

Leveraging Underexplored Marine Environments for the Discovery of Novel Chemistry

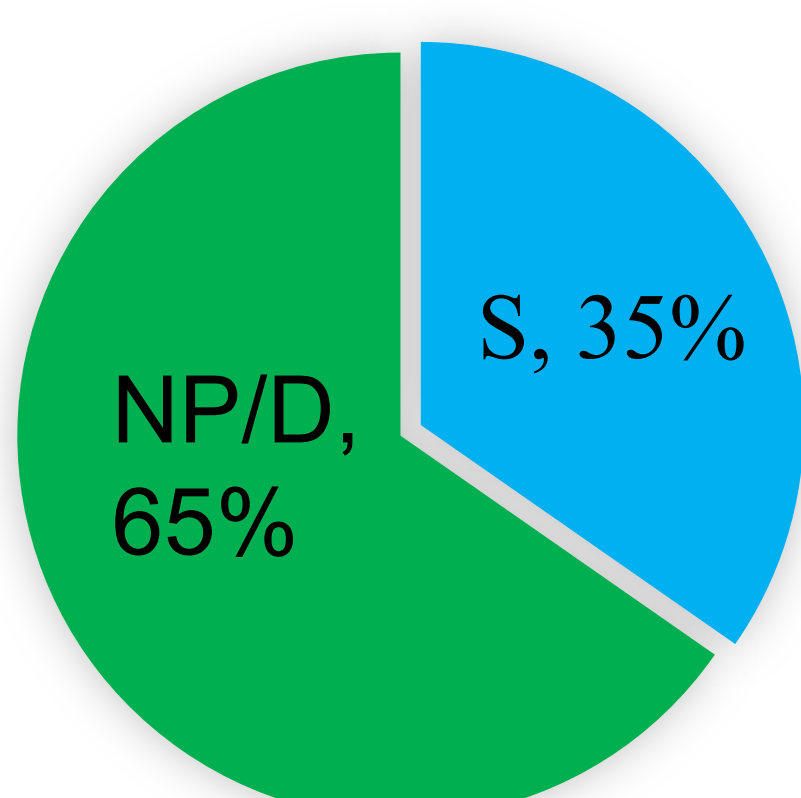
Mevers Lab – Department of Chemistry, Virginia Tech, Blacksburg, VA

Major Goals:

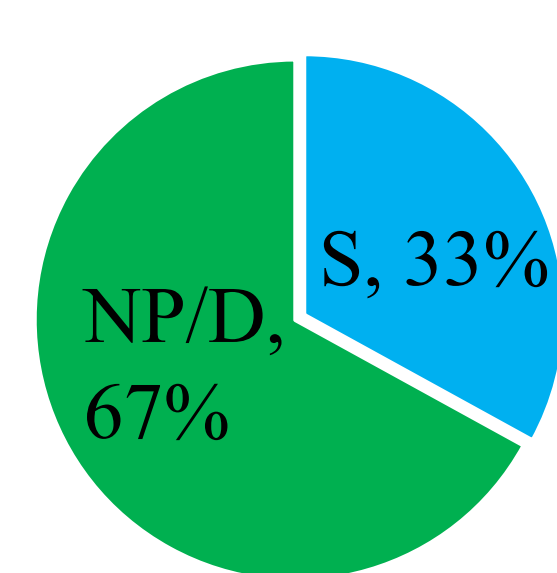
- Elucidation of antibiotics and anticancer agents produced by microbial symbionts of marine egg masses (DOI: 10.1128/mBio.02376-19 and 10.1073/pnas.1807613115)
- Discovery of siderophores and electron shuttles from extremophiles – (DOI: 10.7554/eLife.48054)
- Induction of cryptic bacterial natural products using chemical ecology – (DOI: 10.1021/jacs.6b07588)

Why Natural Products?

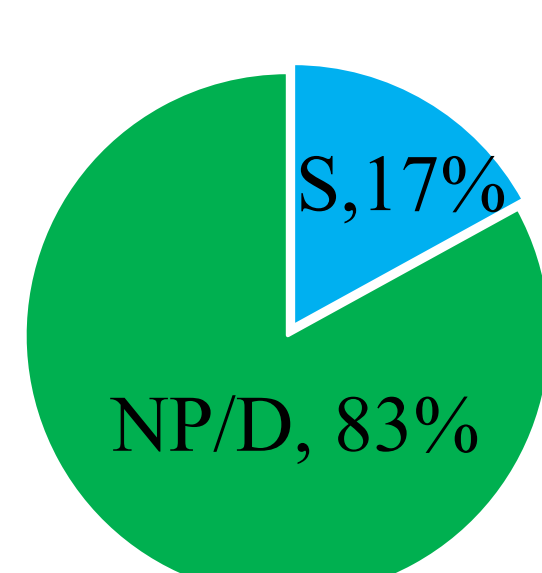
All FDA Approved Drugs



Antimicrobial Agents



Anticancer Agents



NP/D – Natural Product or derivative
S – Synthetic

Unique Ecological Niches

Egg Masses Microbiome



Coral Microbiome



Extremophiles – Hydrothermal vents (Worldwide)



Questions?
Email me!

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Microbiology

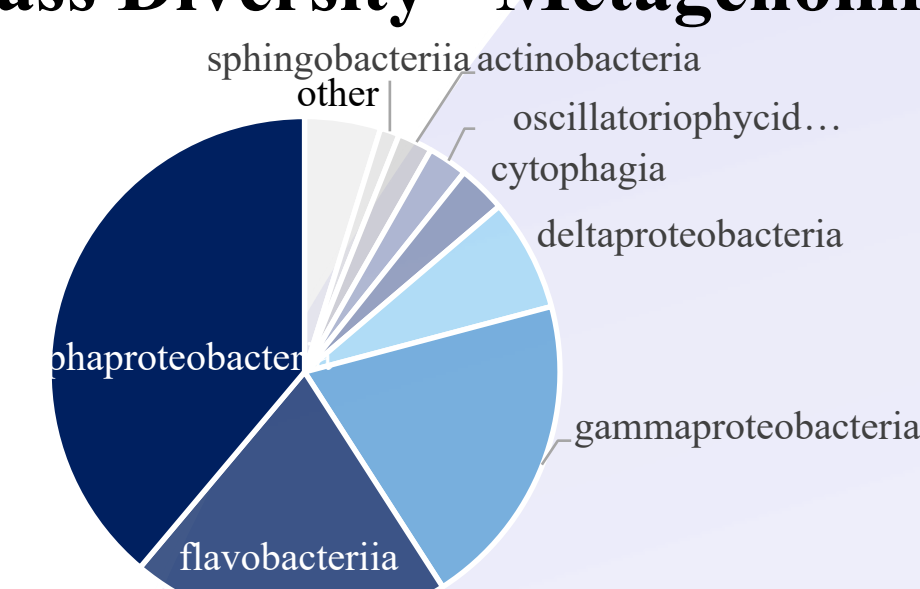
Major Techniques:

- Field collection and microbial culturing
- Development of biological and ecological assays
- Utilization and development of elicitation experiments
- Sequencing and bioinformatic analyses

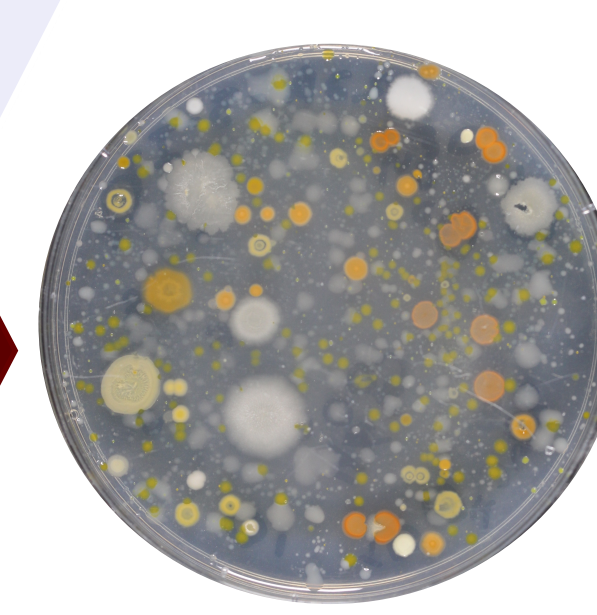
Who is present on the egg masses and coral?

Metagenomics & Microbial Culturing

Class Diversity - Metagenomics

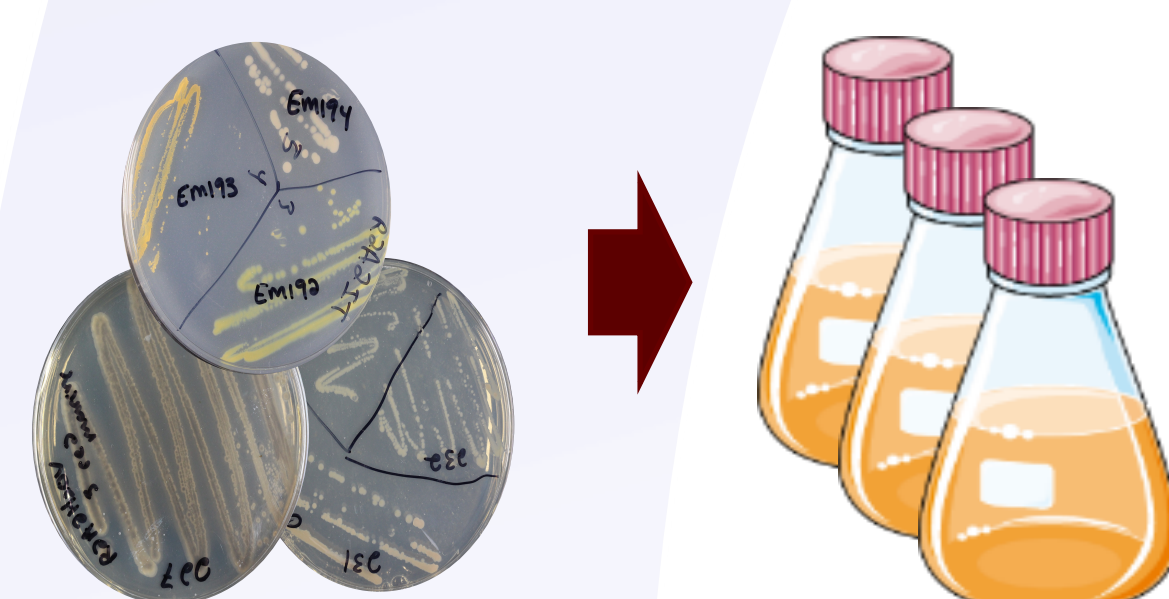


Field collection



What small molecules are they making?

Culturing, Mass Spectrometry, Biological Evaluation & Purification



- MS and NMR-based metabolomics
- Biological evaluation
- Chromatography – Flash and HPLC

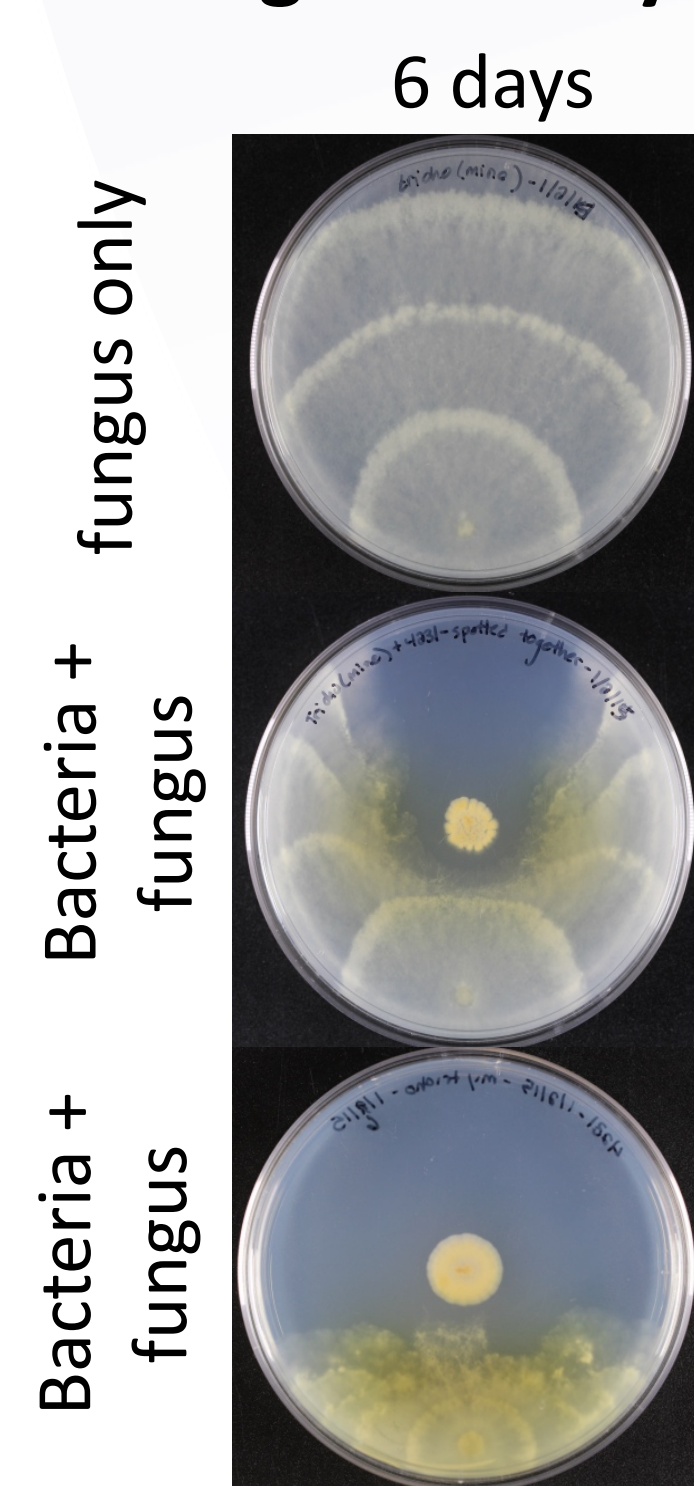
What are their ecological and biological functions?

Biological Assay Development, Bioassay-Guided Isolation, Ecological Assays

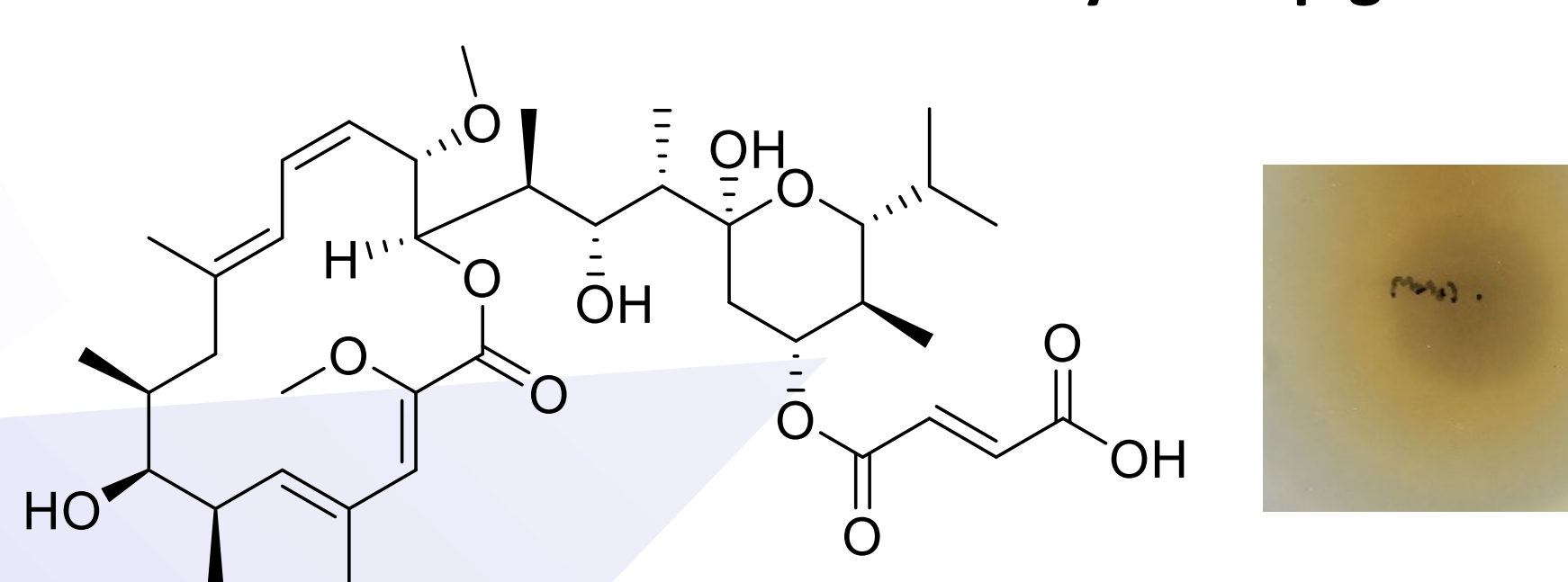
Biological Evaluation

- Non-addictive neuropathic pain
- Anti-HIV migration
- Immune modulation
- Octopus neuronal model
- Antimicrobial
- Cytotoxicity

Ecological Assays

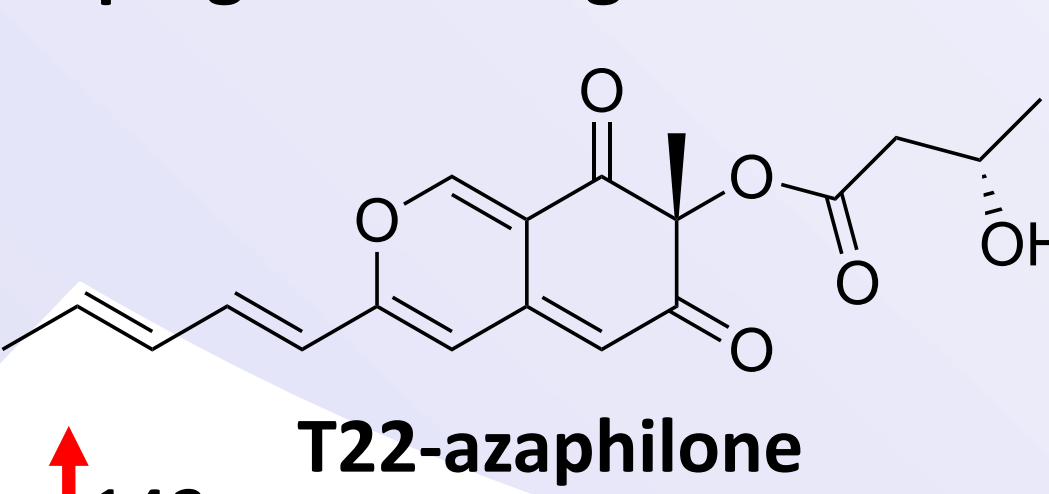


Bacterial metabolite that induces yellow pigment

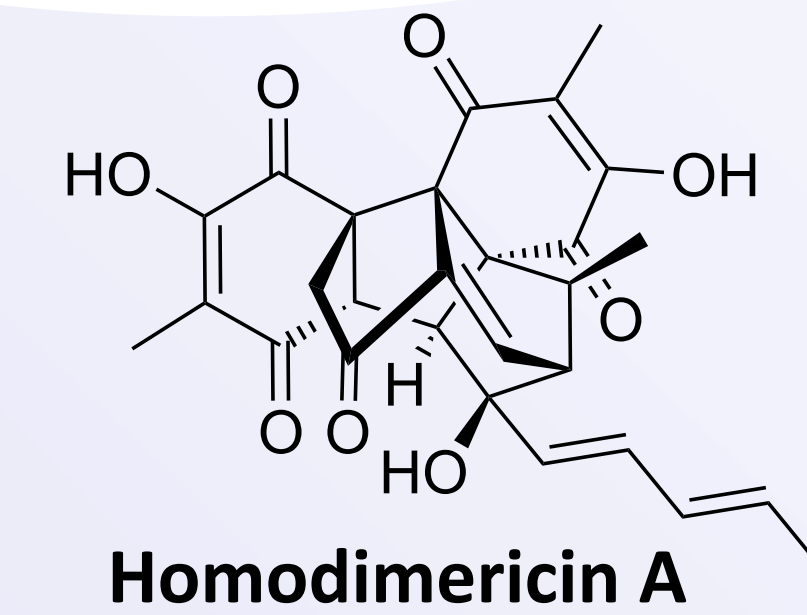


Bafilomycin C1
Antifungal

Upregulated fungal metabolites:



T22-azaphilone
Antibacterial
↑143x



Homodimericin A
Anti-oxidant
↑45x

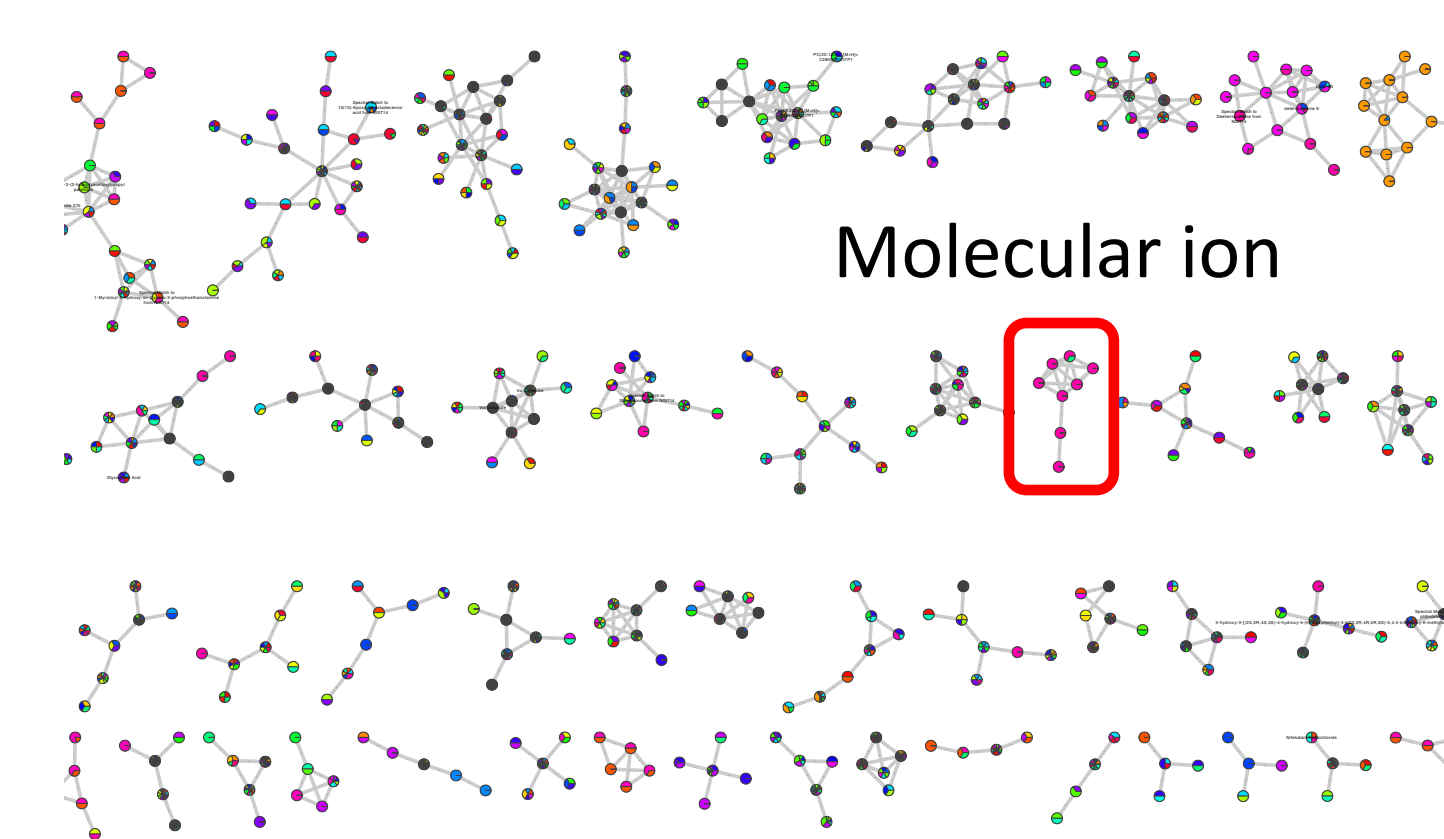
Chemistry

Major Techniques:

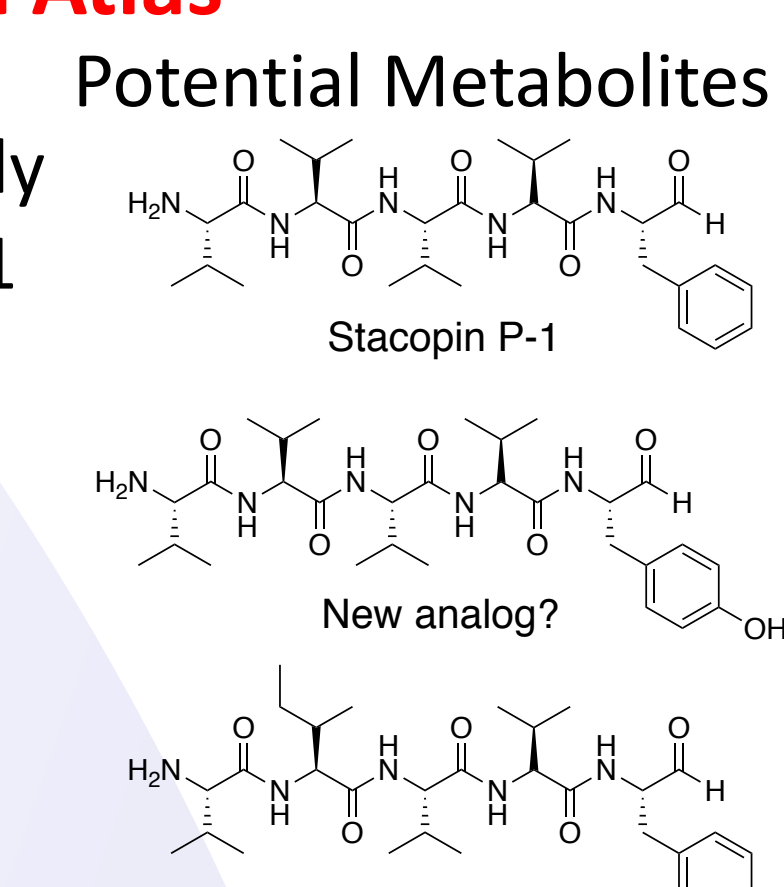
- Metabolomics – untargeted and targeted
 - Purification of complex mixtures
 - Structure elucidation
- Semi-synthesis – stereochemical analyses and SAR

Identifying novel small molecules.

Mass Spectrometry, GNPS, NPAtlas

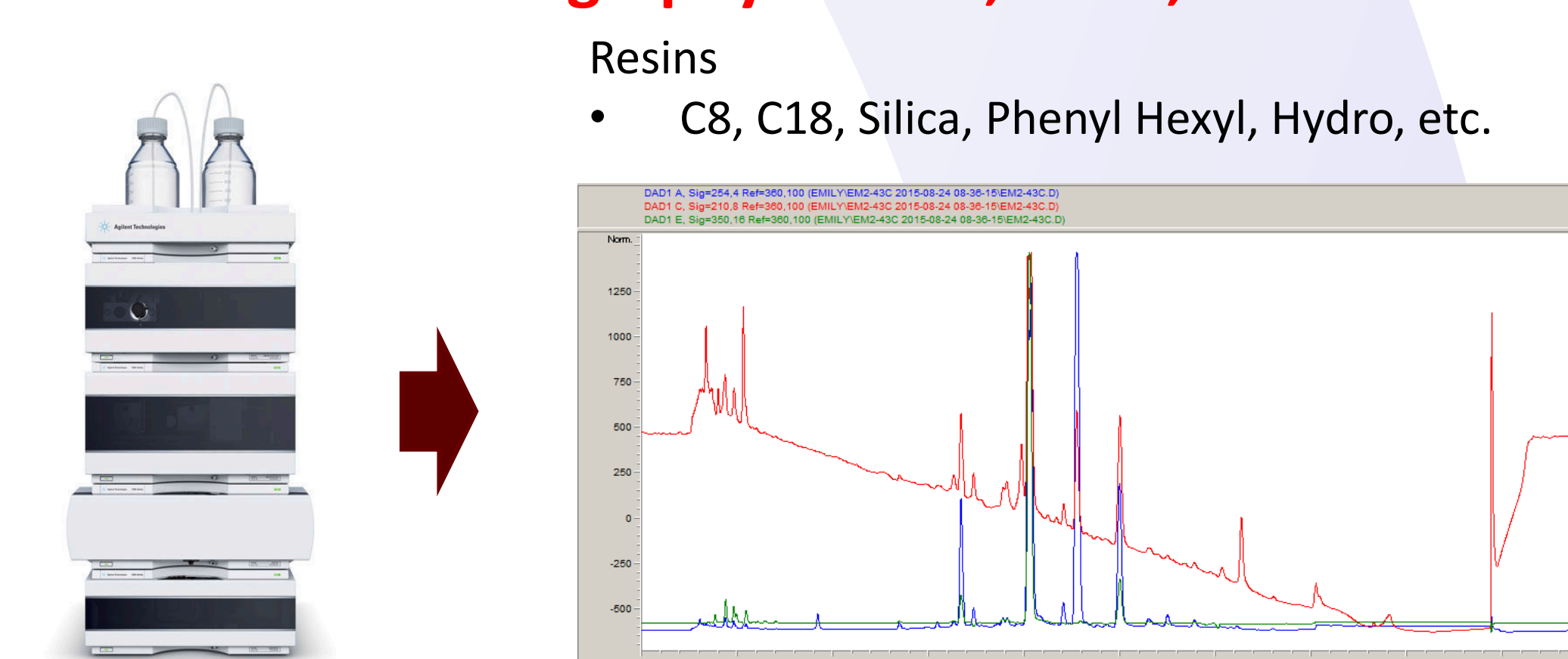


Cluster only found in 1 bacterial strain



Purification of the targeted small molecules

Chromatography – Flash, HPLC, UPLC



Resins

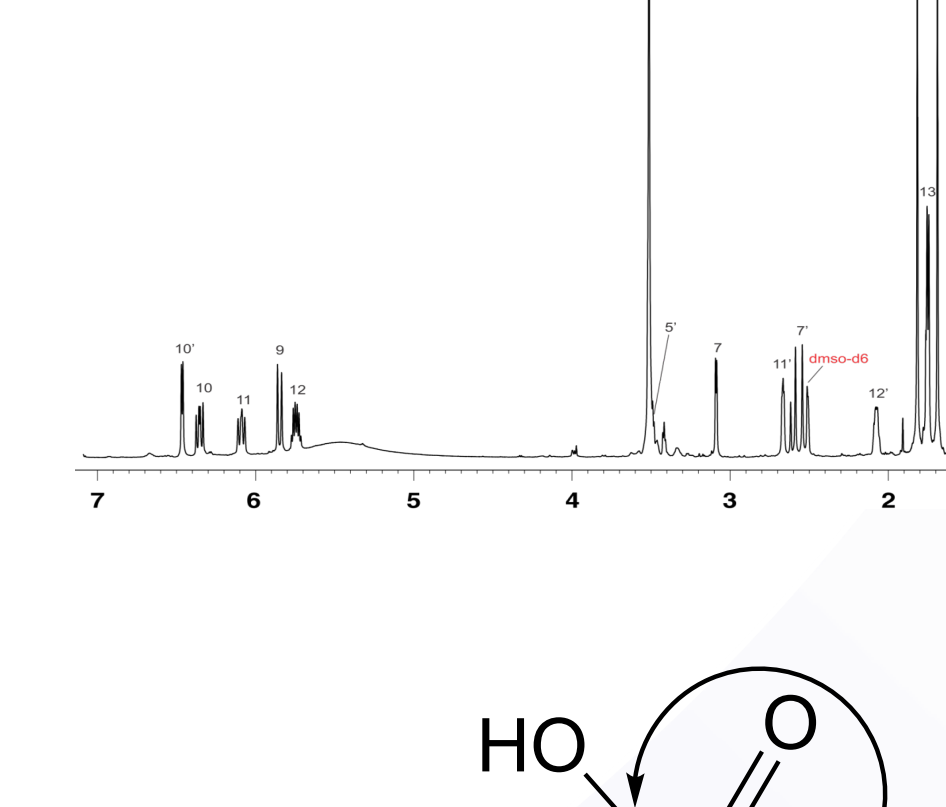
- C8, C18, Silica, Phenyl Hexyl, Hydro, etc.

Structure Elucidation of novel small molecules

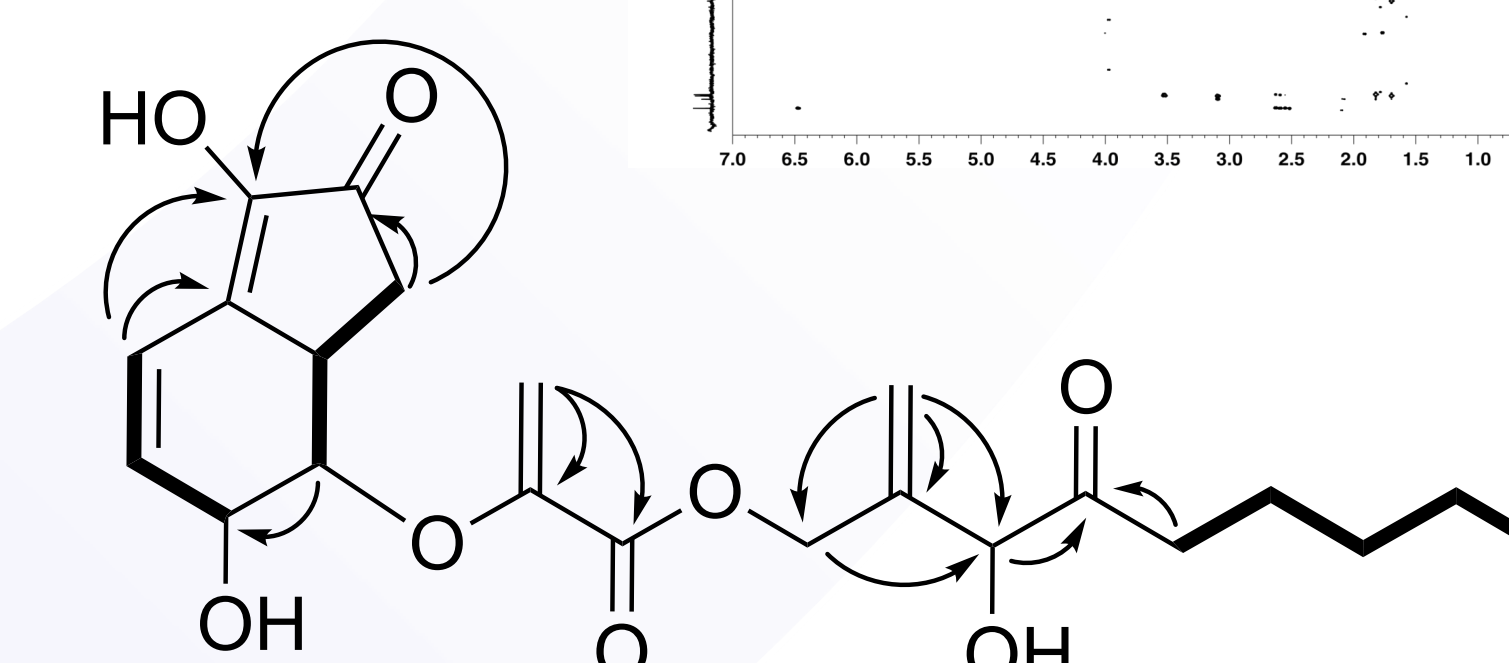
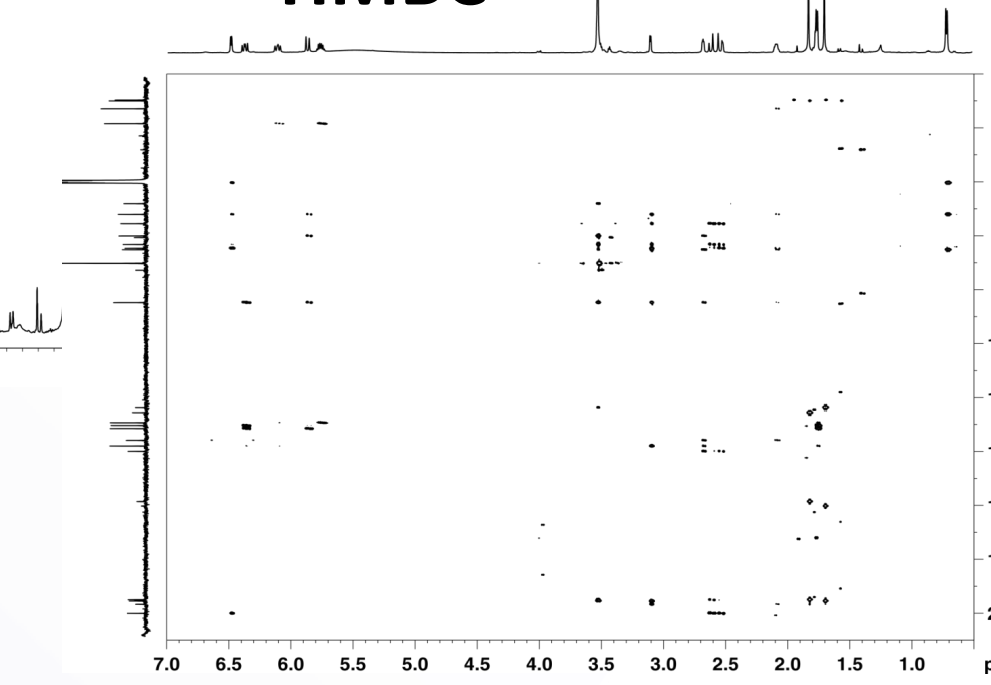
¹H, ¹³C, HSQC, HMBC, COSY, TOCSY, etc.

1D & 2D NMR

¹H NMR



HMBC



Tundrenone

— COSY
— HMBC



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