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Aggregation-Induced Emission Mechanism of Styrene Derivative: A Theoretical Study

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Supporting Information

Table S1. Optimized α, β, γ, and γ' angles of BIM monomer in methanol solution in the S_0 and S_1 states. For the definition of α, β, γ, and γ' angles, see Fig. 1(a). Geometry optimizations are performed using SF-TDDFT/ωB97XD, B3LYP, BHHLYP, CAM-B3LYP, PBE0/cc-pVDZ in the S_0 state and TDωB97XD, TDB3LYP, TDBHHLYP, TDCAM-B3LYP, TDPBE0/cc-pVDZ in the S_1 state.

Functional	State	Angle (^{0})			
		α	β	γ	γ′
ωB97XD	S_0	–9.6	–3.2	–65.7	175.1
	S_1	–86.9	–5.7	–6.0	176.5
B3LYP	S_0	-15.6	-3.1	-65.5	175.9
	S_1	-11.6	-28.9	-27.2	171.9
BHHLYP	S_0	-7.0	-2.7	-68.0	176.0
	S_1	-82.5	-16.0	-2.5	178.1
CAM-B3LYP	S_0	-8.3	-3.6	-62.9	176.0
	S_1	-87.1	-8.0	-6.3	177.1
PBE0	S_0	-14.9	-3.6	-63.5	176.1
	S_1	-14.9	-28.2	-25.8	172.3

Table S2. Calculated vertical $S_0 \rightarrow S_1$ excitation energies for BIM monomer at S_0 optimized geometry. These values were obtained through SF-TDDFT calculations using ωB97XD, B3LYP, BHHLYP, CAM-B3LYP, PBE0 functionals with cc-pVDZ basis set. Experimental absorption wavelength value is provided for comparison.

Functional	Theoretical Calculated Absorption (nm)	Experimental absorption value (nm)
ωB97XD	339	375
B3LYP	401	
BHHLYP	341	
CAM-B3LYP	344	
PBE0	390	

Table S3. Optimized α, β, γ, and γ' angles of BIM monomer in methanol solution in the S_0 and S_1 states. For the definition of α, β, γ, and γ' angles, see Fig. 1(a). Geometry optimizations are performed using DFT/ωB97XD/cc-pVDZ in the S_0 state and TDωB97XD/cc-pVDZ in the S_1 state.

Functional	State	Angle (^{0})			
		α	β	γ	γ′
ωB97XD	S_0	15.2	0.9	69.7	-174.4
	S_1	7.9	38.9	19.6	-173.3

Table S4. $\langle S^2 \rangle$ values for S_0 and S_1 at S_0 and S_1 optimized geometries.

Molecule	$\langle S^2 \rangle_{S_0}$ **at S_0 Opt.**	$\langle S^2 \rangle_{S_1}$ **at S_0 Opt.**	$\langle S^2 \rangle_{S_0}$ **at S_1 Opt.**	$\langle S^2 \rangle_{S_1}$ **at S_1 Opt.**
BIM Monomer	0.0521	0.1427	0.0845	0.6532

Table S5. Tabulated oscillator strength *(f)* values at S_1 -MEP of monomer in methanol solution.

Serial No.	Dihedral Angle (α) value (in degrees)	Oscillator Strength (*f*) (in a.u.) ($S_1 \rightarrow S_0$)
1	**-9.57 (FC)**	1.416
2	**-20**	1.055
3	**-30**	0.897
4	**-40**	0.521
5	**-50**	0.247
6	**-60**	0.107
7	**-70**	0.039
8	**-80**	0.009
9	**-86.9 (S_1-MIN)**	0.002
10	**-90**	0.0005
11	**-100**	0.003
12	**-110**	0.021
13	**-120**	0.066
14	**-130**	0.158
15	**-140**	0.331
16	**-150**	0.681
17	**-160**	1.018
18	**-170**	1.102
19	**-180**	1.101

Table S6. $\langle S^2 \rangle$ values for Excited state 1 [which might be the ground state (i.e., S_0) according to SF-TDDFT], Excited state 2 (i.e., excited triplet state) and Excited state 3 (S_1, first excited singlet state) at S_1-MEP of monomer in methanol solution.

Serial No.	Dihedral Angle (in degrees)	S_1 PES (States)	$\langle S^2 \rangle$ Values
1	**-9.64 (FC)**	1 (might be the ground state)	0.0520
		2	2.0108
		3	0.1426
		4	1.0676
2	**-20**	1 (might be the ground state)	0.0493
		2	2.0229
		3	0.0974
		4	1.0473
3	**-30**	1 (might be the ground state)	0.0535
		2	2.0271
		3	0.0843
		4	1.0475
4	**-40**	1 (might be the ground state)	0.0677
		2	2.0491
		3	0.0689
		4	1.0467
5	**-50**	1 (might be the ground state)	0.0789
		2	2.0503
		3	0.0787
		4	1.0474

6	**-60**	1 (might be the ground state)	0.0835
		2	1.9928
		3	0.1401
		4	1.0479
7	**-70**	1 (might be the ground state)	0.0850
		2	1.8629
		3	0.2712
		4	1.0483
8	**-80**	1 (might be the ground state)	0.0848
		2	1.6503
		3	0.4840
		4	1.0486
9	**-86.9**	1 (might be the ground state)	0.0845
		2	1.4790
		3	0.6550
		4	1.0486
10	**-90**	1 (might be the ground state)	0.0845
		2	1.4280
		3	0.7060
		4	1.0486
11	**-100**	1 (might be the ground state)	0.0849
		2	1.5397
		3	0.5947

		4	1.0486
12	**-110**	1 (might be the ground state)	0.0853
		2	1.7673
		3	0.3665
		4	1.0483
13	**-120**	1 (might be the ground state)	0.0851
		2	1.9188
		3	0.2135
		4	1.0479
14	**-130**	1 (might be the ground state)	0.0827
		2	2.0187
		3	0.1110
		4	1.0474
15	**-140**	1 (might be the ground state)	0.0767
		2	2.0528
		3	0.0712
		4	1.0470
16	**-150**	1 (might be the ground state)	0.0618
		2	2.0399
		3	0.0718
		4	1.0470
17	**-160**	1 (might be the ground state)	0.0504
		2	2.0232

		3	0.0929
		4	1.0480
18	**-170**	1 (might be the ground state)	0.0485
		2	2.0234
		3	0.1052
		4	1.0462
19	**-180**	1 (might be the ground state)	0.0477
		2	2.0272
		3	0.1163
		4	1.0284

Table S7. Tabulated potential energy difference between S_0 and S_1 states vs torsional angle (α) at S_1-MEP for monomer in methanol solution.

Serial No.	Dihedral Angle (α) value (in degrees)	S_0-state Energy (in a.u.)	S_1-state Energy (in a.u.)	Difference in Energy (in kJ/mol)
1	**-9.64**	-899.13106443 (S_0-MIN)	-898.99622825 (FC)	354.01
2	**-20**	-899.11801422	-899.00659519	292.53
3	**-30**	-899.1115150	-899.00761357	271.83
4	**-40**	-899.09114479	-899.00959450	214.11
5	**-50**	-899.07856243	-899.01279065	172.68
6	**-60**	-899.07565185	-899.01576321	157.23
7	**-70**	-899.07703435	-899.01765729	155.89
8	**-80**	-899.07890176	-899.01836044	158.95
9	**-86.9**	-899.07962022	-899.01844133(S_1-MIN)	160.62

10	**-90**	-899.07971420	-899.01842572	160.91
11	**-100**	-899.07937712	-899.01845685	159.94
12	**-110**	-899.07746194	-899.01811446	155.81
13	**-120**	-899.07503044	-899.01677267	152.95
14	**-130**	-899.07482814	-899.01427071	158.99
15	**-140**	-899.08044721	-899.01107749	182.13
16	**-150**	-899.09881095	-899.00816706	237.98
17	**-160**	-899.11643319	-899.00679841	287.84
18	**-170**	-899.11982240	-899.00603338	298.75
19	**-180**	-899.11941638	-899.00522319	299.81

Table S8. Tabulated potential energy difference between S_0 and S_1 states vs torsional angle (α) at S_1-MEP for monomer in methanol solution. Constrained geometry optimizations are performed using SF-LC-TDDFT/ωB97XD/aug-cc-pVDZ in the S_1 state.

Serial No.	**Dihedral Angle (α) value (in degrees)**	**S_0-state Energy (in a.u.)**	**S_1-state Energy (in a.u.)**	**Difference in Energy (in kJ/mol)**
1	**-81.4**	-899.12774906	-899.07787827 (S_1-MIN)	130.93
2	**-90**	-899.12859228	-899.07770790	133.60
3	**-120**	-899.12272498	-899.07609430	122.43
4	**-150**	-899.14376426	-899.06600593	204.15
5	**-180**	-899.17270963	-899.06183321	291.11

Table S9. Tabulated potential energy difference between S_0 and S_1 states vs torsional angle (β) at S_1-MEP for monomer in methanol solution.

Serial No.	**Dihedral Angle (β) value (in**	**S_0-state Energy**	**S_1-state Energy**	**Difference in Energy (in**

	degrees)	(in a.u.)	(in a.u.)	kJ/mol)
1	**-5.7**	-899.07962022	-899.01844133	160.62
2	**-20**	-899.07718841	-899.01810863	155.11
3	**-30**	-899.07334978	-899.01726390	147.25
4	**-40**	-899.06806477	899.01570508	137.47
5	**-50**	-899.05000245	-899.01608685	89.04
6	**-60**	-899.05198129	-899.02102888	81.26
7	**-70**	-899.05600305	-899.02425441	83.36
8	**-80**	-899.05997658	-899.02609363	88.96
9	**-90**	-899.061322151	-899.02666908	90.98
10	**-100**	-899.05990415	-899.03166187	74.15
11	**-110**	-899.05727170	-899.02467005	85.59
12	**-120**	-899.05450125	-899.02169266	109.77
13	**-130**	-899.05193410	-899.01724231	91.08
14	**-140**	-899.05318470	-899.01141818	109.66
15	**-150**	-899.07194714	-899.01624977	146.23
16	**-160**	-899.07639486	-899.01771120	154.07
17	**-170**	-899.07912317	-899.01845069	159.29
18	**-180**	-899.08046821	-899.01872541	162.11

Figure S1. Potential energy profiles for the S_0 and S_1 states calculated for the BIM monomer as a function of the β dihedral angle along the S_1-MEP in methanol solution, using SF-LC-TDDFT with ωB97XD/cc-pVDZ.

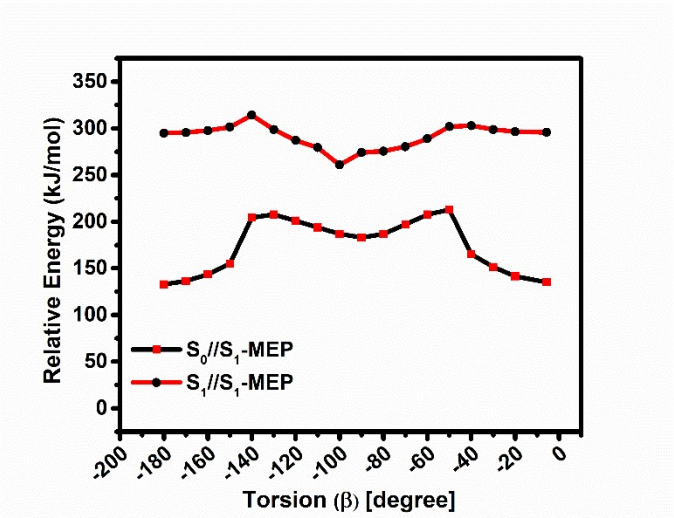
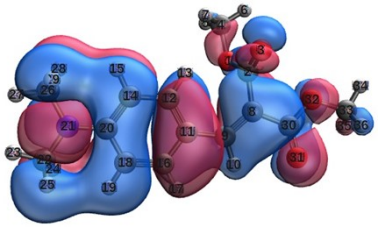
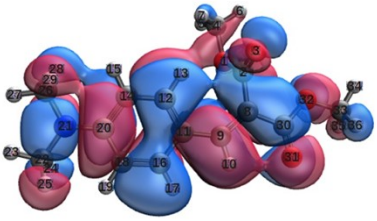
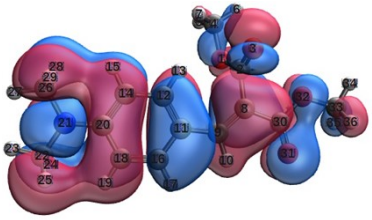
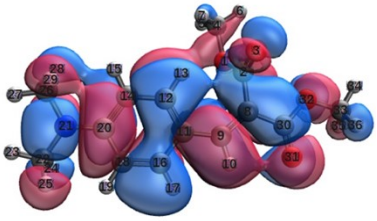
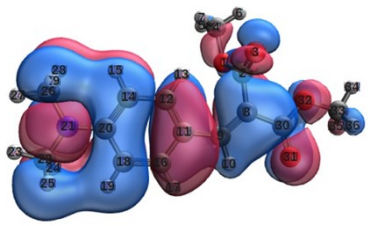
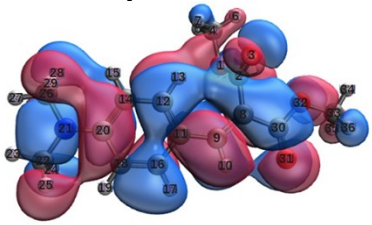
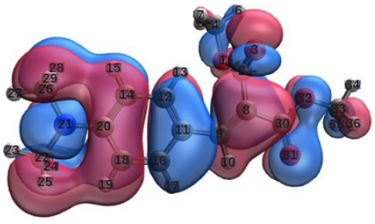
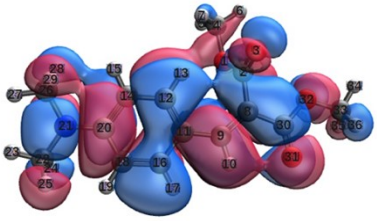
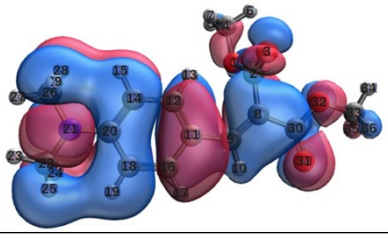
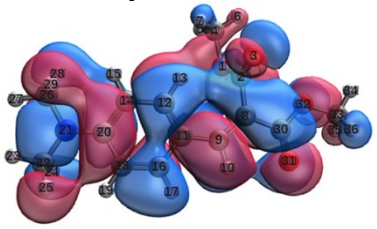
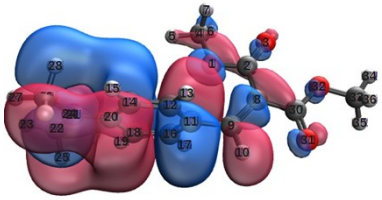
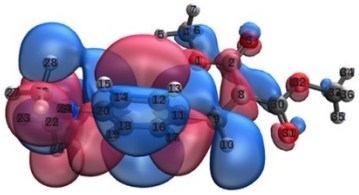
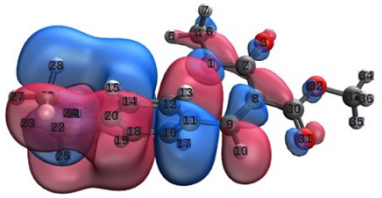
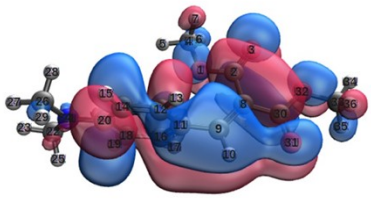
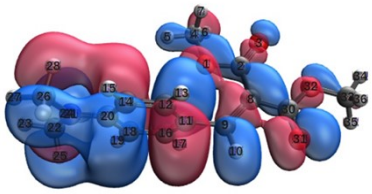
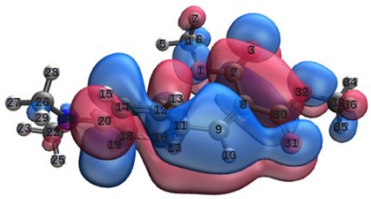
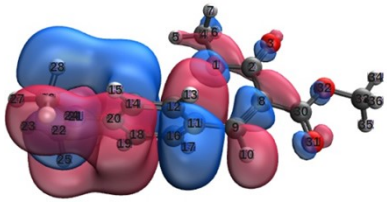
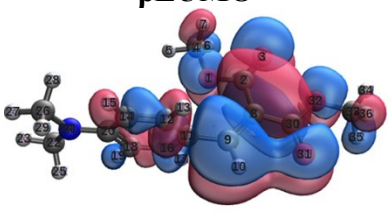


Figure S2. Molecular orbitals of BIM monomer at the S_0 and S_1 optimum geometries, which are calculated using SF-LC-TDDFT with ωB97XD/cc-pVDZ. The response coefficients corresponding to each transition have been placed above the arrows.

Geometry	States	Transitions		
At S_0-Optimized	S_0	Ground (0.9887)		
	T_1	βHOMO 	1.0000 →	αLUMO 
	T_2	αHOMO 	-0.6612 →	αLUMO 
		βHOMO 	0.7322 →	βLUMO 

	S_1	αHOMO 	0.6886 →	αLUMO 
		βHOMO 	0.6411 →	βLUMO 
At S_1-Optimized	S_0	Ground (0.9750)		
		βHOMO 	-0.1749 →	βLUMO+2 
	T_1	βHOMO 	1.0000 →	αLUMO 
	T_2	αHOMO 	0.9533 →	αLUMO 
		βHOMO 	-0.1880 →	βLUMO 
	S_1	αHOMO	0.1945 →	αLUMO

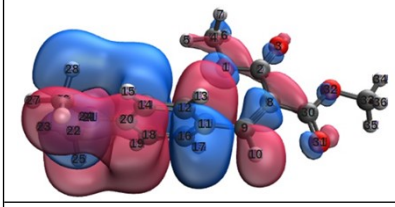
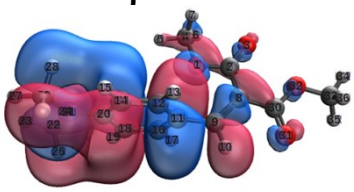
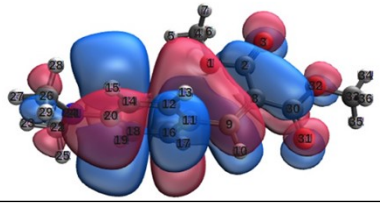
		βHOMO 	0.9046 →	βLUMO
		βHOMO 	-0.3398 →	βLUMO+1 

Table S10. Tabulated potential energy difference between S_0 and S_1 states vs torsional angle (α, β) for 110 optimized points at S_1-MEP for monomer in methanol solution using SF-TDDFT/ωB97XD/cc-pVDZ.

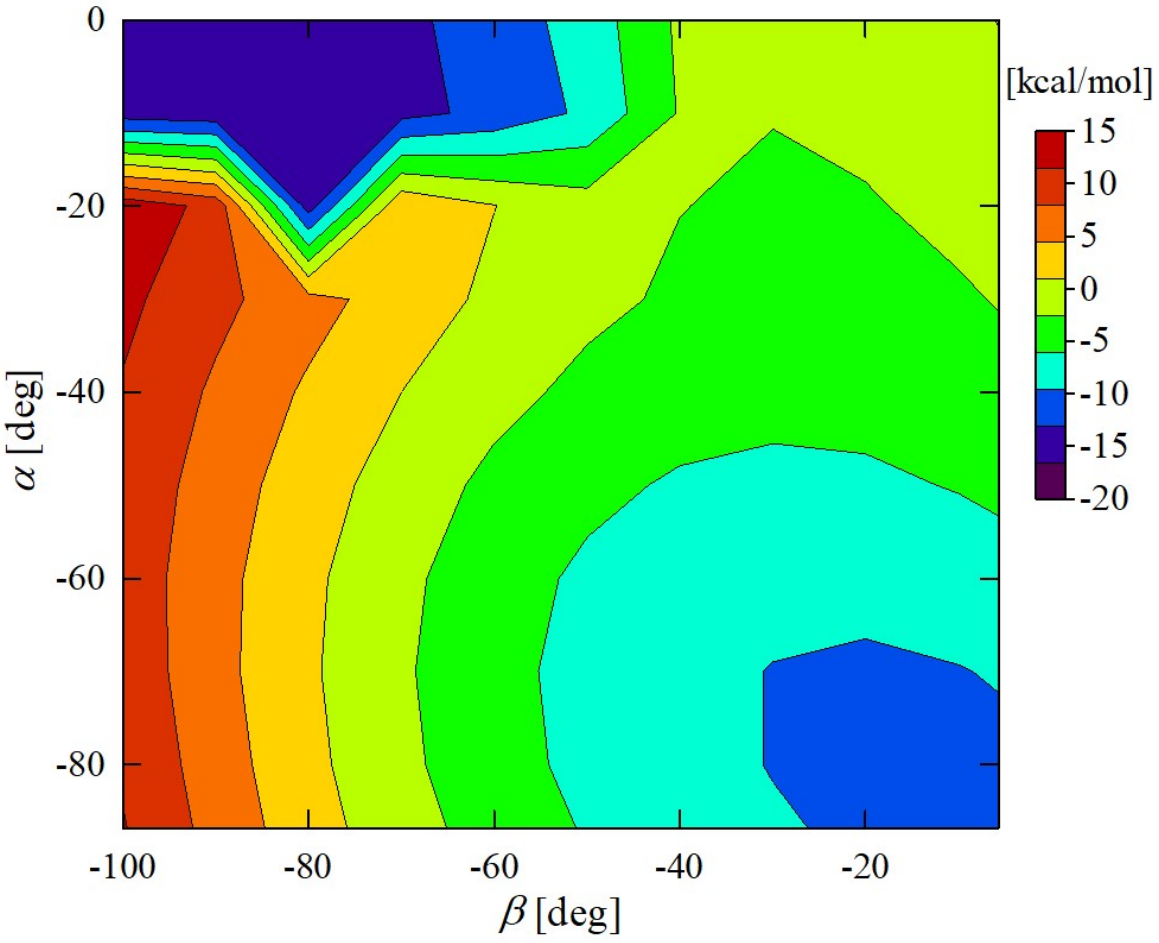
Serial No.	Dihedral Angle (α, β) value (in degrees)	S_0-state Energy (in a.u)	S_1-state Energy (in a.u)	Difference in Energy (in kJ/mol)
1	**(-86.9, -5.7)**	-899.0796202	-899.0184413	160.6252
2	**(-86.9, -10)**	-899.0790333	-899.0183711	159.2685
3	**(-86.9, -20)**	-899.0772557	-899.0177477	156.2385
4	**(-86.9, -30)**	-899.0741227	-899.0164322	151.4664
5	**(-86.9, -40)**	-899.0700738	-899.0144991	145.9112
6	**(-86.9, -50)**	-899.0647498	-899.0117673	139.1056
7	**(-86.9, -60)**	-899.0580769	-899.0081445	131.0976
8	**(-86.9, -70)**	-899.0498723	-899.0035206	121.6963
9	**(-86.9, -80)**	-899.041075	-898.9978547	113.4748
10	**(-86.9, -90)**	-899.0318613	-898.9909626	107.3795
11	**(-86.9, -100)**	-899.0233734	-898.98311	105.7116
12	**(-80, -5.7)**	-899.0800103	-899.0181421	162.4351
13	**(-80, -10)**	-899.0793678	-899.0183189	160.2837
14	**(-80, -20)**	-899.0771766	-899.018101	155.103
15	**(-80, -30)**	-899.0736088	-899.0171238	148.3015
16	**(-80, -40)**	-899.0686767	-899.0153887	139.9077
17	**(-80, -50)**	-899.0628622	-899.0128418	131.3285

18	**(-80, -60)**	-899.0557267	-899.0092449	122.038
19	**(-80, -70)**	-899.0469424	-899.0045545	111.2896
20	**(-80, -80)**	-899.0373388	-898.9987932	101.2014
21	**(-80, -90)**	-899.027857	-898.9919871	94.17621
22	**(-80, -100)**	-899.0175208	-898.9841595	87.59007
23	**(-70, -5.7)**	-899.0805185	-899.0165771	167.8782
24	**(-70, -10)**	-899.079589	-899.0171224	164.0061
25	**(-70, -20)**	-899.0769271	-899.0176373	155.6652
26	**(-70, -30)**	-899.0732177	-899.0170834	147.3807
27	**(-70, -40)**	-899.068	-899.015622	137.5185
28	**(-70, -50)**	-899.061284	-899.0131856	126.2825
29	**(-70, -60)**	-899.0534487	-899.0097208	114.8077
30	**(-70, -70)**	-899.0441961	-899.0050818	102.6946
31	**(-70, -80)**	-899.0339172	-898.9994391	90.5223
32	**(-70, -90)**	-899.0238059	-898.9928986	81.14714
33	**(-70, -100)**	-899.0123285	-898.9854207	70.64648
34	**(-60, -5.7)**	-899.0831315	-899.0137628	182.1275
35	**(-60, -10)**	-899.0814597	-899.0145324	175.7176
36	**(-60, -20)**	-899.0775133	-899.0156183	162.5054
37	**(-60, -30)**	-899.0734162	-899.0155984	151.8007
38	**(-60, -40)**	-899.0678437	-899.0145215	139.9975
39	**(-60, -50)**	-899.061352	-899.0123631	128.6202
40	**(-60, -60)**	-899.0536817	-899.0090365	117.2161
41	**(-60, -70)**	-899.044456	-899.0045502	104.7727
42	**(-60, -80)**	-899.03371	-898.999071	90.94462
43	**(-60, -90)**	-899.0223281	-898.9927895	77.55357
44	**(-60, -100)**	-899.010148	-898.9858178	63.87915
45	**(-50, -5.7)**	-899.0954723	-899.010179	223.9376
46	**(-50, -10)**	-899.0914458	-899.0110266	211.1406
47	**(-50, -20)**	-899.0836955	-899.0124134	187.1512
48	**(-50, -30)**	-899.0773592	-899.0127528	169.624
49	**(-50, -40)**	-899.0707658	-899.0120057	154.2746
50	**(-50, -50)**	-899.0632577	-899.0101019	139.5604
51	**(-50, -60)**	-899.0552208	-899.0071068	126.3232
52	**(-50, -70)**	-899.0459447	-899.0028392	113.1736
53	**(-50, -80)**	-899.0355083	-898.9976514	99.39329
54	**(-50, -90)**	-899.0237946	-898.9917306	84.18411
55	**(-50, -100)**	-899.0115747	-898.9851684	69.32974
56	**(-40, -5.7)**	-899.1125155	-899.0074483	275.8538
57	**(-40, -10)**	-899.1097994	-899.0081438	266.8968
58	**(-40, -20)**	-899.1005781	-899.0092704	239.7285
59	**(-40, -30)**	-899.0897661	-899.0095785	210.5326
60	**(-40, -40)**	-899.0801661	-899.0088936	187.1259
61	**(-40, -50)**	-899.0711239	-899.0070582	168.2044
62	**(-40, -60)**	-899.0611456	-899.0041473	149.6489

63	**(-40, -70)**	-899.0503337	-899.0001912	131.6493
64	**(-40, -80)**	-899.0391364	-898.9954186	114.7811
65	**(-40, -90)**	-899.0269942	-898.9899293	97.31397
66	**(-40, -100)**	-899.0147824	-898.9839054	81.06743
67	**(-30, -5.7)**	-899.1204671	-899.0055311	301.7643
68	**(-30, -10)**	-899.1196049	-899.0063338	297.3932
69	**(-30, -20)**	-899.1152158	-899.0074483	282.9435
70	**(-30, -30)**	-899.1067939	-899.0075136	260.6604
71	**(-30, -40)**	-899.0963786	-899.0065543	235.8336
72	**(-30, -50)**	-899.0854873	-899.0045333	212.5448
73	**(-30, -60)**	-899.0736647	-899.0013717	189.8051
74	**(-30, -70)**	-899.0609736	-898.997253	167.2985
75	**(-30, -80)**	-899.0467608	-898.9925557	142.3155
76	**(-30, -90)**	-899.0321107	-898.9875283	117.0512
77	**(-30, -100)**	-899.017435	-898.9821481	92.64565
78	**(-20, -5.7)**	-899.1242797	-899.0036089	316.8213
79	**(-20, -10)**	-899.123765	-899.0045836	312.9108
80	**(-20, -20)**	-899.1215297	-899.0061659	302.8876
81	**(-20, -30)**	-899.1172205	-899.0065806	290.485
82	**(-20, -40)**	-899.1106228	-899.0056608	275.5778
83	**(-20, -50)**	-899.102075	-899.0034913	258.8316
84	**(-20, -60)**	-899.0916272	-899.0000912	240.328
85	**(-20, -70)**	-899.0816749	-898.9956558	225.8431
86	**(-20, -80)**	-899.0557309	-899.0252216	80.10198
87	**(-20, -90)**	-899.0542057	-898.9851605	181.2782
88	**(-20, -100)**	-899.0243011	-898.9798781	116.6326
89	**(-10, -5.7)**	-899.1257181	-899.0017897	325.3739
90	**(-10, -10)**	-899.1254105	-899.0027579	322.0242
91	**(-10, -20)**	-899.123973	-899.0046786	313.2076
92	**(-10, -30)**	-899.1211383	-899.0056081	303.3244
93	**(-10, -40)**	-899.1175159	-899.0054088	294.3373
94	**(-10, -50)**	-899.0547075	-899.0157966	102.1607
95	**(-10, -60)**	-899.0530863	-899.02091	84.47877
96	**(-10, -70)**	-899.0557369	-899.0242533	82.66032
97	**(-10, -80)**	-899.0583381	-899.0259878	84.93566
98	**(-10, -90)**	-899.0609457	-899.0263704	90.77737
99	**(-10, -100)**	-899.0602493	-899.0253673	91.58274
100	**(0, -5.7)**	-899.1256896	-899.0000972	329.743
101	**(0, -10)**	-899.1254553	-899.0010045	326.7454
102	**(0, -20)**	-899.1241946	-899.0029186	318.4102
103	**(0, -30)**	-899.1218985	-899.0042978	308.7607
104	**(0, -40)**	-899.1185181	-899.0048219	298.5093
105	**(0, -50)**	-899.0587853	-899.0144283	116.4594
106	**(0, -60)**	-899.0560771	-899.0200047	94.70801
107	**(0, -70)**	-899.0579286	-899.023761	89.70701

108	**(0, -80)**	-899.0592815	-899.0259374	87.54486
109	**(0, -90)**	-899.0614271	-899.0267091	91.15216
110	**(0, -100)**	-899.0611121	-899.02613	91.8455

Figure S3. 2D-Contour plot of torsional angle (α, β) for 110 optimized points at S_1-MEP for monomer in methanol solution using SF-TDDFT/ωB97XD/cc-pVDZ. Relative S_1 state energies were plotted by setting the S_1 energy at the optimized ground-state (S_0) geometry as the zero reference.



S1. Cartesian coordinates of S_0-MIN and S_1-MIN optimized structures for BIM monomer in methanol

S_0-MIN of BIM monomer in methanol

O	-0.0335202561	0.1312764120	-0.0116261397
C	-0.0121116196	-0.0181423509	1.3176032477
O	1.0085948906	-0.1313265012	1.9603378612
C	1.2458006736	0.2274767094	-0.6501645326
H	1.0336000191	0.3709335351	-1.7145498925
H	1.8262803820	-0.6919524034	-0.4940020501
H	1.8070912901	1.0856142577	-0.2531922582

C	-1.3927826791	-0.0193574854	1.8881740190
C	-2.2423056345	1.0534074634	1.8746731519
H	-3.2263640981	0.8335378932	2.3023444824
C	-2.0720634506	2.3910088540	1.4182636131
C	-0.8385226745	2.9784324122	1.0175491785
H	0.0914467197	2.4152045274	1.0910614462
C	-0.7608253669	4.2760927942	0.5794324384
H	0.2127452692	4.6766061041	0.3030157277
C	-3.2169744714	3.2353851181	1.3718229739
H	-4.1778416124	2.8300226438	1.6995547295
C	-3.1630373053	4.5314514933	0.9230080259
H	-4.0773616604	5.1215195803	0.9049549879
C	-1.9258883626	5.1030865787	0.4939870754
N	-1.8525295929	6.3725597959	0.0413561820
C	-3.0429899304	7.2047057771	0.0003312998
H	-2.7715700222	8.1929735765	-0.3861218803
H	-3.8147476589	6.7797022063	-0.6625385636
H	-3.4852072379	7.3388827633	1.0018280083
C	-0.5747532722	6.9373412777	-0.3584746875
H	-0.7346502300	7.9617918161	-0.7115359368
H	-0.1145747435	6.3639103577	-1.1796978694
H	0.1403625631	6.9735371367	0.4807096535
C	-1.8852675621	-1.2664945153	2.5051395898
O	-2.9599613429	-1.3979754020	3.0608563161
O	-1.0096606195	-2.2706064370	2.3627695278
C	-1.3943288485	-3.5267153794	2.9292694659
H	-0.5662628554	-4.2112573338	2.7186258019
H	-2.3201423288	-3.8946170125	2.4656479752
H	-1.5437456257	-3.4301782223	4.0137571321

S_1-MIN of BIM monomer in methanol

O	-0.6400183315	0.8809806856	-0.0701783288
C	-0.5735609582	-0.2724032235	0.6624693560
O	0.0972731811	-1.2167111580	0.2572079083
C	0.1477069377	0.9216431016	-1.2503213929
H	-0.0001901220	1.9225174284	-1.6743603464
H	-0.1749811559	0.1584785140	-1.9744987402
H	1.2133818562	0.7639802528	-1.0254984070
C	-1.3544438131	-0.1547639138	1.8875593091

C	-1.9722010540	1.0401919170	2.3041230901
H	-2.5275427648	1.0055002751	3.2429801841
C	-1.8575768444	2.3659958580	1.6842108744
C	-0.8054513066	3.2600273632	2.0319184901
H	-0.0428261522	2.9147133618	2.7311752327
C	-0.7194907353	4.5299468732	1.5186128860
H	0.1070853412	5.1721694910	1.8174783166
C	-2.8359424728	2.8574633681	0.7734162104
H	-3.6520204000	2.1922293647	0.4890229461
C	-2.7846704088	4.1244307322	0.2502937588
H	-3.5611836631	4.4484014546	-0.4402812112
C	-1.7139276314	5.0080815307	0.6046975541
N	-1.6443313521	6.2509068236	0.0950255389
C	-2.6675297834	6.7449513958	-0.8242579927
H	-2.4343770317	7.7800156696	-1.0867091591
H	-2.6834162339	6.1363714566	-1.7394563173
H	-3.6560420395	6.7099014458	-0.3458121788
C	-0.5387697577	7.1427628748	0.4383134773
H	-0.6706973833	8.0885582508	-0.0930531929
H	0.4181407116	6.6935744543	0.1381128852
H	-0.5271827404	7.3370486883	1.5199527179
C	-1.5497854607	-1.3041865504	2.7696485665
O	-2.1682476641	-1.2490600590	3.8331197323
O	-1.0218510611	-2.4765227389	2.3408936730
C	-1.2291239504	-3.5891215076	3.2012609361
H	-0.7573972778	-4.4434508014	2.7012819397
H	-2.3011950242	-3.7876403357	3.3509687664
H	-0.7616827087	-3.4291443027	4.1848530176