An analysis on lipid maps standards database and fragmentation patterns reported for various lipid classes indicated that the ms2 fragmentation of lipid species takes place around very few groups and follows a very predictable pattern. The groups involved in the fragmentations are

1. Alcoholic group (SMART pattern "C(O)")

2. The ether group (SMART pattern "CO", this includes even the pattern present in the ester group, phosphor ester, phosphor diester, thioether)

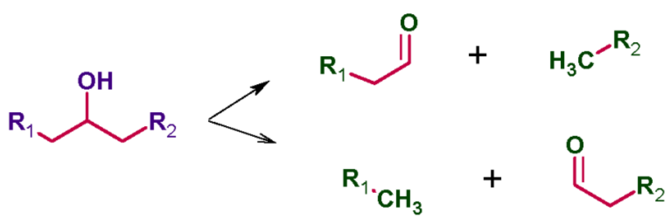
3. Amino are amine group (SMART pattern "CN").

4. The coenzyme group (will find out the smart for this)

5. Other (this fragmentations will occur when there is a adduct added to that)

The following pictures explains the lipid fragmentation rules:

I. The C(O) patterns alcohol_to_aldehyde - DONE

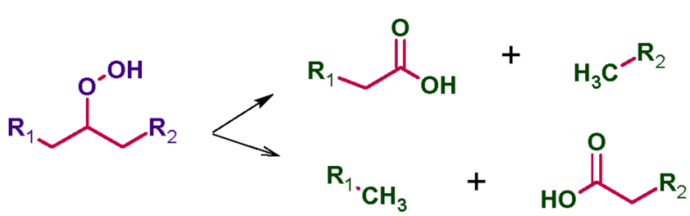


The fragmentation on this group produces two charge unaltered fragments (the fragment with the parental charge will contain the charge here). The fragment containing the oxygen will lose a hydrogen (here we need to reduce an hydrogen) and the other fragment will gain the oxygen (no need to add anything it will be added during bond deletion)

The peroxyl groups will also follow the same pattern

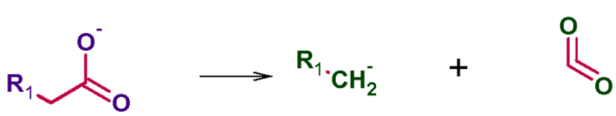
peroxy_to_carboxy

I think for first level fragmentation this is OKAY because masses are correct. TODO: finish.



When the OH is in deprotonated form(as in carboxylic acid) the negative charge will be transferred to the fragment devoid of the oxygen to form a negatively charged ion and a carbon dioxide molecule.

DONE

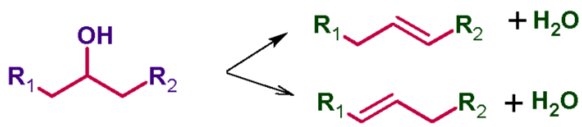


co2_loss

The hydroxyl group present the lipid can also be loosed during the fragmentation as a water molecule as shown below

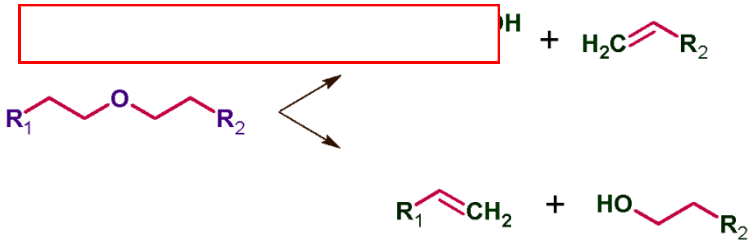
sp3c_oxygen_double_bond

DONE



II. The CO patterns

DONE

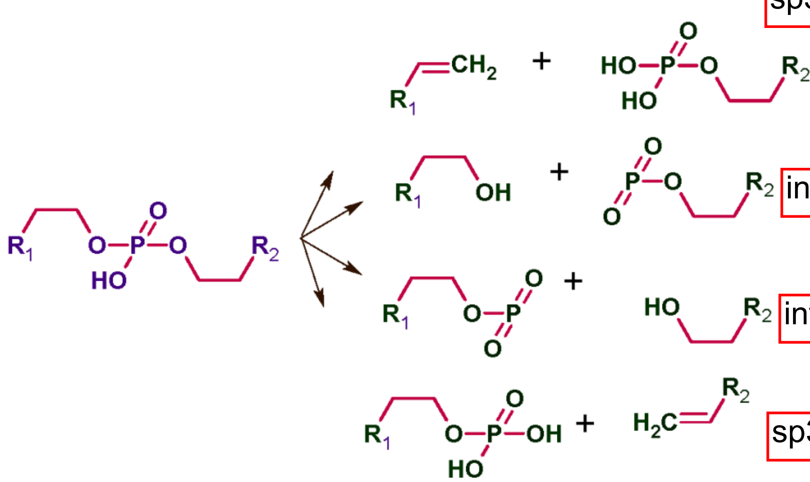


The fragmentation of this group also produces two charge unaltered molecules. However the difference here is the hydrogen is added with the fragment containing the oxygen.

Some examples of these fragmentations are

a. phosphodiesters (as in phospholipids)

sp3c_oxygen_double_bond



internal_phosphodiester

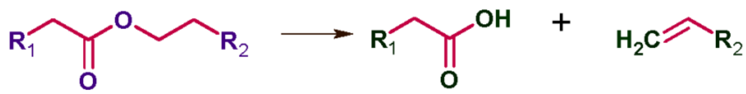
internal_phosphodiester

sp3c_oxygen_double_bond

b. esters

DONE - this is a proper subset of dealing with an ether. the far side

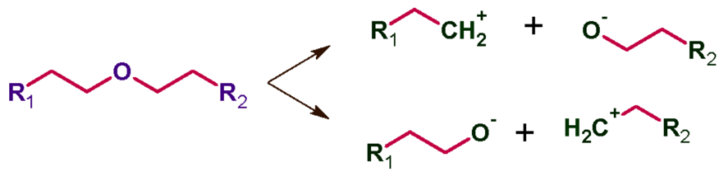
sp3c_oxygen_double_bond



The CO pattern can also produce two charged molecule as shown in the below reaction. (a hydrogen should be removed from both the fragments)

sp3c_oxygen_assymmetric_ether

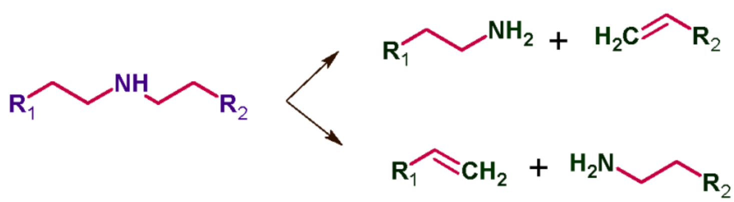
sp3c_nitrogen_assymmetric_non_primary



III. The CN pattern

sp3c_nitrogen_double_bond

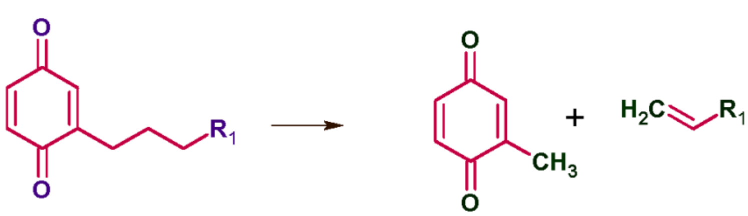
DONE



This group also follows the CO (typeI) fragmentation with hydrogen added to the fragment containing nitrogen

IV. The coenzyme group

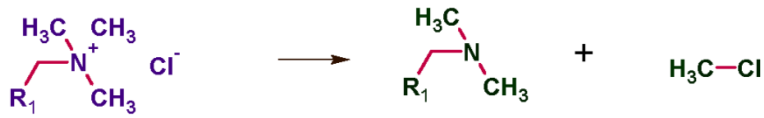
sp3c_coenzyme_double_bond



Here the methyl group attached to the ring gains an electron and the other fragment loses it to form a double bond

V. Other groups

a) When the quandary amine (as in choline) forms an adduct with anions such as chlorine, acetate it lose its charge status as well as methyl chloride and methyl acetate respectively



b) When the carbonyl group formed an adduct with hydrogen containing cations such as ammonium will lose an ammonium molecule.