Notes on the workflow

1. **Get Structure of receptor-agonist complex from Protein Data Bank**
   This is the crystal structure (5C1M) of the agonist interacting with the receptor protein. From this file we can obtain the structures of the receptor and the agonist.

2. **Prepare the files for the ligand and the receptor.**
   Here we need to create the pdbqt files for the two structures. This file format is specifically needed by the docking software smina.

3. **Run docking calculations on for the complex**
   Here we re-dock the agonist-receptor complex. We define the affinity of the agonist for the receptor.

4. **Query PubChem for list of similar compounds**
   Here we want to search for new chemical compound with better affinity and therefore we create a similarity search job on PubChem.
   Similarity Threshold: 75%
   Default Similarity Algorithm:

5. **Download Compounds and Smiles**
   Simply downloading, from PubChem, the compounds returned by the query jobs with their relative SMILES strings.

6. **Run Docking Calculation for new compounds**
   Docking calculations for compounds downloaded from PubChem. The idea is to quantify the affinity for the receptor and check for potential lead compounds with better affinity.

7. **Identify compounds with higher affinity**
   Pick compound(s) with best score for affinity. If desired repeat from query process (step 4) using the newly found ligand as input of the similarity search.

SMINA docking calculation options:

Version: smina 2020.12.10
--Autobox-ligand: Reference ligand for docking site definition: VF1 AGONIST
--Autobox-add
--Exhaustiveness: 8 (Default Value from SMINA)