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Contorted Aromatics via a Palladium-Catalyzed Cyclopentannulation Strategy

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1) DFT minimized chemical structures (Cartesian coordinates supplied at end of SI)

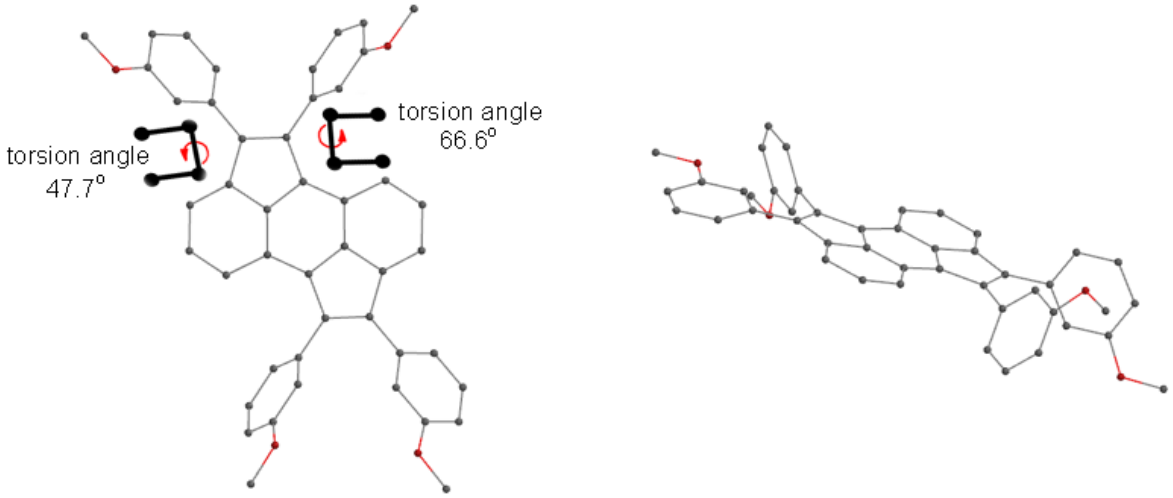


Figure SI-1. DFT energy minimized structure of **1a** at the B3LYP/6-311g(d,p) level.

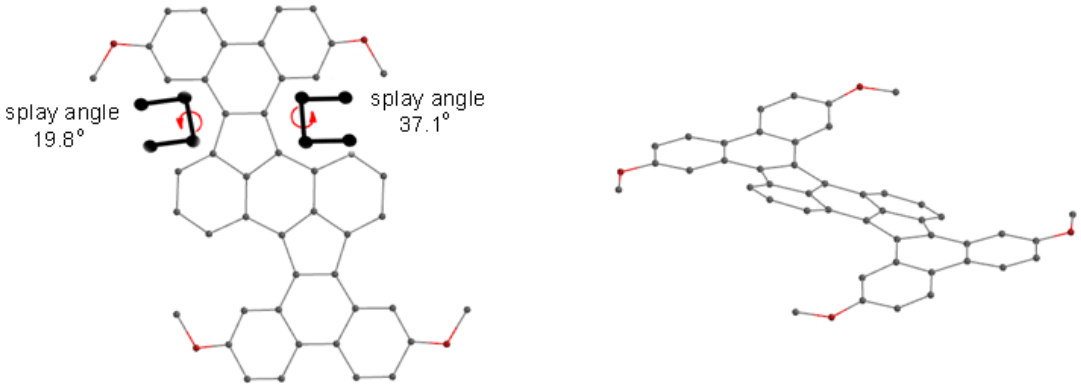


Figure SI-2. DFT energy minimized structure of **2a** at the B3LYP/6-311g(d,p) level. Crystal structure gave slightly different splay angles of 14.34° and 36.83°.

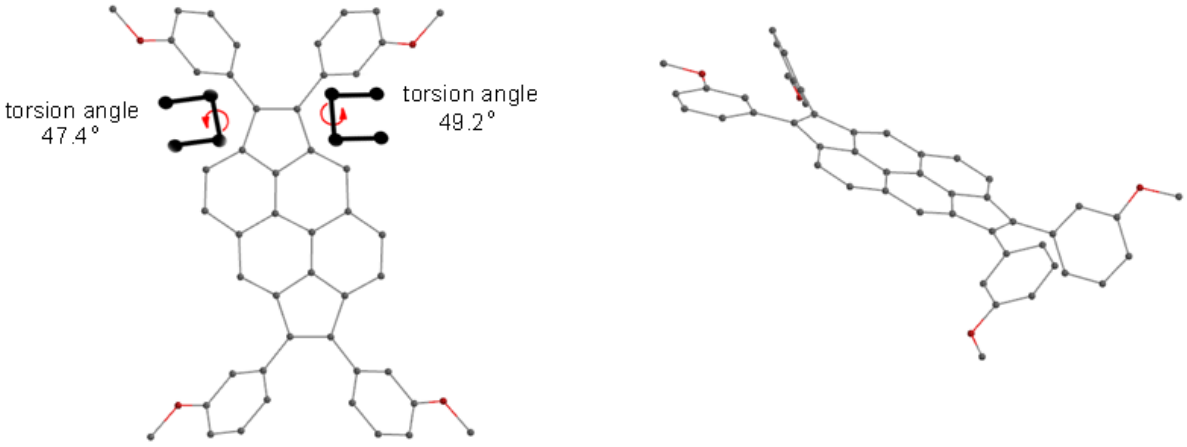


Figure SI-3. DFT energy minimized structure of **3a** at the B3LYP/6-311g(d,p) level.

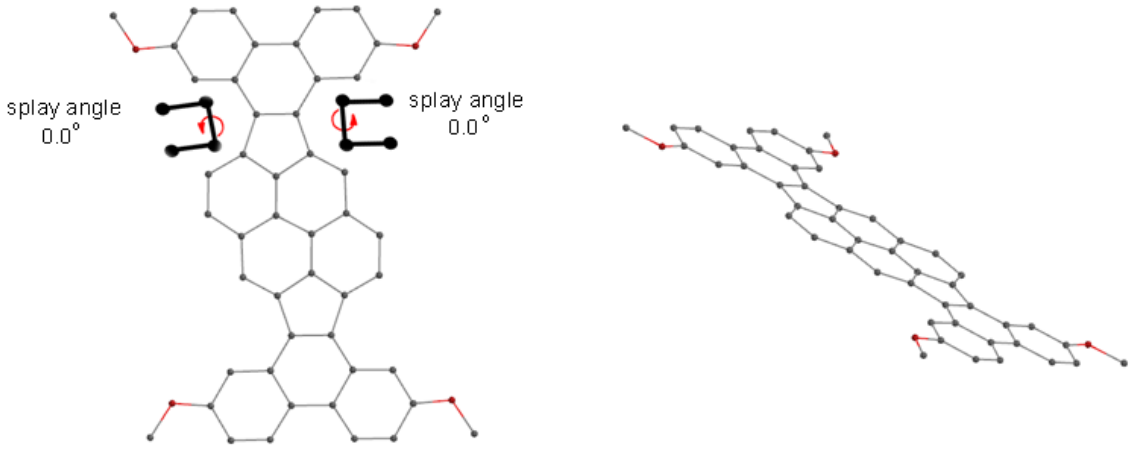


Figure SI-4. DFT energy minimized structure of **4a** at the B3LYP/6-311g(d,p) level.

2) TD-DFT calculated absorption spectra

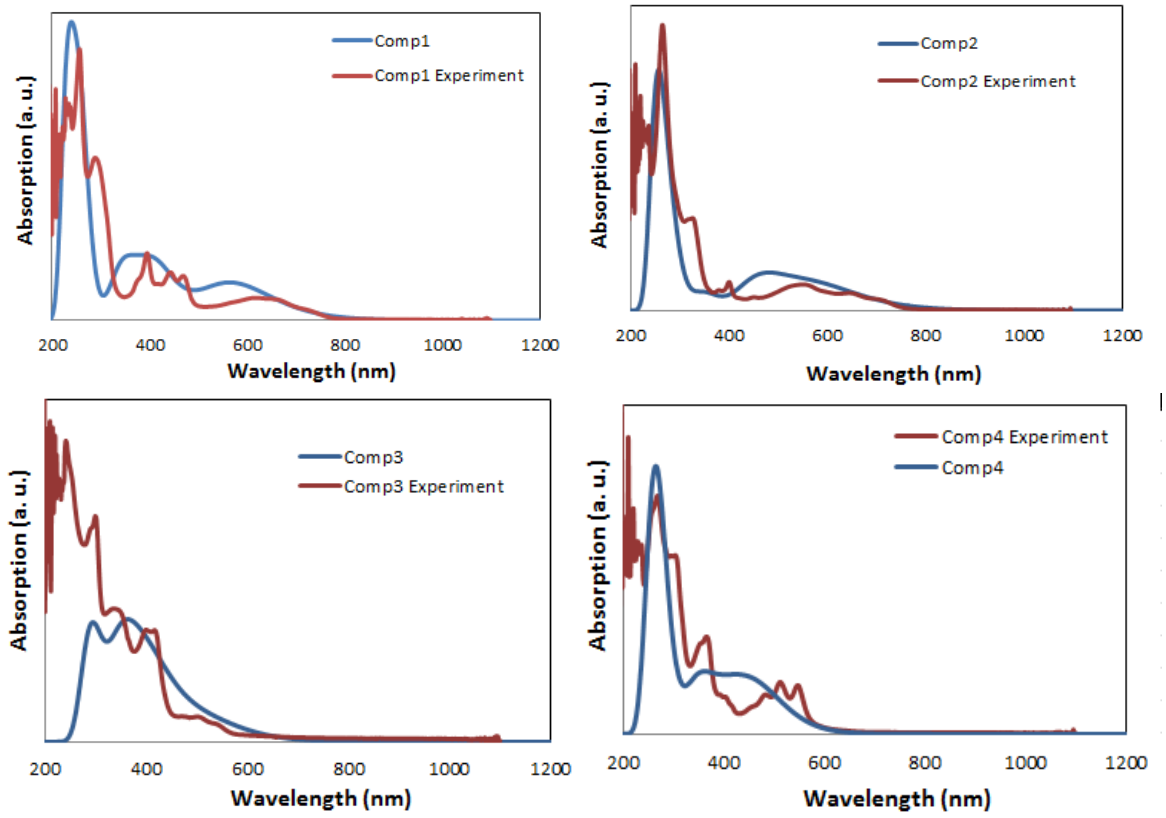


Figure SI-5. Calculated absorption spectra of compounds **1a-4a** obtained from TD-CAMB3LYP/ 6-311g(d,p) with N=24 (states) with the corresponding B3LYP/6-311g(d,p) optimized geometry. For comparison purposes, the experimental spectra are provided in red.

Table SI-1. A comparison between the calculated and experimental λ_{max}

	Experimental λ_{max} (nm)	Calculated λ_{max} (nm)	Error (nm)
1a	625	569	56
2a	551	584	-33
3a	547	534	13
4a	547	538	9

λ_{max} was calculated using TD-CAMB3LYP/6-311g(d,p) with a B3LYP/6-311g(d,p) optimized geometries

3) Association constant determination[1–3]

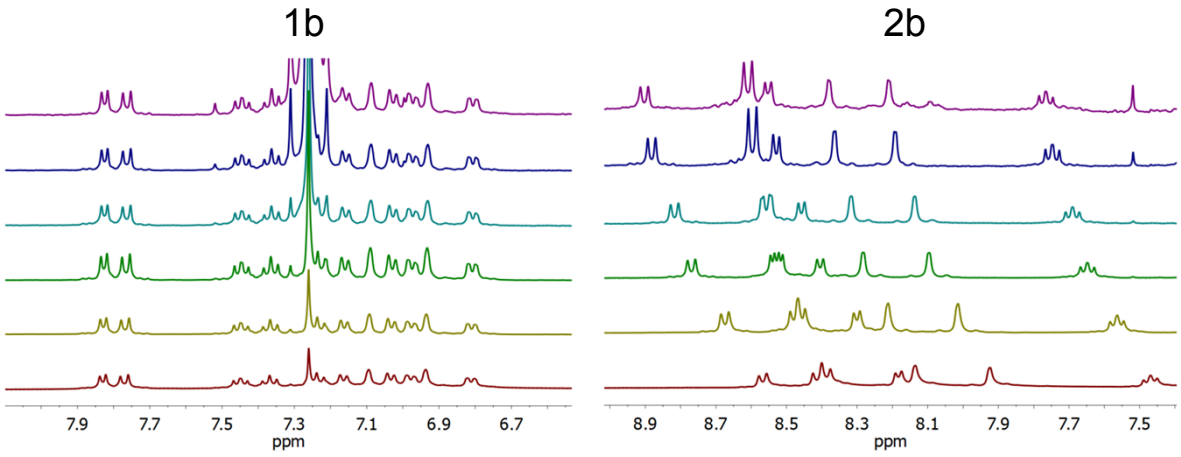


Figure SI-6. Concentration dependent NMR of **1b** and **2b**. General concentrations (for comparison) from top to bottom: 0.5 mM, 1 mM, 3 mM, 6 mM, 12 mM, 25 mM. More specific concentrations in table

A monomer-dimer equilibrium is assumed to be the predominant species for aggregation in solution. The association constant (K2) is found by curve-fitting the chemical shifts of a given proton at various concentrations to eq. 1 where δ is the chemical shift at substrate concentration Ct, and δ_m and δ_d are the chemical shifts of the monomer and dimer, respectively. The data was fit in Origin with K2, δ_m and δ_d being variable. The calculated K2 for each proton was then averaged to give the association constant.

Eq 1. $$\delta = \delta_m + (\delta_d - \delta_m)\left(1 + \frac{1 - (sqrt((8K2Ct) + 1))}{4K2Ct}\right)$$

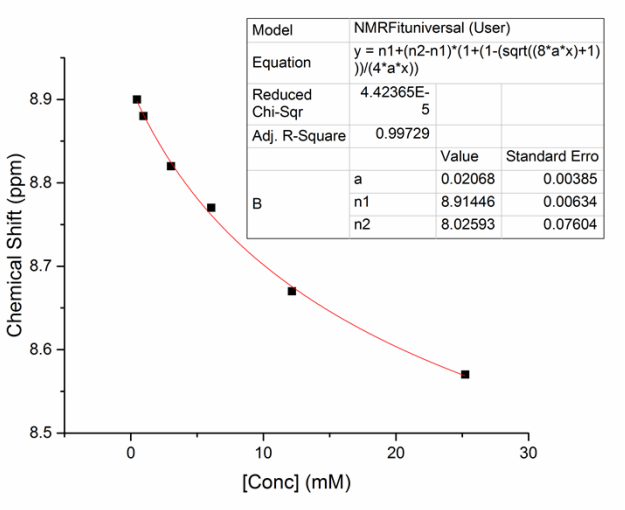
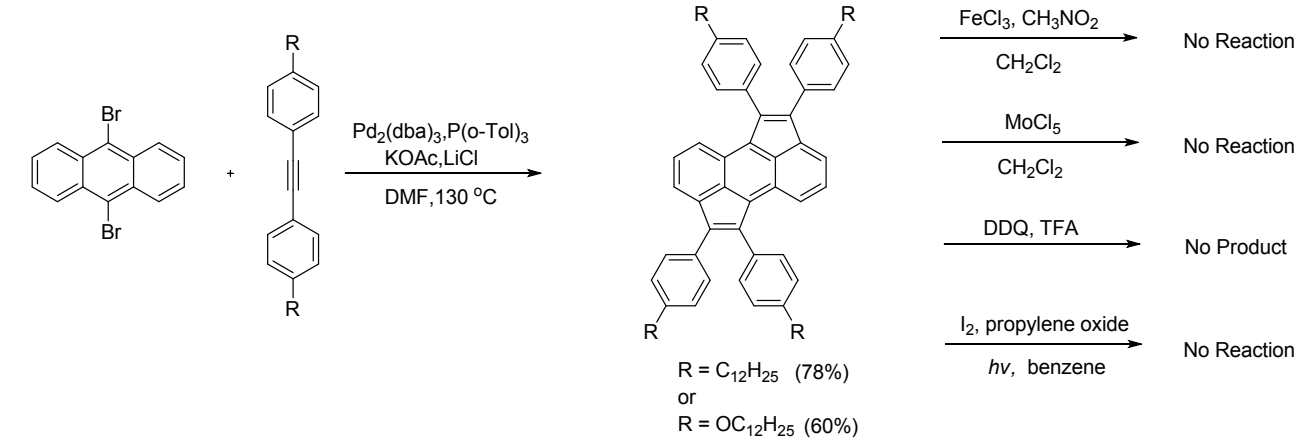


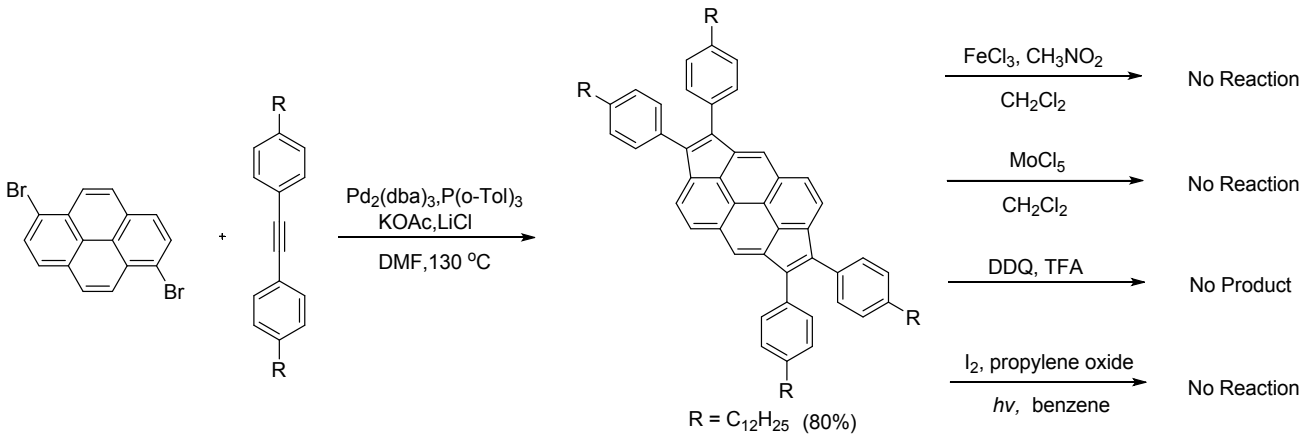
Figure SI-7. Example fit for proton Ha of **2b** at 293 K in $CDCl_3$.

Table SI-2. Concentration dependent NMR shifting of **2b** and **4b** at 293K in $CDCl_3$ or 353K in CD_2Cl_4. Compounds **1b** and **3b** did not show concentration dependent NMR shifts.

Compound 2b @ 293K ($CDCl_3$)							**Compound 2b @ 353K (CD_2Cl_4)**						**Compound 4b @ 353K (CD2Cl4)**			
Conc (mM)	**Ha**	**Hb**	**Hc**	**Hd**	**He**		**Conc. (mM**	**Ha**	**Hb**	**Hc**	**Hd**		**Conc. (mM**	**Ha**	**Hb**	**Hc**
0.47	8.9	8.55	8.38	8.21	7.76		0.608	8.969	8.459	8.271	7.39		0.59	8.50	8.41	7.312
0.95	8.88	8.53	8.37	8.19	7.75		0.719	8.969	8.459	8.271	7.39		0.71	8.49	8.38	7.306
3.04	8.82	8.46	8.32	8.14	7.69		0.879	8.968	8.458	8.269	7.389		0.86	8.48	8.35	7.295
6.07	8.77	8.41	8.28	8.1	7.65		1.318	8.967	8.458	8.269	7.389		1.29	8.45	8.29	7.278
12.15	8.67	8.3	8.21	8.02	7.56		2.637	8.966	8.457	8.268	7.388		2.58	8.40	8.17	7.24
25.23	8.57	8.18	8.14	7.92	7.47		5.697	8.958	8.452	8.263	7.385					
							7.121	8.955	8.45	8.26	7.383					
δd (ppm)	8.03	7.51	7.79	7.36	6.97		9.494	8.951	8.448	8.256	7.381		δd (ppm)	8.13	7.64	7.03
							14.242	8.943	8.444	8.252	7.379					
δm (ppm)	8.91	8.56	8.39	8.22	7.78		28.483	8.92	8.428	8.232	7.368		δm (ppm)	8.58	8.62	7.36
K2 (M^{-1})	20.7	18.1	25.3	16.1	19.8								K2 (M^{-1})	219	304	191
	+/- 3.9	+/- 3.8	+/- 3.6	+/- 3.4	+/- 4.5		δd (ppm)	8.97	8.46	8.27	7.39			+/- 69	+/- 91	+/- 84
K2 avg (M^{-1})	20.0	3.4					δm (ppm)	8.49	7.96	7.62	7.21		K2 avg (M^{-1}	238	58.8	
20.0 +/- 3.4 M^{-1}														**238 +/- 59 M-1**		
							K2 (M^{-1})	2.29	1.25	1.19	2.77					
								+/- 0.058	+/- 0.086	+/- 0.093	+/- 0.13					
							K2 avg (M^{-1}	1.88	0.78							
								1.88 M-1 +/- 0.78 M-1								

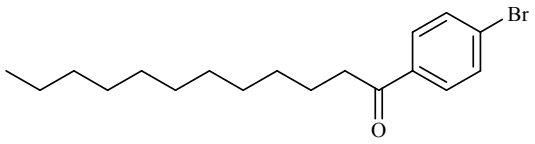
4) Other derivative synthesis with unsuccessful Scholl reactions



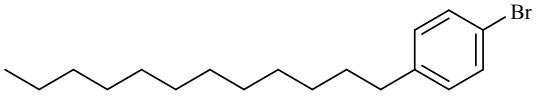


5) Experimental Procedures

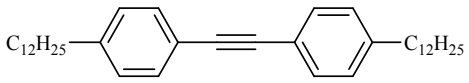
Unless otherwise noted, all reagents were used as received and all reactions were carried out under an argon atmosphere. Column chromatography was performed on a chromatographing system with normal phase silica columns. ^{1}H NMR and ^{13}C NMR were recorded on a 400 MHz NMR station at room temperature, unless otherwise noted.



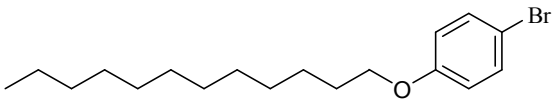
1-(4-bromo-phenyl)-dodecan-1-one (i): To a solution of bromobenzene (31.4 g, 0.217 mol) and $AlCl_3$ (16.0 g, 0.119 mol) was added lauroyl chloride (21.9 g, 0.100 mol) drop wise while stirring. The reaction mixture was stirred for one hour at 50 ^{0}C and then poured into ice water and extracted with dichloromethane. The organic solution was washed with 2N HCl followed by brine and then dried over $MgSO_4$. After removing the dichloromethane in vacuo, the crude product was recrystallized from ethanol to give 23.9 g (35.2 %) of **i** as white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, J = 8.6 Hz, 2H), 7.59 (d, J = 8.6 Hz, 2H), 2.93 (t, J = 7.4 Hz, 2H), 1.72 (p, J = 7.2 Hz, 2H), 1.26 (m, 16H), 0.88 (t, J = 6.7 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 199.5, 135.9, 131.9, 129.7, 128.1, 38.7, 32.0, 29.7, 29.6, 29.6, 29.5, 24.4, 22.8, 14.3. LRMS (EI+): m/z for $C_{18}H_{27}BrO$ calc: 338.1, found 338.1.



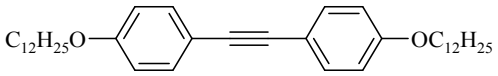
1-bromo-4-dodecyl-benzene (ii): A mixture of **i** (19.0 g, 0.0559 mol), hydrazine hydrate (19.4 g, 0.387 mol) and KOH (14.5 g, 0.259 mol) in diethylene glycol was heated for 4 h at 200 ^{0}C. The reaction mixture was cooled, poured into ice water, acidified with 1N HCl, and then extracted with dichloromethane. The organic layer was washed with brine and dried over $MgSO_4$. Solvent was removed in vacuo and the crude product was purified by column chromatography with hexane to give 5.74 g (31.5%) of **ii** as a clear oil. . ^{1}H NMR (400 MHz, $CDCl_3$) δ7.39 (d, J=8.4Hz, 2H), 7.05 (d, J=8.4Hz, 2H), 2.56 (t, J = 7.6 Hz, 2H), 1.59 (m, 2H), 1.27 (m, 18H), 0.89 (t, J = 6.8 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 141.9, 131.2, 130.2, 119.2, 35.4, 31.9, 31.6, 31.4, 29.7, 29.7, 29.6, 29.5, 29.4, 29.2, 22.7, 14.1.



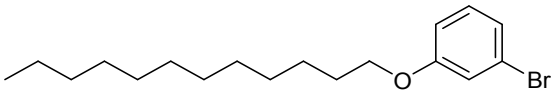
4,4'-didodecyl,1,1'-diphenyl acetylene (iii): In a glove box, **ii** (5.30 g, 16.3 mmol), $PdCl_2(PPh_3)_2$ (345 mg, 0.491 mmol), and CuI (305mg, 1.60 mmol) were dissolved in toluene (22 ml) in a sealed tube. Argon purged H_2O (0.12 ml, 6.5 mmol), DBU (14.8 g, 97.5 mmol) and then trimethylsilylacetylene (0.801 g, 8.15 mmol) were added to the sealed tube outside the glove box and stirred at 70 ^{0}C overnight. The reaction mixture was cooled, acidified with 2N HCl, then extracted with diethyl ether. The organic layer was washed with 2×100 ml 1N HCl, 100 ml brine and dried over $MgSO_4$. The crude product was purified by column chromatography to give 2.70 g (64.5%) of **iii** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, J = 8.0 Hz, 4H), 7.15 (d, J = 8.0 Hz, 4H), 2.61 (t, J= 7.6 Hz, 4H), 1.60 (m, 4H), 1.29 (m, 36H), 0.89 (t, J = 6.8 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.3, 131.6, 128.6, 120.7, 89.1, 36.1, 32.1, 31.4, 29.8, 29.8, 29.8, 29.7, 29.6, 29.5, 29.4, 22.9, 14.3. LRMS (EI+) 514.9 HRMS: m/z for $C_{38}H_{58}$ calc: 514.4539, found 514.4539.



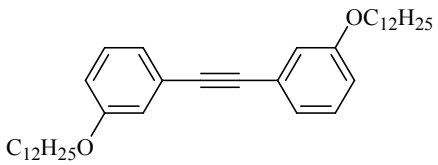
1-Bromo-4-dodecyloxy-benzene (iv): A mixture of 4-Bromo-phenol (5.1 g, 0.029 mmol), dodecylbromide (7.35 g, 0.0295 mmol), KOH (8.27 g, 0.147 mmol) in 50 ml DMSO was stirred at 50 ^{0}C overnight. The reaction mixture was partitioned between 250 ml 1N HCl and dichloromethane. The organic layer was washed with water and dried over MgSO4. The organic layer was concentrated to get 9.66 g (96%) of **iv** as clear oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.6 Hz, 2H), 6.86 (d, *J* = 8.6 Hz, 2H), 3.96 (t, *J* = 6.5 Hz, 2H), 1.83 – 1.74 (m, 2H), 1.52 – 1.25 (m, 18H), 0.90 (t, *J* = 6.7 Hz, 3H).



4,4'-didodecyloxy,1,1'-diphenyl acetylene (v): In a glove box, **(iv)** (9.51 g, 0.0279 mol), $PdCl_2(PPh_3)_2$ (1.37 g, 0.0139 mol), and CuI (531 mg, 0.00279 mol) were dissolved in toluene (135 ml) in a schlenk flask. Argon purged H_2O (0.25 ml, 0.014 mol), DBU (25.48 g, 0.1674 mol) and trimethylsilylacetylene (1.37 g, 0.0139 mol) were added to flask outside the glove box under Ar and stirred at 80 ^{0}C overnight. The reaction mixture was cooled and then acidified with 2N HCl, then extracted with diethyl ether. The organic layer was washed with 2×100 ml 1N HCl, 100ml brine and dried over $MgSO_4$. The crude product was purified by column chromatography to give 4.57 g (60%) of **v** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 9.2 Hz, 4H), 6.85 (d, *J* = 8.8 Hz, 4H), 3.96 (t, *J* = 6.6 Hz, 4H), 1.82 – 1.74 (m, 4H), 1.49 – 1.24 (m, 36H), 0.88 (t, *J* = 6.9 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.1, 132.9, 115.6, 114.6, 88.1, 68.2, 32.1, 29.8, 29.8, 29.7, 29.7, 29.5, 29.5, 29.4, 26.2, 22.8, 14.3. LRMS (EI+): m/z for $C_{38}H_{58}O_2$ calc: 546.44, found 546.50.

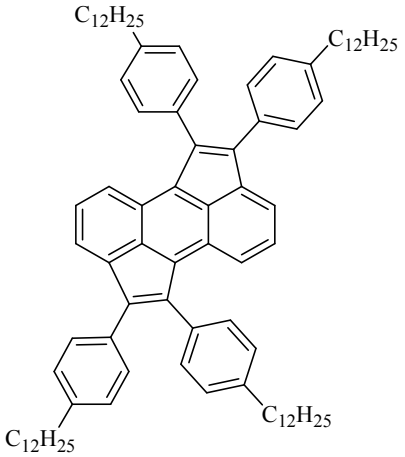


1-Bromo-3-dodecyloxy-benzene (vi): A mixture of 3-Bromo-phenol (5.1 g, 0.029 mol), dodecylbromide (7.35 g, 0.0295 mol), KOH (8.27 g, 0.147 mol) in 50 ml DMSO was stirred at 50 ^{0}C overnight. The reaction mixture was partitioned between 250 ml 1N HCl and dichloromethane. The organic layer was washed with water and dried over MgSO4. The organic layer was concentrated to get 9.56 g (95%) of **vi** as clear oil. . ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 – 7.10 (m, 1H), 7.06 (dd, *J* = 1.7, 1.1 Hz, 1H), 7.05 (dd, *J* = 2.2, 1.6 Hz, 1H), 6.85 – 6.78 (m, 1H), 3.92 (t, *J* = 6.8 Hz, 2H), 1.81 – 1.71 (m, 2H), 1.34 – 1.21 (m, 18H), 0.88 (t, *J* = 6.9 Hz, 3H).

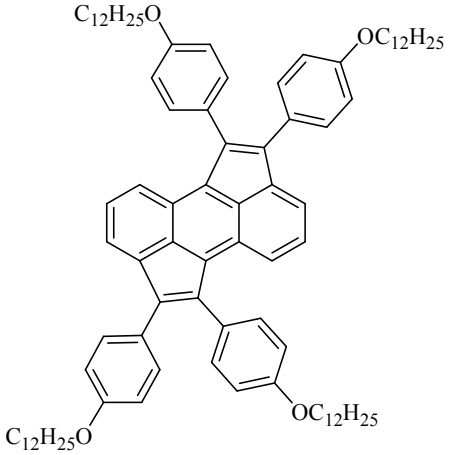


3,3'-didodecyloxy,1,1'-diphenyl acetylene (vii): In a glove box, **(vi)** (9.51 g, 0.0279 mol), $PdCl_2(PPh_3)_2$ (1.37 g, 0.0139 mol), and CuI (531 mg, 0.00279 mol) were dissolved in toluene (135 ml) in a schlenk flask. Argon purged H_2O (0.25 ml, 0.014 mol),DBU (25.48 g, 0.1674 mol) and trimethylsilylacetylene (1.37 g, 0.0139 mol) were added to flask outside the glove box under Ar and stirred at 80 ^{0}C overnight. The reaction mixture was cooled and then acidified with 2N HCl, then extracted with diethyl ether. The organic layer was washed with 2×100 ml 1N HCl, 100

ml brine and dried over $MgSO_4$. The crude product was purified by column chromatography to give 4.26 g (56%) of **vii** as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 – 7.20 (m, 2H), 7.11 (d, *J* = 7.6 Hz, 2H), 7.06 – 7.04 (m, 2H), 6.88 (dd, *J* = 8.3, 2.6 Hz, 2H), 3.96 (t, *J* = 6.6 Hz, 4H), 1.83 – 1.74 (m, 4H), 1.50 – 1.23 (m, 36H), 0.88 (t, *J* = 6.8 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.0, 129.5, 124.3, 124.1, 117.1, 115.7, 89.2, 68.2, 32.1, 29.8, 29.8, 29.8, 29.7, 29.5, 29.5, 29.4, 26.2, 22.8, 14.3. LRMS (EI+) 546.4 HRMS: m/z for $C_{38}H_{58}O_2$ calc: 546.4437, found 546.4431.

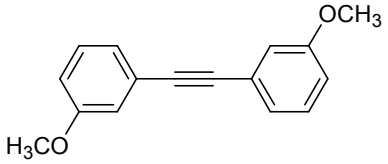


1,2,6,7-tetra(4-dodecylphenyl)cyclopenta[hi]aceanthrylene (viii): In a glove box, **iii** (220.6 mg, 0.4285 mmol), 1,6-dibromoanthracene (60.0 mg, 0.178 mmol), $Pd_2(dba)_3$ (16.3 mg, 0.0178 mmol), P(o-Tol)$_3$ (8.15 mg, 0.0268 mmol), KOAc (87.6 mg, 0.893 mmol), LiCl (15.1 mg, 0.357 mmol) and DMF (15 ml) were combined in a sealed tube and stirred overnight at 130 ^{0}C. The reaction mixture was cooled to room temperature and poured into 75 ml methanol and filtered. The solid was washed with methanol and acetone to give 167 mg (78%) of **viii** as a green solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 6.6 Hz, 2H), 7.70 (d, *J* = 8.6 Hz, 2H), 7.46 (d, *J* = 8.1 Hz, 4H), 7.41 (dd, *J* = 8.7, 6.7 Hz, 2H), 7.33 – 7.29 (m, 4H), 7.27 – 7.24 (m, 4H), 7.12 (d, *J* = 8.2 Hz, 4H), 2.72 (t, *J* = 7.7 Hz, 4H), 2.59 (t, *J* = 7.4 Hz, 4H), 1.71 (m, 4H), 1.61 (m, 4H), 1.44 – 1.15 (m, 72H), 0.91 – 0.85 (m, 12H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.0, 141.5, 140.8, 139.3, 138.2, 138.1, 134.5, 132.4, 130.6, 130.1, 128.7, 128.3, 128.6, 128.2, 128.1, 127.9, 126.0, 125.7, 125.0, 35.9, 35.8, 32.0, 31.9, 31.4, 31.4, 29.8, 29.8, 29.8, 29.7, 29.7, 29.7, 29.7, 29.6, 29.6, 29.5, 29.4, 29.4, 29.4, 22.7, 22.7, 14.2. LRMS (EI+) 1203.9 HRMS: m/z for $C_{90}H_{122}$ calc: 1202.9541, found 1202.9620.

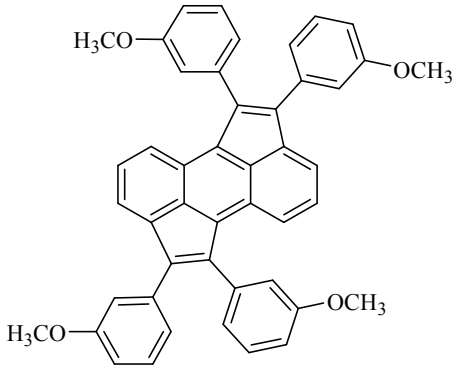


1,2,6,7-tetra(4-dodecyloxyphenyl)cyclopenta[hi]aceanthrylene (ix): In a glove box, **v** (162.76 mg, 0.2976 mmol), 1,6-dibromoanthracene (50.0 mg, 0.148 mmol), $Pd_2(dba)_3$ (13.7 mg, 0.0148 mmol), P(o-Tol)3 (6.79 mg, 0.0223 mmol), KOAc (73.02 mg, 0.7440 mmol), LiCl (12.62 mg, 0.2976 mmol) and DMF (15 ml) were combined in a sealed tube and stirred overnight at 130 ^{0}C. The reaction mixture was cooled to room temperature and poured in to 75 ml methanol and filtered. The solid was washed with methanol and acetone to give 113 mg (60%) of **ix** as a green solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 6.1 Hz, 2H), 7.74 (d, *J* = 3.9 Hz, 2H), 7.45 (d, *J* = 8.7 Hz,

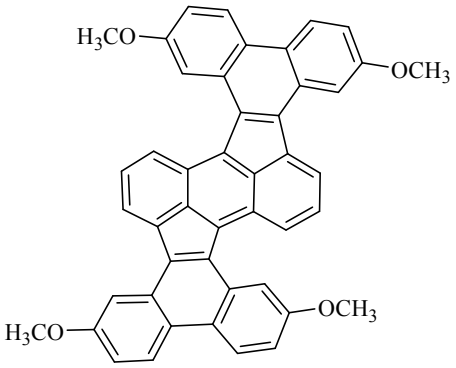
4H), 7.41 (dd, *J* = 8.6, 6.8 Hz, 2H), 7.32 (d, *J* = 8.8 Hz, 4H), 6.98 (d, *J* = 8.7 Hz, 4H), 6.86 (d, *J* = 8.8 Hz, 4H), 4.05 (t, *J* = 6.6 Hz, 4H), 3.96 (t, *J* = 6.6 Hz, 4H), 1.90 – 1.73 (m, 8H), 1.55 – 1.19 (m, 72H), 0.91 - 0.86 (m, 12H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.6, 158.2, 141.0, 138.6, 138.2, 137.9, 132.0, 131.5, 129.4, 128.4, 128.0, 127.6, 127.5, 126.1, 125.6, 125.0, 114.4, 114.3, 77.4, 77.2, 76.9, 68.2, 68.1, 32.09, 32.08, 29.86, 29.83, 29.82, 29.80, 29.79, 29.77, 29.76, 29.67, 29.59, 29.53, 29.52, 29.49, 26.33, 26.25, 22.86, 22.86, 14.30, 14.30. LRMS (EI+) 1267.9 HRMS: m/z for $C_{90}H_{122}O_4$ calc: 1267.9421, found 1267.9392.



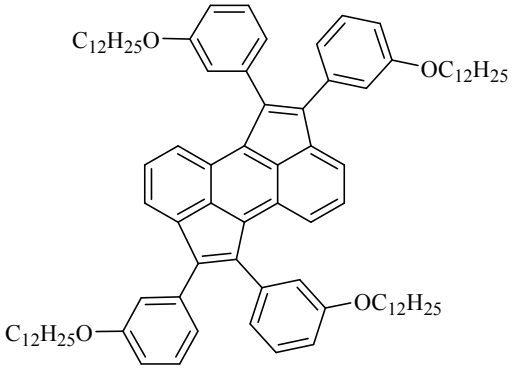
3,3'-dimethoxy,1,1'-diphenyl acetylene (x): In a glove box, 3-bromoanisole (5.22 g, 0.0279 mol), $PdCl_2(PPh_3)_2$ (1.37 g, 0.00139 mol), CuI (531 mg, 0.00279 mol) were dissolved in toluene (70 ml) in a schlenk flask. Argon purged H_2O (0.25 ml, 0.014 mol), DBU (25.48 g, 0.1674 mol) and trimethylsilylacetylene (1.37 g, 0.0139 mol) were added to flask outside the glove box under Ar and stirred at 80 ^{0}C overnight. The reaction mixture was cooled and acidified with 2N HCl, then extracted with diethyl ether. The organic layer was washed with 2×50 ml 1N HCl, 50 ml brine and dried over $MgSO_4$. The crude product was purified by column chromatography to give 1.9 g (58%) of a white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.23 (m, 2H), 7.15 – 7.12 (m, 2H), 7.08 – 7.05 (m, 2H), 6.92 – 6.88 (m, 2H), 3.83 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.5, 129.5, 124.3, 124.3, 116.5, 115.1, 89.2, 55.4. LRMS (EI+): m/z for $C_{16}H_{14}O_2$ calc: 238.1, found 238.1.



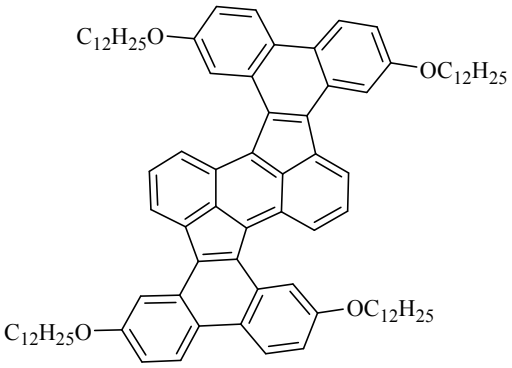
1,2,6,7-tetra(3-methoxyphenyl)cyclopenta[hi]aceanthrylene (1a): In a glove box, **x** (744.58 mg, 3.1250 mmol), 1,6-dibromoanthracene (500 mg, 1.49 mmol), $Pd_2(dba)_3$ (136.4 mg, 0.1488 mmol), P(o-Tol)$_3$ (67.94 mg, 0.2232 mmol), KOAc (730.2 mg, 7.440 mmol), LiCl (126.2 mg, 2.976 mmol) and DMF (120 ml) were combined in a sealed tube and stirred overnight at 130 ^{0}C. The reaction mixture was cooled to room temperature and poured into 250 ml methanol and filtered. The solid was washed with methanol to give 532.6 mg (55%) of **xiii** as a green solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 6.6 Hz, 2H), 7.77 (d, *J* = 8.6 Hz, 2H), 7.45 (dd, *J* = 8.7, 6.7 Hz, 2H), 7.41 – 7.36 (m, 2H), 7.29 – 7.23 (m, 2H), 7.19 (d, *J* = 7.5 Hz, 2H), 7.12 – 7.09 (m, 2H), 7.05 (d, *J* = 7.7 Hz, 2H), 6.99 (dd, *J* = 8.3, 2.6 Hz, 2H), 6.96 – 6.92 (m, 2H), 6.82 (dd, *J* = 7.8, 2.2 Hz, 2H), 3.78 (s, 6H), 3.67 (s, 6H). Too insoluble for ^{13}C NMR. LRMS (EI+) 650.2 HRMS: m/z for $C_{46}H_{34}O_4$ calc: 650.2457, found 650.2450.



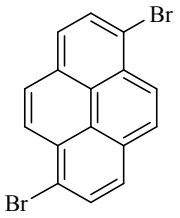
2,7,13,18-tetrakis(methoxy)tetrabenzo[f,h,r,t]rubicene (2a): In a round bottom flask **1a** (234.5 mg, 0.3603 mmol) was dissolved in 250 ml of $CHCl_3$. To this mixture $FeCl_3$ (350.6 mg, 2.162 mmol) in 2ml of CH_3NO_2 was added drop wise under Ar. The reaction mixture was stirred at room temperature overnight. The solvent was reduced to 50 ml by rotovap and methanol (150 ml) was added and the mixture was stirred for 20 min. The product was collected by filtration and washed with methanol to give 210 mg (90%) of **xiv** as a purple solid. ^{1}H NMR (400 MHz, $C_2D_2Cl_4$ (80 ^{o}C)) δ 8.81 (d, *J* = 8.6 Hz, 2H), 8.54 (d, *J* = 9.4 Hz, 4H), 8.48 (d, *J* = 6.7 Hz, 2H), 8.31 – 8.28 (m, 2H), 8.13 – 8.10 (m, 2H), 7.76 -7.70 (m, 2H), 7.31 – 7.24 (m, 4H), 4.03 (s, 6H), 3.96 (s, 6H). Too insoluble for ^{13}C NMR. LRMS (EI+) 646.7 HRMS: m/z for $C_{46}H_{30}O_4$ calc: 646.2144, found 646.2163.



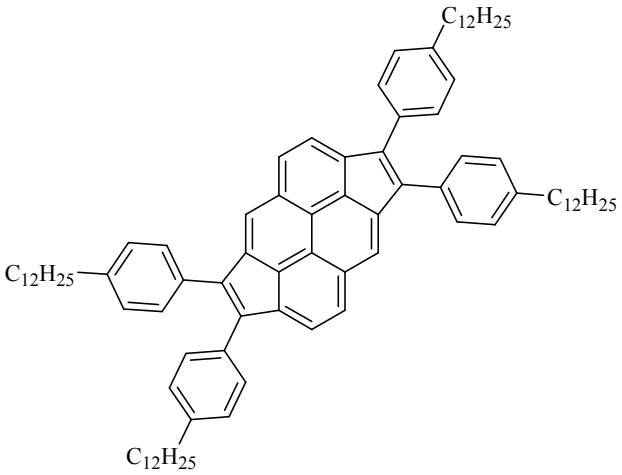
1,2,6,7-tetra(3-dodecyloxyphenyl)cyclopenta[hi]aceanthrylene (1b): In a glove box, **vii** (500 mg, 0.914 mmol), 1,6-dibromoanthracene (153.6 mg, 0.4572 mmol), $Pd_2(dba)_3$ (41.86 mg, 0.04572 mmol), P(o-Tol)$_3$ (20.87 mg, 0.06857mmol), KOAc (224.3 mg, 2.286 mmol), LiCl (38.77 mg, 0.9140 mmol) and DMF (60 ml) were combined in a sealed tube and stirred overnight at 130 ^{0}C. The reaction mixture was cooled to room temperature and poured in to 200 ml methanol and filtered. The solid was washed with methanol and acetone to give 295.6 mg (51.0%) of **x** as a green solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 6.7 Hz, 2H), 7.76 (d, *J* = 8.7 Hz, 2H), 7.44 (dd, *J* = 8.7, 6.7 Hz, 2H), 7.39 – 7.34 (m, 2H), 7.26 – 7.21 (m, 2H), 7.16 (d, *J* = 7.4 Hz, 2H), 7.10 – 7.06 (m, 2H), 7.03 (d, *J* = 7.6 Hz, 2H), 6.97 (dd, *J* = 8.2, 2.5 Hz, 2H), 6.95 – 6.91 (m, 2H), 6.81 (dd, *J* = 8.2, 2.5 Hz, 2H), 3.95 – 3.85 (m, 4H), 3.77 (t, *J* = 6.6 Hz, 4H), 1.80 – 1.65 (m, 8H), 1.45 – 1.20 (m, 72H), 0.90 – 0.81 (m, 12H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.1, 158.9, 140.5, 139.7, 138.7, 138.5, 138.0, 136.3, 136.2, 129.5, 129.2, 128.6, 128.0, 126.4, 126.23, 125.2, 123.2, 122.6, 116.4, 115.8, 114.5, 114.1, 68.2, 68.0, 32.08, 32.07, 29.9, 29.84, 29.82, 29.80, 29.78, 29.76, 29.6, 29.53, 29.51, 29.4, 29.3, 26.19, 26.18, 22.8, 14.3. LRMS (EI+) 1267.9 HRMS: m/z for $C_{90}H_{122}O_4$ calc: 1267.9421, found 1267.9377.



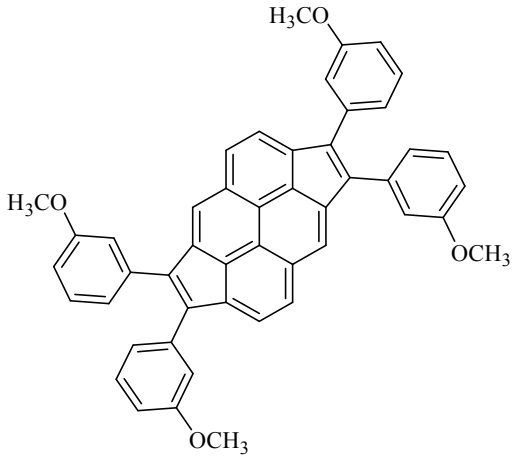
2,7,13,18-tetrakis(dodecyloxy)tetrabenzo[f,h,r,t]rubicene (2b): In a round bottom flask **1b** (504 mg, 0.397 mmol) was dissolved in 300 ml of CH_2Cl_2, To this mixture $FeCl_3$ (386.8 mg, 2.385 mmol) in 2 ml of CH_3NO_2 was added drop wise under Ar. The reaction mixture was stirred at room temperature overnight. The solvent was first reduced to 50 ml by rotovap and methanol (150 ml) was added and the mixture stirred for 20 min. The product was collected by filtration and the solid was washed with methanol to give 452 mg (90%) of **xi** as a purple solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 8.6 Hz, 2H), 8.48 (dd, *J* = 9.3, 6.9 Hz, 4H), 8.32 (d, *J* = 7.1 Hz, 2H), 8.23 (d, *J* = 2.3 Hz, 2H), 8.03 (d, *J* = 2.3 Hz, 2H), 7.61 – 7.55 (m, 2H), 7.25 – 7.18 (m, 4H), 4.17 (t, *J* = 6.5 Hz, 4H), 4.12 (t, *J* = 6.6 Hz, 4H), 1.97 – 1.83 (m, 8H), 1.63 – 1.22 (m, 72H), 0.94 – 0.82 (m, 12H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.7, 157.1, 138.6, 137.3, 136.3, 133.8, 133.0, 129.9, 128.6, 127.8, 127.4, 127.4, 126.1, 125.8, 124.8, 124.7, 124.6, 124.5, 117.2, 116.3, 109.4, 106.3, 68.4, 68.3, 32.12, 32.07, 29.93, 29.90, 29.88, 29.86, 29.8, 29.72, 29.70, 29.63, 29.57, 29.5, 26.5, 26.4, 22.9, 22.8, 14.29, 14.26. LRMS (EI+) 1262.9 HRMS: m/z for $C_{90}H_{118}O_4$ calc: 1262.9030, found 1262.9011.



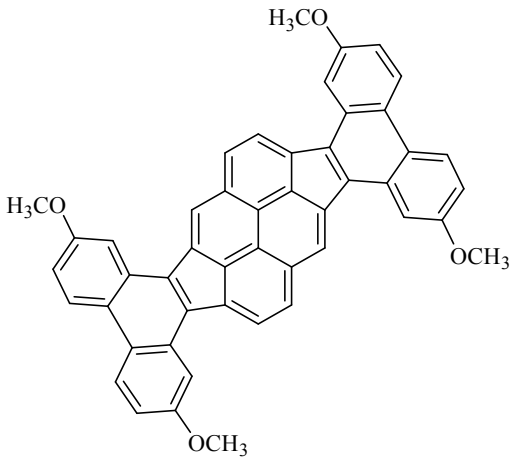
1,6-dibromopyrene (xi): To a solution of pyrene (19.0 g, 0.0941 mol) in dichloromethane (400 ml), a solution of Br_2 (30.11 g, 0.1882 mol) in dichloromethane (100 ml) was added drop wise via addition funnel. The reaction mixture was stirred at room temperature for 24 h. The solvent was removed in vacuo and the crude product was recrystallized from toluene four times (800 ml, 500 ml, 500 ml, 500 ml of toluene respectively) to give 5.07 g (15%) of **xv** as an off white solid. ^{1}H NMR (400 MHz, DMSO) δ 7.58 (d, *J* = 9.2 Hz, 1H), 7.49 (d, *J* = 8.2 Hz, 1H), 7.42 (d, *J* = 9.3 Hz, 1H), 7.37 (d, *J* = 8.2 Hz, 1H). LRMS (EI+): m/z for $C_{16}H_8Br_2$ calc: 360.0, found 359.9.



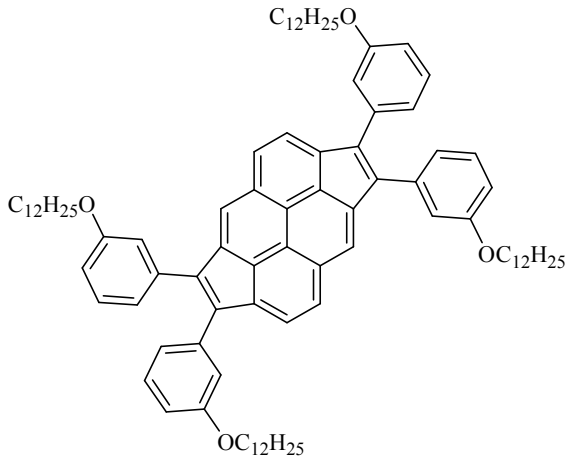
1,2,6,7-tetra(4-dodecylphenyl)dicyclopenta[*cd,jk*]pyrene (xii): In a glove box, **iii** (282.5 mg, 0.5486 mmol), 1,6-dibromopyrene (99.3 mg, 0.276 mmol), $Pd_2(dba)_3$ (25.25 mg, 0.0276 mmol), P(o-Tol)$_3$ (12.6 mg, 0.0414 mmol), KOAc (134.6 mg, 1.372 mmol), LiCl (23.26 mg, 0.5486 mmol) and DMF (25 ml) were combined in a sealed tube and stirred overnight at 130 ^{0}C. The reaction mixture was cooled to room temperature and poured into 200 ml methanol and filtered. The solid was washed with methanol and acetone to give 271 mg (80%) of **xvi** as a red solid. ^{1}H NMR (400 MHz, CDCl3) δ 7.73 (d, *J* = 7.9 Hz, 2H), 7.57 (m, 4H), 7.35 (dd, *J* = 8.1, 6.2 Hz, 8H), 7.17 (dd, *J* = 10.8, 8.3 Hz, 8H), 2.64 (m, 8H), 1.71 – 1.65 (m, 8H), 1.30 (m, 72H), 0.88 (t, *J* = 6.8 Hz, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.2, 142.0, 141.4, 141.3, 140.8, 139.4, 133.0, 132.34, 132.31, 132.28, 131.9, 130.4, 129.4, 129.3, 129.0, 128.4, 128.34, 128.27, 125.2, 121.8, 121.4, 35.9, 31.9, 31.39, 31.35, 29.71, 29.69, 29.67, 29.65, 29.6, 29.5, 29.5, 29.4, 22.7, 14.1. LRMS (EI+) 1228.0 HRMS: m/z for $C_{90}H_{122}$ calc: 1226.9541, found 1226.9480.



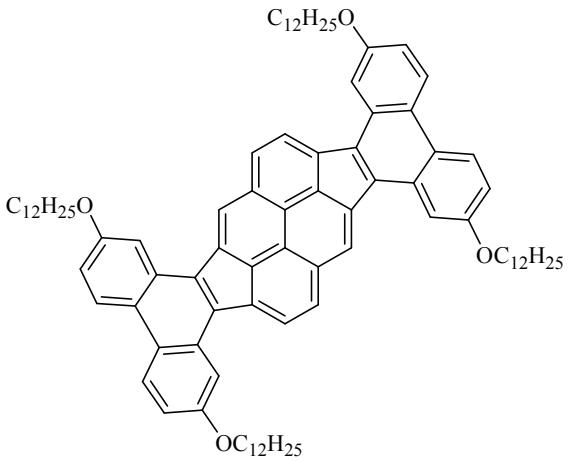
1,2,6,7-tetra(3-methoxyoxyphenyl)dicyclopenta[*cd,jk*]pyrene (3a): In a glove box **x** (138.2 mg, 0.58 mmol), 1,6-dibromopyrene (100 mg, 0.276 mmol), $Pd_2(dba)_3$ (25.25 mg, 0.0276 mmol), P(o-Tol)$_3$ (12.6 mg, 0.0414 mmol), KOAc (134.6 mg, 1.372 mmol), LiCl (23.26 mg, 0.5486 mmol) and DMF (15 ml) were combined in a sealed tube and stirred overnight at 130 ^{0}C. The reaction mixture was cooled to room temperature and poured in to 200 ml methanol and filtered. The solid was washed with methanol and acetone to give 130 mg (70%) of **xix** as a brick red solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.7 Hz, 2H), 7.58 (m, 4H), 7.30 (dd, *J* = 15.0, 7.5 Hz, 4H), 7.07 – 7.02 (m, 4H), 6.98 (m, 4H), 6.88 (dd, *J* = 12.9, 5.3 Hz, 4H), 3.74 (s, 6H), 3.71 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.64, 159.58, 141.99, 141.31, 140.70, 140.13, 136.40, 136.32, 132.17, 130.48, 129.76, 129.57, 129.52, 125.78, 122.27, 122.18, 121.79, 121.69, 115.07, 114.41, 113.76, 113.36, 77.41, 77.16, 76.91, 55.37, 55.31.



2,7,13,18-tetrakis(methoxy)-8b,11b,19b,22b-tetrahydrodibenzo[4,5:6,7]indeno[1,2,3-cd]dibenzo[4,5:6,7]indeno[1,2,3-jk]pyrene (4a): In a round bottom flask **3a** (30 mg, 0.044 mmol) was dissolved in 25 ml of CH_2Cl_2. To this mixture $FeCl_3$ (28.85 mg, 0.1780 mmol) in 0.2 ml of CH_3NO_2 was added drop wise under Ar. The reaction mixture was stirred at room temperature overnight. The solvent was reduced to 5 ml by rotovap, methanol (20 ml) was added and the mixture was stirred for 20 min. The product was collected by filtration and washed with methanol to give 26 mg (87%) of **xx** as a bright red solid. Too insoluble for NMR.



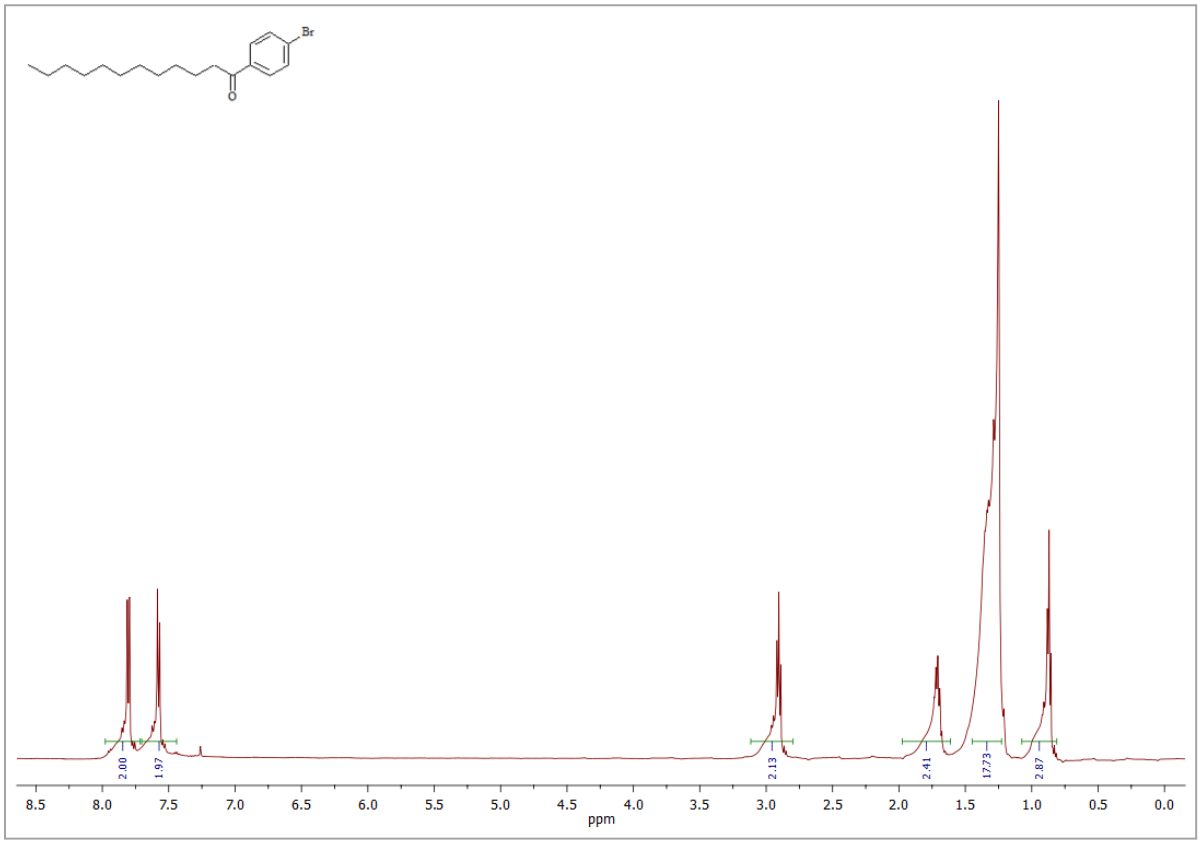
1,2,6,7-tetra(3-dodecyloxyphenyl)dicyclopenta[*cd,jk*]pyrene (3b): In a glove box **vii** (300 mg, 0.548 mmol), 1,6-dibromopyrene (99.3 mg, 0.276 mmol), $Pd_2(dba)_3$ (25.25 mg, 0.0276 mmol), $P(o\text{-}Tol)_3$ (12.6 mg, 0.0414 mmol), KOAc (134.6 mg, 1.372 mmol), LiCl (23.26 mg, 0.5486 mmol) and DMF (30 ml) were combined in a sealed tube and stirred overnight at 130 ^{0}C. The reaction mixture was cooled to room temperature and poured in to 200 ml methanol and filtered. The solid was washed with methanol and acetone to give 221 mg (62%) of **xvii** as a brick red solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 8 Hz, 2H), 7.60 – 7.57 (m, 4H), 7.31 – 7.25 (m, 4H), 7.03 (dd, J = 7.7, 6.5 Hz, 4H), 6.99 – 6.95 (m, 4H), 6.86 (td, J = 7.6, 2.2 Hz, 4H), 3.89 – 3.80 (m, 8H), 1.76 – 1.68 (m, 8H), 1.44 – 1.23 (m, 72H), 0.90 - 0.86 (m, 12H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.2, 159.1, 142.0, 141.4, 140.8, 140.2, 136.4, 136.3, 132.2, 130.5, 129.7, 129.5, 125.8, 122.2, 122.1, 121.7, 121.6, 115.5, 114.8, 114.5, 114.1, 105.1, 77.4, 77.2, 76.9, 68.1, 68.1, 32.1, 29.9, 29.82, 29.80, 29.79, 29.58, 29.56, 29.5, 29.4, 29.3, 26.2, 22.9, 14.3. LRMS (EI+) 1291.9 HRMS: m/z for $C_{92}H_{122}O_4$ calc: 1291.9421, found 1291.9382.

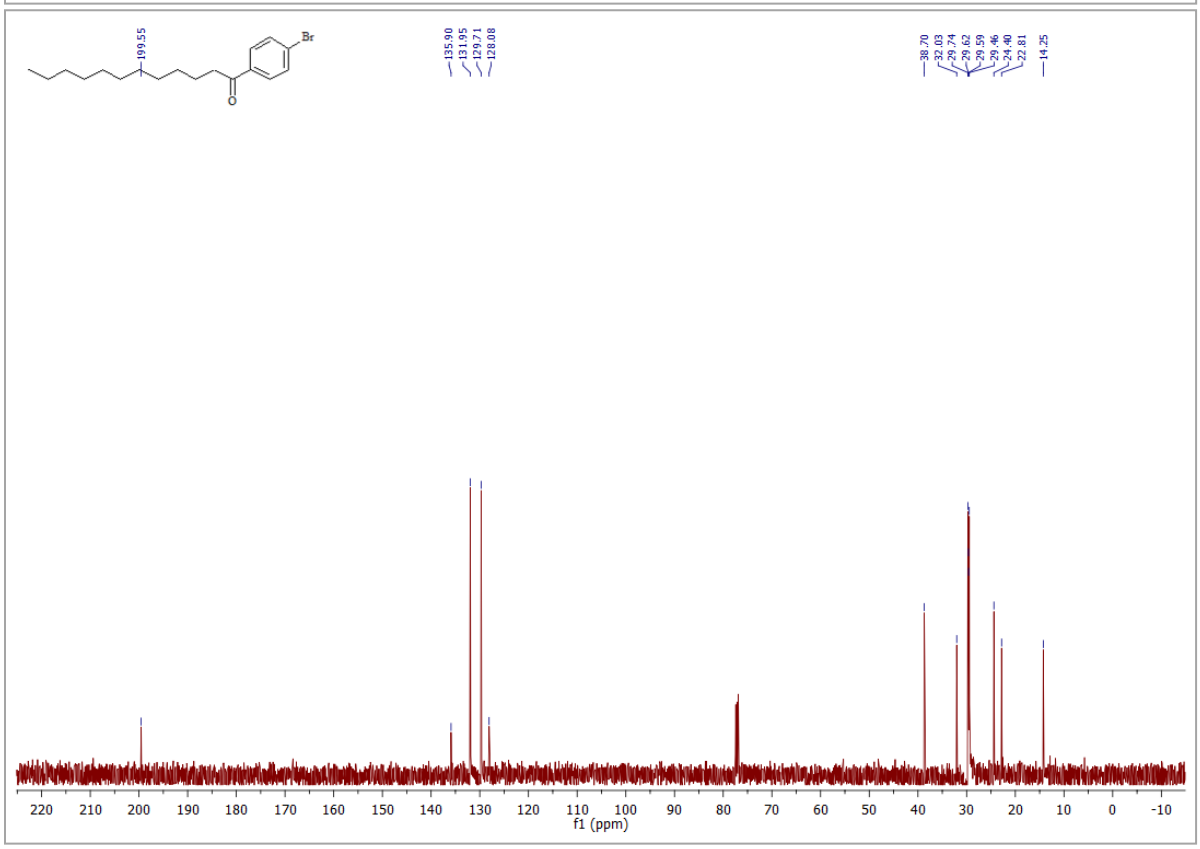


2,7,13,18-tetrakis(dodecyloxy)-8b,11b,19b,22b-tetrahydrodibenzo[4,5:6,7]indeno[1,2,3-cd]dibenzo[4,5:6,7]indeno[1,2,3-jk]pyrene (4b): In a round bottom flask **3b** (100 mg, 0.0774 mmol) was dissolved in 60 ml of CH_2Cl_2. To this mixture $FeCl_3$ (75.32 mg, 0.4644 mmol) in 1ml of CH_3NO_2 was added drop wise under Ar. The reaction mixture was stirred at room temperature overnight. The solvent was reduced to 10 ml by rotovap, methanol (40 ml) was added and the mixture was stirred for 20 min. The product was collected by filtration and washed with methanol to give 90 mg (90%) of **xviii** as a bright red solid. ^{1}H NMR (400 MHz, $C_2D_2Cl_4$ (80^0 C)) δ 8.26 – 8.21 (m, 4H), 7.97 – 7.93 (m, 4H), 7.79 – 7.70 (m, 6H), 7.15 – 7.08 (m, 4H), 4.18 – 4.09 (m, 8H), 1.98 – 1.85 (m, 8H), 1.61 – 1.15 (m, 72H), 0.88 – 0.83 (m, 12H). Too insoluble for ^{13}C NMR. LRMS (EI+) 1287.9 HRMS: m/z for $C_{92}H_{118}O_4$ calc: 1287.9108, found 1287.9073.

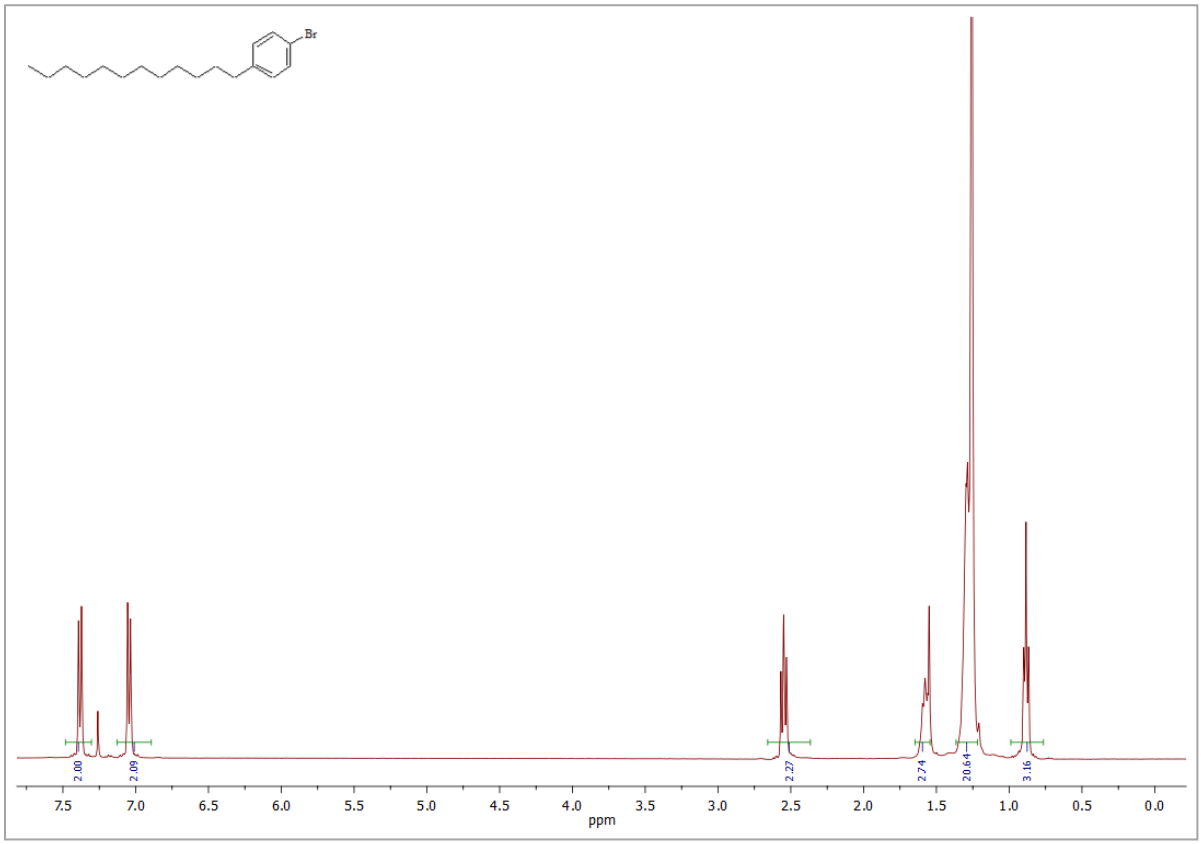
6) NMR Spectra

Compound (i)





Compound (ii)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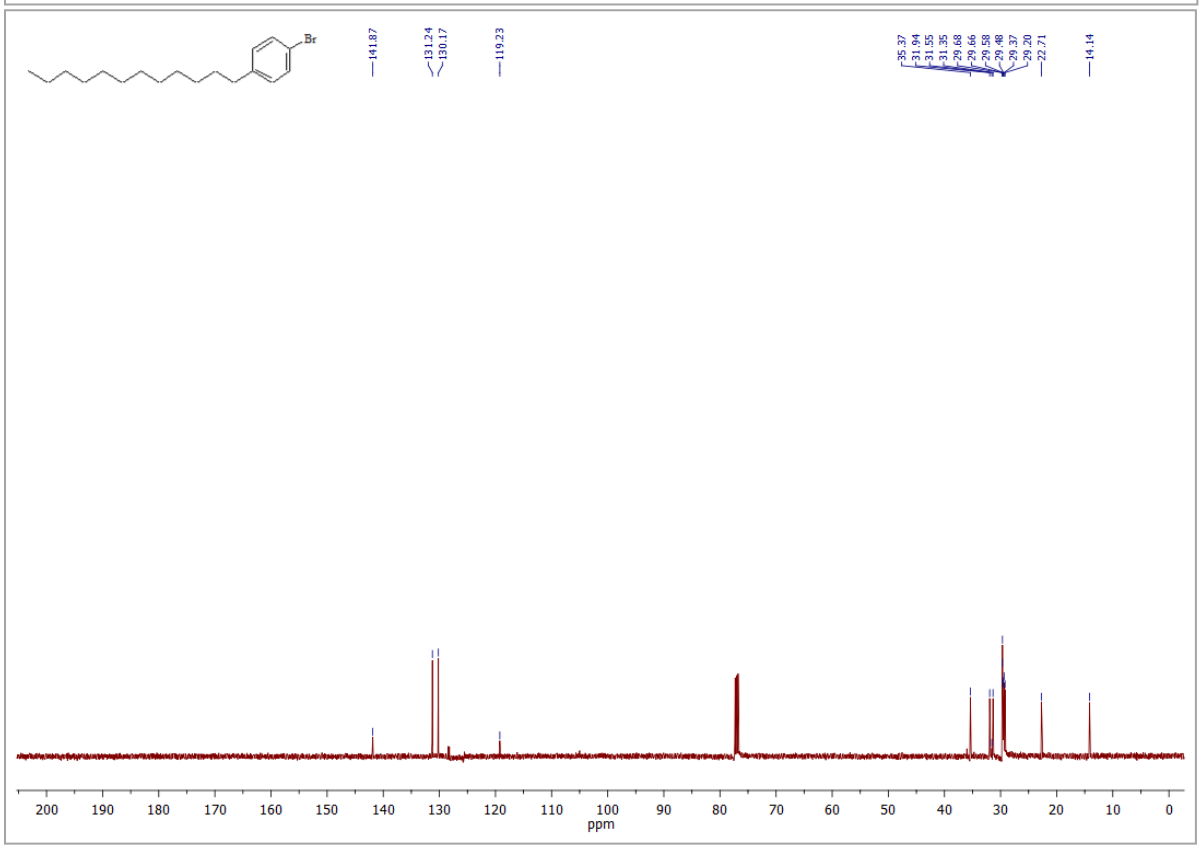
2.09
2.27
2.74
20.64
3.16
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm


Br
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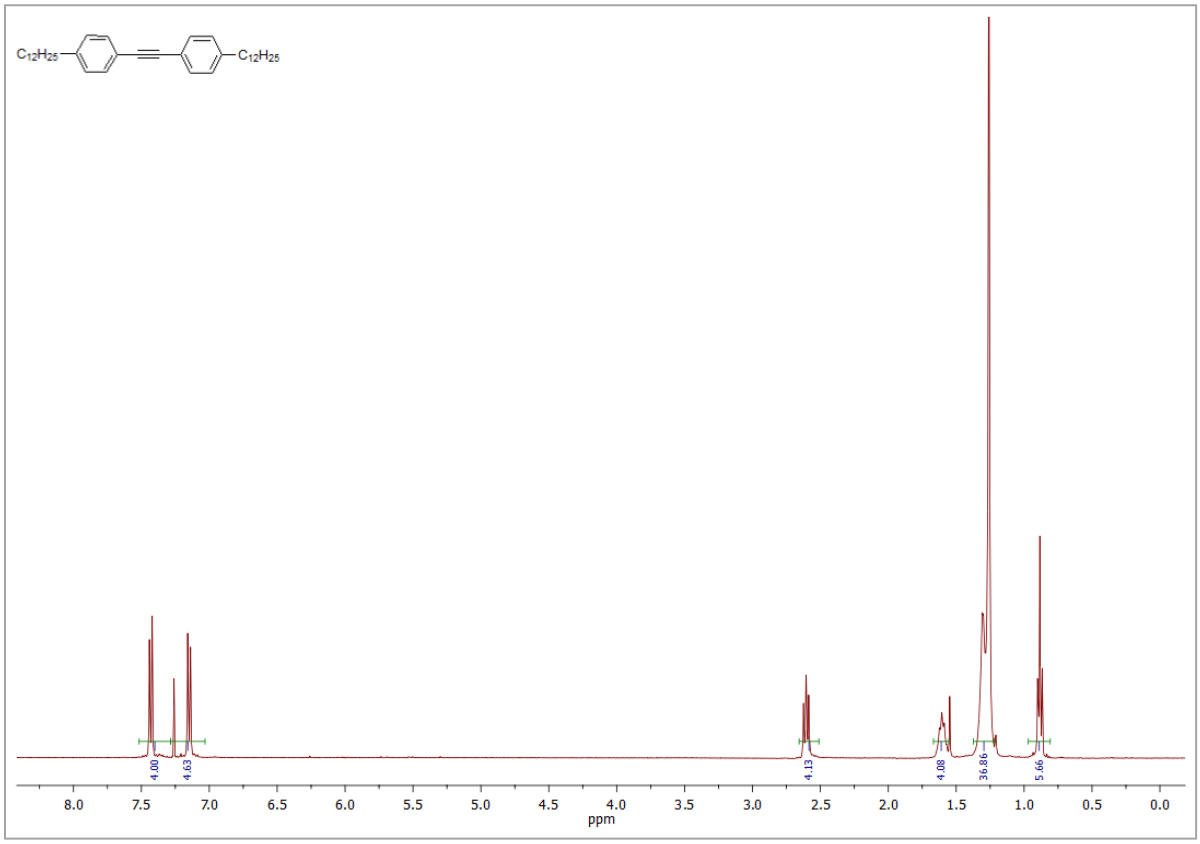
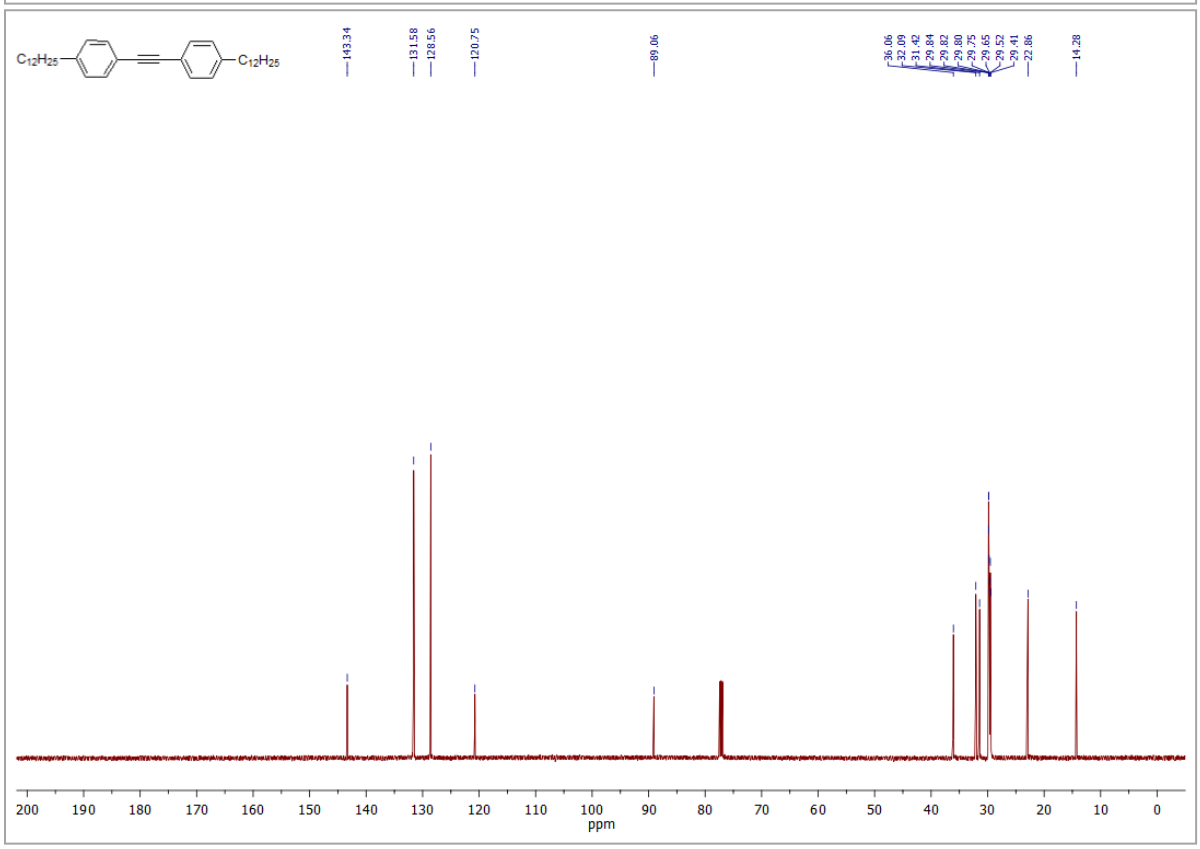
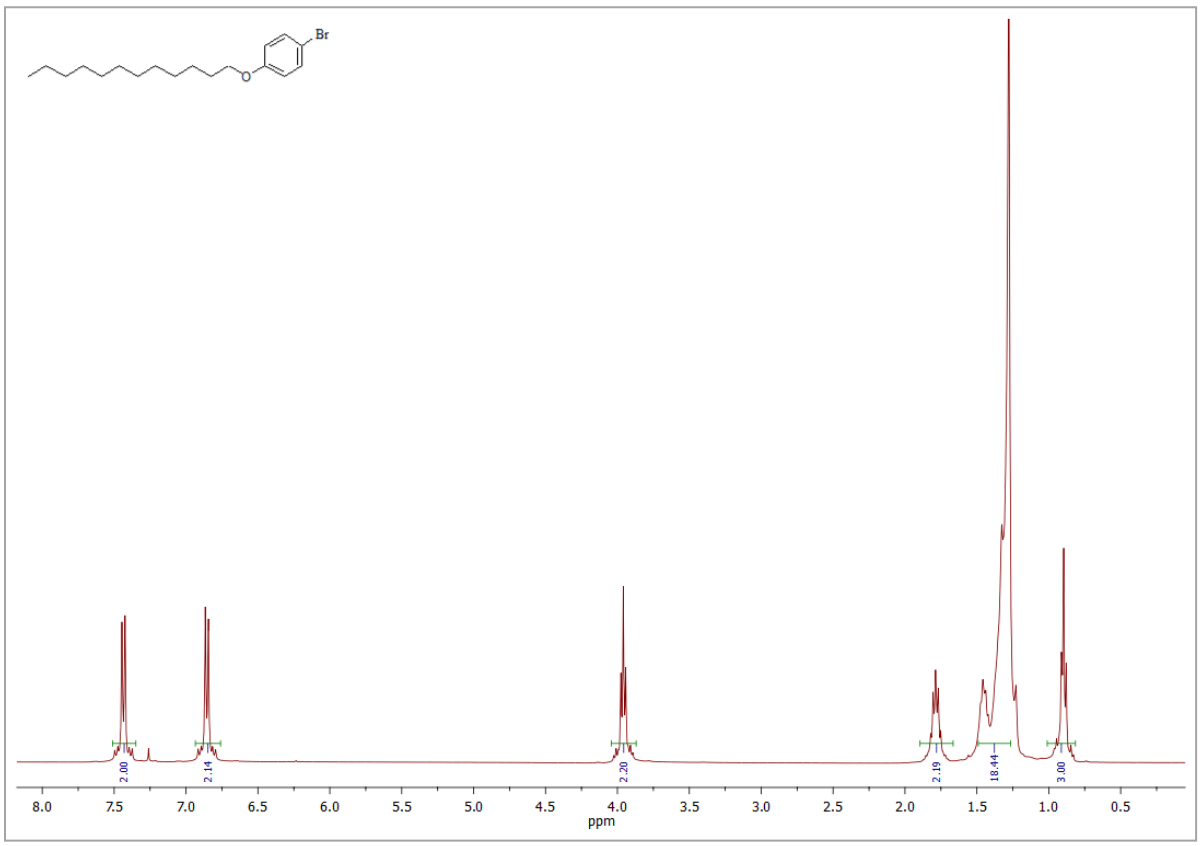
131.24
130.17
119.23
35.37
31.94
31.55
31.35
29.68
29.66
29.58
29.48
29.37
29.20
22.71
14.14
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

Compound (iii)

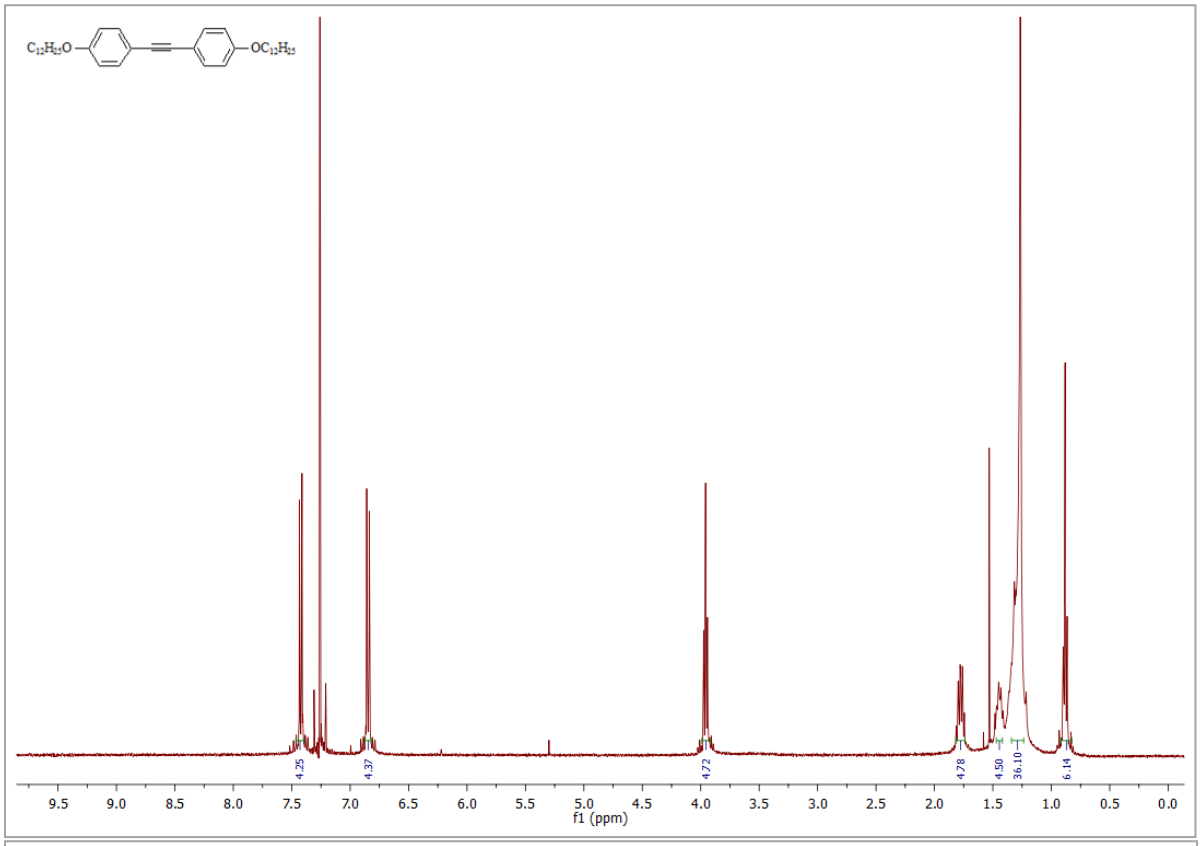


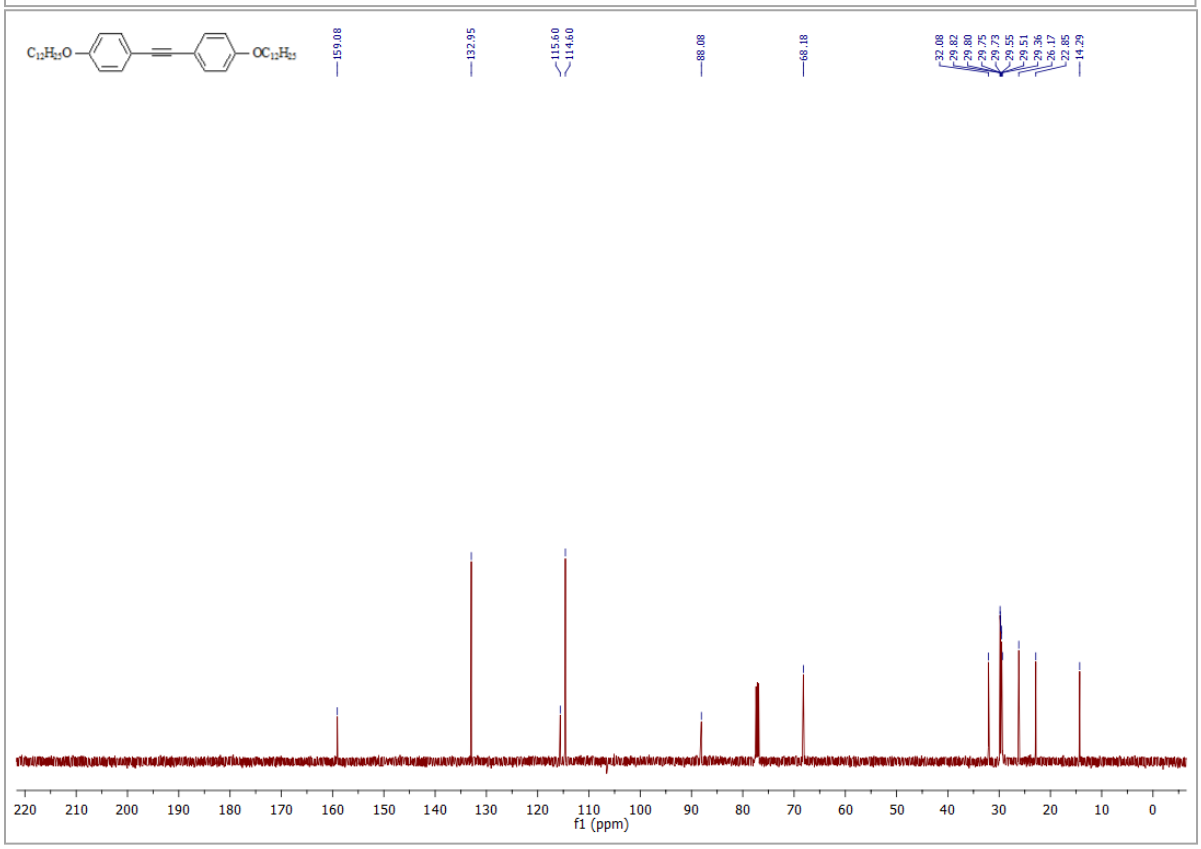


Compound (iv)

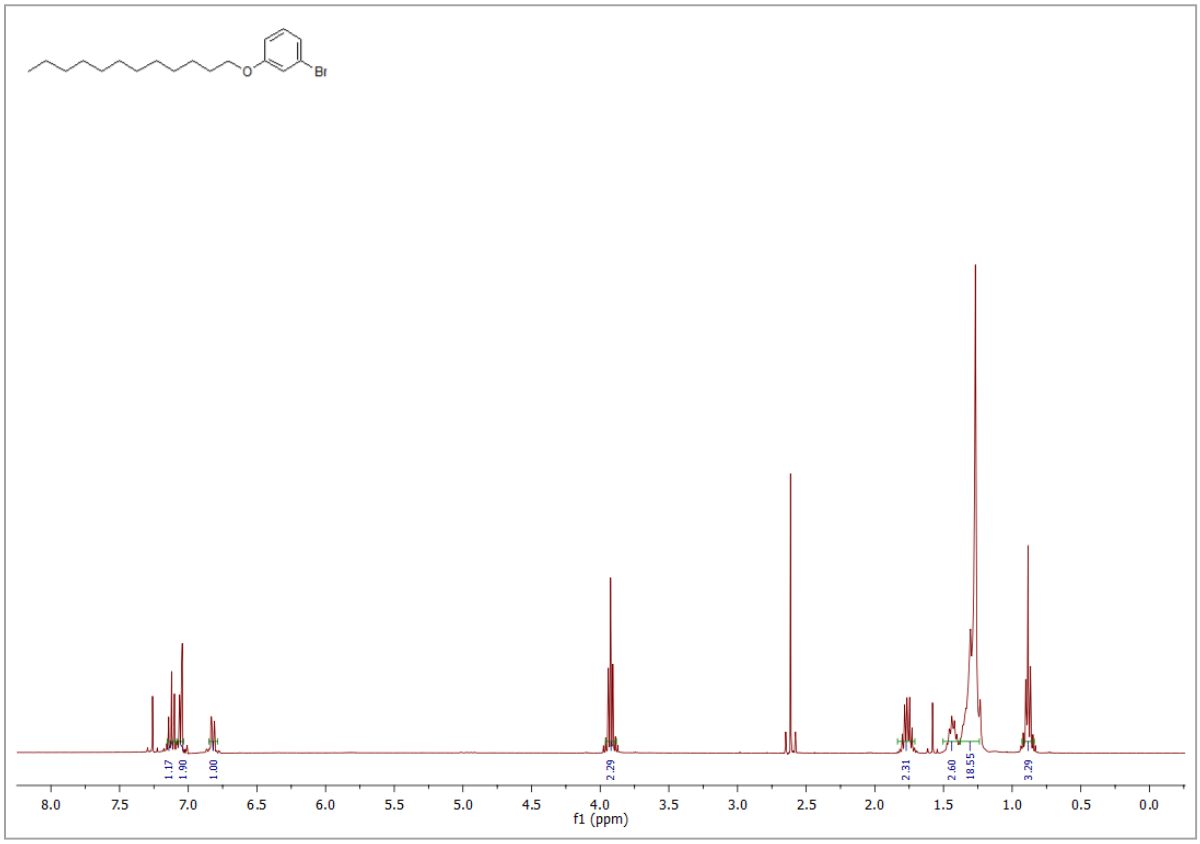

Br
O
2.00
2.14
2.20
2.19
18.44
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

Compound (v)

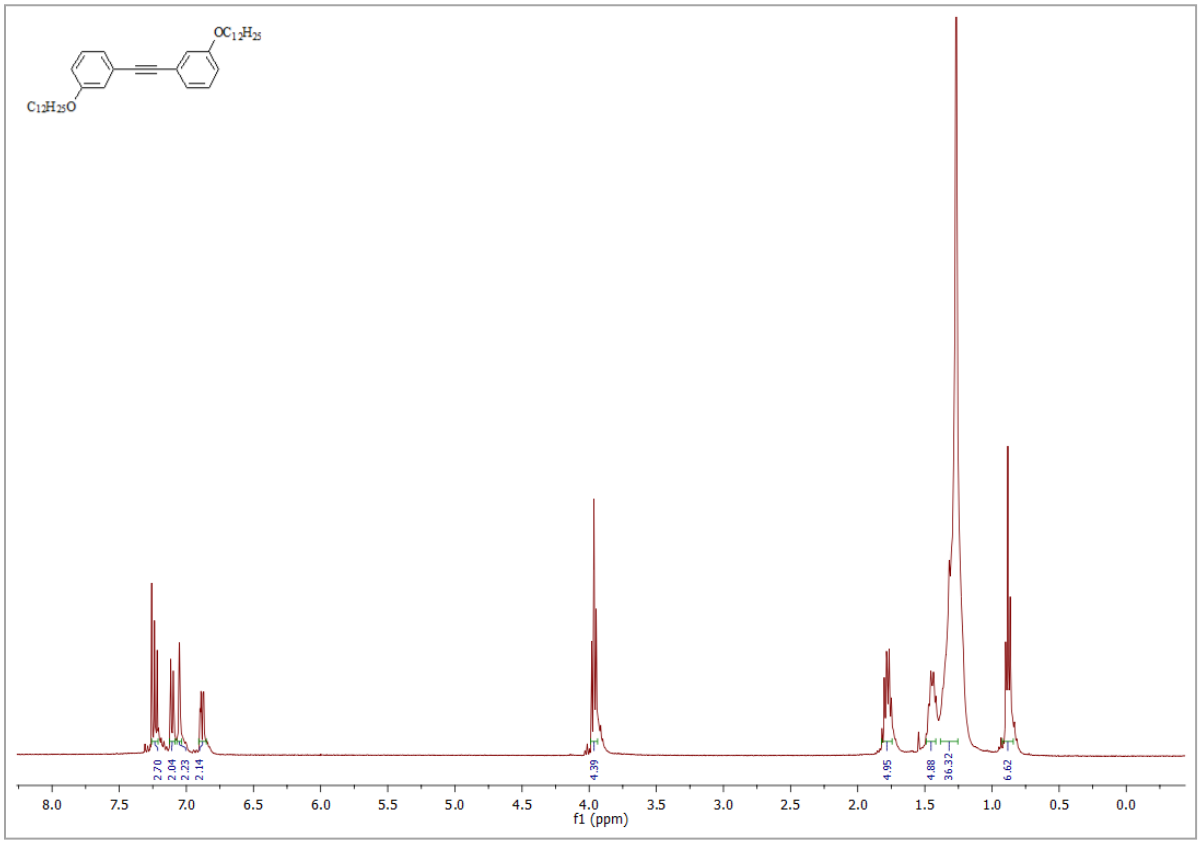

$C_{12}H_{25}O$
$OC_{12}H_{25}$
4.25
4.37
4.72
4.78
4.50
36.10
6.14
f1 (ppm)

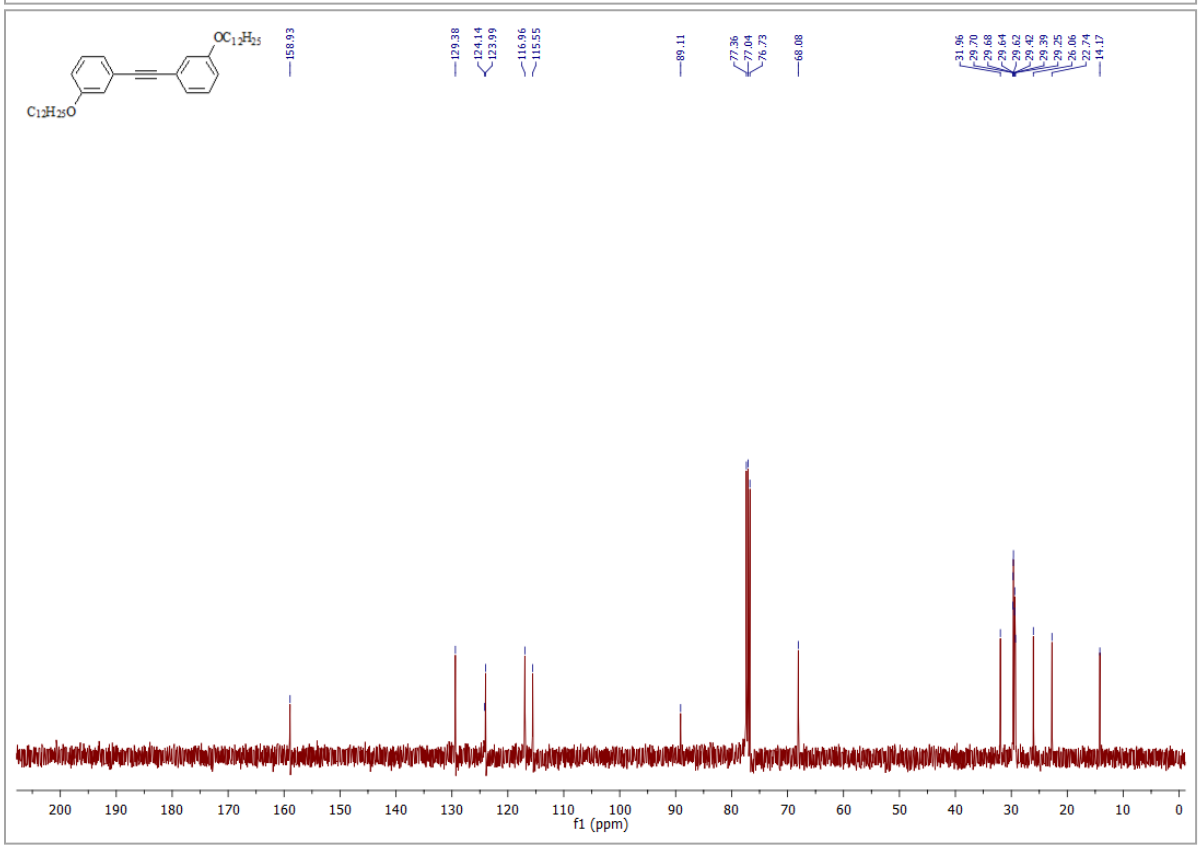

$C_{12}H_{25}O$
$OC_{12}H_{25}$
159.08
132.95
115.60
114.60
88.08
68.18
32.08
29.82
29.80
29.75
29.73
29.55
29.51
29.36
26.17
22.85
14.29
f1 (ppm)

Compound (vi)

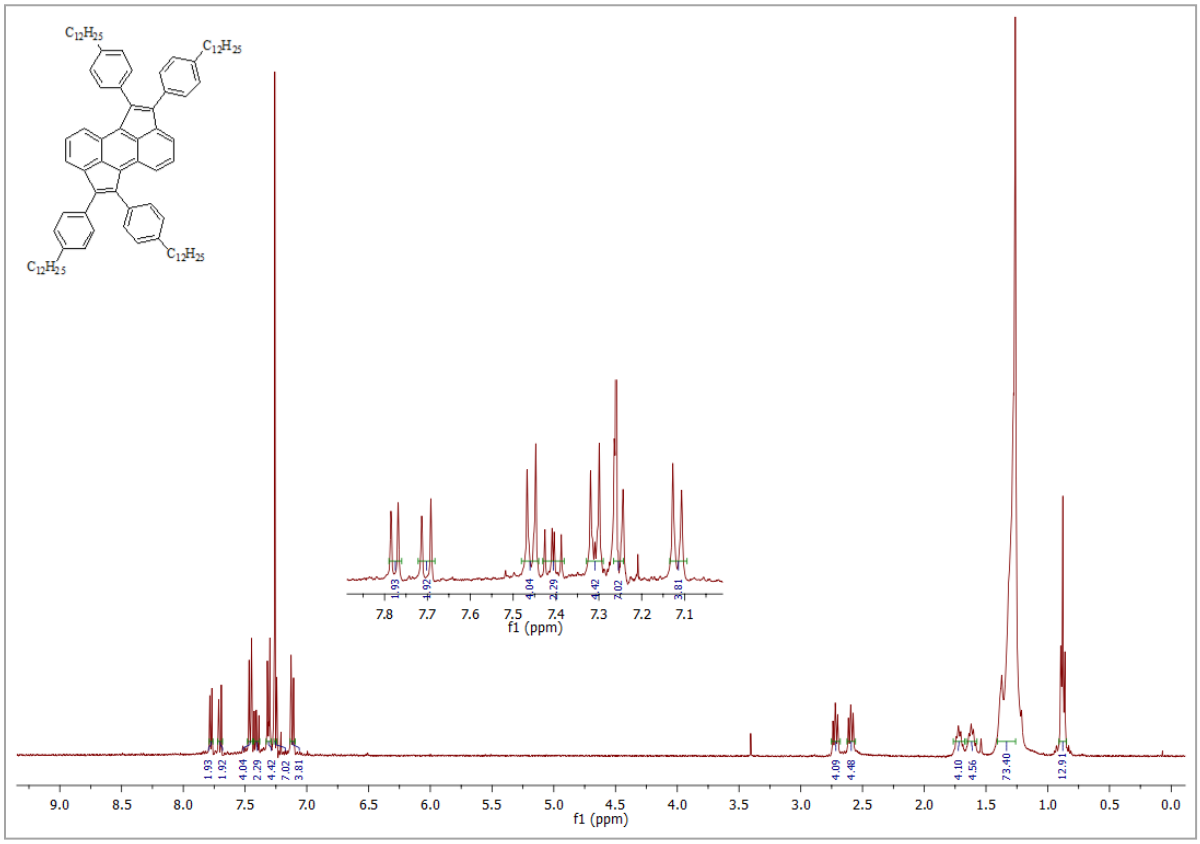

O
Br
1.17
1.90
1.00
2.29
2.31
2.60
18.55
3.29
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

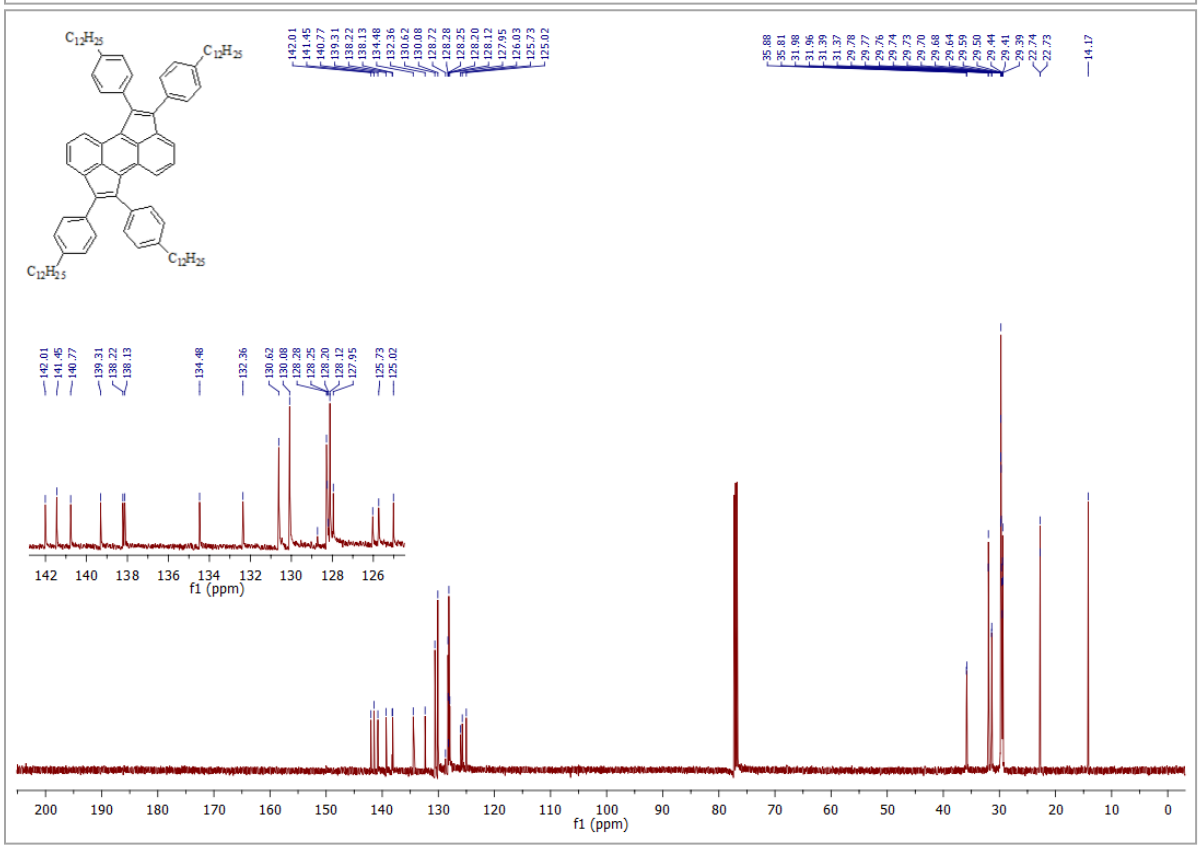
Compound (vii)



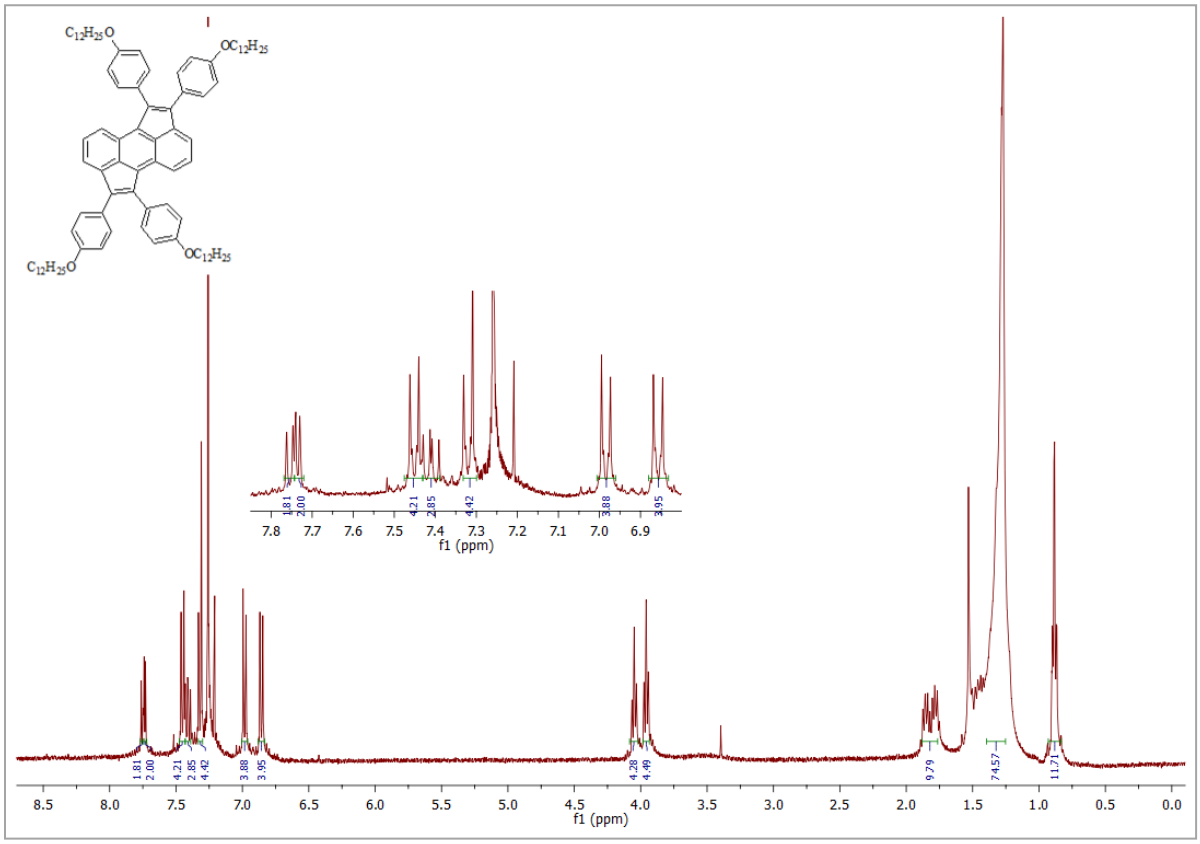


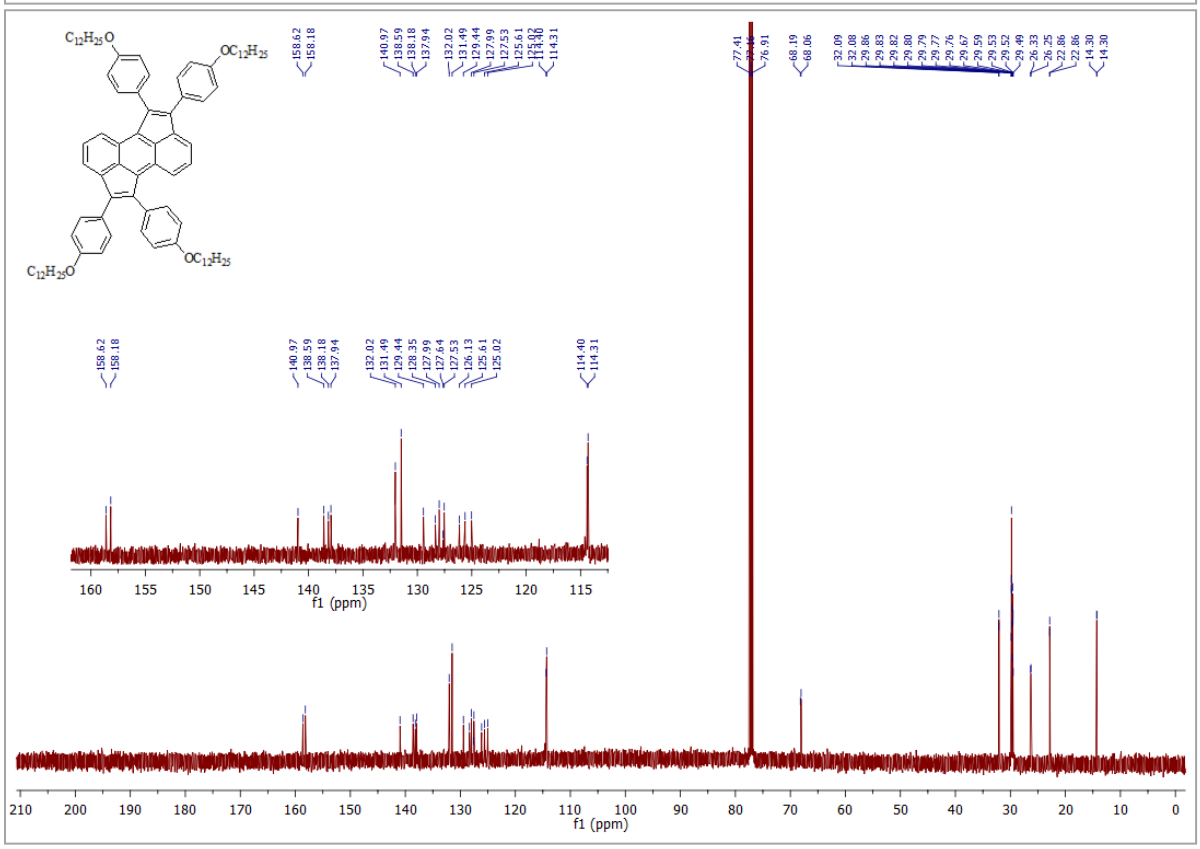
Compound (viii)



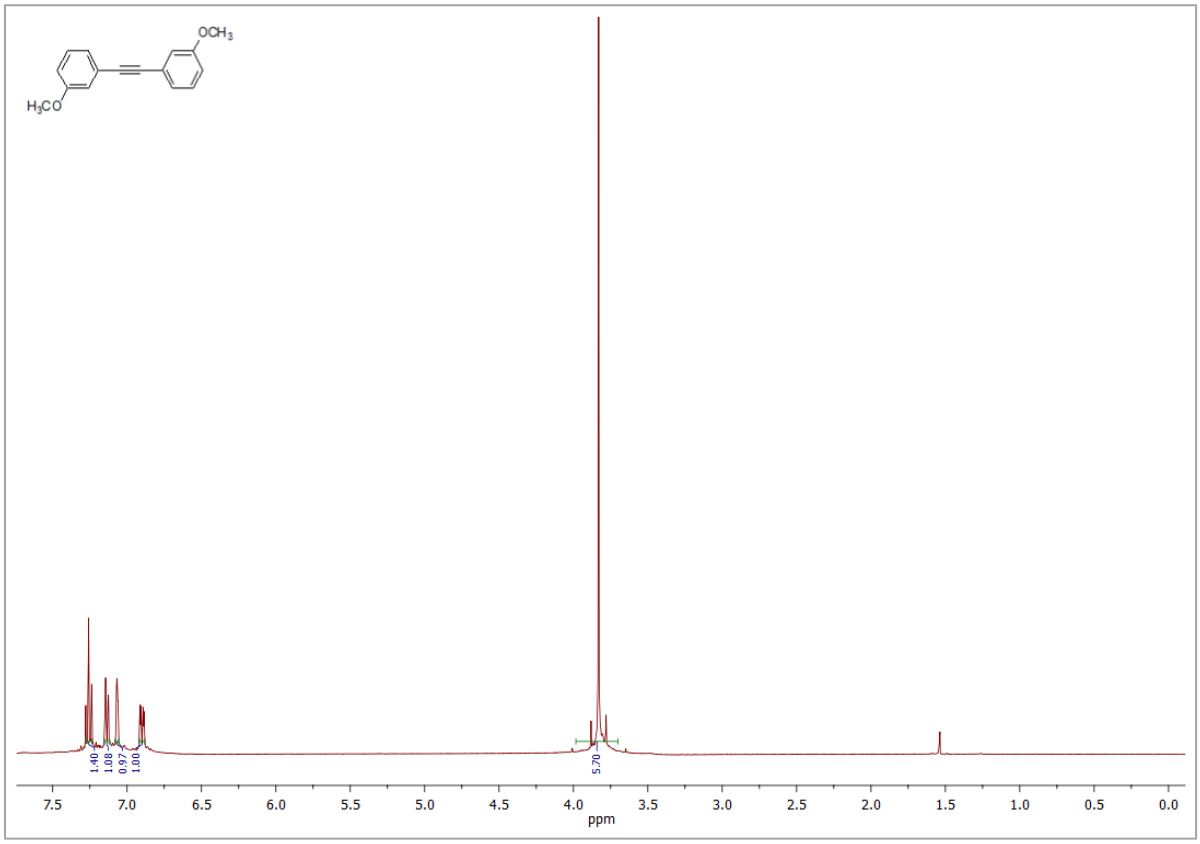


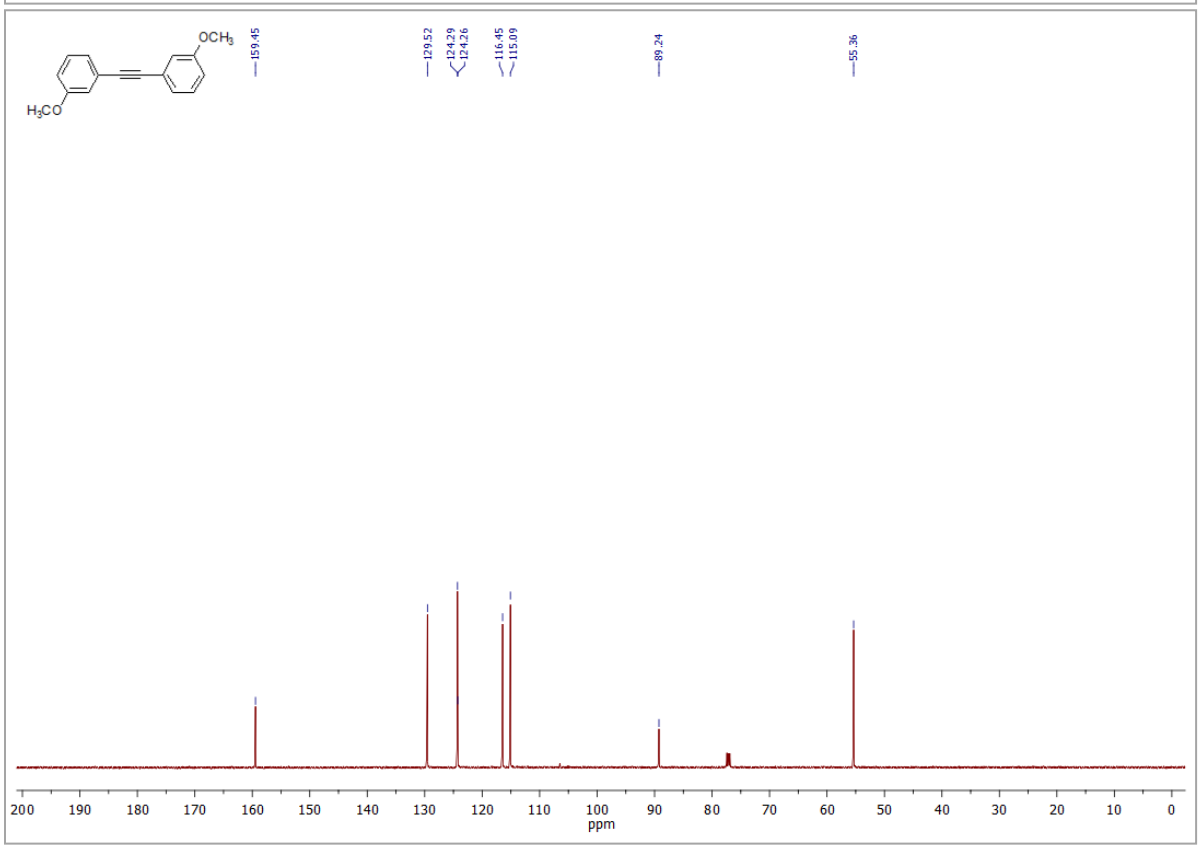
Compound (ix)


$C_{12}H_{25}O$
$OC_{12}H_{25}$
$C_{12}H_{25}O$
$OC_{12}H_{25}$
1.81
2.00
4.21
2.85
4.42
3.88
3.95
4.28
4.49
9.79
74.57
11.21
f1 (ppm)

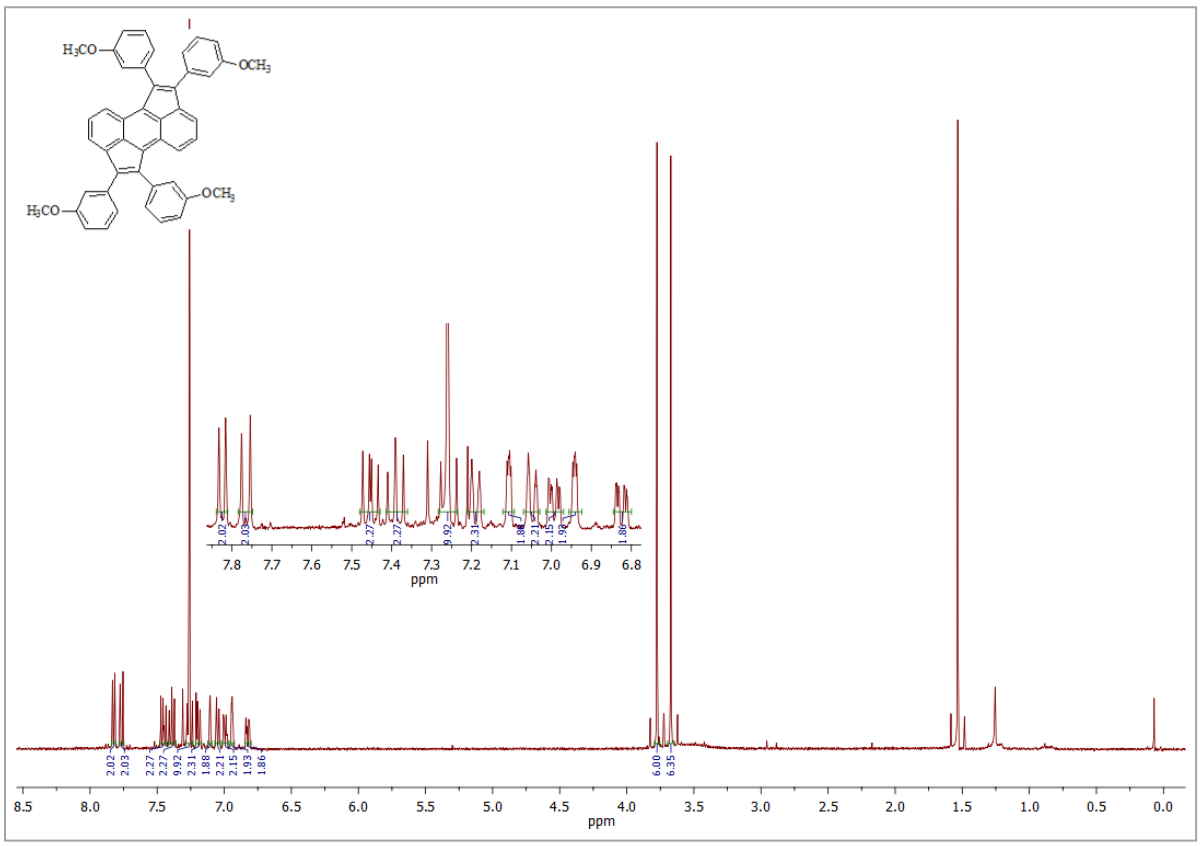

$C_{12}H_{25}O$
$OC_{12}H_{25}$
$C_{12}H_{25}O$
$OC_{12}H_{25}$
158.62
158.18
140.97
138.59
138.18
137.94
132.02
131.49
129.44
127.99
127.53
125.61
125.02
114.40
114.31
77.41
77.16
76.91
68.19
68.06
32.09
32.08
29.86
29.83
29.82
29.80
29.79
29.77
29.76
29.67
29.59
29.53
29.52
29.49
26.33
26.25
22.86
22.86
14.30
14.30
f1 (ppm)

Compound (x)

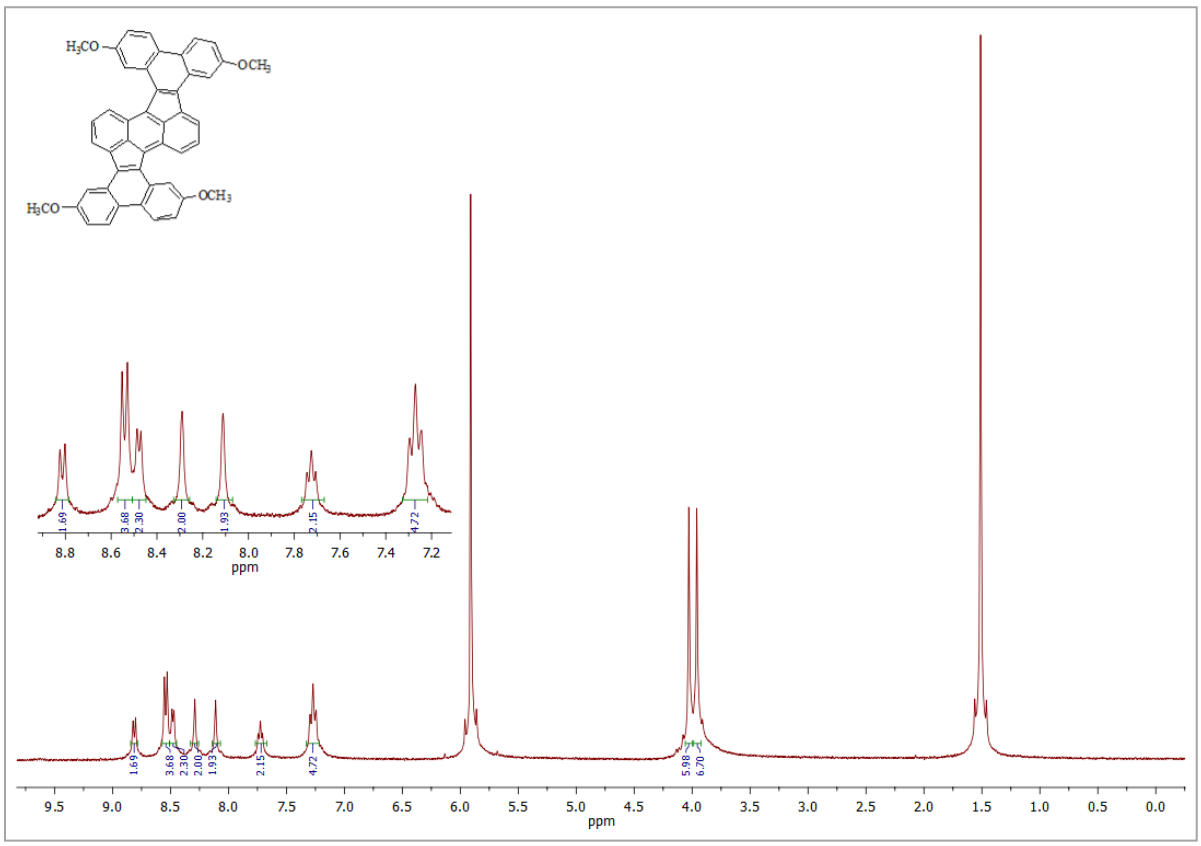

OCH3
H3CO
1.40
1.08
0.97
1.00
5.70
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm


OCH3
H3CO
159.45
129.52
124.29
124.26
116.45
115.09
89.24
55.36
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

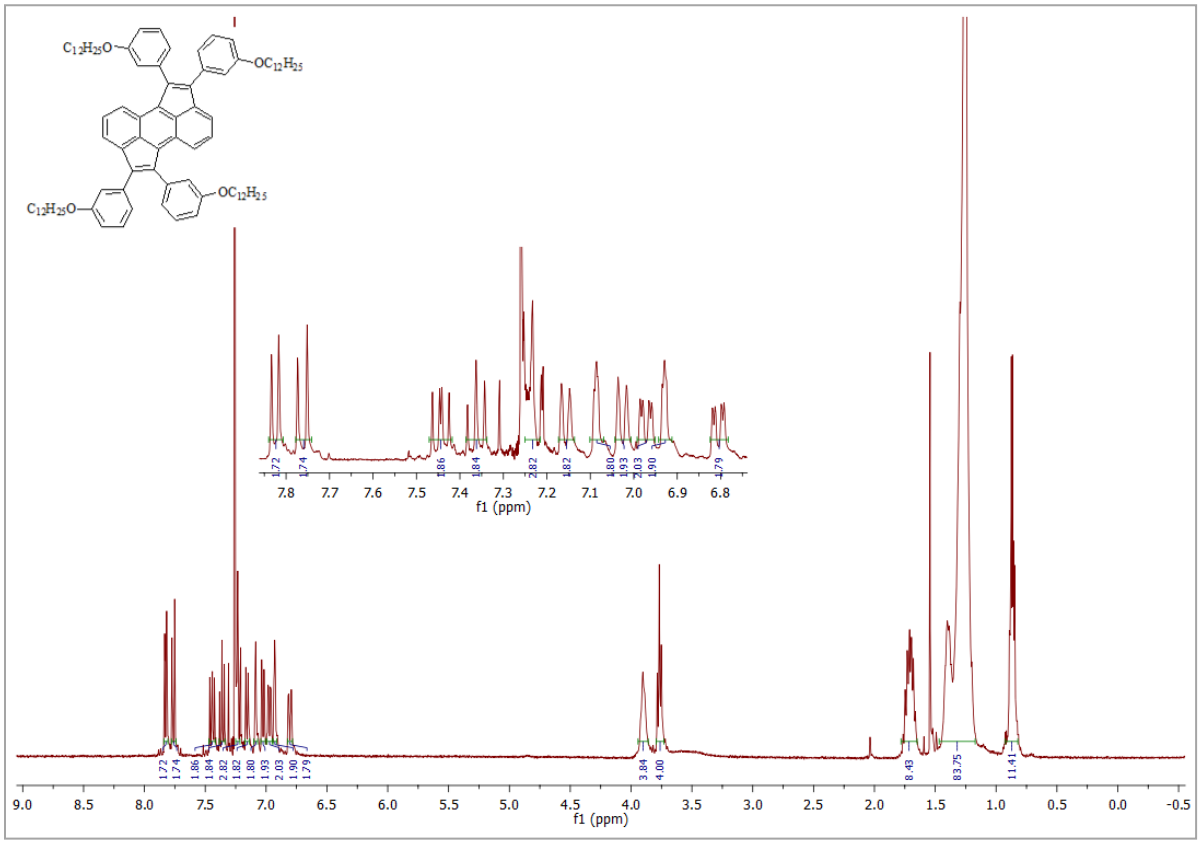
Compound (1a)

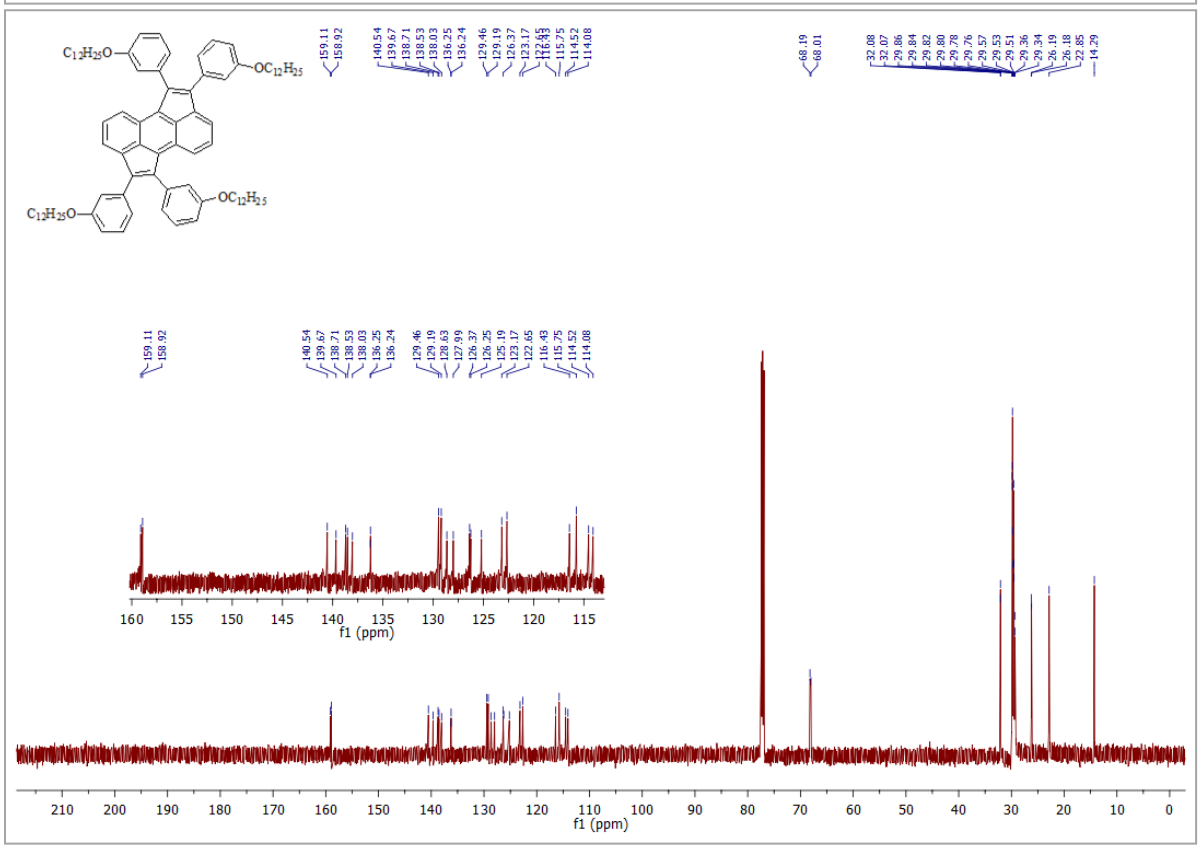


Compound (2a)

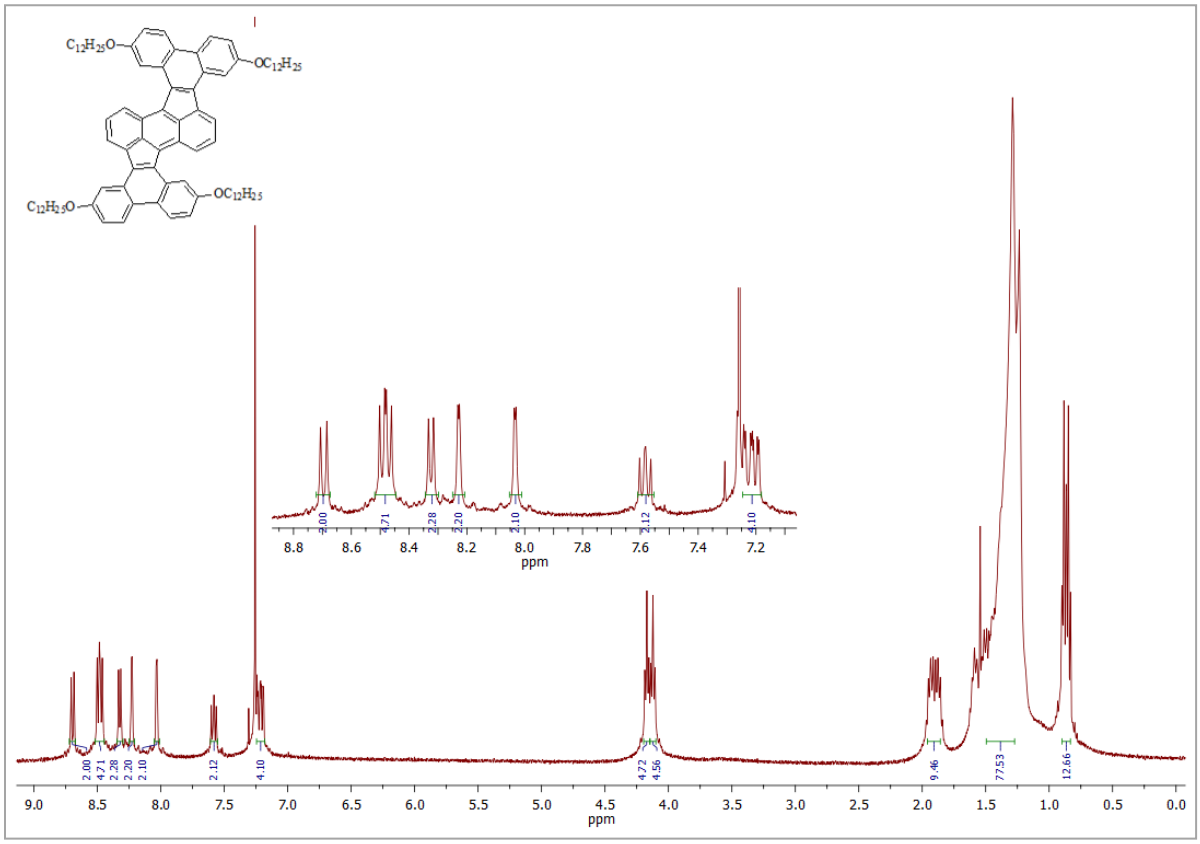

H3CO
OCH3
H3CO
OCH3
1.69
3.68
2.30
2.00
1.93
2.15
4.72
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
ppm
1.69
3.68
2.30
2.00
1.93
2.15
4.72
5.98
6.70
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

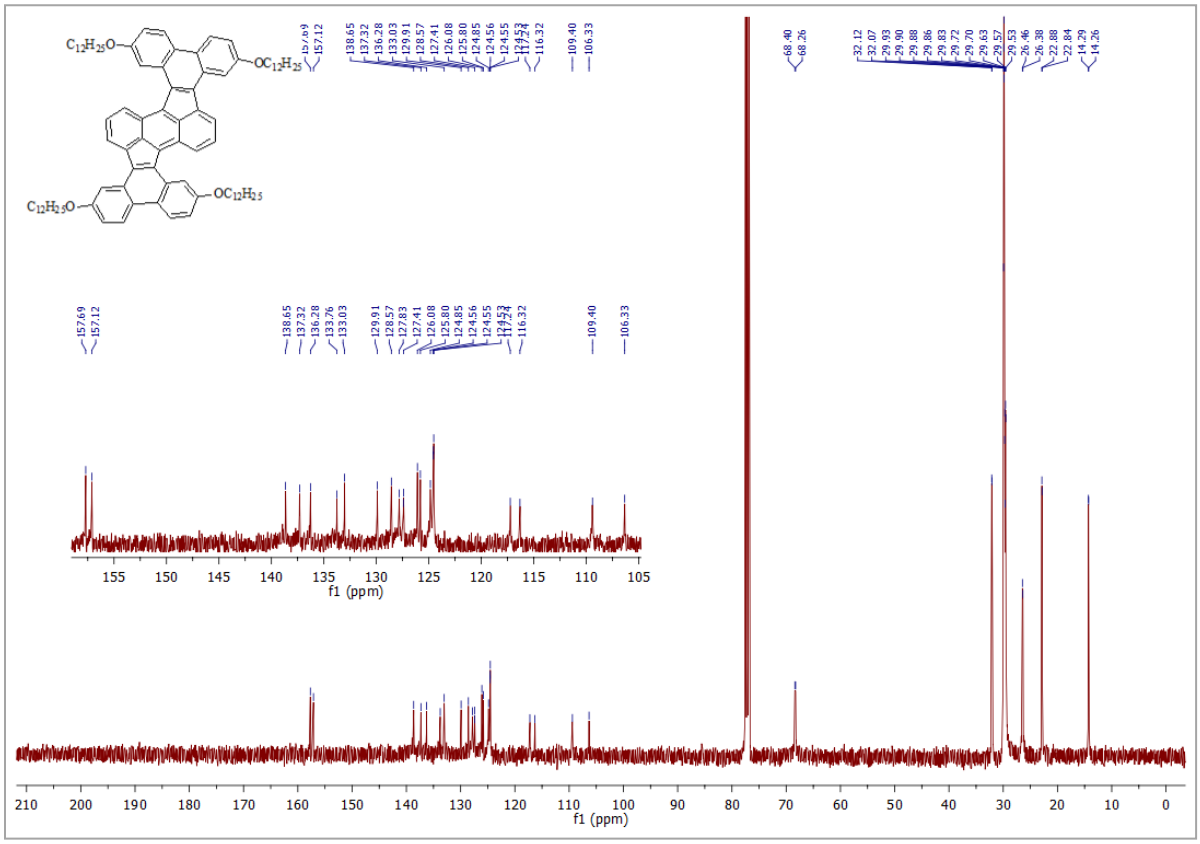
Compound (1b)



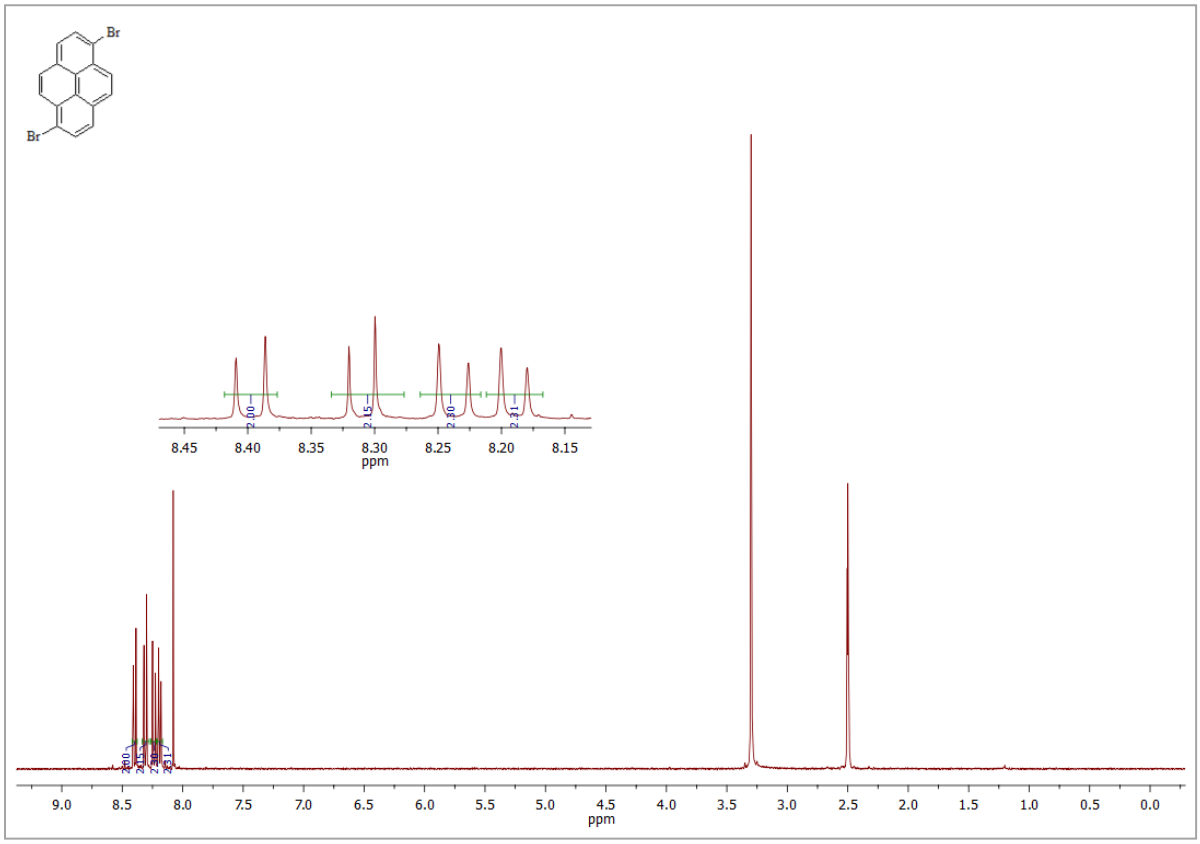


Compound (2b)

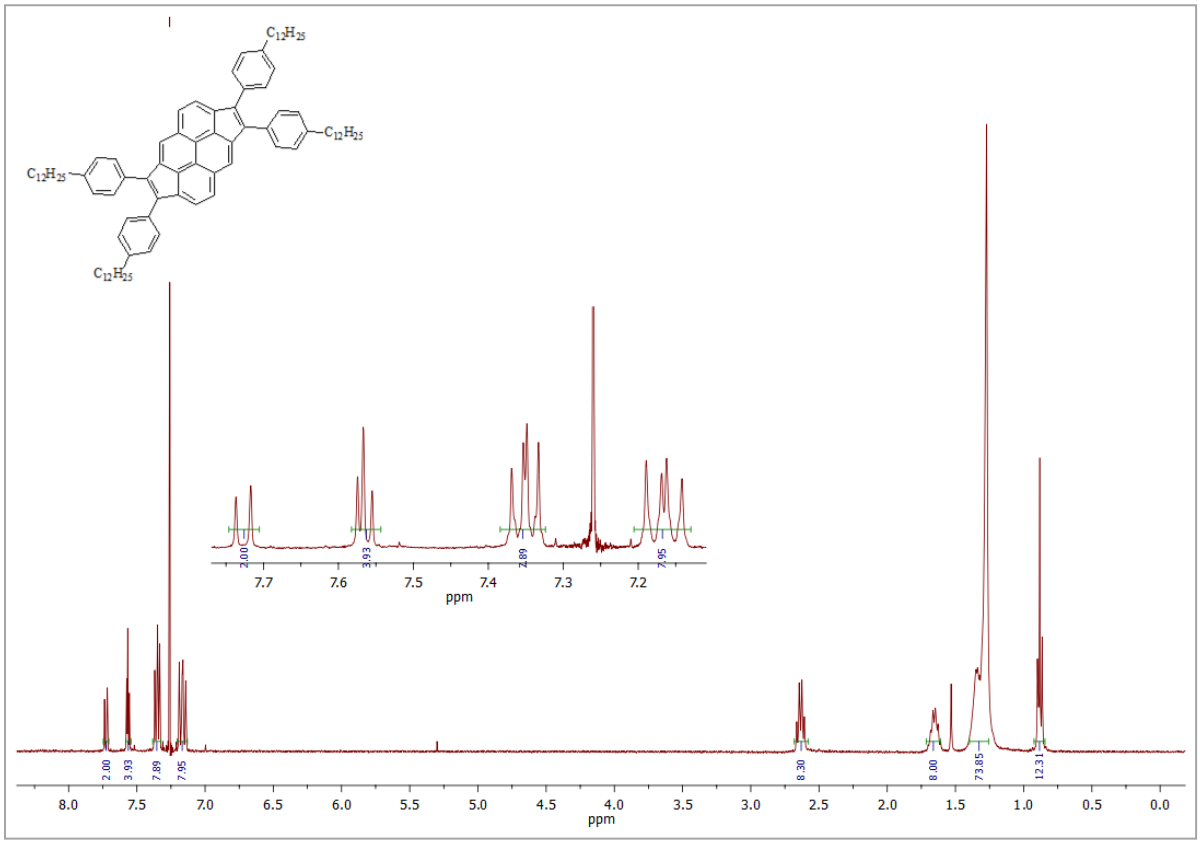


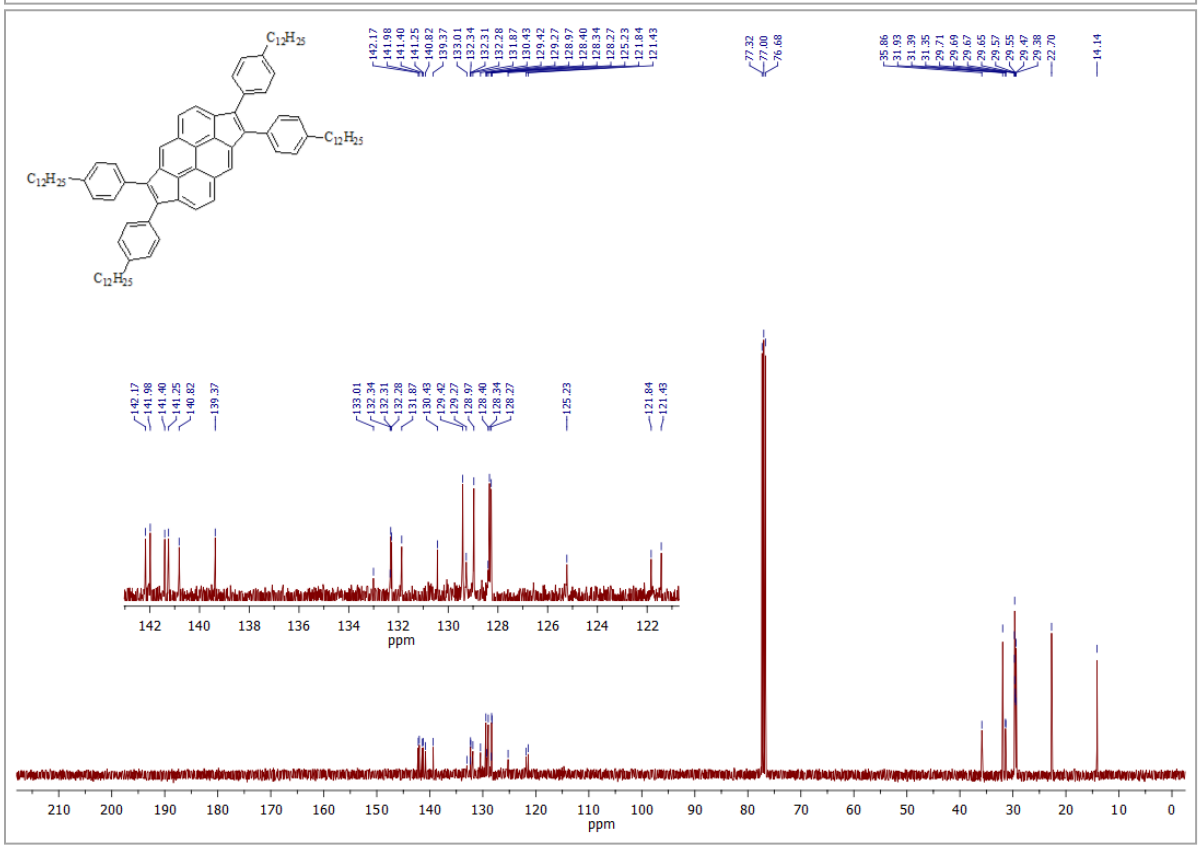


Compound (xi)

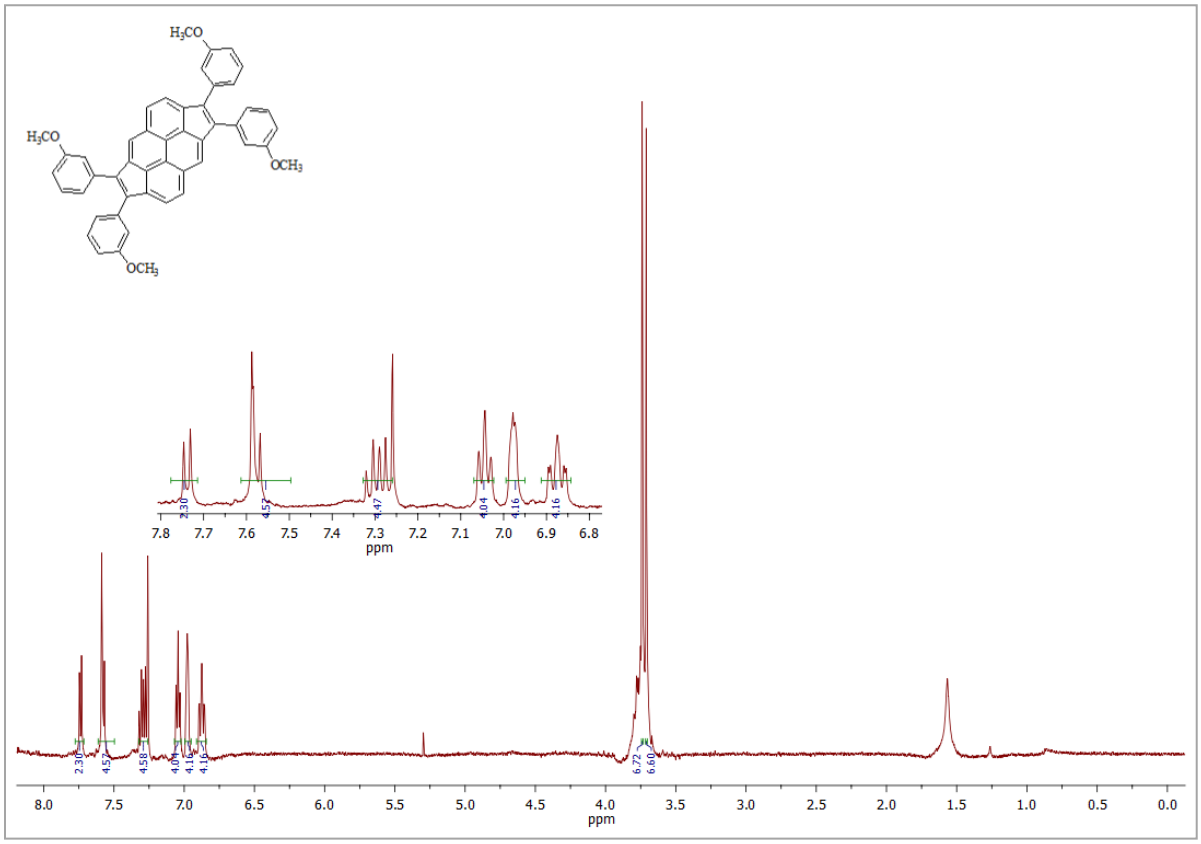

Br
Br
8.45
8.40
8.35
8.30
ppm
8.25
8.20
8.15
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
ppm
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

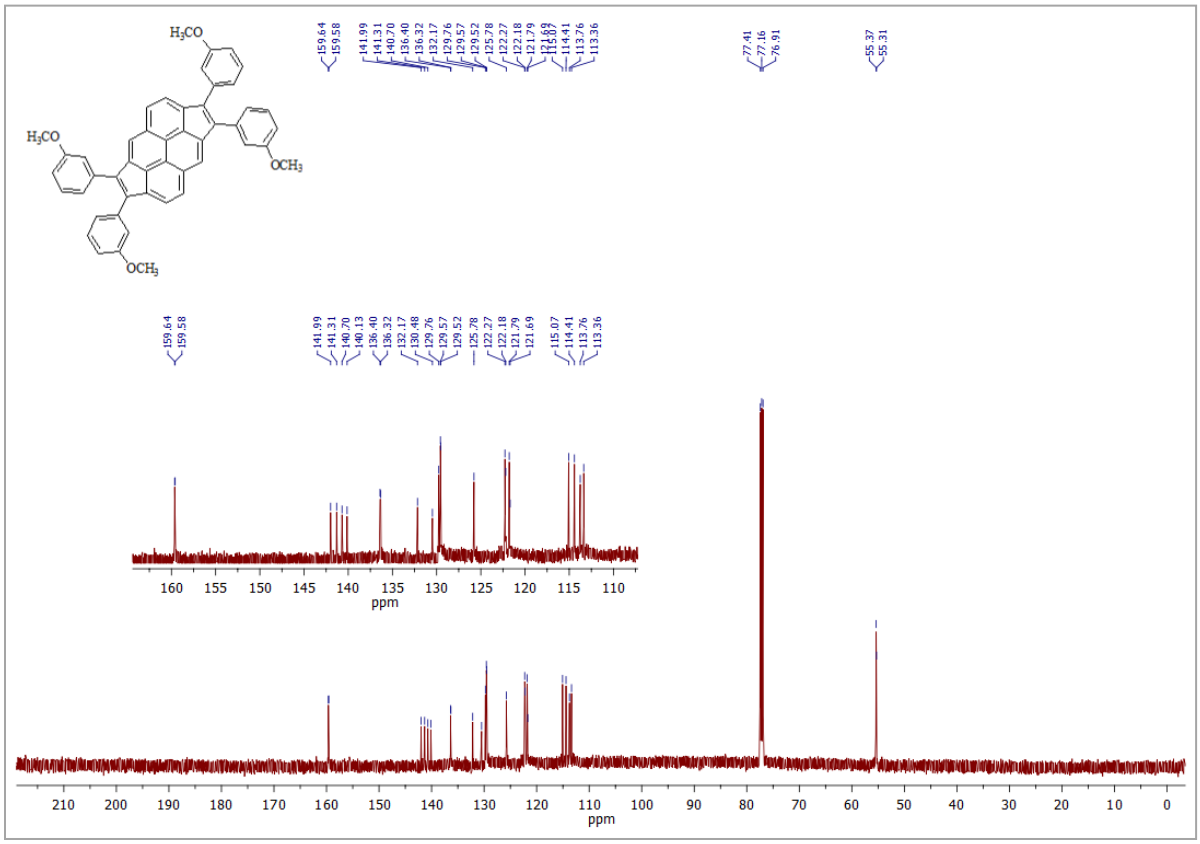
Compound (xii)



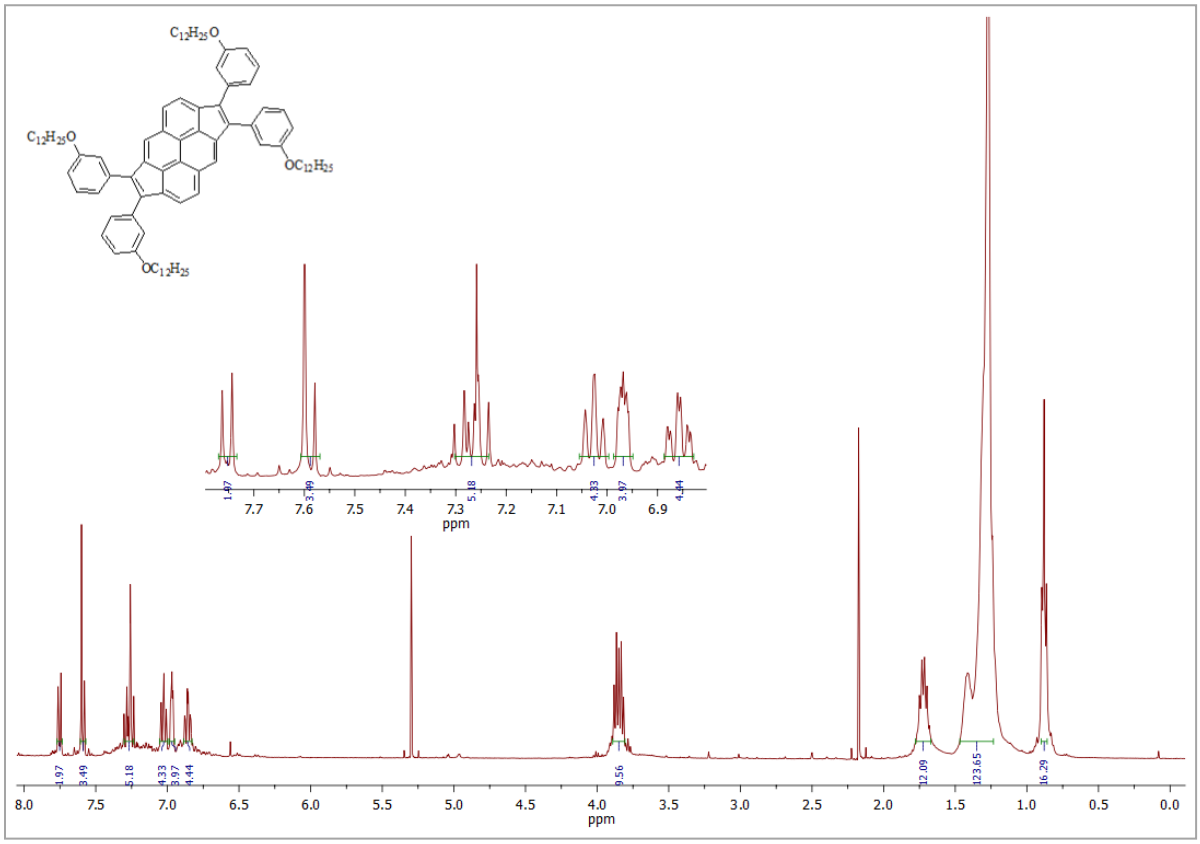


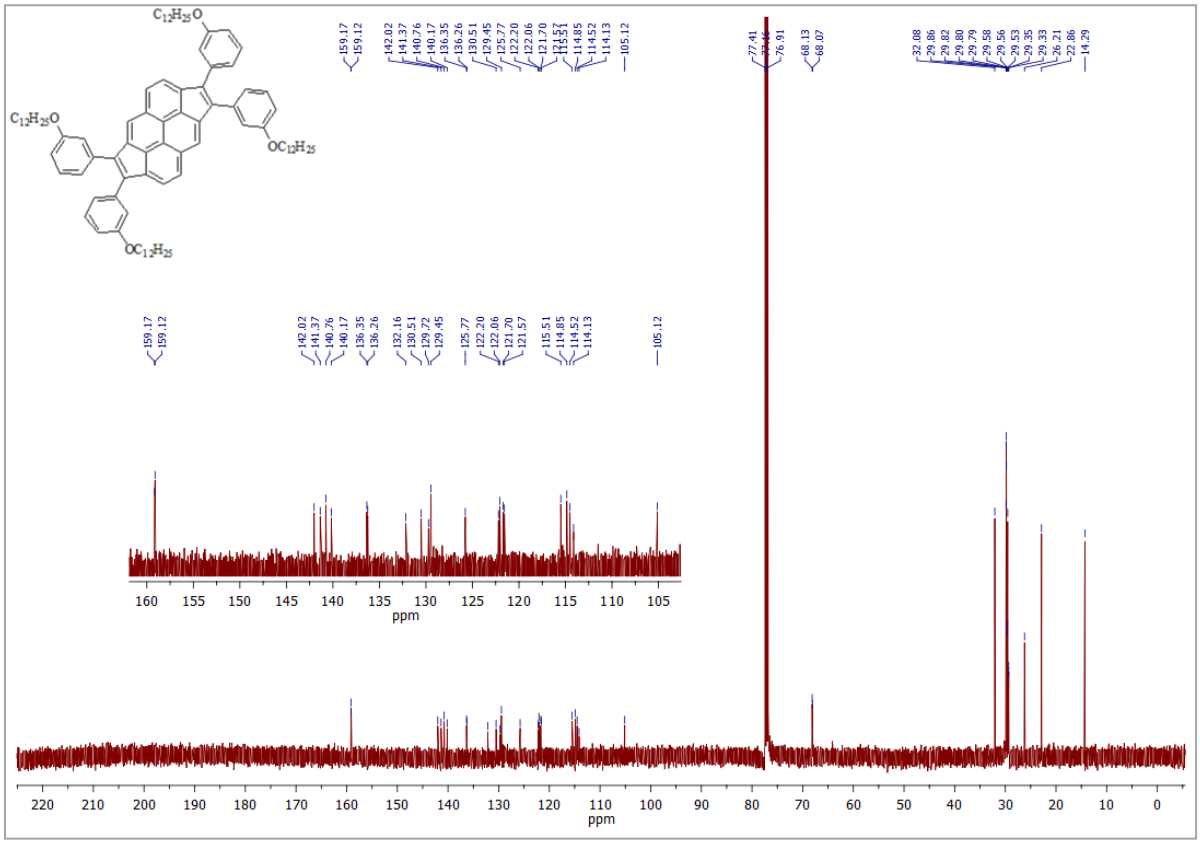
Compound (3a)


H3CO
H3CO
OCH3
OCH3
2.30
4.57
4.58
4.04
4.11
4.16
6.72
6.60
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8
ppm
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

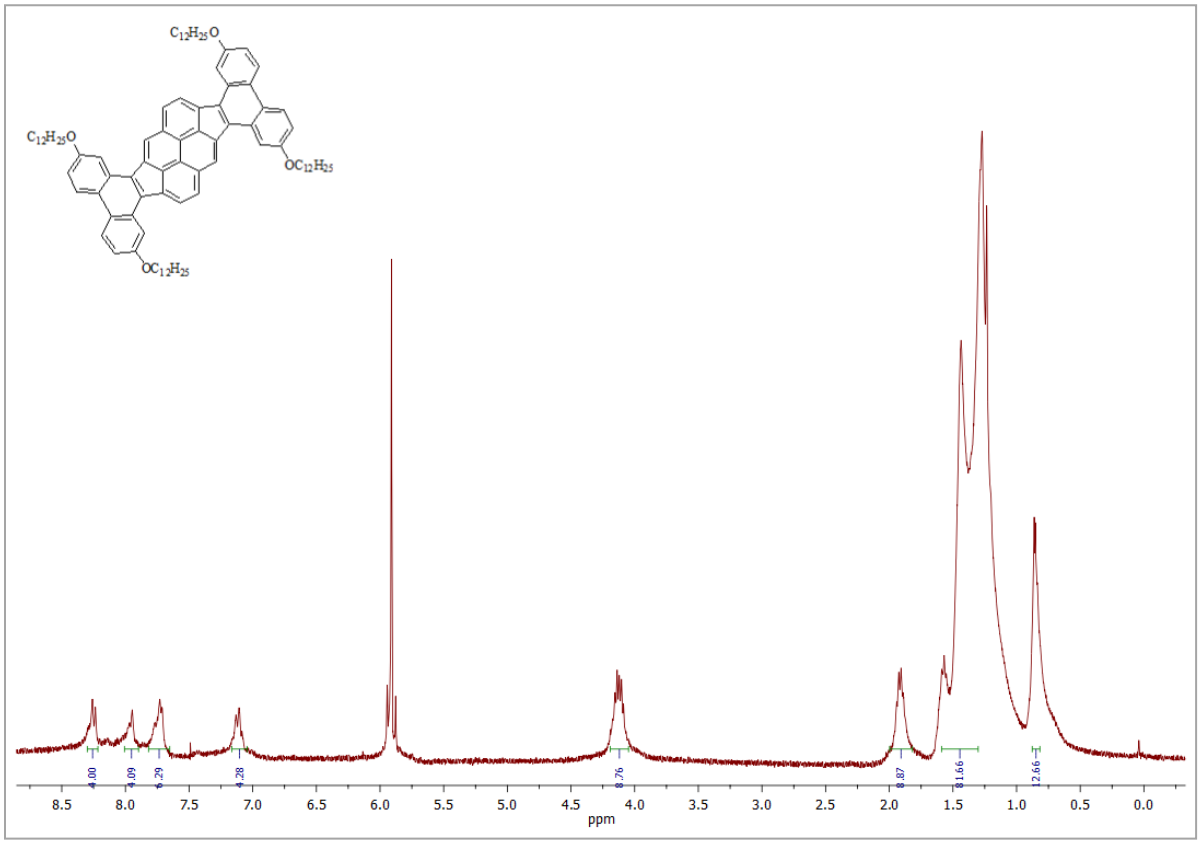

H3CO
H3CO
OCH3
OCH3
159.64
159.58
141.99
141.31
140.70
140.13
136.40
136.32
132.17
130.48
129.76
129.57
129.52
125.78
122.27
122.18
121.79
121.69
115.07
114.41
113.76
113.36
77.41
77.16
76.91
55.37
55.31
160 155 150 145 140 135 130 125 120 115 110
ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

Compound (3b)





Compound (4b)


$C_{12}H_{25}O$
$C_{12}H_{25}O$
$OC_{12}H_{25}$
$OC_{12}H_{25}$
4.00
4.09
6.29
4.28
8.76
8.87
8.166
12.66
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

7) Cartesian coordinates for calculated structures

1a at B3LYP/6-311g(d,p) level

C	**-0.272000**	**-1.288000**	**0.280000**
C	**-0.453000**	**-2.683000**	**0.550000**
H	**-1.451000**	**-3.093000**	**0.621000**
C	**0.637000**	**-3.505000**	**0.718000**
H	**0.477000**	**-4.558000**	**0.924000**
C	**1.979000**	**-3.028000**	**0.626000**
H	**2.800000**	**-3.719000**	**0.775000**
C	**2.193000**	**-1.700000**	**0.345000**
C	**1.070000**	**-0.842000**	**0.188000**
C	**1.520000**	**0.471000**	**-0.067000**
C	**0.540000**	**1.461000**	**-0.323000**
C	**-0.803000**	**1.014000**	**-0.236000**
C	**-1.253000**	**-0.285000**	**0.079000**
C	**0.719000**	**2.840000**	**-0.667000**
H	**1.717000**	**3.246000**	**-0.763000**
C	**-0.371000**	**3.653000**	**-0.878000**
H	**-0.211000**	**4.694000**	**-1.134000**
C	**-1.713000**	**3.177000**	**-0.777000**
H	**-2.534000**	**3.863000**	**-0.946000**
C	**-1.926000**	**1.854000**	**-0.472000**
C	**3.400000**	**-0.865000**	**0.187000**
C	**2.994000**	**0.433000**	**-0.047000**
C	**-2.726000**	**-0.248000**	**0.061000**
C	**-3.133000**	**1.026000**	**-0.278000**
C	**-3.614000**	**-1.407000**	**0.330000**
C	**-3.667000**	**-1.992000**	**1.607000**
C	**-4.415000**	**-1.926000**	**-0.686000**
C	**-4.513000**	**-3.068000**	**1.841000**
H	**-3.055000**	**-1.594000**	**2.408000**
C	**-5.265000**	**-3.013000**	**-0.447000**
H	**-4.394000**	**-1.497000**	**-1.680000**
C	**-5.317000**	**-3.591000**	**0.825000**
H	**-4.557000**	**-3.513000**	**2.828000**
C	**-4.510000**	**1.539000**	**-0.406000**
C	**-5.468000**	**1.279000**	**0.577000**
C	**-4.879000**	**2.321000**	**-1.518000**
C	**-6.770000**	**1.777000**	**0.465000**
H	**-5.219000**	**0.693000**	**1.452000**
C	**-6.173000**	**2.811000**	**-1.625000**
H	**-4.159000**	**2.518000**	**-2.302000**
C	**-7.130000**	**2.550000**	**-0.643000**
H	**-6.453000**	**3.404000**	**-2.489000**

C	**4.778000**	**-1.377000**	**0.304000**
C	**5.150000**	**-2.550000**	**-0.362000**
C	**5.737000**	**-0.721000**	**1.099000**
C	**6.447000**	**-3.063000**	**-0.252000**
H	**4.448000**	**-3.074000**	**-0.999000**
C	**7.020000**	**-1.236000**	**1.207000**
H	**5.464000**	**0.179000**	**1.635000**
C	**7.393000**	**-2.405000**	**0.539000**
H	**7.752000**	**-0.729000**	**1.827000**
C	**3.885000**	**1.595000**	**-0.285000**
C	**4.715000**	**1.636000**	**-1.417000**
C	**3.912000**	**2.664000**	**0.612000**
C	**5.545000**	**2.730000**	**-1.629000**
H	**4.701000**	**0.814000**	**-2.123000**
C	**4.752000**	**3.763000**	**0.397000**
H	**3.288000**	**2.660000**	**1.499000**
C	**5.575000**	**3.799000**	**-0.733000**
H	**6.182000**	**2.760000**	**-2.506000**
H	**6.231000**	**4.638000**	**-0.921000**
H	**8.401000**	**-2.784000**	**0.641000**
H	**-5.966000**	**-4.430000**	**1.033000**
H	**-8.131000**	**2.946000**	**-0.750000**
O	**6.688000**	**-4.207000**	**-0.956000**
O	**4.694000**	**4.742000**	**1.344000**
O	**-5.997000**	**-3.432000**	**-1.518000**
O	**-7.610000**	**1.458000**	**1.491000**
C	**7.991000**	**-4.782000**	**-0.893000**
H	**7.954000**	**-5.669000**	**-1.522000**
H	**8.750000**	**-4.094000**	**-1.281000**
H	**8.250000**	**-5.072000**	**0.130000**
C	**-6.891000**	**-4.530000**	**-1.344000**
H	**-7.362000**	**-4.684000**	**-2.313000**
H	**-6.355000**	**-5.439000**	**-1.053000**
H	**-7.659000**	**-4.304000**	**-0.598000**
C	**5.527000**	**5.890000**	**1.189000**
H	**5.288000**	**6.435000**	**0.270000**
H	**5.321000**	**6.524000**	**2.049000**
H	**6.587000**	**5.617000**	**1.185000**
C	**-8.955000**	**1.930000**	**1.441000**
H	**-9.483000**	**1.542000**	**0.564000**
H	**-9.433000**	**1.557000**	**2.345000**
H	**-8.994000**	**3.024000**	**1.437000**

2a at B3LYP/6-311g(d,p) level

O	**3.648000**	**5.529000**	**0.507000**
O	**7.272000**	**-3.553000**	**-0.230000**
C	**1.049000**	**-0.786000**	**0.282000**
C	**1.338000**	**0.547000**	**-0.090000**

C	**2.811000**	**0.689000**	**-0.030000**
C	**0.238000**	**1.365000**	**-0.458000**
C	**4.767000**	**-0.823000**	**0.037000**
C	**3.175000**	**3.157000**	**0.216000**
H	**2.126000**	**3.289000**	**0.421000**
C	**3.363000**	**-0.582000**	**0.175000**
C	**3.667000**	**1.847000**	**-0.016000**
C	**4.028000**	**4.244000**	**0.262000**
C	**-0.919000**	**3.326000**	**-1.331000**
H	**-0.878000**	**4.298000**	**-1.811000**
C	**2.194000**	**-2.779000**	**1.014000**
H	**3.075000**	**-3.361000**	**1.248000**
C	**0.252000**	**2.662000**	**-1.062000**
H	**1.191000**	**3.108000**	**-1.357000**
C	**5.077000**	**1.642000**	**-0.115000**
C	**2.264000**	**-1.510000**	**0.489000**
C	**6.999000**	**0.044000**	**-0.389000**
H	**7.678000**	**0.865000**	**-0.572000**
C	**5.311000**	**-2.134000**	**0.021000**
H	**4.650000**	**-2.978000**	**0.123000**
C	**5.412000**	**4.054000**	**0.069000**
H	**6.066000**	**4.917000**	**0.099000**
C	**7.512000**	**-1.229000**	**-0.393000**
H	**8.566000**	**-1.410000**	**-0.568000**
C	**5.912000**	**2.786000**	**-0.098000**
H	**6.984000**	**2.672000**	**-0.184000**
C	**5.622000**	**0.299000**	**-0.171000**
C	**6.662000**	**-2.337000**	**-0.186000**
C	**6.475000**	**-4.721000**	**-0.042000**
H	**5.994000**	**-4.719000**	**0.942000**
H	**7.162000**	**-5.563000**	**-0.107000**
H	**5.713000**	**-4.812000**	**-0.822000**
C	**2.271000**	**5.796000**	**0.769000**
H	**2.208000**	**6.867000**	**0.950000**
H	**1.923000**	**5.256000**	**1.654000**
H	**1.644000**	**5.536000**	**-0.089000**
O	**-3.648000**	**-5.529000**	**-0.507000**
O	**-7.272000**	**3.553000**	**0.230000**
C	**-1.049000**	**0.786000**	**-0.282000**
C	**-1.338000**	**-0.547000**	**0.090000**
C	**-2.811000**	**-0.689000**	**0.030000**
C	**-0.238000**	**-1.365000**	**0.458000**
C	**-4.767000**	**0.823000**	**-0.037000**
C	**-3.175000**	**-3.157000**	**-0.216000**
H	**-2.126000**	**-3.289000**	**-0.421000**
C	**-3.363000**	**0.582000**	**-0.175000**
C	**-3.667000**	**-1.847000**	**0.016000**
C	**-4.028000**	**-4.244000**	**-0.262000**
C	**0.919000**	**-3.326000**	**1.331000**
H	**0.878000**	**-4.298000**	**1.811000**
C	**-2.194000**	**2.779000**	**-1.014000**
H	**-3.075000**	**3.361000**	**-1.248000**

C	**-0.252000**	**-2.662000**	**1.062000**
H	**-1.191000**	**-3.108000**	**1.357000**
C	**-5.077000**	**-1.642000**	**0.116000**
C	**-2.264000**	**1.510000**	**-0.489000**
C	**-6.999000**	**-0.044000**	**0.389000**
H	**-7.678000**	**-0.865000**	**0.572000**
C	**-5.311000**	**2.134000**	**-0.021000**
H	**-4.650000**	**2.978000**	**-0.123000**
C	**-5.412000**	**-4.054000**	**-0.069000**
H	**-6.066000**	**-4.917000**	**-0.099000**
C	**-7.512000**	**1.229000**	**0.393000**
H	**-8.566000**	**1.410000**	**0.568000**
C	**-5.912000**	**-2.786000**	**0.098000**
H	**-6.984000**	**-2.672000**	**0.184000**
C	**-5.622000**	**-0.299000**	**0.171000**
C	**-6.662000**	**2.337000**	**0.186000**
C	**-6.475000**	**4.721000**	**0.042000**
H	**-5.994000**	**4.719000**	**-0.942000**
H	**-7.162000**	**5.563000**	**0.107000**
H	**-5.713000**	**4.812000**	**0.822000**
C	**-2.271000**	**-5.796000**	**-0.769000**
H	**-2.208000**	**-6.867000**	**-0.950000**
H	**-1.922000**	**-5.256000**	**-1.654000**
H	**-1.644000**	**-5.536000**	**0.089000**

3a at B3LYP/6-311g(d,p) level

C	**-2.223000**	**2.696000**	**-0.017000**
C	**-2.712000**	**1.380000**	**-0.024000**
C	**-1.766000**	**0.360000**	**0.001000**
C	**-0.408000**	**0.574000**	**0.005000**
C	**0.122000**	**1.895000**	**-0.002000**
C	**-0.834000**	**2.937000**	**-0.009000**
C	**-2.371000**	**-0.935000**	**0.017000**
C	**0.408000**	**-0.574000**	**0.005000**
C	**-0.121000**	**-1.895000**	**-0.002000**
C	**-1.567000**	**-2.053000**	**0.002000**
C	**0.834000**	**-2.937000**	**-0.009000**
H	**0.491000**	**-3.966000**	**-0.008000**
C	**2.223000**	**-2.696000**	**-0.017000**
C	**2.712000**	**-1.380000**	**-0.024000**
C	**1.766000**	**-0.360000**	**0.001000**
C	**2.371000**	**0.935000**	**0.017000**
C	**1.567000**	**2.053000**	**0.002000**
H	**1.984000**	**3.055000**	**-0.006000**
H	**-2.897000**	**3.545000**	**-0.019000**
H	**-0.491000**	**3.966000**	**-0.008000**
H	**-1.984000**	**-3.055000**	**-0.006000**
H	**2.897000**	**-3.545000**	**-0.019000**

C	**4.036000**	**-0.702000**	**-0.016000**
C	**3.833000**	**0.668000**	**0.006000**
C	**-4.036000**	**0.702000**	**-0.016000**
C	**-3.833000**	**-0.668000**	**0.006000**
C	**5.319000**	**-1.430000**	**0.021000**
C	**5.535000**	**-2.506000**	**-0.845000**
C	**6.327000**	**-1.088000**	**0.940000**
C	**6.735000**	**-3.226000**	**-0.816000**
H	**4.786000**	**-2.792000**	**-1.574000**
C	**7.512000**	**-1.809000**	**0.969000**
H	**6.169000**	**-0.270000**	**1.631000**
C	**7.733000**	**-2.879000**	**0.098000**
H	**8.283000**	**-1.546000**	**1.684000**
C	**4.850000**	**1.736000**	**-0.032000**
C	**4.770000**	**2.810000**	**0.859000**
C	**5.894000**	**1.716000**	**-0.976000**
C	**5.713000**	**3.845000**	**0.829000**
H	**3.989000**	**2.853000**	**1.608000**
C	**6.822000**	**2.747000**	**-1.005000**
H	**5.960000**	**0.901000**	**-1.685000**
C	**6.748000**	**3.817000**	**-0.109000**
H	**7.620000**	**2.730000**	**-1.739000**
C	**-4.850000**	**-1.736000**	**-0.032000**
C	**-4.770000**	**-2.810000**	**0.859000**
C	**-5.893000**	**-1.716000**	**-0.976000**
C	**-5.713000**	**-3.844000**	**0.829000**
H	**-3.989000**	**-2.853000**	**1.608000**
C	**-6.821000**	**-2.747000**	**-1.005000**
H	**-5.959000**	**-0.901000**	**-1.685000**
C	**-6.748000**	**-3.817000**	**-0.109000**
C	**-5.318000**	**1.430000**	**0.021000**
C	**-5.535000**	**2.506000**	**-0.845000**
C	**-6.327000**	**1.088000**	**0.940000**
C	**-6.735000**	**3.226000**	**-0.815000**
H	**-4.786000**	**2.793000**	**-1.574000**
C	**-7.512000**	**1.809000**	**0.969000**
H	**-6.169000**	**0.270000**	**1.630000**
C	**-7.733000**	**2.879000**	**0.098000**
H	**7.486000**	**4.606000**	**-0.154000**
H	**8.666000**	**-3.424000**	**0.143000**
H	**-7.486000**	**-4.606000**	**-0.154000**
H	**-8.666000**	**3.424000**	**0.143000**
O	**5.533000**	**4.828000**	**1.757000**
O	**6.830000**	**-4.245000**	**-1.718000**
C	**8.027000**	**-5.019000**	**-1.745000**
H	**7.884000**	**-5.758000**	**-2.531000**
H	**8.898000**	**-4.400000**	**-1.983000**
H	**8.193000**	**-5.531000**	**-0.792000**
C	**6.464000**	**5.908000**	**1.792000**
H	**6.462000**	**6.467000**	**0.850000**
H	**6.132000**	**6.559000**	**2.598000**
H	**7.477000**	**5.554000**	**2.005000**

O	**-5.533000**	**-4.828000**	**1.757000**
O	**-6.830000**	**4.245000**	**-1.718000**
C	**-6.465000**	**-5.908000**	**1.792000**
H	**-7.478000**	**-5.553000**	**2.005000**
H	**-6.463000**	**-6.467000**	**0.851000**
H	**-6.133000**	**-6.559000**	**2.599000**
C	**-8.028000**	**5.019000**	**-1.745000**
H	**-8.898000**	**4.399000**	**-1.983000**
H	**-8.194000**	**5.531000**	**-0.792000**
H	**-7.885000**	**5.757000**	**-2.532000**
H	**-8.283000**	**1.546000**	**1.684000**
H	**-7.620000**	**-2.730000**	**-1.739000**

4a at B3LYP/6-311g(d,p) level

C	**0.131000**	**-1.884000**	**0.000000**
C	**-0.411000**	**-0.571000**	**0.000000**
C	**-1.777000**	**-0.369000**	**0.000000**
C	**-2.712000**	**-1.408000**	**0.000000**
C	**-2.194000**	**-2.716000**	**0.000000**
H	**-2.834000**	**-3.587000**	**0.000000**
C	**-0.806000**	**-2.938000**	**0.000000**
H	**-0.450000**	**-3.963000**	**0.000000**
C	**-2.390000**	**0.930000**	**0.000000**
C	**-1.572000**	**2.040000**	**-0.000000**
H	**-1.956000**	**3.051000**	**-0.000000**
C	**0.411000**	**0.571000**	**0.000000**
C	**-0.131000**	**1.884000**	**0.000000**
C	**0.806000**	**2.938000**	**-0.000000**
H	**0.450000**	**3.963000**	**-0.000000**
C	**2.194000**	**2.716000**	**-0.000000**
H	**2.834000**	**3.587000**	**-0.000000**
C	**2.712000**	**1.408000**	**0.000000**
C	**1.777000**	**0.369000**	**0.000000**
C	**1.572000**	**-2.040000**	**0.000000**
H	**1.956000**	**-3.051000**	**0.000000**
C	**2.390000**	**-0.930000**	**0.000000**
C	**-4.038000**	**-0.741000**	**0.000000**
C	**-3.848000**	**0.647000**	**-0.000000**
C	**4.038000**	**0.741000**	**0.000000**
C	**3.848000**	**-0.647000**	**0.000000**
C	**-5.355000**	**-1.316000**	**-0.000000**
C	**-6.484000**	**-0.437000**	**-0.000000**
C	**-7.765000**	**-1.024000**	**-0.000000**
H	**-8.647000**	**-0.397000**	**-0.000000**
C	**-7.959000**	**-2.391000**	**-0.000000**
H	**-8.967000**	**-2.784000**	**-0.000000**
C	**-6.844000**	**-3.249000**	**0.000000**
C	**-5.569000**	**-2.708000**	**0.000000**
H	**-4.740000**	**-3.398000**	**0.001000**
C	**-4.965000**	**1.553000**	**-0.000000**

C	**-4.803000**	**2.952000**	**-0.000000**
H	**-3.822000**	**3.399000**	**0.000000**
C	**-5.888000**	**3.812000**	**-0.001000**
C	**-7.192000**	**3.282000**	**-0.001000**
H	**-8.059000**	**3.927000**	**-0.001000**
C	**-7.367000**	**1.911000**	**-0.001000**
H	**-8.383000**	**1.540000**	**-0.001000**
C	**-6.287000**	**1.005000**	**-0.001000**
C	**5.355000**	**1.316000**	**0.000000**
C	**6.484000**	**0.437000**	**-0.000000**
C	**7.765000**	**1.024000**	**-0.000000**
H	**8.647000**	**0.397000**	**-0.000000**
C	**7.959000**	**2.391000**	**-0.000000**
H	**8.967000**	**2.784000**	**-0.000000**
C	**6.844000**	**3.249000**	**-0.000000**
C	**5.569000**	**2.708000**	**-0.000000**
H	**4.740000**	**3.398000**	**0.000000**
C	**4.965000**	**-1.553000**	**0.000000**
C	**6.287000**	**-1.005000**	**0.000000**
C	**7.367000**	**-1.911000**	**-0.000000**
H	**8.383000**	**-1.540000**	**-0.000000**
C	**7.192000**	**-3.282000**	**0.000000**
H	**8.059000**	**-3.927000**	**-0.000000**
C	**5.888000**	**-3.812000**	**0.000000**
C	**4.803000**	**-2.952000**	**0.001000**
H	**3.822000**	**-3.399000**	**0.001000**
O	**5.601000**	**-5.144000**	**0.001000**
O	**6.921000**	**4.610000**	**-0.000000**
O	**-6.921000**	**-4.610000**	**0.000000**
O	**-5.601000**	**5.144000**	**-0.001000**
C	**-8.210000**	**-5.224000**	**0.000000**
H	**-8.025000**	**-6.296000**	**0.001000**
H	**-8.780000**	**-4.955000**	**0.895000**
H	**-8.780000**	**-4.955000**	**-0.894000**
C	**-6.679000**	**6.079000**	**-0.001000**
H	**-7.301000**	**5.972000**	**0.893000**
H	**-6.216000**	**7.064000**	**-0.001000**
H	**-7.301000**	**5.972000**	**-0.895000**
C	**8.210000**	**5.224000**	**-0.000000**
H	**8.025000**	**6.296000**	**-0.001000**
H	**8.780000**	**4.955000**	**0.894000**
H	**8.780000**	**4.955000**	**-0.895000**
C	**6.679000**	**-6.079000**	**0.001000**
H	**6.216000**	**-7.064000**	**0.001000**
H	**7.301000**	**-5.972000**	**-0.894000**
H	**7.301000**	**-5.972000**	**0.895000**

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