

Supporting Information

Selective Recognition of Iodide Using Fluorescent Organic Nanoparticles by Displacement Assay

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Figure S1. ¹H NMR spectrum of Compound **1**.

Figure S2. ¹³C NMR spectrum of Compound **1**.

Figure S3. Mass spectrum of Compound **1**.

Figure S4. ¹H NMR spectrum of Compound **2**.

Figure S5. ¹³C NMR spectrum of Compound **2**.

Figure S6. Mass spectrum of Compound **2**.

Figure S7. ¹H NMR spectrum of Compound **3**.

Figure S8. ¹³C NMR spectrum of Compound **3**.

Figure S9. Mass spectrum of Compound **3**.

Figure S10. ¹H NMR spectrum of Compound **4**.

Figure S11. ¹³C NMR spectrum of Compound **4**.

Figure S12. Mass spectrum of Compound **4**.

Figure S13: (A) Changes in the UV-Vis absorption profile of nano-aggregates of **1** at Concentration range from 30 to 100 μ M; (B) Changes in the UV-Vis absorption profile of nano-aggregates of **2** at Concentration range from 30 to 100 μ M; (C) Changes in the UV-Vis absorption profile of nano-aggregates of **3** at concentration range from 10 to 70 μ M; (D) Changes in the UV-Vis absorption profile of nano-aggregates of **4** at concentration range from 10 to 70 μ M.

Figure S14: (A) Changes in the emission profile of nano-aggregates of **1** at concentration range from 10-20 μ M and (B) Changes in the emission profile of nano-aggregates of **2** at concentration range from 10-20 μ M.; (C) Changes in the emission profile of nano-aggregates

of **3** at concentration range from 1-10 μM and (D) Changes in the emission profile of nano-aggregates of **4** at concentration range from 1-9 μM .

Figure S15. Changes in emission profile of nano-aggregates of **1** (17 μM) in aqueous medium upon addition of 5 equivalent of a particular metal nitrate salts.

Figure S16. Changes in emission profile of nano-aggregates of **2** (13 μM) in aqueous medium upon addition of 5 equivalent of a particular metal nitrate salts.

Figure S17. Response Time of receptor **3** for Hg^{2+} ion.

Figure S18. Salt perturbation studies of nano-aggregates of **3** recorded with 6 μM concentration of sensor in aqueous system with the respective fluorescence spectrum recorded upon addition of 100 equiv. of tetrabutylammonium nitrate under the same concentration of sensor and solvent system.

Figure S19. Changes in emission profile of nano-aggregates of **3** (6 μM) in aqueous medium upon addition of a particular tetrabutylammonium anion salt (5 eq.) in aqueous media ($\lambda_{\text{ex}} = 343 \text{ nm}$).

Figure S20. pH effect of receptor **3** (6 μM) in aqueous system ($\lambda_{\text{ex}}=343 \text{ nm}$).

Figure S21. Response time of receptor **4** for Hg^{2+} ion at $\lambda_{\text{ex}} = 321 \text{ nm}$.

Figure S22. Salt perturbation studies of **4** recorded with 1 μM concentration of sensor in aqueous system with the respective fluorescence spectrum recorded upon addition of 100 equiv. of tetrabutyl ammonium nitrate under the same concentration of sensor and solvent system at $\lambda_{\text{ex}} = 321 \text{ nm}$.

Figure S23. Changes in emission profile of nano-aggregates of **4** (1 μM) in aqueous medium upon addition of a particular tetrabutylammonium anion salt (5 eq.) in aqueous media ($\lambda_{\text{ex}} = 321 \text{ nm}$).

Figure S24. pH effect of receptor **4** (1 μM) in aqueous system ($\lambda_{\text{ex}}=321 \text{ nm}$).

Figure S25. pH effect of receptor **3.Hg²⁺** (6 μM) in aqueous system ($\lambda_{\text{ex}}=343 \text{ nm}$).

Figure S26. Response Time of receptor **3.Hg²⁺** for I^- ion at $\lambda_{\text{ex}} = 343 \text{ nm}$.

Figure S27. Changes in emission profile of nano-aggregates of **4** (1 μM) in aqueous medium upon addition of a particular tetrabutylammonium anion salt (5 eq.) in aqueous media ($\lambda_{\text{ex}} = 321 \text{ nm}$).

TableS1 DFT Energies

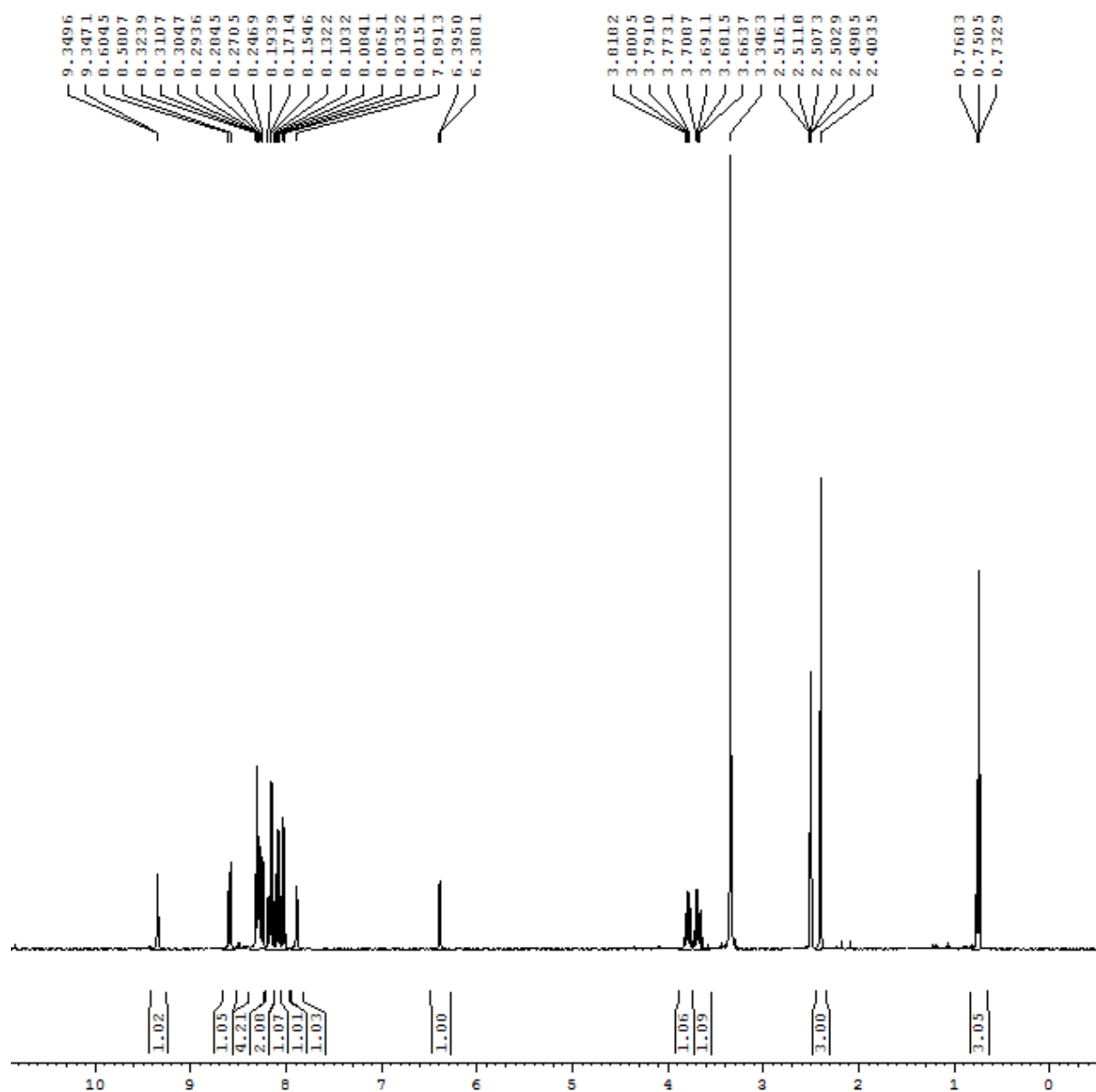


Figure S1. ¹H NMR spectrum of Compound 1.

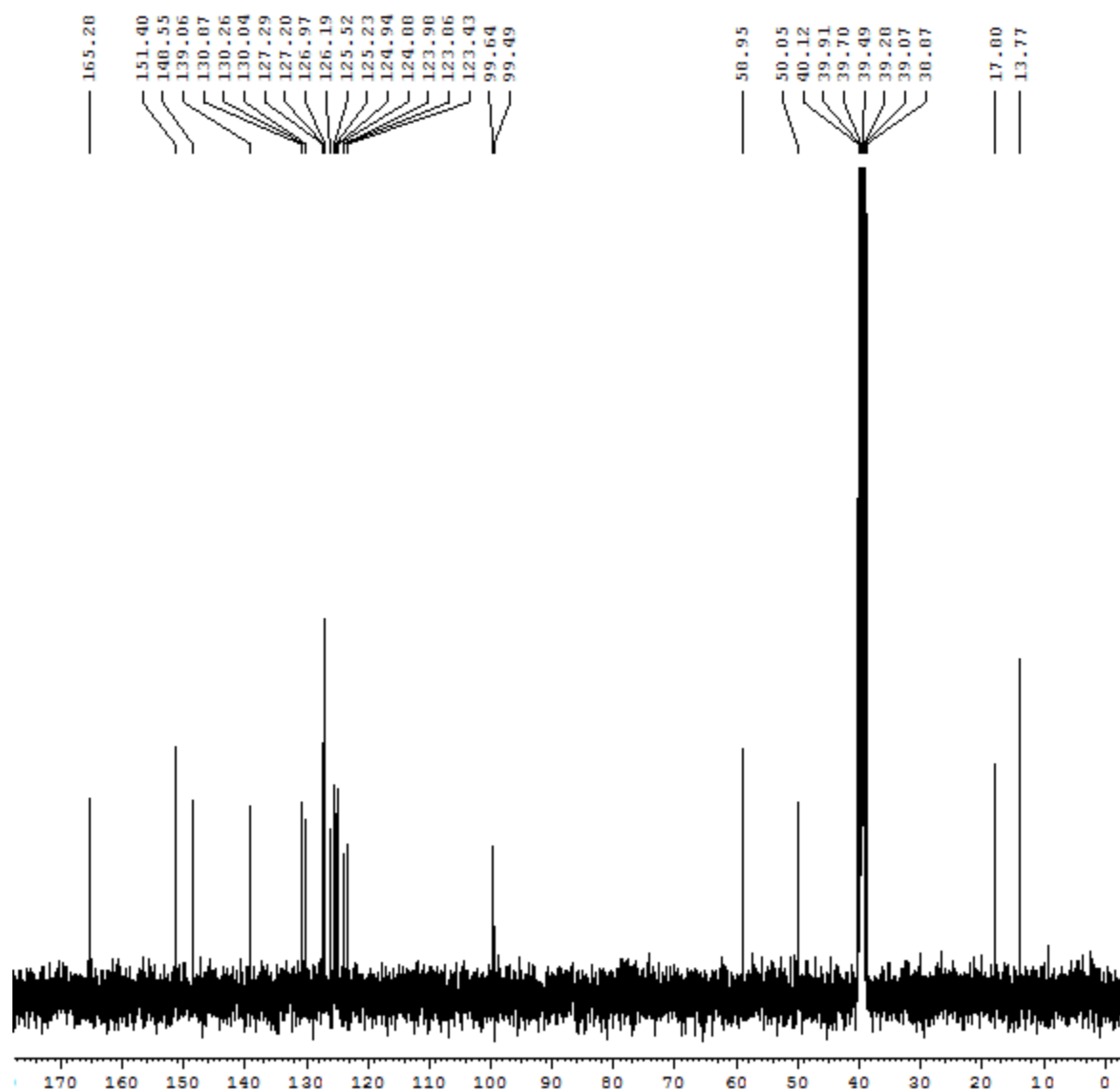


Figure S2. ¹³C NMR spectrum of Compound 1.

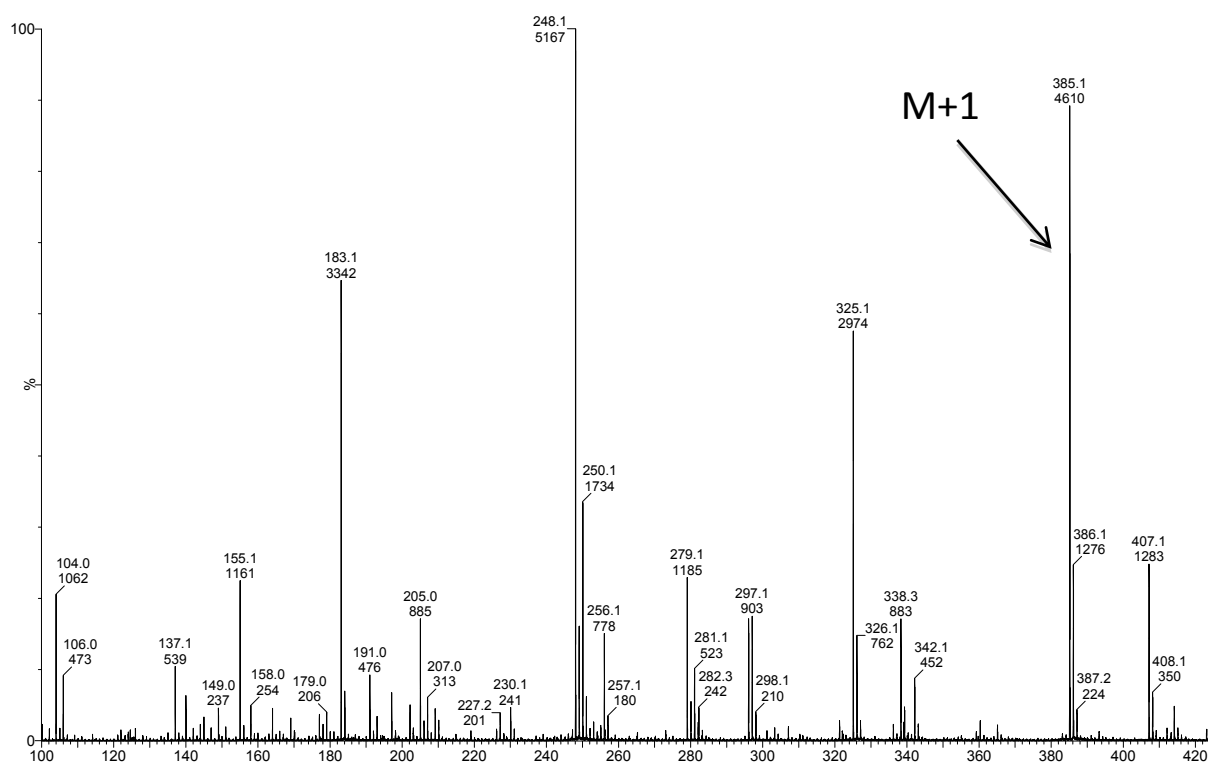


Figure S3. Mass spectrum of Compound 1.

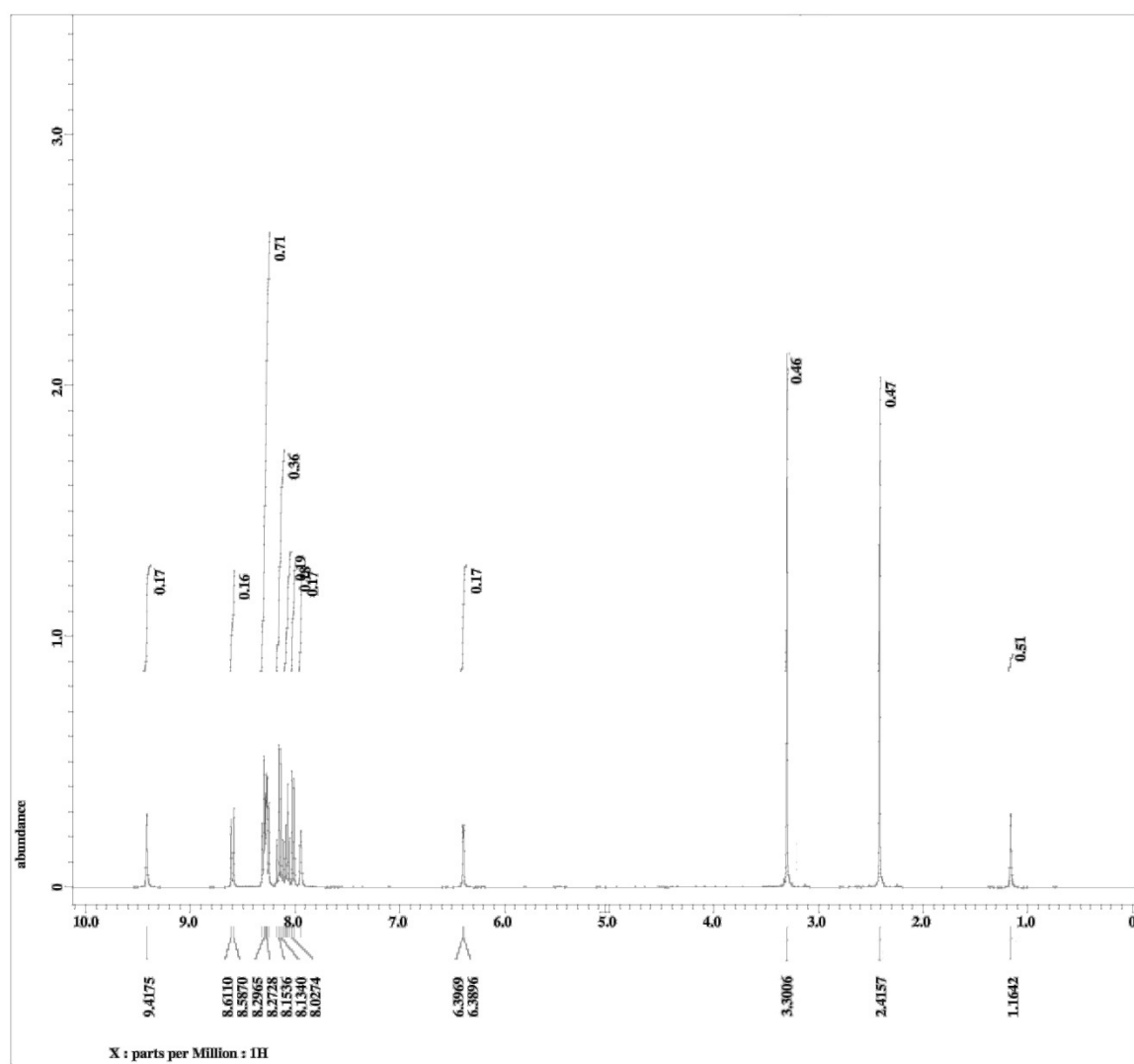


Figure S4. ^1H NMR spectrum of Compound 2.

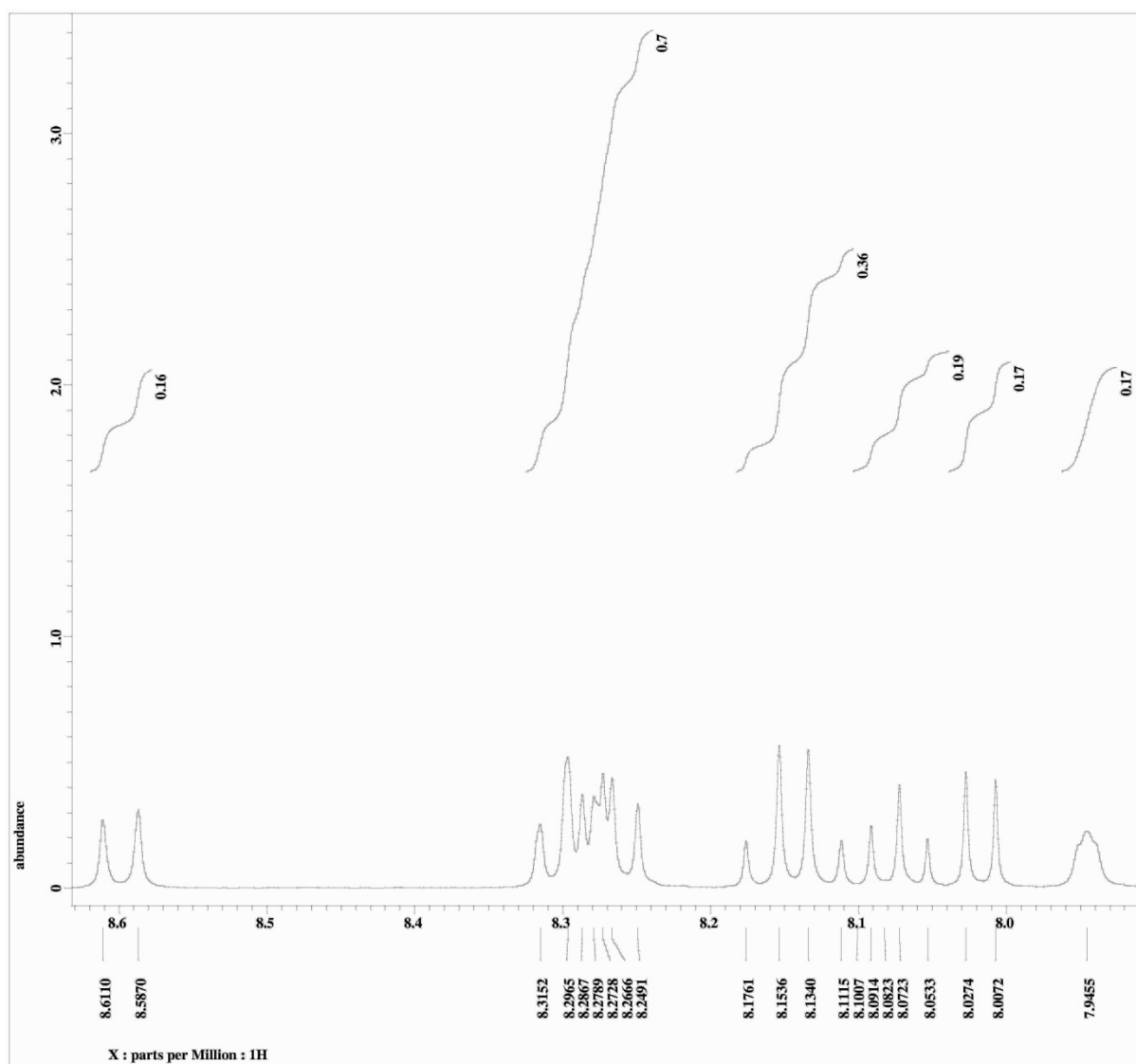


Figure S4A. Expansion ^1H NMR spectrum of Compound 2.

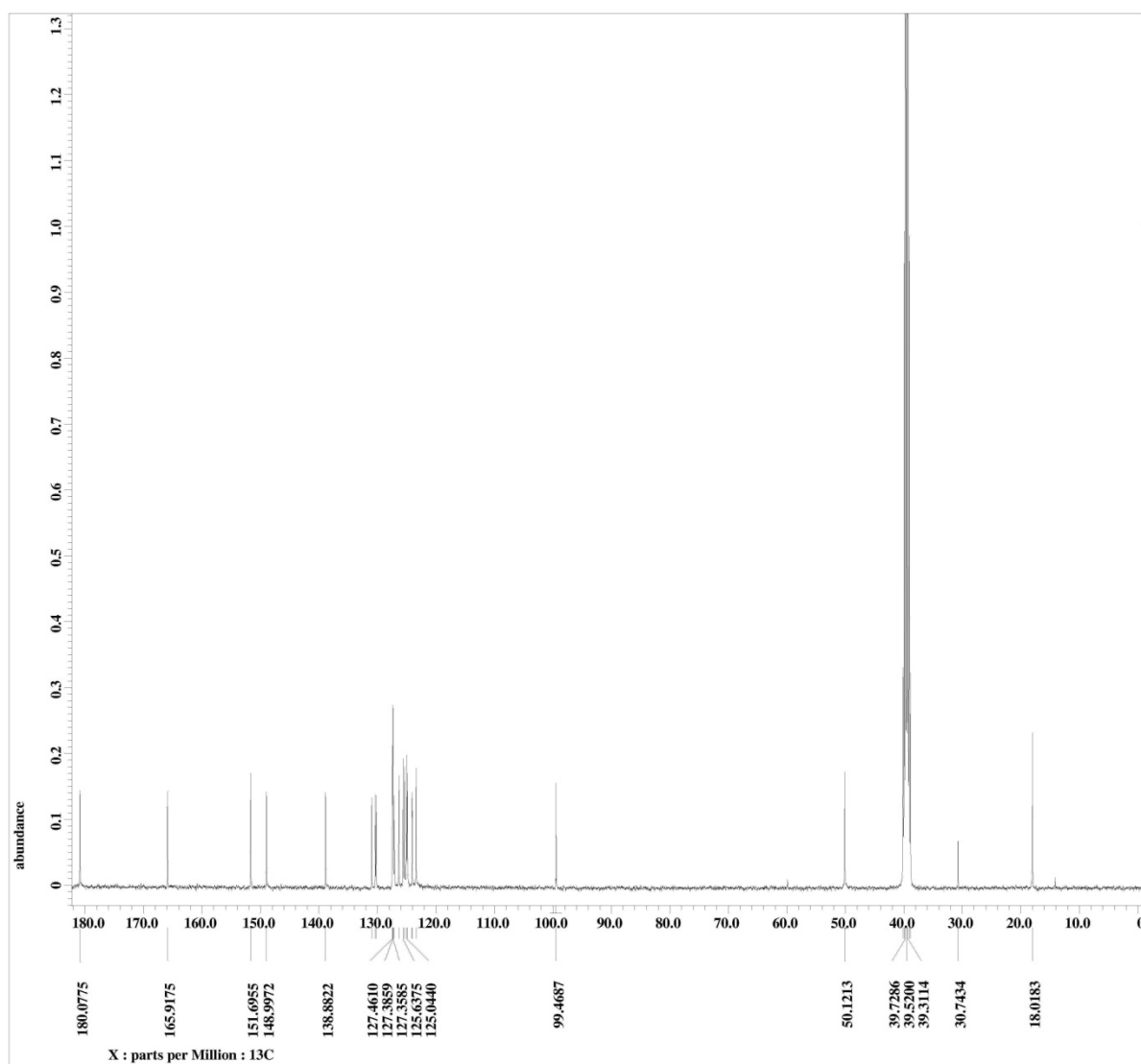


Figure S5. ^{13}C NMR spectrum of Compound 2.

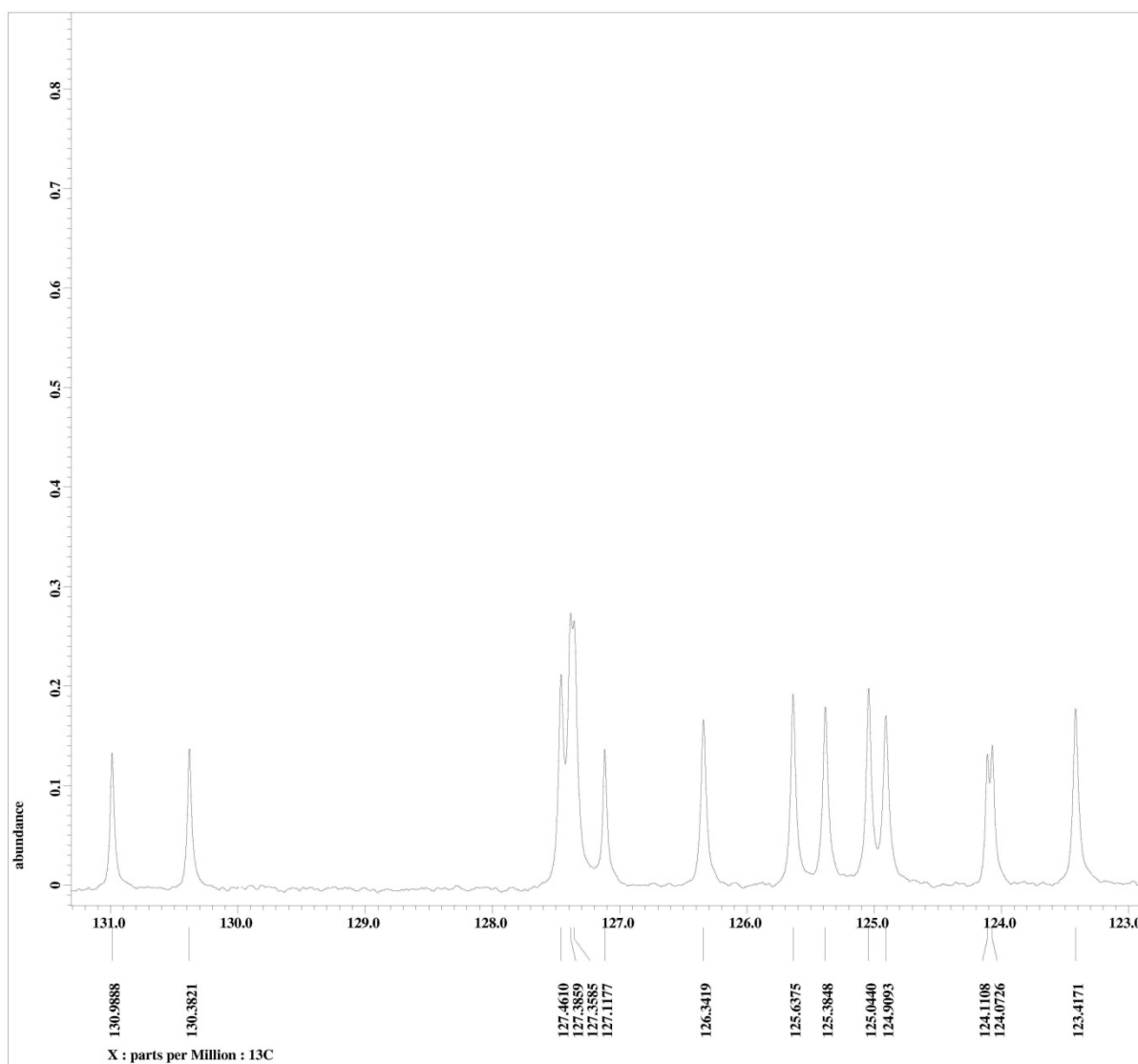


Figure S5A. Expansion ^{13}C NMR spectrum of Compound 2.

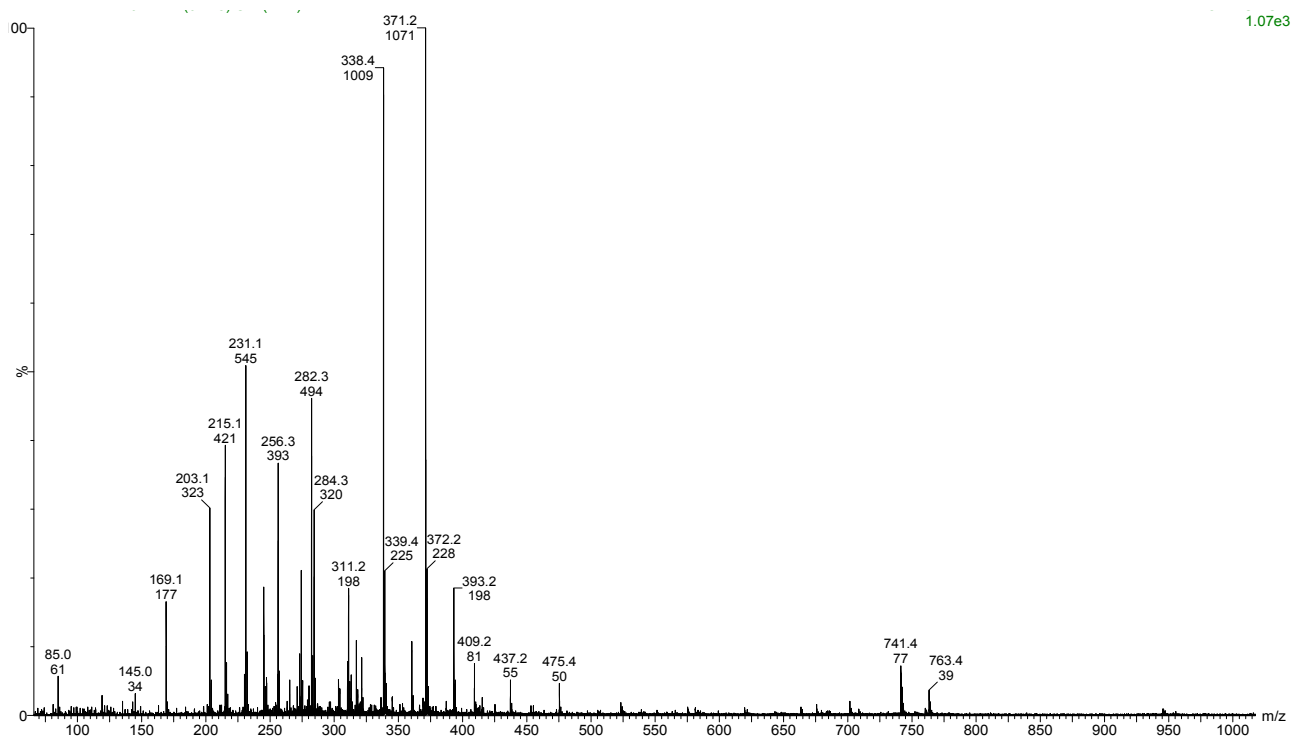


Figure S6. Mass spectrum of Compound 2.

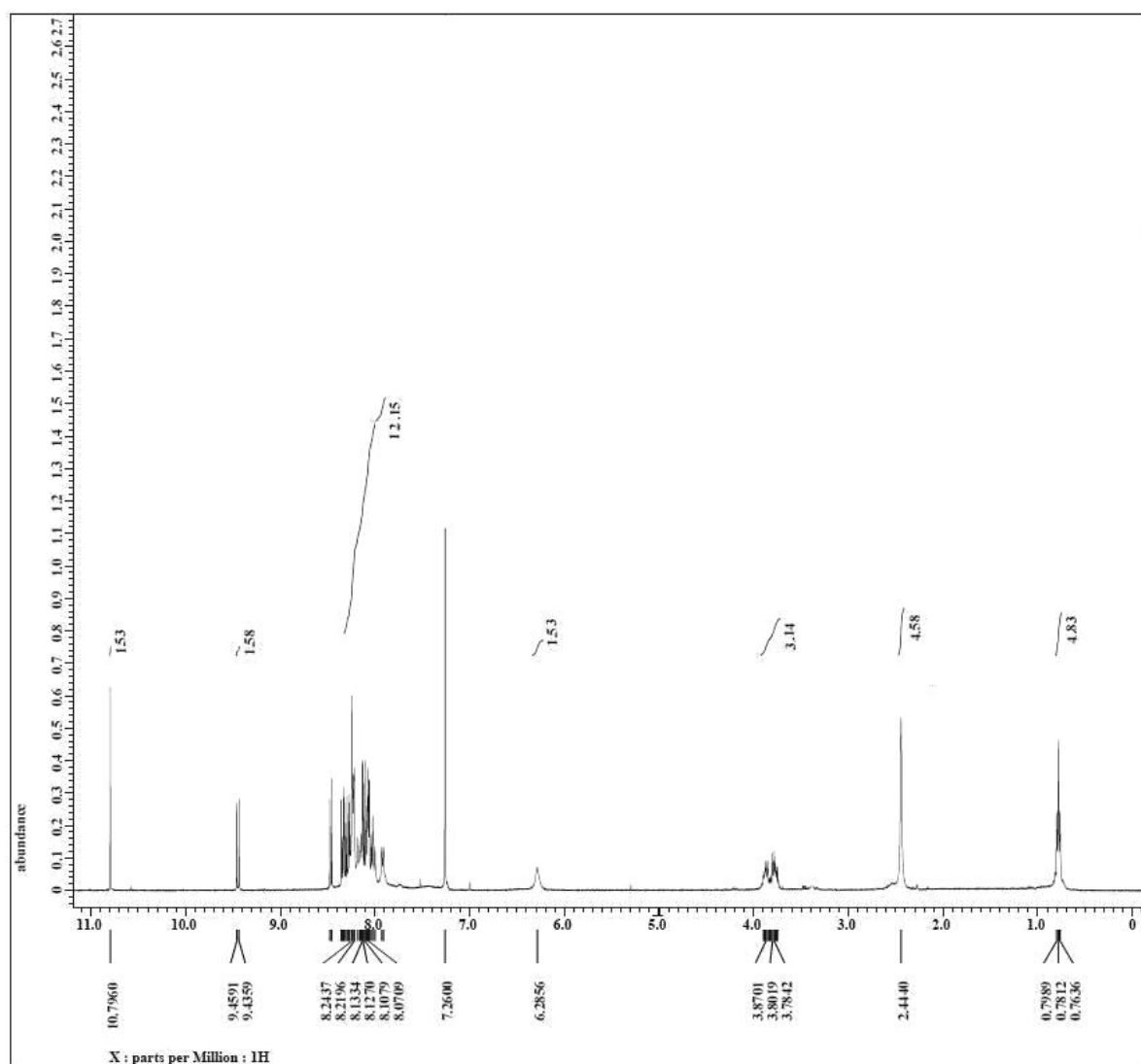


Figure S7. ^1H NMR spectrum of Compound 3.

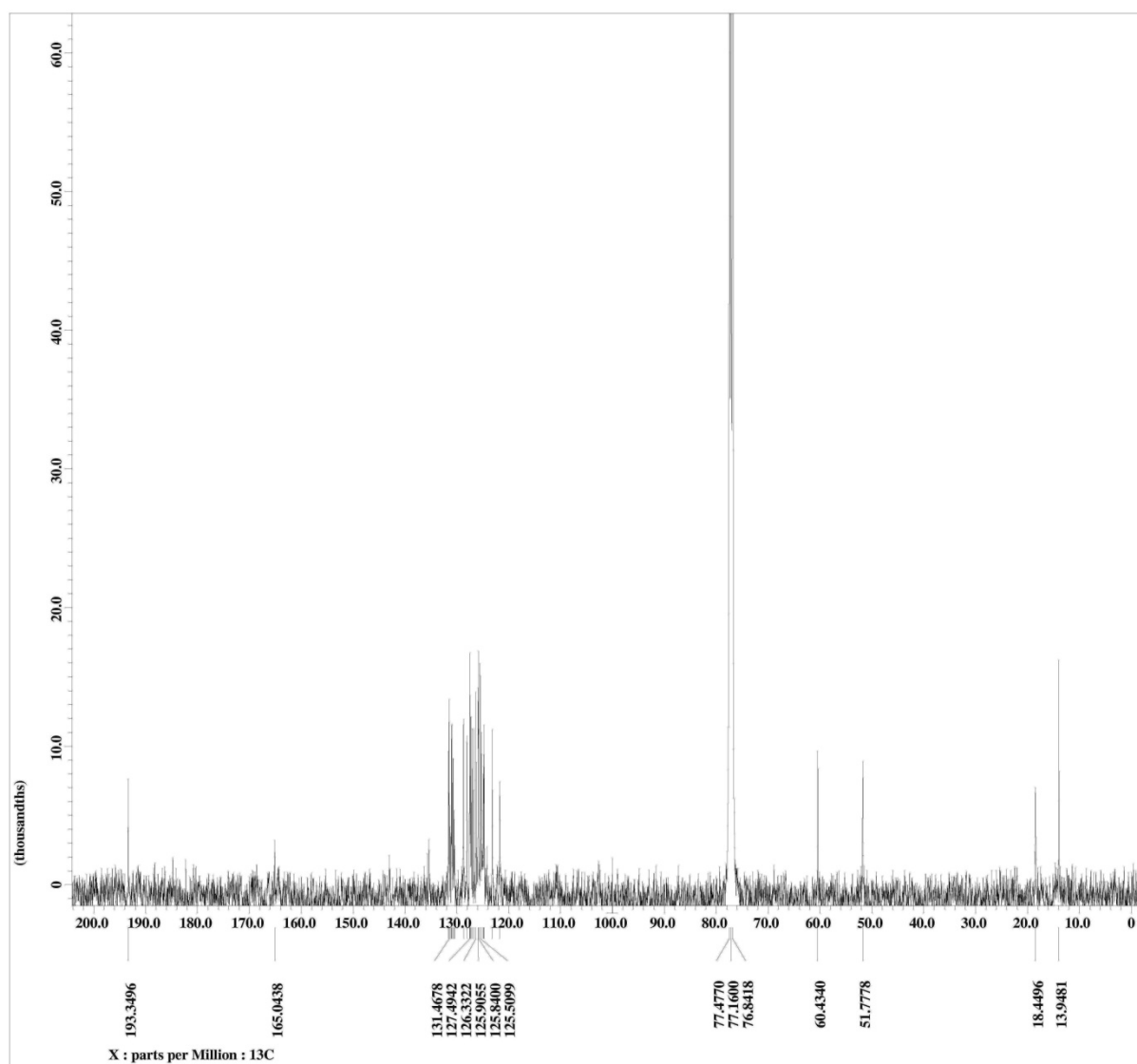


Figure S8. ¹³C NMR spectrum of Compound 3.

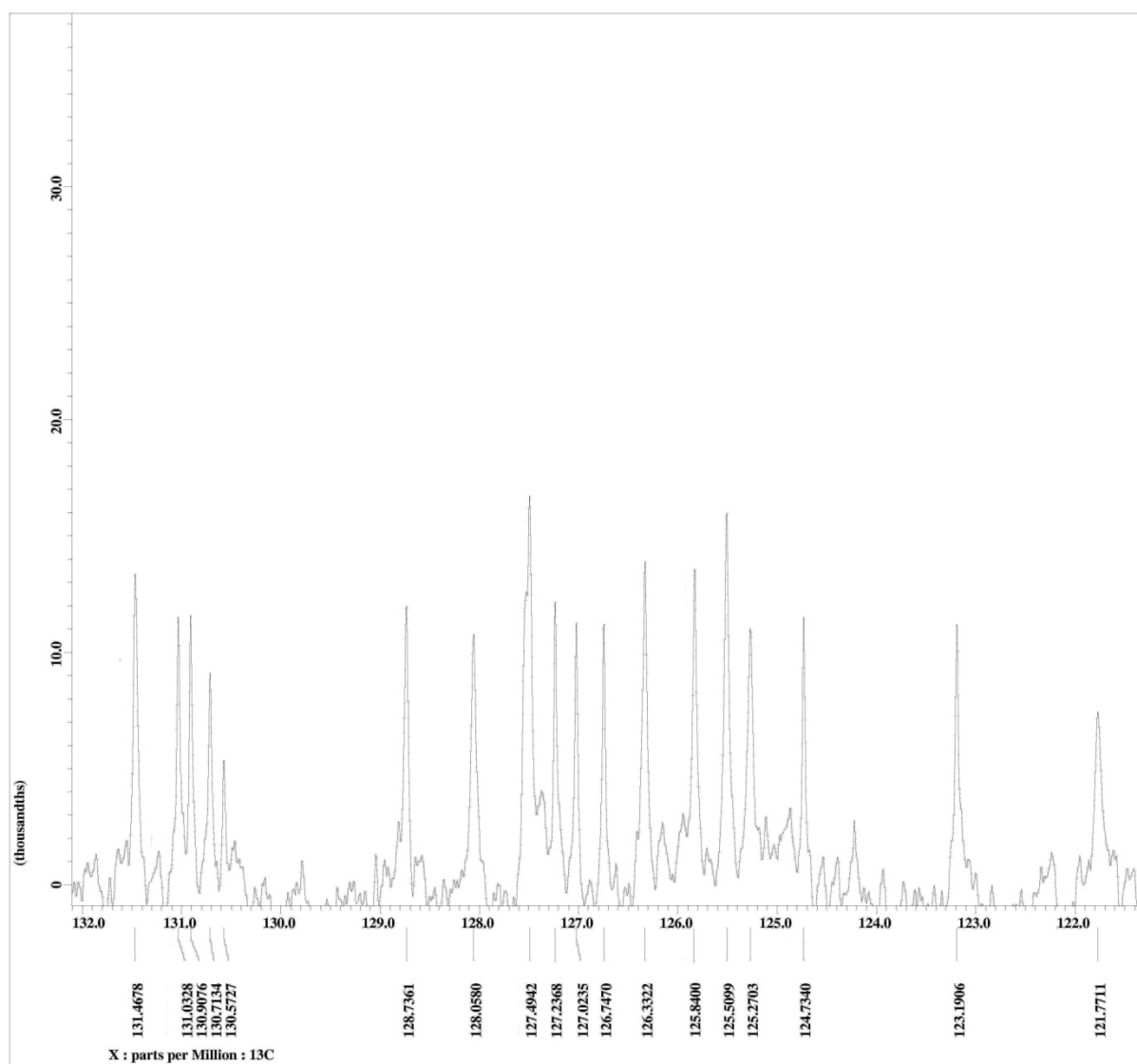


Figure S8B. Expansion ^{13}C NMR spectrum of Compound **3**.

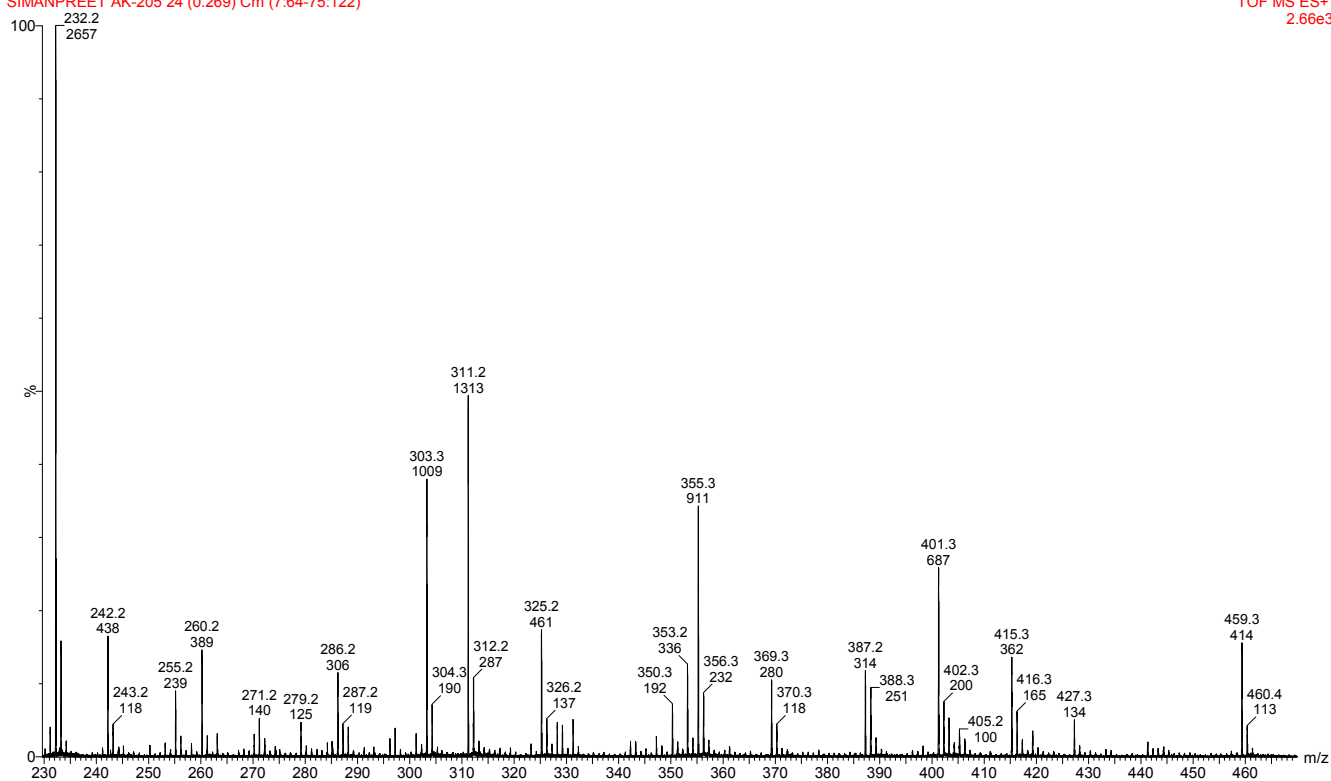


Figure S9. Mass spectrum of Compound 3.

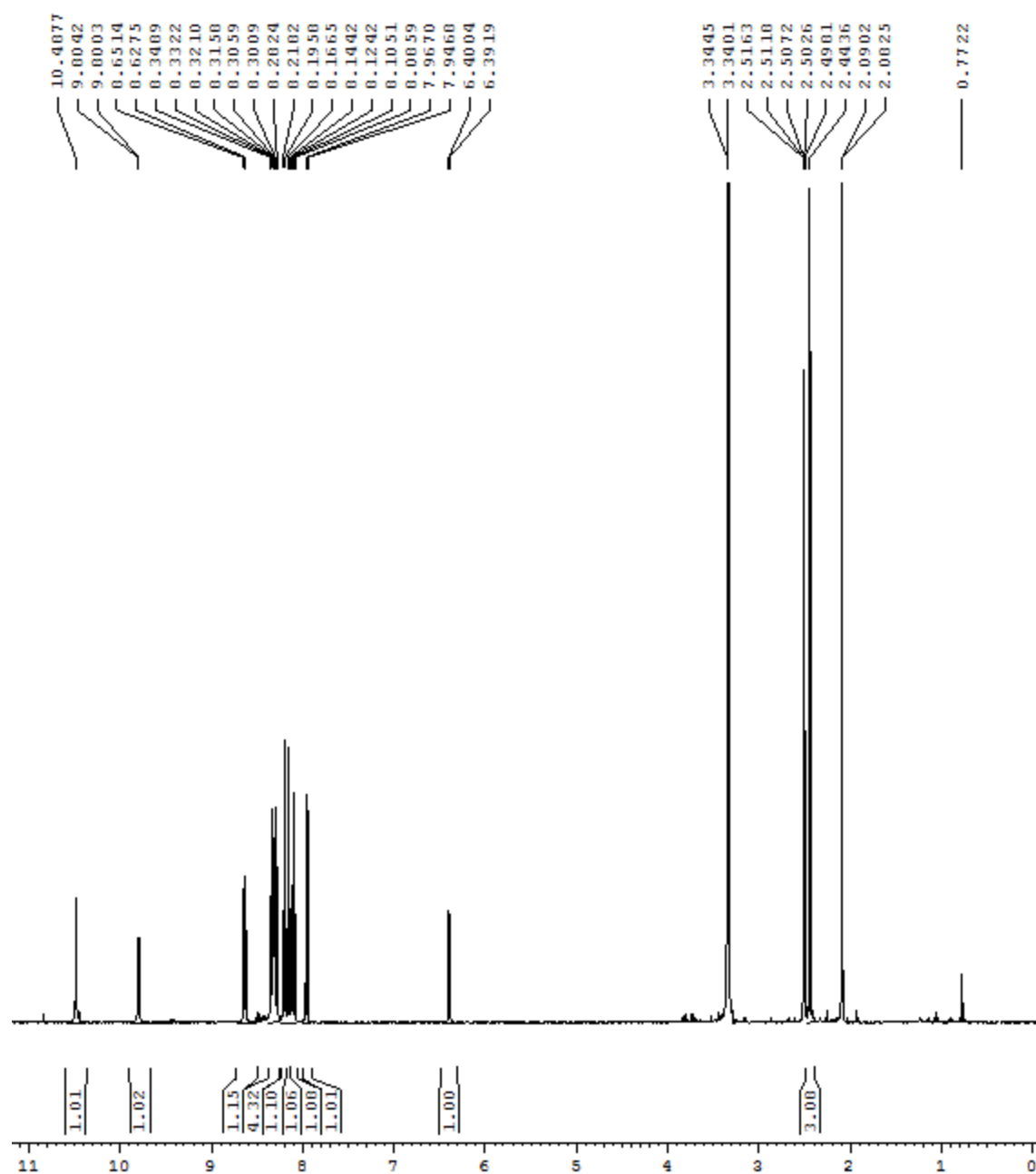


Figure S10. ¹H NMR spectrum of Compound 4.

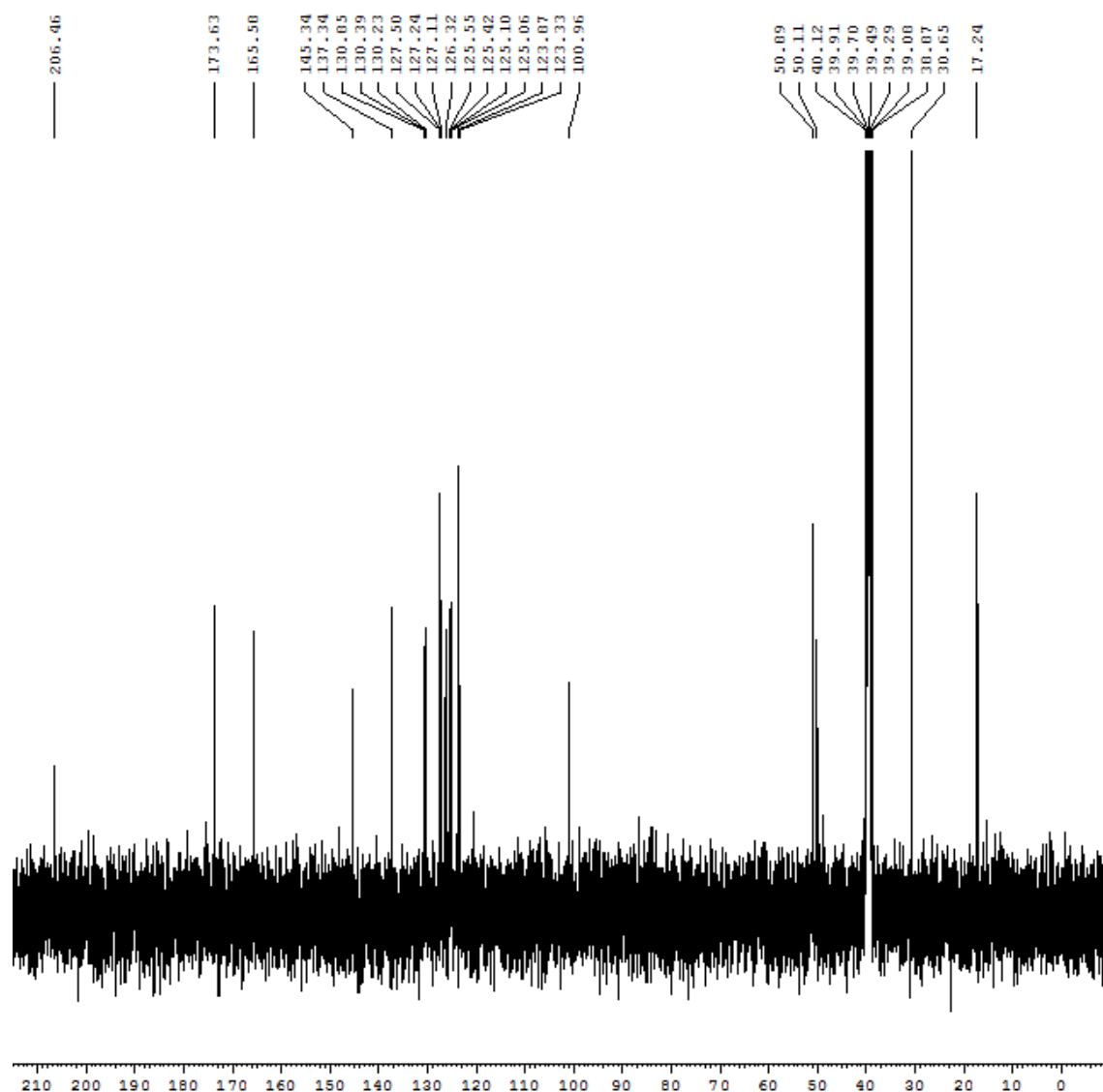


Figure S11. ¹³C NMR spectrum of Compound 4.

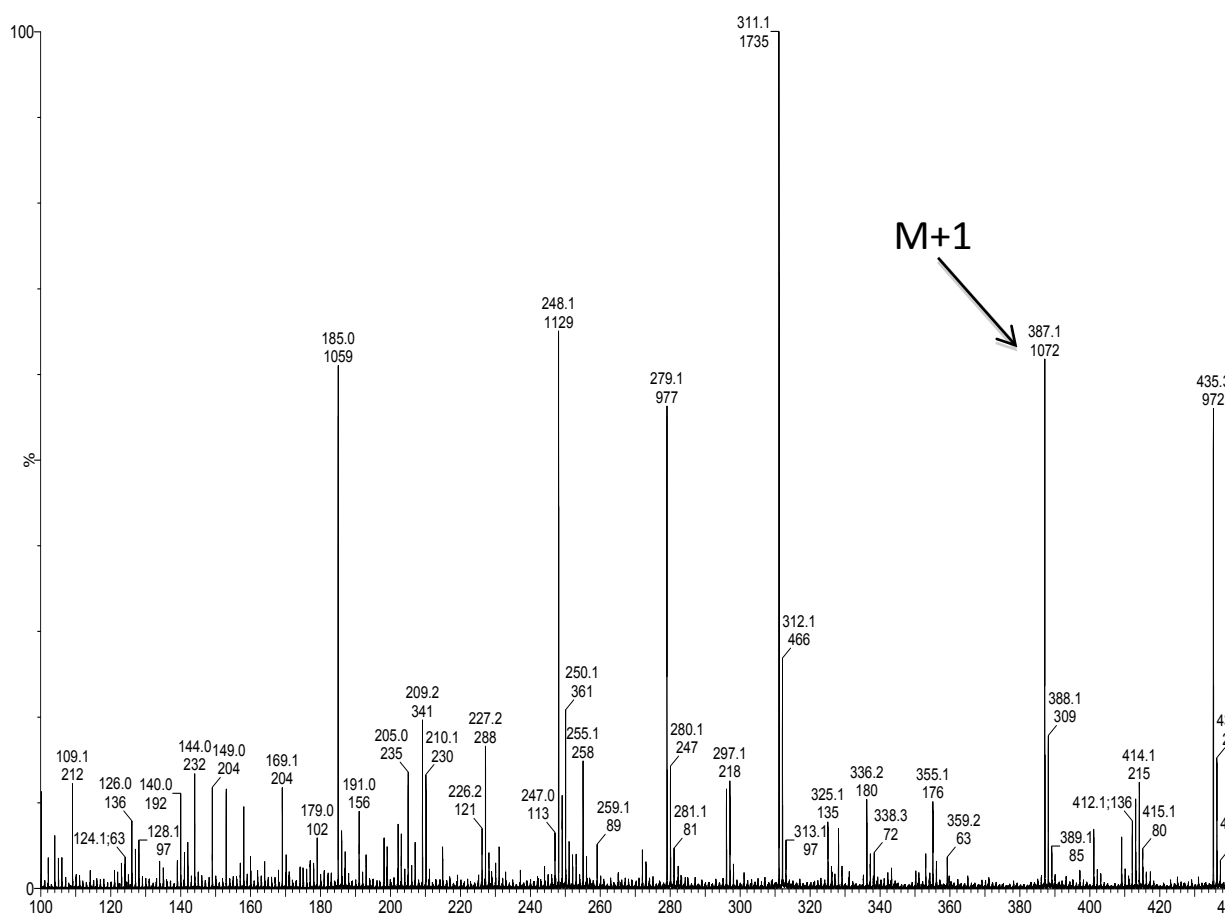


Figure S12. Mass spectrum of Compound 4.

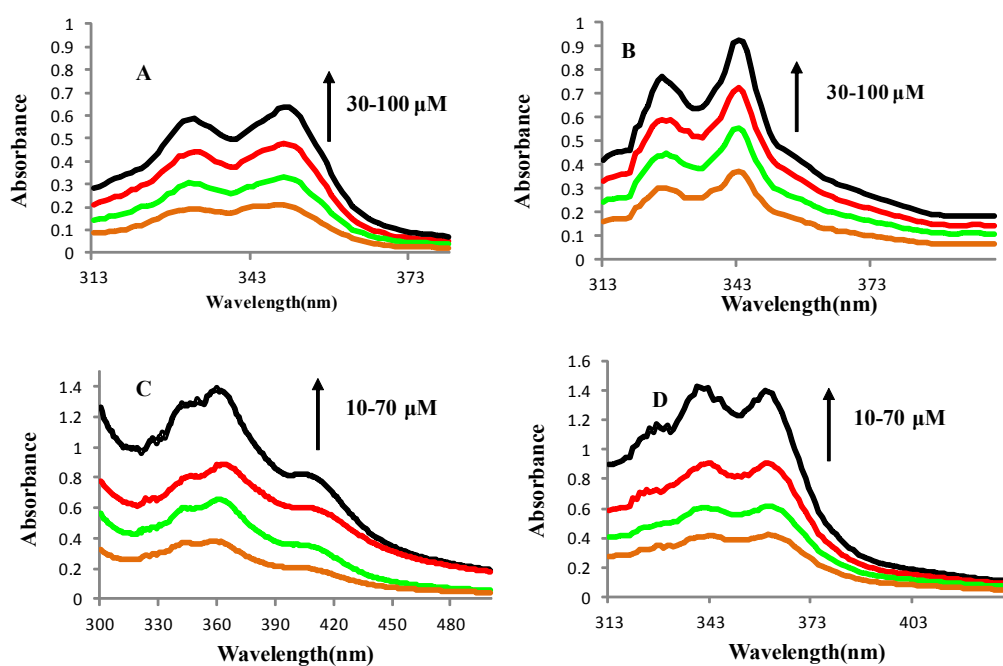


Figure S13: (A) Changes in the UV-Vis absorption profile of nano-aggregates of 1 at Concentration range from 30 to 100 μM ; (B) Changes in the UV-Vis absorption profile of

nano-aggregates of **2** at Concentration range from 30 to 100 μM ; (C) Changes in the UV-Vis absorption profile of nano-aggregates of **3** at concentration range from 10 to 70 μM ; (D) Changes in the UV-Vis absorption profile of nano-aggregates of **4** at concentration range from 10 to 70 μM .

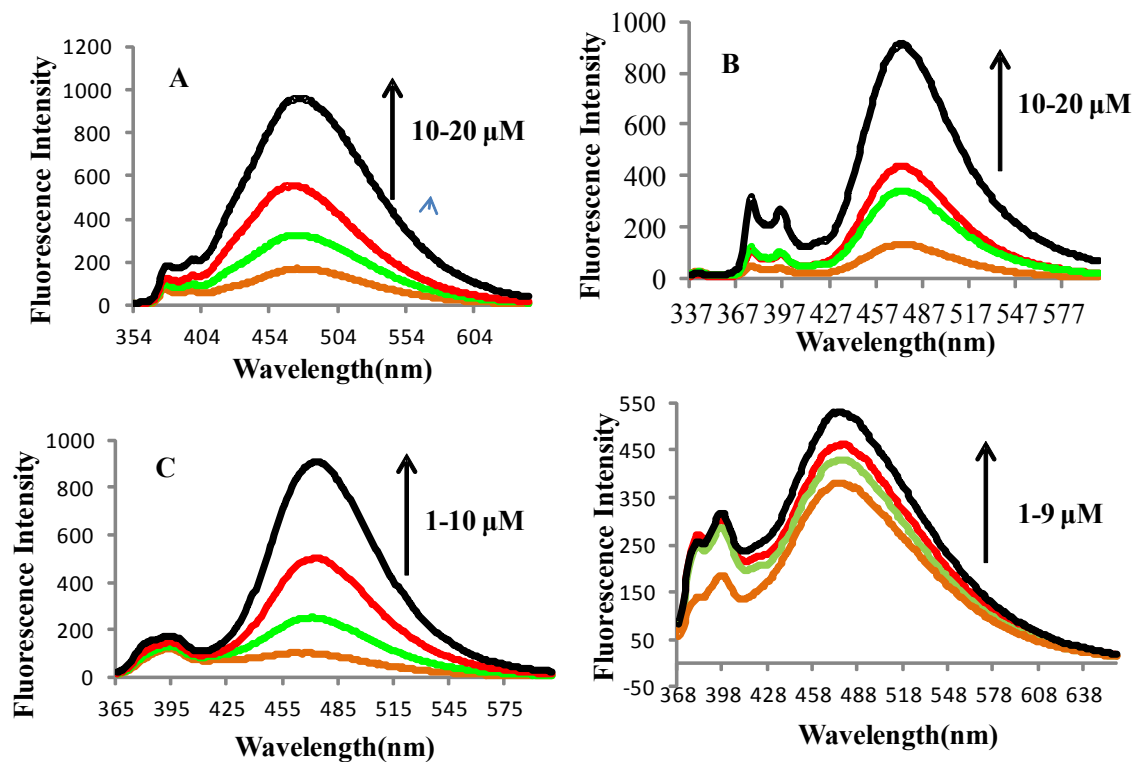


Figure S14: (A) Changes in the emission profile of nano-aggregates of **1** at concentration range from 10-20 μM and (B) Changes in the emission profile of nano-aggregates of **2** at concentration range from 10-20 μM .; (C) Changes in the emission profile of nano-aggregates of **3** at concentration range from 1-10 μM and (D) Changes in the emission profile of nano-aggregates of **4** at concentration range from 1-9 μM .

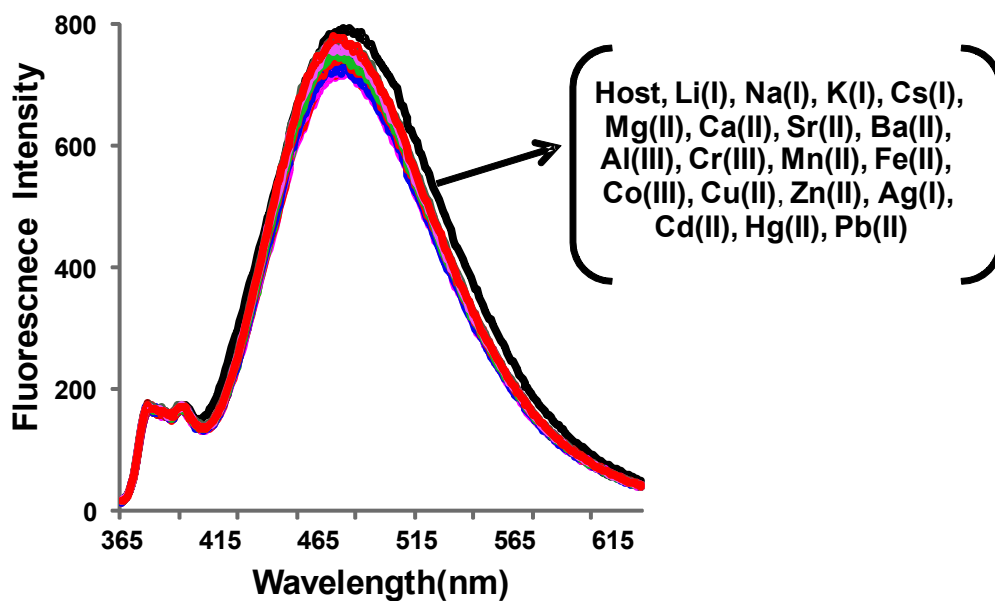


Figure S15. Changes in emission profile of nano-aggregates of **1** (17 μ M) in aqueous medium upon addition of 5 equivalent of a particular metal nitrate salts ($\lambda_{\text{ex}} = 335\text{nm}$).

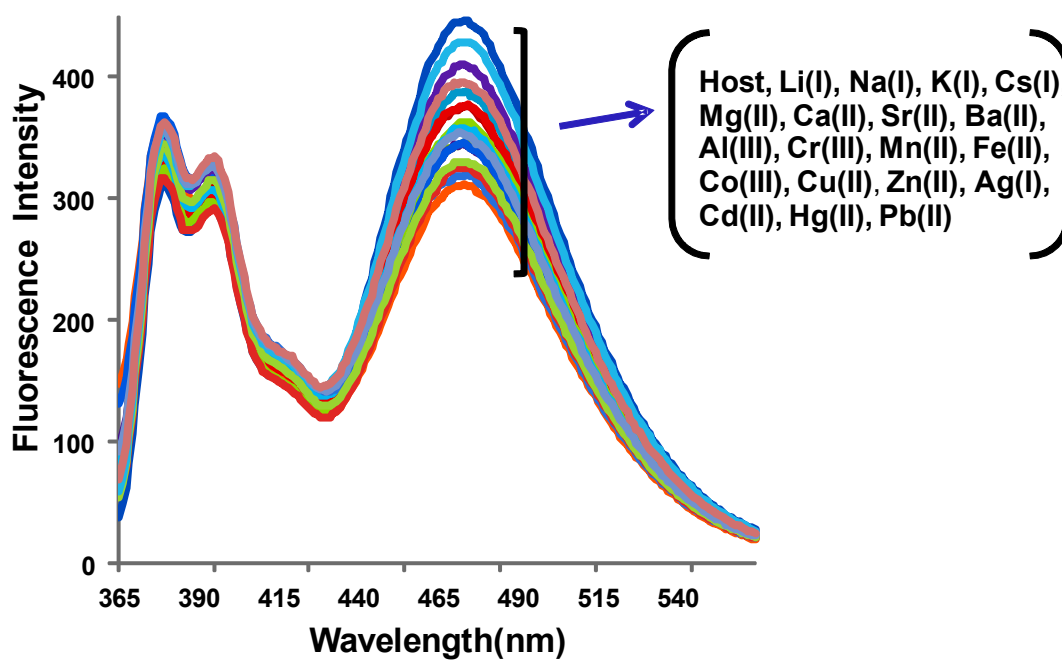


Figure S16. Changes in emission profile of nano-aggregates of **2** (13 μ M) in aqueous medium upon addition of 5 equivalent of a particular metal nitrate salts ($\lambda_{\text{ex}} = 335\text{nm}$).

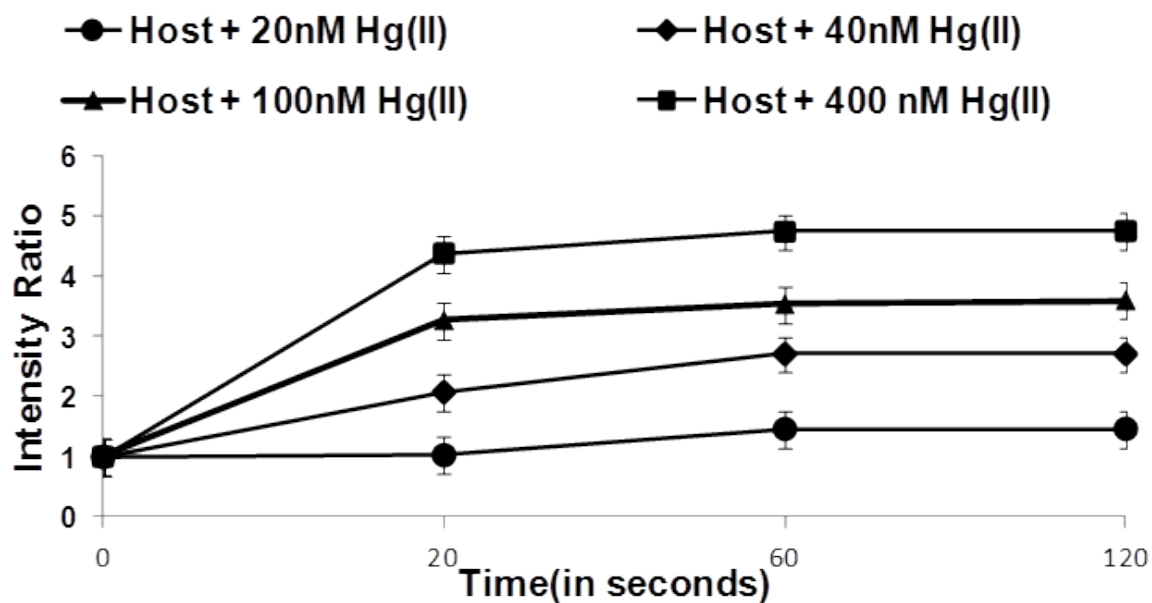


Figure S17. Response Time of receptor **3** for Hg^{2+} ion at $\lambda_{\text{ex}} = 343$ nm.

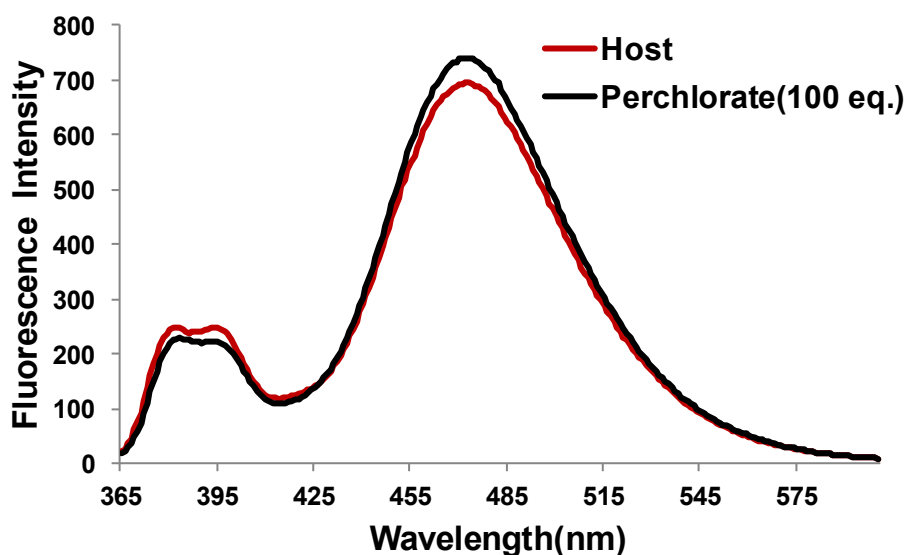


Figure S18. Salt perturbation studies of nano-aggregates of **3** recorded with $6 \mu\text{M}$ concentration of sensor in aqueous system with the respective fluorescence spectrum recorded upon addition of 100 equiv. of tetrabutyl ammonium nitrate under the same concentration of sensor and solvent system at $\lambda_{\text{ex}} = 343$ nm.

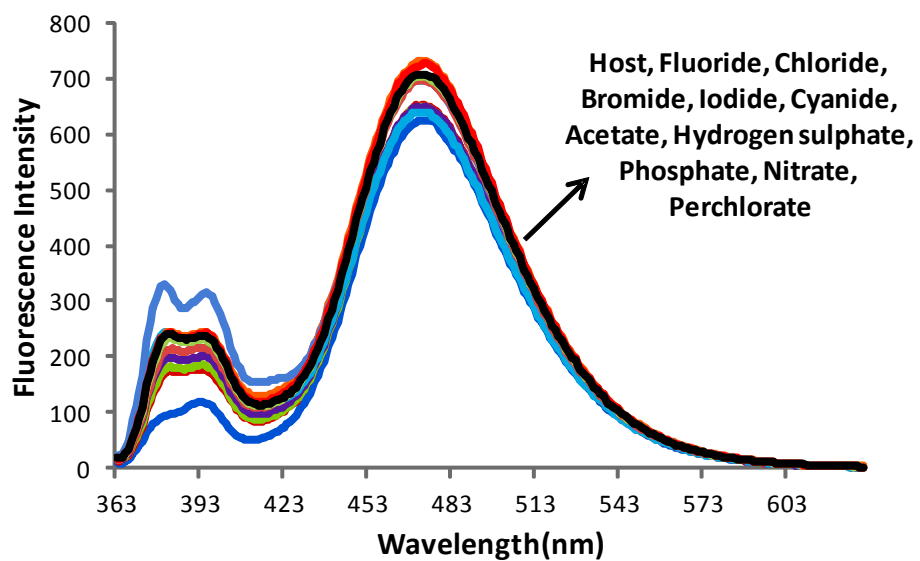


Figure S19. Changes in emission profile of nano-aggregates of **3** (6 μM) in aqueous medium upon addition of a particular tetrabutylammonium anion salt (5 eq.) in aqueous media ($\lambda_{\text{ex}} = 343 \text{ nm}$).

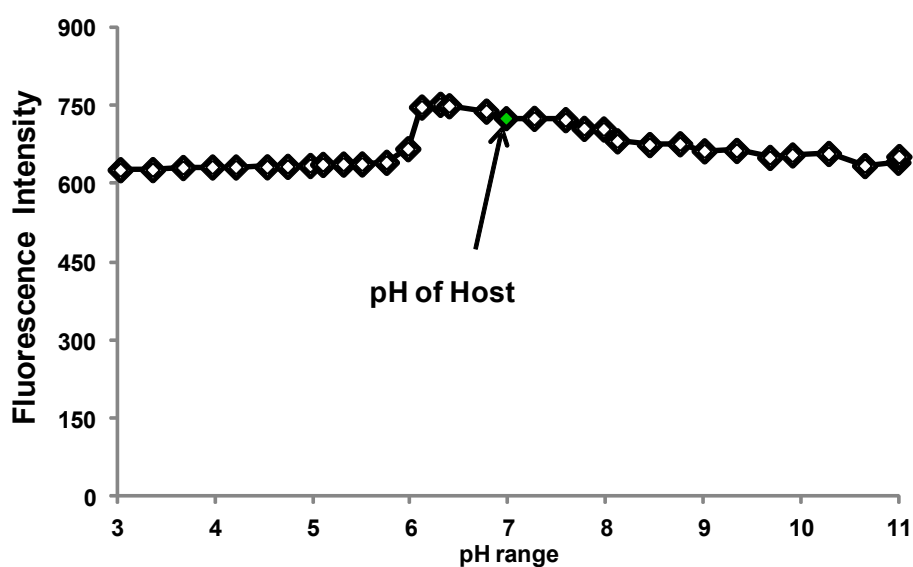


Figure 6. pH effect of receptor **3** (6 μM) in aqueous system ($\lambda_{\text{ex}}=343 \text{ nm}$).

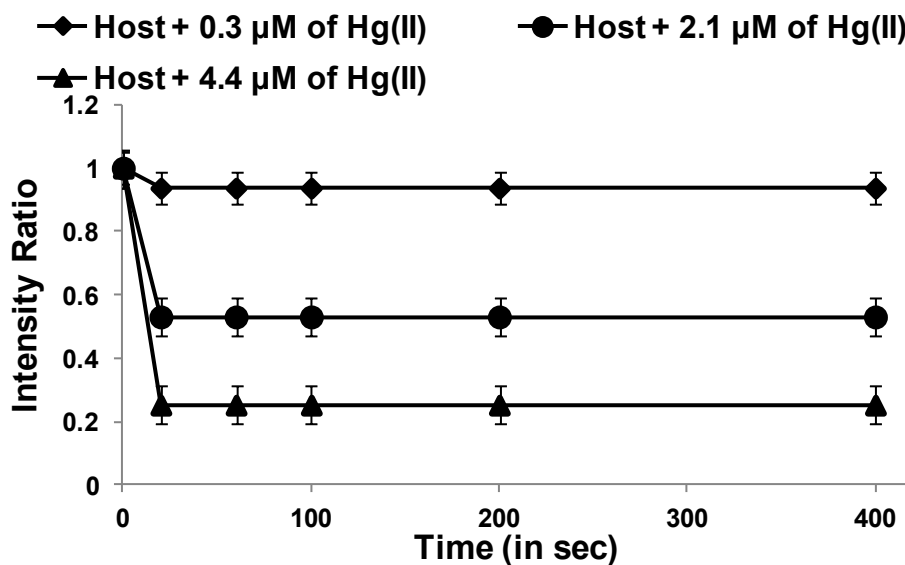


Figure S21. Response time of receptor **4** for Hg^{2+} ion at $\lambda_{\text{ex}} = 321 \text{ nm}$.

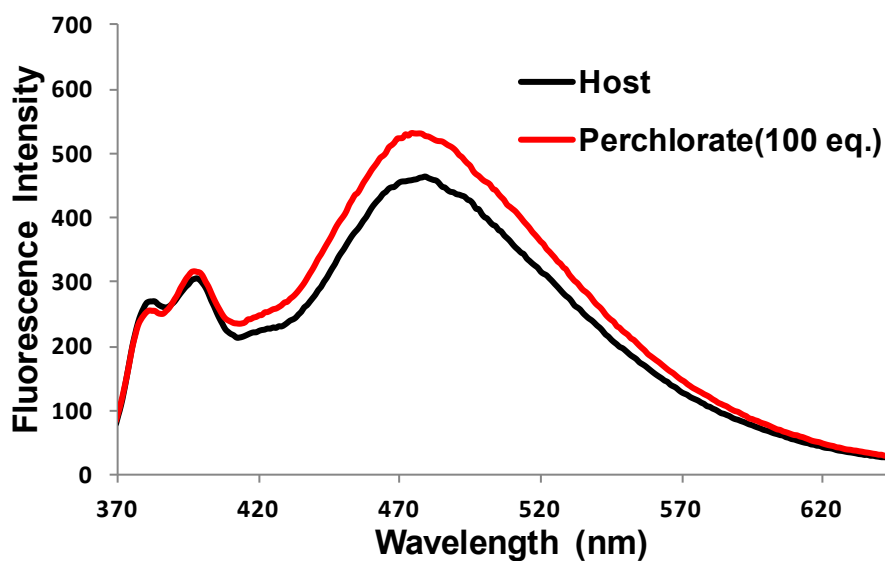


Figure S22. Salt perturbation studies of **4** recorded with $1 \mu\text{M}$ concentration of sensor in aqueous system with the respective fluorescence spectrum recorded upon addition of 100 equiv. of tetrabutyl ammonium nitrate under the same concentration of sensor and solvent system at $\lambda_{\text{ex}} = 321 \text{ nm}$.

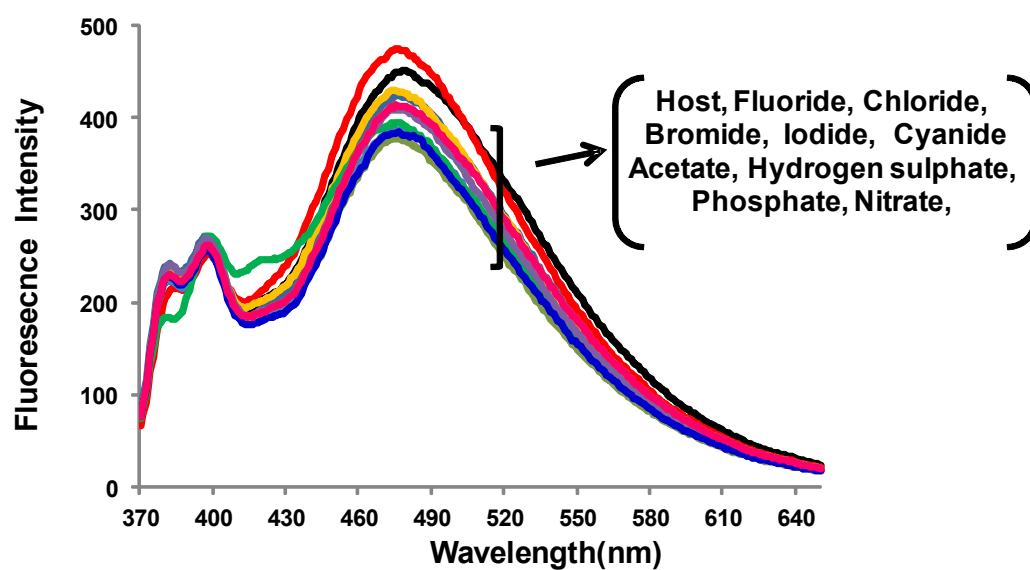


Figure S23. Changes in emission profile of nano-aggregates of **4** ($1\ \mu\text{M}$) in aqueous medium upon addition of a particular tetrabutylammonium anion salt (5 eq.) in aqueous media ($\lambda_{\text{ex}} = 321\ \text{nm}$).

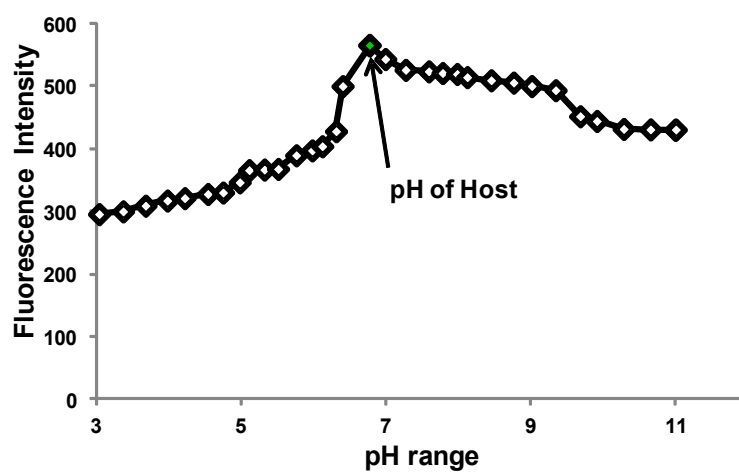


Figure S24. pH effect of receptor **4** ($1\ \mu\text{M}$) in aqueous system ($\lambda_{\text{ex}}=321\ \text{nm}$).

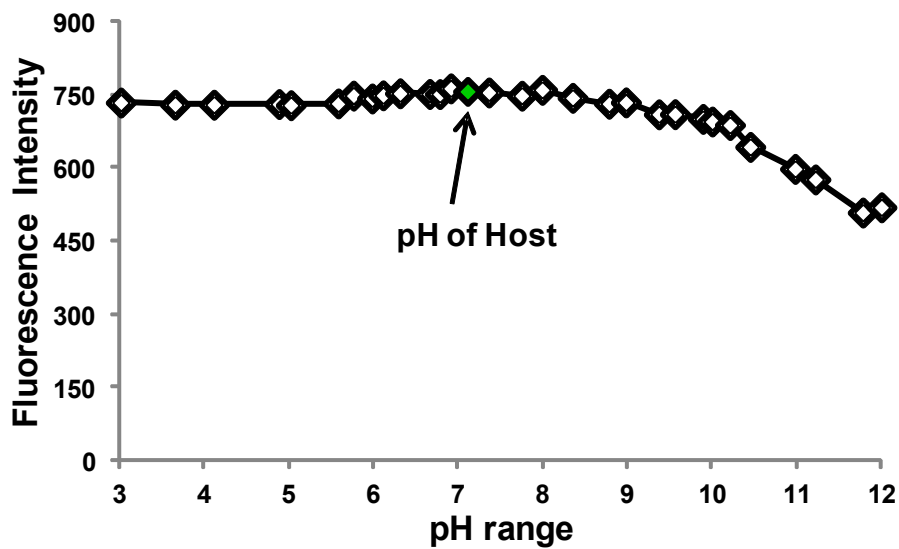


Figure S25. pH effect of receptor **3.Hg²⁺** (6 μM) in aqueous system (λ_{ex} =343 nm).

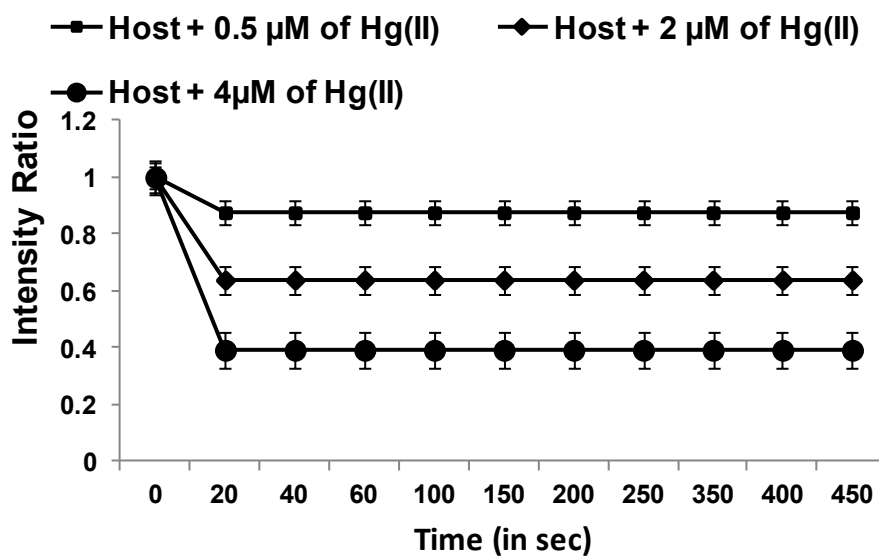


Figure S26. Response Time of receptor **3.Hg²⁺** for I⁻ ion at λ_{ex} = 343 nm.

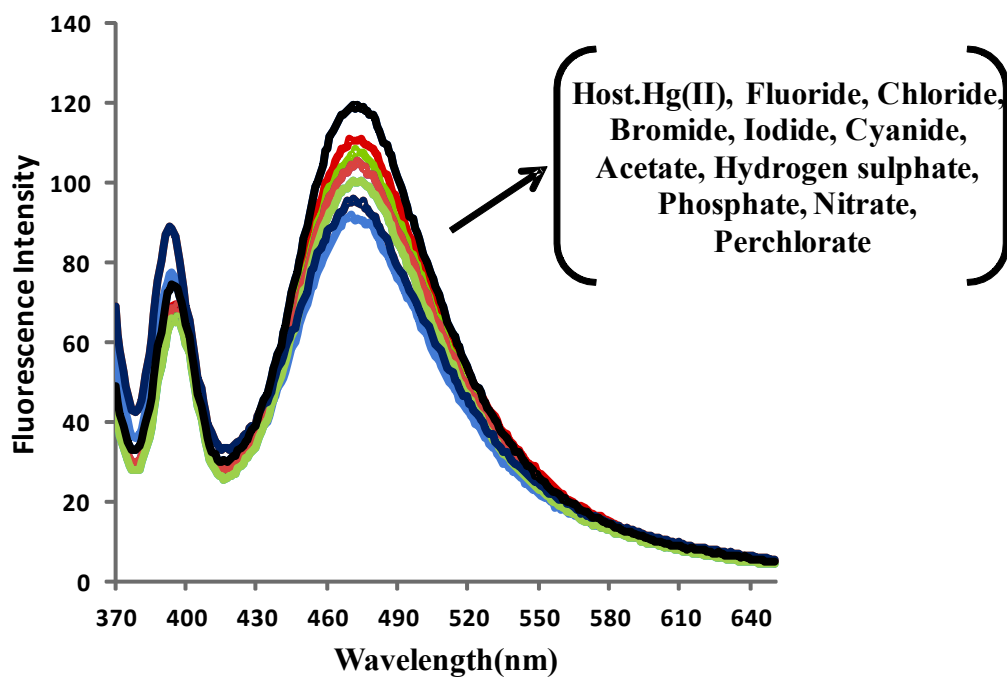


Figure S27. Changes in emission profile of nano-aggregates of **4** (1 μM) in aqueous medium upon addition of a particular tetrabutylammonium anion salt (5 eq.) in aqueous media ($\lambda_{\text{ex}} = 321 \text{ nm}$).

TableS1 DFT Energies

DFT Calculations	1	2	3	4	3. Hg²⁺
E (in eV)	-4.813eV	-4.796eV	-4.476eV	-4.468eV	-10.689