

Mass spectrometry analysis gives a series of peak height readings for various ion masses. For each peak the height  $h_j$  is contributed to by the various constituents. These make different contributions  $c_{ij}$  per unit concentration  $p_i$  with the relation:

$$h_j = \sum_{i=1}^n c_{ij} p_i$$

\* taken, but somewhat modified, from Curtis F. Gerald, Patrick O. Wheatley  
Applied Numerical Analysis

A sample returns peak heights:  
 $h = (5.2, 61.7, 149.2, 79.4, 89.3)$ .

What is concentration  $p_i$  for each component, where the contributions  $c_{ij}$  are given in the following table.

Peak number	Component				
	CH <sub>4</sub>	C <sub>2</sub> H <sub>4</sub>	C <sub>2</sub> H <sub>6</sub>	C <sub>3</sub> H <sub>6</sub>	C <sub>3</sub> H <sub>8</sub>
1	0.165	0.202	0.317	0.234	0.182
2	27.7	0.862	0.062	0.073	0.131
3		22.35	13.05	4.420	6.001
4			11.28	0	1.110
5				9.850	1.684

Mass spectrometry - Wikipedia, the free encyclopedia

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## Mass spectrometry

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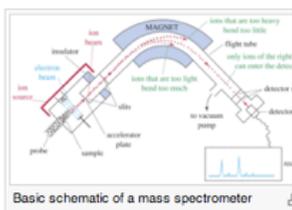
**Mass spectrometry** is an analytical technique used to measure the **mass-to-charge ratio** of ions. It is most generally used to find the composition of a physical sample by generating a **mass spectrum** representing the masses of sample components. The technique has several applications, including:

- identifying unknown **compounds** by the mass of the compound molecules or their fragments
- determining the **isotopic** composition of elements in a compound
- determining the **structure** of a compound by observing its fragmentation
- quantifying the amount of a compound in a sample using carefully designed methods (mass spectrometry is not inherently quantitative)
- studying the fundamentals of **gas phase ion chemistry** (the chemistry of ions and neutrals in vacuum)
- determining other physical, chemical or even biological properties of compounds with a variety of other approaches

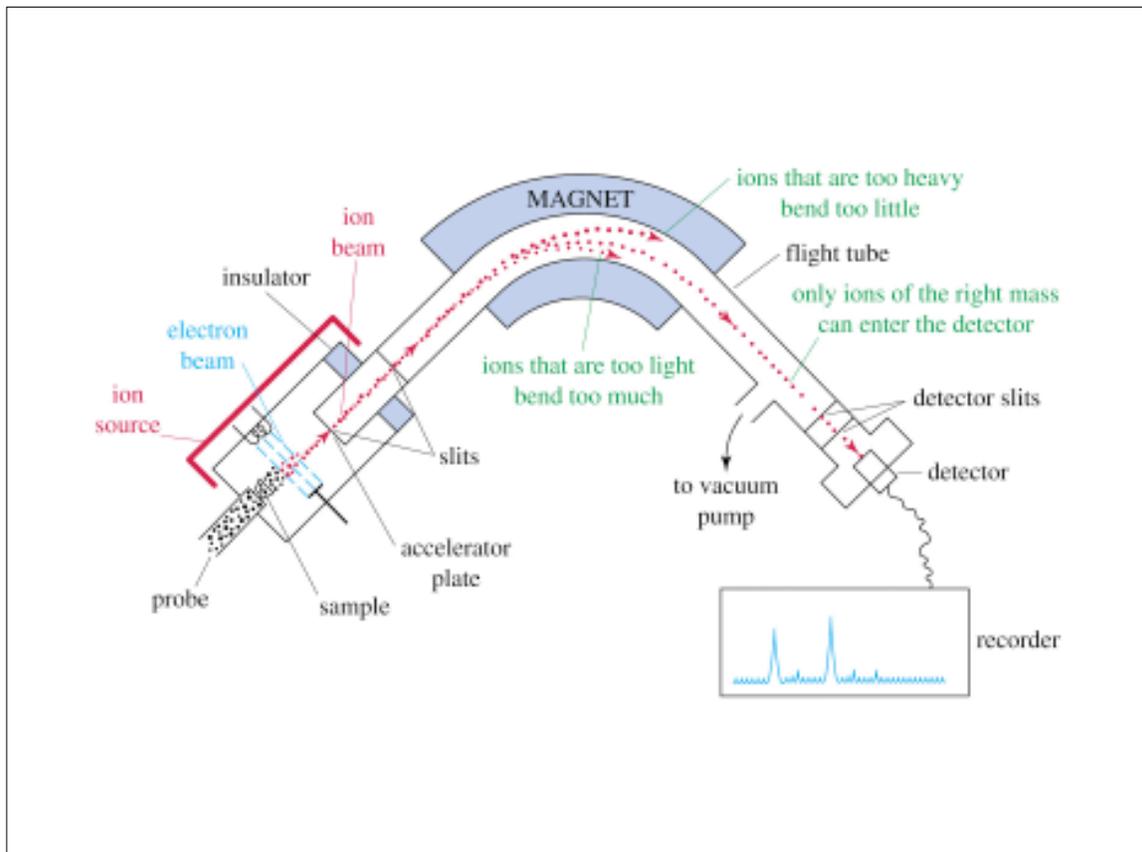
A **mass spectrometer** is a device that measures the **mass-to-charge ratio** of ions. This is achieved by ionizing the sample and separating ions of differing masses and recording their relative abundance by measuring intensities of ion flux. A typical mass spectrometer comprises three parts: an **ion source**, a mass analyzer, and a detector system.

**Contents** [hide]

- Simplified working example
- Instrumentation
  - Ion source
  - Mass analyzer
    - Sector
    - Time-of-flight
    - Quadrupole
    - Quadrupole ion trap
    - Linear quadrupole ion trap
    - Fourier transform ion cyclotron resonance
    - Orbitrap



Basic schematic of a mass spectrometer



# Mass spectrometry facilities and proteomics lab



**Protein Function Discovery Facility**  
6<sup>th</sup> Floor Botterell Hall



## BCHM 410/810 Lecture 3

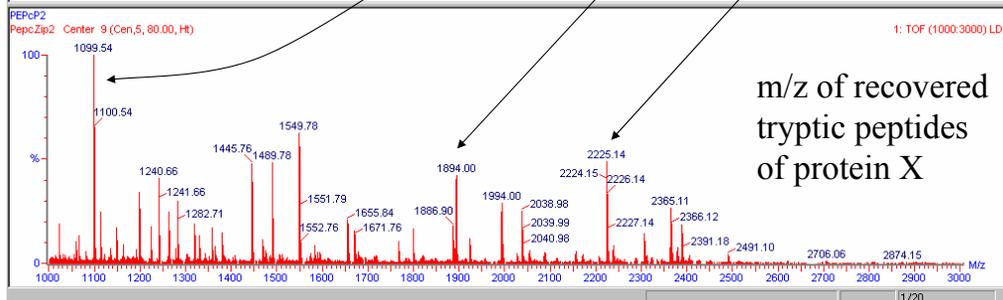
Entry	Score	Match	Coverage	MW	pI	Description	Reading Frame
CAPP_SOYBN	111.72	33	35.93	110742	6.4	PHOSPHOENOLPYRUVATE CARBOXYLASE (EC 4.1)	0
CAPP_SOLTU	107.98	43	44.66	110295	5.7	PHOSPHOENOLPYRUVATE CARBOXYLASE (EC 4.1)	0
CAPP_SORBI	99.87	36	36.98	109529	6.0	PHOSPHOENOLPYRUVATE CARBOXYLASE 2 (EC 4)	0
CAPP_TOBAC	87.24	39	40.25	110145	5.8	PHOSPHOENOLPYRUVATE CARBOXYLASE (EC 4.1)	0

### Best-matched protein sequence

(P51061)

1 MATRNLEKMA SIDAQLR **LA PARVSEDDY** L IEYDALLDR **FLDILQDLHG EDLRTVQEV YELSAEYEGK** HDPKK **LEELG NLITSLDAGD SILVAL** SFSSH  
 101 MLNLANLAE VQISRRRNK LKKGDFADEN NATTESDIEE TLKLVFDLK KSPQVFDAL **KIQIVDLVLT AHTQSTPRS LLOKHGRIRI CLSQLYAKTI**  
 201 **TPDDKQELDE ALQF** IQAAF RTDEIRRTTP TPQDEMRRAG SYFHETIUNG VPFRLRVDV ALNNGIKER **PPTNAPLQF ASUNGDEDC NRPVTEVTE**  
 301 DVCLLAR **MMA ANLYYSQIED LMFELSMG** C NDELVRRAE LHRSSKDEV **AKYIEFHKV VPPNEPVIV LGEVDELYQ TRERSRHLLS NGYSDIPPEA**  
 401 TPTNVEEFLS SLELCYRSLC ACGDRAIADG SLIDFMQVVS TFGLSLVRL **L IQOESDHTD VLDAITKHLV IGSYQEWSEE KREULLSEL SGVRPLFGPD**  
 501 LPQTEEIRDV LDTFHVIAEL PDMFGAYII SMATAPSDVL AVELLQRECH IKHPLRVVFL FEK **ADLEFA PAALAR FSI DUVYNRINGK SEVNIQYSDS**  
 601 **GRDAGRFSAA HOLYIAQEL** INVAKKFGVK LTMFHGRGT VGR **EGGPTHL AILSOPPTDI HGSLRVTVOG** EVIEOSFGEQ HLCFRTLQRF TAATLEHGMH  
 701 PPISPKPEWR ALMDQAVIA TEEYRSIVFK EPRFVEYFL **ATPELEYGM** NIGSFPAKRR PGGQZETLR **IPMIFANTOT RPHLPVULGF GAAPK** VVIEE  
 801 NVKLNMLQE MYNQPFPR **TLDLVENVFA HEDPHIAAL** DRLLVSKDLW PFGDQLRNKY EETKLLQV AGHKEILEGK **PYLKQRLRLR HAPITTLNIV**  
 901 **QAYTLRIPD PNTNWKVRPR** ISKESAEASK SADELV **LNP TSEYAPGLED TLILTRM** CIA AGMQNTG

### Recovered tryptic peptides



m/z of recovered tryptic peptides of protein X

A sample returns peak heights:

$$h = (5.2, 61.7, 149.2, 79.4, 89.3)$$

What is concentration  $p_i$  for each component, where the contributions  $c_{ij}$  are given in the following table.

Peak number	Component				
	CH <sub>4</sub>	C <sub>2</sub> H <sub>4</sub>	C <sub>2</sub> H <sub>6</sub>	C <sub>3</sub> H <sub>6</sub>	C <sub>3</sub> H <sub>8</sub>
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We can formulate this problem as a system of linear equations.

$$A = \begin{matrix} 0.1650 & 0.2020 & 0.3170 & 0.2340 & 0.1820 \\ 27.7000 & 0.8620 & 0.0620 & 0.0730 & 0.1310 \\ 0 & 22.3500 & 13.0500 & 4.4200 & 6.0010 \\ 0 & 0 & 11.2800 & 0 & 1.1100 \\ 0 & 0 & 0 & 9.8500 & 1.6840 \end{matrix}$$

$$h = (5.2, 61.7, 149.2, 79.4, 89.3)^T$$

Given the linear system  $Ap = h$ , we need to solve for  $p$ . We could use Gaussian elimination.

In Matlab this is very easy to do, using the “magic” \ (forward slash also know as left division) operator .

```
A = [ 0.165 0.202 0.317 0.234 0.182 ;  
27.7 0.862 0.062 0.073 0.131 ;  
0 22.35 13.05 4.420 6.001 ;  
0 0 11.28 0 1.110; 0 0 0 9.85 1.684]  
h = [5.2 71.9 149.2 79.4 89.3]'  
p = A\h
```

For the next week or so we will look at various means of solving systems of linear equations.

By the way the concentrations of the components turn out to be:

	<u>CH<sub>4</sub></u>	<u>C<sub>2</sub>H<sub>4</sub></u>	<u>C<sub>2</sub>H<sub>6</sub></u>	<u>C<sub>3</sub>H<sub>6</sub></u>	<u>C<sub>3</sub>H<sub>8</sub></u>
p =	2.5373	0.1288	6.6815	8.4449	3.6329