Predictive Atomistic Modeling of Antitumor Drug Encapsulation within Supramolecular Hosts

Lucija Vrban Đerek and Robert Vianello

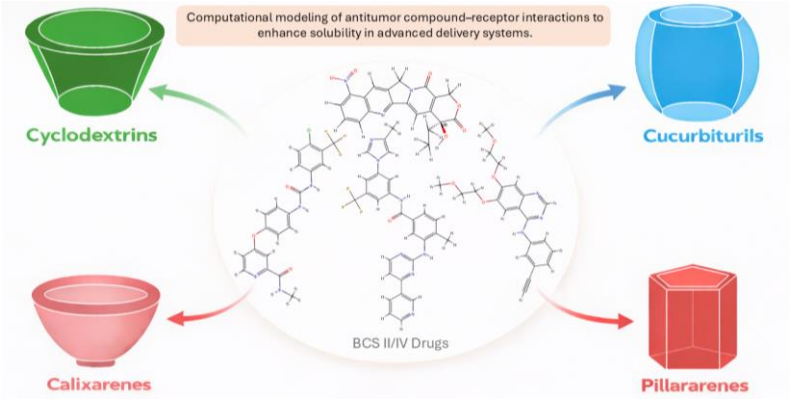
lucija.vrban@irb.hr

Ruđer Bošković Institute, Bijenička cesta 54, 10 000, Zagreb, Croatia

Supramolecular inclusion complexes based on macrocyclic receptors such as cyclodextrins and cucurbiturils offer promising strategies for improving the physicochemical and pharmacokinetic properties of antitumor drugs through non-covalent encapsulation. However, the molecular determinants of binding affinity, selectivity, and stability remain insufficiently understood [1].

In this study, a computational framework combining quantum chemical calculations, restrained electrostatic potential charges, molecular docking, molecular dynamics simulations, and binding free energy analysis was applied to investigate host–guest complexes of representative macrocycles and antitumor drugs [2].

The results provide atomistic insight into binding modes and key interactions, enabling quantitative affinity comparison and supporting predictive design of macrocycle-based drug delivery systems [3].



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