Supporting materials

S1 Effect of concentration on fluorescence intensity

The experiment with different concentrations was performed and the results shows that fluorescence intensity and the concentration of the selected 14 single ring aromatic compounds in water displayed linear co relation with value of R^2 as 0.998–0.999 (Fig. S1).

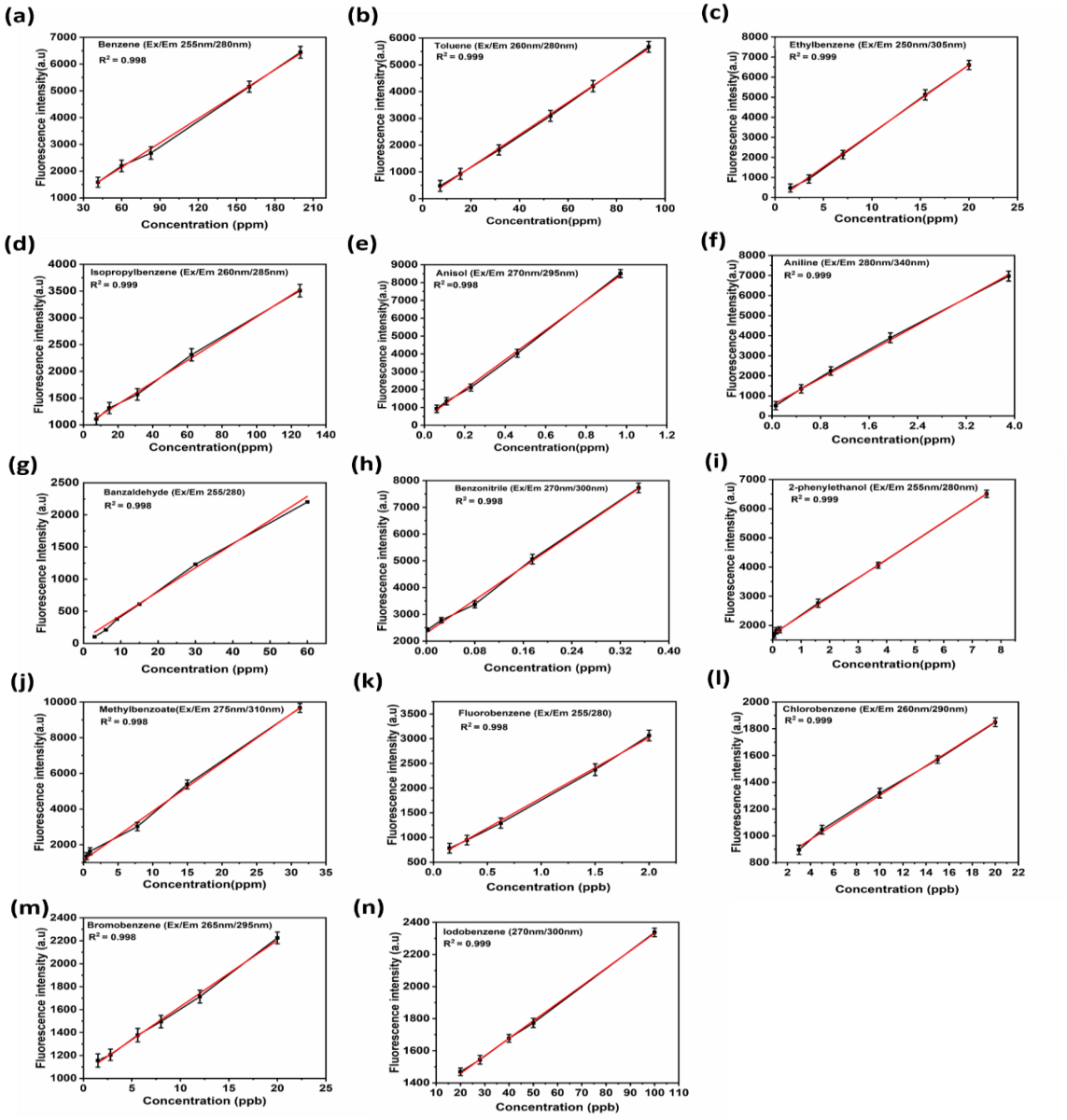


Fig. S1 Fluorescence details of concentration vs fluorescence intensity of (a) benzene, (b) toluene, (c) ethylbenzene, (d) isopropylbenzene, (e) anisole, (f) aniline, (g) benzaldehyde, (h) benzonitrile, (i) 2-phenyl ethanol, (j) methyl benzoate, (k) fluorobenzene, (l) chlorobenzene, (m) bromobenzene, (n) iodobenzene

S2 EEMs of alkyl substituted benzene

The fluorescence Excitation Emission Matrices of alkyl substituted aromatic benzene such as benzene, toluene, Ethylbenzene and isopropyl benzene showed little variation in EX/EM wavelength (Fig. S2) (Cheng et al., 2018).

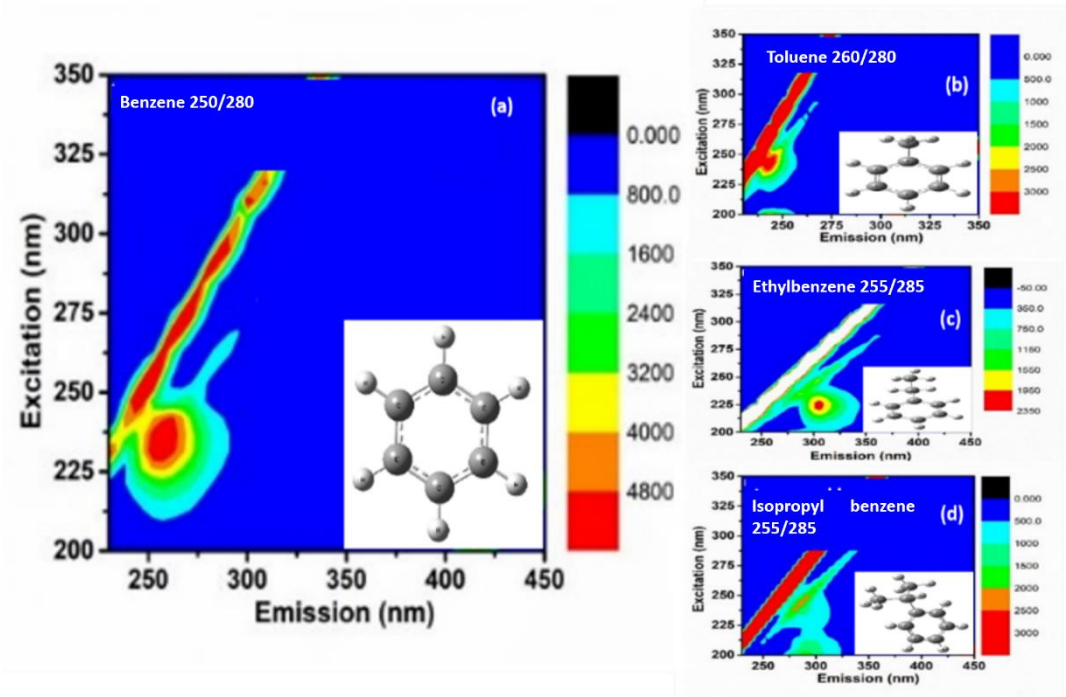


Fig. S2 EEMs of alkyl substituted benzene: (a) benzene, (b) toluene, (c) ethylbenzene and (d) isopropylbenzene

S3 EEMs of nitrogen and oxygen containing substituent with benzene

The fluorescence EX/EM of aniline is compared with other compounds of the same group, which shows longer emission in aniline than the others (Fig. S3). The longer emission is associated to the presence lone pair electrons at nitrogen (-NH_2), which contribute to the ring and make aniline as strong aromatic base.

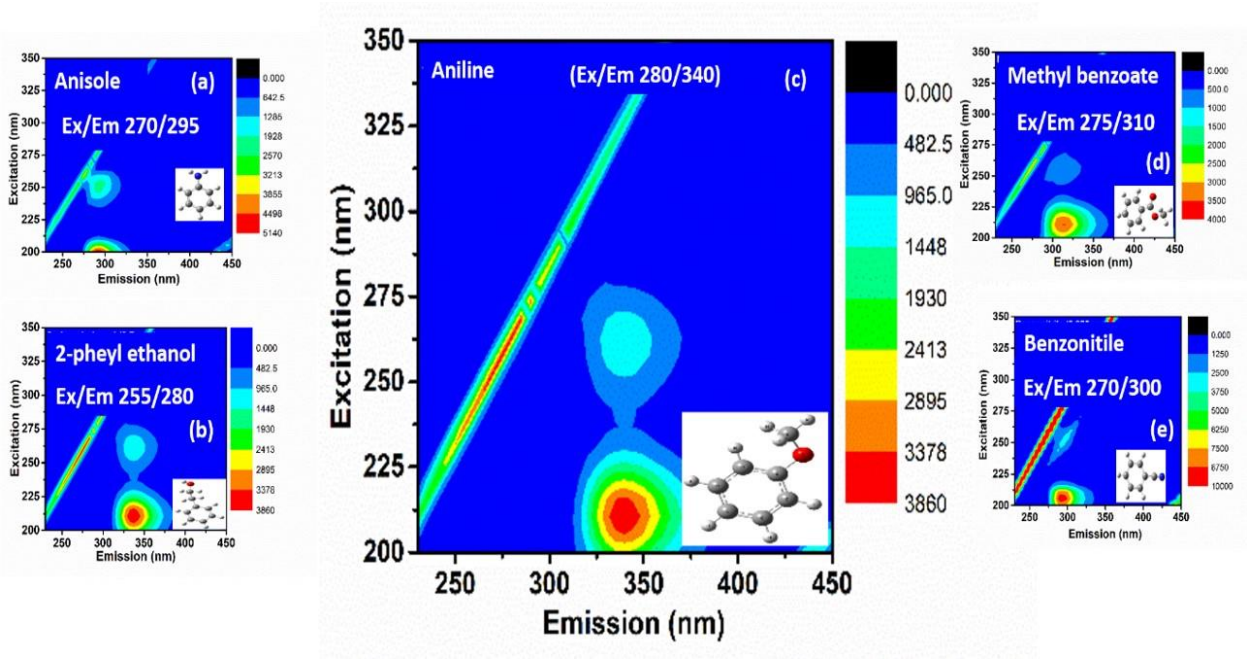


Fig. S3 EEMs of Nitrogen and Oxygen containing substituent with benzene: (a) anisole, (b) 2-phenylethanol, (c) aniline, (d) methyl benzoate, and (e) benzo nitrile

S4 EEMs of halogen substituted benzene

The fluorescence EX/EM of halogen substituted benzene shows decrease in quantum yield with increasing atomic weight with increase in the emission wavelength (Fig. S4).

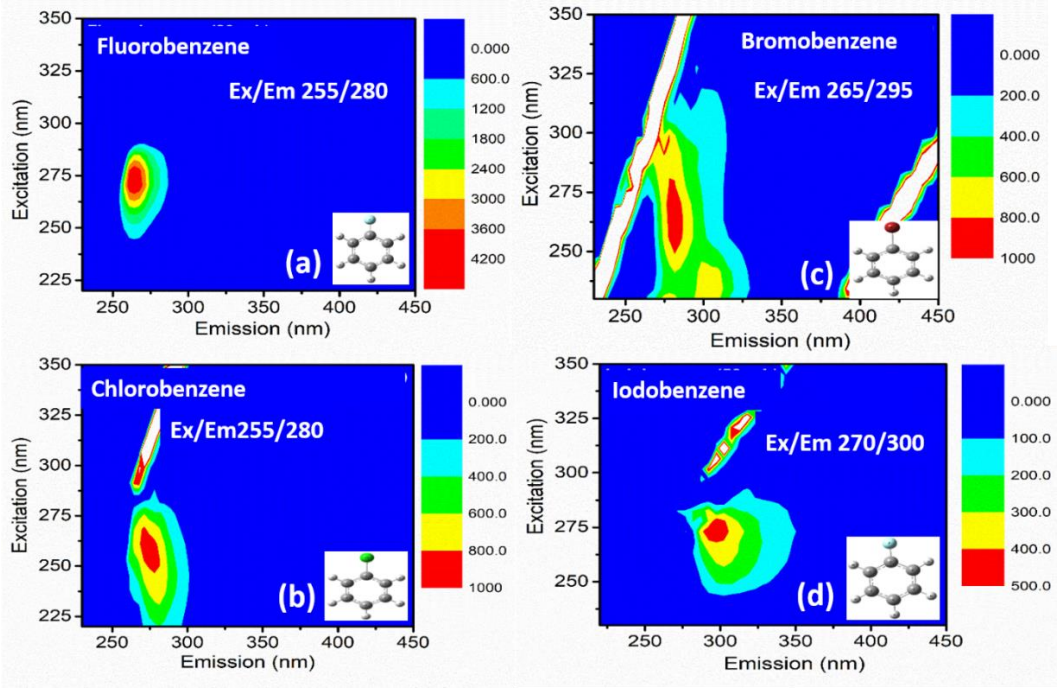


Fig. S4 EEMs of halogen substituted benzene: (a) fluorobenzene, (b) chlorobenzene, (c) bromobenzene and (d) iodobenzene

S5 Chemical softness

The molecular softness of the selected aromatic compounds showed variation in the value with change in substituent on aromatic benzene. The softness at ground absorption and emission is mentioned in Table S1 (Khan et al., 2018). The chemical softness of molecule can be deduced from chemical hardness which can be calculated from the difference of HUMO and LUMO energies as shown in Eqs. (1) and (2) (Akshaya et al., 2017).

$$\eta = \frac{LUMO\ eV - HOMO\ eV}{2} \qquad (1)$$

where E (LUMO) is energy at LUMO, E (HOMO) energy at HOMO and η is symbol for molecular hardness, and

$$S = \frac{1}{\eta} \quad (2)$$

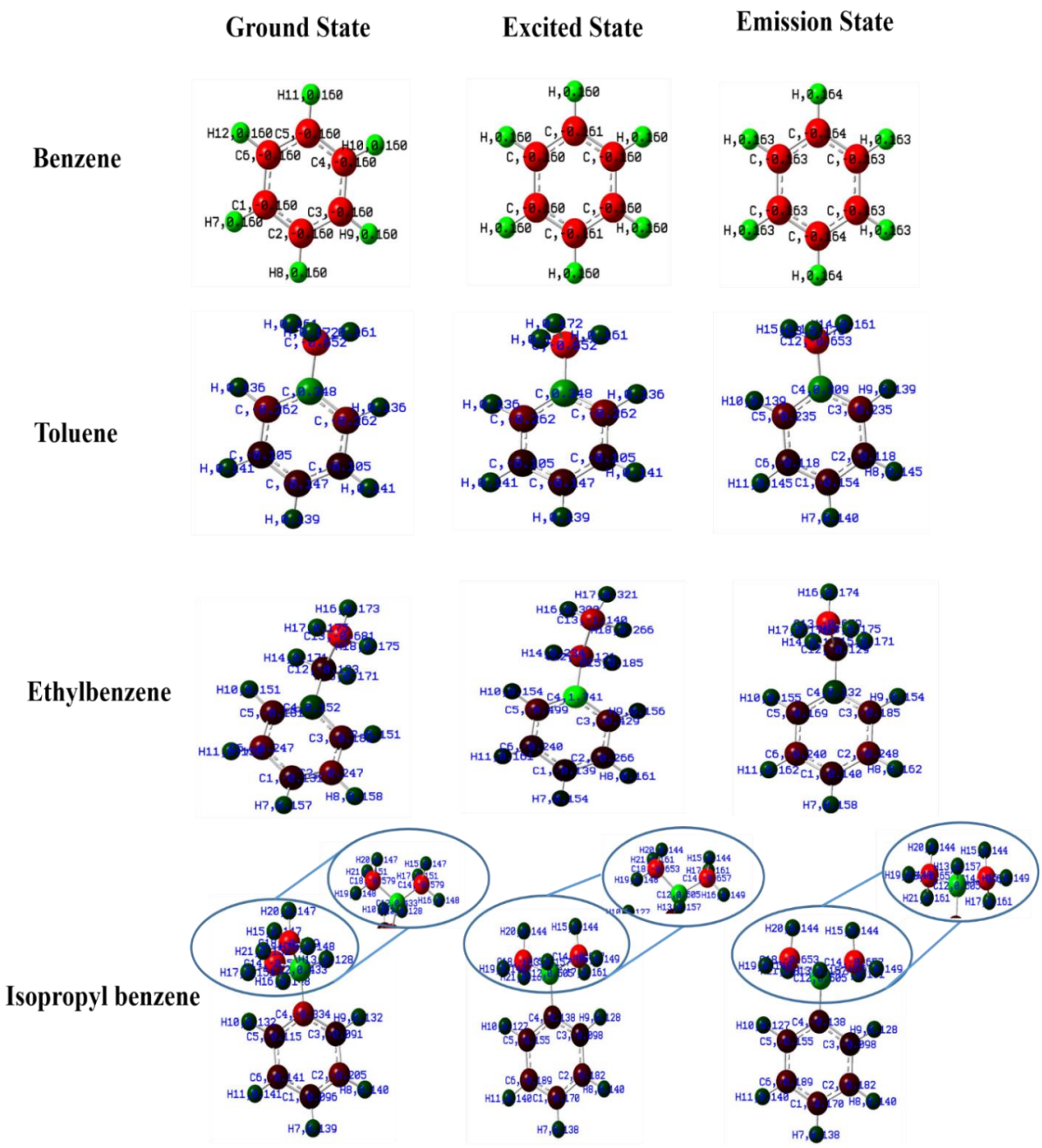
where "*S"* is the chemical softness, eV and "η" is the chemical hardness, eV.

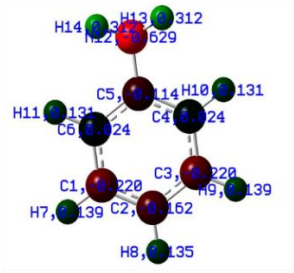
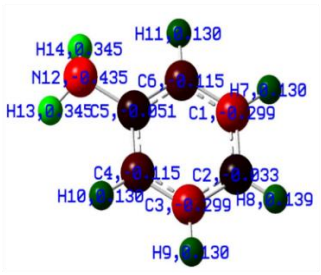
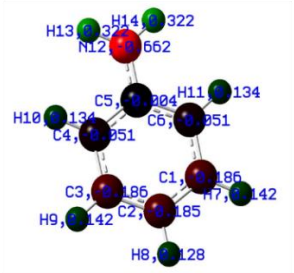
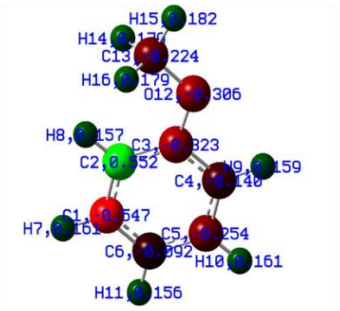
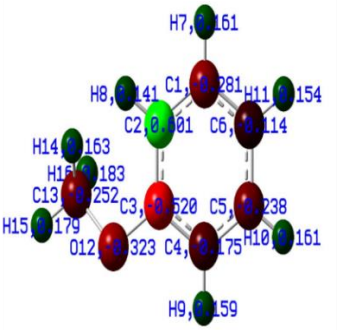
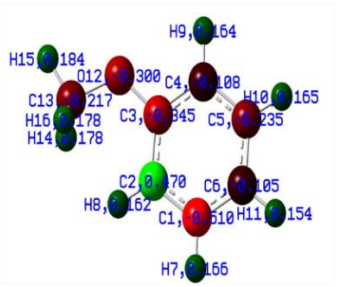
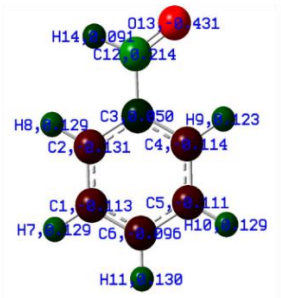
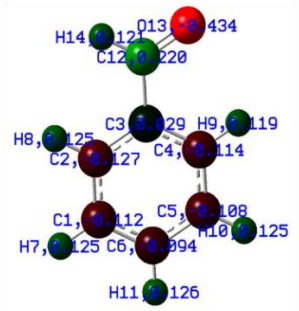
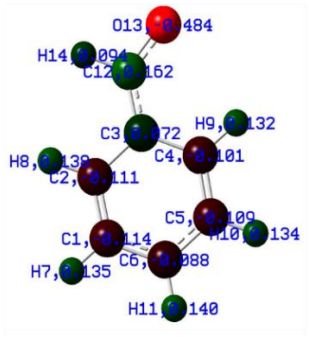
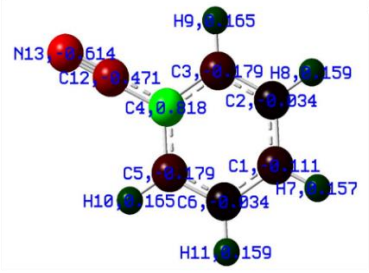
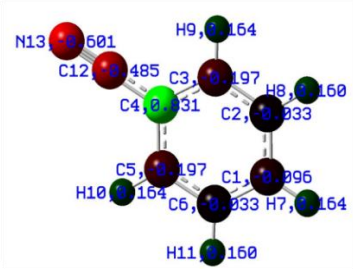
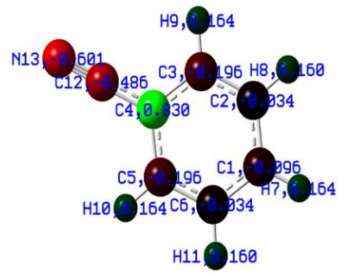
Table S1 Molecular softness of the compounds

Organic compound	Molecular softness		
	Ground state	Excitation state	Emission state
Benzene	5.35	5.35	5.62
Toluene	5.67	5.64	6.06
Ethylbenzene	5.32	5.3	5.84
Isopropylbenzene	5.64	5.54	4.27
Aniline	5.05	4.9	5.6
Anisole	6.48	6.33	7.05
Benzaldehyde	9.5	8.8	11.5
Benzonitrile	4.74	5.01	5.01
2-phenylethanol	5.7	31.2	4.8
Methylbenzoate	4.85	11.4	12.0
Fluorobenzene	5.76	5.66	6.18
Chlorobenzene	5.83	5.78	6.26
Bromobenzene	4.44	4.43	4.70
Iodobenzene	6.62	6.2	4.82

S6 Bond energies

The bond energies changes during fluorescence process in ground, excited and emission state. The substituent effects the change in bond energies which represent a relation with experimental fluorescence results (Bremond et al., 2013). The variation in the bond energies at ground state, excited state and emission for all selected 14 single ring aromatic compounds is mentioned in Fig. S5.


Ground State
Excited State
Emission State
Benzene
Toluene
Ethylbenzene
Isopropyl benzene

	Ground State	Excited State	Emission State
Aniline			
Anisole			
Benzaldehyde			
Benzonitrile			

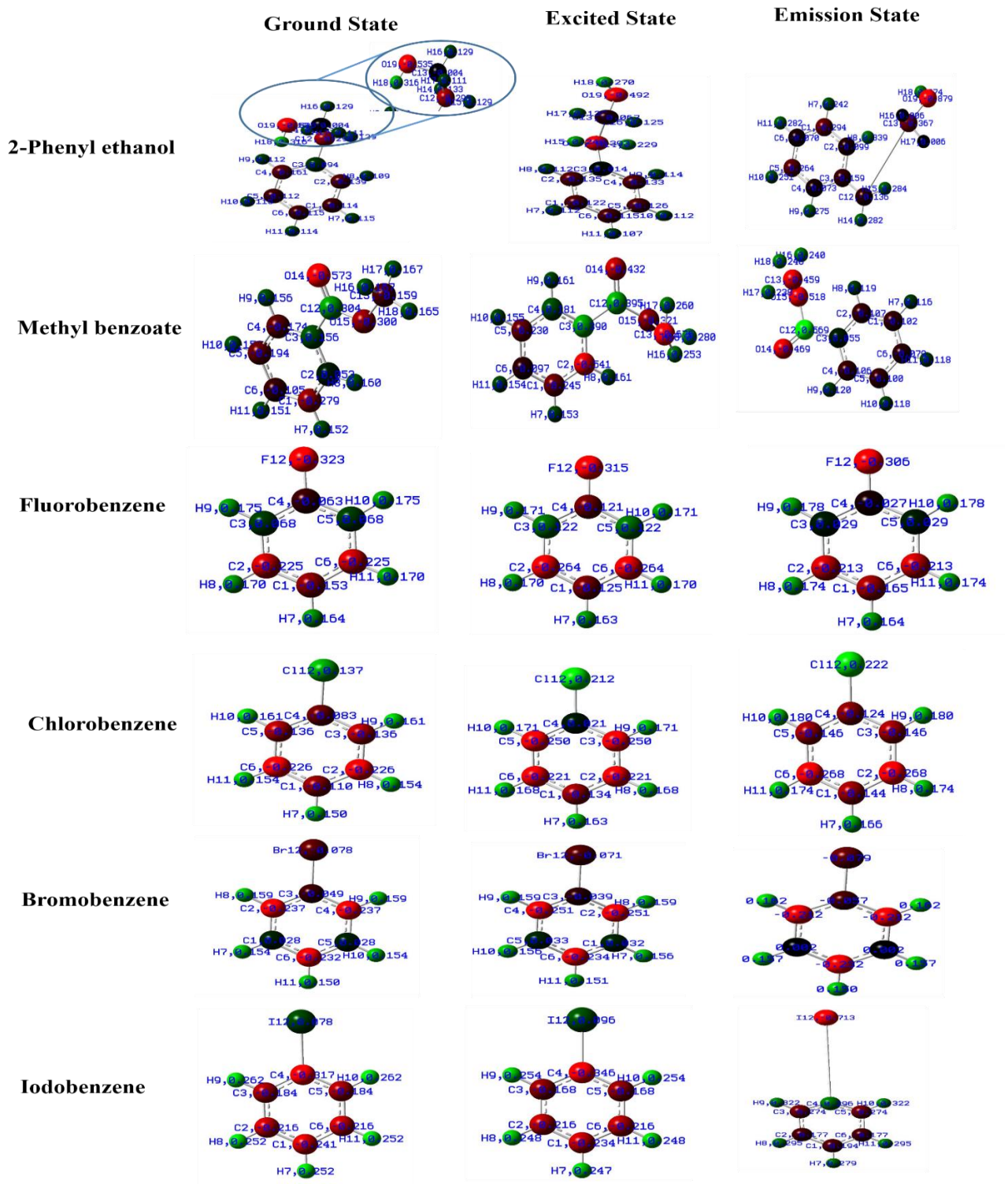


Fig. S5 Electronic charge distribution of compounds during the fluorescence process (Ground state, Excited-state, and Emission state)

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