Supporting Information

A Dual-Function Crystalline Sensor: Tris(2-Carboxyethyl) Isocyanurate for Ultra-Sensitive Detection and Sustainable Degradation of Tetracycline Antibiotics

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S 1. Materials and Instrumentations

The reagents utilized in this study were procured from Sigma-Aldrich (USA), while the metal salts were obtained from Merck (India). All other chemicals and solvents used were of analytical grade and employed without further purification. Spectroscopic-grade solvents were specifically used for analytical purposes. Elemental analysis for carbon, hydrogen, and nitrogen content of **(1)** was conducted using a PerkinElmer 2400 Series II analyzer. Powder X-ray diffraction (PXRD) patterns were recorded with a PANalytical X'Pert PRO instrument equipped with Bragg-Brentano geometry. Fourier transform infrared (FTIR) spectra of the crystalline samples were obtained using a Bruker Optics FTIR Spectrometer (Germany) over the spectral range of 4000–500 cm^{-1}. The solid-state photoluminescence properties were evaluated with a Shimadzu RF-5301PC spectrofluorophotometer. Photocatalytic degradation experiments were monitored using a

Shimadzu UV-1780 UV-Vis spectrophotometer covering a wavelength range of 190–1100 nm. Fluorescence emission spectra were acquired with an Agilent Cary Eclipse atomic absorption spectrophotometer. Density functional theory (DFT) calculations were performed using Quantum ESPRESSO with the Perdew–Burke–Ernzerhof (PBE) functional under the generalized gradient approximation (GGA). A plane-wave basis set (25 Ry for wave functions, 225 Ry for charge density) ensured convergence, while Gaussian smearing (0.01 Ry) facilitated smooth electronic occupation.

S 2. Analysis of the X-ray Crystallography of the (1)

Single crystals of Tris(2-carboxyethyl) isocyanurate crystal **(1)** were mounted on a nylon loop for structural analysis. A suitable crystal was selected, and data collection was performed at ambient temperature using an XtaLAB Synergy, Dualflex, HyPix3000 diffractometer. During the measurement, the crystal was maintained at 100(2) K. The structure was determined using Olex2 software[1], solved by using SHELXT 2018/2 (Sheldrick, 2018)[2] and refined using ShelXL (Sheldrick, 2015).[3] The refinement was carried out using the full-matrix least-squares method on F^2, with anisotropic displacement parameters applied to non-hydrogen atoms. Hydrogen atoms were positioned computationally and refined isotropically using a riding model. Non-hydrogen atoms were refined anisotropically, while hydrogen atoms bonded to carbon were positioned computationally and refined isotropically using a riding model.

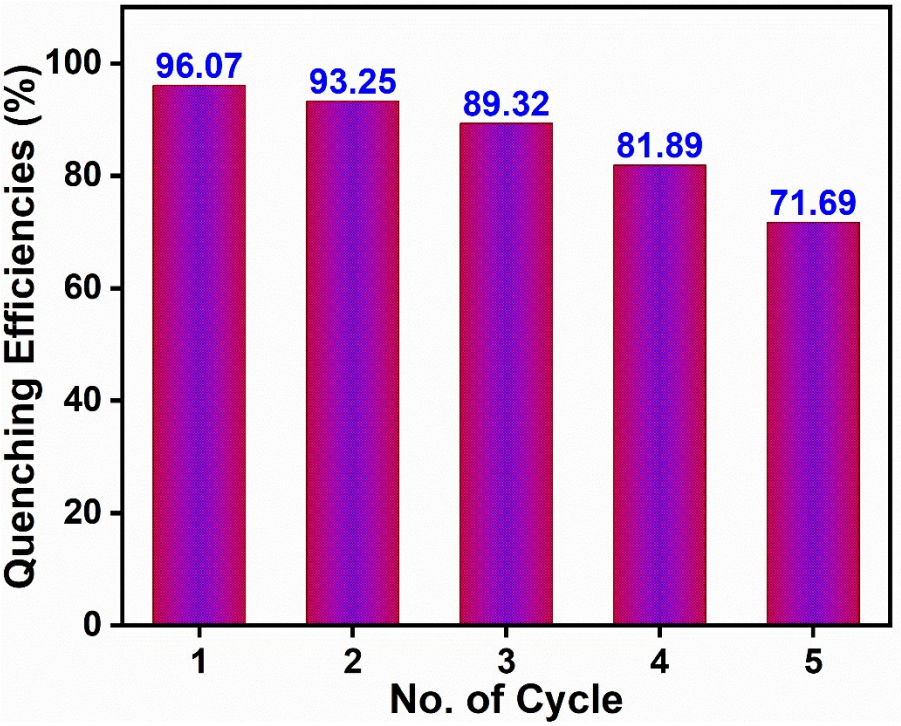


Fig. S1 Reusability study showing the quenching efficiency of the material (**1**) over multiple cycles. The quenching efficiency gradually decreases from 96.07% in the first cycle to 71.69% after the fifth cycle, indicating the material's stability and potential for repeated use.

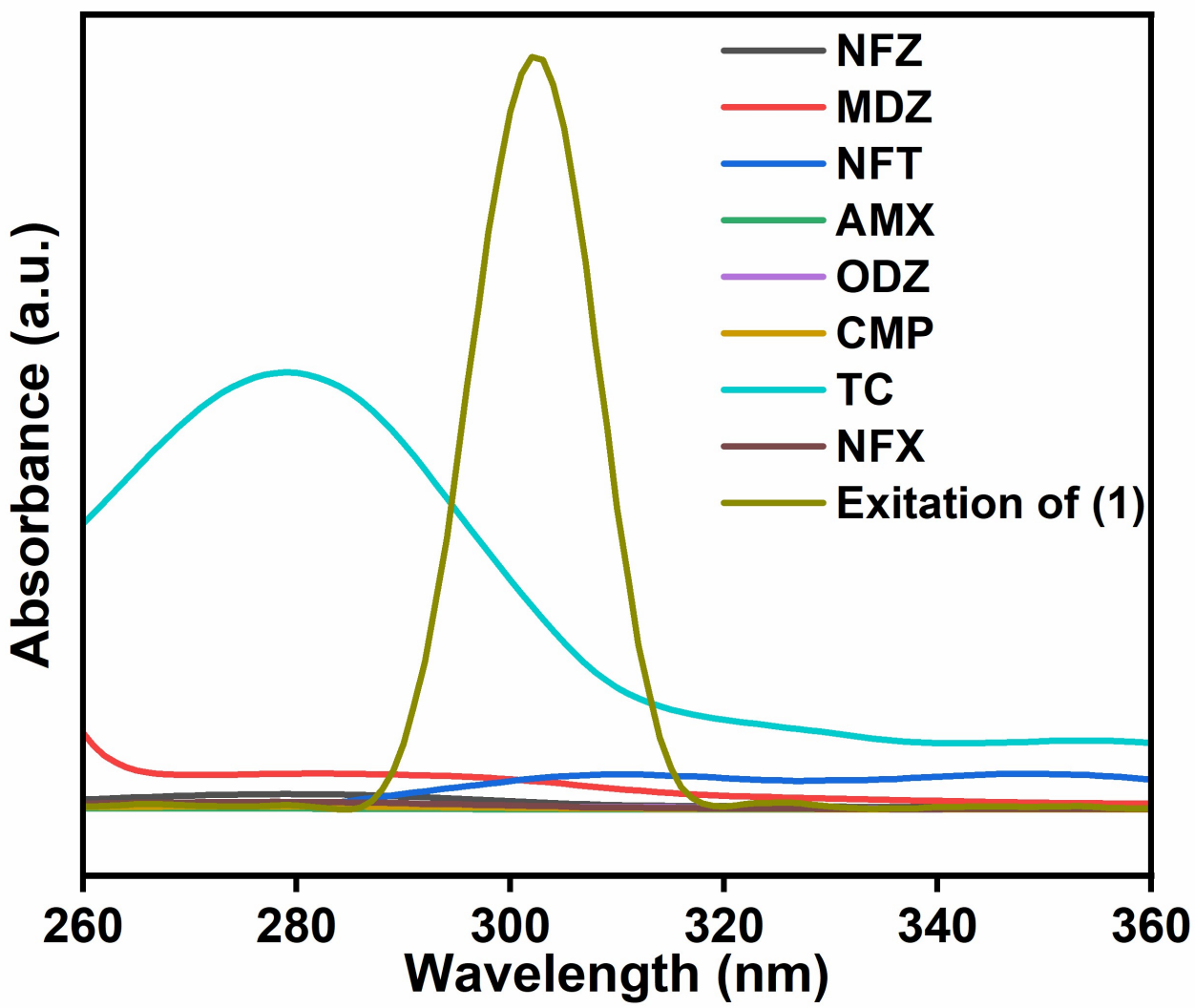


Fig. S2 Spectral overlap between the UV-Vis absorption spectra of various antibiotics analytes and the excitation spectra of (**1**).

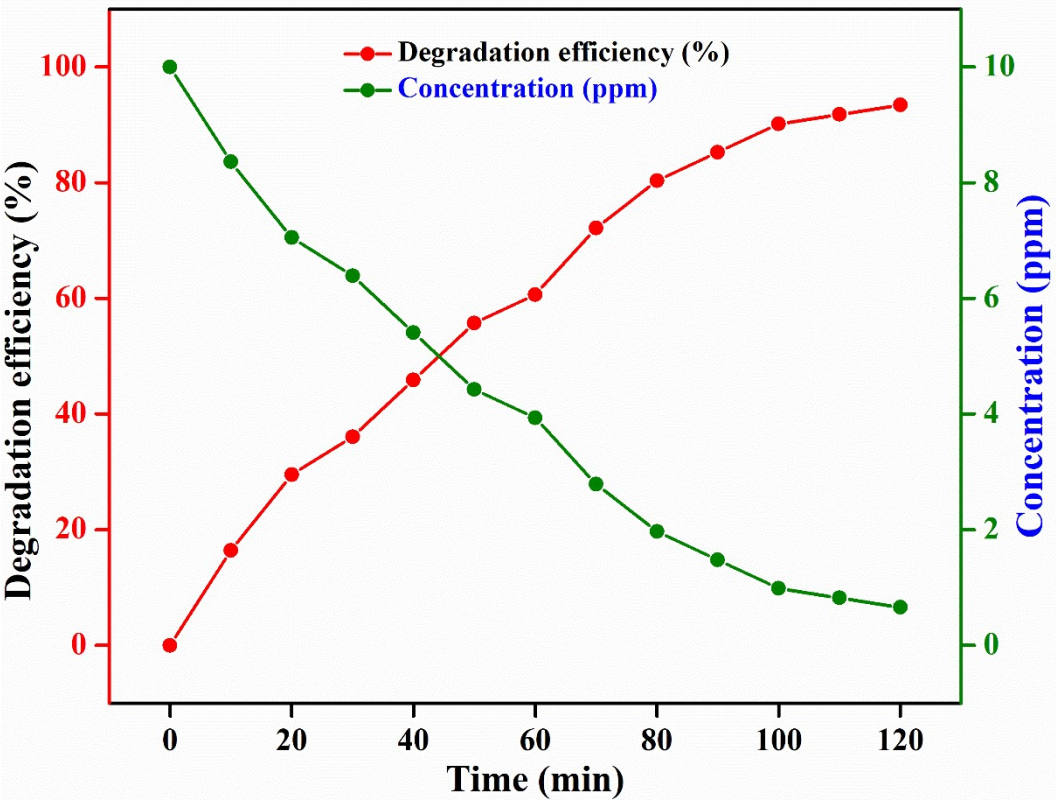


Fig. S3 Photocatalytic breakdown effectiveness of Tetracycline (TC) at different concentrations of (1).

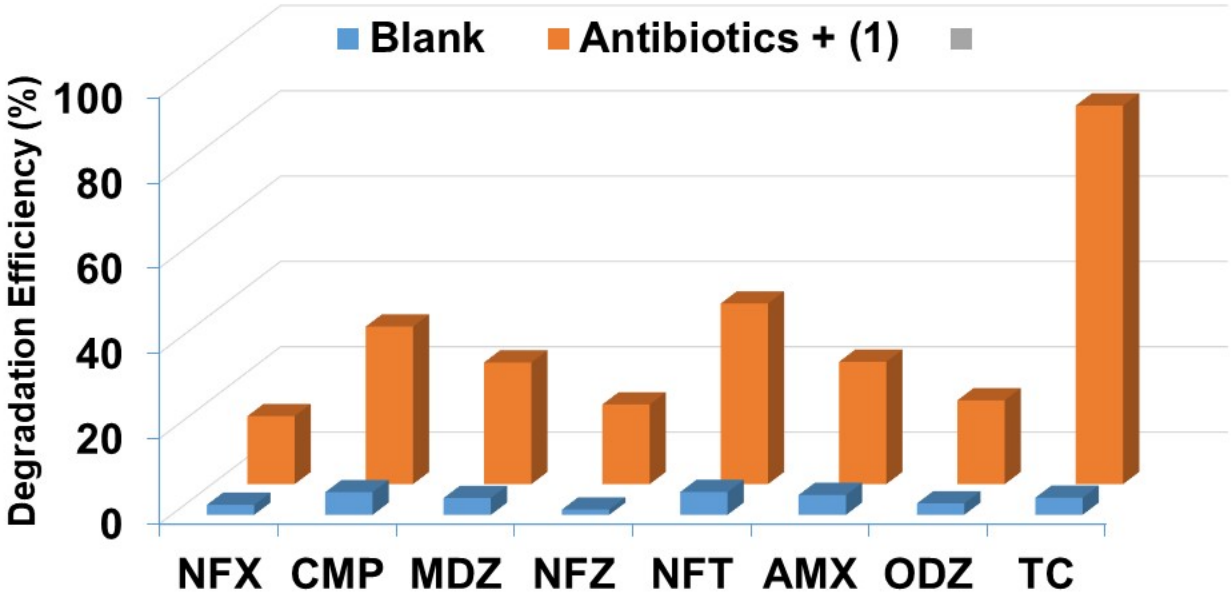


Fig. S4 Comparison of the degradation efficiencies of various antibiotics with and without (**1**).

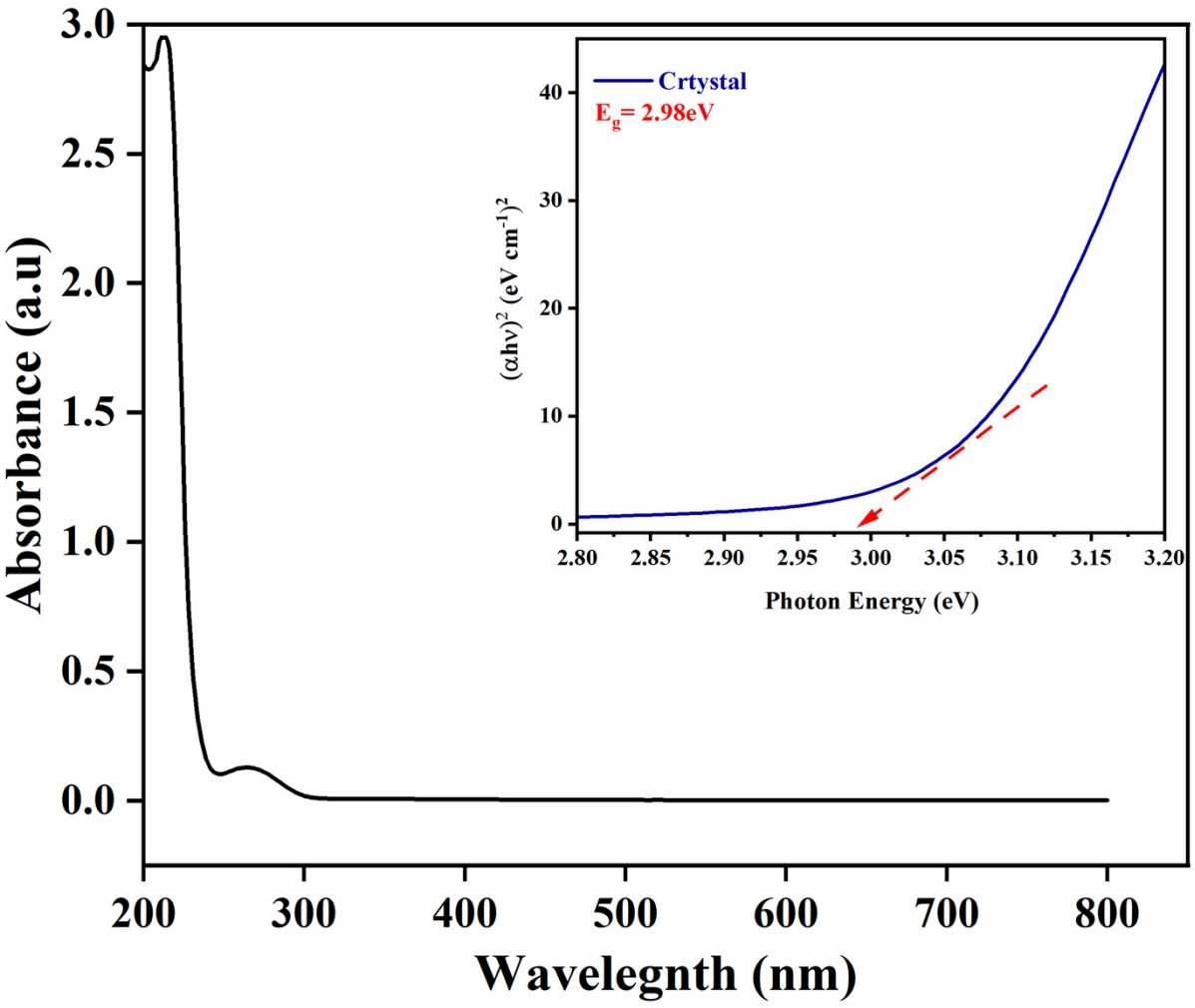


Fig. S5 (a) UV-vis absorption spectra of (**1**) and Tauc plot ($(\alpha h\nu)^2$ vs energy (eV)) for band gap study of (**1**) (inset).

Table S1 Bond Lengths for crystal (1).

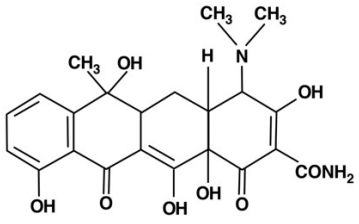
Atom	Atom	Length/Å		Atom	Atom	Length/Å
O(7)	C(9)	1.206(2)		N(4)	C(10)	1.371(2)
O(5)	C(10)	1.218(2)		N(4)	C(11)	1.472(2)
O(6)	C(4)	1.202(2)		O(2)	C(13)	1.306(2)
O(3)	C(1)	1.223(2)		C(1)	C(2)	1.490(2)
O(1)	C(13)	1.224(2)		C(2)	C(3)	1.520(3)
O(4)	C(1)	1.296(2)		C(5)	C(6)	1.492(3)
N(2)	C(3)	1.477(2)		C(6)	C(7)	1.490(3)
N(2)	C(4)	1.386(2)		C(7)	O(9)	1.294(6)
N(2)	C(10)	1.365(2)		C(7)	O(11)	1.212(3)
N(3)	C(4)	1.382(2)		C(7)	O(10)	1.252(8)
N(3)	C(5)	1.472(2)		C(7)	O(8)	1.302(14)

N(3)	C(9)	1.378(2)		C(11)	C(12)	1.520(3)
N(4)	C(9)	1.386(2)		C(12)	C(13)	1.485(2)

Table S2 Bond Angles for (1).

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
C(4)	N(2)	C(3)	119.05(15)		C(7)	C(6)	C(5)	113.23(17)
C(10)	N(2)	C(3)	117.46(15)		O(9)	C(7)	C(6)	112.8(3)
C(10)	N(2)	C(4)	123.41(14)		O(11)	C(7)	C(6)	124.5(2)
C(4)	N(3)	C(5)	117.76(14)		O(11)	C(7)	O(9)	119.5(3)
C(9)	N(3)	C(4)	124.80(14)		O(10)	C(7)	C(6)	117.6(4)
C(9)	N(3)	C(5)	117.37(13)		O(10)	C(7)	O(8)	93.9(8)
C(9)	N(4)	C(11)	118.94(14)		O(8)	C(7)	C(6)	112.4(7)
C(10)	N(4)	C(9)	123.48(14)		O(7)	C(9)	N(3)	122.15(15)
C(10)	N(4)	C(11)	117.55(14)		O(7)	C(9)	N(4)	122.56(15)
O(3)	C(1)	O(4)	123.16(17)		N(3)	C(9)	N(4)	115.29(14)
O(3)	C(1)	C(2)	123.01(17)		O(5)	C(10)	N(2)	121.97(16)
O(4)	C(1)	C(2)	113.82(17)		O(5)	C(10)	N(4)	120.66(17)
C(1)	C(2)	C(3)	114.61(16)		N(2)	C(10)	N(4)	117.37(14)
N(2)	C(3)	C(2)	110.92(15)		N(4)	C(11)	C(12)	112.41(15)
O(6)	C(4)	N(2)	122.17(16)		C(13)	C(12)	C(11)	114.71(16)
O(6)	C(4)	N(3)	122.42(16)		O(1)	C(13)	O(2)	122.90(17)
N(3)	C(4)	N(2)	115.40(14)		O(1)	C(13)	C(12)	123.73(17)
N(3)	C(5)	C(6)	110.65(14)		O(2)	C(13)	C(12)	113.36(16)

Table S3 Quenching efficiencies (Q.E.) and degradation efficiencies (D. E.) of (**1**) with all used antibiotics.

	 Tetracycline (TC) **Q.E. (%) = 96.07 %** **D.E. (%) = 87.50%**

<table>
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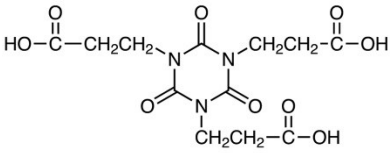
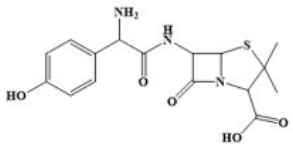
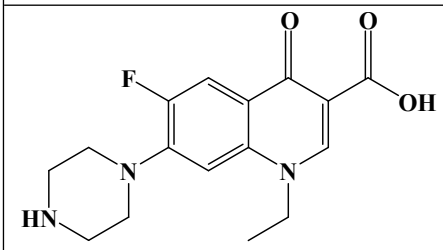
<td rowspan="4"> 
Tris(2-carboxyethyl) isocyanurate crystal (1)

(O–H···O) hydrogen bonding interactions</td>
<td> 
Amoxicillin (AMX)</td>
<td>Q.E. (%) = 68.21%
D.E. (%) = 28.69%</td>
</tr>
<tr>
<td> 
Nitrofurantoin (NFT)</td>
<td>Q.E. (%) =49.64%
D.E. (%) = 42.36%</td>
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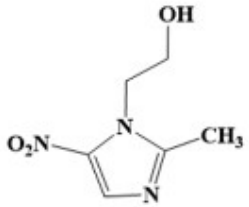
<td> 
Metronidazole (MDZ)</td>
<td>Q.E. (%) = 45.11 %
D.E. (%) = 28.54%</td>
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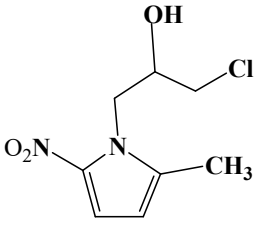
<td> 
Ornidazole (ODZ)</td>
<td>Q.E. (%) = 29.28%
D.E. (%) = 19.66%</td>
</tr>
</table>

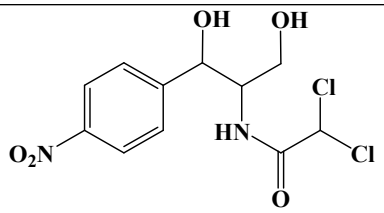
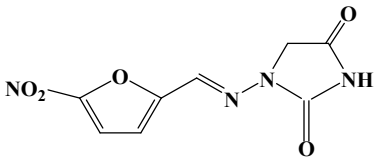
		**Q.E. (%) = 22.14%** **D.E. (%) = 36.95%**
	Chloramphenicol (CMP)	
		**Q.E. (%) = 13.21%** **D.E. (%) = 15.96%**
	Chloramphenicol (NFX)	
		Q.E. (%) = 7.14 % **D.E. (%) = 18.69%**
	Nitrofurazone (NFZ)	

Table S4. LOD values of Tetracycline (TC) with (**1**) and with previously reported materials.

Catalyst	Analyts	LOD	Ref.
MMH-incorporated MNPs	TC	0.16 μM	54
Zr-UiO-66/MWCNTs/AuNPs	TC	1.67×10^{-7} mol L^{-1}	55
TC-Fe(III) complex	TC	931 nM	56
trans-cleavage activity of CRISPR/Cas12a	TC	0.1 μM	57
Eu3+/NH2-MIL-53(Al) nanocomposite	TC	0.16 μM	58
Tris(2-carboxyethyl) isocyanurate crystal (1)	TC	2.109 ppm	**This Study**

Reference

1. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, J. Appl. Crystallogr., 2009, 42, 339–341.

2. G. Sheldrick, *Acta Crystallogr. A*, 1984, 40, C440–C440.

3. G. M. Sheldrick, *Acta Crystallogr. C Struct. Chem.*, 2015, 71, 3–8.