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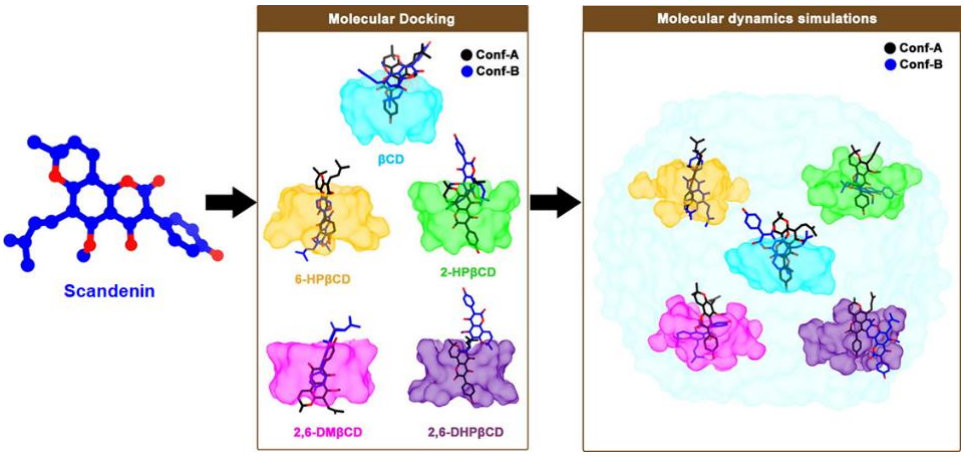
**Molecular insights into complex formation between scandenin and various types of β-cyclodextrin**

Molecular dynamics (MD) simulation of the inclusion complexes formation between scandenin, a phytochemical compound found in *D. scandens* (เถาวัลย์เปรียง), and different types of beta-cyclodextrins (βCDs) were carried out *via* two possible orientations of the guest molecule. The MD results revealed that scandenin preferentially located within all the studied βCDs nanocavities by inserting its hydroxyphenyl ring and pyran terminal close to the narrow and wider rims, respectively. In another feasible orientation, the guest substance was deeply included into the lipophilic cavity of only 6-hydroxypropyl βCD (6-HPβCD) and 2,6-dimethyl βCD (2,6-DMβCD). Altogether, our theoretical data could help in selecting suitable βCD derivatives to enhance the stability of such guest molecules prior to *in vitro* testing.




**Reference:**

Boonma T, Nutho B, Sungthong B, Sripadung P, Rungrotmongkol T, Nunthaboot N. Molecular insights into complex formation between scandenin and various types of β-cyclodextrin. Journal of Molecular Liquids, 2021;344: 117774. https://doi.org/10.1016/j.molliq.2021.117774

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