NPUC Workshop

A Machine Learning/Mass Spectrometry Approach to Understanding Solvent Extractions and Oxidation Reactions of Asphaltenes

or

Introducing our Team/Capabilities and Looking to Develop New Relationships

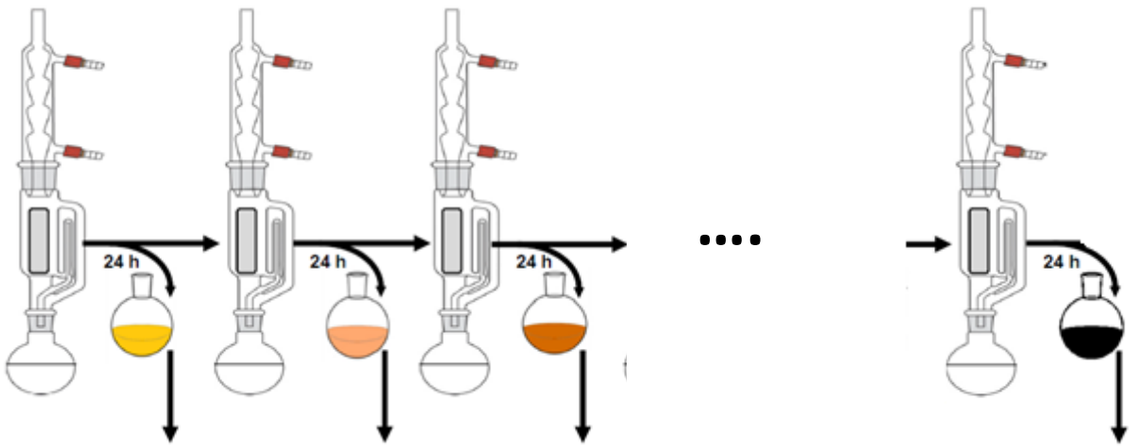
Katelyn Le, Jagos Radovich, Jeff Van Humbeck, Stephen Larter

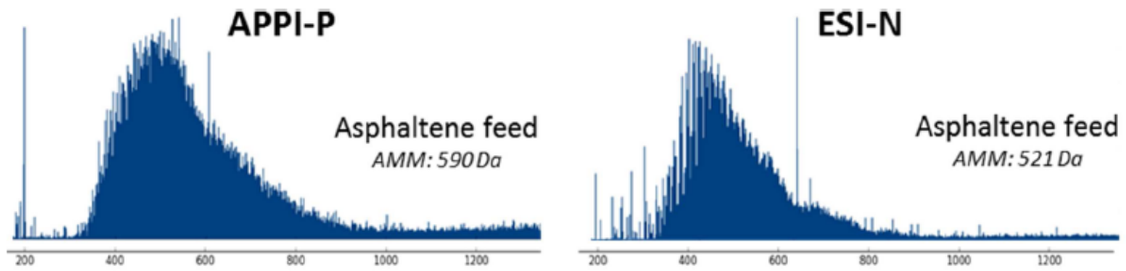
Feb 25, 2021

Radović & Larter (UCalgary PRG)

State-of-the-Art Characterization and Extensive 'Petroleomics' Experience

Silva, Radovic et al., Energy and Fuels, 2015



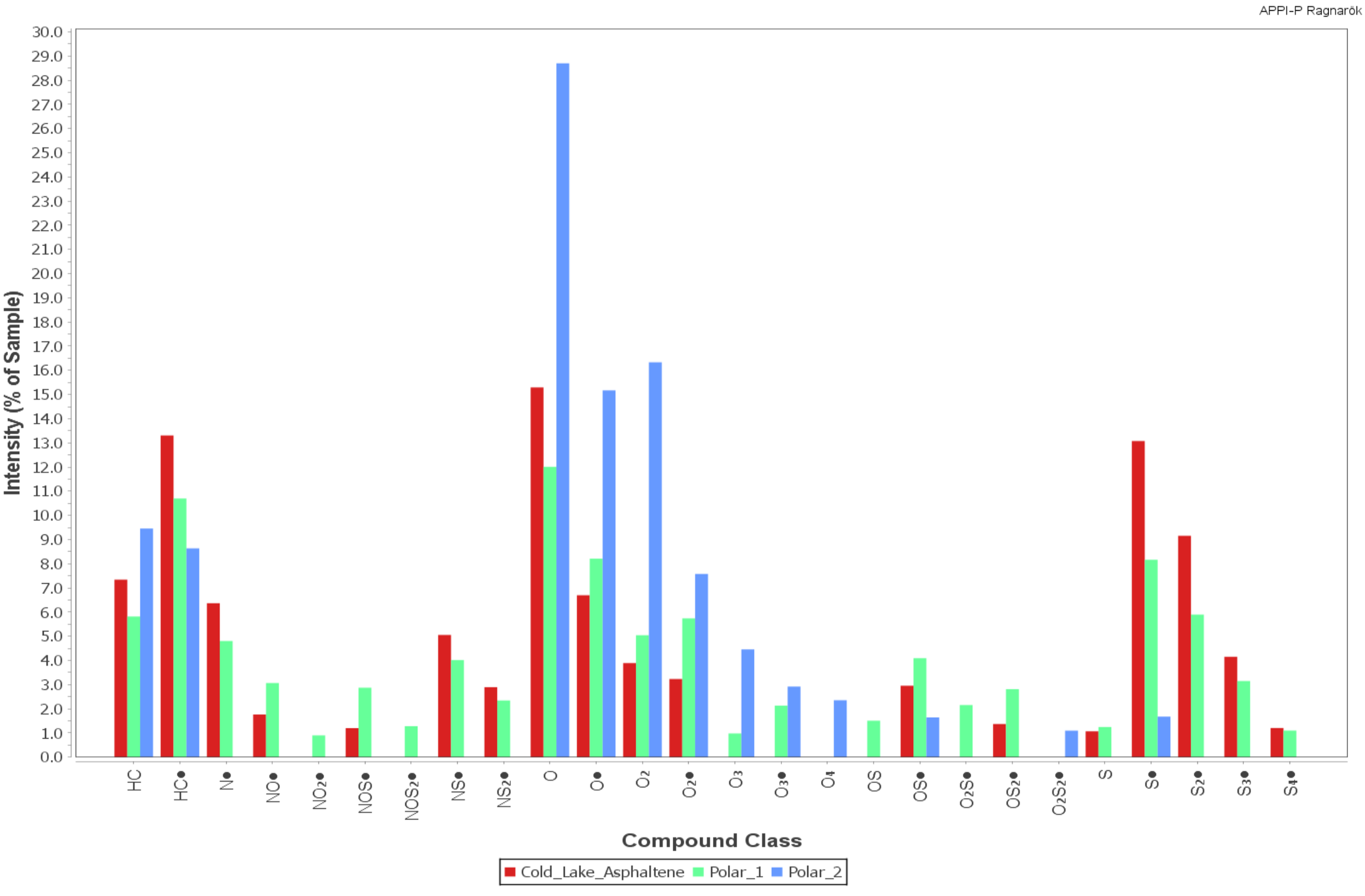


Sequential fractionation based on polarity

Previously applied to wide ranges of heavy oils and environmental samples

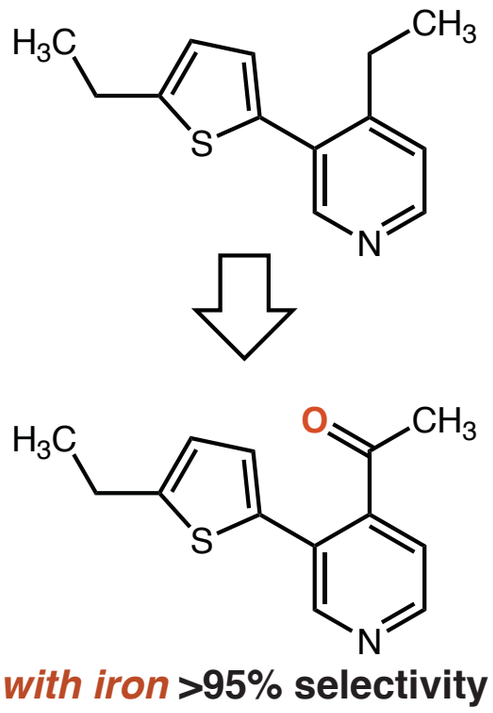
Fourier-Transform Ion Cyclotron Resonance-MS

Data display by class

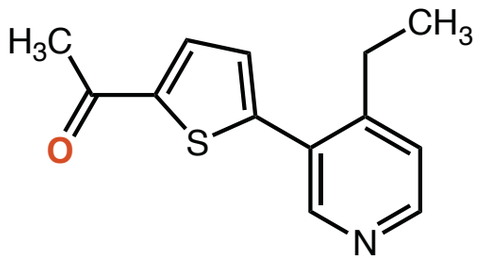


Le & Van Humbeck (UCalgary Chemistry)

New Oxidation Reactions and ML Prediction of Medicinal Chemistry Properties

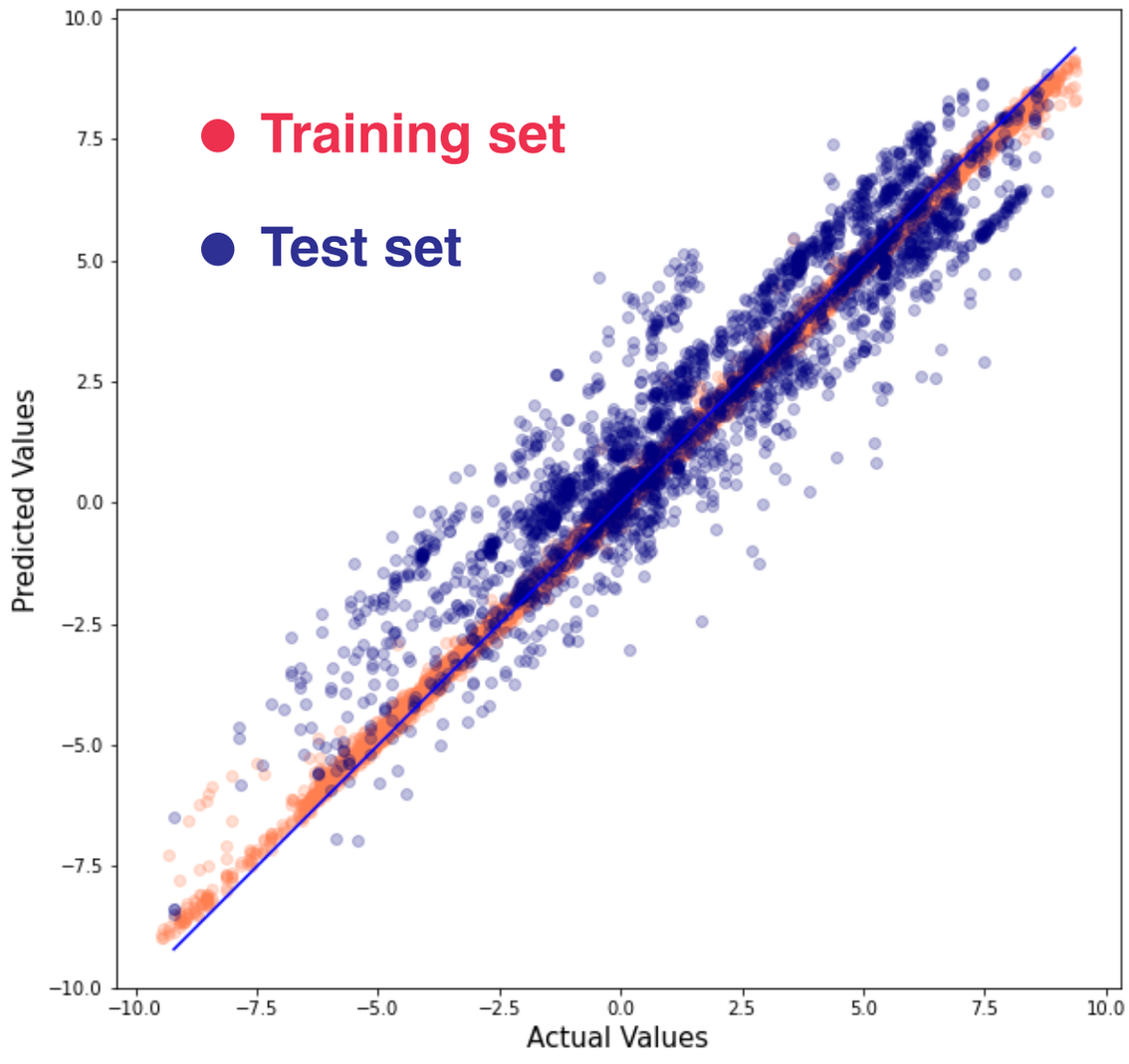


with iron **>95% selectivity**



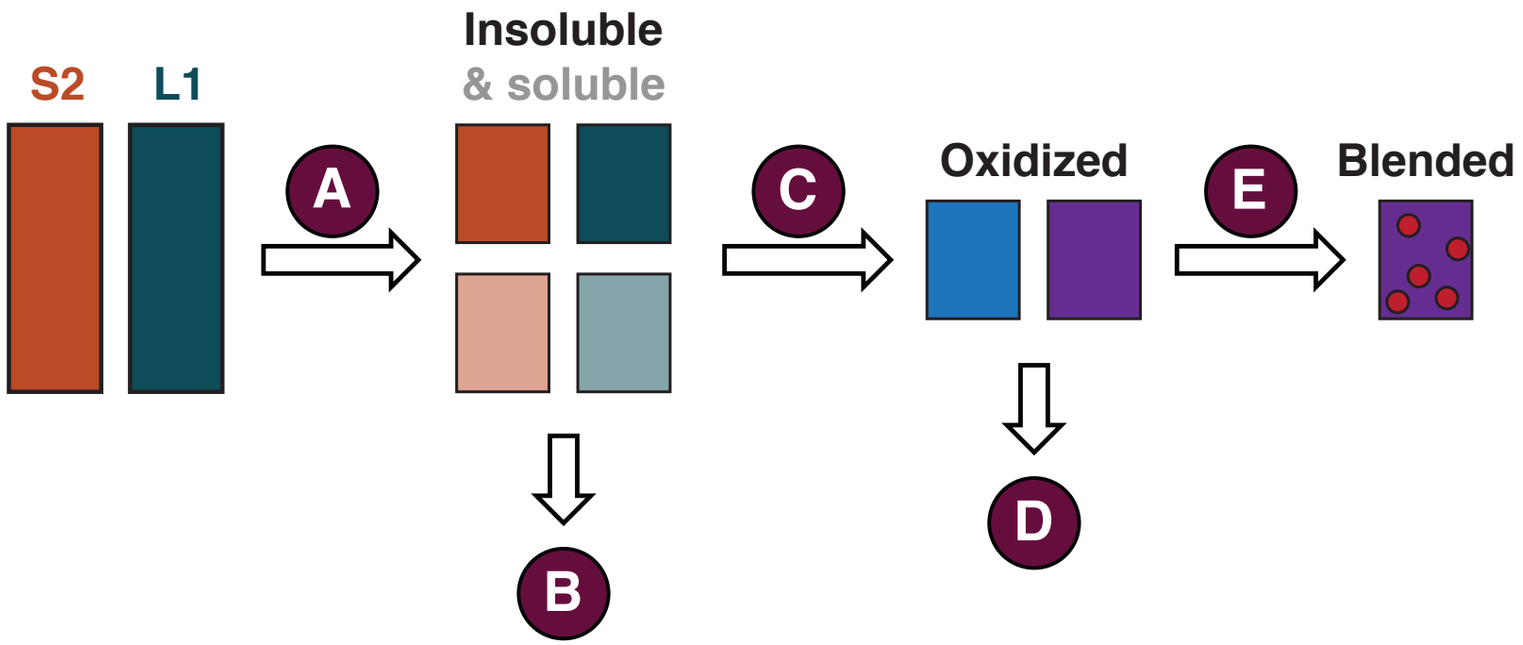
with cobalt **>95% selectivity**

Controlling position of C-H oxidation with catalyst



Prediction of small-molecule binding to CDK9 enzyme

Starting with Alberta Innovates CFGC/PRG



Extract S2 and L1 with various blends selected from:

A Major component {CH_2Cl_2, toluene} Polar modifier {iPrOH, acetone} pH modifier {AcOH, NEt_3}

B Gather HMRS (solubles), %S (all), ppm V (all), DSC (all)
30-40 HRMS, 60-70 %S, 60-70 V, 60-70 DSC

C Oxidize select fractions using conditions developed in CFGC
Room temperature, cheap catalysts and oxidants, ***selective***

D DSC analysis of oxidized products (**30-40 DSC**)

E Preliminary analysis of polymer blending (**~8 DSC**)

Additionally provided MS data for 19 previous heavy oil samples

Part of CFREF-GRI “PHOENIX” team

TEAM

Geochemistry
Electrochemistry
Wood Science
Photochemistry
Catalysis
Analytical chemistry
Ionic liquids
Separations

GOALS

Biomass/bitumen to high value products

New electrochemistry for low-C future

Alternative vectors for carbon storage

We have

Starting data for testing approaches	Initial targets based on AI CFGC	Diverse collaborative team

New collaborations?

You have?

Materials or data for analysis?	Quantifiable goals for a process?	A need for our skills?

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