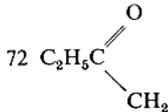
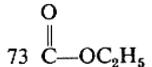
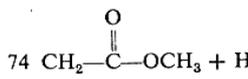
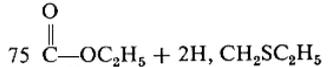
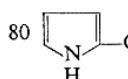
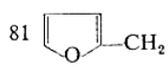
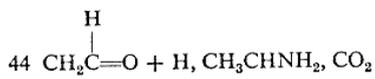
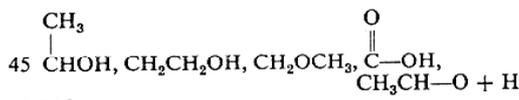
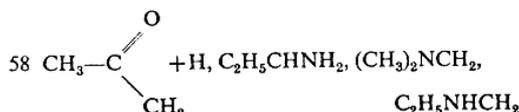
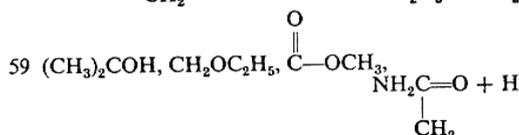
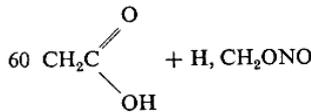
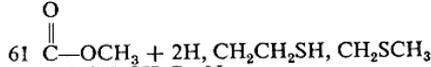
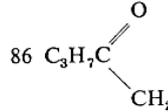
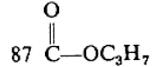
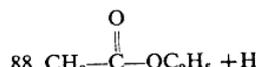
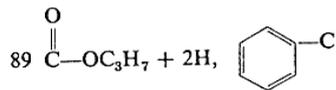
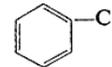
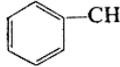
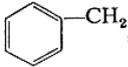
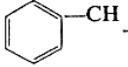
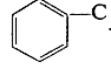
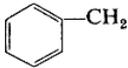
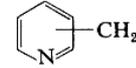
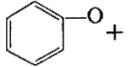
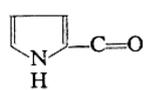


Une liste de ces fragments classés par masse croissante est donnée dans le **Tableau III**.

Tableau III: Fragments fréquemment observés dans les spectres de masse de composés organiques

<i>m/e</i>	Fragments	<i>m/e</i>	Fragments
14	CH ₂	72	 + H, C ₃ H ₇ CHNH ₂
15	CH ₃	73	
16	O	74	 + H
17	OH	75	 + 2H, CH ₂ SC ₂ H ₅
18	H ₂ O, NH ₄	77	C ₆ H ₅
19	F	78	C ₆ H ₅ + H
20	HF	79	C ₆ H ₅ + 2H, Br
26	C≡N	80	 CH ₂ , CH ₃ SS + H, HBr
27	C ₂ H ₃	81	
28	C ₂ H ₄ , CO, N ₂	82	CH ₂ CH ₂ CH ₂ CH ₂ C≡N
29	C ₂ H ₅ , CHO	83	C ₆ H ₁₁
30	CH ₂ NH ₂ , NO	85	C ₆ H ₁₃ , C ₄ H ₉ C=O
31	CH ₂ OH, OCH ₃		
33	SH		
34	H ₂ S		
35	Cl		
36	HCl		
39	C ₃ H ₃		
40	CH ₂ C≡N		
41	C ₃ H ₅ , CH ₂ C≡N + H		
42	C ₃ H ₆		
43	C ₃ H ₇ , CH ₃ C=O		
44	 + H, CH ₃ CHNH ₂ , CO ₂		
45	 CHOH, CH ₂ CH ₂ OH, CH ₂ OCH ₃ , C(=O)OH, CH ₃ CH-O + H		
46	NO ₂		
47	CH ₂ SH, CH ₃ S		
48	CH ₃ S + H		
54	CH ₂ CH ₂ C≡N		
55	C ₄ H ₇		
56	C ₄ H ₈		
57	C ₄ H ₉ , C ₂ H ₅ C=O		
58	 + H, C ₂ H ₅ CHNH ₂ , (CH ₃) ₂ NCH ₂ , C ₂ H ₅ NHCH ₂		
59	 CH ₂ OC ₂ H ₅ , C(=O)OCH ₃ , NH ₂ C(=O)-H + H		
60	 + H, CH ₂ ONO		
61	 + 2H, CH ₂ CH ₂ SH, CH ₂ SCH ₃		
68	CH ₂ CH ₂ CH ₂ C≡N		
69	C ₅ H ₉ , CF ₃		
70	C ₅ H ₁₀		
71	C ₅ H ₁₁ , C ₃ H ₇ C=O		
		86	 + H, C ₄ H ₉ CHNH ₂
		87	
		88	 + H
		89	 + 2H, 
		90	CH ₃ CHONO ₂ , 
		91	 ,  + H,  + 2H
		92	 + H, 
		94	 + H, 

Plus précisément encore, certains modes de fragmentation (coupure de certaines liaisons, apparition de certains types de fragments) peuvent être reliés à la présence de certains groupes fonctionnels (cf. **Tableau IV**).

**Tableau IV: Fragmentations caractéristiques liées
à la nature des composés organiques étudiés.**

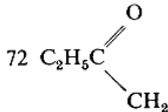
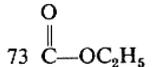
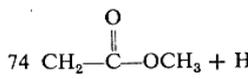
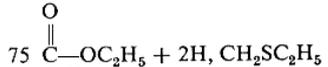
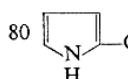
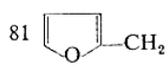
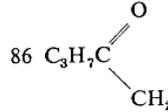
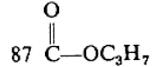
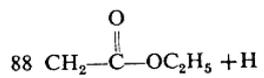
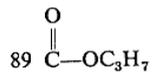
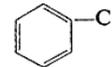
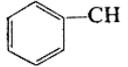
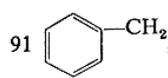
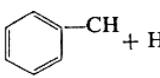
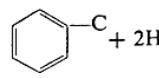
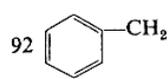
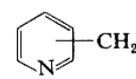
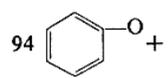
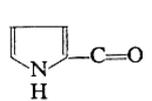
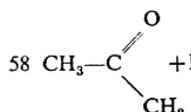
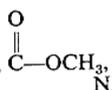
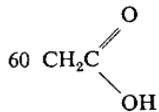
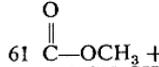
Compound type	Expected peaks (m/z) ^a	Structural unit or fragment
1. Hydrocarbons		
A. Alkanes	15, 29, 43, 57, 71 ...	$C_nH_{2n+1}^+$
B. Cycloalkanes	41, 55, 69, 83 ... $M - 28/M - 42/M - 56 \dots$	$C_nH_{2n-1}^+$ - RCH=CH ₂
C. Alkenes	41, 55, 69, 83 ...	$C_nH_{2n-1}^+$
D. Benzenoid compounds	77 91 65 ↙] - HC≡CH 92	$C_6H_5^+$ $C_7H_7^+$ $C_5H_5^+$ $C_7H_8^+$
2. Halocarbons		
A. Chlorides ^b	$M - 36$ 91	- HCl $C_4H_8Cl^+$
B. Bromides ^b	$M - 80$ 135	- HBr $C_4H_8Br^+$
3. Hydroxy compounds		
A. Alcohols ^b	$M - 2$ $M - 3$ $M - 18$ $M - 33$ $M - 46$ 31 45/59/73 ... 59/73/87 ...	RCH=O ⁺ RC≡O ⁺ - H ₂ O - H ₂ O, - CH ₃ - H ₂ O, - CH ₂ =CH ₂ CH ₂ =OH ⁺ RCH=OH ⁺ R ₂ C=OH ⁺
B. Phenols	$M - 28$ $M - 29$	- CO - CHO
4. Ethers		
A. Aliphatic ^b	31, 45, 59, 73 ... 29, 43, 57 ...	RO ⁺ , ROCH ₂ ⁺ R ⁺
B. Aromatic ^c	92 + mass of ring substituent(s), X 64 + mass of ring substituent(s), X 76 + mass of ring substituent(s), X	X-C ₆ H ₄ O ⁺ X-C ₅ H ₄ ⁺ X-C ₆ H ₄ ⁺

5. Aldehydes			
A. Aliphatic ^b	$M - 1$ $M - 29$ 44/58/72 ...	- H - CHO - $\text{RCH}=\text{CH}_2$ (McLafferty rearrangement)	
B. Aromatic	$M - 1$ $M - 2$	- H - H, - CO	
6. Ketones			
A. Aliphatic ^b	58/72/86 ...	- $\text{RCH}=\text{CH}_2$ (McLafferty rearrangement)	
B. Aromatic	76 + mass of ring substituent(s) 104 + mass of ring substituent(s)	$\text{X}-\text{C}_6\text{H}_4^+$ $\text{X}-\text{C}_6\text{H}_4\text{CO}^+$	
7. Carboxylic acids and esters			
A. Acids ^b	$M - 17$ $M - 45$ $M - 28/M - 42/M - 56 \dots$	- OH - COOH - $\text{RCH}=\text{CH}_2$ (McLafferty rearrangement)	
B. Methyl esters	$M - 31$ $M - 59$ $M - 28/M - 42/M - 56 \dots$	- OCH_3 - CO_2CH_3 - $\text{RCH}=\text{CH}_2$ (McLafferty rearrangement)	
8. Amines			
A. Aliphatic	30, 44, 58, 72 ...	RCHNH_2^+	
B. Aromatic	$M - 1$ $M - 27$ $M - 15/M - 29/M - 43$	- H - HCN alkyl cleavage from N	
9. Amides	$M - 15/M - 29/M - 43 \dots$ $M - 28/M - 42/M - 56 \dots$	alkyl cleavage from N - $\text{RCH}=\text{CH}_2$ (McLafferty rearrangement)	
10. Nitriles			
A. Aliphatic	$M - 1$ $M - 28/M - 42/M - 56 \dots$	- H - $\text{RCH}=\text{CH}_2$ (McLafferty rearrangement)	
B. Aromatic	$M - 1$ $M - 27$	- H - HCN	
11. Nitro compounds (aromatic)	$M - 30$ $M - 46$ $M - 58$ $M - 72$	- NO (with rearrangement) - NO_2 - NO, - CO - NO_2 , - $\text{HC}\equiv\text{CH}$	
12. Thiols and sulfides ^b			
A. Thiols	$M - 34$	- H_2S	
1°	47	$\text{CH}_2=\text{SH}^+$	
2°	61/75/89 ...	$\text{RCH}=\text{SH}^+$	
3°	75/89/103 ...	$\text{R}_2\text{C}=\text{SH}^+$	
B. Sulfides	47/61/75 ...	RS^+	

Tableau IV (suite): Fragmentations caractéristiques liées à la nature des composés organiques étudiés.

Une liste de ces fragments classés par masse croissante est donnée dans le **Tableau III**.

Tableau III: Fragments fréquemment observés dans les spectres de masse de composés organiques

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16	O	74	 + H
17	OH	75	 + 2H, CH ₂ SC ₂ H ₅
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19	F	78	C ₆ H ₅ + H
20	HF	79	C ₆ H ₅ + 2H, Br
26	C≡N	80	 CH ₂ , CH ₃ SS + H, HBr
27	C ₂ H ₃	81	
28	C ₂ H ₄ , CO, N ₂	82	CH ₂ CH ₂ CH ₂ CH ₂ C≡N
29	C ₂ H ₅ , CHO	83	C ₆ H ₁₁
30	CH ₂ NH ₂ , NO	85	C ₆ H ₁₃ , C ₄ H ₉ C=O
31	CH ₂ OH, OCH ₃	86	 + H, C ₄ H ₉ CHNH ₂
33	SH	87	
34	H ₂ S	88	 + H
35	Cl	89	 + 2H, 
36	HCl	90	CH ₃ CHONO ₂ , 
39	C ₃ H ₃	91	 CH ₂ ,  + H,  + 2H
40	CH ₂ C≡N	92	 + H, 
41	C ₃ H ₅ , CH ₂ C≡N + H	94	 + H, 
42	C ₃ H ₆		
43	C ₃ H ₇ , CH ₃ C=O		
44	 + H, CH ₃ CHNH ₂ , CO ₂		
45	 CHO, CH ₂ CH ₂ OH, CH ₂ OCH ₃ ,  + H		
46	NO ₂		
47	CH ₂ SH, CH ₃ S		
48	CH ₃ S + H		
54	CH ₂ CH ₂ C≡N		
55	C ₄ H ₇		
56	C ₄ H ₈		
57	C ₄ H ₉ , C ₂ H ₅ C=O		
58	 + H, C ₂ H ₅ CHNH ₂ , (CH ₃) ₂ NCH ₂ , C ₂ H ₅ NHCH ₂		
59	(CH ₃) ₂ COH, CH ₂ OC ₂ H ₅ ,  + H		
60	 + H, CH ₂ ONO		
61	 + 2H, CH ₂ CH ₂ SH, CH ₂ SCH ₃		
68	CH ₂ CH ₂ CH ₂ C≡N		
69	C ₅ H ₉ , CF ₃		
70	C ₅ H ₁₀		
71	C ₅ H ₁₁ , C ₃ H ₇ C=O		

Plus précisément encore, certains modes de fragmentation (coupure de certaines liaisons, apparition de certains types de fragments) peuvent être reliés à la présence de certains groupes fonctionnels (cf. **Tableau IV**).

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C. Alkenes	41, 55, 69, 83 ...	$C_nH_{2n-1}^+$
D. Benzenoid compounds	77 91] - HC≡CH 65] 92	$C_6H_5^+$ $C_7H_7^+$ $C_5H_5^+$ $C_7H_8^+$
2. Halocarbons		
A. Chlorides ^b	$M - 36$ 91	- HCl $C_4H_8Cl^+$
B. Bromides ^b	$M - 80$ 135	- HBr $C_4H_8Br^+$
3. Hydroxy compounds		
A. Alcohols ^b	$M - 2$ $M - 3$ $M - 18$ $M - 33$ $M - 46$ 31 45/59/73 ... 59/73/87 ...	RCH=O ⁺ RC≡O ⁺ - H ₂ O - H ₂ O, - CH ₃ - H ₂ O, - CH ₂ =CH ₂ CH ₂ =OH ⁺ RCH=OH ⁺ R ₂ C=OH ⁺
B. Phenols	$M - 28$ $M - 29$	- CO - CHO
4. Ethers		
A. Aliphatic ^b	31, 45, 59, 73 ... 29, 43, 57 ...	RO ⁺ , ROCH ₂ ⁺ R ⁺
B. Aromatic ^c	92 + mass of ring substituent(s), X] 64 + mass of ring] - CO substituent(s), X 76 + mass of ring substituent(s), X	X-C ₆ H ₄ O ⁺ X-C ₅ H ₄ ⁺ X-C ₆ H ₄ ⁺

5. Aldehydes			
A. Aliphatic ^b	$M - 1$ $M - 29$ 44/58/72 ...	- H - CHO - $\text{RCH}=\text{CH}_2$ (McLafferty rearrangement)	
B. Aromatic	$M - 1$ $M - 2$	- H - H, - CO	
6. Ketones			
A. Aliphatic ^b	58/72/86 ...	- $\text{RCH}=\text{CH}_2$ (McLafferty rearrangement)	
B. Aromatic	76 + mass of ring substituent(s) 104 + mass of ring substituent(s)	$\text{X}-\text{C}_6\text{H}_4^+$ $\text{X}-\text{C}_6\text{H}_4\text{CO}^+$	
7. Carboxylic acids and esters			
A. Acids ^b	$M - 17$ $M - 45$ $M - 28/M - 42/M - 56 \dots$	- OH - COOH - $\text{RCH}=\text{CH}_2$ (McLafferty rearrangement)	
B. Methyl esters	$M - 31$ $M - 59$ $M - 28/M - 42/M - 56 \dots$	- OCH_3 - CO_2CH_3 - $\text{RCH}=\text{CH}_2$ (McLafferty rearrangement)	
8. Amines			
A. Aliphatic	30, 44, 58, 72 ...	RCHNH_2^+	
B. Aromatic	$M - 1$ $M - 27$ $M - 15/M - 29/M - 43$	- H - HCN alkyl cleavage from N	
9. Amides	$M - 15/M - 29/M - 43 \dots$ $M - 28/M - 42/M - 56 \dots$	alkyl cleavage from N - $\text{RCH}=\text{CH}_2$ (McLafferty rearrangement)	
10. Nitriles			
A. Aliphatic	$M - 1$ $M - 28/M - 42/M - 56 \dots$	- H - $\text{RCH}=\text{CH}_2$ (McLafferty rearrangement)	
B. Aromatic	$M - 1$ $M - 27$	- H - HCN	
11. Nitro compounds (aromatic)	$M - 30$ $M - 46$ $M - 58$ $M - 72$	- NO (with rearrangement) - NO_2 - NO, - CO - NO_2 , - $\text{HC}\equiv\text{CH}$	
12. Thiols and sulfides ^b			
A. Thiols	$M - 34$	- H_2S	
1°	47	$\text{CH}_2=\text{SH}^+$	
2°	61/75/89 ...	$\text{RCH}=\text{SH}^+$	
3°	75/89/103 ...	$\text{R}_2\text{C}=\text{SH}^+$	
B. Sulfides	47/61/75 ...	RS^+	

Tableau IV (suite): Fragmentations caractéristiques liées à la nature des composés organiques étudiés.