Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Computational Evaluation of Optoelectronic and Photophysical Properties of Unsymmetrical Distyrylbiphenyls

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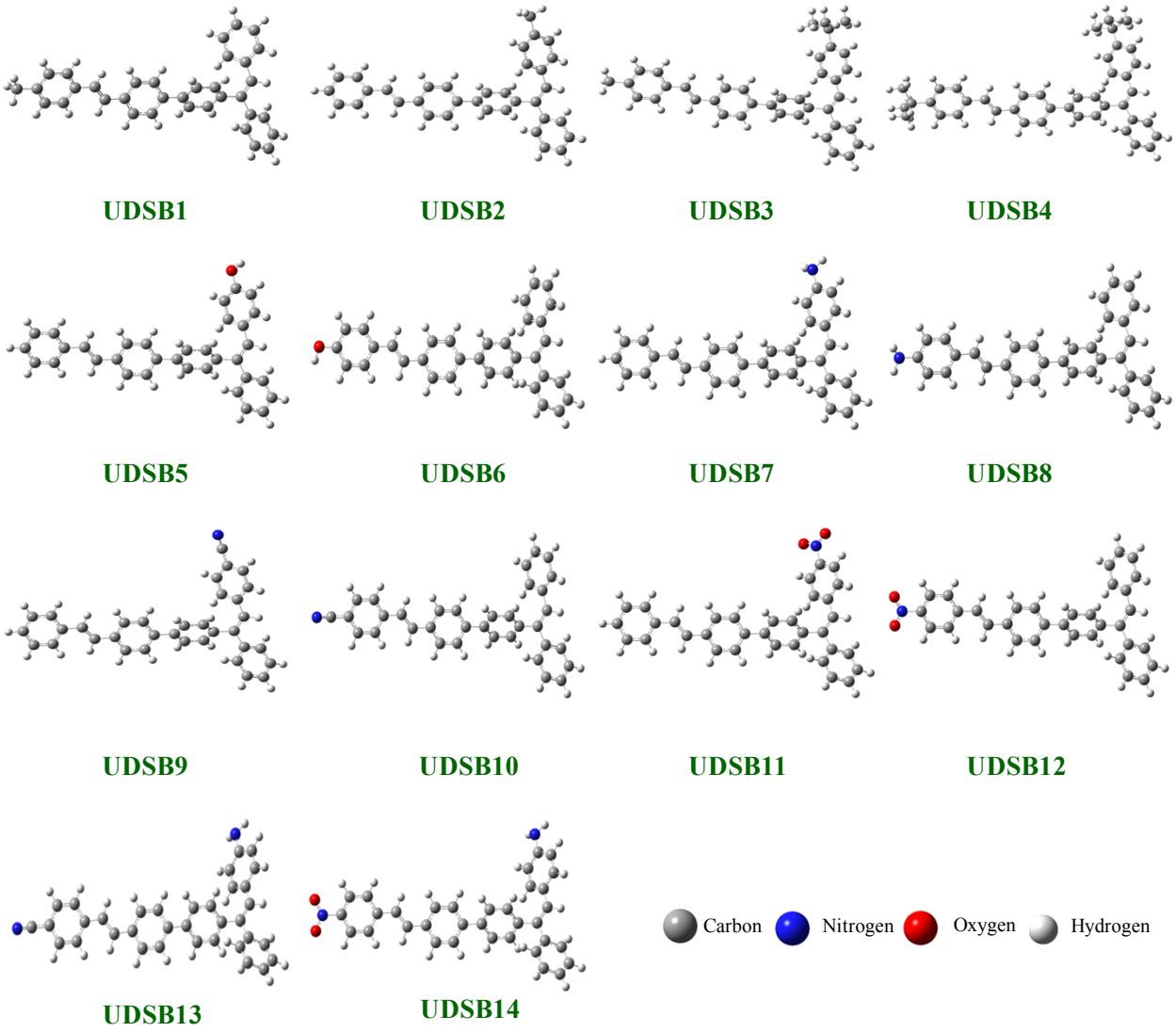
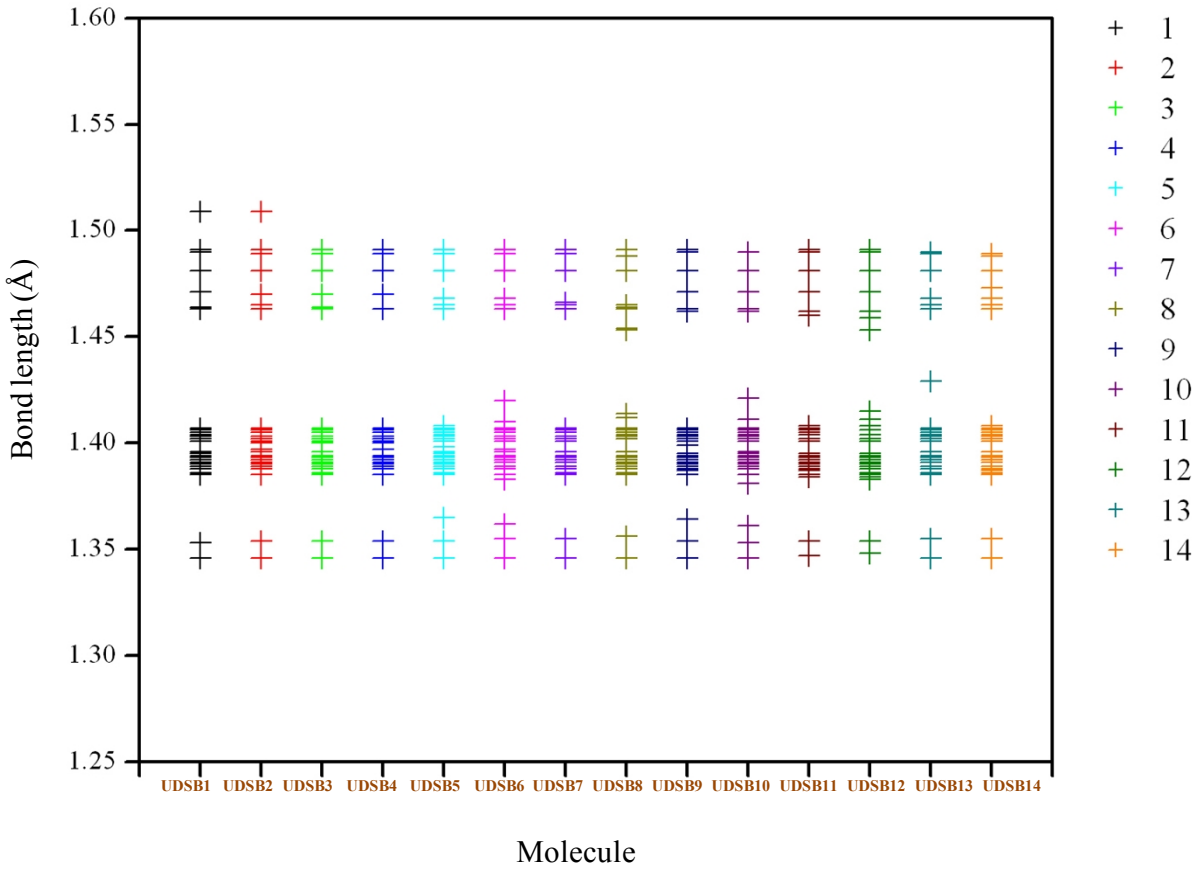
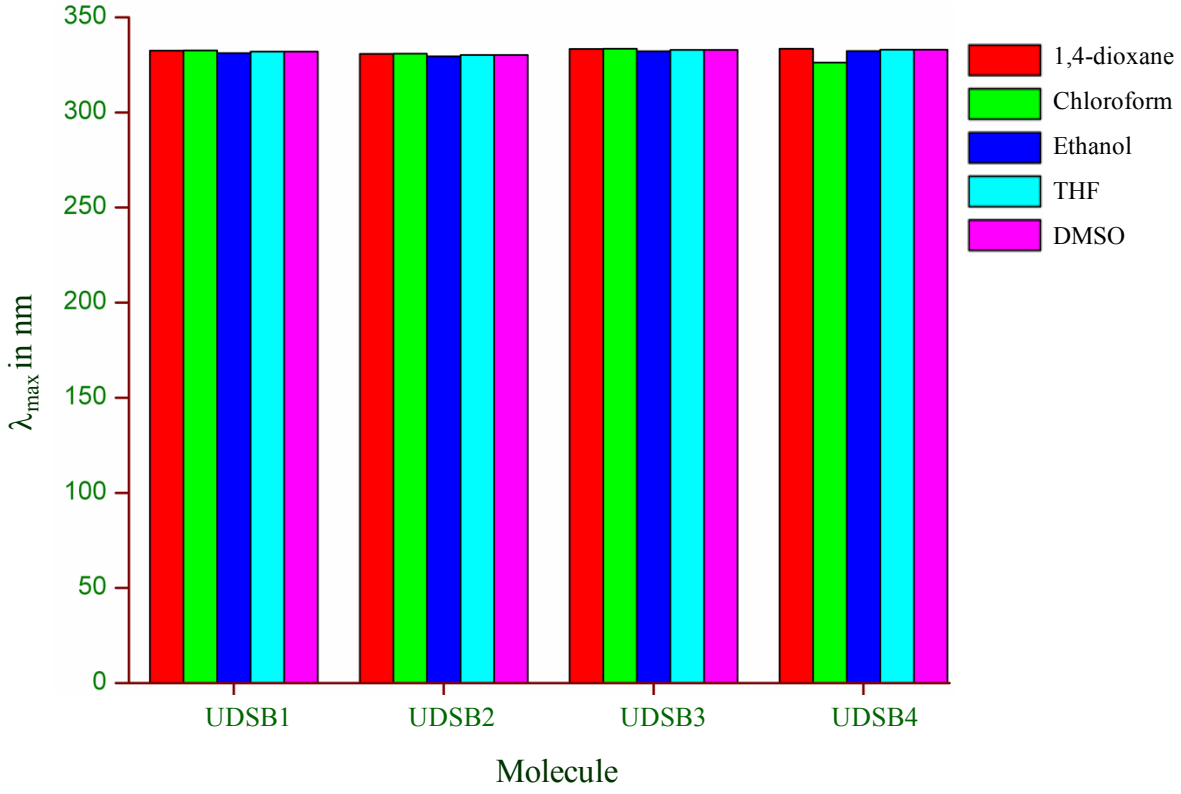
SIF1. Optimized structures of UDB 1-14 at B3LYP/6-311G(d,p) level.



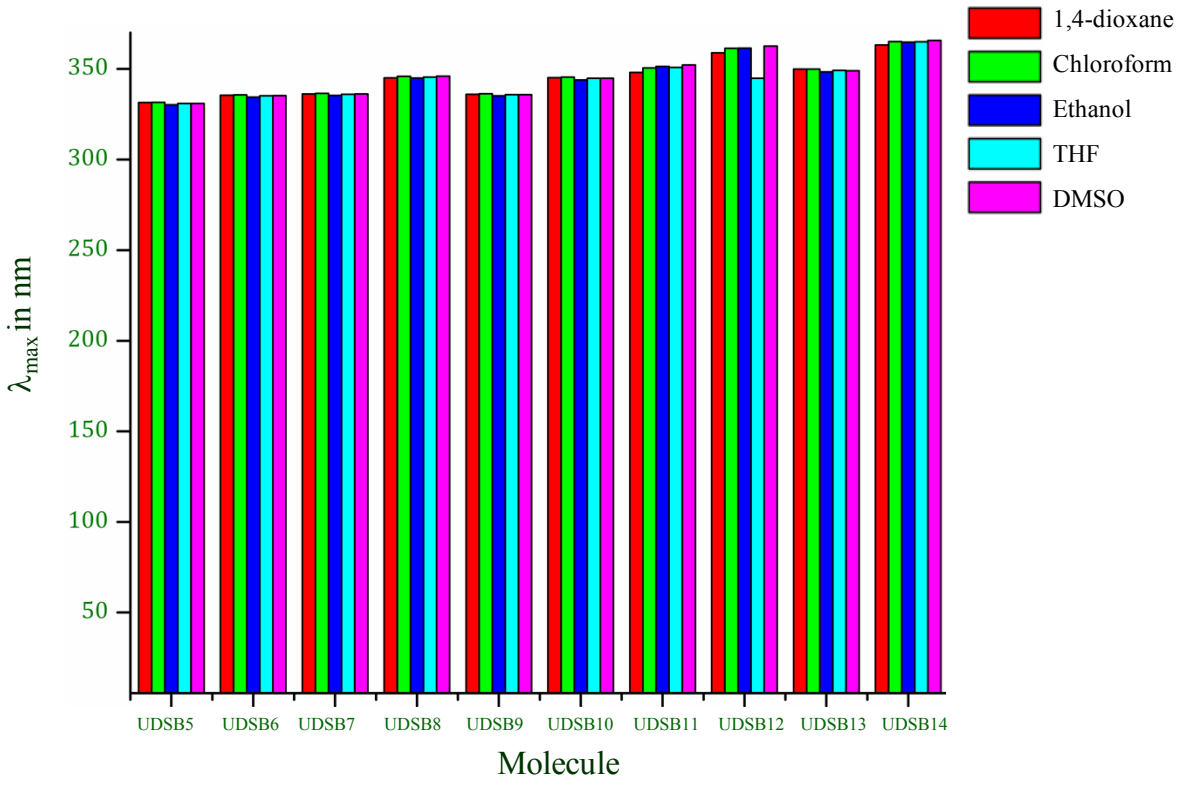
SIF2. Illustration of π-delocalization from calculated C-C bond lengths of UDSB 1-14 at B3LYP/6-311G(d,p) level.



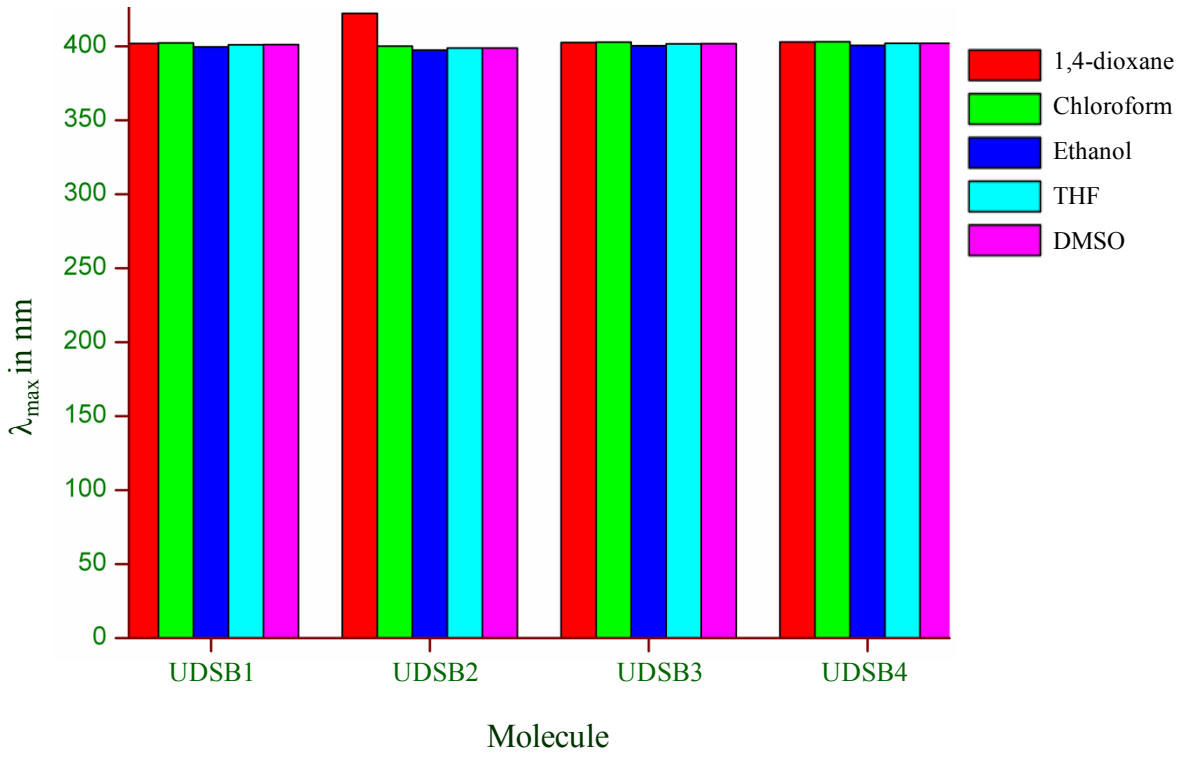
SIF3. Effect of solvent on computed absorption spectra of UDSB 1-4



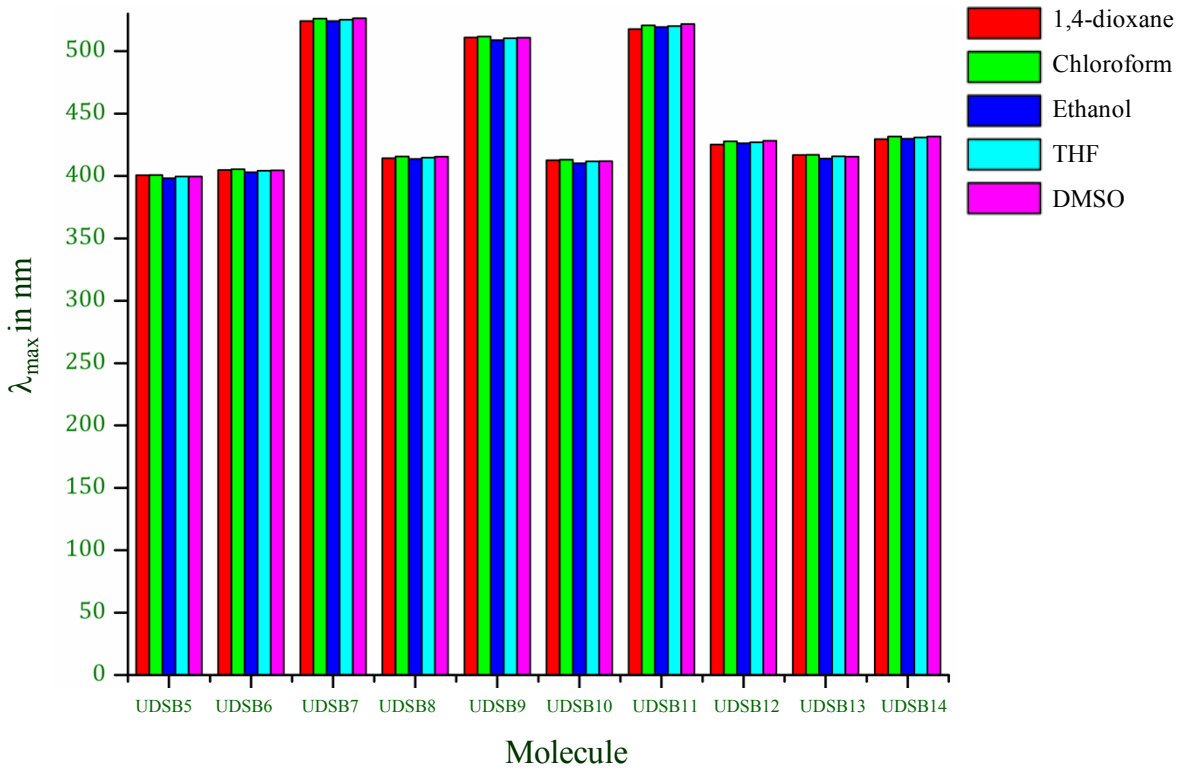
SIF4. Effect of Solvent on Computed Absorption Spectra of UDSB 5-14



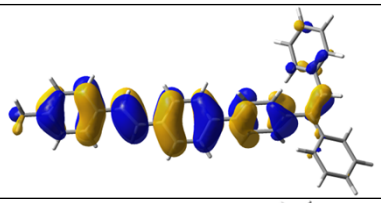
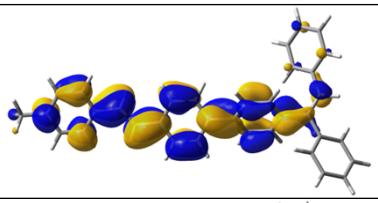
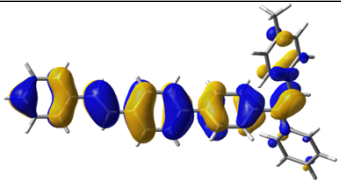
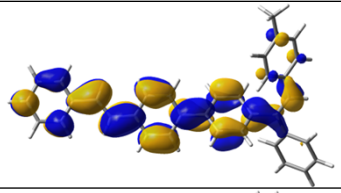
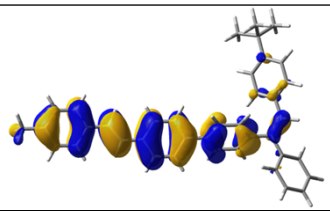
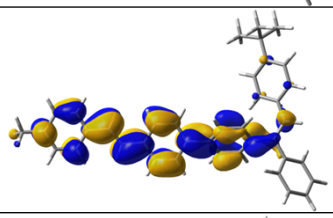
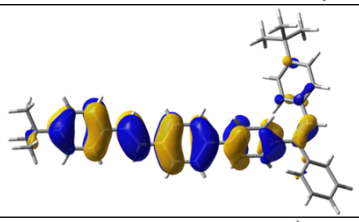
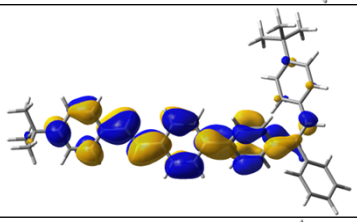
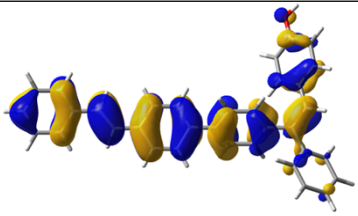
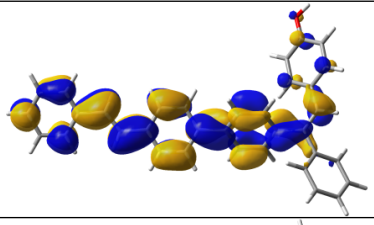
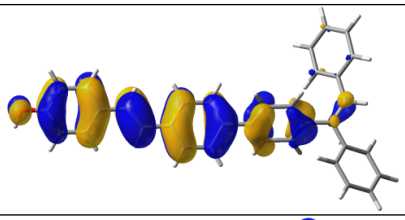
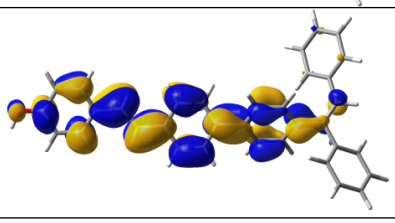
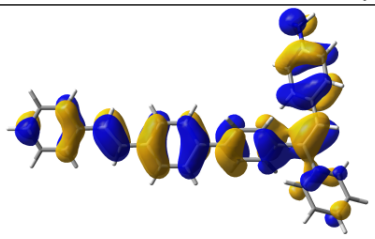
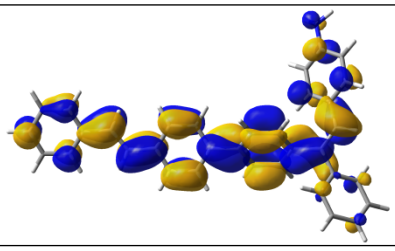
SIF5. Effect of Solvent on Computed Emission Spectra of UDSB 1-4



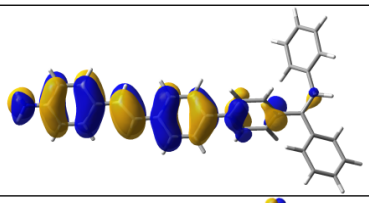
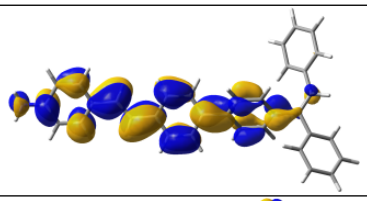
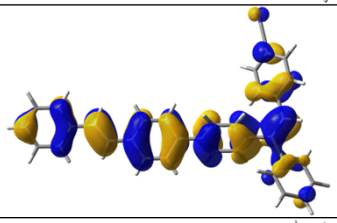
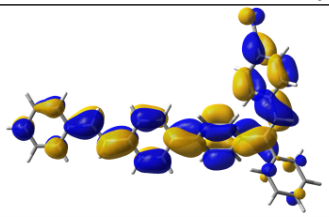
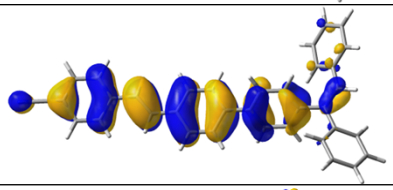
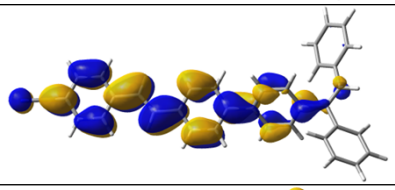
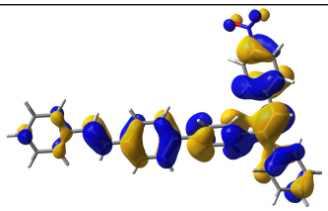
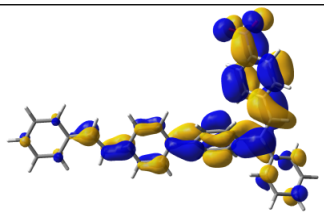
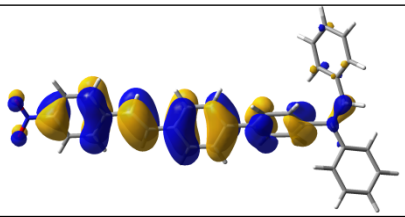
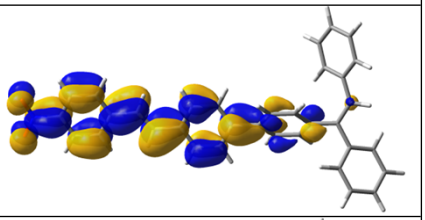
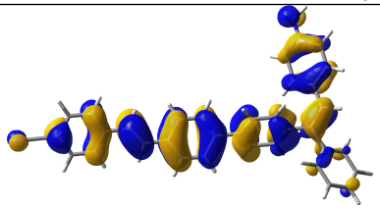
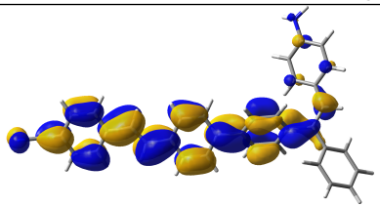
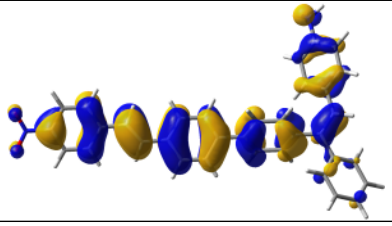
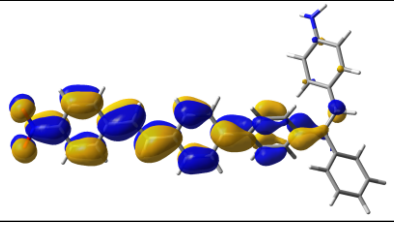
SIF6. Effect of Solvent on Computed Emission Spectra of UDSB 5-14



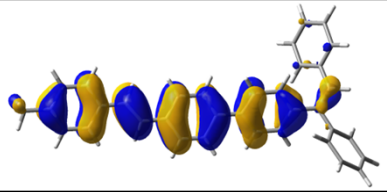
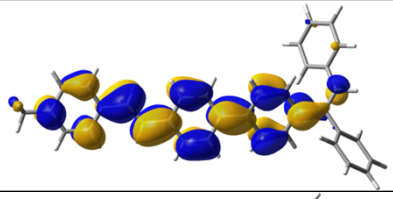
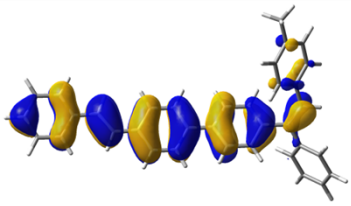
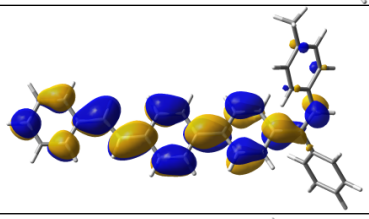
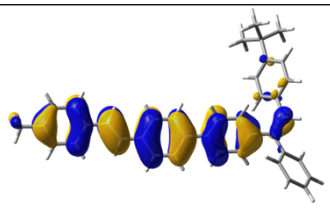
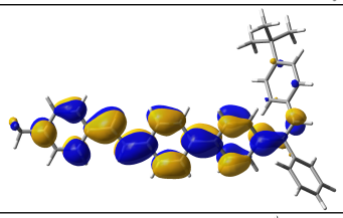
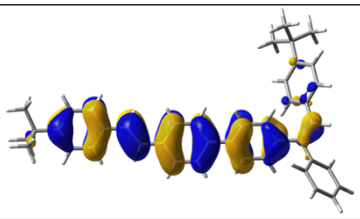
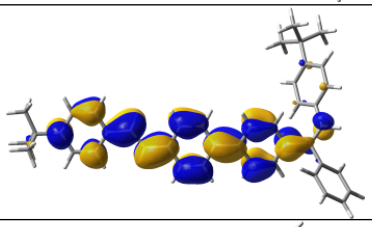
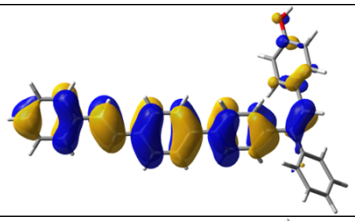
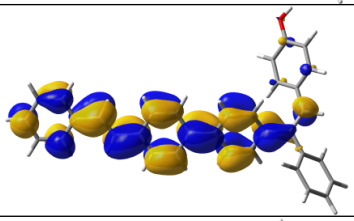
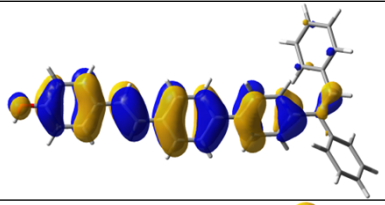
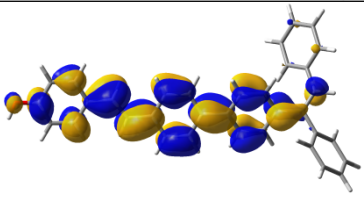
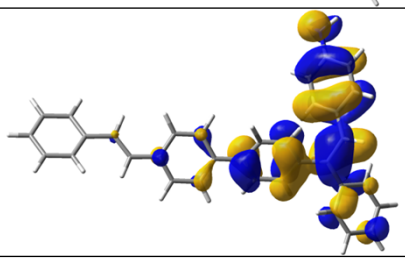
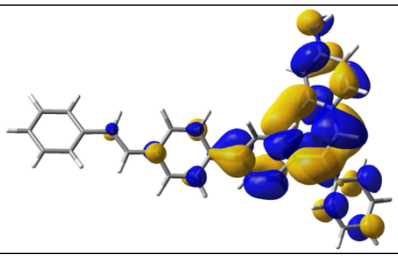
SIF7. Natural Transition Orbitals (NTOs) for the UDSB 1-7 illustrating the nature of optically active singlet excited states in the absorption bands. Shown are only occupied (holes) and unoccupied (electrons) NTO pairs that contribute more than 50% to each excited state. All transitions have π→π* character.

Molecule	λ_{cal} (nm)		Hole	Electron
UDSB1	333	S_1 W= 0.88		
UDSB2	331	S_1 W= 0.85		
UDSB3	334	S_1 W= 0.87		
UDSB4	334	S_1 W= 0.87		
UDSB5	332	S_1 W= 0.84		
UDSB6	336	S_1 W= 0.83		
UDSB7	337	S_1 W= 0.79		

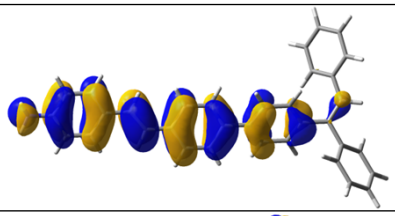
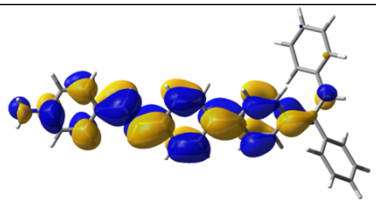
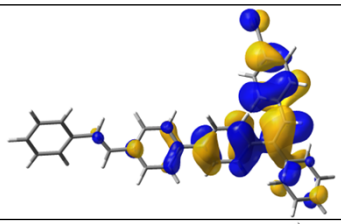
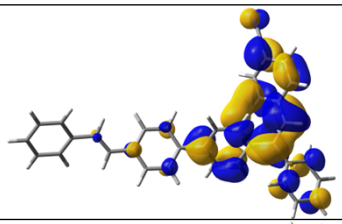
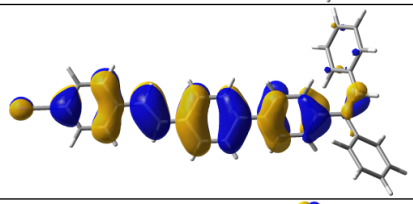
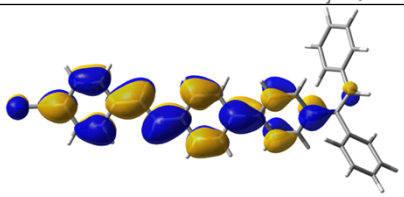
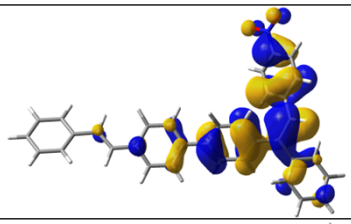
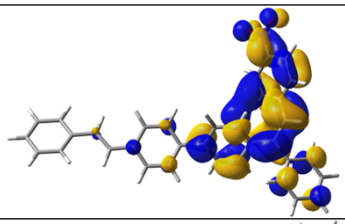
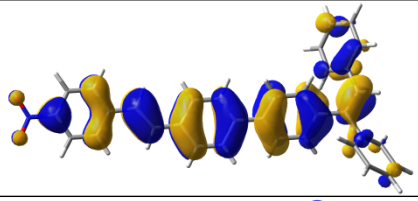
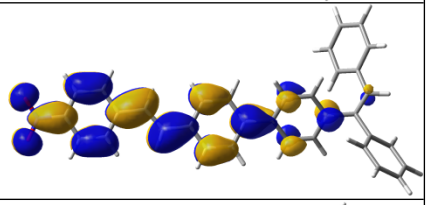
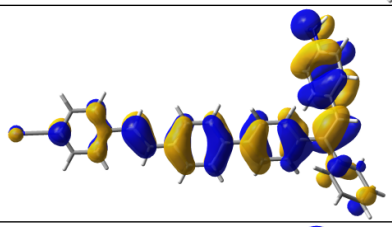
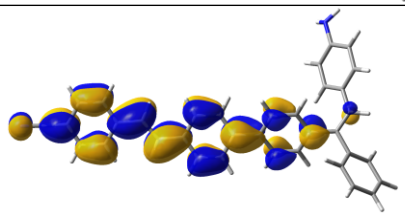
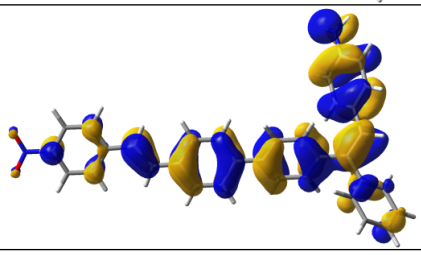
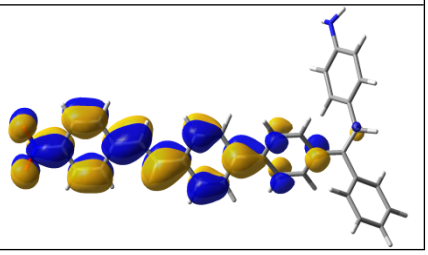
SIF8. Natural Transition Orbitals (NTOs) for the UDSB 8-14 illustrating the nature of optically active singlet excited states in the absorption bands. Shown are only occupied (holes) and unoccupied (electrons) NTO pairs that contribute more than 50% to each excited state. All transitions have π→π* character.

Molecule	λ_{cal} (nm)		Hole	Electron
UDSB8	346	S_1 W= 0.83		
UDSB9	336	S_1 W= 0.90		
UDSB10	346	S_1 W= 0.91		
UDSB11	351	S_1 W= 0.84		
UDSB12	361	S_1 W= 0.92		
UDSB13	350	S_1 W= 0.86		
UDSB14	365	S_1 W= 0.89		

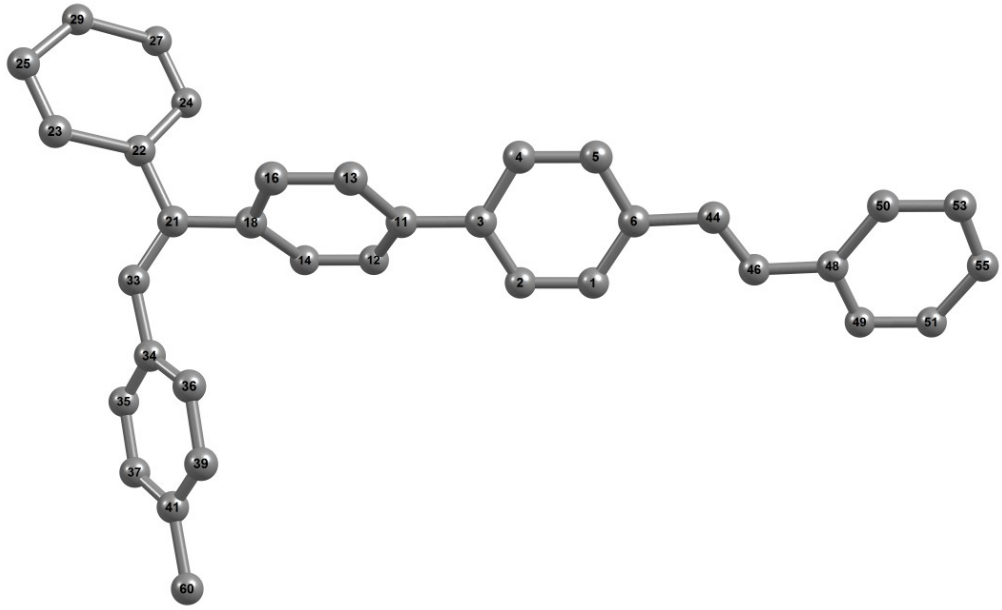
SIF9. Natural Transition Orbitals (NTOs) for the UDSB 1-7 illustrating the nature of optically active singlet excited states in the emission bands. Shown are only occupied (holes) and unoccupied (electrons) NTO pairs that contribute more than 50% to each excited state. All transitions have π→π* character.

Molecule	λ_{cal} (nm)		Hole	Electron
UDSB1	402	S_1 W= 0.95		
UDSB2	400	S_1 W= 0.94		
UDSB3	403	S_1 W= 0.94		
UDSB4	403	S_1 W= 0.94		
UDSB5	401	S_1 W= 0.94		
UDSB6	405	S_1 W= 0.93		
UDSB7	526	S_1 W= 0.99		

SIF10. Natural Transition Orbitals (NTOs) for the UDSB 8-14 illustrating the nature of optically active singlet excited states in the emission bands. Shown are only occupied (holes) and unoccupied (electrons) NTO pairs that contribute more than 50% to each excited state. All transitions have π→π* character.

Molecule	λ_{cal} (nm)		Hole	Electron
UDSB8	416	S_1 W= 0.99		
UDSB9	512	S_1 W= 0.95		
UDSB10	413	S_1 W= 0.95		
UDSB11	521	S_1 W= 0.99		
UDSB12	428	S_1 W= 0.95		
UDSB13	417	S_1 W= 0.94		
UDSB14	432	S_1 W= 0.95		

SIT1. Selected bond lengths (Å) and dihedral angles (°) of UDSB2 and UDSB7 B3LYP/6-311G(d,p) calculations



	UDSB2			UDSB7		
	Neutral	Cationic	Anionic	Neutral	Cationic	Anionic
C1-C2	1.385	1.376	1.378	1.382	1.379	1.377
C2-C3	1.406	1.416	1.420	1.406	1.412	1.421
C3-C4	1.402	1.413	1.419	1.402	1.409	1.420
C4-C5	1.388	1.379	1.379	1.388	1.381	1.378
C5-C6	1.505	1.415	1.418	1.405	1.411	1.420
C6-C1	1.407	1.416	1.421	1.407	1.413	1.423
C3-C11	1.481	1.461	1.456	1.481	1.466	1.455
C11-C12	1.403	1.415	1.419	1.403	1.413	1.420
C12-C14	1.389	1.379	1.380	1.390	1.380	1.380
C14-C18	1.401	1.414	1.416	1.401	1.413	1.415
C18-C16	1.402	1.413	1.416	1.401	1.412	1.415
C16-C13	1.389	1.380	1.381	1.390	1.381	1.382
C13-C11	1.403	1.414	1.419	1.403	1.412	1.419
C18-C21	1.491	1.466	1.464	1.491	1.465	1.467
C21-C22	1.489	1.480	1.487	1.489	1.476	1.487
C22-C23	1.404	1.408	1.408	1.405	1.408	1.408
C23-C25	1.391	1.390	1.392	1.396	1.388	1.392
C25-C29	1.393	1.400	1.394	1.393	1.395	1.394

C29-C27	1.394	1.394	1.340	1.394	1.394	1.396
C27-C24	1.391	1.390	1.390	1.391	1.389	1.390
C24-C22	1.404	1.410	1.409	1.405	1.409	1.408
C21-C33	1.354	1.381	1.383	1.355	1.388	1.379
C33-C34	1.470	1.444	1.452	1.466	1.430	1.456
C34-C35	1.405	1.415	1.414	1.406	1.424	1.412
C35-C37	1.390	1.382	1.390	1.386	1.372	1.388
C37-C41	1.397	1.405	1.400	1.403	1.418	1.401
C41-C(N)60	1.509	1.503	1.510	1.392	1.351	1.410
C34-C36	1.405	1.415	1.416	1.407	1.424	1.414
C36-39	1.389	1.383	1.387	1.385	1.371	1.386
C39-C41	1.400	1.405	1.402	1.405	1.420	1.402
C6-C44	1.463	1.442	1.437	1.463	1.450	1.434
C44-C46	1.346	1.361	1.368	1.346	1.355	1.371
C46-C48	1.465	1.448	1.447	1.465	1.454	1.444
C48-C49	1.405	1.411	1.416	1.405	1.408	1.417
C49-C51	1.391	1.387	1.388	1.391	1.389	1.387
C51-C55	1.392	1.395	1.397	1.392	1.394	1.398
C55-C53	1.396	1.399	1.340	1.340	1.398	1.399
C53-C50	1.388	1.384	1.387	1.388	1.386	1.387
C50-C48	1.407	1.412	1.418	1.407	1.410	1.419
C1-C6-C44-C46	3.94	0.54	0.52	3.57	0.34	0.43
C44-C46-C48-C50	3.58	0.14	0.22	3.08	0.59	0.02
C2-C3-C11-C12	37.56	24.617	19.685	37.32	26.72	18.96
C4-C3-C11-C13	37.00	24.31	18.94	36.789	26.29	18.20
C16-C18-C21-C22	54.85	40.09	39.314	55.616	40.55	40.68
C14-C18-C21-C33	54.46	18.64	36.451	55.319	40.94	38.03
C18-C21-C33-C34	8.30	15.89	18.218	8.675	18.56	16.82

SIT2. Second order perturbation interactions obtained for UDSB 1-14 at B3LYP/6-311g(d,p) from NBO calculations

Molecules	Donor(i)	Acceptor(j)	E(2) (kcal mol^{-1})	E(j)-E(i) (a.u)	$F(i,j)$ (a.u)
UDSB1	π C11 – C12	π* C14 – C18	21.95	0.28	0.070
	π C30 – C34	π* C27 – C28	21.55	0.28	0.070
UDSB2	π C37 – C41	π* C34 – C35	21.98	0.28	0.071
	π C11 – C12	π* C14 – C18	21.83	0.28	0.070
UDSB3	π C47 – C49	π* C42 – C44	21.96	0.28	0.071
	π C11 – C12	π* C14 – C18	21.90	0.28	0.070
UDSB4	π C43 – C45	π* C38 – C40	21.96	0.28	0.071
	π C11 – C12	π* C14 – C18	21.89	0.28	0.070
UDSB5	LP (2) O59	π* C41 – C45	28.80	0.35	0.096
	π C40 – C43	π* C41 – C45	22.97	0.27	0.073
UDSB6	LP (2) O60	π* C30 – C34	27.63	0.35	0.094
	π C30 – C34	π* C27 – C28	23.37	0.29	0.074
UDSB7	LP (1) N 60	π* C41 – C45	27.83	0.33	0.091
	π C41 – C45	π* C38 – C39	24.66	0.29	0.076
UDSB8	LP (1) N 60	π* C30 – C34	28.11	0.33	0.091
	π C30 – C34	π* C27 – C28	24.30	0.29	0.076
UDSB9	π C38 – C39	π* C41 – C45	24.46	0.27	0.073
	π C11 – C12	π* C14 – C18	22.39	0.28	0.071
UDSB10	π C27 – C28	π* C30– C34	24.69	0.27	0.073
	π C3 – C4	π* C5 – C6	22.11	0.28	0.070
UDSB11	LP (3) O61	π* N59 – O60	164.28	0.14	0.140
	π C41 – C45	π* N59 – O60	28.13	0.15	0.062
UDSB12	LP (3) O61	π* N60 – O62	164.23	0.14	0.139
	π C27 – C28	π* C30 – C34	25.00	0.27	0.074
UDSB13	LP (1) N61	π* C41 – C45	28.03	0.33	0.091
	π C27 – C28	π* C30 – C34	24.76	0.27	0.073
UDSB14	LP (3) O60	π* N59 – O61	163.70	0.14	0.139
	LP (1) N 62	π* C41 – C45	28.08	0.33	0.091