



Virtual-screening methodology used in this study. Solid black lines represent the three sets of compounds used to generate the RF model for EC₅₀ β_1 receptor adrenergic, EC₅₀ β_2 receptor adrenergic, IC₅₀ β_1 receptor adrenergic and IC₅₀ β_2 receptor adrenergic and to validate them (solid gray line – external test set). The black dotted lines represent the 786 from the alkaloids of Menispermaceae. The black dash-dot line represents both datasets (CHEMBL). The black dash line represents the five enzyme structures from the PDB databank (4amj, 4qkx, 2ycy, 3nya). The dash-dot border delimits the process performed in the KNIME software.