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Study of 1-H Pyrrolo[3,2-c]pyridine MPS1 Inhibitors by Topomer CoMFA, Virtual screening and Molecular Dynamics Simulation

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SUMMARY. **In this study, 10 potential MPS1 inhibitors were obtained by Topomer CoMFA, virtual screening based on Topomer search and molecular docking. Firstly, the 41 1-H Pyrrolo[3,2-c]pyridine MPS1 inhibitors were carried out to establish a Topomer CoMFA. q^2 and r^2 of the Topomer CoMFA model is 0.501, 0.803, and shows a good prediction ability which lays a foundation for the next virtual screening. Next, 1505384 molecules of ZINC library were selected by Topomer search and molecular docking. Finally 10 potential MPS1 inhibitors were obtained, moreover finding ZINC44324562 is a potential small molecule inhibitor of Mps1 by molecular dynamics simulation.**

RESUMEN. En este estudio fueron obtenidos 10 inhibidores potenciales MPS1 por Topomer CoMFA, el cribado virtual basado en la búsqueda Topomer y acoplamiento molecular. En primer lugar, los 41 inhibidores de MPS1 1-H pirrolo [3,2-c] piridina se utilizaron para establecer un Topomer CoMFA. Los valores q^2 y r^2 del modelo Topomer CoMFA son 0,501 y 0,803, mostrando una buena capacidad de predicción, que establece una base para la próxima selección virtual. A continuación, 1505384 moléculas de la biblioteca ZINC fueron seleccionados por la búsqueda Topomer y acoplamiento molecular. Finalmente se obtuvieron 10 inhibidores potenciales MPS1. Por otra parte por simulación de dinámica molecular se encontró que ZINC44324562 es una molécula pequeña que es un potencial inhibidor de Mps1.

KEY WORDS: molecular dynamics simulation, molecular docking, MPS1, Topomer CoMFA, Topomer search, virtual screening.

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