Electronic Supplementary Material (ESI) for Dalton Transactions

Multifunctional iron-chelators with protective roles against neurodegenerative diseases

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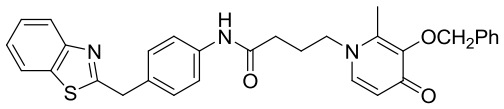
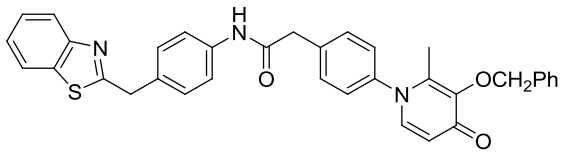
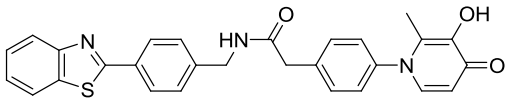
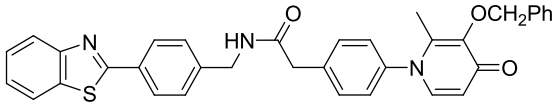
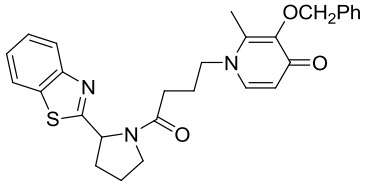
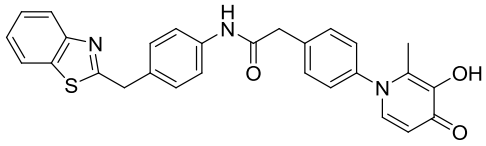
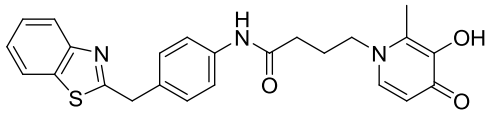
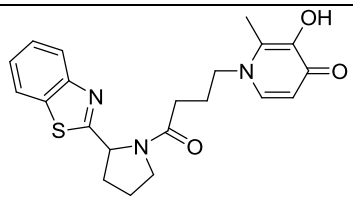
Supplementary Information

Table S1. List of the best docked compounds with AChE and their respective score.[a]

	Structure	**Score**
1a		70.87
1b		69.17
2c		69.14
1c		68.60
1d		65.67
2b		65.05
2a		64.25
2d		57.67

[a] docking calculation using GOLD program[1] and ASP scoring function

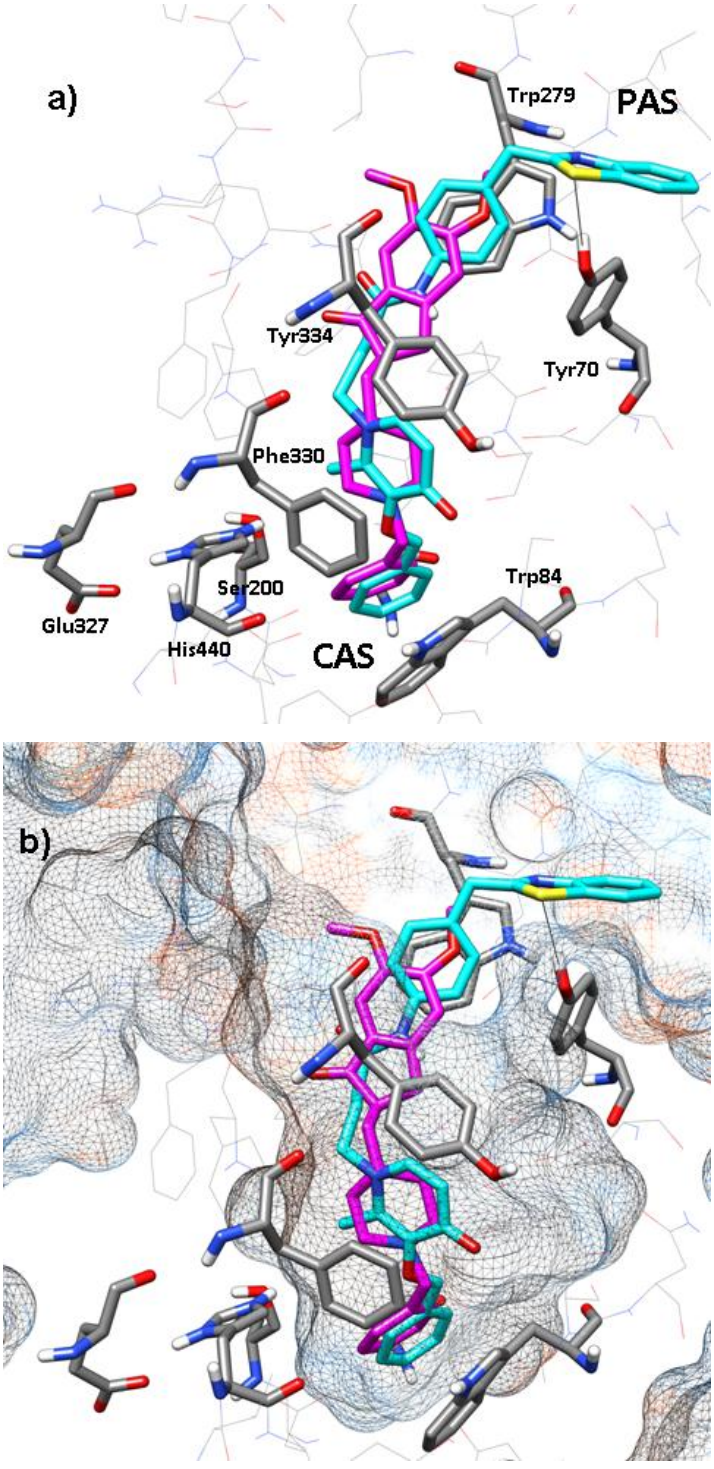


Figure S1. Docking of compound **1a** (cyan) towards AChE, superimposed with the original ligand Dnp (magenta) (a), and cut of the AChE surface showing the same compounds within the gorge of the active site (b). Red surface represents hydrophobic and blue hydrophilic regions of the protein; H-bonds are represented as solid black lines.

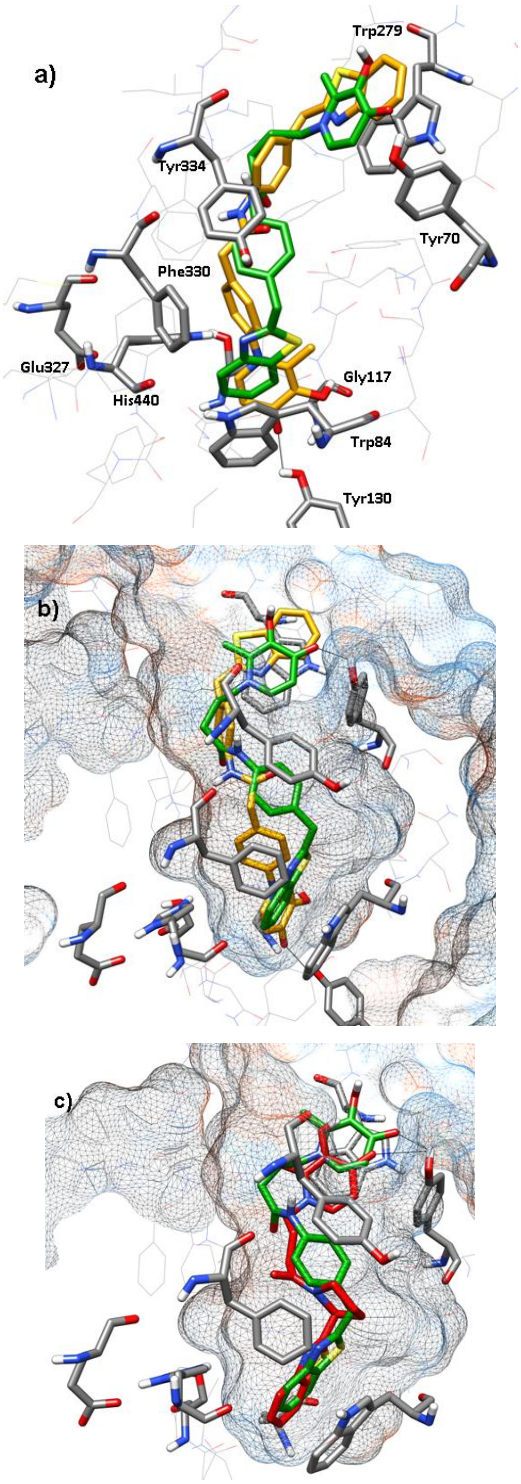


Figure S2. Docking of compounds **2a** (green) and **2b** (orange) into AChE (a), and cut of the AChE surface sowing the same compounds **2a** and **2b** (b), and **2a** and **2d** (red) (c). Red surface represents hydrophobic and blue hydrophilic regions of the protein; H-bonds are represented as solid black lines.

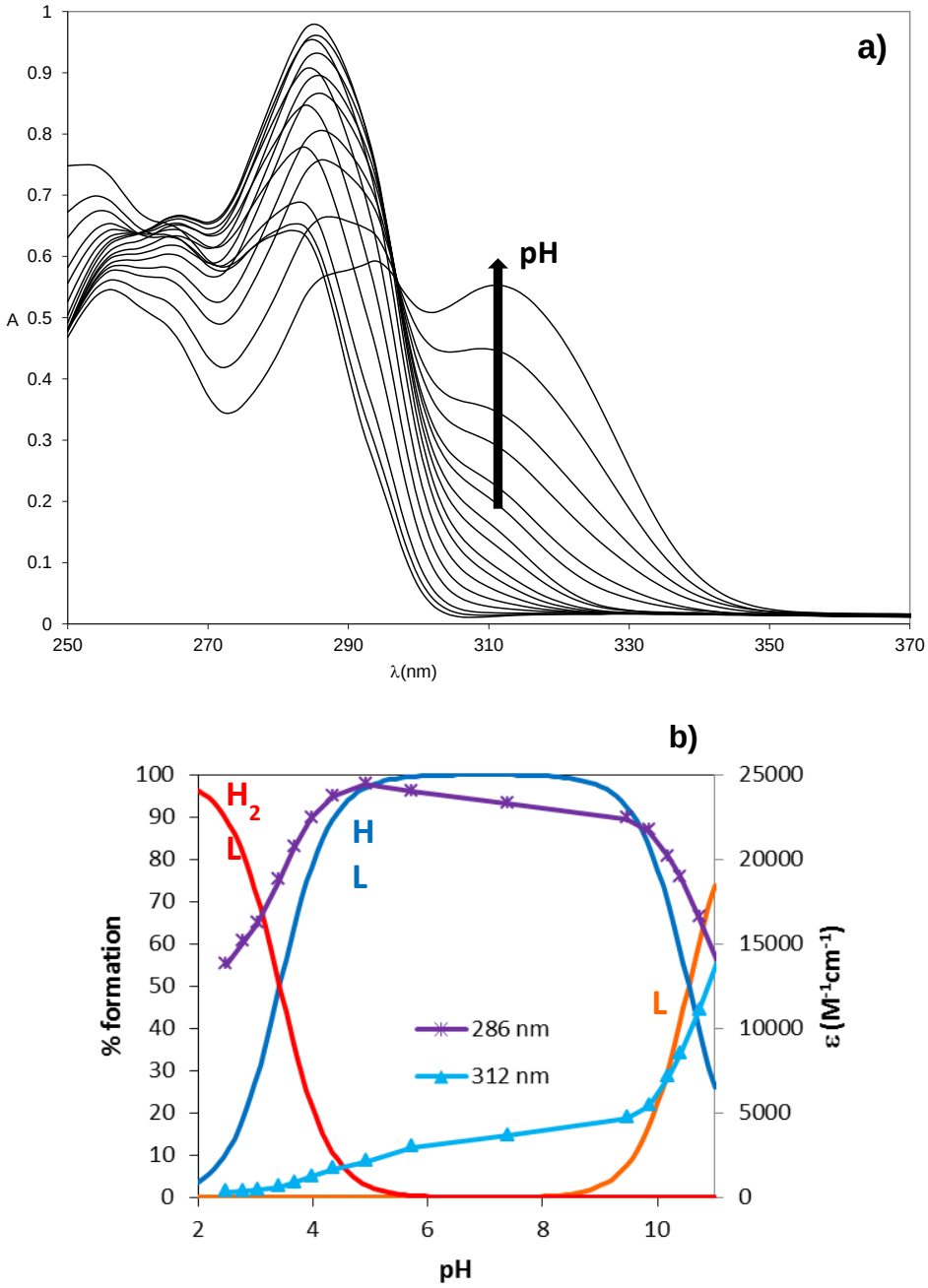


Figure S3. a) Electronic spectra (pH 2.4-11.0) and **b)** species distribution curves with molar extinction coefficients at maximum absorption wavelengths for the system **2d** (C_L = 4 × 10^{-5} M).

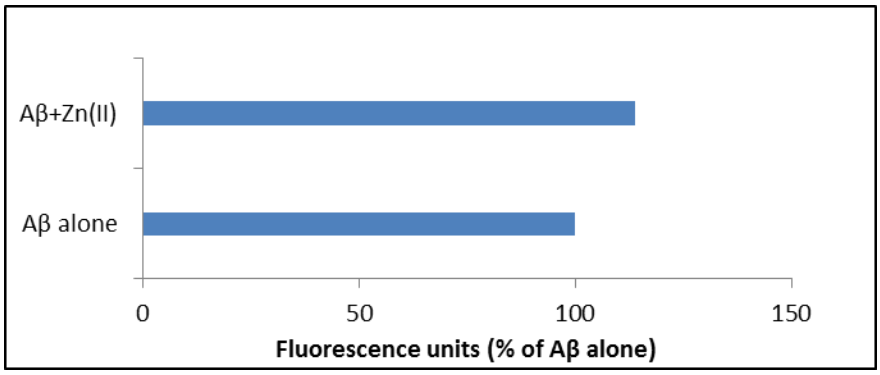
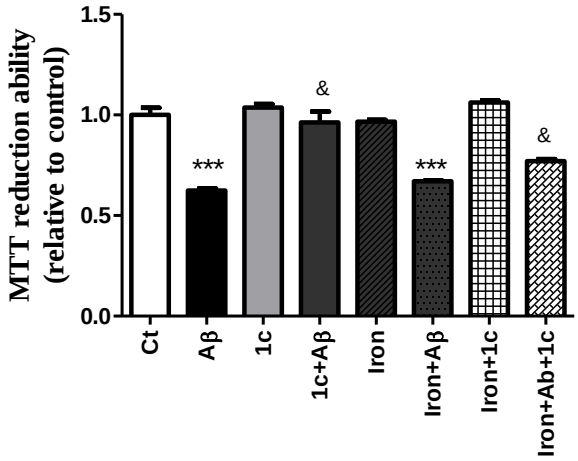


Figure S4. Results of THT assay in metal induced Aβ aggregation

A



B

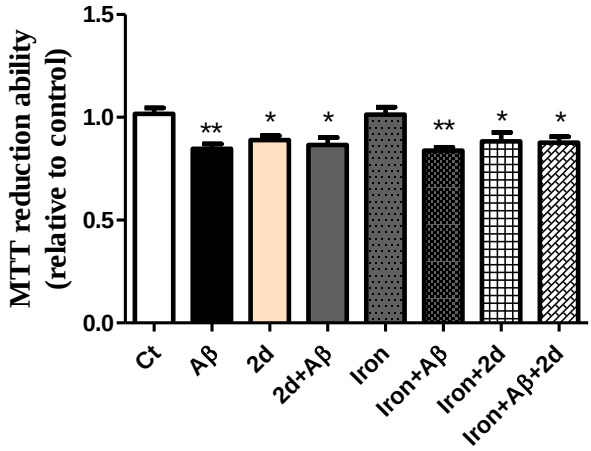


Figure S5. Effect of compound 1c and 2d on iron induce toxicity. SH-SY5Y cells were treated with $A\beta_{42}$ (1 μM) peptides, for 24 h, in the absence or the presence of compound 1c (A) or 2d (B) and with or without iron (2.5 μM)/ascorbate (0.8 mM). Evaluation of cell viability was performed by using MTT reduction test. Results are expressed as the percentage of SH-SY5Y untreated cells, with the mean ± S.E.M. derived from 3 different experiments. ***$p < 0.001$; significantly different when compared with SH-SY5Y untreated cells; $^{\&}p < 0.05$, significantly different when compared with the respective iron/ascorbate treated SH-SY5Y cells.

References

1 G. Jones, P. Willett, R. C. Glen, A. R. Leach, R. Taylor, *J. Mol. Biol.*, 1997, **267**, 727.