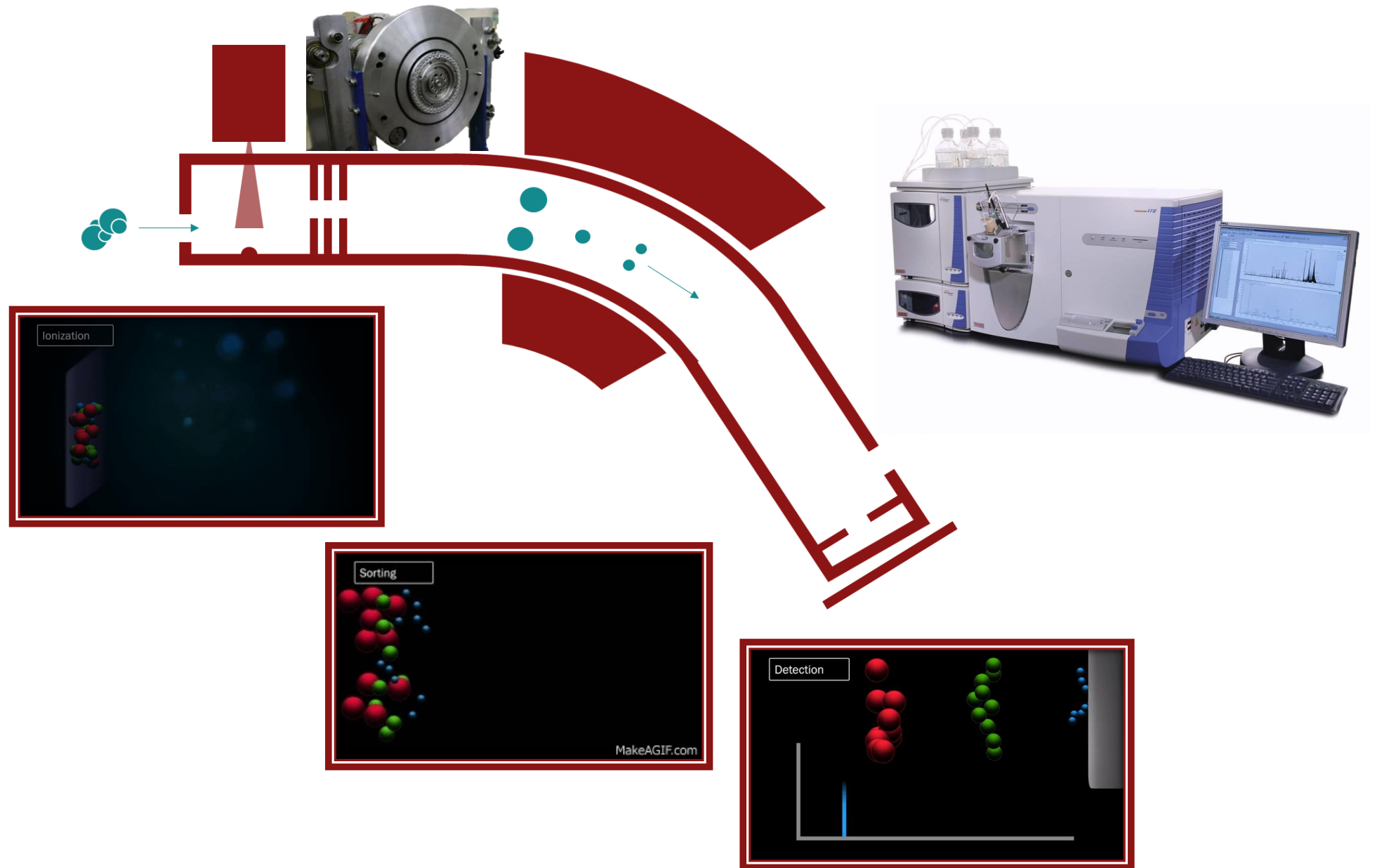


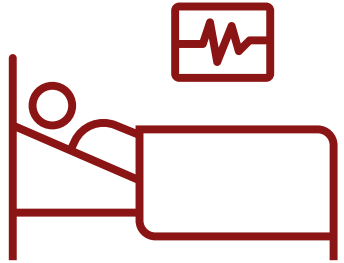
# — MASS — SPECTROMETRY

CHEM242 – AA  
Spring 2021  
Hao Nguyen

# — Instrument



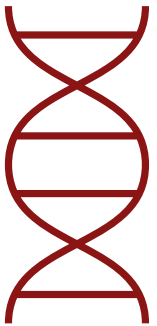
# —Mass Spectrometry Applications



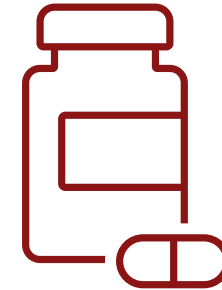
● Anesthesia & clinic



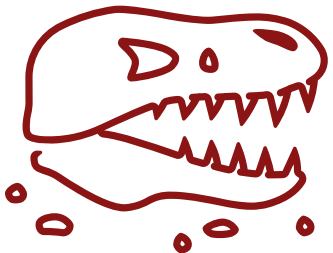
● Forensic



● Genome & epigenesis



● Drug discovery

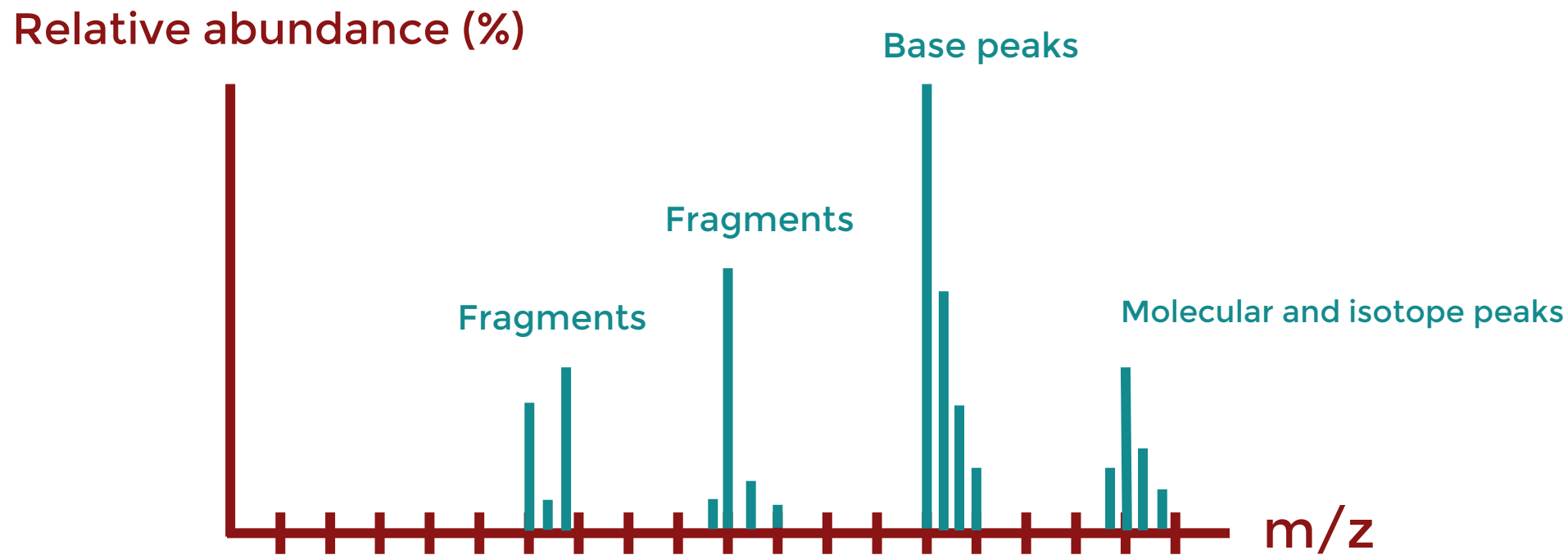


● Archeology & geology



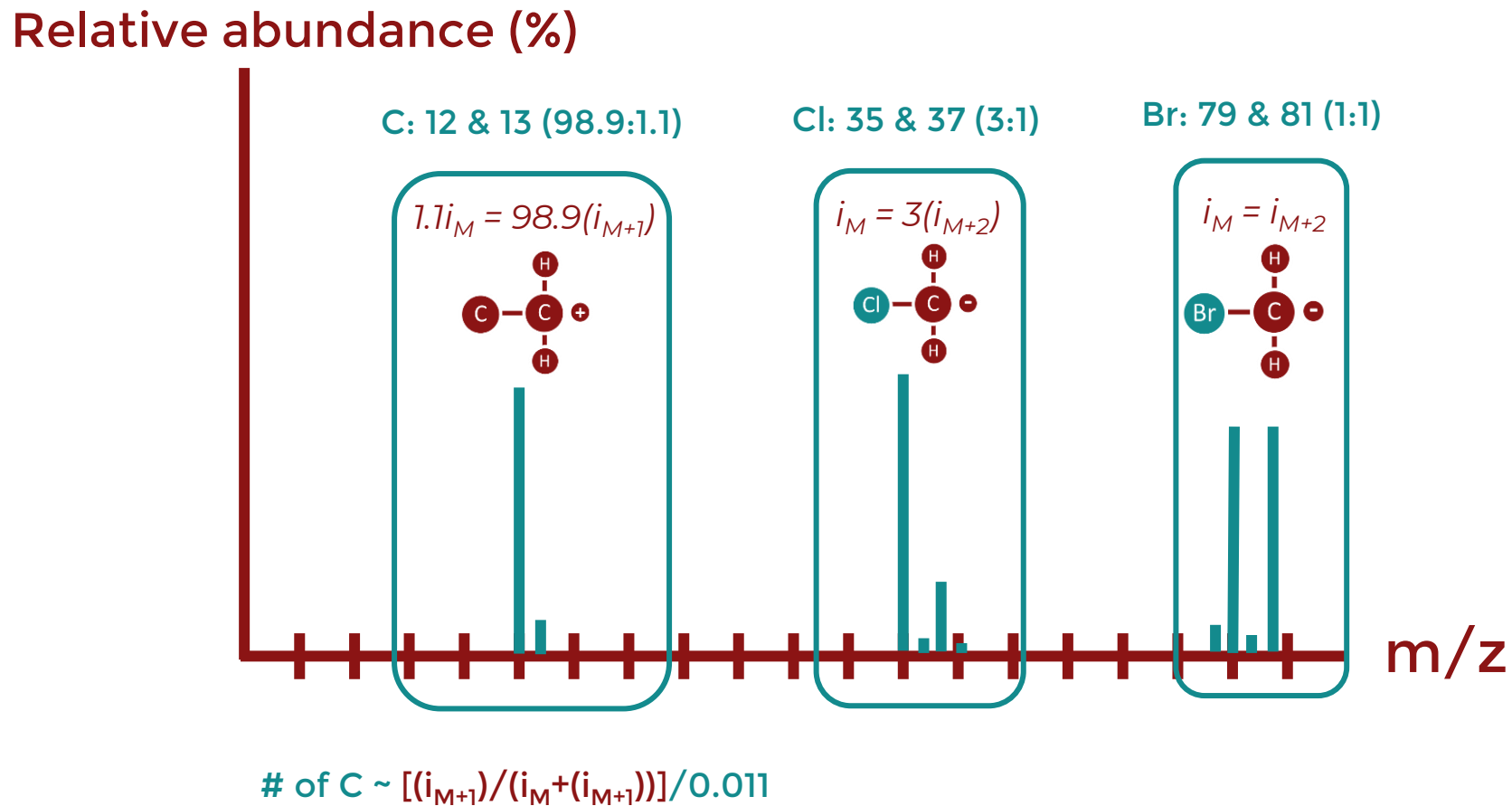
● Food industry

# — Spectral interpretation



# — Spectral interpretation

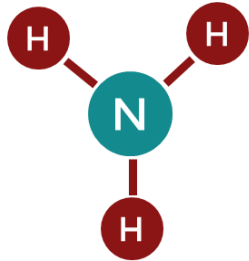
## ● Isotopes:



# — Spectral interpretation

- **Nitrogen rule:** Odd  $m/z$  = odd number of nitrogen atoms  
Even  $m/z$  = zero or even number of nitrogen atoms

*The rule applies when the molecule in question has only hydrogen, carbon, nitrogen, oxygen, fluorine, chlorine, bromine, and iodine*

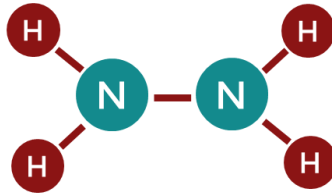


Ammonia



$m/z$

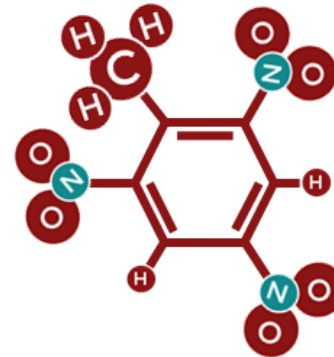
17



Hydrazine



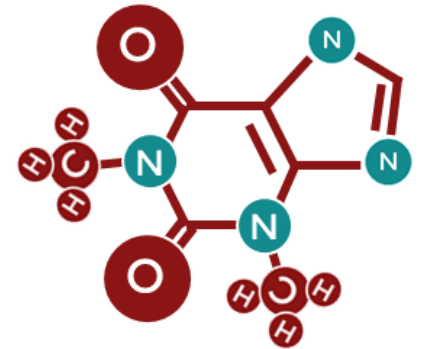
32



TNT



227



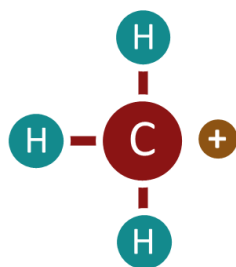
Ammonia



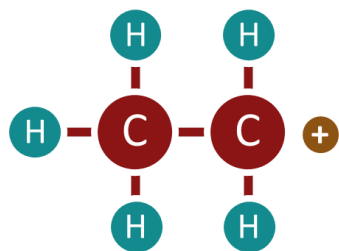
194

# — Spectral interpretation

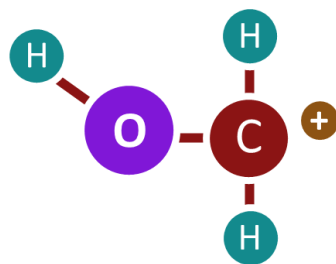
● **Fragments:** Subtract the MW by some common fragments to 'guess' the chemical formula.



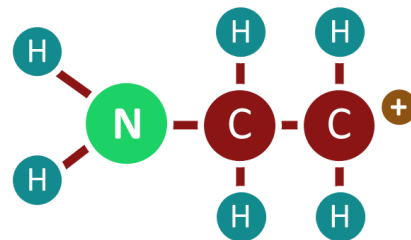
15



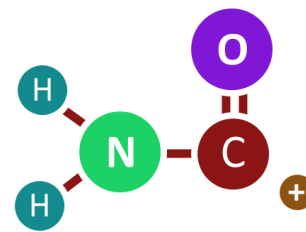
29



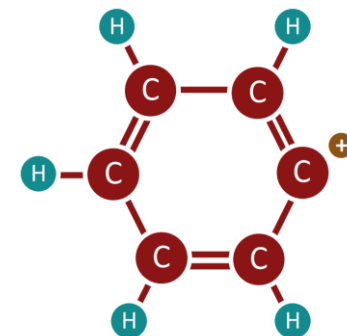
31



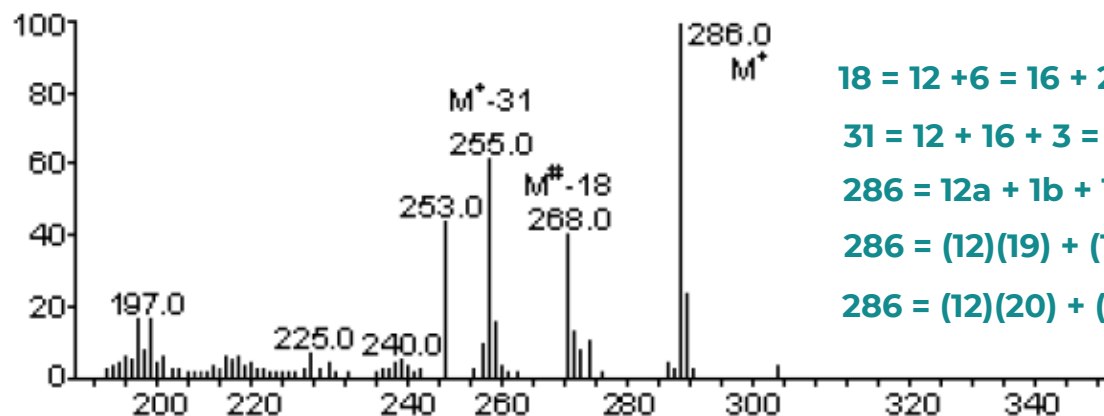
44



44



77



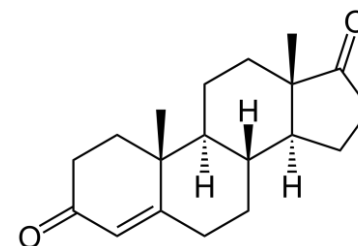
$$18 = 12 + 6 = 16 + 2 = \text{HOH}$$

$$31 = 12 + 16 + 3 = \text{CHHOH}$$

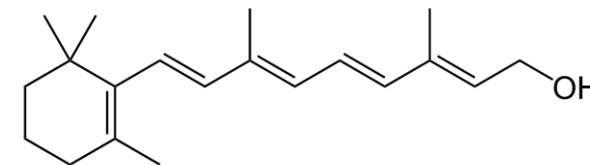
$$286 = 12a + 1b + 16c + \dots$$

$$286 = (12)(19) + (1)(26) + (16)(2)$$

$$286 = (12)(20) + (1)(30) + (16)(1)$$



$\text{C}_{19}\text{H}_{26}\text{O}_2$



$\text{C}_{20}\text{H}_{30}\text{O}$

# — Reading list

**Mass spec for carbon dating**

<https://www.radiocarbon.com/accelerator-mass-spectrometry.htm>

**Mass spec for breath analysis**

<https://www.karger.com/Article/Fulltext/357785>

**Mass spec for forensic science**

<https://www.news-medical.net/life-sciences/Mass-Spectrometry-as-a-Tool-in-Forensic-Science.aspx>

**Mass spec for food safety**

<https://pubs.rsc.org/en/content/articlelanding/2020/ay/c9ay02681a#!divAbstract>

**Mass spec for drug discovery**

<https://www.nature.com/articles/nrd886.pdf?origin=ppub>