

## Novel cyclopentaquinoline and acridine analogs as multifunctional, potent drug candidates in Alzheimer's disease

Karolina Maciejewska <sup>1</sup>, Kamila Czarnecka <sup>1</sup>, Paweł Kręcisz <sup>1</sup>, Dorota Niedziałek <sup>2</sup>, Grzegorz Wieczorek <sup>2</sup>, Robert Skibiński <sup>3</sup>, and Paweł Szymański <sup>1,4,\*</sup>

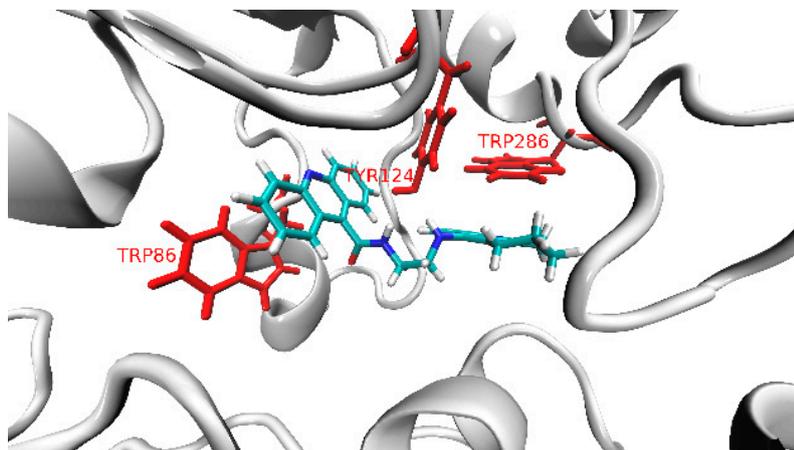
<sup>1</sup> Department of Pharmaceutical Chemistry, Drug Analyses and Radiopharmacy, Faculty of Pharmacy, Medical University of Lodz, Muszyńskiego 1 St., 90-151 Lodz, Poland; karolina.maciejewska@stud.umed.lodz.pl (K.M.); kamila.czarnecka@umed.lodz.pl (K.C); pawel.krecisz@stud.umed.lodz.pl (P.K.); pawel.szymanski@umed.lodz.pl (P.S.)

<sup>2</sup> Institute of Biochemistry and Biophysics, Polish Academy of Sciences, 02-106 Warsaw, Poland; dorotanka@gmail.com (D.N.); wieczorek.grzegorz@gmail.com (G.W.)

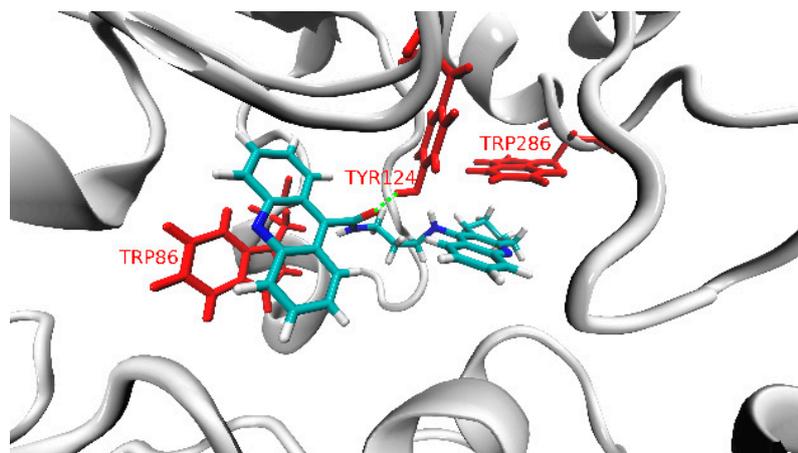
<sup>3</sup> Department of Medicinal Chemistry, Faculty of Pharmacy, Medical University of Lublin, Jaczewskiego 4 St., 20-090 Lublin, Poland; robertskibinski@umlub.pl (R.S.)

<sup>4</sup> Department of Radiobiology and Radiation Protection, Military Institute of Hygiene and Epidemiology, 4 Kozielska St., 01-163 Warsaw, Poland; pawel.szymanski@wihe.pl (P.S.)

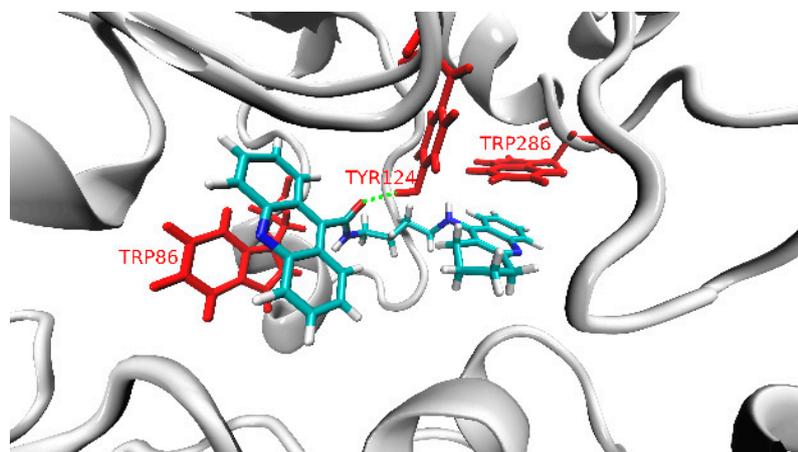
\* pawel.szymanski@umed.lodz.pl; phone: +48-42-677-92-53



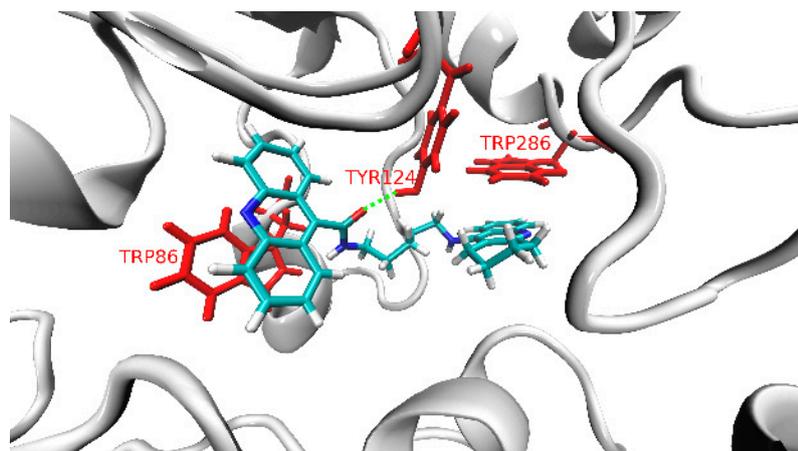
**Figure S1.** The binding mode of the **3a** ligand inside the pocket of AChE. The key ligand-binding aromatic residues in the pocket of AChE are marked in red.



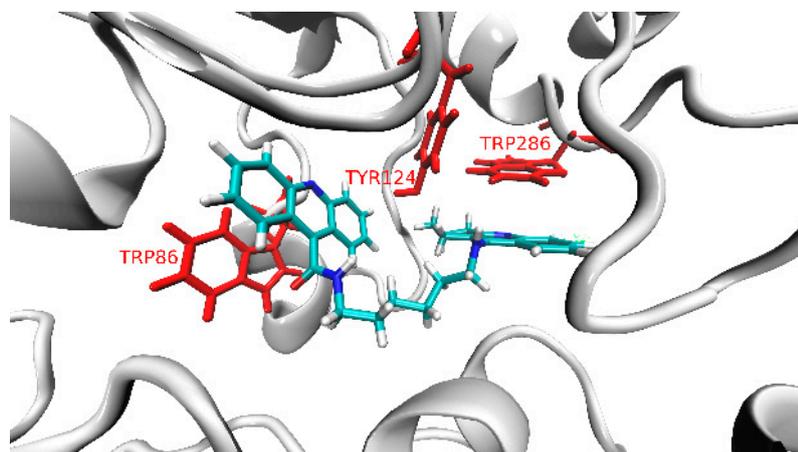
**Figure S2.** The binding mode of the **3b** ligand inside the pocket of AChE. The key ligand-binding aromatic residues in the pocket of AChE are marked in red.



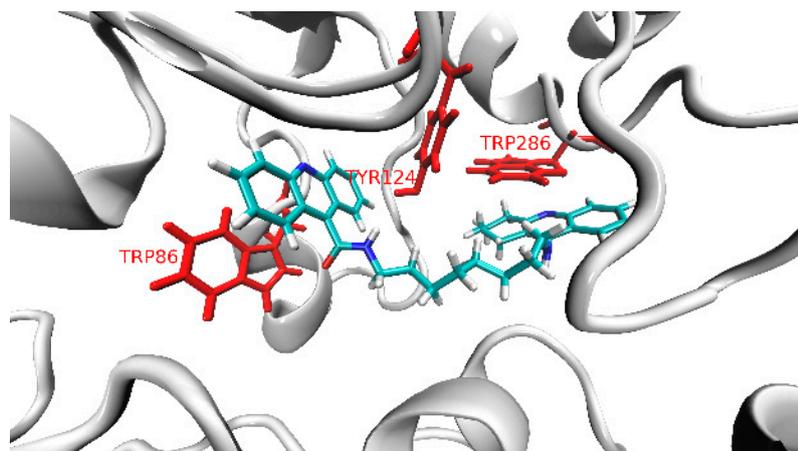
**Figure S3.** The binding mode of the **3c** ligand inside the pocket of AChE. The key ligand-binding aromatic residues in the pocket of AChE are marked in red.



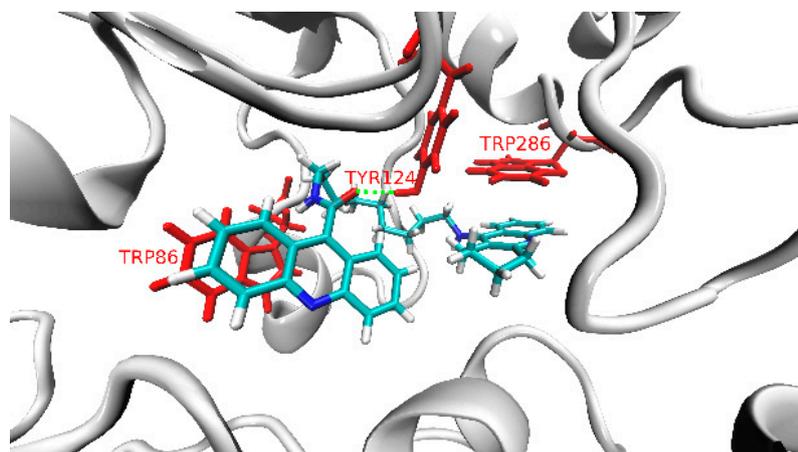
**Figure S4.** The binding mode of the **3d** ligand inside the pocket of AChE. The key ligand-binding aromatic residues in the pocket of AChE are marked in red.



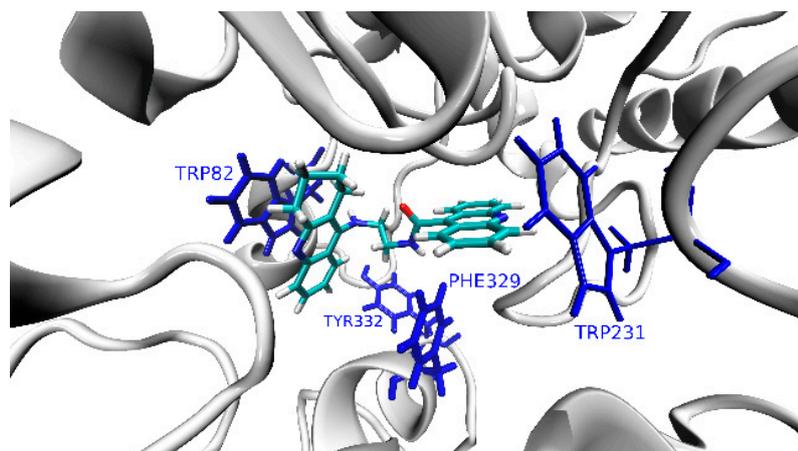
**Figure S5.** The binding mode of the **3e** ligand inside the pocket of AChE. The key ligand-binding aromatic residues in the pocket of AChE are marked in red.



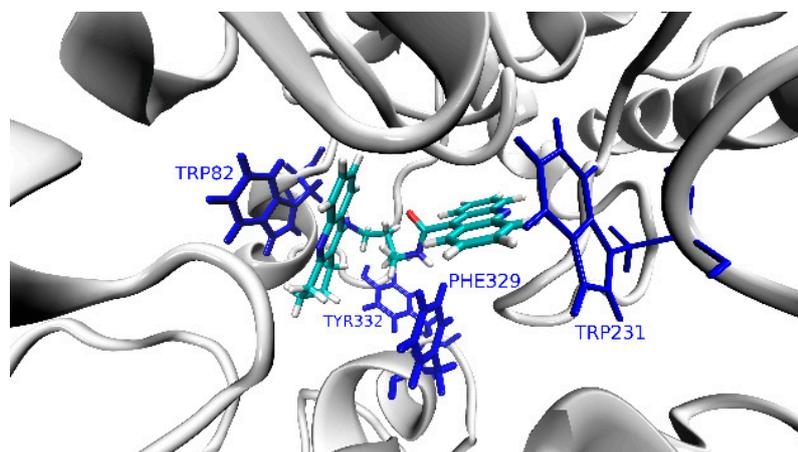
**Figure S6.** The binding mode of the **3g** ligand inside the pocket of AChE. The key ligand-binding aromatic residues in the pocket of AChE are marked in red.



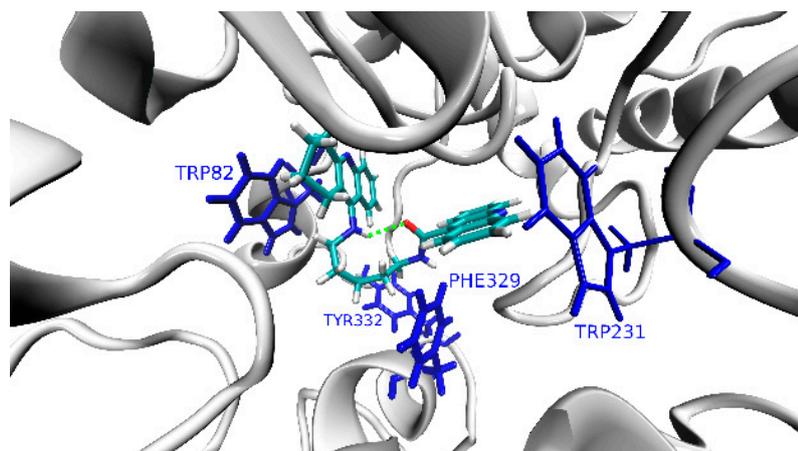
**Figure S7.** The binding mode of the **3h** ligand inside the pocket of AChE. The key ligand-binding aromatic residues in the pocket of AChE are marked in red.



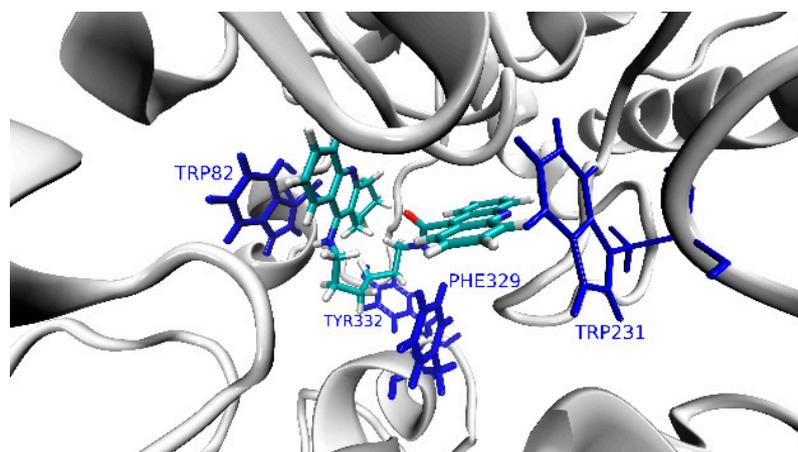
**Figure S8.** The binding mode of the **3a** ligand inside the pocket of BuChE. The key ligand-binding aromatic residues in the pocket of BuChE are marked in blue.



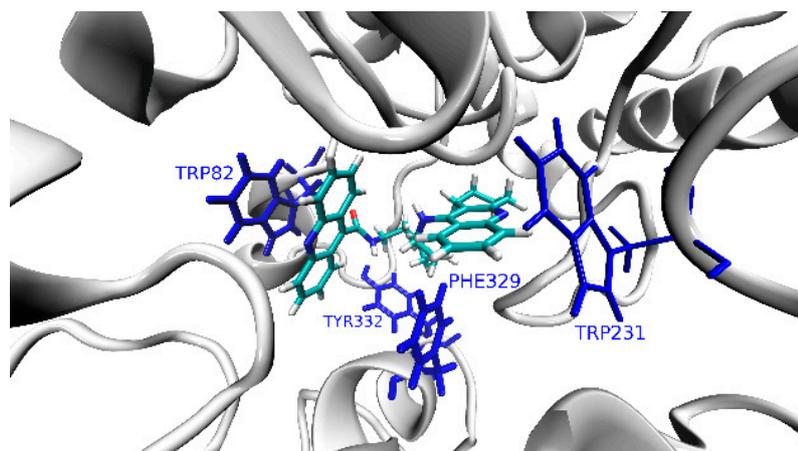
**Figure S9.** The binding mode of the **3c** ligand inside the pocket of BuChE. The key ligand-binding aromatic residues in the pocket of BuChE are marked in blue.



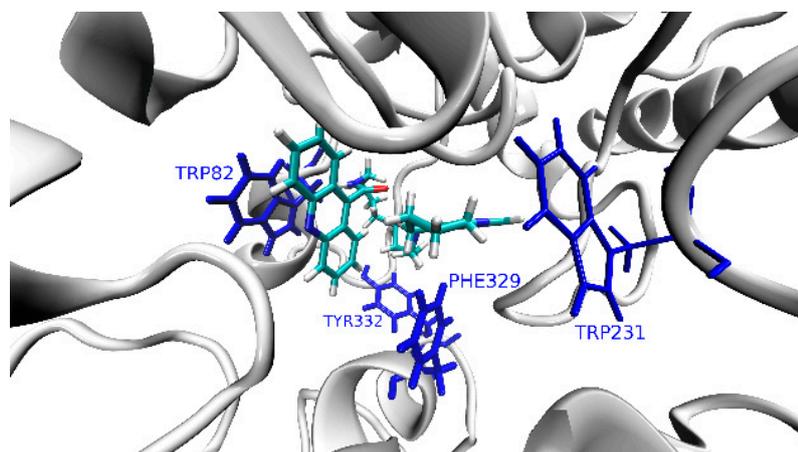
**Figure S10.** The binding mode of the **3d** ligand inside the pocket of BuChE. The key ligand-binding aromatic residues in the pocket of BuChE are marked in blue.



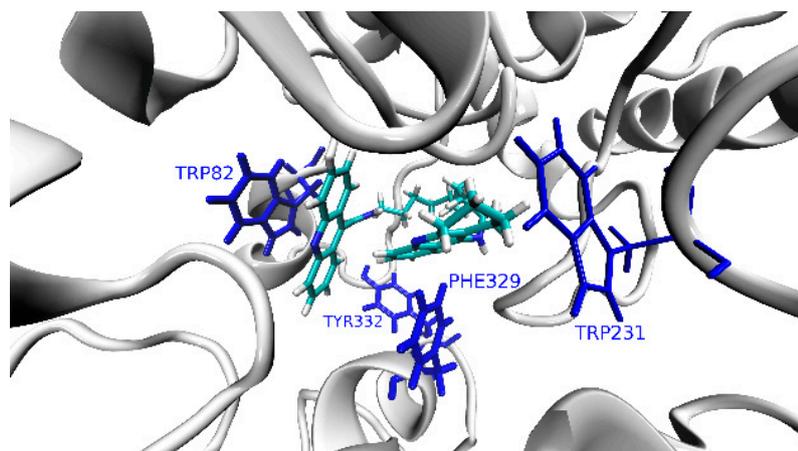
**Figure S11.** The binding mode of the **3e** ligand inside the pocket of BuChE. The key ligand-binding aromatic residues in the pocket of BuChE are marked in blue.



**Figure S12.** The binding mode of the **3f** ligand inside the pocket of BuChE. The key ligand-binding aromatic residues in the pocket of BuChE are marked in blue.



**Figure S13.** The binding mode of the **3g** ligand inside the pocket of BuChE. The key ligand-binding aromatic residues in the pocket of BuChE are marked in blue.



**Figure S14.** The binding mode of the **3h** ligand inside the pocket of BuChE. The key ligand-binding aromatic residues in the pocket of BuChE are marked in blue.