Anti-leishmanial Study of Discrete Tetrahedral Zinc(II) β-oxodithioester Complexes†

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Contents in Supporting Information

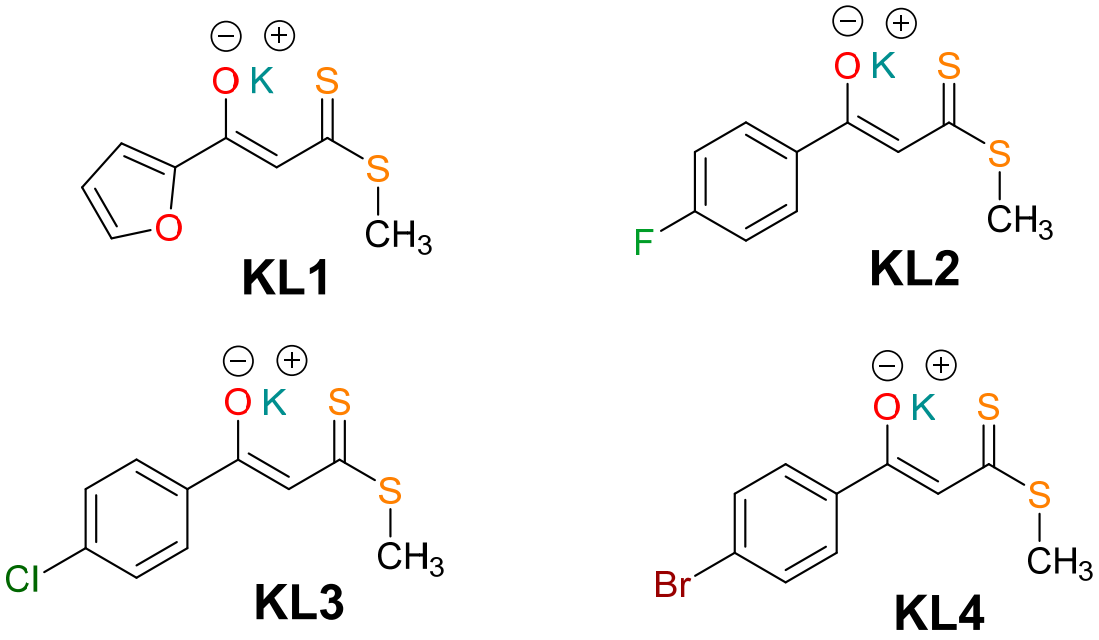


Figure S1. Potassium salts of β-oxodithioester ligands KL1─KL4.

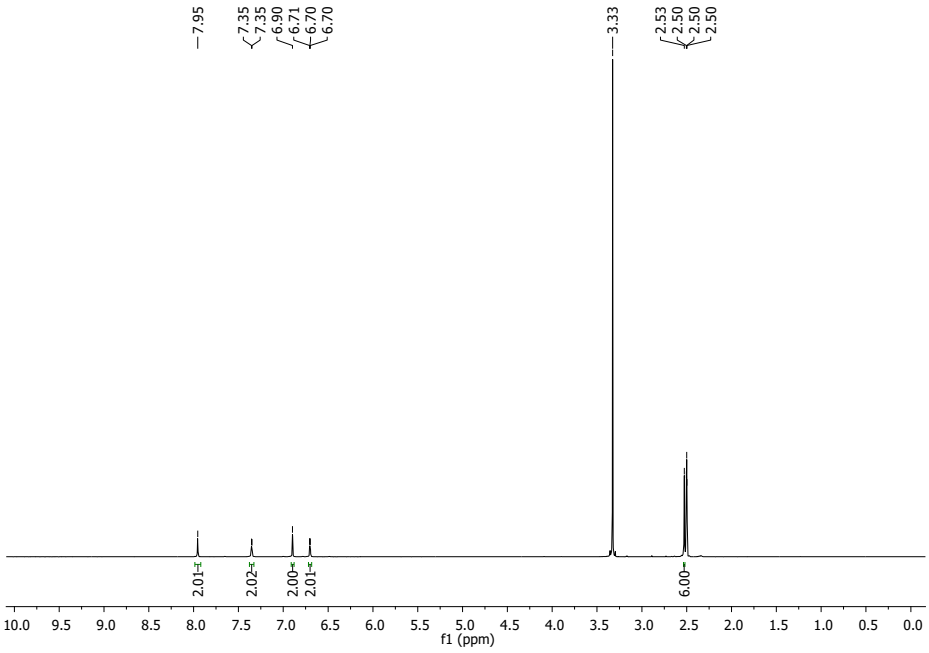


Figure S2. ^{1}H NMR spectrum of complex **1** in DMSO-*d*$_6$.

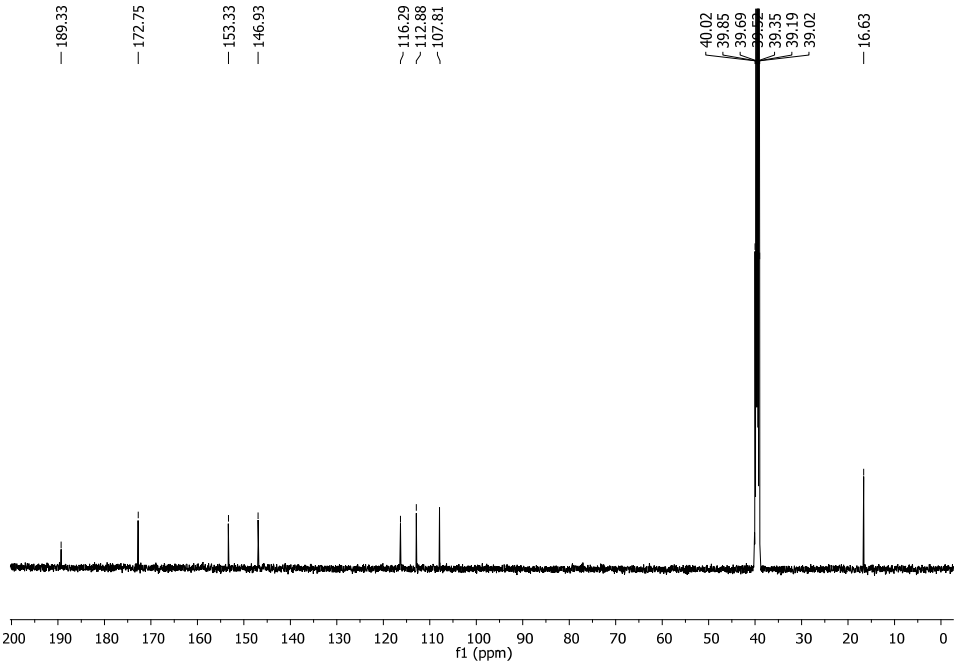


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of complex **1** in DMSO-d_6.

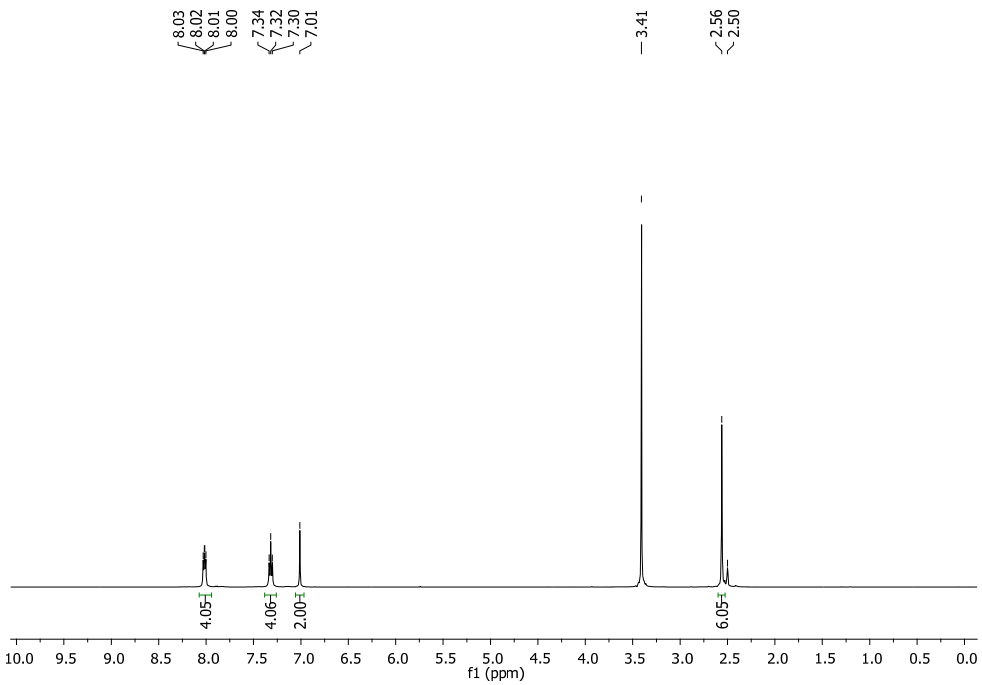


Figure S4. ^{1}H NMR spectrum of complex **2** in DMSO-d_6.

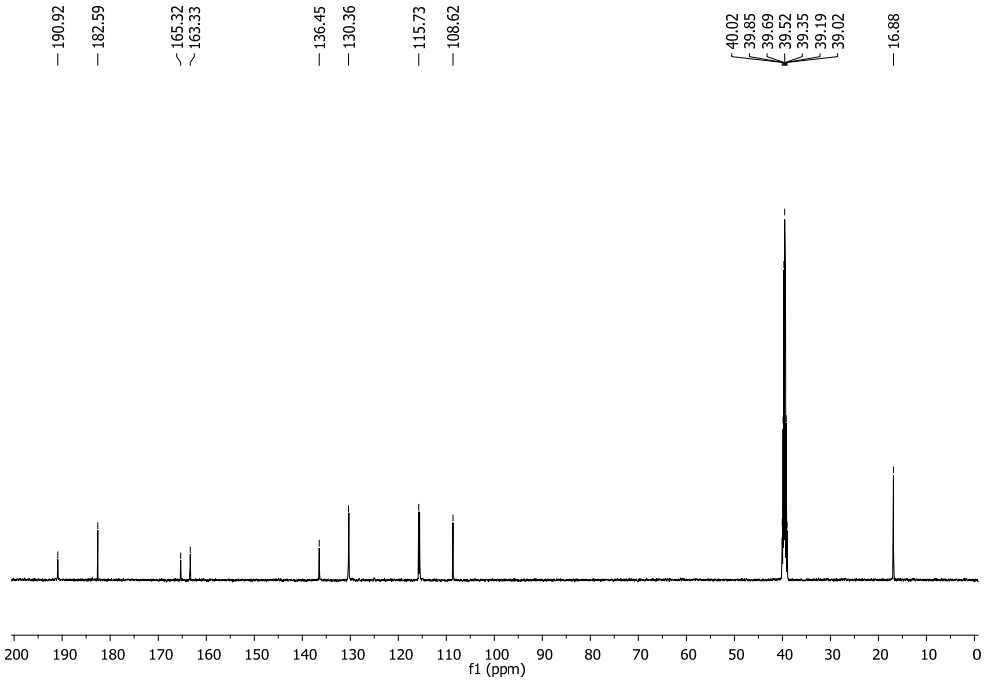


Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of complex **2** in DMSO-d_6.

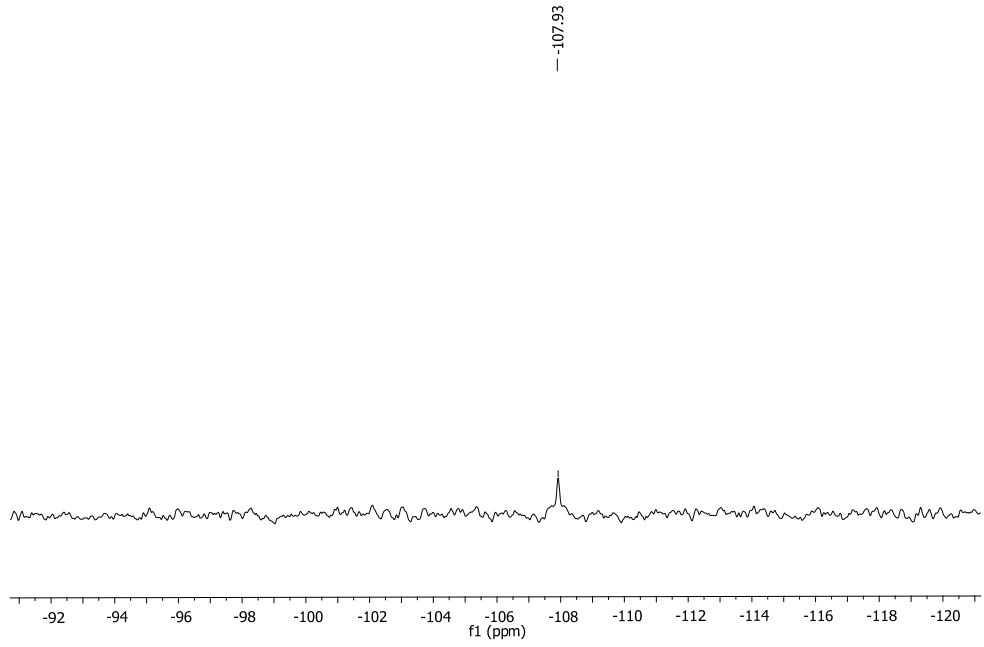


Figure S6. ^{19}F NMR spectrum of complex **2** in DMSO-d_6.

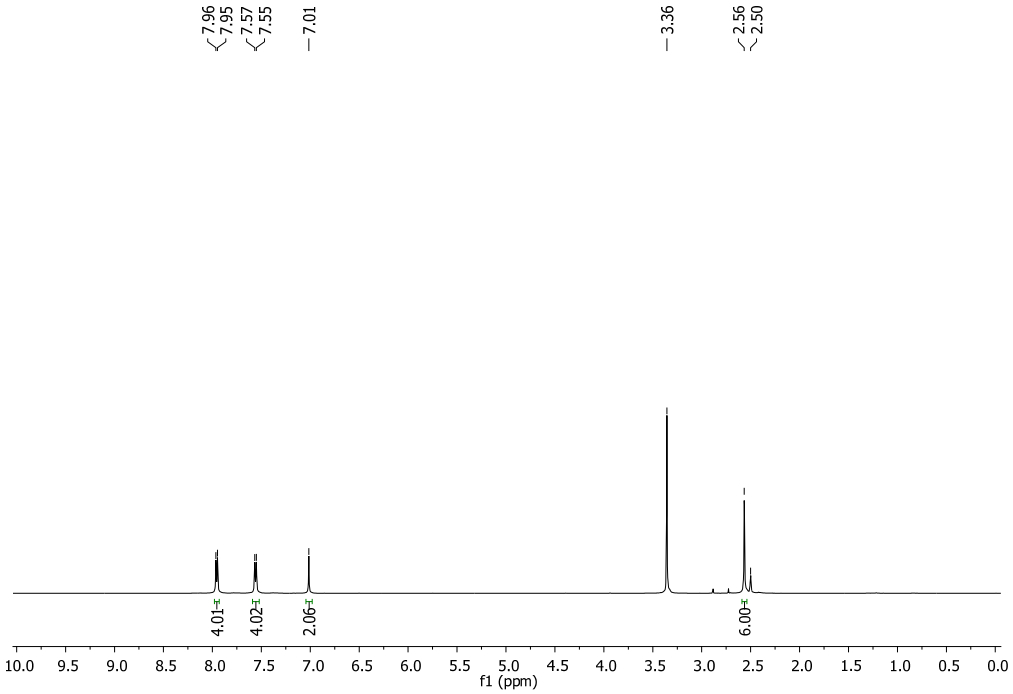


Figure S7. ^{1}H NMR spectrum of complex **3** in DMSO-*d*$_6$.

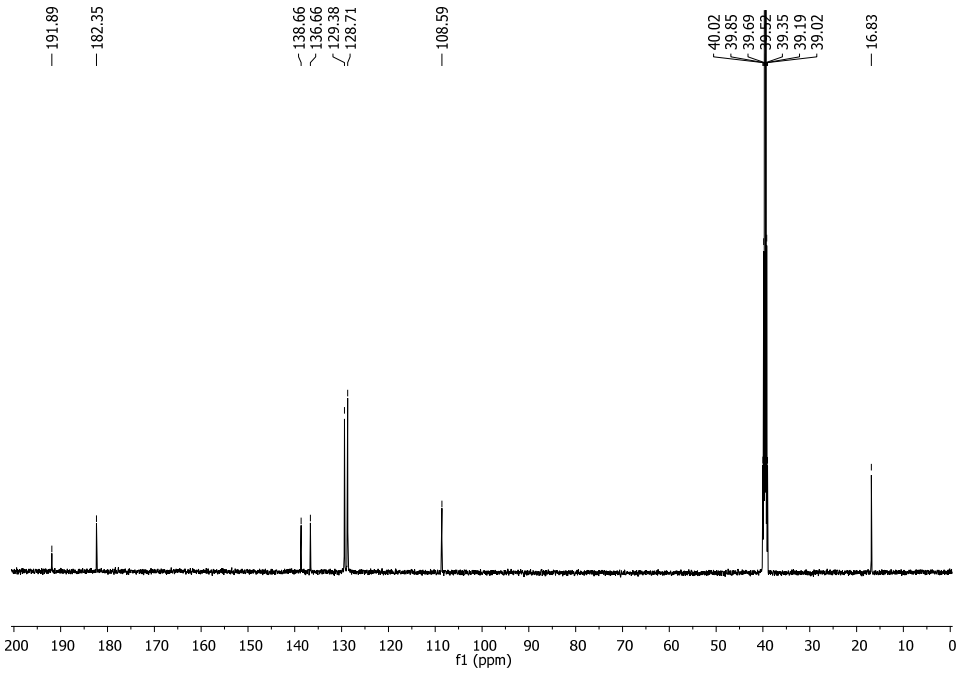


Figure S8. ^{13}C{^{1}H} NMR spectrum of complex **3** in DMSO-*d*$_6$.

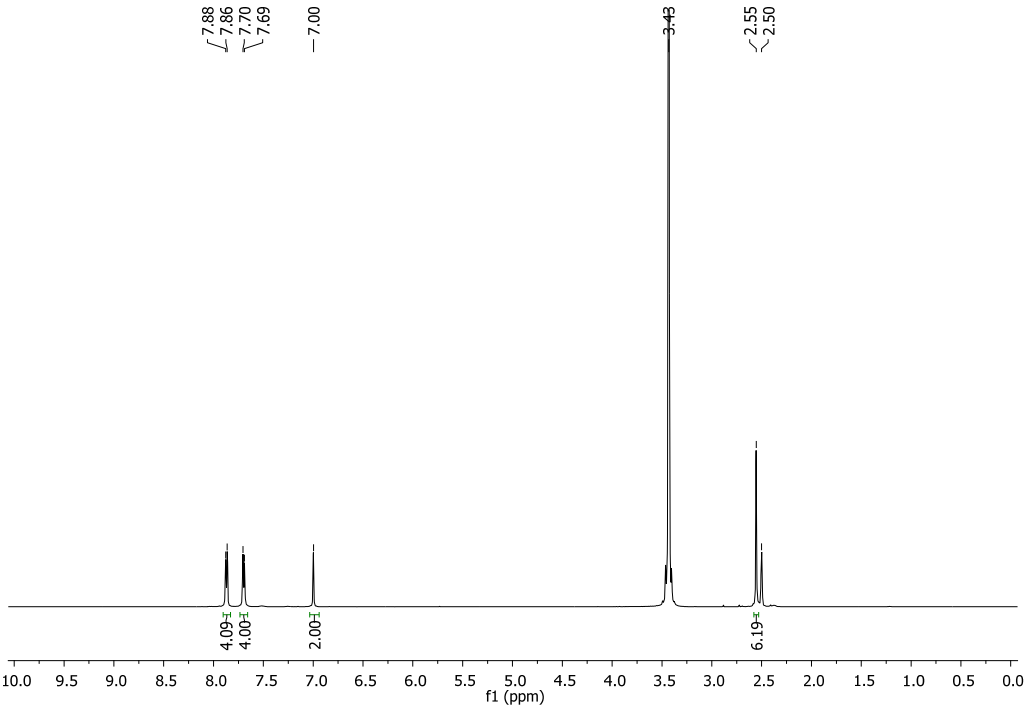


Figure S9. ^{1}H NMR spectrum of complex **4** in DMSO-d_6.

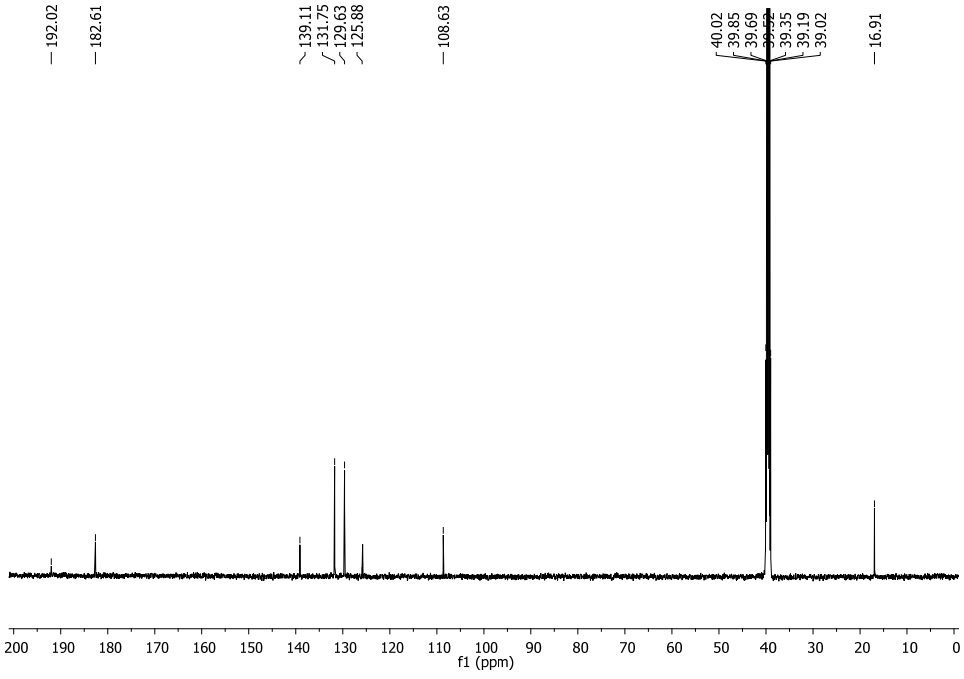


Figure S10. ^{13}C{^{1}H} NMR spectrum of complex **4** in DMSO-d_6.

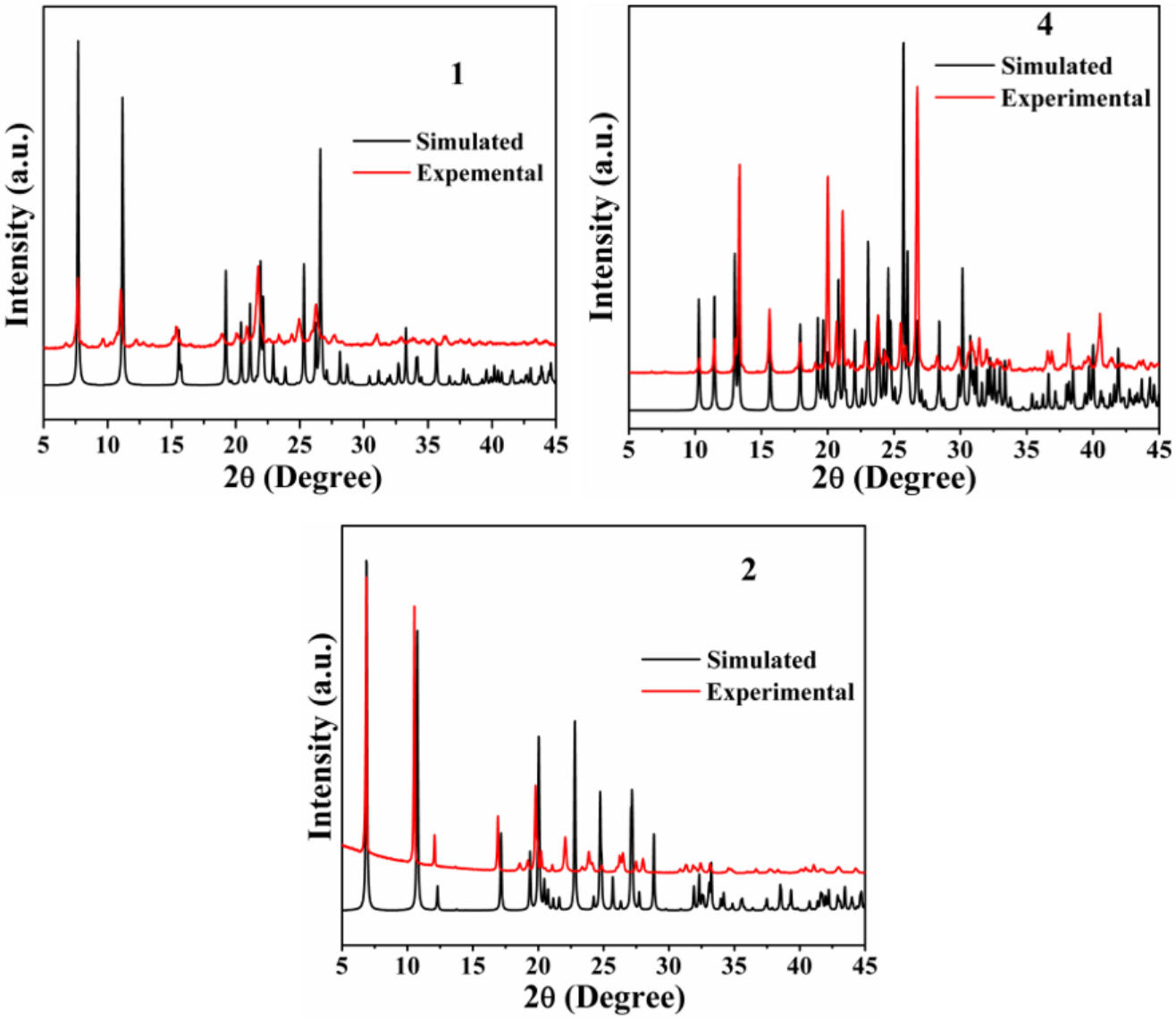


Figure S11. Simulated PXRD (in black, generated from single crystal data) and experimental (in red) patterns of complexes **1**, **2**, and **4**.

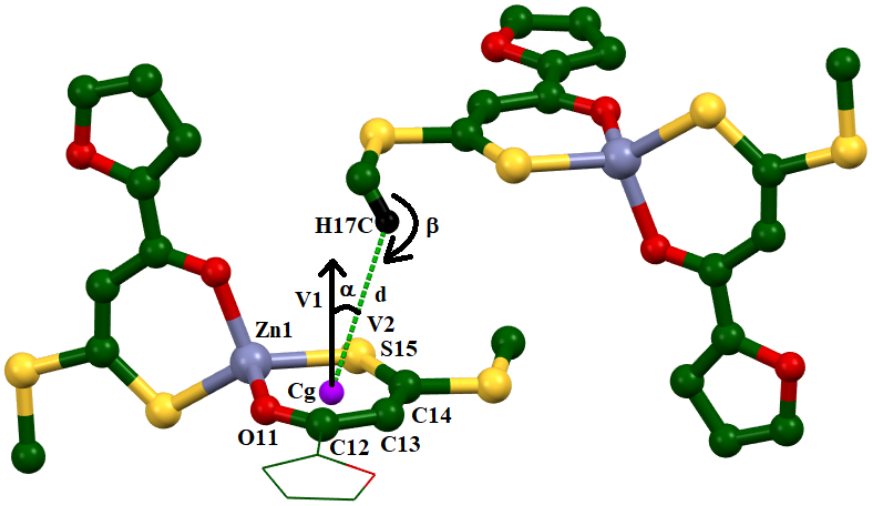


Figure S12. Representation of the C—H···π ($ZnOSC_3$, chelate) interactions with only the major component of the -SMe group shown: *d* is the distance between the ring centroid (Cg) of the chelate ring and the H atom; V1 is the vector normal to the plane through the ring; β is the C—H···CG angle; α is the angle between V1 and V2. All hydrogen atoms have been omitted for clarity except H17C. Color of atoms (C green; O red; S yellow; Zn grey, and H black).

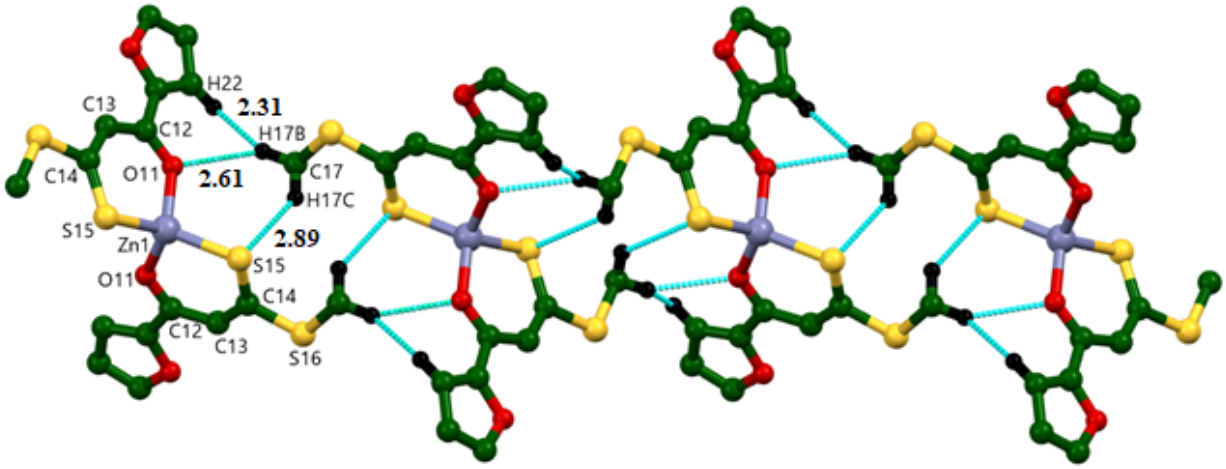
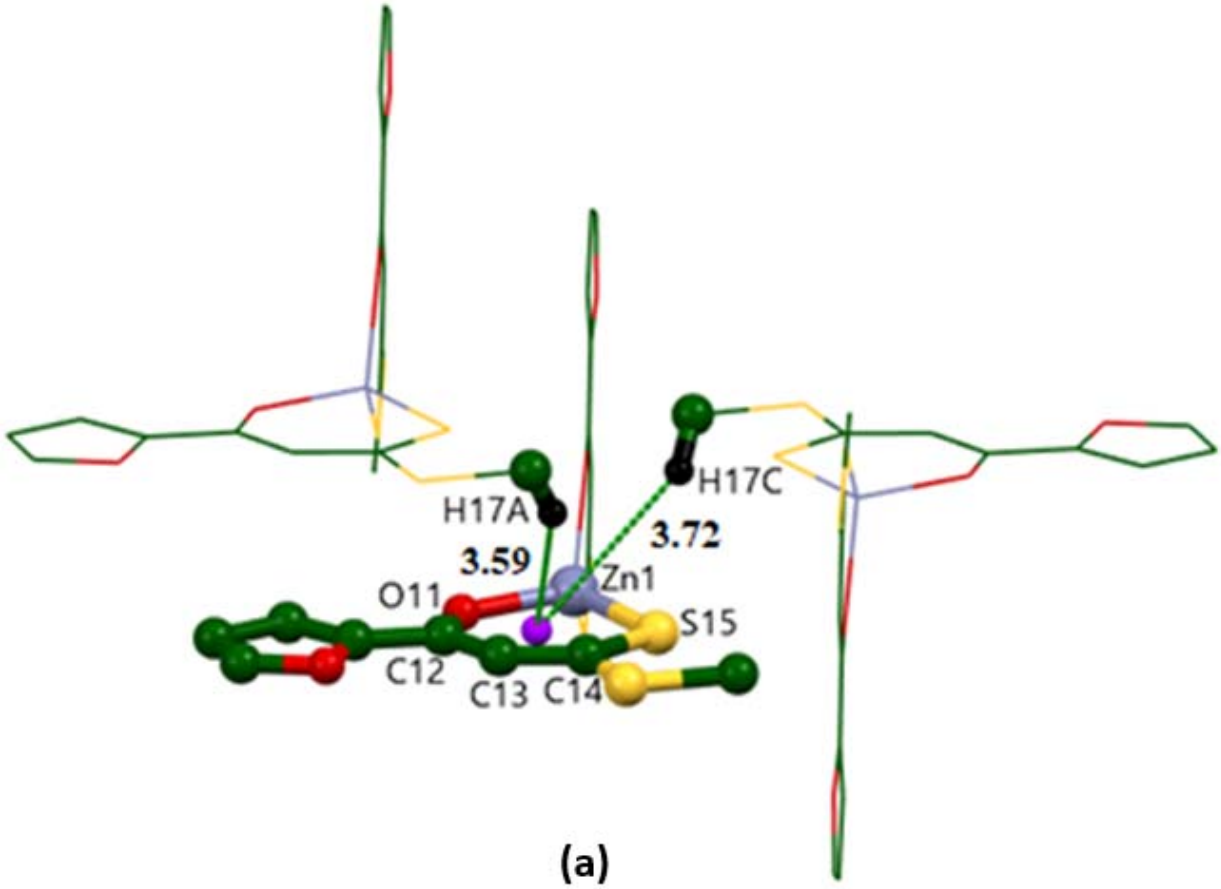
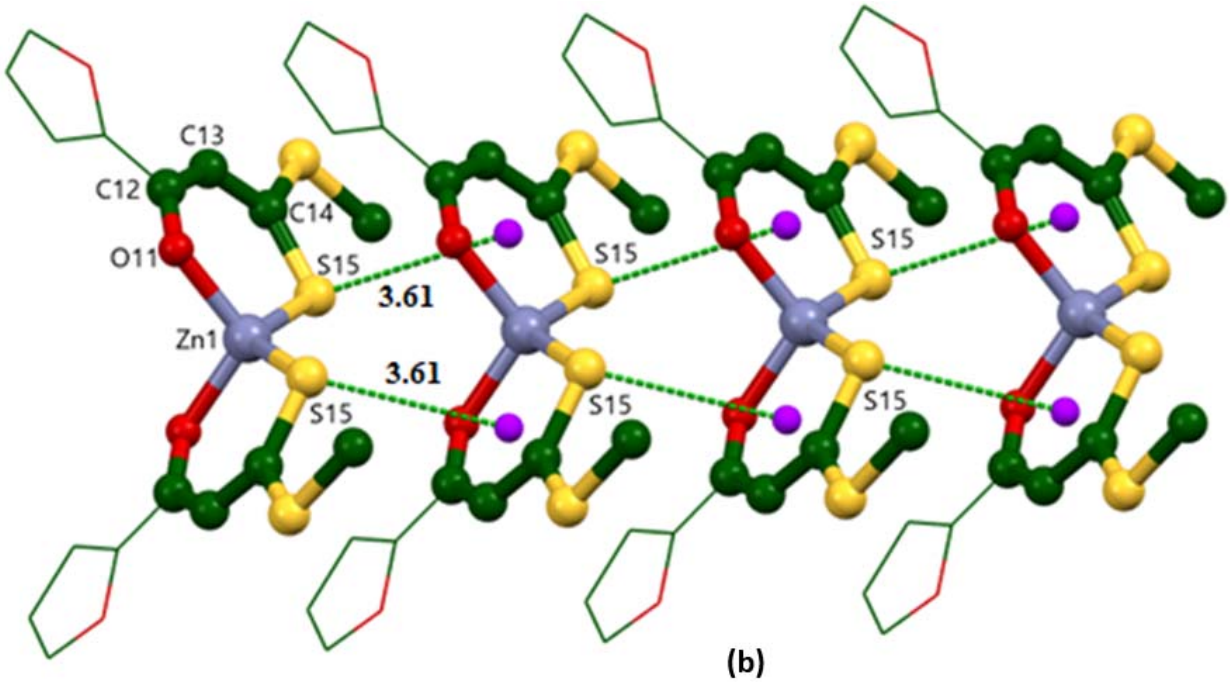


Figure S13. Supramolecular structure of complex **1** sustained by C—H···O, C—H···S and C—H···H—C interactions. Only the major component of the -SMe group is shown. All hydrogen atoms except for H17C and H17B have been omitted for clarity. Colour coding of atoms (C green; O red; S yellow; Zn grey, and H black).


H17A
H17C
3.59
3.72
Zn1
O11
S15
C12
C13
C14

(a)


C13
C12
C14
O11
S15
3.61
Zn1
3.61
S15
S15
S15
S15
S15

(b)

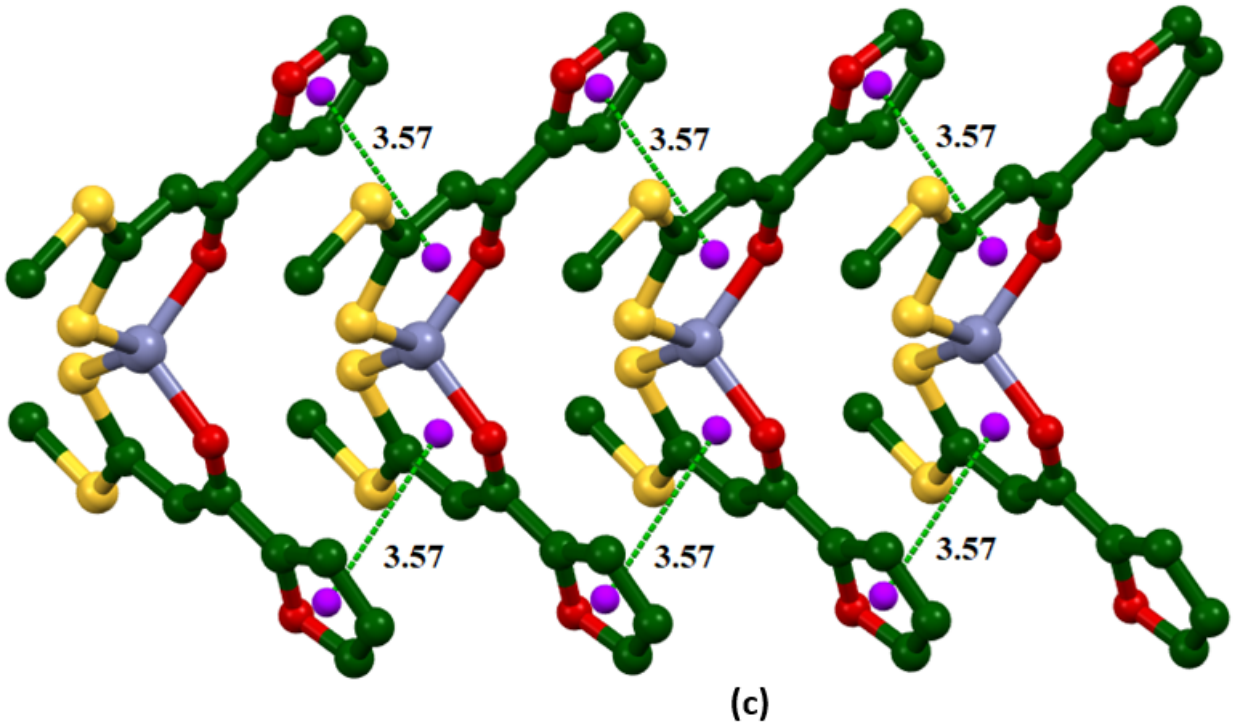


Figure S14. Supramolecular structure of complex **1** sustained by (a) C─H···π ($ZnOSC_3$, chelate), (b) C─S···π ($ZnOSC_3$, chelate), and (c) π···π($ZnOSC_3$,) interactions. Only the major component of the -SMe group is shown. All hydrogen atoms have been omitted for clarity. Colour coding of atoms (C green; O red; S yellow; Zn grey).

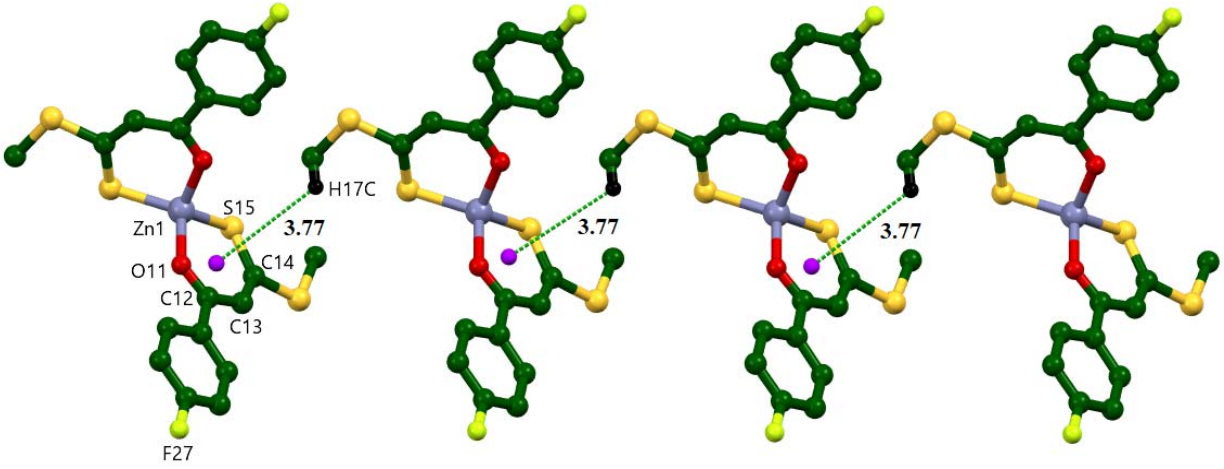


Figure S15. Supramolecular structure of complex **2** sustained by C─H···π ($ZnOSC_3$, chelate) interactions. All hydrogen atoms except for H17C have been omitted for clarity. Colour coding of atoms (C green; O red; S yellow; Zn grey, and H black).

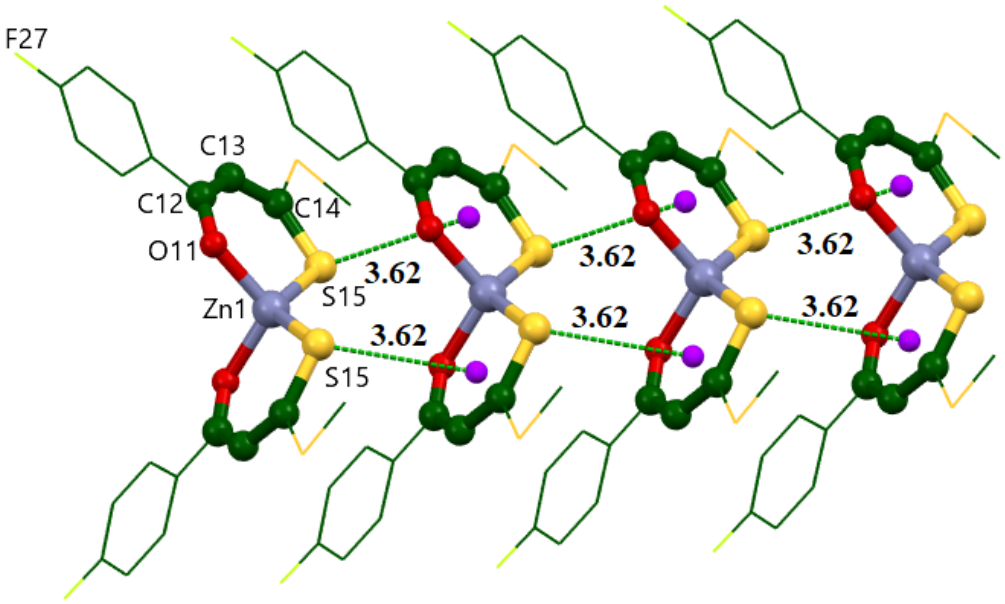


Figure S16. Supramolecular structure of complex **2** sustained by C─S···π ($ZnOSC_3$, chelate) interactions. All hydrogen atoms have been omitted for clarity except H17C. Colour coding of atoms (C green; O red; S yellow; Zn grey).

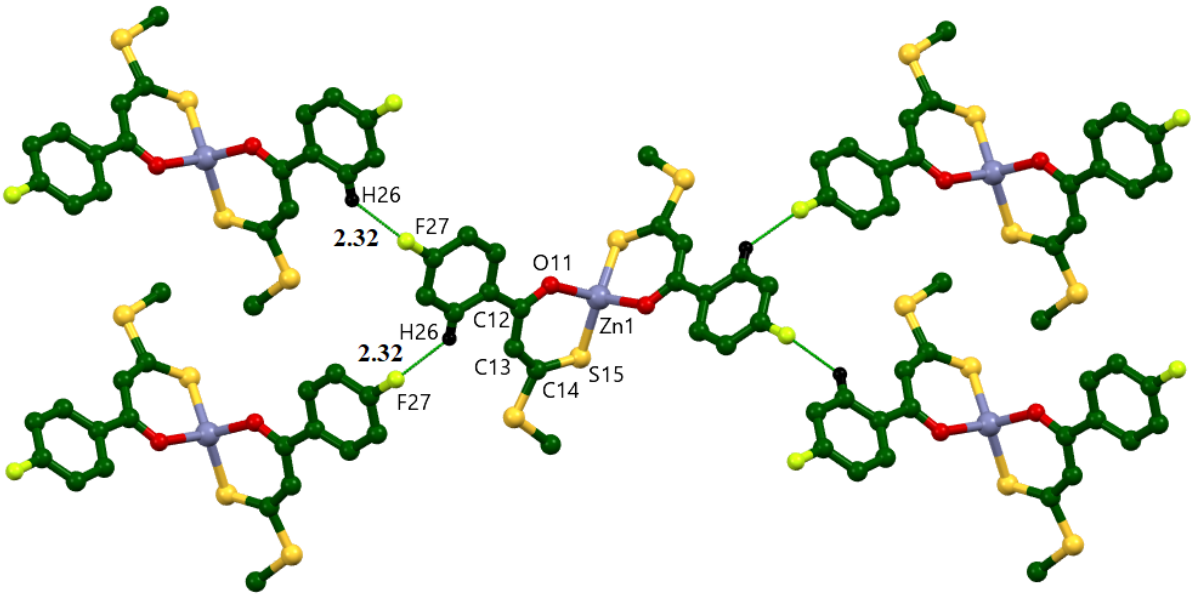


Figure S17. Supramolecular structure of complex **2** sustained by C─H···F─C interactions. All hydrogen atoms except for H26 have been omitted for clarity. Colour coding of atoms (C green; O red; S yellow; F lime green; Zn grey, and H black).

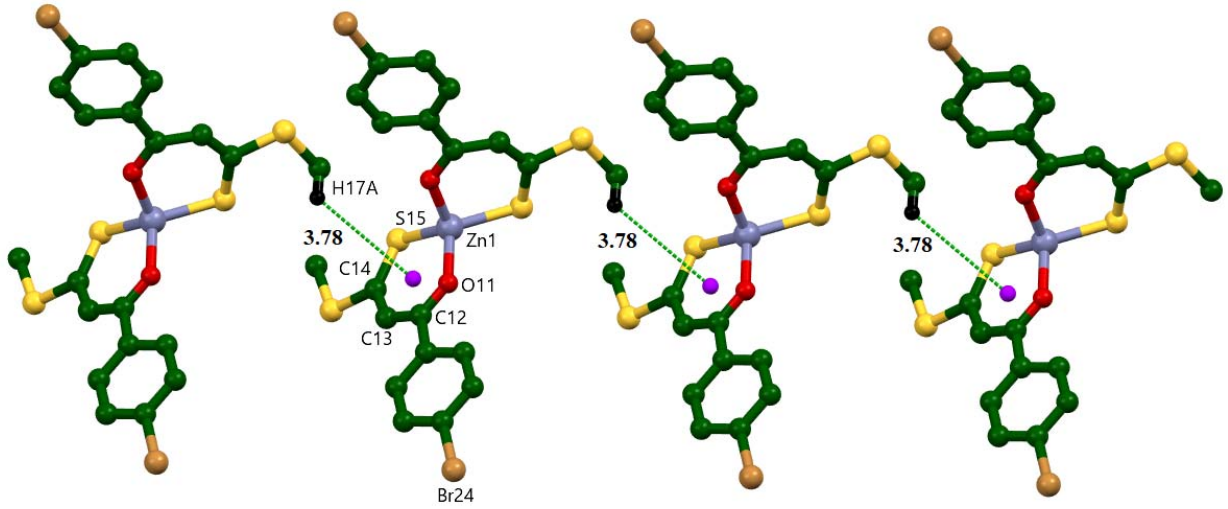
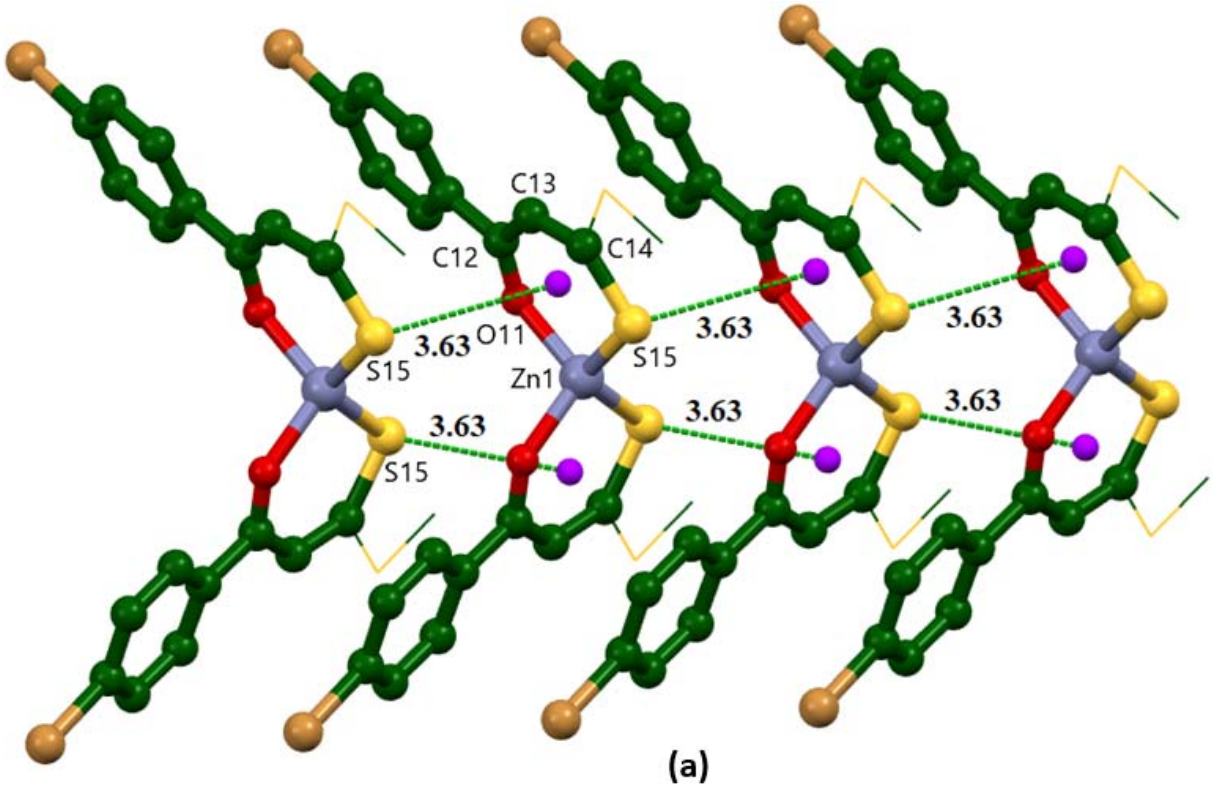


Figure S18. Supramolecular structure of complex **4** sustained by C─H···π ($ZnOSC_3$, chelate) interactions. All hydrogen atoms for except H17A have been omitted for clarity. Colour coding of atoms (C green; O red; S yellow; Br brown; Zn grey, and H black).



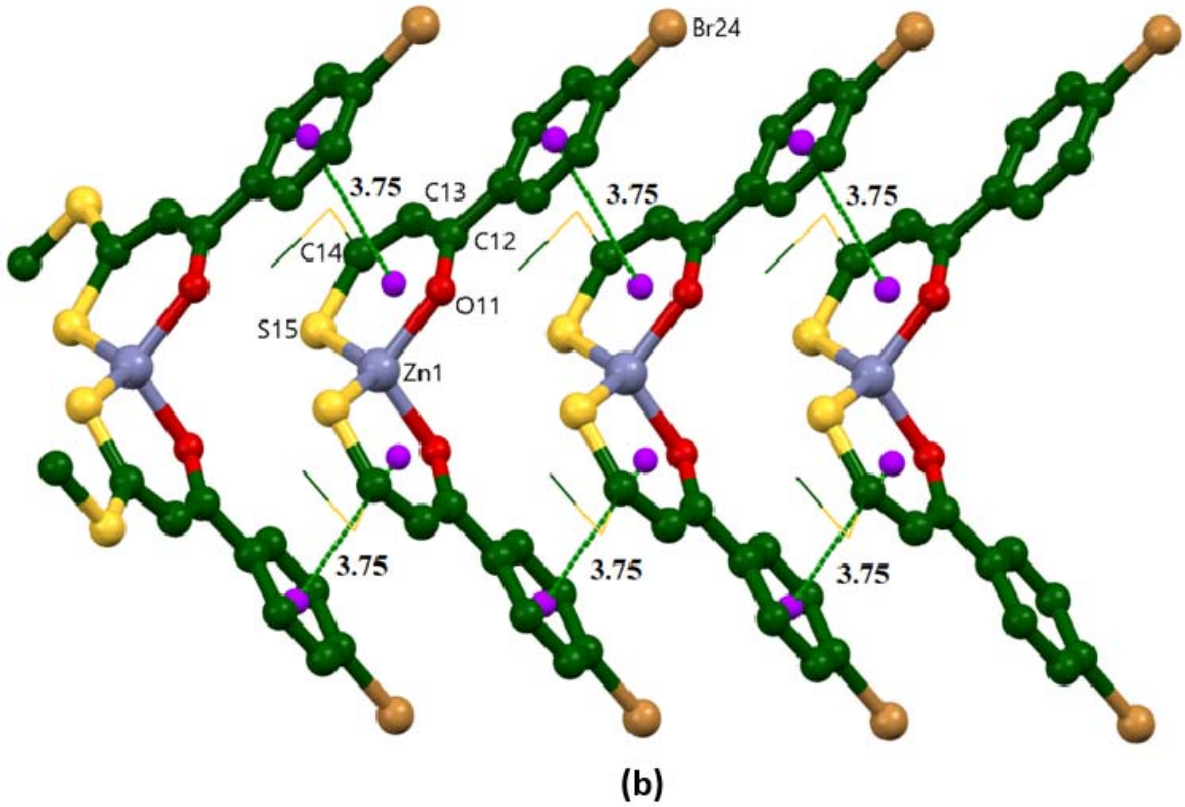


Figure S19. Supramolecular structure of complex **4** sustained by (a) C─S···π ($ZnOSC_3$, chelate) and (b) π···π($ZnOSC_3$) interactions. All hydrogen atoms have been omitted for clarity. Colour coding of atoms (C green; O red; S yellow; Br brown; Zn grey).