Poster #31

Computational Modeling of the Interactions Between Flavonoids and the Human Estrogen Receptor

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Flavonoids, isoflavonoids and related cyclic ether-containing natural products like the glyceollins, can bind to the human estrogen receptor (HER). The present computational study explores the strength and geometry of hydrogen bonds between cyclic ethers and polar, hydrogen-bond donor protein side chains. Interactions of cyclic ethers having various ring sizes with model molecules for serine, threonine, neutral and protonated histamine, and protonated lysine and arginine, have been studied at the ab initio MP2/6-31G* level. Basis set effects have been studied for selected pairs, and the net binding energy has been calculated by considering the basis set superposition error. Results are useful in understanding how the glyceollins may bind to HER and for designing artifical ligands for HER where the ether moiety has been favorably modified for enhanced binding.

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