Supporting Information

Understanding the Regioselectivity in Scholl Reactions for the Synthesis of Oligoarenes

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1) Synthetic details

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1) Synthetic details

Representative procedure
Representative procedure for the $FeCl_3$ mediated Scholl reaction (**8a**): Quinquephenyl **6a** (100 mg, 129 µmol, 1.0 eq) was dissolved in anhydrous CH_2Cl_2 (50 mL). While maintaining a constant flow of argon through the solution anhydrous $FeCl_3$ (167 mg, 1.03 mmol, 8 eq) dissolved in nitromethane (0.6 mL) was added drop wise. After 30 min methanol (20 mL) was added and the solution was stirred additional 5 minutes. After the solution was washed with water (2 x 20 mL) the organic layer was filtered through a short pad of silica gel (eluent: dichloromethane). Recrystallization of the crude product with dichloromethane/methanol afforded the product **8a** (71 mg, 96 µmol, 74%) as a yellowish solid.
^{1}H NMR ($CDCl_3$, 300 MHz): δ = 9.52 (s, 1H), 8.84-8.76 (m, 3H), 8.71 (d, *J* = 7.9 Hz, 1H), 8.51 (s, 1H), 8.38 (s, 1H), 8.37 (s, 1H), 8.27 (s, 1H), 7.92 (t, *J* = 7.9 Hz, 1H), 7.85 (t, *J* = 7.9 Hz, 1H), 4.26 (s, 3H), 2.89 (t, *J* = 7.8 Hz, 4H), 2.81 (t, *J* = 7.9 Hz, 4H), 1.90-1.70 (m, 8H), 1.64-1.38 (m, 24H), 1.03-0.94 (m, 12H). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ = 156.4, 140.4, 140.2, 139.6, 139.5, 130.5, 130.5, 129.3, 129.1, 128.8, 128.5, 128.2, 127.8, 127.8, 127.6, 126.3, 126.1, 125.2, 124.6, 124.3, 123.5, 123.3, 123.0, 121.0, 120.9, 120.9, 120.7, 118.2, 118.0, 104.3, 56.3, 33.3, 33.2, 33.2, 32.0, 31.9, 31.5, 31.4, 31.2, 29.7, 29.6, 22.8, 14.2. **IR**: 2953, 2922, 2855, 1604, 1455, 1383, 1228, 801, 753 cm^{-1}. **MS (APCI)**: m/z = 744 ($M+H^+$, 100), 660 (72), 575 (23). **HRMS (APCI)**: calculated for $C_{55}H_{67}O$ ($M + H^+$): m/z = 743.5186; found: m/z = 743.5183.

Synthesis of starting materials

2-[(Phenyl)ethinyl]-4,4,5,5-tetramethyl-1,3,2-dioxaborolane was prepared according to a procedure reported by Brown[1] and purified by filtration over celites and recrystallization from pentane.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.54-7.51 (m, 2H), 7.39-7.28 (m, 3H), 1.32 (s, 12H). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ = 132.5, 129.4, 128.3, 121.9, 84.4, 24.7.

The analytical data are in accordance with the literature, see H. C. Brown, N .G. Bhat, M. Srebnik, *Tetrahedron Lett.* **1988**, *29*, 2681.

Enyne metathesis

2-[4,5-Dihexyl(1,1'-biphenyl)-2-yl]-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2)

In a glass autoclave 7-tetradecyne (1.17 g, 6.00 mmol, 1.0 equiv) and Grubbs II catalyst(153 mg, 0.18 mmol, 3 mol%) were dissolved in 15 mL CH_2Cl_2 and reacted 5 h at 60 °C with ethene (7.5 bar). The solution was filtered through a short pad of silica gel (pentane/diethyl ether). The solvent was removed and the crude 1,3-diene was used without further purification in the Diels-Alder reaction.

Diels-Alder reaction: $CoBr_2$(dppe) (370 mg, 0.60 mmol, 15 mol%), zinc dust (78 mg, 1.20 mmol, 30 mol%) and anhydrous zinc iodide (383 mg, 1.20 mmol, 30 mol%) were dissolved in 5 mL CH_2Cl_2. 2-[(Phenyl)ethinyl]-4,4,5,5-tetramethyl-1,3,2-dioxaborolan (912 mg, 4.00 mmol, 1.0 equiv) and the crude 1,3-diene (approx. 6.0 mmol, 1.5 equiv) were added subsequent. The mixture was stirred over night at room temperature followed by filtration through a short pad of silica gel (pentane/diethyl

ether). The solvent was removed and the residual dihydroaromatic intermediate was oxidized with DDQ (1.14 g, 5.00 mmol, 1.25 equiv) in toluene (20 mL) to give the corresponding aromatic product. After filtration through a short pad of deactivated silica gel (pentane/diethyl ether) the solvent was removed and the residue was purified by column chromatography (silica gel, eluent pentane/diethyl ether 15:1). The product **2** was isolated as yellowish oil (1.60 g, 3.57 mmol, 89%).

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.50 (s, 1H), 7.41-7.29 (m, 5H), 7.16 (s, 1H), 2.67-2.59 (m, 4H), 1.66-1.53 (m, 4H), 1.45-1.27 (m, 12H), 1.21 (s, 12H), 0.94-0.86 (m, 6H). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ = 145.2, 143.4, 142.8, 138.7, 135.7, 130.1, 129.2, 127.6, 126.4, 83.4, 32.8, 32.5, 31.8, 31.6, 31.2, 29.6, 29.4, 24.6, 22.7, 22.6, 14.1. **IR (cm^{-1})**: 2656, 2928, 2858, 1602, 1545, 1486, 1466, 1397, 1341, 1309, 1270, 1142, 1077, 969, 859, 700. **MS (EI)**: m/z = 448 (M^+, 100), 347(9), 333 (11), 308 (42), 277 (9), 202 (15), 191 (24), 181 (12), 101 (10), 83 (14). **HRMS (EI)**: calculated for $C_{30}H_{45}BO_2$: m/z = 448.3513; found: m/z = 448.3504.

Suzuki reactions

Arylboronic ester **2** (1.2 equiv per coupling), an aryl bromide (1.0 equiv), $Pd(OAc)_2$ (2.5-5 mol% per coupling), S-Phos (2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl) (5-10 mol% per coupling), $K_3PO_4 \cdot H_2O$ (3 equiv per coupling) were added to a sealed tube and shortly evacuated. Toluene and water (10:1) were added and after 3 min at room temperature the sealed tube was heated to 100 °C for 16 h-3 d. After filtration through a short pad of deactivated silica gel the solvent was removed and the residue was purified by column chromatography.

4',5',4''',5'''-Tetrahexyl-1,1':2',1'':4'',1''':2''',1''''-quinquephenyl (**3**):
yield: 98%, yellowish oil, eluent: pentane/CH_2Cl_2 10:1.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.24-7.16 (m, 10H), 7.15-7.09 (m, 4H), 6.97 (s, 4H), 2.66 (t, J = 7.9 Hz, 8H), 1.70-1.57 (m, 8H), 1.49-1.29 (m, 24H), 0.94-0.87 (m, 12H). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ = 141.7, 139.9, 139.8, 139.5, 137.8, 137.6, 131.3, 131.2, 129.9, 129.4, 127.7, 126.1, 32.5, 31.8, 31.4, 31.4, 29.6, 29.6, 22.6, 14.1. **IR (cm^{-1})**: 3005, 2956, 2924, 2855, 1599, 1480, 1465, 1377, 892, 843, 769, 700, 589. **MS (EI)**: m/z = 718 (M^+, 2), 346 (98), 322 (66), 302 (19), 181 (100), 167 (13), 144 (11). **HRMS (EI)**: calculated for $C_{54}H_{70}$: m/z = 718.5478; found: m/z = 718.5475.

4',5',4''',5'''-Tetrahexyl-2'',5''-dimethoxy-1,1':2',1'':4'',1''':2''',1''''-quinquephenyl (**6a**):
yield: 97%, colorless oil, eluent: pentane/CH_2Cl_2 4:1.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.25-7.20 (m, 6H), 7.20-7.13 (m, 8H), 6.56 (s, 2H), 3.13 (s, 6H), 2.70-2.62 (m, 8H), 1.65 (quin, J = 7.5 Hz, 8H), 1.49-1.29 (m, 24H), 0.95-0.87 (m, 12H). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ = 150.1, 142.4, 140.0, 139.5, 138.7, 134.2, 131.6, 130.5, 129.9, 128.9, 127.4, 125.9, 115.2, 55.4, 32.6, 32.4, 31.8, 31.2, 31.2, 29.6, 29.6, 22.7, 14.1. **IR (cm^{-1})**: 3011, 2955, 2927, 2853, 1500, 1484, 1463, 1393, 1212, 1040, 896, 780, 756, 695. **HRMS (APCI)**: calculated for $C_{56}H_{75}O_2$ ($M + H^+$): m/z = 779.5762; found: m/z = 779.5751.

2'',5''-Difluoro-4',5',4''',5'''-tetrahexyl-1,1':2',1'':4'',1''':2''',1''''-quinquephenyl (**6b**):
yield: 98%, white solid, eluent: pentane/CH_2Cl_2 20:1.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.25-7.20 (m, 8H), 7.16-7.11 (m, 6H), 6.71 (t, J = 8.0 Hz, 2H), 2.70-2.61 (m, 8H), 1.69-1.56 (m, 8H), 1.48-1.28 (m, 24H), 0.94-0.86 (m, 12H). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ = 155.1 (dd, J = 244, 3 Hz), 141.3, 141.0, 139.7, 138.9, 131.5, 130.9, 130.6, 129.3 (dd, J = 18, 12 Hz), 129.1, 127.8, 126.5, 118.3 (dd, J = 18, 12 Hz), 32.6, 32.4, 31.8, 31.2, 29.6, 29.5, 22.6, 14.1. **^{19}F NMR** ($CDCl_3$, 282 MHz): δ = -122.0. **IR (cm^{-1})**: 2956, 2924, 2855, 1499, 1483, 1466, 1407, 1269, 1172, 1154, 884, 794, 771, 702. **HRMS (APCI)**: calculated for $C_{54}H_{69}F_2$ ($M + H^+$): m/z = 755.5362; found: m/z = 755.5355.

2,5-Dimethoxy-4',5'-dihexyl-1,1':2',1''-terphenyl (**11**):
yield: 99%, colorless oil, eluent: pentane/CH_2Cl_2 3:1.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.26 (s, 1H), 7.22 (s, 1H), 7.19-7.13 (m, 5H), 6.80-6.72 (m, 2H), 6.62 (d, J = 8.8 Hz, 1H), 3.72 (s, 3H), 3.25 (s, 3H), 2.71-2.62 (m, 4H), 1.72-1.59 (m, 4H), 1.51-1.28 (m, 12H), 0.95-0.88 (m, 6H). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ = 153.3, 150.7, 142.4, 140.0, 139.5, 138.8, 134.2, 131.8, 131.5, 130.4, 128.9, 127.4, 125.9, 117.5, 113.0, 111.9, 55.7, 55.5, 32.6, 32.4, 31.8, 31.2, 31.1, 29.6, 29.6, 22.6, 14.1. **IR (cm^{-1})**: 2954, 2928, 2857, 1603, 1586, 1498, 1485, 1464, 1417, 1273, 1220, 1178, 1049, 1028, 700. **MS (EI)**: m/z = 458 (M^+, 100), 317 (57), 287 (11), 215 (5), 143 (4). **HRMS (EI)**: calculated for $C_{32}H_{42}O_2$: m/z = 458.3185; found: m/z = 458.3168.

Scholl reactions

2,3,12,13-Tetrahexyltribenzo[*fg,ij,rst*]pentaphene (**4**)

Quinquephenyl **3** (100 mg, 139 µmol, 1.0 equiv) was dissolved in anhydrous CH_2Cl_2 (50 mL). While maintaining a constant flow of argon through the solution anhydrous $FeCl_3$ (271 mg, 1.67 mmol, 12 equiv) dissolved in $MeNO_2$ (1.0 mL) was added drop wise. After 1 h methanol (20 mL) was added and the solution was stirred additional 5 min. After the solution was washed with water (2x20 mL) the organic layer was filtered through a short pad of silica gel (eluent: CH_2Cl_2). Recrystallization of the crude product with CH_2Cl_2/methanol afforded the product **4** (94 mg, 132 µmol, 95%) as a white solid.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 8.85 (s, 2H), 8.81 (d, J = 7.9 Hz, 2H), 8.72 (d, J = 8.0 Hz, 2H), 8.39 (d, J = 9.3 Hz, 4H), 7.90 (t, J = 7.9 Hz, 2H), 2.87-2.76 (m, 8H), 1.85-1.71 (m, 8H), 1.60-1.38 (m, 24H), 1.03-0.94 (m, 12H). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ = 140.5, 140.4, 130.2, 129.9, 128.2, 127.9, 127.1, 126.1, 124.4, 123.6, 123.5, 123.2, 121.1, 121.0, 120.5, 33.2, 31.9, 31.5, 31.4, 29.7, 22.7, 14.2. **IR (cm^{-1})**: 2950, 2923, 2853, 1466, 1436, 1377, 874, 791, 751. **HRMS (APCI)**: calculated for $C_{54}H_{65}$ ($M + H^+$): m/z = 713.5081; found: m/z = 713.5071.

15-Methoxy-2,3,12,13-tetrahexyltribenzo-[*fg,ij,rst*]pentaphene (**8a**)

Method A ($FeCl_3$):Quinquephenyl **6a** (100 mg, 129 µmol, 1.0 equiv) was dissolved in anhydrous CH_2Cl_2 (50 mL). While maintaining a constant flow of argon through the solution anhydrous $FeCl_3$ (167 mg, 1.03 mmol, 8 equiv) dissolved in $MeNO_2$ (0.6 mL) was added drop wise. After 30 min methanol (20 mL) was added and the solution was stirred additional 5 min. After the solution was washed with water (2x20 mL) the organic layer was filtered through a short pad of silica gel (eluent: CH_2Cl_2). Recrystallization of the crude product with CH_2Cl_2/methanol afforded the product **8a** (71 mg, 96 µmol, 74%) as a yellowish solid.

Method B (DDQ/$MeSO_3H$): Quinquephenyl **6a** (116 mg, 150 µmol, 1.0 equiv) was dissolved in anhydrous CH_2Cl_2 (45 mL). $MeSO_3H$ (5 mL) and DDQ (103 mg, 450 µmol, 3.0 equiv) were added sequentially at 0 °C. After 30 min the reaction was quenched with saturated $NaHCO_3$ (60 mL). After separation of the organic layer the aqueous phase was extracted with CH_2Cl_2 (20 mL). The combined organic layers were filtered through a short pad of silica gel (eluent: CH_2Cl_2). Recrystallization of the crude product with CH_2Cl_2/methanol afforded the product **8a** (85 mg, 114 µmol, 76%) as a yellowish solid.

Method C ($MoCl_5$/$TiCl_4$): Quinquephenyl **6a** (58 mg, 75 µmol, 1.0 equiv) was dissolved in anhydrous CH_2Cl_2 (25 mL). $MoCl_5$ (41 mg, 150 µmol, 1 equiv) and $TiCl_4$ (17 µL, 150 µmol, 1 equiv) were added at 0 °C. After 30 min the reaction was quenched with saturated $NaHCO_3$ (20 mL). After separation of the organic layer the aqueous phase was extracted with CH_2Cl_2 (10 mL). The combined organic layers were filtered through a short pad of deactivated silica gel (eluent: CH_2Cl_2). Recrystallization of the crude product with CH_2Cl_2/methanol afforded the product **8a** (34 mg, 46 µmol, 61%) as a yellowish solid.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 9.52 (s, 1H), 8.84-8.76 (m, 3H), 8.71 (d, J = 7.9 Hz, 1H), 8.51 (s, 1H), 8.38 (s, 1H), 8.37 (s, 1H), 8.27 (s, 1H), 7.92 (t, J = 7.9 Hz, 1H), 7.85 (t, J = 7.9 Hz, 1H), 4.26 (s, 3H), 2.89 (t, J = 7.8 Hz, 4H), 2.81 (t, J = 7.9 Hz, 4H), 1.90-1.70 (m, 8H), 1.64-1.38 (m, 24H), 1.03-0.94 (m, 12H). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ = 156.4, 140.4, 140.2, 139.6, 139.5, 130.5, 130.5, 129.3, 129.1, 128.8, 128.5, 128.2, 127.8, 127.8, 127.6, 126.3, 126.1, 125.2, 124.6, 124.3, 123.5, 123.3, 123.0, 121.0, 120.9, 120.9, 120.7, 118.2, 118.0, 104.3, 56.3, 33.3, 33.2, 33.2, 32.0, 31.9, 31.5, 31.4, 31.2, 29.7, 29.6, 22.8, 14.2. **IR (cm^{-1})**: 2953, 2922, 2855, 1604, 1455, 1383, 1228, 801, 753. **MS (APCI)**: m/z = 744 ($M+H^+$, 100), 660 (72), 575 (23). **HRMS (APCI)**: calculated for $C_{55}H_{67}O$ ($M + H^+$): m/z = 743.5186; found: m/z = 743.5183.

15-Fluoro-2,3,12,13-tetrahexyltribenzo[*fg,ij,rst*]pentaphene (**8b**)

Quinquephenyl **6b** (100 mg, 132 µmol, 1.0 equiv) was dissolved in anhydrous CH_2Cl_2 (100 mL). While maintaining a constant flow of argon through the solution anhydrous $FeCl_3$ (344 mg, 1.03 mmol, 16 equiv) dissolved in $MeNO_2$ (1.2 mL) was added drop wise. After 2.5 h methanol (50 mL) was added and the solution was stirred additional 5 min. After the solution was washed with water (2x20 mL) the organic layer was filtered through a short pad of silica gel (eluent: CH_2Cl_2). Recrystallization of the crude product with CH_2Cl_2/hexane afforded the product **8b** (53 mg, 72.5 µmol, 55%) as a white solid. Additionally 24 mg (31.8 µmol, 24%) of the starting material (**6b**) were recovered.

^{1}H NMR ($CDCl_3$, 500 MHz): δ = 9.00 (d, J = 3.6 Hz, 1H), 8.80 (d, J = 8.3 Hz, 1H), 8.77 (d, J = 8.0 Hz, 1H), 8.73 (d, J = 7.8 Hz, 1H), 8.66 (d, J = 8.1 Hz, 1H), 8.49 (d, J = 17.0 Hz, 1H), 8.44 (s, 1H), 8.33 (s, 1H), 8.24 (s, 1H), 7.91 (t, J = 7.8 Hz, 1H), 7.86 (t, J = 7.8 Hz, 1H), 2.90-2.84 (m, 4H), 2.84-2.78 (m, 4H), 1.85-1.73 (m, 8H), 1.60-1.50 (m, 8H), 1.49-1.38 (m, 16H), 1.00-0.95 (m, 12H). **^{13}C NMR** ($CDCl_3$, 125 MHz): δ = 159.5 (d, J = 250 Hz), 140.9, 140.6 (d, J = 2 Hz), 140.5, 140.4, 130.3, 130.2, 129.2 (d, J = 23 Hz), 128.6, 128.3, 128.3, 128.1, 128.1, 128.0, 127.1 (d, J = 3 Hz), 126.5, 126.1 (d, J = 8 Hz), 126.1 (d, J = 8 Hz), 125.8, 124.0 (d, J = 3 Hz), 123.7, 123.5, 123.3, 123.1, 121.1, 121.1, 121.0, 120.8, 119.7, 116.1 (d, J = 8 Hz), 33.3, 33.2, 33.2, 31.9, 31.4, 31.4, 31.3, 29.7, 29.7, 29.6, 22.8, 22.7, 14.2. **^{19}F NMR** ($CDCl_3$, 282 MHz): δ = -113.1. **IR (cm^{-1})**: 2951, 2927, 2854, 1614, 1466, 1387, 851, 801, 754. **HRMS (APCI)**: calculated for $C_{54}H_{64}F$ ($M + H^+$): m/z = 731.4987; found: m/z = 731.2978.

3,3'-Dimethoxy-6,6',7,7'-tetrahexyl-2,2'-bistriphenylene (**14'**)

Method A ($FeCl_3$): Terphenyl **11** (115 mg, 250 µmol, 1.0 equiv) was dissolved in anhydrous CH_2Cl_2 (50 mL). While maintaining a constant flow of argon through the solution anhydrous $FeCl_3$ (81 mg, 500 µmol, 2 equiv) dissolved in $MeNO_2$ (0.3 mL) was added drop wise at 0 °C. After 15 min methanol (15 mL) was added and the solution was stirred additional 5 min. After the solution was washed with water (2x10 mL) the organic layer was filtered through a short pad of silica gel (eluent: CH_2Cl_2). The residue was purified by column chromatography (silica gel, eluent: pentane/CH_2Cl_2 3:1). The product **14'** (54 mg, 63 µmol, 51%) was isolated as a white solid. Additionally 21 mg (45 µmol, 18%) of the starting material (**11**) and 8 mg (16 µmol, 7%) of the monomeric cyclisation product **14** could be isolated.

Method B (DDQ/$MeSO_3H$): Terphenyl **11** (115 mg, 250 µmol, 1.0 equiv) was dissolved in anhydrous CH_2Cl_2 (45 mL). $MeSO_3H$ (5 mL) and DDQ (57 mg, 250 µmol, 1.0 equiv) were added sequentially at 0 °C. After 15 min the reaction was quenched with saturated Na_2CO_3 (25 mL). After separation of the organic layer the aqueous phase was extracted with CH_2Cl_2 (20 mL). The combined organic layers were filtered through a short pad of deactivated silica gel (eluent: CH_2Cl_2). The residue was purified by column chromatography (silica gel, eluent: pentane/CH_2Cl_2 3:1). The product **14'** (41 mg, 48 µmol, 39%) was isolated as a white solid. Additionally 23 mg (50 µmol, 20%) of the starting material (**11**) were recovered.

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 8.67-8.63 (m, 4H), 8.62-8.57 (m, 2H), 8.46 (s, 2H), 8.38 (s, 2H), 8.14 (s, 2H), 7.63-7.55 (m, 4H), 4.09 (s, 6H), 2.96-2.86 (m, 8H), 1.86-1.74 (m, 8H), 1.60-1.36 (m, 24H), 0.96 (t, J = 7.0 Hz, 12H). **^{13}C NMR** ($CDCl_3$, 75 MHz): δ = 157.1, 140.3, 140.1, 130.8, 129.7, 129.0, 128.4, 128.2, 127.6, 126.7, 126.6, 126.0, 123.6, 123.4, 123.0, 103.7, 56.1, 33.3, 33.2, 31.9, 31.7, 31.5, 29.6, 29.5, 22.7, 22.7, 14.1. **IR (cm^{-1})**: 2953, 2924, 2853, 1613, 1497, 1465, 1401, 1235, 1202, 1052, 836, 758. **HRMS(APCI)**: calculated for $C_{62}H_{75}O_2$ ($M + H^+$): m/z = 851.5762; found: m/z = 851.5738.

2) Further computational details

Computational Details

Quantum chemical computations have been carried out with the long-range corrected hybrid functional LC-wPBE[1] which has been found to successfully locate all transition states in conjunction with the def2-SVP basis set.[2] Improved energies were obtained with B3LYP[3] in the implementation by *Frisch*[4] in combination with the def2-TZVPP basis set.[2] Standard convergence criteria and an ultrafine integration grid were used. The standard state for all thermodynamic data is 298.15 K and 1 atm. Stationary points have been characterized by calculation of the analytic hessian matrix. Intrinsic reaction coordinate calculations confirmed the nature of the transition states found. All computations were carried out with the program suite Gaussian09. [5]

Cartesian coordinates and SCF-energies of all structures investigated can be found further down.

[1] O. A. Vydrov, G. E. Scuseria *J. Chem. Phys.* **2006**, *125*, 234109.
[2] F. Weigend, R. Ahlrichs *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.
[3] A. D. Becke *J. Chem. Phys.* **1993**, *98*, 5648.
[4] P. J. Stephens, J. F. Devlin, C. F. Chabalowski, M. J. Frisch *J. Phys. Chem.* **1994**, *98*, 11623.
[5] Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Antara- and suprafacial pathway

As mentioned in the manuscript, in addition to the described pathway via an antarafacial arrangement of the rings (transition states discussed in the manuscript is given in Figure S1), a suprafacial arrangement is possible as well. A plot of the transition states **TSA-B1$_H$-supra** and **TSA-B2$_H$-supra** is shown in Figure S2. The energies of this pathway are included in Tables S1a-c and show that this pathway is always less favorable.

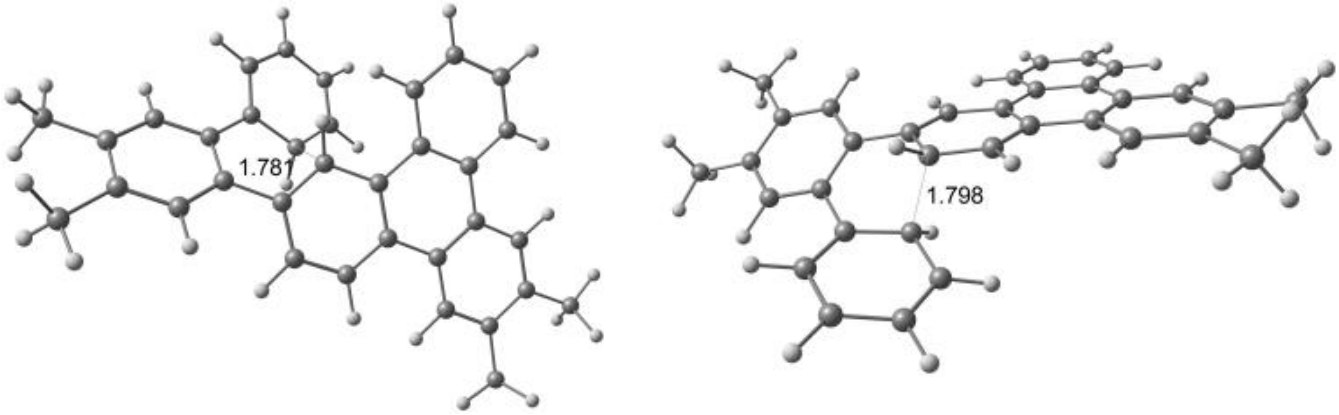


Figure S1. Optimized structures and central bond lengths in Å (LC-ωPBE/def2-SVP) for transition states **TSA-B1$_H$** (left) and **TSA-B2$_H$** (right).

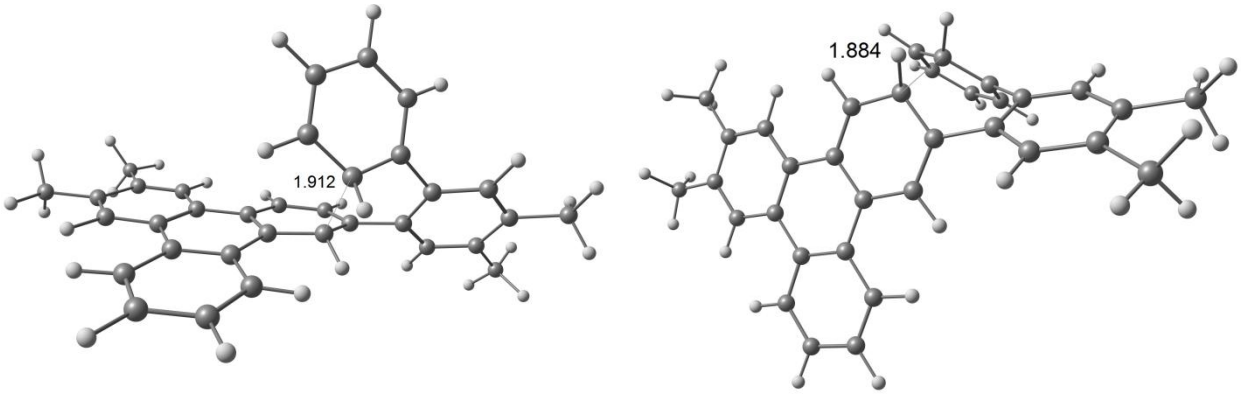


Figure S2. Optimized structures and central bond lengths in Å (LC-ωPBE/def2-SVP) for transition states **TSA-B1$_H$-supra** (left) and **TSA-B2$_H$-supra** (right).

Methodological discussion

In our attempt to elucidate the reaction mechanism of the regioselective Scholl reaction, we employed several density functionals as stated in the manuscript. A full investigation of the reaction path from **A$_x$** to **D1** and **D2$_X$** was possible with BP86/def2-TZVP but neither the crucial transition state **TSA-B1$_x$** nor the intermediate **B1$_X$** could be located as stationary point on the potential energy surface (PES). Instead, the optimization oscillated and forces and displacement stayed constant. In an attempt to investigate this behavior, we reoptimized the complete PES with the hybrid functional B3LYP and the same basis set since B3LYP is widely used for computational investigations of organic compounds and excellent agreement with higher level calculations for radical cation reactions was found[6] although the robustness in comparison to other modern functionals has been found to be below average.[7] Again, we found the same oscillations regarding the optimization of intermediates **B1$_X$** and transition state **TSA-B1$_x$** for X = H, F and OMe. Attempts with increased integration accuracy, tighter convergence criteria, larger basis set and other usual computational parameters tested in such cases have not been successful.

Only the reinvestigation of the complete PES with the recently developed long-range corrected hybrid functional LC-ωPBE lead to the successful identification of stationary points **B1$_X$** and **TSA-B1$_x$** for X = H, F and OMe.

The relative energies of the stationary points computed with B3LYP and LC-ωPBE with different basis sets can be found in Tables S1a-c and show, that the trend is the same for all methods.

The nearly converged structures of **TSA-B1$_x$** which has been found for B3LYP/def2-SVP (Table S1c) is energetically lower lying than **TSA-B2$_x$** for all substituents X. Although these energies cannot strictly be interpreted, since they do not correspond to well-converged stationary points on the PES, the trend is obvious and can be found in Tables S1a-c. This leads us to the conclusion that the results reported in the manuscript are not artefacts of an arbitrary choice of a specific functional and basis set combination.

Further tests with BP86, B97D, TPSS, M06-2X and def2-SVP basis set also could not locate a transition state. In preliminary tests with dispersion correction (PBE-D2) at least the intermediate **B1$_H$** could be located. A further methodological investigation is under way. A discussion of the method dependence of the PES in radical cation reactions can be found in Reference 7.

[6] U. Haberl, O. Wiest, E. Steckhan *J. Am. Chem. Soc.* **1999**, *121*, 6730.
[7] L. Goerigk, S. Grimme *Phys. Chem. Chem. Phys.*, **2011**, *13*, 6670.

Table S1a. LC-ωPBE/def2-SVP energies relative to $\mathbf{A_x}$ (ΔE) for X = H, F, OMe in kcal mol^{-1}. Shown are pathways via supra- and antarafacial arrangement of rings.

	H		**F**		**OMe**	
	antara	supra	antara	supra	antara	supra
D2		-165.9		-182.8		-181.7
$\mathbf{B2_X}$	17.2	22.0	20.6	24.1	20.7	32.5
$\mathbf{TSA\text{-}B2_X}$	22.1	29.8	25.5	32.2	24.8	35.1
$\mathbf{A_X}$		0.0		0.0		0.0
$\mathbf{TSA\text{-}B1_X}$	19.3	27.0	20.6	26.9	18.7	24.3
$\mathbf{B1_X}$	17.3	21.3	16.4	19.8	18.0	18.0
$\mathbf{C1_X}$		12.3		12.0		5.3
$\mathbf{D1_X}$		-166.4		-167.6		-164.6

Table S1b. B3LYP/def2-TZVPP//LC-ωPBE/def2-SVP energies relative to $\mathbf{A_x}$ (ΔE) for X = H, F, OMe in kcal mol^{-1}. Shown are pathways via supra- and antarafacial arrangement of rings.

	H		**F**		**OMe**	
	antara	supra	antara	supra	antara	supra
D2		-153.2		-176.9		-175.4
$\mathbf{B2_X}$	31.8	36.6	33.2	35.6	35.0	43.8
$\mathbf{TSA\text{-}B2_X}$	30.2	27.3	33.4	39.5	33.5	43.3
$\mathbf{A_X}$		0.0		0.0		0.0
$\mathbf{TSA\text{-}B1_X}$	29.5	35.8	30.8	35.5	28.2	31.9
$\mathbf{B1_X}$	32.6	34.0	32.2	34.1	32.2	30.5
$\mathbf{C1_X}$		13.0		14.1		7.9
$\mathbf{D1_X}$		-152.9		-153.7		-151.8

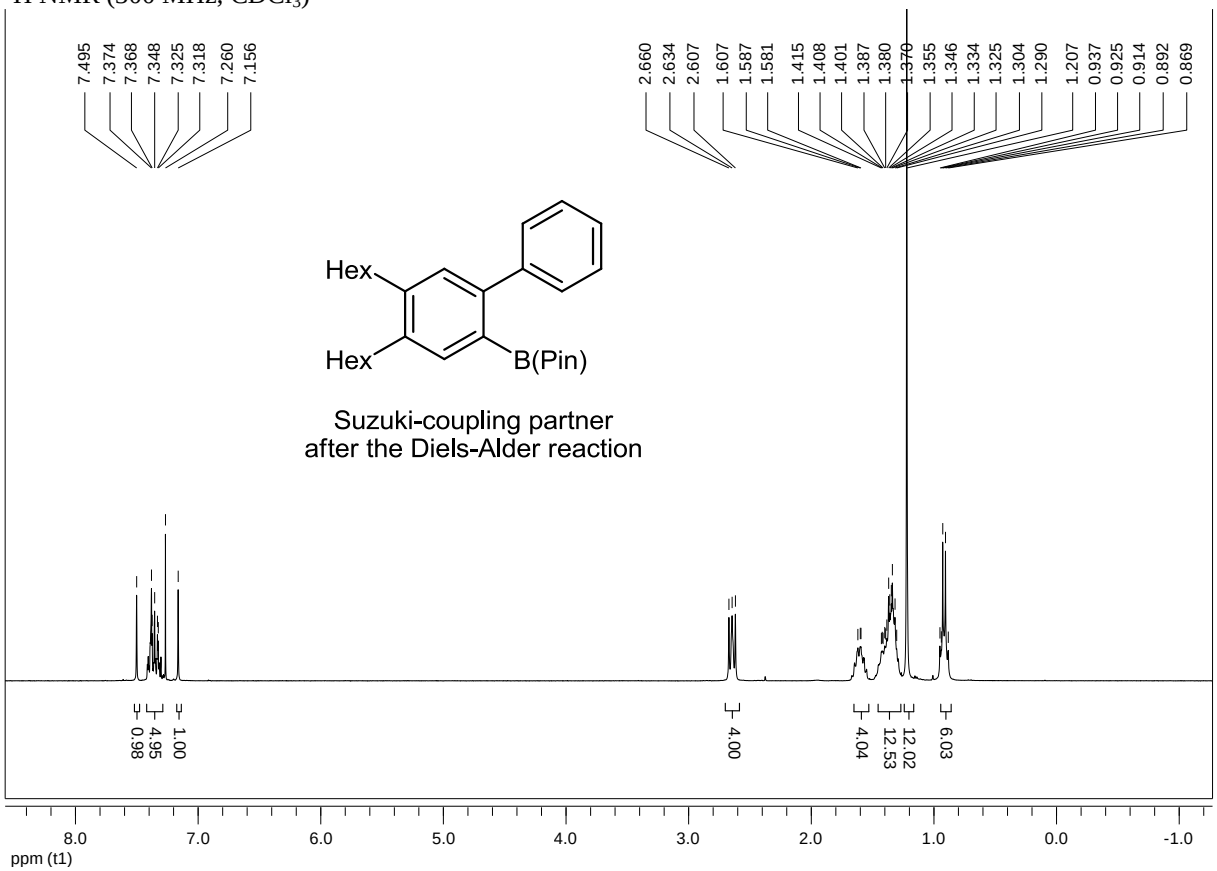
Table S1c. B3LYP/def2-SVP energies relative to $\mathbf{A_x}$ (ΔE) for X = H, F, OMe in kcal mol^{-1}. Shown are pathways via supra- and antarafacial arrangement of rings.

	H		**F**		**OMe**	
	antara	supra	antara	supra	antara	supra
D2		-153.1		-168.3		-169.8
$\mathbf{B2_X}$	28.5	33.3	31.3	34.1	32.0	41.4
$\mathbf{TSA\text{-}B2_X}$	30.3	36.0	33.9	38.5	33.9	42.1
$\mathbf{A_X}$		0.0		0.0		0.0
$\mathbf{TSA\text{-}B1_X}$	28.1[a]	34.3	28.9[a]	34.3	26.4[a]	30.4
$\mathbf{B1_X}$	-	31.0	-	30.9	-	27.4
$\mathbf{C1_X}$		13.0		13.6		7.2
$\mathbf{D1_X}$		-153.5		-154.3		-152.6

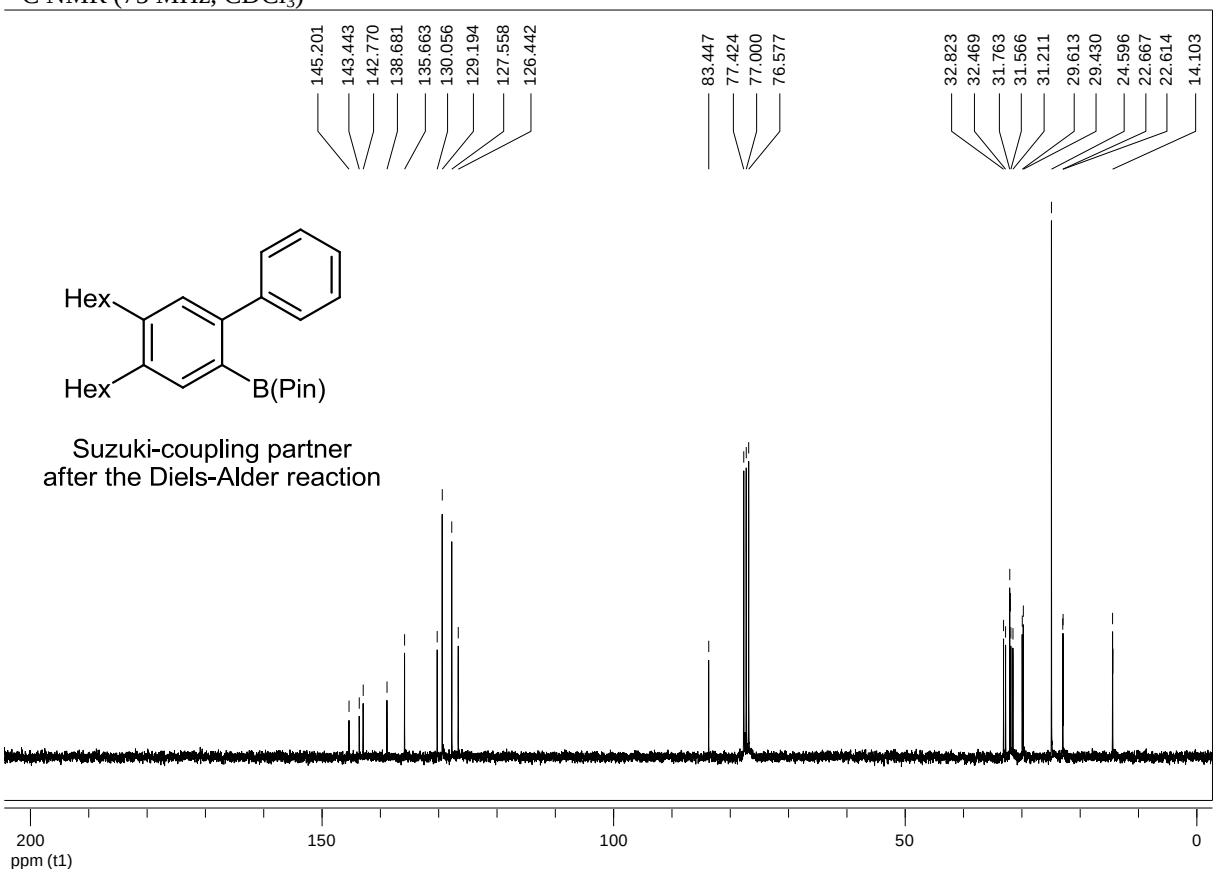
[a] Not fully converged structure. See text for discussion.

3) NMR spectra

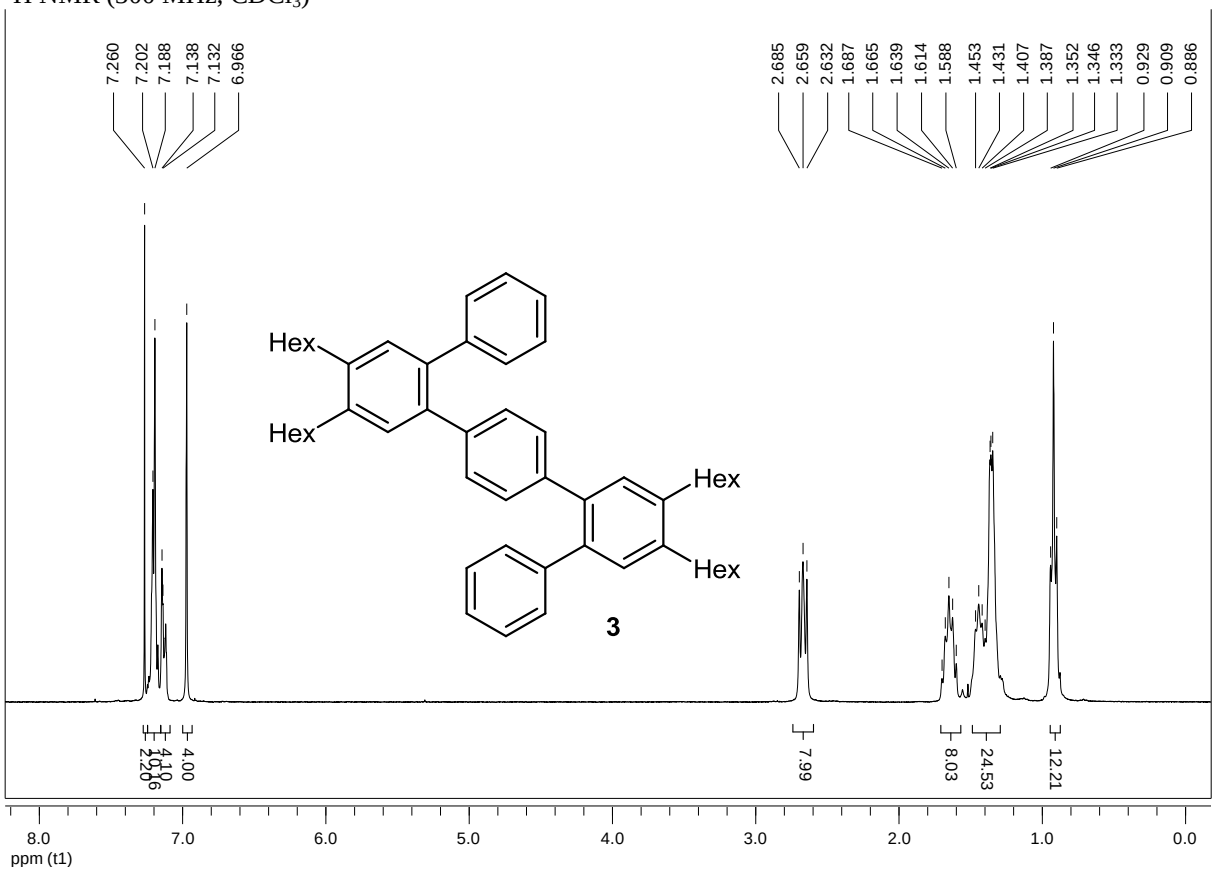
^{1}H NMR (300 MHz, $CDCl_3$)



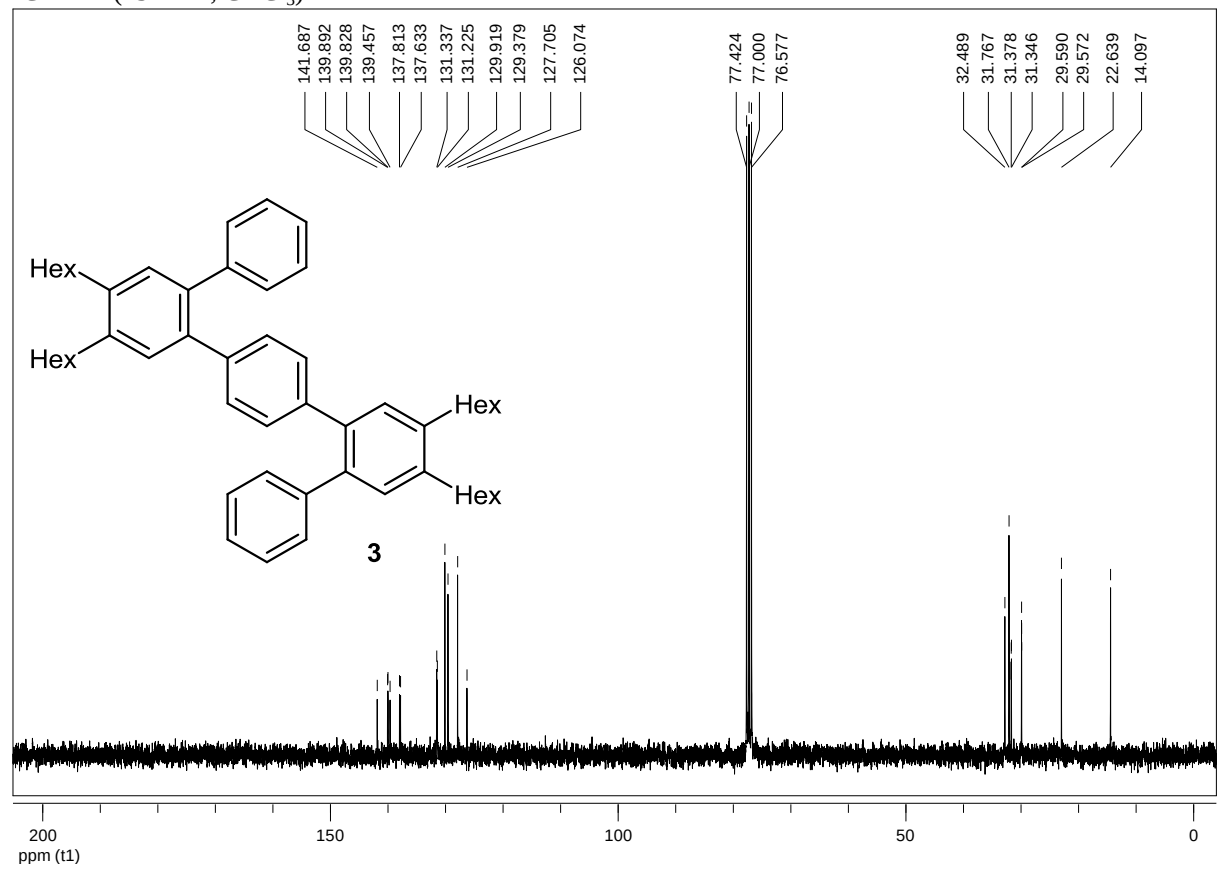
^{13}C NMR (75 MHz, $CDCl_3$)



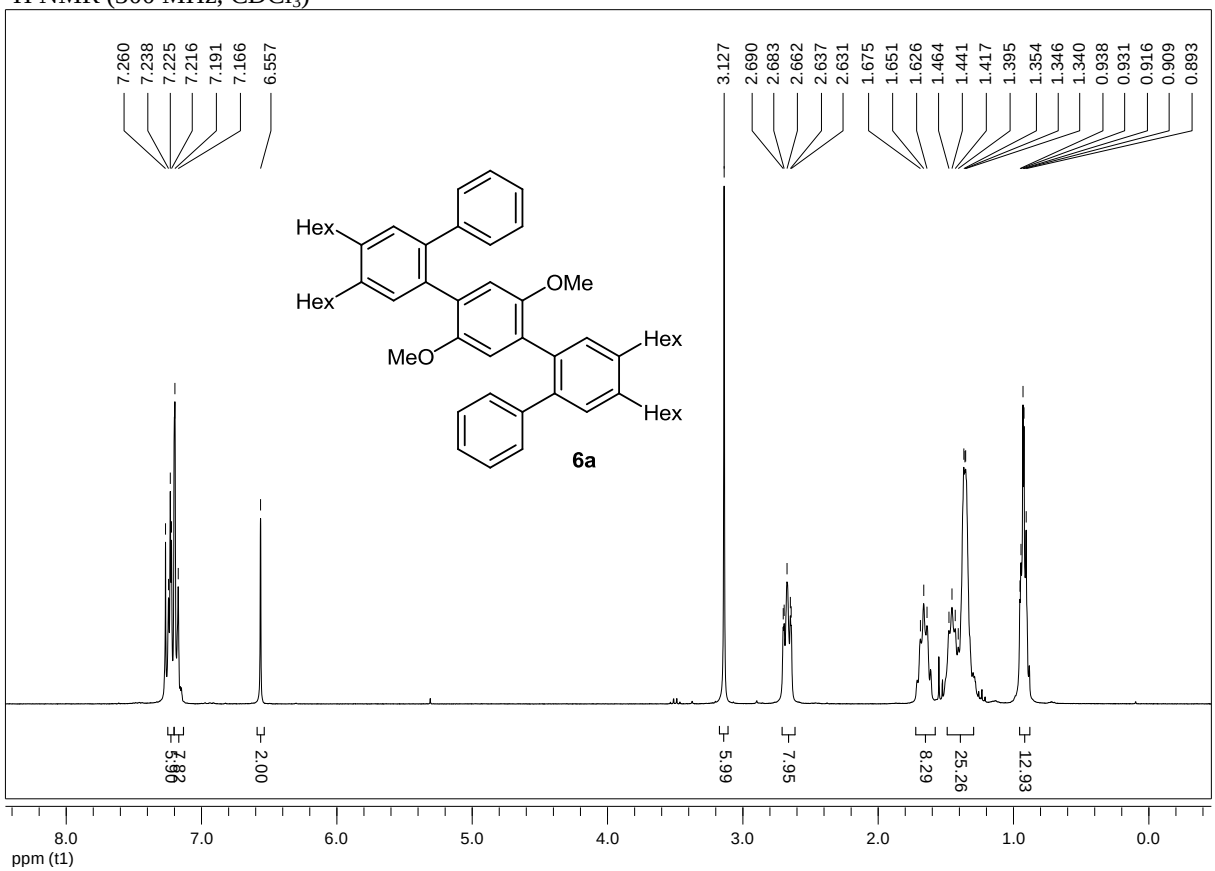
^{1}H NMR (300 MHz, $CDCl_3$)



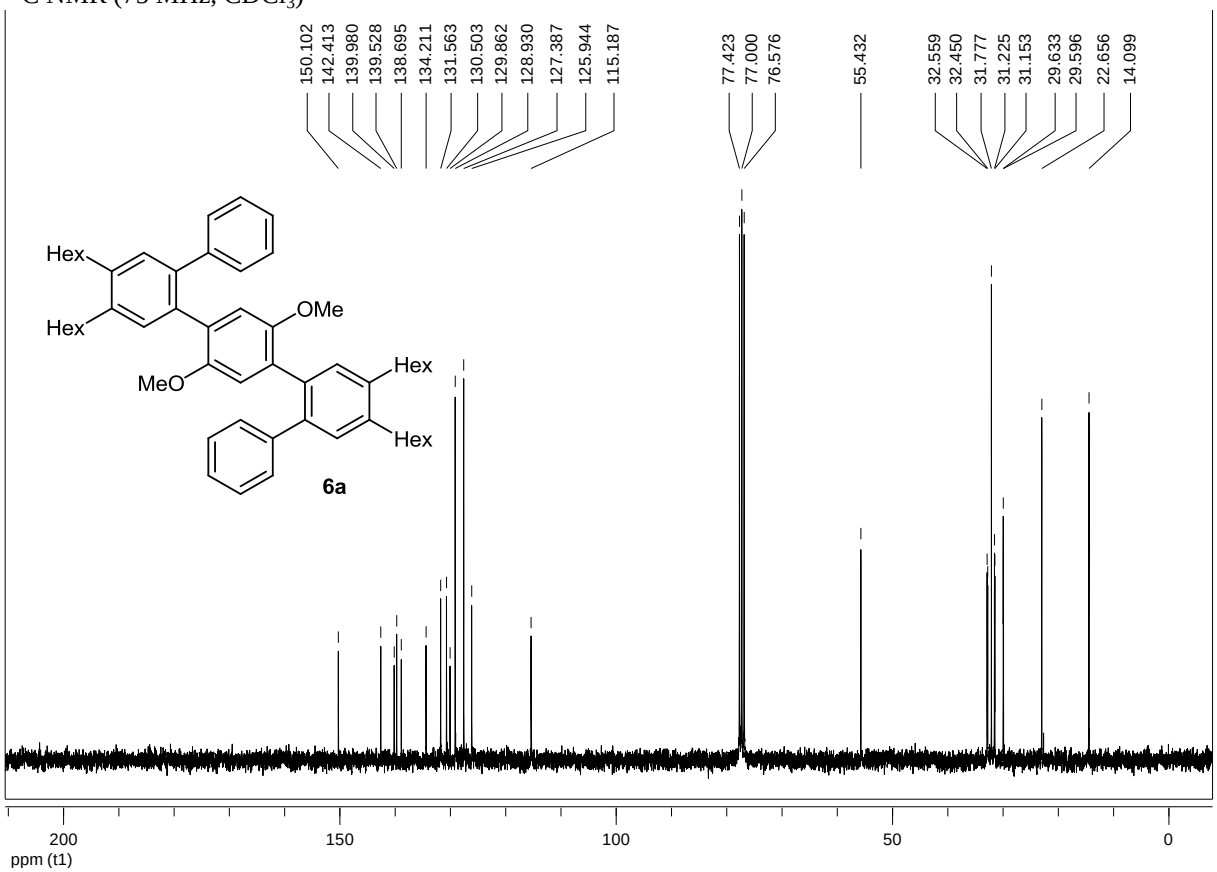
^{13}C NMR (75 MHz, $CDCl_3$)



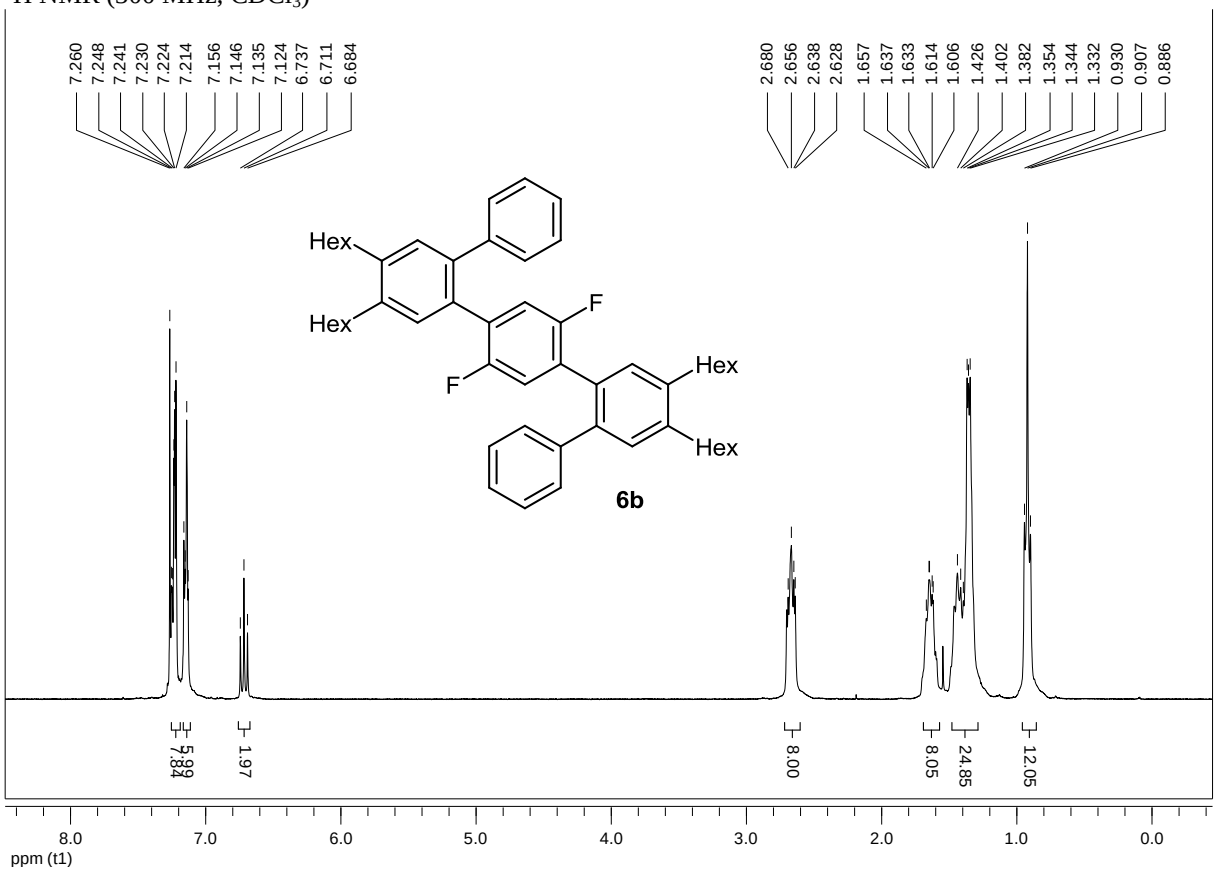
^{1}H NMR (300 MHz, $CDCl_3$)



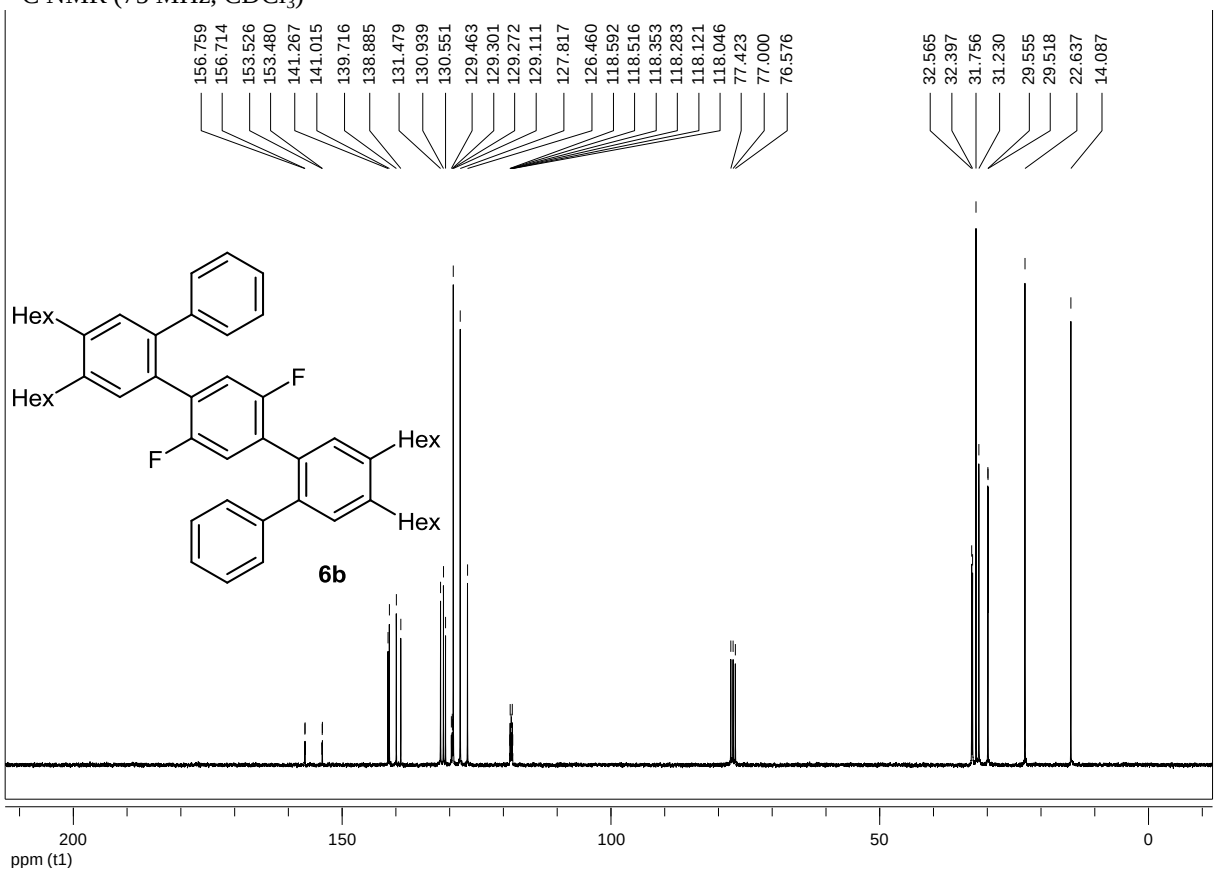
^{13}C NMR (75 MHz, $CDCl_3$)



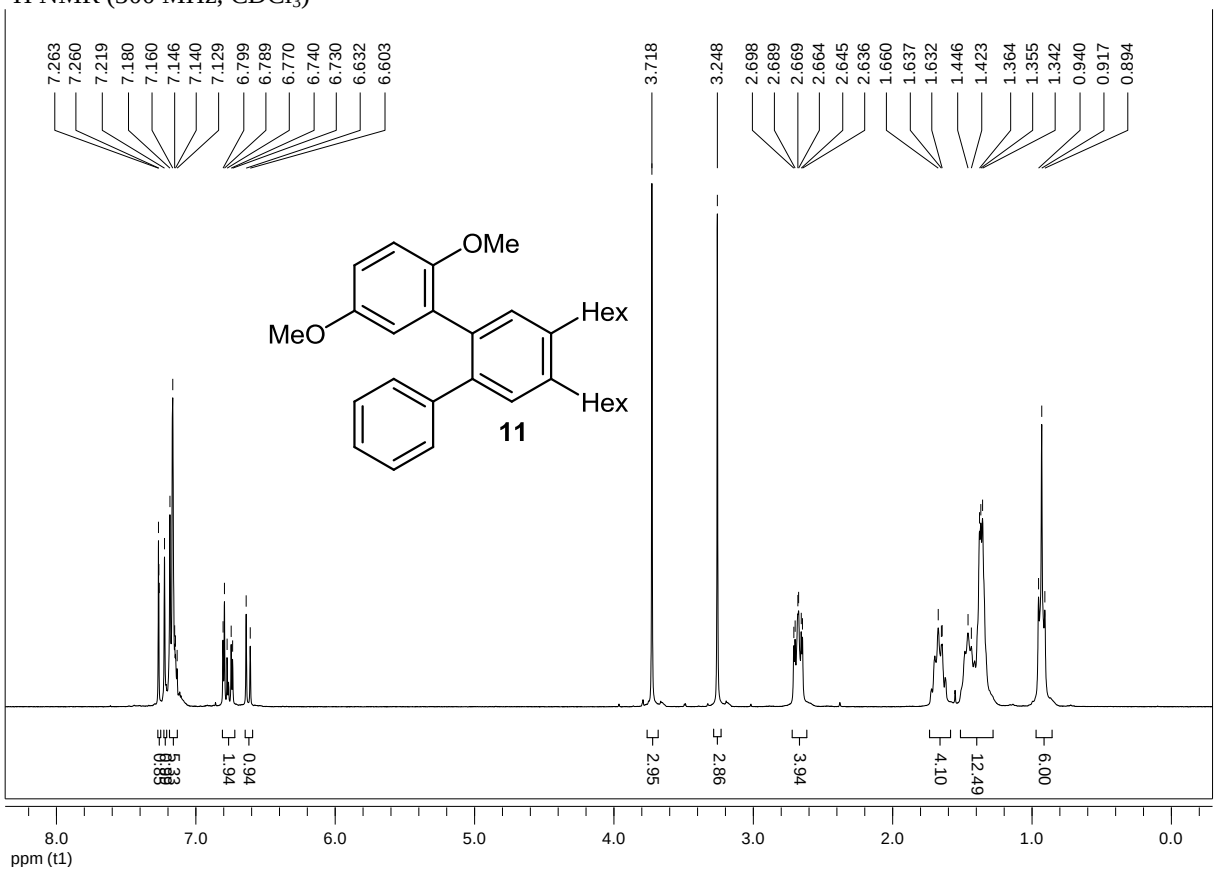
^{1}H NMR (300 MHz, $CDCl_3$)



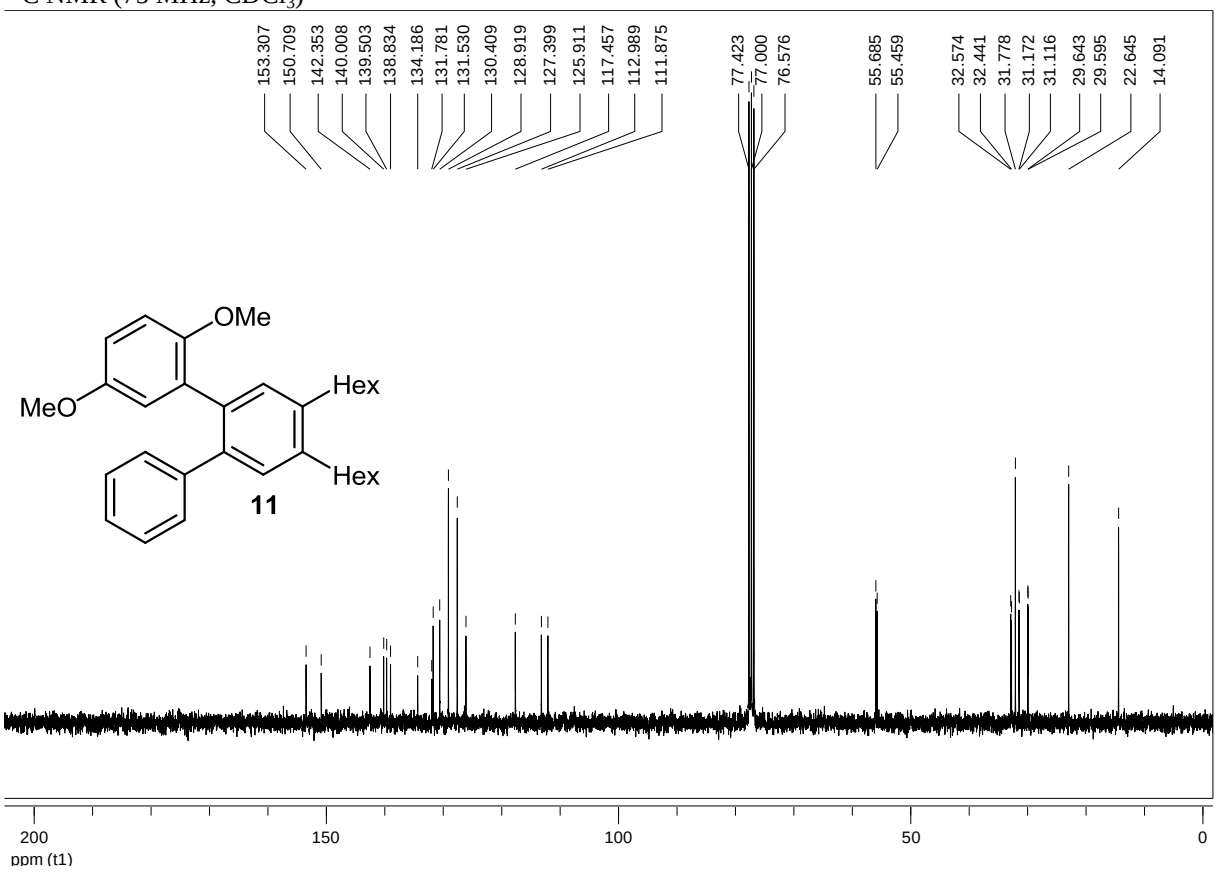
^{13}C NMR (75 MHz, $CDCl_3$)



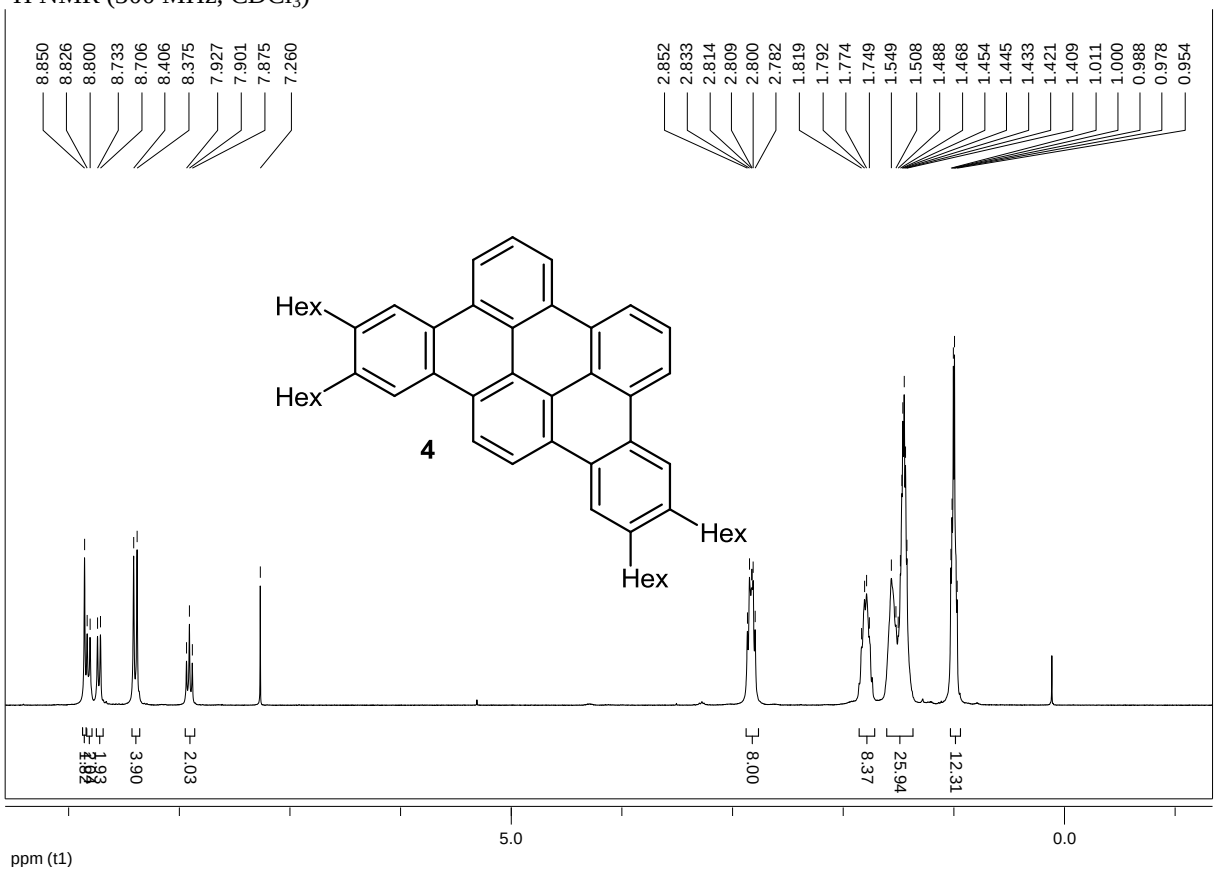
^{1}H NMR (300 MHz, $CDCl_3$)



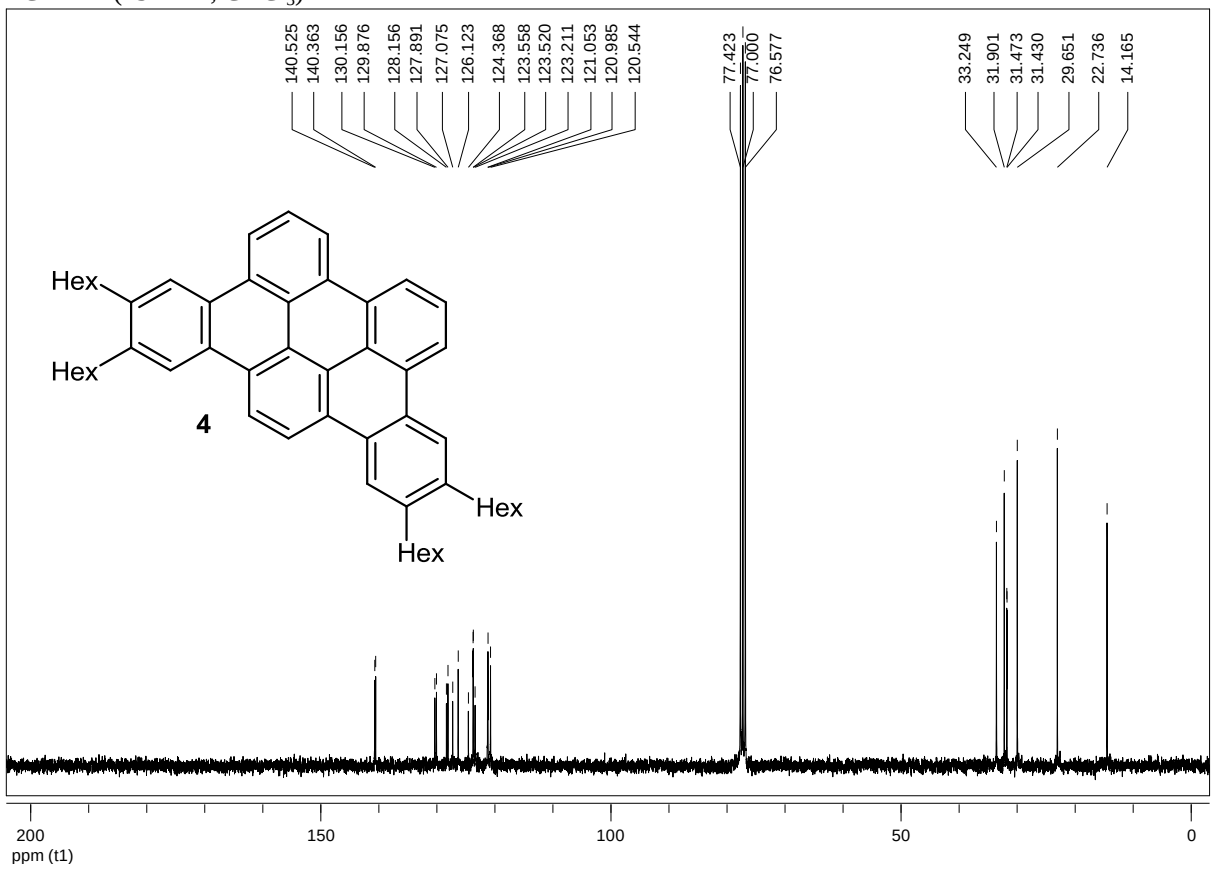
^{13}C NMR (75 MHz, $CDCl_3$)



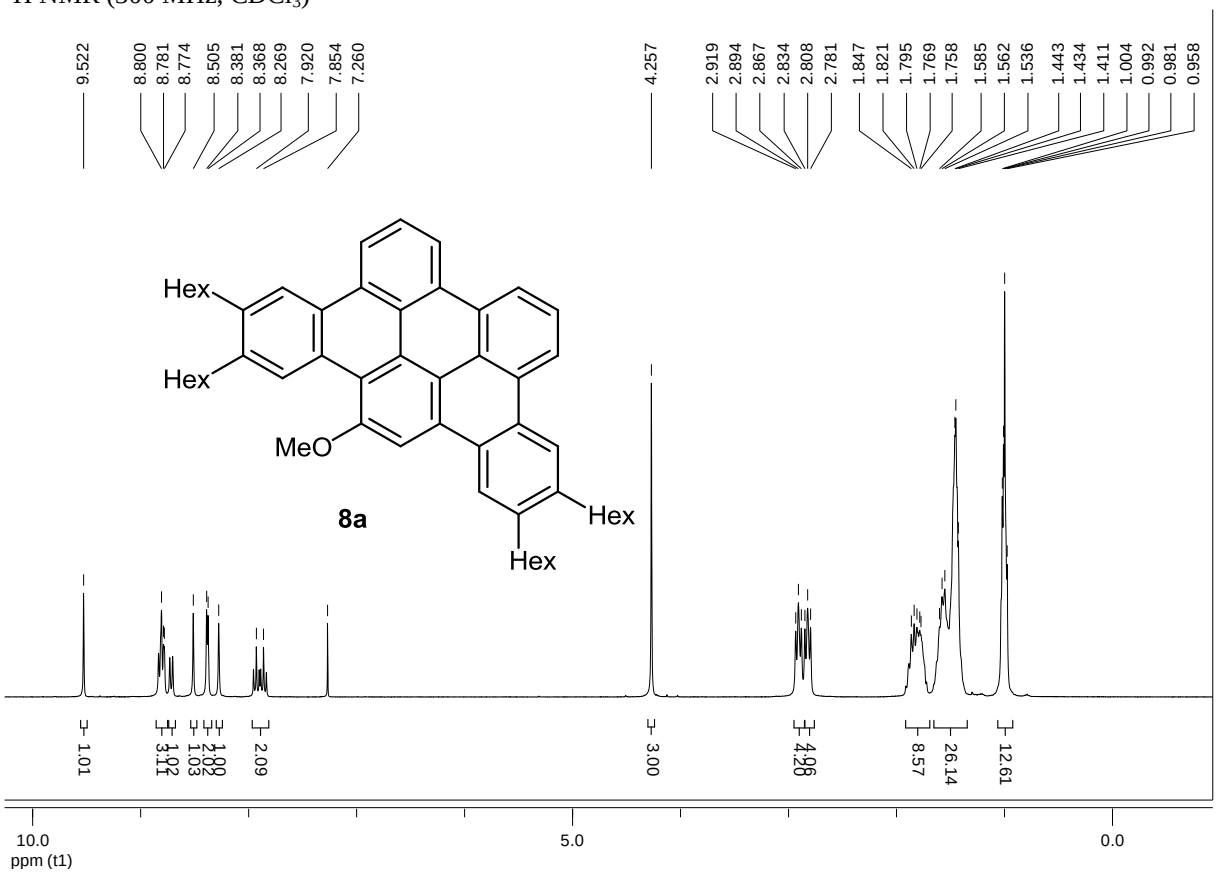
^{1}H NMR (300 MHz, $CDCl_3$)



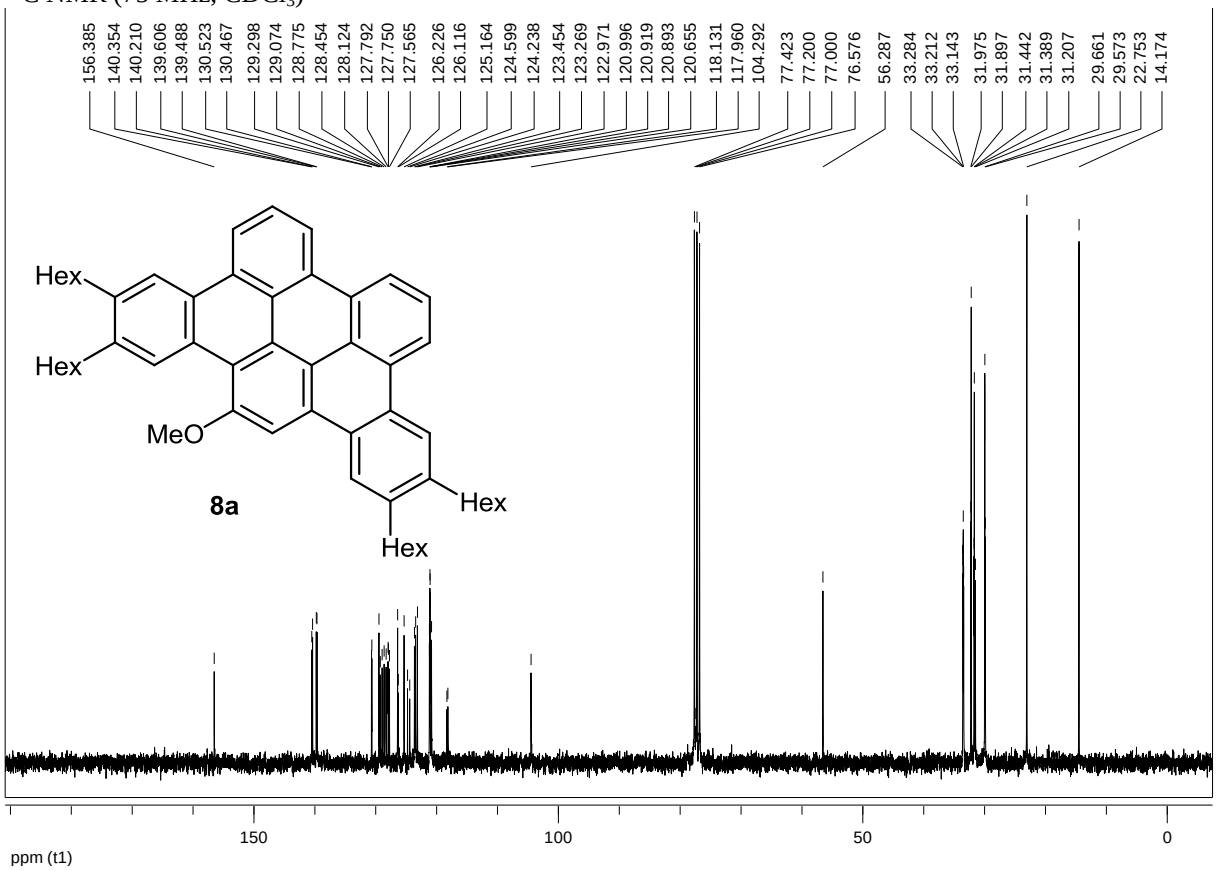
^{13}C NMR (75 MHz, $CDCl_3$)



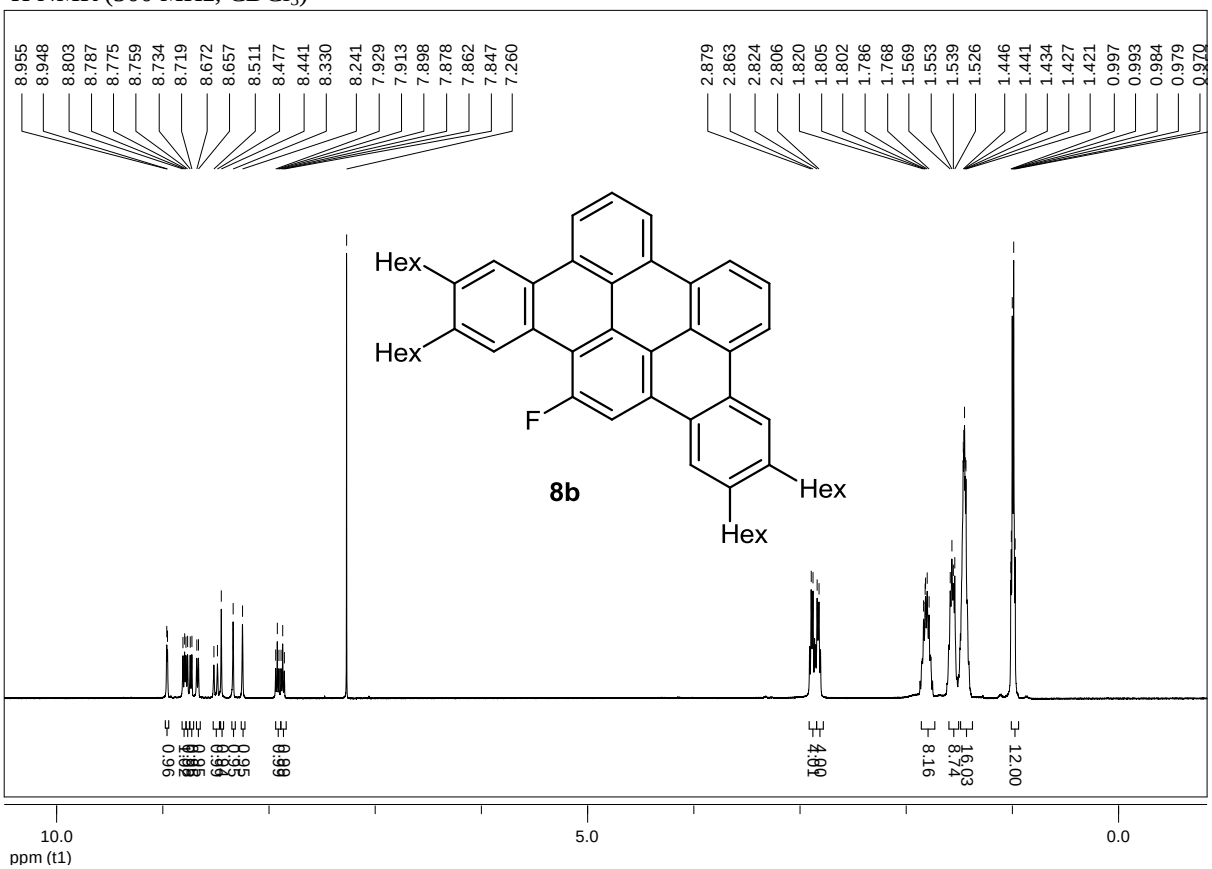
^{1}H NMR (300 MHz, $CDCl_3$)



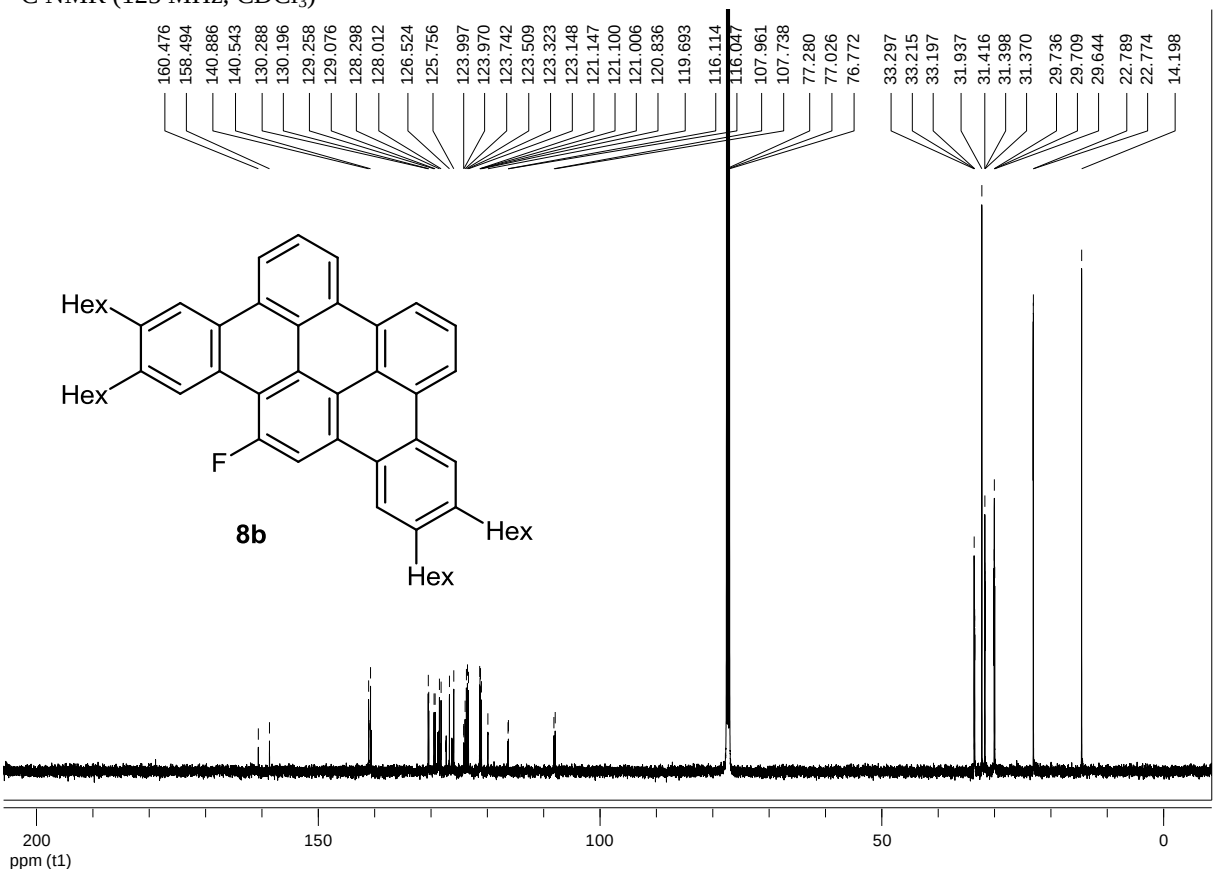
^{13}C NMR (75 MHz, $CDCl_3$)



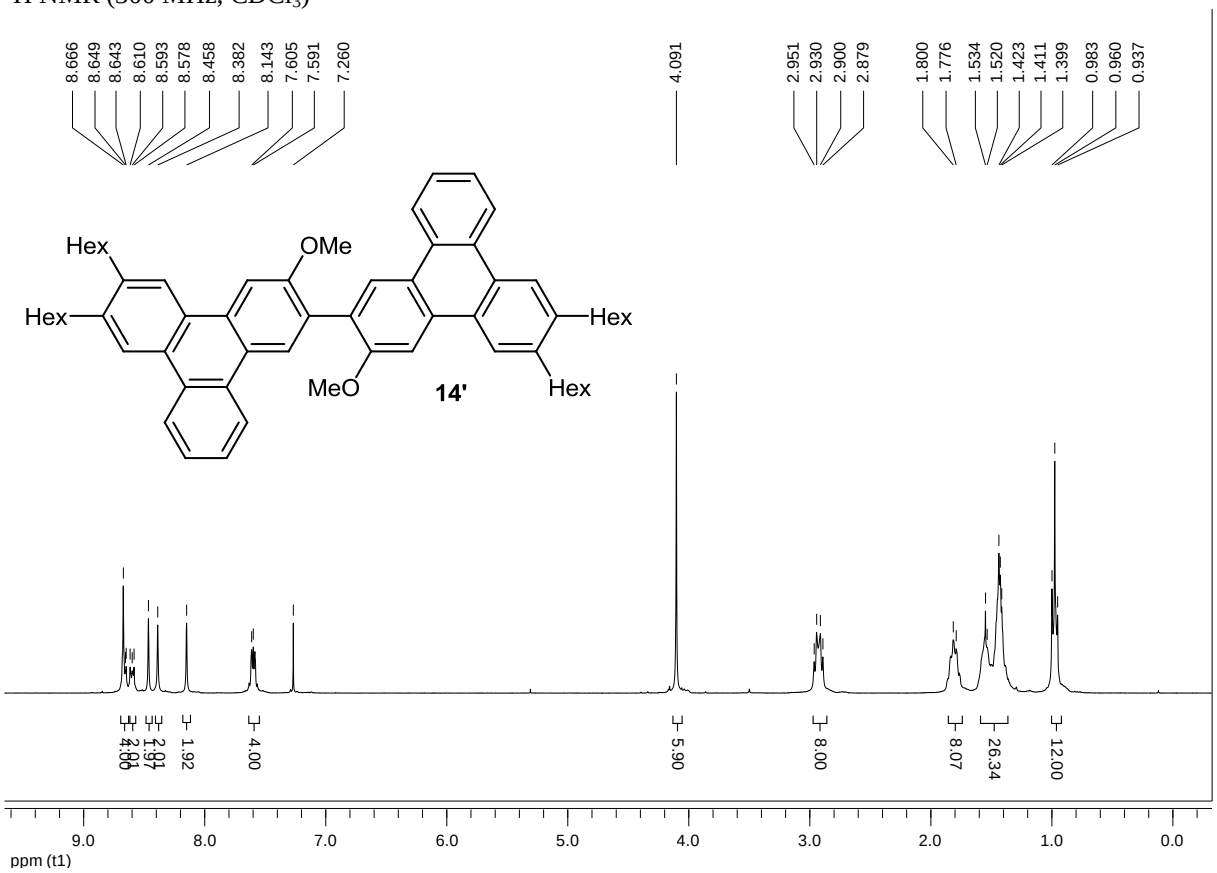
^{1}H NMR (500 MHz, $CDCl_3$)



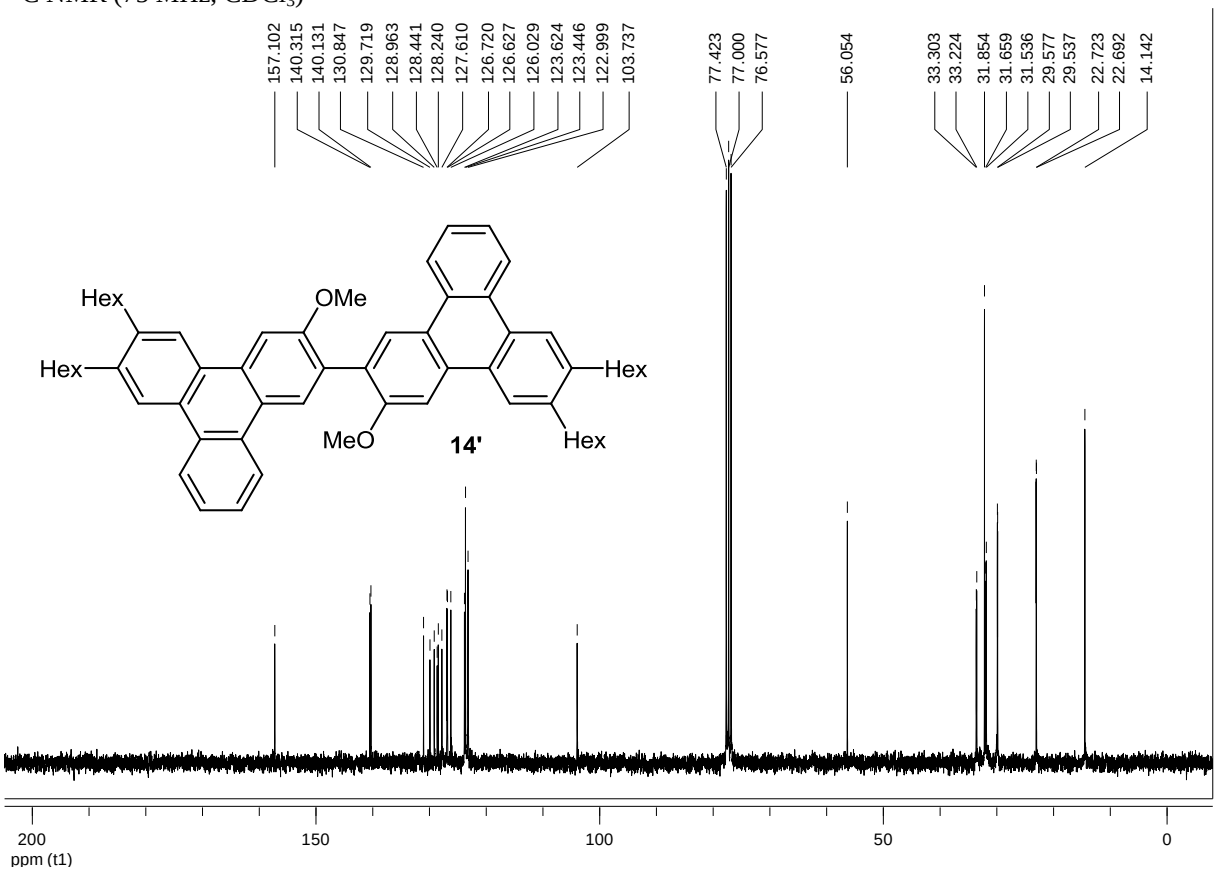
^{13}C NMR (125 MHz, $CDCl_3$)



^{1}H NMR (300 MHz, $CDCl_3$)



^{13}C NMR (75 MHz, $CDCl_3$)



4) Cartesian coordinates and SCF energies of computed compounds

Table S2a. Cartesian coordinates and SCF energies (LC-ωPBE/def2-SVP) for compounds investigated with X = H.

A

62

SCF-energy = -1310.4066

C	-2.9435772	-1.7567475	-0.5682319
C	-4.0657819	-0.8874305	-0.3767974
C	-3.8387233	0.46552194	-0.233624
H	-4.6834028	1.14405328	-0.153298
C	-2.5462668	1.03755214	-0.2361622
C	-1.4378811	0.16036101	-0.4080164
C	-1.6333909	-1.1751569	-0.5549768
H	-0.7596673	-1.8146895	-0.6615987
C	-1.3019302	3.06062773	-0.867088
C	-1.0916022	4.42531946	-0.9230618
C	-1.9453017	5.26618161	-0.176945
C	-2.9558866	4.69252356	0.59167384
H	-3.5814822	5.34441912	1.20601144
C	-3.1796029	3.32076415	0.64904638
C	0.01056208	4.99994021	-1.7628571
H	-0.6643821	2.41811683	-1.4780357
C	-2.345978	2.4740332	-0.1226091
C	-6.5008056	2.8569268	2.39363271
C	-6.1795309	1.91321651	3.36283037
H	-6.9425796	1.56325284	4.06142941
C	-4.8799866	1.42648293	3.44843462
C	-3.9074228	1.87390247	2.56409343
C	-4.2223982	2.81522616	1.5796174
H	-4.6179691	0.69925761	4.21996971
H	-7.5178273	3.24986951	2.32710064
C	-5.5278879	3.3094083	1.51055859
H	-5.785564	4.0490294	0.74815349
C	-1.7575304	6.75089619	-0.1937974
H	0.57678708	4.21265483	-2.2752186
H	0.71626116	5.57912664	-1.1500287
H	-0.385741	5.68285018	-2.5280872
H	-0.755698	7.0256937	0.16739427
H	-2.4981219	7.25938568	0.43460366
H	-1.8458701	7.14623591	-1.2163178
H	-3.2643691	-7.9670202	-0.85111
C	-3.1413802	-3.1459577	-0.7978465
C	-4.4636007	-3.6784143	-0.8426278
C	-2.0471189	-4.0320356	-1.0110769
H	-0.9982418	-7.0760596	-0.743111
H	-1.0293876	-3.6469787	-0.9741701
C	-4.6072241	-5.0401855	-1.1116943
C	-2.2056923	-5.3681483	-1.2661679
C	-3.5303858	-5.8894273	-1.3236086
C	-3.7568172	-7.3386871	-1.6077269
C	-1.0233473	-6.2635456	-1.4833339
H	-0.0813275	-5.7075866	-1.405267
H	-5.603025	-5.4774688	-1.1629235
H	-3.325159	-7.6184228	-2.5799365
H	-4.8238505	-7.58923	-1.6207779
H	-1.05693	-6.7333802	-2.4767503
C	-5.4270646	-1.441487	-0.3529141
C	-6.5380995	-0.6352187	-0.0711766
C	-5.6211744	-2.8121601	-0.5990277
H	-6.411679	0.42169193	0.16279579
C	-7.8163872	-1.1576632	-0.0587866
C	-6.9283956	-3.322635	-0.5839842
C	-8.0136961	-2.5108057	-0.3240054
H	-8.6662034	-0.5095903	0.16384578
H	-7.1094387	-4.3797398	-0.7723585
H	-9.020217	-2.9334537	-0.3175495
H	-0.4231786	0.55865091	-0.3821063
H	-2.8824482	1.50468125	2.65084733

D2

60

SCF-energy = -1309.4978

H	2.2697542	3.07233843	1.70510845
C	2.23578506	2.94630392	0.6272895
C	1.00231804	3.06007214	-0.0087118
C	0.95704935	2.89653222	-1.4086522
C	2.14813293	2.63023732	-2.0788694
H	2.11415991	2.50417698	-3.1566852
C	3.38159839	2.51645902	-1.4428669
C	3.42687218	2.68003169	-0.0429306
C	7.09842199	2.19786257	0.66000243
C	7.15666512	2.35575187	2.02745537
H	8.11397312	2.27123465	2.54629884
C	5.9870981	2.62331248	2.73958036
C	4.79042663	2.72596734	2.06473636
C	4.709034	2.56844927	0.67026312
H	3.89078286	2.93548214	2.6421803
H	6.01537136	2.75120172	3.82380439
H	8.02428384	1.98968535	0.12541088
C	5.88778063	2.29849245	-0.0476904
C	-0.3251042	3.00816868	-2.1218525
C	-0.4064735	2.85080167	-3.5163442
C	-1.6031347	2.95352357	-4.1911963
C	-2.7727128	3.22101233	-3.4790626
C	-2.714491	3.37876276	-2.1115926
H	-3.6403576	3.58690918	-1.5769972
H	-3.7300109	3.30559379	-3.9979138
H	-1.6313895	2.8257534	-5.2754349
H	0.49318282	2.64136886	-4.0937982
C	-1.5038624	3.27805068	-1.4038899
C	5.83708553	2.12776066	-1.5084314
C	4.61636703	2.23386304	-2.1891838
C	4.61546201	2.06349771	-3.5835966
C	5.75657644	1.79720528	-4.3133146
C	6.9853984	1.6902433	-3.6284304
H	3.67801021	2.14149812	-4.1344406
C	6.99408392	1.85651687	-2.2579389
H	7.95477294	1.76937029	-1.7505428
C	-2.6015392	3.88592224	2.17689589
C	-2.6102114	3.71973237	0.8063939
C	-1.4531881	3.44864916	0.05686727
C	-0.232463	3.34258895	0.73761477
C	-0.2315688	3.51288712	2.13203564
H	0.70589095	3.43493958	2.68287358
H	-3.570912	3.80680377	0.29900693
C	-3.872369	4.17431203	2.92324279
C	-1.3727043	3.77904595	2.86176977
C	-1.3081637	3.95128797	4.35218021
C	5.69202475	1.62489258	-5.8037164
C	8.25620012	1.40167417	-4.3747559
H	-4.7318515	4.22482486	2.24287184
H	-3.8126571	5.13158581	3.46219888
H	-4.0819696	3.3975416	3.67364826
H	-0.2816354	3.83733721	4.72291555
H	-1.9370543	3.21124062	4.86909287
H	-1.6679664	4.94526602	4.65702116
H	8.19637929	0.44438608	-4.9136742
H	9.11567135	1.3510877	-3.6943762
H	8.46589853	2.17839006	-5.1251907
H	6.32103881	2.36480997	-6.3206639
H	4.66551841	1.73898498	-6.174469
H	6.05167207	0.63083946	-6.1084975

C1

60

SCF-energy = -1309.2137

C	2.23462775	2.95655444	0.72249975
C	1.04169682	3.21305561	-0.0240649
C	1.0850811	3.09846932	-1.451301
H	0.20745213	3.34995395	-2.0433755
C	2.22550463	2.74202144	-2.0800444
H	2.25286031	2.73323579	-3.1677982
C	3.36974629	2.31327369	-1.332448
C	3.27659345	2.25573956	0.09382454
C	6.37920013	0.26359042	0.85388068
C	6.09082075	-0.2418858	2.10576766
H	6.81023297	-0.8905148	2.60952176
C	4.86221111	0.04147371	2.7013659
C	3.96075941	0.86356048	2.05662218
C	4.26250117	1.43315786	0.80988361
H	4.60454147	-0.3959278	3.66784349
H	7.31743846	-0.020298	0.37770558
C	5.4680509	1.08728558	0.17703857
C	1.20788794	4.35688659	4.06276114
C	2.43092339	4.59537461	4.65709929
C	3.60615741	4.3268268	3.95624637
C	3.54045737	3.78059023	2.69077596
C	2.30616211	3.47735504	2.09544758
H	4.57672521	4.56060457	4.39799199
H	2.47392024	5.02659345	5.6592208
H	0.30124858	4.63211731	4.6011689
C	1.12237034	3.81741648	2.77107464
C	5.70140397	1.51752331	-1.2039679
C	4.61686887	2.02555634	-1.9667522
C	4.83508975	2.3153452	-3.3392508
C	6.05633214	2.15962483	-3.948312
C	7.14644732	1.69145913	-3.1658362
H	4.01705526	2.70562694	-3.9438147
C	6.9404886	1.38135839	-1.8277566
H	7.79453565	1.02338693	-1.2526938

C	-2.6017219	3.79735025	2.07248195
C	-1.3822003	3.81823348	2.73685104
C	-0.1613857	3.68709811	2.07698998
C	-0.1748433	3.49225709	0.67056351
C	-1.4266629	3.49747567	0.0010334
H	-1.4607797	3.35028249	-1.0779288
H	-1.3967285	3.93675745	3.82035698
C	-3.8801168	3.93534445	2.83567536
C	-2.6228713	3.64617402	0.65951413
C	-3.9233785	3.63246383	-0.0869368
C	6.2448825	2.490661	-5.3986828
C	8.50110733	1.53177344	-3.7783754
H	-4.4465343	4.81474304	2.49581227
H	-3.7013561	4.03809398	3.91235336
H	-4.5279797	3.06088952	2.6767942
H	-3.7645565	3.50719422	-1.164811
H	-4.4791723	4.56878226	0.06544049
H	-4.5718086	2.81347343	0.25605586
H	5.30971592	2.83755621	-5.8545898
H	6.59117404	1.61408936	-5.9648318
H	6.99885245	3.27949937	-5.5332722
H	8.86305157	2.48772536	-4.1843141
H	8.47024185	0.82262728	-4.618518
H	9.23585065	1.16863334	-3.0503456
H	2.99242153	1.05640702	2.51871949
H	4.46437865	3.6001387	2.1410679

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SCF-energy	=	-1308.3253	
C	2.14759112	2.73019871	0.6783767
C	1.00842554	3.0756579	-0.0671519
C	1.10743257	3.08620748	-1.4653338
H	0.24496983	3.34900031	-2.0755475
C	2.27858431	2.77005899	-2.10317
H	2.29391285	2.79586777	-3.1914554
C	3.43207469	2.42137691	-1.3871284
C	3.36436596	2.4016551	0.01567969
C	6.86581224	1.37799466	0.89681304
C	6.80305145	1.35736627	2.27715565
H	7.6862774	1.0889355	2.86052298
C	5.62047707	1.67700504	2.92076442
C	4.47876355	2.02301284	2.19928351
C	4.53997793	2.04484448	0.78756314
H	5.60010133	1.65244875	4.00891772
H	7.80777089	1.12258225	0.41414099
C	5.75000029	1.71790465	0.13008804
C	0.83323628	3.00823001	4.18259095
C	1.95192935	2.66883482	4.91951521
C	3.13411426	2.34938837	4.27509539
C	3.2221134	2.36265046	2.88375208
C	2.07970387	2.70943985	2.12755814
H	3.99933474	2.08590643	4.88095334
H	1.90363345	2.65253493	6.01032432
H	-0.0849103	3.2554311	4.71305414
C	0.87092259	3.03597973	2.78751067
C	5.81554683	1.74027856	-1.3351276
C	4.68023894	2.08484564	-2.0766576
C	4.77820598	2.09643992	-3.4800132
C	5.93909012	1.78445565	-4.155953
C	7.08528424	1.43652379	-3.4070831
H	3.90690195	2.361817	-4.0784885
C	6.99593247	1.42327507	-2.030808
H	7.89270454	1.1519653	-1.4739555
C	-2.6683949	4.06951704	1.90496509
C	-1.5376709	3.72754354	2.61687645
C	-0.3159286	3.39604939	2.0043079
C	-0.2473417	3.41502088	0.60701022
C	-1.4042413	3.76466536	-0.1130436
H	-1.3746399	3.78621489	-1.202277
H	-1.6144983	3.71951668	3.70404119
C	-3.9467626	4.41447802	2.61343657
C	-2.5993413	4.08863997	0.49412378
C	-3.8029607	4.45430505	-0.3261253
C	5.98522752	1.81359152	-5.6566974
C	8.37336351	1.0887035	-4.0963045
H	-4.277917	5.43485532	2.36938226
H	-3.8287445	4.35093806	3.70256058
H	-4.7622904	3.735648	2.32274561
H	-3.579154	4.41998485	-1.3998531
H	-4.157634	5.46816921	-0.0880875
H	-4.6420515	3.76896866	-0.1347545
H	5.01489895	2.10256029	-6.0799165
H	6.25297492	0.82935046	-6.0689589
H	6.73807126	2.52831825	-6.0210624
H	8.24982523	0.22363987	-4.7647299
H	9.15993463	0.84366943	-3.3714443
H	8.73452489	1.9227105	-4.7163073

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SCF-energy	=	-1310.3792	
C	1.36477528	3.02580762	0.75472644
C	1.64880446	1.8040821	0.23800115
H	0.92365642	0.99663897	0.33592423
C	2.85286383	1.47827587	-0.5388557
H	2.45931887	1.36114316	-1.5751448
C	3.862627	2.55963217	-0.6287062
C	4.51723618	-1.3774058	-1.9613794
C	3.61566178	-2.3924639	-1.6298159
H	3.63711304	-3.3399412	-2.1699506
C	2.66257962	-2.1839213	-0.5916389
C	2.59755122	-1.0056865	0.0731956
C	3.53921055	0.12591297	-0.2045828
H	1.98120897	-2.9940795	-0.3225064
H	5.21373053	-1.5479466	-2.7839785
C	4.52014564	-0.1556895	-1.3127553
C	0.70177191	6.90763279	2.38787905
C	1.63168209	7.91193928	2.22773643
C	2.81203669	7.67642904	1.5165791
C	3.03476649	6.43042282	0.98687045
H	3.54697863	8.47184141	1.38303181
H	1.4401279	8.89749902	2.65782966
H	-0.2061923	7.13136694	2.94405532
C	0.90105782	5.6255479	1.85386961
C	5.4248862	0.93048742	-1.6619513
C	5.11908741	2.26334511	-1.2948998
C	6.02773826	3.28326823	-1.633151
C	7.20762494	3.04112737	-2.3069005
C	7.51621666	1.70653116	-2.6677498
H	5.79509879	4.31937635	-1.3839624
C	6.62815529	0.69534264	-2.3422707
H	6.8984448	-0.3296444	-2.6002188
C	-2.2818121	3.83209237	2.86722942
C	-1.3089759	4.80074198	2.70909846
C	-0.1088416	4.5708786	2.01949075
C	0.10896038	3.30147555	1.47368238
C	-0.8802449	2.32235406	1.6300107
H	-0.7404639	1.32744998	1.20574477
H	-1.5052681	5.77886404	3.14629056
C	-3.5472118	4.1326309	3.61405703
C	-2.062346	2.55473063	2.30861171
C	-3.0911659	1.47273049	2.44730232
C	8.14196352	4.16247704	-2.6517957
C	8.7928162	1.39286804	-3.3855947
H	-4.4298264	3.99112185	2.97363951
H	-3.5606089	5.1652765	3.98320462
H	-3.6673068	3.46315801	4.47806751
H	-2.7704826	0.54507898	1.95756762
H	-4.0491274	1.77692068	2.00133726
H	-3.288963	1.2466058	3.50508169
H	7.75335323	5.12898817	-2.3082614
H	8.30111711	4.22983369	-3.7376934
H	9.12960474	4.01370761	-2.1917545
H	9.66542752	1.70735089	-2.7949462
H	8.84700808	1.92856524	-4.3444642
H	8.88839261	0.31980644	-3.5893636
H	1.89338215	-0.8939911	0.90087392
H	3.95832811	6.27167765	0.4337149
H	4.30642953	4.57064024	-0.1509742
C	2.1008856	5.3793428	1.14239172
C	2.35660964	4.0671706	0.5898526
C	3.56002216	3.78660796	-0.0872877
H	4.11609081	0.31089968	0.72500674

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SCF-energy	=	-1310.379	
C	1.016738	3.177133	0.090091
C	1.080185	3.038229	-1.317279
H	0.153064	3.13467	-1.885158
C	2.238646	2.829463	-2.043996
H	2.177825	2.74613	-3.128575
C	3.436782	2.621437	-1.380251
C	3.466555	2.698657	0.104874
C	6.401301	0.712327	0.919579
C	6.112498	0.305596	2.221982
H	6.912204	-0.05771	2.869
C	4.773347	0.367239	2.708596
C	3.770111	0.851384	1.93983
C	3.984658	1.264273	0.518192
H	4.555559	0.017905	3.720211
H	7.438597	0.67998	0.583032
C	5.419633	1.17643	0.05743
C	1.128238	4.357184	4.156004
C	2.334166	4.495472	4.800577
C	3.532713	4.190258	4.138492
C	3.491298	3.743655	2.844158
H	4.49044	4.316562	4.646336
H	2.357771	4.857368	5.83075
H	0.218789	4.620511	4.693266

C	1.052308	3.905184	2.824151
C	5.678843	1.589096	-1.310228
C	4.659249	2.246832	-2.044467
C	4.871721	2.556061	-3.401515
C	6.058852	2.273043	-4.044736
C	7.086147	1.625639	-3.310305
H	4.094719	3.083462	-3.958192
C	6.875268	1.297581	-1.980958
H	7.667105	0.764325	-1.453577
C	-2.668126	3.895854	2.138455
C	-1.454204	3.993791	2.782987
C	-0.224982	3.775551	2.132523
C	-0.245597	3.439041	0.770605
C	-1.487356	3.341258	0.11652
H	-1.532777	3.062026	-0.937065
H	-1.466292	4.24534	3.843111
C	-3.95031	4.135348	2.878822
C	-2.68572	3.559412	0.761741
C	-3.98636	3.434813	0.025805
C	6.26324	2.64369	-5.483227
C	8.385543	1.288019	-3.97373
H	-4.518676	4.963612	2.431548
H	-3.765762	4.382483	3.931268
H	-4.599147	3.248096	2.848351
H	-3.830495	3.167118	-1.026445
H	-4.550233	4.378345	0.055116
H	-4.627486	2.665325	0.479546
H	6.475529	1.756144	-6.096623
H	7.116225	3.327321	-5.601967
H	5.376488	3.136495	-5.900012
H	8.87786	2.19362	-4.356821
H	8.227211	0.623144	-4.835178
H	9.075992	0.791326	-3.281956
H	2.748005	0.871159	2.323014
H	4.432814	3.521408	2.342307
H	4.274574	3.39939	0.368581
H	3.38767	0.556892	-0.094743
C	2.260717	3.583746	2.158099
C	2.21735	3.146822	0.790802

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SCF-energy = -1310.3714

C	1.36523653	-0.2529206	0.24122363
C	0.46029614	-1.2666387	0.43838401
H	0.81552919	-2.283035	0.6099645
C	-0.9630568	-1.0851018	0.42299418
H	-1.4831728	-1.721644	1.14863225
C	-1.4510347	0.28156182	0.32029782
C	-3.778816	-2.9833643	-0.6082623
C	-3.1482373	-4.2032487	-0.8738941
H	-3.705854	-5.1357511	-0.7688553
C	-1.7989308	-4.2324299	-1.2878571
C	-1.089414	-3.0723889	-1.4091945
C	-1.6778836	-1.7815349	-1.0721431
H	-1.3324604	-5.1862468	-1.5432675
H	-4.8180641	-2.983469	-0.274249
C	-3.107484	-1.7812646	-0.7295847
C	4.02309265	3.02810805	-0.3515336
C	3.53901228	4.3062383	-0.5253269
C	2.16180298	4.54709595	-0.5061254
C	1.29987366	3.49655268	-0.3110432
H	1.77459945	5.55778944	-0.6458444
H	4.23693448	5.13194549	-0.6797421
H	5.10073655	2.87825605	-0.3739165
C	3.16486927	1.93522018	-0.1506183
C	-3.7134012	-0.5004666	-0.3331119
C	-2.9038982	0.50087744	0.23345725
C	-3.494222	1.68613963	0.66884207
C	-4.8590622	1.92184924	0.54691896
C	-5.6660001	0.93465201	-0.0493648
H	-2.8734566	2.44589231	1.15008553
C	-5.0780942	-0.2529803	-0.4723497
H	-5.7083085	-1.0063181	-0.9504851
C	5.59514263	-0.9538113	0.18690044
C	5.0710934	0.31332882	0.02217476
C	3.69213095	0.57734659	0.03256167
C	2.81408172	-0.4971256	0.21979214
C	3.34911773	-1.7836134	0.38325053
H	2.68773677	-2.6383467	0.5293339
H	5.77755888	1.13023284	-0.1194591
C	7.07812647	-1.1771764	0.16942333
C	4.70705825	-2.0364212	0.37258558
C	5.22935088	-3.4302685	0.55619129
C	-5.4574746	3.20568051	1.04001246
C	-7.1385911	1.15624522	-0.2248318
H	7.42464918	-1.6182707	1.1152407
H	7.62403027	-0.2385542	0.01520241
H	7.36642086	-1.8718002	-0.6328203
H	4.41429979	-4.1526511	0.68755632
H	5.88375583	-3.4958905	1.43743853
H	5.82770325	-3.7481034	-0.3099219
H	-4.696849	3.86126264	1.48115325
H	-6.2258481	3.01836919	1.80398575
H	-5.9466158	3.75582997	0.22307166
H	-7.3354799	2.04629804	-0.8398172
H	-7.632399	1.32141149	0.74377043
H	-7.6204766	0.29796189	-0.708269
H	-0.0618664	-3.0898736	-1.7800511
H	0.23206834	3.7074726	-0.3037702
H	-0.9367096	2.29336692	-0.0229074
C	1.77089572	2.17620739	-0.1283591
C	0.85329654	1.07631991	0.08292886
C	-0.5480846	1.29004839	0.1322536
H	-1.3818044	-0.989168	-1.7726807

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SCF-energy = -1310.3758

C	1.034458	3.207919	0.067907
C	1.080731	3.000015	-1.321695
H	0.146979	3.007656	-1.884968
C	2.255776	2.800651	-2.04164
H	2.205321	2.636787	-3.118763
C	3.462279	2.737215	-1.38158
C	3.478004	2.862199	0.068871
C	6.336686	0.887189	0.937373
C	6.045387	0.591447	2.276589
H	6.858395	0.380593	2.973739
C	4.708774	0.555805	2.720509
C	3.684119	0.837153	1.860307
C	3.930534	1.186033	0.46391
H	4.487161	0.280326	3.753648
H	7.379804	0.93035	0.618795
C	5.338275	1.138535	0.020005
C	1.143972	4.301168	4.173069
C	2.349006	4.439178	4.824915
C	3.549379	4.188454	4.151324
C	3.513802	3.800564	2.834504
H	4.505724	4.310832	4.662884
H	2.36469	4.755526	5.870094
H	0.230194	4.516222	4.72419
C	1.075901	3.905597	2.825929
C	5.61865	1.523257	-1.371825
C	4.704458	2.345807	-2.055272
C	4.978431	2.735354	-3.365874
C	6.133564	2.334855	-4.027023
C	7.03889	1.491158	-3.355306
H	4.281385	3.400034	-3.882011
C	6.762224	1.102944	-2.047887
H	7.457376	0.424797	-1.548218
C	-2.649427	3.842802	2.15343
C	-1.43144	3.95868	2.790042
C	-0.204008	3.764922	2.131829
C	-0.227684	3.436012	0.768506
C	-1.471635	3.318246	0.124068
H	-1.518745	3.051932	-0.932377
H	-1.44215	4.20918	3.850313
C	-3.929542	4.060203	2.904001
C	-2.670793	3.512215	0.777214
C	-3.973266	3.371922	0.047117
C	6.404412	2.787699	-5.430777
C	8.283777	1.011883	-4.039425
H	-4.513228	4.881659	2.463909
H	-3.741497	4.305935	3.95618
H	-4.56548	3.163623	2.874069
H	-3.81852	3.110986	-1.007004
H	-4.550589	4.307096	0.082728
H	-4.601196	2.591345	0.50043
H	6.4909	1.931099	-6.11487
H	7.351051	3.343684	-5.49323
H	5.605464	3.439308	-5.804792
H	8.917564	1.857184	-4.344473
H	8.042434	0.448185	-4.952199
H	8.877885	0.361134	-3.386722
H	2.648482	0.766514	2.199004
H	4.460726	3.62758	2.323689
H	4.36705	3.383009	0.433807
H	3.238135	0.654383	-0.204747
C	2.288978	3.647636	2.143596
C	2.253042	3.250286	0.758934

Table S2b. Cartesian coordinates and SCF energies (LC-ωPBE/def2-SVP) for compounds investigated with X = F.

A

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SCF-energy = -1409.5096

C	-2.9379334	-1.7639663	-0.5483432
C	-4.0569426	-0.8784767	-0.3891562

C	-3.8154029	0.47098508	-0.2351474
H	-4.6523857	1.16089974	-0.1745905
C	-2.5250805	1.0418591	-0.2079668
C	-1.4353809	0.12305708	-0.3340094
C	-1.6275597	-1.2088025	-0.4899121
H	-0.7375844	-1.8300657	-0.5595
C	-1.3038861	3.0763438	-0.8798747
C	-1.1381844	4.4444207	-0.9600921
C	-2.0026866	5.27365818	-0.2106815
C	-2.9839969	4.68562809	0.58613888
H	-3.6142246	5.33004751	1.20337055
C	-3.1678369	3.31087677	0.66739147
C	-0.0676626	5.03689939	-1.8276232
H	-0.6503081	2.44304459	-1.4796725
C	-2.3219263	2.47365371	-0.107704
C	-6.4336149	2.79220023	2.4961631
C	-6.0725227	1.85059355	3.45345654
H	-6.8116532	1.48708678	4.17057622
C	-4.7640537	1.38348614	3.50376405
C	-3.8222264	1.84719152	2.59515963
C	-4.1772681	2.78654839	1.62223687
H	-4.470685	0.6591124	4.26660953
H	-7.4579665	3.16943753	2.45771544
C	-5.491462	3.26213329	1.58972344
H	-5.7805554	4.00017587	0.83707915
C	-1.854648	6.76137316	-0.2518427
H	0.51164259	4.25707892	-2.3363939
H	0.63188493	5.64423323	-1.2353763
H	-0.4957915	5.69651819	-2.5961211
H	-0.8546823	7.06608506	0.09017936
H	-2.5990289	7.26054919	0.37941015
H	-1.9661315	7.13779936	-1.2792361
H	-3.3211178	-7.9703618	-0.8194488
C	-3.1479401	-3.1539106	-0.7816678
C	-4.4714553	-3.6681622	-0.8611703
C	-2.0585546	-4.0489549	-0.961836
H	-1.0469522	-7.1034523	-0.6564628
H	-1.038469	-3.6726526	-0.8993021
C	-4.6234176	-5.0287897	-1.1282259
C	-2.223958	-5.3858977	-1.2170364
C	-3.5501903	-5.8915733	-1.3073256
C	-3.7861187	-7.3396968	-1.5913113
C	-1.0449048	-6.2934814	-1.3998943
H	-0.0998858	-5.7463004	-1.2989675
H	-5.6222699	-5.4554534	-1.2049448
H	-3.3326185	-7.6287791	-2.5507456
H	-4.8552984	-7.57806	-1.6313094
H	-1.0566906	-6.7666259	-2.3922439
C	-5.4241988	-1.4158094	-0.4096178
C	-6.5340851	-0.5940607	-0.1707856
C	-5.6269847	-2.7850697	-0.6559512
H	-6.4027957	0.46311682	0.05906672
C	-7.8189038	-1.1001849	-0.197616
C	-6.9389631	-3.2786438	-0.6806456
C	-8.0231127	-2.4519174	-0.4607163
H	-8.6675513	-0.4402622	-0.0079932
H	-7.1267263	-4.334486	-0.8695839
H	-9.0341728	-2.8629511	-0.4852827
F	-0.1975775	0.58404449	-0.2553382
H	-2.7893555	1.49523742	2.65586258

C1

60

SCF-energy = -1408.3172

C	2.17391484	2.90716221	0.72187583
C	0.95556968	3.10606367	-0.0043801
C	1.03425645	3.06286646	-1.3792386
H	0.18211995	3.28546793	-2.0206861
C	2.25331146	2.81354797	-2.0125681
F	2.22309419	2.87197856	-3.3236256
C	3.43392126	2.42862782	-1.3450842
C	3.29997408	2.27646069	0.04444124
C	6.28394433	0.14100034	0.78039299
C	5.97479219	-0.341071	2.03043984
H	6.66158837	-1.0275391	2.53022221
C	4.76370491	0.01045723	2.64675316
C	3.90846466	0.87140221	2.01189365
C	4.22662379	1.42166793	0.74210197
H	4.49439102	-0.416236	3.61453619
H	7.20643232	-0.1909302	0.30672665
C	5.41758789	1.01232755	0.09302899
C	1.23144848	4.49177416	3.96399237
C	2.4780141	4.71418271	4.52515485
C	3.64639145	4.37648287	3.82757849
C	3.54571661	3.78104649	2.5977362
C	2.27559497	3.49503905	2.01535994
H	4.62639017	4.60247774	4.25084372
H	2.54788764	5.18641438	5.50763292
H	0.34802189	4.81000769	4.51585686
C	1.092001	3.9087226	2.70284254
C	5.70061071	1.46616699	-1.2614355
C	4.69638028	2.11195794	-2.0060492
C	4.98654573	2.49560455	-3.3292934
C	6.21505215	2.26451087	-3.915343
C	7.22744867	1.62062435	-3.1645519
H	4.23952641	3.01771952	-3.9210826
C	6.94854594	1.24215985	-1.8686717
H	7.74433068	0.76261235	-1.2989636
C	-2.6576707	3.85053414	2.14280826
C	-1.4197391	3.951338	2.75840326
C	-0.219136	3.73903926	2.07179867
C	-0.2810108	3.40195056	0.71371456
C	-1.5288471	3.30922317	0.08834172
H	-1.5888303	3.02591107	-0.9639434
H	-1.4014156	4.19794272	3.82042061
C	-3.9166253	4.07892298	2.92414917
C	-2.7148346	3.52653993	0.77055929
C	-4.033482	3.40431119	0.06787029
C	6.47742014	2.70451602	-5.3246128
C	8.57720474	1.36444522	-3.765014
H	-4.5006664	4.90868329	2.50046543
H	-3.7027317	4.31679712	3.97307334
H	-4.5628748	3.18951841	2.90325786
H	-3.9043152	3.14572492	-0.9900517
H	-4.5984617	4.34619744	0.11985284
H	-4.6603107	2.62922738	0.53198958
H	5.59748287	3.18893936	-5.7647326
H	6.74821523	1.85025492	-5.9619146
H	7.31523661	3.41530651	-5.3700668
H	9.0570907	2.30259657	-4.0791142
H	8.4989399	0.72989041	-4.6596146
H	9.24536697	0.86446449	-3.0533941
H	2.95143052	1.10550485	2.47709424
H	4.45193504	3.55358157	2.03764951

D1

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SCF-energy = -1407.4301

C	2.12930101	2.70369946	0.67316602
C	0.97242496	3.02194339	-0.0567484
C	1.03975548	2.97882905	-1.4488737
H	0.18276437	3.19370267	-2.0834299
C	2.20485176	2.65901413	-2.0889619
F	2.13045322	2.63852092	-3.4268348
C	3.4038245	2.36126081	-1.4199493
C	3.33468353	2.36698131	-0.0083326
C	6.80125072	1.22180327	0.87269192
C	6.73731816	1.18912985	2.25186692
H	7.60232214	0.86129159	2.83213335
C	5.57615974	1.57361285	2.89710158
C	4.45517202	1.98575231	2.1781344
C	4.50919255	1.99896025	0.76461411
H	5.55144089	1.53820344	3.98460542
H	7.72727815	0.91692299	0.38927778
C	5.70572399	1.62839943	0.10841033
C	0.87963603	3.14265063	4.18654072
C	2.01039762	2.83017199	4.91754438
C	3.17196779	2.45776626	4.26554713
C	3.22753035	2.39484225	2.87329597
C	2.08081196	2.73160778	2.12323391
H	4.0485047	2.21922674	4.86524671
H	1.98689958	2.876165	6.00825944
H	-0.0243538	3.42840386	4.72187149
C	0.888197	3.10031645	2.79192196
C	5.7865145	1.68667871	-1.3541617
C	4.66460892	2.05613404	-2.110168
C	4.81572588	2.13321508	-3.5105708
C	6.00050949	1.84886856	-4.1590664
C	7.12116166	1.46267758	-3.3964146
H	3.97448889	2.43526824	-4.1243201
C	6.98633712	1.39645592	-2.0258481
H	7.86767141	1.11162326	-1.4525787
C	-2.6686589	4.09559463	1.93012553
C	-1.5252329	3.78720424	2.63771528
C	-0.3143213	3.42919503	2.01898317
C	-0.2729395	3.38560576	0.62238169
C	-1.4409935	3.70084103	-0.0943275
H	-1.4287263	3.67291265	-1.1838529
H	-1.5836873	3.82706269	3.725251
C	-3.9350337	4.47092116	2.64456418
C	-2.6256853	4.0509191	0.51866456
C	-3.8443649	4.37774317	-0.2955772
C	6.09144534	1.95413879	-5.654615
C	8.43001382	1.14145702	-4.0579929
H	-4.2718777	5.47883976	2.36006847
H	-3.7981703	4.45682	3.73320873
H	-4.7540336	3.77877743	2.39865416
H	-3.6394536	4.29521803	-1.3704222
H	-4.1966195	5.40090481	-0.0972124
H	-4.6783841	3.7005886	-0.058558

H	5.13441956	2.26874143	-6.0891894
H	6.3677062	0.99062659	-6.1084013
H	6.8572337	2.68275894	-5.9600172
H	8.32540667	0.30708798	-4.7673553
H	9.19286138	0.8624754	-3.3200687
H	8.81139141	2.00064469	-4.6295437

B2

62			
SCF-energy	=	-1409.4768	
C	-1.2996674	0.33651325	0.60658174
C	-1.0939693	-0.8552663	-0.0379949
H	-1.8970316	-1.5867775	-0.1106899
C	0.12936759	-1.2034923	-0.8056004
F	-0.26344	-1.4945153	-2.114546
C	1.14115731	-0.1010629	-0.8300134
C	2.32276834	-4.1513759	-1.4349037
C	1.5126922	-5.1464169	-0.9544244
H	1.7780925	-6.1851953	-1.1712118
C	0.32744013	-4.8886812	-0.1985017
C	-0.0015005	-3.6133301	0.0733977
C	0.85931945	-2.47671	-0.3267756
H	-0.2897199	-5.7206498	0.14337614
H	3.18844462	-4.4292994	-2.0326498
C	2.01231441	-2.7939186	-1.2188563
C	-1.7037515	3.9741462	2.83040448
C	-0.6670085	4.88287738	2.90357278
C	0.52562039	4.63394511	2.21984698
C	0.65423992	3.48111449	1.47986779
H	1.35239589	5.34468284	2.27422801
H	-0.7820062	5.7918488	3.4974011
H	-2.6190637	4.19380455	3.37739451
C	-1.6009137	2.79295624	2.08096748
C	2.76948428	-1.7245113	-1.784501
C	2.3582101	-0.3799779	-1.5753405
C	3.14396105	0.64270364	-2.1106544
C	4.30040137	0.39313588	-2.8333212
C	4.71921139	-0.9481478	-3.047853
H	2.81810309	1.67743168	-1.9931465
C	3.95147234	-1.9624107	-2.5273841
H	4.28809436	-2.9851447	-2.696002
C	-5.0164948	1.21595687	2.56277154
C	-3.9459238	2.08798963	2.62290988
C	-2.7143102	1.83591402	1.9983471
C	-2.5708008	0.63848386	1.2824746
C	-3.6617832	-0.2422165	1.22135808
H	-3.5791627	-1.1713319	0.65662801
H	-4.0874545	3.0126246	3.18137938
C	-6.310153	1.54391515	3.24800146
C	-4.8713145	0.01341747	1.83777557
C	-6.0084765	-0.9598232	1.73315768
C	5.09414125	1.52642637	-3.3992583
C	5.96433167	-1.2436492	-3.8293504
H	-7.1406059	1.5917658	2.52858539
H	-6.2566997	2.50961567	3.76532257
H	-6.5735956	0.77673285	3.9906298
H	-5.7332481	-1.8371417	1.13452076
H	-6.8881804	-0.4954339	1.26426222
H	-6.3249342	-1.3125668	2.72561026
H	4.64827783	2.49743319	-3.1548952
H	5.16397802	1.44517398	-4.4937416
H	6.12416626	1.51191483	-3.0143101
H	6.84697263	-0.7823923	-3.3636313
H	5.89532762	-0.8472752	-4.8525556
H	6.14613789	-2.3228595	-3.899244
H	-0.8852691	-3.3837783	0.67215761
H	1.59945063	3.30732804	0.96724269
H	1.7167526	1.79885894	-0.1464059
C	-0.3925146	2.53608907	1.3892258
C	-0.2493872	1.31776048	0.62345873
C	0.9250111	1.052358	-0.1384404
H	1.35162342	-2.1813494	0.63016639

B1

62			
SCF-energy	=	-1409.4834	
C	0.964886	3.078078	0.087599
C	0.960173	2.772173	-1.305628
H	0.038926	2.734764	-1.882853
C	2.143797	2.579313	-2.012674
F	2.034055	2.365496	-3.32202
C	3.382722	2.551069	-1.411761
C	3.449395	2.699722	0.082526
C	6.327538	0.416997	0.769874
C	6.014955	-0.010126	2.036585
H	6.772552	-0.561521	2.601085
C	4.753671	0.237241	2.652879
C	3.818003	0.923491	1.965682
C	4.030946	1.341369	0.56276
H	4.56213	-0.121771	3.664884
H	7.319554	0.202659	0.376793
C	5.395911	1.138346	-0.000637
C	1.138769	4.4631	4.111402
C	2.352403	4.637124	4.737339
C	3.536589	4.323199	4.059854
C	3.475348	3.834338	2.776572
H	4.504071	4.477153	4.542011
H	2.389007	5.03034	5.755197
H	0.233466	4.730948	4.654257
C	1.045312	3.966414	2.797362
C	5.673354	1.62872	-1.314103
C	4.632526	2.246678	-2.068691
C	4.880963	2.55537	-3.412845
C	6.111729	2.330062	-4.006069
C	7.169505	1.755041	-3.247429
H	4.091478	3.020125	-4.001475
C	6.9263	1.415614	-1.93828
H	7.740914	0.961756	-1.373605
C	-2.684552	3.928252	2.154868
C	-1.460967	4.057242	2.776818
C	-0.24008	3.798997	2.125999
C	-0.278814	3.384294	0.784495
C	-1.532113	3.259032	0.154317
H	-1.587795	2.935042	-0.884954
H	-1.458914	4.37237	3.820023
C	-3.955554	4.217266	2.897393
C	-2.721863	3.517511	0.799591
C	-4.031985	3.364801	0.084755
C	6.333799	2.705969	-5.436314
C	8.513584	1.520852	-3.86909
H	-4.523966	5.024565	2.413128
H	-3.755648	4.519712	3.93259
H	-4.611591	3.335049	2.92298
H	-3.887752	3.040031	-0.953088
H	-4.588523	4.313095	0.067509
H	-4.675245	2.625773	0.584123
H	5.431278	3.134834	-5.886589
H	6.630786	1.828277	-6.028633
H	7.147601	3.440056	-5.527007
H	8.955535	2.461758	-4.227142
H	8.439976	0.849526	-4.736631
H	9.213013	1.071682	-3.15371
H	2.833493	1.115221	2.397101
H	4.414116	3.618149	2.264711
H	4.219841	3.460083	0.295676
H	3.429478	0.568401	0.020661
C	2.239385	3.636077	2.114841
C	2.175593	3.127217	0.764841

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62			
SCF-energy	=	-1409.4767	
C	1.012969	3.193103	0.062503
C	1.055441	2.970333	-1.318185
H	0.137842	2.943675	-1.907498
C	2.235593	2.794912	-2.033994
F	2.127906	2.624337	-3.346983
C	3.456935	2.737095	-1.407854
C	3.462369	2.849958	0.051771
C	6.336877	0.908547	0.934761
C	6.051132	0.607864	2.275329
H	6.865654	0.383938	2.966355
C	4.714913	0.583506	2.725079
C	3.689585	0.887247	1.875824
C	3.925756	1.237131	0.469834
H	4.49523	0.301311	3.75689
H	7.379059	0.942438	0.612409
C	5.339309	1.173958	0.02237
C	1.136386	4.29607	4.159201
C	2.344842	4.448511	4.802837
C	3.544468	4.211731	4.122928
C	3.505729	3.821311	2.8072
H	4.502103	4.347617	4.628461
H	2.363202	4.767029	5.847352
H	0.224085	4.502158	4.716124
C	1.063899	3.898062	2.814028
C	5.618796	1.547965	-1.37227
C	4.696704	2.345887	-2.079176
C	4.981159	2.723858	-3.39292
C	6.151295	2.334028	-4.033005
C	7.060103	1.511825	-3.341513
H	4.27601	3.357717	-3.931129
C	6.773737	1.135631	-2.032244
H	7.473222	0.473472	-1.51793
C	-2.664521	3.810902	2.156485
C	-1.444954	3.932181	2.790121
C	-0.219134	3.745998	2.127568
C	-0.247946	3.417294	0.76471
C	-1.491356	3.297023	0.121755
H	-1.538545	3.036421	-0.936303
H	-1.45384	4.181451	3.850705

C	-3.943146	4.02005	2.911623
C	-2.689428	3.484551	0.779282
C	-3.993266	3.342259	0.052492
C	6.429085	2.772203	-5.440104
C	8.317869	1.039533	-4.005753
H	-4.531861	4.840005	2.475511
H	-3.753296	4.263399	3.963988
H	-4.574782	3.120513	2.880479
H	-3.840725	3.086003	-1.003045
H	-4.573801	4.275177	0.093673
H	-4.616718	2.557593	0.504856
H	5.623619	3.406642	-5.829098
H	6.532749	1.907948	-6.112095
H	7.368308	3.340724	-5.501916
H	8.942402	1.88904	-4.318083
H	8.092208	0.459458	-4.912287
H	8.91453	0.406665	-3.33797
H	2.656054	0.825093	2.22246
H	4.451171	3.661851	2.28915
H	4.334883	3.414345	0.394516
H	3.249796	0.659959	-0.180361
C	2.277385	3.651222	2.124699
C	2.238014	3.246688	0.746238

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62			
SCF-energy	=	-1409.469	
C	1.335659	2.994861	0.572893
C	1.513489	1.836609	-0.148998
H	0.710879	1.109612	-0.265791
C	2.742557	1.499427	-0.836793
F	2.481418	0.879618	-2.020985
C	3.752979	2.571921	-0.916716
C	4.63339	-1.408343	-1.490237
C	3.723003	-2.337689	-1.021612
H	3.721685	-3.341215	-1.456122
C	2.785946	-2.030191	-0.007902
C	2.77975	-0.778934	0.520512
C	3.665052	0.258601	0.029341
H	2.09865	-2.797988	0.35072
H	5.315556	-1.682841	-2.295389
C	4.642472	-0.110929	-0.984772
C	0.947193	6.618133	2.804969
C	1.98033	7.531023	2.860357
C	3.168876	7.283609	2.167647
C	3.296007	6.127635	1.434195
H	3.991944	7.999341	2.209391
H	1.866395	8.444366	3.447756
H	0.035705	6.838828	3.357739
C	1.04897	5.431115	2.063795
C	5.491922	0.926387	-1.563569
C	5.024099	2.253325	-1.585005
C	5.788611	3.220692	-2.225655
C	7.0189	2.925781	-2.808958
C	7.50533	1.604882	-2.758181
H	5.405132	4.241494	-2.29242
C	6.725205	0.630789	-2.149826
H	7.110133	-0.390517	-2.103593
C	-2.33187	3.811275	2.635105
C	-1.274148	4.699707	2.666238
C	-0.057076	4.466075	2.006343
C	0.081764	3.272484	1.283972
C	-0.993439	2.370358	1.258278
H	-0.907909	1.436736	0.701247
H	-1.412941	5.62052	3.23156
C	-3.610479	4.11879	3.356596
C	-2.187966	2.608244	1.908956
C	-3.310274	1.614923	1.843215
C	7.811051	4.002365	-3.485709
C	8.834071	1.253404	-3.358633
H	-4.461593	4.150325	2.660902
H	-3.559007	5.086471	3.87025
H	-3.839125	3.348817	4.107741
H	-3.037773	0.738932	1.241501
H	-4.211059	2.061776	1.398019
H	-3.591293	1.263068	2.846515
H	7.296732	4.969808	-3.443969
H	7.9878	3.756412	-4.54281
H	8.798629	4.119753	-3.016437
H	9.645932	1.832042	-2.894902
H	8.855231	1.47688	-4.435068
H	9.064144	0.188722	-3.230988
H	2.090475	-0.521093	1.328866
H	4.235338	5.955078	0.91098
H	4.369975	4.429137	-0.179214
C	2.251481	5.177881	1.360302
C	2.389198	3.962858	0.590395
C	3.560991	3.701048	-0.186472
H	4.061355	0.893876	0.832138

Table S2c. Cartesian coordinates and SCF energies (LC-ωPBE/def2-SVP) for compounds investigated with X =OMe.

A

66			
SCF-energy	=	-1424.775065	
C	-1.564251	-0.174237	-0.758995
C	-0.766331	-0.754057	-1.785243
H	-1.218691	-1.215864	-2.659884
C	0.595040	-0.769969	-1.733954
O	1.270622	-1.329770	-2.755298
C	1.278342	-0.160547	-0.619763
C	3.144871	0.089447	3.052711
C	2.648986	-0.395656	4.256610
H	2.810987	0.170360	5.176670
C	1.954688	-1.599672	4.291789
C	1.761949	-2.318846	3.117921
C	2.252995	-1.832604	1.913606
H	1.570867	-1.984013	5.239263
H	3.686379	1.038619	3.030035
C	2.944613	-0.619010	1.864570
C	-3.817632	1.500118	2.474495
C	-3.195274	1.926114	3.632509
C	-1.812271	1.826392	3.750978
C	-1.070722	1.313060	2.704326
H	-1.312038	2.145722	4.667168
H	-3.791755	2.329966	4.452835
H	-4.902476	1.574878	2.415659
C	-3.083779	0.975834	1.402549
C	3.494532	-0.102028	0.583911
C	2.725442	0.014535	-0.598697
C	3.368762	0.418426	-1.786427
C	4.710321	0.752097	-1.831367
C	5.470157	0.651010	-0.647456
H	2.776660	0.507829	-2.698144
C	4.846422	0.219906	0.521600
H	5.449321	0.101106	1.425018
C	-5.778234	0.128837	-1.130993
C	-5.123623	0.589902	0.005097
C	-3.744192	0.496410	0.179980
C	-2.982326	-0.092528	-0.867370
C	-3.665383	-0.564096	-2.021694
H	-3.096495	-1.017625	-2.831968
H	-5.736709	1.044394	0.781877
C	-7.261633	0.262830	-1.252273
C	-5.024844	-0.470781	-2.176766
C	-5.702248	-0.980049	-3.413518
C	5.340359	1.216277	-3.111621
C	6.929420	0.985527	-0.646521
H	-7.528870	0.858805	-2.137282
H	-7.701070	0.742390	-0.369957
H	-7.733996	-0.722133	-1.380606
H	-4.978675	-1.409114	-4.117079
H	-6.241107	-0.174712	-3.932999
H	-6.440357	-1.758177	-3.171653
H	4.612666	1.233587	-3.931955
H	6.170006	0.558718	-3.409110
H	5.755655	2.229080	-3.007322
H	7.093757	2.026919	-0.959781
H	7.480633	0.350480	-1.355349
H	7.374030	0.853336	0.346928
H	1.233211	-3.274140	3.142355
H	0.008046	1.223490	2.831510
H	1.003894	0.819730	1.251852
C	-1.684913	0.893714	1.516641
C	-0.898317	0.351002	0.402235
C	0.480890	0.351024	0.422518
H	2.116579	-2.415103	0.999036
C	1.964617	-2.539428	-2.498336
H	2.451501	-2.829125	-3.435904
H	2.733224	-2.413241	-1.720796
H	1.259639	-3.330727	-2.198958

C1

64			
SCF-energy	=	-1423.593381	
C	2.203403	2.973619	0.717037
C	1.015326	3.122968	0.005673
C	1.128092	3.047853	-1.432573
O	0.062273	3.333001	-2.135635
C	2.358746	2.785633	-2.066387
H	2.408197	2.810622	-3.151734
C	3.470620	2.420654	-1.342849
C	3.329119	2.311219	0.078515
C	6.212305	0.056242	0.814510
C	5.862325	-0.432593	2.062563
H	6.516550	-1.150230	2.562421

C	4.663238	-0.039648	2.667231
C	3.850309	0.864920	2.029266
C	4.204555	1.411321	0.766688
H	4.366993	-0.459250	3.630040
H	7.131528	-0.302764	0.353121
C	5.398277	0.962889	0.132623
C	1.282343	4.598526	3.967179
C	2.516731	4.818948	4.527966
C	3.679731	4.437709	3.842914
C	3.576659	3.815179	2.625633
C	2.313510	3.541872	2.047112
H	4.662827	4.653512	4.265408
H	2.591691	5.318892	5.495915
H	0.397257	4.948028	4.496783
C	1.147595	3.971400	2.711794
C	5.731808	1.436479	-1.216611
C	4.756084	2.107915	-1.964051
C	5.053364	2.507204	-3.272379
C	6.286173	2.270869	-3.856866
C	7.274860	1.605144	-3.102238
H	4.311295	3.057388	-3.853872
C	6.977157	1.204578	-1.808580
H	7.760176	0.700190	-1.241514
C	-2.590129	3.824788	2.226612
C	-1.344483	3.978826	2.793550
C	-0.149477	3.781767	2.079209
C	-0.223712	3.414708	0.720186
C	-1.505926	3.249771	0.152434
H	-1.598138	2.928420	-0.879950
H	-1.297158	4.245125	3.849269
C	-3.834411	4.038724	3.035163
C	-2.669546	3.442488	0.865685
C	-4.004359	3.233033	0.213540
C	6.570989	2.729237	-5.256157
C	8.629813	1.340910	-3.687154
H	-4.459690	4.830900	2.598437
H	-3.598363	4.324869	4.067275
H	-4.449206	3.127568	3.068042
H	-3.895539	2.930403	-0.835086
H	-4.608049	4.151900	0.239942
H	-4.584069	2.455360	0.731647
H	5.702425	3.230179	-5.700867
H	6.841661	1.882823	-5.903771
H	7.415510	3.433035	-5.280116
H	9.125452	2.278196	-3.978800
H	8.556508	0.722390	-4.593396
H	9.281880	0.821293	-2.974857
H	2.901563	1.145417	2.485620
H	4.487355	3.558387	2.085027
C	0.075927	3.411933	-3.552910
H	-0.945596	3.672006	-3.847856
H	0.349840	2.444242	-3.996045
H	0.763103	4.199855	-3.891098

D1

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SCF-energy = -1422.690817

C	2.172335	2.826170	0.677901
C	1.039870	3.210310	-0.067145
C	1.214201	3.364312	-1.469899
O	0.196566	3.886205	-2.190016
C	2.397667	3.011521	-2.078923
H	2.479339	3.119781	-3.155292
C	3.490416	2.524517	-1.355710
C	3.395391	2.464455	0.038978
C	6.786743	1.130422	0.938355
C	6.706859	1.094267	2.317508
H	7.547470	0.719001	2.904830
C	5.560007	1.537247	2.953638
C	4.473125	2.015455	2.223856
C	4.537159	2.020590	0.814404
H	5.518411	1.494894	4.040965
H	7.702741	0.786437	0.460520
C	5.718296	1.589367	0.165469
C	0.962562	3.425489	4.181573
C	2.097044	3.142042	4.915887
C	3.232713	2.676082	4.276699
C	3.264408	2.514168	2.892927
C	2.120813	2.851098	2.131647
H	4.114856	2.456827	4.876000
H	2.097671	3.281764	5.998971
H	0.078083	3.784403	4.704998
C	0.945769	3.271173	2.793238
C	5.802435	1.632315	-1.297581
C	4.713969	2.100008	-2.041952
C	4.829887	2.132148	-3.443680
C	5.964489	1.728328	-4.115540
C	7.063803	1.257859	-3.363413
H	3.993355	2.484875	-4.046871
C	6.956202	1.221244	-1.988886
H	7.816319	0.854430	-1.429010
C	-2.696557	3.865364	1.984092
C	-1.504610	3.721805	2.661732
C	-0.275013	3.500206	2.018393
C	-0.242244	3.443977	0.616452
C	-1.473278	3.558659	-0.063304
H	-1.484984	3.471565	-1.143923
H	-1.540196	3.760876	3.750086
C	-3.981790	4.097735	2.724853
C	-2.678021	3.763305	0.578540
C	-3.951410	3.867332	-0.212048
C	6.030936	1.784594	-5.614877
C	8.322028	0.806158	-4.047642
H	-4.457569	5.040138	2.414956
H	-3.814871	4.145735	3.808504
H	-4.708152	3.294462	2.530748
H	-3.760699	3.755540	-1.286790
H	-4.442984	4.839428	-0.056084
H	-4.674269	3.092682	0.084927
H	5.096584	2.171236	-6.041319
H	6.211132	0.788729	-6.046358
H	6.850874	2.433921	-5.956187
H	8.126337	-0.028837	-4.736784
H	9.073384	0.472777	-3.320689
H	8.766996	1.616074	-4.644680
C	0.366648	4.160627	-3.551259
H	-0.562467	4.632675	-3.892688
H	0.533598	3.243565	-4.140306
H	1.203406	4.856950	-3.724833

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SCF-energy = -1424.742041

C	-1.289851	0.354417	0.661189
C	-1.092138	-0.826123	-0.009697
H	-1.902005	-1.550540	-0.087709
C	0.128787	-1.185008	-0.793645
O	-0.224759	-1.565234	-2.112123
C	1.157615	-0.084934	-0.766804
C	2.319648	-4.133165	-1.363625
C	1.487825	-5.124062	-0.907783
H	1.745721	-6.163636	-1.130465
C	0.293485	-4.861282	-0.172783
C	-0.026436	-3.582812	0.100408
C	0.851337	-2.452593	-0.272396
H	-0.339786	-5.688889	0.149384
H	3.192503	-4.415431	-1.948762
C	2.020030	-2.777739	-1.138240
C	-1.708384	4.002852	2.868727
C	-0.678940	4.920576	2.930146
C	0.514026	4.672360	2.247033
C	0.650038	3.512151	1.519607
H	1.335337	5.390217	2.290698
H	-0.800201	5.835673	3.513197
H	-2.625002	4.222351	3.413632
C	-1.597279	2.813411	2.133229
C	2.811001	-1.709587	-1.671890
C	2.399920	-0.365986	-1.476025
C	3.207283	0.652933	-1.984301
C	4.390928	0.398482	-2.662301
C	4.810829	-0.942457	-2.858546
H	2.883102	1.689470	-1.875654
C	4.017065	-1.954146	-2.367070
H	4.356682	-2.978537	-2.519868
C	-4.989494	1.202846	2.667643
C	-3.927692	2.086267	2.708219
C	-2.702076	1.845135	2.066921
C	-2.555861	0.646850	1.352841
C	-3.637967	-0.246683	1.313863
H	-3.551063	-1.180688	0.757877
H	-4.070291	3.010661	3.266803
C	-6.276068	1.519077	3.371745
C	-4.841004	-0.001928	1.946970
C	-5.966983	-0.990659	1.867695
C	5.212567	1.529079	-3.194704
C	6.085554	-1.245914	-3.588183
H	-7.118819	1.552500	2.665912
H	-6.226023	2.488486	3.882476
H	-6.518010	0.753457	4.123284
H	-5.690318	-1.868128	1.269838
H	-6.861108	-0.541097	1.411727
H	-6.261447	-1.341703	2.867512
H	4.759441	2.501768	-2.970765
H	5.331171	1.447244	-4.284911
H	6.224367	1.512825	-2.764139
H	6.951110	-0.789643	-3.086748
H	6.061862	-0.850193	-4.613738
H	6.263981	-2.326257	-3.649716
H	-0.921044	-3.347676	0.680379
H	1.594210	3.341984	1.003966

H	1.752159	1.789678	-0.035737
C	-0.388784	2.557410	1.441696
C	-0.240216	1.333813	0.684083
C	0.946020	1.058731	-0.060163
H	1.315408	-2.153807	0.696664
C	-0.806129	-0.559445	-2.908219
H	-1.043221	-1.018143	-3.875272
H	-1.734458	-0.167313	-2.462222
H	-0.111863	0.281056	-3.074744

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SCF-energy = -1424.746383

C	1.096251	3.175850	0.063992
C	1.116579	2.953944	-1.347122
H	0.179016	2.995563	-1.892776
C	2.293642	2.774625	-2.077119
O	2.294122	2.660968	-3.412120
C	3.520623	2.646149	-1.412065
C	3.550586	2.668823	0.098238
C	6.294542	0.311834	0.745746
C	5.899675	-0.214780	1.944791
H	6.597047	-0.852772	2.494354
C	4.611529	0.043829	2.511914
C	3.745278	0.832303	1.849880
C	4.034487	1.359711	0.486464
H	4.346849	-0.393806	3.475513
H	7.294936	0.089099	0.378498
C	5.433445	1.144744	-0.005794
C	1.223263	4.396342	4.140017
C	2.427180	4.492838	4.799803
C	3.612553	4.144046	4.141267
C	3.561988	3.700690	2.841615
H	4.573246	4.234069	4.652210
H	2.456167	4.851335	5.830674
H	0.317908	4.689767	4.669409
C	1.141379	3.946312	2.808377
C	5.796009	1.728212	-1.244532
C	4.783315	2.377217	-2.026482
C	5.111618	2.744431	-3.349701
C	6.375423	2.572526	-3.869278
C	7.403126	1.976306	-3.072368
H	4.349521	3.223040	-3.959549
C	7.091978	1.567103	-1.803676
H	7.879217	1.104790	-1.207828
C	-2.571578	4.073396	2.087571
C	-1.357693	4.132931	2.737708
C	-0.132761	3.856349	2.101864
C	-0.154894	3.498033	0.743879
C	-1.399306	3.442235	0.086262
H	-1.449179	3.157237	-0.964842
H	-1.366174	4.404100	3.793147
C	-3.847398	4.377733	2.815844
C	-2.593332	3.716873	0.717117
C	-3.892818	3.635954	-0.028538
C	6.683338	3.027093	-5.261358
C	8.786057	1.802998	-3.623521
H	-4.377977	5.222593	2.353155
H	-3.658561	4.632874	3.865755
H	-4.533535	3.518565	2.794709
H	-3.738497	3.345740	-1.075252
H	-4.417442	4.602414	-0.020081
H	-4.570589	2.900864	0.429285
H	7.485535	3.779247	-5.261783
H	5.802756	3.464552	-5.745654
H	7.034557	2.187702	-5.878970
H	9.225342	2.770522	-3.906087
H	8.779183	1.177232	-4.527490
H	9.452300	1.331463	-2.891133
H	2.750857	1.027275	2.255095
H	4.501801	3.452329	2.346898
H	4.326231	3.409301	0.365974
H	3.465574	0.610723	-0.127306
C	2.335636	3.584211	2.143952
C	2.282417	3.133507	0.772638
C	1.086209	2.704735	-4.137297
H	1.355602	2.583370	-5.192109
H	0.413047	1.883464	-3.846813
H	0.572396	3.669915	-4.008928

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SCF-energy = -1424.745303

C	1.147472	3.316673	0.068689
C	1.233591	3.154127	-1.327545
H	0.292986	3.169468	-1.885245
C	2.392998	2.993875	-2.092221
O	2.391821	2.879507	-3.419546
C	3.598606	2.789222	-1.412046
C	3.592704	2.665001	0.115510
C	6.288576	0.694348	0.905261
C	5.954084	0.327693	2.238025
H	6.717746	0.008594	2.940135
C	4.558874	0.344103	2.598004
C	3.592131	0.822153	1.796027
C	3.865766	1.432715	0.354220
H	4.269171	-0.048883	3.577638
H	7.343732	0.669153	0.617954
C	5.379088	1.128143	-0.004708
C	1.219890	4.200032	4.208595
C	2.418623	4.253582	4.876449
C	3.627912	3.992964	4.208312
C	3.604811	3.681550	2.880078
H	4.575180	4.050404	4.744164
H	2.428503	4.509345	5.941336
H	0.305603	4.415770	4.761363
C	1.156280	3.877866	2.837958
C	5.722954	1.590392	-1.334342
C	4.833560	2.443279	-2.042828
C	5.205617	2.922002	-3.321844
C	6.403365	2.574606	-3.910012
C	7.245730	1.653809	-3.240872
H	4.547078	3.615473	-3.841216
C	6.879966	1.176925	-1.988302
H	7.526094	0.446430	-1.493215
C	-2.547774	3.987450	2.106093
C	-1.341467	4.024013	2.766133
C	-0.106367	3.815803	2.119141
C	-0.123078	3.559470	0.740587
C	-1.355262	3.525120	0.067972
H	-1.399666	3.314054	-1.002161
H	-1.360656	4.222038	3.837322
C	-3.831376	4.216496	2.847333
C	-2.557808	3.728337	0.714784
C	-3.851705	3.677464	-0.042111
C	6.788657	3.125256	-5.247611
C	8.522888	1.192598	-3.875437
H	-4.375969	5.080978	2.440845
H	-3.651904	4.401732	3.913290
H	-4.500240	3.347791	2.762676
H	-3.688620	3.466276	-1.106153
H	-4.393840	4.631069	0.038258
H	-4.516846	2.899126	0.363227
H	7.749764	3.661959	-5.207248
H	6.035663	3.826826	-5.622181
H	6.900957	2.324189	-5.996938
H	9.191295	2.040495	-4.070380
H	8.327099	0.712748	-4.844057
H	9.055207	0.476634	-3.237844
H	2.548021	0.793741	2.113105
H	4.548258	3.477729	2.373607
H	4.408269	3.423441	0.387982
H	3.346823	0.591408	-0.294012
C	2.374177	3.598939	2.161202
C	2.335540	3.253899	0.788030
C	1.187430	2.929799	-4.149328
H	1.464095	2.809385	-5.203100
H	0.513876	2.100647	-3.870865
H	0.673654	3.893364	-4.021153

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SCF-energy = -1424.735510

C	1.346146	3.029658	0.541541
C	1.513619	1.899099	-0.228293
H	0.703649	1.180075	-0.350577
C	2.730907	1.563620	-0.952066
O	2.488643	0.932666	-2.166022
C	3.759677	2.633382	-0.956326
C	4.631123	-1.333876	-1.650570
C	3.709254	-2.273757	-1.229160
H	3.719011	-3.266226	-1.688203
C	2.748162	-1.991673	-0.230796
C	2.730306	-0.755477	0.330620
C	3.630485	0.293587	-0.107172
H	2.052179	-2.767829	0.091132
H	5.333555	-1.588112	-2.444757
C	4.626034	-0.050086	-1.112805
C	0.970442	6.594129	2.870890
C	2.001512	7.508073	2.939656
C	3.185998	7.277875	2.234436
C	3.310867	6.138037	1.475443
H	4.007705	7.994610	2.285695
H	1.889088	8.408604	3.546791
H	0.061508	6.801139	3.433118
C	1.070651	5.422915	2.104109
C	5.496850	1.000445	-1.636715
C	5.039065	2.330525	-1.619011
C	5.824879	3.314625	-2.207518
C	7.065257	3.031852	-2.775797
C	7.540331	1.706721	-2.762680

H	5.453116	4.341646	-2.239847
C	6.740100	0.717205	-2.205968
H	7.117181	-0.307905	-2.188599
C	-2.294250	3.772451	2.682058
C	-1.240218	4.664601	2.720509
C	-0.032357	4.455131	2.035371
C	0.100734	3.282922	1.277657
C	-0.971151	2.376485	1.245278
H	-0.888825	1.456998	0.664719
H	-1.373260	5.568055	3.314517
C	-3.562051	4.052973	3.433306
C	-2.155989	2.590212	1.921416
C	-3.273323	1.591527	1.849324
C	7.881180	4.126937	-3.392984
C	8.879860	1.366214	-3.345788
H	-4.425583	4.097724	2.753797
H	-3.506972	5.007090	3.971434
H	-3.773195	3.262291	4.167913
H	-3.006220	0.733541	1.219800
H	-4.185229	2.043731	1.433039
H	-3.533547	1.210912	2.847744
H	8.084014	3.919265	-4.453621
H	8.857035	4.220788	-2.894730
H	7.372030	5.095963	-3.328307
H	9.685507	1.919886	-2.842341
H	8.928235	1.629178	-4.412411
H	9.098509	0.295538	-3.252569
H	2.023851	-0.520046	1.130770
H	4.246145	5.980128	0.940506
H	4.399305	4.451254	-0.140670
C	2.268539	5.187648	1.387741
C	2.402491	3.990515	0.586975
C	3.577924	3.738482	-0.187037
H	4.014824	0.896457	0.725395
C	1.894221	1.754714	-3.150796
H	1.766768	1.132036	-4.043520
H	0.909873	2.129885	-2.829300
H	2.541473	2.611477	-3.398969