Supporting Information

(Oligo-)Thiophene Functionalized Tetraazaperopyrenes: Donor-Acceptor Dyes and Ambipolar Organic Semiconductors

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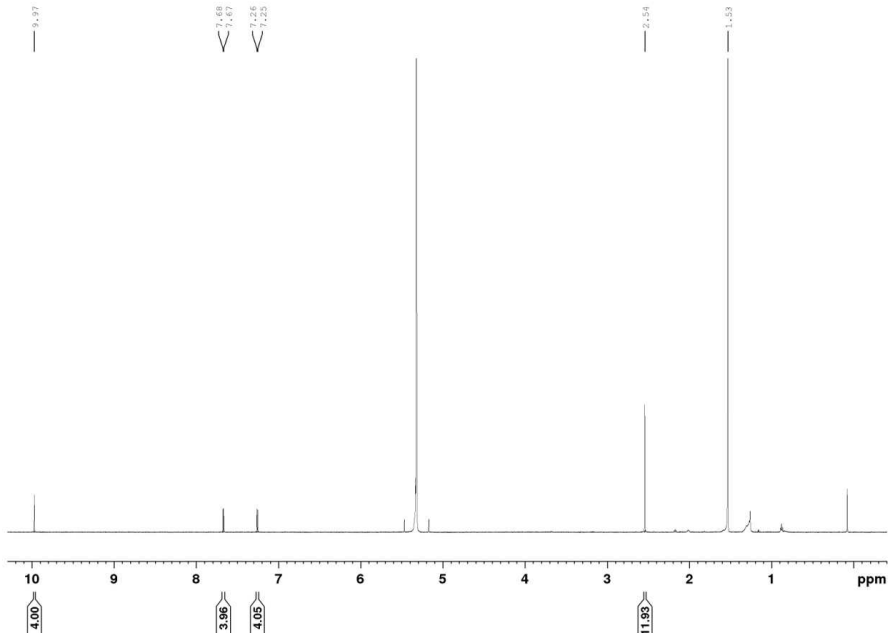
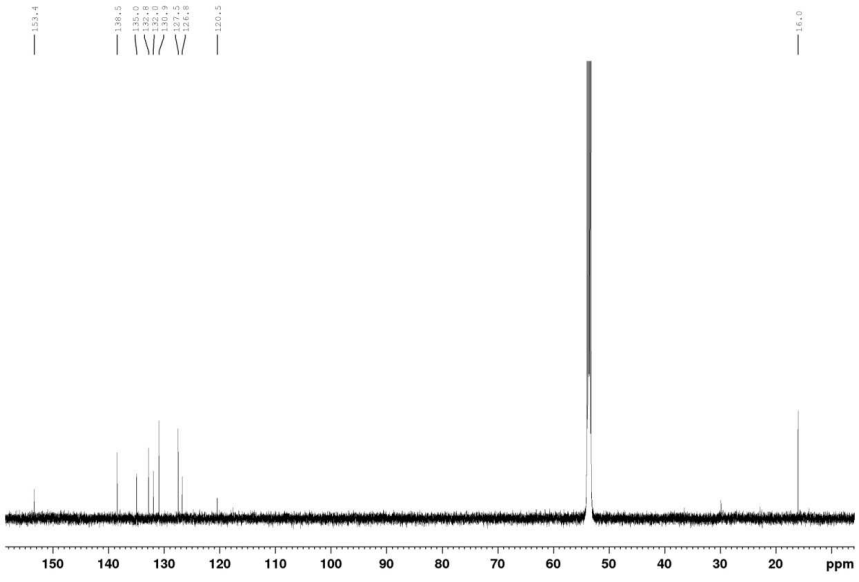
The ^{1}H, ^{13}C and ^{19}F NMR Spectra of Compounds 2-5, 8-12

Compound 2:

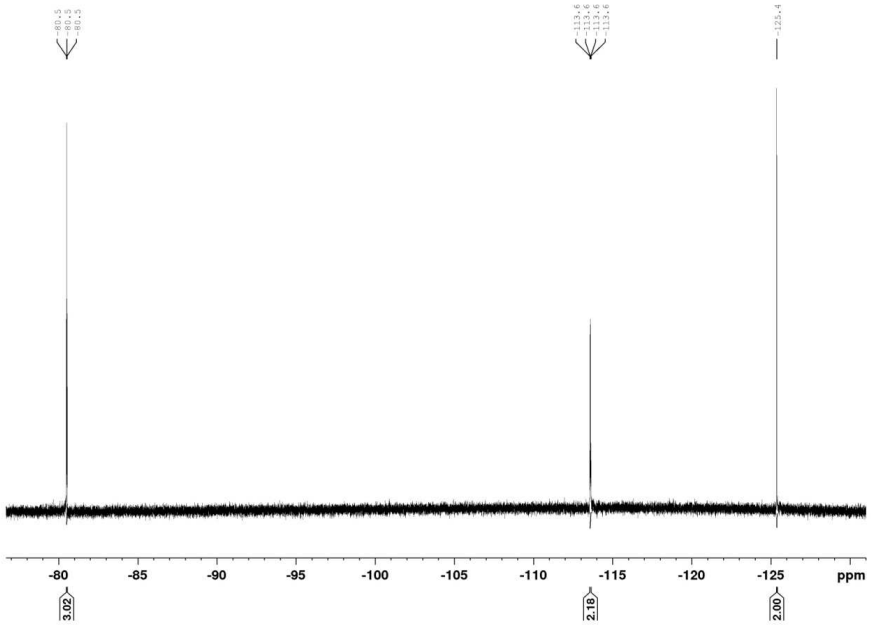
^{1}H-NMR (600.13 MHz, CD_2Cl_2, 295 K):



^{13}C-NMR (150.90 MHz, CD_2Cl_2, 295 K):

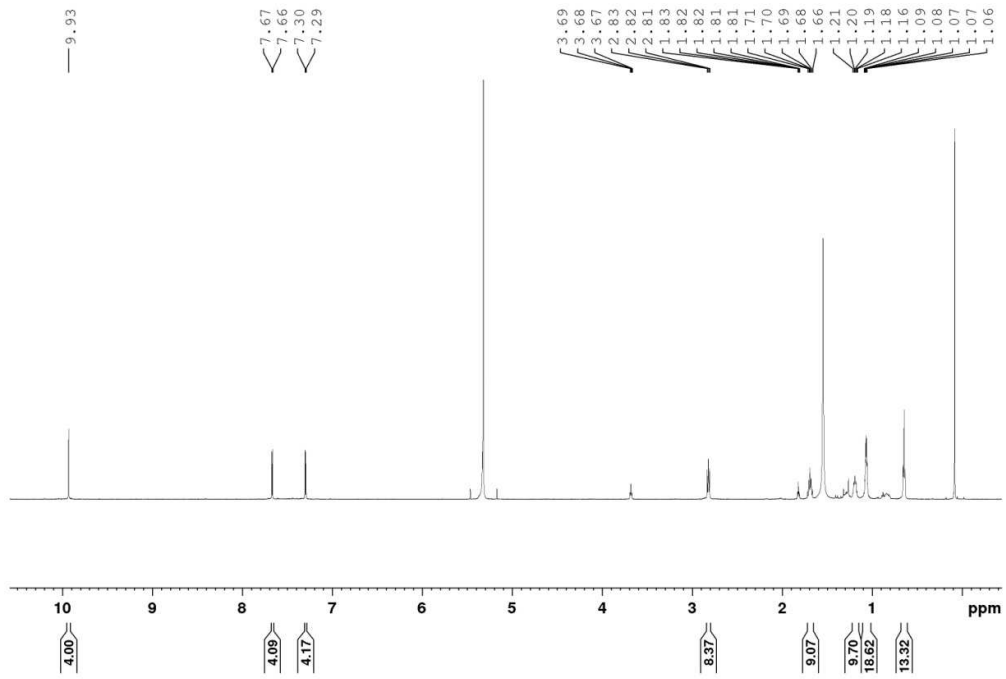


^{19}F-NMR (376.27 MHz, CD_2Cl_2, 295 K):

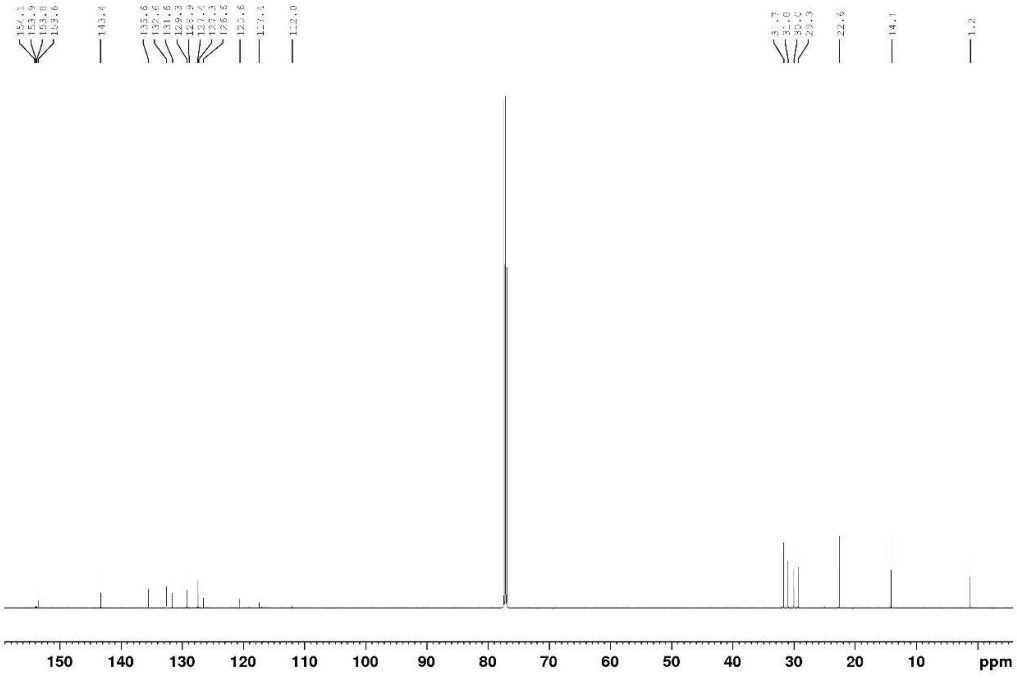


Compound 3:

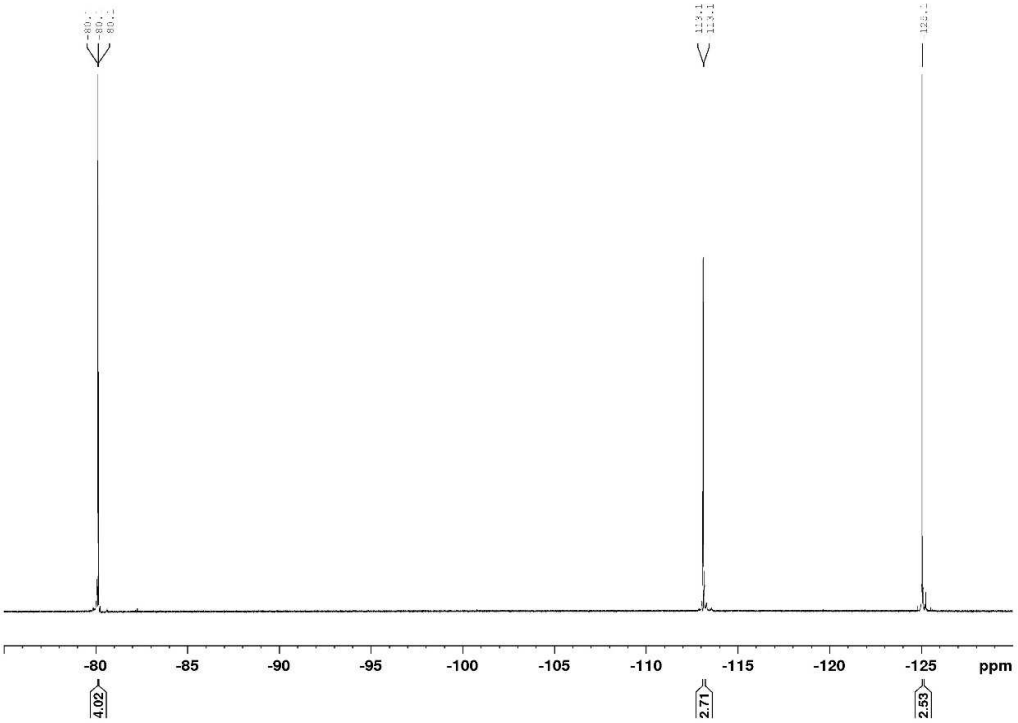
^{1}H-NMR (600.13 MHz, CD_2Cl_2, 295 K):



^{13}C-NMR (150.90 MHz, CD_2Cl_2, 295 K):

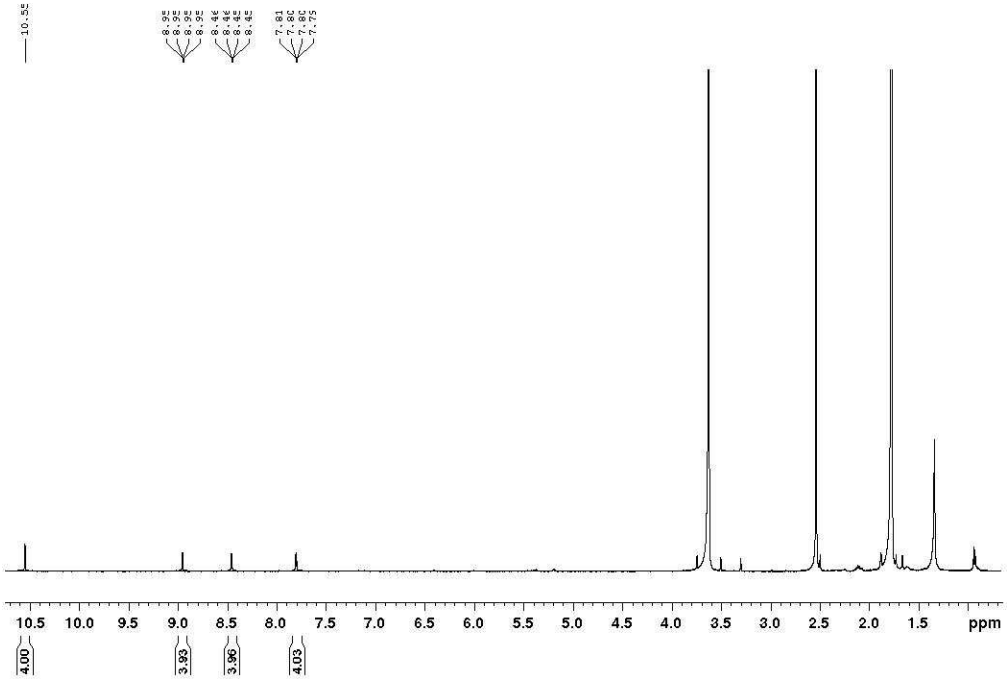


^{19}F-NMR (376.27 MHz, CD_2Cl_2, 295 K):

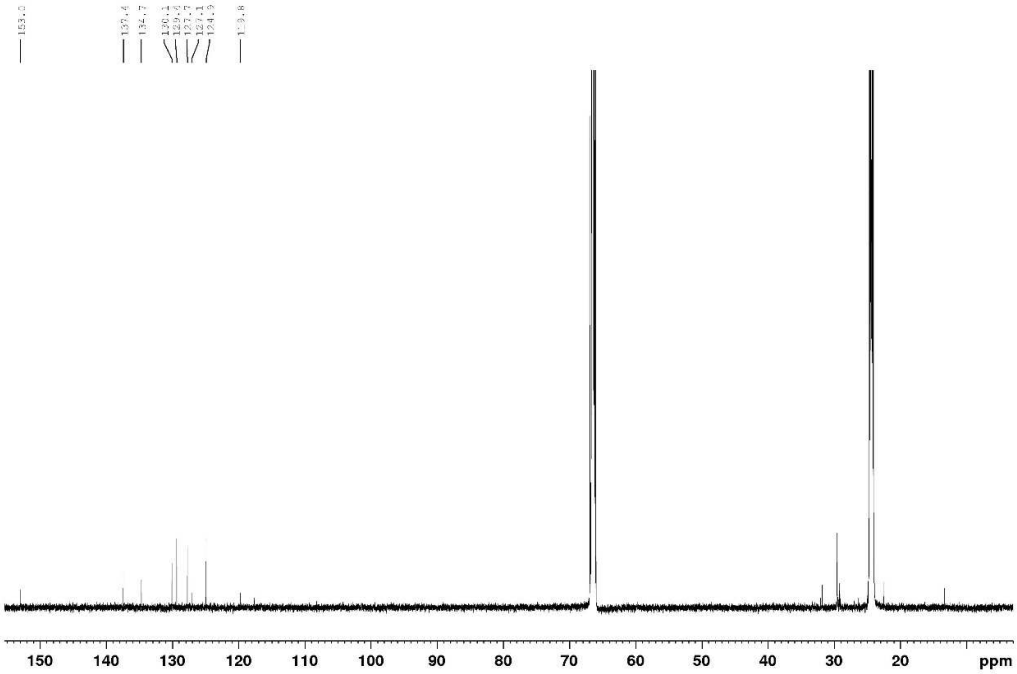


Compound 4:

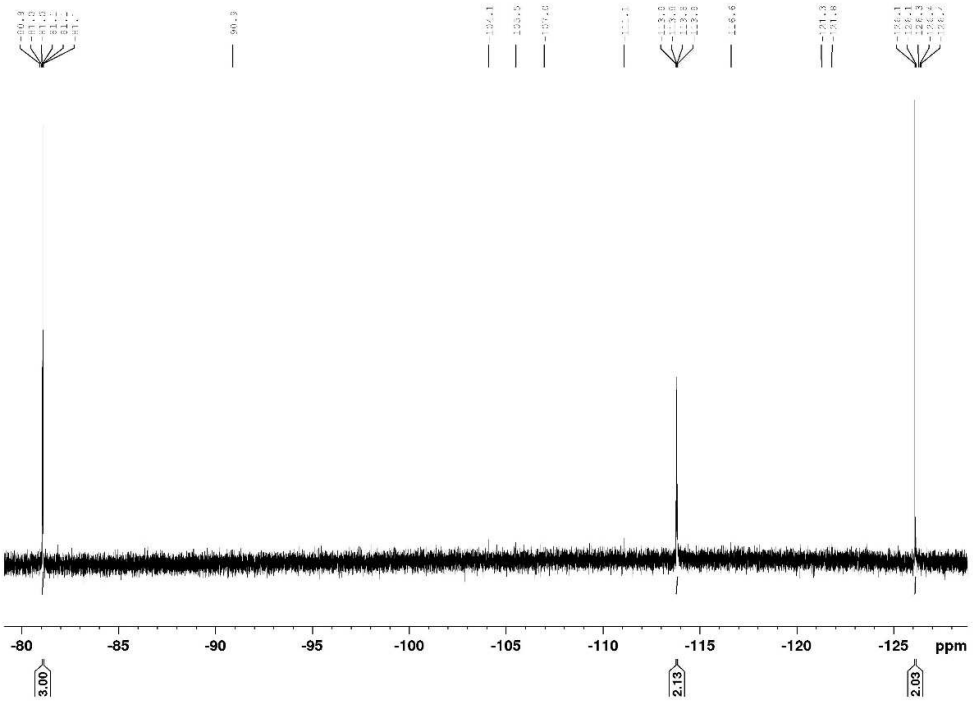
^{1}H-NMR (600.13 MHz, THF-d_8, 295 K):



^{13}C-NMR (150.90 MHz, THF-d_8, 295 K):

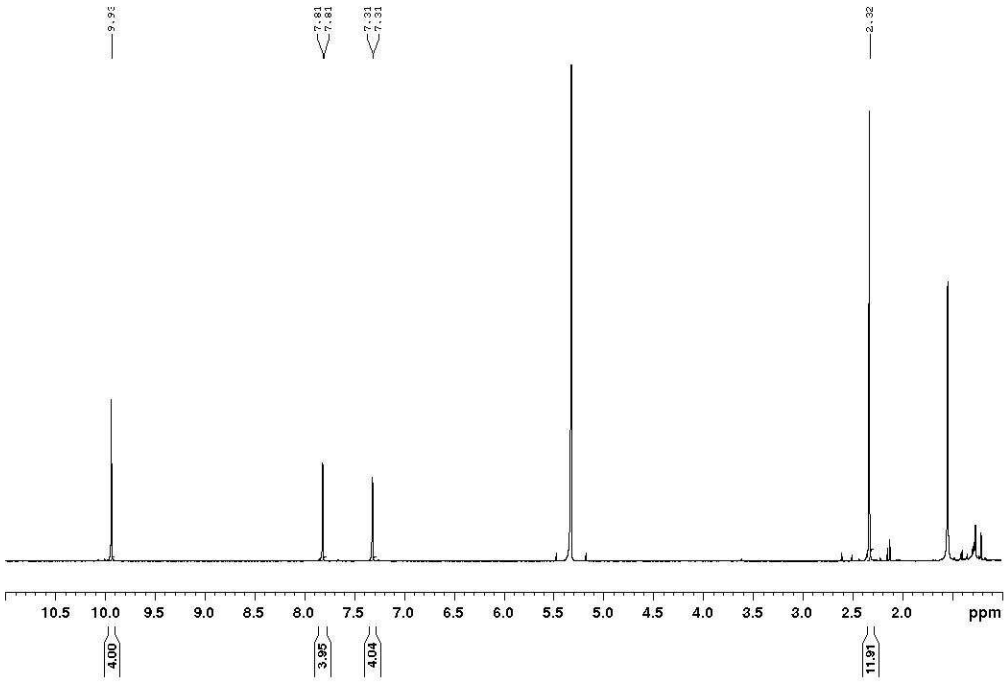


^{19}F-NMR (376.27 MHz, THF-d_8, 295 K):

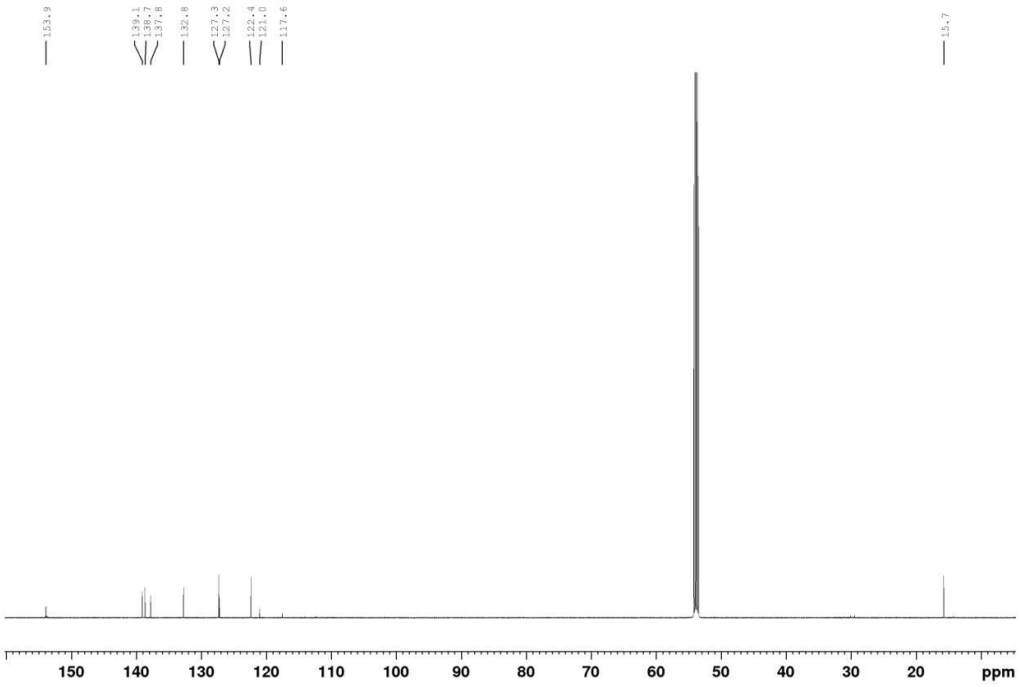


Compound 5:

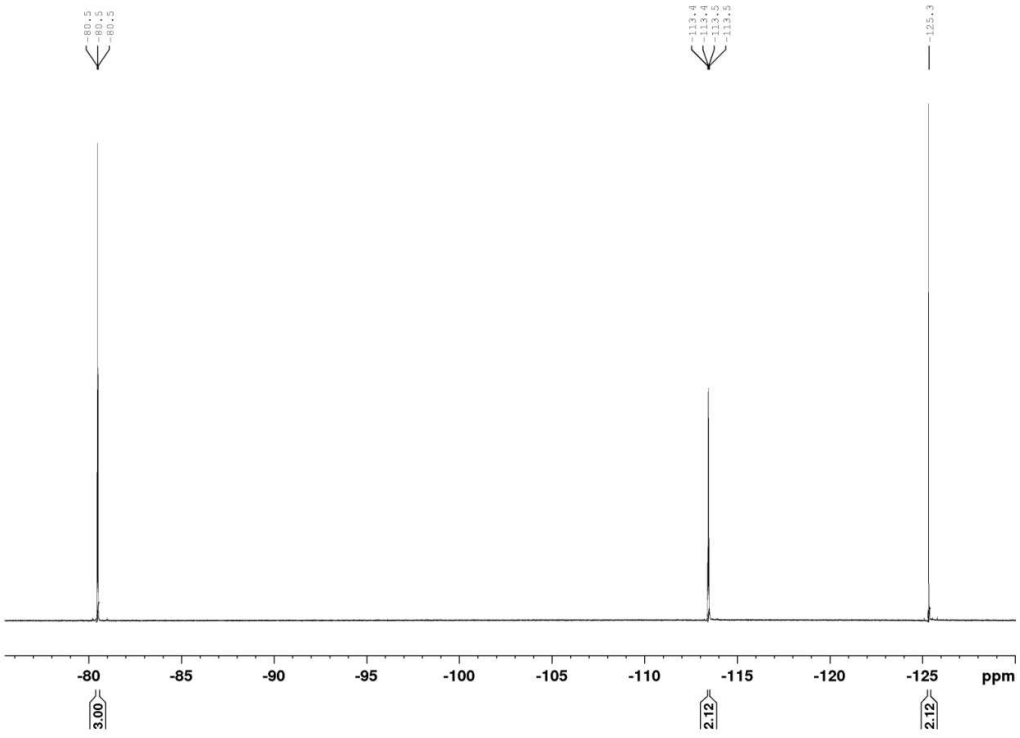
^{1}H-NMR (600.13 MHz, CD_2Cl_2, 295 K):



^{13}C-NMR (150.90 MHz, CD_2Cl_2, 295 K):

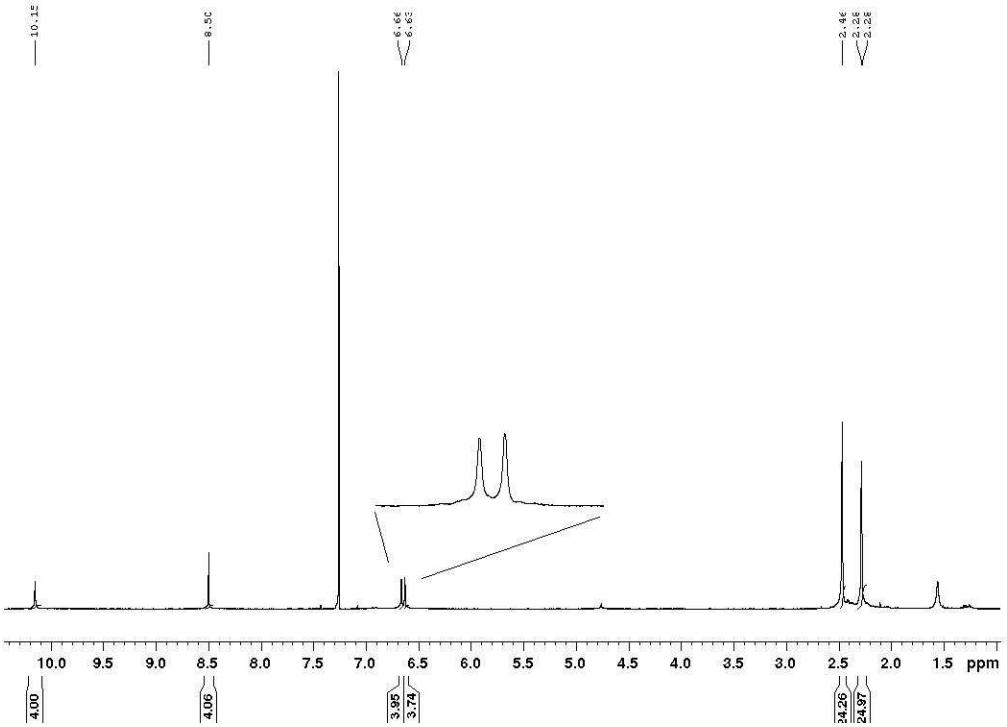


^{19}F-NMR (376.27 MHz, CD_2Cl_2, 295 K):

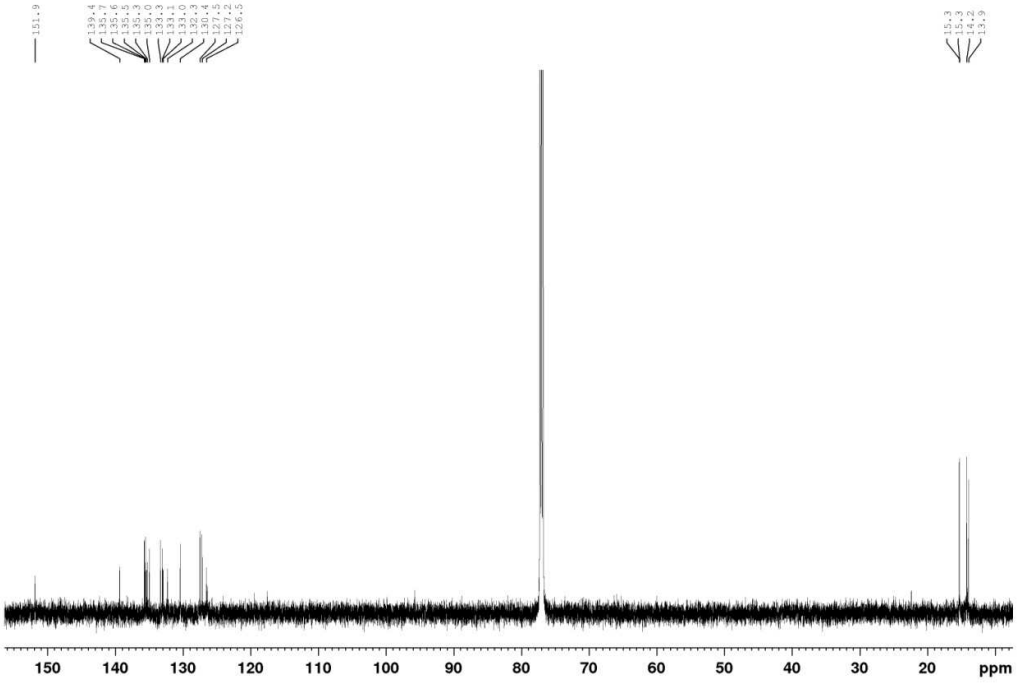


Compound 8:

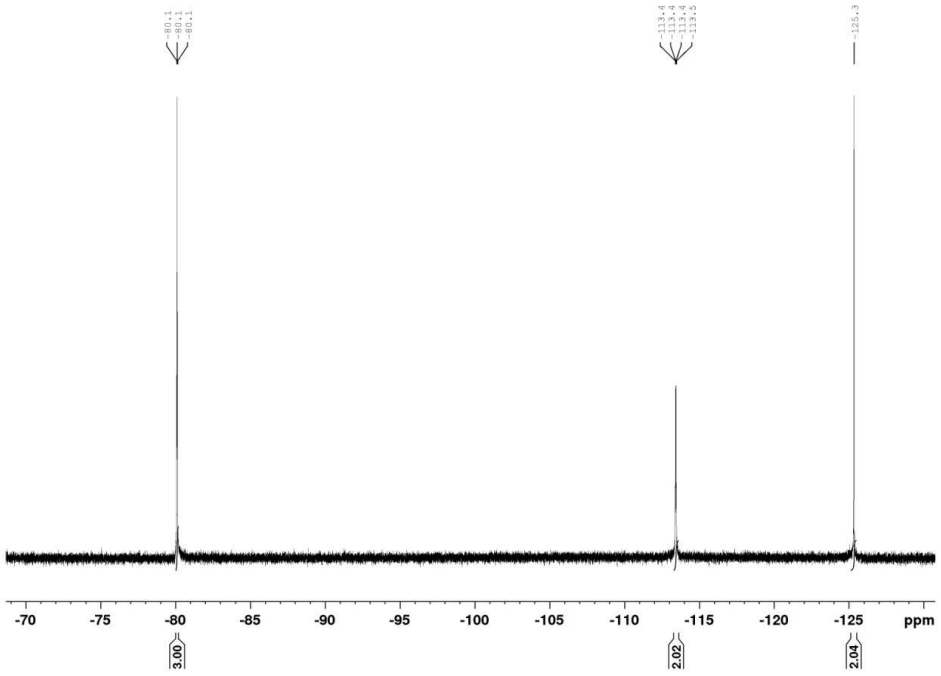
^{1}H-NMR (600.13 MHz, $CDCl_3$, 295 K):



^{13}C-NMR (150.90 MHz, $CDCl_3$, 295 K):

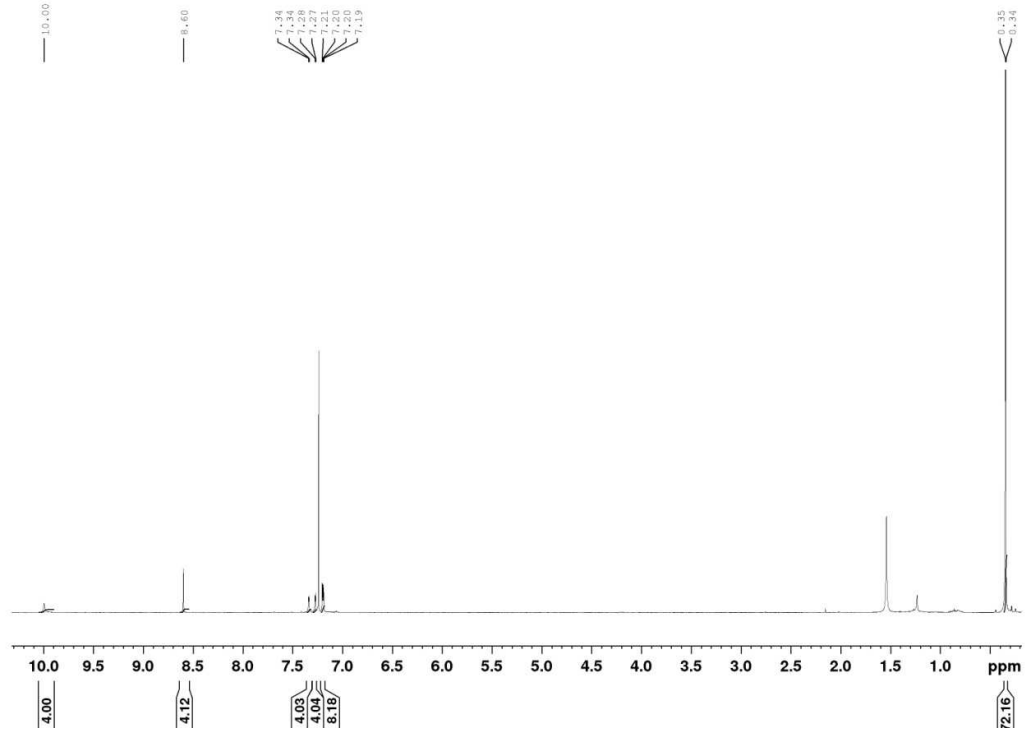


^{19}F-NMR (376.27 MHz, $CDCl_3$, 295 K):

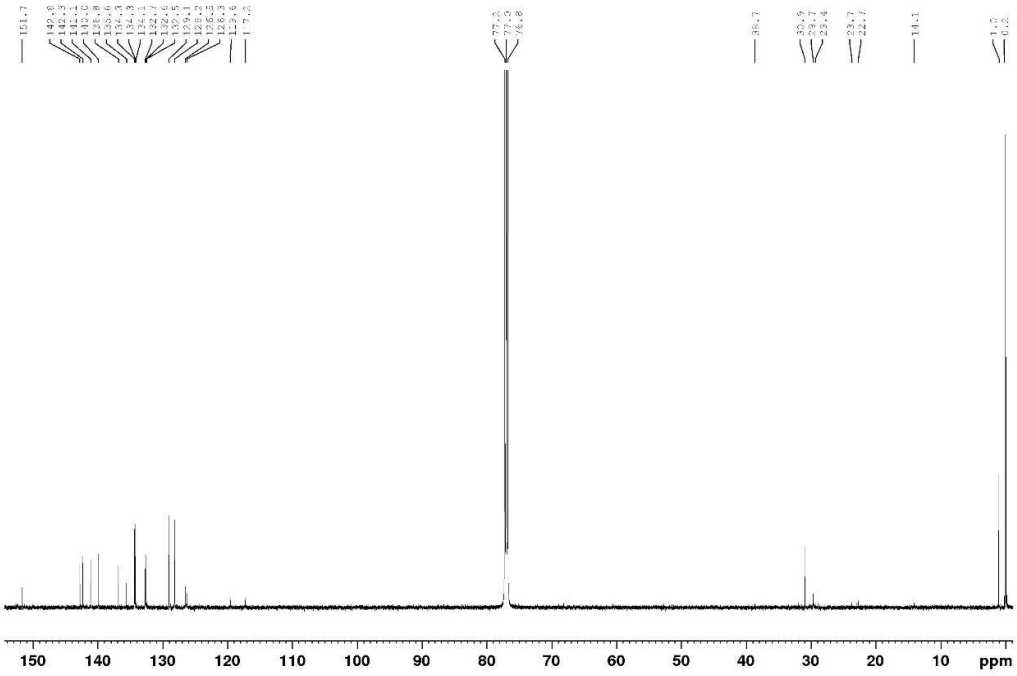


Compound 9:

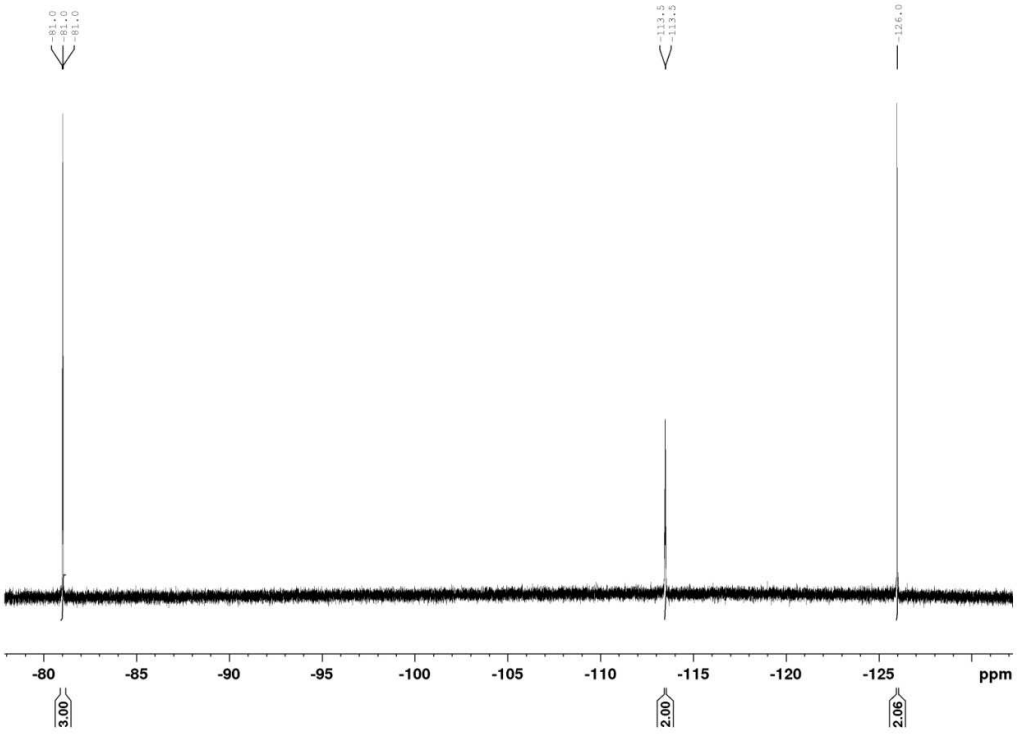
^{1}H-NMR (600.13 MHz, $CDCl_3$, 295 K):



^{13}C-NMR (150.90 MHz, $CDCl_3$, 295 K):

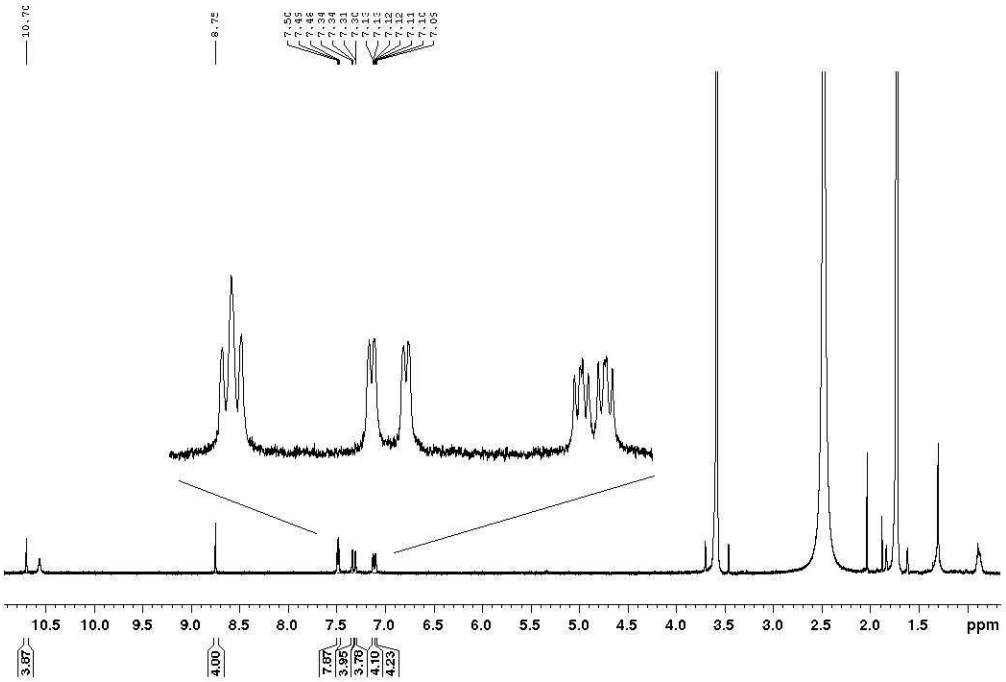


^{19}F-NMR (376.27 MHz, $CDCl_3$, 295 K):

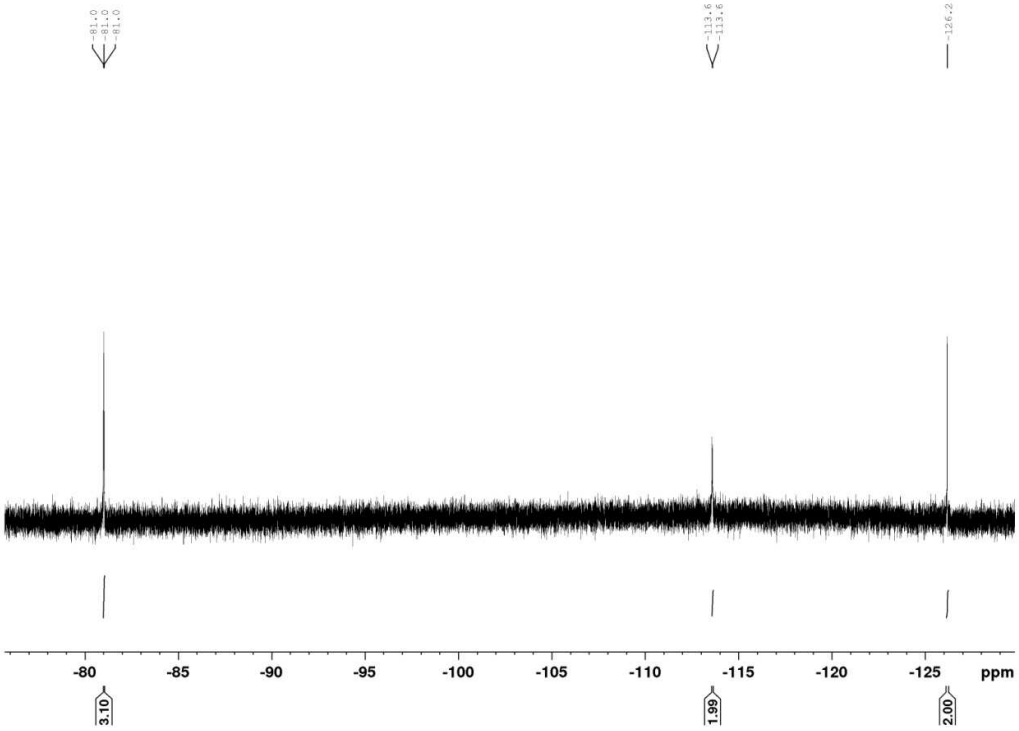


Compound 10:

^{1}H-NMR (600.13 MHz, THF-d_8, 295 K):

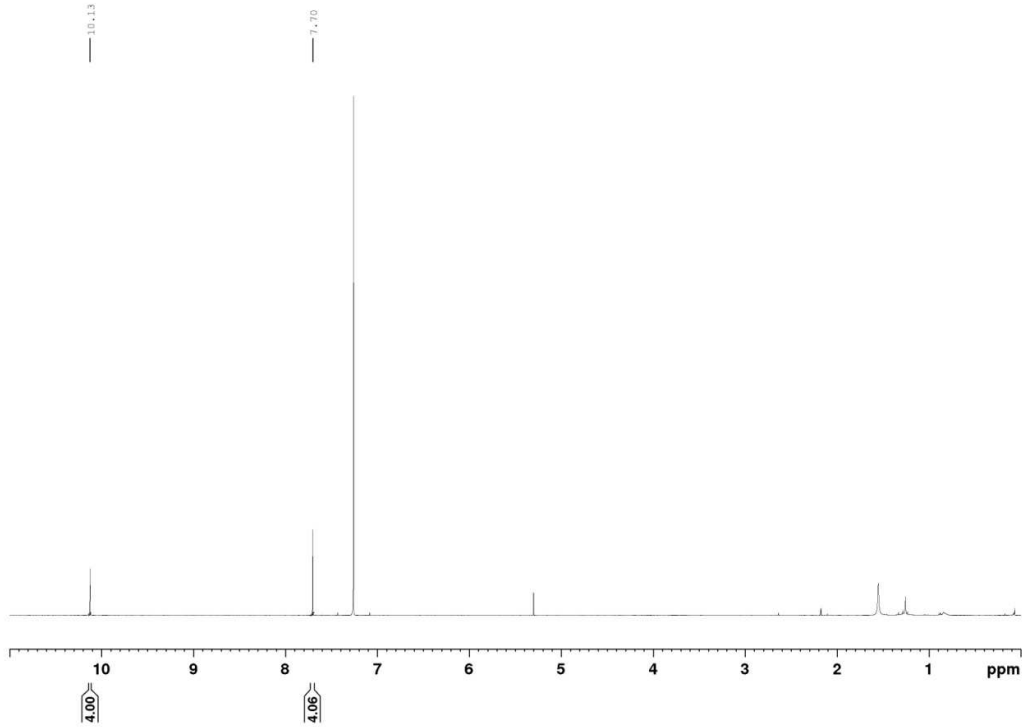


^{19}F-NMR (376.27 MHz, THF-d_8, 295 K):

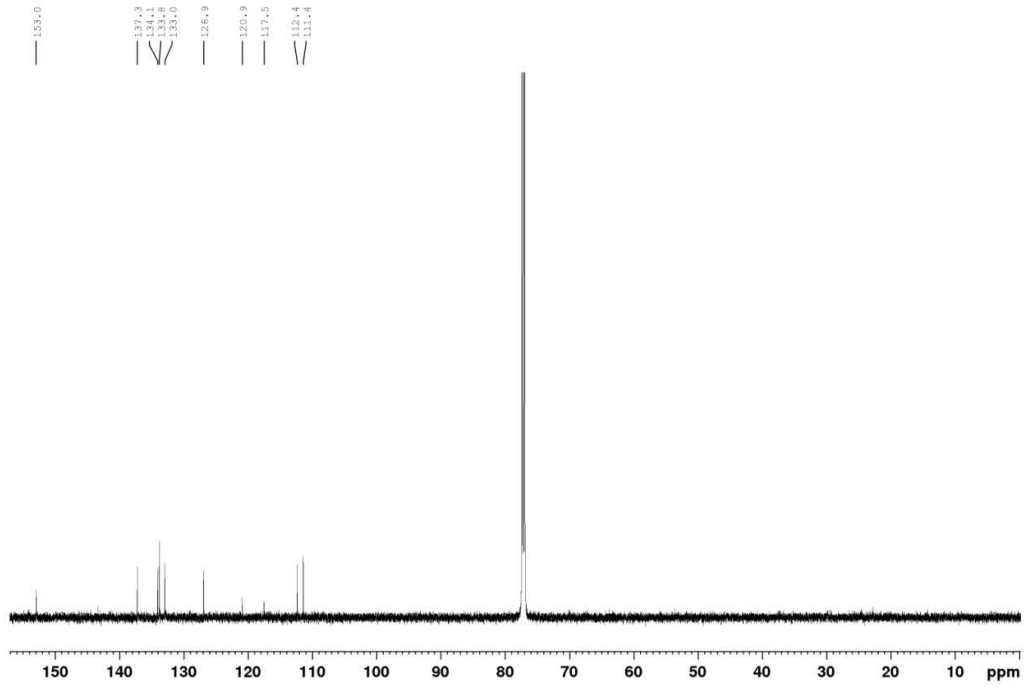


Compound 11:

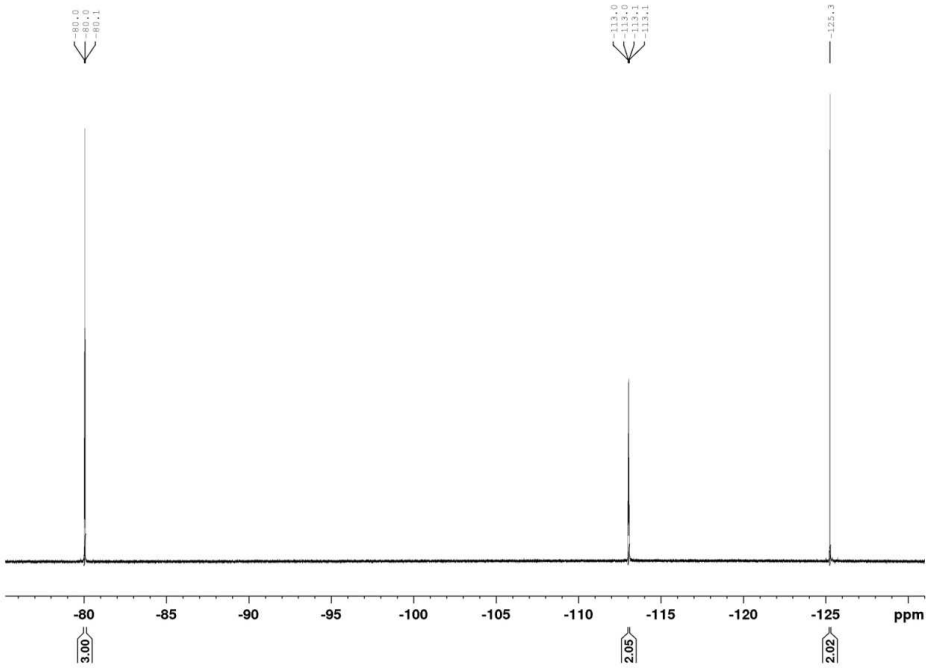
^{1}H-NMR (600.13 MHz, $CDCl_3$, 295 K):



^{13}C-NMR (150.90 MHz, $CDCl_3$, 295 K):

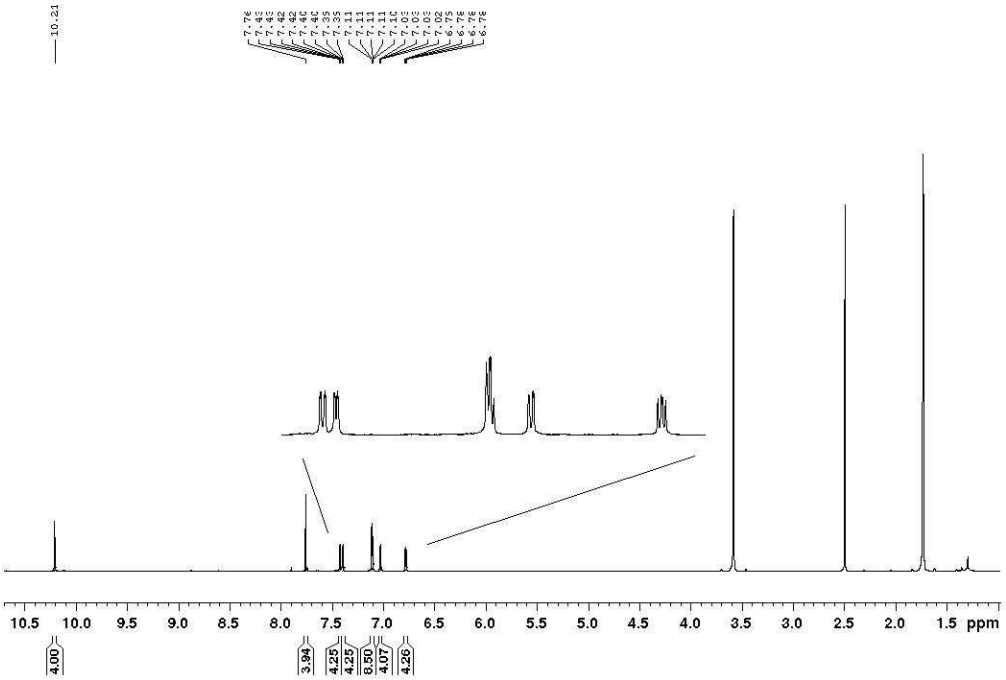


^{19}F-NMR (376.27 MHz, $CDCl_3$, 295 K):

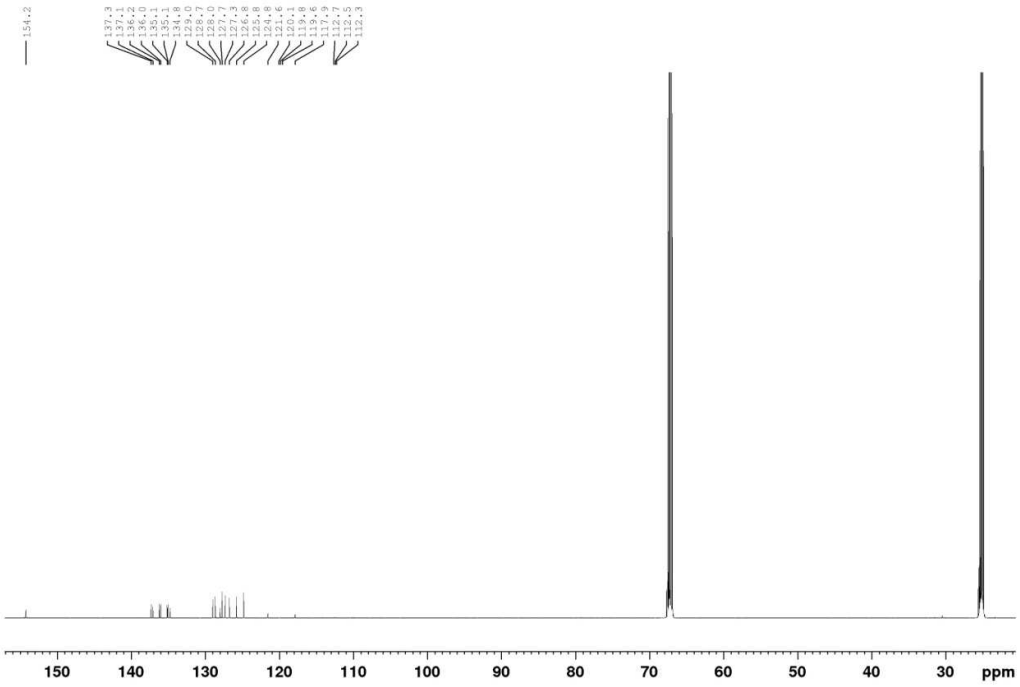


Compound 12:

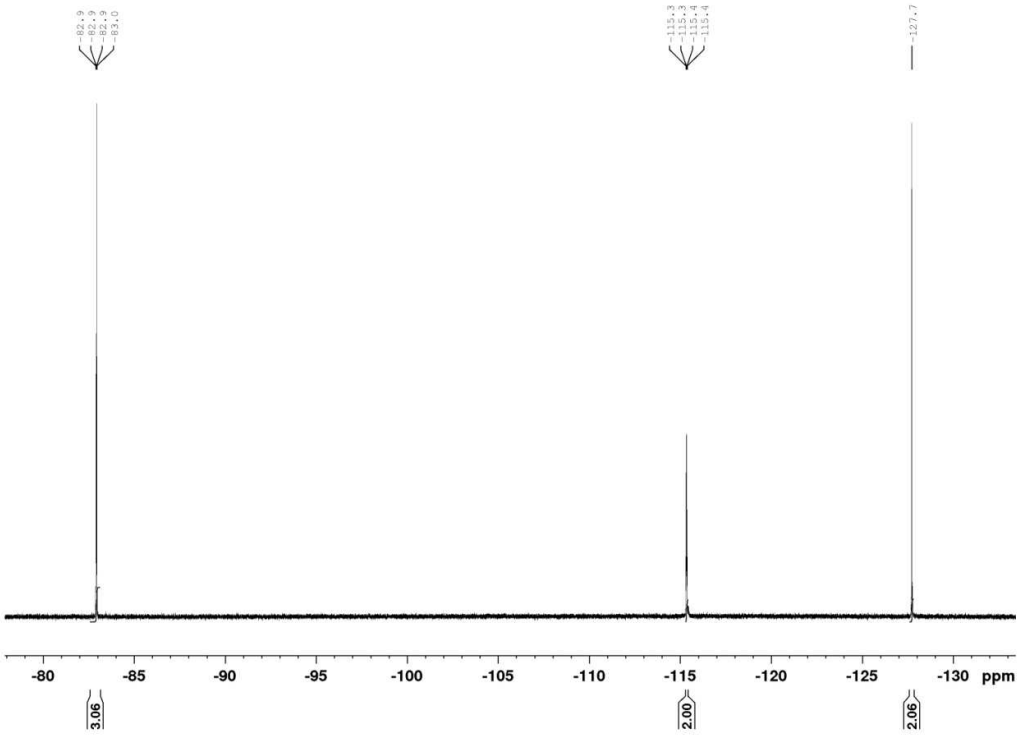
^{1}H-NMR (600.13 MHz, THF-d_8, 295 K):



^{13}C-NMR (150.90 MHz, THF-d_8, 295 K):

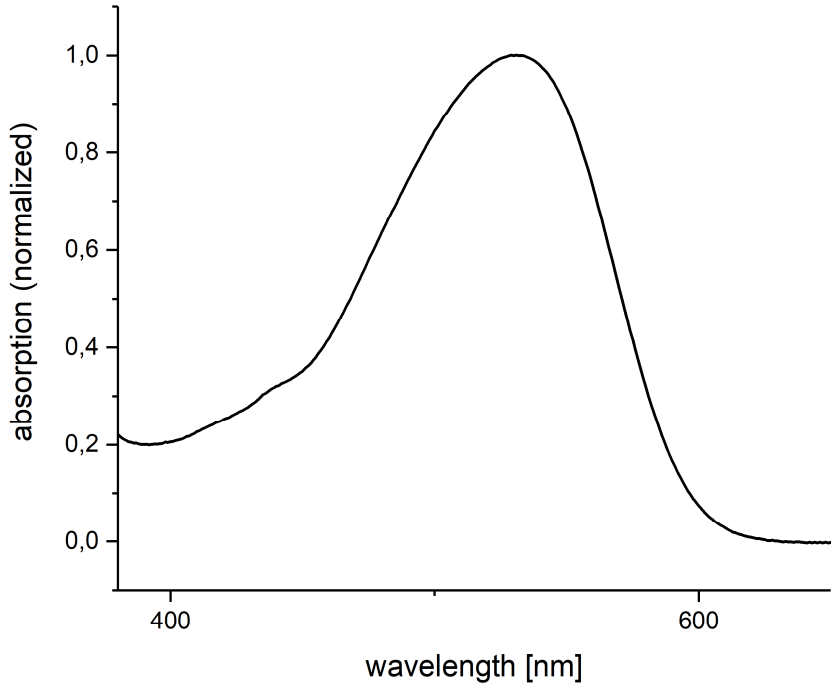


^{19}F-NMR (376.27 MHz, THF-d_8, 295 K):

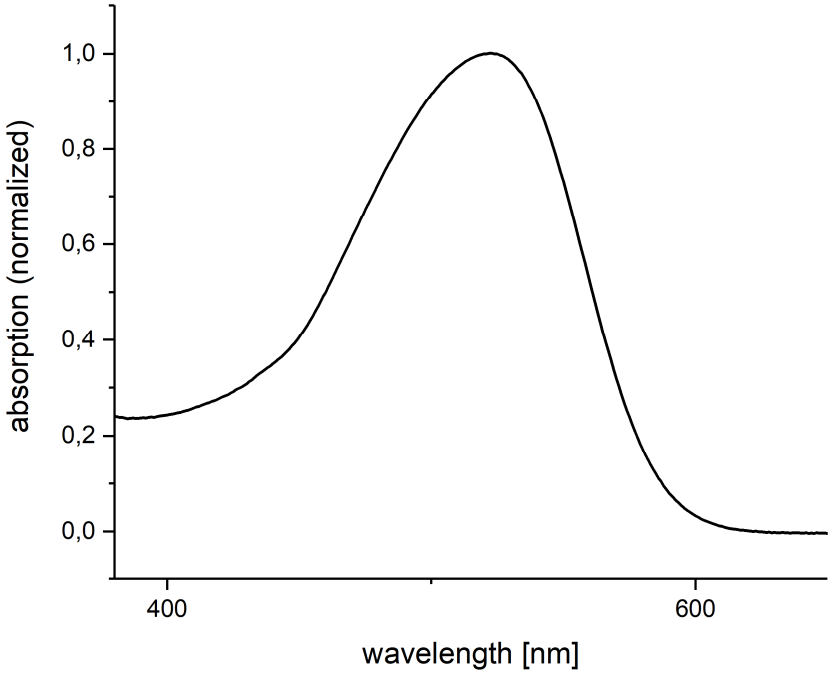


Absorption Spectra of Compounds 2-5, 8, 10, 12

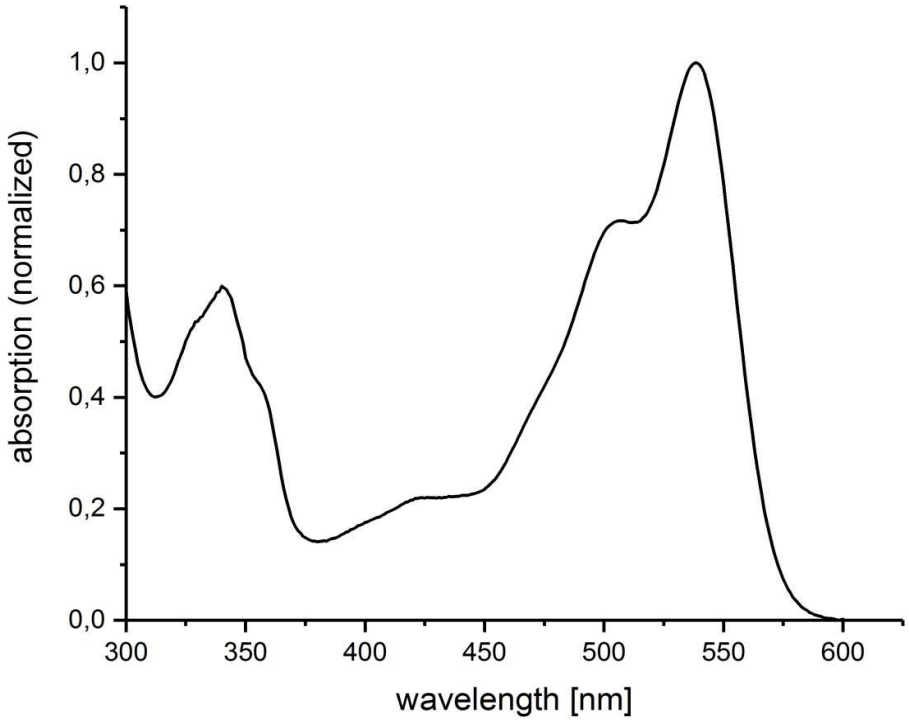
Compound 2:



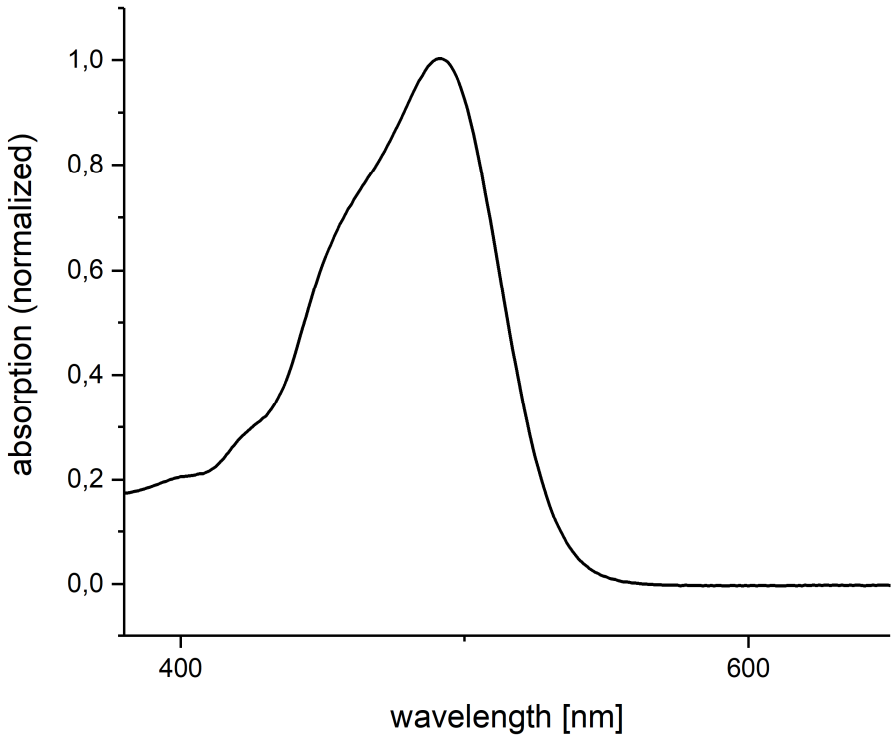
Compound 3:



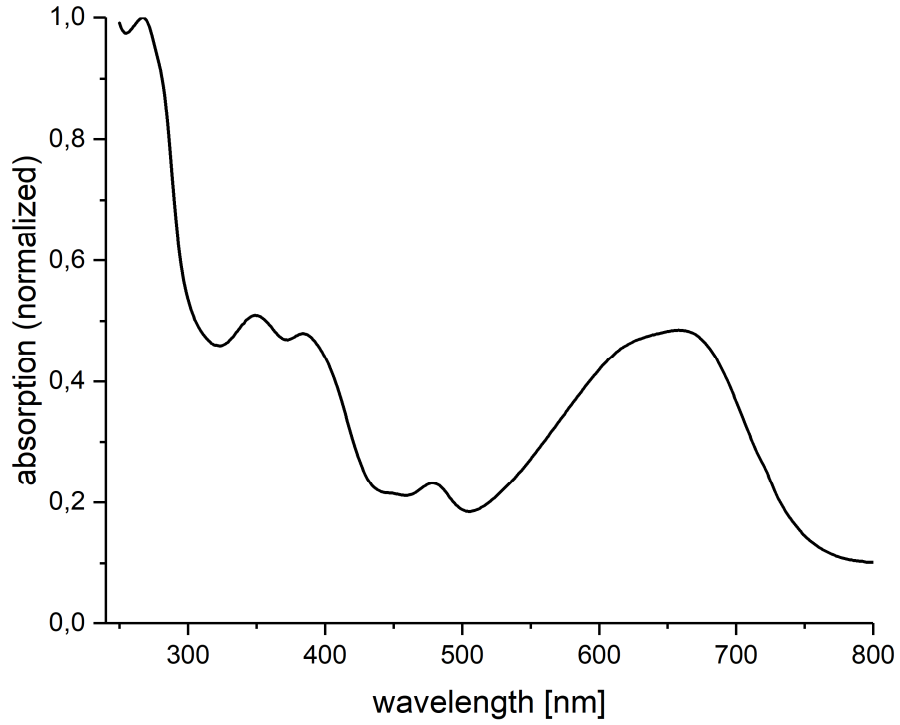
Compound 4:



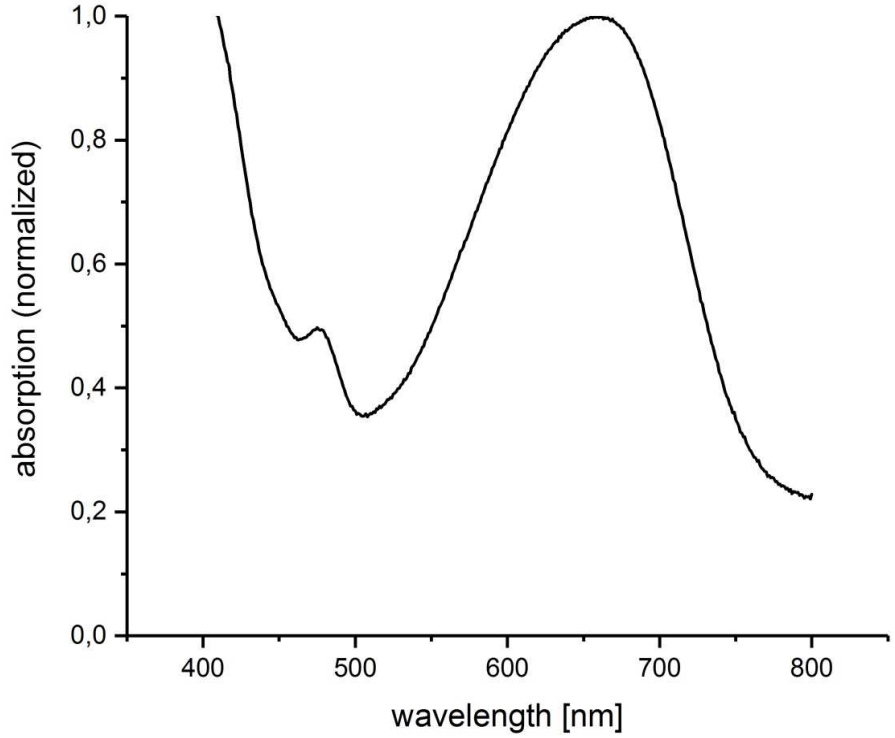
Compound 5:



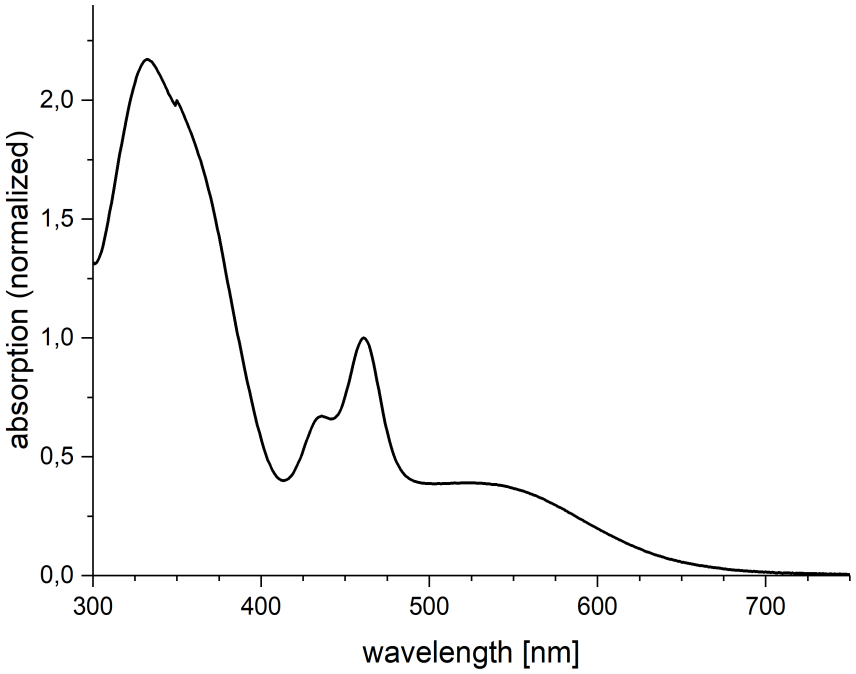
Compound 8:



Compound 10:

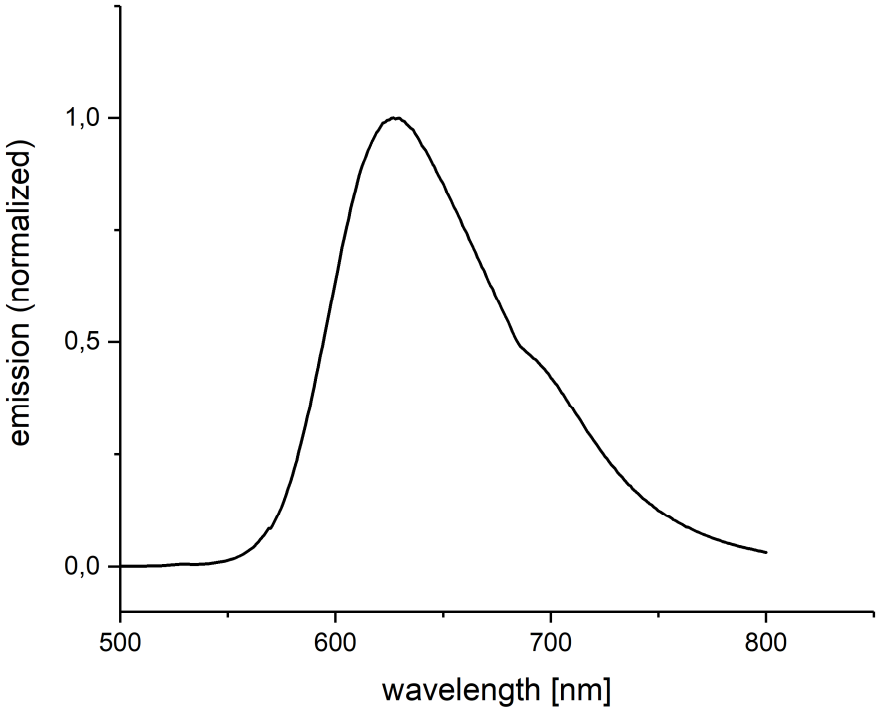


Compound 12:


absorption (normalized)
2,0
1,5
1,0
0,5
0,0
300
400
500
600
700
wavelength [nm]

Emission Spectra of Compounds 2-5

Compound 2:



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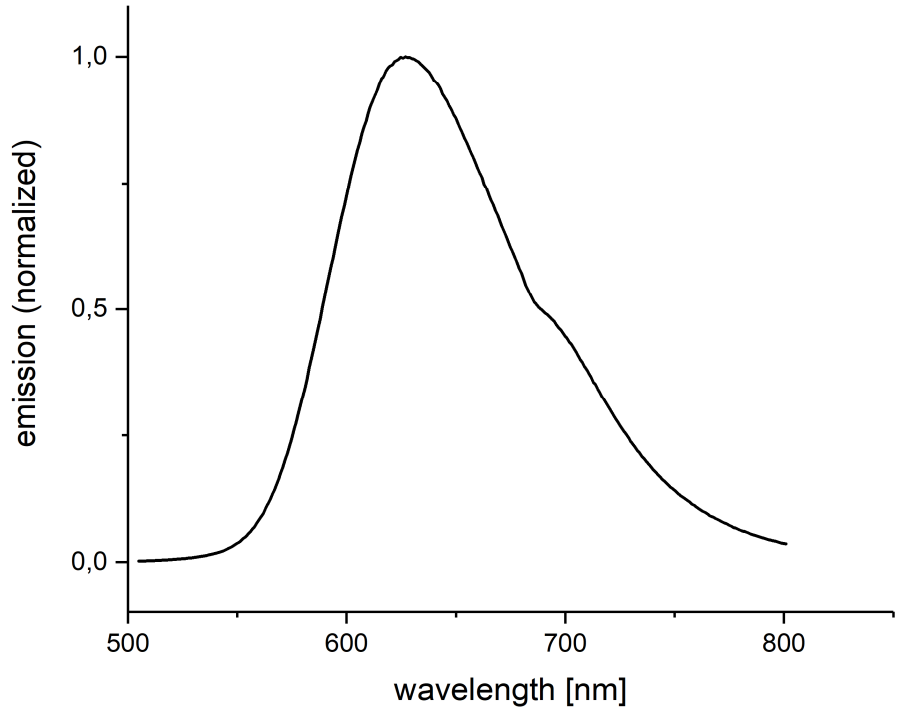
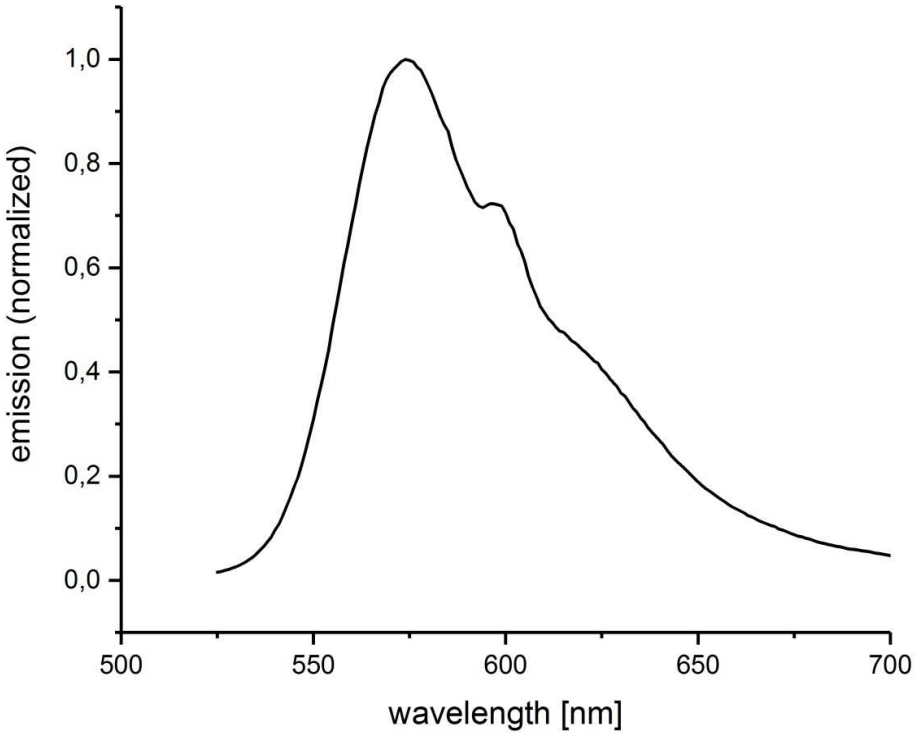
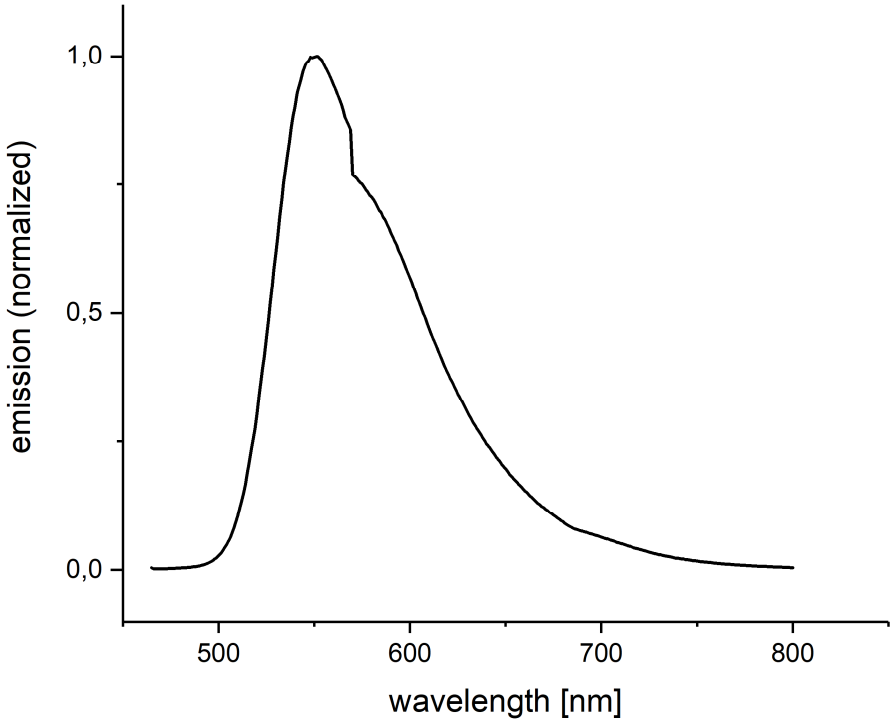


Compound 4:

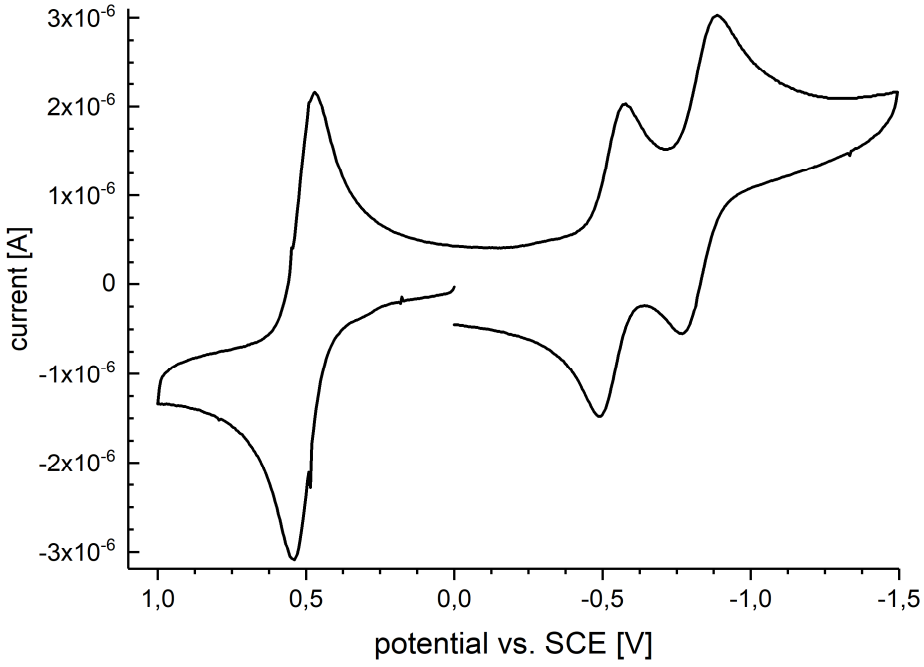


Compound 5:

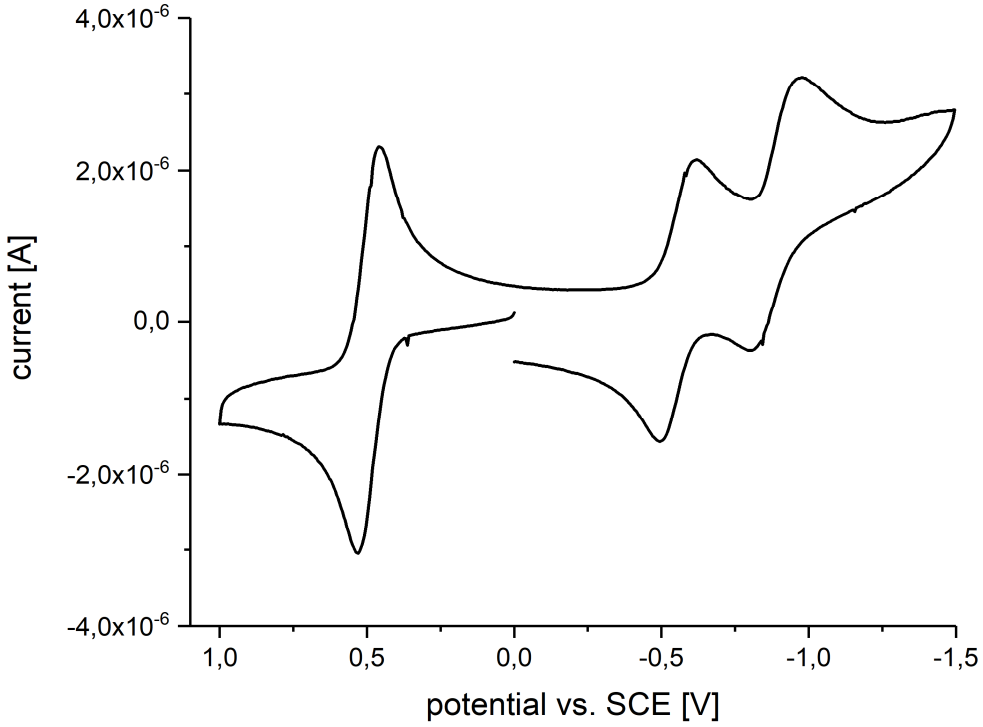


Cyclic Voltammograms of Compounds 2-5, 8, 10, 12

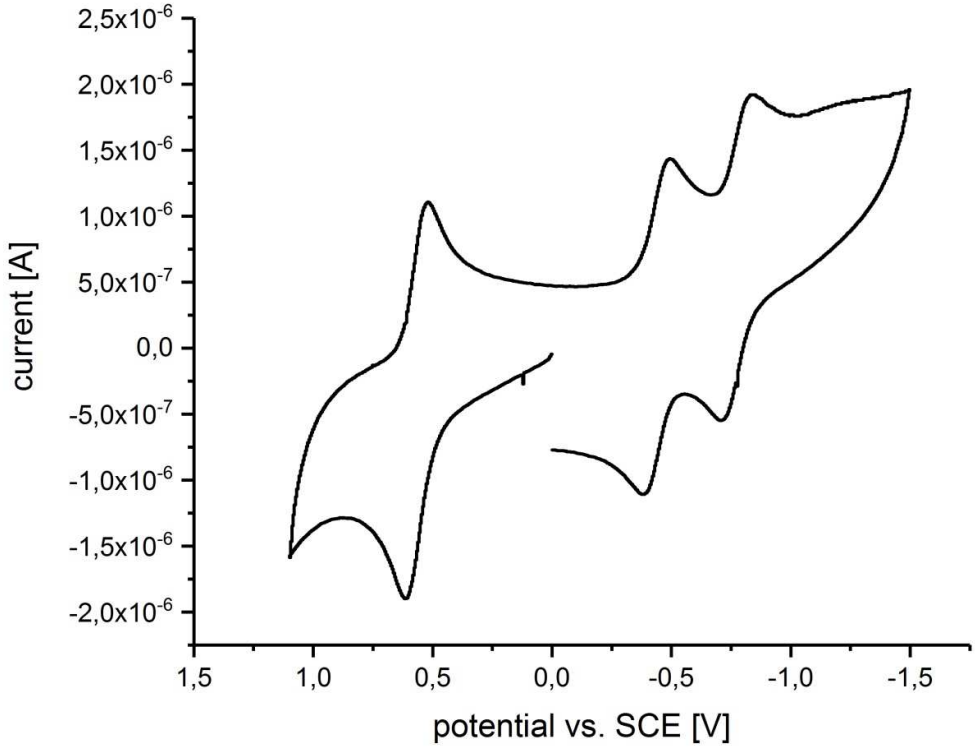
Compound 2:



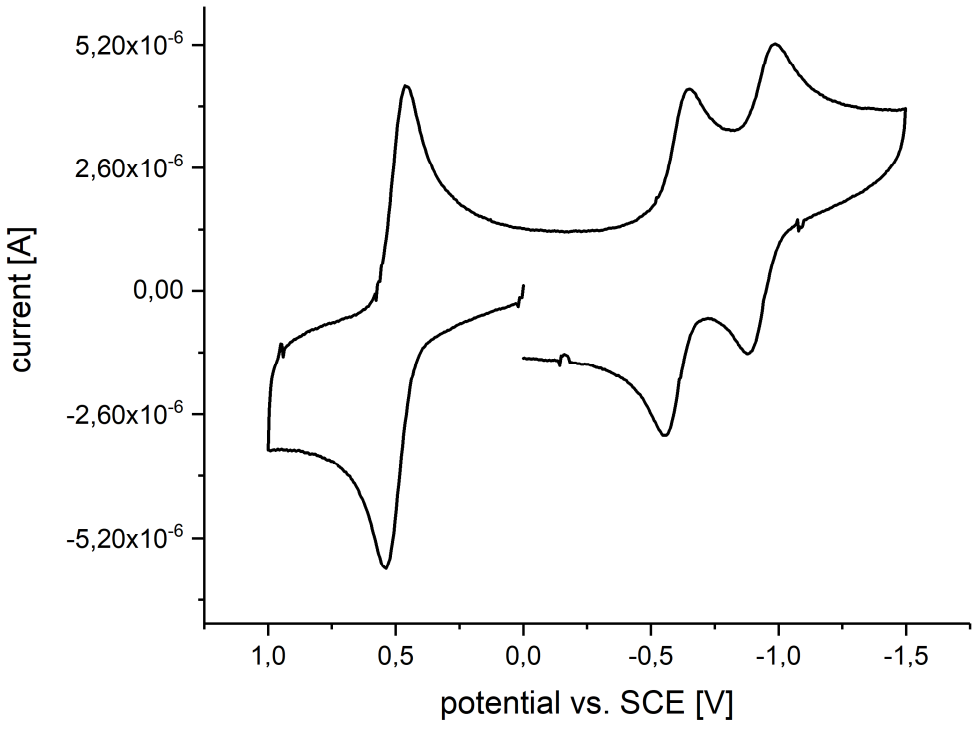
Compound 3:



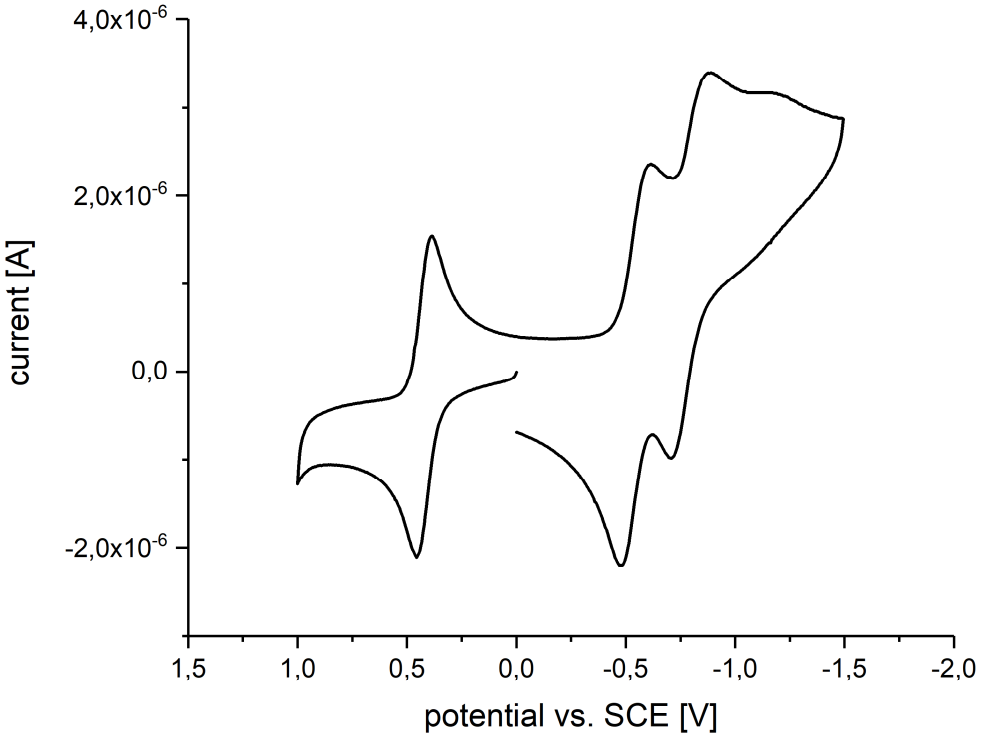
Compound 4:



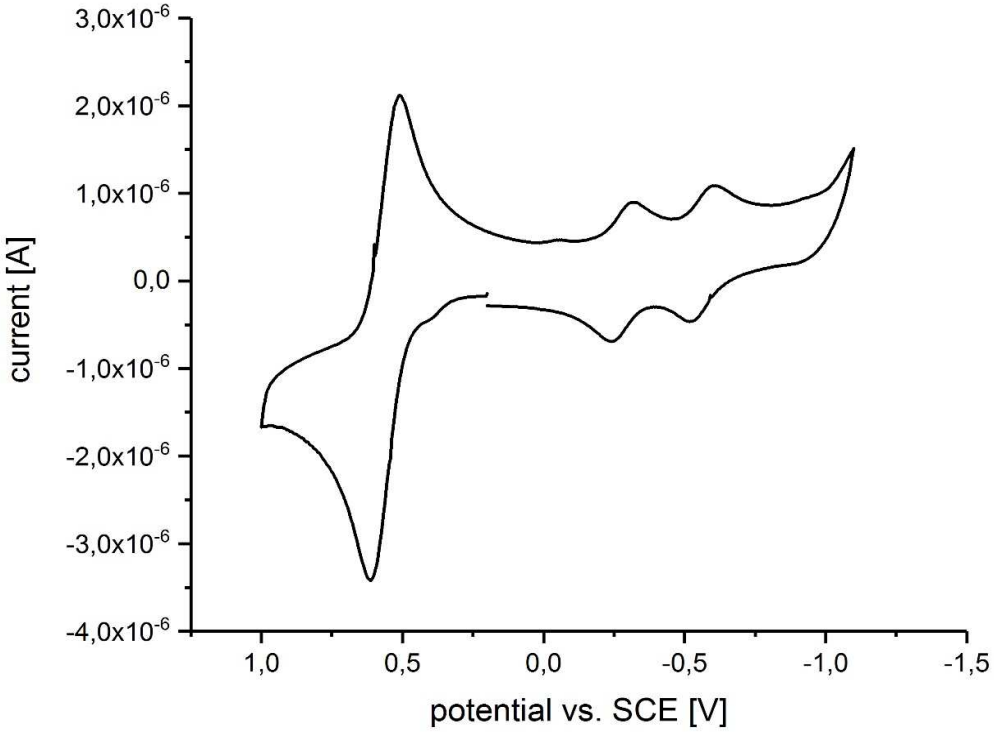
Compound 5:



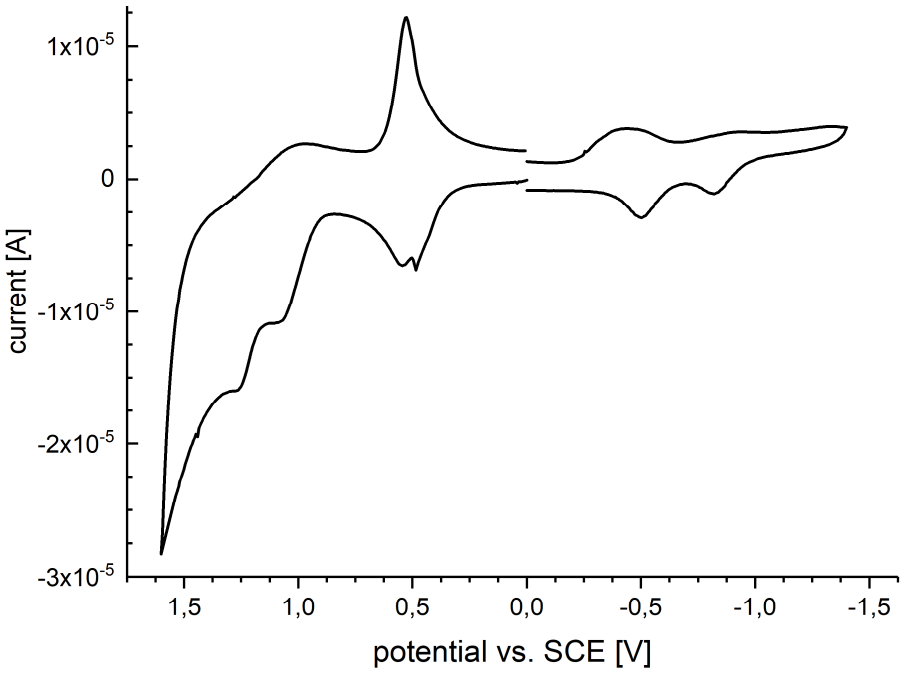
Compound 8:



Compound 10:



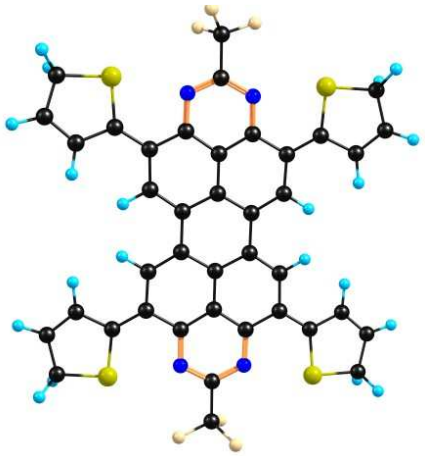
Compound 12:


1x10-5
0
-1x10-5
-2x10-5
-3x10-5
current [A]
1,5
1,0
0,5
0,0
-0,5
-1,0
-1,5
potential vs. SCE [V]

Computational Methods.

The DFT calculations were carried out using ORCA 3.0.1 program package.[1] B3LYP was employed as functional[2]a def2-SVP basis set was used for all atoms during geometry optimizations[3]. All other properties were calculated using a def2-QZVPP basis set.[4]

Compound 1:



Coordinates of 1:

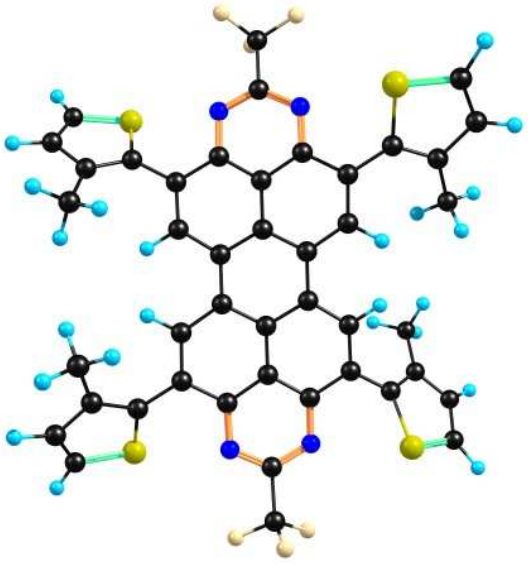
	Coordinates (Angstroms)		
Atomic Type	X	Y	Z
F	4.688535	2.874021	10.315876
F	5.319944	4.862439	10.898074
N	2.001917	3.658746	10.464108
N	2.904407	5.360417	11.842306
C	0.779579	3.848929	10.984107
C	-0.340634	3.074653	10.482427
C	4.356652	4.174235	10.280981
C	-2.164417	6.184619	14.260426
C	-0.720158	5.017685	12.599149
C	0.563954	4.819669	12.006402
C	-1.604160	3.303740	11.109491
H	-2.447965	2.712676	10.764302
C	1.557982	6.636145	13.388567
C	1.700257	5.586541	12.395730
C	-0.845074	6.012139	13.622761
C	0.258627	6.784009	13.969967
H	0.135532	7.549002	14.733414

C	2.991630	4.412701	10.922134
C	-0.187722	2.151107	9.428791
C	-0.913948	0.572754	7.813418
H	-1.624872	-0.027608	7.240793
C	-1.271986	1.433557	8.791722
H	-2.310619	1.602024	9.077968
C	2.643890	7.466151	13.741546
C	3.736700	9.251880	14.864937
H	3.833239	10.117593	15.524850
C	2.580300	8.579568	14.666498
H	1.648566	8.862404	15.156511
F	-8.666354	7.521522	16.084014
F	-9.297353	5.532981	15.501782
N	-5.979498	6.737425	15.935026
N	-6.881987	5.035781	14.556791
C	-4.757219	6.547454	15.414807
C	-3.637015	7.321778	15.916434
C	-8.334081	6.221401	16.118667
C	-1.813281	4.211963	12.138280
C	-3.257538	5.378892	13.799563
C	-4.541619	5.576809	14.392411
C	-2.373521	7.092788	15.289269
H	-1.529728	7.683892	15.634421
C	-5.535653	3.760367	13.010183
C	-5.677902	4.809875	14.003135
C	-3.132629	4.384463	12.775923
C	-4.236323	3.612592	12.428708
H	-4.113239	2.847645	11.665210
C	-6.969177	5.983366	15.477101
C	-3.789891	8.245277	16.970120
C	-3.063579	9.823516	18.585568
H	-2.352624	10.423819	19.158219
C	-2.705592	8.962763	17.607200
H	-1.666969	8.794271	17.320926
C	-6.621536	2.930330	12.657179
C	-7.714252	1.144588	11.533713
H	-7.810738	0.278884	10.873780
C	-6.557882	1.816942	11.732197
H	-5.626123	1.534159	11.242199
F	-8.323127	5.845332	17.410354
F	4.346187	4.550169	8.989250
C	-4.529610	9.893659	18.847465

H	-4.788983	9.633541	19.890246
H	-4.947423	10.899449	18.653252
C	4.902492	8.727029	14.097998
H	5.339287	9.480239	13.416462
H	5.720918	8.378375	14.755020
C	0.552094	0.502631	7.551571
H	0.969924	-0.503134	7.745879
H	0.811493	0.762673	6.508778
C	-8.880081	1.669369	12.300639
H	-9.698506	2.018015	11.643609
H	-9.316865	0.916120	12.982140
S	-5.329159	8.683283	17.707469
S	4.281570	7.300416	13.105205
S	1.351575	1.713122	8.691492
S	-8.259237	3.095974	13.293488

Final Single Point Energy	--3944.464735431668 E_h	
HOMO:	-0.209466 E_h	-5.6999 eV
LUMO:	-0.136821 E_h	-3.7231 eV

Compound 2:



Coordinates of 2:

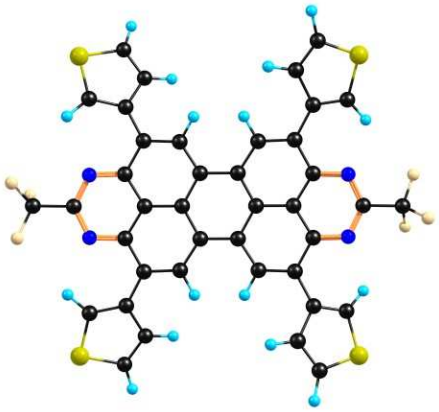
Atomic Type	Coordinates (Angstroms) X	Y	Z
S	7.594461	14.333895	13.108886
S	8.852790	6.234278	12.493954
F	10.055340	11.479518	14.399920

F	10.096072	9.322575	14.577673
N	7.872543	11.416961	12.829522
N	7.971585	9.038532	12.970254
C	6.915659	11.351276	11.874713
C	6.399754	12.551879	11.275221
C	5.308000	12.424663	10.411244
H	4.870772	13.336018	10.006078
C	4.753081	11.187303	10.016925
C	5.367796	9.985180	10.484779
C	6.413509	10.082594	11.446419
C	7.012539	8.916931	12.020558
C	6.574220	7.617943	11.590425
C	5.591418	7.559090	10.598440
H	5.290871	6.574409	10.245524
C	3.605118	11.078657	9.134632
C	8.315177	10.268801	13.314351
C	9.285824	10.385213	14.485342
C	7.011706	13.867729	11.521456
C	7.219734	14.897247	10.603391
C	7.816347	16.048388	11.208014
H	8.082130	16.945493	10.642719
C	8.053193	15.899285	12.551074
H	8.520579	16.610742	13.231477
C	6.938541	14.836437	9.124039
H	7.032518	13.813752	8.729594
H	7.645227	15.477836	8.574787
H	5.924567	15.192645	8.867975
C	7.137286	6.379706	12.153519
C	6.483883	5.178746	12.423698
C	7.386166	4.158803	12.862586
H	7.056430	3.155470	13.142885
C	8.692016	4.574429	12.927061
H	9.560896	4.004408	13.254579
C	4.997745	4.943176	12.339554
H	4.426918	5.867372	12.514488
H	4.684965	4.202154	13.092330
H	4.683364	4.548109	11.356625
S	2.233776	5.854310	4.928609
S	-0.908728	13.016640	7.441685
F	-1.237239	8.406797	4.454259
F	-1.324948	10.570100	4.387750
N	1.071731	8.456650	5.917119

N	0.579146	10.771697	6.227099
C	1.990074	8.490331	6.911568
C	2.689478	7.296949	7.300971
C	3.650895	7.402589	8.308735
H	4.211536	6.505204	8.564419
C	3.978694	8.607659	8.967418
C	3.300226	9.801646	8.572076
C	2.281808	9.721557	7.579932
C	1.504133	10.865737	7.213992
C	1.703621	12.107697	7.913294
C	2.760554	12.167398	8.827937
H	2.909818	13.093290	9.378820
C	4.974454	8.691752	10.022792
C	0.449448	9.592275	5.641941
C	-0.491736	9.524569	4.441948
C	2.429961	5.994392	6.666238
C	2.380098	4.739512	7.266592
C	2.217788	3.688907	6.308896
H	2.136261	2.636585	6.593245
C	2.146469	4.135101	5.013686
H	1.993054	3.546997	4.109344
C	2.436822	4.461614	8.746862
H	2.133092	5.334467	9.342770
H	1.766070	3.626603	9.007042
H	3.449522	4.171553	9.081027
C	0.808017	13.260831	7.727908
C	1.087697	14.620833	7.859780
C	-0.089367	15.428063	7.761718
H	-0.067658	16.518960	7.829270
C	-1.236428	14.703902	7.562337
H	-2.250405	15.081230	7.429939
C	2.450354	15.241357	8.037566
H	3.248168	14.601793	7.633451
H	2.495919	16.209971	7.514221
H	2.690791	15.439674	9.098047
F	8.601015	10.471999	15.648170
F	0.216378	9.514969	3.290717

Final Single Point Energy	-4101.623171767360 E_h	
Homo	-0.210617 E_h	-5.7312 eV
Lumo	-0.131061 E_h	-3.5664 eV

Compound 4:



Coordinates of 4:

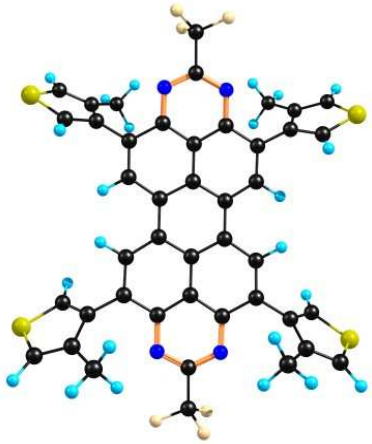
Atomic Type	Coordinates (Angstroms) X	Y	Z
S	0.572072	0.404774	7.615285
S	4.930936	8.669956	14.181776
F	4.614767	2.878741	10.275444
F	5.288907	4.834817	10.917777
N	1.965509	3.683384	10.432042
N	2.867434	5.409407	11.790986
C	0.742450	3.865861	10.953845
C	-0.383347	3.065700	10.491075
C	4.318868	4.188665	10.263443
C	-2.152577	6.187446	14.230936
C	-0.737461	5.033112	12.581436
C	0.537326	4.850454	11.972778
C	-1.595045	3.259793	11.126592
H	-2.428050	2.634978	10.815298
C	1.514178	6.682899	13.360375
C	1.668355	5.639095	12.354710
C	-0.876582	6.023740	13.597234
C	0.263421	6.812076	13.937281
H	0.142205	7.561927	14.714429
C	2.946491	4.446118	10.889149
C	-0.283090	2.091585	9.384929
C	0.878352	1.520472	8.889267
H	1.892237	1.712210	9.226185
C	-1.133434	0.685207	7.702112
H	-1.815463	0.179322	7.020111
C	-1.439877	1.595084	8.675324
H	-2.460487	1.933922	8.854652

C	2.612841	7.582746	13.773701
C	3.962379	7.427341	13.489040
H	4.417355	6.640205	12.896417
C	3.545866	9.447111	14.867703
H	3.650935	10.373028	15.431278
C	2.396996	8.768903	14.572180
H	1.420676	9.129046	14.896088
S	-4.552912	10.002016	18.771801
S	-8.905496	1.715899	12.229670
F	-8.592729	7.516464	16.123895
F	-9.266017	5.559807	15.482478
N	-5.943335	6.714293	15.964985
N	-6.844374	4.985221	14.609402
C	-4.720477	6.532204	15.442614
C	-3.595218	7.334069	15.903564
C	-8.296023	6.206717	16.136147
C	-1.825519	4.210123	12.165778
C	-3.240439	5.363951	13.815859
C	-4.515041	5.546381	14.424960
C	-2.383371	7.139254	15.268666
H	-1.550670	7.765010	15.578872
C	-5.490910	3.710861	13.040876
C	-5.645499	4.756034	14.045040
C	-3.101210	4.372833	12.800504
C	-4.240673	3.582735	12.462503
H	-4.119281	2.831836	11.686378
C	-6.923832	5.949833	15.509789
C	-3.696257	8.310586	17.007429
C	-4.858065	8.883529	17.500006
H	-5.871592	8.691466	17.162167
C	-2.847454	9.720268	18.688172
H	-2.166117	10.227274	19.370031
C	-2.540163	8.808017	17.717453
H	-1.519530	8.468035	17.540401
C	-6.588670	2.808260	12.631185
C	-7.938138	2.962402	12.917033
H	-8.393655	3.750625	13.507780
C	-7.520008	0.938879	11.544407
H	-7.624251	0.011012	10.983904
C	-6.371881	1.619954	11.836196
H	-5.395365	1.260412	11.512166
F	-8.316468	5.801275	17.414929

F	4.340197	4.594439	8.984783

Final Single Point Energy	-3941.040844369229 E_h	
HOMO	-0.211787 E_h	-5.7630 eV
LUMO	-0.130715 E_h	-3.5569 eV

Compound 5:



Coordinates of 5:

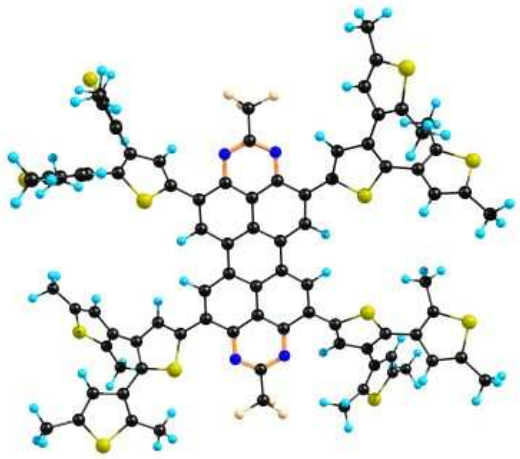
	Coordinates (Angstroms)		
Atomic Type	X	Y	Z
S	-0.582908	9.470236	2.025635
S	5.373558	4.181412	11.608226
F	3.823082	5.625870	3.878891
F	4.148794	4.216346	5.489557
N	2.388615	7.142972	5.512337
N	3.487630	6.144481	7.377304
C	1.577839	7.836582	6.331390
C	0.600803	8.763191	5.789346
C	-0.283954	9.351152	6.669045
H	-1.004027	10.054594	6.252163
C	-0.109195	8.625390	10.916200
C	0.729634	8.277872	8.630910
C	1.653724	7.654536	7.745086
C	2.694063	6.807143	8.231971
C	2.874443	6.653651	9.663973
C	1.946746	7.238513	10.496343
H	2.090580	7.110752	11.569281
C	0.845593	8.033205	10.032977
C	3.265953	6.329016	6.081602
C	4.175645	5.514004	5.160371

C	0.503215	9.063455	4.339565
C	-0.703036	8.978615	3.672147
H	-1.648118	8.611458	4.070142
C	1.100454	9.820985	2.216863
H	1.672764	10.216647	1.378376
C	1.564719	9.557940	3.483214
C	2.989935	9.797410	3.900319
H	3.046240	10.352032	4.851616
H	3.528592	10.381186	3.139415
H	3.519439	8.843552	4.043653
C	4.019164	5.889236	10.218320
C	3.862173	4.829099	11.086696
H	2.927523	4.376437	11.415456
C	6.240688	5.355706	10.681258
H	7.330364	5.375000	10.709308
C	5.414019	6.203030	9.985143
C	5.908269	7.336418	9.130869
H	5.850982	7.073789	8.062141
H	6.952075	7.586421	9.372774
H	5.301405	8.243905	9.285061
S	0.185387	8.267730	16.973028
S	-5.767621	13.564787	7.391742
F	-4.218103	12.117882	15.121065
F	-4.542249	13.528436	13.510990
N	-2.784322	10.600526	13.487254
N	-3.882448	11.600361	11.622478
C	-1.973845	9.906716	12.668071
C	-0.997390	8.979360	13.209902
C	-0.112595	8.391586	12.330134
H	0.607185	7.687741	12.746846
C	-0.286990	9.117960	8.083107
C	-1.125596	9.465768	10.368473
C	-2.049438	10.089305	11.254413
C	-3.089244	10.937425	10.767681
C	-3.269617	11.091167	9.335702
C	-2.342380	10.505755	8.503186
H	-2.486198	10.633760	7.430277
C	-1.241535	9.710517	8.966407
C	-3.660980	11.415332	12.918153
C	-4.570250	12.230640	13.839550
C	-0.900277	8.678018	14.659493
C	0.306030	8.760995	15.327049

H	1.251523	9.127485	14.929416
C	-1.498334	7.918895	16.781397
H	-2.071082	7.522999	17.619475
C	-1.962300	8.183723	15.515307
C	-3.387735	7.946122	15.097868
H	-3.444527	7.391875	14.146377
H	-3.927242	7.362749	15.858476
H	-3.916041	8.900674	14.954734
C	-4.413962	11.856308	8.781558
C	-4.256512	12.916158	7.912921
H	-3.321653	13.368024	7.583661
C	-6.635272	12.391478	8.319468
H	-7.724977	12.373070	8.291929
C	-5.808959	11.543706	9.015469
C	-6.303681	10.411064	9.870467
H	-6.245540	10.674061	10.939064
H	-7.347841	10.161849	9.629279
H	-5.697671	9.503006	9.716279
F	-5.844658	11.809044	13.722447
F	5.449753	5.936699	5.276962

Final Single Point Energy:	-4101.587009188829 E_h	
Homo	-0.226115 E_h	-6.1529 eV
Lumo	-0.133879 E_h	-3.6430 eV

Compound 8:



Coordinates of 8:

	Coordinates (Angstroms)		
Atomic Type	X	Y	Z
C	19.680741	-1.230747	4.142699

F	26.372634	-4.887019	1.851326
F	25.252403	-5.965863	3.360193
N	23.031918	-4.100198	1.821851
N	24.082322	-5.919162	0.703860
C	21.974350	-4.170077	0.995840
C	20.829232	-3.297485	1.195363
C	19.819849	-3.335723	0.246068
H	18.988674	-2.642774	0.374895
C	19.817832	-4.212176	-0.883396
C	20.896364	-5.138540	-1.026849
C	21.962726	-5.101068	-0.085335
C	23.067944	-6.002537	-0.169168
C	23.075144	-7.017322	-1.210456
C	22.043753	-7.005071	-2.129071
H	22.051985	-7.780401	-2.894965
C	18.755386	-4.245639	-1.848149
C	24.020509	-4.957875	1.614169
C	25.227683	-4.887683	2.550768
C	20.700974	-2.437420	2.375447
C	19.520197	-2.094020	3.016526
C	21.018559	-0.876823	4.333532
N	16.633854	-6.388870	-5.659542
N	15.523162	-4.615344	-4.525005
C	17.710602	-6.262392	-4.873603
C	18.897230	-7.069814	-5.112650
C	19.903546	-6.997915	-4.167087
H	20.794532	-7.602288	-4.336589
C	19.895901	-6.117848	-3.049518
C	18.799042	-5.220672	-2.889658
C	17.710076	-5.317273	-3.801358
C	16.572038	-4.460030	-3.696915
C	16.584323	-3.398002	-2.696674
C	17.650890	-3.339736	-1.819091
H	17.639734	-2.548125	-1.068736
C	20.954025	-6.088739	-2.089305
C	15.611232	-5.585256	-5.427552
F	25.209671	-3.796207	3.319166
H	18.554451	-2.515419	2.732933
S	22.048495	-1.665787	3.169759
S	16.009588	-0.684564	-2.464662
C	14.358412	-0.126114	-2.574824
C	13.487019	-1.197342	-2.748508

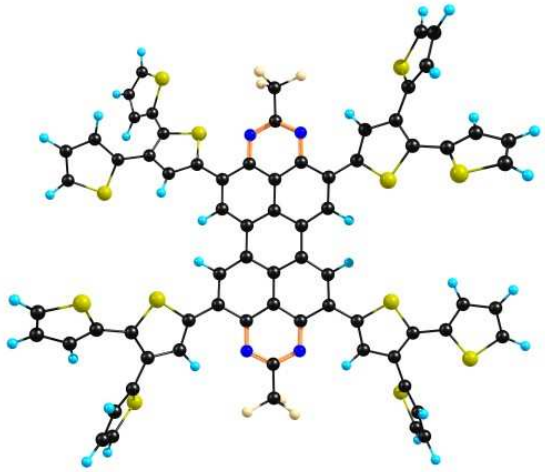
C	15.546706	-2.354839	-2.675470
C	14.180427	-2.450820	-2.809070
H	13.672608	-3.396379	-2.988708
S	24.627349	-8.713610	-2.802277
C	25.697143	-9.860710	-2.035579
C	25.682125	-9.698049	-0.649459
C	24.124459	-8.032418	-1.275264
C	24.794937	-8.653304	-0.242549
H	24.618815	-8.394170	0.798661
S	20.401188	-9.001699	-6.448654
C	20.094816	-9.311652	-8.139908
C	19.023186	-8.551277	-8.600097
C	19.079564	-7.854580	-6.332302
C	18.447511	-7.752711	-7.559747
H	17.608228	-7.081199	-7.726341
C	14.362972	-5.840767	-6.268952
F	14.640583	-6.598028	-7.337469
F	13.442400	-6.492018	-5.539352
F	13.809688	-4.703934	-6.698090
C	27.972395	-10.824425	-2.686182
C	28.609887	-11.587622	-3.626727
S	27.451058	-12.207865	-4.776634
C	26.108537	-11.431270	-3.984337
C	26.546803	-10.709670	-2.883041
H	28.496476	-10.324372	-1.870540
C	26.371309	-10.559951	0.335693
C	27.022980	-10.090881	1.465153
S	27.558355	-11.424172	2.454435
C	26.895801	-12.618460	1.366905
C	26.319024	-11.999655	0.291025
H	25.824916	-12.548272	-0.512959
C	22.412631	-10.137930	-8.793048
C	23.078699	-11.096544	-9.505559
S	21.935996	-12.216144	-10.210879
C	20.560877	-11.373194	-9.543253
C	20.977230	-10.266083	-8.823916
H	22.920563	-9.317624	-8.280927
C	17.105715	-8.487139	-10.290548
C	16.808451	-8.375174	-11.623050
S	18.282133	-8.246827	-12.551437
C	19.290932	-8.330330	-11.130714
C	18.516999	-8.478555	-9.991580
H	16.336336	-8.571981	-9.519344

C	12.012023	-1.145223	-2.882156
C	11.301660	-0.406344	-3.809328
S	9.587659	-0.702443	-3.647813
C	9.816739	-1.837345	-2.340511
C	11.152315	-1.956992	-2.057586
H	11.532345	-2.611962	-1.270535
C	20.992711	1.395167	5.491026
C	21.711911	2.219985	6.312687
S	23.162060	1.408432	6.851025
C	22.791054	-0.043005	5.961546
C	21.598936	0.103410	5.265221
H	20.054629	1.694907	5.021609
C	14.781628	2.280028	-3.335636
C	14.502611	3.588937	-3.045085
S	13.411392	3.674322	-1.682385
C	13.367294	1.940046	-1.491886
C	14.130708	1.327334	-2.470431
H	15.442677	1.981240	-4.151605
C	17.348546	-0.199615	4.539081
C	16.425607	0.071939	5.515968
S	17.023656	-0.464687	7.065384
C	18.517517	-1.052309	6.383601
C	18.555344	-0.826388	5.019515
H	17.189867	0.059163	3.489655
C	26.964329	-14.080922	1.687348
H	26.343262	-14.337692	2.562420
H	26.596071	-14.671371	0.834889
H	27.992451	-14.410726	1.913008
C	27.307829	-8.680693	1.897839
H	28.279370	-8.608726	2.412736
H	27.330272	-8.000887	1.034077
H	26.546153	-8.290008	2.594586
C	30.074592	-11.866204	-3.780420
H	30.500617	-11.335498	-4.649425
H	30.619003	-11.527933	-2.886181
H	30.282434	-12.939499	-3.923554
C	24.717978	-11.633607	-4.515232
H	24.600021	-12.638397	-4.953134
H	23.973457	-11.521014	-3.713593
H	24.461354	-10.904063	-5.302825
C	8.659411	-2.535539	-1.690618
H	8.101250	-3.162504	-2.407466
H	9.024558	-3.192171	-0.886803
H	7.939766	-1.827125	-1.245981
C	11.812472	0.505691	-4.882245
H	11.790726	1.565190	-4.571744
H	12.856289	0.253158	-5.120828

H	11.219808	0.410109	-5.806236
C	23.729635	-1.211731	6.035782
H	24.186688	-1.295197	7.034660
H	23.202350	-2.152154	5.821368
H	24.554877	-1.128892	5.307550
C	21.433569	3.641149	6.702216
H	22.159546	4.335161	6.245420
H	20.430523	3.935832	6.359326
H	21.481348	3.791737	7.793903
C	15.001745	4.825408	-3.731653
H	15.505292	5.511750	-3.029349
H	15.727097	4.551868	-4.512897
H	14.186048	5.391637	-4.213859
C	12.616254	1.316043	-0.355203
H	11.553905	1.150120	-0.603067
H	13.050338	0.335221	-0.113973
H	12.662344	1.944257	0.548532
C	19.513764	-1.743340	7.262778
H	19.016677	-2.452896	7.945086
H	20.230056	-2.307317	6.648516
H	20.094841	-1.033840	7.876359
C	15.082389	0.728256	5.398496
H	14.995384	1.608912	6.055956
H	14.909464	1.064052	4.365107
H	14.265085	0.039888	5.674762
C	15.468239	-8.363837	-12.293446
H	15.352471	-9.200537	-13.002954
H	14.671165	-8.448507	-11.539295
H	15.299356	-7.432357	-12.860798
C	20.778200	-8.212251	-11.279614
H	21.043387	-7.495801	-12.073487
H	21.231339	-7.858929	-10.343051
H	21.252441	-9.176807	-11.527857
C	24.552257	-11.230447	-9.731590
H	24.812694	-11.167002	-10.801913
H	25.086592	-10.422892	-9.209820
H	24.942788	-12.191345	-9.355761
C	19.173728	-11.891897	-9.768957
H	19.101224	-12.964978	-9.522838
H	18.460340	-11.350211	-9.136178
H	18.849019	-11.760835	-10.814907

Final Single Point Energy	-8987.436927424180 E_h	
Homo:	-0.197201 E_h	-5.3661 eV
Lumo:	-0.129350 E_h	-3.5198 eV

Compound 10:



Coordinates of 10:

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	11.438156	6.292075	5.657586
F	16.097756	3.603912	8.946321
F	17.620238	2.094229	8.638208
N	15.783726	3.964395	6.234759
N	17.876707	2.853118	6.083147
C	15.909318	4.435925	4.986645
C	14.843054	5.238278	4.408221
C	14.995317	5.646428	3.088949
H	14.206538	6.259399	2.651872
C	16.146016	5.360163	2.293999
C	17.225952	4.643354	2.894311
C	17.074268	4.143081	4.217612
C	18.059287	3.306714	4.830325
C	19.239549	2.929877	4.063304
C	19.410347	3.543755	2.830787
H	20.316185	3.312528	2.271155
C	16.278885	5.755665	0.916324
C	16.765574	3.209770	6.708461
C	16.521765	2.645394	8.112634
C	13.648182	5.587667	5.180855
C	12.414733	5.964887	4.674016
C	11.958979	6.207687	6.953360
N	19.105244	6.512022	-2.962574
N	16.793799	7.063991	-3.054504
C	18.978555	6.031998	-1.717938
C	20.125763	5.448628	-1.031991

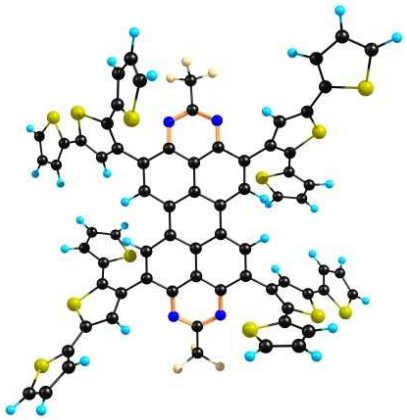
C	19.902692	4.936323	0.237958
H	20.750883	4.500403	0.765089
C	18.653703	4.975658	0.916351
C	17.545719	5.604087	0.275954
C	17.710073	6.081780	-1.056009
C	16.609286	6.604807	-1.803898
C	15.282803	6.603716	-1.200123
C	15.191761	6.246252	0.138583
H	14.209513	6.297227	0.609697
C	18.453671	4.395826	2.213865
C	18.021403	7.004149	-3.545501
F	15.570551	1.697178	8.066329
H	12.176642	5.950982	3.608850
S	13.606244	5.642773	6.932967
C	10.542312	6.588225	10.603064
C	10.045365	7.635769	9.864877
C	10.483971	7.610957	8.510480
C	11.318163	6.544263	8.221913
S	11.551805	5.558314	9.653155
H	9.389055	8.403503	10.278868
H	10.201970	8.354128	7.764240
C	7.972419	5.462450	-2.715434
S	9.582087	4.988684	-2.302958
C	7.941856	6.712072	-3.285431
H	7.024737	7.198440	-3.622226
C	10.243515	6.505032	-2.886990
C	9.231569	7.306443	-3.384231
S	12.556717	6.176123	-1.418190
C	11.671587	6.775279	-2.792127
H	9.416123	8.299835	-3.792333
C	12.511385	7.498102	-3.642873
C	14.068241	6.874004	-1.975463
C	13.859876	7.541794	-3.170232
H	14.668062	8.014792	-3.723617
C	24.417118	-2.401468	2.695068
S	22.928182	-1.565678	2.429988
C	24.913008	-2.166483	3.955212
H	25.844411	-2.599329	4.324225
C	22.963417	-0.866078	4.040123
C	24.089864	-1.292127	4.719876
S	21.272354	1.187802	3.329948
C	21.908664	0.041533	4.477230

H	24.320647	-0.966348	5.734260
C	21.292905	0.197331	5.722570
C	20.175517	1.894116	4.504888
C	20.327494	1.253033	5.721265
H	19.719819	1.507513	6.586466
C	27.597684	3.502087	-2.227172
S	26.529793	4.562627	-3.070640
C	26.986401	2.894827	-1.156207
H	27.488032	2.186059	-0.495701
C	25.209595	4.201630	-1.973296
C	25.631119	3.291964	-1.010945
S	22.684720	4.364568	-0.903563
C	23.887657	4.791682	-2.094563
H	24.975683	2.916208	-0.223398
C	23.347749	5.682774	-3.026478
C	21.453176	5.376887	-1.641264
C	21.983359	5.999405	-2.759204
H	21.396925	6.661540	-3.390519
C	18.267328	7.616582	-4.925843
F	18.939782	8.774347	-4.785392
F	19.011454	6.808403	-5.694075
F	17.129610	7.874679	-5.574492
C	25.056959	6.533824	-6.290731
C	25.298294	7.770866	-5.746071
S	24.675769	7.893157	-4.139001
C	24.076003	6.250548	-4.181471
C	24.353739	5.669753	-5.400243
H	25.369399	6.246498	-7.296331
H	25.805975	8.620018	-6.203043
H	24.054823	4.650211	-5.648053
C	21.646137	-2.033191	6.956245
C	21.522735	-0.659754	6.895167
S	21.630862	0.030618	8.500467
C	21.838361	-1.526317	9.222087
C	21.825866	-2.525849	8.281798
H	21.594182	-2.667448	6.070684
H	21.961512	-1.621407	10.300547
H	21.937395	-3.582595	8.532792
C	7.692989	6.568645	5.322204
C	7.928466	7.443999	4.290497
S	9.622872	7.682922	4.034205
C	10.036681	6.585610	5.332040
C	8.893321	6.080419	5.915764
H	6.694365	6.272118	5.648728
H	7.202994	7.960142	3.662968

H	8.922767	5.373382	6.746093
C	11.112406	8.460013	-7.018045
C	11.517866	9.739550	-6.729687
S	12.292341	9.829235	-5.186591
C	12.071289	8.116454	-4.906785
C	11.428311	7.535711	-5.979772
H	10.605565	8.181275	-7.943842
H	11.410377	10.635048	-7.340772
H	11.177851	6.474248	-6.015144
H	10.365008	6.356098	11.652741
H	24.843544	-3.019295	1.905360
H	28.621011	3.376850	-2.580427
H	7.139141	4.790102	-2.514305

Final Single Point Energy: 8358.560644524268 E_h
Homo: -0.197049 E_h -5.3620 eV
Lumo: -0.134977 E_h -3.6729 eV

Compound 12:



Coordinates of 12:

Atomic Type	Coordinates (Angstroms) X	Y	Z
S	-17.209399	25.007113	16.550027
S	-13.788104	31.852640	26.130237
F	-15.472020	30.503427	18.912436
F	-15.186600	31.658214	20.720541
N	-15.900130	28.224225	20.300363
N	-15.449905	29.489080	22.271623
C	-15.874533	27.078269	21.001377
C	-16.106179	25.806621	20.342926
C	-16.145564	24.668354	21.117484

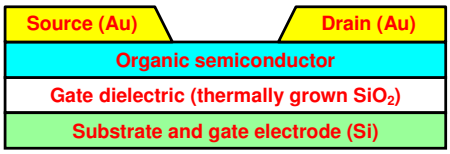
H	-16.320813	23.723880	20.604851
C	-15.654432	24.811907	25.398064
C	-15.704638	25.901526	23.191712
C	-15.648787	27.092626	22.410879
C	-15.406036	28.365353	23.007323
C	-15.128759	28.433683	24.427359
C	-15.195713	27.273553	25.162960
H	-15.003695	27.350679	26.233077
C	-15.503254	25.990129	24.602120
C	-15.704323	29.351076	20.977133
C	-15.872265	30.648716	20.179956
C	-16.311354	25.713147	18.875980
C	-17.393327	25.060440	18.286731
C	-15.676547	25.844804	16.607328
C	-15.362887	26.175253	17.910497
C	-14.863356	29.727842	25.115312
C	-13.676428	30.456164	25.079989
C	-15.405949	31.447016	26.641996
C	-15.826120	30.296518	26.003332
S	-15.491358	24.669443	31.537870
S	-17.780874	17.356863	22.358267
F	-17.806357	19.505485	29.126919
F	-18.495594	18.554179	27.307054
N	-16.549830	21.426029	27.727261
N	-17.050974	20.184787	25.757199
C	-16.190230	22.489145	26.986145
C	-15.754160	23.717681	27.624939
C	-15.504325	24.810117	26.823118
H	-15.176348	25.723815	27.315753
C	-15.990170	24.661416	22.541131
C	-16.006670	23.587471	24.754257
C	-16.267277	22.442995	25.560731
C	-16.677195	21.208445	24.980974
C	-16.747419	21.082969	23.536310
C	-16.493149	22.204536	22.778308
H	-16.580706	22.109538	21.695737
C	-16.148584	23.482461	23.335957
C	-16.985136	20.359028	27.068245
C	-17.449114	19.155300	27.889156
C	-15.571240	23.803199	29.095201
C	-16.061588	24.836732	29.894529
C	-14.556735	23.245610	31.153392

C	-14.737615	22.900278	29.829871
C	-17.242426	19.826429	22.922940
C	-16.795926	18.532008	23.192087
C	-18.829581	18.582149	21.692272
C	-18.385249	19.834829	22.062028
F	-16.459898	18.245623	27.982053
F	-17.171408	31.004037	20.161421
H	-18.920213	20.748310	21.797967
H	-14.239346	22.046643	29.371217
H	-16.818077	29.867378	26.149763
H	-14.464490	26.730255	18.180324
C	-15.693458	18.041291	24.007342
C	-15.681482	16.935571	24.837838
S	-14.129975	18.828962	24.023542
C	-14.434403	16.737056	25.495975
H	-16.563877	16.314976	25.001848
C	-13.501533	17.686087	25.159258
H	-14.239081	15.930713	26.205062
H	-12.478286	17.780786	25.520964
C	-19.996685	18.252884	20.887507
C	-20.535223	18.977881	19.840153
S	-20.978959	16.841160	21.217203
C	-21.722999	18.400185	19.306297
H	-20.067597	19.886191	19.458199
C	-22.082164	17.238843	19.945593
H	-22.284880	18.822597	18.471301
H	-22.928766	16.586622	19.734122
C	-18.607872	24.496994	18.868217
C	-19.301428	23.371330	18.458039
S	-19.464895	25.285594	20.178183
C	-20.498404	23.140948	19.197172
H	-18.947688	22.727389	17.650751
C	-20.712691	24.089920	20.167222
H	-21.173976	22.302366	19.017963
H	-21.537543	24.155230	20.876738
C	-14.876887	26.045981	15.406948
C	-13.503707	26.190592	15.318301
S	-15.596060	26.111530	13.810680
C	-13.037190	26.341985	13.981035
H	-12.850908	26.156859	16.191714
C	-14.052135	26.311045	13.057849
H	-11.986872	26.459887	13.707520

H	-13.978411	26.399553	11.974193
C	-13.736867	22.587886	32.162915
C	-13.478408	21.238310	32.315210
S	-12.871075	23.512556	33.374739
C	-12.593483	20.953483	33.396652
H	-13.936015	20.479143	31.678826
C	-12.187655	22.082779	34.064895
H	-12.276388	19.948421	33.680755
H	-11.531721	22.156832	34.931657
C	-16.987279	25.930193	29.616896
C	-17.000661	27.187630	30.197569
S	-18.373264	25.741805	28.559839
C	-18.105135	27.989359	29.788971
H	-16.226522	27.523087	30.890244
C	-18.926139	27.345723	28.895982
H	-18.284144	29.004076	30.147315
H	-19.828051	27.724377	28.415945
C	-12.395552	30.200997	24.436170
C	-11.143279	30.552077	24.917129
S	-12.232222	29.379377	22.898197
C	-10.073133	30.149930	24.071806
H	-11.001692	31.060849	25.871859
C	-10.508634	29.494003	22.946305
H	-9.021704	30.335568	24.300032
H	-9.913877	29.073370	22.136215
C	-16.130088	32.240042	27.623405
C	-17.154873	31.829451	28.459073
S	-15.789128	33.937921	27.877806
C	-17.658300	32.870326	29.289589
H	-17.520751	30.802184	28.486047
C	-17.010611	34.065241	29.095093
H	-18.466082	32.734642	30.011082
H	-17.186657	35.017695	29.593494

Final Single Point Energy:	-8358.150806246387 E_h	
Homo:	-0.202699 E_h	-5.5157 eV
Lumo:	-0.130190 E_h	-3.5427 eV

Schematic Cross-Section of the TFTs



X-ray Crystal Structure Determinations

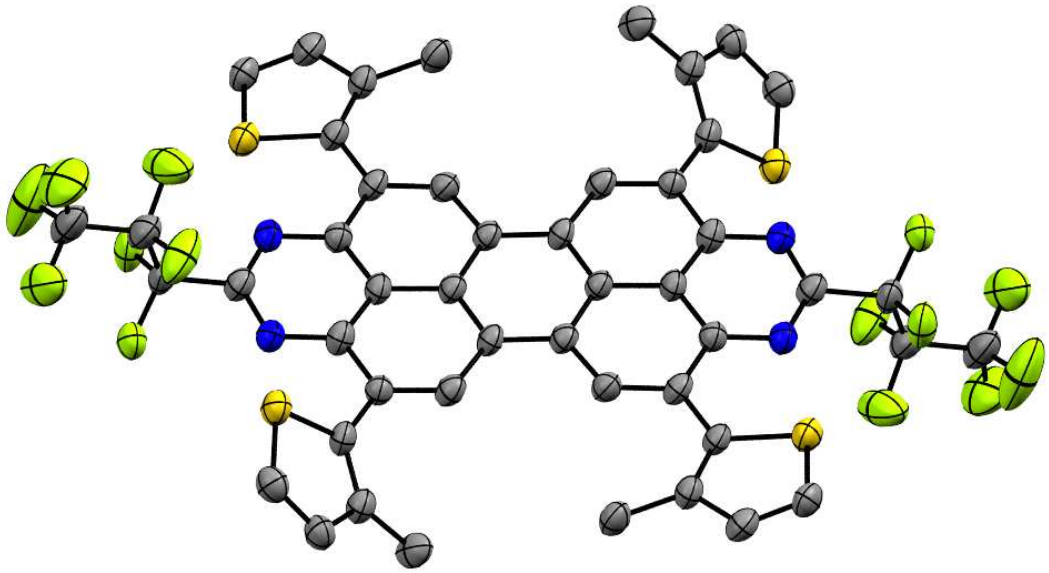
Crystal data and details of the structure determinations are compiled in Tables S1 and S2. Full shells of intensity data were collected at low temperature with a Bruker AXS Smart 1000 CCD diffractometer (Mo-K_a radiation, sealed X-ray tube, graphite monochromator, compound **5**·2 $CHCl_3$) or an Agilent Technologies Supernova-E CCD diffractometer (Mo- or Cu-K_a radiation, microfocus X-ray tube, multilayer mirror optics, all other compounds). Detector frames (typically w-, occasionally j-scans, scan width 0.4...1°) were integrated by profile fitting.[5-7] Data were corrected for air and detector absorption, Lorentz and polarization effects[5] and scaled essentially by application of appropriate spherical harmonic functions.[7-10] Absorption by the crystal was treated with a semiempirical multiscan method (as part of the scaling process), (and) augmented by a spherical correction (compounds **2**, **5**·2 $CHCl_3$, **11**·0.75 $CHCl_3$),[8-10] or numerically (Gaussian grid, all other compounds).[7,11] For datasets collected with the microfocus tube(s) an illumination correction was performed as part of the numerical absorption correction.[10]

The structures were solved by "intrinsic" phasing[12] (compound **11**·0.75 $CHCl_3$) or by the charge flip procedure[13] (all other compounds) and refined by full-matrix least squares methods based on F^2 against all unique reflections.[14] All non-hydrogen atoms were given anisotropic displacement parameters. Hydrogen atoms were generally input at calculated positions and refined with a riding model. When justified by the quality of the data the positions of some hydrogen atoms were taken from difference Fourier syntheses and refined. When found necessary, disordered groups and/or solvent molecules were subjected to suitable geometry and adp restraints.

Crystal Structures of Compounds 2-5, 11

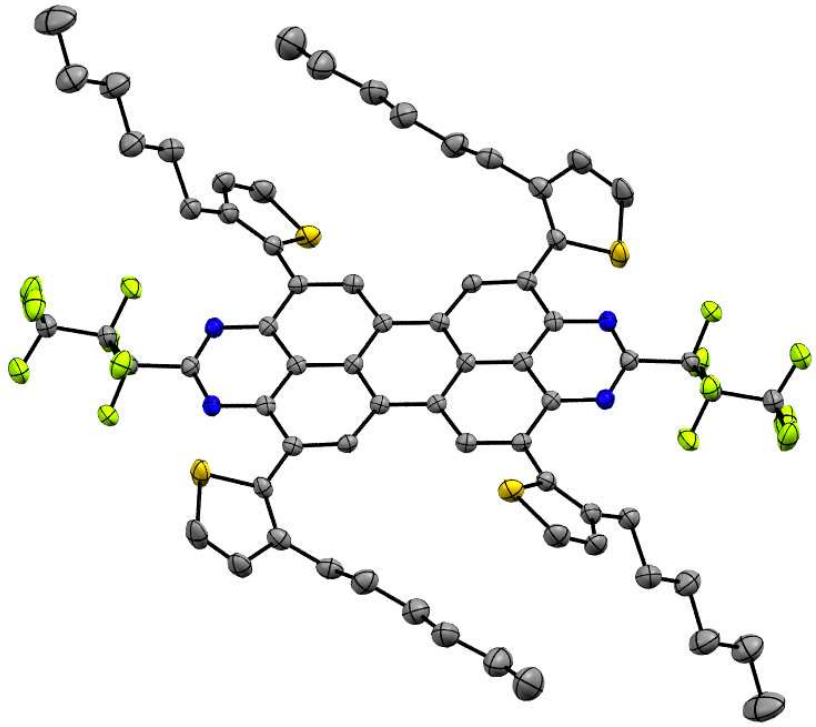
Crystals of compounds **2**-**5** and **11** were grown by slow evaporation of saturated solutions of the compounds in THF (**2**-**4**) or $CHCl_3$ (**5**, **11**), respectively. Crystals of **11** could also be grown by slow evaporation of a pentane solution.

Compound 2:



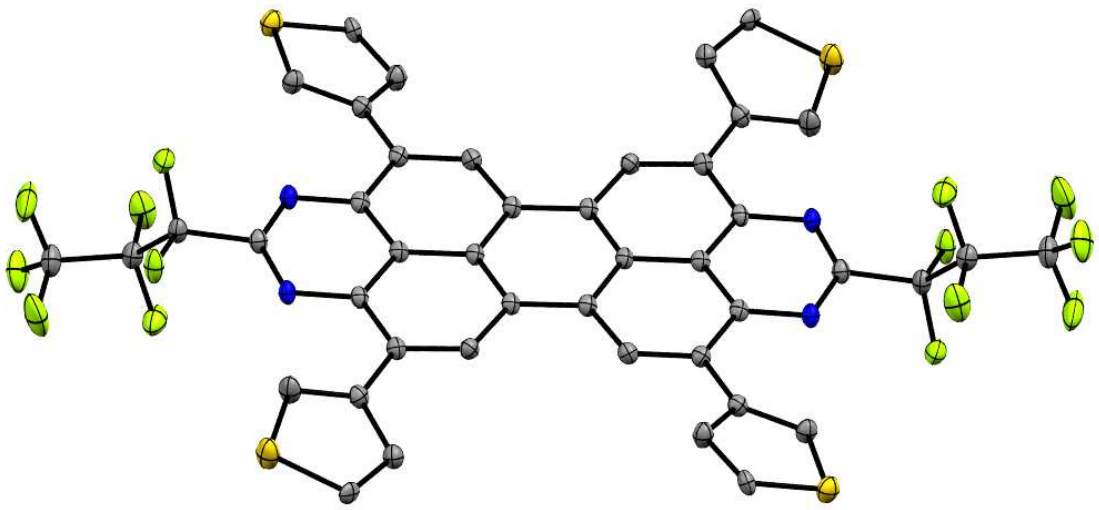
Ortep view (50% probability level) of **2** (C = grey ,N = blue, F = green, S = yellow). Hydrogen atoms are omitted for clarity. Only one of the independent molecules is shown.

Compound 3:



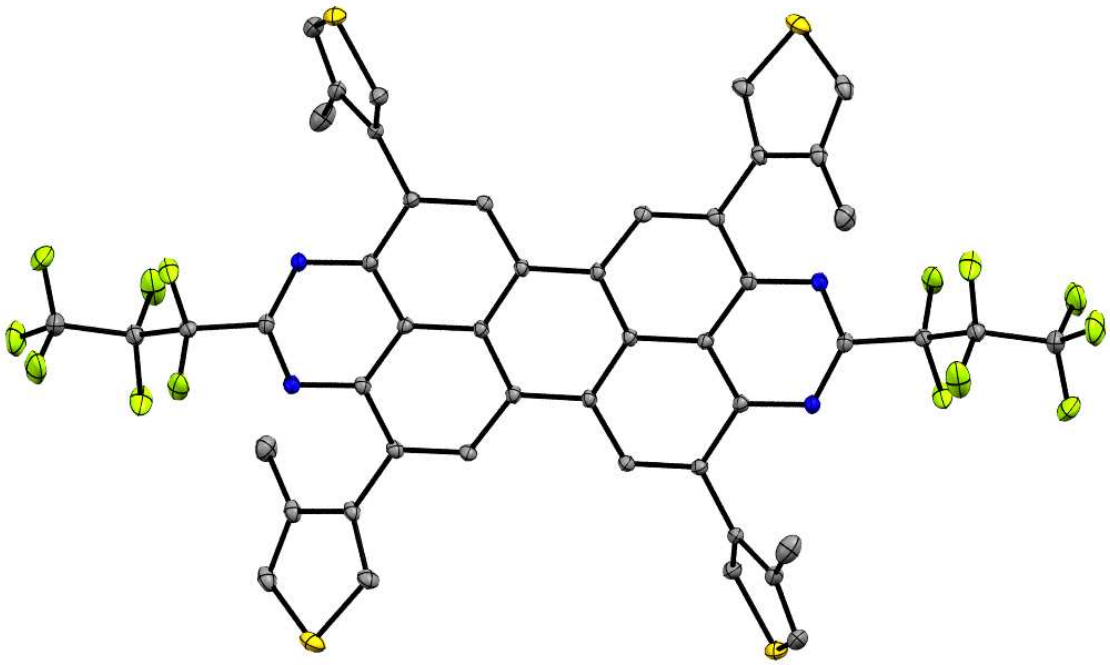
Ortep view (50% probability level) of **3** (C = grey ,N = blue, F = green, S = yellow). Hydrogen atoms are omitted for clarity. Only one of the independent molecules is shown.

Compound 4:



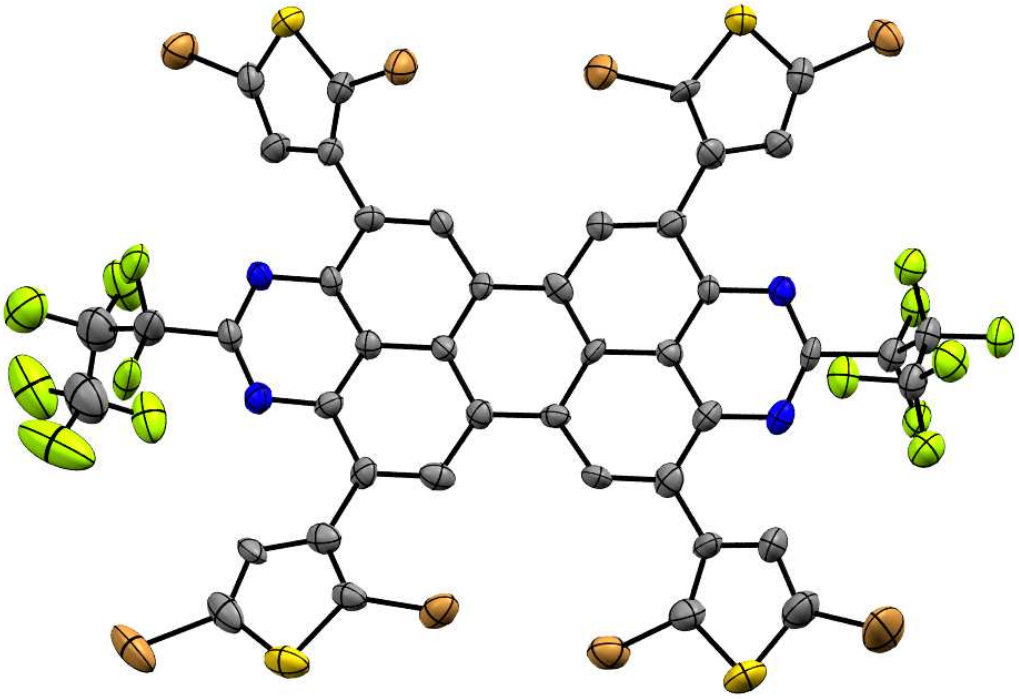
Ortep view (50% probability level) of **4** (C = grey ,N = blue, F = green, S = yellow). Hydrogen atoms and solvent molecules are omitted for clarity.

Compound 5:



Ortep view (50% probability level) of **5** (C = grey ,N = blue, F = green, S = yellow). Hydrogen atoms and solvent molecules are omitted for clarity.

Compound 11:



Ortep view (50% probability level) of **11** (C = grey ,N = blue, F = green, S = yellow, Br = brown). Hydrogen atoms and solvent molecules are omitted for clarity. **O**nly one of the independent molecules is shown.

Table S1. Details of the crystal structure determinations of compounds **2**, **3**, **4**·2 thf and **5**·2 $CHCl_3$.

	2	**3**	**4**·2 thf	**5**·2 $CHCl_3$
formula	$C_{48}H_{24}F_{14}N_4S_4$	$C_{68}H_{64}F_{14}N_4S_4$	$C_{52}H_{32}F_{14}N_4O_2S_4$	$C_{50}H_{26}Cl_6F_{14}N_4S_4$
crystal system	monoclinic	triclinic	monoclinic	monoclinic
space group	$P2_1/n$	$P\bar{1}$	$P2_1/c$	$P2_1/c$
a /Å	16.6520(8)	15.3304(3)	16.1364(3)	14.764(8) [a]
b /Å	19.7591(6)	17.3728(4)	5.19816(7)	8.872(5) [a]
c /Å	20.6578(11)	21.0398(4)	26.6969(5)	19.004(9) [a]
α /°		107.5526(18)		
β /°	112.774(6)	100.5745(16)	98.5684(17)	91.194(15) [a]
γ /°		111.0829(18)		
V /Å^3	6267.1(6)	4708.83(17)	2214.33(6)	2489(2)
Z	6	3	2	2
M_r	1050.95	1331.47	1139.05	1289.69
F_{000}	3180	2070	4146	1292
d_c /Mgm^{-3}	1.671	1.409	1.708	1.721
μ /mm^{-1}	3.052	2.147	2.967	0.610
max., min. transmission factors	1.000, 0.606 [b]	0.909, 0.808 [c]	0.925, 0.554 [c]	0.746, 0.709 [b]
X-radiation, λ /Å	Cu-$K\alpha$, 1.54184	Cu- $K\alpha$, 1.54184	Cu- $K\alpha$, 1.54184	Mo- $K\alpha$, 0.71073
data collect. temperat. /K	120(1)	120(1)	120(1)	100(1)
θ range /°	3.6 to 69.6	4.0 to 71.0	4.0 to 71.0	1.4 to 31.5
index ranges h,k,l	±19, ±23, -25 ... 24	±18, ±21, ±25	±19, ±6, -32 ... 30	±21, -12 ... 13, ±27
reflections measured	220936	126219	168031	60977
unique (R_{int})	11252 (0.2395)	17947 (0.0641)	4258 (0.0860)	8212 (0.0419)
observed ($I \geq 2\sigma(I)$)	5632	13532	4146	6564
data / restraints /parameters	11252 / 284 / 1007	17947 / 0 / 1240	4258 / 18 / 357	8212 / 0 / 354
GooF on F^2	0.966	1.024	1.125	1.032
R indices ($F>4\sigma(F)$) $R(F)$, $wR(F^2)$	0.0758, 0.1728	0.0533, 0.1368	0.0403, 0.0938	0.0430, 0.1072
R indices (all data) $R(F)$, $wR(F^2)$	0.1595, 0.2277	0.0751, 0.1507	0.0415, 0.0945	0.0580, 0.1164
largest residual peaks /eÅ^{-3}	0.534, -0.574	0.865, -0.509	0.434, -0.391	0.954, -0.520

[a] su include systematic error contributions from Monte Carlo simulations. [b] empirical absorption correction. [c] numerical absorption correction.

Table S2. Details of the crystal structure determinations of compounds **11**·0.75 $CHCl_3$ and **11**·0.667 *n*-pentane.

	11·0.75 $CHCl_3$	**11**·0.667 *n*-pentane
formula	$C_{44.50}H_{8.75}Br_8Cl_{2.25}F_{14}N_4S_4$	$C_{47.33}H_{16}Br_8F_{14}N_4S_4$
crystal system	triclinic	monoclinic
space group	*P* -1	$P\,2_1/n$
a /Å	15.2196(7)	15.36041(17)
b /Å	15.3694(5)	25.7224(2)
c /Å	24.0731(6)	20.8946(2)
α /°	101.545(2)	
β /°	102.351(3)	110.8723(13)
γ /°	105.027(3)	
V /Å^3	5113.9(3)	7713.83(16)
Z	4	6
M_r	1712.59	1674.16
F_{000}	3248	4788
d_c /Mgm^{-3}	2.224	2.162
μ /mm^{-1}	10.950	6.493
max., min. transmission factors	0.7500, 0.7359 [a]	1.000, 0.290 [b]
X-radiation, λ /Å	Cu-$K\alpha$, 1.54184	Mo-$K\alpha$, 0.71073
data collect. temperat. /K	120(1)	120(1)
θ range /°	3.6 to 71.2	2.6 to 26.4
index ranges *h,k,l*	±18, -18 ... 17, ±29	±19, ±32, ±26
reflections measured	101070	413499
unique (R_{int})	18912 (0.1438)	15801 (0.1026)
observed ($I \geq 2\sigma(I)$)	10069	13021
data / restraints /parameters	18912 / 476 / 1396	15801 / 24 / 1047
GooF on F^2	1.019	1.022
R indices ($F>4\sigma(F)$) $R(F)$, $wR(F^2)$	0.0783, 0.1761	0.0369, 0.0840
R indices (all data) $R(F)$, $wR(F^2)$	0.1579, 0.2191	0.0500, 0.0894
largest residual peaks /eÅ^{-3}	1.403, -1.309	2.437, -1.008

[a] empirical absorption correction. [b] numerical absorption correction.

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