

# Supporting Information

## Experimental and DFT Studies: Novel Structural Modifications Greatly Enhance the Solvent Sensitivity of Live Cell Imaging Dyes

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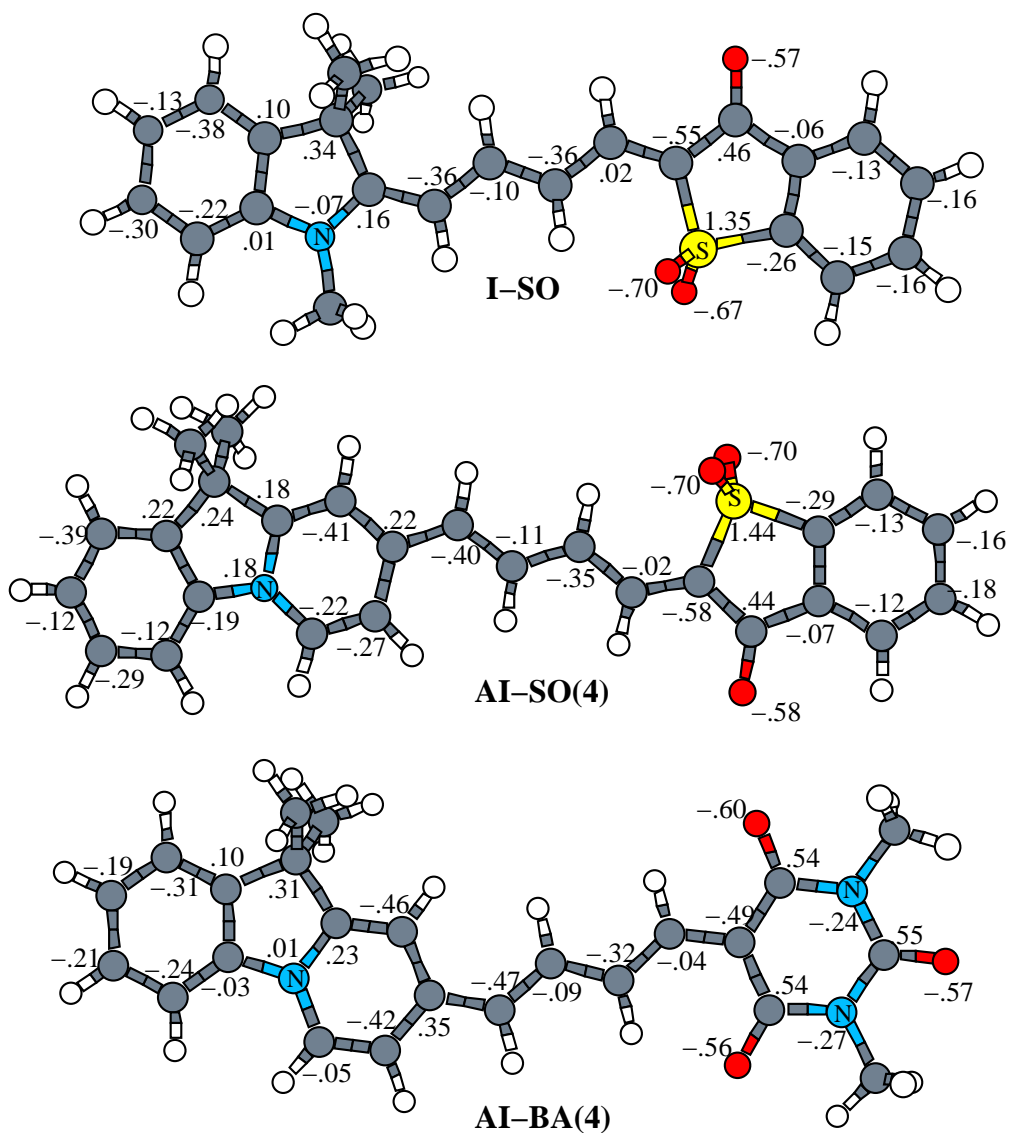
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**Figure S1.** Atomic ESP charges of the ground state I-SO, AI-SO(4) and AI-BA(4) dyes in MeOH.

Cartesian coordinates of COSMO optimized  $S_0$  state I-SO in  $C_6H_6$ :

C	3.770719	-0.064592	-5.335505	C	-1.076782	-0.357886	-4.516484
C	2.607601	-0.117777	-4.575924	C	3.097539	-1.281894	-2.388573
C	1.362787	-0.223022	-5.212411	C	2.932351	1.256965	-2.485240
C	1.239937	-0.282096	-6.602351	H	4.748102	0.019202	-4.856840
C	2.420626	-0.227312	-7.356427	H	4.575568	-0.077658	-7.344792
C	3.672170	-0.119311	-6.736758	H	2.357106	-0.269966	-8.443918
C	2.403644	-0.076042	-3.068242	H	0.271339	-0.367181	-7.094245
C	0.875825	-0.171937	-2.965562	H	-1.008043	-0.279260	-1.999155
N	0.350854	-0.249888	-4.230852	H	1.545371	-0.022484	-0.256278
C	0.068484	-0.191306	-1.838943	H	-1.473909	-0.246733	0.316177
C	0.484585	-0.115175	-0.495468	H	1.029798	0.002111	2.161751
C	-0.412603	-0.156173	0.556133	H	-0.937168	0.066333	7.195769
C	-0.032438	-0.089689	1.905903	H	-5.167418	-0.321979	4.510671
C	-0.910535	-0.123068	2.972765	H	-3.170491	-0.041683	8.345163
C	-0.569433	-0.020064	4.386588	H	-5.259178	-0.242652	7.015784
C	-1.809767	-0.060324	5.227660	H	-1.233234	-0.316704	-5.598411
C	-3.004286	-0.159290	4.499276	H	-1.475891	-1.309218	-4.132741
S	-2.671667	-0.184578	2.743788	H	-1.621402	0.474778	-4.048248
C	-4.255940	-0.231322	5.104285	H	4.181383	-1.231357	-2.572923
C	-4.295732	-0.188589	6.505242	H	2.933123	-1.273733	-1.301605
C	-3.112488	-0.076978	7.255199	H	2.720259	-2.235183	-2.788842
C	-1.864076	-0.014631	6.624695	H	2.766988	1.310680	-1.399707
O	0.579142	0.093390	4.846612	H	4.014177	1.333688	-2.672600
O	-3.130843	1.058477	2.076452	H	2.436011	2.120027	-2.954488
O	-3.142087	-1.473370	2.138678				

Cartesian coordinates of COSMO optimized  $S_1$  state I-SO in  $C_6H_6$ :

C	3.773368	-0.054528	-5.352390	S	-2.691802	-0.176536	2.763959
C	2.612591	-0.109769	-4.591179	C	-4.273958	-0.223942	5.130442
C	1.361520	-0.226030	-5.228601	C	-4.307217	-0.185766	6.535604
C	1.240887	-0.293365	-6.624469	C	-3.117509	-0.072657	7.274443
C	2.418929	-0.235956	-7.374230	C	-1.872280	-0.009237	6.636981
C	3.672973	-0.117278	-6.752679	O	0.577031	0.048032	4.849297
C	2.414392	-0.064279	-3.085547	O	-3.132336	1.064955	2.084655
C	0.894791	-0.169977	-2.981239	O	-3.135343	-1.463667	2.148942
N	0.359380	-0.255903	-4.255012	C	-1.067235	-0.376987	-4.542492
C	0.087199	-0.194505	-1.837629	C	3.123227	-1.264168	-2.405262
C	0.511207	-0.116431	-0.504045	C	2.945159	1.272178	-2.503917
C	-0.400182	-0.165348	0.568242	H	4.750903	0.036210	-4.875827
C	-0.029983	-0.096606	1.912102	H	4.575473	-0.073836	-7.361889
C	-0.930065	-0.122103	2.990531	H	2.359570	-0.284863	-8.461559
C	-0.592361	-0.034165	4.398254	H	0.273918	-0.387551	-7.117174
C	-1.821440	-0.056076	5.236702	H	-0.990394	-0.288398	-1.995695
C	-3.028174	-0.150337	4.518844	H	1.569683	-0.015166	-0.265322

H	-1.460029	-0.261942	0.320202	H	-1.617798	0.456421	-4.083292
H	1.028746	-0.007163	2.181575	H	4.206590	-1.203212	-2.588930
H	-0.942258	0.070247	7.203596	H	2.957724	-1.258425	-1.318851
H	-5.189442	-0.312968	4.542740	H	2.754659	-2.220638	-2.806545
H	-3.166143	-0.040198	8.365344	H	2.777279	1.326359	-1.419164
H	-5.266635	-0.245082	7.053024	H	4.027662	1.346857	-2.688055
H	-1.221026	-0.348321	-5.624972	H	2.450140	2.134373	-2.975894
H	-1.457281	-1.328085	-4.149824				

Cartesian coordinates of COSMO optimized  $S_0$  state I-SO in MeOH:

C	3.782573	-0.060421	-5.351389	C	-1.063730	-0.362770	-4.521541
C	2.621188	-0.114303	-4.586551	C	3.120389	-1.274543	-2.401053
C	1.375445	-0.222549	-5.218722	C	2.941585	1.265719	-2.499492
C	1.240864	-0.283845	-6.607450	H	4.762766	0.025674	-4.879530
C	2.418070	-0.229120	-7.367076	H	4.573662	-0.076561	-7.365471
C	3.673653	-0.118164	-6.752076	H	2.349643	-0.273911	-8.454126
C	2.419575	-0.071748	-3.079845	H	0.269484	-0.370802	-7.092774
C	0.893737	-0.175448	-2.976425	H	-0.997640	-0.296339	-2.014667
N	0.366486	-0.251670	-4.229652	H	1.543001	-0.031334	-0.257233
C	0.076431	-0.202837	-1.843141	H	-1.484939	-0.269689	0.294508
C	0.485081	-0.129719	-0.507053	H	1.014286	-0.017363	2.139429
C	-0.426940	-0.174305	0.548388	H	-0.932585	0.060001	7.203877
C	-0.050725	-0.100986	1.890493	H	-5.184687	-0.311435	4.545349
C	-0.926138	-0.120810	2.976932	H	-3.152360	-0.058337	8.362464
C	-0.584119	-0.020453	4.378903	H	-5.252609	-0.253252	7.050221
C	-1.814918	-0.056114	5.233772	H	-1.212850	-0.323201	-5.603699
C	-3.018319	-0.151721	4.516902	H	-1.455466	-1.315539	-4.138141
S	-2.683251	-0.174424	2.765437	H	-1.607411	0.470123	-4.055778
C	-4.266236	-0.226181	5.128721	H	4.202047	-1.217906	-2.594668
C	-4.293705	-0.193353	6.532202	H	2.965054	-1.260789	-1.312915
C	-3.104406	-0.085634	7.271841	H	2.742122	-2.229042	-2.797899
C	-1.859139	-0.017646	6.631520	H	2.783862	1.315673	-1.412697
O	0.574433	0.084271	4.841990	H	4.021570	1.345449	-2.694464
O	-3.155929	1.062088	2.085543	H	2.437078	2.124998	-2.967644
O	-3.148404	-1.456570	2.144359				

Cartesian coordinates of COSMO optimized  $S_1$  state I-SO in MeOH:

C	3.780386	-0.053181	-5.356241	C	0.092651	-0.209337	-1.851104
C	2.621250	-0.108933	-4.592328	C	0.510019	-0.130920	-0.502484
C	1.367293	-0.226657	-5.227859	C	-0.407665	-0.175091	0.547202
C	1.239389	-0.292922	-6.624845	C	-0.044035	-0.101794	1.907110
C	2.414659	-0.235718	-7.376673	C	-0.934197	-0.116208	2.983551
C	3.672228	-0.116968	-6.756741	C	-0.600694	-0.032942	4.393290
C	2.425257	-0.063311	-3.087353	C	-1.816760	-0.057740	5.235579
C	0.904932	-0.178088	-2.981959	C	-3.032955	-0.151251	4.526441
N	0.368591	-0.260938	-4.257284	S	-2.700224	-0.167162	2.775445

C	-4.276301	-0.225679	5.142399	H	-1.464760	-0.271125	0.286453
C	-4.302439	-0.191723	6.549300	H	1.016953	-0.019634	2.168258
C	-3.107254	-0.080645	7.280959	H	-0.936846	0.065132	7.209135
C	-1.864706	-0.014181	6.638810	H	-5.196810	-0.309978	4.562005
O	0.580143	0.046620	4.842527	H	-3.149040	-0.051601	8.372129
O	-3.161516	1.078586	2.105864	H	-5.258784	-0.252461	7.071647
O	-3.151426	-1.447047	2.142998	H	-1.211845	-0.350824	-5.627723
C	-1.059024	-0.381454	-4.546045	H	-1.443922	-1.333512	-4.153150
C	3.145804	-1.255773	-2.407665	H	-1.605948	0.451075	-4.082794
C	2.946074	1.278300	-2.509393	H	4.226609	-1.186246	-2.602073
H	4.760186	0.038191	-4.884985	H	2.992120	-1.241739	-1.319489
H	4.572411	-0.074391	-7.369585	H	2.778476	-2.216039	-2.801221
H	2.353344	-0.284598	-8.463867	H	2.785961	1.327577	-1.423074
H	0.269766	-0.386241	-7.111669	H	4.026478	1.360524	-2.701240
H	-0.982847	-0.306447	-2.017084	H	2.439442	2.135489	-2.978838
H	1.567084	-0.030127	-0.256082				

Cartesian coordinates of COSMO optimized  $S_0$  state I-TBA in  $C_6H_6$ :

C	0.021860	-0.113643	-0.020694	H	3.927601	3.021219	-0.208514
C	1.411080	-0.047037	0.001792	H	-0.493692	-1.075417	-0.008958
C	2.049591	1.199454	-0.015784	H	-1.805016	1.045924	-0.077804
C	1.338980	2.401025	-0.049751	H	-0.644192	3.240982	-0.099567
C	-0.060671	2.320418	-0.072378	H	1.837639	3.369817	-0.056482
C	-0.715773	1.082191	-0.059293	H	5.864250	-0.022037	0.103579
C	2.456533	-1.151166	0.046802	H	4.755279	-2.914576	0.127808
C	3.760423	-0.337947	0.052956	H	7.636805	-1.785540	0.155785
N	3.447369	0.992915	0.005962	H	6.294414	-4.583888	0.192430
C	5.080574	-0.782369	0.095354	H	5.169078	1.894084	-0.814867
C	5.504100	-2.120017	0.127898	H	4.962003	2.134888	0.950638
C	6.836983	-2.523287	0.157393	H	10.546008	-8.519615	0.341059
C	7.140013	-3.886680	0.188572	H	8.970562	-8.436459	1.213726
C	8.386036	-4.528575	0.220479	H	8.989647	-8.473598	-0.569009
C	9.649337	-3.814840	0.218768	H	11.891539	-2.836477	0.252353
N	10.836080	-4.622137	0.267119	H	12.679985	-4.160715	1.189669
C	10.849599	-6.003284	0.299923	H	12.720552	-4.197683	-0.591250
N	9.611549	-6.652661	0.290627	C	2.347957	-2.046838	-1.212341
C	8.361272	-5.986826	0.255268	C	2.292070	-1.992867	1.335741
O	9.759579	-2.579186	0.179520	H	1.304283	-2.478133	1.328214
O	7.324006	-6.670704	0.255783	H	3.058937	-2.777265	1.403627
C	9.527659	-8.123617	0.321242	H	2.361401	-1.360653	2.233974
S	12.332081	-6.860895	0.348285	H	1.362855	-2.537547	-1.225689
C	12.122543	-3.904259	0.280306	H	2.451309	-1.451290	-2.132171
C	4.438070	2.073587	-0.014764	H	3.120853	-2.828181	-1.216707

Cartesian coordinates of COSMO optimized  $S_1$  state I-TBA in  $C_6H_6$ :

C	-0.008740	0.074435	-0.080964	C	1.379142	0.031633	-0.027569
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C	2.117142	1.231966	-0.036805	H	-0.597202	-0.844679	-0.074530
C	1.493732	2.487539	-0.094918	H	-1.739843	1.370363	-0.184199
C	0.097336	2.511362	-0.148502	H	-0.416141	3.472054	-0.193770
C	-0.651789	1.323433	-0.142853	H	2.063426	3.416140	-0.095446
C	2.331803	-1.151424	0.045229	H	5.803136	-0.269725	0.203572
C	3.686939	-0.443236	0.088640	H	4.570629	-3.114230	0.227444
N	3.478036	0.927606	0.021303	H	7.470767	-1.992918	0.326452
C	4.975089	-0.983358	0.180040	H	6.255362	-4.843896	0.347197
C	5.337127	-2.338388	0.243747	H	5.282269	1.693039	-0.757970
C	6.685805	-2.749049	0.314646	H	5.050538	1.951291	1.001798
C	7.050514	-4.093189	0.355167	H	10.787064	-8.476013	0.340259
C	8.362300	-4.645040	0.378565	H	9.228871	-8.514608	1.250013
C	9.573437	-3.847632	0.389759	H	9.208916	-8.508136	-0.532059
N	10.807092	-4.570622	0.350019	H	11.732276	-2.714235	0.325199
C	10.916174	-5.945606	0.333250	H	12.650669	-3.989260	1.208438
N	9.732390	-6.672162	0.360560	H	12.620164	-4.002795	-0.573687
C	8.443296	-6.097301	0.382627	C	2.188980	-2.046005	-1.214268
O	9.594994	-2.602163	0.425887	C	2.066583	-1.987928	1.322824
O	7.448936	-6.847791	0.401080	H	1.050743	-2.409743	1.279944
C	9.745487	-8.146156	0.354578	H	2.779591	-2.820107	1.407356
S	12.460057	-6.700838	0.282385	H	2.148180	-1.366942	2.227912
C	12.039818	-3.763028	0.325711	H	1.175309	-2.474262	-1.245755
C	4.546805	1.928665	0.023675	H	2.350638	-1.464222	-2.134462
H	4.115782	2.912562	-0.181691	H	2.911594	-2.874221	-1.194700

Cartesian coordinates of COSMO optimized  $S_0$  state I-TBA in MeOH:

C	3.146891	-0.242862	-5.788235	C	0.544509	0.267925	6.557778
C	2.049386	-0.200437	-4.933194	S	-2.471214	0.251694	7.172420
C	0.753482	-0.266842	-5.460824	C	-4.019870	0.132328	4.642417
C	0.503184	-0.384824	-6.829224	C	-1.629904	-0.228382	-4.577184
C	1.616416	-0.429718	-7.680146	H	-1.855125	-0.131623	-5.642291
C	2.921465	-0.357798	-7.171386	H	4.165404	-0.191510	-5.400131
C	1.970953	-0.090783	-3.419324	H	3.769637	-0.394143	-7.855007
C	0.454553	-0.119310	-3.191908	H	1.458523	-0.523850	-8.754743
N	-0.173082	-0.200873	-4.394559	H	-0.507632	-0.445561	-7.231064
C	-0.270954	-0.075808	-1.993753	H	-1.358652	-0.121785	-2.075252
C	0.252788	0.008574	-0.703188	H	1.333625	0.055583	-0.554737
C	-0.553907	0.033537	0.443636	H	-1.635160	-0.004664	0.333281
C	0.015916	0.098114	1.709988	H	1.108713	0.127930	1.762350
C	-0.619875	0.127186	2.973910	H	-2.086182	0.611485	-4.038025
C	-2.055668	0.113030	3.135242	H	-2.041006	-1.175826	-4.202029
N	-2.554563	0.149416	4.478871	H	-0.051200	0.302500	7.472657
C	-1.763735	0.202047	5.602400	H	1.186098	-0.622362	6.551365
N	-0.380591	0.213558	5.409938	H	1.173629	1.163184	6.475194
C	0.241187	0.175971	4.139532	H	-4.455280	0.089124	3.641526
O	-2.871758	0.073485	2.194006	H	-4.317445	-0.744923	5.229841
O	1.489477	0.186818	4.094408	H	-4.345851	1.040174	5.164639

C	2.585717	1.248609	-2.941219	H	2.264273	-2.247856	-3.105846
C	2.683039	-1.292870	-2.752556	H	3.657681	1.260867	-3.190344
H	3.752655	-1.263204	-3.010286	H	2.101006	2.104173	-3.436591
H	2.593182	-1.253519	-1.657729	H	2.482539	1.368103	-1.853118

Cartesian coordinates of COSMO optimized  $S_1$  state I-TBA in MeOH:

C	3.136689	-0.251689	-5.797133	H	-1.870239	-0.126922	-5.665974
C	2.041932	-0.197641	-4.943457	H	4.155080	-0.206860	-5.408034
C	0.734948	-0.258764	-5.472532	H	3.761825	-0.417120	-7.862629
C	0.492330	-0.378330	-6.851310	H	1.452299	-0.529056	-8.769473
C	1.604585	-0.431902	-7.694295	H	-0.517310	-0.433931	-7.256117
C	2.912976	-0.369983	-7.180672	H	-1.342390	-0.111161	-2.073110
C	1.972974	-0.084104	-3.430655	H	1.369011	0.066142	-0.560228
C	0.460852	-0.107163	-3.198800	H	-1.596175	-0.021129	0.338200
N	-0.182053	-0.189335	-4.427872	H	1.136008	0.126373	1.802946
C	-0.252657	-0.067402	-2.003449	H	-2.091637	0.620052	-4.060653
C	0.288569	0.014265	-0.698392	H	-2.044470	-1.166054	-4.219810
C	-0.514299	0.024795	0.447483	H	-0.063239	0.293480	7.492754
C	0.045801	0.088383	1.736099	H	1.184294	-0.610706	6.561950
C	-0.614237	0.113324	2.988335	H	1.151352	1.174252	6.499086
C	-2.056175	0.084081	3.148432	H	-4.454791	0.120245	3.633821
N	-2.557020	0.149733	4.481733	H	-4.338569	-0.723305	5.217761
C	-1.773527	0.208405	5.614347	H	-4.337101	1.062588	5.162560
N	-0.391289	0.213700	5.428193	C	2.606758	1.249235	-2.954353
C	0.235033	0.173841	4.168506	C	2.689205	-1.287665	-2.766904
O	-2.860761	0.008838	2.193890	H	3.761708	-1.250123	-3.010522
O	1.486262	0.190097	4.119825	H	2.586424	-1.259235	-1.673209
C	0.532026	0.271566	6.577493	H	2.279592	-2.242172	-3.132353
S	-2.490402	0.270954	7.183692	H	3.682851	1.243069	-3.185361
C	-4.024321	0.152378	4.637112	H	2.142991	2.109863	-3.460773
C	-1.636052	-0.219282	-4.602402	H	2.489920	1.377150	-1.868811

Cartesian coordinates of COSMO optimized  $S_0$  state AI-SO(4) in  $C_6H_6$ :

C	7.636499	-12.427668	-1.011976	C	4.235371	-3.096818	-0.067858
C	7.616310	-11.038856	-0.855477	C	4.547717	-1.703143	0.100943
C	8.824664	-10.342401	-0.737909	C	3.564359	-0.754511	0.174681
C	10.062466	-10.976047	-0.769610	N	2.227198	-1.125367	0.084618
C	10.070673	-12.368540	-0.926795	C	1.871490	-2.443534	-0.075527
C	8.869996	-13.085097	-1.046576	C	2.831156	-3.413883	-0.150469
C	6.398659	-10.172191	-0.797418	C	1.381723	0.011639	0.187227
C	6.764898	-8.774368	-0.627920	C	2.186219	1.150474	0.344673
S	8.528051	-8.583546	-0.549254	C	3.662766	0.757760	0.351551
C	5.856773	-7.731083	-0.539526	C	1.581257	2.401434	0.467368
C	6.116758	-6.364406	-0.376672	C	0.178124	2.486366	0.431011
C	5.084745	-5.430470	-0.304221	C	-0.606118	1.332693	0.274694
C	5.268411	-4.057045	-0.142463	C	-0.014014	0.067019	0.149268

C	4.436547	1.404080	-0.822932	H	10.990346	-10.412429	-0.675989
C	4.347628	1.118602	1.692256	H	8.902099	-14.168306	-1.168442
O	9.059301	-7.848190	-1.707911	H	11.022619	-12.899073	-0.956042
O	8.979773	-8.126775	0.774522	H	4.411805	2.500453	-0.726622
O	5.236575	-10.609056	-0.884624	H	5.488295	1.079476	-0.811856
H	2.182991	3.305783	0.590536	H	3.993559	1.128451	-1.792212
H	-0.306697	3.459899	0.525881	H	5.400807	0.798367	1.679840
H	-1.694464	1.416047	0.249847	H	4.320636	2.209261	1.840712
H	-0.626050	-0.828604	0.027961	H	3.842632	0.636785	2.543120
H	5.592801	-1.393690	0.172591	H	2.497739	-4.444228	-0.276209
H	6.293469	-3.682893	-0.066059	H	0.805363	-2.656316	-0.134442
H	4.066763	-5.823381	-0.381869	H	7.148936	-6.014766	-0.303719
H	6.696445	-12.971540	-1.104184	H	4.809650	-8.047885	-0.609444

Cartesian coordinates of COSMO optimized  $S_1$  state AI-SO(4) in  $C_6H_6$ :

c	0.005204	0.079633	0.034860	o	9.040157	-7.814494	-1.719767
c	1.402917	0.043564	0.008364	o	9.015005	-8.048436	0.770680
c	2.197613	1.201283	0.056198	o	5.293281	-10.644948	-0.718189
c	1.579601	2.445619	0.132234	c	4.396119	1.416981	-1.214249
c	0.175020	2.510202	0.159426	c	4.406349	1.266128	1.312892
c	-0.597384	1.339506	0.111880	h	2.169588	3.362782	0.170941
c	3.676506	0.825849	0.020854	h	-0.319543	3.479347	0.219653
c	3.591491	-0.692393	-0.065514	h	-1.685054	1.407466	0.135502
n	2.247040	-1.080586	-0.064505	h	-0.595474	-0.828608	-0.002067
c	4.572108	-1.645912	-0.133656	h	5.617482	-1.334350	-0.134218
c	4.249804	-3.039402	-0.203769	h	6.310840	-3.667126	-0.262528
c	2.855488	-3.373932	-0.195862	h	4.053301	-5.802304	-0.379106
c	1.887776	-2.412735	-0.127455	h	6.803659	-12.995226	-0.869397
c	5.279970	-4.028481	-0.274835	h	11.059203	-10.328121	-0.673415
c	5.076016	-5.413830	-0.358418	h	9.034381	-14.149923	-0.940917
c	6.114401	-6.368192	-0.420961	h	11.137889	-12.830319	-0.845571
c	5.858406	-7.742723	-0.511230	h	4.392256	2.516364	-1.158690
c	6.795134	-8.777927	-0.576594	h	5.443108	1.078022	-1.242962
s	8.561692	-8.546048	-0.536680	h	3.902925	1.111447	-2.149108
c	8.891275	-10.306856	-0.681908	h	5.453125	0.925852	1.294369
c	7.687551	-11.029863	-0.735297	h	4.401465	2.364369	1.388669
c	6.460055	-10.193768	-0.680329	h	3.918162	0.851176	2.207449
c	10.140581	-10.916015	-0.718956	h	2.532466	-4.412054	-0.242318
c	10.174815	-12.317138	-0.814158	h	0.824649	-2.632620	-0.119041
c	8.983585	-13.061101	-0.868192	h	7.149885	-6.013241	-0.399354
c	7.735792	-12.428254	-0.829623	h	4.814134	-8.077646	-0.538121

Cartesian coordinates of COSMO optimized  $S_0$  state AI-SO(4) in MeOH:

C	7.639216	-12.429535	-1.011998	C	10.068693	-10.977636	-0.768772
C	7.617650	-11.041158	-0.855498	C	10.076409	-12.372261	-0.926506
C	8.829469	-10.348849	-0.737761	C	8.875533	-13.086805	-1.046448



C	6.406218	-10.166256	-0.796633	O	8.982415	-8.121186	0.768675
C	6.764385	-8.781953	-0.629664	O	5.235164	-10.613606	-0.885029
S	8.516358	-8.597504	-0.551672	H	2.181066	3.308728	0.590175
C	5.856103	-7.715587	-0.538605	H	-0.308997	3.455348	0.526334
C	6.119969	-6.362743	-0.375806	H	-1.694992	1.409489	0.250640
C	5.079245	-5.414646	-0.302969	H	-0.622042	-0.835508	0.027533
C	5.271299	-4.056057	-0.141083	H	5.593503	-1.397106	0.170656
C	4.225081	-3.085015	-0.066226	H	6.294128	-3.676550	-0.062741
C	4.547918	-1.703593	0.100050	H	4.060118	-5.803613	-0.382898
C	3.560291	-0.750726	0.173779	H	6.703680	-12.980895	-1.105002
N	2.232185	-1.124842	0.083902	H	10.997745	-10.416114	-0.675322
C	1.869528	-2.434854	-0.074128	H	8.906652	-14.169684	-1.168700
C	2.831790	-3.409005	-0.148197	H	11.028180	-12.902314	-0.955873
C	1.381530	0.015126	0.186997	H	4.418692	2.497688	-0.718437
C	2.186814	1.151509	0.344130	H	5.486893	1.070337	-0.811231
C	3.661103	0.758056	0.350936	H	3.990618	1.132791	-1.792738
C	1.581122	2.403473	0.467287	H	5.398378	0.787020	1.678632
C	0.177869	2.482777	0.431128	H	4.326726	2.205107	1.836300
C	-0.606626	1.327273	0.274835	H	3.837205	0.636066	2.542925
C	-0.013213	0.062210	0.148802	H	2.499270	-4.439961	-0.271705
C	4.437717	1.402281	-0.823495	H	0.803310	-2.645183	-0.133158
C	4.347590	1.114004	1.692935	H	7.149886	-6.005687	-0.300038
O	9.062812	-7.845368	-1.702127	H	4.806201	-8.021826	-0.608418

Cartesian coordinates of COSMO optimized S<sub>1</sub> state Al-SO(4) in MeOH:

C	-3.890585	0.302786	5.788583	C	5.979984	-1.098950	-6.801756
C	-2.678006	0.247921	5.083164	C	5.308429	-1.221181	-8.033495
C	-1.472317	0.323914	5.806170	C	3.906928	-1.122259	-8.103475
C	-1.418967	0.450916	7.187179	C	3.138294	-0.909041	-6.951020
C	-2.641918	0.505511	7.877726	C	6.423865	-1.934553	-3.642771
C	-3.859098	0.431430	7.180455	C	6.539073	0.566828	-4.011038
S	-0.082203	0.230897	4.690892	O	-3.463359	0.038182	2.797368
C	-1.106420	0.099570	3.245530	O	0.702332	-0.997689	4.922005
C	-2.512635	0.118818	3.623193	O	0.692587	1.486999	4.701001
C	-0.630547	0.004387	1.943262	H	7.069657	-1.174057	-6.760534
C	0.711435	-0.014302	1.506650	H	5.882323	-1.394969	-8.945844
C	1.024763	-0.106873	0.149827	H	3.404584	-1.215635	-9.068507
C	2.332675	-0.154640	-0.357633	H	2.050912	-0.833798	-7.004691
C	2.659322	-0.275309	-1.738381	H	4.831945	-0.349049	-1.437399
C	1.653516	-0.313189	-2.767977	H	3.168007	-0.115448	0.347941
C	1.978712	-0.472199	-4.086040	H	0.183003	-0.159503	-0.543446
N	3.301666	-0.606219	-4.445431	H	-4.834803	0.245094	5.247627
C	4.325554	-0.554684	-3.497347	H	-0.469432	0.506772	7.718516
C	4.023920	-0.386596	-2.171658	H	-4.796185	0.475452	7.736192
C	3.830252	-0.801077	-5.738841	H	-2.641358	0.606054	8.962487
C	5.231732	-0.884092	-5.644555	H	7.366105	-2.074409	-4.193036
C	5.670166	-0.703818	-4.192647	H	6.663290	-1.784752	-2.579052

H	5.817588	-2.847899	-3.742286	H	0.596821	-0.210559	-2.522306
H	6.782725	0.707239	-2.946942	H	1.243503	-0.500668	-4.887456
H	7.479944	0.451715	-4.570300	H	1.526084	0.039716	2.233056
H	6.017977	1.464674	-4.376681	H	-1.411604	-0.061165	1.179364

Cartesian coordinates of COSMO optimized  $S_0$  state AI-BA(4) in  $C_6H_6$ :

C	0.171884	-0.689805	-7.897467	H	-4.734973	0.792477	-7.666667
C	-1.002257	-0.639937	-7.147949	H	-4.890444	0.813960	-5.891455
C	-2.276839	-0.597248	-7.727572	H	-3.524745	1.656550	-6.676406
C	-2.392972	-0.607263	-9.115579	H	-5.019158	-1.705070	-5.861324
C	-1.226393	-0.658930	-9.895763	H	-4.867157	-1.737707	-7.637476
C	0.037975	-0.698584	-9.291588	H	-3.748155	-2.697239	-6.628734
C	-3.347008	-0.536095	-6.642487	H	0.292981	-0.625491	-2.710653
C	-2.489973	-0.561049	-5.381742	H	0.863295	-0.685384	-5.128013
N	-1.146765	-0.619626	-5.735800	H	-2.763770	-0.447500	1.009003
C	-0.162922	-0.641539	-4.775775	H	-5.758539	-0.356141	0.209563
C	-0.502261	-0.607730	-3.454604	C	-6.725042	-0.290626	2.515199
C	-1.871652	-0.549138	-3.020771	N	-7.116684	-0.257500	3.868058
C	-2.858162	-0.527819	-4.066626	C	-6.228427	-0.271105	4.951236
C	-2.160628	-0.515248	-1.639664	N	-4.868089	-0.320829	4.655964
C	-3.429418	-0.458282	-1.042021	C	-4.318526	-0.357509	3.349892
C	-3.628543	-0.427883	0.344359	O	-7.590333	-0.276677	1.624366
C	-4.909910	-0.374581	0.902701	C	-8.557166	-0.205055	4.160065
C	-5.286743	-0.341176	2.254225	O	-6.619959	-0.241162	6.124671
C	-4.170769	0.767678	-6.722504	C	-3.951634	-0.335050	5.807413
C	-4.301492	-1.748916	-6.693950	O	-3.079881	-0.400514	3.218791
H	-3.372285	-0.574712	-9.595749	H	-8.672901	-0.185585	5.247168
H	-1.304368	-0.667307	-10.982760	H	-8.995515	0.696348	3.712245
H	0.933983	-0.736487	-9.911233	H	-9.055182	-1.087615	3.737589
H	1.155164	-0.719754	-7.429258	H	-2.935664	-0.374403	5.404468
H	-3.919227	-0.482563	-3.823771	H	-4.089532	0.571730	6.410683
H	-1.300868	-0.535591	-0.965144	H	-4.148764	-1.213428	6.435328
H	-4.321652	-0.437115	-1.678161				

Cartesian coordinates of COSMO optimized  $S_1$  state AI-BA(4) in  $C_6H_6$ :

C	0.172576	-0.690649	-7.906905	C	-1.842942	-0.550630	-3.035664
C	-1.003007	-0.640373	-7.150212	C	-2.843871	-0.528560	-4.069460
C	-2.281913	-0.597945	-7.732940	C	-2.157236	-0.515184	-1.640471
C	-2.399555	-0.607918	-9.118700	C	-3.431150	-0.457889	-1.062387
C	-1.232196	-0.659775	-9.902777	C	-3.635595	-0.427343	0.341217
C	0.033922	-0.699676	-9.299203	C	-4.913815	-0.374521	0.901915
C	-3.349967	-0.535807	-6.645588	C	-5.282511	-0.341290	2.267799
C	-2.489504	-0.561288	-5.387786	C	-4.173526	0.769042	-6.726102
N	-1.140198	-0.619689	-5.750581	C	-4.308297	-1.746522	-6.696856
C	-0.139166	-0.642352	-4.789378	H	-3.379687	-0.574987	-9.597628
C	-0.483175	-0.608168	-3.462898	H	-1.311495	-0.667749	-10.989598

H	0.928296	-0.737664	-9.921461	N	-7.120320	-0.258165	3.875633
H	1.156276	-0.720454	-7.440081	C	-6.238399	-0.270945	4.961940
H	-3.902079	-0.482920	-3.814238	N	-4.876564	-0.320113	4.670799
H	-1.304686	-0.535083	-0.955690	C	-4.320694	-0.356741	3.369657
H	-4.318597	-0.437031	-1.701909	O	-7.578684	-0.276592	1.628717
H	-4.737889	0.794359	-7.670540	C	-8.562824	-0.207060	4.153890
H	-4.892859	0.816969	-5.894632	O	-6.635625	-0.240599	6.133296
H	-3.526179	1.656973	-6.680938	C	-3.965145	-0.333988	5.825574
H	-5.026044	-1.701142	-5.864095	O	-3.081082	-0.398873	3.236584
H	-4.874062	-1.733991	-7.640493	H	-8.690597	-0.186954	5.239228
H	-3.757621	-2.696287	-6.631882	H	-8.996340	0.693182	3.699142
H	0.313128	-0.624759	-2.718905	H	-9.054569	-1.090131	3.725444
H	0.883731	-0.686201	-5.147933	H	-2.947383	-0.372548	5.428278
H	-2.769311	-0.446561	1.005553	H	-4.107410	0.572330	6.427923
H	-5.765577	-0.356520	0.215291	H	-4.165255	-1.212491	6.452266
C	-6.721694	-0.291051	2.529164				

Cartesian coordinates of COSMO optimized  $S_0$  state AI-BA(4) in MeOH:

C	0.194560	-0.684869	-7.880888	H	-4.723858	0.777684	-7.696681
C	-0.989907	-0.638021	-7.149515	H	-4.896601	0.792353	-5.922363
C	-2.259162	-0.599836	-7.738119	H	-3.527911	1.648682	-6.691701
C	-2.362371	-0.611031	-9.128471	H	-5.009503	-1.715081	-5.890181
C	-1.185689	-0.659552	-9.893246	H	-4.841765	-1.755759	-7.665355
C	0.074514	-0.695160	-9.276364	H	-3.726680	-2.706984	-6.642138
C	-3.338024	-0.542953	-6.663648	H	0.261941	-0.613888	-2.701769
C	-2.492077	-0.561849	-5.399465	H	0.853557	-0.674765	-5.119269
N	-1.150376	-0.616050	-5.733427	H	-2.796941	-0.448125	0.979562
C	-0.174901	-0.633897	-4.774779	H	-5.789649	-0.351525	0.204540
C	-0.527109	-0.599599	-3.451972	C	-6.727801	-0.284819	2.545862
C	-1.896017	-0.545125	-3.043325	N	-7.110284	-0.252400	3.902040
C	-2.874524	-0.527741	-4.083521	C	-6.209956	-0.271480	4.967502
C	-2.201861	-0.510772	-1.649938	N	-4.858447	-0.327007	4.657865
C	-3.467797	-0.455718	-1.072575	C	-4.334424	-0.363543	3.341011
C	-3.671557	-0.426638	0.328280	O	-7.613040	-0.263440	1.662572
C	-4.937319	-0.372961	0.892574	C	-8.548904	-0.194904	4.208765
C	-5.306234	-0.340796	2.264326	O	-6.588414	-0.240289	6.152349
C	-4.169174	0.756625	-6.746993	C	-3.923117	-0.347888	5.795441
C	-4.285360	-1.762168	-6.716715	O	-3.089152	-0.412078	3.195786
H	-3.336200	-0.582260	-9.619384	H	-8.658447	-0.175785	5.295774
H	-1.251422	-0.668544	-10.981107	H	-8.988019	0.710438	3.770566
H	0.976477	-0.730723	-9.887113	H	-9.054245	-1.077023	3.795306
H	1.171594	-0.711314	-7.399973	H	-2.912895	-0.391688	5.380906
H	-3.937374	-0.485153	-3.848794	H	-4.043064	0.560237	6.399707
H	-1.343836	-0.529961	-0.973120	H	-4.111334	-1.228131	6.423067
H	-4.355501	-0.434372	-1.714548				

Cartesian coordinates of COSMO optimized  $S_1$  state AI-BA(4) in MeOH:

C	0.191287	-0.684868	-7.893279	H	-4.730140	0.775778	-7.707985
C	-0.992596	-0.637880	-7.149580	H	-4.904147	0.796518	-5.932898
C	-2.266607	-0.600594	-7.743555	H	-3.534357	1.648621	-6.704599
C	-2.372123	-0.612002	-9.131324	H	-5.020488	-1.713089	-5.899263
C	-1.196363	-0.660243	-9.902853	H	-4.852408	-1.748747	-7.675276
C	0.065624	-0.695408	-9.287199	H	-3.740335	-2.706005	-6.654328
C	-3.344785	-0.542843	-6.667207	H	0.291398	-0.614819	-2.714283
C	-2.496721	-0.562057	-5.401610	H	0.874738	-0.674843	-5.136339
N	-1.144119	-0.615753	-5.750164	H	-2.782116	-0.449134	0.968684
C	-0.150611	-0.634025	-4.783873	H	-5.792902	-0.350196	0.225554
C	-0.501140	-0.600406	-3.461879	C	-6.724916	-0.284448	2.554386
C	-1.870228	-0.546511	-3.044034	N	-7.115635	-0.251947	3.899794
C	-2.865666	-0.528902	-4.086933	C	-6.223753	-0.271259	4.974061
C	-2.185222	-0.511458	-1.658325	N	-4.866978	-0.326158	4.675661
C	-3.471234	-0.455906	-1.075974	C	-4.325888	-0.362599	3.370912
C	-3.660782	-0.427247	0.320713	O	-7.591667	-0.265451	1.655852
C	-4.937039	-0.372287	0.906413	C	-8.558122	-0.194799	4.188860
C	-5.292078	-0.340308	2.274811	O	-6.612343	-0.241594	6.154205
C	-4.176229	0.756592	-6.757247	C	-3.948216	-0.346468	5.827783
C	-4.296079	-1.759115	-6.726044	O	-3.082573	-0.410698	3.227760
H	-3.347446	-0.583237	-9.619960	H	-8.683180	-0.175571	5.273841
H	-1.265278	-0.669154	-10.990486	H	-8.990002	0.709932	3.742392
H	0.965845	-0.730759	-9.901040	H	-9.055821	-1.077044	3.766503
H	1.170344	-0.711073	-7.416469	H	-2.931098	-0.389833	5.431392
H	-3.926458	-0.486938	-3.841581	H	-4.080939	0.561461	6.429549
H	-1.334514	-0.529549	-0.971566	H	-4.148617	-1.226474	6.451903
H	-4.357023	-0.434873	-1.717692				

Cartesian coordinates of COSMO optimized  $S_0$  state AI-TBA(4) in  $C_6H_6$ :

C	0.186144	-0.685566	-7.889256	C	-4.170206	0.759209	-6.736185
C	-0.990659	-0.635197	-7.144301	C	-4.284727	-1.758288	-6.698370
C	-2.263474	-0.599245	-7.728270	H	-3.352886	-0.589065	-9.600103
C	-2.375182	-0.615681	-9.116534	H	-1.280236	-0.678193	-10.979715
C	-1.205765	-0.666163	-9.892255	H	0.954590	-0.737396	-9.900841
C	0.056706	-0.699981	-9.283927	H	1.167944	-0.711515	-7.417741
C	-3.337708	-0.538845	-6.648010	H	-3.924960	-0.481083	-3.836885
C	-2.484618	-0.552673	-5.384385	H	-1.337790	-0.534056	-0.958153
N	-1.141080	-0.609771	-5.731488	H	-4.349766	-0.429051	-1.706775
C	-0.163992	-0.631135	-4.765901	H	-4.730906	0.776641	-7.682864
C	-0.512240	-0.598753	-3.445939	H	-4.893665	0.802847	-5.908182
C	-1.883941	-0.542654	-3.022400	H	-3.530693	1.653081	-6.690427
C	-2.862317	-0.521689	-4.072120	H	-5.007439	-1.715066	-5.869979
C	-2.189067	-0.511956	-1.643021	H	-4.845852	-1.752804	-7.644783
C	-3.465170	-0.454743	-1.061940	H	-3.727509	-2.703962	-6.627439
C	-3.673078	-0.429402	0.325231	H	0.278665	-0.616087	-2.697385
C	-4.950106	-0.374959	0.887254	H	0.864415	-0.674807	-5.111725
C	-5.308981	-0.345930	2.248391	H	-2.808473	-0.454075	0.988332

H	-5.804861	-0.350513	0.203540	C	-3.863629	-0.354680	5.740480
C	-6.726583	-0.289021	2.545092	O	-3.101098	-0.420792	3.153292
N	-7.099298	-0.254855	3.911806	H	-8.710021	-0.178527	5.238258
C	-6.198644	-0.270886	4.971385	H	-8.963273	0.707566	3.688792
N	-4.853424	-0.330730	4.649426	H	-9.031379	-1.075432	3.707113
C	-4.332146	-0.369964	3.318371	H	-2.877354	-0.400924	5.270711
O	-7.608146	-0.269075	1.670110	H	-3.961221	0.550256	6.353248
C	-8.551489	-0.196243	4.156481	H	-4.032522	-1.231271	6.378556
S	-6.690801	-0.220805	6.586556				

Cartesian coordinates of COSMO optimized  $S_0$  state AI-TBA(4) in MeOH

C	0.199719	-0.682575	-7.880090	H	-4.718626	0.782253	-7.701620
C	-0.986121	-0.635750	-7.151092	H	-4.887870	0.801636	-5.926818
C	-2.254511	-0.598319	-7.741295	H	-3.518003	1.652139	-6.701008
C	-2.355645	-0.610952	-9.131732	H	-5.007051	-1.709231	-5.893607
C	-1.177656	-0.659683	-9.894360	H	-4.842381	-1.748978	-7.669279
C	0.081756	-0.693928	-9.275812	H	-3.727274	-2.703304	-6.648306
C	-3.334644	-0.540087	-6.668679	H	0.254367	-0.618692	-2.700256
C	-2.491139	-0.560595	-5.403766	H	0.852628	-0.675455	-5.117504
N	-1.149708	-0.614655	-5.734381	H	-2.806265	-0.451584	0.971195
C	-0.176585	-0.634718	-4.775230	H	-5.797344	-0.357441	0.198405
C	-0.532402	-0.603207	-3.452463	C	-6.716985	-0.292931	2.562023
C	-1.900588	-0.547693	-3.048088	N	-7.095495	-0.255156	3.928617
C	-2.876353	-0.528758	-4.087596	C	-6.196148	-0.268919	4.981759
C	-2.210235	-0.513274	-1.652463	N	-4.855988	-0.327802	4.662753
C	-3.475119	-0.458044	-1.082050	C	-4.342850	-0.366842	3.326588
C	-3.681618	-0.429885	0.321955	O	-7.610975	-0.277667	1.687524
C	-4.945186	-0.377817	0.884881	C	-8.548681	-0.195969	4.171104
C	-5.310992	-0.345917	2.262896	S	-6.690745	-0.215684	6.608210
C	-4.162336	0.761929	-6.752870	C	-3.862967	-0.351207	5.752141
C	-4.284495	-1.757386	-6.721502	O	-3.104078	-0.416549	3.162369
H	-3.328616	-0.583483	-9.624196	H	-8.711973	-0.175160	5.251026
H	-1.242099	-0.670163	-10.982482	H	-8.959690	0.708272	3.704523
H	0.984590	-0.729318	-9.885364	H	-9.028119	-1.077975	3.727994
H	1.176088	-0.708292	-7.397979	H	-2.876302	-0.397729	5.284857
H	-3.939562	-0.485574	-3.854560	H	-3.955809	0.555656	6.362327
H	-1.353190	-0.532279	-0.974460	H	-4.027612	-1.229278	6.388819
H	-4.360235	-0.435362	-1.725471				