BIFX-550

ChemSketch Hands-on

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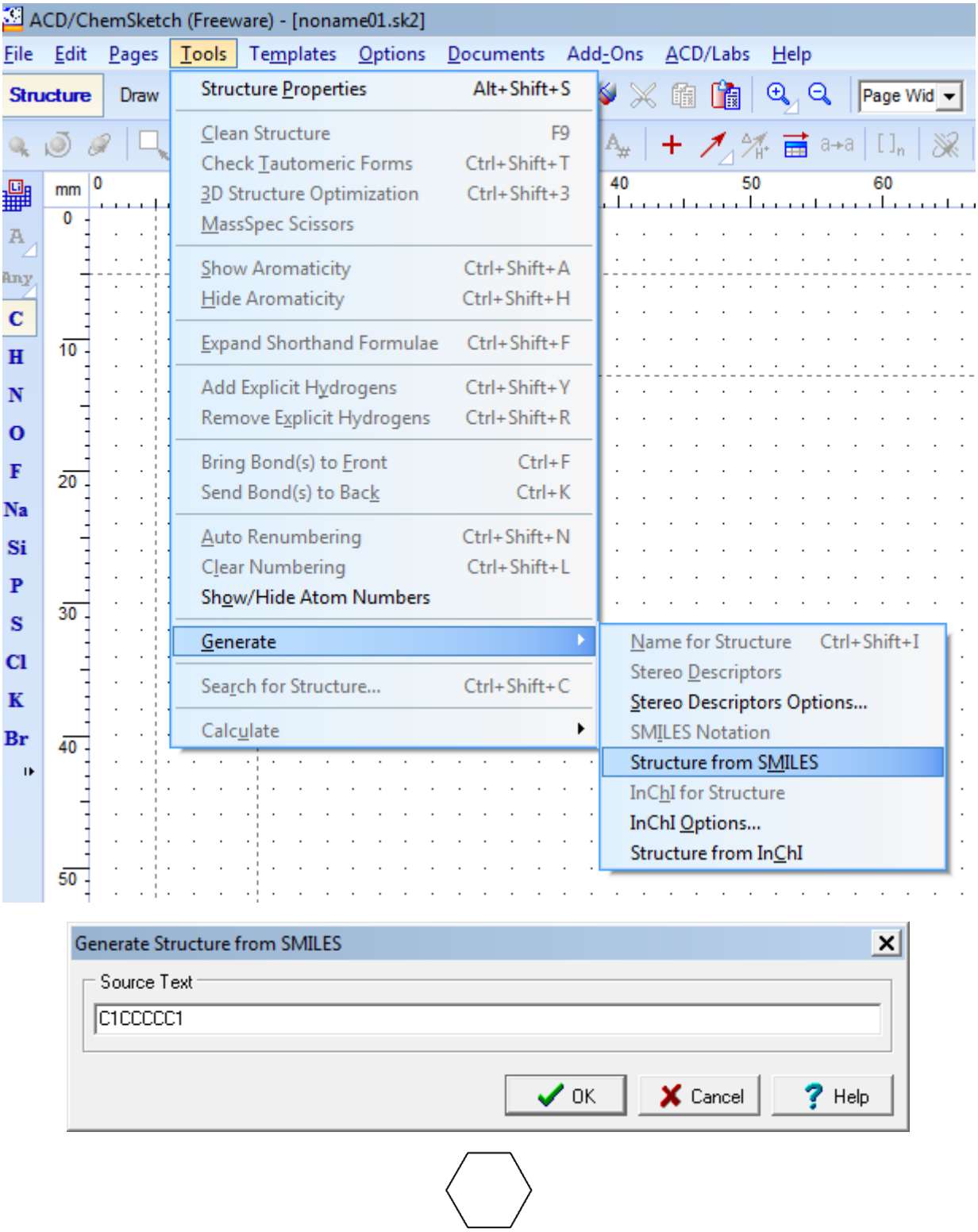
S. Ravichandran, Ph.D.

How to draw small molecules (< 900 Daltons; most drug molecules are small molecules) on a computer? (Need ACD ChemSketch software)

You can use the following link to download the software (ACD/ChemSketch free for Academic and Personal Use).
http://www.acdlabs.com/resources/freeware/chemsketch/

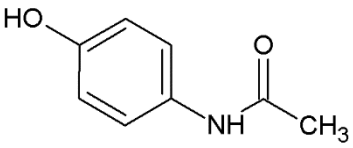
Start ACD/ChemSketch from your computer



For example, C1CCCCC1, should create cyclohexane (shown above). Lower case version of the same will create benzene.

For example, Tylenol (Acetoaminophen) has the following Molecular Input formats:
SMILES: **CC(=O)NC1=CC=C(C=C1)O**
InChi: **InChI=1S/C8H9NO2/c1-6(10)9-7-2-4-8(11)5-3-7/h2-5,11H,1H3,(H,9,10)**

To create the molecular structure of Tylenol, follow the steps shown here: Tools → Generate → Structure from SMILES or Structure from InChi will create a pop-in radio box. Copy the appropriate string shown above to create the molecular form of Tylenol. Molecular formula of Tylenol is shown below for your convenience.



In the previous classes, we had discussed the genetic aspects of the Lactose intolerance/persistence in humans. Let us take a look at the chemical structure of Lactose. Lactose is a disaccharide of Glucose and Galactose and is present in human and cow's milk.

You can learn about the chemistry (& properties) of Lactose in the following PubChem entry, https://pubchem.ncbi.nlm.nih.gov/compound/6134

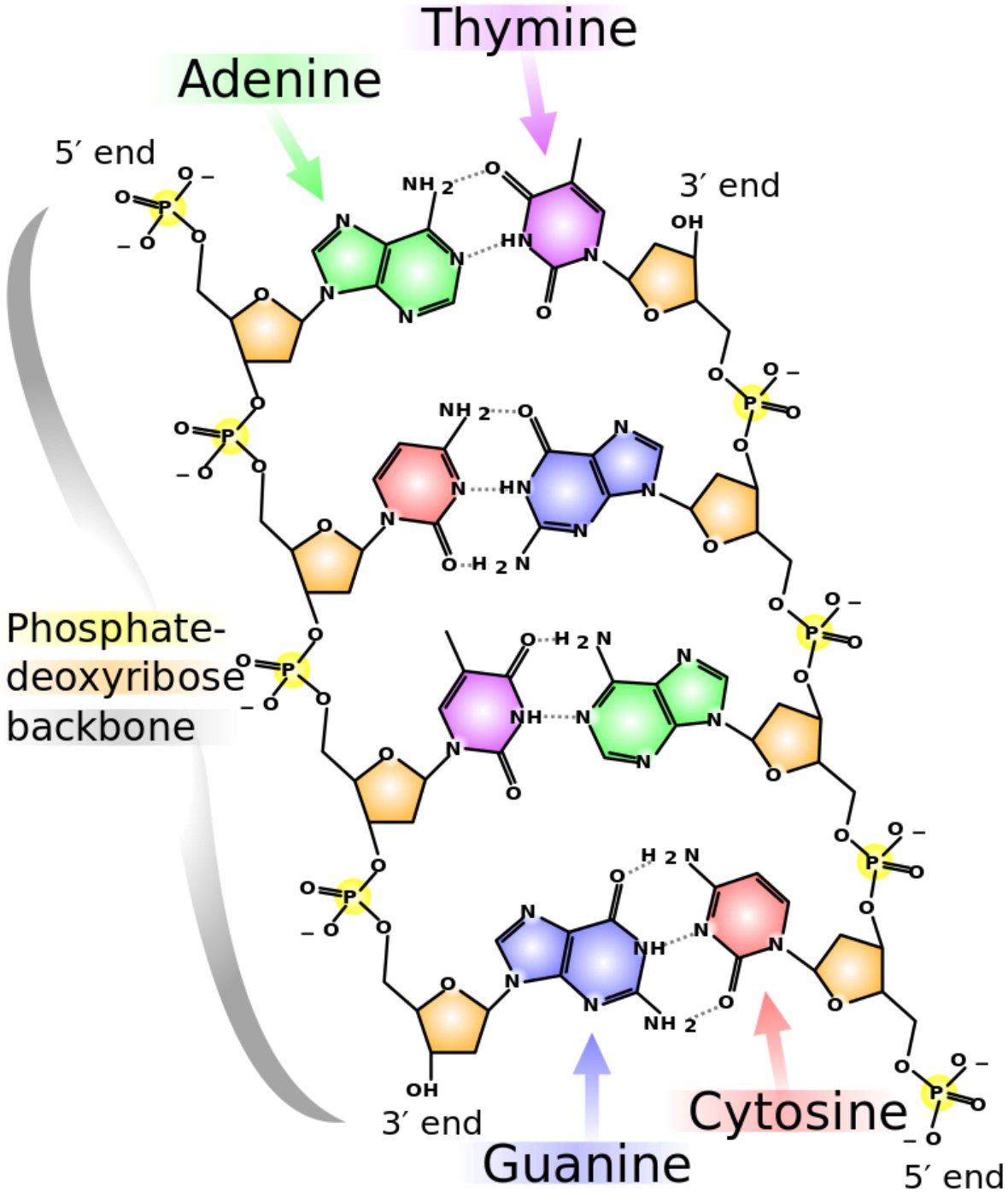
To create Lactose, use either one of the following SMILES strings:

Cannonical SMILES: C(C1C(C(C(C(O1)OC2C(OC(C(C2O)O)O)CO)O)O)O)O
Isomeric SMILES:
C([C@@H]1[C@@H]([C@@H]([C@H]([C@@H](O1)O[C@@H]2[C@H](O[C@H]([C@@H]([C@H]2O)O)O)CO)O)O)O)O

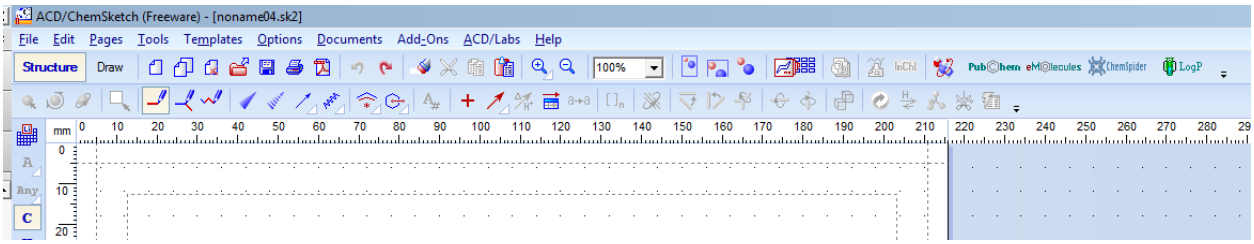
Exploring the chemistry of the Single-stranded DNA molecule

How to draw a Single stranded DNA using ChemSketch?

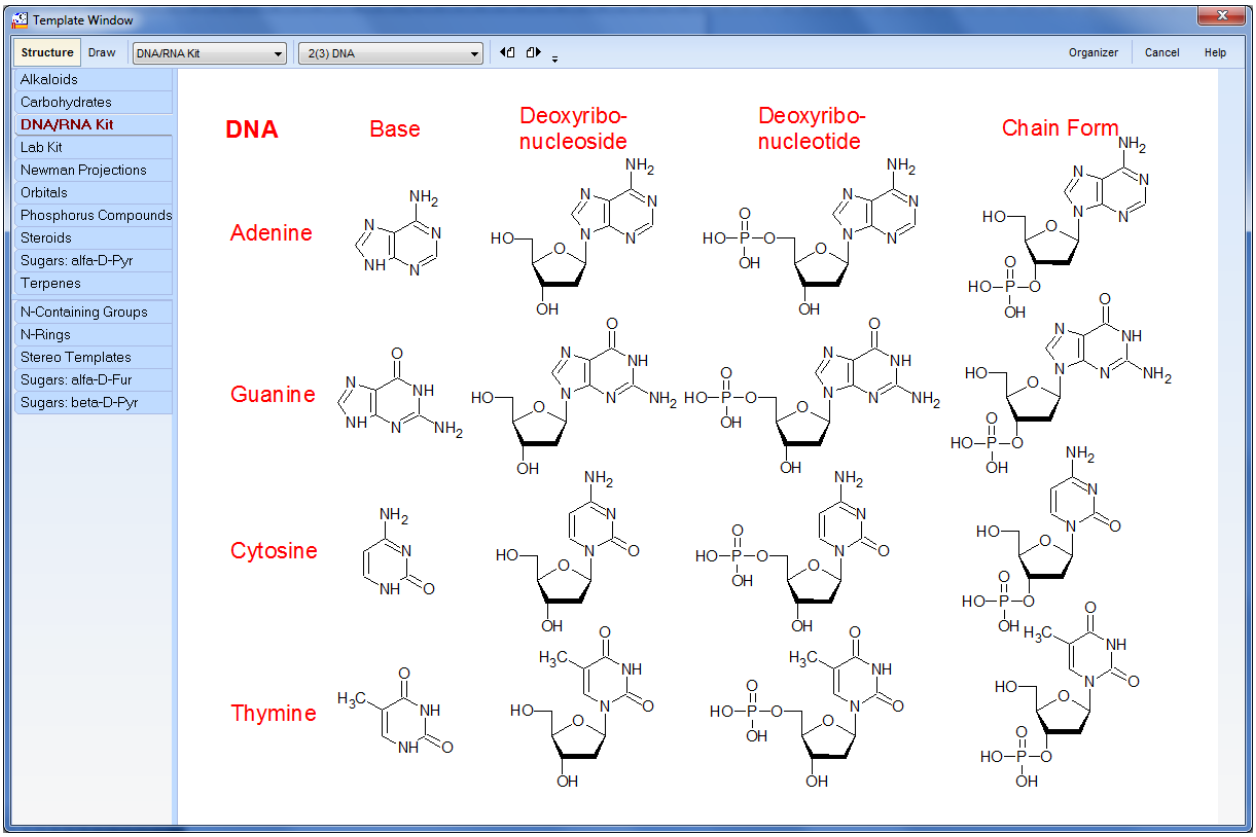
1. Here is a dsDNA molecule, you can use this as a guidance to draw ssDNA using ChemSketch



2. Start ChemSketch (Windows-Start → ACDLabs Freeware 2015 → ChemSketch)
3. From the top menu of ACD ChemSketch, Click on **Templates** (see below) → **Templates Window**



4. Click on DNA/RNA kit on the left-hand side menu



Click on the base of your interest and take it to the main window. Without clicking Escape/Right-click, continue to string the bases to build the single stranded DNA.