

Supplementary Information

Investigations of Oral Pathogens on Copper(II) Complexes with Thiosemicarbazone: Antimicrobial and Antibiofilm Activities in Addition to *in vitro* and *in vivo* Toxicity

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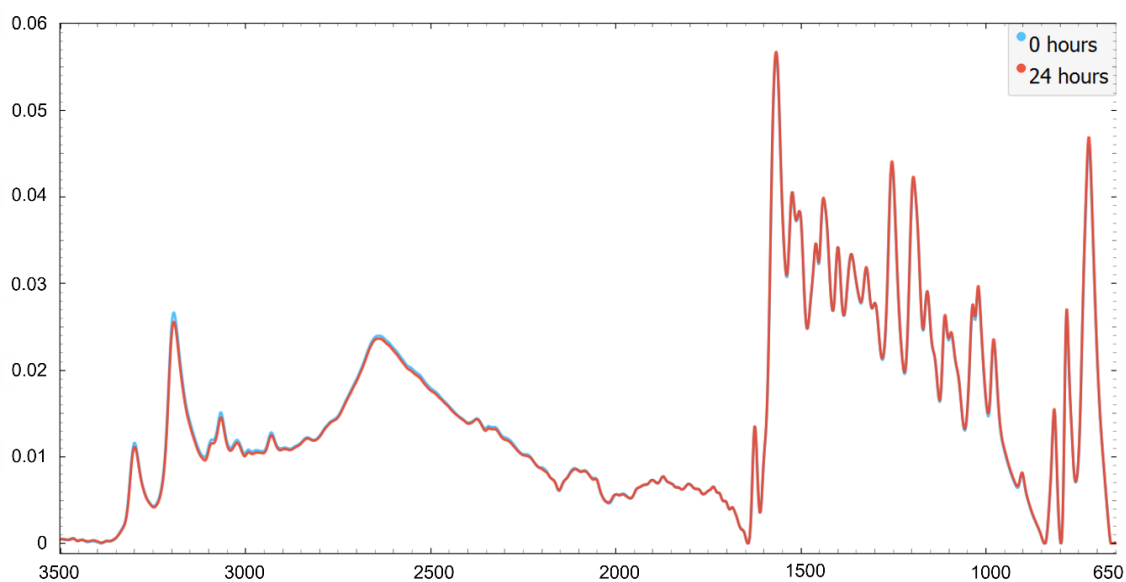


Figure S1. Representative average ATR-FTIR spectra (3500-650 cm^{-1}) for 0 h, and 24 h of compound **1** at powder in pure concentration.

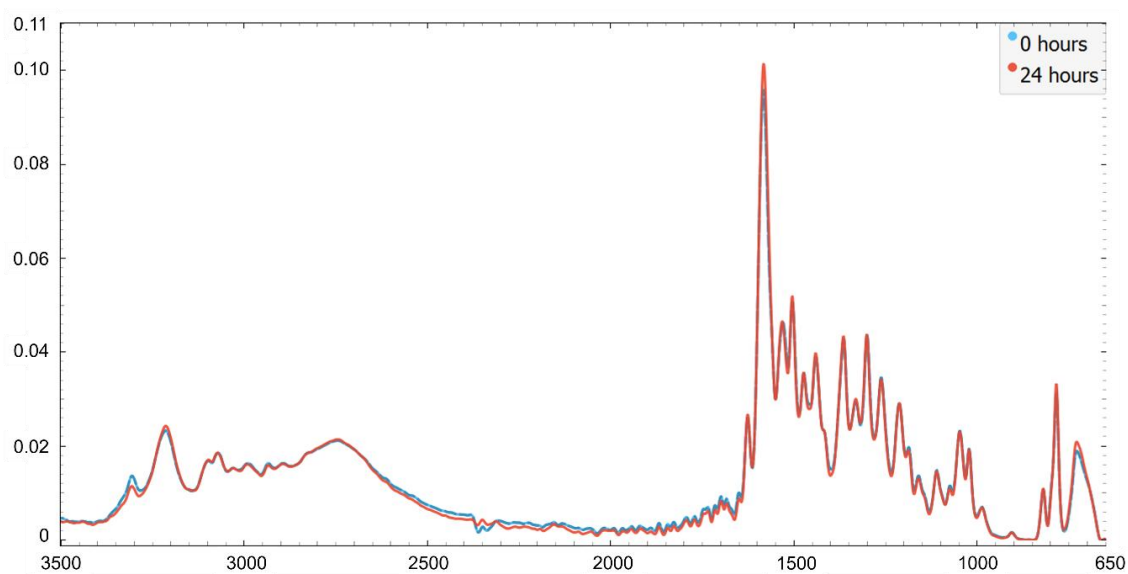


Figure S2. Representative average ATR-FTIR spectra (3500-650 cm^{-1}) for 0 h, and 24 h of compound **1** at 200 $\mu\text{g mL}^{-1}$ concentration.

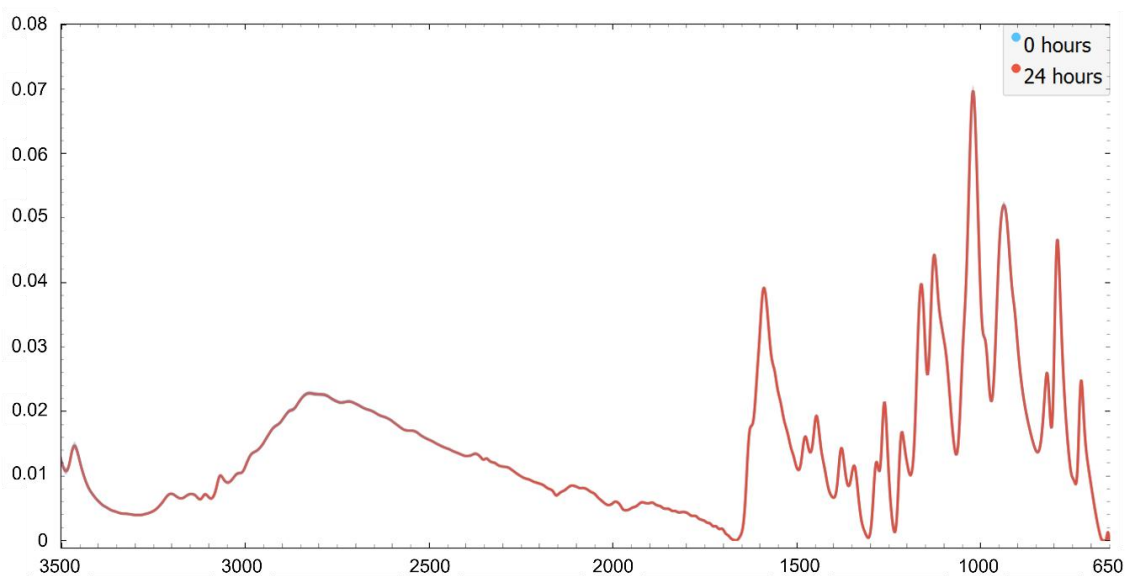


Figure S3. Representative average ATR-FTIR spectra (3500-650 cm^{-1}) for 0 h, and 24 h of compound **2** at powder in pure concentration.

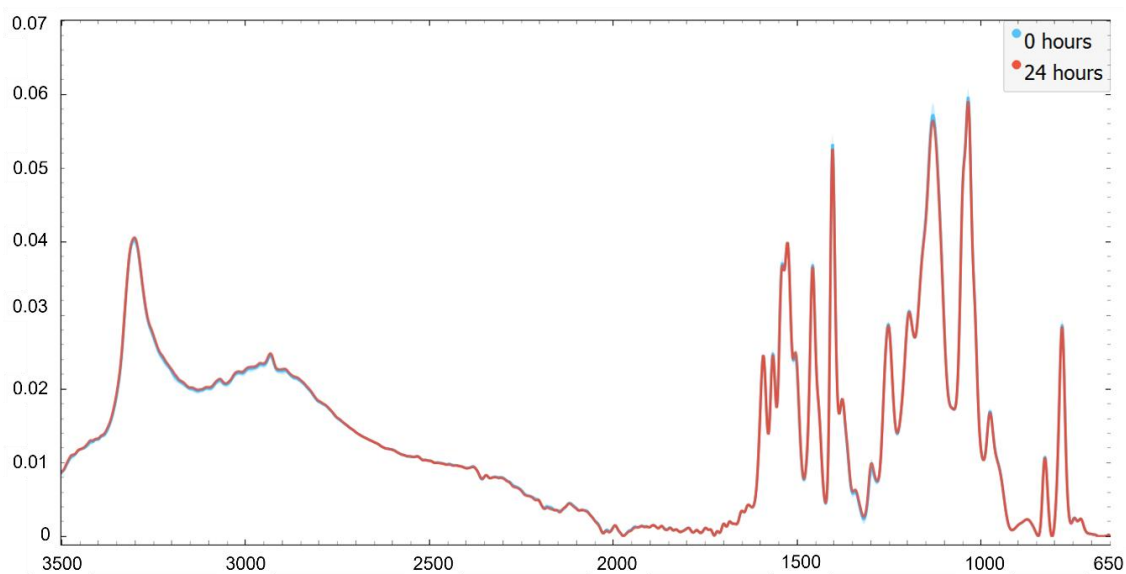


Figure S4. Representative average ATR-FTIR spectra (3500-650 cm^{-1}) for 0 h, and 24 h of compound **2** at 200 $\mu\text{g mL}^{-1}$ concentration.

Table S1. Infrared vibrational modes associated with interaction between *S. mutans* and metallic complexes

Vibrational mode / cm^{-1}	Assignment	Biomolecular components
2925	stretching C–H	lipids
2917	stretching C–H	lipids
1734	stretching C=O	fatty acid ester
932	phosphodiester region	nucleic acids

Table S2. Binding affinities (ΔG) of free ligand, complexes and the standard drug

Bacterial proteins	$\Delta G / (\text{kcal mol}^{-1})$			
	1	2	5	Chlorhexidine
<i>S. mutans</i> deoxycytidylate deaminase	−4.78	−6.71	−5.07	−7.92
<i>S. mitis</i> lectinolysin	−5.35	−5.01	−6.85	−3.03
<i>S. sanguinis</i> oxireductase	−6.53	−7.58	−6.10	−9.49
<i>L. paracasei</i> transcriptional regulator	−6.10	−7.79	−5.21	−8.46
<i>E. faecalis</i> hydrolase domain	−5.02	−7.32	−5.78	−11.24

