Electronic Supplementary Material (ESI) for RSC Advances.

Amide-containing Luminescent Metal−organic Complexes as Bifunctional Materials for Selective Sensing of Amino Acid and Reaction Prompting

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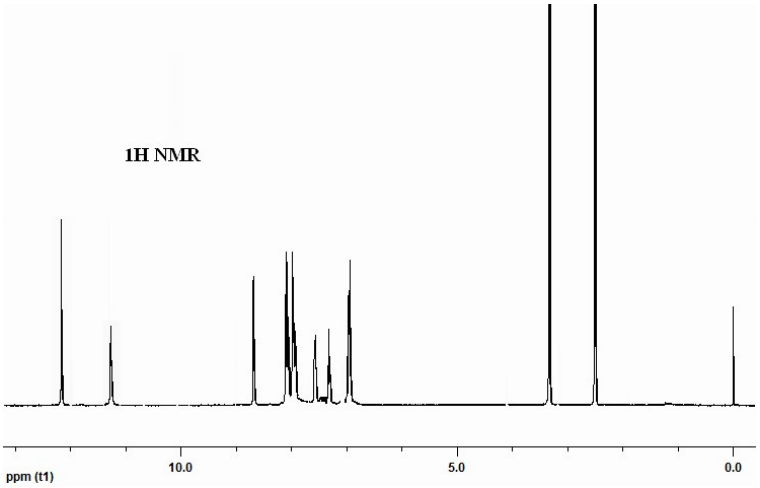
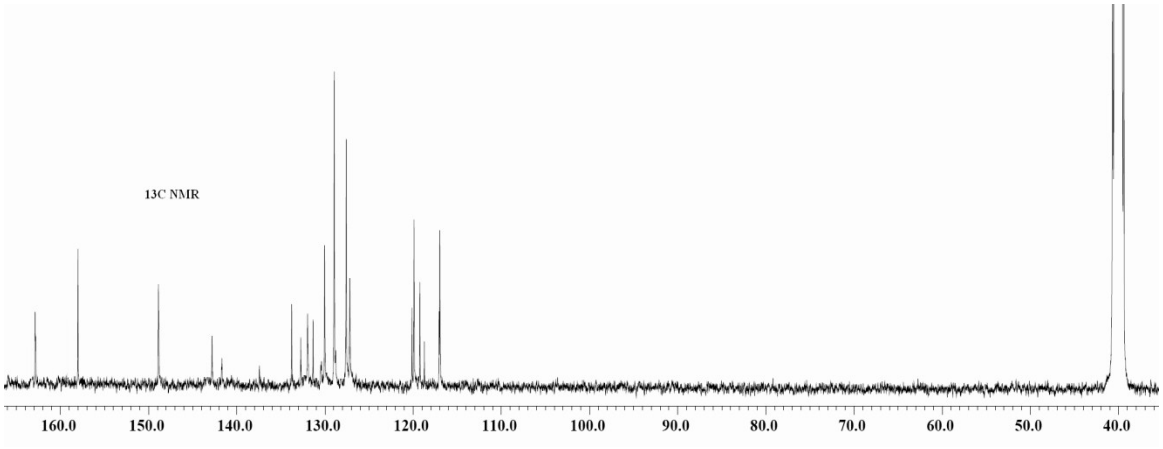
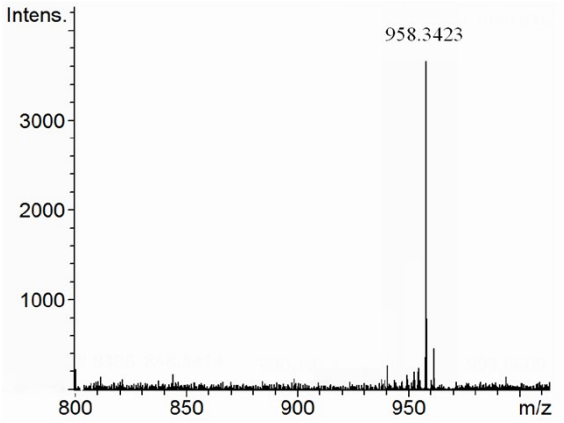
1. NMR, MS Data of ligands and Characterization of Ce−TBAS.

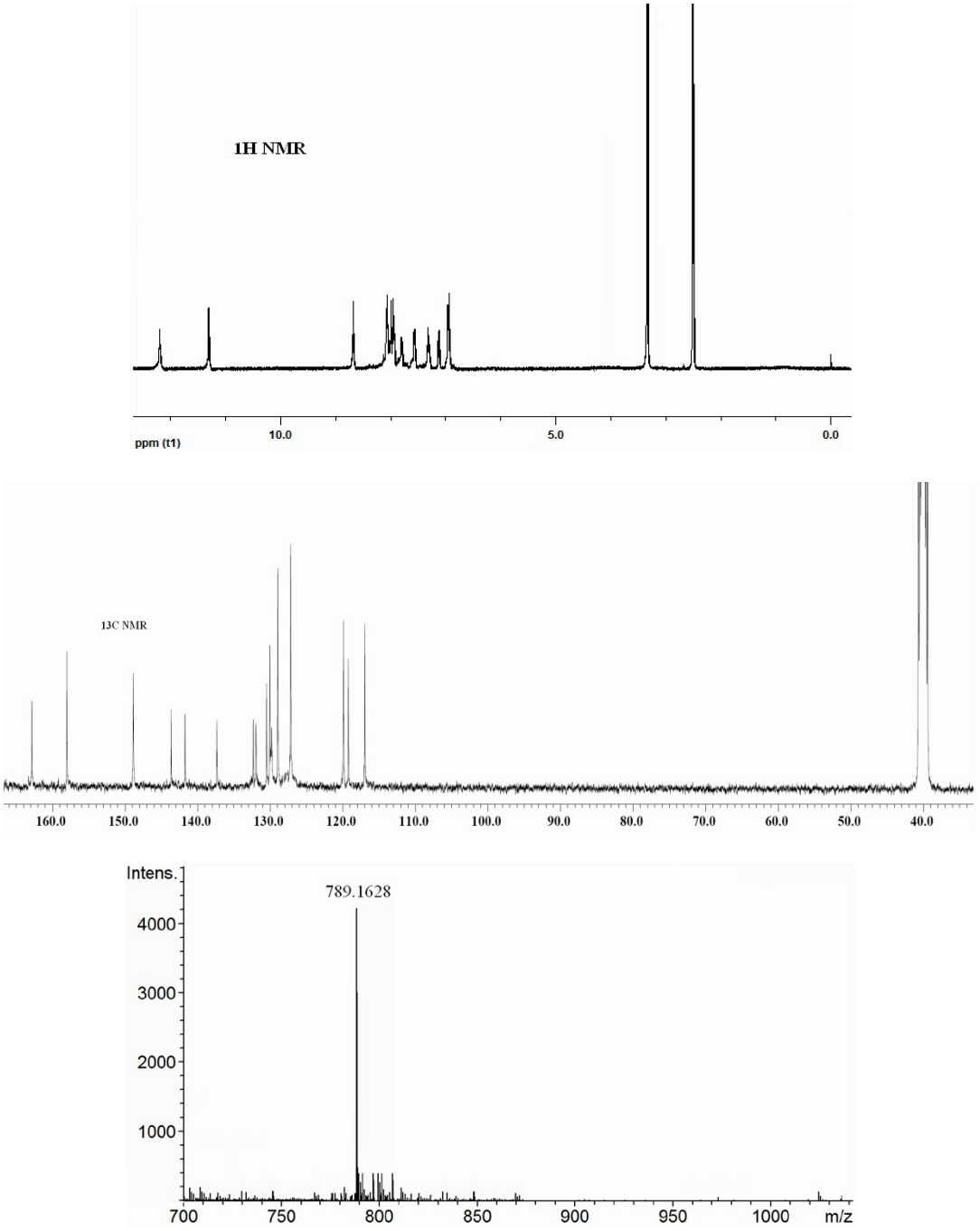
1.1 Figure S1 NMR and MS data of H_4BBAS.





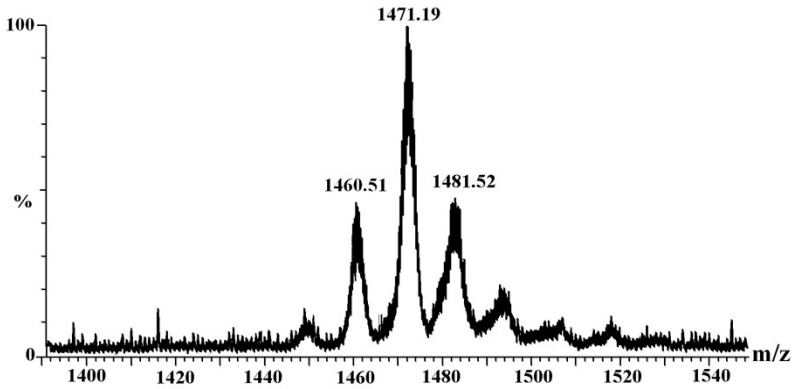


1.2 Figure S2 NMR and MS data of H_6TBAS.



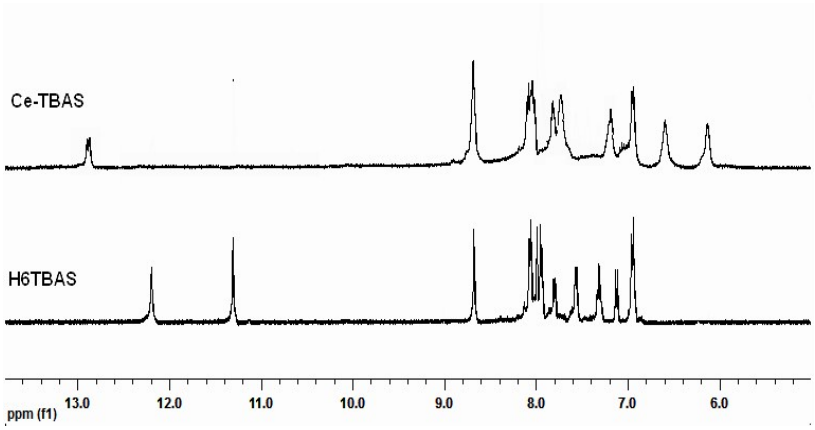
1.3. Characterization of Ce−TBAS.

1.3.1 Figure S3 ESI-MS of Ce−**TBAS** (0.1 mM) in DMF/CH_3OH in present of KOH (0.1 *m*M).



Peak number	value	Specie Assigned
1	1460.51	$[Ce(IV)_4(H\mathbf{TBAS})_3(H_2\mathbf{TBAS})]^{3-}$
2	1471.19	$[Ce(IV)_4(H\mathbf{TBAS})_3(H_2\mathbf{TBAS})(CH_3OH)]^{3-}$
3	1481.52	$[Ce(IV)_4(H\mathbf{TBAS})_3(H_2\mathbf{TBAS})(HNO_3)]^{3-}$

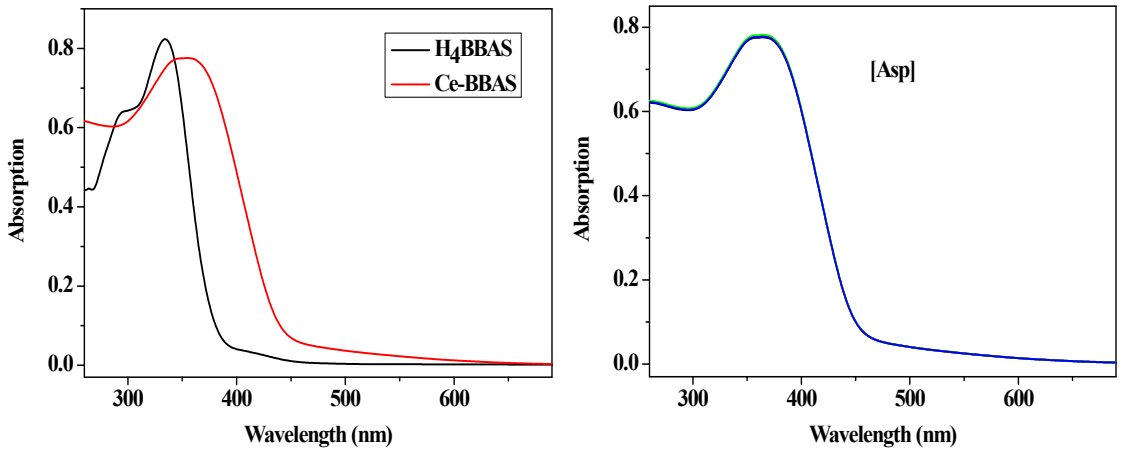
1.3.2 Figure S4 The relative ^1H NMR spectra of H_6**TBAS** and Ce−**TBAS** in DMSO-d_6.



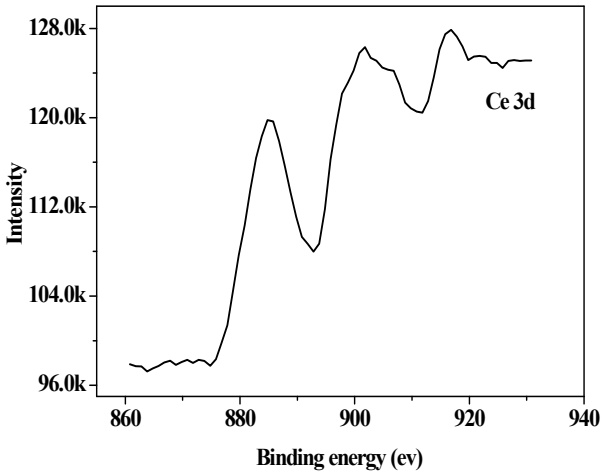
The disappearance of the phenolic proton signal at ~11.31 *ppm* and the significant upfield shift of aromatic protons in the phenol ring suggested the coordination occurred between the deprotonated phenolic groups and the metal ions. The downfield shift from 12.20 to 12.91 *ppm* and the reduction of the proton portion of the amide signal were indicative of the coordination of amide groups to the metal ions and the partial deprotonation of amide groups during the coordination process.

2. Studies on the amino acids sensing based on Ce−BBAS.

2.1 Figure S5 Uv-vis absorption spectra of H_4**BBAS**, **Ce−BBAS** and **Ce−BBAS** upon the addition of Asp up to 0.13 *m*M.

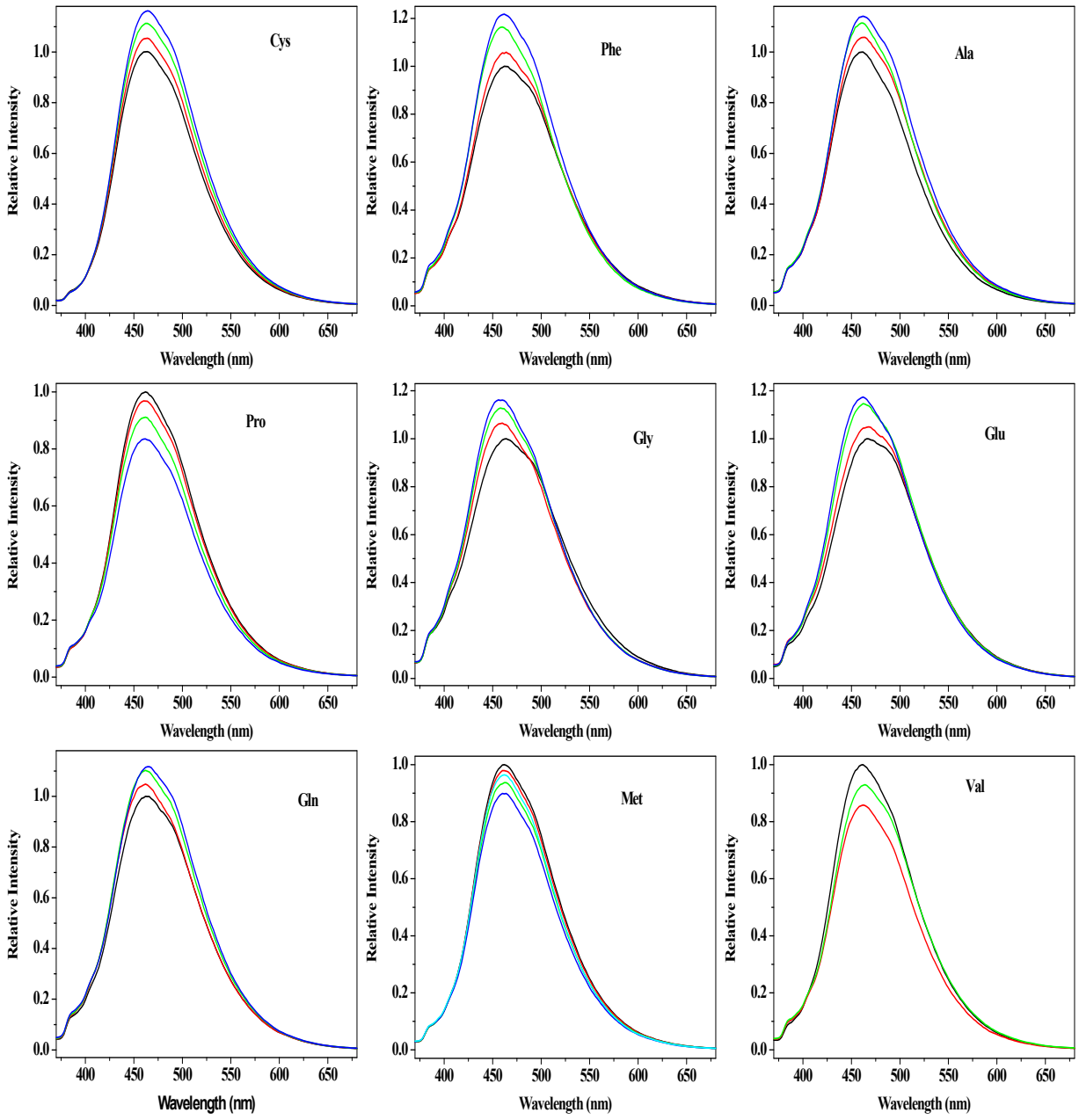


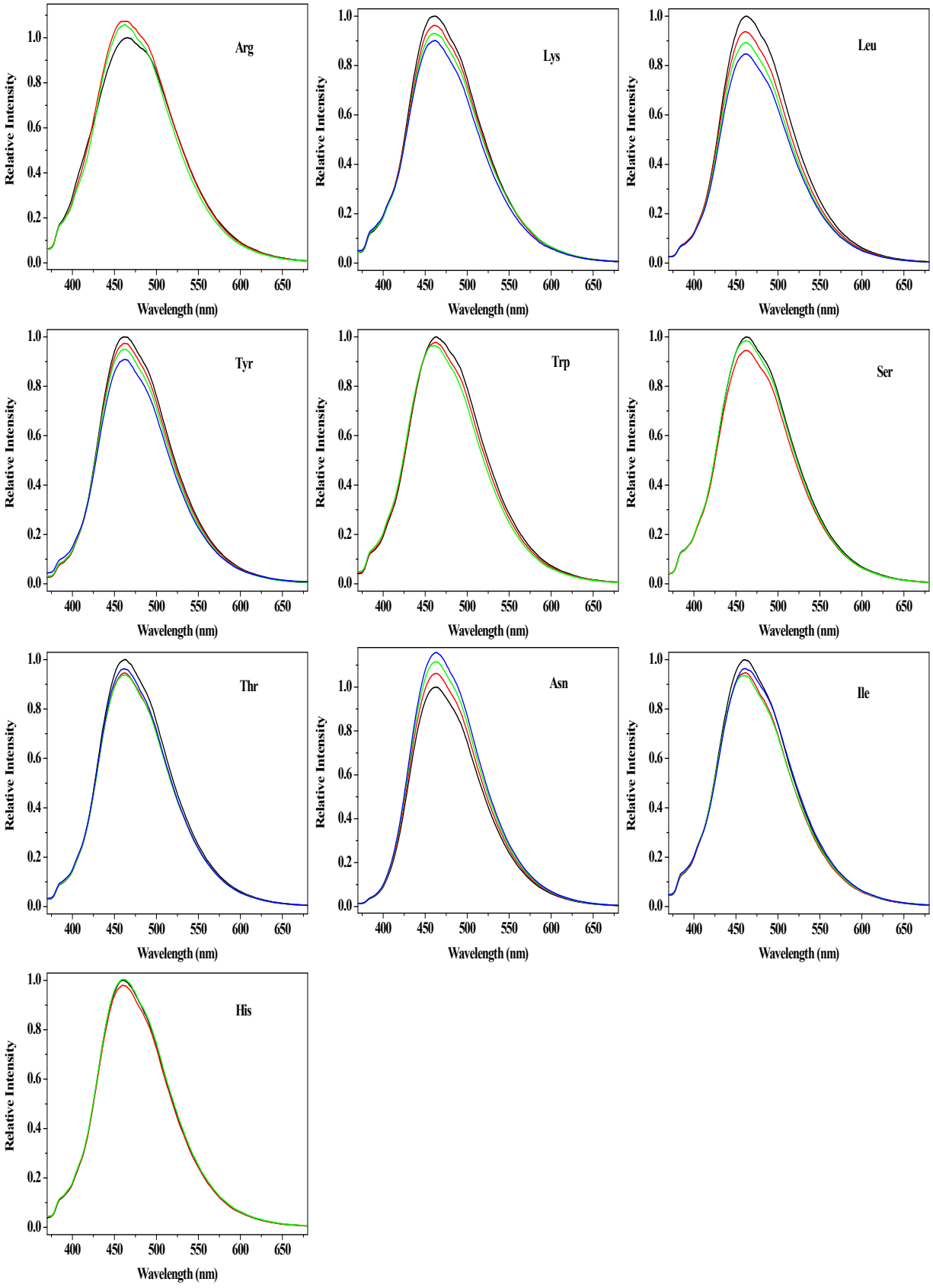
2.2 Figure S6 XPS spectra of Ce 3d from surface and near surface region of **Ce−BBAS**.



Ce 3d: 885.2, 901.4, 906.6, 916.5 eV. Typically the Ce 3d core level XPS spectrum exhibits three distinct regions of envelopes (around 880-890 eV, 895-910 eV and approximately 916 eV). The peak at a binding energy of 916 eV is normally used as the spectroscopic marker to detect the presence of the Ce^{IV} state and is usually assigned to $4f^0$ orbital transitions. The Ce 3d picture show the multiplet peaks of Ce 3d with the peak at 885.2, 901.4, 906.6, 916.5 eV are assigned to the presence of two Ce^{IV} ions of **Ce−BBAS** in the solid state. (F. Larachi, J. Pierre, A. Adnot, A. Bernis, *Appl. Surf. Sci.* 2002, **195**, 236; P. Datta, P. Majewski, F. Aldinger, *Mater. Charact.* 2009, **60**, 138.)

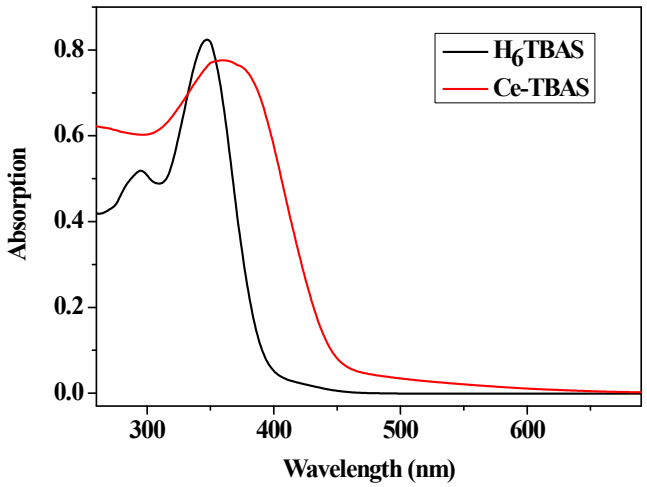
2.3 Figure S7 Families of various fluorescence spectra of Ce−**BBAS** in DMF/H_2O = 8/2 solution upon the addition of 0.13 mM of different selected analytes.



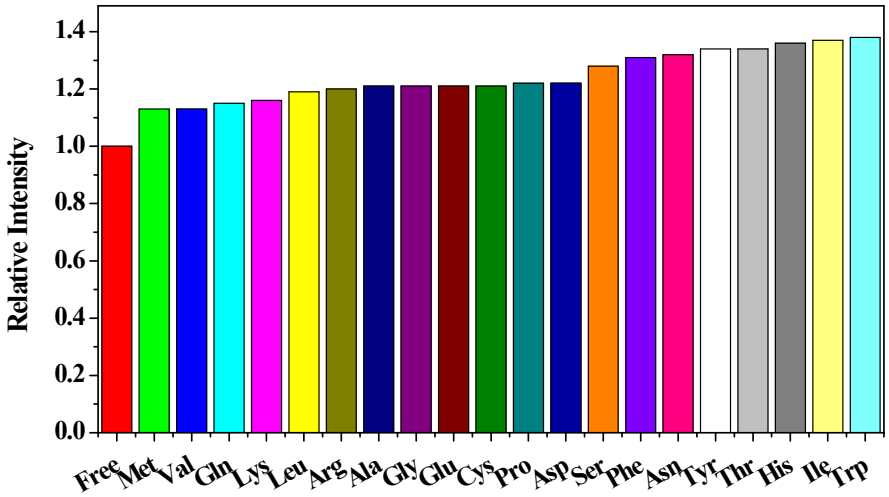

Arg
Lys
Leu
Tyr
Trp
Ser
Thr
Asn
Ile
His
Relative Intensity
Wavelength (nm)
0.0
0.2
0.4
0.6
0.8
1.0
400
450
500
550
600
650

3. Studies on the amino acids sensing based on Ce−TBAS.

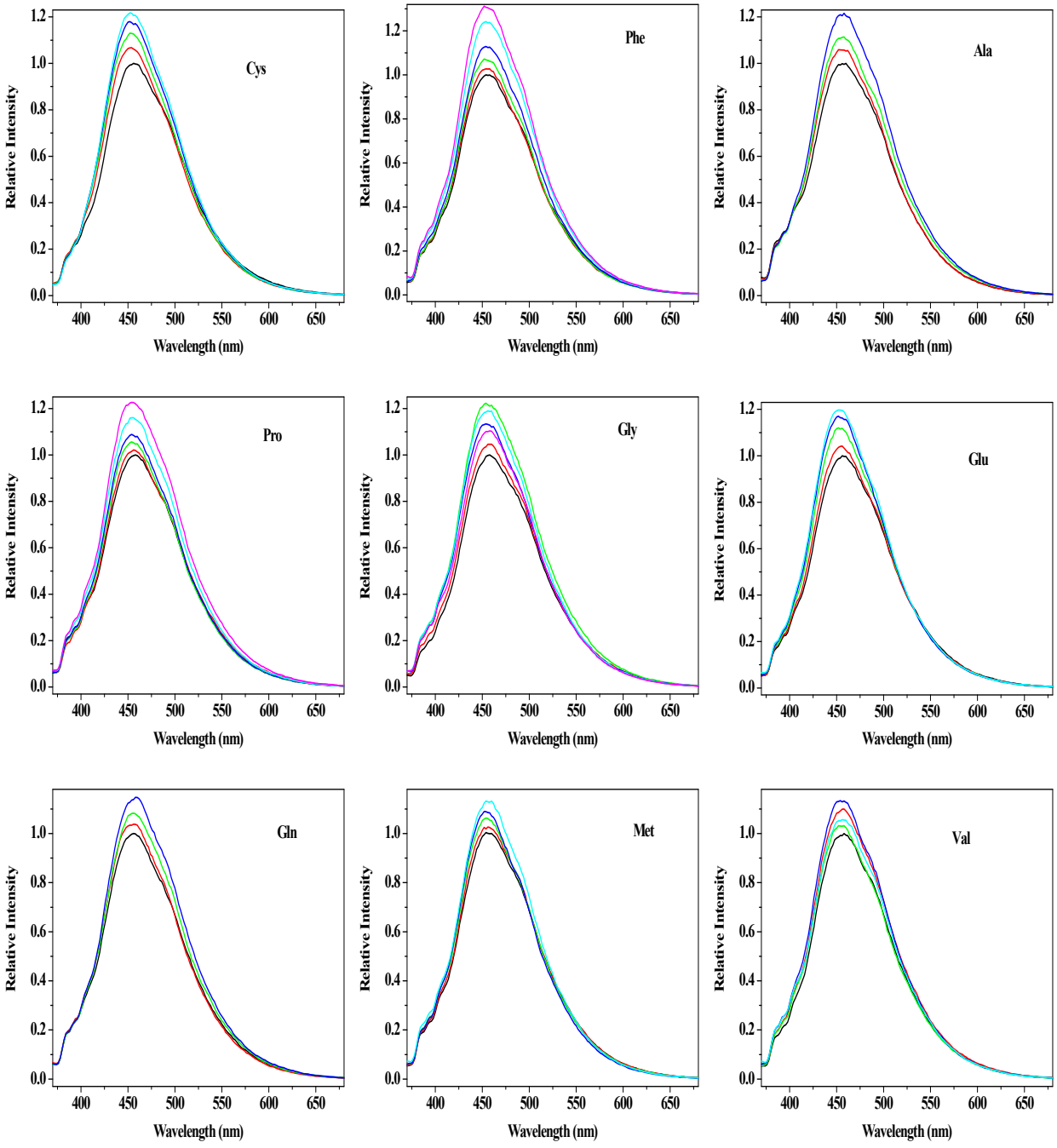
3.1 Figure S8 Uv-vis absorption spectra of H_6**TBAS** and **Ce−TBAS**.

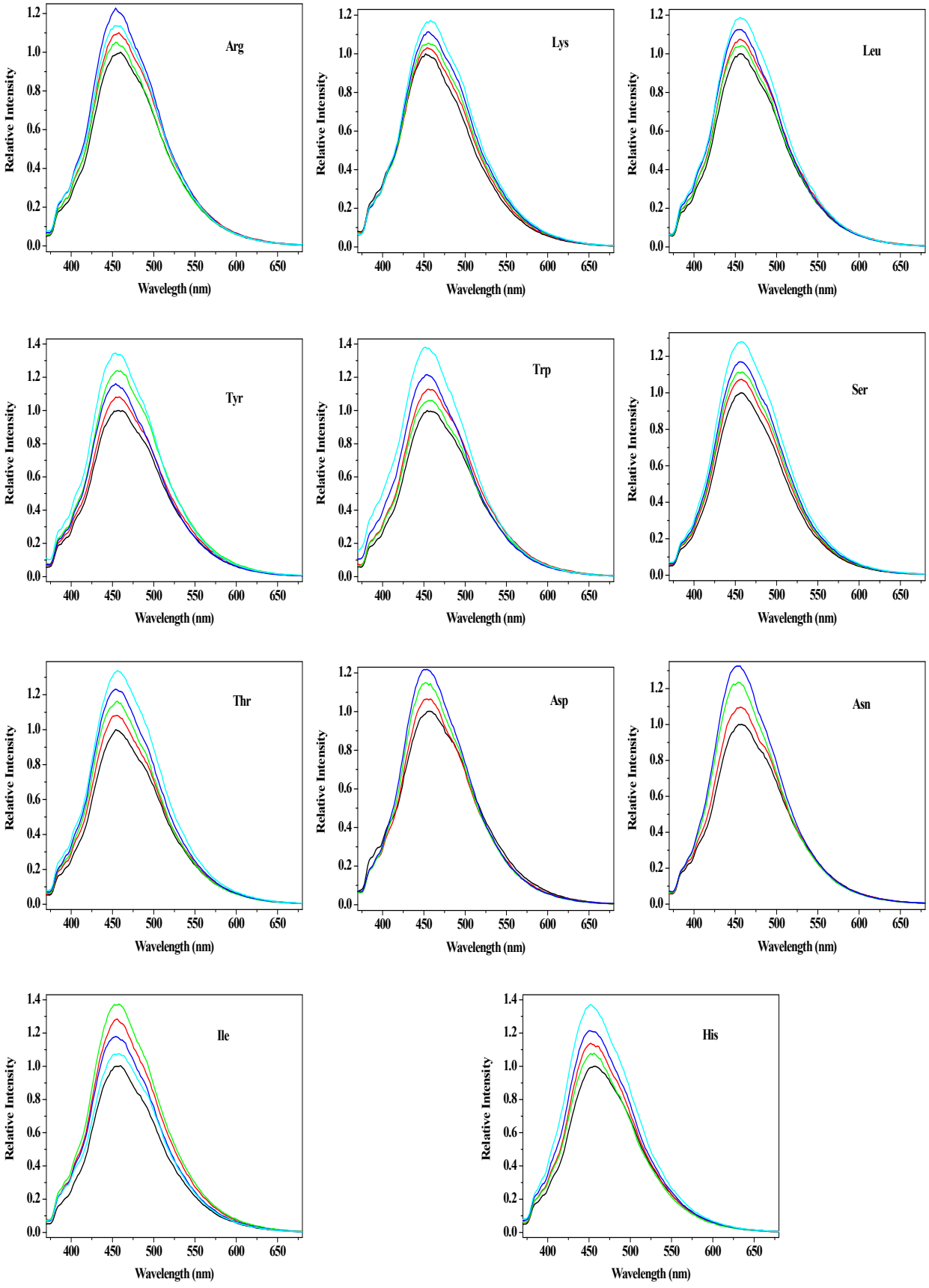


3.2 Figure S9 The fluorescence spectra of **Ce−TBAS** (15 μM) in DMF/H_2O = 8/2 solution upon the addition of 0.13 mM of various amino acids.



3.3 Figure S10 Families of various fluorescence spectra of Ce−**TBAS** in DMF/H_2O = 8/2 solution upon the addition of 0.13 mM of different selected analytes.




Arg
Lys
Leu
Tyr
Trp
Ser
Thr
Asp
Asn
Ile
His
Relative Intensity
Wavelength (nm)
Wavelength (nm)
Wavelength (nm)
Wavelength (nm)
Wavelength (nm)
Wavelength (nm)
Wavelength (nm)
Wavelength (nm)
Wavelength (nm)
Wavelength (nm)
Wavelength (nm)

4. Association Constant Calculations and **Figure S11**.

Generally, for the formation of Host-Guest complexation species formed by the cage compound host (H) and the guest (G), if we assume xC_0 to the concentration of complexes species Host-Guest (H-G), when the concentration of the added guest is an nC_0 with the original concentration of the cage being fixed at C_0:

$$\mathbf{1} + nG \rightleftharpoons \mathbf{1}-G$$

cage only	C_0		
G is added	$(1-x)C_0$	[G]-xC_0	xC_0

While [G]>>xC_0, $K = \mathbf{x}/[1-\mathbf{x}][G]^n$ (1)

The measurements are performed under the conditions where the luminescence intensity of the free host (H) in such a concentration is F_0; after addition of a given amount (nC_0) of G, the fluorescent intensity becomes:

$$F = F_1 x + F_0 (1-x) \qquad (2)$$

Where F_1 is the luminescence of the saturated value in the presence of excess guest.

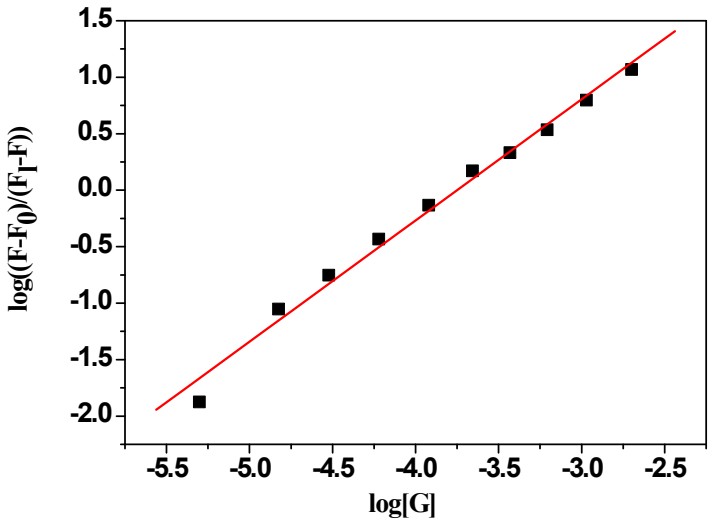
It is easy to derive the usual equation:

$$(F-F_0) / (F_1-F_0) = x \qquad (3)$$

From eqs (1) and (3), we can obtain the equation:

$$\log[(F-F_0)/(F_1-F)] = \log\boldsymbol{K} + n\log[G] \qquad (4)$$

K_s can be obtained by a linear analysis of (X) log[G] versus (Y). log[$(F-F_0)/(F_1-F)$]



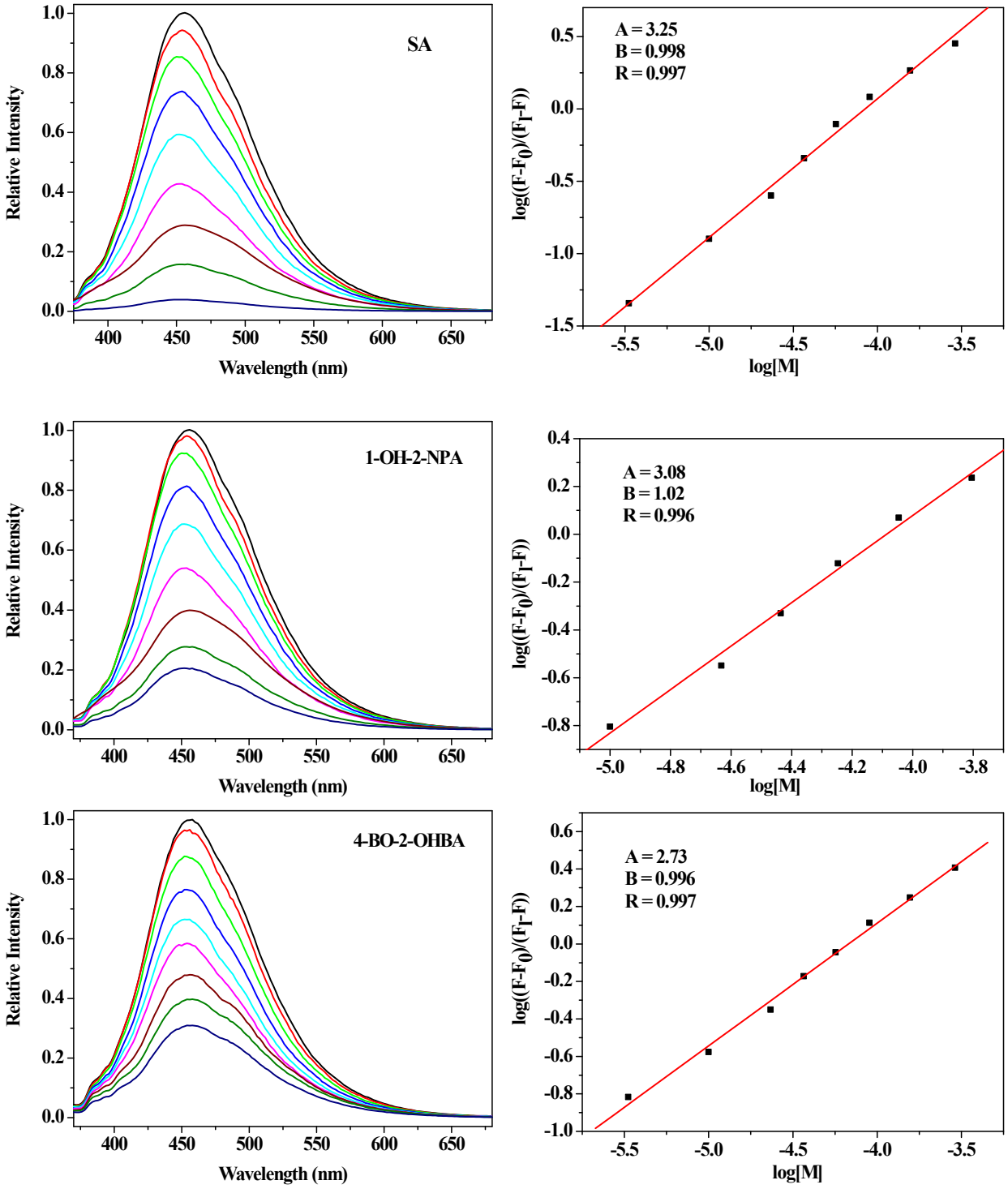
R = 0.994;

logK = 4.03 ± 0.11;

n = 1.03.

5. Studies on the aldehydes sensing based on Ce−TBAS.

5.1 Figure S12 Families of various fluorescence spectra of Ce−**TBAS** in DMF solution upon the addition of 0.3 mM of different selected aldehydes.



6. Studies on the aldehydes sensing based on Ce−BBAS.

6.1 Figure S13 Families of various fluorescence spectra of Ce−**BBAS** in DMF solution upon the addition of 0.3 mM of different selected aldehydes.