Supporting Information for

"Studies Leading to the Development of a Highly Selective Colorimetric and Fluorescent Chemosensor for Lysine"

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Experimental Section

General methods

Unless otherwise noted, materials were obtained from commercial suppliers and were used without further purification. Flash chromatography was carried out on silica gel (230-400 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded using 250 MHz. Chemical shifts were expressed in ppm and coupling constants (*J*) in Hz. Mass spectra were obtained using JEOL JMS-700 Mstation spectrometers.

Preparation of amino acids and other testing target solutions

Stock solutions (0.1 M) of the amino acids, such as lysine(Lys), histidine (His), leucine (Leu), isoleucine (Ile), methionine (Met), threonine (Thr), tryptophan (Trp), tyrosine (Tyr), valine (Val), asparagines (Asn), aspartic acid (Asp), arginine (Arg), alanine (Ala), serine (Ser), glutamine (Gln), glutamic acid (Glu), glycine (Gly), phenylalanine (Phe) and cysteine (Cys), and butylamine, ethylenediamine, 1, 3-diaminopropane, 4-aminobutyric acid, N-(tert-butoxycarbonyl) – D – lysine, peptide (Lys-Gly-Lys), 2-hydroxy-1-naphthaldehyde were prepared in DW. Stock solutions of host **1** were prepared in CH_3CN/HEPES (0.01 M, pH = 7.4) (1: 9). For all measurements, excitation and emission slit widths were 5 and 10 nm, respectively.

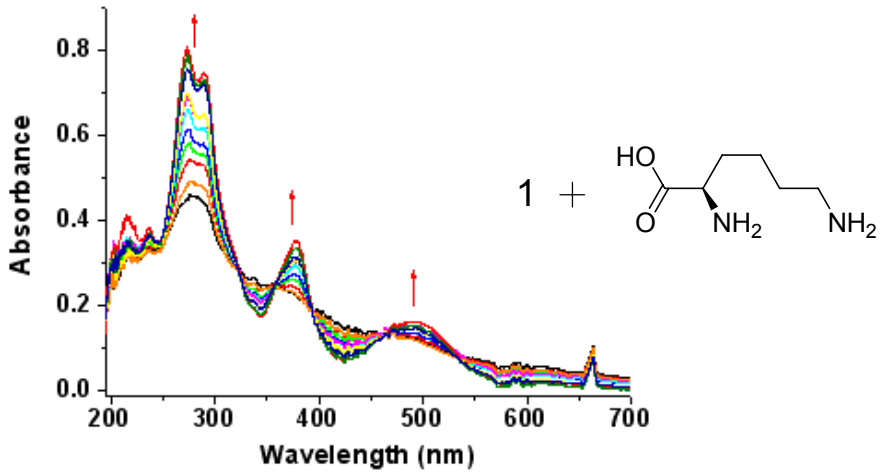


Figure S1. UV spectra of **1** (20 μM) in CH_3CN-HEPES buffer (0.01 M, pH=7.4) (1: 9, v/v) upon addition of 100 equiv. of D-lysine (0.1M in DW).

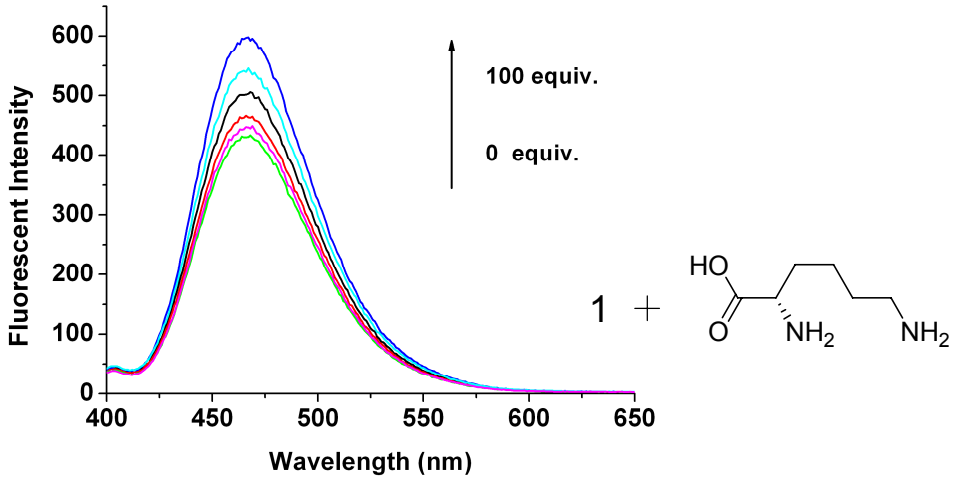


Figure S2. Fluorescent spectra of 1 (20 μM) in CH3CN-HEPES buffer (0.01 M, pH=7.4) (1: 9, v/v) upon addition 100 equiv. of L-lysine (0.1M in DW). Excitation wavelength was 380 nm.

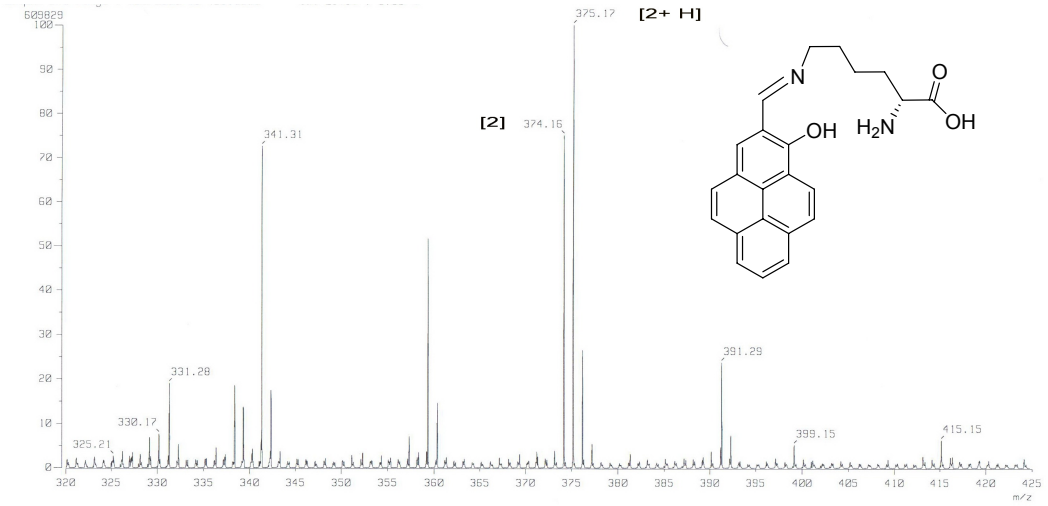


Figure S3. HRFAB mass spectrum of compound **2.**

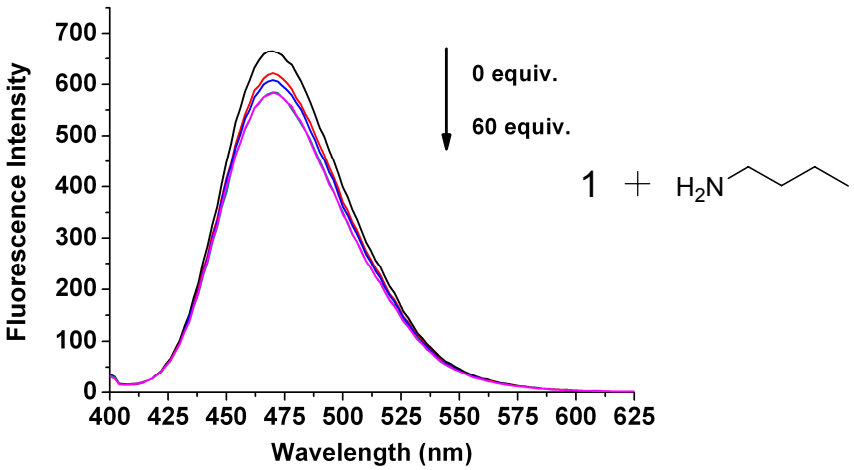


Figure S4. Fluorescent spectra of **1** (20 μM) in CH3CN-HEPES buffer (0.01 M, pH=7.4) (1: 9, v/v) upon addition 10 equiv. of butylamine (0.1M in DW). Excitation wavelength was 390 nm.

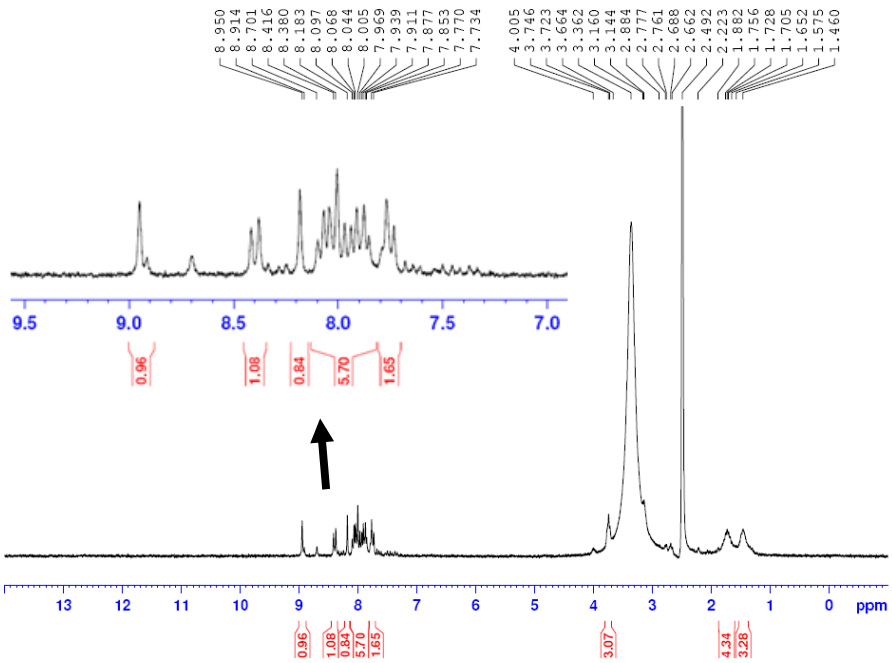


Figure S5. ^{1}H NMR spectra of **2** in DMSO.

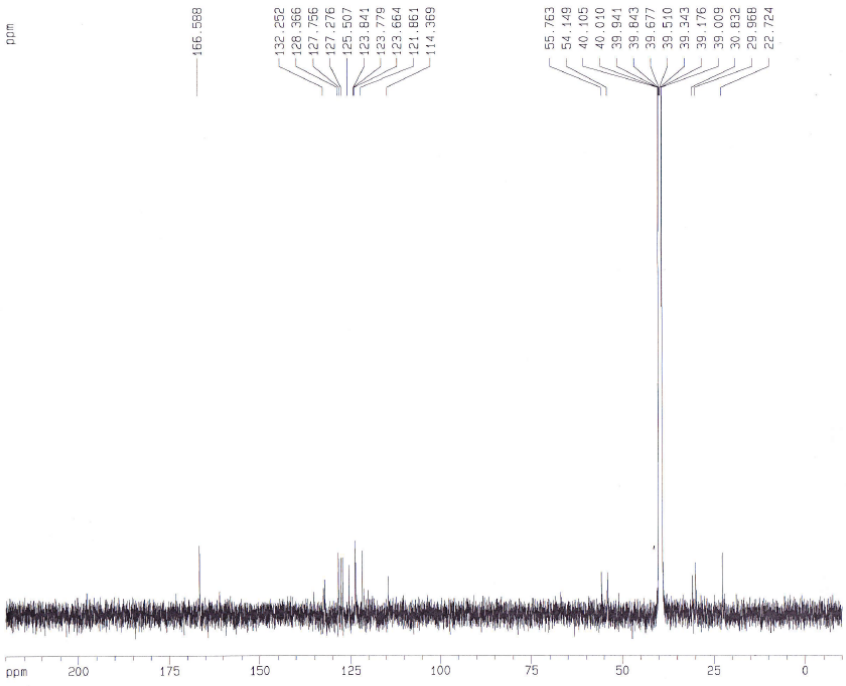


Figure S6. ^{13}C NMR spectra of **2** in DMSO.

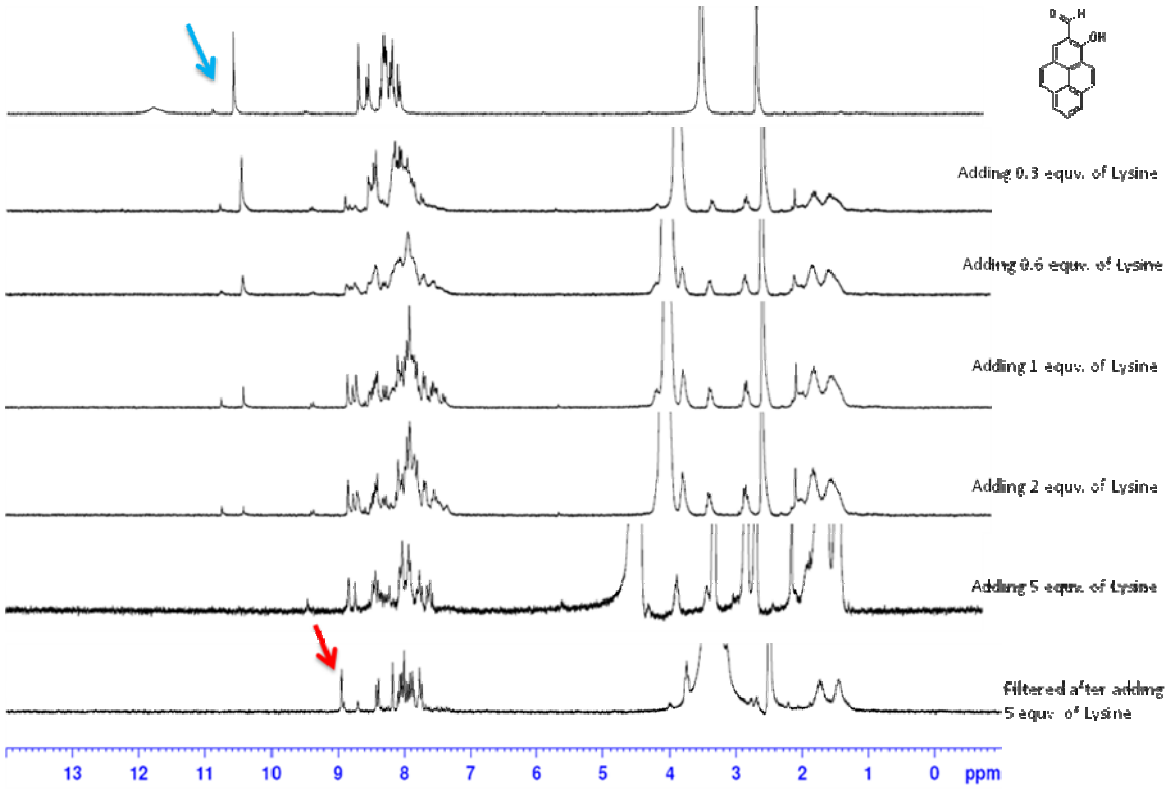


Figure S7. ^{1}H NMR spectra of **1** in DMSO in the presence of a different amount of lysinein D2O.

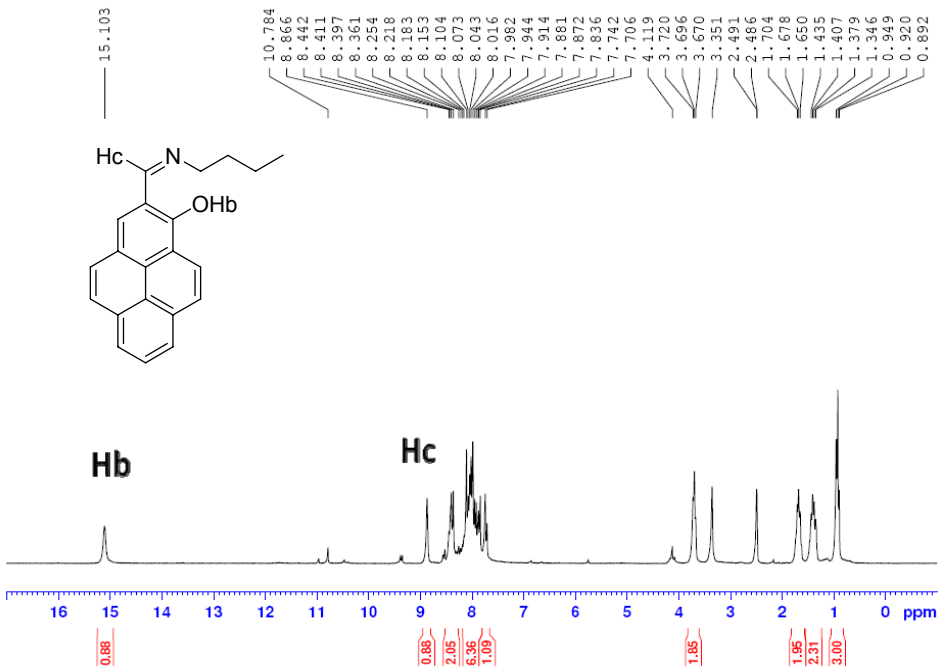


Figure S8. ^{1}H NMR spectra of **1-BA** in DMSO.

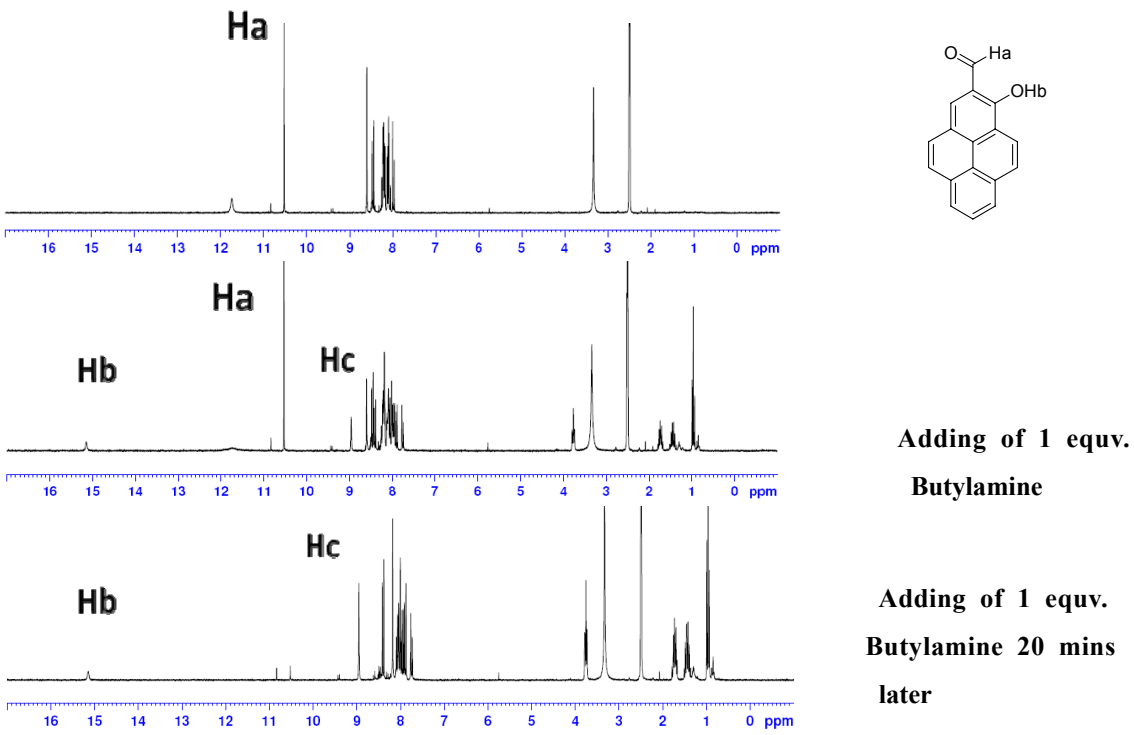
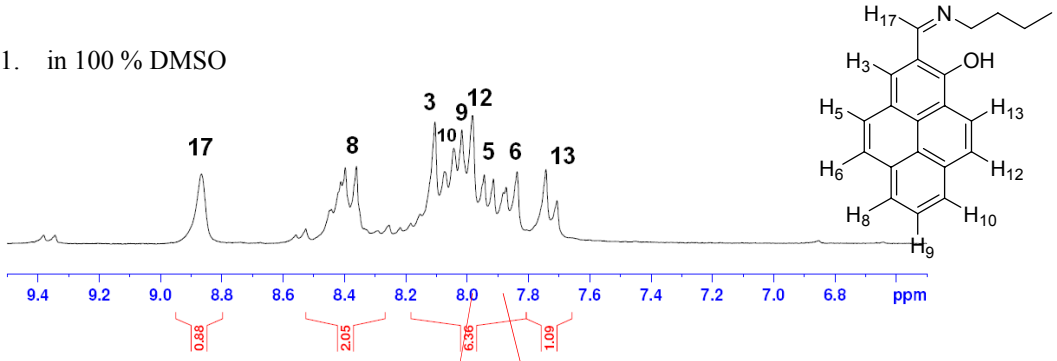
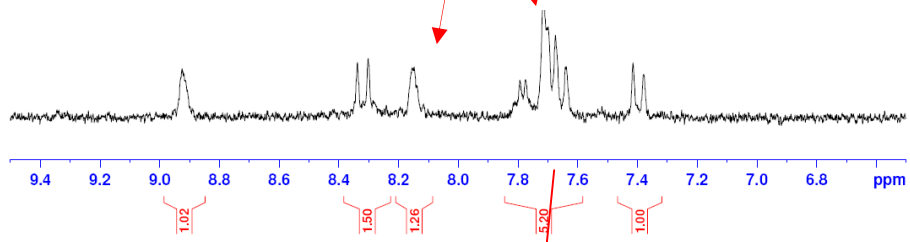


Figure S9. ^{1}H NMR spectra of **1** in DMSO in the presence of butylamine.

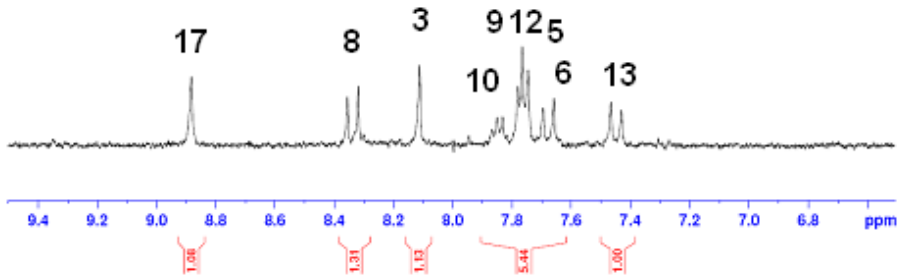
1. in 100 % DMSO



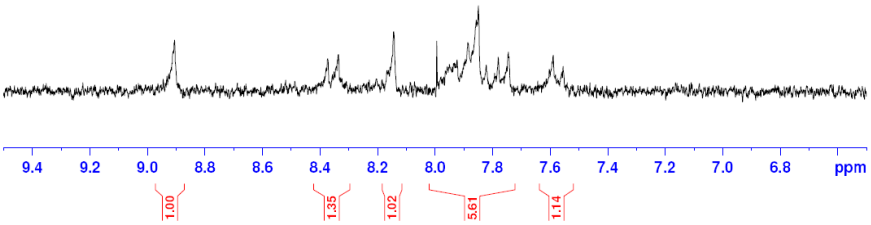
2. in DMSO : D2O = 1: 1



3. in DMSO : D2O ≅ 2: 1



4. the sample of 3 (12 hours later) with more DMSO



5. add NaOH solid to sample 4

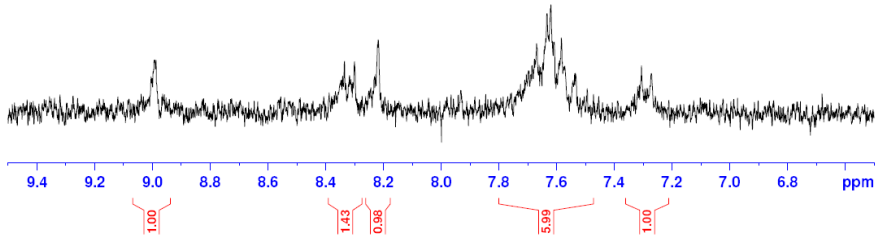


Figure S10. The NMR data of compound **1** with butylamine in different systems.

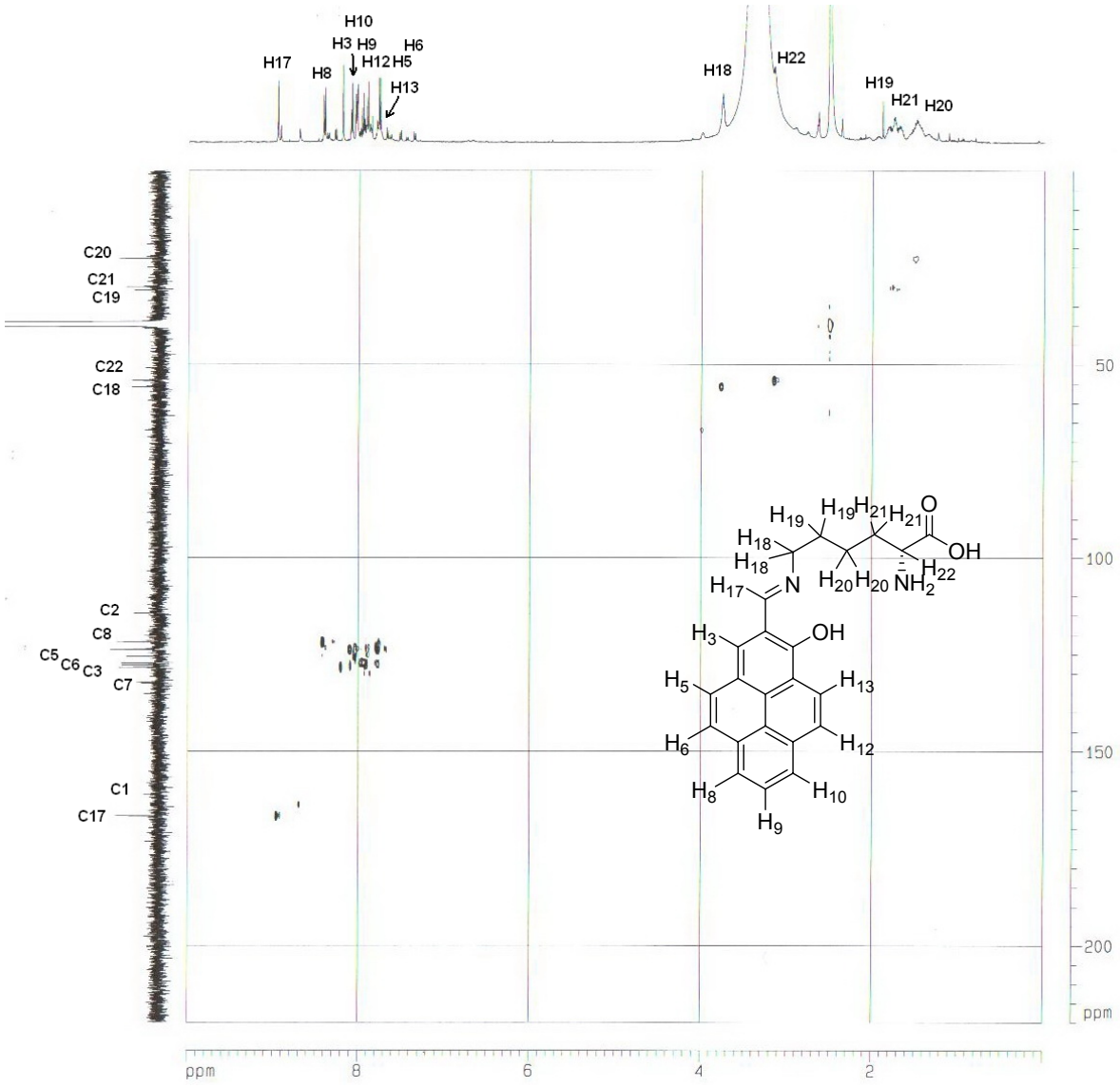


Figure S11. 500 MHz HSQC spectrum of **1** in DMSO.

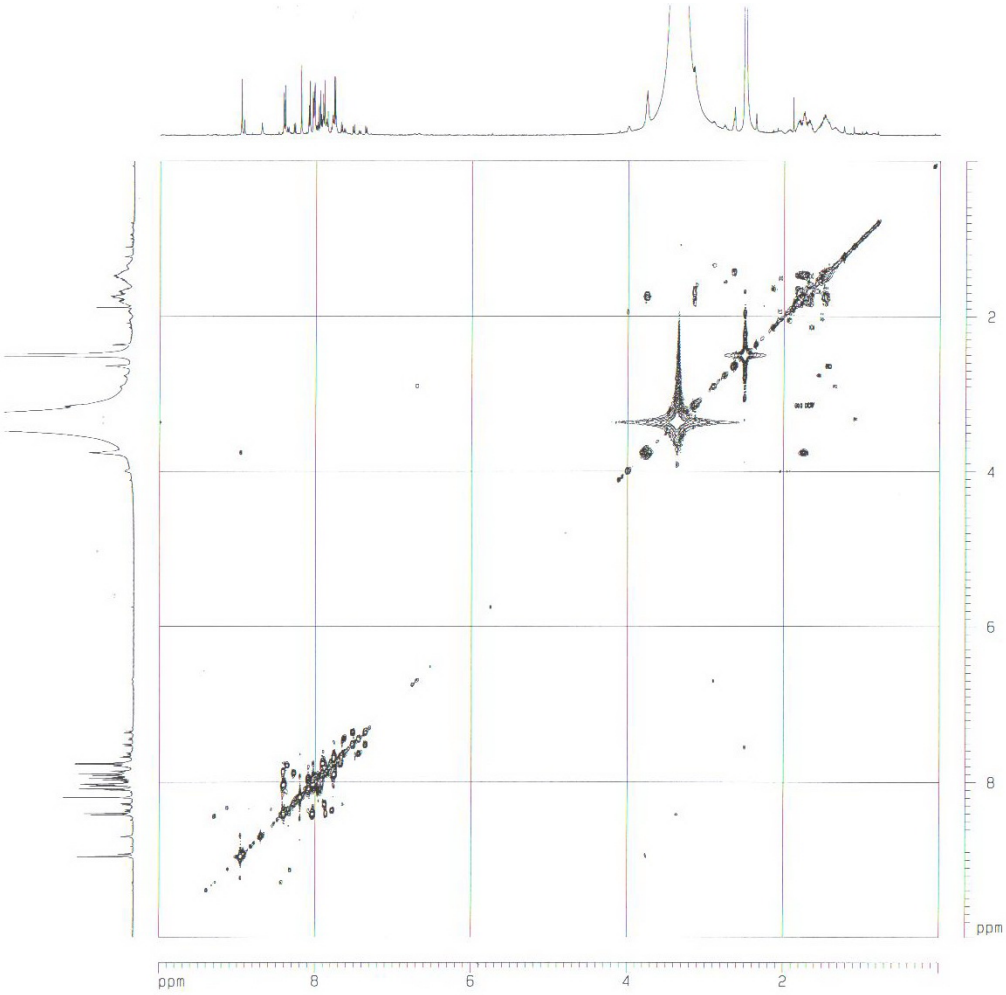


Figure S12. 500 MHz COSY spectrum of **1** in DMSO.

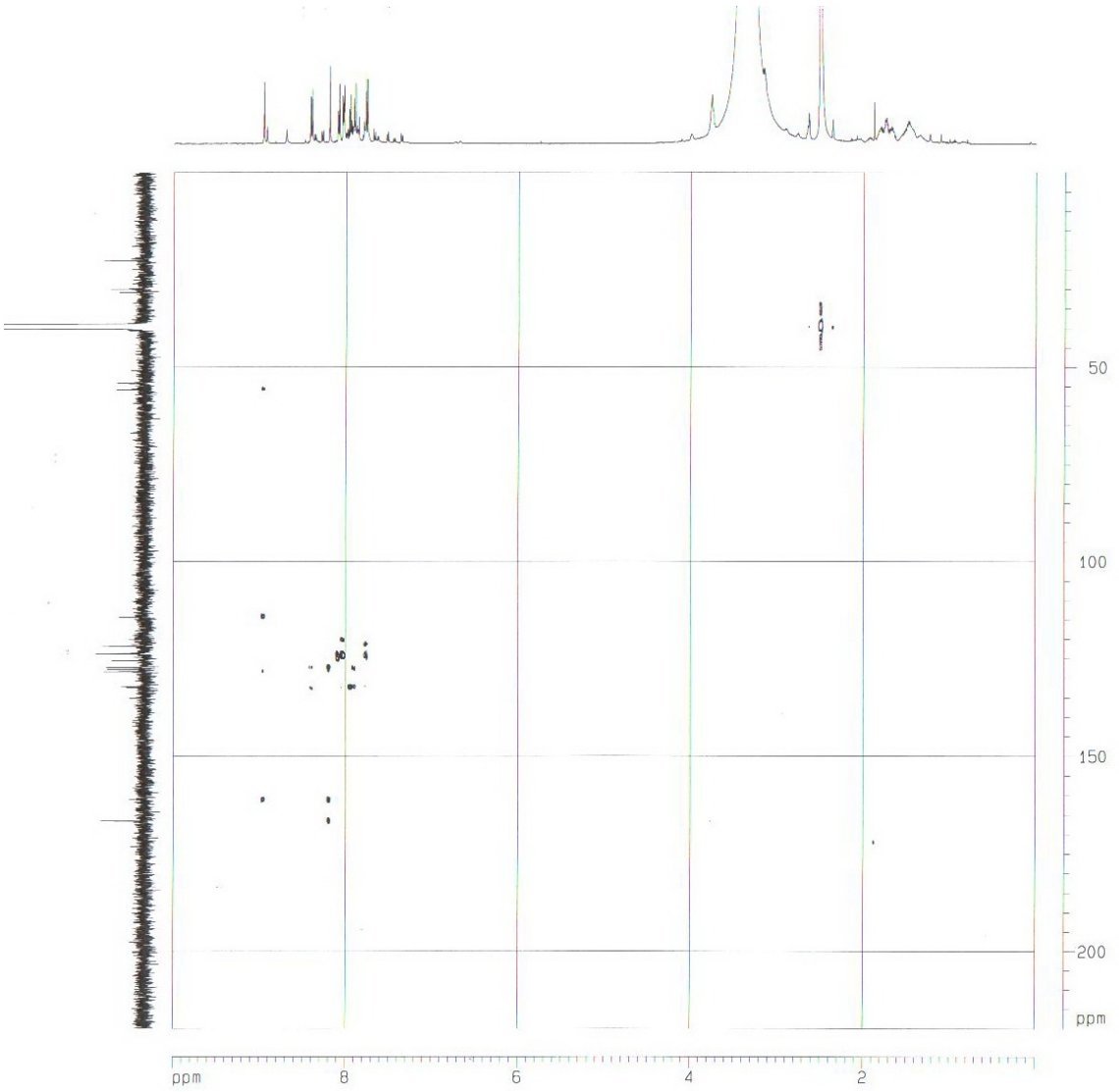


Figure S13. 500 MHz HMBC spectrum of **1** in DMSO.

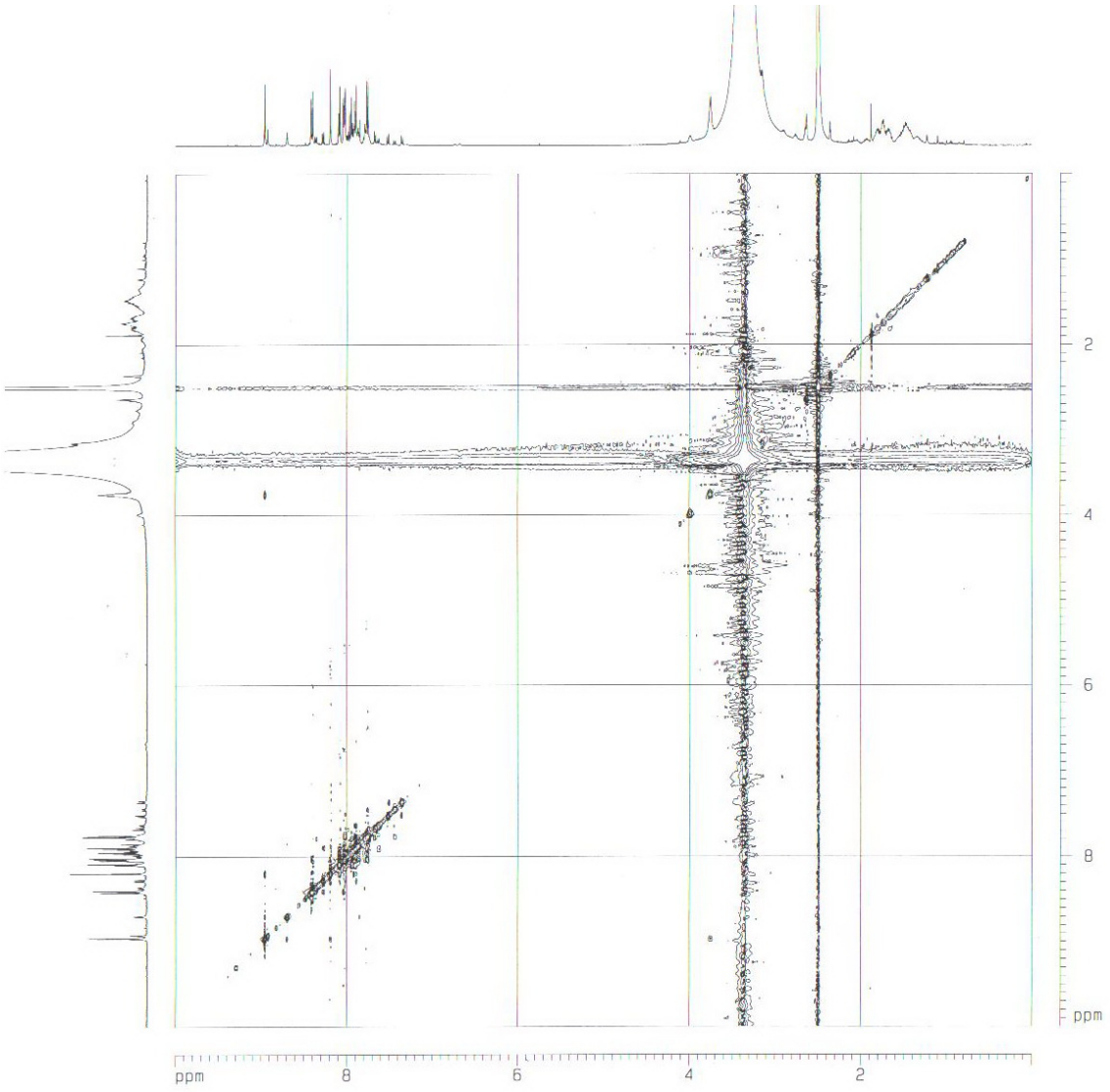


Figure S14. 500 MHz NOESY spectrum of **1** in DMSO.

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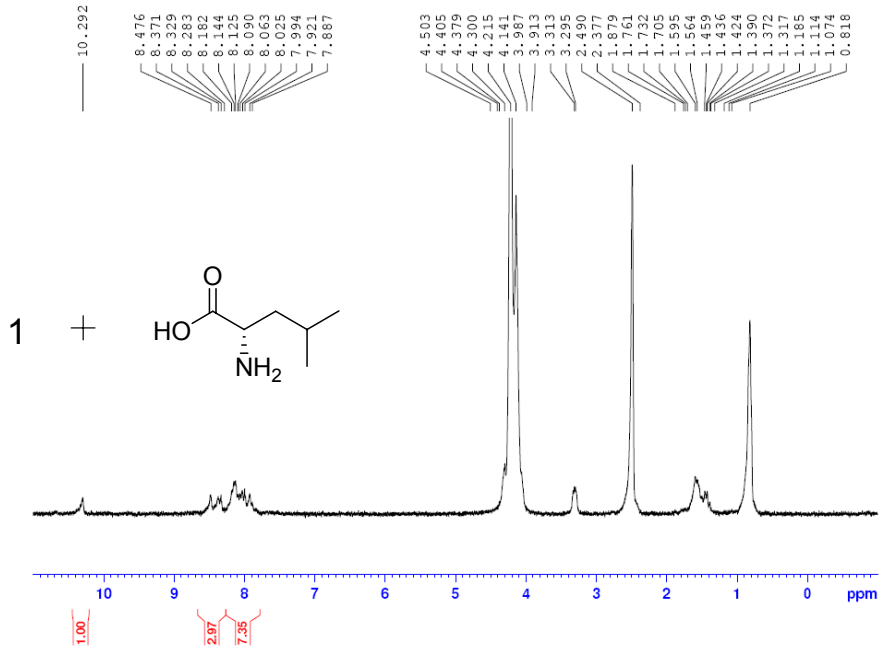

Figure S15. The NMR of compound **1** with excess leucine (Leu) in DMSO-D_2O (2:1).

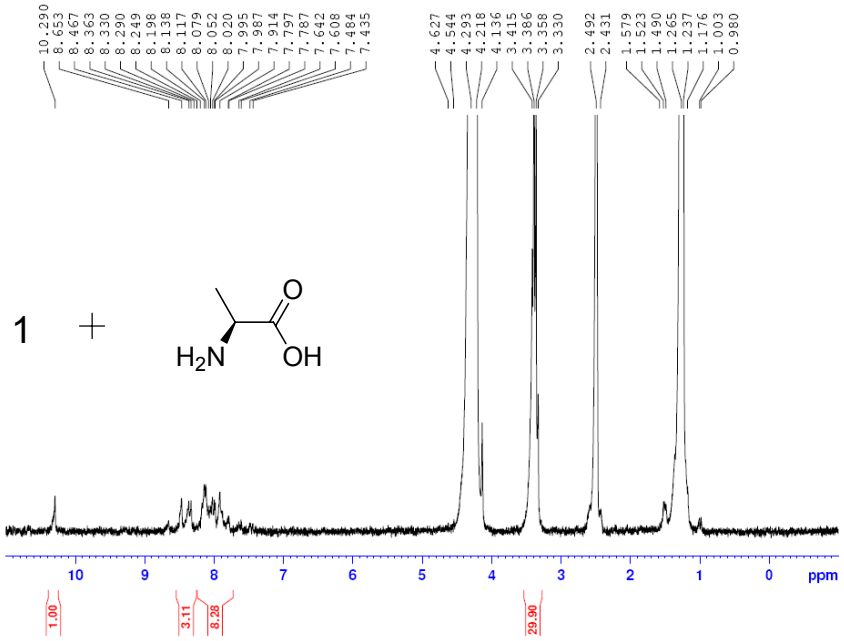

Figure S16. The NMR of compound **1** with excess alanine (Ala) in DMSO-D_2O (2:1).

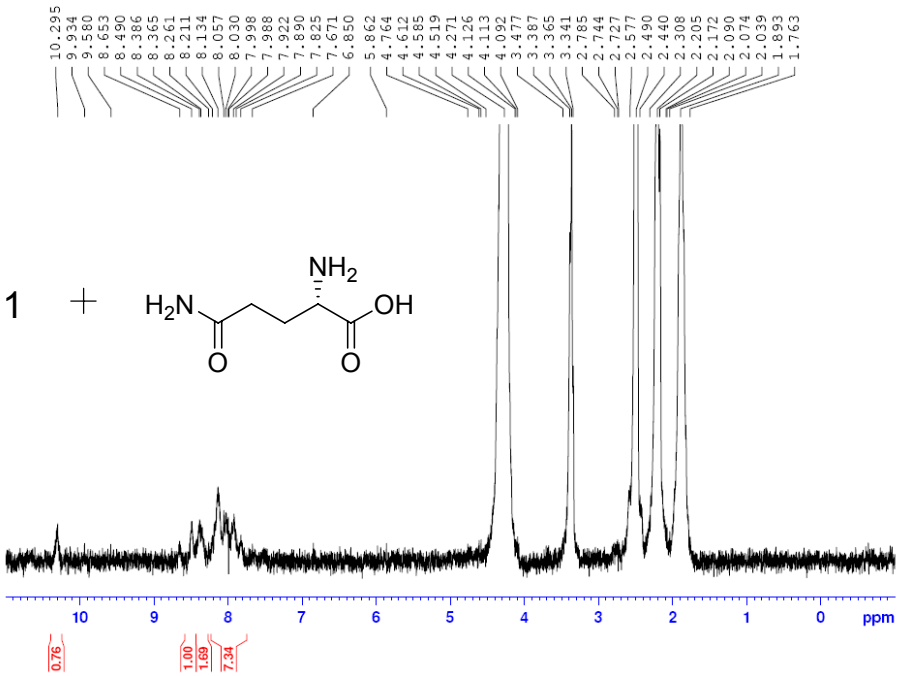

Figure S17. The NMR of compound **1** with excess glutamine (Gln) in DMSO-D_2O (2:1).

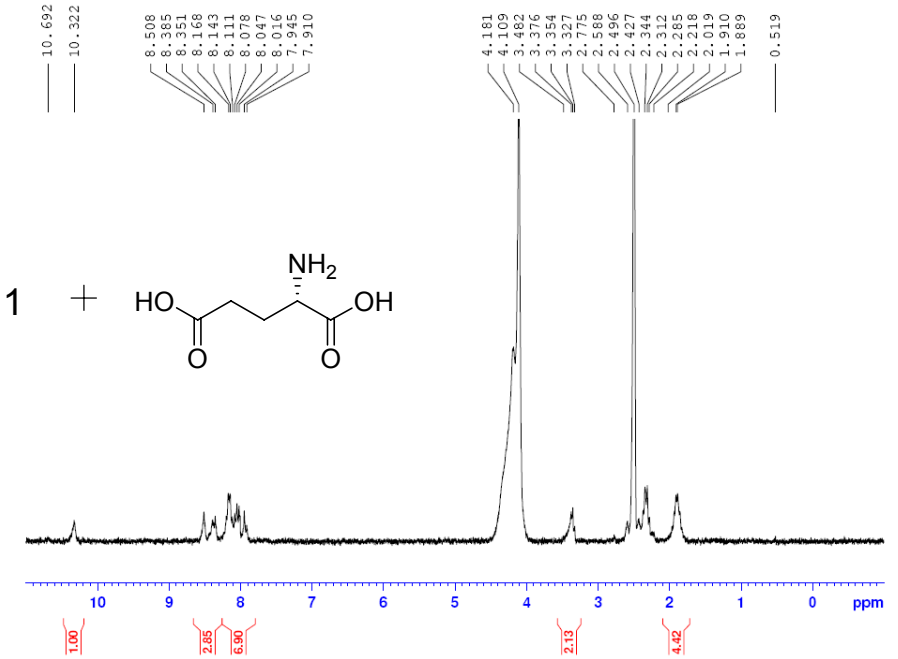

Figure S18. The NMR of compound **1** with excess glutamic acid (Glu) in DMSO-D_2O (2: 1).

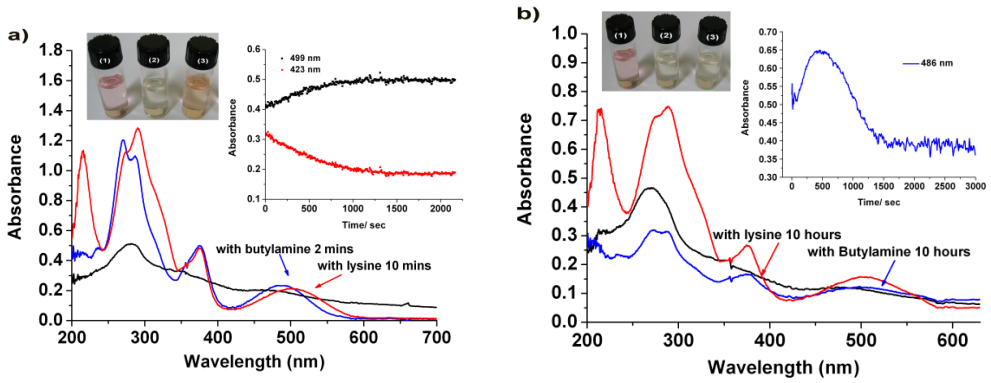

Figure S19. The UV spectra of 1 (20 μM) in CH_3CN-HEPES buffer (0.01 M, pH 7.4) (1: 9, v/v) after addition of 50 equiv. of L-Lys (0.1 M in DW), 10 equiv. of butylamine. Inset: picture of a solution of 1 only (2), and after addition of 50 equiv. of L-Lys (1), 10 equiv. of butylamine (3). (a) Within 10 min after the addition. Inset: The time dependent change in the absorbance of 1 (100 μM) upon addition of 70 equiv of L-Lys. (b) After 10 h of the addition. Inset: The time dependent change in the absorbance of 1 (100 μM) at 486 nm upon addition of 70 equiv of butylamine.

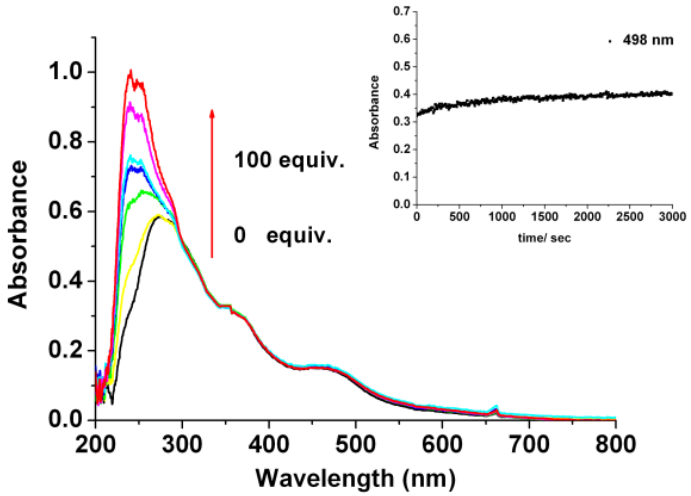

Figure S20. UV spectra of **1** (20 μM) in CH_3CN-HEPES buffer (0.01 M, pH=7.4) (1:9, v/v) upon addition of 100 equiv. of *N*-(*tert*-butoxycarbonyl)-D-Lys. Inset: an absorbance versus time plot following addition of 70 equiv of *N*-(*tert*-butoxycarbonyl)-D-Lys to **1** (100 μM) in CH_3CN-HEPES buffer (0.01 M, pH=7.4) (1:9, v/v).

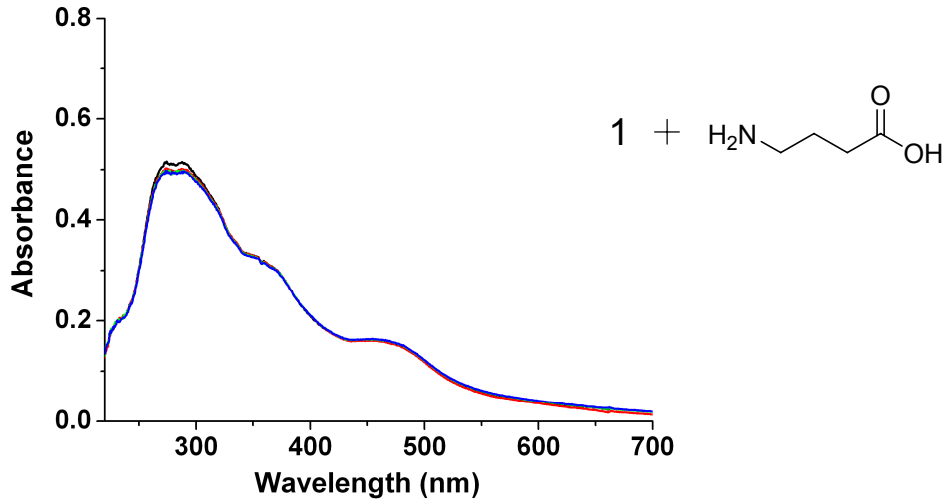

Figure S21. UV spectra of **1** (20 μM) in CH_3CN-HEPES buffer (0.02 M, pH=7.4) (1: 9, v/v) upon addition of 30 equiv. of 4-aminobutyric acid (0.1M in DW).

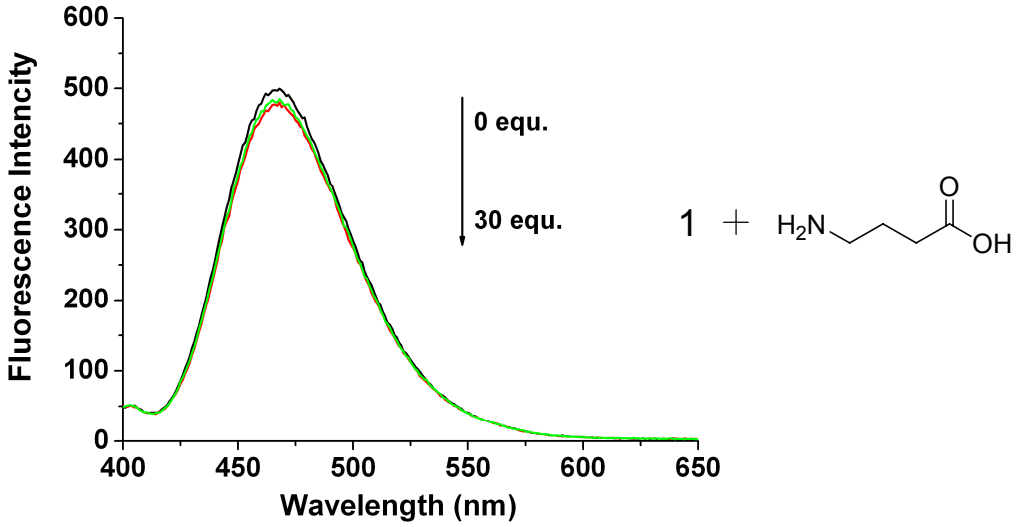

Figure S22. Fluorescent spectra of **1** (20 μM) in CH3CN-HEPES buffer (0.01 M, pH=7.4) (1: 9, v/v) upon addition of 30 equiv. of 4-aminobutyric acid (0.1M in DW). Excitation wavelength was 390 nm.

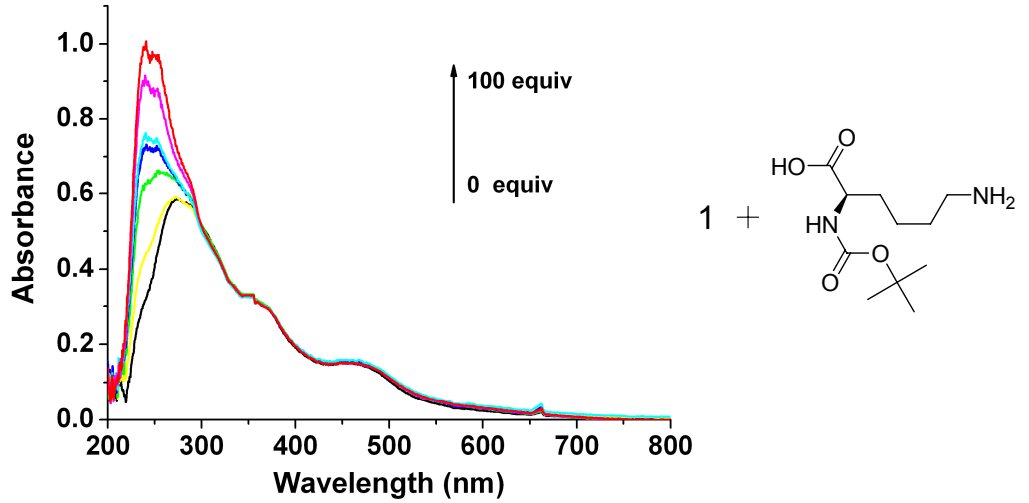

Figure S23. UV spectra of **1** (20 μM) in CH3CN-HEPES buffer (0.01 M, pH=7.4) (1: 9, v/v) upon addition of 100 equiv. of N-(tert-butoxycarbonyl)-D-lysine (0.1M in DW).

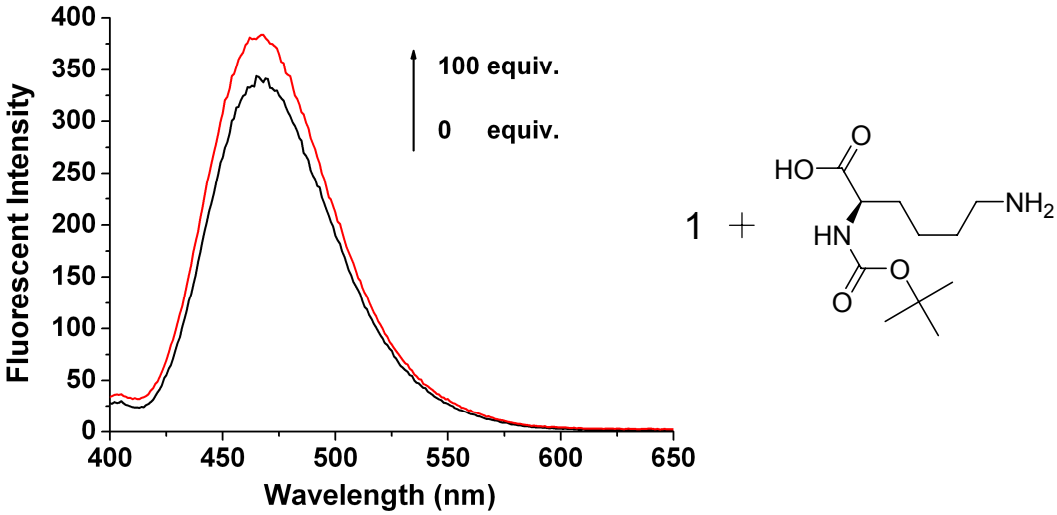

Figure S24. Fluorescent spectra of **1** (20 μM) in CH_3CN-HEPES buffer (0.01 M, pH=7.4) (1: 9, v/v) upon addition of 100 equiv. of N-(tert-butoxycarbo nyl)-D-lysine (0.1M in DW). Excitation wavelength was 380 nm.

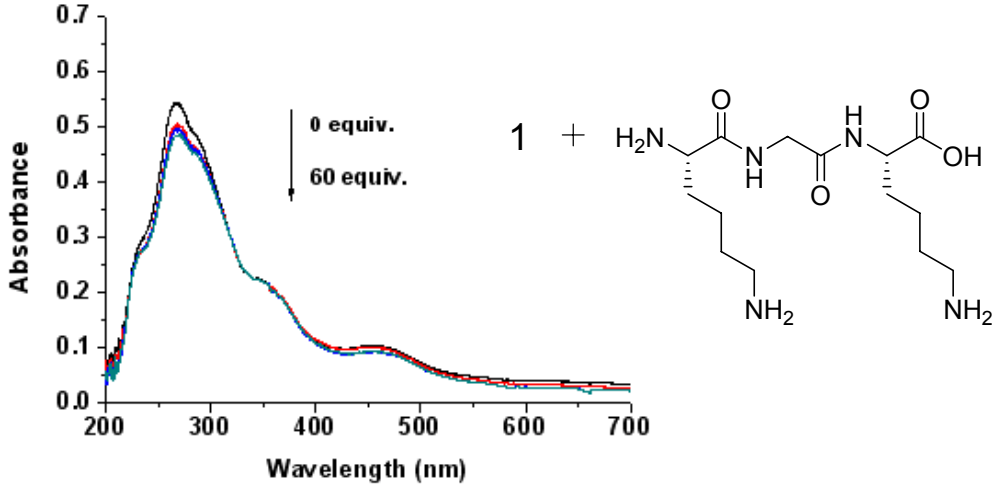

Figure S25. The UV spectra of **1** (10 μM) in CH_3CN-HEPES buffer (0.01 M, pH=7.4) (1: 9, v/v) upon addition of 60 equiv. of Lys-Gly-Lys (KGK) (0.1M in DW)

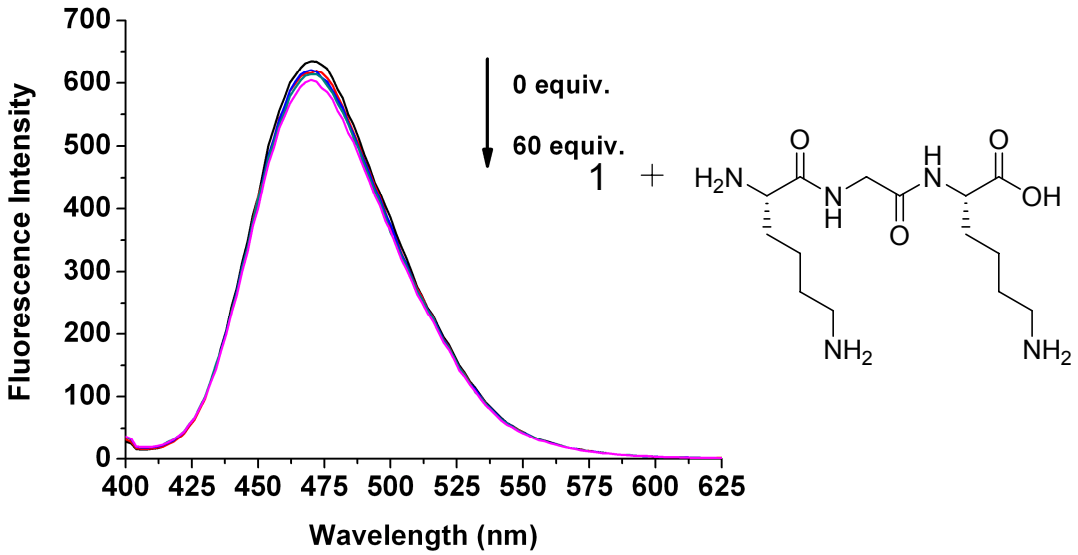

Figure S26. Fluorescent spectra of **1** (20 μM) in CH_3CN-HEPES buffer (0.01 M, pH=7.4) (1: 9, v/v) upon addition of 60 equiv. of Lys-Gly-Lys (KGK) (0.1M in DW). Excitation wavelength was 390 nm.

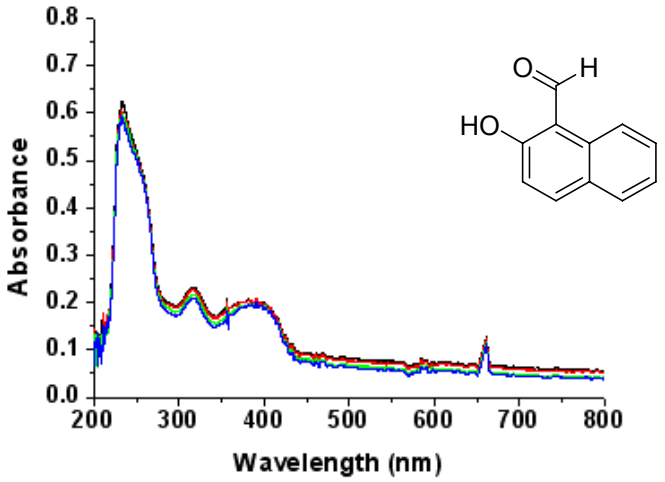

Figure S27. The UV spectra of 2-hydroxy-1-naphthaldehyde (10 μM) in CH_3CN-HEPES buffer (0.01 M, pH=7.4) (1: 9, v/v) upon addition of 50 equiv of L-Lysine (0.1M in DW).

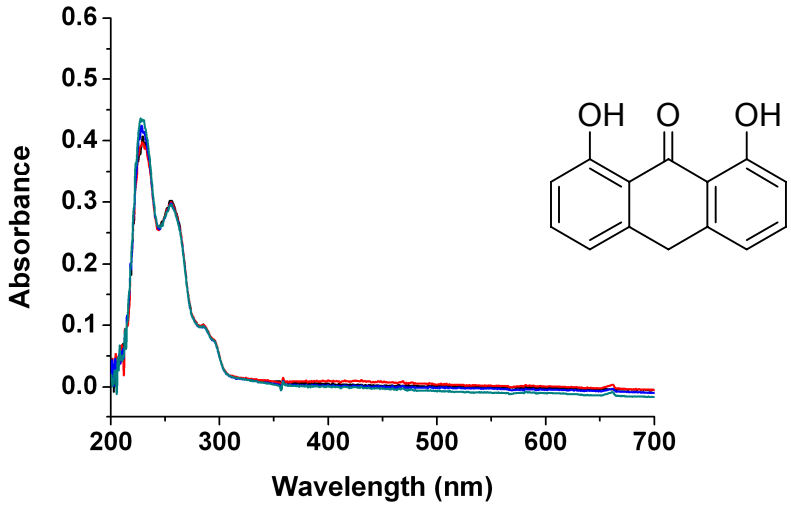

Figure S28. The UV spectra of 1, 8-Dihydroxyanthrone (10 μM) in CH_3CN-HEPES buffer (0.01 M, pH=7.4) (2: 8, v/v) upon addition of 50 equiv of L-Lysine (0.1M in DW).

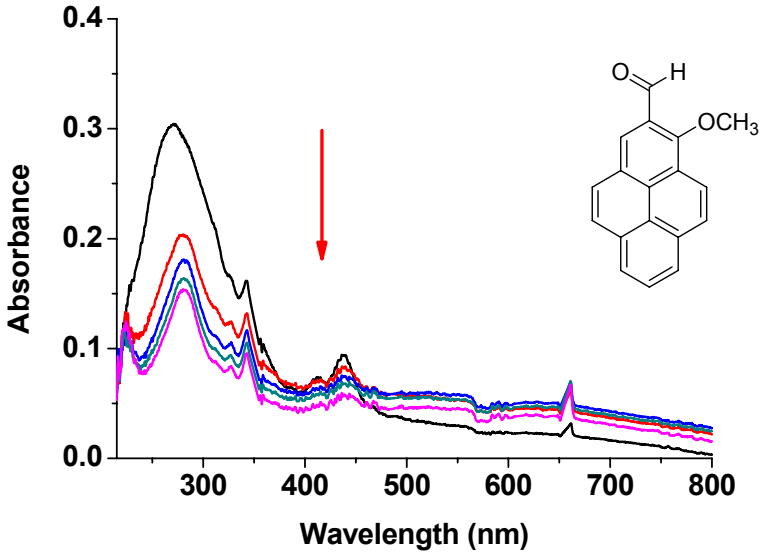

Figure S29. The UV spectra of 1-methoxypyrene-2-carbaldehyde (20 μM) in CH3CN-HEPES buffer (0.01 M, pH=7.4) (1: 9, v/v) upon addition of 50 eq uiv of L-Lysine (0.1M in DW).

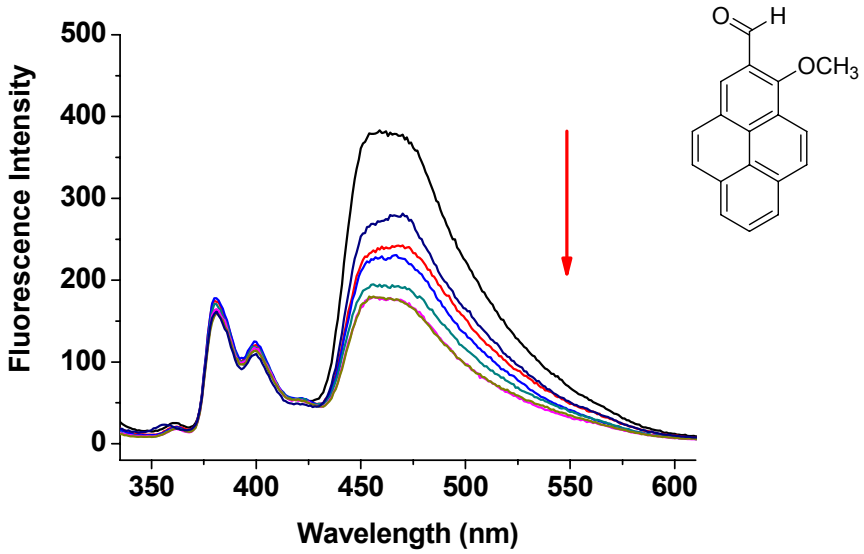

Figure S30. Fluorescent spectra of 1-methoxypyrene-2-carbaldehyde (20 μM) in CH3CN-HEPES buffer (0.01 M, pH=7.4) (1: 9, v/v) upon addition of 50 equiv. of Lys (0.1M in DW). Excitation wavelength was 330 nm.

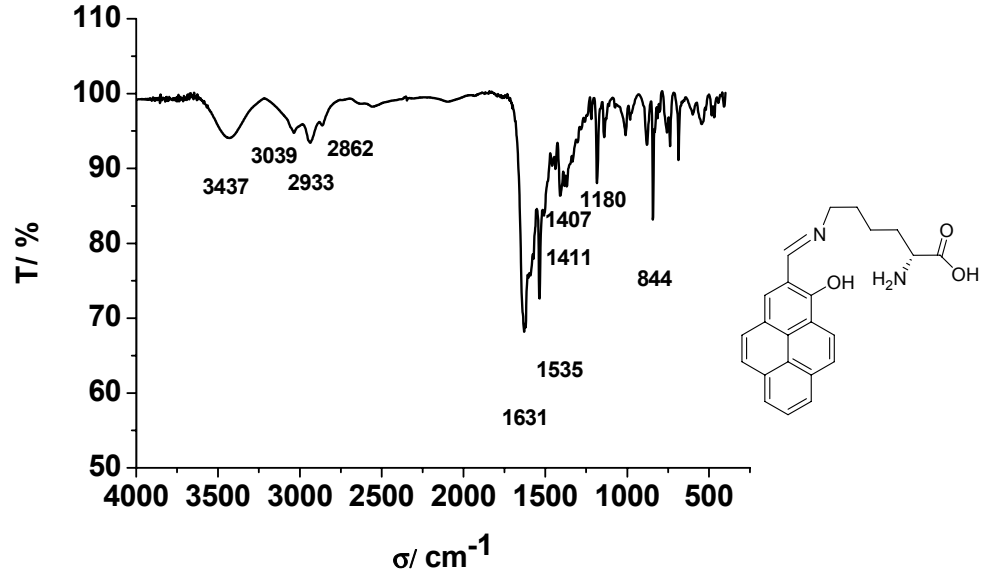

Figure S31. IR spectrum of compound **2**.

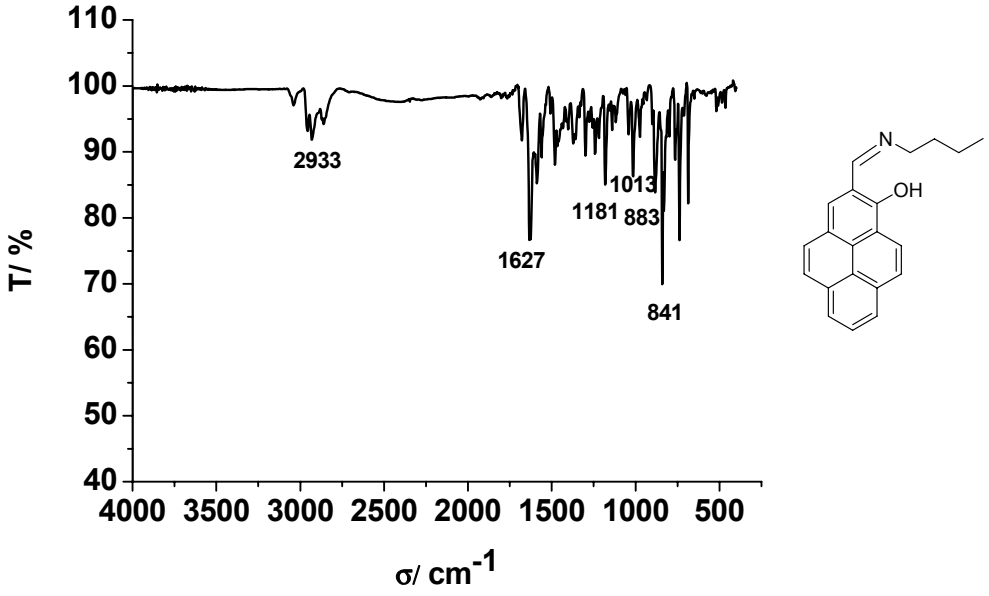

Figure S32. IR spectrum of compound **1-BA**.

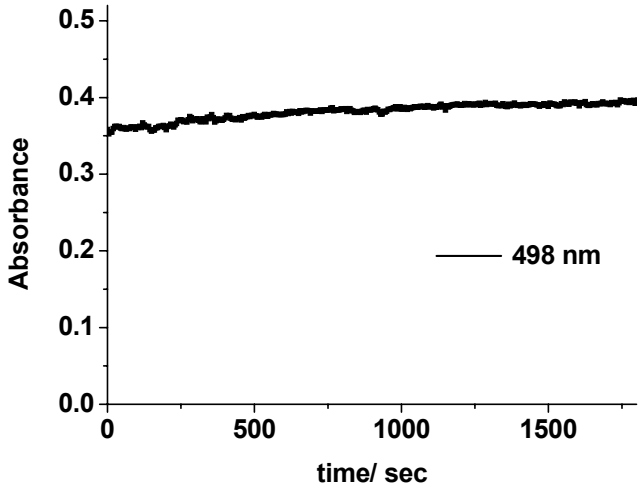

Figure S33. The kinetics upon addition of 70 equiv of 4-aminobutyric acid to **1** (100 uM) in CH_3CN-HEPES buffer (0.01 M, pH=7.4) (1: 9, v/v).

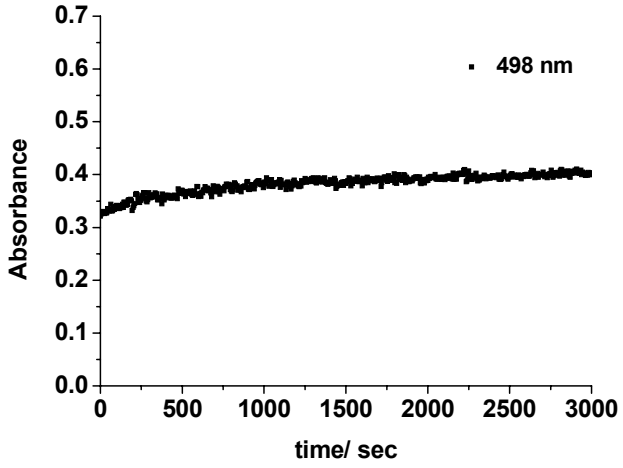

Figure S34. The kinetics upon addition of 70 equiv of N-(tert-butoxycarbonyl)-D-lysine to 1 (100 uM) in CH_3CN-HEPES buffer (0.01 M, pH=7.4) (1: 9, v/v).

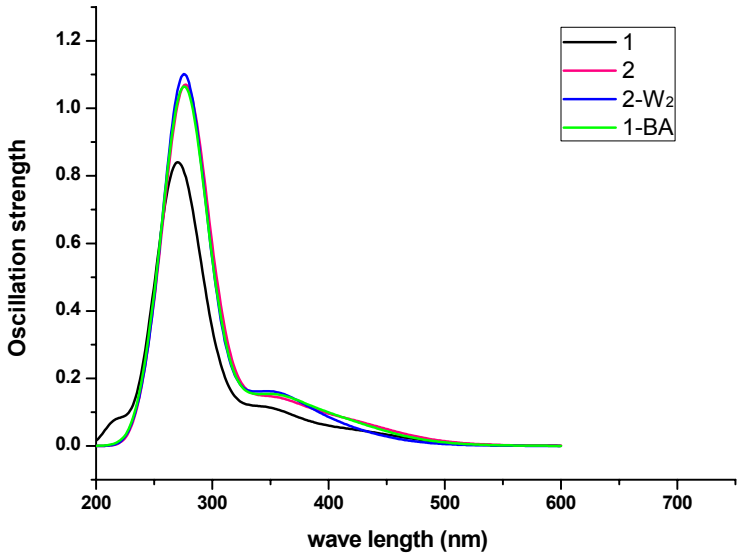

Figure S35. Calculated absorption spectra of **1**, **2**, **2-W$_2$**, and **1-BA**.

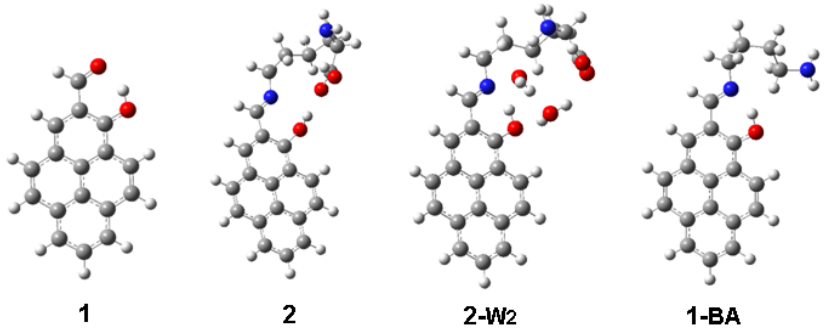

Figure S36. Structures of **1**, **2**, **2-W$_2$** and **1-BA.**

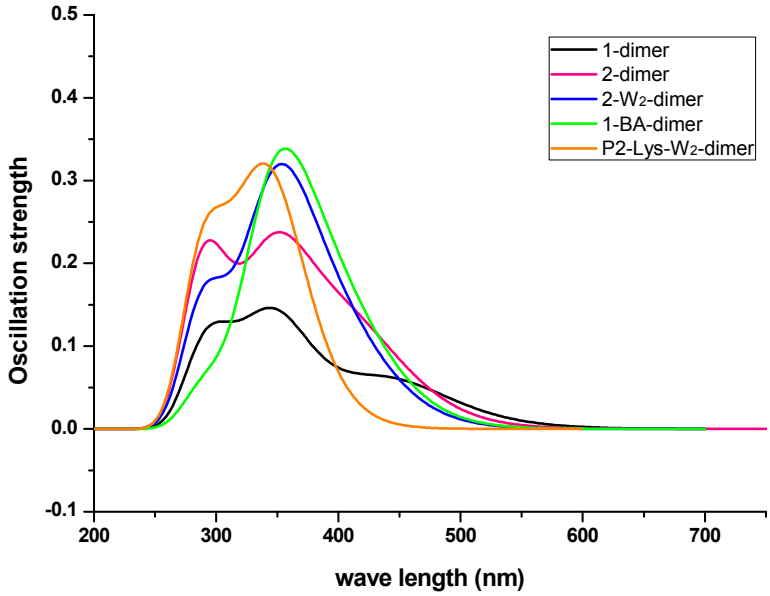

Figure S37. Calculated absorption spectra of the stacked dimers of **1**, **2**, **2-W$_2$**, **1-BA**, and **P2-Lys-W$_2$**.

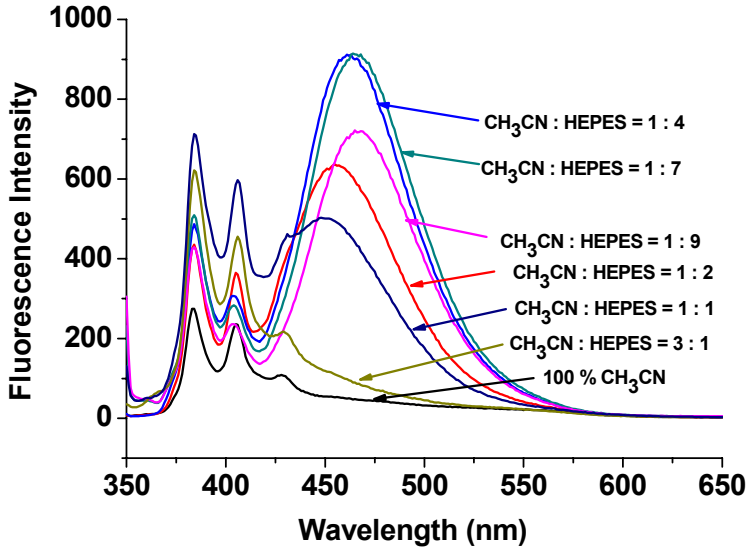

Figure S38. The fluorescence spectra of compound **1** (20 μM) in different ratios CH_3CN and HEPES buffer (0.01 M, pH 7.4). Excitation wavelength = 340 nm.