NATIONAL HIGH MAGNETIC FIELD LABORATORY

Analytical Chemistry: How do you know if you're right?

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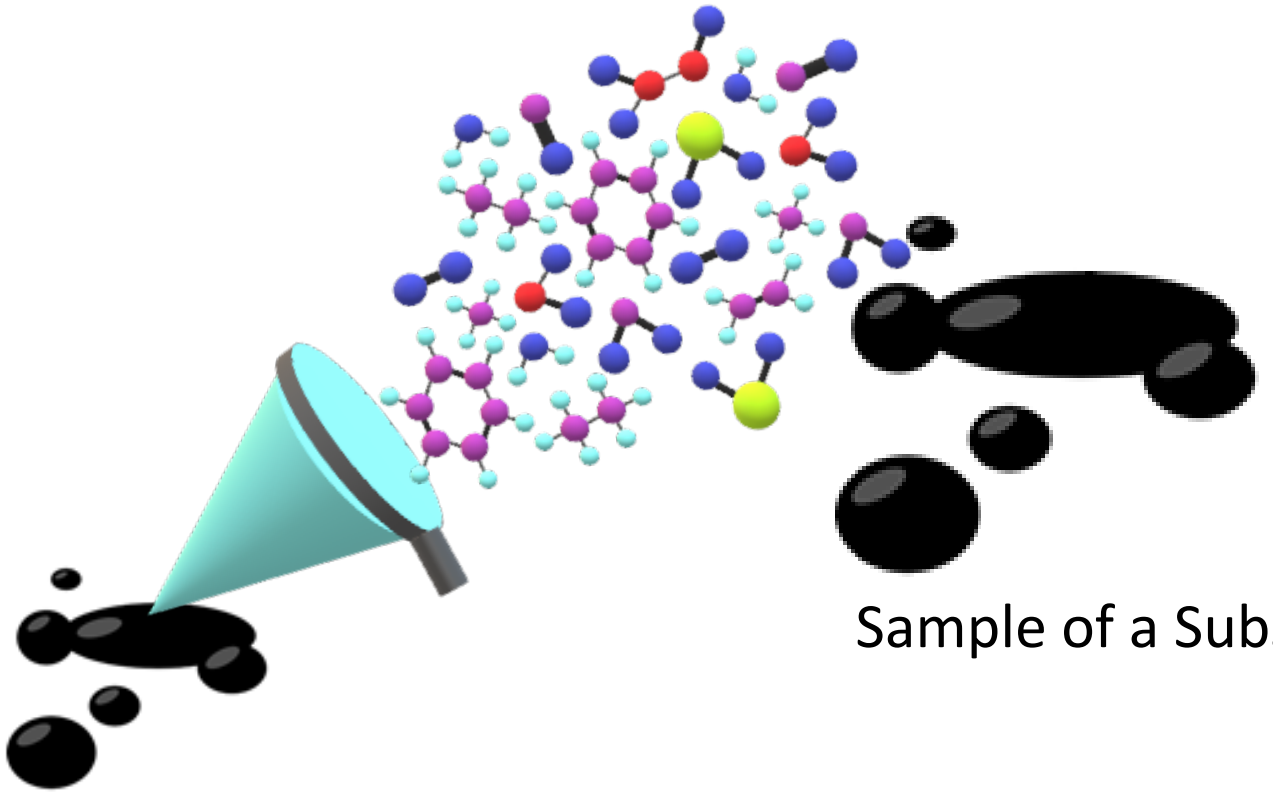
Analytical Chemistry

Exams substances by separating them into their chemical components and identifying each one and their abundances.



Sample of a Substance

Sample of a Substance

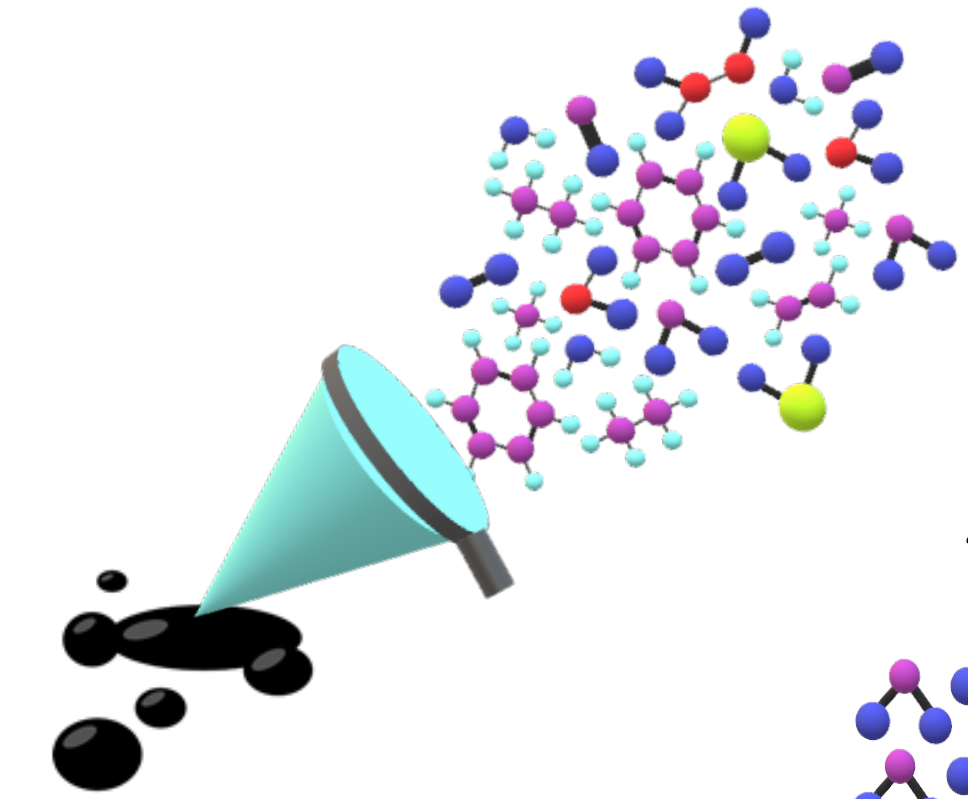
H_2

N_2O_2

C

How to identify Chemical Compositions ?

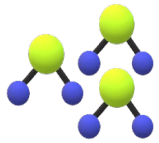
Mass Spectrometry Analysis



Sample of a Substance

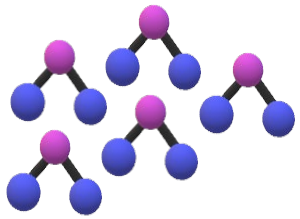
64 m/z

SO_2 ?



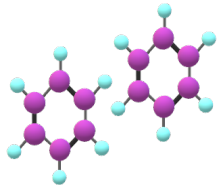
44 m/z

CO_2 ?



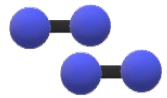
78 m/z

C_6H_6 ?



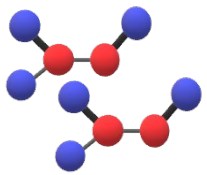
32 m/z

O_2 ?



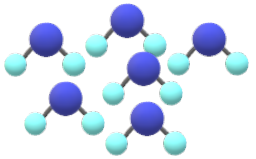
76 m/z

N_2O_3 ?



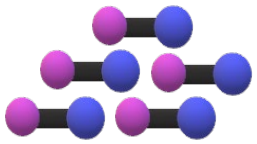
18 m/z

H_2O ?



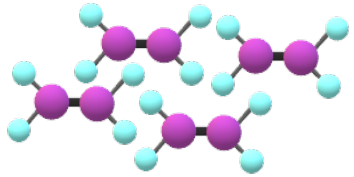
28 m/z

CO ?



28 m/z

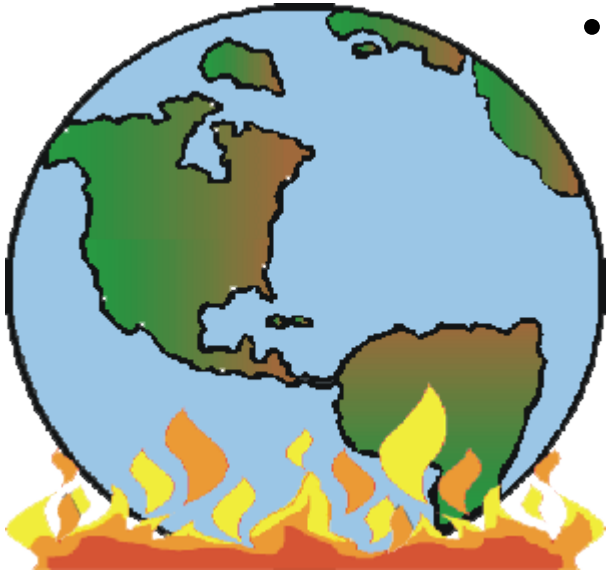
C_2H_4 ?



Applications

- Climate Change:

Analyze the effects of Global Warming



http://kpe-kastor.kas.sch.gr/energy1/eikones/backgrounds/earth_on_fire_an.gif

- Carbon dioxide and pollution monitoring

- Carbon dating

https://upload.wikimedia.org/wikipedia/commons/4/4c/August_1,_2012_-_Masiakasaurus_knopfleri_Fossil_Partial_Skeleton_on_Display_at_the_Royal_Ontario_Museum_(FMNH_PR_2481).jpg

https://upload.wikimedia.org/wikipedia/commons/0/05/Carnotaurus_LA.jpg

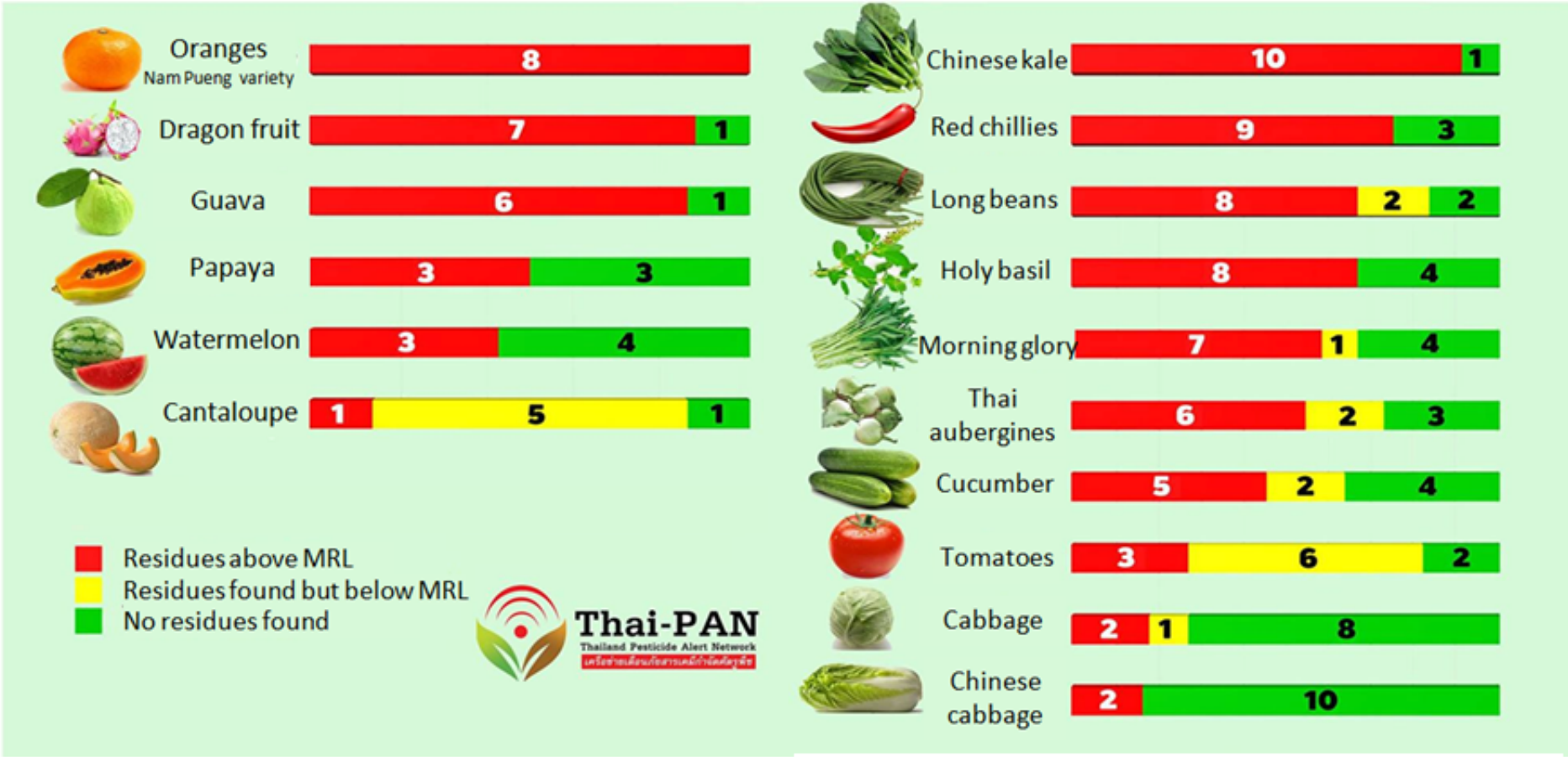
http://www.soil-net.com/album/Soils_Rocks/slides/Fossil%20Amonite.jpg

- Soil contamination assessment
- Food contamination detection
- Pesticides Control
- Drinking water quality

https://www.ag.ndsu.edu/williamscounty/extension/little-bit-country/pesticide-certification-trainings-scheduled-cow-nutrition-requirements-increase/image_mini

2nd Report on pesticide contamination monitoring on fruits and vegetables 2016

Comparison of fruit and vegetables with residues above maximum limit (MRL)



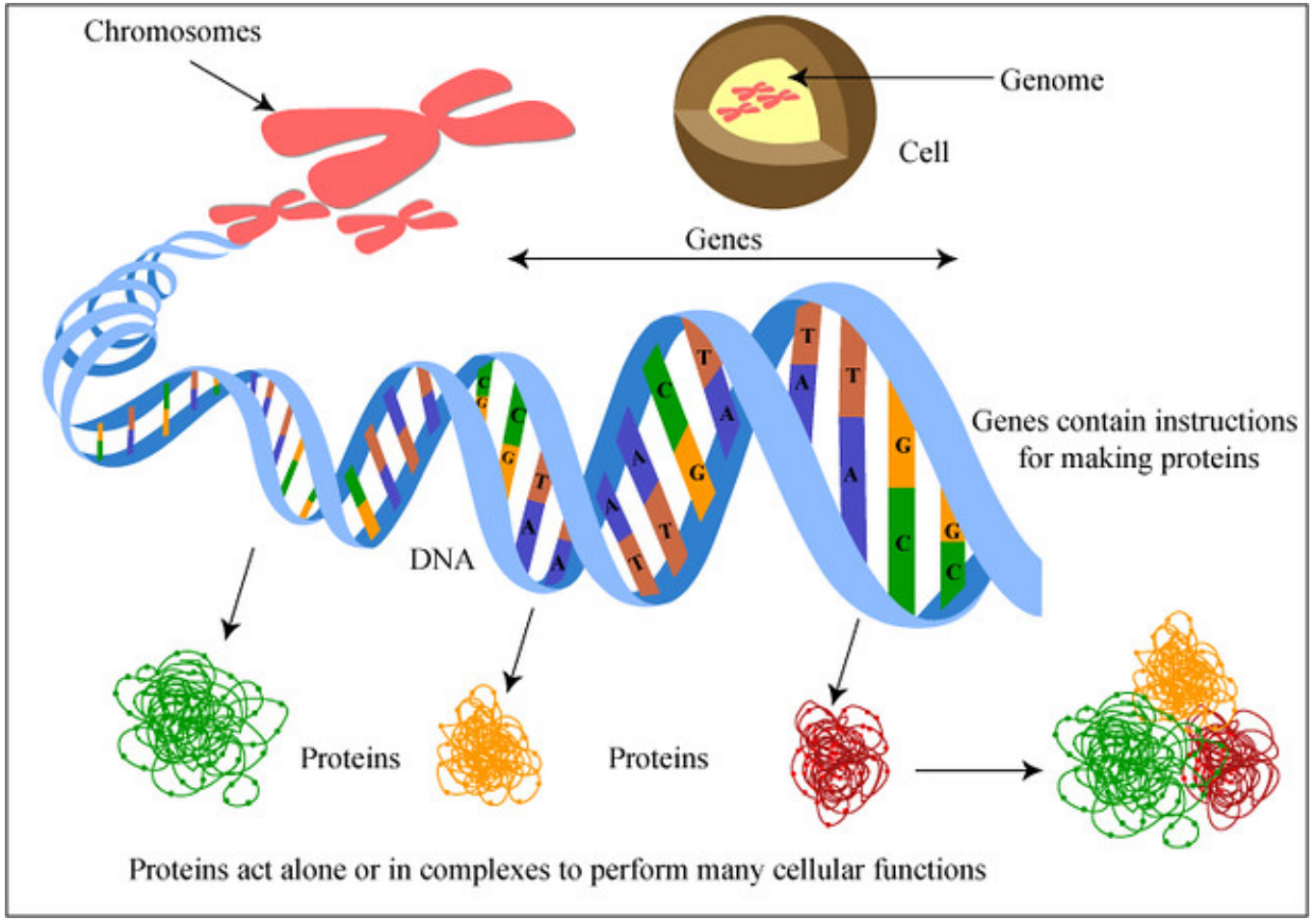
158 samples were collected on 23-29 August 2016, sent to laboratory certified to ISO/IEC 17025:2005 standard, tested for over 450 different chemicals

- Drug testing and discovery
- Drug abuse confirmation

Forensic analysis:

- Trace evidence:
  - Fibers in carpet
  - Polymers in paint
- Explosive residues:
  - Bombing investigation
  - Fire Accelerants

- Genetics: Protein identification and Mutations
- Disease screening
- Cancer screening and diagnostics



https://farm5.staticflickr.com/4138/4814933459_29822f41f9_z.jpg

FTICR-Mass Spectrometry

(Fourier Transform Ion Cyclotron Mass Spectrometry)

Measures the ‘weight’ (in *m*/*z*) of ions based on the cyclotron frequency of the ions in a fixed magnetic field.

World visitors

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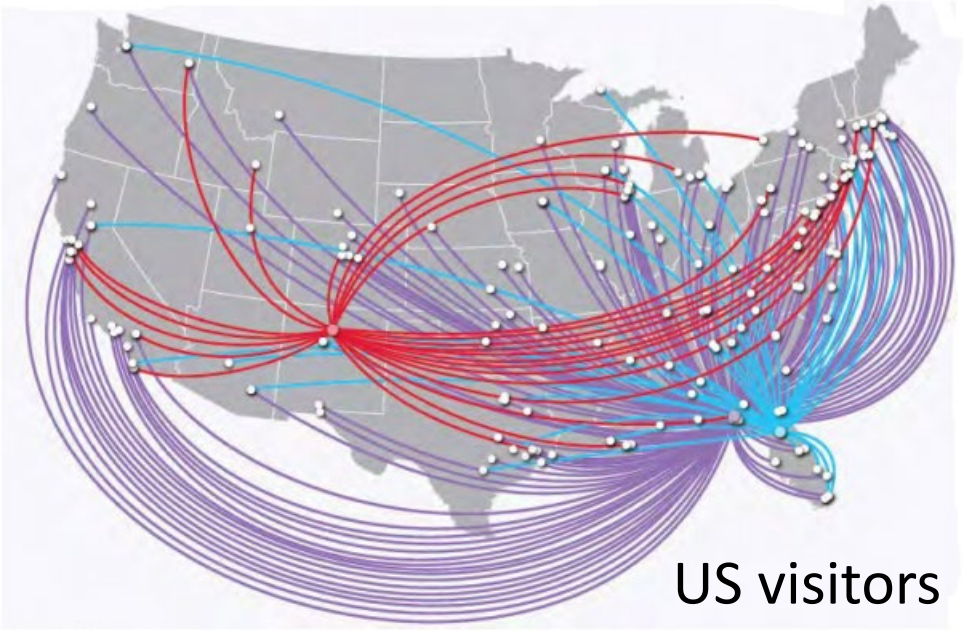
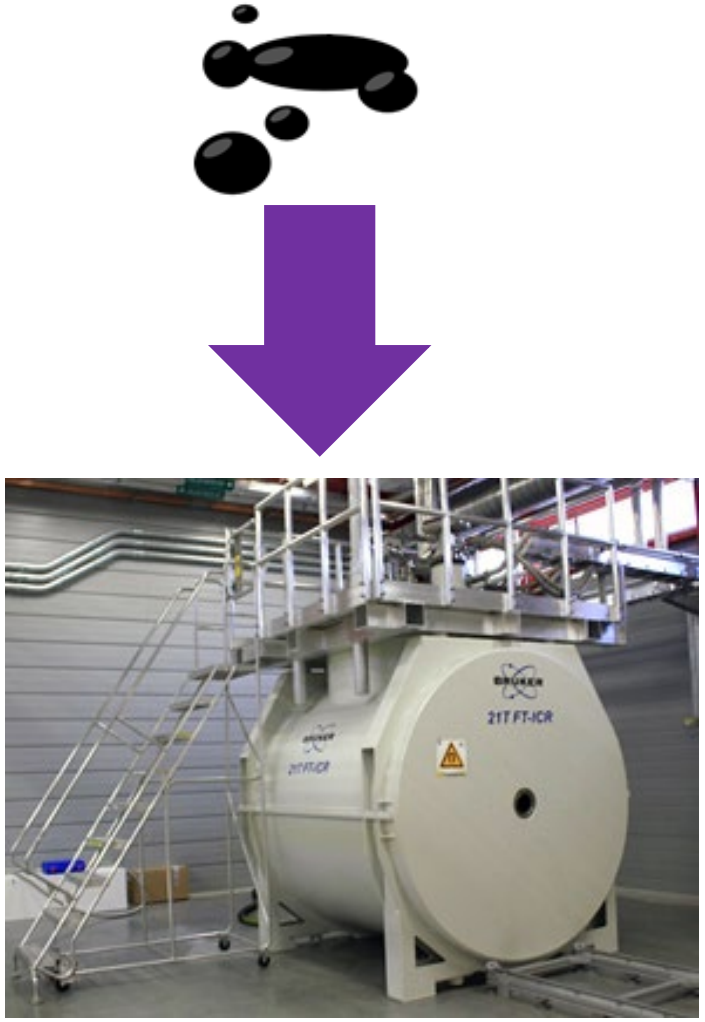
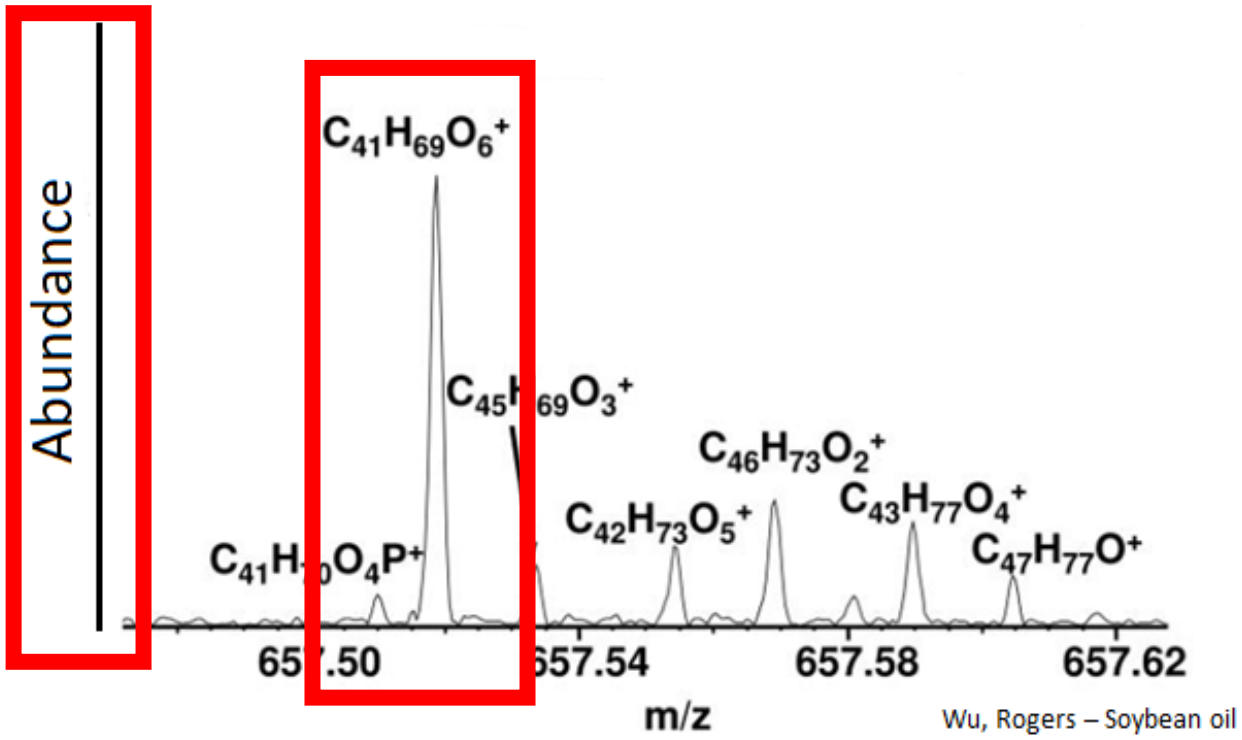


US visitors

Mass Spectrometry Analysis

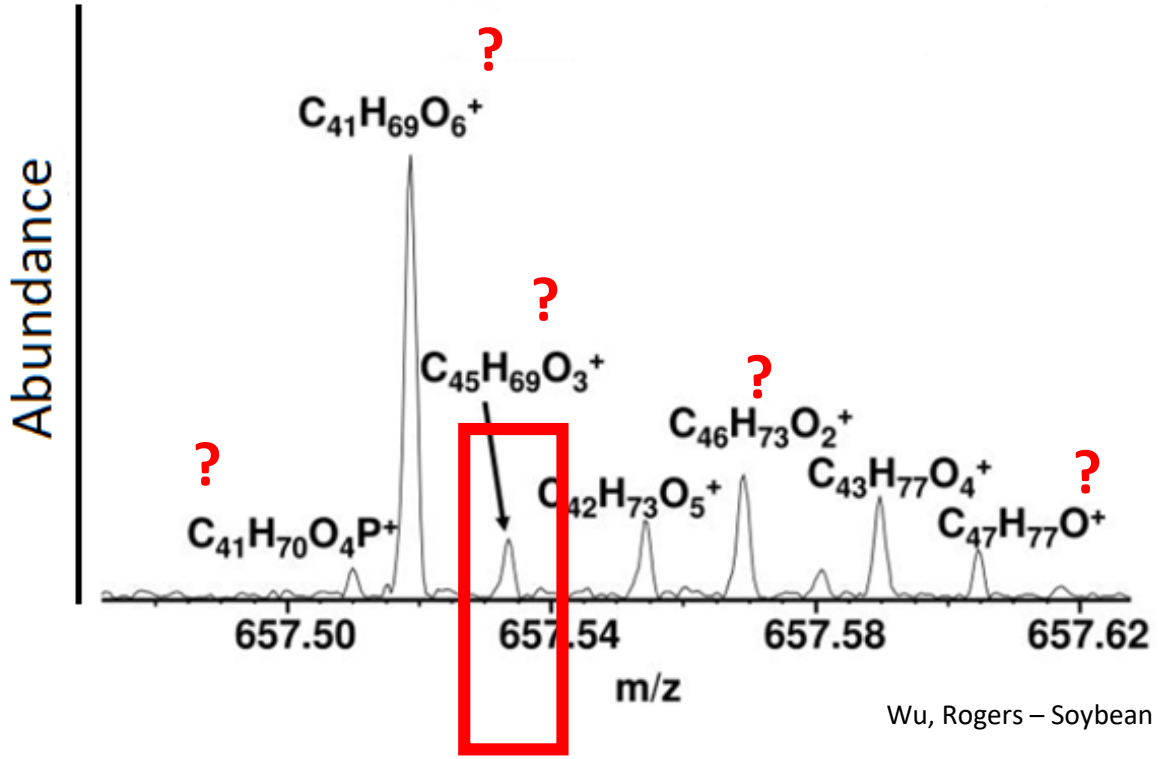
Assigning a molecular formula for each component/peak by their ‘weight’ (m/z)





How do you know if your molecular formula assignments are correct?

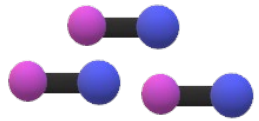
There is uncertainty and noise in the process



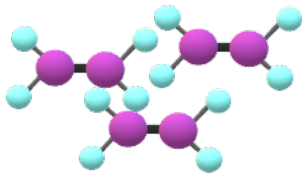
Wu, Rogers – Soybean Oil

28 m/z ? =

CO



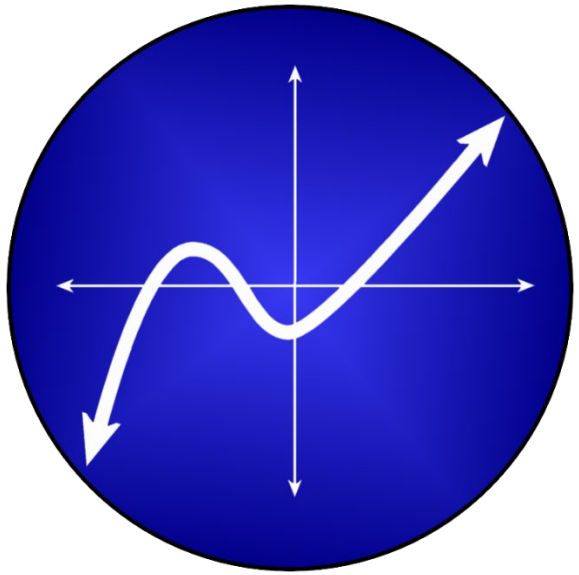
C_2H_4



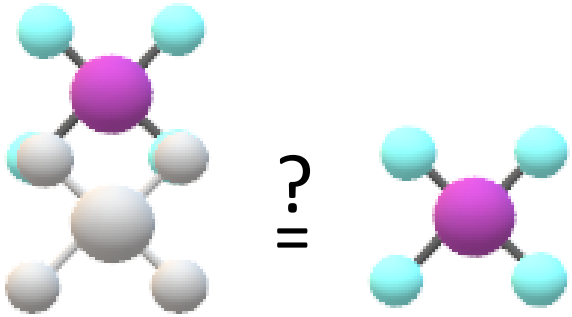
Goal

To measure the uncertainty of substance identification

Statistical Model

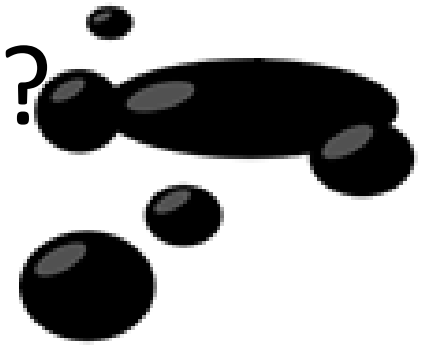


$P(CH_4 \text{ is correct}) = ?$



?

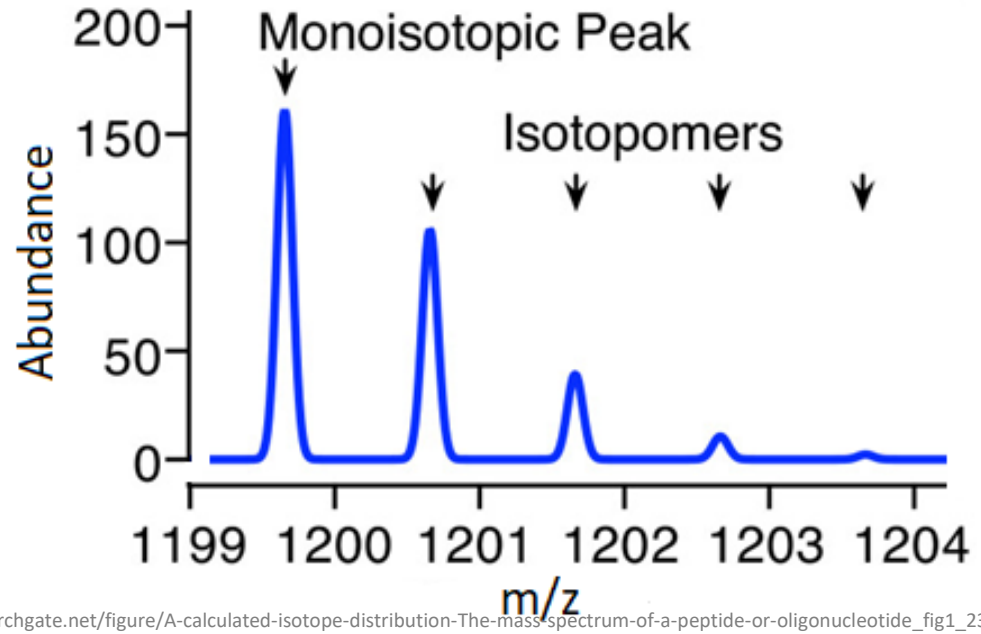
=

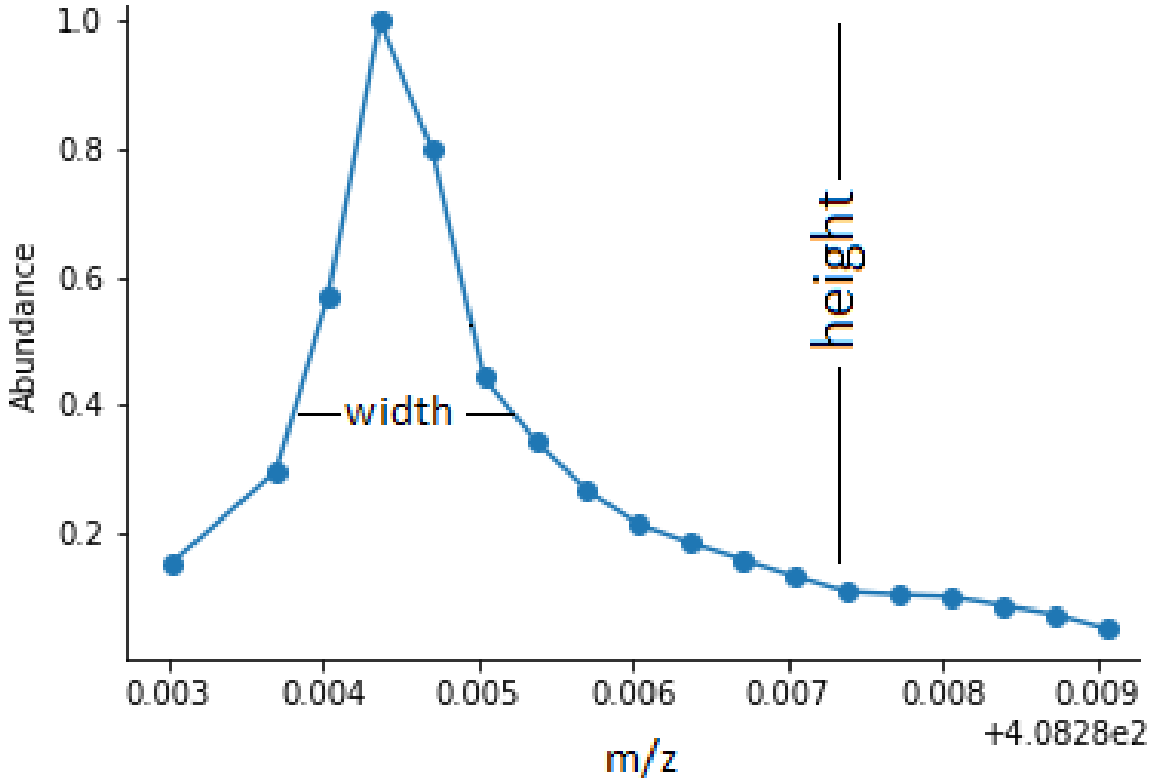


Statistical Approach

Capture the uncertainty of molecular formula assignments

Theoretical m/z	Identified Component	Observed m/z
214.159026066	$C_{15}H_{20}N_1$	214.15902
466.252926451	$C_{35}H_{32}N_1$	466.25292
523.379767240	$C_{33}H_{52}N_1O_1S_1{}^{13}C_1$	523.37927
⋮	⋮	⋮

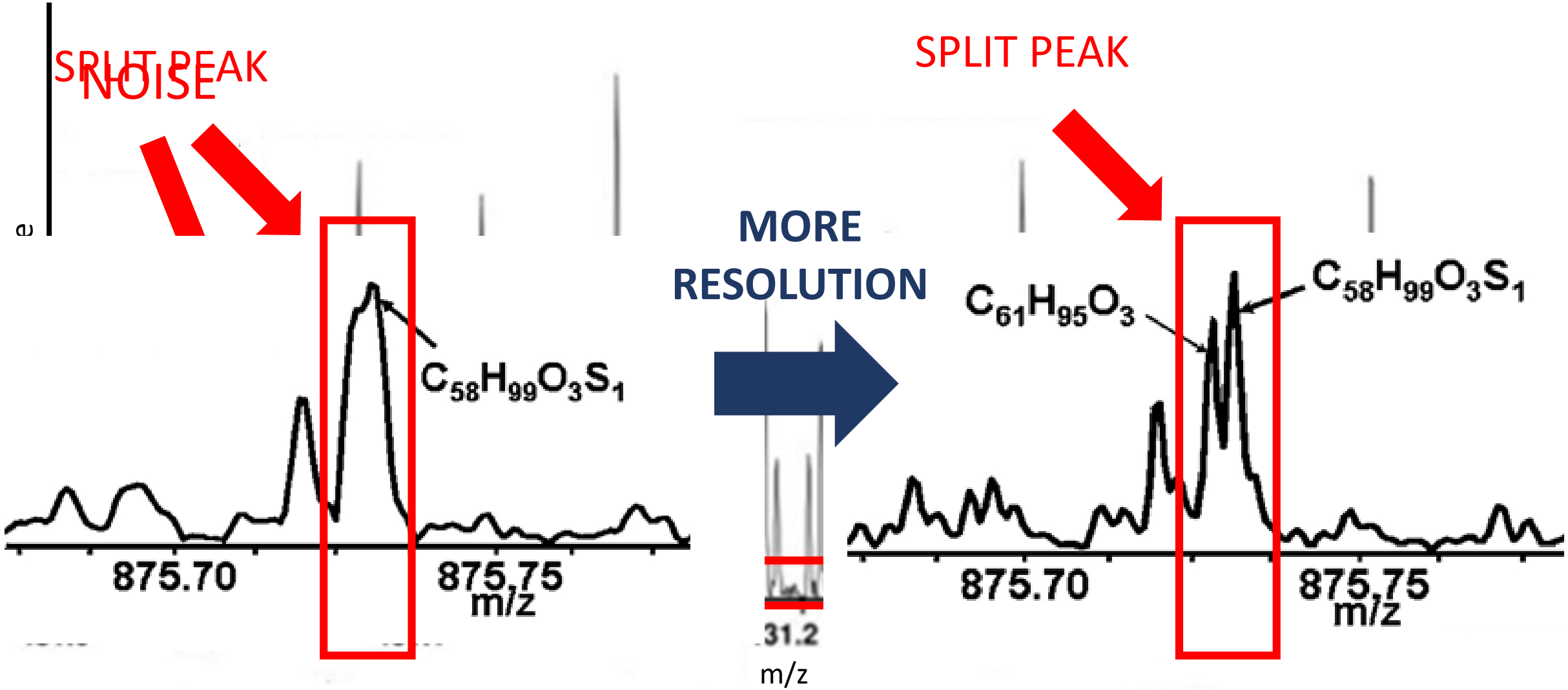




https://www.researchgate.net/figure/A-calculated-isotope-distribution-The-mass-spectrum-of-a-peptide-or-oligonucleotide_fig1_23401650

Uncertainty of assignments

(noise, split peaks = non-unique theoretical candidate)



Published in: Feng Xian; Christopher L. Hendrickson; Greg T. Blakney; Steven C. Beu; Alan G. Marshall; *Anal. Chem.* **2010,** 82, 8807-8812. DOI: 10.1021/ac101091w.

Direct Contributions of our Model

- Gives the confidence in each chemical component identified
- Improve research in several fields
- How much resolution is enough?

Thank you!

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