Supplementary Material

for

Insights into inhibition of human amyloid beta protein precursor (APP: PDB ID 3UMI) by (*E*)-*N*-(pyridin-2-ylmethylene)arylamine (L_R) models: Structure elucidation of a family of ZnX_2-L_R complexes†

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Table S1. Docking score (Kcal/mol) of the L_R during their docking in the peptide[a]

S. No.	No. of iterations	Docking score (Kcal/mol) after each cycle of 10,000 iterations			
		L_H	$L_{2\text{-Me}}$	$L_{2\text{-OMe}}$	$L_{4\text{-Me}}$
1	10000	-13.326	-15.221	-17.406	-14.213
2	10000	-14.113	-15.587	-17.612	-14.480
3	10000	-14.104	-15.892	-17.809	-14.539
4	10000	-14.118	-15.890	-17.800	-14.530
5	10000	-14.115	-15.890	-17.805	-14.532
6	10000	-14.115	-15.884	-17.805	-14.529
7	10000	-14.110	-15.889	-17.805	-14.530
8	10000	-14.112	-15.889	-17.801	-14.530
9	10000	-14.113	-15.887	-17.804	-14.528
10	10000	-14.112	-15.889	-17.804	-14.530

[a]In each case, the docking is repeated 10 times to obtain the maximum possible interactions between the ligand and the peptide.

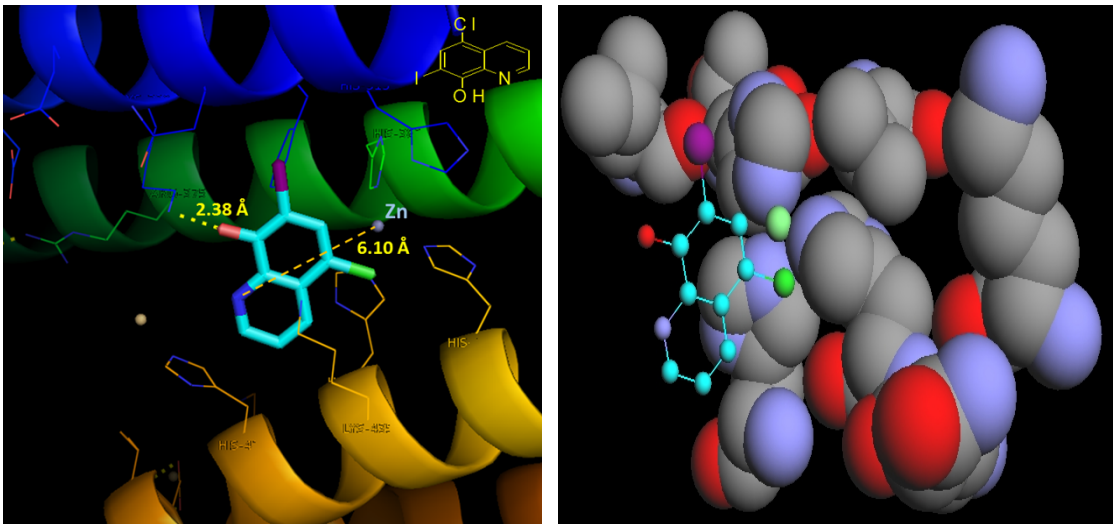

Fig. S1. Clioquinol docked (PyMOL and CPK views) in the amyloid beta protein precursor (APP; PDB ID: 3UMI) showing the ligating sites of the molecule have a remote possibility of interaction with Zn.

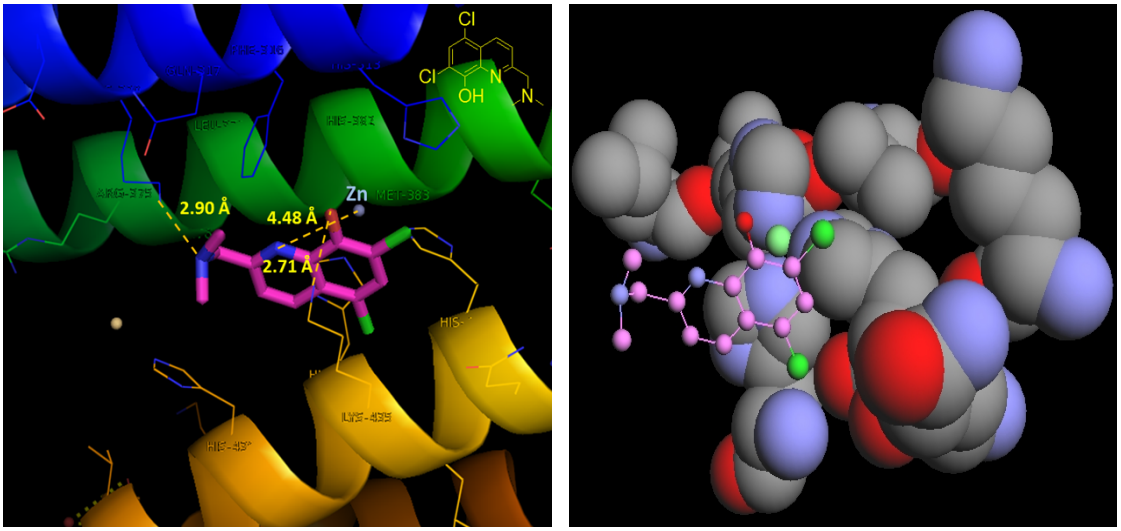

Fig. S2. PBT2 docked (PyMOL and CPK views) in the amyloid beta protein precursor (APP; PDB ID: 3UMI) showing the ligating sites of the molecule have a remote possibility of interaction with Zn.

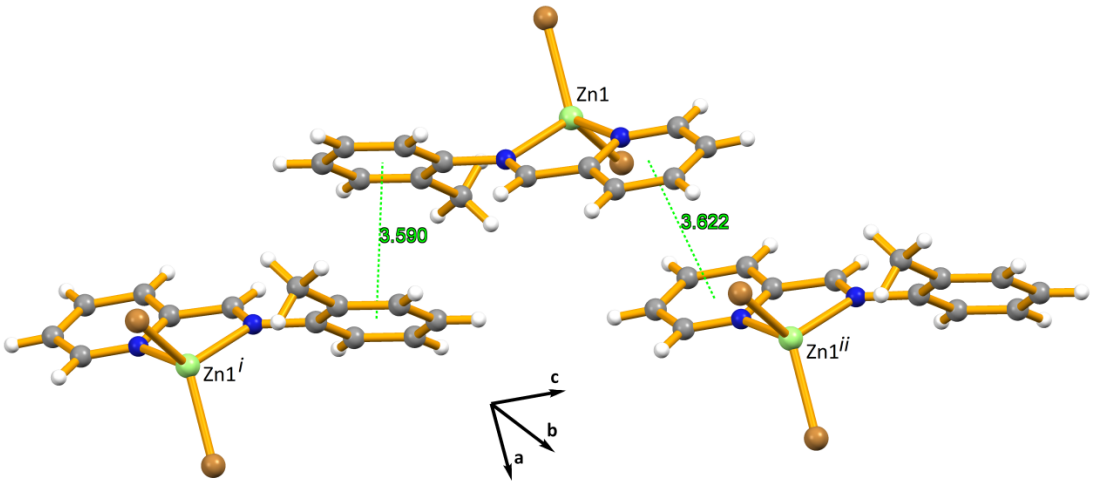

Fig. S3 The π···π stacking interactions in compound **1**. Symmetry codes: *i*) 2-*x*,-*y*,-*z*; *ii*) 2-*x*,-*y*,1-*z*.

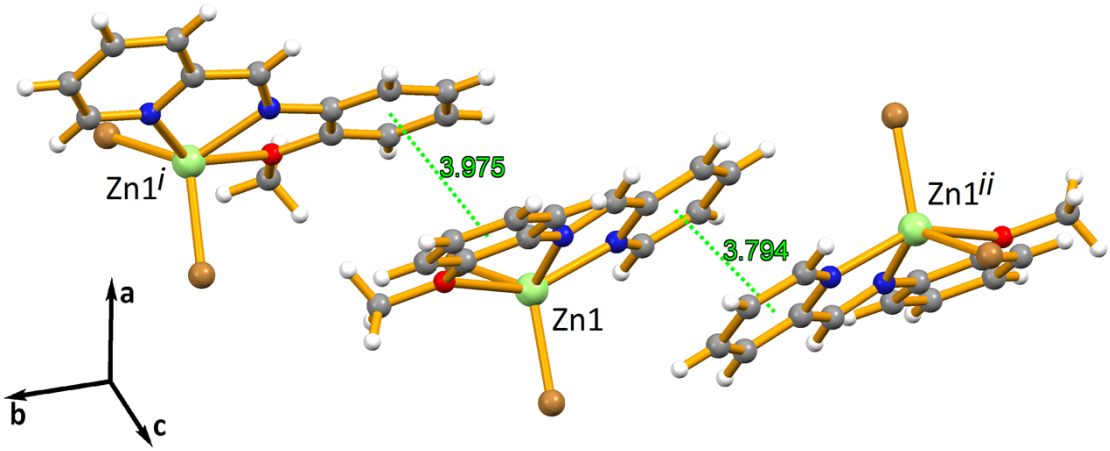

Fig. S4 The π···π stacking interactions in compound **2**. Symmetry codes: *i*) *x*,1/2-*y*,-1/2+*z*; 1-*x*,-*y*,1-*z*.

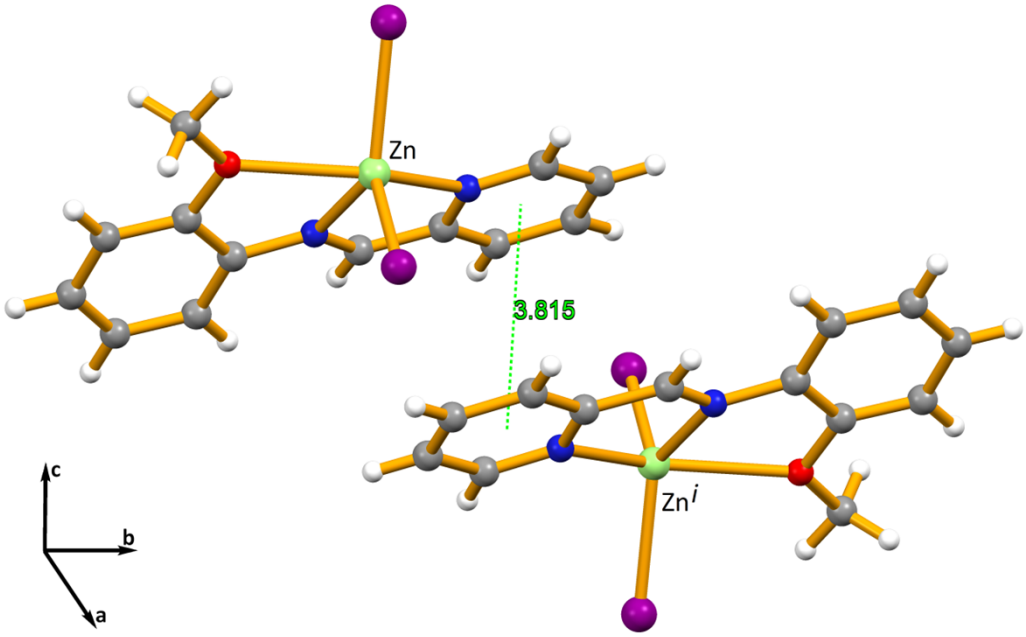

Fig. S5 The π···π stacking interaction in compound **3**. Symmetry code: *i*) -*x*,1-*y*,1-*z*.

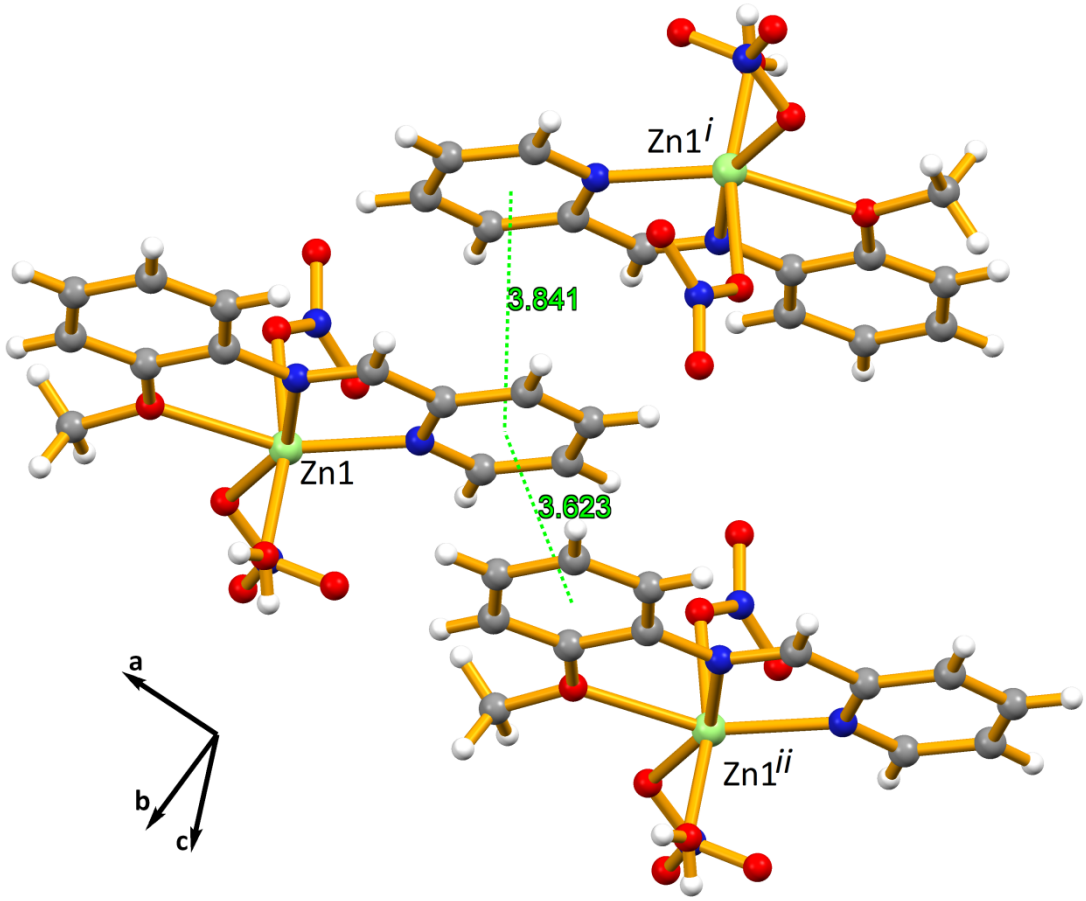

Fig. S6 The π···π stacking interactionsin compound **4**. Symmetry codes: *i*) 1-*x*,1-*y*,-*z*; *ii*) -1+*x*,*y*,*z*.