Calculation of Polymer Hydrophobicity

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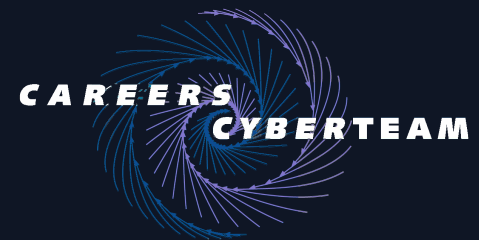
7/13/2022

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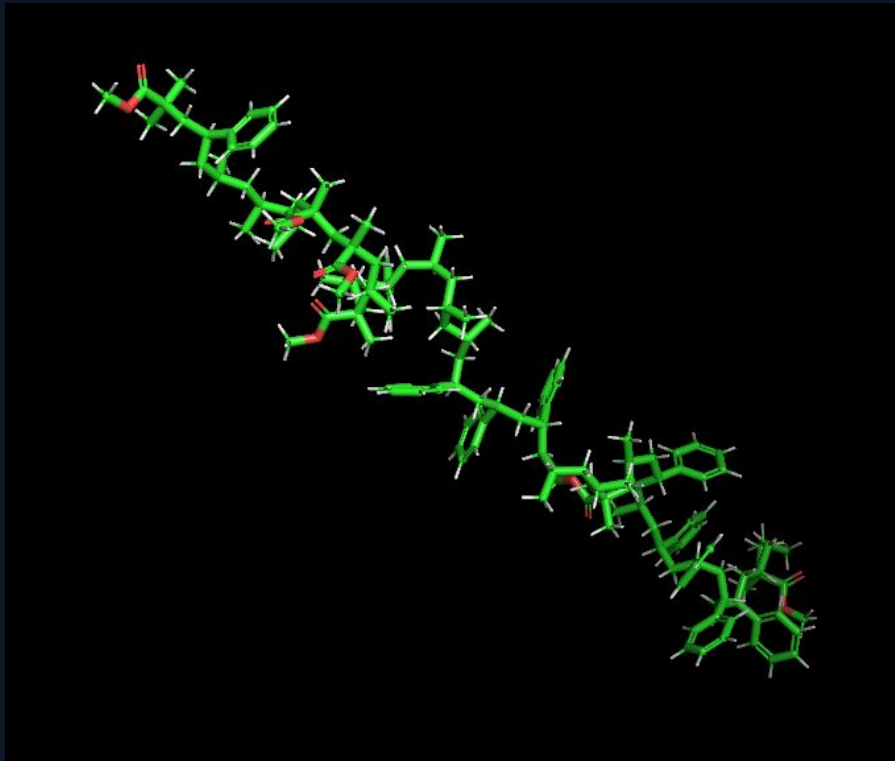
Calculation of Polymer Hydrophobicity

- Create a tool that can calculate several properties of a polymer
- Track size dependance
- Accommodate any desired composition

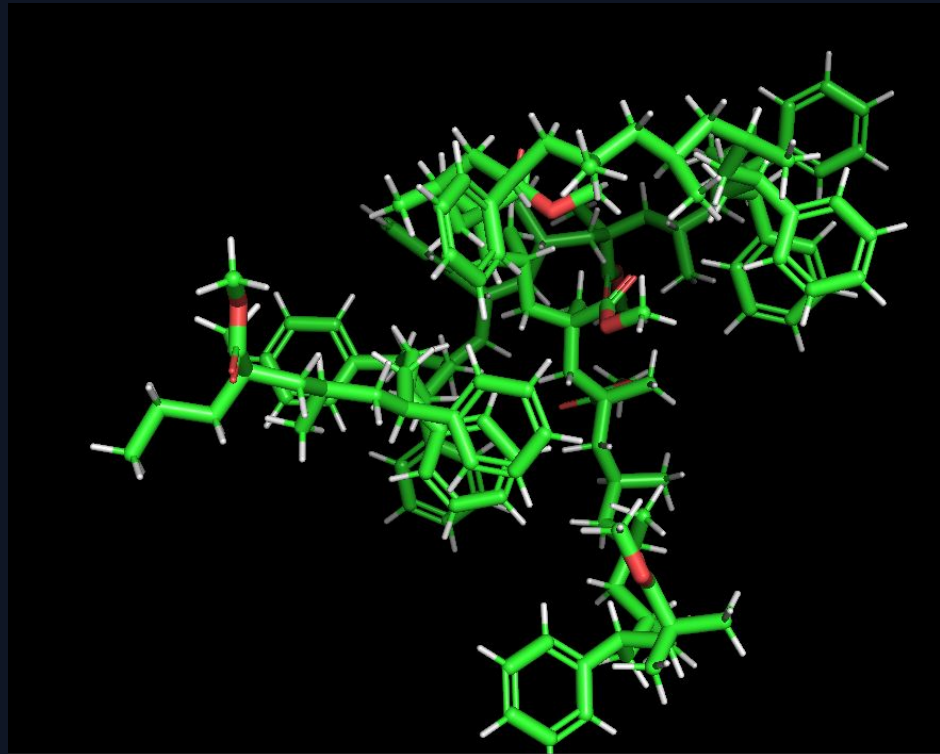# Calculation of Polymer Hydrophobicity

- Goals
  - Improve versatility of existing code
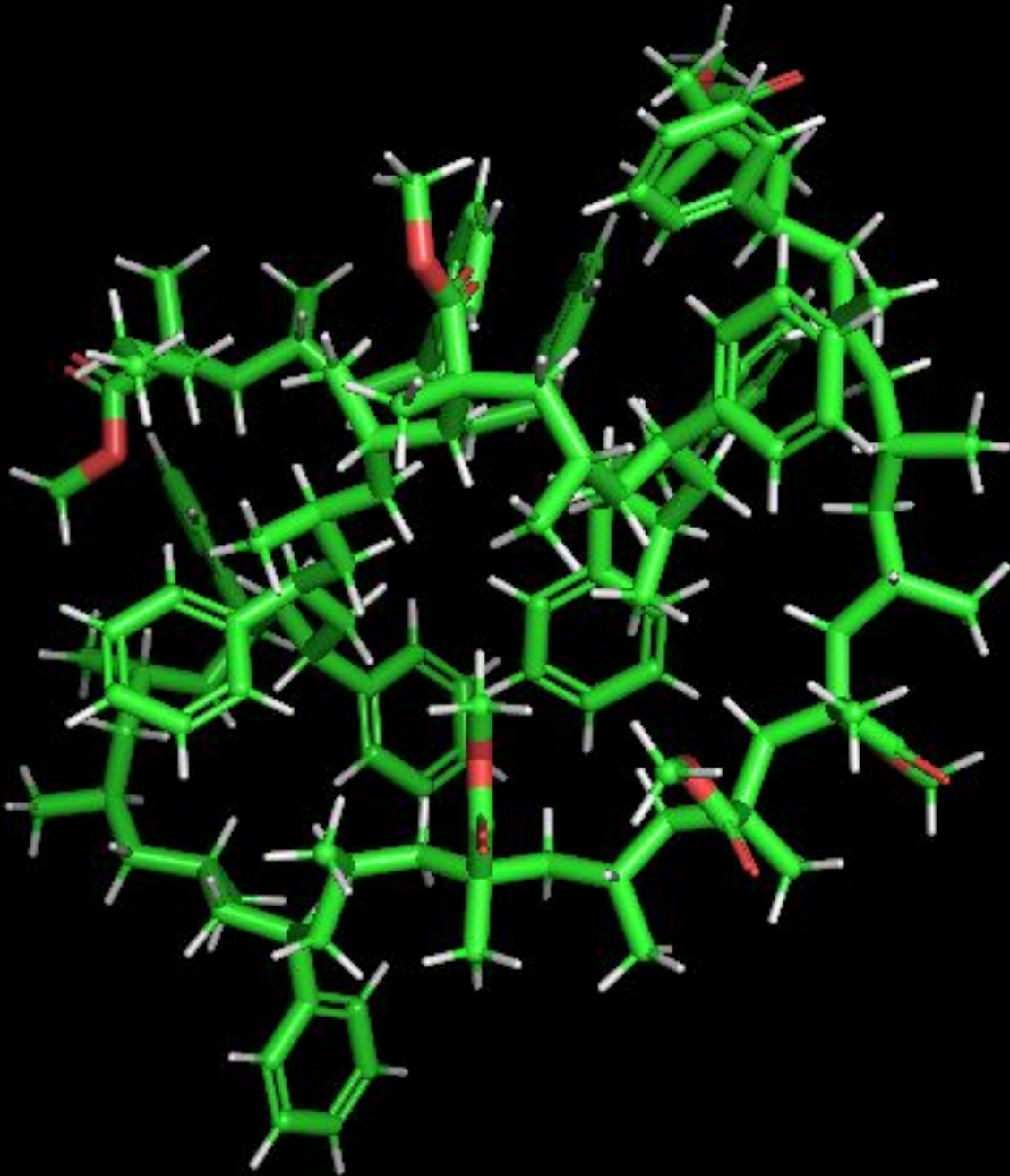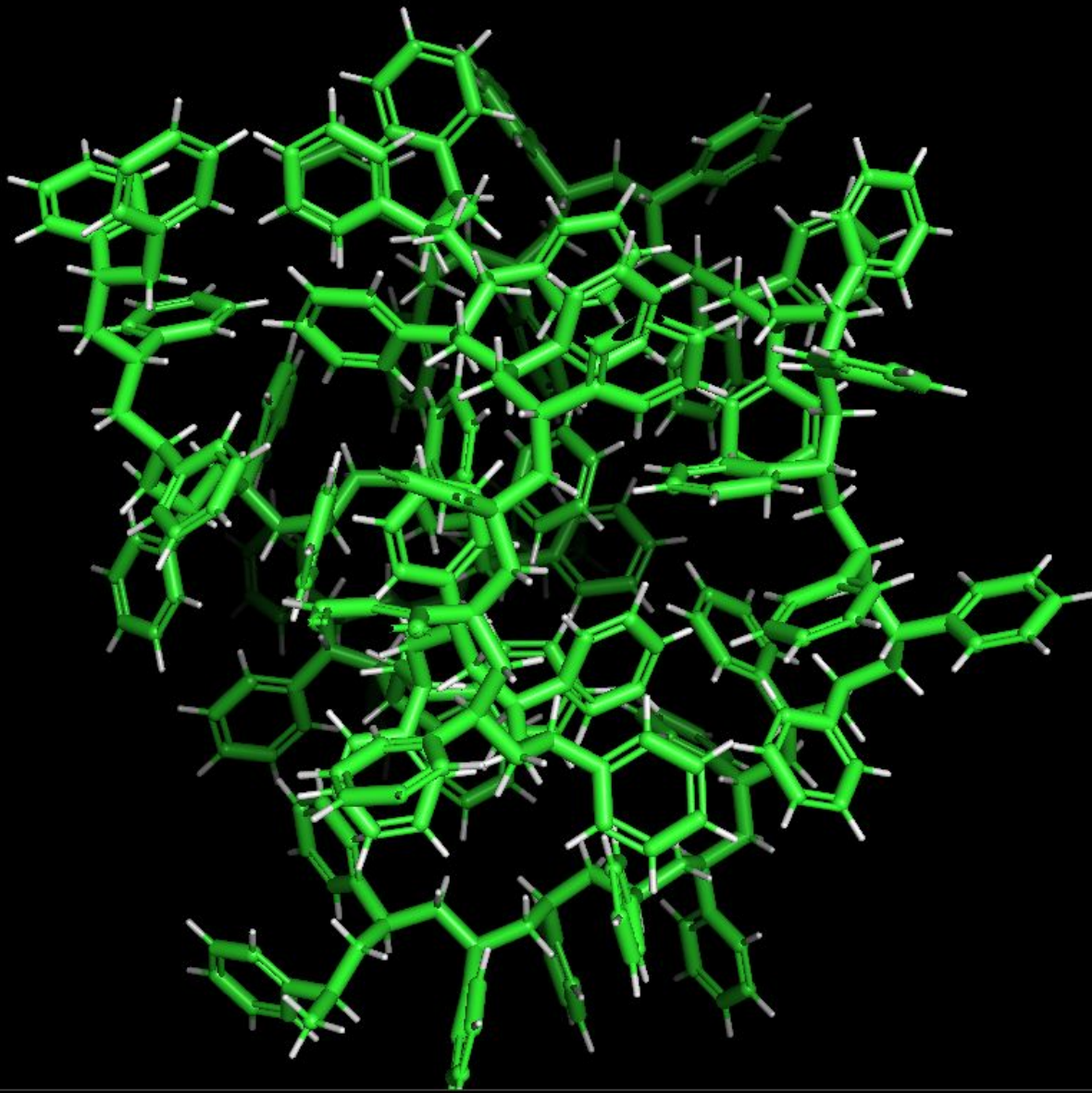 - Improve efficiency
  - Make accessible

Old method: Poor coiling behavior, ~10 minutes for ~20 monomers

Iteration 2: Good coiling behavior, ~10 minutes for ~20 monomers.

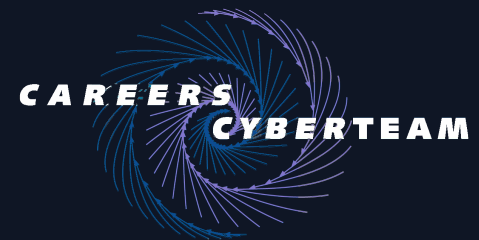Iteration 3: Only 25 seconds while coiling as expected

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Pushing harder with Iteration 2: 50 Styrene monomers in under 4 minutes.

This would have taken multiple hours with previous methods.

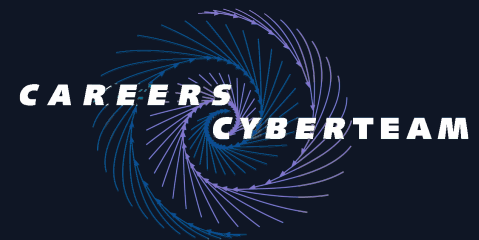# Calculation of Polymer Hydrophobicity

- Timeframe
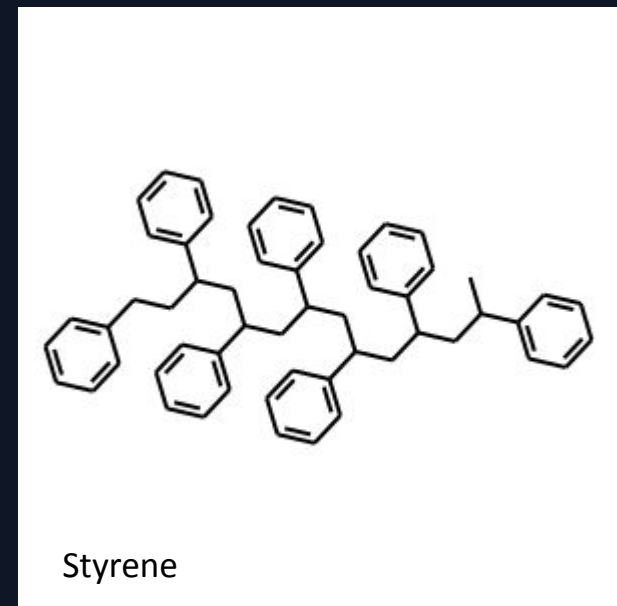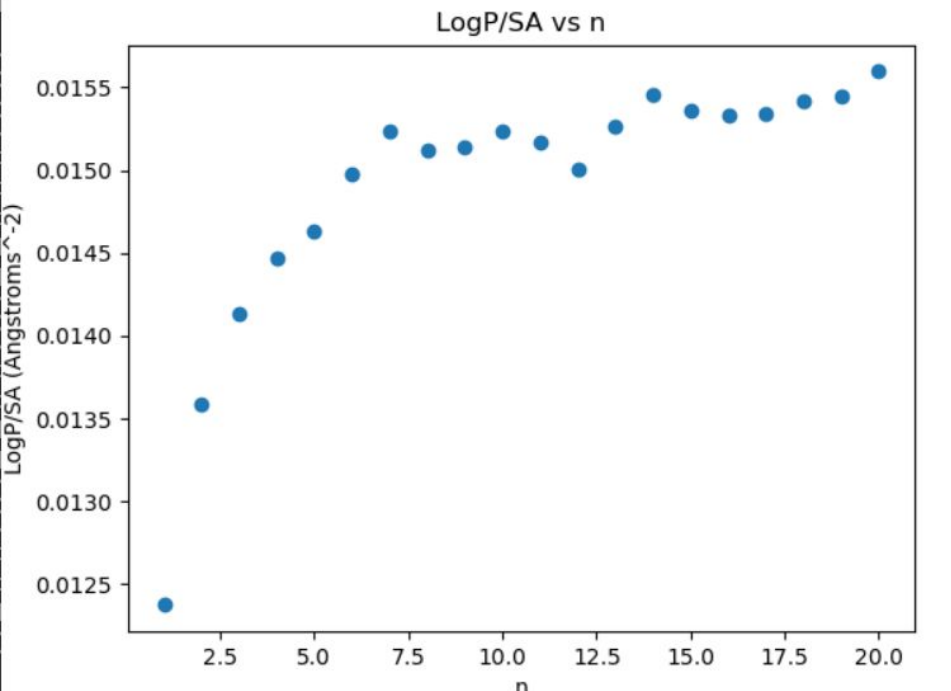 - June 1
  - Oct 30

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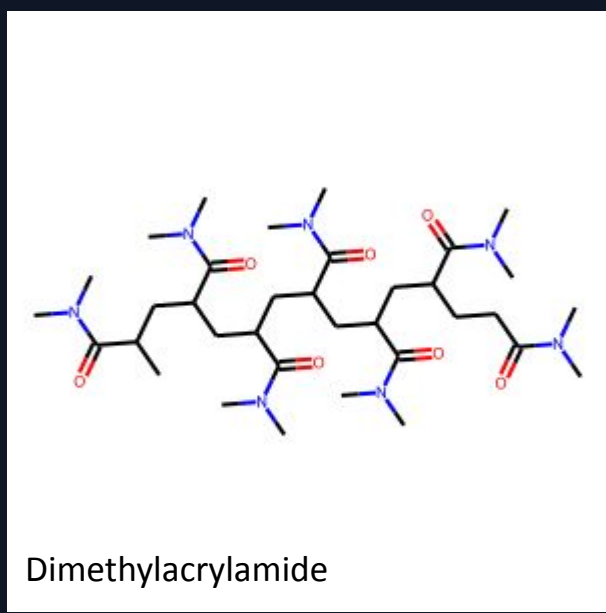# Calculation of Polymer Hydrophobicity

- What I hope to learn
  - Publishing Python Packages
  - Polymer Properties
  - RDkit

LogP/SA vs n

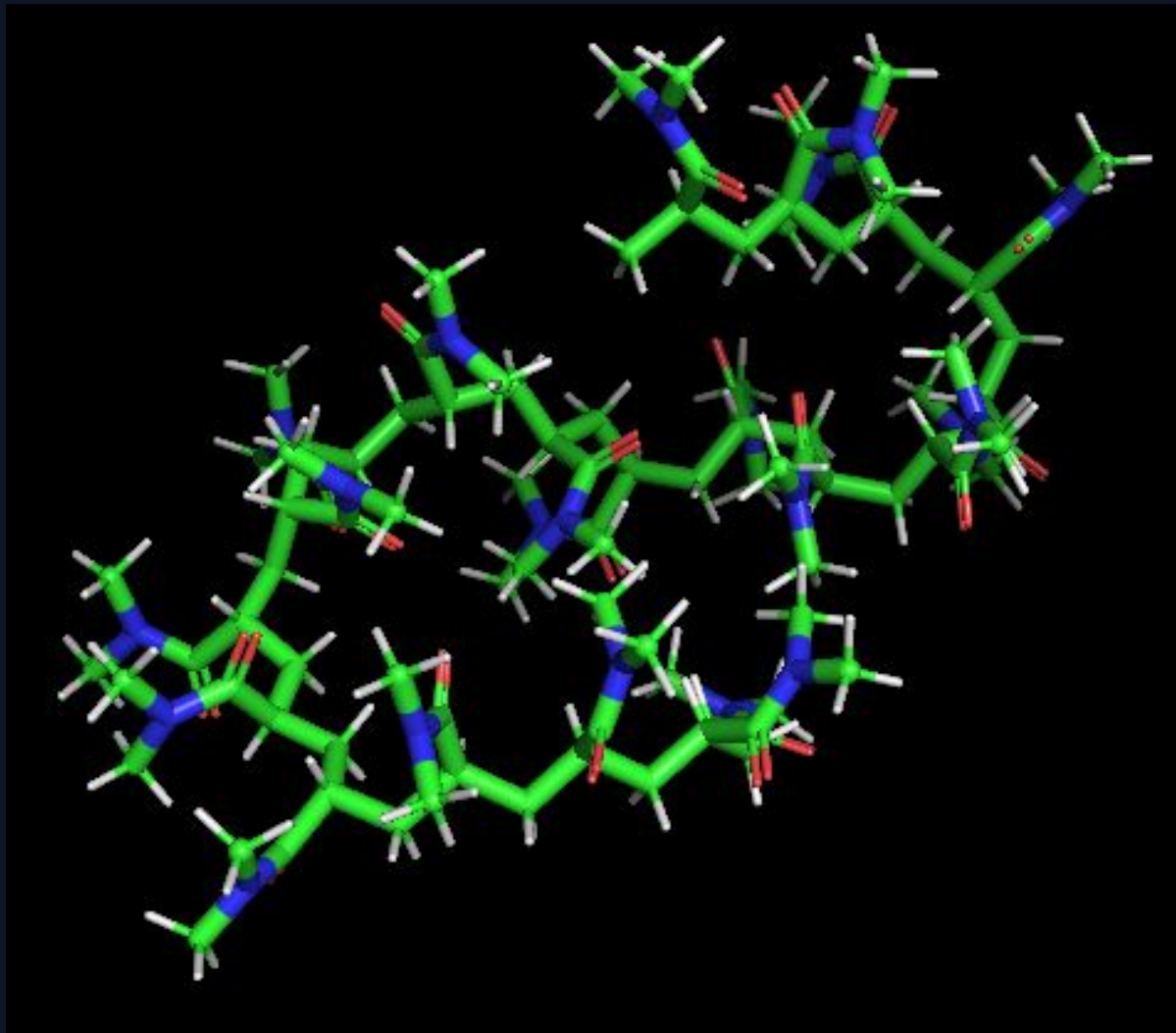Styrene

LogP/SA has different trends based on polymer composition.


Dimethylacrylamide

LogP/SA vs n
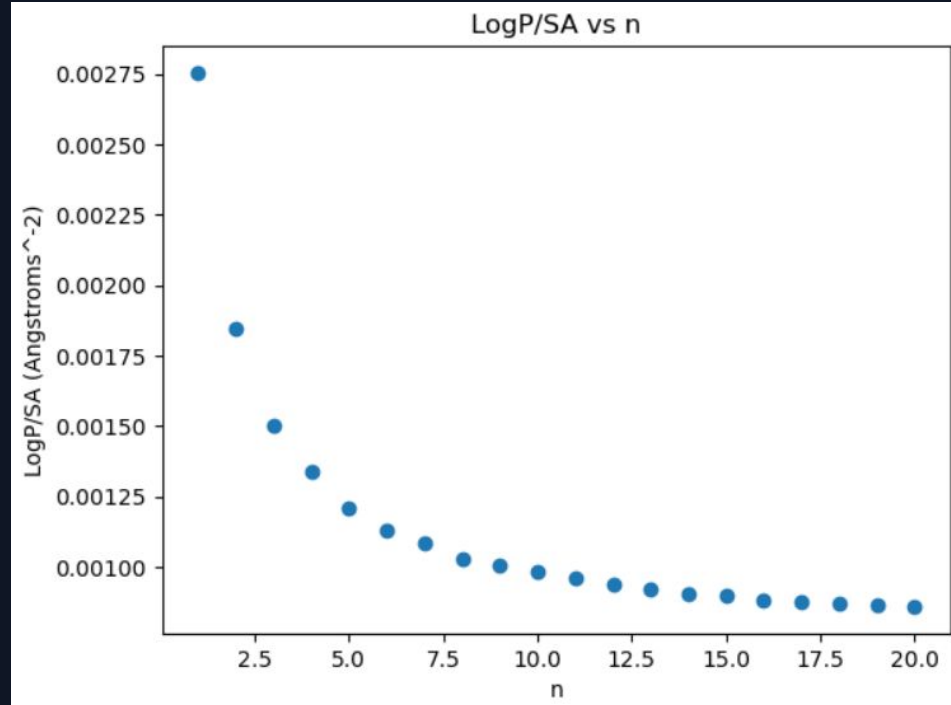
Dimethylacrylamide is far less hydrophobic than styrene, so it is not surprising that it is less coiled, though other factors have effects as well.

The radius of gyration (RMS distance from center of mass) scales in a predictable way with size, so the accuracy of these models can be quantitatively assessed.

Calculation of Polymer Hydrophobicity

- Goals for Next Month
  - Improve Random Polymer Generation
  - Use finer steps when comonomers are defined
  - Make clearer visualizations

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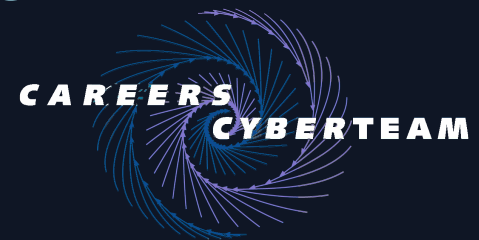
Calculation of Polymer Hydrophobicity

- Help needed (if any)
  - Working with mentors to learn about packaging