



学术讲座



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Computational Study and Design of Small-Molecule & Peptide-based MDM2 Inhibitors

报告摘要:

As the “guardian of the genome”, p53 plays a very important role in biological systems. It acts as transcription factor and more importantly as a tumor suppressor protein. The level of p53 in cells is negatively regulated by MDM2 via an autoregulatory feedback loop. However, in many tumor cells, MDM2 is overexpressed and highly impair the function of p53 to suppress tumor. This study was to design effective inhibitors to block p53 and MDM2 interactions using computational methods, to offer a novel strategy to conquer cancer. With analysis using molecular dynamics simulation, we were focusing on better understanding the interactions of small-molecule and peptide-based MDM2 inhibitors. In addition, accurate binding free energy and energetic contribution of single residue were calculated using GBVI/WSA method. Furthermore, optimized small-molecule and peptide-based MDM2 inhibitors were designed and evaluated to have improved binding affinities.

个人简介:

Yujing ZHOU is currently a PhD candidate in the NUS Graduate School of Integrative Sciences & Engineering under the supervision of Prof Richard Wong and is going to obtain her PhD degree in 2015. She earned her Bachelor of Science with Honors degree from National University of Singapore in 2011. The topic of her research is the computational study of interactions of small-molecule and peptide-based inhibitors.

