阅读日期：20190506

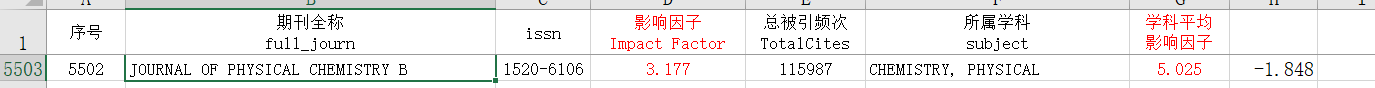
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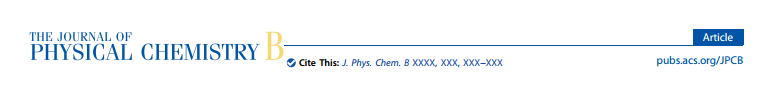
发表杂志：PHYSICAL CHEMISTRY

影响因子：

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| 文章名 Ensemble Docking in Drug Discovery How Many Protein Configurations from Molecular Dynamics Simulations are Needed To Reproduce Known Ligand Binding？ | |
| 中文译名 | 药物发现中的集成对接:从分子动力学模拟中需要多少种蛋白质构型才能复制已知的配体结合? |
| 网址 |  |
| 关键词 |  |
| 摘要 | Ensemble docking in drug discovery or chemical biology uses dynamical simulations of target proteins to generate binding site conformations for docking campaigns. We show that 600 ns molecular dynamics simulations of four G-proteincoupled receptors in their membrane environments generate ensembles of protein configurations that, collectively, are selected by 70−99% of the known ligands of these proteins. Therefore, the process of ligand recognition by conformational selection can be reproduced by combining molecular dynamics and docking calculations. Clustering of the molecular dynamics trajectories, however, does not necessarily identify the protein conformations that are most often selected by the ligands.  因此，结合分子动力学和对接计算，可以再现构象选择识别配体的过程。然而，分子动力学轨迹的聚类不一定能确定配体最常选择的蛋白质构象。 |
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