

Hands-on exercises to the lecture „Modern Methods in Drug Discovery“ WS24/25

The “Draw Structure” option of the PubChem database allows you to depict your SMILES and SMARTS, which opens a separate window:

<https://pubchem.ncbi.nlm.nih.gov/#draw=true>

The screenshot shows the PubChem homepage. At the top, there is the NIH National Library of Medicine logo and the PubChem logo. Below the logo, there are navigation links: About, Blog, Submit, and Contact. The main heading is "Explore Chemistry" with the subtitle "Quickly find chemical information from authoritative sources". A search bar is present with a magnifying glass icon. Below the search bar, there are several search suggestions: "Try covid-19 aspirin EGFR C9H8O4 57-27-2 C1=CC=C(C=C1)C=O InChI=1S/C3H6O/c1-3(2)4/h1-2H3". There are also radio buttons for "Use Entrez", "Compounds", "Substances", and "BioAssays". At the bottom, there are four icons with labels: "Draw Structure", "Upload ID List", "Browse Data", and "Periodic Table".

The screenshot shows the "DRAW STRUCTURE" window in PubChem. The window title is "DRAW STRUCTURE". At the top, there is a dropdown menu for "Broadband" and a dropdown menu for "SMILES". The SMILES string is C1(=CC=CC=C1)C[N]C(C)=O. Below the SMILES string, there is a toolbar with various drawing tools. A periodic table is visible in the background, with the element Nitrogen (N) highlighted in yellow. The chemical structure of N-acetylbenzylamine is shown in the center of the window. At the bottom, there is a button labeled "Search for This Structure".

Try to find correct SMILES for the following structures:

Tip: Type your SMILES in a text editor program first and then copy/paste them into the PubChem editor. Hit the "NEW" button to delete the input before each new try.

