Electronic Supplementary Material (ESI) for CrystEngComm.
This journal is © The Royal Society of Chemistry 2023

<Electronic Supplementary Information>

Single crystals of cyclodimeric zinc(II) complexes containing 9,10-bis((isoquinolin-5-yloxy)methyl)anthracene: reversible adsorption of targeting molecules and recognition of CH_2I_2 in SCSC mode

Gyeongwoo Kim, Jihun Han, Dongwon Kim, and Ok-Sang Jung*

Department of Chemistry, Pusan National University, Busan 46241, Republic of Korea Fax: (+82) 51-5163522; Tel: (+82) 51-5103240; E-mail: oksjung@pusan.ac.kr

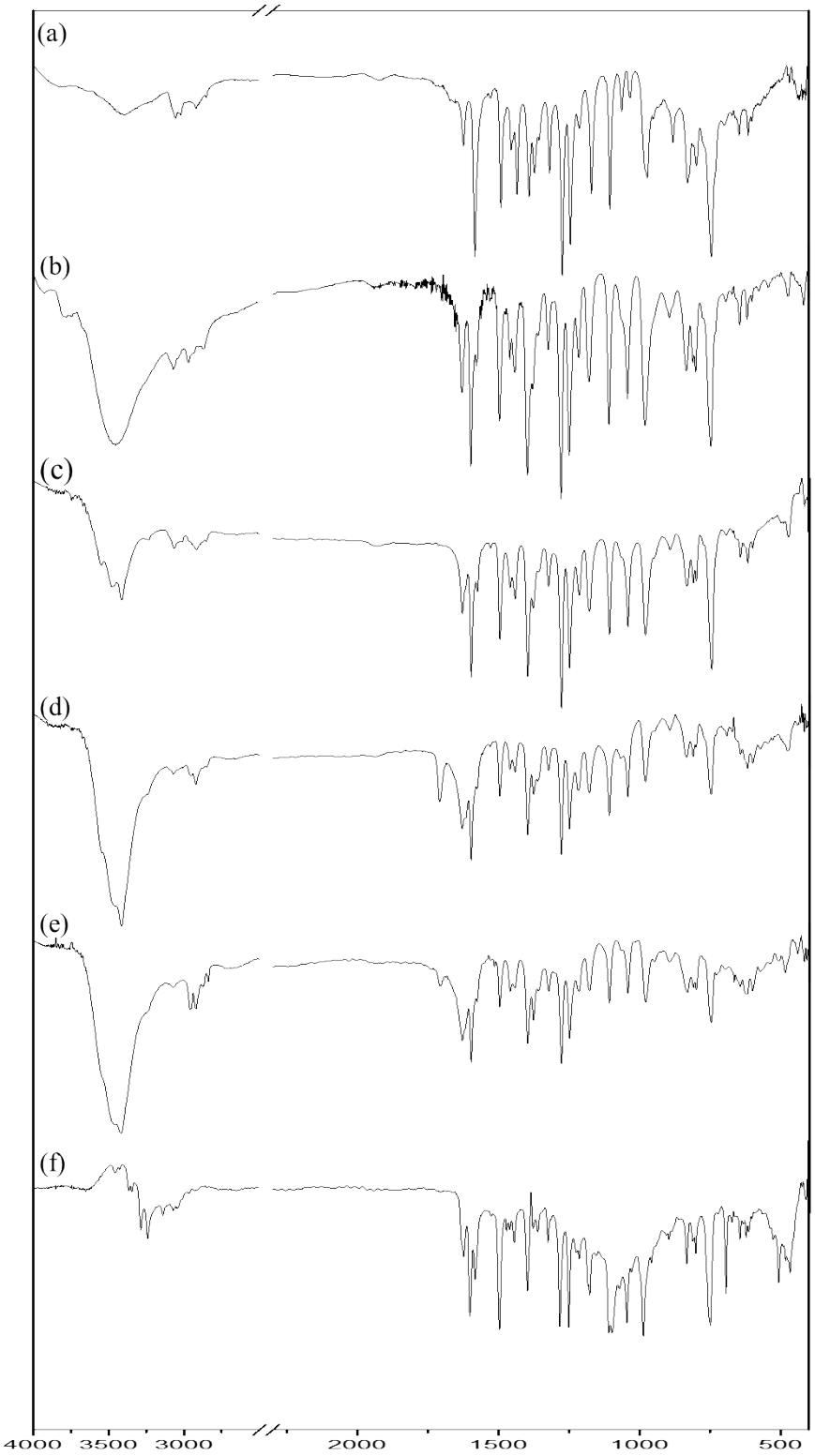

Fig. S1. IR spectra of L (a), $[ZnCl_2L]_2 \cdot 5C_4H_8O$ (b), $[ZnCl_2L]_2 \cdot 4o\text{-X} \cdot 2C_4H_8O \cdot 0.5CH_2Cl_2$ (c), $[ZnCl_2L]_2 \cdot 4m\text{-X}$ (d), $[ZnCl_2L]_2 \cdot 4p\text{-X}$ (e), and $[Zn_2Cl_4L(C_6H_5NH_2)_2] \cdot 2C_6H_5NH_2$ (f).

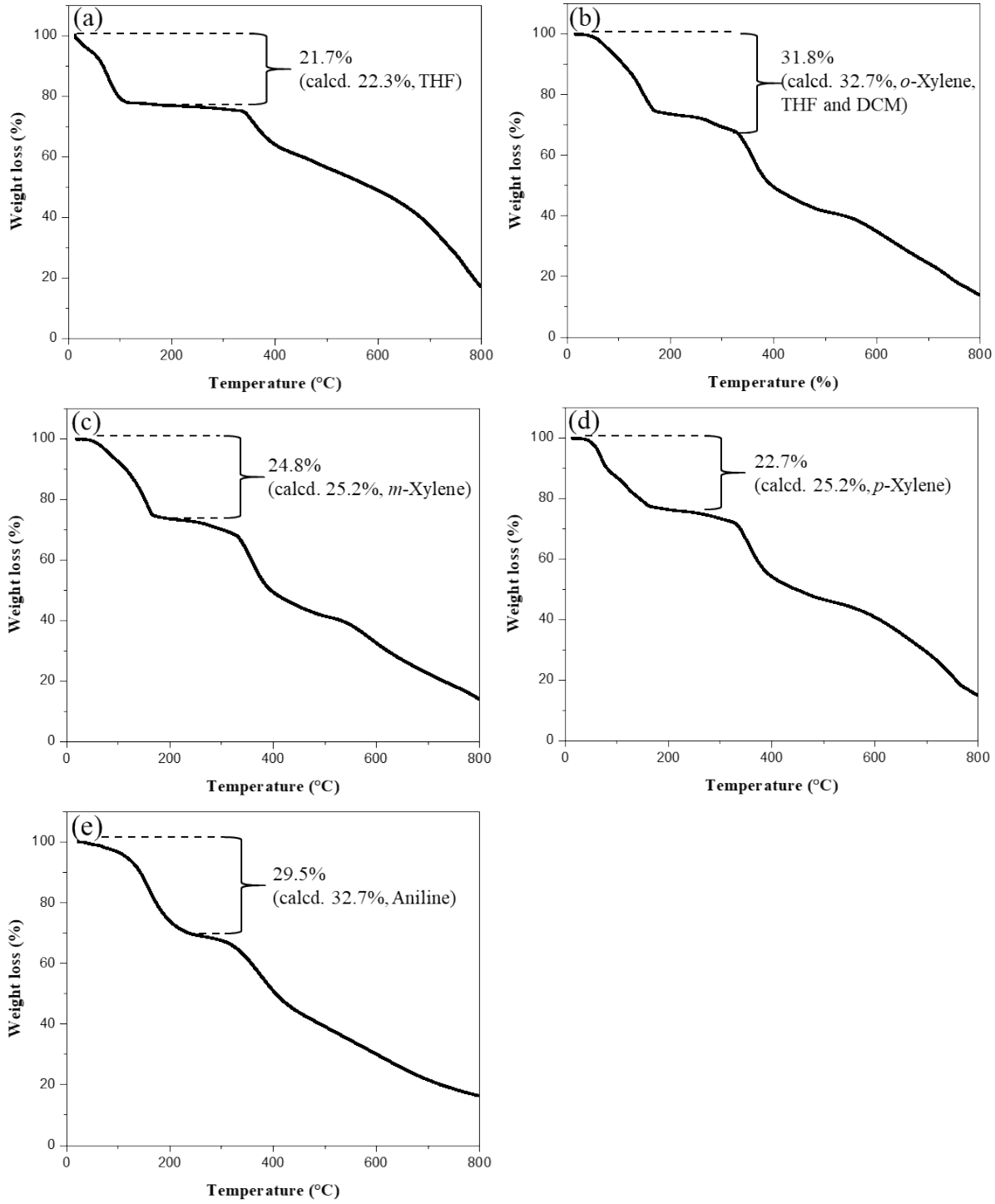

Fig. S2. TG curves of $[ZnCl_2L]_2 \cdot 5C_4H_8O$ (a), $[ZnCl_2L]_2 \cdot 4o\text{-X} \cdot 2C_4H_8O \cdot 0.5CH_2Cl_2$ (b), $[ZnCl_2L]_2 \cdot 4m\text{-X}$ (c), $[ZnCl_2L]_2 \cdot 4p\text{-X}$ (d), and $[Zn_2Cl_4L(C_6H_5NH_2)_2] \cdot 2C_6H_5NH_2$ (e).

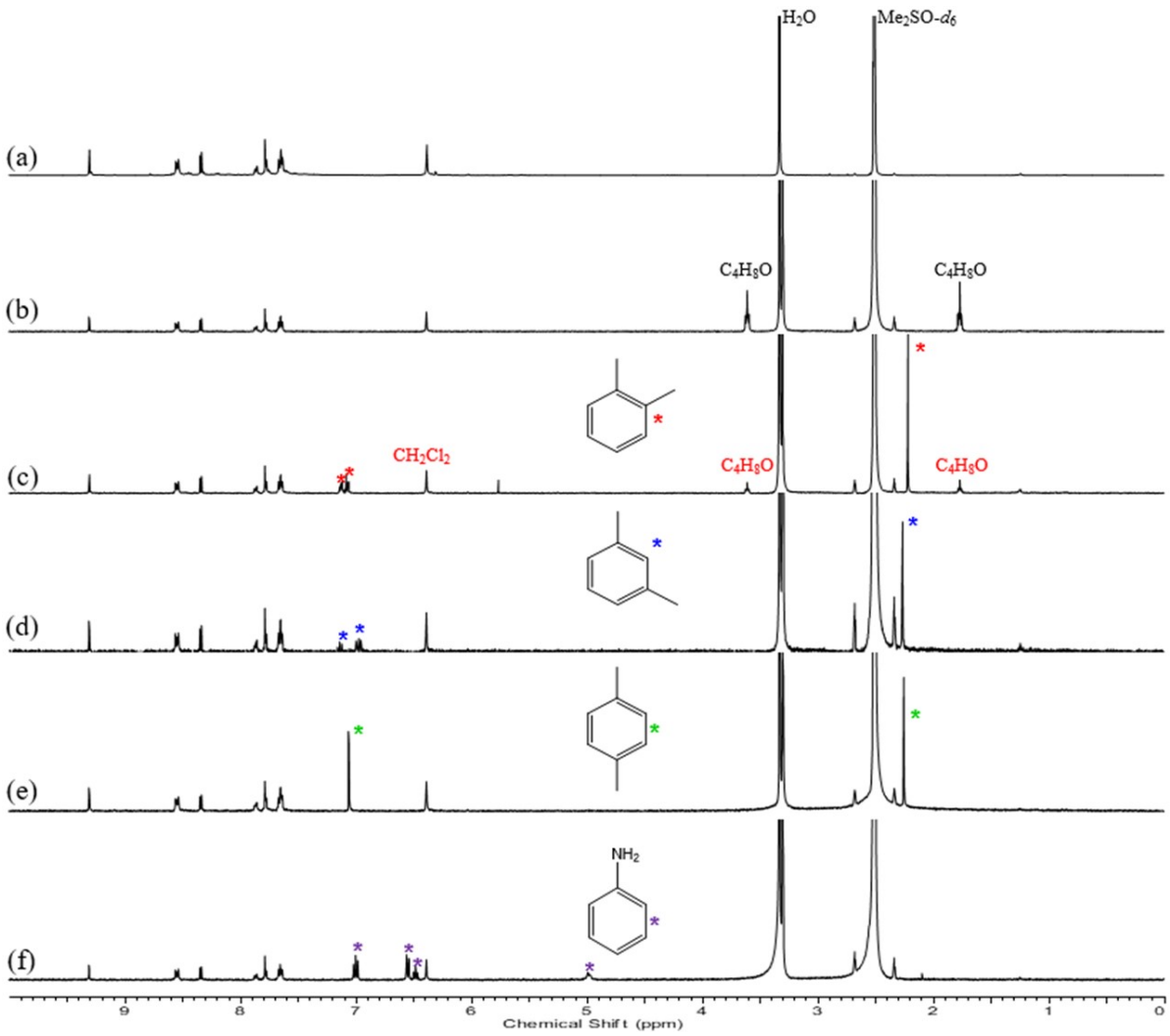

Fig. S3. ^{1}H NMR spectra (dissociated in Me_2SO-d^6) of L (a), $[ZnCl_2L]_2 \cdot 5C_4H_8O$ (b), $[ZnCl_2L]_2 \cdot 4o\text{-}X \cdot 2C_4H_8O \cdot 0.5CH_2Cl_2$ (c), $[ZnCl_2L]_2 \cdot 4m\text{-}X$ (d), $[ZnCl_2L]_2 \cdot 4p\text{-}X$ (e), and $[Zn_2Cl_4L(C_6H_5NH_2)_2] \cdot 2C_6H_5NH_2$ (f).

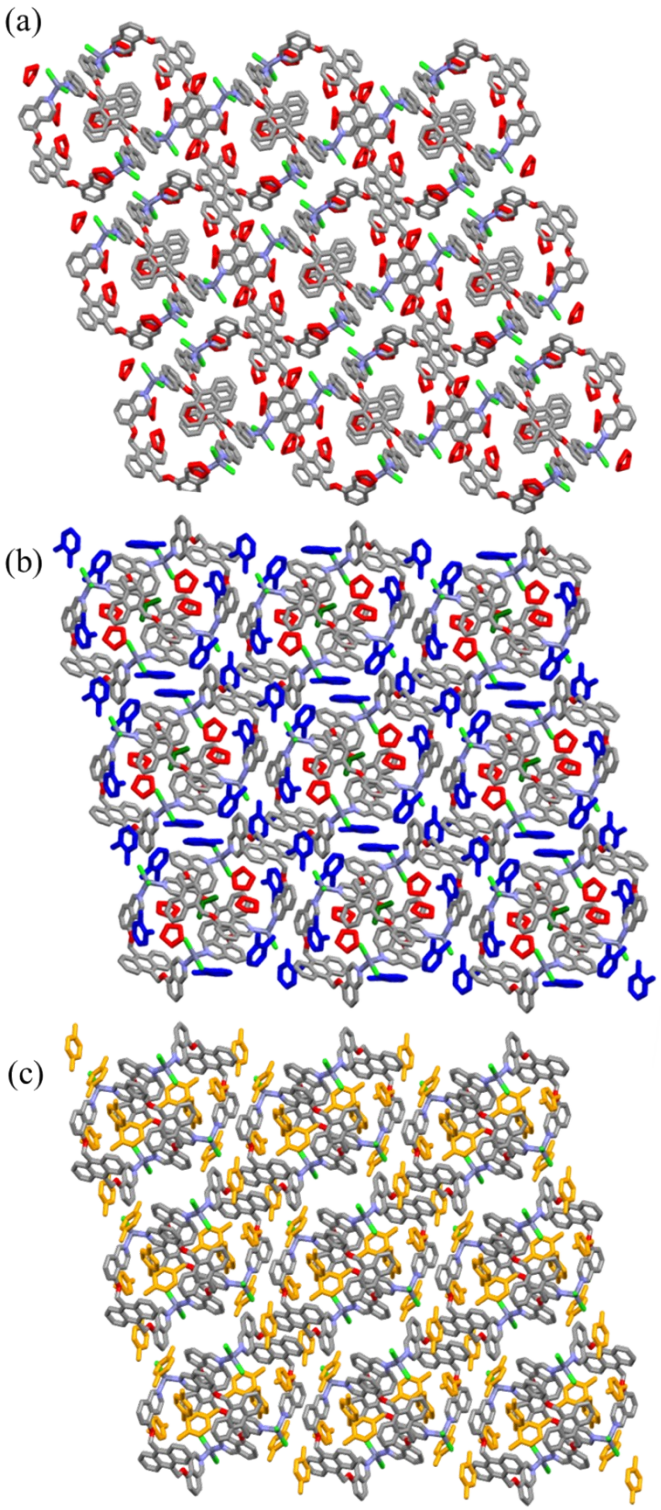

Fig. S4. Packing structures of $[ZnCl_2L]_2 \cdot 5C_4H_8O$ (a), $[ZnCl_2L]_2 \cdot 4o\text{-X} \cdot 2C_4H_8O \cdot 0.5CH_2Cl_2$ (b), and $[ZnCl_2L]_2 \cdot 4p\text{-X}$ (c). C_4H_8O (red), CH_2Cl_2 (green), *o*-X (blue), and *p*-X (yellow).

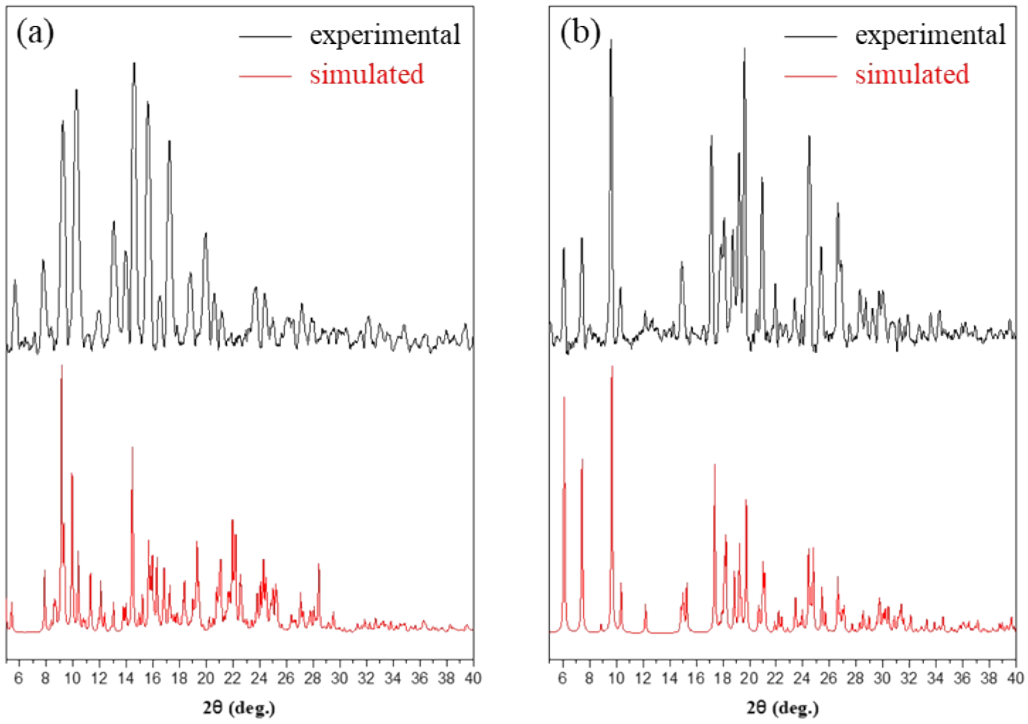

Fig. S5. PXRD patterns of $[ZnCl_2L]_2 \cdot 5C_4H_8O$ (a) and $[Zn_2Cl_4L(C_6H_5NH_2)_2] \cdot 2C_6H_5NH_2$ (b).

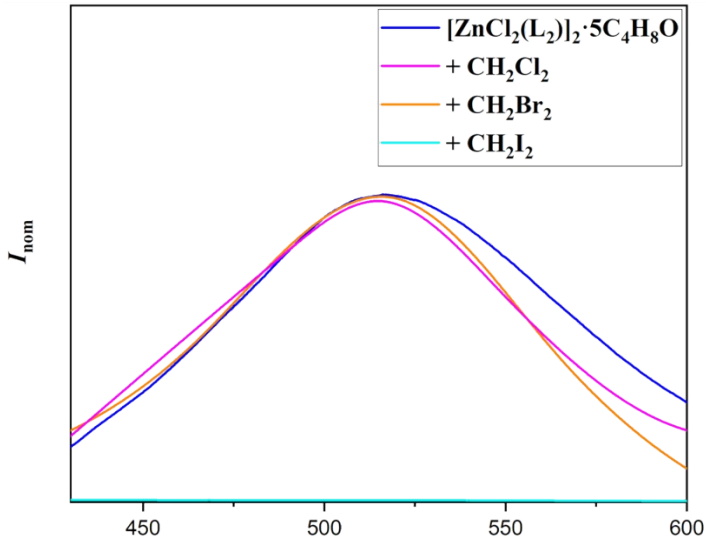

Fig. S6. Solid PL spectra at λ_{ex} = 350 nm of crystals of $[ZnCl_2L]_2 \cdot 5C_4H_8O$ (blue line), the crystals + one drop (20 μL) of the CH_2Cl_2 (pink line), the crystals + one drop of the CH_2Br_2 (orange line), and the crystals + one drop of the CH_2I_2 (sky blue line).