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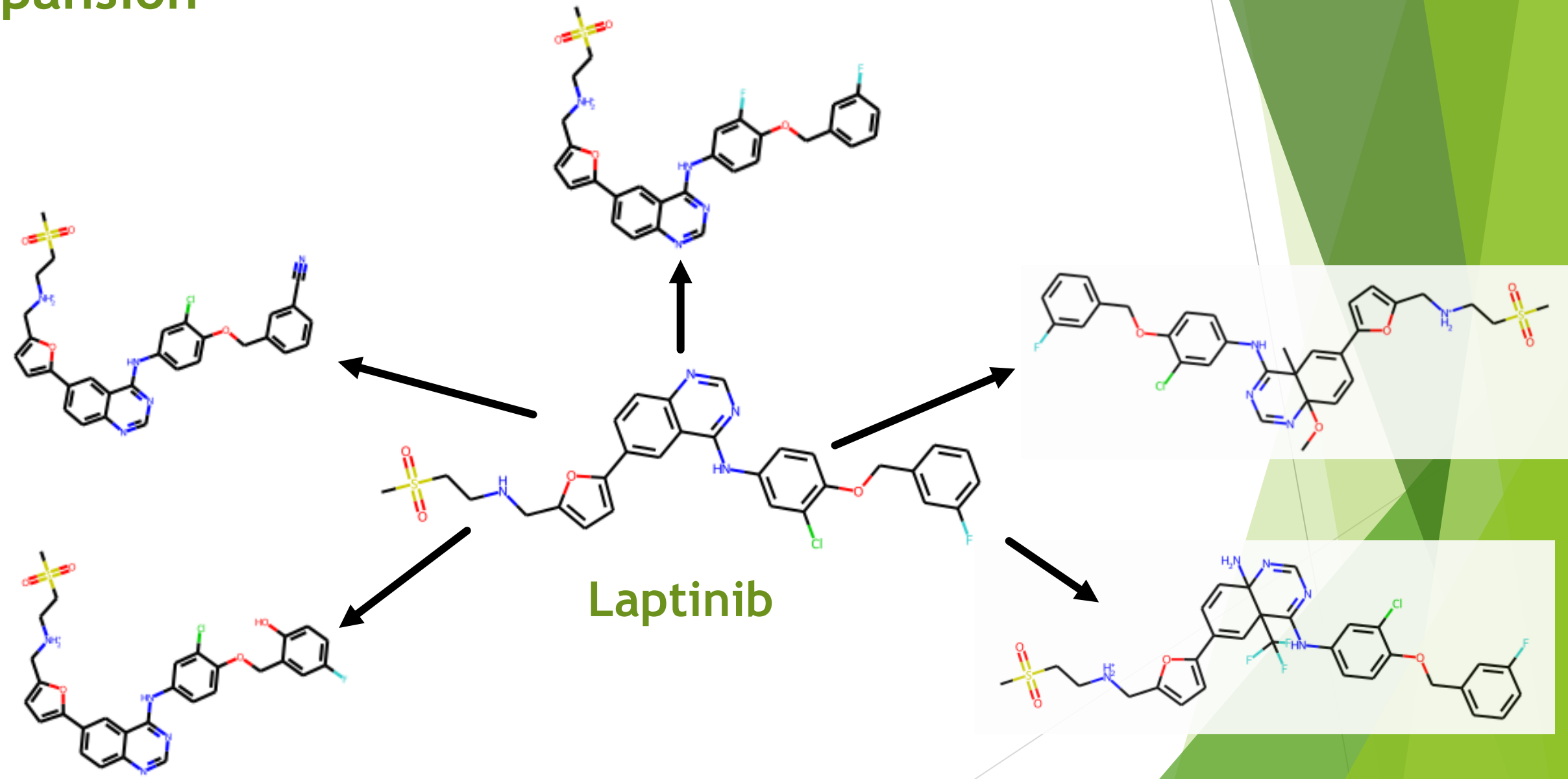
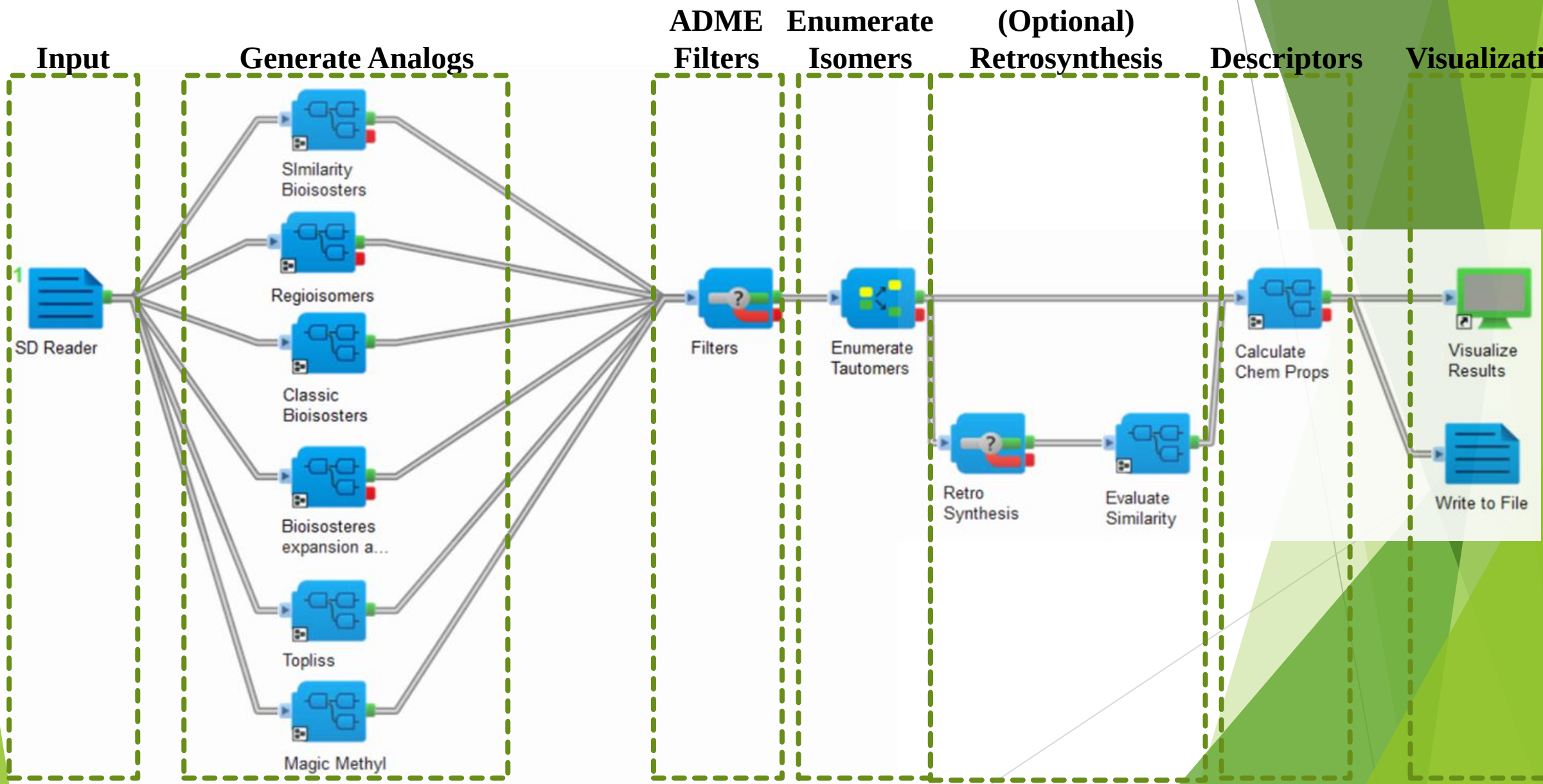
Automated Analog Generation and Retrosynthesis Predictions

Jacob Spiegel

Analog generation as a method for lead expansion



Analog Generator in Pipeline Pilot



Analog Generator in Pipeline Pilot

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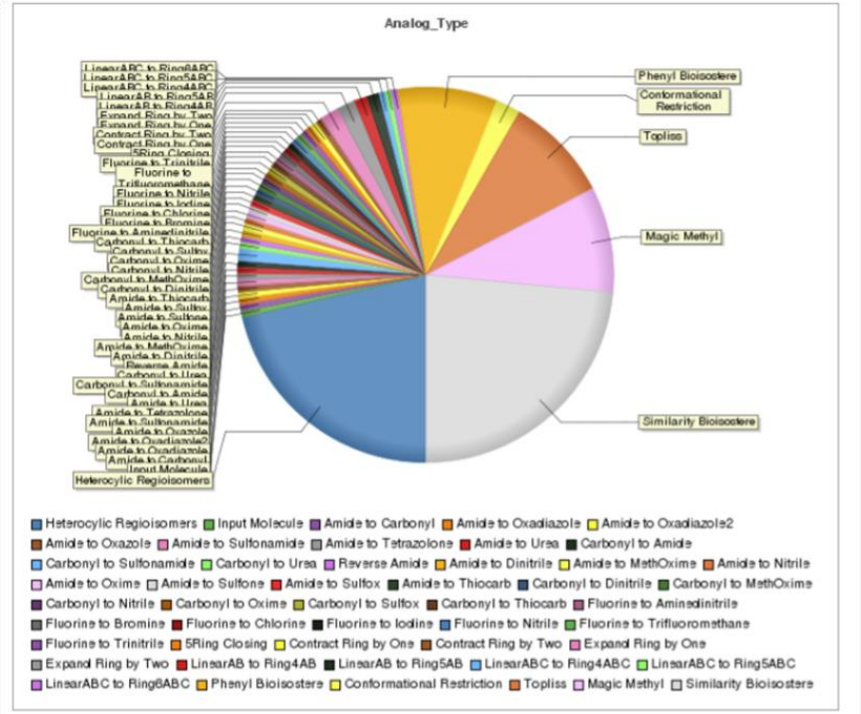
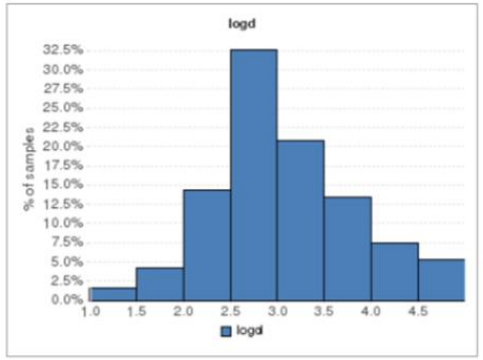
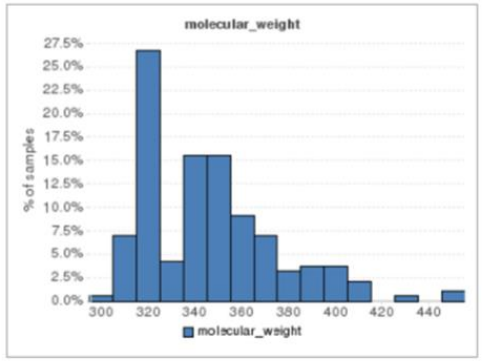
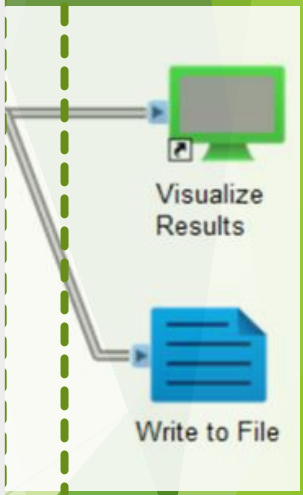
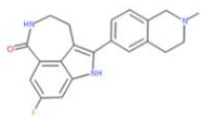
Input | **Generate Analogs** | **ADME Filters** | **Enumerate Isomers** | **(Optional) Retrosynthesis** | **Descriptors** | **Visualization**









Molecule	Total Fragments	Chembl Fragment Score	eMolecules Fragment Score	Chembl Weighted Fragment Score	eMolecules Weighted Fragment Score	Consensus_Score	Tag	Analog_Type	description	Nasty	Molecular_Solubility	LogD	ADMET_BBB	ADMET_BBB_Level	ADMET_Unknown_AlogP98	ADMET_Absorption_Level	ADMET_Solubility	ADMET_Solubility_Level	Source_Mol	cmpd_ID	Undesirability	Canonical_SMILES
	1 1	0 0	0 0	0 0	0 0			5Ring Closing Conformational Restriction		false false	-5.2680 -5.2680	3.5690 3.5690	0.18200 0.18200	1 1		0 0	0 0	-5.7890 -5.7890	2 2	CNCc1ccc(cc1)c2[nH]c3cc(F)cc4C(=O)NCCc2c34			CNCc1ccc(cc1)c2[nH]c3cc(F)cc4C(=O)NCCc2c34

Pythonizing the Analog Generator

- The Pythonized version of the code does not require a requires a commercial Pipeline Pilot license

Pythonizing the Analog Generator

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- The Pythonized version of the code does not require a requires a commercial Pipeline Pilot license
- Codebase was modeled on AutoGrow4's modular plugin architecture
- Features:
  - More extensive stereochemistry sampling
  - Expansion of the ADME-PK filters options
  - Addition of compound fitness functions
    - Synthetic Accessibility Scoring (SAScore)
    - Protein-ligand docking score

Future Directions

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- Improving the GUI
- Expanding out-of-the-box options
  - Filters
  - Fitness functions
  - Reactions
  - Analysis tools

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- Hunter Phillips (Accounts Manager)
- Garrett Meek (Research Informatics Consultant)
- Ryan Moore (Informatics Scientist)

Workflow Informatics provides world class consulting services specializing in research informatics and cheminformatics.

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- **Our primary areas of expertise are:**
  - Data modeling and management
  - Cheminformatics
  - Laboratory informatics
  - Scientific Integrations
- **Example solutions (often utilizing RDKIT)**
  - Assay Data Autoloaders
  - Custom Assay data parsers
  - Sample and Inventory logistics tracking systems
  - Software Specific API integration tools
  - Plate Mapping Solutions
  - Custom Datawarehouses

If interested, please contact our Account Manager (Hunter Philips):

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