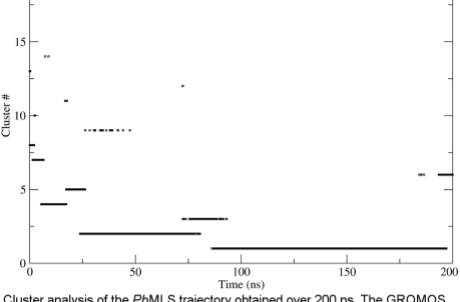
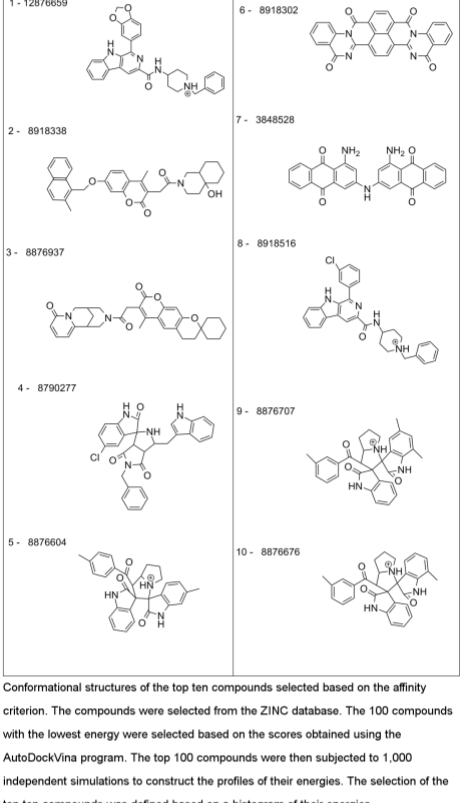


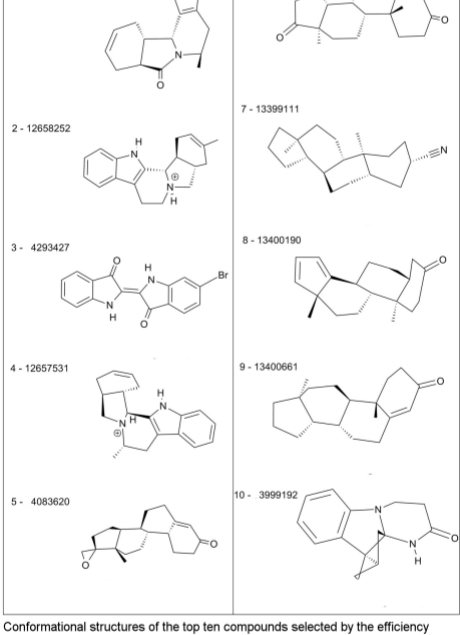
Flowchart to screening of compounds by affinity and efficiency.



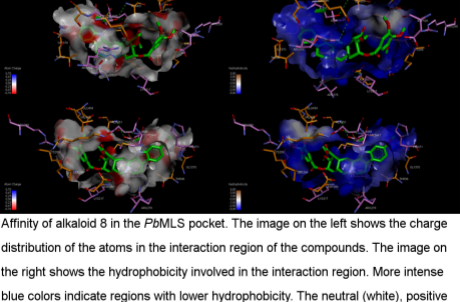
Cluster analysis of the *PbMLS* trajectory obtained over 200 ns. The GROMOS algorithm with a cutoff of 0.3 nm was selected. The clusters were determined using the non-hydrogen-atom RMSD values



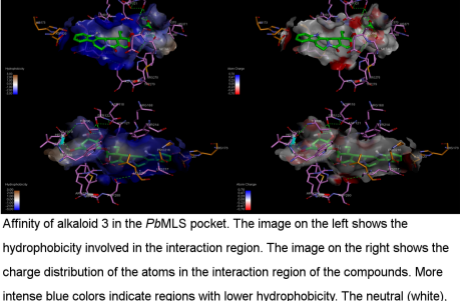
Conformational structures of the top ten compounds selected based on the affinity criterion. The compounds were selected from the ZINC database. The 100 compounds with the lowest energy were selected based on the scores obtained using the AutoDockVina program. The top 100 compounds were then subjected to 1,000 independent simulations to construct the profiles of their energies. The selection of the top ten compounds was defined based on a histogram of their energies.



Conformational structures of the top ten compounds selected by the efficiency criterion. The compounds were selected from the ZINC database. The 100 compounds with the lowest energy were selected based on the scores obtained with the AutoDockVina program. The top 100 compounds were then subjected to 1,000 independent simulations to construct the profile of their energies. The selection of the top ten compounds was based on a histogram of their energies.



Affinity of alkaloid 8 in the *PbMLS* pocket. The image on the left shows the charge distribution of the atoms in the interaction region of the compounds. The image on the right shows the hydrophobicity involved in the interaction region. More intense blue colors indicate regions with lower hydrophobicity. The neutral (white), positive (blue) and negative (red) atoms are indicated.



Affinity of alkaloid 3 in the *PbMLS* pocket. The image on the left shows the hydrophobicity involved in the interaction region. The image on the right shows the charge distribution of the atoms in the interaction region of the compounds. More intense blue colors indicate regions with lower hydrophobicity. The neutral (white), positive (blue) and negative (red) atoms are indicated.