9541141633
C,0,6.815991368,-2.0432794735,-0.9952929858
H,0,7.8173182279,-0.6080211683,0.2600828057
H,0,5.5551333903,-3.2983990661,-2.2124787182
H,0,7.6886404607,-2.6804617736,-1.0999627659
C,0,3.2359904835,1.3517698544,0.553021482
C,0,3.4479673685,0.8264205408,1.8372583857
C,0,2.9548483718,2.7151286372,0.4162533165
C,0,3.3621217822,1.6452681334,2.955992059
H,0,3.65007621,-0.2343501586,1.9454192763
C,0,2.8733948158,3.5364452879,1.5394223758
H,0,2.8110783018,3.1305073868,-0.5755920151
C,0,3.07401847,3.0041675765,2.8101754591
H,0,3.5147853354,1.2242672004,3.9446830464
H,0,2.6565444589,4.5929682702,1.418248016
H,0,3.0097999902,3.6436054874,3.6851140996
C,0,-3.3852478954,0.9424913724,-0.6853693916
C,0,-3.6667442955,2.2039928525,-1.2432861555
C,0,-4.4550910501,0.1586340142,-0.2228215684
C,0,-4.9638854917,2.6670409958,-1.3869782924

C,0,-5.7627469025,0.6408420427,-0.381469501
C,0,-6.0287074236,1.8728739004,-0.9605432841
H,0,-5.1446233008,3.6448346504,-1.8222866424
H,0,-7.0529430873,2.215529949,-1.0675233974
C,0,-0.1294350958,-2.4375483011,0.9672611703
H,0,0.9060364172,-2.731304016,1.0986774959
C,0,-2.7952606282,-1.5861909815,0.6180585247
C,0,-4.2643134791,-1.2002837495,0.449237225
C,0,-4.9565315868,-2.2785616507,-0.4154788652
H,0,-4.4962587872,-2.3249330149,-1.4066666063
H,0,-4.8712752618,-3.2645298246,0.0501399895
H,0,-6.019712213,-2.0544467108,-0.5397545416
C,0,-4.9253886893,-1.155433614,1.8457861375
H,0,-4.4494101646,-0.3916879954,2.467340675
H,0,-5.9906434939,-0.922916098,1.7703734458
H,0,-4.8315838814,-2.1191205911,2.3531489171
H,0,-1.110126407,1.975953876,-1.7708856004
H,0,-2.8529502608,2.8463573784,-1.559299305
H,0,-6.598392157,0.0363948307,-0.04159286
Zero-point correction= 0.499237 (Hartree/Particle)
Thermal correction to Energy= 0.526021
Thermal correction to Enthalpy= 0.526965
Thermal correction to Gibbs Free Energy= 0.442018
Sum of electronic and zero-point Energies= -1385.468865
Sum of electronic and thermal Energies= -1385.442082
Sum of electronic and thermal Enthalpies= -1385.441137
Sum of electronic and thermal Free Energies= -1385.526084

5/6NP-a -TS

C,0,2.2811683807,3.4907133781,0.5200769505
C,0,1.5630780577,1.2963071674,-0.0502414488
C,0,0.2160027103,1.6938245071,-0.0762520439
C,0,0.9389311453,3.9168323075,0.4821760138
C,0,1.8471247446,-0.0557481747,-0.346452597
C,0,-0.8342478049,0.6698116379,-0.2857607826
C,0,-0.4497838132,-0.6810325544,-0.7097679592
C,0,0.9525920987,-1.0124941725,-0.6959703368
C,0,-1.3912809739,-1.4296786395,-1.4469654333
C,0,-2.7528233678,-1.1728959318,-1.4753972172
H,0,3.0476696855,4.2227692055,0.7621861533
H,0,0.7128836366,4.9586408986,0.6872147473
H,0,-3.3252281897,-1.4097449907,-2.367676094
O,0,-2.0303083125,1.0391330149,-0.1261384085
H,0,-0.9933894996,-2.1299046728,-2.1782645974

C,0,-3.3970419307,-0.4907019869,-0.4209482869
C,0,-4.6487405287,0.2413276108,-0.7448086722
C,0,-5.822149991,0.0594638712,-0.001850507
C,0,-4.6704302651,1.0970517308,-1.8545900227
C,0,-6.9974906427,0.7082512799,-0.3740321235
H,0,-5.818055042,-0.6061399497,0.8555979942
C,0,-5.8410666594,1.7539780101,-2.2167572798
H,0,-3.7489257718,1.2623066305,-2.4047202599
C,0,-7.0090638687,1.5577528462,-1.4785268704
H,0,-7.9042001181,0.549574207,0.201004669
H,0,-5.8419639633,2.4252961145,-3.0696041738
H,0,-7.9237129789,2.0694998965,-1.761467706
C,0,-3.1993902402,-0.9183895193,0.9938687541
C,0,-3.43075823,-0.015335747,2.0425152036
C,0,-2.8311148395,-2.2325615872,1.3001586259
C,0,-3.2761262635,-0.4157375447,3.3640414272
H,0,-3.7028146085,1.008343308,1.8058117993
C,0,-2.6794704919,-2.6340125728,2.6260929329
H,0,-2.6724603009,-2.9406879273,0.493552062
C,0,-2.8984261207,-1.7272084212,3.6599693958
H,0,-3.4450438214,0.2961146045,4.1657969428
H,0,-2.3936799616,-3.6572407795,2.8486914153
H,0,-2.7794668644,-2.0393735028,4.6929067755
C,0,3.1802932678,-0.559198449,-0.2941265649
C,0,3.1645013106,-1.9180403191,-0.60671612
C,0,4.2888244224,0.2030950356,0.0228284461
C,0,4.3753979038,-2.5927710103,-0.6036781639
C,0,5.5035892806,-0.496904077,0.0249479433
C,0,5.535364902,-1.8634429689,-0.2806672027
H,0,4.4501697501,-3.6518404984,-0.8387528838
H,0,6.4918256293,-2.3772494515,-0.269330692
C,0,-0.0925793718,3.0331755869,0.2072954708
H,0,-1.1291014537,3.3532902399,0.2091841433
C,0,2.6304057948,2.1707817634,0.2638052254
C,0,1.7161542954,-2.3388302956,-0.9210872091
C,0,1.6483767141,-2.8522166391,-2.3708967158
H,0,2.3673694965,-3.6670716608,-2.5051469214
H,0,0.6587953948,-3.2479162464,-2.6151342527
H,0,1.8963578514,-2.0560936697,-3.078584602
C,0,1.2209590953,-3.4201520572,0.0504011195
H,0,1.3078982655,-3.0793571341,1.0858762318
H,0,0.1687365544,-3.653843361,-0.1481860427
H,0,1.8065755449,-4.3381013689,-0.0672003952
C,0,4.1095972658,1.7006879102,0.3258087145

C,0,4.9260387818,2.5050779817,-0.7070058502
H,0,4.5529002982,2.3225576124,-1.7186903697
H,0,4.8640276604,3.5785050076,-0.5034923974
H,0,5.9801194729,2.2124414913,-0.6699488515
C,0,4.6582477265,1.982817173,1.7394229119
H,0,4.0907907624,1.426239374,2.4905291368
H,0,5.7084924913,1.6823290084,1.8076374224
H,0,4.5954023359,3.0488682275,1.9779110191
H,0,6.4379531417,0.0067163832,0.2615143386

Zero-point correction=	0.561281 (Hartree/Particle)
Thermal correction to Energy=	0.591422
Thermal correction to Enthalpy=	0.592366
Thermal correction to Gibbs Free Energy=	0.500999
Sum of electronic and zero-point Energies=	-1502.097828
Sum of electronic and thermal Energies=	-1502.067687
Sum of electronic and thermal Enthalpies=	-1502.066743
Sum of electronic and thermal Free Energies=	-1502.158110

5NP-b -TS

C,0,-2.408000124,-3.189780404,3.1427547581
C,0,-2.2721494166,-1.7518597275,1.1837675951
C,0,-0.8605711269,-1.8117891261,1.2743306738
C,0,-1.0077011978,-3.2222268788,3.2388578817
C,0,-2.8569430219,-0.9994256351,0.0978577914
C,0,-0.0052319302,-1.0838920543,0.3222778347
C,0,-0.6330038893,-0.5777400579,-0.8829244981
C,0,-2.0671994934,-0.531415994,-0.9252548609
C,0,0.1742485121,-0.4603202272,-2.0399221046
C,0,1.5535928239,-0.3732211681,-2.0340356397
H,0,-3.013131226,-3.7411330682,3.8562125729
H,0,-0.5273084004,-3.7907491387,4.0286492851
H,0,2.1166314636,-0.7427713568,-2.8864644223
O,0,1.2295757147,-1.0118829514,0.565617016
H,0,-0.3076934548,-0.6327586826,-2.9983060445
C,0,2.2712884049,0.0888263528,-0.9027283143
C,0,3.6565973111,-0.3899520519,-0.7226627239
C,0,4.7087226477,0.4742743843,-0.4084195732
C,0,3.9490384171,-1.7525174915,-0.9186116269
C,0,6.0206609026,0.0127034474,-0.3056018896
H,0,4.5099605894,1.5318411857,-0.2664786208
C,0,5.2409924719,-2.227597889,-0.8066152723
H,0,3.1320212347,-2.4375535496,-1.1243102827
C,0,6.2881476002,-1.3440545523,-0.5024870291
H,0,6.8136290298,0.7142135383,-0.0773059485

H,0,5.473772148,-3.2789339176,-0.9368196356
C,0,1.8747210457,1.3478331552,-0.2291521917
C,0,2.1999520887,1.5705303313,1.1136836867
C,0,1.1822128934,2.3543488538,-0.9202973939
C,0,1.8346661778,2.7451205477,1.7633549239
H,0,2.7113240958,0.7893571756,1.6672298596
C,0,0.8189308826,3.5328866507,-0.2909253037
H,0,0.9393085822,2.2070637378,-1.9674171244
C,0,1.1371616962,3.7326323384,1.0576606815
H,0,2.0844396802,2.8732819548,2.8094692281
H,0,0.2875159888,4.3166432488,-0.8200543819
C,0,-4.2532422012,-0.590756071,-0.1405674185
C,0,-4.2923941916,0.0933883683,-1.3689441027
C,0,-5.4251429655,-0.7019839435,0.6135874162
C,0,-5.4728117205,0.6225642742,-1.864817567
C,0,-6.6124591435,-0.1598259198,0.116331933
H,0,-5.4364843918,-1.1725537473,1.5884750065
C,0,-6.6456432295,0.4920427982,-1.1150021742
H,0,-5.4897428708,1.1438369969,-2.8193999043
H,0,-7.5774972633,0.9073237065,-1.4854145072
C,0,-0.2472158996,-2.5311923869,2.3152813924
H,0,0.8366218505,-2.5332250369,2.361959509
C,0,-3.0263863575,-2.4667930192,2.1395408353
H,0,-4.1055535175,-2.4833448193,2.0672899793
C,0,-2.9158626686,0.1379684392,-2.005896344
C,0,-2.9685703066,-0.666140502,-3.3228622955
H,0,-3.7584811957,-0.2607495371,-3.9631961277
H,0,-2.0343745055,-0.6073156882,-3.8856996064
H,0,-3.1954072367,-1.7172325602,-3.1236090326
C,0,-2.4682407677,1.5820978869,-2.2736077054
H,0,-2.4519465672,2.1598647737,-1.3448938976
H,0,-1.4624960566,1.5996525959,-2.7066980931
H,0,-3.1509307781,2.0690531179,-2.9776972064
O,0,0.7358467121,4.9119454386,1.5920703864
C,0,1.0155313887,5.1511477847,2.9574374531
H,0,0.6029526682,6.1341799339,3.1802115479
H,0,0.536744505,4.3997400233,3.5955228673
H,0,2.0956634586,5.1568981245,3.1442355884
O,0,7.5202357096,-1.9001589786,-0.4163169564
C,0,8.6084414483,-1.0560098363,-0.0947112704
H,0,8.4666635435,-0.586962601,0.8856602074
H,0,9.4879984454,-1.6976180132,-0.0679173569
H,0,8.7443347814,-0.2800484122,-0.8567606141
H,0,-7.5211371281,-0.2442095895,0.7045922123

Zero-point correction= 0.564676 (Hartree/Particle)
Thermal correction to Energy= 0.596874
Thermal correction to Enthalpy= 0.597818
Thermal correction to Gibbs Free Energy= 0.500751
Sum of electronic and zero-point Energies= -1614.367908
Sum of electronic and thermal Energies= -1614.335711
Sum of electronic and thermal Enthalpies= -1614.334766
Sum of electronic and thermal Free Energies= -1614.431833

5NP-c- TS

C,0,-2.8267619631,-2.4441044248,3.7080957546
C,0,-2.3946412929,-1.5395188103,1.4911908779
C,0,-1.0541092,-1.9788504256,1.6056498987
C,0,-1.4887888628,-2.8520950786,3.8225605746
C,0,-2.8006344874,-0.8907726861,0.2641578777
C,0,-0.0803948223,-1.7341295863,0.5279210619
C,0,-0.6077933683,-1.3467085005,-0.7686065045
C,0,-1.970966209,-0.8953954864,-0.8299613103
C,0,0.1218326721,-1.7405969561,-1.9111456114
C,0,1.4649547369,-2.0834383559,-1.9030646949
H,0,-3.5245352587,-2.6414780839,4.5162867369
H,0,-1.1467532993,-3.3577528146,4.7197331143
H,0,1.8359685027,-2.8113673668,-2.6190063088
O,0,1.1366281066,-1.9548249524,0.7657435309
H,0,-0.4469816544,-1.9676727544,-2.8085185478
C,0,2.3448126136,-1.6053249235,-0.9093442659
C,0,3.5542945019,-2.4130867126,-0.6127237138
C,0,4.8303489273,-1.8370937712,-0.5645890923
C,0,3.4221909042,-3.7954104349,-0.4213953048
C,0,5.9528940582,-2.6329731269,-0.3478129897
H,0,4.9441219553,-0.7684676477,-0.7174744471
C,0,4.5424025605,-4.5860721142,-0.1918779572
H,0,2.4271851755,-4.2303083131,-0.4213347268
C,0,5.8115122643,-4.0061847491,-0.1584745051
H,0,6.9381311502,-2.1783312798,-0.325893137
H,0,4.4266333323,-5.6530523044,-0.0304229872
H,0,6.6866715651,-4.6232607295,0.0197719123
C,0,2.3813218714,-0.1591637755,-0.5608414281
C,0,2.8411262291,0.258321336,0.6970174211
C,0,2.0054437621,0.8140854376,-1.4921242944
C,0,2.8962778236,1.6068210479,1.0170998797
H,0,3.1308965271,-0.4894541575,1.4283173499
C,0,2.0657749089,2.1662528652,-1.1705675708
H,0,1.6650578834,0.5053202755,-2.4750548761

C,0,2.5069220447,2.5850878532,0.0893596312
H,0,3.2638131121,1.9119947555,1.9924819301
H,0,1.744418279,2.9047996405,-1.8994456693
C,0,-4.0343307575,-0.1530241054,-0.0651381025
C,0,-3.9454063513,0.2426455558,-1.4117655398
C,0,-5.1436835329,0.2403255152,0.6889849107
C,0,-4.9518760559,0.9777189113,-2.0169799668
C,0,-6.1527514889,0.9892903287,0.07969022
H,0,-5.2323484985,0.0065503085,1.7423307826
C,0,-6.0681207717,1.3522008075,-1.2633807126
H,0,-4.8735243519,1.2724043407,-3.0610866888
H,0,-6.8619883866,1.9347704315,-1.7198148018
C,0,-0.6129025607,-2.6108102719,2.781272488
H,0,0.4283306139,-2.9095503809,2.8394972855
C,0,-3.2688727994,-1.7971078858,2.5685259189
H,0,-4.3115719244,-1.5197868354,2.4908993686
C,0,-2.6506848186,-0.2456242112,-2.034249533
C,0,-3.0006303618,-1.2492938458,-3.1540012151
H,0,-3.6820764829,-0.7732601498,-3.8661223089
H,0,-2.1205801422,-1.5704196825,-3.7156023282
H,0,-3.4987472168,-2.1309892556,-2.7411399823
C,0,-1.8231966256,0.9195241556,-2.5963243365
H,0,-1.595748414,1.6466999967,-1.811457114
H,0,-0.8774560132,0.5542808951,-3.0108814102
H,0,-2.3728605078,1.4269096017,-3.395832938
C,0,2.5672771002,4.026284875,0.4358448451
C,0,3.0015951522,4.9715367883,-0.5023033819
C,0,2.1887962617,4.4701535696,1.709469174
C,0,3.0566139389,6.32400771,-0.1759661274
H,0,3.3214920322,4.6391967076,-1.4858790875
C,0,2.2429639758,5.8225154954,2.0360047156
H,0,1.8244050114,3.7518324474,2.4383549153
C,0,2.6774731462,6.7543871911,1.094600366
H,0,3.4041659014,7.0417410526,-0.912571804
H,0,1.9363119071,6.1498353365,3.0245629583
H,0,2.7197887577,7.8086207959,1.3491267691
H,0,-7.0123922264,1.297561448,0.6666553833
Zero-point correction= 0.579877 (Hartree/Particle)
Thermal correction to Energy= 0.611712
Thermal correction to Enthalpy= 0.612656
Thermal correction to Gibbs Free Energy= 0.515622
Sum of electronic and zero-point Energies= -1616.356767
Sum of electronic and thermal Energies= -1616.324932
Sum of electronic and thermal Enthalpies= -1616.323988

Sum of electronic and thermal Free Energies= -1616.421022

NP-a-CC

C,0,-5.5695707177,-2.5172973527,-0.2014213485
C,0,-3.567986111,-1.141472359,-0.116645081
C,0,-2.7959392152,-2.3223796443,-0.1468856041
C,0,-4.7955340391,-3.6778447098,-0.2579775498
C,0,-2.8993438843,0.1679981889,0.0031881471
C,0,-1.3081579004,-2.2771603751,-0.0674560903
C,0,-0.6853761862,-0.920581283,0.0215986929
C,0,-1.5543107016,0.2324374726,0.1322854216
C,0,0.6682378403,-0.8533456024,-0.0830152993
C,0,1.5393585662,0.3155469263,-0.1229719443
H,0,-6.6532507358,-2.586123673,-0.2071687591
H,0,-5.2710769278,-4.6513793462,-0.3184360833
H,0,2.4791739003,0.1781159137,0.4109487835
O,0,-0.6414863932,-3.3008840613,-0.088236624
H,0,1.1760462683,-1.8180023783,-0.1012408916
C,0,1.3939483419,1.4881092728,-0.7922314446
C,0,2.4042212203,2.5649277922,-0.6204812432
C,0,2.7445278192,3.396540652,-1.6970432489
C,0,3.0429079412,2.7700068705,0.6107646476
C,0,3.7169135601,4.3822045903,-1.5543297503
H,0,2.249019654,3.2578809334,-2.6537029902
C,0,4.0123797312,3.7582290153,0.7543425634
H,0,2.7581166967,2.1651306575,1.4668697465
C,0,4.3560734033,4.5655720799,-0.329123149
H,0,3.9752795691,5.0084293832,-2.4026518384
H,0,4.4908448123,3.9064174758,1.7175955029
H,0,5.1097490283,5.3385804576,-0.2163107056
C,0,0.2809309065,1.7490073992,-1.7447159435
C,0,-0.4871646559,2.9152677381,-1.6160044602
C,0,-0.0527505423,0.8237193273,-2.7371331004
C,0,-1.6030630734,3.1205090928,-2.4199032475
H,0,-0.2251180292,3.6427154964,-0.8511671477
C,0,-1.1580629506,1.0392693214,-3.5581339626
H,0,0.5474928662,-0.0746943181,-2.8500012166
C,0,-1.9425890444,2.1791473838,-3.3918681022
H,0,-2.2192197232,4.00324733,-2.2748950103
H,0,-1.4105077023,0.3114924653,-4.3233232056
H,0,-2.8170234716,2.3351898506,-4.0166718302
C,0,-3.667404097,1.4392341532,-0.061524879
C,0,-3.4667668372,2.4454431476,0.8901059891
C,0,-4.0901817325,3.6849500071,0.7587006026

C,0,-5.1433915114,2.9370389783,-1.2755159577
C,0,-4.9306962105,3.9351776785,-0.3243421063
H,0,-3.9246969585,4.4533924667,1.5077399391
H,0,-5.4189523236,4.8994782084,-0.4256991754
C,0,-3.4111020101,-3.5738750719,-0.2205723771
H,0,-2.7741638046,-4.4525767248,-0.2414283209
H,0,-1.0864408819,1.2010661771,0.2588619577
H,0,-2.8178256198,2.2484620899,1.7391346553
H,0,-5.7899554034,3.1259911065,-2.1274382899
C,0,-4.5167585123,1.7010705368,-1.1453552102
H,0,-4.6548399664,0.9393544145,-1.9084280649
C,0,-4.9655255016,-1.2666919709,-0.1278525757
H,0,-5.5839111196,-0.3783101805,-0.0597069297
Zero-point correction= 0.436736 (Hartree/Particle)
Thermal correction to Energy= 0.461495
Thermal correction to Enthalpy= 0.462439
Thermal correction to Gibbs Free Energy= 0.380583
Sum of electronic and zero-point Energies= -1268.856737
Sum of electronic and thermal Energies= -1268.831979
Sum of electronic and thermal Enthalpies= -1268.831034
Sum of electronic and thermal Free Energies= -1268.912891

NP-a-TT

C,0,-2.9666352358,-1.0817943722,3.2325721986
C,0,-2.4601318974,-0.6322727944,0.9004367465
C,0,-1.1815019589,-1.1886792426,1.1045904716
C,0,-1.706054373,-1.6538026102,3.4169962582
C,0,-2.8176506344,-0.1038389919,-0.4293866371
C,0,-0.1758021955,-1.2253318792,0.0075377845
C,0,-0.4786219786,-0.3870187456,-1.1908284377
C,0,-1.8668456363,0.0063502583,-1.3848471432
C,0,0.4523713295,0.0042608964,-2.1021016443
C,0,1.9058390573,-0.0843125439,-2.0903107675
H,0,-3.6641167409,-1.0264522912,4.0629827666
H,0,-1.4206611777,-2.0488290662,4.3867717997
H,0,2.3507776392,-0.262221078,-3.0684626785
O,0,0.8232846512,-1.9200251486,0.0923615277
H,0,0.0496077027,0.4819363042,-2.998502255
C,0,2.757014515,0.137513466,-1.0601590573
C,0,4.2157046056,-0.0592093844,-1.2498931982
C,0,5.1375061146,0.7838058511,-0.612551919
C,0,4.701586582,-1.0912436742,-2.0647478534
C,0,6.5049848045,0.6192058209,-0.8113966293
H,0,4.7735034901,1.577966976,0.0331248816

C,0,6.0696852878,-1.2587668805,-2.2590390992
H,0,3.9989656936,-1.783432918,-2.519358899
C,0,6.9759268425,-0.4010319574,-1.6371144812
H,0,7.2049881657,1.2877806599,-0.3198615351
H,0,6.4289967007,-2.0700790042,-2.8845645028
H,0,8.0430229365,-0.5340622193,-1.7858881498
C,0,2.2983127529,0.5941467764,0.2767156095
C,0,2.719126491,-0.0853638689,1.4268901915
C,0,1.4169246605,1.6721173738,0.4126252455
C,0,2.2340053811,0.2800512717,2.6798487717
H,0,3.4020931153,-0.9241057239,1.3270211231
C,0,0.9325982221,2.0390982726,1.6653941439
H,0,1.1013489396,2.2141442657,-0.4743719532
C,0,1.3333035387,1.3374674538,2.8018167807
H,0,2.5538919291,-0.2672924286,3.5614841137
H,0,0.2424934596,2.8723830896,1.7540169369
H,0,0.9471719965,1.6153046115,3.7776911269
C,0,-4.2135125284,0.3164090904,-0.7230929103
C,0,-4.4835936545,1.5903432146,-1.2345297702
C,0,-5.786839986,1.9668922209,-1.5555414744
C,0,-6.5817273252,-0.1981103927,-0.8562132636
C,0,-6.8394217311,1.074347596,-1.3668823434
H,0,-5.9799039494,2.9612322358,-1.9465311292
H,0,-7.8547564569,1.3669257205,-1.6155880825
C,0,-0.818132232,-1.7053741794,2.3498952564
H,0,0.1751608302,-2.1312600362,2.4544000324
H,0,-2.1355383009,0.4227505265,-2.3541824766
H,0,-3.6642647175,2.2918434782,-1.365983306
H,0,-7.3955916256,-0.9025411772,-0.7140852109
C,0,-5.2808537976,-0.5724786289,-0.5343542666
H,0,-5.0801840809,-1.5680846799,-0.147254309
C,0,-3.3420116252,-0.5802239198,1.9905606962
H,0,-4.3237685949,-0.1355205932,1.8660219198
Zero-point correction= 0.436491 (Hartree/Particle)
Thermal correction to Energy= 0.461347
Thermal correction to Enthalpy= 0.462291
Thermal correction to Gibbs Free Energy= 0.379519
Sum of electronic and zero-point Energies= -1268.849988
Sum of electronic and thermal Energies= -1268.825132
Sum of electronic and thermal Enthalpies= -1268.824188
Sum of electronic and thermal Free Energies= -1268.906960

8. Reference

1. M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E.R. Scuseria, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. , Gaussian 09, revision B01, Gaussian Inc.: Wallingford, CT, 2013.
2. A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* 2009**, 113**, 6378-6396.
3. J. P. Foster, F. Weinhold, *J. Am. Chem. Soc.* 1980, **102**, 7211-7218.
4. A. E. Reed, R. B. Weinstock, F. Weinhold, *J. Chem. Phys.* 1985**, 83**, 735-746.
5. E. R. Johnson, S. Keinan, P. Mori-Sánchez, J. Contreras-García, A. J. Cohen, W. Yang, *J. Am. Chem. Soc.* 2010**, 132**, 6498-6506.
6. J. Contreras-García, E. R. Johnson, S. Keinan, R. Chaudret, J.-P. Piquemal, D. N. Beratan, W. Yang, *J. Chem. Theory Comput.* 2011**, 7**, 625-632.
7. T. Lu, F. Chen, *J. Comput. Chem.* 2012**, 33**, 580-592.
8. T. Lu, F. Chen, *J. Mol. Graphics Modell.* 2012**, 38**, 314-323.
9. C. Legault, Y. Universitede Sherbrooke: Que bec, Montreal, Canada, 2009;http://www.cylview.org.
10. W. Humphrey, A. Dalke, K. Schulten, *J. Mol. Graphics*, 1996**, 14**, 33-38.
11. I. Olaizola, T. E. Campano, I. Iriarte, S. Vera, A. Mielgo, J. M. García, J.M. Odriozola, M. Oiarbide, C. Palomo, *Chem. Eur. J.* 2018, **24**, 3893-3901.
12. C. J. Blackwell, C. D. Gabbutt, J. T. Guthrie, M. HeronB, *Dyes Pigments*, 2012, **95**, 408-420.
13. F. Ercole, N. Malic, T. Davis, R.Evans, *J. Mater. Chem.,* 2009*,* **19***,* 5612-5623.
14. T. Ishiyama, H. Isou, T. Kikuchia, N. Miyaura, *Chem. Commun.*, 2010, **46**, 159-161.
15. S. Kawamorita, H. Ohmiya, K. Hara, A. Fukuoka, M. Sawamura, *J. Am. Chem. Soc.* 2009, **131**, 5058–5059.
16. K. Mutoh, Y. Kobayashi, Y. Hirao, T. Kubob, J. Abe, *Chem. Commun*., 2016, **52**, 6797-6800.
17. A. H. Choon, S. M. Ran, C. Y. Jun, K. H. Joo, K. B. Ok, K. S. Min, WO2011/115378.