

PyoFuel - Using Python and Pathway Tools to engineer synthetic Biofuel

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Background

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 -- as a precursor to more detailed modeling or wet-lab work.

Methods and Results

PyoFuel 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

Conclusions

PyoFuel's design of Python scripts using Pathway Tools can effectively automate preliminary identification and evaluation of biofuel metabolites, pathways, and gene edits.