## Hands-on exercises to the lecture "Modern Methods in Drug Discovery" WS13/14

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: http://pubchem.ncbi.nlm.nih.gov//search/search.cgi# menu item: Substructure/Superstructure , Launch the PubChem editor

| S NCBI        |                          |                          |                                 |                   |              |                |
|---------------|--------------------------|--------------------------|---------------------------------|-------------------|--------------|----------------|
|               | hem<br>cture Search      | PubChem C<br>Limits Adva |                                 |                   |              | Search<br>Help |
| Search<br>By: | Name/<br>Text            | Identity/<br>Similarity  | Substructure/<br>Superstructure | Molecular Formula | 3D Conformer | Saved Search   |
| æ             | Draw a Structu<br>Launch |                          | CID, SMILES/SMARTS, InChI       | Structure File    |              | 2              |
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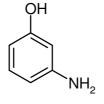
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You may use alternatively DEPICT from the Daylight website: http://www.daylight.com/daycgi\_tutorials/depict.cgi

## Try to find correct SMILES for the following structures:







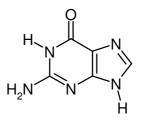
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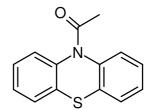
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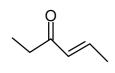
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