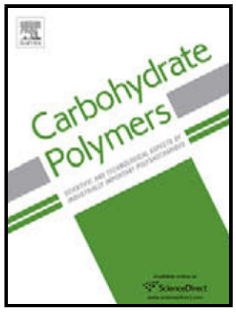


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# Mechanism and structure studies of cinnamaldehyde/cyclodextrins inclusions by computer simulation and NMR technology

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**Highlights**

- Inclusion mechanisms and structures of CNMA-CDs were investigated.
- Docking and molecule dynamics predicted detailed inclusion information.
- The inclusion abilities followed the order: DM > HP > β-CD.
- The benzene ring of CNMA inserted into hydrophobic cavity of CDs.
- The solubility and dissolution rate of CNMA were improved after inclusion.

## Abstract

This work aims to explore the inclusion mechanism and structure of cinnamaldehyde