

## Hands-on exercises to the lecture „Modern Methods in Drug Discovery“ WS21/22

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 following elements:

- NIH National Library of Medicine logo and text: "National Center for Biotechnology Information".
- PubChem logo and navigation links: "About", "Blog", "Submit", "Contact".
- Header text: "Explore Chemistry" and "Quickly find chemical information from authoritative sources".
- A search bar with a magnifying glass icon.
- Below the search bar, a row of 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".
- Radio buttons for search filters: "Use Entrez" (checked), "Compounds", "Substances", "BioAssays".
- Four main navigation icons: "Draw Structure" (pencil and flask), "Upload ID List" (upload arrow), "Browse Data" (grid), and "Periodic Table" (periodic table grid).

The screenshot shows the "DRAW STRUCTURE" window with the following elements:

- NIH National Library of Medicine logo and text: "National Center for Biotechnology Information".
- PubChem logo.
- Window title: "DRAW STRUCTURE".
- Input fields: "Broadband" (dropdown), "SMILES" (dropdown), and a text box containing the SMILES string: C1(=CC=CC=C1)C[N](C)C=O.
- A toolbar with various drawing tools: "New", "Undo", "Cln", "Sty", "Del", "Qry", "↕", "↻", "↶", "↷", "S/A", "D/A", "S/D", "△", "□", "○", "⊕", "⊖", "⊙", "⌒", "⌒", "⌒", "⌒", "⌒", "⌒", "⌒", "⌒", "CHO", "CO<sub>2</sub>H", "NO<sub>2</sub>", "SO<sub>3</sub>H".
- A periodic table with the element Nitrogen (N) highlighted in yellow.
- Export options: "Export" (dropdown), "MDL Molfile" (dropdown), "Done".
- Hydrogen options: "Hydrogen" (dropdown), "Keep AsIs", "Help".
- Import options: "Import" (dropdown), "Durchsuchen...", "Keine Datei ausgewählt".
- A central area displaying the chemical structure of N-(benzyl)acetamide.
- A blue button at the bottom: "Search for This Structure".
- Navigation icons at the bottom: "Draw Structure", "Upload ID List", "Browse Data", "Periodic Table".

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.

