SUPPLEMENTARY MATERIAL

Fluorescence studies and photocatalytic application for hydrogen production of Zn^{II} and Cd^{II} complexes with isophthaloylbis(thioureas)

Vânia Denise Schwade [a,*], Estefane Isis Teixeira [b], Fábio Alencar dos Santos [b], Tanize Bortolotto [a], Bárbara Tirloni [a], Ulrich Abram [c]

[a] Department of Chemistry, Natural and Exact Sciences Centre, Federal University of Santa Maria, Av. Roraima, n.1000, 97105-900, Santa Maria/RS, Brazil

[b] Faculty of Exact Sciences and Technology, Federal University of Grande Dourados, Rod. Dourados/Itahum, Km 12, 79804-970, Dourados/MS, Brazil

[c] Institute of Chemistry and Biochemistry, Freie Universität Berlin, Fabeckstr. 34-36, D-14195, Berlin, Germany

Corresponding author

* vaniaschwade@gmail.com and vania.schwade@ufsm.br

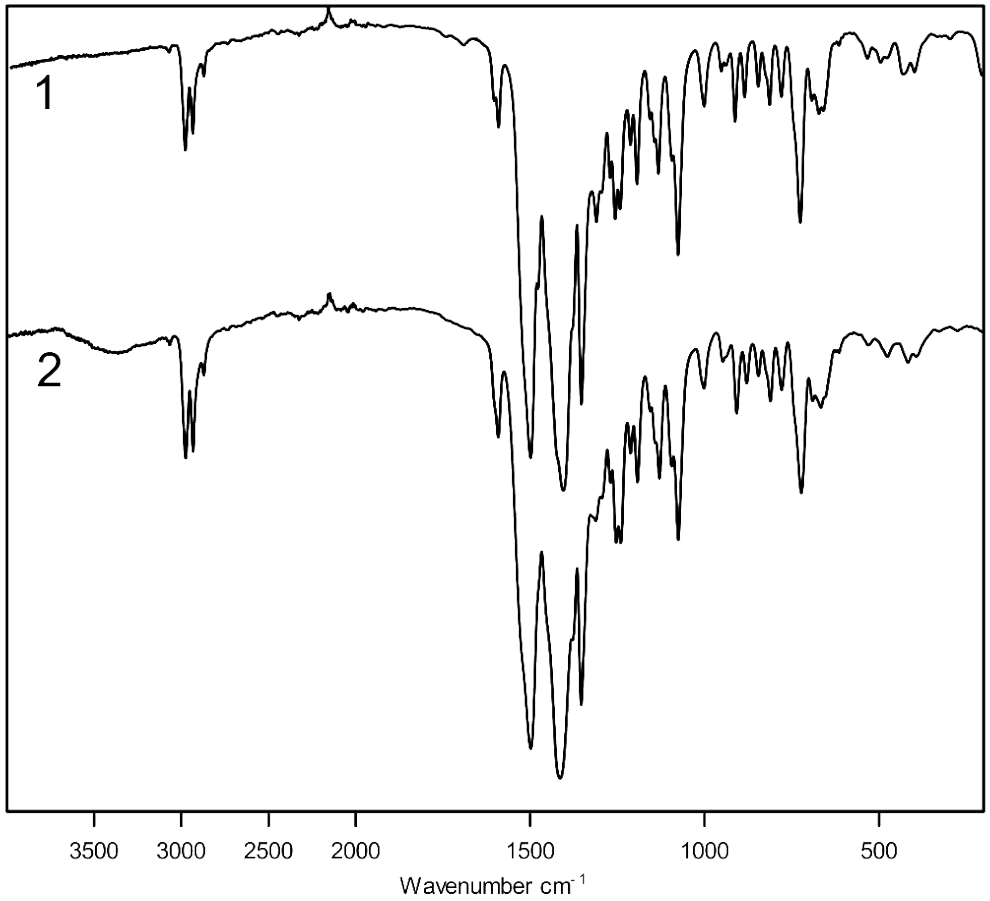

Figure S1. FT-IR spectra of compounds **1** and **2** in the 4000–200 cm^{-1} range.

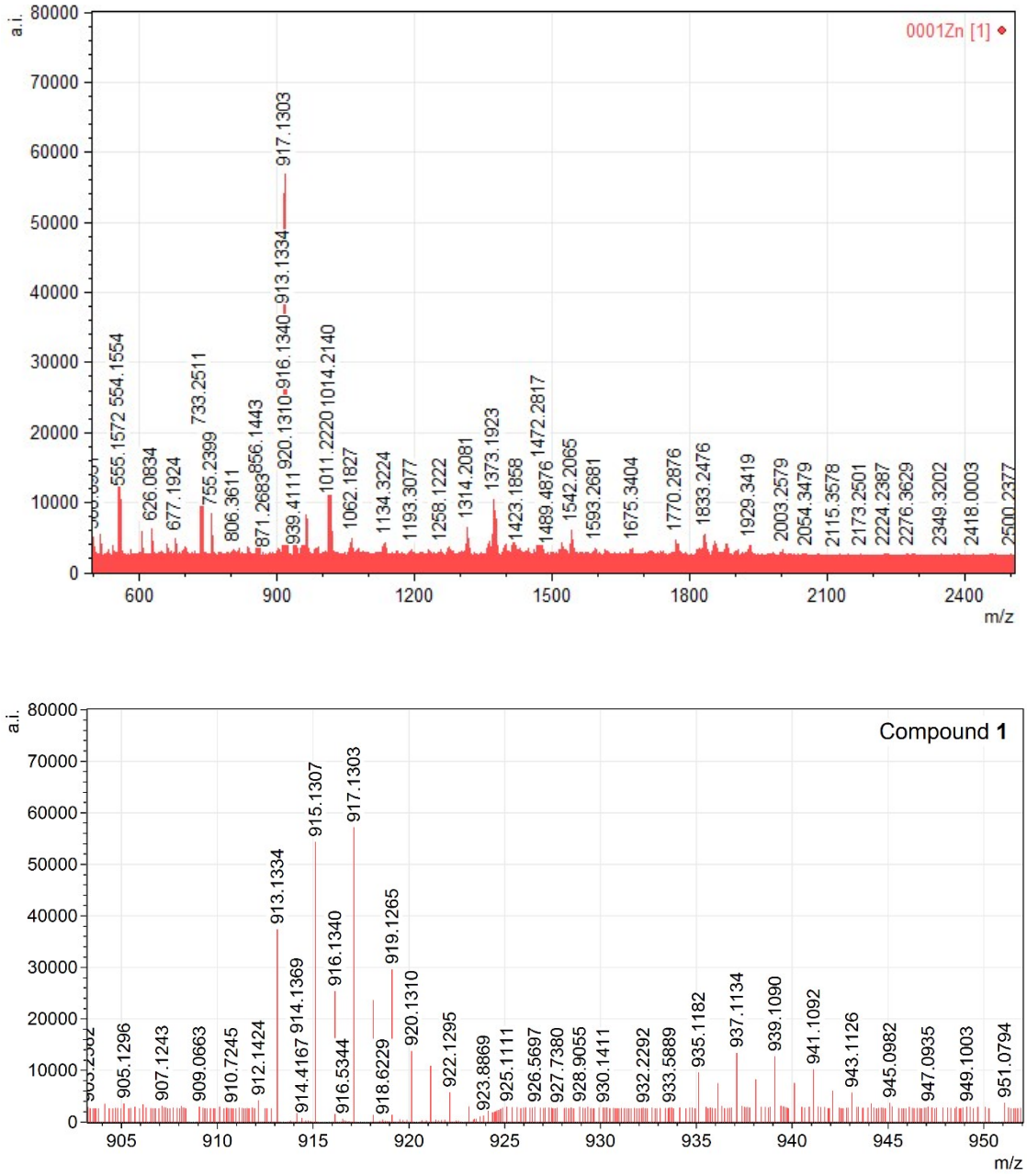

Figure S2. ESI-MS spectrum of compound **1** in the positive mode.

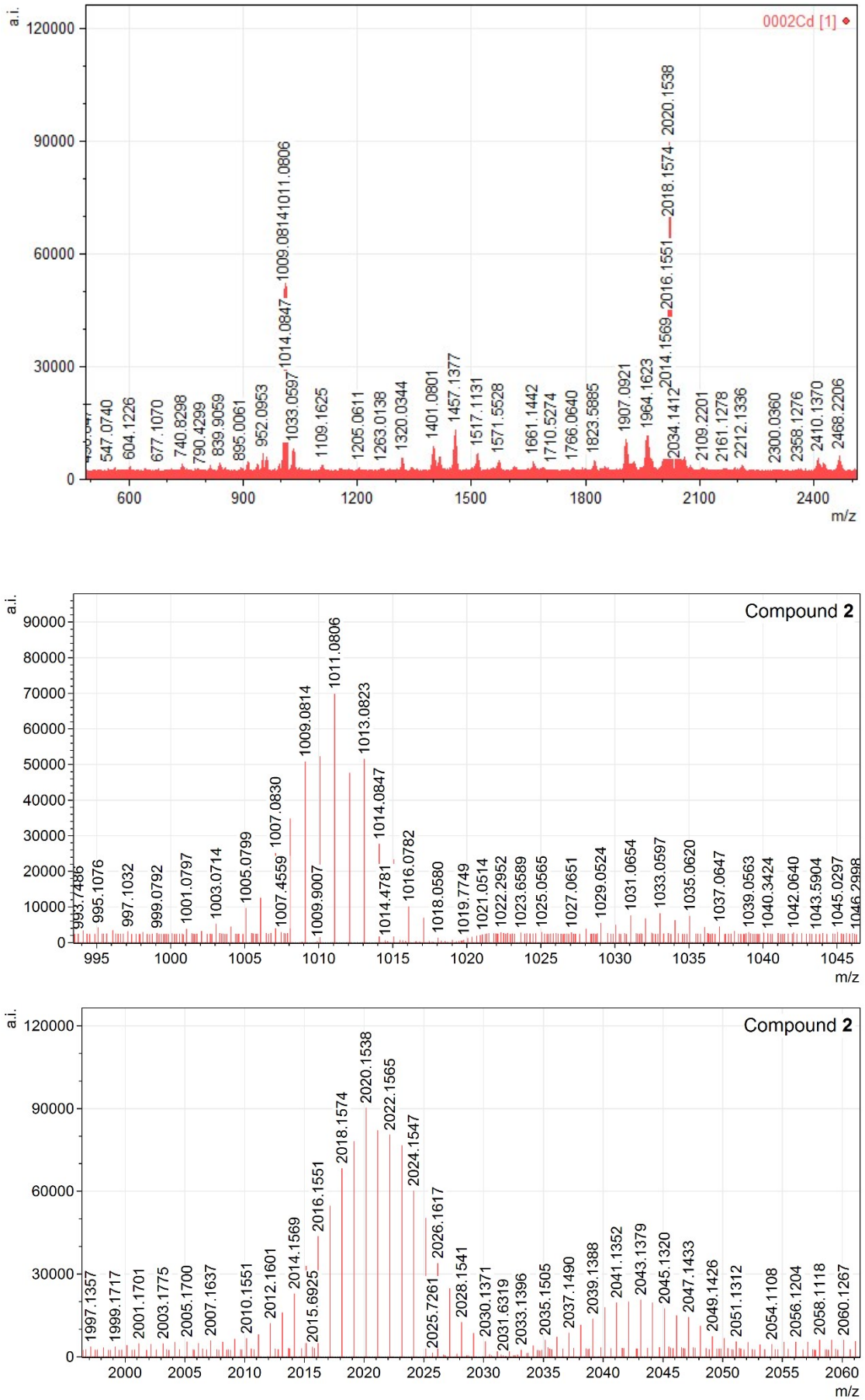

Figure S3. ESI-MS spectrum of compound **2** in the positive mode.

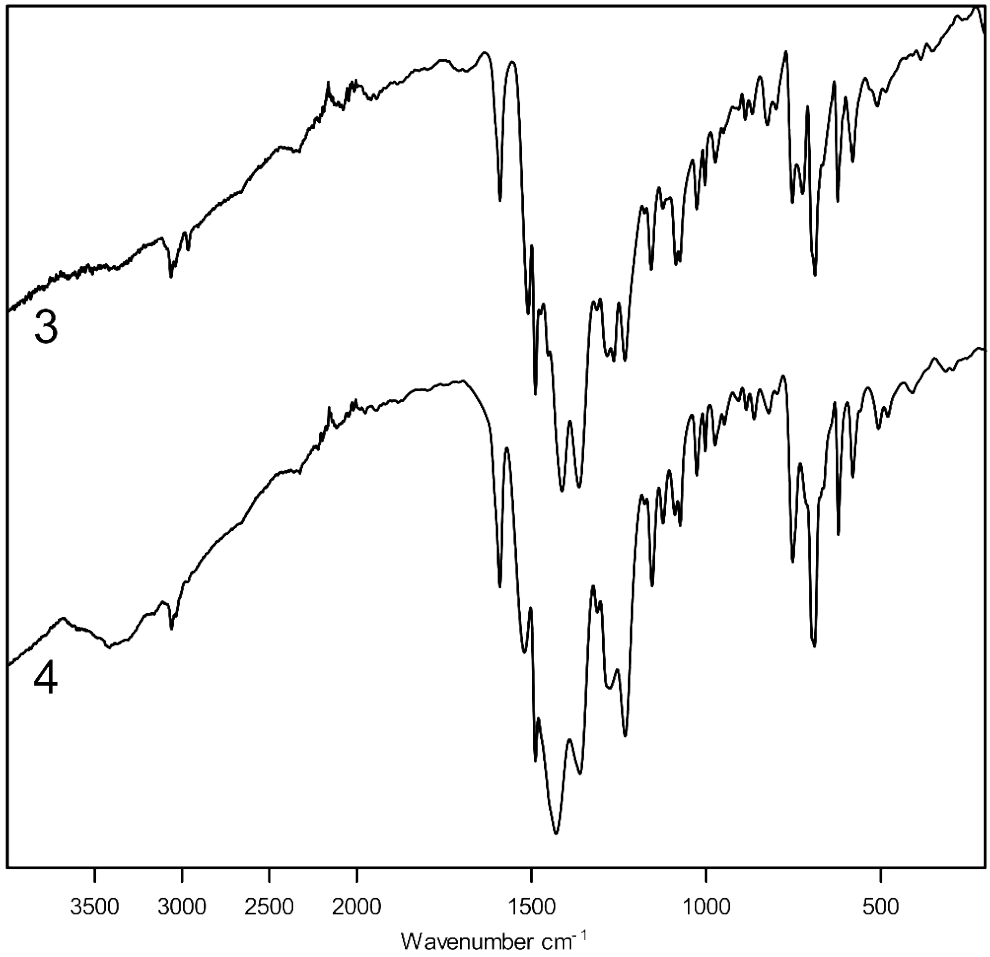

Figure S4. FT-IR spectra of compounds **3** and **4** in the 4000–200 cm^{-1} range.

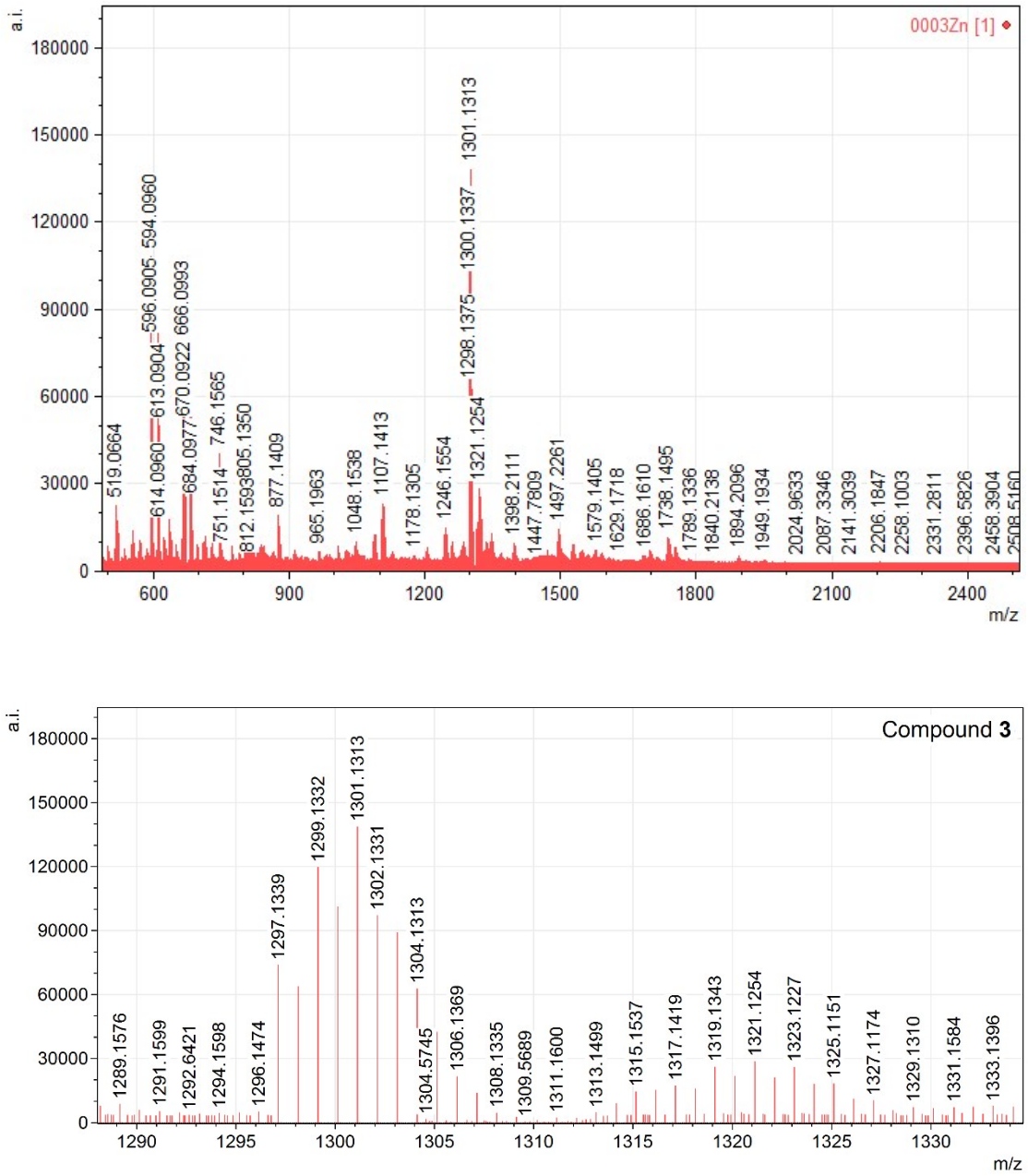

Figure S5. ESI-MS spectrum of compound **3** in the positive mode.

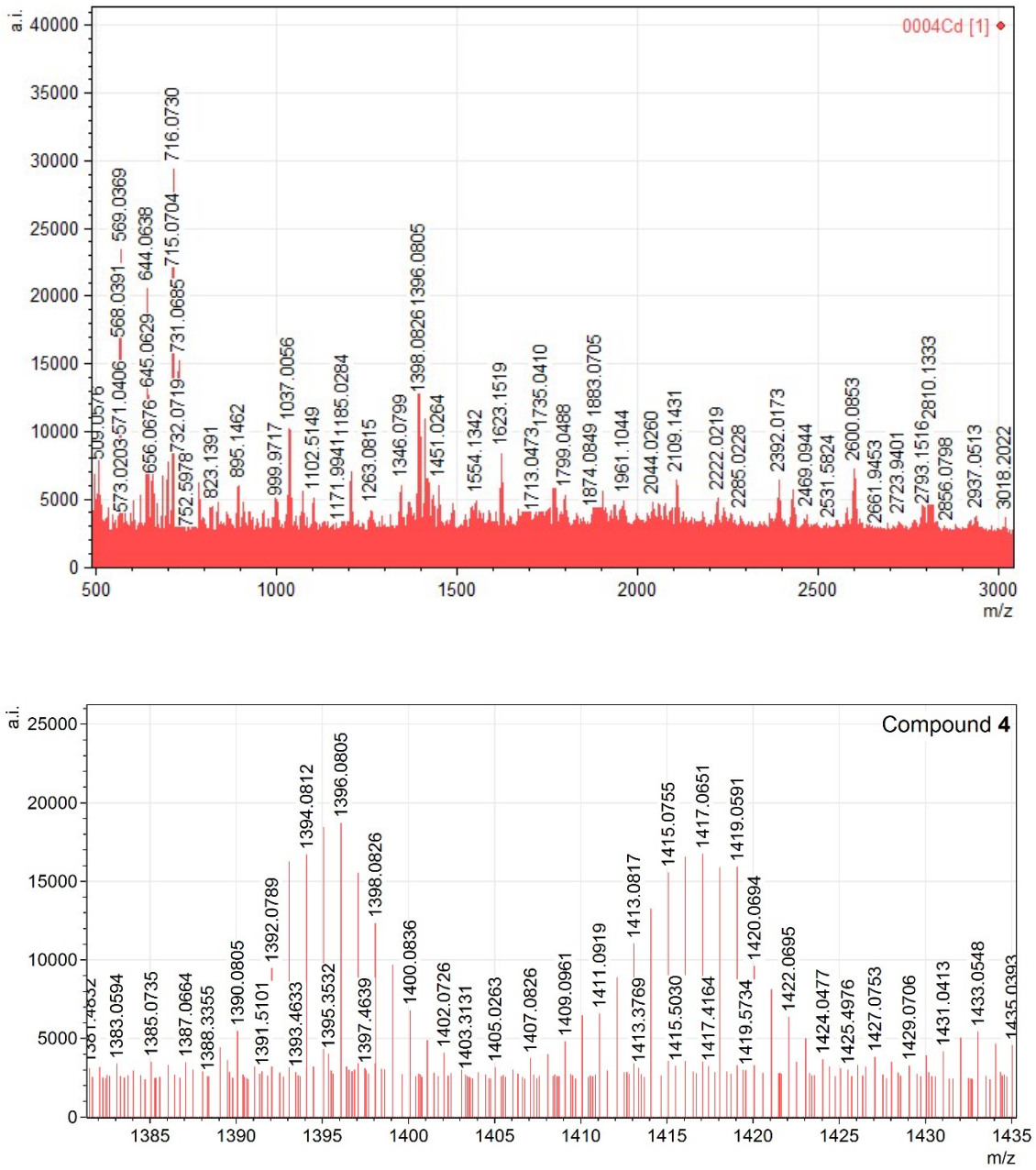

Figure S6. ESI-MS spectrum of compound **4** in the positive mode.

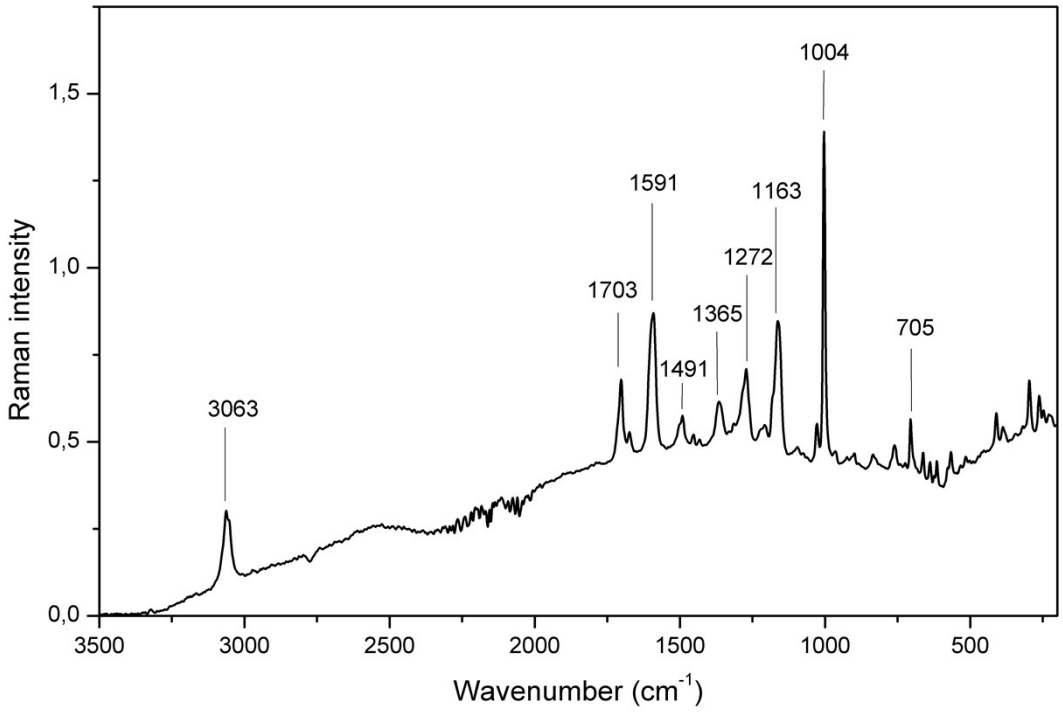

Figure S7. Raman spectrum of H_2L^{Ph} in the 3500–200 cm^{-1} range.

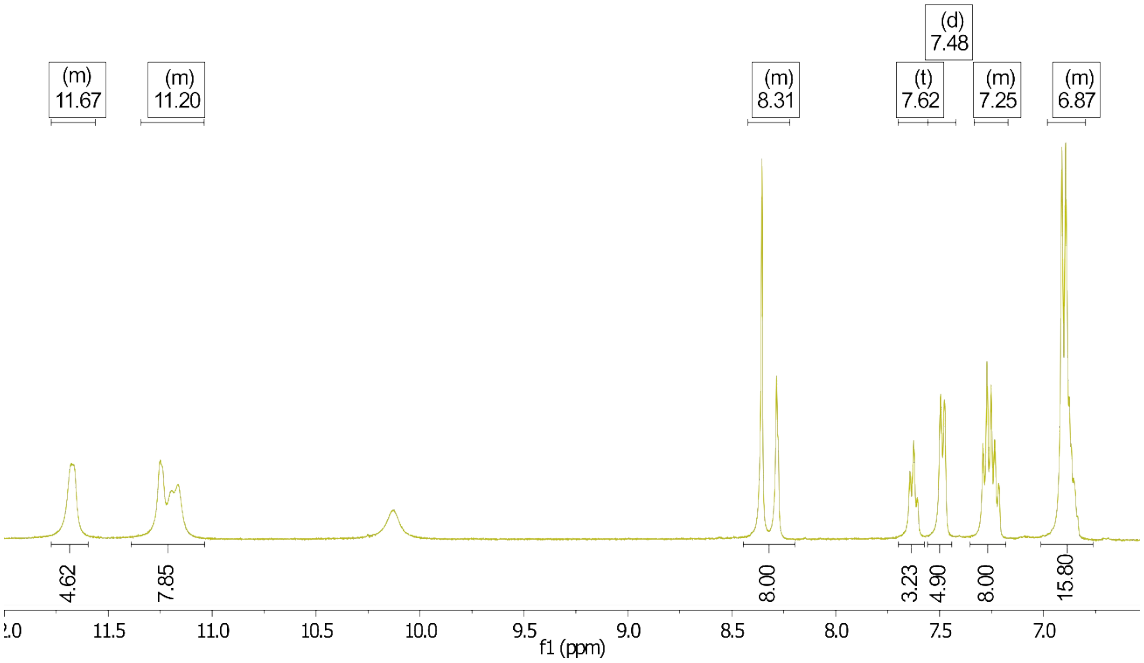

Figure S8. ^1H NMR spectrum of complex **3** in DMSO-d_6.

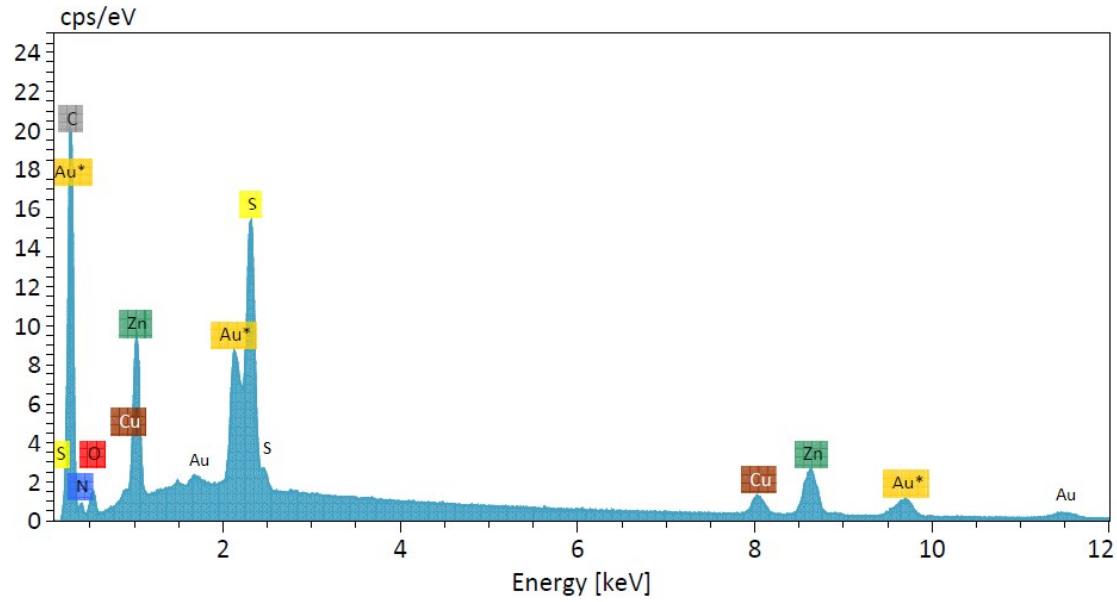

Figure S9. EDS spectrum of the **[$Zn_2(L^{Et})_2$]** compound. The elements Cu and Au come from the stub and the metallization process, respectively.

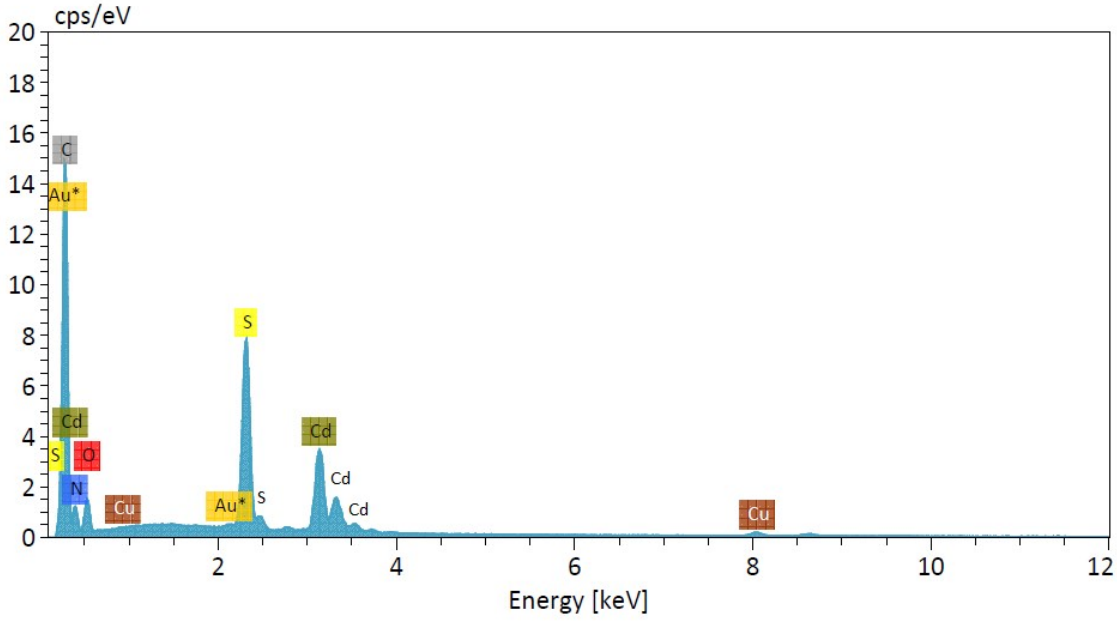

Figure S10. EDS spectrum of the **[$Cd_2(L^{Et})_2$]** compound. The elements Cu and Au come from the stub and the metallization process, respectively.

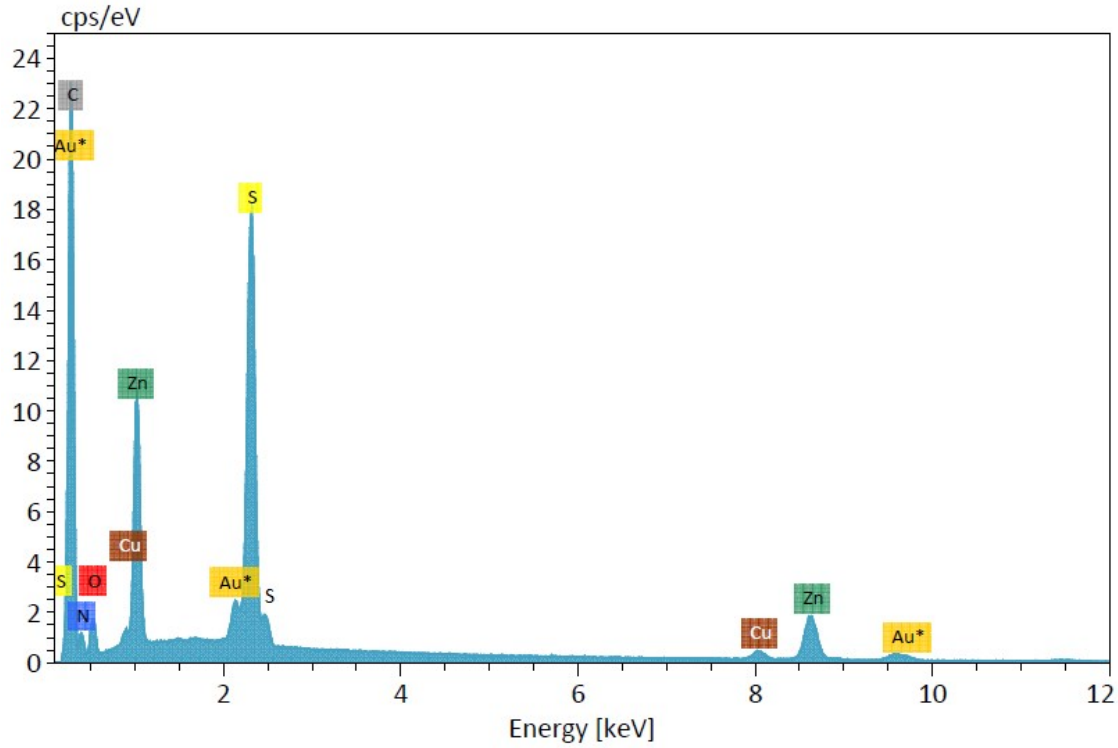

Figure S11. EDS spectrum of the **[Zn(HL^{Ph})$_2$(H$_2$O)]** compound. The elements Cu and Au come from the stub and the metallization process, respectively.

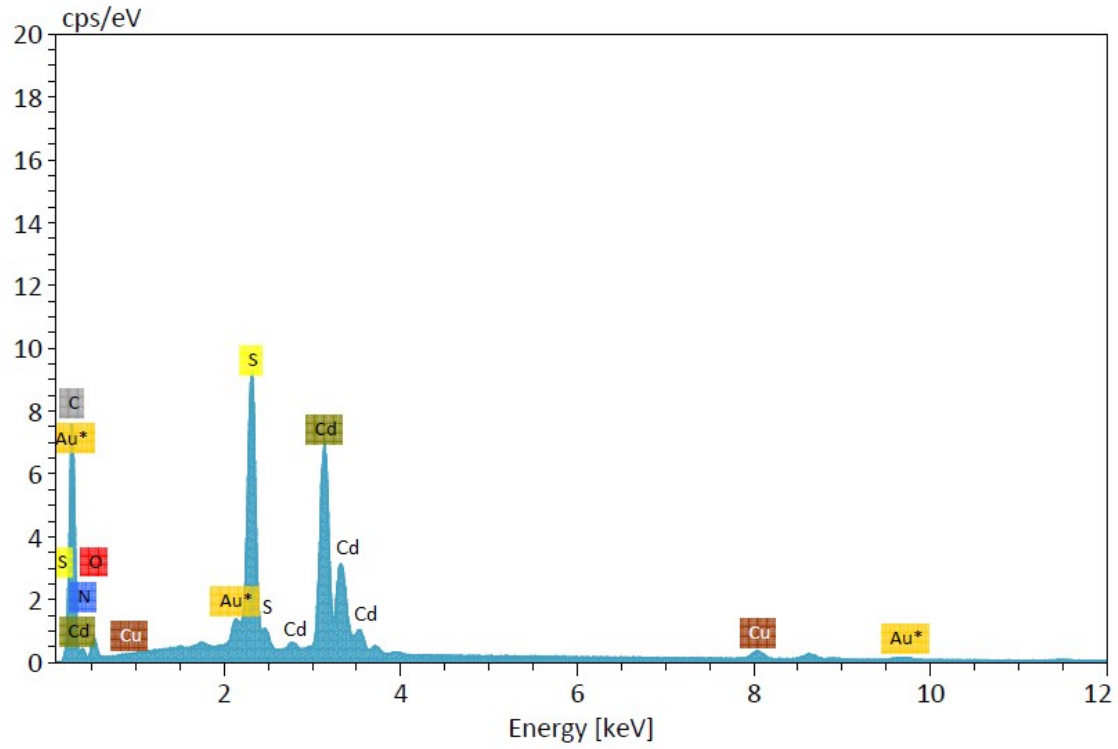

Figure S12. EDS spectrum of the **[Cd$_2$(L^{Ph})$_2$]** compound. The elements Cu and Au come from the stub and the metallization process, respectively.

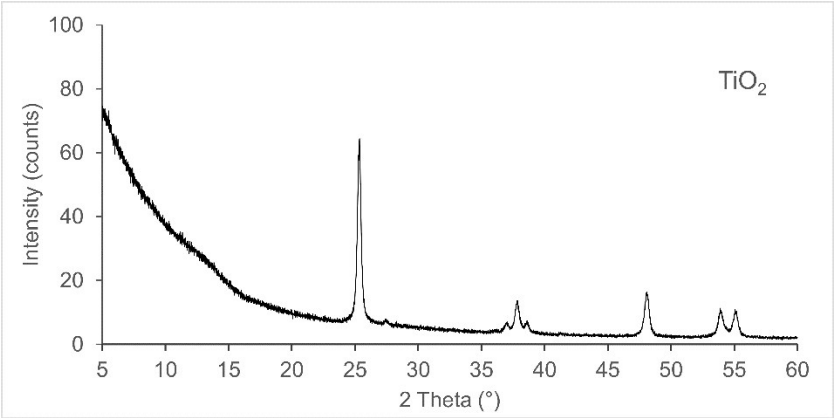

Figure S13. PXRD diffractogram of the prepared TiO_2.

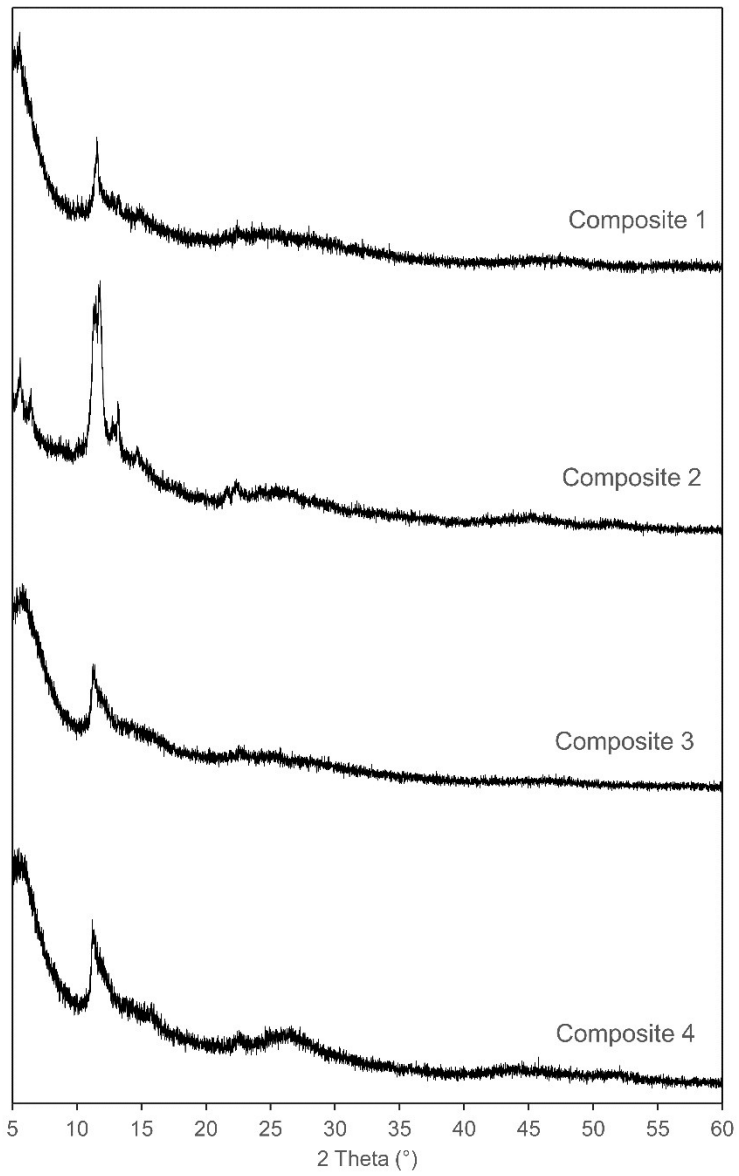

Figure S14. PXRD diffractograms of composites TiO_2**-1**–TiO_2**-4** using acrylic sample holder.

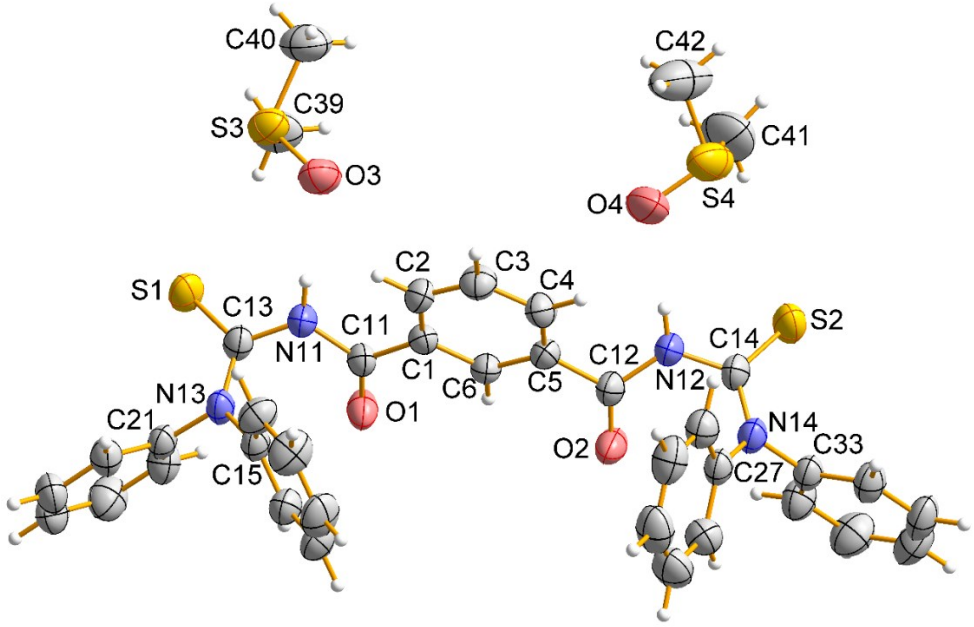

Figure S15. Anisotropic thermal ellipsoids plot at 50% probability of the H_2L^{Ph} ligand as a dimethyl sulfoxide solvate crystallization.

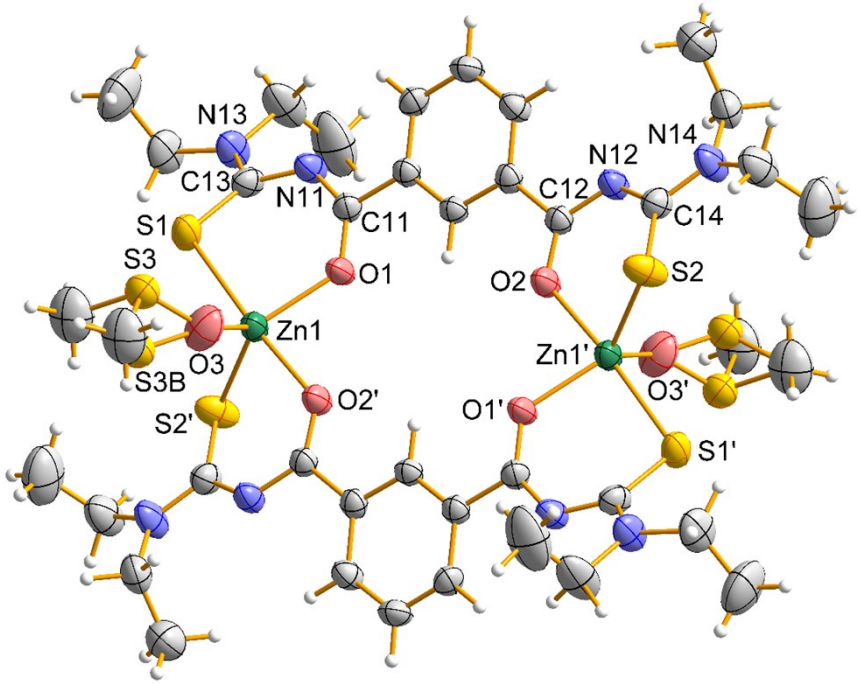

Figure S16. Anisotropic thermal ellipsoids plot at 50% probability of **[$Zn_2(L^{Et})_2(dmso)_2$]** (adduct of complex **1**). The coordinated dimethyl sulfoxide molecule is disordered at the sulfur atom (S3/S3B). Symmetry code: ' $-x+1, -y+2, -z+1$.

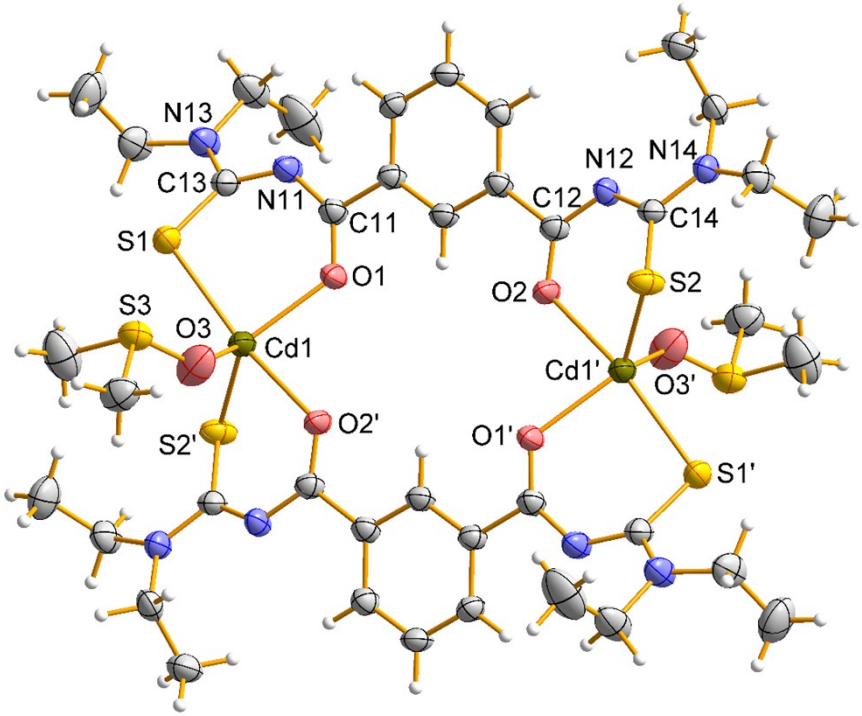

Figure S17. Anisotropic thermal ellipsoids plot at 50% probability of **[$Cd_2(L^{Et})_2(dmso)_2$]** (adduct of complex **2**). Symmetry code: ‘ –*x*+1, –*y*+1, –*z*+1.

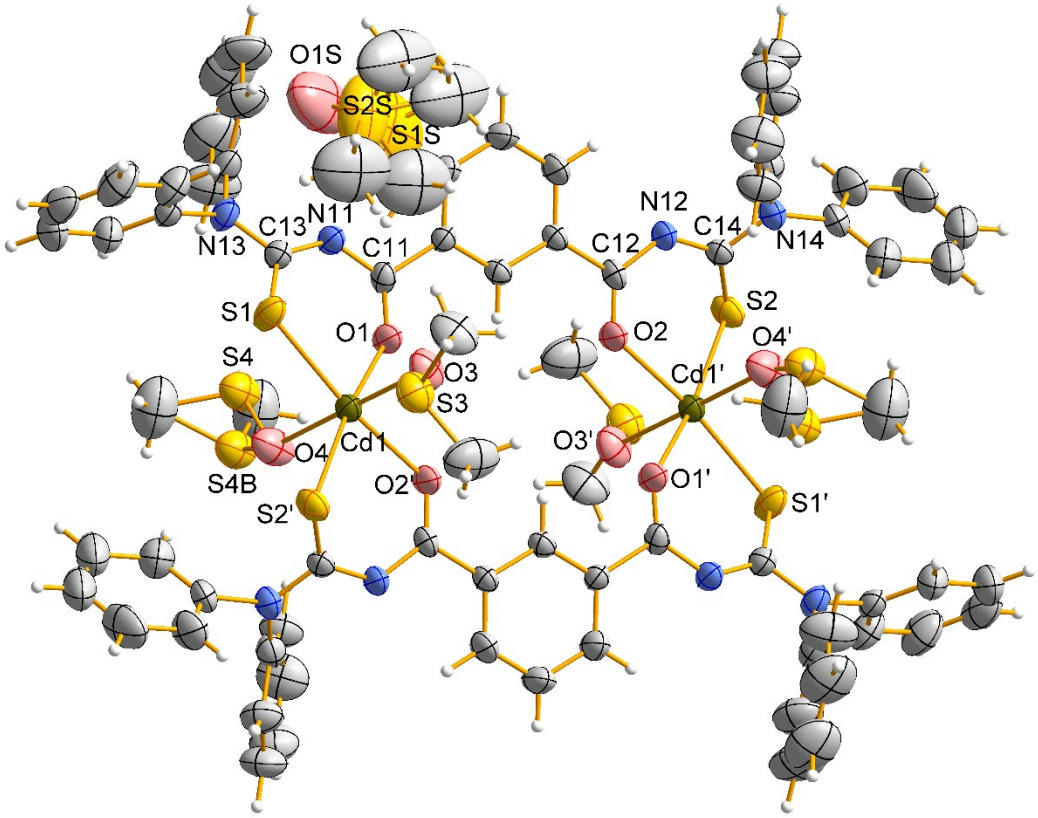

Figure S18. Anisotropic thermal ellipsoids plot at 50% probability of **[$Cd_2(L^{Ph})_2(dmso)_4$]·2DMSO** (adduct of complex **4**). One of the coordinated dimethyl sulfoxide molecules is disordered at the sulfur atom (S4/S4B). The solvate dimethyl sulfoxide molecule is fully disordered. Symmetry code: ‘ –*x*+1, –*y*+1, –*z*+1.

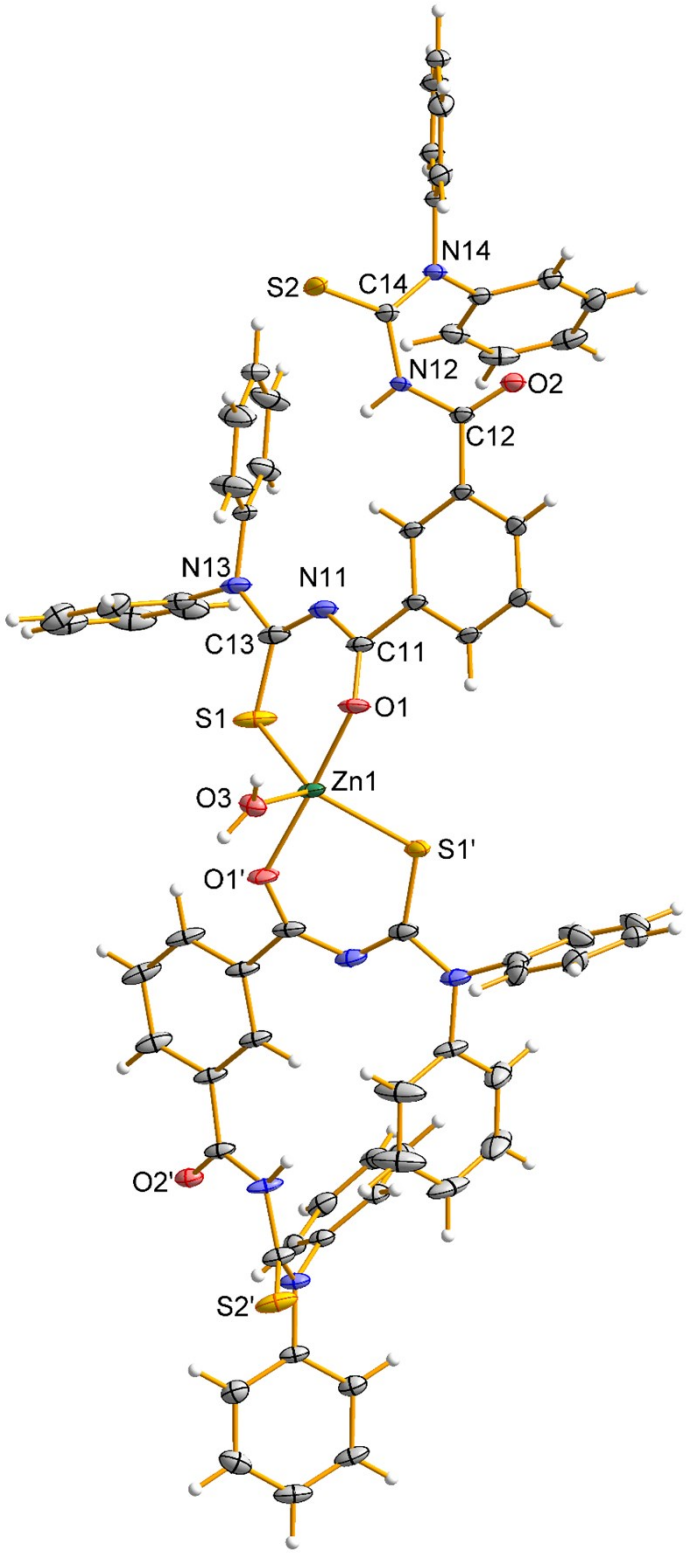

Figure S19. Anisotropic thermal ellipsoids plot at 50% probability of **[Zn(HL^{Ph})$_2$(H$_2$O)]**. Symmetry code: ‘ –*x*+1, *y*, –*z*+3/2.