ROCKY 2016
Aspen/Snowmass Colorado
December 8 - 10, 2016
iSCB INTERNATIONAL SOCIETY FOR COMPUTATIONAL BIOLOGY

Bioinformatics Conference

JOIN ISCB   KEY DATES   REGISTER

▶ HOME
▶ GENERAL INFORMATION

POSTER PRESENTATIONS

top

P19
PyoFuel - Using Python and Pathway Tools to engineer synthetic Biofuel

Subject: Simulation and numeric computing

Presenting Author: Ashley D'Souza, Westwood High School, Austin, Texas

Abstract:
Pathway Tools is a collection of biological modeling tools with databases of organism models, metabolic flux analysis, and query and visualization tools. Pythoncyc is a Python programming interface to Pathway Tools. In two earlier projects I had experimented with flux balance analysis on models of bacteria that had been modified with pathways to synthesize biofuel, and with wet-lab recombineering of the DHX35 gene using E.coli. The former was quick, easy, and fun; the latter was slow, painful, and fun. So I wanted to use Python to script Pathway Tools, to help find candidate biofuel pathways across organisms, identify the corresponding gene-edits to engineer biofuel-friendly E.coli, and evaluate how effective each engineered organism might be -- all as a precursor to either more detailed modeling or wet-lab work.

PyoFuel is the resulting project. It is ongoing work, and my poster will report on the following using flowcharts, relevant Pythoncyc API calls, PyoFuel code snippets, and Pathway visualizations:

- Find candidate biofuel metabolites in MetaCyc, a multi-organism database
- Identify the pathways that produce those metabolites
- Generate a modified organism database to evaluate via FBA
- Run MetaFlux on the modified organism with suitable objectives and constraints
- Filter out those organisms if key flux numbers are poor
- Identify enzymes and corresponding genes for the modified pathways

I am currently a senior in high school. If accepted, I plan to open-source the current Jupyter notebook and pgdb databases. My info is at http://ashdza.github.io/.

top