Supporting Information

The enhanced ultrafast dissociation of *meso*-hydrogen of bis(indolyl)methane derivatives under acidic conditions

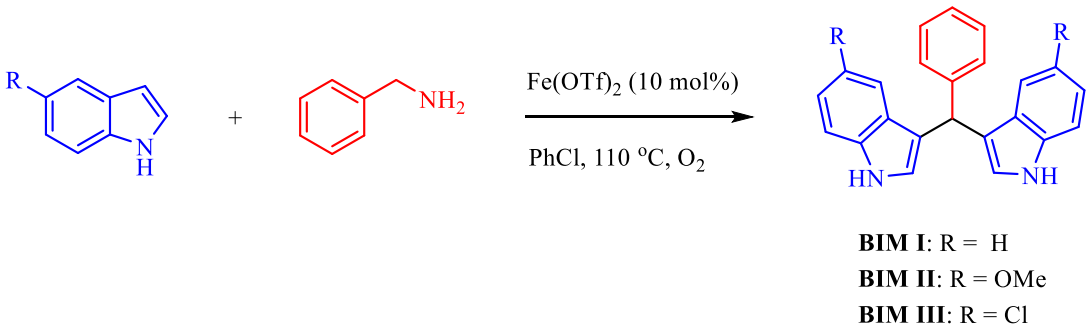
Vikas Kumar Jha,[1] Sunil Kumar Patel,[1] Devarapalli Chenna Rao,[2] Kovuru Gopalaiah,[2] E. Siva Subramaniam Iyer*[1]

1. School of chemical and materials science, Indian Institute of Technology Goa, Farmagudi, Ponda, Goa 403 401, India. E-mail: vikas19251104@iitgoa.ac.in, sunil21251103@iitgoa.ac.in, and essiyer@iitgoa.ac.in

2. Department of Chemistry, University of Delhi, Delhi 110 007, India. E-mail: dchennarao@yahoo.co.in, gopal@chemistry.du.ac.in

Synthesis

A 10 mL oven-dried Schlenk tube equipped with a magnetic stir bar, benzylamine (1.3 mmol), indole (2.0 mmol), iron(II) triflate (10 mol %), and anhydrous chlorobenzene (1 mL) were added under oxygen atmosphere. The Schlenk tube was immersed in a silicon oil bath placed over a magnetic stirrer and heated at 110 °C with constant stirring until complete consumption of indole. After completion of the reaction, as monitored by TLC, the reaction mixture was allowed to cool at room temperature. The crude compound was diluted with dichloromethane and absorbed over silica gel to dry. The dried, finely crushed residue was purified by column chromatography using hexane and ethyl acetate as eluents to afford the compounds BIM I, BIM II and BIM III.[3]



BIM I: R = H
BIM II: R = OMe
BIM III: R = Cl

Scheme S1. Synthesis of Bis(indolyl)methanes

BIM I: 3,3'-Benzylidenebis(1*H*-indole)

Pinkish solid; yield: 92%; mp 149–151 °C (Lit.[1] 147–150 °C).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.68 (br s, 2 H, NH), 7.36 (d, *J* = 8.0 Hz, 2H), 7.32-7.30 (m, 2H), 7.28-7.22 (m, 4H), 7.20-7.12 (m, 3H), 6.99-6.96 (m, 2H), 6.52 (s, 2H), 5.85 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 144.0, 136.6, 128.7, 128.2, 126.9, 126.1, 123.6, 121.9, 119.9, 119.6, 119.2, 111.0, 40.1.

BIM II: 3,3'-Benzylidenebis(5-methoxy-1*H*-indole)

Pale yellow solid; yield: 84%; mp 215–218 °C (Lit.[1] 212–215 °C).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.83 (br s, 2 H, NH), 7.35–7.34 (m, 2 H), 7.29–7.18 (m, 5 H), 6.84-6.79 (m, 4 H), 6.65 (d, *J* = 1.6 Hz, 2 H), 5.77 (s, 1 H), 3.68 (s, 6 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ = 153.7, 143.9, 131.8, 128.7, 128.2, 127.5, 126.1, 124.4, 119.3, 111.9, 111.6, 101.9, 55.8, 40.3.

BIM III 3,3'-Benzylidenebis(5-chloro-1*H*-indole)

White solid; yield: 86%; mp 192–194 °C (Lit.[2] 190–193 °C).

^{1}H NMR (400 MHz, CD_3OD): δ = 7.21-7.15 (m, 7H), 7.12-7.07 (m, 4H), 6.91 (dd, *J* = 8.4, 2.0 Hz, 2H), 6.59 (s, 2H), 5.63 (s, 1H).

^{13}C NMR (100 MHz, CD_3OD): δ = 145.4, 136.9, 129.7, 129.3, 129.2, 127.3, 126.4, 125.2, 122.4, 119.7, 119.5, 113.4, 41.4.

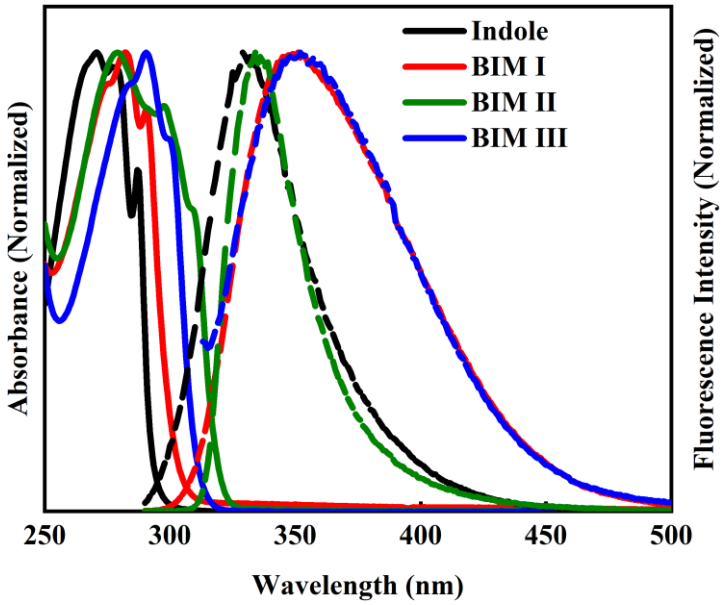


Figure S1. Steady state absorption (solid lines) and fluorescence (dash lines) spectra of indole (black), BIM I (red), BIM II (green) and BIM III (blue) in methanol.

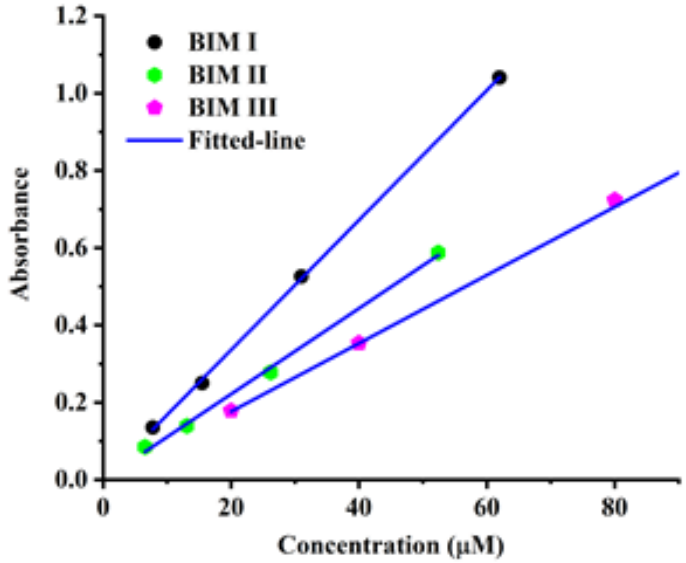


Figure S2: Beer-Lambert plots of BIM-I (black dots), BIM II (green dots), BIM III (pink dots). Blue lines are the linear fit.

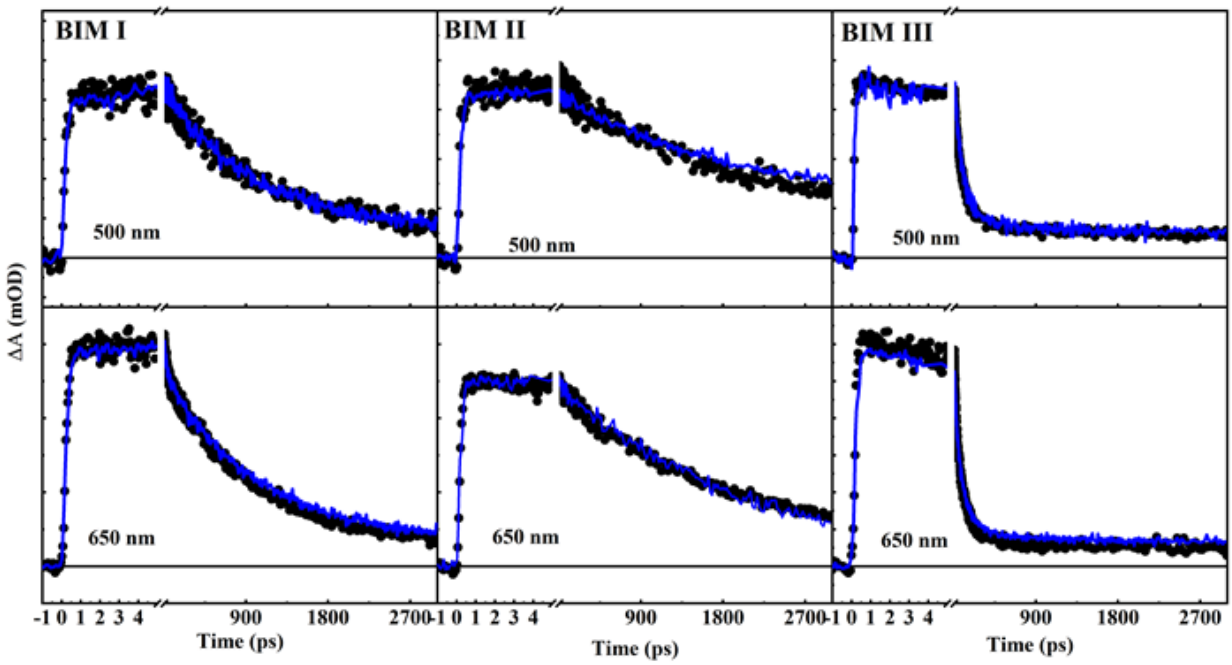


Figure S3: The kinetic traces for BIM I-III under VH(blue line) and VV (black dots) polarizations at 500 nm (top panel) and 650 nm (bottom panel).

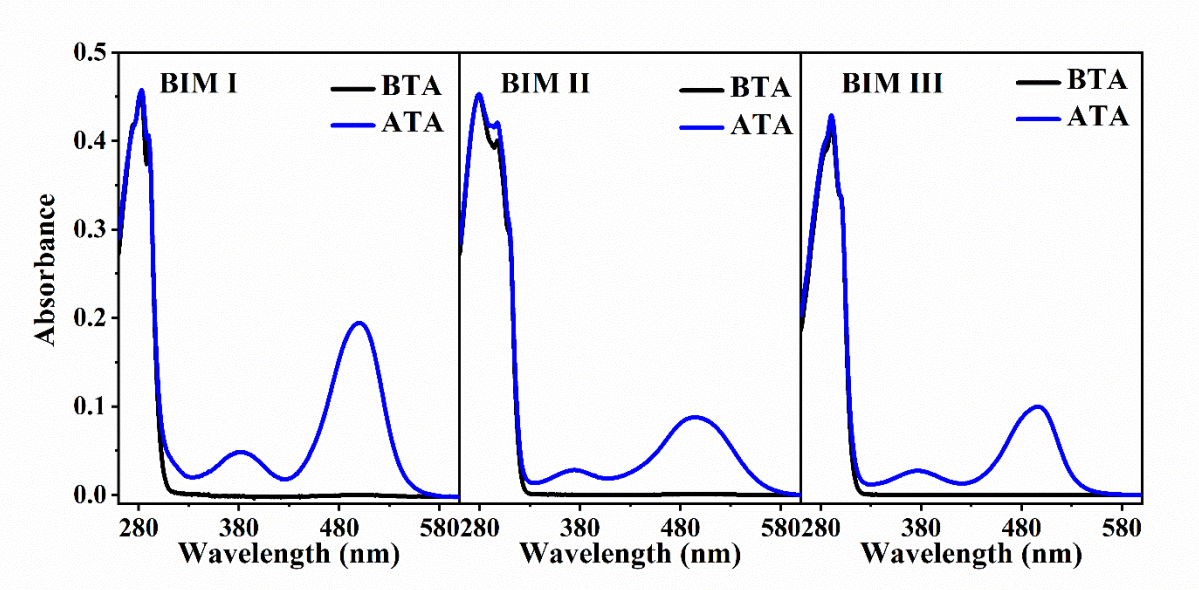


Figure S4. The absorption spectra of BIM derivatives in the presence of HCl before TA (black) and after TA (blue) measurements.

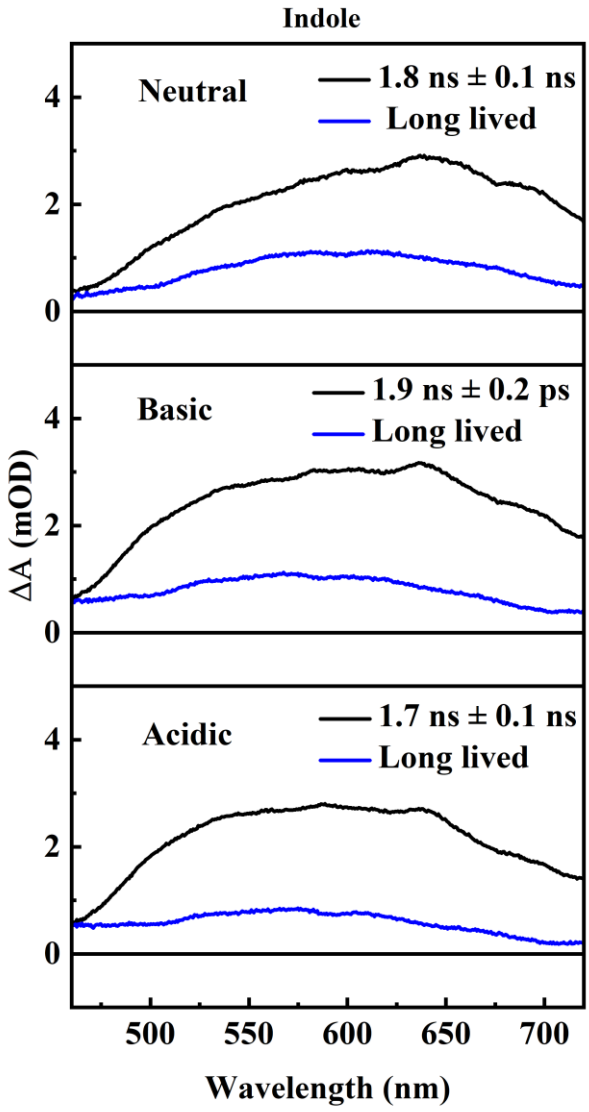


Figure S5. EADS of Indole in neutral, alkaline, and acidic medium (from top to bottom).

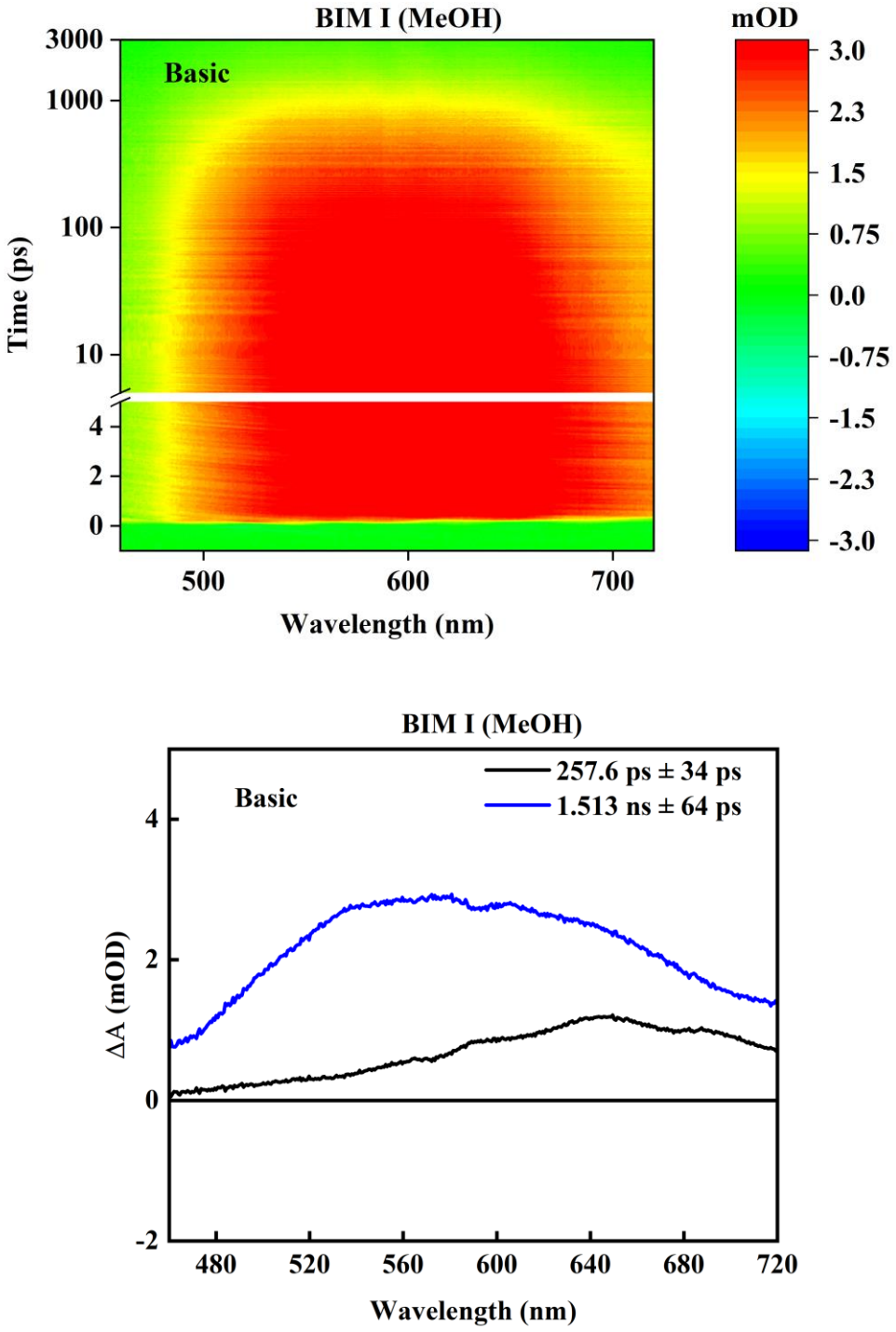


Figure S6. 2D contour plot (above) and EADS spectrum (below) of BIM I in alkaline medium.

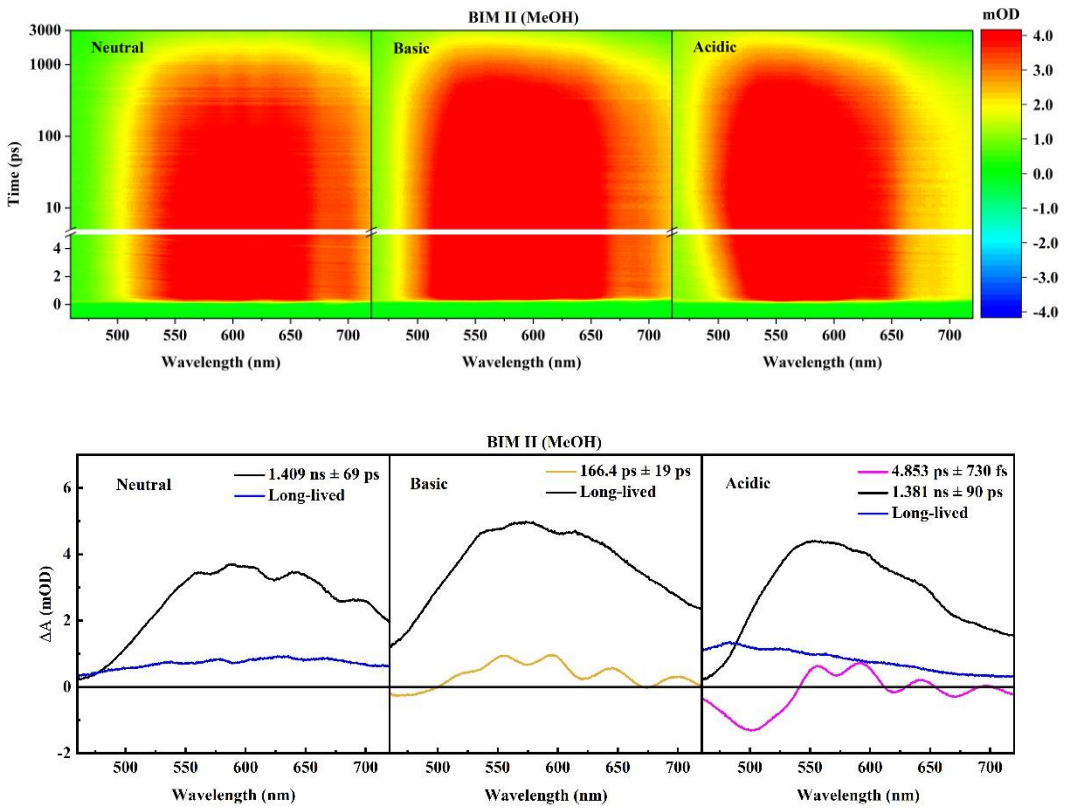


Figure S7. 2D contour plots (above) and EADS spectra (below) of BIM II in neutral, alkaline and acidic mediums (from left to right).

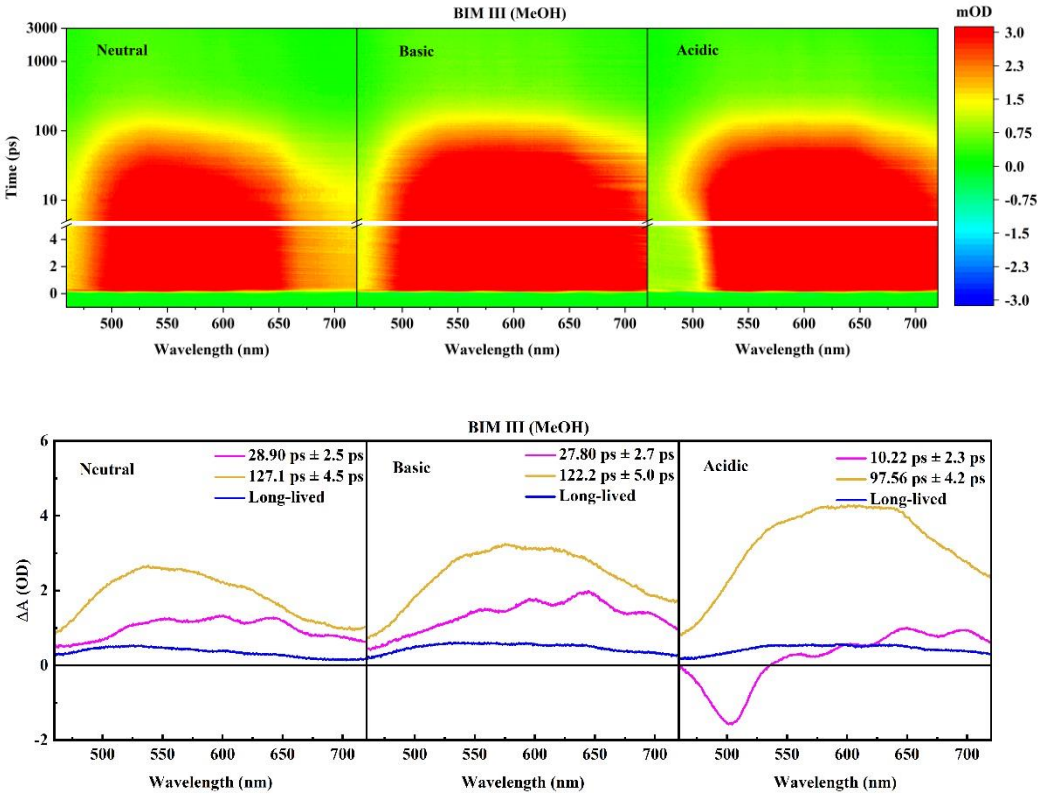


Figure S8. 2D contour plots (above) and EADS spectra (below) of BIM III in neutral, alkaline and acidic mediums (from left to right).

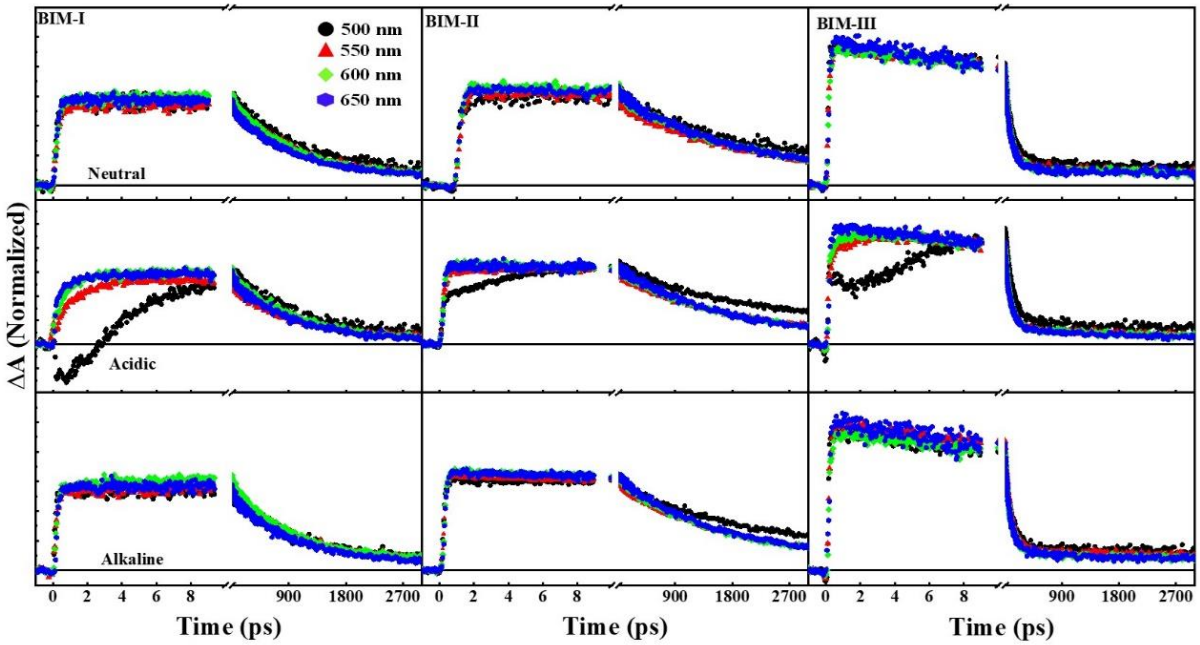


Figure S9: The kinetic traces of BIM I (coloum 1), BIM II (column 2), and BIM III (coloumn 3) at 500 nm (black), 550 nm (red), 600 nm (green) and 650 nm (dark blue) in neutral (row 1), acidic (row 2) and alkaline (row 3) medium.

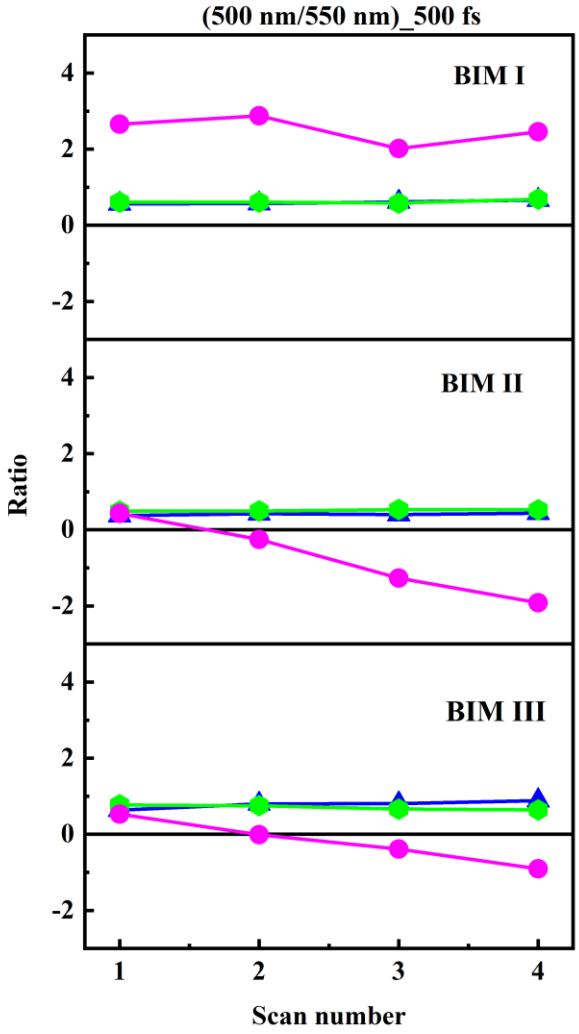


Figure S10. The ratio of 500 nm to 550 nm of BIM I, BIM II, and BIM III (from top to bottom) at 500 fs delay between pump and probe signals after completion of every scan where blue, green, and magenta lines represent the neutral, basic and acidic conditions, respectively.

DFT calculations of BIM derivatives

Compounds	E (a.u)	E_{HOMO}	E_{LUMO}	E_{LUMO+1}	$E_{HOMO-LUMO}$	λ_{H-L}, $\lambda_{H-(L+1)}$ (nm)	λ_{exp}	μ(D)
BIM I	-996.79	-0.307	-0.174	-0.171	-0.133	342.6, 335	282	3.027
BIM II	-1225.83	-0.293	-0.172	-0.169	-0.121	376.5, 367	279	3.557
BIM III	-1915.99	-0.303	-0.173	-0.172	-0.130	350.5, 348	291	6.30

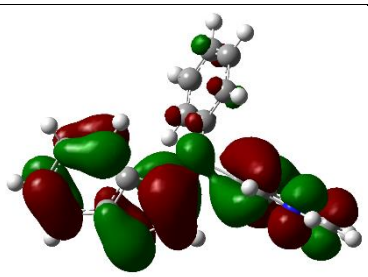
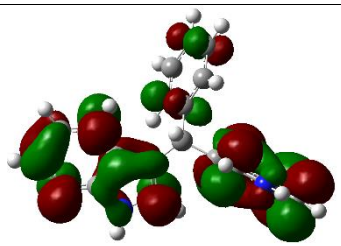
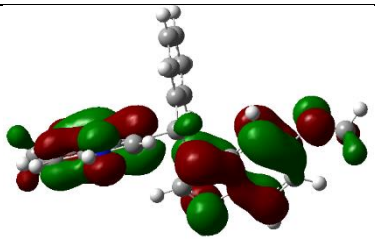
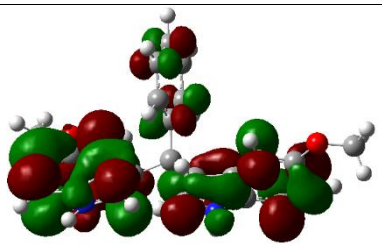
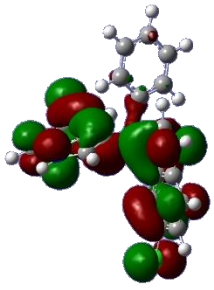
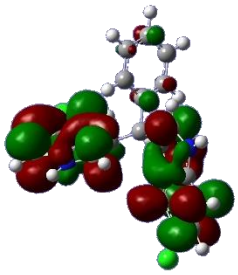
Compound	HOMO	LUMO
BIM I		
BIM II		
BIM III		

Figure S11. Frontier molecular orbitals (FMOs) and energies of BIM I, BIM II, and BIM III.

Compounds	E (a.u)	E_{HOMO}	E_{LUMO}	E_{LUMO+1}	$E_{HOMO-LUMO}$	λ_{H-L}, $\lambda_{H-(L+1)}$ (nm)	λ_{exp}	μ (D)
BIM I_ox	-995.58	-0.307	-0.222	-0.173	-0.085	536, 340	500, 380	4.93
BIM II_ox	-1224.62	-0.298	-0.219	-0.171	-0.079	577, 359	517, 370	4.92
BIM III_ox	-1914.77	-0.304	-0.221	-0.172	-0.083	549, 345	497, 375	5.69

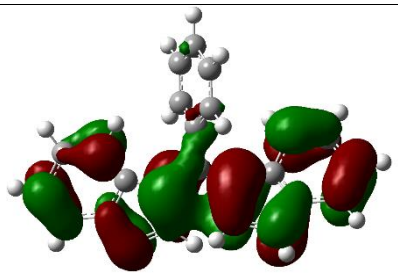
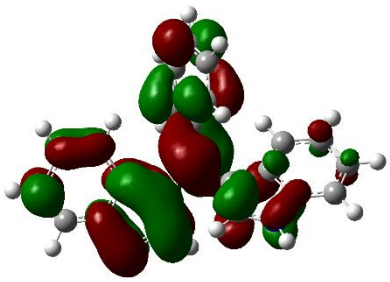
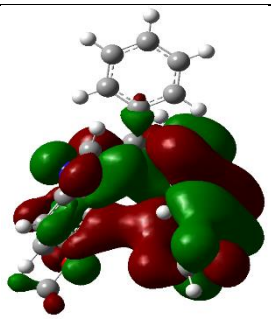
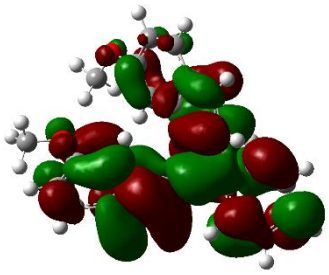
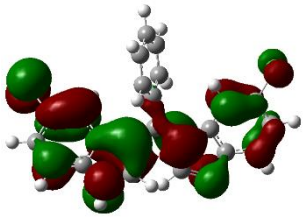
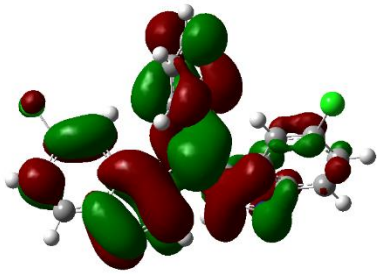
Compound	HOMO	LUMO
BIM I_ox		
BIM II_ox		
BIM III_ox		

Figure S12. Frontier molecular orbitals (FMOs) and energies of oxidised BIM I, BIM II, and BIM III.

Compounds	E (a.u)	E_{HOMO}	E_{LUMO}	E_{LUMO+1}	$E_{HOMO-LUMO}$	λ_{H-L}, $\lambda_{H-(L+1)}$ (nm)	μ (D)
BIM I_pro	-997.75	-0.213	-0.187	-0.166	-0.026	1752, 969	6.37
BIM II_pro	-1226.78	-0.204	-0.186	-0.165	-0.018	2531, 1168	7.12
BIM III_pro	-1916.99	-0.207	-0.189	-0.166	-0.018	2531, 1111	10.10

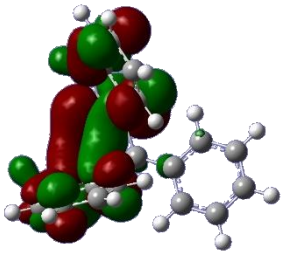
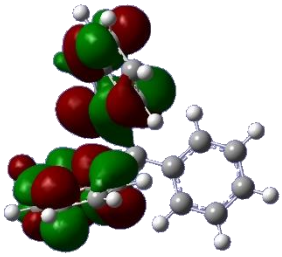
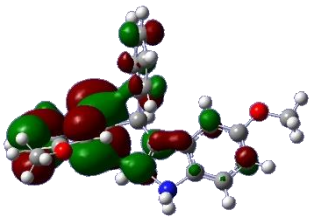
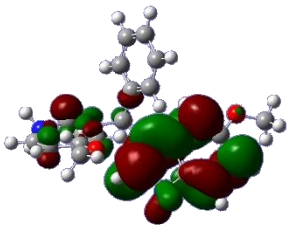
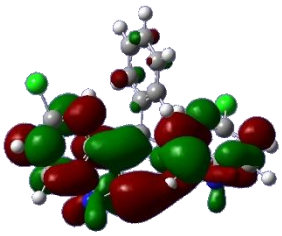
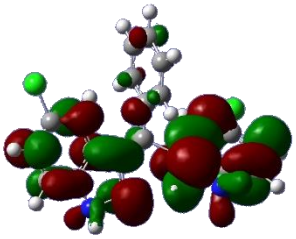
Compound	HOMO	LUMO
BIM I_pro		
BIM II_pro		
BIM III_pro		

Figure S13. Frontier molecular orbitals (FMOs) and energies of protonated BIM I, BIM II, and BIM III.

Compounds	E (a.u)	E_{HOMO}	E_{LUMO}	E_{LUMO+1}	$E_{HOMO-LUMO}$	λ_{H-L}, $\lambda_{H-(L+1)}$ (nm)	μ (D)
BIM I_ox_pro	-996.07	-0.234	-0.182	-0.171	-0.052	876, 723	13.09
BIM II_ox_pro	-1225.12	-0.233	-0.180	-0.167	-0.053	859, 690	11.02
BIM III_ox_pro	-1915.27	-0.234	-0.182	-0.169	-0.052	876, 701	13.36

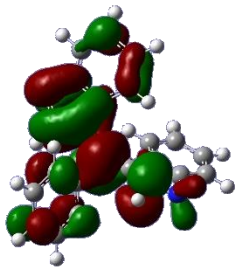
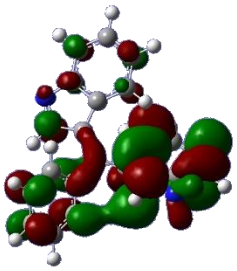
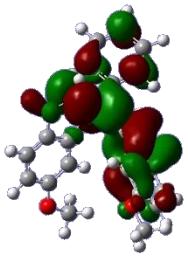
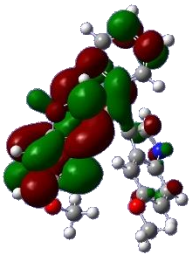
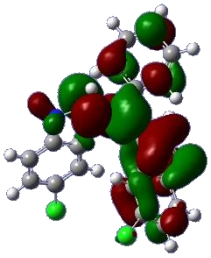
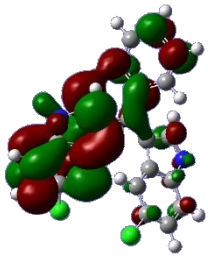
Compounds	HOMO	LUMO
BIM I_ox_pro		
BIM II_ox_pro		
BIM III_ox_pro		

Figure S14. Frontier molecular orbitals (FMOs) and energies of oxidised protonated BIM I, BIM II, and BIM III derivatives.

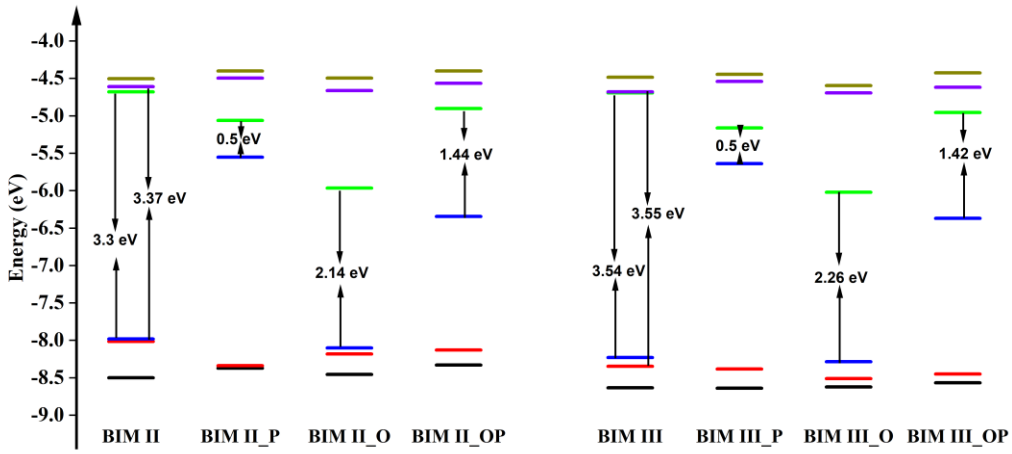


Figure S15. Energy level diagram of BIM-II(left) and BIM-III (right) in native, protonated, oxidised and protonated-oxidised forms, respectively, from left to right.

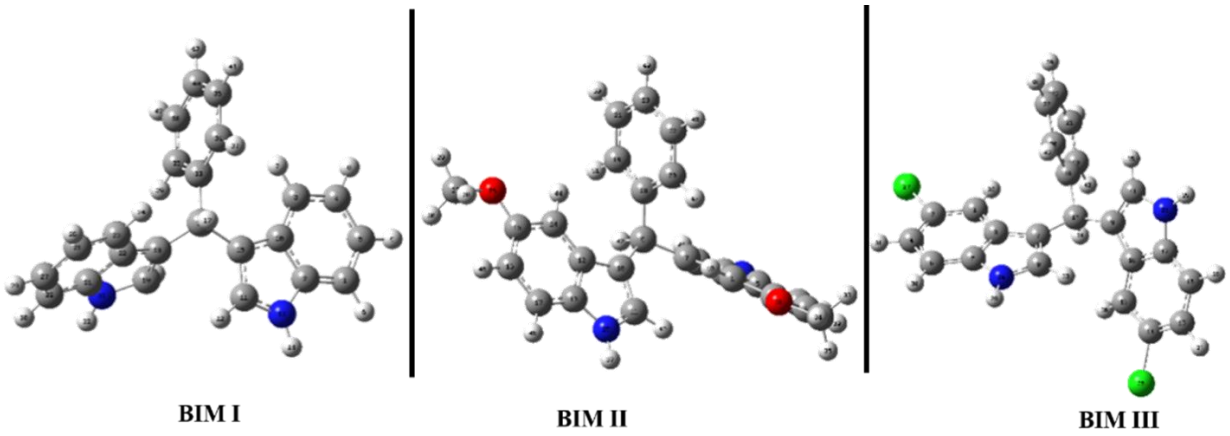


Figure S16: Optimised TD-DFT structure of the excited state of BIM I to III.

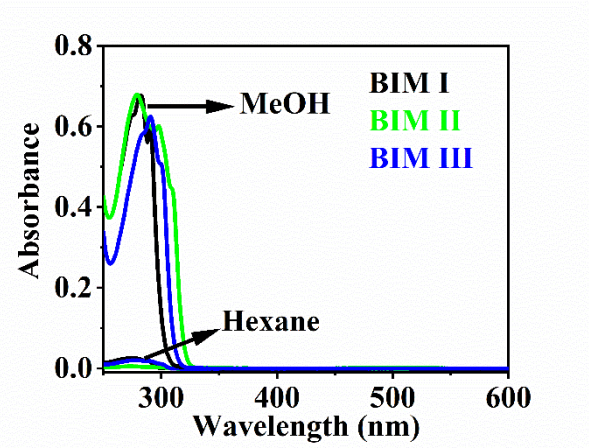


Figure S17. Comparison of absorbance of BIMs in Hexane (nonpolar) and Methanol (polar).

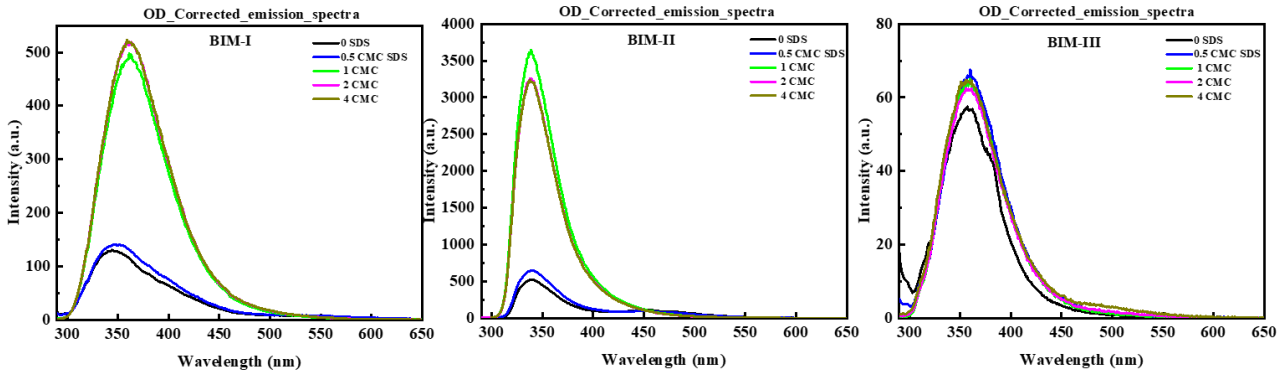


Figure S18. OD corrected emission spectra of BIM I (left), BIM II (middle) and BIM III (right) in SDS.

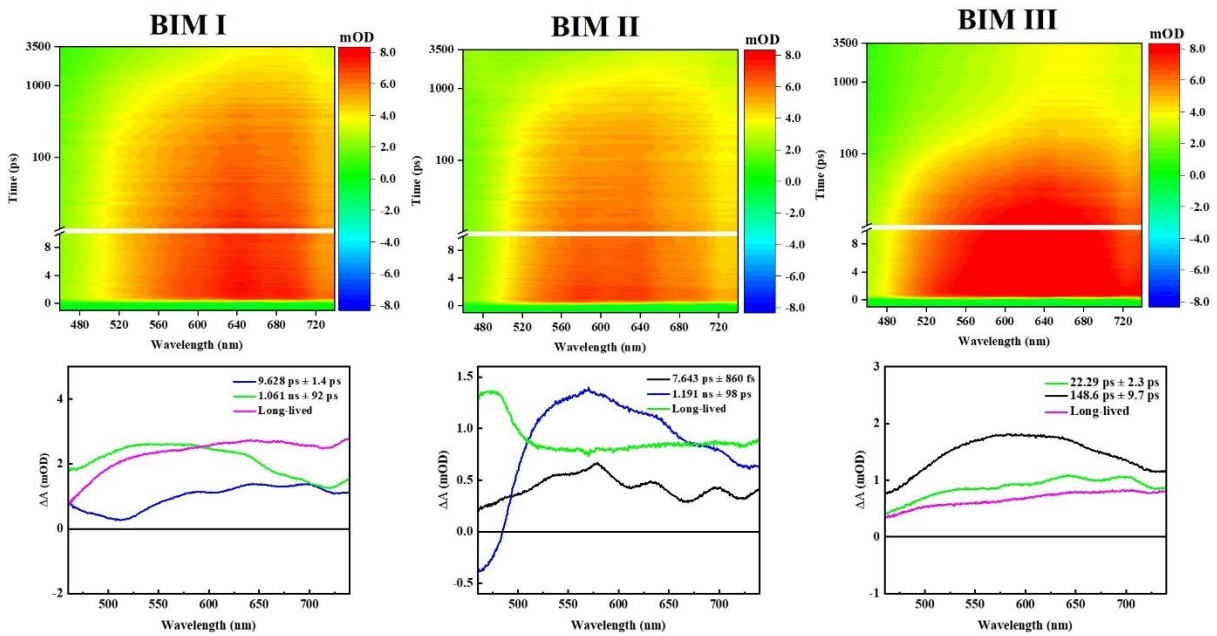


Figure S19: 2D contour plots (above) and EADS spectra (below) of BIM I to III in SDS.

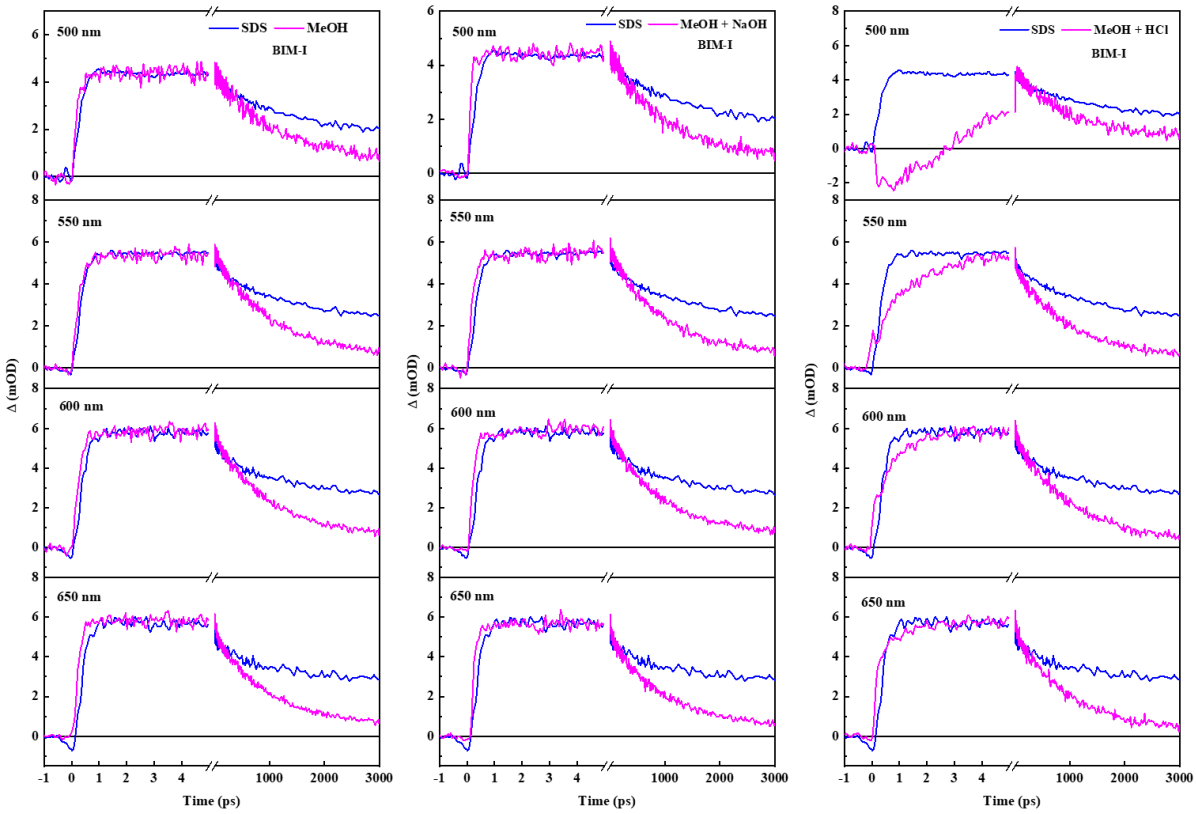


Figure S20. Comparison of Kinetic traces of BIM-I in SDS with neutral, alkaline and acidic media.

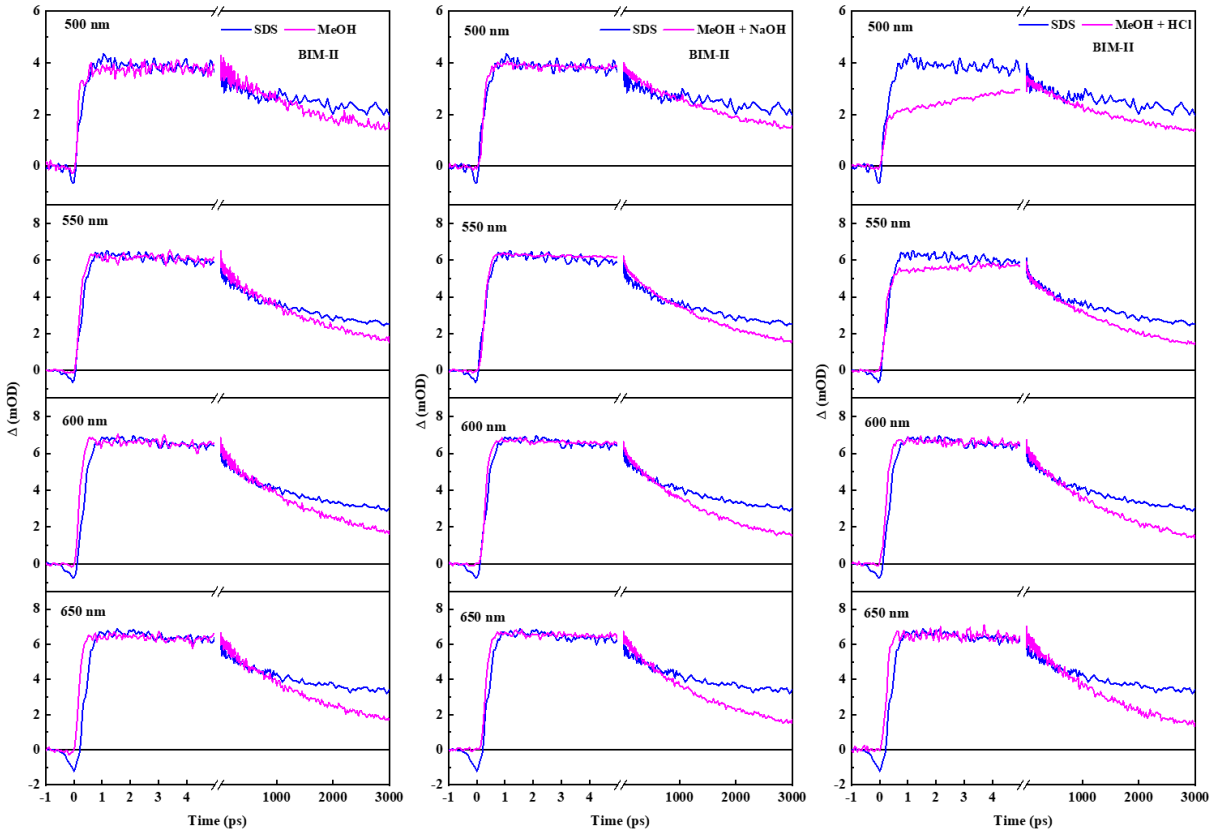


Figure S21. Comparison of Kinetic traces of BIM-II in SDS with neutral, alkaline and acidic media.

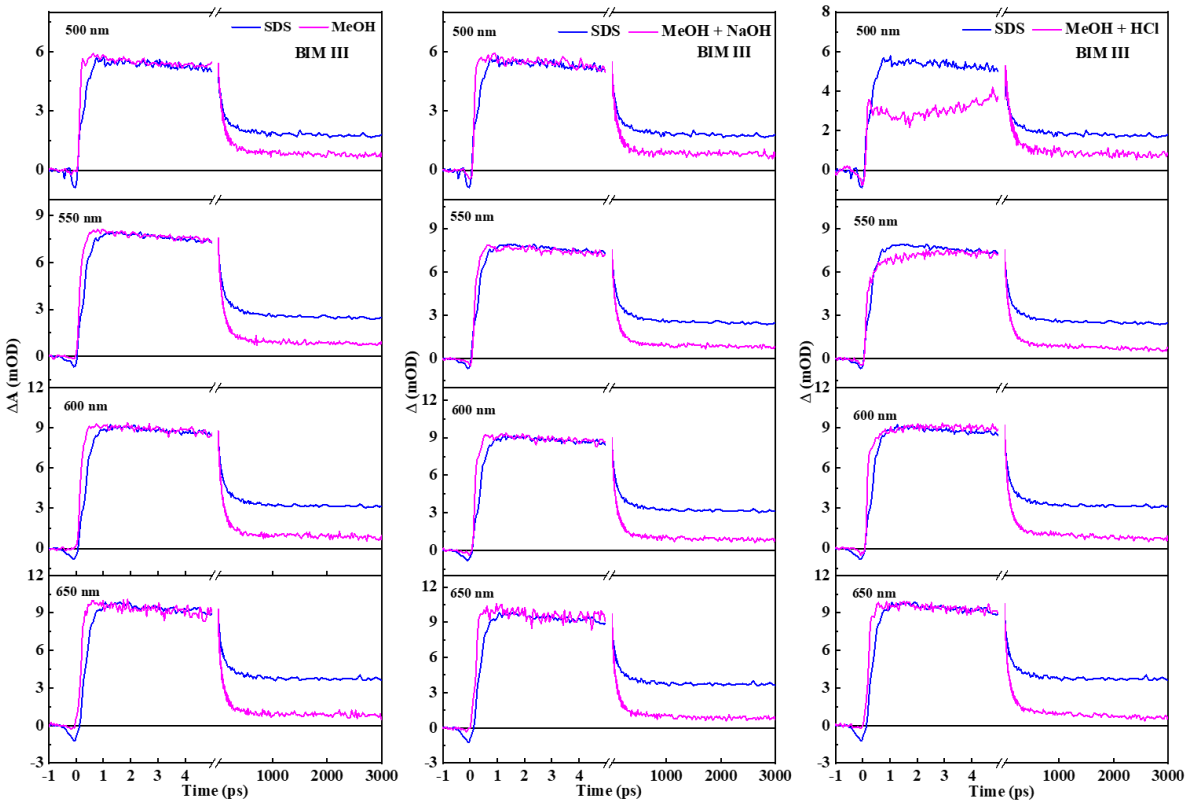


Figure S22. Comparison of Kinetic traces of BIM-III in SDS with neutral, alkaline and acidic media.

Table ST1: Lifetimes obtained by fitting kinetic traces at 550 nm for Indole, BIM I, BIM II and BIM III.

Name	**Solvent**	τ_1**(ps)**	τ_2**(ps)**	τ_3**(ns)**
Indole	Neutral		1840 ± 130	> 3
	Basic		1860 ± 150	> 3
	Acidic		1710 ± 110 ps	> 3
BIM I	Neutral	135.5 ± 19	1420 ± 36	
	Basic	257.6 ± 34	1510 ± 64	
	Acidic	2.9 ± 0.3	33.39 ± 9.3	1.22 ± 0.03
BIM II	Neutral		1410 ± 69	> 3
	Basic	166.4 ± 19	2330 ± 19	
	Acidic	4.85 ± 0.7	1380 ± 90	> 3
BIM III	Neutral	28.90 ± 2.5	127.1 ± 4.5	> 3
	Basic	27.8 ± 2.7	122.2 ± 5.0	> 3
	Acidic	10.22 ± 2.3	97.56 ± 4.2	> 3

Table ST2: Vibrational frequency of *meso* CH bond in the ground state.

Compound	C-H frequency (cm^{-1})
BIM I	2995.06
BIM II	2994.65
BIM III	2990.42
BIM I_pro	2970.77
BIM II_pro	3002.83
BIM III_pro	2966.15

Table ST3: The computed dihedral angle for the ground and excited states for BIM I, BIM II and BIM III.

Compound		Dihedral angle	
		Ground State	Excited State
BIM I	C3C9C16C33	-57.58355	6.70579
	C8C9C16C33	122.36151	-171.74662
	C19C18C16C33	116.75826	94.23080
	C22C18C16C33	-66.54589	-90.66604
BIM II	C3C9C16C33	58.28880	78.85317
	C8C9C16C33	-121.28754	-98.94507
	C19C18C16C33	-116.08047	-143.62470
	C22C18C16C33	67.15799	39.61384
BIM III	C3C9C16C33	66.43676	38.91048
	C8C9C16C33	-113.94213	-146.35655
	C19C18C16C33	12.92436	18.09717
	C22C18C16C33	-165.26765	-163.13480

Table ST4: Vibrational frequency of *meso* CH bond in the first excited state.

Compound	C-H frequency (cm^{-1})
BIM I	2961.44
BIM II	2988.24
BIM III	2966.92

Table ST5: The optimised energies of different molecules.

Compound	Energy (Hartree)
BIM I	-996.79
BIM III	-1225.83
BIM II	-1915.99
BIM I_pro	-997.75
BIM III_pro	-1226.78
BIM II_pro	-1916.99
BIM I_ox	-995.58
BIM II_ox	-1224.62
BIM III_ox	-1914.77
BIM I_ox_pro	-996.07
BIM II_ox_pro	-1225.12
BIM II_ox_pro	-1915.27

Cartesian coordinates of optimised structures:

1. BIM I

		X	Y	Z
1	C	-4.6191870	-1.4498160	0.0436950
2	C	-3.4523300	-1.1219960	-0.6550260
3	C	-2.3097070	-0.5599290	-0.0175260
4	C	-2.3652850	-0.3243750	1.3694830
5	C	-3.5219030	-0.6485850	2.0669950
6	C	-4.6385470	-1.2068880	1.4116430
7	N	-3.1522900	-1.2501570	-1.9952530
8	C	-1.8696440	-0.7860860	-2.2176510
9	C	-1.3070240	-0.3578310	-1.0413440
10	H	-5.4794080	-1.8782780	-0.4646880
11	H	-5.5296570	-1.4492670	1.9843700
12	H	-3.5709920	-0.4655130	3.1370190
13	H	-1.5167890	0.1141990	1.8845210
14	H	-1.4449370	-0.8023540	-3.2126610
15	H	-3.7770100	-1.6007980	-2.7039520
16	C	0.0945010	0.2064950	-0.9110510
17	H	0.4600380	0.3316950	-1.9418870
18	C	1.0622090	-0.7408950	-0.2331160
19	C	0.7709940	-1.8944130	0.4514210
20	N	1.9386280	-2.5041600	0.8725380
21	C	3.0203310	-1.7548520	0.4572740
22	C	2.5038470	-0.6298040	-0.2431430
23	C	3.4069370	0.3046630	-0.7800450
24	C	4.7711540	0.0988210	-0.6148300
25	C	5.2592190	-1.0246570	0.0832770
26	C	4.3924000	-1.9647930	0.6291590
27	H	-0.1896190	-2.3380350	0.6691460
28	H	1.9876590	-3.3696140	1.3863320
29	H	4.7685230	-2.8306990	1.1683940
30	H	6.3315060	-1.1581140	0.1985350
31	H	5.4763180	0.8162940	-1.0257380
32	H	3.0421310	1.1815190	-1.3080090
33	C	0.0738800	1.6241430	-0.3083580
34	C	-0.4793300	2.6699290	-1.0612670
35	C	-0.5333470	3.9681300	-0.5581700
36	C	-0.0335530	4.2466120	0.7167780

37	C	0.5195080	3.2155660	1.4745930
38	C	0.5748510	1.9152500	0.9644620
39	H	1.0213870	1.1223680	1.5566200
40	H	0.9156630	3.4196950	2.4662470
41	H	-0.0734450	5.2582640	1.1120660
42	H	-0.9650920	4.7634320	-1.1607710
43	H	-0.8804850	2.4572920	-2.0500480

2. BIM II

1	C	-4.7675600	0.9098270	-1.2726590
2	C	-3.4691590	0.6307170	-1.6957150
3	C	-2.4337870	0.2916900	-0.7778870
4	C	-2.7349340	0.2381320	0.5917730
5	C	-4.0327990	0.5176760	1.0164740
6	C	-5.0454040	0.8525800	0.0910290
7	N	-2.9186130	0.6143580	-2.9640800
8	C	-1.5848650	0.2726640	-2.8675440
9	C	-1.2329990	0.0704750	-1.5556910
10	H	-5.5509210	1.1671110	-1.9810890
11	H	-6.0517040	1.0681160	0.4302840
12	O	-4.2379440	0.4448610	2.3741440
13	H	-1.9875620	-0.0272830	1.3306890
14	H	-0.9705970	0.2033240	-3.7557110
15	H	-3.4164180	0.7892220	-3.8221860
16	C	0.1563730	-0.3153370	-1.0862250
17	H	0.7316610	-0.5195980	-2.0023820
18	C	0.8848330	0.8037200	-0.3725560
19	C	0.3659670	1.9863870	0.0945740
20	N	1.3675990	2.7667150	0.6377100
21	C	2.5738030	2.0988670	0.5253300
22	C	2.3055520	0.8529130	-0.1071760
23	C	3.3651490	-0.0313260	-0.3517940
24	C	4.6562080	0.3344170	0.0269220
25	C	4.9049770	1.5745890	0.6545650
26	C	3.8627010	2.4645440	0.9084000
27	H	-0.6553650	2.3381050	0.0770410
28	H	1.2365950	3.6794810	1.0430970
29	H	4.0622010	3.4172230	1.3925270
30	H	5.9110810	1.8498530	0.9481590
31	O	5.6377370	-0.5875380	-0.2515110

32	H	3.2088690	-0.9993490	-0.8169500
33	C	0.1344690	-1.6465520	-0.3110020
34	C	-0.1438390	-2.8305950	-1.0086810
35	C	-0.1890660	-4.0586730	-0.3520550
36	C	0.0425070	-4.1256810	1.0243670
37	C	0.3209260	-2.9554000	1.7287700
38	C	0.3692510	-1.7262310	1.0651610
39	H	0.6017780	-0.8223430	1.6198820
40	H	0.5064330	-2.9943000	2.7992790
41	H	0.0087260	-5.0820130	1.5397930
42	H	-0.4040230	-4.9642420	-0.9141000
43	H	-0.3356100	-2.7834670	-2.0787200
44	C	-5.5401550	0.6817730	2.8717010
45	H	-5.4755490	0.5563680	3.9547820
46	H	-6.2690910	-0.0361120	2.4701090
47	H	-5.8857060	1.7014560	2.6492860
48	C	6.9677290	-0.2879400	0.1230620
49	H	7.5673110	-1.1482480	-0.1826010
50	H	7.0664770	-0.1494910	1.2090230
51	H	7.3448940	0.6106760	-0.3855530

3. BIM III

1	C	-2.9192950	2.7972050	-1.6555100
2	C	-1.8530510	1.8992400	-1.5530400
3	C	-1.7414320	0.9760820	-0.4774480
4	C	-2.7382370	0.9545390	0.5132180
5	C	-3.7887450	1.8521920	0.4002090
6	C	-3.8917850	2.7685280	-0.6635140
7	N	-0.7625140	1.6997530	-2.3736950
8	C	0.0299160	0.6998460	-1.8425810
9	C	-0.5265080	0.2223140	-0.6816520
10	H	-2.9934410	3.5000820	-2.4808820
11	H	-4.7357090	3.4483110	-0.7023910
12	Cl	-5.0556550	1.8521440	1.6307690
13	H	-2.6992940	0.2527010	1.3391020
14	H	0.9499130	0.4104640	-2.3293960
15	H	-0.5406690	2.2405080	-3.1947540
16	C	0.0082370	-0.8677750	0.2249920
17	H	-0.0058990	-0.4602490	1.2481020
18	C	1.4511440	-1.2260000	-0.0765910

19	C	1.9357440	-2.4224360	-0.5449370
20	N	3.3110550	-2.3643180	-0.6677240
21	C	3.7511860	-1.1209400	-0.2653880
22	C	2.6018320	-0.3723870	0.1105860
23	C	2.7636670	0.9485630	0.5642750
24	C	4.0495940	1.4626620	0.6296120
25	C	5.1844360	0.7167830	0.2577070
26	C	5.0419760	-0.5885370	-0.1964890
27	H	1.3996290	-3.3265270	-0.7944280
28	H	3.8998120	-3.1283510	-0.9598930
29	H	5.9129920	-1.1704120	-0.4856220
30	H	6.1672960	1.1693820	0.3282560
31	Cl	4.2853680	3.1192550	1.1945950
32	H	1.9110260	1.5555720	0.8483090
33	C	-0.8867050	-2.1115680	0.2511970
34	C	-1.4728180	-2.6171540	-0.9157720
35	C	-2.2521230	-3.7748980	-0.8784850
36	C	-2.4614840	-4.4432820	0.3291320
37	C	-1.8843680	-3.9463580	1.4991180
38	C	-1.1022290	-2.7913980	1.4568990
39	H	-0.6517940	-2.4111080	2.3714790
40	H	-2.0459650	-4.4545030	2.4462950
41	H	-3.0749900	-5.3397880	0.3595010
42	H	-2.7033400	-4.1498080	-1.7937090
43	H	-1.3281710	-2.0894260	-1.8544300

4. BIM l_pro

1	C	3.7205140	-1.6877230	0.8024680
2	C	2.7635040	-1.4355100	-0.1551380
3	C	0.9989540	-1.2239220	1.4582450
4	C	1.9497250	-1.4750370	2.4394080
5	C	3.3073400	-1.7024400	2.1438810
6	H	4.7602290	-1.8701390	0.5350440
7	H	-0.0344600	-1.0655290	1.7378760
8	H	1.6292600	-1.4956280	3.4787740
9	H	4.0240940	-1.8915980	2.9360570
10	C	1.3842570	-1.1902670	0.0874440
11	C	1.6691290	-0.9355210	-2.2290840
12	H	1.4706660	-1.4458740	-3.1718960
13	N	2.9869390	-1.4182310	-1.6255360

14	H	3.7728380	-0.8103790	-1.8773760
15	C	0.7213930	-0.9743080	-1.1540920
16	C	-0.6783790	-0.4709920	-1.4118500
17	H	-0.8864650	-0.6411770	-2.4810120
18	C	-0.4820380	1.0113640	-1.2465360
19	C	0.0186640	1.7730540	-2.3275080
20	H	0.6964450	1.3160570	-3.0545100
21	C	0.1141910	3.0440820	-0.2970420
22	C	-0.4860800	1.7880000	-0.0398150
23	C	-0.9748120	1.5995190	1.2772060
24	H	-1.4771970	0.6789840	1.5472760
25	C	-0.8424120	2.6204070	2.2146290
26	H	-1.2294920	2.4596700	3.2181460
27	C	-0.2363490	3.8499180	1.9097420
28	H	-0.1566390	4.6288140	2.6610130
29	C	0.2624580	4.0653300	0.6144080
30	H	0.7479660	5.0028820	0.3501580
31	N	0.6081480	3.0410690	-1.6985490
32	H	0.2982230	3.8714420	-2.2087420
33	C	-1.8353660	-1.1225960	-0.6626520
34	C	-3.0597960	-0.4497170	-0.5402110
35	C	-1.7464280	-2.4320270	-0.1737490
36	C	-4.1594800	-1.0631650	0.0597640
37	H	-3.1423340	0.5656730	-0.9191400
38	C	-2.8453990	-3.0489820	0.4281850
39	H	-0.8055690	-2.9661790	-0.2667170
40	C	-4.0566980	-2.3672880	0.5496640
41	H	-5.0982880	-0.5211020	0.1451510
42	H	-2.7514940	-4.0647050	0.8051090
43	H	-4.9112710	-2.8452660	1.0220070
44	H	3.2463570	-2.3593850	-1.9594460
45	H	1.6401700	3.0604820	-1.7133750

5. BIM III_pro

1	C	3.2317940	-0.3018370	-0.2380990
2	C	4.6113080	-0.1862960	-0.2530110
3	C	2.4400060	0.8754930	-0.3974340
4	C	5.3097770	1.0250200	-0.4194420
5	C	3.1808010	2.0814940	-0.5698860
6	C	4.5509930	2.1920300	-0.5940710

7	C	1.0538630	1.1688770	-0.4192700
8	C	0.8496970	2.5863870	-0.4754610
9	C	-1.2940000	0.8553760	0.3650930
10	C	-2.6745680	0.5990200	0.1370070
11	C	-1.1194340	1.7860930	1.3970470
12	C	-3.4553680	1.4141170	0.9969640
13	C	-3.3884470	-0.2904540	-0.7080200
14	C	-4.7723240	-0.2997990	-0.6374230
15	C	-5.5227830	0.5267040	0.2218590
16	C	-4.8288850	1.4141960	1.0613200
17	C	-0.1341680	0.2363710	-0.3738350
18	C	0.1529200	-1.1644460	0.1667400
19	C	0.1836070	-2.2613130	-0.7020560
20	C	0.3770670	-1.3844040	1.5335850
21	C	0.4437980	-3.5494770	-0.2234980
22	C	0.6422510	-2.6651960	2.0121560
23	C	0.6784080	-3.7549000	1.1346190
24	N	2.2123580	3.1809350	-0.8108360
25	N	-2.5186030	2.2693790	1.7758630
26	Cl	-5.6590500	-1.4070420	-1.6897400
27	Cl	5.5737670	-1.6574790	-0.0485250
28	H	2.4151050	3.9997280	-0.2323930
29	H	-2.6691040	2.1682090	2.7841380
30	H	5.0448390	3.1501510	-0.7451650
31	H	6.3917630	1.0482440	-0.4173540
32	H	2.7738560	-1.2716000	-0.1032560
33	H	0.0566940	3.0323790	-1.0758550
34	H	-0.4841260	0.1068140	-1.4127560
35	H	-0.3268800	2.5374120	1.4385090
36	H	-2.8696340	-0.9557360	-1.3881610
37	H	-6.6036390	0.4712760	0.2351710
38	H	-5.3756270	2.0712810	1.7343270
39	H	0.8867180	-4.7533360	1.5099680
40	H	0.8217240	-2.8170770	3.0736650
41	H	0.4646150	-4.3878040	-0.9152540
42	H	0.0145030	-2.1065810	-1.7657860
43	H	0.3411690	-0.5382400	2.2140730
44	H	2.2718810	3.5021950	-1.7930290
45	H	-2.6582070	3.2690000	1.5651530

6. BIM II_pro

1	C	-2.8849270	-0.5526430	-0.8399630
2	C	-4.1844920	-1.0600470	-0.8183460
3	C	-2.5931100	0.7869850	-0.5401080
4	C	-5.2405380	-0.2128420	-0.4742510
5	C	-3.6730970	1.6412000	-0.1726060
6	C	-4.9690700	1.1168720	-0.1506390
7	C	-1.2044730	1.2554890	-0.6039000
8	C	-0.7266880	2.4918460	-0.9237960
9	C	-0.0000710	0.3441610	-0.3505960
10	C	1.2042730	1.2555470	-0.6038920
11	C	0.7264170	2.4918970	-0.9237520
12	C	2.5928780	0.7870330	-0.5401240
13	C	3.6727910	1.6413110	-0.1725270
14	C	2.8847700	-0.5525190	-0.8401450
15	C	4.1843780	-1.0598310	-0.8185150
16	C	5.2403480	-0.2125900	-0.4742330
17	C	4.9687890	1.1170790	-0.1504790
18	C	0.0001060	-0.2949880	1.0345630
19	C	-0.0001220	0.5097840	2.1825020
20	C	0.0006510	-1.6840380	1.1929350
21	C	0.0001630	-0.0602030	3.4534750
22	C	0.0008760	-2.2600470	2.4659700
23	C	0.0006650	-1.4503240	3.6003360
24	N	-3.4679790	2.9978300	0.1367850
25	N	3.4674400	2.9978940	0.1368400
26	O	4.3142110	-2.3852060	-1.1526450
27	C	5.6151370	-2.9415760	-1.1478930
28	H	6.0748920	-2.8947190	-0.1506370
29	H	5.4975750	-3.9875400	-1.4388970
30	H	6.2758770	-2.4392940	-1.8684570
31	O	-4.3142090	-2.3854940	-1.1522010
32	C	-5.6150850	-2.9419670	-1.1472610
33	H	-6.2758550	-2.4400070	-1.8680260
34	H	-5.4974330	-3.9880300	-1.4378740
35	H	-6.0748620	-2.8947710	-0.1500320
36	H	-4.2126200	3.3853310	0.7064380
37	H	2.5643620	3.1781630	0.5645090
38	H	-5.7932580	1.7698780	0.1295570
39	H	-6.2647950	-0.5666290	-0.4456170
40	H	-2.0904210	-1.2332350	-1.1239970

41	H	-1.3297060	3.3453660	-1.2118230
42	H	-0.0000460	-0.4606830	-1.0987930
43	H	1.3293800	3.3454750	-1.2117000
44	H	2.0903030	-1.2330800	-1.1243670
45	H	6.2646140	-0.5663360	-0.4454740
46	H	5.7929270	1.7700830	0.1298800
47	H	0.0007990	-2.3256000	0.3148570
48	H	0.0012140	-3.3422700	2.5662430
49	H	0.0009230	-1.8957670	4.5916390
50	H	0.0000250	0.5801200	4.3321160
51	H	-0.0005230	1.5916090	2.0722760
52	H	-2.5649760	3.1782910	0.5645550
53	H	4.2119530	3.3856340	0.7064950

7. BIM I_ox

1	C	-4.7942110	-1.4785210	-0.1133870
2	C	-3.4199840	-1.4914410	-0.3671530
3	C	-2.5379070	-0.4929440	0.1222760
4	C	-3.0692760	0.5436100	0.9091910
5	C	-4.4349510	0.5643230	1.1643880
6	C	-5.2904630	-0.4337310	0.6570170
7	N	-2.6565190	-2.4033280	-1.0789680
8	C	-1.3416740	-2.0234660	-1.0501250
9	C	-1.1991030	-0.8551210	-0.3181910
10	H	-5.4480400	-2.2561510	-0.4993100
11	H	-6.3538660	-0.3891220	0.8746000
12	H	-4.8531230	1.3646020	1.7684990
13	H	-2.4232440	1.3180880	1.3089310
14	H	-0.5885050	-2.5817330	-1.5874650
15	H	-3.0182760	-3.1979670	-1.5842030
16	C	0.0632310	-0.1549570	-0.0940820
17	C	1.2294940	-0.8505770	0.1297340
18	C	1.3151000	-2.2627400	0.5398680
19	N	2.5281050	-2.7018340	0.7054410
20	C	3.3745650	-1.6220510	0.3718810
21	C	2.6439160	-0.4505220	0.0423530
22	C	3.3318670	0.6983790	-0.3558030
23	C	4.7300240	0.6702730	-0.3901890
24	C	5.4401760	-0.4854090	-0.0410330
25	C	4.7653860	-1.6482500	0.3409940

26	H	0.4565540	-2.8829560	0.7772660
27	H	5.2977880	-2.5585660	0.6000390
28	H	6.5265970	-0.4788690	-0.0742260
29	H	5.2721580	1.5627760	-0.6915710
30	H	2.8040870	1.6052730	-0.6306670
31	C	0.0270670	1.3311930	-0.1408500
32	C	-0.6391920	1.9996640	-1.1822540
33	C	-0.6878960	3.3919490	-1.2173160
34	C	-0.0935110	4.1405040	-0.1988100
35	C	0.5560720	3.4879520	0.8517110
36	C	0.6205510	2.0955940	0.8785710
37	H	1.1252080	1.5876490	1.6946820
38	H	1.0121100	4.0634190	1.6527890
39	H	-0.1404890	5.2259590	-0.2208900
40	H	-1.1949540	3.8930620	-2.0374600
41	H	-1.1108020	1.4184090	-1.9690950

8. BIM II_ox

1	C	1.0519710	-3.9789510	0.7384150
2	C	0.0916140	-2.9816680	0.9384430
3	C	0.0557210	-1.8016230	0.1579680
4	C	0.9996610	-1.6271250	-0.8712800
5	C	1.9589480	-2.6164640	-1.0686340
6	C	1.9841620	-3.7827150	-0.2658980
7	N	-0.9723310	-2.9248990	1.8280680
8	C	-1.6757910	-1.7730790	1.6239810
9	C	-1.0822300	-1.0223370	0.6168600
10	H	1.0687810	-4.8811930	1.3439140
11	H	2.7565540	-4.5186950	-0.4634560
12	O	2.9387710	-2.5616940	-2.0210670
13	H	0.9771040	-0.7315990	-1.4771580
14	H	-2.5462460	-1.5398010	2.2204260
15	H	-1.1828160	-3.6164280	2.5313950
16	C	-1.6086430	0.2438720	0.1136500
17	C	-0.8246800	1.3106000	-0.2676640
18	C	-1.2695410	2.4369490	-1.1092050
19	N	-0.3453040	3.3162910	-1.3635950
20	C	0.7992420	2.8815960	-0.6631300
21	C	0.5804840	1.6476220	0.0086500

22	C	1.5830830	1.1032210	0.8038840
23	C	2.8136310	1.7777920	0.9012610
24	C	3.0342850	2.9812520	0.2158480
25	C	2.0157190	3.5402660	-0.5677870
26	H	-2.2563030	2.5161820	-1.5541890
27	H	2.1669350	4.4835420	-1.0842190
28	H	3.9856120	3.4948920	0.2934440
29	O	3.7433670	1.1655920	1.7022110
30	H	1.4609840	0.1771530	1.3521770
31	C	-3.0916610	0.3469110	0.0208400
32	C	-3.8578070	-0.7115220	-0.5037180
33	C	-5.2443420	-0.6129730	-0.5938160
34	C	-5.8985870	0.5358360	-0.1411670
35	C	-5.1549850	1.5865790	0.3985310
36	C	-3.7657500	1.4946790	0.4772590
37	H	-3.1912870	2.3046840	0.9157360
38	H	-5.6564510	2.4777880	0.7662170
39	H	-6.9810550	0.6084590	-0.2042290
40	H	-5.8159490	-1.4332200	-1.0200530
41	H	-3.3527890	-1.6035610	-0.8612400
42	C	3.0186050	-1.3944630	-2.8246450
43	H	2.1168920	-1.2638470	-3.4379880
44	H	3.1689900	-0.4955680	-2.2129970
45	H	3.8804540	-1.5398360	-3.4788270
46	C	5.0081010	1.7830130	1.8533790
47	H	5.5800780	1.1368600	2.5225760
48	H	5.5372790	1.8672630	0.8940470
49	H	4.9222930	2.7823990	2.3018240

9. BIM III_ox

1	C	-4.8115570	-1.7484580	0.6381820
2	C	-5.3730210	-0.6558940	-0.0094020
3	C	-4.5443620	0.3499810	-0.5412070
4	C	-3.1612760	0.3087270	-0.4457390
5	C	-2.5770560	-0.7837290	0.2174560
6	C	-3.4194660	-1.7981670	0.7415160
7	N	-2.6017720	-2.7601130	1.3113730
8	C	-1.2918570	-2.3959690	1.1606520
9	C	-1.2059600	-1.1876880	0.4858200
10	H	-5.4406280	-2.5352400	1.0447860

11	H	-6.4490040	-0.5720760	-0.1132080
12	Cl	-5.3051860	1.7122660	-1.3607400
13	H	-2.5567590	1.1016170	-0.8691530
14	H	-0.4957780	-2.9948090	1.5792720
15	H	-2.9216360	-3.5781420	1.8078320
16	C	0.0362460	-0.4904310	0.1636390
17	C	1.1579220	-1.1884360	-0.2225270
18	C	1.1784770	-2.5772120	-0.7114580
19	N	2.3609190	-3.0193840	-1.0258320
20	C	3.2527760	-1.9686080	-0.7301170
21	C	2.5795850	-0.8084590	-0.2663330
22	C	3.3142490	0.3156020	0.1153070
23	C	4.7041630	0.2572160	-0.0058600
24	C	5.3725390	-0.8749410	-0.4828960
25	C	4.6386000	-2.0058650	-0.8469490
26	H	0.2908660	-3.1760180	-0.8887470
27	H	5.1326920	-2.9032200	-1.2061620
28	H	6.4544060	-0.8670770	-0.5604690
29	Cl	5.6526370	1.6720890	0.4575340
30	H	2.8432590	1.2162630	0.4890880
31	C	0.0315270	0.9904480	0.2908790
32	C	-0.5022240	1.6093670	1.4345970
33	C	-0.5208500	2.9980640	1.5468810
34	C	-0.0303860	3.7922630	0.5077870
35	C	0.4857530	3.1898500	-0.6419210
36	C	0.5214580	1.8003910	-0.7485100
37	H	0.9205780	1.3315420	-1.6427680
38	H	0.8597470	3.8019510	-1.4578410
39	H	-0.0548680	4.8752440	0.5912480
40	H	-0.9234930	3.4610080	2.4435340
41	H	-0.8917640	0.9930890	2.2395320

10. BIM l_ox_pro

1	C	-2.3650820	-3.7528440	0.0327490
2	C	-1.2718640	-2.9711910	-0.2920200
3	C	-1.0337740	-1.6691540	0.1650840
4	C	-1.9839860	-1.1274480	1.0464190
5	C	-3.1019390	-1.8860480	1.3928070
6	C	-3.3071900	-3.1801620	0.8930680

7	H	-2.4905550	-4.7620130	-0.3518840
8	H	-1.8485820	-0.1311470	1.4461610
9	H	-3.8355940	-1.4581320	2.0699960
10	H	-4.1908750	-3.7429840	1.1763610
11	C	0.2707670	-1.2039060	-0.3272840
12	C	0.8150100	-2.2468690	-1.0853030
13	N	-0.1202760	-3.3999320	-1.1304590
14	C	0.9267410	0.0247100	-0.0121740
15	H	-0.4224360	-3.6204710	-2.0917050
16	H	1.7260010	-2.3258410	-1.6542300
17	C	-1.1472280	3.0456740	0.3608050
18	C	-2.2538770	3.8543630	0.1052980
19	C	-3.2590760	3.3689300	-0.7348230
20	C	-3.1502350	2.0987710	-1.3221460
21	C	-2.0466810	1.2808090	-1.0675350
22	C	-1.0412460	1.7389510	-0.2056430
23	H	-2.3114960	4.8459120	0.5459160
24	H	-4.1298200	3.9849470	-0.9463040
25	H	-3.9351200	1.7459390	-1.9871340
26	H	-1.9763820	0.3074610	-1.5450010
27	C	0.2547140	1.2402030	0.2357660
28	C	0.7820990	2.3451460	1.0197130
29	N	-0.0244890	3.3783820	1.1272060
30	C	2.4182370	0.0208400	0.0036130
31	C	3.1448320	-0.9931700	0.6582140
32	C	4.5370520	-0.9778090	0.6882110
33	C	5.2437060	0.0505190	0.0577200
34	C	4.5411890	1.0630070	-0.5971210
35	C	3.1465240	1.0493730	-0.6225150
36	H	2.6029360	-1.7876550	1.1633410
37	H	5.0736990	-1.7632610	1.2150700
38	H	6.3302790	0.0625580	0.0804850
39	H	5.0791710	1.8666130	-1.0936080
40	H	2.6040030	1.8357260	-1.1379280
41	H	1.7372670	2.3299760	1.5370530
42	H	0.2887040	-4.2729370	-0.7612250

11. BIM III_ox_pro

1	C	-1.2328880	-1.3362580	0.8662490

2	C	-2.3223310	-2.1777380	1.0834320
3	C	-0.2968390	-1.6957270	-0.1157920
4	C	-2.5262680	-3.3655190	0.3660650
5	C	-0.5178900	-2.8979820	-0.7997910
6	C	-1.5912420	-3.7448820	-0.5996050
7	C	0.9884980	-1.1206280	-0.5327800
8	C	1.5435880	-2.0002950	-1.4688660
9	C	0.9154630	1.1888090	0.4291560
10	C	-0.3925230	1.7133950	0.0625510
11	C	1.4064170	2.1714590	1.3818110
12	C	-0.5389050	2.9119060	0.8247020
13	C	-1.3744090	1.3595120	-0.8711180
14	C	-2.4896760	2.1858980	-0.9929170
15	C	-2.6581780	3.3465990	-0.2278260
16	C	-1.6682510	3.7166490	0.6850600
17	C	1.6200590	0.0508710	-0.0134870
18	C	3.1101090	0.0789190	0.0060520
19	C	3.8593870	-1.0192890	0.4719070
20	C	3.8129800	1.2193190	-0.4250320
21	C	5.2507430	-0.9772130	0.5091760
22	C	5.2068370	1.2597760	-0.3930110
23	C	5.9324530	0.1630400	0.0740590
24	N	0.6222620	-3.1392330	-1.7210740
25	N	0.5692450	3.1517120	1.6418120
26	Cl	-3.7440730	1.7484810	-2.1663060
27	Cl	-3.4934770	-1.7401650	2.3126310
28	H	1.0523240	-4.0584750	-1.5343190
29	H	-1.7148550	-4.6696860	-1.1569570
30	H	-3.3958750	-3.9799250	0.5661830
31	H	-1.1141940	-0.4288360	1.4424320
32	H	2.4392220	-1.9466890	-2.0646620
33	H	2.3593360	2.1026400	1.8984340
34	H	-1.2846420	0.4812400	-1.5000060
35	H	-3.5490160	3.9517250	-0.3577190
36	H	-1.7634130	4.6254560	1.2720430
37	H	7.0183690	0.1956720	0.1023180
38	H	5.7259710	2.1505390	-0.7371550
39	H	5.8059700	-1.8311680	0.8894920
40	H	3.3365630	-1.9031150	0.8260040
41	H	3.2525140	2.0716990	-0.7959110
42	H	0.3067450	-3.1735300	-2.7028590

12. BIM II_ox_pro

1	C	1.0528290	-1.5209400	-0.8540250
2	C	2.0649440	-2.4571950	-1.1006720
3	C	0.0601680	-1.8257750	0.0857850
4	C	2.0867130	-3.7057060	-0.4426670
5	C	0.1153950	-3.0756470	0.7086100
6	C	1.0902800	-4.0308600	0.4724080
7	C	-1.1564020	-1.1144000	0.5133800
8	C	-1.8309500	-1.9632060	1.3972220
9	C	-1.6306900	0.1471830	0.0443000
10	C	-0.7932940	1.2048700	-0.3775390
11	C	-1.1682400	2.2511590	-1.3146700
12	C	0.5706550	1.5647810	-0.0126890
13	C	0.8578380	2.7430090	-0.7696660
14	C	1.5104240	1.0842450	0.9029370
15	C	2.7369080	1.7501340	1.0359950
16	C	3.0301780	2.8890510	0.2664960
17	C	2.0805840	3.3900840	-0.6331400
18	C	-3.1055280	0.3690940	0.0420820
19	C	-3.9967140	-0.6001850	-0.4591600
20	C	-3.6514470	1.5730520	0.5250600
21	C	-5.3710130	-0.3753160	-0.4781700
22	C	-5.0280740	1.7972580	0.5108740
23	C	-5.8951770	0.8252220	0.0097860
24	N	-1.0676680	-3.2234490	1.5932210
25	N	-0.2202510	3.1253680	-1.5753000
26	O	3.6002420	1.2013410	1.9603760
27	C	4.8428270	1.8406880	2.1697440
28	H	4.7175150	2.8752900	2.5190380
29	H	5.3554710	1.2618180	2.9418720
30	H	5.4591780	1.8484710	1.2592100
31	O	3.0858180	-2.2512670	-1.9706320
32	C	3.1858370	-0.9784750	-2.6089230
33	H	3.2542920	-0.1690620	-1.8733180
34	H	4.1014170	-1.0193960	-3.2008440
35	H	2.3313720	-0.7970200	-3.2722170
36	H	-0.7861620	-3.3553730	2.5764330

37	H	1.0919600	-4.9953240	0.9741280
38	H	2.8927740	-4.3956720	-0.6655620
39	H	1.0311630	-0.5683190	-1.3610530
40	H	-2.7281830	-1.8328870	1.9785970
41	H	-2.1275150	2.3047680	-1.8218020
42	H	1.3294790	0.2157080	1.5272590
43	H	3.9817100	3.3978520	0.3718560
44	H	2.2867690	4.2865460	-1.2114850
45	H	-2.9809670	2.3297370	0.9202940
46	H	-5.4232530	2.7340020	0.8957580
47	H	-6.9676930	1.0008430	-0.0043800
48	H	-6.0356580	-1.1333450	-0.8858750
49	H	-3.5967480	-1.5298120	-0.8538300
50	H	-1.6082690	-4.0655970	1.3423840

13. BIM I excited state

		X	Y	Z
1	C	4.265941	-2.34469	0.104342
2	C	2.923622	-2.07186	0.26269
3	C	3.269908	0.329658	0.048176
4	C	4.63021	0.065993	-0.11398
5	C	5.123642	-1.2432	-0.08696
6	H	4.654039	-3.35838	0.122598
7	H	2.897961	1.345426	0.025438
8	H	5.317659	0.891573	-0.26536
9	H	6.186426	-1.42081	-0.21683
10	C	2.382322	-0.75235	0.244391
11	C	0.706679	-2.25882	0.566467
12	H	-0.25188	-2.72985	0.707622
13	N	1.850395	-2.95275	0.469112
14	H	1.922219	-3.96025	0.50882
15	C	0.971159	-0.86149	0.441478
16	C	-0.15358	0.139563	0.502413
17	H	-0.43006	0.160764	1.571747
18	C	-1.35761	-0.38942	-0.23896
19	C	-1.31935	-1.16848	-1.44532
20	H	-0.6133	-1.02065	-2.26675
21	C	-3.51749	-0.91129	-0.78075
22	C	-2.69711	-0.27402	0.206831
23	C	-3.32973	0.257386	1.367293
24	H	-2.75305	0.762631	2.138356
25	C	-4.72304	0.125399	1.497336
26	H	-5.2083	0.529824	2.384153
27	C	-5.49838	-0.51005	0.530115
28	H	-6.57246	-0.60213	0.668493
29	C	-4.897	-1.04821	-0.64194
30	H	-5.49245	-1.54743	-1.4024
31	N	-2.67962	-1.34975	-1.79134
32	H	-2.98564	-2.0043	-2.49569
33	C	0.271394	1.569275	0.153924
34	C	0.653855	2.459709	1.165871
35	C	0.284208	2.015235	-1.17423
36	C	1.063119	3.76058	0.859583
37	H	0.626409	2.135273	2.204461
38	C	0.700854	3.30979	-1.48386
39	H	-0.05531	1.344295	-1.95754

40	C	1.096456	4.18666	-0.46837
41	H	1.346187	4.440458	1.659287
42	H	0.704289	3.640447	-2.51937
43	H	1.411268	5.198309	-0.71068

14. BIM II excited state

1	C	-2.50802	-0.64634	-0.52019
2	C	-3.74815	-1.16321	-0.94985
3	C	-2.49856	0.321868	0.545509
4	C	-4.95948	-0.78479	-0.38378
5	C	-3.75868	0.713088	1.10208
6	C	-4.97602	0.184576	0.67639
7	C	-1.49786	0.995645	1.303133
8	C	-2.1179	1.753636	2.313384
9	C	0.004597	1.001667	1.109368
10	C	0.594951	-0.38523	1.005891
11	C	-0.09943	-1.56311	1.316334
12	C	1.938378	-0.81199	0.653118
13	C	1.986743	-2.22791	0.780211
14	C	3.08727	-0.14482	0.246493
15	C	4.273159	-0.89908	-0.01444
16	C	4.292972	-2.29065	0.122067
17	C	3.13071	-2.96829	0.524931
18	C	0.500575	1.929687	-0.00781
19	C	1.389174	2.97266	0.287012
20	C	0.055245	1.780481	-1.32983
21	C	1.842478	3.837684	-0.71362
22	C	0.510487	2.640652	-2.32907
23	C	1.409493	3.667965	-2.02822
24	N	-3.49873	1.636091	2.102578
25	N	0.725389	-2.63111	1.183195
26	O	5.322297	-0.14616	-0.39588
27	C	6.559106	-0.78607	-0.70832
28	H	6.437132	-1.48415	-1.54418
29	H	7.239866	0.015356	-0.99373
30	H	6.956507	-1.31655	0.164573
31	O	-3.64013	-2.09407	-1.98129
32	C	-4.8349	-2.59036	-2.53408
33	H	-5.47082	-1.7846	-2.92972
34	H	-4.54552	-3.25522	-3.35382
35	H	-5.42476	-3.16305	-1.80164

36	H	-4.19152	1.904717	2.784158
37	H	0.432743	-3.59145	1.310659
38	H	-5.91572	0.497998	1.121861
39	H	-5.89631	-1.21432	-0.71667
40	H	-1.61839	-0.94962	-1.05963
41	H	-1.72222	2.60995	2.848249
42	H	0.439289	1.400573	2.04056
43	H	-1.14203	-1.66513	1.566658

15. BIM III excited state

1	C	-2.91651	-0.79293	-0.29117
2	C	-3.97266	-1.69613	-0.13659
3	C	-1.67408	-1.12099	0.283089
4	C	-3.82498	-2.89214	0.570294
5	C	-1.54847	-2.34232	0.998472
6	C	-2.58798	-3.23262	1.154511
7	C	-0.39973	-0.46468	0.312249
8	C	0.461075	-1.33094	1.059066
9	C	1.415134	1.271772	0.168741
10	C	2.654708	0.596705	-0.04351
11	C	1.653036	2.403536	0.953504
12	C	3.652476	1.343596	0.638479
13	C	3.022098	-0.63364	-0.70983
14	C	4.390231	-0.98295	-0.63551
15	C	5.354544	-0.26561	0.04175
16	C	5.00121	0.955808	0.704271
17	C	0.069621	0.807415	-0.35691
18	C	-1.01161	1.885971	-0.34574
19	C	-1.4214	2.489106	-1.54125
20	C	-1.60496	2.303351	0.855025
21	C	-2.40266	3.482752	-1.5413
22	C	-2.58468	3.296627	0.857556
23	C	-2.98962	3.887491	-0.34134
24	N	-0.21879	-2.41314	1.451088
25	N	3.018205	2.431623	1.209938
26	Cl	4.879917	-2.50531	-1.44754
27	Cl	-5.52613	-1.31395	-0.84359
28	H	0.185707	-3.18858	1.960253
29	H	3.491796	3.158677	1.721594
30	H	-2.47686	-4.16589	1.696911

31	H	-4.67027	-3.56312	0.669616
32	H	-3.05541	0.13404	-0.83283
33	H	1.518457	-1.20161	1.23295
34	H	0.202033	0.510516	-1.41232
35	H	1.021931	3.241179	1.202389
36	H	2.37654	-1.11729	-1.43525
37	H	6.372442	-0.63617	0.090707
38	H	5.749509	1.555863	1.210597
39	H	-3.75415	4.659496	-0.3395
40	H	-3.03083	3.610528	1.797615
41	H	-2.70512	3.940618	-2.47921
42	H	-0.96071	2.18561	-2.47844
43	H	-1.28429	1.85927	1.793684