Electronic Supplementary Material (ESI) for Dalton Transactions.

A real-time fluorescent sensor specific to Mg^{2+}: crystallographic evidence, DFT calculation and its use for quantitative determination of magnesium in drinking water†

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(Electronic Supplementary Information)

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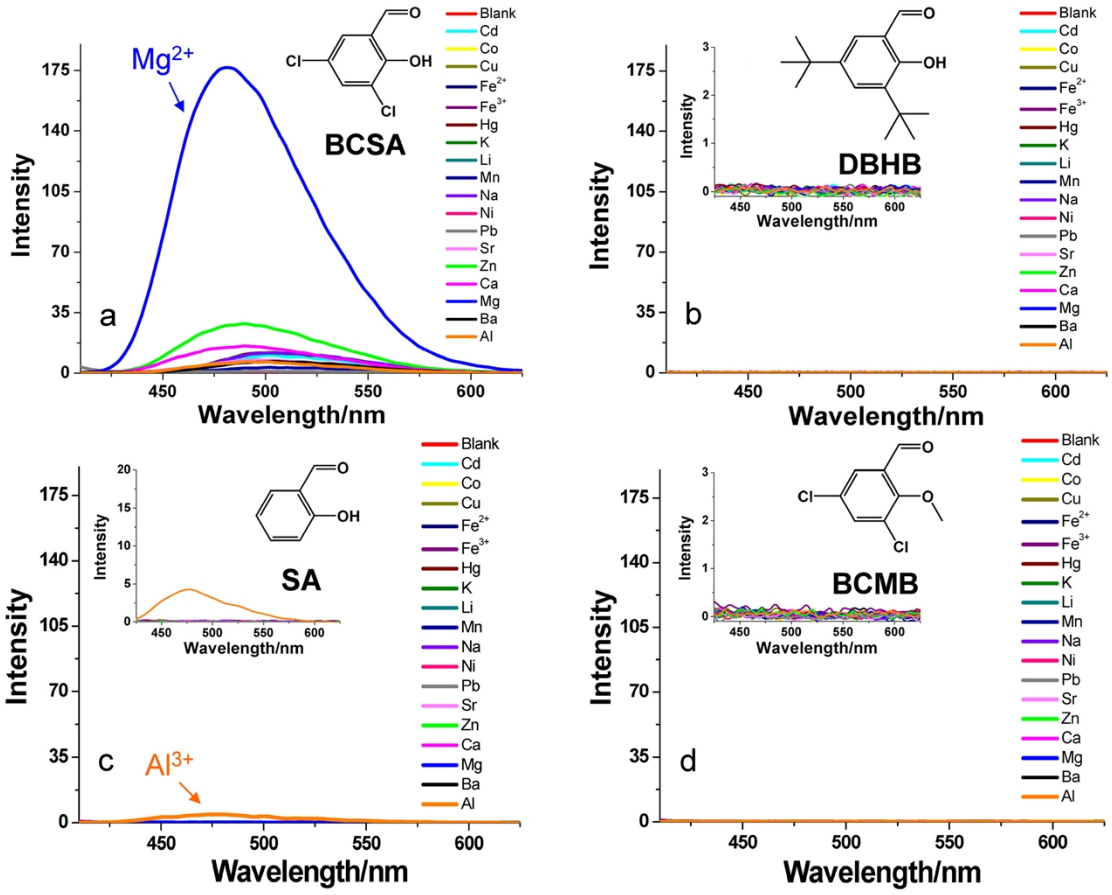

Fig. S1 Fluorescence emission spectra of four receptors (50 μM) in the presence of 8 equiv. of various metal ions in a 95:5 (v/v) ethanol-HEPES (0.05 M, pH = 7.0) solution. Inset: the magnification of the region between 425 and 625 nm (λ_{ex} = 400 nm).

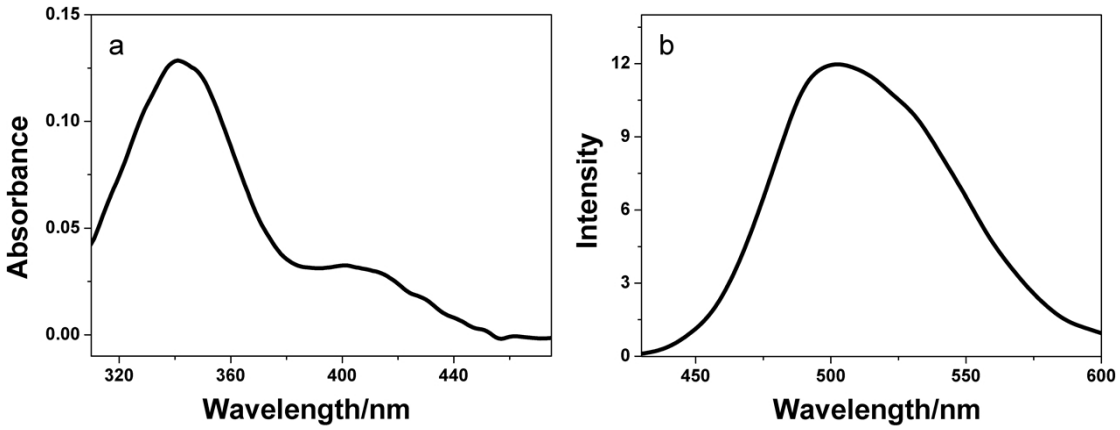

Fig. S2 (a) Absorption and (b) fluorescence spectra of **BCSA** in 95:5 (v/v) different organic solvents-HEPES (0.05 M, pH = 7.0) solutions (λ_{ex} = 400 nm).

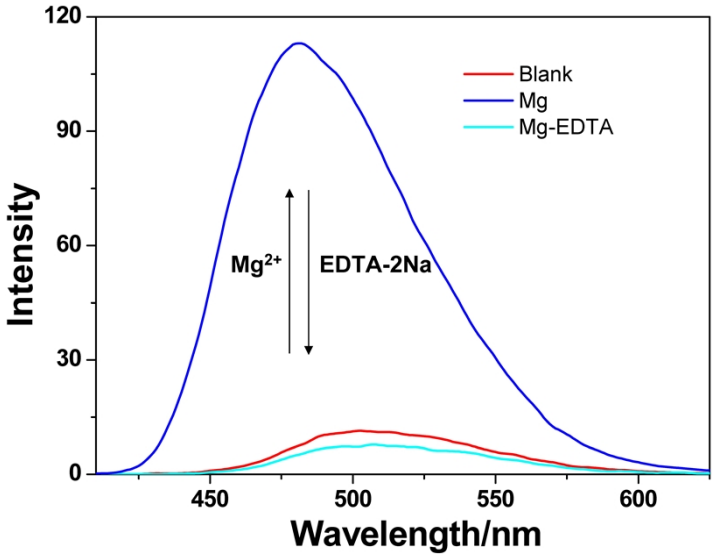

Fig. S3 Fluorescence emission spectra of probe **BCSA** in the presence of Mg^{2+} (2.0 equiv.) or EDTA-2Na (4.0 equiv.) in a 95:5 (v/v) ethanol-HEPES (0.05 M, pH = 7.0) solution (λ_{ex} = 400 nm).

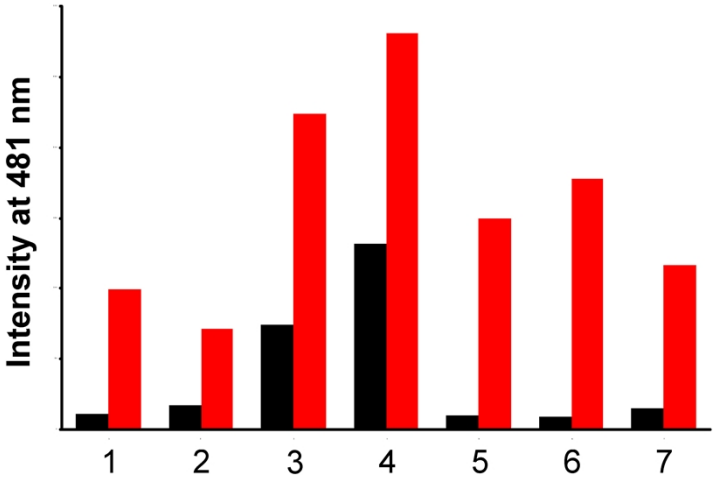

Fig. S4 Fluorescence intensity changes of bands at 481 nm of **BCSA** (black bar) and **BCSA**-Mg^{2+} (red bar) in 95:5 (v/v) different organic solvents-HEPES (0.05 M, pH = 7.0) solutions (1:THF, 2:acetone, 3:DMF, 4:DMSO, 5:acetonitrile, 6:ethanol, 7:methanol, λ_{ex} = 400 nm).

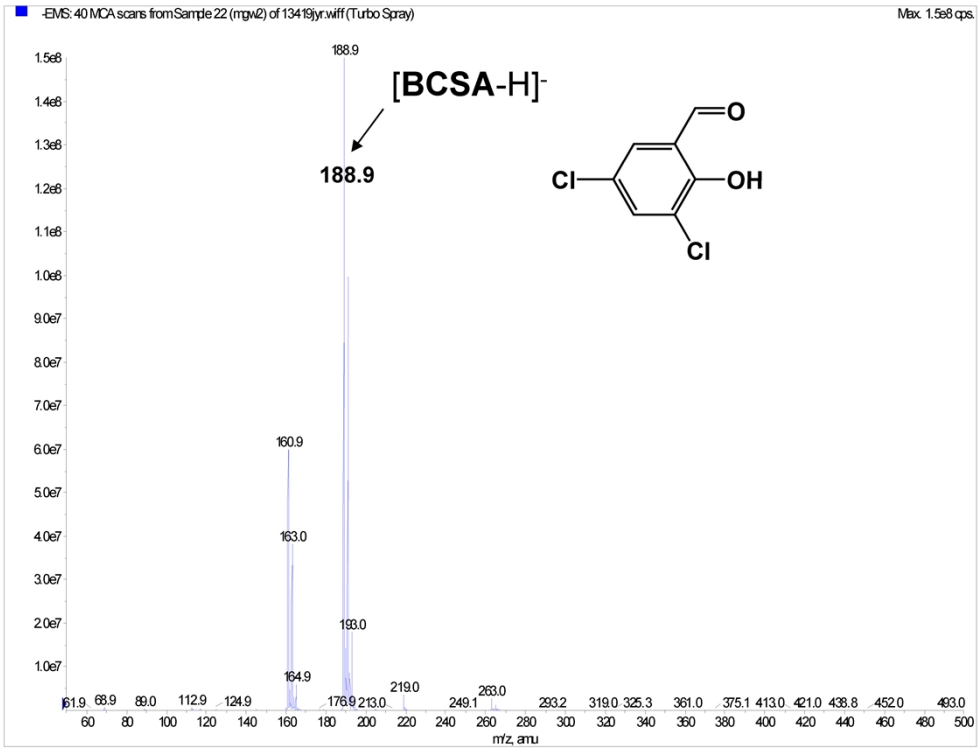

Fig. S5 ESI mass spectrum of 50 μM **BCSA** in a 95:5 (v/v) ethanol-water (pH = 7.0) solution under negative ion mode.

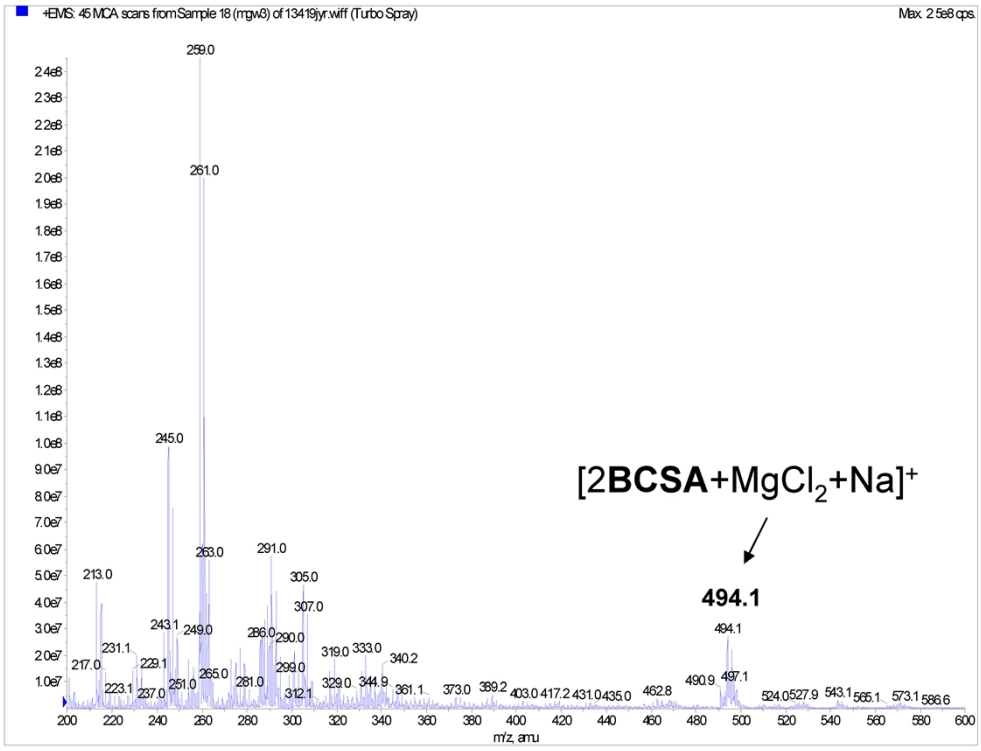

Fig. S6 ESI mass spectrum of 50 μM **BCSA** in a 95:5 (v/v) ethanol-water (pH = 7.0) solution after adding 200 μM Mg^{2+} under positive ion mode.

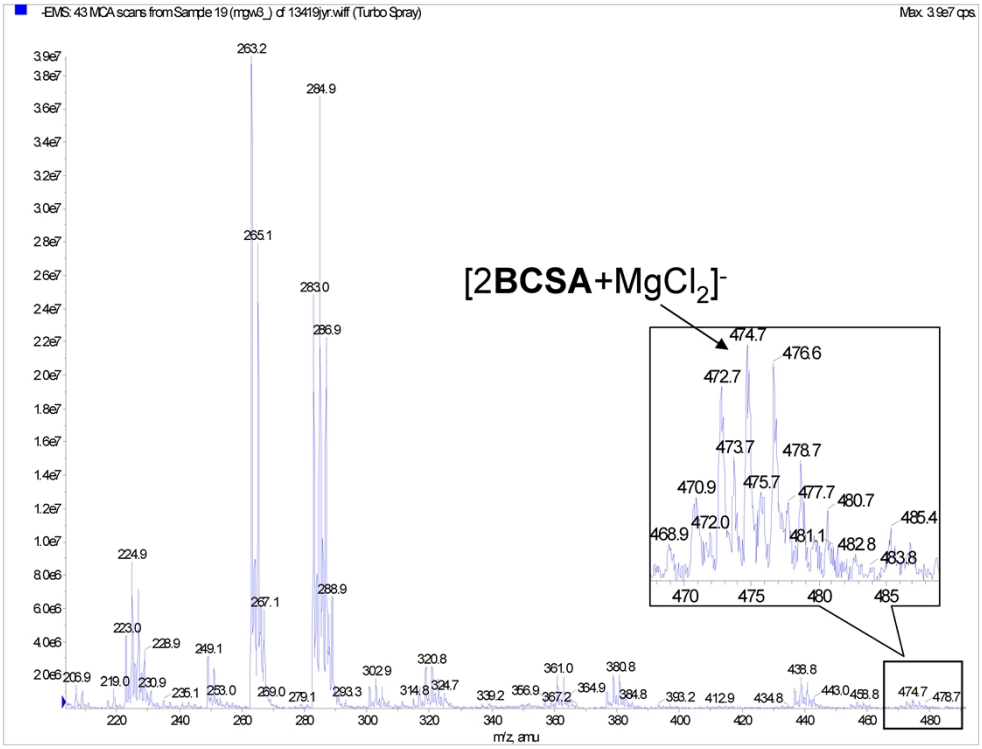

Fig. S7 ESI mass spectrum of 50 μM **BCSA** in a 95:5 (v/v) ethanol-water (pH = 7.0) solution after adding 200 μM Mg^{2+} under negative ion mode.

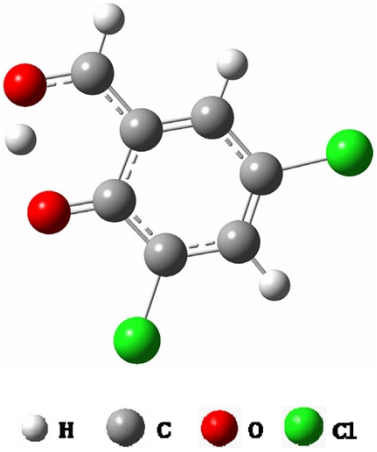

Fig. S8 DFT optimized excited-state geometry of the enol form of **BCSA**.

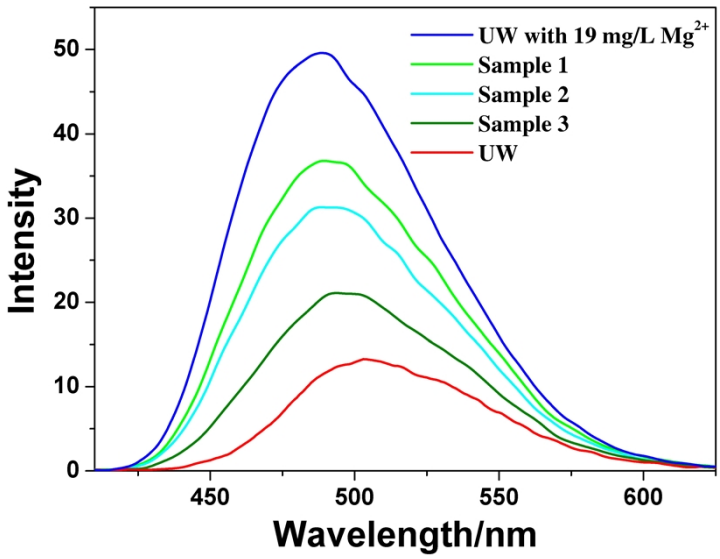

Fig. S9 Fluorescence spectra of 50 μM **BCSA** in different 95:5 (v/v) ethanol-HEPES (0.05 M, pH = 7.0) solutions. The HEPES buffer were prepared by ultrapure water (UW), bottled drinking water sample **1-3** and UW containing 19 mg/L Mg^{2+}, respectively (λ_{ex} = 400 nm).

Table. S1 Crystal data and structure refinement for **BCSA-**Mg^{2+}.

Identification code	**BCSA-**Mg^{2+}
Empirical formula	C22 H26 Cl4 Mg O8
Formula weight	584.54
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 10.477(2) Å α = 91.500(4)° b = 11.673(2) Å β = 106.143(3)° c = 12.937(2) Å γ = 115.291(3)°
Volume	1354.8(3) $Å^3$
Z, Calculated density	2, 1.433 Mg/m^3
Absorption coefficient	0.503 mm^{-1}
F(000)	604
Theta range for data collection	1.66 to 28.22°
Limiting indices	$-13 \le h \le 13$, $-15 \le k \le 13$, $-17 \le l \le 17$
Reflections collected / unique	11157 / 6618 [R(int) = 0.0251]
Completeness to theta = 28.22	99.1 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6618 / 0 / 353
Goodness-of-fit on F^2	1.045
Final R indices [I>2sigma(I)]	$R_1 = 0.0539$, $wR_2 = 0.1456$
R indices (all data)	$R_1 = 0.0922$, $wR_2 = 0.1657$
Largest diff. peak and hole	0.422 and -0.347 e. $Å^{-3}$