Electronic Supplementary Information (ESI)

Neutral Mononuclear Rhenium(I) Complex with Rare *in-situ* Generated Triazolyl Ligand for Luminescence "Turn-On" Detection of Histidine

(On the occasion of the 85th birthday anniversary of Retired Senior Professor Chockalingam Srinivasan)

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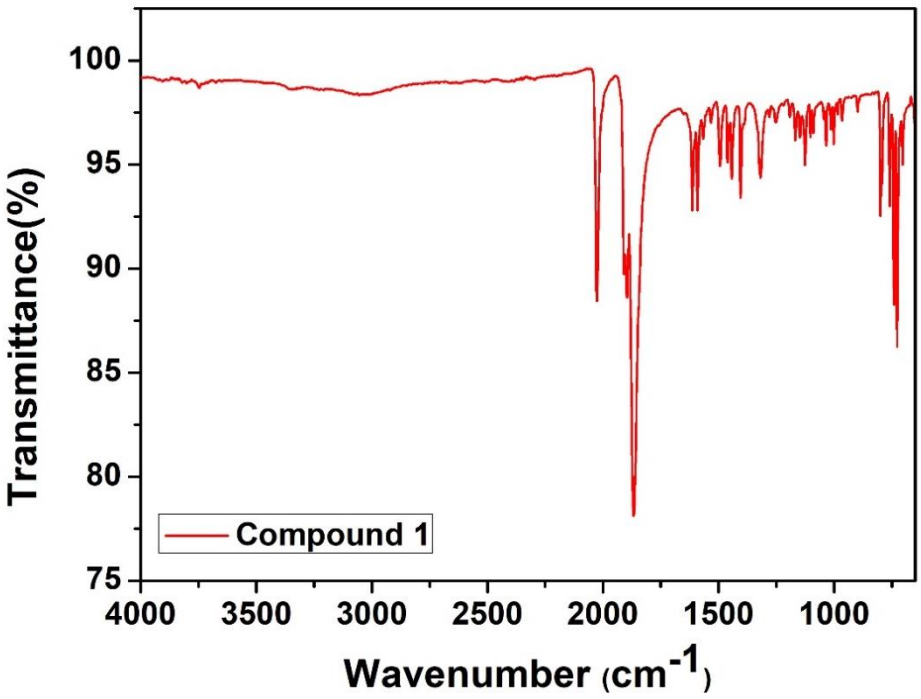


Fig. S1. FTIR spectrum of compound **1**.

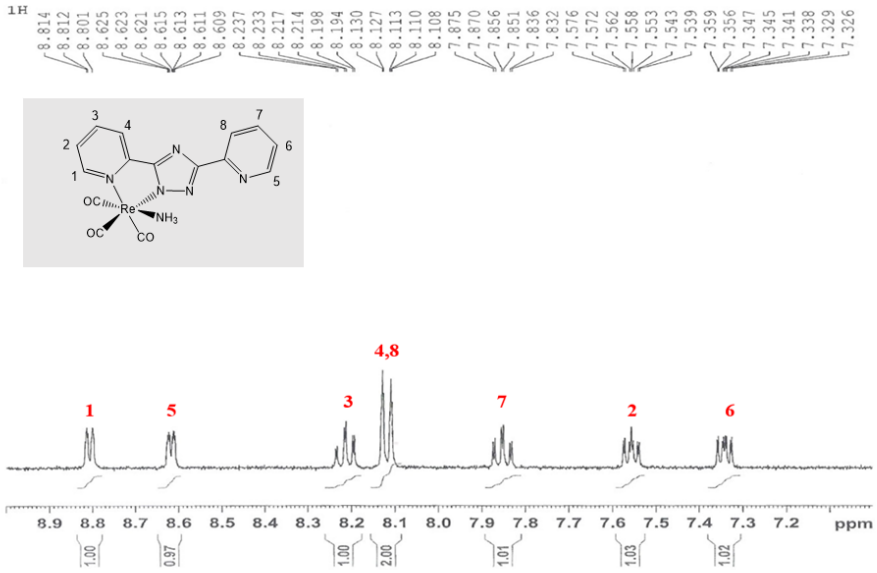


Fig. S2. ^{1}H NMR spectrum of compound **1**.

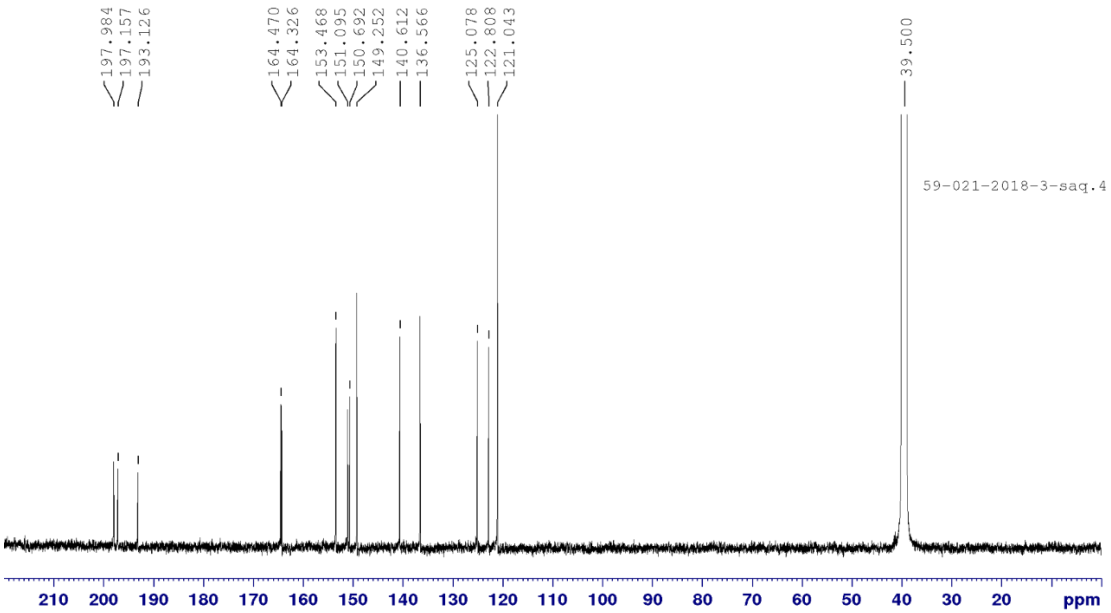


Fig. S3. ^{13}C NMR spectrum of compound **1**.

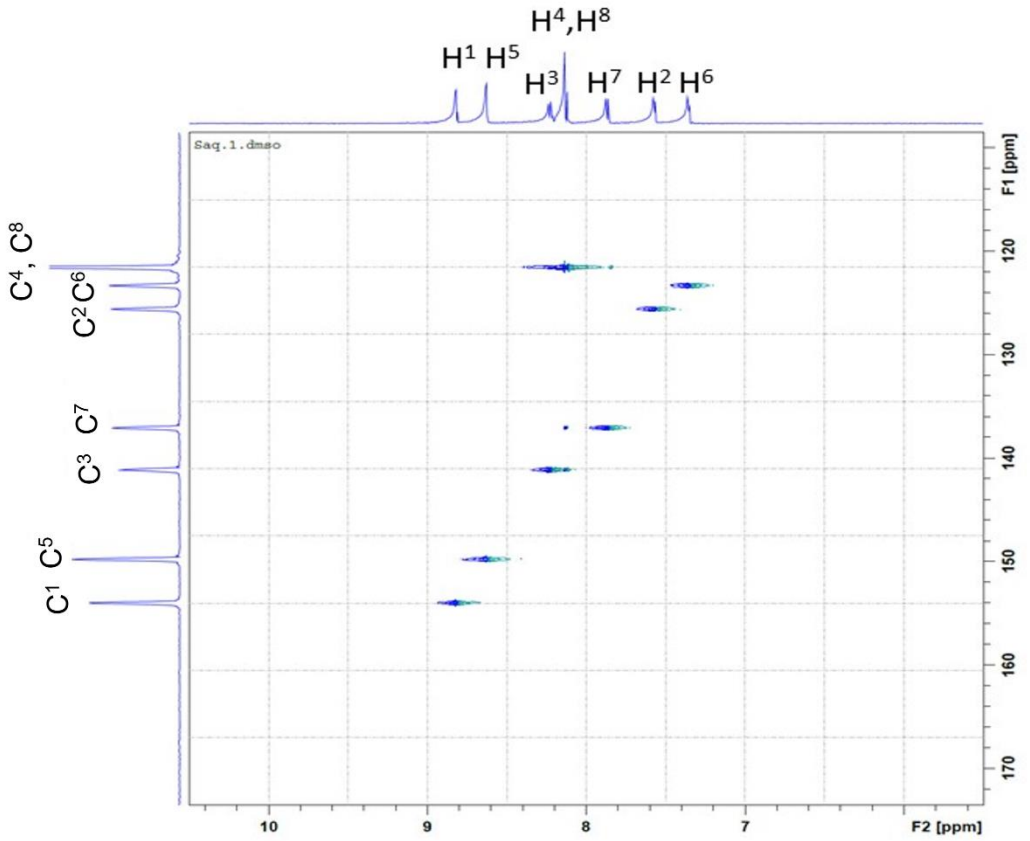


Fig. S4. [^{1}H–^{13}C]-HSQC 2D NMR spectrum of compound **1**.

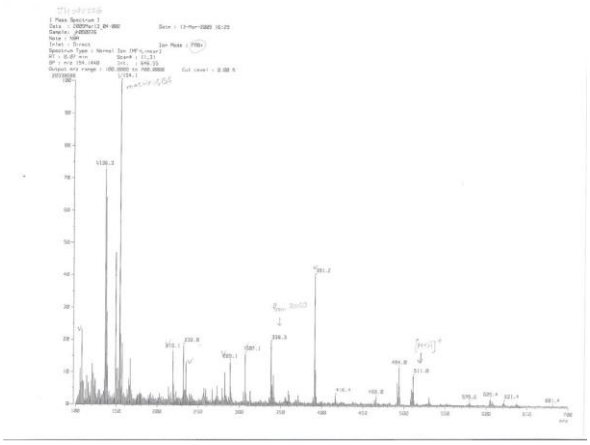
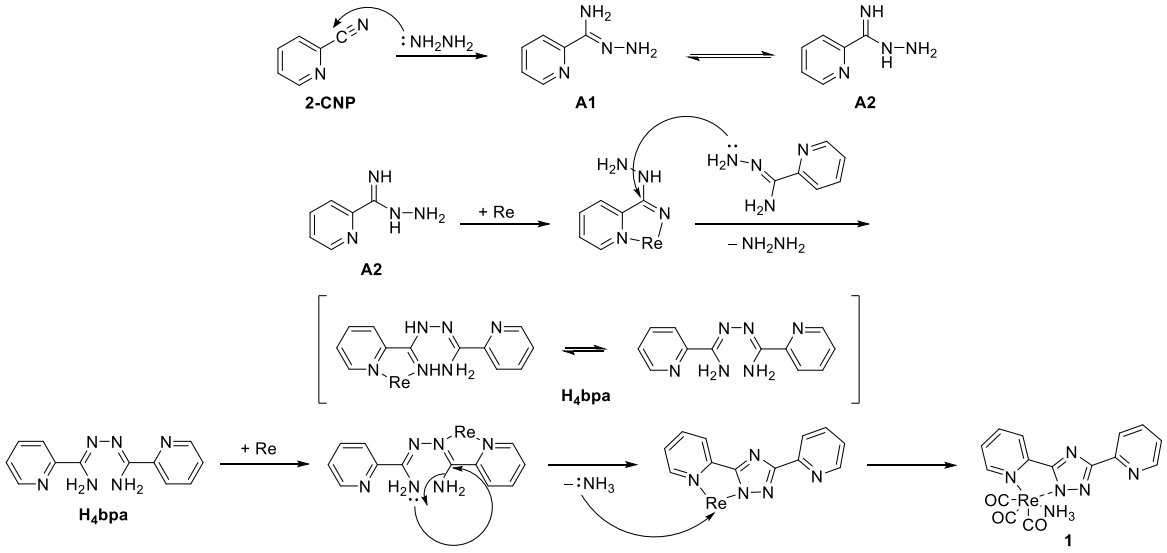


Fig. S5. FAB-Mass spectrum of compound **1**.



Scheme S1. Proposed reaction pathway for the formation of compound **1**, where the 3,5-bis(2-pyridyl)-1,2,4-triazolate (bpt) ligand was *in situ* generated from the reaction of 2-cyanopyridine (2-CNP) and hydrazine.[1] The NH_3 produced in the reaction as a byproduct is trapped in the metal center. H_4bpa = *N*,*N*'-bis(picolinamide)azine.

Reference (for Scheme S1)

[1] L. Cheng, W.-X. Zhang, B.-H. Ye, J.-B. Lin, X.-M. Chen, *Inorg. Chem.* 2007, **46**, 1135-1143.

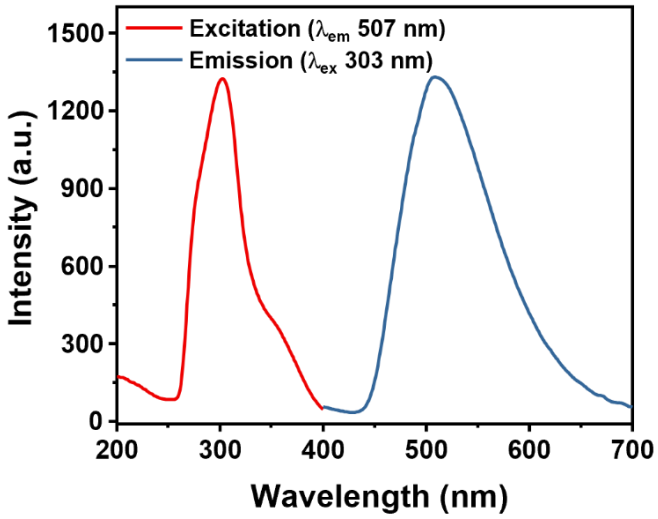


Fig. S6. Excitation and emission spectra of the compound **1** in DMF.

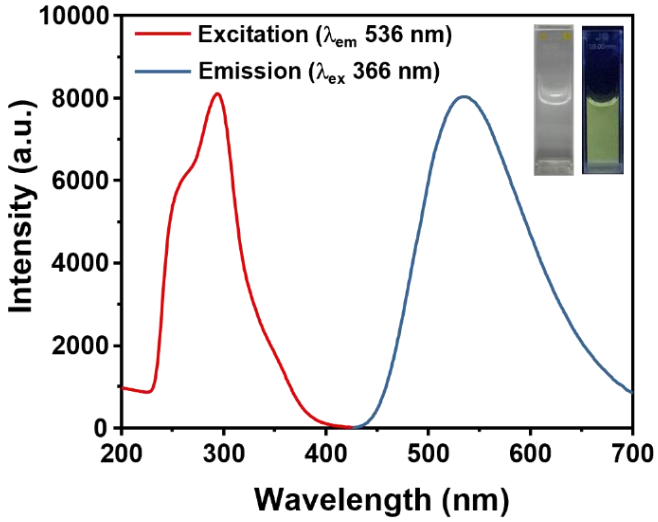


Fig. S7. The excitation and emission spectra of compound **1** in Tris–HCl buffer solution.

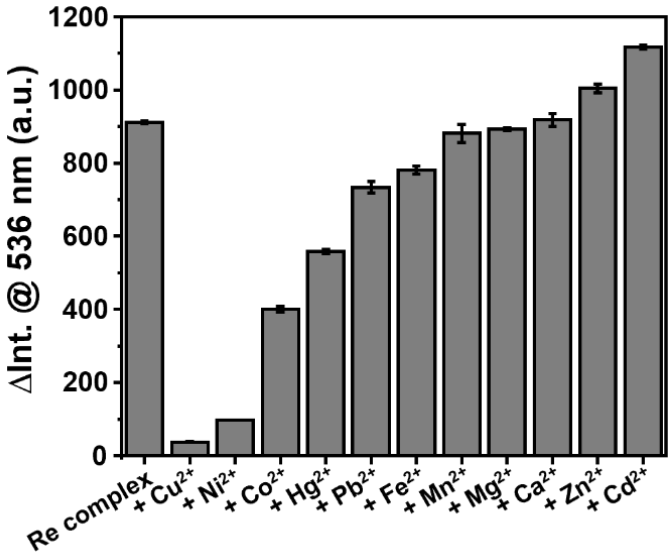


Fig. S8. The change in relative emission intensity (at 536 nm) of compound **1** in the presence of various metal ions with equivalent concentration (250 μM).

Table S1. K_{SV} values at different temperatures.

T (K)	Linear equation[a]	K_{SV} (μM^{-1})
293.15	$(F_0/F) = 0.0372 \times [Ni^{2+}] + 1$	0.0372
303.15	$(F_0/F) = 0.0285 \times [Ni^{2+}] + 1$	0.0285
313.15	$(F_0/F) = 0.0223 \times [Ni^{2+}] + 1$	0.0223

[a] $[Ni^{2+}]$ in μM.

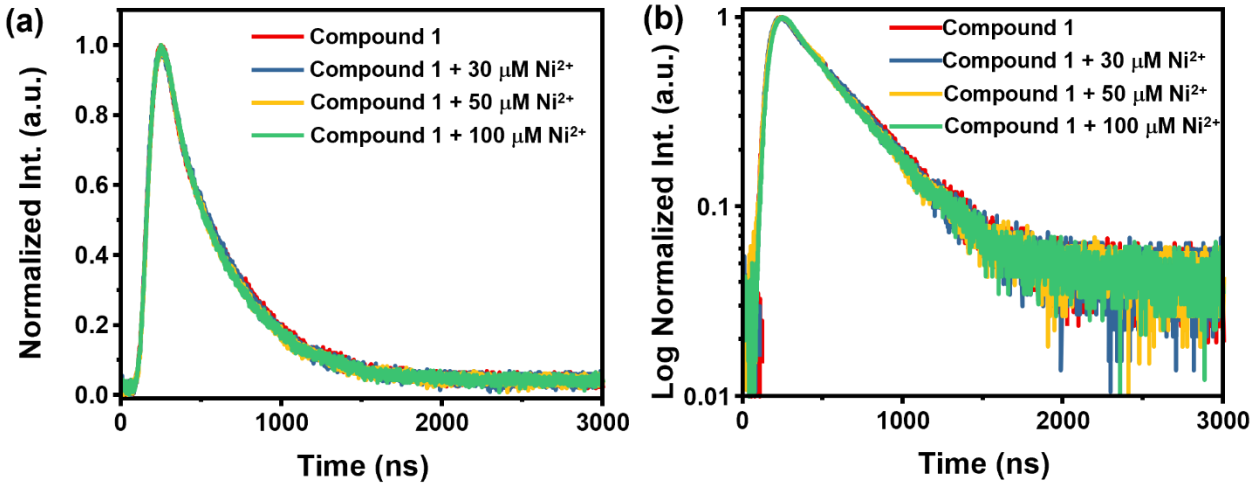


Fig. S9. Time-resolved luminescence decay (a) and the corresponding profiles with the logarithmic scale (b) of compound **1** in the absence and presence of Ni^{2+}.

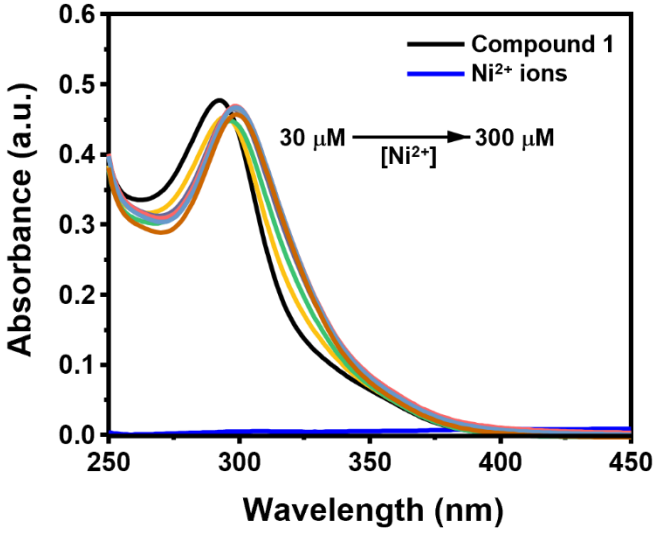


Fig. S10. The UV-vis absorption spectra of compound **1** in the absence and presence of Ni^{2+}.

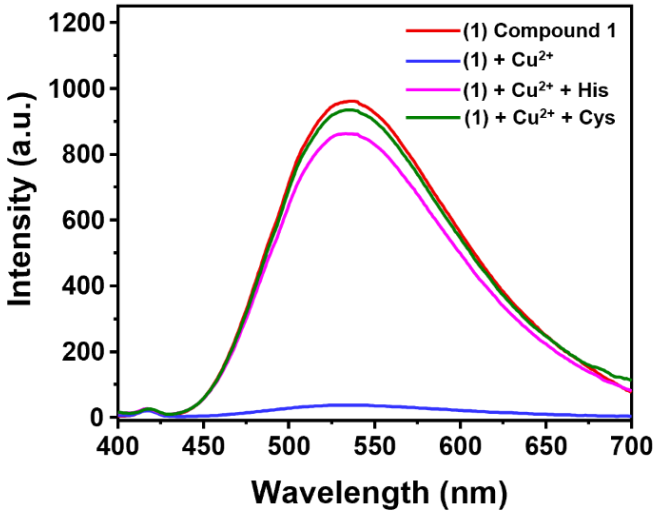
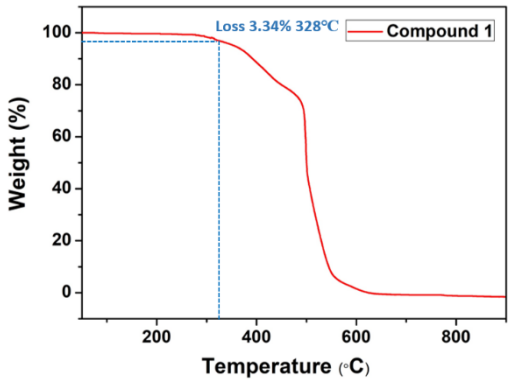


Fig. S11. The emission spectra of compound **1**. Compound **1** mixed with Cu^{2+} followed by the addition of either histidine or cysteine, respectively.

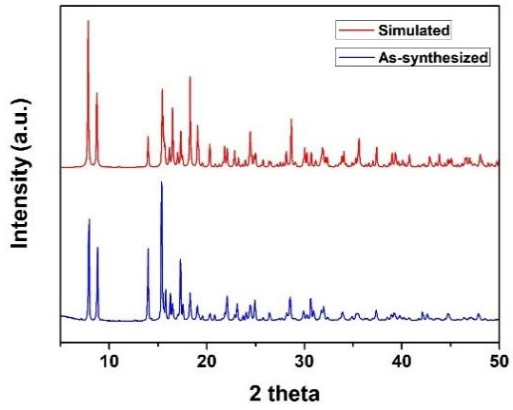
Table S1. Comparison of methods using other compounds or nanomaterials for the detection of histidine with that for compound **1**.

Compound or nanomaterials	Linear range (μM)	LOD (μM)	Reference*
DNA-scaffolded Ag nanoclusters	0–100	1.4	12b
ds-DNA-templated Cu nanoclusters	0.2–100	0.02	12c
IF@SiQDs	2800–5000	2200	12d
BSA-AuNCs	0.1–26	0.03	12e
ZnS QDs	1.25–30	0.74	12f
CdTe QDs	1–30	0.3	12g
Dumbbell DNA-templated Cu nanoclusters	0.05–40	0.0016	12h
SSA/AMP-Tb	0.2–150	0.07	12i
Ru-PDA	18–143	1.4	12j
Re complex	200–2000	1.2	This work

*As referred in main text.



(a)



(b)

Fig. S12. (a) Thermogravimetric plot and (b) powder X-ray diffraction patterns of compound **1**.

Cyrstallographic information

Table S2. Crystal data and structure refinement for compound **1**.

Identification code	**1**	
Empirical formula	$C_{15}H_{11}N_6O_3Re$	
Formula weight	509.50	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	*Pbca*	
Unit cell dimensions	a = 6.07770(10) Å	α = 90°
	b = 22.5621(5) Å	β = 90°
	c = 22.9459(6) Å	γ = 90°
Volume	3146.47(12) Å^3	
Z	8	
Density (calculated)	2.151 Mg/m^3	
Absorption coefficient	7.753 mm^{-1}	
F(000)	1936	
Crystal size	0.34 x 0.20 x 0.06 mm^3	
Theta range for data collection	2.53 to 25.13°	
Index ranges	-7<=h<=7, -26<=k<=26, -27<=l<=25	
Reflections collected	13787	
Independent reflections	2779 [R(int) = 0.0316]	
Completeness to theta = 25.13°	98.9 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.6534 and 0.1780	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2779 / 0 / 227	
Goodness-of-fit on F^2	1.071	
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0193, wR2 = 0.0428	
R indices (all data)	R1 = 0.0219, wR2 = 0.0440	
Largest diff. peak and hole	0.486 and –0.693 e.Å^{-3}	