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Benzimidazolium-based new flexible cleft built on piperazine unit: A case of selective fluorometric sensing of ATP

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1. Change in emission of receptor 1 with various anions of sodium salt in CH_3CN-H_2O (1:1/v/v, using 10 mM HEPES, pH 6.4).

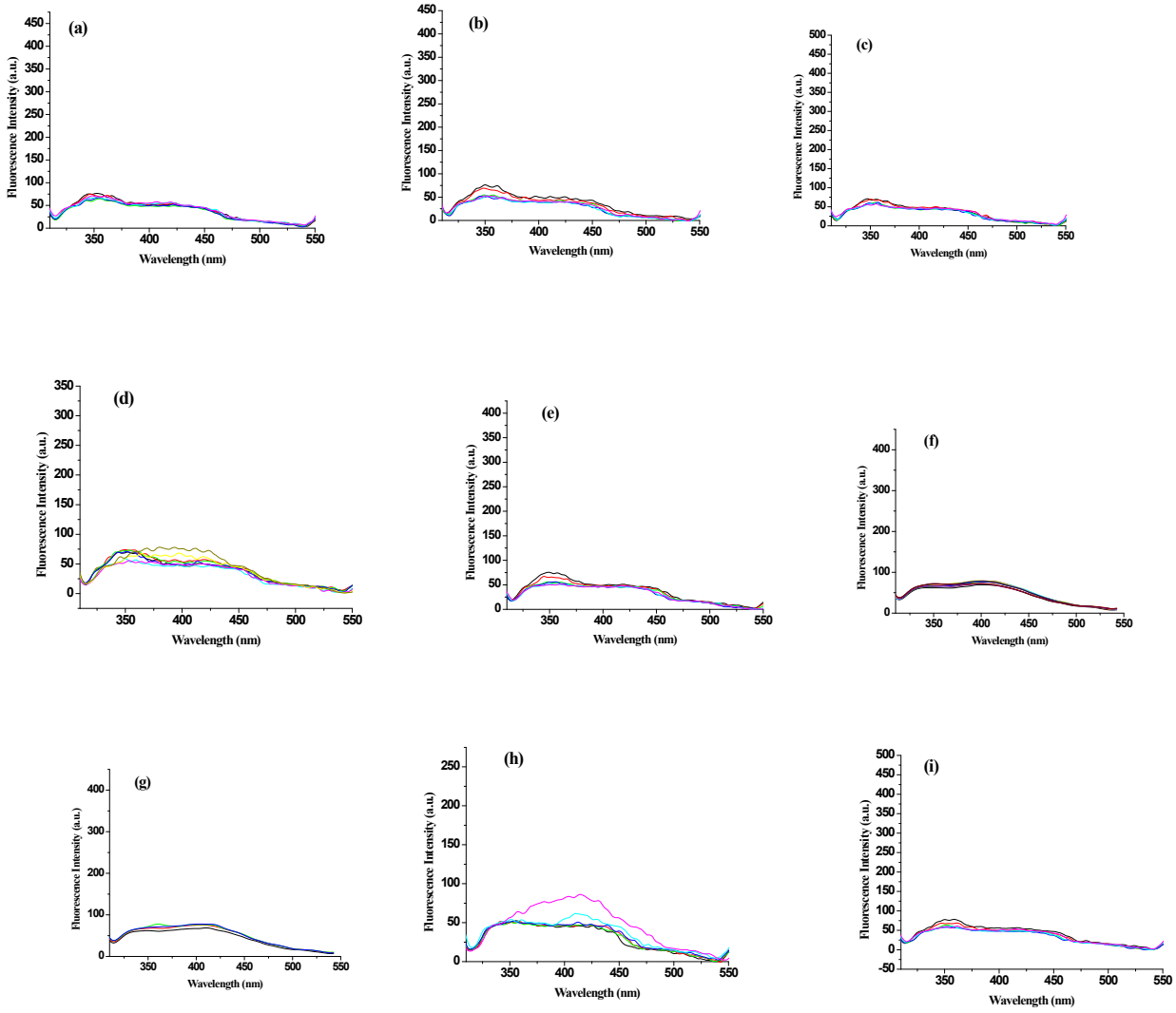


Figure 1S. Change in emission of **1** (c = 2.5 x 10^{-5} M) in CH_3CN-H_2O (1:1/v/v, using 10 mM HEPES, pH 6.4) upon addition of (a) Na_3PO_4 , (b) Na_2HPO_4, (c) NaH_2PO_4, (d) ADP, (e) AMP, (f) $Na_3HP_2O_7$, (g) $Na_4P_2O_7$, (h) G1P, (i) G6P; [concentration of anions of sodium salts were 1 x 10^{-3} M].

2. Change in absorbance of receptor 1 with various anions of sodium salt in CH_3CN-H_2O (1:1/v/v, using 10 mM HEPES, pH 6.4).

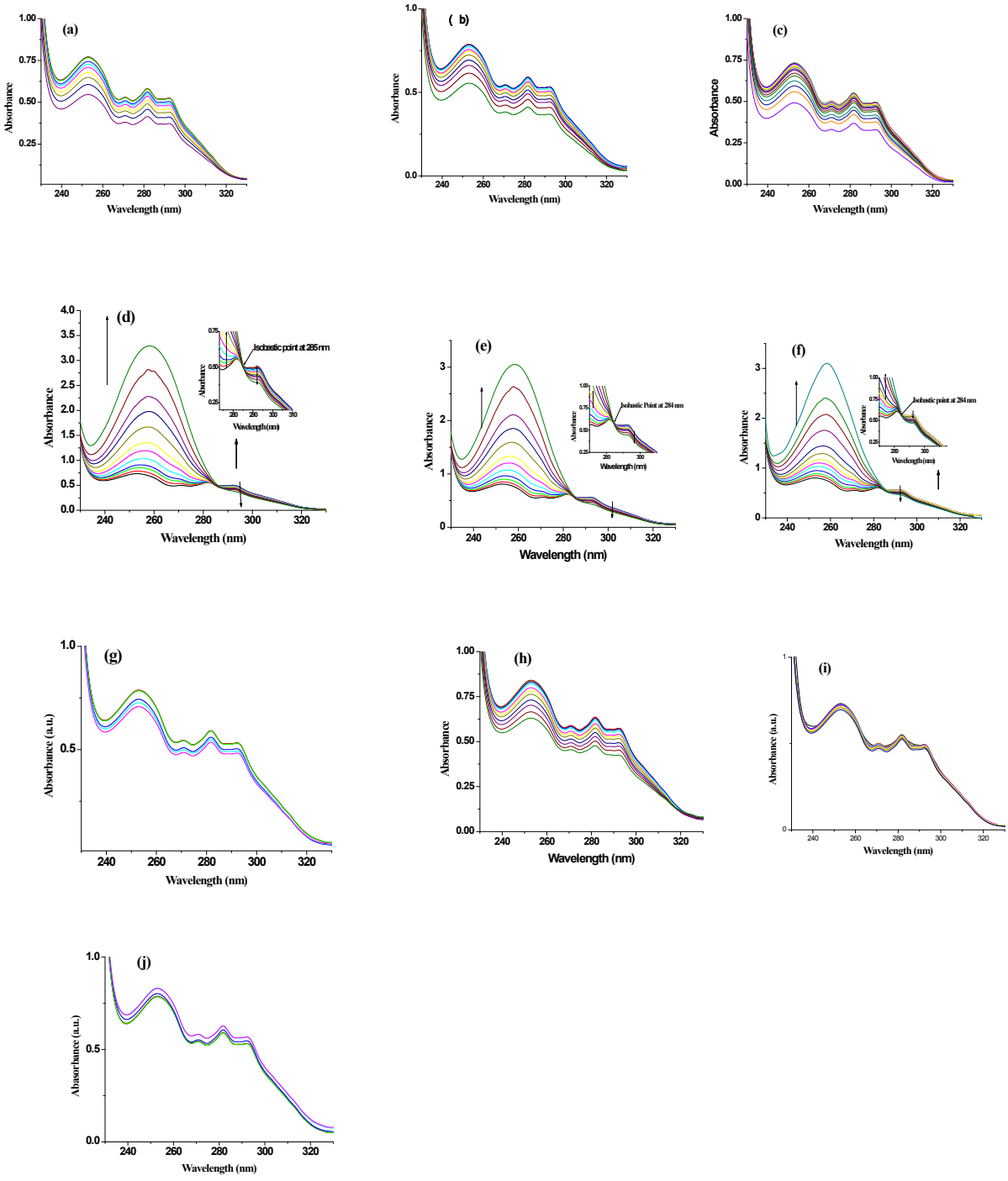


Figure 2S. Change in absorbance of **1** (c = 2.5 x 10^{-5} M) in CH_3CN-H_2O (1:1/v/v, using 10 mM HEPES, pH 6.4) upon addition of (a) Na_3PO_4 , (b) Na_2HPO_4, (c) NaH_2PO_4, (d) ADP, (e) AMP, (f) ATP, (g) $Na_3HP_2O_7$, (h) $Na_4P_2O_7$, (i) G1P, (j) G6P; [concentration of anions of sodium salts were 1 x 10^{-3} M].

3. Change in emission of receptor 1 with various anions of tetrabutylammonium salts in CH_3CN-H_2O (1:1/v/v, using 10 mM HEPES, pH 6.4).

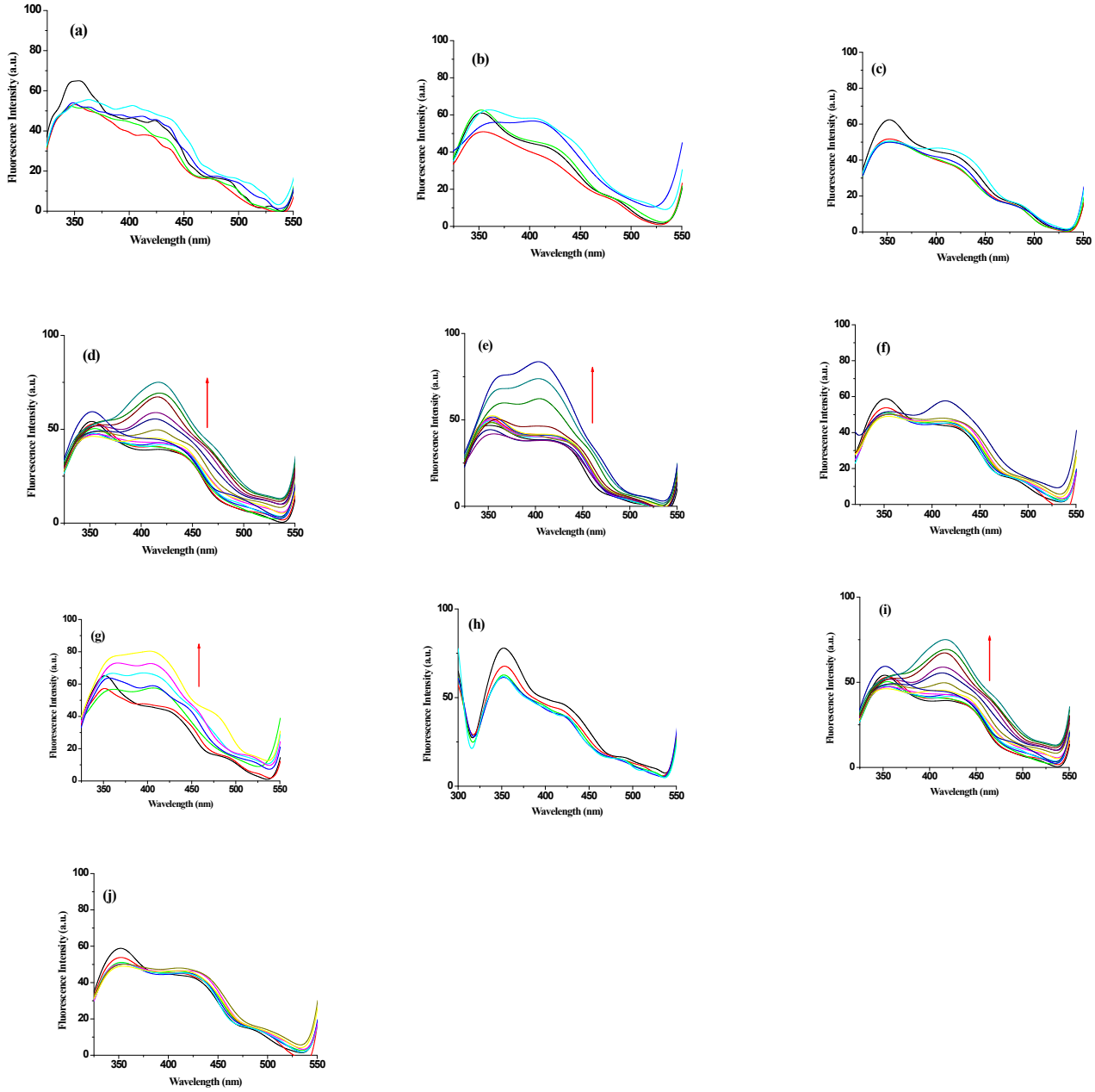


Figure 3S. Change in emission of **1** (c = 2.5 x 10^{-5} M) in CH_3CN-H_2O (1:1/v/v, using 10 mM HEPES, pH 6.4) upon addition of (a) OAc^-, (b) HSO_4^-, (c) NO_3^-, (d) $HP_2O_7^{3-}$, (e) F^-, (f) Cl^-, (g) Br^-, (h) I^-, (i) $H_2PO_4^-$ and (j) ClO_4^-; [anions were taken as their tetrabutylammonium salts and their concentrations were 1 x 10^{-3} M].

4. NOESY spectrum of the complex of 1.ATP

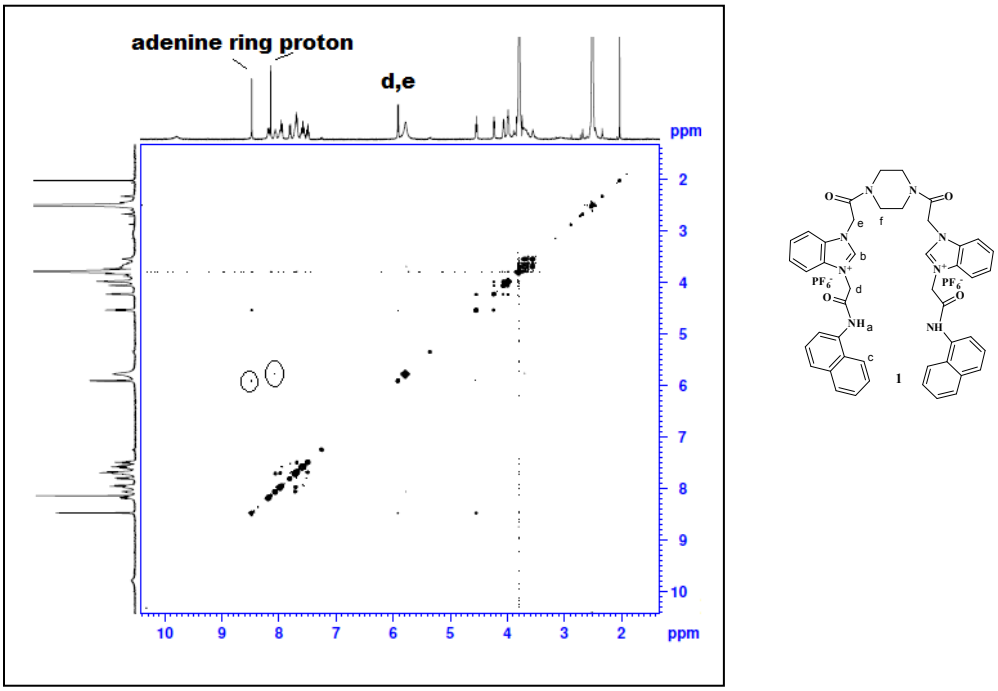


Figure 4S. NOESY spectrum of **1** in the presence of equivalent amount of ATP.

5. MTT assay for receptor 1.

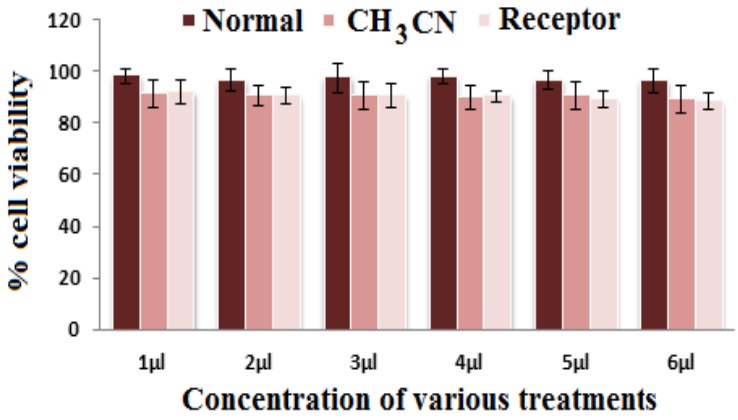
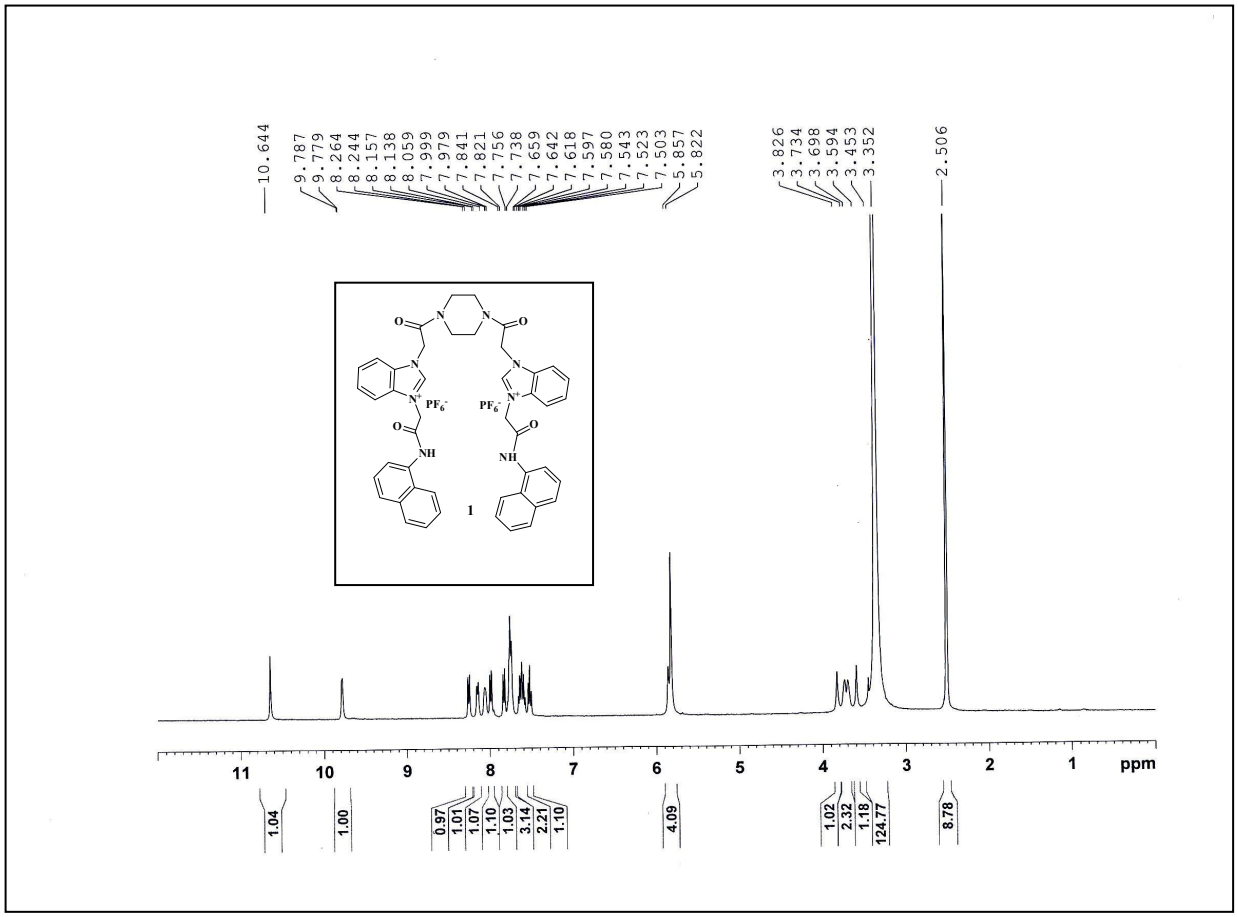


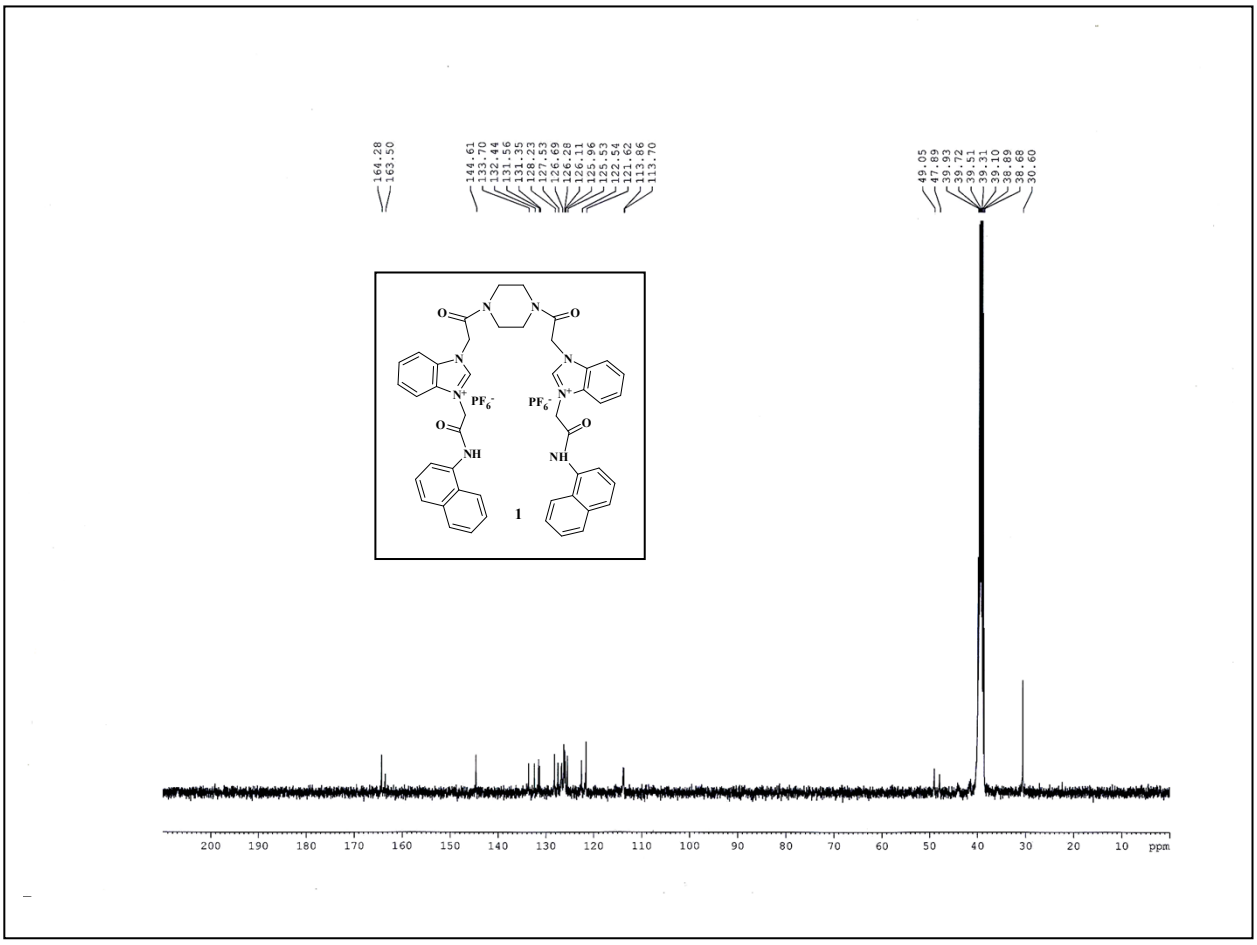
Figure 5S. MTT assay of receptor **1**

Spectral data

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



^{13}C NMR of 1 (100 MHz, d_6-DMSO):



Mass (HRMS) of 1: