

Molecular docking studies of the antitumoral activity and characterization of new chalcone

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© 2015, Bentham Science Publishers. Phytochemical investigation of *Azorella madreporica* led to the isolation of four known compounds and an unknown chalcone. The structure of the new compound was identified by spectroscopy, including two-dimensional NMR techniques and comparison with published spectral data. The antioxidant activity of chalcone (compound 1) was measured using the 1,2-diphenyl-2-picryl-hydrazyl (DPPH) free radical scavenging assay, and the bioactivity was evaluated against five bacteria (*Mycobacterium smegmatis* ATCC 14468, clinical isolates of *Staphylococcus aureus*, *Klebsiella granulomatis*, *Morganella morganii* and *Escherichia coli*) and four cancer cell lines. Docking studies with the tested cancer related proteins revealed nearby values of energy between doxorubicin and compound 1. Besides, protein-ligand interactions correlate with these energy values.