# Binding Properties of Cucurbit[7]uril to Neutral and Protonated Amino Acids: A Computational Study

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## Abstract

We systematically investigate the binding nature of CB[7] towards 20 amino acids in both neutral (AAs) and protonated ($AAs^+$) states by quantum chemistry methods. The result indicates molecular recognition process are enthalpy-driven. Among AAs, Arg and Asn shows the largest binding strength to CB[7], and for $AAs^+$, $Gln^+$ and $Asn^+$ bind to CB[7] the strongest. The binding strength of protonated CB[7]/$AA^+$ is much stronger than that of neutral CB[7]/AA counterpart, due to the introduction of ion-dipole interaction and the increase number and strength of hydrogen bonds. Energy decomposition analysis (EDA) indicates that electrostatic interactions play major roles in both CB[7]/AAs and CB[7]/$AAs^+$ complexes. Moreover, we analyzed the dependence of binding strength on single AA volume and dipole moment. This study is benefit for providing valuable information in predicting the recognition sites for sequence-based peptide or protein by CB[7] and rationally designing synthetic host molecule for specific peptide or protein recognition.

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