Supporting Information

Innocent BN Bond Substitution *in* Anthracene Derivatives

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I. General Information

General Experimental Procedures: All reactions were conducted under a positive pressure of inert atmosphere (nitrogen or argon), unless stated otherwise. Standard Schlenk techniques were used in all syntheses conducted under inert atmosphere and all glassware was oven-dried overnight in a 175 °C oven.

Instrumentation: ^{1}H NMR, ^{11}B NMR, ^{13}C {^{1}H} NMR, and ^{19}F {^{1}H} NMR spectra were recorded on a Bruker Avance III 400 MHz Spectrometer and chemical shifts are reported in parts per million (ppm). Spectra were recorded in chloroform-*d*, dichloromethane-d_2, or DMSO-d_6, with the residual solvent peak as the internal standard (^{1}H NMR: $CHCl_3$, δ = 7.26 ppm; CH_2Cl_2, δ = 5.32 ppm. ^{13}C NMR: $CHCl_3$, δ = 77.16 ppm; CH_2Cl_2, δ = 53.84 ppm; DMSO, δ = 39.52 ppm). ^{11}B NMR spectra are externally referenced to boron trifluoride diethyl etherate ($BF_3 \bullet Et_2O$, δ = 0 ppm). ^{19}F {^{1}H} NMR spectra are reported as collected. Carbons bound to boron are not observed due to the quadrupolar relaxation of boron. Broad signals at ~ δ = 2.7 ppm in the ^{11}B NMR spectra are due to the borosilicate glass NMR tube. Multiplicities are as indicated: s (singlet), d (doublet), t (triplet), q (quartet), p (pentet), m (multiplet), and br (broad). Coupling constants, *J*, are reported in Hertz and integration is provided, along with assignments, as indicated. UV-Vis spectroscopy was performed on a Varian Cary50 Bio UV-Visible spectrophotometer. Cyclic voltammetry was performed on a CH Instruments, Inc. 600E Electrochemical Analyzer. Low-resolution Mass Spectrometry and High Resolution Mass Spectrometry were performed in the Department of Chemistry at Johns Hopkins University using a VG Instruments VG70S/E magnetic sector mass spectrometer with EI (70 eV). The UNIlab Plus Glove Box by MBRAUN was maintained under nitrogen atmosphere. All column chromatography was performed on a Teledyne ISCO Combiflash Rf using Redisep Rf silica columns.

Materials: Unless otherwise specified, all chemicals were used as purchased without further purification. Solvents used for extraction and column chromatography were reagent grade and used as received. Reaction solvents tetrahydrofuran (THF) (Fisher, HPLC grade), diethyl ether (Fisher, anhydrous, BHT stabilized, certified ACS), methylene chloride (Fisher, cyclohexane stabilized, HPLC grade), pentane (Fisher, certified ACS), and toluene (Fisher, certified ACS) were dried on a J. C. Meyer Solvent Dispensing System (SDS) using stainless steel columns packed with neutral alumina (except for toluene which is dried with neutral alumina and Q5 reactant, a copper(II) oxide oxygen scavenger), following the manufacturer's recommendations for solvent preparation and dispensation unless otherwise noted. Cyclopentyl methyl ether (CPME) (Sigma Aldrich, SureSeal, anhydrous, BHT inhibited, ≥99.9%) was dried on 3 Å molecular sieves overnight, degassed by the freeze-pump-thaw method and stored under an atmosphere of nitrogen in a glove box before use. Triethylamine (Sigma Aldrich, >99%) was dried over potassium hydroxide overnight, distilled under argon, degassed by the freeze-pump-thaw method, and stored under an atmosphere of nitrogen in glove box before use. UV-Vis studies were performed in THF dried on the J.C. Meyer SDS as described above. Electrochemical studies were performed in dimethylformamide (DMF) (Sigma Aldrich, anhydrous, 99.8%), dried on 3 Å molecular sieves overnight then vacuum distilled and stored in the absence of light, under argon. All water used was house deionized water.

2-Amino-3-naphthoic acid, concentrated hydrochloric acid, diphenyl phosphoryl azide (DPPA), SPhos, 2-chloroanthraquinone, 4-fluorophenylboronic acid, 4-tolylboronic acid, boron trichloride, concentrated

sulfuric acid, dichloromethane, dimethylformamide (DMF) (for synthesis of **5**), dioxane (SureSeal), ethyl acetate, hexanes, hydrogen chloride solution in ethyl ether, lithium aluminum hydride powder, palladium(II) acetate, potassium 4-(trifluoromethyl)phenyltrifluoroborate, potassium 4-chlorophenyltrifluoroborate, potassium 4-cyanophenyltrifluoroborate, potassium 4-fluorophenyltrifluoroborate, potassium 4-methoxyphenyltrifluoroborate, potassium carbonate, potassium hydroxide, potassium phenyltrifluoroborate, potassium p-tolyltrifluoroborate, sodium bicarbonate, sodium chloride, sodium hydroxide, toluene (for workup of **5**), and vinylboronic acid MIDA ester were purchased from Sigma Aldrich.

Copper(I) chloride, 2-mesitylmagnesium bromide, phenylboronic acid, potassium 4-nitrophenyltrifluoroborate, silicon tetrachloride, and tribasic potassium phosphate were purchased from Acros Organics, concentrated acetic acid, ethyl ether, and anhydrous sodium sulfate were purchased from Fisher Scientific, silica was purchased from Silicycle, tetrakis(triphenylphosphine)palladium(0) was purchased from Strem Chemicals Inc., and sodium nitrate was purchased from J.T. Baker Chemical Company.

Computational Characterization: All Density Functional Theory (DFT) calculations were done using Gaussian 09.[1] Geometries were optimized using the restricted CAM-B3LYP functional with the 6-311G(d,p) basis set with forced non-symmetry and from these optimizations the energies and orbital density maps of the frontier molecular orbitals are reported. Energies and orbital density maps of the frontier molecular orbitals of some compounds with X-ray diffraction determined geometries were also calculated using the restricted CAM-B3LYP functional with the 6-311G(d,p) basis set, without geometry optimization. All structural and orbital density map visualization were created with GaussView 5.0 by Gaussian, Inc. with hydrogens omitted for clarity and the following color scheme: grey = carbon; blue = nitrogen; pink = boron; red = oxygen; light blue = fluorine; green = chlorine.

Hammett Parameters: Hammett parameters used were given by a review by Taft and coworkers[2], with values shown below:

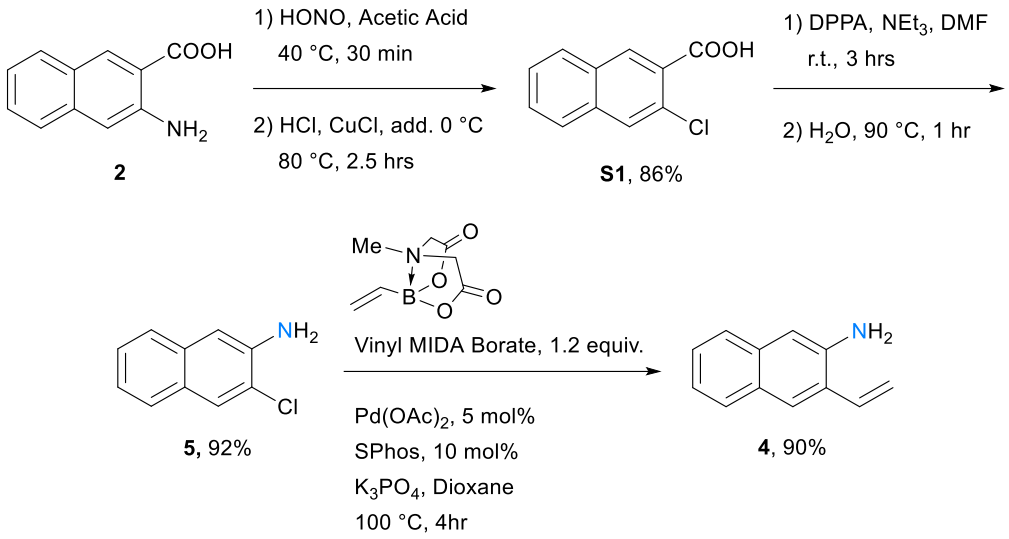
Group	**σ(para)**
OMe	-0.27
Me	-0.17
F	0.06
Cl	0.23
CF_3	0.54
CN	0.66
NO_2	0.78

[1] 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, T. Keith, 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, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

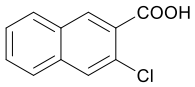
[2] C. Hansch, A. Leo, R. W. Taft, *Chem. Rev.* 1991, **91**, 165-195.

II. Experimental Procedures

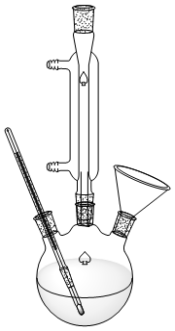
A. Synthesis of Intermediate 4



3-Chloro-2-Naphthoic Acid (S1)



This synthesis was adapted from van Koten *et al*.[3] and Tucker *et al*.[4]



In air, a 1000 mL 3-neck round bottom flask equipped with a thermometer, unsealed reflux condenser (no water was used to cool), a powder funnel and a stir bar was charged with concentrated sulfuric acid (86 mL). Sodium nitrite (1.1 equiv., 117.7 mmol, 8.12 g) was slowly added to the sulfuric acid over 20 minutes through the powder funnel. The heterogeneous, colorless mixture was heated to 70 °C for 20 minutes, or until all of sodium nitrite dissolved, then was cooled to room temperature then to 0 °C in an ice-water bath. A slurry of 2-amino-3-naphthoic acid (1 equiv., 107.0 mmol, 20.02 g) in glacial acetic acid (214 mL) was poured in portions through the powder funnel into the cooled HONO solution, ensuring the temperature did not exceed 40 °C.[5] The viscous mixture was warmed to room temperature then heated to 40 °C, and stirred at 40 °C for 30 minutes.

Separately, in air, a 1000 mL round bottom flask equipped with a stir bar and a 125 mL addition funnel was charged with copper(I) chloride (2.2 equiv., 235.4 mmol, 23.38 g) and the copper salt was dissolved in concentrated hydrochloric acid (214 mL). The copper solution was cooled to 0 °C with an ice water bath. The thick, brown solution of diazonium ion, which had been cooled to room temperature, was transferred to the addition funnel and added in a slow stream to the cooled solution of copper salt. Following the complete addition of diazonium salt, the ice water bath was removed and the reaction mixture was warmed to room temperature. The addition funnel was replaced with an unsealed reflux

[3] J. –M. Valk, R. van Belzen, J. Boersma, A. L. Spek, G. J. van Koten, *Chem. Soc. Dalton Trans.* 1994, **15**, 2293-2302.
[4] F. D. Gunstone, S. H. Tucker, *Org. Synth.* 1952, **32**, 23.
[5] The Sandmeyer reaction is mildly exothermic and Tucker *et al.* note "The temperature of diazotization is critical. Lower yields are obtained if the temperature rises above 40 °C."

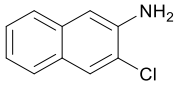
condenser (no cooling). The solution was slowly warmed to 80 °C. At 50 °C effervescence began and heating continued until effervescence ceased, about 2.5 hours. The flocculent reaction mixture was cooled to room temperature, water was slowly added (357 mL), and the mixture was allowed to slowly stir for 5 minutes causing more solids to form. The reaction mixture was filtered through a coarse fritted funnel, washing with water (500 mL) which was collected and subsequently properly disposed of. The solid product was dissolved in ethyl acetate (850 mL), passed through the fritted funnel, and separately collected. The dissolved mixture of **S1** was washed with a saturated sodium chloride solution, and dried over anhydrous sodium sulfate. Solvent was removed by rotary evaporation under reduced pressure and dried on high vacuum overnight. 3-Chloro-2-naphthoic acid (**S1**) was used without further purification (unpurified yield 19.05 g, 86%).

δ_H (400 MHz, $CDCl_3$) 8.62 (1 H, s), 7.97 (1 H, s), 7.87 (2 H, dd, *J* 52.3, 8.3), 7.61 (2 H, dt, *J* 28.9, 7.3).

δ_C (101 MHz, DMSO) 166.73, 134.25, 131.56, 130.59, 128.94, 128.90, 128.83, 128.61, 127.82, 127.26, 126.84.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{11}H_7ClO_2$ 206.0135; Found 206.01373.

3-Chloronaphthalen-2-Amine (5)



This reaction is adapted from Liu *et al.*[6]

CAUTION: This reaction was performed behind a blast shield due to the potential explosion risk associated with acyl azides.[7]

An oven-dried 1000 mL Schlenk flask equipped with a stir bar was cooled under vacuum and backfilled with nitrogen. To the flask was added **S1** (1 equiv., 50 mmol, 10.33 g). The flask was purged and backfilled three times with nitrogen. Dimethylformamide (DMF) (400 mL) was added via cannula transfer and triethylamine (1.5 equiv., 75 mmol, 10.5 mL) and diphenyl posphoryl azide (DPPA) (1.5 equiv., 75 mmol, 16.2 mL) were added via syringe. The brown solution was allowed to stir for 3 hours at room temperature under a positive pressure of nitrogen. Nitrogen-sparged water (33.3 mL) was added via cannula transfer and the reaction mixture was heated to 90 °C with stirring for 1 hour. The reaction mixture was cooled to room temperature, opened to atmosphere, and water (350 mL) was added. The biphasic mixture was poured into a 1000 mL separatory funnel and the aqueous layer was washed with diethyl ether (3 x 150 mL). The combined organic layers were washed sequentially with saturated sodium bicarbonate (2 x 175 mL) then saturated sodium chloride solutions (2 x 175 mL) and dried over sodium sulfate. The organic solvent was removed by rotary evaporation under reduced pressure. The brown solid was dissolved in 150 mL warm toluene and hot filtered through a fritted funnel to remove insoluble materials. The organic solvent was removed by rotary evaporation under reduced pressure. This product was used without further purification (unpurified yield 8.13 g, 92%).

δ_H (400 MHz, $CDCl_3$) 7.97 (1 H, s), 7.78 (2 H, dd, *J* 12.1, 8.3), 7.60 – 7.39 (2 H, m), 7.18 (1 H, s), 4.27 (2 H, s).

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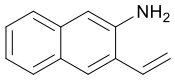
[6] J. S. A. Ishibashi, J. L. Marchall, A. Mazière, G. J. Lovinger, B. Li, L. N. Zakharov, A. Dargelos, A. Graciaa, A. Chrostowska, S.–Y. Liu, *J. Am. Chem. Soc.* 2014, **136**, 15414-15421.

[7] S. Bräse, C. Gil, K. Knepper, V. Zimmermann, *Angew. Chem. Int. Ed.* 2005, **44**, 5188–5240.

δ_C (101 MHz, $CDCl_3$) 140.89, 133.52, 127.99, 127.92, 126.86, 126.49, 125.58, 123.21, 122.25, 109.72.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{10}H_8ClN$ 177.0345; Found 177.03418.

3-Vinylnaphthalen-2-Amine (4)



This procedure was adapted from Burke *et al.*[8]

An oven dried 250 mL Schlenk flask equipped with a condenser and stir bar was cooled under vacuum. The flask was charged with **5** (1 equiv., 10 mmol, 1.78 g), palladium(II) acetate (5 mol%, 0.5 mmol, 112.3 mg), SPhos (10 mol%, 1 mmol, 410.5 mg), and vinylboronic acid MIDA ester (1.2 equiv., 12 mmol, 2.05 g). The reaction vessel was purged and backfilled three times with nitrogen. The solids were dissolved in dioxane (100 mL) and a nitrogen-sparged aqueous solution of tribasic potassium phosphate (3 M, 20 mL) was added. The reaction was heated to 100 °C with stirring under a positive pressure of nitrogen for 4 hours. The reaction was cooled to room temperature, transferred to a 250 mL round bottom flask, and concentrated by rotary evaporation under reduced pressure. The solids were dissolved in ethyl acetate (50 mL) and added to a separatory funnel, along with an aqueous solution of sodium hydroxide (1 M, 40 mL). The aqueous layer was extracted with ethyl acetate (3 x 50 mL) and the combined organic layers were dried over sodium sulfate. After filtration, the organic solvents were removed by rotary evaporation under reduced pressure. **4** was purified by automated silica gel column chromatography (40 g column) eluting with 10% ethyl acetate in hexanes (yield 1.52 g, 90%).

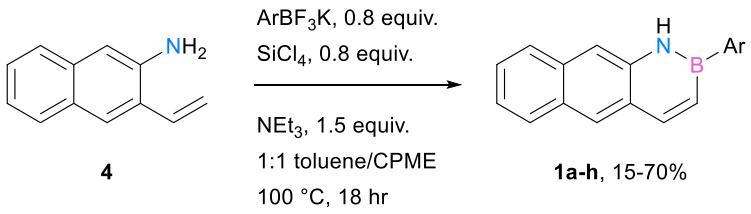
δ_H (400 MHz, $CDCl_3$) 7.76 (1 H, s), 7.70 (1 H, dd, *J* 8.2, 1.1), 7.58 (1 H, dd, *J* 8.2, 1.1), 7.35 (1 H, ddd, *J* 8.2, 6.8, 1.3), 7.28 – 7.19 (1 H, m), 7.02 (1 H, s), 6.92 (1 H, ddd, *J* 17.4, 11.0, 0.8), 5.80 (1 H, dd, *J* 17.3, 1.5), 5.45 (1 H, dd, *J* 11.0, 1.5), 4.042 (2 H, s).

δ_C (101 MHz, $CDCl_3$) 142.29, 134.58, 133.05, 128.26, 127.89, 127.54, 126.62, 126.33, 125.50, 122.82, 117.57, 109.67.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{12}H_{11}N$ 169.0891; Found 169.08868.

[8] D. M. Knapp, E. P. Gillis, M. D. Burke, *J. Am. Chem. Soc.* 2009, **131**, 6961-6963.

B. Synthesis of BN Anthracenes 1a-h



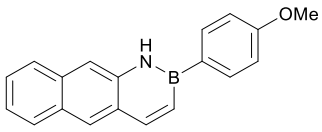
4 **1a-h**, 15-70%

General Procedure A

This procedure was adapted from Molander *et al.*[9]

An oven dried 15 mL heavy walled cylindrical pressure vessel equipped with a stir bar was charged with **4** (1 equiv., 1.8 mmol, 304 mg) and the appropriate potassium aryltrifluoroborate (0.8 equiv., 1.5 mmol). The vessel and contents were brought into a nitrogen atmosphere glove box. Toluene (6 mL), cyclopentyl methyl ether (CPME) (6 mL), triethylamine (1.5 equiv., 2.3 mmol, 0.32 mL), and silicon tetrachloride (1 equiv., 1.5 mmol, 175 µL) were added to the reaction vessel. The vessel was sealed with a PTFE screw cap, brought out of the glove box and heated to 100 °C for 18 hours with stirring. The reaction mixture was cooled to room temperature, added to a separatory funnel, and diluted with an aqueous hydrochloric acid solution (1M, 30 mL) and ethyl acetate (25 mL). The organic layer was collected and the aqueous layer was washed with ethyl acetate (3 x 25 mL). The combined organic layers were washed with a saturated aqueous sodium bicarbonate solution (1 x 50 mL) then a saturated aqueous sodium chloride solution (1 x 50 mL), dried over anhydrous sodium sulfate, and concentrated by rotary evaporation under reduced pressure. The products were recrystallized from hot chlorobenzene. (In exception to this procedure was the work-up of **1h**, as detailed below)

2-(4-Methoxyphenyl)-1,2-Dihydronaphtho[2,3-*e*][1,2]Azaborinine (4-MeO Ph BN Anthracene, 1a)



Synthesized according to General Procedure A using potassium 4-methoxyphenyltrifluoroborate (0.8 equiv., 1.5 mmol, 0.32 g). Yield 0.11 g, 25%.

δ_H (400 MHz, $CDCl_3$) 8.24 (1 H, d, *J* 11.7), 8.17 (1 H, s), 8.05 (1 H, s), 7.99 – 7.92 (3 H, m), 7.88 (1 H, d, *J* 8.4), 7.73 (1 H, s), 7.50 (1 H, ddd, *J* 8.3, 6.7, 1.3), 7.41 (1 H, ddd, *J* 8.0, 6.7, 1.2), 7.10 – 7.04 (2 H, m), 3.92 (3 H, s).

δ_C (101 MHz, DMSO) 160.99, 144.90, 139.20, 135.33, 132.98, 127.99, 127.97, 126.50, 126.27, 126.13, 123.45, 113.59, 113.25, 54.97.

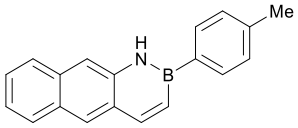
δ_B (128 MHz, $CDCl_3$) 34.10.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{19}H_{16}BNO$ 285.1325; Found 285.13217.

Melting point: 263.8°C

[9] S. R. Wisniewski, C. L. Guenther, O. A. Argintaru, G. A. Molander, *J. Org. Chem*. 2014, **79**, 365-378.

2-(p-Tolyl)-1,2-Dihydronaphtho[2,3-*e*][1,2]Azaborinine (4-Me Ph BN Anthracene, 1b)



Synthesized according to General Procedure A using potassium p-tolyltrifluoroborate (0.8 equiv., 1.5 mmol, 0.30 g). Yield 0.077 g, 19%.

δ_H (400 MHz, $CDCl_3$) 8.23 (1 H, d, *J* 11.6), 8.16 (1 H, s), 8.09 (1 H, s), 7.94 (1 H, d, *J* 8.2), 7.88 (2 H, d, *J* 7.9), 7.89 – 7.82 (1 H, m), 7.72 (1 H, s), 7.48 (1 H, ddd, *J* 8.2, 6.7, 1.3), 7.39 (1 H, ddd, *J* 8.1, 6.7, 1.2), 7.35 – 7.27 (3 H, m), 2.43 (3 H, s).

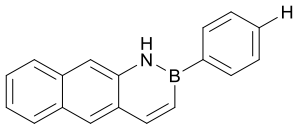
δ_C (101 MHz, DMSO) 145.14, 139.45, 139.10, 133.69, 132.97, 128.68, 128.05, 128.03, 128.02, 126.56, 126.31, 126.19, 123.54, 113.45, 21.22.

δ_B (128 MHz, $CDCl_3$) 34.84.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{19}H_{16}BN$ 269.1376; Found 269.13806.

Melting point: 252.6 °C

2-Phenyl-1,2-Dihydronaphtho[2,3-*e*][1,2]Azaborinine (4-H Ph BN Anthracene, 1c)



Synthesized according to General Procedure A using potassium phenyltrifluoroborate (0.8 equiv., 1.5 mmol, 0.28 g). Yield 0.17 g, 44%.

δ_H (400 MHz, $CDCl_3$) 8.26 (1 H, d, *J* 11.6), 8.18 (1 H, s), 8.13 (1 H, s), 8.01 – 7.84 (4 H, m), 7.74 (1 H, s), 7.55 – 7.46 (4 H, m), 7.40 (1 H, ddd, *J* 8.1, 6.7, 1.2), 7.29 (1 H, dd, *J* 11.7, 1.9).

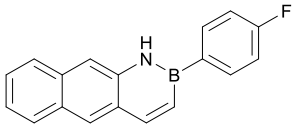
δ_C (101 MHz, DMSO) 145.34, 139.02, 133.59, 133.59, 130.28, 129.89, 128.11, 128.09, 128.03, 127.96, 126.591, 126.35, 126.19, 123.60, 113.60.

δ_B (128 MHz, $CDCl_3$) 34.62.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{18}H_{14}BN$ 255.1219; Found 255.12272.

Melting point: 232.5 °C

2-(4-Fluorophenyl)-1,2-Dihydronaphtho[2,3-*e*][1,2]Azaborinine (4-F Ph BN Anthracene, 1d)



Synthesized according to General Procedure A using potassium 4-fluorophenyltrifluoroborate (0.8 equiv., 1.5 mmol, 0.30 g). Yield 0.22 g, 54%.

δ_H (400 MHz, $CDCl_3$) 8.25 (1 H, d, *J* 11.6), 8.17 (1 H, s), 8.06 (1 H, s), 7.98 – 7.91 (3 H, m), 7.89 – 7.84 (1 H, m), 7.73 (1 H, s), 7.50 (1 H, ddd, *J* 8.2, 6.7, 1.3), 7.40 (1 H, ddd, *J* 8.1, 6.7, 1.2), 7.26 – 7.16 (3 H, m).

δ_C (101 MHz, DMSO) 164.20 (d, *J* 246.9), 145.88, 139.42, 136.50, 136.42, 133.46, 128.62, 128.57, 128.50, 127.07, 126.85, 126.57, 124.11, 115.49, 115.29, 114.02.

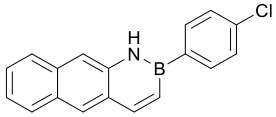
δ_B (128 MHz, $CDCl_3$) 34.42.

δ_F (376 MHz, $CDCl_3$) –110.75.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{18}H_{13}BFN$ 273.1125; Found 273.11224.

Melting point: 247.1 °C

2-(4-Chlorophenyl)-1,2-Dihydronaphtho[2,3-*e*][1,2]Azaborinine (4-Cl Ph BN Anthracene, 1e)



Synthesized according to General Procedure A using potassium 4-chlorophenyltrifluoroborate (0.8 equiv., 1.5 mmol, 0.33 g). Yield 0.30 g, 70%.

δ_H (400 MHz, $CDCl_3$) 8.26 (1 H, d, *J* 11.7), 8.18 (1 H, s), 8.09 (1 H, s), 7.95 (1 H, ddd, *J* 8.3, 1.4, 0.7), 7.91 – 7.84 (3 H, m), 7.74 (1 H, s), 7.54 – 7.45 (3 H, m), 7.41 (1 H, ddd, *J* 8.1, 6.7, 1.2), 7.23 (1 H, dd, *J* 11.6, 2.0).

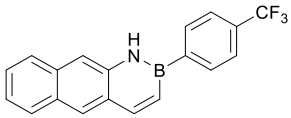
δ_C (101 MHz, $CDCl_3$) 150.81, 144.07, 140.67, 140.19, 138.21, 133.46, 133.39, 133.36, 133.26, 133.23, 131.85, 131.63, 131.36, 128.92, 118.90.

δ_B (128 MHz, $CDCl_3$) 34.31.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{18}H_{13}BClN$ 289.083; Found 289.08337.

Melting point: 254.7 °C

2-(4-(Trifluoromethyl)Phenyl)-1,2-Dihydronaphtho[2,3-*e*][1,2]Azaborinine (4-CF_3 Ph BN Anthracene, 1f)



Synthesized according to General Procedure A using potassium 4-(trifluoromethyl)phenyltrifluoroborate (0.8 equiv., 1.5 mmol, 0.38 g). Yield 0.22 g, 46%.

δ_H (400 MHz, $CDCl_3$) 8.31 (1 H, d, *J* 11.6), 8.21 (1 H, d, *J* 1.0), 8.17 (1 H, s), 8.08 – 8.02 (2 H, m), 7.99 – 7.94 (1 H, m), 7.92 – 7.86 (1 H, m), 7.78 (1 H, s), 7.77 – 7.71 (2 H, m), 7.54 – 7.48 (1 H, m), 7.42 (1 H, ddd, *J* 8.1, 6.7, 1.2), 7.26 (1 H, dd, *J* 11.6, 2.0).

δ_C (101 MHz, DMSO) 146.39, 139.17, 134.67, 133.47, 130.48, 130.16, 128.77, 128.72, 128.54, 127.16, 126.95, 126.65, 126.28, 124.92, 124.88, 124.30, 123.57, 114.37.

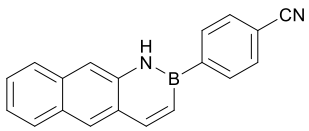
δ_B (128 MHz, $CDCl_3$) 34.53.

δ_F (376 MHz, $CDCl_3$) –62.76.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{19}H_{13}BF3N$ 323.1093; Found 323.10941.

Melting point: 256.3 °C

4-(Naphtho[2,3-e][1,2]Azaborinin-2(1H)-yl)Benzonitrile (4-CN Ph BN Anthracene, 1g)



Synthesized according to General Procedure A using potassium 4-cyanophenyltrifluoroborate (0.8 equiv., 1.5 mmol, 0.31 g). Yield 0.062 g, 15%.

δ_H (400 MHz, $CDCl_3$) 8.36 – 8.28 (1 H, m), 8.21 (1 H, s), 8.16 (1 H, s), 8.04 – 7.99 (2 H, m), 7.92 (2 H, dddt, *J* 32.0, 8.4, 1.3, 0.8), 7.80 – 7.73 (3 H, m), 7.48 (2 H, dddd, *J* 34.5, 8.1, 6.7, 1.2), 7.22 (1 H, dd, *J* 11.6, 2.0).

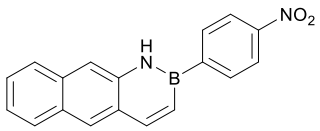
δ_C (101 MHz, DMSO) 146.01, 138.61, 134.18, 132.99, 131.44, 128.32, 128.28, 128.06, 126.70, 126.50, 126.17, 123.88, 119.09, 113.95, 112.05.

δ_B (128 MHz, $CDCl_3$) 34.06.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{19}H_{13}BN_2$ 280.1172; Found 280.11689.

Melting point: 239.2 °C

2-(4-Nitrophenyl)-1,2-Dihydronaphtho[2,3-e][1,2]Azaborinine (4-NO_2 Ph BN Anthracene, 1h)



Synthesized according to General Procedure A using potassium 4-nitrophenyltrifluoroborate (0.8 equiv., 1.5 mmol, 0.34 g) and an alternative workup procedure. Once the reaction was cooled to room temperature the reaction mixture was diluted with hexanes (100 mL) then filtered through a fritted funnel and washed with hexanes (10 mL). The product was eluted with dichloromethane (200 mL), washed with a saturated aqueous sodium chloride solution (1 x 50 mL), dried over magnesium sulfate, and concentrated by rotary evaporation under reduced pressure. The product was recrystallized from hot chlorobenzene. Yield 0.27 g, 59%.

δ_H (400 MHz, $CDCl_3$) 8.37 – 8.30 (3 H, m), 8.23 (1 H, s), 8.21 (1 H, s), 8.12 – 8.07 (2 H, m), 8.00 – 7.86 (2 H, m), 7.80 (1 H, s), 7.48 (2 H, dddd, *J* 34.4, 8.1, 6.7, 1.2), 7.25 (1 H, dd, *J* 11.8, 1.8).

δ_C (101 MHz, DMSO) 148.38, 146.07, 138.58, 134.70, 133.00, 130.25, 128.36, 128.34, 128.31, 128.06, 126.98, 126.71, 126.51, 126.16, 123.90, 122.50, 122.48, 114.05.

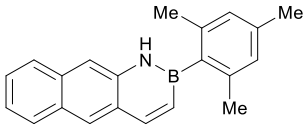
δ_B (128 MHz, $CDCl_3$) 34.26.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{18}H_{13}BN_2O_2$ 300.107; Found 300.10714.

Melting point: 256.3 °C

C. Synthesis of Mes BN Anthracene 1i

2-Mesityl-1,2-Dihydronaphtho[2,3-*e*][1,2]Azaborinine (Mes BN Anthracene, 1i)



This procedure was adapted from Liu *et al.*6

An oven dried 250 mL Schlenk flask equipped with a condenser and stir bar was cooled under vacuum and purged with argon. The flask was charged with **4** (1 equiv., 1.9 mmol, 0.32 g). The reaction flask was purged and backfilled three times with argon. The solid was dissolved in toluene (40 mL) and the brown solution was cooled to −40 °C in an acetonitrile/dry ice bath.

Separately, an oven dried 5 mL heart-shaped flask, purged and backfilled with argon three times, was cooled to −78 °C in an isopropanol/dry ice bath. The flask was charged with boron trichloride (1M in hexanes, 4 mL). The chilled boron trichloride (1M in hexanes, 2 equiv., 3.8 mmol, 3.8 mL) was added dropwise, via syringe in two portions, to the chilled and stirred solution of **4**. The reaction mixture stirred for 1 hour at −40 °C. While under a high positive pressure of argon and still cool, an oven-dried condenser was fit to the reaction flask, then the reaction mixture was brought to reflux (120 °C) for 18 hours.

The reaction was cooled to room temperature and solvent removed under reduced pressure with stirring. Once dried, the flask was backfilled with argon and the condenser was replaced with a septum. The reaction mixture was redissolved in diethyl ether (40 mL) and cooled to −40 °C in an acetonitrile/dry ice bath. 2-Mesitylmagnesium bromide (1M in THF, 2 equiv., 3.8 mmol, 3.8 mL) was added dropwise via syringe to the cooled reaction mixture with stirring. Following addition, the solution was warmed to room temperature and allowed to stir under argon for 18 hours.

The reaction was cooled to 0 °C in an ice water bath and water (10 mL) was added dropwise by syringe to quench excess Grignard reagent then the biphasic mixture was warmed to room temperature for 30 minutes. Ethyl acetate (15 mL) and water (10 mL) were added and the biphasic mixture transferred to a separatory funnel. The organic layer was collected. The aqueous layer was extracted with ethyl acetate (3 x 15 mL) and the combined organic layers were washed with a saturated aqueous solution of sodium chloride and dried over sodium sulfate. Organic solvents were removed by rotary evaporation under reduced pressure then passed through a silica gel column, eluting with 50% dichloromethane in hexanes. The product fractions were collected, concentrated by rotary evaporation, and dried on vacuum overnight (yield 0.25 g, 46%).

δ_H (400 MHz, $CDCl_3$) 8.22 (2 H, d, *J* 11.8), 7.97 (1 H, d, *J* 8.3), 7.86 (1 H, d, *J* 8.4), 7.82 (1 H, s), 7.62 (1 H, s), 7.50 (1 H, ddd, *J* 8.2, 6.7, 1.3), 7.42 (1 H, ddd, *J* 8.1, 6.7, 1.2), 6.97 (1 H, dd, *J* 11.5, 1.8), 6.94 (2 H, s), 2.36 (3 H, s), 2.26 (6 H, s).

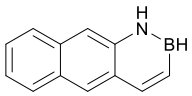
δ_C (101 MHz, DMSO) 144.42, 139.08, 138.95, 137.980, 136.33, 132.77, 131.00, 128.15, 128.02, 126.85, 126.44, 126.33, 125.80, 123.51, 113.24, 40.15, 39.94, 39.86, 39.73, 39.52, 39.40, 39.31, 39.10, 38.90, 22.62, 20.83.

δ_B (128 MHz, $CDCl_3$) 37.71.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{21}H_{20}BN$ 297.1689; Found 297.1689.

D. Synthesis of BN Anthracene

1,2-Dihydronaphtho[2,3-*e*][1,2]Azaborinine (BN Anthracene)



BN anthracene was synthesized as reported by Liu *et al.*6 on a 2.0 mmol scale (yield 0.096 g, 27%). Characterization data matched the reported spectra.

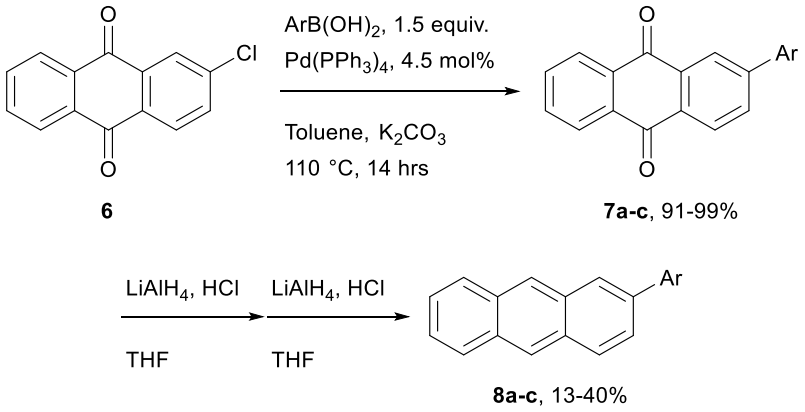
δ_H (400 MHz, $CDCl_3$) 8.25 – 8.12 (3 H, m), 7.94 (1 H, ddt, *J* 8.3, 1.4, 0.7), 7.89 – 7.84 (1 H, m), 7.68 (1 H, s), 7.49 (1 H, ddd, *J* 8.3, 6.7, 1.3), 7.41 (1 H, ddd, *J* 8.1, 6.7, 1.3), 6.98 (1 H, ddd, *J* 11.5, 2.5, 1.7).

δ_C (101 MHz, $CDCl_3$) 144.97, 137.95, 133.15, 128.83, 128.81, 128.16, 126.56, 126.47, 126.46, 123.91, 113.40.

δ_B (128 MHz, $CDCl_3$) 32.87 (d, *J* 95.7).

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{12}H_{10}BN$ 179.0906; Found 179.09095.

E. Synthesis of 2-Arylanthracenes 8a-c



General Procedure B (Suzuki Coupling)

This procedure was adapted from Yamashita *et al.*[10]

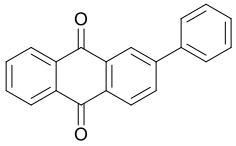
An oven dried 100 mL Schlenk flask equipped with a condenser and stir bar was cooled under vacuum. The nitrogen-filled flask was charged with 2-chloroanthraquinone, **6,** (1 equiv., 2.1 mmol, 0.50 g), the appropriate arylboronic acid (1.5 equiv., 3.1 mmol), and tetrakis(triphenylphosphine)palladium(0) (4.5 mol%, 0.09 mmol, 0.11 g). The flask was purged and backfilled three times with argon. The solids were dissolved in toluene (10.3 mL) and an argon-sparged aqueous solution of potassium carbonate (2 M, 4.1 mL) was added. The biphasic reaction mixture was heated to reflux (110 °C) with stirring under a positive pressure of argon for 14 hours.

The reaction was cooled to room temperature and diluted with ethyl acetate (10 mL). The biphasic mixture was transferred to a separatory funnel and the organic layer was collected. The aqueous layer was

[10] H. Chiba, J. Nishida, Y. Yamashita, *Chem. Lett*. 2012, **41**, 482-484.

washed with ethyl acetate (3 x 15 mL) and the combined organic layers were washed with a saturated aqueous sodium chloride solution then dried over sodium sulfate. The mixture was filtered and concentrated by rotary evaporation under reduced pressure. Products **7a-c** were purified by dissolving in a minimal quantity of dichloromethane, passing through a silica plug and eluting with 50% dichloromethane in hexanes.

2-Phenylanthracene-9,10-Dione (7a)



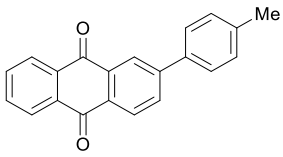
Synthesized according to General Procedure B using phenylboronic acid (1.5 equiv., 3.1 mmol, 0.38 g). Yield 0.53 g, 91%.

δ_H (400 MHz, $CDCl_3$) 8.46 (1 H, dd, *J* 1.9, 0.5), 8.33 – 8.24 (3 H, m), 7.96 (1 H, dd, *J* 8.1, 2.0), 7.80 – 7.73 (2 H, m), 7.71 – 7.66 (2 H, m), 7.52 – 7.39 (3 H, m).

δ_C (101 MHz, $CDCl_3$) 183.13, 182.80, 146.77, 138.90, 134.17, 134.05, 133.86, 133.62, 133.59, 132.32, 132.12, 129.17, 128.90, 128.04, 127.34, 127.28, 127.21, 125.52.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{20}H_{12}O_2$ 284.0837; Found 284.08341.

2-(p-Tolyl)Anthracene-9,10-Dione (7b)



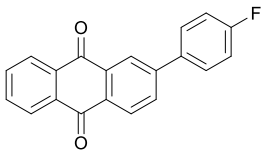
Synthesized according to General Procedure B using 4-tolylboronic acid (1.5 equiv., 3.1 mmol, 0.42 g). Yield 0.61 g, 99%.

δ_H (400 MHz, $CDCl_3$) 8.51 (1 H, dd, *J* 2.0, 0.5), 8.36 (0 H, d, *J* 0.5), 8.35 – 8.31 (3 H, m), 8.00 (1 H, dd, *J* 8.1, 2.0), 7.84 – 7.77 (2 H, m), 7.66 – 7.60 (2 H, m), 7.35 – 7.29 (2 H, m), 2.43 (3 H, s).

δ_C (101 MHz, $CDCl_3$) 183.41, 183.01, 146.91, 139.14, 136.13, 134.27, 134.13, 134.00, 133.80, 133.75, 132.21, 132.02, 129.99, 128.15, 127.39, 127.32, 127.28, 125.37, 21.37.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{21}H_{14}O_2$ 298.0994; Found 298.09976.

2-(4-Fluorophenyl)Anthracene-9,10-Dione (7c)



Synthesized according to General Procedure B using 4-fluorophenylboronic acid (1.5 equiv., 3.1 mmol, 0.43 g). Yield 0.61 g, 98%.

δ_H (400 MHz, $CDCl_3$) 8.46 (1 H, d, *J* 1.9), 8.35 (1 H, dd, *J* 8.1, 0.5), 8.34 – 8.29 (2 H, m), 7.95 (1 H, dd, *J* 8.1, 2.0), 7.84 – 7.78 (2 H, m), 7.73 – 7.66 (2 H, m), 7.23 – 7.16 (2 H, m).

δ_C (101 MHz, $CDCl_3$) 183.24, 182.88, 163.45 (d, *J* 249.1), 145.86, 135.19, 135.16, 134.34, 134.20, 134.01, 133.70, 133.65, 132.24, 129.23, 128.23, 127.40, 127.34, 125.44, 116.27 (d, *J* 21.6).

δ_F (376 MHz, $CDCl_3$) –112.81.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{20}H1_1FO_2$ 302.0743; Found 302.07418.

General Procedure C (Reduction of Quinone)

This procedure was adapted from Tao *et al.* [11]

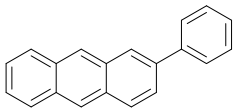
An oven dried 100 mL Schlenk flask equipped with a stir bar and sealed with a rubber septum was cooled under vacuum. The flask was charged with lithium aluminum hydride (4 equiv., 4.4 mmol, 0.17 g). The flask was purged and backfilled three times with argon and the LAH was suspended in THF (5.5 mL). The heterogeneous suspension was cooled to 0 °C in an ice water bath. The appropriate anthraquinone (1 equiv., 1.1 mmol) was dissolved in THF (8.8 mL) and added dropwise via syringe to the cooled lithium aluminum hydride suspension under a positive pressure of argon. The reaction mixture was allowed to stir for 1 hour at 0 °C, after which a second portion of lithium aluminum hydride (2 equiv., 2.2 mmol, 0.08 g) was added by quickly removing the septum, pouring in reagent, and resealing. The ice bath was removed and the reaction mixture was allowed to warm to room temperature and stirred for 2 hours.

The reaction was quenched by cooling to 0 °C with an ice water bath, followed by opening the reaction to air and the very slow dropwise addition of an aqueous solution of hydrochloric acid (6M, 5.5 mL) via syringe. The mixture was stirred 30 minutes at 0 °C then warmed to room temperature. The reaction mixture was diluted with dichloromethane (20 mL) and the biphasic mixture was transferred to a separatory funnel. The organic layer was collected and the aqueous layer was washed with dichloromethane (3 x10 mL). The combined organic layers were washed with a saturated aqueous sodium chloride solution and dried over sodium sulfate. After filtration, the organic solvents were removed by rotary evaporation under reduced pressure.

The product mixture was subjected to the reduction conditions for a second time using the same procedure.

The desired product was obtained after purification by silica gel chromatography (40 g column) eluting with a 20% dichloromethane in hexanes,

2-Phenylanthracene (4-H Ph Anthracene, 8a)



Synthesized according to General Procedure C using **7a** (1 equiv., 1.1 mmol, 0.31 g). Yield 0.093 g, 33% yield.

δ_H (400 MHz, $CDCl_3$) 8.48 (1 H, s), 8.45 (1 H, s), 8.21 (1 H, t, *J* 1.2), 8.12 – 8.07 (1 H, m), 8.05 – 7.99 (2 H, m), 7.78 (3 H, td, *J* 8.5, 1.7), 7.55 – 7.37 (5 H, m).

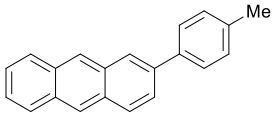
δ_C (101 MHz, $CDCl_3$) 141.18, 137.93, 132.19, 132.00, 131.94, 130.99, 129.04, 128.90, 128.36, 128.29, 127.57, 127.57, 126.70, 126.15, 125.80, 125.67, 125.63, 125.53.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{21}H_{16}$ 254.1096; Found 254.10991.

Melting point: 213.6 °C

2-(p-Tolyl)Anthracene (4-Me Ph Anthracene, 8b)

[11] F. Valiyev, W. -S. Hu, H. -Y. Chen, M. -Y. Kuo, I. Chao, Y. -T. Tao, *Chem. Mater.* 2007, **19**, 3018-3026.



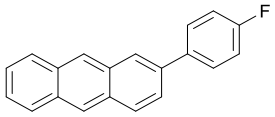
Synthesized according to General Procedure C using **7b** (1 equiv., 1.1 mmol, 0.33 g). Yield 0.12 g, 40% yield.

δ_H (400 MHz, $CDCl_3$) 8.48 – 8.42 (2 H, m), 8.19 (1 H, dq, *J* 1.6, 0.8), 8.08 (1 H, dq, *J* 8.9, 0.8), 8.04 – 7.99 (2 H, m), 7.76 (1 H, dd, *J* 8.8, 1.8), 7.72 – 7.66 (2 H, m), 7.50 – 7.44 (2 H, m), 7.36 – 7.30 (2 H, m), 2.44 (3 H, s).

δ_C (101 MHz, $CDCl_3$) 138.25, 137.83, 137.40, 132.16, 132.06, 131.84, 130.93, 129.76, 128.80, 128.35, 128.26, 127.30, 126.56, 126.11, 125.67, 125.57, 125.42, 125.33, 21.31.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{20}H_{14}$ 268.1252; Found 268.12554.

2-(4-Fluorophenyl)Anthracene (4-F Ph Anthracene, 8c)



Synthesized according to General Procedure C using **7c** (1 equiv., 1.1 mmol, 0.33 g). Yield 0.040 g, 13% yield.

δ_H (400 MHz, $CDCl_3$) 8.47 (1 H, s), 8.45 (1 H, s), 8.15 (1 H, d, *J* 1.7), 8.11 – 8.06 (1 H, m), 8.05 – 7.98 (2 H, m), 7.77 – 7.67 (3 H, m), 7.51 – 7.44 (2 H, m), 7.24 – 7.14 (2 H, m).

δ_C (101 MHz, CD_2Cl2) 163.04 (d, *J* 246.2), 137.58 (d, *J* 3.3), 137.19, 132.58, 132.32, 132.25, 131.21, 129.38, 129.30, 129.26, 128.58, 128.49, 126.90, 126.41, 126.05, 125.93, 125.84, 125.83, 125.69, 116.12 (d, *J* 21.7).

δ_F (376 MHz, $CDCl_3$) –114.89.

HRMS (EI) m/z: $[M]^+$ Calcd for $C_{20}H_{13}F$ 272.1001; Found 272.10074.

III. UV-Vis Spectroscopy

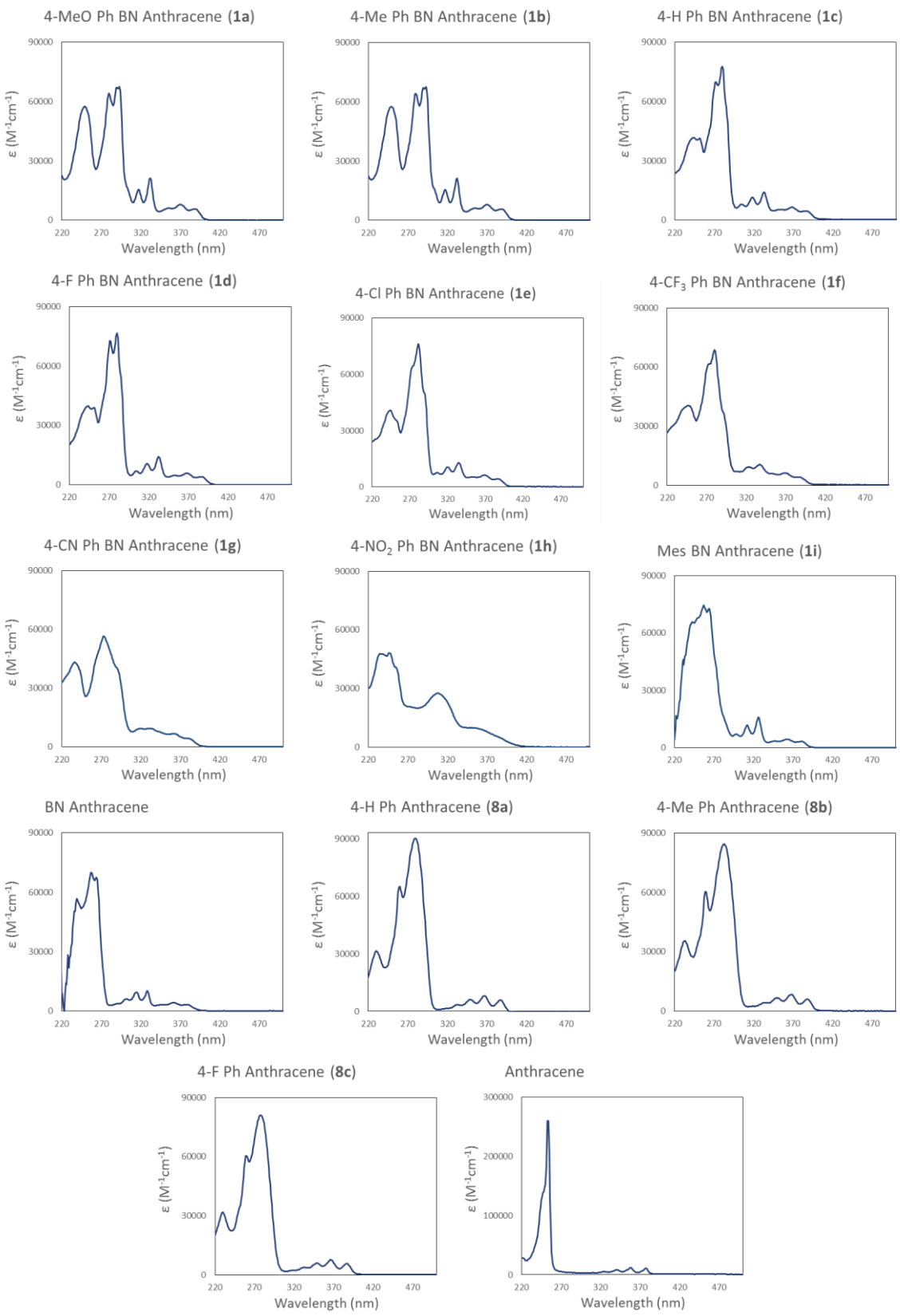
All UV-Vis measurements were collected in THF at room temperature using a Varian Cary50 Bio UV-Visible spectrophotometer with quartz cuvettes. All solutions were prepared in air with exception to BN anthracene. A stock solution of BN anthracene was prepared in the glove box and diluted just prior to spectrum collection in air.

UV-Vis Data

Table S-1: Tabulated data from all UV-Vis studies. [a] λ_{onset} = onset of absorption; [b] E_g = optical bandgap, calculated from the onset of absorption.

Compound	**Substituent**	**λ_{onset}[a] (nm)**	**E_g[b] (eV)**
1a	4-MeO	401	3.09
1b	4-Me	400	3.10
1c	4-H	400	3.10
1d	4-F	399	3.10
1e	4-Cl	400	3.10
1f	4-CF_3	401	3.09
1g	4-CN	396	3.13
1h	4-NO_2	411	3.01
1i	Mes	393	3.15
BN Anthracene	n/a	392	3.17
8a	4-H	398	3.12
8b	4-Me	399	3.11
8c	4-F	398	3.12
Anthracene	n/a	383	3.24

UV-Vis Spectra of Products



IV. Cyclic Voltammetry (CV)

All CV measurements were performed in an oven dried single chamber cell cooled on vacuum and solutions were made using standard Schlenk techniques. All voltammograms were obtained using an analyte concentration of 3.5 mM and a tetrabutylammonium hexafluorophosphate (*n*-Bu_4NPF_6 or $TBAPF_6$, recrystallized from ethanol and dried on vacuum) concentration of 0.1 M in dimethylformamide (DMF). DMF was dried on 3 Å molecular sieves overnight then vacuum distilled and stored in the absence of light under argon. Ferrocene (sublimed) was used as an internal standard. All voltammograms were obtained using a CH Instruments, Inc. 600E Electrochemical Analyzer with a 2 mm diameter platinum button working electrode, platinum wire counter electrode, and a quasi-internal silver wire reference electrode submersed in 0.01 M $AgNO_3$/0.1 M $TBAPF_6$ in anhydrous acetonitrile. All voltammograms were collected at room temperature with a scan rate of 0.1 Vs^{-1} and internally referenced to the ferrocene/ferrocenium (Fc/Fc^+) redox couple ($E_{1/2}$ = 0 V).

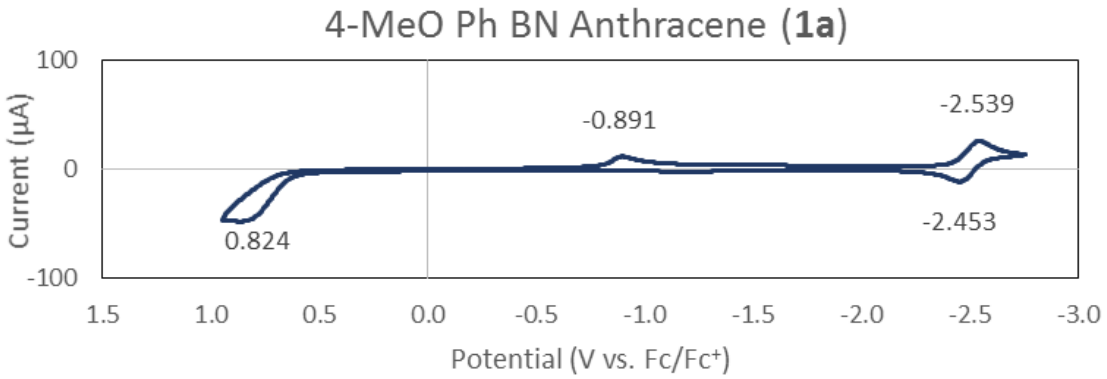
CV Data

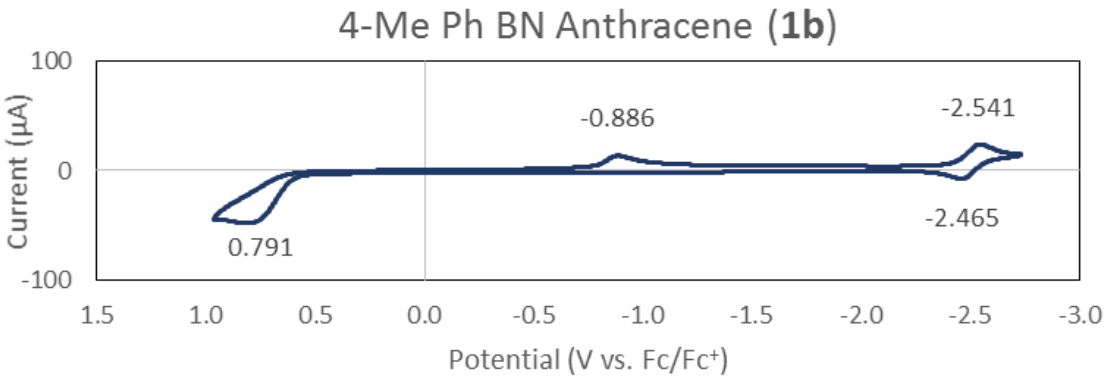
Table S-2: Tabulated data from all CV studies. [a] $E_{p,a}$ = anodic peak potential; [b] OSP = oxidation side product; [c] $E_{p,c}$ = cathodic peak potential; [d] $E_{1/2} = (E_{pc} + E_{pa})/2$.

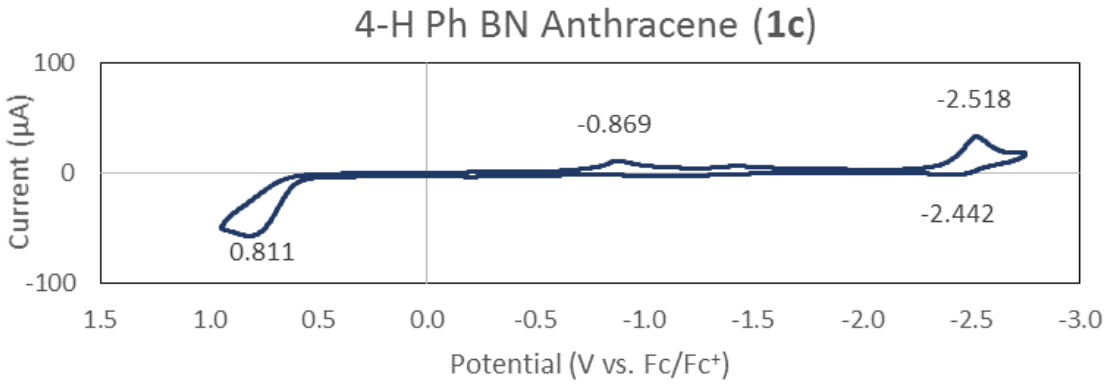
Compound	Substituent	Oxidation $E_{p,a}$[a] (V)	Reduction $E_{p,c}$[c] (V)	Reduction $E_{p,a}$[a] (V)	Reduction $E_{1/2}$[d] (V)
1a	4-MeO	0.82	-2.54	-2.45	-2.50
1b	4-Me	0.79	-2.54	-2.47	-2.50
1c	4-H	0.81	-2.52	-2.44	-2.48
1d	4-F	0.91	-2.53	-2.44	-2.48
1e	4-Cl	0.74	-2.48	n/a	n/a
1f	4-CF_3	0.85	-2.41	n/a	n/a
1g	4-CN	0.88	-2.33	-2.25	-2.29
1h	4-NO_2	0.82	-2.27	n/a	n/a
1i	Mes	0.93	-2.59	-2.50	-2.54
BN Anthracene	n/a	0.77	-2.53	n/a	n/a
8a	4-H	0.82	-2.37	-2.28	-2.33
8b	4-Me	0.80	-2.39	-2.30	-2.35
8c	4-F	0.81	-2.37	-2.28	-2.33
Anthracene	n/a	0.86	-2.46	-2.36	-2.41

Cyclic Voltammograms of Products

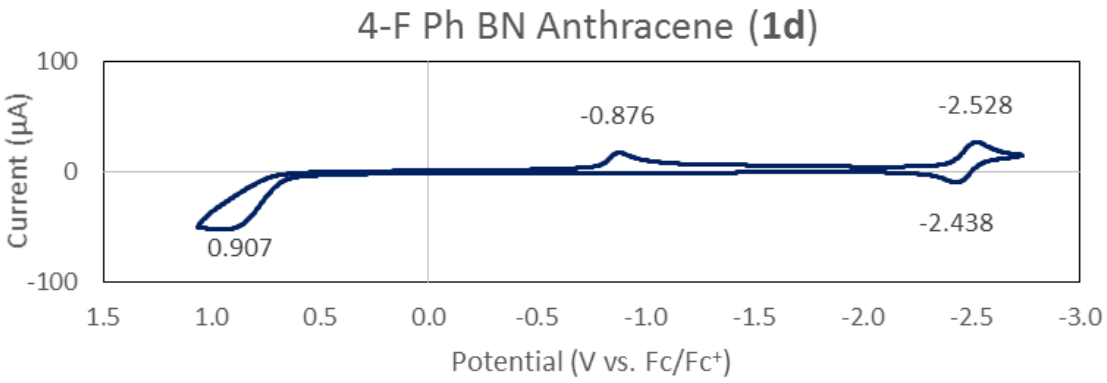
All CVs were taken in triplicate and the third scan is reported.

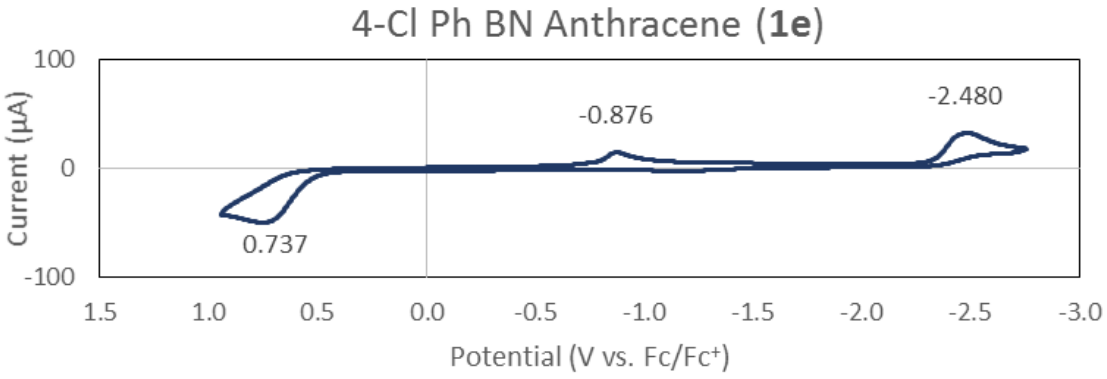


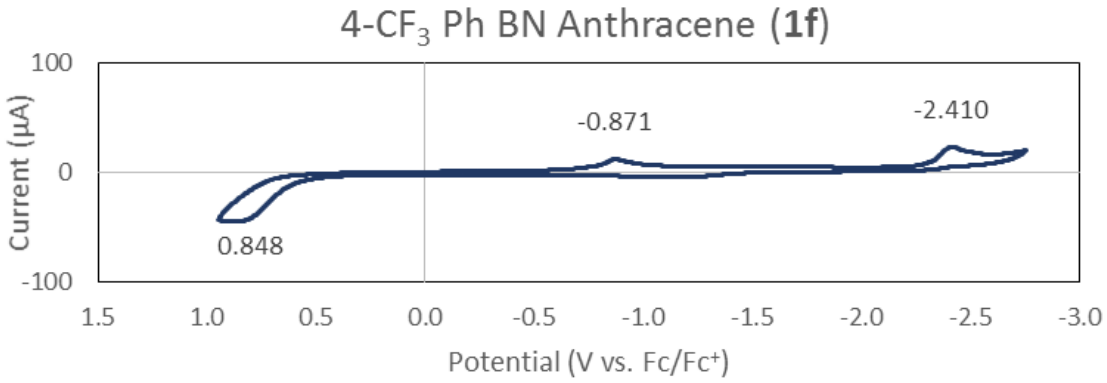




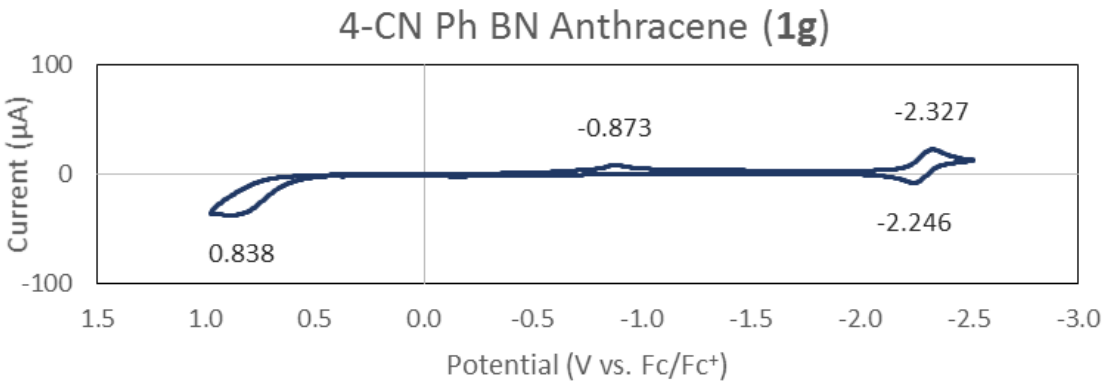
Cyclic Voltammograms of Products, con't

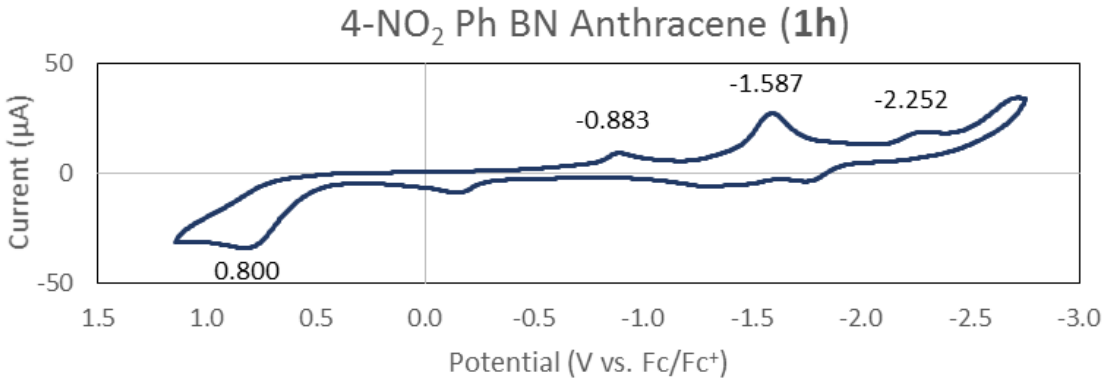


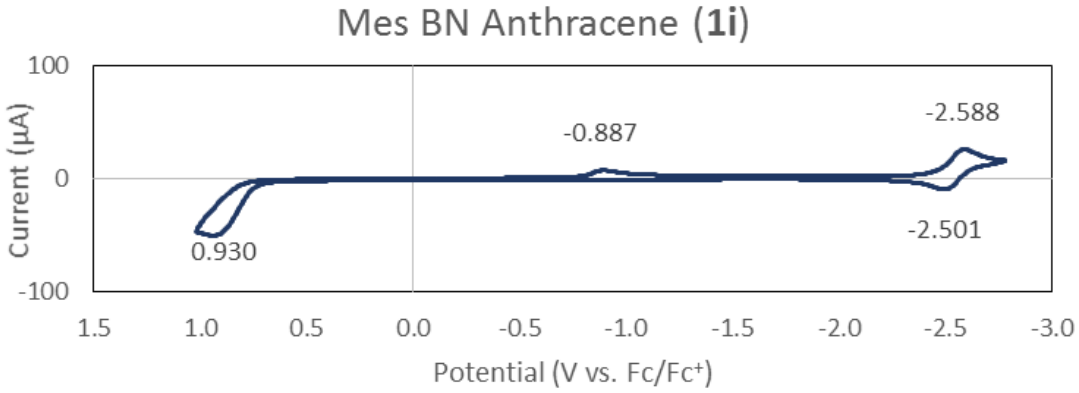




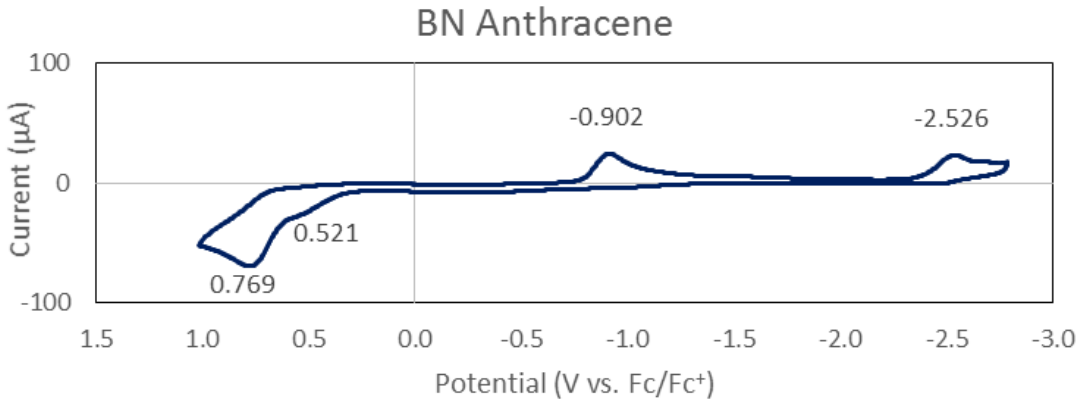
Cyclic Voltammograms of Products, con't

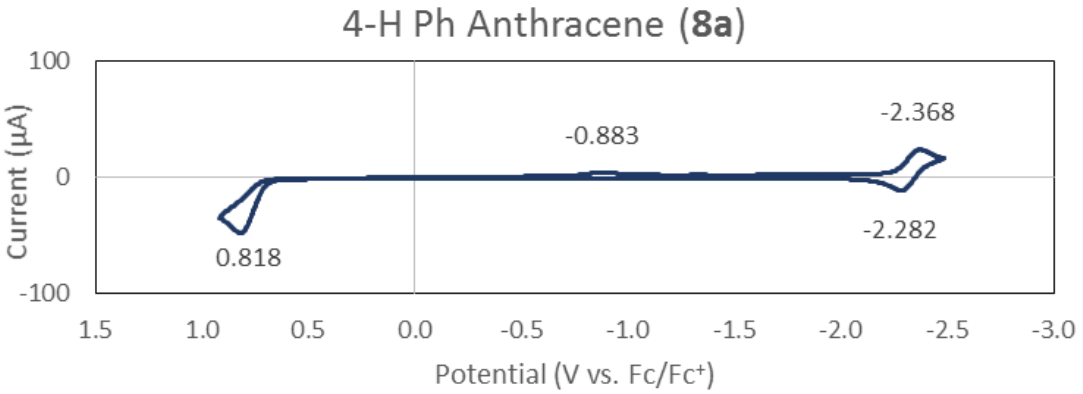


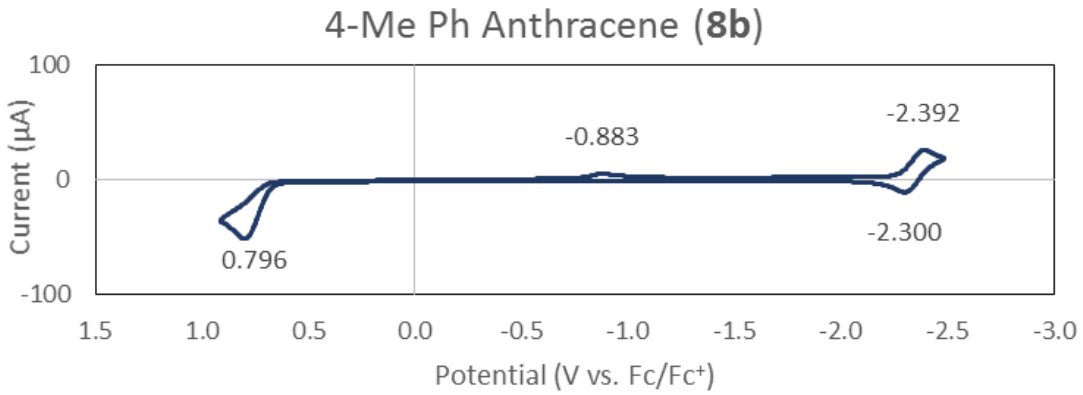




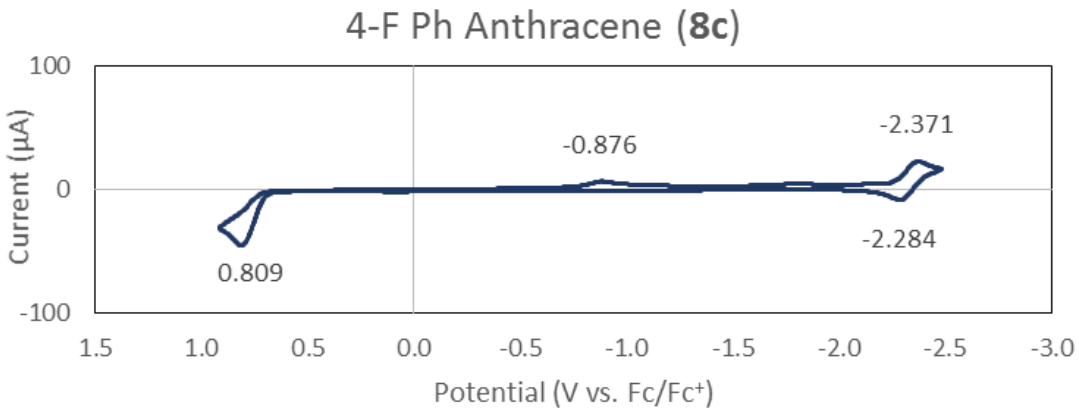
Cyclic Voltammograms of Products, con't

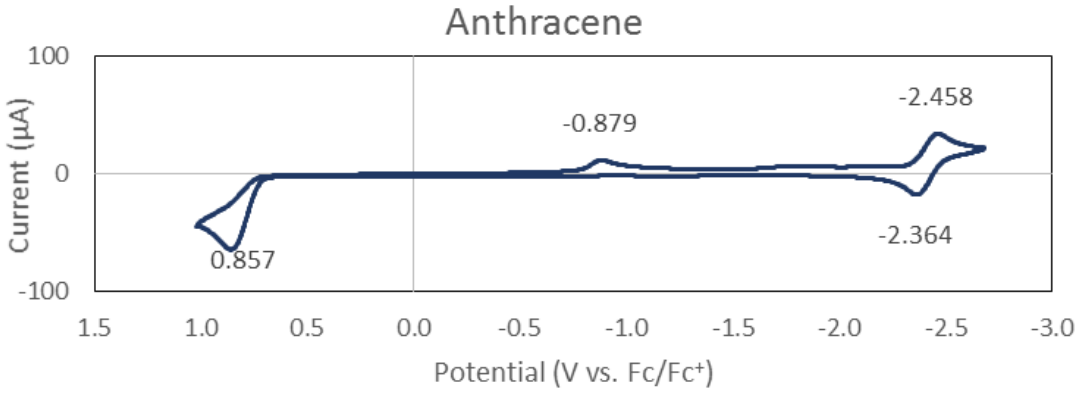






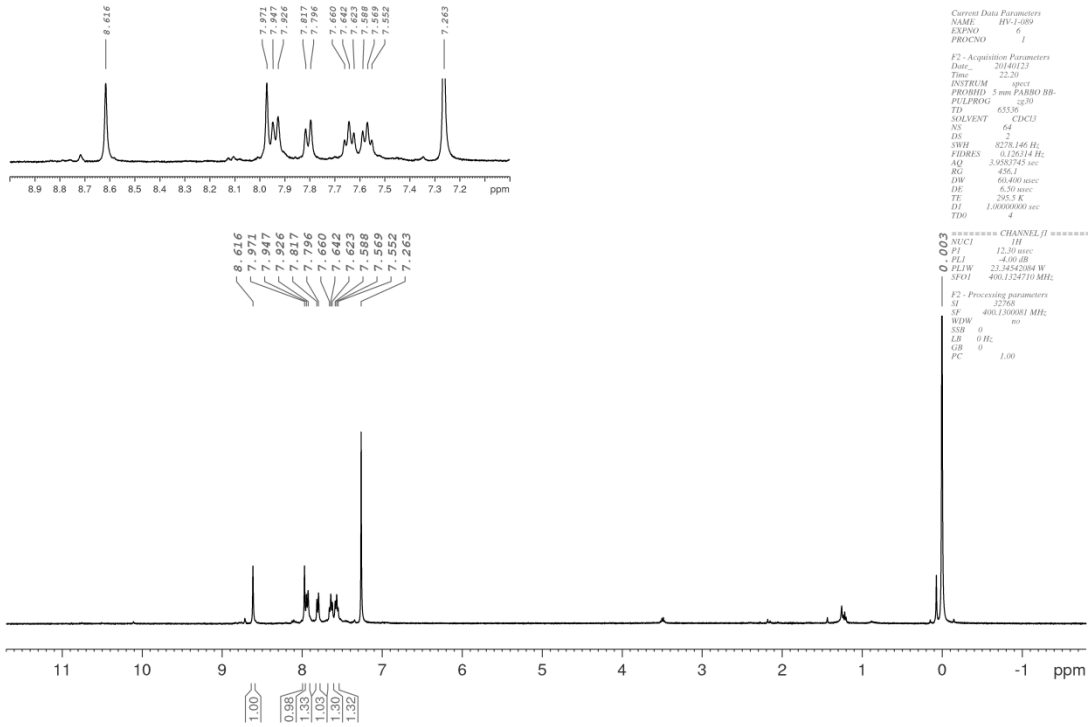
Cyclic Voltammograms of Products, con't



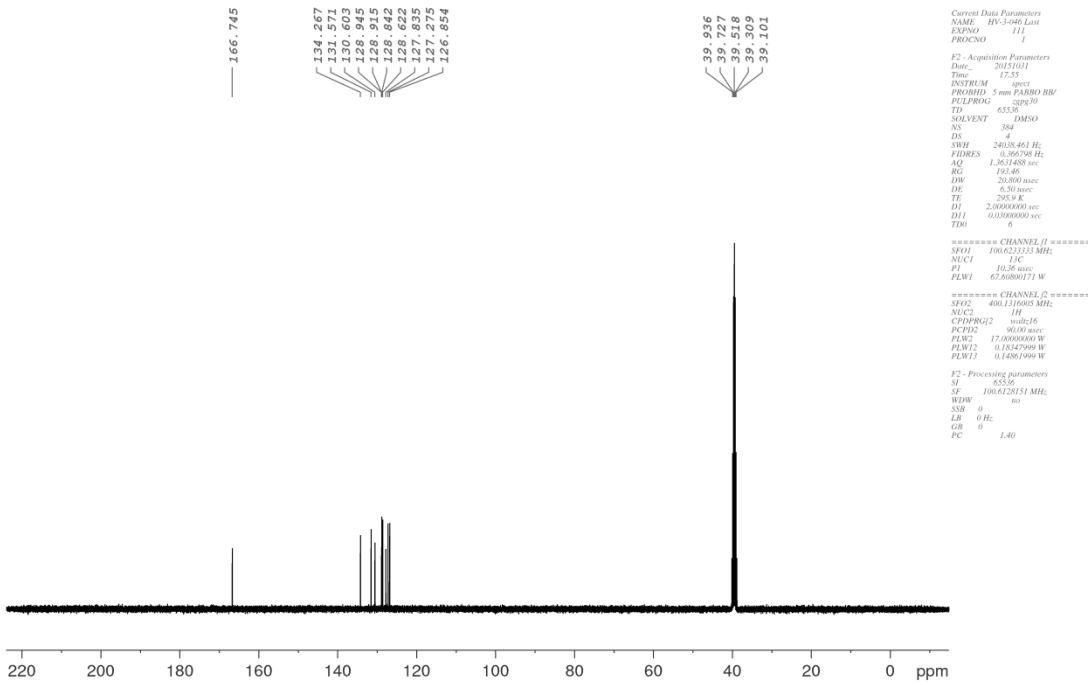


V. NMR Spectra

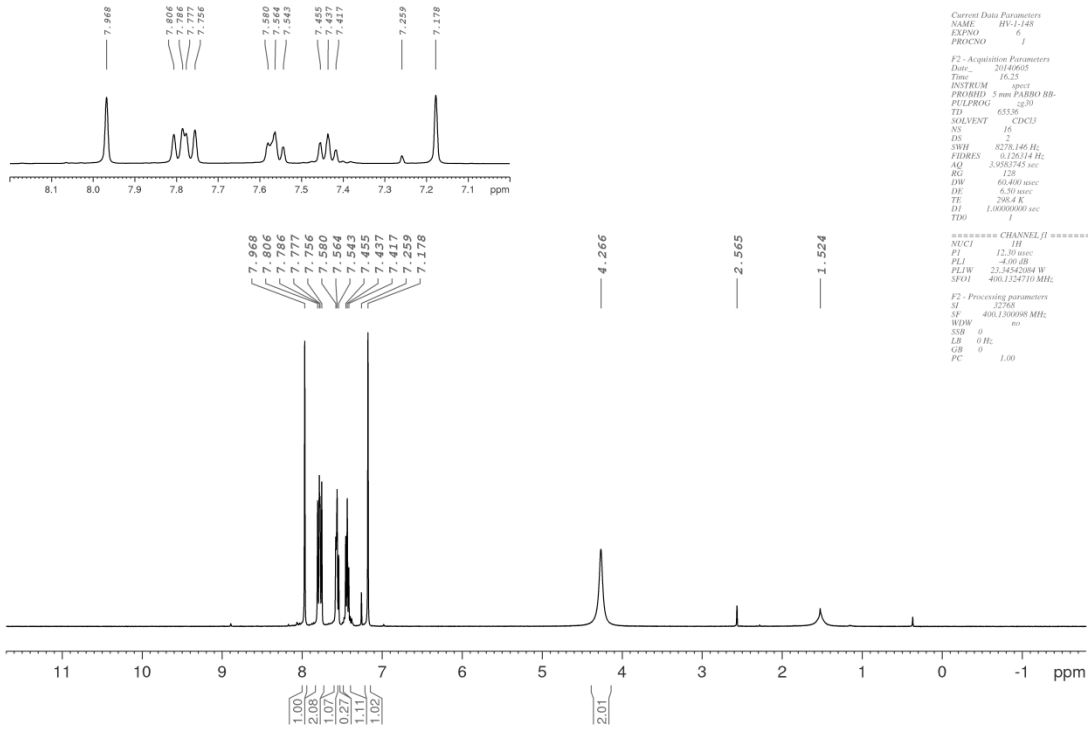
^{1}H NMR ($CDCl_3$, 400 MHz) 3-Chloro-2-Naphthoic Acid (S1)



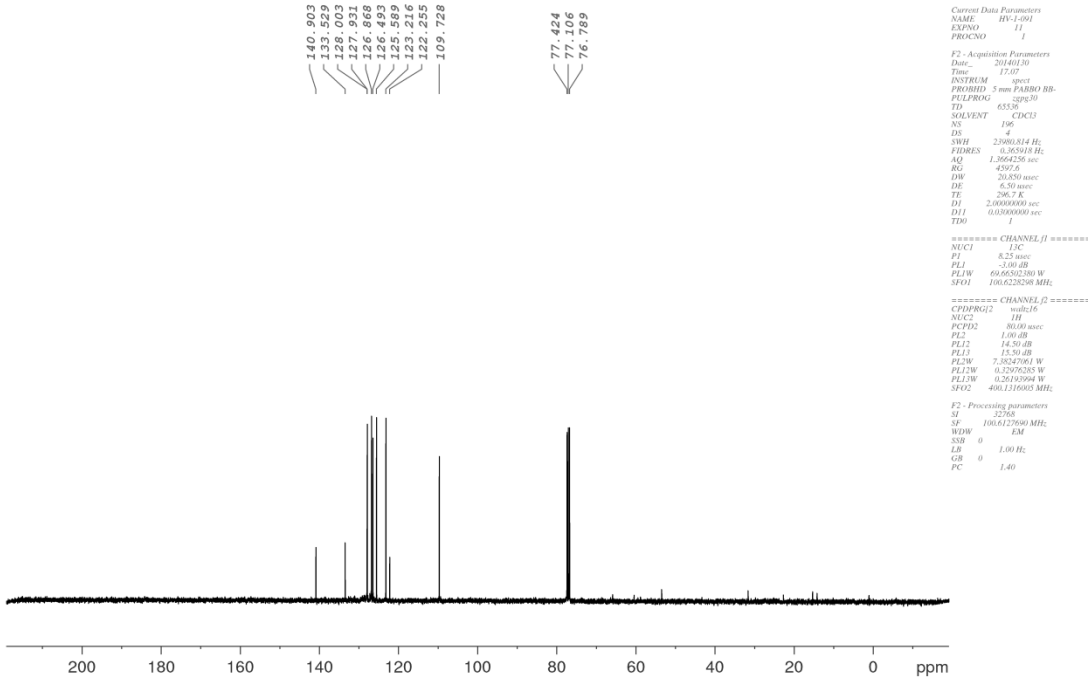
^{13}C NMR (DMSO, 101 MHz) 3-Chloro-2-Naphthoic Acid (S1)



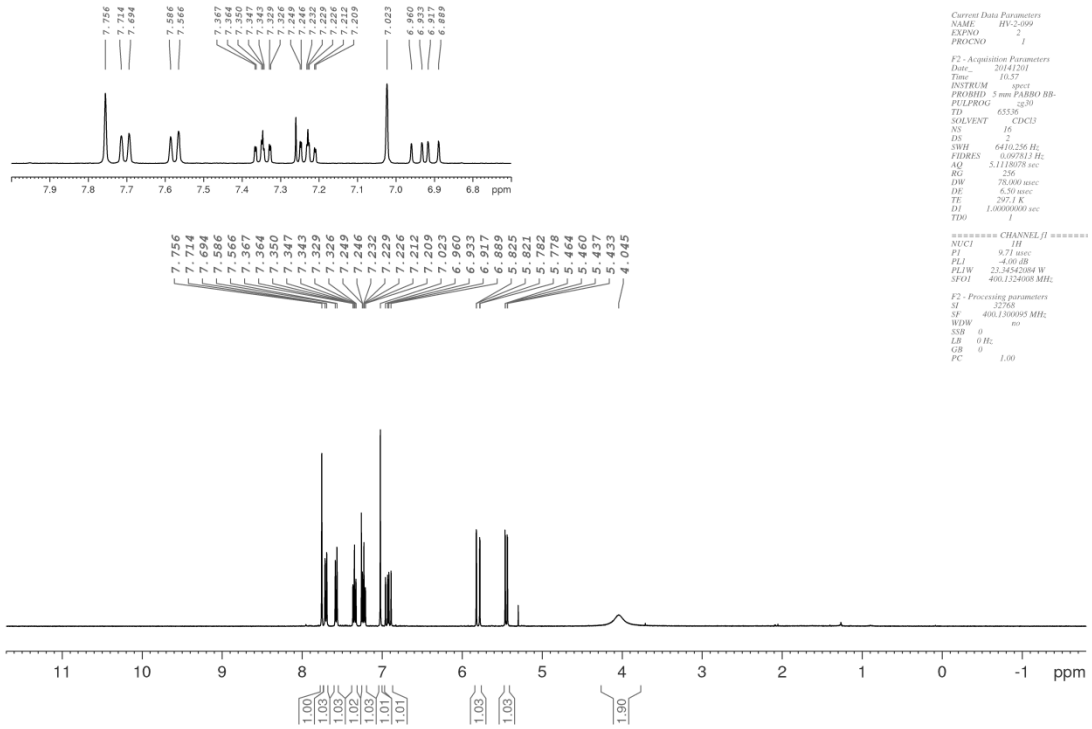
^{1}H NMR ($CDCl_3$, 400 MHz) 3-Chloronaphthalen-2-Amine (5)



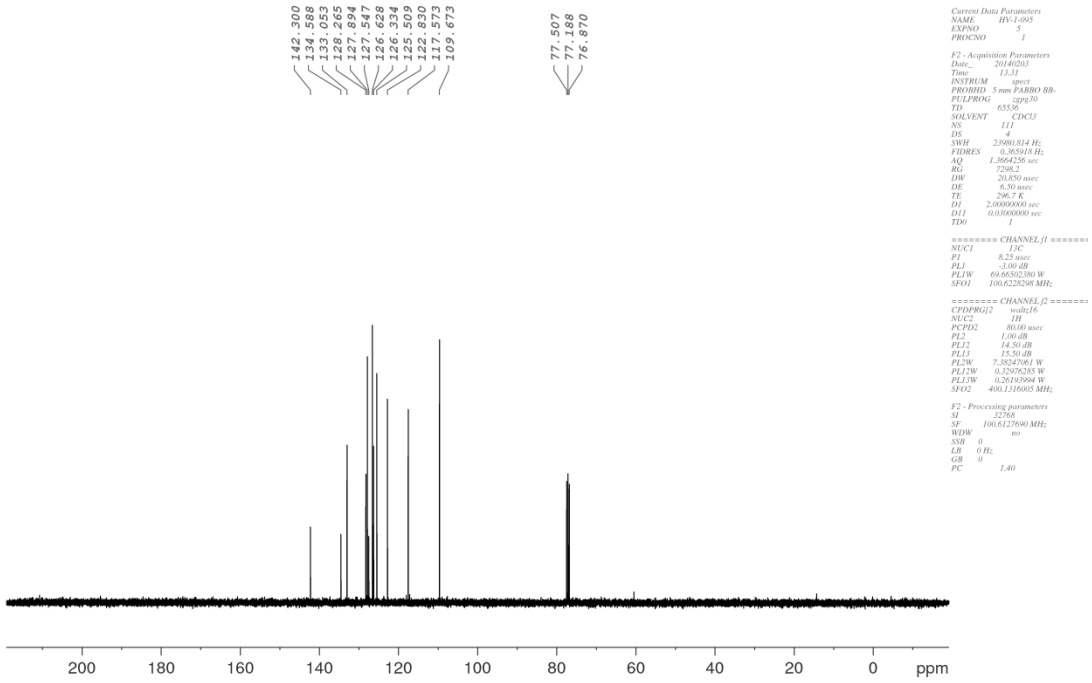
^{13}C NMR ($CDCl_3$, 101 MHz) 3-Chloronaphthalen-2-Amine (5)



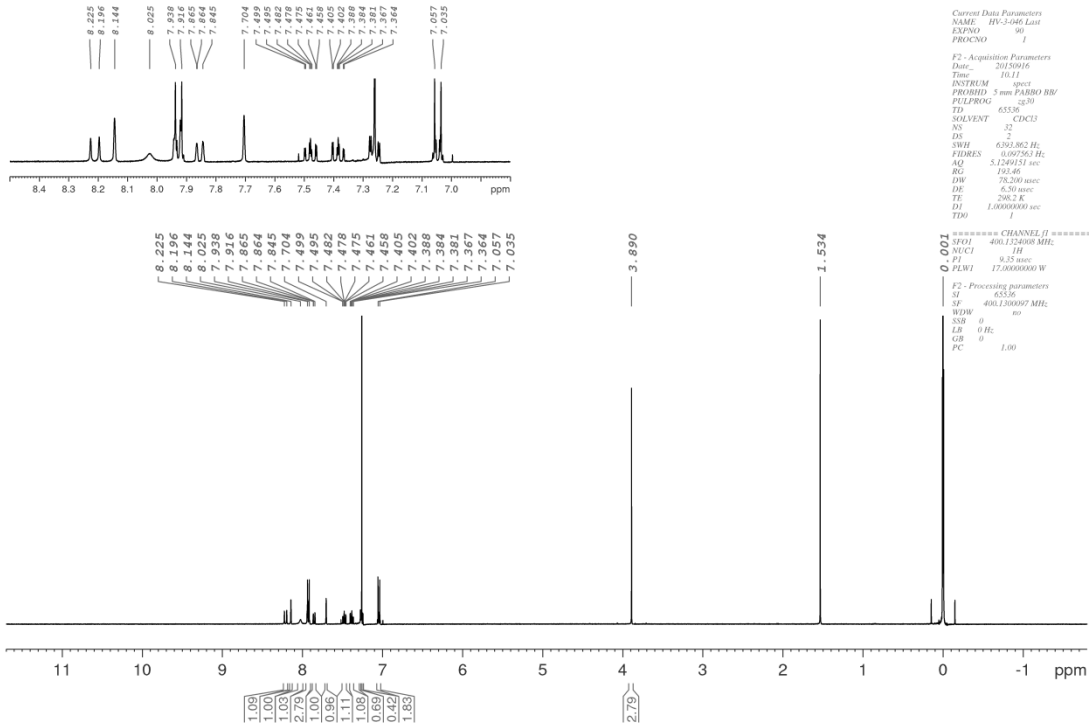
^{1}H NMR ($CDCl_3$, 400 MHz) 3-Vinylnaphthalen-2-Amine (4)



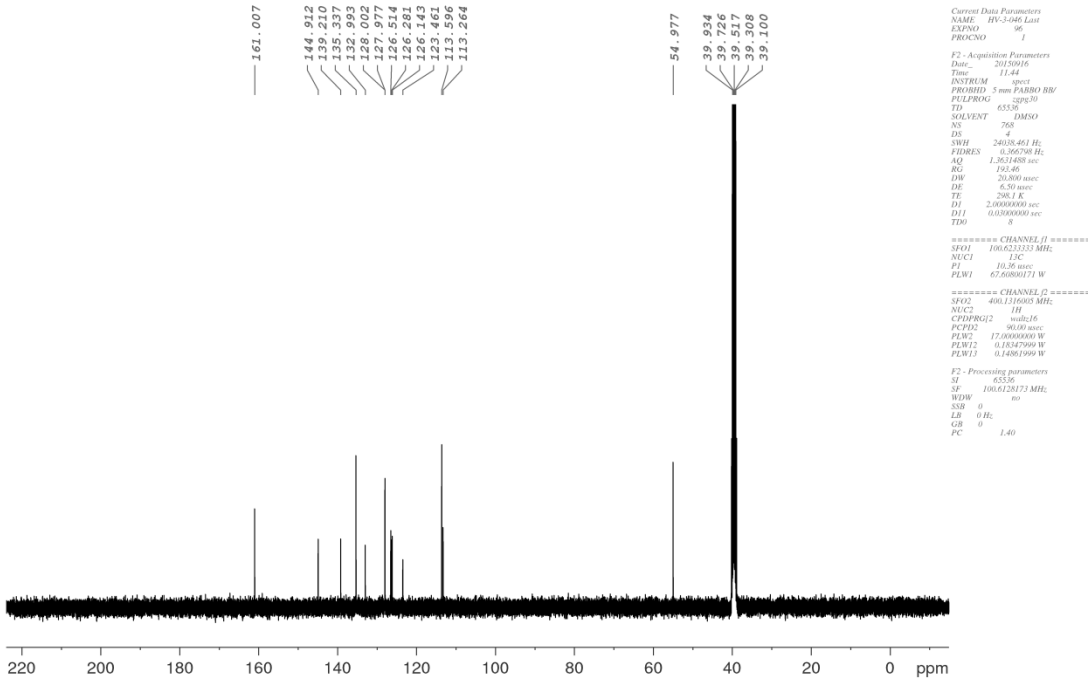
^{13}C NMR ($CDCl_3$, 101 MHz) 3-Vinylnaphthalen-2-Amine (4)



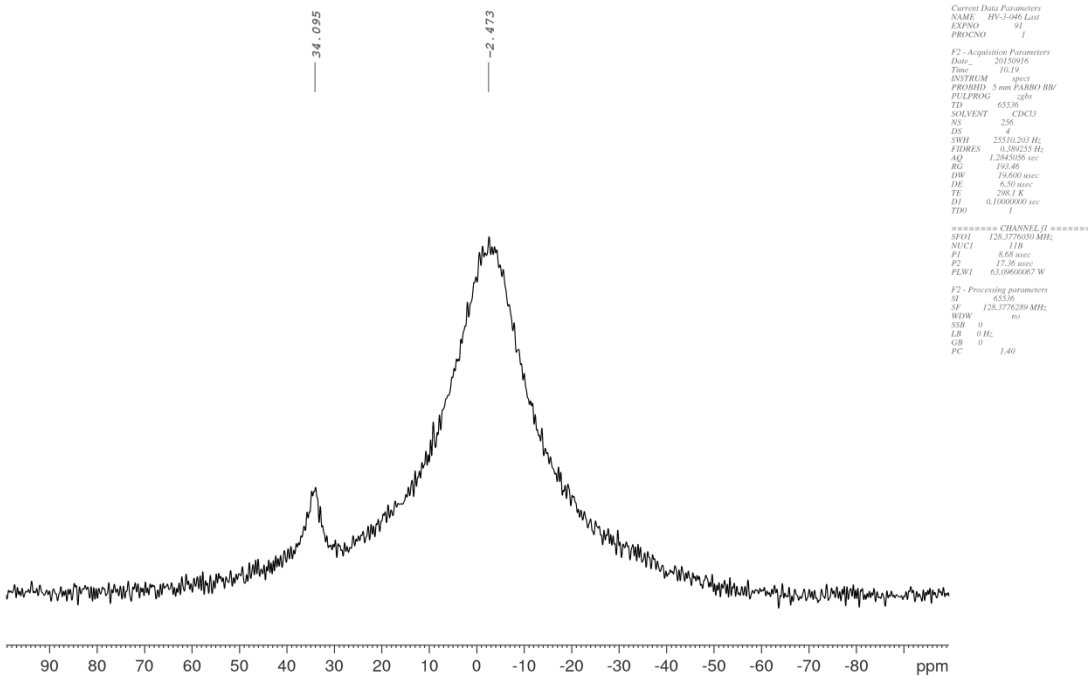
^{1}H NMR ($CDCl_3$, 400 MHz) 4-MeO Ph BN Anthracene (1a)



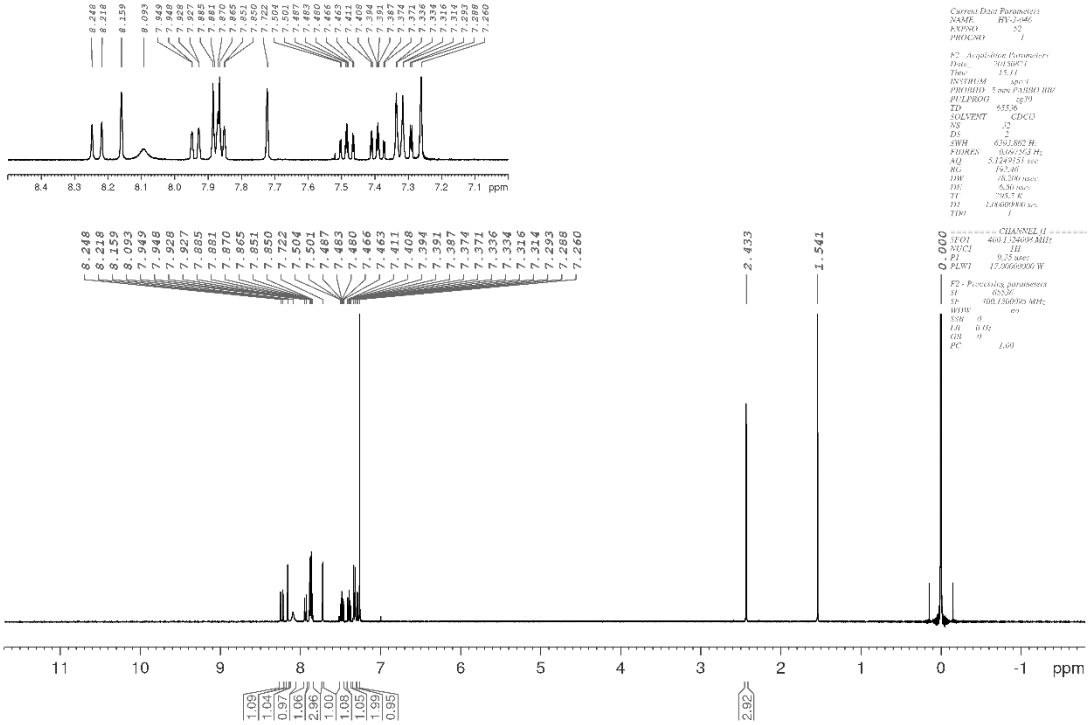
^{13}C NMR (DMSO, 101 MHz) 4-MeO Ph BN Anthracene (1a)



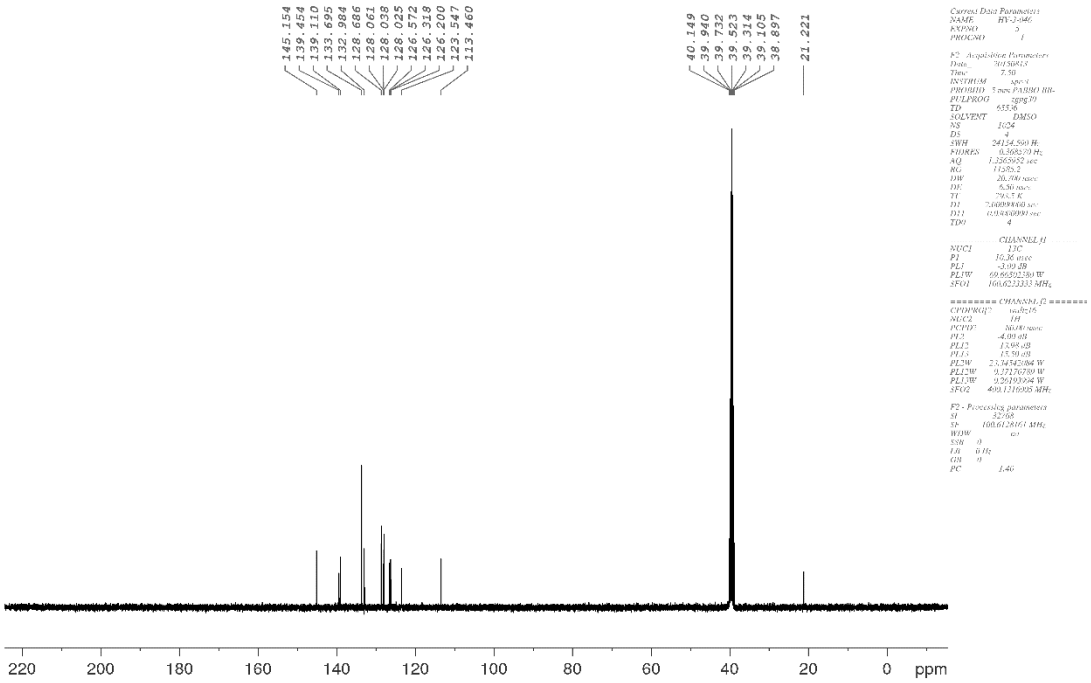
^{11}B NMR ($CDCl_3$, 128 MHz) 4-MeO Ph BN Anthracene (1a)



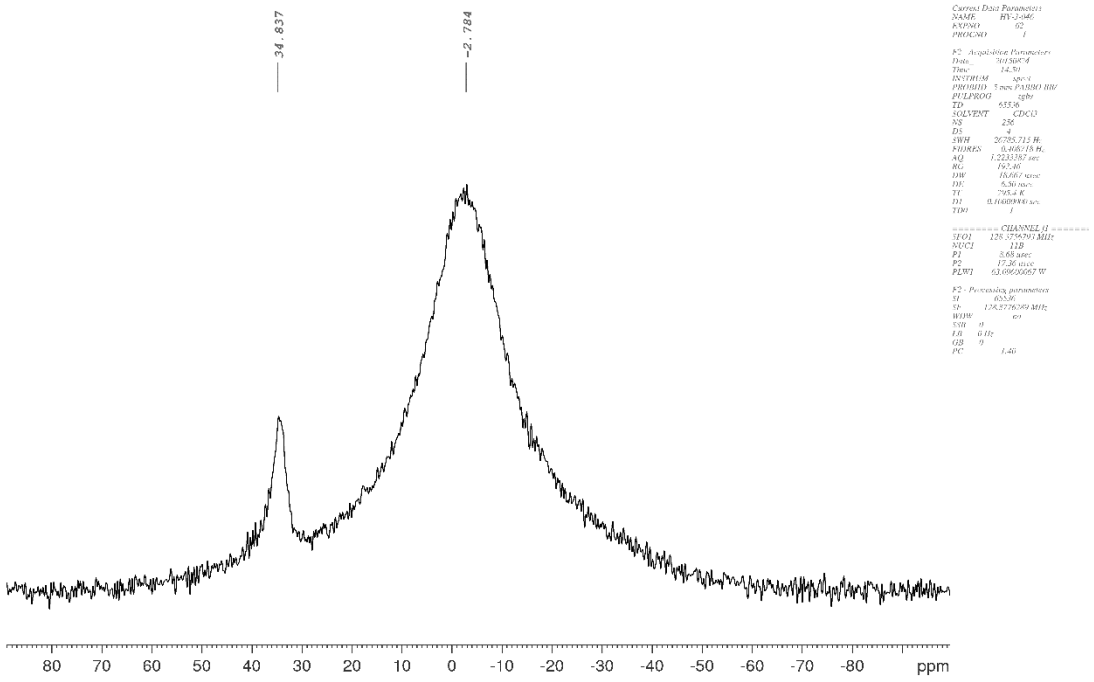
^{1}H NMR ($CDCl_3$, 400 MHz) 4-Me Ph BN Anthracene (1b)



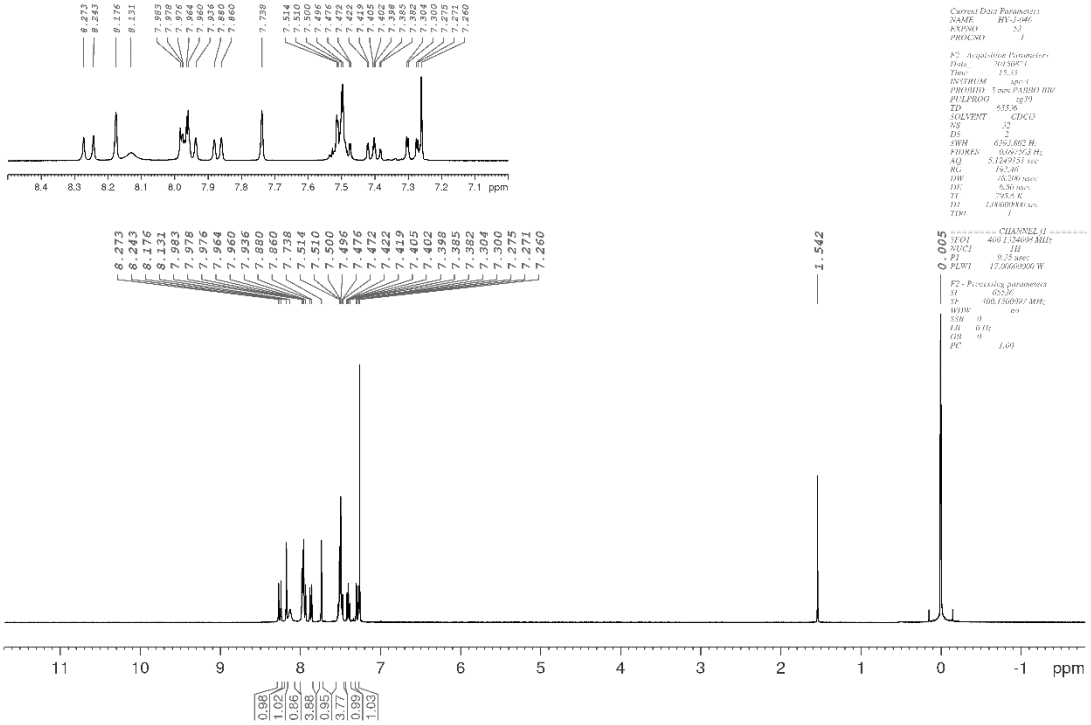
^{13}C NMR (DMSO, 101 MHz) 4-Me Ph BN Anthracene (1b)



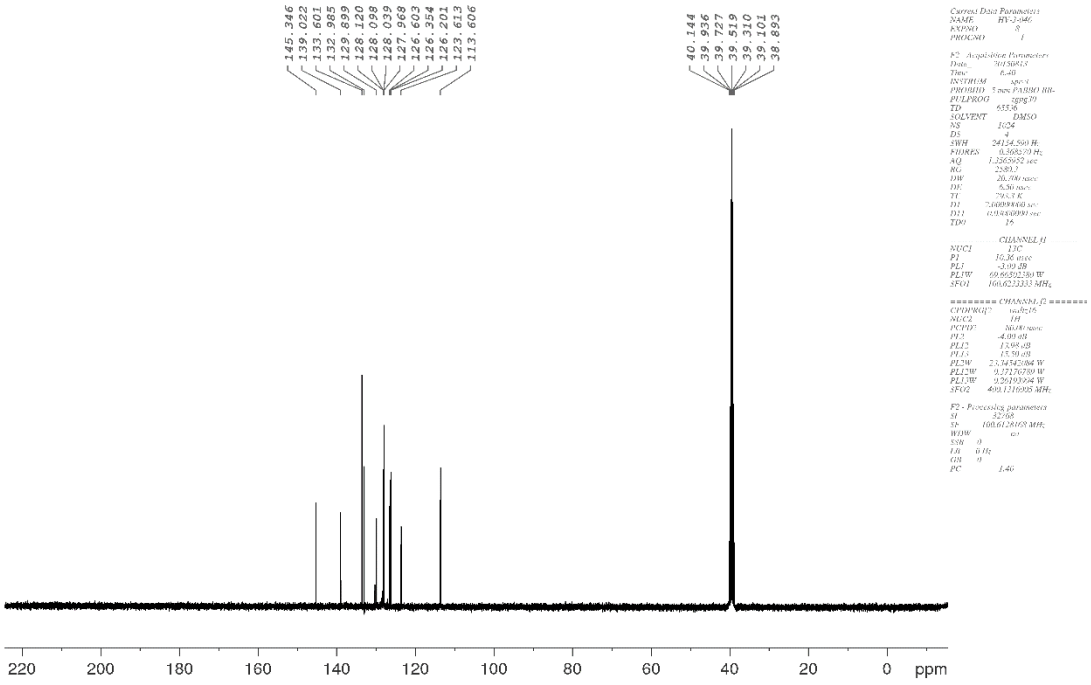
^{11}B NMR ($CDCl_3$, 128 MHz) 4-Me Ph BN Anthracene (1b)



^{1}H NMR ($CDCl_3$, 400 MHz) 4-H Ph BN Anthracene (1c)



^{13}C NMR (DMSO, 101 MHz) 4-H Ph BN Anthracene (1c)



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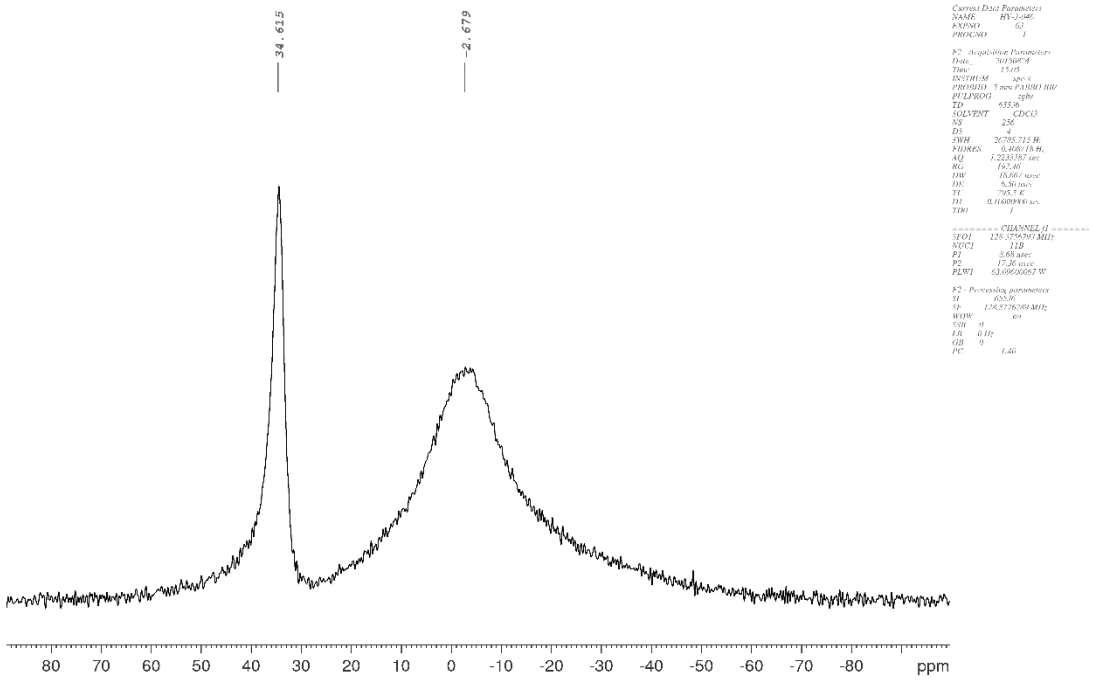
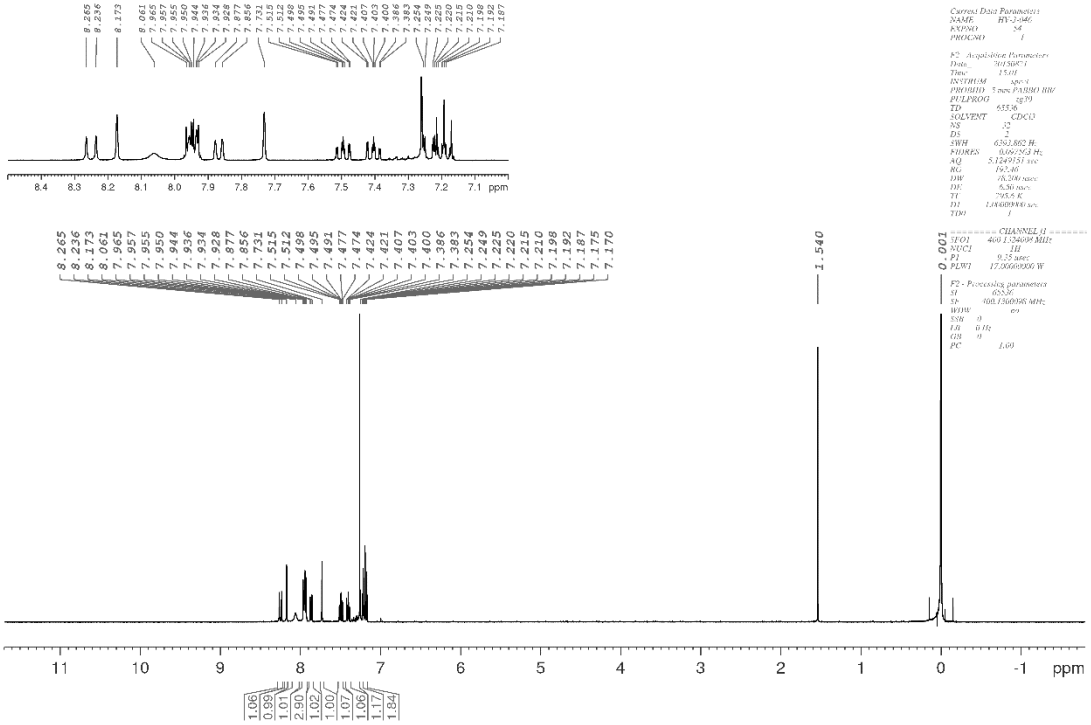
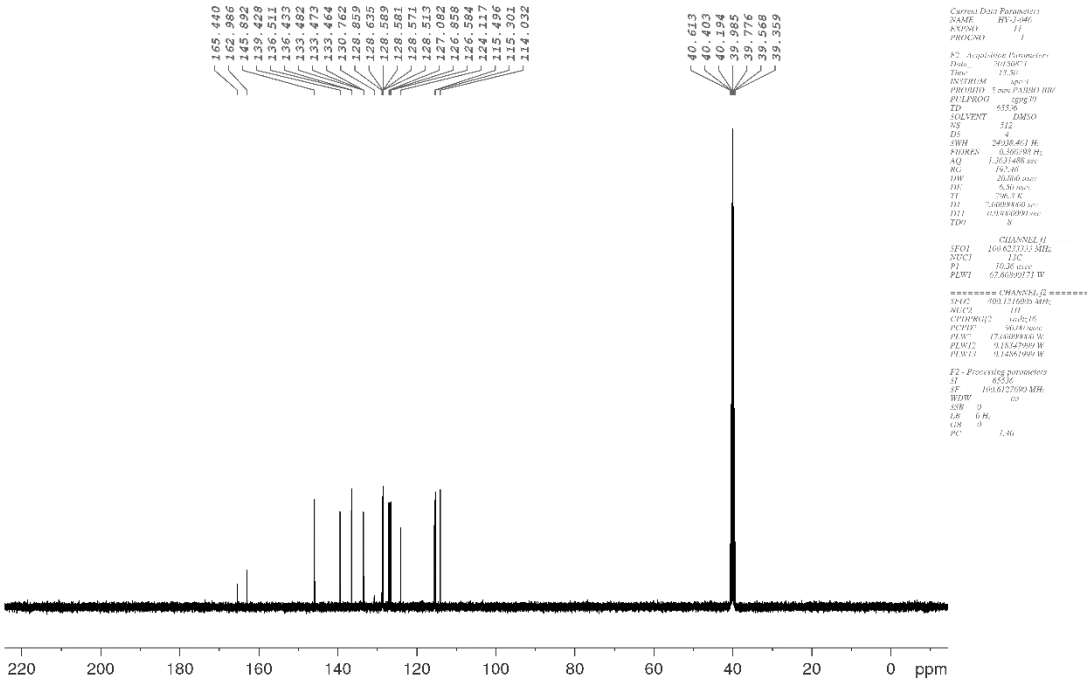


^{1}H NMR ($CDCl_3$, 400 MHz) 4-F Ph BN Anthracene (1d)



^{13}C NMR (DMSO, 101 MHz) 4-F Ph BN Anthracene (1d)



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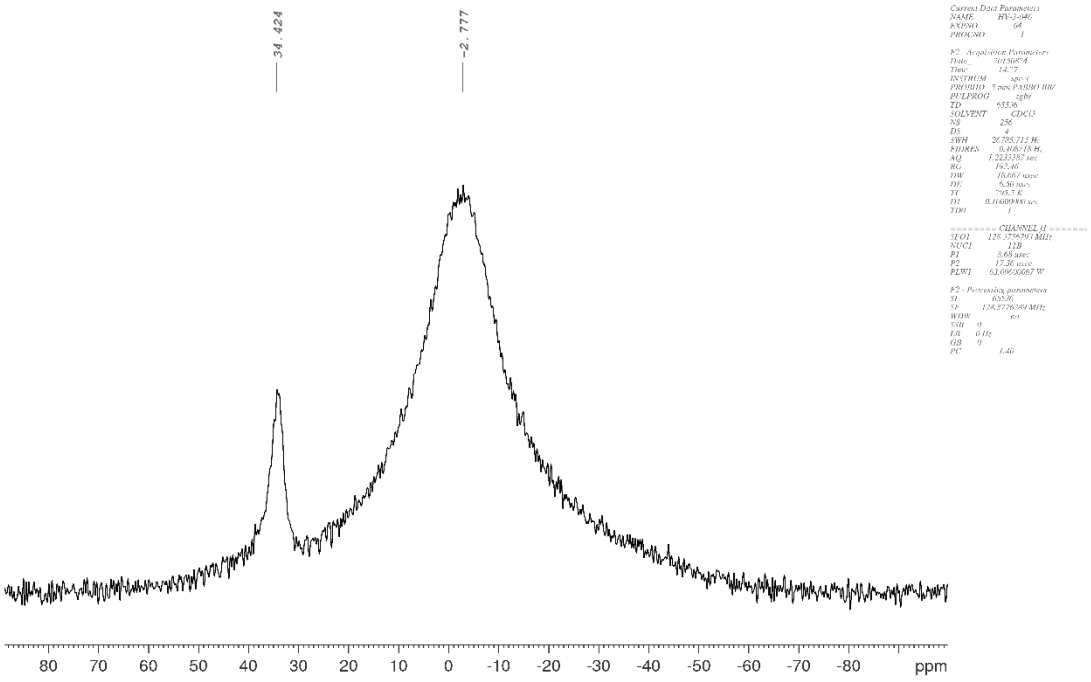
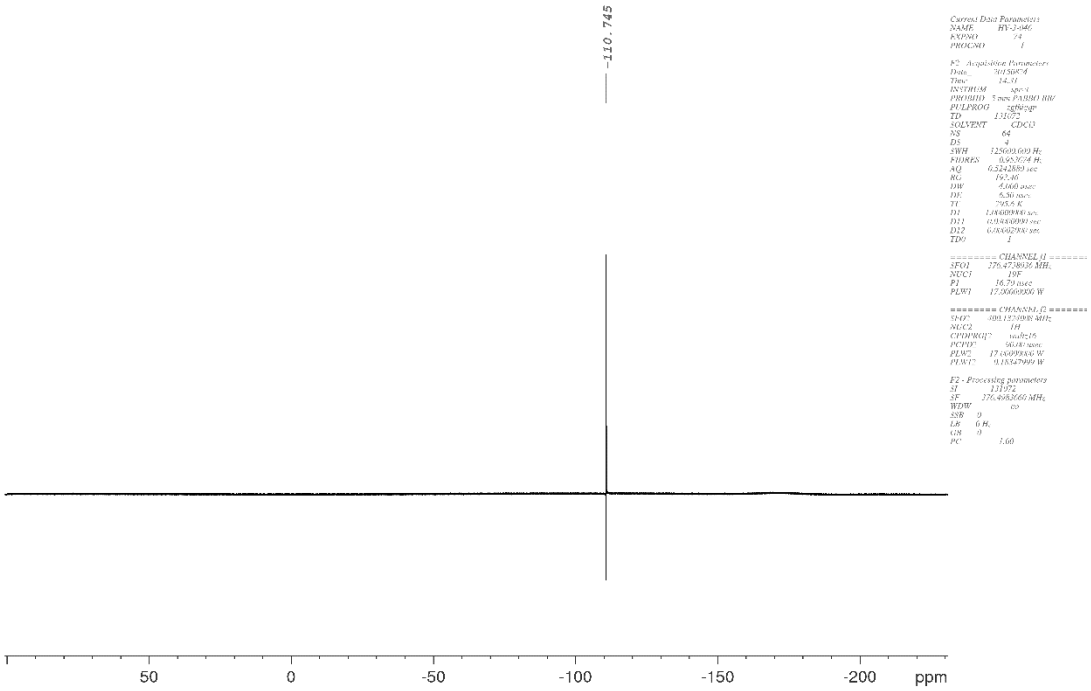
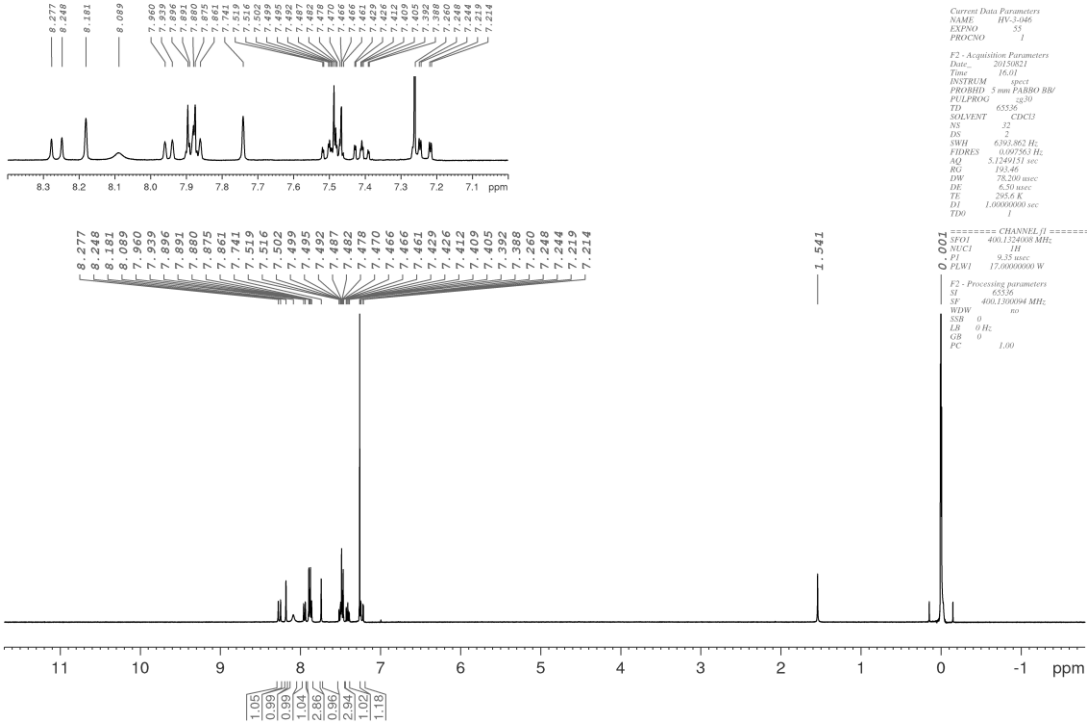


^{19}F NMR ($CDCl_3$, 376 MHz) 4-F Ph BN Anthracene (1d)



^{1}H NMR ($CDCl_3$, 400 MHz) 4-Cl Ph BN Anthracene (1e)



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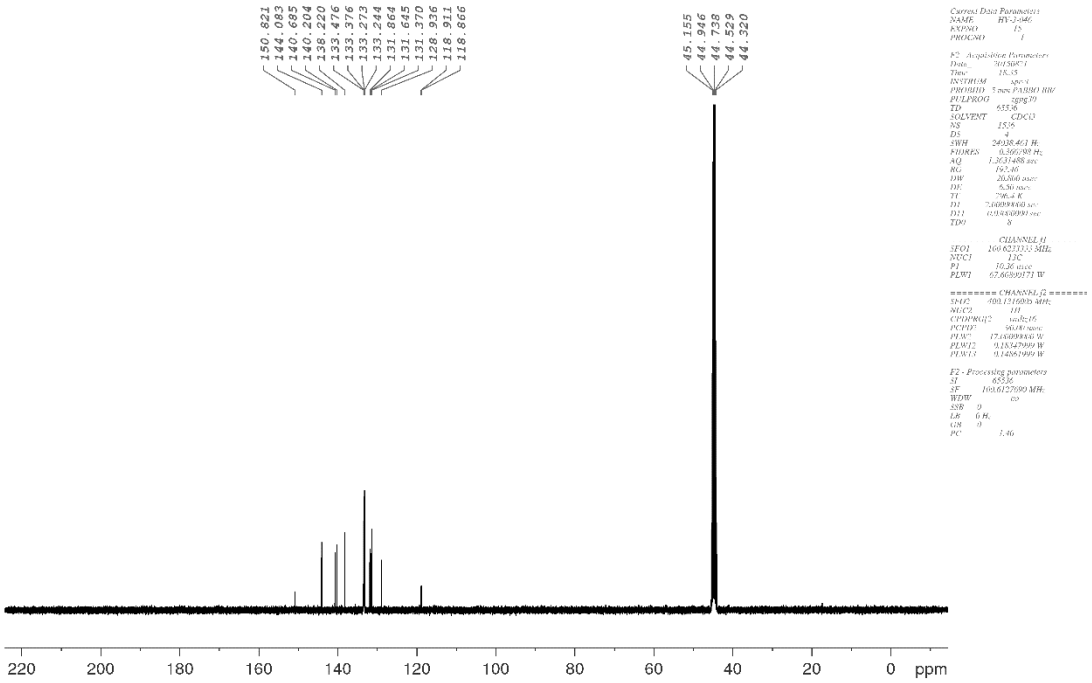
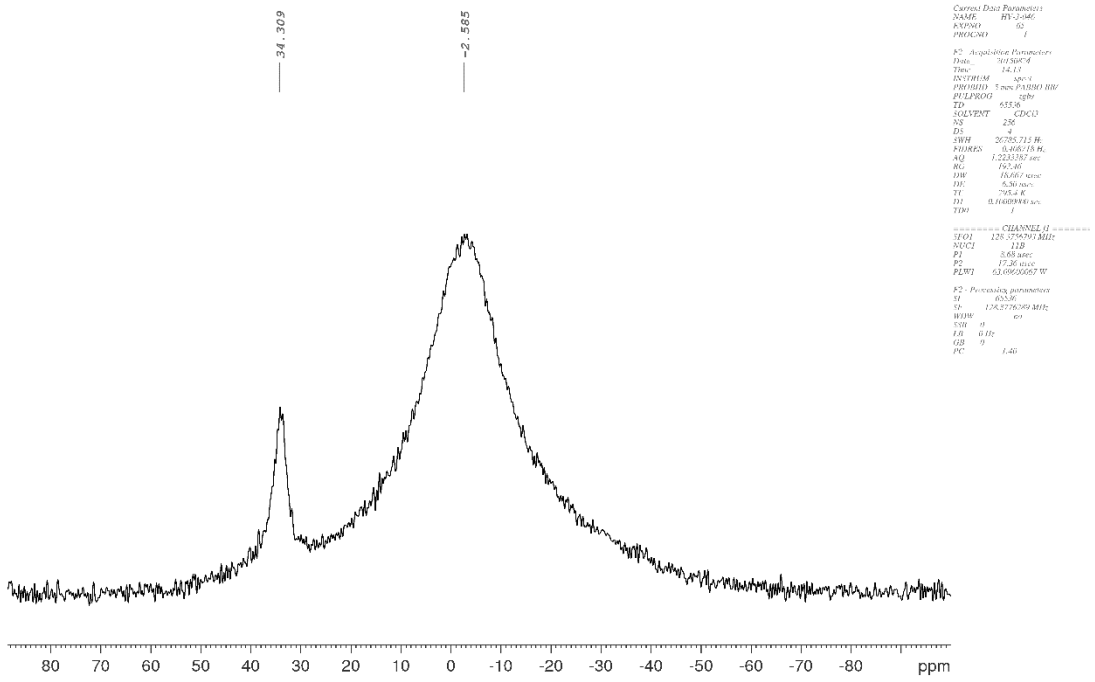
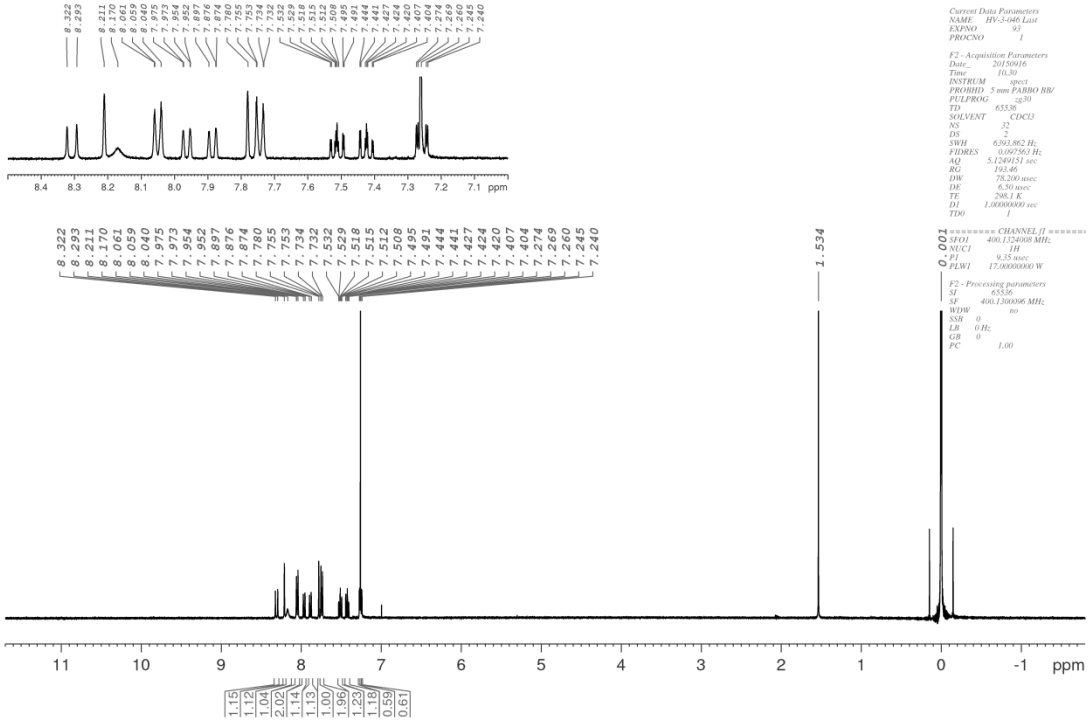


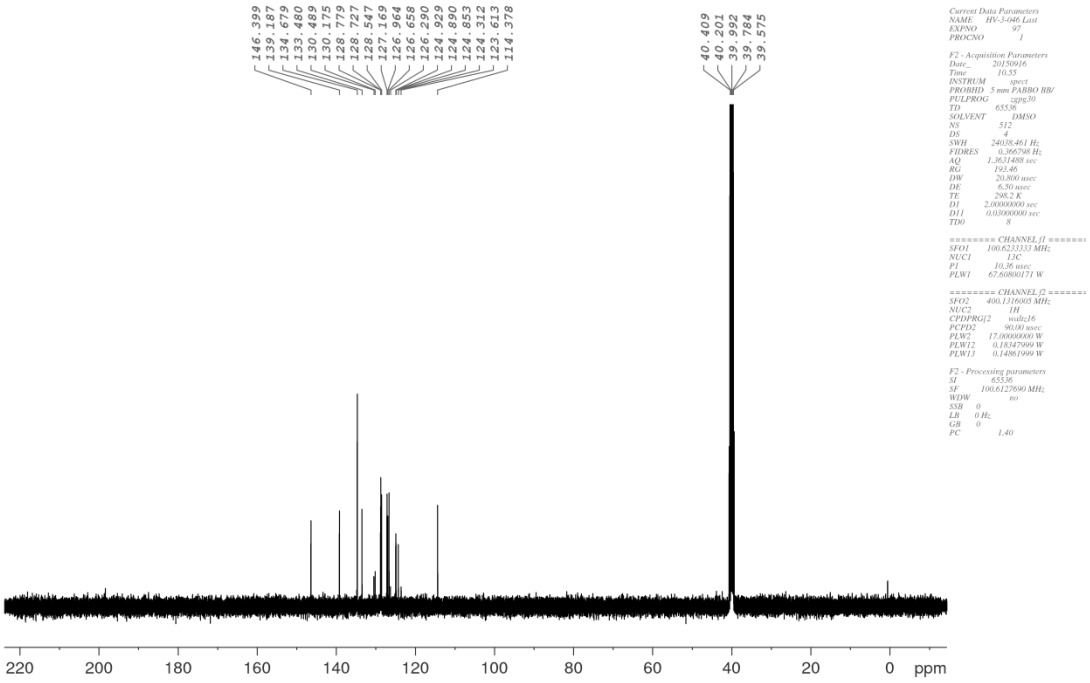
^{11}B NMR ($CDCl_3$, 128 MHz) 4-Cl Ph BN Anthracene (1e)



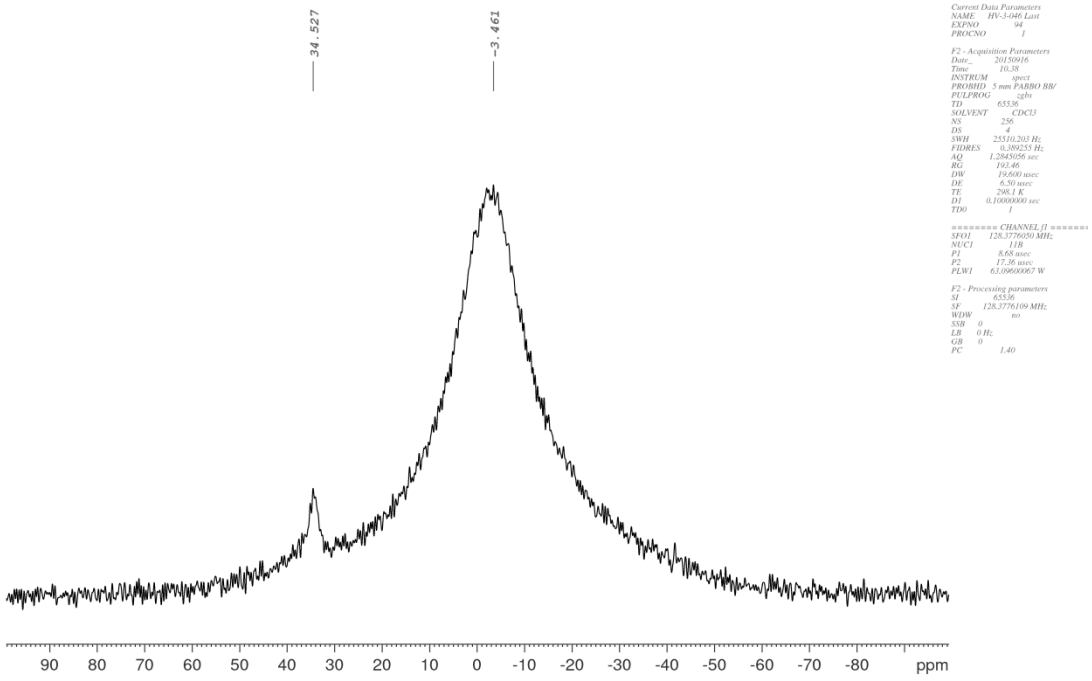
^{1}H NMR ($CDCl_3$, 400 MHz) 4-CF_3 Ph BN Anthracene (1f)



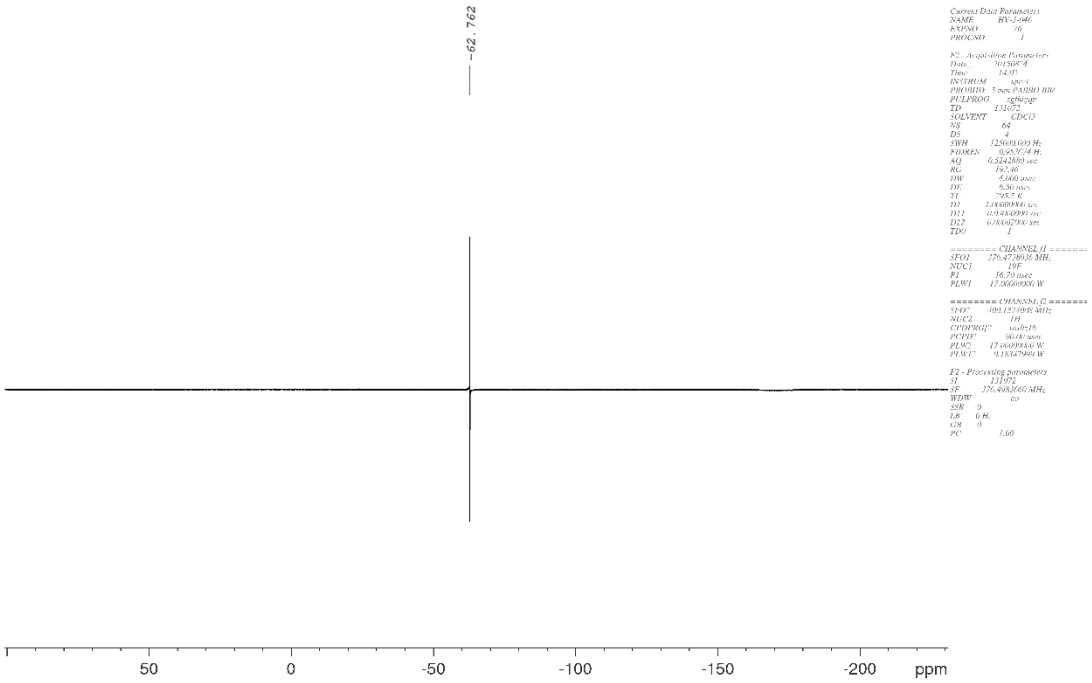
^{13}C NMR (DMSO, 101 MHz) 4-CF_3 Ph BN Anthracene (1f)



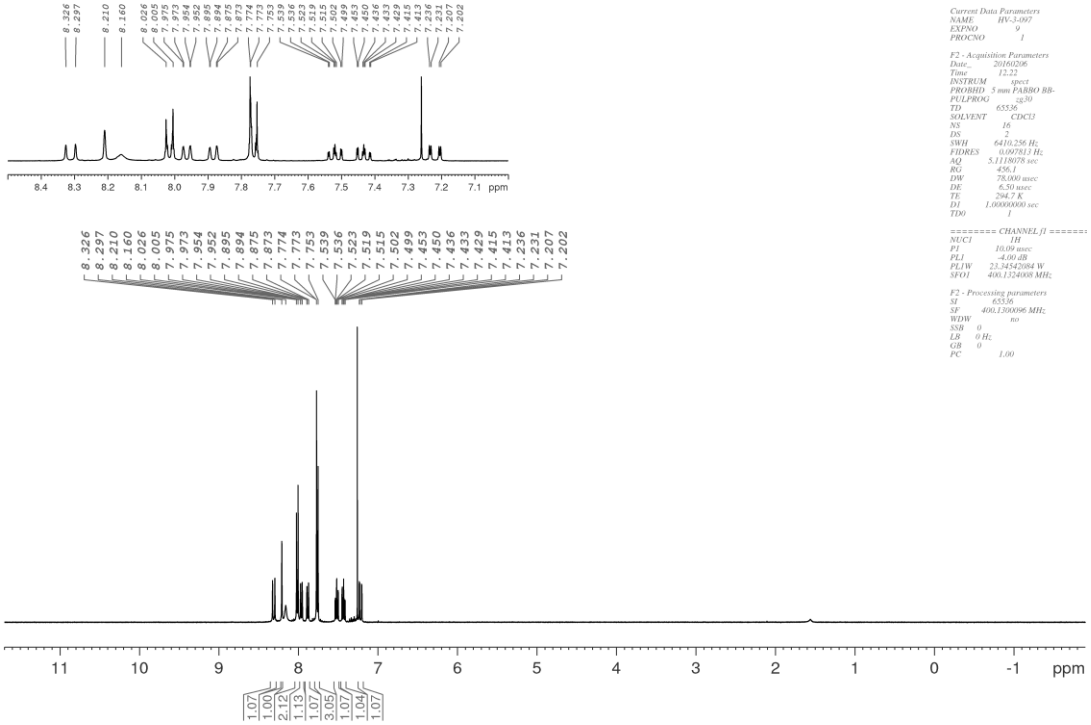
^{11}B NMR ($CDCl_3$, 128 MHz) 4-CF_3 Ph BN Anthracene (1f)



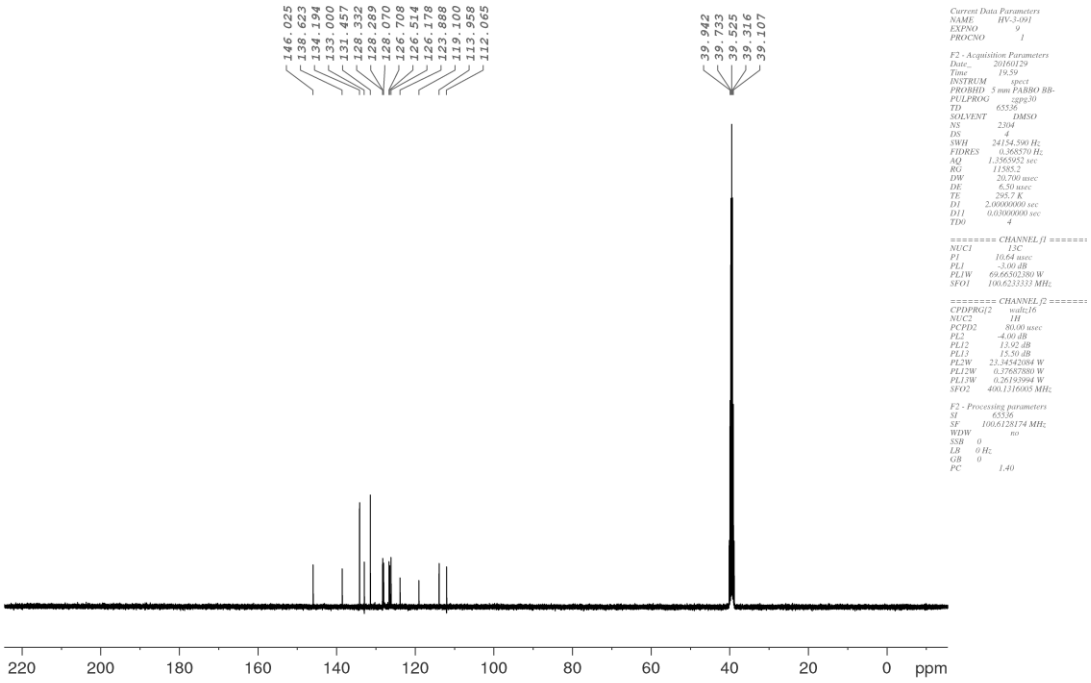
^{19}F NMR ($CDCl_3$, 376 MHz) 4-CF_3 Ph BN Anthracene (1f)



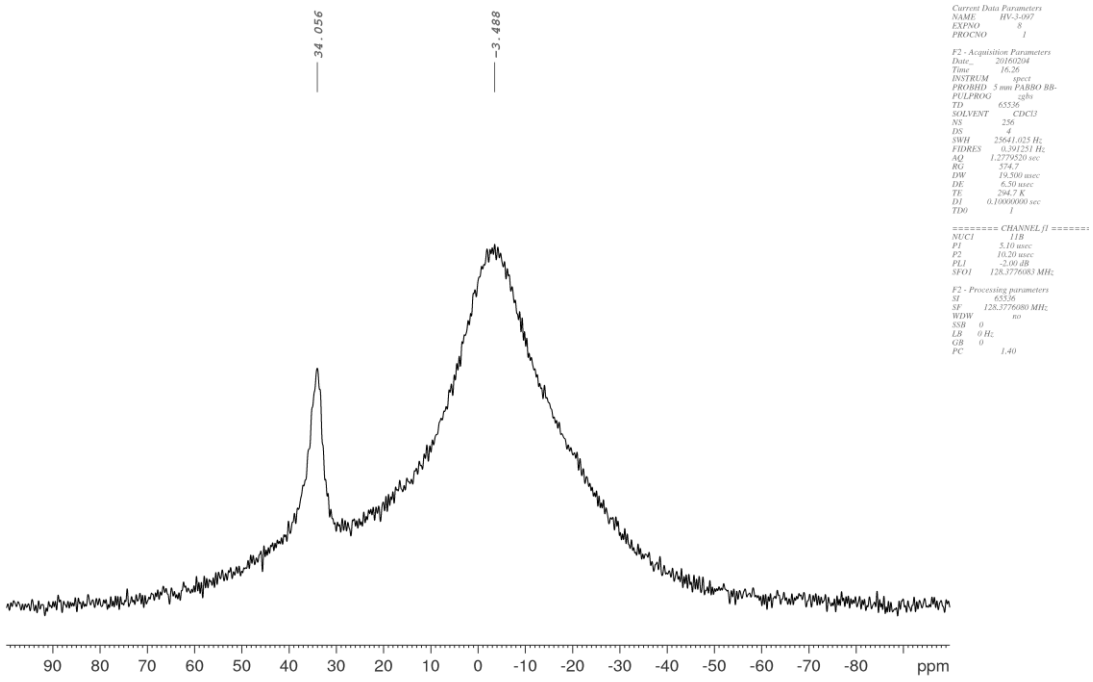
^{1}H NMR ($CDCl_3$, 400 MHz) 4-CN Ph BN Anthracene (1g)



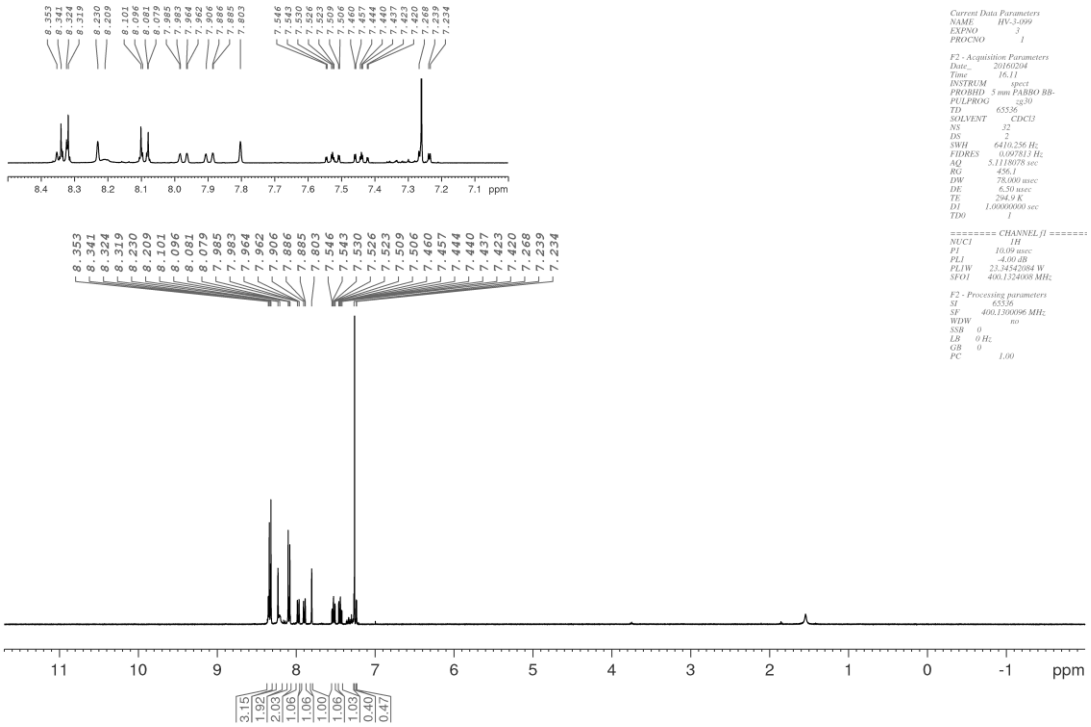
^{13}C NMR (DMSO, 101 MHz) 4-CN Ph BN Anthracene (1g)



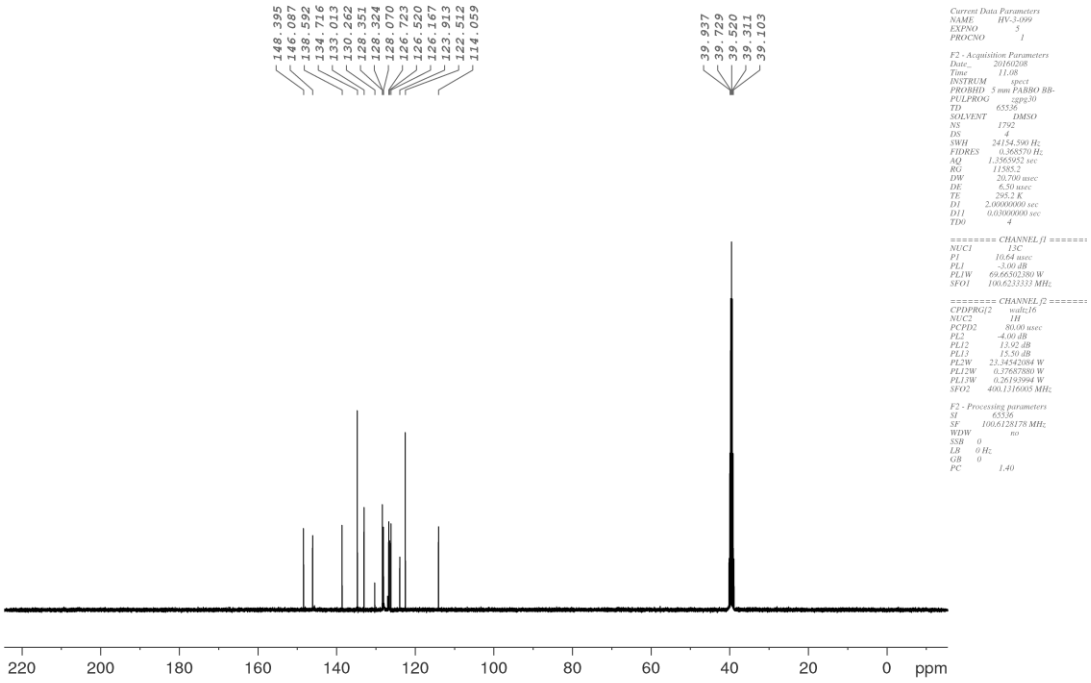
^{11}B NMR ($CDCl_3$, 128 MHz) 4-CN Ph BN Anthracene (1g)



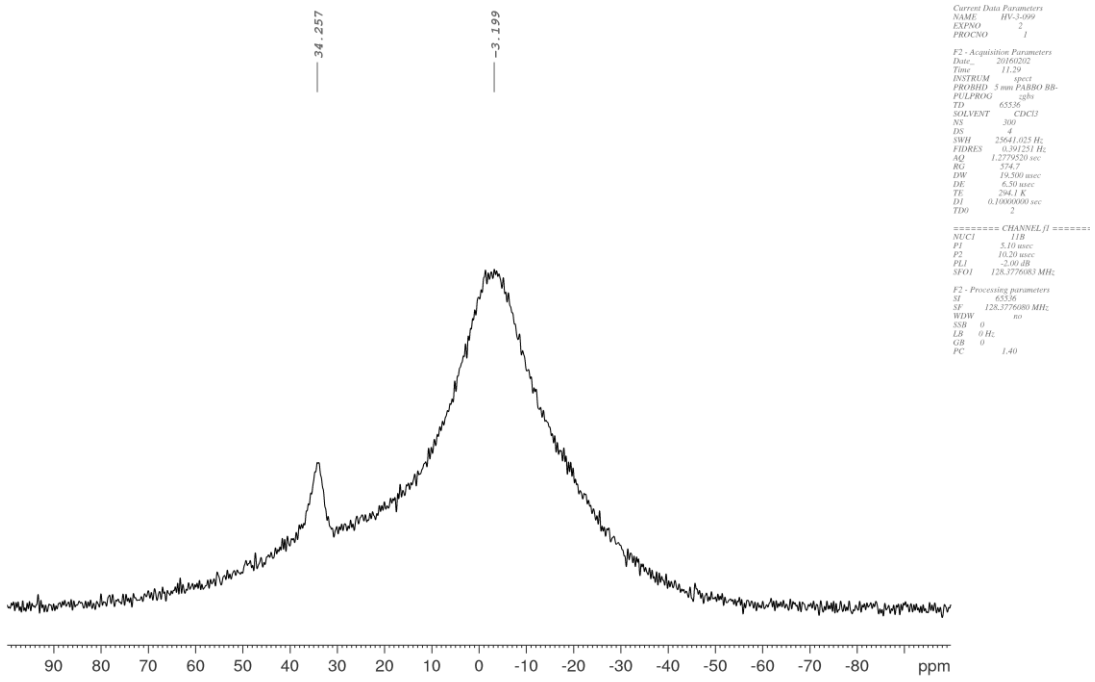
^{1}H NMR ($CDCl_3$, 400 MHz) 4-NO_2 Ph BN Anthracene (1h)



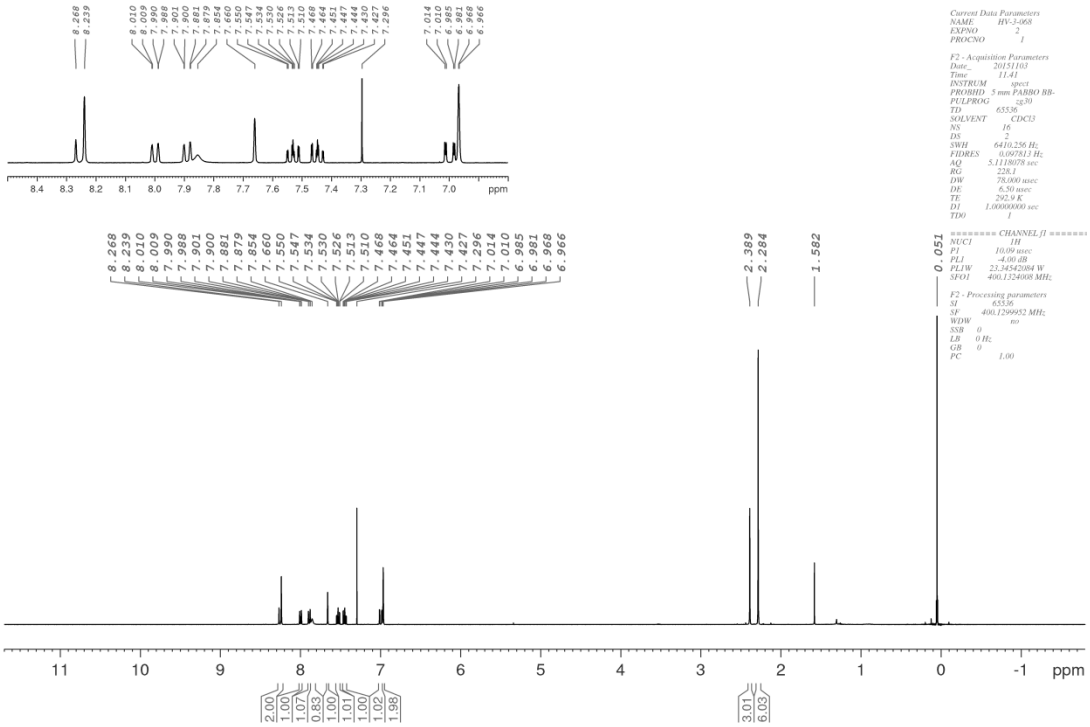
^{13}C NMR (DMSO, 101 MHz) 4-NO_2 Ph BN Anthracene (1h)



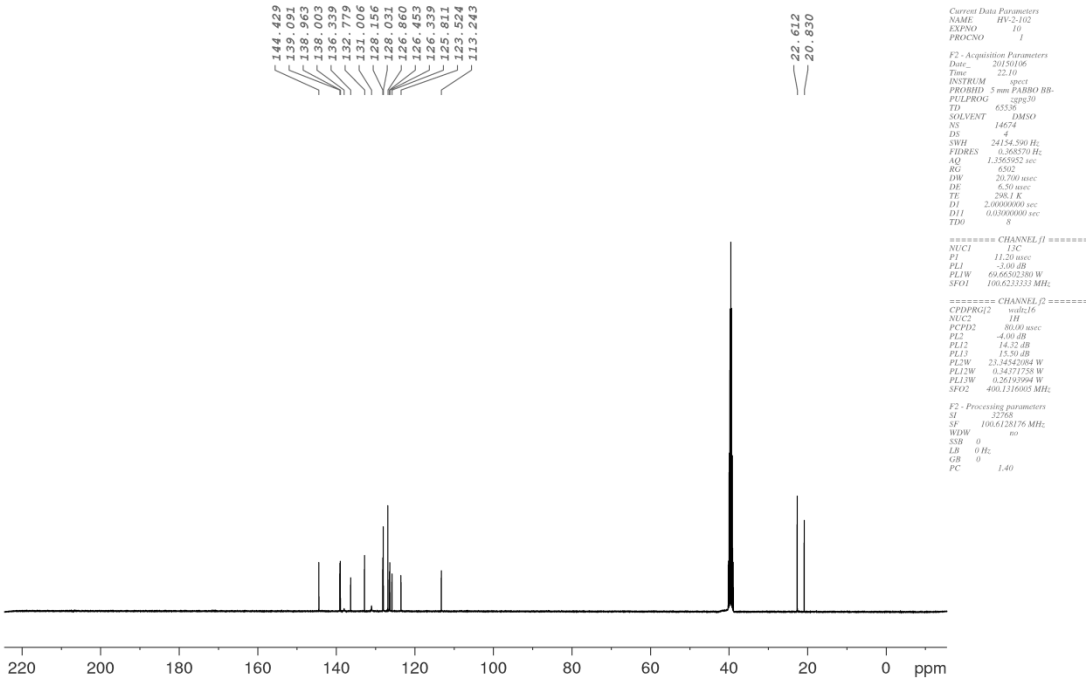
^{11}B NMR ($CDCl_3$, 128 MHz) 4-NO_2 Ph BN Anthracene (1h)



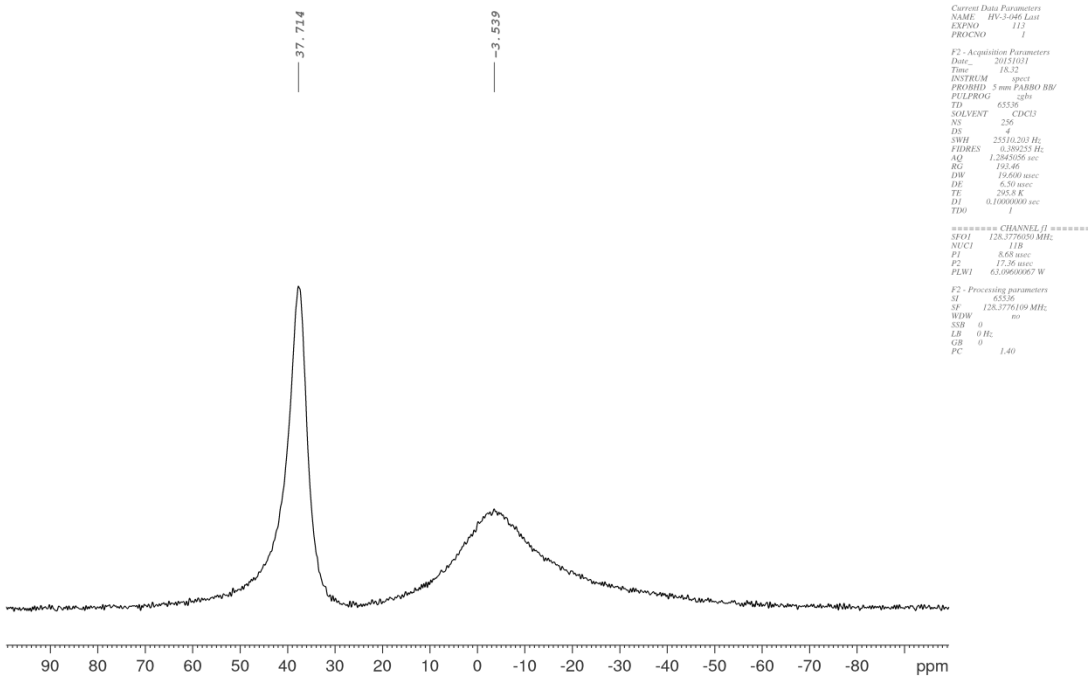
^{1}H NMR ($CDCl_3$, 400 MHz) Mes BN Anthracene (1i)



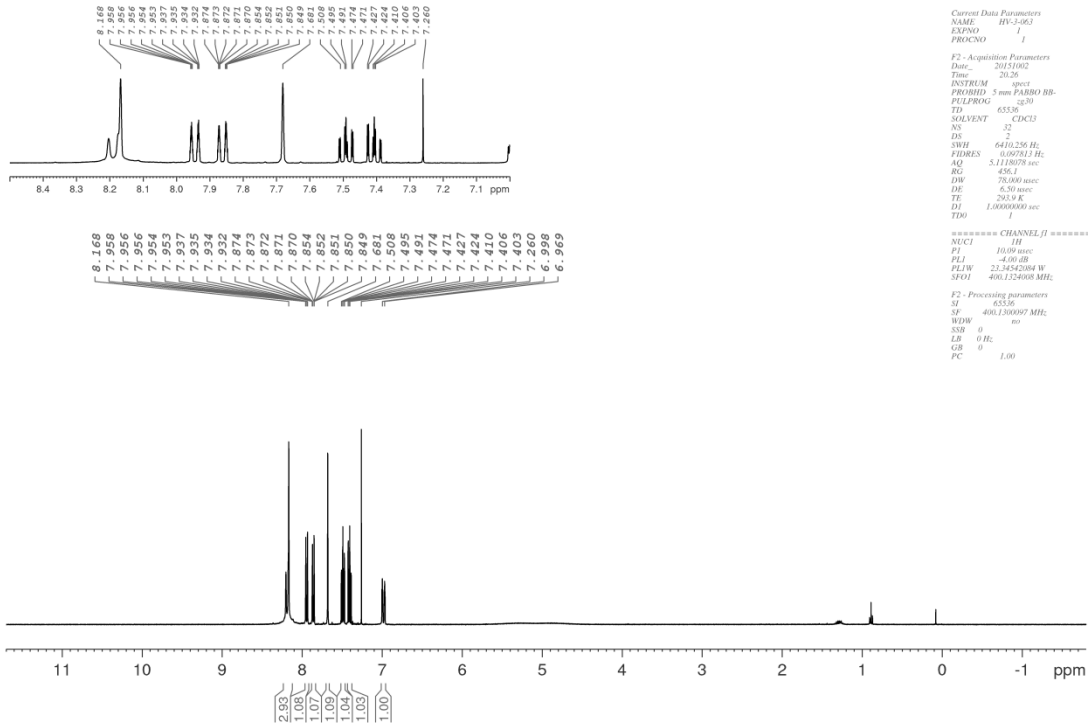
^{13}C NMR (DMSO, 101 MHz) Mes BN Anthracene (1i)



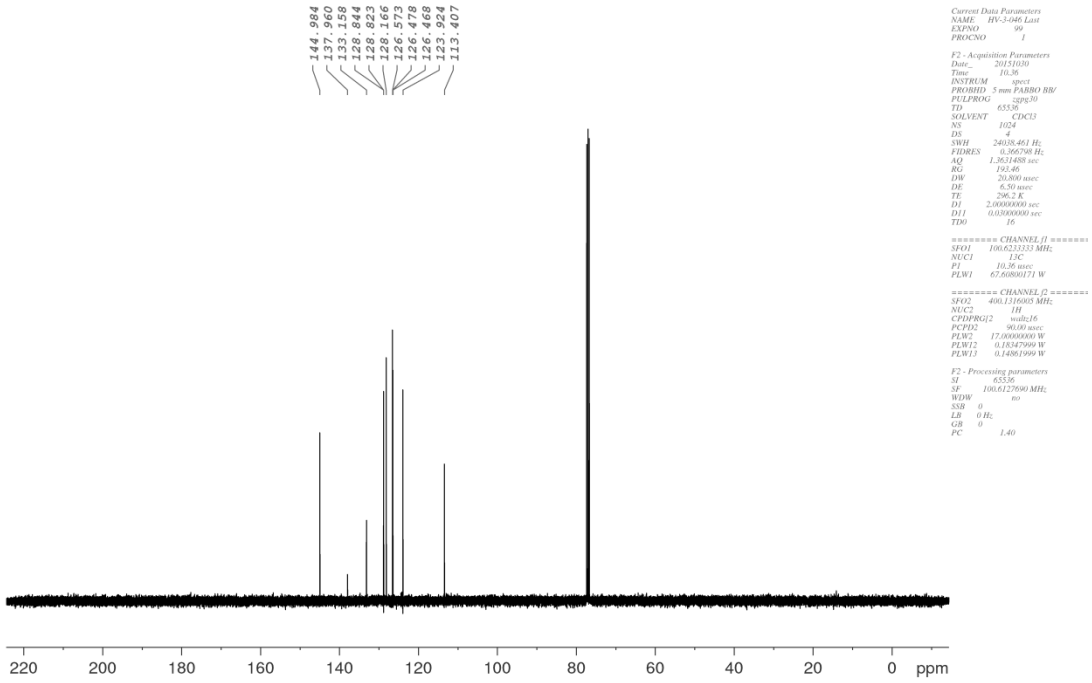
^{11}B NMR ($CDCl_3$, 128 MHz) Mes BN Anthracene (1i)



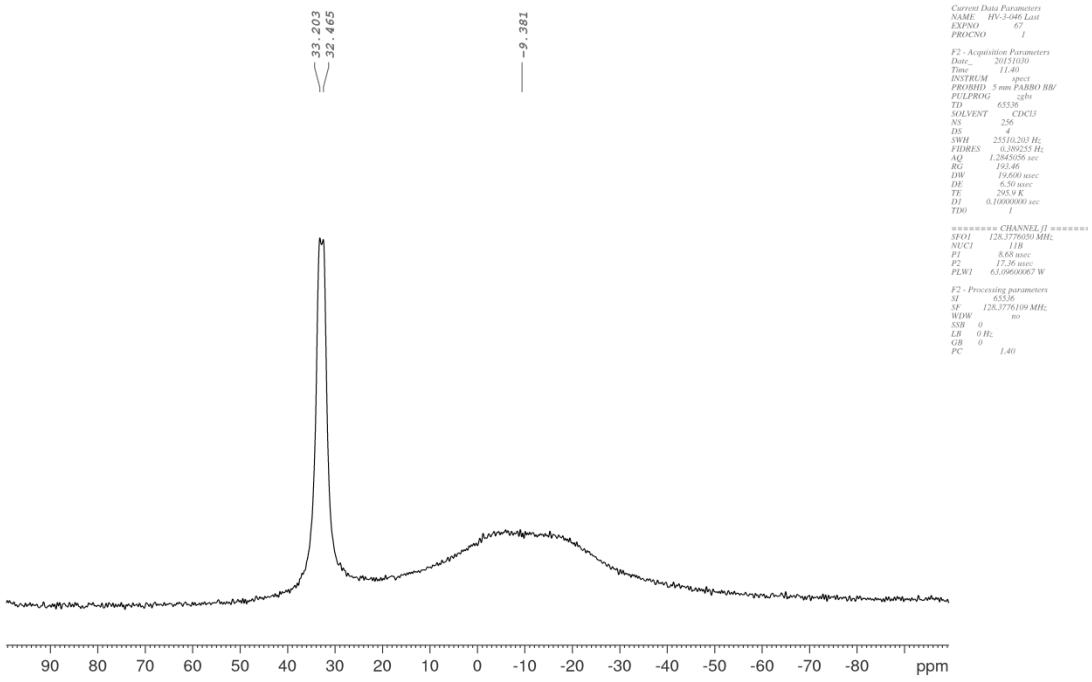
^{1}H NMR ($CDCl_3$, 400 MHz) BN Anthracene



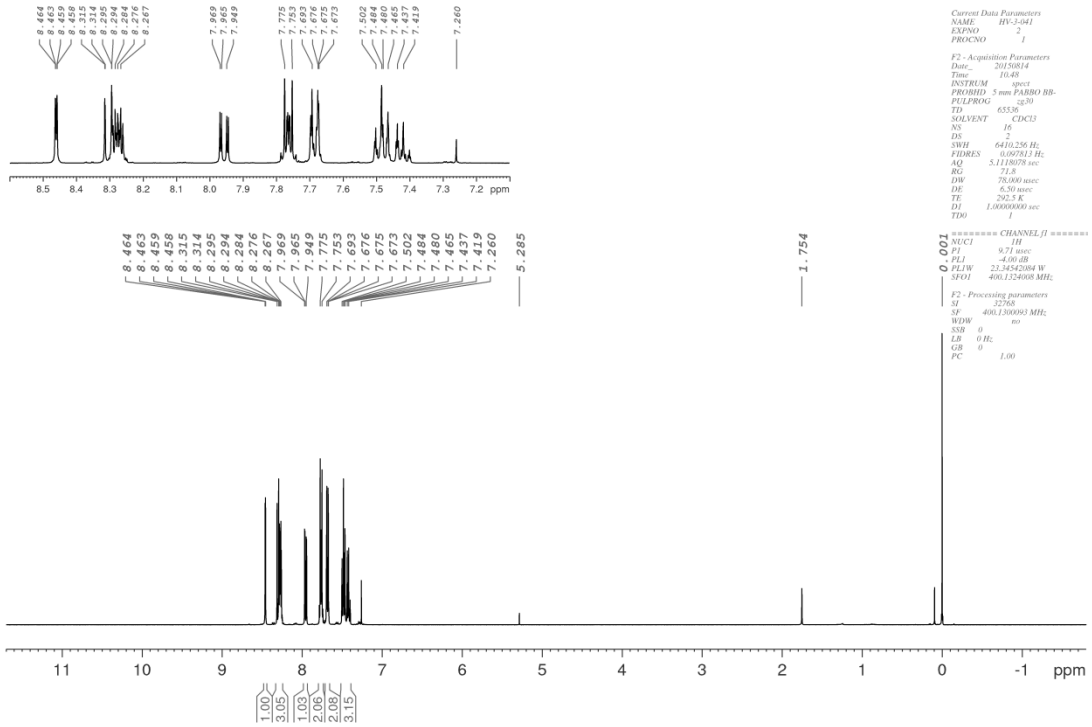
^{13}C NMR ($CDCl_3$, 101 MHz) BN Anthracene



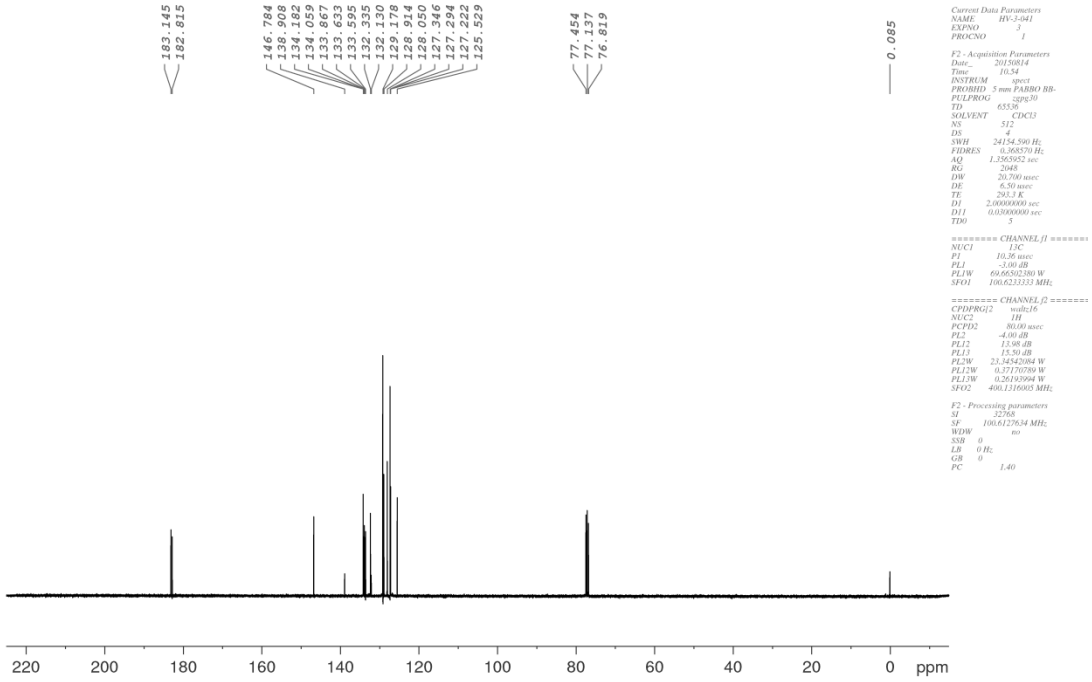
^{11}B NMR ($CDCl_3$, 128 MHz) BN Anthracene



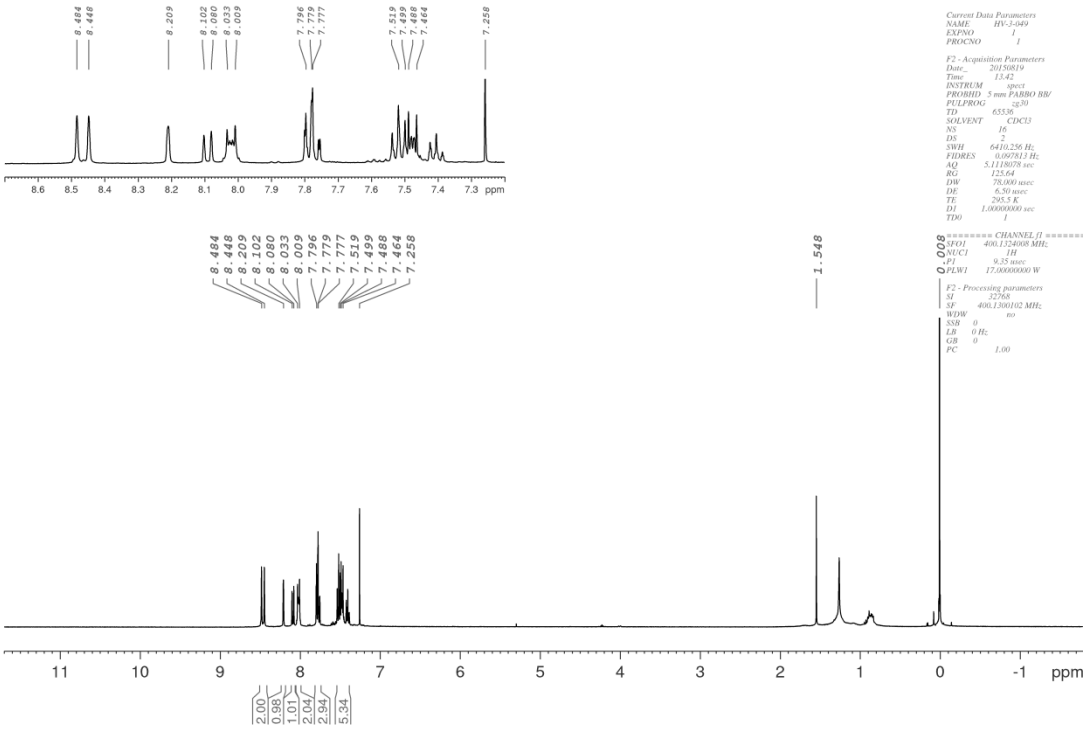
^{1}H NMR ($CDCl_3$, 400 MHz) 2-Phenylanthracene-9,10-Dione (7a)



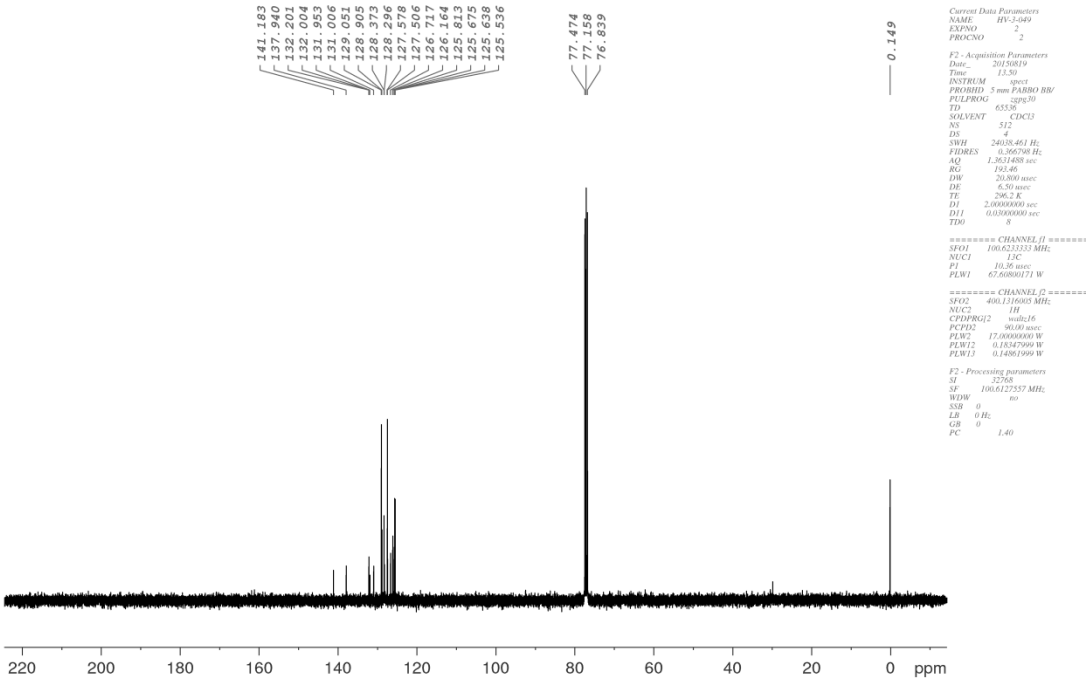
^{13}C NMR ($CDCl_3$, 101 MHz) 2-Phenylanthracene-9,10-Dione (7a)



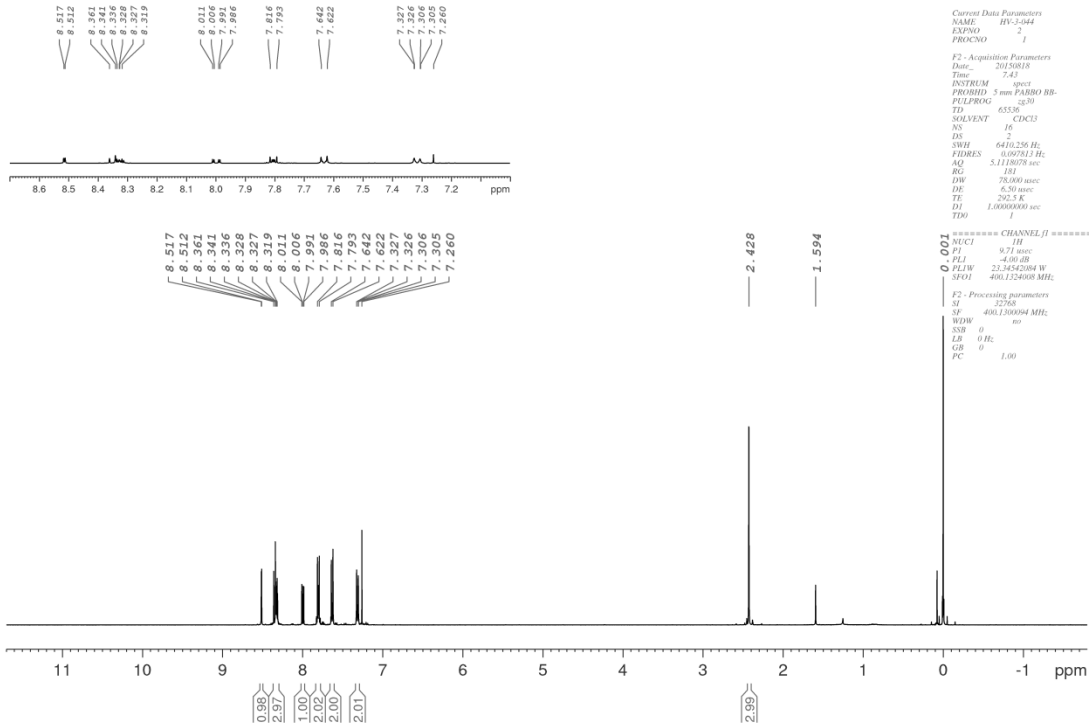
^{1}H NMR ($CDCl_3$, 400 MHz) 4-H Ph Anthracene (8a)



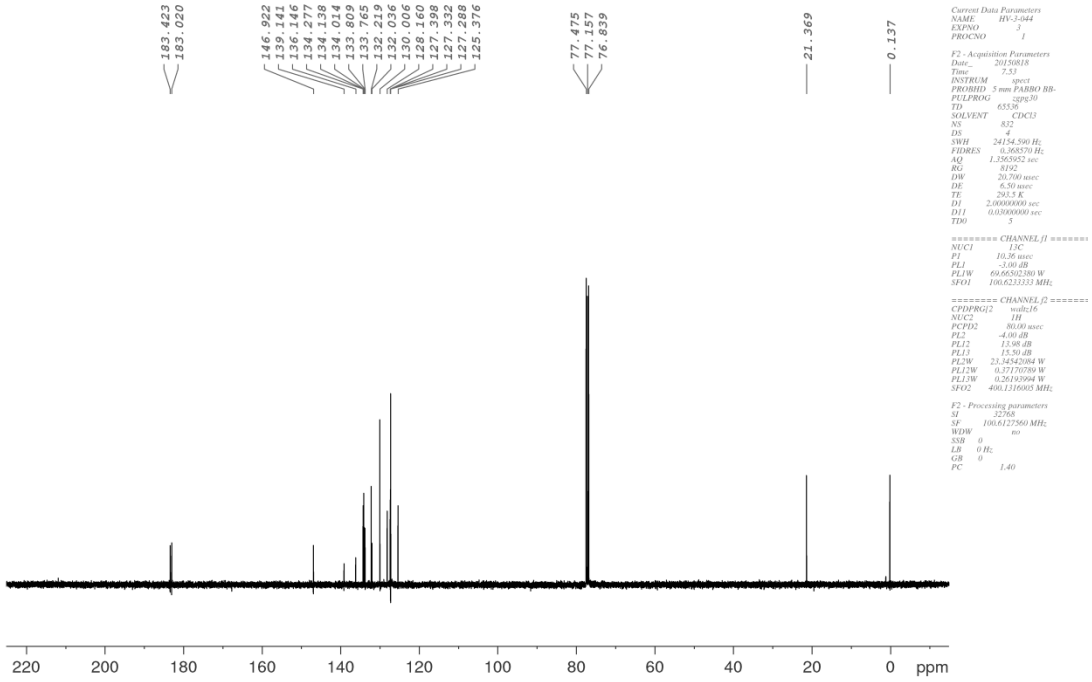
^{13}C NMR ($CDCl_3$, 101 MHz) 4-H Ph Anthracene (8a)



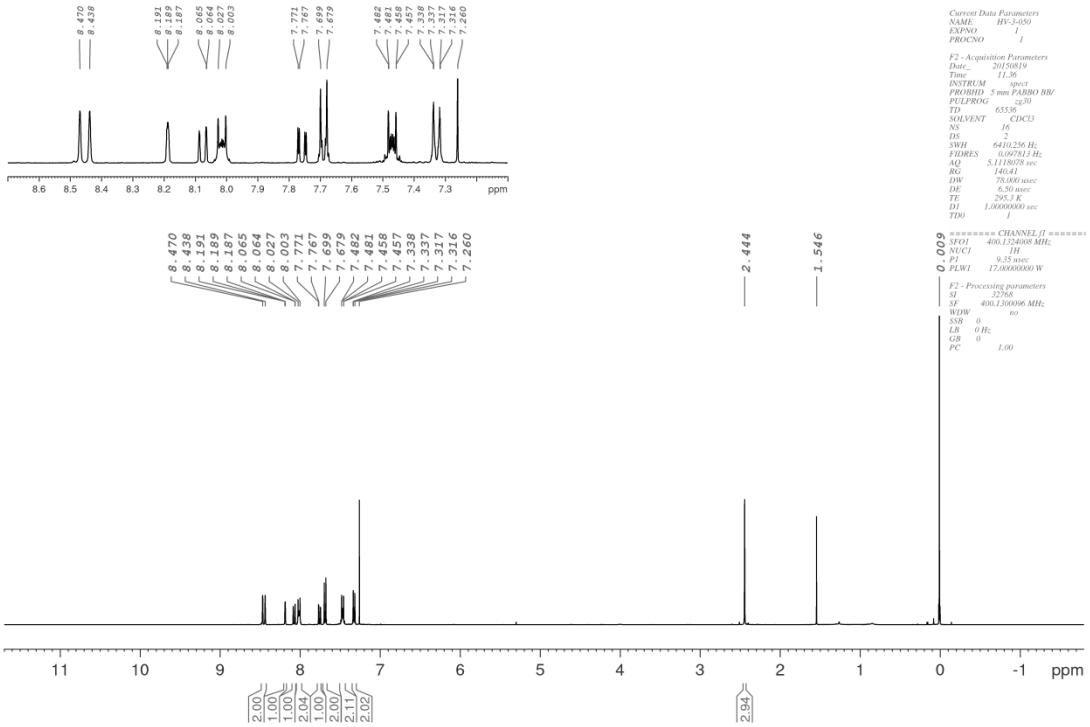
^{1}H NMR ($CDCl_3$, 400 MHz) 2-(p-Tolyl)Anthracene-9,10-Dione (7b)



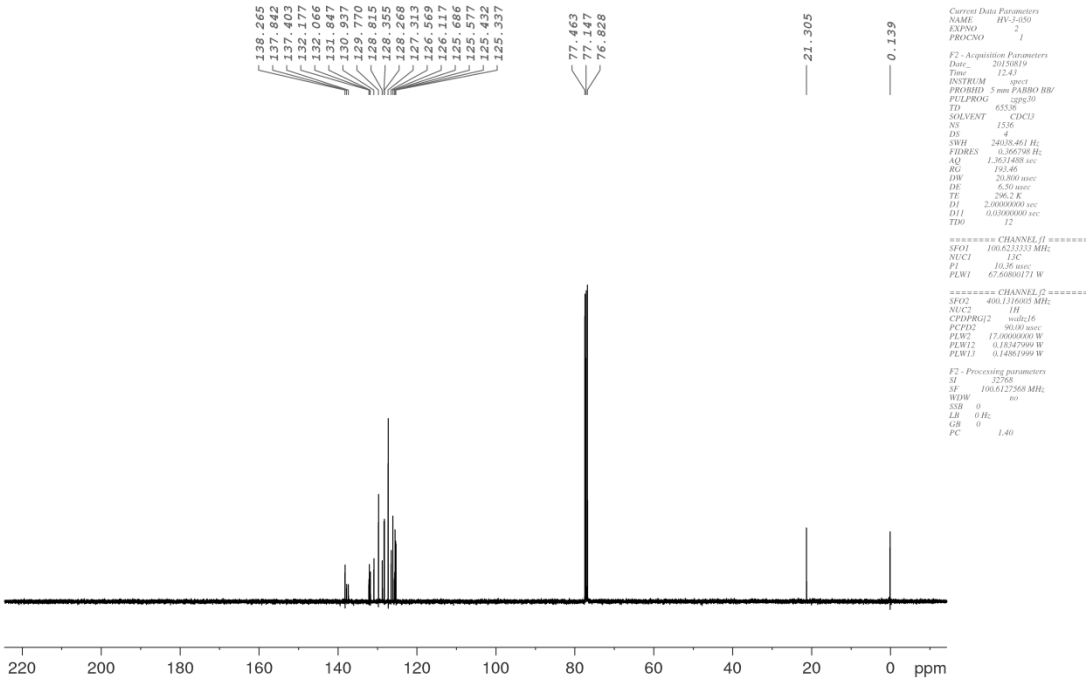
^{13}C NMR ($CDCl_3$, 101 MHz) 2-(p-Tolyl)Anthracene-9,10-Dione (7b)



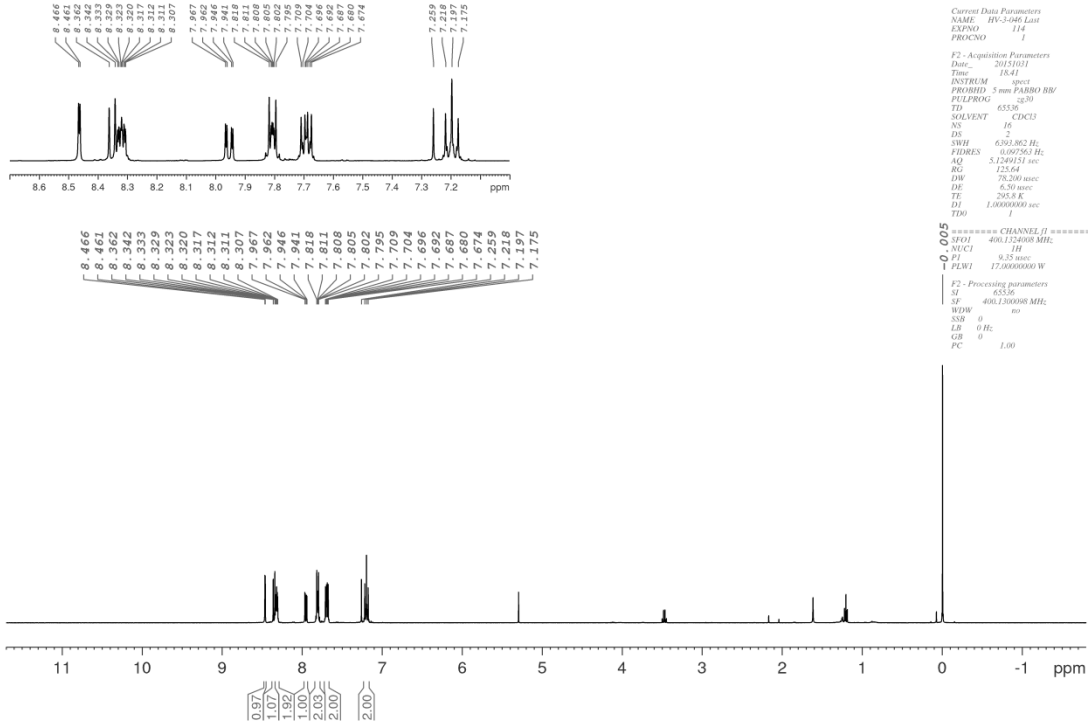
^{1}H NMR ($CDCl_3$, 400 MHz) 4-Me Ph Anthracene (8b)



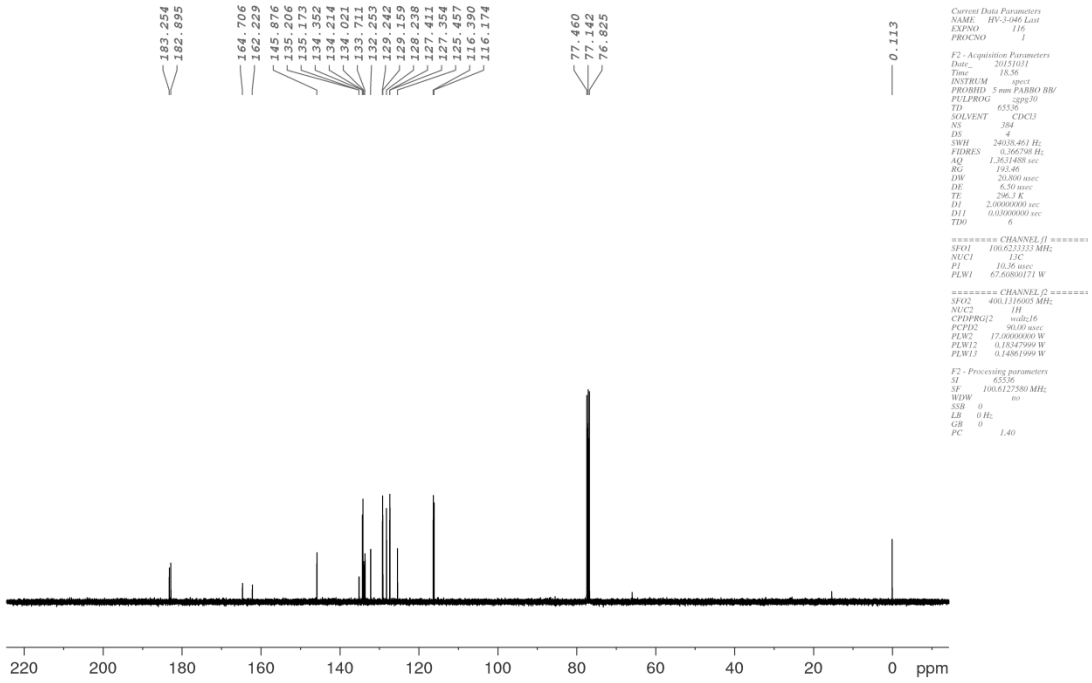
^{13}C NMR ($CDCl_3$, 101 MHz) 4-Me Ph Anthracene (8b)



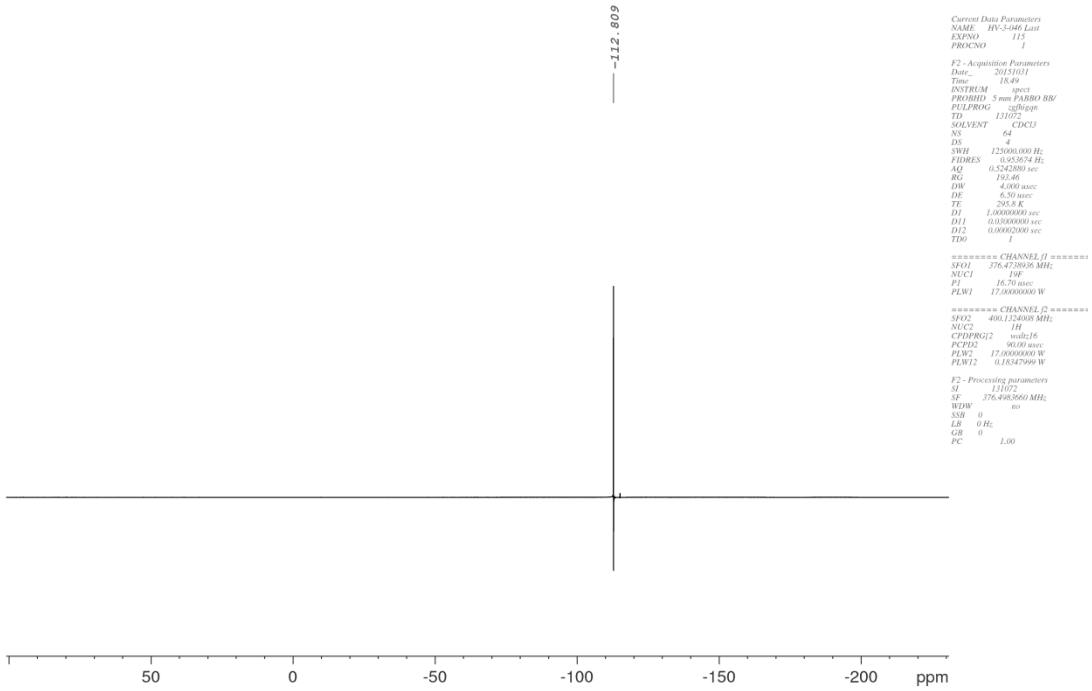
^{1}H NMR ($CDCl_3$, 400 MHz) 2-(4-Fluorophenyl)Anthracene-9,10-Dione (7c)



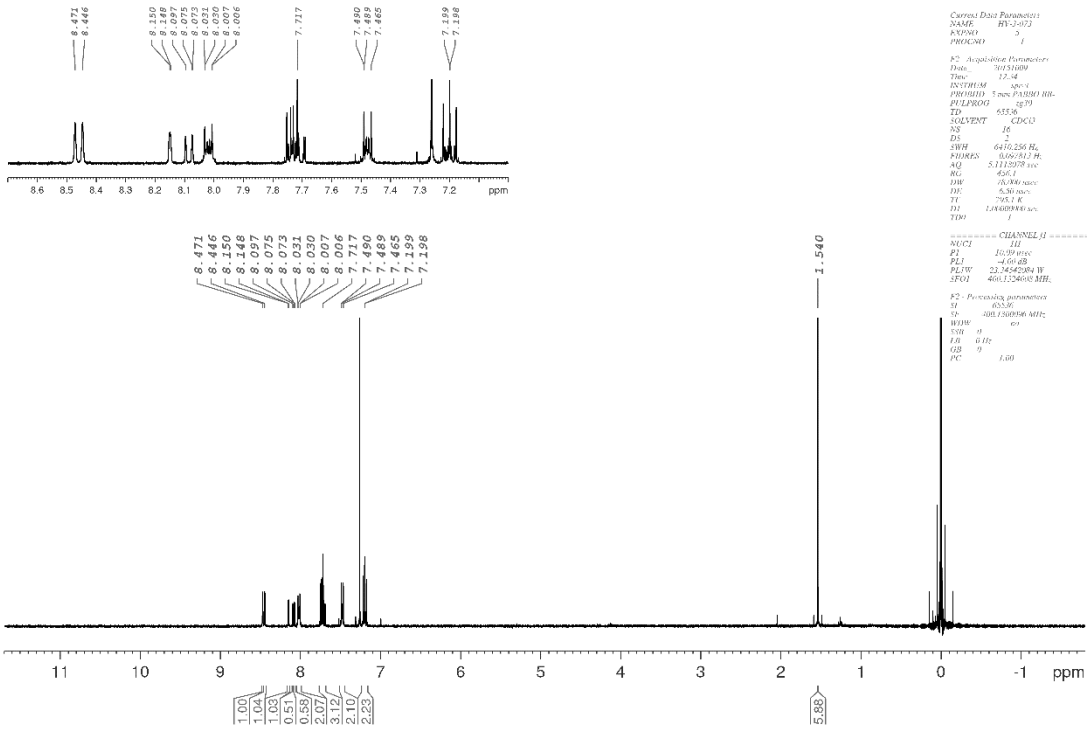
^{13}C NMR ($CDCl_3$, 101 MHz) 2-(4-Fluorophenyl)Anthracene-9,10-Dione (7c)



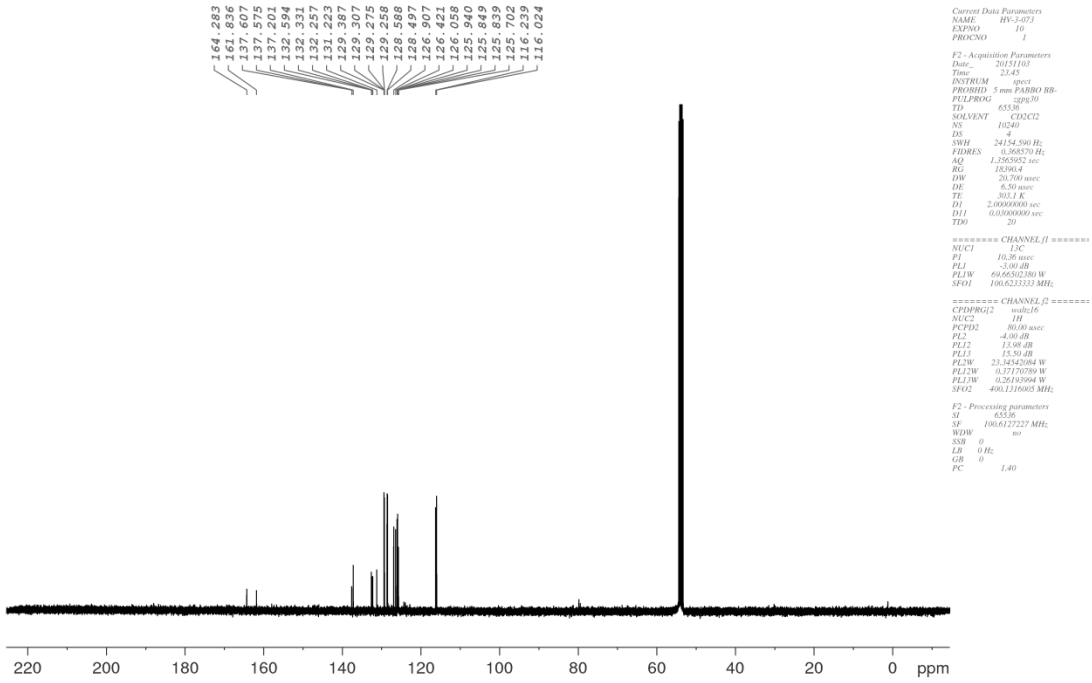
^{19}F NMR ($CDCl_3$, 376 MHz) 2-(4-Fluorophenyl)Anthracene-9,10-Dione (7c)



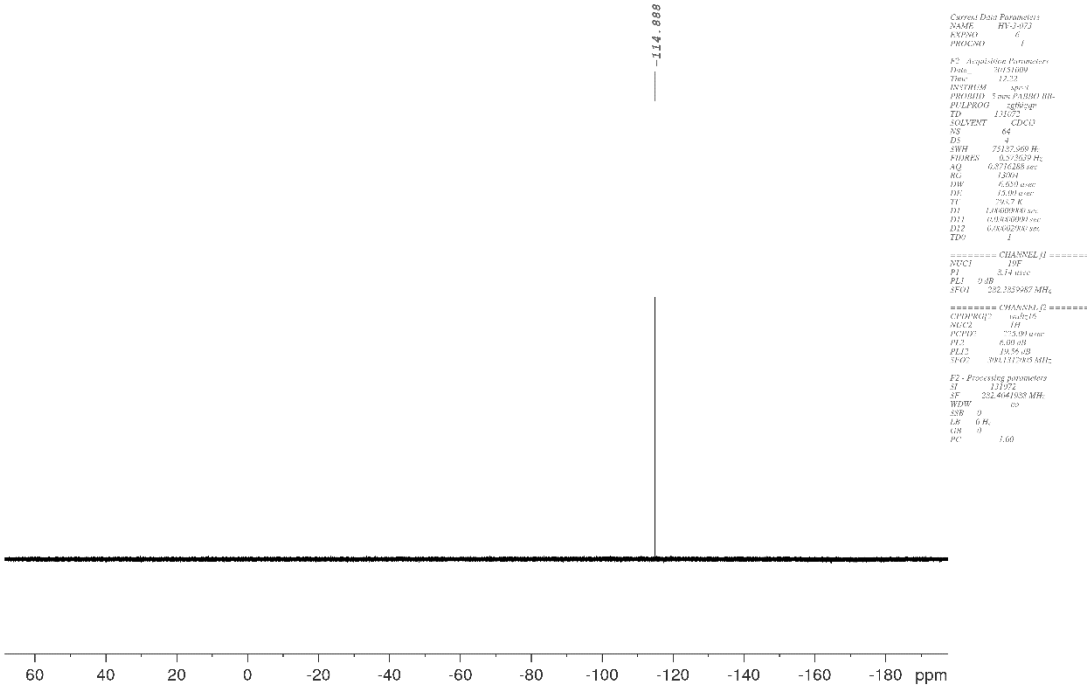
^{1}H NMR ($CDCl_3$, 400 MHz) 4-F Ph Anthracene (8c)



^{13}C NMR (CD_2Cl_2, 101 MHz) 4-F Ph Anthracene (8c)



^{19}F NMR ($CDCl_3$, 376 MHz) 4-F Ph Anthracene (8c)



VI. Single Crystal X-Ray Crystallography

All crystals suitable for X-ray structure determination were obtained as follows: (i) Crystals of **1b** were grown by slow evaporation of toluene; (ii) Crystals of **1c** were grown by solvent diffusion by layering hexanes over a concentrated solution of dichloromethane; (iii) Crystals of **1d**, **1f**, and **1i** were grown by slow evaporation of chlorobenzene; (iv) Crystals of **1g** were grown by slow evaporation of 20% ethyl acetate in hexanes; (v) Crystals of **1h** were grown by slow evaporation of chloroform; (vi) Crystals of Crystals of **8a** were grown by solvent diffusion by layering ethyl ether over a concentrated solution of toluene. Graphical representations of crystal structures were created using Mercury Version 3.5.1 by CCDC,[12] with ellipsoids shown at a probability level of 30%, hydrogens omitted for clarity, and the following color scheme: grey = carbon; blue = nitrogen; pink = boron; yellow = fluorine.
All reflection intensities were measured at 110(2) K using a SuperNova diffractometer (equipped with Atlas detector) with Cu *K*α radiation (λ = 1.54178 Å) under the program CrysAlisPro (Versions 1.171.36.32 / 1.171.37.33 / 1.171.37.35 Agilent Technologies, 2013-2014). The same program was used to refine the cell dimensions and for data reduction. The structure was solved with the program SHELXS-2013 and was refined on F^2 with SHELXL-2013. [13] Analytical numeric absorption corrections based on a multifaceted crystal model was applied using CrysAlisPro. The temperature of the data collection was controlled using the system Cryojet (manufactured by Oxford Instruments). The H atoms were placed at calculated positions (unless otherwise specified) using the instructions AFIX 43 or AFIX 137 with isotropic displacement parameters having values 1.2 or 1.5 *U*eq of the attached C or N atoms. For compounds **1f** and **1i**, the H atom attached to N1 was found from difference Fourier map, and its coordinates and isotropic temperature factor were refined freely. All important X-ray data are summarized in Table S3.

4-Me Ph BN Anthracene (1a)

The asymmetric unit contains two crystallographically independent molecules (Z' = 2). The structure is ordered. The crystal was non-merohedrally twinned, and the twin relationship corresponds to a twofold axis along the reciprocal vector –0.0015a* +0.9573b* – 0.2892c*. The BASF scale factor refines to 0.253(4).

4-H Ph BN Anthracene (1b)

The structure is disordered. The molecule is disordered over two orientations (the two orientations are related by a pseudo-twofold axis), and the occupancy factor of the major component of the disorder refines to 0.8954(15). In order to keep the data/parameter ratio to an acceptable level, all atoms of the minor component of the disorder follow a rigid group model. Furthermore, the anisotropic displacement parameters are set to be the same (EADP instruction) for all atoms of the minor and major components of

[12] C. F. Macrae, P. R. Edgington, P. McCabe, E. Pidcock, G. P. Shields, R. Taylor, M. Towler, J. van de Streek, *J. Appl. Cryst.* 2006, **39**, 453-457.
[13] Sheldrick, G. M. (2015). Acta Cryst. C**71**, 3-8.

the disorder related by a pseudo symmetry. The absolute configuration has not been established by anomalous-dispersion effects in diffraction measurements on the crystal.

4-F Ph BN Anthracene (1d)

The structure is disordered. The molecule is disordered over two orientations (the two orientations are related by a pseudo-twofold axis), and the occupancy factor of the major component of the disorder refines to 0.9619(15).

4-CF_3 Ph BN Anthracene (1f)

The structure is mostly ordered. The $–CF_3$ group is disordered over two orientations and the occupancy factor of the major component of the disorder refines to 0.917(6).

4-CN Ph BN Anthracene (1g)

The structure is ordered. The crystal that was mounted on the diffractometer was (slightly) twinned. The two twin components are related by a twofold axis along the reciprocal vector 0.0003a* + 0.0001b* + 1.0000c*. The BASF scale factor refines to 0.0711(9).

4-NO_2 Ph BN Anthracene (1h)

The structure is ordered.

Mes BN Anthracene (1i)

The structure is ordered. The absolute structure configuration might be established by anomalous-dispersion effects in diffraction measurements on the crystal. Although the value of the Flack parameter of -0.2(5) remains uninformative, the Bayesian statistics suggest that the absolute structure has been potentially correctly assigned as P2(true) = 1.000, and the Hooft parameter refines to -0.14(17).

Bayesian Statistics

Student_T Nu	11	P3(rac-twin)	0.001
Select Pairs	1416	P3(false)	0.2E-09
Theta_Min.	6.82	G	1.2735
Theta_Max.	71.86	G (su)	0.3366
P2(true)	1.000	Hooft y	-0.14(17)
P3(true)	0.999		

4-H Ph Anthracene (8a)

The structure is disordered. The molecule is disordered over two orientations (the two orientations are related by a pseudo-twofold axis), and the occupancy factor of the major component of the disorder refines to 0.873(2).

Table S-3: Experimental details for X-ray crystallographic studies.

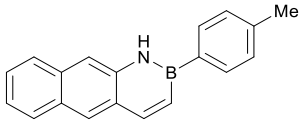
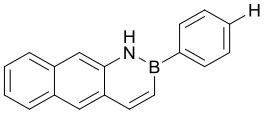
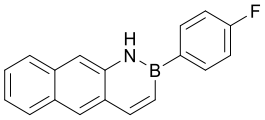
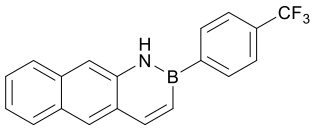
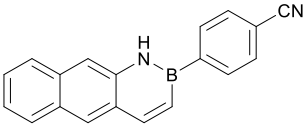
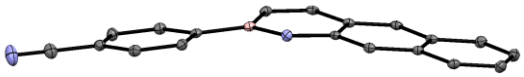
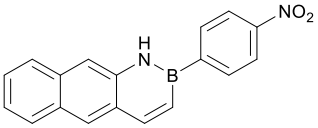
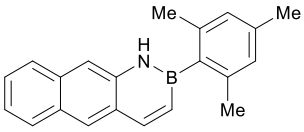
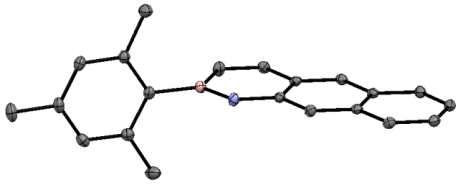
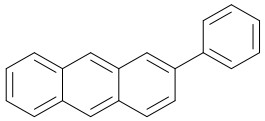
	1b	**1c**	**1d**	**1f**
Crystal data				
Chemical formula	$C_{19}H_{16}BN$	$C_{18}H_{14}BN$	$C_{18}H_{13}BFN$	$C_{19}H_{13}BF_3N$
M_r	269.14	255.11	273.10	323.11
Crystal system, space group	Triclinic, *P*-1	Monoclinic, $P2_1$	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/n$
a, *b*, *c* (Å)	5.9219 (3), 7.4968 (3), 31.3180 (19)	7.5827 (3), 5.8864 (3), 14.3622 (7)	7.5086 (3), 5.9024 (3), 29.5225 (17)	7.54619 (13), 5.86945 (11), 32.5219 (5)
α, β, γ (°)	94.271 (4), 91.188 (4), 90.053 (3)	90, 93.408 (4), 90	90, 93.266 (5), 90	90, 94.2129 (15), 90
V (Å^3)	1386.21 (12)	639.92 (5)	1306.28 (11)	1436.57 (4)
Z	4	2	4	4
μ (mm^{-1})	0.56	0.58	0.72	0.95
Crystal size (mm)	0.27 × 0.22 × 0.02	0.50 × 0.40 × 0.02	0.58 × 0.51 × 0.05	0.48 × 0.31 × 0.05
Data collection				
Absorption correction	Analytical	Analytical	Analytical	Analytical
T_{min}, T_{max}	0.895, 0.990	0.816, 0.986	0.782, 0.971	0.751, 0.958
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15319, 5846, 4038	7322, 2277, 2191	8531, 2569, 2276	9494, 2815, 2523
R_{int}	0.032	0.022	0.026	0.030
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.598	0.617	0.616	0.616
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.073, 0.247, 1.10	0.034, 0.096, 1.05	0.050, 0.143, 1.06	0.039, 0.109, 1.06
No. of reflections	5846	2277	2569	2815
No. of parameters	382	188	380	249
No. of restraints	0	757	794	42
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.38, -0.31	0.17, -0.15	0.27, -0.25	0.32, -0.28

Table S-3 con't: Experimental details for X-ray crystallographic studies.

	1g	**1h**	**1i**	**8a**
Crystal data				
Chemical formula	$C_{19}H_{13}BN_2$	$C_{18}H_{13}BN_2O_2$	$C_{21}H_{20}BN$	$C_{20}H_{14}$
M_r	280.12	300.11	297.19	254.31
Crystal system, space group	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/n$	Monoclinic, $P2_1$	Monoclinic, $P2_1/n$
a, b, c (Å)	7.46841 (17), 5.90109 (11), 32.1078 (10)	7.35557 (13), 5.95525 (11), 31.4266 (6)	7.44538 (9), 7.11221 (8), 15.95865 (19)	7.5423 (2), 5.9013 (2), 28.5913 (9)
α, β, γ (°)	90, 91.971 (3), 90	90, 90.5796 (17), 90	90, 94.8062 (11), 90	90, 94.099 (3), 90
V (Å^3)	1414.21 (6)	1376.55 (4)	842.09 (2)	1269.33 (7)
Z	4	4	2	4
μ (mm^{-1})	0.60	0.76	0.50	0.57
Crystal size (mm)	0.65 × 0.28 × 0.09	0.29 × 0.11 × 0.09	0.33 × 0.26 × 0.07	0.39 × 0.30 × 0.02
Data collection				
Absorption correction	Analytical	Analytical	Analytical	Analytical
T_{min}, T_{max}	0.769, 0.955	0.859, 0.940	0.901, 0.971	0.855, 0.988
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7449, 3487, 3146	8815, 2703, 2390	8578, 3204, 3130	8823, 2491, 2298
R_{int}	0.018	0.030	0.019	0.025
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.616	0.616	0.616	0.616
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.052, 0.153, 1.09	0.040, 0.114, 1.03	0.030, 0.081, 1.04	0.062, 0.152, 1.16
No. of reflections	3487	2703	3204	2491
No. of parameters	200	208	216	362
No. of restraints	--	--	1	829
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.36, -0.30	0.27, -0.27	0.19, -0.15	0.29, -0.20

Computer programs: *CrysAlis PRO*, Agilent Technologies, Version 1.171.37.33 (release 3/27/2014 CrysAlis171 .NET) (compiled 3/27/2014, 17:12:48), Version 1.171.36.32 (release 8/2/2013 CrysAlis171 .NET) (compiled 8/2/2013, 16:46:58), Version 1.171.37.35 (release 8/13/2014 CrysAlis171 .NET) (compiled 8/13/2014, 18:06:01), *SHELXS2013* (Sheldrick, 2013), *SHELXL2013* (Sheldrick, 2013), *SHELXTL* v6.10 (Sheldrick, 2008).

Table S-4: Solved single crystal XDR molecular structures of B-aryl anthracenes and 2-aryl anthracenes. Ellipsoids shown at 30% probability. Disorder and hydrogens omitted for clarity. Grey = carbon; blue = nitrogen; pink = boron; yellow = fluorine; red = oxygen.

Compound	*XRD Results*
4-Me Ph BN Anthracene (1b)	
	 Torsional ∠ = -7.5(5)º BN bond length = 1.418(5) Å
4-H Ph BN Anthracene (1c)	
	 Torsional ∠ = 5.0(3) BN bond length = 1.426(3) Å
4-F Ph BN Anthracene (1d)	
	 Torsional ∠ = -5.3(2)º BN bond length = 1.423(2) Å
4-CF_3 Ph BN Anthracene (1f)	
	 Torsional ∠ = 5.4(2)º BN bond length = 1.4175(18) Å
4-CN Ph BN Anthracene (1g)	
	 Torsional ∠ = 5.4(2)º BN bond length = 1.419(2) Å
4-NO_2 Ph BN Anthracene (1h)	
	 Torsional ∠ = -2.7(2)º BN bond length = 1.4207(16) Å
Mes BN Anthracene (1i)	
	 Torsional ∠ = -84.7(2)º BN bond length = 1.418(2) Å
4-H Ph Anthracene (8a)	
	 Torsional ∠ = -6.7(4) º $CC_{BN\ equiv.}$ bond length = 1.380(4) Å

VII. Computational Details

All DFT calculations were done using Gaussian 09.[1] Geometries were optimized using the restricted CAM-B3LYP functional with the 6-311G(d,p) basis set with forced non-symmetry and from these optimizations the energies and orbital density maps of the frontier molecular orbitals are reported. Energies and orbital density maps of the frontier molecular orbitals of X-ray diffraction determined geometries were also calculated using the restricted CAM-B3LYP functional with the 6-311G(d,p) basis set, without geometry optimization. All structural and orbital density map visualization were created with GaussView 5.0 by Gaussian, Inc.

Table S-5: Calculated optimized geometries of B-aryl anthracenes and 2-aryl anthracenes. Hydrogens omitted for clarity. Grey = carbon; blue = nitrogen; pink = boron; red = oxygen; light blue = fluorine; green = chlorine.

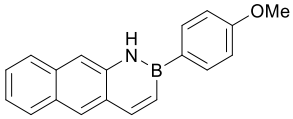
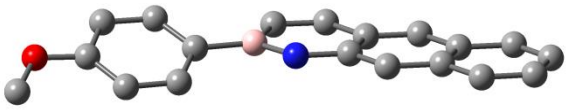
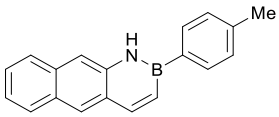
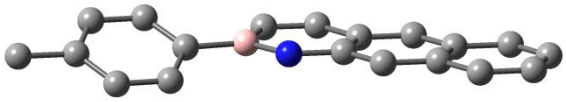
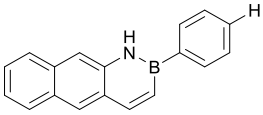
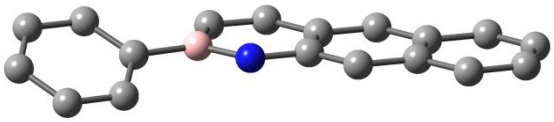
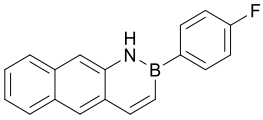
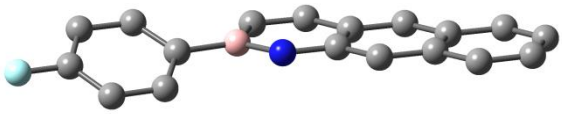
Compound	*Calculated Geometry*
4-MeO Ph BN Anthracene (1a)	
	 Torsional ∠ = -24º BN bond length = 1.420 Å
4-Me Ph BN Anthracene (1b)	
	 Torsional ∠ = -25º BN bond length = 1.419 Å
4-H Ph BN Anthracene (1c)	
	 Torsional ∠ = -27º BN bond length = 1.418 Å
4-F Ph BN Anthracene (1d)	
	 Torsional ∠ = -26º BN bond length = 1.418 Å

Table S-5 con't: Calculated optimized geometries of B-aryl anthracenes and 2-aryl anthracenes. Hydrogens omitted for clarity. Grey = carbon; blue = nitrogen; pink = boron; red = oxygen; light blue = fluorine; green = chlorine.

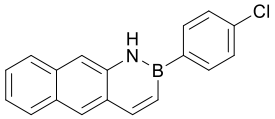
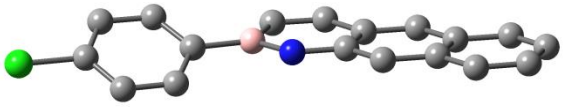
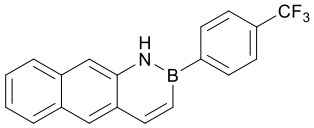
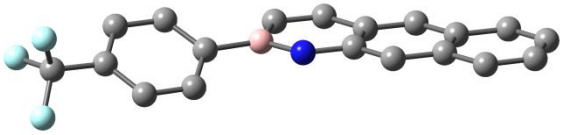
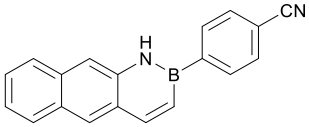
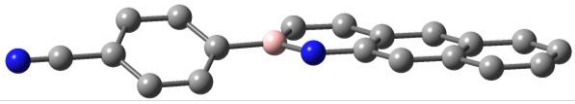
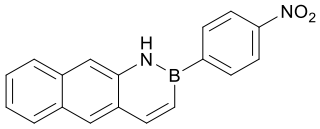
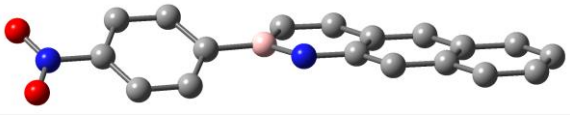
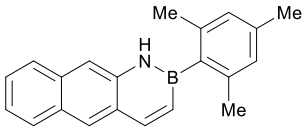
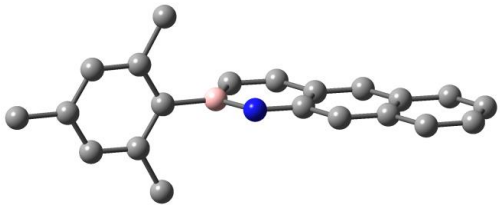
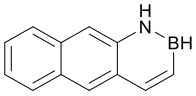
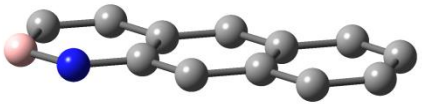
4-Cl Ph BN Anthracene (1e)	
	 Torsional ∠ = -27º BN bond length = 1.417 Å
4-CF_3 Ph BN Anthracene (1f)	
	 Torsional ∠ = -29º BN bond length = 1.416 Å
4-CN Ph BN Anthracene (1g)	
	 Torsional ∠ = -30º BN bond length = 1.415 Å
4-NO_2 Ph BN Anthracene (1h)	
	 Torsional ∠ = -31º BN bond length = 1.415 Å
2,4,6-MePh BN Anthracene (1i)	
	 Torsional ∠ = -90º BN bond length = 1.417 Å
BN Anthracene	
	 BN bond length = 1.411 Å

Table S-5 con't: Calculated optimized geometries of B-aryl anthracenes and 2-aryl anthracenes. Hydrogens omitted for clarity. Grey = carbon; blue = nitrogen; pink = boron; red = oxygen; light blue = fluorine; green = chlorine.

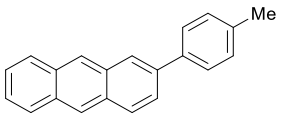
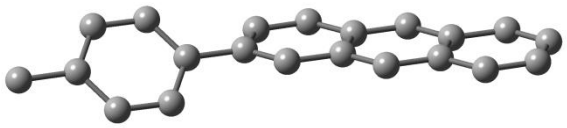
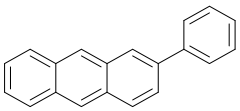
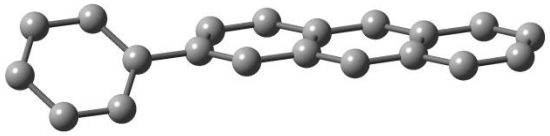
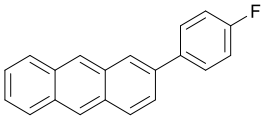
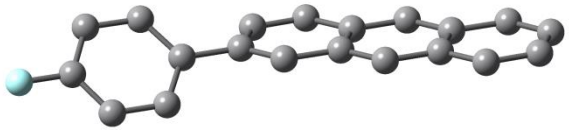
4-Me Ph Anthracene (8b)	
	 Torsional ∠ = -40º $CC_{BN\ equiv.}$ bond length = 1.364 Å
4-H Ph Anthracene (8a)	
	 Torsional ∠ = -41º $CC_{BN\ equiv.}$ bond length = 1.364 Å
4-F Ph Anthracene (8c)	
	 Torsional ∠ = -41º $CC_{BN\ equiv.}$ bond length = 1.364 Å

Table S-6: Calculated orbital density maps and energies of the frontier molecular orbitals for B-aryl anthracenes and 2-aryl anthracenes.

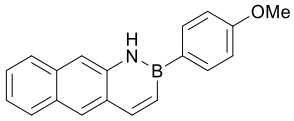
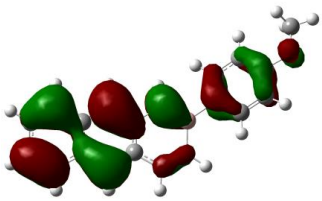
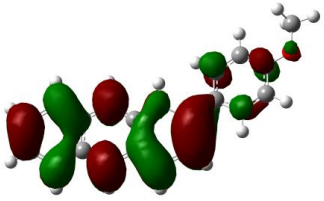
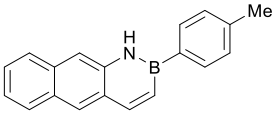
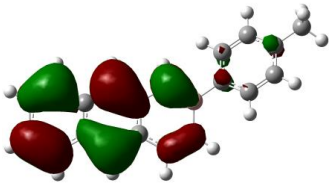
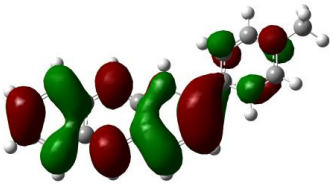
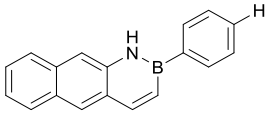
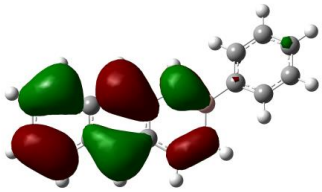
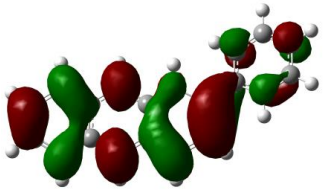
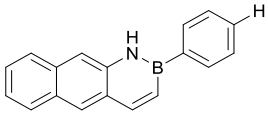
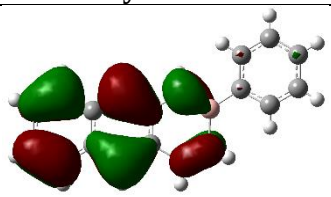
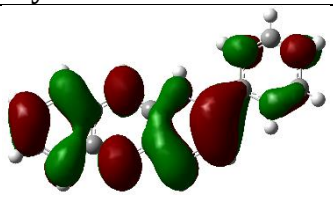
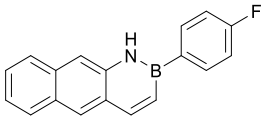
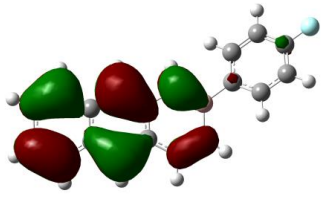
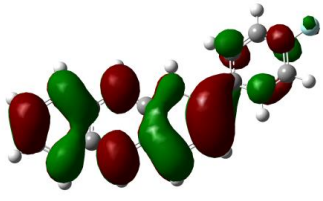
Compound / HOMO-LUMO gap	HOMO/ HOMO Energy	LUMO/ LUMO Energy
4-MeO Ph BN Anthracene (1a)		
 6.30 eV	 -6.93 eV	 -0.63 eV
4-Me Ph BN Anthracene (1b)		
 6.31 eV	 -6.98 eV	 -0.67 eV
4-H Ph BN Anthracene (1c)		
 6.31 eV	 -7.02 eV	 -0.71 eV
4-H Ph BN Anthracene (1c) – Geometry Abstracted from Crystal Structure		
 6.25 eV	 -6.96 eV	 -0.71 eV
4-F Ph BN Anthracene (1d)		
 6.30 eV	 -7.08 eV	 -0.78 eV

Table S-6 con't: Calculated orbital density maps and energies of the frontier molecular orbitals for B-aryl anthracenes and 2-aryl anthracenes.

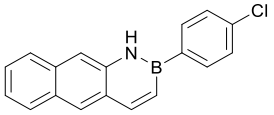
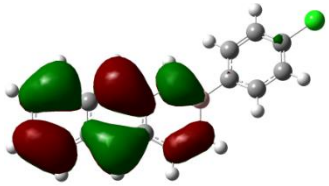
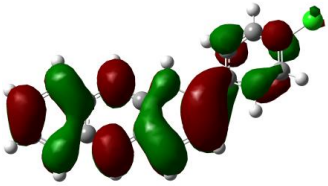
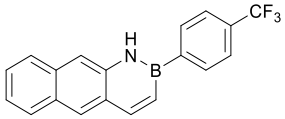
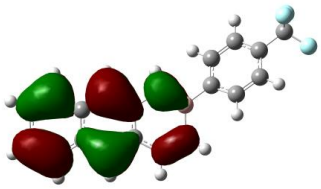
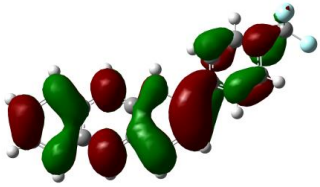
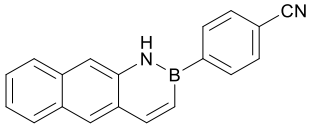
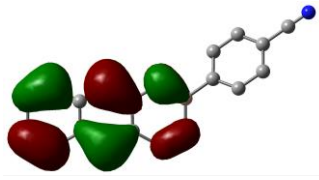
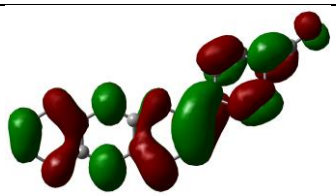
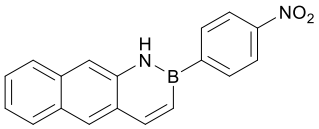
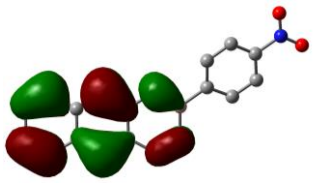
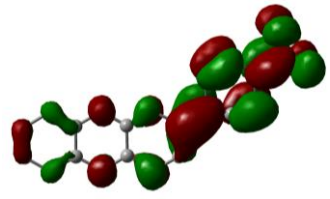
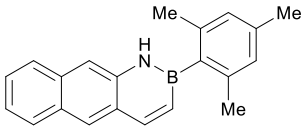
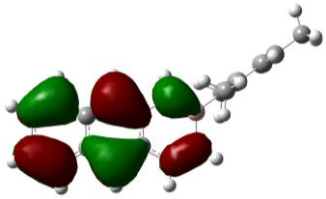
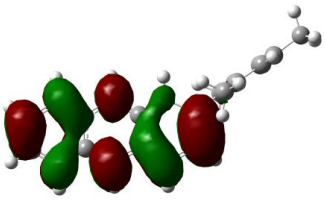
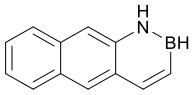
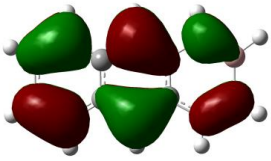
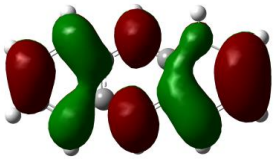
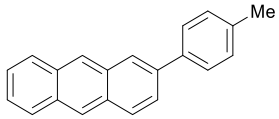
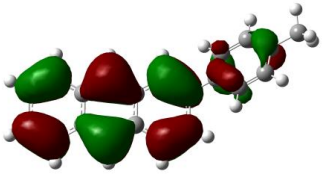
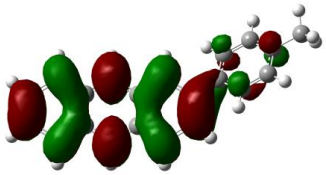
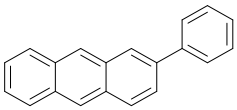
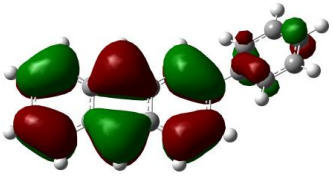
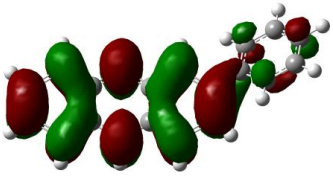
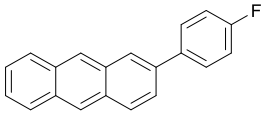
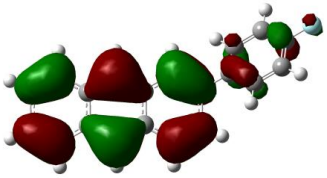
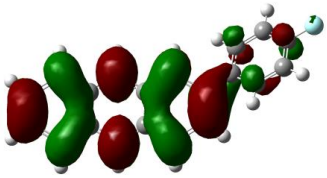
4-Cl Ph BN Anthracene (1e)		
		
6.27 eV	-7.12 eV	-0.85 eV
4-CF_3 Ph BN Anthracene (1f)		
		
6.24 eV	-7.19 eV	-0.95 eV
4-CN Ph BN Anthracene (1g)		
		
6.14 eV	-7.26 eV	-1.11 eV
4-NO_2 Ph BN Anthracene (1h)		
		
5.86 eV	-7.28 eV	-1.42 eV
Mes BN Anthracene (1i)		
		
6.40 eV	-7.05 eV	-0.65 eV
BN Anthracene		
		
6.39 eV	-7.07 eV	-0.68 eV

Table S-6 con't: Calculated orbital density maps and energies of the frontier molecular orbitals for B-aryl anthracenes and 2-aryl anthracenes.

4-Me Ph Anthracene (8b)		
		
5.85 eV	-6.64 eV	-0.79 eV
4-H Ph Anthracene (8a)		
		
5.86 eV	-6.68 eV	-0.83 eV
4-F Ph Anthracene (8c)		
		
5.86 eV	-6.75 eV	-0.89 eV

4-MeO Ph BN Anthracene (1a) Coordinates

E(RCAM-B3LYP)= -888.27701176 E_h No. Imaginary Frequencies= 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.716423	-1.853544	-2.188152
2	6	0	4.056270	-0.589372	-2.117385
3	6	0	2.609604	-0.542350	-2.101569
4	6	0	1.846636	-1.650293	-2.151517
5	6	0	6.093157	-1.909832	-2.195587
6	6	0	4.820293	0.557895	-2.063077
7	6	0	6.223277	0.522617	-2.071935
8	6	0	6.872346	-0.742539	-2.138451
9	6	0	8.293049	-0.777410	-2.146363
10	1	0	8.790321	-1.739657	-2.196943
11	6	0	9.020636	0.373414	-2.091720
12	6	0	8.374237	1.632146	-2.025600
13	6	0	7.013920	1.701586	-2.016034
14	1	0	6.590069	-2.873503	-2.248570
15	1	0	2.164335	0.448521	-2.050630
16	1	0	0.768267	-1.527720	-2.148008
17	1	0	4.319333	1.519124	-2.010417
18	1	0	10.103335	0.330698	-2.098524
19	1	0	8.968214	2.536931	-1.982605
20	1	0	6.511685	2.661355	-1.965307
21	7	0	3.940749	-2.999142	-2.245872
22	1	0	4.468366	-3.860242	-2.258529
23	5	0	2.521053	-3.029017	-2.242514
24	6	0	1.768049	-4.392789	-2.332742
25	6	0	2.347654	-5.535823	-2.883876
26	6	0	0.453930	-4.526254	-1.858444
27	6	0	1.679321	-6.751019	-2.962904
28	1	0	3.351293	-5.487549	-3.295558
29	6	0	-0.227705	-5.723638	-1.914699
30	1	0	-0.044108	-3.667746	-1.421822
31	6	0	0.382005	-6.848435	-2.470158
32	1	0	2.172040	-7.603174	-3.409733
33	1	0	-1.238446	-5.821958	-1.539100
34	8	0	-0.365205	-7.979248	-2.489521
35	6	0	0.199602	-9.149805	-3.042638
36	1	0	-0.561530	-9.921610	-2.953019
37	1	0	0.451261	-9.012981	-4.099095
38	1	0	1.094474	-9.460726	-2.494269

4-Me Ph BN Anthracene (1b) Coordinates

E(RCAM-B3LYP)= -813.07015919 E_h No. Imaginary Frequencies= 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.783919	-1.894465	-2.133627
2	6	0	4.071654	-0.666092	-2.283074
3	6	0	2.629499	-0.689624	-2.403277
4	6	0	1.917519	-1.832113	-2.378932
5	6	0	6.156300	-1.882756	-2.011019
6	6	0	4.782472	0.516159	-2.306243
7	6	0	6.180049	0.549964	-2.184743
8	6	0	6.880879	-0.679799	-2.032833
9	6	0	8.296309	-0.644480	-1.909338
10	1	0	8.832632	-1.579699	-1.793502
11	6	0	8.970445	0.539295	-1.935481
12	6	0	8.272564	1.762873	-2.086493
13	6	0	6.915920	1.765116	-2.207458
14	1	0	6.692453	-2.819641	-1.896496
15	1	0	2.143806	0.276436	-2.519584
16	1	0	0.839699	-1.765459	-2.486954
17	1	0	4.242328	1.450365	-2.421040
18	1	0	10.049757	0.550371	-1.840343
19	1	0	8.824624	2.694634	-2.105092
20	1	0	6.374587	2.697575	-2.323439
21	7	0	4.061518	-3.075941	-2.114353
22	1	0	4.619566	-3.905944	-1.972904
23	5	0	2.651100	-3.174276	-2.231474
24	6	0	1.964720	-4.578775	-2.206005
25	6	0	2.634159	-5.747678	-2.582689
26	6	0	0.634112	-4.720478	-1.800146
27	6	0	2.015013	-6.986687	-2.550087
28	1	0	3.658498	-5.693174	-2.939274
29	6	0	0.013767	-5.958734	-1.755344
30	1	0	0.070836	-3.842405	-1.503445
31	6	0	0.694158	-7.114693	-2.128323
32	1	0	2.562331	-7.869914	-2.862487
33	1	0	-1.018983	-6.030621	-1.430333
34	6	0	0.028825	-8.462388	-2.058507
35	1	0	0.458669	-9.156227	-2.782628
36	1	0	0.150750	-8.905871	-1.065900
37	1	0	-1.042214	-8.387436	-2.253655

4-Me Ph BN Anthracene (1b) Coordinates- Geometry Abstracted from Crystal Structure

E(RCAM-B3LYP)= -812.83529032 E_h No. Imaginary Frequencies= N/A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.531500	7.711400	9.088100
2	6	0	6.350200	8.045300	10.167500
3	1	0	7.193600	8.449800	10.001100
4	6	0	5.962300	7.800100	11.483000
5	6	0	6.802300	8.108700	12.589900
6	1	0	7.657900	8.492500	12.439700
7	6	0	6.385000	7.854700	13.872000
8	1	0	6.949300	8.082200	14.600500
9	6	0	5.132000	7.262600	14.121800
10	1	0	4.858300	7.087800	15.015700
11	6	0	4.308400	6.937200	13.078000
12	1	0	3.466000	6.536400	13.254700
13	6	0	4.687700	7.186700	11.746200
14	6	0	3.866300	6.888700	10.657800
15	1	0	3.009200	6.513500	10.822300
16	6	0	4.247500	7.117600	9.349200
17	6	0	3.410200	6.764500	8.226300
18	1	0	2.538000	6.433900	8.405600
19	6	0	3.790800	6.876900	6.952100
20	1	0	3.208200	6.613900	6.248000
21	6	0	5.812100	7.515100	5.212900
22	6	0	7.045300	8.142200	4.947500
23	1	0	7.517300	8.549700	5.664100
24	6	0	7.593000	8.183700	3.670100
25	1	0	8.427500	8.616600	3.534600
26	6	0	6.941500	7.603700	2.592500
27	6	0	5.717700	6.967100	2.835800
28	1	0	5.253400	6.556700	2.117000
29	6	0	5.172400	6.926500	4.111600
30	1	0	4.340400	6.487000	4.243400
31	6	0	7.534400	7.667000	1.223700
32	1	0	7.438500	8.574500	0.868000
33	1	0	7.068700	7.034600	0.637000
34	1	0	8.484700	7.432100	1.267700
35	5	0	5.198500	7.443100	6.638000
36	7	0	5.925300	7.890500	7.774800
37	1	0	6.683000	8.314300	7.631200

4-H Ph BN Anthracene (1c) Coordinates

E(RCAM-B3LYP)= -773.76735731 E_h No. Imaginary Frequencies= 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.789752	-1.897573	-2.127563
2	6	0	4.072158	-0.673514	-2.285746
3	6	0	2.630311	-0.703747	-2.405934
4	6	0	1.922867	-1.849068	-2.373429
5	6	0	6.161981	-1.879506	-2.004738
6	6	0	4.778113	0.511643	-2.317130
7	6	0	6.175329	0.552033	-2.195617
8	6	0	6.881416	-0.673756	-2.034874
9	6	0	8.296674	-0.631662	-1.911357
10	1	0	8.836910	-1.563758	-1.788838
11	6	0	8.965729	0.554736	-1.945710
12	6	0	8.262695	1.774312	-2.105491
13	6	0	6.906145	1.770133	-2.226743
14	1	0	6.701941	-2.813348	-1.883521
15	1	0	2.140594	0.259378	-2.529298
16	1	0	0.844783	-1.788573	-2.482259
17	1	0	4.234077	1.442729	-2.438587
18	1	0	10.044954	0.571046	-1.850433
19	1	0	8.810854	2.708216	-2.130536
20	1	0	6.360988	2.699496	-2.349362
21	7	0	4.072136	-3.082166	-2.100220
22	1	0	4.633134	-3.909218	-1.952707
23	5	0	2.662787	-3.185735	-2.215987
24	6	0	1.982181	-4.595083	-2.180446
25	6	0	2.653014	-5.755788	-2.581996
26	6	0	0.663693	-4.738711	-1.736281
27	6	0	2.043221	-7.000173	-2.538502
28	1	0	3.667868	-5.687947	-2.962132
29	6	0	0.048414	-5.980440	-1.678273
30	1	0	0.110718	-3.861667	-1.418188
31	6	0	0.737691	-7.115400	-2.081127
32	1	0	2.583655	-7.881171	-2.864760
33	1	0	-0.971519	-6.063677	-1.321261
34	1	0	0.257964	-8.086403	-2.043382

4-H Ph BN Anthracene (ld) Coordinates – Geometry Abstracted from Crystal Structure

E(RCAM-B3LYP)= -773.54847954 E_h No. Imaginary Frequencies= N/A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.303500	3.236300	8.009100
2	6	0	1.056600	4.137000	9.021600
3	1	0	0.595000	4.944600	8.828600
4	6	0	1.481600	3.875000	10.340400
5	6	0	1.262200	4.801500	11.401800
6	1	0	0.804600	5.616200	11.230000
7	6	0	1.707000	4.526600	12.667400
8	1	0	1.550900	5.151800	13.366200
9	6	0	2.395500	3.324100	12.948100
10	1	0	2.704700	3.151600	13.829300
11	6	0	2.617500	2.406400	11.957900
12	1	0	3.080200	1.601100	12.157600
13	6	0	2.159900	2.650100	10.626300
14	6	0	2.352000	1.726500	9.590200
15	1	0	2.774400	0.897700	9.780600
16	6	0	1.939600	1.993100	8.290000
17	6	0	2.198100	1.045400	7.221900
18	1	0	2.581200	0.202500	7.435100
19	6	0	1.908900	1.329700	5.928700
20	1	0	2.087300	0.689300	5.250100
21	6	0	1.044300	3.169200	4.084600
22	6	0	0.419000	4.387100	3.761100
23	1	0	0.134000	4.964000	4.460200
24	6	0	0.207500	4.766200	2.435800
25	1	0	-0.221500	5.591500	2.242300
26	6	0	0.622000	3.942100	1.396400
27	1	0	0.472600	4.197600	0.493200
28	6	0	1.261200	2.733100	1.690900
29	1	0	1.556300	2.166800	0.987800
30	6	0	1.463700	2.362800	3.014000
31	1	0	1.899200	1.539300	3.200000
32	5	0	1.290100	2.692400	5.560400
33	7	0	0.983400	3.525400	6.676600
34	1	0	0.560600	4.280000	6.516100

4-F Ph BN Anthracene (1d) Coordinates

E(RCAM-B3LYP)= -873.01555113 E_h No. Imaginary Frequencies= 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.791561	-1.898412	-2.126480
2	6	0	4.072570	-0.674842	-2.280282
3	6	0	2.630488	-0.705994	-2.395646
4	6	0	1.923788	-1.851832	-2.362957
5	6	0	6.163975	-1.879758	-2.007846
6	6	0	4.777445	0.510977	-2.312080
7	6	0	6.174998	0.552101	-2.194982
8	6	0	6.882450	-0.673338	-2.038300
9	6	0	8.297998	-0.630566	-1.919067
10	1	0	8.839297	-1.562411	-1.799576
11	6	0	8.965999	0.556388	-1.953737
12	6	0	8.261616	1.775701	-2.109556
13	6	0	6.904749	1.770849	-2.226605
14	1	0	6.705170	-2.813292	-1.889794
15	1	0	2.139505	0.256822	-2.515775
16	1	0	0.845415	-1.790509	-2.468790
17	1	0	4.232382	1.441845	-2.430289
18	1	0	10.045474	0.573408	-1.861771
19	1	0	8.809116	2.709952	-2.134924
20	1	0	6.358572	2.699978	-2.346162
21	7	0	4.074836	-3.084124	-2.098780
22	1	0	4.638406	-3.909409	-1.951748
23	5	0	2.665279	-3.187947	-2.211297
24	6	0	1.983624	-4.596012	-2.178157
25	6	0	2.655318	-5.760134	-2.568930
26	6	0	0.659372	-4.737744	-1.749175
27	6	0	2.049843	-7.006125	-2.532007
28	1	0	3.674111	-5.698734	-2.937650
29	6	0	0.034189	-5.973698	-1.692450
30	1	0	0.102353	-3.860979	-1.439421
31	6	0	0.745016	-7.088990	-2.087720
32	1	0	2.565166	-7.905538	-2.843524
33	1	0	-0.987370	-6.085518	-1.352614
34	9	0	0.147634	-8.292936	-2.044121

4-Cl Ph BN Anthracene (1e) Coordinates

E(RCAM-B3LYP)= -1233.39320376 E_h No. Imaginary Frequencies= 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.790654	-1.898377	-2.127269
2	6	0	4.072707	-0.675113	-2.287618
3	6	0	2.631382	-0.705564	-2.409461
4	6	0	1.923573	-1.851009	-2.376614
5	6	0	6.162445	-1.880346	-2.002184
6	6	0	4.778404	0.510427	-2.319247
7	6	0	6.175214	0.551027	-2.195633
8	6	0	6.881479	-0.674370	-2.032385
9	6	0	8.296499	-0.631983	-1.906469
10	1	0	8.836821	-1.563721	-1.781966
11	6	0	8.965046	0.554596	-1.941002
12	6	0	8.261896	1.773866	-2.103367
13	6	0	6.905688	1.769468	-2.226918
14	1	0	6.702584	-2.813824	-1.879079
15	1	0	2.141470	0.257134	-2.534536
16	1	0	0.845708	-1.790255	-2.487473
17	1	0	4.234367	1.441227	-2.442430
18	1	0	10.044058	0.571454	-1.843870
19	1	0	8.809965	2.707780	-2.128499
20	1	0	6.360557	2.698535	-2.351472
21	7	0	4.073056	-3.083931	-2.099920
22	1	0	4.635047	-3.909611	-1.948512
23	5	0	2.664625	-3.185301	-2.217258
24	6	0	1.982147	-4.594804	-2.181805
25	6	0	2.645284	-5.755760	-2.592396
26	6	0	0.666937	-4.739945	-1.730454
27	6	0	2.039475	-7.001454	-2.553252
28	1	0	3.657398	-5.693441	-2.979133
29	6	0	0.043422	-5.976540	-1.671217
30	1	0	0.114071	-3.866329	-1.404294
31	6	0	0.739492	-7.099030	-2.086096
32	1	0	2.563312	-7.888521	-2.883904
33	1	0	-0.972056	-6.072954	-1.310464
34	17	0	-0.036960	-8.665037	-2.025701

4-CF_3 Ph BN Anthracene (1f) Coordinates

E(RCAM-B3LYP)= -1110.83368392 E_h No. Imaginary Frequencies= 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.779964	-1.898082	-2.133331
2	6	0	4.070474	-0.672445	-2.311041
3	6	0	2.631566	-0.696163	-2.457030
4	6	0	1.917227	-1.838102	-2.431141
5	6	0	6.149498	-1.886495	-1.985378
6	6	0	4.782523	0.509764	-2.335941
7	6	0	6.177063	0.543881	-2.189388
8	6	0	6.874654	-0.684169	-2.009143
9	6	0	8.287703	-0.648163	-1.860215
10	1	0	8.821316	-1.581920	-1.722849
11	6	0	8.962340	0.534972	-1.889011
12	6	0	8.267826	1.756989	-2.068200
13	6	0	6.913970	1.758793	-2.213948
14	1	0	6.682883	-2.821998	-1.849174
15	1	0	2.148626	0.268399	-2.593894
16	1	0	0.841593	-1.773531	-2.559470
17	1	0	4.245259	1.442645	-2.472096
18	1	0	10.039662	0.547218	-1.774323
19	1	0	8.820927	2.688028	-2.088367
20	1	0	6.375526	2.689892	-2.351438
21	7	0	4.055983	-3.080383	-2.113355
22	1	0	4.610848	-3.908865	-1.950712
23	5	0	2.650244	-3.173087	-2.253495
24	6	0	1.960651	-4.582107	-2.220784
25	6	0	2.616580	-5.740086	-2.651020
26	6	0	0.649135	-4.721697	-1.756530
27	6	0	2.002519	-6.980893	-2.613744
28	1	0	3.623169	-5.674138	-3.050704
29	6	0	0.025145	-5.957052	-1.703238
30	1	0	0.105291	-3.845988	-1.421553
31	6	0	0.704821	-7.088214	-2.133299
32	1	0	2.520456	-7.863472	-2.966290
33	1	0	-0.990795	-6.045550	-1.340243
34	6	0	0.051870	-8.432923	-2.035783
35	9	0	0.513549	-9.287440	-2.963981
36	9	0	0.272023	-9.007660	-0.838393
37	9	0	-1.280732	-8.358995	-2.187804

4-CF_3 Ph BN Anthracene (1f) Coordinates– Geometry Abstracted from Crystal Structure

E(RCAM-B3LYP= -1110.62149968 E_h No. Imaginary Frequencies= N/A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.025000	0.357400	8.943400
2	1	0	2.349800	-0.721900	7.540900
3	6	0	2.807100	-0.538800	9.969600
4	1	0	2.350000	-1.352300	9.791800
5	6	0	3.252200	-0.267100	11.282500
6	6	0	3.065500	-1.189200	12.351500
7	1	0	2.613900	-2.009700	12.191900
8	6	0	3.530700	-0.903300	13.606700
9	1	0	3.399700	-1.528400	14.309900
10	6	0	4.206500	0.315200	13.868800
11	1	0	4.530800	0.498900	14.741300
12	6	0	4.392500	1.226100	12.868800
13	1	0	4.842100	2.042000	13.054700
14	6	0	3.919400	0.967300	11.549800
15	6	0	4.084000	1.885900	10.501800
16	1	0	4.501400	2.719900	10.683800
17	6	0	3.655900	1.614700	9.211600
18	6	0	3.886300	2.549700	8.132800
19	1	0	4.263100	3.397800	8.335500
20	6	0	3.585400	2.260300	6.846800
21	1	0	3.750800	2.897200	6.162500
22	6	0	2.699600	0.400900	5.031500
23	6	0	2.068500	-0.816400	4.730500
24	1	0	1.783700	-1.379300	5.442400
25	6	0	1.850700	-1.217900	3.419500
26	1	0	1.420200	-2.044900	3.236900
27	6	0	2.267700	-0.400900	2.373800
28	6	0	2.898000	0.804700	2.631000
29	1	0	3.180100	1.360500	1.913600
30	6	0	3.114600	1.194400	3.947900
31	1	0	3.554900	2.018500	4.119100
32	5	0	2.972700	0.891000	6.502400
33	7	0	2.688900	0.061400	7.616500
34	6	0	2.035100	-0.862200	0.964600
35	9	0	0.808400	-1.334700	0.776500
36	9	0	2.878400	-1.842400	0.610700
37	9	0	2.213900	0.102100	0.053200

4-CN Ph BN Anthracene (1g) Coordinates

E(RCAM-B3LYP)= -865.99180613 E_h No. Imaginary Frequencies= 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.783575	-1.903169	-2.130148
2	6	0	4.068620	-0.680002	-2.301793
3	6	0	2.628894	-0.708029	-2.435763
4	6	0	1.917924	-1.852214	-2.403724
5	6	0	6.154114	-1.887568	-1.992896
6	6	0	4.776791	0.504623	-2.332161
7	6	0	6.172149	0.542933	-2.196583
8	6	0	6.875119	-0.682951	-2.021991
9	6	0	8.289158	-0.642584	-1.883845
10	1	0	8.826806	-1.574609	-1.750709
11	6	0	8.959615	0.542712	-1.917528
12	6	0	8.259812	1.762596	-2.091194
13	6	0	6.904982	1.760298	-2.226594
14	1	0	6.691562	-2.821362	-1.861072
15	1	0	2.141743	0.254924	-2.568562
16	1	0	0.841072	-1.790903	-2.523002
17	1	0	4.235574	1.435824	-2.463840
18	1	0	10.037711	0.558484	-1.811029
19	1	0	8.809866	2.695320	-2.115397
20	1	0	6.362607	2.689707	-2.359768
21	7	0	4.063429	-3.088165	-2.104930
22	1	0	4.622579	-3.914614	-1.946514
23	5	0	2.657256	-3.183563	-2.232592
24	6	0	1.971363	-4.595187	-2.194124
25	6	0	2.622176	-5.749237	-2.644177
26	6	0	0.670350	-4.740206	-1.701467
27	6	0	2.014875	-6.991352	-2.602277
28	1	0	3.621352	-5.678028	-3.060798
29	6	0	0.049110	-5.974944	-1.640642
30	1	0	0.133740	-3.867758	-1.347119
31	6	0	0.721991	-7.108926	-2.093537
32	1	0	2.530271	-7.872453	-2.962743
33	1	0	-0.955124	-6.070235	-1.247756
34	6	0	0.085778	-8.391175	-2.041195
35	7	0	-0.423540	-9.419732	-1.998804

4-NO_2 Ph BN Anthracene (1h) Coordinates

E(RCAM-B3LYP)= -978.26118211 E_h No. Imaginary Frequencies= 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.763101	-1.887146	-2.171310
2	6	0	4.071684	-0.659328	-1.945503
3	6	0	2.637130	-0.671271	-1.763711
4	6	0	1.908993	-1.804662	-1.799949
5	6	0	6.128305	-1.886668	-2.354685
6	6	0	4.797345	0.514635	-1.910093
7	6	0	6.187692	0.537487	-2.091897
8	6	0	6.866909	-0.692956	-2.320446
9	6	0	8.275963	-0.668157	-2.505503
10	1	0	8.795491	-1.603677	-2.679672
11	6	0	8.963926	0.506817	-2.465409
12	6	0	8.287790	1.731247	-2.238001
13	6	0	6.938424	1.743811	-2.056781
14	1	0	6.647630	-2.823998	-2.527539
15	1	0	2.168415	0.294492	-1.591140
16	1	0	0.837651	-1.732070	-1.643397
17	1	0	4.274208	1.449456	-1.737488
18	1	0	10.037928	0.510826	-2.608100
19	1	0	8.851602	2.655590	-2.209505
20	1	0	6.414183	2.676788	-1.882415
21	7	0	4.025680	-3.061551	-2.200896
22	1	0	4.567425	-3.891521	-2.397127
23	5	0	2.623701	-3.140222	-2.028541
24	6	0	1.916941	-4.542215	-2.079761
25	6	0	2.563642	-5.712478	-1.665461
26	6	0	0.603564	-4.657714	-2.548148
27	6	0	1.940600	-6.947515	-1.718908
28	1	0	3.571874	-5.661432	-1.268882
29	6	0	-0.037998	-5.882575	-2.621103
30	1	0	0.072419	-3.770972	-2.873361
31	6	0	0.646090	-7.009727	-2.202778
32	1	0	2.430357	-7.854286	-1.394126
33	1	0	-1.048896	-5.981137	-2.989832
34	7	0	-0.027058	-8.319689	-2.270279
35	8	0	-1.164791	-8.346449	-2.694718
36	8	0	0.597587	-9.292947	-1.898096

Mes BN Anthracene (1i) Coordinates

E(RCAM-B3LYP)= -891.66835405 E_h No. Imaginary Frequencies= 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.739066	-1.853051	-2.010126
2	6	0	4.327148	-0.869524	-2.959113
3	6	0	3.141020	-1.099870	-3.755336
4	6	0	2.395222	-2.215851	-3.640427
5	6	0	5.866959	-1.644022	-1.247256
6	6	0	5.077304	0.281464	-3.091250
7	6	0	6.228480	0.514363	-2.324156
8	6	0	6.630919	-0.473173	-1.380820
9	6	0	7.797574	-0.236015	-0.604307
10	1	0	8.106128	-0.986585	0.114785
11	6	0	8.516948	0.910763	-0.757248
12	6	0	8.116098	1.893382	-1.696051
13	6	0	7.003426	1.698188	-2.456500
14	1	0	6.174619	-2.396047	-0.527533
15	1	0	2.879038	-0.314873	-4.461093
16	1	0	1.518080	-2.321001	-4.270874
17	1	0	4.765814	1.030366	-3.812192
18	1	0	9.404155	1.077714	-0.158069
19	1	0	8.700194	2.799116	-1.804317
20	1	0	6.690359	2.445541	-3.177165
21	7	0	3.977376	-3.005068	-1.885051
22	1	0	4.313172	-3.665579	-1.198026
23	5	0	2.806822	-3.296921	-2.628080
24	6	0	2.044936	-4.651423	-2.372024
25	6	0	2.377131	-5.806890	-3.095866
26	6	0	1.005765	-4.719199	-1.432476
27	6	0	1.683962	-6.990634	-2.869949
28	6	0	0.330996	-5.918272	-1.228541
29	6	0	0.657917	-7.067694	-1.936055
30	1	0	1.948281	-7.875072	-3.441861
31	1	0	-0.474852	-5.953691	-0.501698
32	6	0	-0.062852	-8.365302	-1.684243
33	1	0	-0.147371	-8.956886	-2.597659
34	1	0	0.471404	-8.973944	-0.948709
35	1	0	-1.068715	-8.192512	-1.298116
36	6	0	3.480256	-5.773497	-4.125671
37	1	0	3.304438	-4.995327	-4.873083
38	1	0	4.449686	-5.560267	-3.667420
39	1	0	3.562137	-6.727252	-4.648302
40	6	0	0.609322	-3.497165	-0.639975
41	1	0	1.415982	-3.170255	0.021759
42	1	0	0.375722	-2.654829	-1.296262
43	1	0	-0.267665	-3.694252	-0.022298

Mes BN Anthracene (1i) Coordinates- Geometry Abstracted from Crystal Structure

E(RCAM-B3LYP)= - 891.41622676 E_h No. Imaginary Frequencies= N/A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.456600	3.571000	14.270800
2	6	0	1.560200	4.014100	15.580400
3	1	0	2.145900	4.732500	15.786400
4	6	0	0.810200	3.414600	16.610000
5	6	0	0.894000	3.849800	17.968900
6	1	0	1.474200	4.566000	18.197300
7	6	0	0.148000	3.246700	18.942900
8	1	0	0.220600	3.544700	19.841600
9	6	0	-0.734400	2.179900	18.625500
10	1	0	-1.254400	1.775900	19.310400
11	6	0	-0.837000	1.734000	17.340100
12	1	0	-1.426900	1.017800	17.138200
13	6	0	-0.070600	2.330700	16.297400
14	6	0	-0.153700	1.889000	14.965100
15	1	0	-0.729800	1.164300	14.754400
16	6	0	0.579800	2.480700	13.950000
17	6	0	0.474000	2.025600	12.586400
18	1	0	-0.108800	1.301500	12.389700
19	6	0	1.172300	2.588800	11.578200
20	1	0	1.090300	2.252400	10.692900
21	6	0	2.931500	4.578800	10.790700
22	6	0	2.411400	5.756600	10.220100
23	6	0	3.182400	6.496300	9.321700
24	1	0	2.822100	7.288600	8.940400
25	6	0	4.466000	6.097300	8.975400
26	6	0	4.947500	4.900300	9.492100
27	1	0	5.808500	4.594500	9.231400
28	6	0	4.195700	4.137200	10.384500
29	6	0	1.016100	6.202600	10.575500
30	1	0	0.751000	6.943700	9.991600
31	1	0	0.995700	6.499100	11.508700
32	1	0	0.393900	5.454400	10.457500
33	6	0	5.327100	6.950800	8.076300
34	1	0	6.024100	6.396000	7.668200
35	1	0	5.744400	7.664100	8.603300
36	1	0	4.772100	7.347600	7.372400
37	6	0	4.746700	2.834900	10.914500
38	1	0	5.642800	2.685600	10.546600
39	1	0	4.157100	2.098100	10.648300
40	1	0	4.797100	2.875500	11.891900
41	5	0	2.100700	3.778700	11.870800
42	7	0	2.171900	4.165500	13.233000
43	1	0	2.708200	4.850500	13.482200

BN Anthracene Coordinates

E(RCAM-B3LYP)= -542.78164322 E_h No. Imaginary Frequencies= 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.831231	-1.916416	-2.148587
2	6	0	4.083841	-0.700317	-2.151873
3	6	0	2.638070	-0.749110	-2.154098
4	6	0	1.950979	-1.908919	-2.153186
5	6	0	6.209170	-1.878582	-2.146458
6	6	0	4.769160	0.499147	-2.152846
7	6	0	6.169273	0.559460	-2.150717
8	6	0	6.905130	-0.660506	-2.147452
9	6	0	8.326029	-0.597462	-2.145302
10	1	0	8.888190	-1.524691	-2.142808
11	6	0	8.971688	0.601368	-2.146340
12	6	0	8.239255	1.815158	-2.149589
13	6	0	6.878342	1.792125	-2.151710
14	1	0	6.770196	-2.808123	-2.143951
15	1	0	2.127482	0.211232	-2.156581
16	1	0	0.866930	-1.868670	-2.154981
17	1	0	4.202380	1.424758	-2.155353
18	1	0	10.054816	0.633610	-2.144681
19	1	0	8.770029	2.759456	-2.150375
20	1	0	6.311188	2.716445	-2.154207
21	7	0	4.134948	-3.114863	-2.147625
22	1	0	4.715530	-3.940778	-2.145265
23	5	0	2.728027	-3.226838	-2.149672
24	1	0	2.249967	-4.317409	-2.148546

4-Me Ph Anthracene (8b) Coordinates

E(RCAM-B3LYP)= -809.61124113 E_h No. Imaginary Frequencies= 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.323709	-5.801957	0.938624
2	6	0	-1.978967	-5.797258	0.752767
3	6	0	-1.236596	-4.578641	0.793465
4	6	0	-1.939268	-3.354735	1.035027
5	6	0	-3.353601	-3.405068	1.225215
6	6	0	-4.022589	-4.585300	1.178922
7	6	0	0.143348	-4.542870	0.607768
8	6	0	-1.227075	-2.158958	1.077123
9	6	0	0.152418	-2.123252	0.888799
10	6	0	0.853446	-3.347510	0.651318
11	6	0	2.267488	-3.288786	0.466153
12	1	0	2.803588	-4.211526	0.274132
13	6	0	2.932263	-2.108733	0.516396
14	6	0	2.243865	-0.875129	0.753377
15	6	0	0.891909	-0.904971	0.932808
16	1	0	0.677225	-5.469921	0.425900
17	1	0	-3.875462	-6.733721	0.905342
18	1	0	-1.443920	-6.722423	0.569774
19	1	0	-3.883667	-2.477044	1.408091
20	1	0	-5.095847	-4.609446	1.324900
21	1	0	-1.760424	-1.231958	1.260543
22	1	0	4.002548	-2.084523	0.351496
23	1	0	0.352698	0.012545	1.139911
24	6	0	3.003494	0.396389	0.803378
25	6	0	2.497702	1.563937	0.231383
26	6	0	4.245535	0.466748	1.433548
27	6	0	3.204337	2.753415	0.294338
28	1	0	1.546684	1.533780	-0.287048
29	6	0	4.948360	1.659413	1.495237
30	1	0	4.656446	-0.417284	1.906882
31	6	0	4.443469	2.824112	0.925284
32	1	0	2.787768	3.644454	-0.163345
33	1	0	5.905900	1.686835	2.004177
34	6	0	5.222575	4.111018	0.963157
35	1	0	5.818620	4.234361	0.054232
36	1	0	4.559986	4.974917	1.039083
37	1	0	5.908688	4.134827	1.811101

4-H Ph Anthracene (8a) Coordinates

E(RCAM-B3LYP)= -770.30869066 E_h No. Imaginary Frequencies= 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.322239	-5.801462	0.912772
2	6	0	-1.976041	-5.796384	0.737476
3	6	0	-1.234387	-4.577578	0.784601
4	6	0	-1.939388	-3.354037	1.021365
5	6	0	-3.355102	-3.404760	1.200431
6	6	0	-4.023362	-4.585198	1.148220
7	6	0	0.146981	-4.541433	0.609667
8	6	0	-1.227846	-2.158090	1.069741
9	6	0	0.152974	-2.122115	0.892080
10	6	0	0.856448	-3.345927	0.659321
11	6	0	2.271869	-3.286662	0.485369
12	1	0	2.809959	-4.209017	0.297131
13	6	0	2.936106	-2.106478	0.542097
14	6	0	2.244784	-0.873700	0.773451
15	6	0	0.891537	-0.903451	0.941708
16	1	0	0.682390	-5.468329	0.431537
17	1	0	-3.873357	-6.733429	0.874644
18	1	0	-1.439442	-6.721383	0.558224
19	1	0	-3.886907	-2.477020	1.379698
20	1	0	-5.097733	-4.609642	1.285755
21	1	0	-1.762824	-1.231306	1.249525
22	1	0	4.007799	-2.081983	0.386587
23	1	0	0.350445	0.014011	1.144161
24	6	0	3.002789	0.399238	0.832412
25	6	0	2.502992	1.560474	0.241087
26	6	0	4.234235	0.466726	1.485724
27	6	0	3.207069	2.752657	0.308792
28	1	0	1.563268	1.520453	-0.296628
29	6	0	4.938603	1.658894	1.554624
30	1	0	4.633423	-0.418795	1.965995
31	6	0	4.427658	2.807122	0.966732
32	1	0	2.804666	3.641224	-0.163183
33	1	0	5.888284	1.691793	2.075422
34	1	0	4.978806	3.738355	1.018214

4-H Ph Anthracene (8a) Coordinates- Geometry Abstracted from Crystal Structure

E(RCAM-B3LYP)= -770.09420845 E_h No. Imaginary Frequencies= N/A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.875500	2.607200	7.999600
2	6	0	6.633100	3.497700	9.045400
3	1	0	6.180600	4.313300	8.866300
4	6	0	7.040300	3.217400	10.351500
5	6	0	6.812000	4.129700	11.432900
6	1	0	6.363800	4.951200	11.267500
7	6	0	7.230800	3.832300	12.692600
8	1	0	7.066200	4.444900	13.400700
9	6	0	7.913100	2.614300	12.959800
10	1	0	8.206600	2.421900	13.842700
11	6	0	8.147900	1.718500	11.956500
12	1	0	8.606300	0.908800	12.148700
13	6	0	7.713800	1.985200	10.625900
14	6	0	7.921600	1.070500	9.588900
15	1	0	8.346600	0.241400	9.773200
16	6	0	7.514200	1.356700	8.286200
17	6	0	7.740100	0.458500	7.206500
18	1	0	8.100000	-0.402500	7.383400
19	6	0	7.449800	0.810200	5.921200
20	1	0	7.637200	0.195900	5.221700
21	6	0	6.866900	2.088500	5.594100
22	6	0	6.566800	2.930000	6.645300
23	1	0	6.137400	3.756800	6.459400
24	6	0	6.657500	2.469100	4.169100
25	6	0	7.123100	1.662400	3.123000
26	1	0	7.579100	0.855100	3.328100
27	6	0	6.934100	2.014100	1.792700
28	1	0	7.252000	1.444000	1.103700
29	6	0	6.282300	3.197300	1.468700
30	1	0	6.149200	3.437500	0.559000
31	6	0	5.828700	4.024700	2.483400
32	1	0	5.393000	4.840800	2.270000
33	6	0	6.008400	3.663500	3.817400
34	1	0	5.685500	4.237100	4.503000

4-F Ph Anthracene (8c) Coordinates

E(RCAM-B3LYP)= -869.55600437 E_h No. Imaginary Frequencies= 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.320047	-5.803868	0.898455
2	6	0	-1.974465	-5.797093	0.719111
3	6	0	-1.233385	-4.578175	0.771990
4	6	0	-1.938254	-3.356558	1.018693
5	6	0	-3.353397	-3.409039	1.201702
6	6	0	-4.021047	-4.589484	1.143898
7	6	0	0.147440	-4.540312	0.593358
8	6	0	-1.227292	-2.160511	1.072669
9	6	0	0.152940	-2.122902	0.891359
10	6	0	0.856311	-3.344742	0.648834
11	6	0	2.271218	-3.283954	0.471239
12	1	0	2.808827	-4.204911	0.275261
13	6	0	2.935285	-2.104019	0.532953
14	6	0	2.244011	-0.873345	0.775385
15	6	0	0.891425	-0.904486	0.947930
16	1	0	0.682795	-5.465700	0.407705
17	1	0	-3.870965	-6.735717	0.855993
18	1	0	-1.437924	-6.720567	0.532255
19	1	0	-3.885099	-2.482781	1.388524
20	1	0	-5.094941	-4.615540	1.284517
21	1	0	-1.762313	-1.235298	1.260042
22	1	0	4.006299	-2.078402	0.372613
23	1	0	0.350408	0.010980	1.159751
24	6	0	3.001582	0.399142	0.839016
25	6	0	2.500933	1.564050	0.255505
26	6	0	4.234323	0.465313	1.490709
27	6	0	3.197689	2.759863	0.324843
28	1	0	1.560716	1.528984	-0.280767
29	6	0	4.943602	1.653065	1.569176
30	1	0	4.636829	-0.421032	1.965637
31	6	0	4.410319	2.783461	0.983555
32	1	0	2.820856	3.665603	-0.132194
33	1	0	5.894789	1.715478	2.081594
34	9	0	5.093717	3.939950	1.053600