Quercetin in water, studied with molecular simulations

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Quercetin, or 3,3',4',5,7-Pentahydroxyflavone, is an important molecule in biological photochemistry [1,2], belonging to the class of flavonoids. Quercetin has five hydroxyl groups at different kind of sites that can interact with the water molecules around it. It is therefore interesting to study how the solvation around the four OH groups differ. Here we want to study the quercetin solvated in the aqueous environment. This system has been widely studied experimentally. We report atomistic simulations to investigate the solvation of quercetin in liquid water. Both models of microsolvation and full solvation in explicit water are used. We characterise the solvation dynamics and describe spectroscopic quantities obtained from the simulations, and compare these to the available experimental results.

REFERENCES

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FIGURES