Electronic Supplementary Material (ESI) for Analytical Methods.

Supplementary documents

Exploitation of a simple Schiff base as a ratiometric and colorimetric chemosensor for glutamic acid

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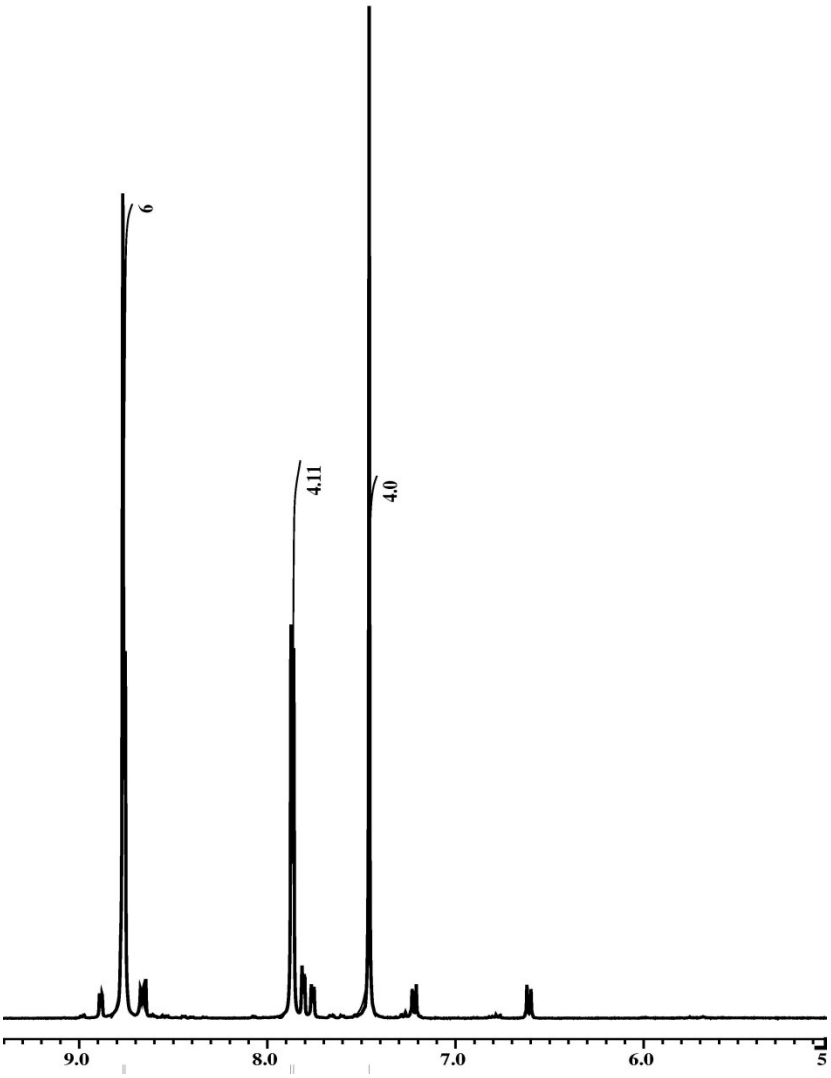


Fig. S1 ^{1}H NMR spectra of **L** in d_6-DMSO

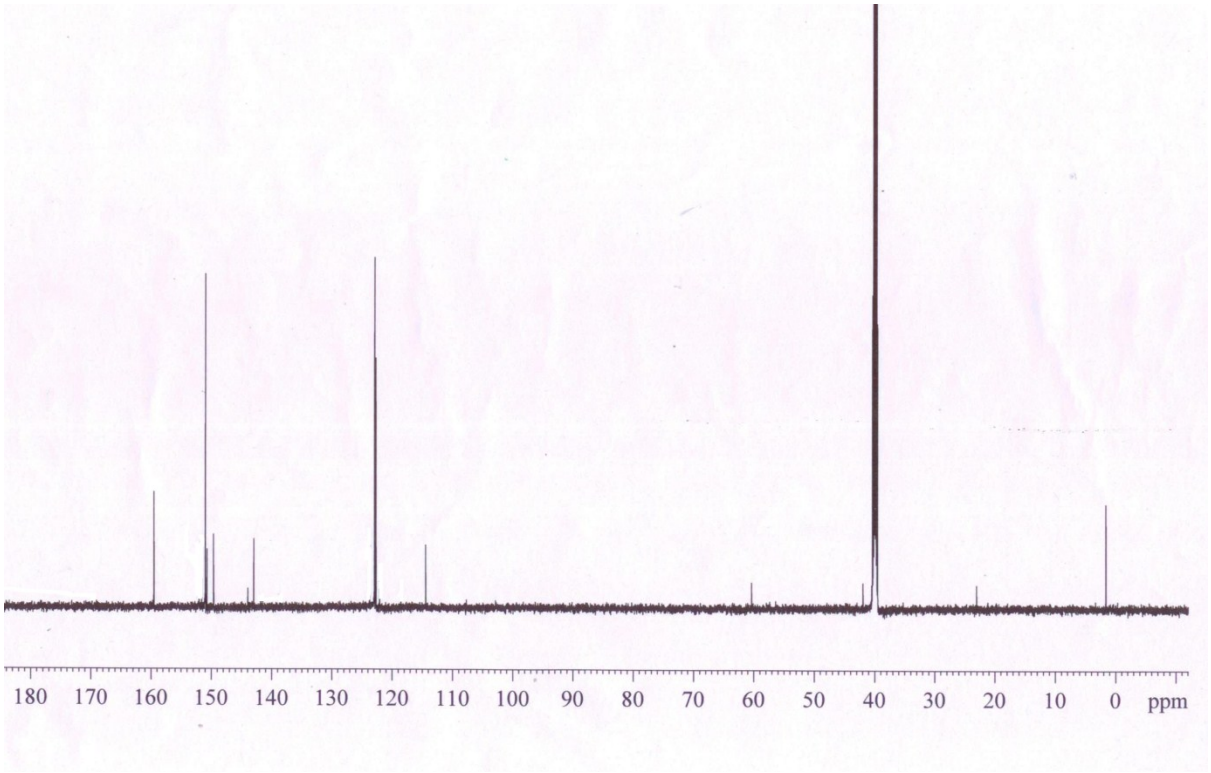


Fig. S2 ^{13}C NMR Spectra of **L** in d_6-DMSO

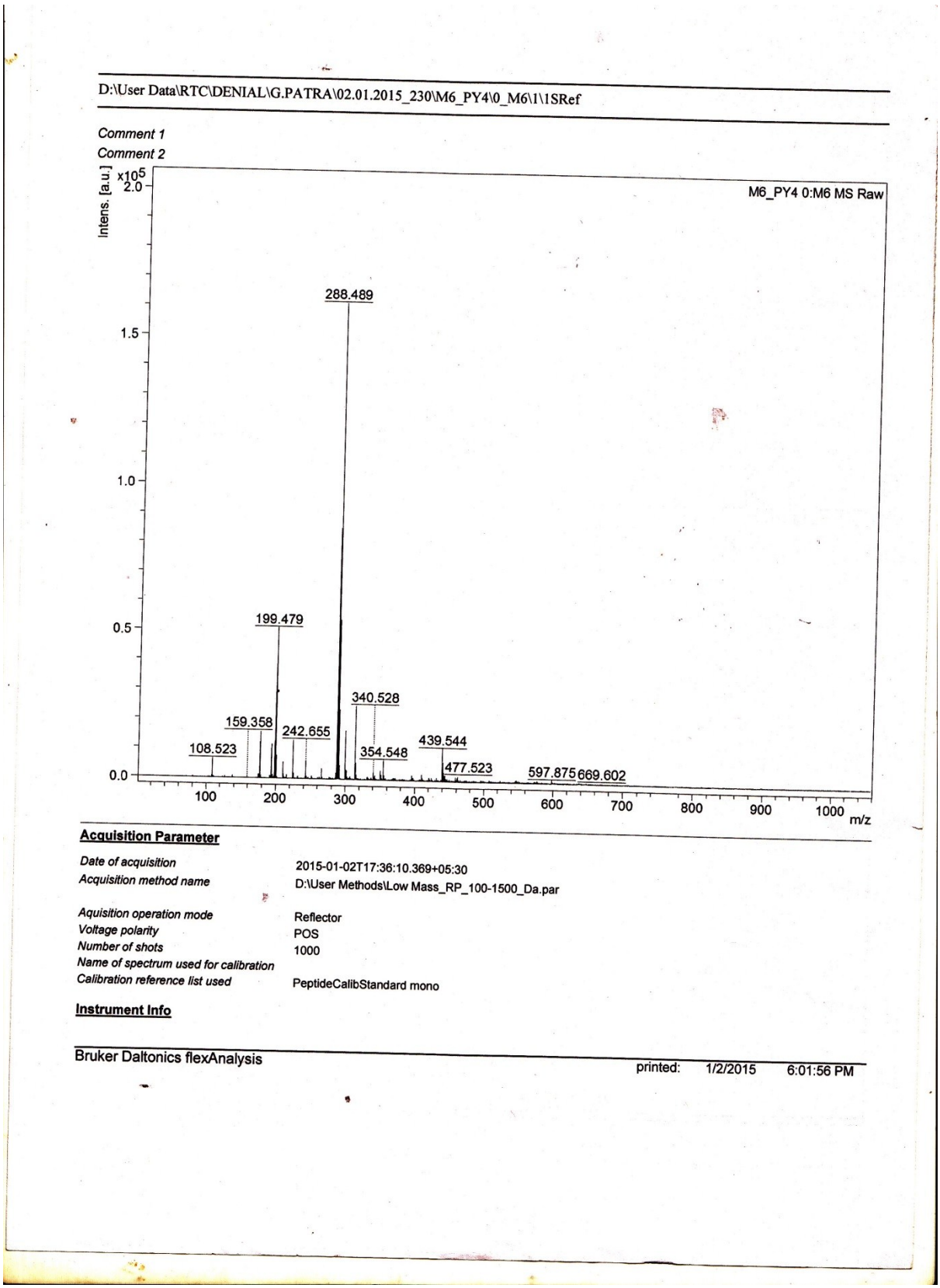


Fig. S3 Mass spectra of **L**

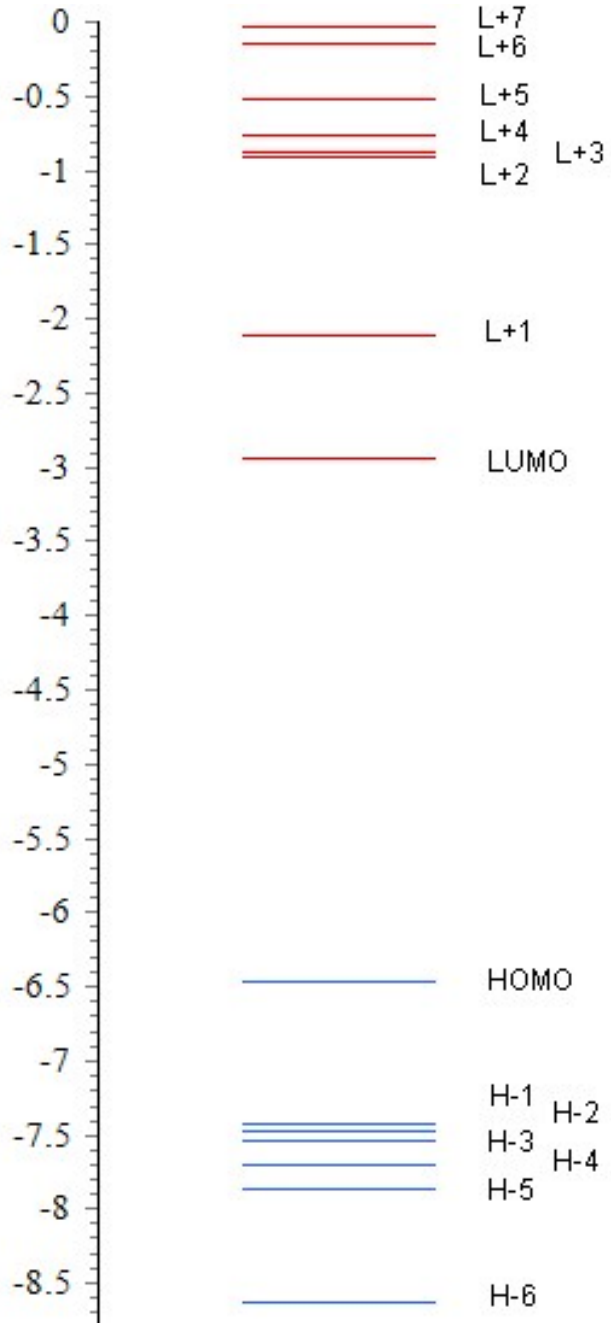


Fig. S4 Schematic representation of the energy levels of **L**.

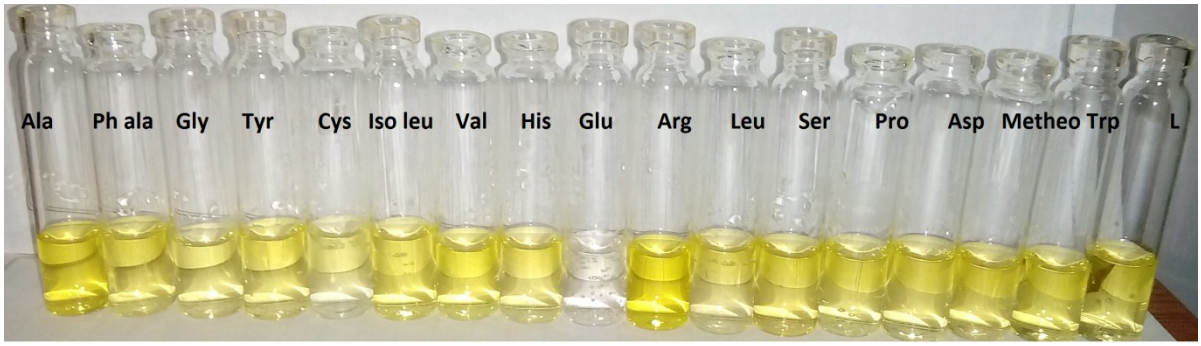
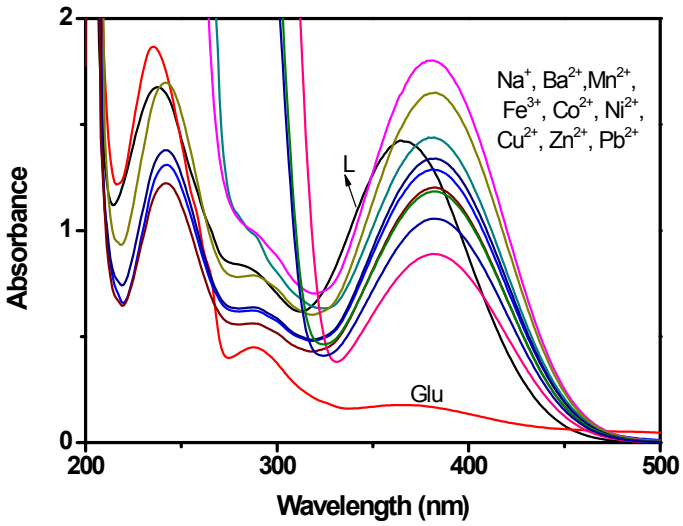
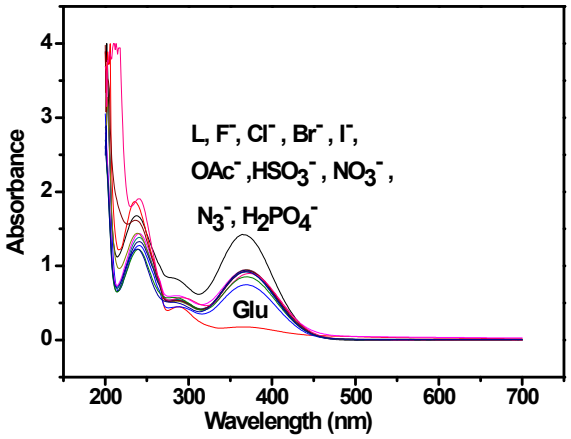


Fig. S5 The colour changes of L in presence of different amino acids



(a)



(b)

Fig. S6 Absorption spectra of **L** (1 μM) changes in presence of 10 equiv. of different (a) metal cations and (b) anions

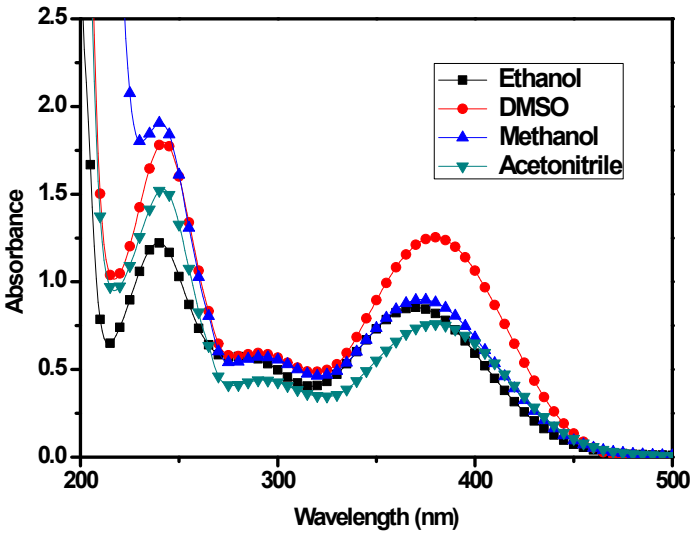


Fig. S7 Absorption behavior of **L** in different solvents

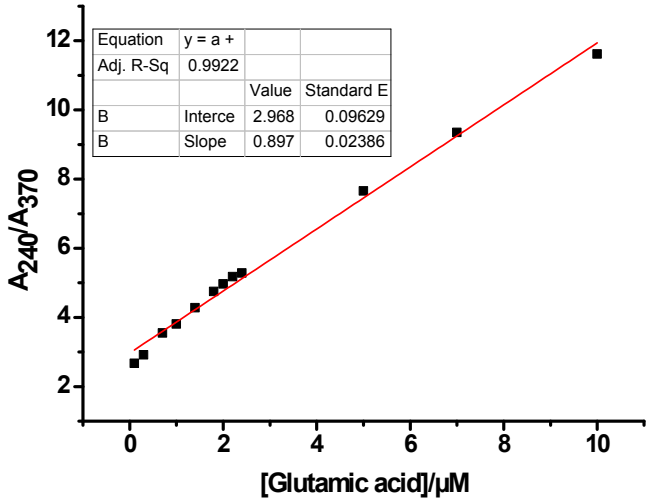


Fig. S8 Detection limit of the chemosensor **L** for glutamic acid

The detection limit DL of the probe for glutamic acid was determined from the following equation[1]:

DL = K* Sb1/S

Where K = 2 or 3 (we take 3 in this case); Sb1 is the standard deviation of the blank solution;

S is the slope of the calibration curve.

From the graph we get slope, S = 0.8971, and Sb1 value is 0.23818.

Thus using the formula we get the Detection Limit = 7.96×10^{-7} M i.e. the probe can detect glutamic acid in this minimum concentration.

Ref.

1. M. Zhu, M. Yuan, X. Liu, J. Xu, J. Lv, C. Huang, H. Liu, Y. Li, S. Wang and D. Zhu, *Org. Lett.* 2008**, 10***,* 1481-1484.

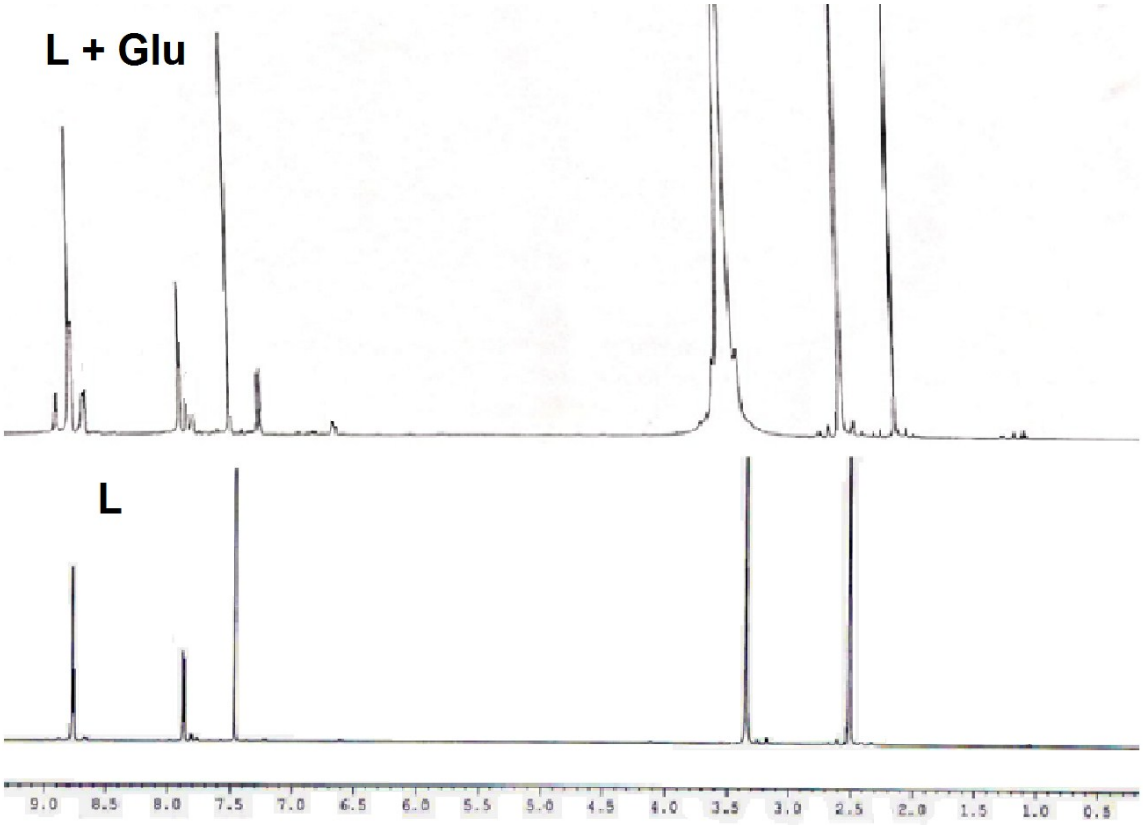


Fig. S9 ^{1}H NMR spectra of the probe **L** and **L- Glu** in d_6-DMSO (in 400 MHz NMR spectrometer).

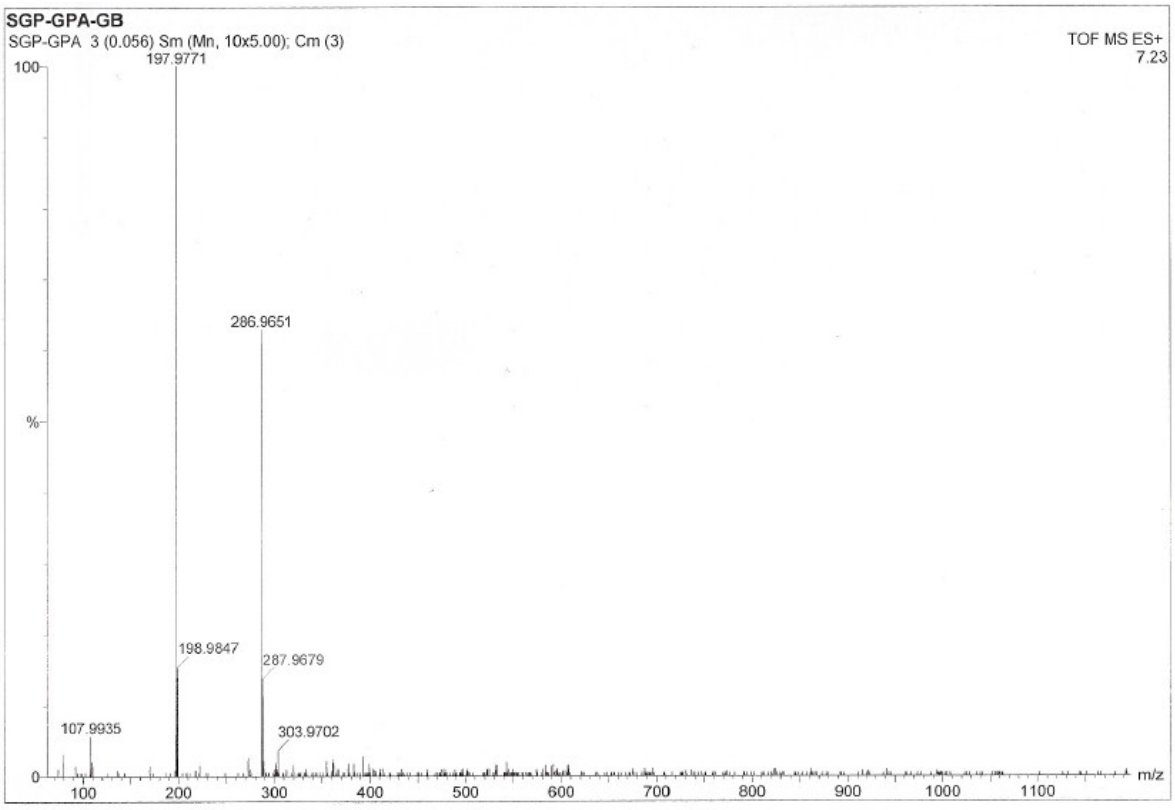


Fig. S10 HRMS spectra of **L-Glu**.

Table S1 Selected optimized bond distances (Å) and angles (°) for **L**.

Bond Length (Å)		Bond Angle (°)	
C1-C2	1.39226	C31-N35-C3	123.99968
C2-C3	1.40971	N35-C3-C4	125.72900
C3-C4	1.41146	C3-C2-C1	121.15751
C4-C5	1.39219	C2-C1-C6	120.16781
C5-C6	1.40957	C1-C6-C5	118.67060
C3-N35	1.41658	C6-C5-C4	121.16137
C6-N36	1.41644	C6-N36-C33	124.00061
C31-N35	1.29209	N36-C33-C11	121.78535
C31-C21	1.46748	C33-C11-C13	122.21780
C21-C22	1.40737	C11-C13-C16	118.98698
C22-C24	1.39841	C13-C16-N20	123.36042
C24-N30	1.35268	C16-N20-C14	117.49344

N30-C26	1.35796	N20-C14-C12	123.03788
C26-C23	1.39445	C14-C12-C11	119.27926
C23-C21	1.40901	N35-C31-C21	121.78172
N36-C33	1.29200	C31-C21-C22	119.94187
C33-C11	1.46749	C21-C22-C24	119.28066
C11-C12	1.40736	C22-C24-N30	123.03711
C12-C14	1.39841	C24-N30-C26	117.49321
C14-N20	1.35268	N30-C26-C23	123.36137
N20-C16	1.35796	C26-C23-C21	118.98691
C13-C16	1.39445	C23-C21-C31	122.21738
C13-C11	1.40901		

Table S2 The energy and molar absorption coefficients of experimental absorption bands and the electronic transitions calculated with the TD-DFT method for **L**

Most important orbital excitations	λ [nm]	f	Experimental λ [nm] (log ε)
H→L	389.43	1.6748	370 (6.92)
H-2→L, H-1→L+1	325.54	0.0041	
H-5→L	311.81	0.0239	
H-7→L	291.21	0.0531	287(4.44)
H-3→L+1, H-4→L	267.17	0.0012	
H-1→L+1, H-2→L	259.38	0.0027	
H→L+2, H-6→L+1,	247.73	0.0178	
H→L+4, H-6→L+1	242.01	0.0460	
H-9→L, H→L+5, H→L+2	238.37	0.207	
H-6→L+1, H→L+4, H→L+2	235.35	0.0333	239 (11.76)
H-8→L+1, H→L+5	230.63	0.2503	

H→L+5, H-9→L	218.38	0.0417	
H→L+7	207.96	0.0017	
H-2→L+4, H-2→L+5, H-4→L+5	203.31	0.0017	
H-4→L+5, H-2→L+4, H-4→L+4	202.76	0.0045	

ε – molar absorption coefficient [$dm^3\ mol^{-1}\ cm^{-1}$]; f – oscillator strength; H – highest occupied molecular orbital; L – lowest unoccupied molecular orbital.