Adduct transformations

Simon Rogers

October 23, 2014

A given precursor mass will be oberved with the addition of an adduct. For example, rather than measuring M, we might measure $M + H$, or $M + ACN$, or $M + ACN + H$ etc. Because we measure the mass per unit charge, working out the mass of the particlar ionization product (molecule of interest plus adduct) is not as easy as you might think.

In general, an adduct is of the form:

$$nM + \sum_i h_i A_i$$

where n is the multiplicity of the original molecule (how many of them are stuck together), A_i is an adduct and h_i is the count of the adducts. For example $M + ACN + 2H$ has a multiplicty of 1 and then $A_1 = ACN, h_1 = 1$, $A_2 = H, h_2 = 2$.

The total mass observed can now be calculated. Using G_i to denote the molecular mass of adduct A_i, we first compute:

$$nM + \sum_i h_i G_i$$

Now, the molecule will be charged (i.e. it will have gained or lost some electrons). Assume that the (integer) charge of the complete molecule is c. We must therefore substract c times the mass of an electron (e):

$$nM - ce + \sum_i h_i G_i$$

i.e. if the charge is +2, we subtract the masses of the missing two electrons.

Finally, we measure mass per unit charge, so we need to divide this by the absolute value of the charge $|c|$:

$$O = \frac{nM - ce + \sum_i h_i G_i}{|c|}$$

To compute the precursor mass M from an ion mass O due to a known adduct, we re-arrange:

$$M = \frac{O|c| + ce - \sum_i h_i G_i}{n}$$

1 Common adducts

Adduct	n	c
M+3H	1	3
M+2H+Na	1	3
M+H+2Na	1	3
M+3Na	1	3
M+2H	1	2
M+H+NH4	1	2
M+H+Na	1	2
M+H+K	1	2
M+ACN+2H	1	2
M+2Na	1	2
M+2ACN+2H	1	2
M+3ACN+2H	1	2
M+H	1	1
M+NH4	1	1
M+Na	1	1
M+CH3OH+H	1	1
M+K	1	1
M+ACN+H	1	1
M+2Na-H	1	1
M+IsoProp+H	1	1
M+ACN+Na	1	1
M+2K-H	1	1
M+DMSO+H	1	1
M+2ACN+H	1	1
M+IsoProp+Na+H	1	2
2M+H	2	1
2M+NH4	2	1
2M+Na	2	1
2M+3H2O+2H	2	2
2M+K	2	1
2M+ACN+H	2	1
2M+ACN+Na	2	1

2 Exotic adducts

Note that in the list of common ones we see ACN, Isoprop and DMSO. These are:

Molecule	Formula
ACN	C2H3N
IsoProp	C3H8O
DMSO	C2H6OS
FA	CH2O2

3 Charges

Only some of the adduct components have charge. These are:

Adduct	Charge
H	1
Na	1
NH4	1
K	1
Cl	-1
Br	-1

4 Atomic masses

To compute the adduct masses, we require various atomic masses. Most accurate ones seem to be available from `http://dx.doi.org/10.1351/pac200375060683`.

Atom	Mass
O	15.9949146223
H	1.0078250319
C	12.0 (by definition)
N	14.0030740074
Na	22.98976966
K	38.9637069
S	31.97207073
e	0.00054857990924