Electronic Supplementary Material (ESI) for CrystEngComm.

Effect of functionalities on the crystal structures of new zinc(II) dithiocarbamates; A combined anti-leishmanial and thermal decomposition study

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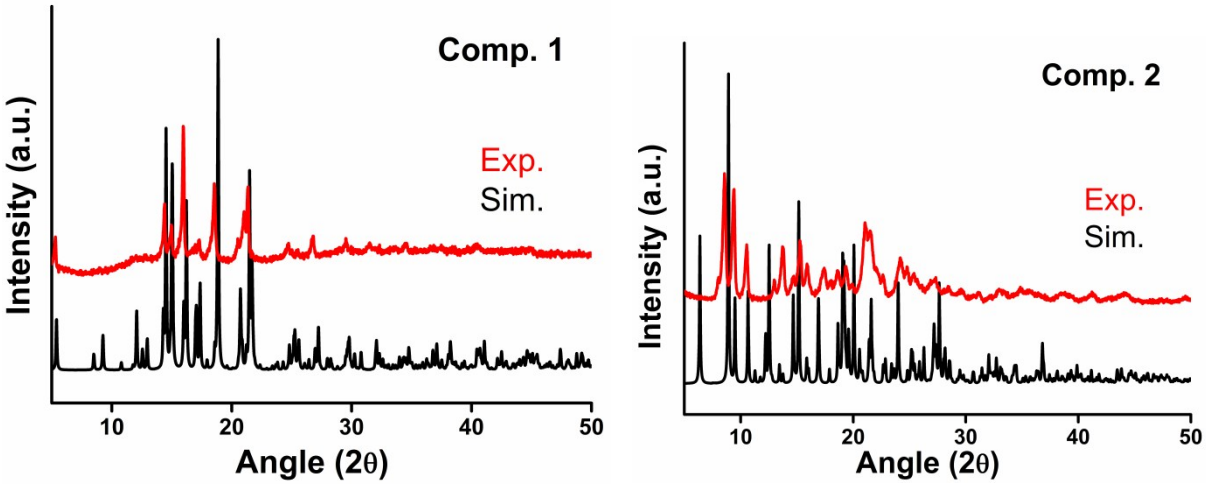
Table S1. Dimensions (Å, deg) in complex **6**

Zn1- S11	2.349(1)
Zn1 - S13	2.334(1)
Zn1 - S41	2.338(1)
Zn1 -S43	2.331(1)
S13 - Zn - S11	77.93(4)
S43 - Zn - S41	78.05(4)
S43 - Zn - S13	130.22(4)
S13 - Zn - S41	121.94(5)
S43 - Zn - S11	126.13(5)
S41 - Zn - S11	130.52(4)



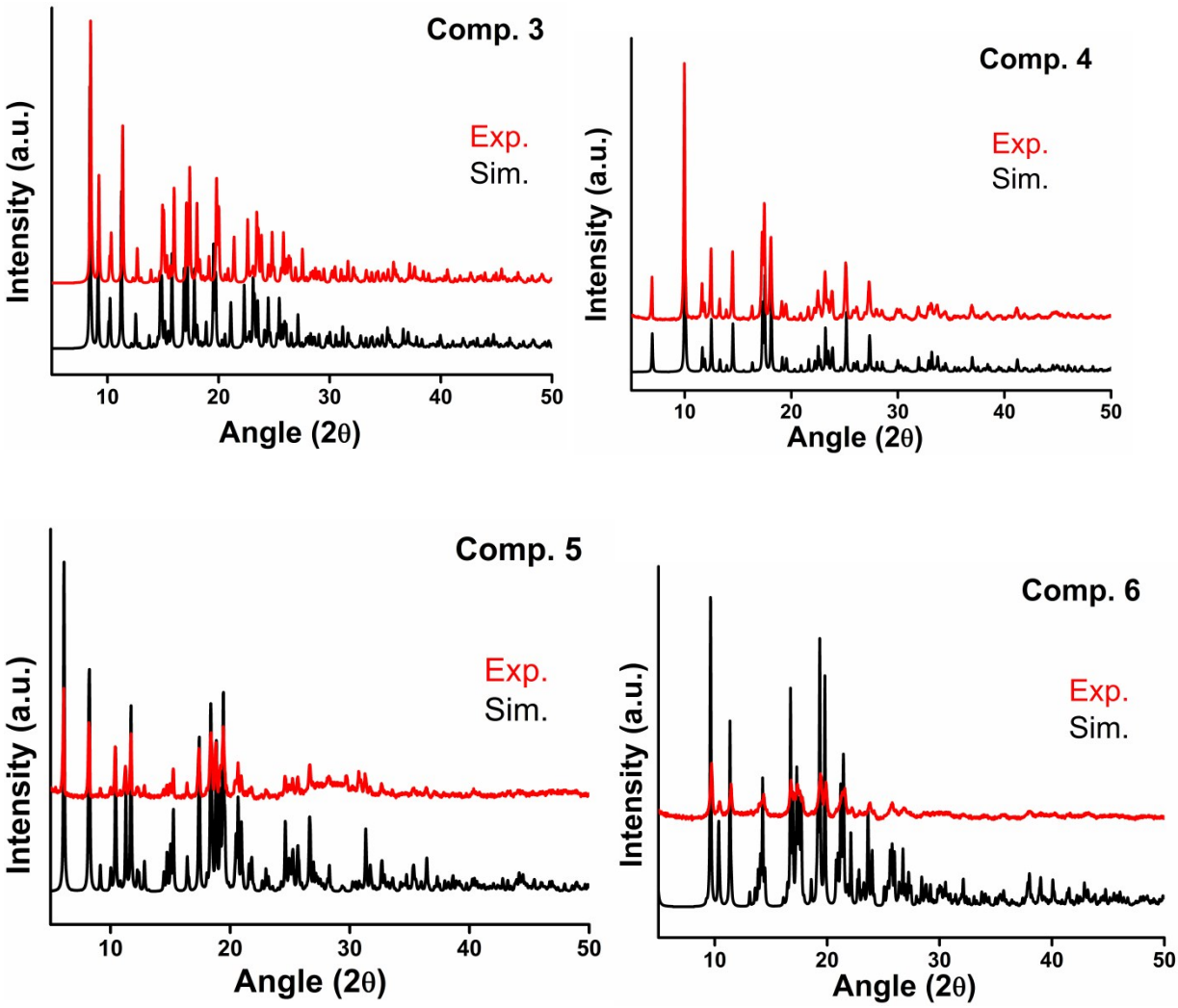
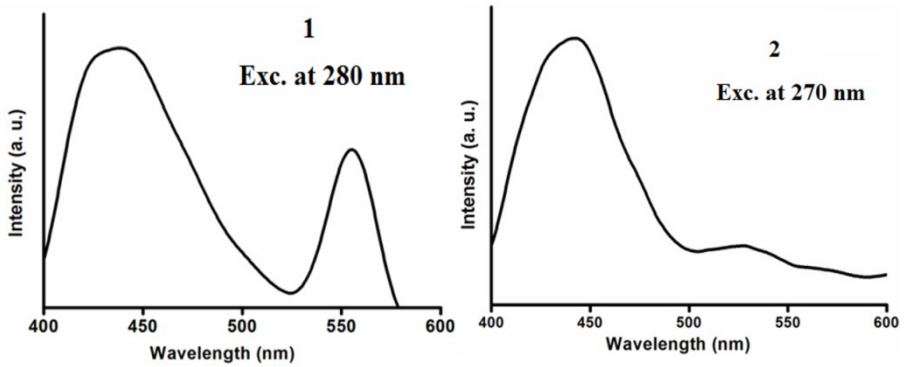


Figure S1. Simulated in black, generated from single crystal data and experimental in red from PXRD patterns of **1-6.**



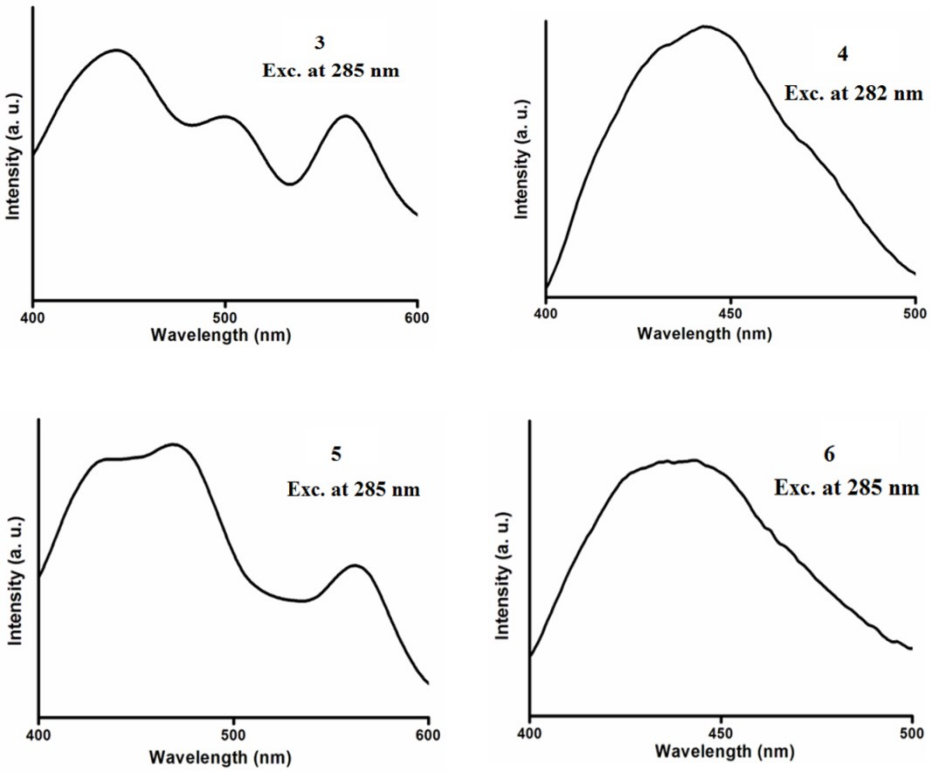


Figure S2. Photoluminescence spectra of **1-6** in CH_2Cl_2 solution.

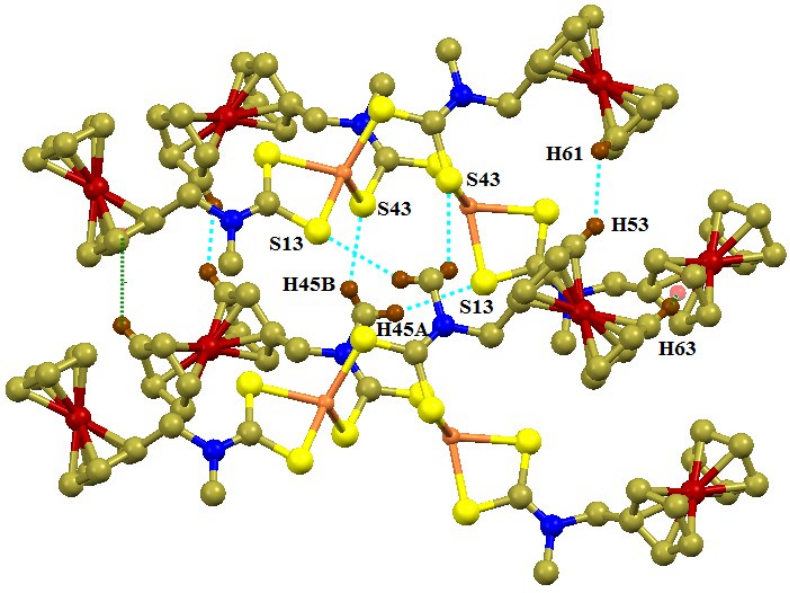
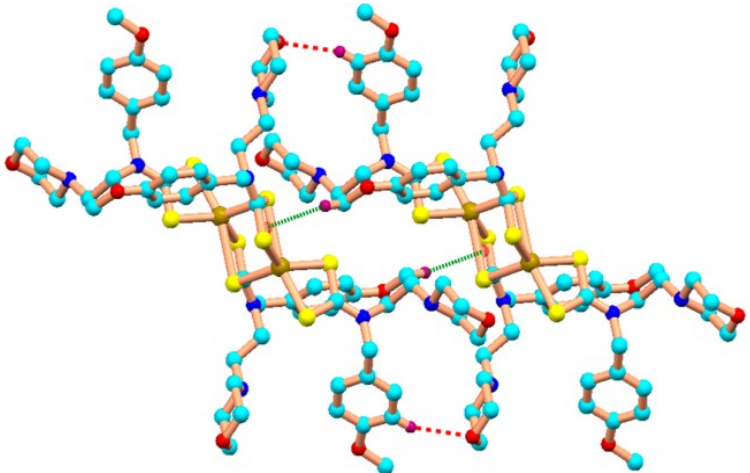
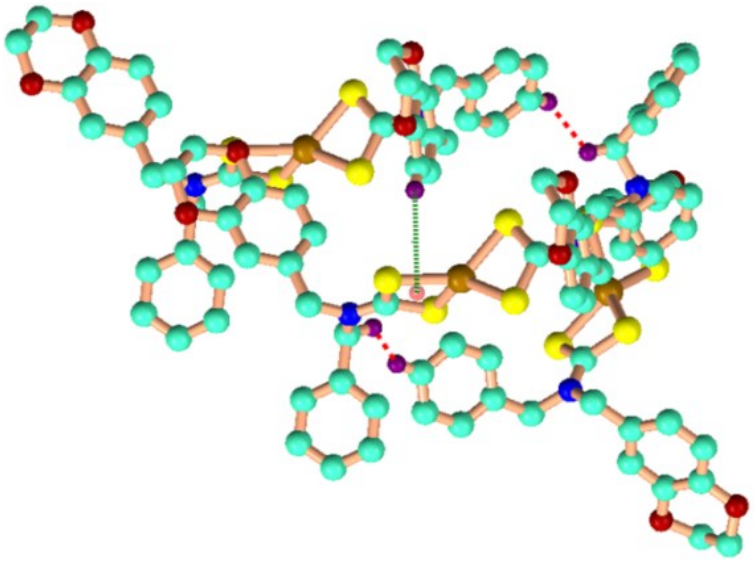


Figure S3. Supramolecular structure of **1** sustained via H···H, C-H···S and C-H···π interactions.



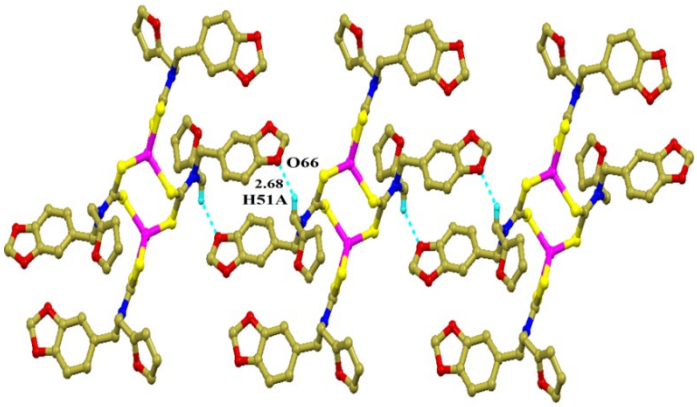
(a)



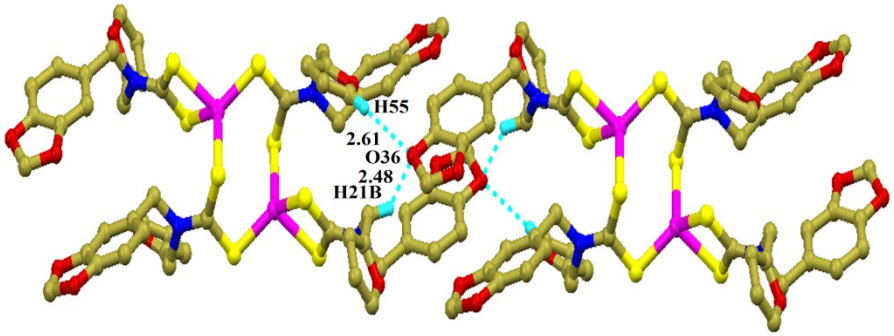
(b)

Figure S4. C-H···π (ZnS_2C, chelate) and C-H···O interactions in **5** (a) and C-H···π (ZnS_2C, chelate) and C-H···H-C interactions in **6** (b).

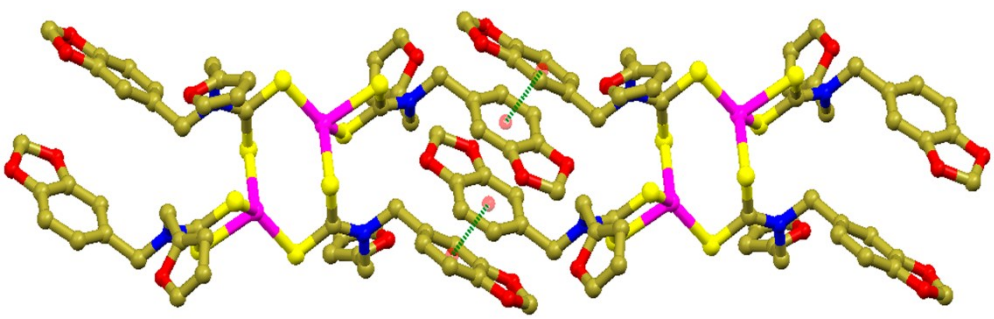
Figure S5. Supramolecular structure of **2** sustained via C-H···S interactions.



(a)



(b)



(c)

Figure S6. Supramolecular structure of **2** (a), (b) and (c) sustained via C-H···O and π···π interactions respectively.

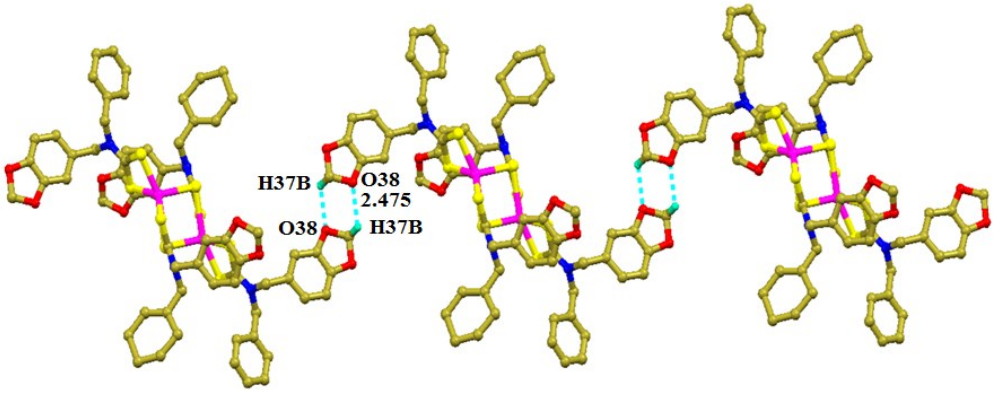


Figure S7. Wave like structure of **3** via C–H···O interactions.

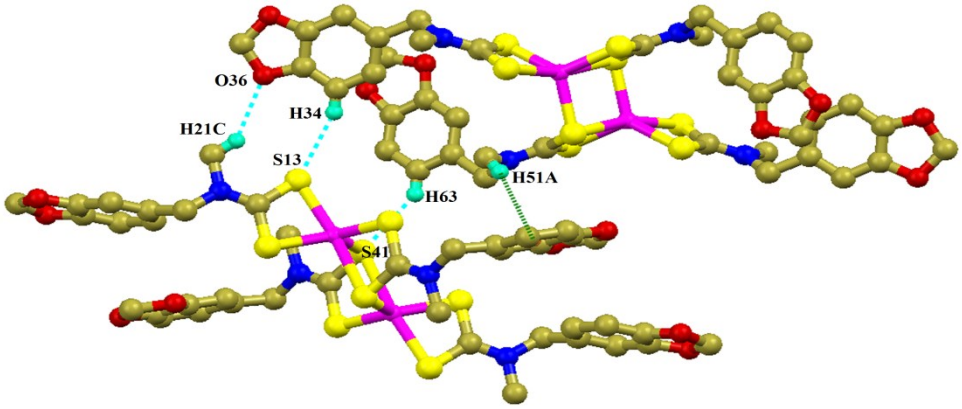


Figure S8. Supramolecular structure of **4** supported by C–H···O, C–H···S and C–H···π interactions.

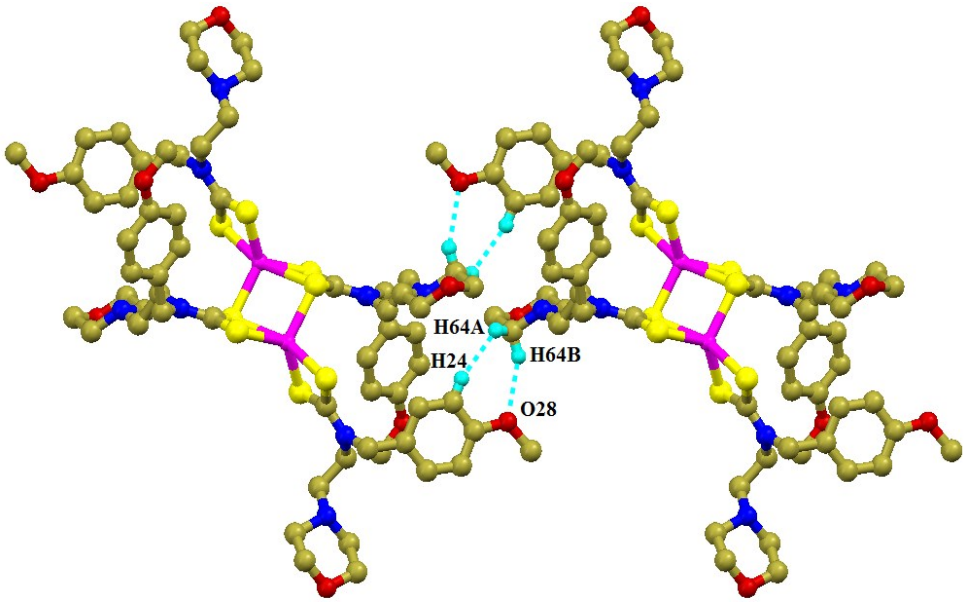


Figure S9. Supramolecular structure of **5** supported by C–H···H–C and C–H···O interactions.

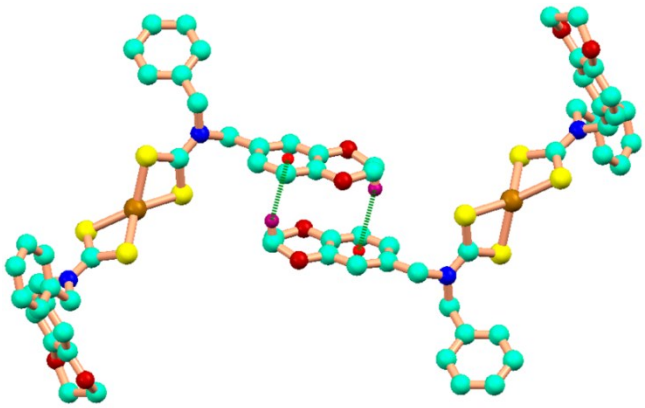


Figure S10. Supramolecular structure of **6** stabilished by C–H···π interactions.

PXRD patterns

The d-spacing observed at (2θ) 28.40, 47.63, 56.25 corresponds to the [111, 220, 311] planes of cubic ZnS for **2**; 31.67, 47.12, 56.46, 62.73, 67.90, [101, 110, 112, 202, 104] **3**; 26.84, 28.38, 30.44, 39.46, 47.75, 52.08, 56.44 [100, 002, 101, 102, 110, 103, 112] **4**; 26.21,28.83, 30.63, 4036, 47.93, 56.50 [100, 002, 101, 102, 110, 112] **5;** 28.47, 29.80, 56.46, 62.29 [002, 102, 112, 202] **6**, planes of hexagonal phase of zinc sulphide. In **1** the d-spacing observed at (2θ) 28.59, 30.98, 47.75, 56.87, 63.04 [002, 101, 110, 112, 202], correspond to hexagonal phase of zinc iron sulphide which is similar to zinc sulphide.

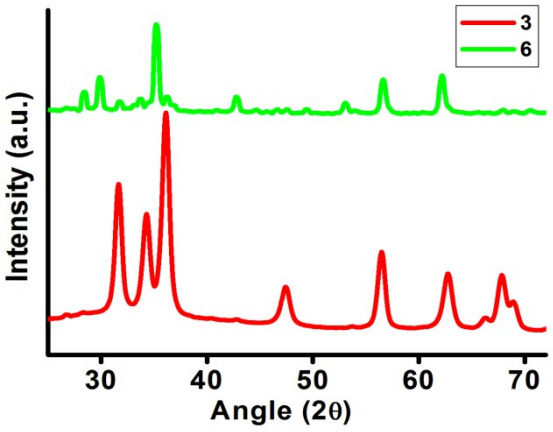
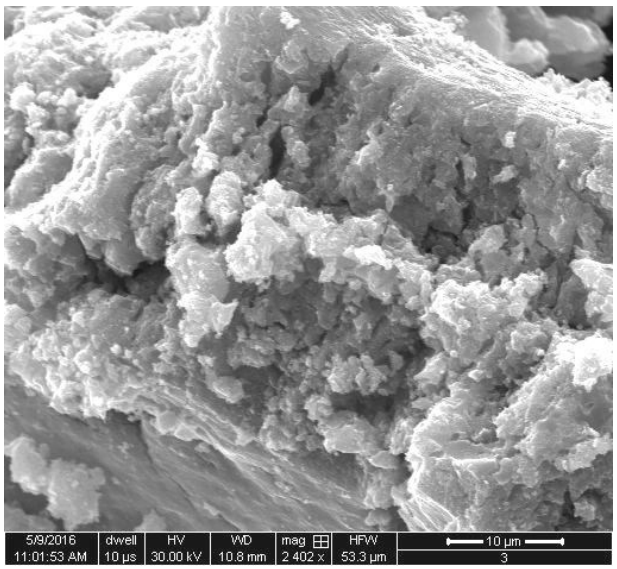
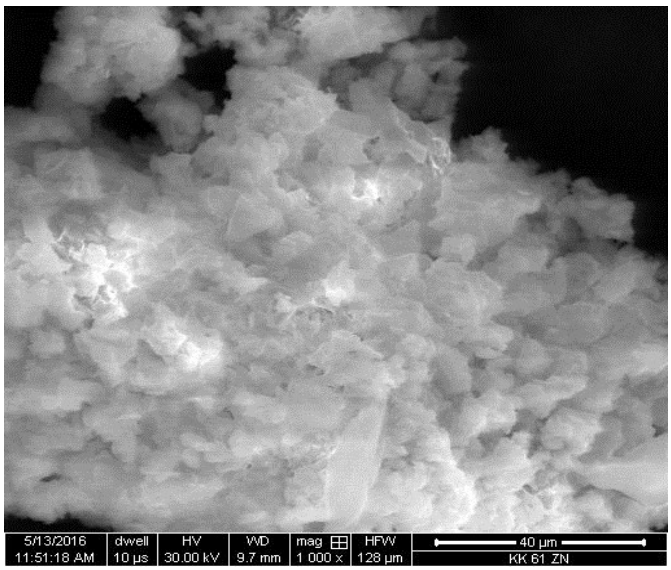
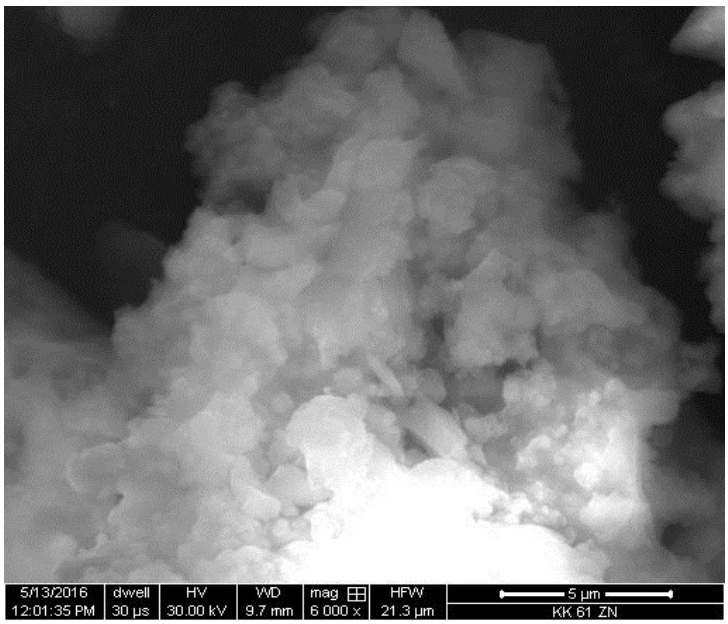


Figure S11. PXRD patterns of TG residue of **3** and **6**.



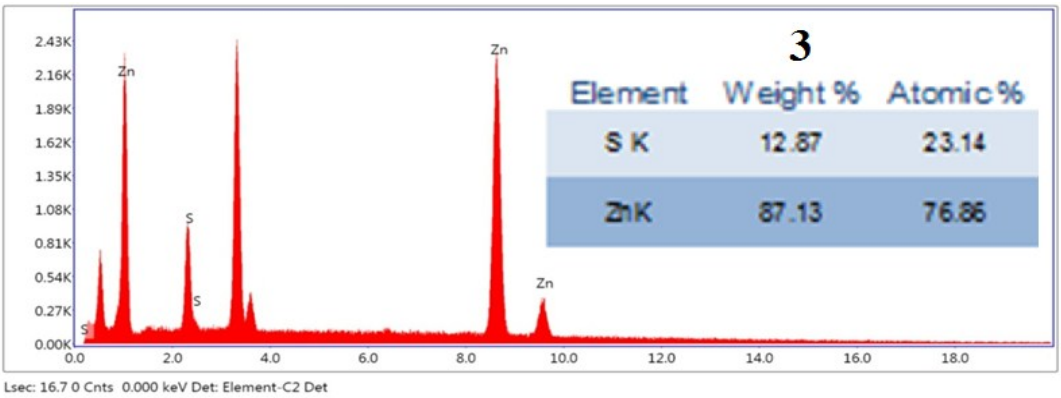


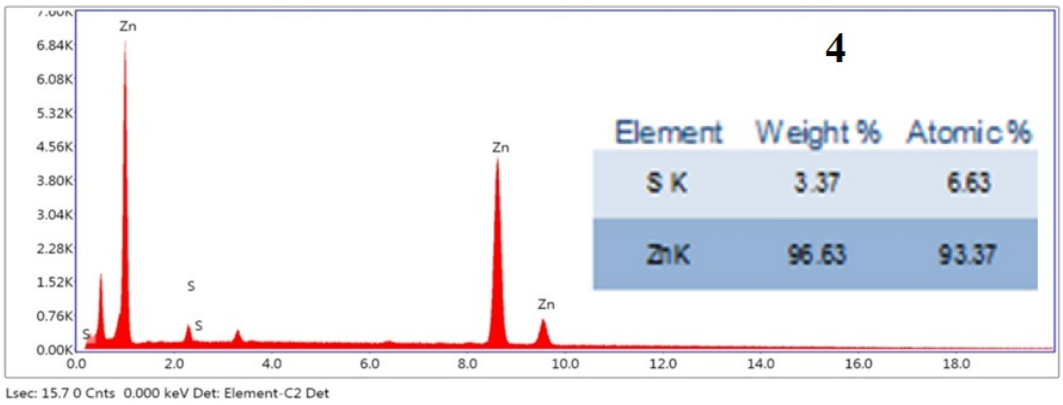
3 **5**

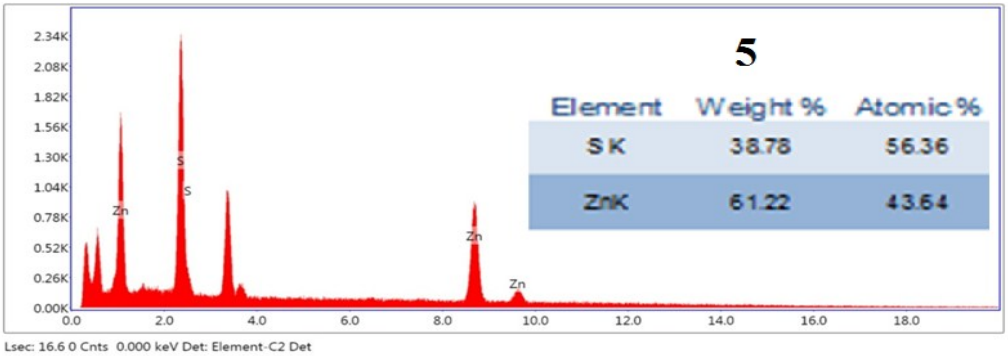


6

Figure S12. SEM images of and zinc sulfide (**3, 5** and **6)**.







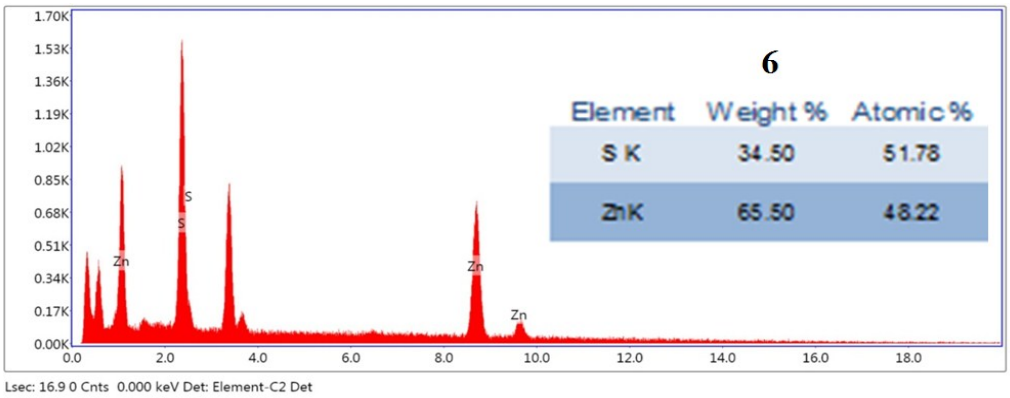


Figure S13. EDAX images of **3**-**6**.