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# Title: Naturally occurring plant-based anticancerous candidates as prospective ABCG2 inhibitors: an in silico drug discovery study

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ATP-binding cassette transporter G2 (ABCG2) is an efflux transporter related to the clinical multidrug resistance (MDR) phenomenon. Identifying ABCG2 inhibitors could help discover extraordinary curative strategies for carcinoma remediation. Hitherto, there is no medication drug inhibiting ABCG2 transporter, notwithstanding that a considerable number of drugs have been submitted to clinical-trial and investigational phases. In the search for unprecedented chemical compounds that could inhibit the ABCG2 transporter, an in silico screening was conducted on the Naturally Occurring Plant-based Anticancer Compound-Activity-Target (NPACT) database containing 1574 compounds. Inhibitor-ABCG2 binding affinities were estimated based on molecular docking and molecular minimization (MM) calculations and compared to a co-crystallized inhibitor (BWQ) acting as a reference inhibitor. Molecular dynamics (MD) simulations pursued by molecular mechanics-generalized Born surface area (MM-GBSA) binding energy estimations were further executed for compounds with MM-GBSA//MM binding energies lower than BWQ (calc. ☐ 60.5 kcal/mol). Two compounds demonstrated auspicious inhibitory activities according to binding affinities (ΔGbinding) over the 100 ns MD simulations that were nearly one and a half folds compared to BWQ. Throughout the 100 ns MD simulations, structural and energetical analyses unveiled outstanding stability of the ABCG2 transporter when bound with the identified inhibitors. In silico calculations hold a promise for those two inhibitors as drug candidates of ABCG2 transporter and emphasize that further in vitro and in vivo experiments are guaranteed.