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SUPPLEMENTARY MATERIAL TO

Reaction of a 3-aryilidene-2-thiohydantoin derivative with polymeric *trans*-$[CuCl_2(DMSO)_2]_n$ complex: unexpected isomerization to dinuclear *cis*-$[\{CuCl(DMSO)_2\}(\mu\text{-}Cl)]_2$

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TABLE S-I. Crystallographic and refinement details of *cis*-$[(DMSO)_2ClCu(\mu\text{-}Cl)_2CuCl(DMSO)_2]$

Crystal data	
Chemical formula	$C_4H_{12}Cl_2CuO_2S_2$
M_r	290.70
Crystal system	Monoclinic
Space group	$P2_1/c$
Temperature, K	295
a / Å	8.1773 (3)
b / Å	16.6064 (8)
c / Å	8.4323 (3)
β / °	109.356 (4)
V / Å^3	1080.35 (8)
Z	4
Radiation type	Mo $K\alpha$
μ / mm^{-1})	2.86
Crystal size, mm	0.58 × 0.47 × 0.38
Data collection	
Diffractometer	Gemini S (Oxford Diffraction)
Absorption correction	Multi-scan

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Crystal data	
T_{min}, T_{max}	0.822, 1.000
No. of measured reflections	6720
No. of independent reflections	2209
No. of observed [$I > 2\sigma(I)$] reflections	2000
R_{int}	0.018
$(\sin \theta/\lambda)_{max}$ / Å^{-1}	0.626

Refinement	
$R[F^2 > 2\sigma(F^2)]$	0.027
$wR(F^2)$	0.058
S	1.17
No. of reflections	2209
No. of parameters	104
H-atom treatment	Constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ / e Å^{-3}	0.25, −0.40

3-[(2-hydroxybenzylidene)amino]-2-thioxo-imidazolidin-4-one. Yield: 2.103 g (89 %). IR (KBr): 3441*m*, 3318*m*, 3031*w*, 2958*m*, 2776*m*, 1718*s*, 1640*s*, 1623*s*, 1568*w*, 1492*w*, 1469*w*, 1334*m*, 1317*m*, 1266*m*, 1254*m*, 1204*m*, 1149*w*, 890*w*, 838*w*, 757*m*, 735*m*, 710*m*, 637*w*, cm^{-1}. ^{1}H-NMR (200 MHz, DMSO-d_6, δ / ppm): 12.10 (*bs*, NH, exchangeable with D_2O), 10.88 (*s*, OH, exchangeable with D_2O), 8.64 (*s*, 1H, H-7), 7.58 (*dd*, 1H, J = 8.0 and 1.9 Hz, H-6), 7.32 (*dt*, 1H, J = 7.8 and 1.8 Hz, H-1), 6.95 (*m*, 2H, H-4, H-5), 3.97 (*s*, 2H, CH_2-8). ^{13}C-NMR (50 MHz, DMSO-d_6, δ / ppm): 173.77, 164.44, 158.01, 157.76, 132.17, 130.62, 119.54, 118.50, 116.38, 33.46. Combustion analysis for $C_{10}H_9N_3O_2S$: Cald. C 51.05, H 3.86, N 17.86; found C 51.10, H 3.89, N 17.88.

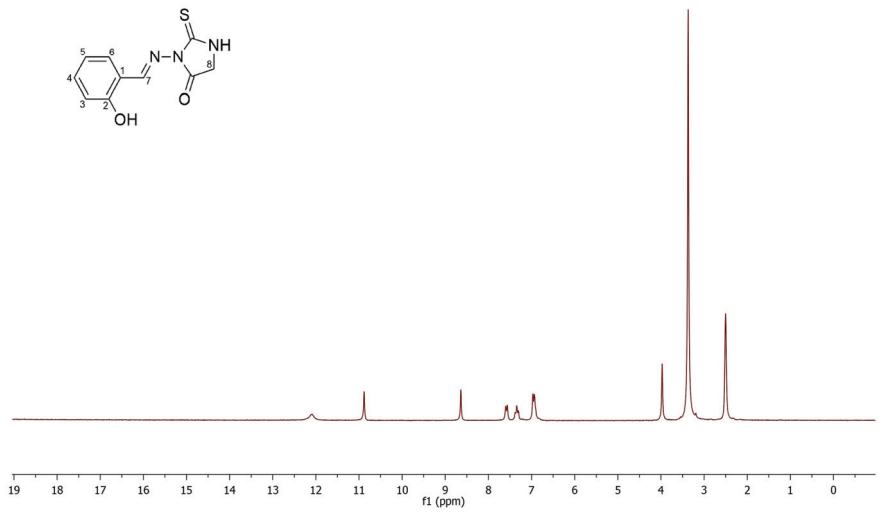

Fig. S-1. ^{1}H-NMR spectra of 3-[(2-hydroxybenzylidene)amino]-2-thioxoimidazolidin-4-one.

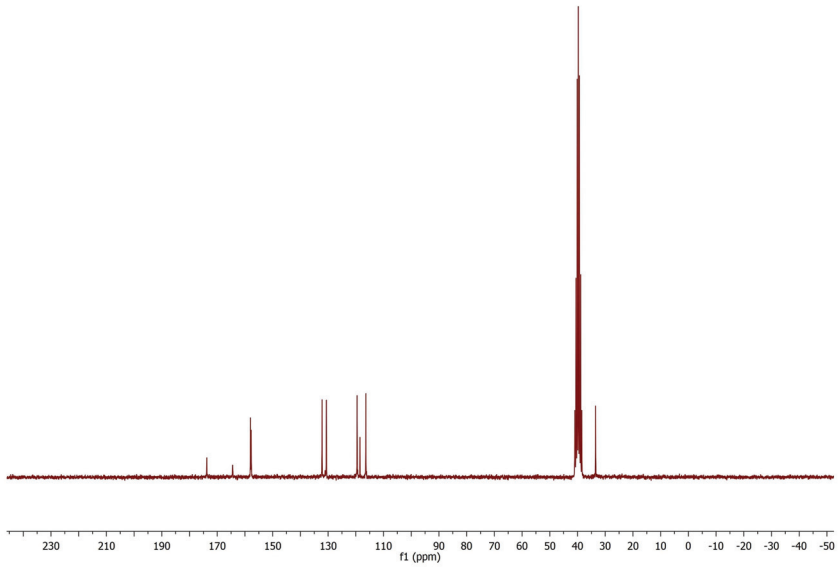

Fig. S-2. ^{13}C-NMR spectra of 3-[(2-hydroxybenzylidene)amino]-2-thioxoimidazolidin-4-one.

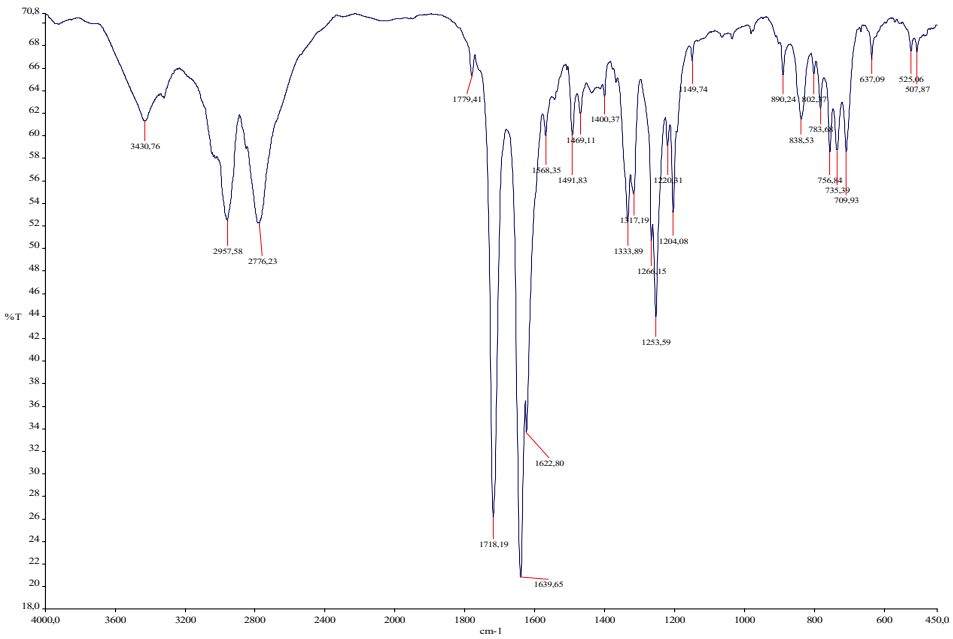

Fig. S-3. IR spectra of 3-[(2-hydroxybenzylidene)amino]-2-thioxoimidazolidin-4-one.