

Mass spectral fragments of common hydrocarbons

Mass Spectral peaks can be identified to have originated from the fragmentation of specific hydrocarbon sources including:

Some common ions

Alkanes: 57 / 43.

Alkenes: 55 / 41

Per fluorinated hydrocarbons: 69

Aromatics: 75-78, /130-138.

Compound type	Common lines
Alkanes	29, 43, 57, 71, 85, 99
Alkenes/cycloalkanes	27, 41, 55, 69, 83, 97
Aliphatic alcohols	31, 45, 59, 73, 87, 101
Aromatics	38, 39, 50-2, 63-5, 75-8
Acids/esters	45, 59, 73, 87, 101
Alkyl amines	30, 44, 58, 72, 86, 100
Chloroalkyl	49, 63, 77, 91, 105
Alkyl silanes	31, 45, 59, 73, 87, 101

Some Common Fragments at m/z include:

14 CH ₂	39 C ₃ H ₃	58 CH ₃ C(=O)CH ₂ + H, C ₂ H ₅ CHNH ₂
15 CH ₃	41 C ₃ H ₅	59 C ₃ H ₆ OH, CH ₂ OC ₂ H ₅
16 O	42 C ₃ H ₆ , C ₂ H ₂ O	60 CH ₂ COOH
17 OH	43 C ₃ H ₇ , CH ₃ C=O	61 CH ₃ COO
18 H ₂ O, NH ₄	44 CH ₂ CHO	65 C ₅ H ₅
19 F	45 CH ₃ CHOH, CH ₂ CH ₂ OH, CH ₂ OCH ₂	66 C ₅ H ₆
26 CN, C ₂ H ₂	46 NO ₂	67 C ₅ H ₇
27 C ₂ H ₃	47 CH ₂ SH	68 CH ₂ CH ₂ CH ₂ CN
28 C ₂ H ₄ , CO	48 CH ₃ S + H	69 C ₅ H ₉ , CF ₃
29 C ₂ H ₅ , CHO	49 CH ₂ Cl	70 C ₅ H ₁₀
30 CH ₂ NH ₂	51 CHF ₂ , C ₃ H ₃	71 C ₅ H ₁₁ , C ₃ H ₇ C=O
31 CH ₂ OH	53 C ₄ H ₅	76 C ₆ H ₄
32 O ₂	54 CH ₂ CH ₂ CN	77 C ₆ H ₅
33 SH	55 C ₄ H ₇	78 C ₆ H ₅ + H
34 H ₂ S	56 C ₄ H ₈	79 C ₆ H ₅ + 2H Br
35 Cl	57 C ₄ H ₉ , C ₂ H ₅ C=O	
36 HCl		

References:

Hamming, M and N. Foster. Interpretation of Mass Spectra of Organic Compounds. New York, NY. Academic Press.

McLafferty, F. W. Interpretation of Mass Spectra. Mill Valley, CA. University Scientific Books.

Silverstein, R, G. Bassler and T. Morrill. Spectrometric Identification of Organic Compounds. New York, NY. John Wiley and Sons. Inc.