

$$DOU (C_nH_m) = n - \frac{m}{2} + 1; \text{ for } m: Br, H = 1, S = 0, N = -1$$

Equation 1. Degrees of unsaturation

$$C_nH_{n+r}; \frac{M}{13} = n + \frac{r}{13}; DOU = \frac{n - r + 2}{2}$$

Equation 2. Rule of 13

Common mass fragments	
H	1
CH ₃	15
NH ₂ ; O (rare)	16
OH; NH ₃ (rare)	17
H ₂ O	18
F	19
HF	20
CH≡CH; CN	26
HCN; CH ₂ =CH	27
CH ₂ =CH ₂ ; CO	28
C ₂ H ₅ ; CHO	29
NO; CH ₂ O	30
OCH ₃ ; CH ₂ OH;	31
CH ₃ OH; S	32
HS	33
Cl	35
HCl	36
CH ₂ =C=O; CH ₂ =CH=CH ₃	42
C ₃ H ₇ ; CH ₃ C=O	43
CO ₂	44
OCH ₂ CH ₃ ; COOH;;	45
NO ₂	46
CH ₃ CH ₂ C=O; C ₄ H ₉	57
CH ₃ COOH	60
C ₅ H ₁₁	71
Ph-	77
Br	79
C ₆ H ₁₃	85
Ph-CH ₂	91
Py-CH ₂	92
C ₇ H ₁₅	99
Ph-C=O	105
I	127

Halogen intensities (M+2,+4,+6, etc. peaks)	
Cl	100: 32.6
Cl ₂	100: 65.3: 10.6
Cl ₃	100: 98.1: 31.9: 3.5
Cl ₄	76.6: 100: 48.9: 10.6: 0.9
Cl ₅	61.3: 100: 65.2: 21.3: 3.5
Br	100: 97.7
Br ₂	51.2: 100: 48.9
Br ₃	34.1: 100: 97.8: 31.9
BrCl	76.7: 100: 24.5

Rule of 13 substitution

Add	Remove	Unsaturation
C	H ₁₂	7
H ₁₂	C	-7
N	CH ₂	0.5
O	CH ₄	1
F	CH ₇	2
N ₂	C ₂ H ₄	1
Si	C ₂ H ₄	1
P	C ₂ H ₇	2
³² S	C ₂ H ₈	2
O ₂	C ₂ H ₈	2
³⁵ Cl	C ₂ H ₁₁	3
O ₃	C ₃ H ₁₂	3
⁷⁹ Br	C ₅ H ₁₉	4
⁷⁹ Br	C ₆ H ₇	-3
I	C ₉ H ₁₉	0
I	C ₁₀ H ₇	7

*Unsaturation can not be less than 0 and is unlikely to be fractional; An odd number of nitrogens will show an odd MW; Be aware of the isotopes used in this table