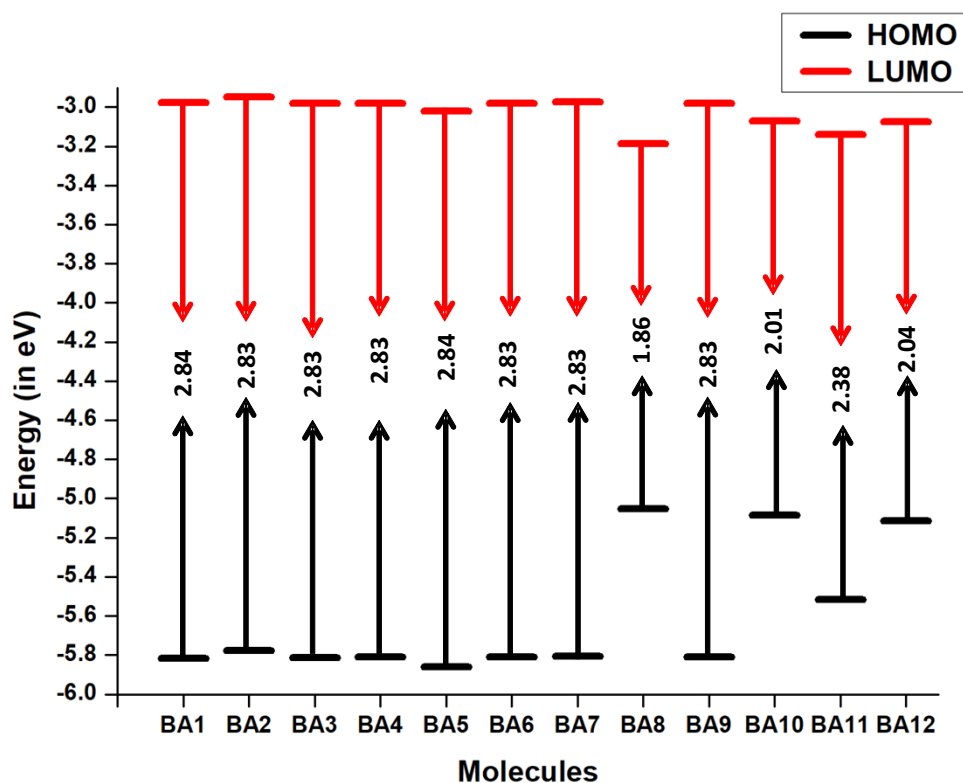
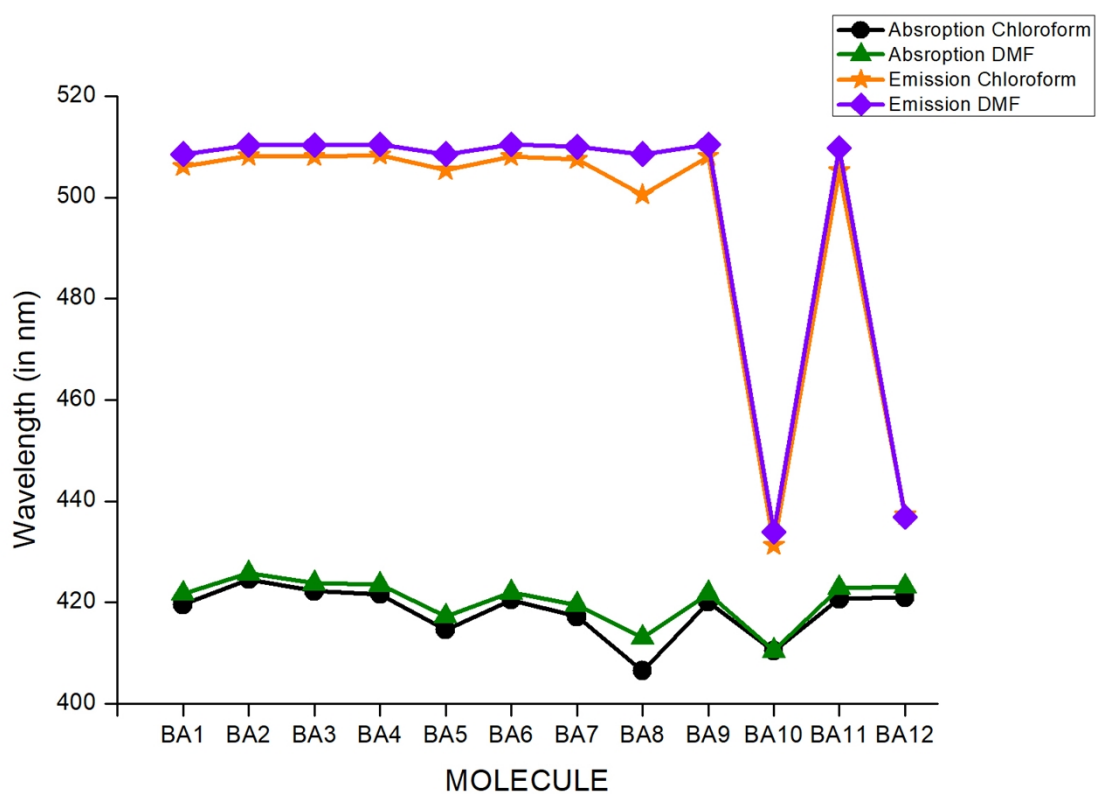
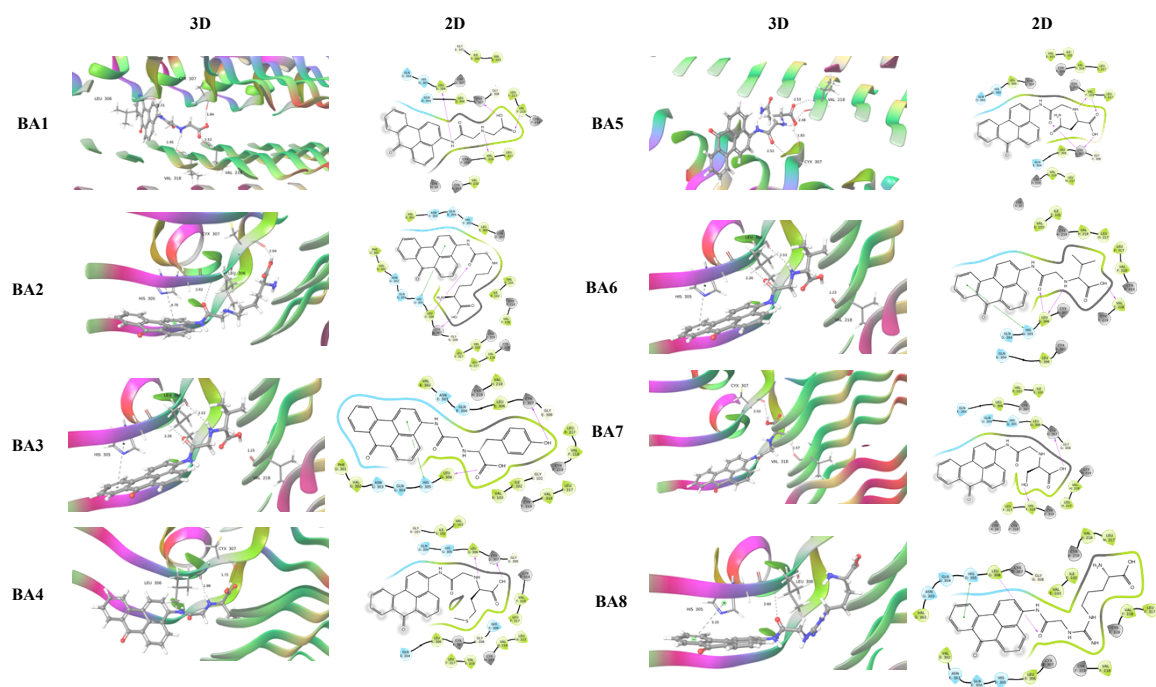




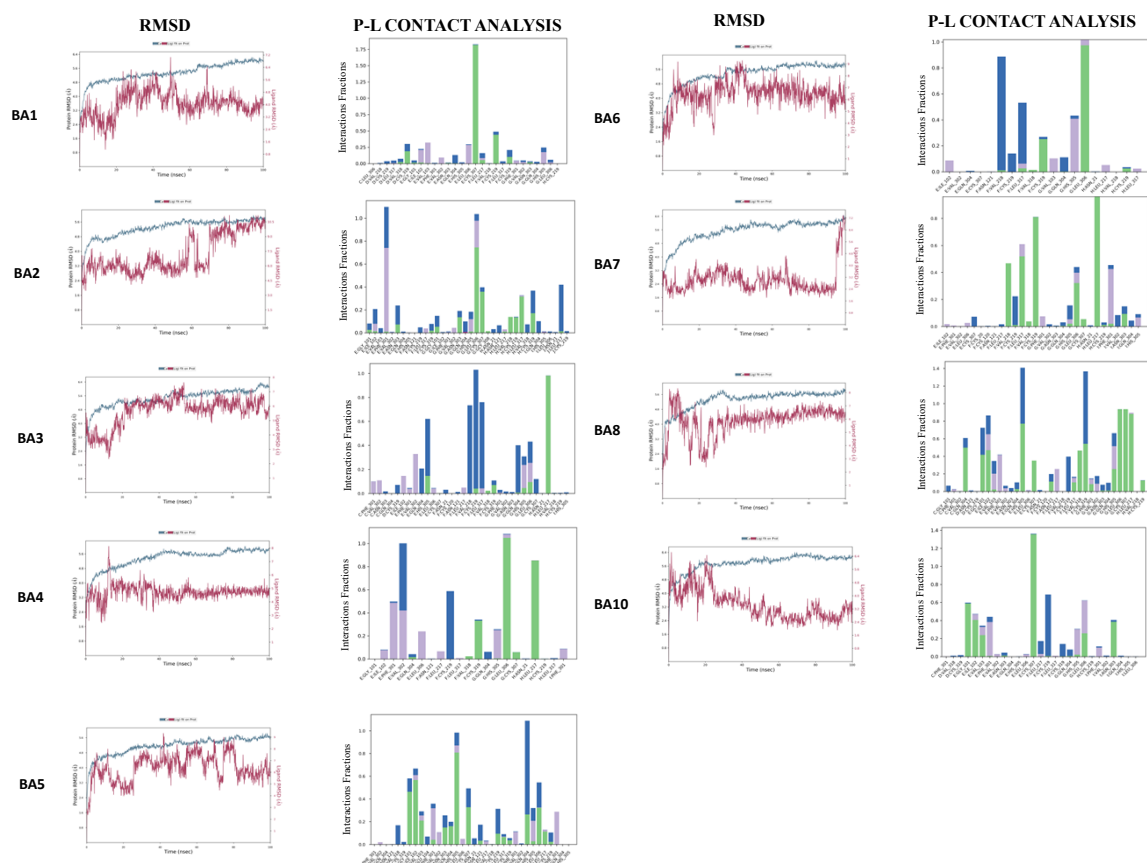
Supporting Figure 1: Excited State frontier molecular energy along with the HOMO-LUMO gap of the benzanthrone-2-aminoacetamide



Supporting Figure 2: Absorption and emission spectra of the benzanthrone-2-aminoacetamide in Chloroform and DMF



Supporting Figure 3: 2D and 3D schematic representation of interaction made by benzanthrone-2-aminoacetamide derivatives with insulin amyloid fibrils.



Supporting Figure 4: RMSD plot for the benzanthrone-2-aminoacetamide derivatives with insulin amyloid fibrils. The blue colour represents the evolution of backbone C α atoms of the protein, whereas red indicates the molecule's heavy atoms

Supporting Table 1: Calculated absorption properties of benzanthrone-2-aminoacetamide derivatives in gas phase and solvent phase

Molecules	Solvent	$\lambda_{\max}$ (nm)	f_o	eV	Assignment	Contribution (in %)
BA1	Chloroform	419.57	0.335	2.955	HOMO→LUMO	96.70
	DMF	421.72	0.330	2.940	HOMO→LUMO	96.80
	Gas	409.35	0.243	3.029	HOMO→LUMO	91.60
BA2	Chloroform	424.51	0.299	2.921	HOMO→LUMO	96.30
	DMF	425.73	0.313	2.912	HOMO→LUMO	96.70
	Gas	410.02	0.216	3.024	HOMO-1→LUMO	75.50
BA3	Chloroform	422.22	0.332	2.937	HOMO→LUMO	97.00
	DMF	423.75	0.327	2.926	HOMO→LUMO	97.00
	Gas	413.52	0.243	2.998	HOMO→LUMO	90.10
BA4	Chloroform	421.62	0.321	2.941	HOMO-1→LUMO	86.80
	DMF	423.48	0.326	2.928	HOMO→LUMO	97.00
	Gas	411.39	0.248	3.014	HOMO-1→LUMO	94.00
BA5	Chloroform	414.60	0.336	2.990	HOMO→LUMO	96.50
	DMF	417.23	0.330	2.972	HOMO→LUMO	96.70
	Gas	404.82	0.219	3.063	HOMO→LUMO	80.00
BA6	Chloroform	420.44	0.316	2.949	HOMO→LUMO	97.00
	DMF	421.94	0.316	2.939	HOMO→LUMO	97.00
	Gas	413.84	0.203	2.996	HOMO→LUMO	94.00
BA7	Chloroform	417.17	0.332	2.972	HOMO→LUMO	96.70
	DMF	419.50	0.326	2.956	HOMO→LUMO	96.80
	Gas	407.31	0.244	3.044	HOMO→LUMO	91.40
BA8	Chloroform	406.49	0.228	3.050	HOMO-1→LUMO	95.00
	DMF	413.02	0.268	3.002	HOMO→LUMO	96.80
	Gas	401.10	0.140	3.091	HOMO-1→LUMO	57.00
BA9	Chloroform	420.07	0.320	2.952	HOMO→LUMO	96.90
	DMF	421.77	0.319	2.940	HOMO→LUMO	97.00
	Gas	412.07	0.202	3.009	HOMO→LUMO	93.50
BA10	Chloroform	410.39	0.183	3.021	HOMO-1→LUMO	97.40
	DMF	410.43	0.161	3.020	HOMO-1→LUMO	97.70
	Gas	406.28	0.187	3.052	HOMO-1→LUMO	90.30
BA11	Chloroform	420.72	0.327	2.947	HOMO-1→LUMO	96.30
	DMF	422.86	0.323	2.932	HOMO-1→LUMO	70.70
	Gas	412.17	0.249	3.008	HOMO-1→LUMO	94.20
BA12	Chloroform	420.98	0.329	2.945	HOMO-2→LUMO	96.60
	DMF	423.09	0.325	2.931	HOMO-1→LUMO	97.00
	Gas	410.71	0.242	3.019	HOMO-2→LUMO	93.70

Supporting Table 2: Calculated emission properties of benzanthrone-2-aminoacetamide derivatives in gas phase and solvent phase

Molecules	Solvent	$\lambda_{\max}$ (nm)	f_o	eV	Assignment	Contribution (in %)
BA1	Chloroform	506.16	0.317	2.450	HOMO-LUMO	97.75
	DMF	508.59	0.317	2.438	HOMO-LUMO	97.76
	Gas	493.81	0.225	2.511	HOMO-LUMO	96.60
BA2	Chloroform	508.21	0.319	2.440	HOMO-LUMO	97.76
	DMF	510.37	0.320	2.429	HOMO-LUMO	97.78
	Gas	416.76	0.231	2.975	HOMO-1-LUMO	94.00
BA3	Chloroform	508.11	0.315	2.440	HOMO-LUMO	97.79
	DMF	510.37	0.318	2.429	HOMO-LUMO	97.80
	Gas	495.70	0.225	2.501	HOMO-LUMO	96.68
BA4	Chloroform	508.43	0.322	2.439	HOMO-LUMO	97.79
	DMF	510.52	0.315	2.429	HOMO-LUMO	97.80
	Gas	415.16	0.112	2.986	HOMO-2-LUMO	68.92
BA5	Chloroform	505.36	0.321	2.453	HOMO-LUMO	97.74
	DMF	508.57	0.321	2.438	HOMO-LUMO	97.77
	Gas	492.42	0.230	2.518	HOMO-LUMO	96.57
BA6	Chloroform	508.14	0.315	2.440	HOMO-LUMO	97.80
	DMF	510.45	0.316	2.429	HOMO-LUMO	97.81
	Gas	416.67	0.230	2.976	HOMO-1-LUMO	94.03
BA7	Chloroform	507.55	0.318	2.443	HOMO-LUMO	97.78
	DMF	510.01	0.319	2.431	HOMO-LUMO	97.80
	Gas	494.47	0.227	2.507	HOMO-LUMO	96.64
BA8	Chloroform	429.57	0.284	2.886	HOMO-1-LUMO	95.30
	DMF	508.59	0.315	2.438	HOMO-LUMO	97.76
	Gas	422.48	0.113	2.935	HOMO-2-LUMO	66.25
BA9	Chloroform	508.15	0.314	2.440	HOMO-LUMO	97.80
	DMF	510.48	0.315	2.429	HOMO-LUMO	97.81
	Gas	416.58	0.234	2.976	HOMO-1-LUMO	94.10
BA10	Chloroform	431.30	0.293	2.875	HOMO-1-LUMO	95.45
	DMF	433.94	0.289	2.857	HOMO-1-LUMO	95.47
	Gas	425.93	0.208	2.911	HOMO-1-LUMO	93.45
BA11	Chloroform	452.29	0.135	2.741	HOMO-1-LUMO	87.90
	DMF	509.73	0.320	2.432	HOMO-LUMO	97.79
	Gas	418.27	0.143	2.964	HOMO-2-LUMO	71.49
BA12	Chloroform	437.26	0.255	2.836	HOMO-2-LUMO	93.29
	DMF	436.83	0.145	2.838	HOMO-2-LUMO	74.26
	Gas	438.89	0.080	2.825	HOMO-2-LUMO	76.64