**Supplementary data**

**Figure S1:** Two-dimensional representations of the observed interactions between both enzymes and both ligands after docking procedure; residues in a green frame: van der Waals interaction, residues in a magenta frame: electrostatic interaction, Orange lines: $\pi-\pi$ interaction, blue dashed line with arrow at H-bond acceptor: hydrogen bond with amino acid side-chain; (a) AChE-bis(7)tacrine, (b) AChE- bis(7)tacrine(7)-SAC, (c) AChE-bis(7)tacrine, (d) BChE-bis(7)tacrine-SAC.
Figure S2: Two-dimensional representations of the observed interactions between both enzymes and both ligands after MD simulation; residues in a green frame: van der Waals interaction, residues in a magenta frame: electrostatic interaction, cyan small rectangles: water molecules, Orange lines: π–π interaction, blue dashed line with arrow at H-bond acceptor: hydrogen bond with amino acid side-chain, green dashed line with arrow at H-bond acceptor: hydrogen bond with amino acid main chain, black dashed line with arrow at H-bond acceptor: hydrogen bond with non-amino acid; (a) AChE-bis(7)tacrine, (b) AChE-bis(7)tacrine(7)-SAC, (c) AChE-bis(7)tacrine, (d) BChE-bis(7)tacrine-SAC.