Spectral features

- Signal intensity/absorbance
- Absorptivity
- Peak frequency
- Peak width
- Peak height ratios

Physical/molecular properties

- Phase state
- Hydrogen bonding
- Indicator of acid, alcohol etc.
- Molecular weight
- Electron withdrawing atoms
- Indicator of oxygen, etc.
- Ring strain
- Chain length
- Degree of branching
- Number of carbon atoms

Previous approaches (Beer-Lambert law)

Organic matter
OC and EC
OM/OC ratio
O/C ratio

Current approach

Causality
Predictions