Title: Comparison of AutoDock 4.2.6, AutoDock Vina 1.1.2 and Glide 6.6

docking methods to reproduce the binding energy of twelve macrolides

to their receptors.

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Evaluation of the docking performance of AutoDock 4.2.6, AutoDock Vina 1.1.2 and Glide 6.6, using crystallographic data of eight macrolides, has been carried out by means of self-docking and conformational docking. Then, a docking protocol has been suggested which has been applied on four amphidinolides that are being investigated in the research group.