Virtual screening of natural compounds from Brazilian semiarid plants targeting GABA receptor inhibitors

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Different Brazilian semiarid plant species are widely used in popular medicine because they have sedative, anxiolytic, anticonvulsant and central analgesic effects. This study investigated in silico psychopharmacological action of these plant compounds by docking them human GABAA receptor.The ligands used in this work are deposited in The SAM Database, hosted at the Laboratory of Bioinformatics and Computational Chemistry from Universidade Estadual do Sudoeste da Bahia, Jequié, Brazil. All compounds were isolated from brazilian semiarid plant species with psychopharmacological activity. The molecular structures of the ligands were prepared in Marvin Sketch (Chemaxon) for verification of the valences and structural errors, and then saved in mol2 format. The AutoDock tools was used to prepare the ligands for docking studies and convert them to pdbqt format. Furthermore, it was defined the region of interaction with potential inhibitors (gridbox) and recorded coordinates. The molecular docking calculation was performed using the AutoDock Vina program. Ligand docking poses with better energy values were choosed using PyMOL 1.7, as well as for obtaining the complexes in pdb format. The interaction maps for each best energy complex were generated using Discovery Studio 4.0 program. We tested 78 chemical structures in molecular docking studies described for Brazilian semiarid plants against GABA receptor. Even different structures have presented good interactions with the receptor, SAM2800 and SAM 3201 compounds showed the highest interaction with the target, and presented better affinity energies (-10,2 kcal/Mol) in comparison to Diazepam® (-9,0kcal/Mol). Therefore, this study reports the need for further research on the extracts and isolated compounds *in vitro* and *in vivo* in order to validate the therapeutic properties of these plants, and thus its chemical constituents can become future drug candidates.