Electronic Supplementary Material (ESI) for New Journal of Chemistry
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Supporting Information

Design and synthesis of anthracene-based bispyridinium amides: Anion binding, cell staining and their DNA interaction studies

Kumaresh Ghosh,*[a] Avik Ranjan Sarkar, [a] Atanu Ghorai, [b] Utpal Ghosh [b]

[a]*Department of Chemistry, University of Kalyani, Kalyani-741235, India.*
[b]*Department of Biochemistry and Biophysics, University of Kalyani, Kalyani-741235, India.*
E-mail : *ghosh_k2003@yahoo.co.in*

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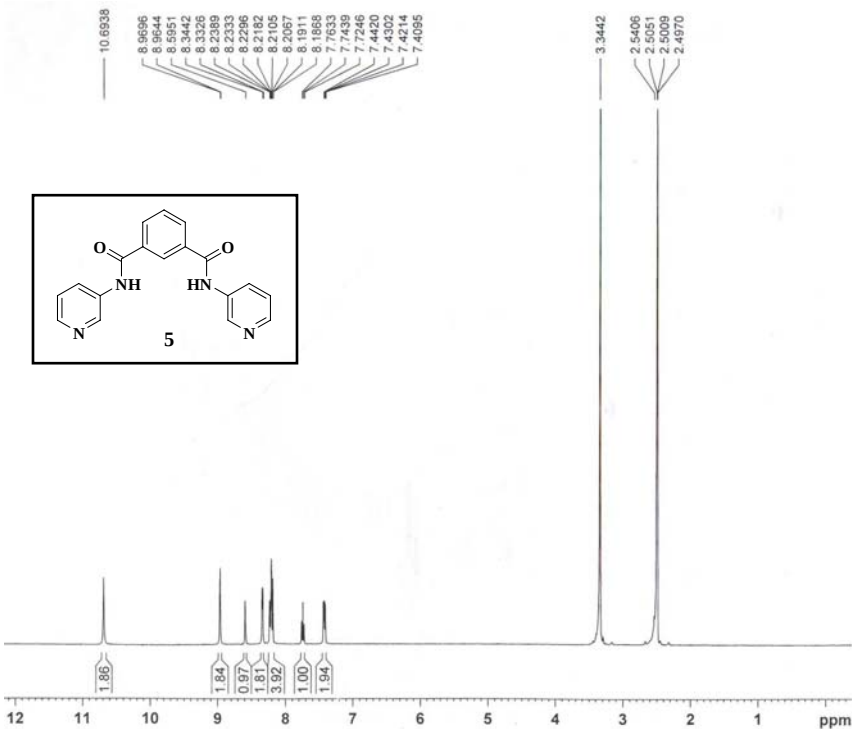

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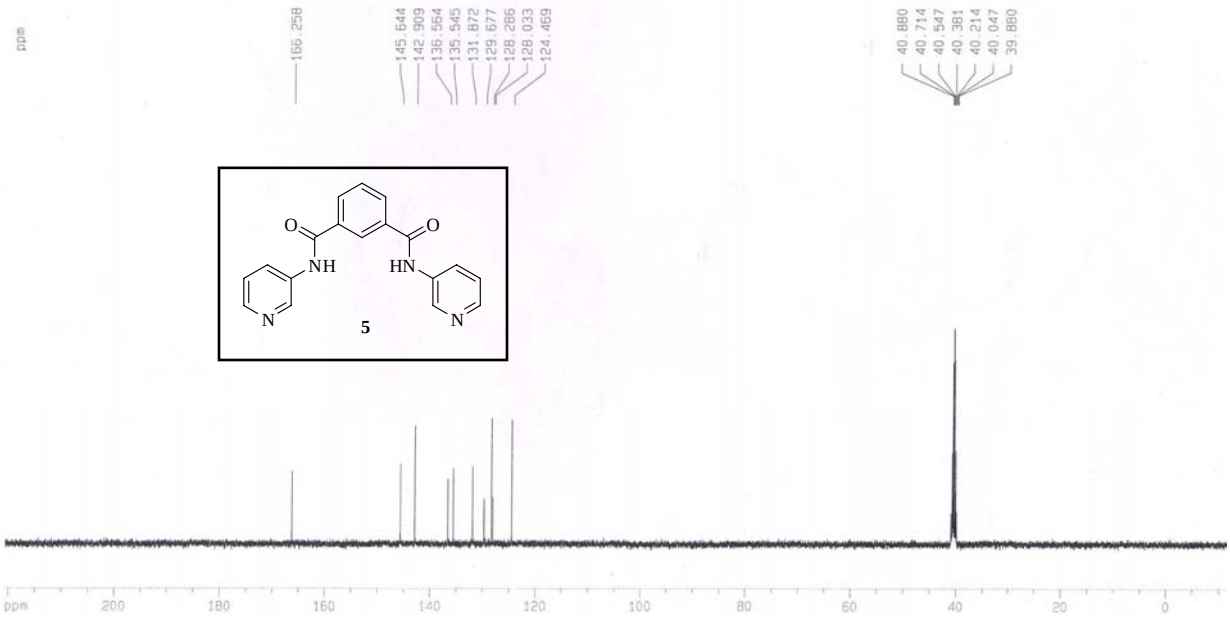

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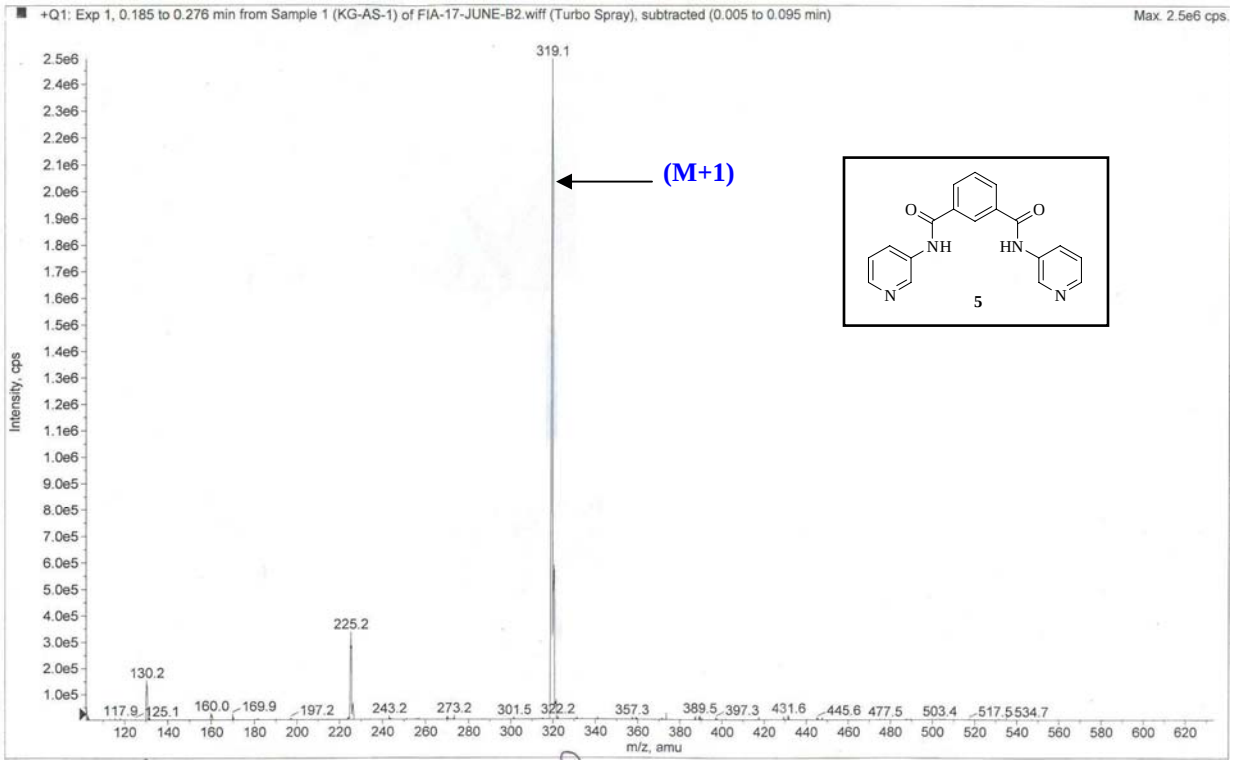

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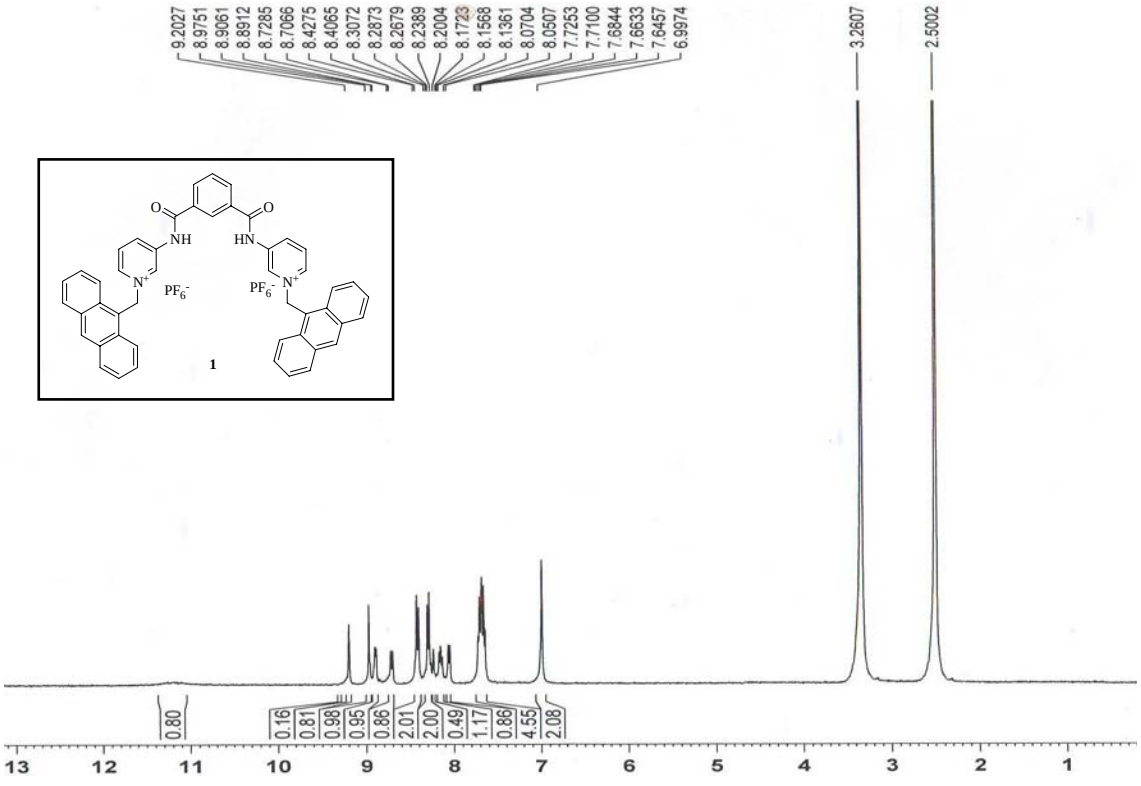

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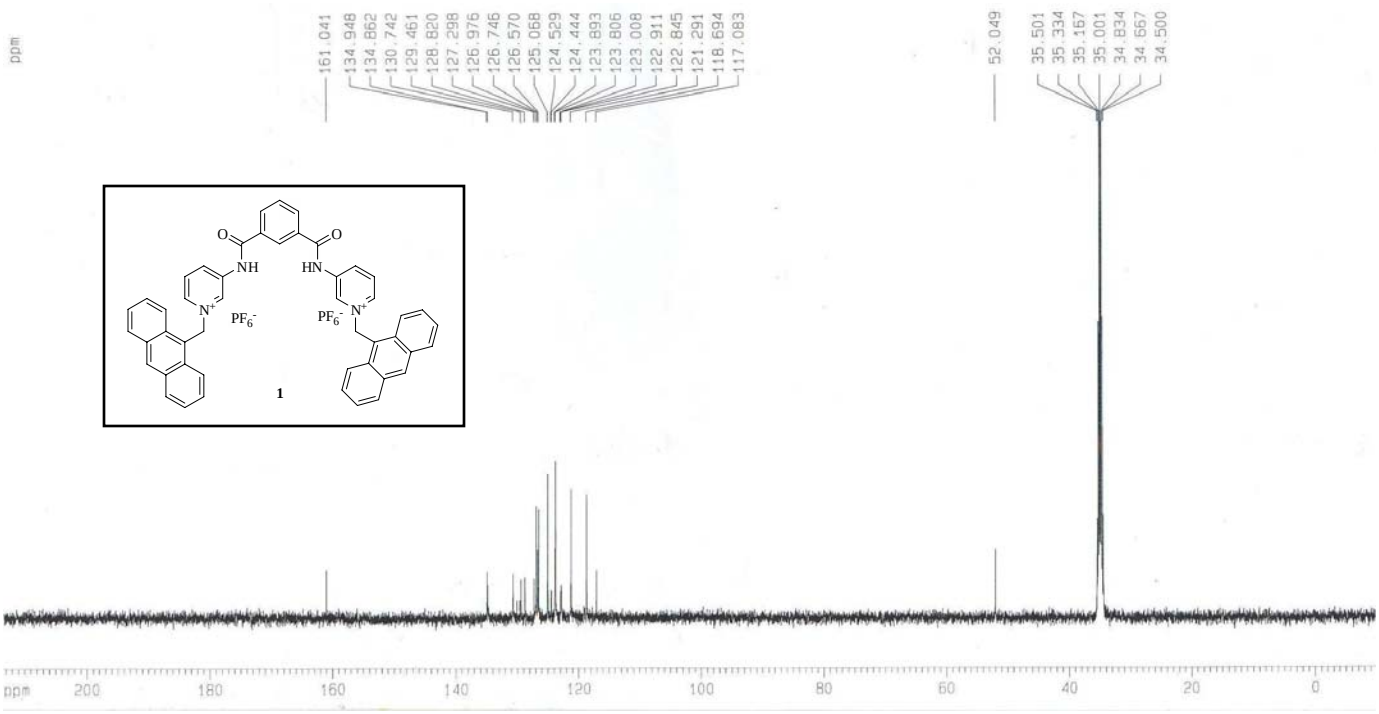

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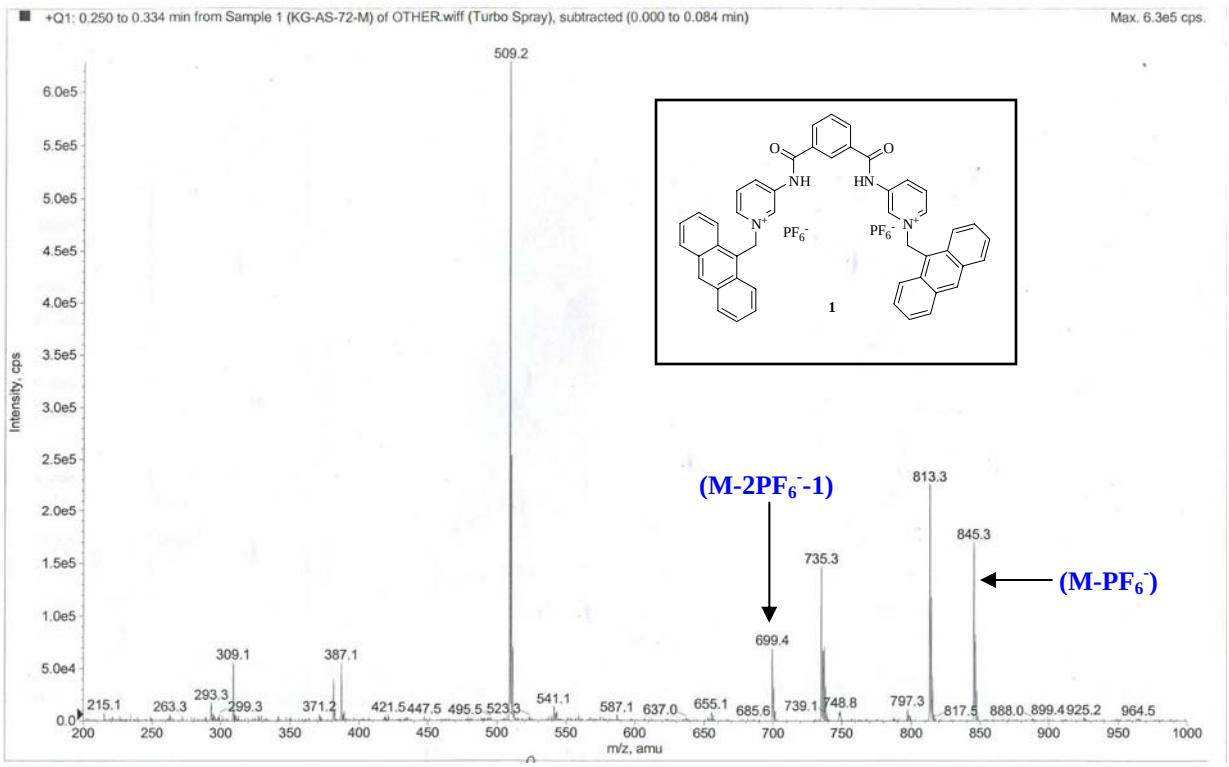

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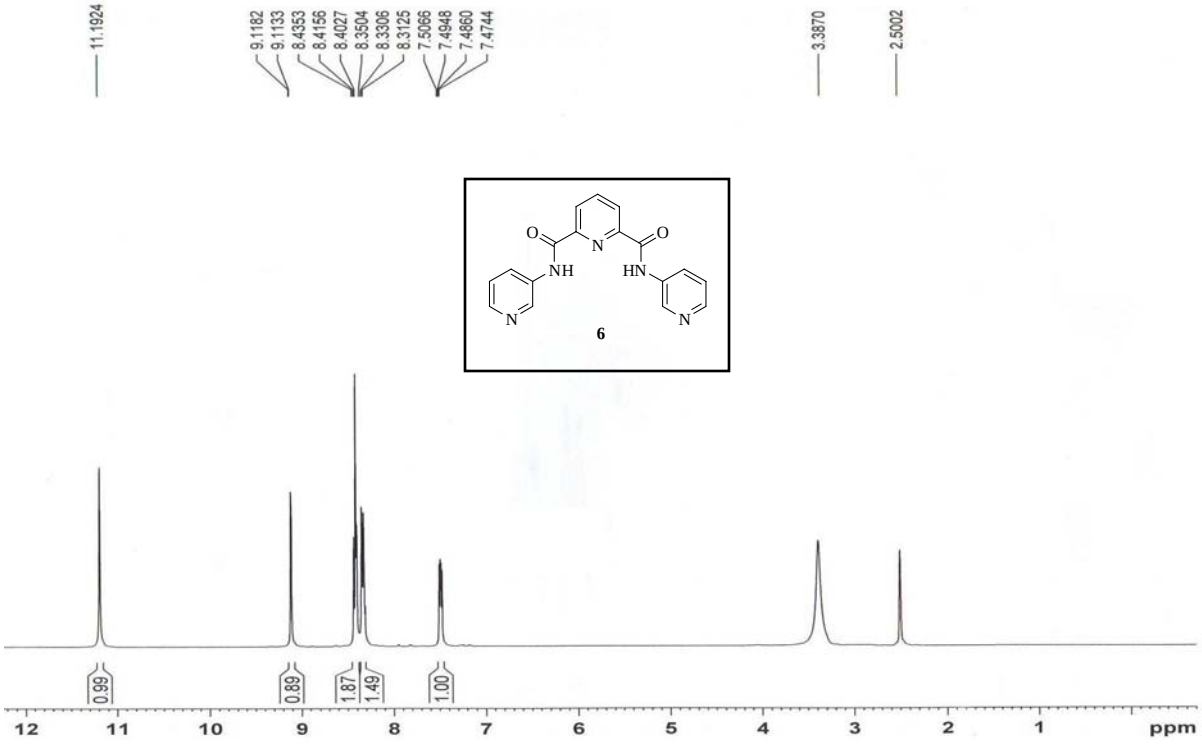

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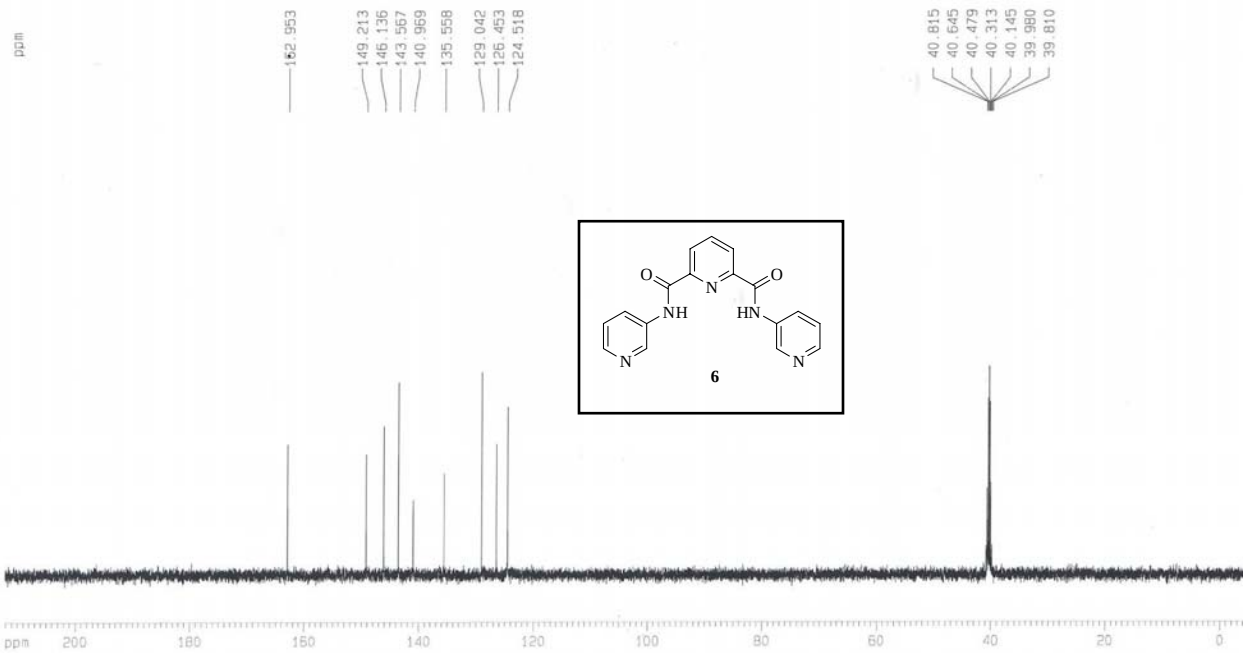

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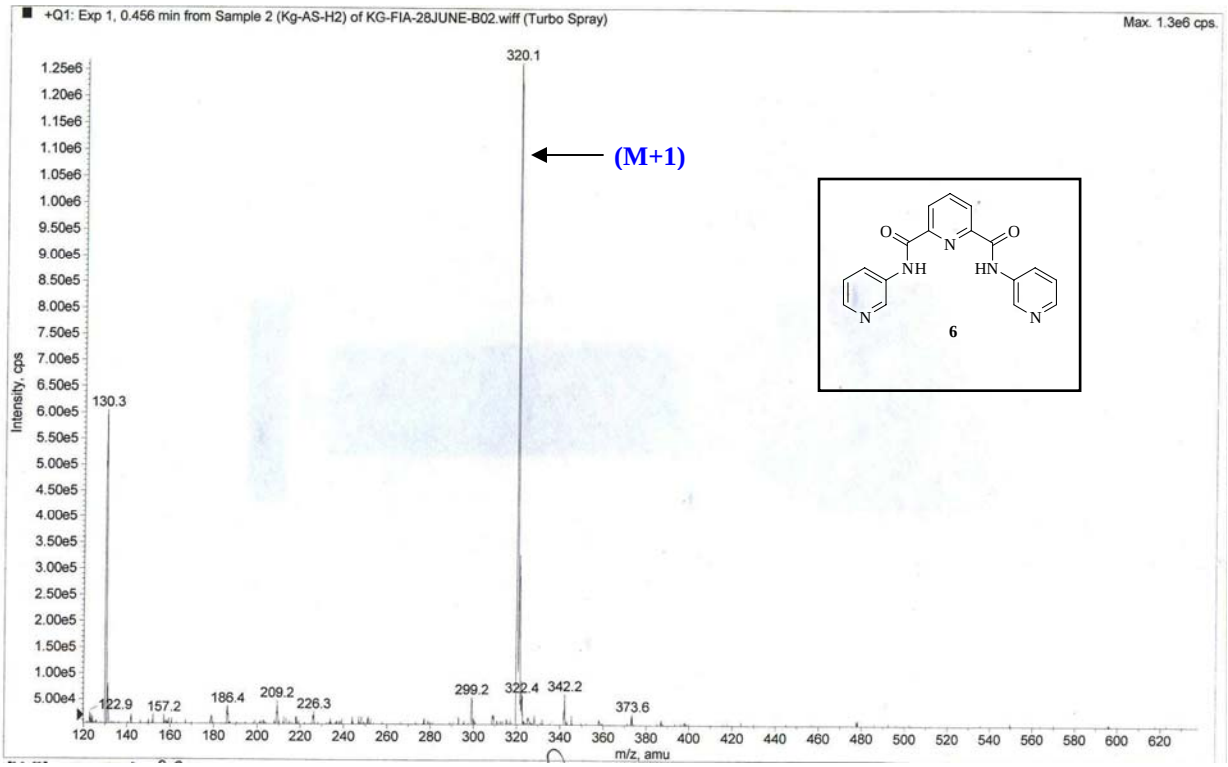

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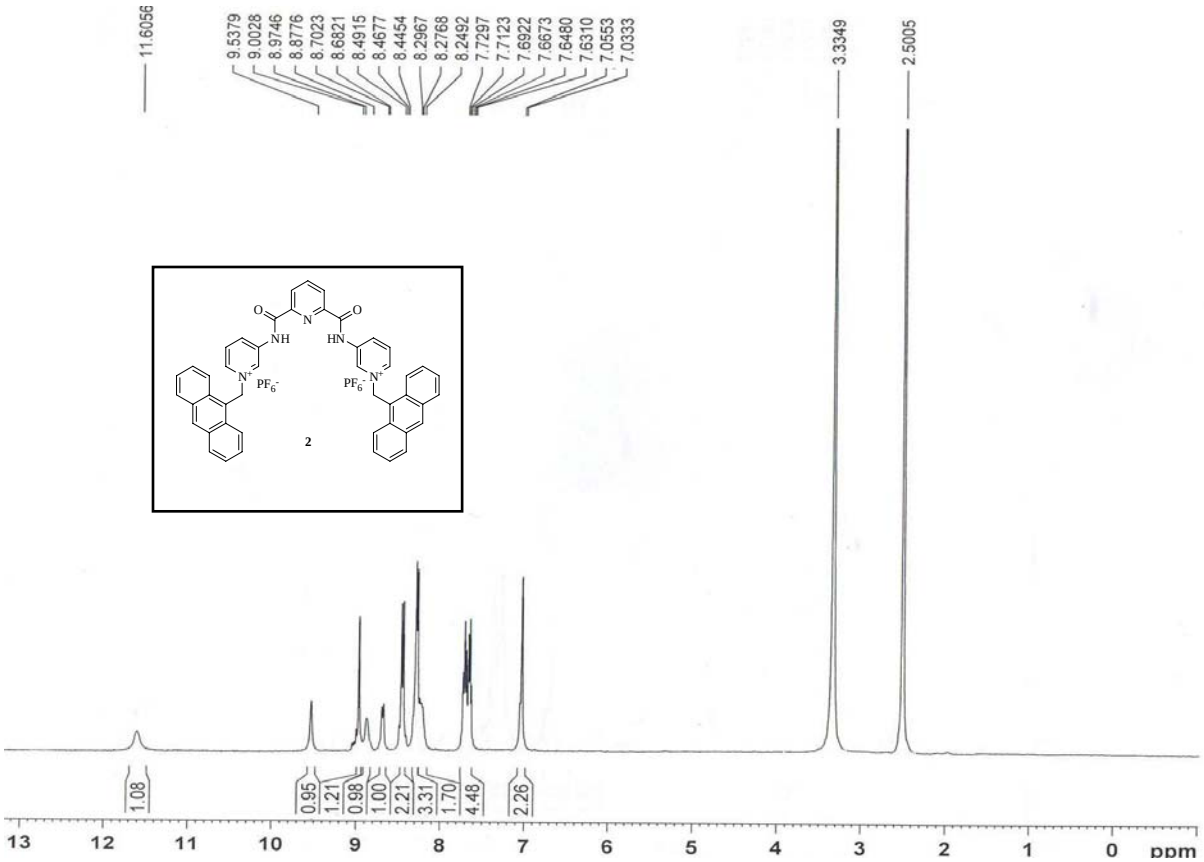

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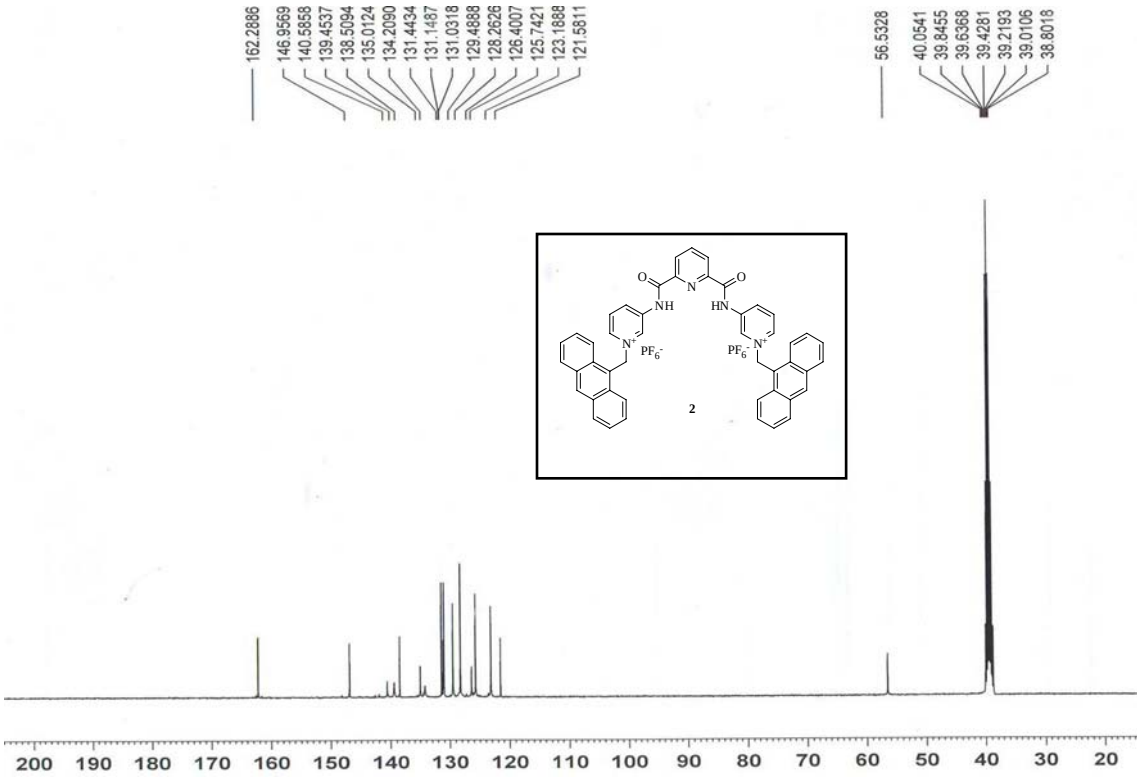

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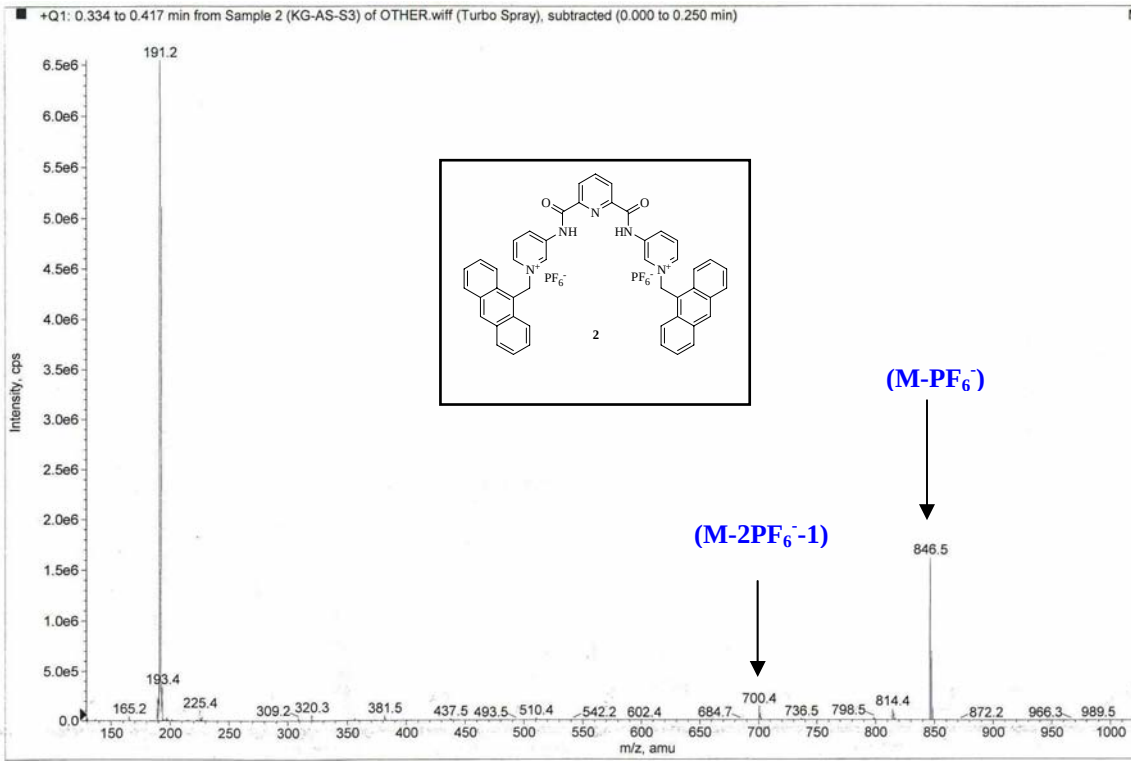

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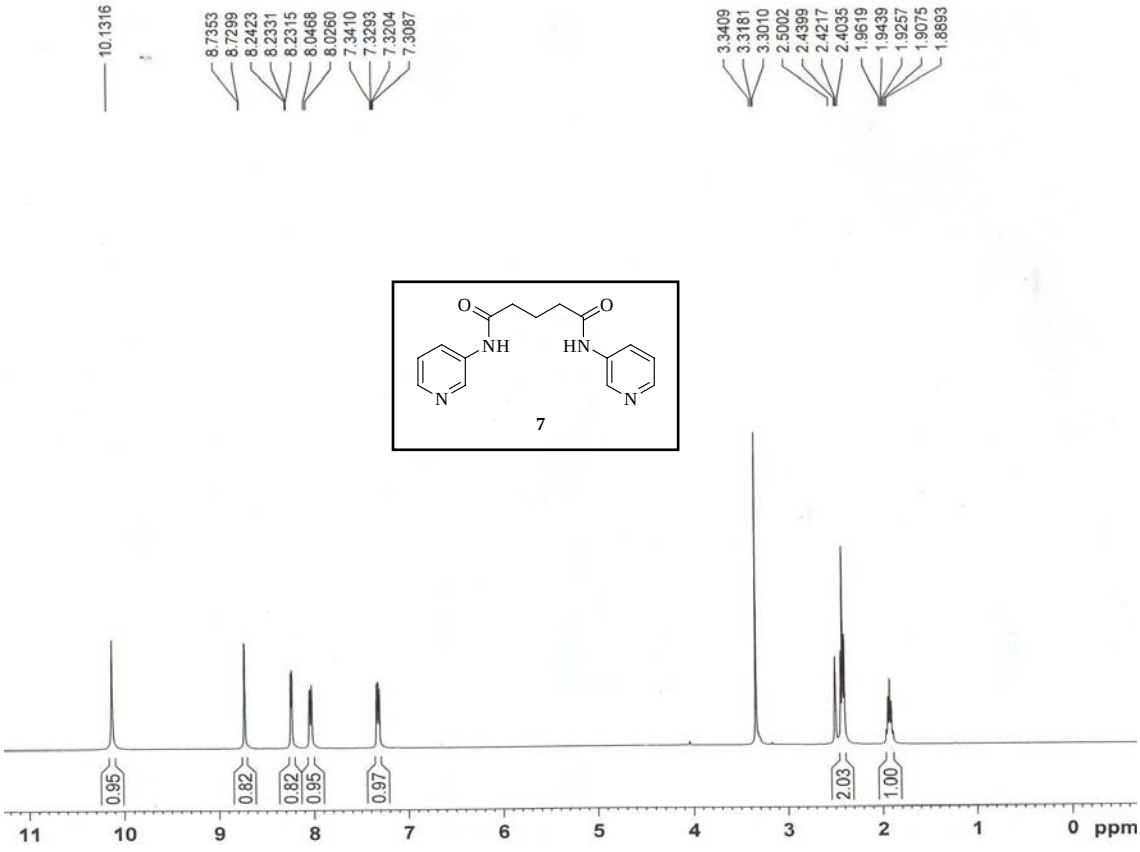

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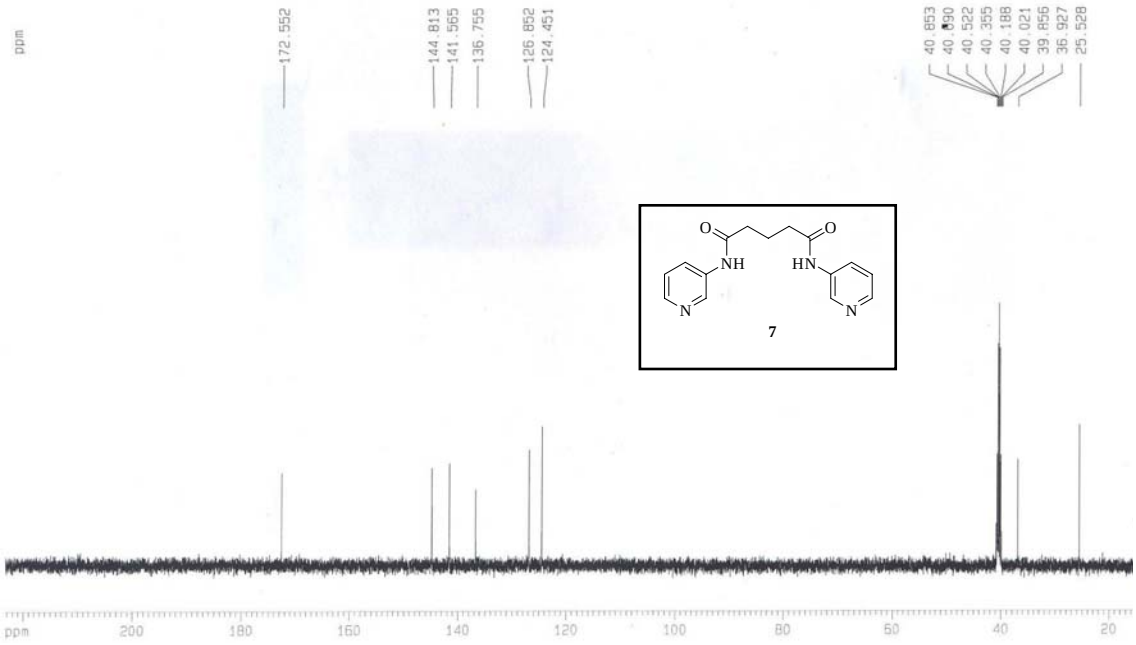

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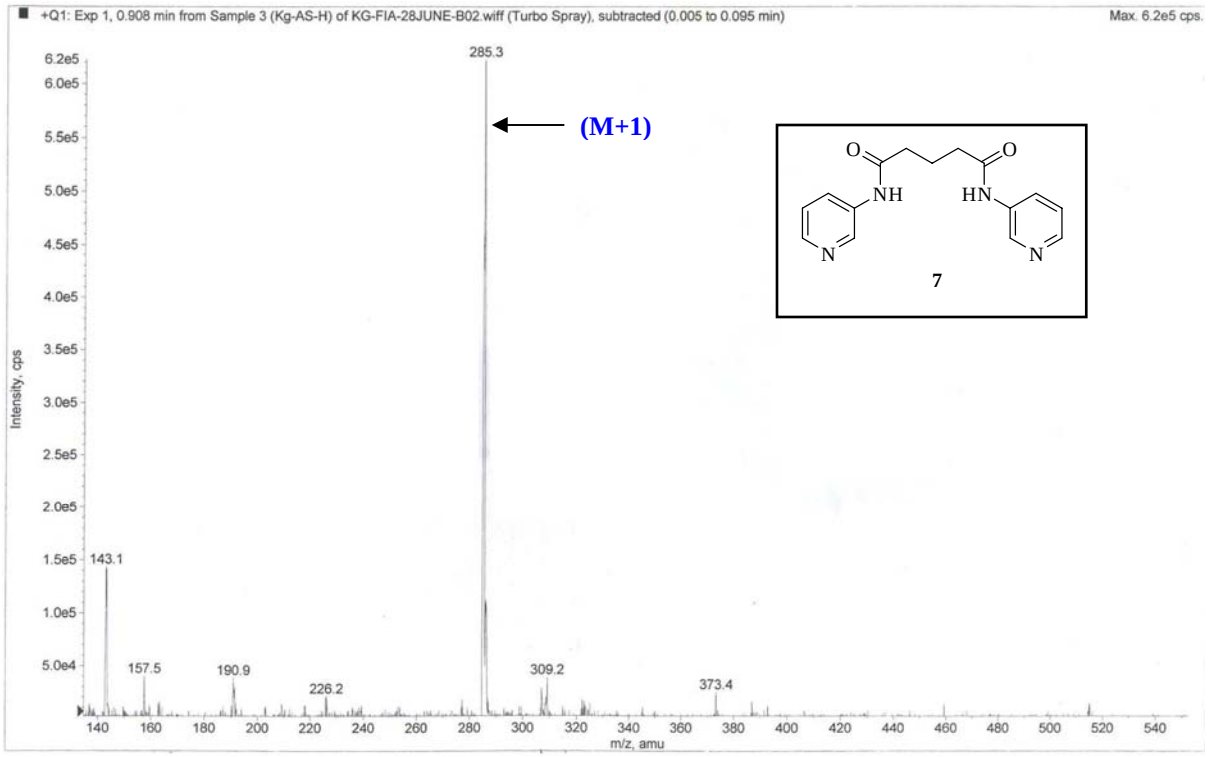

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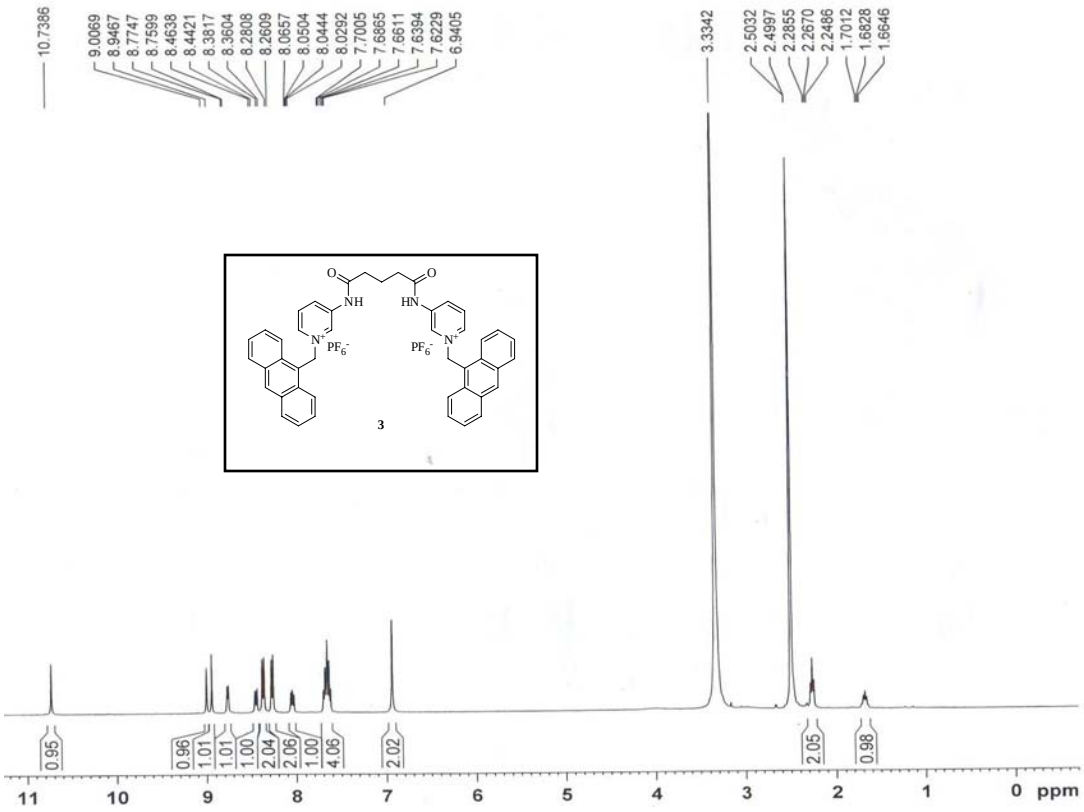

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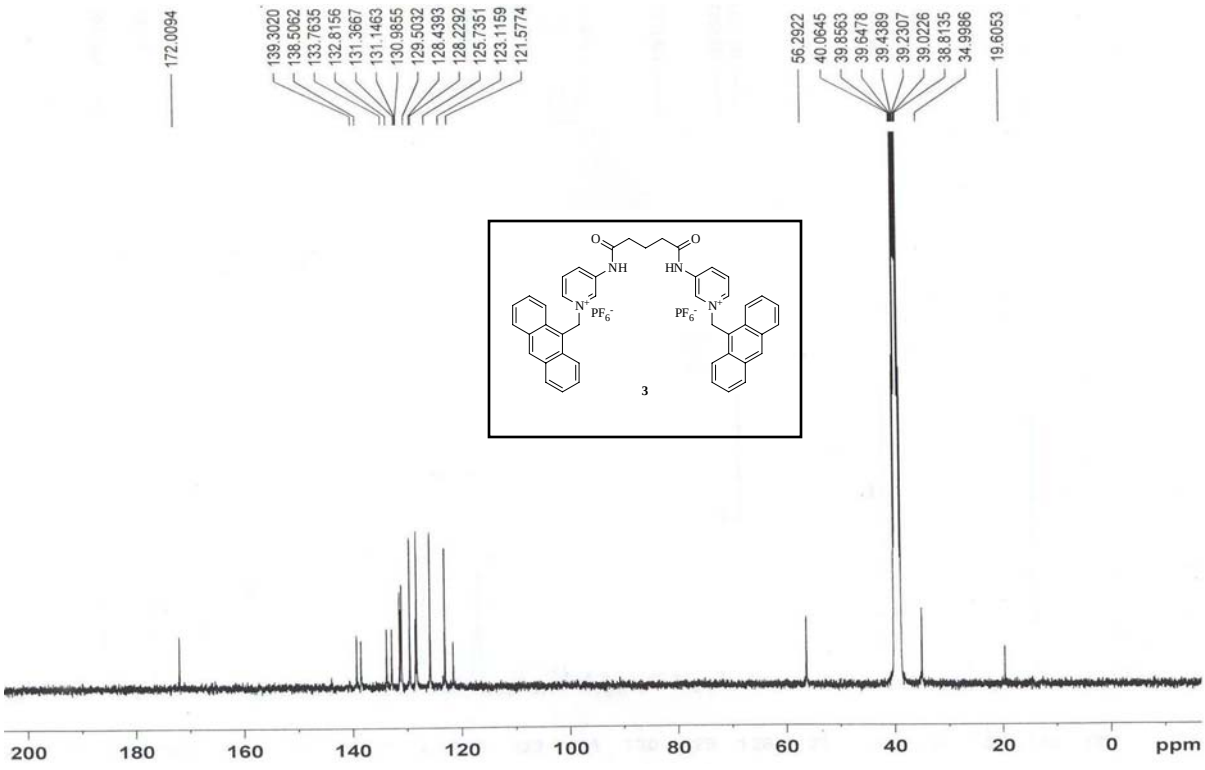

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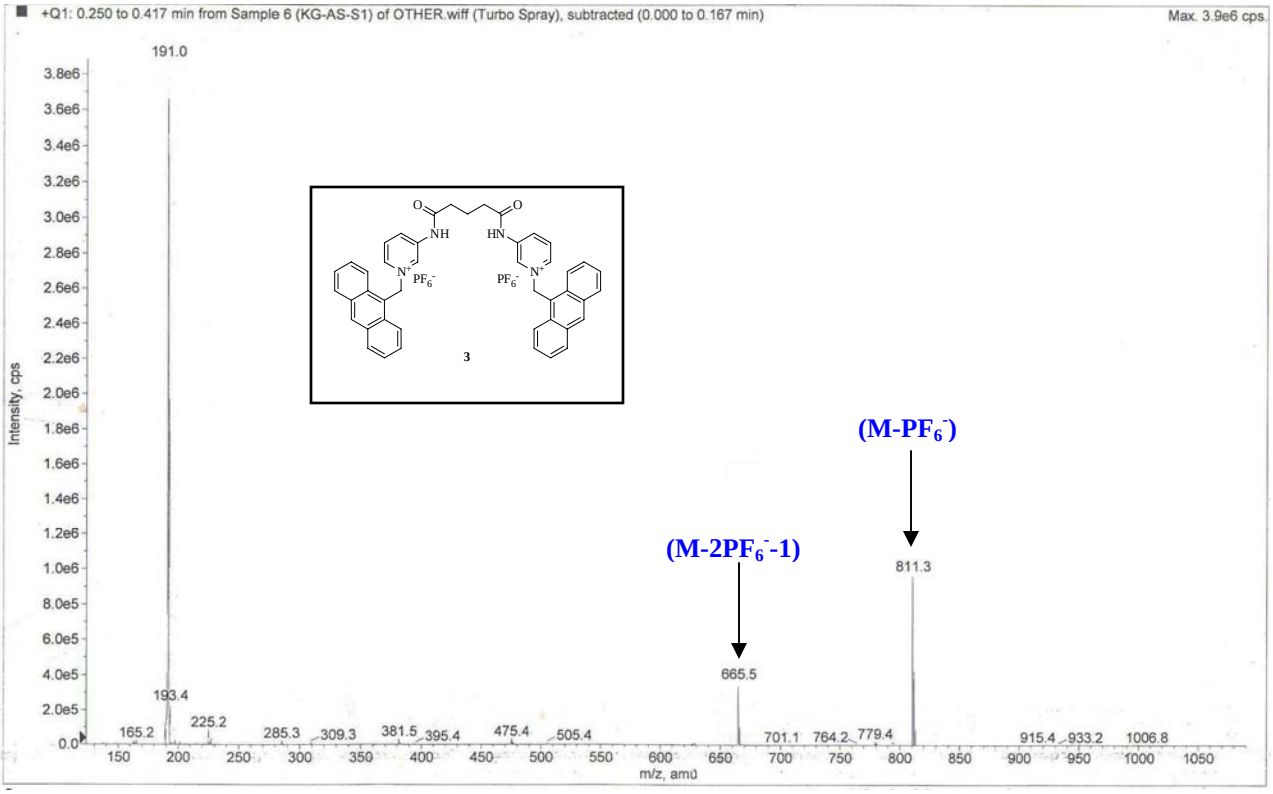

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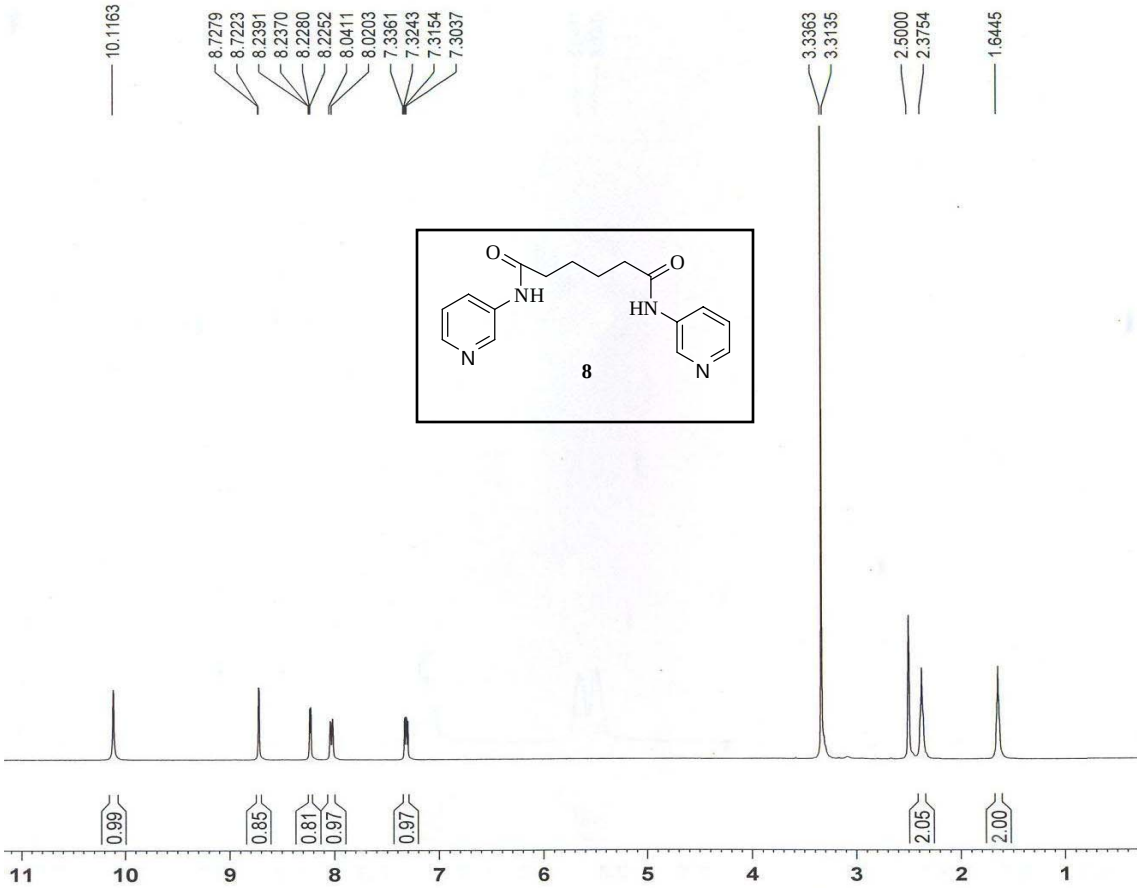
^{1}H NMR of 8 (400 MHz, d_6-DMSO):



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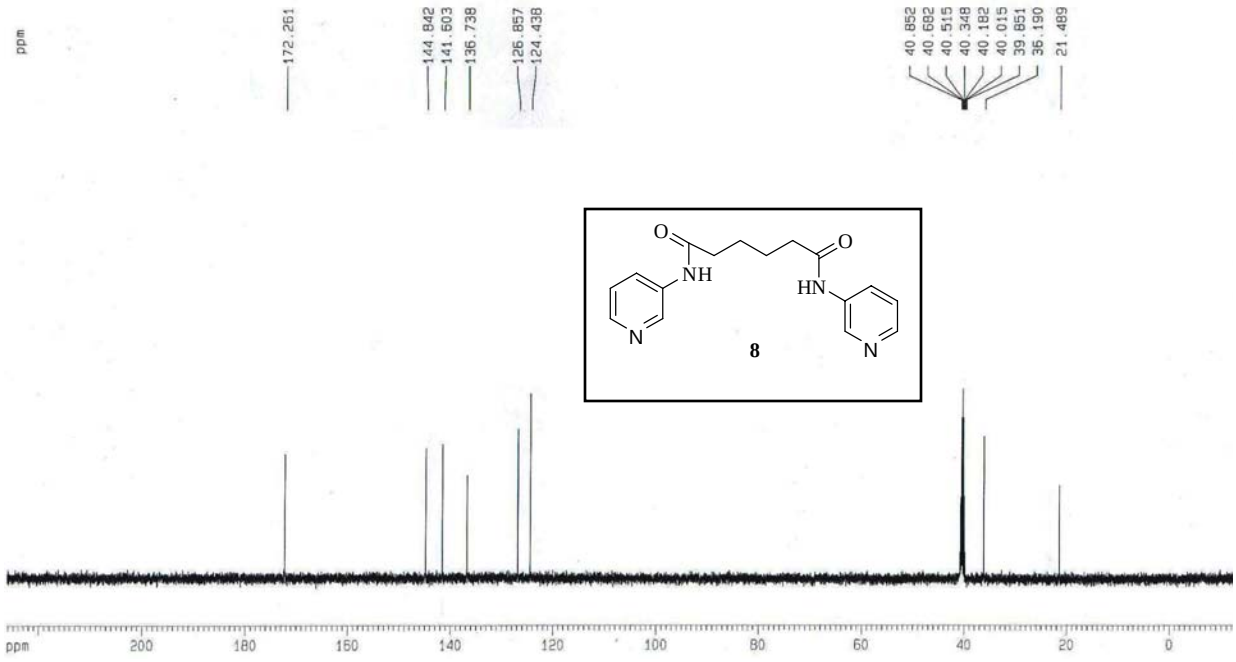

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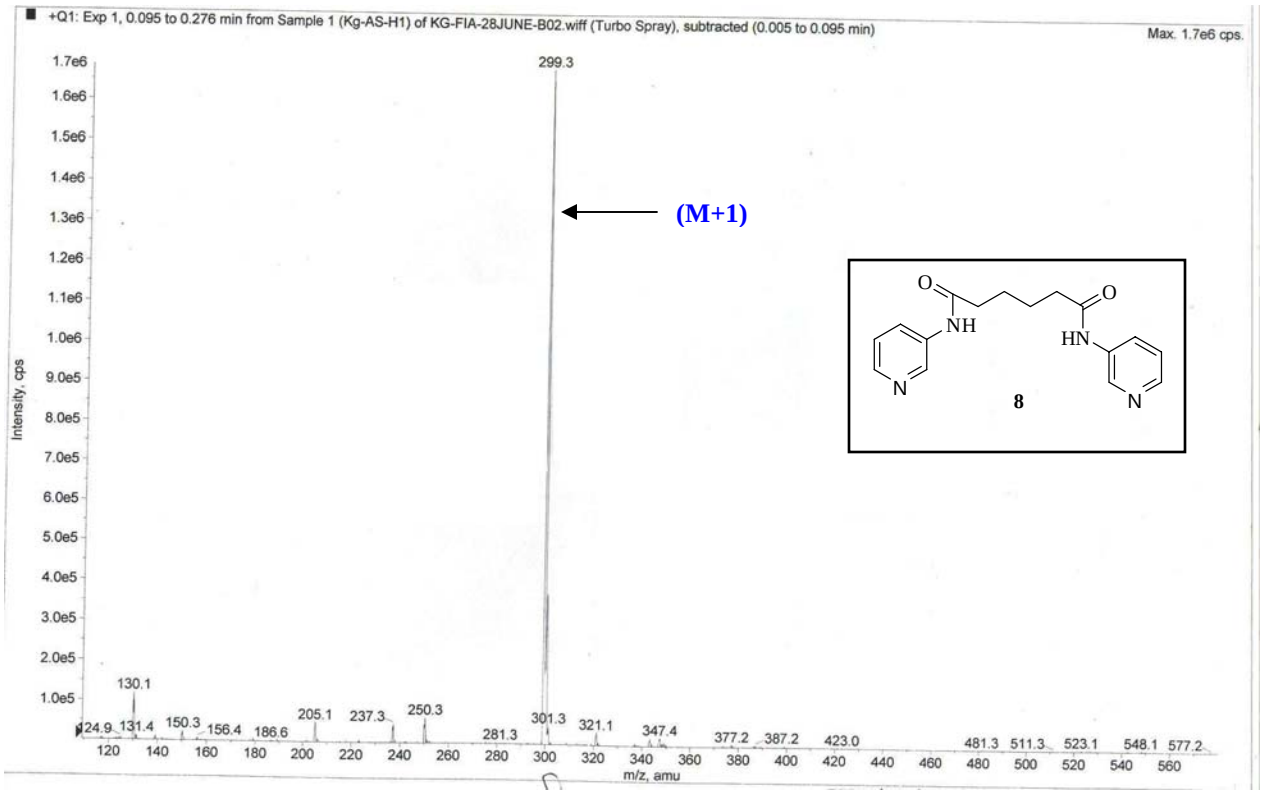

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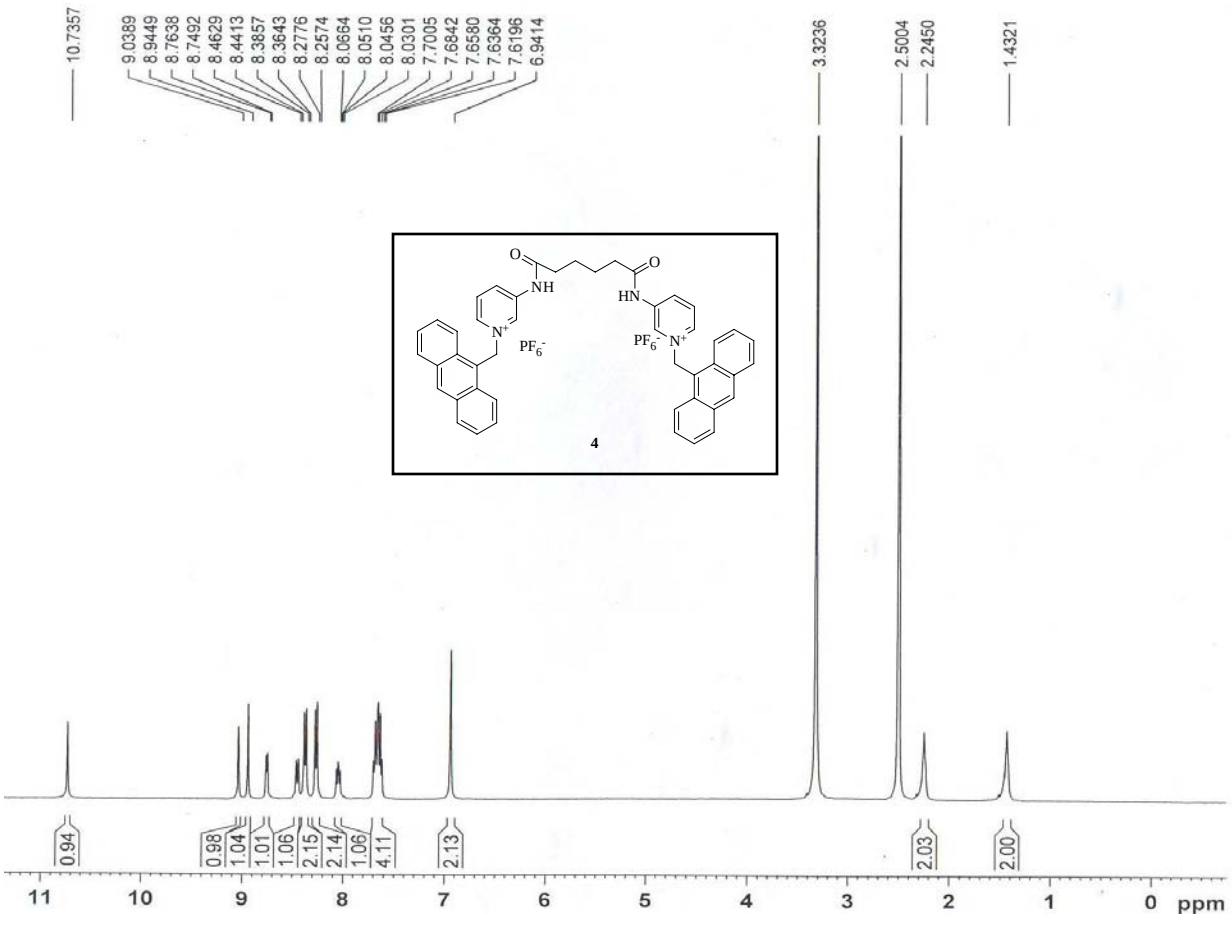

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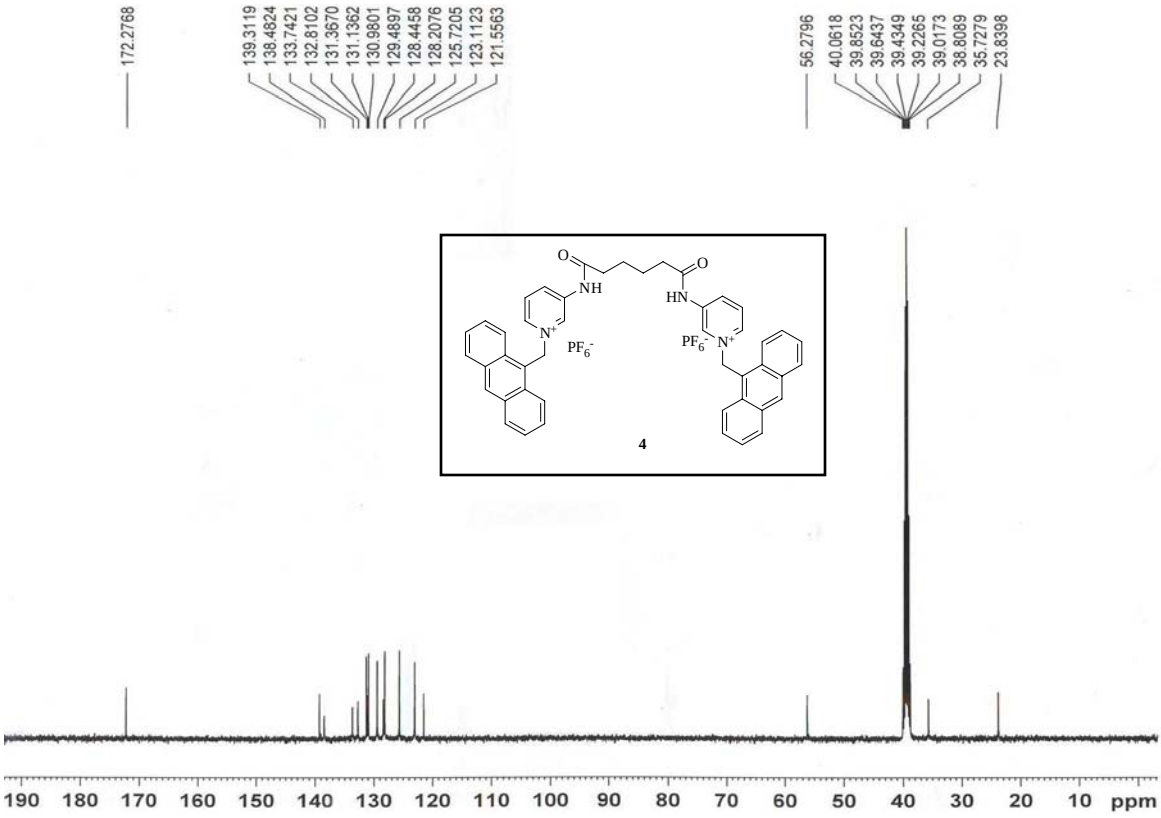
^{13}C NMR of 4 (100 MHz, d_6-DMSO):



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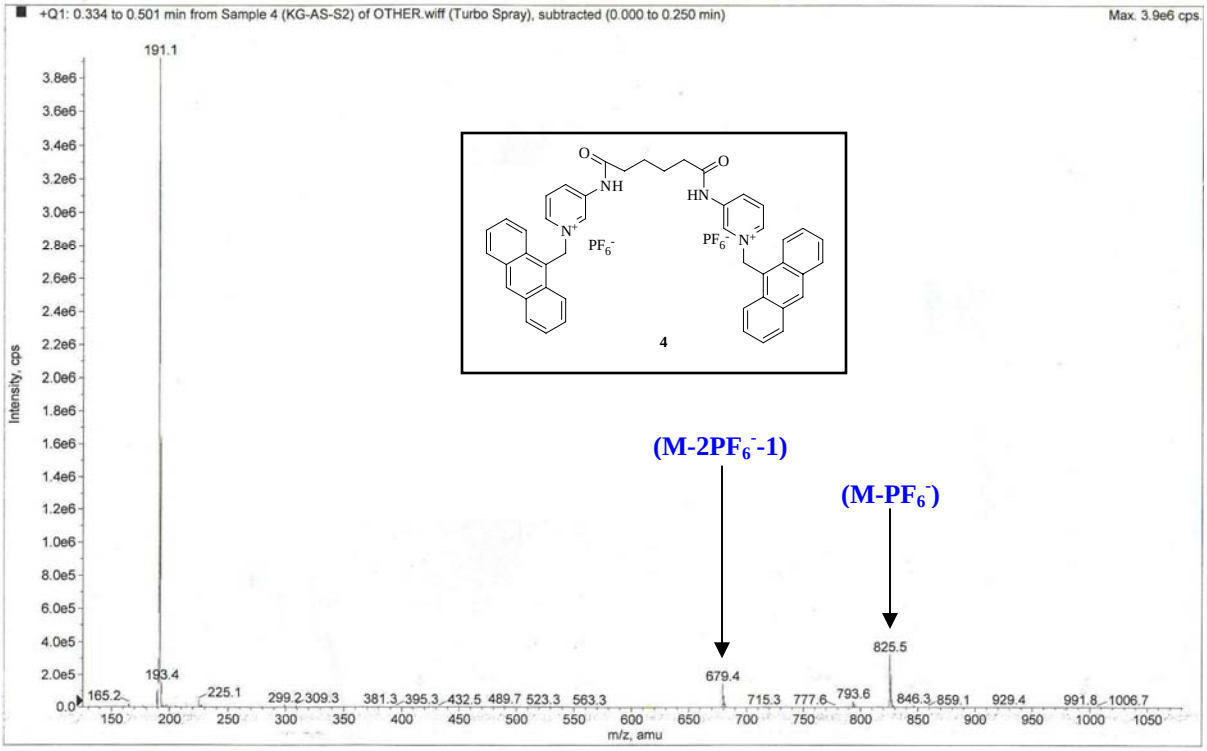

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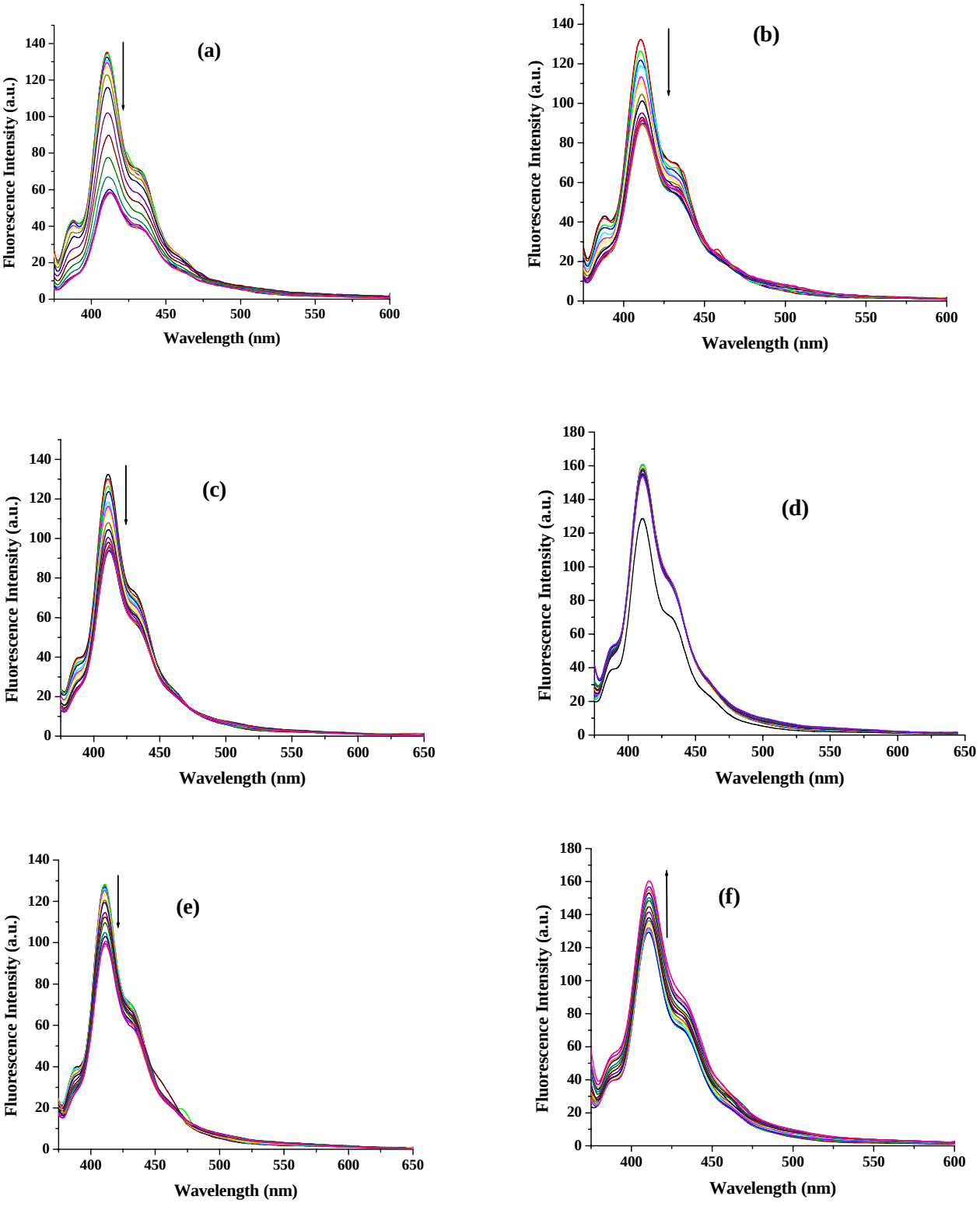
2a. Selected emission titration curves for receptor 1 in CH_3CN with following anions.



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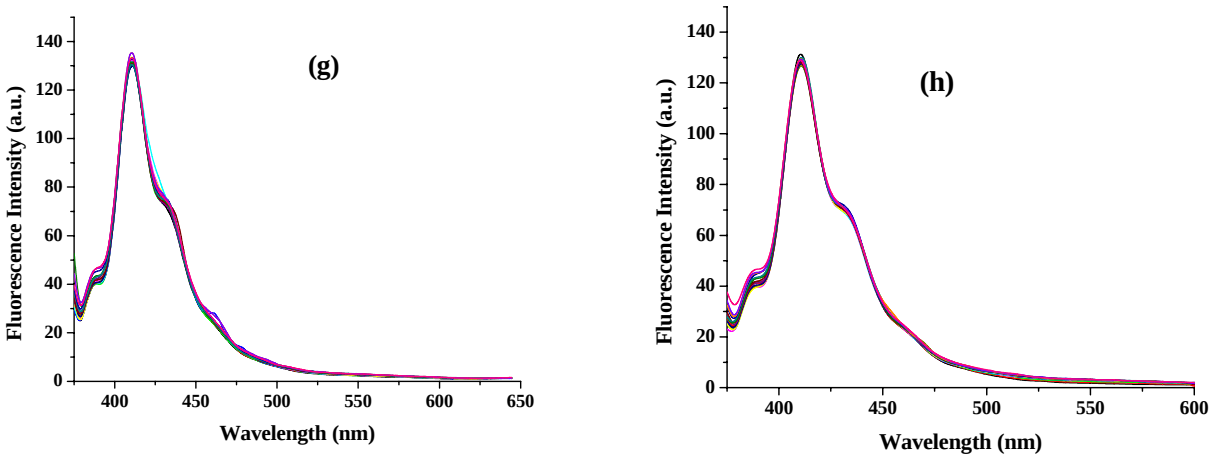
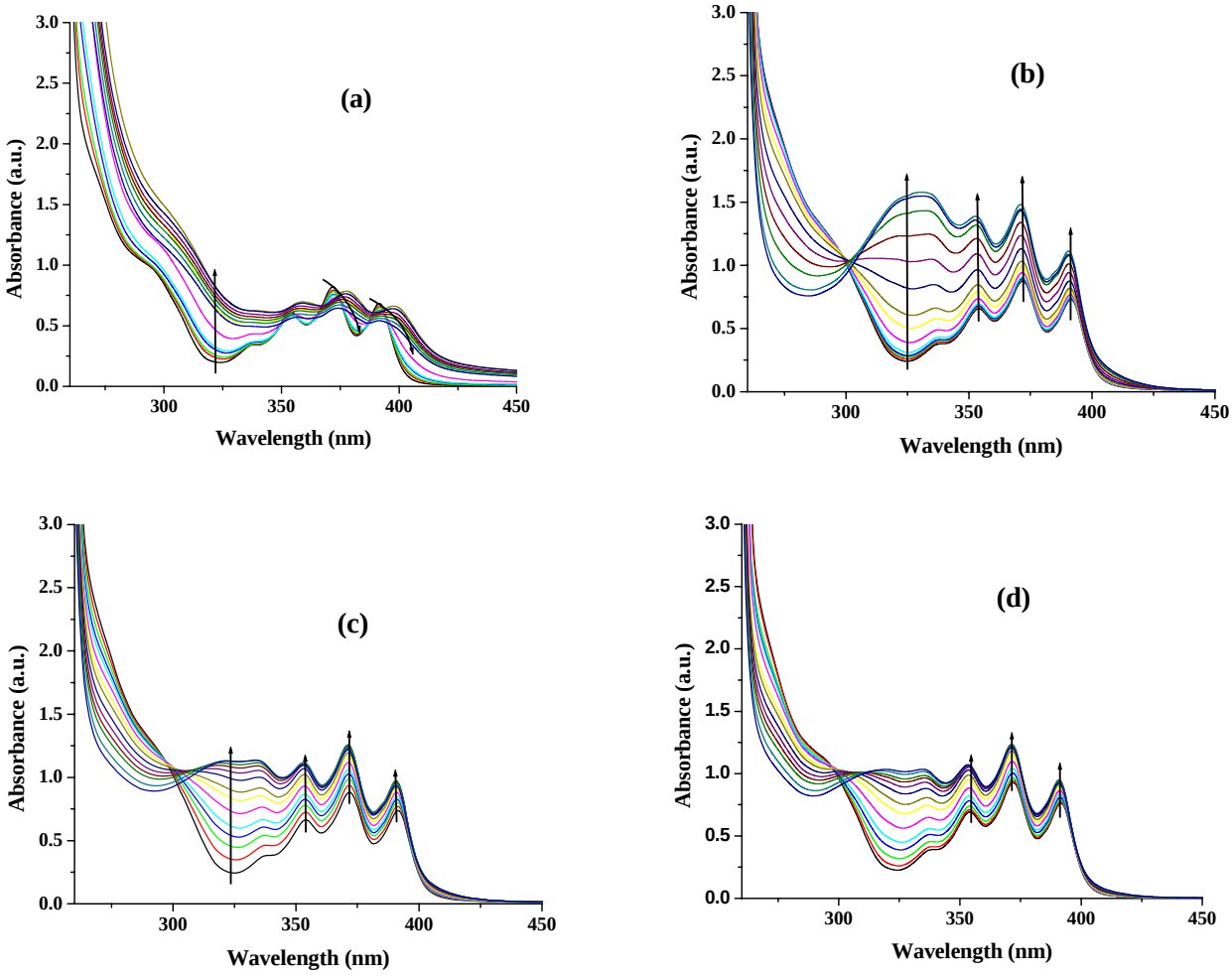


FigureS1a: Fluorescence titration curve of receptor **1** (c = 5.65 x 10^{-5} M) with the tetrabutylammonium (a) fluoride, (b) acetate, (c) propanoate, (d) hydrogensulphate, (e) salt of ibuprofen, (f) benzoate, (g) chloride, (h) bromide in CH_3CN(concentration of all guests c = 2.5 x 10^{-4} M, $\lambda_{Excitation}$ = 370 nm).

2b. Selected UV-vis titration curves for receptor 1 in CH_3CN:



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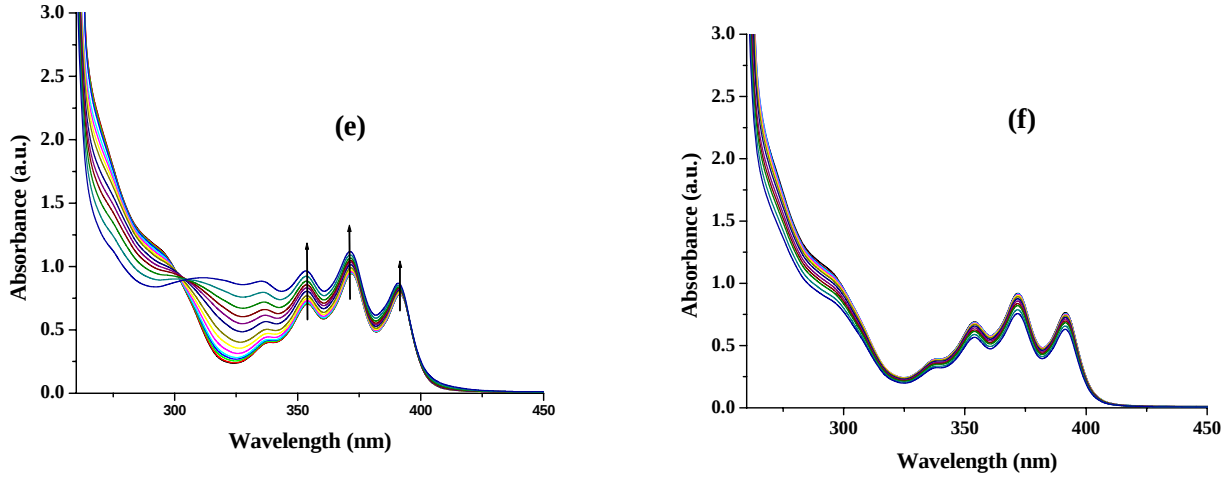
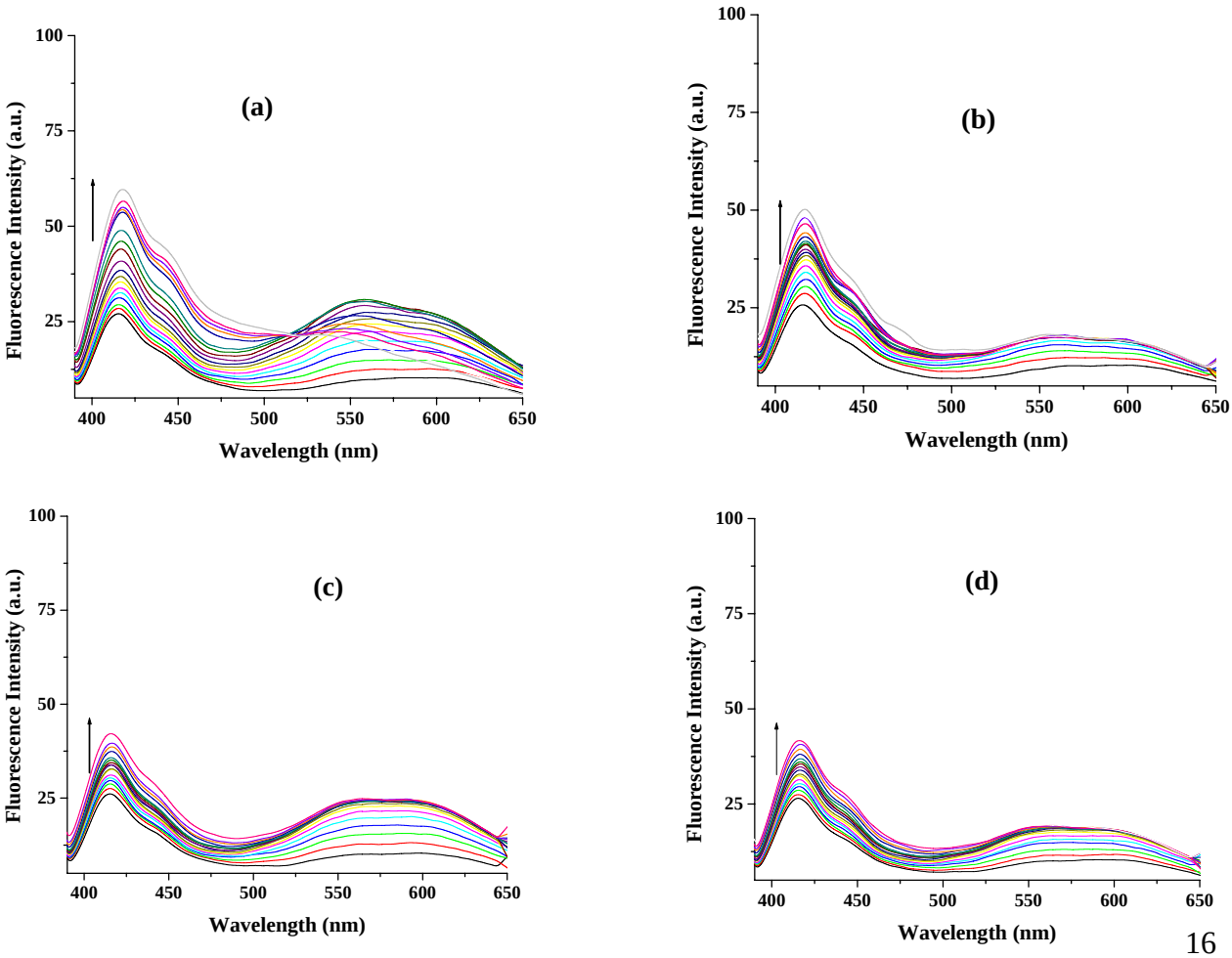


Figure S1b: UV-vis titration curve of receptor **1** (c = 5.65 x 10^{-5} M) with the tetrabutylammonium (a) $H_2PO_4^-$, (b) fluoride, (c) acetate, (d) propanoate, (e) salt of ibuprofen, (f) hydrogensulphate in CH_3CN (concentration of all guests c = 2.5 x 10^{-3} M λ_{max} = 371 nm).

2c. Selected emission titration curves for receptor 2 in CH_3CN with following anions



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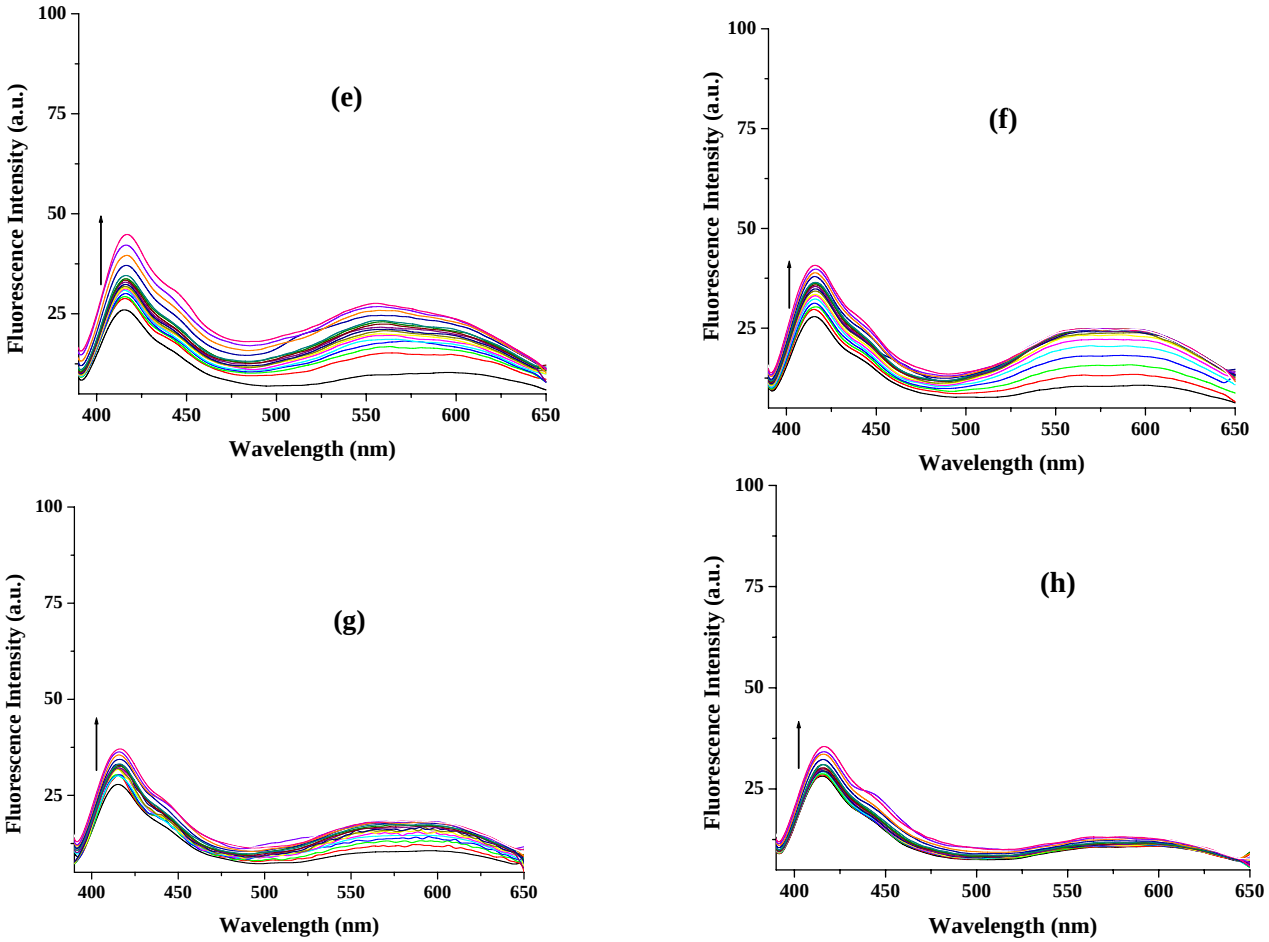
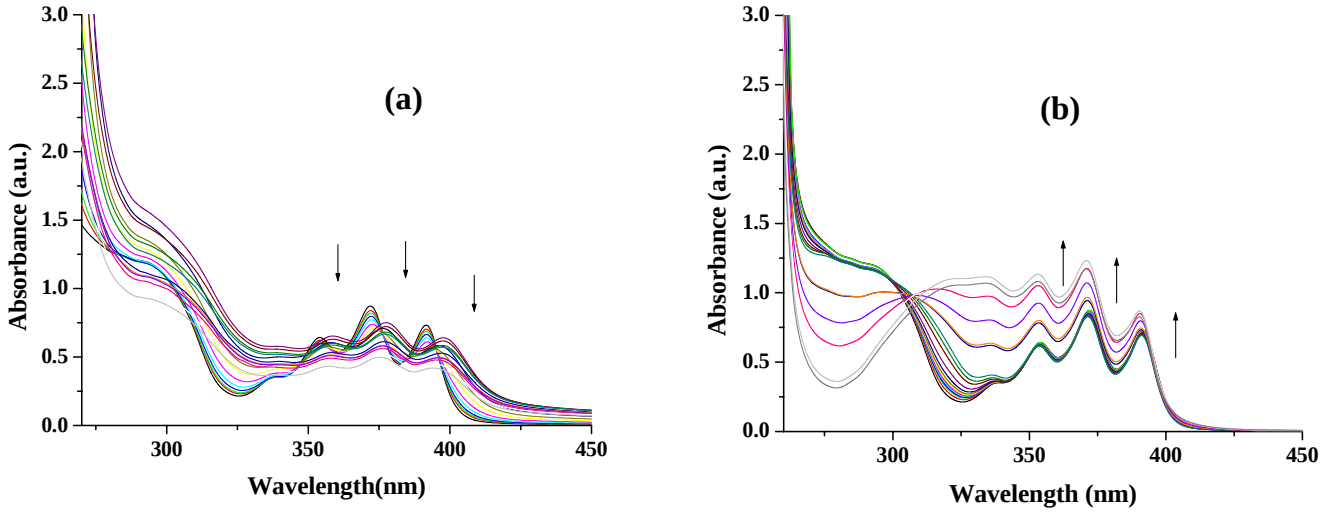


Figure S1c: Fluorescence titration curve of receptor **2** (c = 5.65 x 10^{-5} M) with the tetrabutylammonium (a) fluoride, (b) acetate, (c) propanoate, (d) hydrogensulphate, (e) salt of ibuprofen, (f) benzoate, (g) chloride, (h) bromide in CH_3CN (concentration of all guests c = 2.5 x 10^{-3} M, $\lambda_{Excitation}$ = 370 nm).

2d. Selected UV-vis titration curves for receptor 2 in CH_3CN:



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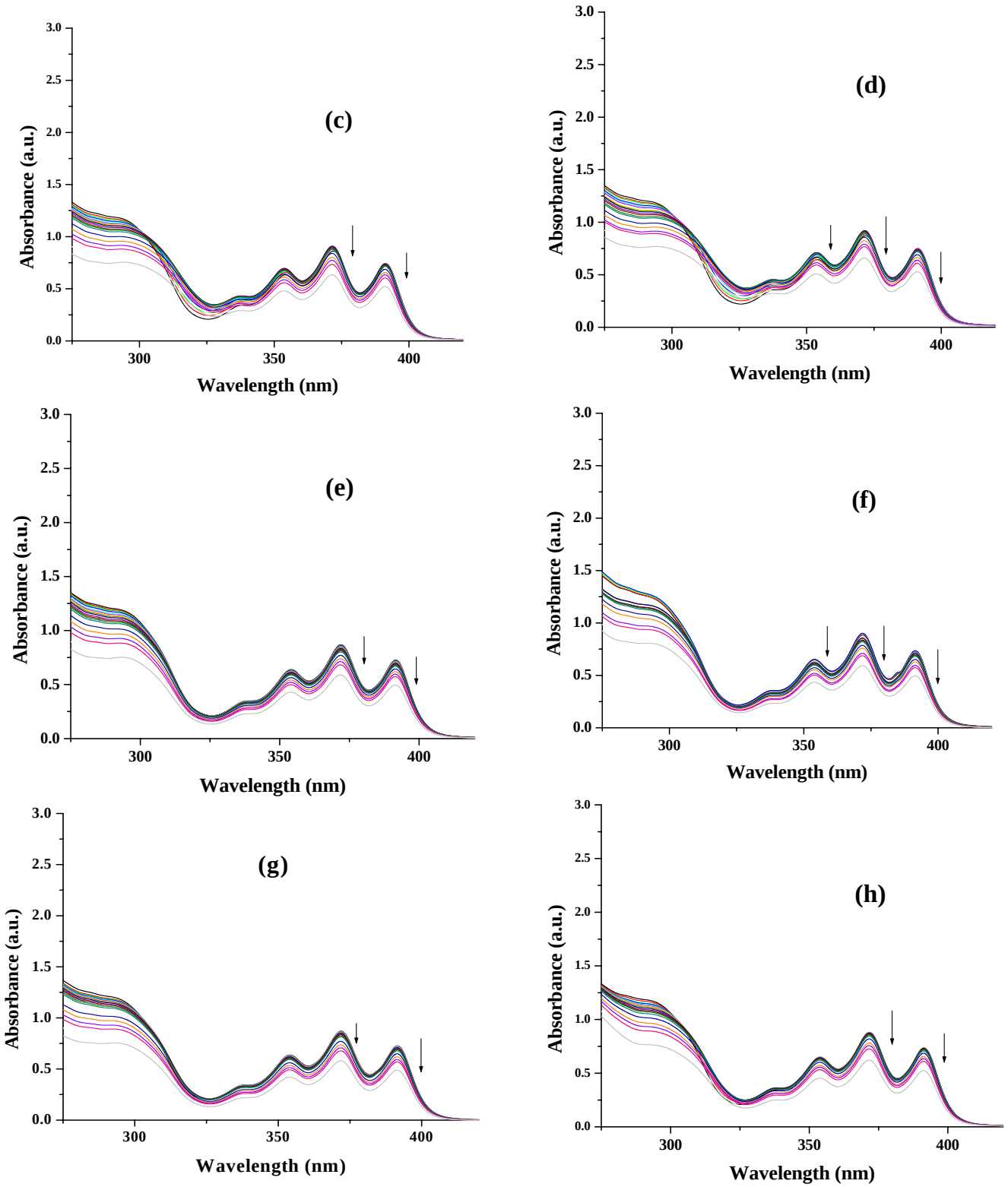

Figure S1d. UV-vis titration curve of receptor **2** (c = 5.65 x 10^{-5} M) with the tetrabutylammonium (a) $H_2PO_4^-$, (b) fluoride, (c) acetate, (d) propanoate, (e) salt of ibuprofen, (f) hydrogensulphate (g) chloride, (h) benzoate in CH_3CN (concentration of all guests c = 2.5 x 10^{-4} M, λ_{max} = 371 nm).

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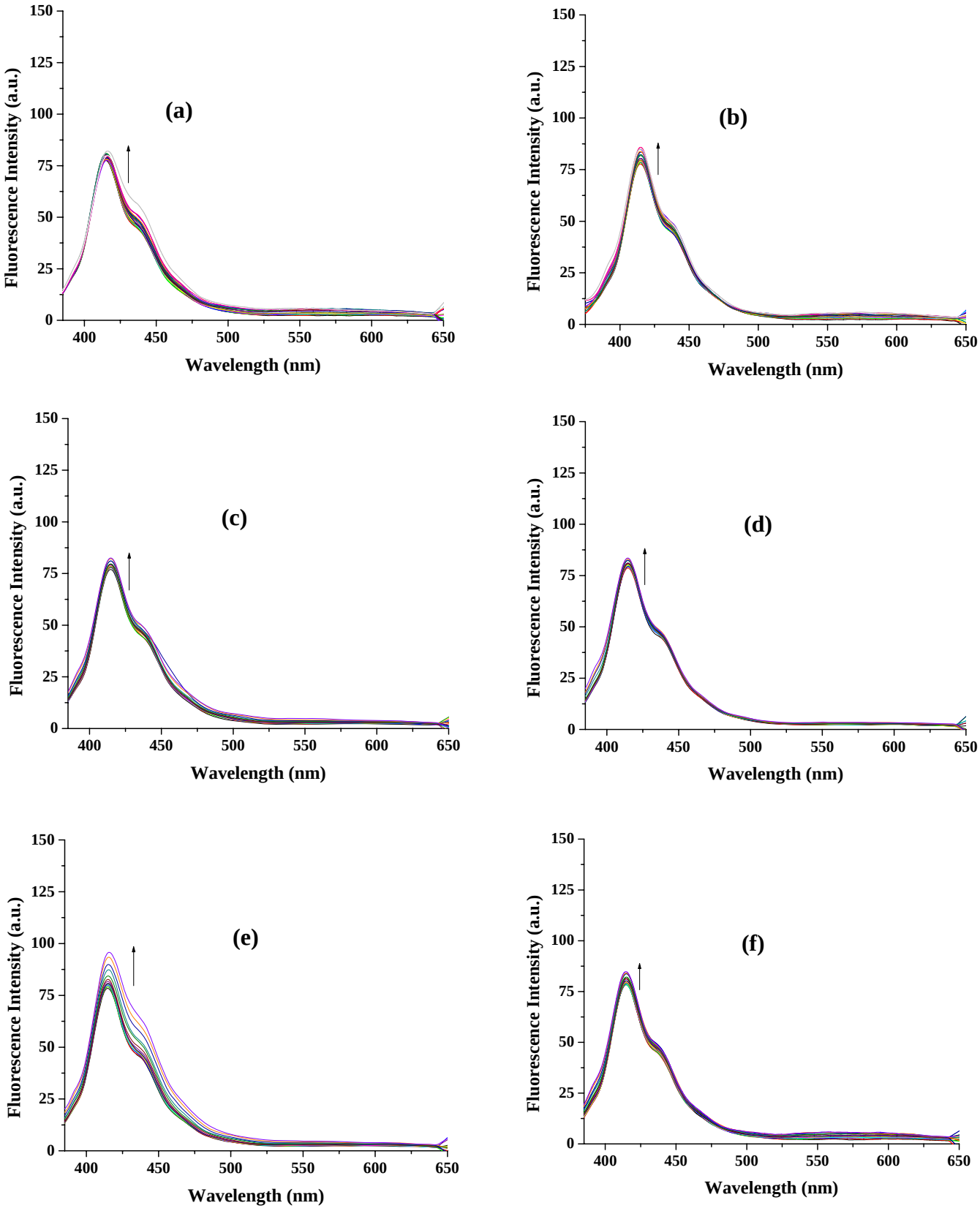
2e. Selected emission titration curves for receptor 3 in CH_3CN with following anions



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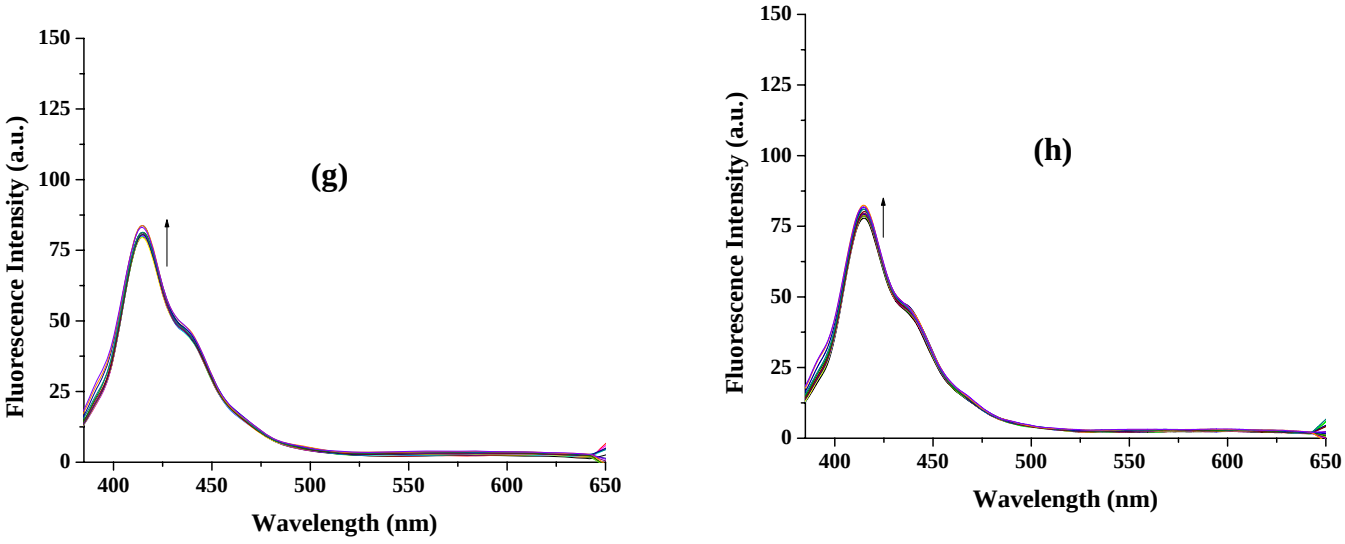
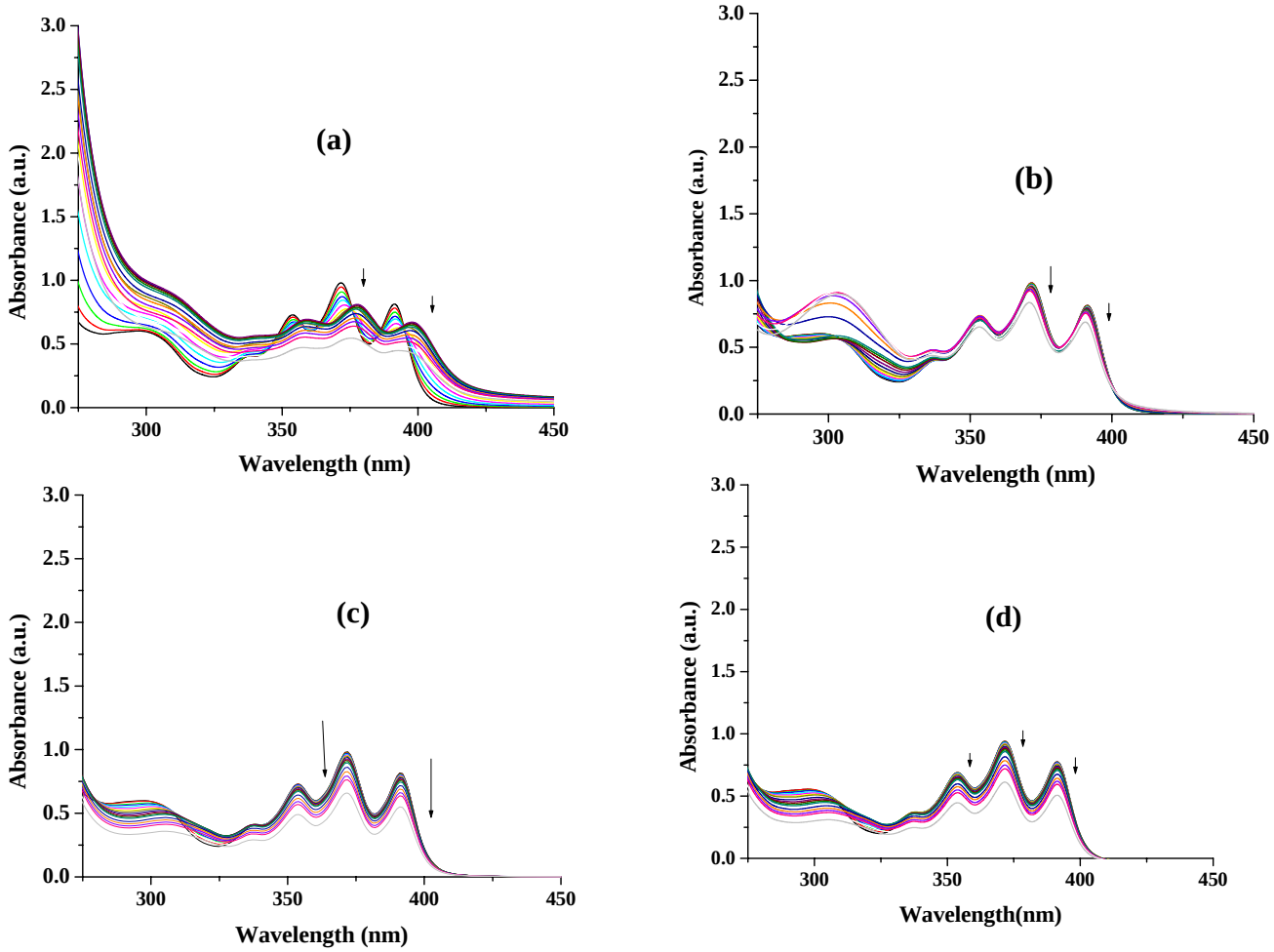


Figure S1e. Fluorescence titration curve of receptor **3** (c = 5.65 x 10^{-5} M) with the tetrabutylammonium (a) fluoride, (b) acetate, (c) propanoate, (d) hydrogensulphate, (e) salt of ibuprofen, (f) benzoate, (g) chloride, (h) bromide in CH_3CN(concentration of all guests c = 2.5 x 10^{-3} M, $\lambda_{Excitation}$ = 370 nm).

2f. Selected UV-vis titration curves for receptor 3 in CH_3CN:



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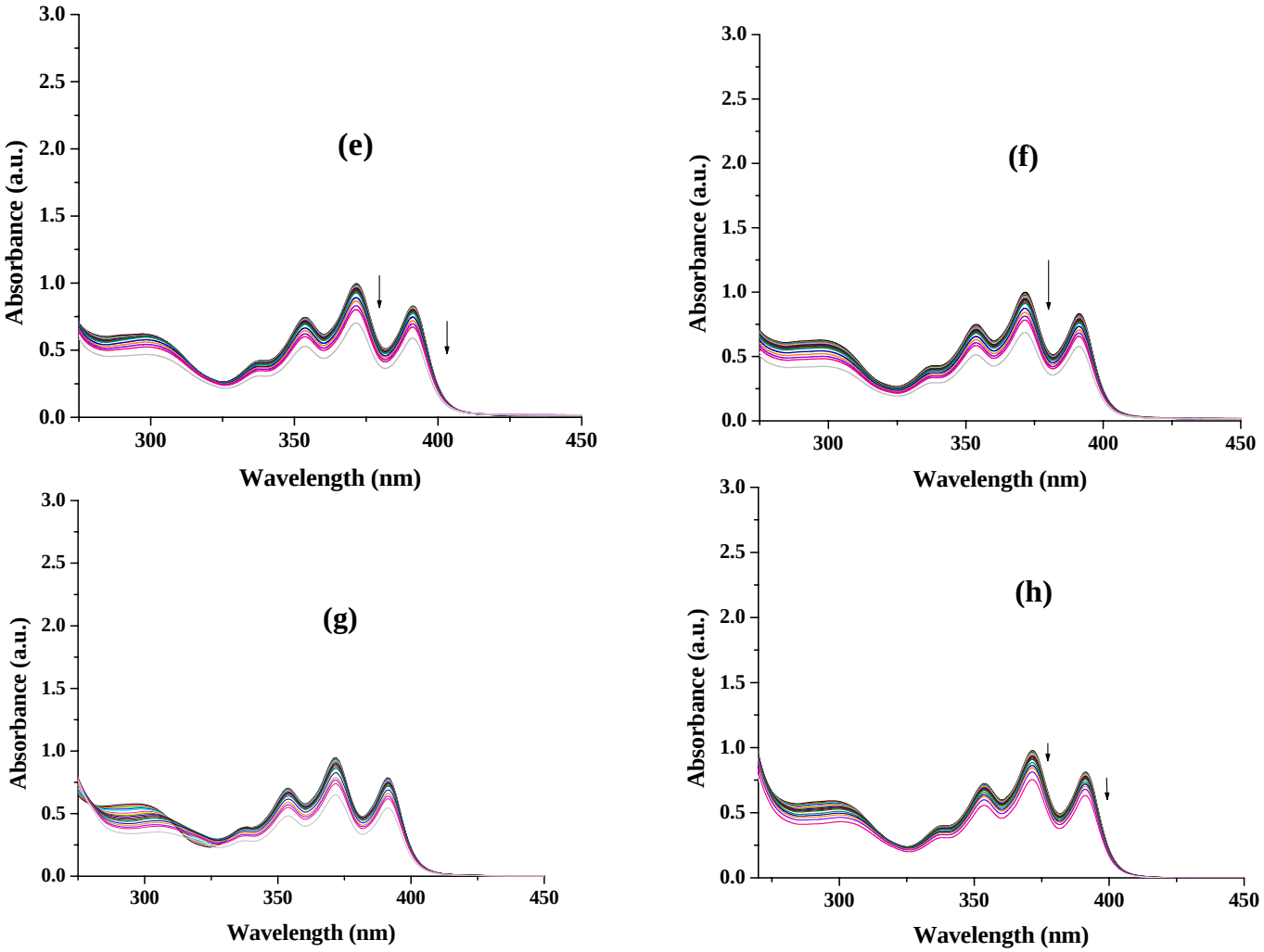
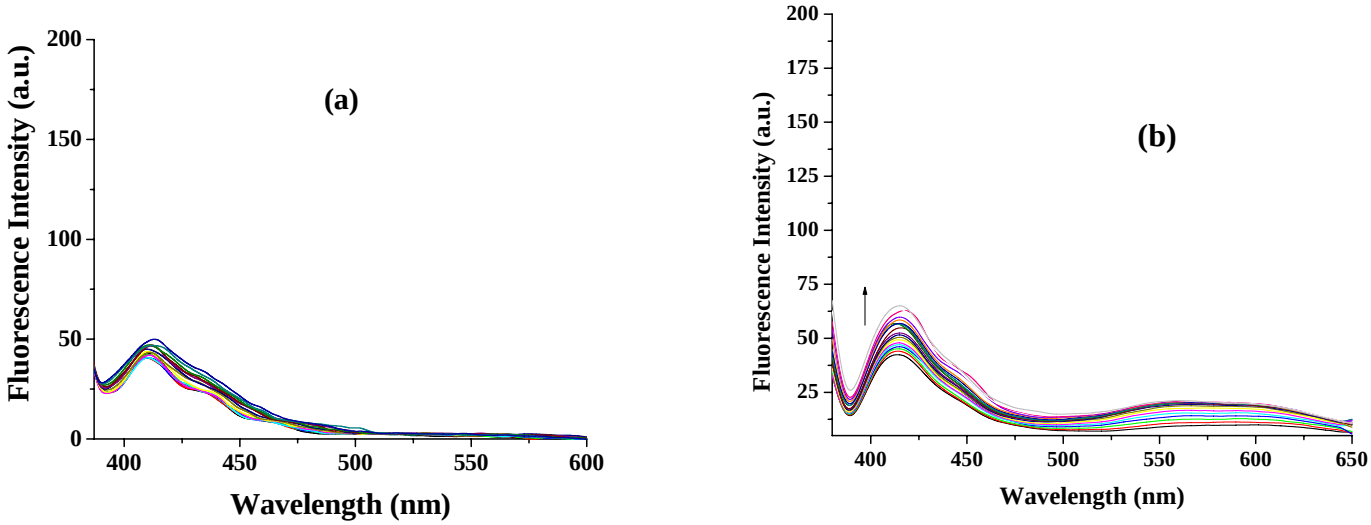


Figure S1f: UV-vis titration curve of receptor **3** (c = 5.65 x 10^{-5} M) with the tetrabutylammonium (a) $H_2PO_4^-$, (b) fluoride, (c) acetate, (d) propanoate, (e) salt of ibuprofen, (f) hydrogensulphate (g) chloride, (h) benzoate in CH_3CN(concentration of all guests c = 2.5 x 10^{-3} M, λ_{max} = 371 nm).

2g. Selected emission titration curves for receptor 4 in CH_3CN with following anions



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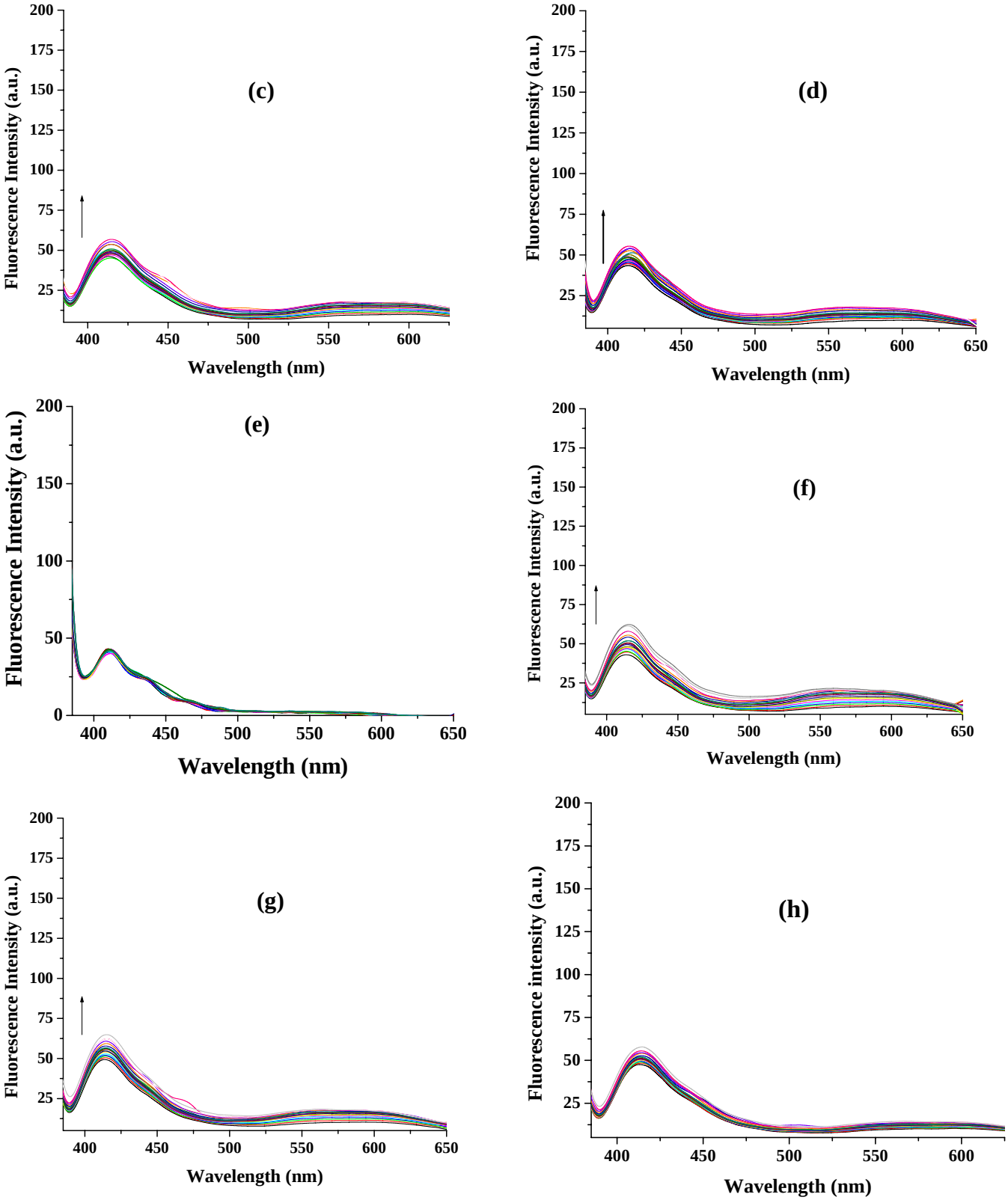

Figure S1g. Fluorescence titration curve of receptor **4** (c = 5.65 x 10^{-5} M) with the tetrabutylammonium (a) fluoride, (b) acetate, (c) propanoate, (d) hydrogensulphate, (e) salt of ibuprofen, (f) benzoate, (g) chloride, (h) bromide in CH_3CN(concentration of all guests c = 2.5 x 10^{-3} M, $\lambda_{Excitation}$ = 370 nm).

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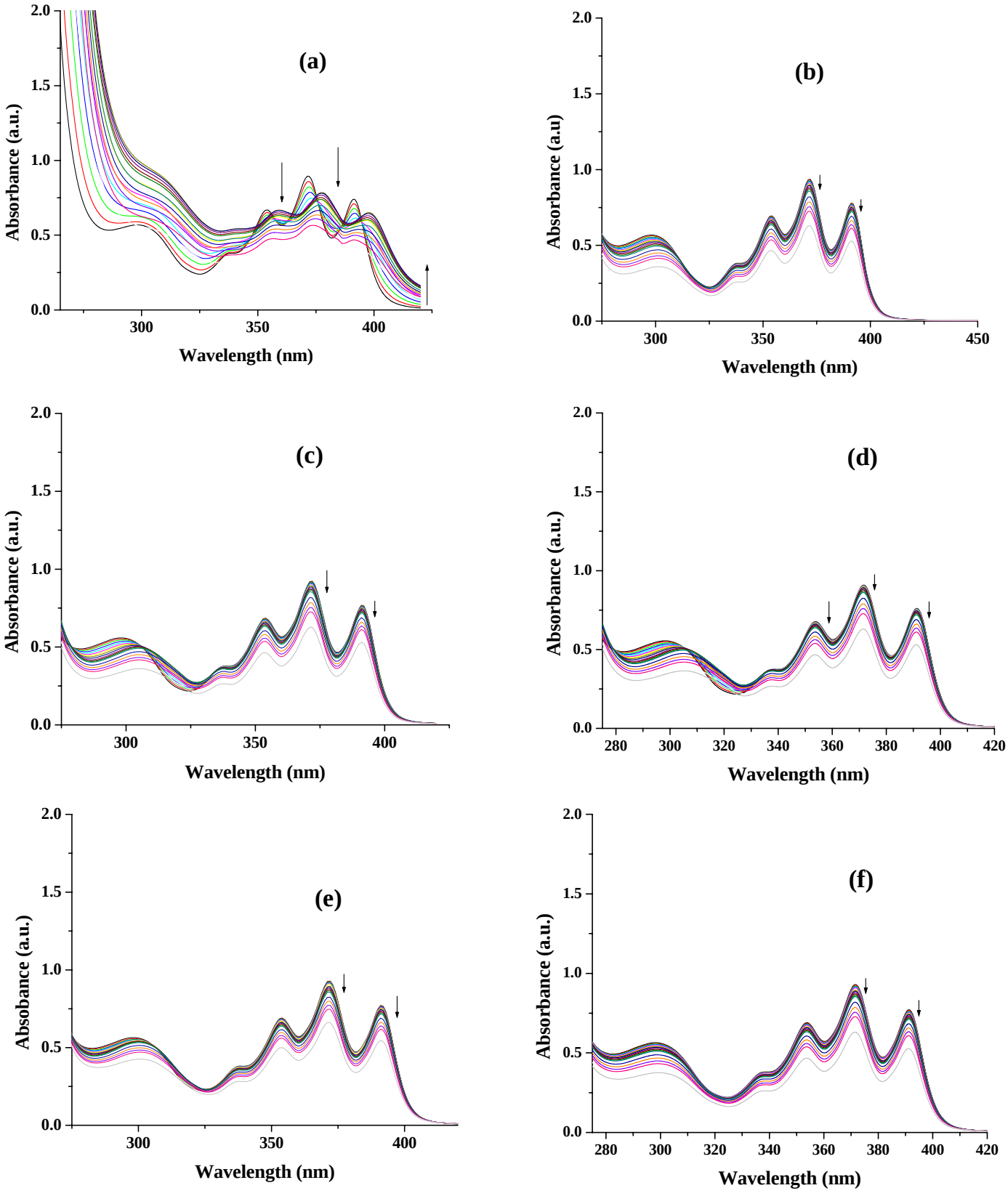
2h. Selected UV-vis titration curves for receptor 4 in CH_3CN:



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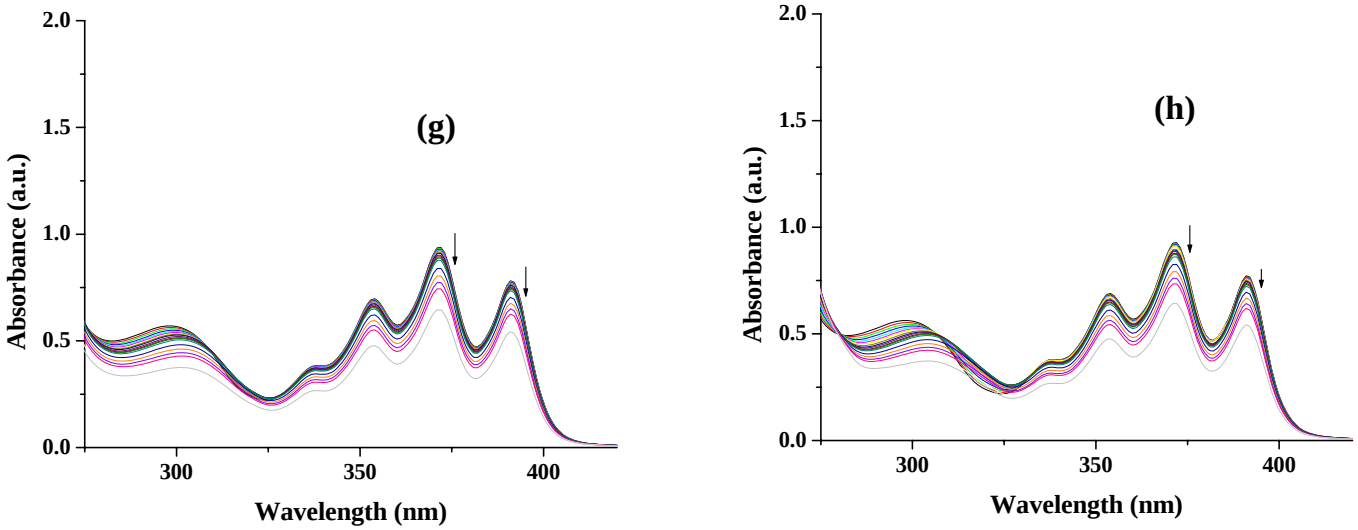

Figure S1h: UV-vis titration curve of receptor **3** (c = 5.65 x 10^{-5} M) with the tetrabutylammonium (a) $H_2PO_4^-$, (b) fluoride, (c) acetate, (d) propanoate, (e) salt of ibuprofen, (f) hydrogensulphate (g) chloride, (h) benzoate in CH_3CN (concentration of all guests c = 2.5 x 10^{-3} M, λ_{max} = 371 nm).

3a. Job plots from fluorescence of 1 and 2.

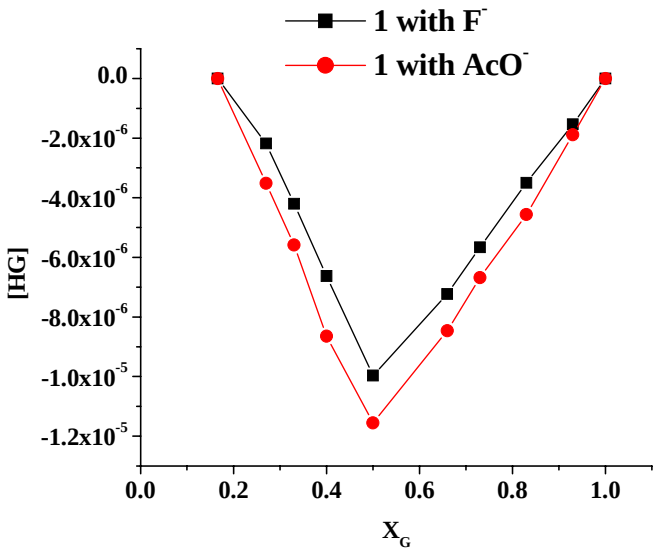

Figure S2a. Job plot of **1** (c = 5.65 x 10^{-5} M) with tetrabutylammonium F^- (c = 5.65 x 10^{-5} M) and AcO^- (c = 5.65 x 10^{-5} M) at 412 nm from fluorescence in CH_3CN at 25 ^{0}C

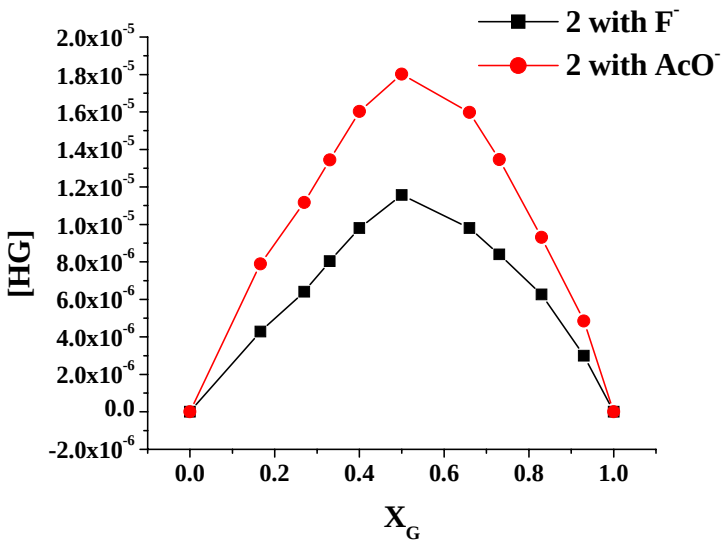

Figure S2b. Job plot of **2** (c = 5.65 x 10^{-5} M) with tetrabutylammonium F^- (c = 5.65 x 10^{-5} M) and AcO^- (c = 5.65 x 10^{-5} M) at 412 nm from fluorescence in CH_3CN at 25 ^{0}C

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3b. Job plots from UV-vis.

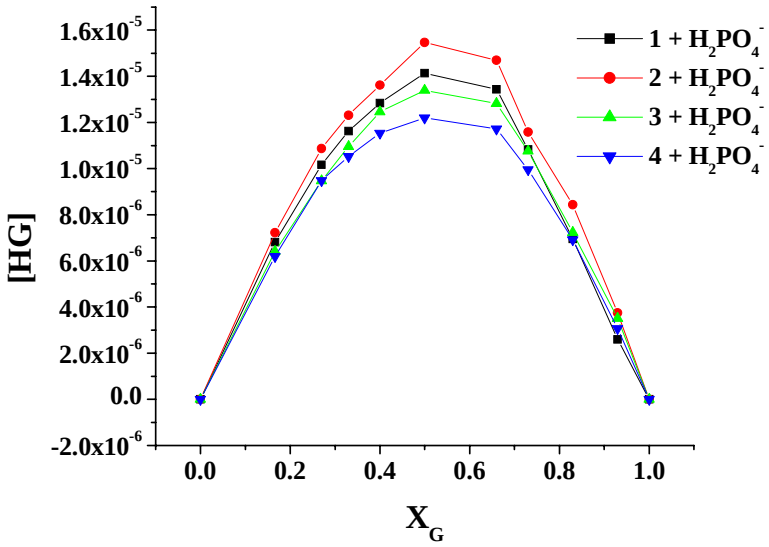

Figure S2c. Job plots of **1** to **4** with tetrabutylammonium $H_2PO_4^-$ at 371 nm from UV-vis in CH_3CN ([G] = [H] = 5.65 x 10^{-5} M).

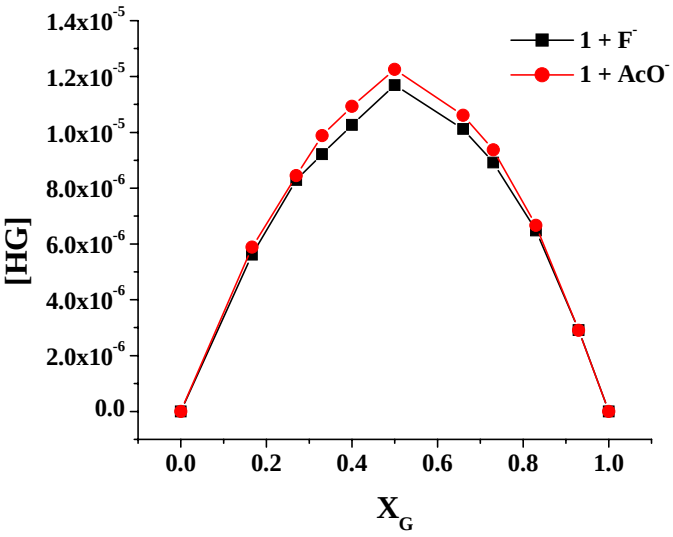

Figure S2d. Job plot of **1** (c = 5.65 x 10^{-5} M) with tetrabutylammonium F^- (c = 5.65 x 10^{-5} M) and AcO^- (c = 5.65 x 10^{-5} M) at 371 nm from UV-vis in CH_3CN.

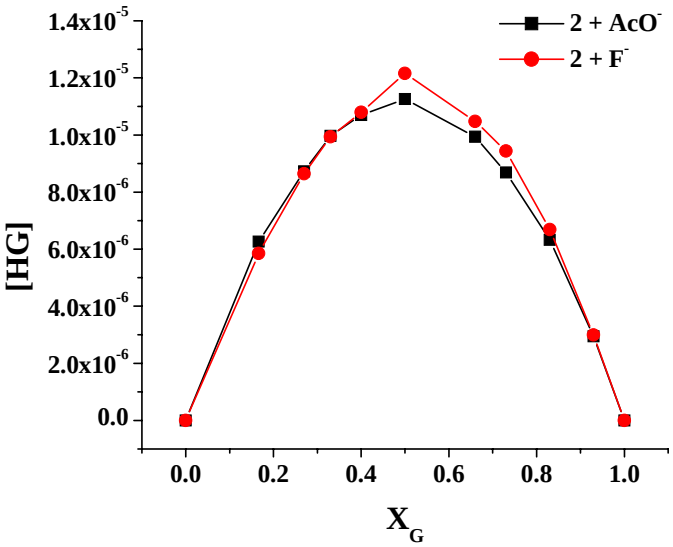

Figure S2e. Job plot of **2** (c = 5.65 x 10^{-5} M) with tetrabutylammonium F^- (c = 5.65 x 10^{-5} M) and AcO^- (c = 5.65 x 10^{-5} M) at 371 nm from UV-vis in CH_3CN.

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4a. Binding constant curves for receptor 1-4 with tetrabutylammonium dihydrogenphosphate from fluorescence in CH_3CN:

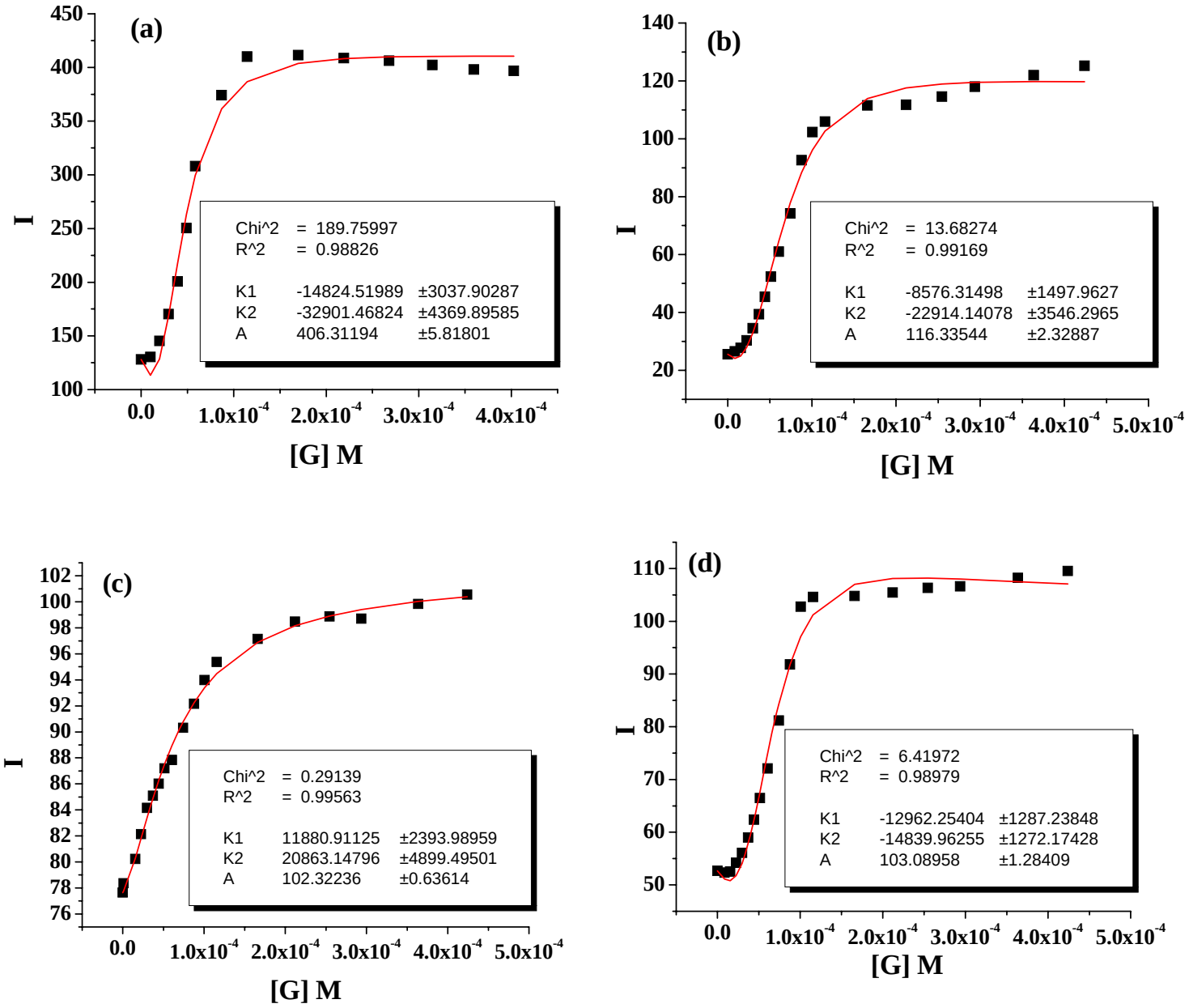

Figure S3a: Binding constant curves of receptor (a) **1,** (b) **2,** (c) **3** and (d) **4** with the tetrabutylammonium $H_2PO_4^-$ from fluorescence titration in CH_3CN. Working formula
$I = (I_0 + K_1 \times C_G \times I_{[1:1]} + K_1 \times K_2 \times I_{lim} \times C_G^2) / (1 + K1x\ C_G + K_1 \times K_2 \times C_G^2)$ where I_0 = intensity of receptor solution, I = intensity after successive addition of guest into the receptor solution, $I_{(1:1)}$ = intensity at 1:1, I_{lim} = represent the intensity at infinite guest concentration C_G = [G].(λ_{max} = 412 nm, [H] = 5.65 x 10^{-5} M and [G] = 2.5 x 10^{-3} M).

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4b.Binding constant curves for receptor 1 and 2 with F^- and AcO^- from fluorescence in CH_3CN:

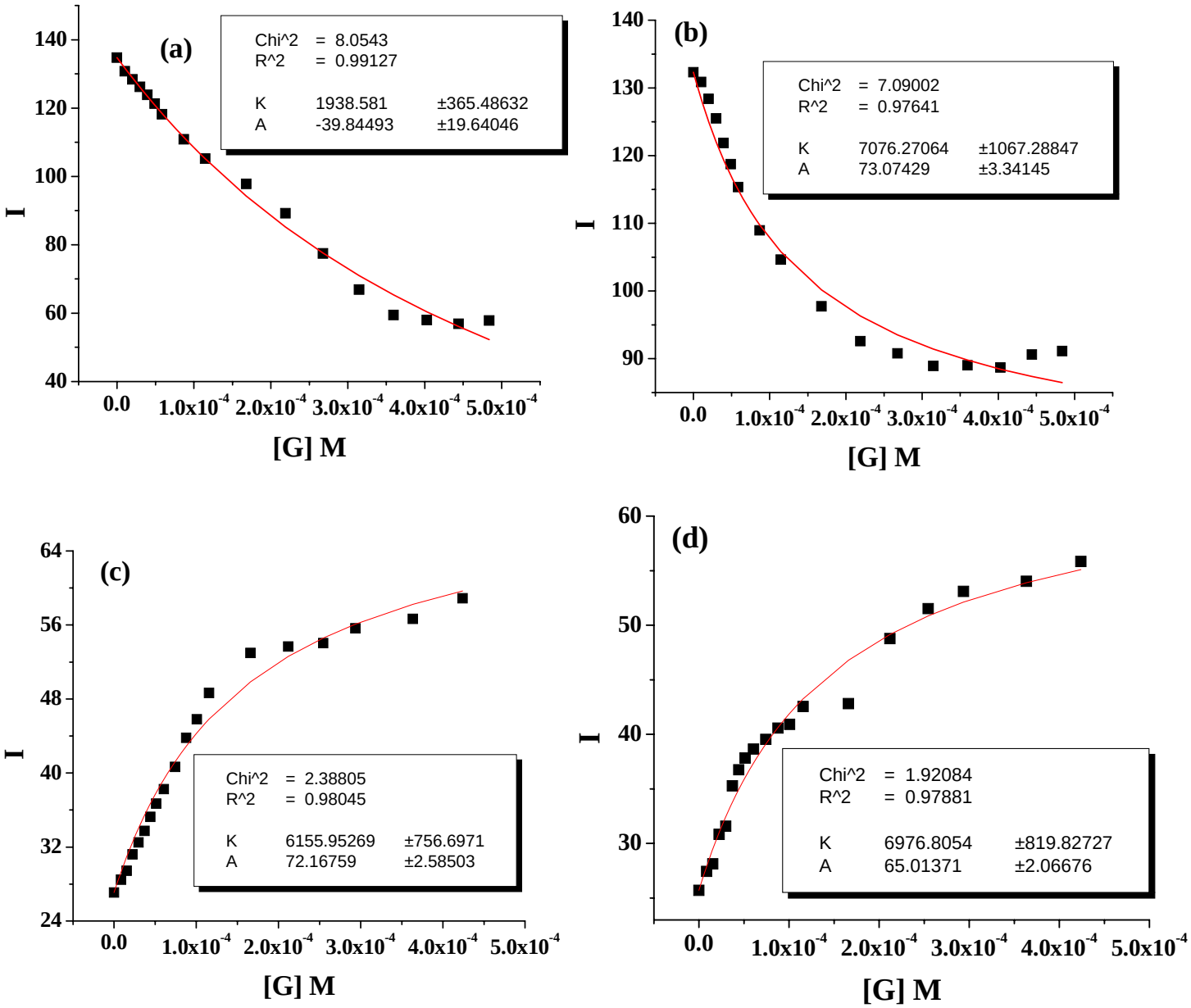

Figure S3b: Binding constant curves of receptor (a) **1,** (b) **2,** (c) **3** and (d) **4** with the tetrabutylammonium dihydrogenphosphate from UV-vis titration in CH_3CN.Working formula
$I = I_0 + (I-I_0) / (2 \times C_H) \{(C_G + C_H + 1/K - [(C_G + C_H + 1/K)^2 - 4 \times C_G \times C_H]^{0.5}\}$, where I_0 = emission intensity of receptor, I = emission intensity after succive addition of guest, C_G = [G], C_H = [H]. (λ_{max} = 371 nm, [H] = 5.65 x 10^{-5} M and [G] = 2.5 x 10^{-3} M).

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4c. Binding constant curves for receptor 1-4 with tetrabutylammonium dihydrogenphosphate from UV-vis in CH_3CN:

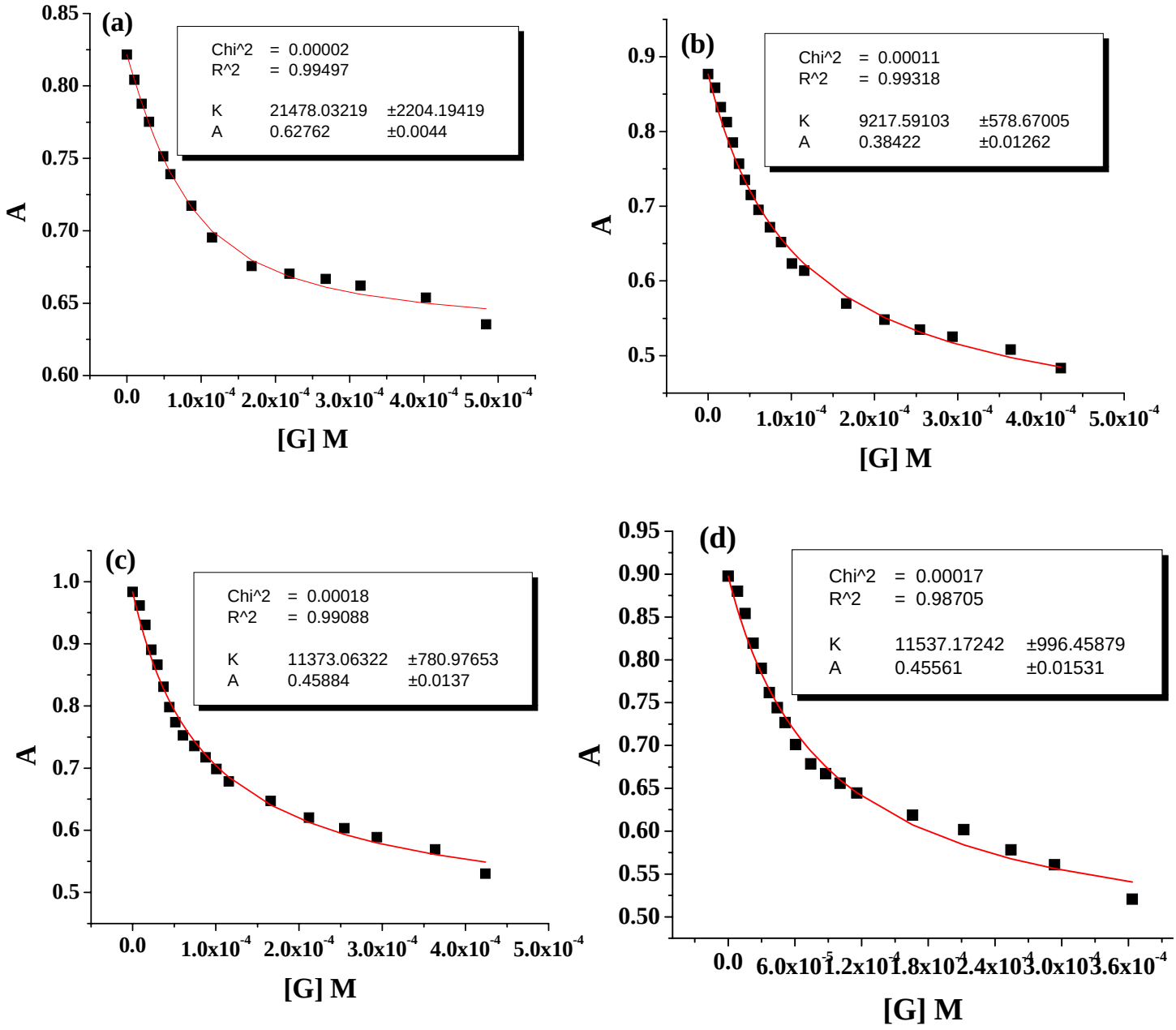

Figure S3c: Binding constant curves of receptor **1** with (a) fluoride**,** (b) acetate and receptor **2** with (c) fluoride and (d) acetate from fluorescence titration in CH_3CN. Working formula
$A = A_0 + (A - A_0) / 2 \times C_H \times \{C_G + C_H + 1/K - [(C_G + C_H + 1/K)^2 - 4 \times C_G \times C_H]^{0.5}\}$ where A_0 = absorption of receptor, A = absorption after succive addition of guest, C_G = [G], C_H = [H]. (λ_{max} = 412 nm, [H] = 5.65 x 10^{-5} M and [G] = 2.5 x 10^{-3} M).

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5. Reversibility experiment of receptor 2 -4 for $H_2PO_4^-$ in CH_3CN from fluorescence.

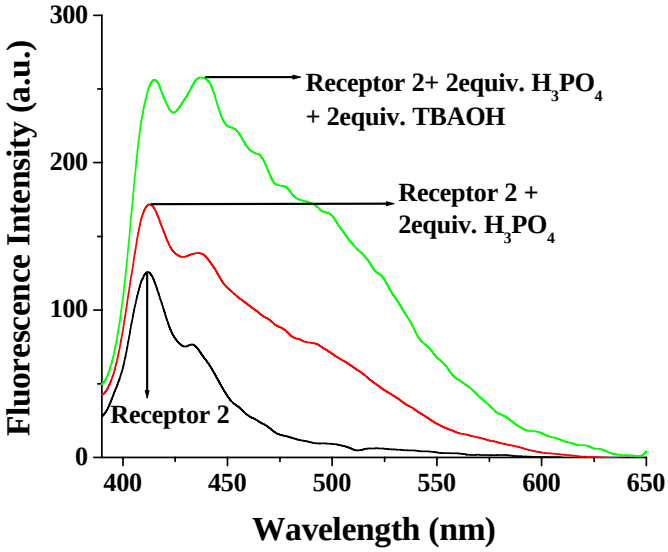

Figure S4a. Emission profile for sensitivity of $H_2PO_4^-$ over H_3PO_4 receptor **2** and the reversibility in the process.

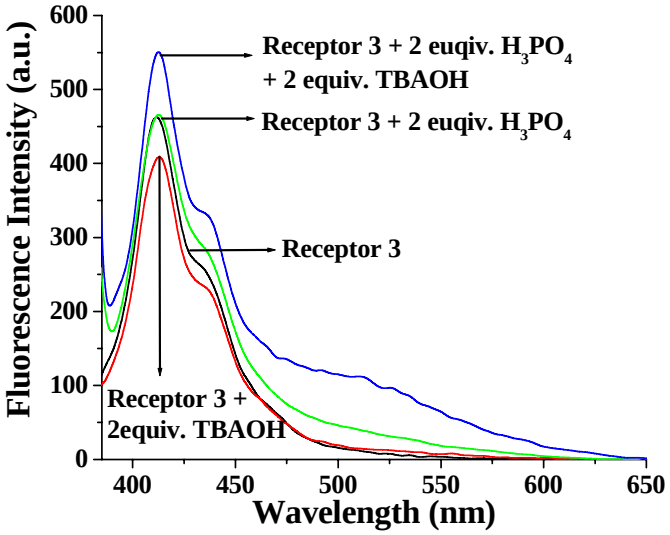

Figure S4b. Emission profile for sensitivity of $H_2PO_4^-$ over H_3PO_4 receptor **3** and the reversibility in the process.

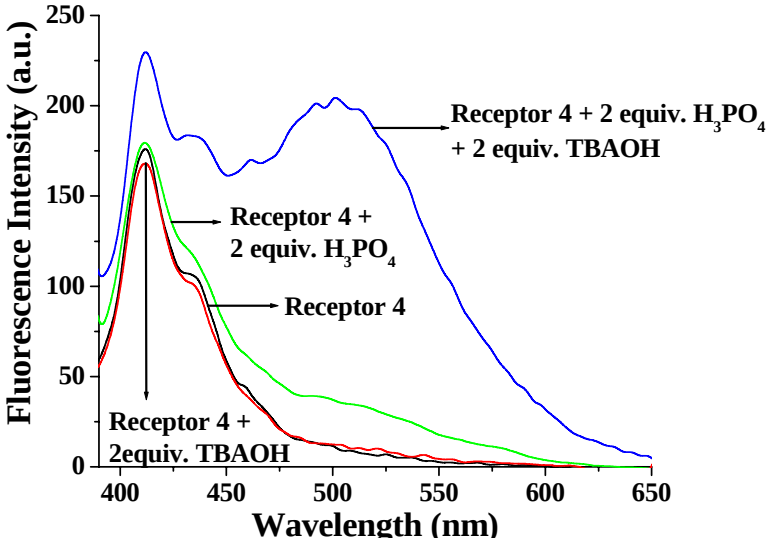

Figure S4c. Emission profile for sensitivity of $H_2PO_4^-$ over H_3PO_4 receptor **4** and the reversibility in the process.

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6a. Emission titration curves for receptor 3 in CH_3CN with dicarboxylate.

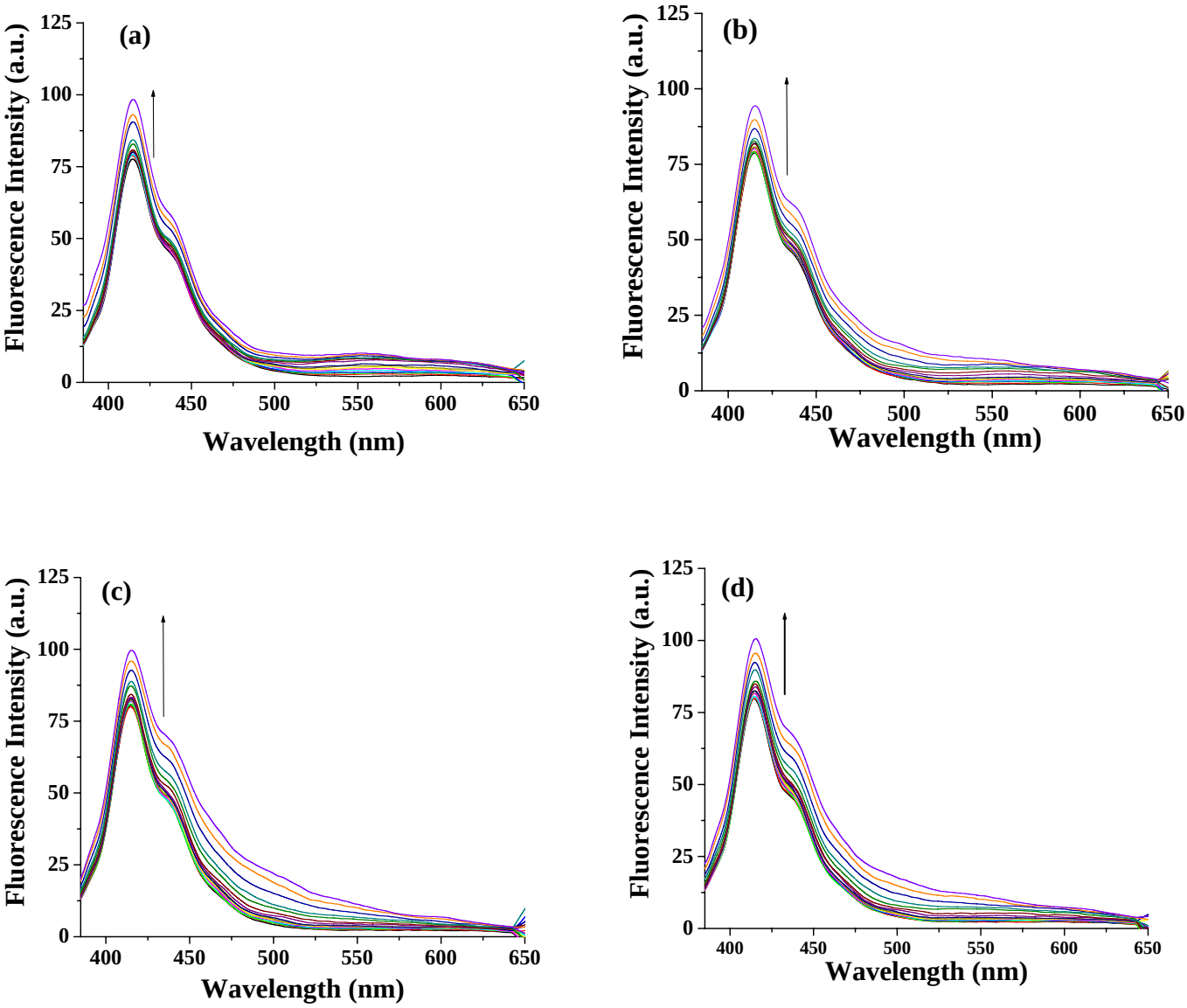

Figure S5a. Fluorescence titration curve of receptor **3** (c = 5.65 x 10^{-5} M) with the tetrabutylammonium (a) Adipate, (b) Glutarate, (c) Malonate and (d) Succinate in CH_3CN (concentration of all guests c = 2.5 x 10^{-3} M, λ_{max} = 412 nm).

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6b. Emission titration curves for receptor 4 with dicarboxylate in CH_3CN.

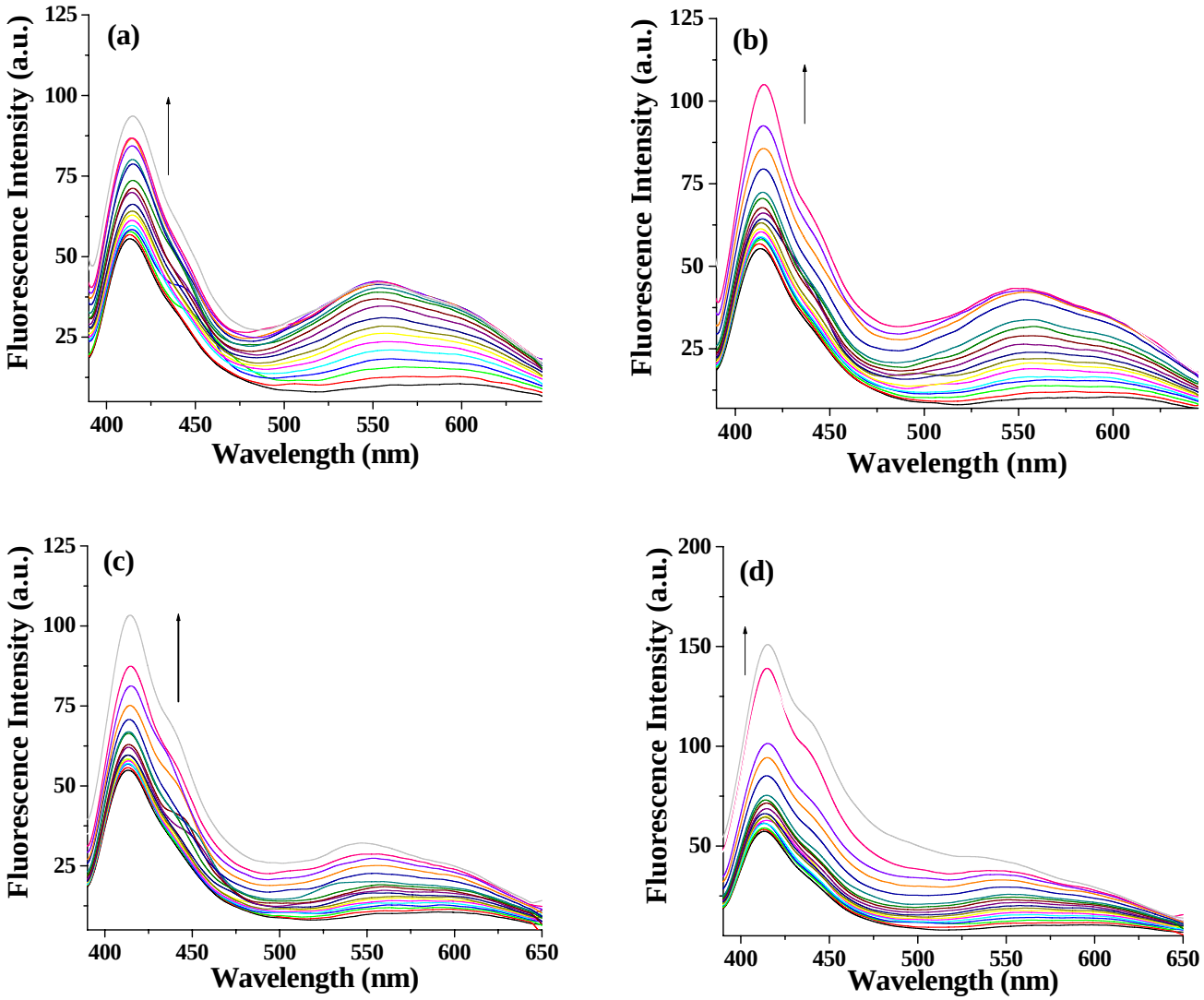

Figure S5b. Fluorescence titration curve of receptor **4** (c = 5.65 x 10^{-5} M) with the tetrabutylammonium (a) Adipate, (b) Glutarate, (c) Malonate and (d) Succinate in CH_3CN (concentration of all guests c = 2.5 x 10^{-3} M, λ_{max} = 412 nm).

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6c. UV-vis titration curves for receptor 3 with dicarboxylate in CH_3CN.

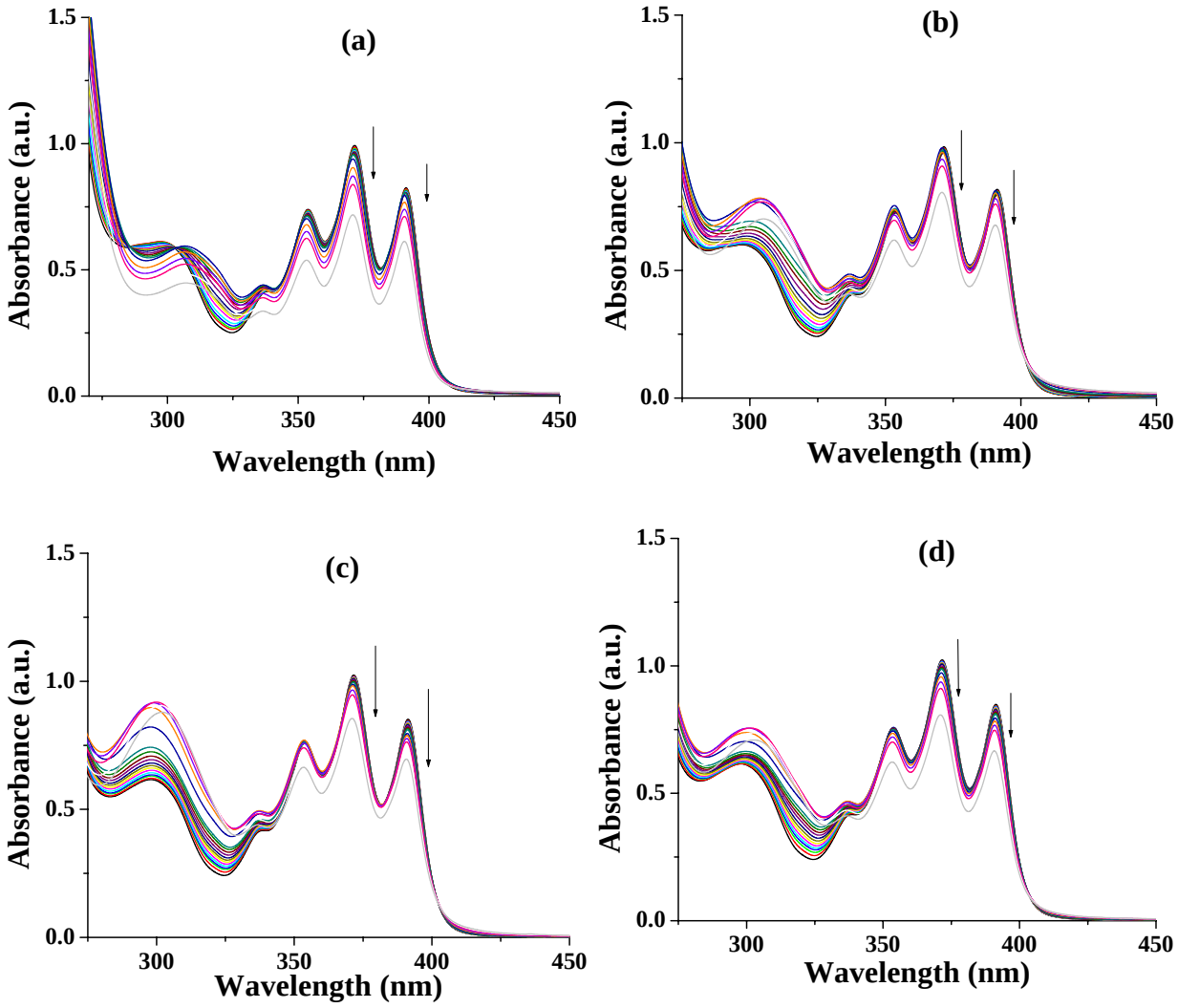

Figure S5c: UV-vis titration curve of receptor **3** (c = 5.65 x 10^{-5} M) with the tetrabutylammonium (a) Adipate, (b) Glutarate, (c) Malonate and (d) Succinate in CH_3CN (concentration of all guests c = 2.5 x 10^{-3} M, λ_{max} = 371 nm).

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6d.UV-vis titration curves for receptor 4 with dicarboxylate in CH_3CN.

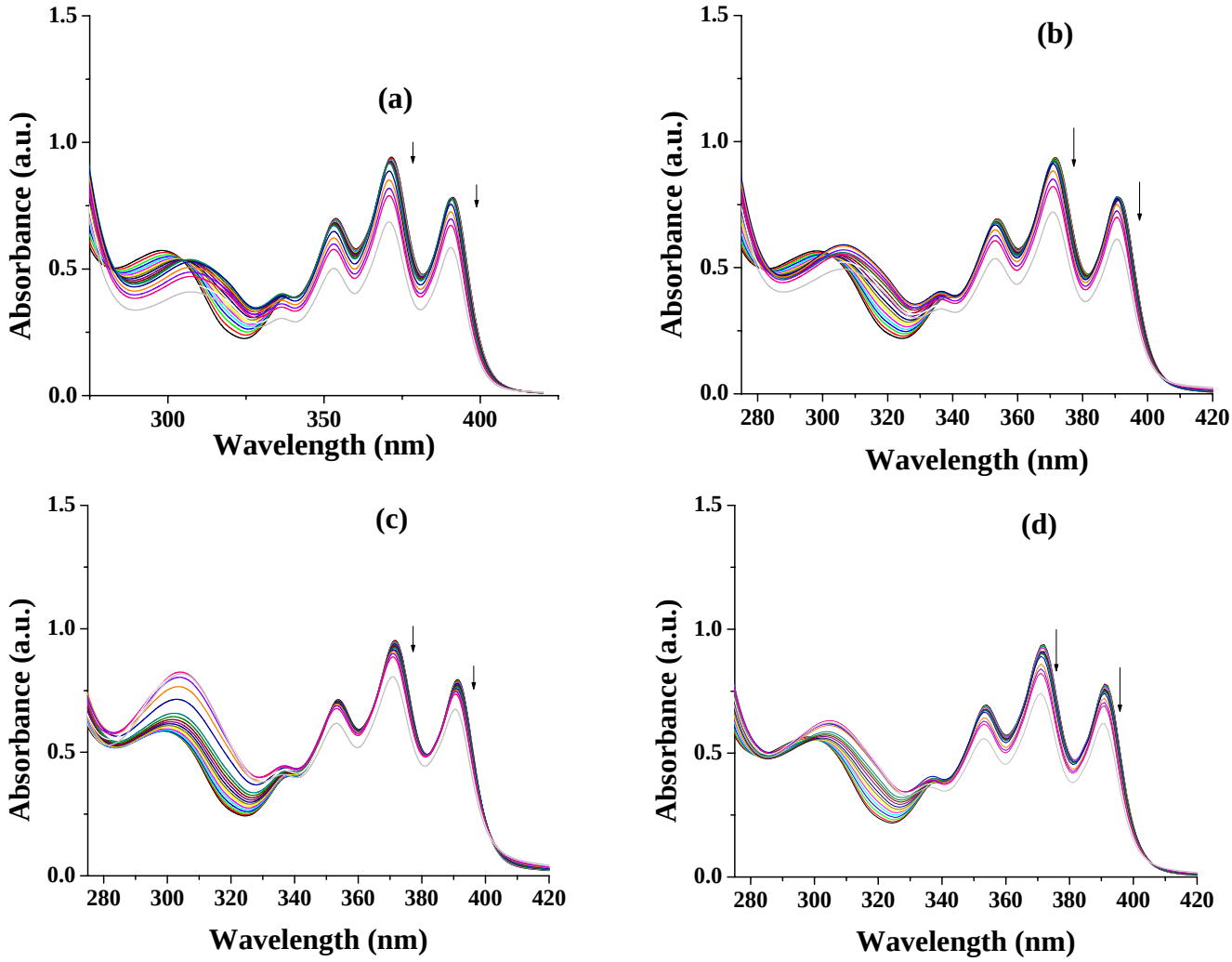

Figure S5d. UV-vis titration curve of receptor **4** (c = 5.65 x 10^{-5} M) with the tetrabutylammonium (a) Adipate, (b) Glutarate, (c) Malonate and (d) Succinate in CH_3CN (concentration of all guests c = 2.5 x 10^{-3} M, λ_{max} = 371 nm).

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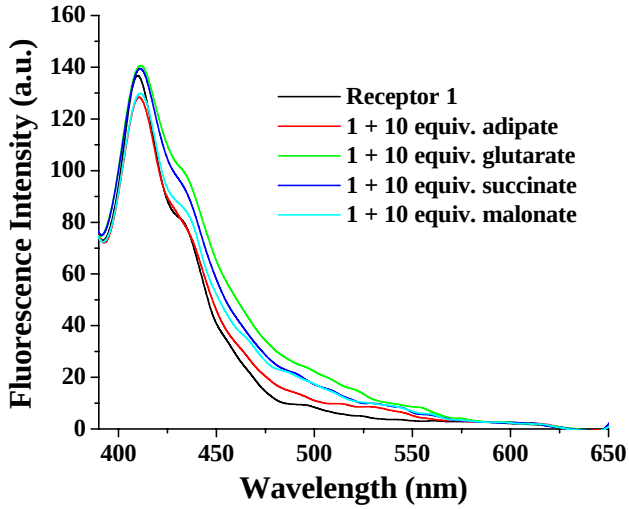

Figure S5e: Fluorescence emission change of **1** (c = 5.65 x 10^{-5}M) with addition of 10 equiv. amounts of tetrabutylammonium (a) adipate, (b) glutarate (c) succinate and (d) malonate CH_3CN.$\lambda_{Excitation}$ = 370 nm.

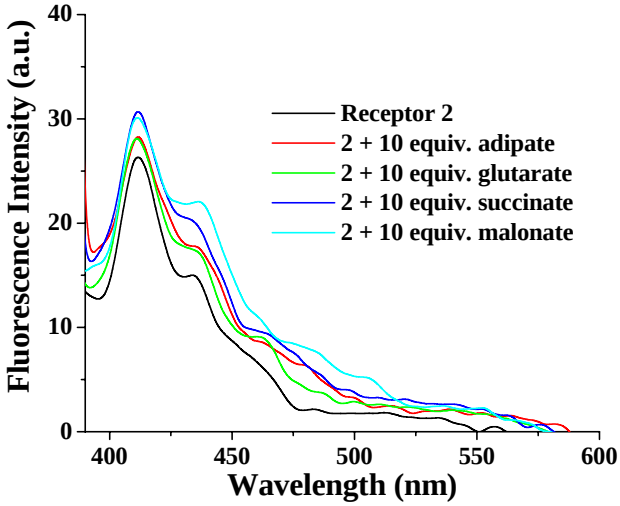

Figure S5f: Fluorescence emission change of **2** (c = 5.65 x 10^{-5}M) with addition of 10 equiv. amounts of tetrabutylammonium (a) adipate, (b) glutarate (c) succinate and (d) malonate CH_3CN.$\lambda_{Excitation}$ = 370 nm.

7. Change in absorption with guest to host ration for receptor 1 - 4 with various anions at 371 nm in CH_3CN.

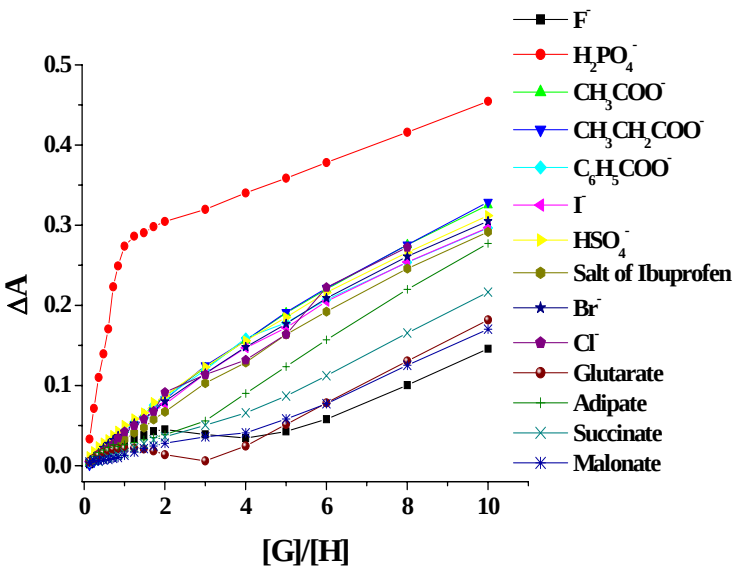

Figure S6a. UV-vis titration curves ([Guest]/[Host] vs change in absorbance) for **3** (measured at 371 nm) with various anions.

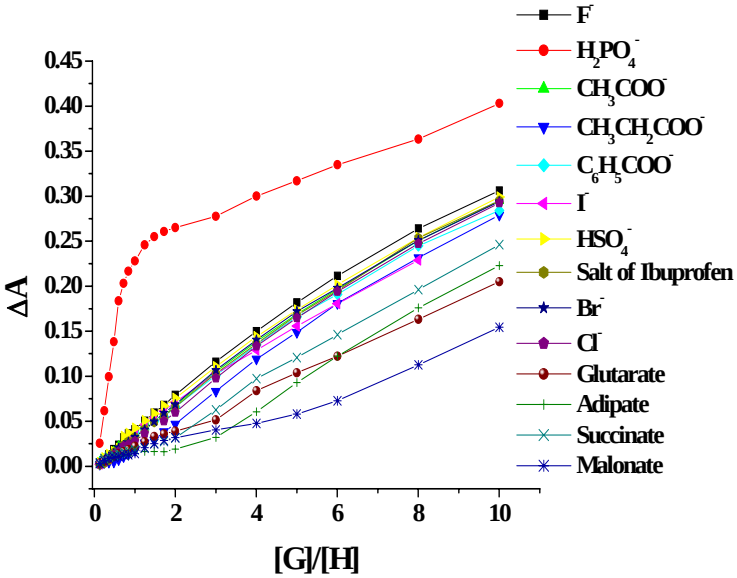

Figure S6b. UV-vis titration curves ([Guest]/[Host] vs change in absorbance) for **4** (measured at 371 nm) with various anions.

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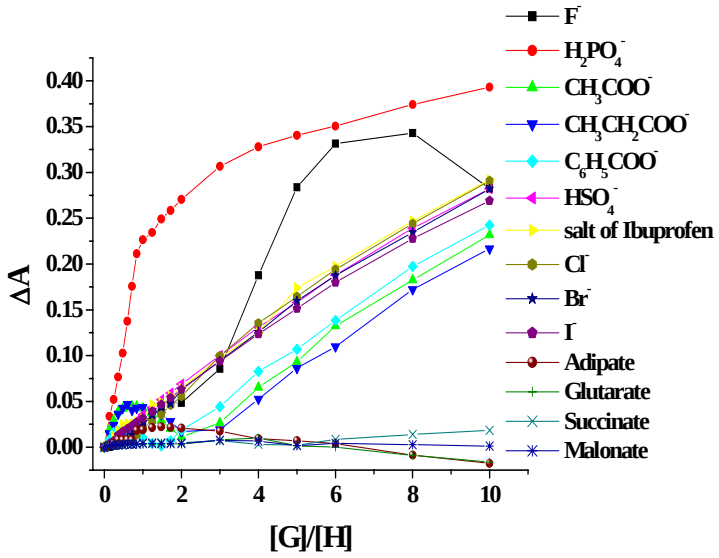

Figure S6c: UV-vis titration curves ([Guest]/[Host] vs change in absorbance) for **2** (measured at 371 nm) with various anions.

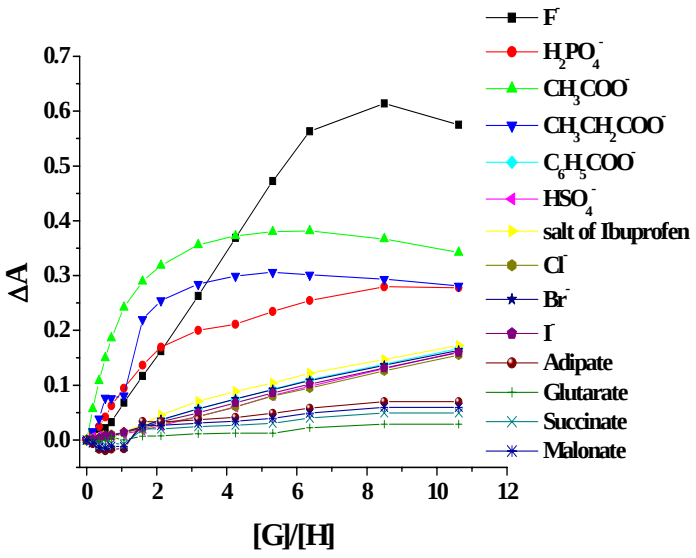

Figure S6d: UV-vis titration curves ([Guest]/[Host] vs change in absorbance) for **1** (measured at 371 nm) with various anions.

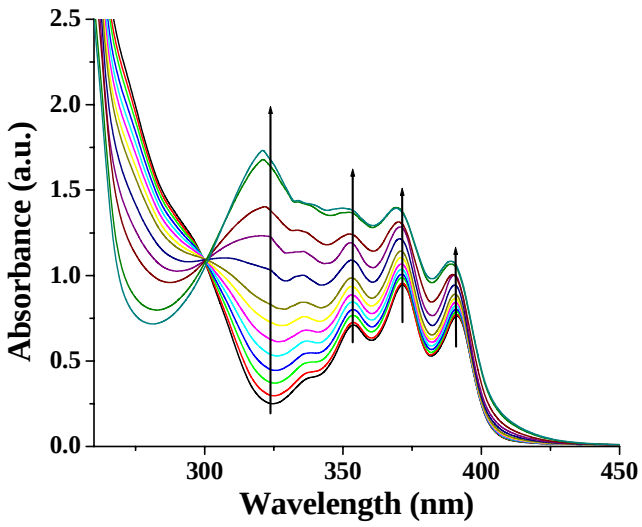

Figure S6e: UV-vis titration curve of receptor **1** (c = 5.65 x 10^{-5} M) with the tetrabutylammonium hydroxide (TBAOH) in CH_3CN (concentration of guest c = 2.5 x 10^{-3} M, λ_{max} = 371 nm).

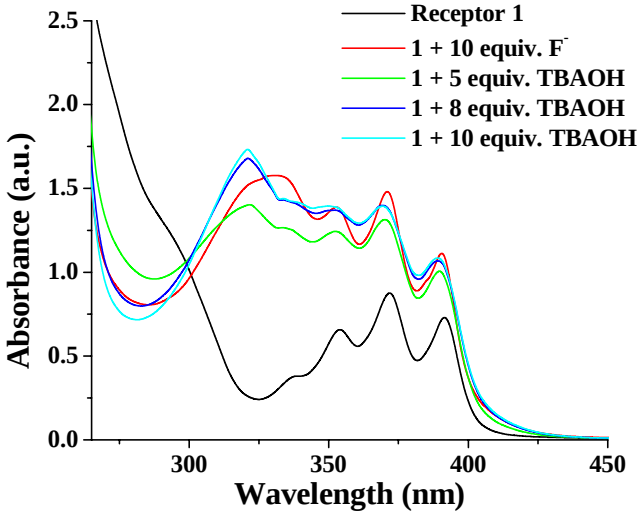

Figure S6f: Effect of addition of TBA OH and TBA F on UV-vis spectrum of receptor **1**.

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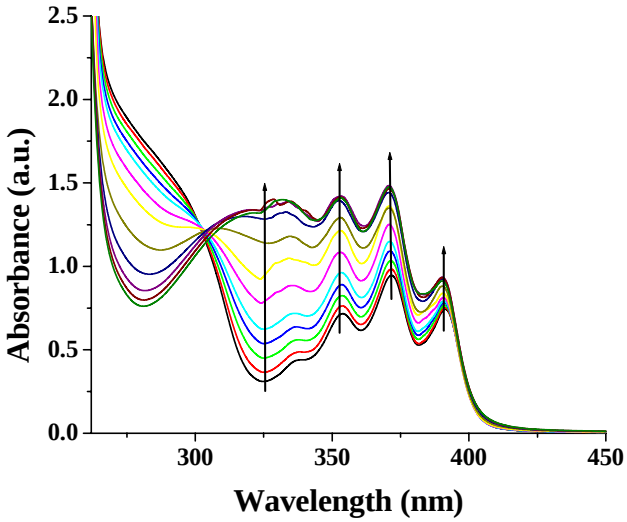


Figure S6g: UV-vis titration curve of receptor **2** (c = 5.65 x 10^{-5} M) with the tetrabutylammonium hydroxide (TBAOH) in CH_3CN (concentration of guest c = 2.5 x 10^{-3} M, λ_{max} = 371 nm).

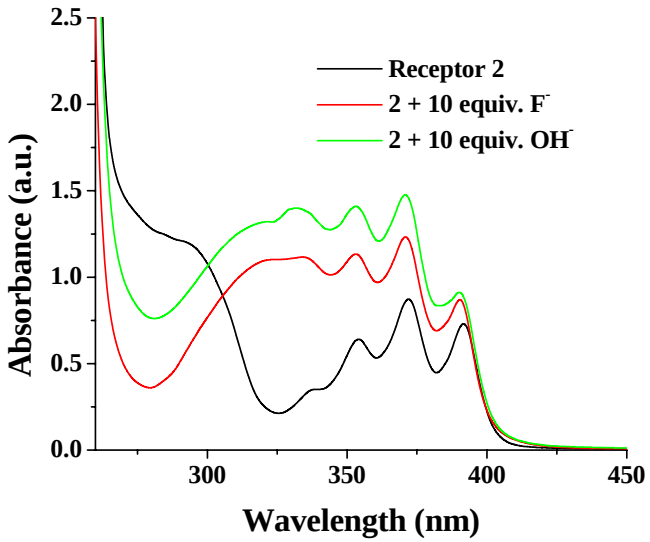
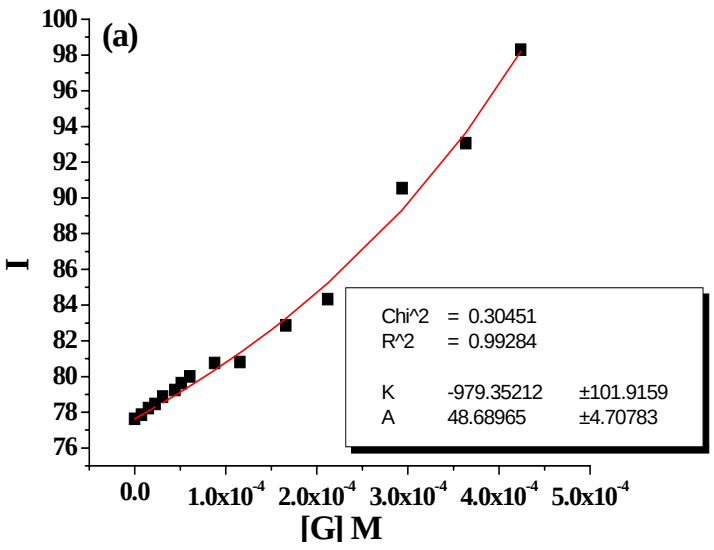
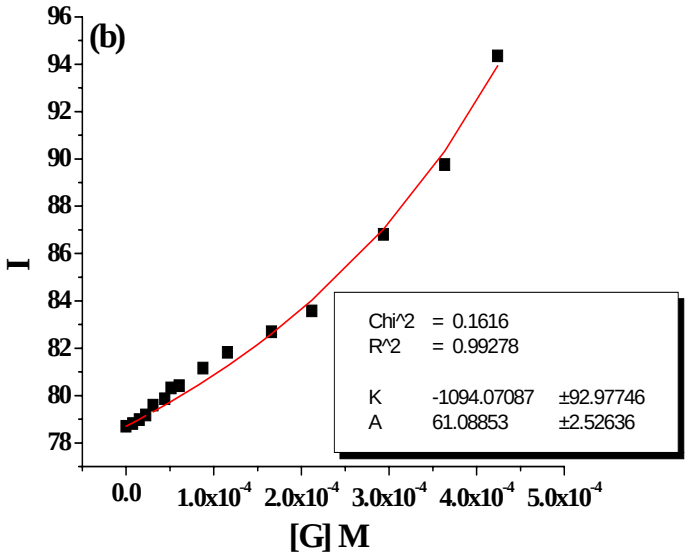


Figure S6h: Effect of addition of TBA OH and TBA F on UV-vis spectrum of receptor **2**.

8a. Binding constant curves for receptor 3 with dicarboxylates from fluorescence in CH_3CN:





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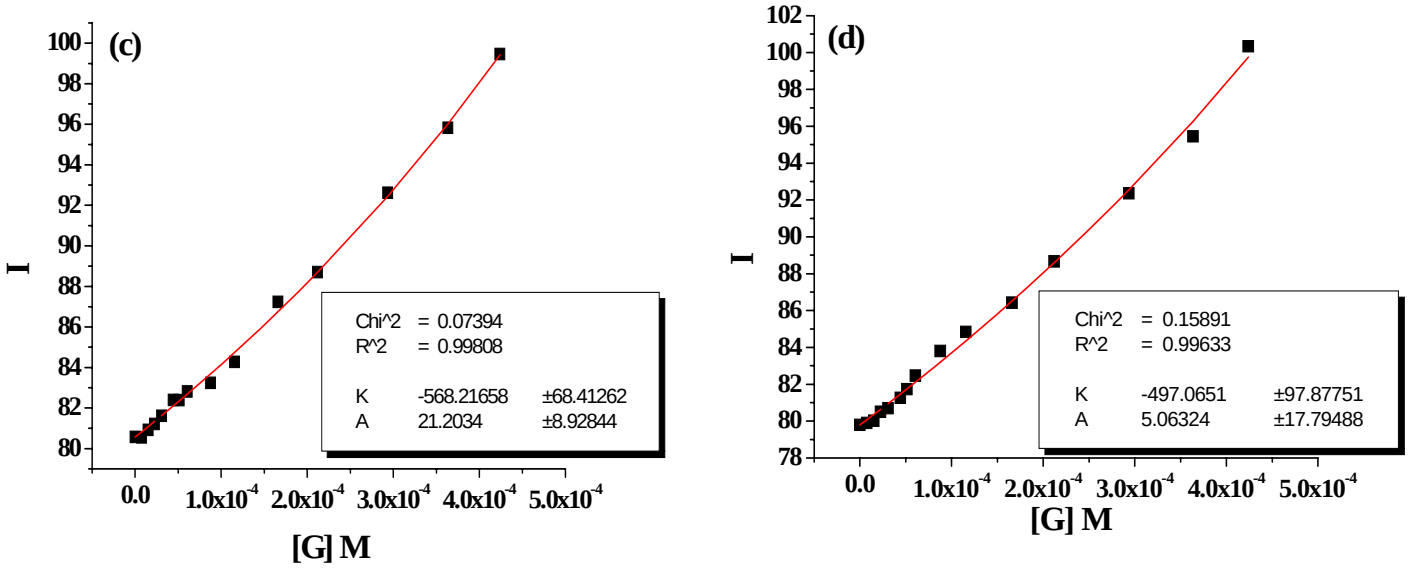
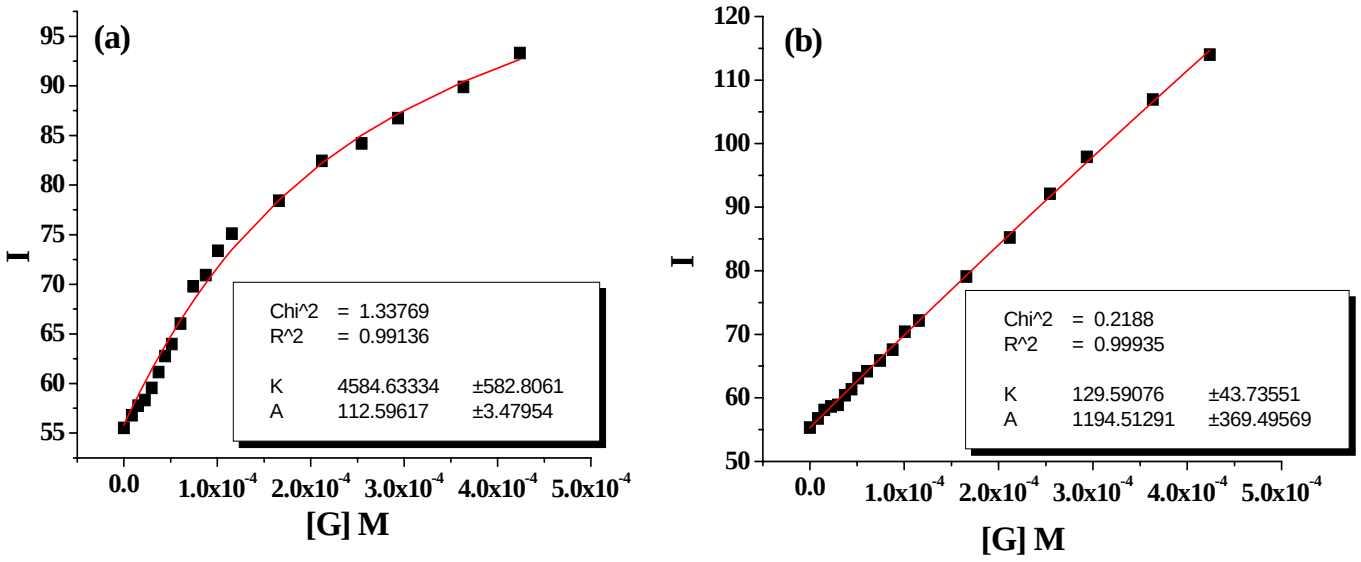


Figure S7a: Binding constant curves of receptor **3** with tetrabutylammonium salt of (a) Adipate**,** (b) Glutarate, (c) Malonate and (d) Succinate from fluorescence titration in CH_3CN. Working formula
$I= (I_0+I \times K \times C_G)/ (1+K \times C_G)$, I_0 = initial intensity, I = intensity after successive addition of guest. C_G = [G]. (λ_{max} = 412 nm, [H] = 5.65 x 10^{-5} M and [G] = 2.5 x 10^{-3} M).

8b. Binding constant curves for receptor 4 with dicarboxylates from fluorescence in CH_3CN:



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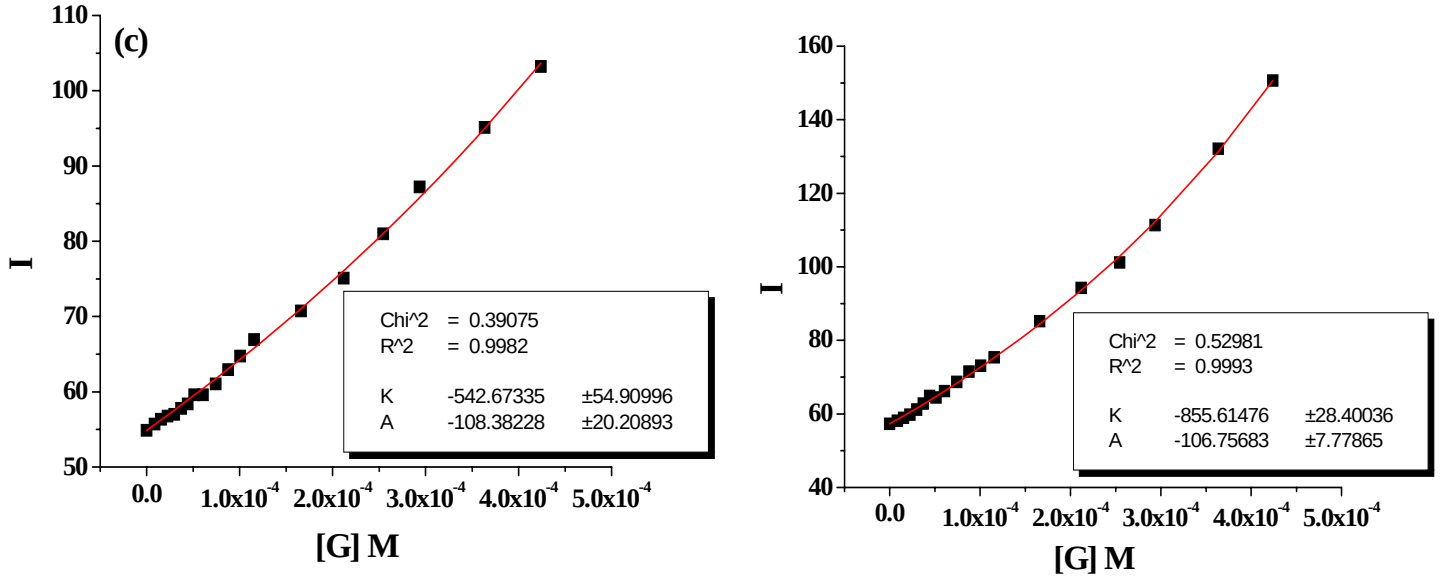

Figure S7b: Binding constant curves of receptor **4** with tetrabutylammonium salt of (a) Adipate**,** (b) Glutarate, (c) Malonate and (d) Succinate from fluorescence titration in CH_3CN. Working formula
$I= (I_0+I \times K \times C_G)/ (1+K \times C_G)$, I_0 = initial intensity, I = intensity after successive addition of guest. C_G = [G]. (λ_{max} = 412 nm, [H] = 5.65 x 10^{-5} M and [G] = 2.5 x 10^{-3} M).

9a. Emission titration curves for receptor 1-4 with sodium salt of $H_2PO_4^-$, HPO_4^{2-}, PO_4^- in 4:1 (v/v) $CH_3CN:H_2O$ containing 10 mM HEPES buffer (pH= 7.2) at 25 ^{0}C

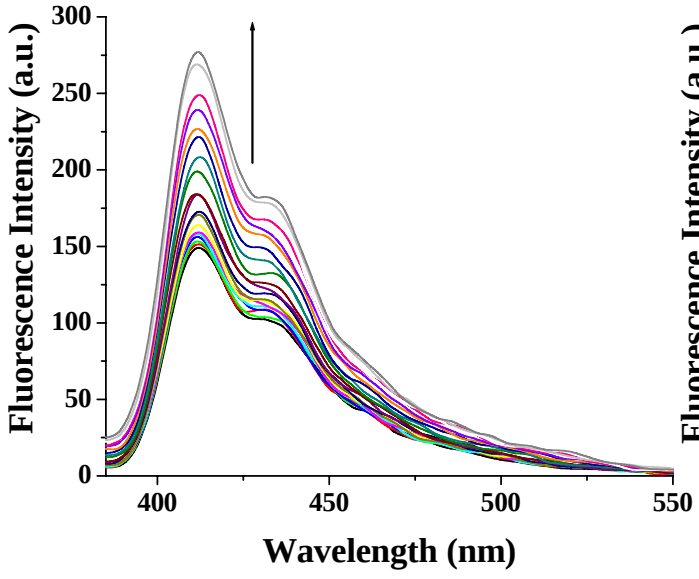

Figure S8a: Fluorescence titration of **1** (c = 2.01 x 10^{-5}M) with addition of 50 equiv. amounts of NaH_2PO_4 (c = 9.84 x 10^{-2} M) in 4:1 (v/v) $CH_3CN:H_2O$ containing 10 mM HEPES buffer (pH= 7.2).$\lambda_{Excitation}$ = 380 nm.

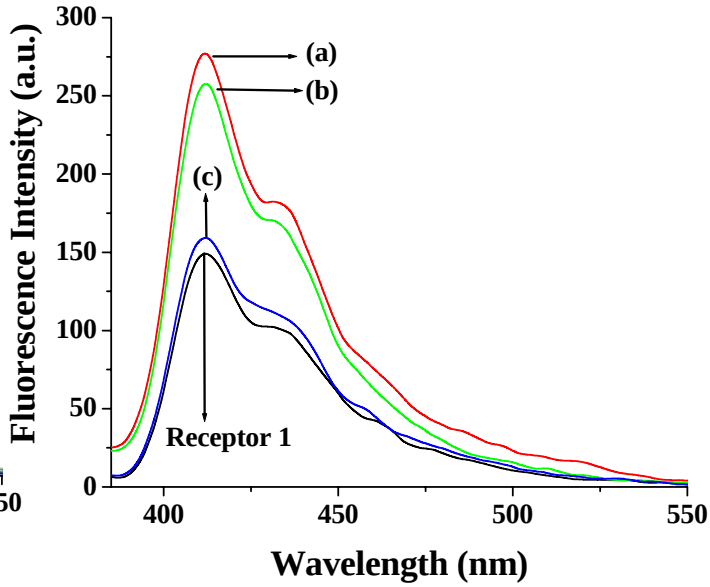

Figure S8b: Fluorescence emission change of **1** (c = 2.01 x 10^{-5}M) with addition of 50 equiv. amounts of (a) NaH_2PO_4, (b) Na_2HPO_4 and (c) Na_3PO_4 in 4:1 (v/v) $CH_3CN:H_2O$ containing 10 mM HEPES buffer (pH= 7.2).$\lambda_{Excitation}$ = 380 nm.

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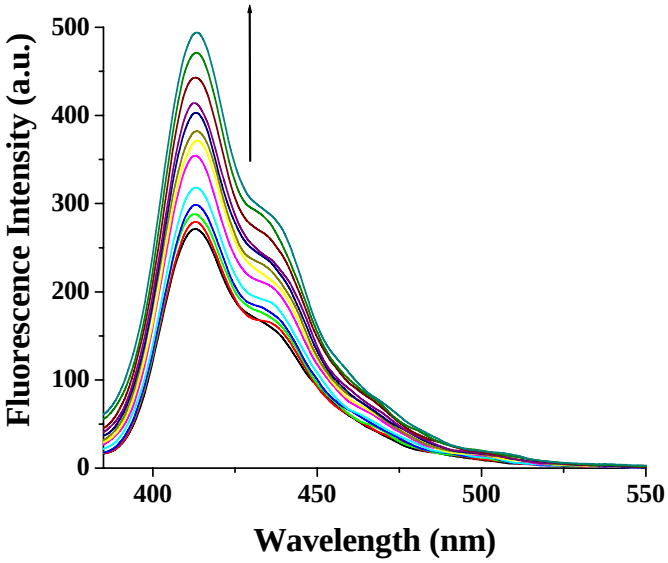

Figure S8c: Fluorescence titration of **3** (c = 2.01 x 10^{-5}M) with addition of 50 equiv. amounts of Na_2HPO_4 (c = 9.84 x 10^{-2} M) in 4:1 (v/v) CH_3CN:H_2O containing 10 mM HEPES buffer (pH= 7.2).$\lambda_{Excitation}$ = 380 nm.

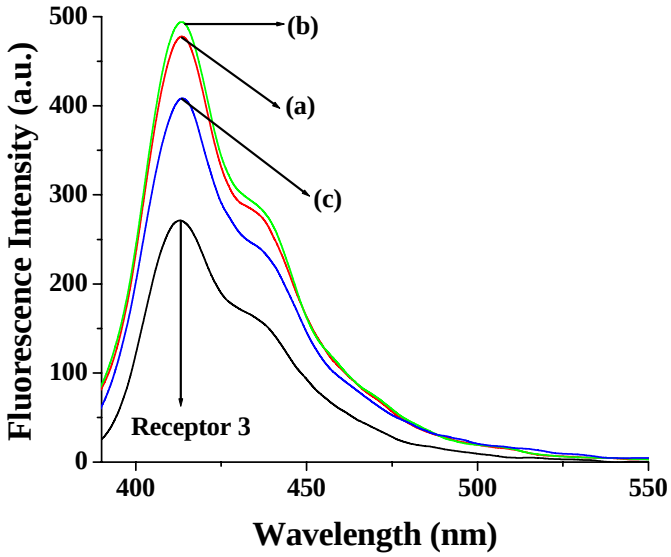

Figure S8d: Fluorescence emission change of **3** (c = 2.01 x 10^{-5}M) with addition of 50 equiv. amounts of (a) NaH_2PO_4, (b) Na_2HPO_4 and (c) Na_3PO_4 in 4:1 (v/v) CH_3CN:H_2O containing 10 mM HEPES buffer (pH= 7.2).$\lambda_{Excitation}$ = 380 nm.

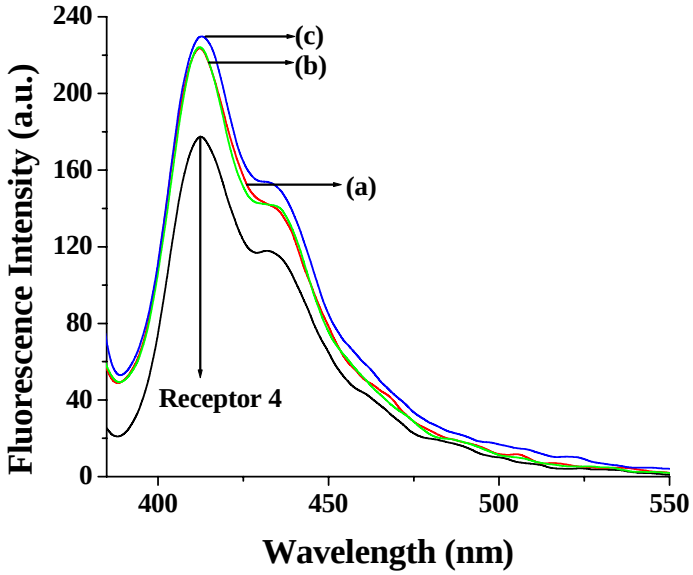

Figure S8e: Fluorescence emission change of **4** (c = 2.01 x 10^{-5}M) with addition of 50 equiv. amounts of (a) NaH_2PO_4, (b) Na_2HPO_4 and (c) Na_3PO_4 in 4:1 (v/v) CH_3CN:H_2O containing 10 mM HEPES buffer (pH= 7.2).$\lambda_{Excitation}$ = 380 nm.

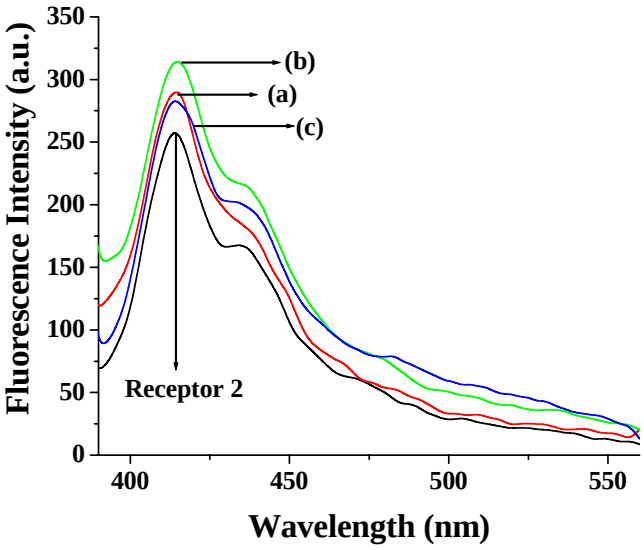

Figure S8f: Fluorescence emission change of **2** (c = 2.01 x 10^{-5}M) with addition of 50 equiv. amounts of (a) NaH_2PO_4, (b) Na_2HPO_4 and (c) Na_3PO_4 in 4:1 (v/v) CH_3CN:H_2O containing 10 mM HEPES buffer (pH= 7.2).$\lambda_{Excitation}$ = 380 nm.

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9b. UV-vis titration curves for receptor 1-4 with sodium salt of $H_2PO_4^-$ and HPO_4^{2-} in 4:1 (v/v) $CH_3CN:H_2O$ containing 10 mM HEPES buffer (pH= 7.2) at 25 ^{0}C

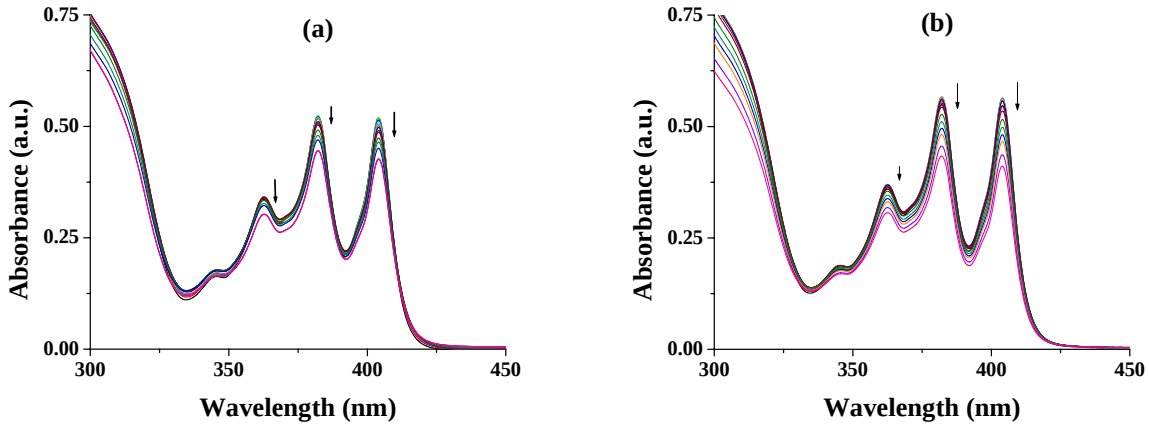

Figure S8g: UV-vis titration of **1** (c = 2.01 x 10^{-5}M) with addition of 50 equiv. amounts of (a) NaH_2PO_4 (c = 9.84 x 10^{-2} M) and (b) Na_2HPO_4 (c = 9.84 x 10^{-2} M) in 4:1 (v/v) $CH_3CN:H_2O$ containing 10 mM HEPES buffer (pH= 7.2).λ_{Max} = 380 nm.

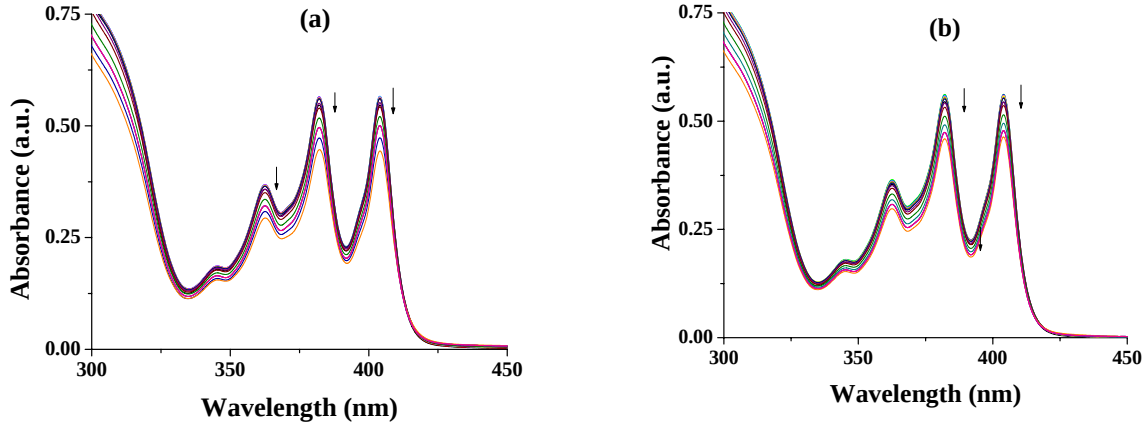

Figure S8h: UV-vis titration of **2** (c = 2.01 x 10^{-5}M) with addition of 50 equiv. amounts of (a) NaH_2PO_4 (c = 9.84 x 10^{-2} M) and (b) Na_2HPO_4 (c = 9.84 x 10^{-2} M) in 4:1 (v/v) $CH_3CN:H_2O$ containing 10 mM HEPES buffer (pH= 7.2).λ_{Max} = 380 nm.

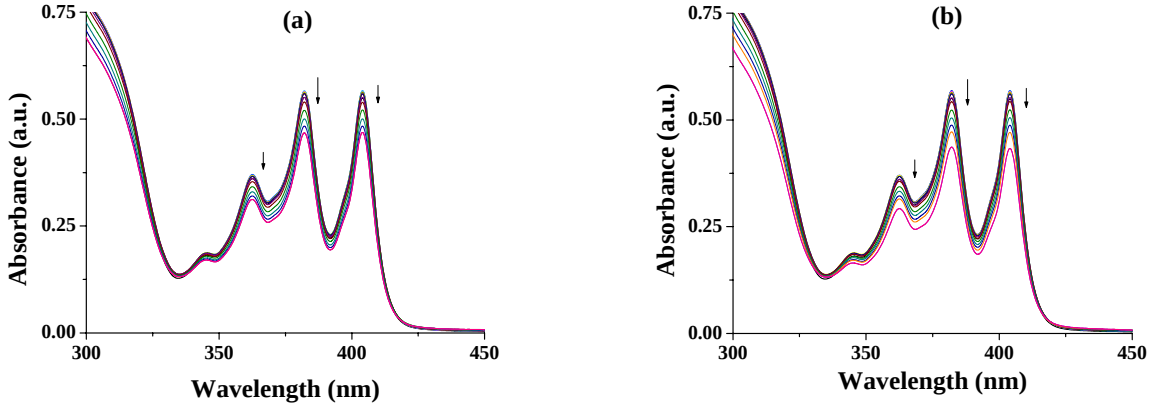

Figure S8i: UV-vis titration of **3** (c = 2.01 x 10^{-5}M) with addition of 50 equiv. amounts of (a) NaH_2PO_4 (c = 9.84 x 10^{-2} M) and (b) Na_2HPO_4 (c = 9.84 x 10^{-2} M) in 4:1 (v/v) $CH_3CN:H_2O$ containing 10 mM HEPES buffer (pH= 7.2).λ_{Max} = 380 nm.

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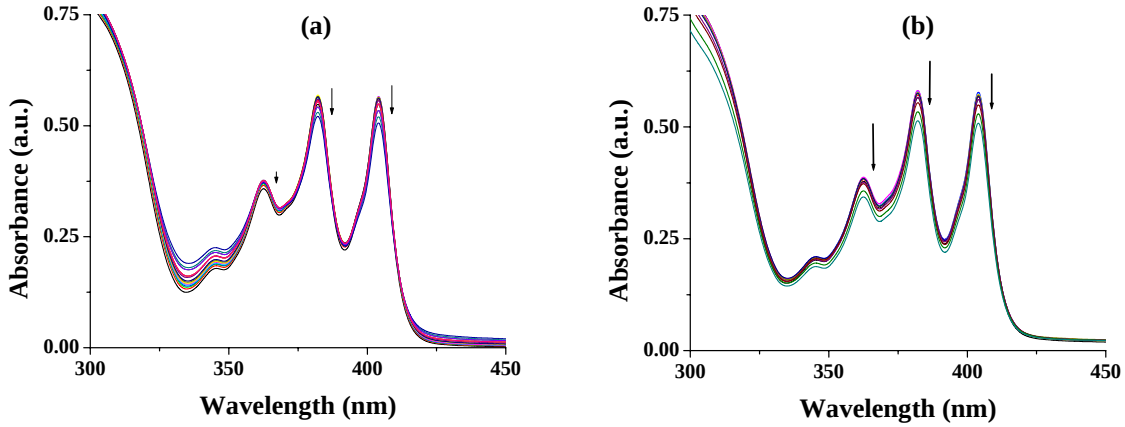

Figure S8j: UV-vis titration of **4** (c = 2.01 x 10^{-5}M) with addition of 50 equiv. amounts of (a) NaH_2PO_4 (c = 9.84 x 10^{-2} M) and (b) Na_2HPO_4 (c = 9.84 x 10^{-2} M) in 4:1 (v/v) CH_3CN:H_2O containing 10 mM HEPES buffer (pH= 7.2).λ_{Max} = 380 nm.

10. Anion binding studies of receptors 1 – 4 with sodium salt of $H_2PO_4^-$, HPO_4^{2-} and PO_4^{3-} in CH_3CN:H_2O (4:1, v/v)

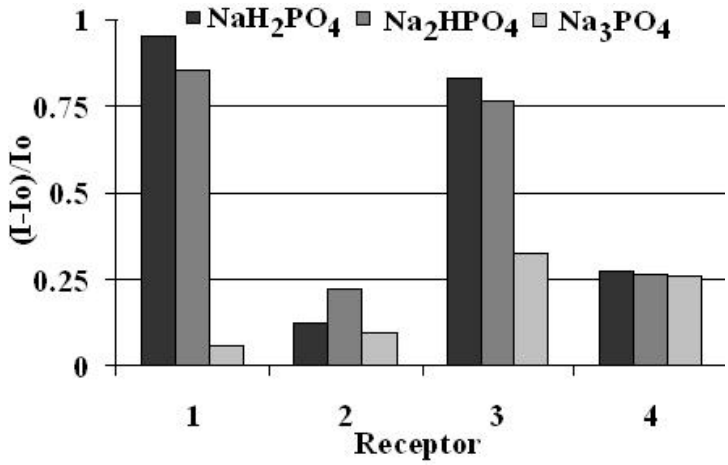

Figure S8k. Fluorescence ratio [$(I-I_0)/I_0$] of receptors **1** – **4** in CH_3CN: H_2O (4:1 v/v) at 412 nm upon addition of 50 equiv. amounts of a particular anion (dissolved in H_2O).

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11. Binding constant curves for receptors 1 and 3 with NaH_2PO_4 and Na_2HPO_4 from fluorescence in 4:1 (v/v) $CH_3CN:H_2O$ containing 10 mM HEPES buffer (pH= 7.2)

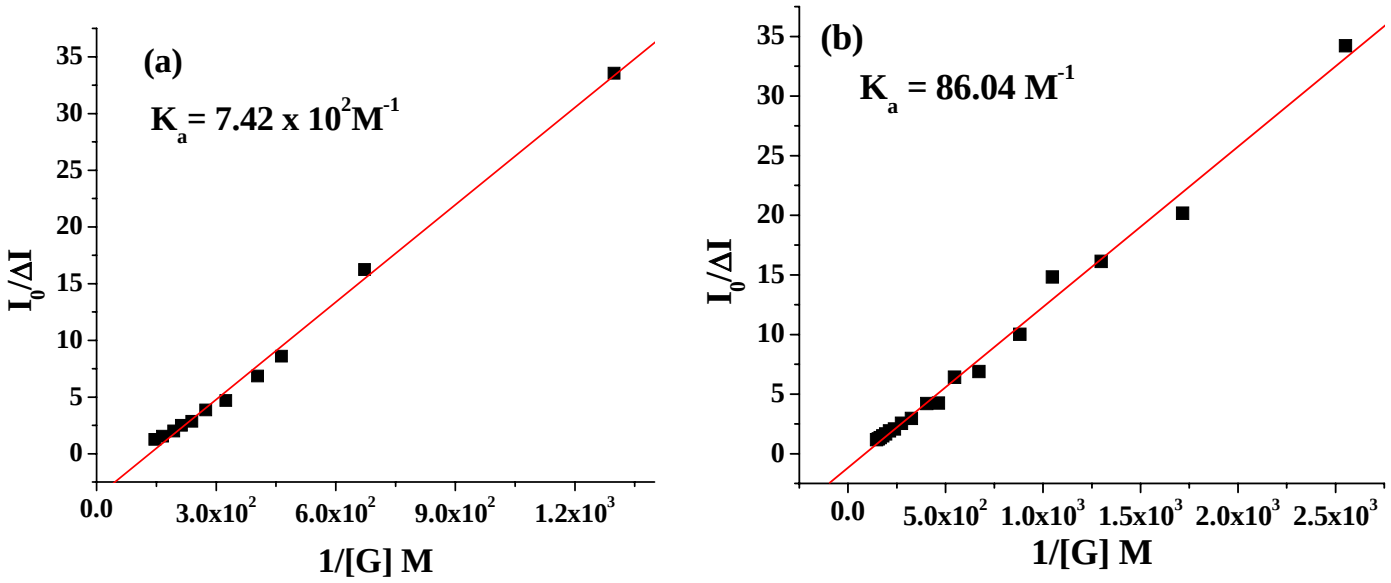

Figure S9a : Benesi–Hilderband plot for **1** (c = 2.01 x 10^{-5}M) with (a) $NaH_2PO_4^-$ and (b) Na_2HPO_4 at 412 nm.

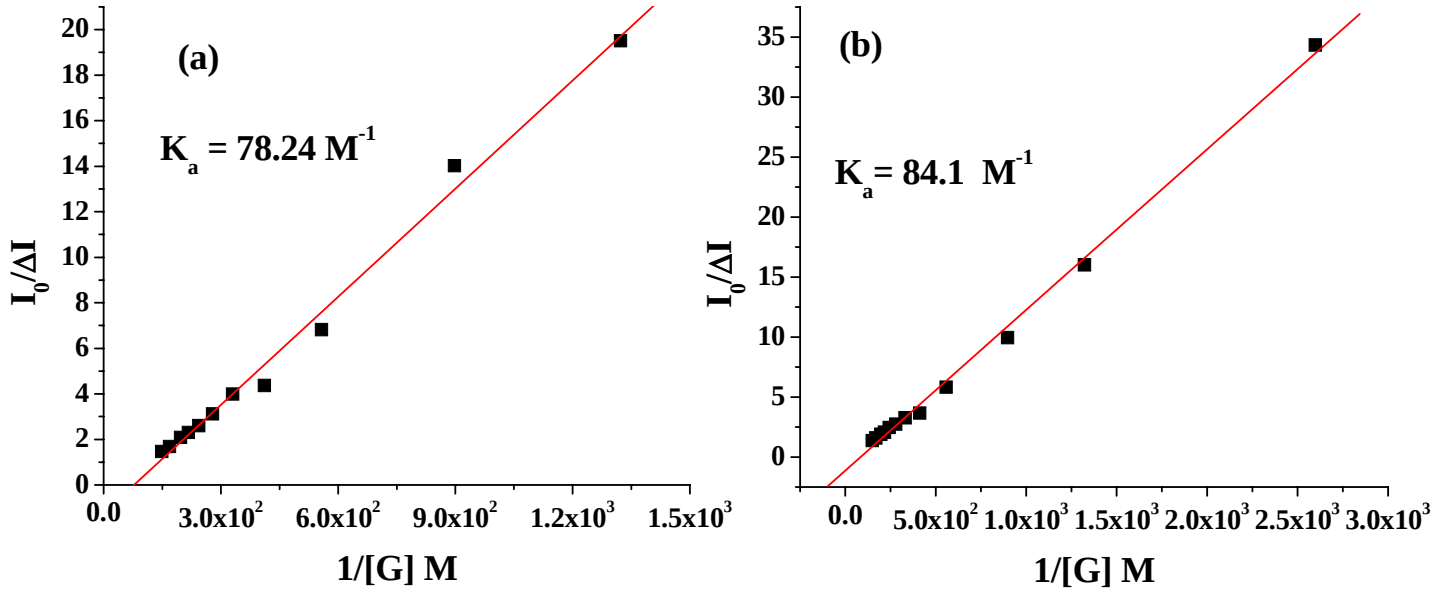

Figure S9b: Benesi–Hilderband plot for **3** (c = 2.01 x 10^{-5}M) with (a) $NaH_2PO_4^-$ and (b) Na_2HPO_4 at 412 nm.

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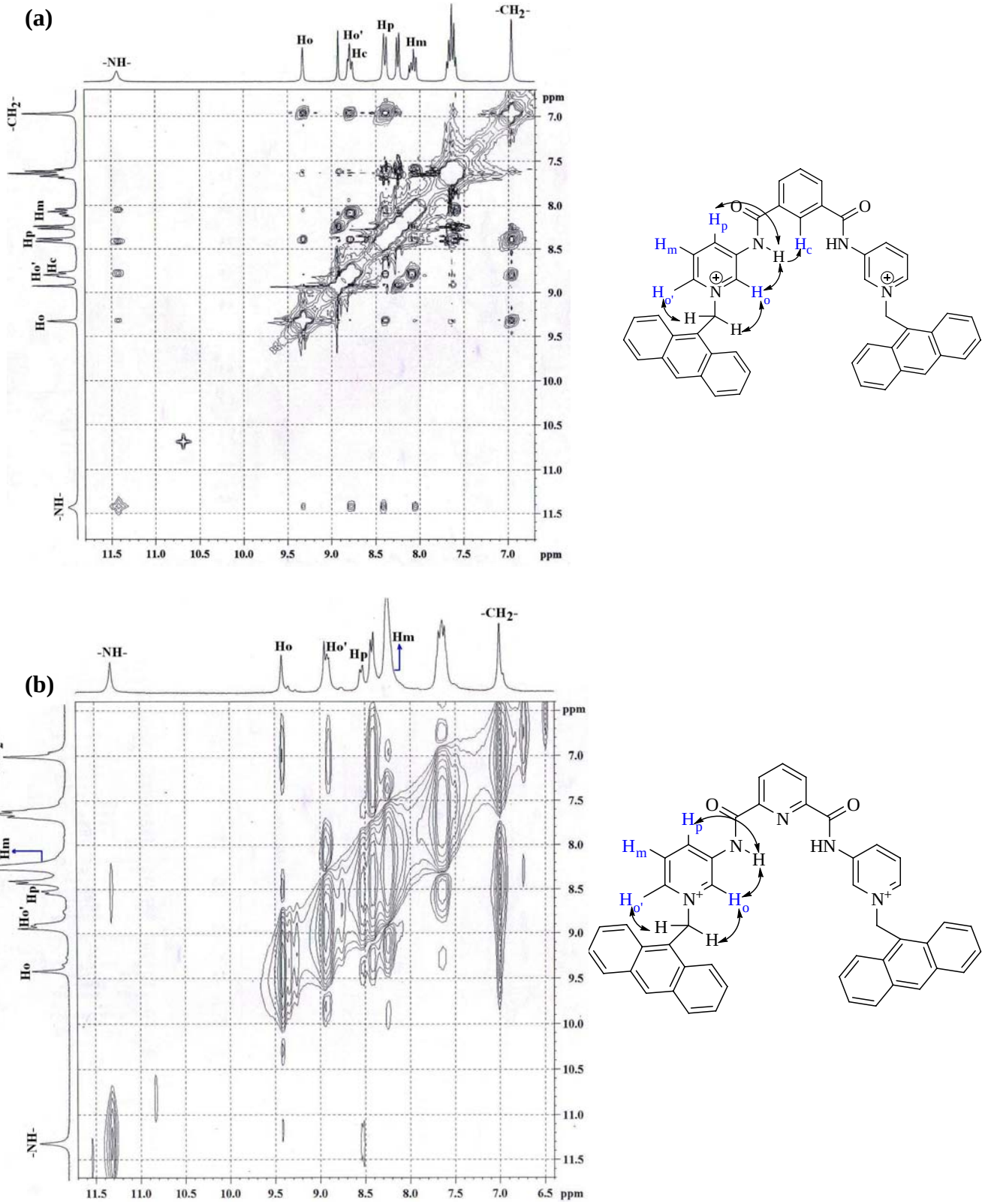
12. ROESY spectrum in d_6-DMSO of receptors 1-4



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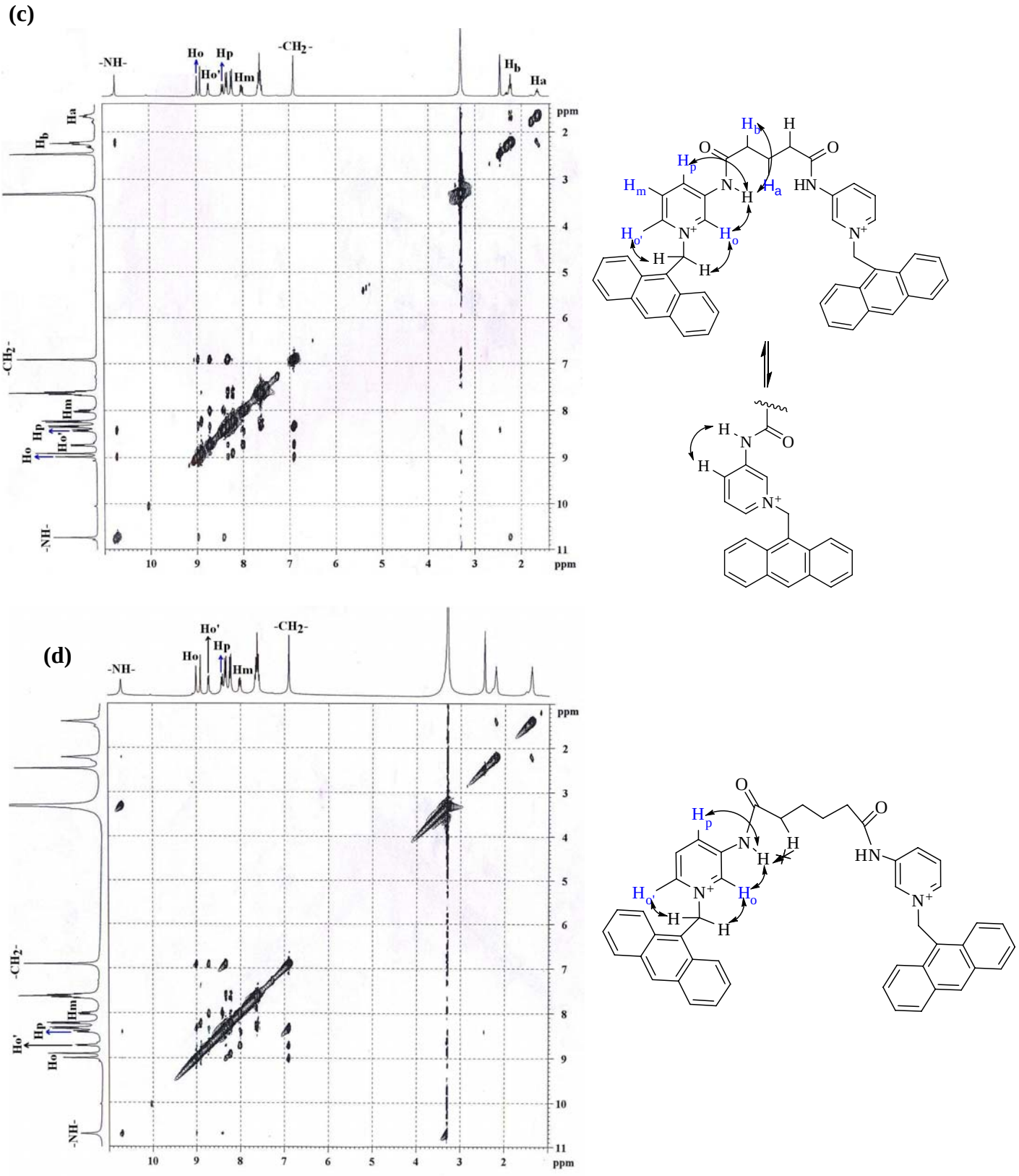

Figure S10. ROSEY spectrum of receptors (a) **1**, (b) **2**, (c) **3** and (d) **4** in d_6-DMSO.

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13a. ^{1}H NMR of the receptors 2 – 4 itself and in presence of equiv. amount of F^-, AcO^- and $H_2PO_4^-$ in $CDCl_3$ containing 6% d_6-DMSO

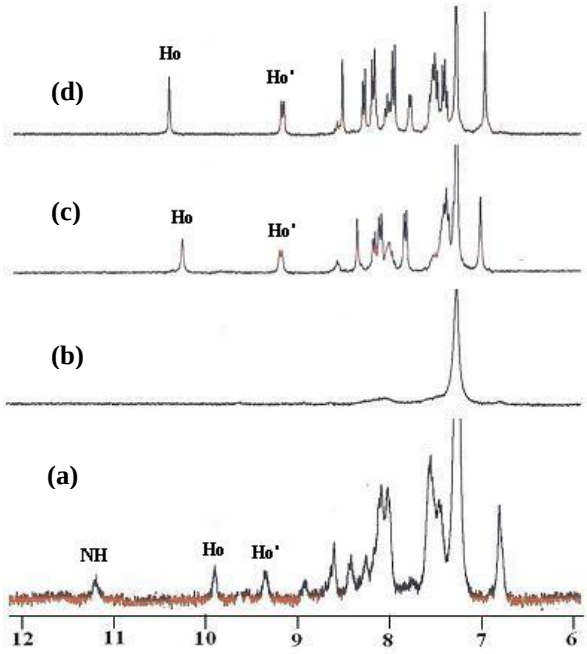

Figure S11a. Partial ^{1}H NMR of (a) receptor **2** (c = 2.64 x 10^{-3} M) and with equiv. amount of (b) $H_2PO_4^-N^+Bu_4$, (c) $F^-N^+Bu_4$, (d) AcO^- N^+Bu_4 in $CDCl_3$ containing 6% d_6-DMSO.

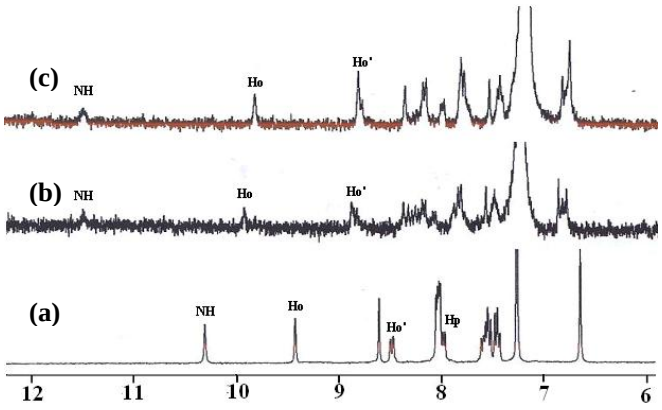

Figure S11b. Partial ^{1}H NMR of (a) receptor **3** (c = 2.64 x 10^{-3} M) and with (b) 1 equiv. amount of $H_2PO_4^-$ N^+Bu_4, (c) 2 equiv. amount of $H_2PO_4^-$ N^+Bu_4 in $CDCl_3$ containing 6% d_6-DMSO.

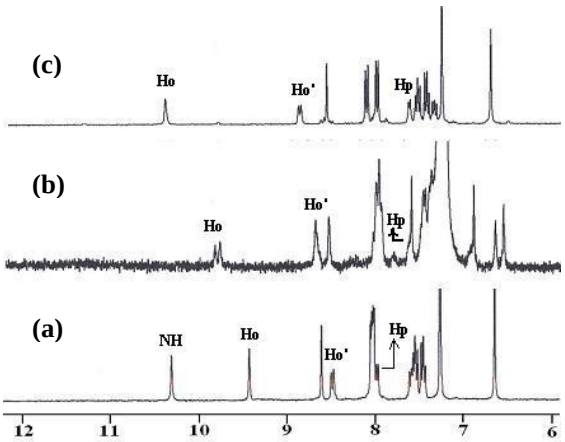

Figure S11c. Partial ^{1}H NMR of receptor **3** (c = 2.64 x 10^{-3} M) and with tetrabutylammonium salts of (b) F^- (1:1), (c) AcO^- (1:1) in $CDCl_3$ containing 6% d_6-DMSO.

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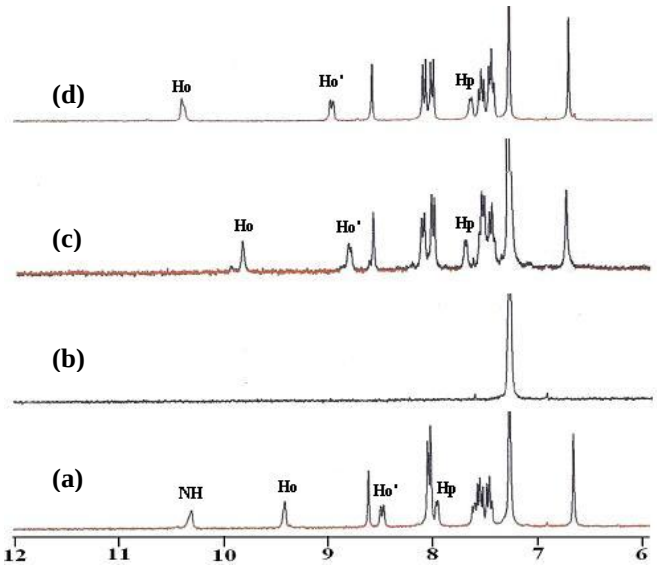

Figure S11d. Partial ^{1}H NMR of (a) receptor **4** (c = 2.64 x 10^{-3} M) and with tetrabutylammonium salts of (b) $H_2PO_4^-$ (1:1), (c) F^- (1:1), (d) AcO^- (1:1) in $CDCl_3$ containing 6% d_6-DMSO.

13b. ^{1}H NMR titration spectra (partial) of the receptors 3 – 4 and in presence of glutarate and adipate in $CDCl_3$ containing 6% d_6-DMSO

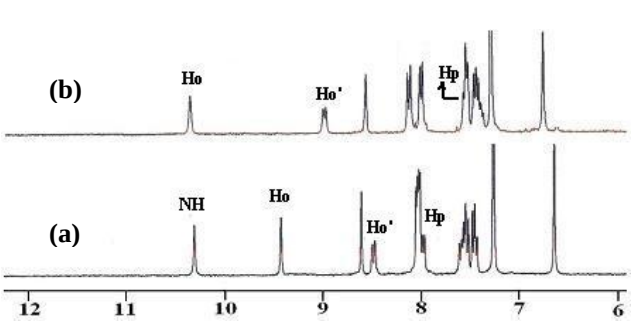

Figure S11e. (a) Partial ^{1}H NMR spectrum of receptor **3** (c = 2.64 x 10^{-3} M) only, with tetrabutylammonium (b) Glutarate (1:1) in $CDCl_3$ containing 6% d_6-DMSO.

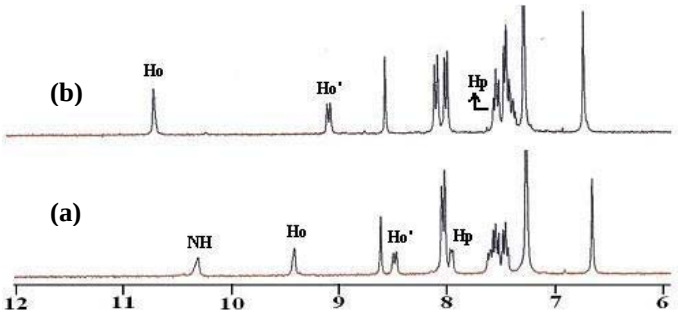

Figure S11f. (a) Partial ^{1}H NMR spectrum of receptor **4** (c = 2.64 x 10^{-3} M) only, with tetrabutylammonium (b) Adipate (1:1) in $CDCl_3$ containing 6% d_6-DMSO.

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14. ^{31}P of $H_2PO_4^-$ in the presence of 1-4 in d_6-DMSO (Brucker 500 MHz).

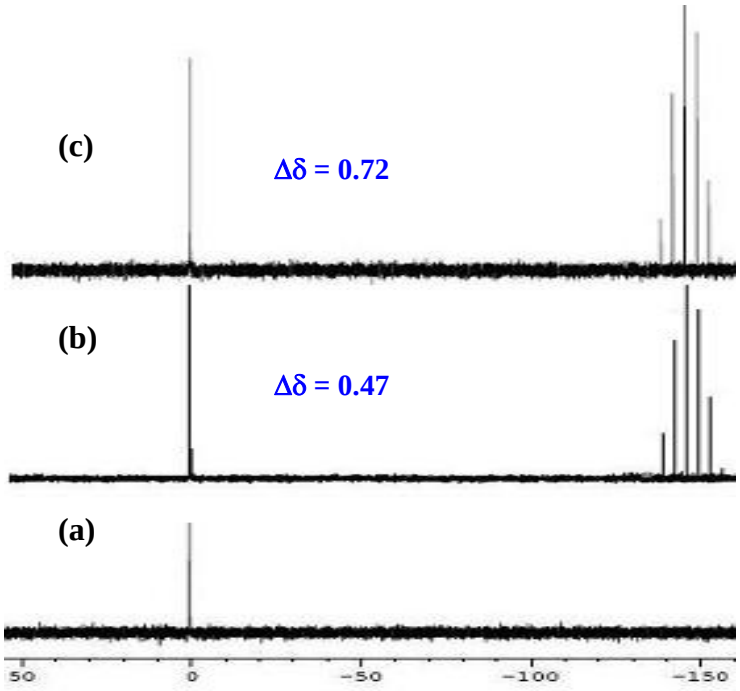

Figure S12a. ^{31}P NMR (500 MHz, in d_6-DMSO) of (a) $\mathbf{H_2PO_4^-}$ (*c* = 8.66x 10^{-3} M), (b) $\mathbf{1.H_2PO_4^-}$ (1:1) and (c) $\mathbf{1.H_2PO_4^-}$ (1:2).

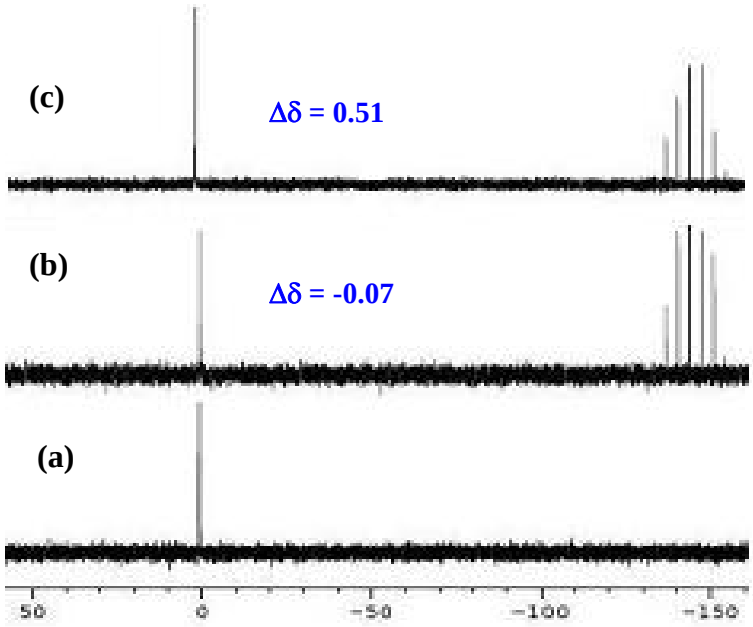

Figure S12b. ^{31}P NMR (500 MHz, in d_6-DMSO) of (a) $\mathbf{H_2PO_4^-}$ (*c* = 8.66x 10^{-3} M), (b) $\mathbf{2.H_2PO_4^-}$ (1:1) and (c) $\mathbf{2.H_2PO_4^-}$ (1:2).

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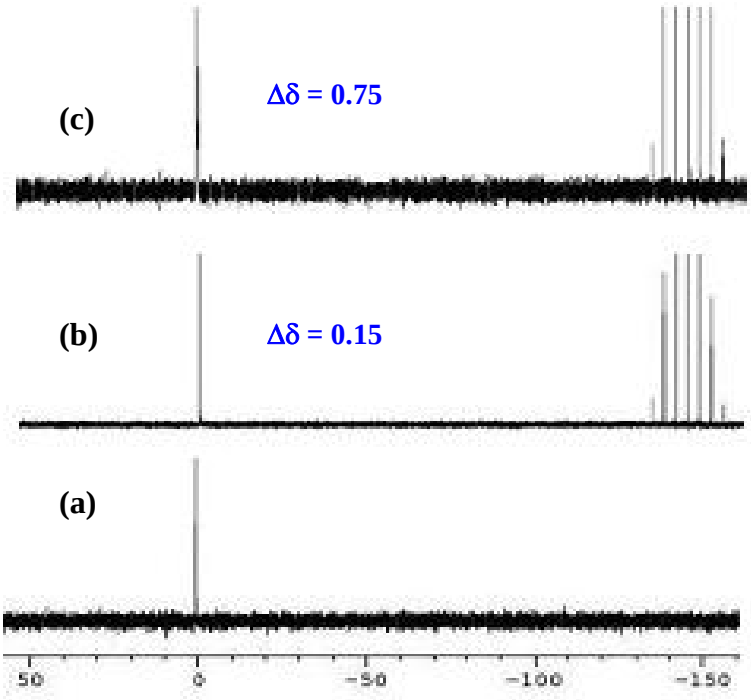

Figure S12c. ^{31}P NMR (500 MHz, in d_6-DMSO) of (a) $\mathbf{H_2PO_4^-}$ (*c* = 8.66x 10^{-3} M), (b) $\mathbf{3.H_2PO_4^-}$ (1:1) and (c) $\mathbf{3.H_2PO_4^-}$ (1:2).

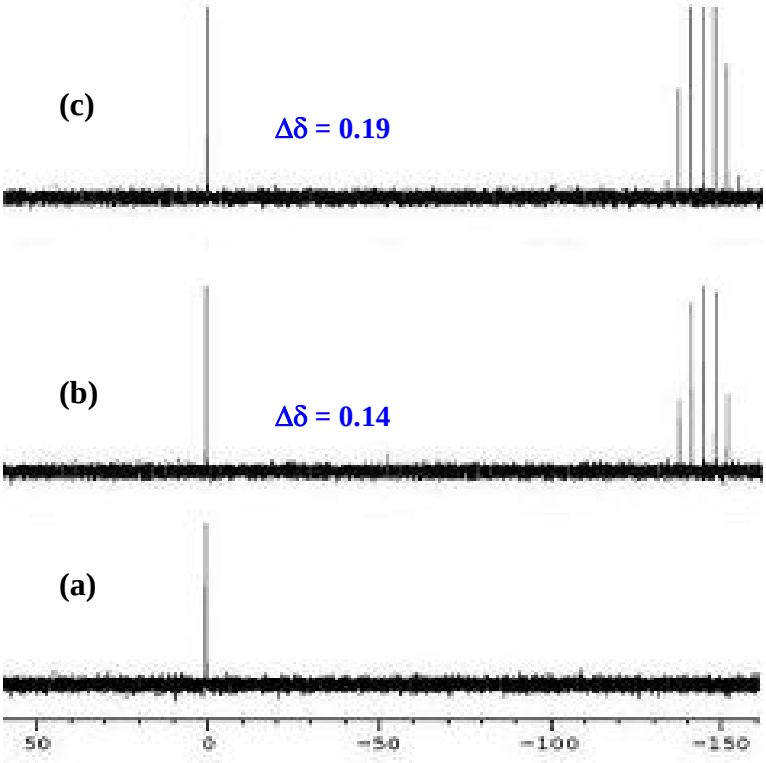

Figure S12d. ^{31}P NMR (500 MHz, in d_6-DMSO) of (a) $\mathbf{H_2PO_4^-}$ (*c* = 8.66x 10^{-3} M), (b) $\mathbf{4.H_2PO_4^-}$ (1:1) and (c) $\mathbf{4.H_2PO_4^-}$ (1:2).

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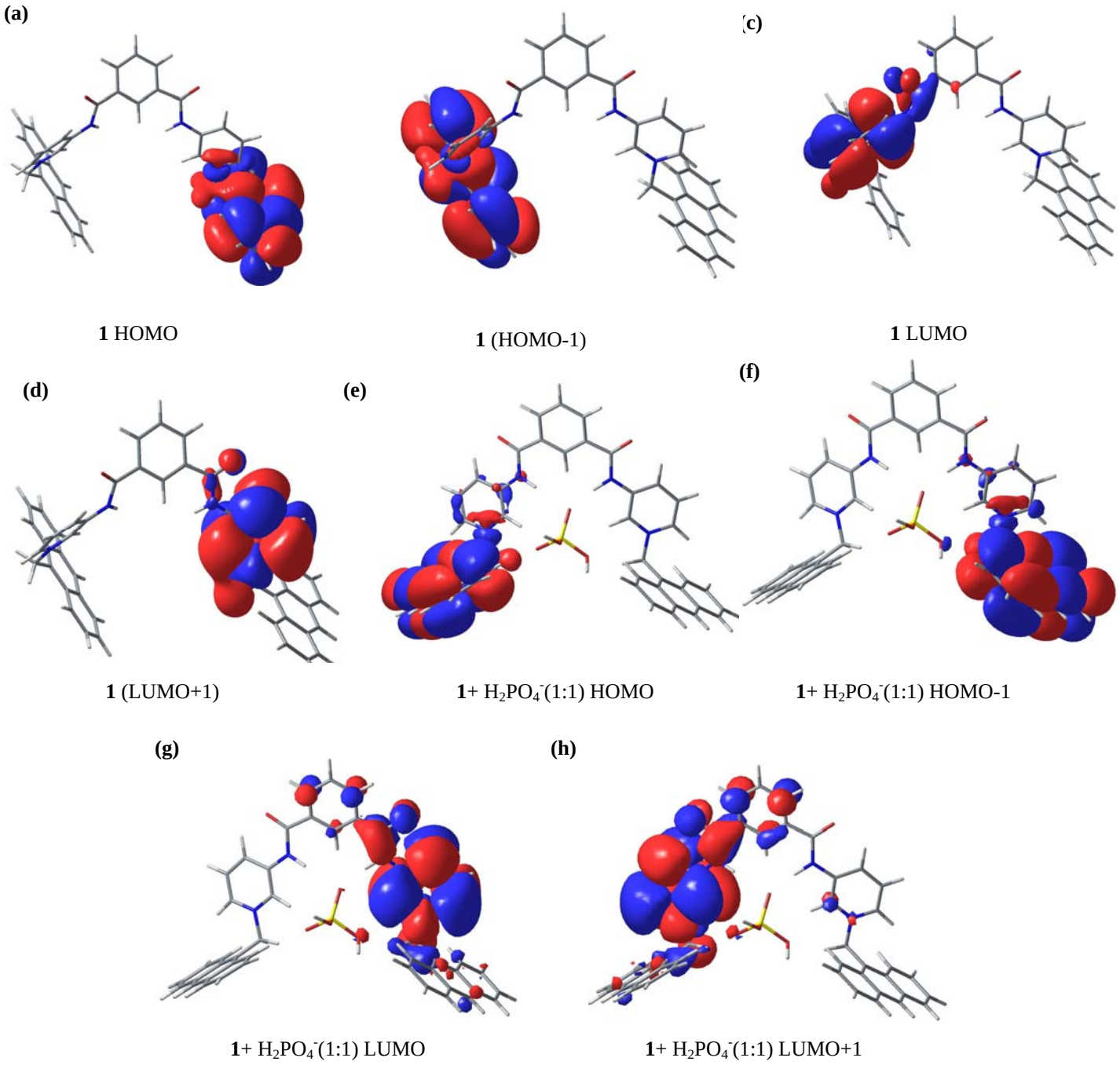
15. The distribution of the MO's of the receptors (1-4) itself and in their complexes with $H_2PO_4^-$ ([G]/ [H] = 1:1)



1 HOMO

1 (HOMO-1)

1 LUMO

1 (LUMO+1)

1+ $H_2PO_4^-$(1:1) HOMO

1+ $H_2PO_4^-$(1:1) HOMO-1

1+ $H_2PO_4^-$(1:1) LUMO

1+ $H_2PO_4^-$(1:1) LUMO+1

Figure S13a. MO picture of receptor **1** and 1:1 complex with $H_2PO_4^-$.

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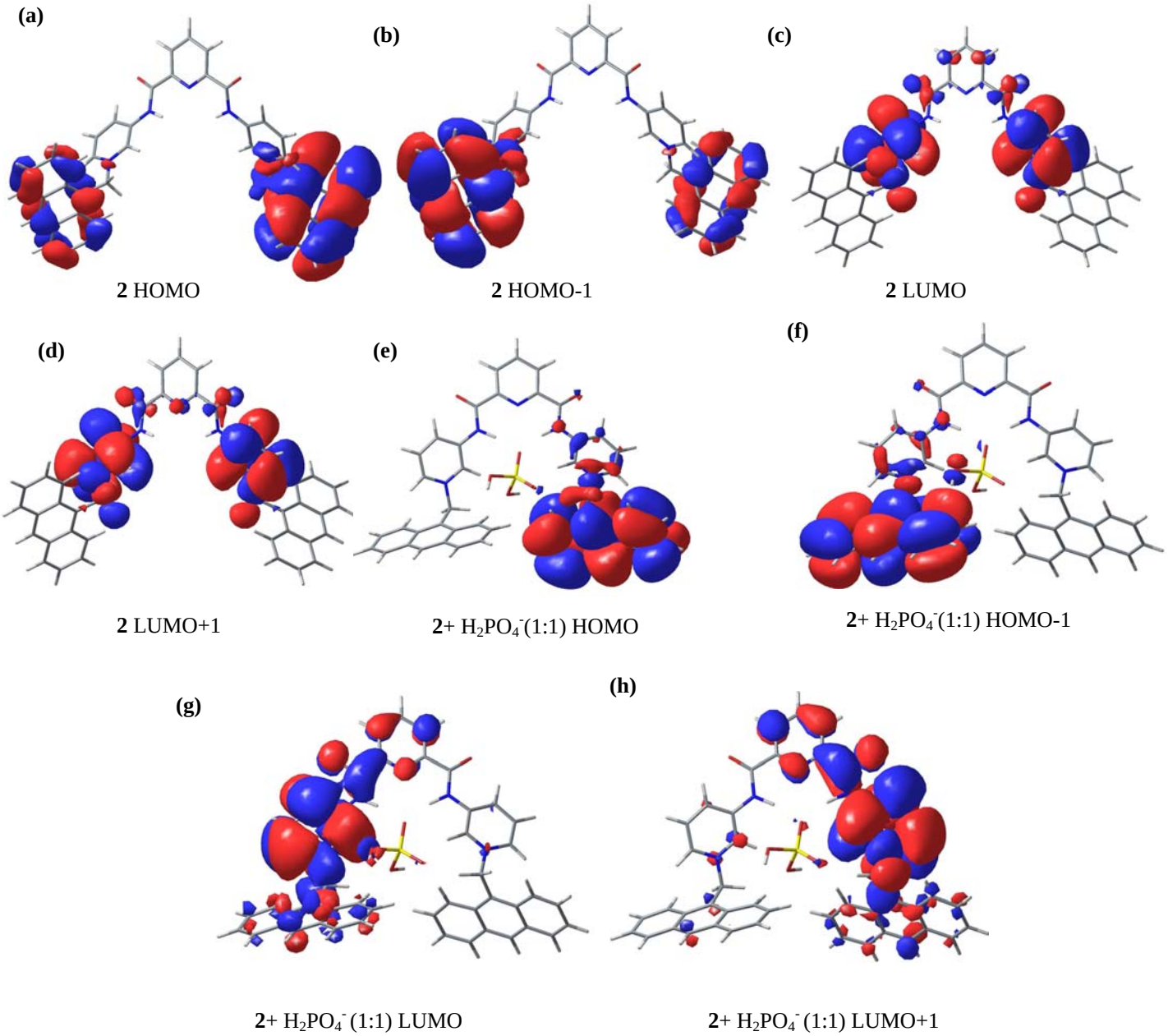

2 HOMO | **2** HOMO-1 | **2** LUMO

2 LUMO+1 | **2**+ $H_2PO_4^-$(1:1) HOMO | **2**+ $H_2PO_4^-$(1:1) HOMO-1

2+ $H_2PO_4^-$ (1:1) LUMO | **2**+ $H_2PO_4^-$ (1:1) LUMO+1

Figure S13b. MO picture of receptor **2** and 1:1 complex with $H_2PO_4^-$.

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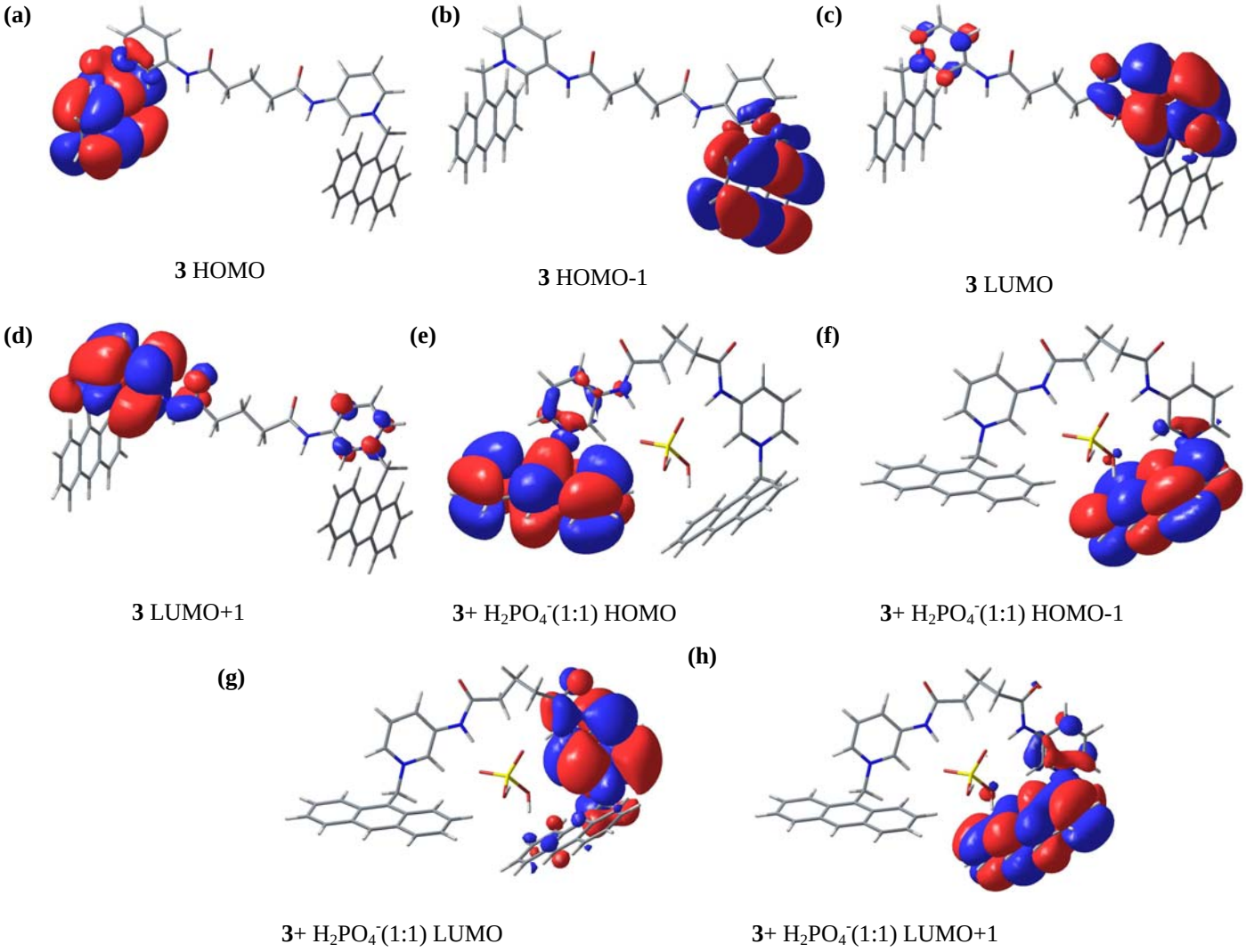

Figure S13c. MO picture of receptor **3** and 1:1 complex with $H_2PO_4^-$.

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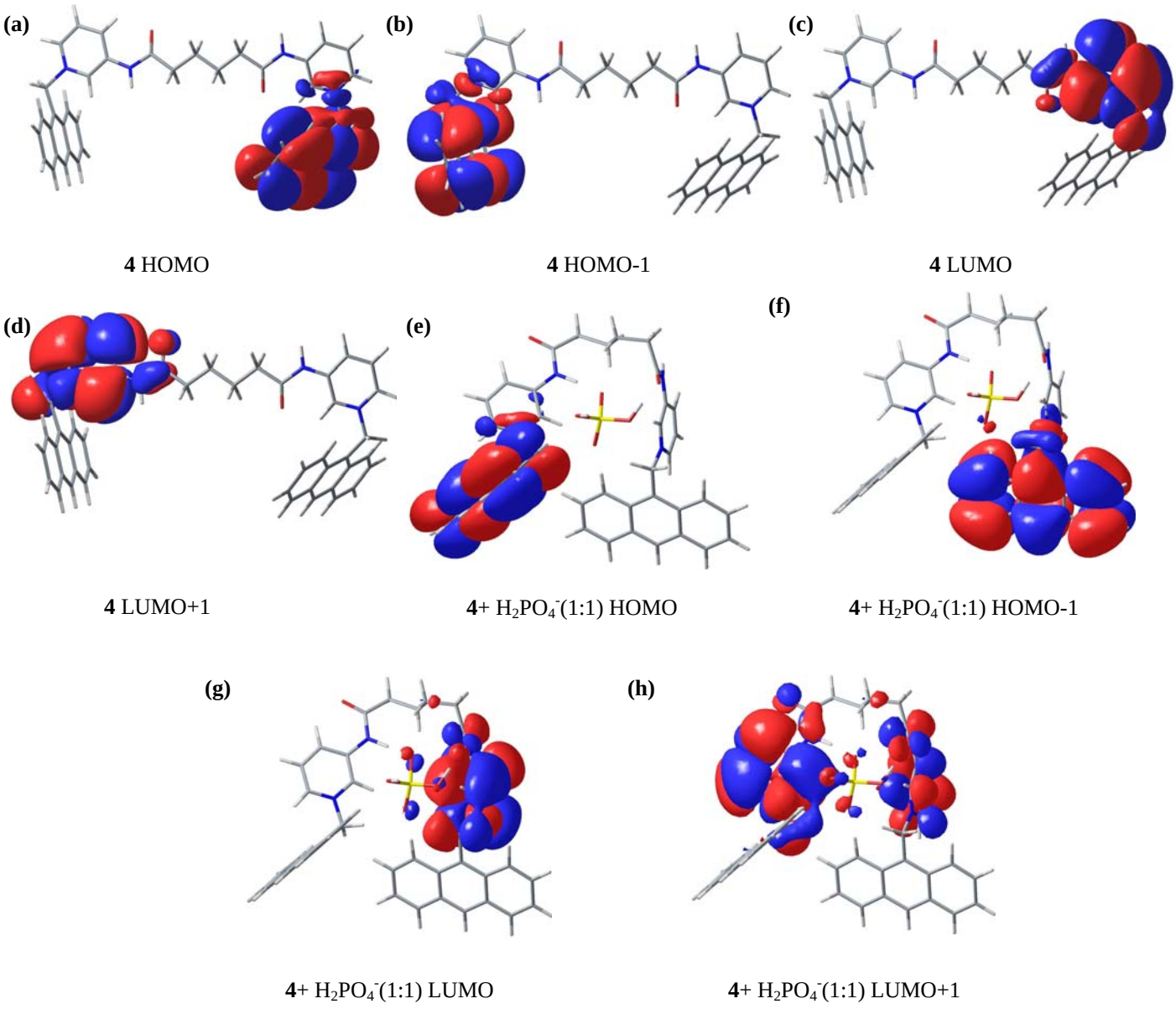

4 HOMO | **4** HOMO-1 | **4** LUMO

4 LUMO+1 | **4**+ $H_2PO_4^-$(1:1) HOMO | **4**+ $H_2PO_4^-$(1:1) HOMO-1

4+ $H_2PO_4^-$(1:1) LUMO | **4**+ $H_2PO_4^-$(1:1) LUMO+1

Figure S13d. MO picture of receptor **4** and 1:1 complex with $H_2PO_4^-$.

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16. Cell Staining.

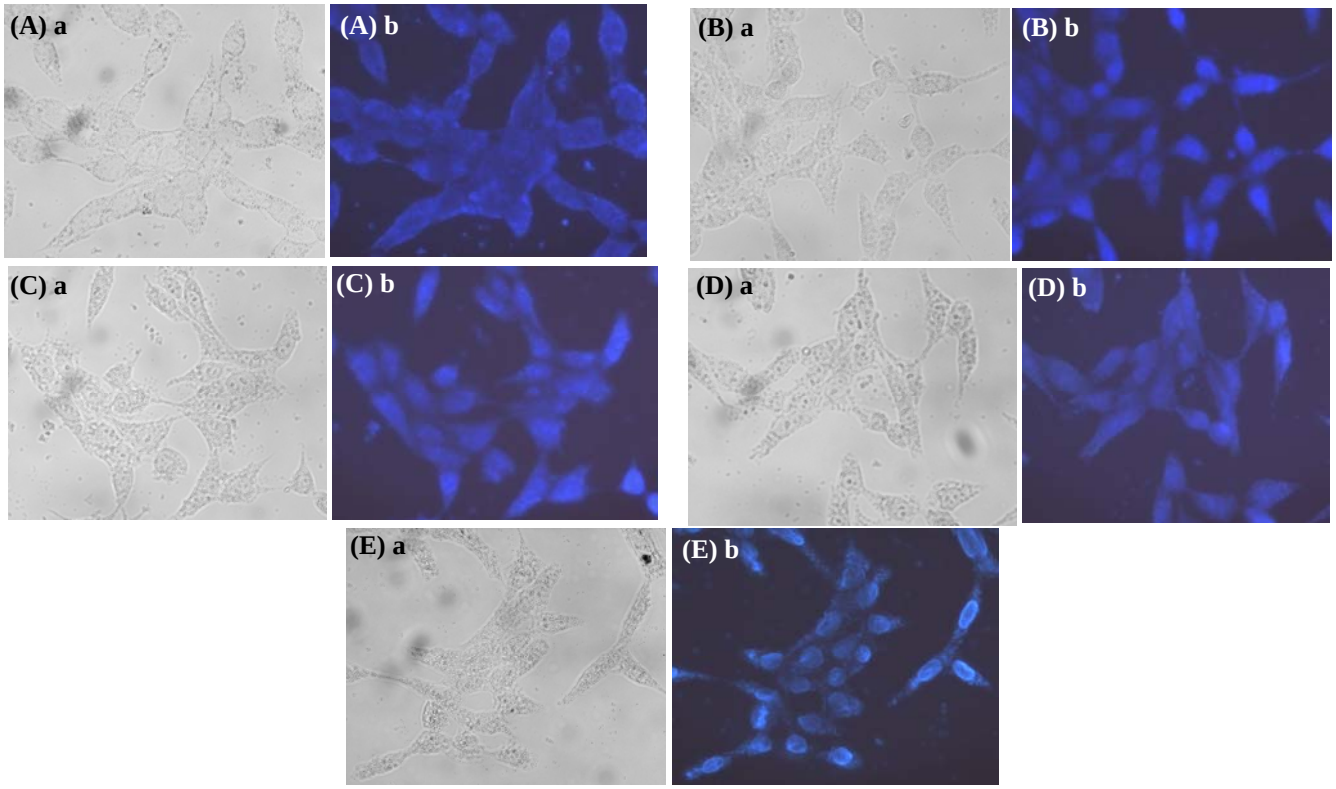
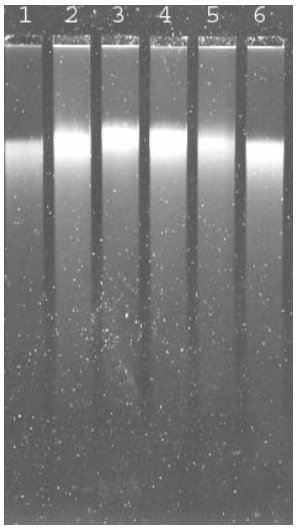


Figure S14. Fixed HeLa cells stained with – (A) receptor **1**, (B) receptor **3**, (C) receptor **4**, (D) receptor **2** and (E) Hoechst dye. a- bright-field mode, b- fluorescence mode.

17. Gel Retardation Assay (taking calf-thymus DNA)



Experimental procedure:
20 μM of each receptors **1 - 4** was mixed with 0.46 μg of calf-thymus DNA in Tris-EDTA (TE) buffer, pH-8 in separate microcentrifuge tubes and incubated for 25 minutes. All samples were loaded in 1.15% normal agarose gel after adding 1X gel loading dye and run in 1X Tris-acetate EDTA (TAE) buffer at constant 60 volt for 3 hrs. After staining with ethidium bromide (20 μg/μl) for 5 minutes it was observed under Typhon 9210 (Variable Mode Imager), GE Healthcare.

Figure S15.. Changes in the agarose gel electrophoretic pattern of calf thymus DNA induced by all the four receptors. Lanes 1 and 6, DNA alone; lane 2 for receptor **1** (20μM); lane 3 for receptor **3** (20μM); lane 4 for receptor **4** (20μM) and lane 5, receptor **2** (20μM) respectively. The concentration of DNA used is 0.046μg/μl.

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18. CD spectra of receptors 1 – 4.

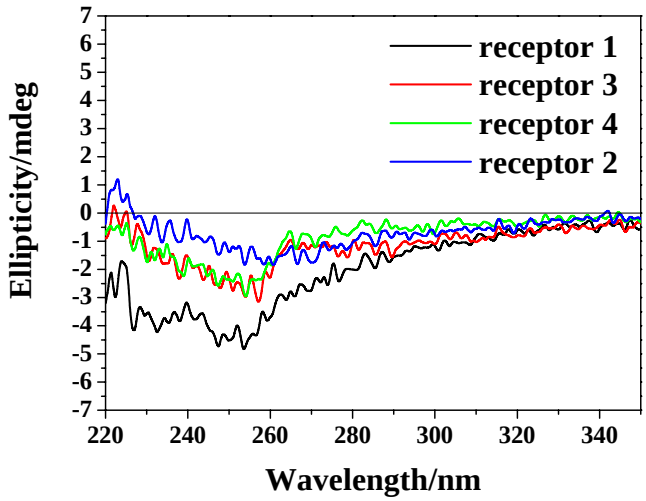

Figure S16. CD spectra of receptors **1** - **4** after buffer subtraction (20 μM of each compound has been used for analysis).