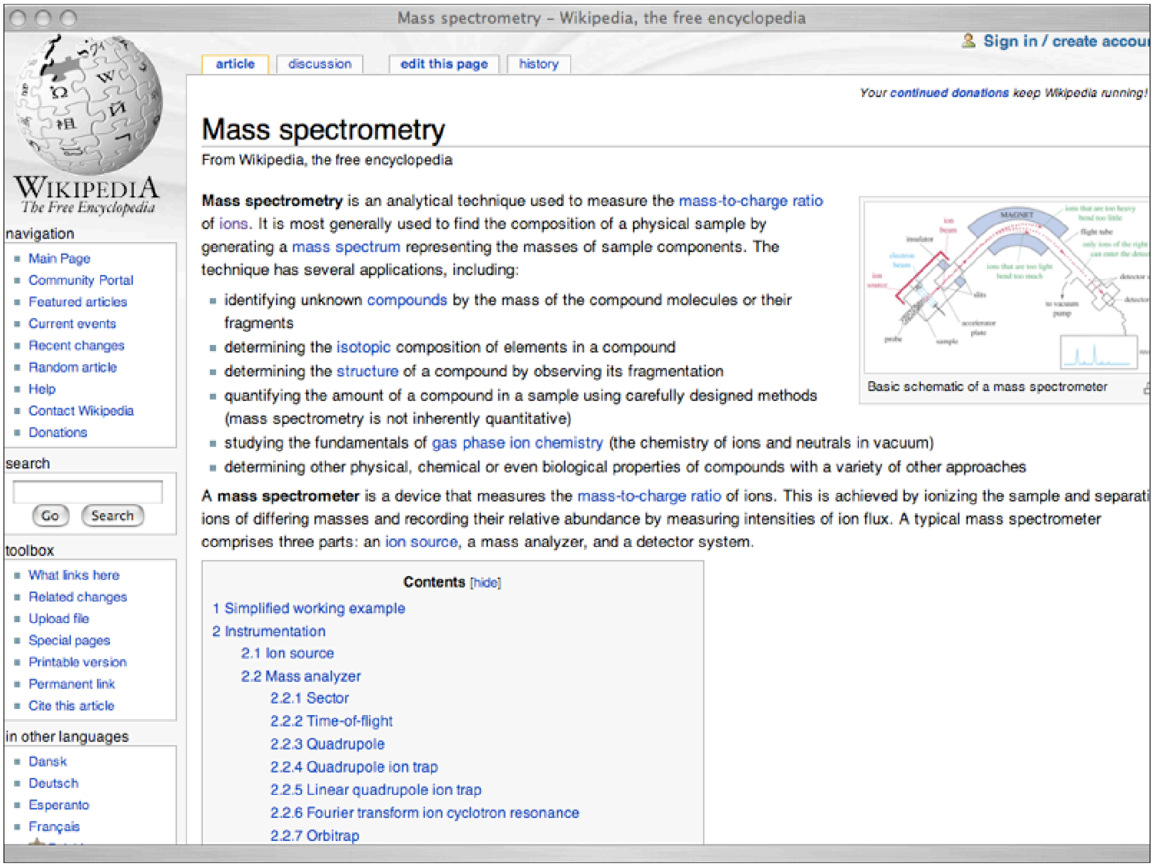
Mass spectrometry analysis gives a series of peak height readings for various ion masses. For each peak the height h_j is contributed to by the various constituents. These make different contributions c_{ij} per unit concentration p_i with the relation:

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

* 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_4	C_2H_4	C_2H_6	C_3H_6	C_3H_8
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



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Mass spectrometry

From Wikipedia, the free encyclopedia

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

Basic schematic of a mass spectrometer

A **mass spectrometer** is a device that measures the mass-to-charge ratio of ions. This is achieved by ionizing the sample and separati 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.

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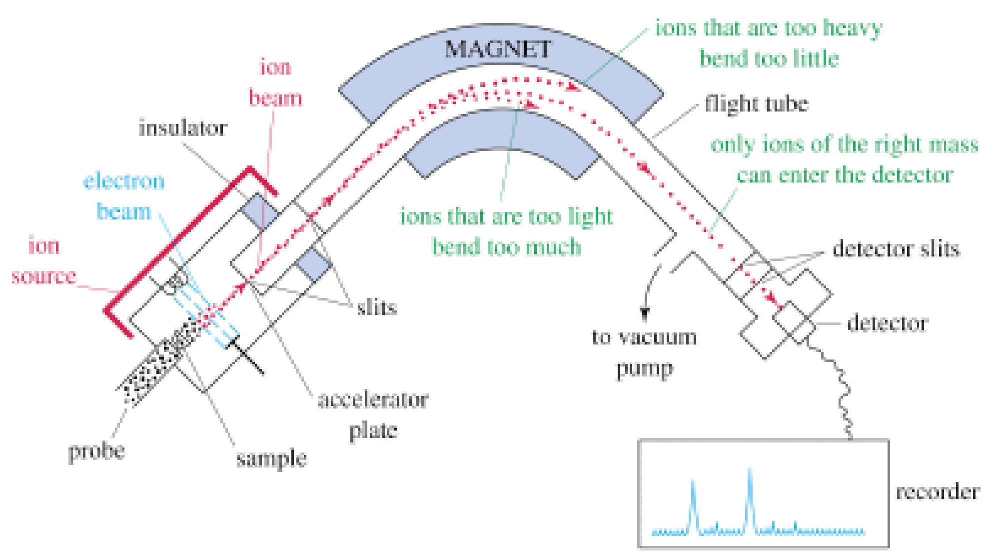
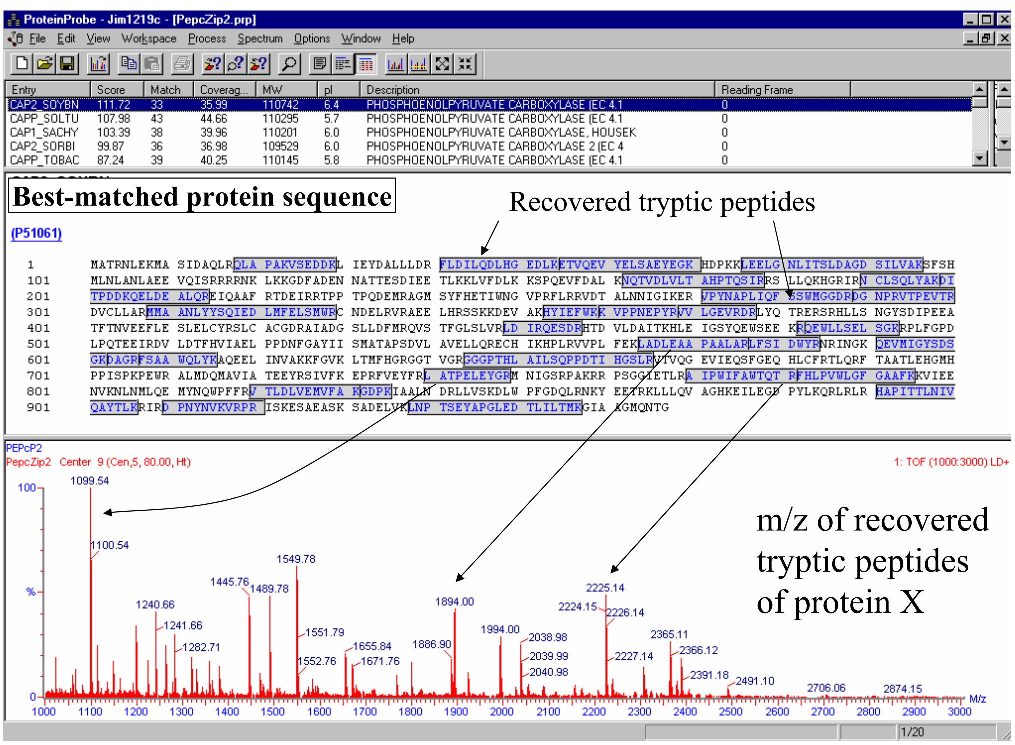
1 Simplified working example
2 Instrumentation
2.1 Ion source
2.2 Mass analyzer
2.2.1 Sector
2.2.2 Time-of-flight
2.2.3 Quadrupole
2.2.4 Quadrupole ion trap
2.2.5 Linear quadrupole ion trap
2.2.6 Fourier transform ion cyclotron resonance
2.2.7 Orbitrap



Mass spectrometry facilities
and proteomics lab

Protein Function Discovery Facility
6th Floor Botterell Hall

BCHM 410/810 Lecture 3



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5				9.850	1.684

We can formulate this problem as a system of linear equations.

```
A = 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
```

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

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:

	CH_4	C_2H_4	C_2H_6	C_3H_6	C_3H_8
p =	2.5373	0.1288	6.6815	8.4449	3.6329