

SUPPORTING INFORMATION

GLUCOPYRANOSYL-1,4-DIHYDROPYRIDINE AS A NEW FLUORESCENT CHEMOSENSOR FOR SELECTIVE DETECTION OF 2,4,6-TRINITROPHENOL

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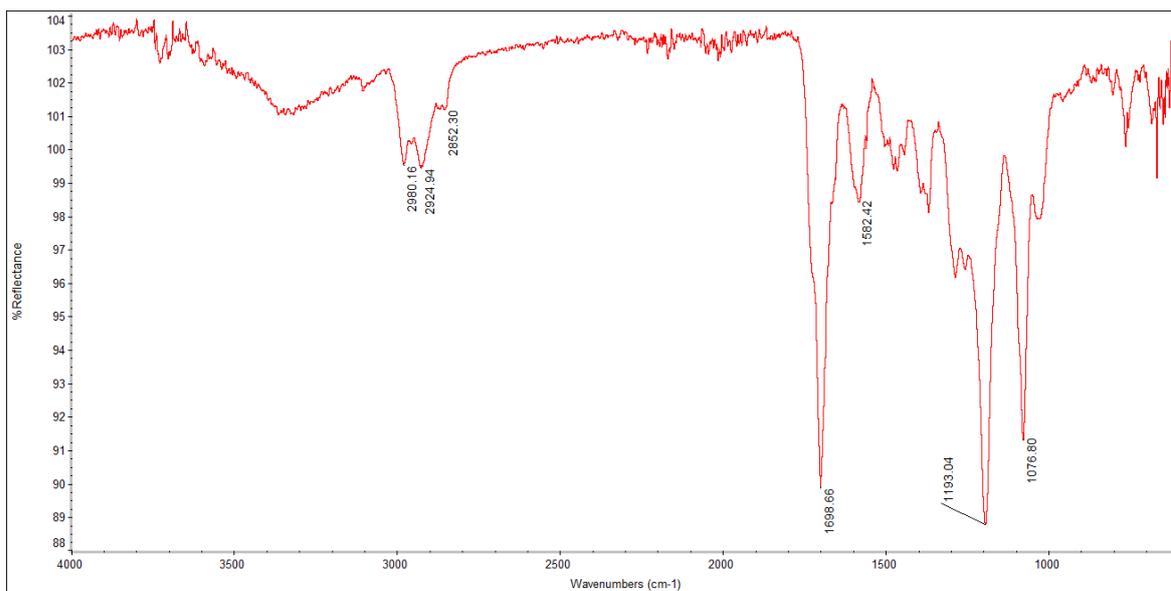
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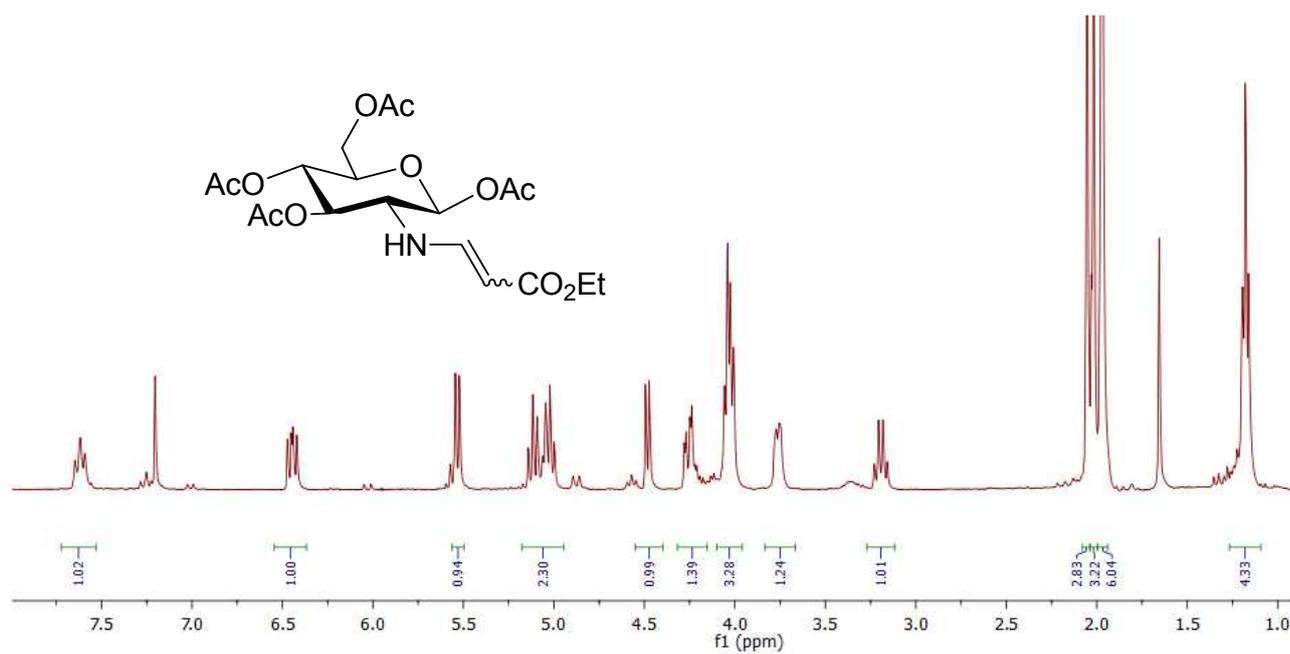
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- S1.** The IR of glucopyranosyl-1,4-dihydropyridine (Glc-DHP).
- S2.** The ¹H NMR of ethyl β-amino acrylate **2** in CDCl₃.
- S3.** The ¹H NMR of glucopyranosyl-1,4-dihydropyridine (Glc-DHP) in CDCl₃.
- S4.** The ¹³C NMR ethyl β-amino acrylate **2** in CDCl₃.
- S5.** The ¹³C NMR of glucopyranosyl-1,4-dihydropyridine (Glc-DHP) in CDCl₃.
- S6.** The HRMS of ethyl β-amino acrylate **2** and glucopyranosyl-1,4-dihydropyridine (Glc-DHP).
- S7.** Fluorescence quenching effects of 14 metal ions
- S8.** Fluorescence intensity of Glc-DHP 1 μM in various pHs.
- S9.** Absorption spectra of TNP in various pHs.
- S10.** Absorption spectra of DNP in various pHs.
- S11.** Absorption spectra of 4NP in various pHs.
- S12.** Absorption spectra of 3NP in various pHs.
- S13.** Absorption spectra of 2NP in various pHs.
- S14.** Calculation of the critical distance (R_0) between fluorescent donor (Glc-DHP) and acceptor (TNP) when the efficiency of transfer = 50%.
- S15.** (A) Change in fluorescence spectra of Glc-DHP (1 μM) with the addition of 4NP at pH 3. (B) Stern-Volmer plot in response to 4NP at pH 3.

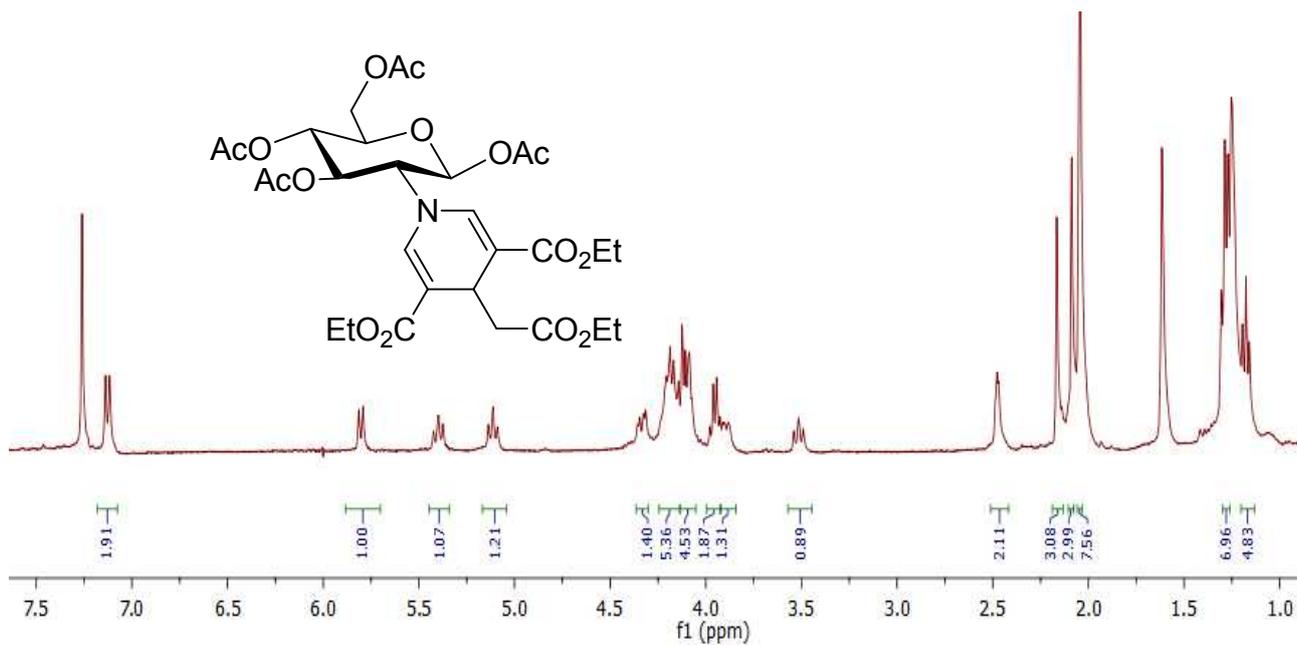
- S16.** (A) Change in fluorescence spectra of Glc-DHP (1 μM) with the addition of DNP at pH 3. (B) Stern-Volmer plot in response to DNP at pH 3.
- S17.** (A) Change in fluorescence spectra of Glc-DHP (1 μM) with the addition of TNP at pH 3. (B) Stern-Volmer plot in response to TNP at pH 3.
- S18.** (A) Change in fluorescence spectra of Glc-DHP (1 μM) with the addition of 4NP at pH 5. (B) Stern-Volmer plot in response to 4NP at pH 5.
- S19.** (A) Change in fluorescence spectra of Glc-DHP (1 μM) with the addition of DNP at pH 5. (B) Stern-Volmer plot in response to DNP at pH 5.
- S20.** (A) Change in fluorescence spectra of Glc-DHP (1 μM) with the addition of TNP at pH 5. (B) Stern-Volmer plot in response to TNP at pH 5.
- S21.** (A) Change in fluorescence spectrum of Glc-DHP (1 μM) with the addition of 4NP at pH 8. (B) Stern-Volmer plot in response to 4NP at pH 8.
- S22.** (A) Change in fluorescence spectra of Glc-DHP (1 μM) with the addition of DNP at pH 8. (B) Stern-Volmer plot in response to DNP at pH 8.
- S23.** (A) Change in fluorescence spectra of Glc-DHP (1 μM) with the addition of TNP at pH 8. (B) Stern-Volmer plot in response to TNP at pH 8.
- S24.** Stern-Volmer plot in response to various NPs at pH 3.
- S25.** Stern-Volmer plot in response to various NPs at pH 5.
- S26.** Stern-Volmer plot in response to various NPs at pH 8.
- S27.** Stern-Volmer plot in response to various NPs at pH 3, 5, 8.



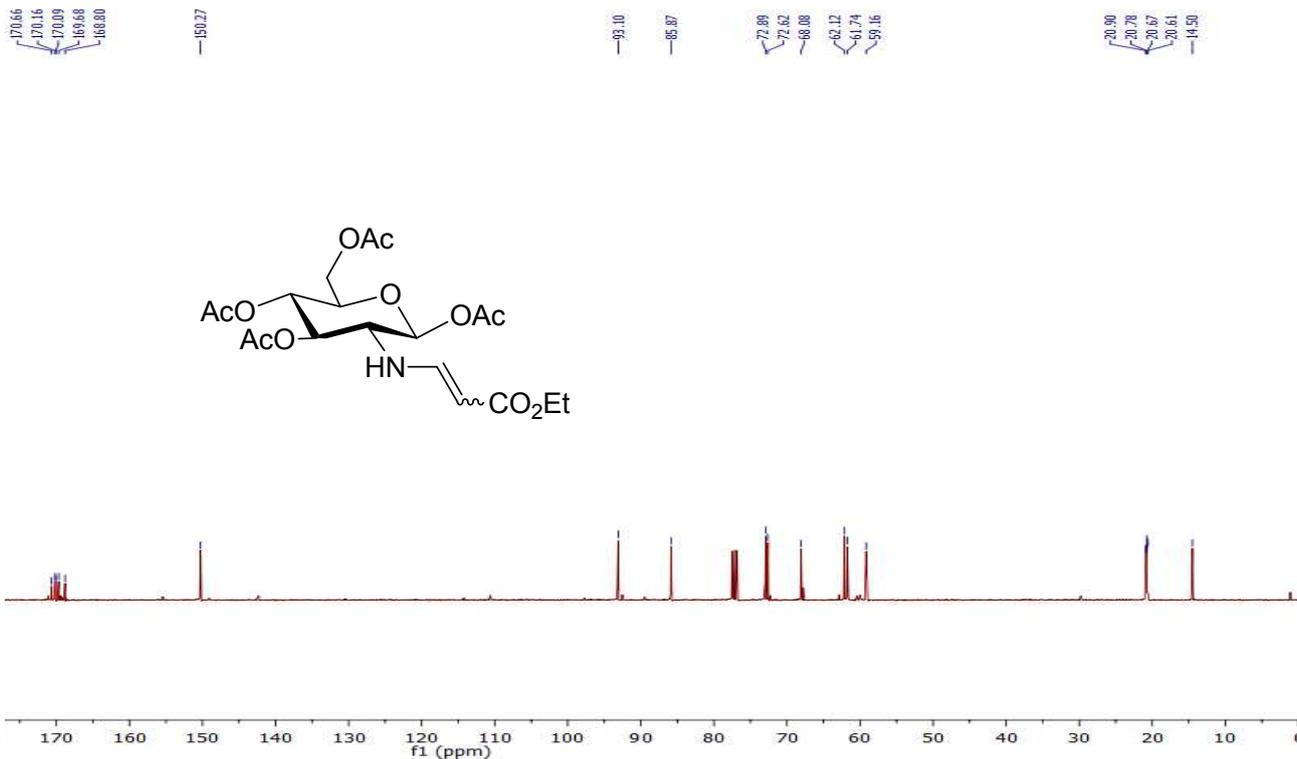
S1. The IR of glucopyranosyl-1,4-dihydropyridine (Glc-DHP).



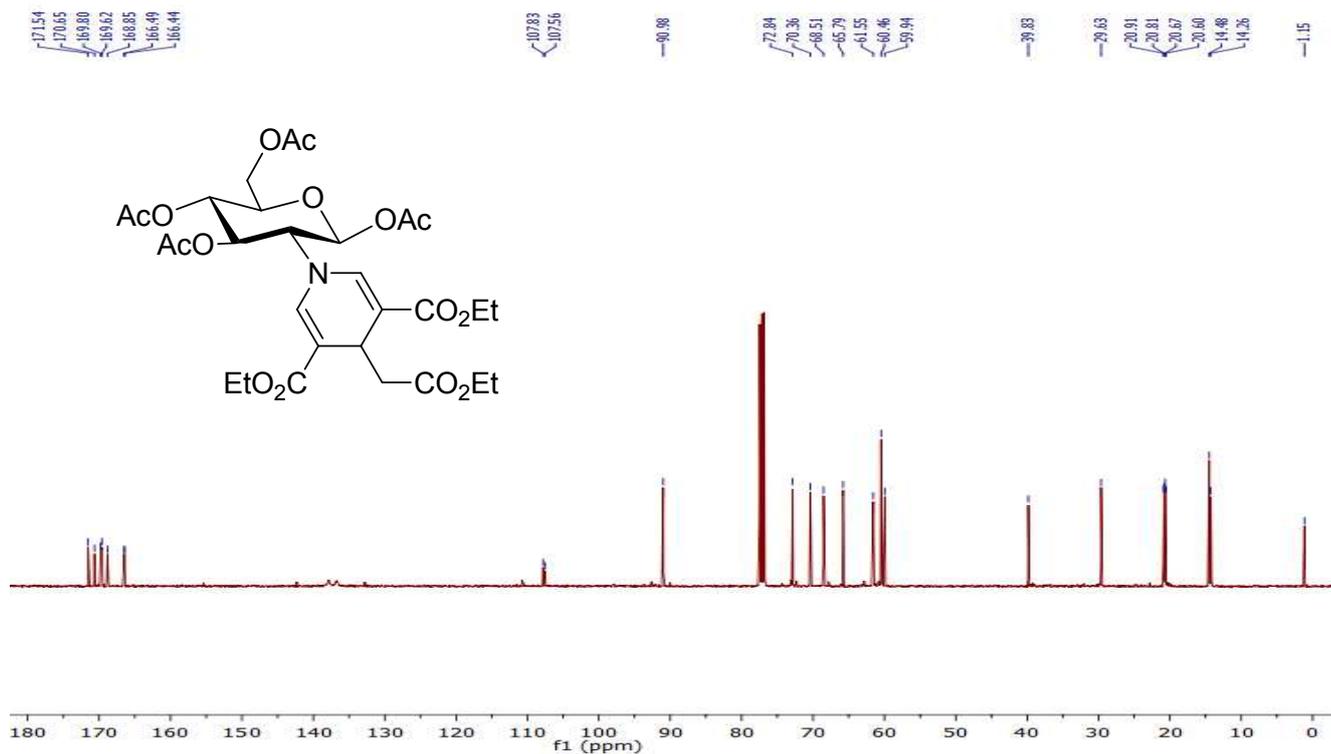
S2. The ^1H NMR of ethyl β -amino acrylate **2** in CDCl_3 .



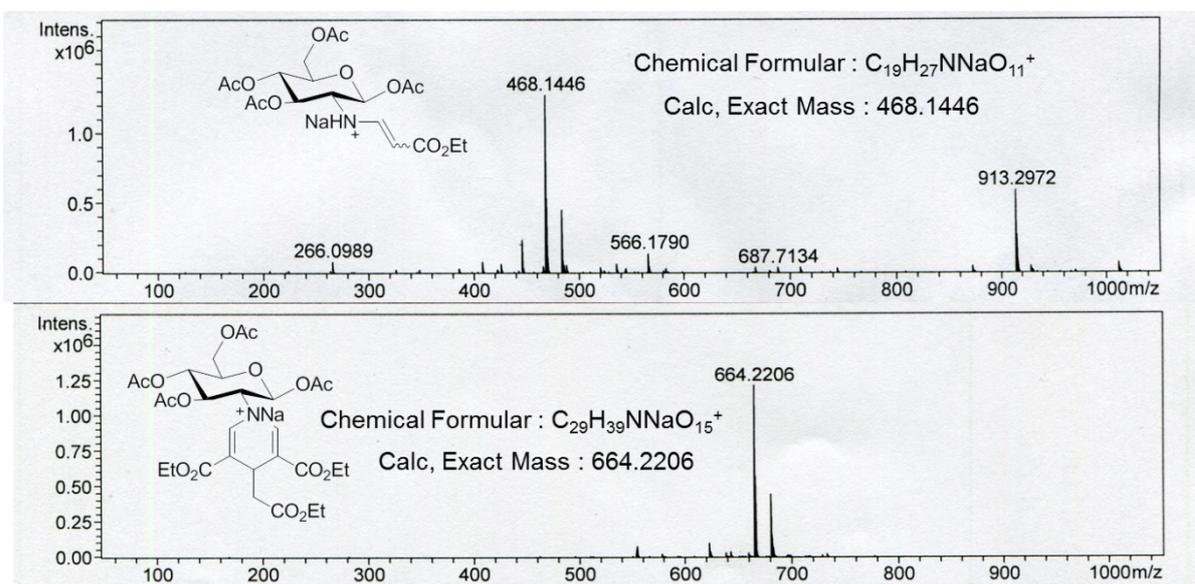
S3. The ¹H NMR of glucopyranosyl-1,4-dihydropyridine (Glc-DHP) in CDCl₃.



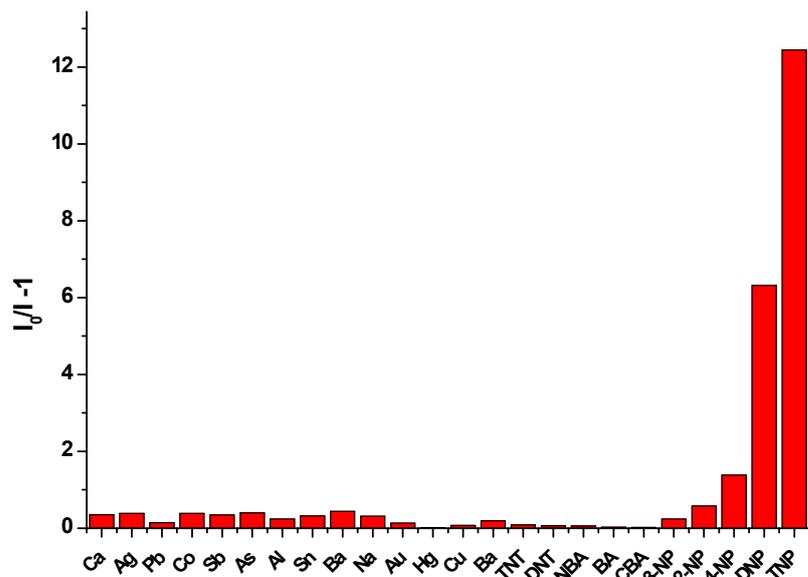
S4. The ¹³C NMR ethyl β-amino acrylate 2 in CDCl₃.



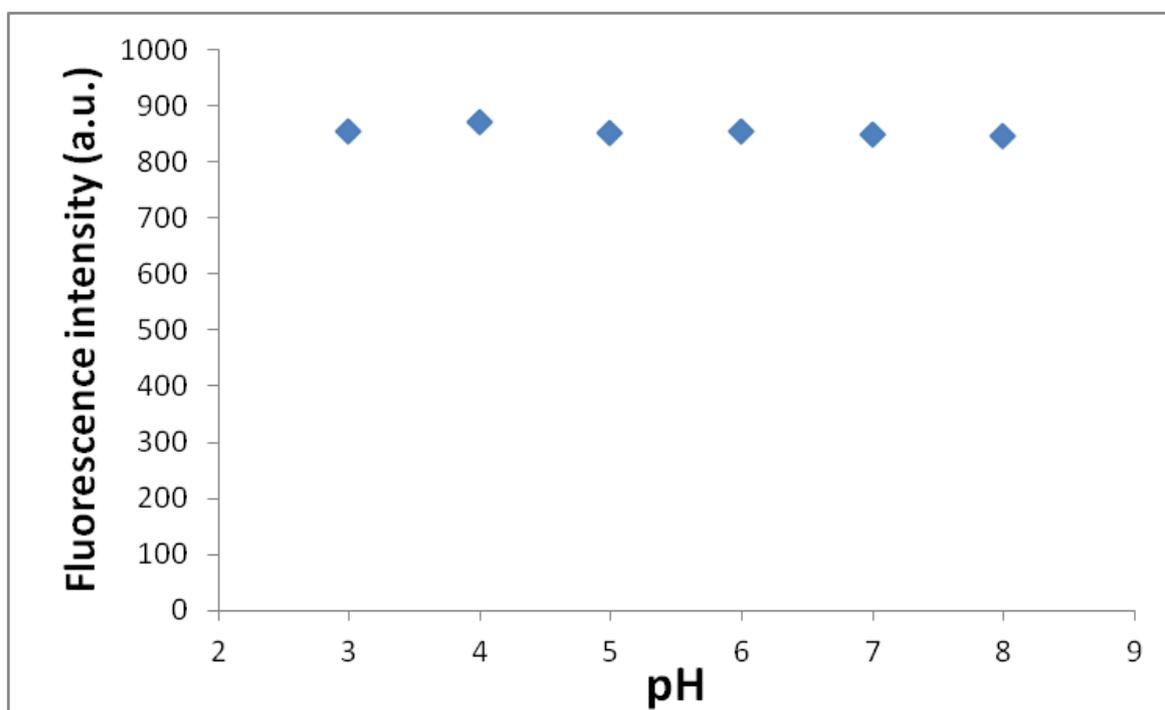
S5. The ^{13}C NMR of glucopyranosyl-1,4-dihydropyridine (Glc-DHP) in CDCl_3 .



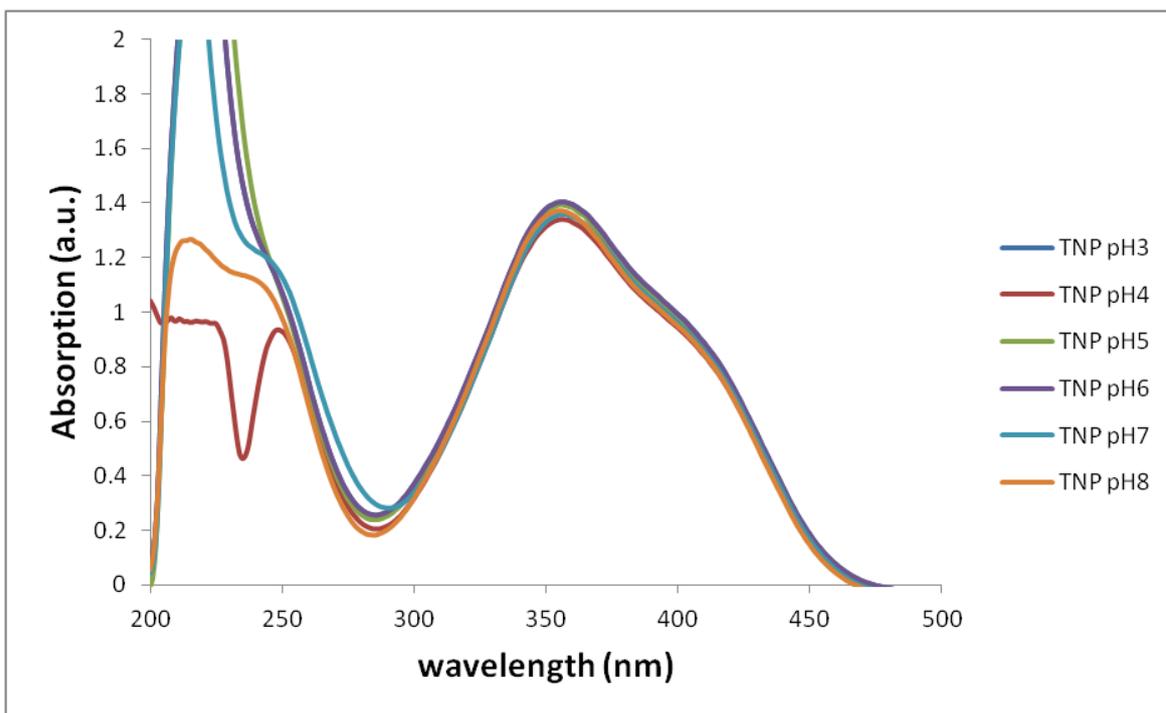
S6. The HRMS of ethyl β -amino acrylate **2** and glucopyranosyl-1,4-dihydropyridine (Glc-DHP).



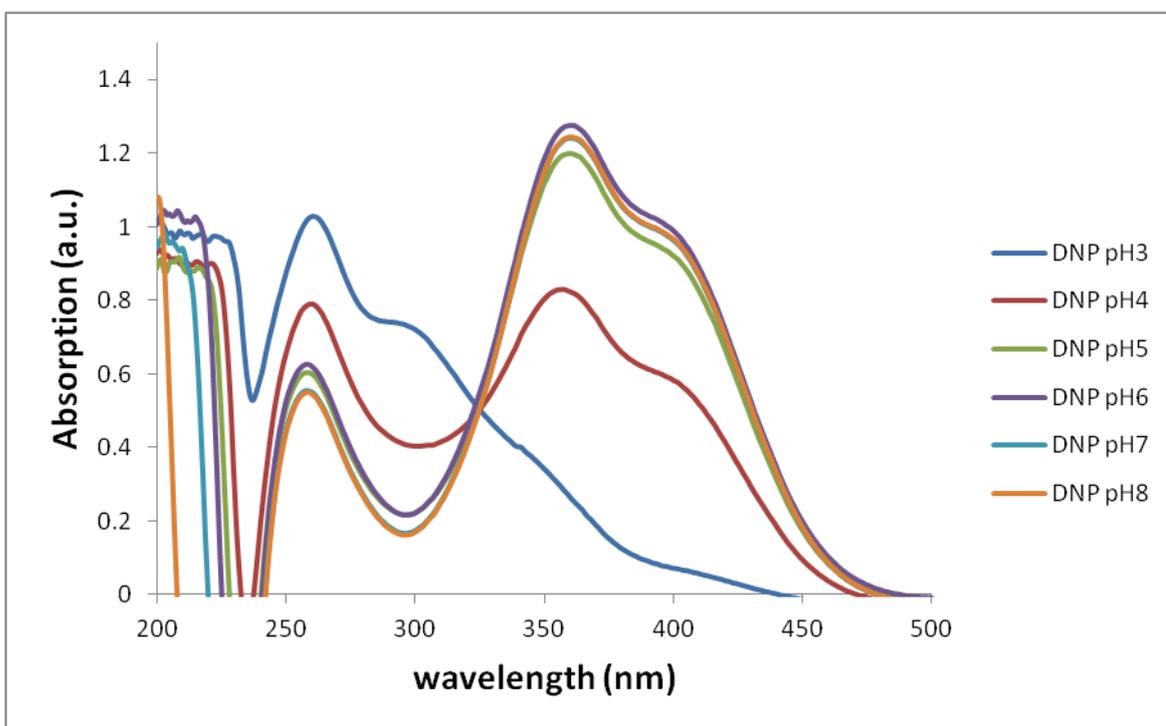
S7. Fluorescence quenching effects of 14 metal ions (Ca^{2+} , Ag^+ , Pb^{2+} , Co^{2+} , Sb^{5+} , As^{3+} , Al^{3+} , Sn^{2+} , Ba^{2+} , Na^+ , Au^+ , Hg^{2+} , Cu^{2+} , Ba^+) and 10 electron deficient aromatic compounds (TNT, DNT, NBA, BA, CBA, 3-NP, 2-NP, 4-NP, DNP, TNP) ($100\mu\text{M}$) on the fluorophores ($1\mu\text{M}$) in aqueous solution.



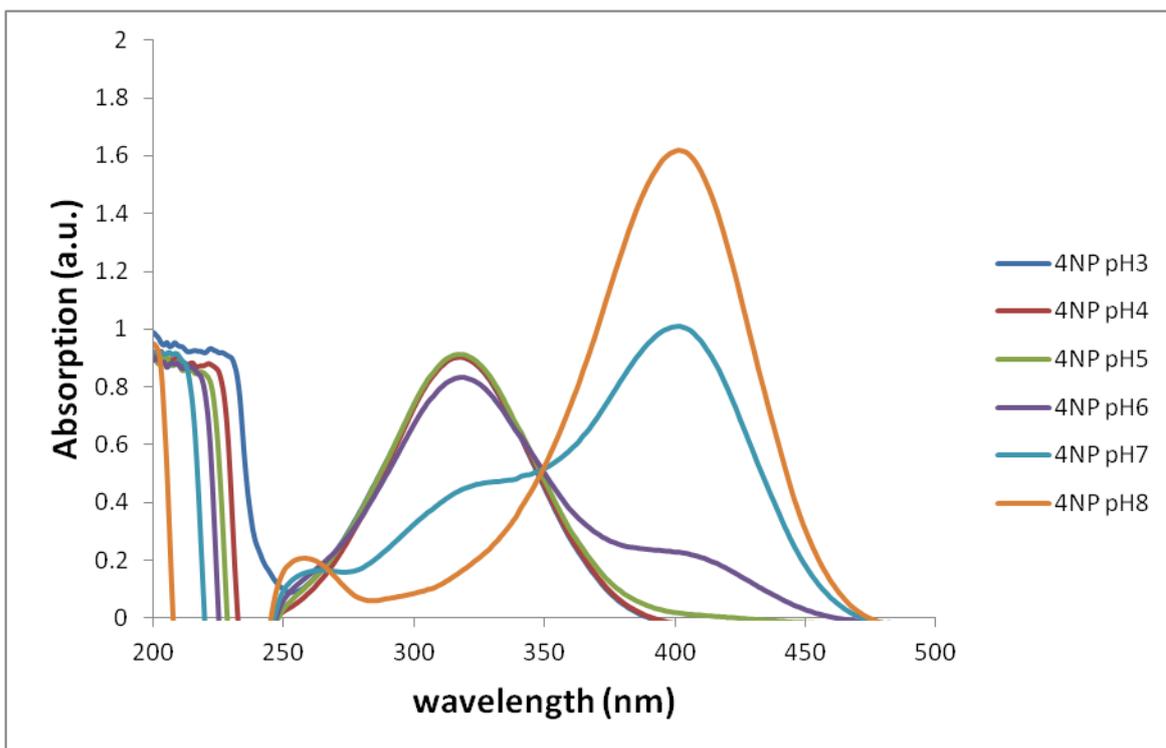
S8. Fluorescence intensity of Glc-DHP $1\mu\text{M}$ at $\lambda_{\text{max}} = 450\text{ nm}$ in various pHs.



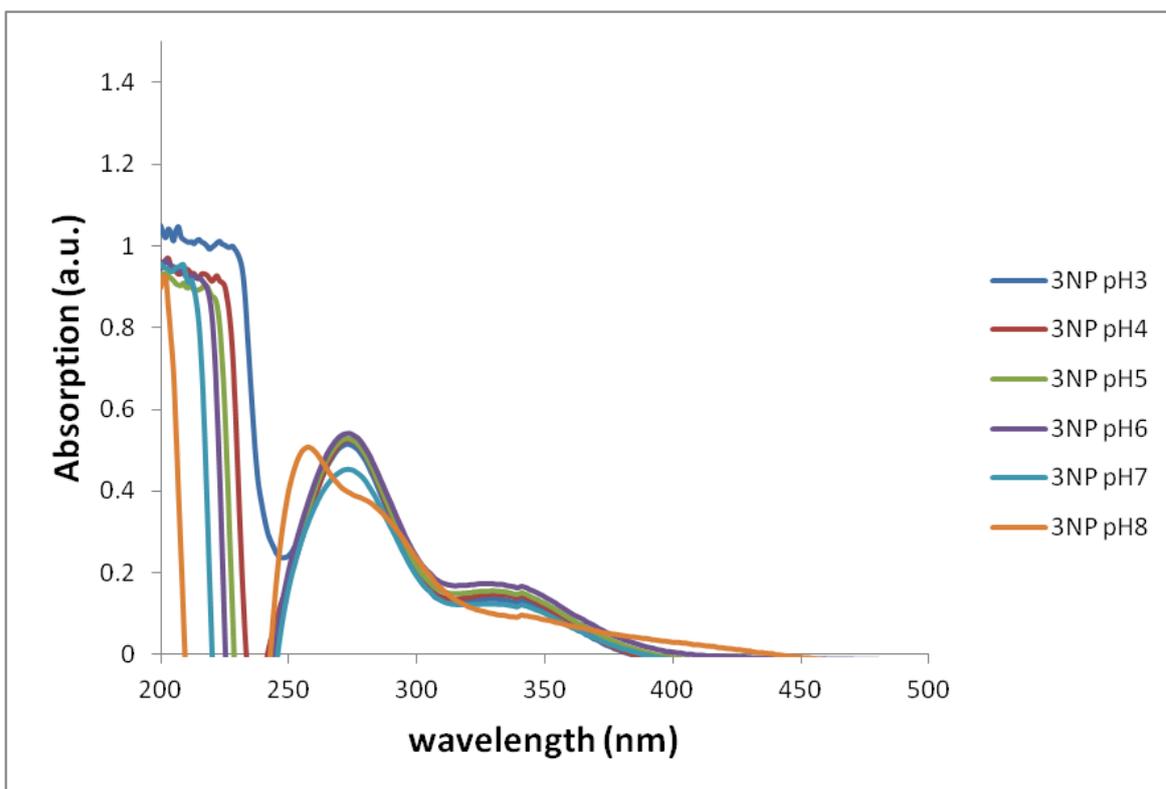
S9. Absorption spectra of TNP in various pHs.



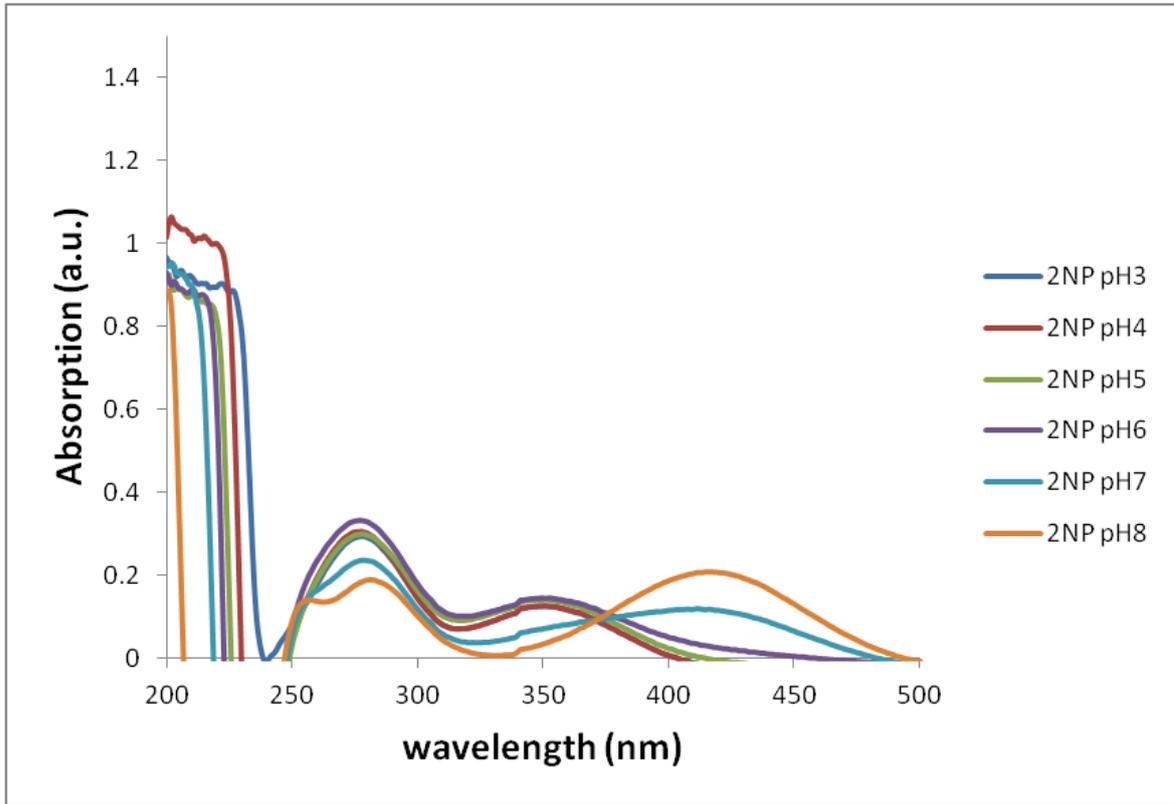
S10. Absorption spectra of DNP in various pHs.



S11. Absorption spectra of 4NP in various pHs.



S12. Absorption spectra of 3NP in various pHs.



S13. Absorption spectra of 2NP in various pHs.

S14. Calculation of the critical distance (R_0) between fluorescent donor (Glc-DHP) and acceptor (TNP) when the efficiency of transfer = 50%

According to the Förster theory, the efficiency of FRET between donor and acceptor also depends on the distance between the fluorescent donor and the acceptor, which is lower than 8 nm. The critical distance (R_0) between fluorescent donor (Glc-DHP) and acceptor (TNP) when the efficiency of transfer = 50% was estimated by the calculation using the following equation (eq. [5]).

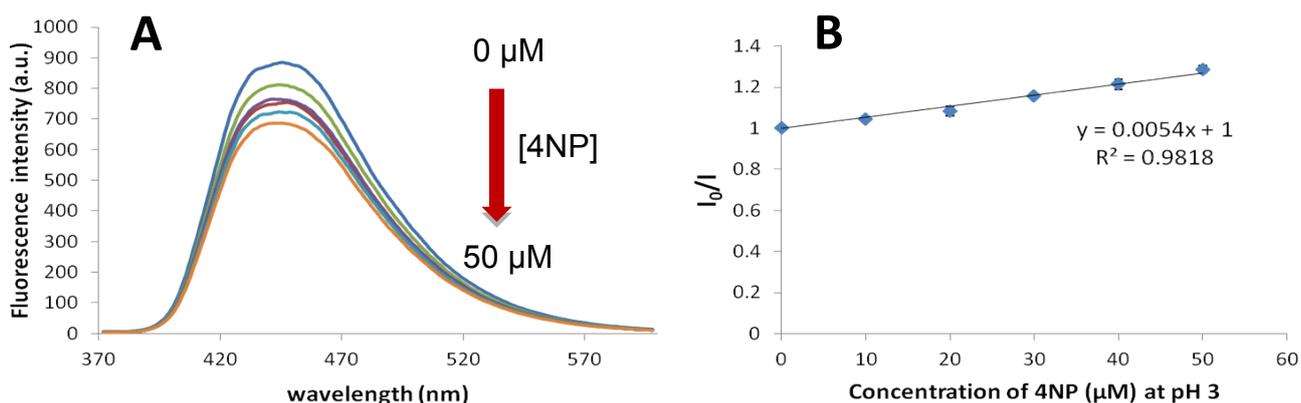
$$R_0^6 = 8.79 \times 10^{-25} K^2 N^{-4} \Phi J \quad [5]$$

In eq. [5], K^2 is the orientation related to the dipole geometry of the donor and the acceptor and $K^2 = 2/3$ for random orientation as in fluid solution; N is the average refracted index of medium in the wavelength range where spectral overlap is significant; Φ is the fluorescence quantum yield of the donor; J is the effect of the spectral overlap between the emission spectrum of the donor and the absorption spectrum of the acceptor, which could be calculated by the eq. [6]:

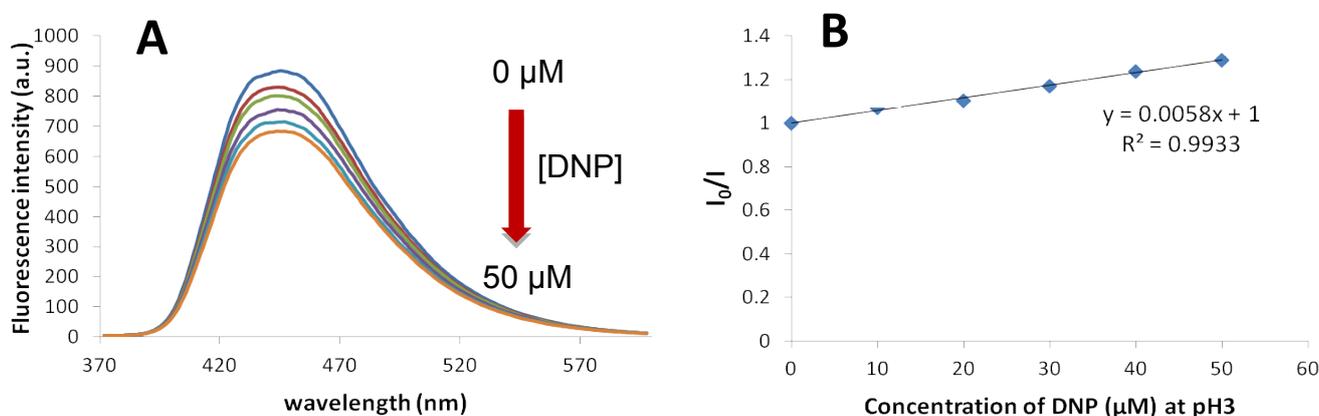
$$J = \frac{\int_0^{\infty} F(\lambda)\varepsilon(\lambda)\lambda^4 d\lambda}{\int_0^{\infty} F(\lambda)d\lambda} \quad [6]$$

where $F(\lambda)$ is the corrected fluorescence intensity of the donor in the wavelength range, from λ to $\lambda + \Delta\lambda$; $\varepsilon(\lambda)$ is the extinction coefficient of the acceptor at λ .

In the present case, $N = 1.33$, $\Phi = 0.29$ for Glc-DHP, according to eqs. [5]–[6], $J = 1.3264 \times 10^{-15} \text{ cm}^3 \text{ Lmol}^{-1}$ and $R_0 = 2.039 \text{ nm}$ could be determined. The critical average distance between a donor fluorophore and acceptor when the efficiency of transfer = 50% are 2-8 nm, which indicate that the energy transfer from Glc-DHP to TNP occurs with high probability.

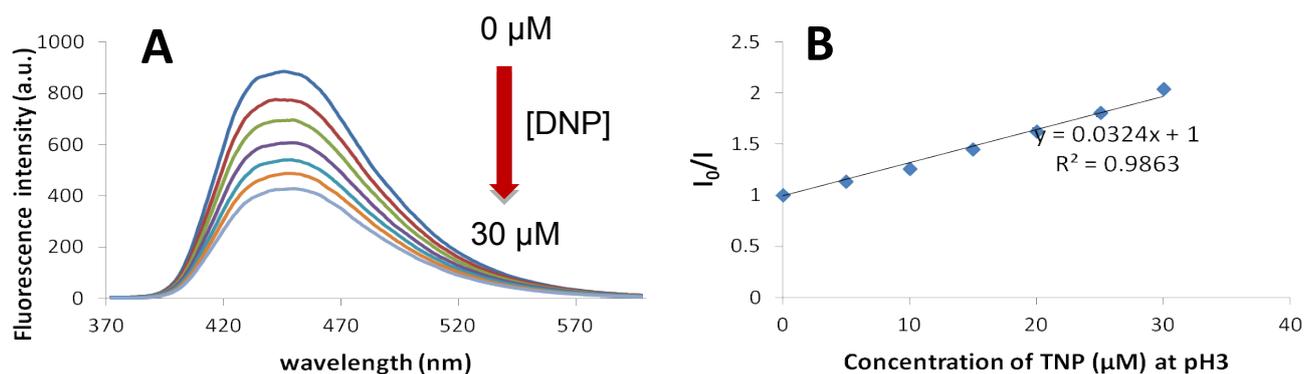


S15. (A) Change in fluorescence spectra of Glc-DHP (1 μM) with the addition of 4NP at pH 3. (B) Stern-Volmer plot in response to 4NP at pH 3.

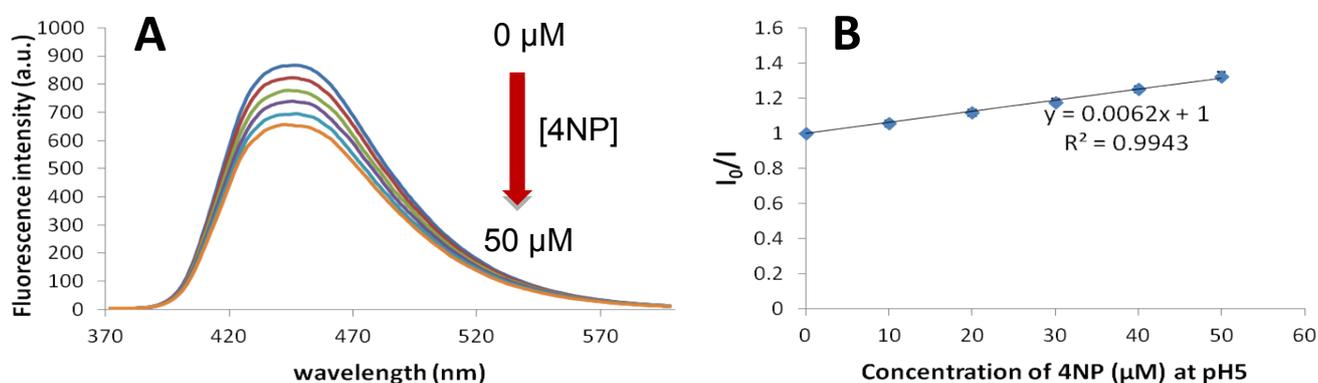


S16. (A) Change in fluorescence spectra of Glc-DHP (1 μM) with the addition

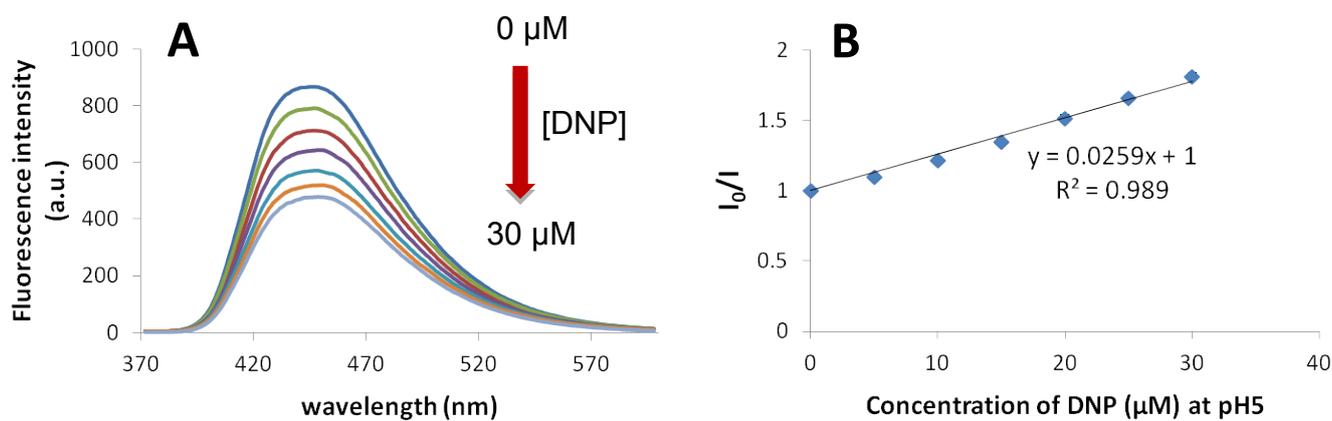
of DNP at pH 3. (B) Stern-Volmer plot in response to DNP at pH 3.



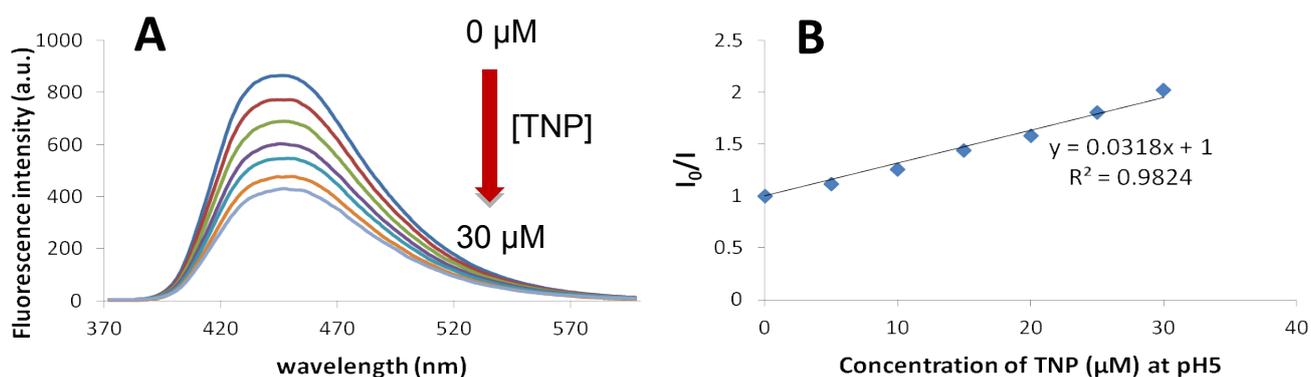
S17. (A) Change in fluorescence spectra of Glc-DHP (1 μM) with the addition of TNP at pH 3. (B) Stern-Volmer plot in response to TNP at pH 3.



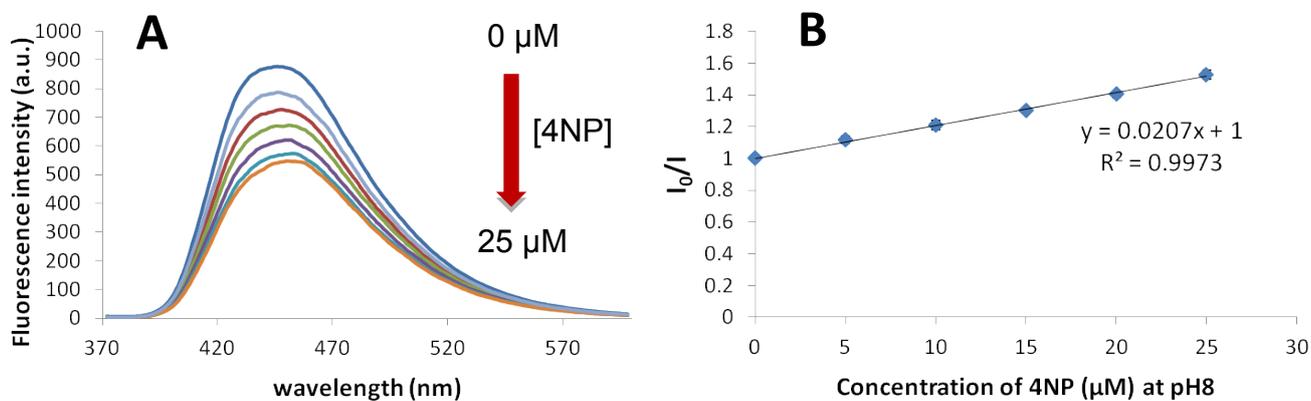
S18. (A) Change in fluorescence spectra of Glc-DHP (1 μM) with the addition of 4NP at pH 5. (B) Stern-Volmer plot in response to 4NP at pH 5.



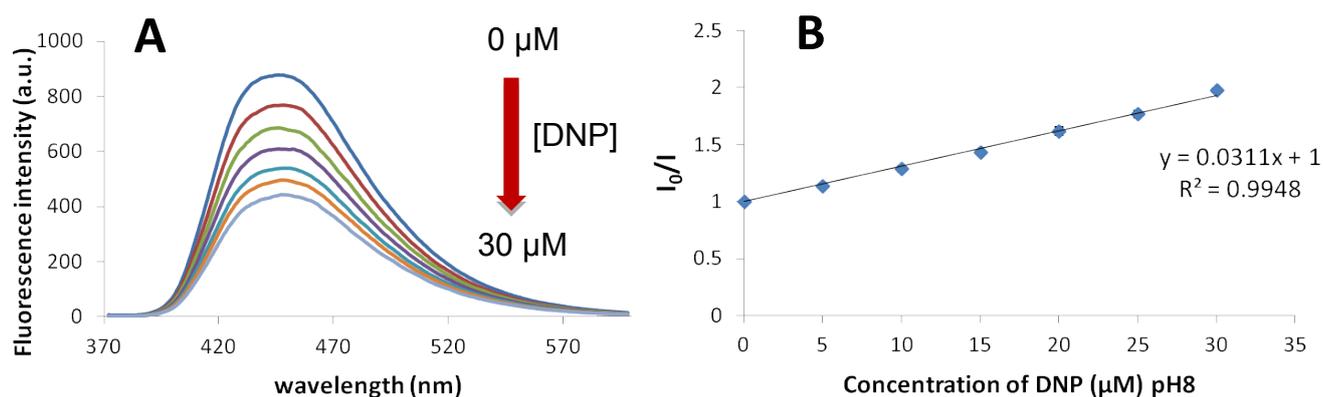
S19. (A) Change in fluorescence spectra of Glc-DHP (1 μM) with the addition of DNP at pH 5. (B) Stern-Volmer plot in response to DNP at pH 5.



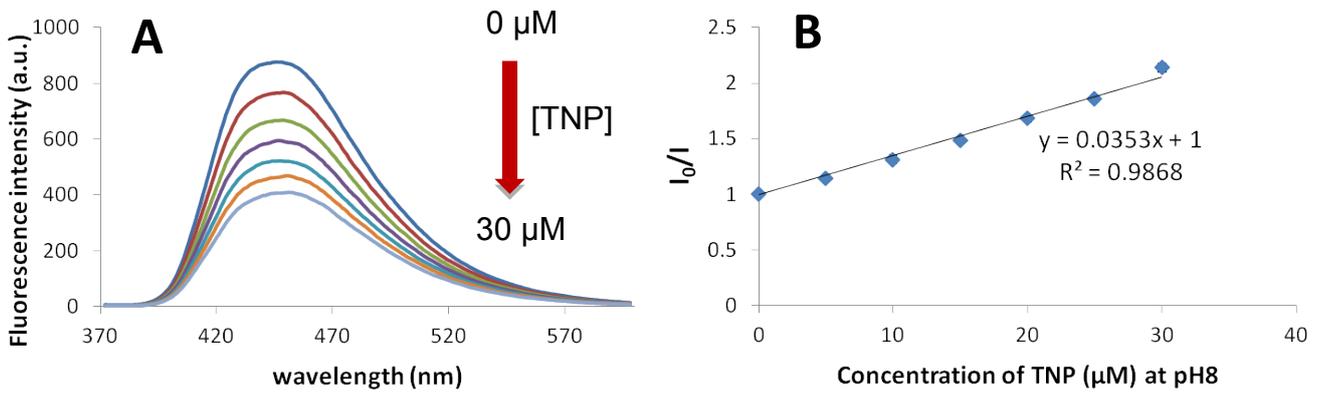
S20. (A) Change in fluorescence spectra of Glc-DHP (1 μM) with the addition of TNP at pH 5. (B) Stern-Volmer plot in response to TNP at pH 5.



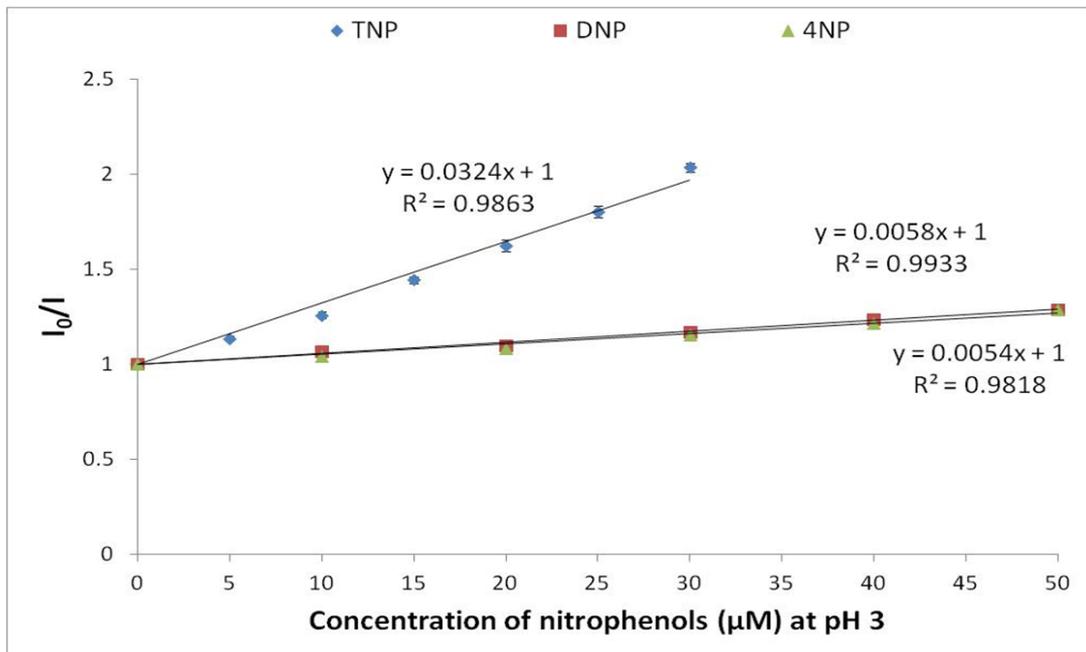
S21. (A) Change in fluorescence spectra of Glc-DHP (1 μM) with the addition of 4NP at pH 8. (B) Stern-Volmer plot in response to 4NP at pH 8.



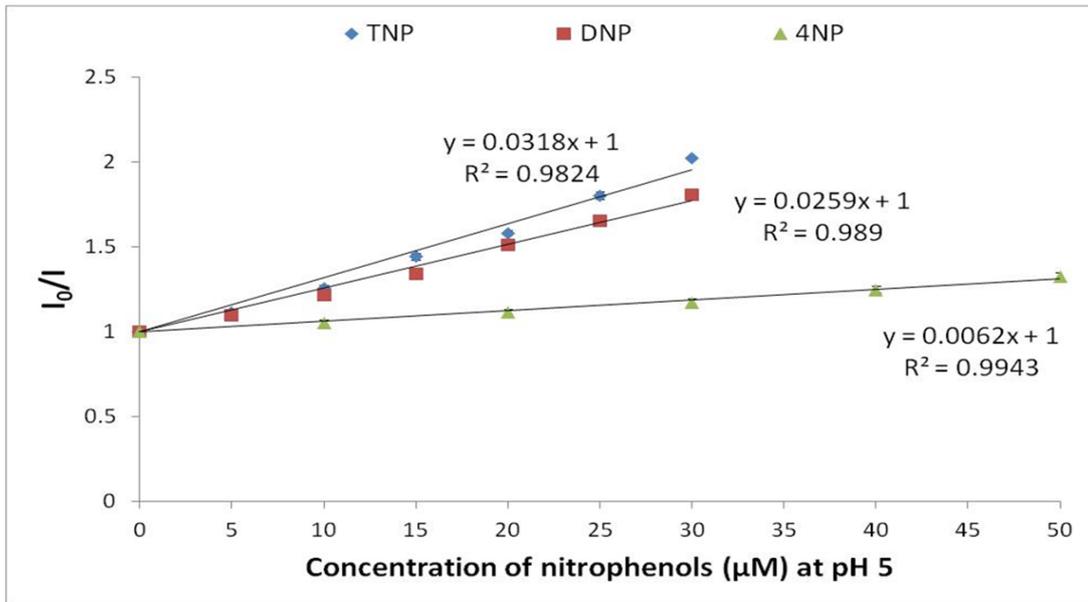
S22. (A) Change in fluorescence spectra of Glc-DHP (1 μM) with the addition of DNP at pH 8. (B) Stern-Volmer plot in response to DNP at pH 8.



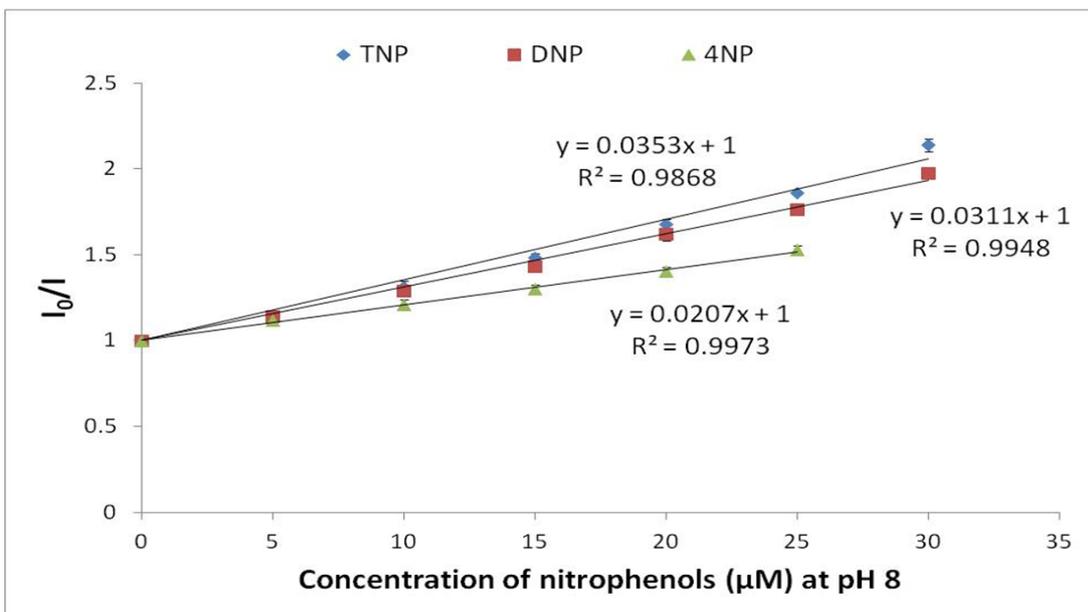
S23. (A) Change in fluorescence spectra of Glc-DHP (1 μM) with the addition of TNP at pH 8. (B) Stern-Volmer plot in response to TNP at pH 8.



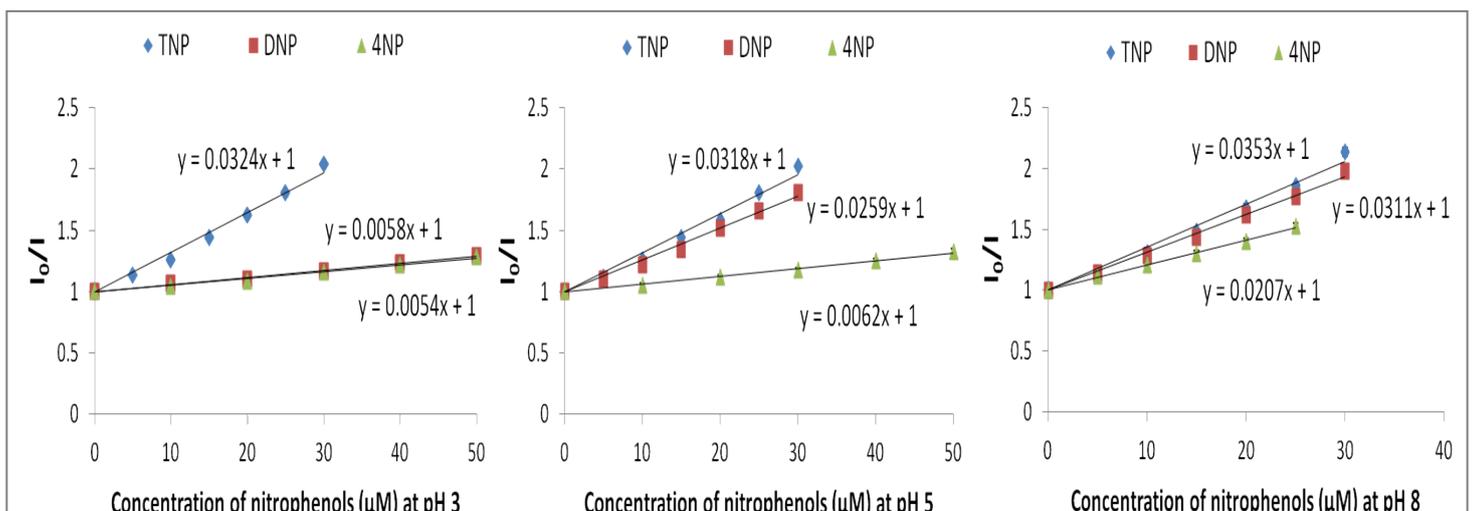
S24. Stern-Volmer plot in response to various NPs at pH 3.



S25. Stern-Volmer plot in response to various NPs at pH 5.



S26. Stern-Volmer plot in response to various NPs at pH 8.



S27. Stern-Volmer plot in response to various NPs at pH 3, 5, 8.