

Table S11. Corresponding SMILES of the top 3 predicted compounds.

Term	SMILES
phenoxybenzamine CTD 00006514	<chem>CC(COC1=CC=CC=C1)N(CCCl)CC2=CC=CC=C2</chem>
rimexolone HL60 UP	<chem>CCC(=O)[C@]1([C@@H](C[C@@H]2[C@@]1(C[C@@H]([C@H]3[C@H]2CCC4=CC(=O)C=C[C@]34C)O)C)C)C</chem>
NSC321521 CTD 00005452	<chem>CC[PH+](CC)CC.CC(=O)OCC1C(C(C(O1)[S-])OC(=O)C)OC(=O)C)OC(=O)C.[Au+]</chem>