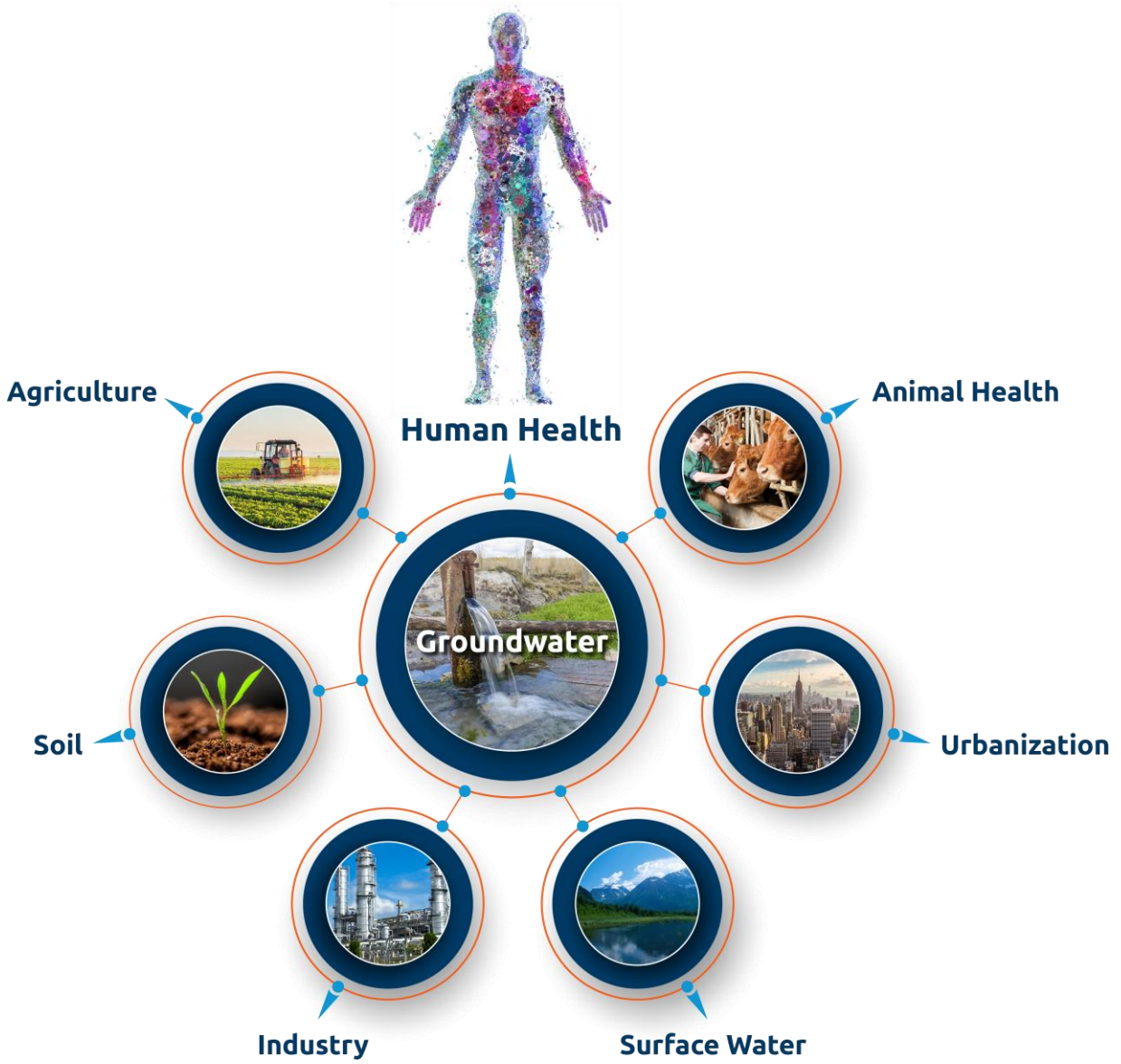
Using Environmental Metabolomics to Improve Decision Making at Chlorinated Solvent Sites

Molecular Tools to Navigate Your Diagnostic Exploration

microbialinsights


Human Health
Agriculture
Animal Health
Groundwater
Soil
Urbanization
Industry
Surface Water

ONE DEGREE RULE

- A small change can help correct our course and get us to our goal.
- Understanding the black box of microbiology allows us to correct quickly and cost effectively.
  - What are the dominant organisms present?
  - What is the genetic potential for complete reductive dechlorination?
  - What organisms are competing for available donors?
  - Are compounds biodegrading?
  - What is likely to happen in the future?
  - What is the rate of degradation?

STATE OF REMEDIATION IN THE 1990'S

In situ bioremediation of chlorinated solvents

Microbiology (1998), 144, 599–608 Printed in Great Britain

REVIEW ARTICLE

Bioremediation: towards a credible technology

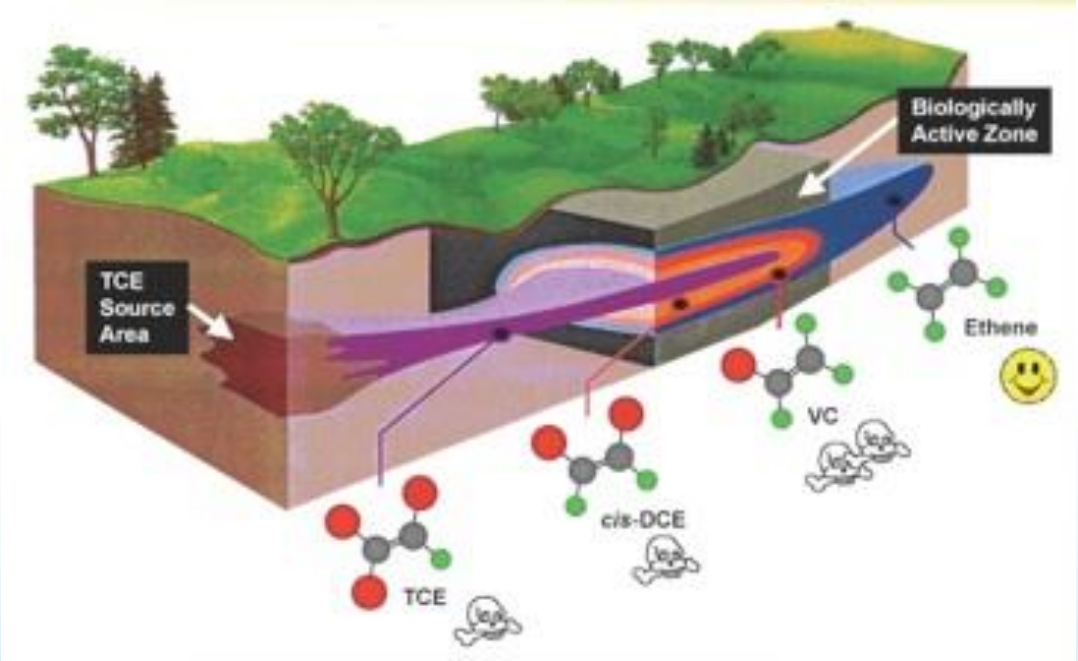
Ian M. Head

of chlorinated solvents and chlorinated aliphatic hydrocarbon contaminants in groundwater may soon become a reality. Both anaerobic reductive dehalogenation to non-chlorinated products and complete aerobic oxidation offer greatly increased promise for potential applications.

Current Opinion in Biotechnology 1993, **4**:323–330

REMEDIATION EFFORTS MUST LEAD TO COMPLETE DECHLORINATION

The toxicity of TCE transformation products increase as dechlorination proceeds.



This is problematic if the process stalls once *cis*-DCE and/or VC is produced.

DATA GAPS

- qPCR and QuantArray provide quantitative data for microorganisms and gene targets
  - What about activity?
- Next Generation Sequencing provides a bigger picture of the overall microbiome
  - What about the health of the microbiome?
- Compound Specific Isotope Analysis and Stable Isotope Probing provide proof of contaminant degradation
  - What about predicting future degradation trends?

METABOLOMICS

nature COMMUNICATIONS

ARTICLE

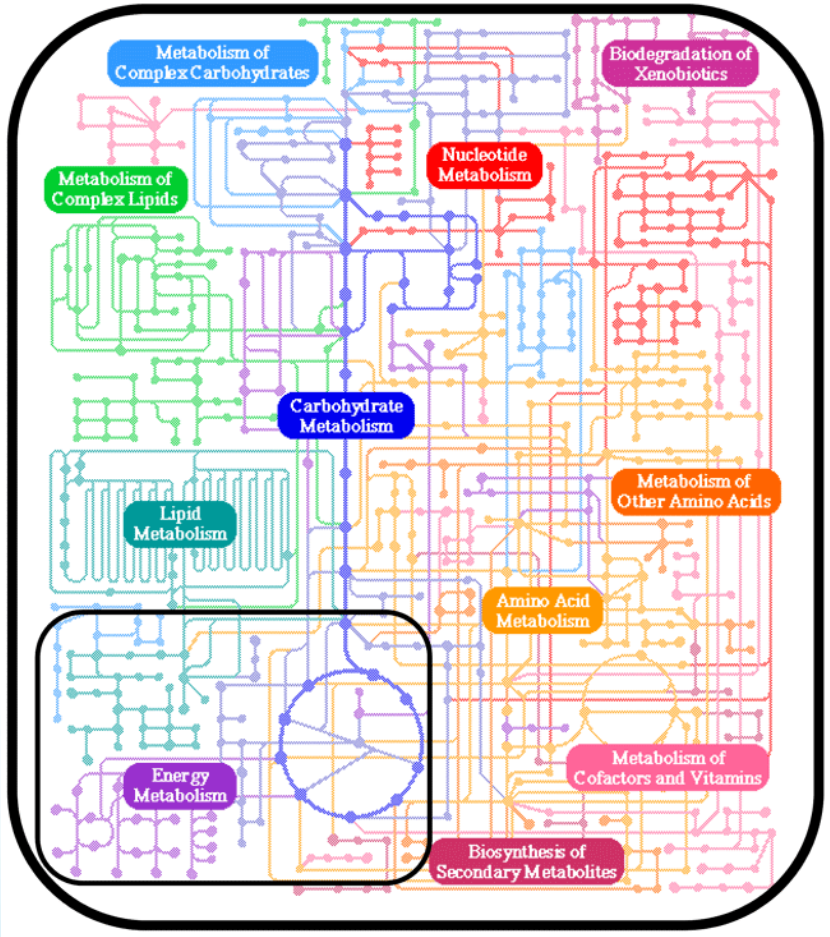
https://doi.org/10.1038/s41467-019-11311-9 OPEN

A metabolic profile of all-cause mortality risk identified in an observational study of 44,168 individuals

Joris Deelen et al.#

METABOLOMICS

- Systematic study of the unique chemical fingerprints as the result specific cellular processes.
- Metabolome: the collection of all metabolites in a biological cell, tissue, organ or organism.
- Metabolic profiling: instantaneous snapshot of the cell physiology.



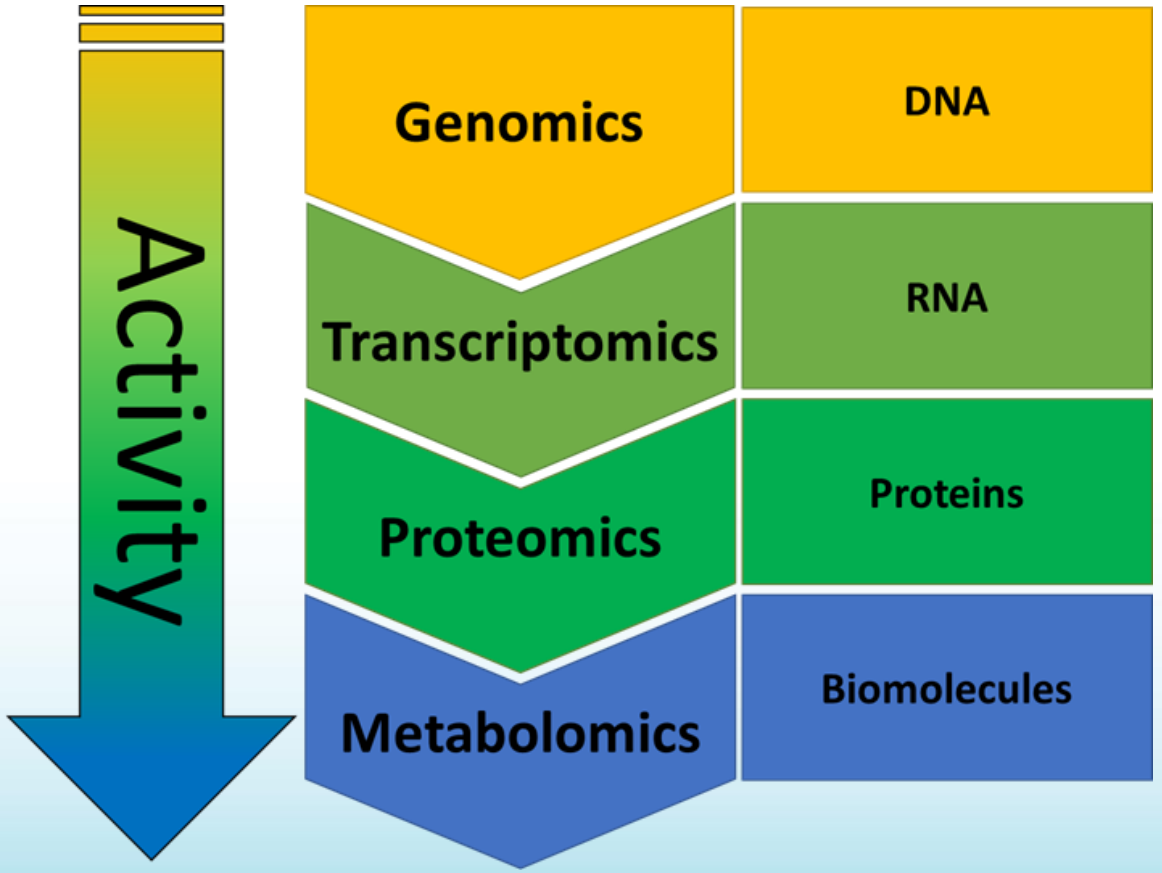
http://www.urmc.rochester.edu/labs/Munger-Lab/

METABOLOMICS

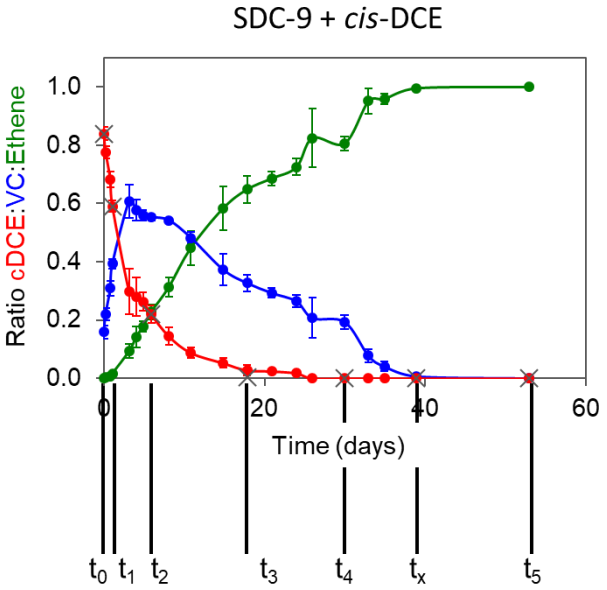
- Analysis of all small molecules (MW<1100) within an environmental sample
- Identification of 80-100 known compounds
- Comparison of the overall metabolic profile
- Statistical Analysis and pattern recognition
  - Predictive capabilities
  - Activity of key degraders

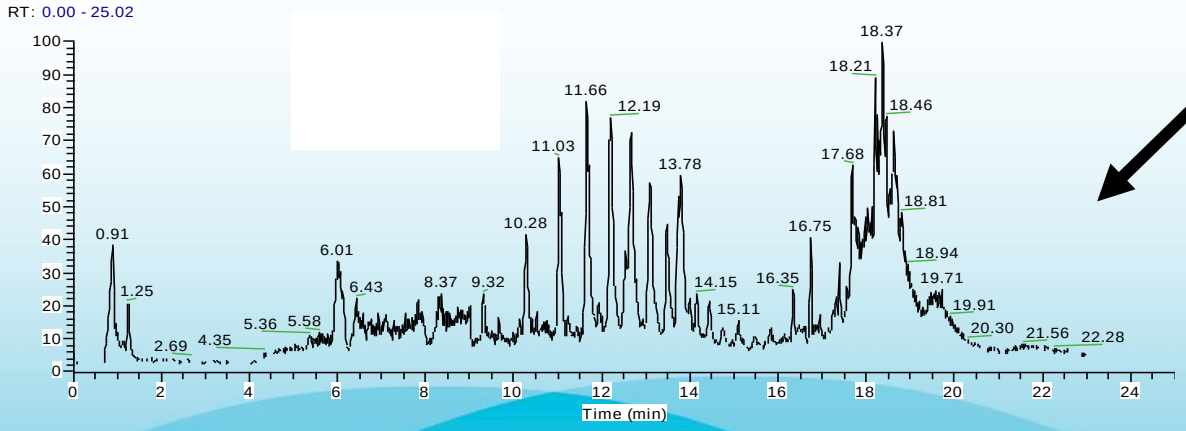
Metabolomics

- Metabolomics - analysis of thousands of small molecules from a biological sample
- Trends and patterns can be used to predict the health and activity of the entire microbiome
- Allows for a broad screening of reductive dechlorination potential

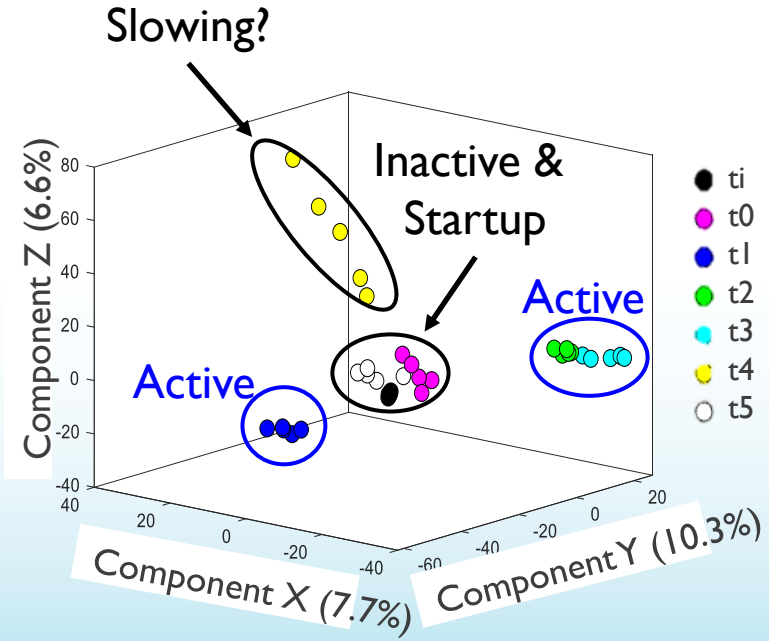


SBIR METABOLOMICS STUDY

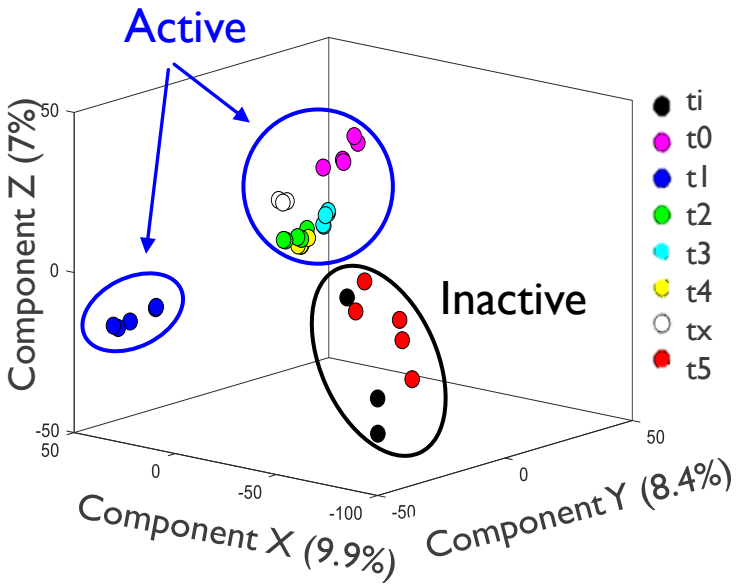




SBIR METABOLOMICS STUDY



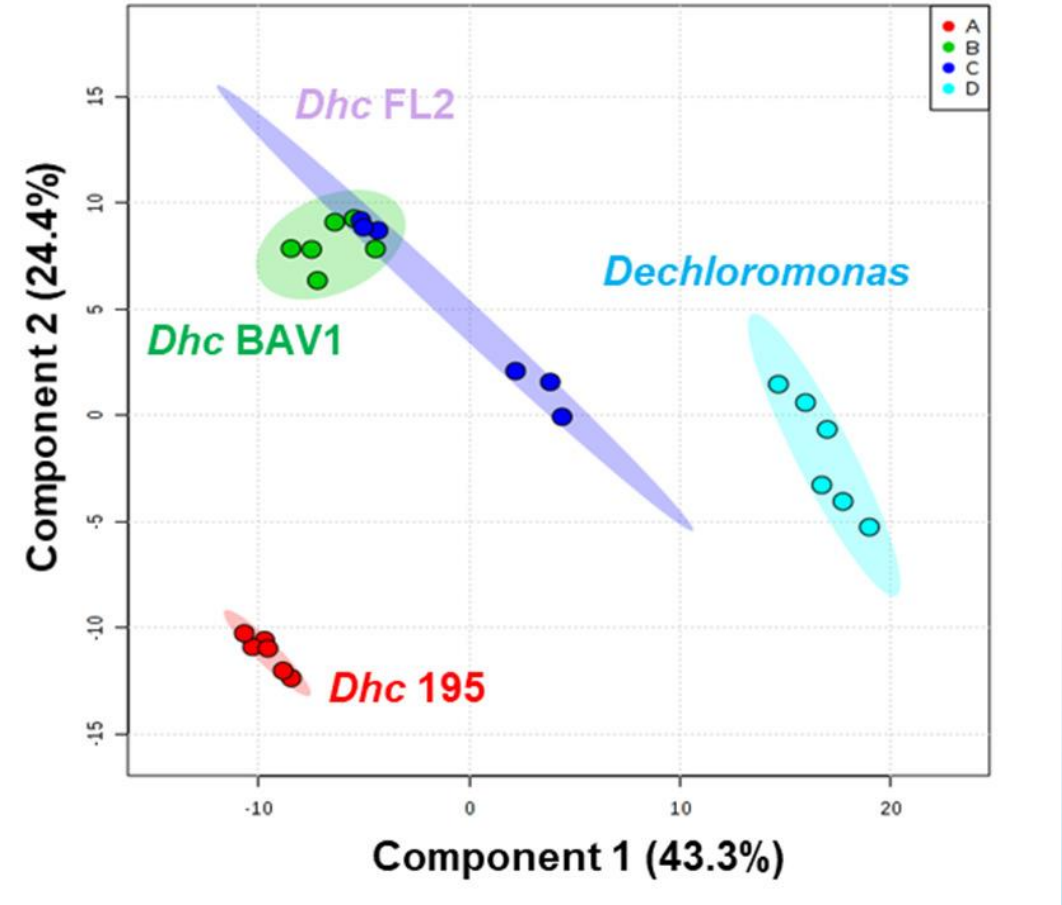
Vinyl chloride



cis-DCE

- Commercial Bioaugmentation consortium (SDC-9)
- Sampling performed in intervals to capture stage of dechlorination
- Over 10,000 metabolites identified
- Both the known and unknown metabolites were analyzed using PLS-DA plots
- Differences in stages of dechlorination

SBIR METABOLOMICS STUDY



SBIR METABOLOMICS STUDY

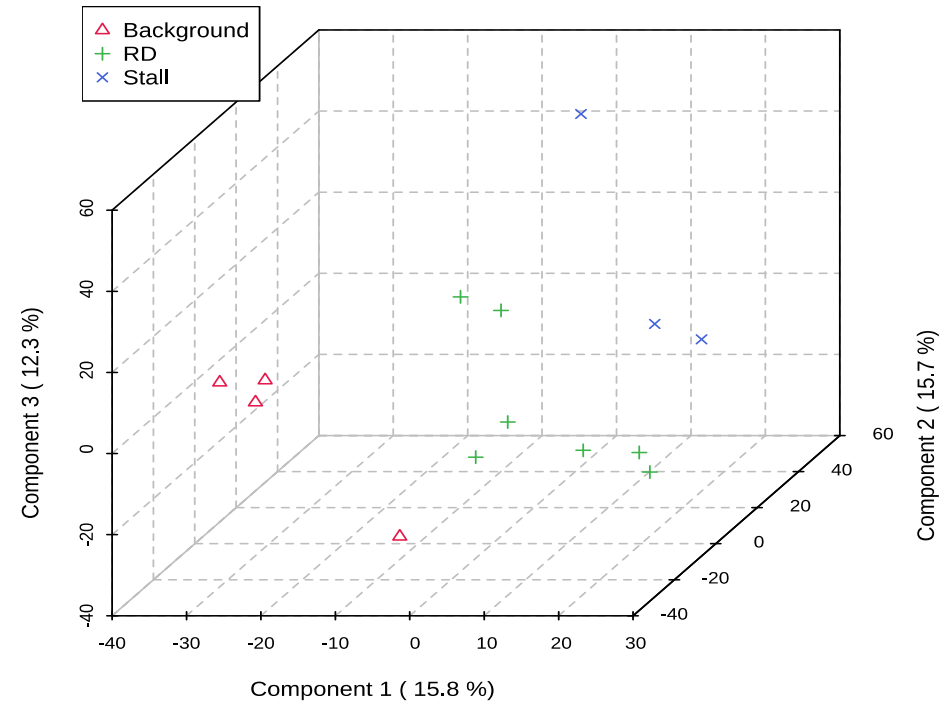


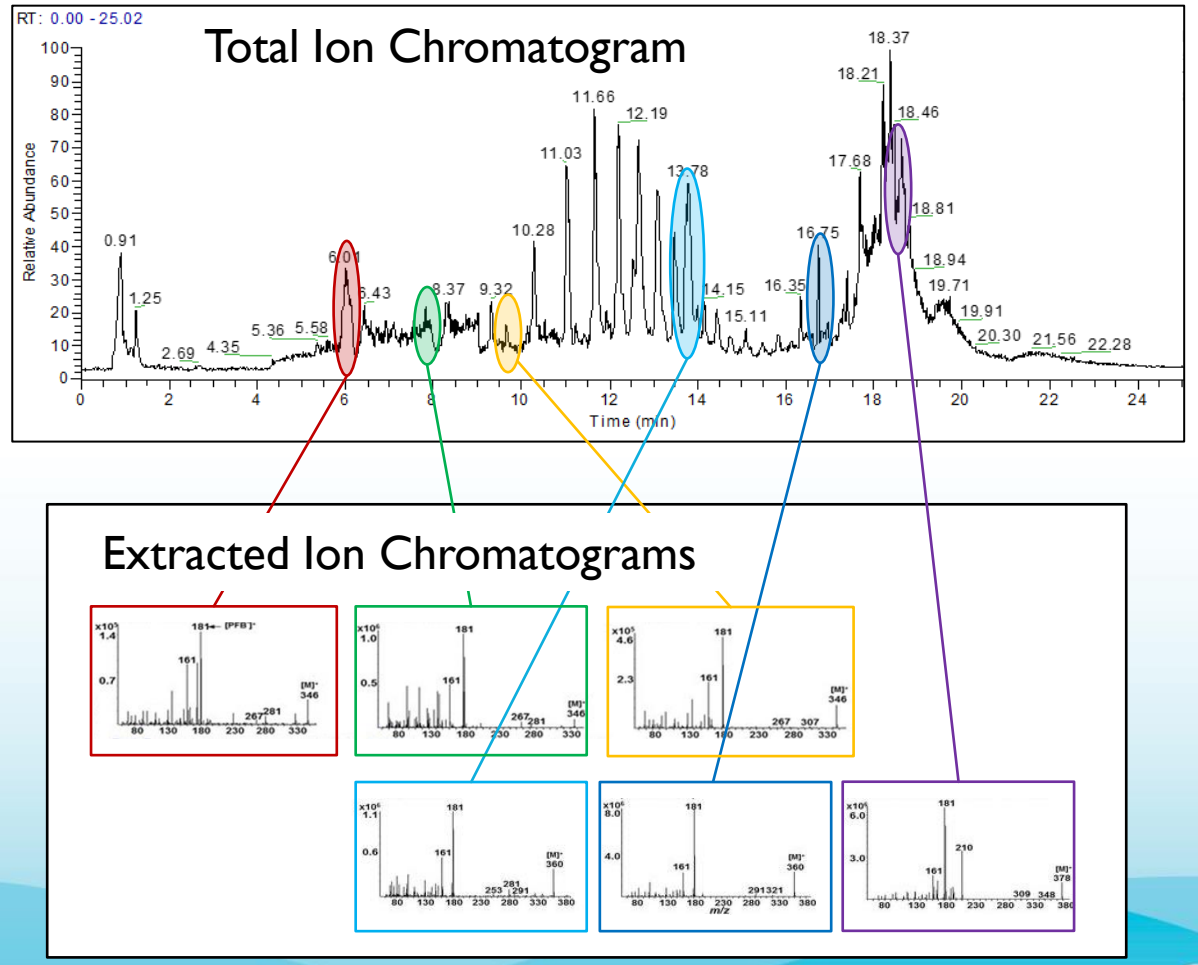
Figure 10: 3D scores plot between the selected PCs. The explained variances are shown in brackets.

- Three chlorinated sites
  - Belleville Industrial (NJ)
  - Former Vickers Facility (MO)
  - Earnhart Site (TN)
- Different stages of Dechlorination
  - Active RD
  - Stall
  - Background
- Over 12,000 metabolites identified
- PLS-DA plot clearly distinguishes each stage
- VIP scoring identified 5 metabolites that could be sentinel for robust RD!

Metabolomics

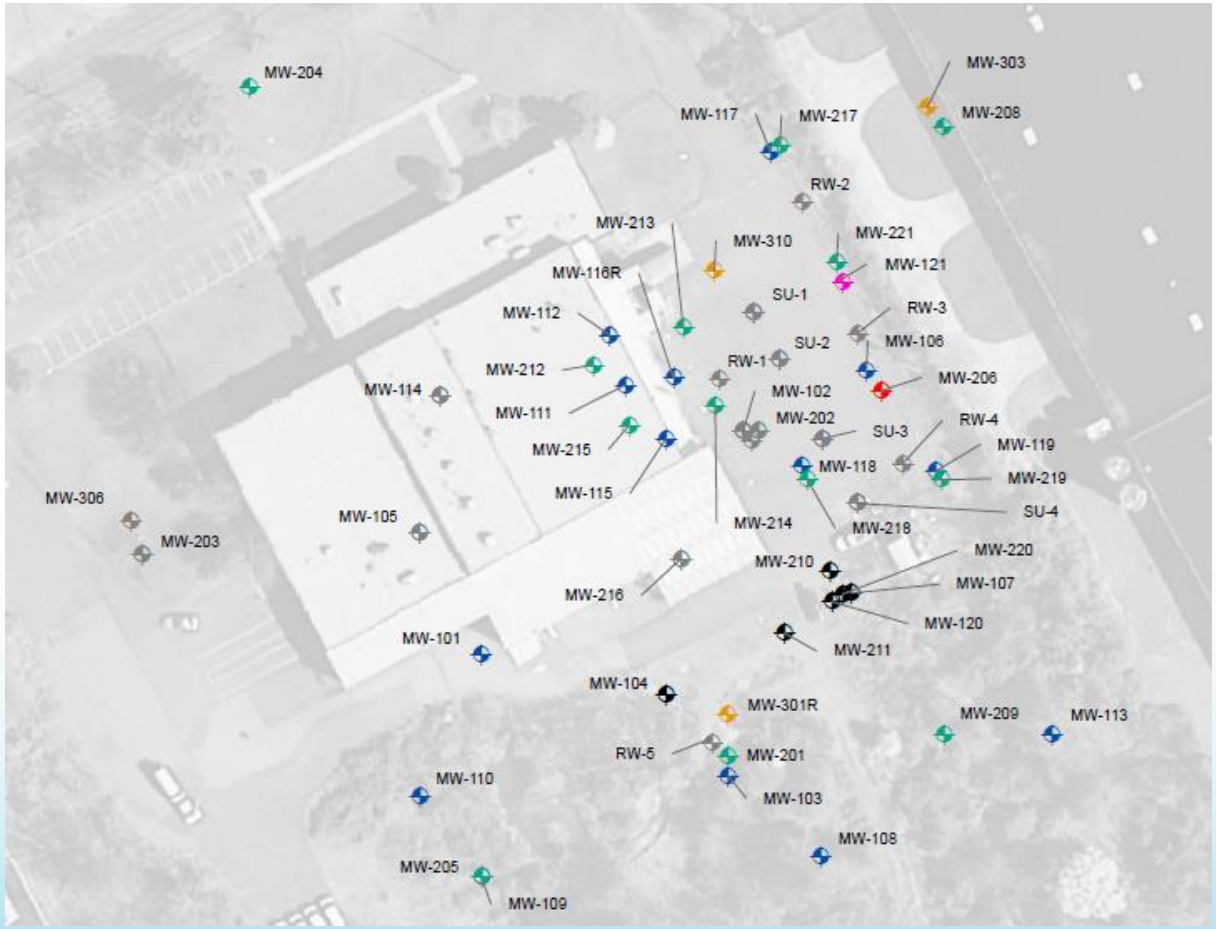
- Each sample's pattern is compared against a database
  - MI's in-house database
  - Made up of well-characterized samples with known reductive dechlorination classifications
  - Incorporation of machine learning to predict unknown samples based on the database

Thousands of features per sample



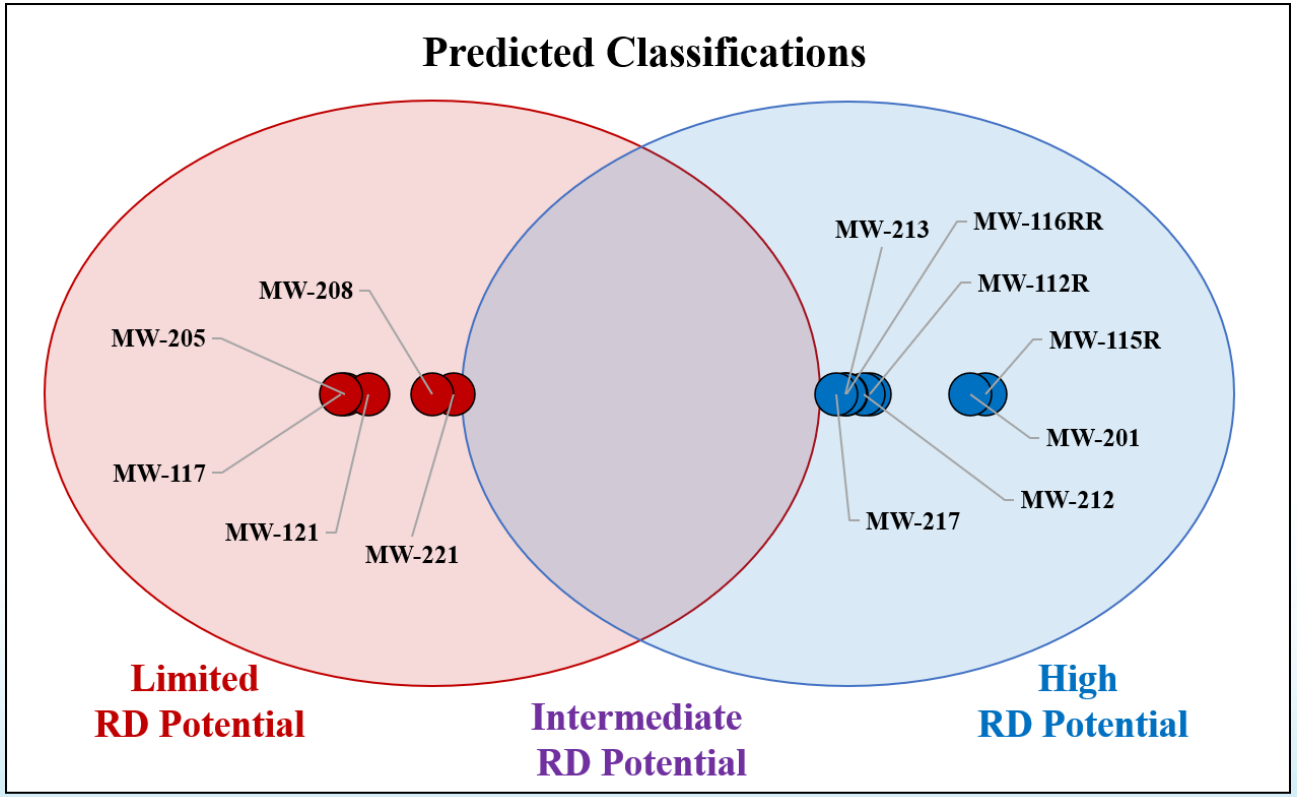
Metabolomics Case Study

- Chlorinated solvent site
- QuantArray-Chlor and MetaArray
- Site chemistry, geochem, and history were not shared before analysis

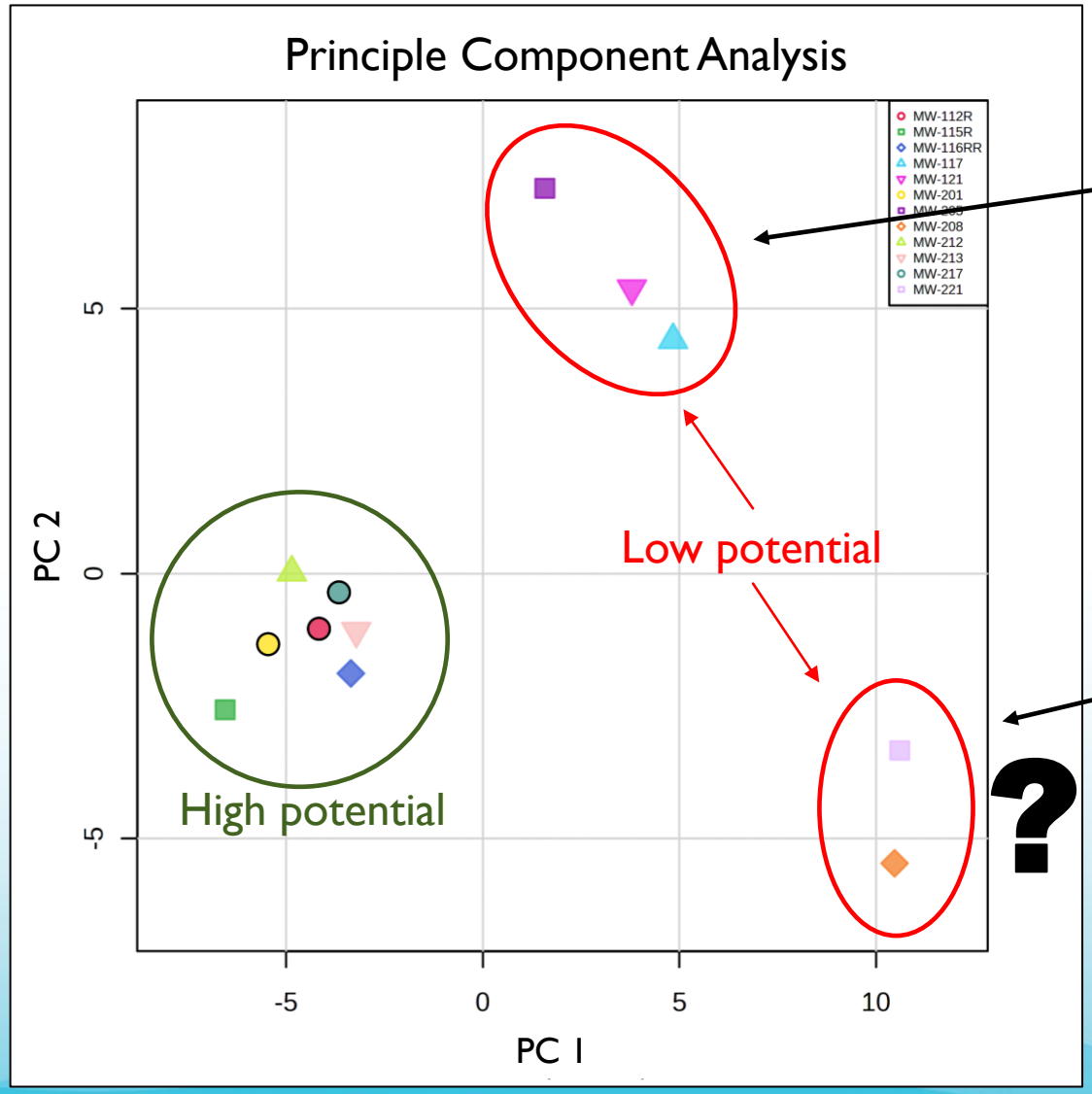


Metabolomics Case Study

Sample Name	Predicted Class	SVM Model Accuracy[1]
MW-115R	High Reductive Dechlorination Potential	80%
MW-212	High Reductive Dechlorination Potential	80%
MW-121	Limited Reductive Dechlorination Potential	80%
MW-221	Limited Reductive Dechlorination Potential	80%
MW-116RR	High Reductive Dechlorination Potential	80%
MW-213	High Reductive Dechlorination Potential	80%
MW-117	Limited Reductive Dechlorination Potential	80%



Metabolomics Case Study



Low Potential & Low DHC

Low Potential &10^3 cell/mL DHC

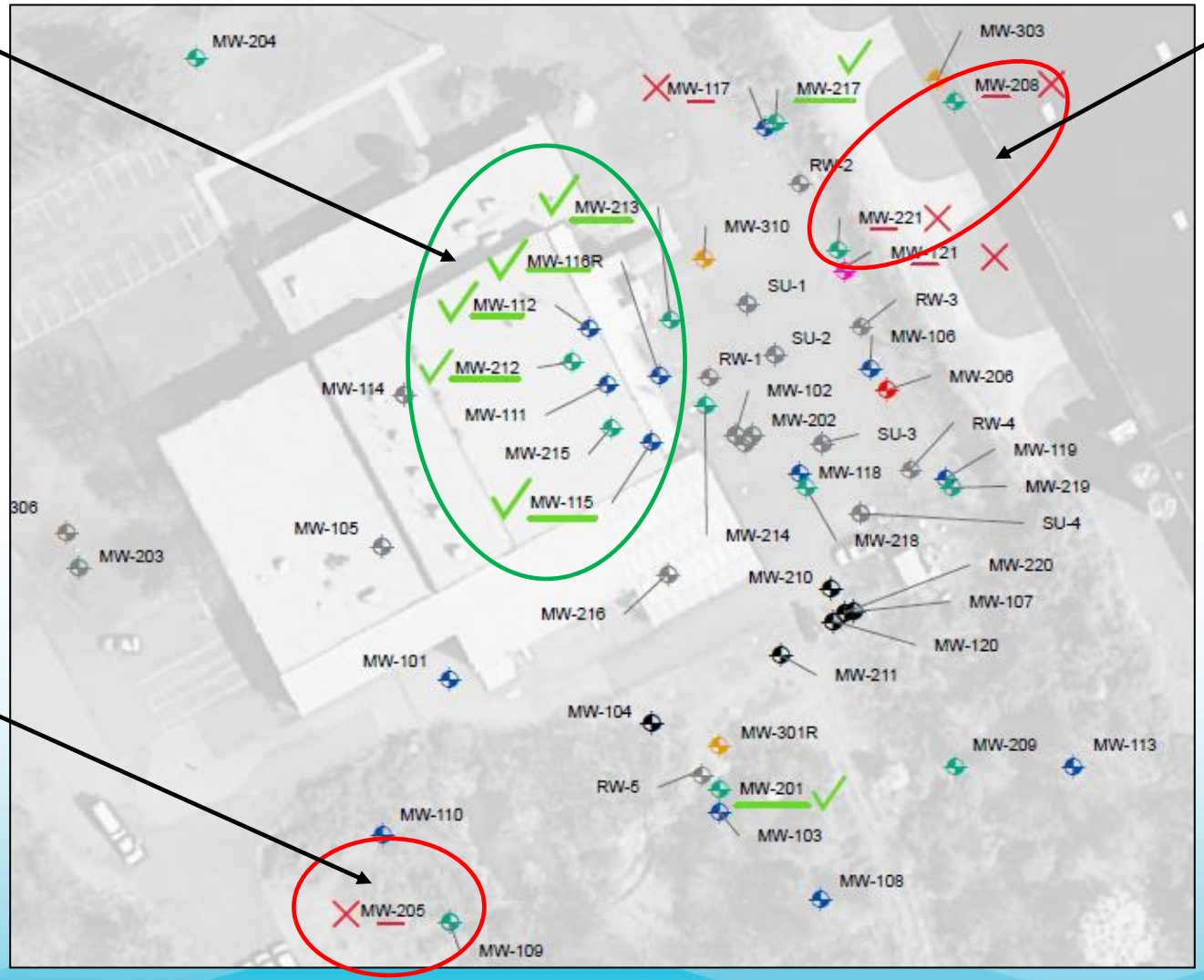
?

Metabolomics Case Study

High Potential

Heavy treatment Area
Excavation
EVO Soil Mixing
ZVI/Hydraulic Fracking

Background

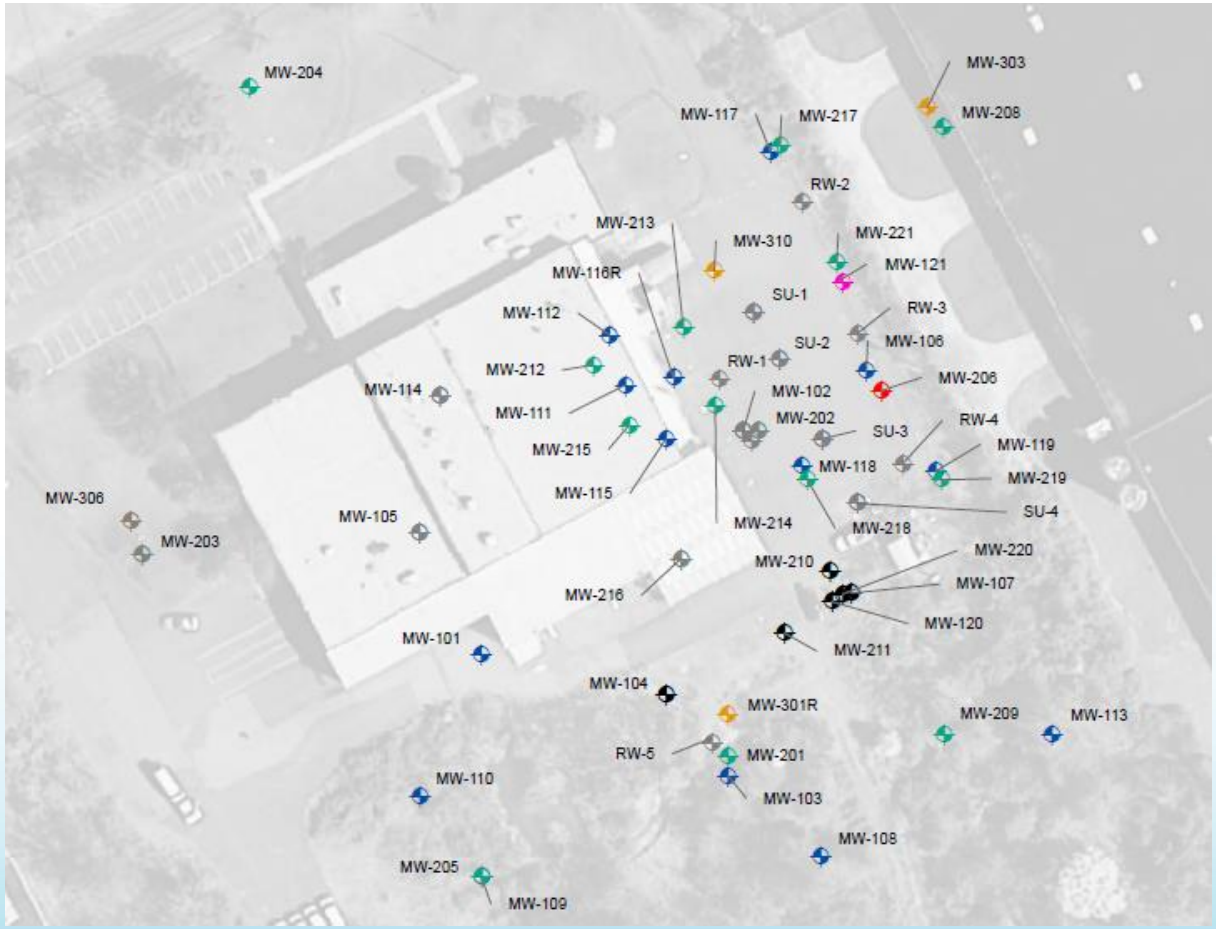


Low Potential &10^3 cell/mL DHC

Bedrock wells
Share the same fracture line

Metabolomics Case Study

- Next steps
  - Second sampling event
  - Compare results
    - Has the DHC and functional gene abundance changed
    - Does MetaArray indicate in the lower potential wells
  - Use the MBT results to identify the locations with issues
    - Reassess strategy in these locations



CONCLUSIONS

- Machine learning will continue to grow our databases and understanding of the biological metabolome.
- Metabolomics has the ability to help us get closer to rates of degradation.
- Key sentinel metabolites likely exist to help us define degradation potential and predict processes or community health.

THANK YOU!

srosolina@microbe.com
(865) 573-8188
www.microbe.com