

Electronic Supplementary Information

1,7-Naphthodiyne: a new platform for the synthesis of novel, sterically congested PAHs

Iago Pozo, Agustín Cobas, Diego Peña, Enrique Guitián and Dolores Pérez*

*Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares (CIQUS) and
Departamento de Química Orgánica, Universidade de Santiago de Compostela,
15782-Santiago de Compostela, Spain
dolores.perez@usc.es*

SUPPORTING INFORMATION

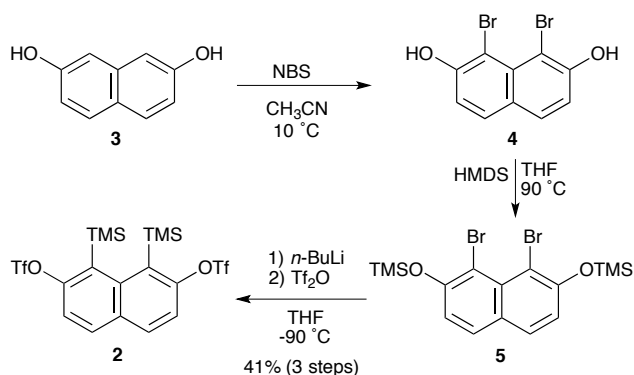
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1. Experimental details and spectroscopic data

1.1 General methods

All reactions were carried out under argon using oven-dried glassware. THF and CH₃CN were purified by a MBraun SPS-800 Solvent Purification System. TMSCl was dried by distillation from CaH₂. Finely powdered CsF was dried under vacuum at 100 °C, cooled under argon and stored in a glove-box. Other commercial reagents were purchased from ABCR GmbH, Sigma-Aldrich or Acros Organics, and were used without further purification. TLC was performed on Merck silica gel 60 F₂₅₄ and chromatograms were visualized with UV light (254 and 365 nm). Column chromatography was performed on Merck silica gel 60 (ASTM 230-400 mesh). Centrifugation was performed in a Hettich EBA21 centrifuge. ¹H and ¹³C NMR spectra were recorded at 300 and 75 MHz (Varian Mercury-300 instrument) or 500 and 125 MHz (Varian Inova 500) respectively. Low-resolution mass spectra (EI) were obtained at 70 eV on a HP-5988A instrument, while high-resolution mass spectra (HRMS) were obtained on a Micromass Autospec spectrometer. HPLC was performed with CHIRALPAK IA.

1.2 Experimental procedures



1.2.1 Synthesis of 1,8-dibromonaphthalene-2,7-diol (4)

N-Bromosuccinimide (NBS, 1.2 g, 6.7 mmol) was added in portions to a solution of 2,7-naphthalenediol (**3**, 0.5 g, 0.1 M in MeCN) at 10 °C and the mixture was stirred under argon at this temperature for 2 h. The reaction was quenched by adding H₂SO₄ to pH=1 and the reaction mixture was extracted with dichloromethane (3 x 100 mL). The solution was quickly filtered through a pad of SiO₂ (CH₂Cl₂) to isolate diol **4** (1 g, >95%) as a brown solid, which was used without further purification. Spectroscopic data were coincident with those described in the literature for this compound.¹

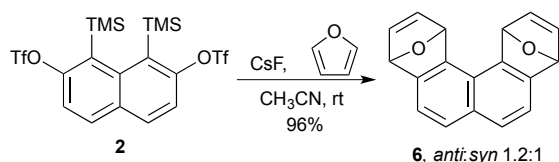
1.2.2 Synthesis of 1,8-bis(trimethylsilyl)naphthalene-2,7-diyl bistriflate (2)

1,8-Dibromonaphthalene-2,7-diol (**4**, 1 g, 3.1 mmol) and hexamethyldisilazane (HMDS, 3.4 mL, 15 mmol) in THF were placed in a round bottom flask and the resulting solution was refluxed for 2 h. The reaction mixture was dried in vacuum to remove NH₃ and excess HMDS. The crude product was dissolved in THF (22 mL, 0.1 M) and cooled to -90 °C. Then, *n*-BuLi (2.7 mL, 2.5 M in hexane) was added dropwise and the reaction mixture was stirred at -90 °C for 60 min and allowed to warm up to -80 °C. The reaction mixture

¹ K. C. Majumdar, S. Mondal, D. Ghosh, *Tetrahedron Letters*, 2009, **50**, 4781.

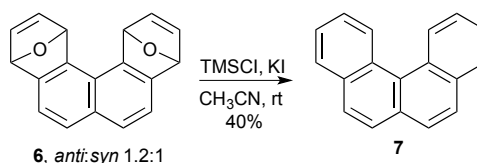
was cooled again at $-90\text{ }^{\circ}\text{C}$ and trifluoromethanesulfonic anhydride (Tf_2O , 1.3 mL, 7.5 mmol) was added dropwise. The reaction mixture was allowed to warm up to $-80\text{ }^{\circ}\text{C}$ and diluted with cold 5% aq NaHCO_3 (30 mL). After the mixture reached rt, the layers were separated, and the aqueous layer was further extracted with diethyl ether (2 x 20 mL). The combined organic layers were dried (anhydrous Na_2SO_4) and concentrated under vacuum. The crude residue was purified by column chromatography (SiO_2 ; 39:1 hexane/ Et_2O) to isolate bistriflate **2** (0.720 g, 41%, m.p.: $72\text{--}74\text{ }^{\circ}\text{C}$) as a white solid. ^1H RMN (300 MHz, CDCl_3), δ : 7.85 (d, $J = 8.8\text{ Hz}$, 2H), 7.36 (d, $J = 8.8\text{ Hz}$, 2H), 0.36 (s, 18H; TMS) ppm. ^{13}C RMN-DEPT (CDCl_3), δ : 155.3 (C), 143.2 (C), 134.0 (C), 132.4 (CH), 130.1 (C), 118.5 (CH), 118.0 (q, $J = 320.1\text{ Hz}$, CF_3), 2.1 (CH_3) ppm. EM (IE^+), m/z (%): 553 ($\text{M}^+ - 15$, 23), 73 (100).

1.2.3 Synthesis of 1,4,9,12-tetrahydro-1,4:9,12-diepoxybenzo[*c*]phenanthrene (**6**)



To a solution of furan (75 μL , 1.1 mmol) and naphthodiyne precursor **2** (30 mg, 0.05 mmol) in CH_3CN (0.5 mL, 0.1 M), finely powdered anhydrous CsF (64 mg, 0.4 mmol) was added. The mixture was stirred at rt under argon for 16 h. Then, the solvent was evaporated under reduced pressure and the residue was purified by preparative TLC (SiO_2 ; hexane/ CH_2Cl_2 / Et_2O 3:2:1) to isolate *syn*-**6** (5.6 mg, 42%, m.p.: $142\text{--}144\text{ }^{\circ}\text{C}$) as a white solid, and the *anti*-**6** isomer (7.7 mg, 54%, m.p.: $183\text{--}185\text{ }^{\circ}\text{C}$) as a yellow solid. Both enantiomers of chiral *anti*-**6** can be separated by Chiral HPLC (9:1, Hex:*i*-PrOH, 0.5 mL/min). *Syn*-**6**: ^1H RMN (300 MHz, CDCl_3), δ : 7.59 (d, $J = 8.2\text{ Hz}$, 2H), 7.44 (d, $J = 7.9\text{ Hz}$, 2H), 7.19 (dd, $J = 5.5, 1.8\text{ Hz}$, 2H), 7.15 (dd, $J = 5.5, 1.8\text{ Hz}$, 2H), 6.39 (s, 2H), 5.90 (d, $J = 1.0\text{ Hz}$, 2H) ppm. EM (IE^+), m/z (%): 260 (M^+ , 90), 206 (100). HRMS, found 260.0837 (calcd. for $\text{C}_{16}\text{H}_{12}\text{O}_2$, 260.0837). *Anti*-**6**: ^1H RMN (300 MHz, CDCl_3), δ : 7.58 (d, $J = 8.3\text{ Hz}$, 2H), 7.44 (d, $J = 8.0\text{ Hz}$, 2H), 7.29 (dd, $J = 5.5, 1.8\text{ Hz}$, 2H), 7.23 (dd, $J = 5.5, 1.8\text{ Hz}$, 2H), 6.25 – 6.18 (m, 2H), 5.90 (d, $J = 1.8\text{ Hz}$, 2H) ppm. EM (IE^+), m/z (%): 260 (M^+ , 90), 206 (100). HRMS, found 260.0837 (calcd. $\text{C}_{16}\text{H}_{12}\text{O}_2$, 260.0837).

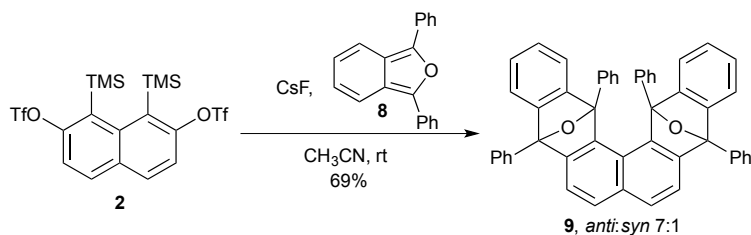
1.2.4 Synthesis of benzo[*c*]phenanthrene (**7**)



To a solution of **6** (mixture of isomers, 100 mg, 0.4 mmol) and KI (230 mg 2.2 mmol) in MeCN (3.8 mL), TMSCl (0.2 mL, 2.2 mmol) was dropwise added. The mixture was stirred under argon for 4 h. Then, the solvent was evaporated under reduced pressure and the residue was purified by column chromatography (SiO_2 ; hexane) to isolate benzo[*c*]phenanthrene (**7**, 33 mg, 40%) as a white solid. Spectroscopic data were identical to those described in the literature for this compound.²

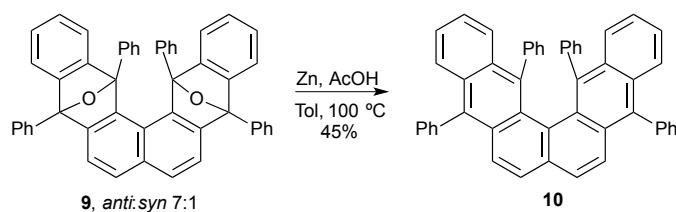
² M. Murai, N. Hosokawa, D. Roy, K. Taka, *Org. Lett.*, 2014, **16**, 4134.

1.2.5 Synthesis of 5,10,15,16-tetraphenyl-5,10,15,16-tetrahydro-5,16:10,15-diepoxy-naphtho[2,3-*a*]tetraphene (**9**)



To a solution of 1,3-diphenylisobenzofuran (**8**, 150 mg, 0.6 mmol) and naphthodiyne precursor **2** (100 mg, 0.18 mmol) in CH₃CN (1.5 mL, 0.1 M), finely powdered anhydrous CsF (230 mg, 1.4 mmol) was added. The mixture was stirred at rt under argon for 16 h. Then, the solvent was evaporated under reduced pressure. The resulting solid residue was washed with water (3 x 10 mL), MeOH (3 x 10 mL), hexane (3 x 10 mL) and finally Et₂O (3 x 10 mL) to isolate *anti*-**9** (72 mg, 61%, m.p.: 267-269 °C) as a brown solid. The organic ethereal phase was evaporated under reduced pressure to isolate the minor diastereomer *syn*-**9** (10 mg, 8%, m.p.: 273-275 °C) as a brown solid. *Syn*-**9**: ¹H RMN (300 MHz, CDCl₃), δ: 7.70 – 7.61 (m, 6 H), 7.54 – 7.44 (m, 6 H), 7.41 (dd, *J* = 8.1, 3.1 Hz, 4 H), 7.36 – 7.23 (m, 8 H), 7.22 – 7.16 (m, 2 H), 6.93 (t, *J* = 7.4 Hz, 2 H), 6.71 (t, *J* = 7.4 Hz, 2 H), 5.89 (d, *J* = 7.2 Hz, 2 H) ppm. ¹³C RMN-DEPT (75 MHz, CDCl₃), δ: 153.6 (C), 151.7 (C), 145.3 (C), 145.3 – 145.2 (C), 145.2 – 145.0 (C), 136.2 (C), 135.5 (C), 132.3 – 131.8 (C), 129.5 (CH), 129.1 (CH), 128.5 (CH), 127.8 (CH), 127.7 (CH), 127.1 (CH), 126.7 (C), 126.1 (CH), 125.8 (CH), 124.0 (CH), 122.5 (CH), 119.3 (CH), 118.0 (CH), 96.5 – 94.3 (C), 90.6 – 88.9 (C), 88.6 (C). EM (IE⁺), *m/z* (%): 664 (M⁺, 100), 648 (M⁺-16, 15). HRMS, found 664.2404 (calcd. for C₅₀H₃₂O₂, 664.2402). *Anti*-**9**: ¹H RMN (300 MHz, CDCl₃), δ: 7.69 – 7.63 (m, 8 H), 7.53 – 7.45 (m, 8 H), 7.44 – 7.36 (m, 6 H), 7.34 (d, *J* = 7.3 Hz, 4 H), 6.93 (td, *J* = 7.7, 0.7 Hz, 2 H), 6.71 (td, *J* = 7.6, 0.9 Hz, 2 H), 5.90 (d, *J* = 7.2 Hz, 2 H) ppm. ¹³C RMN-DEPT (75 MHz, CDCl₃), δ: 153.7 (C), 151.9 (C), 145.5 (C), 145.3 (C), 136.4 (C), 135.7 (C), 129.7 (CH), 129.3 (CH), 128.6 (CH), 127.8 (CH), 126.3 (CH), 125.9 (CH), 124.2 (CH), 122.7 (CH), 119.5 (CH), 118.2 (CH), 95.3 (C), 88.7 (C). EM (IE⁺), *m/z* (%): 664 (M⁺, 100), 648 (M⁺-16, 15). HRMS found: 664.2409 (calcd. C₅₀H₃₂O₂, 664.2402).

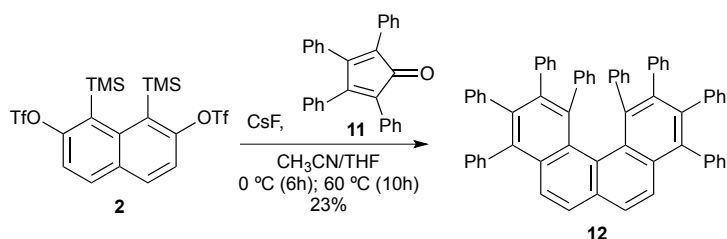
1.2.6 Synthesis of naphtho[2,3-*a*]tetraphene (**10**)



To a suspension of Zn (50 mg, 0.8 mmol, previously activated³) in AcOH (0.5 mL), a solution of **9** (mixture of isomers, 20 mg, 0.03 mmol) in toluene (10 mL) was added. The mixture was heated at 100 °C under argon for 4 days. Then, the solvent was evaporated under reduced pressure and the residue was purified by column chromatography (SiO₂; 4:1 hexane/CH₂Cl₂) to isolate naphtho[2,3-*a*]tetraphene (**10**, 8.6 mg, 45%, m.p.: 280-282 °C) as a yellow solid. ¹H RMN (500 MHz, CDCl₃), δ: 8.02 (d, *J* = 8.2 Hz, 4H), 7.68 – 7.61 (m, 2H), 7.62 – 7.52 (m, 6H), 7.45 – 7.39 (m, 4H), 7.38 – 7.37 (m, 4H), 7.36 – 7.27 (m, 4H), 6.71 (s, 6H), 5.88 (s, 2H) ppm. ¹³C RMN-DEPT (126 MHz, CDCl₃), δ: 140.2 (C), 139.6 (C), 136.1 (C), 133.8 (C), 132.9 (C), 132.1 (CH), 131.8 (CH), 131.6 (C), 131.2 (C), 130.6 (C), 129.5 (C), 129.5 (C), 128.6 (CH), 128.5 (CH), 128.1, 127.8 (CH), 127.3 (CH), 126.4 (CH), 126.1 (CH), 125.6 (CH), 125.5 (CH), 124.7 (CH), 124.5 (CH) ppm. EM (IE⁺), *m/z* (%): 632 (M⁺, 100). HRMS found: 632.2504 (calcd. for C₅₀H₃₂, 632.2504).

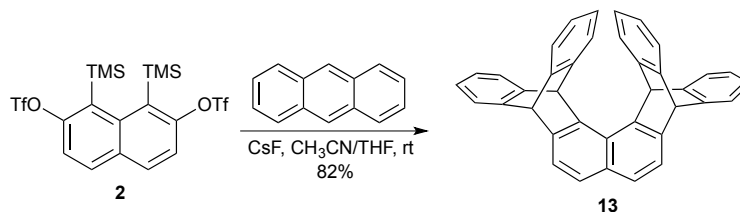
³ G. Thanasis, K. Masato, *J. Org. Chem.*, 1993, **58**, 7158.

1.2.7 Synthesis of 1,2,3,4,9,10,11,12-octaphenylbenzo[*c*]phenanthrene (**12**)



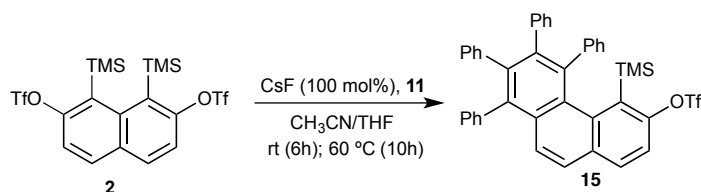
To a solution of naphthodiyne precursor **2** (100 mg, 0.18 mmol) and 2,3,4,5-tetraphenylcyclopentadienone (**11**, 150 mg, 0.4 mmol) in CH₃CN/THF (1:1, 5 mL) cooled to 0 °C, finely powdered anhydrous CsF (160 mg, 1.1 mmol) was added. The mixture was stirred at 0 °C under argon for 6 h. Then, the mixture was heated at 60 °C for 10 h. The solvent was evaporated under reduced pressure and the residue was purified by column chromatography (SiO₂; CH₂Cl₂) to isolate 1,2,3,4,9,10,11,12-octaphenylbenzo[*c*]phenanthrene (**12**, 34 mg, 23%) as an orange solid. ¹H RMN (500 MHz, CDCl₃), δ: 7.96 (d, *J* = 7.9 Hz, 1H), 7.82 (d, *J* = 8.1 Hz, 1H), 7.52 (d, *J* = 8.9 Hz, 1H), 7.46 – 7.30 (m, 4H), 7.22 – 7.08 (m, 10H), 7.07 – 6.89 (m, 8H), 6.89 – 6.72 (m, 6H), 6.72 – 6.62 (m, 4H), 6.59 – 6.48 (m, 6H), 6.26 (d, *J* = 7.7 Hz, 1H), 6.13 (s, 1H), 5.76 (s, 1H), 5.60 (d, *J* = 7.9 Hz, 1H) ppm. EM (IE⁺), *m/z* (%): 836 (M⁺, 100). HRMS found: 836.3475 (calcd. for C₆₆H₄₄, 836.3443).

1.2.8 Synthesis of 5,10,15,16-tetrahydro-5,16:10,15-bis([1,2]benzeno)naphtho[2,3-*a*]tetrapiene (**13**)



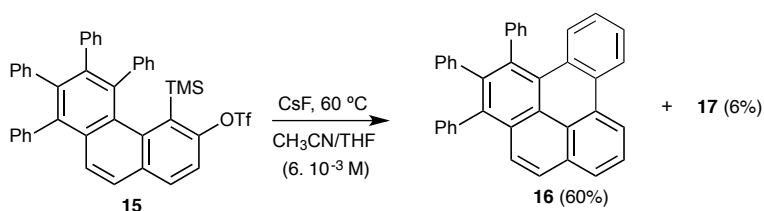
To a solution of anthracene (70 mg, 0.4 mmol) and naphthodiyne precursor **2** (100 mg, 0.18 mmol) in CH₃CN/THF (1:1, 2 mL), finely powdered anhydrous CsF (160 mg, 1.1 mmol) was added. The mixture was stirred at rt under argon for 16 h. Then, the solvent was evaporated under reduced pressure and the residue was purified by column chromatography (SiO₂; 1:1 hexane/CH₂Cl₂) to afford pentaitycene **13** (69 mg, 82%, m.p.: 363-365 °C) as a white solid. ¹H RMN (300 MHz, CDCl₃), δ: 7.70 (d, *J* = 6.7 Hz, 4H), 7.50 – 7.41 (m, 8H), 7.21 (s, 2H), 7.12 – 7.00 (m, 8H), 5.61 (s, 2H) ppm. ¹³C RMN-DEPT (75 MHz, CDCl₃), δ: 146.20 (C), 145.39 (C), 141.20 (C), 131.14 (C), 126.79 (CH), 126.54 (C), 125.25 (CH), 125.10 (CH), 123.62 (CH), 123.45 (CH), 122.11 (CH), 55.35 (CH), 53.00 (CH) ppm. EM (IE⁺), *m/z* (%): 480 (M⁺, 100). HRMS, found: 480.1871 (calcd. for C₃₈H₂₄, 480.1878).

1.2.9 Synthesis of 5,6,7,8-tetraphenyl-4-(trimethylsilyl)phenanthren-3-yl trifluoromethanesulfonate (**15**)



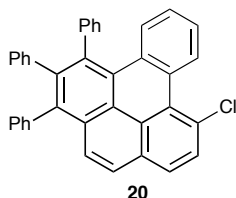
To a solution of cyclopentadienone **11** (60 mg, 0.2 mmol) and naphthodiyne precursor **2** (100 mg, 0.2 mmol) in CH₃CN/THF (1:1, 5 mL), finely powdered anhydrous CsF (26 mg, 0.2 mmol) was added. The mixture was stirred at rt under argon for 6 h. Then, the mixture was heated at 60 °C for 10 h. The solvent was evaporated under reduced pressure and the residue was purified by column chromatography (SiO₂; 3:2 hexane/CH₂Cl₂) to isolate unreacted **2** (30 mg, 30%) and triflate **15** [27 mg, 24% (34% based on an unrecovered starting material), m.p.: 232-233 °C] as a white solid. ¹H RMN (500 MHz, CDCl₃), 7.76 (d, *J* = 8.7 Hz, 1H), 7.42 (t, *J* = 8.9 Hz, 2H), 7.39 – 7.30 (m, 3H), 7.20 (tt, *J* = 7.3, 1.3 Hz, 1H), 7.16 – 7.09 (m, 1H), 7.05 – 6.90 (m, 11H), 6.87 (tt, *J* = 7.3, 1.4 Hz, 1H), 6.84 – 6.76 (m, 2H), 6.57 (d, *J* = 7.7 Hz, 1H), 6.23 (d, *J* = 7.9 Hz, 1H), -0.11 (s, 9H) ppm. ¹³C RMN-DEPT (126 MHz, CDCl₃), δ: 154.6 (C), 141.0 (C), 140.7 (C), 140.4 (C), 140.3 (C), 139.5 (C), 138.9 (C), 138.9 (C), 137.8 (C), 136.7 (C), 134.7 (C), 134.3 (CH), 132.8 (C), 132.2 (CH), 132.1 (CH), 131.7 (C), 131.5 (CH), 131.1 (CH), 131.2 (CH), 130.9 (C), 130.5 (CH), 130.3 (CH), 127.9 (CH), 127.6 (CH), 127.1 (CH), 127.0 (CH), 126.8 (CH), 126.8 – 126.7 (C), 126.6 (CH), 126.4 (CH), 126.2 (CH), 125.7 (C), 125.6 (CH), 118.3 (CH), 2.3 (CH). EM (IE⁺), *m/z* (%): 702 (M⁺, 40), 495 (M⁺-207, 100). HRMS, found: 702.1850 (calcd. for C₄₂H₃₃O₃F₃SiS, 702.1872).

1.2.10 Synthesis of 1,2,3-triphenylbenzo[e]pyrene (**16**)

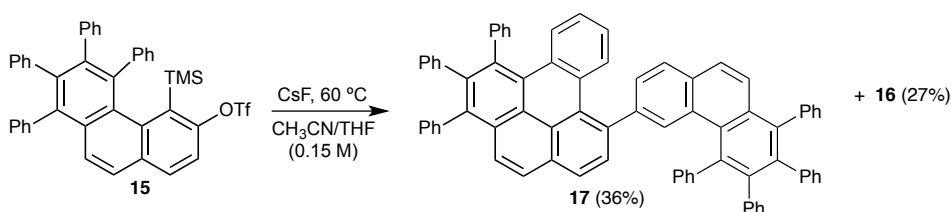


To a solution of phenanthryne precursor **15** (20 mg, 0.03 mmol) in CH₃CN/THF (1:1, 5 mL) at 60 °C, finely powdered anhydrous CsF (23 mg, 0.15 mmol) was added. The mixture was stirred under argon at 60 °C for 16 h. Then, the solvent was evaporated under reduced pressure and the residue was purified by column chromatography (SiO₂; 3:2 hexane/CH₂Cl₂) to afford 1,2,3-triphenylbenzo[e]pyrene (**16**) (8.2 mg, 60%, m.p.: 230-231 °C) as a white solid, and the 8-(3'-phenanthryl)-derivative **17** (0.82 mg, 6%, see characterization data in section 1.2.11). Data for **16**: ¹H RMN (500 MHz, CDCl₃), δ: 8.90 (d, *J* = 7.7 Hz, 1H), 8.78 (d, *J* = 7.8 Hz, 1H), 8.17 (d, *J* = 7.6 Hz, 1H), 8.05 (t, *J* = 7.8 Hz, 1H), 7.93 (d, *J* = 9.2 Hz, 1H), 7.78 (d, *J* = 8.5 Hz, 1H), 7.75 (d, *J* = 9.1 Hz, 1H), 7.58 – 7.48 (m, 1H), 7.27 – 7.23 (m, 2H), 7.22 (d, *J* = 1.7 Hz, 1H), 7.21 (s, 1H), 7.20 – 7.16 (m, 4H), 7.16 – 7.11 (m, 2H), 7.11 – 7.04 (m, 1H), 6.93 (dd, *J* = 4.2, 2.3 Hz, 3H), 6.83 (d, *J* = 3.6 Hz, 1H), 6.81 (d, *J* = 2.4 Hz, 1H) ppm. ¹³C RMN-DEPT (126 MHz, CDCl₃), δ: 143.6 (C), 140.8 (C), 140.7 (C), 140.3 (C), 138.3 (C), 137.3 (C), 132.0 (C), 131.8 (CH), 131.7 (CH), 131.6 (C), 131.4 (CH), 131.0 (C), 130.8 (CH), 130.1 (C), 129.5 (C), 128.3 (CH), 127.7 (C), 127.7 (CH), 127.3 (CH), 126.8 (CH), 126.6 (CH), 126.6 (CH), 126.5 (CH), 126.4 (CH), 126.2 (CH), 125.6 (C), 125.4 (CH), 125.4 (CH), 124.5 (C), 123.5 (CH), 120.3 (CH) ppm. EM (IE⁺), *m/z* (%): 480 (M⁺, 100). EM found: 480.1860 (calcd. C₃₈H₂₄, 480.1878).

When the reaction was performed in CH₃CN/CCl₄ (4:1, 5 mL), using similar amounts and procedure, 8-chloro-1,2,3-triphenylbenzo[e]pyrene (**20**) (1 mg, 6%) was isolated as a white solid, together with **16** (2.4 mg, 17%, see characterization data in section 1.2.10), and **17** (0.82 mg, 6%, see characterization data in section 1.2.11). Data for **20**: ¹H RMN (500 MHz, CDCl₃), δ: 9.42 (d, *J* = 8.2 Hz, 1H), 8.00 (d, *J* = 8.3 Hz, 1H), 7.96 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 9.1 Hz, 1H), 7.75 (d, *J* = 8.7 Hz, 1H), 7.67 (d, *J* = 9.2 Hz, 1H), 7.40 (t, *J* = 7.2 Hz, 1H), 7.30 – 7.21 (m, 7H), 7.17 – 7.12 (m, 4H), 7.07 (t, *J* = 7.8 Hz, 1H), 6.95 – 6.89 (m, 2H), 6.80 – 6.75 (m, 2H) ppm. EM (IE⁺), *m/z* (%): 514 (M⁺, 100). EM found: 514.1484 (calcd. C₃₈H₂₃Cl, 514.1488).

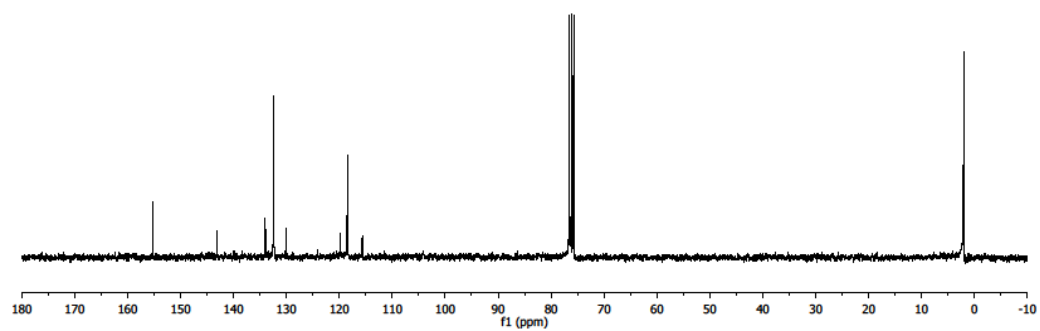
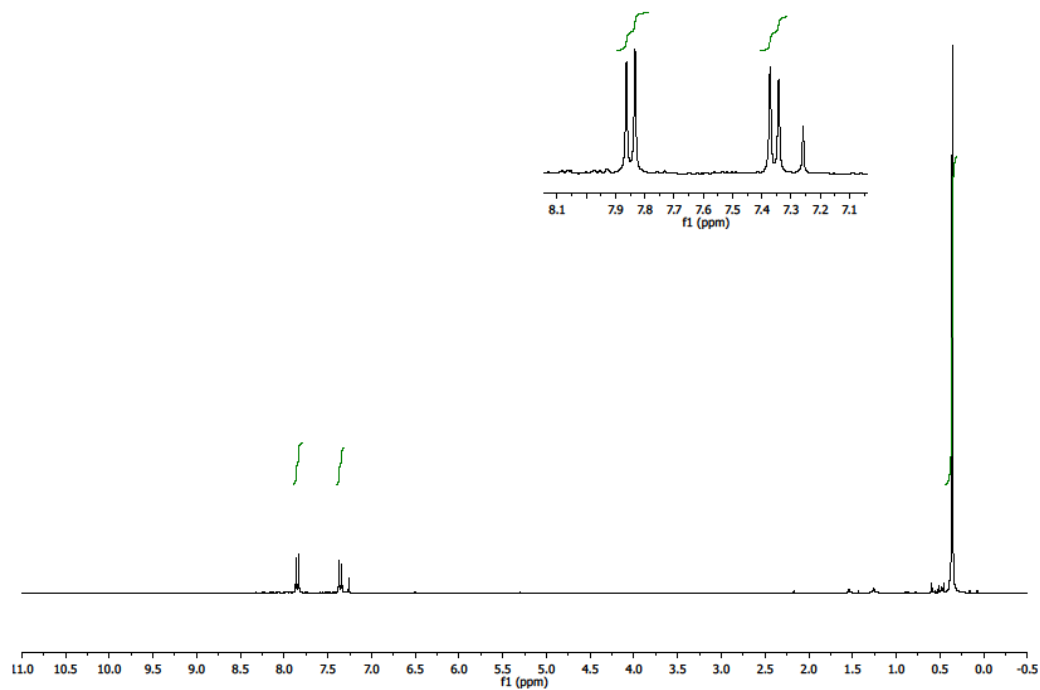
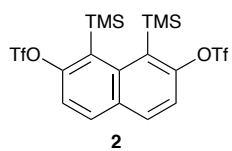


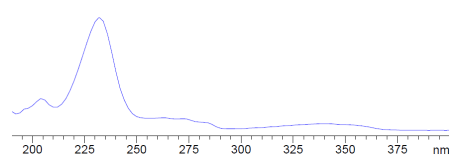
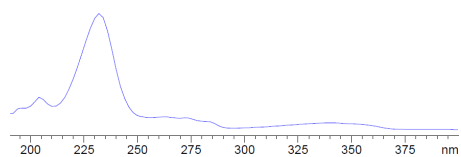
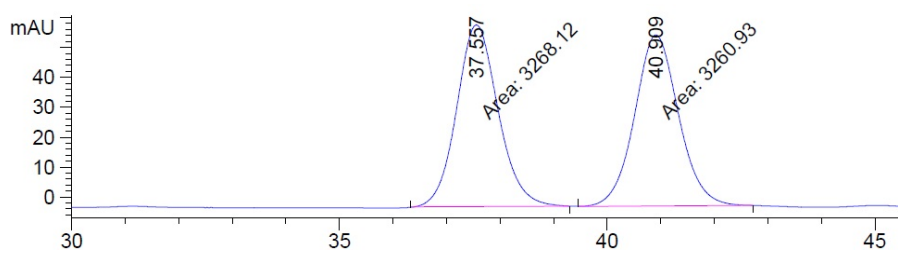
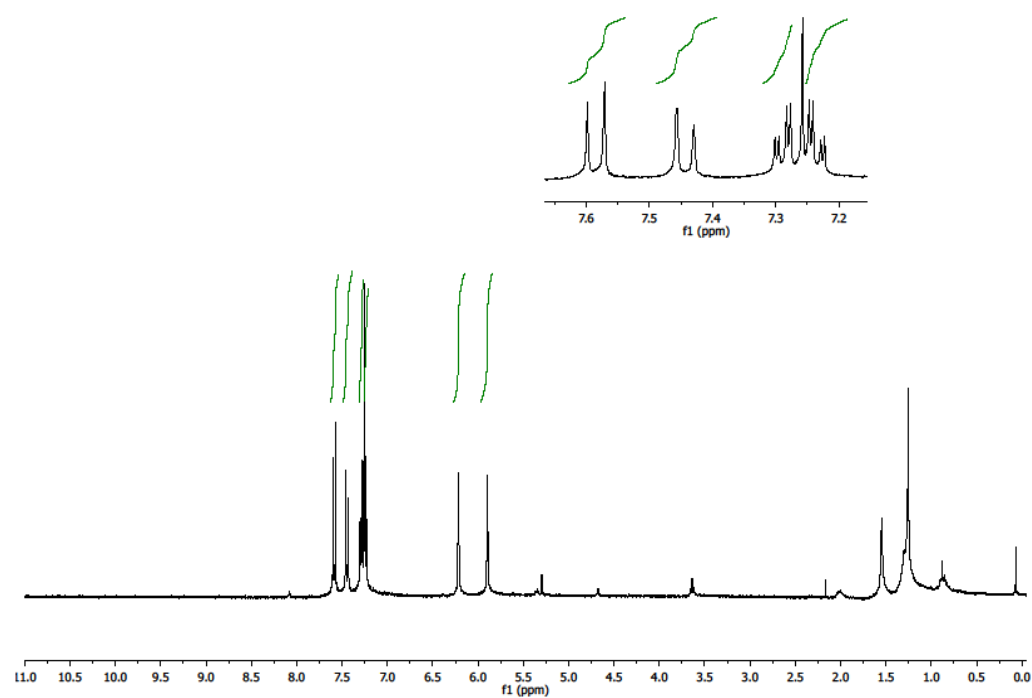
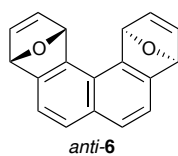
1.2.11 Synthesis of 1,2,3-triphenyl-8-(5',6',7',8'-tetraphenylphenanthren-3'-yl)benzo[e]pyrene (**17**)



To a solution of phenanthryne precursor **15** (20 mg, 0.03 mmol) in CH₃CN/THF (1:1, 0.2 mL) placed in a 1 mL vial at 60 °C, finely powdered anhydrous CsF (23 mg, 0.15 mmol) was added. The mixture was stirred under argon at 60 °C for 16 h. Then, the solvent was evaporated under reduced pressure and the residue was purified by column chromatography (SiO₂; 3:2 hexane/CH₂Cl₂) to isolate 1,2,3-triphenyl-8-(5',6',7',8'-tetraphenylphenanthren-3'-yl)benzo[e]pyrene **17** (4.9 mg, 36%, m.p.: 392-394 °C) as a white solid, and compound **16** (3.7 mg, 27%, see characterization data in section 1.2.10). Data for **17**: ¹H RMN (400 MHz, CDCl₃), δ: 8.40 (s, 1H), 7.97 (d, *J* = 7.8 Hz, 1H), 7.87 (t, *J* = 13.0 Hz, 1H), 7.77 (d, *J* = 7.9 Hz, 1H), 7.72 (d, *J* = 8.9 Hz, 1H), 7.66 (d, *J* = 9.2 Hz, 1H), 7.62 (d, *J* = 7.8 Hz, 4H), 7.55 (d, *J* = 8.3 Hz, 1H), 7.53 – 7.46 (m, 4H), 7.43 (d, *J* = 6.9 Hz, 2H), 7.40 (d, *J* = 8.1 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.25 – 7.21 (m, 6H), 7.18 (d, *J* = 8.5 Hz, 4H), 7.15 (d, *J* = 7.0 Hz, 4H), 7.10 (d, *J* = 7.9 Hz, 2H), 7.08 – 7.03 (m, 2H), 6.93 (dd, *J* = 19.3, 7.1 Hz, 14H), 6.87 (d, *J* = 8.3 Hz, 2H), 6.82 (d, *J* = 6.9 Hz, 2H), 6.78 (d, *J* = 7.3 Hz, 3H), 6.73 (d, *J* = 6.8 Hz, 3H), 6.45 (d, *J* = 7.6 Hz, 2H). ppm. ¹³C RMN-DEPT (101 MHz, CDCl₃), δ: 143.8 (C), 142.9 (C), 141.0 (C), 140.9 (C), 140.5 (C), 140.5 (C), 140.2 (C), 140.1 (C), 140.0 (C), 139.8 – 139.8 (C), 139.3 – 139.3 (C), 138.4 – 138.4 (C), 138.3 – 138.2 (C), 137.0 (C), 136.0 – 135.9 (C), 132.4 – 132.3 (C), 132.2 – 132.1 (CH), 131.9 – 131.8 (C), 131.8 – 131.7 (C), 131.6 – 131.5 (C), 131.4 (CH), 131.2 (CH), 130.1 (CH), 129.9 (CH), 129.8 (C), 129.3 – 129.2 (CH), 129.1 (CH), 129.1 – 129.0 (C), 128.9 – 128.8 (C), 128.3 (CH), 127.9 (C), 127.7 – 127.4 (C), 127.3 (CH), 126.7 (CH), 126.5 (CH), 126.4 (CH), 126.3 (CH), 126.1 (CH), 125.8 (C), 125.7 (CH), 125.5 (CH), 125.3 (CH), 125.3 – 125.2 (CH), 125.1 (CH), 124.8 (CH), 124.6 (CH). ppm. EM (IE⁺), *m/z* (%): 960 (M⁺, 100). EM found: 960.3744 (calcd. C₇₆H₄₈, 960.3756).

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

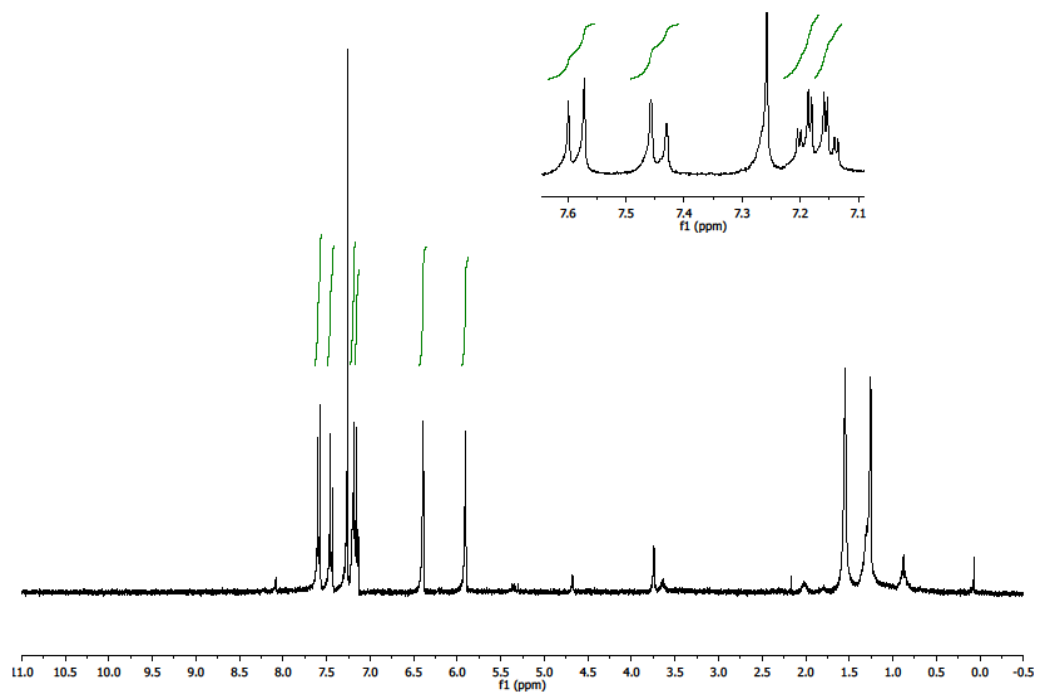
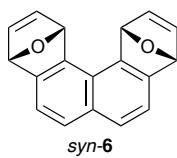


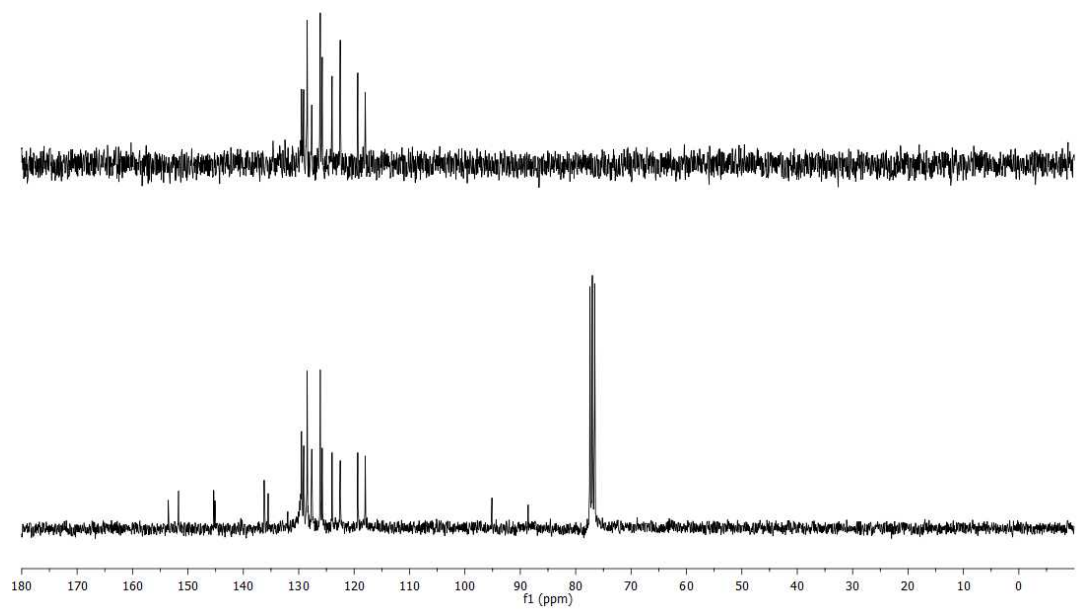
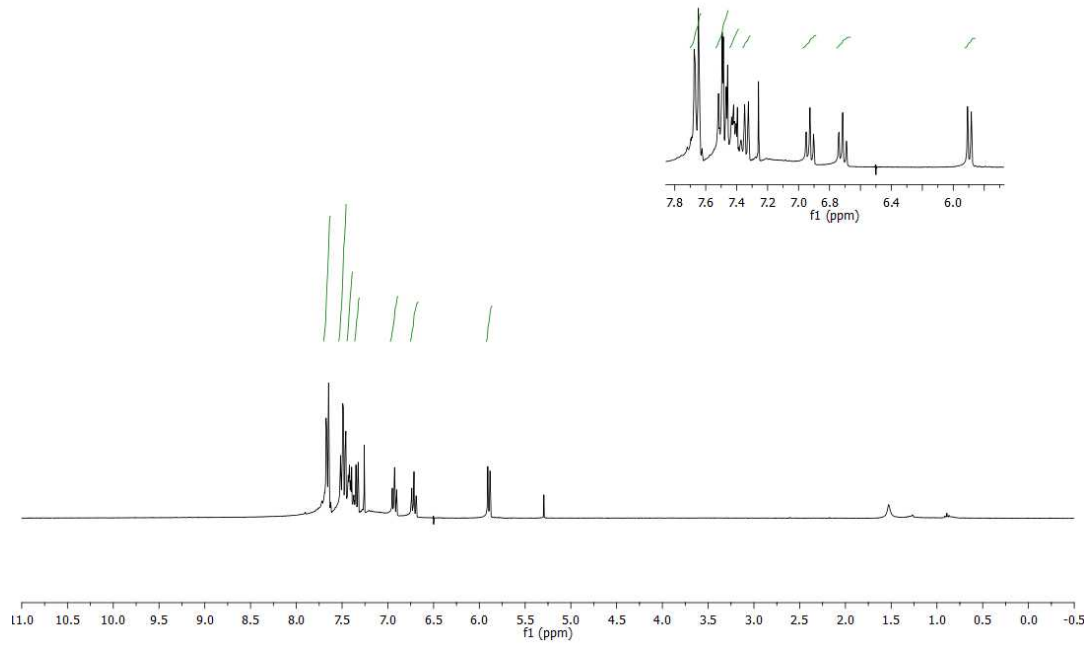
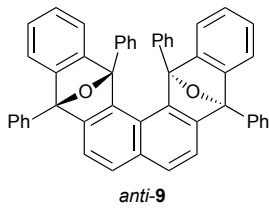


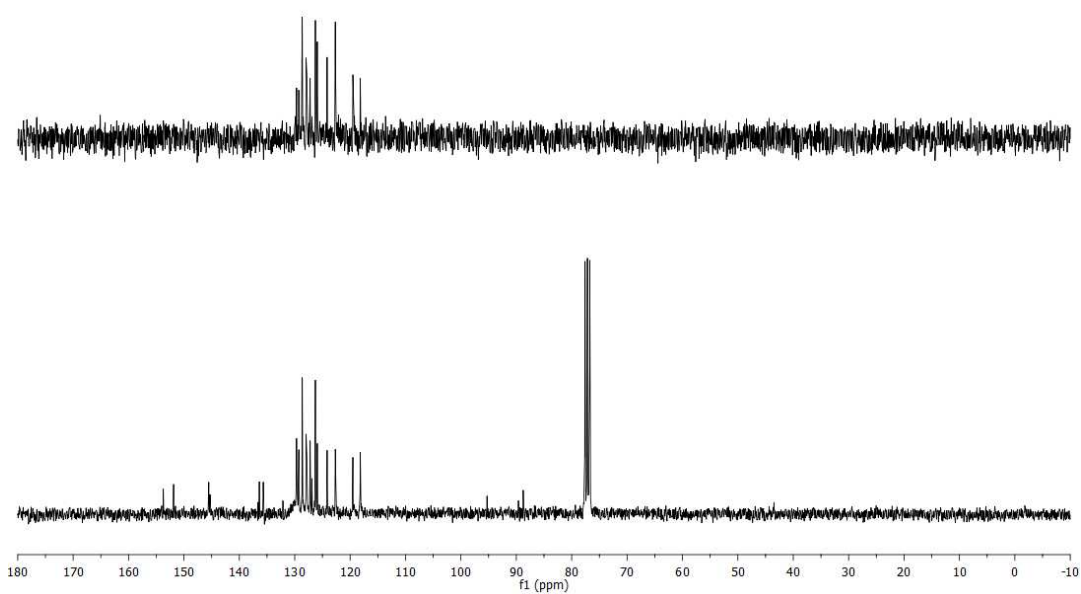
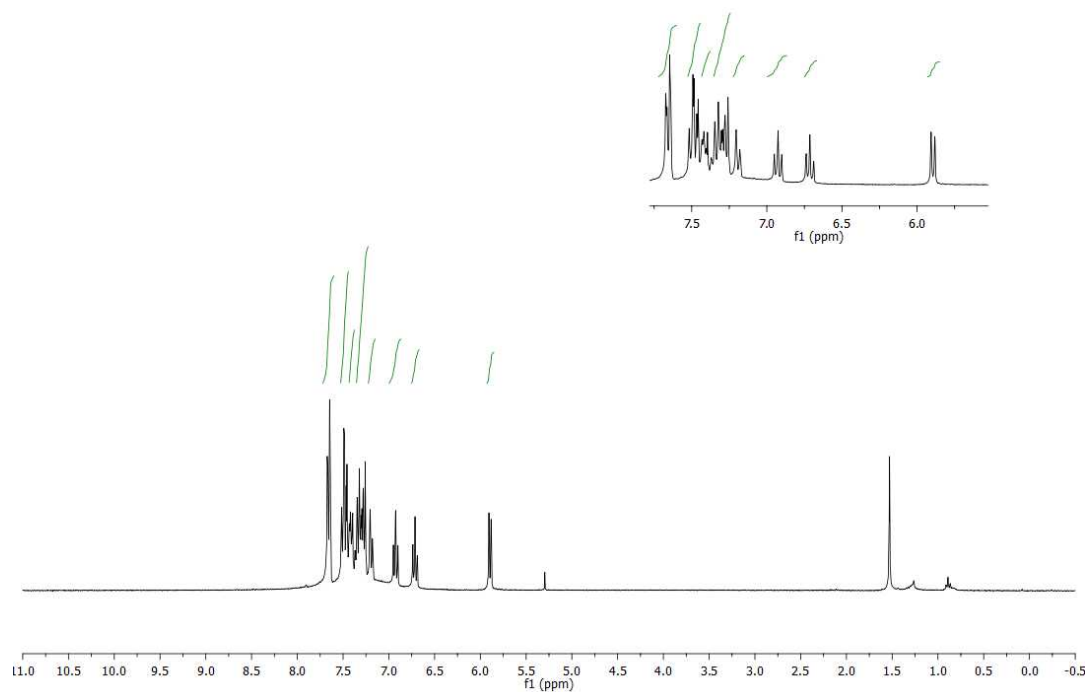
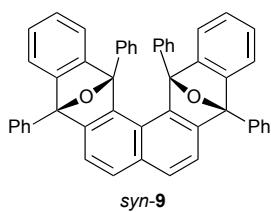
UV-Vis spectrum at 37.557 min.

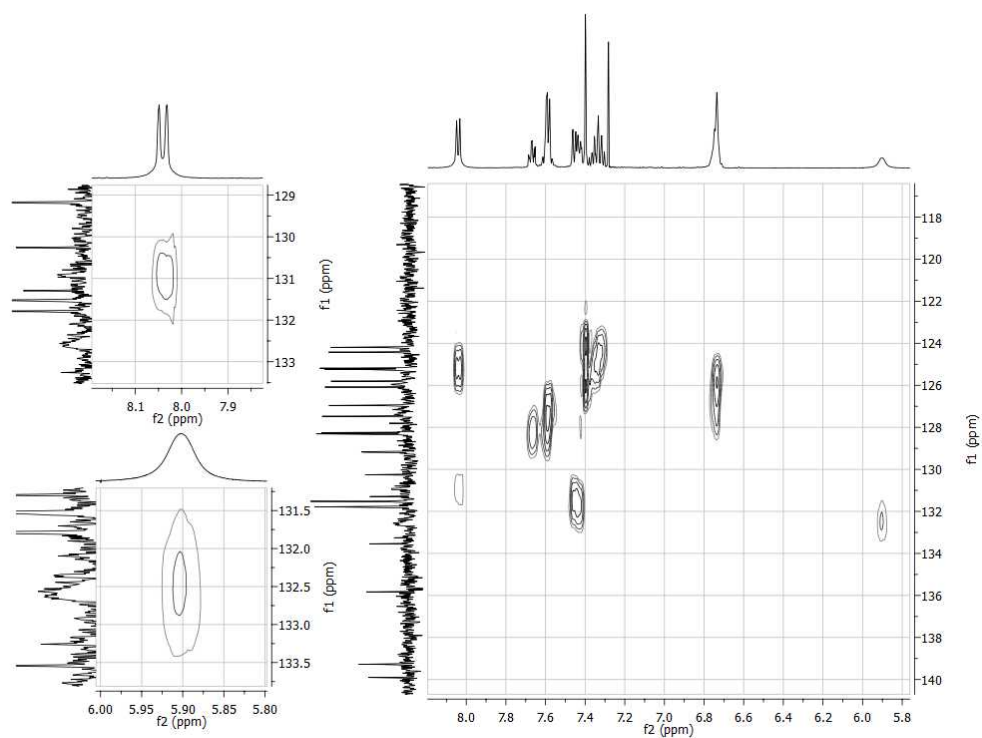
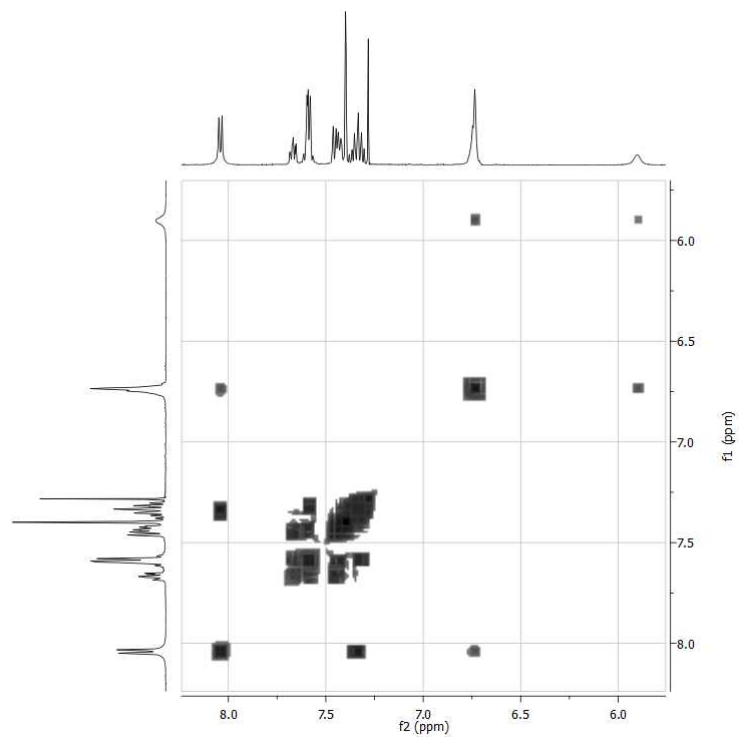
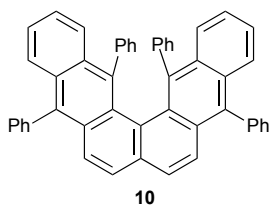
UV-Vis spectrum at 40.909 min.

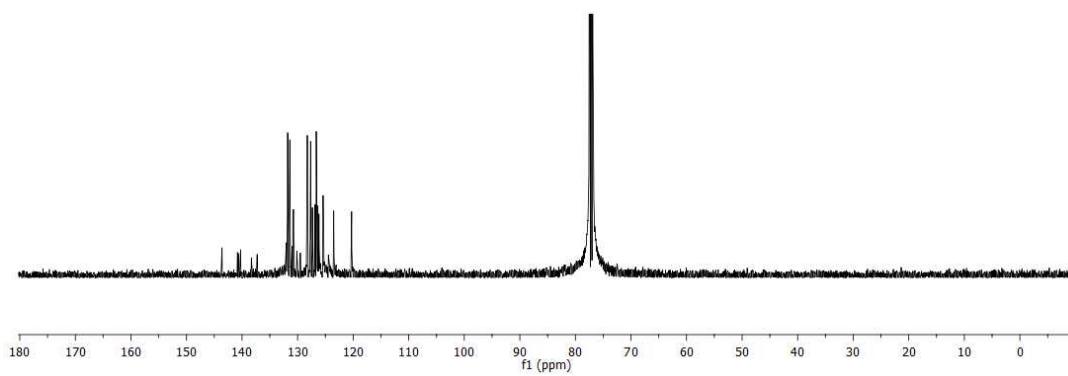
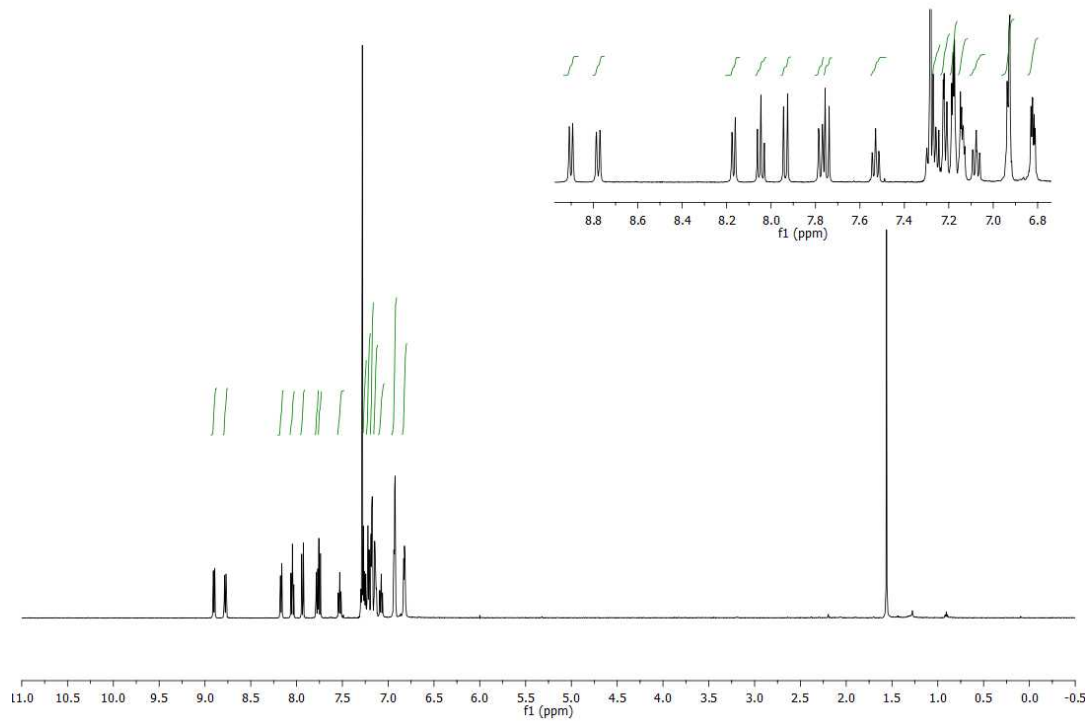
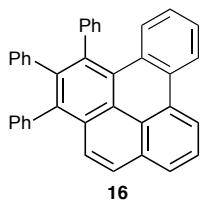
Figure S1. Chiral chromatogram (9:1, Hex:*i*-PrOH, 0.5 ml/min) and UV-Vis absorption spectra of *anti*-6 enantiomers.

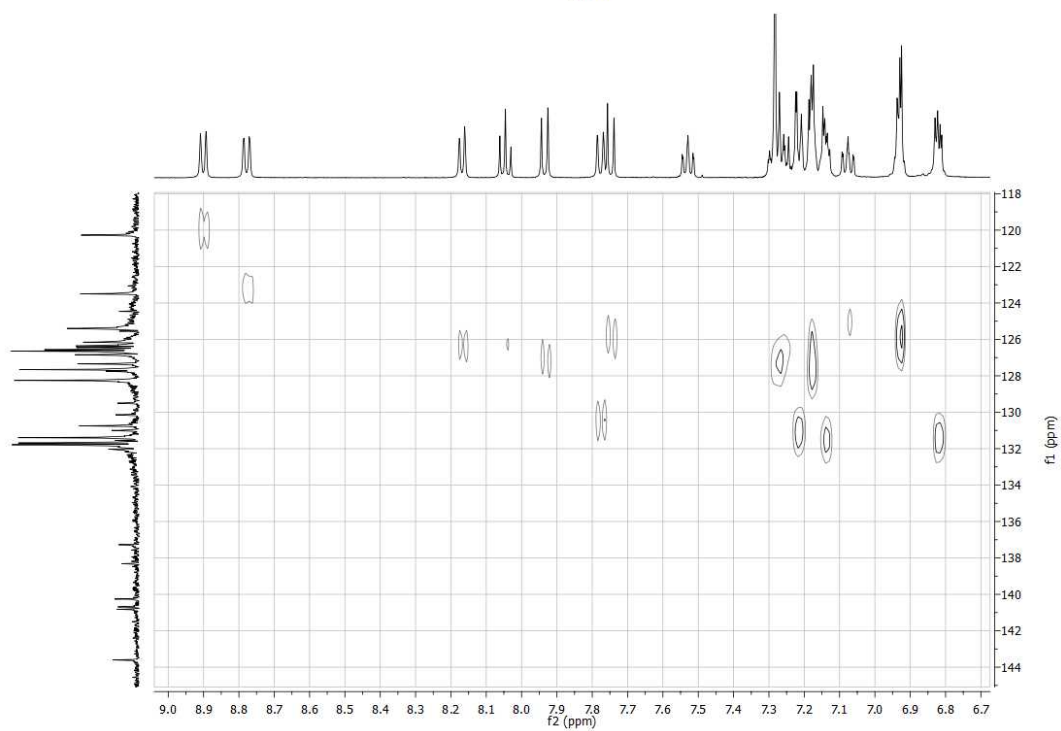
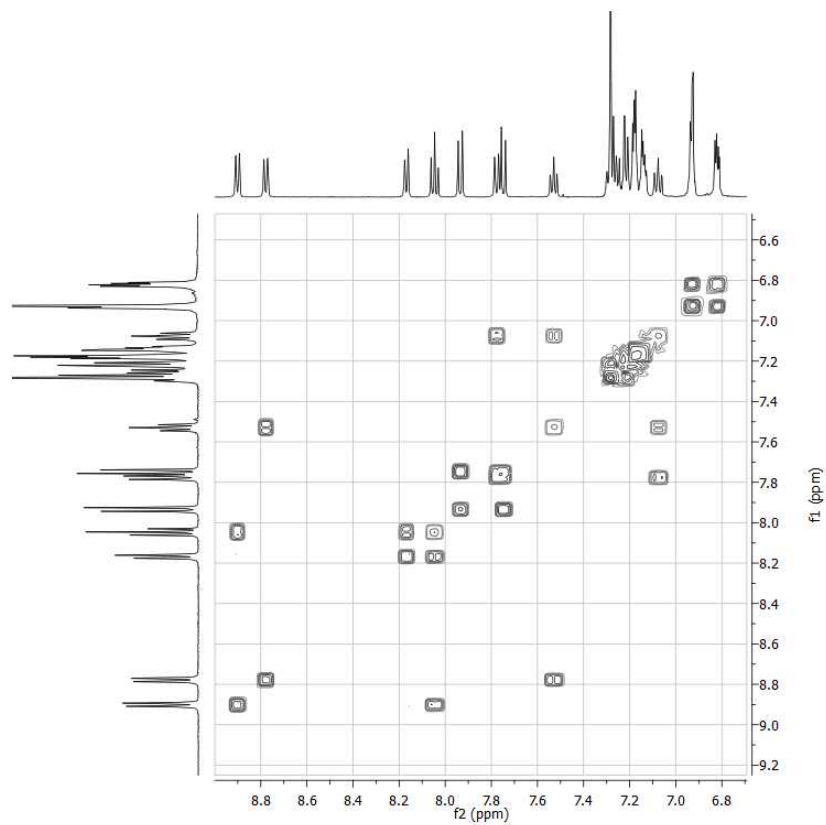
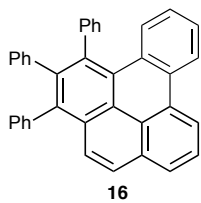


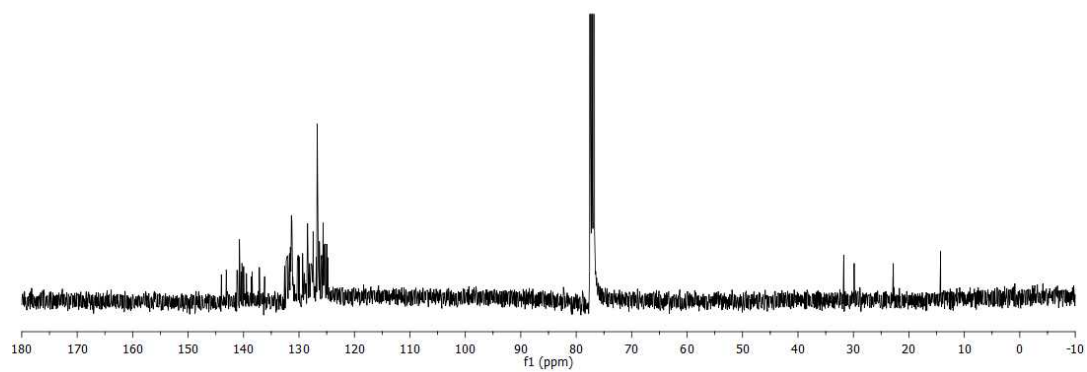
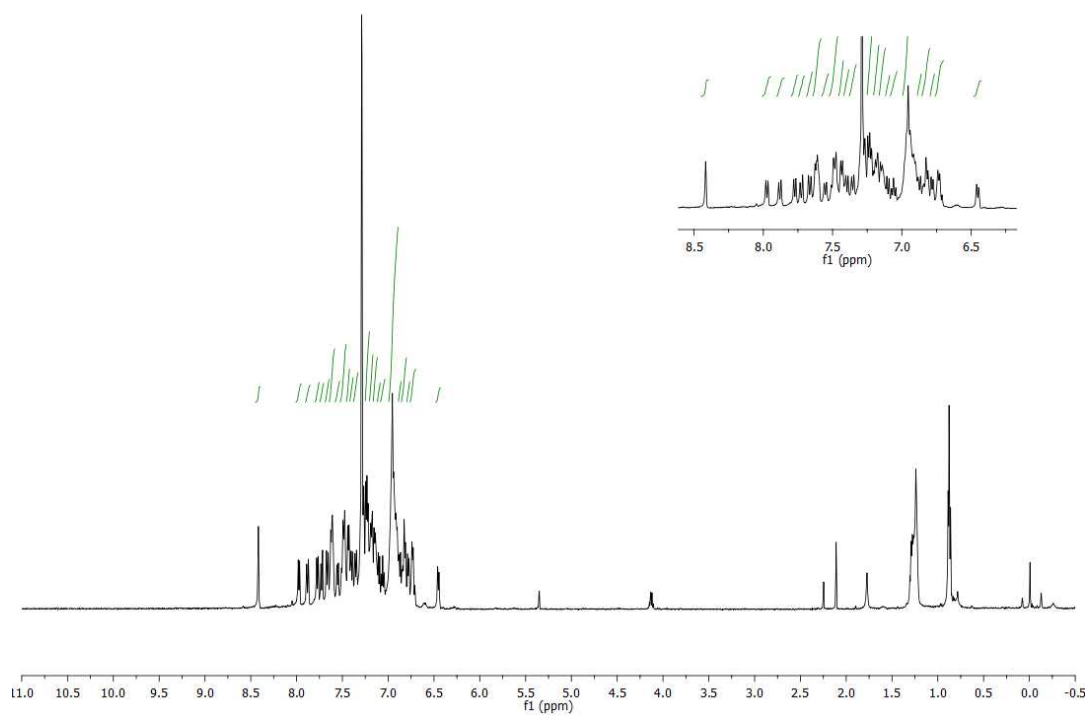
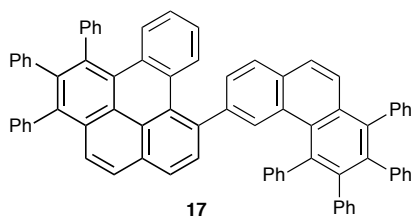


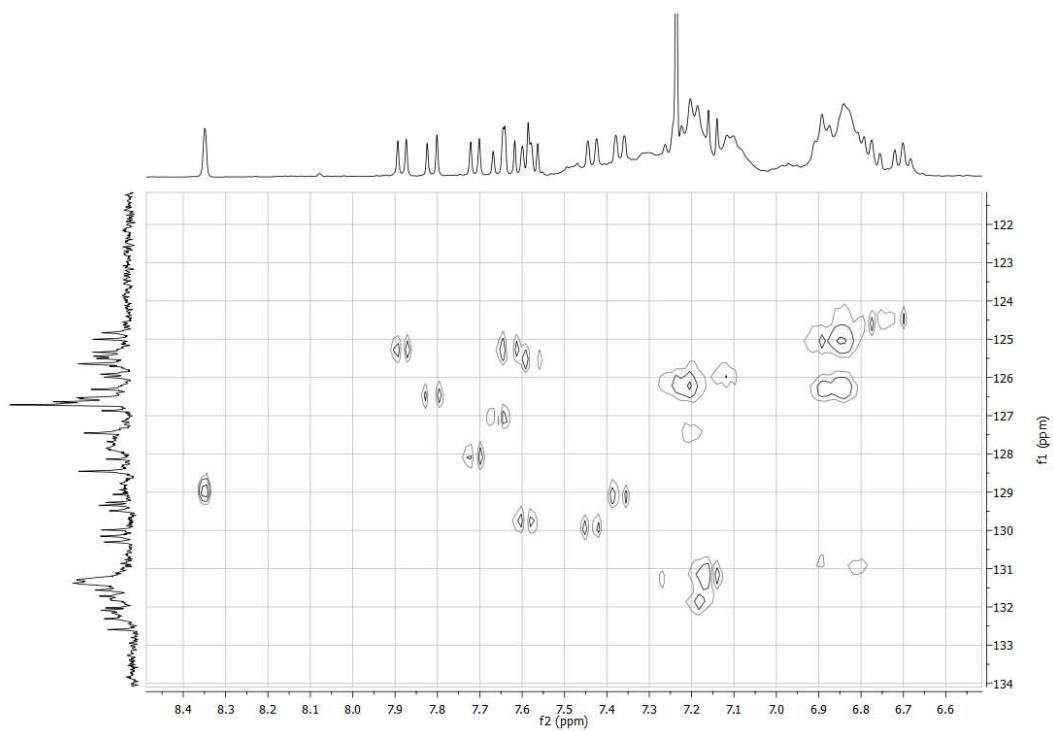
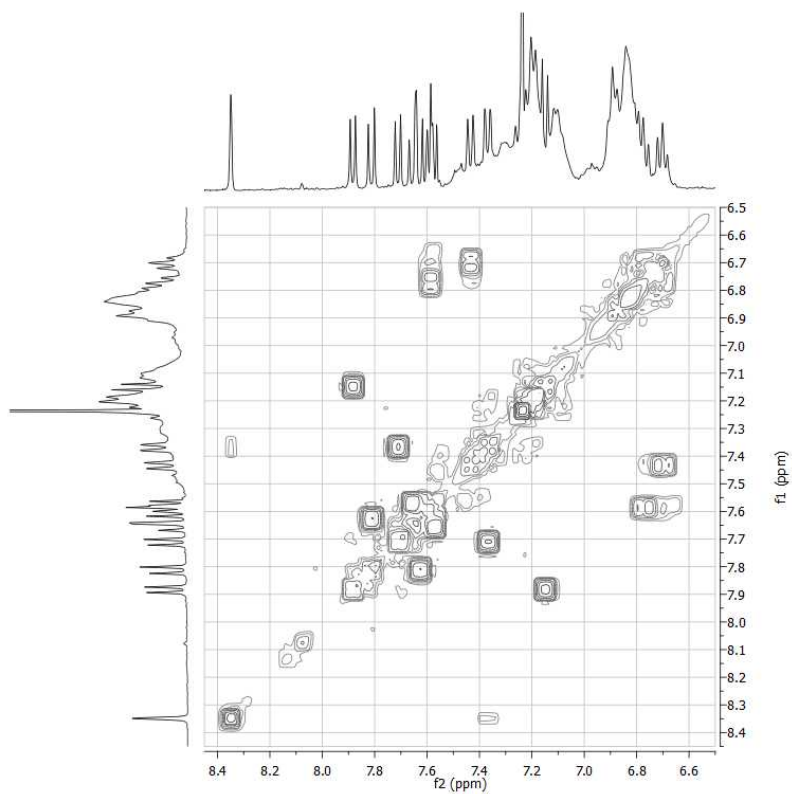
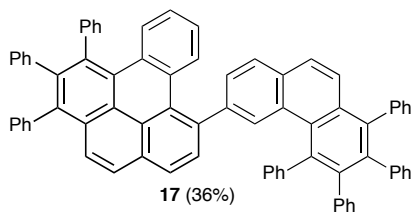


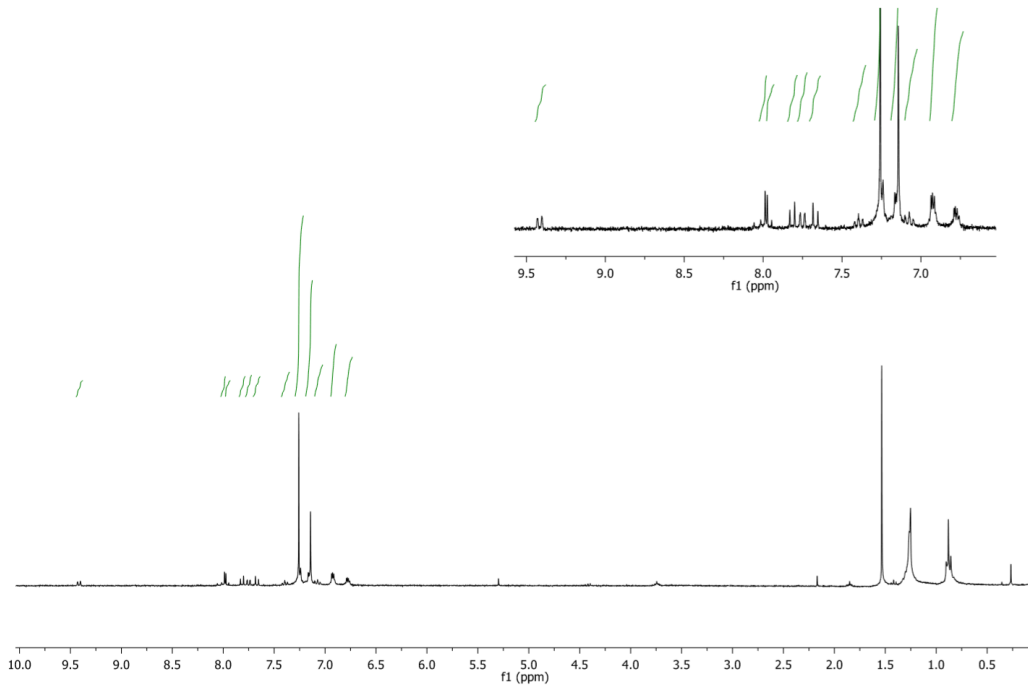
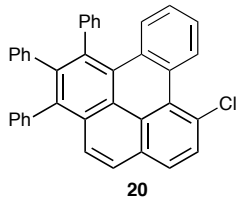












3. X-ray structures

Cambridge Crystallographic Data Centre (CCDC) 1443038 and 1443039 records contain the supplementary crystallographic data for compounds **9** and **13**, respectively. These data can be obtained free of charge from <http://www.ccdc.cam.ac.uk>

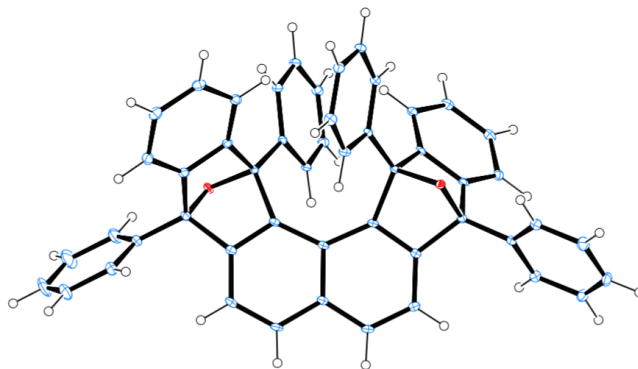


Figure S2

Summary of Data CCDC 1443038

Formula: $C_{50} H_{32} O_2$

Unit cell parameters: a 8.8161(4) b 13.0764(6) c 29.5577(14)

space group P21/c

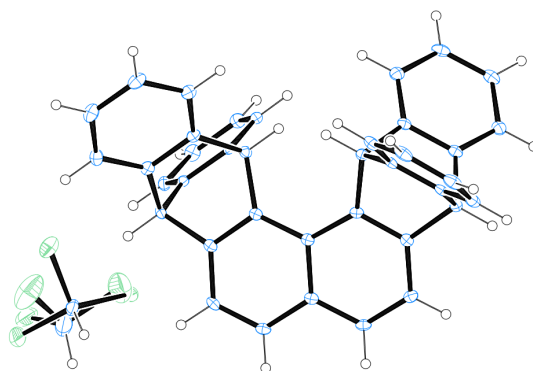


Figure S3

Summary of Data CCDC 1443039

Formula: $C_{38} H_{24}, CHCl_3$

Unit cell parameters: a 14.0105(5) b 13.0164(5) c 16.1008(6)

space group P21/c

4. Computational details

All the calculations were performed using the Gaussian 09 program package.⁴ Geometries of intermediates and transition states were optimized at the density functional level using the b3lyp functional⁵ and 6-31G(d) basis set. Frequency calculations were performed at this level to confirm the nature of the stationary points and to obtain the thermal and entropic contribution to the free energy. Single-point calculations were carried out for all optimized gas-phase geometries using the M062x functional⁶ and the 6-31++G(d,p) basis set. Solvation corrections for acetonitrile with a dielectric constant ϵ of 35.688 were computed using CPCM⁷ polarizable conductor calculation model.

4.1 Relative Electronic Energies (ΔE) and Free Energies (ΔG) at M062x/6-31++G(d,p) level for the intramolecular arylation of aryne 18

	ΔE (Kcal/mol)	ΔG (Kcal/mol)
Aryne 18	0.0	0.0
Triplet arine 18	34.7	33.4
Zwitterion-TS	18.4	20.1
Zwitterion 22	18.1	19.5
Singlet radical-TS	15.9	16.8
Singlet radical 21	1.5	3.2
Triplet radical-TS	37.8	38.5
Triplet radical 21	1.6	2.8
16	-93.5	-89.4
Triplet 16	-34.4	-34.6

⁴ Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

⁵ B3lyP: (a) A.D. Becke, *J.Chem.Phys.*, 1993, **98** 5648; (b) C. Lee, W. Yang, R.G. Parr, *Phys. Rev. B*, 1988, **37**, 785.

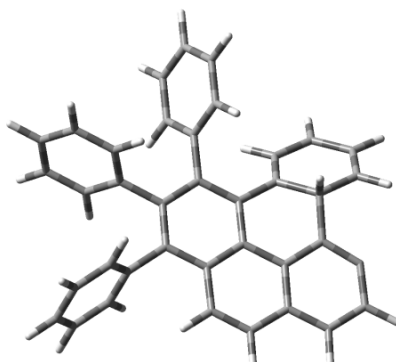
⁶ M062x: Y. Zhao and D. G. Truhlar *Theor. Chem. Acc.*, 2008, **120**, 215.

⁷ CPCM: (a) M. Cossi, N. Rega, G. Scalmani, V. Barone, *J. Comp. Chem.*, 2003, **24**, 669; (b) V. Barone M. Cossi, *J. Phys. Chem. A*, 1998, **102**, 1995.

4.2 Cartesian coordinates (in Angstroms) for the b3lyp/6-31G(d) calculated geometries and energies (in Hartrees) for M062x/6-31++G(d,p) single point calculations

Singlet closed shell 22

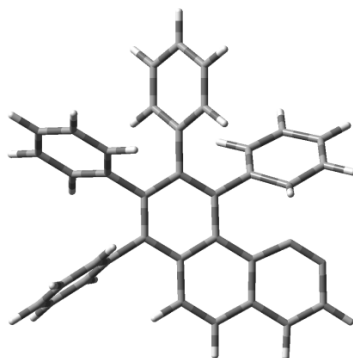
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Singlet closed shell TS

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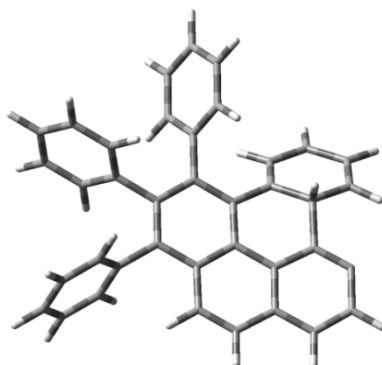


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H	4.23430700	-3.99778800	2.24526100
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Singlet open shell 21

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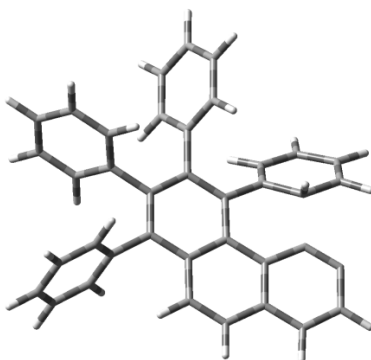


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C	4.71294100	-3.68703600	0.14070000
C	4.34331600	-3.03017300	-1.03420200
C	3.19192000	-2.24309400	-1.06673600
C	-3.70090300	0.47047800	-0.52210600
C	-4.99765200	1.17193300	-0.21884500
C	-5.06404100	2.25307400	0.60077600
C	-3.89548300	2.75324300	1.24355100
C	-2.65505700	2.13177300	1.04087800
C	-0.33881500	3.11003500	-1.16910000
C	-0.22260900	4.49634100	-1.26474500
C	0.38753000	5.22164300	-0.23979700
C	0.88411900	4.54788500	0.87738000
C	0.77340700	3.16038800	0.96786600
C	2.97853800	1.45939100	-1.22356600
C	4.23175100	2.06688900	-1.29737000
C	5.09413800	2.03237600	-0.20031800
C	4.69427800	1.38357000	0.96883500
C	3.44218500	0.77241000	1.03907200
H	-3.95213300	-4.95116700	-0.12962700
H	-6.06024700	-3.62518300	-0.36490700
H	0.67100100	-3.92764000	0.02883000
H	-1.50333400	-5.04495800	-0.00708700
H	2.15445600	-2.66640400	2.13918400
H	4.20006000	-4.06083200	2.20266500
H	5.61046200	-4.29933700	0.16599600
H	4.95175300	-3.13048100	-1.92925200
H	2.91061400	-1.73275400	-1.98332500
H	-3.50300400	0.59609000	-1.60977800
H	-5.89101300	0.76855000	-0.68802700
H	-6.02162100	2.73352800	0.78800000
H	-3.96733800	3.60011000	1.91886300
H	-1.79388900	2.51570400	1.57522300
H	-0.81736700	2.55041900	-1.96833800
H	-0.60954800	5.00993100	-2.14113700
H	0.47701500	6.30231400	-0.31198100
H	1.36187900	5.10230900	1.68099200
H	1.16676800	2.64453900	1.83868600
H	2.30896300	1.49654400	-2.07822400
H	4.53344400	2.56872700	-2.21313500
H	6.07026400	2.50697900	-0.25629300
H	5.35822500	1.35035400	1.82885500
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Singlet open shell TS

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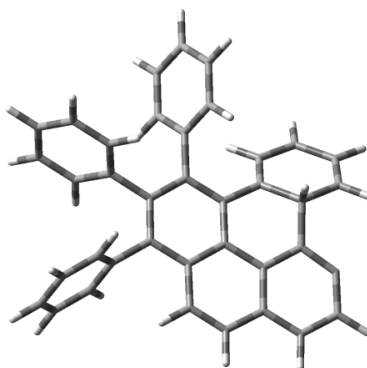


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C	-5.06059700	-3.25671500	-0.20380100
C	-4.95304700	-1.86239300	-0.31400400
C	-3.81821700	-1.23603600	-0.27828300
C	-1.28635500	-1.15136400	-0.06378400
C	-0.08590200	-1.91334500	0.00108900
C	-0.17550500	-3.34753800	0.03283200
C	-1.37669400	-3.99010300	0.03575000
C	-1.21678400	0.27403200	-0.01335600
C	0.02625100	0.91980300	-0.00990200
C	1.23116600	0.15200000	-0.01290700
C	1.17509400	-1.24444600	0.02300900
C	-2.49759500	1.00624300	0.13100000
C	0.09292100	2.41643500	-0.03298100
C	2.55892000	0.84776000	-0.07173100
C	2.43351900	-2.05984600	0.04315700
C	2.84095700	-2.71877200	1.21334500
C	4.00796600	-3.48371900	1.23355800
C	4.78485200	-3.60705600	0.08041300
C	4.38592800	-2.96183500	-1.09129100
C	3.21983000	-2.19619400	-1.10959400
C	-3.59053300	0.64976800	-0.73330300
C	-4.82209300	1.37703200	-0.59811800
C	-5.01272100	2.25983300	0.43937400
C	-3.96683300	2.50977500	1.35196000
C	-2.72968700	1.88836600	1.19042100
C	-0.43645400	3.13119300	-1.11838300
C	-0.38420400	4.52456600	-1.15282400
C	0.19451600	5.23065000	-0.09725000
C	0.72390400	4.53200800	0.98947900
C	0.67725400	3.13864300	1.01885400
C	2.94569200	1.54287700	-1.22710500
C	4.18203400	2.18452300	-1.29528400
C	5.05310800	2.14705400	-0.20522900
C	4.67899800	1.46086800	0.95105200
C	3.44402000	0.81537000	1.01550200
H	-3.86329500	-5.03099300	0.00462300
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H	0.74134500	-3.92353200	0.06455300

H	-1.41056600	-5.07630600	0.07484400
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H	4.30938300	-3.98270400	2.15101400
H	5.69384600	-4.20253300	0.09460300
H	4.98294900	-3.05436200	-1.99480300
H	2.91539900	-1.69460900	-2.02368300
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H	1.09653300	2.60329100	1.86557500
H	2.26951700	1.58184100	-2.07652800
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Triplet-21

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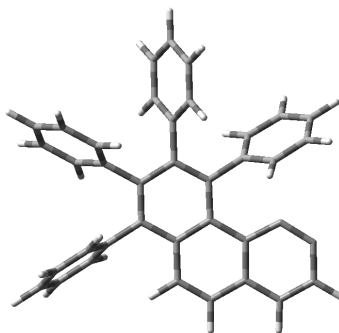


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C	-5.09243600	-3.13132700	-0.28663500
C	-4.95548400	-1.75302700	-0.37520700
C	-3.78876600	-1.04340300	-0.32819800
C	-1.30726100	-1.12122800	-0.05841200
C	-0.12184400	-1.90357700	-0.00700000
C	-0.23517900	-3.33780900	-0.00347800
C	-1.44536900	-3.95937600	-0.01943500
C	-1.23179300	0.30626700	0.03636500
C	0.03505000	0.92759500	0.02087000
C	1.22252100	0.13802600	0.00892000
C	1.14899600	-1.25957500	0.03708200
C	-2.49973700	1.03328500	0.20212000
C	0.15588000	2.41977400	-0.04719200
C	2.56622400	0.80446100	-0.05467800
C	2.39327500	-2.09514200	0.06964100

C	2.77121400	-2.76812300	1.24192100
C	3.92357000	-3.55458300	1.27542600
C	4.71581200	-3.68564500	0.13367600
C	4.34666100	-3.02646700	-1.04007400
C	3.19493400	-2.23983400	-1.07171300
C	-3.69689000	0.46629100	-0.53644800
C	-4.99733800	1.16689000	-0.24397900
C	-5.07100900	2.24511300	0.57972500
C	-3.90789400	2.74606400	1.23015700
C	-2.66307400	2.12820700	1.03342200
C	-0.33570400	3.11370400	-1.16361400
C	-0.22036600	4.50045500	-1.25363700
C	0.38559100	5.22240700	-0.22383800
C	0.87892400	4.54490100	0.89249600
C	0.76905000	3.15695400	0.97739200
C	2.97908400	1.46359000	-1.22171200
C	4.23176100	2.07243500	-1.29352100
C	5.09355400	2.03642400	-0.19605100
C	4.69364100	1.38478800	0.97150800
C	3.44209100	0.77229800	1.03974000
H	-3.95389000	-4.94928900	-0.10858100
H	-6.06185300	-3.62035400	-0.32745600
H	0.67246300	-3.92859100	0.02374000
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H	2.15563300	-2.67028900	2.13266600
H	4.20175800	-4.06399800	2.19452000
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H	4.95571300	-3.12463700	-1.93494300
H	2.91398600	-1.72770200	-1.98741300
H	-3.49148400	0.58843700	-1.62305600
H	-5.88517400	0.76592900	-0.72565800
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H	-0.81115800	2.55667300	-1.96650200
H	-0.60474200	5.01702900	-2.12940200
H	0.47439100	6.30341800	-0.29165400
H	1.35346600	5.09671200	1.69980500
H	1.15986700	2.63810300	1.84758700
H	2.30997900	1.50188700	-2.07668800
H	4.53349800	2.57650600	-2.20804400
H	6.06925000	2.51209100	-0.25045900
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Triplet-TS

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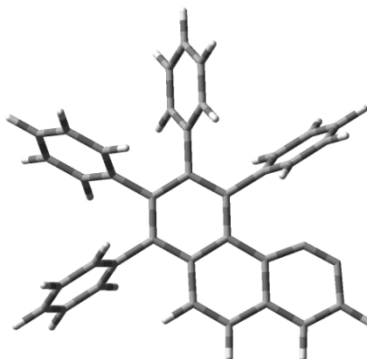


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C	-4.94075100	-3.49202200	-0.15528100
C	-4.93821700	-2.10205100	-0.23528500
C	-3.78077200	-1.35456300	-0.19149700
C	-1.27166700	-1.21727200	-0.03789800
C	-0.04161200	-1.93532500	-0.00560500
C	-0.06811300	-3.37499200	0.00642300
C	-1.23569200	-4.07048800	0.01295000
C	-1.24376000	0.20906900	-0.00212300
C	-0.01973200	0.89129700	-0.00915800
C	1.20994500	0.16803700	-0.01609300
C	1.19748200	-1.22899300	0.01068800
C	-2.52398800	0.97117500	0.11314600
C	0.00084200	2.39084000	-0.01573300
C	2.51330100	0.90883100	-0.06747800
C	2.48286200	-2.00209200	0.02501900
C	2.92193500	-2.64049300	1.19509000
C	4.11492000	-3.36427300	1.21005100
C	4.88698800	-3.46608800	0.05153900
C	4.45710100	-2.84085600	-1.12002300
C	3.26488400	-2.11629100	-1.13302500
C	-3.49805300	0.89254200	-0.91153900
C	-4.70724500	1.60013600	-0.80265800
C	-4.98822100	2.32099700	0.35426600
C	-4.05044800	2.36595400	1.39044100
C	-2.82849400	1.69983500	1.26612600
C	-0.49857400	3.10515000	-1.11489900
C	-0.48241200	4.49973300	-1.12970200
C	0.02987300	5.20657700	-0.04081600
C	0.52878800	4.50774900	1.05983300
C	0.51755000	3.11330000	1.06987400
C	2.88333000	1.61603000	-1.22092100
C	4.09787800	2.29867800	-1.28230100
C	4.96318000	2.29102100	-0.18709400
C	4.60535000	1.59337400	0.96744100
C	3.39242900	0.90670900	1.02495400
H	-3.66593100	-5.21946600	-0.01515300
H	-5.86816200	-4.06008200	-0.17344600
H	0.87462100	-3.90827200	0.01539300
H	-1.22453400	-5.15808800	0.03083100
H	2.32170200	-2.56570000	2.09845000

H	4.44046800	-3.84791000	2.12748200
H	5.81631600	-4.02940100	0.06146500
H	5.05039600	-2.91680500	-2.02753900
H	2.93631800	-1.62988100	-2.04700200
H	-3.23926200	0.42048000	-1.85438100
H	-5.42256800	1.56681400	-1.61944000
H	-5.92985800	2.85525800	0.44897100
H	-4.26638000	2.92705300	2.29556500
H	-2.10456000	1.74392600	2.07380600
H	-0.90098600	2.56053900	-1.96462200
H	-0.87174400	5.03353700	-1.99281300
H	0.04114900	6.29327200	-0.05000100
H	0.92980700	5.04852500	1.91317100
H	0.91288400	2.57687900	1.92760100
H	2.21131900	1.63171300	-2.07434200
H	4.36684500	2.83836500	-2.18665800
H	5.90884400	2.82468700	-0.23297200
H	5.27163500	1.58141400	1.82619800
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Aryne 18

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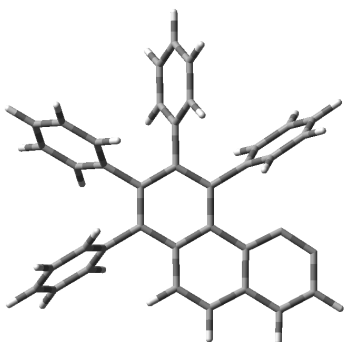


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C	-4.96090700	-3.55408300	0.09930100
C	-4.88038300	-2.15105000	0.10932900
C	-3.79159900	-1.54388200	0.06866300
C	-1.24949200	-1.23270900	-0.03042300
C	-0.01733000	-1.94780900	-0.04824200
C	-0.04780100	-3.38478200	-0.09896900
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C	-1.24626900	0.19130700	-0.02455700
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C	1.20658000	0.17030300	-0.01825200
C	1.21406600	-1.22747600	-0.03352700
C	-2.54641200	0.93701900	-0.00183600
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C	3.30720700	-2.01292700	-1.20481800
C	4.50488200	-2.72798800	-1.22466300

C	4.92342900	-3.42967800	-0.09289000
C	4.13458300	-3.41372500	1.05864400
C	2.93555600	-2.70030400	1.07612400
C	3.34914200	0.89107800	1.10539800
C	4.55277400	1.59602300	1.11193900
C	4.93147400	2.34831000	-0.00083900
C	4.09631300	2.39230800	-1.11839100
C	2.89058300	1.69160300	-1.12078200
C	0.38629200	3.06171500	1.18249700
C	0.38662500	4.45537400	1.23197200
C	-0.02057900	5.19718300	0.12189800
C	-0.43016000	4.53438500	-1.03583100
C	-0.43499100	3.14010700	-1.08144100
C	-3.28913200	1.11882300	-1.18047200
C	-4.48808700	1.83040400	-1.16437700
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C	-4.24034300	2.18952100	1.21032000
C	-3.03803300	1.48398800	1.19330900
H	-3.64717900	-5.25084200	0.01171000
H	-5.87852600	-4.13453700	0.13559200
H	0.89410300	-3.91732100	-0.15185400
H	-1.19129700	-5.17476300	-0.12338000
H	5.85729300	-3.98529900	-0.10830800
H	4.45179800	-3.95653000	1.94536300
H	2.32257700	-2.69237800	1.97390900
H	3.06252200	0.30345400	1.97283100
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H	4.38193400	2.97486000	-1.99046100
H	2.24256700	1.73570400	-1.99145100
H	0.71063500	2.49034900	2.04765600
H	0.70712100	4.96159000	2.13886600
H	-0.01847600	6.28335200	0.15888100
H	-0.74855400	5.10233400	-1.90620900
H	-0.75830200	2.63078100	-1.98472500
H	-2.92029700	0.69646800	-2.11148300
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H	-5.90463800	2.91634800	0.04618700
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H	-2.47141000	1.35221200	2.11066000
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Triplet Aryne 18

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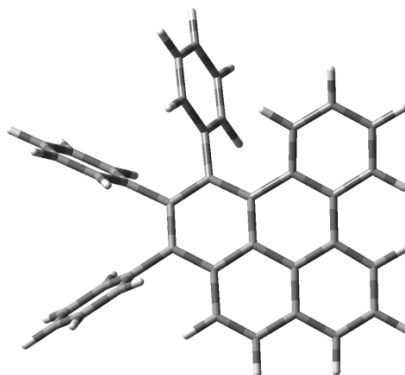


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C	4.82841100	-3.66695100	-0.10437800
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C	3.72796000	-1.50279000	-0.13152200
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C	-0.03700100	-3.40531100	0.11648600
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C	0.06816800	0.85847100	0.00856800
C	-1.18785600	0.18184200	0.01368800
C	-1.23065500	-1.21551800	0.03377600
C	2.57282700	0.86595500	-0.00665900
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C	-2.46135400	0.97443300	0.00448000
C	-2.54420400	-1.93825700	0.05710900
C	-3.34497400	-1.93895400	1.20815900
C	-4.56294900	-2.61886400	1.22972500
C	-5.00178300	-3.31076000	0.09960400
C	-4.21269600	-3.32043800	-1.05187300
C	-2.99342400	-2.64230700	-1.07092200
C	-3.30572800	0.96357600	-1.11505600
C	-4.49093900	1.69909200	-1.12358700
C	-4.85557700	2.45530000	-0.00876800
C	-4.02496900	2.47218700	1.11287600
C	-2.83773900	1.74050500	1.11734200
C	-0.29258800	3.05068400	-1.18302900
C	-0.26398000	4.44427300	-1.22581900
C	0.15087100	5.17235300	-0.10949800
C	0.53812200	4.49572300	1.04790800
C	0.51356100	3.10142800	1.08688400
C	3.30637000	1.05025000	1.18149400
C	4.48356000	1.79569000	1.18341000
C	4.95000200	2.37059300	-0.00038100
C	4.22994500	2.19943100	-1.18473500
C	3.04905000	1.45986400	-1.18750700
H	3.50873200	-5.36187200	0.02276500
H	5.73960400	-4.26047700	-0.13613300
H	-0.99509400	-3.90626400	0.18358800
H	1.06240900	-5.22383200	0.16666700
H	-5.95145900	-3.83887700	0.11620300

H	-4.54554500	-3.85588200	-1.93735100
H	-2.38026100	-2.65446500	-1.96852500
H	-3.03009600	0.37308700	-1.98417000
H	-5.13021400	1.67944800	-2.00249300
H	-5.77964300	3.02737700	-0.01406100
H	-4.29973700	3.05753400	1.98658200
H	-2.19299100	1.76332400	1.99127200
H	-0.62339100	2.49002000	-2.05273100
H	-0.56823300	4.96124800	-2.13225900
H	0.17138100	6.25850700	-0.14120600
H	0.86143800	5.05284200	1.92347400
H	0.81881500	2.58147800	1.99040800
H	2.94387700	0.60150700	2.10237300
H	5.03674400	1.92748200	2.10953100
H	5.86806000	2.95210400	0.00041300
H	4.58619600	2.64817400	-2.10820600
H	2.48594800	1.33573600	-2.10781400
H	-3.00957600	-1.39957500	2.08922200
H	-5.16957400	-2.60734300	2.13150200

1,2,3-Triphenylbenzo[e]pyrene (16)

Electronic Energy=-1462.044025 Free Energy=-1461.606042

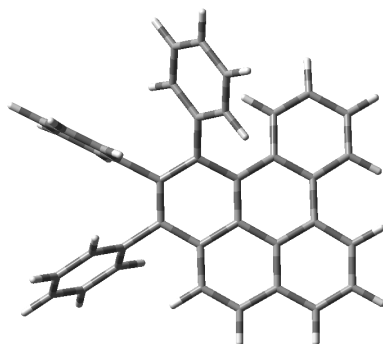


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C	-5.04348500	-3.05900700	0.72173700
C	-5.00856400	-1.68240800	0.49377100
C	-3.81507100	-1.02093900	0.17419000
C	-1.33446300	-1.11557200	-0.04727900
C	-0.14143200	-1.90009500	-0.03825200
C	-0.24210900	-3.32797100	0.10401200
C	-1.43993100	-3.93806100	0.29519200
C	-1.25980800	0.30729100	-0.17227200
C	0.01392500	0.92485900	-0.06803200
C	1.19574900	0.13453400	-0.06244200
C	1.12272400	-1.26499700	-0.11248500
C	-2.52158800	1.03665000	-0.42265800
C	0.16874800	2.40134500	0.14734500
C	2.54715300	0.78521600	0.02352800
C	2.36456300	-2.10269800	-0.17008300
C	-3.77223500	0.39486900	-0.19647100
C	-4.96464100	1.11523000	-0.42599800

C	-4.95467700	2.41260300	-0.90523400
C	-3.73052900	3.01894400	-1.20688500
C	-2.54723900	2.33856700	-0.97430800
C	-0.33269900	2.98170700	1.32283300
C	-0.17714300	4.34548300	1.57078300
C	0.48039500	5.15673600	0.64461400
C	0.98573600	4.59139300	-0.52784800
C	0.83627700	3.22639400	-0.77126300
C	3.40690200	0.80148200	-1.08381100
C	4.66925300	1.38970000	-0.99961800
C	5.09609000	1.96686000	0.19717400
C	4.25065500	1.95263200	1.30788300
C	2.98752100	1.36788000	1.22055000
C	2.70762700	-2.77401000	-1.35380200
C	3.85469400	-3.56612800	-1.42019700
C	4.67535900	-3.70570800	-0.29984300
C	4.33995700	-3.04930500	0.88569000
C	3.19424900	-2.25600200	0.94993400
H	-3.90074200	-4.88325700	0.79375300
H	-5.98772500	-3.53930600	0.96357700
H	-5.93553200	-1.12602400	0.57004200
H	0.66861200	-3.91444900	0.08998600
H	-1.49335000	-5.01541400	0.43243000
H	-5.92143800	0.63300900	-0.26349600
H	-5.89075200	2.93681600	-1.07797500
H	-3.69972000	4.01694300	-1.63543300
H	-1.62192800	2.82149300	-1.24691500
H	-0.85074900	2.35515500	2.04377400
H	-0.57121800	4.77383600	2.48880600
H	0.60047200	6.21983400	0.83553500
H	1.50148000	5.21327600	-1.25493100
H	1.23542500	2.79531300	-1.68421700
H	3.08346900	0.34687500	-2.01609200
H	5.32018200	1.39386600	-1.87016200
H	6.08013100	2.42335000	0.26416900
H	4.57360500	2.39824800	2.24523900
H	2.33103100	1.36733400	2.08603400
H	2.06853600	-2.67047600	-2.22711900
H	4.10586900	-4.07401500	-2.34786900
H	5.56879800	-4.32246000	-0.34975300
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H	2.94014100	-1.74631200	1.87464000

Triplet 1,2,3-Triphenylbenzo[e]pyrene (16)

Electronic Energy=-1461.950060 Free Energy=-1461.518179

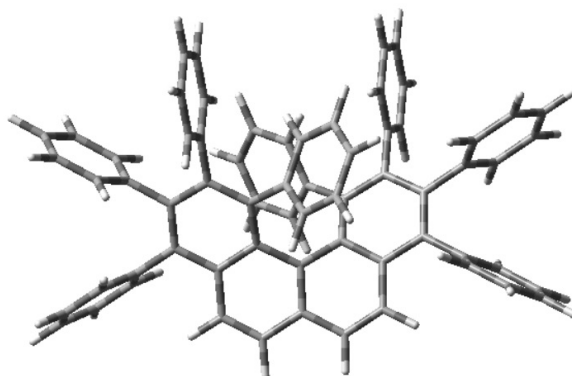


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C	5.00968700	-1.64181700	0.50230000
C	3.81423500	-0.99620700	0.18189500
C	1.34151500	-1.11753400	-0.07172400
C	0.16317500	-1.91100300	-0.06873900
C	0.27540900	-3.34244300	0.05854500
C	1.47532900	-3.93882600	0.24014700
C	1.25451700	0.30022600	-0.18024500
C	-0.01635900	0.90236500	-0.08056300
C	-1.18600300	0.10476800	-0.07114100
C	-1.10232400	-1.28768300	-0.12454500
C	2.50954500	1.05077000	-0.40616300
C	-0.18933100	2.37329600	0.12285500
C	-2.53416600	0.74922400	0.01743000
C	-2.34405200	-2.11790800	-0.15006500
C	-2.68263800	-2.85030900	-1.29206900
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C	-3.18993900	-2.16654800	0.96217800
C	3.75736500	0.42820500	-0.16579000
C	4.94266700	1.16205600	-0.36506800
C	4.92122900	2.46145000	-0.83161300
C	3.69621900	3.05003500	-1.15578900
C	2.52083000	2.35191300	-0.95183700
C	0.32212100	2.96640700	1.28065600
C	0.14967900	4.32823400	1.51475600
C	-0.53362900	5.11484100	0.59000300
C	-1.04898700	4.53054400	-0.56653700
C	-0.88284800	3.16794200	-0.79575900
C	-2.93304100	1.40148700	1.18758100
C	-4.18903200	1.99522700	1.27277600
C	-5.06105100	1.94598000	0.18632000
C	-4.67190500	1.29516200	-0.98270200
C	-3.41660700	0.69720800	-1.06446900
H	3.93961100	-4.85783700	0.73655700
H	6.00638600	-3.49256700	0.94938000
H	-0.63040600	-3.93746900	0.03924900
H	1.54557200	-5.01608200	0.36407300
H	-2.02744000	-2.81874000	-2.15901800

H	-4.10691800	-4.16599700	-2.22127600
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H	-5.00589900	-2.95100100	1.80043800
H	-2.93157900	-1.59817800	1.85153700
H	5.90373900	0.69459600	-0.18797500
H	5.85144300	3.00026900	-0.98131700
H	3.65997700	4.04761700	-1.58207000
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H	0.85934000	2.35202800	1.99870400
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H	-1.58333000	5.13720100	-1.29138200
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H	-2.24909900	1.44741200	2.03117000
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1,2,3,4,9,10,11,12-Octaphenylbenzo[c]phenanthrene (12)

Electronic Energy=-2540.638943



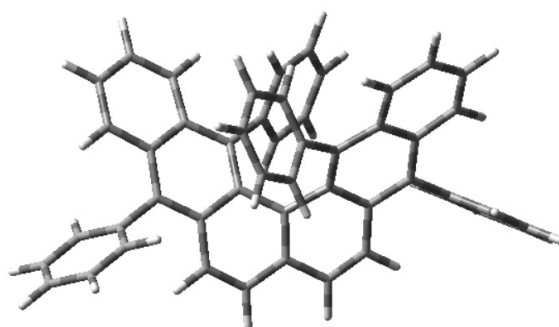
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C	1.22631500	4.19767200	-0.20191200
C	2.39492200	3.51223800	-0.34212300
C	2.44769700	2.10350300	-0.08512300
C	1.25494400	1.42008300	0.25997700
C	-1.36987400	0.17856600	-0.95750500
C	-2.59398300	-0.48870900	-0.97349200
C	-3.74738500	0.10314000	-0.38579100
C	-3.68895900	1.40969500	0.08318800
C	3.68896600	1.40937000	-0.08401600
C	3.74731400	0.10305700	0.38560300
C	2.59387300	-0.48839000	0.97363700
C	1.36983100	0.17899900	0.95735500
C	-4.88873900	2.09892700	0.57600500
C	-5.89629400	2.49775600	-0.31228000
C	-7.02698000	3.16113500	0.16144600
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C	-6.16600000	3.03106000	2.41259800
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C	-5.00296600	-0.65849100	-0.31724100
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C	-6.53409500	-2.06304500	0.92869300
C	-7.39616300	-2.10380500	-0.16660300
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C	-1.75359200	-1.12449500	3.57169100
C	-1.24791200	0.17308400	3.65271300
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C	-0.26558200	-0.28738100	-1.80827800
C	0.24274300	-1.59016500	-1.74108000
C	1.24974700	-2.00406200	-2.61238300
C	1.75361000	-1.12679000	-3.57083500
C	1.24811500	0.17081200	-3.65261900

C	0.24844400	0.58993100	-2.77861100
C	2.73985300	-1.80006400	1.62319000
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C	2.75166500	-4.21911200	1.47881200
C	3.06295500	-4.30279100	2.83594800
C	3.21076100	-3.13764400	3.58734800
C	3.05270400	-1.88979700	2.98575300
C	-2.74002300	-1.80073800	-1.62231500
C	-2.58827400	-2.97522000	-0.87141000
C	-2.75206900	-4.21970100	-1.47655900
C	-3.06313500	-4.30412500	-2.83370100
C	-3.21072800	-3.13939600	-3.58578600
C	-3.05268000	-1.89121800	-2.98487200
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C	5.87354600	-0.70080400	1.41443000
C	7.06425300	-1.42111800	1.33742100
C	7.39616800	-2.10387000	0.16757900
C	6.53319200	-2.06528000	-0.92708400
C	5.34114500	-1.34632200	-0.85567800
C	4.88881600	2.09837700	-0.57702200
C	5.03352500	2.36662900	-1.94537400
C	6.16861500	3.02522800	-2.41448900
C	7.16456200	3.42706600	-1.52459200
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H	-5.79481200	2.27623700	-1.38538600
H	-7.81343000	3.47079600	-0.54225700
H	-8.05876700	3.94833800	1.89539200
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H	-6.79394200	-2.59845900	1.85345200
H	-8.33593100	-2.67144400	-0.10752000
H	-7.74034200	-1.45452800	-2.20350300
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H	-1.63829600	0.86968800	4.40888000
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H	-0.16615400	-2.29804600	-1.00349800
H	1.64098800	-3.02979900	-2.54402800
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H	1.63865700	0.86695000	-4.40913200
H	-0.14355000	1.61646400	-2.84312200
H	2.33835000	-2.90678900	-0.19837300
H	2.63671800	-5.13650700	0.88337000
H	3.19228500	-5.28554200	3.31174600
H	3.45391900	-3.20041100	4.65806500
H	3.17210300	-0.97238000	3.58077300
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H	-2.63729900	-5.13676800	-0.88057700
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H	5.61089300	-0.16657200	2.33956000
H	7.74194200	-1.45071300	2.20296400
H	8.33596200	-2.67149400	0.10878200
H	6.79236100	-2.60238400	-1.85105300
H	4.66219700	-1.31630400	-1.72082200
H	4.24724500	2.05192700	-2.64770300
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H	8.05896300	3.94722500	-1.89683500
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5,10,15,16-Tetraphenylnaphtho[2,3-*a*]tetraphene (10)

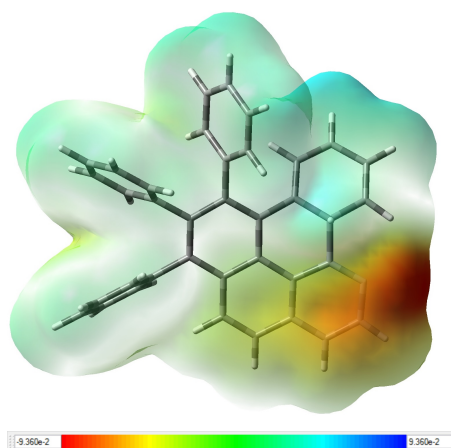
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C	-2.47531300	-1.26006900	-0.17868000
C	-2.43007300	-2.67720000	0.07357700
C	-1.24947300	-3.35409600	0.03677200
C	-1.23948600	0.63393000	-1.15417400
C	-2.48435500	1.28472100	-1.40213300
C	-3.70974700	0.72204100	-0.88465500
C	-3.69823800	-0.58279900	-0.33253100
C	-2.58513300	2.48894900	-2.16771300
C	-3.77517800	3.15861500	-2.30803300
C	-4.95443300	2.66022400	-1.69907100
C	-4.92047700	1.46998200	-1.01878200
C	3.69825900	-0.58281500	0.33240300
C	3.70972700	0.72192600	0.88473400
C	2.48430200	1.28451100	1.40224800
C	1.23946800	0.63372900	1.15416800
C	4.92043600	1.46988500	1.01899700
C	4.95433200	2.66004800	1.69942100
C	3.77503400	3.15835000	2.30838800
C	2.58501600	2.48866800	2.16795700
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C	-7.10715000	-2.26829300	-0.55818500
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C	1.64170700	2.81576600	-2.43759000
C	0.51714800	2.40854400	-1.71844400
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C	0.00140800	1.11036700	1.85225800
C	5.25667800	-1.53594700	-1.39329800
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H	-1.23224700	-4.43946400	0.10143700
H	-1.69660800	2.88431500	-2.64313300
H	-3.81225100	4.07782000	-2.88681800
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H	5.82684500	1.07273500	0.57603600
H	5.88643300	3.21184600	1.78776000
H	3.81206200	4.07750700	2.88725200
H	1.69645400	2.88396300	2.64336700
H	-5.71545700	-1.42614400	-1.97157000
H	-7.82297700	-2.55582800	-1.32395900
H	-8.29881500	-3.03110100	1.07120800
H	-6.64609200	-2.37063200	2.80969200
H	-4.53507200	-1.24438500	2.15158700
H	0.24926100	-0.76421900	-2.88327700
H	2.23099100	-0.04754300	-4.16806200
H	3.14510100	2.25323100	-3.87959300
H	2.02663600	3.82346100	-2.30493900
H	0.03471400	3.10808300	-1.04504300
H	4.53521700	-1.24417800	-2.15176000
H	6.64624100	-2.37039500	-2.80985900
H	8.29888700	-3.03102500	-1.07135200
H	7.82296200	-2.55592000	1.32382500
H	5.71541200	-1.42628200	1.97143800
H	-0.24893400	-0.76484400	2.88318100
H	-2.23063200	-0.04861500	4.16827700
H	-3.14507800	2.25207700	3.88022500
H	-2.02699900	3.82267300	2.30566600
H	-0.03511000	3.10773900	1.04545800

4.3 Electrostatic potential map for the closed shell singlet **22** (zwitterion)



4.4 Spin density map for diradical **21**

