Electronic Supplementary Information

A highly specific 'Turn–On' fluorescent detection of Mg^{2+} through a xanthene based fluorescent molecular probe

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EXPERIMENTAL SECTION

Instrumentation:

The IR Spectra for the **B-XAN, N-XAN** and **(**B-XAN)$_2$Mg were recorded on JASCO-FTIR Spectrophotometer while ^{1}H NMR spectra were recorded on JEOL AL 300 FT NMR Spectrometer Mass spectrometric analysis was carried out on a Brukar Compass data analysis spectrometer. Electronic spectra were recorded at room temperature (298 K) on a UV-1800 pharmaspec spectrophotometer with quartz cuvette (path length=1 cm). Emission spectra were recorded on Varian Cary Eclipse Fluorescence spectrophotometer and JY HORIBA Fluorescence spectrophotometer. The ^{1}H NMR spectra were recorded by using tetramethylsilane (TMS) as an internal reference standard.

Materials and methods:

All reagents for synthesis were purchased from Sigma-Aldrich and were used without any further purification. All titration experiments were carried at room temperature. All the cations were used as their chloride salts. The ^{1}H NMR spectra were recorded by using tetramethylsilane (TMS) as an internal reference standard.

X-ray crystallographic studies:

Single crystal X-ray diffraction measurements were carried out on an Oxford Diffraction Xcalibur system with a Ruby CCD detector. All the determinations of unit cell and intensity data were performed with graphite-mono-chromated Mo-Kα radiation (λ= 0.71073 A°). Data for the ligand and metal complex were collected at room temperature. The structures were solved by direct methods, using Fourier techniques, and refined by full-matrix least-squares on F2 using the SHELXTL-97 program package [1]. Crystal data and details of the structure determination for ligand and complex are summarized in Table 1. **CCDC 1059288** contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/cgi-bin/catreq.cgi.

References:

1. (a) G. M. Sheldrick, SHELXL-97, Program for X-ray Crystal Structure Refinement, Göttingen University, Göttingen, Germany, 1997; (b) G. M. Sheldrick, SHELXS-97, Program for X-ray Crystal Structure Solution, Göttingen University, Göttingen, Germany, 1997.

Electronic Supplementary Information

Table 1: Crystal data and details of the structure determination of **B-XAN:**

Identification code	**B-XAN**
CCDC No.	CCDC 1059288
Empirical formula	$C_{21}H_{16}N_2O_3$
Formula weight	344.36
Temperature	293(2) K
Wavelength	0.71073A
Crystal system	Monoclinic
space group	P21/c
Unit cell dimensions	a=16.7245(10)Å , alpha=90deg. b=11.3341(6) Å, beta=105.028(5) deg. c=9.6962(5) Å, gamma=90deg.
Volume	1775.12(17) Å3
Z	4
Density (calculated)	1.288 mg/m^3
Absorption coefficient	0.087 mm-1
F(000)	720.0
Crystal size	0.028 x 0.023 x 0.016 mm
Crystal color and habit	Colourless, needle
Diffractometer	'Xcalibur, Eos'
Theta range for data collection	3.31 to 29.16 deg.
Limiting indices	-22<=h<=22, -9<=k<=15, -12<=l<=13
Reflections collected / unique	8177 / 4800 [R(int) = 0.0196]
Completeness to theta = 25.00	99.8 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Max. and min. transmission	1.00000 and 0.93478
Data / restraints / parameters	4034 / 0 / 236

Goodness-of-fit on F^2	1.053
Final R indices [I>2sigma(I)]	R1 = 0.0515, wR2 = 0.1104
R indices (all data)	R1 = 0.0856, wR2 = 0.1321
Largest diff. peak and hole	0.170 and -0.218 $e.A^{-3}$

Figure S1: IR spectrum of **B-XAN**

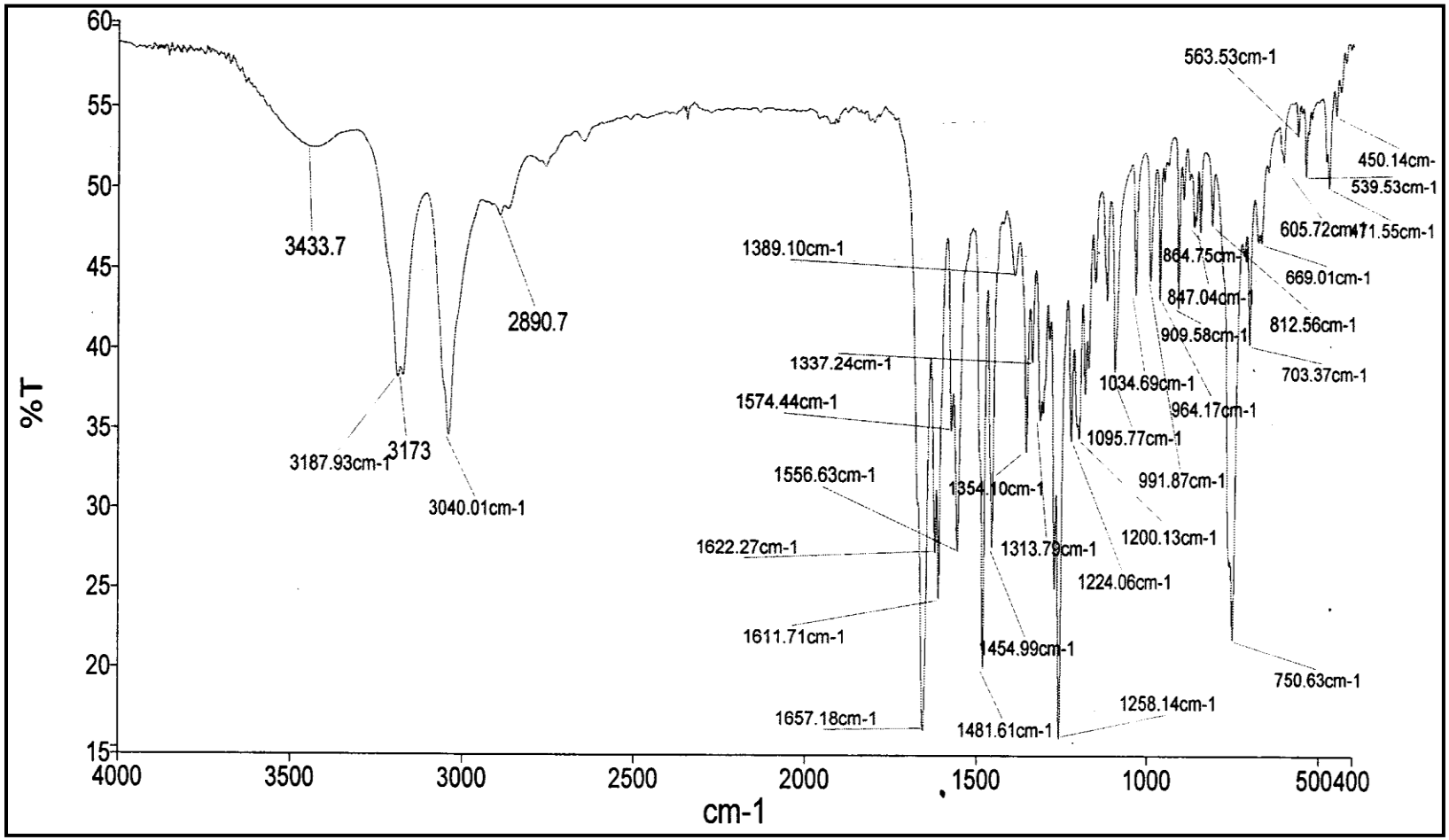

Figure S2: ^{1}H NMR spectrum of **B-XAN** (in CD_3CN)

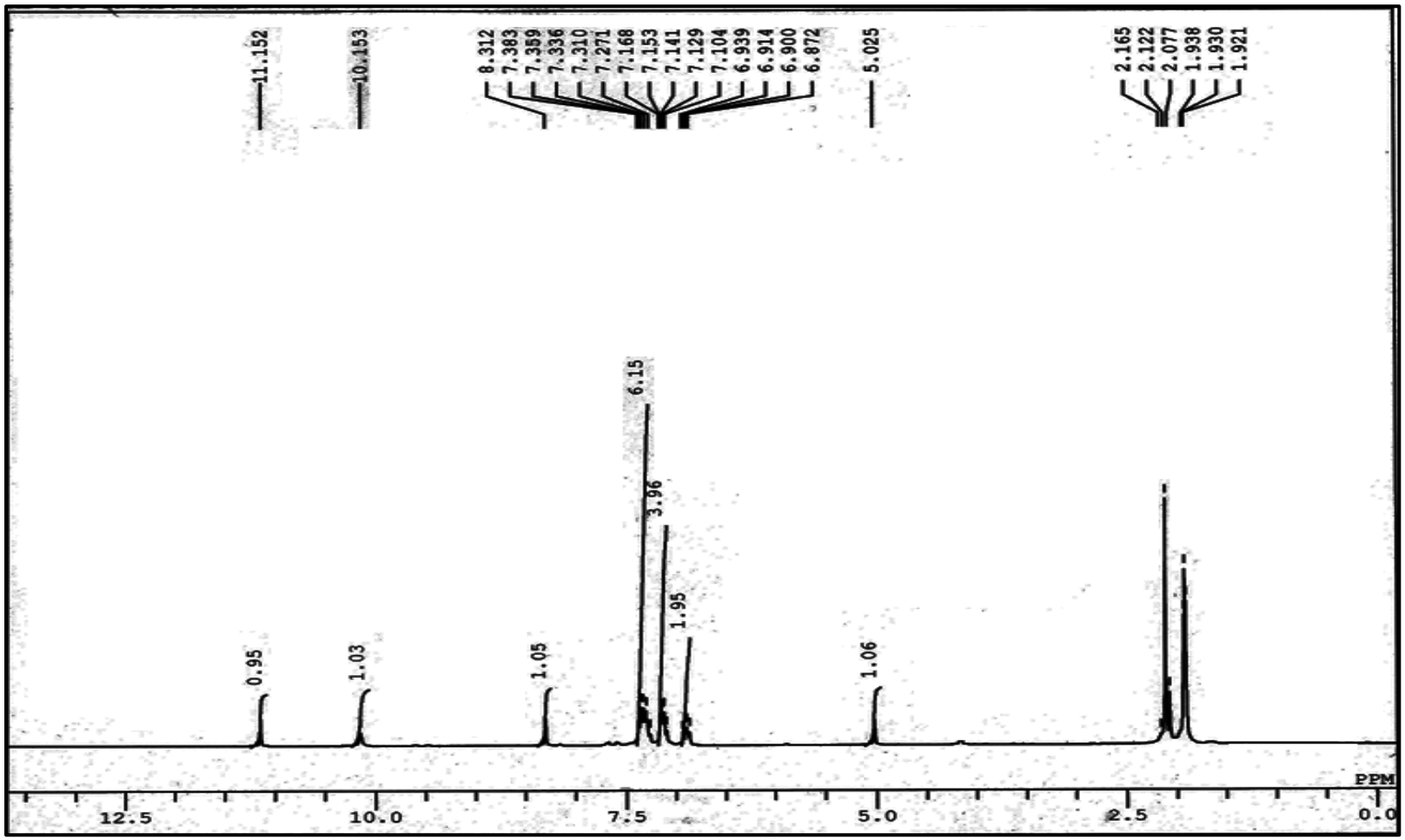

Figure S3: ^{13}C NMR spectrum of **B-XAN** (in DMSO–d_6)

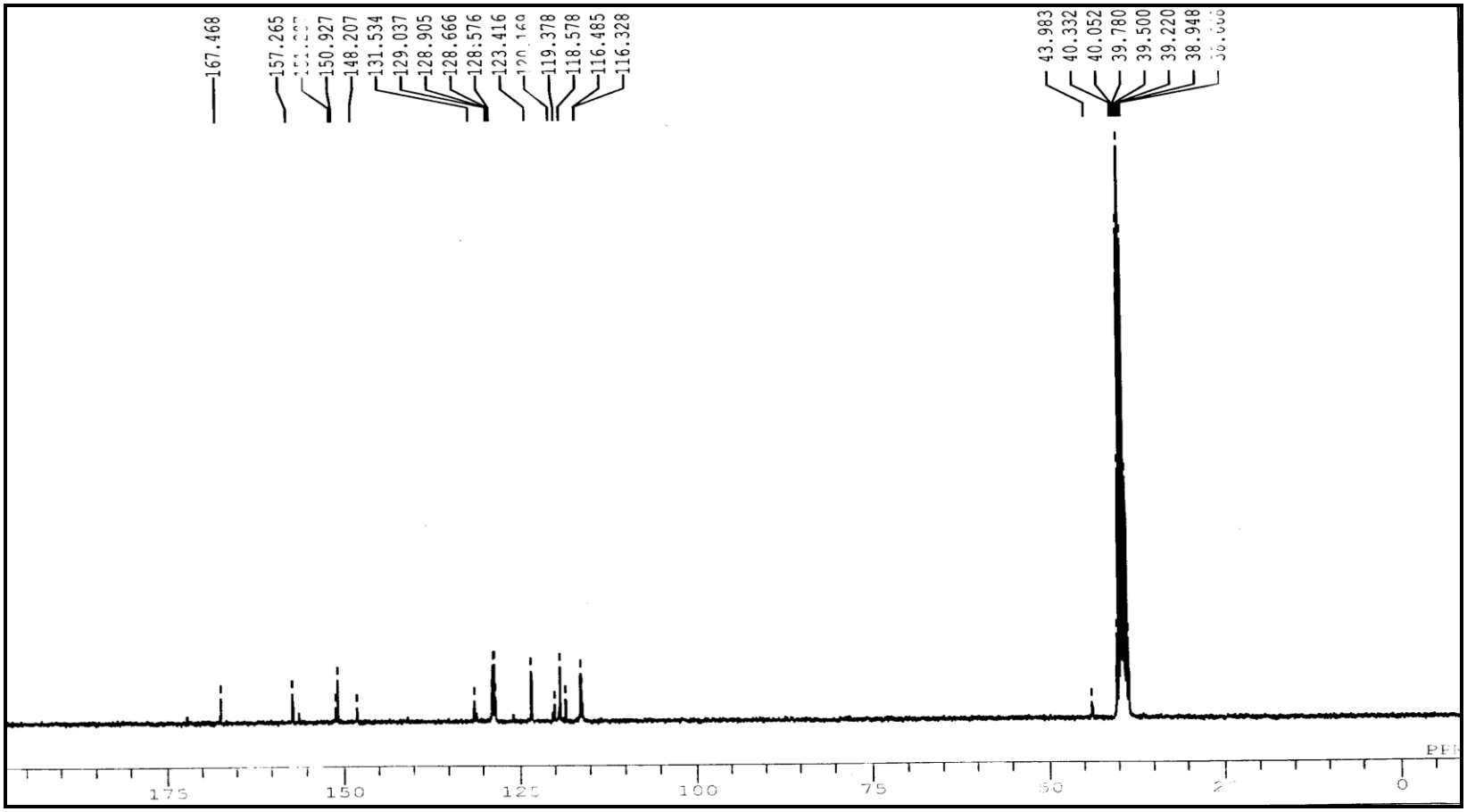

Figure S4: ESI-MS spectrum of **B-XAN**

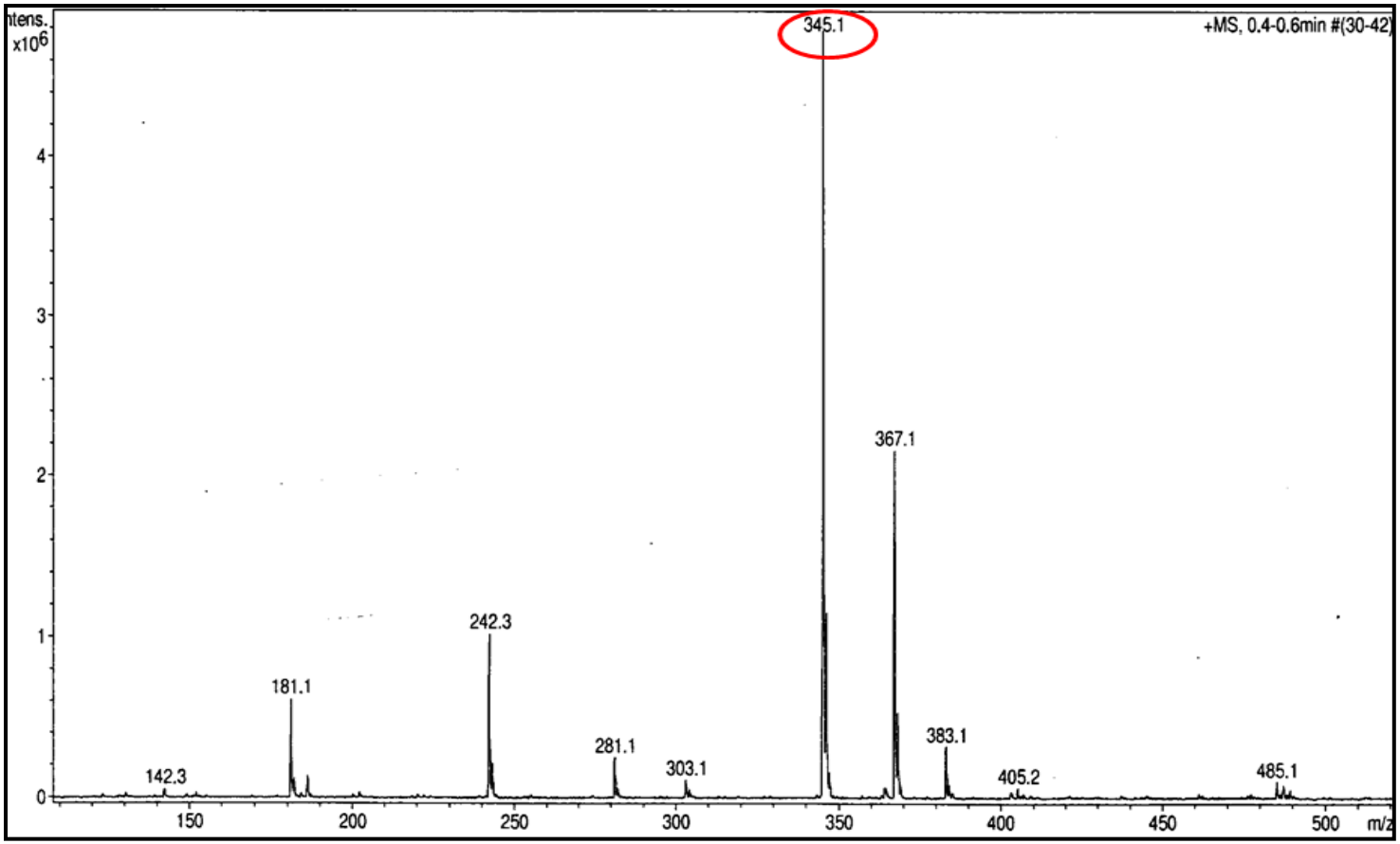

Figure S5: IR spectrum of **N-XAN**

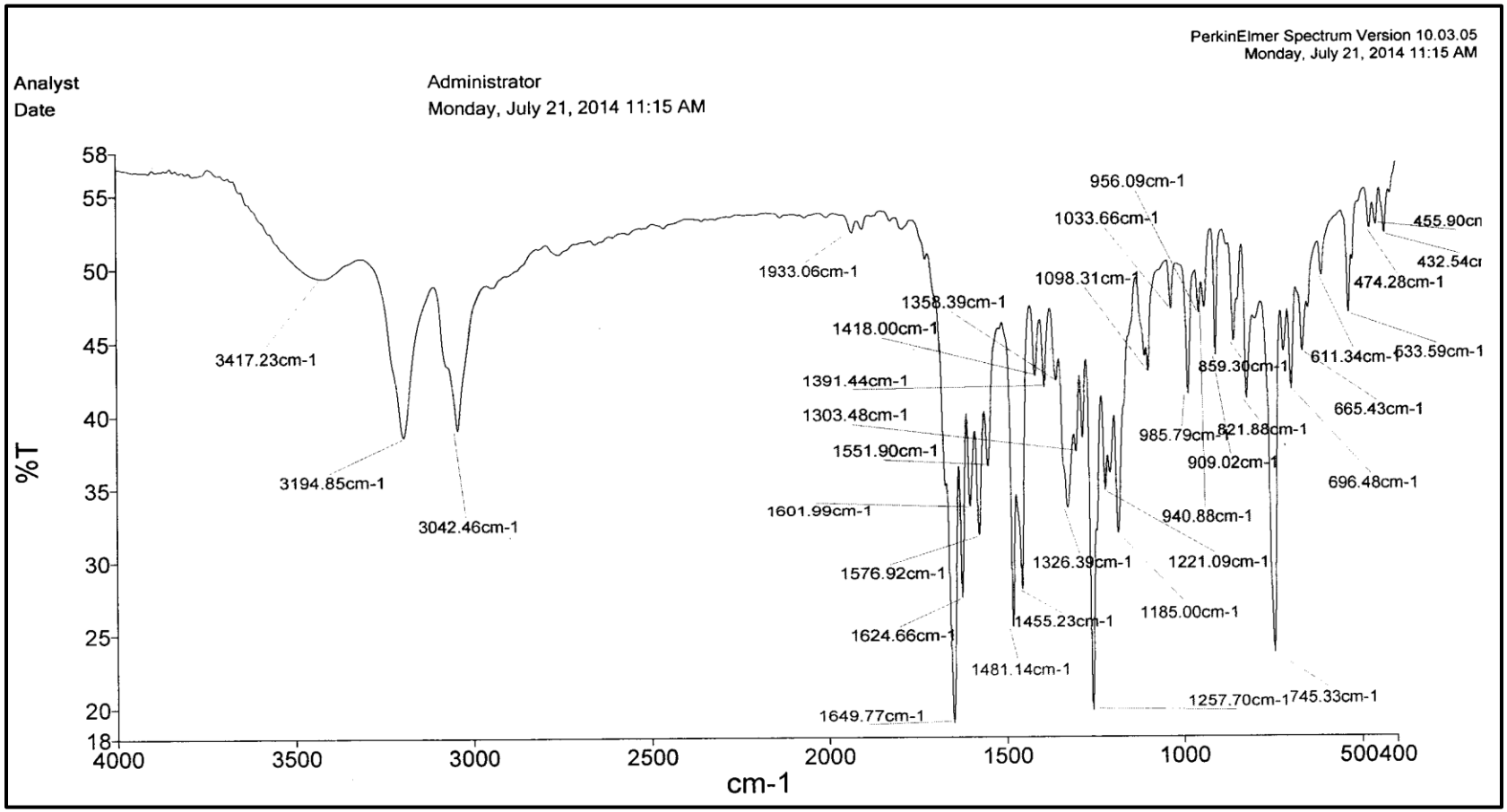

Figure S6: ^{1}H NMR spectrum of **N-XAN** (in DMSO–d_6)

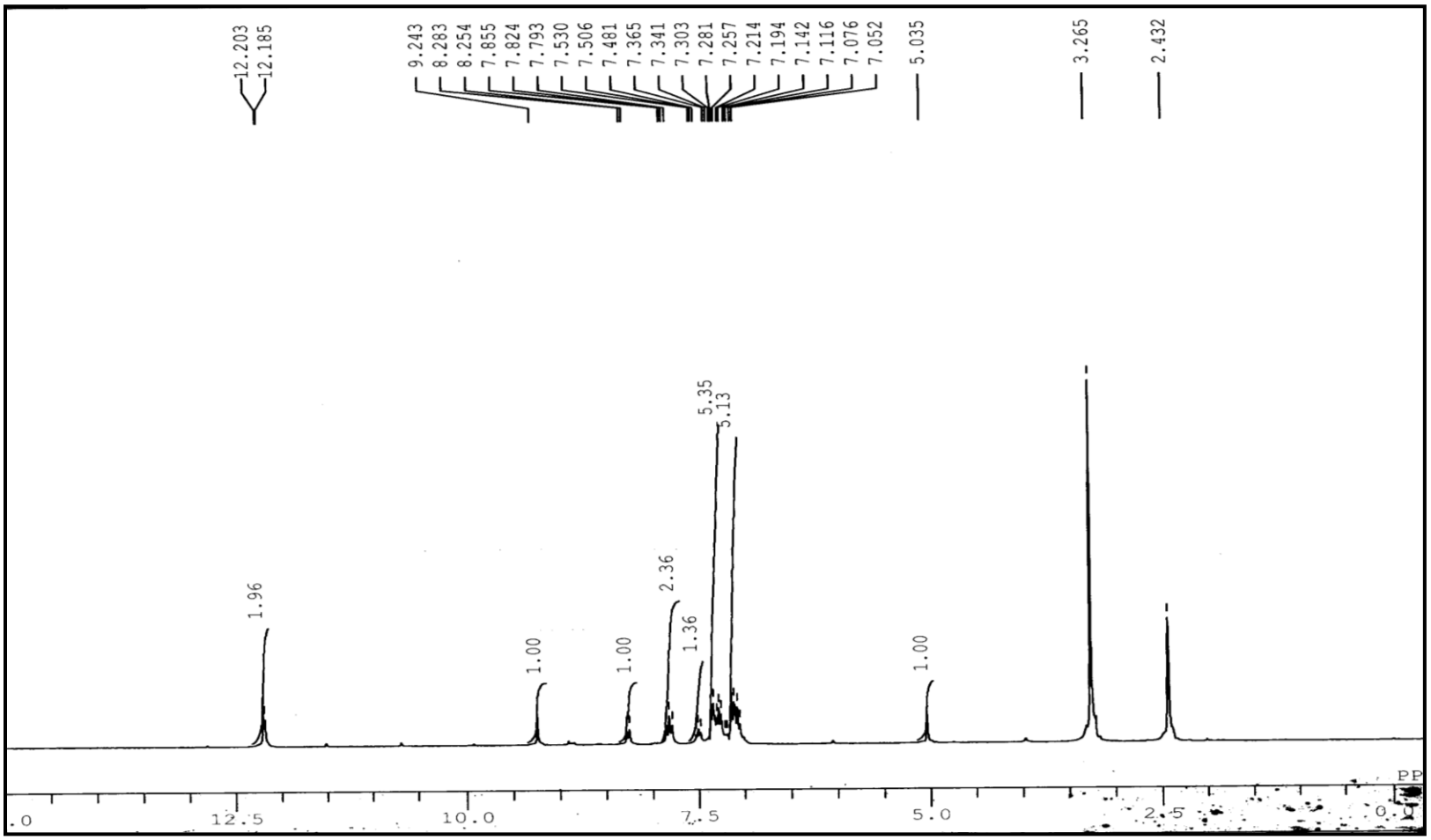

Figure S7: ^{13}C NMR spectrum of **N-XAN** (in DMSO–d_6)

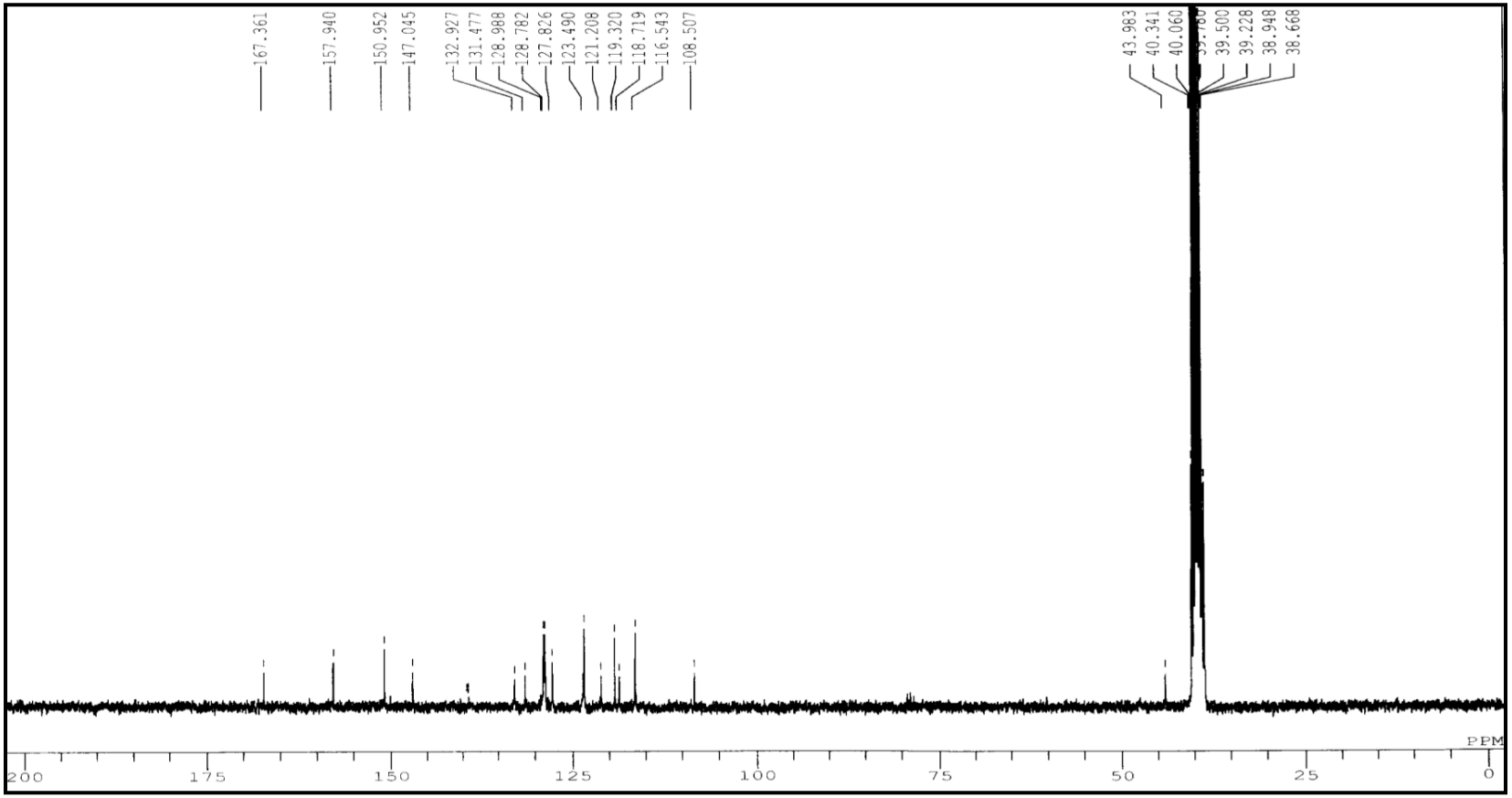

Figure S8: ESI-MS spectrum of **N-XAN**

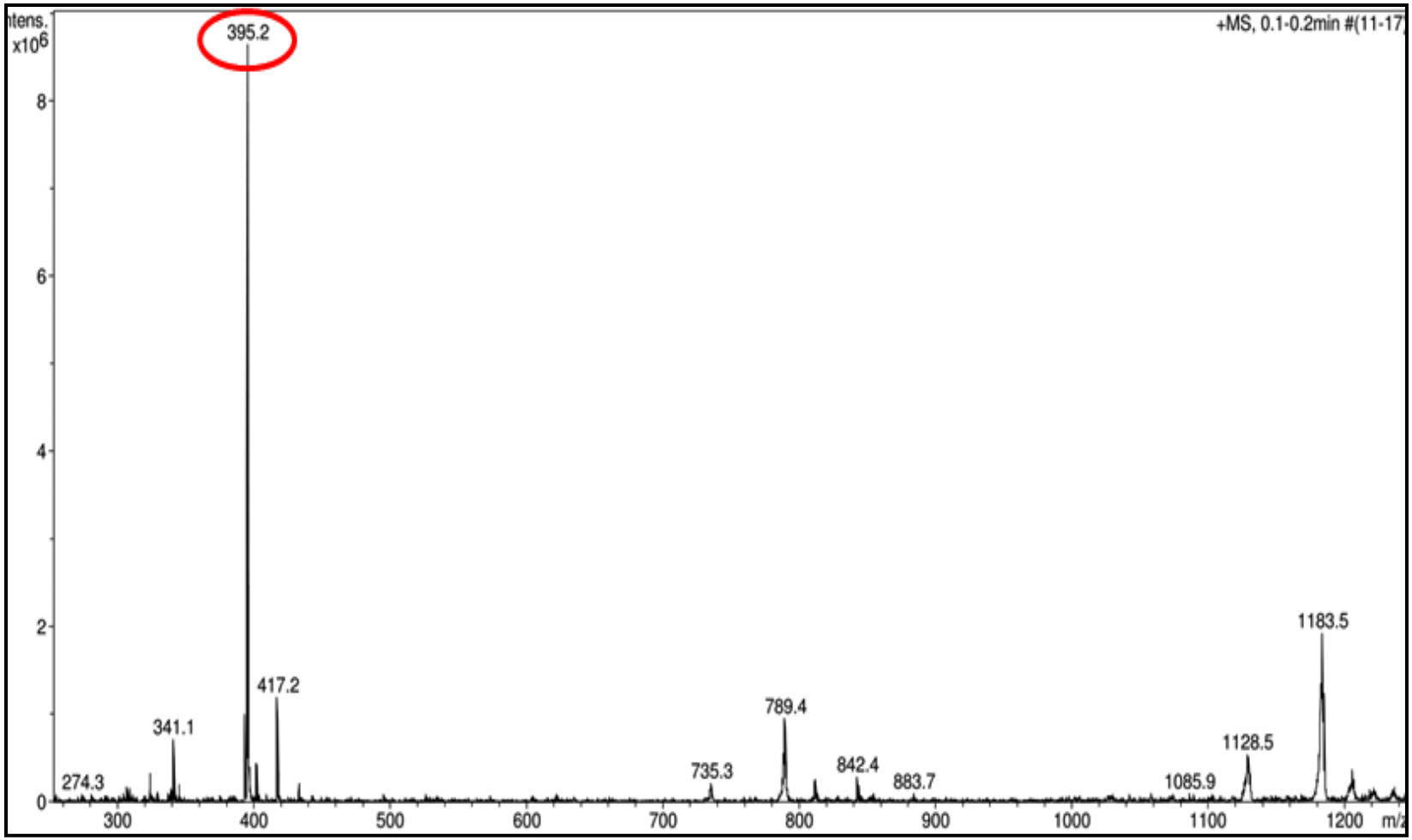

Figure S9: IR spectrum of $(B\text{-}XAN)_2Mg$

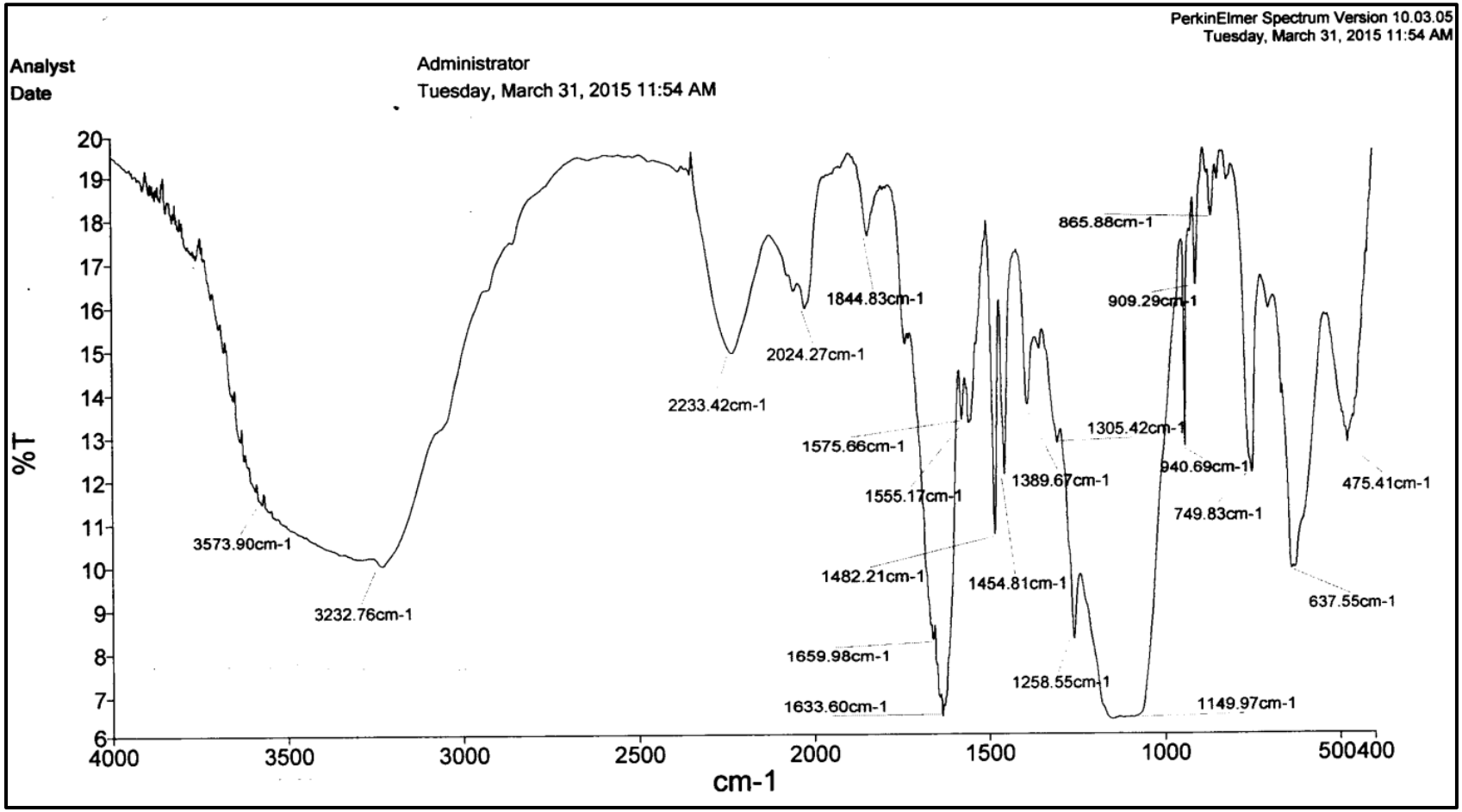

Figure S10: ^{1}H NMR spectrum of (B-XAN)$_2$Mg (in CD_3CN)

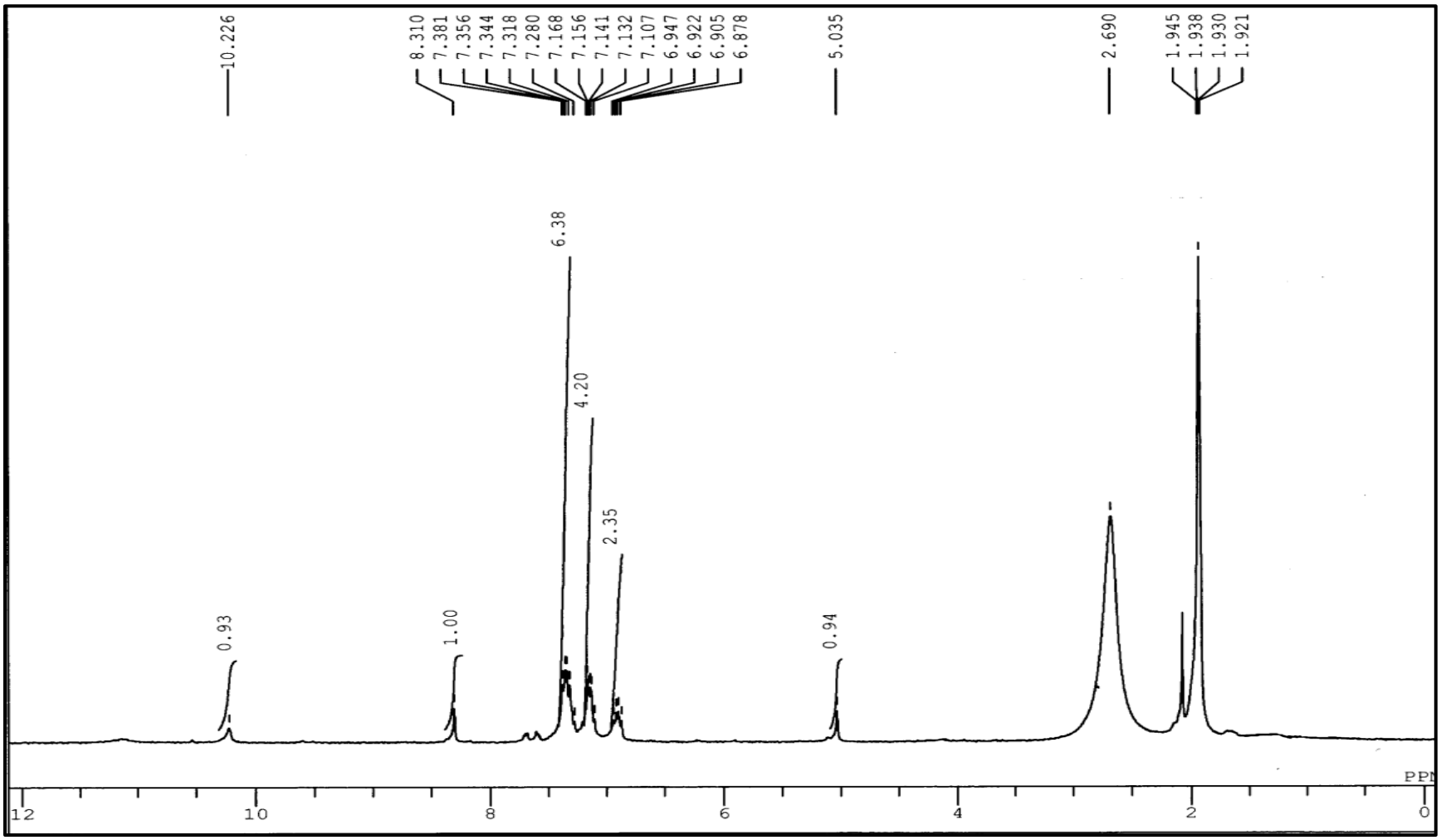

Figure S11: ^{13}C NMR spectrum of (B-XAN)$_2$Mg (in DMSO–d_6)

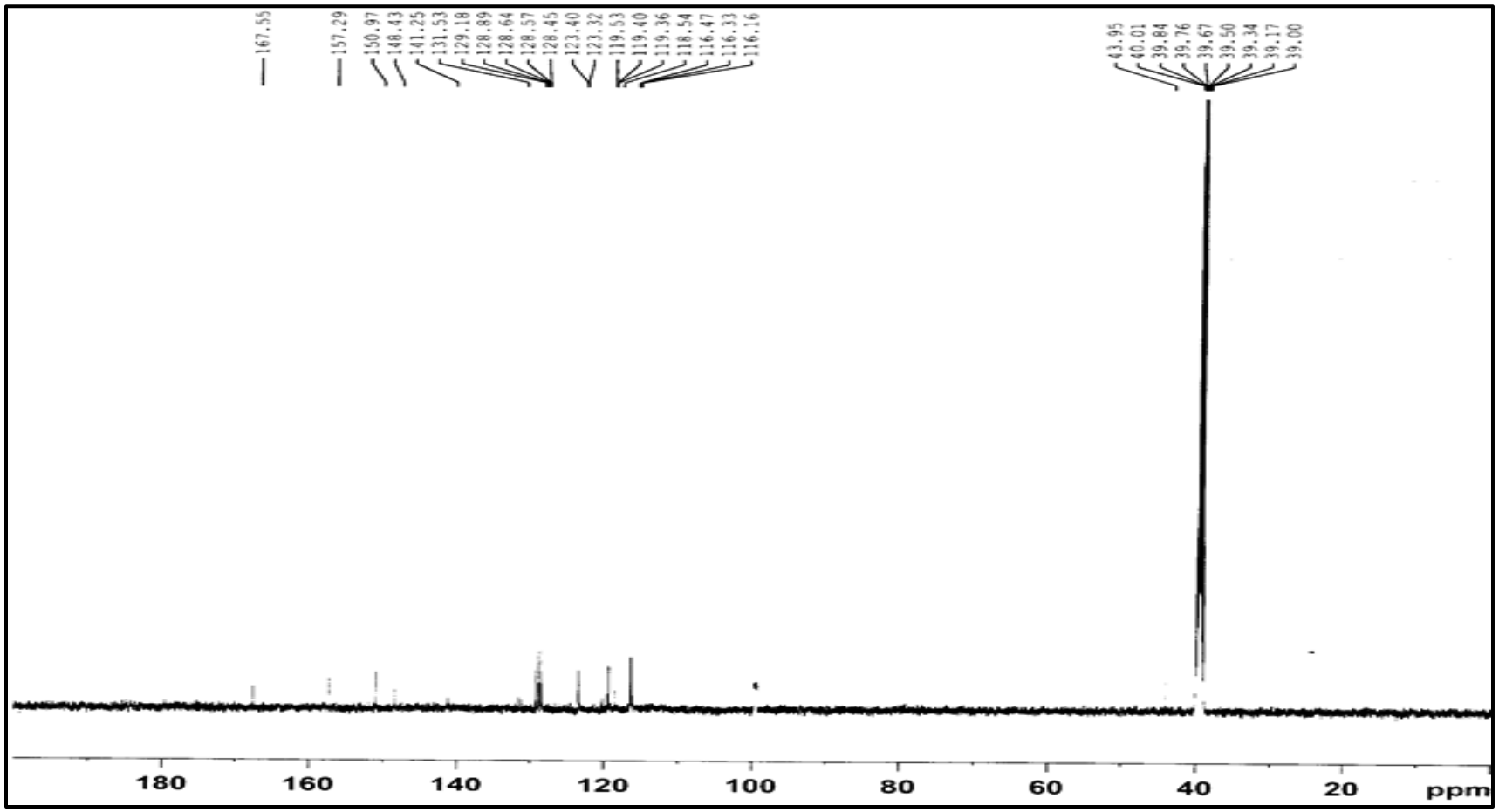

Figure S12: Mass spectrum of $(B\text{-}XAN)_2Mg$

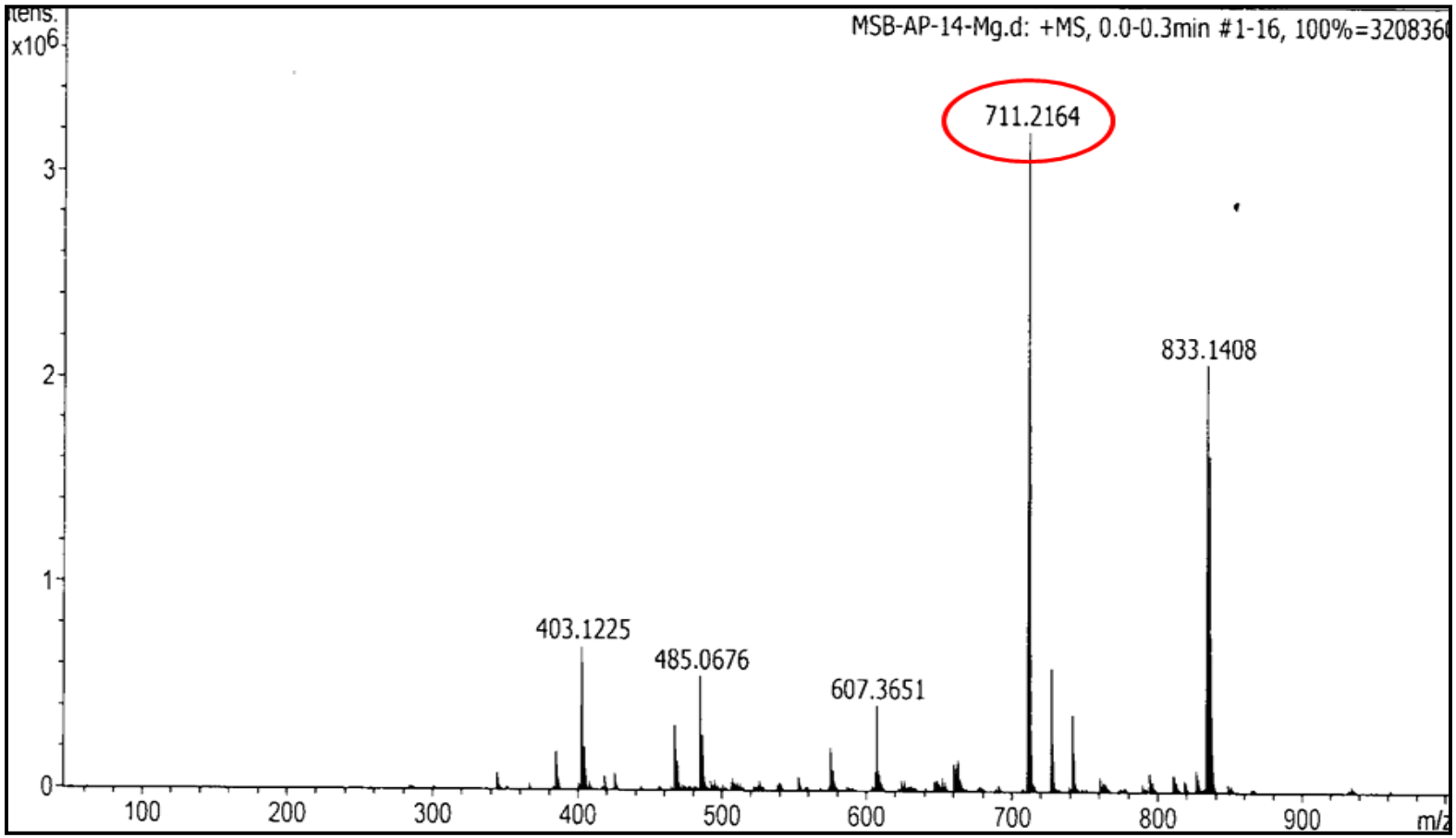

Figure S13 (a): UV-visible spectrum of **B-XAN** with different metal ions (10 equiv.) at 10 μM in acetonitrile

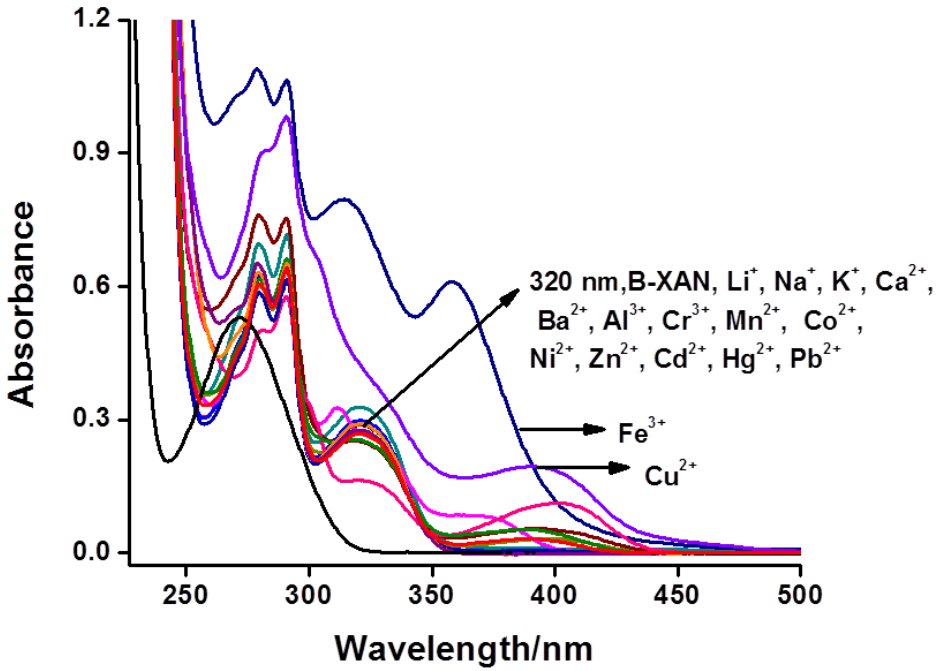

Figure S13 (b): Photograph showing naked eye color change of **B-XAN** (under visible light) in presence of different metal ions in acetonitrile

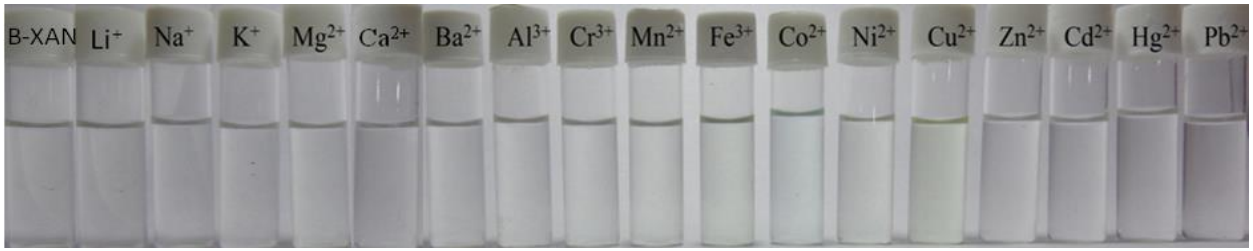

Figure S14 (a): UV-visible spectrum of **N-XAN** with different metal ions (10 equiv.) at 10 μM in acetonitrile

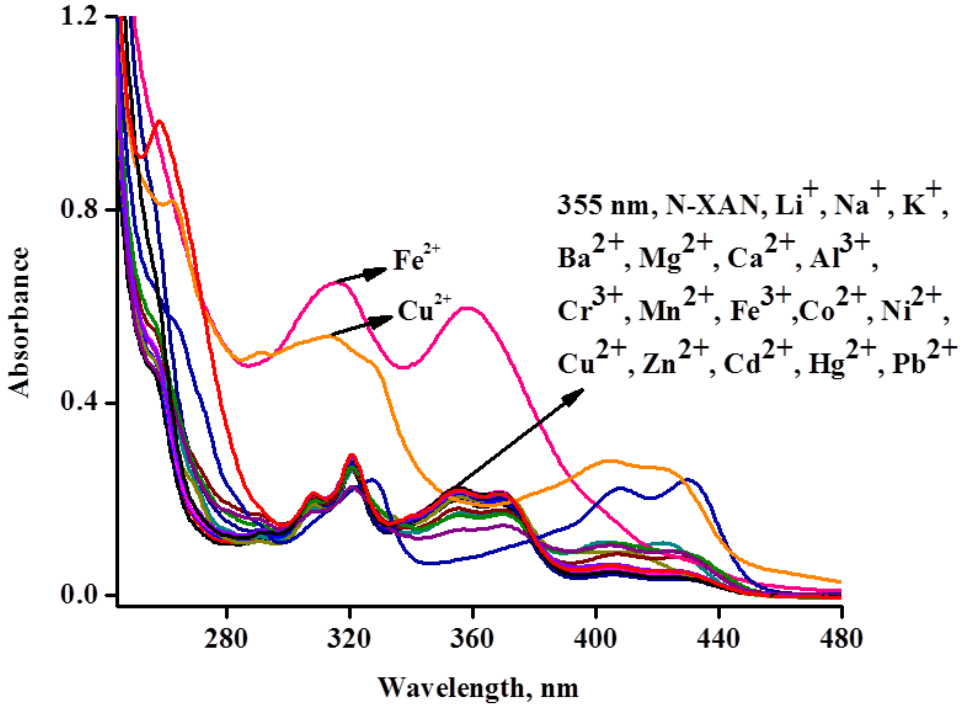

Figure S14 (b): Photograph showing naked eye colour change of **N-XAN** (under visible light) in presence of different metal ions in acetonitrile

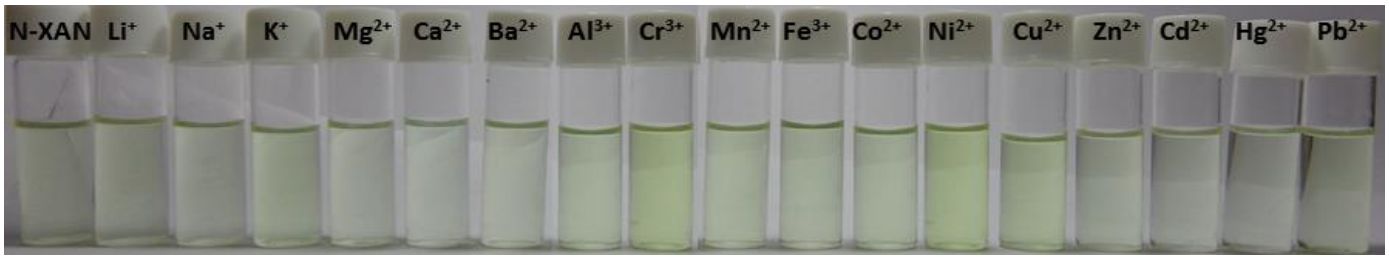

Figure S15 (a): Relative fluorescence changes of **N-XAN** (1.0 μM) after addition of 10 equiv. of various metal ions in acetonitrile at 458 nm along with inset fluorescence spectral graph.

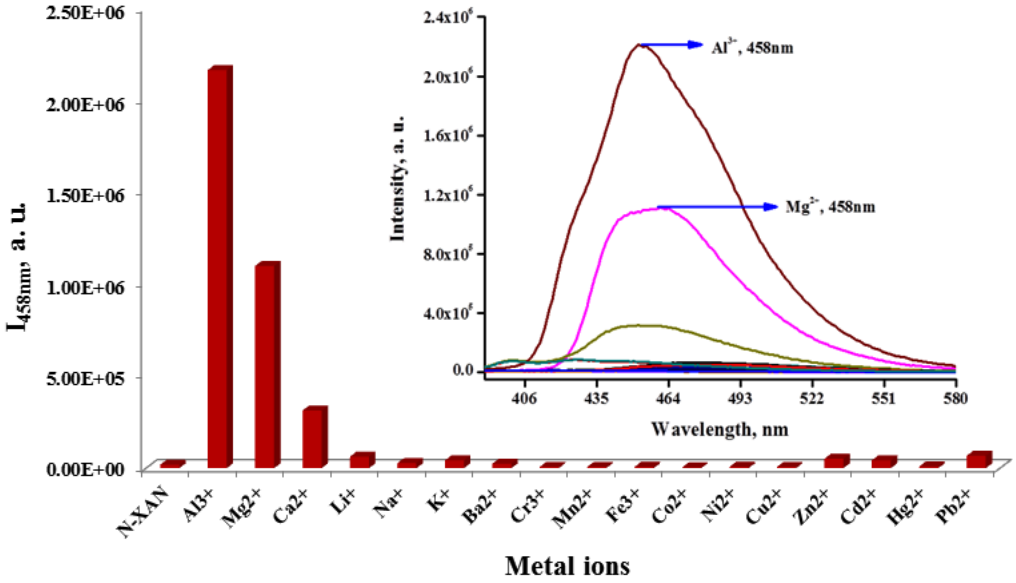

Figure S15 (b): Naked eye fluorescence response of **N-XAN** in the presence of different metal ions (under UV light of 365 nm)

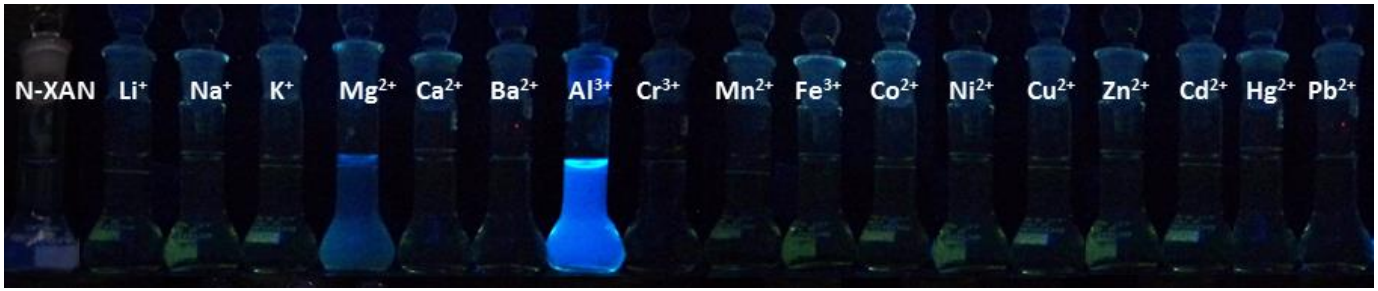

Figure S16: Fluorescence responses of **B-XAN** (1μM) at λex=458 nm in the presence of various cations in acetonitrile solution. The red bars represent the emission intensities of **B-XAN** in the presence of various cations (10.0 eq.). The blue bars represent the change of emission upon subsequent addition of Mg^{2+} (10.0 eq.) to the above solution.

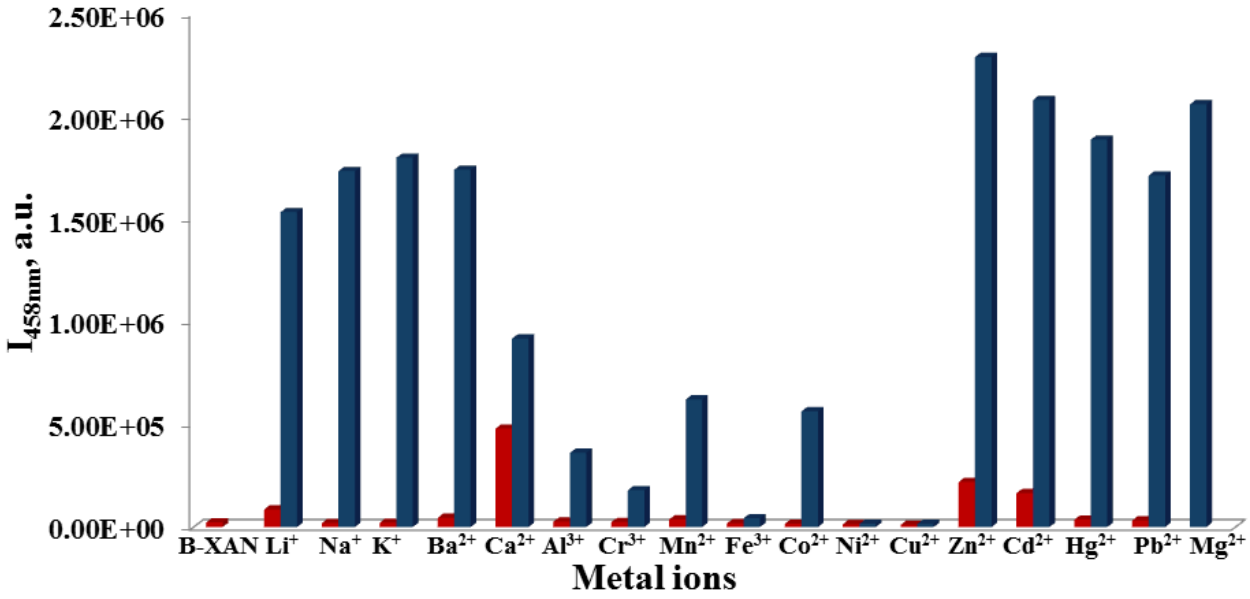

Figure S17: Calibration curve for determination of detection limit of **B-XAN** for Mg^{2+} by fluorescence titration data

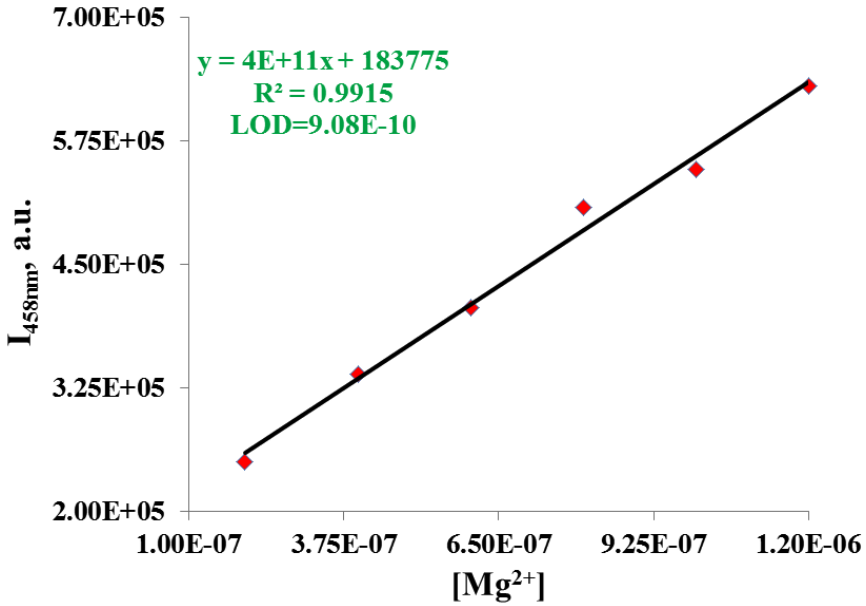

Figure S18: Job's Plot between **B-XAN** and Mg^{2+} showing 2:1 binding stoichiometry

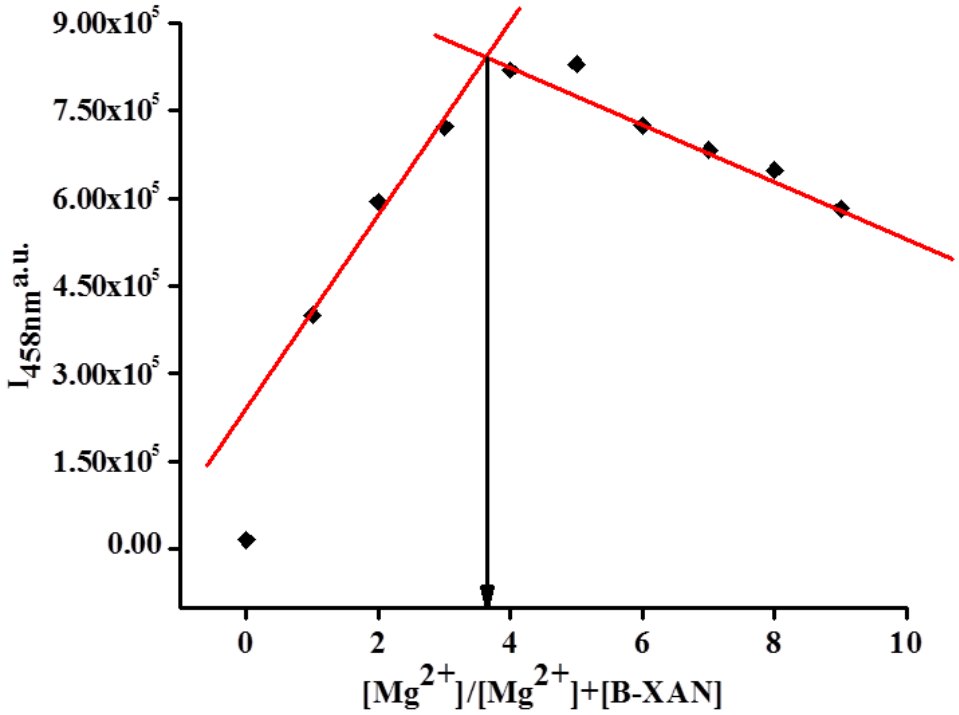

Figure S19: Reaction-time profile of **B-XAN** in presence of Mg^{2+}

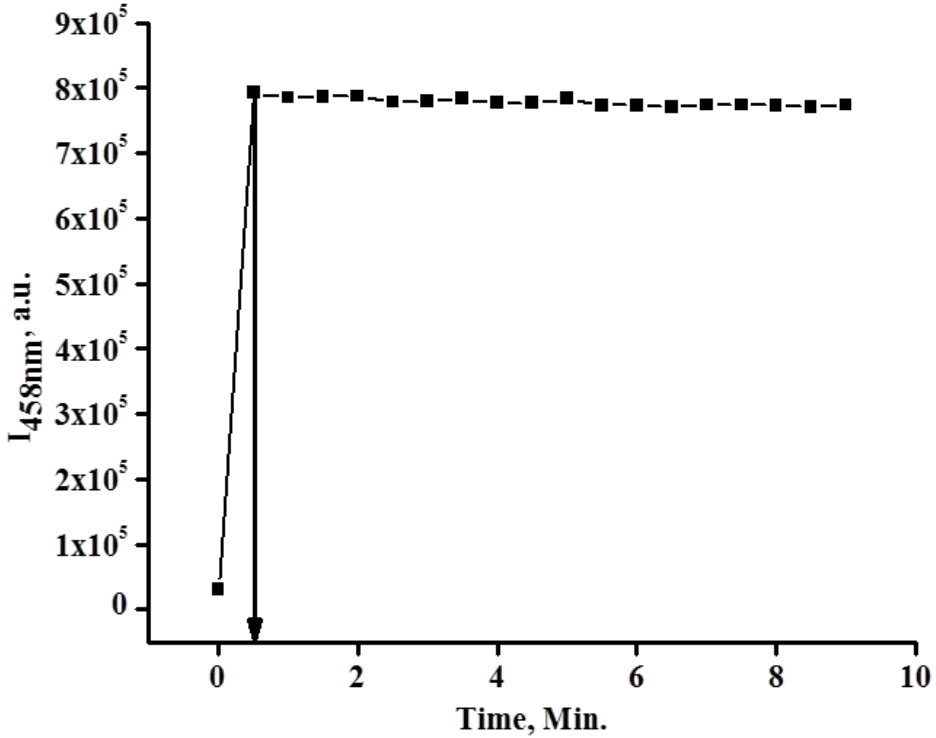

Figure S20: Fluorescence emission spectra showing reversibility of **B-XAN** in the presence of Mg^{2+} and EDTA in acetonitrile solution

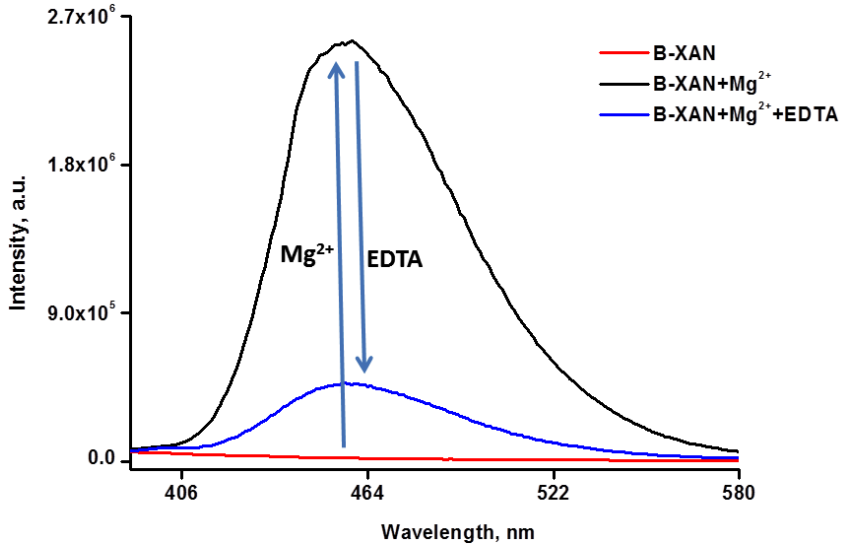

Figure S21: Non-linear fit plot of fluorescence titration data for determination of binding constants