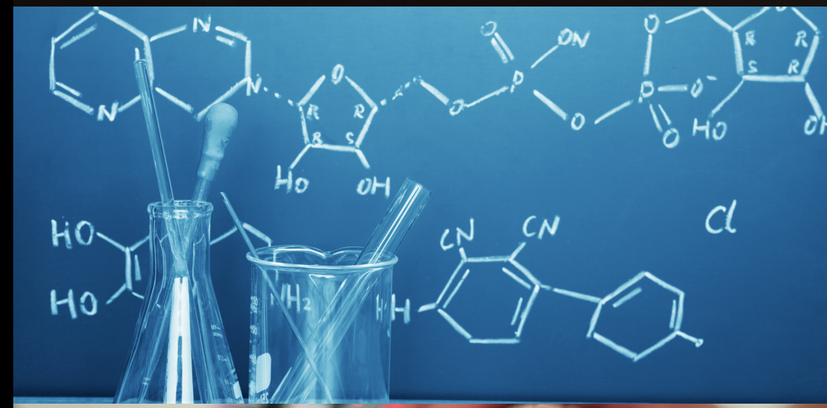
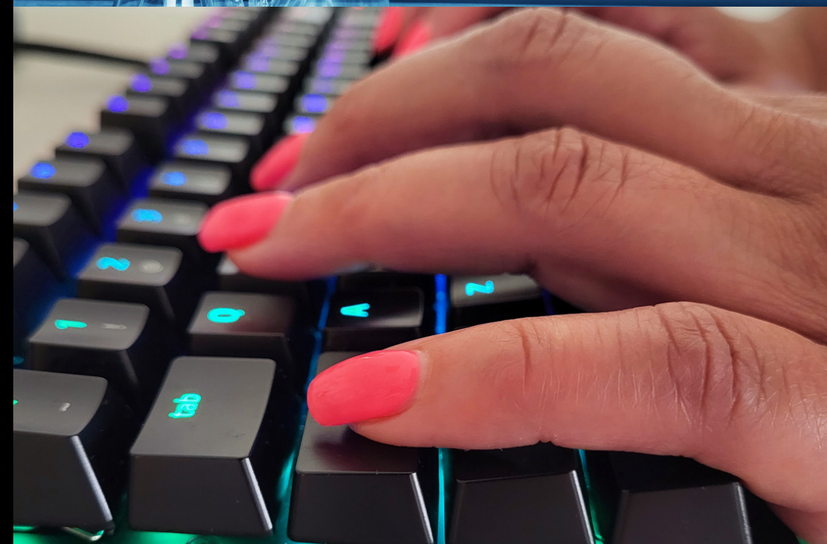
Cheminformatics

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

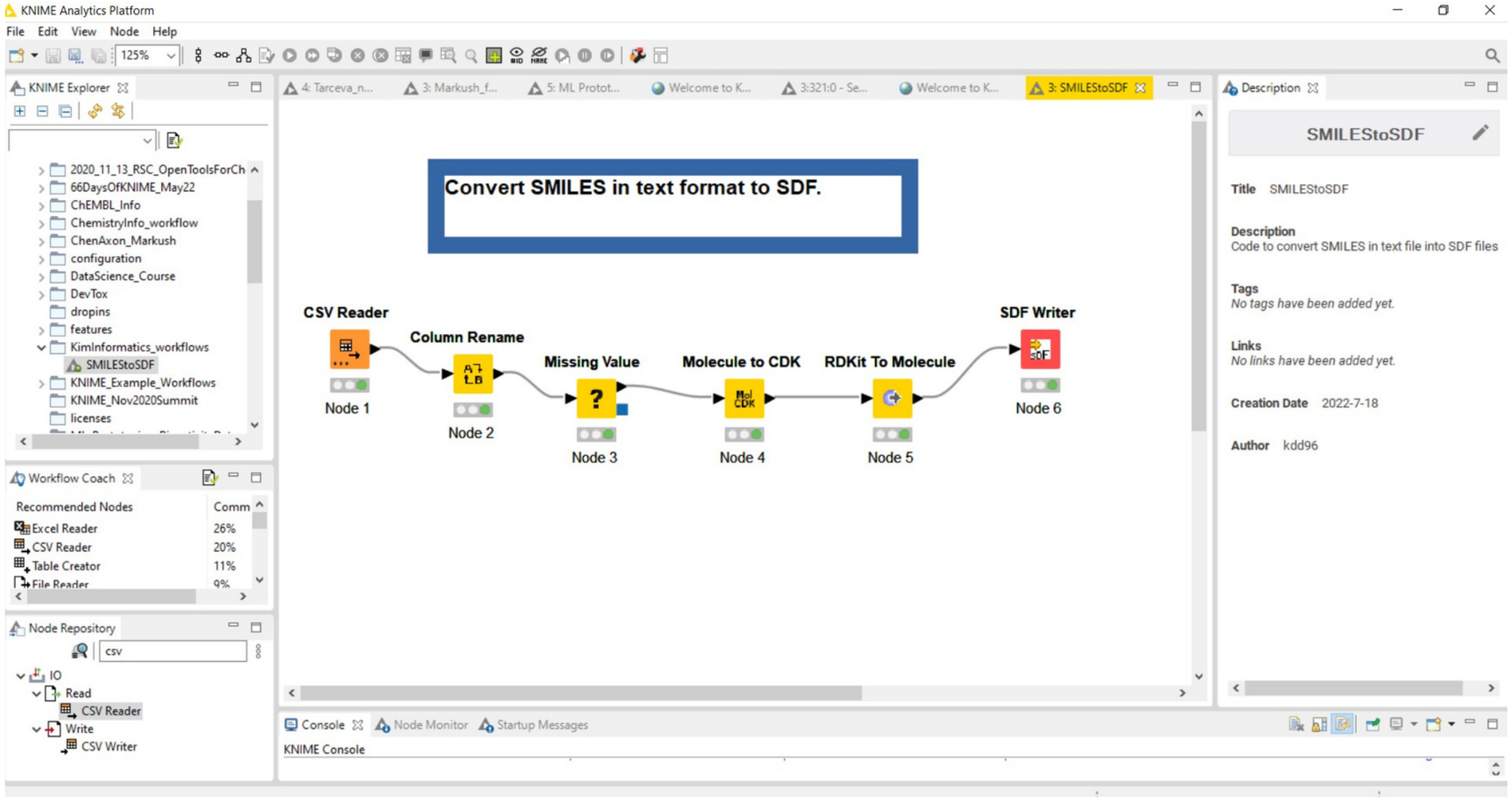
2) Introduction to Cheminformatics, David Wild, PhD, http://david-wild-knzl.squarespace.com/david-wilds-blog/2018/5/1/introducing-cheminformatics

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



Transition to KNIME