Calculation of Polymer Hydrophobicity

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• Create a tool that can calculate several properties of a polymer
• Track size dependance
• Accommodate any desired composition
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• Goals
  – Improve versatility of existing code
  – Improve efficiency
  – Make accessible
Iteration 2: Good coiling behavior, ~10 minutes for ~20 monomers.

Old method: Poor coiling behavior, ~10 minutes for ~20 monomers.
Iteration 3: Only 25 seconds while coiling as expected
Pushing harder with Iteration 2: 50 Styrene monomers in under 4 minutes.

This would have taken multiple hours with previous methods.
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• Timeframe
  – June 1
  – Oct 30
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- What I hope to learn
  - Publishing Python Packages
  - Polymer Properties
  - RDkit
LogP/SA has different trends based on polymer composition.
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.

Dimethylacrylamide is far less hydrophobic than styrene, so it is not surprising that it is less coiled, though other factors have effects as well.
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• Goals for Next Month
  – Improve Random Polymer Generation
  – Use finer steps when comonomers are defined
  – Make clearer visualizations
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• Help needed (if any)
  – Working with mentors to learn about packaging