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Exploring the quantum mechanical/molecular mechanical replica path method: a pathway optimization of the chorismate to prephenate Claisen rearrangement catalyzed by chorismate mutase

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#	Paper	IF	Citations
96	A DFT-Based QM-MM Approach Designed for the Treatment of Large Molecular Systems: Application to Chorismate Mutase. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 13728-13736	3.4	110
95	Parallel iterative reaction path optimization in ab initio quantum mechanical/molecular mechanical modeling of enzyme reactions. <i>Journal of Chemical Physics</i> , 2004 , 121, 697-706	3.9	43
94	Adapting the nudged elastic band method for determining minimum-energy paths of chemical reactions in enzymes. <i>Journal of Chemical Physics</i> , 2004 , 120, 8039-52	3.9	65
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