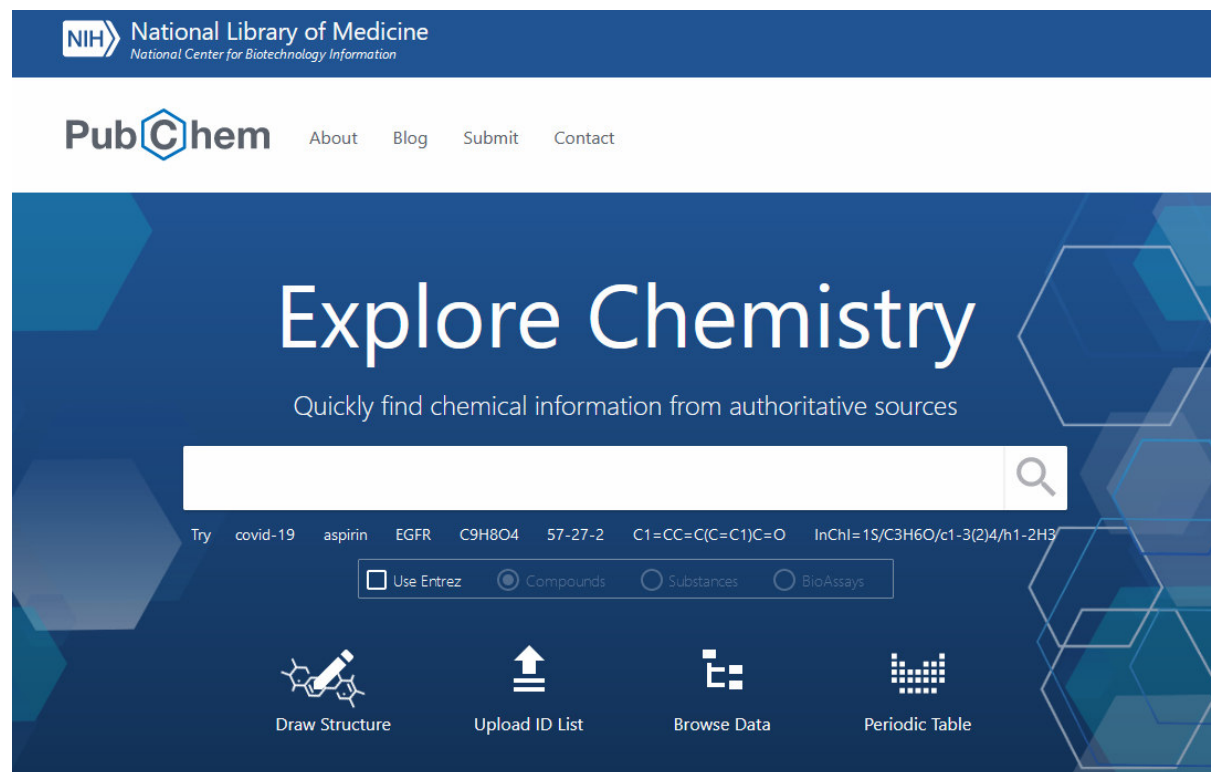


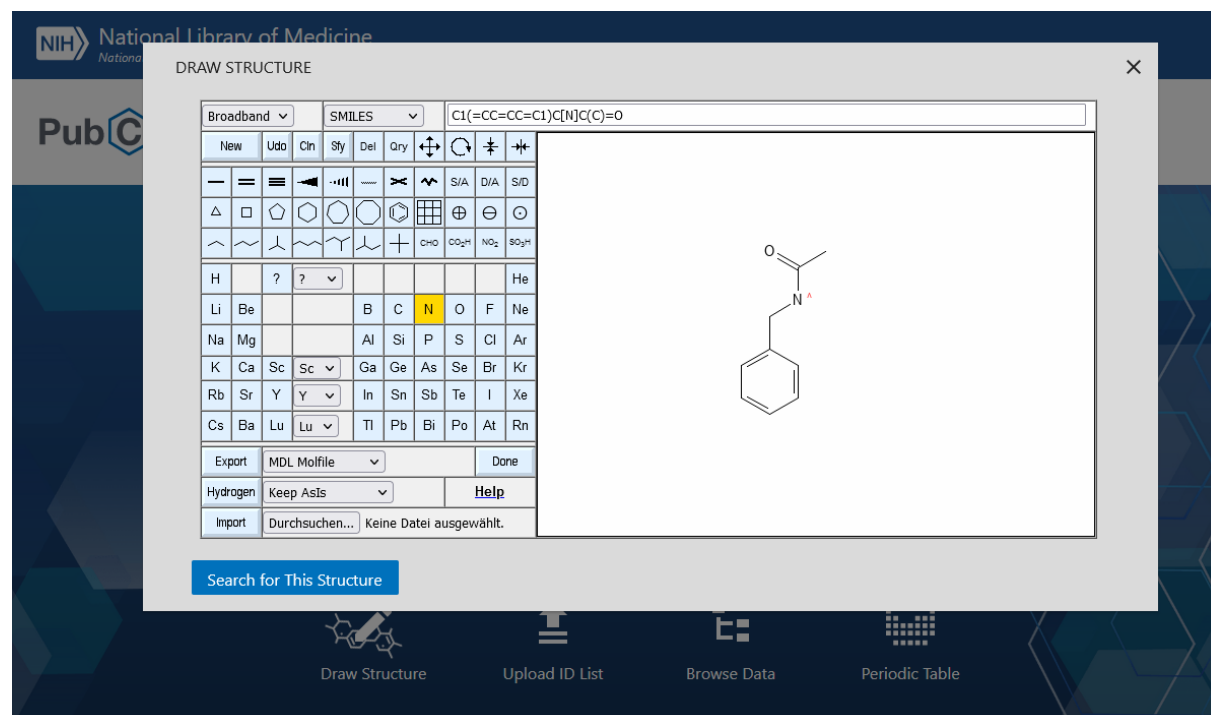
Hands-on exercises to the lecture „Modern Methods in Drug Discovery“ WS25/26

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 with the NIH logo and the text "National Library of Medicine" and "National Center for Biotechnology Information". The main heading is "Explore Chemistry" with the subtitle "Quickly find chemical information from authoritative sources". A search bar is present, and below it, a row of buttons includes "Try", "covid-19", "aspirin", "EGFR", "C9H8O4", "57-27-2", "C1=CC=C(C=C1)C=O", and "InChI=1S/C3H6O/c1-3(2)4/h1-2H3". Below these are four radio buttons: "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 has a title bar with "DRAW STRUCTURE" and a close button. It features a toolbar with various drawing tools like lines, polygons, and rings. Below the toolbar is a periodic table with elements color-coded by groups. The main area displays the chemical structure of N-methylbenzamide, which was generated from the SMILES string CN(C)C(=O)c1ccccc1 entered in the input field. The input field also shows the SMILES string C1(=CC=CC=C1)C[N]C(C)=O. At the bottom, there are buttons for "Export", "MDL Molfile", "Done", "Hydrogen", "Keep AsIs", "Help", and "Import". A "Search for This Structure" button is also visible.

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.

