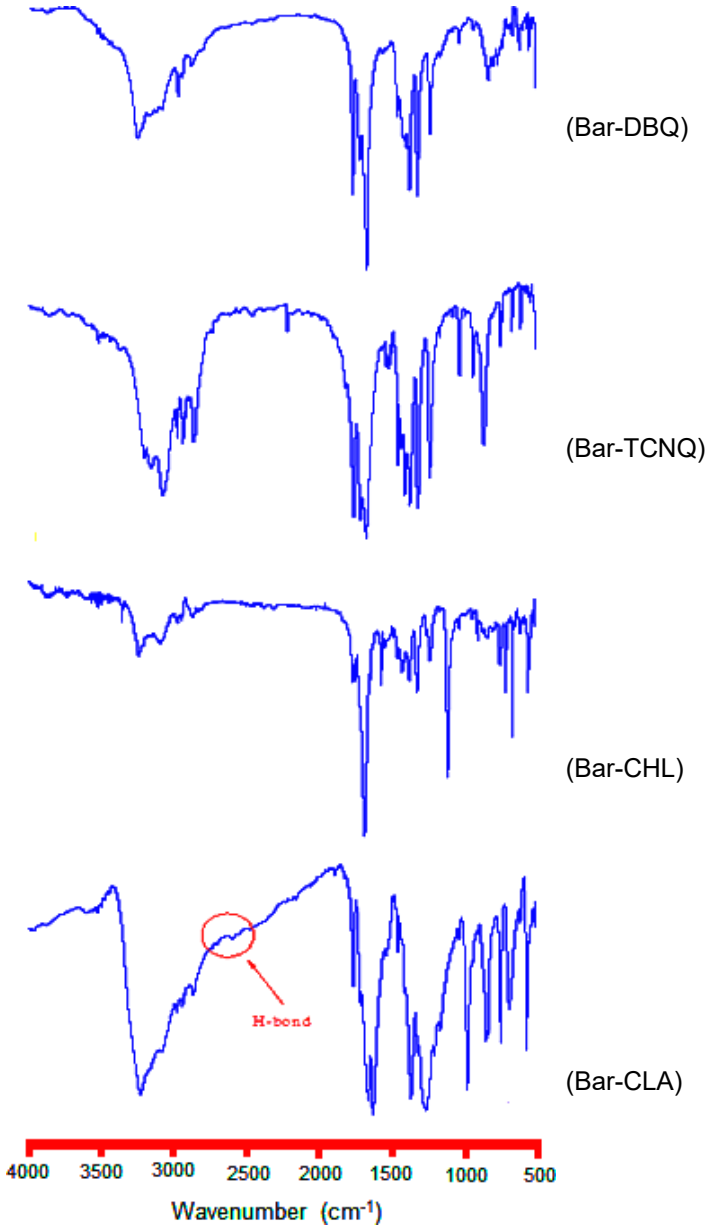

Figure S1. The IR spectra of Bar-CT complexes [56].

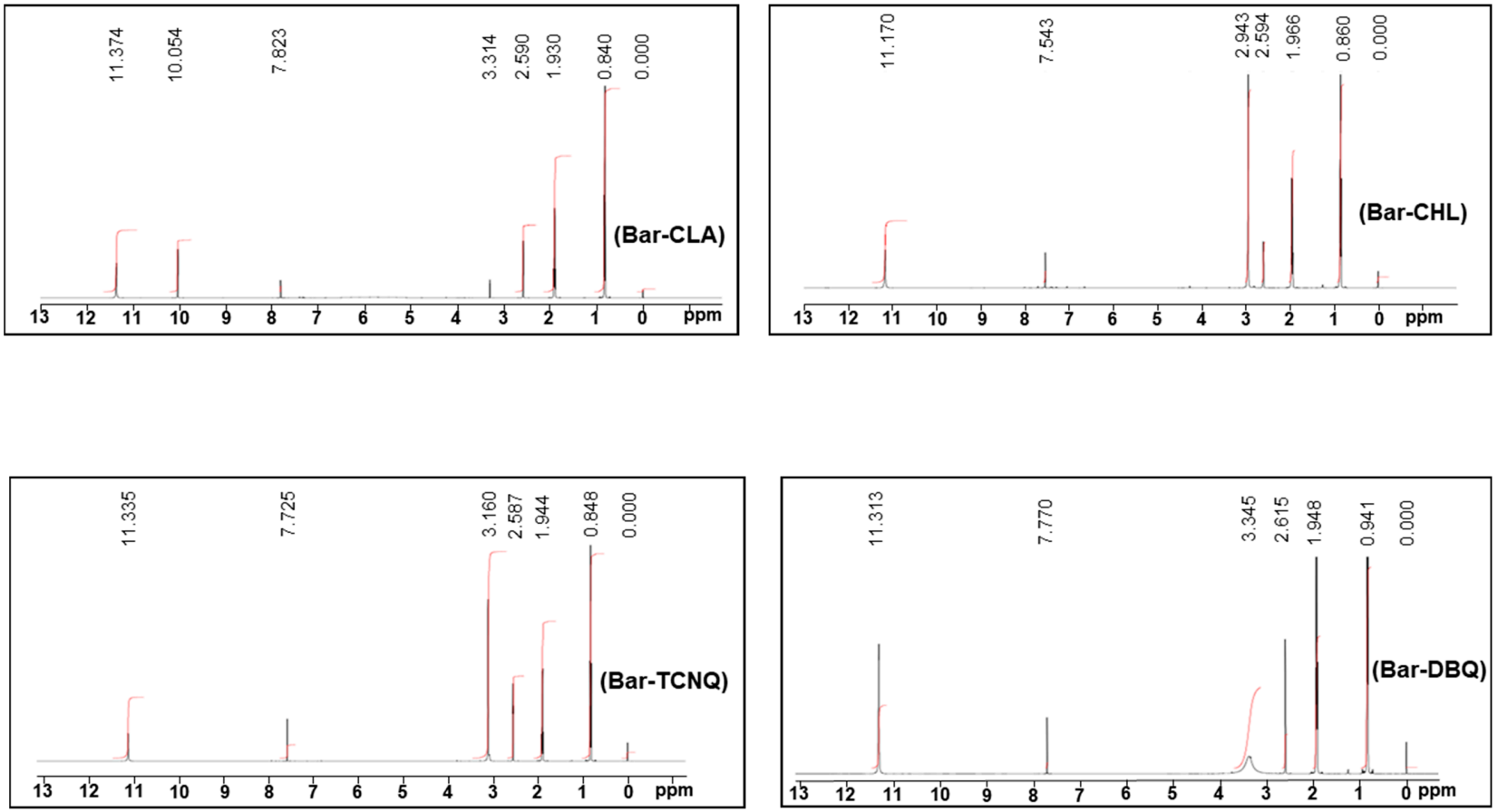

Figure S2. The ^{1}H NMR spectra of Bar-CT complexes [56].

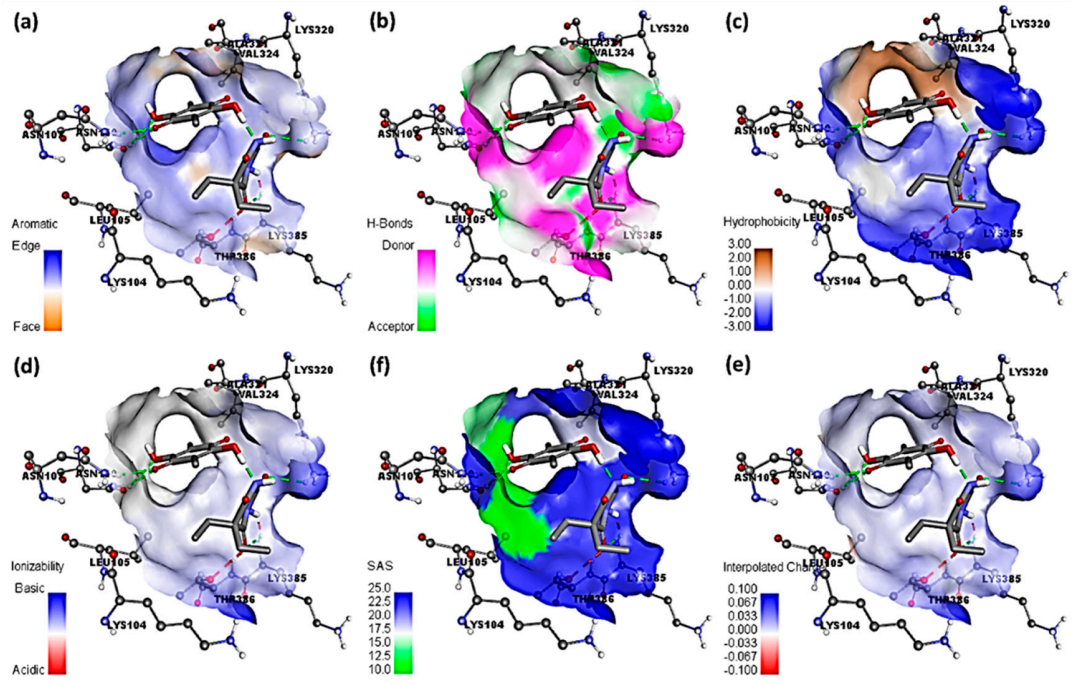

Figure S3. The docking results of (Bar-CLA)-serotonin complex. **a:**aromatic surface, **b:** hydrogen binding surface, **c:** hydrophobic surface, **d:** ionizability surface, **e:**solvent accessible surface, and **f:** Interpolated charge.

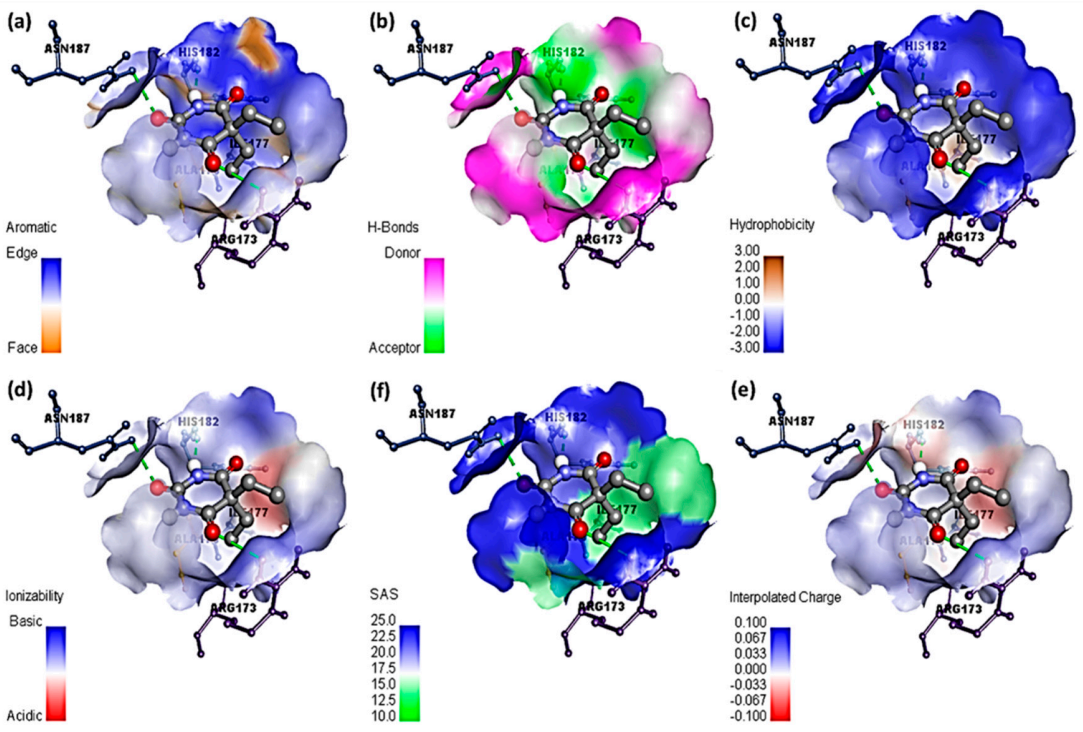

Figure S4. The docking results of (Bar)-serotonin complex. **a:**aromatic surface, **b:** hydrogen binding surface, **c:** hydrophobic surface, **d:** ionizability surface, **e:**solvent accessible surface, and **f:** Interpolated charge.

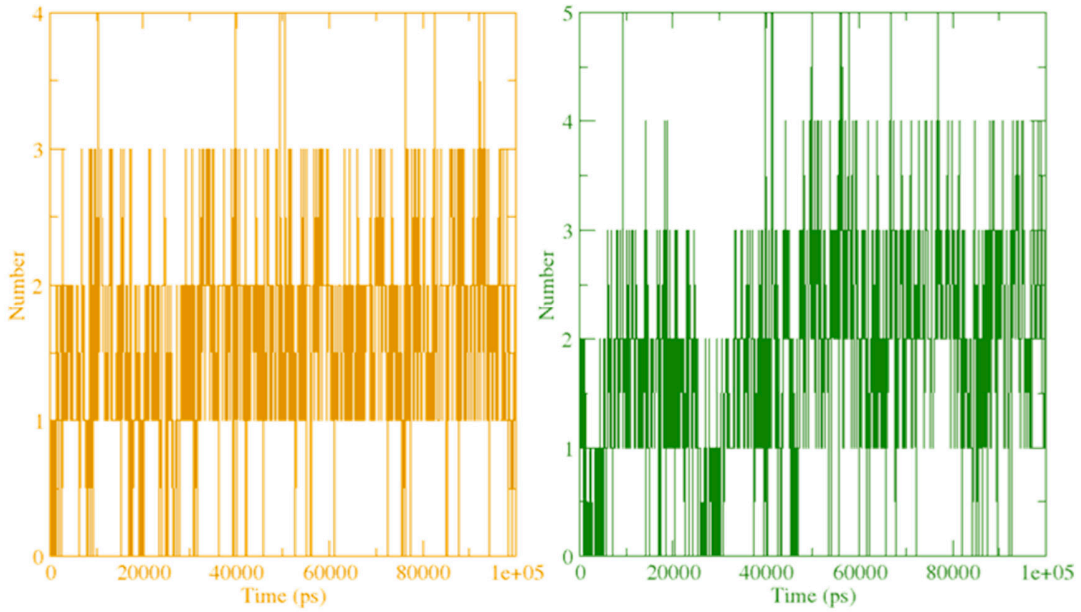

Figure S5. Number of average hydrogen bonding interactions between (a) BarScomplex and (b) BarCS complex during 100 ns simulation time.

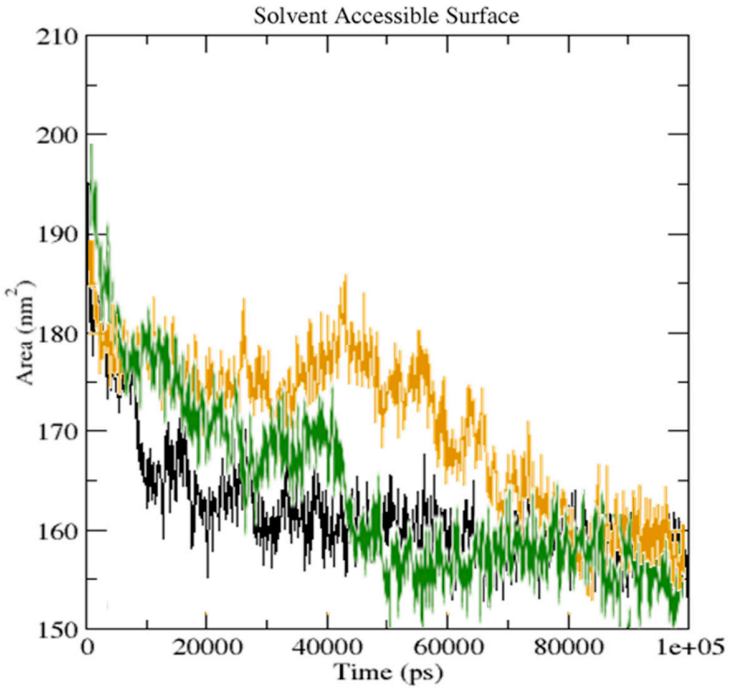

Figure S6. Solvent accessible surface area analysis for unbound serotonin receptor (black), BarS complex (orange) and BarCS complex (green) during 100 ns simulation time.

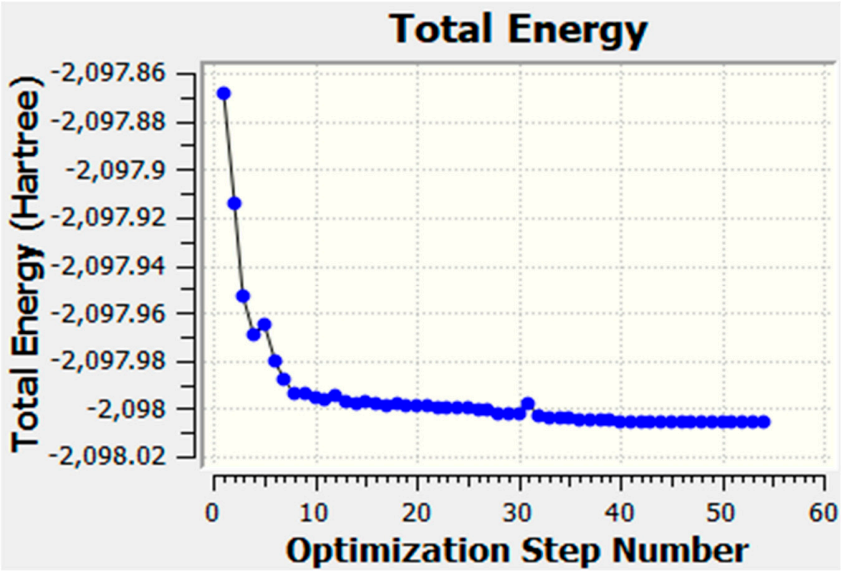

Figure S7. Optimization Steps for (Bar-CLA)(B3LYP/6-311G++).

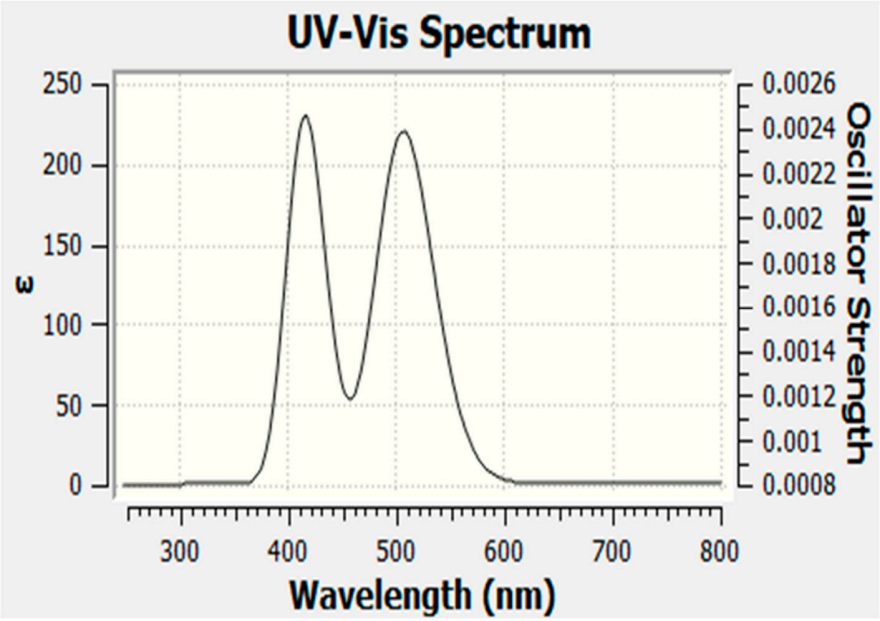

Figure S8. UV-visible spectrum of (Bar-CLA) obtained through TD-DFT calculations.

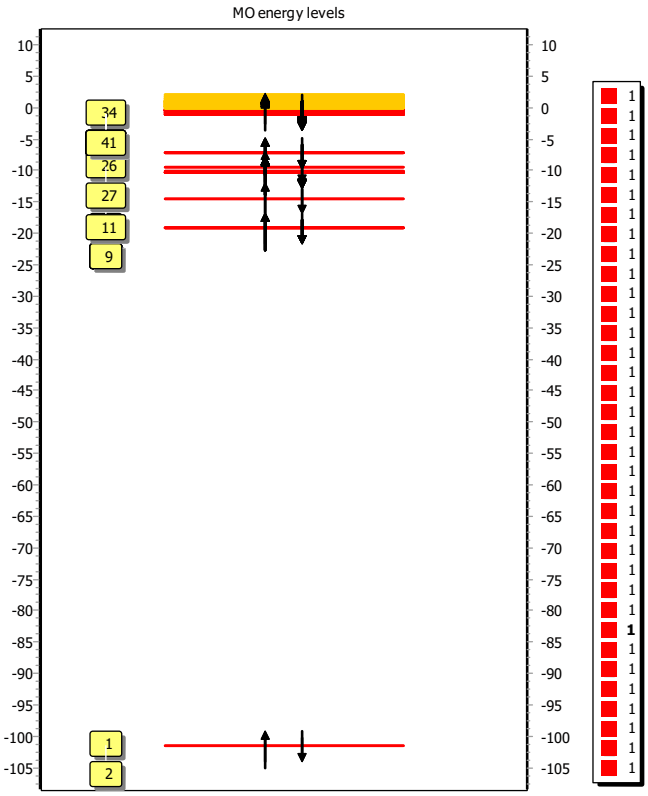

Figure S9. MO energy level diagram of the CT complex (Bar-CLA).

Table S1. (Bar-CLA)-dopamine interactions results by DS.

Name	Distance	Category	Type
ASN107:H - (Bar-CLA):O	2.16368	Hydrogen Bond	Conventional Hydrogen Bond
ASN110:H - (Bar-CLA):O	2.23611	Hydrogen Bond	Conventional Hydrogen Bond
ASN110:H - (Bar-CLA):O	2.7051	Hydrogen Bond	Conventional Hydrogen Bond
LYS320:H - (Bar-CLA):O	2.59336	Hydrogen Bond	Conventional Hydrogen Bond
LYS385:HN - (Bar-CLA):O	2.59495	Hydrogen Bond	Conventional Hydrogen Bond
THR386:HN - (Bar-CLA):O	1.96306	Hydrogen Bond	Conventional Hydrogen Bond
(Bar-CLA):H - (Bar-CLA):N	1.50033	Hydrogen Bond	Conventional Hydrogen Bond
(Bar-CLA):Cl - VAL324	4.25141	Hydrophobic	Alkyl
(Bar-CLA):C - LYS104	4.44711	Hydrophobic	Alkyl
(Bar-CLA):C - LEU105	5.45535	Hydrophobic	Alkyl
(Bar-CLA) - ALA321	4.19839	Hydrophobic	Pi-Alkyl

Table S2. Bar-dopamine interactions results by DS.

Name	Distance	Category	Type
ARG173:H - Bar:O6	2.72974	Hydrogen Bond	Conventional Hydrogen Bond
ASN187:H - Bar:O2	2.72666	Hydrogen Bond	Conventional Hydrogen Bond
UNK1:H - Bar:O	2.33497	Hydrogen Bond	Conventional Hydrogen Bond
ALA176 - Bar:C10	4.31947	Hydrophobic	Alkyl
Bar:C10 - ARG173	4.11553	Hydrophobic	Alkyl
Bar:C10 - ILE177	5.1821	Hydrophobic	Alkyl

Table S3. The bond lengths of the CT complex (Bar-CLA) obtained through DFT.

S. No.	(Bar-CLA) (B3LYP/ 6-311G++)			
	Atom No.	Bond length (Å)	Atom No.	Bond length (Å)
1	R(1-9)	1.258	R(11-19)	1.07
2	R(2-10)	1.259	R(11-20)	1.07
3	R(3-13)	1.258	R(12-21)	1.07
4	R(4-9)	1.476	R(12-22)	1.07
5	R(4-13)	1.482	R(12-23)	1.07
6	R(4-24)	1	R(26-34)	1.76
7	R(5-10)	1.464	R(27-35)	1.76
8	R(5-13)	1.476	R(28-32)	1.43
9	R(5-25)	1	R(28-38)	0.96
10	R(6-7)	1.54	R(29-33)	1.43
11	R(6-8)	1.54	R(29-39)	0.96
12	R(6-9)	1.535	R(30-36)	1.258
13	R(6-10)	1.528	R(31-37)	1.258
14	R(7-11)	1.54	R(32-34)	1.355
15	R(7-14)	1.07	R(32-37)	1.54
16	R(7-15)	1.07	R(33-35)	1.355
17	R(8-12)	1.54	R(33-36)	1.54
18	R(8-16)	1.07	R(34-36)	1.54
19	R(8-17)	1.07	R(35-37)	1.539
20	R(11-18)	1.07	R(4-38)	1.5

Table S4. The bond angles of the CT complex (Bar-CLA) obtained through DFT.

S. No.	(Bar-CLA) (B3LYP/ 6-311G++)			
	Atom No.	Bond Angle (Å)	Atom No.	Bond Angle (Å)
1	A(1-9-4)	117.7	A(14-7-15)	109.5
2	A(1-9-6)	117.7	A(12-8-16)	109.5
3	A(2-10-5)	119.8	A(12-8-17)	109.5
4	A(2-10-6)	119.8	A(8-12-21)	109.4
5	A(3-13-4)	117	A(8-12-22)	109.5
6	A(3-13-5)	117	A(8-12-23)	109.5
7	A(9-4-13)	113.8	A(16-8-17)	109.5
8	A(9-4-24)	107.7	A(18-11-19)	109.5
9	A(4-9-6)	124.5	A(18-11-20)	109.5
10	A(9-4-38)	108.7	A(19-11-20)	109.4
11	A(13-4-24)	107.6	A(21-12-22)	109.5
12	A(4-13-5)	126	A(21-12-23)	109.5
13	A(13-4-38)	108.9	A(22-12-23)	109.5
14	A(24-4-38)	110.1	A(26-34-32)	120
15	A(10-5-13)	113.3	A(26-34-36)	120
16	A(10-5-25)	109.1	A(27-35-33)	120
17	A(5-10-6)	120.3	A(27-35-37)	120
18	A(13-5-25)	107.6	A(32-28-38)	109.4
19	A(7-6-8)	109.7	A(28-32-34)	120
20	A(7-6-9)	108.5	A(28-32-37)	120
21	A(7-6-10)	109.9	A(28-38-4)	179.9
22	A(6-7-11)	109.5	A(33-29-39)	109.5
23	A(6-7-14)	109.5	A(29-33-35)	120

24	A(6-7-15)	109.5	A(29-33-36)	120
25	A(8-6-9)	109.6	A(30-36-33)	120
26	A(8-6-10)	108.2	A(30-36-34)	120
27	A(6-8-12)	109.5	A(31-37-32)	120
28	A(6-8-16)	109.5	A(31-37-35)	120
29	A(6-8-17)	109.5	A(34-32-37)	120
30	A(9-6-10)	110.9	A(32-34-36)	120
31	A(11-7-14)	109.5	A(32-37-35)	120
32	A(11-7-15)	109.5	A(35-33-36)	120
33	A(7-11-18)	109.5	A(33-35-37)	120
34	A(7-11-19)	109.5	A(33-36-34)	120
35	A(7-11-20)	109.5		

Table S5. Mulliken atomic charges of the CT complex (Bar-CLA) atoms.

S.No.	Synthesized complex			
	Mulliken atomic numbers	**Mulliken atomic charges**	**Mulliken atomic numbers**	**Mulliken atomic charges**
1	1O	-0.39605	21H	0.16819
2	2O	-0.4134	22H	0.15527
3	3O	-0.37655	23H	0.15026
4	4N	-0.73014	24H	0.40593
5	5N	-0.51945	25H	0.35518
6	6C	-0.10352	26Cl	0.20931
7	7C	-0.22869	27Cl	0.21513
8	8C	-0.24093	28O	-0.59099
9	9C	0.48745	29O	-0.56989
10	10C	0.45428	30O	-0.40156
11	11C	-0.44066	31O	-0.43624
12	12C	-0.417	32C	0.30859
13	13C	0.56652	33C	0.32137
14	14H	0.17528	34C	-0.34899
15	15H	0.16892	35C	-0.33435
16	16H	0.15877	36C	0.34696
17	17H	0.1732	37C	0.39147
18	18H	0.15941	38H	0.48295
19	19H	0.14673	39H	0.39692
20	20H	0.15035		

Table S6. Theoretical molecular properties of (Bar-CLA) complex and their constituents.

Parameters	B3LYP/ 6-311G++
Minimum SCF energy (a.u.)	-2097.881963
Polarizability (α) (a.u.)	201.790198
Dipole Moment (Debye)	4.931296
Zero point vibrational energy (kcal/mol)	174.56503
Total thermal energy (kcal/mol)	187.763
Electronic spatial extent (a.u.)	11030.3027
Frontier MO energies (eV)	
LUMO	-3.9623
HOMO	-6.4029
HOMO-1	-6.9533
Gap (HOMO – LUMO)	2.4406
Gap (HOMO-1 – LUMO)	2.9533