Supporting Information

Active Components of Essential Oils as Anti-Obesity Potential Drugs investigated by *in silico* techniques

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Table 1S: Theoretical affinity values "G-score" in Kcal/mol of the best docked poses of compounds **1-10**, due to the ligand-target interactions within the CA I, CA II and CA VA catalytic sites by using the PDB X-ray crystal structures 1AZM, 4CQ0 and 1DMY, respectively. The Gscore values of AZA (**11**) best poses were computed by re-docking simulations.

COMPOUND	TARGET		
	CA I	CA II	CA VA
1	-7.53	-7.64	-7.68
2	-7.83	-7.17	-7.83
3	-8.11	-8.48	-8.26
4	-6.51	-6.64	-5.96
5	-7.87	-8.12	-8.21
6	-6.18	-5.52	-6.08
7	-6.16	-6.33	-5.85
8	-6.24	-6.06	-5.84
9	-7.56	-7.73	-7.35
10	-7.73	-7.60	-7.60
11	-5.99	-6.70	-6.69

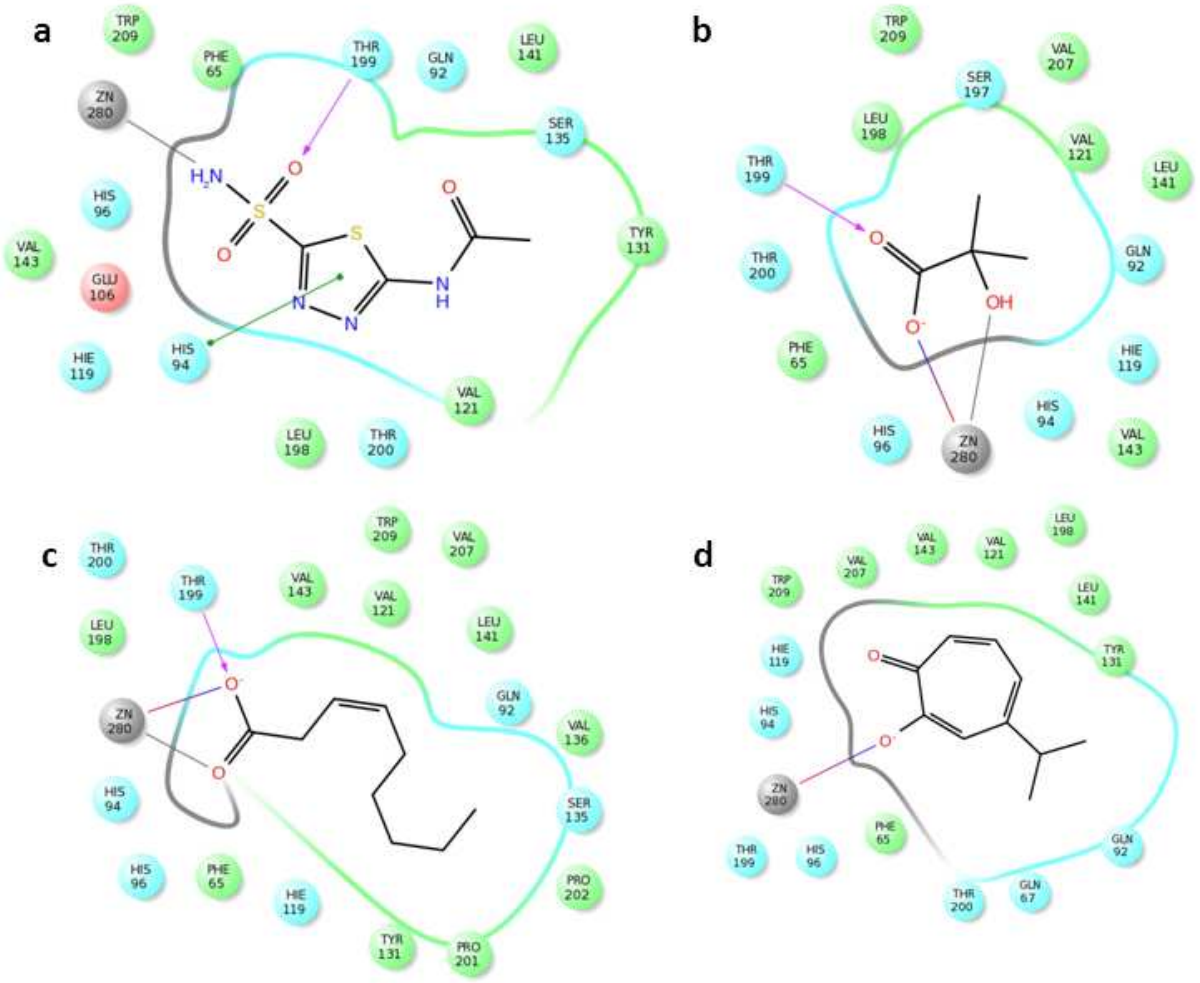

Figure 1S. Best docked poses of ligands **1** (d), **2** (b), **6** (c) and AZA **11** (a) in complex with CA VA. Ligand-target interactions were analyzed using the Maestro graphical interface. 2D depictions show hydrogen bonds (magenta arrows), π-π stacking interactions (green arrows), interacting hydrophobic and polar residues are respectively depicted as green and cyan spheres. Metal Zn ion is represented as grey sphere.

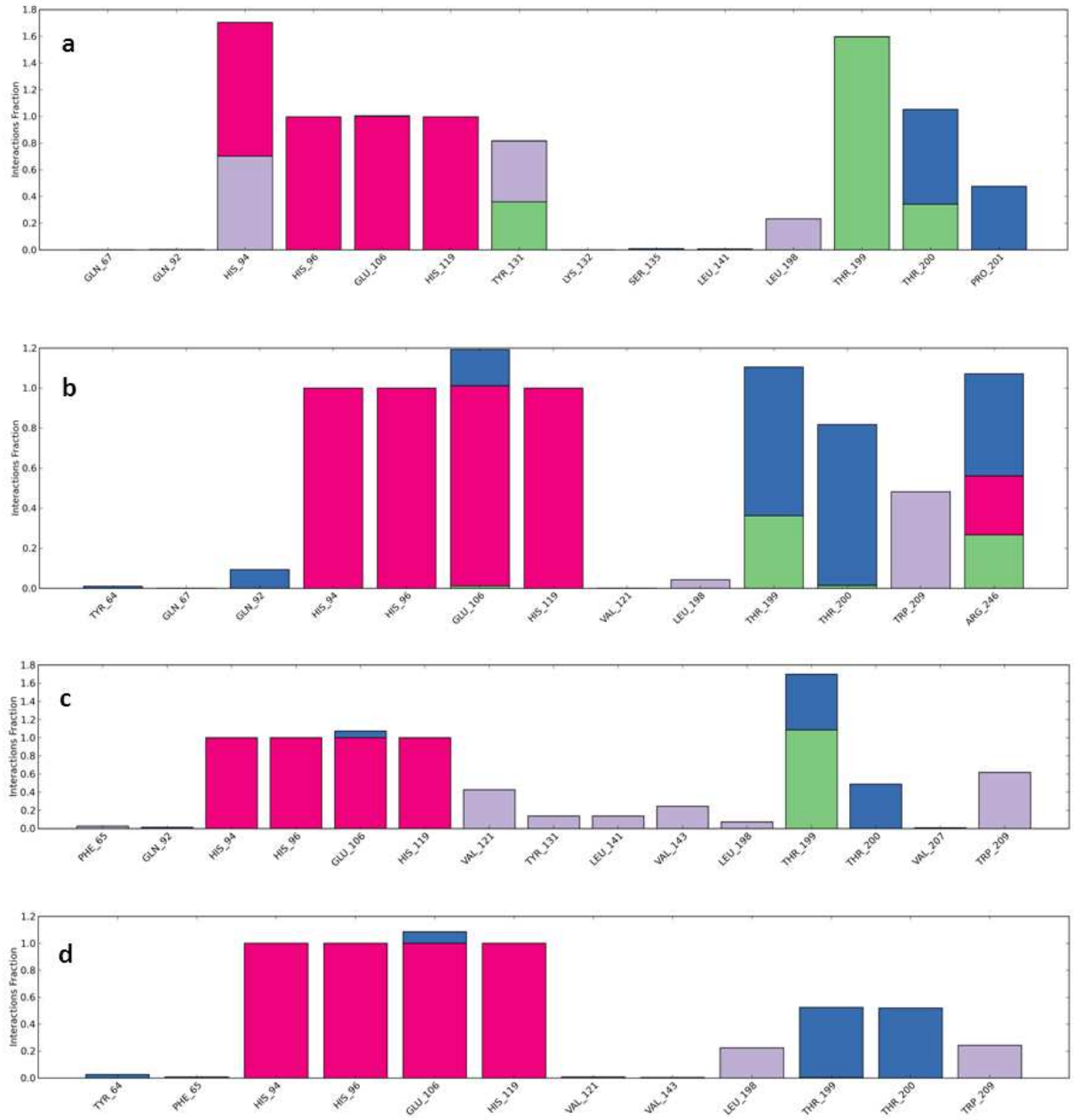

Figure 2S. Plots showing the protein-ligand interactions, established during the MD simulations, between the amino acid residues of CA VA binding site and the compounds **1** (d), **2** (b), **6** (c) and AZA **11** (a). The stacked bar charts are categorized as follow: hydrogen bond (green), hydrophobic (violet), ionic (pink) and water bridge (blue).