Supporting Information

Silindeno-Fused *3H*-Naphthopyrans with Fast Thermal Fading Rate and High Optical Density

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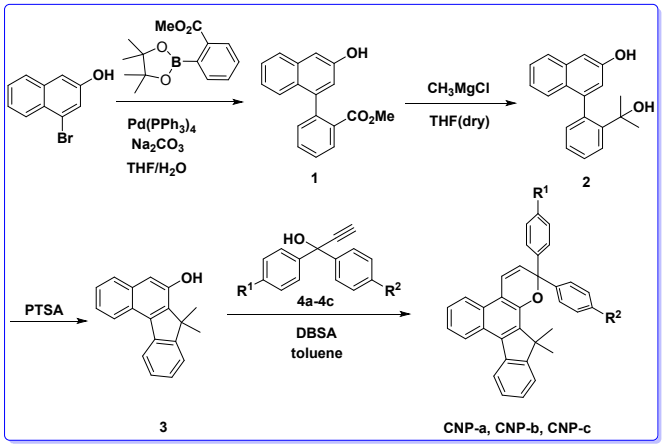
1. Synthesis of compounds CNPs, SiNPs and NP-Ph



Scheme S1. Synthetic route to CNPs.

Synthesis of methyl 2-(3-hydroxynaphthalen-1-yl)benzoate (1).[S1] A mixture of 4-bromonaphthalen-2-ol (0.50 g, 2.2 mmol), methyl 2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzoate (0.70 g, 2.64 mmol), $Pd(PPh_3)_4$ (0.25 g, 0.22 mmol) and Na_2CO_3 (1.12 g, 10.56 mmol) in THF (20 mL) and water (8 mL) was stirred at 80 °C under nitrogen for 12 h. After cooling down to room temperature, the reaction mixture was extracted by ethyl acetate twice (2×10 mL). The organic phase was combined and washed with brine and water, then dried with anhydrous $MgSO_4$, filtered and the solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography using petroleum ether/ethyl acetate (v/v = 20:1) as an eluent affording **1** as orange solid. Yield, 72%. m.p. 151.6 - 152.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.0 Hz, 1H), 7.77 – 7.45 (m, 3H), 7.44 – 7.30 (m, 3H), 7.21 – 7.10 (m, 1H), 7.03 (s, 1H), 6.92 (s, 1H), 5.66 (s, 1H), 3.42 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.34, 152.86, 141.54,140.95, 134.73, 131.91, 131.88, 131.57, 130.15, 127.87, 127.79, 126.31, 125.46, 123.74, 118.20, 109.40, 52.17.

Synthesis of 4-(2-(2-hydroxypropan-2-yl)phenyl)naphthalen-2-ol (2).[S1] To a three-neck flask under a nitrogen atmosphere was added **1** (1.05 g,3.8 mmol) and anhydrous THF (10 mL). Methyl magnesium bromide (5 mL of 3.0M in 2-methyltetrahydrofuran) was added to the reaction mixture over 15 min. The reaction mixture was stirred at 40 °C under nitrogen for 6 h, then cooled to room temperature, and poured in saturated aqueous NH_4Cl solution (20 mL). The mixture was extracted with ethyl acetate twice (2 × 10 mL). The organic extracts were combined and washed with brine and water, then dried with anhydrous $MgSO_4$, filtered and the solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography using petroleum ether/ethyl acetate (v/v = 5:1) as an eluent affording **2** as a viscous white oil. Yield, 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.4 Hz, 1H), 7.41 (t, *J* = 8.0 Hz, 1H), 7.3 (t, *J* = 8.0 Hz, 1H), 7.29 - 7.23 (m, 2H), 7.17 - 7.13 (m, 1H), 7.04 (d, *J* = 7.6 Hz, 1H), 6.97 (s, 1H), 6.96 (s, 1H),1.391 (s,3H), 1.386 (s,3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.72, 146.70, 143.00, 136.94, 134.95, 132.67, 128.60, 127.97, 126.89, 126.85, 126.57, 126.47, 126.40, 123.69, 119.38, 109.51, 74.90, 32.36, 32.17.

Synthesis of 7,7-dimethyl-7H-benzo[c]fluoren-6-ol (3).[S2] To a 100 mL of round bottom flask **2** (0.3 g, 1.15 mmol) and xylene (20 mL) were added under a nitrogen atmosphere. After *p*-toluenesulfonic acid (27 mg, 0.14 mmol) was added, the reaction mixture was refluxed for 2 h, and cooled to room temperature. The solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography using petroleum ether/ethyl acetate

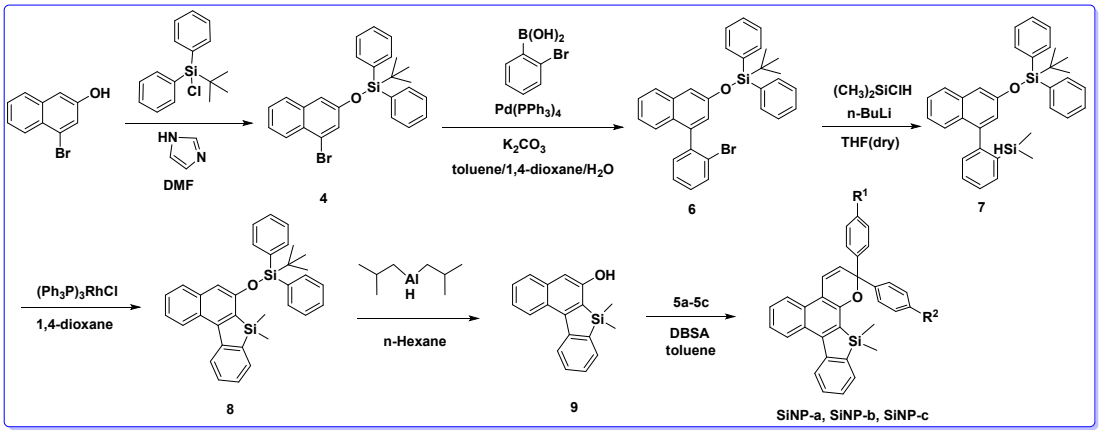
(v/v = 5:1) as an eluent affording **3** as a viscous brown oil. Yield, 63%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 8.0 Hz, 1H), 8.32 (d, *J* = 7.6 Hz,1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.42 - 7.33 (m, 5H), 6.89 (s, 1H), 5.02 (s,1H), 1.65 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.73, 151.19, 141.28, 139.92, 136.23, 135.16, 127.29, 127.12, 126.83, 125.66, 124.29, 124.00, 123.34, 122.35, 110.38, 47.47, 24.36.

Synthesis of 13,13-dimethyl-2,2-diphenyl-2,13-dihydrobenzo[f]indeno[1,2-h] chromene (CNP-a). A solution of 7,7-dimethyl-7H-benzo[c]fluoren-6-ol **3** (0.20 g, 0.77 mmol), 1,1-diphenylprop-2-yn-1-ol **5a** (0.21 g, 1.00 mmol), and dodecylbenzenesulphonic acid (cat. amount) in dry toluene (20 mL) was stirred at 40 °C for 3h. Then the reaction mixture was washed with water and the organic phase was separated. After evaporation of toluene, the product was isolated by column chromatography (silica gel, eluent petroleum ether : ethylacetate 100 : 1). Yield, 87%. Yellow solids, m.p. 83.0 - 84.1 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 8.0 Hz, 1H), 8.27 (d, *J* = 7.6 Hz, 1H), 8.11 (d, *J* = 8.4 Hz, 1H), 7.57-7.37 (m, 10H), 7.33-7.28 (m,5H), 7.25-7.20 (m, 1H), 6.07 (d, *J* = 10.0 Hz, 1H), 1.62 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.77, 148.12, 144.56, 140.98, 139.77, 136.56, 130.55, 128.123, 127.68, 127.63, 126.85, 126.46, 125.90, 125.77, 124.51, 124.25, 123.30, 122.38, 122.29, 120.08, 113.78, 83.61, 47.47, 24.98. HRMS-ESI calcd for $C_{34}H_{26}O$ $[M+Na]^+$ 473.1881; found 473.1880.

The chromemes **CNP-b** and **CNP-c** were synthesized according to the same procedure as that for **CNP-a**.

2-([1,1'-biphenyl]-4-yl)-13,13-dimethyl-2-phenyl-2,13-dihydrobenzo[f]indeno[1,2-h]chromene (CNP-b). Yield, 46%. Pale yellow solids, m.p. 91.6 – 92.4 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 8.0 Hz, 1H), 8.27 (d, *J* =7.6 Hz, 1H), 8.11 (d, *J* = 8.0 Hz, 1H), 7.62 - 7.18 (m, 20H), 6.08 (d, *J* = 10.0 Hz, 1H), 1.64 (s, 3H), 1.63 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ155.67,148.04, 144.43, 143.45, 140.90, 140.65,140.41, 139.68, 136.53, 130.47, 128.79, 128.22, 128.05, 127.66, 127.59,127.38,127.14, 127.04, 126.89, 126.79, 126.29, 125.85, 125.71, 124.44, 124.21, 123.23, 122.32, 122.23, 120.10, 113.73, 83.41, 47.41, 24.94. HRMS-ESI calcd for $C_{40}H_{30}O$ $[M+H]^+$527.2375; found 527.2373.

2,2-bis(4-methoxyphenyl)-13,13-dimethyl-2,13-dihydrobenzo[f]indeno[1,2-h]chromene (CNP-c). Pale yellow solids, m.p. 165.6-166.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 7.9 Hz, 1H), 8.27 (d, *J* = 7.6 Hz, 1H), 8.11 (d, *J* = 8.1 Hz, 1H), 7.47 - 7.35 (m, 10H), 6.90 - 6.76 (m, 4H), 6.01 (d, *J* = 10.0 Hz, 1H), 3.76 (s, 6H), 1.60 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ159.02, 155.78, 148.15, 141.08, 139.83, 136.94, 136.39, 130.55, 128.99, 127.08, 126.95, 126.79, 125.83, 125.72, 124.50, 124.16, 123.27, 122.37, 122.28, 119.60, 113.85, 113.50, 83.12. 55.37, 47.41, 24.95. HRMS-ESI calcd for $C_{36}H_{30}O_3$ $[M+Na]^+$533.2093; found 533.2090.



Scheme S2. Synthetic route to **SiNPs**.

Synthesis of ((4-bromonaphthalen-2-yl)oxy)(tert-butyl)diphenylsilane 5. To a 50 mL of round bottom flask 4-bromonaphthalen-2-ol (1.1 g, 4.93 mmol), 1*H*-imidazole (0.62 g, 9.07 mmol), *tert*-butylchlorodiphenylsilane (1.08 mL, 4.14 mmol) and DMF (15 mL) were added, and the reaction mixture was stirred at room temperature for 14 h. Then, the mixture was poured in water (20 mL) and extracted with ethyl acetate twice (3 × 20 mL). The organic extracts were combined and washed with brine and water, then dried with anhydrous $MgSO_4$, filtered and the solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography using petroleum ether as an eluent affording **5** as white solid. Yield, 85%. Mp 129.8 – 130.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.0 Hz, 1H), 8.10 – 7.99 (d, *J* = 8.0 Hz, 4H), 7.82 (d, *J* = 2.4 Hz, 1H), 7.66 –7.46 (m, 9H), 7.24 (d, *J* = 2.4 Hz, 1H), 1.43 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.99, 132.97, 135.63, 135.55, 134.91, 132.27, 130.27, 128.07, 127.83, 125.76, 125.17, 123.17, 114.76, 114.72, 26.68, 19.62.

Synthesis of ((4-(2-bromophenyl)naphthalen-2-yl)oxy)(tert-butyl)diphenylsilane 6. A mixture of **4** (0.97 g, 2.1 mmol), (2-bromophenyl)boronic acid (0.42 g, 2.1 mmol), $Pd(PPh_3)_4$ (0.12 g, 0.10 mmol) and K_2CO_3(1.46 g, 10.54 mmol) in 1,4-dioxane (20 mL) and water (10 mL) was stirred at 95 °C under argon for 20 h. After cooling down to room temperature, the reaction mixture was extracted by ethyl acetate twice (2 × 50 mL). The organic phase was combined and washed with brine and water, then dried with anhydrous $MgSO_4$, filtered and the solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography using petroleum ether as an eluent affording **4** as white solid. Yield, 74%. Mp 135.3 – 135.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (m, 4H), 7.78 (dd, *J* = 8.4, 1.3 Hz, 1H), 7.66 – 7.62 (m, 1H), 7.55 – 7.51 (m, 2H), 7.50 – 7.46 (m, 4H), 7.42 (m, 4H), 7.32 (m, 3H), 7.16 (d, *J* = 2.4 Hz, 1H), 1.28 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.66, 140.88, 140.53, 135.72, 135.71, 134.67, 132.85, 132.76, 131.91, 130.09, 129.19, 127.99, 127.26, 127.14, 126.19, 125.81, 124.28, 124.08, 123.10, 115.03, 26.73, 19.70. HRMS (ESI) Calcd. for $C_{32}H_{29}BrOSi$ $[M+H]^+$ 537.1123, found 537.1124.

Synthesis of tert-butyl((4-(2-(dimethylsilyl)phenyl)naphthalen-2-yl)oxy)diphenylsilane 7. To a 100 mL of Schlenk flask was added **6** (2.64 g, 4.92 mmol), and the Schlenk flask was sealed and evacuated with argon. Absolute THF (30 mL) was injected into the Schlenk flask, and the mixture was cooled to -78 °C under magnetic stirring. Then, chlorodimethylsilane (2.5 M, 2.40 mL, 5.90 mmol) was added slowly to the reaction mixture, which was stirred at -78 °C for 1 h, and then stirred at room temperature for 9 h. The reaction mixture was extracted by ethyl acetate (2 × 70 mL). The organic phase was combined and washed with brine and water, then dried with anhydrous $MgSO_4$, filtered and the solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography using petroleum ether as an eluent affording **7** as pale yellow crystals. Yield, 83%. Mp 138.5 – 139.1 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (dd, *J* = 8.0, 2.2 Hz, 2H), 8.13 (dd, *J* = 8.0, 2.2 Hz, 2H), 7.99 (dd, *J* = 8.0, 2.4 Hz, 1H), 7.75 (d, *J* = 8.2 Hz, 1H), 7.72 – 7.60 (m, 9H), 7.58 – 7.52 (m, 2H), 7.50 (d, *J* = 2.4 Hz, 1H), 7.44 – 7.39 (m, 2H), 4.40 (m, 1H), 1.50 (s, 9H), 0.21 (d, *J* = 3.5 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.4, 146.5, 142.5, 135.7, 135.0, 134.5, 133.1, 132.6, 130.0, 128.8, 128.6, 127.9, 127.0, 126.8, 126.5, 126.0, 123.7, 123.1, 114.3, 27.3, 19.6, -3.0. HRMS (ESI) Calcd. for $C_{34}H_{36}OSi_2$ $[M+H]^+$ 536.8310, found 536.8310.

Synthesis of 6-((tert-butyldiphenylsilyl)oxy)-7,7-dimethyl-7H-benzo[b]naphtho[1,2-d]silole 8. To a 50 mL of Schlenk flask was added **7** (0.40 g, 0.78 mmol) and triphenylphosphine rhodium chloride (35 mg, 0.04 mmol), and the Schlenk flask was sealed and evacuated with argon. Absolute dry 1,4-

dioxane (10 mL) was injected into the Schlenk flask, and the mixture was stirred at 115 °C for 24 h. After cooling down to room temperature, the reaction mixture was extracted by ethyl acetate (3 × 20 mL). The organic phase was combined and washed with brine and water, then dried with anhydrous $MgSO_4$, filtered and the solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography using petroleum ether/ethyl acetate (v/v = 5:1) as an eluent affording **8** as white crystals. Yield, 51%. Mp 168.7 – 168.1 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.81 (m, 2H), 7.80 – 7.74 (m, 3H), 7.47 (d, *J* = 8.2 Hz, 1H), 7.45 – 7.28 (m, 9H), 7.21 – 7.10 (m, 3H), 7.04 (d, *J* = 2.4 Hz, 1H), 1.15 (s, 9H), -0.01 (s, 3H), -0.23 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.1, 144.2, 141.6, 137.7, 134.4, 134.3, 133.3, 133.0, 131.7, 131.2, 128.9, 128.8, 127.8, 127.4, 126.7, 125.9, 125.6, 125.1, 125.0, 122.7, 121.9, 113.2, 25.3, 18.3, -0.1. HRMS (ESI) Calcd. for $C_{34}H_{34}OSi_2$ $[M+H]^+$ 535.1876, found 535.1888.

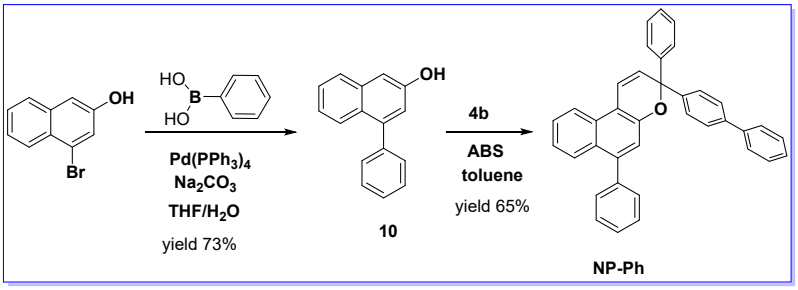
Synthesis of 7,7-dimethyl-7H-benzo[b]naphtho[1,2-d]silol-6-ol 9. To a 50 mL of Schlenk flask was added **8** (0.15 g, 0.30 mmol), and the Schlenk flask was sealed and evacuated with argon. Then, absolute dry hexane (b mL) and diisobutyl aluminium hydride (0.72 mL, 0.86 mmol) were injected into the Schlenk flask, and the mixture was stirred at 50 °C for 7 h. After cooling down to room temperature, the reaction mixture was extracted by ethyl acetate (2 × 10 mL). The organic phase was combined and washed with brine and water, then dried with anhydrous $MgSO_4$, filtered and the solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography using petroleum ether/ethyl acetate (v/v = 2:1) as an eluent affording **9** as pale yellow solid. Yield, 87%. Mp 180.5 – 181.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.0 Hz, 1H), 7.62 (s, 1H), 7.49 – 7.33 (m, 4H), 7.24 (s, 1H), 7.19 – 7.10 (m, 2H), 6.98 (s, 1H), 0.03 (s, 3H), -0.27 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.7, 144.8, 141.9, 137.2, 134.0, 133.6, 129.5, 128.4, 127.3, 126.0, 125.6, 125.5, 122.7, 118.9, 109.0, -0.3. HRMS (ESI) Calcd. for $C_{18}H_{17}OSi$ $[M+H]^+$, found 277.1042.

Synthesis of 13,13-dimethyl-2,2-diphenyl-2,13-dihydrobenzo[f]benzo[4,5]silolo[3,2-h]chromene SiNP-a. A solution of **9** (0.13 g, 0.46 mmol), 1,1-diphenylprop-2-yn-1-ol **5a** (0.11 g, 0.52 mmol), and two drops of dodecylbenzenesulphonic acid in dry toluene (8 mL) was stirred at 40 °C for 3 h. Then the reaction mixture was washed with water and the organic phase was separated. After evaporation of toluene, the product was isolated by column chromatography (silica gel, eluent petroleum ether : ethylacetate 40 : 1). Yield, 62%. Pale yellow solids. Mp 170.6 – 171.1 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 8.4, 2.8 Hz, 1H), 7.67 – 7.58 (m, 1H), 7.43 – 7.35 (m, 4H), 7.34 – 7.26 (m, 4H), 7.23 – 6.97 (m, 9H), 6.19 (dd, *J* = 10 Hz, 1H), -0.34 (d, *J* = 20 Hz, 3H), -0.76 (d, *J* = 20 Hz, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 149.5, 145.1, 145.0, 144.4, 143.4, 139.5, 139.5, 134.9, 134.8, 130.0, 129.8, 129.1, 128.5, 128.2, 128.1, 127.9, 127.5, 127.1, 126.7, 126.6, 123.5, 121.4, 121.3, 119.9, 119.7, 113.9, 82.5, 2.8, 1.4. HRMS (ESI) Calcd. for $C_{33}H_{27}OSi$ $[M+H]^+$ 467.1753, found 467.1831.

Synthesis of 2-([1,1'-biphenyl]-4-yl)-13,13-dimethyl-2-phenyl-2,13-dihydrobenzo[f]benzo[4,5]silolo[3,2-h]chromene SiNP-b. This compound was prepared according to the same procedure as that of **SiNP-b**, except that the eluent for column chromatography is petroleum ether : ethylacetate 10 : 1. Yield, 72%. Pale yellow solids. Mp 180.6 – 181.1 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 – 8.09 (m, 1H), 8.00 – 7.85 (m, 1H), 7.79 – 7.63 (m, 8H), 7.61 – 7.48 (m, 8H), 7.48 – 7.41 (m, 2H), 7.41 – 7.32 (m, 2H), 7.31 – 7.28 (m, 1H), 6.52 – 6.47 (m, 1H), 0.00 – -0.13 (m, 3H), -0.40 – -0.52 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.1, 143.7, 143.5, 142.9, 142.6, 142.0, 139.3, 138.9, 138.1, 138.0, 133.4, 133.3, 128.6, 128.5, 128.3, 127.7, 127.3, 127.1, 126.8, 126.7, 126.4, 126.3, 126.2,

126.1, 125.9, 125.8, 125.7, 125.6, 125.5, 125.2, 125.1, 122.1, 119.9, 118.5, 118.4, 112.5, 112.4, 81.0, 1.4. HRMS (ESI) Calcd. for $C_{39}H_{30}OSi$ $[M+H]^+$ 543.2066, found 543.2142.

Synthesis of 2,2-bis(4-methoxyphenyl)-13,13-dimethyl-2,13-dihydrobenzo[f]benzo[4,5]silolo [3,2-h]chromene SiNP-c. This compound was prepared according to the same procedure as that of **SiNP-a**, except that the eluent for column chromatography is petroleum ether : ethylacetate 8 : 1. Yield, 75%. Pale yellow solids. Mp 182.1 – 182.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (dd, *J* = 8.4, 2.8 Hz, 1H), 7.76 – 7.69 (m, 1H), 7.47 – 7.29 (m, 8H), 7.20 (d, *J* = 8.0 Hz, 1H), 7.14 (m, 1H), 7.03 (d, *J* = 3.6 Hz, 1H), 6.86 (d, *J* = 8.8 Hz, 2H), 6.81 – 6.75 (m, 2H), 6.23 (d, *J* = 10.0 Hz, 1H), 3.79 (s, 3H), 3.71 (s, 3H), -0.22 (d, *J* = 12 Hz, 3H), , -0.65 (d, *J* = 12 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.4, 148.1, 143.7, 141.8, 138.0, 135.9, 135.3, 135.3, 133.3, 128.5, 128.3, 127.6, 127.0, 126.9, 126.8, 126.0, 125.1, 125.0, 121.9, 119.8, 118.5, 118.4, 117.9, 112.3, 112.0, 111.9, 80.7, 53.8, 53.7, 1.3, -0.7. HRMS (ESI) Calcd. for $C_{35}H_{30}O_3Si$ $[M+H]^+$ 527.1964, found 527.2042.



Scheme S3. Synthetic route to **NP-Ph**.

Synthesis of 4-phenylnaphthalen-2-ol (10)

A mixture of 4-bromonaphthalen-2-ol (1g, 4.50 mmol), phenylboronic acid (0.66 g, 5.40 mmol), $Pd(PPh_3)_4$ (0.52 g, 0.45 mmol) and Na_2CO_3(2.3 g, 21.6 mmol) in THF(50 mL) and water (20 mL) was stirred for 12 h at 80 °C under nitrogen. After cooling down to room temperature, the reaction mixture was extracted by ethyl acetate twice (2 × 10 mL). The organic extracts were combined and washed with brine and water, then dried with anhydrous $MgSO_4$, filtered and concentrated at reduced pressure. The crude product was purified by silica gel column chromatography using petroleum ether/ethyl acetate (v/v = 30 : 1) as an eluent affording **10** as a thick brown oil which thickened on standing. Yield: 73%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.4 Hz, 1H), 7.68 (d, *J* = 8.4 Hz, 1H), 7.45 – 7.42 (m, 6H), 7.26 – 7.20 (m, 1H), 7.14(t, *J* = 2.4 Hz, 1H), 7.04 (d, *J* = 2.4 Hz, 1H), 5.64 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.7, 142.5, 140.1, 135.2, 130.0, 128.4, 128.3, 127.5, 126.9, 126.6, 126.1, 123.8, 118.8, 109.3.

Synthesis of 3-([1,1'-biphenyl]-4-yl)-3,6-diphenyl-3H-benzo[f]chromene (NP-Ph). A solution of 7,7-dimethyl-7H-benzo[c]fluoren-6-ol **4** (0.24 g, 1.1 mmol), **4b** (0.4 g, 1.38 mmol), and 1-2 drops of dodecylbenzenesulphonic acid (cat. amount) in dry toluene (20 mL) was stirred for 3h at 40 ºC.

Then the reaction mixture was washed with water and the organic phase was separated. After evaporation of toluene, the product **NP-Ph** was isolated by column chromatography (silica gel, eluent petroleum ether : ethylacetate 100 : 1).

Yield, 65%. Yellow solid, m.p. 83.1-84.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.8 Hz, 1H), 7.79 (d, *J* = 8.8 Hz, 1H), 7.59 – 7.51 (m, 8H), 7.49 – 7.30 (m, 12H), 7.29 – 7.22 (m, 2H), 7.20 (s, 1H), 6.31 (d, *J* = 9.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.0, 144.9, 144.0, 142.4, 140.7, 140.4, 140.3, 130.3, 130.0, 128.8, 128.3, 128.2, 127.8, 127.6, 127.5, 127.4, 127.2, 127.1, 126.9, 126.8, 126.6, 123.7, 121.6, 119.6, 119.3, 113.5, 82.5. HRMS-ESI calcd for $C_{37}H_{26}O$ [M+Na]$^{+}$ 509.1876; found 509.1881.

2. ^{1}H NMR, ^{13}C NMR, and MS spectra

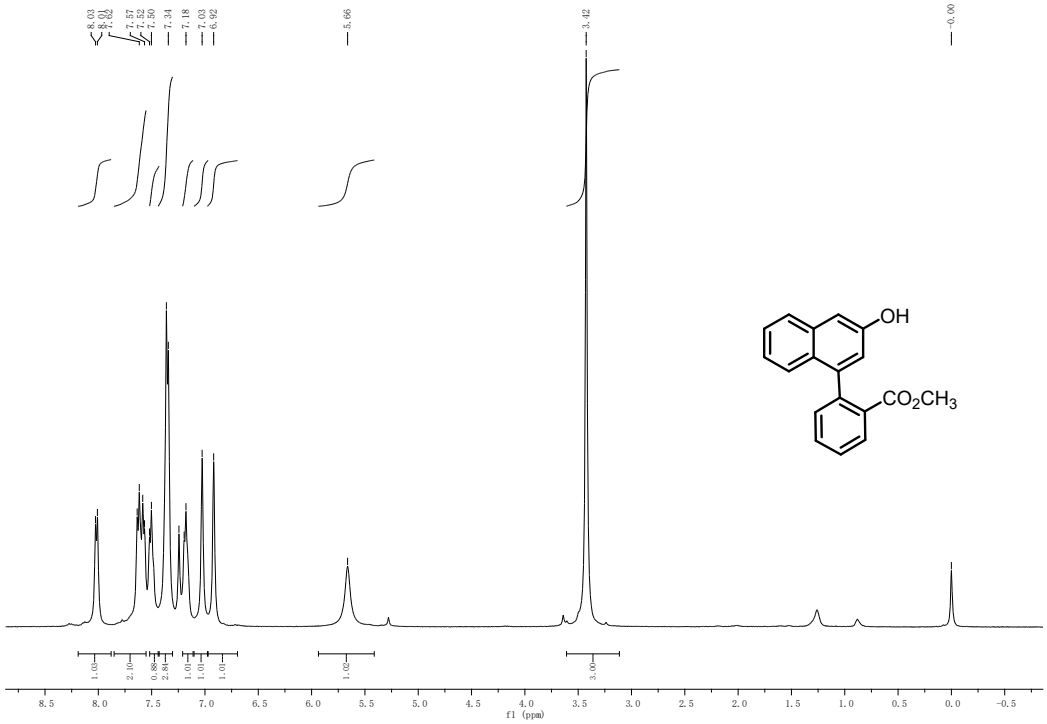


Figure S1. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **1**.

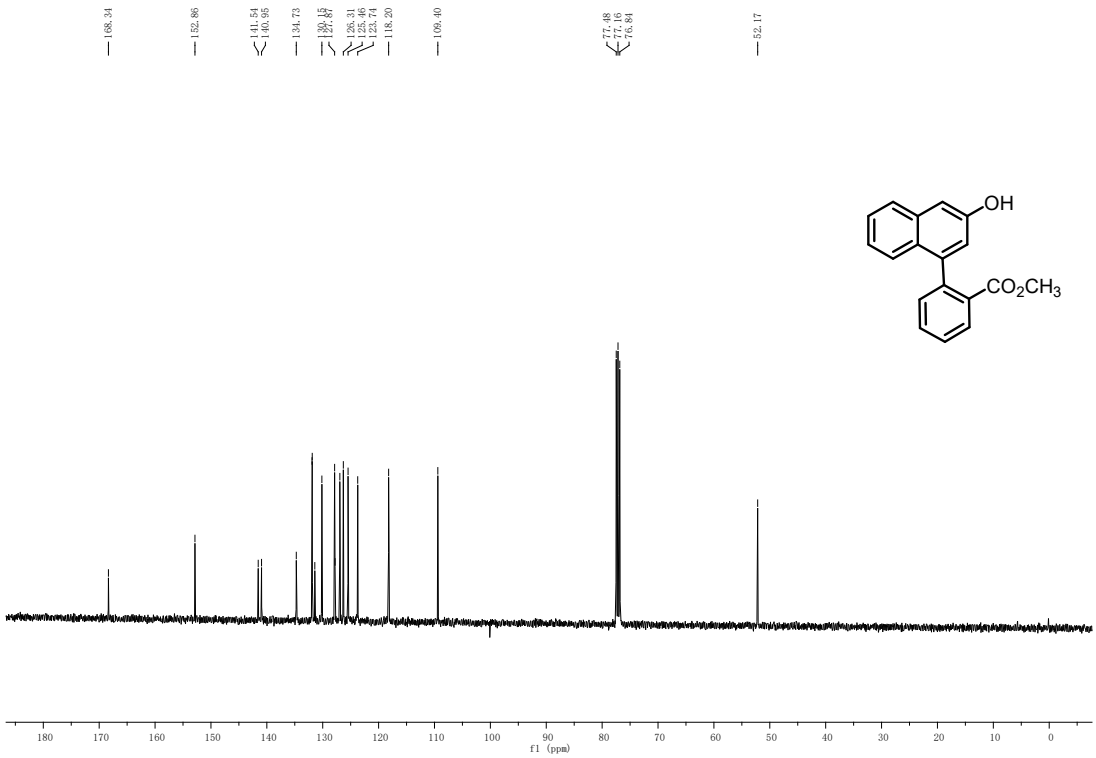


Figure S2. ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of **1.**

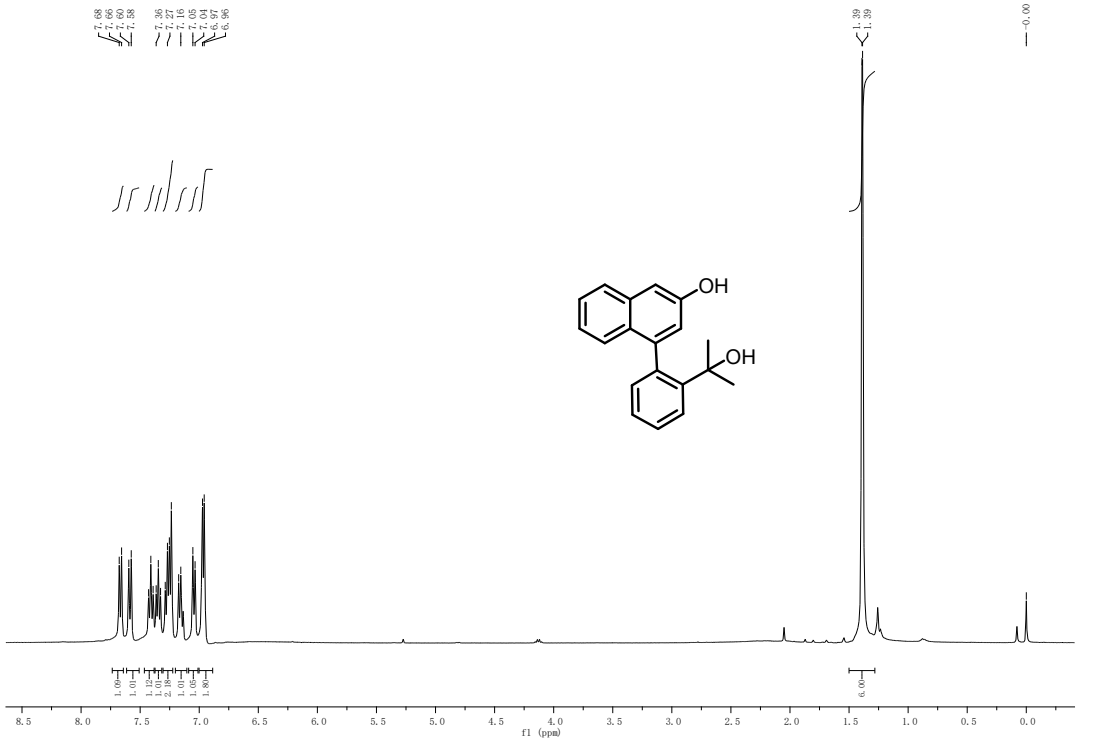


Figure S3. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **2**.

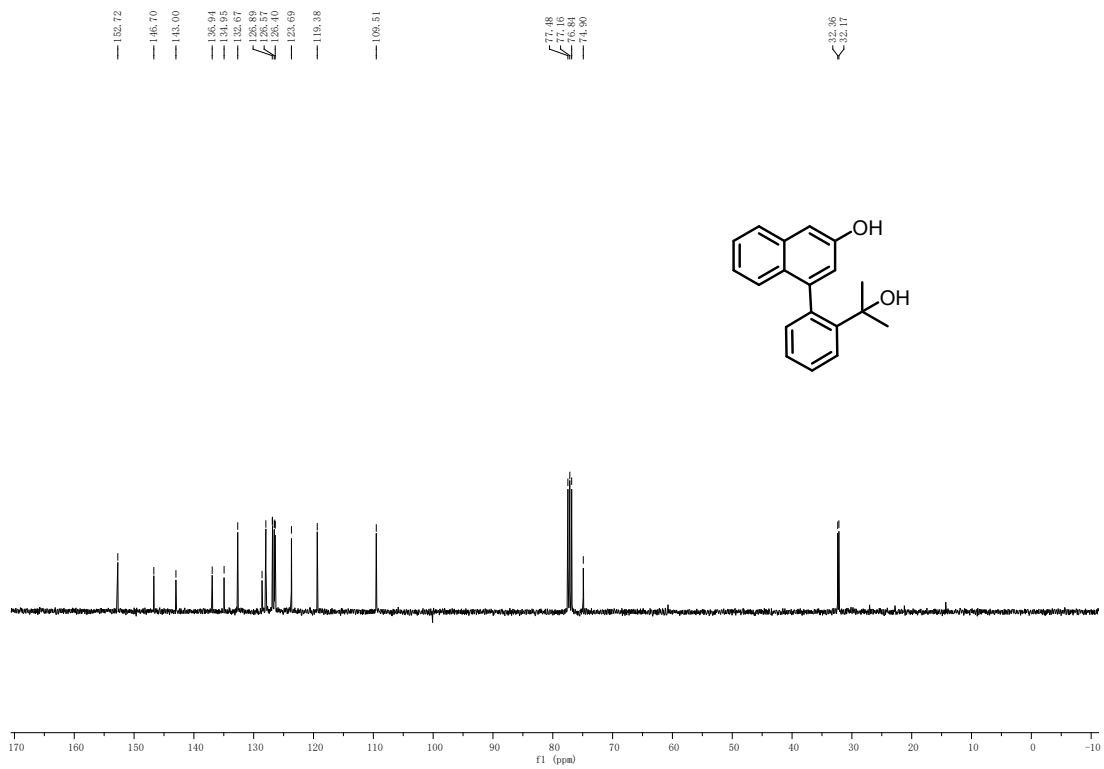


Figure S4. ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of **2.**

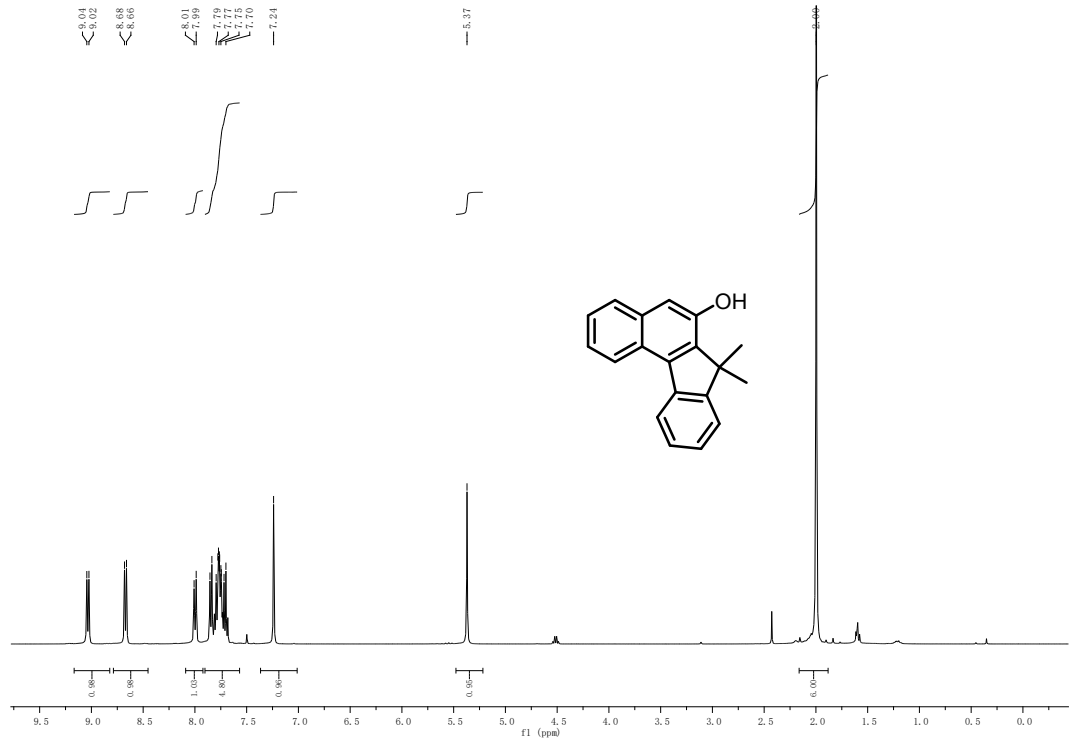


Figure S5. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **3**.

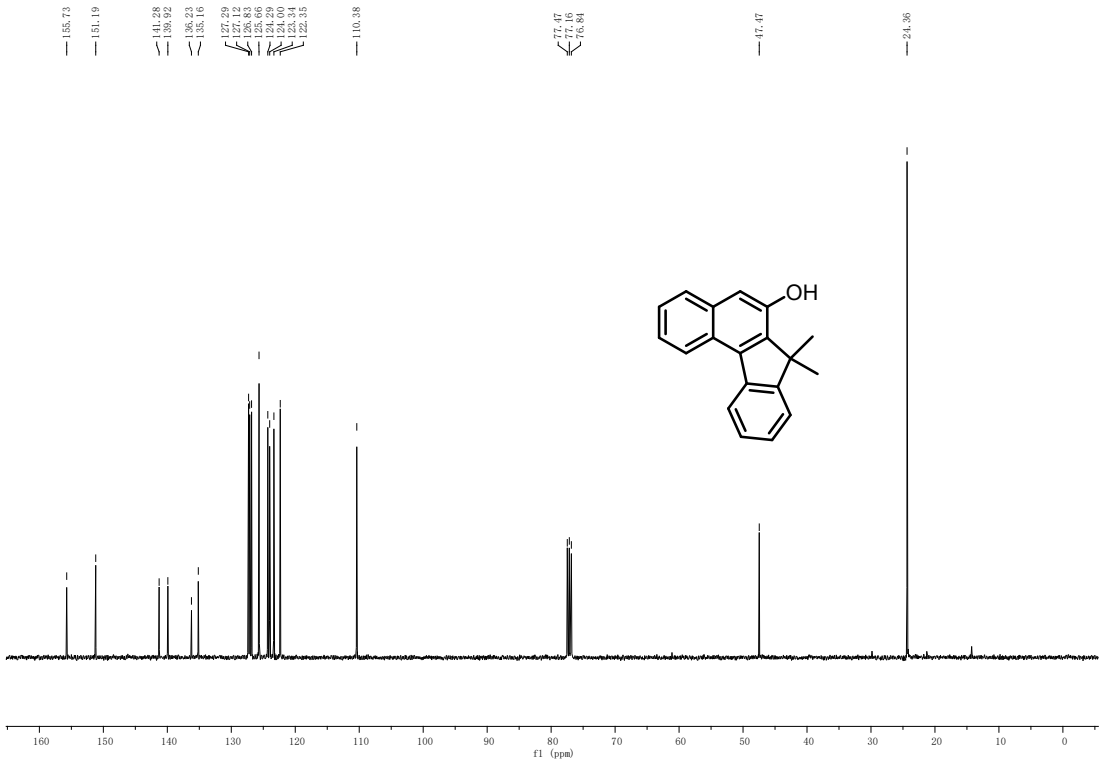


Figure S6. ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of **3.**

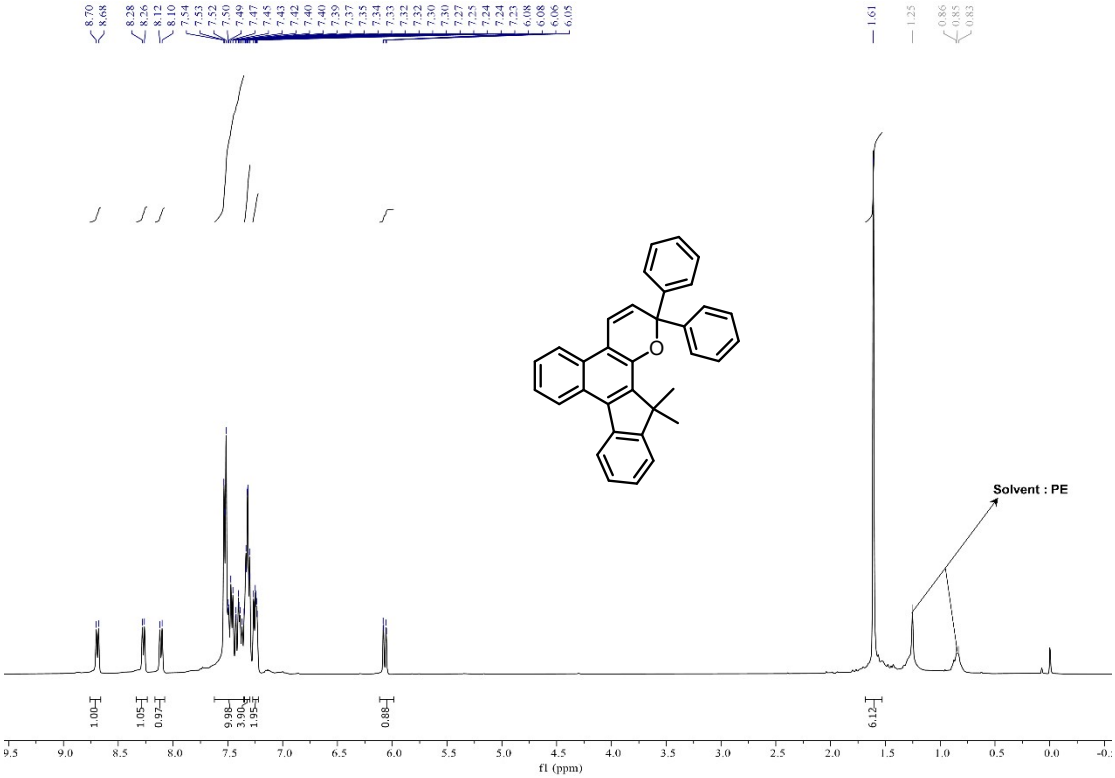


Figure S7. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **CNP-a**.

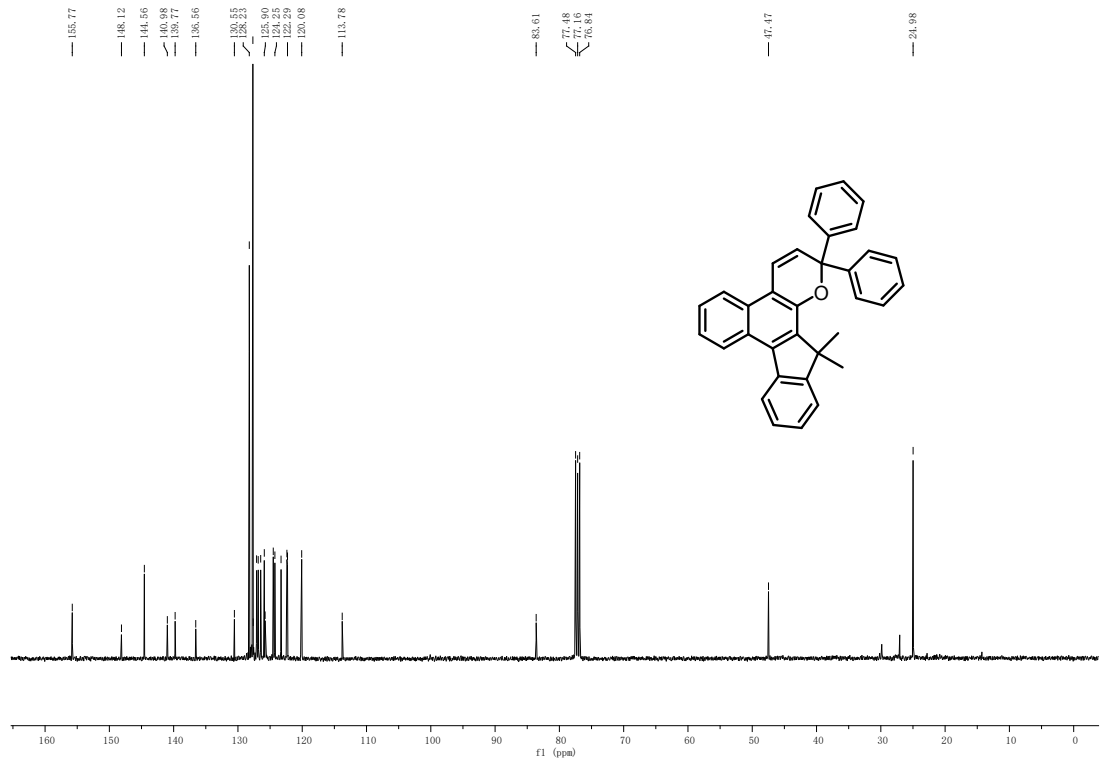


Figure S8. ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of **CNP-a.**

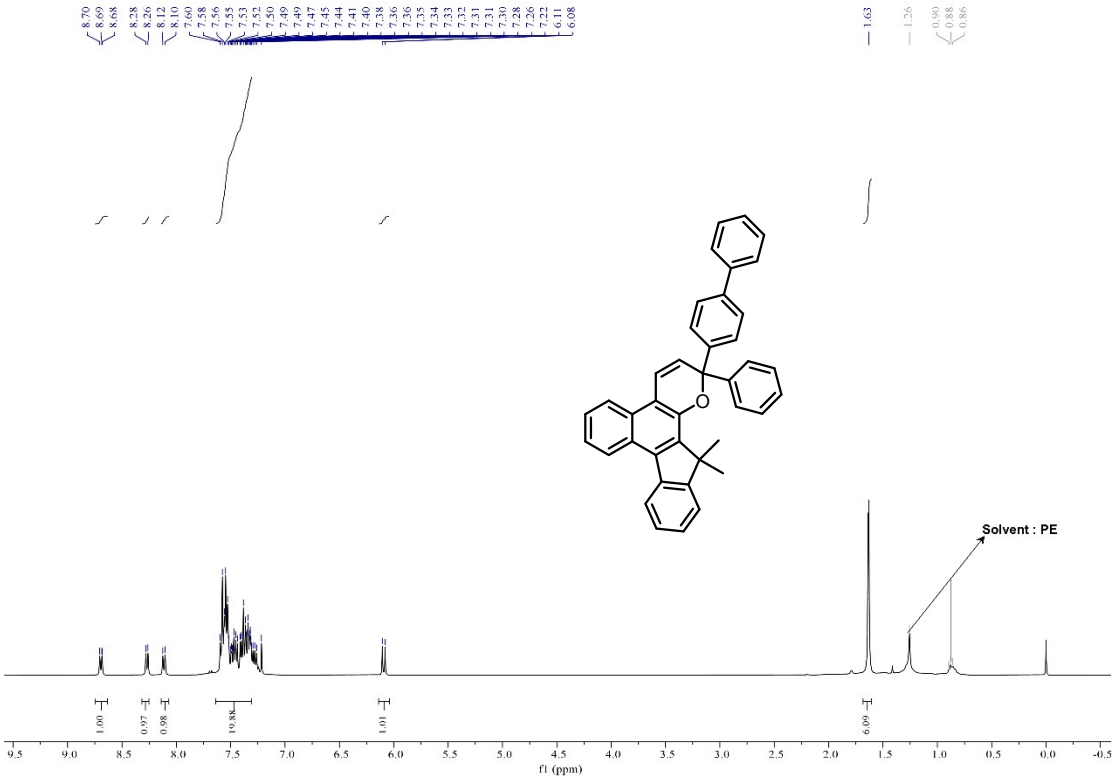


Figure S9. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **CNP-b**.

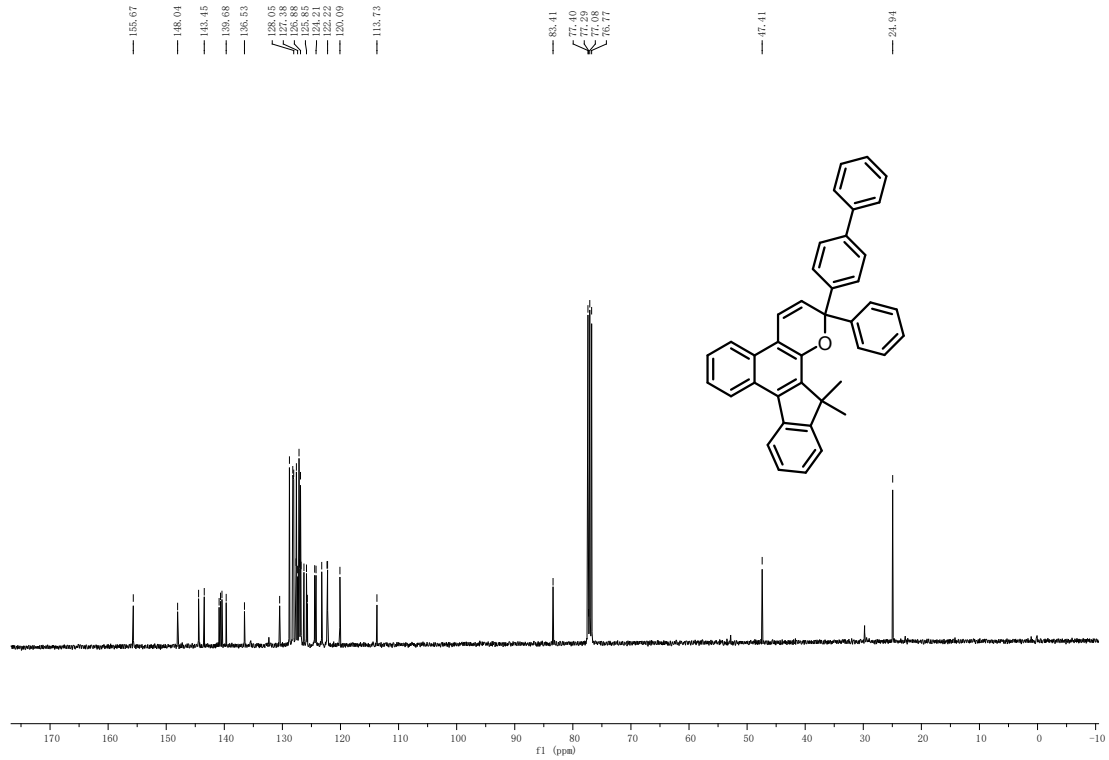


Figure S10. ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of **CNP-b**.

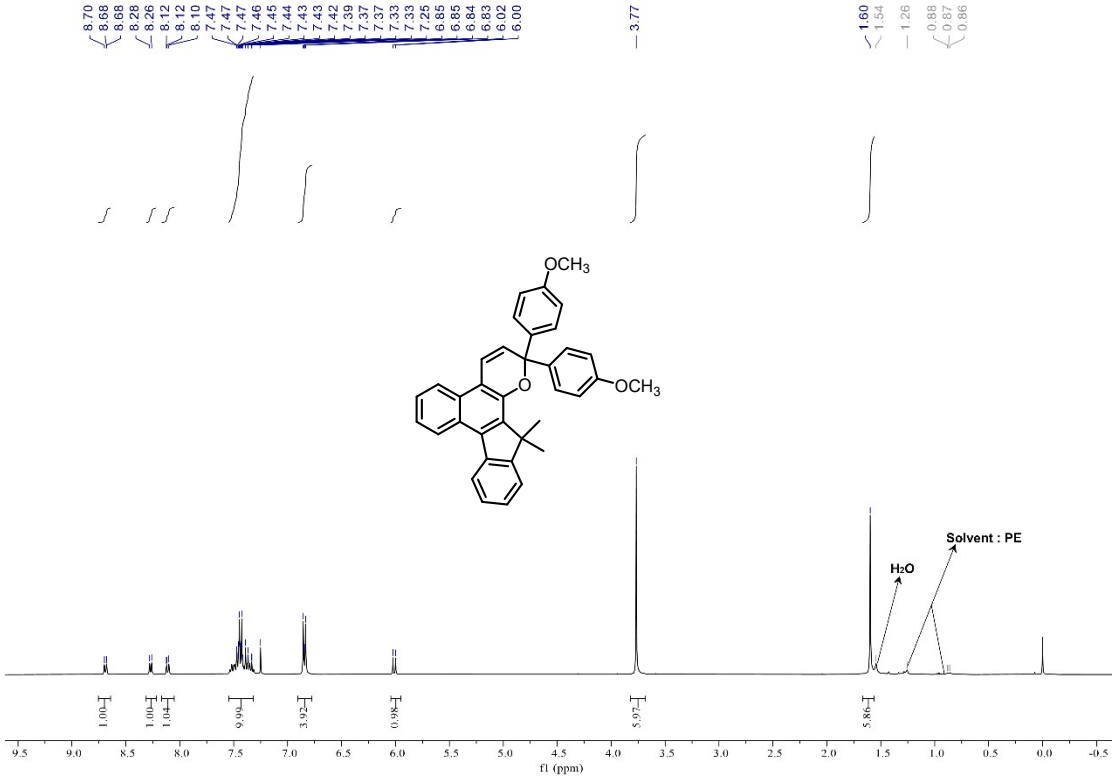


Figure S11. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **CNP-c**.

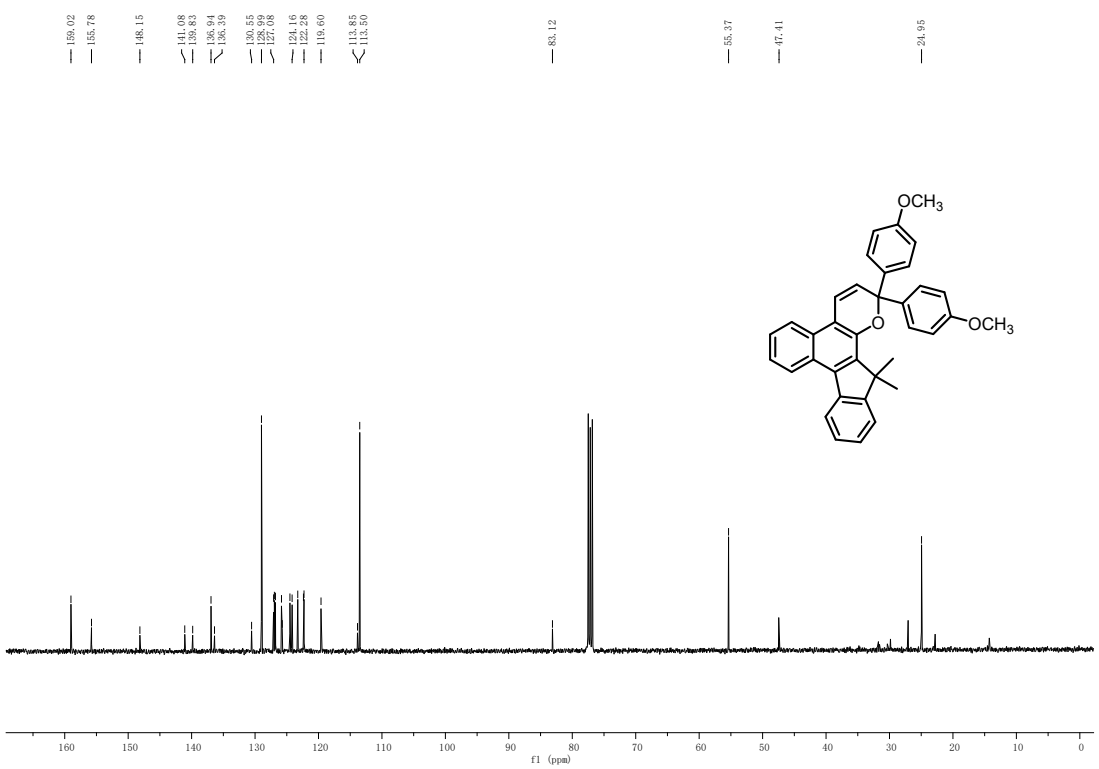


Figure S12. ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of **CNP-c**.

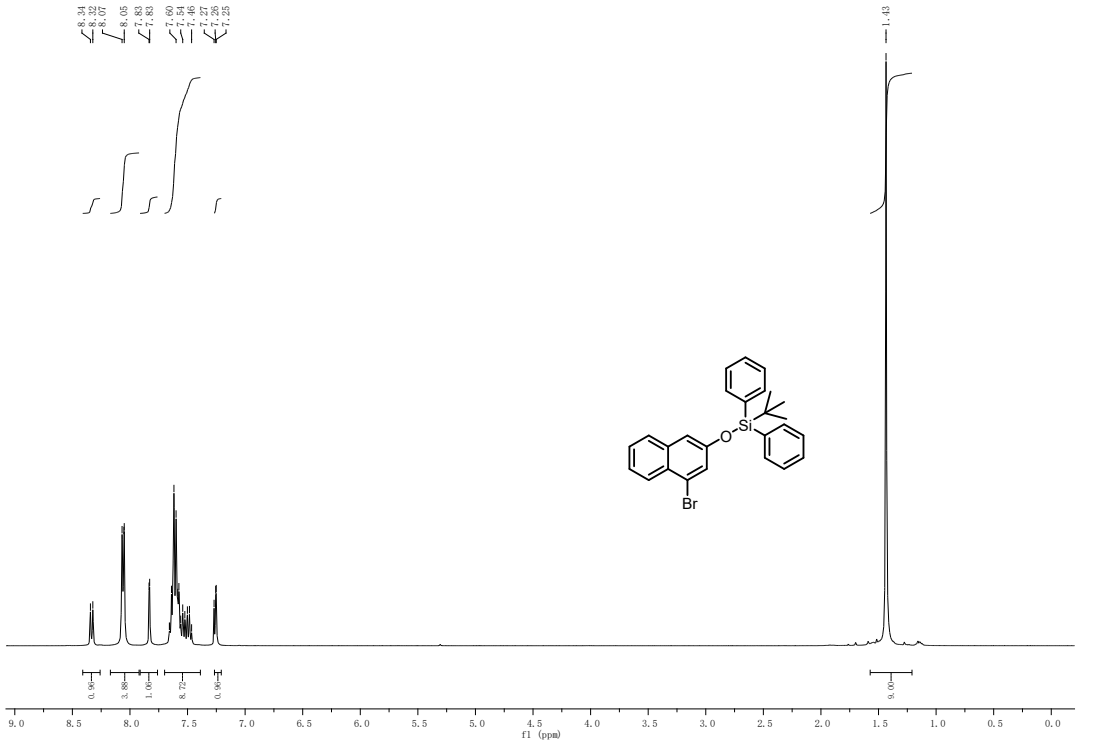


Figure S13. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **4**.

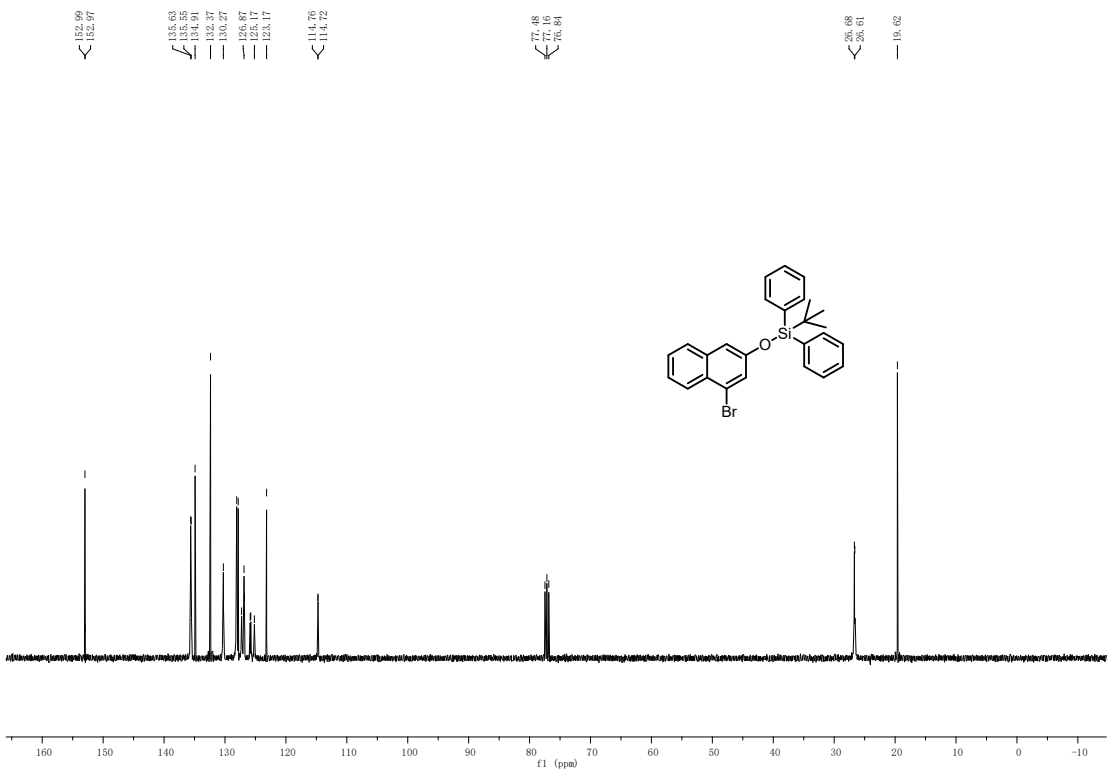


Figure S14. ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of **4.**

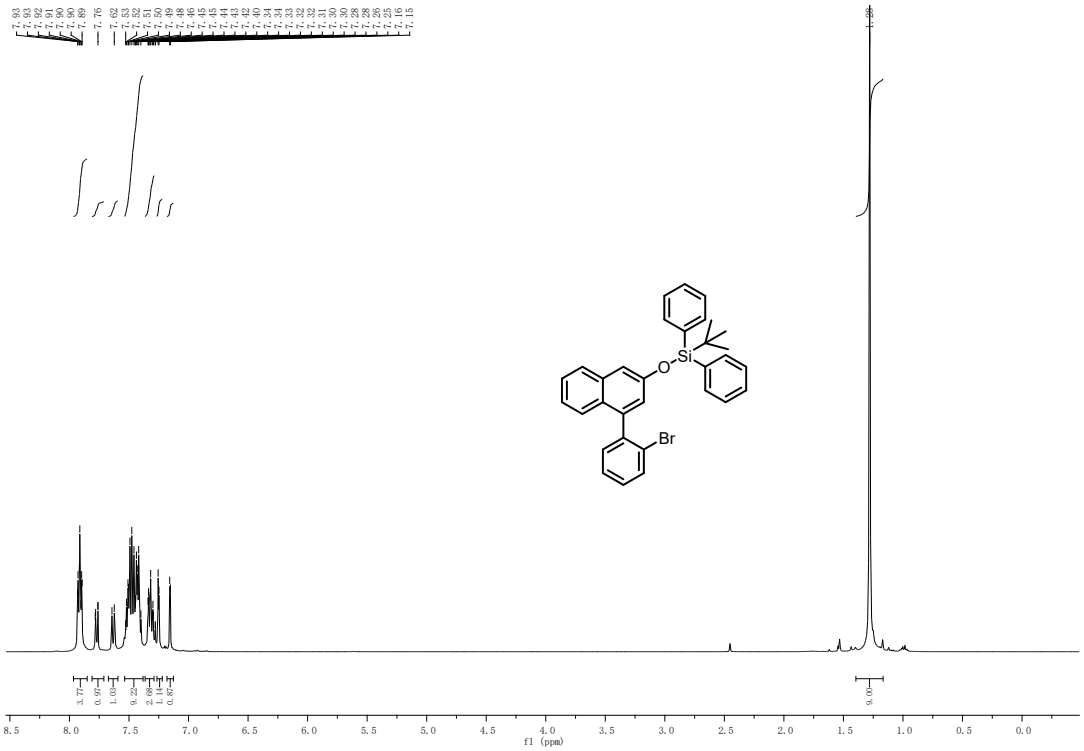


Figure S15. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **6**.

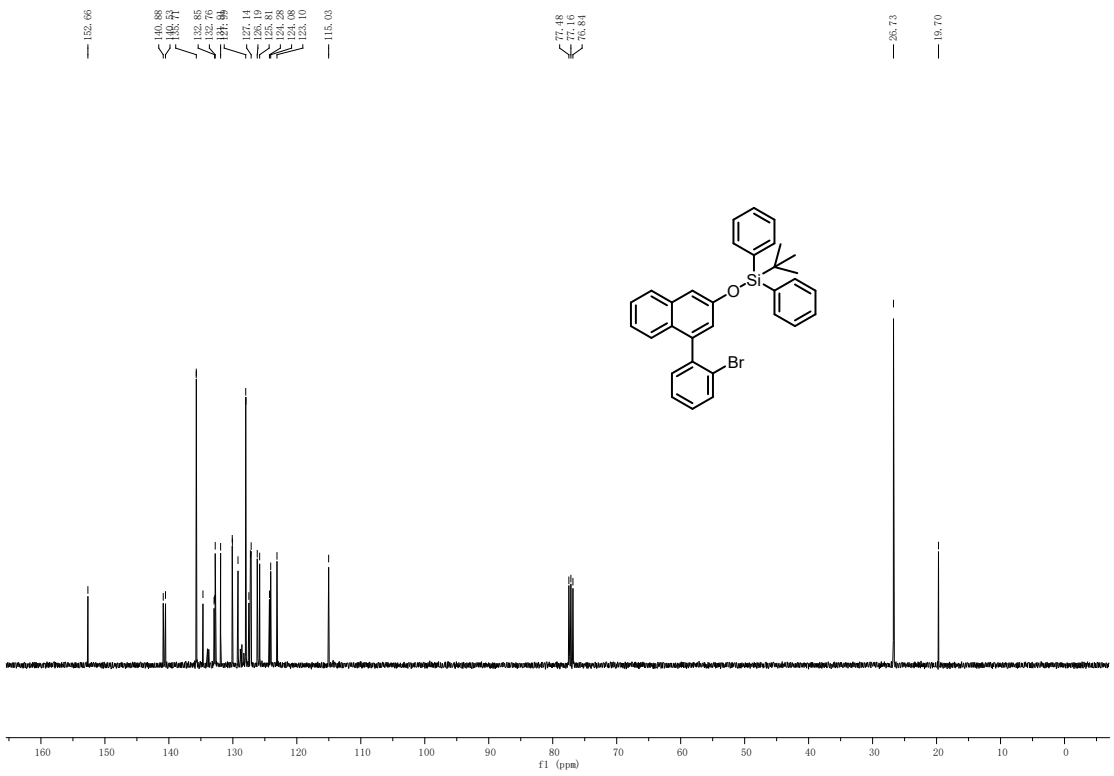


Figure S16. ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of **6.**

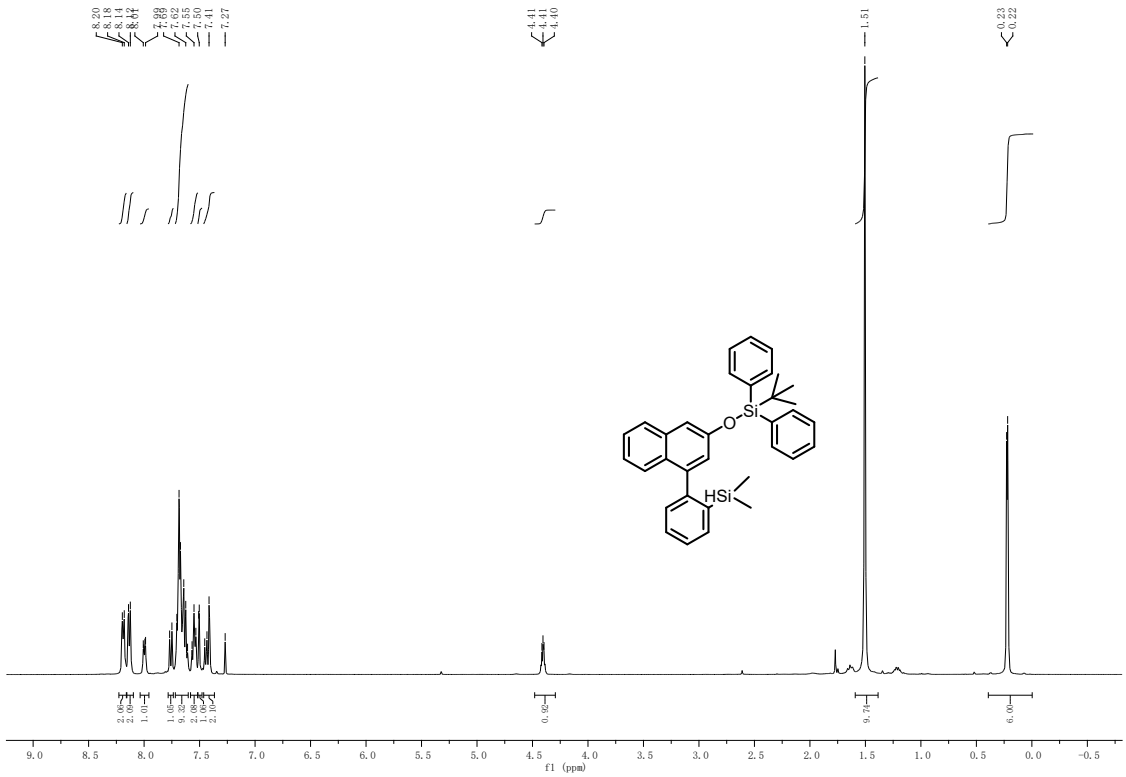


Figure S17. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **7**.

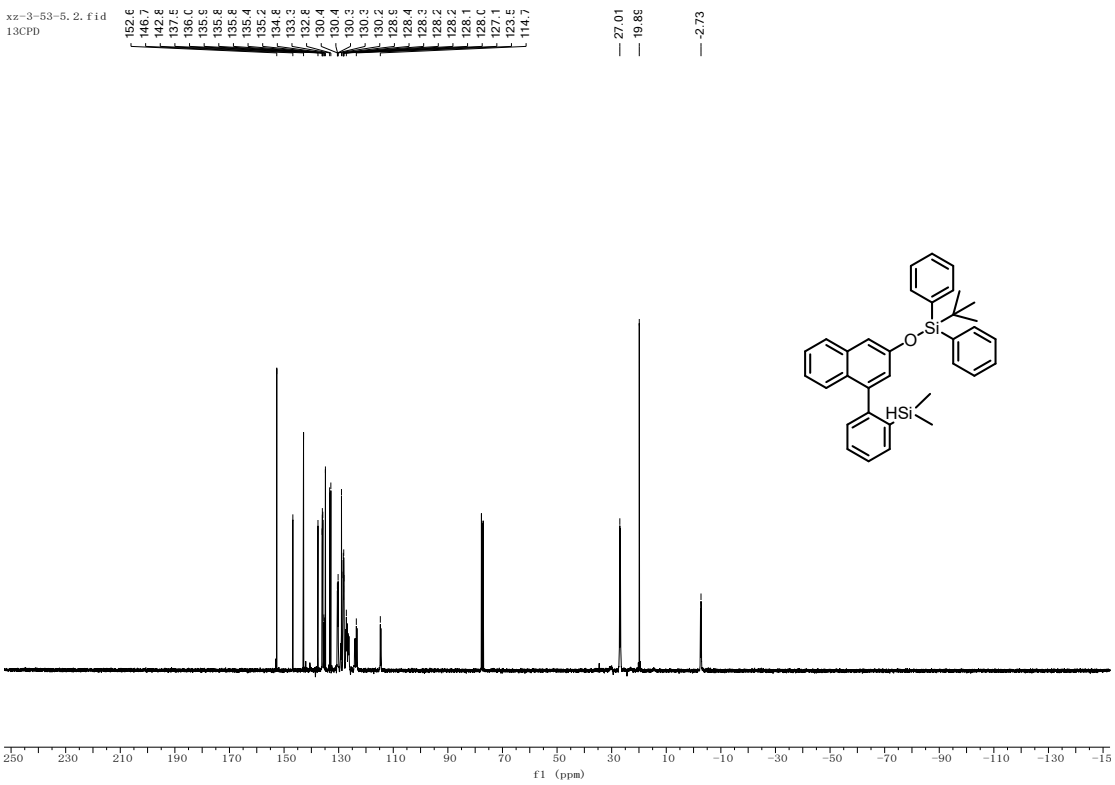


Figure S18. ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of **7.**

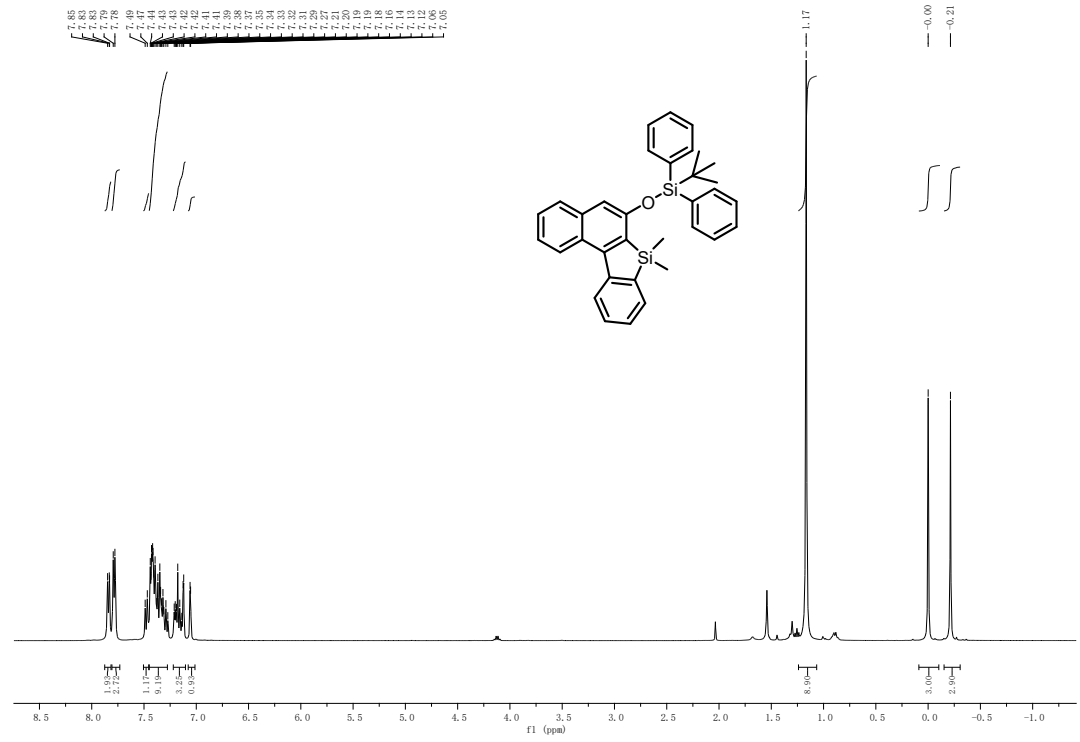


Figure S19. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **8**.

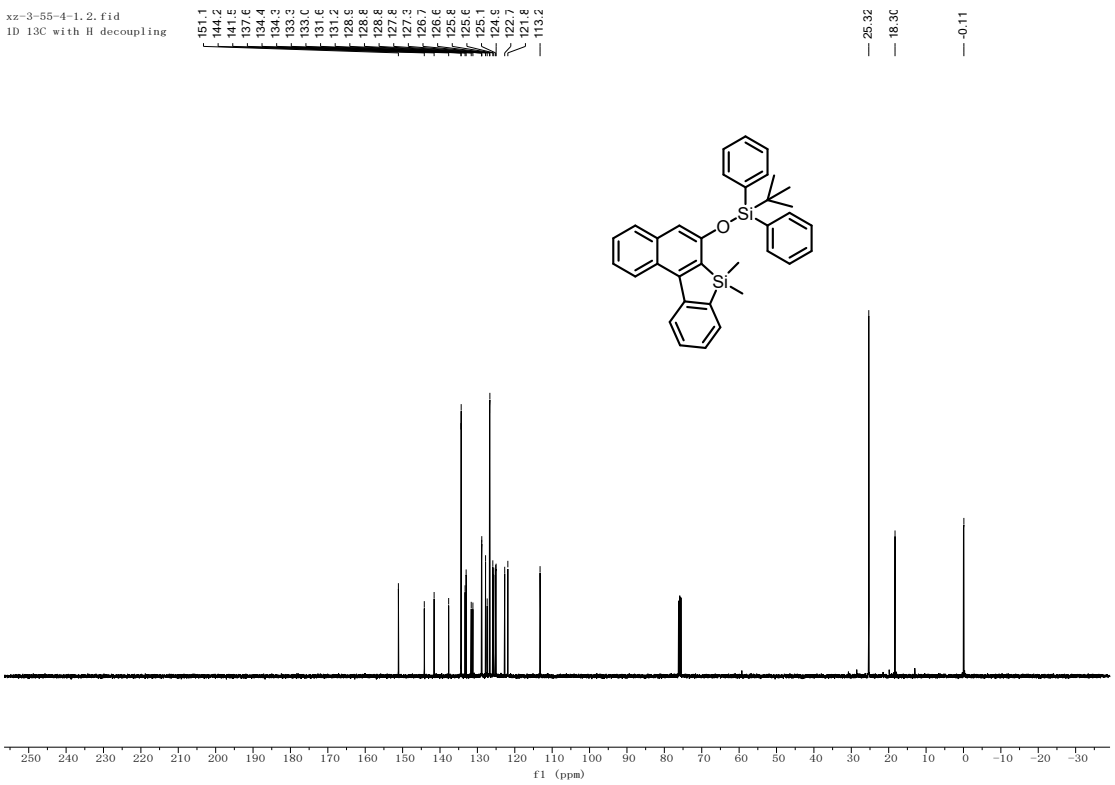


Figure S20. ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of **8.**

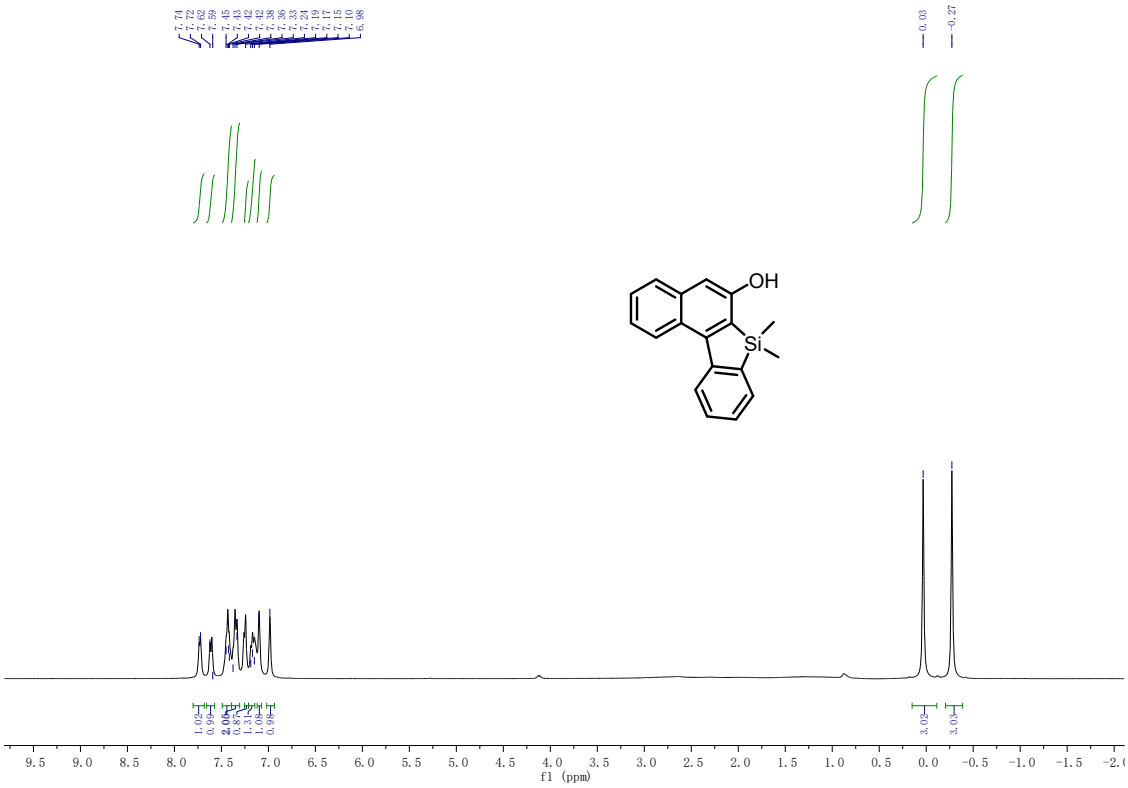


Figure S21. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **9**.

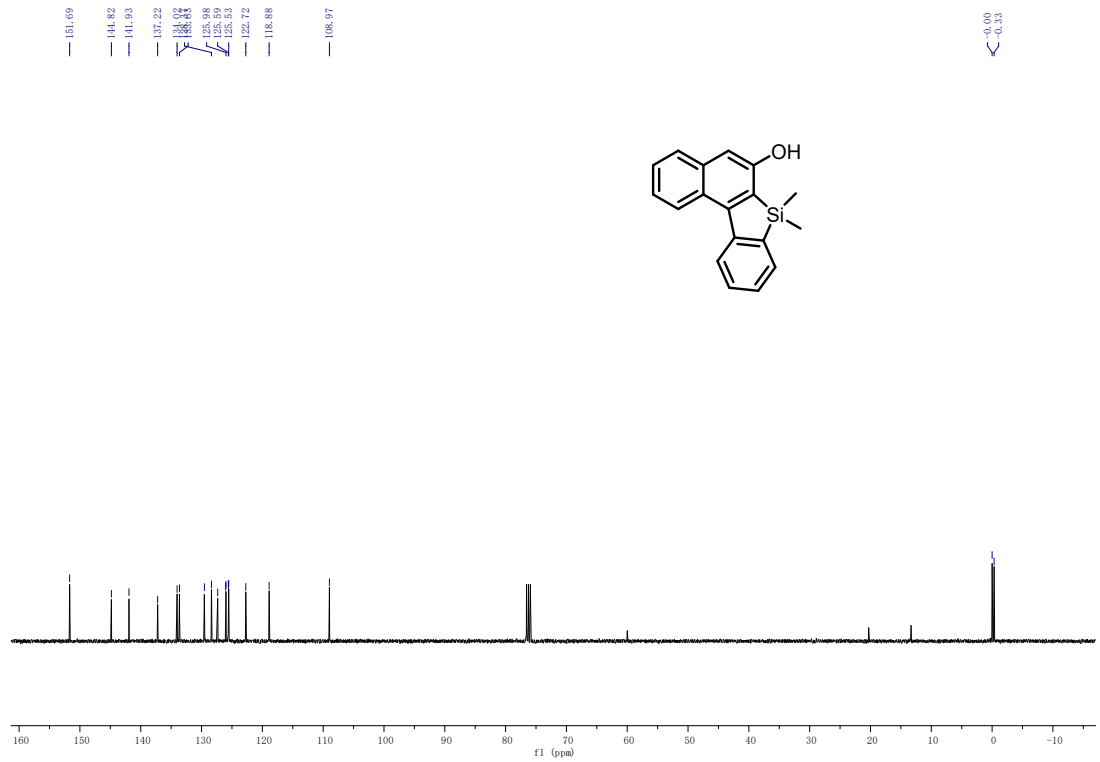


Figure S22. ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of **9.**

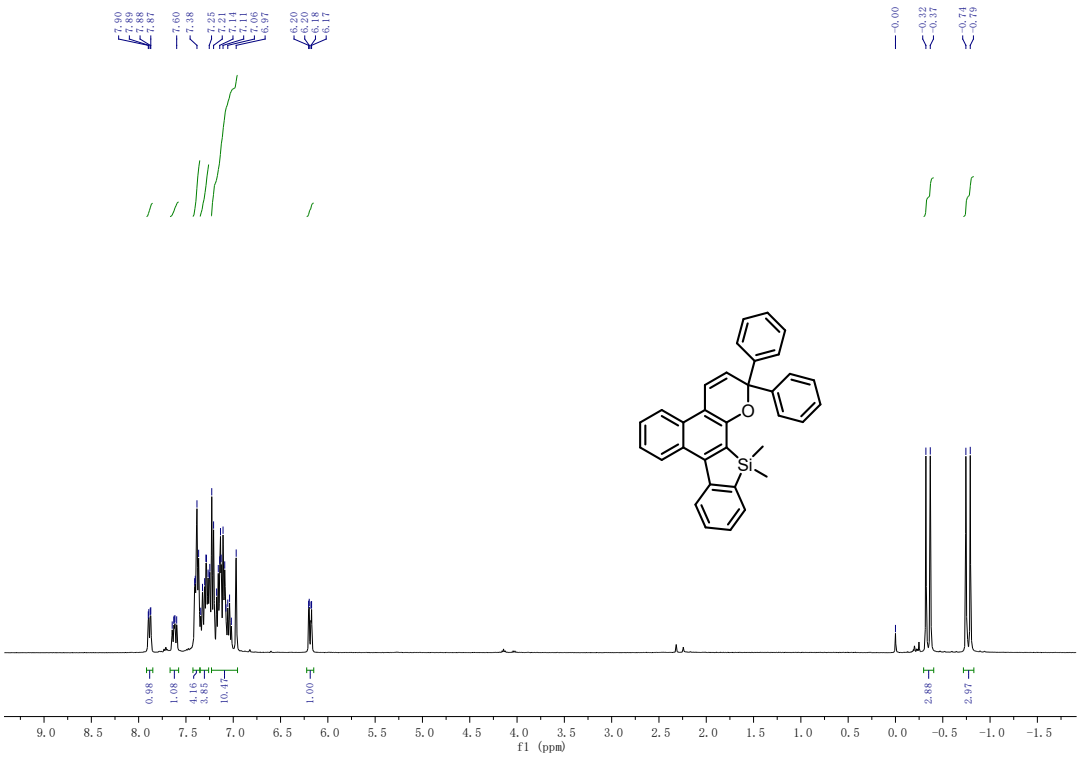


Figure S23. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **SiNP-a**.

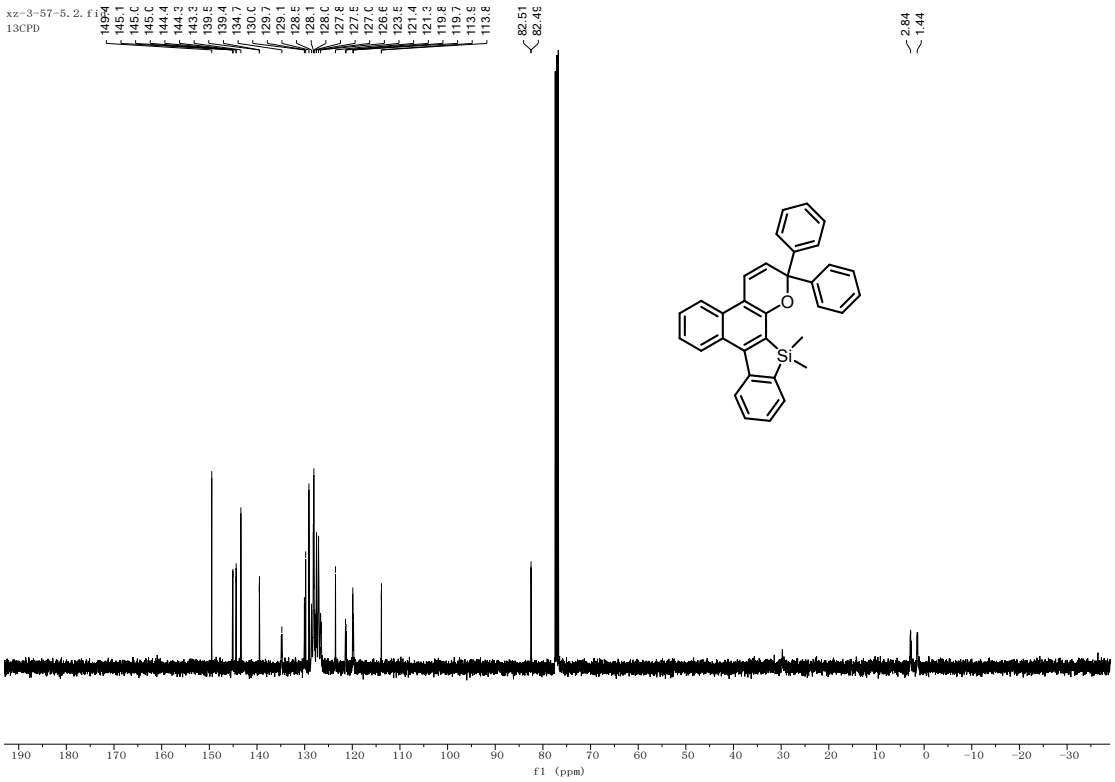


Figure S24. ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of **SiNP-a.**

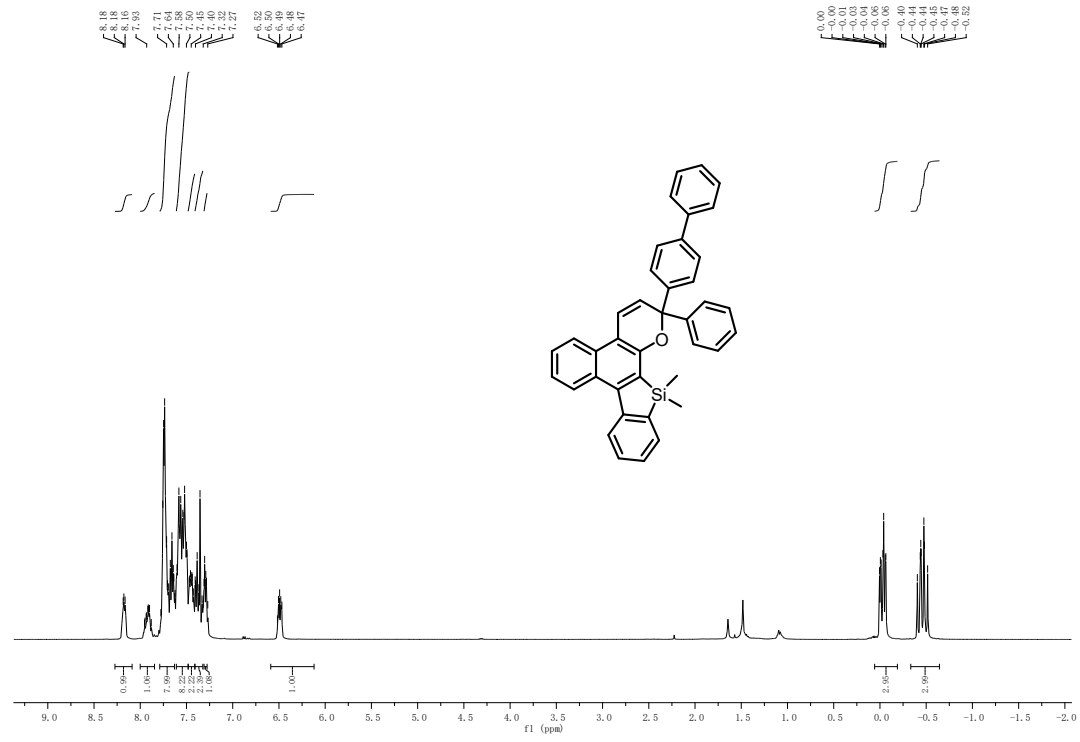


Figure S25. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **SiNP-b**.

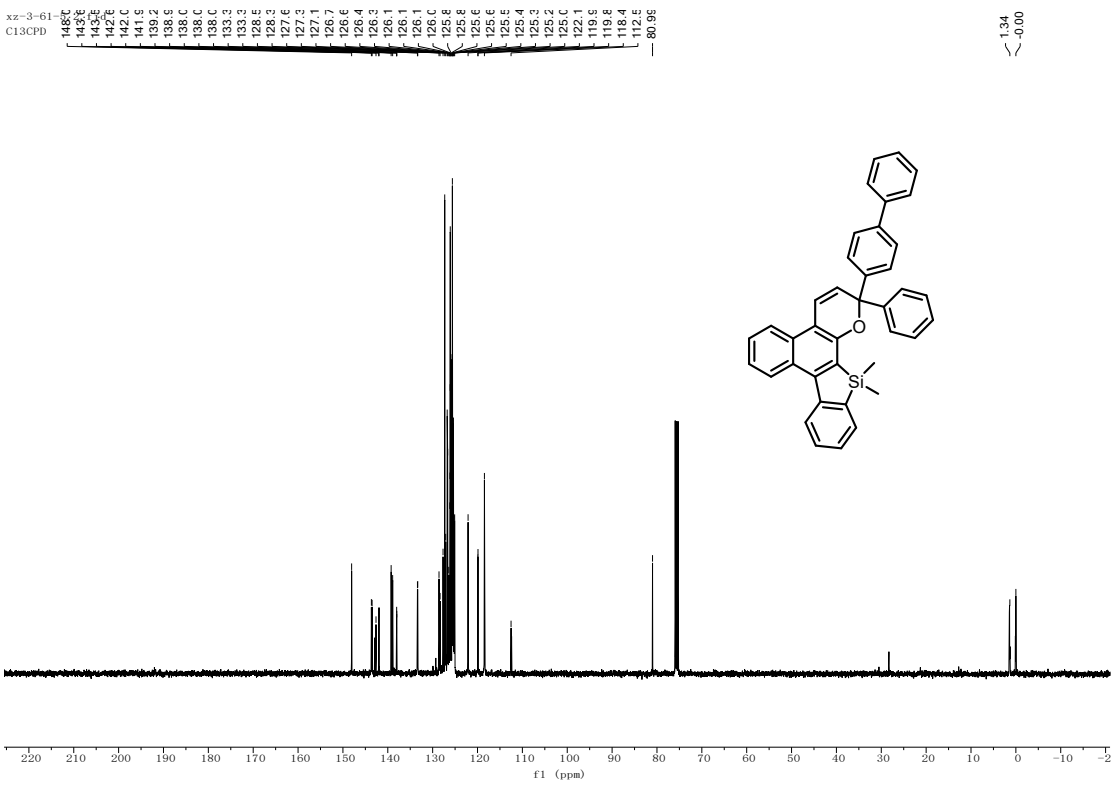


Figure S26. ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of **SiNP-b.**

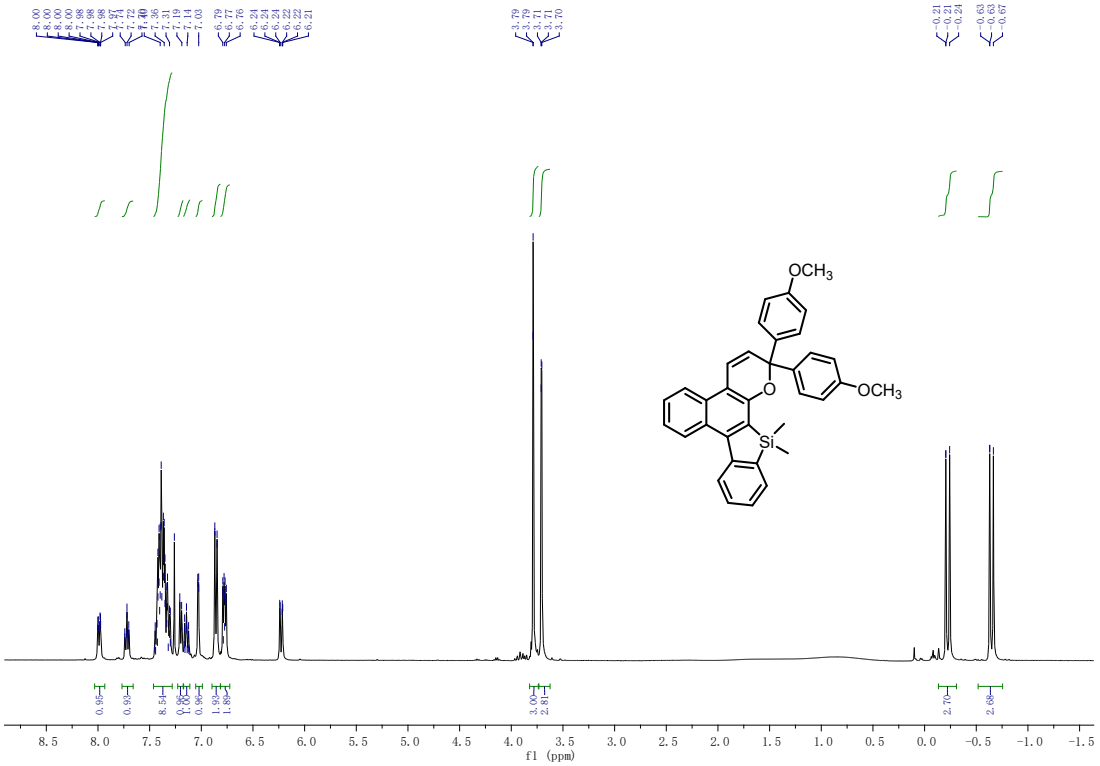


Figure S27. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **SiNP-c**.

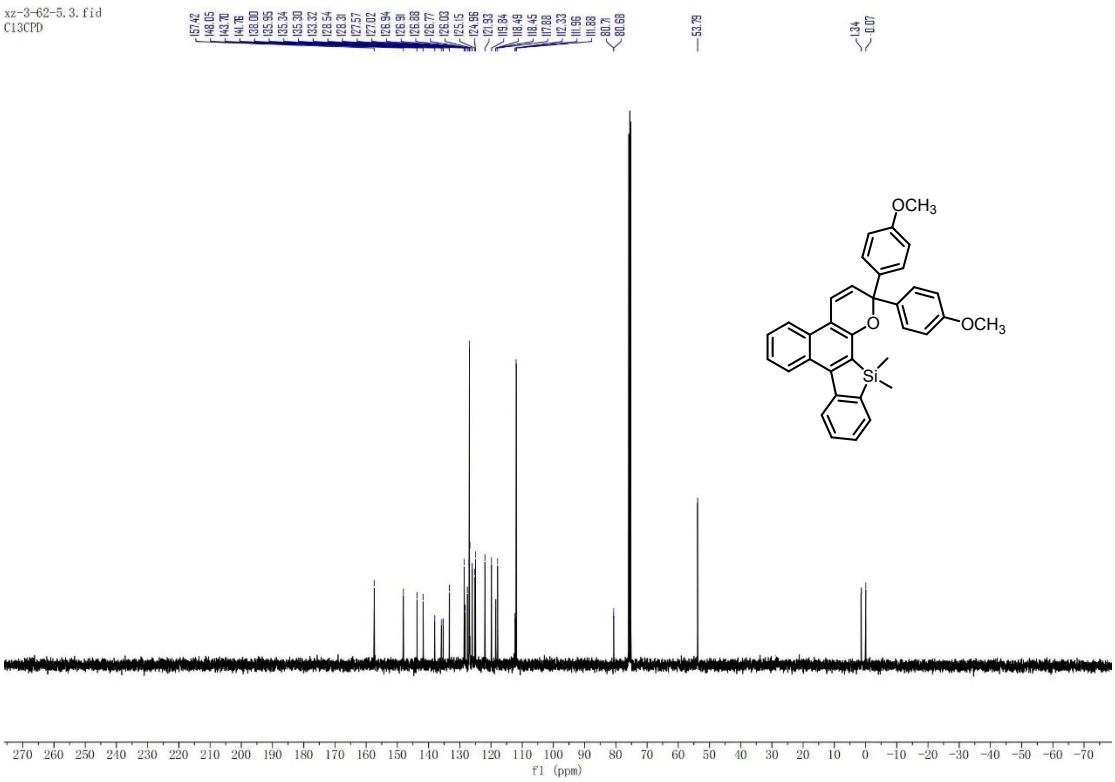


Figure S28. ^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298 K) of **SiNP-c.**

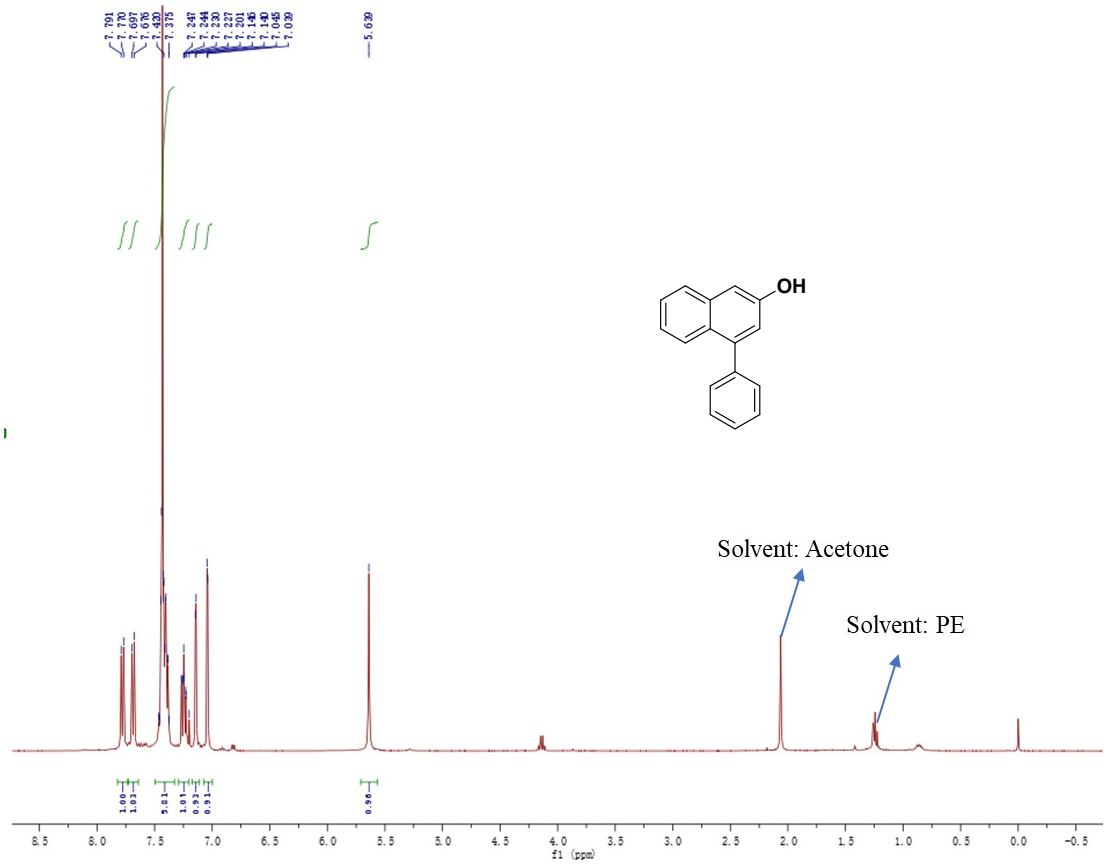


Figure S29. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **10**.

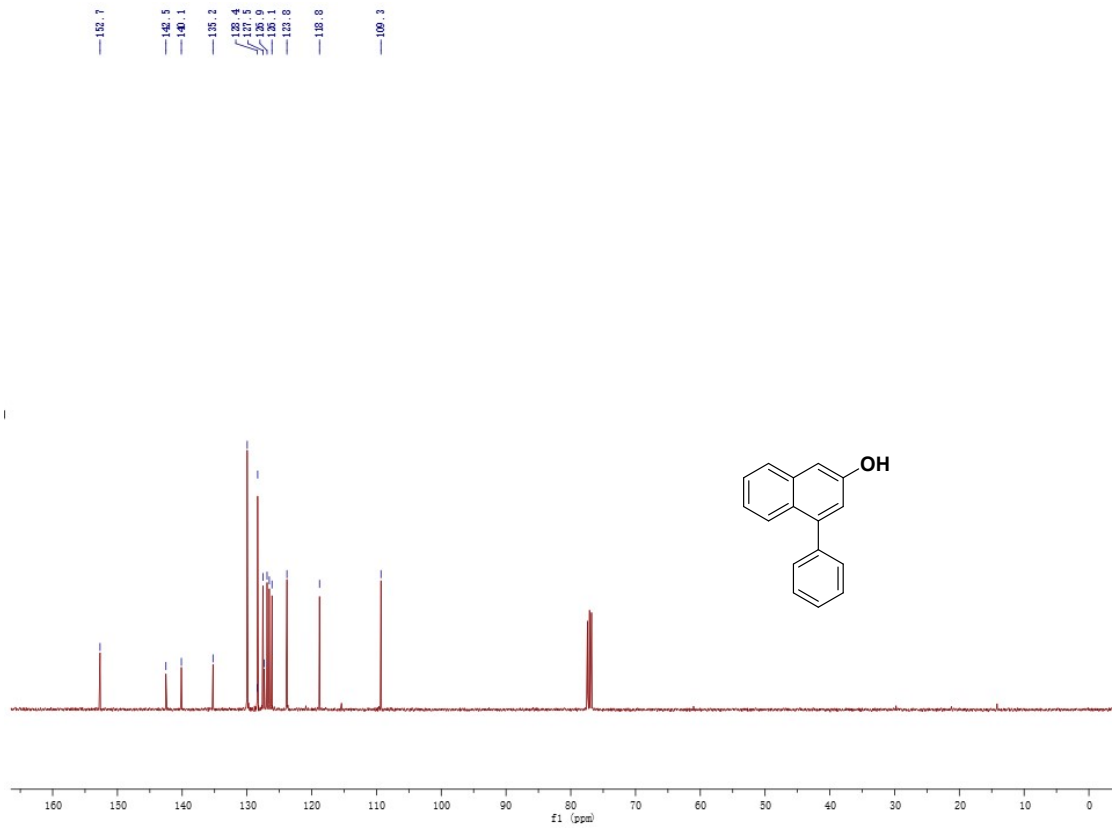


Figure S30. ^{13}C NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **10**.

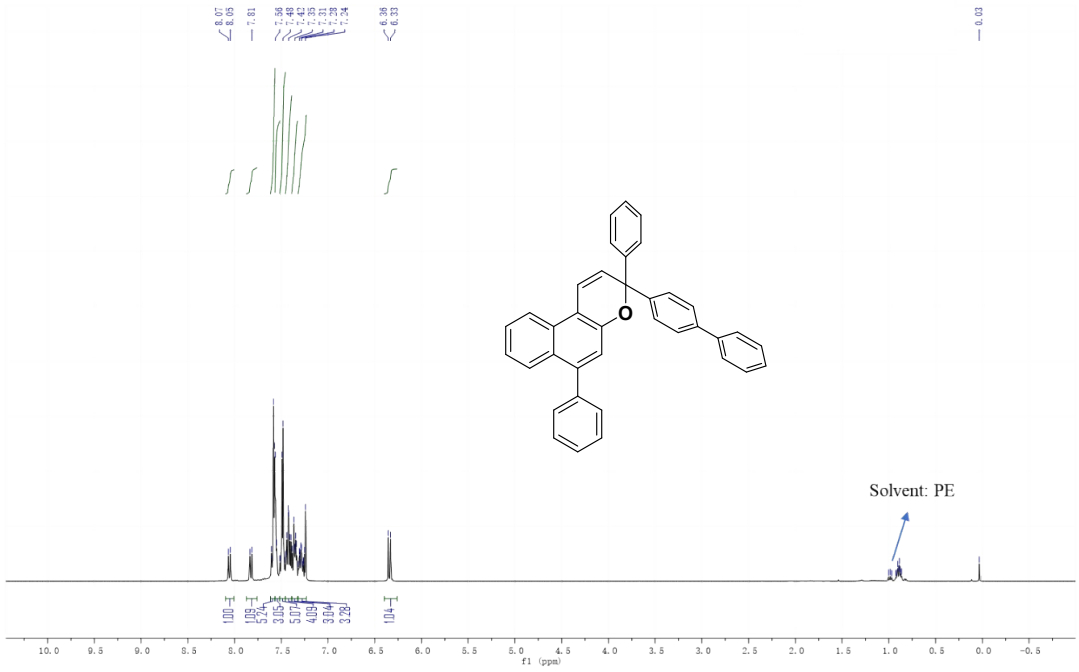


Figure S31. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of **NP-Ph**.

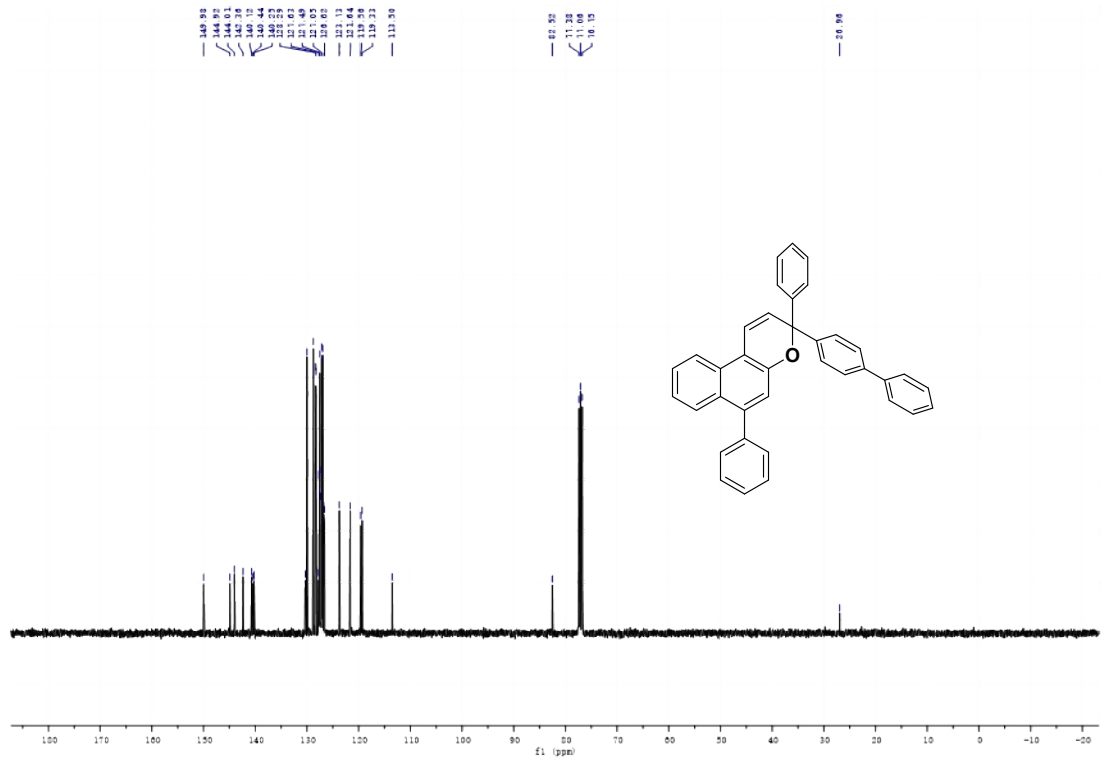


Figure S32. ^{13}C NMR spectrum (400 MHz, $CDCl_3$, 298 K) of NP-Ph.

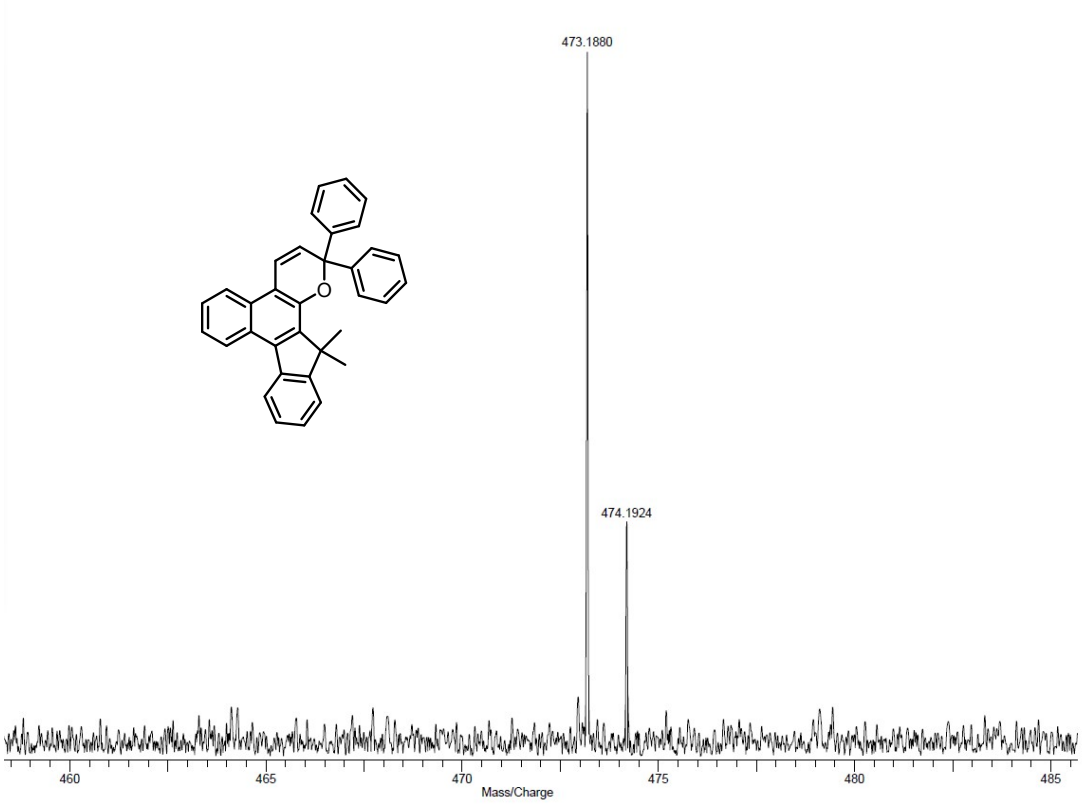


Figure S33. HRMS (ESI) of **CNP-a**.

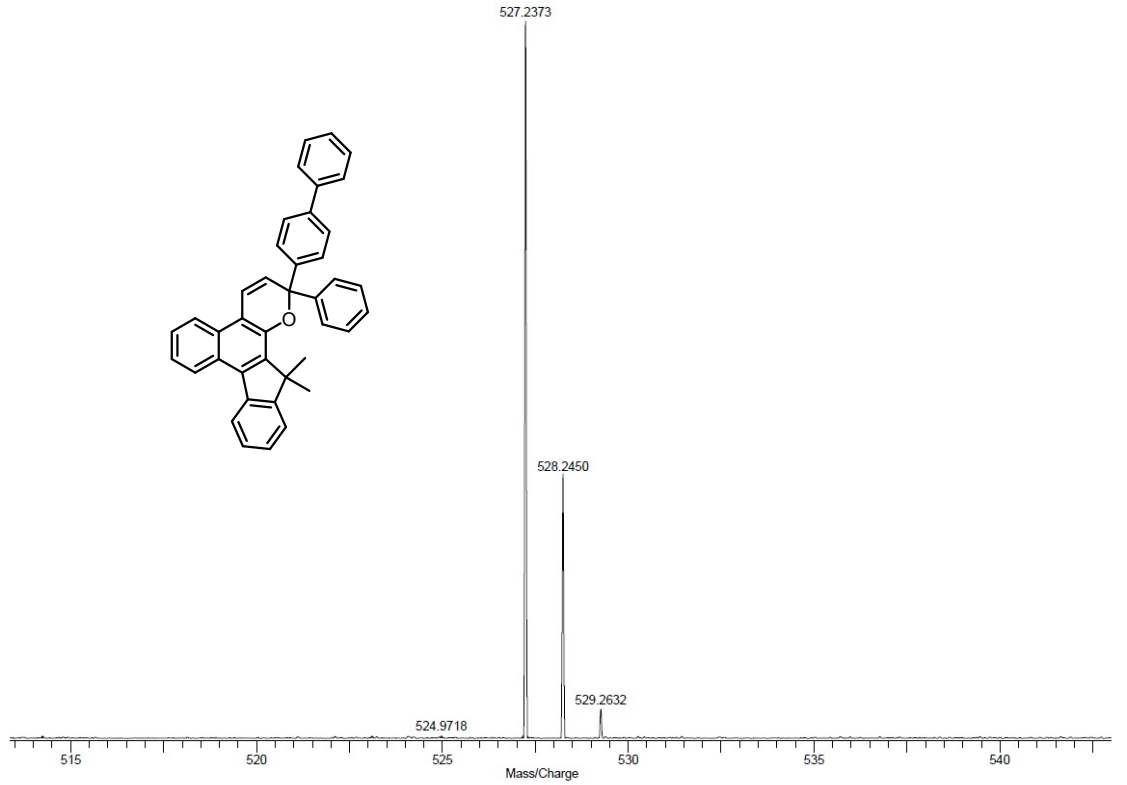


Figure S34. HRMS (ESI) of **CNP-b**.

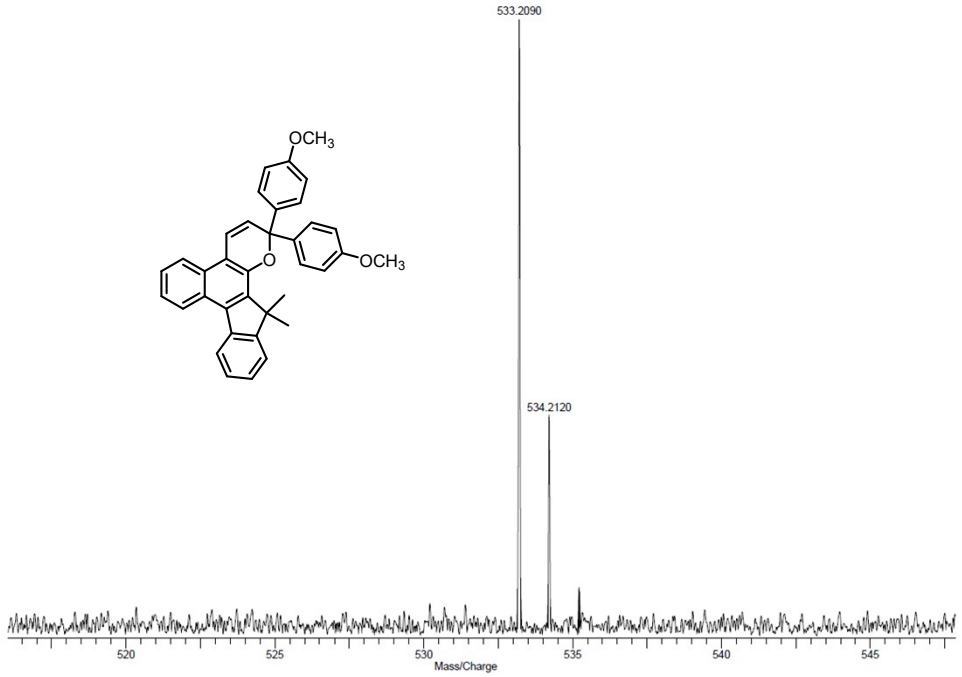


Figure S35. HRMS (ESI) of **CNP-c**.

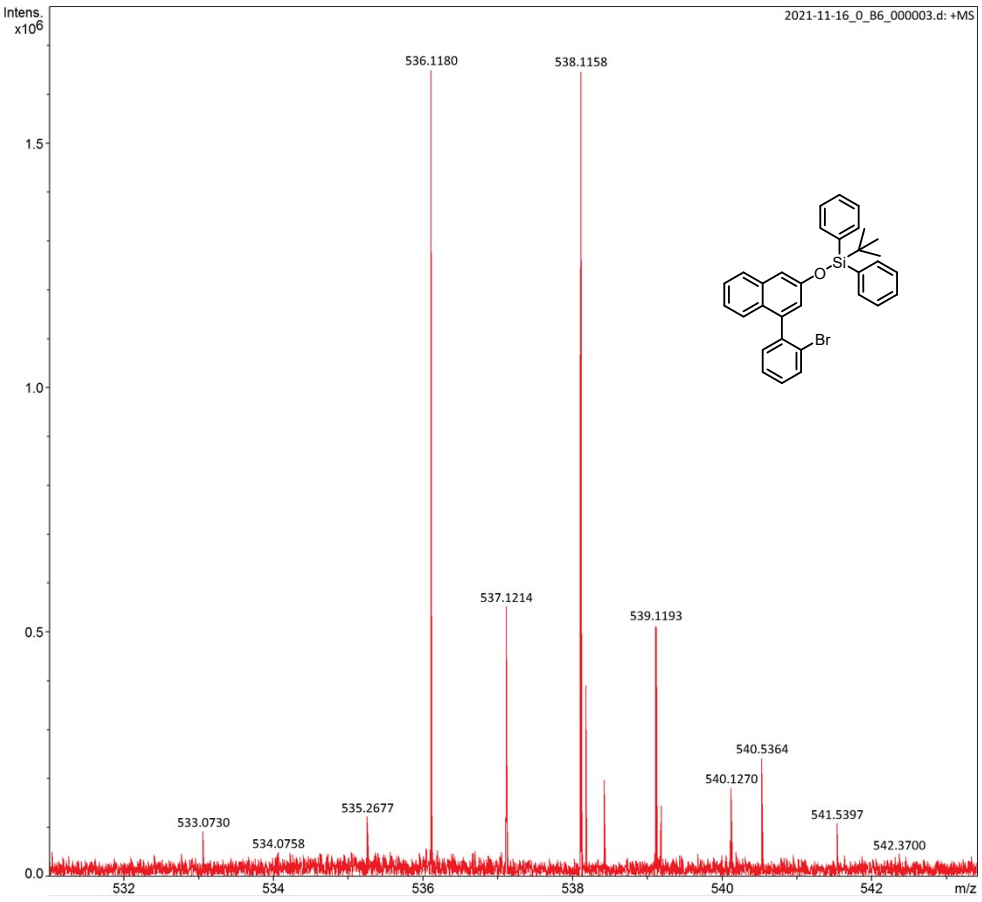


Figure S36. HRMS (ESI) of **6**.

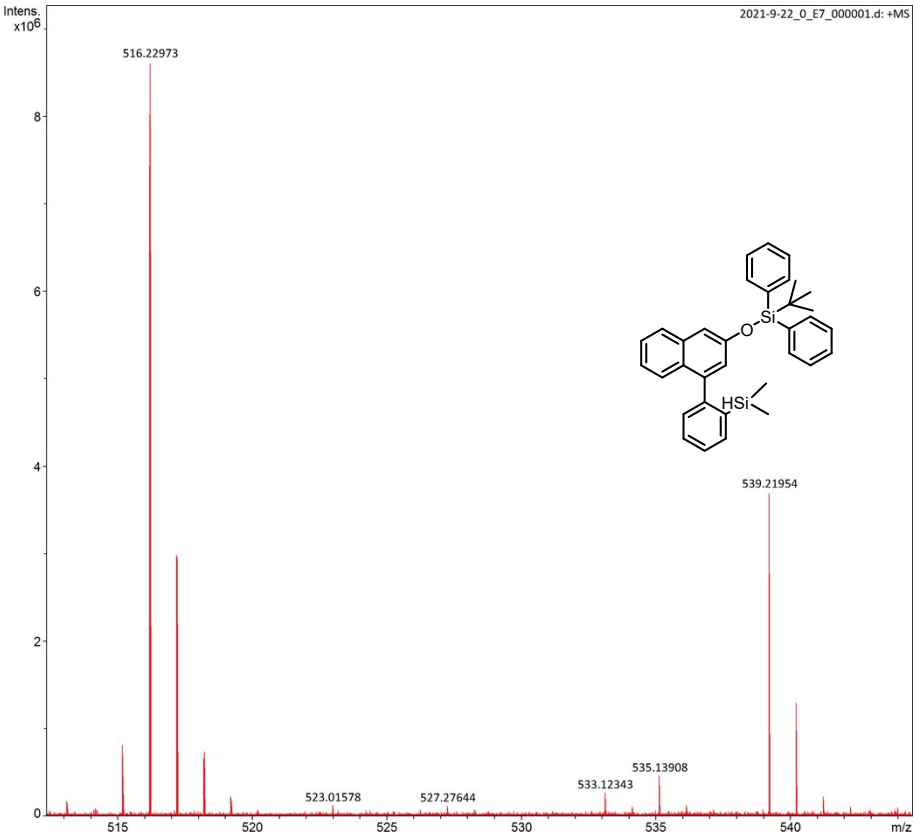


Figure S37. HRMS (ESI) of **7**.

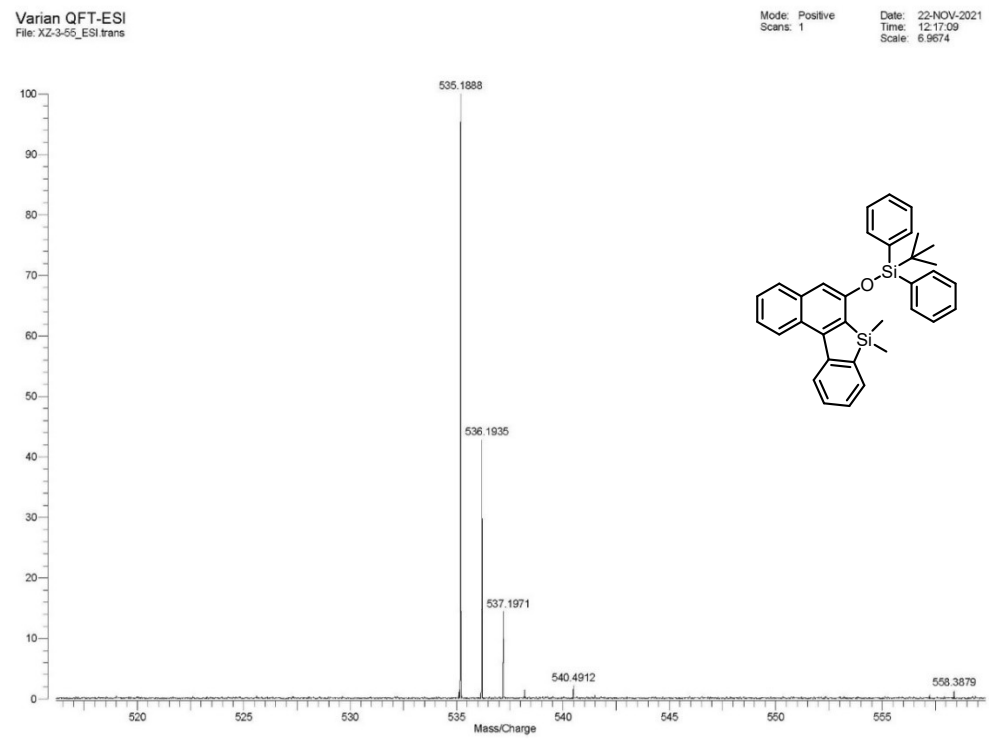


Figure S38. HRMS (ESI) of **8**.

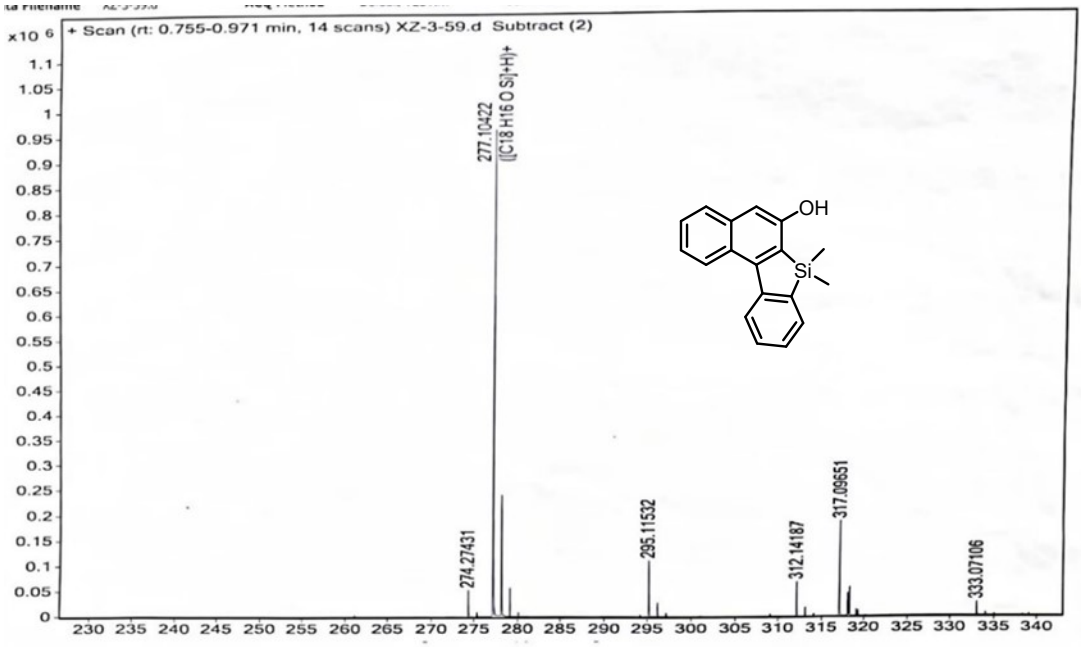


Figure S39. HRMS (ESI) of **9**.

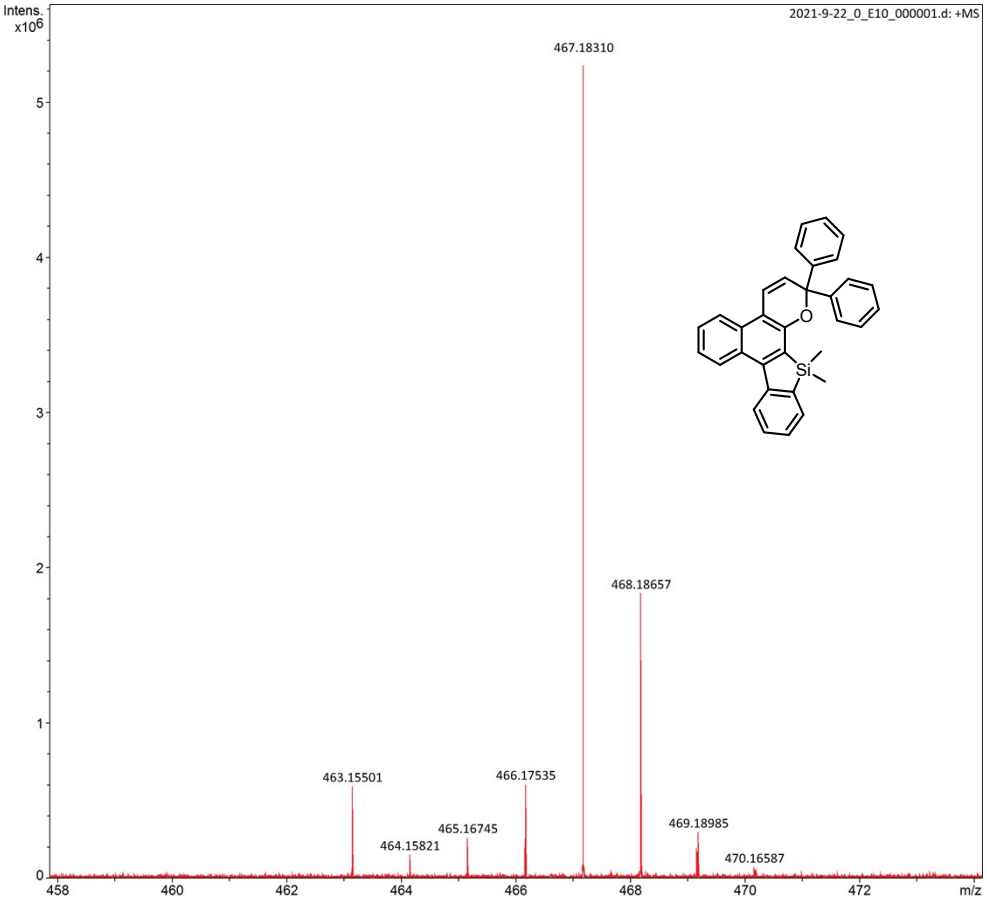


Figure S40. HRMS (ESI) of **SiNP-a**.

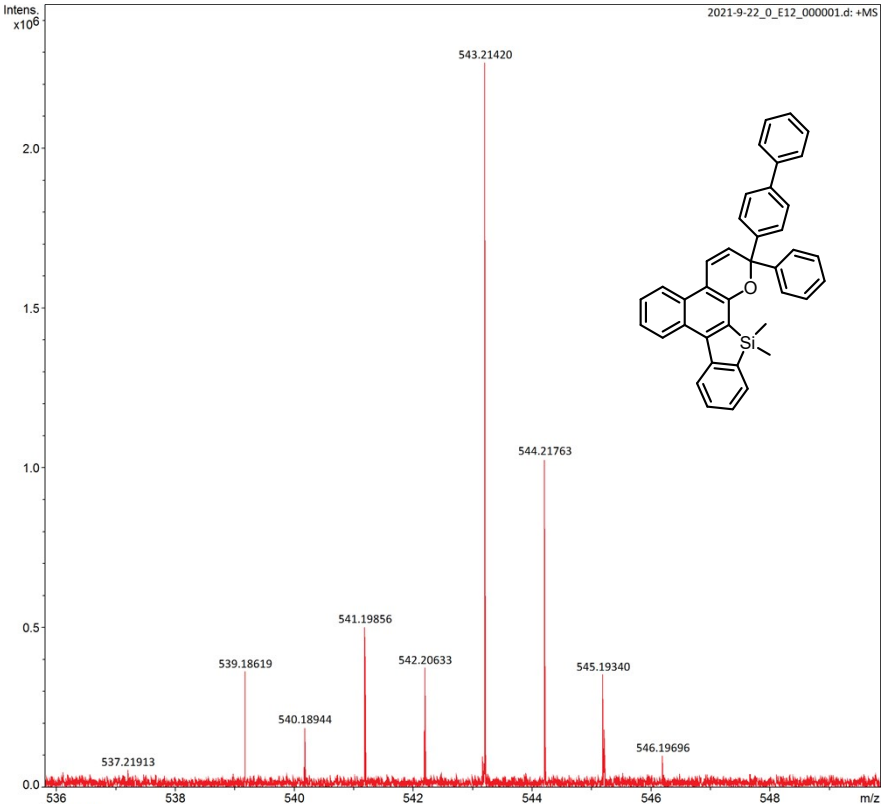


Figure S41. HRMS (ESI) of **SiNP-b**.

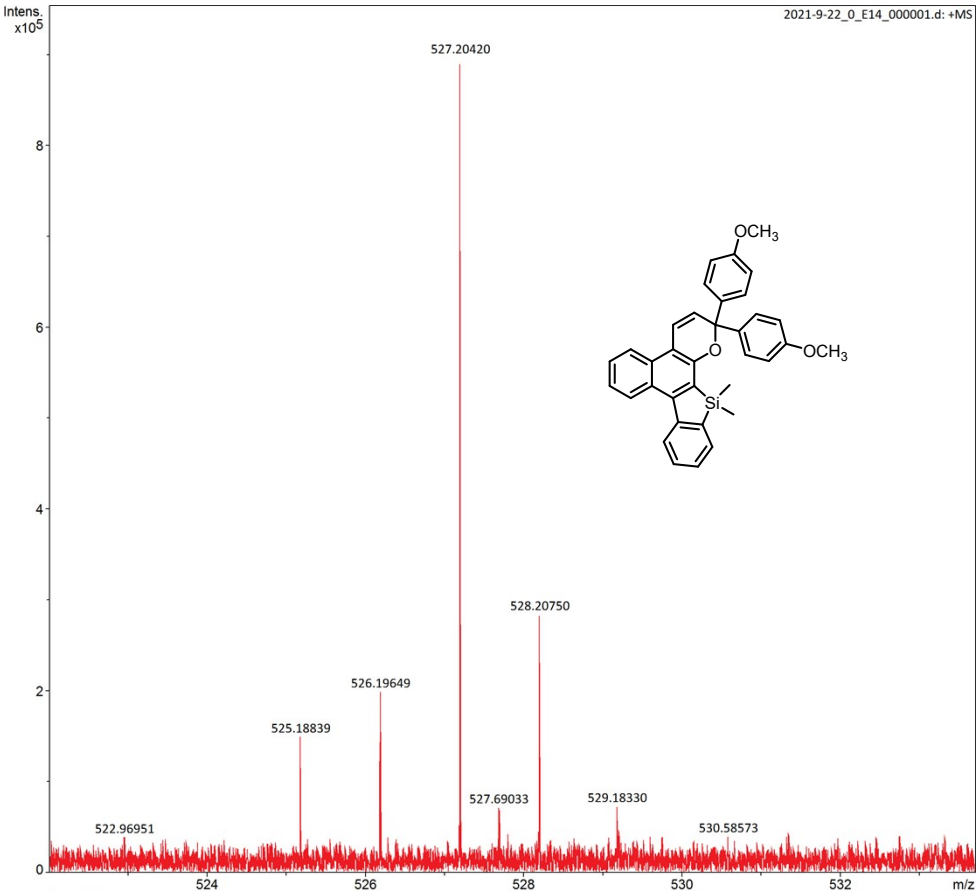


Figure S42. HRMS (ESI) of **SiNP-c**.

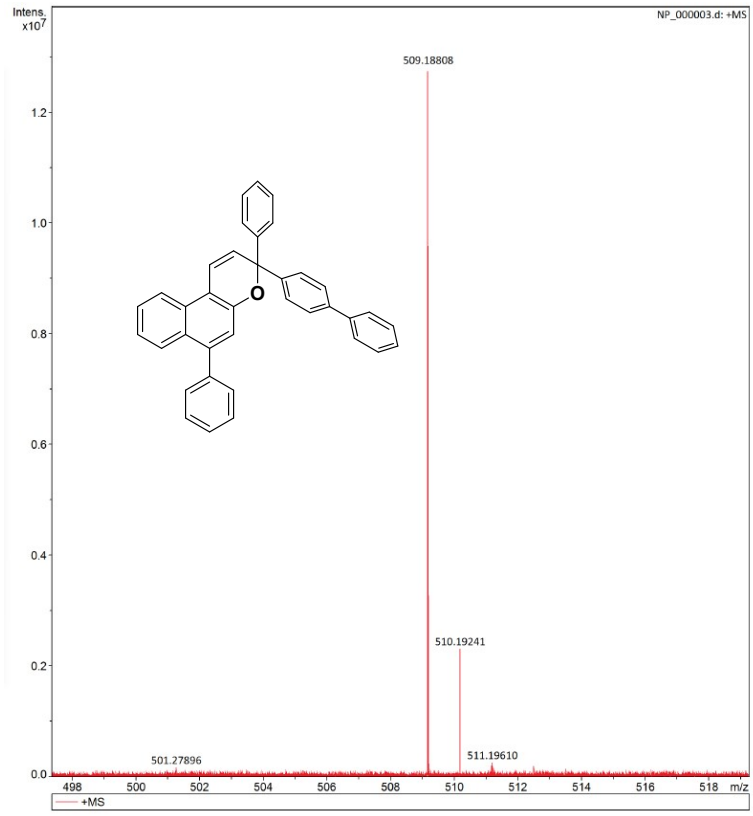


Figure S43. HRMS (ESI) of NP-Ph.

3. X-ray crystal structure refinement data for CNP-a.

Table S1. X-ray crystal structure refinement data for **CNP-a.**

Identification code	**CNP-a**
Empirical formula	$C_{34}H_{26}O$
Formula weight	450.55
Temperature	113(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 9.6418(19) A, alpha = 90 deg. b = 26.613(5) A, beta = 98.63(3) deg. c = 9.4683(19) A, gamma = 90 deg.
Volume	2402.0(8) A^3
Z, Calculated density	4, 1.246 Mg/m^3
Absorption coefficient	0.073 mm^-1
F(000)	952
Crystal size	0.200 x 0.180 x 0.120 mm
Theta range for data collection	1.530 to 25.017 deg.
Limiting indices	-11<=h<=11, -31<=k<=31, -11<=l<=11
Reflections collected / unique	18867 / 4229 [R(int) = 0.0571]
Completeness to theta = 27.89	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1 and 0.7957
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4229 / 0 / 319
Goodness-of-fit on F^2	1.011
Final R indices [I>2sigma(I)]	R_1 = 0.0601, wR_2 = 0.1746
R indices (all data)	R_1 = 0.0731, wR_2 = 0.2022
Extinction coefficient	0.030(4)
Largest diff. peak and hole	0.516 and -0.423 e.A^-3

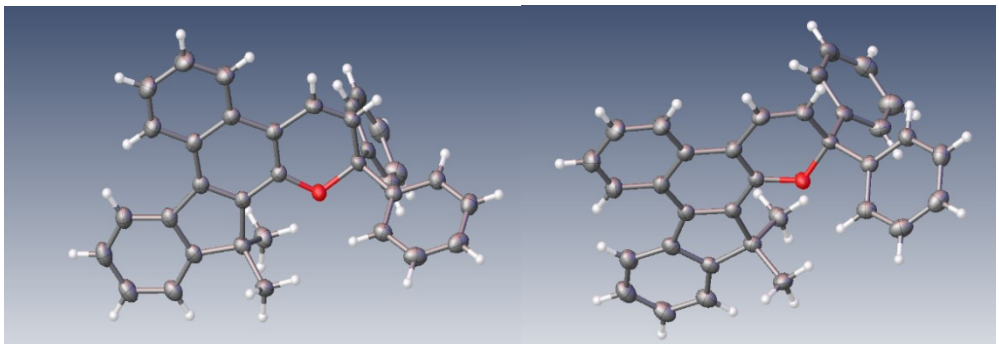


Figure S44. Crystal structure of **CNP-a**

4. Fatigue resistance of SiNP-b in toluene at 298 K.

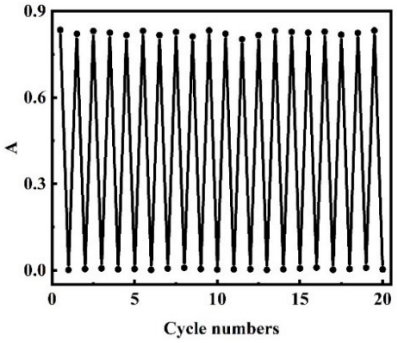


Figure S45. UV–vis irradiation/dark cycles for **SiNP-b** in toluene (8.0×10^{-5} M) at 298 K.

5. Calculated cartesian coordinates and thermodynamic energy

CNP-a-CF

C,0,0.7964899767,2.4697589093,-1.3866294574
C,0,1.3878764016,0.3550720335,-0.3491056738
C,0,0.0506671768,-0.0937047765,-0.4996612403
C,0,-0.5114324682,2.0262197673,-1.5532540913
C,0,2.3797506042,-0.5875383256,0.1762395607
C,0,-0.313915049,-1.4576960676,-0.0816074918
C,0,0.7774445298,-2.4739448713,0.0739119597
C,0,2.1106616658,-1.9156372446,0.2912916233
C,0,-1.5561137564,-1.8936978661,0.254475262
C,0,-2.748601741,-1.103526813,0.4670625105
H,0,1.092697406,3.4530194618,-1.7378641333
H,0,-1.2473769488,2.6583165197,-2.0404122598
H,0,-2.6129246242,-0.0371713277,0.6311103436
O,0,0.5562276315,-3.6790319007,0.1160081712
H,0,-1.6275677656,-2.9609200301,0.4607344175
C,0,-4.0107875207,-1.5997608937,0.5371021273
C,0,-5.1361943623,-0.7133864929,0.9247250867
C,0,-6.3968467253,-0.8676181073,0.3310342442
C,0,-4.9632118736,0.3067685061,1.870119665
C,0,-7.4444969932,-0.014088978,0.6555309246
H,0,-6.5452931057,-1.656603765,-0.4005416825
C,0,-6.0127812966,1.1576806873,2.197134526
H,0,-4.0038433962,0.4137822231,2.368239937
C,0,-7.256085534,1.0029558096,1.5885224918
H,0,-8.4105998727,-0.142924523,0.177062311
H,0,-5.863082865,1.9371505949,2.9380380204
H,0,-8.0760097877,1.6665748549,1.8457389367

C,0,-4.3260886816,-3.0090997687,0.1987478227
C,0,-5.2171652866,-3.7447334134,0.9939293461
C,0,-3.7511079868,-3.6319040369,-0.9161580824
C,0,-5.4983303785,-5.0726625712,0.6987196237
H,0,-5.6787824534,-3.2679755209,1.8541748338
C,0,-4.0381255897,-4.960250577,-1.2146638554
H,0,-3.0865094879,-3.061969622,-1.5590294057
C,0,-4.9084491651,-5.6848169039,-0.4064035349
H,0,-6.1788890107,-5.6327726817,1.3326707049
H,0,-3.5821578964,-5.42585872,-2.0826898218
H,0,-5.1311067628,-6.7218141865,-0.6382066506
C,0,-0.8707903515,0.7515139712,-1.1310806073
H,0,-1.8706287996,0.3871842634,-1.340204791
C,0,1.7382976743,1.6288653753,-0.8061008149
H,0,2.7707747623,1.949500459,-0.7559273694
C,0,3.7851713629,-0.3640398569,0.5784187495
C,0,4.5470942739,0.7916309534,0.7628734393
C,0,4.3476325643,-1.6229028781,0.8618701845
C,0,5.8715971917,0.6694744622,1.1768398677
C,0,5.6677267614,-1.7391253255,1.2689616963
C,0,6.4346137263,-0.5838798701,1.4155991489
H,0,6.0959010417,-2.7157087023,1.4817163802
H,0,7.4700258177,-0.6578856118,1.7340629884
H,0,4.1263806479,1.7806395019,0.6265913345
H,0,6.4696815607,1.5637969993,1.3221495562
C,0,3.3213533347,-2.7220110183,0.6963814282
C,0,3.7161277272,-3.7119370278,-0.4133369865
H,0,2.9123209605,-4.4378450289,-0.5600445746
H,0,3.8978740397,-3.186330941,-1.3555699904
H,0,4.6307791051,-4.2457206321,-0.1332097879
C,0,3.088384133,-3.4731433927,2.0176562461
H,0,3.9962801626,-4.0102723173,2.3122337107
H,0,2.8254350358,-2.7756490883,2.8186312928
H,0,2.2760665107,-4.193333217,1.8908520789

Zero-point correction = 0.502701 (Hartree/Particle)
Thermal correction to Energy = 0.530492
Thermal correction to Enthalpy = 0.531436
Thermal correction to Gibbs Free Energy = 0.442258
Sum of electronic and zero-point Energies = -1385.424600
Sum of electronic and thermal Energies = -1385.396809
Sum of electronic and thermal Enthalpies = -1385.395865
Sum of electronic and thermal Free Energies = -1385.485043

CNP-a-TC

C,0,1.1384803737,-2.9293626774,-1.3137212403
C,0,1.3972877507,-0.6021672606,-0.6719841243
C,0,-0.0031827693,-0.4144020534,-0.7661651677
C,0,-0.2411478249,-2.7534482264,-1.3915239341
C,0,2.2263479128,0.5578302267,-0.344911922
C,0,-0.5953166469,0.9199472951,-0.5285821492
C,0,0.3045388879,2.1108510609,-0.5651562854
C,0,1.7222089901,1.8208734567,-0.3622384133
C,0,-1.9118538942,1.0414484321,-0.1987330653
C,0,-2.6527799459,2.2446736569,0.0923909232
H,0,1.584417443,-3.8913881336,-1.5448862683
H,0,-0.8829054378,-3.5796485058,-1.68152589
H,0,-2.0944273273,3.1708394172,0.1566290641
O,0,-0.1042492475,3.2647279652,-0.675314222
H,0,-2.4705463295,0.1177213925,-0.0714157707
C,0,-3.996267366,2.266457147,0.2995515227
C,0,-4.66099134,3.5113808993,0.7542201327
C,0,-5.9729203193,3.8054345483,0.3564037889
C,0,-3.9930715741,4.4266845465,1.5801933694
C,0,-6.5890508093,4.9866098002,0.7538355128
H,0,-6.5045753296,3.1058623479,-0.2817916363
C,0,-4.6114568104,5.6050271006,1.9805554286
H,0,-2.9893922101,4.1984284206,1.9258638856
C,0,-5.9105974038,5.8911375179,1.5667573756
H,0,-7.6012828444,5.2015267552,0.4252549772
H,0,-4.0797435282,6.2987370912,2.624594369
H,0,-6.3929627369,6.8118009828,1.8803334038
C,0,-4.8607654429,1.081381054,0.0610678845
C,0,-5.784880991,0.678532275,1.0345518314
C,0,-4.7857753743,0.356468219,-1.1349354222
C,0,-6.5872698553,-0.4377102697,0.8307000822
H,0,-5.8606593742,1.2455133061,1.9583714487
C,0,-5.5966604543,-0.7561128118,-1.3427870979
H,0,-4.0985181785,0.6862697702,-1.9098402698
C,0,-6.4949774885,-1.1589288888,-0.358343792
H,0,-7.2884135471,-0.7449856891,1.60059757
H,0,-5.5335540879,-1.3016801967,-2.2794735107
H,0,-7.1273236821,-2.0266986956,-0.5190880838
C,0,-0.7977327226,-1.5080810517,-1.1362664686
H,0,-1.8679190776,-1.3772722304,-1.2654238158
C,0,1.9456779772,-1.8558261534,-0.9672771873
H,0,3.0206831637,-1.9807083482,-0.96877263
C,0,3.6639952935,0.6364864928,-0.0075842426

C,0,3.9965256989,1.9997181222,0.101538574
C,0,4.6323209139,-0.3343892686,0.257985445
C,0,5.2867975363,2.3972873984,0.4163990853
C,0,5.9261014721,0.07035772,0.5783019252
C,0,6.257809839,1.4233344888,0.6453691247
H,0,6.6828156354,-0.6798089172,0.7866102351
H,0,7.2729832485,1.7175420627,0.8937322739
H,0,4.3973822887,-1.3918333778,0.2561811583
H,0,5.5359413271,3.452761054,0.495181362
C,0,2.7818006806,2.8721488687,-0.1278780777
C,0,2.4696656504,3.7315332922,1.1080855885
H,0,1.5436443732,4.2881754836,0.9425781936
H,0,2.3564882137,3.1048862276,1.9979370241
H,0,3.2820841031,4.4435527307,1.2887901336
C,0,2.9545769685,3.7686071532,-1.3667234327
H,0,3.1929328446,3.1681092424,-2.2495814437
H,0,2.0313907525,4.3230612708,-1.55177031
H,0,3.7707529229,4.4808974426,-1.20330011
Zero-point correction = 0.502858 (Hartree/Particle)
Thermal correction to Energy = 0.530674
Thermal correction to Enthalpy = 0.531618
Thermal correction to Gibbs Free Energy = 0.443539
Sum of electronic and zero-point Energies = -1385.425079
Sum of electronic and thermal Energies = -1385.397263
Sum of electronic and thermal Enthalpies = -1385.396319
Sum of electronic and thermal Free Energies = -1385.484398

CNP-a-TS

C,0,-1.8739836075,-2.6572517102,2.7066090159
C,0,-1.3267936729,-0.7817867483,1.2606283482
C,0,0.0518412255,-0.9695202694,1.5410706472
C,0,-0.5173036105,-2.8253085247,3.0071370374
C,0,-1.6791611162,0.2974050775,0.3614323973
C,0,1.0701669543,-0.1494265282,0.9073265633
C,0,0.6996497968,0.7440085016,-0.1733273777
C,0,-0.7171739295,1.0070035527,-0.3065176812
C,0,2.2873139876,0.1012441933,1.5630283854
C,0,3.3386436568,0.809141018,0.9959109839
H,0,-2.6160144998,-3.3216786373,3.1377247415
H,0,-0.2018697051,-3.6195549562,3.6770102191
H,0,3.9854661802,1.4085601966,1.6303509081
O,0,1.5132759234,1.370265471,-0.9103537323
H,0,2.3222284999,-0.1061782822,2.632905496

C,0,3.4879783142,0.8973983602,-0.3990915556
C,0,4.2423386421,2.0589206514,-0.9365414208
C,0,5.2891588254,1.8941244363,-1.8503869797
C,0,3.9283048362,3.3468585997,-0.4849303056
C,0,6.016732993,2.9951243559,-2.2912291193
H,0,5.541857171,0.8990455477,-2.2027770768
C,0,4.6472871361,4.4464370794,-0.9365714867
H,0,3.0924894464,3.4704398554,0.1977595206
C,0,5.6963303718,4.271835547,-1.8382216593
H,0,6.8342353316,2.8540521787,-2.9913333166
H,0,4.3867022887,5.4419761624,-0.5908056526
H,0,6.2593659336,5.1306289911,-2.1908688718
C,0,3.4065076876,-0.3164964446,-1.2613015822
C,0,3.0793222216,-0.1922213115,-2.6191578461
C,0,3.7184429113,-1.580405801,-0.7536161659
C,0,3.0448079522,-1.3101266744,-3.4407885199
H,0,2.8295801405,0.7889420479,-3.0105116625
C,0,3.6866417336,-2.7005465251,-1.5795947527
H,0,3.9944728115,-1.6782243444,0.291195719
C,0,3.3475505841,-2.5692607812,-2.9223797091
H,0,2.778082125,-1.20162807,-4.4875045355
H,0,3.931395362,-3.6763601337,-1.171721321
H,0,3.3233676984,-3.4433543597,-3.5662027471
C,0,0.4263763264,-2.004800604,2.4192754918
H,0,1.4824203553,-2.1855554662,2.5983567539
C,0,-2.2653370851,-1.6548149424,1.8394797404
H,0,-3.3108997396,-1.5663211102,1.5763060043
C,0,-3.0014665087,0.8394505308,-0.0261343681
C,0,-2.7833987816,1.8505095758,-0.9796991041
C,0,-4.3038493128,0.5724323465,0.4027685831
C,0,-3.8399325253,2.559921735,-1.5293469788
C,0,-5.3632031333,1.2880352997,-0.1517046086
C,0,-5.139475485,2.2683928419,-1.1169584711
H,0,-6.3757886241,1.0811417239,0.1810766384
H,0,-5.9780355134,2.8139597145,-1.5388873048
H,0,-3.6572235014,3.3382212233,-2.2666983889
H,0,-4.5156306976,-0.1538971644,1.1770683698
C,0,-1.3064619562,2.0285389994,-1.2547206242
C,0,-0.97582995,1.6920295434,-2.7192850742
H,0,-1.3003629507,0.6765307674,-2.9651419751
H,0,-1.490085483,2.3906782627,-3.3884626018
H,0,0.1016202841,1.7704479142,-2.883591584
C,0,-0.8410774732,3.4549359063,-0.9202125841
H,0,-1.0949898717,3.712600769,0.1123784424

H,0,0.2414835303,3.5291010988,-1.0520541751
H,0,-1.3273546641,4.1773472531,-1.584819796
Zero-point correction = 0.501175 (Hartree/Particle)
Thermal correction to Energy = 0.528060
Thermal correction to Enthalpy = 0.529005
Thermal correction to Gibbs Free Energy = 0.444410
Sum of electronic and zero-point Energies = -1385.400383
Sum of electronic and thermal Energies = -1385.373497
Sum of electronic and thermal Enthalpies = -1385.372553
Sum of electronic and thermal Free Energies = -1385.457148

CNP-a-TT

C,0,-2.4388979161,-1.3112031246,3.4855448342
C,0,-1.478160243,-0.2011968166,1.543037929
C,0,-0.1661753148,-0.5056441181,2.0236375456
C,0,-1.1451709602,-1.591882425,3.9704615844
C,0,-1.5949203051,0.5146671108,0.3108185394
C,0,0.9879422309,-0.1314141141,1.2625265364
C,0,0.8137642132,0.4692503491,0.0295155909
C,0,-0.4683665171,0.8174494212,-0.4340723365
C,0,2.3644115149,-0.2735030241,1.7277744705
C,0,3.3893768308,-0.0528598257,0.9007747645
H,0,-3.3111691338,-1.6390522878,4.0422031697
H,0,-1.021488591,-2.1310329702,4.9046795487
H,0,4.4205505465,-0.134827987,1.2306342872
O,0,1.8579407503,0.8192585994,-0.7706282173
H,0,2.5544663445,-0.5138660849,2.768324076
C,0,3.1567709583,0.2306805695,-0.5678229495
C,0,4.116248929,1.2800275647,-1.1266858081
C,0,4.3651401665,1.3387340824,-2.4993291937
C,0,4.665515262,2.2551524176,-0.2947428931
C,0,5.1636276891,2.3474601304,-3.0283766203
H,0,3.9324650769,0.5872875193,-3.1538081706
C,0,5.4714852812,3.261240655,-0.8219828137
H,0,4.4522663744,2.2353599088,0.7704798849
C,0,5.7238243094,3.3082008987,-2.1896101569
H,0,5.3503015672,2.3812111353,-4.0974382127
H,0,5.8981257682,4.0109439176,-0.1626029955
H,0,6.353075347,4.0912567988,-2.6015904952
C,0,3.2604114089,-1.0981527665,-1.318707023
C,0,2.1449144055,-1.7263679954,-1.8686317824

C,0,4.5080882143,-1.7250935297,-1.4099561879
C,0,2.2758427791,-2.9646637268,-2.4978758312
H,0,1.1708794975,-1.2534955703,-1.8133079817
C,0,4.6369015639,-2.9571748482,-2.0376575651
H,0,5.3863731795,-1.2332903667,-0.9980671503
C,0,3.5168970248,-3.5837075005,-2.5838824475
H,0,1.3978853161,-3.4415572844,-2.9230777049
H,0,5.6130884753,-3.428048018,-2.1041194831
H,0,3.6156678281,-4.5460324397,-3.0765105473
C,0,-0.0419597108,-1.2044431547,3.2524783691
H,0,0.9447529566,-1.4615050039,3.6218323644
C,0,-2.5942324581,-0.6364025592,2.300593029
H,0,-3.5920241622,-0.4612197401,1.9231937943
C,0,-2.7706238276,1.0551225303,-0.4116306323
C,0,-4.136102337,1.0988471317,-0.1189675406
C,0,-2.3071156253,1.6510519161,-1.5992768112
C,0,-5.0104524367,1.7003896399,-1.0221584549
C,0,-3.179260638,2.2475255183,-2.4959429047
C,0,-4.5430916298,2.2650188381,-2.2070819416
H,0,-2.8046923157,2.7013474188,-3.4105763233
H,0,-5.2403441081,2.727253555,-2.8990286999
H,0,-4.540545403,0.6989032897,0.8016401718
H,0,-6.0712353353,1.7313210989,-0.7927563626
C,0,-0.7988369298,1.5661388589,-1.7091078118
C,0,-0.3735664973,0.7992314472,-2.9711276395
H,0,0.7165049586,0.7323920497,-3.0278196469
H,0,-0.7954437392,-0.2110929657,-2.9750414003
H,0,-0.7349544763,1.3223310922,-3.8631260422
C,0,-0.1744935455,2.9729166427,-1.7120863462
H,0,-0.4853645402,3.5340622901,-0.8259552933
H,0,0.916459967,2.9038218982,-1.7237027186
H,0,-0.5009482185,3.5243100938,-2.600524893
Zero-point correction = 0.503610 (Hartree/Particle)
Thermal correction to Energy = 0.530578
Thermal correction to Enthalpy = 0.531522
Thermal correction to Gibbs Free Energy = 0.445361
Sum of electronic and zero-point Energies = -1385.442174
Sum of electronic and thermal Energies = -1385.415206
Sum of electronic and thermal Enthalpies = -1385.414262
Sum of electronic and thermal Free Energies = -1385.500423

SiNP-a-CF

C,0,0.9567454982,2.2437443683,-1.5698945503

C,0,1.4135965181,0.1475446609,-0.4245918132
C,0,0.0652629593,-0.2472191195,-0.6242131463
C,0,-0.3700508945,1.8658013345,-1.7471526198
C,0,2.3505274205,-0.8251289485,0.1705325184
C,0,-0.3609554257,-1.6004771301,-0.2343109183
C,0,0.7035814716,-2.6473145292,-0.1324197621
C,0,2.0417221212,-2.1517680026,0.1890891225
C,0,-1.6150061924,-1.9949357804,0.1043631302
C,0,-2.7646516432,-1.1516296951,0.3433709895
H,0,1.3139640456,3.1934531188,-1.9552079894
H,0,-1.0615370512,2.5180008654,-2.2716703816
H,0,-2.5784980133,-0.0869147961,0.4621917454
O,0,0.4596406963,-3.8465582015,-0.1937304143
H,0,-1.7300743404,-3.0618734525,0.2899506075
C,0,-4.0414816109,-1.5889708271,0.4926816611
C,0,-5.1075513087,-0.6374590118,0.8950282622
C,0,-6.4037026214,-0.7640143917,0.37545749
C,0,-4.8440471615,0.41460772,1.7825090518
C,0,-7.3972886564,0.1469133757,0.7137204417
H,0,-6.62381823,-1.5788314797,-0.3081493961
C,0,-5.8396014941,1.3228382742,2.1239897969
H,0,-3.8563325512,0.502319315,2.2257630299
C,0,-7.118924522,1.1948453476,1.5881942765
H,0,-8.3919327246,0.0381725541,0.2921780706
H,0,-5.618497059,2.1268265405,2.8194156698
H,0,-7.8967177197,1.9029897789,1.8573461007
C,0,-4.4378756833,-2.9976109968,0.2468787103
C,0,-5.2985519212,-3.6467946494,1.1443516741
C,0,-3.979262952,-3.7031243987,-0.8723039844
C,0,-5.6645508226,-4.9712827112,0.9429726749
H,0,-5.6682818179,-3.1042407283,2.0099369899
C,0,-4.3525714672,-5.0282296773,-1.0772861595
H,0,-3.3377819401,-3.2016702225,-1.5913135525
C,0,-5.1921029524,-5.6664104653,-0.1693121126
H,0,-6.3207090751,-5.4627521623,1.6547843648
H,0,-3.9891382726,-5.5597369117,-1.9511869464
H,0,-5.4827530614,-6.70013609,-0.329354356
C,0,-0.8004720158,0.622695066,-1.29856299
H,0,-1.8098139734,0.2959566297,-1.5251618688
C,0,1.8396103848,1.3816533875,-0.9301658412
H,0,2.8867562566,1.6514845647,-0.8706510373
C,0,3.7017281674,-0.4964721076,0.7273876117
C,0,4.1429129363,0.767964063,1.123597377
C,0,4.521920498,-1.6280081279,0.9620992377

C,0,5.4159424134,0.9201876745,1.6737517678
C,0,5.7885524167,-1.4535788842,1.5077942238
C,0,6.2486874647,-0.1792977729,1.8463307993
H,0,6.4248219505,-2.3163553197,1.6936543075
H,0,7.2396222919,-0.0500005869,2.2712306751
H,0,3.4938530084,1.6332931936,1.0511674476
H,0,5.7495509918,1.9070818127,1.9802778467
Si,0,3.5257461737,-3.1960284995,0.6357033399
C,0,4.1199213109,-4.2337515491,-0.8104180603
H,0,5.0558258181,-4.7498018525,-0.5736035226
H,0,3.3630115144,-4.9865874836,-1.0519578665
H,0,4.2829609388,-3.6146559565,-1.6969416776
C,0,3.319584735,-4.2425287853,2.1777336209
H,0,2.556089847,-5.0069842234,2.0028132418
H,0,4.2540494833,-4.7463251641,2.4457104855
H,0,3.0042608627,-3.6307716536,3.0274021758
Zero-point correction = 0.493352 (Hartree/Particle)
Thermal correction to Energy = 0.523169
Thermal correction to Enthalpy = 0.524113
Thermal correction to Gibbs Free Energy = 0.430816
Sum of electronic and zero-point Energies = -1636.816712
Sum of electronic and thermal Energies = -1636.786896
Sum of electronic and thermal Enthalpies = -1636.785951
Sum of electronic and thermal Free Energies = -1636.879248

SiNP-a-TC

C,0,1.2784851281,-2.7079260421,-1.5364049729
C,0,1.4123330149,-0.4116666919,-0.747387145
C,0,0.0019809221,-0.3033304244,-0.835393379
C,0,-0.1111168128,-2.6193862077,-1.5681970857
C,0,2.1819576722,0.7830287755,-0.3605774435
C,0,-0.6628057408,0.9906100267,-0.5821760289
C,0,0.1831966245,2.2150979107,-0.6764291773
C,0,1.6093847977,2.0175831923,-0.4275836023
C,0,-1.9721577143,1.0516355728,-0.2165914917
C,0,-2.7426052179,2.2329144987,0.0909979627
H,0,1.7783965422,-3.6223178945,-1.8394440846
H,0,-0.7071891138,-3.4685037933,-1.8879676781
H,0,-2.2053529703,3.1730562247,0.1446897658
O,0,-0.2730676724,3.3416049991,-0.8579415714
H,0,-2.4881322939,0.1059065738,-0.0657113207
C,0,-4.0801221285,2.2231165481,0.33042115
C,0,-4.7588149006,3.4486504861,0.8171441924

C,0,-6.0840869167,3.7260578681,0.4528737327
C,0,-4.0901800626,4.3605362137,1.6460641989
C,0,-6.7126451304,4.8876457854,0.8867380903
H,0,-6.616617855,3.0285524021,-0.1868662932
C,0,-4.7203973655,5.5197123757,2.0821985689
H,0,-3.0758791834,4.1429744613,1.9666354764
C,0,-6.0333154884,5.7891781287,1.702288991
H,0,-7.7356646319,5.0902781049,0.5847938357
H,0,-4.1875024992,6.2105634445,2.7283408692
H,0,-6.5257202221,6.6944563533,2.0440764857
C,0,-4.9228943077,1.0220117438,0.0969621539
C,0,-5.8332833056,0.5979158851,1.0745437393
C,0,-4.8425290728,0.3030489285,-1.102555008
C,0,-6.6172490917,-0.5312597222,0.8705079988
H,0,-5.9136887391,1.1594001368,2.0012699948
C,0,-5.6345087622,-0.8229850819,-1.3102209718
H,0,-4.1674902455,0.64936259,-1.8809551751
C,0,-6.5199265509,-1.2455824083,-0.3224822505
H,0,-7.3087192642,-0.8537988007,1.6429137908
H,0,-5.5675162413,-1.3633127855,-2.2496520122
H,0,-7.1387848722,-2.1229297505,-0.483841099
C,0,-0.7349969673,-1.423637192,-1.2415330637
H,0,-1.8127291954,-1.344668333,-1.3501487312
C,0,2.0271951413,-1.6090865107,-1.1392831216
H,0,3.1077633938,-1.6657000003,-1.1783719307
C,0,3.615223164,0.7904964296,0.0779407898
C,0,4.2016867665,2.0800063422,0.1150179939
C,0,4.3417547513,-0.3084421748,0.5430225296
C,0,5.5202311723,2.2213383969,0.5322275492
C,0,5.6624110616,-0.1439068977,0.9615680794
C,0,6.2625048816,1.1096176289,0.9357934282
H,0,6.2183359859,-1.0042956067,1.3219795409
H,0,7.2927013766,1.2272181092,1.2582838855
H,0,3.882316369,-1.2864859146,0.6268223326
H,0,5.9785895605,3.2076110483,0.5636752702
Si,0,2.8786021264,3.3756237655,-0.2400603694
C,0,2.5995077742,4.52041102,1.2205249989
H,0,1.6830470677,5.0975819329,1.0623701848
H,0,2.4939451205,3.9525701821,2.1490524457
H,0,3.4307404091,5.2231256394,1.3401111526
C,0,3.1150425727,4.3502575675,-1.8249643289
H,0,2.2026632838,4.913625171,-2.0436972094
H,0,3.946208233,5.0576037034,-1.739735312
H,0,3.3156347727,3.6832672057,-2.6679359506

Zero-point correction = 0.493387 (Hartree/Particle)
Thermal correction to Energy = 0.523292
Thermal correction to Enthalpy = 0.524236
Thermal correction to Gibbs Free Energy = 0.430686
Sum of electronic and zero-point Energies = -1636.817237
Sum of electronic and thermal Energies = -1636.787332
Sum of electronic and thermal Enthalpies = -1636.786388
Sum of electronic and thermal Free Energies = -1636.879938

SiNP-a-TS

C,0,-1.9215991828,-2.778302368,2.2370612626
C,0,-1.3221491308,-0.7407961125,1.0478029838
C,0,0.0391323973,-0.947389146,1.4001454666
C,0,-0.5944111043,-2.9313750241,2.655388333
C,0,-1.6366965476,0.4278581923,0.23719251
C,0,1.093371309,-0.1088392465,0.8612284273
C,0,0.7696272035,0.7909265701,-0.2254994403
C,0,-0.6287602613,1.1222341028,-0.3819470154
C,0,2.2812809375,0.1259736412,1.5706522704
C,0,3.3545004445,0.831013549,1.0392752614
H,0,-2.6711265435,-3.511718238,2.5171279634
H,0,-0.3128342893,-3.7743120158,3.2793119419
H,0,3.9805801847,1.4340550722,1.6907608032
O,0,1.6124765393,1.3948492172,-0.9487750112
H,0,2.2740297063,-0.0917269832,2.6393565837
C,0,3.5531448172,0.9041226114,-0.3509335928
C,0,4.341247901,2.0510804101,-0.8726035401
C,0,5.4217628426,1.8641419184,-1.7414622812
C,0,4.0244640593,3.3475074451,-0.4484738368
C,0,6.1795096156,2.9518252237,-2.1645602674
H,0,5.6771003863,0.8621408632,-2.0718379779
C,0,4.7744812864,4.4336222625,-0.8818436239
H,0,3.1626959174,3.4885364803,0.1975190506
C,0,5.8570095612,4.2370369259,-1.738129737
H,0,7.0230169863,2.7934045225,-2.8293069548
H,0,4.5113284765,5.4358806794,-0.5580264463
H,0,6.4448770663,5.0851191237,-2.0758713996
C,0,3.497811751,-0.3234279114,-1.1980516765
C,0,3.2220094391,-0.2209820172,-2.568545907
C,0,3.7873753556,-1.5800857606,-0.6594359717
C,0,3.2127793075,-1.3528145097,-3.372289121
H,0,2.9907441148,0.7540986663,-2.9853557355
C,0,3.7800035863,-2.7141095197,-1.4667969785

H,0,4.0269523354,-1.661857784,0.3957619604
C,0,3.4899910834,-2.6045626313,-2.8227288253
H,0,2.9851281179,-1.2605534396,-4.4298283862
H,0,4.0059977053,-3.6835784929,-1.0336363092
H,0,3.4841862275,-3.4891978869,-3.4523606451
C,0,0.3695707487,-2.0415525865,2.2224721001
H,0,1.4136372759,-2.2149865831,2.4679844355
C,0,-2.2719704829,-1.7034368527,1.4416429778
H,0,-3.2882220139,-1.629414358,1.0758606067
C,0,-3.0042128427,0.9901198786,-0.0142178707
C,0,-3.0531877636,1.9751659918,-1.0332138883
C,0,-4.1588643131,0.7182455441,0.7245925634
C,0,-4.2608578242,2.5924153489,-1.3382621703
C,0,-5.3614634949,1.3470019997,0.4009565469
C,0,-5.4250641698,2.2645503956,-0.6411132987
H,0,-6.2512438226,1.1232879344,0.982060723
H,0,-6.3665881874,2.7451509971,-0.8897473766
H,0,-4.3025487714,3.3500433008,-2.1182684367
H,0,-4.1309461392,0.0576233477,1.5824585281
Si,0,-1.3006445617,2.3674932072,-1.6004860804
C,0,-0.9050519675,1.9012284612,-3.3757686538
H,0,-1.2082091218,0.8716821121,-3.585286065
H,0,-1.4106363919,2.5619161395,-4.0874835235
H,0,0.1748010284,1.9797030248,-3.5370186831
C,0,-0.8254439058,4.1513908861,-1.2576493338
H,0,0.2519431416,4.2803566684,-1.4024223702
H,0,-1.3465568371,4.8389731336,-1.9320011646
H,0,-1.071691026,4.4287590589,-0.2289275535
Zero-point correction = 0.491248 (Hartree/Particle)
Thermal correction to Energy = 0.520239
Thermal correction to Enthalpy = 0.521184
Thermal correction to Gibbs Free Energy = 0.431028
Sum of electronic and zero-point Energies = -1636.792690
Sum of electronic and thermal Energies = -1636.763699
Sum of electronic and thermal Enthalpies = -1636.762755
Sum of electronic and thermal Free Energies = -1636.852911

SiNP-a-TT

C,0,-2.3908248203,-0.6540835956,3.6451412881
C,0,-1.3852071145,0.0277255824,1.5251172218
C,0,-0.101118441,-0.366614715,2.0244487924
C,0,-1.1430904239,-1.142982109,4.0877879938
C,0,-1.465771615,0.5974006694,0.2076792196

C,0,1.0852393853,-0.1031398404,1.266898779
C,0,0.9524433393,0.5443208546,0.0546972969
C,0,-0.2956194887,0.9065277614,-0.4749124679
C,0,2.446427381,-0.3496884063,1.734907849
C,0,3.4852932672,-0.1748050349,0.9106756733
H,0,-3.2599947473,-0.7141431525,4.2933796283
H,0,-1.0585573613,-1.6172574569,5.0613937519
H,0,4.5089435409,-0.3281803473,1.2403259915
O,0,2.034872306,0.9165584717,-0.6931813788
H,0,2.6225736764,-0.6365620928,2.7664867956
C,0,3.2666066445,0.1861858625,-0.5475647385
C,0,4.3328408382,1.1554020145,-1.0604067709
C,0,4.7978494799,1.103228364,-2.3753922204
C,0,4.7921153784,2.171723234,-0.2178021279
C,0,5.716878703,2.0454252205,-2.8366389125
H,0,4.4445099594,0.3233648171,-3.0439857379
C,0,5.712099866,3.1111508086,-0.675525751
H,0,4.4176490999,2.2308785749,0.8014256945
C,0,6.1793529831,3.0482513172,-1.9879515715
H,0,6.0708846886,1.9927923325,-3.8622232392
H,0,6.0632196507,3.8928640508,-0.0080126999
H,0,6.8997757871,3.7780558981,-2.346174976
C,0,3.2125145989,-1.1037444888,-1.3690645836
C,0,2.0990812276,-1.4415723823,-2.1362321884
C,0,4.3120351742,-1.9702071681,-1.3482114024
C,0,2.0833245899,-2.6295973508,-2.8710424516
H,0,1.2417392782,-0.7778038471,-2.1670738286
C,0,4.2985267511,-3.1502429452,-2.08295877
H,0,5.192830804,-1.7094967444,-0.7649271805
C,0,3.1792734885,-3.4855950443,-2.8478880059
H,0,1.2071980204,-2.8805805988,-3.4626044205
H,0,5.1623308312,-3.8086632477,-2.062754963
H,0,3.1664939882,-4.407836189,-3.4213715572
C,0,-0.028930141,-0.9873974379,3.3010032303
H,0,0.9283993238,-1.3428573917,3.6664571441
C,0,-2.502267753,-0.0888683709,2.3980977586
H,0,-3.4541930576,0.3289201322,2.0990462648
C,0,-2.7084426505,0.923488979,-0.5686427446
C,0,-3.9944703948,0.4221454162,-0.3377726371
C,0,-2.4878871986,1.7327763849,-1.7128283717
C,0,-5.0552459816,0.7945403439,-1.1656503424
C,0,-3.5581457545,2.0963809386,-2.5251016075
C,0,-4.8516651188,1.6513411767,-2.2429048182
H,0,-3.3876652868,2.7180126045,-3.4025549062

H,0,-5.6842722443,1.940754695,-2.8778105759
H,0,-4.183770577,-0.2997491525,0.4471686638
H,0,-6.0466528641,0.3952224882,-0.9698571548
Si,0,-0.6405322556,1.9389474429,-1.9990993902
C,0,-0.0984628382,1.1908967521,-3.6361599371
H,0,0.9951989736,1.1689971329,-3.704394069
H,0,-0.4762885706,0.1699152262,-3.7535986188
H,0,-0.4774232505,1.7891453521,-4.4729600066
C,0,0.0225417627,3.6853797595,-1.8225428873
H,0,-0.3082065262,4.134940919,-0.8812874165
H,0,1.1179862216,3.6723969809,-1.8316819752
H,0,-0.319485173,4.3216049013,-2.6464532942
Zero-point correction = 0.493022 (Hartree/Particle)
Thermal correction to Energy = 0.521021
Thermal correction to Enthalpy = 0.521965
Thermal correction to Gibbs Free Energy = 0.434969
Sum of electronic and zero-point Energies = -1636.870955
Sum of electronic and thermal Energies = -1636.842957
Sum of electronic and thermal Enthalpies = -1636.842013
Sum of electronic and thermal Free Energies = -1636.929008

6. References

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[S2] J. Han, J. Sun, S. Liu, Z. Xi, J. Meng, Z. Liu, China, CN111440193A **2020**.