Efficient blue light emitting materials based on *m*-carborane-anthracene dyads. Structure, photophysics and bioimaging studies.

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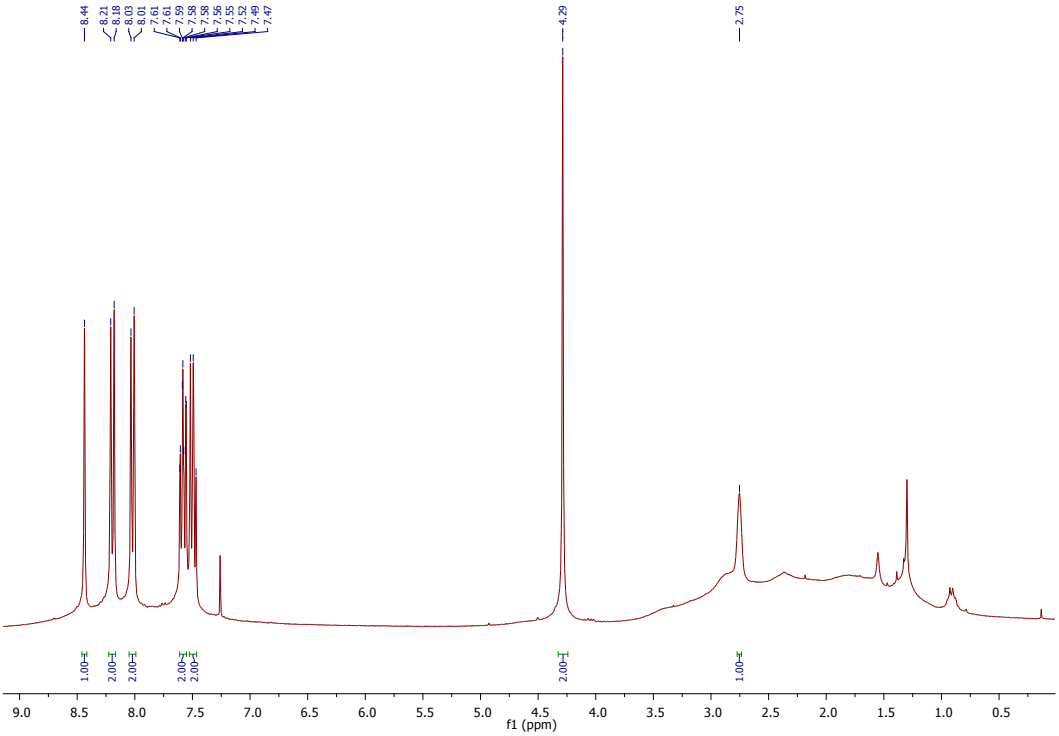
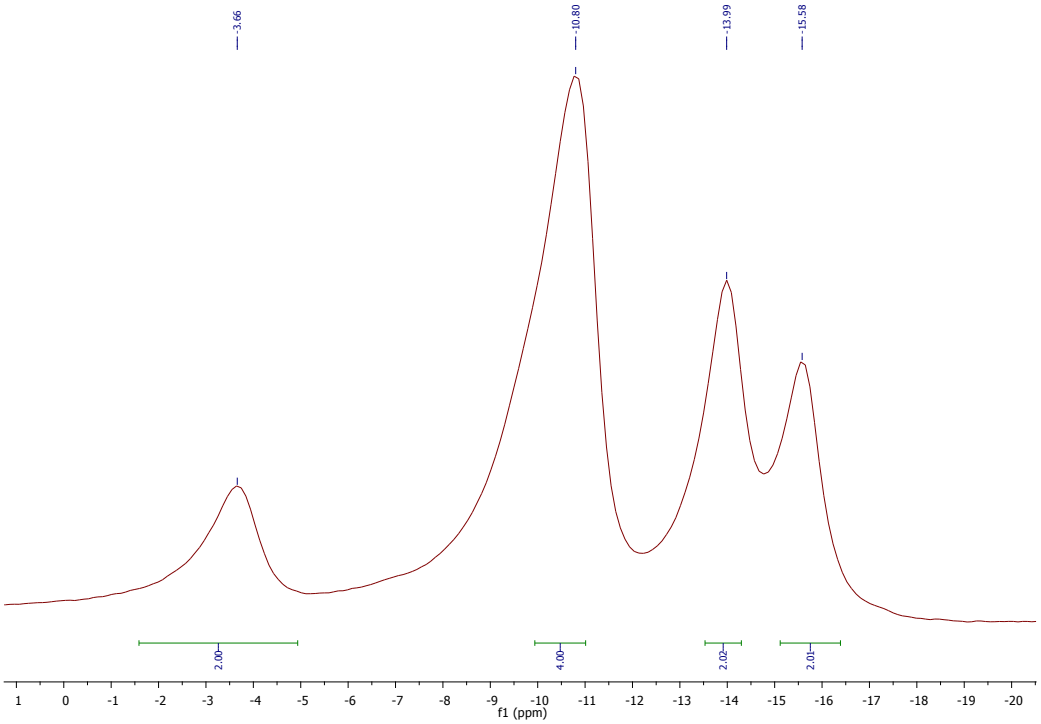
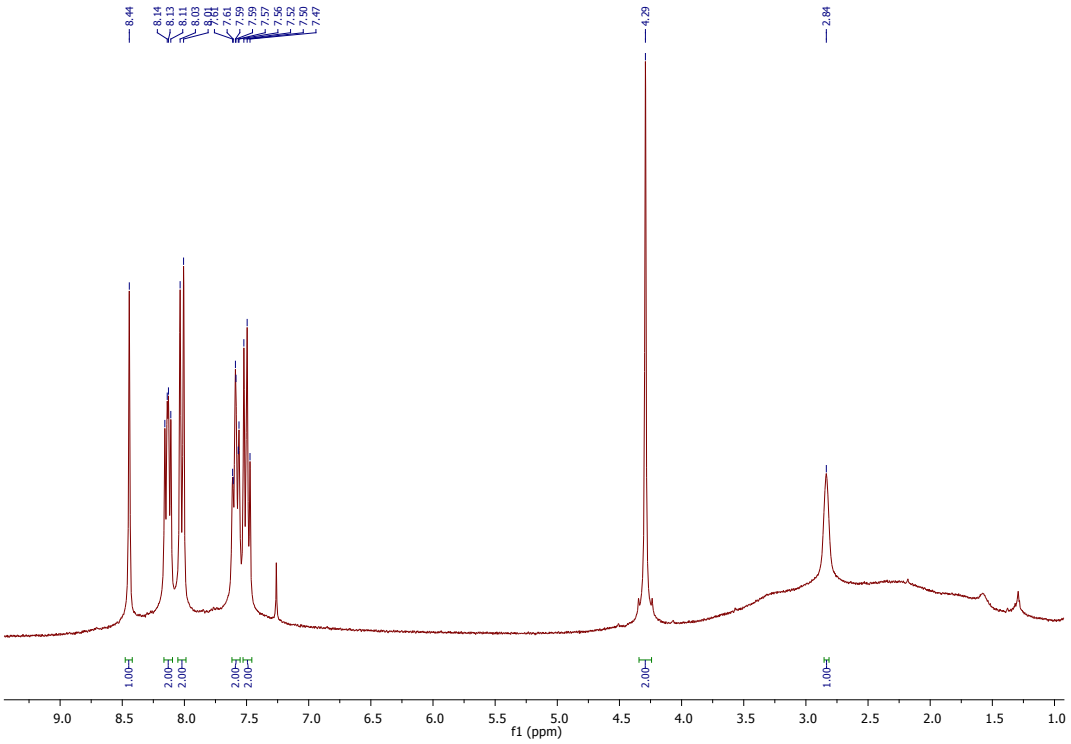
^{1}H and $^{11}B\{^{1}H\}$ NMR spectra for compounds 4-6



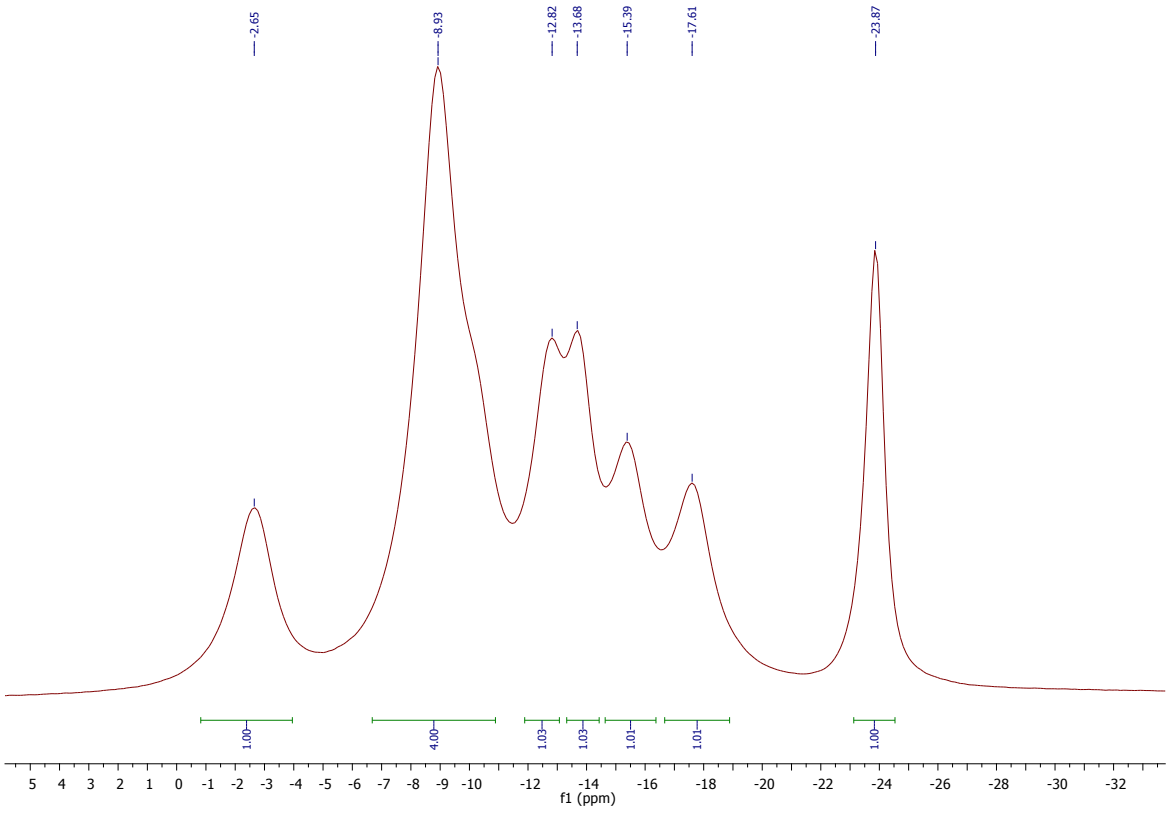
^{1}H NMR spectrum of **4**.



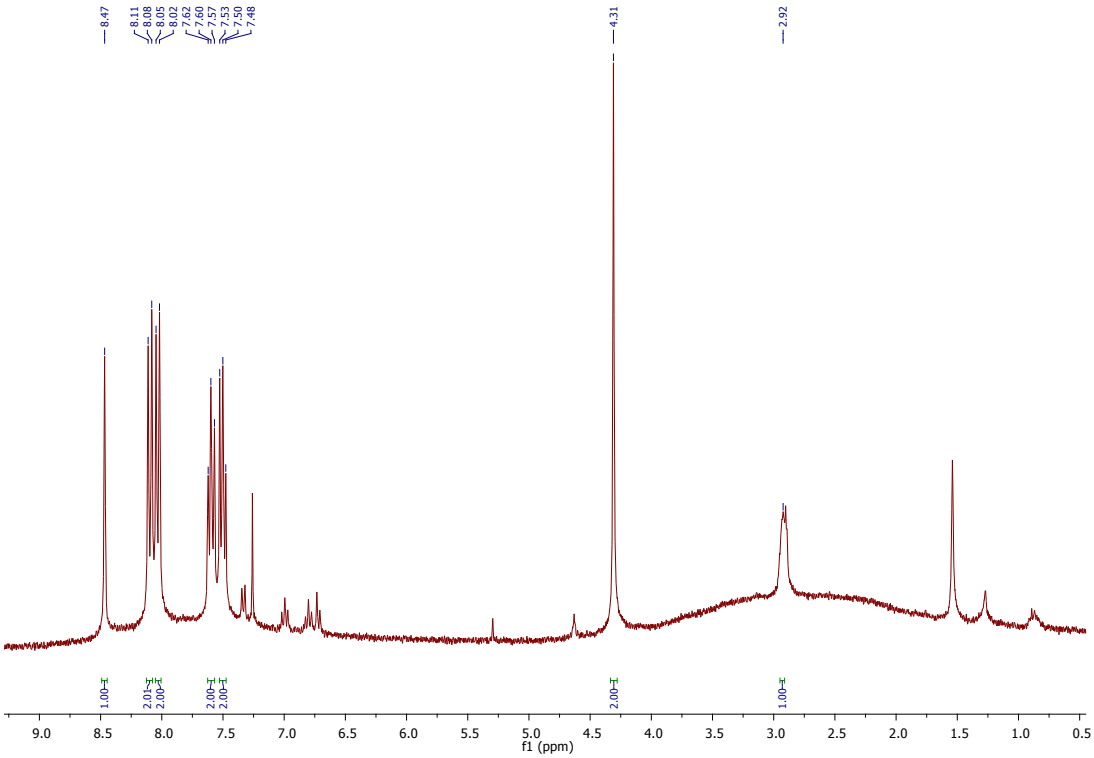
$^{11}B\{^{1}H\}$ NMR spectrum of **4**.



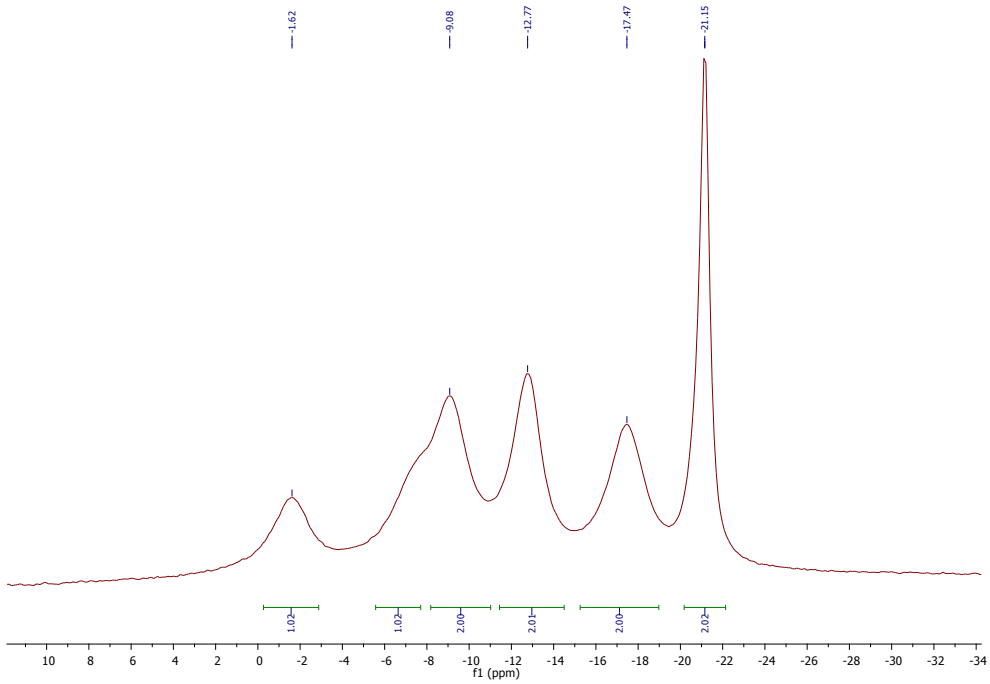
^{1}H NMR spectrum of **5**.



^{11}B{^{1}H} NMR spectrum of **5**.



^{1}H NMR spectrum of **6**.



^{11}B{^{1}H} NMR spectrum of **6**.

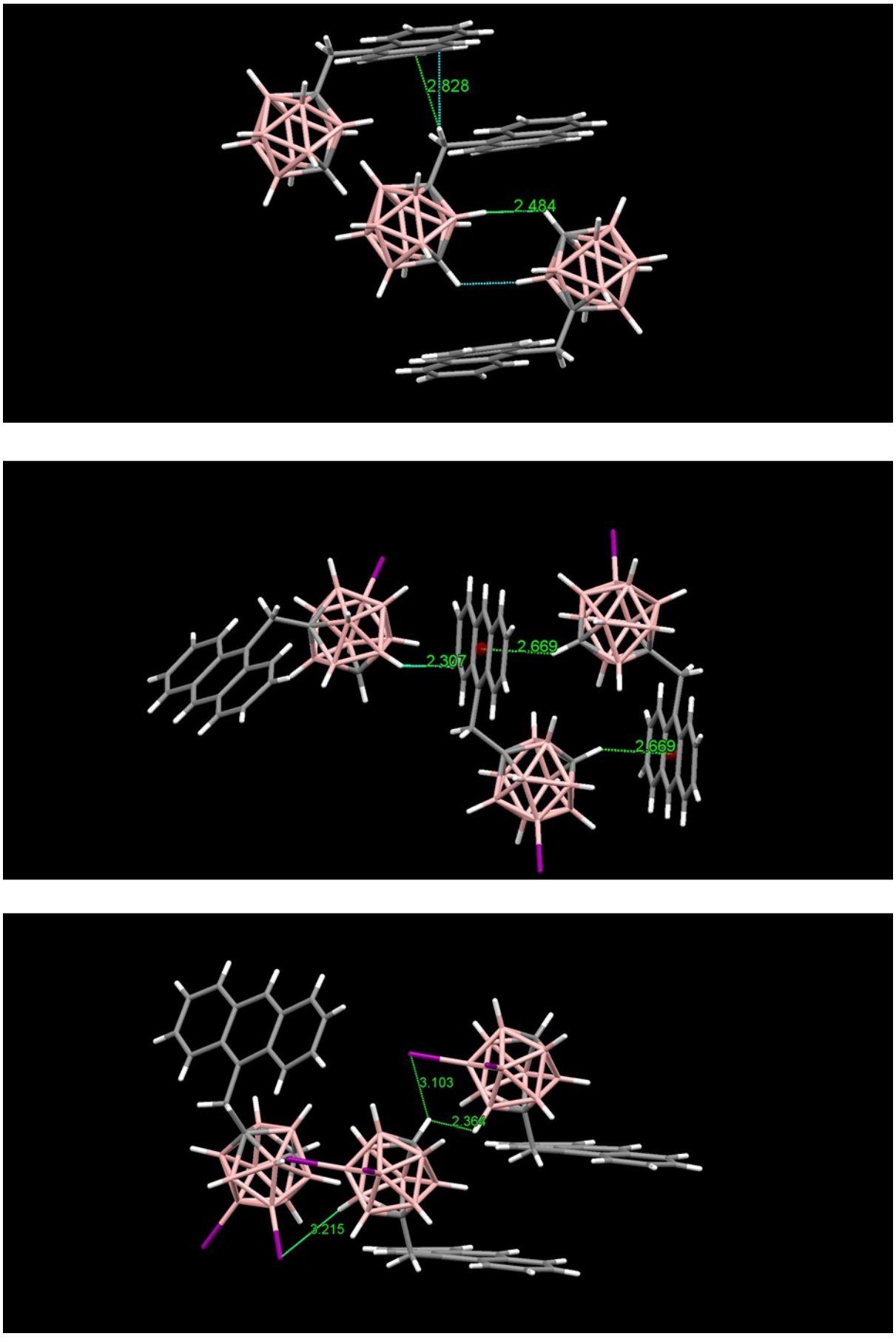


Figure S1. Picture indicating the intermolecular C–H···A interactions

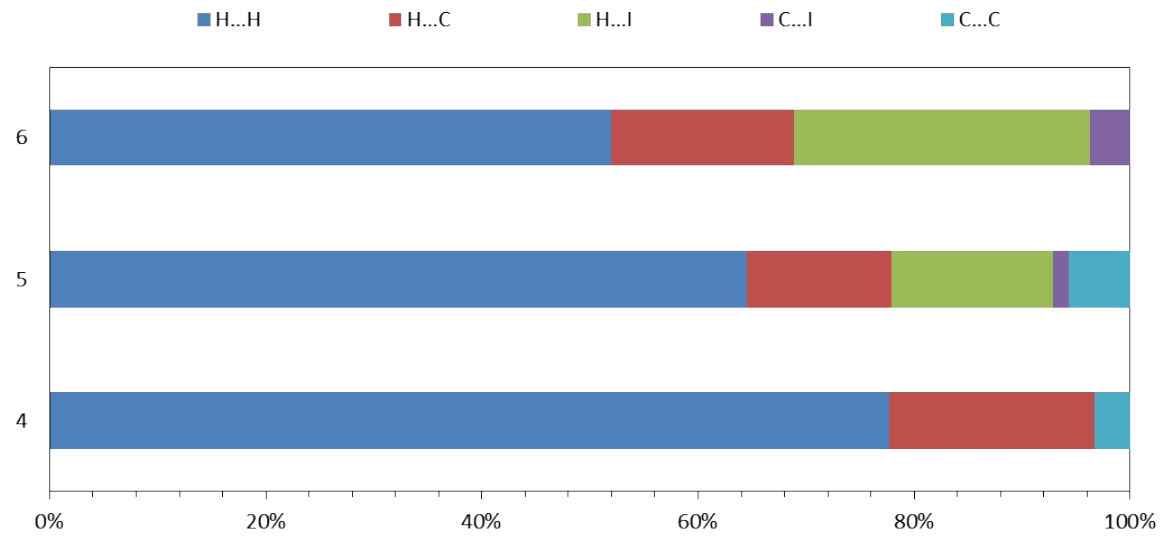
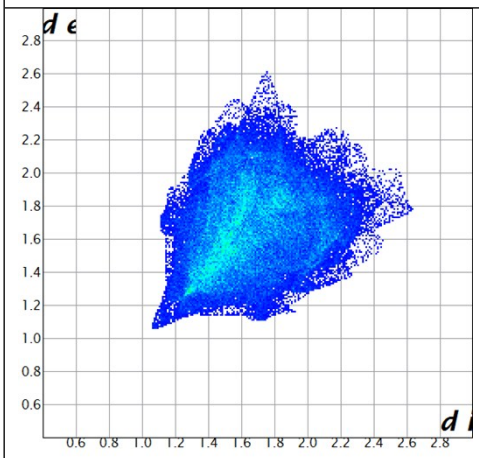
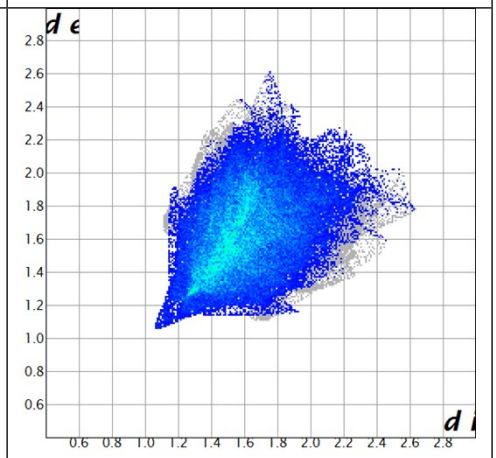
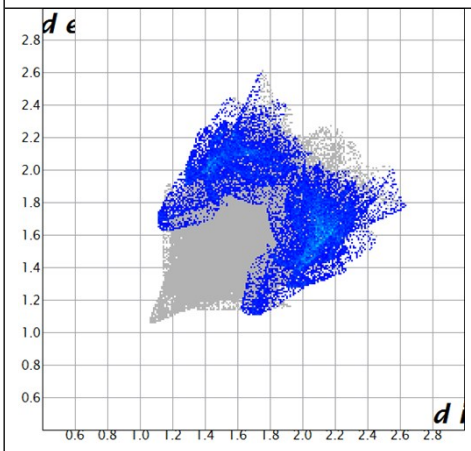
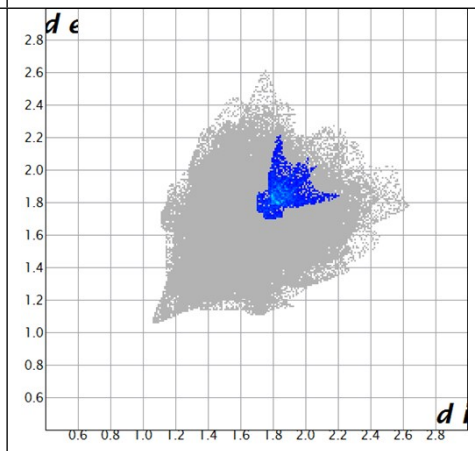


Figure S2. Hirshfeld Surface Analyses: Relative contributions of various intermolecular contacts to the Hirshfeld surface area in all compounds **4–6**.

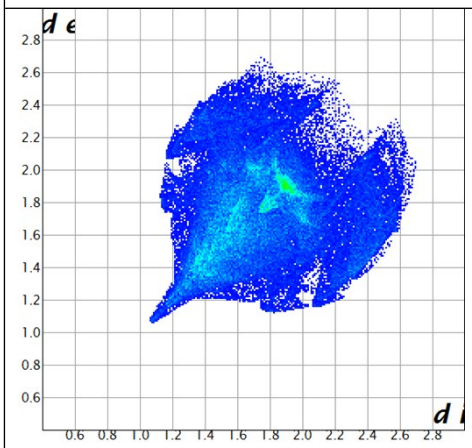
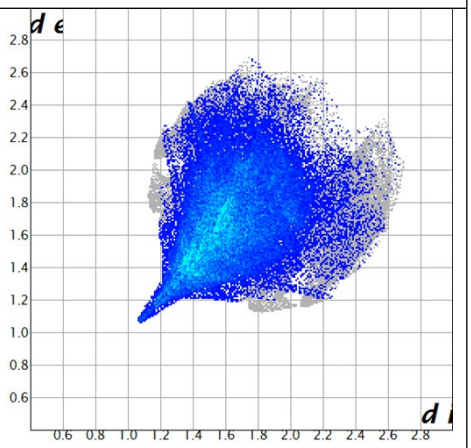
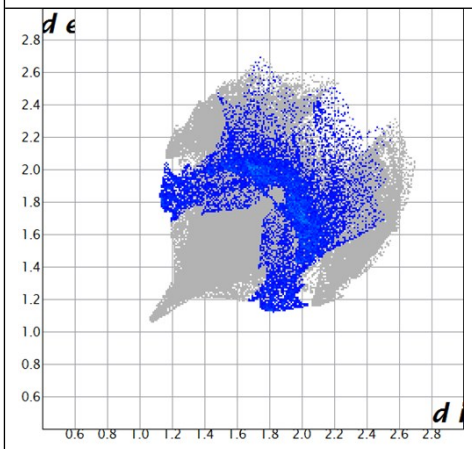
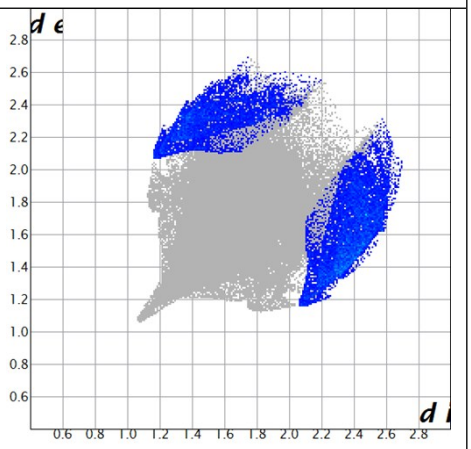
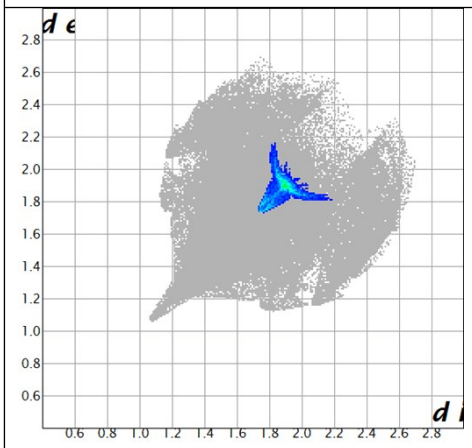
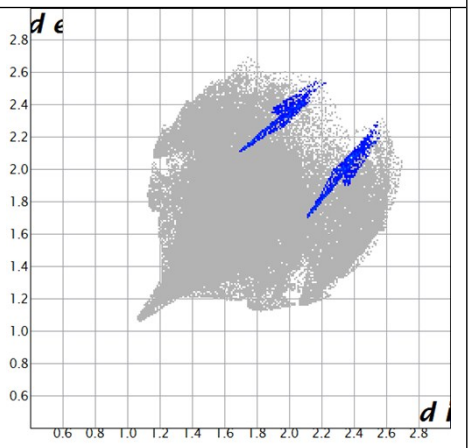
Fingerprints for compounds 4-6

Full and decomposed fingerprints for each compound were done by using CrystalExplorer17 (2017).[1] Legend: Close Contacts X···Y, where: X = atom inside the surface, Y = atom outside the surface.

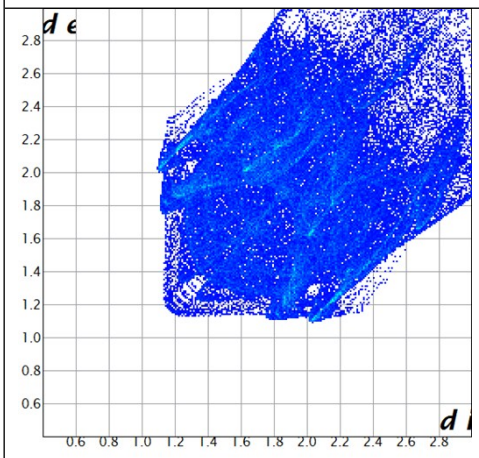
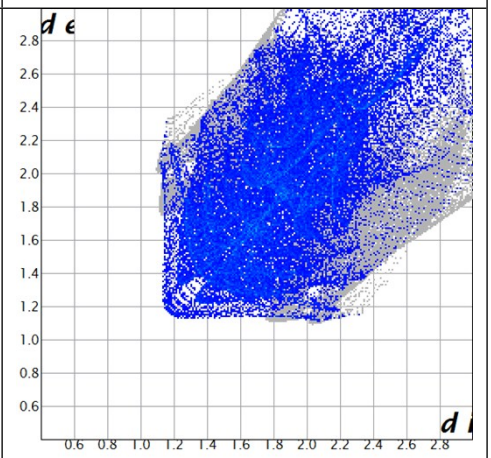
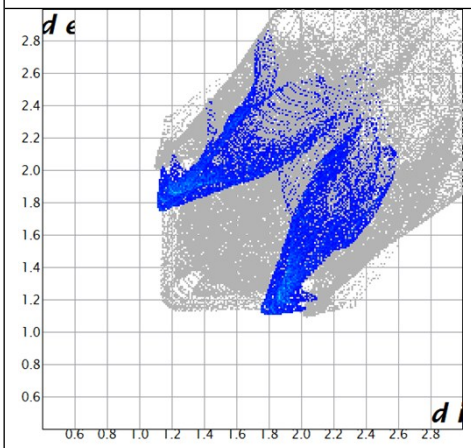
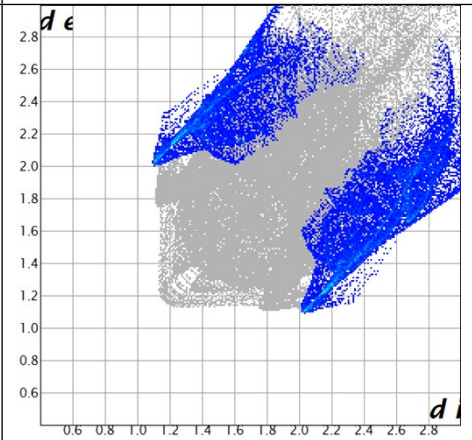
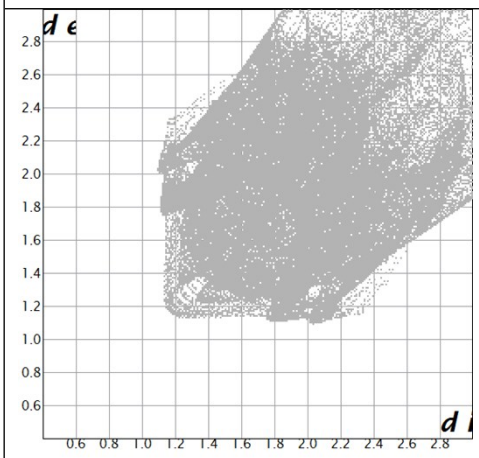
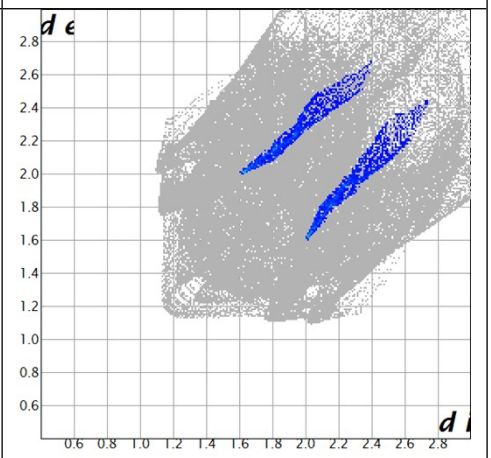
Compound 4

Full Plot	**H…H Contacts (77.7%)**
	
H…C Contacts (19.0%)	**C…C Contacts (3.3%)**
	

Compound 5

Full Plot	H…H Contacts (64.6%)
	
H…C Contacts (13.4%)	**H…I Contacts (14.9%)**
	
C…C Contacts (5.7%)	**C…I Contacts (1.5%)**
	

Compound 6

Full Plot	H…H Contacts (52.0%)
	
H…C Contacts (16.9%)	**H…I Contacts (27.5%)**
	
C…C Contacts (0%)	**C…I Contacts (3.7%)**
	

Computational details

All calculations were carried out with the Gaussian 09 program package[2] at B3LYP/6-31G* level of theory (for the iodine atoms LANL2DZ basis was applied) as it was implemented in G09. Full geometry optimization calculations were carried out and harmonic vibrational frequencies were calculated to establish the nature of the stationary points obtained, as characterized by none negative eigenvalue of the Hessian for minima structures. For the visualization of the molecules and orbitals the MOLDEN[3] program was used.

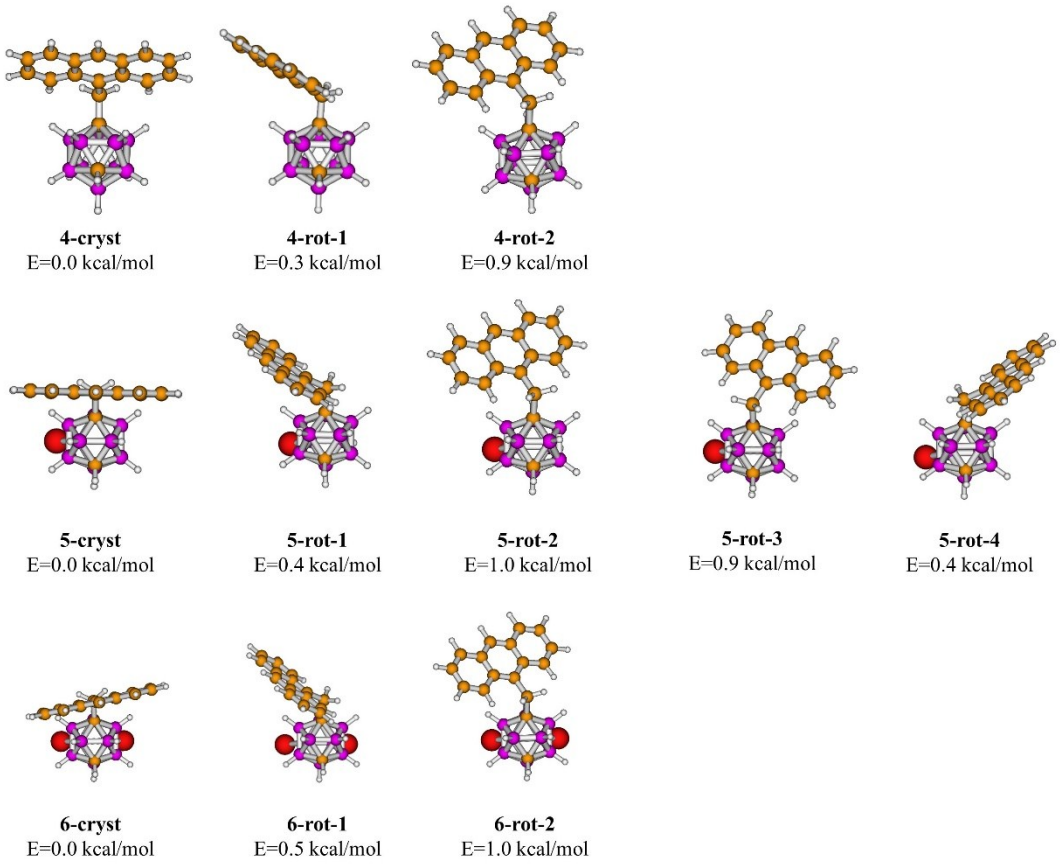


Figure S3. The different rotamers of **4**, **5** and **6** and their relative energies in kcal/mol and at B3LYP/6-31G* level of theory (Note that the number of the rotamers depend on the symmetry of the system.)

Table S1. TD-DFT results of the investigated isomers

Isomer	Excitation	λ_{abs} (nm) Calculated	Intensity (*f*)	Transition	%
4-cryst	S0→S1	389	0.1030	HOMO→ LUMO	98
4-rot-1	S0→S1	389	0.1019	HOMO→ LUMO	98
4-rot-2	S0→S1	389	0.1028	HOMO→ LUMO	98
5-cryst	S0→S1	390	0.1115	HOMO → LUMO	98
	S0→S3	293	0.0008	HOMO-1→ LUMO	100
	S0→S4	291	0.0010	HOMO-2→ LUMO	99
5-rot-1	S0→S1	390	0.1007	HOMO → LUMO	98
	S0→S3	296	0.0001	HOMO-1→ LUMO	99
	S0→S4	293	0.0004	HOMO-2→ LUMO	99
5-rot-2	S0→S1	390	0.1115	HOMO → LUMO	98
	S0→S3	291	0.0000	HOMO-1→ LUMO	100
	S0→S4	288	0.0012	HOMO-2→ LUMO	99
5-rot-3	S0→S1	390	0.1045	HOMO → LUMO	98
	S0→S3	294	0.0004	HOMO-1→ LUMO	100
	S0→S4	292	0.0000	HOMO-2→ LUMO	98
5-rot-4	S0→S1	390	0.1051	HOMO → LUMO	98
	S0→S3	295	0.0006	HOMO-1→ LUMO	99
	S0→S4	292	0.0000	HOMO-2→ LUMO	99
6-cryst	S0→S1	391	0.1196	HOMO → LUMO	98
	S0→S3	299	0.0001	HOMO-1→ LUMO	100
	S0→S4	291	0.0004	HOMO-1→ LUMO	99
6-rot-1	S0→S1	390	0.1028	HOMO → LUMO	98
	S0→S3	296	0.0000	HOMO-1→ LUMO	99
	S0→S4	291	0.0005	HOMO-1→ LUMO	97
6-rot-2	S0→S1	390	0.1128	HOMO → LUMO	98
	S0→S3	297	0.0005	HOMO-2→ LUMO	98
	S0→S4	291	0.0001	HOMO-2→ LUMO	94

In order to get some information about the possible formation of excimers, calculations at M06-2X/6-31G* level of theory were carried out. Previously it was demonstrated that this method with similar basis set properly describes the properties of anthracene containing dimers and excimers. Since **4**, **5** and **6** exhibit similar properties only **4** was investigated to save computational time. The geometry optimizations of the dimer in the ground state and the first singlet excited state (S_1) were started from a dimeric structure, which was taken from the crystal structure of **4**. The ground state geometry is similar to the crystal structure, the two aromatic moieties do not exhibit perfect face to face π-π stacking, they were shifted along both the short and long axis of the anthracenes (Figure S4, A). During the geometry optimization the distance of the two anthracene units decreased by ~0.15 Å (the distance is around ~3.30 Å, in the crystal structure it is 3.461 Å). The perfect cofacial π-π stacked structure was attempted to optimized, but during the optimization the same structure was obtained as starting from the crystal structure, which indicates that it is a less stable geometry. TD-M06-2X/6-31G* calculation suggest absorption at 356 nm for the dimeric structure. Investigation of the energy minimum of the first excited state it can be established that it exhibits similar geometry to the ground state, but the distance between the two anthracene unit decreased to ~3.11 Å, similar shortening (0.17 Å) was published for thiantrene functionalized anthracene. Based on the optimized S_1 geometry the vertical emission was calculated to be 501 nm. In contrast to the ground state, the perfect face to face π-π stacked geometry is a minimum as well (Figure S4, B), but it is less stable by 2.2 kcal/mol. This can be considered as a metastable excited state, similar behaviour was observed for other anthracene and naphthalene containing systems.[4] DFT calculations do not rule out the possible formation of excimers, thus it is difficult to establish a relationship between the emission spectra and the structure of our compounds, since the crystal packing and the possibility of the excimer (or dimer) formation from a diluted solution are slightly different.

During the formation of the crystal lattice, the first dimers can change the geometry when they start connecting with other molecules.

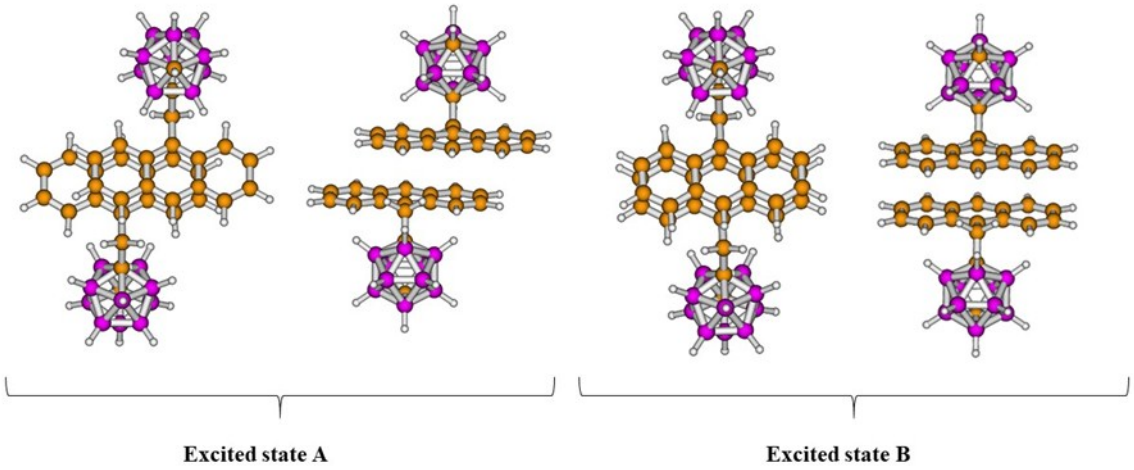


Figure S4. The optimized S1 excited state of **4**.

XYZ coordinates and total energies (in a.u.) of the investigated systems

4-cryst

E(B3LYP/6-31G*) = -909.764000

C	0.063890	-0.138012	0.037683
C	0.028864	-0.062069	1.469408
C	1.303581	-0.046662	2.153907
C	2.514916	-0.109993	1.396530
C	2.494052	-0.181991	0.030715
C	1.246581	-0.194737	-0.653325
C	-1.173489	0.003455	2.219483
C	-1.118903	0.097203	3.633988
C	0.163832	0.111471	4.303372
C	1.334962	0.035889	3.547193
C	0.217613	0.208715	5.729063
C	-0.924295	0.292275	6.477481
C	-2.191154	0.282270	5.830008
C	-2.283922	0.187785	4.465481
C	-2.516356	0.041228	1.504635
C	-3.237900	-1.305536	1.221321
B	-3.330475	-1.846667	-0.422843
B	-4.759166	-1.197086	0.406395
B	-4.896349	-2.673367	-0.573281
B	-5.733620	-2.557023	1.005319
B	-4.678452	-1.659444	2.118304
B	-3.196835	-2.584470	2.350345
B	-4.752053	-3.420122	2.211720
B	-4.883766	-4.047920	0.550358
B	-3.401809	-3.607678	-0.333876
C	-3.370886	-3.934725	1.344370
B	-2.361487	-2.700481	0.775671
H	-6.915615	-2.495297	1.097885
H	-2.889091	-4.850407	1.667455
H	-5.481290	-2.694782	-1.606168
H	-2.521660	-2.584110	3.317231
H	-1.184430	-2.770006	0.796444
H	-2.894371	-4.367491	-1.088054
H	-5.363182	-5.117278	0.374754
H	-5.023849	-0.900835	2.960725
H	-2.404449	0.548889	0.544912
H	-2.784524	-1.212052	-1.261693
H	-5.155543	-0.117115	0.116440
H	-3.268790	0.170164	4.015209
H	-3.097295	0.348203	6.426024
H	-0.870943	0.366570	7.559980
H	-5.133976	-4.056229	3.135358
H	1.195323	0.216187	6.204999
H	2.296578	0.047140	4.056262
H	3.458046	-0.097685	1.937678

H	3.420851	-0.228823	-0.534100
H	1.231737	-0.252537	-1.738276
H	-0.862757	-0.163743	-0.522388
H	-3.213586	0.661377	2.070844

4-rot-1

E(B3LYP/6-31G*) = -909.762516

C	-0.018288	-0.001764	-0.001399
C	-0.012122	-0.008220	1.432682
C	1.282220	-0.005597	2.079022
C	2.471034	-0.003859	1.284312
C	2.410651	0.000761	-0.082155
C	1.143518	0.003902	-0.729020
C	-1.191476	-0.009661	2.220787
C	-1.096034	0.010250	3.635768
C	0.205961	0.015785	4.266556
C	1.354502	0.002767	3.473162
C	0.301876	0.041258	5.693122
C	-0.817857	0.064926	6.478226
C	-2.103565	0.062038	5.868906
C	-2.236474	0.033908	4.504891
C	-2.555536	0.044114	1.549606
C	-3.266343	-1.298317	1.215639
B	-4.695016	-1.701981	2.110957
B	-3.210703	-2.664811	2.271100
B	-4.787287	-3.473787	2.098889
B	-3.353138	-4.090365	1.220242
H	-2.839535	-5.126500	1.488236
B	-4.929548	-3.993528	0.406931
B	-3.448435	-3.513716	-0.458763
B	-2.384188	-2.691952	0.695888
B	-3.362003	-1.753427	-0.428499
B	-4.784396	-1.135688	0.447231
B	-5.760135	-2.516981	0.959791
C	-4.856704	-2.540179	-0.493203
H	-5.404526	-2.479561	-1.426656
H	-5.290701	-4.070223	2.993486
H	-2.951009	-1.076112	-1.306692
H	-5.213470	-0.089599	0.098773
H	-6.940345	-2.423052	0.913410
H	-5.574253	-4.896832	-0.008800
H	-1.206110	-2.640564	0.621377
H	-2.477780	0.608001	0.617582
H	-5.048579	-0.969801	2.973650
H	-2.570626	-2.597745	3.262628
H	-3.234255	0.013579	4.084079
H	-2.992025	0.077133	6.494261

H	-0.732856	0.084708	7.561077
H	-3.106012	-4.082073	-1.440383
H	1.293476	0.042707	6.139433
H	2.330856	0.005389	3.953457
H	3.429614	-0.004824	1.797726
H	3.320691	0.002286	-0.675431
H	1.097121	0.007181	-1.814669
H	-0.960571	-0.012693	-0.535466
H	-3.241471	0.621924	2.172028

4-rot-2

E(B3LYP/6-31G*) = -909.763469

C	-0.144034	-0.260708	-0.038577
C	-0.047003	-0.143703	1.387580
C	1.283040	-0.187398	1.955827
C	2.416695	-0.330064	1.095934
C	2.270076	-0.434038	-0.260041
C	0.966784	-0.401301	-0.829688
C	1.442727	-0.097594	3.339748
C	0.348080	0.026074	4.197288
C	-0.988166	0.075604	3.644812
C	-1.171848	-0.000882	2.240200
C	0.532242	0.098436	5.613520
C	-0.534904	0.210162	6.461768
C	-1.853658	0.257852	5.929891
C	-2.070719	0.195067	4.577817
C	-2.576821	-0.001107	1.655771
C	-3.211812	1.361964	1.264436
B	-2.268444	2.627871	0.617426
C	-3.373969	3.382604	-0.426746
B	-3.073746	4.131519	1.081627
B	-4.702646	4.125085	0.355104
B	-4.896425	2.614401	-0.568604
B	-3.396900	1.697114	-0.401499
B	-4.797198	1.267069	0.574145
B	-5.621648	2.771734	1.046311
B	-4.492790	3.714399	2.069446
B	-4.548101	1.947929	2.194551
B	-2.980465	2.782846	2.223160
H	-6.799070	2.805653	1.194681
H	-2.964929	3.856629	-1.311555
H	-4.865494	4.423991	2.945222
H	-2.928795	1.021718	-1.251589
H	-1.117856	2.533289	0.375599
H	-2.432909	5.126972	1.123330
H	-5.140617	5.133436	-0.087376
H	-5.283796	0.195031	0.432538
H	-3.263719	-0.476550	2.358148
H	-2.274347	2.738967	3.169398

H	-4.890720	1.315687	3.137812
H	-1.116085	-0.231909	-0.515329
H	0.851352	-0.488294	-1.906730
H	3.138834	-0.543533	-0.903016
H	-5.452391	2.601719	-1.614834
H	3.403862	-0.356567	1.551196
H	2.445344	-0.131605	3.761113
H	1.547855	0.060511	6.000226
H	-0.383101	0.263541	7.536141
H	-2.699908	0.349911	6.605148
H	-3.089754	0.253188	4.215527
H	-2.600797	-0.635505	0.767238

5-cryst

E(B3LYP/6-31G*) = -920.557019

C	0.059689	-0.153892	0.041105
C	0.020214	-0.069047	1.472403
C	1.292775	-0.055593	2.161216
C	2.506633	-0.131867	1.408604
C	2.490170	-0.213991	0.042937
C	1.244772	-0.223131	-0.645484
C	-1.184024	0.006571	2.218908
C	-1.134470	0.109641	3.633122
C	0.146408	0.123693	4.306508
C	1.319755	0.036808	3.554354
C	0.196220	0.231078	5.731838
C	-0.948065	0.324428	6.476129
C	-2.213148	0.314362	5.824585
C	-2.301979	0.210671	4.460079
C	-2.524172	0.045584	1.499213
C	-3.243521	-1.302791	1.214375
B	-3.355443	-1.828753	-0.432798
B	-4.775405	-1.193813	0.420693
B	-4.916393	-2.663328	-0.573385
B	-5.723965	-2.569217	1.019610
B	-4.665174	-1.673115	2.129790
B	-3.176633	-2.591459	2.328864
B	-4.726564	-3.438335	2.206998
B	-4.880198	-4.053182	0.537625
B	-3.414856	-3.590121	-0.361504
C	-3.358789	-3.934575	1.313033
B	-2.365618	-2.688347	0.742401
I	-7.918583	-2.476450	1.230165
H	-2.868814	-4.851400	1.620665
H	-5.523376	-2.677705	-1.591537
H	-2.491507	-2.597426	3.288409
H	-1.188744	-2.752614	0.744358
H	-2.916300	-4.339117	-1.131462
H	-5.364772	-5.118290	0.361267

H	-5.014402	-0.928169	2.980297
H	-2.408081	0.551382	0.538838
H	-2.827909	-1.181839	-1.273358
H	-5.192270	-0.118310	0.150768
H	-3.285541	0.196114	4.007054
H	-3.120885	0.388808	6.417042
H	-0.898039	0.406874	7.558124
H	-5.101855	-4.082869	3.125338
H	1.172404	0.238533	6.210759
H	2.279701	0.046528	4.066488
H	3.447871	-0.121381	1.952950
H	3.418480	-0.270850	-0.518338
H	1.233443	-0.287370	-1.730096
H	-0.865068	-0.175566	-0.522503
H	-3.224960	0.665445	2.061180

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E(B3LYP/6-31G*) = -920.555333

C	-0.018188	0.021904	-0.006312
C	-0.011272	0.005271	1.427778
C	1.283589	0.004673	2.073486
C	2.472281	0.015536	1.278401
C	2.411346	0.031980	-0.088315
C	1.143687	0.036479	-0.734506
C	-1.189583	-0.000616	2.217720
C	-1.094048	0.009855	3.633055
C	0.208668	0.008200	4.262774
C	1.356619	0.001084	3.467937
C	0.306524	0.020621	5.689595
C	-0.812439	0.039941	6.476480
C	-2.098846	0.046765	5.868266
C	-2.233511	0.031372	4.503799
C	-2.553768	0.062645	1.548293
C	-3.274673	-1.274346	1.210095
B	-4.712925	-1.659200	2.097487
B	-3.240143	-2.635585	2.271942
B	-4.827796	-3.428725	2.093006
B	-3.397071	-4.056649	1.220470
I	-2.465293	-5.992507	1.723064
B	-4.967397	-3.954302	0.399641
B	-3.473159	-3.490611	-0.461886
B	-2.403676	-2.675408	0.698641
B	-3.366396	-1.732568	-0.432926
B	-4.785996	-1.098169	0.432374
B	-5.780757	-2.465559	0.943805
C	-4.869146	-2.504356	-0.503623
H	-5.410798	-2.443415	-1.440838
H	-5.334216	-4.022694	2.985066
H	-2.941582	-1.065961	-1.311984

H	-5.201943	-0.049607	0.077793
H	-6.959399	-2.362001	0.892114
H	-5.610822	-4.857175	-0.014138
H	-1.225454	-2.648268	0.634427
H	-2.476011	0.628520	0.617492
H	-5.063065	-0.923351	2.957517
H	-2.603949	-2.581873	3.264845
H	-3.232386	0.021163	4.085178
H	-2.986572	0.059950	6.494667
H	-0.726451	0.049282	7.559302
H	-3.129114	-4.073818	-1.432080
H	1.298621	0.015267	6.134543
H	2.333296	-0.001140	3.947385
H	3.430964	0.012365	1.791423
H	3.320945	0.041404	-0.682019
H	1.096820	0.048303	-1.820048
H	-0.960265	0.013621	-0.540796
H	-3.237106	0.640907	2.173380

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E(B3LYP/6-31G*) = -920.556402

C	-0.021777	0.028085	-0.013309
C	-0.005990	0.014423	1.420722
C	1.291880	0.030453	2.060335
C	2.476348	0.057411	1.259209
C	2.407253	0.071787	-0.107124
C	1.136296	0.057025	-0.746979
C	-1.180998	-0.005470	2.215817
C	-1.078264	0.005879	3.630859
C	0.227458	0.016624	4.254657
C	1.371746	0.024982	3.454431
C	0.331536	0.026859	5.681082
C	-0.783536	0.033931	6.473887
C	-2.072932	0.032667	5.871879
C	-2.213371	0.018292	4.507793
C	-2.549111	0.038925	1.551346
C	-3.247256	-1.307523	1.211215
B	-2.354895	-2.685788	0.666099
B	-3.384777	-1.766374	-0.450719
B	-3.435217	-3.539735	-0.464000
H	-3.007132	-4.175121	-1.368584
B	-3.131182	-2.657494	2.248771
B	-4.640481	-1.722199	2.110357
B	-4.793141	-1.160022	0.450612
B	-4.946582	-2.591948	-0.593454
B	-5.727480	-2.561090	1.000982
B	-4.884368	-4.032413	0.439942
B	-3.282475	-4.086021	1.219839
C	-4.637171	-3.405006	2.013023

I	-6.143074	-2.521618	-2.446474
H	-5.052705	-3.949610	2.853277
H	-4.997255	-1.119399	3.062361
H	-2.579068	-2.641639	3.290280
H	-2.834804	-5.113136	1.602922
H	-5.502714	-5.031770	0.301064
H	-5.224345	-0.077260	0.241536
H	-2.484622	0.601249	0.618224
H	-1.176973	-2.629938	0.600241
H	-2.895078	-1.068527	-1.272746
H	-3.213785	0.009679	4.092499
H	-2.957688	0.043039	6.502722
H	-0.692099	0.043219	7.556269
H	-6.887378	-2.575106	1.234200
H	1.325714	0.031598	6.121439
H	2.350608	0.034497	3.929373
H	3.437752	0.068213	1.767041
H	3.313411	0.093778	-0.705796
H	1.083373	0.065436	-1.832152
H	-0.966439	0.001594	-0.542060
H	-3.238420	0.610328	2.176826

5-rot-3

E(B3LYP/6-31G*) = -920.555613

C	-0.016134	0.102328	-0.021093
C	0.002776	0.054755	1.412282
C	1.301911	0.076698	2.049362
C	2.484048	0.138385	1.246637
C	2.411758	0.182101	-0.118762
C	1.139569	0.164630	-0.756239
C	-1.168956	-0.002965	2.209918
C	-1.063013	-0.020837	3.624562
C	0.243755	-0.000292	4.245442
C	1.385537	0.043463	3.442719
C	0.351797	-0.017281	5.671423
C	-0.761060	-0.046959	6.466825
C	-2.051609	-0.061376	5.867786
C	-2.195464	-0.050063	4.504082
C	-2.539420	0.032748	1.550822
C	-3.214534	-1.318898	1.178419
B	-3.014269	-2.740031	2.143451
B	-2.322546	-2.637496	0.508352
B	-3.184142	-4.107302	1.017759
B	-3.438291	-3.437745	-0.620627
B	-3.420210	-1.668855	-0.504249
B	-4.776691	-1.180495	0.501810
B	-4.963914	-2.528102	-0.624747
B	-4.817997	-4.038707	0.318305
B	-4.557603	-3.605124	2.025994

C	-5.507754	-2.625111	0.992811
B	-4.530864	-1.846184	2.133045
I	-2.720787	-4.458231	-2.441405
H	-6.578457	-2.603204	1.161839
H	-2.619047	-5.133493	1.198689
H	-5.349576	-0.148976	0.422666
H	-4.969479	-1.214554	3.030557
H	-5.078516	-4.221803	2.892458
H	-5.514963	-4.955488	0.046047
H	-2.999621	-0.905105	-1.304913
H	-2.484961	0.622575	0.633805
H	-2.323118	-2.703161	3.100264
H	-1.154890	-2.537048	0.367036
H	-3.196978	-0.072935	4.092357
H	-2.934698	-0.084351	6.500575
H	-0.666973	-0.058697	7.548957
H	-5.744357	-2.434586	-1.509097
H	1.347065	-0.003746	6.109120
H	2.365467	0.058627	3.915288
H	3.446314	0.150854	1.752757
H	3.316076	0.228772	-0.718767
H	1.084032	0.195447	-1.840829
H	-0.961309	0.073445	-0.549309
H	-3.237208	0.573975	2.193685

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E(B3LYP/6-31G*) = -920.556425

C	-0.082382	0.098768	-0.015548
C	-0.023566	0.069224	1.417322
C	1.292749	0.125677	2.016031
C	2.450460	0.194675	1.179125
C	2.340075	0.216682	-0.184455
C	1.050778	0.171067	-0.784649
C	-1.171447	-0.000923	2.248693
C	-1.025078	0.011109	3.660073
C	0.298467	0.070078	4.242286
C	1.416178	0.119080	3.406900
C	0.447377	0.081914	5.664715
C	-0.642077	0.043769	6.491204
C	-1.948760	-0.009415	5.930049
C	-2.132172	-0.026199	4.571298
C	-2.561076	-0.020325	1.628722
C	-3.204767	-1.399785	1.312786
B	-4.743584	-1.337784	0.522588
B	-4.607511	-1.866623	2.210572
B	-5.635566	-2.773187	1.077873
B	-4.586633	-3.635543	2.243346
B	-3.062789	-2.728554	2.407706
B	-2.258447	-2.736917	0.839794

B	-3.124247	-4.176204	1.390078
B	-4.712094	-4.206400	0.569482
B	-4.812407	-2.781994	-0.495079
C	-3.320540	-3.565773	-0.193792
B	-3.302384	-1.884403	-0.324836
I	-5.404190	-4.783129	3.941813
H	-2.874098	-4.130420	-1.004414
H	-6.817702	-2.775041	1.165110
H	-1.093964	-2.689078	0.661880
H	-2.770451	-1.302258	-1.204474
H	-5.309749	-2.856886	-1.567316
H	-5.151055	-5.243460	0.205930
H	-2.420144	-2.619662	3.391015
H	-2.554758	0.552853	0.699067
H	-5.197180	-0.275539	0.256908
H	-4.988501	-1.150356	3.073602
H	-3.143929	-0.084148	4.188946
H	-2.812703	-0.042518	6.587930
H	-0.517540	0.052989	7.570264
H	-2.520760	-5.177745	1.569782
H	1.453988	0.123329	6.073716
H	2.408485	0.160345	3.851239
H	3.425978	0.232790	1.657909
H	3.226396	0.271505	-0.810098
H	0.963899	0.193890	-1.867620
H	-1.042005	0.059124	-0.515880
H	-3.260062	0.507811	2.279687

6-cryst

E(B3LYP/6-31G*) = -931.364997

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.435089
C	1.292222	0.000000	2.086734
C	2.484936	-0.007153	1.297216
C	2.430334	-0.014532	-0.069714
C	1.165580	-0.010937	-0.722195
C	1.358895	0.007656	3.481153
C	0.207089	0.004167	4.270877
C	-1.093418	0.003382	3.635623
C	-1.182701	0.011739	2.219202
C	0.300067	-0.004934	5.697855
C	-0.821689	-0.026426	6.480963
C	-2.105201	-0.044953	5.867509
C	-2.234608	-0.031092	4.502089
C	-2.536829	-0.016121	1.526301
C	-3.125467	1.332123	1.023224
B	-2.793715	2.806834	1.814609
C	-2.864338	3.913890	0.530385
B	-4.215967	3.831310	1.573979

B	-4.410867	4.092619	-0.182356
B	-3.091887	3.231007	-1.022334
B	-2.104039	2.440655	0.212099
B	-3.282450	1.500442	-0.696291
B	-4.709846	2.517142	-0.943660
I	-5.911076	2.300334	-2.753443
B	-4.406450	2.099672	1.893206
B	-5.405886	2.889309	0.659432
I	-7.542614	3.177735	1.003590
B	-4.713200	1.289449	0.339840
H	-2.231706	4.791180	0.603233
H	-0.933790	2.314760	0.143754
H	-2.043881	2.914305	2.717541
H	-4.426738	4.708058	2.339006
H	-4.754406	5.153354	-0.574526
H	-2.907712	0.616743	-1.388502
H	-3.286274	-0.493841	2.162520
H	-4.791163	1.631343	2.906548
H	-5.292122	0.257712	0.323895
H	-0.938983	0.016467	-0.540939
H	1.123473	-0.015302	-1.807868
H	3.342640	-0.019810	-0.659248
H	-2.556562	3.708030	-1.962659
H	3.441154	-0.006252	1.814754
H	2.333465	0.012324	3.964876
H	1.290709	0.001561	6.146014
H	-0.739603	-0.036323	7.564037
H	-2.995458	-0.071014	6.489809
H	-3.230699	-0.043887	4.079768
H	-2.467561	-0.653775	0.644799

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E(B3LYP/6-31G*) = -931.363301

C	-0.030620	0.028304	-0.004254
C	-0.021832	0.005442	1.429817
C	1.274089	-0.008637	2.073168
C	2.461679	-0.009273	1.276501
C	2.398982	0.009937	-0.090119
C	1.130421	0.031647	-0.734072
C	-1.198425	0.004291	2.222413
C	-1.100780	0.011711	3.637799
C	0.203279	0.000449	4.264691
C	1.349442	-0.015210	3.467531
C	0.304386	0.010332	5.691289
C	-0.812645	0.035428	6.480646
C	-2.100302	0.050569	5.875400
C	-2.237988	0.037845	4.511188
C	-2.563719	0.067971	1.555452

C	-3.279085	-1.271879	1.215360
B	-4.712731	-1.659687	2.102705
B	-3.233574	-2.631859	2.283106
B	-4.818115	-3.429292	2.102777
B	-3.377333	-4.060841	1.232616
I	-2.408659	-5.975312	1.705506
B	-4.955184	-3.968788	0.413384
B	-3.466004	-3.494342	-0.449591
B	-2.401161	-2.668792	0.707650
B	-3.369441	-1.735627	-0.426633
B	-4.791701	-1.107213	0.436275
B	-5.778683	-2.478363	0.950486
C	-4.867608	-2.517467	-0.493938
H	-5.412323	-2.465674	-1.429993
I	-5.804909	-4.478395	3.763407
H	-2.948260	-1.071655	-1.308618
H	-5.218489	-0.063044	0.082907
H	-6.957303	-2.388618	0.908023
H	-5.596147	-4.876738	0.010841
H	-1.223512	-2.637073	0.643451
H	-2.489623	0.635643	0.625512
H	-5.070073	-0.931564	2.964457
H	-2.605435	-2.574755	3.279775
H	-3.238124	0.033434	4.095575
H	-2.986636	0.066698	6.503480
H	-0.724325	0.042152	7.563235
H	-3.119397	-4.080563	-1.416608
H	1.297289	-0.002281	6.134179
H	2.326768	-0.027485	3.945461
H	3.420814	-0.024164	1.788415
H	3.307593	0.009668	-0.685330
H	1.082125	0.048873	-1.819481
H	-0.973293	0.036379	-0.537919
H	-3.248781	0.641359	2.182816

6-rot-2

E(B3LYP/6-31G*) = -931.364256

C	-0.178177	-0.266448	-0.036177
C	-0.069633	-0.145097	1.389014
C	1.265415	-0.182459	1.946059
C	2.393059	-0.316882	1.076615
C	2.235874	-0.421322	-0.278534
C	0.927241	-0.399766	-0.836857
C	1.435873	-0.092837	3.329098
C	0.348042	0.024546	4.196758
C	-0.993306	0.072037	3.655900
C	-1.186747	-0.002960	2.252211
C	0.544729	0.095004	5.611563
C	-0.515483	0.203310	6.469456

C	-1.839031	0.249596	5.949096
C	-2.068012	0.188260	4.598489
C	-2.595762	0.005665	1.678855
C	-3.214480	1.376956	1.286648
B	-2.262303	2.617192	0.605130
C	-3.376144	3.382516	-0.421219
B	-3.025704	4.141036	1.068345
B	-4.673070	4.163964	0.378446
B	-4.913418	2.643192	-0.524099
B	-3.430133	1.698707	-0.377501
B	-4.813800	1.304557	0.633366
B	-5.600265	2.829136	1.103033
B	-4.426093	3.763518	2.094308
B	-4.519629	1.996898	2.243753
B	-2.932086	2.799066	2.223909
I	-7.778165	2.905831	1.382819
H	-2.981061	3.843590	-1.319379
I	-5.006568	5.119108	3.723966
H	-2.998841	1.005530	-1.231231
H	-1.119361	2.503761	0.340970
H	-2.374172	5.127655	1.092772
H	-5.108103	5.174187	-0.054593
H	-5.335802	0.248340	0.518812
H	-3.284667	-0.458887	2.386326
H	-2.217064	2.759224	3.161425
H	-4.861611	1.393316	3.202052
H	-1.154602	-0.250207	-0.504979
H	0.803193	-0.490891	-1.912563
H	3.099793	-0.524105	-0.928914
H	-5.503698	2.634688	-1.549015
H	3.384070	-0.336646	1.523581
H	2.442113	-0.121736	3.741933
H	1.563655	0.058465	5.989286
H	-0.354792	0.255348	7.542452
H	-2.679568	0.339267	6.631515
H	-3.091233	0.242285	4.247357
H	-2.634314	-0.628437	0.790640

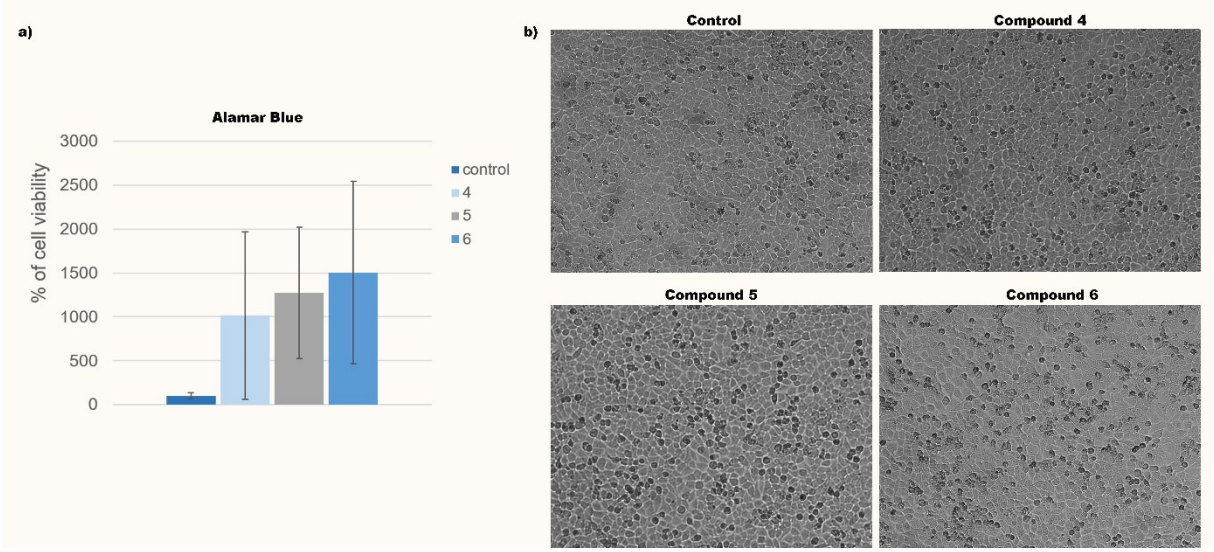

Figure S5. Cytotoxicity of compounds 4-6 by Alamar Blue assay (a) and optical images of cell density in cultures incubated with each compound (b). None of the compounds is cytotoxic but results obtained based on resazurin reduction are unreliable since no differences in cell density among the compounds and control cultures were observed under the inverted microscope. Magnification: 10x

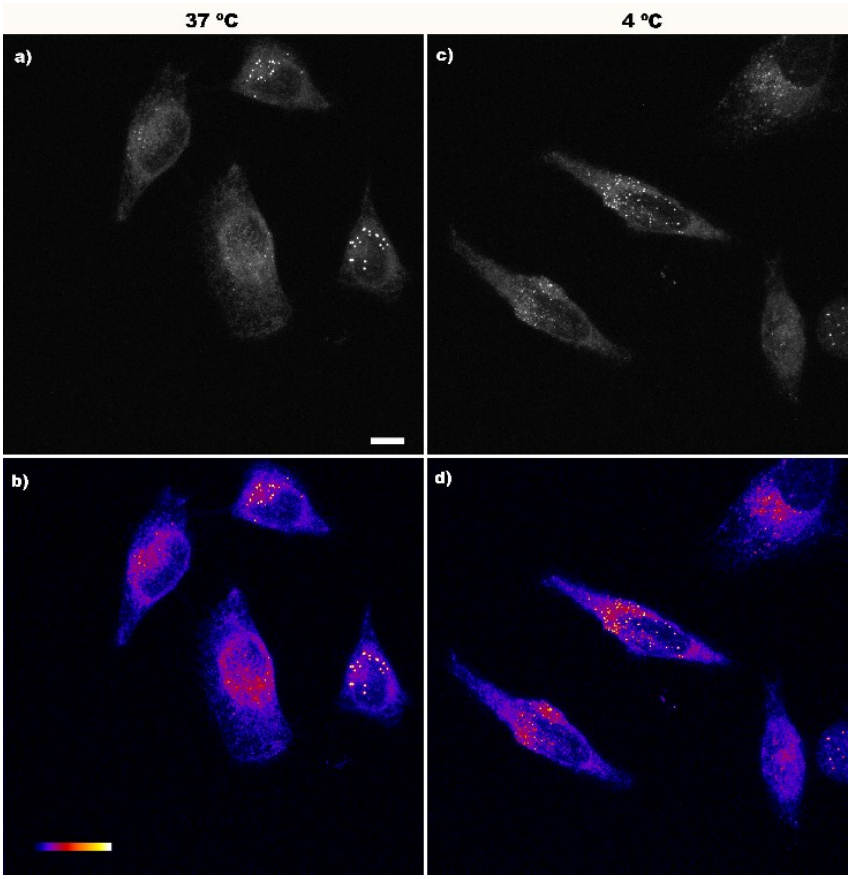

Figure S6. Photostability of compound 6 depending on the temperature. There were no differences in fluorescence intensity of compound **6** after their incubation with cells for 4 h at 37 ºC (a-b) followed by 1 extra h at 4 ºC (c-d). Images were obtained by confocal laser scanning microscopy (CLSM) applying a greyscale (upper panel) and a colour palette scale (lower panel) to better appreciate differences in fluorescence intensity.

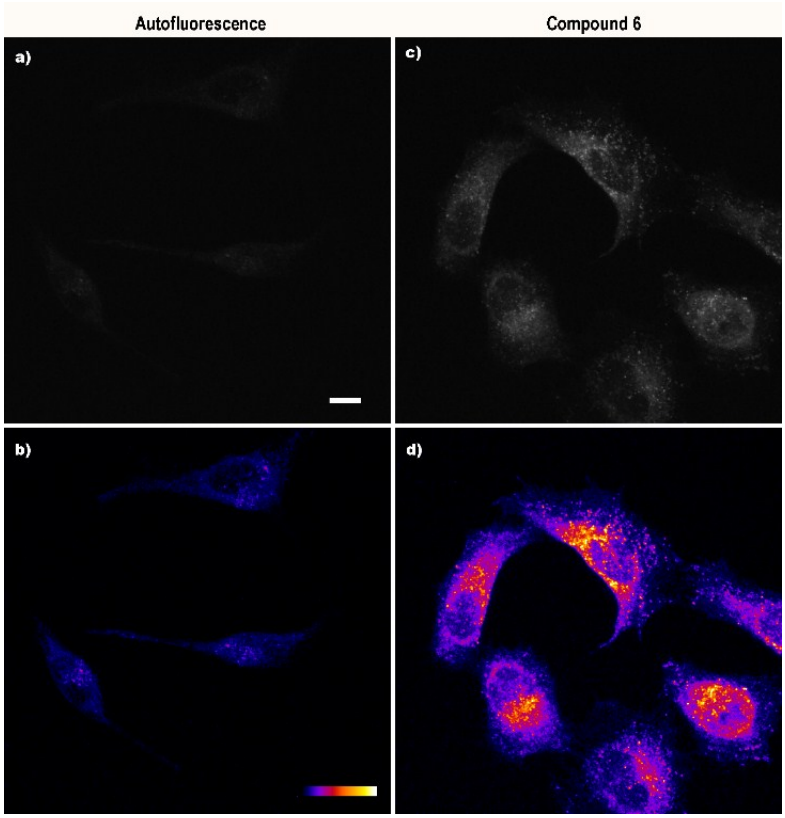

Figure S7. Autofluorescence of Hela cells. Comparison of the fluorescence intensity emitted by untreated cells (a-b) and cells incubated with **6** for 4 h (c-d) using the same CLSM settings for both conditions. Autofluorescence of HeLa cells is almost undetectable. A greyscale (upper panel) and a colour palette scale (lower panel) were applied.

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