Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting information

Novel di styryl BODIPY NIR derivatives

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1. NMR spectra

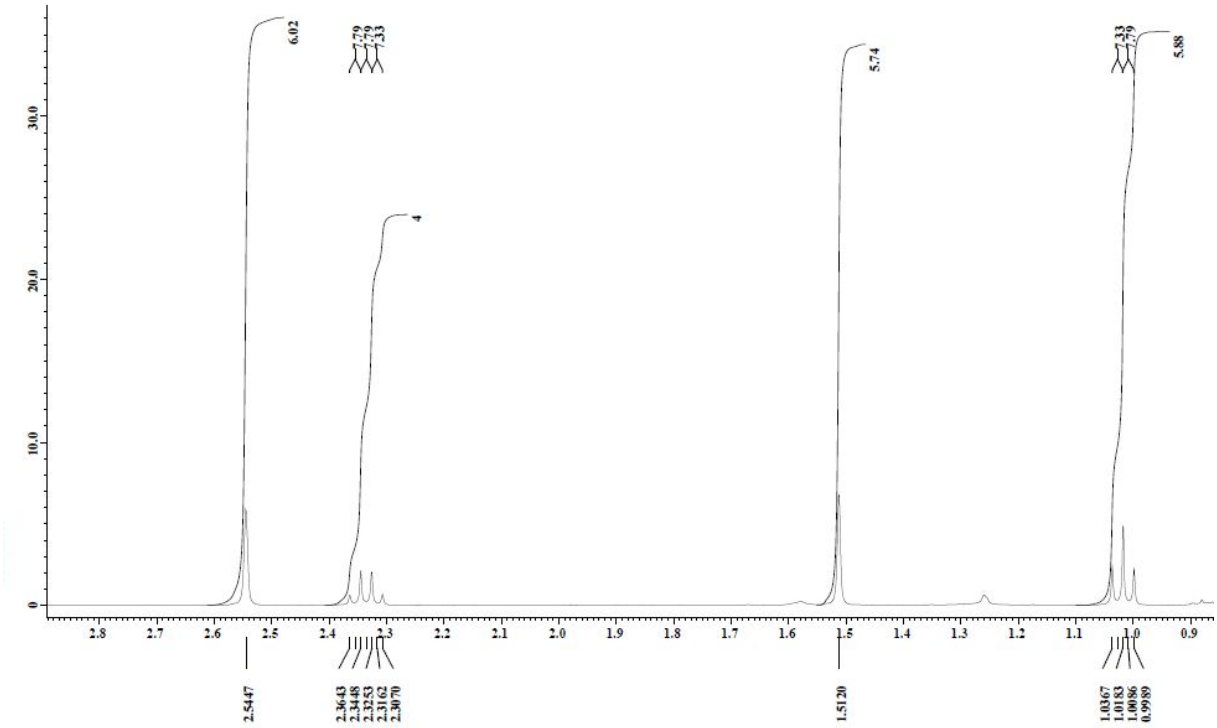

Figure S1 ^{1}H NMR spectra of compound **1**

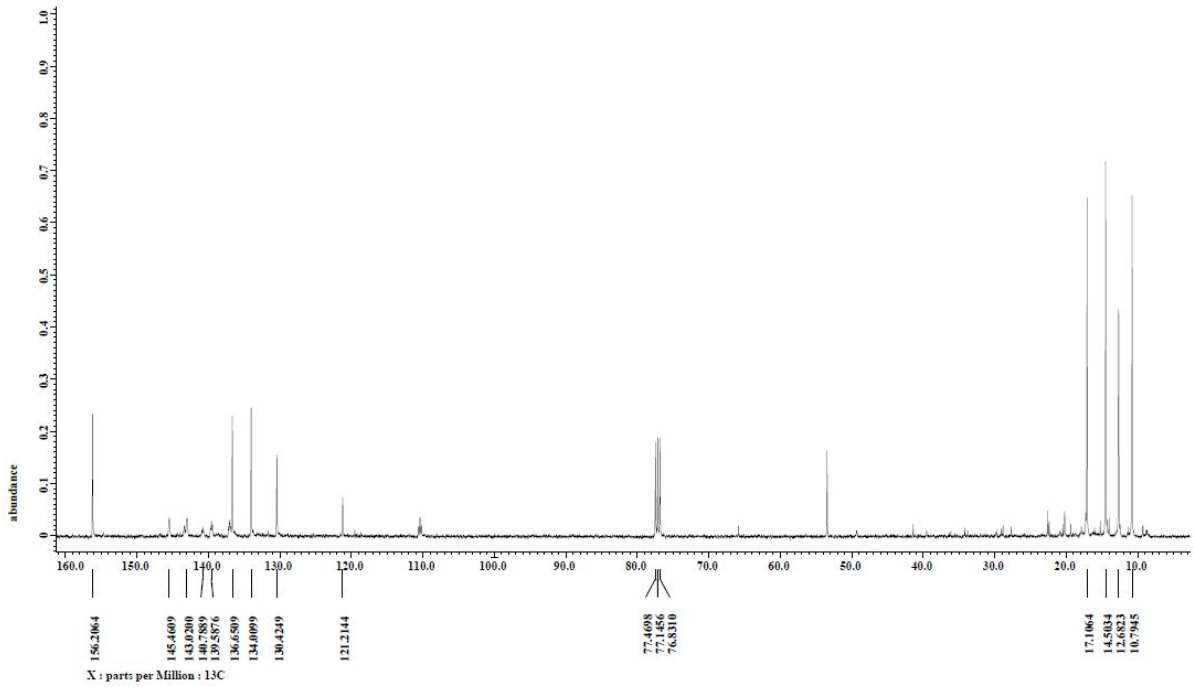

Figure S2 ^{13}C NMR spectra of compound **1**

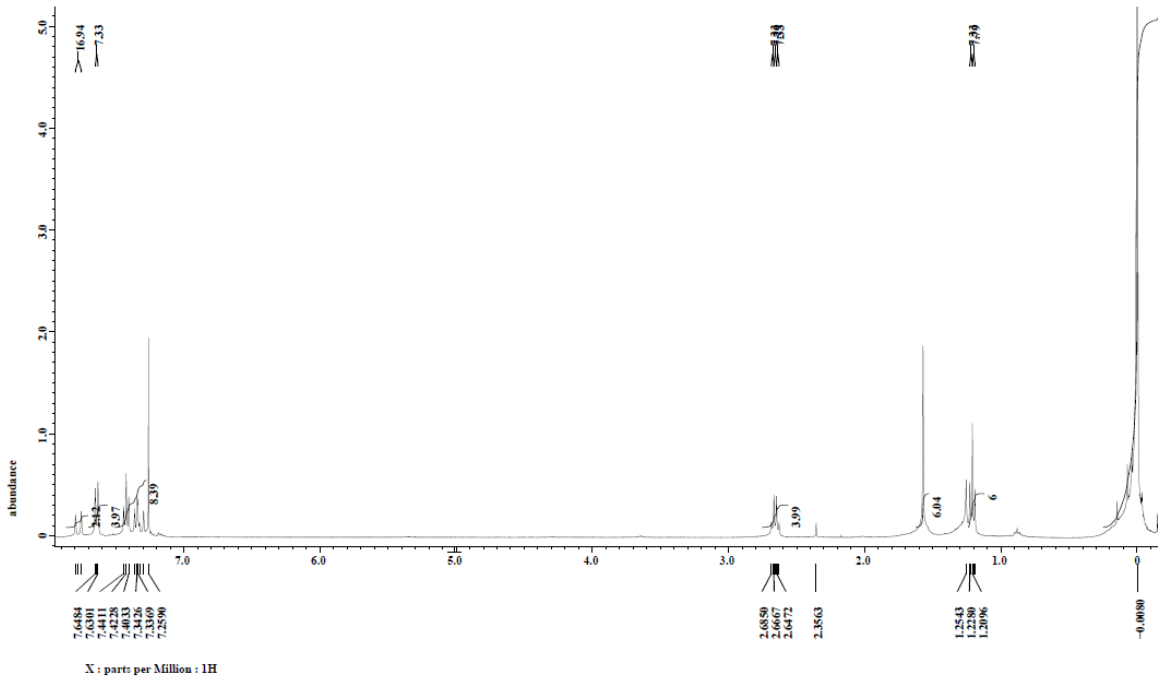

Figure S3 ^{1}H NMR spectra of compound **4a**

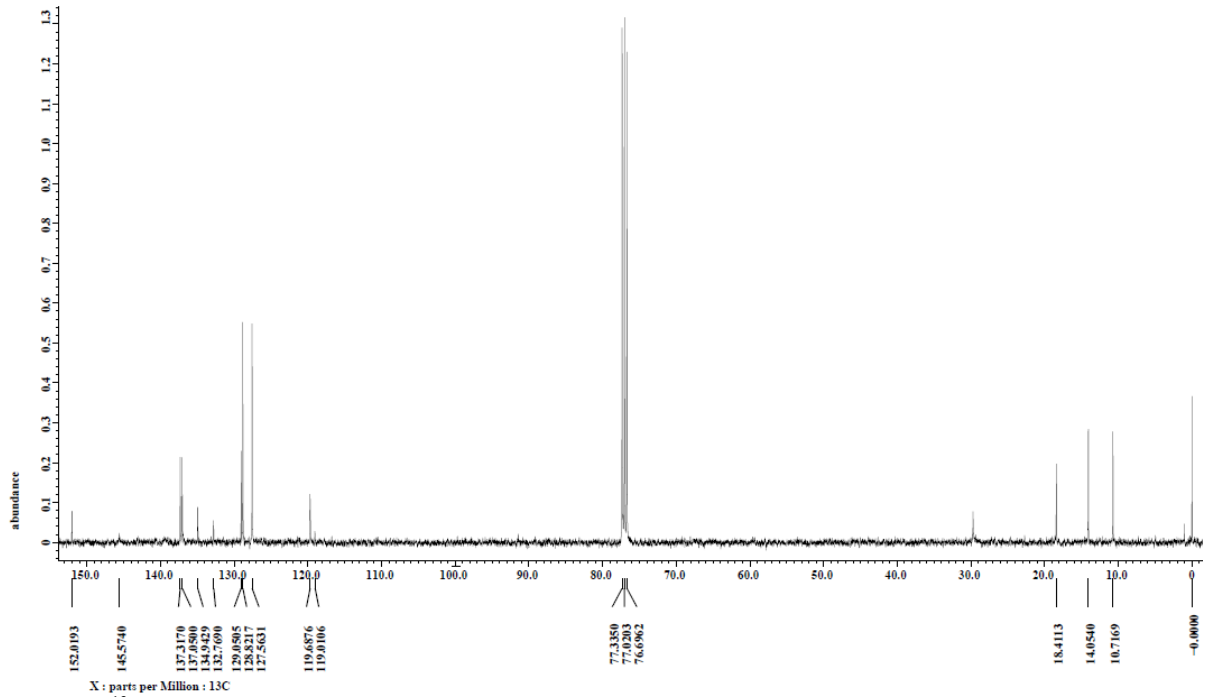

Figure S4 ^{13}C NMR spectra of compound **4a**

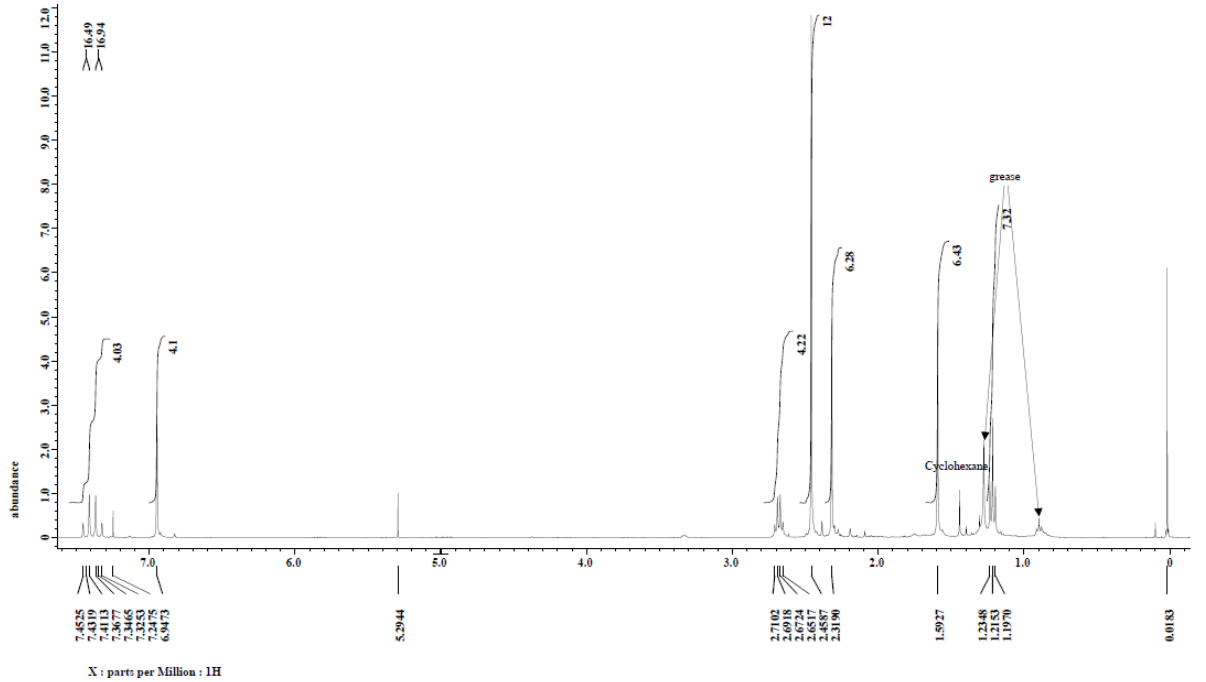

Figure S5 ^{1}H NMR spectra of compound **4b**

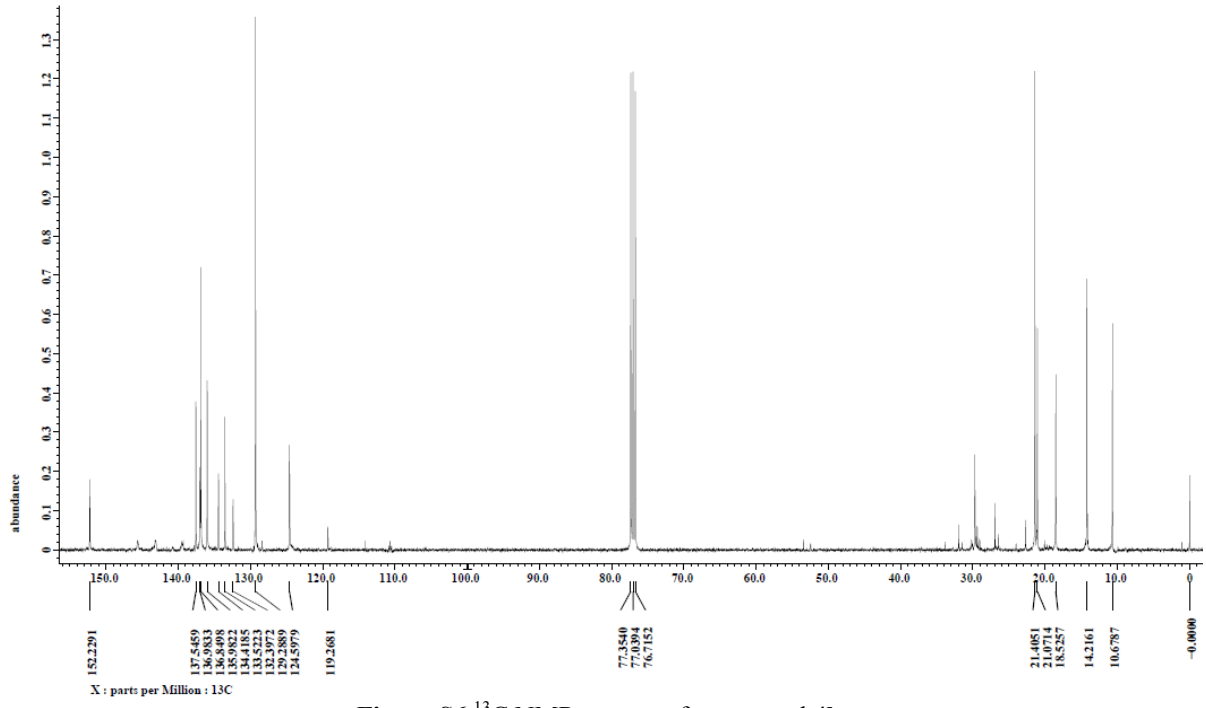

Figure S6 ^{13}C NMR spectra of compound **4b**

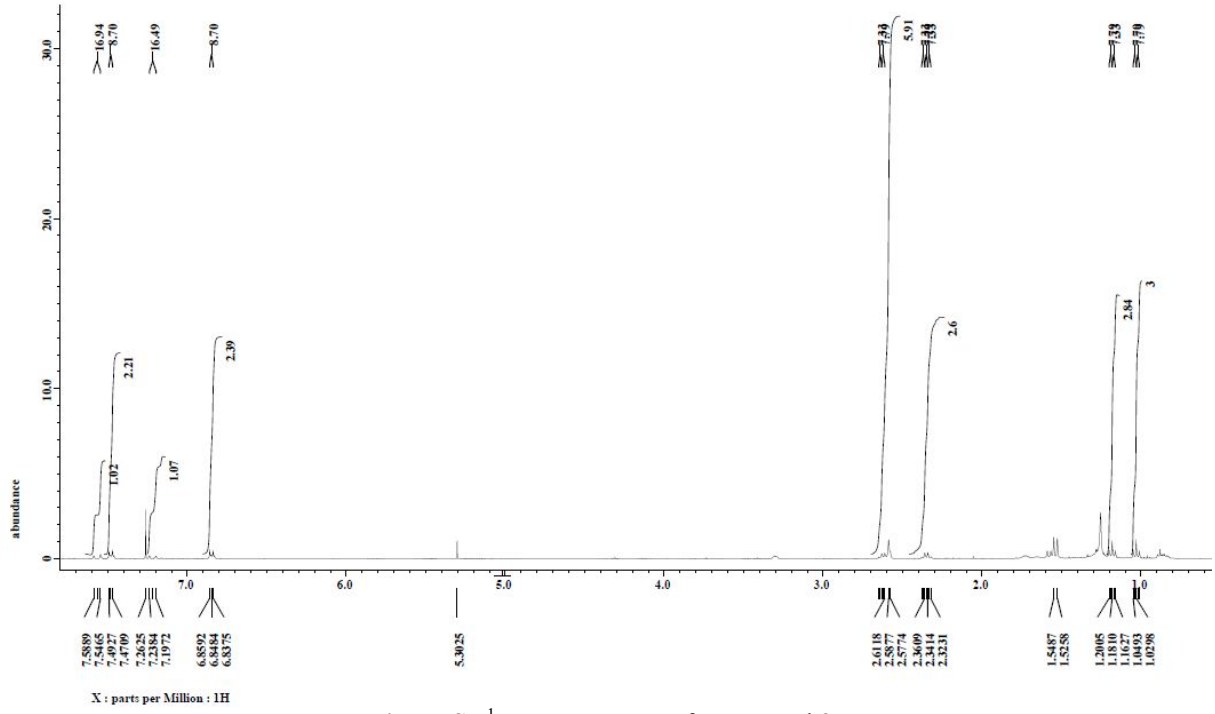

Figure S7 ^{1}H NMR spectra of compound **3c**

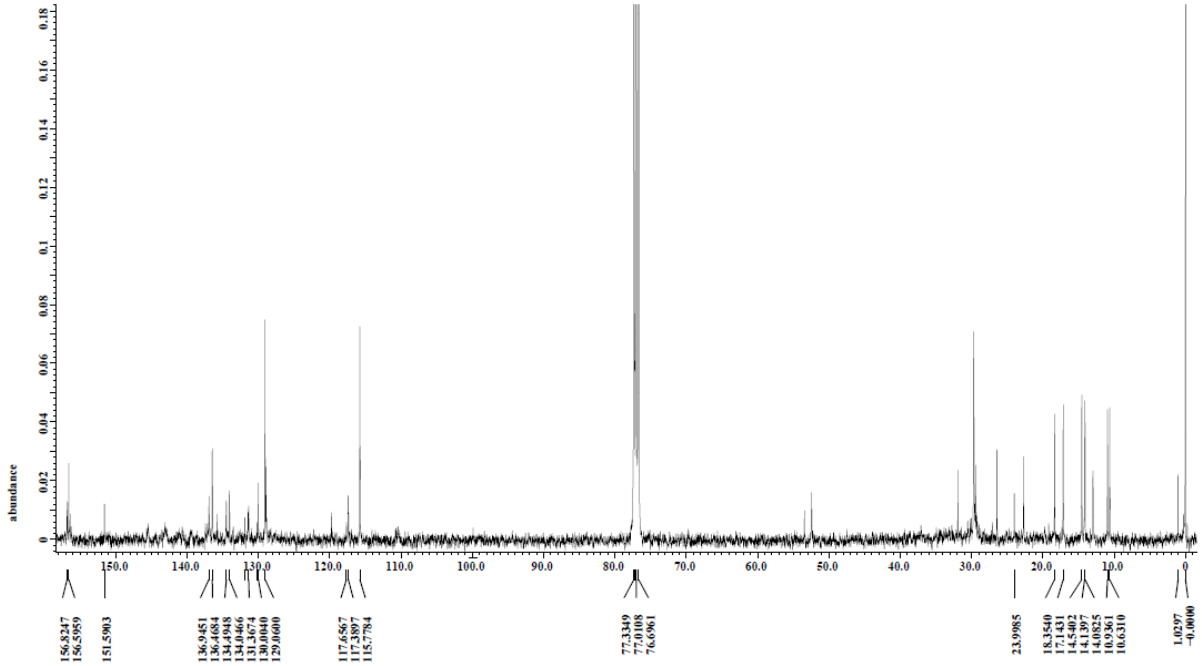

Figure S8 ^{13}C NMR spectra of compound **3c**

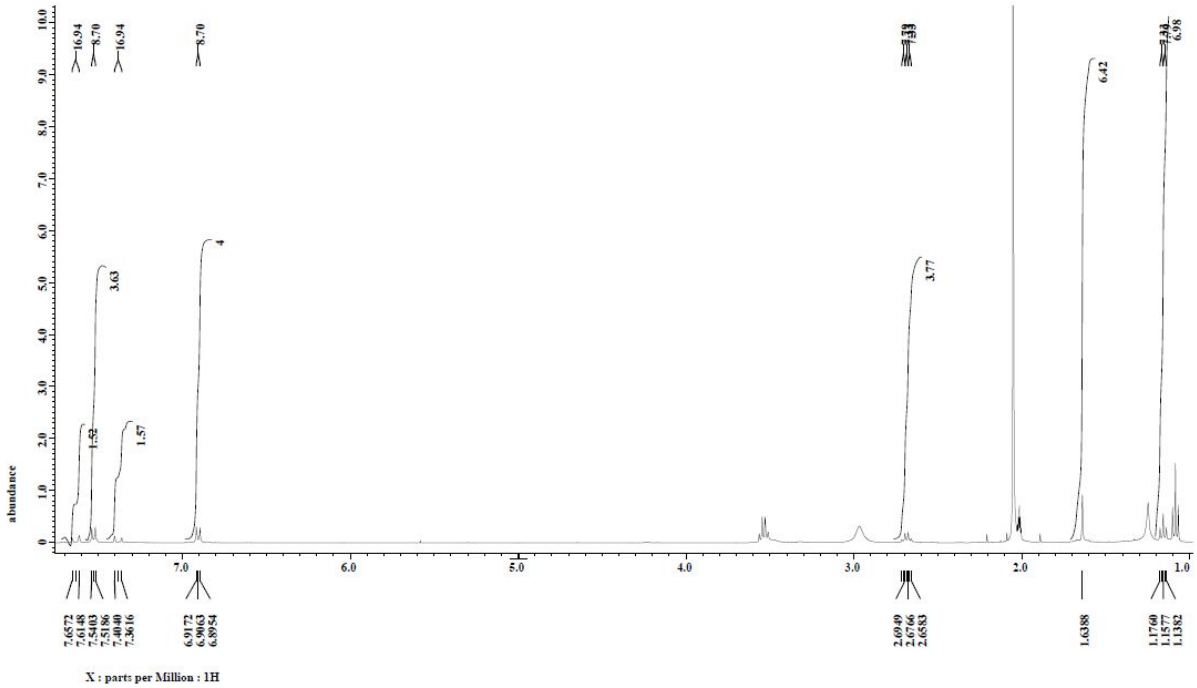

Figure S9 ^{1}H NMR spectra of compound **4c**

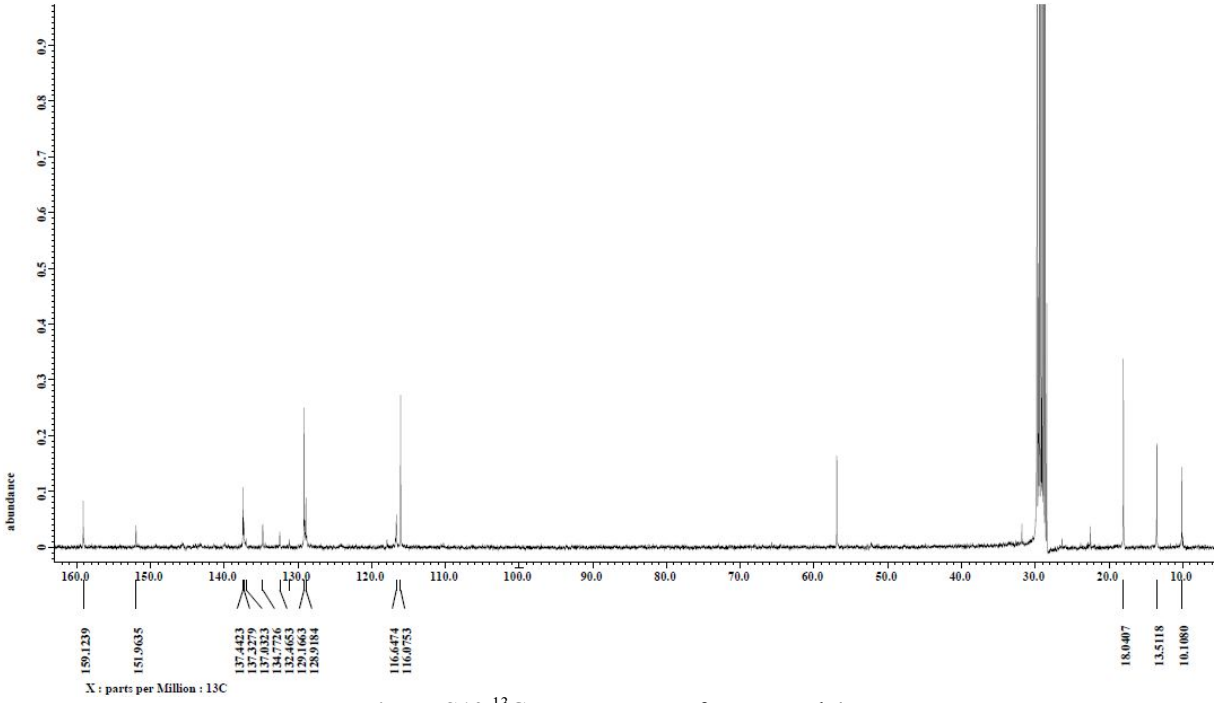

Figure S10 ^{13}C NMR spectra of compound **4c**

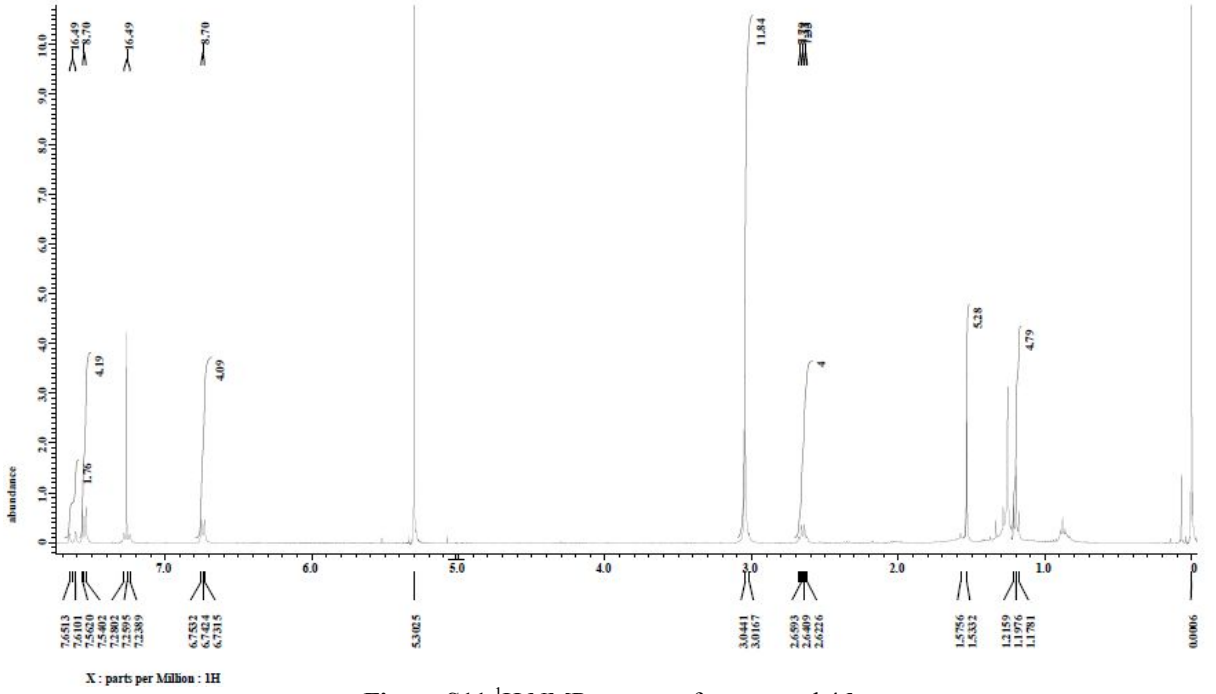

Figure S11 ^{1}H NMR spectra of compound **4d**

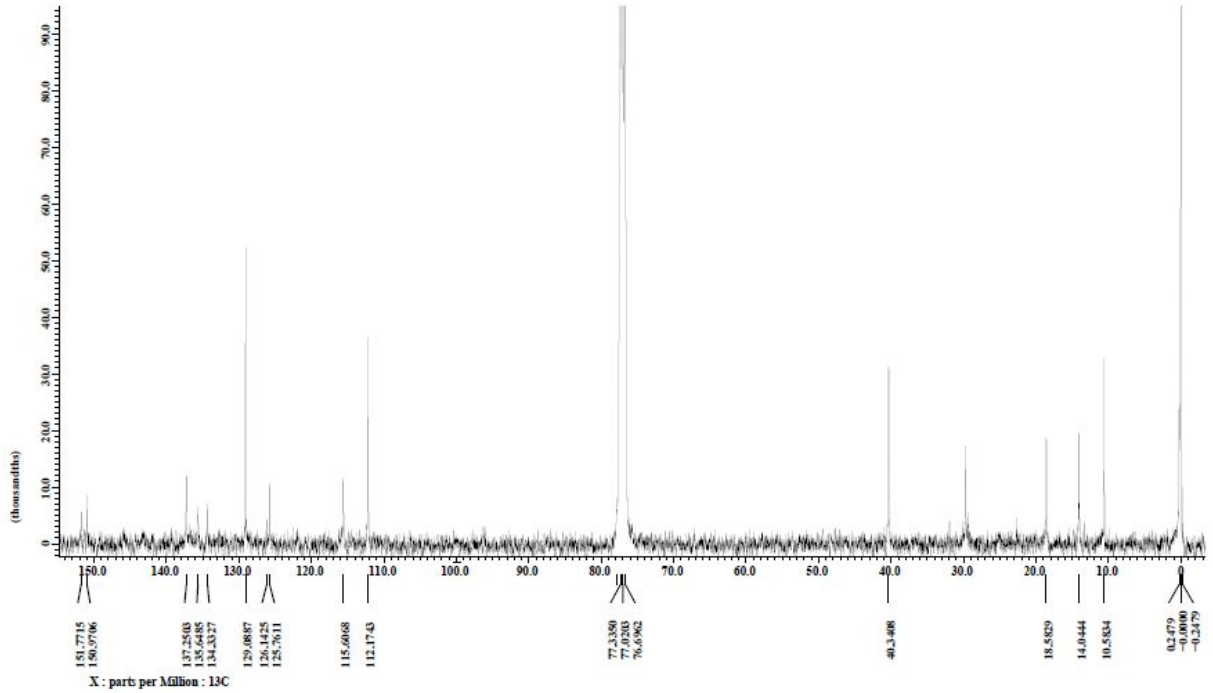

Figure S12 ^{13}C NMR spectra of compound **4d**

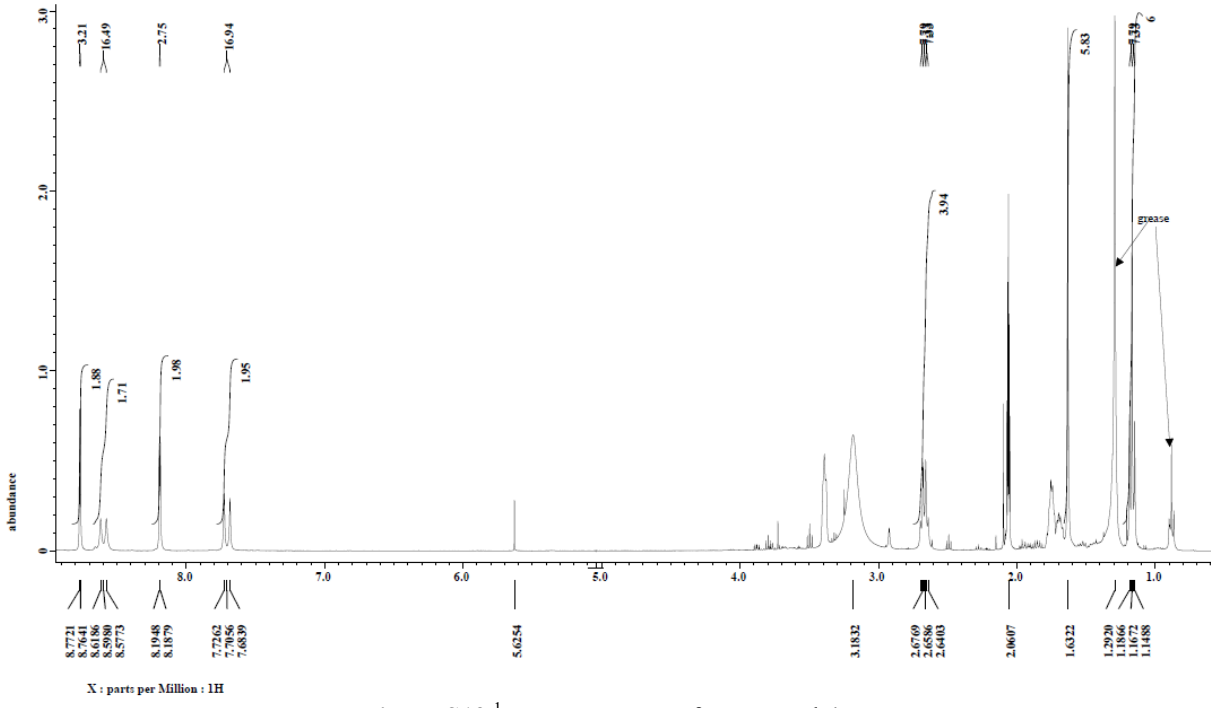

Figure S13 ^{1}H NMR spectra of compound **4e**

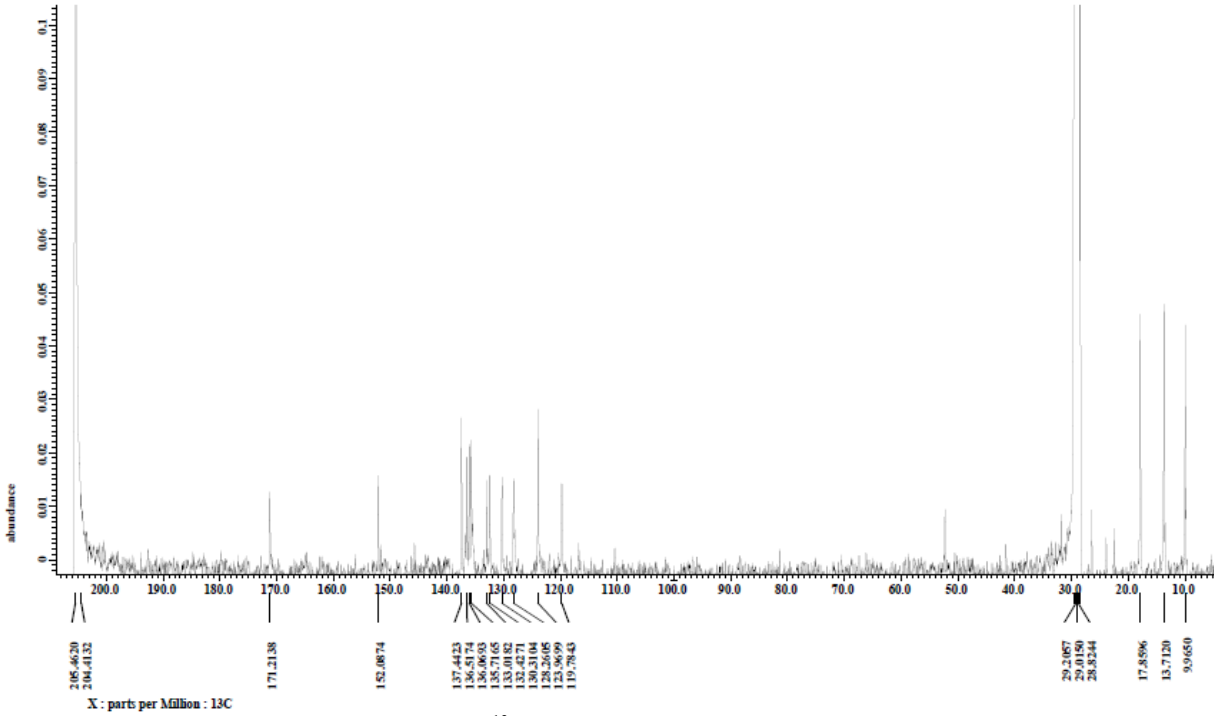

Figure S14 ^{13}C NMR spectra of compound **4e**

2. Spectroscopic results

2.1. Absorption and fluorescence excitation spectra

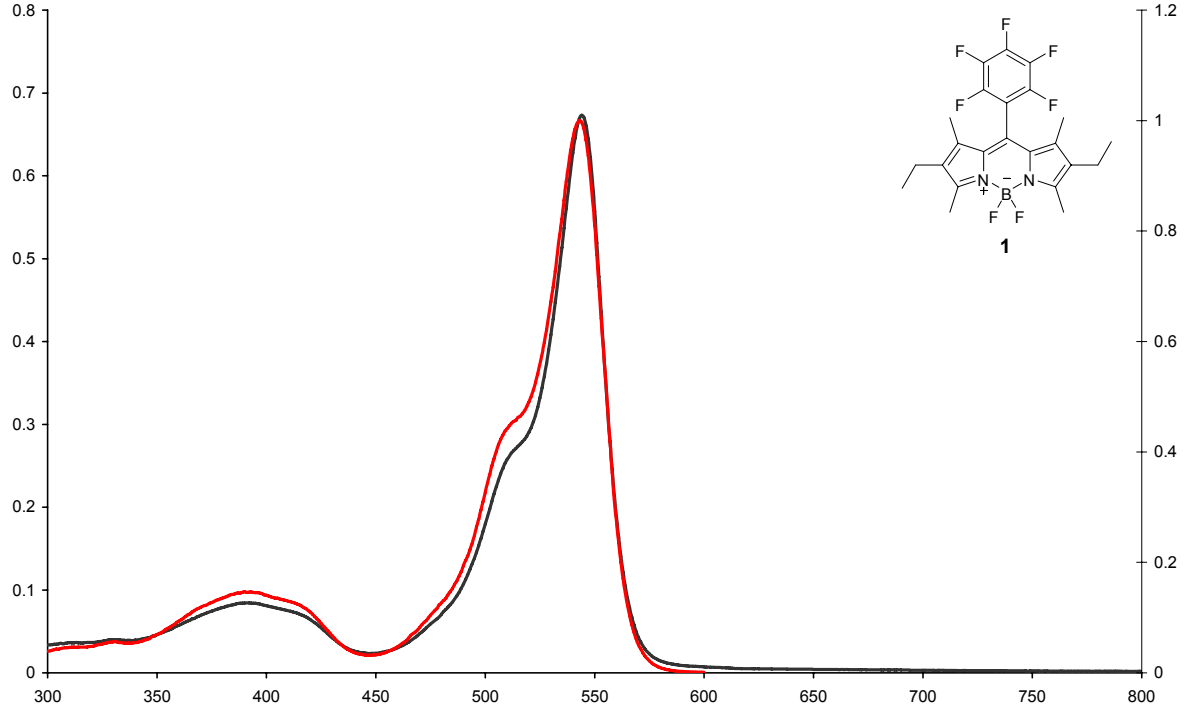

Figure S15 Absorption (black) and fluorescence excitation (red) spectra of compound **1**.

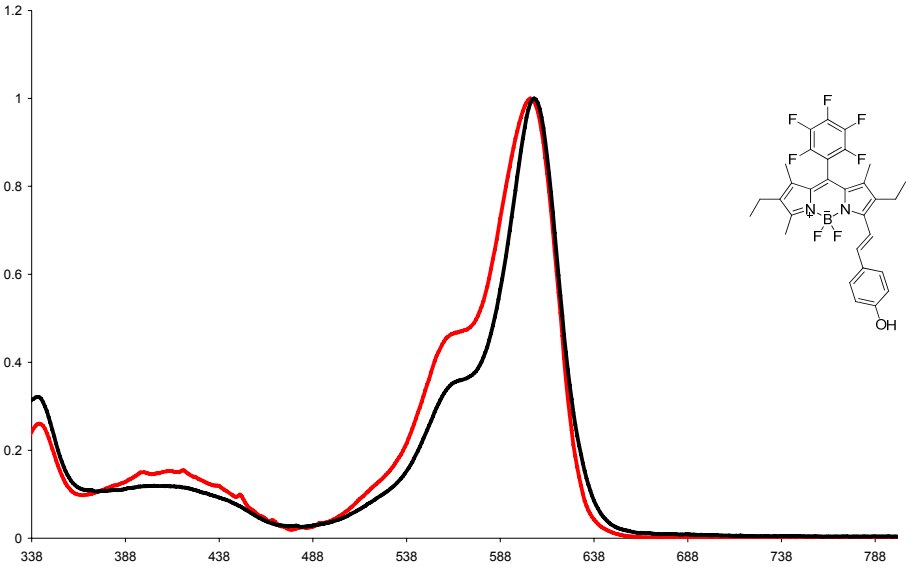

Figure S16 Absorption (black) and fluorescence excitation (red) spectra of compound **3c**.

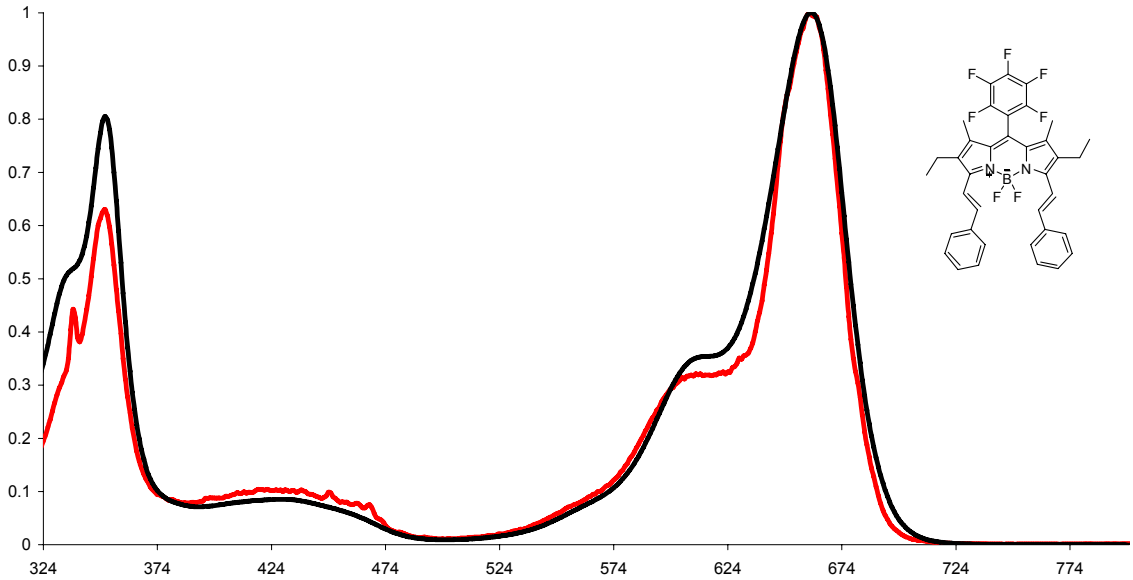

Figure S17 Absorption (black) and fluorescence excitation (red) spectra of compound **4a**.

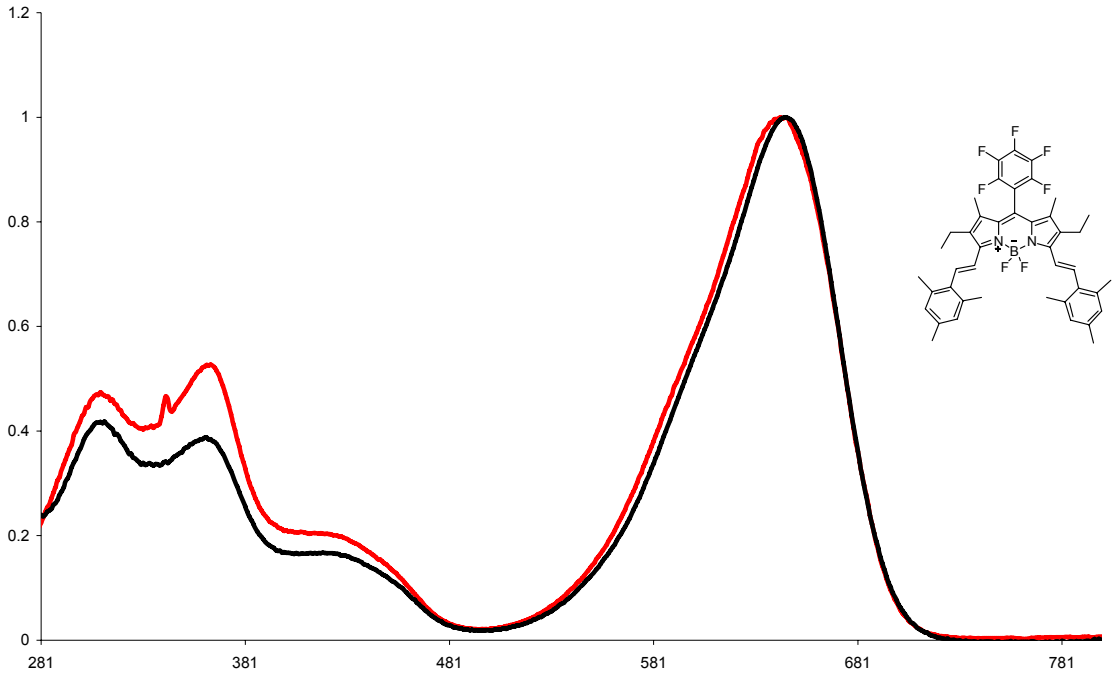

Figure S18 Absorption (black) and fluorescence excitation (red) spectra of compound **4b**.

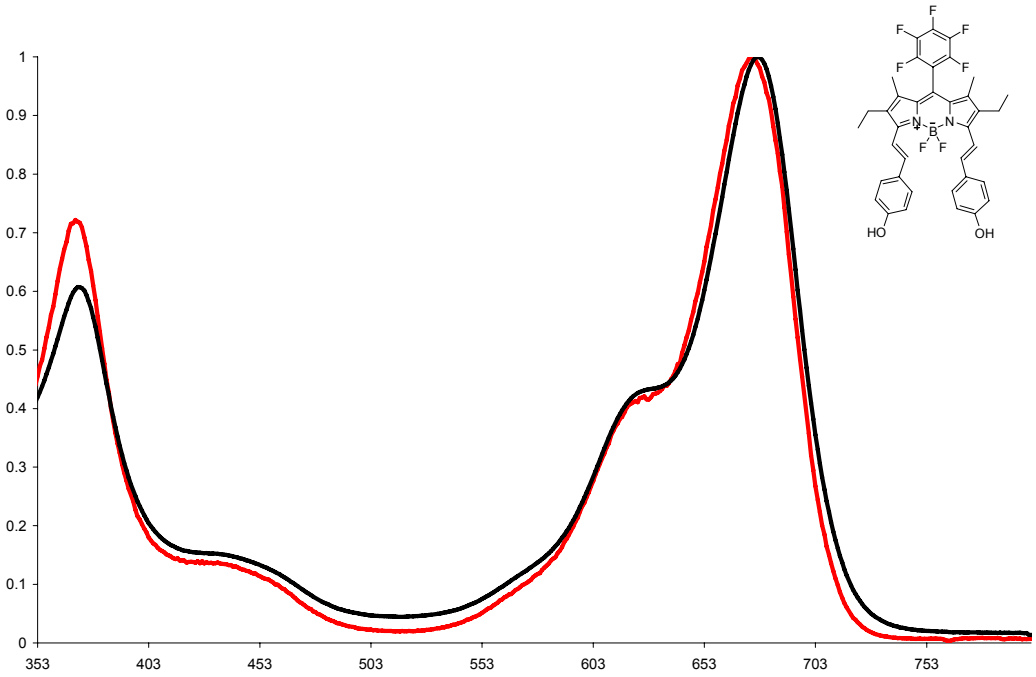

Figure S19 Absorption (black) and fluorescence excitation (red) spectra of compound **4c** (red, solid).

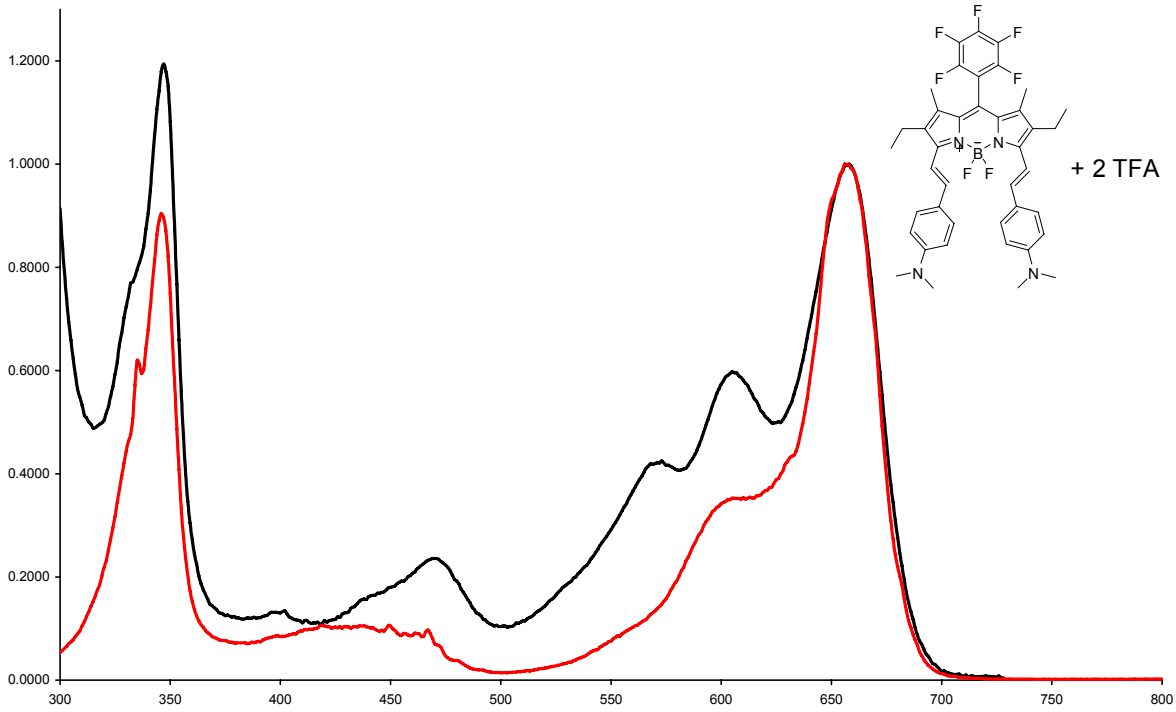

Figure S20: absorption (black) and fluorescence (red) excitation spectra of compound **4d** + $2H^+$.

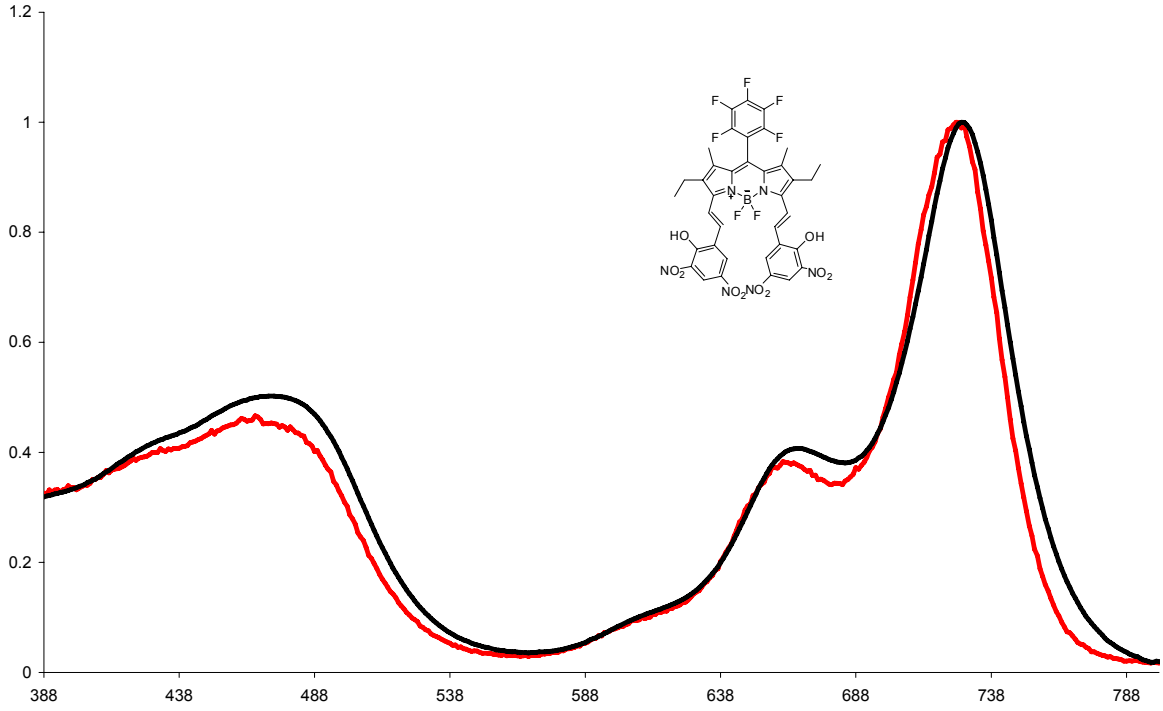

Figure S21 absorption (black) and fluorescence (red) excitation spectra of compound **4e**.

2.2. Solvatochromism

According to Catalán treatment,[1] the observable (here the absorption wavenumber) can be fitted with 4 independent solvent parameters according to the equation:

$$\bar{\nu} = \bar{\nu}^{\circ} + aSP + bSdP + cSA + dSB$$

where $\bar{\nu}$ is the measured wavenumber, $\bar{\nu}^{\circ}$ the gas phase wavenumber, SP the solvent polarizability, SdP the solvent dipolarity, SA the solvent acidity, SB the solvent basicity and a, b, c and d are the regression coefficients describing the sensitivity of $\bar{\nu}$ to the different parameters.

The equation was solved by minimizing the value:

$$\sum_i (\bar{\nu}_{\exp} - \bar{\nu}_{calc})_i^2$$

where $\bar{\nu}_{\exp}$ is the experimental value $\bar{\nu}_{calc}$ is the calculated value using the Catalán equation and i is the solvent with the solver of Excel software and keeping $\bar{\nu}^{\circ}$, a, b, c and d equal for all solvents.

4a

Solvent	Wavelength (nm)	$\bar{\nu}_{\exp}$ (cm^{-1})	SP	SdP	SA	SB
acetonitrile	653	15314	0.645	0.974	0.044	0.286
methanol	654	15291	0.608	0.904	0.605	0.545
cyclohexane	656	15244	0.683			0.073
dichloromethane	661	15129	0.761	0.769	0.04	0.178
dimethyl sulfoxide	663	15083	0.83	1	0.072	0.647
toluene	664	15060	0.782	0.284		0.128

The best fit found is:

$$\bar{\nu} = 16337 - 1636.6 \times SP - 1.5 \times SdP - 249.9 \times SA + 187.5 \times SB$$

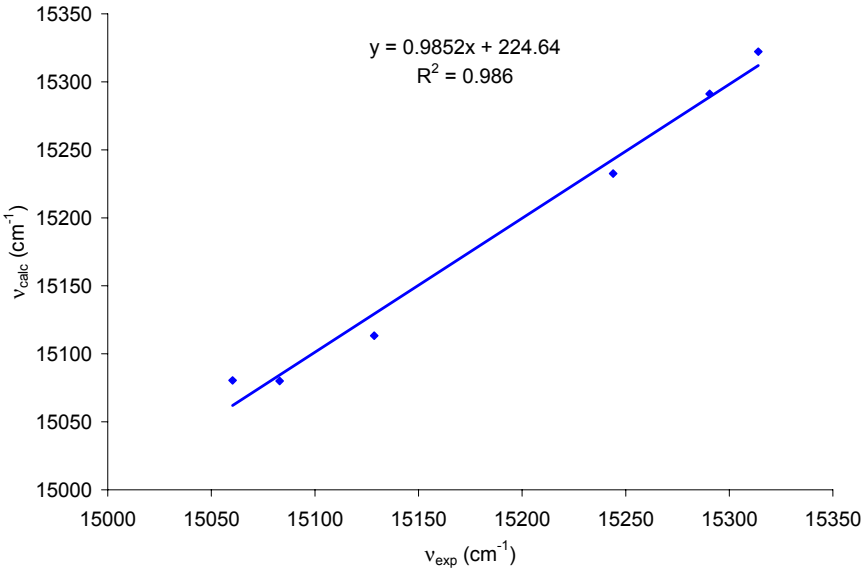

Figure S22 $\bar{\nu}_{calc}$ =f($\bar{\nu}_{\exp}$) plot for **4a**.

4b

Solvent	Wavelength (nm)	$\bar{\nu}_{exp}$ (cm^{-1})	SP	SdP	SA	SB
methanol	590	16949	0.608	0.904	0.605	0.545
acetonitrile	603	16584	0.645	0.974	0.044	0.286
cyclohexane	642	15576	0.683			0.073
tetrhydrofuran	644	15528	0.714	0.634		0.591
dichloromethane	646	15480	0.761	0.769	0.04	0.178
dimethyl sulfoxide	649	15408	0.83	1	0.072	0.647

The best fit found is:

$$\bar{\nu} = 19744 - 6194.7 \times SP + 821.5 \times SdP + 665.6 \times SA - 297.0 \times SB$$

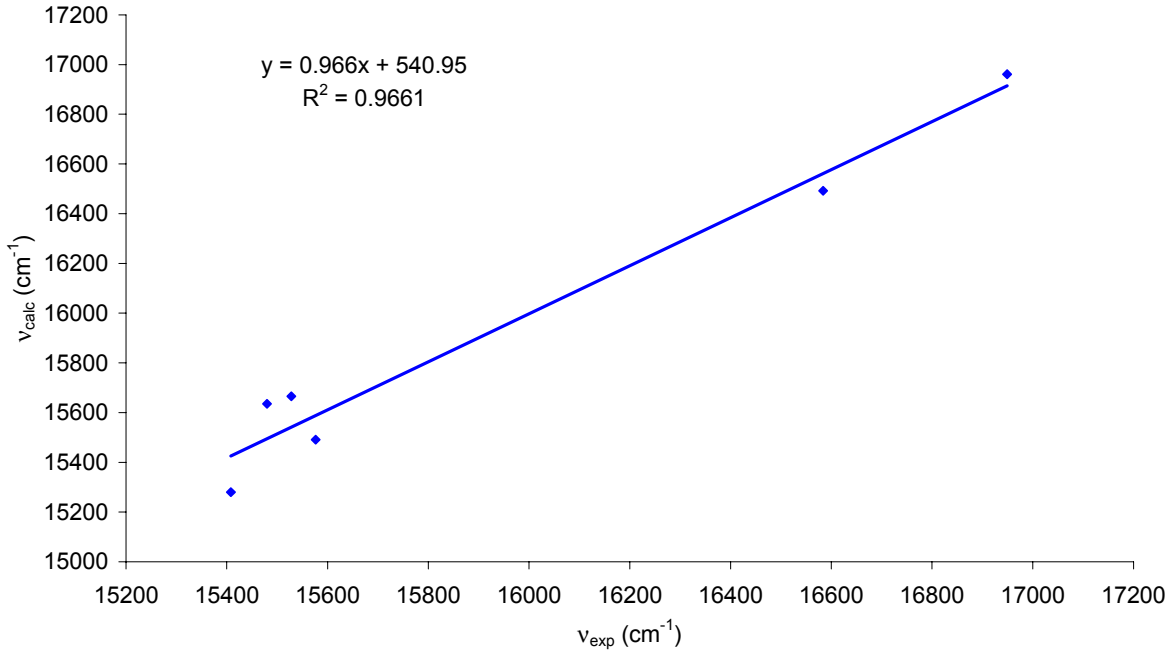

Figure S23 $\bar{\nu}_{calc}$ =f($\bar{\nu}_{exp}$) plot for **4b**.

3. Molecular modelling

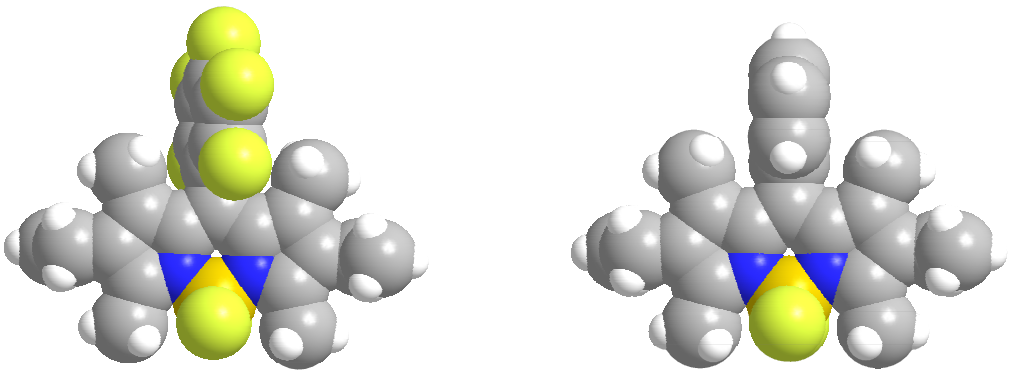

Figure S24 optimized geometry (B3LYP/ 6-31g(d)) of BODIPY **4e** (left) and a model non fluorinated BODIPY (right).

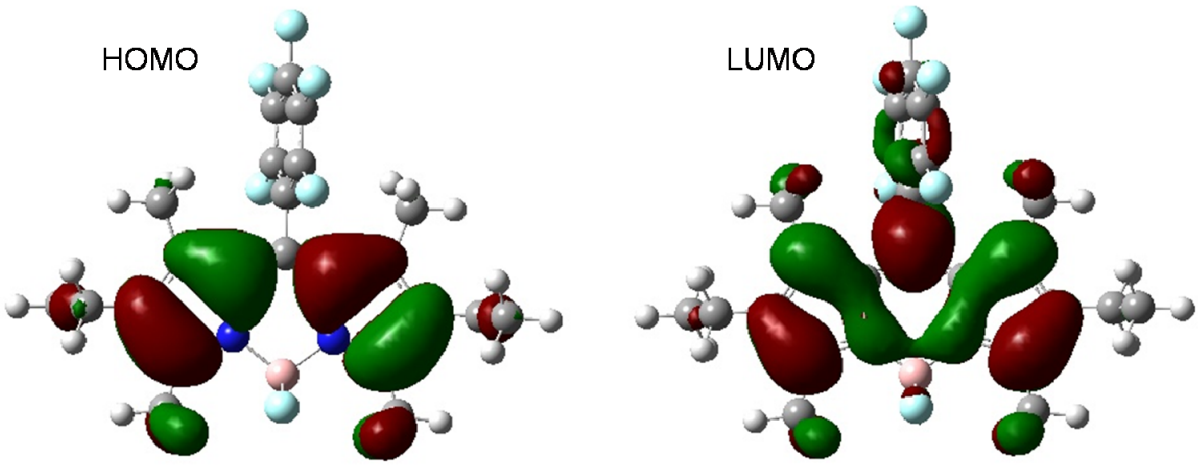

Figure S25 HOMO (left) and LUMO (right) of BODIPY **1** (B3LYP/ 6-31g(d)).

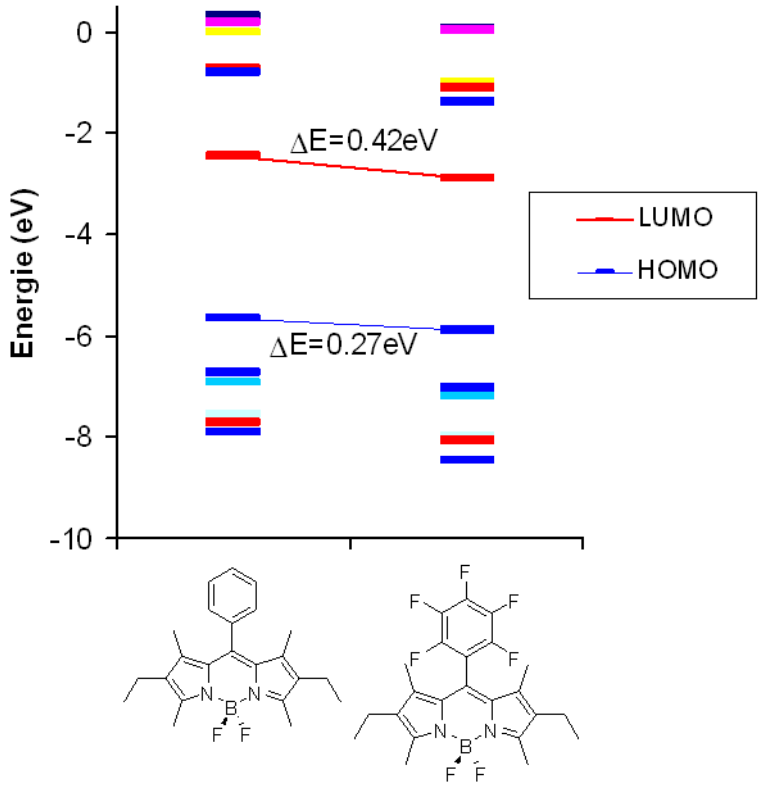

Figure S26 calculated energy (PBE0/6-311+g(d,p)) of the molecular orbital for BODIPY **4e** and its non fluorinated model.

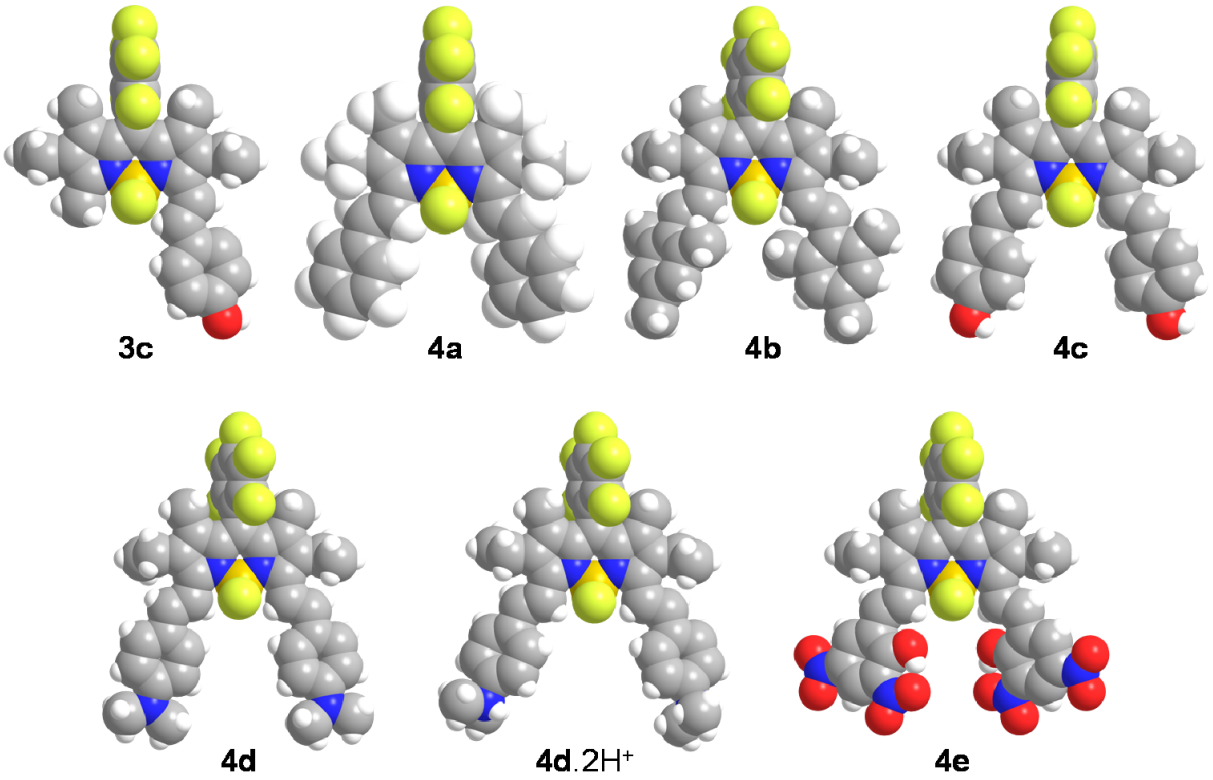

Figure S27 optimized geometry (B3LYP/ 6-31g(d)) of styryl-BODIPY.

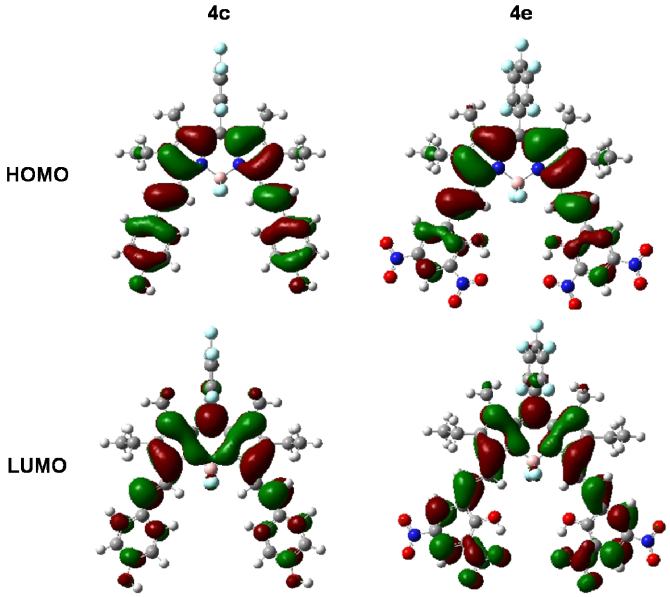

Figure S28 HO (upper) and LUMOs (bottom) of styryl BODIPY **4c** and **4e** (B3LYP/ 6-31g(d)).

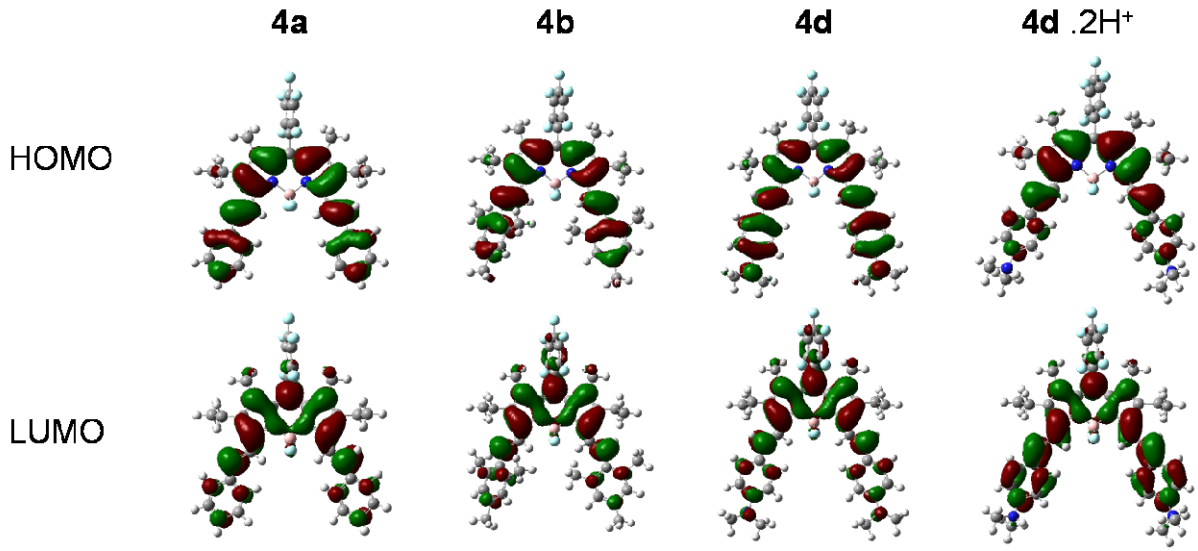

Figure S29 HO (upper) and LUMOs (bottom) of styryl BODIPY **4a**, **4b**, **4d** and **4d**.2H$^+$ (B3LYP/ 6-31g(d)).

Cartesian coordinates of the optimised structures

1

Atomic number	X	Y	Z
6	-1.524441	-0.000415	0.000004
6	-2.252883	-0.435438	-1.109546
6	-3.645346	-0.439322	-1.122408
6	-4.34397	-0.000806	0.000109
6	-3.645378	0.437871	1.122589
6	-2.25292	0.434403	1.109629
6	-0.031391	-0.000088	-0.000049
6	0.651659	1.215276	-0.171523
6	2.46288	2.500803	-0.354377
6	1.33874	3.358067	-0.490569
6	0.652253	-1.215093	0.171391
6	0.19814	-2.561678	0.375974
7	2.047944	-1.233316	0.169796
6	1.340331	-3.357569	0.490457
6	2.464063	-2.499752	0.354413
7	2.047336	1.234149	-0.169856
6	0.196925	2.561631	-0.376156
9	-1.612881	0.888016	2.195722
9	-4.312292	0.868521	2.198387
9	-5.678409	-0.00099	0.000169
9	-4.3122	-0.870169	-2.19816
9	-1.6128	-0.8889	-2.195696
5	2.983519	0.000668	0.000062
9	3.776642	0.16105	1.134124
9	3.776942	-0.159274	-1.133887
6	3.91476	2.853222	-0.392219
1	4.43489	2.242896	-1.137146
1	4.059497	3.909922	-0.62688
1	4.384811	2.636298	0.573421
6	1.403016	-4.848506	0.688185
1	2.299302	-5.104839	1.266219
1	0.555095	-5.176217	1.302137

6	1.408668	-5.646713	-0.62917
1	2.26846	-5.37447	-1.251439
1	1.45843	-6.724147	-0.433444
1	0.503205	-5.448534	-1.213463
6	-1.212105	-3.071668	0.446757
1	-1.840913	-2.477265	1.116913
1	-1.691675	-3.073563	-0.539763
1	-1.225873	-4.102205	0.812052
6	-1.21354	3.070985	-0.447143
1	-1.842188	2.475898	-1.116828
1	-1.69302	3.073341	0.53943
1	-1.227763	4.101278	-0.81311
6	1.400747	4.84903	-0.688365
1	2.296959	5.105749	-1.266339
1	0.552725	5.176329	-1.302395
6	1.405944	5.647306	0.628953
1	2.265835	5.375496	1.251273
1	1.455207	6.724752	0.433171
1	0.500547	5.448736	1.213216
6	3.916105	-2.851476	0.392388
1	4.386166	-2.634203	-0.573182
1	4.435855	-2.240984	1.137451
1	4.061333	-3.908143	0.626943

3c

Atomic number	X	Y	Z
6	2.931093	-0.59642	0.022393
6	3.494741	-1.066803	1.202551
6	4.759504	-1.634111	1.234889
6	5.490843	-1.738992	0.061048
6	4.954042	-1.277499	-1.131546
6	3.687936	-0.71238	-1.136902
6	1.581862	0.024691	0.012585
6	1.486404	1.413178	0.121843
6	0.396203	3.338887	0.213571
6	1.77477	3.646833	0.286715
6	0.451658	-0.787237	-0.106133
6	0.343241	-2.198573	-0.310064
7	-0.825549	-0.245495	-0.078771
6	-1.005858	-2.478343	-0.420673
6	-1.717135	-1.25067	-0.25692
6	-3.150882	-1.189964	-0.285985
1	-3.597743	-2.126353	-0.606696
7	0.23926	2.009902	0.116471
6	2.46961	2.441641	0.229146
9	3.201289	-0.279148	-2.295075
9	5.654205	-1.377905	-2.25362
9	6.69886	-2.279337	0.078962
9	5.273291	-2.076228	2.374758
9	2.81861	-0.98072	2.342693
5	-1.116531	1.269759	0.090281
9	-1.888216	1.741114	-0.970229
9	-1.782449	1.507262	1.303535

6	-3.978479	-0.180024	0.062346
1	-3.55597	0.740501	0.44454
6	-5.428452	-0.211267	0.008991
6	-6.175279	-1.262071	-0.543689
6	-6.141041	0.8767	0.538948
6	-7.557818	-1.23336	-0.553885
1	-5.672113	-2.116294	-0.983885
6	-7.523189	0.917593	0.53594
1	-5.585346	1.706336	0.965374
6	-8.240509	-0.142693	-0.011372
1	-8.115607	-2.058034	-0.991135
1	-8.063721	1.761311	0.949774
8	-9.592852	-0.063317	0.003372
1	-9.966594	-0.848084	-0.40454
6	-0.753382	4.277332	0.228352
1	-1.518347	3.938263	0.930546
1	-0.429553	5.2807	0.507157
1	-1.223649	4.324306	-0.758904
6	-1.634782	-3.822029	-0.615798
1	-2.504577	-3.732348	-1.275537
1	-0.936919	-4.473589	-1.150576
6	-2.051844	-4.490178	0.695864
1	-2.772548	-3.873156	1.239787
1	-2.508985	-5.467053	0.51182
1	-1.187348	-4.636916	1.349586
6	1.439027	-3.208611	-0.394462
1	2.149136	-2.983658	-1.194706
1	2.005161	-3.278324	0.538915
1	1.025196	-4.198303	-0.593707
6	3.95535	2.306977	0.261511
1	4.293842	1.603412	1.02661
1	4.355588	1.966644	-0.699149
1	4.416484	3.272769	0.476749
6	2.350798	5.024797	0.369708
1	1.670061	5.67116	0.93382
1	3.278076	4.999652	0.951959
6	2.626139	5.649063	-0.999313
1	1.707484	5.724322	-1.588395
1	3.046478	6.654134	-0.897428
1	3.33328	5.041362	-1.571425

4a

Atomic number	X	Y	Z
6	-1.718895	2.562853	-0.213021
6	-0.597735	3.375711	-0.284045
6	0.544491	2.523559	-0.215868
7	0.128484	1.240062	-0.118886
6	-1.249733	1.21624	-0.101267
6	-1.249708	-1.21631	0.101053
6	-1.718869	-2.562903	0.213055
7	0.128509	-1.240128	0.118607
6	-0.597711	-3.375748	0.284207
6	0.54452	-2.523616	0.215803

6	-1.931289	-0.000041	-0.000112
5	1.050508	-0.000048	-0.000422
9	1.856594	-0.113252	-1.135752
9	1.857309	0.113143	1.134411
6	-3.12912	-3.048884	0.260384
1	-3.734969	-2.501896	0.986491
1	-3.621177	-2.962284	-0.713985
1	-3.155962	-4.103944	0.538737
6	-3.129142	3.048859	-0.260229
1	-3.735116	2.501753	-0.986138
1	-3.621049	2.962455	0.714235
1	-3.155995	4.103869	-0.538775
6	-0.598847	-4.862205	0.451971
1	-1.44828	-5.149528	1.080938
1	0.291777	-5.164471	1.010665
6	-0.678613	-5.629987	-0.869518
1	-0.665464	-6.710333	-0.697109
1	-1.598694	-5.384876	-1.407735
1	0.155797	-5.379898	-1.53126
6	-0.59887	4.862198	-0.451544
1	-1.448216	5.149619	-1.080586
1	0.291838	5.164574	-1.010045
6	-0.678837	5.629746	0.870068
1	-0.666246	6.710123	0.697814
1	-1.598721	5.384103	1.40838
1	0.155791	5.379977	1.531657
6	-3.416084	-0.000042	-0.000052
6	-4.139098	0.248156	1.160631
6	-4.139196	-0.248216	-1.16068
6	-5.525481	0.249385	1.174285
6	-5.525579	-0.2494	-1.174228
6	-6.22039	0.000006	0.000055
9	-3.502234	0.493014	2.300839
9	-6.189606	0.489521	2.296691
9	-7.543571	0.000028	0.000106
9	-6.189799	-0.489512	-2.296583
9	-3.502427	-0.493095	-2.300938
6	1.949394	2.823244	-0.295486
6	2.530194	4.012869	-0.03814
1	2.571537	1.977638	-0.566991
1	1.92006	4.844222	0.30052
6	3.954096	4.306626	-0.130829
6	4.398624	5.587792	0.224606
6	4.909147	3.372543	-0.5611
6	5.74213	5.928374	0.155644
1	3.672912	6.323426	0.560252
6	6.249723	3.712997	-0.630036
1	4.601683	2.37226	-0.846564
6	6.674534	4.991204	-0.272735
1	6.061472	6.926687	0.436533
1	6.972453	2.976627	-0.966353
1	7.726138	5.252198	-0.329288
6	1.949425	-2.823281	0.295281
6	2.530207	-4.013058	0.038562

1	2.571653	-1.977511	0.566072
1	1.92008	-4.844619	-0.299589
6	3.954146	-4.306656	0.131171
6	4.399011	-5.5873	-0.225721
6	4.908913	-3.372904	0.56279
6	5.742595	-5.927633	-0.15706
1	3.67351	-6.322701	-0.562335
6	6.249565	-3.713114	0.631438
1	4.601143	-2.373115	0.849655
6	6.67473	-4.990759	0.272552
1	6.062207	-6.925524	-0.439137
1	6.97207	-2.977016	0.968835
1	7.72639	-5.25157	0.328901

4b

Atomic number	X	Y	Z
6	-2.451998	2.567613	-0.237379
6	-1.324332	3.385369	-0.298676
6	-0.183087	2.530395	-0.242985
7	-0.592843	1.242527	-0.151393
6	-1.982955	1.213845	-0.127295
6	-1.96134	-1.227615	0.117398
6	-2.406993	-2.588999	0.232012
7	-0.570935	-1.232338	0.140493
6	-1.265605	-3.386927	0.296731
6	-0.138816	-2.512732	0.23672
6	-2.658469	-0.012949	-0.00492
5	0.352772	0.013689	-0.004598
9	1.153389	-0.117895	-1.140657
9	1.148228	0.159852	1.133166
6	-3.813965	-3.110462	0.286037
1	-4.442101	-2.550061	0.985072
1	-4.298768	-3.072448	-0.697179
1	-3.818992	-4.156083	0.605934
6	-3.86755	3.065395	-0.290712
1	-4.486893	2.493722	-0.988439
1	-4.350937	3.020637	0.692978
1	-3.89009	4.110437	-0.611893
6	-4.151184	-0.025724	-0.003628
6	-4.882171	0.353601	1.124729
6	-4.877708	-0.416938	-1.130778
6	-6.274567	0.34589	1.138832
6	-6.270068	-0.432039	-1.142527
6	-6.970918	-0.048814	-0.001267
9	-6.93459	-0.820865	-2.235488
9	-4.235053	-0.817996	-2.235936
9	-8.305191	-0.05975	-0.000189
9	-6.943509	0.723855	2.232903
9	-4.244353	0.765316	2.22876
6	1.287478	-2.795052	0.314546
6	1.910845	-3.87812	-0.182362
1	1.887466	-2.005575	0.758838
1	1.332631	-4.652039	-0.688584

6	3.388428	-4.064555	-0.127847
6	3.981602	-4.788725	0.924781
6	4.188994	-3.545236	-1.167865
6	5.369015	-4.968764	0.928845
6	5.5711	-3.74933	-1.124082
6	6.182162	-4.460109	-0.086601
1	5.824172	-5.52093	1.749076
1	6.186557	-3.338562	-1.922557
6	3.572376	-2.76558	-2.308897
1	2.865949	-3.382091	-2.880564
1	3.009928	-1.89409	-1.955591
1	4.344219	-2.417452	-3.002451
6	3.143492	-5.363114	2.04513
1	2.598245	-4.58107	2.586152
1	2.391141	-6.068568	1.668423
1	3.768421	-5.899263	2.766184
6	7.675894	-4.689829	-0.07956
1	8.040805	-4.924464	0.925867
1	7.95404	-5.528274	-0.732356
1	8.218794	-3.80851	-0.439202
6	1.238067	2.838847	-0.320483
6	1.841868	3.920871	0.201722
1	1.850736	2.07007	-0.78356
1	1.249299	4.666186	0.733914
6	3.316277	4.132689	0.152347
6	3.912321	4.811657	-0.929109
6	4.116767	3.632159	1.200633
6	5.299592	4.988622	-0.937806
6	5.499938	3.830968	1.150895
6	6.112605	4.504139	0.090429
1	5.755701	5.518458	-1.772242
1	6.114294	3.44443	1.962046
6	3.076233	5.355067	-2.066465
1	2.54463	4.556495	-2.596856
1	2.31272	6.058441	-1.709576
1	3.701155	5.883632	-2.793116
6	3.497324	2.881966	2.359494
1	2.785913	3.509989	2.91216
1	2.940051	2.000095	2.023334
1	4.266462	2.553039	3.065313
6	7.613142	4.677589	0.042187
1	7.894788	5.592489	-0.490399
1	8.044037	4.725268	1.048101
1	8.094923	3.838384	-0.477631
6	-1.223833	-4.883684	0.450174
1	-0.26594	-5.172254	0.895996
1	-1.994876	-5.199173	1.165133
6	-1.428392	-5.654231	-0.868052
1	-1.379084	-6.735933	-0.698049
1	-2.403294	-5.425278	-1.312394
1	-0.663913	-5.391057	-1.607606
6	-1.307419	4.883394	-0.44433
1	-2.075703	5.18921	-1.166581
1	-0.349433	5.19106	-0.876939

6	-1.540746	5.64275	0.875601
1	-0.779068	5.390202	1.621732
1	-1.510415	6.726095	0.711822
1	-2.515683	5.392613	1.308252

4c

Atomic number	X	Y	Z
6	2.098956	2.565556	0.125977
6	0.981429	3.383388	0.177092
6	-0.165653	2.533266	0.144902
7	0.247998	1.245127	0.086326
6	1.625955	1.216953	0.066085
6	1.62091	-1.219097	-0.068509
6	2.088562	-2.568982	-0.127534
7	0.243098	-1.241532	-0.090701
6	0.967302	-3.382544	-0.179592
6	-0.175734	-2.528136	-0.149192
6	2.305351	-0.002055	-0.00067
5	-0.673744	0.003473	-0.002002
9	-1.483797	-0.080896	1.135507
9	-1.484005	0.0909	-1.139054
6	3.500472	-3.05282	-0.145156
1	4.053793	-2.680387	-1.012117
1	4.048864	-2.748034	0.750774
1	3.528509	-4.142905	-0.1842
6	3.512893	3.043204	0.14403
1	4.064082	2.668885	1.011533
1	4.060173	2.735191	-0.751448
1	3.545762	4.133151	0.182149
6	0.970666	-4.874597	-0.291862
1	1.8453	-5.186525	-0.872192
1	0.105172	-5.195693	-0.879325
6	0.988908	-5.593458	1.059031
1	0.964658	-6.679474	0.927034
1	1.892743	-5.341899	1.621384
1	0.135773	-5.305709	1.680372
6	0.990715	4.875505	0.288152
1	1.869778	5.184629	0.863169
1	0.130114	5.200402	0.880642
6	1.003854	5.593023	-1.063527
1	0.984032	6.679164	-0.932277
1	1.903801	5.337767	-1.630427
1	0.146277	5.307952	-1.679901
6	3.790679	-0.005318	0.000554
6	4.514915	0.034149	-1.184892
6	4.512724	-0.048305	1.187199
6	5.901544	0.03185	-1.19731
6	5.899322	-0.052499	1.201953
6	6.595047	-0.011937	0.002911
9	3.879704	0.076247	-2.351098
9	6.567156	0.070566	-2.343896
9	7.918582	-0.015079	0.004044
9	6.562815	-0.094437	2.349681

9	3.875361	-0.087595	2.352374
6	-1.567965	2.83404	0.216728
1	-2.19281	1.980805	0.455036
6	-1.579426	-2.824262	-0.22413
1	-2.200468	-1.971623	-0.474519
6	-2.168696	-4.017189	0.006194
1	-1.564536	-4.861071	0.323209
6	-2.153183	4.031369	-0.002203
1	-1.545749	4.878057	-0.304831
6	-3.574907	4.315396	0.092251
6	-4.528842	3.373399	0.505356
6	-4.036648	5.598123	-0.240974
6	-5.870947	3.698197	0.57739
1	-4.221351	2.370104	0.77967
6	-5.376533	5.935042	-0.173439
1	-3.319891	6.348287	-0.563056
6	-6.303584	4.981453	0.237762
1	-6.591877	2.951795	0.902148
1	-5.722653	6.928799	-0.434085
6	-3.590886	-4.298769	-0.091861
6	-4.056996	-5.570384	0.264747
6	-4.541719	-3.361754	-0.532122
6	-5.40161	-5.900379	0.194803
1	-3.346852	-6.317743	0.607029
6	-5.882908	-3.678535	-0.606991
1	-4.225895	-2.366856	-0.827084
6	-6.322536	-4.952273	-0.241836
1	-6.611703	-2.952791	-0.950315
8	-7.606205	5.350617	0.292348
1	-8.138889	4.608303	0.587702
8	-7.650626	-5.205888	-0.336086
1	-5.735173	-6.895196	0.479295
1	-7.826218	-6.108834	-0.06077

4d

Atomic number	X	Y	Z
6	-2.850422	2.57176	-0.343367
6	-1.715871	3.387719	-0.39848
6	-0.561783	2.544284	-0.222781
7	-1.001882	1.244043	-0.089146
6	-2.398598	1.217552	-0.143274
6	-2.398516	-1.217747	0.142794
6	-2.85024	-2.571989	0.343041
7	-1.001811	-1.24417	0.088474
6	-1.715646	-3.387876	0.398025
6	-0.561612	-2.544359	0.222159
6	-3.089997	-0.000123	-0.000163
5	-0.097265	-0.00004	-0.000487
9	0.757523	-0.079599	-1.158638
9	0.757844	0.079526	1.157472
6	-4.581159	-0.000127	0.000067
6	-5.316651	0.447924	1.10194
6	-5.317008	-0.448144	-1.101589

6	-6.70844	0.453434	1.114196
6	-6.708798	-0.453592	-1.113427
6	-7.40853	-0.000059	0.00049
9	-4.659878	-0.925528	-2.215099
9	-7.394878	-0.910242	-2.214205
9	-8.781574	-0.000024	0.000698
9	-7.394165	0.910118	2.21518
9	-4.659168	0.925287	2.215254
6	-4.268299	-3.053518	0.459441
1	-4.861408	-2.440802	1.145547
1	-4.77779	-3.055098	-0.512356
1	-4.300027	-4.078616	0.836737
6	-4.268501	3.053274	-0.459583
1	-4.861849	2.440231	-1.145178
1	-4.777697	3.055385	0.512374
1	-4.300293	4.078181	-0.83741
6	-1.716978	-4.887104	0.547688
1	-2.672986	-5.207827	0.977015
1	-0.958252	-5.196512	1.276549
6	-1.500636	-5.642003	-0.784943
1	-1.495977	-6.726357	-0.622033
1	-2.301831	-5.406366	-1.494005
1	-0.550944	-5.360494	-1.250903
6	-1.717348	4.886939	-0.548174
1	-2.673354	5.207557	-0.977596
1	-0.958576	5.19639	-1.276956
6	-1.50122	5.641908	0.784454
1	-1.496687	6.726253	0.621495
1	-2.302463	5.406186	1.49344
1	-0.551539	5.360539	1.250523
6	0.842062	2.833205	-0.124692
6	1.469997	4.02198	-0.354346
1	1.442907	1.988237	0.186616
1	0.893827	4.884329	-0.672592
6	0.842249	-2.833193	0.124099
6	1.470259	-4.021845	0.354178
1	1.44302	-1.988277	-0.187486
1	0.894116	-4.88411	0.67271
6	2.895053	4.275171	-0.221161
6	3.400314	5.562371	-0.514943
6	3.835619	3.303851	0.198098
6	4.748922	5.874714	-0.402053
1	2.709223	6.33546	-0.841033
6	5.185632	3.598799	0.317596
1	3.503698	2.299173	0.437119
6	5.685151	4.896237	0.0207
1	5.076085	6.878302	-0.641371
1	5.860472	2.81857	0.645247
6	2.895333	-4.274998	0.221145
6	3.400636	-5.562113	0.515231
6	3.835881	-3.303712	-0.198237
6	4.74926	-5.874422	0.402449
1	2.709566	-6.335161	0.841461
6	5.18591	-3.598626	-0.317624

1	3.503935	-2.299069	-0.437374
6	5.685464	-4.895997	-0.020487
1	5.076459	-6.877944	0.641993
1	5.860737	-2.818422	-0.645358
7	7.035308	5.192537	0.140598
7	7.035628	-5.192283	-0.140313
6	7.979721	4.165833	0.579983
1	7.993957	3.306477	-0.1045
1	8.983582	4.59177	0.607832
1	7.739763	3.794759	1.585959
6	7.521967	6.536735	-0.166962
1	7.320141	6.813611	-1.211039
1	7.059654	7.294898	0.480294
1	8.600921	6.572108	-0.010668
6	7.52237	-6.536329	0.167791
1	8.6013	-6.571748	0.011337
1	7.320695	-6.812765	1.212019
1	7.059982	-7.294768	-0.479078
6	7.980059	-4.165553	-0.579611
1	7.99432	-3.306238	0.104927
1	8.983908	-4.591514	-0.607523
1	7.740083	-3.794418	-1.585554

4d.2H$^+$

Atomic number	X	Y	Z
6	0	0	0
6	0	0	1.392124
6	1.368392	0	1.810783
7	2.176942	0.025468	0.714825
6	1.376451	-0.003607	-0.416704
6	3.351762	0.029213	-1.869171
6	4.160535	-0.003588	-3.05945
7	4.191232	0.141877	-0.771874
6	5.48743	0.09357	-2.650949
6	5.479948	0.184049	-1.218528
6	1.955756	-0.026053	-1.698447
5	3.736872	-0.018794	0.718459
9	4.231265	1.047446	1.487774
9	4.191862	-1.22042	1.232766
6	1.06775	-0.102978	-2.893131
6	0.421658	-1.291729	-3.24274
6	0.841081	1.012857	-3.703152
6	-0.410369	-1.376172	-4.355848
6	0.009334	0.956397	-4.817757
6	-0.618149	-0.245444	-5.145581
9	1.457329	2.171016	-3.427291
9	-0.177686	2.036951	-5.575106
9	-1.41245	-0.313023	-6.208451
9	-1.016442	-2.523728	-4.658937
9	0.57839	-2.383393	-2.481612
6	3.697029	-0.106423	-4.483451
1	2.930749	-0.874541	-4.613636
1	3.281928	0.843352	-4.83955

1	4.526407	-0.36216	-5.145593
6	-1.236331	0.019645	-0.850035
1	-1.169151	0.73942	-1.669855
1	-1.43599	-0.965262	-1.287833
1	-2.109201	0.285832	-0.249143
6	6.678734	0.172627	-3.572126
1	6.381083	-0.174431	-4.565345
1	7.4584	-0.531076	-3.25851
6	7.26319	1.591797	-3.710539
1	8.118797	1.589368	-4.394418
1	6.512309	2.279552	-4.112428
1	7.595783	1.991487	-2.747159
6	-1.22533	0.065766	2.266245
1	-1.95333	0.743365	1.804774
1	-0.969204	0.5258	3.226389
6	-1.907706	-1.295988	2.50061
1	-2.787205	-1.181022	3.14326
1	-2.238186	-1.738406	1.555344
1	-1.230755	-2.018402	2.97202
6	1.917309	0.029337	3.148964
6	1.278122	-0.456386	4.242027
1	2.910603	0.460681	3.231873
1	0.334333	-0.972526	4.104928
6	6.564846	0.35509	-0.27841
6	7.883798	0.188154	-0.550572
1	6.252095	0.652453	0.717285
1	8.180305	-0.155038	-1.533545
6	1.72541	-0.395789	5.628239
6	0.970005	-1.08527	6.602801
6	2.84724	0.337396	6.06977
6	1.300243	-1.04986	7.951524
1	0.101355	-1.657418	6.291376
6	3.190794	0.381536	7.416459
1	3.446697	0.89365	5.357205
6	2.412428	-0.308759	8.34545
1	0.687948	-1.590756	8.667063
1	4.054363	0.964128	7.732932
6	9.00457	0.427751	0.348801
6	10.302147	0.115767	-0.111101
6	8.886886	0.986917	1.641547
6	11.429578	0.35415	0.665235
1	10.42649	-0.316688	-1.099135
6	10.00536	1.231384	2.429129
1	7.908733	1.249115	2.030223
6	11.270299	0.914943	1.928953
1	12.415569	0.106715	0.276093
1	9.87864	1.673615	3.413258
7	2.782727	-0.226571	9.787628
7	12.494729	1.189176	2.734805
6	3.172575	-1.564654	10.374772
1	3.95864	-1.994679	9.754111
1	3.522938	-1.410925	11.397038
1	2.297129	-2.213222	10.371346
6	1.732275	0.467931	10.627203

1	1.524253	1.439804	10.17964
1	0.83076	-0.143833	10.629545
1	2.113914	0.581391	11.643525
6	12.553984	0.391291	4.016768
1	13.51939	0.566174	4.49517
1	11.745563	0.722475	4.667801
1	12.429238	-0.663033	3.769557
6	12.721578	2.664646	2.979119
1	11.910977	3.040606	3.602593
1	13.680235	2.793948	3.484858
1	12.719942	3.174559	2.015705
1	13.280924	0.868663	2.159463
1	3.620117	0.36346	9.827995

4e

Atomic number	X	Y	Z
6	0	0	0
6	0	0	1.392333
6	1.368877	0	1.813341
7	2.17004	0.004184	0.716559
6	1.376182	-0.008378	-0.420083
6	3.366911	-0.024429	-1.856897
6	4.199159	-0.025226	-3.030681
7	4.195304	-0.059473	-0.745652
6	5.520489	-0.043546	-2.592112
6	5.488661	-0.062112	-1.160426
6	1.969282	-0.010818	-1.695896
5	3.730386	-0.035097	0.744402
9	4.223448	1.101898	1.375582
9	4.163383	-1.184697	1.396469
6	3.777973	-0.015024	-4.47164
1	2.9997	-0.75333	-4.686181
1	3.394401	0.967341	-4.772389
1	4.629568	-0.238104	-5.119573
6	-1.234841	0.012768	-0.853737
1	-1.18629	0.761403	-1.649998
1	-1.408559	-0.961774	-1.325645
1	-2.116007	0.235969	-0.246676
6	6.744609	-0.096954	-3.467504
1	6.535226	-0.724348	-4.342582
1	7.554118	-0.603723	-2.931241
6	7.227485	1.281755	-3.957724
1	8.127076	1.181208	-4.575288
1	6.457441	1.777026	-4.559174
1	7.461366	1.950022	-3.121159
6	-1.215983	0.053283	2.279003
1	-1.974477	0.694154	1.812962
1	-0.95732	0.54517	3.222847
6	-1.846498	-1.323382	2.564616
1	-2.715089	-1.223282	3.225141
1	-2.179337	-1.803304	1.63785
1	-1.132655	-2.00483	3.041248
6	1.096004	0.001362	-2.905982

6	0.438416	-1.15175	-3.341166
6	0.901294	1.166367	-3.651855
6	-0.378261	-1.153699	-4.468941
6	0.088447	1.191055	-4.782127
6	-0.55364	0.024383	-5.19192
9	-0.06906	2.320362	-5.478681
9	1.527299	2.297723	-3.300714
9	-1.333904	0.035272	-6.273146
9	-1.000433	-2.272127	-4.852803
9	0.56355	-2.293592	-2.651462
6	6.557458	-0.160134	-0.186622
6	7.824813	0.278752	-0.383705
1	6.277086	-0.601343	0.759588
1	8.059322	0.783766	-1.315653
6	8.968282	0.225271	0.524471
6	8.96973	-0.433882	1.7947
6	10.14687	0.85802	0.120614
6	10.153924	-0.404905	2.581047
6	11.289946	0.86428	0.921767
1	10.1877	1.364413	-0.836688
6	11.31444	0.241513	2.154523
1	12.20093	0.248868	2.773475
7	12.497622	1.547851	0.443965
8	13.4853	1.537947	1.176444
8	12.443776	2.087009	-0.661329
7	10.203045	-1.061247	3.879323
8	11.238563	-1.016622	4.526043
8	9.17582	-1.65107	4.285645
6	1.957132	0.075071	3.135675
6	1.366617	-0.373384	4.270498
1	2.947553	0.506607	3.173501
1	0.403593	-0.868465	4.192781
6	1.868596	-0.342705	5.642448
6	3.07974	0.299791	6.052684
6	1.107982	-0.981409	6.625333
6	3.452475	0.249253	7.423817
6	1.507949	-1.009047	7.962409
1	0.181913	-1.475661	6.355815
6	2.675911	-0.402636	8.382236
1	2.983821	-0.42653	9.418403
7	4.675165	0.888151	7.888102
8	4.962077	0.825254	9.07396
8	5.390039	1.482405	7.049058
7	0.667523	-1.697889	8.948934
8	1.051448	-1.706982	10.117117
8	-0.369438	-2.222098	8.542508
8	3.805337	0.924186	5.134364
1	4.600157	1.305191	5.59367
8	7.863601	-1.052882	2.185837
1	8.045326	-1.447309	3.079858

[1] Catalan, J. *J. Phys. Chem. B* **2009**, *113*, 5951.