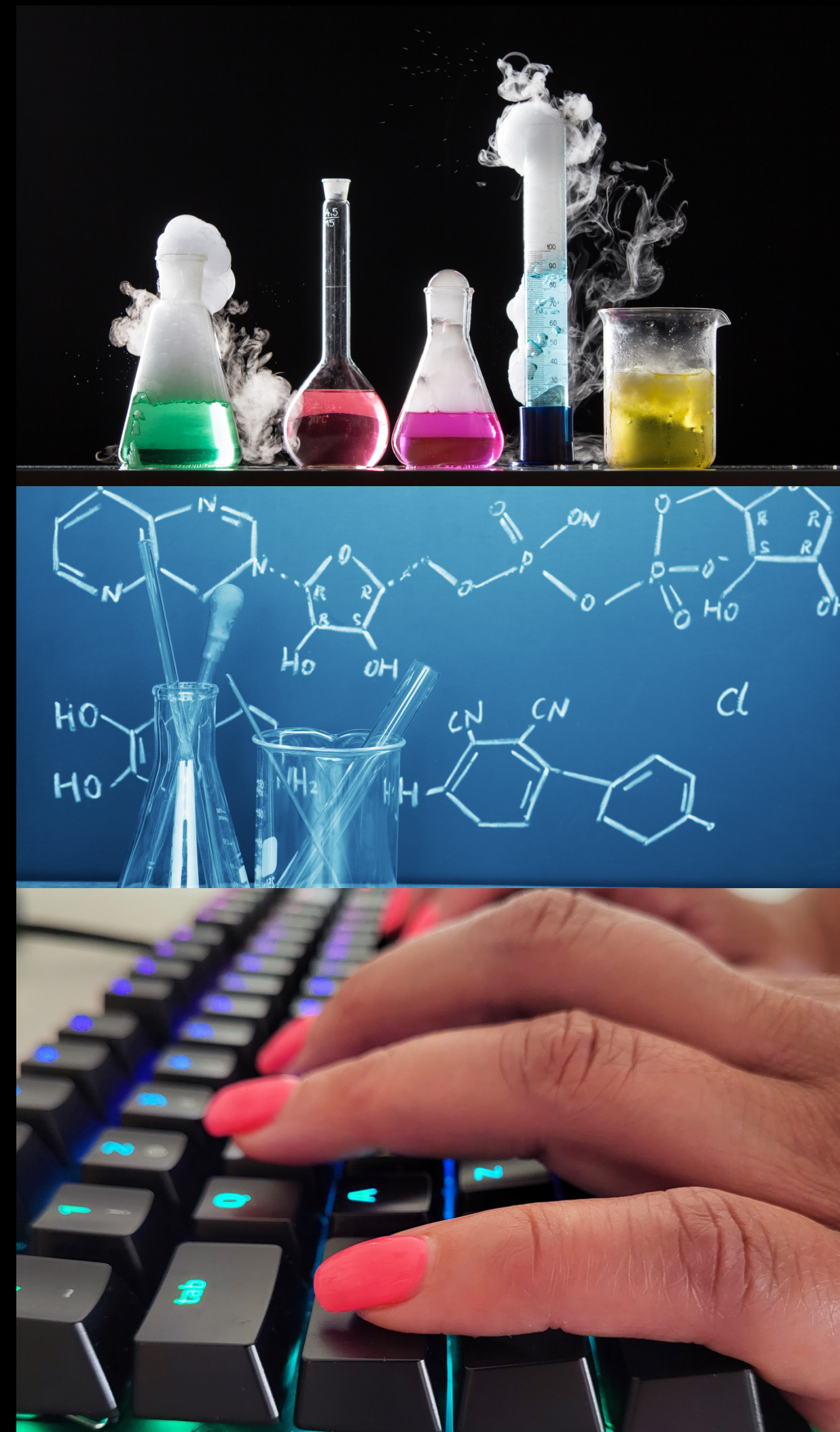


Cheminformatics

with Kimberly Deas, MS, PhD Candidate



Converting SMILES to SDF Using KNIME

Prerequisites

- 1) Basic Chemistry and data knowledge.
- 2) Familiarity with KNIME is helpful.
- 3) Willingness to learn!

Resources

- 1) KNIME Website, [knime.com](https://www.knime.com)
- 2) Introduction to Cheminformatics, David Wild, PhD,
<http://david-wild-knzi.squarespace.com/david-wilds-blog/2018/5/1/introducing-cheminformatics>
- 3) Chemistry Library / LibreTexts Project website,
chem.libretextx.org

Important Terms

- **CDK:** Chemical Development Kit (<https://cdk.github.io/>)
- **RDKit:** Open source cheminformatics and machine learning tools (<https://www.rdkit.org/>)
- **SDF:** Structured Data Files consist of atom and bond tables that are used to convey chemical structural information. Molfiles are examples.
- **SMILES:** Defined as The Simplified Molecular-Input Line-Entry System (SMILES), are short ASCII strings for describing chemical structures.

SMILES to SDF Workflow in KNIME

The screenshot displays the KNIME Analytics Platform interface with a workflow titled "SMILEStoSDF". A blue box highlights the workflow's purpose: "Convert SMILES in text format to SDF."

The workflow consists of the following nodes:

- Node 1: CSV Reader** (Orange icon)
- Node 2: Column Rename** (Yellow icon)
- Node 3: Missing Value** (Yellow icon with a question mark)
- Node 4: Molecule to CDK** (Yellow icon with "Mol CDK")
- Node 5: RDKit To Molecule** (Yellow icon with a plus sign)
- Node 6: SDF Writer** (Red icon)

The workflow is connected as follows: CSV Reader (Node 1) → Column Rename (Node 2) → Missing Value (Node 3) → Molecule to CDK (Node 4) → RDKit To Molecule (Node 5) → SDF Writer (Node 6).

The right sidebar shows the "Description" tab for the "SMILEStoSDF" workflow:

- Title:** SMILEStoSDF
- Description:** Code to convert SMILES in text file into SDF files
- Tags:** No tags have been added yet.
- Links:** No links have been added yet.
- Creation Date:** 2022-7-18
- Author:** kdd96

The bottom of the interface shows the "Console" tab with the text "KNIME Console".

Transition to KNIME