Supplementary Information

Exploration of Interesting Photovoltaic Behavior for Fused Benzothiophene dioxide Moiety as Core Donor with Modification in Acceptors for High Efficacy Organic Solar Cells

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Table S1: Cartesian coordinates of **R1** compound.

Atom	X-axis	Y-axis	Z-axis
C	-0.00896	1.429041	0.114513
C	-1.19959	0.720531	0.115042
C	-1.18877	-0.69926	0.078634
C	0.008345	-1.4296	0.049893
C	1.198957	-0.72105	0.049135
C	1.188161	0.69871	0.086499
H	-0.00012	2.514109	0.132387
H	-0.00034	-2.51468	0.031643
C	2.567377	1.126216	0.097887

C	3.426332	0.04077	0.091556
C	6.24527	2.286751	0.124138
C	4.918941	1.856524	0.10461
C	4.775912	0.452481	0.084849
H	6.57091	3.320611	0.121644
S	3.363082	2.679248	0.10593
S	6.316186	-0.34413	0.108812
C	7.156614	1.220743	0.11542
C	2.643394	-1.27214	0.037783
C	-3.42704	-0.04144	0.078546
C	-4.77667	-0.45311	0.075985
C	-4.9195	-1.85726	0.067186
C	-7.15723	-1.22182	0.060547
C	-6.24592	-2.28777	0.06339
H	-6.57131	-3.32149	0.042345
S	-3.36364	-2.67984	0.064339
S	-6.31737	0.34306	0.097172
C	-2.56801	-1.12681	0.07177
C	-2.64415	1.271612	0.126098
C	3.013877	-1.99898	-1.27556
C	2.278761	-1.81481	-2.45344
C	4.172237	-2.78971	-1.32861
C	2.685418	-2.41097	-3.6484
H	1.383463	-1.20312	-2.44431
C	4.581143	-3.38057	-2.52354
H	4.75467	-2.95788	-0.42853
C	3.837447	-3.19523	-3.68936
H	2.097208	-2.25765	-4.5485
H	5.484152	-3.9831	-2.53946
H	4.153859	-3.65666	-4.61991
C	2.838443	-2.15663	1.287629
C	2.479896	-3.51282	1.256694
C	3.290872	-1.61499	2.497062
C	2.574607	-4.30281	2.401665
H	2.142982	-3.95965	0.326886
C	3.390192	-2.40679	3.642227
H	3.570098	-0.56796	2.549243
C	3.031968	-3.75333	3.600241
H	2.296002	-5.35147	2.353182
H	3.752716	-1.96681	4.566547
H	3.112817	-4.37026	4.490075
C	-3.01205	2.004026	1.437169
C	-2.27987	1.816872	2.616535
C	-4.16394	2.804269	1.486981

C	-2.68227	2.420075	3.809337
H	-1.38961	1.197817	2.609661
C	-4.56837	3.4027	2.679782
H	-4.7442	2.974482	0.585959
C	-3.8272	3.214964	3.846771
H	-2.09599	2.264646	4.710374
H	-5.46549	4.014094	2.692432
H	-4.13954	3.68309	4.775401
C	-2.8411	2.151585	-1.1268
C	-3.30455	1.608391	-2.33124
C	-2.47378	3.505685	-1.10318
C	-3.4063	2.396751	-3.47864
H	-3.59109	0.563186	-2.37843
C	-2.57069	4.292041	-2.25036
H	-2.12829	3.95406	-0.17723
C	-3.03923	3.741027	-3.44395
H	-3.77817	1.955784	-4.39868
H	-2.28509	5.339064	-2.20759
H	-3.12208	4.355159	-4.33549
C	8.554486	1.478912	0.067559
C	9.677485	0.699686	-0.04926
H	8.744483	2.54381	0.139377
C	-8.55468	-1.47974	-0.00106
C	-9.67704	-0.6999	-0.11837
H	-8.74492	-2.54545	0.057354
C	11.99889	-0.00187	0.116497
C	11.36511	-1.25346	0.103067
C	12.02942	-2.4595	0.263869
C	13.40963	-2.42073	0.462685
C	14.07299	-1.19082	0.498661
C	13.38779	0.012196	0.329573
H	11.48501	-3.3976	0.243688
H	13.96455	-3.34378	0.595997
H	15.14502	-1.16318	0.66543
H	13.94072	0.938577	0.376188
C	-13.4136	2.411646	0.408773
C	-14.0752	1.180555	0.43526
C	-13.3883	-0.0201	0.256514
C	-11.9995	-0.0021	0.043316
C	-11.3672	1.250321	0.040357
C	-12.0333	2.454056	0.210538
H	-13.9698	3.332808	0.549419
H	-15.1471	1.150103	0.602273
H	-13.9395	-0.94785	0.296324

H	-11.4903	3.393078	0.198171
S	9.613664	-1.10022	-0.14772
S	-9.61494	1.100535	-0.20811
C	-11.0638	-1.14171	-0.16616
C	11.06475	1.140844	-0.08399
C	11.4847	2.445649	-0.31552
C	-11.4815	-2.44339	-0.41766
C	10.59912	3.529819	-0.60042
N	9.912916	4.442791	-0.83398
C	12.84972	2.864764	-0.33649
N	13.94185	3.270473	-0.36539
C	-10.5932	-3.52207	-0.71483
N	-9.9042	-4.42988	-0.95984
C	-12.8463	-2.86257	-0.45158
N	-13.9383	-3.26752	-0.49173
O	8.883102	-1.6604	1.00181
O	9.241824	-1.54175	-1.50099
O	-9.24003	1.545547	-1.55927
O	-8.8886	1.658877	0.945089

Table S2: Cartesian coordinates of **D2** compound.

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	0.216561	-1.412763	0.027499
C	1.291018	-0.537958	0.038603
C	1.074207	0.865163	0.007166
C	-0.216609	1.41267	-0.027336
C	-1.291068	0.537865	-0.038434
C	-1.074256	-0.865256	-0.007006
H	0.366283	-2.48752	0.041787
H	-0.36633	2.487427	-0.041621
C	-2.377044	-1.489035	-0.008738
C	-3.385008	-0.54117	-0.017743
C	-5.84813	-3.170326	-0.000889
C	-4.59793	-2.551774	-0.012518
C	-4.662701	-1.143161	-0.025188
H	-6.017921	-4.240865	0.009142
S	-2.939071	-3.141283	-0.006288
S	-6.305465	-0.575991	-0.024147
C	-6.907409	-2.251062	-0.002483
C	-2.801009	0.871891	-0.059359
C	3.384958	0.541074	0.01792
C	4.662653	1.14306	0.025326

C	4.597886	2.551673	0.01263
C	6.907366	2.250955	0.002661
C	5.848088	3.17022	0.001028
H	6.017881	4.240759	-0.008996
S	2.939028	3.141187	0.006419
S	6.305415	0.575883	0.024262
C	2.376996	1.488941	0.008903
C	2.800959	-0.871985	0.059532
C	-3.260238	1.54322	-1.374538
C	-2.503539	1.451884	-2.549833
C	-4.508461	2.181869	-1.433706
C	-2.976326	1.990933	-3.747359
H	-1.538122	0.958348	-2.535986
C	-4.981546	2.718431	-2.630845
H	-5.111408	2.274687	-0.536263
C	-4.21624	2.627052	-3.793764
H	-2.369518	1.91176	-4.644691
H	-5.950503	3.20824	-2.650364
H	-4.582491	3.047645	-4.725433
C	-3.132984	1.713947	1.190548
C	-2.955998	3.105933	1.171212
C	-3.532111	1.110668	2.389536
C	-3.1737	3.870152	2.3168
H	-2.664219	3.598614	0.249305
C	-3.75377	1.876003	3.535811
H	-3.672514	0.035896	2.432595
C	-3.574918	3.258137	3.505285
H	-3.034556	4.946586	2.277118
H	-4.069846	1.386643	4.45238
H	-3.750456	3.853753	4.396015
C	3.260181	-1.543316	1.374712
C	2.503379	-1.452132	2.549953
C	4.5085	-2.181774	1.43396
C	2.976149	-1.991157	3.747497
H	1.537891	-0.958736	2.536047
C	4.981569	-2.718308	2.631118
H	5.11154	-2.274457	0.536566
C	4.216154	-2.627092	3.793978
H	2.369257	-1.912106	4.644782
H	5.950601	-3.207967	2.650699
H	4.582393	-3.047665	4.72566
C	3.132926	-1.714023	-1.190393
C	3.532248	-1.110725	-2.389307

C	2.955702	-3.10598	-1.171172
C	3.753883	-1.876016	-3.535616
H	3.672829	-0.035973	-2.432279
C	3.173377	-3.870155	-2.316795
H	2.663748	-3.598676	-0.249329
C	3.574802	-3.258124	-3.505202
H	4.070116	-1.386644	-4.452124
H	3.034047	-4.946568	-2.277201
H	3.750319	-3.853705	-4.395958
C	-8.251191	-2.717502	0.011185
C	-9.478733	-2.098857	0.016263
H	-8.274833	-3.80225	0.021538
C	8.251148	2.717406	-0.010915
C	9.478719	2.0988	-0.015957
H	8.274769	3.802156	-0.021247
C	-11.790754	-1.714209	0.03623
C	-11.202367	-0.472163	0.018458
C	11.790757	1.714279	-0.03614
C	11.202442	0.4722	-0.018507
C	10.785118	2.777983	-0.035834
C	-10.785166	-2.777966	0.036256
C	-11.090369	-4.126475	0.05351
C	11.090239	4.12652	-0.05283
C	-10.117333	-5.170415	0.055467
N	-9.340541	-6.039064	0.057982
C	-12.445415	-4.576962	0.07204
N	-13.549468	-4.949331	0.087347
C	10.117135	5.170394	-0.054483
N	9.340147	6.038868	-0.056738
C	12.445256	4.577084	-0.071427
N	13.549307	4.949457	-0.0868
C	9.736641	0.63028	-0.004163
C	-9.736572	-0.630323	0.004419
O	8.912203	-0.276171	0.01384
O	-8.912073	0.276081	-0.013361
C	14.543966	-0.998992	-0.042865
C	13.457272	-0.126158	-0.038277
C	12.124737	-0.614172	-0.019201
C	11.890222	-1.998109	-0.004941
C	12.970209	-2.867558	-0.009403
C	14.296125	-2.369032	-0.028344
H	15.566424	-0.639937	-0.057365
H	10.875143	-2.376226	0.008938

C	-11.890027	1.998182	0.004404
C	-12.969974	2.867682	0.008599
C	-14.295917	2.369221	0.027448
C	-14.543825	0.999195	0.042144
C	-13.457171	0.126312	0.037834
C	-12.124609	0.614257	0.01885
H	-10.87493	2.376251	-0.009409
H	-15.566301	0.64019	0.056565
S	13.533231	1.641786	-0.054789
S	-13.533205	-1.641628	0.054625
Cl	15.661322	-3.453472	-0.034276
Cl	12.661297	-4.585487	0.00867
Cl	-15.661062	3.453727	0.033044
Cl	-12.66098	4.585594	-0.009686

Table S3: Cartesian coordinates of **D3** compound.

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	0.253018	-1.407275	0.023532
C	1.304522	-0.505456	0.035974
C	1.051203	0.892072	0.008442
C	-0.253017	1.407286	-0.023521
C	-1.304522	0.505468	-0.035959
C	-1.051203	-0.892061	-0.008432
H	0.430407	-2.477797	0.034713
H	-0.430405	2.477808	-0.034699
C	-2.337014	-1.548951	-0.011264
C	-3.369192	-0.626111	-0.017046
C	-5.760512	-3.318129	-0.009936
C	-4.528372	-2.668801	-0.019217
C	-4.629559	-1.260459	-0.027398
H	-5.903406	-4.392639	-0.002651
S	-2.85468	-3.215261	-0.01442
S	-6.284727	-0.734037	-0.026663
C	-6.844565	-2.424544	-0.009525
C	-2.822179	0.801435	-0.054252
C	3.369193	0.626122	0.017062
C	4.62956	1.26047	0.027358
C	4.528372	2.668812	0.019128
C	6.844566	2.424559	0.009437
C	5.760511	3.318143	0.009805
H	5.903405	4.392652	0.002463
S	2.85468	3.215271	0.014363

S	6.28473	0.734053	0.026628
C	2.337014	1.548962	0.011266
C	2.822179	-0.801423	0.054279
C	-3.299622	1.464395	-1.367469
C	-2.545765	1.385549	-2.54555
C	-4.559278	2.080534	-1.42186
C	-3.032257	1.915909	-3.741383
H	-1.571783	0.908919	-2.535384
C	-5.045695	2.608995	-2.617393
H	-5.16022	2.163889	-0.522144
C	-4.283085	2.53073	-3.783001
H	-2.427595	1.847261	-4.640977
H	-6.022391	3.08321	-2.633221
H	-4.65969	2.945508	-4.713083
C	-3.173889	1.630064	1.19945
C	-3.033654	3.026253	1.184252
C	-3.554606	1.012365	2.397078
C	-3.270104	3.780686	2.332598
H	-2.757267	3.529673	0.263456
C	-3.794797	1.767881	3.546147
H	-3.665748	-0.065985	2.437724
C	-3.653103	3.15437	3.519623
H	-3.160749	4.860586	2.296013
H	-4.096238	1.267499	4.461648
H	-3.843819	3.742344	4.412219
C	3.299618	-1.464378	1.367499
C	2.545765	-1.385521	2.545582
C	4.559274	-2.080517	1.42189
C	3.03226	-1.915871	3.741417
H	1.571785	-0.908885	2.535415
C	5.045693	-2.60897	2.617426
H	5.160213	-2.163879	0.522173
C	4.283086	-2.530695	3.783036
H	2.427601	-1.847216	4.641012
H	6.022389	-3.083186	2.633254
H	4.659694	-2.945467	4.713119
C	3.173894	-1.630055	-1.199418
C	3.554622	-1.012356	-2.397042
C	3.033642	-3.026242	-1.184225
C	3.794812	-1.767872	-3.546111
H	3.665775	0.065993	-2.437685
C	3.27009	-3.780675	-2.332572
H	2.757239	-3.529661	-0.263433

C	3.653105	-3.15436	-3.519592
H	4.096265	-1.267491	-4.461609
H	3.160722	-4.860573	-2.295989
H	3.84382	-3.742333	-4.412188
C	-8.172556	-2.92425	0.004435
C	-9.418346	-2.335618	0.011787
H	-8.170159	-4.009328	0.013592
C	8.172559	2.924263	-0.004582
C	9.418347	2.335622	-0.011989
H	8.170165	4.009341	-0.013769
C	-11.740105	-2.008113	0.03704
C	-11.182137	-0.753613	0.01901
C	11.740102	2.008094	-0.037195
C	11.182129	0.7536	-0.019066
C	10.703643	3.047722	-0.034405
C	-10.703637	-3.047735	0.034124
C	-10.9805	-4.401908	0.051338
C	10.980518	4.401888	-0.051763
C	-9.984099	-5.42353	0.049904
N	-9.185195	-6.27164	0.04957
C	-12.326434	-4.878087	0.073657
N	-13.425758	-5.263992	0.092285
C	9.98412	5.423513	-0.050486
N	9.185289	6.271691	-0.050309
C	12.326459	4.878042	-0.074169
N	13.425766	5.263994	-0.09286
C	9.710219	0.875639	-0.000121
C	-9.710233	-0.875639	-0.000047
O	8.913262	-0.053891	0.02299
O	-8.913288	0.0539	-0.023189
C	14.564623	-0.627425	-0.048666
C	13.452903	0.216739	-0.036
C	12.132038	-0.306586	-0.020871
C	11.933298	-1.697873	0.002866
C	13.03817	-2.526753	0.004943
C	14.345682	-1.996058	-0.037031
H	15.582347	-0.257436	-0.083666
H	10.934783	-2.11622	0.038866
C	-11.933316	1.697857	-0.002633
C	-13.038193	2.526732	-0.004593
C	-14.345705	1.996025	0.037324
C	-14.564634	0.627387	0.048823
C	-13.452911	-0.216768	0.036048

C	-12.132049	0.306566	0.02096
H	-10.934799	2.116203	-0.038616
H	-15.582359	0.257397	0.083805
S	13.48317	1.980981	-0.055588
S	-13.483164	-1.981015	0.055441
N	15.531049	-2.855728	-0.205928
O	16.568602	-2.483613	0.335344
O	15.403429	-3.842293	-0.921986
N	12.789786	-3.969254	0.190308
O	13.528302	-4.561764	0.968775
O	11.825225	-4.446334	-0.399111
N	-12.789782	3.969251	-0.189833
O	-13.528105	4.561773	-0.96847
O	-11.825432	4.446331	0.399921
N	-15.531068	2.855668	0.206334
O	-16.568677	2.483531	-0.334818
O	-15.403381	3.842306	0.922287

Table S4: Cartesian coordinates of **D4** compound.

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	0.299377	-1.39799	0.004511
C	1.320437	-0.461715	0.026791
C	1.021337	0.926575	0.018105
C	-0.299496	1.397808	-0.004421
C	-1.320556	0.461534	-0.026696
C	-1.021455	-0.926757	-0.018022
H	0.512312	-2.462101	0.001247
H	-0.512426	2.46192	-0.001163
C	-2.285135	-1.62582	-0.027192
C	-3.347363	-0.738561	-0.020098
C	-5.648794	-3.509232	-0.040543
C	-4.438412	-2.817814	-0.045399
C	-4.586808	-1.414689	-0.036838
H	-5.755081	-4.587992	-0.044033
S	-2.747673	-3.308158	-0.049728
S	-6.260188	-0.945843	-0.028465
C	-6.761287	-2.653982	-0.028156
C	-2.847502	0.706849	-0.038091
C	3.347247	0.738375	0.020126
C	4.586695	1.414505	0.036705
C	4.438295	2.817631	0.045207
C	6.761178	2.653811	0.027962

C	5.648675	3.509052	0.04025
H	5.754957	4.587813	0.043716
S	2.747557	3.307974	0.049652
S	6.260078	0.945669	0.028136
C	2.285019	1.625635	0.027238
C	2.84738	-0.707035	0.038169
C	-3.349439	1.373982	-1.339797
C	-2.593769	1.34275	-2.518883
C	-4.630563	1.94497	-1.383701
C	-3.099489	1.875995	-3.705425
H	-1.603501	0.901012	-2.516036
C	-5.136323	2.476078	-2.569949
H	-5.233827	1.989429	-0.482803
C	-4.371673	2.445934	-3.736506
H	-2.493179	1.844795	-4.606016
H	-6.130104	2.913617	-2.578147
H	-4.76356	2.862693	-4.659411
C	-3.222834	1.505113	1.22846
C	-3.128423	2.905215	1.234095
C	-3.580156	0.857633	2.417538
C	-3.385495	3.634248	2.394366
H	-2.871005	3.430994	0.32034
C	-3.841199	1.58755	3.57851
H	-3.656287	-0.224204	2.441895
C	-3.744253	2.978126	3.572829
H	-3.310624	4.717559	2.37393
H	-4.12348	1.063784	4.48705
H	-3.950544	3.546039	4.47496
C	3.349339	-1.374134	1.33989
C	2.593708	-1.342867	2.518998
C	4.630465	-1.945126	1.38377
C	3.099465	-1.876085	3.70554
H	1.603444	-0.901124	2.516174
C	5.13626	-2.476204	2.570013
H	5.233695	-1.989617	0.482852
C	4.371646	-2.446027	3.736595
H	2.493183	-1.844857	4.606148
H	6.130039	-2.913748	2.578193
H	4.763562	-2.862762	4.659499
C	3.222679	-1.505332	-1.228369
C	3.580083	-0.857868	-2.417433
C	3.128127	-2.905423	-1.234027
C	3.841084	-1.587793	-3.578408

H	3.656314	0.223962	-2.441771
C	3.385157	-3.634464	-2.394304
H	2.870621	-3.431191	-0.320291
C	3.744008	-2.978361	-3.572747
H	4.123435	-1.064042	-4.486935
H	3.310175	-4.717768	-2.373887
H	3.950266	-3.54628	-4.474882
C	-8.073063	-3.200342	-0.013497
C	-9.337075	-2.657582	0.001338
H	-8.03092	-4.28459	-0.010986
C	8.072942	3.20021	0.01336
C	9.336997	2.657533	-0.001459
H	8.030737	4.28445	0.010756
C	-11.668384	-2.415246	0.034272
C	-11.157796	-1.139773	0.013254
C	11.668325	2.415333	-0.034482
C	11.15782	1.139834	-0.013259
C	10.597112	3.416049	-0.027422
C	-10.597228	-3.416026	0.027058
C	-10.820955	-4.780037	0.043836
C	10.820829	4.780063	-0.044422
C	-9.786357	-5.763114	0.037914
N	-8.957469	-6.582067	0.033808
C	-12.146357	-5.311184	0.069561
N	-13.22649	-5.747762	0.090631
C	9.78626	5.76317	-0.03858
N	8.957517	6.582269	-0.034563
C	12.146241	5.311172	-0.070355
N	13.226368	5.747757	-0.091609
C	9.68375	1.207669	0.007487
C	-9.683723	-1.207696	-0.007498
O	8.917141	0.252418	0.028475
O	-8.917039	-0.252503	-0.028434
C	14.582468	-0.120531	-0.050867
C	13.444426	0.685658	-0.04319
C	12.149088	0.115533	-0.016086
C	12.01323	-1.281817	0.006595
C	13.140555	-2.090827	-0.000894
C	14.438642	-1.504661	-0.024887
H	15.574266	0.312783	-0.071848
H	11.022442	-1.71692	0.028261
C	-12.01304	1.281936	-0.00629
C	-13.140312	2.091021	0.001278

C	-14.438437	1.50494	0.025151
C	-14.582358	0.120815	0.050929
C	-13.44437	-0.685449	0.043188
C	-12.148994	-0.115406	0.0162
H	-11.022221	1.716972	-0.02787
H	-15.574185	-0.312435	0.071814
S	13.411177	2.451748	-0.062701
S	-13.411244	-2.451545	0.062456
C	12.914705	-3.589831	0.086316
C	15.715908	-2.324739	-0.085525
C	-12.914367	3.590022	-0.085803
C	-15.715645	2.32511	0.085829
F	15.721284	-3.33093	0.807939
F	15.904669	-2.857222	-1.309475
F	16.797994	-1.557126	0.179176
F	13.682988	-4.277066	-0.780159
F	11.630047	-3.904522	-0.191143
F	13.173606	-4.055945	1.325256
F	-15.720564	3.331857	-0.807012
F	-15.904822	2.856857	1.310032
F	-16.797716	1.55778	-0.179755
F	-13.172994	4.056221	-1.324766
F	-11.629752	3.904643	0.191938
F	-13.682798	4.277253	0.780543

Table S5: Cartesian coordinates of **D5** compound.

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	0.336027	1.389733	-0.01361
C	1.332416	0.42723	-0.02597
C	0.996636	-0.95282	-0.00816
C	-0.33602	-1.38978	0.013866
C	-1.33241	-0.42727	0.026225
C	-0.99663	0.952774	0.008419
H	0.576461	2.447956	-0.01741
H	-0.57646	-2.448	0.017652
C	-2.24119	1.684619	0.009528
C	-3.32641	0.824629	0.005655
C	-5.55247	3.654692	0.012103
C	-4.36163	2.932888	0.019357
C	-4.54678	1.53284	0.017985
H	-5.63119	4.735851	0.010896

S	-2.65843	3.378743	0.022247
S	-6.23063	1.106374	0.013154
C	-6.688	2.827396	0.005393
C	-2.86484	-0.63327	0.033663
C	3.326415	-0.82467	-0.00543
C	4.546786	-1.53287	-0.01779
C	4.361646	-2.93292	-0.01917
C	6.688018	-2.8274	-0.00528
C	5.552496	-3.65471	-0.01196
H	5.63123	-4.73587	-0.01078
S	2.658453	-3.37879	-0.02203
S	6.230632	-1.10639	-0.01299
C	2.241192	-1.68466	-0.00929
C	2.864835	0.633231	-0.03342
C	-3.38911	-1.27959	1.337177
C	-2.63915	-1.25656	2.52011
C	-4.68302	-1.82123	1.377692
C	-3.16303	-1.77026	3.707385
H	-1.63927	-0.8369	2.519792
C	-5.20679	-2.33311	2.564662
H	-5.28219	-1.85927	0.473809
C	-4.44768	-2.3118	3.735032
H	-2.56114	-1.74639	4.611149
H	-6.20967	-2.74927	2.569978
H	-4.85351	-2.71387	4.658395
C	-3.25547	-1.42834	-1.23049
C	-3.1991	-2.83049	-1.22748
C	-3.58893	-0.77821	-2.425
C	-3.4713	-3.55895	-2.38464
H	-2.96066	-3.35807	-0.30964
C	-3.86481	-1.50754	-3.58291
H	-3.63465	0.305205	-2.4564
C	-3.8067	-2.9002	-3.56845
H	-3.42722	-4.64375	-2.35736
H	-4.1284	-0.98171	-4.49584
H	-4.02532	-3.46764	-4.46793
C	3.389085	1.27955	-1.33695
C	2.639139	1.256457	-2.51989
C	4.682978	1.821251	-1.37747
C	3.162998	1.770151	-3.70717
H	1.639277	0.836759	-2.51957
C	5.206726	2.33312	-2.56445

H	5.28214	1.859335	-0.47358
C	4.447628	2.31175	-3.73482
H	2.561119	1.746231	-4.61094
H	6.209594	2.749328	-2.56977
H	4.853453	2.713822	-4.65819
C	3.255488	1.4283	1.230721
C	3.588984	0.778178	2.425223
C	3.199098	2.830451	1.227716
C	3.864884	1.507508	3.58313
H	3.634719	-0.30524	2.456616
C	3.471321	3.558911	2.384866
H	2.960634	3.358023	0.309883
C	3.806761	2.900166	3.568674
H	4.128495	0.981675	4.496051
H	3.427236	4.643706	2.357595
H	4.025391	3.467603	4.468141
C	-7.98311	3.40645	-0.00785
C	-9.26232	2.894106	-0.01603
H	-7.91485	4.489392	-0.01503
C	7.983135	-3.40645	0.007869
C	9.262341	-2.89409	0.015987
H	7.914881	-4.48939	0.014999
C	-11.5996	2.706312	-0.03928
C	-11.118	1.420847	-0.01562
C	11.59961	-2.70629	0.039068
C	11.11802	-1.42083	0.015517
C	10.50208	-3.68204	0.039588
C	-10.5021	3.682054	-0.03976
C	-10.6972	5.050263	-0.06119
C	10.69727	-5.05024	0.060953
C	-9.64122	6.010131	-0.06356
N	-8.79289	6.808785	-0.06624
C	-12.0121	5.606623	-0.08391
N	-13.086	6.058284	-0.10256
C	9.64125	-6.01011	0.063372
N	8.792913	-6.80877	0.066085
C	12.01209	-5.60662	0.083572
N	13.08606	-6.0583	0.102132
C	9.641078	-1.45415	0.001176
C	-9.64106	1.454167	-0.00114
O	8.901234	-0.47882	-0.01906
O	-8.90122	0.478837	0.019216

C	14.57763	-0.24622	0.042666
C	13.4159	-1.02163	0.038132
C	12.13127	-0.42076	0.014044
C	12.01844	0.980447	-0.00885
C	13.16924	1.750969	-0.00195
C	14.45245	1.137308	0.018135
H	15.56718	-0.6887	0.06663
H	11.04284	1.452216	-0.03255
C	-12.0184	-0.98042	0.008819
C	-13.1693	-1.75093	0.001861
C	-14.4525	-1.13726	-0.0184
C	-14.5776	0.246268	-0.04304
C	-13.4159	1.02167	-0.03842
C	-12.1313	0.420791	-0.01418
H	-11.0428	-1.45219	0.032639
H	-15.5672	0.688757	-0.06715
S	13.34112	-2.78381	0.062365
S	-13.3411	2.783838	-0.06275
S	12.90583	3.53783	-0.075
O	13.82088	4.069813	-1.10351
O	11.48334	3.795093	-0.17761
S	16.01132	2.050526	0.070355
O	15.86155	3.105778	1.090231
O	17.10046	1.099269	0.173657
S	-12.9059	-3.5378	0.075043
O	-11.4834	-3.7951	0.177829
O	-13.8211	-4.06971	1.103522
S	-16.0113	-2.05048	-0.07075
O	-17.1004	-1.09921	-0.17425
O	-15.8615	-3.10581	-1.09053
O	16.11173	2.720713	-1.37977
O	13.37139	4.052439	1.36862
O	-13.3713	-4.05251	-1.36857
O	-16.1119	-2.72054	1.379427
H	-14.3499	-3.89356	-1.44098
H	-15.3732	-3.38273	1.453968
H	14.34995	3.893507	1.440943
H	15.37311	3.382919	-1.4542

Table S6: Cartesian coordinates of **D6** compound.

Atom	**X-axis**	**Y-axis**	**Z-axis**

C	0.295625	-1.41374	0.018661
C	1.311659	-0.47173	0.042606
C	1.005324	0.914746	0.034444
C	-0.31816	1.378361	0.009573
C	-1.33396	0.436451	-0.01506
C	-1.02783	-0.9502	-0.00579
H	0.514447	-2.47665	0.015382
H	-0.53692	2.441315	0.012575
C	-2.28815	-1.65598	-0.01635
C	-3.35477	-0.77465	-0.00998
C	-5.64436	-3.55638	-0.03648
C	-4.43631	-2.85849	-0.03775
C	-4.5915	-1.45708	-0.02746
H	-5.74523	-4.63562	-0.04454
S	-2.74323	-3.3405	-0.04067
S	-6.2678	-0.99717	-0.01606
C	-6.76011	-2.70736	-0.02285
C	-2.86218	0.673364	-0.03196
C	3.332358	0.739617	0.03776
C	4.568347	1.422664	0.054606
C	4.412316	2.824567	0.066505
C	6.73615	2.67448	0.04503
C	5.619118	3.522965	0.062719
H	5.719309	4.602286	0.070065
S	2.718838	3.305515	0.07166
S	6.244739	0.963612	0.039469
C	2.265233	1.620675	0.045781
C	2.839989	-0.70856	0.057037
C	-3.36282	1.330882	-1.33923
C	-2.60092	1.302109	-2.51434
C	-4.64899	1.8896	-1.39219
C	-3.10563	1.825298	-3.7058
H	-1.60662	0.869746	-2.50455
C	-5.15388	2.410255	-2.58337
H	-5.25745	1.93106	-0.49466
C	-4.38315	2.382485	-3.74599
H	-2.49446	1.795724	-4.60317
H	-6.15252	2.836519	-2.59895
H	-4.77463	2.790495	-4.67301
C	-3.24691	1.476826	1.227978
C	-3.1586	2.877372	1.22639
C	-3.6078	0.834482	2.418752
C	-3.42414	3.611726	2.381385

H	-2.89849	3.398987	0.310972
C	-3.87766	1.569691	3.574377
H	-3.67993	-0.24749	2.448204
C	-3.78608	2.960608	3.561669
H	-3.35269	4.695219	2.355589
H	-4.16251	1.049735	4.484306
H	-3.99862	3.5325	4.459877
C	3.342282	-1.36912	1.362118
C	2.583937	-1.33741	2.539505
C	4.625613	-1.93466	1.410676
C	3.08903	-1.86487	3.728864
H	1.591796	-0.89999	2.53287
C	5.130583	-2.46028	2.59969
H	5.231075	-1.97918	0.511294
C	4.363342	-2.42975	3.764512
H	2.480446	-1.83341	4.62793
H	6.125948	-2.89424	2.61109
H	4.754549	-2.84244	4.689591
C	3.223461	-1.50866	-1.20558
C	3.585016	-0.86322	-2.39445
C	3.134194	-2.90915	-1.20781
C	3.85558	-1.59552	-3.55176
H	3.65759	0.218797	-2.42127
C	3.400692	-3.64053	-2.36443
H	2.873598	-3.43338	-0.29404
C	3.763978	-2.98641	-3.54262
H	4.141759	-1.0734	-4.46001
H	3.330032	-4.72407	-2.3413
H	3.978407	-3.55615	-4.44167
C	-8.07128	-3.26052	-0.0183
C	-9.3362	-2.72407	-0.00261
H	-8.02325	-4.34445	-0.02733
C	8.045345	3.229016	0.030185
C	9.311804	2.694271	-0.00074
H	7.996236	4.312896	0.040181
C	-11.6683	-2.492	0.027964
C	-11.163	-1.21311	0.031612
C	11.64388	2.465855	-0.07923
C	11.13895	1.186452	-0.07931
C	10.56832	3.459757	-0.02725
C	-10.5955	-3.48772	0.004641
C	-10.8108	-4.85325	-0.00648
C	10.78336	4.825373	-0.00841

C	-9.7704	-5.83008	-0.02718
N	-8.93765	-6.64506	-0.04348
C	-12.1323	-5.39475	0.001786
N	-13.2075	-5.84387	0.007843
C	9.742929	5.800941	0.043652
N	8.909903	6.614702	0.085755
C	12.104	5.368148	-0.03832
N	13.17851	5.818273	-0.06129
C	9.666671	1.246051	-0.0243
C	-9.68968	-1.27493	0.013715
O	8.903847	0.28734	-7.2E-05
O	-8.92403	-0.3183	0.01409
C	14.5653	-0.05434	-0.23228
C	13.42784	0.74376	-0.17329
C	12.1314	0.165292	-0.13221
C	11.99567	-1.23297	-0.15805
C	13.1285	-2.03762	-0.21136
C	14.41941	-1.44348	-0.24151
H	15.56649	0.360142	-0.27428
H	11.001	-1.66646	-0.1559
C	-12.02	1.206777	0.083401
C	-13.156	2.008741	0.113837
C	-14.4491	1.417208	0.096234
C	-14.5961	0.032616	0.098625
C	-13.4534	-0.76708	0.074369
C	-12.1562	-0.19073	0.056261
H	-11.0318	1.64926	0.102111
H	-15.5931	-0.39383	0.109988
S	13.38373	2.513139	-0.14376
S	-13.4111	-2.53409	0.056985
C	12.89794	-3.52624	-0.38598
C	15.69224	-2.2269	-0.28766
C	-13.0069	3.484205	0.317247
C	-15.7231	2.212173	0.039716
O	15.50283	-3.5241	0.025206
O	16.77732	-1.74985	-0.5495
O	12.83222	-4.02568	-1.48159
O	12.65327	-4.27398	0.713531
O	-11.8435	3.945861	-0.18782
O	-13.8067	4.182024	0.905317
O	-15.6808	3.150642	-0.92242
O	-16.6968	1.967721	0.718891
C	16.66561	-4.36887	-0.06463

H	17.08177	-4.33184	-1.07325
H	17.42588	-4.04424	0.649314
H	16.31349	-5.37202	0.170499
C	12.86423	-3.7312	2.024583
H	13.90564	-3.42733	2.157591
H	12.20251	-2.88393	2.22411
H	12.63066	-4.54309	2.713962
C	-11.5879	5.342079	0.044248
H	-11.5534	5.55349	1.115635
H	-10.6227	5.543293	-0.41911
H	-12.3696	5.95378	-0.41181
C	-16.8331	4.009037	-0.9914
H	-16.667	4.65266	-1.85456
H	-17.7446	3.420689	-1.11605
H	-16.9088	4.604315	-0.07842

Table S7: Cartesian coordinates of **D7** compound.

Atom	X-axis	Y-axis	Z-axis
C	-0.19658	1.416103	0.025932
C	-1.2835	0.55715	0.036258
C	-1.08602	-0.84922	0.006459
C	0.196594	-1.4161	-0.02572
C	1.283512	-0.55715	-0.03604
C	1.086034	0.849224	-0.00625
H	-0.33055	2.492924	0.039056
H	0.330566	-2.49292	-0.03885
C	2.396978	1.454473	-0.00711
C	3.391643	0.491528	-0.01364
C	5.888325	3.086666	0.000301
C	4.631188	2.486348	-0.0107
C	4.676459	1.075462	-0.02112
H	6.073358	4.15472	0.008802
S	2.980609	3.098885	-0.00675
S	6.309916	0.484317	-0.01944
C	6.936056	2.151342	0.000043
C	2.788167	-0.91322	-0.05334
C	-3.39163	-0.49153	0.013857
C	-4.67644	-1.07546	0.021304
C	-4.63117	-2.48635	0.010861
C	-6.93604	-2.15134	0.000138
C	-5.88831	-3.08667	-0.00012
H	-6.07334	-4.15472	-0.00864

S	-2.98059	-3.09888	0.006915
S	-6.3099	-0.48432	0.019616
C	-2.39696	-1.45447	0.007322
C	-2.78815	0.913222	0.053554
C	3.24072	-1.59383	-1.36614
C	2.489944	-1.49062	-2.54425
C	4.478144	-2.25362	-1.41993
C	2.957841	-2.03908	-3.73942
H	1.532956	-0.98071	-2.53484
C	4.946231	-2.79977	-2.61474
H	5.075637	-2.35686	-0.51998
C	4.186812	-2.69649	-3.7805
H	2.355801	-1.95074	-4.63906
H	5.905945	-3.30751	-2.63
H	4.548886	-3.12493	-4.71016
C	3.105353	-1.75629	1.199985
C	2.910471	-3.14592	1.183429
C	3.507705	-1.15486	2.398837
C	3.115074	-3.90985	2.331641
H	2.615738	-3.63754	0.261903
C	3.716024	-1.92001	3.547742
H	3.66102	-0.08174	2.440281
C	3.520205	-3.29989	3.519854
H	2.963182	-4.98457	2.294093
H	4.034993	-1.43243	4.464225
H	3.685806	-3.89552	4.412405
C	-3.24071	1.593854	1.366341
C	-2.49003	1.490516	2.5445
C	-4.47803	2.253836	1.420042
C	-2.95794	2.03902	3.739645
H	-1.53312	0.98047	2.535157
C	-4.94613	2.800034	2.614826
H	-5.07543	2.357195	0.520043
C	-4.18682	2.696611	3.780645
H	-2.35598	1.950576	4.639329
H	-5.90577	3.307922	2.630016
H	-4.5489	3.125089	4.71028
C	-3.10533	1.756284	-1.19978
C	-3.50755	1.154844	-2.39867
C	-2.91059	3.145928	-1.18318
C	-3.71586	1.919993	-3.54757
H	-3.66076	0.081711	-2.44015
C	-3.11519	3.909865	-2.33139
H	-2.61597	3.637559	-0.26162

C	-3.52018	3.299895	-3.51964
H	-4.03472	1.432403	-4.46409
H	-2.9634	4.984599	-2.2938
H	-3.68577	3.895527	-4.41219
C	8.283256	2.598461	0.013074
C	9.504503	1.961516	0.01809
H	8.323359	3.682774	0.022647
C	-8.28324	-2.59846	-0.0129
C	-9.5045	-1.96152	-0.01795
H	-8.32334	-3.68278	-0.02245
C	11.81159	1.543321	0.036502
C	11.20508	0.311689	0.019506
C	-11.8116	-1.54335	-0.03659
C	-11.2051	-0.31171	-0.01964
C	-10.8174	-2.62262	-0.03674
C	10.81742	2.622601	0.036895
C	11.14639	3.965111	0.053561
C	-11.1464	-3.96513	-0.05324
C	10.1903	5.024577	0.05595
N	9.425181	5.903313	0.05873
C	12.50965	4.389593	0.070922
N	13.62251	4.734708	0.085257
C	-10.1903	-5.02462	-0.05539
N	-9.42515	-5.90332	-0.05798
C	-12.5097	-4.3896	-0.07066
N	-13.6225	-4.73461	-0.08504
C	-9.73953	-0.49108	-0.00641
C	9.739515	0.491074	0.006538
O	-8.90588	0.406257	0.010662
O	8.905853	-0.40626	-0.01032
C	-14.5306	1.200753	-0.04094
C	-13.4536	0.31616	-0.03741
C	-12.1119	0.786673	-0.01955
C	-11.8557	2.166087	-0.00531
C	-12.9252	3.05791	-0.00844
C	-14.2698	2.573764	-0.0264
H	-15.5562	0.849733	-0.05456
H	-10.8336	2.526005	0.007693
C	11.85571	-2.16612	0.004873
C	12.92512	-3.05794	0.007795
C	14.26975	-2.57381	0.025605
C	14.53054	-1.2008	0.040215
C	13.4536	-0.3162	0.036912
C	12.11183	-0.7867	0.019193

H	10.8336	-2.52603	-0.00802
H	15.55617	-0.84978	0.053714
S	-13.5526	-1.44743	-0.05376
S	13.55258	1.44739	0.053402
C	-15.3714	3.488279	-0.02988
N	-16.2838	4.209361	-0.0331
C	-12.663	4.466731	0.006964
N	-12.4241	5.60451	0.02025
C	12.66298	-4.46676	-0.00769
N	12.42402	-5.60454	-0.02102
C	15.37134	-3.48833	0.028846
N	16.2838	-4.20942	0.031881

Table S8: Cartesian coordinates of **D8** compound.

Atom	X-axis	Y-axis	Z-axis
C	0.021311	1.428918	0.018947
C	-1.18387	0.744876	0.024571
C	-1.20344	-0.67456	0.001293
C	-0.02132	-1.42893	-0.01881
C	1.183858	-0.74489	-0.02443
C	1.203426	0.674541	-0.00115
H	0.052565	2.513748	0.027025
H	-0.05258	-2.51376	-0.02688
C	2.592075	1.072867	0.004757
C	3.428564	-0.02887	0.00768
C	6.295323	2.154373	0.018552
C	4.959195	1.751706	0.007605
C	4.789195	0.35227	0.003709
H	6.640989	3.181771	0.021618
S	3.421297	2.60867	0.001374
S	6.315902	-0.4792	0.01213
C	7.186637	1.072627	0.023768
C	2.617244	-1.32547	-0.02895
C	-3.42858	0.028846	-0.00755
C	-4.78921	-0.3523	-0.00365
C	-4.9592	-1.75174	-0.00761
C	-7.18665	-1.07267	-0.02386
C	-6.29533	-2.15441	-0.01861
H	-6.64098	-3.18181	-0.02174
S	-3.4213	-2.60869	-0.00132
S	-6.31592	0.47916	-0.01204
C	-2.59209	-1.07289	-0.00464
C	-2.61726	1.325451	0.029077

C	2.96825	-2.07969	-1.33201
C	2.242736	-1.88347	-2.51414
C	4.096262	-2.91361	-1.3733
C	2.62702	-2.51078	-3.70039
H	1.371074	-1.23853	-2.51377
C	4.481531	-3.53809	-2.55913
H	4.672259	-3.08892	-0.47059
C	3.746663	-3.34126	-3.72859
H	2.04588	-2.3472	-4.6033
H	5.358453	-4.17853	-2.56472
H	4.043921	-3.82994	-4.65162
C	2.792562	-2.19646	1.233436
C	2.398717	-3.54328	1.224515
C	3.260675	-1.64858	2.434104
C	2.474402	-4.31793	2.381328
H	2.047392	-3.99533	0.302603
C	3.34025	-2.42485	3.591439
H	3.566467	-0.60837	2.469602
C	2.947196	-3.76218	3.570991
H	2.16755	-5.35935	2.349403
H	3.713736	-1.97962	4.508951
H	3.011967	-4.36685	4.470549
C	-2.96828	2.079706	1.332104
C	-2.24291	1.883392	2.51431
C	-4.09615	2.913823	1.373269
C	-2.62722	2.510773	3.700511
H	-1.37135	1.238315	2.51404
C	-4.48144	3.538383	2.559054
H	-4.672	3.089236	0.470493
C	-3.74673	3.341437	3.72859
H	-2.04619	2.347107	4.603486
H	-5.35825	4.17897	2.564544
H	-4.044	3.830174	4.65158
C	-2.79256	2.196441	-1.23331
C	-3.2604	1.64852	-2.43407
C	-2.39901	3.543342	-1.22427
C	-3.33997	2.42483	-3.59138
H	-3.56598	0.60825	-2.46966
C	-2.4747	4.318035	-2.38106
H	-2.04793	3.995428	-0.30228
C	-2.9472	3.762241	-3.57081
H	-3.71324	1.979569	-4.50897
H	-2.16807	5.35952	-2.34904
H	-3.01197	4.366942	-4.47035

C	8.590333	1.310504	0.031735
C	9.698888	0.499633	0.032671
H	8.791781	2.376752	0.037718
C	-8.59034	-1.31055	-0.0319
C	-9.69889	-0.49966	-0.03276
H	-8.7918	-2.37679	-0.03801
C	11.91466	-0.25059	0.030878
C	11.13488	-1.39243	0.020695
C	-11.9147	0.250578	-0.03096
C	-11.1349	1.392415	-0.02062
C	-11.0994	-0.95939	-0.04025
C	11.09944	0.959369	0.040111
C	11.61671	2.242408	0.053946
C	-11.6167	-2.24244	-0.05424
C	10.82726	3.430595	0.065685
N	10.20237	4.41435	0.075899
C	13.02768	2.460191	0.058396
N	14.18025	2.632575	0.061971
C	-10.8272	-3.43059	-0.06622
N	-10.2023	-4.41432	-0.07662
C	-13.0277	-2.46025	-0.05881
N	-14.1802	-2.63275	-0.06247
C	-9.71063	0.993542	-0.02208
C	9.710643	-0.99357	0.022238
O	-8.74393	1.743663	-0.01584
O	8.74395	-1.74371	0.016294
C	-13.2199	2.343751	-0.0158
C	-11.8715	2.599721	-0.01197
C	13.21996	-2.34375	0.015809
C	11.87149	-2.59974	0.012146
S	-13.6018	0.642085	-0.03018
S	13.60183	-0.64208	0.030064
H	-11.4362	3.590847	-0.00357
H	-14.0316	3.059287	-0.01103
H	14.0316	-3.05928	0.011066
H	11.43621	-3.59087	0.003935

Table S9: Cartesian coordinates of **D9** compound.

Atom	X-axis	Y-axis	Z-axis
C	-0.08607	-1.42649	-0.01364
C	-1.23654	-0.6539	-0.02489
C	-1.14941	0.76306	-0.00682
C	0.086087	1.42645	0.01382

C	1.236553	0.653861	0.02507
C	1.149426	-0.7631	0.006992
H	-0.13636	-2.51063	-0.01786
H	0.13638	2.51059	0.018036
C	2.504179	-1.26493	0.005464
C	3.420969	-0.22929	0.000907
C	6.116403	-2.6215	-0.00486
C	4.813957	-2.11957	0.006019
C	4.749154	-0.71161	0.006766
H	6.384075	-3.67197	-0.00665
S	3.216065	-2.85862	0.013326
S	6.334132	0.002856	-0.00318
C	7.086133	-1.60994	-0.01297
C	2.709567	1.124916	0.030807
C	-3.42095	0.229248	-0.00073
C	-4.74914	0.711571	-0.0066
C	-4.81394	2.119523	-0.00587
C	-7.08612	1.609896	0.012998
C	-6.11639	2.621457	0.004942
H	-6.38406	3.671925	0.006672
S	-3.21605	2.858578	-0.01316
S	-6.33411	-0.0029	0.003395
C	-2.50416	1.264886	-0.00529
C	-2.70955	-1.12496	-0.03062
C	3.114762	1.855547	1.331481
C	2.372137	1.725266	2.511966
C	4.306512	2.59561	1.372546
C	2.803275	2.324541	3.696672
H	1.450454	1.154066	2.512032
C	4.738661	3.191569	2.556841
H	4.896863	2.720118	0.47064
C	3.987311	3.060293	3.725072
H	2.208038	2.213232	4.598373
H	5.664826	3.758468	2.562084
H	4.321277	3.526764	4.647032
C	2.953577	1.975448	-1.23393
C	2.658735	3.347418	-1.2314
C	3.38706	1.390633	-2.43017
C	2.796239	4.110226	-2.39036
H	2.336797	3.827285	-0.31276
C	3.528599	2.154827	-3.58967
H	3.617582	0.331074	-2.46017
C	3.233386	3.517169	-3.57568
H	2.565839	5.171328	-2.36355

H	3.873727	1.680403	-4.50364
H	3.346418	4.11229	-4.47685
C	-3.11475	-1.8556	-1.33128
C	-2.3721	-1.72536	-2.51176
C	-4.30652	-2.59563	-1.37236
C	-2.80324	-2.32464	-3.69646
H	-1.4504	-1.15419	-2.51182
C	-4.73867	-3.19159	-2.55665
H	-4.89689	-2.7201	-0.47046
C	-3.9873	-3.06035	-3.72487
H	-2.20799	-2.21336	-4.59816
H	-5.66485	-3.75846	-2.5619
H	-4.32127	-3.52683	-4.64683
C	-2.95355	-1.97547	1.23413
C	-3.38708	-1.39065	2.430357
C	-2.65865	-3.34743	1.231645
C	-3.52861	-2.15482	3.58987
H	-3.61764	-0.3311	2.460327
C	-2.79614	-4.11022	2.390613
H	-2.33667	-3.8273	0.313025
C	-3.23334	-3.51715	3.575916
H	-3.87377	-1.68039	4.503826
H	-2.5657	-5.17131	2.363836
H	-3.34636	-4.11226	4.477093
C	8.468441	-1.95327	-0.02364
C	9.634014	-1.22782	-0.02811
H	8.588449	-3.03152	-0.02914
C	-8.46843	1.953234	0.023498
C	-9.63402	1.227816	0.027864
H	-8.58842	3.031493	0.028931
C	11.90305	-0.6469	-0.03244
C	11.20212	0.54758	-0.01988
C	-11.9031	0.646949	0.032117
C	-11.2022	-0.54755	0.019744
C	-10.9997	1.789056	0.039071
C	10.99966	-1.78903	-0.0395
C	11.4156	-3.10967	-0.05518
C	-11.4156	3.109709	0.054555
C	10.53631	-4.23261	-0.06511
N	9.83834	-5.16611	-0.07392
C	12.80432	-3.43978	-0.06389
N	13.93856	-3.70789	-0.07104
C	-10.5362	4.232622	0.064415
N	-9.83829	5.166136	0.073165

C	-12.8043	3.439848	0.063155
N	-13.9385	3.708022	0.070208
C	-9.75592	-0.2577	0.017484
C	9.75588	0.257695	-0.01764
O	-8.85485	-1.08675	0.008581
O	8.854789	1.086723	-0.0087
C	-14.2797	-2.44029	0.01338
C	-13.3986	-1.32391	0.020303
C	-12.0435	-1.67545	0.013056
C	-13.577	-3.6154	0.001062
H	-15.3609	-2.38473	0.017214
C	13.5769	3.615485	-0.00081
C	14.27961	2.440388	-0.01334
C	13.39849	1.323988	-0.02039
C	12.04343	1.675507	-0.01305
H	15.36083	2.384851	-0.01722
S	-13.6347	0.415188	0.036087
S	13.63462	-0.4151	-0.03645
H	-13.9816	-4.61839	-0.00626
H	13.98144	4.618478	0.006653
S	-11.8412	-3.40194	-0.00231
S	11.8411	3.401991	0.002585

Table S10: Wavelength (λ), transition energy (E_g), oscillator strength (f_{os}) and nature of molecular orbital contributions of **R1** in chloroform**.**

NO	λ (*nm*)	E_g(*eV*)	f_{os}	MO contributions
1	719.082	1.724	2.739	H→L (99%),
2	607.349	2.041	0.001	H→L+1 (98%),
3	504.904	2.456	0.003	H-1→L (97%),
4	463.233	2.677	0.340	H-1→L+1 (91%), H→L+2 (6%)
5	451.706	2.745	0.009	H-2→L (91%), H-4→L (4%), H-3→L+1 (3%)
6	448.763	2.763	0.014	H-3→L (89%), H-4→L+1 (5%), H-2→L+1 (3%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}=oscillator strength

Table S11: Wavelength (λ), transition energy (E_g), oscillator strength (f_{os}) and nature of molecular orbital contributions of **D2** in chloroform**.**

NO	λ (*nm*)	E_g(*eV*)	f_{os}	MO contributions
1	737.562	1.681	1.786	H→L (97%), H-1→L+1 (3%)
2	681.531	1.819	0.000	H→L+1 (96%),
3	567.615	2.184	1.393	H→L+2 (96%),

4	524.313	2.365	0.000	H-1→L (83%), H→L+3 (11%), H→L+1 (2%)
5	498.890	2.485	0.109	H-1→L+1 (90%), H-2→L (2%), H→L (3%)
6	482.129	2.572	0.000	H-1→L (11%), H→L+3 (87%),

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}=oscillator strength

Table S12: Wavelength (λ), transition energy (E_g), oscillator strength (f_{os}) and nature of molecular orbital contributions of **D3** in chloroform**.**

NO	λ (*nm*)	E_g(*eV*)	f_{os}	MO contributions
1	794.516	1.561	1.663	H→L (98%),
2	733.417	1.691	0.000	H→L+1 (97%),
3	581.158	2.133	1.375	H→L+2 (97%),
4	553.328	2.241	0.000	H-1→L (56%), H→L+3 (36%), H→L+5 (3%)
5	538.476	2.303	0.000	H-1→L (38%), H→L+3 (61%),
6	537.799	2.305	0.233	H-1→L+1 (11%), H→L+4 (86%),

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}=oscillator strength

Table S13: Wavelength (λ), transition energy (E_g), oscillator strength (f_{os}) and nature of molecular orbital contributions of **D4** in chloroform**.**

NO	λ (*nm*)	E_g(*eV*)	f_{os}	MO contributions
1	747.839	1.658	1.781	H→L (97%), H-1→L+1 (2%),
2	689.606	1.798	0.000	H→L+1 (96%),
3	568.970	2.179	1.374	H→L+2 (96%),
4	527.817	2.349	0.000	H-1→L (85%), H→L+3 (10%),
5	501.514	2.472	0.098	H-1→L+1 (92%), H→L (3%)
6	483.784	2.563	0.000	H-1→L (11%), H→L+3 (87%),

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}=oscillator strength

Table S14: Wavelength (λ), transition energy (E_g), oscillator strength (f_{os}) and nature of molecular orbital contributions of **D5** in chloroform**.**

NO	λ (*nm*)	E_g(*eV*)	f_{os}	MO contributions
1	778.257	1.593	1.738	H→L (98%),
2	716.672	1.730	0.000	H→L+1 (97%),
3	577.503	2.147	1.438	H→L+2 (97%),
4	541.463	2.290	0.000	H-1→L (88%), H→L+3 (8%)
5	515.227	2.406	0.088	H-1→L+1 (94%), H→L (2%)
6	491.202	2.524	0.000	H→L+3 (90%), H-1→L (8%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}=oscillator strength

Table S15: Wavelength (λ), transition energy (E_g), oscillator strength (f_{os}) and nature of molecular orbital contributions of **D6** in chloroform**.**

NO	λ (*nm*)	E_g(*eV*)	f_{os}	MO contributions
1	747.929	1.658	1.750	H→L (97%), H-1→L+1 (2%)
2	687.960	1.802	0.035	H→L+1 (96%),
3	566.889	2.187	1.400	H→L+2 (96%),
4	528.605	2.346	0.004	H-1→L (86%), H→L+3 (9%)
5	501.940	2.470	0.100	H-1→L+1 (89%), H→L (2%)
6	482.579	2.569	0.002	H→L+3 (88%), H-1→L (9%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}=oscillator strength

Table S16: Wavelength (λ), transition energy (E_g), oscillator strength (f_{os}) and nature of molecular orbital contributions of **D7** in chloroform**.**

NO	λ (*nm*)	E_g(*eV*)	f_{os}	MO contributions
1	778.795	1.592	1.711	H→L (97%), H-1→L+1 (2%)
2	718.707	1.725	0.000	H→L+1 (97%),
3	577.961	2.145	1.476	H→L+2 (97%),
4	542.102	2.287	0.000	H-1→L (88%), H→L+3 (8%)
5	516.687	2.400	0.090	H-1→L+1 (93%), H→L (2%)
6	491.825	2.521	0.000	H→L+3 (90%), H-1→L (8%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}=oscillator strength

Table S17: Wavelength (λ), transition energy (E_g), oscillator strength (f_{os}) and nature of molecular orbital contributions of **D8** in chloroform**.**

NO	λ (*nm*)	E_g(*eV*)	f_{os}	MO contributions
1	682.657	1.816	2.229	H→L (98%),
2	617.359	2.008	0.000	H→L+1 (96%),
3	538.476	2.303	0.803	H→L+2 (95%),
4	495.976	2.500	0.000	H-1→L (64%), H→L+3 (31%),
5	466.439	2.658	0.000	H-1→L (33%), H→L+3 (65%),
6	460.394	2.693	0.160	H-1→L+1 (92%), H→L (2%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}=oscillator strength

Table S18: Wavelength (λ), transition energy (E_g), oscillator strength (f_{os}) and nature of molecular orbital contributions of **D9** in chloroform**.**

NO	λ (*nm*)	E_g(*eV*)	f_{os}	MO contributions
1	700.555	1.770	1.930	H→L (96%), H-1→L+1 (3%)
2	646.829	1.917	0.000	H→L+1 (95%),

3	561.091	2.210	1.177	H→L+2 (95%), H-1→L+3 (2%)
4	508.883	2.436	0.000	H-1→L (70%), H→L+3 (23%), H→L+1 (3%)
5	481.417	2.575	0.158	H-1→L+1 (87%), H-2→L (3%), H→L (3%), H→L+2 (2%)
6	477.542	2.596	0.000	H-1→L (23%), H→L+3 (75%),

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}=oscillator strength

Table S19: Wavelength (λ), transition energy (E_g), oscillator strength (f_{os}) and nature of molecular orbital contributions of **R1** in gas phase.

NO	λ (*nm*)	E_g(*eV*)	f_{os}	MO contributions
1	673.242	1.842	2.375	H→L (100%),
2	589.559	2.103	0.001	H→L+1 (93%), H-1→L (6%)
3	486.346	2.549	0.003	H-1→L (90%), H→L+1 (6%)
4	458.386	2.705	0.339	H-1→L+1 (87%), H→L+2 (7%)
5	445.554	2.783	0.103	H-2→L (75%), H-4→L (4%), H-3→L (6%), H-2→L+1 (6%), H→L+2 (5%)
6	443.466	2.796	0.009	H-4→L (24%), H-3→L (59%), H-4→L+1 (3%), H-2→L (9%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}=oscillator strength

Table S20: Wavelength (λ), transition energy (E_x), oscillator strength (f_{os}) and nature of molecular orbital contributions of **D2** in gas phase.

NO	λ (*nm*)	E_g(*eV*)	f_{os}	MO contributions
1	693.928	1.787	1.498	H→L (96%), H-1→L+1 (2%)
2	650.153	1.907	0.000	H→L+1 (95%),
3	548.773	2.259	1.389	H→L+2 (95%),
4	512.289	2.420	0.000	H-1→L (73%), H→L+3 (21%),
5	484.616	2.558	0.102	H-1→L+1 (89%), H-2→L (2%), H→L (2%)
6	465.546	2.663	0.000	H-1→L (19%), H→L+3 (75%), H-1→L+2 (4%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}=oscillator strength

Table S21: Wavelength (λ), transition energy (E_x), oscillator strength (f_{os}) and nature of molecular orbital contributions of **D3** in gas phase.

NO	λ (*nm*)	E_g(*eV*)	f_{os}	MO contributions
1	744.784	1.665	1.343	H→L (97%),
2	699.290	1.773	0.000	H→L+1 (97%),
3	563.693	2.200	1.487	H→L+2 (96%),
4	535.014	2.317	0.000	H-1→L (78%), H→L+3 (16%), H→L+5 (2%)
5	509.510	2.433	0.100	H-1→L+1 (91%), H→L+4 (3%)

6	494.276	2.508	0.000	H-1→L (14%), H→L+3 (79%), H→L+5 (4%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}=oscillator strength

Table S22: Wavelength (λ), transition energy (E_x), oscillator strength (f_{os}) and nature of molecular orbital contributions of **D4** in gas phase.

NO	λ (*nm*)	E_g(*eV*)	f_{os}	MO contributions
1	705.217	1.758	1.465	H→L (97%),
2	660.650	1.877	0.000	H→L+1 (96%),
3	551.384	2.249	1.390	H→L+2 (96%),
4	516.708	2.400	0.000	H-1→L (75%), H→L+3 (20%),
5	488.665	2.537	0.096	H-1→L+1 (92%),
6	468.130	2.649	0.000	H-1→L (19%), H→L+3 (75%), H-1→L+2 (3%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}=oscillator strength

Table S23: Wavelength (λ), transition energy (E_x), oscillator strength (f_{os}) and nature of molecular orbital contributions of **D5** in gas phase.

NO	λ (*nm*)	E_g(*eV*)	f_{os}	MO contributions
1	738.749	1.678	1.387	H→L (97%),
2	692.533	1.790	0.000	H→L+1 (97%),
3	562.440	2.204	1.491	H→L+2 (96%),
4	531.596	2.332	0.000	H-1→L (81%), H→L+3 (16%),
5	505.007	2.455	0.080	H-1→L+1 (94%),
6	478.482	2.591	0.000	H-1→L (15%), H→L+3 (78%), H-1→L+2 (2%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}=oscillator strength

Table S24: Wavelength (λ), transition energy (E_x), oscillator strength (f_{os}) and nature of molecular orbital contributions of **D6** in gas phase.

NO	λ (*nm*)	E_g(*eV*)	f_{os}	MO contributions
1	701.030	1.769	1.433	H→L (97%),
2	649.438	1.909	0.109	H→L+1 (95%),
3	546.619	2.268	1.358	H→L+2 (95%),
4	515.013	2.407	0.015	H-1→L (77%), H→L+3 (17%),
5	485.375	2.554	0.086	H-1→L+1 (83%), H-1→L (2%), H→L+3 (5%)
6	464.586	2.669	0.010	H-1→L (14%), H→L+3 (74%), H-1→L+1 (6%), H-1→L+2 (3%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}=oscillator strength

Table S25: Wavelength (λ), transition energy (E_x), oscillator strength (f_{os}) and nature of molecular orbital contributions of **D7** in gas phase.

NO	λ (*nm*)	E_g(*eV*)	f_{os}	MO contributions
1	734.504	1.688	1.374	H→L (97%),
2	689.567	1.798	0.000	H→L+1 (96%),
3	561.828	2.207	1.517	H→L+2 (96%),
4	529.847	2.340	0.000	H-1→L (80%), H→L+3 (16%),
5	503.898	2.461	0.083	H-1→L+1 (93%),
6	477.505	2.597	0.000	H-1→L (15%), H→L+3 (79%), H-1→L+2 (3%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}=oscillator strength

Table S26: Wavelength (λ), transition energy (E_x), oscillator strength (f_{os}) and nature of molecular orbital contributions of **D8** in gas phase.

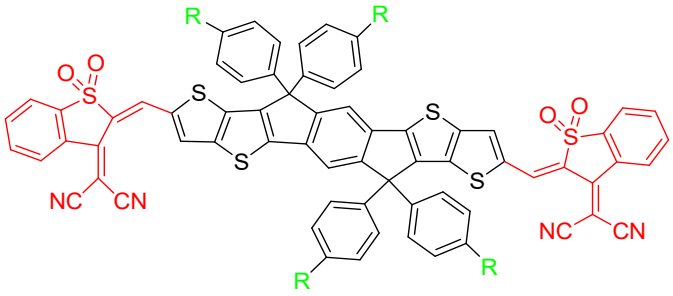
NO	λ (*nm*)	E_g(*eV*)	f_{os}	MO contributions
1	643.773	1.926	1.885	H→L (98%),
2	592.659	2.092	0.000	H→L+1 (95%), H-1→L+2 (2%)
3	521.139	2.379	0.812	H→L+2 (95%),
4	488.781	2.537	0.000	H-1→L (57%), H→L+3 (39%),
5	449.903	2.756	0.159	H-1→L+1 (92%),
6	447.306	2.772	0.000	H-1→L (39%), H→L+3 (56%),

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}=oscillator strength

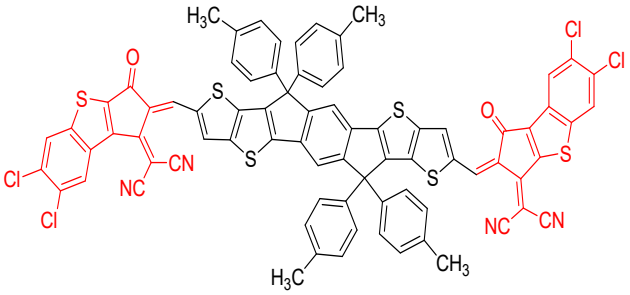
Table S27: Wavelength (λ), transition energy (E_x), oscillator strength (f_{os}) and nature of molecular orbital contributions of **D9** in gas phase.

NO	λ (*nm*)	E_g(*eV*)	f_{os}	MO contributions
1	661.955	1.873	1.618	H→L (96%), H-1→L+1 (2%)
2	619.085	2.003	0.000	H→L+1 (94%), H-1→L+2 (2%)
3	540.472	2.294	1.176	H→L+2 (94%),
4	498.930	2.485	0.000	H-1→L (61%), H→L+3 (33%), H→L+1 (2%)
5	467.177	2.654	0.127	H-1→L+1 (88%), H-2→L (2%), H→L (2%), H→L+2 (2%)
6	457.810	2.708	0.000	H-1→L (30%), H→L+3 (63%), H-1→L+2 (5%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}=oscillator strength



R1



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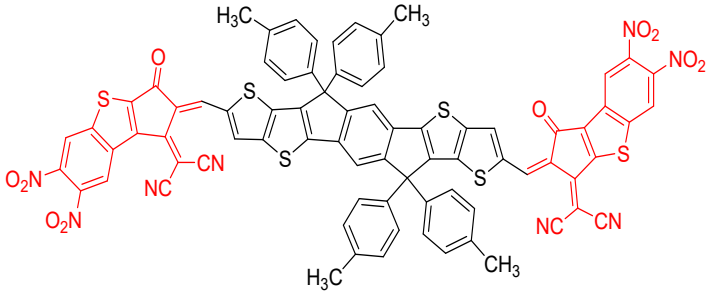
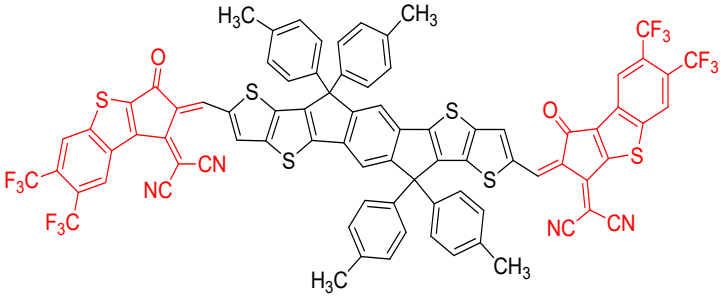
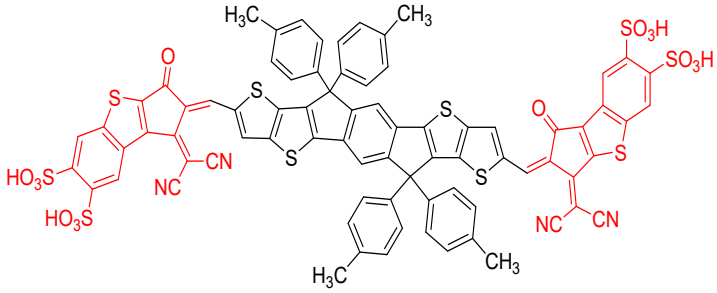


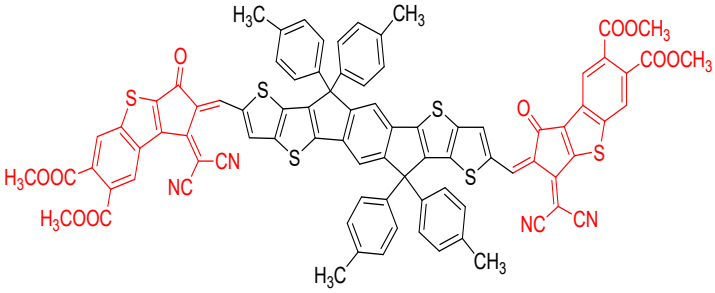
D3



D4



D5



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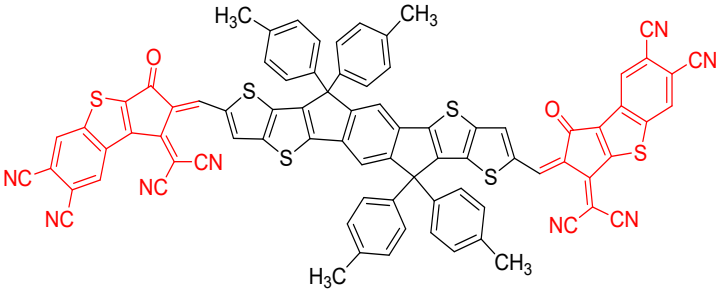

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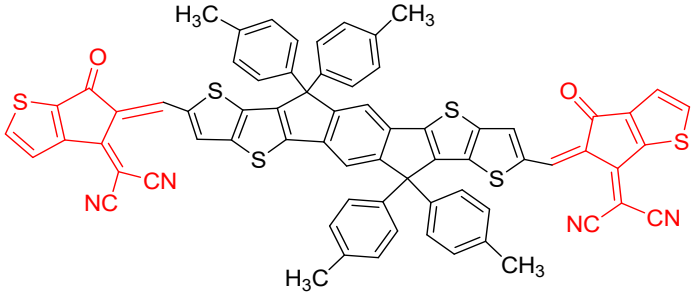

D8

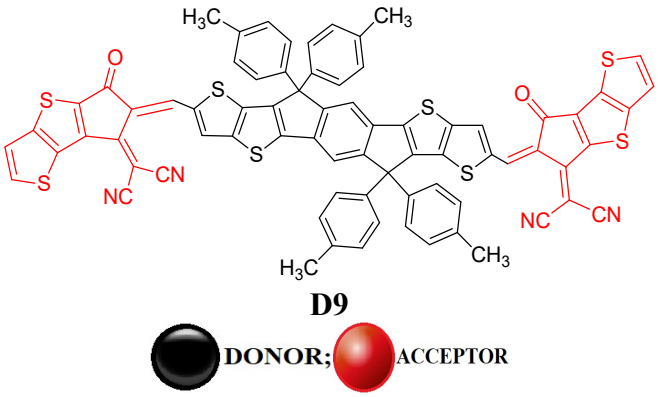

Fig. S1. 2D structural representations of the reference and designed chromophores.

The **R1** molecule has been modified with end-capped acceptor substitutions 2-(6,7-dichloro-2-methylene-3-oxo-2,3-dihydro-1H-benzo[b] cyclopenta [d]thiophen-1-ylidene)malononitrile (**D2**), 2-(2-methylene-6,7-dinitro-3-oxo-2,3-dihydro-1H-benzo[b]cyclopenta[d]thiophen-1-ylidene) malononitrile (**D3**), 2-(2-methylene-3-oxo-6,7-bis(trifluoromethyl)-2,3-dihydro-1H-benzo[b] cyclopenta[d]thiophen-1-ylidene)malononitrile (**D4**), 1-(dicyanomethylene)-2-methylene-3-oxo-2,3-dihydro-1H-benzo[b] cyclopenta[d] thiophene-6,7-disulfonic acid (**D5**), dimethyl 1-(dicyanomethylene)-2-methylene-3-oxo-2,3-dihydro-1H-benzo[b]cyclopenta[d] thiophene-6,7-dicarboxylate (**D6**), 1-(dicyano-methylene)-2-methylene-3-oxo-2,3-dihydro-1H-benzo[b] cyclopenta[d]thiophene-6,7-dicarbo-nitrile (**D7**), 2-(5-methylene-6-oxo-5,6-dihydro-4H-cyclopenta[b] thiophen-4-ylidene)malononitrile (**D8**), 2-(6-methylene-5-oxo-5H-cyclopenta [b] thieno[2,3-d]thiophen-7(6H)-ylidene) malononitrile (**D9**), as shown in Scheme 1 & Fig. S1.