

Supporting Information:

Recognition Study of Substituted Benzoic Acids by 7-Substituted Pterin Receptors in Solution and Solid Phases

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1. UV-vis titration spectra and Association constant determination curve:

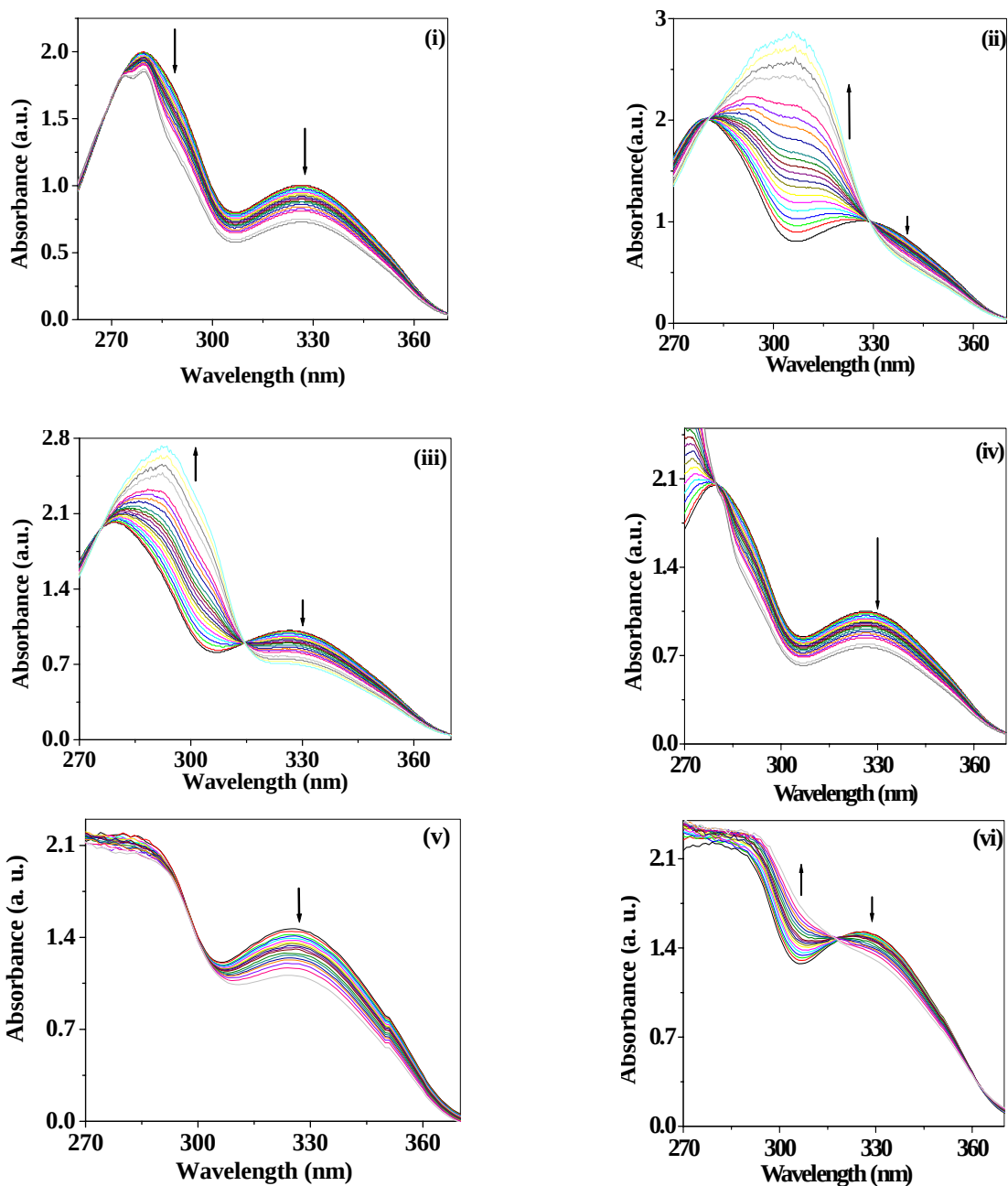


Figure 1: UV-vis titration spectra of receptor **1** ($1.69 \times 10^{-4} \text{ mL}^{-1}$) with substituted benzoic acids: (i) benzoic acid; (ii) 2-hydroxybenzoic acid; (iii) 3-hydroxybenzoic acid; (iv) 4-hydroxybenzoic acid; (v) 3-nitrobenzoic acid and (vi) 4-nitrobenzoic acid.

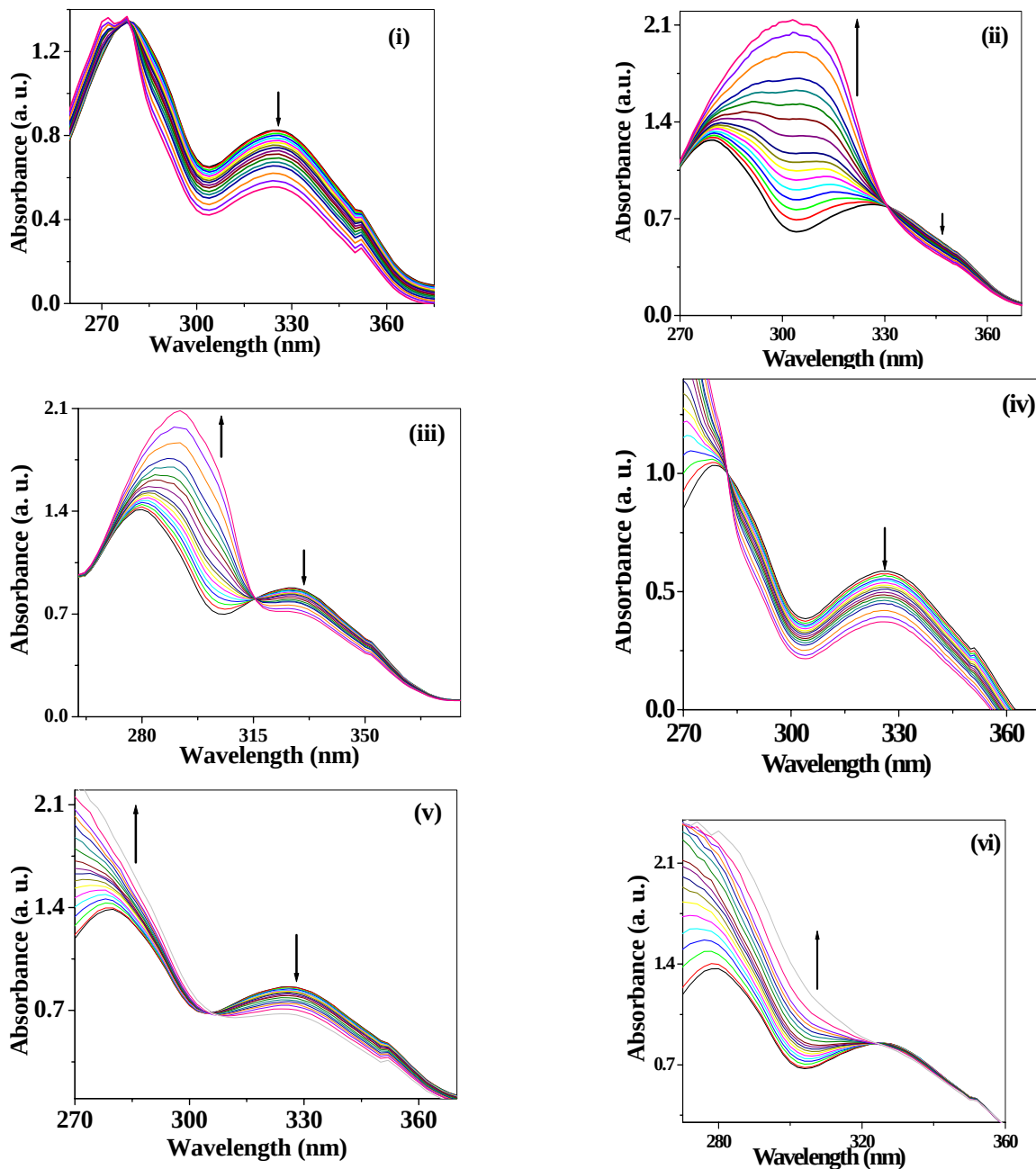
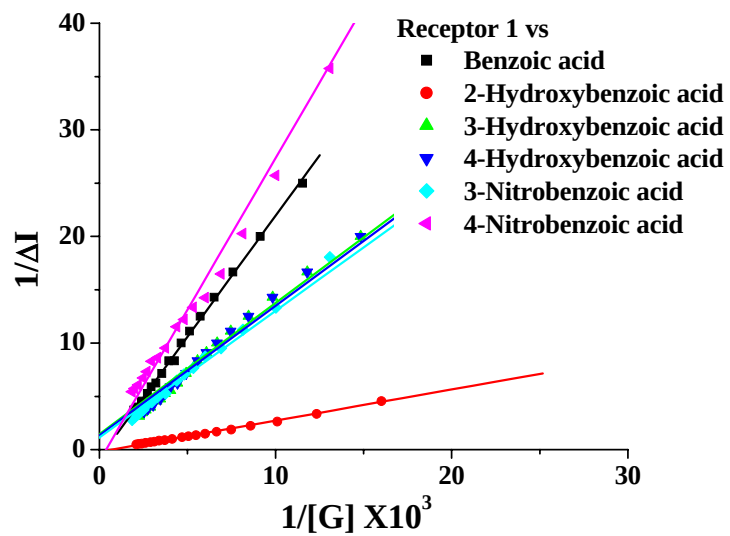
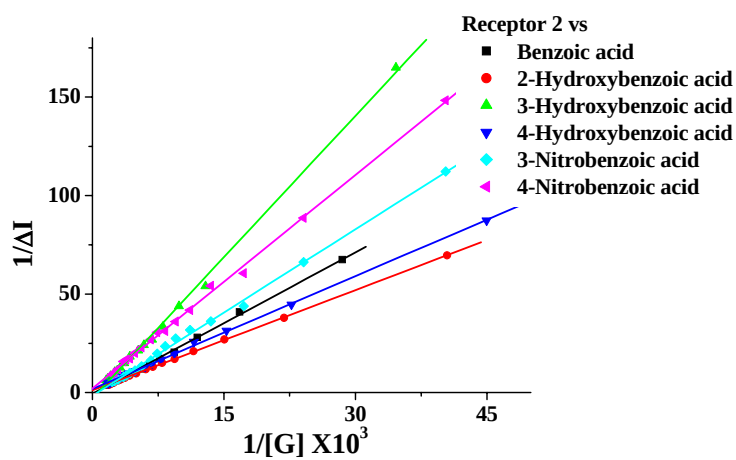


Figure 2: UV-vis titration spectra of receptor **2** ($1.12 \times 10^{-4} \text{ mL}^{-1}$) with substituted benzoic acids: (i) benzoic acid; (ii) 2-hydroxybenzoic acid; (iii) 3-hydroxybenzoic acid; (iv) 4-hydroxybenzoic acid; (v) 3-nitrobenzoic acid and (vi) 4-nitrobenzoic acid.



(i)



(ii)

Figure 3: Binding constant calculation curve of (i) receptor 1; (ii) receptor 2 with different aromatic acids by UV-vis titration method in acetonitrile.

2. Fluorescence titration spectra and association constants determination curves:

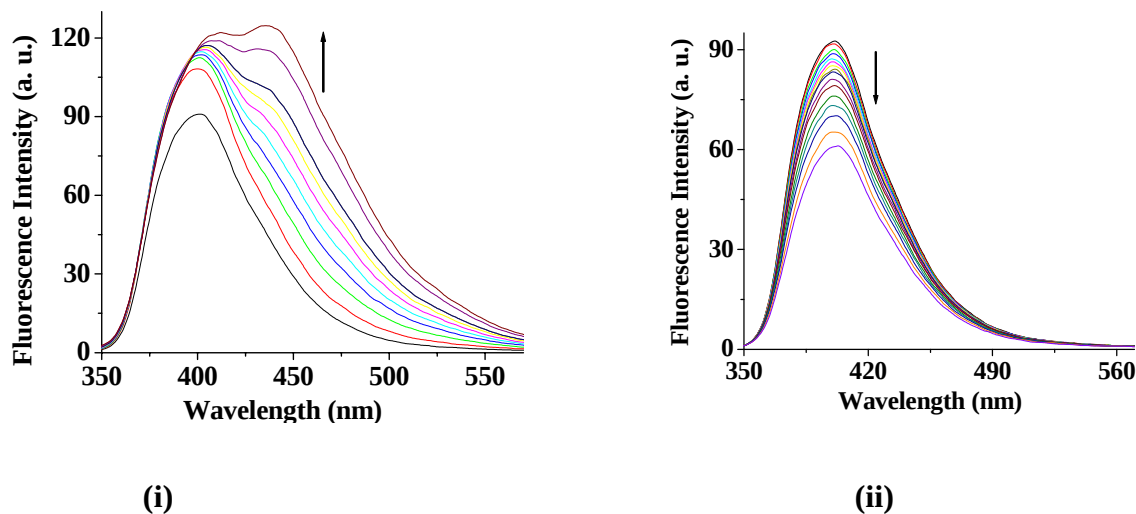


Figure 4: Fluorescence titration spectra of receptor **1** ($1.53 \times 10^{-4} \text{ mL}^{-1}$) with aromatic acids: (i) 2-hydroxybenzoic acid and (ii) 4-nitrobenzoic acid in acetonitrile solution.

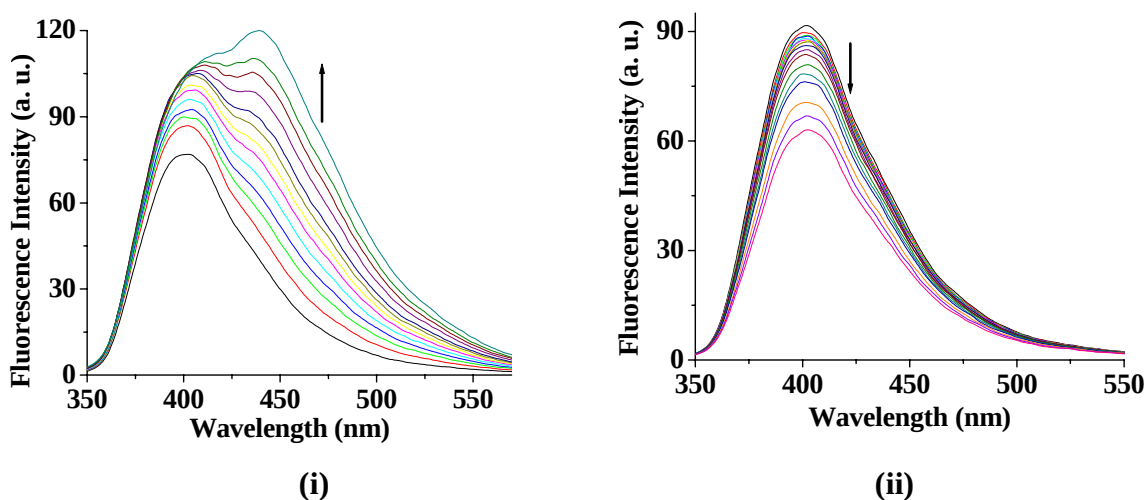
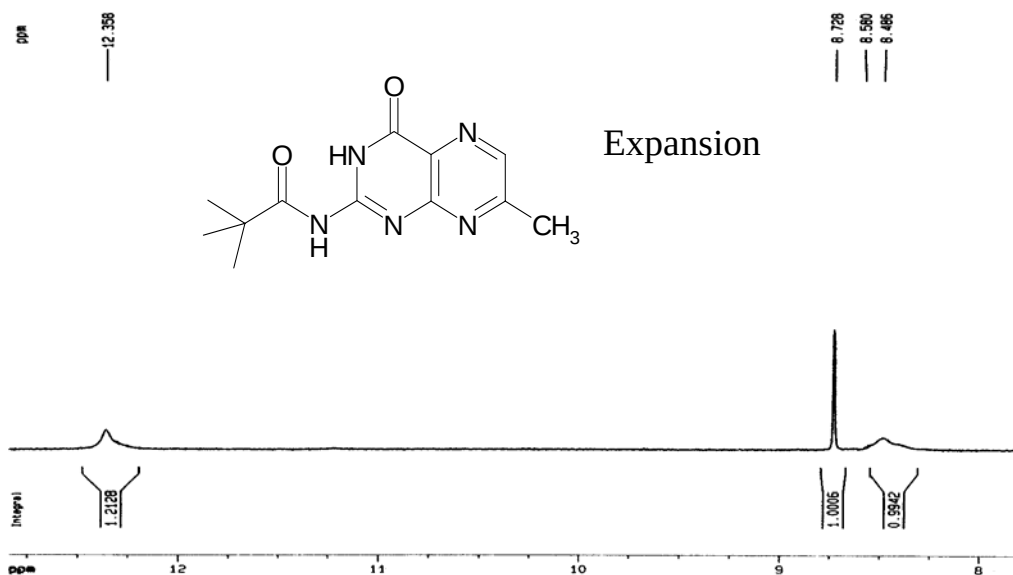
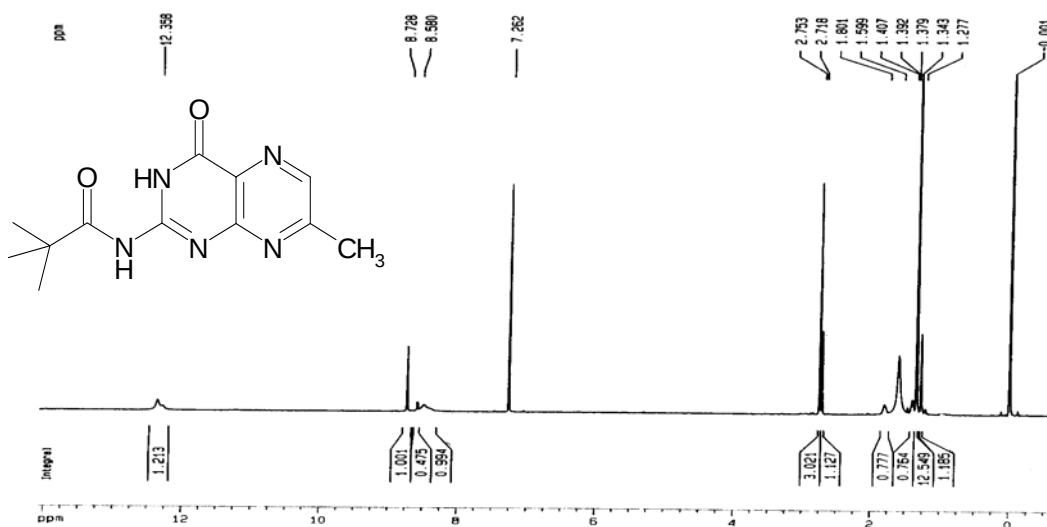
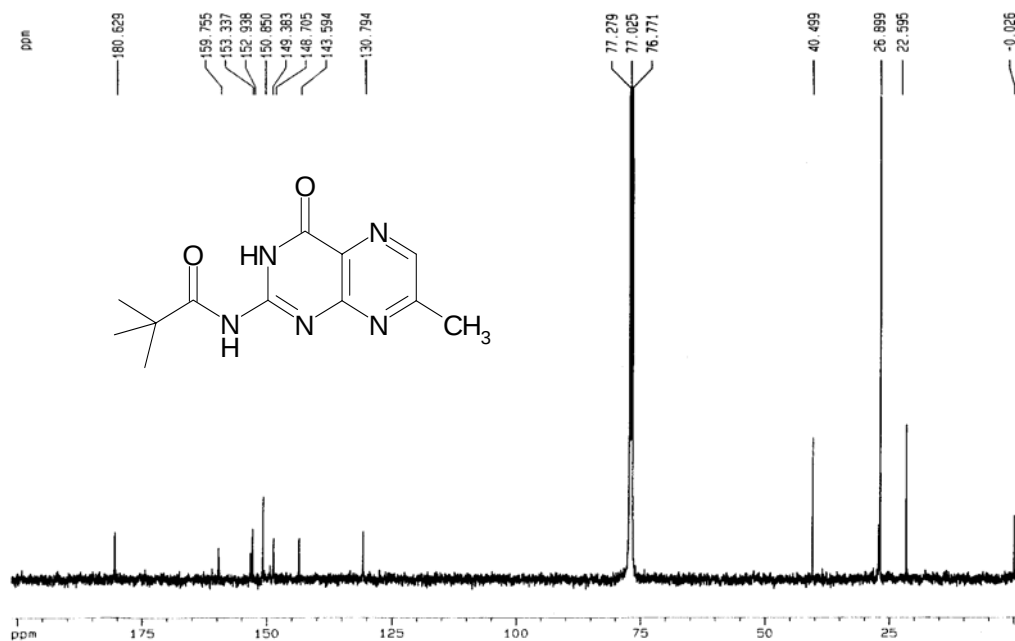


Figure 5: Fluorescence titration spectra of receptor **2** ($1.12 \times 10^{-4} \text{ mL}^{-1}$) with aromatic acids: (i) 2-hydroxybenzoic acid; (ii) 4-nitrobenzoic acid in acetonitrile solvent.

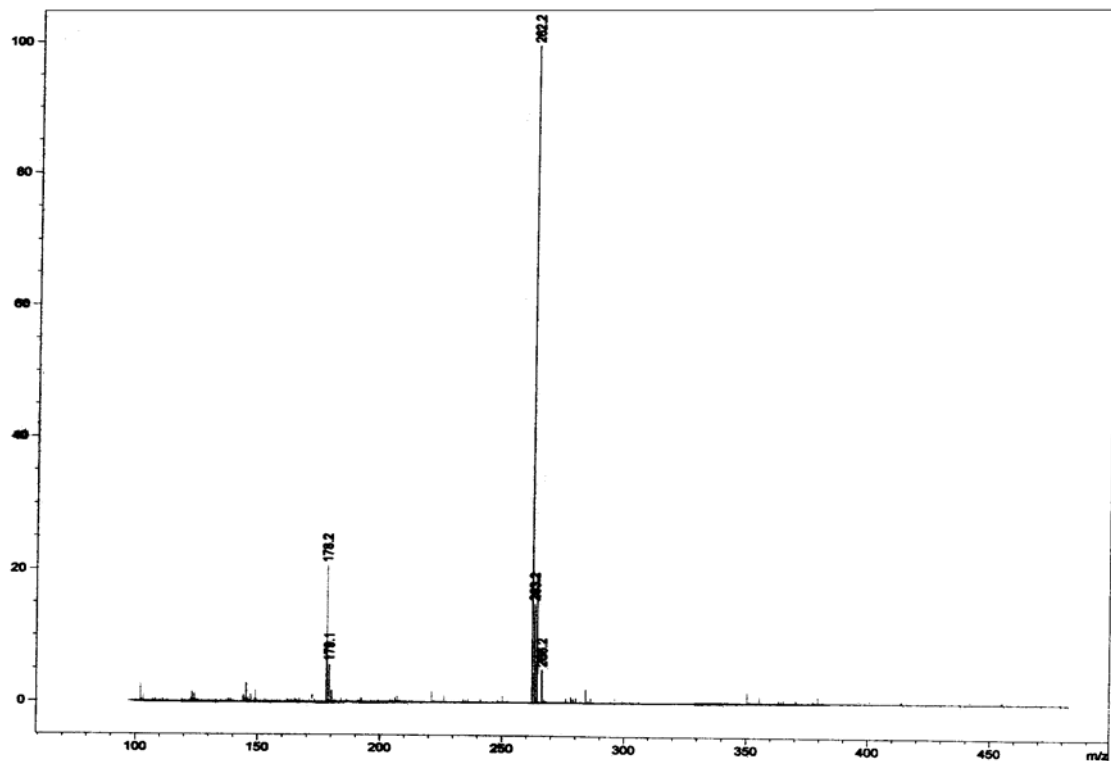
3. ^1H NMR (500 MHz) of receptor 1:



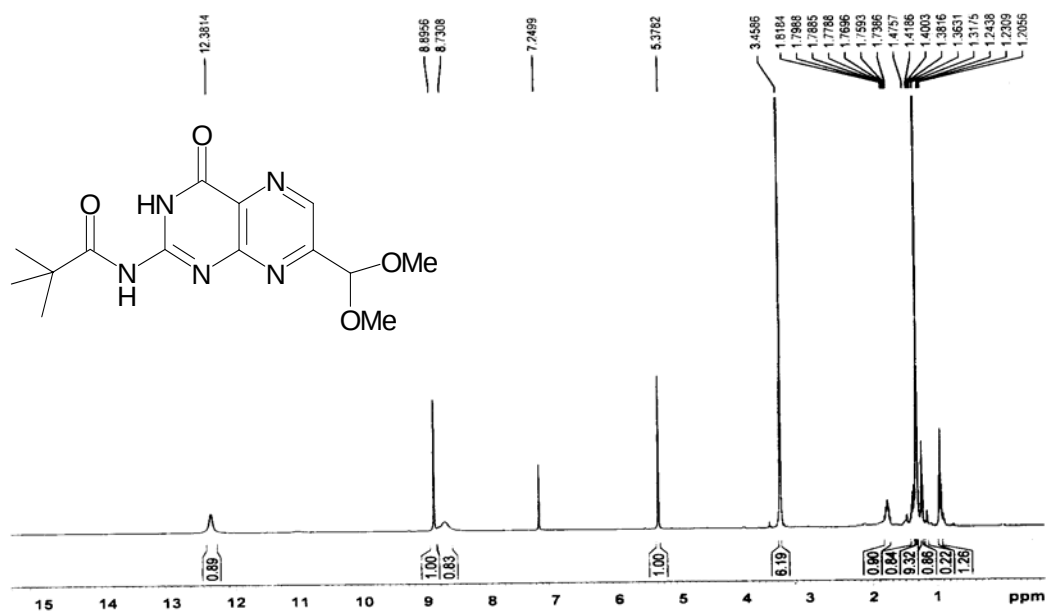
4. ^{13}C NMR (125 MHz) of receptor 1:



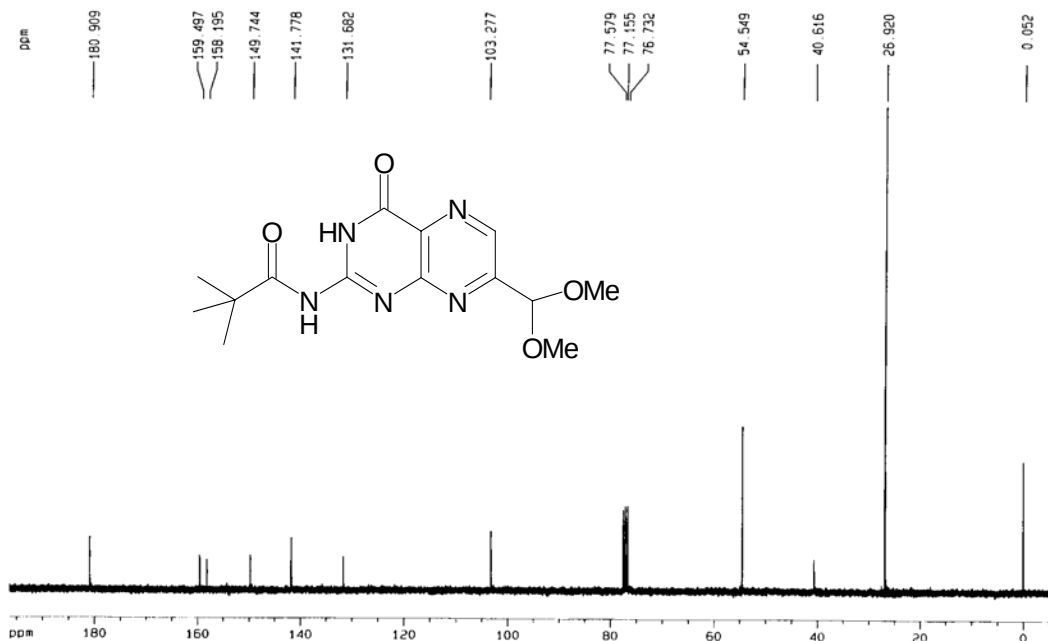
5. Mass spectra of receptor 1:



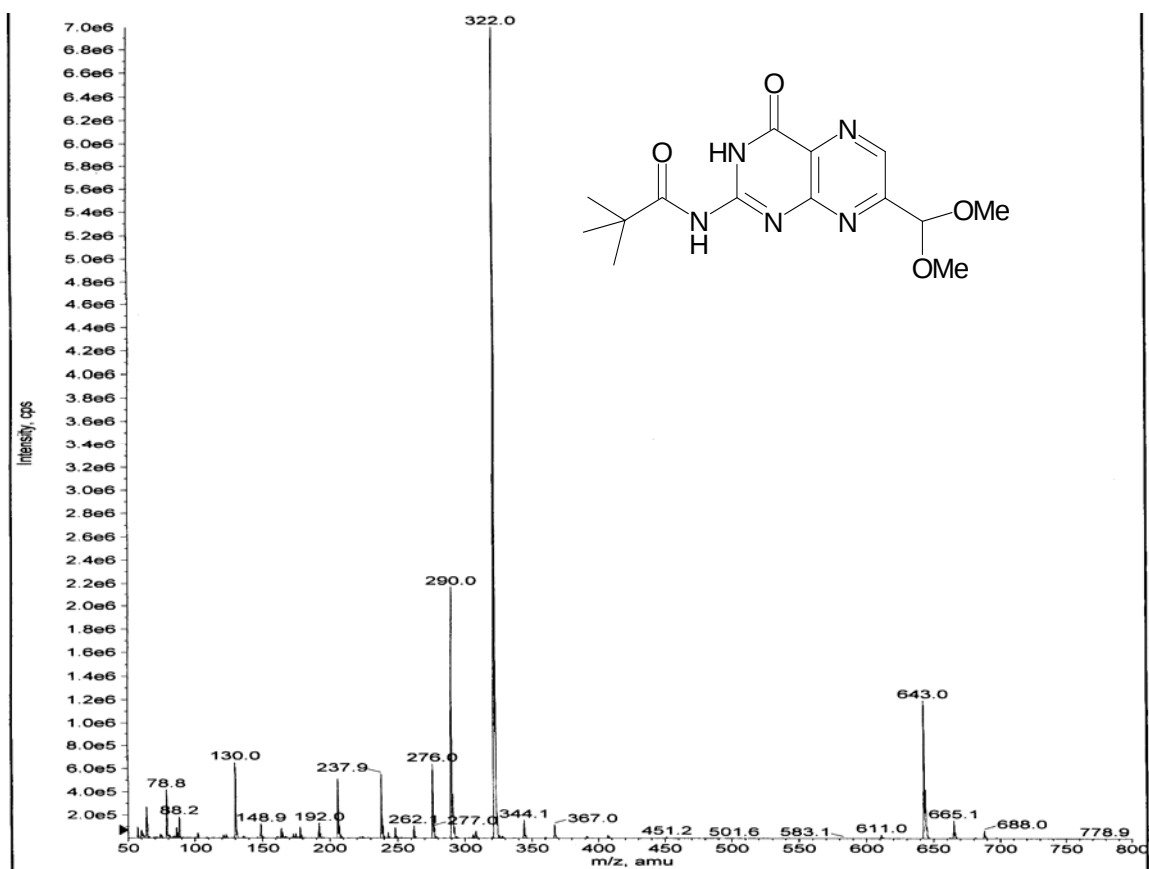
6. ^1H NMR (500 MHz) of receptor 2:



7. ^{13}C NMR (75 MHz) of receptor 2:



8. Mass spectra of receptor 2: 322.0 (M+H)⁺



9. ^1H NMR (500 MHz) of receptor 1 with 3-hydroxybenzoic acid:

