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SIZE DEPENDENCE OF HOST-GUEST INTERACTIONS OF *β*-CYCLODEXTRIN *IN SILICO*

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Cyclodextrins (CDs) are cyclic oligosaccharides with glucopyranose units bonded together with 1-4 linkages to form a truncated cone. The cavity within this cone can make inclusion complexes with various molecules; either engulfing part or the whole molecule. The outer surface of CDs is more hydrophilic than the interior. *β*-CDs, which consist of seven glucopyranose units, are used extensively in oral pharmaceutical formulations as a functional excipient. Measurements of the cavity size have been reported using molecular visualization software, however, the actual size range of guests that *β*-CD can accommodate has not been systematically studied. The glucopyranose rings can distort depending on the functional groups of the guest molecule and the nature of the surrounding environment (solvent, temperature, etc.). Therefore, a novel approach was taken to measure the size range of the guest molecules that *β*-CDs can accommodate irrespective of their geometry and chemistry. Molecular dynamic simulations were carried out using spherical implicit continuum particles with different sizes to observe complex-forming behaviour and to determine the maximum size of the guest molecule. The results revealed that the actual size range of the guest molecules that the *β*-CDs can complex is greater than expected, with the reported cavity size of 6.0 − 6.5 Å. Particles with the radius of 0.9 − 1.9 Å range make the complexes with *β*-CD. However, the full inclusion complexes only form for sizes 0.9 − 1.2 Å. From size 1.6 Å above they can make only partial complexes up to 1.9 Å. It should be noted that radial distribution plots of water around the probe particles show that the effective radius of particles is approximately 2.4 Å greater than the radius. Interestingly, some larger particles above the cavity size remain in close contact with the broader ring of the *β*-CD throughout a majority of the simulation time even though they did not make inclusion complexes. These results may help in the development of formulations and understanding the interaction of guest molecules with cyclodextrins.

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