Navigating Potentials and Pitfalls in using Artificial Intelligence for Expedited Decision Making in Pharmaceutical Problems

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Prime Labs

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My Background

- CS undergrad, MS in CS (AI focus), PhD in CS (AI focus ~ applications in computational mass spectrometry)
- 8 years teaching AI, conducting academic research in AI for computational mass spectrometry.
- Many papers and grants evaluating existing algorithms, creating data sets to facilitate evaluations, creating new ones.
- Prime Labs: 4 years. We build software that leverages AI for computational mass spectrometry.

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AI Crash Course

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AI is not a complicated idea

- You might need deep knowledge to advance it, but not to use or understand it.
- In a nutshell:
  - A program is a recipe to solve a problem.
  - AI is a recipe that creates a recipe to solve a problem.

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Obfuscation makes it harder

- There is a lot of jargon.
  - AI
  - Machine learning
  - Deep learning
  - Big data
  - Knowledge discovery
- Mostly marketing / job security.

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In a nutshell

- You are building a *model.*
- A putative relationship between caus(es) and effect(s).
- Can be used to predict the future or understand the past.
  - Prediction ex: Test the toxicological properties of an a new molecule.
  - Understand ex: Devise plausible explanations for observed toxicological response of a tested molecule.

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AI: The good and bad

- The good news: It is straightforward to apply AI to well-understood problems.
- The bad news: It is extraordinarily difficult to do something new.
- Why? Surprisingly, not because of lack of tools.
- Instead, the problem lies in *data* and *representation*.

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Representation

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Representation

- Standard approaches to AI funnel problems into a specific representation. Example: spreadsheet for off-the-shelf machine learning techniques.

- But nature is not found in spreadsheets…

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Representation

- Machines do well with defined, repetitive tasks.
- People do well with creativity and intuition.

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Representation

- Everything is simple if you know the representation that makes it so.

- Discovery isn't so much about solving problems as it is finding the representation that makes the solution obvious.

- Discovery isn't so much about doing what others can't do, but about seeing what others haven't seen. More often than not, this requires *not* seeing what others see.

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Representation

- Take away: In order to succeed in applying AI to a novel task, you will need at least one *very* clever human.

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Data

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Data

- Things AI does well:
  - Problems for which the answer is known.
  - Problems for which there exist large quantities of data.
- Why is this a problem?

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The AI Data Paradox

- The more complex the problem, the more useful AI is, BUT ALSO:
- The more expensive data is.
- The less accessible data is.
- The less certain you are of the content, completeness, and meaning of your observations.

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Obstacles to Data

- Must be digital.
- Must be scalable.
- Must have sufficient *breadth* (data sets) and *depth* (observed variables) to capture causative components.

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Data

- Take aways:
  - You need AI because it is hard to generate large volumes of correct data, and you need large volumes of correct data to create AI.
  - In order to create large volumes of correct data, you will need *quite a few* clever humans.

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The Way Forward

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Practical Approaches

- Digitize the manual process.
- Create innovative tools to expedite human decisions.
- Automate or semi-automate where possible.
- Facilitate fast human feedback.

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- Extract information from data.
- Apply state of the art algorithms.
- Provide fast/easy ways for humans to find and correct discrepancies.

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Prometheus by Prime Labs

- Ever-increasing volumes of training data, supplied by doing what needs doing anyway.
- Feedback loop for better solutions over time.
- Unlimited data storage and processing.

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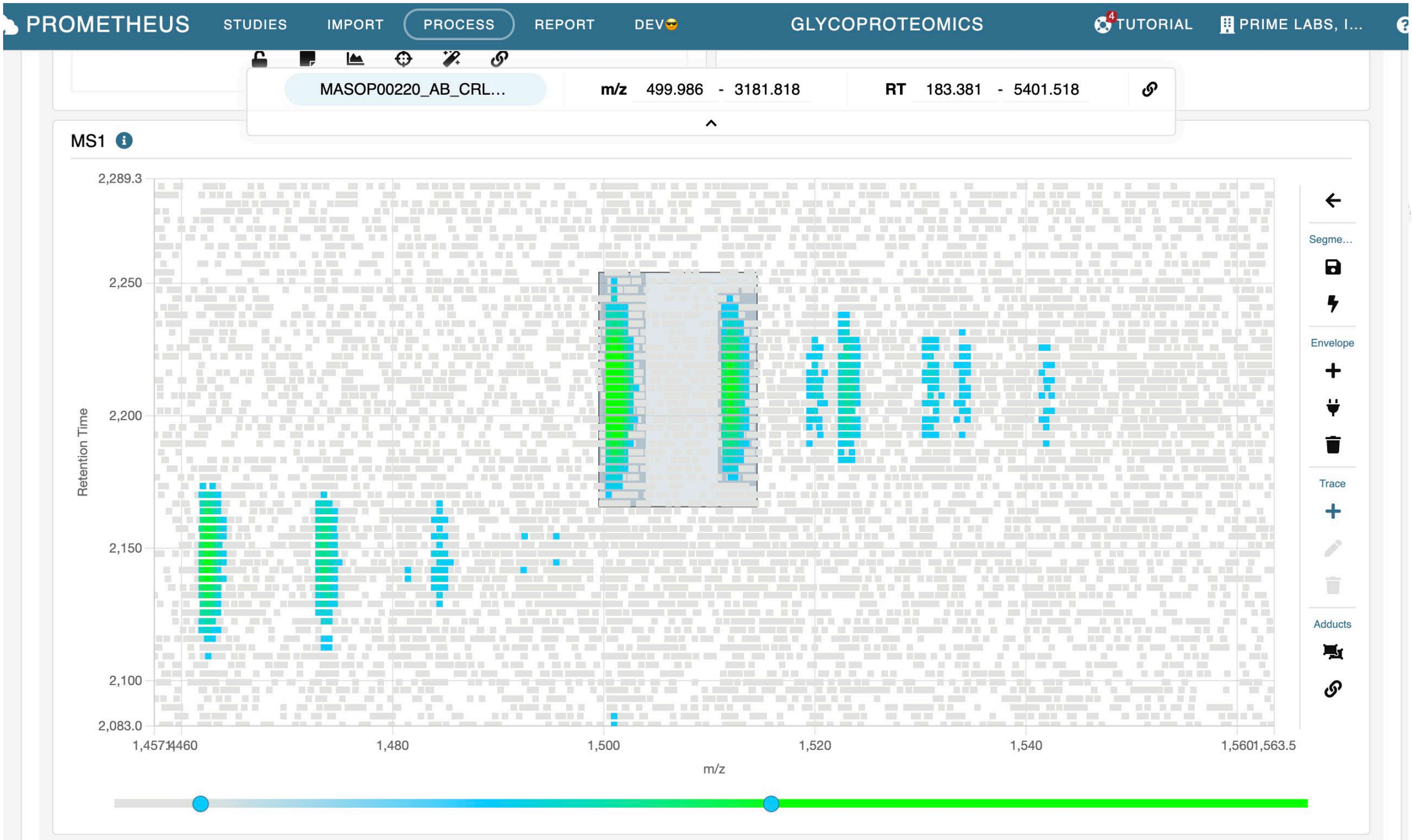
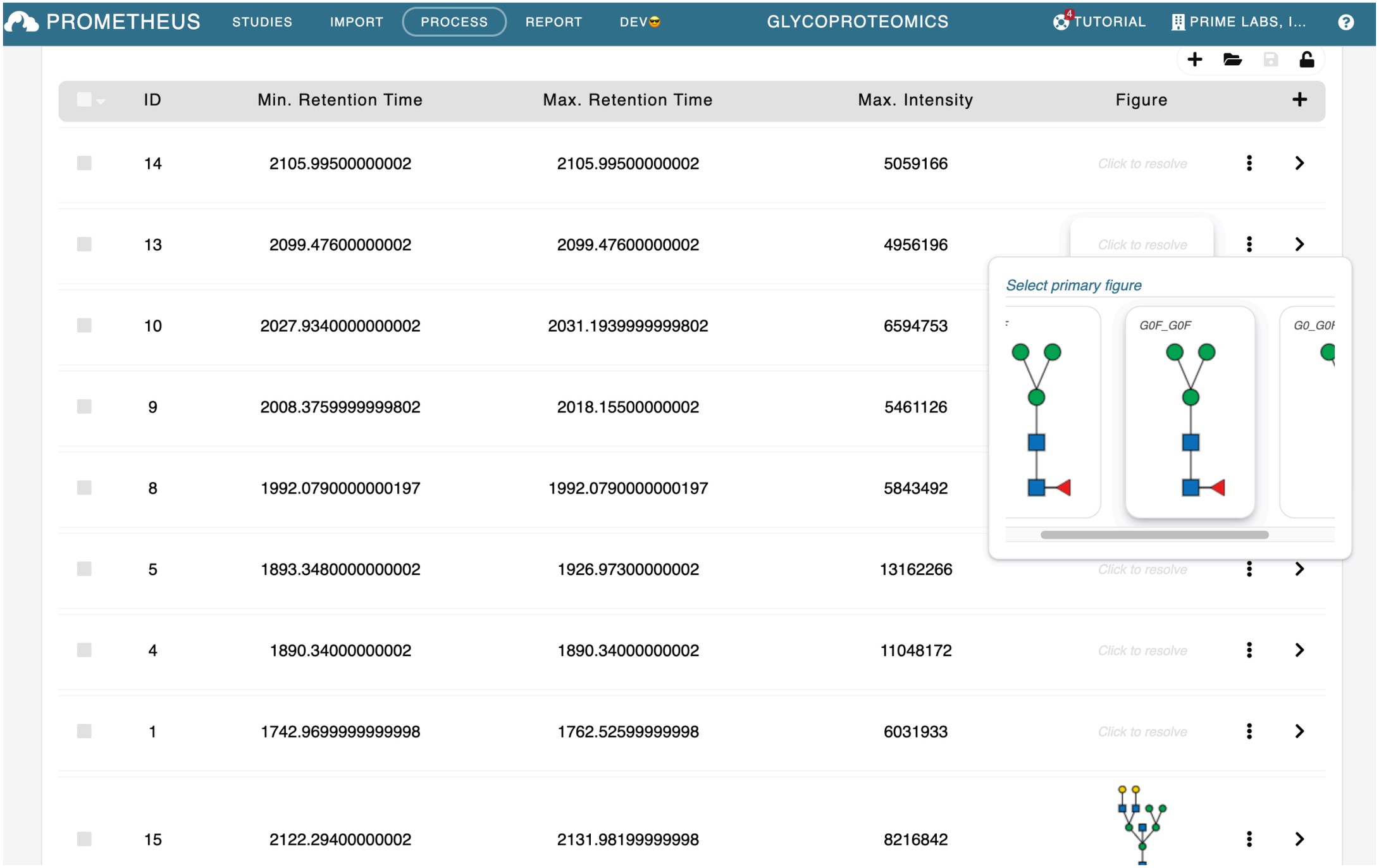
Example: MS1 feature detection



Example: Glycan Structure Elucidation



In Summary

- AI *is* amazing, and it will continue to drive innovation.
- But:
  - You can’t get something for nothing.
  - Good AI isn’t cheap or easy.
  - The next advancement in AI will probably not come from institutional sources.

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Questions?

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