Electronic Supplementary Material (ESI) for CrystEngComm.

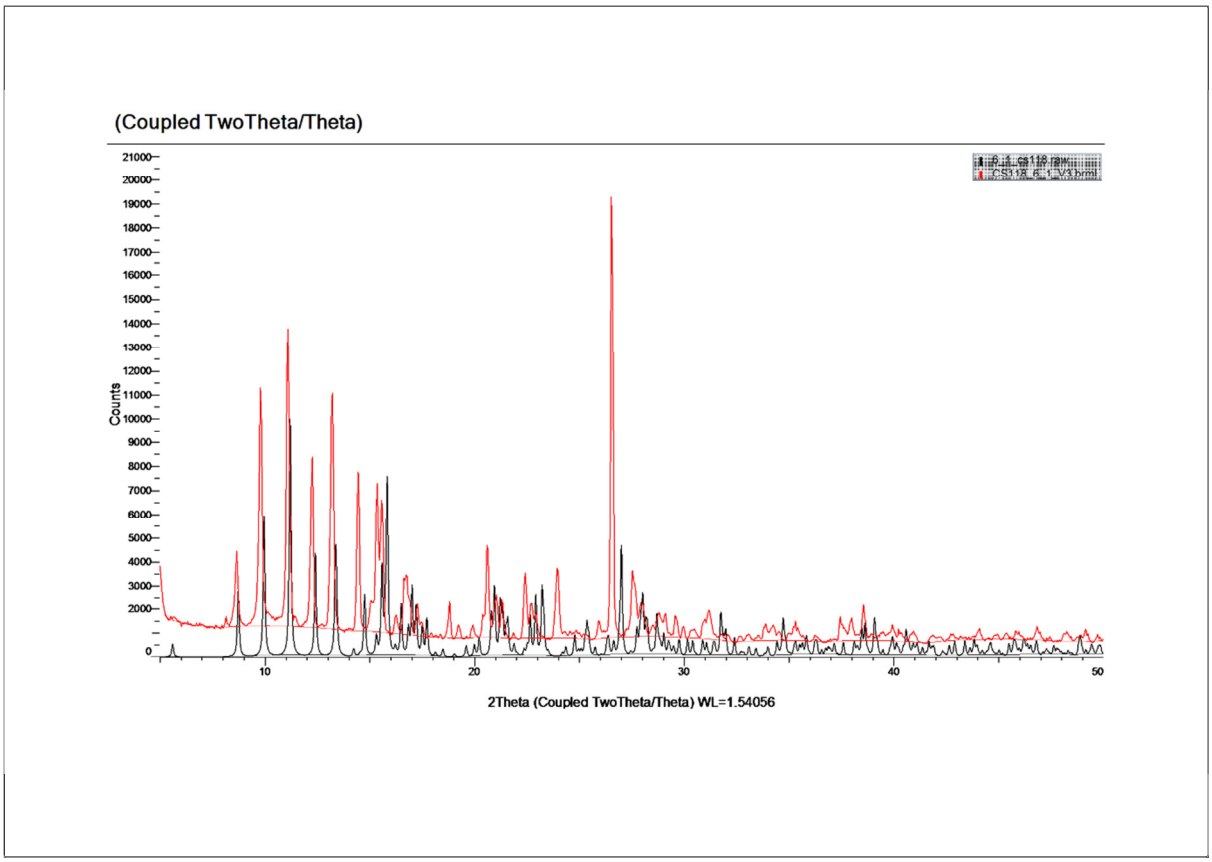
Supplementary Material

Experimental and Simulated Powder Patterns

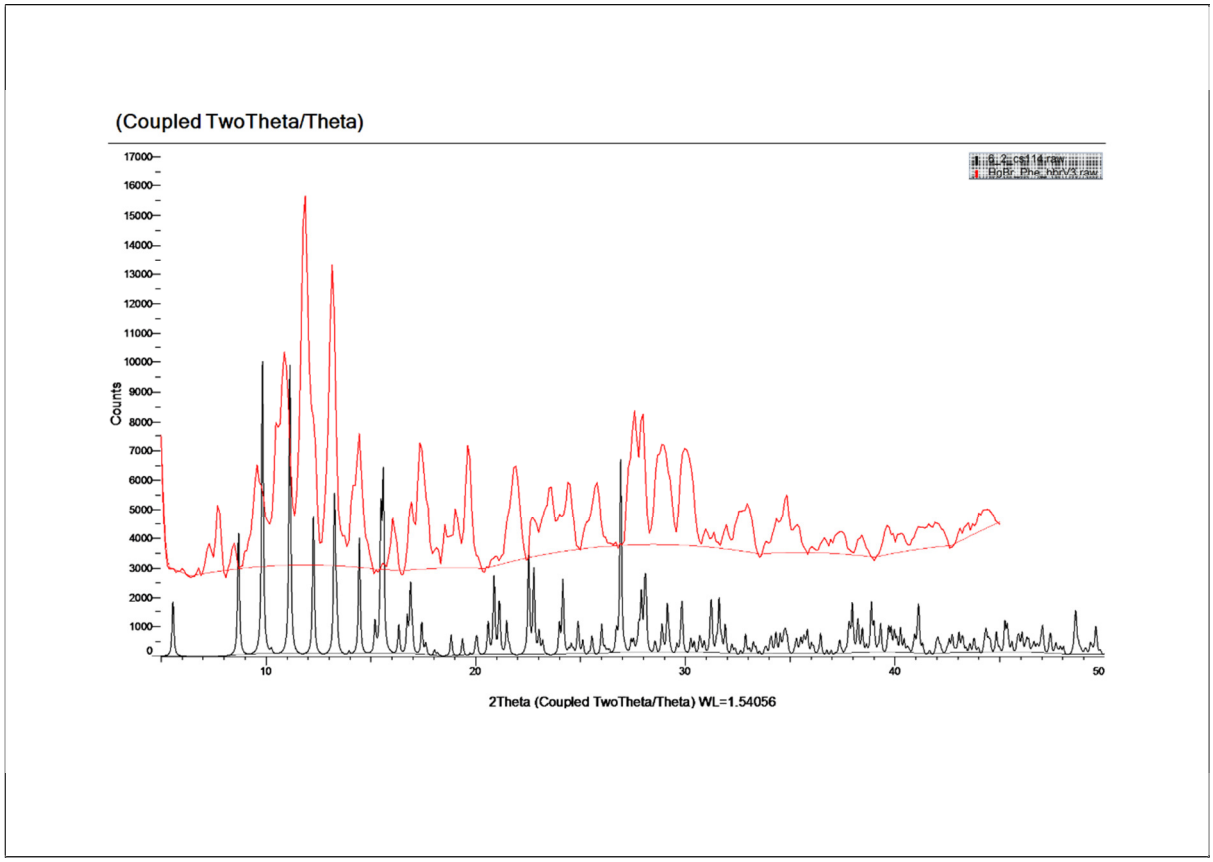
Comparison of the experimental X-ray powder patterns of the bulk samples with powder patterns calculated from the single crystal structures reported, to determine if the single crystal selected for single crystal X-ray diffraction is representative of the bulk sample, was carried out. The experimental powder patterns are shown in red, while the calculated patterns are given in black.

Compounds **5** and **14** decomposed upon preparative grinding of powder X-ray diffraction samples. For all other compounds the single crystal was found to be representative of the bulk sample.

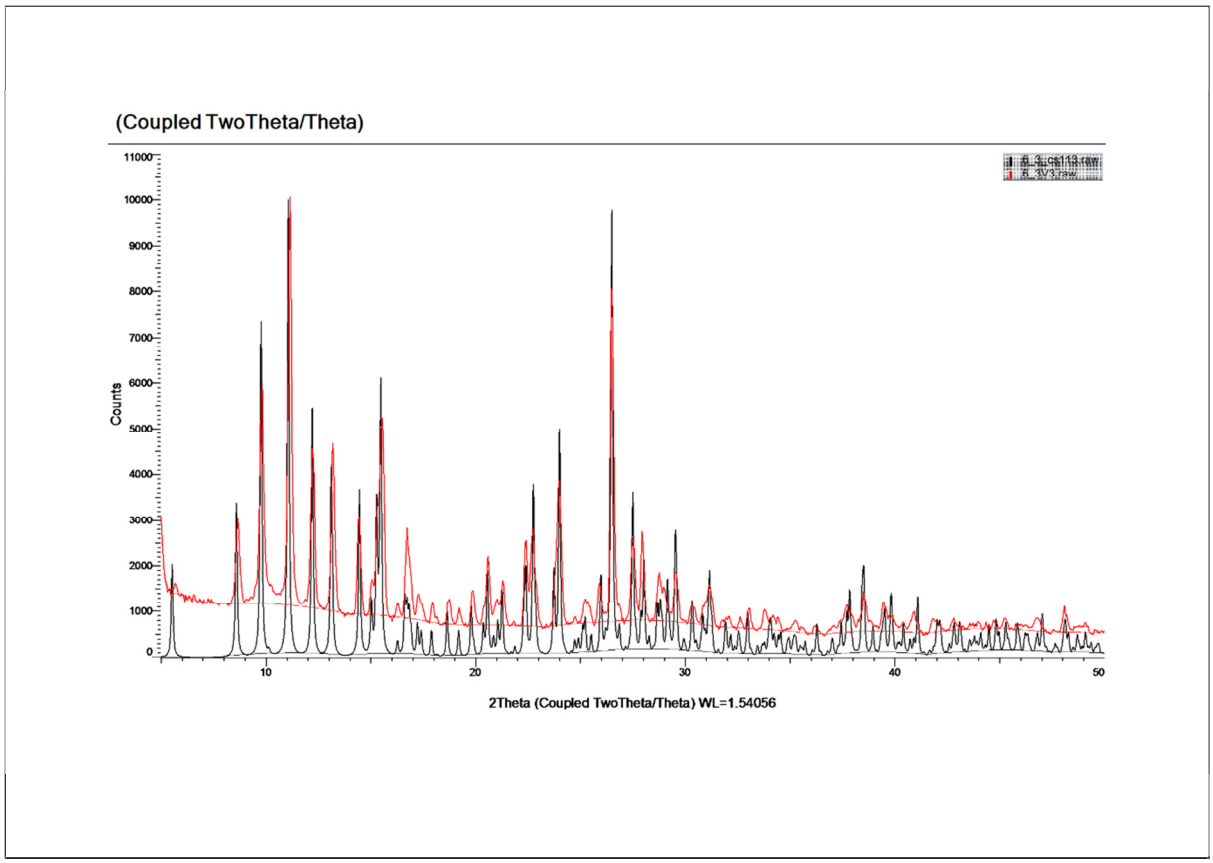
Compound 1: $[phe\text{-}H]_2[HgCl_4]\cdot 2H_2O$



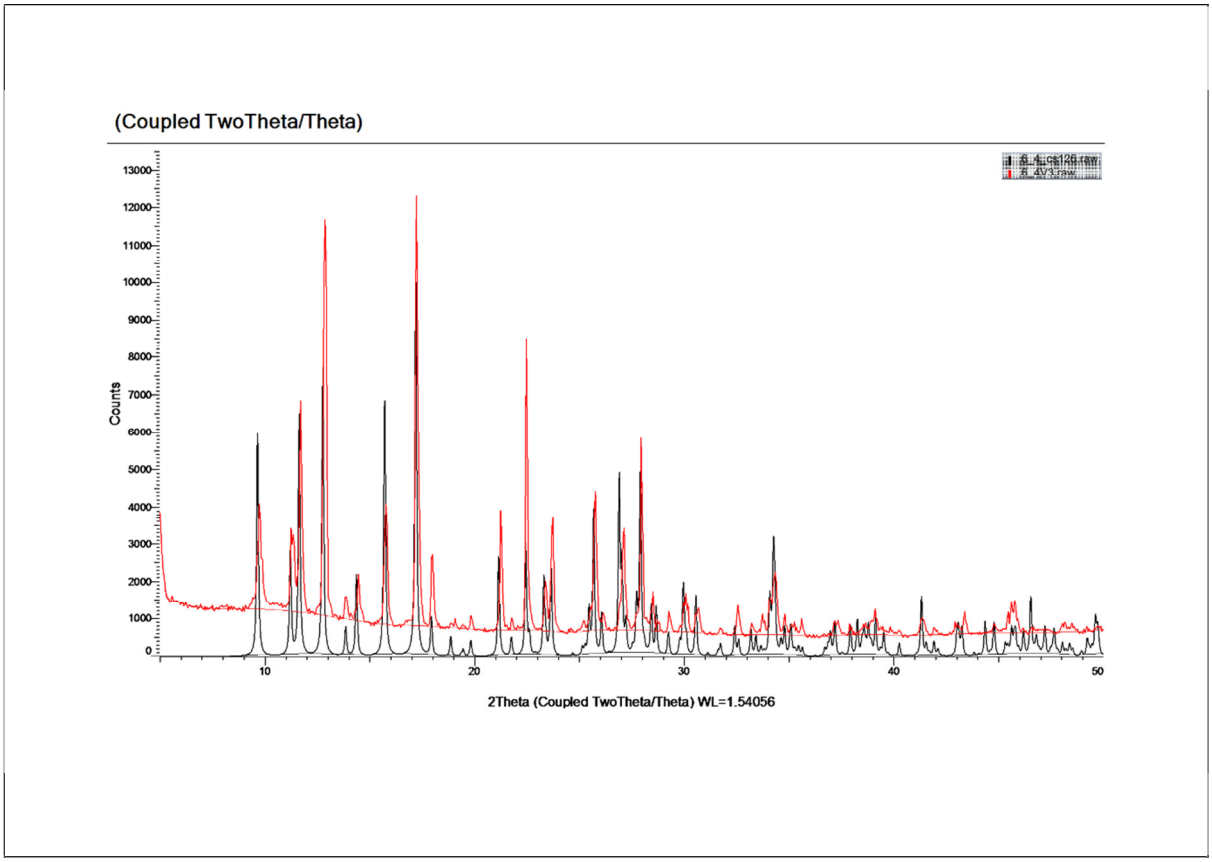
Compound 2: $[phe\text{-}H]_2[HgBr_4]\cdot 2H_2O$



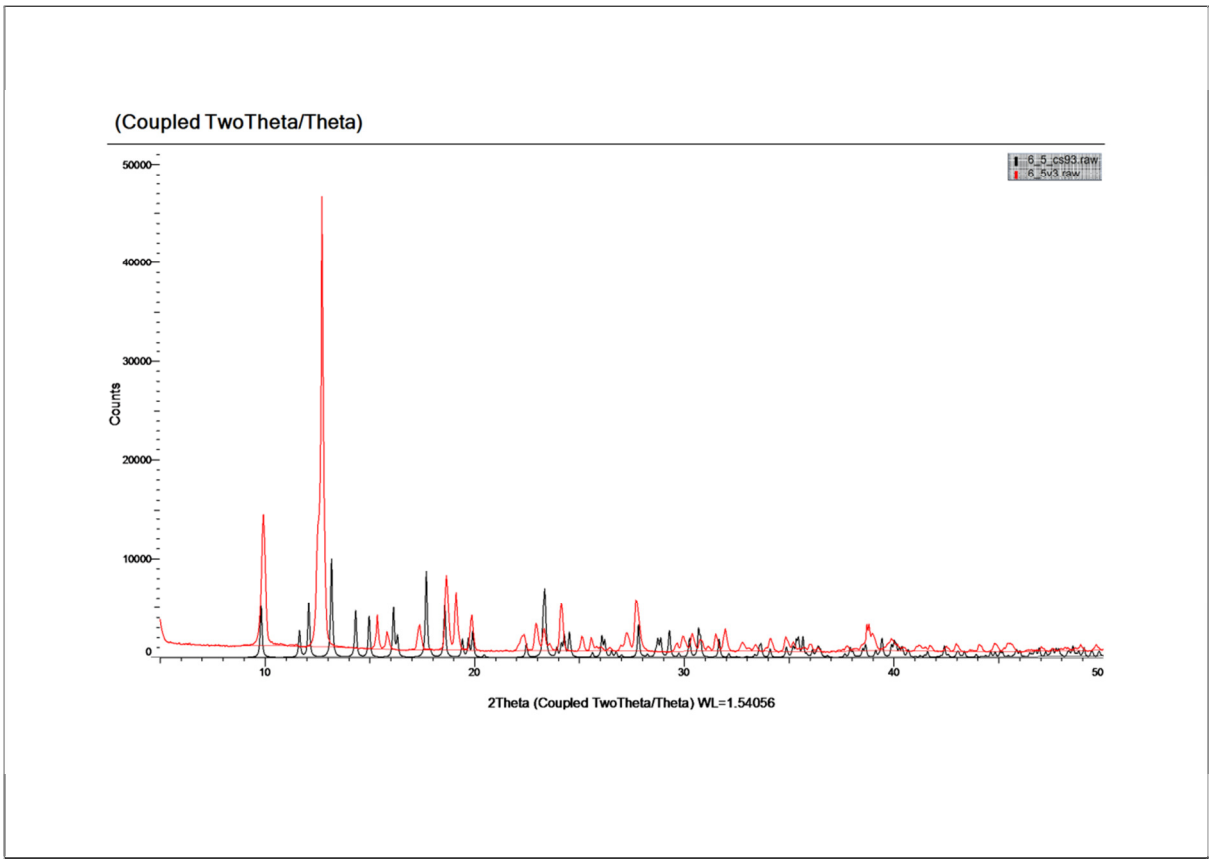
Compound 3: $[phe\text{-}H]_2[CdBr_4]\cdot 2H_2O$



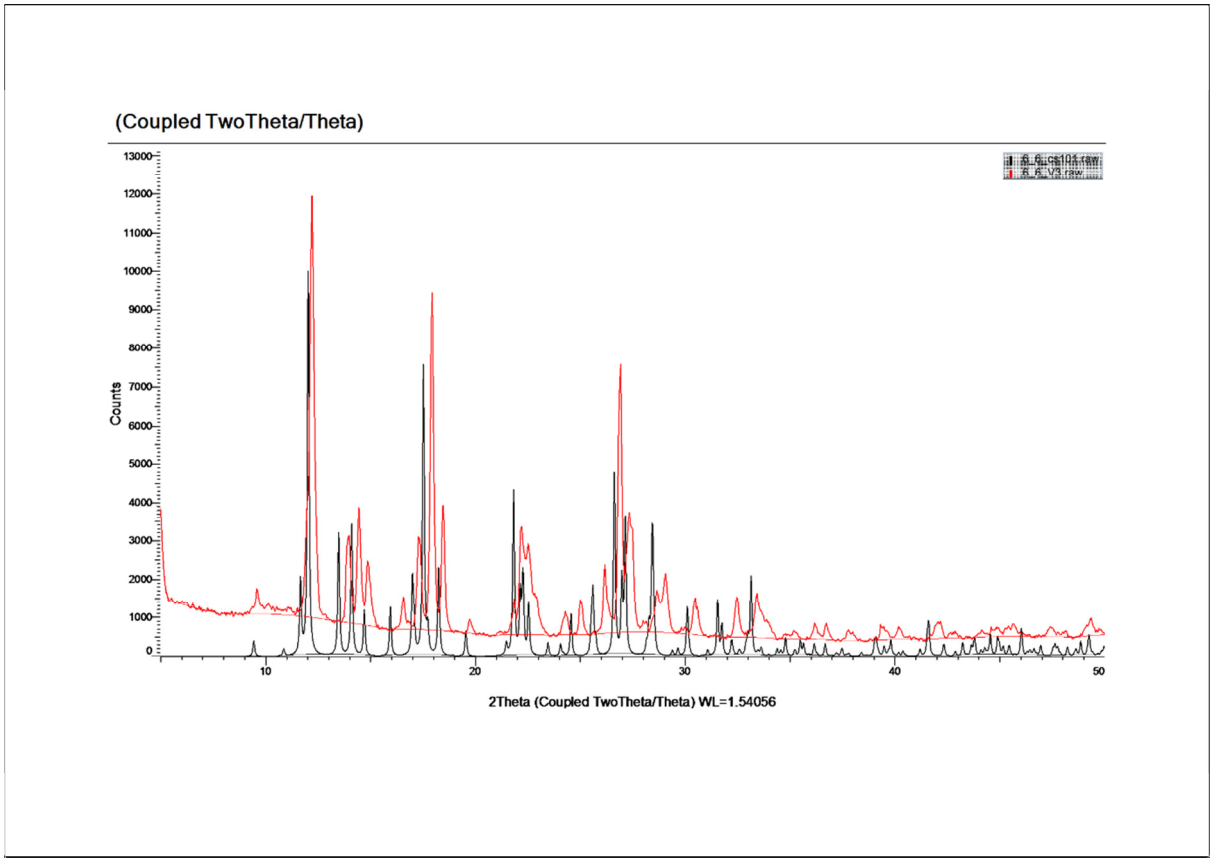
Compound 4: $[quin\text{-}H]_2[CdBr_4]\cdot H_2O$



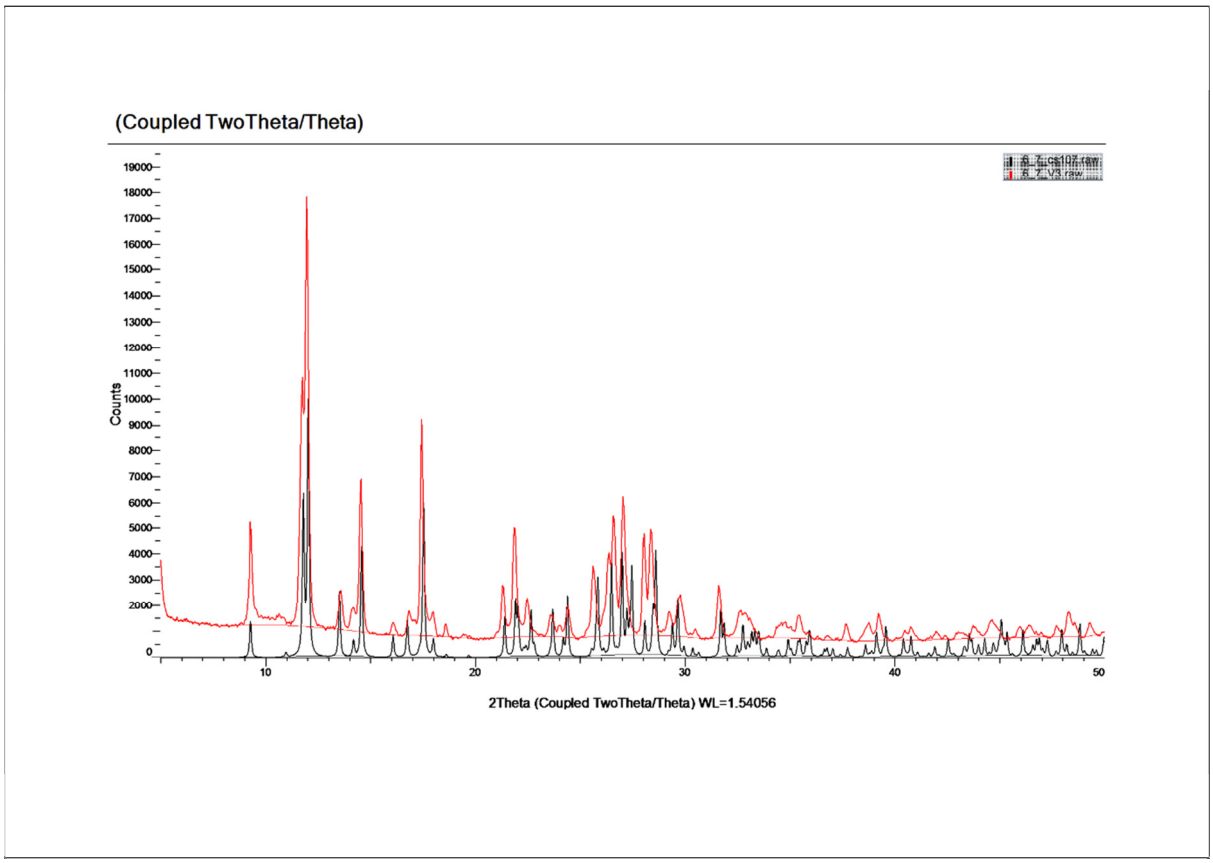
Compound 5: $[quin\text{-}H]_2[HgCl_4]\cdot H_2O$



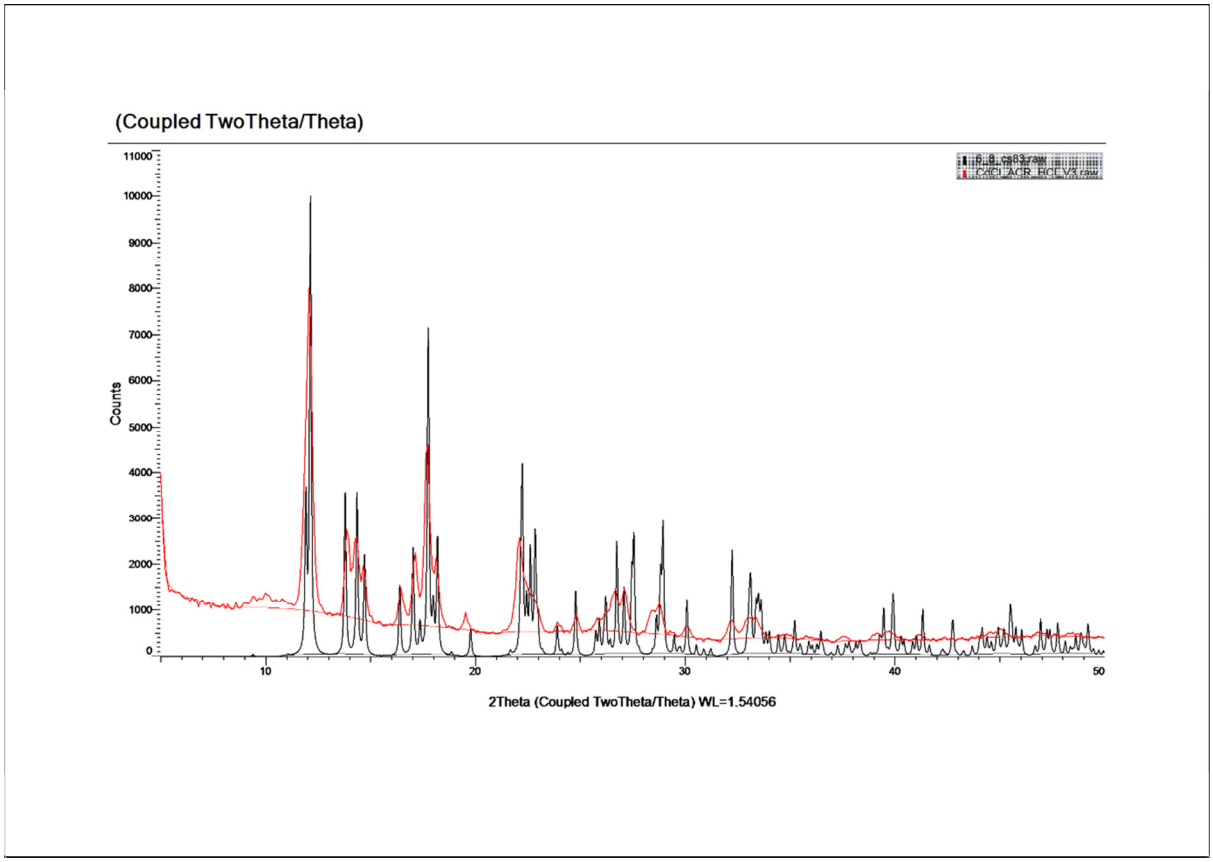
Compound 6: $[acr\text{-}H]_2[ZnCl_4]$



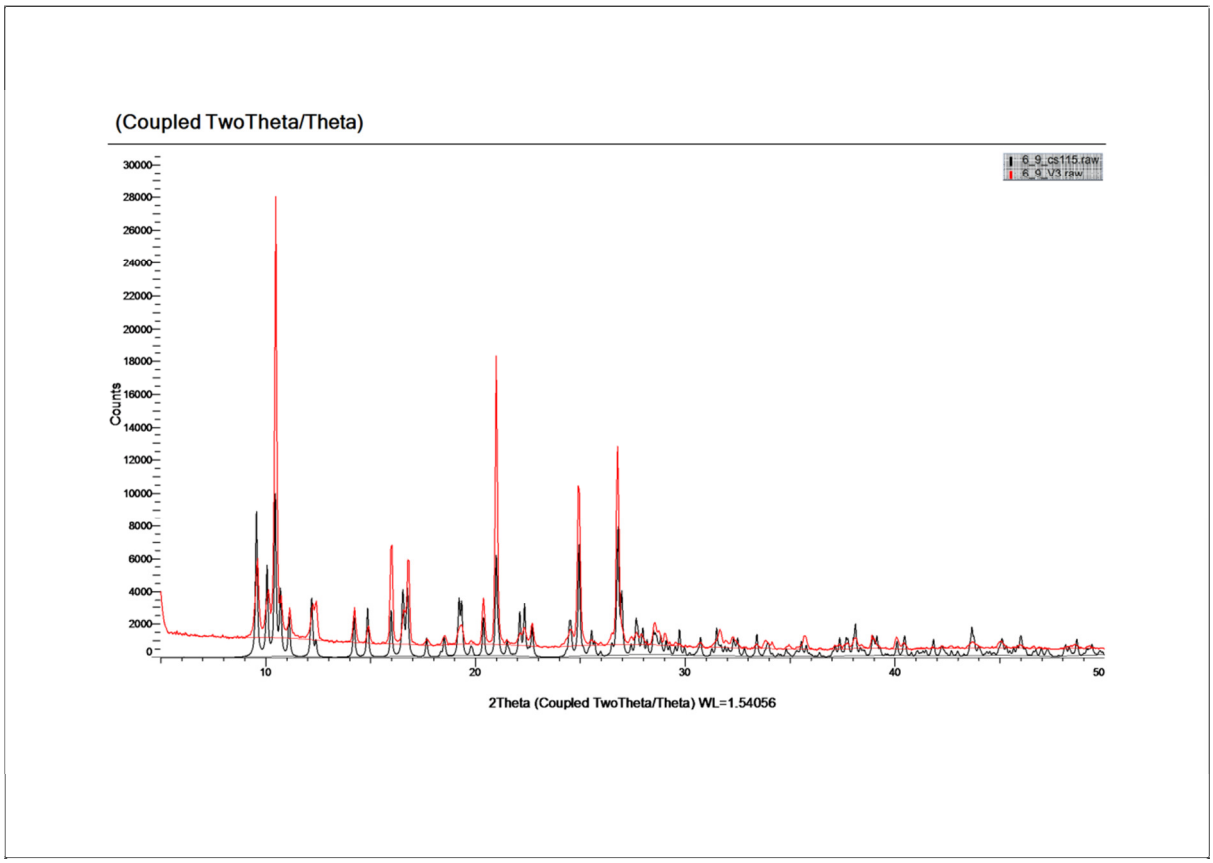
Compound 7: $[acr\text{-}H]_2[ZnBr_4]$



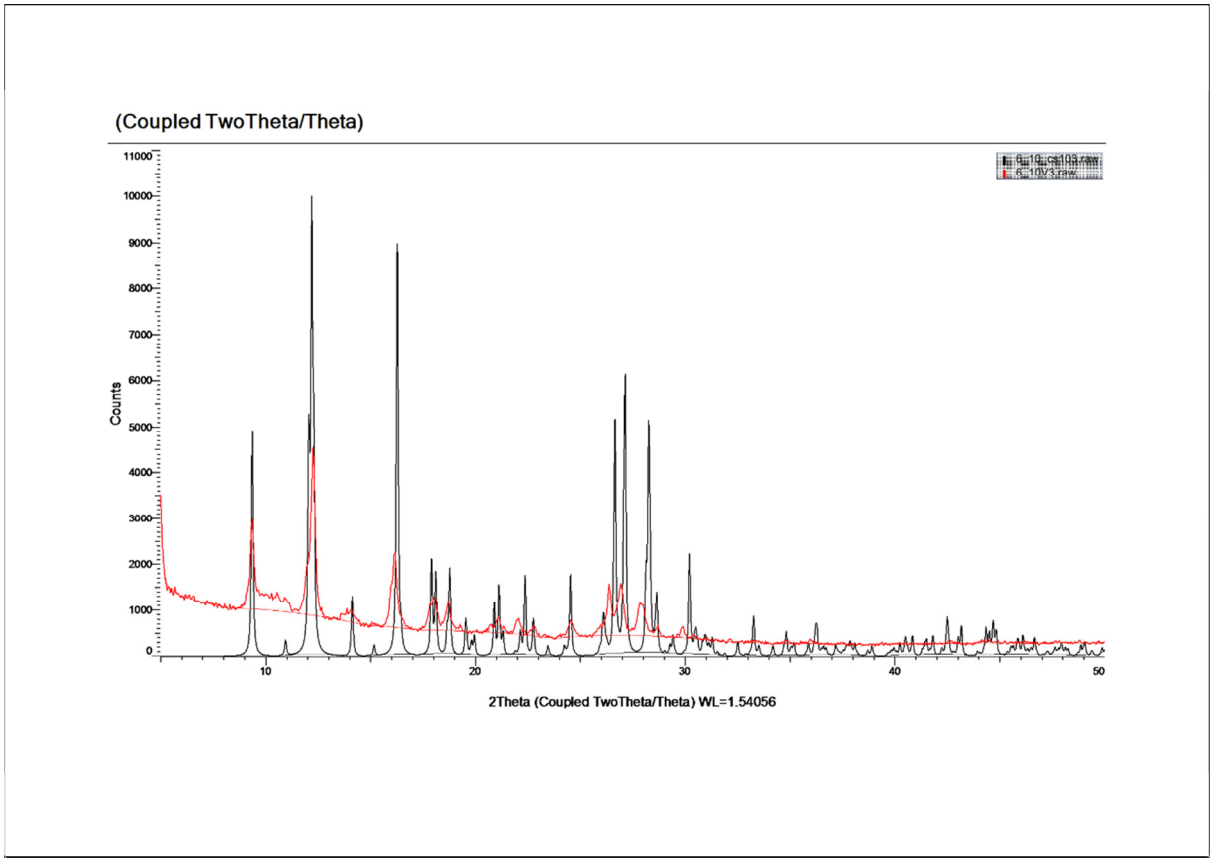
Compound 8: $[acr\text{-}H]_2[CdCl_4]$



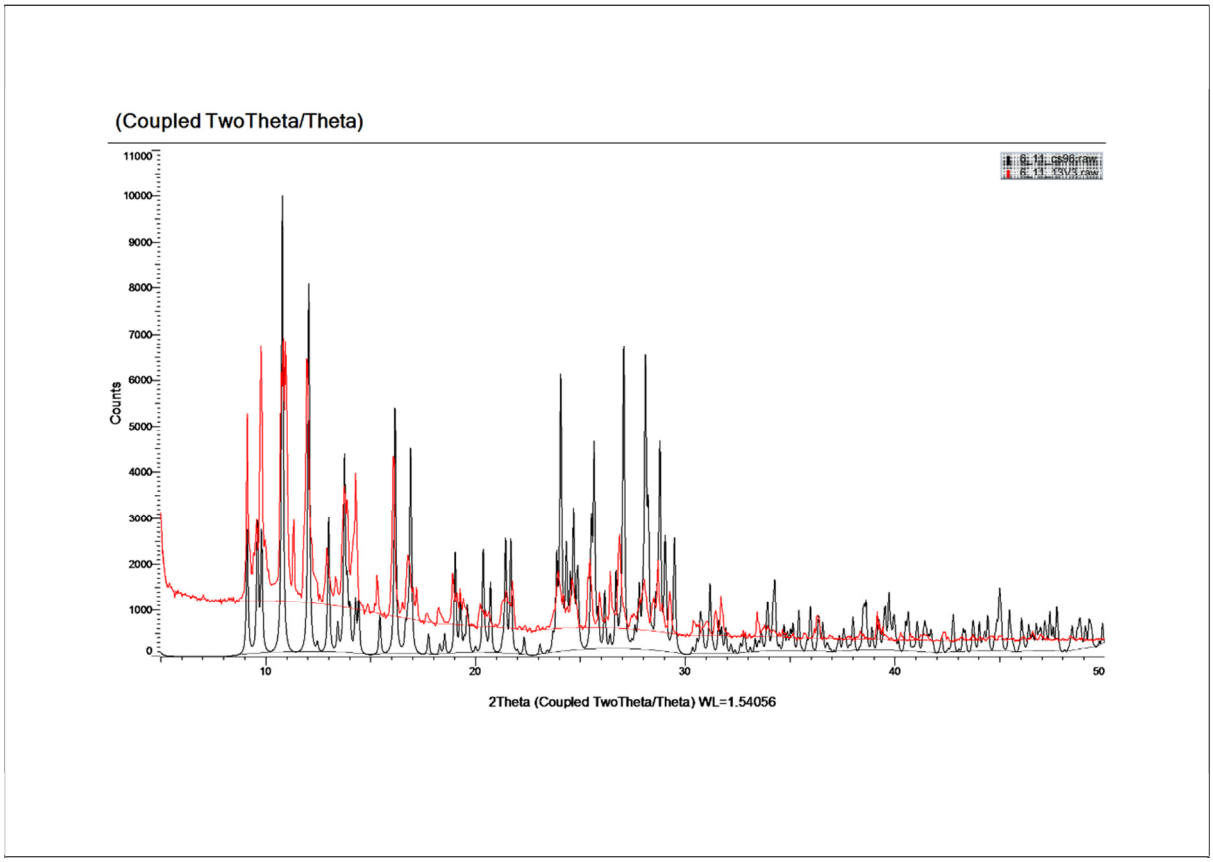
Compound 9: $[acr\text{-}H]_2[CdBr_4]$



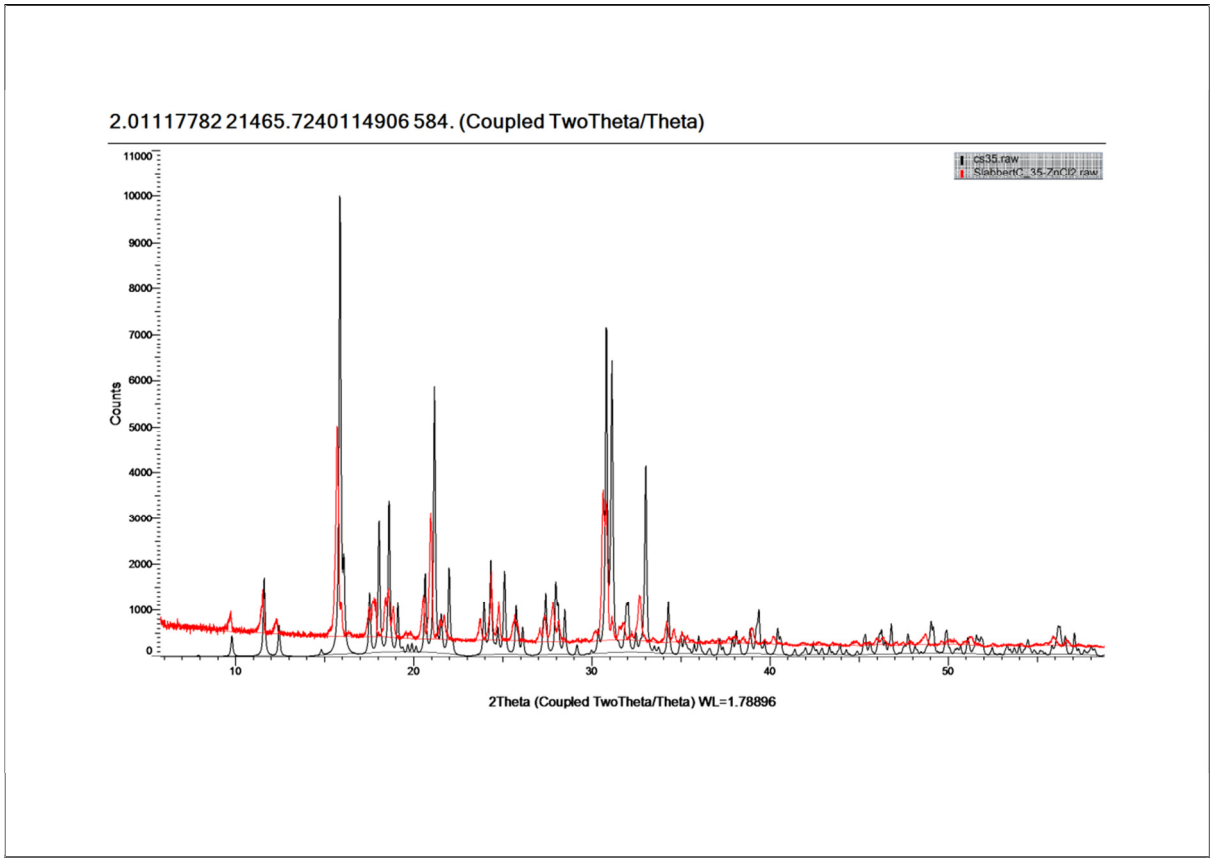
Compound 10: [phe-H_2]phe[$ZnCl_4$]



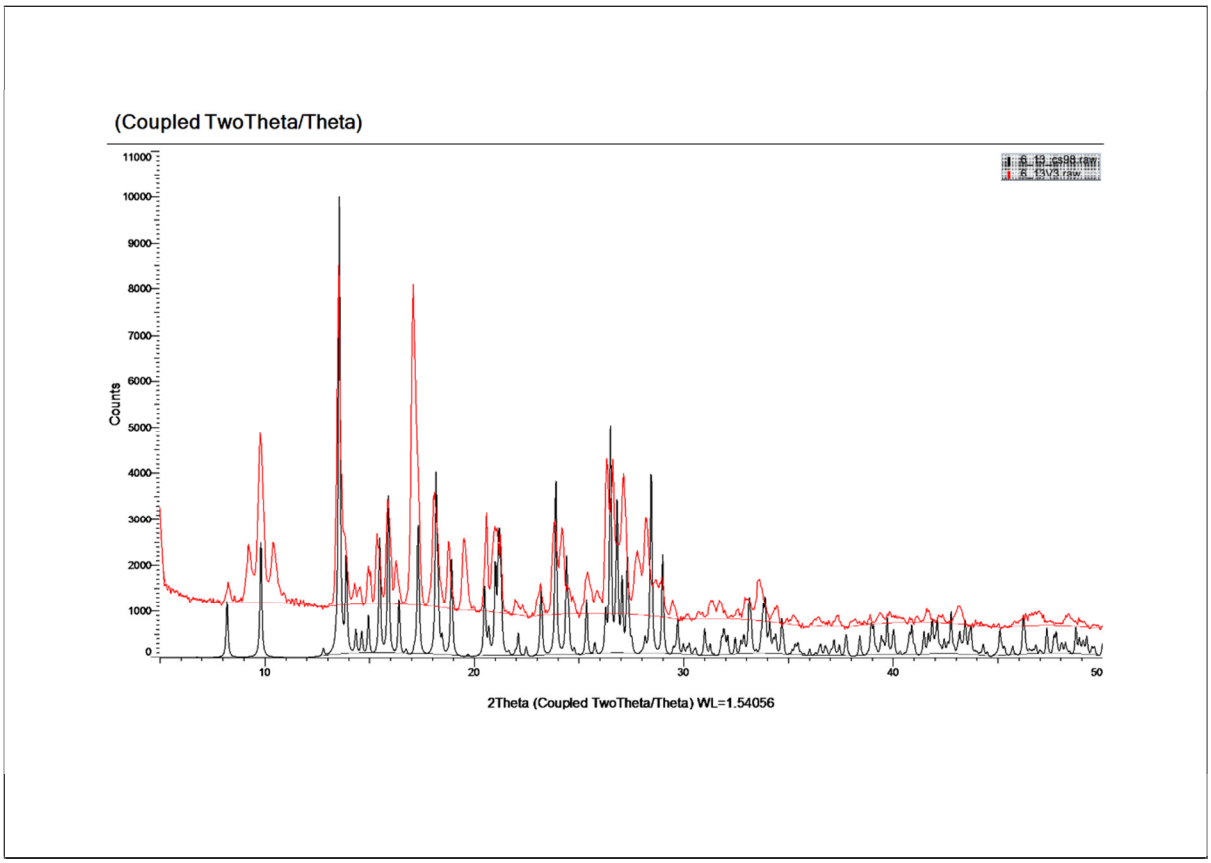
Compound 11: [phe-H](phe)$_2$ [$Zn(OH_2)X_3$]·EtOH·H_2O



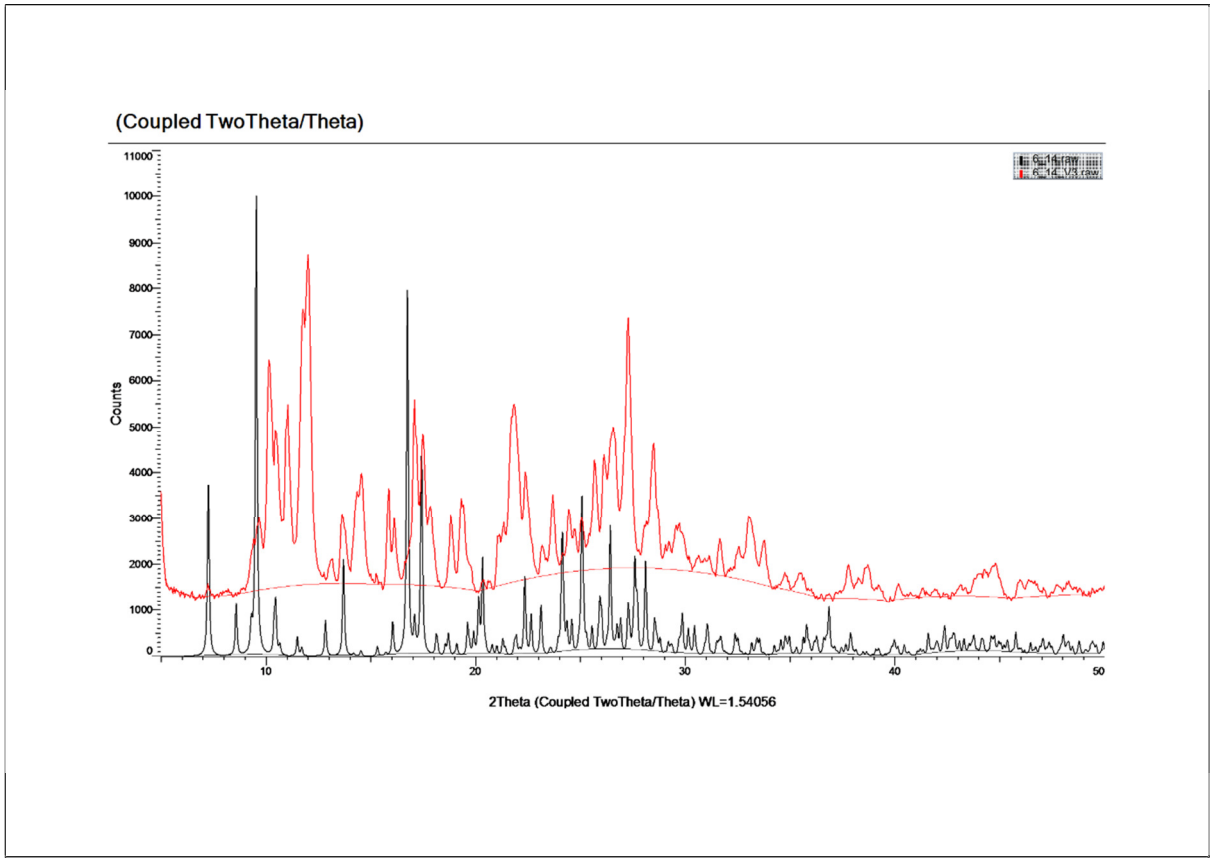
Compound 12: $(phe)_2[Zn(OH_2)_2Cl_2]\cdot H_2O$



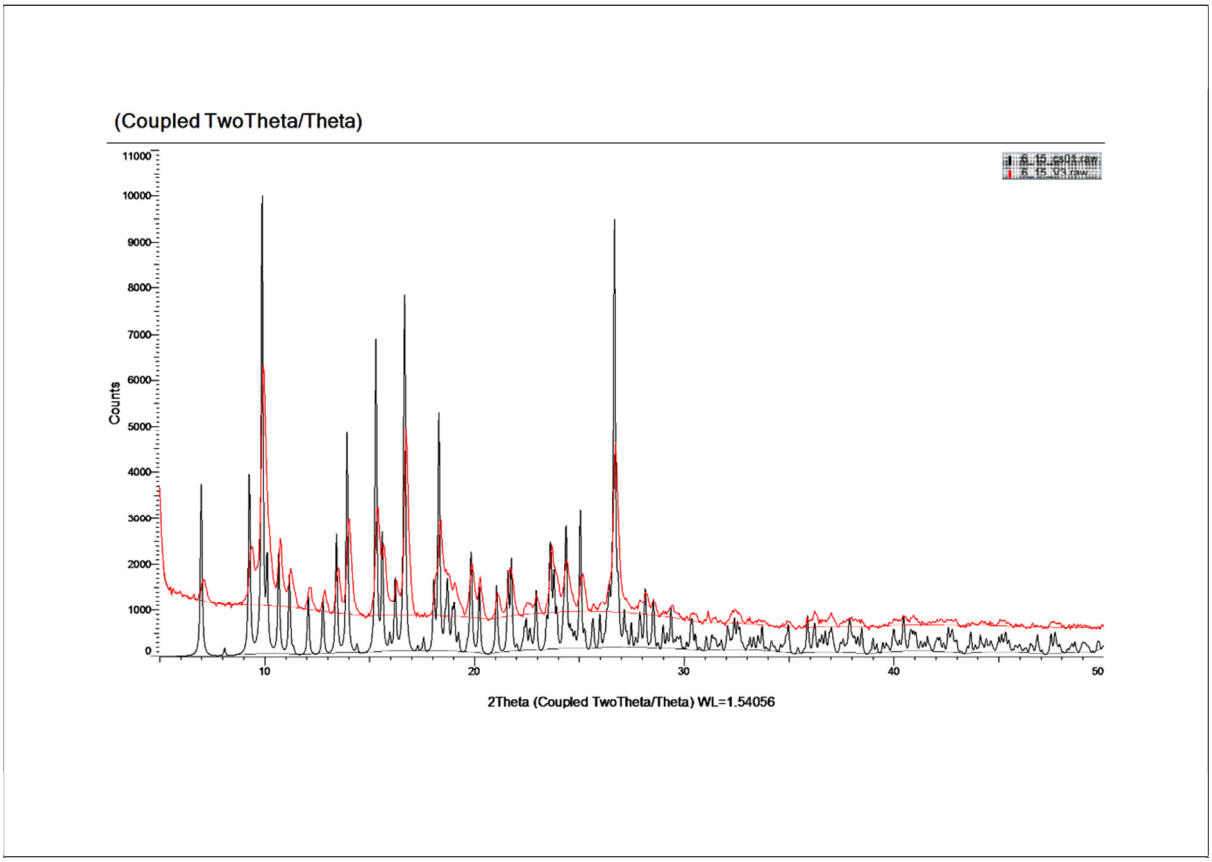
Compound 13: $(phe)_2[Zn(OH_2)_2Br_2]\cdot H_2O$



Compound 14: $(acr)_3[Zn(OH_2)_2Br_2]\cdot H_2O$



Compound 15: $(acr)_2[Zn(OH_2)I_2(O\text{-}^{i}prop)]$



Compound 16: $(phe)_2[Zn(OH_2)I_2(O\text{-}EtOH)]$