Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information:

Computational investigation of photoswitch conjugates for molecular solar energy storage

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Supplementary figures

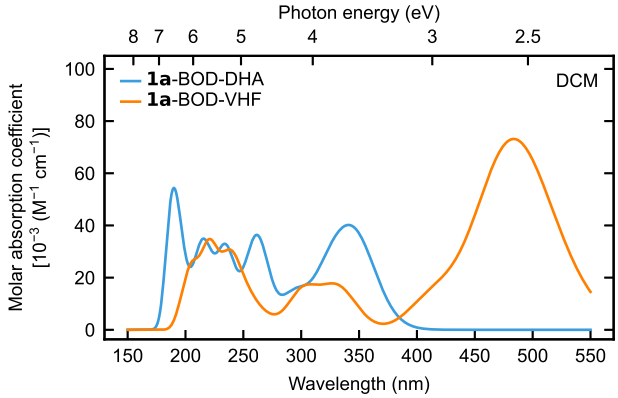

Figure S1: ωB97-XD[S1]/6-311++G(d,p)[S2]-predicted one-photon absorption for **1a**-BOD-DHA and **1a**-BOD-VHF in DCM.

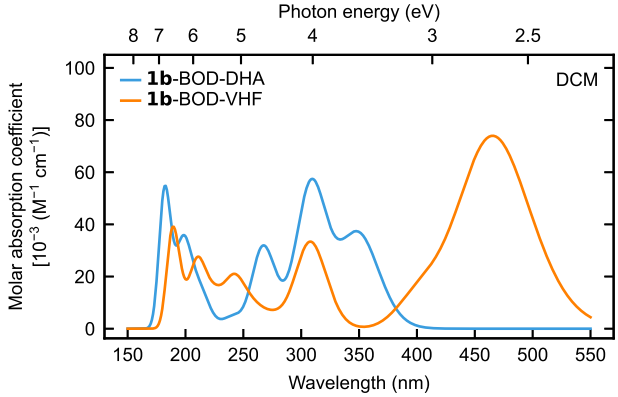

Figure S2: ωB97-XD/6-311++G(d,p)-predicted one-photon absorption for **1b**-BOD-DHA and **1b**-BOD-VHF in DCM.

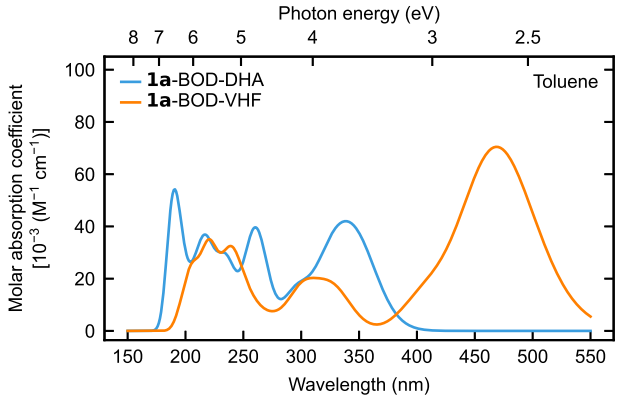

Figure S3: ωB97-XD/6-311++G(d,p)-predicted one-photon absorption for **1a**-BOD-DHA and **1a**-BOD-VHF in toluene.

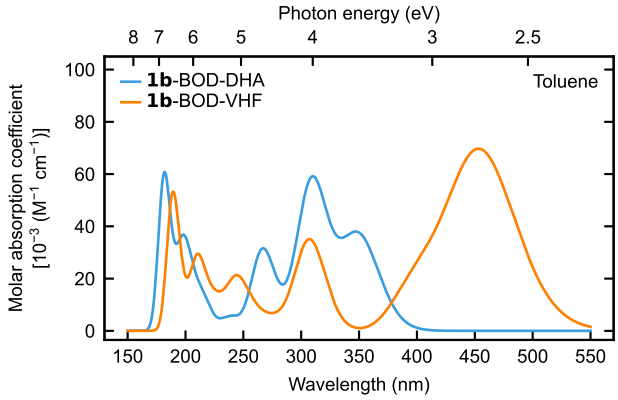

Figure S4: ωB97-XD/6-311++G(d,p)-predicted one-photon absorption for **1b**-BOD-DHA and **1b**-BOD-VHF in toluene.

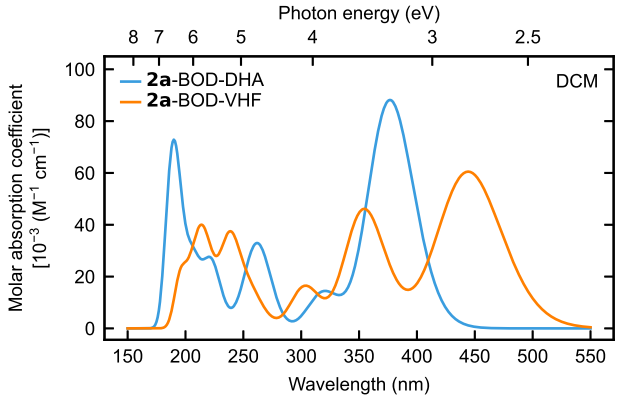

Figure S5: ωB97-XD/6-311++G(d,p)-predicted one-photon absorption for **2a**-BOD-DHA and **2a**-BOD-VHF in DCM.

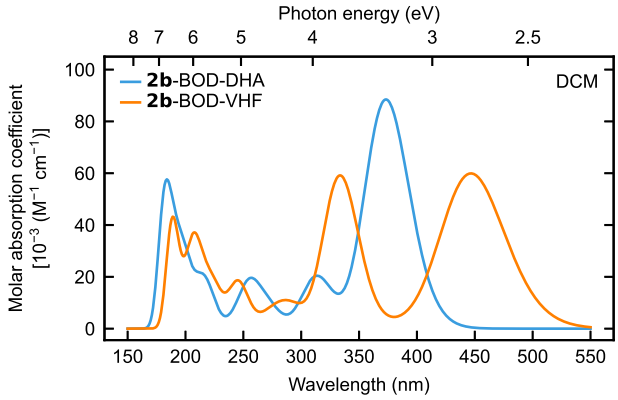

Figure S6: ωB97-XD/6-311++G(d,p)-predicted one-photon absorption for **2b**-BOD-DHA and **2b**-BOD-VHF in DCM.

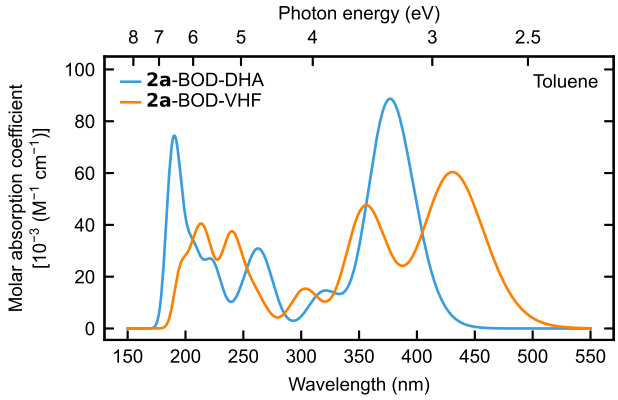

Figure S7: ωB97-XD/6-311++G(d,p)-predicted one-photon absorption for **2a**-BOD-DHA and **2a**-BOD-VHF in toluene.

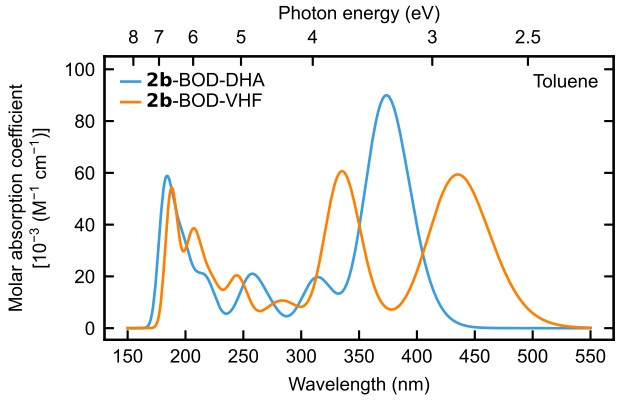

Figure S8: ωB97-XD/6-311++G(d,p)-predicted one-photon absorption for **2b**-BOD-DHA and **2b**-BOD-VHF in toluene.

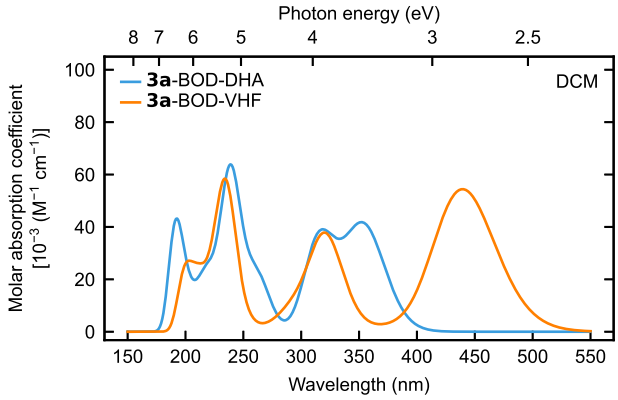

Figure S9: ωB97-XD/6-311++G(d,p)-predicted one-photon absorption for **3a**-BOD-DHA and **3a**-BOD-VHF in DCM.

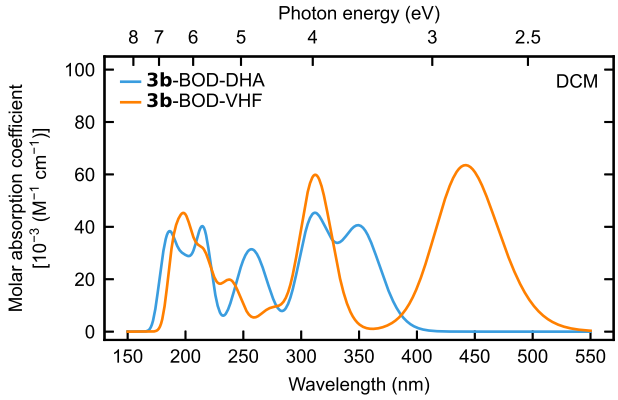

Figure S10: ωB97-XD/6-311++G(d,p)-predicted one-photon absorption for **3b**-BOD-DHA and **3b**-BOD-VHF in DCM.

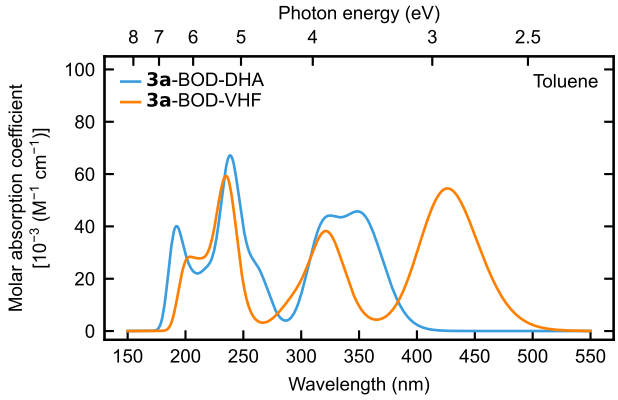

Figure S11: ωB97-XD/6-311++G(d,p)-predicted one-photon absorption for **3a**-BOD-DHA and **3a**-BOD-VHF in toluene.

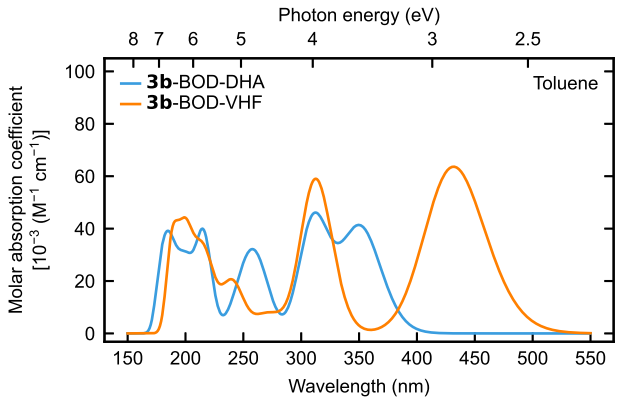

Figure S12: ωB97-XD/6-311++G(d,p)-predicted one-photon absorption for **3b**-BOD-DHA and **3b**-BOD-VHF in toluene.

Supplementary tables

Storage energies and storage densities

The presented storage densities were determined using the following molecular masses: **a**-systems (460.58 g/mol), **b**-systems (409.49 g/mol), DHA/VHF (256.31 g/mol), BOD/TCO (106.17 g/mol), BOD(CN)/TCO(CN) (131.18 g/mol), and BOD(Ph)/TCO(Ph) (182.27 g/mol).

Table S1: Storage energies (kJ/mol) for the different conjugate systems, obtained using the M06-2X[S3] functional in combination with the 6-311+G(d) basis set. The storage energy is defined as the energy difference between the BOD-DHA and the TCO-VHF isomers of each system.

System	Vacuum	DCM	Toluene
1a	186.02	181.42	184.66
1b	190.24	183.53	189.30
2a	195.00	191.12	196.00
2b	193.02	186.65	193.12
3a	191.38	186.97	189.80
3b	192.56	186.28	193.39

Table S2: Storage densities (MJ/kg) for the different conjugate systems, obtained using the M06-2X functional in combination with the 6-311+G(d) basis set. The storage density is defined as the ratio between the storage energy and the molecular weight.

System	Vacuum	DCM	Toluene
1a	0.404	0.394	0.401
1b	0.465	0.448	0.462
2a	0.423	0.415	0.426
2b	0.471	0.456	0.471
3a	0.416	0.406	0.412
3b	0.470	0.455	0.472

Table S3: Storage energies (kJ/mol) for the DHA/VHF and BOD/TCO photoswitch pairs, obtained using the M06-2X and ωB97-XD functionals in combination with the 6-311+G(d) basis set. The storage energies are defined as the energy difference between the DHA and VHF molecules and the difference between the BOD and TCO molecules.

Method	System	Vacuum	DCM	Toluene
M06-2X	DHA/VHF	32.4485	21.7890	26.6619
-	BOD/TCO	163.0094	164.8157	163.8837
-	BOD/TCO(CN)	160.3104	163.0094	159.8588
-	BOD/TCO(Ph)	162.0537	162.8230	162.3740
ωB97-XD	DHA/VHF	31.3327	18.5465	24.6744
-	BOD/TCO	169.3789	171.3112	170.3057
-	BOD/TCO(CN)	166.4803	166.0156	166.1180
-	BOD/TCO(Ph)	168.3077	169.2345	168.6778

Table S4: Storage densities (kJ/mol) for the DHA/VHF and BOD/TCO photoswitch pairs, obtained using the M06-2X and ωB97-XD functionals in combination with the 6-311+G(d) basis set. The storage densities are defined as the ratios between the storage energies and the molecular weights of the respective photoswitch pairs.

Method	System	Vacuum	DCM	Toluene
M06-2X	DHA/VHF	0.1266	0.0850	0.1040
-	BOD/TCO	1.5353	1.5523	1.5435
-	BOD/TCO(CN)	1.2220	1.2426	1.2186
-	BOD/TCO(Ph)	0.8891	0.8933	0.8908
ωB97-XD	DHA/VHF	0.1222	0.0724	0.0963
-	BOD/TCO	1.5953	1.6135	1.6040
-	BOD/TCO(CN)	1.2690	1.2655	1.2663
-	BOD/TCO(Ph)	0.9234	0.9285	0.9254

Optimized geometries

All the presented geometries are optimized *in vacuo* at the ωB97-XD/6-311+G(d) level in Gaussian 16.[S4]

Table S5: Cartesian coordinates of **1a**-BOD-DHA.

Atom	x	y	z	Continued			
N	-4.36872	0.70395	3.22300	C	5.85979	-0.96344	-0.50766
C	-3.79182	0.54562	2.24170	C	6.32681	-0.27777	-1.77400
C	-3.04853	0.39721	0.97698	C	6.03568	1.01775	-1.82111
C	-3.98756	0.61645	-0.23141	C	5.29778	1.51734	-0.59998
C	-5.01513	-0.35285	-0.63392	C	6.24402	1.26534	0.61958
C	-5.42723	-0.40383	-1.97175	C	6.58647	-0.23772	0.67422
C	-6.40698	-1.29506	-2.38009	H	-4.95600	0.24182	-2.70533
C	-6.98809	-2.16338	-1.46185	H	-6.70788	-1.32212	-3.42203
C	-6.57707	-2.13436	-0.13560	H	-7.75051	-2.86560	-1.78176
C	-5.59758	-1.24069	0.27622	H	-7.01936	-2.81088	0.58755
C	-3.69281	1.78491	-0.81992	H	-5.30725	-1.23538	1.32058
C	-2.45555	-0.94836	0.93932	H	-4.23948	2.19903	-1.65897
N	-2.00432	-2.00306	0.87687	H	-1.95967	2.11061	1.82221
C	-1.99399	1.56835	0.87104	H	-2.60841	4.30610	-1.19635
C	-2.56664	2.45629	-0.21005	H	-0.82307	5.31489	0.16536
C	-2.08214	3.68187	-0.47856	H	1.06257	4.09048	0.86571
C	-0.88965	4.23079	0.12525	H	-0.36679	0.12806	0.29648
C	0.19519	3.53114	0.52752	H	1.85889	-1.00808	-1.28435
C	-0.60052	1.17182	0.48128	H	0.24059	-2.77711	-0.69256
C	0.38873	2.08826	0.39360	H	0.88183	-4.57386	0.87880
C	1.71946	1.63820	0.13255	H	3.16985	-4.60586	1.84435
C	2.81467	1.18753	-0.09909	H	4.77684	-2.83366	1.27618
C	4.08627	0.62525	-0.36097	H	6.08017	-2.03064	-0.50970
C	4.37645	-0.69119	-0.31977	H	6.87467	-0.81713	-2.53831
C	3.42637	-1.77724	-0.03031	H	6.31529	1.68490	-2.62858
C	2.14249	-1.78794	-0.58673	H	5.01633	2.56762	-0.66915
C	1.23656	-2.78849	-0.26369	H	5.74073	1.58987	1.53346
C	1.59748	-3.80171	0.61756	H	7.14490	1.87292	0.50635
C	2.87786	-3.81704	1.15842	H	6.26382	-0.67983	1.62028
C	3.78593	-2.81798	0.83212	H	7.66278	-0.40272	0.58521

Table S6: Cartesian coordinates of **1a**-TCO-VHF.

Atom	x	y	z	Continued			
N	7.20422	2.18326	-0.92571	C	3.65421	-0.90124	0.44587
C	6.57737	1.27050	-0.60361	C	2.94680	-0.90575	1.64999
C	5.78035	0.15683	-0.20153	C	2.25422	-2.03889	2.04973
C	6.47447	-1.08126	-0.05534	C	2.24740	-3.17364	1.24483
N	7.05912	-2.06911	0.05358	C	2.93452	-3.16919	0.03726
C	4.43618	0.30270	0.06128	C	3.63925	-2.04015	-0.35952
C	3.85240	1.61525	0.06278	H	4.56828	2.42681	0.15539
C	2.53440	1.99210	-0.04980	H	1.80752	0.11201	-0.80242
C	1.47273	1.06892	-0.42033	H	-0.43677	0.34589	-0.71164
C	0.13166	1.21024	-0.38057	H	-5.76216	2.45132	0.83367
C	-0.69511	2.32326	0.04952	H	-5.71631	1.96011	-1.61454
C	-2.08374	2.01226	0.12040	H	-5.78328	-0.67308	-2.30254
C	-3.21913	1.60331	0.11255	H	-5.80093	-2.28778	-0.38047
C	-4.45662	0.91825	0.04887	H	-7.72553	-1.18676	0.80753
C	-5.78784	1.39487	0.57998	H	-6.43034	-1.57881	1.91681
C	-5.64922	1.15787	-0.89143	H	-6.19458	0.63621	2.51764
C	-5.64478	-0.33138	-1.28434	H	-7.62573	0.98460	1.57206
C	-5.80555	-1.23889	-0.09369	H	-2.74557	-1.40810	1.51098
C	-6.69968	-0.92411	1.08318	H	-0.52466	-2.44946	1.18664
C	-6.62314	0.55119	1.51474	H	0.30103	-2.92882	-1.09316
C	-4.47134	-0.59409	-0.36280	H	-1.11200	-2.36864	-3.05818
C	-3.19027	-1.30384	-0.58820	H	-3.31962	-1.30115	-2.72918
C	-2.39089	-1.63299	0.50938	H	-1.00761	4.31929	0.57991
C	-1.14516	-2.21656	0.32844	H	1.18029	5.14464	0.37844
C	-0.67929	-2.48488	-0.95565	H	3.15209	4.03426	0.10265
C	-1.46974	-2.16738	-2.05353	H	2.95253	-0.01954	2.27574
C	-2.71558	-1.57354	-1.86922	H	1.72237	-2.03778	2.99544
C	-0.25357	3.58407	0.31672	H	1.70775	-4.06124	1.55903
C	1.08873	4.06929	0.24876	H	2.93495	-4.05152	-0.59390
C	2.26170	3.41054	0.08836	H	4.18033	-2.04359	-1.29952

Table S7: Cartesian coordinates of **1b**-BOD-DHA.

Atom	x	y	z	Continued			
N	-4.22434	1.28628	3.01930	C	6.75367	-0.65959	-0.29310
C	-3.65893	0.82256	2.13276	C	6.56074	-1.72114	-1.35533
C	-2.92227	0.27665	0.97792	C	5.42288	-2.39711	-1.23930
C	-3.79614	0.34321	-0.29569	C	4.56397	-1.96108	-0.07172
C	-4.94473	-0.54234	-0.52480	C	5.42341	-2.18677	1.21820
C	-5.34715	-0.82405	-1.83665	C	6.74881	-1.40956	1.08118
C	-6.43882	-1.64103	-2.08464	H	-4.78316	-0.42138	-2.67143
C	-7.14507	-2.20361	-1.02644	H	-6.73110	-1.85102	-3.10802
C	-6.74680	-1.94518	0.27867	H	-7.99598	-2.84799	-1.21980
C	-5.65498	-1.12514	0.52966	H	-7.28710	-2.38313	1.11081
C	-3.33102	1.30606	-1.10568	H	-5.37729	-0.93333	1.55987
C	-2.52442	-1.10464	1.28750	H	-3.80030	1.59735	-2.03790
N	-2.19975	-2.18543	1.50309	H	-1.57639	1.94645	1.47755
C	-1.70311	1.22662	0.66197	H	-1.88834	3.53023	-1.94404
C	-2.13115	1.93706	-0.60101	H	0.01055	4.53453	-0.74030
C	-1.46936	3.00021	-1.09254	H	1.69002	3.22259	0.26463
C	-0.21688	3.48699	-0.56215	H	-0.32452	-0.52765	0.39547
C	0.75014	2.73868	0.01652	H	7.66584	-0.07974	-0.42538
C	-0.38991	0.55529	0.39347	H	7.31722	-1.90882	-2.10825
C	0.72452	1.28508	0.17137	H	5.12061	-3.21362	-1.88444
C	1.98605	0.62526	0.04924	H	3.61505	-2.49155	-0.01257
C	3.08100	0.12868	-0.04574	H	5.60175	-3.25757	1.33420
C	4.35958	-0.45738	-0.15493	H	4.85507	-1.85244	2.08898
C	5.51788	0.22207	-0.27292	H	7.60831	-2.08199	1.11740
C	5.60643	1.63796	-0.30583	H	6.86635	-0.68156	1.88684
N	5.70170	2.78744	-0.33146				

Table S8: Cartesian coordinates of **1b**-TCO-VHF.

Atom	x	y	z	Continued			
N	-7.26355	1.52637	-0.31158	C	-3.13089	-1.09417	0.00115
C	-6.47449	0.68704	-0.26930	C	-3.19799	-2.04697	1.01803
C	-5.47513	-0.33272	-0.21758	C	-2.18118	-2.98253	1.16422
C	-5.94701	-1.67701	-0.31673	C	-1.10069	-2.98326	0.28966
N	-6.35496	-2.75189	-0.39656	C	-1.04767	-2.05787	-0.74780
C	-4.14607	-0.01695	-0.10294	C	-2.05464	-1.11653	-0.88964
C	-3.72353	1.36590	-0.15144	H	-4.43036	2.06227	-0.59510
C	-2.53623	1.88099	0.27520	H	-2.01221	0.41145	1.77412
C	-1.57938	1.14317	1.10102	H	0.28977	0.53263	1.75037
C	-0.23826	1.22813	1.10498	H	5.56114	2.23556	0.26236
C	0.61604	2.08685	0.30508	H	5.27633	1.40039	-2.08568
C	1.96121	1.62999	0.15531	H	5.44700	-1.28914	-2.40313
C	3.06209	1.15641	0.02529	H	5.91563	-2.60502	-0.32803
C	4.32031	0.52163	-0.14331	H	7.83586	-1.25855	0.53320
C	5.66205	1.16057	0.14308	H	6.64307	-1.51134	1.78859
C	5.36126	0.71512	-1.25333	H	7.66309	1.01884	0.83568
C	5.46868	-0.80903	-1.43425	H	6.45258	0.76888	2.07483
C	5.86191	-1.52910	-0.18623	H	1.00647	3.85915	-0.73226
C	6.82310	-0.98917	0.84552	H	-1.09225	4.93294	-0.44224
C	6.70458	0.53275	1.03774	H	-3.14576	3.92772	-0.05089
C	4.43923	-1.02380	-0.31910	H	-4.03087	-2.03834	1.71341
C	3.30681	-1.88458	-0.34427	H	-2.23293	-3.70863	1.96850
N	2.39080	-2.58422	-0.36982	H	-0.29108	-3.69418	0.41081
C	0.23603	3.27555	-0.23724	H	-0.20179	-2.06206	-1.42547
C	-1.06725	3.87627	-0.18905	H	-1.99954	-0.37470	-1.67961
C	-2.26624	3.29338	0.03197				

Table S9: Cartesian coordinates of **2a**-BOD-DHA.

Atom	x	y	z
N	4.10012	-1.74172	2.61708
C	4.35642	-1.45645	1.53401
C	4.68453	-1.05904	0.15676
C	6.05825	-0.29122	0.03334
C	5.71246	0.90915	-0.81463
C	6.64505	1.72399	-1.34415
C	8.05461	1.65395	-1.04196
C	8.59522	1.24496	0.13244
C	7.85776	0.82929	1.30848
C	6.67314	0.20049	1.31522
C	3.64151	-0.06969	-0.41094
C	2.19550	-0.29305	-0.32000
C	1.64606	-1.57212	-0.17817
C	0.27518	-1.75519	-0.11205
C	-0.59396	-0.66180	-0.17855
C	-2.00561	-0.82782	-0.10093
C	-3.20845	-0.88926	-0.01877
C	-4.61783	-0.96744	0.06586
C	-5.45868	0.08271	0.15945
C	-5.07360	1.50053	0.24458
C	-4.00597	1.91651	1.04759
C	-3.64615	3.25606	1.11104
C	-4.34291	4.20635	0.37270
C	-5.41098	3.80730	-0.42310
C	-5.77714	2.46928	-0.47967
C	-6.91829	-0.33548	0.08547
C	-7.17173	-1.40963	1.12179
C	-6.34046	-2.44253	1.03746
C	-5.32267	-2.31147	-0.07226
C	-6.13360	-2.21743	-1.40619
C	-7.10319	-1.02170	-1.30945
C	-0.04885	0.62357	-0.30784
C	1.31992	0.80045	-0.37080
C	4.27606	0.97318	-0.96890
C	4.74461	-2.27276	-0.67852
N	4.81464	-3.19816	-1.35645
H	6.78300	-0.92627	-0.48637
H	6.32461	2.49927	-2.03586
H	8.72931	2.07375	-1.78356
H	9.66943	1.35841	0.25301
H	8.30833	1.07218	2.26755
H	6.16359	0.02103	2.25658
H	2.28230	-2.44855	-0.13359
H	-0.13152	-2.75436	-0.00629
H	-3.46690	1.18485	1.63831
H	-2.82244	3.55981	1.74936
H	-4.06079	5.25292	0.42324
H	-5.96220	4.54094	-1.00249
H	-6.60842	2.17215	-1.11184
H	-7.59151	0.51384	0.19909
H	-7.98607	-1.32655	1.83248
H	-6.38234	-3.32293	1.66851
H	-4.61144	-3.13609	-0.10200
H	-5.43633	-2.09612	-2.23850
H	-6.67385	-3.15372	-1.56344
H	-6.90656	-0.29156	-2.09878
H	-8.14196	-1.34396	-1.41227
H	-0.71413	1.47927	-0.34631
H	1.71756	1.80763	-0.43567
H	3.77771	1.78110	-1.49157

Table S10: Cartesian coordinates of **2a**-TCO-VHF.

Atom	x	y	z
N	-4.09678	-4.59835	0.63829
C	-4.43721	-3.50716	0.48931
C	-4.89244	-2.16666	0.30677
C	-6.30626	-1.97580	0.36910
N	-7.44449	-1.79887	0.41869
C	-4.04252	-1.10353	0.11843
C	-4.56855	0.24076	0.11735
C	-4.00009	1.37890	-0.38812
C	-4.70965	2.62940	-0.14904
C	-4.24576	3.89830	-0.15615
C	-2.92361	4.38754	-0.43890
C	-1.91302	3.71192	-1.02914
C	-1.94469	2.35950	-1.51495
C	-2.82897	1.37181	-1.25943
C	-2.58284	-1.33485	0.01009
C	-1.70904	-0.59130	0.80910
C	-0.34254	-0.74916	0.69185
C	0.18933	-1.65429	-0.23915
C	1.60794	-1.73514	-0.35275
C	2.81073	-1.65084	-0.33411
C	4.17382	-1.27804	-0.20767
C	5.37977	-1.97008	-0.79027
C	5.25945	-1.86990	0.70093
C	5.57140	-0.46743	1.25700
C	5.95523	0.50599	0.17531
C	6.78227	0.13659	-1.03428
C	6.40894	-1.23752	-1.61934
C	4.50533	0.14283	0.37012
C	3.40583	1.09066	0.66401
C	3.04455	1.42802	1.96574
C	1.95778	2.26494	2.20758
C	1.21003	2.76272	1.14752
C	1.56499	2.42971	-0.15649
C	2.65282	1.60386	-0.39551
C	-0.68304	-2.40658	-1.03007
C	-2.05481	-2.25137	-0.90053
H	-5.54063	0.35597	0.58866
H	-5.75292	2.50496	0.13185
H	-4.96514	4.66214	0.12749
H	-2.74781	5.43120	-0.19357
H	-0.99584	4.26202	-1.22255
H	-1.12364	2.08873	-2.17378
H	-2.63706	0.43080	-1.76176
H	-2.10925	0.12384	1.51963
H	0.33303	-0.16254	1.30482
H	5.13345	-2.96259	-1.15814
H	5.13523	-2.74121	1.33037
H	5.75763	-0.27681	2.30675
H	6.17086	1.49381	0.57592
H	7.83641	0.15110	-0.74092
H	6.66558	0.91728	-1.79147
H	6.01091	-1.12761	-2.63242
H	7.29790	-1.86888	-1.70633
H	3.60754	1.01742	2.79828
H	1.68796	2.51526	3.22859
H	0.35127	3.40023	1.33330
H	0.98833	2.81163	-0.99229
H	2.91496	1.33168	-1.41344
H	-0.28215	-3.10950	-1.75136
H	-2.71875	-2.83115	-1.53227

Table S11: Cartesian coordinates of **2b**-BOD-DHA.

Atom	x	y	z	Continued			
N	-3.39689	-2.24862	2.15004	C	7.78002	0.09922	-1.17346
C	-3.66570	-1.70920	1.17186	C	0.54576	1.18048	0.07928
C	-4.00975	-0.99164	-0.06480	C	-0.83294	1.24281	0.01843
C	-5.45073	-0.34752	-0.03905	C	-3.78658	1.29592	-0.59623
C	-5.21166	1.06238	-0.52315	C	-3.93452	-1.94003	-1.19153
C	-6.21040	1.90251	-0.85553	N	-3.89767	-2.65421	-2.09122
C	-7.61113	1.62738	-0.64293	H	-6.09962	-0.88384	-0.73903
C	-8.12770	0.87121	0.35702	H	-5.95588	2.86085	-1.30161
C	-7.37259	0.22313	1.41042	H	-8.31129	2.16870	-1.27379
C	-6.13263	-0.27570	1.30001	H	-9.20964	0.85108	0.45845
C	-3.06121	0.20380	-0.30904	H	-7.86074	0.15817	2.37954
C	-1.60074	0.09626	-0.22889	H	-5.62426	-0.65536	2.18058
C	-0.93505	-1.12431	-0.38722	H	-1.48533	-2.03794	-0.57939
C	0.44618	-1.19445	-0.32262	H	0.94497	-2.14806	-0.45199
C	1.20553	-0.04362	-0.09312	H	8.08318	1.62665	0.39306
C	2.62672	-0.10193	-0.02420	H	8.57662	-0.24774	1.98755
C	3.83144	-0.10635	0.03945	H	7.13116	-2.34761	1.70686
C	5.23989	-0.10138	0.11199	H	5.42143	-2.25125	-0.12521
C	6.00581	0.99855	0.25973	H	7.51605	-2.04791	-1.51156
C	5.49067	2.31658	0.36366	H	6.22923	-1.05978	-2.19732
N	5.09535	3.39720	0.44722	H	7.56101	0.84208	-1.94356
C	7.49843	0.72174	0.23517	H	8.84209	-0.14424	-1.24382
C	7.79545	-0.36588	1.24586	H	1.12651	2.07497	0.27431
C	7.04688	-1.45364	1.10029	H	-1.32283	2.19484	0.19075
C	6.05874	-1.37225	-0.04360	H	-3.36366	2.25630	-0.86652
C	6.90439	-1.15915	-1.34441				

Table S12: Cartesian coordinates of **2b**-TCO-VHF.

Atom	x	y	z	Continued			
N	-3.22960	-4.58324	0.42218	C	6.55756	-0.66894	-1.75723
C	-3.75885	-3.56437	0.31817	C	5.17566	0.66941	0.63110
C	-4.44032	-2.31732	0.18607	C	4.40533	1.68686	1.26009
C	-5.86645	-2.38252	0.17460	N	3.77706	2.50887	1.76872
N	-7.01902	-2.41190	0.16534	C	-0.21985	-0.26341	0.97640
C	-3.78423	-1.11185	0.10595	C	-1.60079	-0.32521	1.00977
C	-4.53270	0.11782	0.13696	H	-5.54429	0.02992	0.52327
C	-4.13832	1.37373	-0.24735	H	-2.51432	0.78375	-1.53437
C	-2.91985	1.63702	-1.00383	H	-1.30333	2.70952	-1.71235
C	-2.21475	2.78331	-1.12466	H	-1.65912	4.79868	-0.65300
C	-2.47392	4.08468	-0.57488	H	-3.67999	5.56656	0.26251
C	-3.63806	4.52662	-0.04866	H	-5.73024	4.38652	0.35461
C	-4.86165	3.78750	0.09352	H	-6.09958	2.12814	0.18668
C	-5.08015	2.45690	-0.00154	H	-2.11954	-2.40703	-1.61889
C	-2.30082	-1.09390	0.07687	H	0.33961	-2.28245	-1.69646
C	-1.58876	-1.80816	-0.88690	H	5.04883	-2.20716	-1.34960
C	-0.20596	-1.73633	-0.93542	H	5.42680	-2.39358	1.12154
C	0.49482	-0.96107	-0.00608	H	6.53035	-0.21495	2.30821
C	1.91820	-0.86763	-0.05084	H	7.07241	1.69624	0.78710
C	3.11840	-0.76386	-0.06575	H	8.27906	0.42369	-0.99179
C	4.52579	-0.57832	-0.04149	H	7.04874	1.45255	-1.69245
C	5.51640	-1.33961	-0.89252	H	6.08719	-0.38398	-2.70200
C	5.60460	-1.46499	0.59657	H	7.32208	-1.41047	-2.00545
C	6.23717	-0.23308	1.26734	H	0.31957	0.33329	1.70321
C	6.64477	0.82642	0.29595	H	-2.14788	0.23281	1.76195
C	7.19750	0.55726	-1.08326				

Table S13: Cartesian coordinates of **3a**-BOD-DHA.

Atom	x	y	z	Continued			
N	1.80075	-1.33370	-2.08734	C	-6.19380	1.19308	-1.24653
C	2.30759	-0.89046	-1.15614	C	-6.44291	-0.32817	-1.29290
C	3.02044	-0.30814	-0.00432	C	0.59857	1.58596	-0.00985
C	4.53231	-0.75752	-0.07437	C	4.31739	1.60125	-0.48183
C	5.24615	0.49350	-0.52448	C	2.34834	-0.72687	1.23419
C	6.53223	0.49834	-0.92410	N	1.85243	-1.04380	2.22086
C	7.42108	-0.63392	-0.81912	H	4.64210	-1.54813	-0.82369
C	7.36850	-1.59750	0.13362	H	6.94377	1.41468	-1.34025
C	6.42887	-1.65299	1.23541	H	8.27131	-0.64593	-1.49615
C	5.16072	-1.21694	1.21287	H	8.17779	-2.32277	0.15410
C	3.07147	1.23003	-0.14908	H	6.80498	-2.07122	2.16570
C	1.89750	2.09259	0.03656	H	4.57288	-1.21837	2.12517
C	2.07361	3.46345	0.27074	H	3.07279	3.87579	0.35718
C	0.98007	4.29989	0.42516	H	1.13437	5.35778	0.60861
C	-0.30991	3.79108	0.36530	H	-1.16698	4.44212	0.49514
C	-0.51031	2.42437	0.15333	H	-4.29851	-2.92818	1.40326
C	-1.82143	1.86740	0.10910	H	-2.57996	-4.69002	1.30169
C	-2.90044	1.32825	0.07631	H	-0.65424	-4.46434	-0.24614
C	-4.16849	0.70195	0.05434	H	-0.47246	-2.46096	-1.69735
C	-4.38566	-0.62686	0.00775	H	-2.18675	-0.69528	-1.58870
C	-3.35983	-1.67946	-0.07866	H	-6.03017	-2.05153	0.00711
C	-3.46340	-2.82522	0.71663	H	-7.17676	-0.81620	1.86540
C	-2.49292	-3.81643	0.66364	H	-6.75027	1.71171	1.93868
C	-1.41121	-3.68819	-0.20074	H	-5.22793	2.59956	0.15153
C	-1.30580	-2.56332	-1.01113	H	-5.58574	1.52106	-2.09302
C	-2.27031	-1.56602	-0.94770	H	-7.13348	1.74922	-1.28151
C	-5.86561	-0.97432	0.01187	H	-7.50990	-0.55381	-1.35704
C	-6.54609	-0.27549	1.16847	H	-5.95838	-0.78433	-2.15953
C	-6.32542	1.03437	1.20652	H	0.40724	0.53221	-0.17766
C	-5.44487	1.53408	0.08241	H	4.61329	2.61893	-0.70678

Table S14: Cartesian coordinates of **3a**-TCO-VHF.

Atom	x	y	z	Continued			
N	0.27558	3.70555	2.06520	C	-2.02008	1.81177	-1.18614
C	1.08550	3.22557	1.40013	C	-0.75292	2.18512	-1.62699
C	2.08656	2.66760	0.54982	C	0.13464	1.22392	-2.09481
C	2.63999	3.54961	-0.42629	C	-0.25220	-0.11374	-2.12006
N	3.08729	4.23769	-1.23651	C	-1.51920	-0.48188	-1.68606
C	2.48190	1.35574	0.61585	C	0.42131	0.24988	1.42834
C	3.57457	0.88899	-0.19952	H	4.26112	1.65980	-0.53885
C	3.83781	-0.39000	-0.61548	H	5.50600	0.32795	-1.75709
C	5.06316	-0.58994	-1.37732	H	6.68503	-1.59280	-2.17383
C	5.75549	-1.72364	-1.62578	H	6.27176	-3.79122	-1.40419
C	5.47075	-3.07708	-1.23505	H	4.25362	-4.62466	-0.54645
C	4.30888	-3.55687	-0.73894	H	2.21714	-3.43333	-0.32768
C	3.09666	-2.82029	-0.50809	H	1.86192	-1.18354	-0.29093
C	2.88716	-1.48643	-0.46507	H	3.58026	-0.17708	2.58048
C	1.79157	0.43152	1.54822	H	2.39622	-1.78693	4.03949
C	2.50762	-0.31111	2.48957	H	-0.03452	-2.16958	3.76467
C	1.84181	-1.22158	3.29810	H	-5.33022	-1.86704	1.76957
C	0.47498	-1.43390	3.15219	H	-5.36920	0.63011	1.86372
C	-0.24570	-0.70353	2.20580	H	-5.15597	1.91622	-0.52492
C	-1.62945	-0.88928	1.91244	H	-4.87331	0.42749	-2.52735
C	-2.73896	-0.87478	1.44069	H	-5.45292	-1.98580	-2.45478
C	-3.90033	-0.70484	0.64429	H	-6.84579	-1.03707	-1.98372
C	-5.24160	-1.37396	0.80505	H	-6.95816	-2.29399	-0.05641
C	-5.16195	0.11792	0.93342	H	-5.44286	-3.08781	-0.42821
C	-5.00180	0.85028	-0.41228	H	-2.69862	2.56387	-0.79655
C	-4.98705	-0.09667	-1.58136	H	-0.45468	3.22797	-1.59081
C	-5.84358	-1.33889	-1.66396	H	1.12531	1.51497	-2.42967
C	-5.91628	-2.10607	-0.33164	H	0.43630	-0.87067	-2.48352
C	-3.75418	0.04984	-0.72562	H	-1.81592	-1.52664	-1.69960
C	-2.42200	0.47781	-1.21949	H	-0.14119	0.81045	0.69185

Table S15: Cartesian coordinates of **3b**-BOD-DHA.

Atom	x	y	z
N	-5.02380	2.48827	-1.70288
C	-4.54849	1.80140	-0.91345
C	-3.94382	0.88222	0.06856
C	-4.72827	-0.48767	0.03444
C	-3.75762	-1.42951	-0.63691
C	-4.10101	-2.66227	-1.05555
C	-5.37086	-3.29150	-0.78182
C	-6.13711	-3.08598	0.31759
C	-5.81010	-2.21935	1.43207
C	-5.11280	-1.07588	1.36466
C	-2.50727	0.50997	-0.36010
C	-1.38335	1.45436	-0.30060
C	-1.57053	2.84092	-0.30196
C	-0.48182	3.70249	-0.25934
C	0.81022	3.20509	-0.21251
C	1.01772	1.82121	-0.20047
C	2.32961	1.26513	-0.14396
C	3.40630	0.72299	-0.10733
C	4.64240	0.04497	-0.06608
C	4.78446	-1.29319	-0.15580
C	3.69608	-2.19054	-0.31006
N	2.81955	-2.93036	-0.43519
C	6.21610	-1.77554	-0.00899
C	7.07764	-1.00579	-0.98791
C	6.94481	0.31310	-0.89939
C	5.96136	0.76364	0.15983
Continued			
C	6.49911	0.21349	1.52434
C	6.66207	-1.31702	1.42003
C	-0.07915	0.95915	-0.23593
C	-2.47977	-0.76592	-0.77327
C	-3.95865	1.53543	1.38630
N	-3.95418	2.02969	2.42354
H	-5.62953	-0.37312	-0.57664
H	-3.37574	-3.23672	-1.62644
H	-5.67619	-4.08037	-1.46425
H	-7.01102	-3.72021	0.44164
H	-6.15080	-2.54826	2.41059
H	-4.84305	-0.55523	2.27795
H	-2.56552	3.26771	-0.35112
H	-0.64883	4.77377	-0.26495
H	1.66108	3.87601	-0.17904
H	6.29668	-2.85556	-0.12225
H	7.75514	-1.51467	-1.66343
H	7.49847	1.03092	-1.49305
H	5.82880	1.84383	0.19321
H	5.80080	0.48481	2.31922
H	7.45180	0.69932	1.74410
H	7.70021	-1.61665	1.57706
H	6.05433	-1.83180	2.16734
H	0.10262	-0.10863	-0.19058
H	-1.60369	-1.26071	-1.17596

Table S16: Cartesian coordinates of **3b**-TCO-VHF.

Atom	x	y	z	Continued			
N	-4.69117	4.24306	-1.12131	C	7.23682	0.55125	-0.06403
C	-3.87309	3.62872	-0.58969	C	6.28620	1.72524	-0.35597
C	-2.87608	2.84374	0.06483	C	5.17480	-1.11901	-0.08992
C	-1.77411	3.56510	0.61516	C	4.76374	-2.27211	0.63513
N	-0.89267	4.16986	1.04666	N	4.42711	-3.20591	1.22152
C	-3.00326	1.47956	0.17015	C	-0.61519	0.75998	0.35029
C	-4.20923	0.83159	-0.27430	H	-5.06676	1.48863	-0.38886
C	-4.41685	-0.49192	-0.56999	H	-6.43419	-0.03834	-1.13783
C	-5.78161	-0.87577	-0.90228	H	-7.42940	-2.10211	-1.12941
C	-6.36688	-2.09434	-0.90054	H	-6.52160	-4.19180	-0.49410
C	-5.80567	-3.38120	-0.59644	H	-4.24750	-4.73620	-0.29882
C	-4.49579	-3.69463	-0.48189	H	-2.41398	-3.30739	-0.74692
C	-3.37668	-2.81098	-0.65528	H	-2.35336	-1.03390	-0.86300
C	-3.33629	-1.46112	-0.70588	H	-3.24503	-0.16727	2.28042
C	-1.92158	0.70060	0.82557	H	-1.46636	-1.50940	3.35902
C	-2.22583	-0.12101	1.91230	H	0.85047	-1.43484	2.48332
C	-1.22864	-0.87721	2.51050	H	4.26451	2.09348	-1.11968
C	0.07123	-0.83516	2.02641	H	4.16879	0.17673	-2.73668
C	0.38919	-0.01211	0.94042	H	5.82225	-1.90590	-2.18533
C	1.72580	0.03615	0.44269	H	7.27225	-1.63984	-0.16387
C	2.86054	0.06946	0.04055	H	7.53882	0.55297	0.98641
C	4.20914	0.06367	-0.40261	H	8.15608	0.64722	-0.64873
C	4.95285	1.28018	-0.90822	H	6.73919	2.41421	-1.07434
C	4.76056	0.11917	-1.83322	H	6.10299	2.30473	0.55246
C	5.70512	-1.05666	-1.52585	H	-0.37063	1.39262	-0.49562
C	6.62590	-0.79327	-0.37899				

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