Comparative Network Pharmacology Analysis of Ethyl Acetate, n-Butanol and Residual Fractions of Stachytarpheta jamaicensis Against Lung Cancer

In Silico Pharmacology

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Online Resource 6 Superimposition of the crystallographic and redocked poses of the co-crystallized ligand MPZ in the SRC kinase ATP site (PDB 1Y57). The crystallographic pose and the redocked pose are shown overlaid within the binding site, with surrounding residues displayed. The central binding scaffold is closely reproduced (regional RMSD 0.76 Å) while the solvent-exposed peripheral and piperazine-containing portions diverge (5.00 Å and 6.98 Å respectively), accounting for the elevated whole-ligand RMSD of 3.38 Å. The hinge hydrogen bond to Met341 observed in the crystal structure is retained in the redocked pose. Image generated in Maestro (Schrödinger Suite, Release 2024-1).

