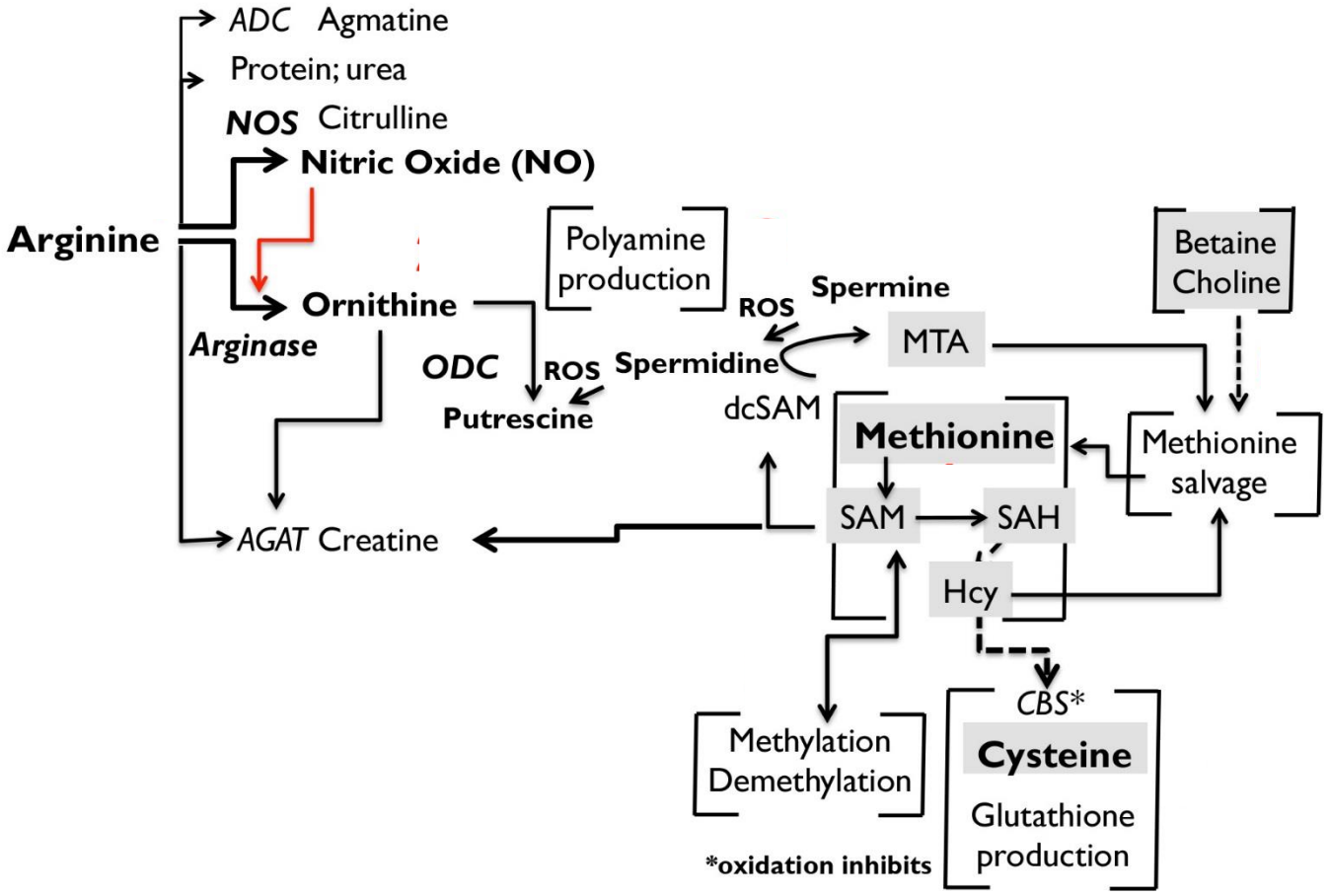
Skyline for Small Molecules, a Sneak Peek at Emerging Capabilities

Brian Pratt, Laura G. Dubois, and J. Will Thompson

Targeting a Metabolite Pathway of Interest: Arginine and Methionine



Courtesy of Dr. Carol Colton, Department of Neurology, Duke University Medical Center and Dr. Ashley Chi, Center for Genomics and Computational Biology, Duke

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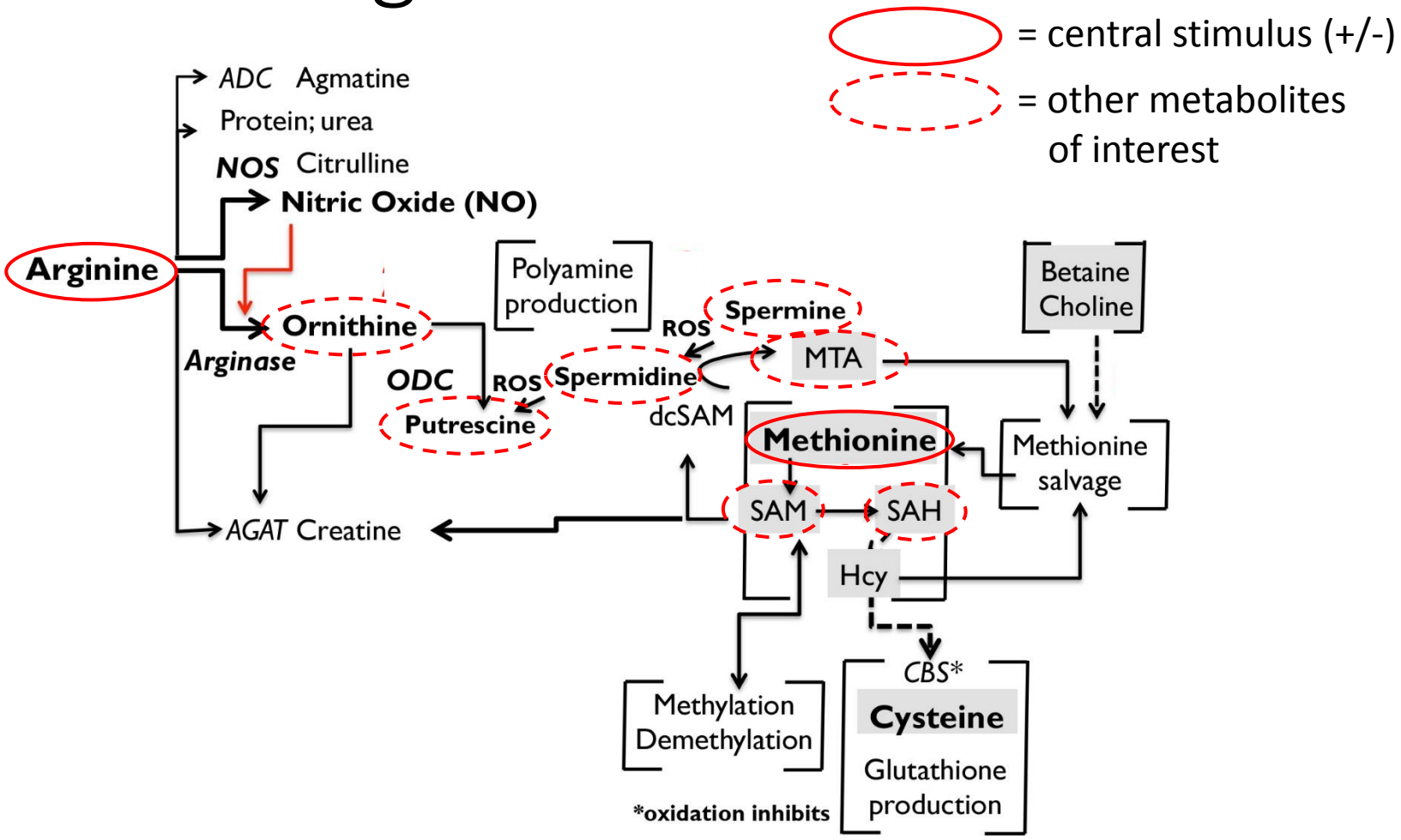

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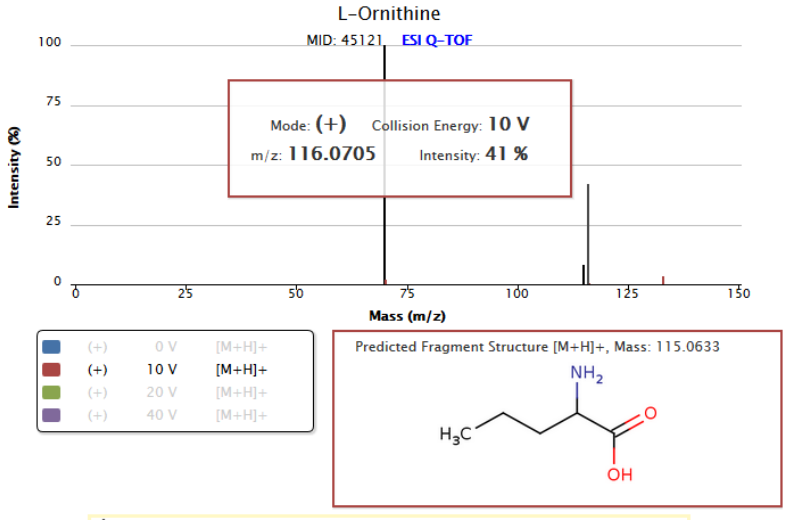
Precursor and Product Ion Calculations

- Experimental Data
- Fragmentation Databases
  - Metlin
  - MassBank
  - NIST
  - In-silico
- Currently flat-file support for transition lists, including:
  - Precursor and product m/z
  - Retention time
  - Ion Mobility Drift Time
- Future Support for fragmentation libraries

http://metlin.scripps.edu/

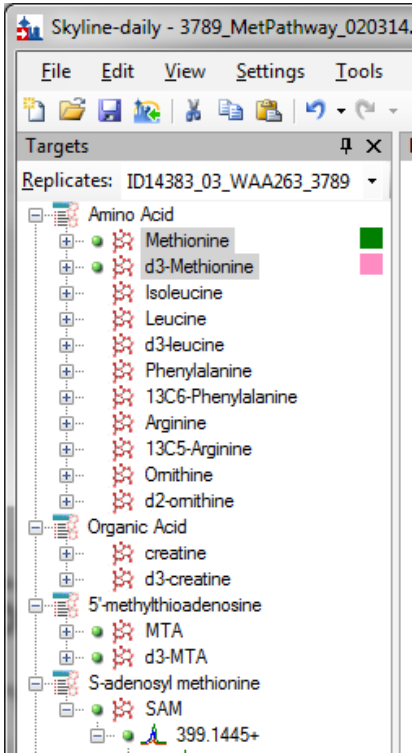


Skyline Small Molecule Workflow Summary

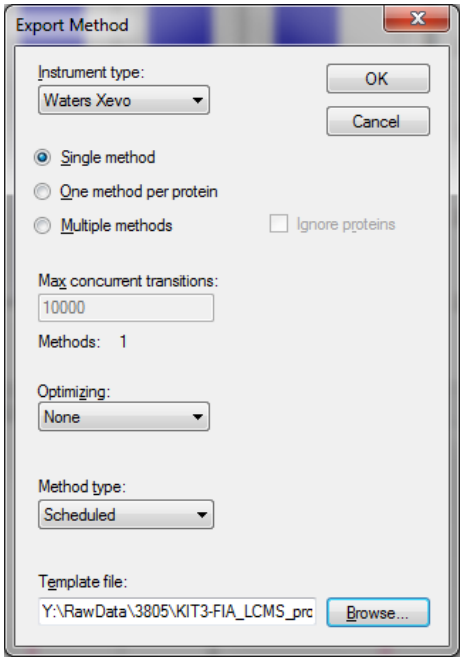
Flat File “Library”

Precursor Name	Precursor Formula
Methionine	C5H12NO2S
d3-Methionine	C5H9H'3NO2S
Isoleucine	C6H13NO2
Leucine	C6H13NO2
d3-leucine	C6H10H'3NO2
Phenylalanine	C9H11NO2
13C6-Phenylalanine	C3C'6H11NO2
Arginine	C6H14N4O2
13C5-Arginine	C1C'5H14N4O2
Ornithine	C5H13N2O2
Ornithine	C5H13N2O2
d2-ornithine	C5H11H'2N2O2
d2-ornithine	C5H11H'2N2O2
creatine	C4H10N3O2
d3-creatine	C4H7H'3N3O2
MTA	C11H16N5O3S
d3-MTA	C11H13H'3N5O3S
SAM	C15H23N6O5S
SAH	C14H21N6O5S
Spermidine	C7H20N3
Spermine	CH27N4

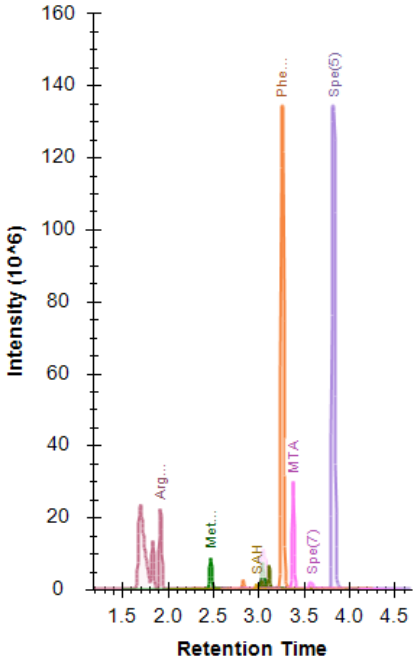
Skyline Document



Export Transition List/Method



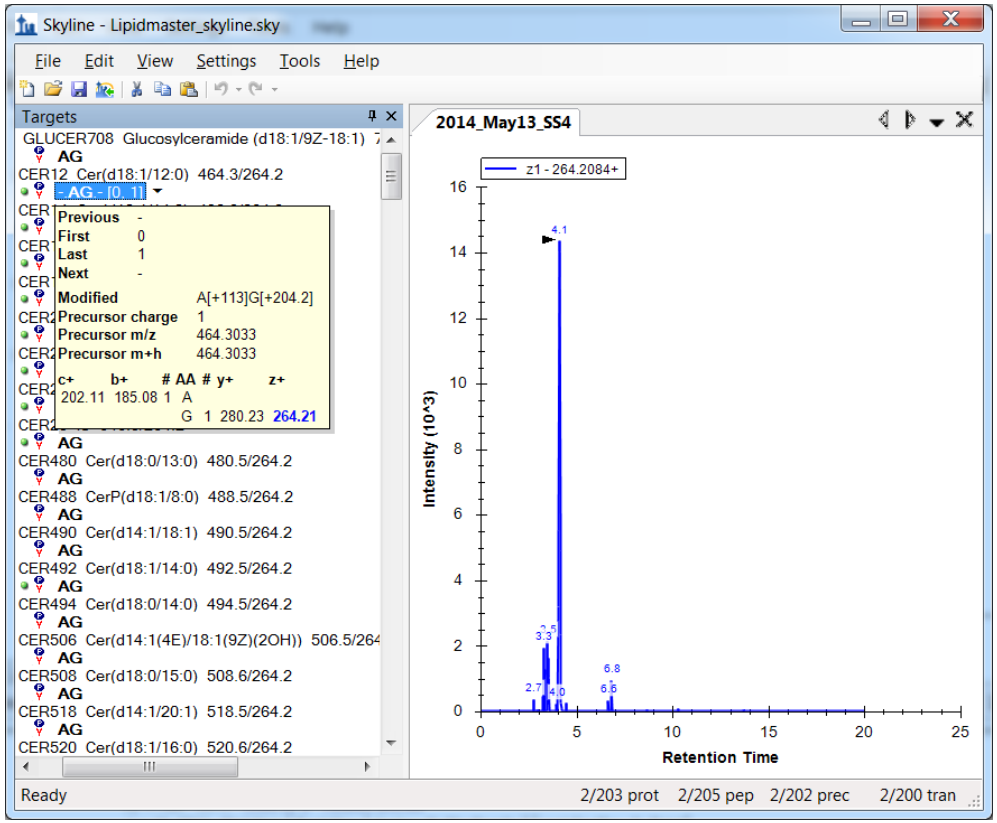
Import and Integrate Raw Data



Small Molecules in Previous Skyline Versions

It was always possible to trick Skyline into creating the masses you needed for lipidomics or metabolomics by means of clever peptide modifications, but this was inconvenient and lacked support for negative ions.

The Skyline document pictured here was prepared using a previous version of Skyline for a lipidomics experiment by **Hari Nair** of the Hoofnagle lab at the University of Washington. Constructing this document was a lot of work!



Using Skyline for Targeted Lipidomics is a presentation from the 2013 Skyline User Group meeting in which **Andy Hoofnagle** (ahoof@u.washington.edu) explains how his group used this approach for practical work.

Recent Skyline-daily versions would greatly simplify this experiment today.