

Supporting Information

Photophysics of Faecal Pigments Stercobilin and Urobilin in Aliphatic Alcohols:

Introduction of a Sensitive Method for their Detection using Solvent Phase Extraction and Fluorometry

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Figure S6. Extraction of FP-Zn(II) in 1-hexanol and 1-butanol (Comparison of absorption and fluorescence)

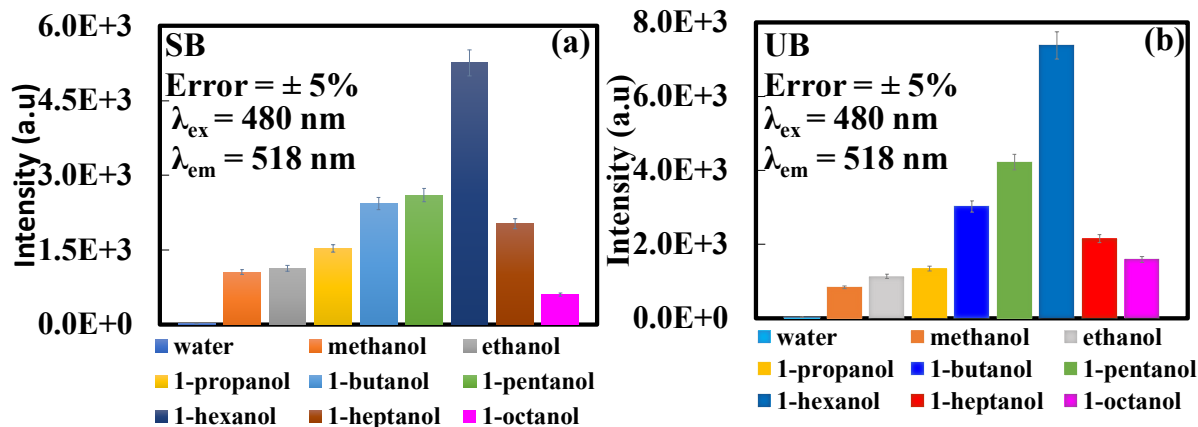
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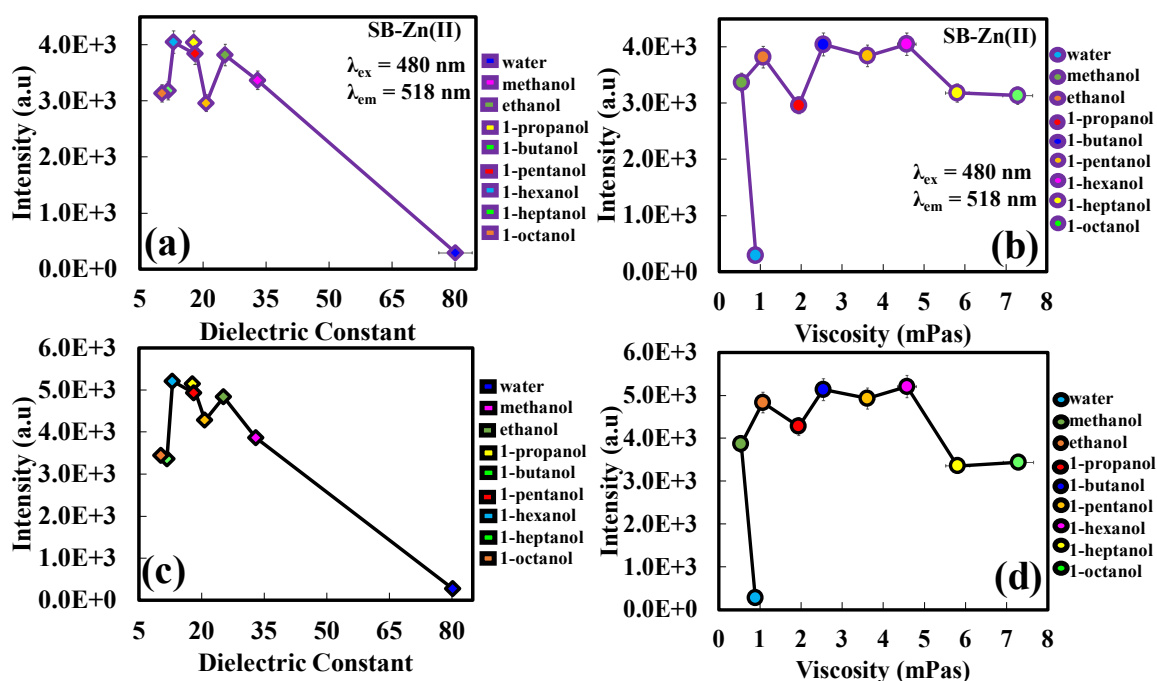
Figure S10. Theoretically predicted transition energies (TDDFT) of FPs and their ground state coordinates.

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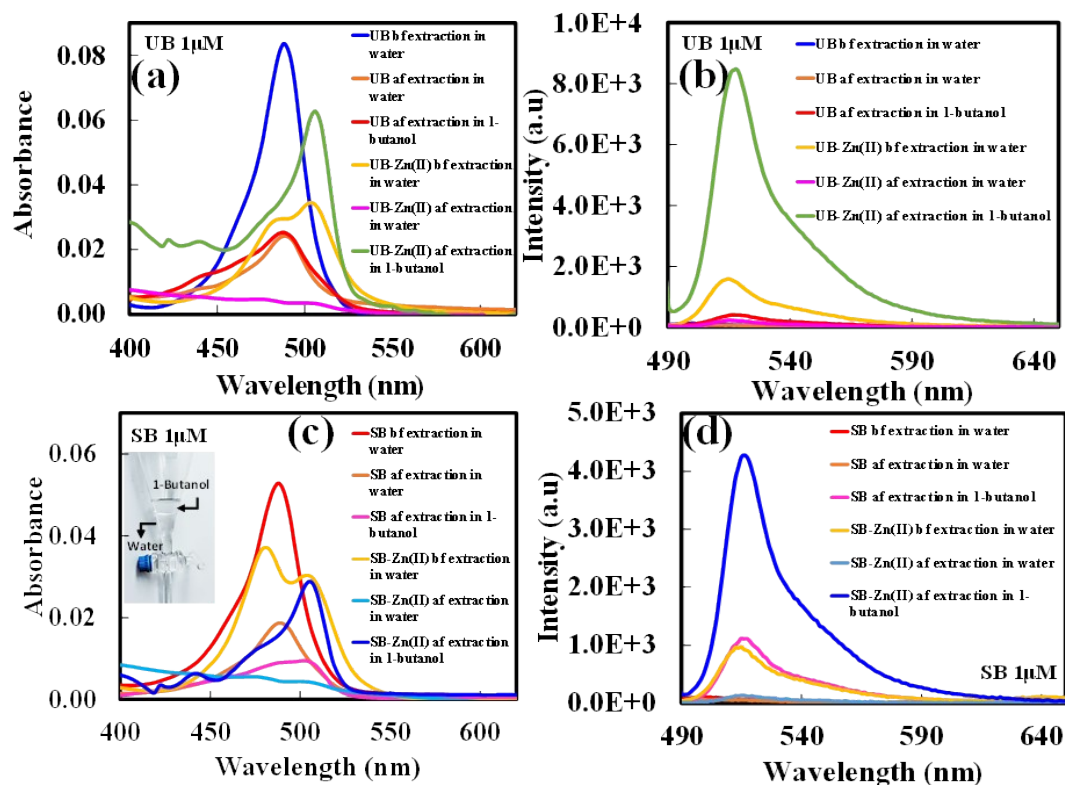
24 **Figure S1.** Emission intensity at 518 nm of excitation 480 nm of FPs (1μM) in various
 25 primary alcohol (a) SB (1μM) and (b) UB (1μM)



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27 **Figure S2.** Emission intensity at 518 nm of excitation 480 nm of FPs (1μM)-Zn(II) (20 mM)
 28 in various primary alcohol (a) Correlation of fluorescence Intensity of SB-Zn(II) with
 29 dielectric constant, (b) Correlation of fluorescence Intensity of SB-Zn(II) with viscosity, (c)
 30 Correlation of fluorescence Intensity of UB-Zn(II) with dielectric constant and (d) Correlation
 31 of fluorescence Intensity of UB-Zn(II) with viscosity.

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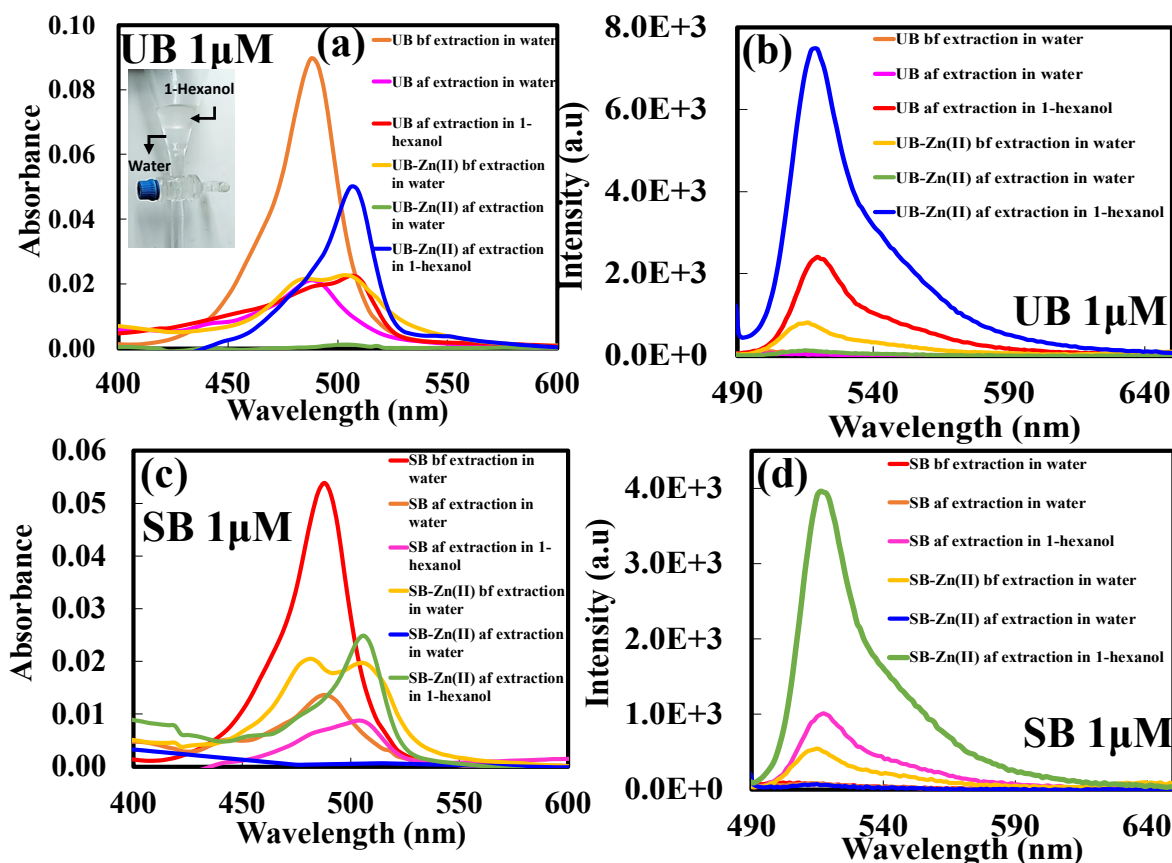
33 **Figure S3.** Extraction of FP-Zn(II) in 1-butanol

34 (a) Steady-state absorption spectra of UB (1 μ M) and UB (1 μ M) -Zn(II) (20 mM) in water
 35 before and after extract with 1-butanol (b) Steady-state emission spectra of UB (1 μ M) and
 36 UB (1 μ M) -Zn(II) (20 mM) in water before and after extract with 1-butanol at excitation
 37 wavelength of 480 nm, (c) Steady-state absorption spectra of SB (1 μ M) and SB (1 μ M) -
 38 Zn(II) (20 mM) in water before and after extract with 1-butanol (d) Steady-state emission
 39 spectra of SB(1 μ M) and SB (1 μ M) -Zn(II) (20 mM) in water before and after extract with 1-
 40 butanol at excitation wavelength of 480 nm, Instrument parameters were kept constant at IT =
 41 1 sec and CCD sensitivity kept high.

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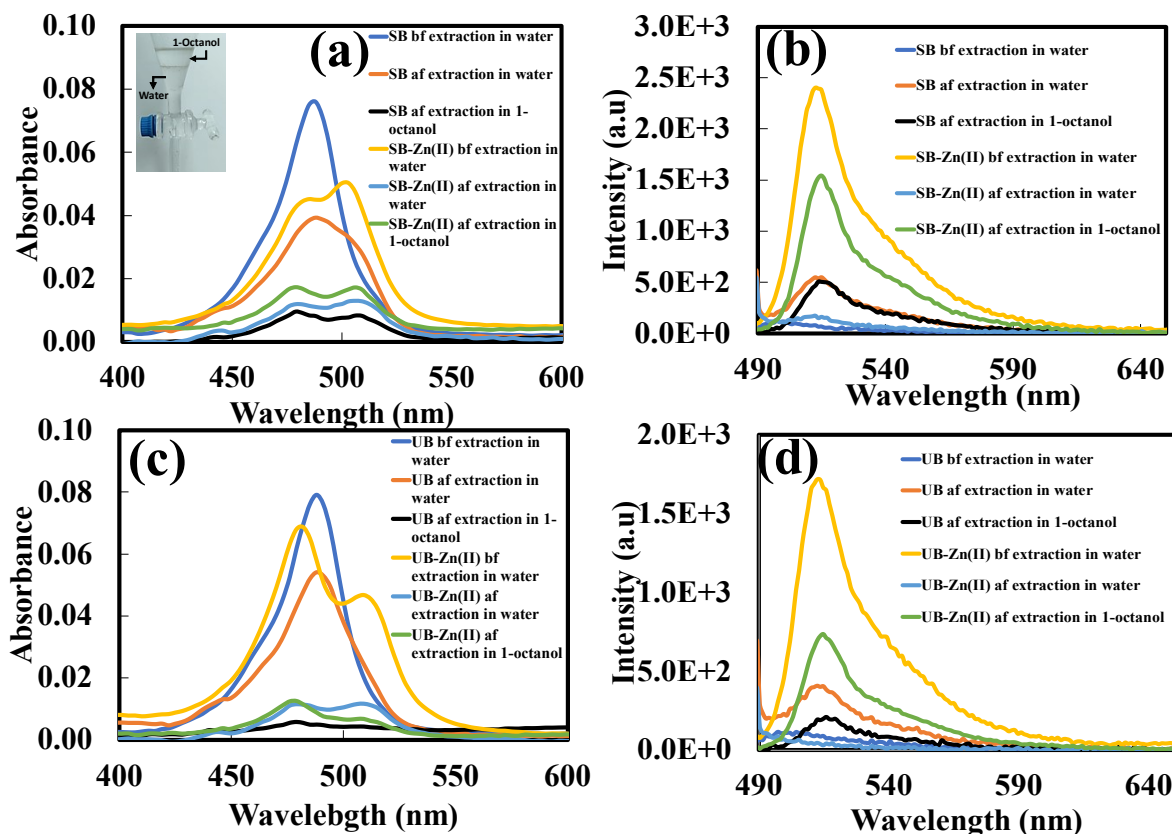


44

45 **Figure S4.** Extraction of FP-Zn(II) in 1-hexanol

46 (a) Steady-state absorption spectra of UB (1 μM) and UB (1 μM)-Zn(II) (20mM) in water
 47 before and after extract with 1-hexanol (b) Steady-state emission spectra of UB (1 μM) and
 48 UB (1 μM)-Zn(II) (20 mM) in water before and after extract with 1-hexanol with excitation
 49 wavelength at 480 nm, (c)) Steady-state absorption spectra of SB (1 μM) and SB (1 μM) -
 50 Zn(II) (20 mM) in water before and after extract with 1-hexanol (d) Steady-state emission
 51 spectra of SB (1 μM) and SB(1 μM)-Zn(II) (20 mM) in water before and after extract with 1-
 52 hexanol with excitation wavelength at 480 nm, Instrument parameters were kept constant at IT
 53 = 1 sec and CCD sensitivity kept high.

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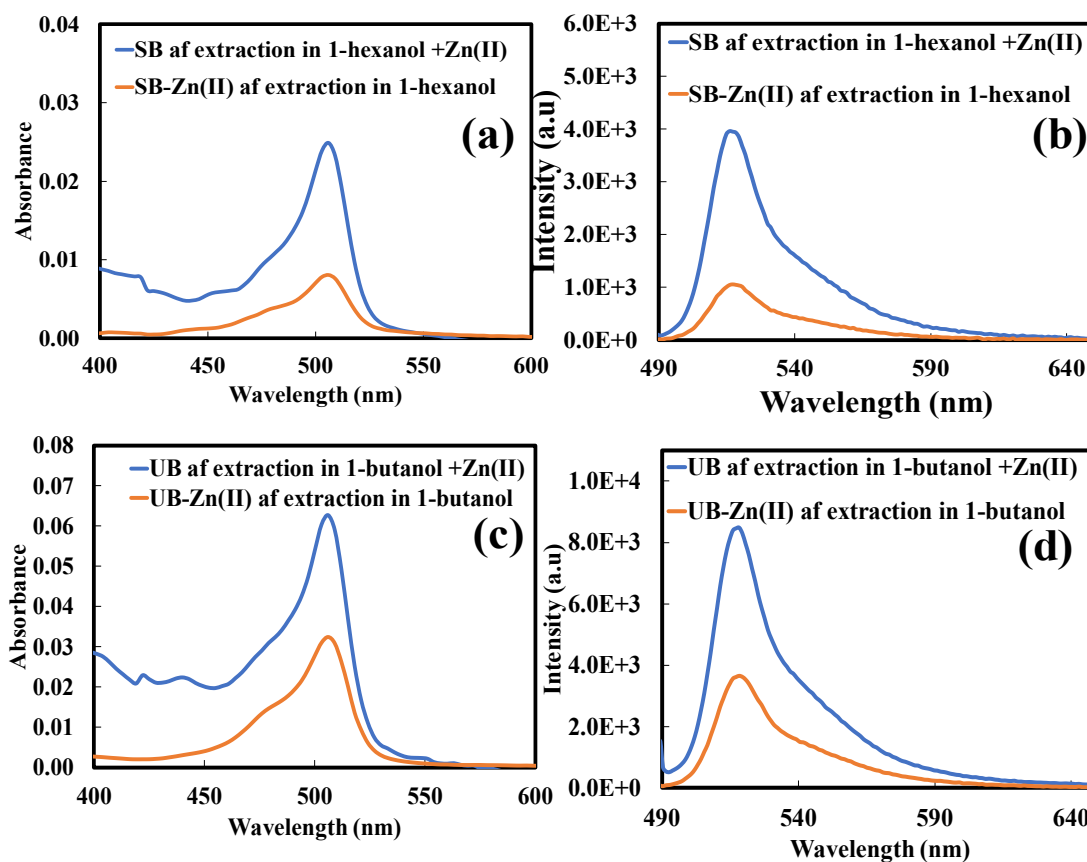
54

55 **Figure S5.** Extraction of FP-Zn(II) in 1-octanol

56 (a) Steady-state absorption spectra of SB (1 μM) and SB (1 μM)-Zn(II) (20 mM) in water
 57 before and after extract with 1-hexanol (b) Steady-state emission spectra of SB (1 μM) and
 58 SB (1 μM)-Zn(II) (20 mM) in water before and after extract with 1-hexanol with excitation
 59 wavelength at 480 nm, (c) Steady-state absorption spectra of UB (1 μM) and UB (1 μM) -
 60 Zn(II) (20 mM) in water before and after extract with 1-hexanol (d) Steady-state emission
 61 spectra of UB (1 μM) and UB (1 μM)-Zn(II) (20 mM) in water before and after extract with
 62 1-hexanol with excitation wavelength at 480 nm, Instrument parameters were kept constant at
 63 IT = 1 sec and CCD kept high.

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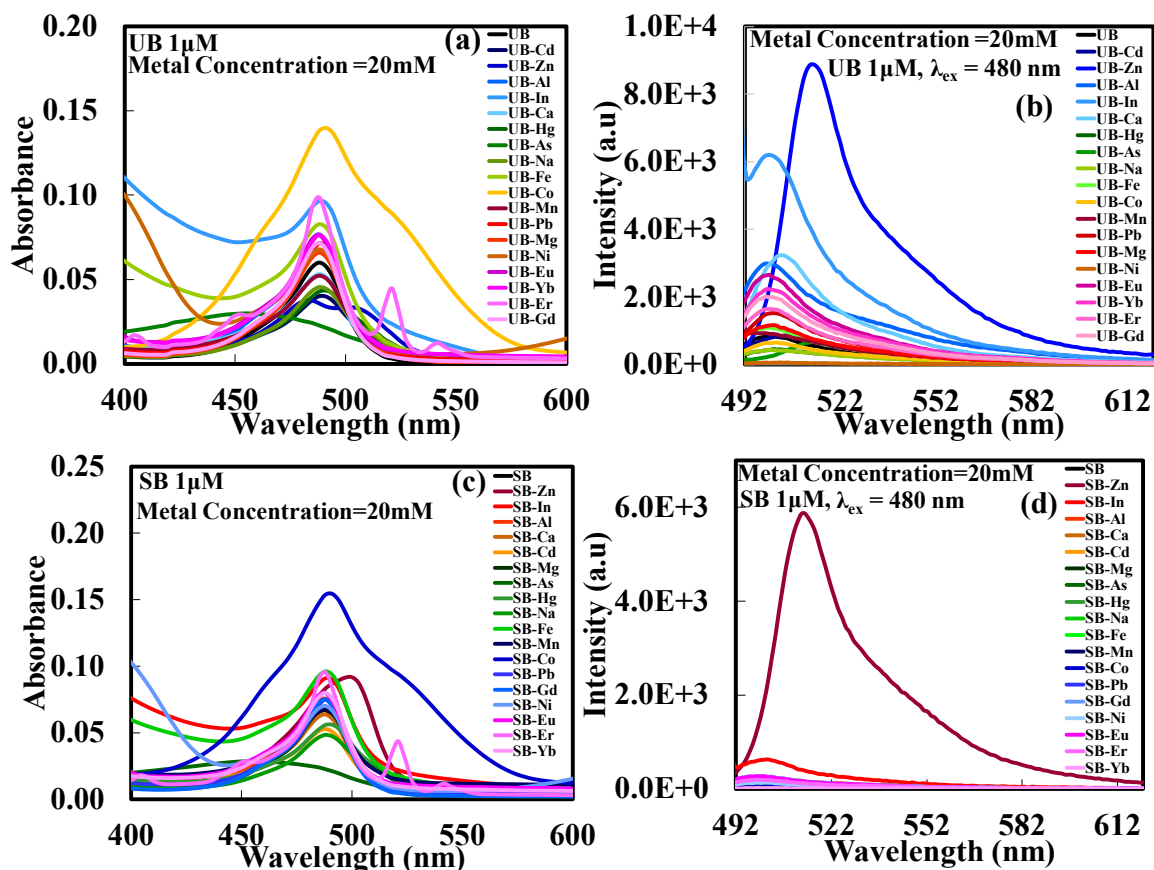
65

Fig

66 **ure S6.** Extraction of FP-Zn(II) in 1-hexanol and 1-butanol (Comparison of absorption and
 67 fluorescence) (a) Steady-state absorption of SB-Zn(II) by 1-hexanol, (b) Steady-state emission
 68 of SB-Zn(II) by 1-Hexanol, (c) Steady-state absorption of SB-Zn(II) by 1-butanol, (b)
 69 Steady-state emission of SB-Zn(II) by 1-butanol

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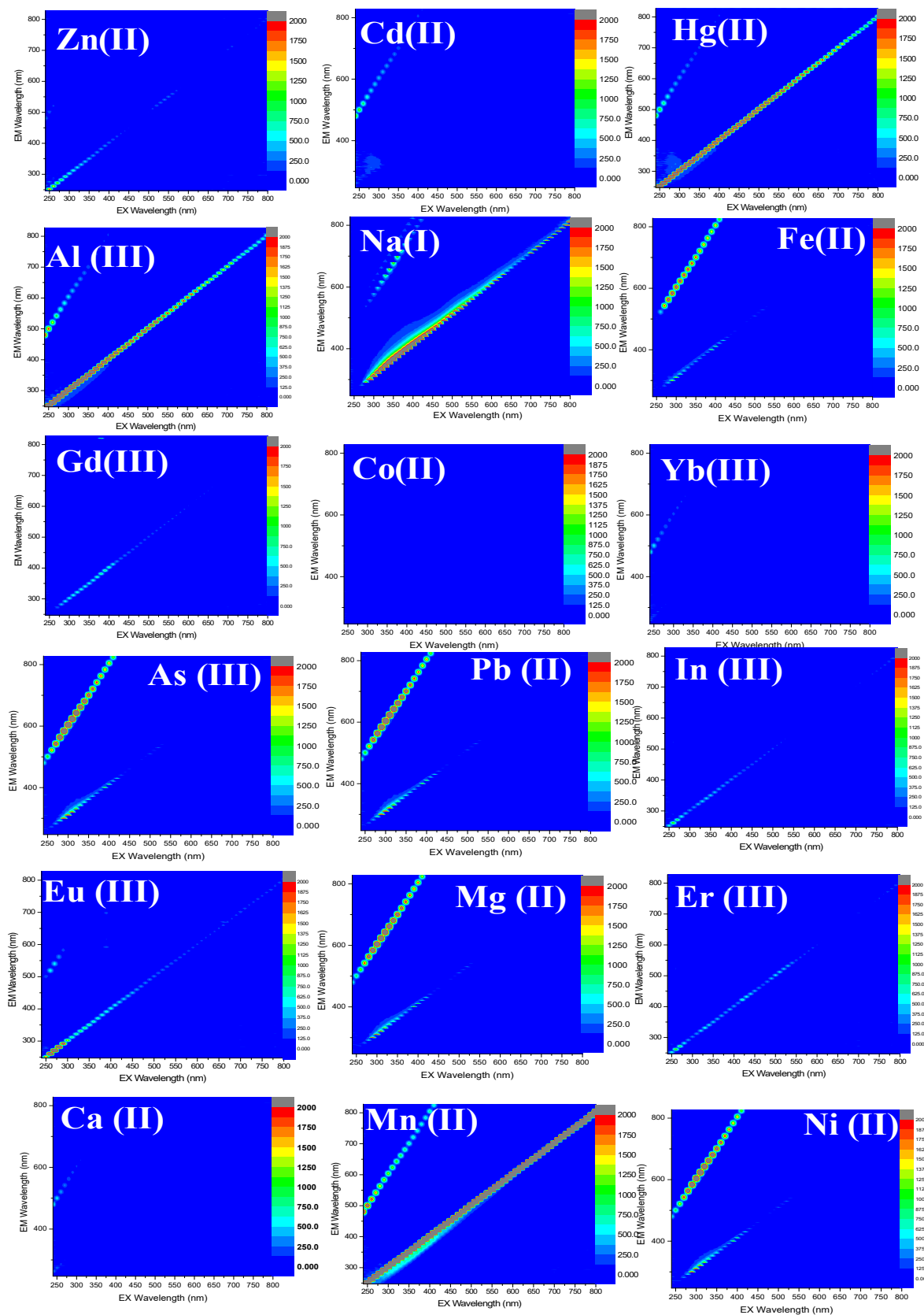


71

72 **Figure S7.** a) Steady-state absorption spectra of UB (1 μ M) and metal ions of (20 mM)
 73 concentration in water (b) Steady-state emission spectra of UB (1 μ M) and metal ions of (20
 74 mM) concentration in water at an excitation wavelength of 480 nm, (c) Steady-state absorption
 75 spectra of SB (1 μ M) and metal ions of (20 mM) concentration in water (b) Steady-state
 76 emission spectra of SB (1 μ M) and metal ions of (20 mM) concentration in water at an
 77 excitation wavelength of 480 nm, Instrument parameters were kept constant at IT = 0.1 sec and
 78 CCD sensitivity kept high.

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81 **Figure S8.** EEMF of various metal ions in Mili Q water.

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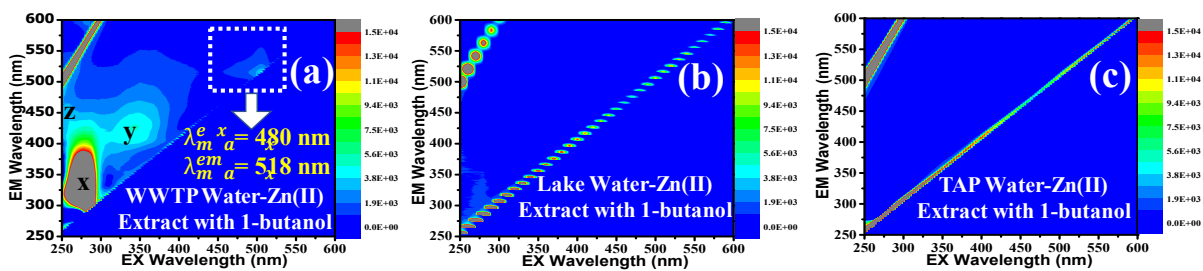


Figure S9. EEMF of various real water samples (a) WWTP water extracted with 1-butanol in the presence of 20 mM Zn(II), (b) lake water extracted with 1-butanol in the presence of 20 mM Zn(II), (c) tap water extracted with 1-butanol in the presence of 20 mM Zn(II)

SB Implicit 1-hexanol

Charge = 0, Multiplicity = 1

TDDFT

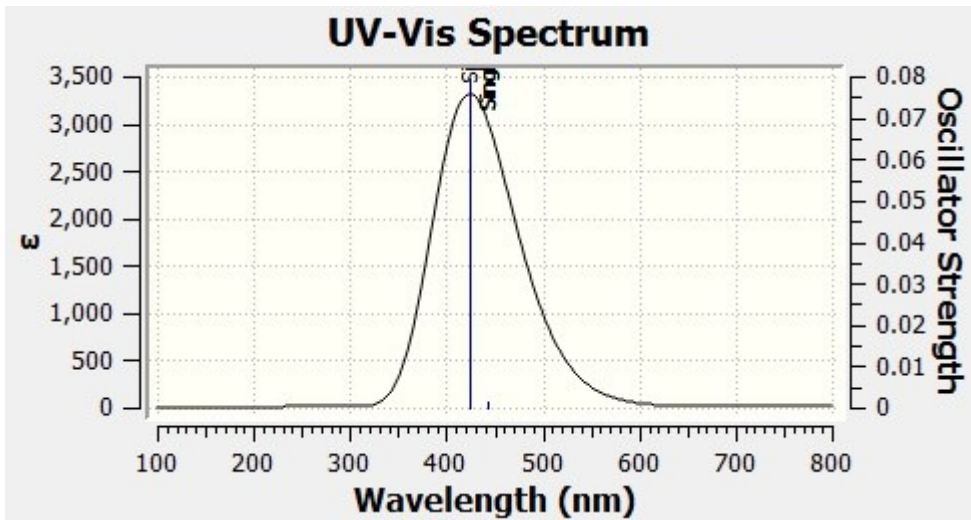


Figure S10a TDDFT of SB Implicit model in 1-hexanol. Wavelength maximum = 443.05 (nm)

Cartesian coordinates of the optimized ground state geometry

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

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95	-----					
96	1	6	0	-2.454005	-2.986526	1.208388
97	2	6	0	-3.324999	-4.107763	0.855517
98	3	6	0	-4.511670	-3.546200	0.392427
99	4	6	0	-4.339095	-2.095704	0.468326
100	5	7	0	-3.046227	-1.796299	0.983449
101	6	6	0	-5.094549	0.280509	0.147317
102	7	6	0	-6.049137	1.316689	-0.080554
103	8	6	0	-5.397036	2.557690	0.153285
104	9	6	0	-4.047073	2.271608	0.501006
105	10	7	0	-3.893800	0.907782	0.494357
106	11	6	0	-0.140986	-0.317578	3.624366
107	12	6	0	0.915788	-1.251418	4.075608
108	13	6	0	0.423830	-2.589578	3.819192
109	14	6	0	-0.955079	-2.481151	3.210028
110	15	7	0	-1.212305	-1.034252	3.181179
111	16	8	0	-0.075431	0.958262	3.650001
112	17	6	0	-5.755423	-4.267132	-0.062940
113	18	6	0	-6.744486	-4.517529	1.122500
114	19	1	0	-5.495848	-5.234649	-0.506022
115	20	1	0	-6.273189	-3.691104	-0.840237

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116	21	1	0	-6.246124	-5.139171	1.875649
117	22	1	0	-7.027652	-3.570167	1.588877
118	23	6	0	-7.500773	1.111600	-0.438965
119	24	6	0	-8.405456	1.055744	0.816177
120	25	1	0	-7.629941	0.184886	-1.009991
121	26	1	0	-7.845980	1.922491	-1.090446
122	27	1	0	-8.103019	0.236074	1.480534
123	28	1	0	-8.309668	1.974926	1.409073
124	29	6	0	1.108529	-3.865649	4.100291
125	30	1	0	2.025053	-3.739004	4.684517
126	31	1	0	1.378327	-4.373239	3.163069
127	32	6	0	2.221144	-0.841532	4.641630
128	33	1	0	2.070332	0.092066	5.199542
129	34	1	0	2.590332	-1.586464	5.357999
130	35	6	0	-2.970833	-5.566546	0.992098
131	36	1	0	-3.751877	-6.207866	0.568997
132	37	1	0	-2.031079	-5.806683	0.475828
133	38	1	0	-2.842031	-5.858704	2.044349
134	39	6	0	-6.023730	3.927611	0.073256
135	40	1	0	-5.657099	4.494056	-0.791715
136	41	1	0	-7.112918	3.859071	-0.017940

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137	42	1	0	-5.807402	4.524251	0.969497
138	43	6	0	-1.062433	-3.098512	1.782971
139	44	6	0	-5.262989	-1.124853	0.104366
140	45	6	0	-8.008252	-5.215031	0.677351
141	46	6	0	-9.868884	0.870143	0.481590
142	47	8	0	-9.162059	-4.747556	0.709876
143	48	8	0	-10.643401	0.779242	1.626411
144	49	8	0	-7.756785	-6.488369	0.192524
145	50	8	0	-10.372126	0.801762	-0.654329
146	51	1	0	-8.581713	-6.935698	-0.107561
147	52	1	0	-0.339159	-2.579400	1.140600
148	53	1	0	-0.766304	-4.151364	1.835764
149	54	1	0	-6.232094	-1.471342	-0.248484
150	55	1	0	-1.683998	-2.982519	3.863849
151	56	1	0	0.439998	-4.543044	4.648566
152	57	6	0	-2.921286	3.182133	0.911783
153	58	6	0	-1.980144	3.364348	-2.407382
154	59	6	0	-2.730697	4.635345	-2.386287
155	60	6	0	-2.814382	4.979458	-0.980302
156	61	6	0	-2.101019	3.865310	-0.230544
157	62	7	0	-1.613124	2.883999	-1.237999

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158	63	6	0	-3.345575	6.230836	-0.391485
159	64	6	0	-3.226815	5.379120	-3.561151
160	65	1	0	-3.888541	4.741711	-4.162616
161	66	1	0	-3.778542	6.285646	-3.289537
162	67	1	0	-2.391708	5.670626	-4.212548
163	68	1	0	-4.060661	6.716788	-1.067989
164	69	1	0	-3.895001	5.993988	0.529598
165	70	6	0	-2.219507	7.243025	-0.041785
166	71	6	0	3.300465	-0.606341	3.551219
167	72	1	0	-1.669427	7.542613	-0.942597
168	73	1	0	-2.646383	8.144470	0.416258
169	74	1	0	-1.502289	6.810454	0.667189
170	75	1	0	3.508298	-1.532771	3.001411
171	76	1	0	2.974054	0.150433	2.828535
172	77	1	0	4.235636	-0.259612	4.009158
173	78	8	0	-1.703177	2.799983	-3.612745
174	79	1	0	-3.314829	3.975391	1.561302
175	80	1	0	-2.207652	2.605725	1.512603
176	81	1	0	-1.219932	4.299574	0.267768
177	82	6	0	2.453766	-2.986594	-1.208155
178	83	6	0	3.324734	-4.107846	-0.855281

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179	84	6	0	4.511451	-3.546311	-0.392279
180	85	6	0	4.338929	-2.095811	-0.468215
181	86	7	0	3.046019	-1.796376	-0.983223
182	87	6	0	5.094519	0.280388	-0.147413
183	88	6	0	6.049188	1.316524	0.080316
184	89	6	0	5.397148	2.557547	-0.153568
185	90	6	0	4.047125	2.271524	-0.501110
186	91	7	0	3.893764	0.907713	-0.494354
187	92	6	0	0.140987	-0.317707	-3.624312
188	93	6	0	-0.915022	-1.253724	-4.075088
189	94	6	0	-0.424746	-2.587466	-3.819512
190	95	6	0	0.954960	-2.481306	-3.209880
191	96	7	0	1.212296	-1.034414	-3.181130
192	97	8	0	0.075453	0.958132	-3.649886
193	98	6	0	5.755193	-4.267278	0.063054
194	99	6	0	6.744081	-4.518008	-1.122480
195	100	1	0	5.495577	-5.234693	0.506343
196	101	1	0	6.273123	-3.691160	0.840171
197	102	1	0	6.245561	-5.139747	-1.875436
198	103	1	0	7.027292	-3.570753	-1.589044
199	104	6	0	7.500840	1.111378	0.438623

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200	105	6	0	8.405414	1.055417	-0.816588
201	106	1	0	7.630013	0.184684	1.009683
202	107	1	0	7.846141	1.922283	1.090039
203	108	1	0	8.102902	0.235707	-1.480862
204	109	1	0	8.309608	1.974560	-1.409541
205	110	6	0	-1.108683	-3.865729	-4.100172
206	111	1	0	-2.025131	-3.739066	-4.684516
207	112	1	0	-1.378634	-4.373226	-3.162942
208	113	6	0	-2.221169	-0.841574	-4.641557
209	114	1	0	-2.070314	0.092027	-5.199452
210	115	1	0	-2.590362	-1.586487	-5.357943
211	116	6	0	2.970524	-5.566624	-0.991805
212	117	1	0	3.751380	-6.207941	-0.568347
213	118	1	0	2.030575	-5.806636	-0.475839
214	119	1	0	2.842079	-5.858907	-2.044066
215	120	6	0	6.023923	3.927440	-0.073713
216	121	1	0	7.113108	3.858850	0.017476
217	122	1	0	5.807614	4.523982	-0.970028
218	123	1	0	5.657342	4.494015	0.791193
219	124	6	0	1.062194	-3.098530	-1.782739
220	125	6	0	5.262898	-1.124979	-0.104406

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221	126	6	0	8.007799	-5.215537	-0.677250
222	127	6	0	9.868867	0.869803	-0.482113
223	128	8	0	9.161559	-4.747908	-0.709220
224	129	8	0	10.643297	0.778933	-1.626999
225	130	8	0	7.756319	-6.489076	-0.192949
226	131	8	0	10.372197	0.801395	0.653765
227	132	1	0	8.581194	-6.936404	0.107285
228	133	1	0	0.338947	-2.579271	-1.140461
229	134	1	0	0.765968	-4.151360	-1.835432
230	135	1	0	6.232021	-1.471488	0.248374
231	136	1	0	1.683876	-2.982790	-3.863609
232	137	1	0	-0.440133	-4.543212	-4.648312
233	138	6	0	2.921363	3.182121	-0.911795
234	139	6	0	1.980476	3.364237	2.407406
235	140	6	0	2.731411	4.635834	2.383391
236	141	6	0	2.814604	4.978640	0.983348
237	142	6	0	2.101241	3.865347	0.230602
238	143	7	0	1.613262	2.884039	1.238022
239	144	6	0	3.346039	6.230749	0.391644
240	145	6	0	3.227580	5.378714	3.561227
241	146	1	0	3.889282	4.741162	4.162567

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242	147	1	0	3.779402	6.285188	3.289633
243	148	1	0	2.392581	5.670277	4.212737
244	149	1	0	4.061289	6.716527	1.068098
245	150	1	0	3.895287	5.993948	-0.529556
246	151	6	0	2.220038	7.243122	0.042249
247	152	6	0	-3.300517	-0.606375	-3.551177
248	153	1	0	1.670138	7.542659	0.943187
249	154	1	0	2.646953	8.144575	-0.415743
250	155	1	0	1.502660	6.810731	-0.666669
251	156	1	0	-3.508395	-1.532813	-3.001405
252	157	1	0	-2.974116	0.150372	-2.828460
253	158	1	0	-4.235662	-0.259608	-4.009143
254	159	8	0	1.703511	2.799829	3.612753
255	160	1	0	3.314918	3.975363	-1.561326
256	161	1	0	2.207644	2.605769	-1.512563
257	162	1	0	1.220194	4.299772	-0.267644
258	163	1	0	11.597904	0.657297	-1.414503
259	164	1	0	-11.597993	0.657619	1.413842
260	165	1	0	-1.054118	2.009836	-3.586704
261	166	1	0	1.054278	2.009826	3.586703
262	167	1	0	-3.055289	0.365332	0.699085

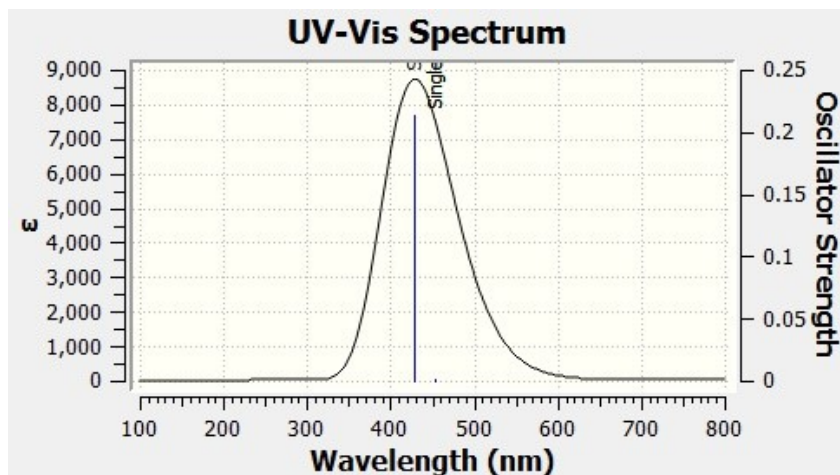
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263	168	1	0	-1.994028	-0.662395	2.647452
264	169	1	0	1.993937	-0.662604	-2.647241
265	170	1	0	3.055189	0.365305	-0.698937
266	171	1	0	3.674181	4.131015	2.348133
267	172	1	0	3.775443	4.521230	0.871706
268	173	1	0	-0.886052	-2.590599	-2.854065
269	174	1	0	-0.526323	-1.276345	-5.071733
270	175	1	0	-3.673316	4.130183	-2.351927
271	176	1	0	-3.775166	4.522101	-0.867959
272	177	1	0	0.527104	-1.273319	5.072275
273	178	1	0	0.884721	-2.593244	2.853550
274	-----					

275 **UB Implicit 1-hexanol**

276 Charge = 0, Multiplicity = 1

277 **TDDFT**



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279 **Figure S10b** TDDFT of UB Implicit model in 1-hexanol. Wavelength maximum = 452.68 (nm)

280 Cartesian coordinates of the optimized ground state geometry

281 -----

282 Center Atomic Atomic Coordinates (Angstroms)

283 Number Number Type X Y Z

284 -----

285 1 6 0 3.797893 -3.016762 -0.202361

286 2 6 0 4.911917 -3.907380 0.129696

287 3 6 0 5.993490 -3.085132 0.428845

288 4 6 0 5.515059 -1.707974 0.272870

289 5 7 0 4.144899 -1.717480 -0.117464

290 6 6 0 5.825740 0.792616 0.290588

291 7 6 0 6.614677 1.978034 0.257282

292 8 6 0 5.737667 3.074560 0.034104

293 9 6 0 4.419465 2.552117 -0.050091

294 10 7 0 4.497938 1.186679 0.097236

295 11 6 0 0.963786 -1.041505 -2.858334

296 12 6 0 0.197393 -2.300430 -3.375220

297 13 6 0 0.587763 -3.323068 -2.589359

298 14 6 0 2.054909 -3.003678 -2.065042

299 15 7 0 2.012763 -1.529293 -2.161469

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300	16	8	0	0.716030	0.200636	-3.008086
301	17	6	0	7.382301	-3.518856	0.833199
302	18	6	0	8.384847	-3.689268	-0.358705
303	19	1	0	7.320501	-4.490565	1.336888
304	20	1	0	7.821302	-2.823223	1.557704
305	21	1	0	7.991247	-4.464183	-1.028471
306	22	1	0	8.472216	-2.754650	-0.919099
307	23	6	0	8.118499	2.024482	0.343399
308	24	6	0	8.775155	1.835209	-1.070431
309	25	1	0	8.488661	1.239648	1.013749
310	26	1	0	8.447257	2.982946	0.760668
311	27	1	0	8.354408	0.941937	-1.543916
312	28	1	0	8.565595	2.701722	-1.701477
313	29	6	0	0.504147	-4.733232	-3.194625
314	30	1	0	-0.520167	-4.964674	-3.512813
315	31	1	0	0.798306	-5.487962	-2.453719
316	32	6	0	0.499006	-2.484485	-4.891912
317	33	1	0	1.577927	-2.638191	-5.041007
318	34	1	0	0.002592	-3.406422	-5.220554
319	35	6	0	4.848439	-5.413061	0.125437
320	36	1	0	5.779232	-5.854412	0.498129

Supporting Information

321	37	1	0	4.029580	-5.786280	0.755925
322	38	1	0	4.680817	-5.810126	-0.886180
323	39	6	0	6.137428	4.523902	-0.092736
324	40	1	0	6.275505	4.998474	0.889256
325	41	1	0	7.082689	4.631480	-0.638513
326	42	1	0	5.381018	5.104898	-0.632249
327	43	6	0	2.416057	-3.449934	-0.627425
328	44	6	0	6.257582	-0.550783	0.438034
329	45	6	0	9.769213	-4.124574	0.075234
330	46	6	0	10.262720	1.633991	-0.952693
331	47	8	0	10.817195	-3.452500	-0.055470
332	48	8	0	11.005413	2.729822	-1.283995
333	49	8	0	9.765568	-5.367451	0.649797
334	50	8	0	10.812900	0.575182	-0.560623
335	51	1	0	10.673890	-5.709947	0.942446
336	52	1	0	1.666324	-3.025843	0.055175
337	53	1	0	2.333566	-4.540869	-0.571464
338	54	1	0	7.305577	-0.675567	0.700790
339	55	1	0	2.808412	-3.399437	-2.762073
340	56	1	0	1.163003	-4.844824	-4.063851
341	57	6	0	3.117150	3.263747	-0.283734

Supporting Information

342	58	6	0	1.728594	2.530061	2.911150
343	59	6	0	2.341948	3.889041	3.332030
344	60	6	0	2.947457	4.342701	2.205411
345	61	6	0	2.266727	3.587424	0.978083
346	62	7	0	1.729404	2.346167	1.622002
347	63	6	0	3.075598	5.877698	2.017021
348	64	6	0	1.219132	4.755711	3.954067
349	65	1	0	0.833087	4.267322	4.856666
350	66	1	0	1.601718	5.742700	4.240472
351	67	1	0	0.379434	4.897825	3.263398
352	68	1	0	3.362098	6.318934	2.983647
353	69	1	0	3.920675	6.071631	1.341427
354	70	6	0	1.847994	6.638400	1.461843
355	71	6	0	0.013897	-1.315815	-5.774768
356	72	1	0	0.955208	6.497971	2.079716
357	73	1	0	2.063939	7.714774	1.426195
358	74	1	0	1.603567	6.321063	0.439904
359	75	1	0	-1.064137	-1.148479	-5.647971
360	76	1	0	0.528118	-0.380503	-5.528457
361	77	1	0	0.199197	-1.538530	-6.833613
362	78	8	0	1.211260	1.661452	3.822620

Supporting Information

363	79	1	0	3.321881	4.208971	-0.801452
364	80	1	0	2.485641	2.663502	-0.952337
365	81	1	0	1.400399	4.155876	0.610355
366	82	6	0	-3.814453	-3.029739	0.200714
367	83	6	0	-4.933233	-3.911804	-0.137899
368	84	6	0	-6.007597	-3.081472	-0.440254
369	85	6	0	-5.520180	-1.707952	-0.279639
370	86	7	0	-4.151679	-1.727709	0.116452
371	87	6	0	-5.817872	0.795099	-0.294448
372	88	6	0	-6.602300	1.983499	-0.261183
373	89	6	0	-5.721918	3.075991	-0.032310
374	90	6	0	-4.405835	2.548550	0.054760
375	91	7	0	-4.489125	1.183610	-0.095874
376	92	6	0	-0.958347	-1.075291	2.851418
377	93	6	0	-0.208488	-2.341575	3.375033
378	94	6	0	-0.612286	-3.363673	2.595276
379	95	6	0	-2.074193	-3.027222	2.066737
380	96	7	0	-2.013030	-1.553121	2.156236
381	97	8	0	-0.695570	0.164402	2.995710
382	98	6	0	-7.397714	-3.505100	-0.850868
383	99	6	0	-8.405069	-3.673500	0.337247

Supporting Information

384	100	1	0	-7.340191	-4.475469	-1.357651
385	101	1	0	-7.829982	-2.804398	-1.574521
386	102	1	0	-8.018513	-4.453274	1.005474
387	103	1	0	-8.488277	-2.740353	0.900706
388	104	6	0	-8.105665	2.036345	-0.351881
389	105	6	0	-8.767301	1.849630	1.059891
390	106	1	0	-8.477201	1.253364	-1.023628
391	107	1	0	-8.429000	2.996315	-0.769928
392	108	1	0	-8.353351	0.953319	1.533647
393	109	1	0	-8.554217	2.714211	1.692406
394	110	6	0	-0.549693	-4.770874	3.210069
395	111	1	0	0.470832	-5.014862	3.531059
396	112	1	0	-0.853716	-5.526141	2.473706
397	113	6	0	-0.512297	-2.513130	4.892792
398	114	1	0	-1.593198	-2.651276	5.042786
399	115	1	0	-0.028503	-3.439969	5.226398
400	116	6	0	-4.880437	-5.417906	-0.135970
401	117	1	0	-5.812789	-5.851980	-0.513242
402	118	1	0	-4.061674	-5.795871	-0.763742
403	119	1	0	-4.719786	-5.817859	0.875640
404	120	6	0	-6.116878	4.526284	0.098367

Supporting Information

405	121	1	0	-7.068877	4.634428	0.632057
406	122	1	0	-5.365232	5.100412	0.651818
407	123	1	0	-6.239734	5.007892	-0.882193
408	124	6	0	-2.437983	-3.475262	0.630515
409	125	6	0	-6.255170	-0.546096	-0.445791
410	126	6	0	-9.790690	-4.098609	-0.102598
411	127	6	0	-10.255758	1.657661	0.938038
412	128	8	0	-10.835027	-3.420721	0.027593
413	129	8	0	-10.992686	2.757299	1.269377
414	130	8	0	-9.792722	-5.339189	-0.682123
415	131	8	0	-10.811309	0.602783	0.542828
416	132	1	0	-10.702339	-5.675533	-0.978117
417	133	1	0	-1.682199	-3.062502	-0.052392
418	134	1	0	-2.367096	-4.567228	0.578983
419	135	1	0	-7.302789	-0.665013	-0.712812
420	136	1	0	-2.834299	-3.409704	2.763987
421	137	1	0	-1.211116	-4.867397	4.079131
422	138	6	0	-3.102705	3.256114	0.296975
423	139	6	0	-1.706925	2.566080	-2.904650
424	140	6	0	-2.322038	3.929005	-3.309782
425	141	6	0	-2.929503	4.368442	-2.178588

Supporting Information

426	142	6	0	-2.250897	3.597991	-0.959357
427	143	7	0	-1.709586	2.366457	-1.617922
428	144	6	0	-3.057151	5.901199	-1.971775
429	145	6	0	-1.199774	4.804633	-3.920257
430	146	1	0	-0.812765	4.328072	-4.828717
431	147	1	0	-1.583118	5.794790	-4.194419
432	148	1	0	-0.360565	4.938777	-3.227408
433	149	1	0	-3.341362	6.354282	-2.933573
434	150	1	0	-3.903411	6.087596	-1.295677
435	151	6	0	-1.830265	6.654400	-1.404860
436	152	6	0	-0.011166	-1.346480	5.769313
437	153	1	0	-0.936041	6.520420	-2.022098
438	154	1	0	-2.045458	7.730468	-1.357321
439	155	1	0	-1.588641	6.325142	-0.386027
440	156	1	0	1.069026	-1.194464	5.641574
441	157	1	0	-0.512617	-0.405592	5.518063
442	158	1	0	-0.199348	-1.561022	6.829341
443	159	8	0	-1.185765	1.709525	-3.825351
444	160	1	0	-3.307201	4.194147	0.827862
445	161	1	0	-2.471383	2.646406	0.957133
446	162	1	0	-1.386427	4.163026	-0.582119

Supporting Information

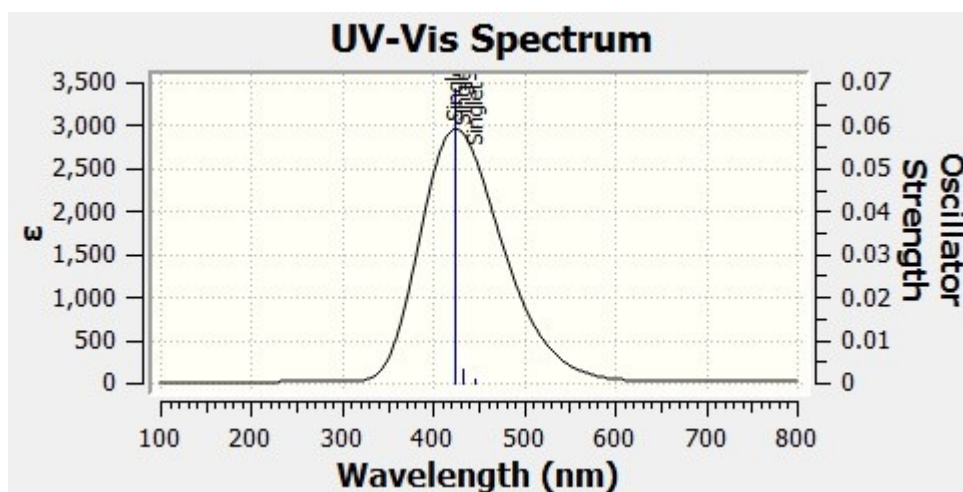
447	163	1	0	-11.962480	2.614542	1.159037
448	164	1	0	11.974586	2.581072	-1.176211
449	165	1	0	0.547781	0.977459	3.449028
450	166	1	0	-0.523690	1.021071	-3.457148
451	167	1	0	3.731479	0.518021	0.083235
452	168	1	0	2.701701	-0.968345	-1.661037
453	169	1	0	-2.695486	-0.986085	1.653835
454	170	1	0	-3.726219	0.511042	-0.078177

455 -----

456 **SB Explicit 1-hexanol**

457 Charge = 0, Multiplicity = 1

458 **TDDFT**



459

460 **Figure S10c** TDDFT of SB Explicit model in 1-hexanol. Wavelength maximum = 445.06 (nm)

461 Cartesian coordinates of the optimized ground state geometry

462 -----

Supporting Information

463 Center Atomic Atomic Coordinates (Angstroms)

464 Number Number Type X Y Z

465 -----

466 1 6 0 3.580368 -2.818750 -0.292710

467 2 6 0 4.709440 -3.708678 -0.016533

468 3 6 0 5.805605 -2.887277 0.215180

469 4 6 0 5.323195 -1.508376 0.068195

470 5 7 0 3.935616 -1.517923 -0.245735

471 6 6 0 5.678028 0.988781 0.072209

472 7 6 0 6.491765 2.158301 0.035306

473 8 6 0 5.639239 3.271787 -0.184014

474 9 6 0 4.306688 2.780189 -0.261874

475 10 7 0 4.356350 1.413882 -0.115545

476 11 6 0 0.592007 -0.903410 -2.826966

477 12 6 0 -0.224576 -2.093301 -3.349217

478 13 6 0 0.289346 -3.267574 -2.441923

479 14 6 0 1.739964 -2.844497 -2.060985

480 15 7 0 1.684930 -1.371377 -2.182935

481 16 8 0 0.320633 0.331647 -2.968807

482 17 6 0 7.229408 -3.287219 0.502813

483 18 6 0 8.098386 -3.309625 -0.799577

Supporting Information

484	19	1	0	7.257463	-4.283344	0.963560
485	20	1	0	7.687200	-2.594919	1.222107
486	21	1	0	7.715433	-4.085420	-1.473089
487	22	1	0	8.039346	-2.347755	-1.308474
488	23	6	0	7.996015	2.180328	0.146824
489	24	6	0	8.695902	1.903978	-1.239276
490	25	1	0	8.335070	1.429057	0.875324
491	26	1	0	8.330511	3.155634	0.524847
492	27	1	0	8.335420	0.957996	-1.686704
493	28	1	0	8.448263	2.709540	-1.946622
494	29	6	0	0.186682	-4.688205	-3.020805
495	30	1	0	-0.851735	-4.937765	-3.270231
496	31	1	0	0.534523	-5.428013	-2.287520
497	32	6	0	0.006176	-2.298016	-4.876370
498	33	1	0	1.072468	-2.450300	-5.080838
499	34	1	0	-0.503371	-3.228603	-5.164843
500	35	6	0	4.645134	-5.215263	0.004203
501	36	1	0	5.608494	-5.652963	0.288609
502	37	1	0	3.892651	-5.580433	0.716587
503	38	1	0	4.378366	-5.623334	-0.981316
504	39	6	0	6.068474	4.711109	-0.330880

Supporting Information

505	40	1	0	6.202119	5.197730	0.648040
506	41	1	0	7.023619	4.789509	-0.862403
507	42	1	0	5.331598	5.297135	-0.887905
508	43	6	0	2.177430	-3.255310	-0.634991
509	44	6	0	6.086392	-0.361166	0.200934
510	45	6	0	9.555727	-3.605558	-0.499573
511	46	6	0	10.189753	1.806873	-1.056091
512	47	8	0	10.018761	-4.730217	-0.227231
513	48	8	0	10.803994	3.048966	-1.080700
514	49	8	0	10.347654	-2.488911	-0.604048
515	50	8	0	10.833188	0.761727	-0.849159
516	51	1	0	1.463748	-2.807741	0.072455
517	52	1	0	2.095105	-4.343320	-0.541252
518	53	1	0	7.144873	-0.498228	0.411610
519	54	1	0	2.461714	-3.248395	-2.790725
520	55	1	0	0.794884	-4.803823	-3.925467
521	56	6	0	3.019226	3.511574	-0.500296
522	57	6	0	1.753272	3.130941	2.809336
523	58	6	0	2.321256	4.506775	3.143667
524	59	6	0	2.984287	4.883945	1.778448
525	60	6	0	2.225082	3.968634	0.752167

Supporting Information

526	61	7	0	1.716344	2.802849	1.549551
527	62	6	0	3.105400	6.384984	1.412613
528	63	6	0	1.198623	5.436643	3.678929
529	64	1	0	0.833336	5.057975	4.642156
530	65	1	0	1.581410	6.453801	3.846429
531	66	1	0	0.350258	5.495546	2.993631
532	67	1	0	3.386431	6.929012	2.330323
533	68	1	0	3.942632	6.513882	0.719985
534	69	6	0	1.868510	7.069706	0.783387
535	70	6	0	-0.528690	-1.144431	-5.750342
536	71	1	0	0.977032	6.991092	1.415348
537	72	1	0	2.073686	8.137639	0.630655
538	73	1	0	1.627275	6.637050	-0.193980
539	74	1	0	-1.602502	-0.984200	-5.579390
540	75	1	0	-0.013687	-0.203778	-5.533769
541	76	1	0	-0.390115	-1.379030	-6.812832
542	77	8	0	1.270713	2.373620	3.828685
543	78	1	0	3.223395	4.407624	-1.100067
544	79	1	0	2.350520	2.875758	-1.098577
545	80	1	0	1.341979	4.493685	0.360982
546	81	6	0	-3.272801	-3.198164	0.991185

Supporting Information

547	82	6	0	-4.253632	-4.251646	0.721284
548	83	6	0	-5.443431	-3.602403	0.384282
549	84	6	0	-5.157068	-2.165163	0.463101
550	85	7	0	-3.794592	-1.964856	0.834597
551	86	6	0	-5.796109	0.266403	0.338735
552	87	6	0	-6.738849	1.342922	0.363894
553	88	6	0	-5.997878	2.549175	0.496587
554	89	6	0	-4.623063	2.214258	0.504088
555	90	7	0	-4.525203	0.843539	0.418162
556	91	6	0	-0.644133	-0.587522	3.260285
557	92	6	0	0.316648	-1.574647	3.956374
558	93	6	0	-0.015419	-2.913552	3.215604
559	94	6	0	-1.499285	-2.756961	2.782455
560	95	7	0	-1.650339	-1.291385	2.694431
561	96	8	0	-0.559332	0.682936	3.236499
562	97	6	0	-6.747718	-4.257525	-0.003398
563	98	6	0	-7.828713	-4.312873	1.140046
564	99	1	0	-6.540375	-5.288493	-0.308442
565	100	1	0	-7.192402	-3.772215	-0.883344
566	101	1	0	-8.377544	-5.266684	1.038464
567	102	1	0	-7.357471	-4.269249	2.111868

Supporting Information

568	103	6	0	-8.237966	1.197903	0.406529
569	104	6	0	-8.752036	1.066591	1.850872
570	105	1	0	-8.575376	0.341567	-0.177824
571	106	1	0	-8.693888	2.093185	-0.059871
572	107	1	0	-8.371244	0.138668	2.313039
573	108	1	0	-8.408199	1.887642	2.492168
574	109	6	0	0.261291	-4.214234	4.003035
575	110	1	0	1.318451	-4.278728	4.297520
576	111	1	0	0.045944	-5.094704	3.379337
577	112	6	0	0.105340	-1.582392	5.488782
578	113	1	0	-0.953367	-1.828606	5.716061
579	114	1	0	0.705666	-2.388951	5.911645
580	115	6	0	-3.977184	-5.728187	0.807043
581	116	1	0	-4.856573	-6.322314	0.531675
582	117	1	0	-3.150023	-6.032586	0.159683
583	118	1	0	-3.703986	-6.026780	1.836444
584	119	6	0	-6.581317	3.939958	0.588276
585	120	1	0	-7.494227	3.947077	1.201380
586	121	1	0	-5.874764	4.638950	1.052952
587	122	1	0	-6.847843	4.344499	-0.392640
588	123	6	0	-1.844492	-3.425009	1.423761

Supporting Information

589	124	6	0	-6.051674	-1.126456	0.268821
590	125	6	0	-8.868011	-3.215390	1.035461
591	126	6	0	-10.257912	0.992340	1.958681
592	127	8	0	-8.954450	-2.251030	1.823479
593	128	8	0	-10.720036	1.410557	3.159938
594	129	8	0	-9.646539	-3.331493	-0.072814
595	130	8	0	-11.038363	0.600206	1.067441
596	131	1	0	-10.361996	-2.566709	-0.230625
597	132	1	0	-1.161612	-3.008481	0.667460
598	133	1	0	-1.641078	-4.494274	1.496969
599	134	1	0	-7.082616	-1.394488	0.060977
600	135	1	0	-2.178664	-3.154348	3.550680
601	136	1	0	-0.350040	-4.281731	4.904234
602	137	6	0	-3.412515	3.096215	0.626867
603	138	6	0	-2.235283	2.552360	-2.689561
604	139	6	0	-2.986964	3.807479	-3.124095
605	140	6	0	-3.632993	4.235045	-1.758592
606	141	6	0	-2.725316	3.527909	-0.698328
607	142	7	0	-2.098461	2.362885	-1.408423
608	143	6	0	-3.924668	5.742032	-1.539336
609	144	6	0	-2.021374	4.804816	-3.812566

Supporting Information

610	145	1	0	-1.647956	4.374223	-4.748766
611	146	1	0	-2.537093	5.743324	-4.056826
612	147	1	0	-1.157431	5.041397	-3.180841
613	148	1	0	-4.326442	6.155180	-2.474675
614	149	1	0	-4.736099	5.830651	-0.802406
615	150	6	0	-2.756421	6.637307	-1.061436
616	151	6	0	0.483749	-0.259049	6.188691
617	152	1	0	-1.902130	6.605014	-1.743019
618	153	1	0	-3.092879	7.680726	-0.994302
619	154	1	0	-2.404055	6.344317	-0.063489
620	155	1	0	1.528663	0.004945	5.976633
621	156	1	0	-0.146476	0.577215	5.860543
622	157	1	0	0.370530	-0.359701	7.276370
623	158	8	0	-1.704969	1.752592	-3.650098
624	159	1	0	-3.695611	4.014395	1.156648
625	160	1	0	-2.655920	2.593379	1.239455
626	161	1	0	-1.895927	4.186416	-0.400694
627	162	1	0	-11.712573	1.318410	3.236703
628	163	1	0	11.756411	2.951631	-0.833374
629	164	1	0	0.631101	1.623293	3.549051
630	165	1	0	-0.976724	1.106770	-3.338871

Supporting Information

631	166	1	0	3.576577	0.759011	-0.107237
632	167	1	0	2.383689	-0.798516	-1.721694
633	168	1	0	-2.429176	-0.897276	2.158335
634	169	1	0	-3.677381	0.286075	0.407660
635	170	6	0	12.785685	-2.277917	-0.269809
636	171	8	0	12.099620	-0.997113	0.004555
637	172	1	0	12.666683	-2.558836	-1.333012
638	173	6	0	14.276809	-2.098982	0.027046
639	174	1	0	14.386231	-1.788994	1.075966
640	175	1	0	14.768845	-3.078830	-0.070002
641	176	6	0	14.985577	-1.086178	-0.901905
642	177	1	0	14.478099	-0.115005	-0.828094
643	178	1	0	14.879208	-1.419218	-1.947274
644	179	6	0	16.483950	-0.913630	-0.571411
645	180	1	0	16.588512	-0.577279	0.473310
646	181	1	0	16.989142	-1.890607	-0.637298
647	182	6	0	17.200425	0.091529	-1.500002
648	183	1	0	16.695494	1.067591	-1.433687
649	184	1	0	17.095831	-0.243406	-2.543501
650	185	6	0	18.696867	0.263514	-1.162467
651	186	1	0	18.827470	0.627152	-0.133711

Supporting Information

652	187	1	0	19.231035	-0.692699	-1.249616
653	188	1	0	19.180549	0.982188	-1.837483
654	189	1	0	12.346891	-3.076525	0.343487
655	190	6	0	-12.695230	-1.782592	-0.986839
656	191	8	0	-11.314583	-1.527092	-0.521953
657	192	6	0	-14.207412	-1.560164	-1.130609
658	193	1	0	-11.243417	-0.696127	0.022758
659	194	1	0	-14.710053	-2.539239	-1.121632
660	195	1	0	-14.379331	-1.112307	-0.138550
661	196	6	0	-14.822016	-0.660423	-2.221792
662	197	1	0	-14.632611	-1.102558	-3.209083
663	198	1	0	-14.314868	0.318113	-2.211203
664	199	6	0	-16.339878	-0.449554	-2.034281
665	200	1	0	-16.846597	-1.427638	-2.037923
666	201	1	0	-16.527994	-0.003816	-1.043085
667	202	6	0	-16.966785	0.449943	-3.121985
668	203	1	0	-16.777921	0.005166	-4.110809
669	204	1	0	-16.460707	1.427881	-3.118005
670	205	6	0	-18.484450	0.655612	-2.931025
671	206	1	0	-19.016987	-0.304950	-2.961317
672	207	1	0	-18.698427	1.126382	-1.961216

Supporting Information

673	208	1	0	-18.903878	1.298662	-3.716440
674	209	1	0	-1.291146	-1.906101	-3.188627
675	210	1	0	-0.308912	-3.230404	-1.518392
676	211	1	0	4.007938	4.483438	1.835221
677	212	1	0	3.079170	4.424870	3.927435
678	213	1	0	-3.768965	3.545121	-3.849646
679	214	1	0	-4.605437	3.715101	-1.729316
680	215	1	0	0.591345	-2.935690	2.301847
681	216	1	0	1.346374	-1.254870	3.748797
682	217	1	0	-12.750706	-2.798829	-0.656559
683	218	1	0	-12.472488	-1.797239	-2.033296
684	219	1	0	10.521671	-2.136916	0.271976
685	220	1	0	12.318648	-0.062978	0.036490

686 -----

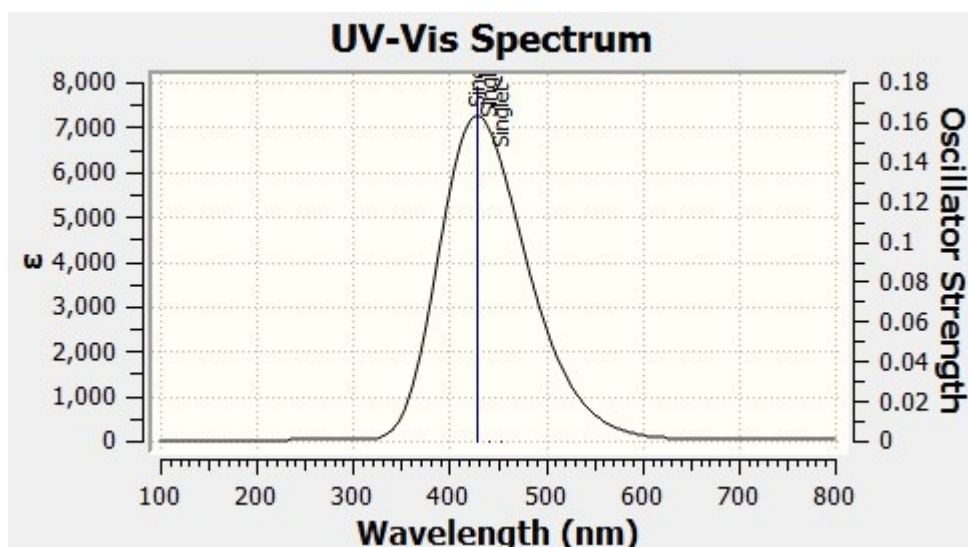
687

688 **UB Implicit 1-hexanol**

689 Charge = 0, Multiplicity = 1

690 **TDDFT**

Supporting Information



691

692 **Figure S10d** TDDFT of UB Explicit model in 1-hexanol. Wavelength maximum = 452.24 (nm)

693 Cartesian coordinates of the optimized ground state geometry

694 -----

695 Center Atomic Atomic Coordinates (Angstroms)

696 Number Number Type X Y Z

697 -----

698 1 6 0 3.333149 -3.117892 -0.275517

699 2 6 0 4.375922 -4.114348 -0.012653

700 3 6 0 5.571999 -3.411093 0.062580

701 4 6 0 5.237488 -1.999719 -0.150043

702 5 7 0 3.831410 -1.869735 -0.356058

703 6 6 0 5.792100 0.444640 -0.295167

704 7 6 0 6.647997 1.579442 -0.388383

705 8 6 0 5.821065 2.728924 -0.542949

Supporting Information

706	9	6	0	4.472030	2.288596	-0.528117
707	10	7	0	4.478715	0.921643	-0.383565
708	11	6	0	0.573769	-1.359233	-3.148758
709	12	6	0	-0.398659	-2.570598	-3.315082
710	13	6	0	-0.085448	-3.436485	-2.344457
711	14	6	0	1.452023	-3.239871	-1.981974
712	15	7	0	1.604578	-1.834184	-2.415802
713	16	8	0	0.483548	-0.158171	-3.569827
714	17	6	0	6.966215	-3.934127	0.299155
715	18	6	0	7.803127	-4.072330	-1.018605
716	19	1	0	6.926104	-4.910687	0.794382
717	20	1	0	7.497372	-3.257265	0.976534
718	21	1	0	7.810152	-5.105843	-1.375725
719	22	1	0	7.345252	-3.455060	-1.802715
720	23	6	0	8.156565	1.587970	-0.362083
721	24	6	0	8.764999	1.622003	-1.808712
722	25	1	0	8.552396	0.713949	0.166093
723	26	1	0	8.499440	2.475673	0.184409
724	27	1	0	8.663236	0.631200	-2.265137
725	28	1	0	8.229305	2.344844	-2.426798
726	29	6	0	-0.411558	-4.915692	-2.602713

Supporting Information

727	30	1	0	-1.481894	-5.053432	-2.800765
728	31	1	0	-0.156897	-5.524540	-1.725361
729	32	6	0	-0.264410	-3.122060	-4.765178
730	33	1	0	0.768668	-3.455273	-4.943465
731	34	1	0	-0.899548	-4.013515	-4.843514
732	35	6	0	4.143724	-5.595939	0.135408
733	36	1	0	5.076152	-6.124175	0.362836
734	37	1	0	3.432194	-5.817187	0.943533
735	38	1	0	3.731913	-6.037593	-0.783432
736	39	6	0	6.297461	4.153979	-0.680920
737	40	1	0	6.625924	4.569893	0.282564
738	41	1	0	7.147376	4.231556	-1.370232
739	42	1	0	5.506399	4.806872	-1.065292
740	43	6	0	1.869770	-3.404549	-0.498686
741	44	6	0	6.120086	-0.930152	-0.150115
742	45	6	0	9.240473	-3.596926	-0.881590
743	46	6	0	10.225596	1.996125	-1.781097
744	47	8	0	10.241855	-4.255791	-1.261557
745	48	8	0	10.476218	3.228840	-2.325810
746	49	8	0	9.336785	-2.360274	-0.338294
747	50	8	0	11.156745	1.313427	-1.297605

Supporting Information

748	51	1	0	1.258817	-2.718332	0.102404
749	52	1	0	1.635087	-4.428158	-0.185513
750	53	1	0	7.177489	-1.161752	-0.032245
751	54	1	0	2.081797	-3.891024	-2.606302
752	55	1	0	0.146347	-5.314455	-3.458260
753	56	6	0	3.201042	3.079126	-0.664102
754	57	6	0	1.992319	2.417728	2.618585
755	58	6	0	2.724517	3.734839	2.988616
756	59	6	0	3.271431	4.147506	1.845049
757	60	6	0	2.464385	3.451251	0.655177
758	61	7	0	1.888799	2.244702	1.331955
759	62	6	0	3.489370	5.672323	1.654996
760	63	6	0	1.702302	4.667043	3.684990
761	64	1	0	1.340484	4.194454	4.605967
762	65	1	0	2.165997	5.623693	3.954208
763	66	1	0	0.833128	4.871489	3.048492
764	67	1	0	3.866052	6.084821	2.603244
765	68	1	0	4.300719	5.815828	0.927625
766	69	6	0	2.282476	6.518091	1.184193
767	70	6	0	-0.682688	-2.115209	-5.857110
768	71	1	0	1.425078	6.434889	1.859906

Supporting Information

769	72	1	0	2.568533	7.577564	1.136221
770	73	1	0	1.949438	6.224707	0.180293
771	74	1	0	-1.719330	-1.783949	-5.708625
772	75	1	0	-0.043861	-1.225282	-5.853368
773	76	1	0	-0.615707	-2.580499	-6.849134
774	77	8	0	1.488441	1.579252	3.563419
775	78	1	0	3.422209	4.011252	-1.198635
776	79	1	0	2.486691	2.518832	-1.281902
777	80	1	0	1.615533	4.079868	0.349177
778	81	6	0	-3.780869	-3.415916	0.779338
779	82	6	0	-4.908354	-4.303424	0.490603
780	83	6	0	-5.954304	-3.486939	0.070244
781	84	6	0	-5.442717	-2.111666	0.114501
782	85	7	0	-4.084540	-2.123361	0.552156
783	86	6	0	-5.661737	0.389634	-0.097051
784	87	6	0	-6.394886	1.610923	-0.082927
785	88	6	0	-5.457661	2.672850	0.062580
786	89	6	0	-4.161707	2.096571	0.109227
787	90	7	0	-4.310247	0.731696	0.024589
788	91	6	0	-0.802442	-1.131186	2.977109
789	92	6	0	-0.093378	-2.308365	3.725041

Supporting Information

790	93	6	0	-0.541471	-3.431229	3.163308
791	94	6	0	-2.007114	-3.151252	2.605622
792	95	7	0	-1.889952	-1.691268	2.407060
793	96	8	0	-0.487044	0.100687	2.867576
794	97	6	0	-7.332209	-3.936826	-0.354443
795	98	6	0	-8.449749	-3.758874	0.730910
796	99	1	0	-7.285603	-5.001354	-0.607863
797	100	1	0	-7.655412	-3.419348	-1.265221
798	101	1	0	-9.208014	-4.537385	0.574732
799	102	1	0	-8.039736	-3.879072	1.737211
800	103	6	0	-7.896211	1.765835	-0.087099
801	104	6	0	-8.460063	1.761227	1.369734
802	105	1	0	-8.380366	0.970753	-0.664419
803	106	1	0	-8.162008	2.713356	-0.571144
804	107	1	0	-8.421146	0.736813	1.766338
805	108	1	0	-7.856967	2.397260	2.022270
806	109	6	0	-0.507473	-4.699838	4.030226
807	110	1	0	0.512354	-4.913658	4.374120
808	111	1	0	-0.850316	-5.568792	3.453702
809	112	6	0	-0.387835	-2.180007	5.248970
810	113	1	0	-1.470333	-2.263106	5.426210

Supporting Information

811	114	1	0	0.078624	-3.037360	5.750702
812	115	6	0	-4.883862	-5.802149	0.649803
813	116	1	0	-5.821674	-6.258198	0.315456
814	117	1	0	-4.069178	-6.258390	0.070364
815	118	1	0	-4.734368	-6.095522	1.698888
816	119	6	0	-5.790071	4.140678	0.172264
817	120	1	0	-6.689931	4.302248	0.778205
818	121	1	0	-4.975444	4.701539	0.643583
819	122	1	0	-5.976776	4.596958	-0.810345
820	123	6	0	-2.428303	-3.851583	1.292714
821	124	6	0	-6.144016	-0.946056	-0.154041
822	125	6	0	-9.166800	-2.422654	0.645256
823	126	6	0	-9.894846	2.214797	1.450031
824	127	8	0	-9.250695	-1.597045	1.592041
825	128	8	0	-10.141483	3.041377	2.514319
826	129	8	0	-9.709675	-2.202246	-0.574078
827	130	8	0	-10.817340	1.901672	0.661756
828	131	1	0	-10.248971	-1.304395	-0.719666
829	132	1	0	-1.657834	-3.640533	0.537677
830	133	1	0	-2.428599	-4.934097	1.460370
831	134	1	0	-7.192476	-1.047710	-0.421129

Supporting Information

832	135	1	0	-2.760805	-3.360467	3.379276
833	136	1	0	-1.151553	-4.610245	4.913000
834	137	6	0	-2.816321	2.749398	0.268527
835	138	6	0	-1.783571	2.265104	-3.105708
836	139	6	0	-2.342212	3.696199	-3.321313
837	140	6	0	-2.787368	4.068740	-2.121227
838	141	6	0	-2.063029	3.146605	-1.034251
839	142	7	0	-1.675524	1.950182	-1.847235
840	143	6	0	-2.761464	5.582931	-1.780791
841	144	6	0	-1.230273	4.545570	-3.985433
842	145	1	0	-0.980014	4.121936	-4.965308
843	146	1	0	-1.565885	5.578347	-4.138208
844	147	1	0	-0.313599	4.565373	-3.384163
845	148	1	0	-3.100503	6.138847	-2.667954
846	149	1	0	-3.516433	5.775919	-1.005729
847	150	6	0	-1.423666	6.186522	-1.291116
848	151	6	0	0.143552	-0.879811	5.886981
849	152	1	0	-0.610275	6.036344	-2.008381
850	153	1	0	-1.539055	7.268164	-1.138309
851	154	1	0	-1.111437	5.753424	-0.332196
852	155	1	0	1.224129	-0.773788	5.723799

Supporting Information

853	156	1	0	-0.344013	0.007081	5.468173
854	157	1	0	-0.036449	-0.889088	6.969883
855	158	8	0	-1.407573	1.464297	-4.141685
856	159	1	0	-2.936119	3.659110	0.871424
857	160	1	0	-2.152772	2.080388	0.832373
858	161	1	0	-1.128223	3.616260	-0.696531
859	162	1	0	-11.090104	3.305401	2.573225
860	163	1	0	11.430115	3.475000	-2.278384
861	164	1	0	0.780759	0.914158	3.236707
862	165	1	0	-0.748541	0.723659	-3.885022
863	166	1	0	3.679274	0.289778	-0.333743
864	167	1	0	2.389077	-1.273471	-2.086319
865	168	1	0	-2.575841	-1.211396	1.823811
866	169	1	0	-3.578848	0.026483	0.054178
867	170	6	0	12.817241	-1.754061	-0.477946
868	171	8	0	11.490120	-1.137518	-0.308600
869	172	1	0	13.209381	-1.482685	-1.468142
870	173	6	0	13.788026	-1.336073	0.633007
871	174	1	0	13.352309	-1.608888	1.605253
872	175	1	0	14.705481	-1.934503	0.516037
873	176	6	0	14.149257	0.164877	0.621268

Supporting Information

874	177	1	0	13.236090	0.765423	0.747640
875	178	1	0	14.568390	0.430068	-0.362984
876	179	6	0	15.159758	0.544759	1.725135
877	180	1	0	14.742625	0.275368	2.708797
878	181	1	0	16.077521	-0.052582	1.601063
879	182	6	0	15.526676	2.045027	1.723204
880	183	1	0	14.609513	2.641470	1.847979
881	184	1	0	15.942309	2.314219	0.739641
882	185	6	0	16.537377	2.418412	2.828282
883	186	1	0	16.133624	2.186843	3.823796
884	187	1	0	17.474628	1.857182	2.708772
885	188	1	0	16.780704	3.489218	2.804239
886	189	1	0	12.636424	-2.833265	-0.459913
887	190	6	0	-11.962101	-0.053449	-2.139275
888	191	8	0	-10.976801	-0.120193	-1.047873
889	192	6	0	-13.385209	-0.380805	-1.666425
890	193	1	0	-10.958175	0.675543	-0.446514
891	194	1	0	-14.025222	-0.443858	-2.560789
892	195	1	0	-13.385476	-1.379114	-1.204513
893	196	6	0	-13.977586	0.652969	-0.684708
894	197	1	0	-13.957213	1.650873	-1.152295

Supporting Information

895	198	1	0	-13.347379	0.713430	0.214649
896	199	6	0	-15.424827	0.315217	-0.265469
897	200	1	0	-16.061337	0.257058	-1.163337
898	201	1	0	-15.445494	-0.684696	0.197122
899	202	6	0	-16.027406	1.341792	0.718448
900	203	1	0	-16.005339	2.341306	0.256660
901	204	1	0	-15.391495	1.398750	1.615518
902	205	6	0	-17.473742	0.999134	1.134197
903	206	1	0	-18.136282	0.964407	0.258057
904	207	1	0	-17.518247	0.017368	1.626128
905	208	1	0	-17.877623	1.744357	1.832635
906	209	1	0	-11.620769	-0.780861	-2.882919
907	210	1	0	-11.914254	0.948896	-2.585737
908	211	1	0	10.297876	-1.912857	-0.317304
909	212	1	0	11.419155	-0.205117	-0.650884

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