Discovery of new antioxidant molecules enhancing the Nrf2-mediated pathway: docking studies and biological evaluation

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Table S1. Calculated properties and descriptors according to the QikProp software of the selected compounds 1-4. 2

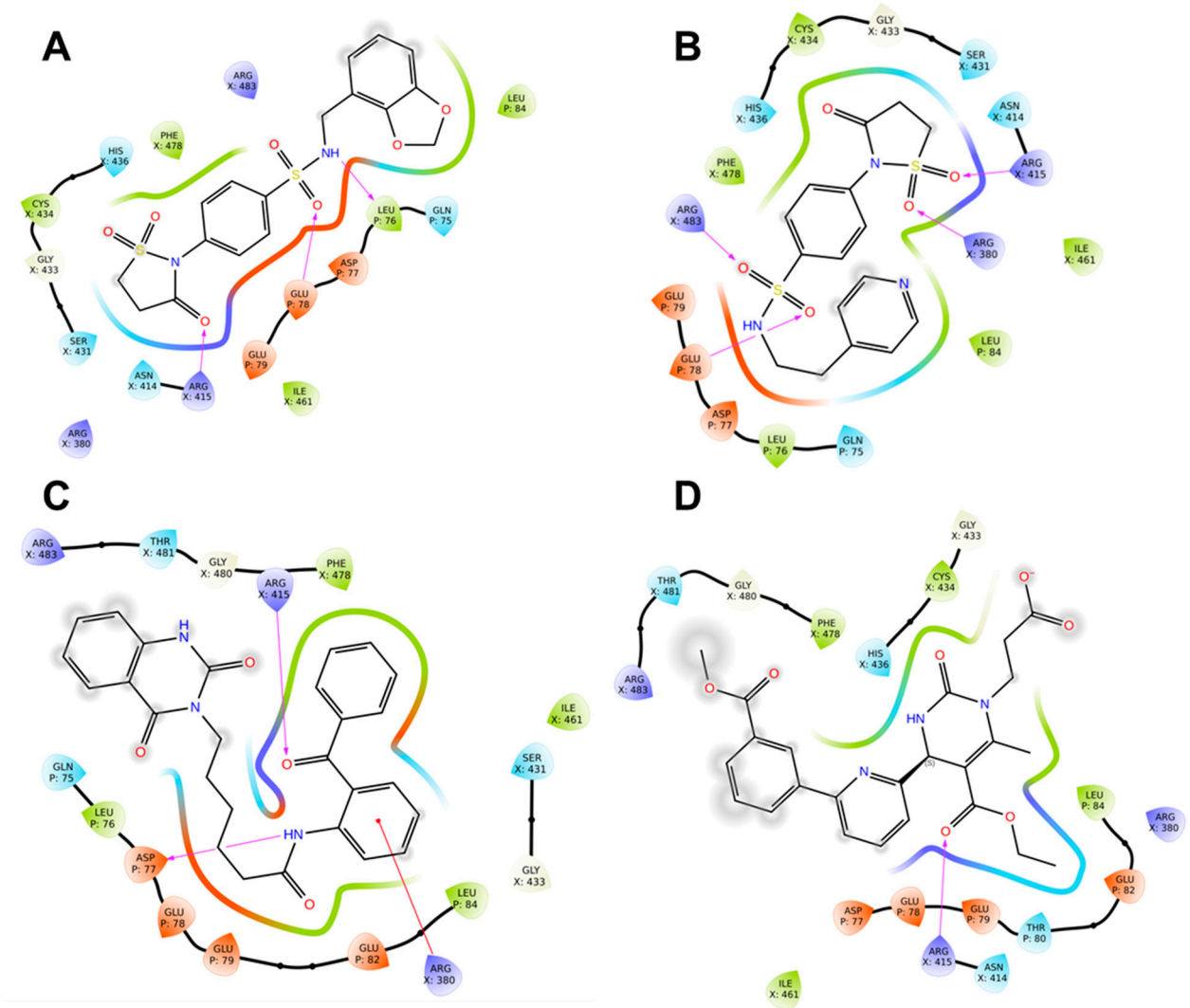


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Compound	1	2	3	4
#stars	0	0	2	0
#rtvFG	1	0	0	2
mol_MW	424.44	439.50	455.51	467.48
QPPlogBB	-1.589	-2.251	-1.195	-1.724

#stars: Number of property or descriptor values that fall outside the 95% range of similar values for known drugs (**Range or recommended values: 0-5**); **#rtvFG:** number of reactive functional groups, which can lead to false-positive in high-throughput screening (HTS) assays and to decomposition, reactivity, or toxicity problem *in vivo* (**Range or recommended values: 0-2**); **mol_MW:** Molecular weight of the molecule (**Range or recommended values: 130.0 - 725.0**); **QPPlogBB:** Predicted brain/blood partition coefficient (**Range or recommended values: -3.0 – 1.2**).