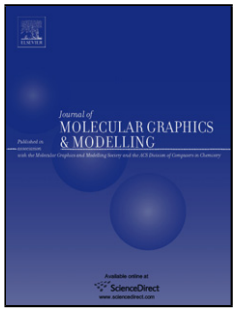

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PII: S1093-3263(17)30308-X
DOI: http://dx.doi.org/doi:10.1016/j.jmgm.2017.07.016
Reference: JMG 6975

To appear in: *Journal of Molecular Graphics and Modelling*

Received date: 26-4-2017
Revised date: 14-7-2017
Accepted date: 17-7-2017

Please cite this article as: Lihua Dong, Shujun Zhang, Yongjun Liu, A water-assisted nucleophilic mechanism utilized by BphD, the meta-cleavage product hydrolase in biphenyl degradation, Journal of Molecular Graphics and Modellinghttp://dx.doi.org/10.1016/j.jmgm.2017.07.016

A water-assisted nucleophilic mechanism utilized by BphD, the *meta*-cleavage product hydrolase in biphenyl degradation

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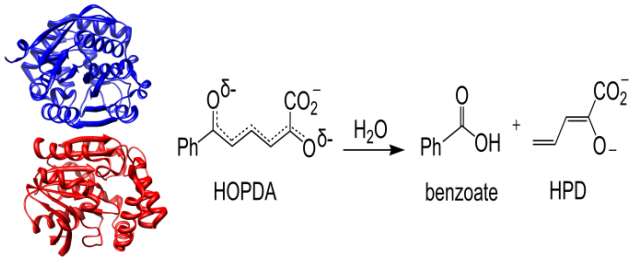
Graphical abstract



Highlights:

- The catalytic mechanism of BphD has been elucidated by using QM/MM calculations.
- The hydrolysis of C-C bond contains two half-reactions: acylation and deacylation.
- An active site water molecule is suggested to play important roles for the deprotonation of Ser112.
- The mechanism of BphD may highlight the versatility of Ser-His-Asp triad.

Abstract: As members of the *α/β*-hydrolase superfamily, *Meta*-cleavage product (MCP) hydrolases generally utilize a Ser-His-Asp catalytic triad to hydrolyze the cleavage of C-C bond during the aerobic catabolism of aromatic compounds by bacteria. BphD is one kind of MCP hydrolase that catalyzes the hydrolysis of 2-hydroxy-6-oxo-6-phenylhexa-2,4-dienoic acid (HOPDA) to 2-hydroxypenta-2,4-dienoic acid (HPD) and benzoate. In this article, a combined quantum mechanics and molecule mechanics (QM/MM) approach has been employed to explore the reaction mechanism of BphD from *Burkholderia*