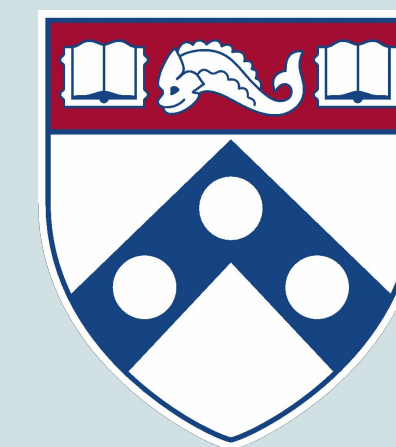


Untargeted Metabolomics using Marine Sponges

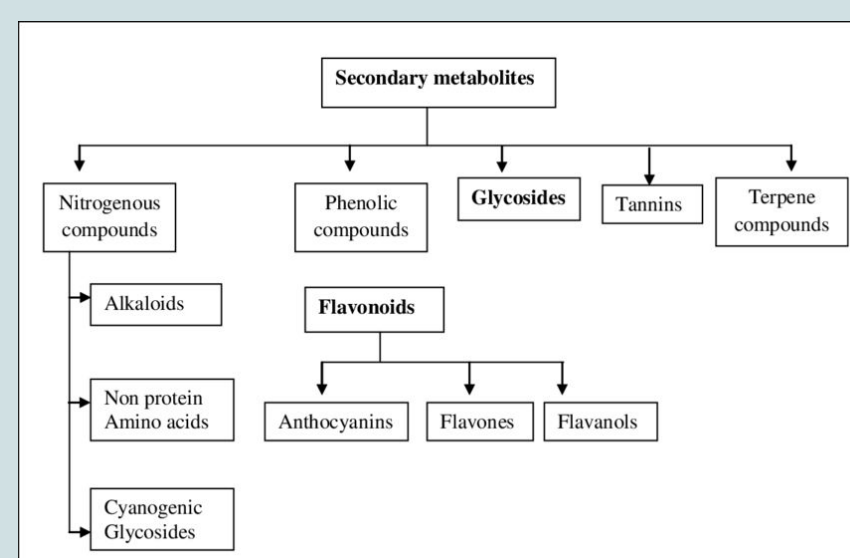
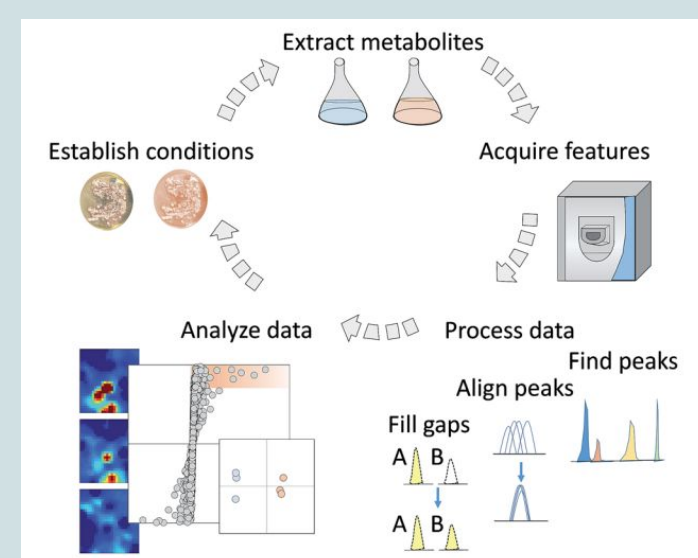
Jacob Isaac, Monica E. McCallum*

Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104



WHAT IS METABOLOMICS?

Metabolomics is the large scale study of the totality of small molecules, or metabolites, produced by a biological specimen. Within recent decades, the field of metabolomics has been used to yield biochemical insights with broad implications, from drug discovery to toxicology to nutrition.

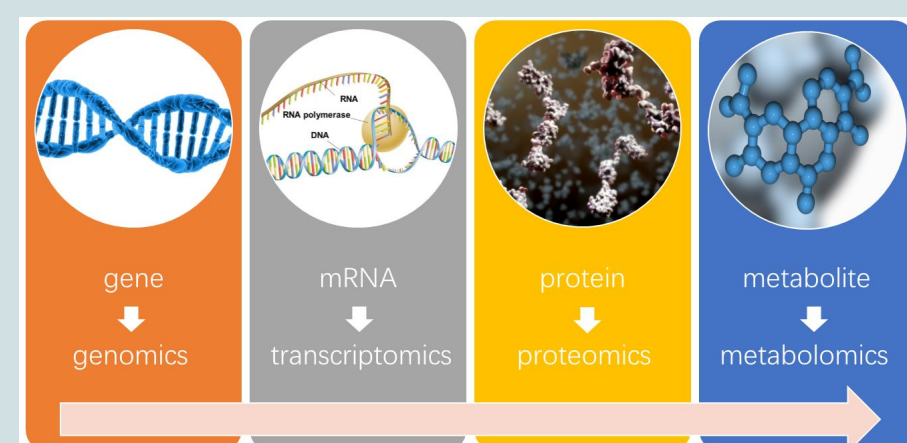


Covington, B. C.; McLean, J. A.; Bachmann, B. O. Comparative Mass Spectrometry-Based Metabolomics Strategies for the Investigation of Microbial Secondary Metabolites. *Nat. Prod. Rep.* 2017, 34 (1), 6-24.

Das, Kuntal & Gezici, Sevgi. (2018). Secondary plant metabolites, their separation and identification, and role in human disease prevention. *Annals of Phytomedicine: An International Journal*. 7, 13-24. 10.21276/ap.2018.7.2.3.

OTHER "OMICS" STRATEGIES

Metabolomics is just a single discipline in the much larger field of "Omics". The suffix "ome" means "all constituents considered collectively." Therefore fields such as genomics, transcriptomics, and proteomics attempt to holistically characterize the collective gene, RNA, and protein activity within biological samples.



WHY SPONGES?

Marine sponges are structurally diverse, prolific sources for a wide variety of natural products. Up to 35% of the biomass of a marine sponge is comprised of microbial life, which make it a prime specimen for the study of the microbial interactions that produce metabolites.



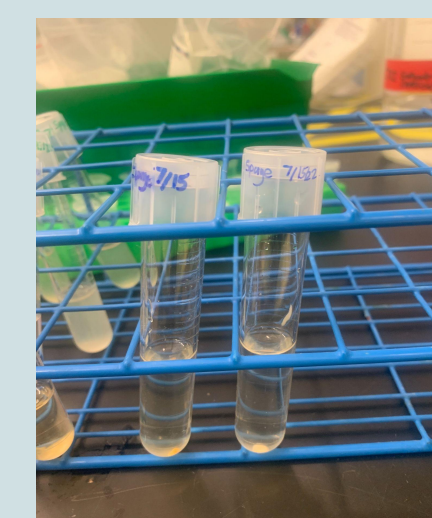
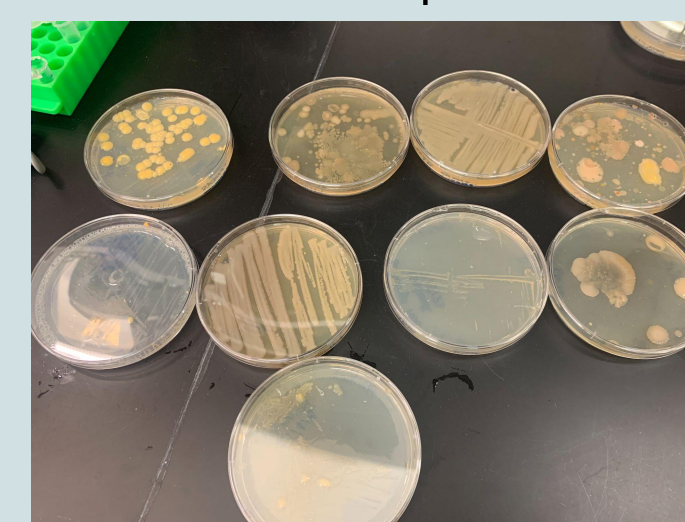
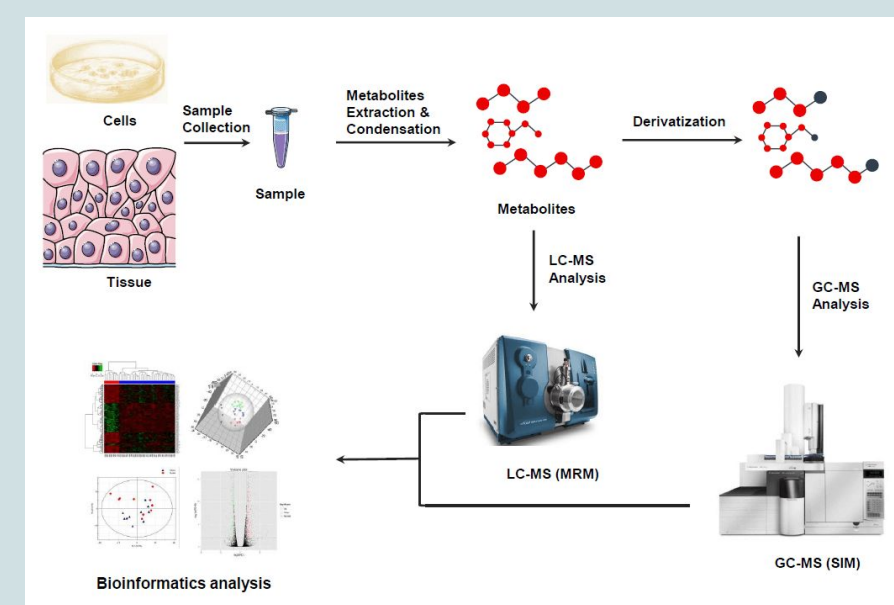
Red beard Sponge; *Microciona prolifera*. Chesapeake Bay Program. 2022.



Engelberts, J.P., Robbins, S.J., de Goeij, J.M. *et al.* Characterization of a sponge microbiome using an integrative genome-centric approach. *ISME J* 14, 1100-1110 (2020). <https://doi.org/10.1038/s41396-020-0591-9>

UNTARGETED METABOLOMICS

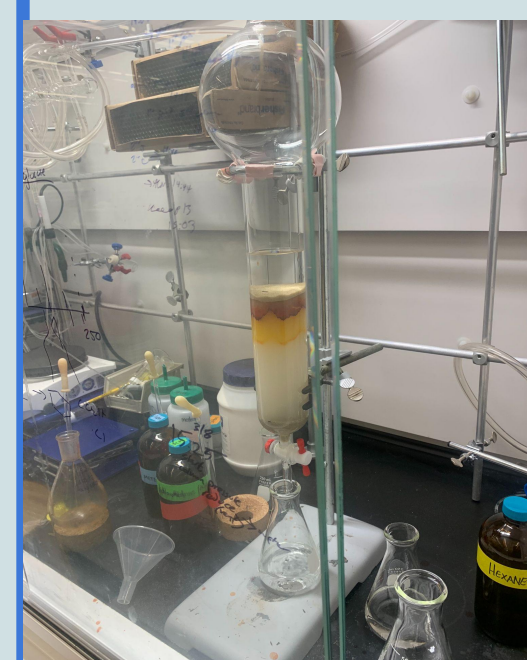
My project took an untargeted approach to characterizing the metabolome of the sponge. Untargeted metabolomics is hypothesis generating, and is solely focused on the large scale identification the full diversity of metabolite compounds from the sample.



Untargeted Metabolomics. *MtoZ Biolabs*. 2018.

RUNNING LC-MS

Liquid Chromatography-Mass Spectrometry is a technique that involves the separation of biological extracts into individual compounds and the analysis of the mass to charge ratio of each compound.



Liquid Chromatography Column



Separated samples from the sponge extract

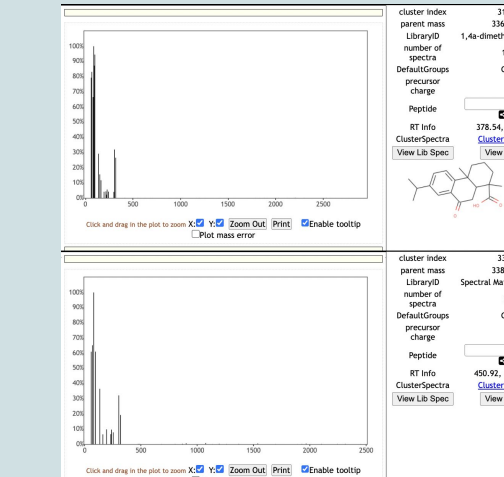
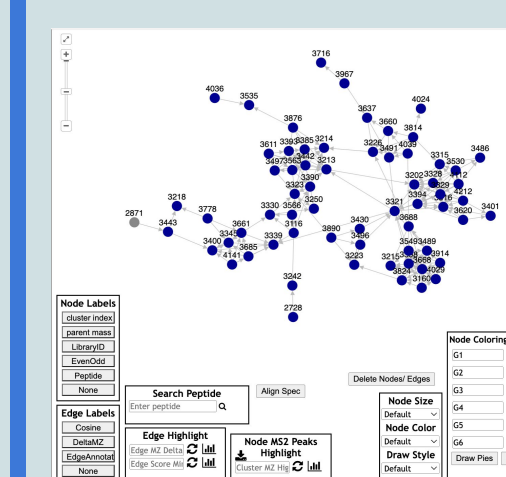


Scaled down samples prepared from mass spectrometry

Using samples of sponge extract collected within the lab, I set up a column to separate the extract into samples of different polarities and colors. The flasks of separated sponge extract had the solvents removed and were scaled down into smaller vials. These different samples were then placed into the mass spectrometer for the analysis of the mass to charge ratios of the ions within the samples.

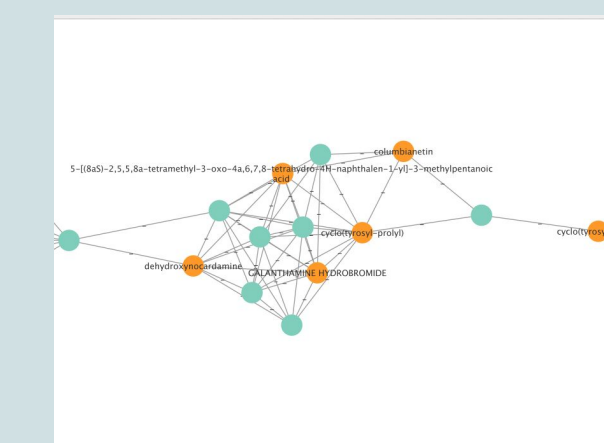
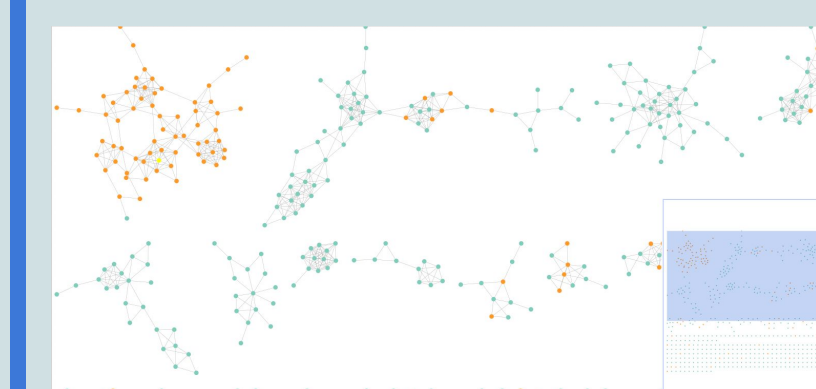
DATA ANALYSIS

GNPS

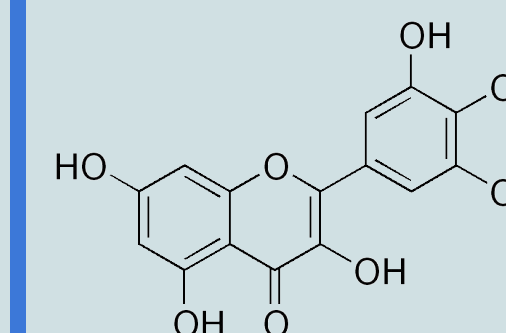


Wang, M., Carver, J., Phelan, V. *et al.* Sharing and community curation of mass spectrometry data with Global Natural Products Social Molecular Networking. *Nat Biotechnol* 34, 828-837 (2016). <https://doi.org/10.1038/nbt.3597>

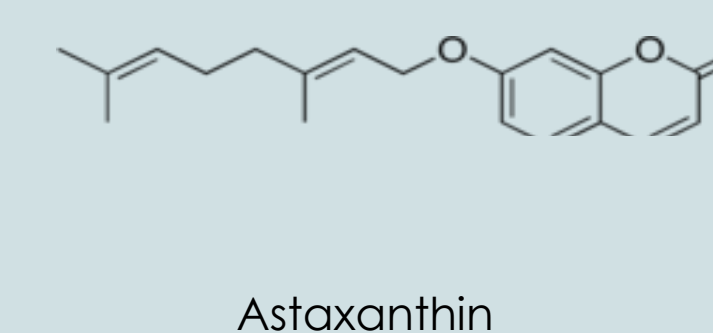
Cytoscape



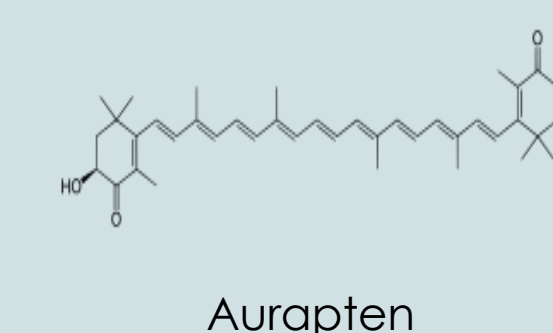
Some Discoveries



Chemical Structure of Myricetin. Wikipedia.



Chemical Structure of Astaxanthin. Wikipedia.



Chemical Structure of Auraptene. Wikipedia.

ACKNOWLEDGEMENTS



A Massive Thank You to All of My Labmates!!!

- Gail Calimaran
- Mason Singer
- Sabina Maurer
- Steven Cheng
- Jordan Artzy
- Percular Adimauba

MEM Lab | June 2022

L to R: Jacob Isaac (Penn UG), Steven Cheng (Penn G2), Gail Calimaran (Penn UG), Monica McCallum (PI), Sabina Maurer (Penn G2), Mason Singer (Penn UG)

And Especially Our Wonderful PI, **Monica McCallum!!**

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