

**Supporting information for**  
**C-H Arylation of Unsubstituted Furan and Thiophene with**  
**Acceptor Bromides: Access to Donor-Acceptor-Donor-Type**  
**Building Blocks for Organic Electronics**

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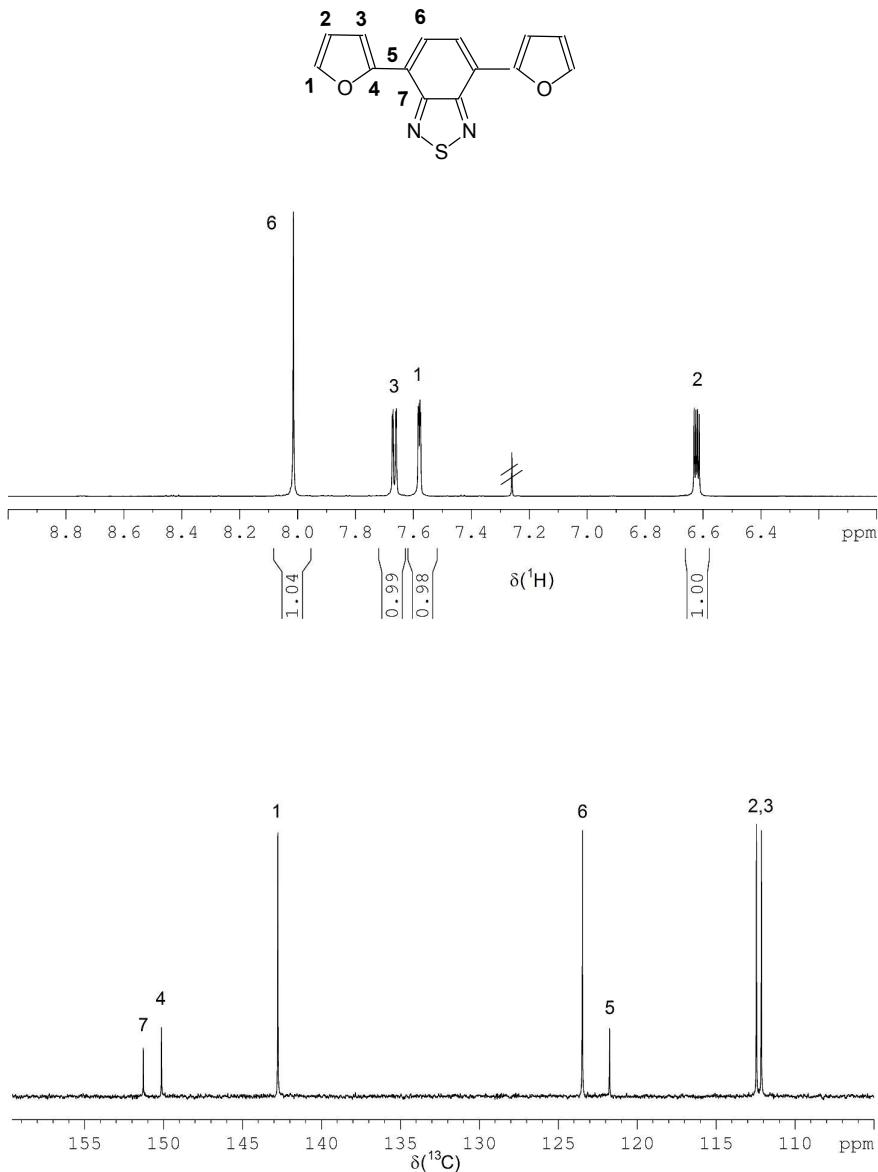
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<sup>⊥</sup>Universität Freiburg, Freiburger Materialforschungszentrum (FMF), Stefan-Meier-Str. 21, 79104 Freiburg, Germany

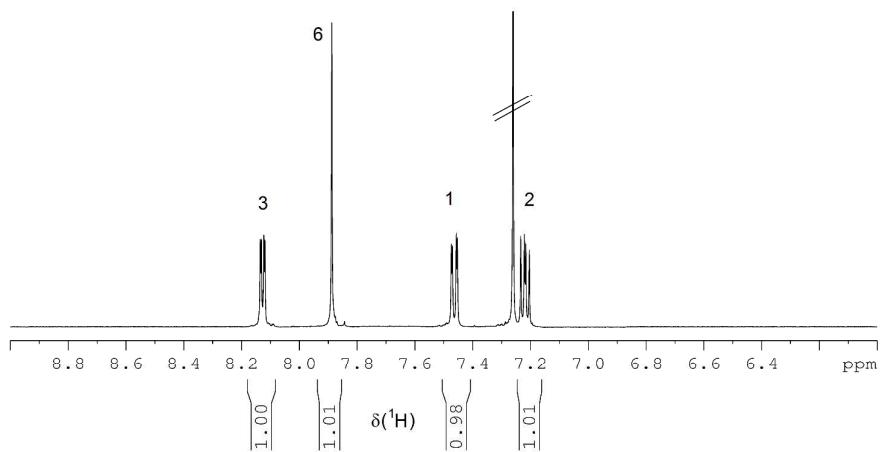
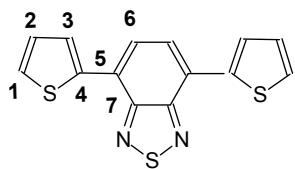
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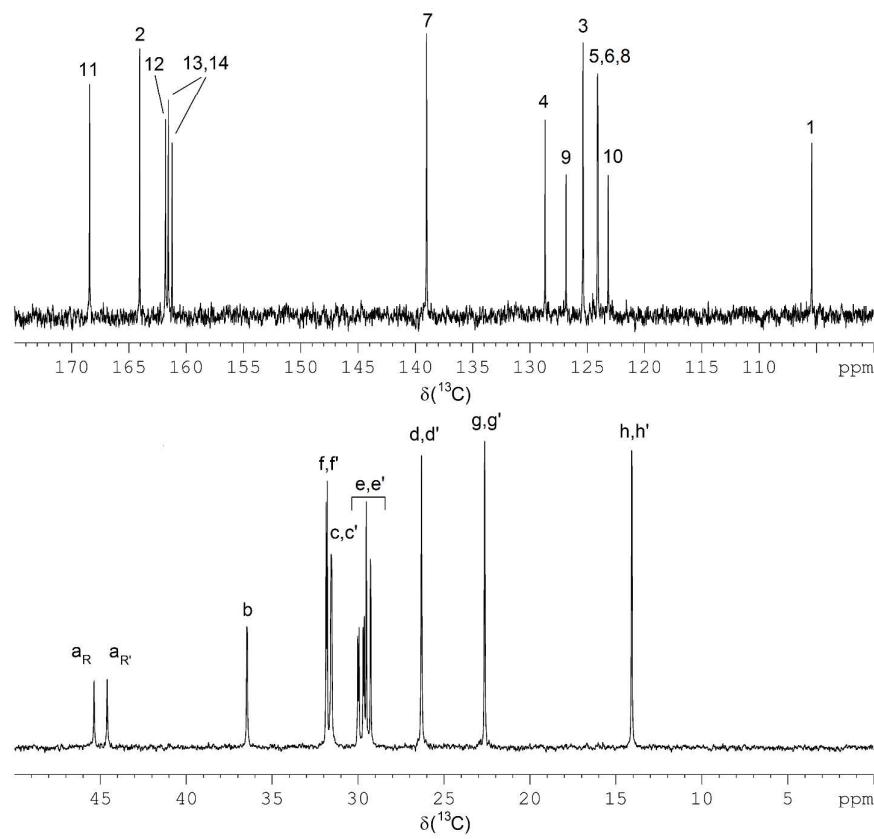
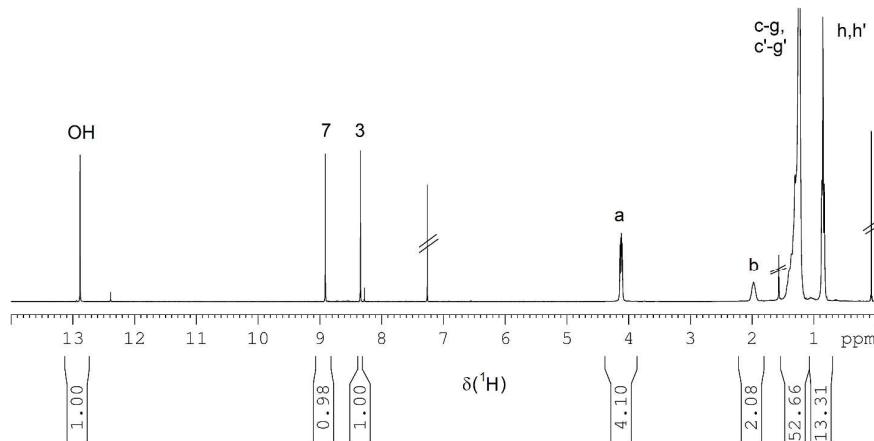
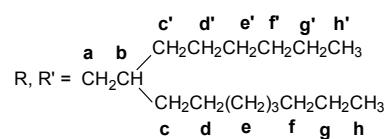
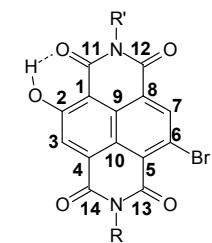
**4,7-Bis(2-furanyl) 2,1,3-benzothiadiazole (BTFu<sub>2</sub>)**



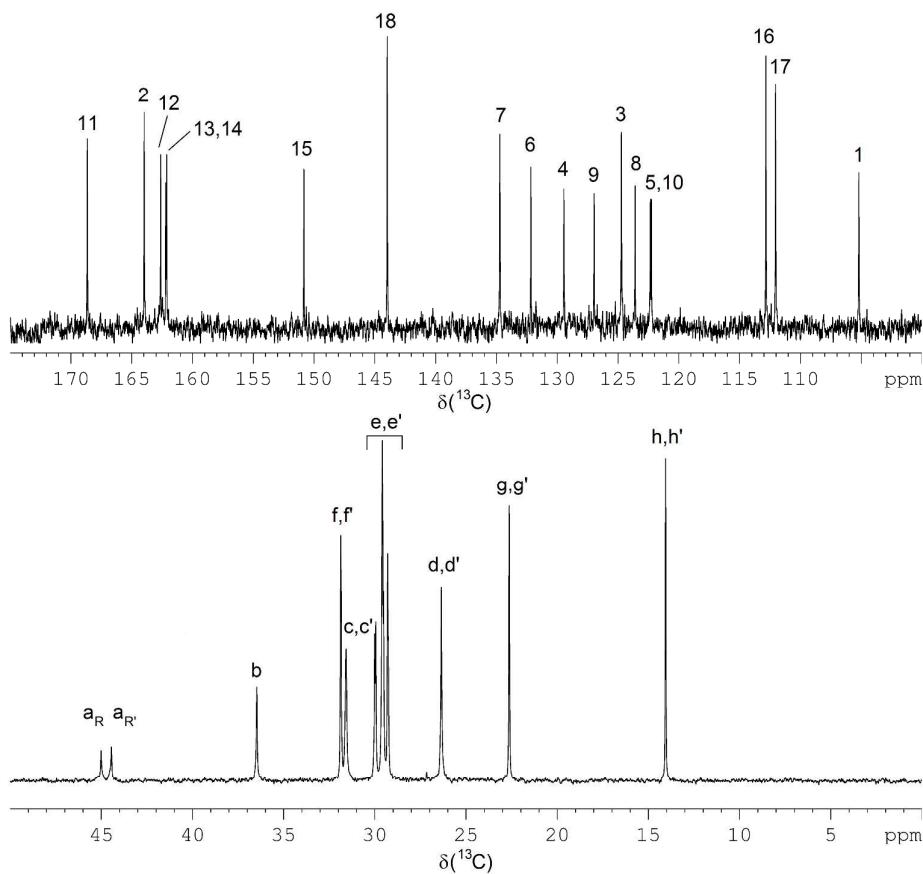
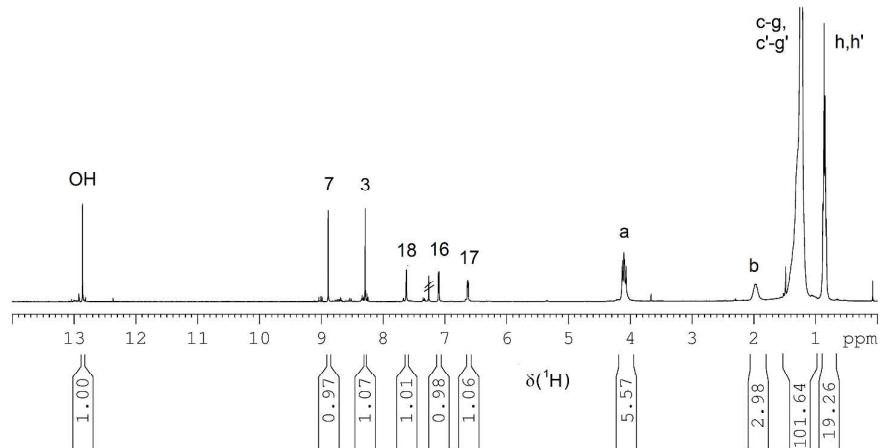
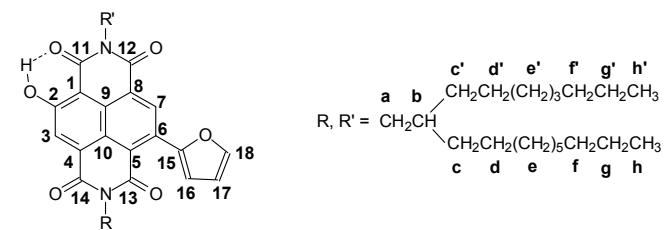
**4,7-Bis(2-thienyl) 2,1,3-benzothiadiazole (BTTh<sub>2</sub>)**



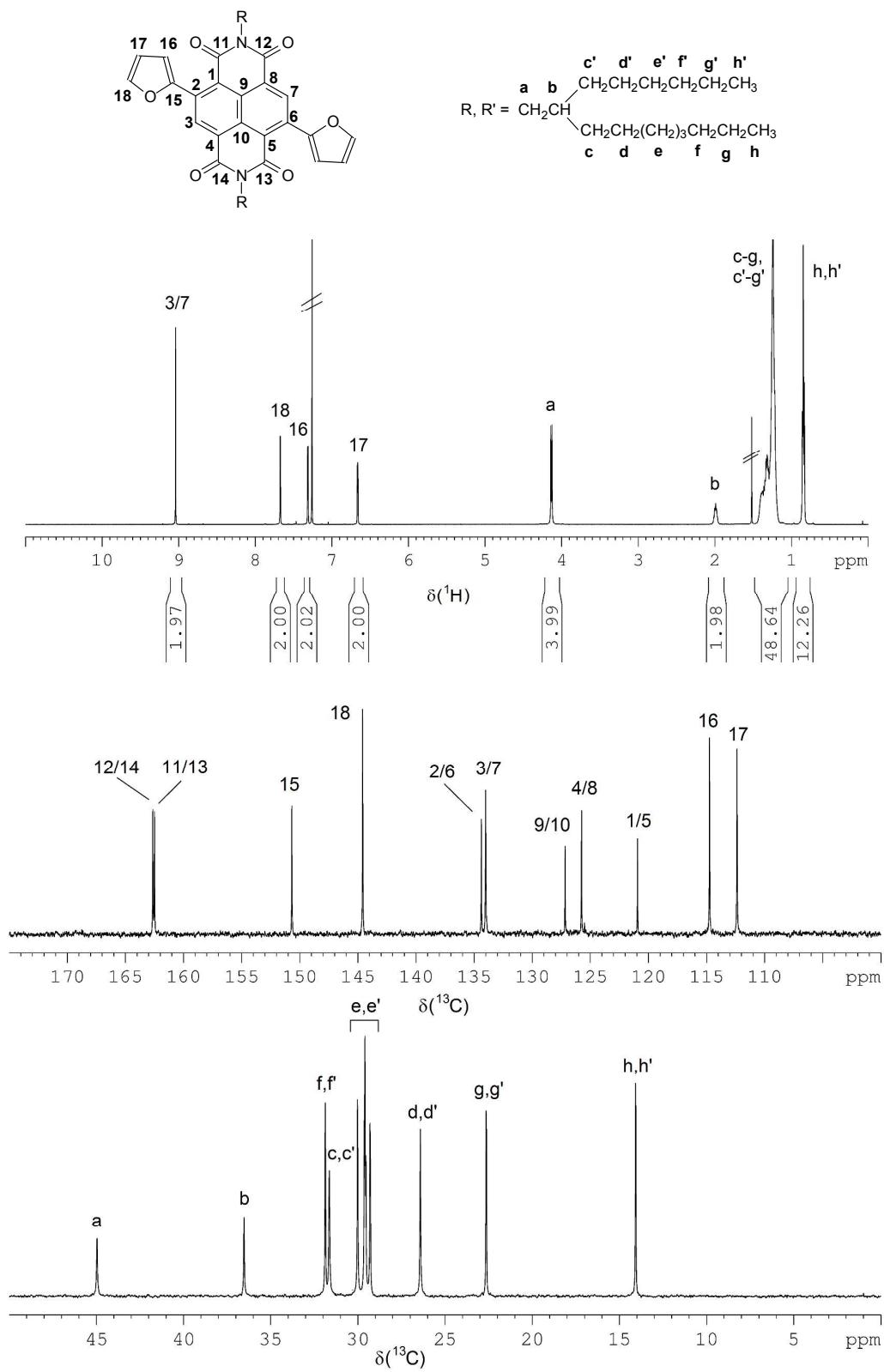
**2-Hydroxy-6-bromonaphthalene-1,4,5,8-tetracarboxylic-N,N'-bis(2-hexyldecyl) diimide  
(HO-NDI-Br)**



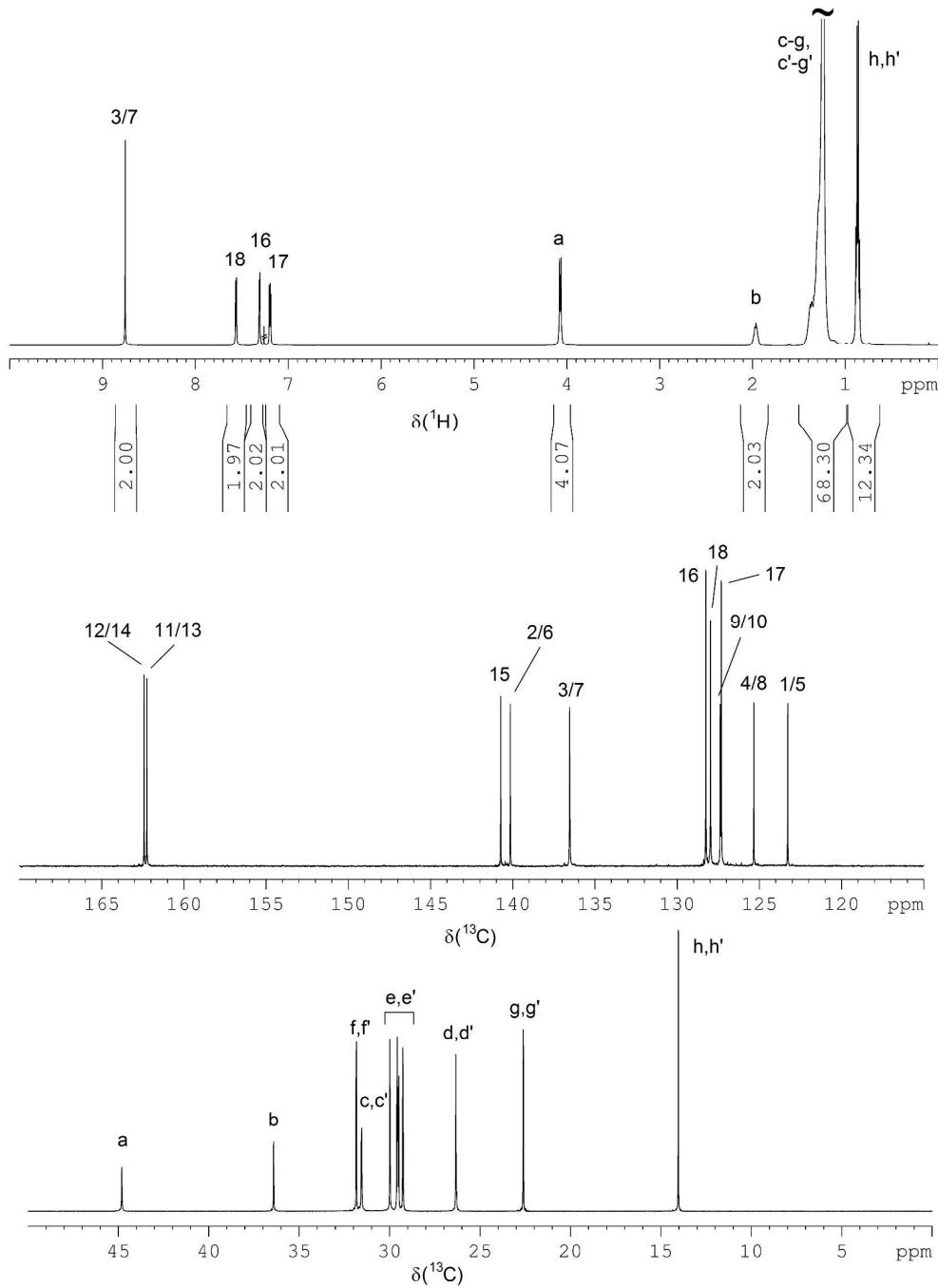
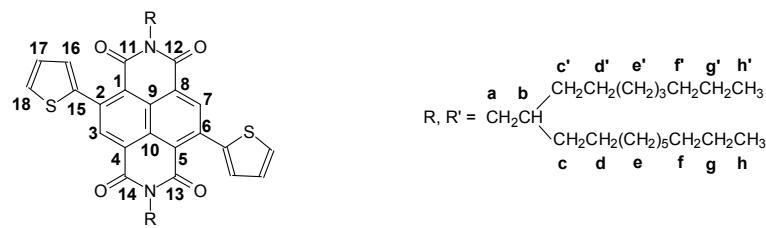
**2-Hydroxy-6-(2-furanyl)naphthalene-1,4,5,8-tetracarboxylic-N,N'-bis(2-octyldodecyl) diimide (HO-NDI-Fu)**



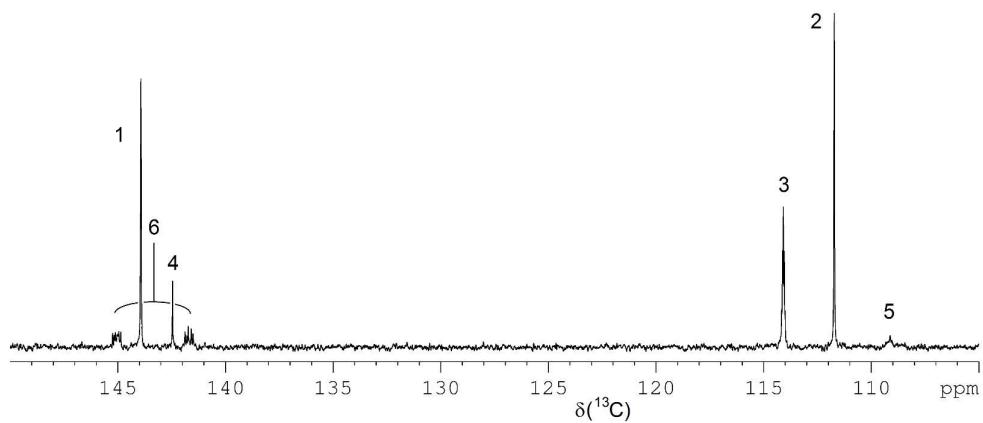
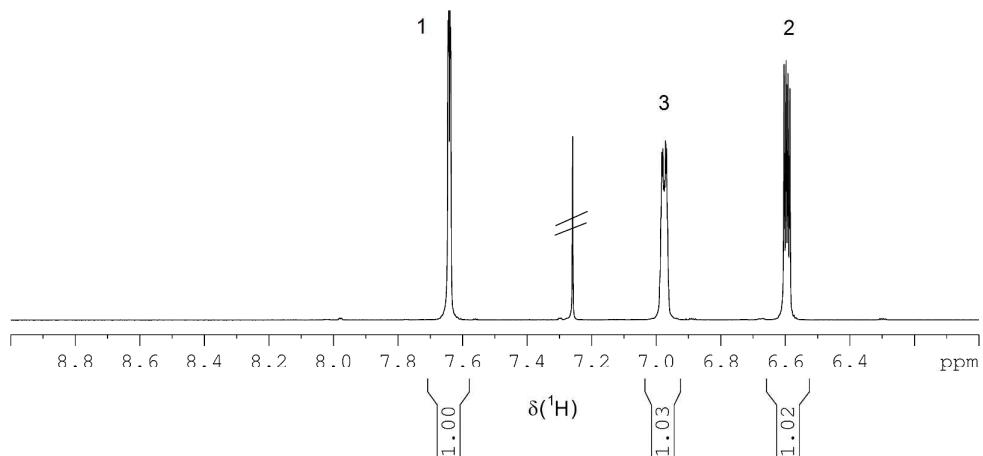
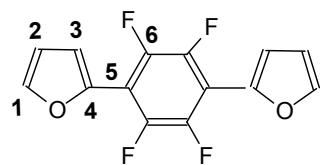
**2,6-Bis(2-furanyl)naphthalene-1,4,5,8-tetracarboxylic-*N,N'*-bis(2-hexyldecyl)diimide  
(NDIFu<sub>2</sub>)**



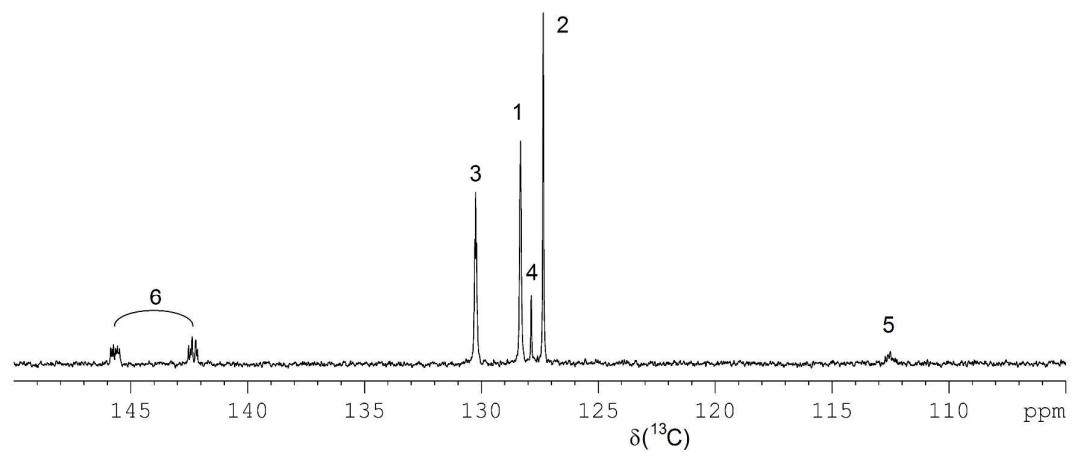
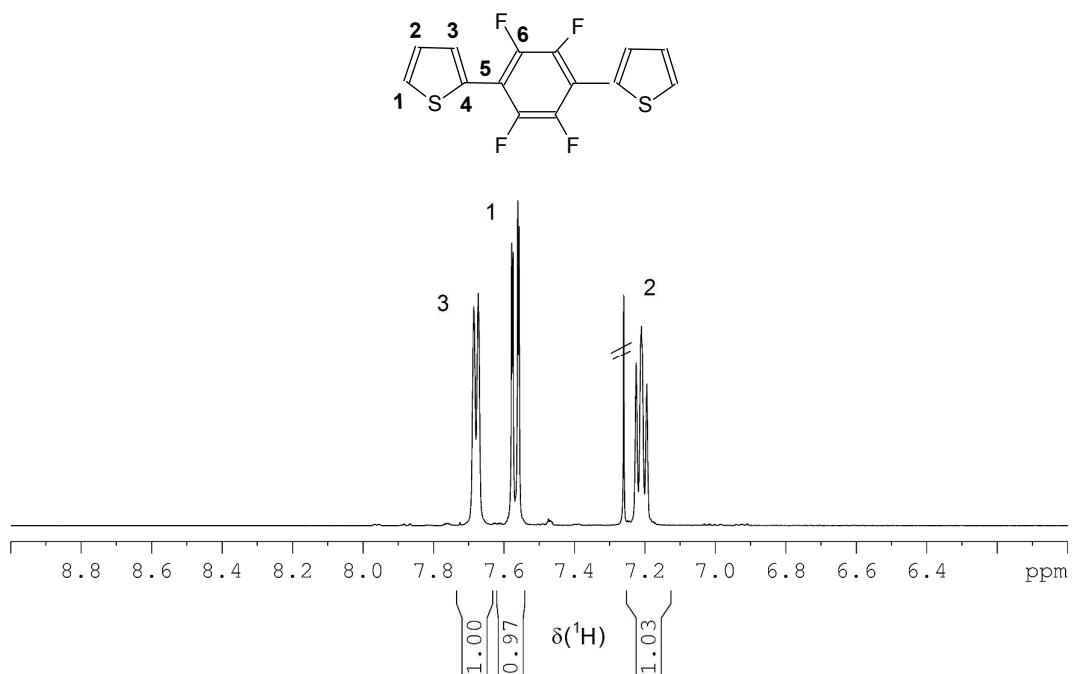
**2,6-Bis(2-thienyl)naphthalene-1,4,5,8-tetracarboxylic-*N,N'*-bis(2-octyldodecyl)diimide  
(NDITH<sub>2</sub>)**



**1,4-Bis(2-furanyl)-2,3,5,6-tetrafluorobenzene ( $F_4Fu_2$ )**



**1,4-Bis(2-thienyl)-2,3,5,6-tetrafluorobenzene ( $F_4Th_2$ )**



<sup>1</sup> Guo, X.; Watson, M. D. *Org. Lett.* **2008**, 10 (23), 5333.

## DFT (B3LYP/6-31G\*\*) NDIFu<sub>2</sub> optimized molecular structure

Atom type / x, y, z Cartesian coordinates

C	-5.106506	0.196127	0.447679
C	-4.017403	-0.528930	0.012080
O	-4.472679	-1.770999	-0.406325
C	-5.813034	-1.801872	-0.239077
C	-6.256128	-0.626291	0.290892
C	-2.557465	-0.413158	-0.007544
C	-1.752513	0.752774	-0.001621
C	-0.329028	0.631699	0.000871
C	0.329027	-0.631695	-0.001205
C	-0.504615	-1.779198	-0.007457
C	-1.873518	-1.661789	-0.016425
C	1.752491	-0.752762	0.001405
C	2.327470	-2.123794	0.050137
N	1.451309	-3.220782	0.074328
C	0.060171	-3.149616	0.023844
C	0.504604	1.779199	0.006950
C	1.873524	1.661784	0.016046
C	2.557463	0.413155	0.007513
C	-2.327469	2.123840	-0.050658
N	-1.451307	3.220810	-0.074660
C	-0.060150	3.149614	-0.024681
C	2.081152	-4.545864	0.129133
O	-0.637545	-4.154524	0.014676
O	3.528694	-2.357929	0.078806
C	4.017378	0.528878	-0.011481
O	-3.528669	2.358011	-0.079701
C	-2.081123	4.545901	-0.129571
O	0.637593	4.154508	-0.016013
H	2.443999	2.579855	0.013033
H	-2.698212	4.624829	-1.026369
H	-2.724119	4.688280	0.741199
H	-1.285070	5.285568	-0.142836
H	1.285077	-5.285439	0.145831
H	2.721371	-4.689744	-0.743478
H	2.701059	-4.623400	1.024064
H	-2.444017	-2.579845	-0.013555
H	-5.079038	1.199900	0.828681
H	-7.277400	-0.370091	0.531763
C	5.106716	-0.196137	-0.446561
C	6.256240	0.626243	-0.289178
C	5.812839	1.801830	0.240594
O	4.472457	1.770969	0.407170
H	5.079409	-1.199906	-0.827589
H	7.277641	0.370083	-0.529531
H	6.304703	2.710385	0.552763
H	-6.304966	-2.710586	-0.550660

## DFT (B3LYP/6-31G\*\*) NDITh<sub>2</sub> optimized molecular structure

Atom type / x, y, z Cartesian coordinates

S	-4.940840	-1.511308	0.797737
C	-4.029180	-0.332806	-0.139027
C	-4.880040	0.368392	-0.962253
C	-6.239688	-0.024713	-0.847432
C	-6.429724	-1.022310	0.071916
C	-2.558791	-0.320838	-0.047826
C	-1.721007	0.813299	0.002327
C	-0.303406	0.645195	0.008882
C	0.303379	-0.644940	-0.009210
C	-0.565355	-1.764415	-0.029627
C	-1.931030	-1.595006	-0.045844
C	0.565353	1.764649	0.029448
C	1.931048	1.595226	0.045847
C	2.558723	0.321061	0.047737
C	1.720955	-0.813044	-0.002718
C	-0.040861	-3.151868	-0.070066
N	1.346562	-3.268899	-0.136380
C	2.262413	-2.201509	-0.131053
C	-2.262424	2.201808	0.130141
N	-1.346523	3.269145	0.136219
C	0.040898	3.152102	0.070019
C	4.029091	0.332787	0.139403
C	4.879379	-0.368344	0.963241
C	6.239208	0.024297	0.848742
C	6.429863	1.021491	-0.070909
S	4.941359	1.510582	-0.797490
O	-3.449611	2.465607	0.239458
C	-1.929567	4.612996	0.239112
O	0.773361	4.131663	0.060677
O	3.449525	-2.465151	-0.241380
C	1.929607	-4.612735	-0.239471
O	-0.773301	-4.131441	-0.060545
H	-2.539504	-2.490594	-0.092405
H	2.482445	-4.706150	-1.176171
H	2.625464	-4.777444	0.585141
H	1.112629	-5.328335	-0.202359
H	-1.112519	5.328550	0.202701
H	-2.624833	4.777901	-0.585961
H	-2.483063	4.706264	1.175436
H	2.539552	2.490786	0.092619
H	4.536702	-1.148189	1.629179
H	7.043831	-0.420779	1.422224
H	-4.537858	1.148646	-1.627938
H	-7.044660	0.420412	-1.420384
H	-7.356982	-1.486850	0.377191
H	7.357380	1.485595	-0.376059