

Insights into structure and biological activity of copper(II) and zinc(II) complexes with triazolopyrimidine ligands

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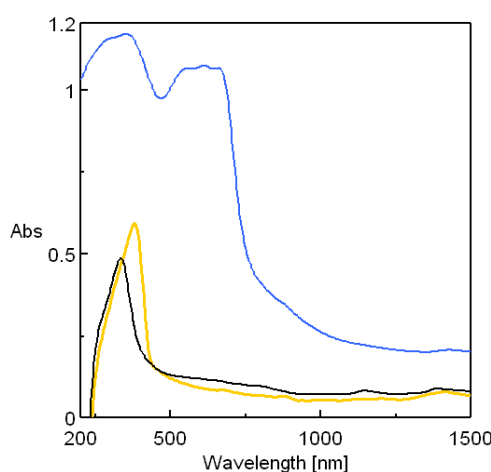


Figure S1. UV-Vis spectra of complexes (1) (dark blue), (2) (yellow) and pmtip (black).

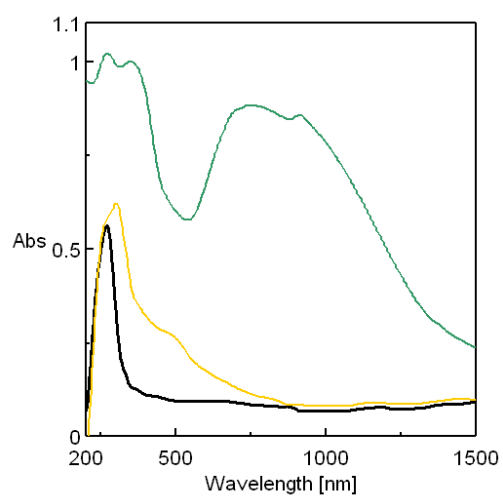


Figure S2. UV-Vis spectra of complexes (3) (green), (4) (yellow) and dmtp (black).

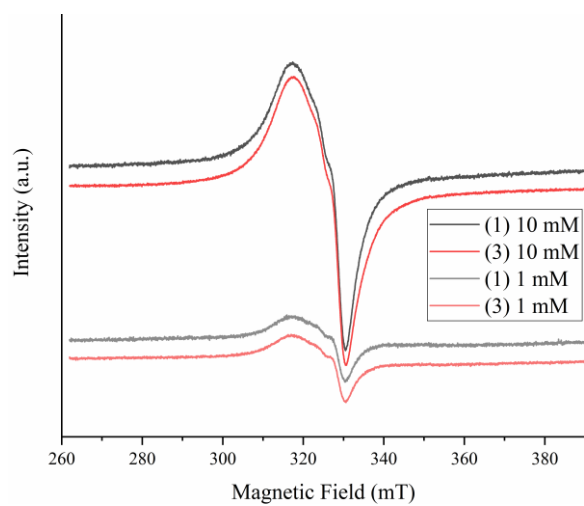


Figure S3. EPR spectra of complexes (1) and (3) in 1 and 10 mM DMSO solution.

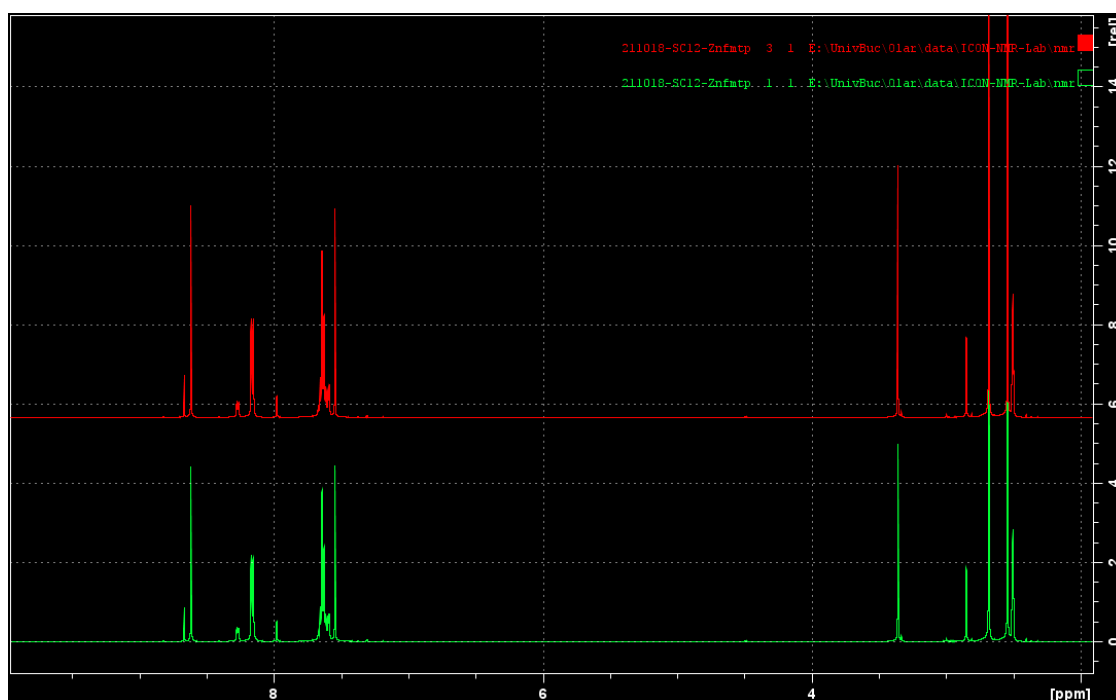
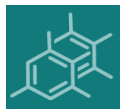


Figure S4. ¹H NMR spectra of fresh prepared complex (2) (green) and after 72 h (red).

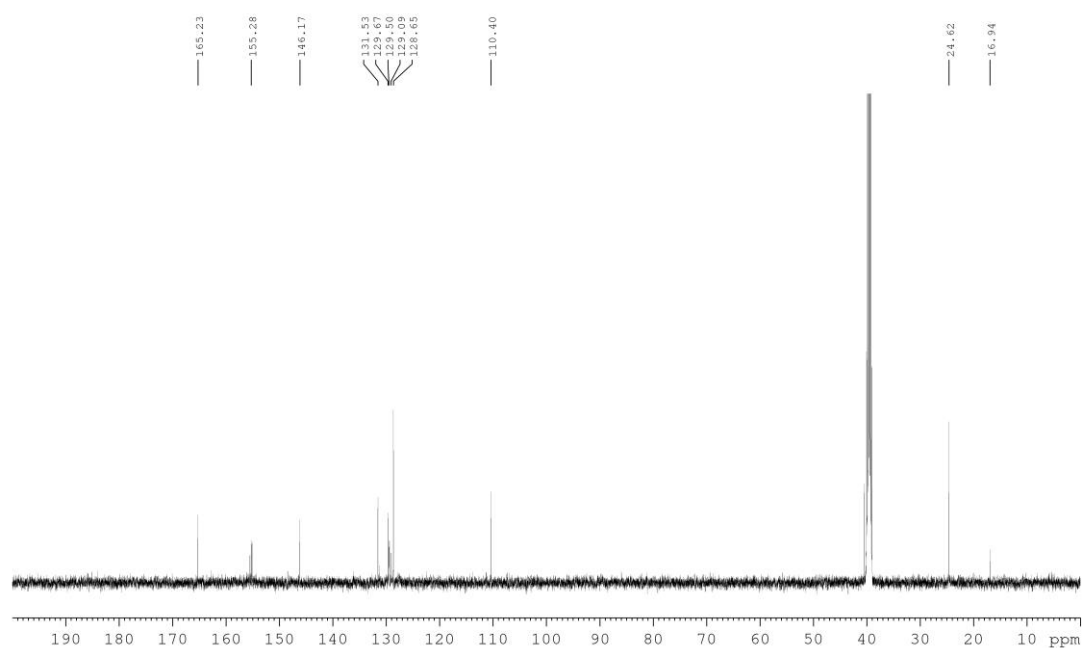


Figure S5. ¹³C NMR spectrum of complex (2).

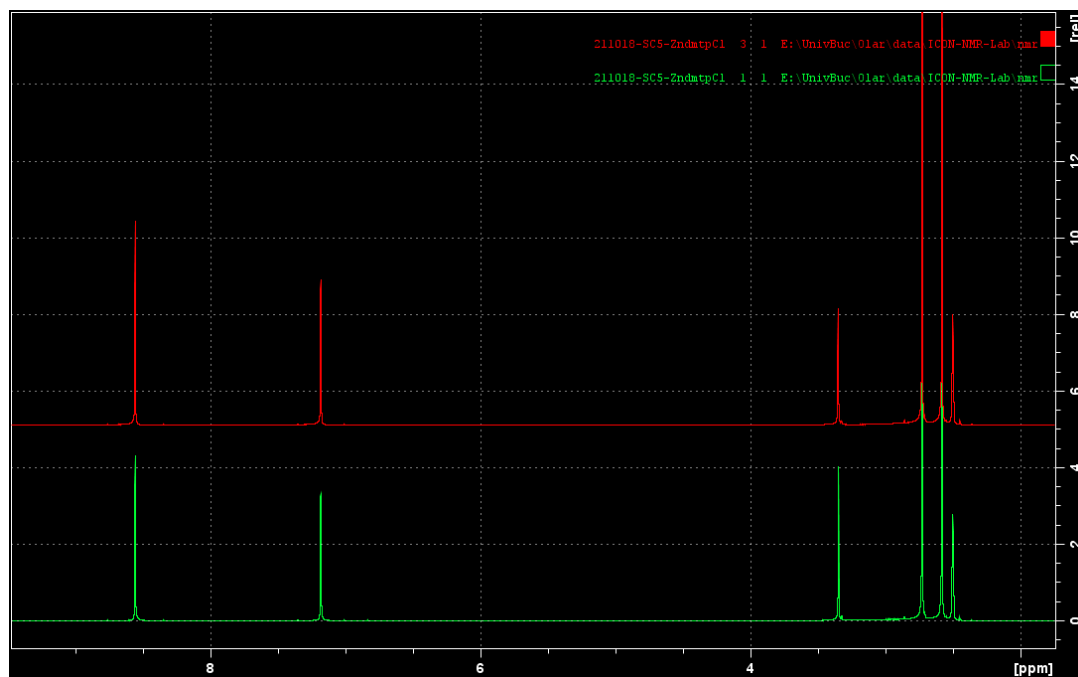
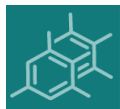


Figure S6. ^1H NMR spectra of fresh prepared complex (4) (green) and after 72 h (red).

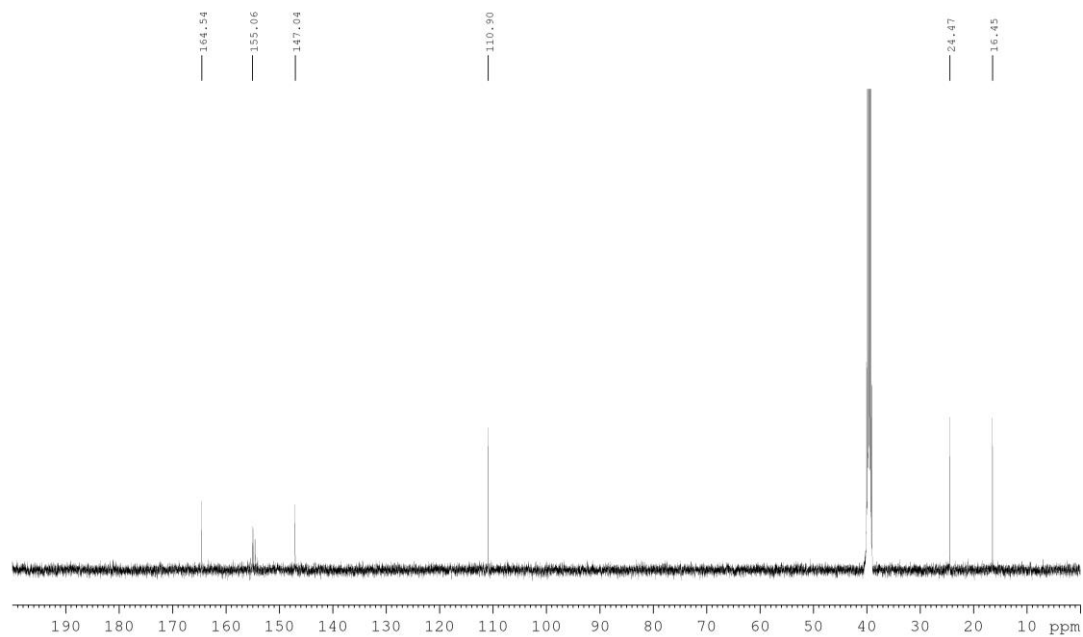


Figure S7. ^{13}C NMR spectrum of complex (4).

Table S1. Selected geometric parameters-angles (°) in compounds (1) and (2).

(1)					(2)		
Cl1	Cu1	Cl1 ¹	180.0	O1	Zn1	Cl1	107.95(7)
N1	Cu1	Cl1	88.38(8)	O1	Zn1	N1	106.65(8)
N1 ¹	Cu1	Cl1 ¹	88.38(8)	C6	S1	C4	99.30(19)
N1	Cu1	Cl1 ¹	91.62(8)	O1	S1	C4	103.79(16)
N1 ¹	Cu1	Cl1	91.62(8)	O1	S1	C6	104.19(15)
N1 ¹	Cu1	N1	180.0	C12	N1	Zn1	129.18(18)
N2	N3	C2	110.5(2)	C14	N1	Zn1	124.95(17)
N2	N3	C7	127.5(2)	C14	N1	C12	103.9(2)
C7	N3	C2	122.0(2)	C14	N2	N3	103.0(2)
C4	C3	C2	115.8(2)	N1	C12	N3	107.5(2)
C1	N2	N3	102.2(2)	N4	C12	N1	128.0(2)
C2	N1	Cu1	132.41(19)	N4	C12	N3	124.5(2)
C2	N1	C1	104.4(2)	C10	N4	C12	115.4(2)
C1	N1	Cu1	122.97(19)	N2	N3	C12	110.07(19)
C3	C2	N3	123.5(2)	N2	N3	C8	128.2(2)

Symmetry transformations used to generate equivalent atoms: ¹1-x, 1-y, -z