Electronic Supplementary Information (EIS)

Electrogenerated chemiluminescence (ECL) of triazole-modified deoxycytidine analogues in *N*,*N*-dimethylformamide

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Cyclic voltammetry and ECL experimental parameters

In annihilation systems, the CV potential window was 2.069 to -1.889 V for **1**, 1.861 to -2.435 V for **2**, 1.787 to -2.231 V for **3**, and 1.828 to -2.940 V for **4**. In coreactant systems, the CV potential window was 0.000 to -2.278 V for **1**, 0.000 to -2.452 V for **2**, 0.000 to -2.517 V for **3**, and 0.000 to -2.126 V for **4**.)"

Curve-fitting for ECL spectra

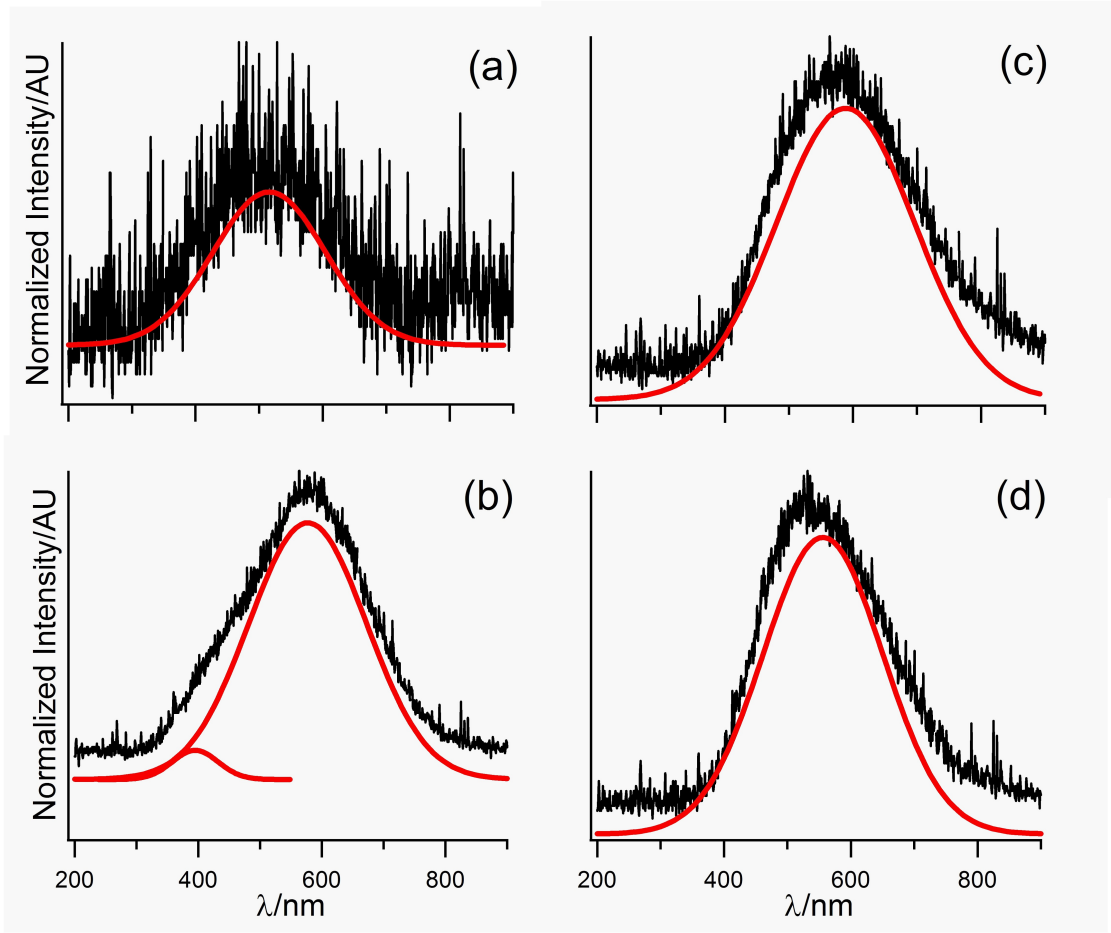

Figure S1. ECL spectra and their curve-fitting for **1-4** in DMF containing 5.0×10^{-3} M BPO and 0.1 M TBAP as supporting electrolyte and pulsing between potential ranges from (a) 0.000 to -2.278 V, t = 60 s for **1**, (b) 0.000 to -2.452 V, t = 60 s for **2**, (c) 0.000 to -2.517 V, t = 60 s for **3**, and (d) 0.000 to -2.126 V, t = 60 s for **4**.

Crystallographic details for 1 • 2 H_2O

Crystals of $[C_{15}H_{16}N_6O_4S]$ • 2 H_2O were grown from a concentrated aqueous solution (refer to Figure S2 for crystal structure of **1**). A colourless needle was mounted on a glass fibre. Data were collected at low temperature (-123°C) on a Nonius Kappa-CCD area detector diffractometer with COLLECT (Nonius B.V., 1997-2002). The unit cell parameters were calculated and refined from the full data set. Crystal cell refinement and data reduction were carried out using HKL2000 DENZO-SMN (Otwinowski & Minor, 1997). The absorption correction was applied using HKL2000 DENZO-SMN (SCALEPACK). The crystal data and refinement parameters for $[C_{15}H_{16}N_6O_4S]$ • 2 H_2O are listed in Table S1. The reflection data and systematic absences were consistent with an orthorhombic space group: P2(1)2(1)2(1). Bond lengths and angles are listed in Table S2.

The SHELXTL/PC V6.14 for Windows NT (Sheldrick, G.M., 2001) suite of programs was used to solve the structure by direct methods. Subsequent difference Fourier syntheses allowed the remaining atoms to be located. Independent molecules were formed and are interconnected via H-bonding interactions involving the molecule itself and the two water molecules of solvation. All of the non-hydrogen atoms were refined with anisotropic thermal parameters. Some soft restraints were used for the thermal parameters and the disordered thiophene rings. The hydrogen atom positions were calculated geometrically and were included as riding on their respective carbon atoms.

The largest residue electron density peak (0.244 e/Å^3) was associated with the disordered thiophene ring (Table S1). Full-matrix least squares refinement on F^2 gave R_1 = 5.26 for 2σ data and wR_2 = 11.96 for all data as seen in Table S1 (GOOF = 1.086). The final solution was submitted to the IUCR checkCIF program and had some Alert level A's or B's associated with the lack of complete data.

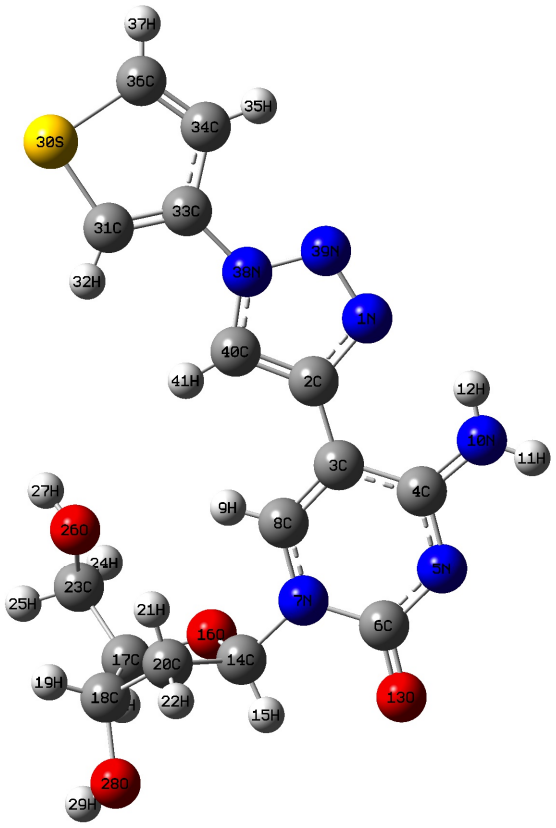

Figure S2: Ball-and-stick representation of **1**. Carbon atoms are in grey, sulfur in yellow, nitrogen in blue, oxygen in red, and hydrogen in white. The final solution was submitted to the IUCR CIF checking program and had some Alert level A's or B's associated with the lack of complete data, however the general structure can be observed for **1**, similar to our previously reported solid state structure of **2**.

Table S1: Crystal data and structure refinement for **1** • 2 H2O

Empirical formula	$C_{15}H_{20}N_6O_6S$	
Formula weight	412.43	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 2_1 2_1 2_1	
Unit cell dimensions	a = 4.8367(6) Å	
	b = 12.1128(18) Å	a= 90°.
	c = 30.967(5) Å	b= 90°.

Volume	1814.2(5) $Å^3$	g = 90°.
Z	4	
Density (calculated)	1.510 Mg/m3	
Absorption coefficient	0.227 mm-1	
F(000)	864	
Crystal size	0.75 x 0.13 x 0.03 mm3	
Theta range for data collection	2.59 to 18.84°.	
Index ranges	-4<=h<=4, -11<=k<=10, -27<=l<=27	
Reflections collected	6165	
Independent reflections	1347 [R(int) = 0.0910]	
Completeness to θ = 18.84°	97.80%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9943 and 0.8482	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	1347 / 366 / 279	
Goodness-of-fit (GOOF) on F^2	1.086	
Final R indices [I>2σ(I)]	R_1 = 0.0526, wR_2 = 0.1052	
R indices (all data)	R_1 = 0.0752, wR_2 = 0.1196	
Absolute structure parameter	0.0(3)	
Largest diff. peak and hole	0.244 and -0.211 $eÅ^{-3}$	

Table S2: Hydrogen bonds for **7** • 2 H_2O [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(17)-H(17A)...O(41)#1	0.88	2.54	3.261(8)	139.5
N(17)-H(17B)...N(8)	0.88	2.08	2.764(10)	134.4
O(25)-H(25A)...O(31)#2	0.84	1.98	2.813(8)	171.4
O(26)-H(26A)...O(18)#3	0.84	1.82	2.625(7)	160.8
O(31)-H(31A)...O(26)	0.87(4)	1.90(5)	2.724(8)	157(9)
O(31)-H(31B)...O(41)	0.87(4)	2.59(9)	2.778(10)	93(6)
O(41)-H(41A)...N(13)#2	0.88(4)	2.05(6)	2.833(8)	147(8)
O(41)-H(41B)...O(31)#4	0.87(4)	2.12(5)	2.968(9)	162(9)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y-1/2,-z+3/2 #2 -x+1,y+1/2,-z+3/2 #3 -x+2,y+1/2,-z+3/2
#4 x-1,y,z