

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