

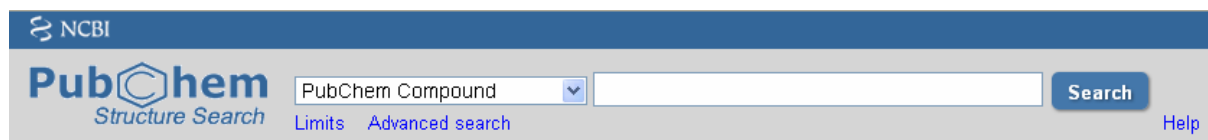
Hands-on exercises to the lecture „Modern Methods in Drug Discovery“ WS19/20

The Chemical Structure Search option of the PubChem database allows you to depict your SMILES and SMARTS using the Sketch button that opens a separate window:

<https://pubchem.ncbi.nlm.nih.gov/edit3/index.html> or

<https://pubchem.ncbi.nlm.nih.gov/search/search.cgi>

menu item: Substructure/Superstructure , Launch the PubChem editor



NCBI
PubChem
Structure Search
PubChem Compound [v] [input field] Search
Limits Advanced search Help

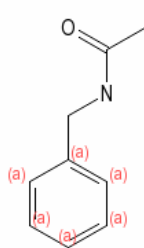
Search By: Name/Text Identity/Similarity **Substructure/Superstructure** Molecular Formula 3D Conformer Saved Search

Draw a Structure CID, SMILES/SMARTS, InChI Structure File
Launch the PubChem editor to make a structure

Options +
Substructure [v] [?]

Broadband [v] SMILES [v] CC(=O)NCc1=cc=cc=c1

| | | | | | | | | | |
|------------|-----------------|---------------|-----------|------------|-----------|-----------|--------|---------|----------------|
| New | Undo | Cln | Del | Qry | [arrow] | [refresh] | [undo] | [redo] | [grid] |
| [line] | [double line] | [triple line] | [arrow] | [dotted] | [cross] | [wavy] | S/A | D/A | S/D |
| [triangle] | [square] | [pentagon] | [hexagon] | [heptagon] | [octagon] | [circle] | [plus] | [minus] | |
| [wavy] | [zigzag] | [branch] | [zigzag] | [zigzag] | [zigzag] | [plus] | NO2 | COOH | COOMe |
| H | | [?] | [?] | | | | | | He |
| Li | Be | | | B | C | N | O | F | Ne |
| Na | Mg | | | Al | Si | P | S | Cl | Ar |
| K | Ca | Sc | Sc [v] | Ga | Ge | As | Se | Br | Kr |
| Rb | Sr | Y | Y [v] | In | Sn | Sb | Te | I | Xe |
| Cs | Ba | Lu | Lu [v] | Tl | Pb | Bi | Po | At | Rn |
| Export | MDL Molfile [v] | | | | | | | | Done |
| Hydrogen | Keep AsIs [v] | | | | | | | | |
| Import | | | | | | | | | Durchsuchen... |



(a) (a) (a) (a) (a) (a)

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.

