

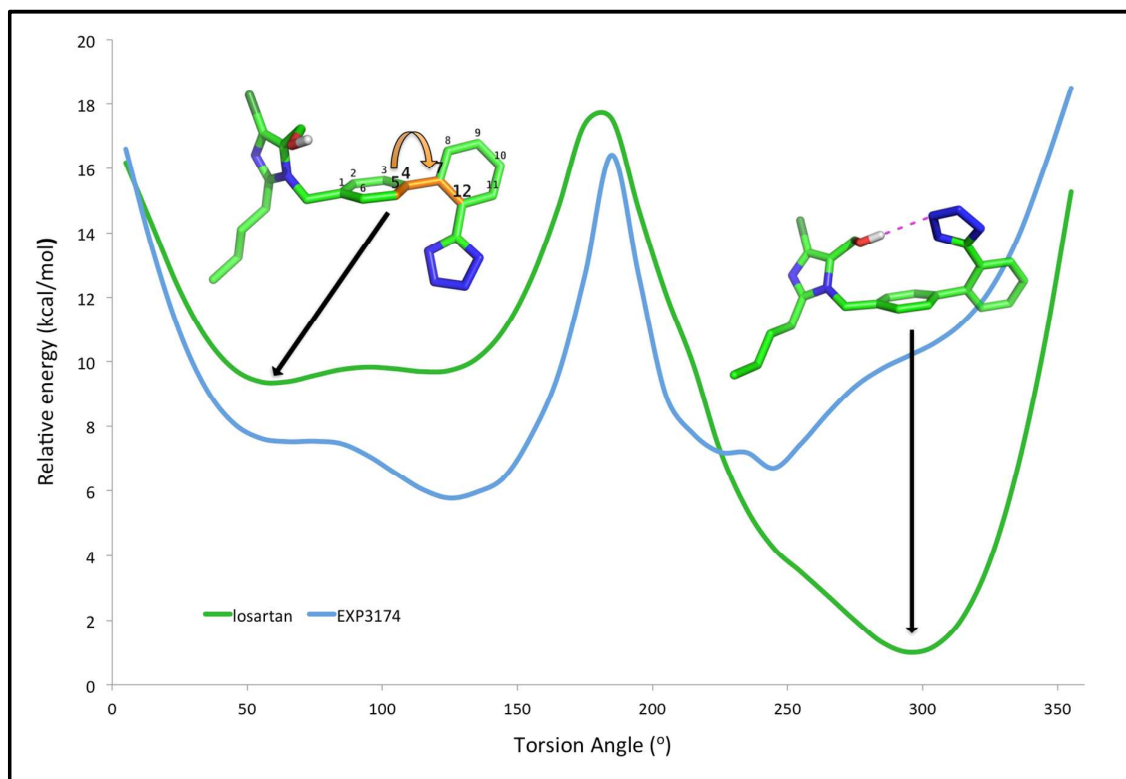
SUPPLEMENTARY INFORMATION

Ligand Binding Determinants for Angiotensin II type 1 Receptor from Computer Simulations

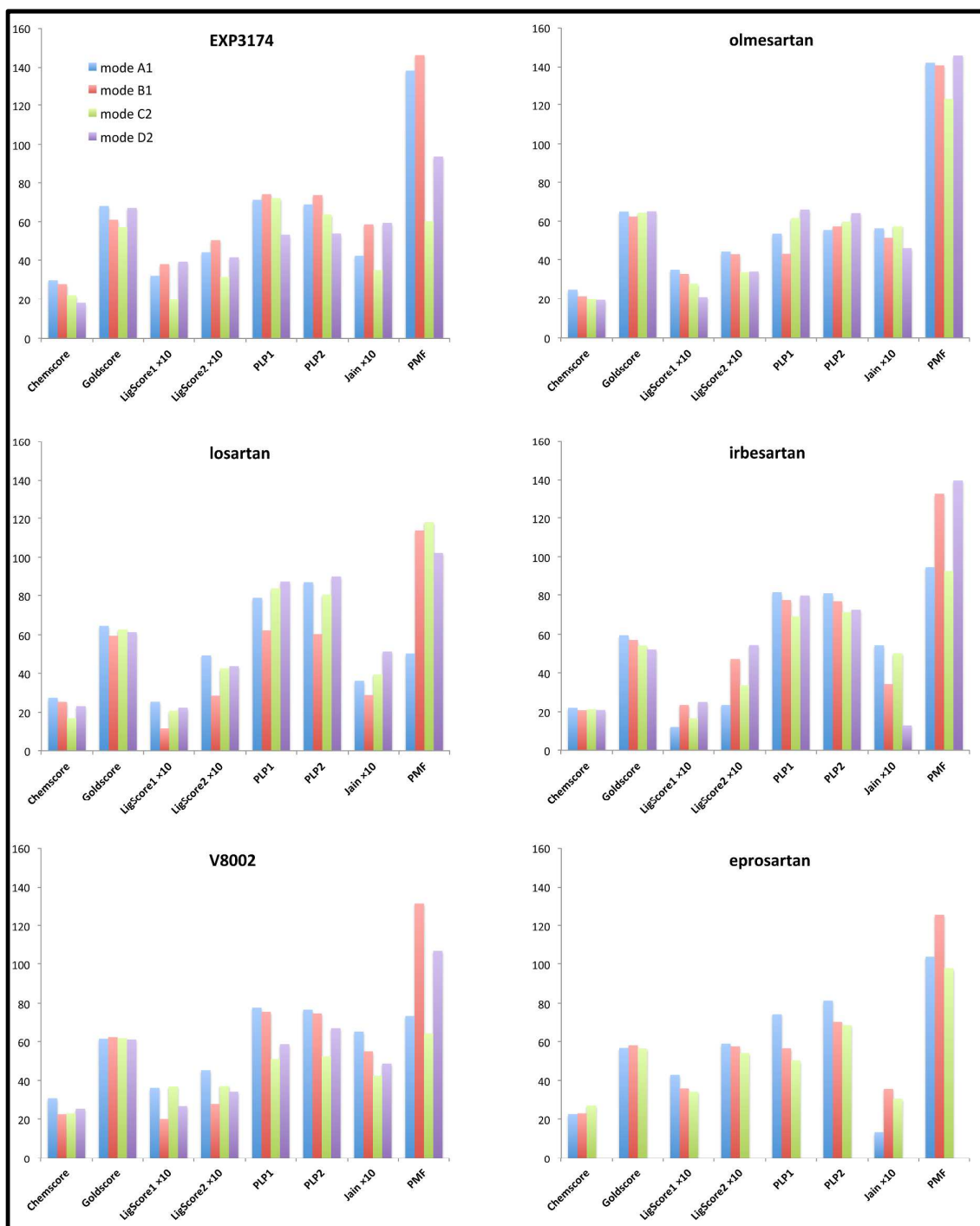
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Supplementary Figure 1. Relative energies (kcal/mol), calculated at the B3LYP/6–31G* level of theory, of losartan (green) and EXP3174 (blue) corresponding to a full rotation of the torsional angle C12-C7-C4-C5 (in orange).



Supplementary Figure 2. Docking scores for binding modes A1, B1, C2 and D2, evaluated with several scoring functions. Functions LigScore1, LigScore2 and Jain are multiplied by a factor of 10 for comparison and clarity reasons. For eprosartan, mode of binding D2 was not found as a docking solution.