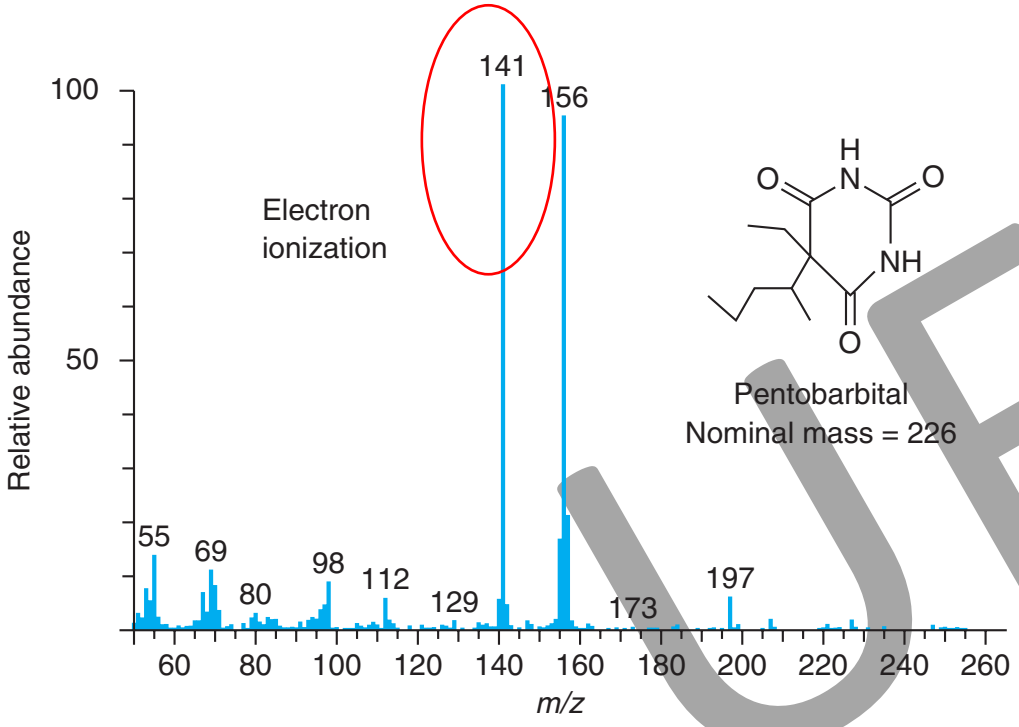
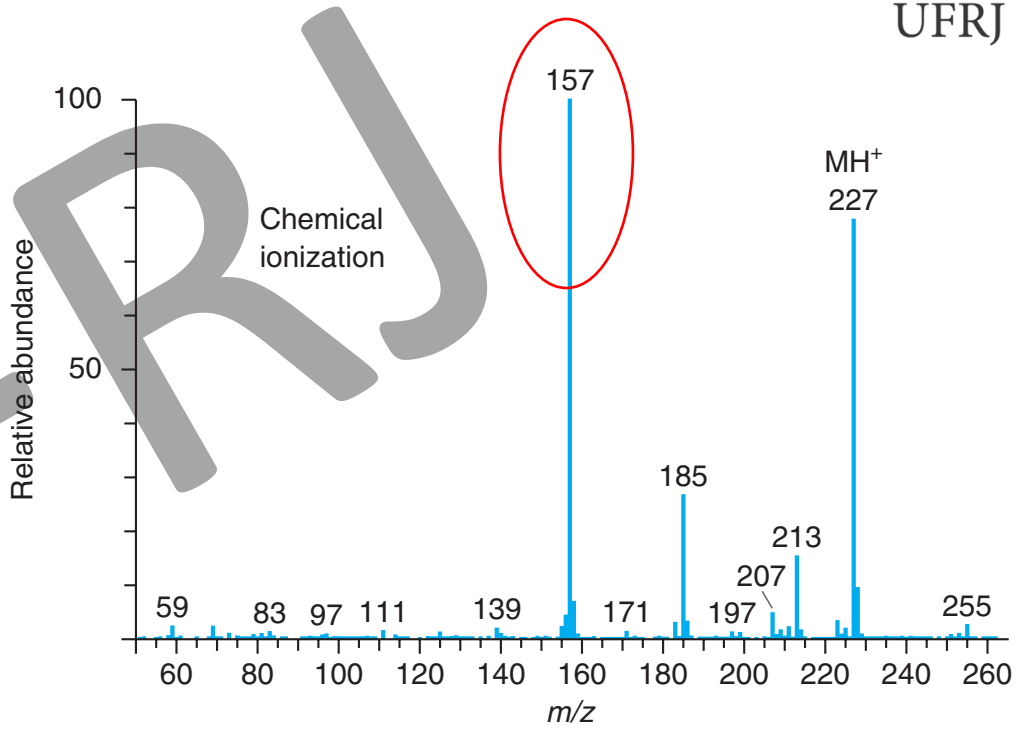
Pico base

É o pico mais intenso do espectro

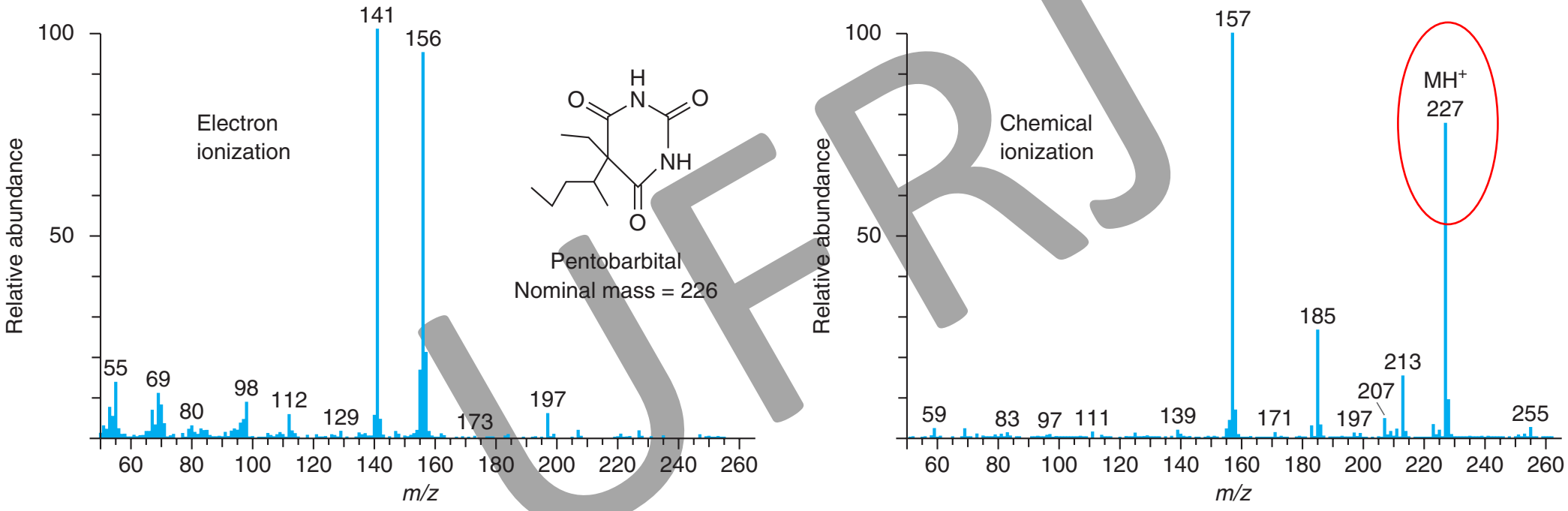


Pentobarbital
Nominal mass = 226

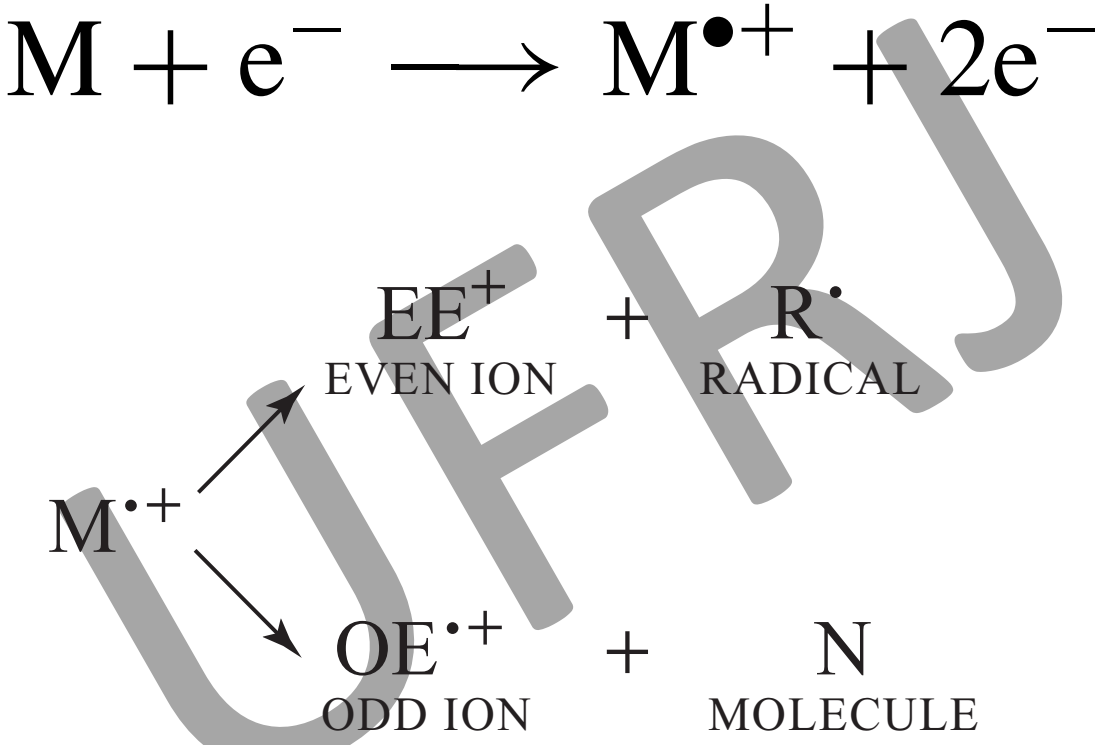


Pico do íon molecular

É pequeno ou inexistente dependendo da molécula e do modo de ionização



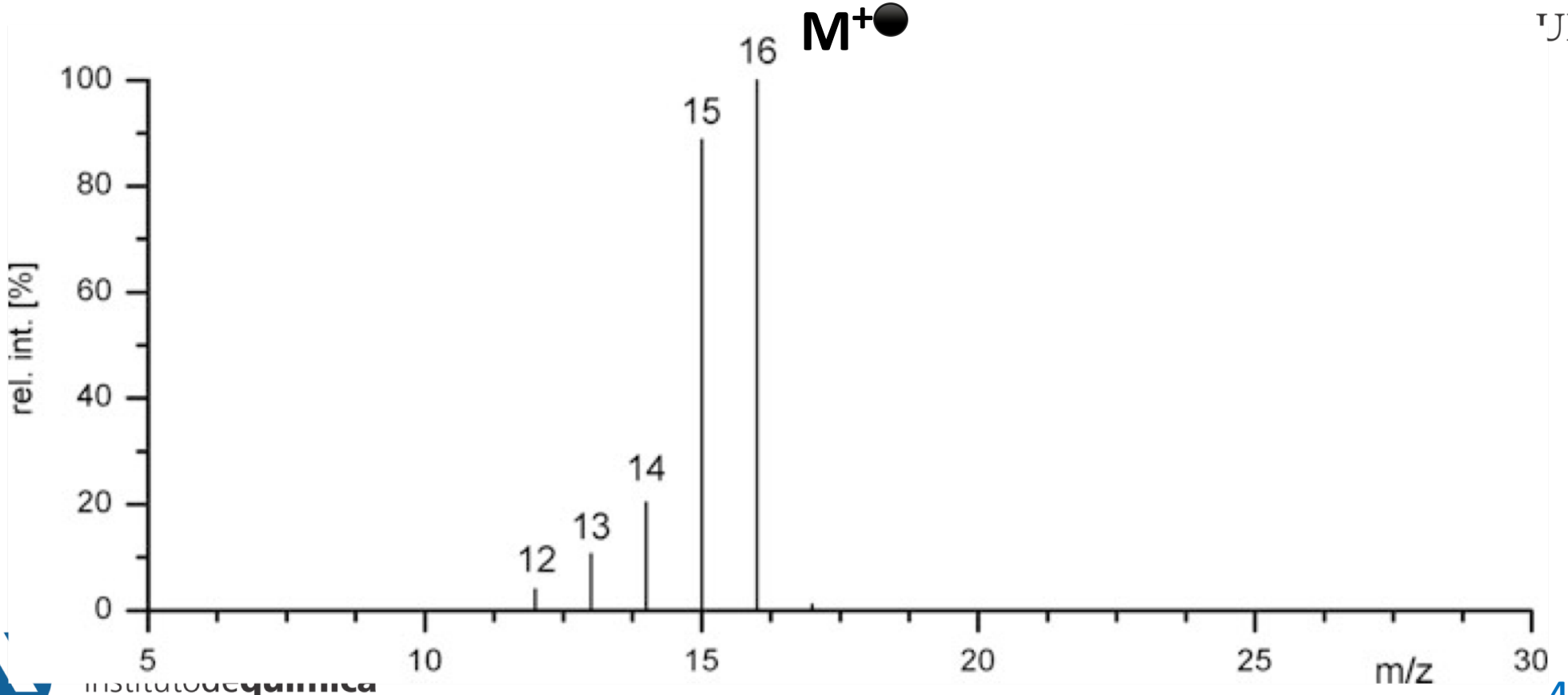
Formação e íons



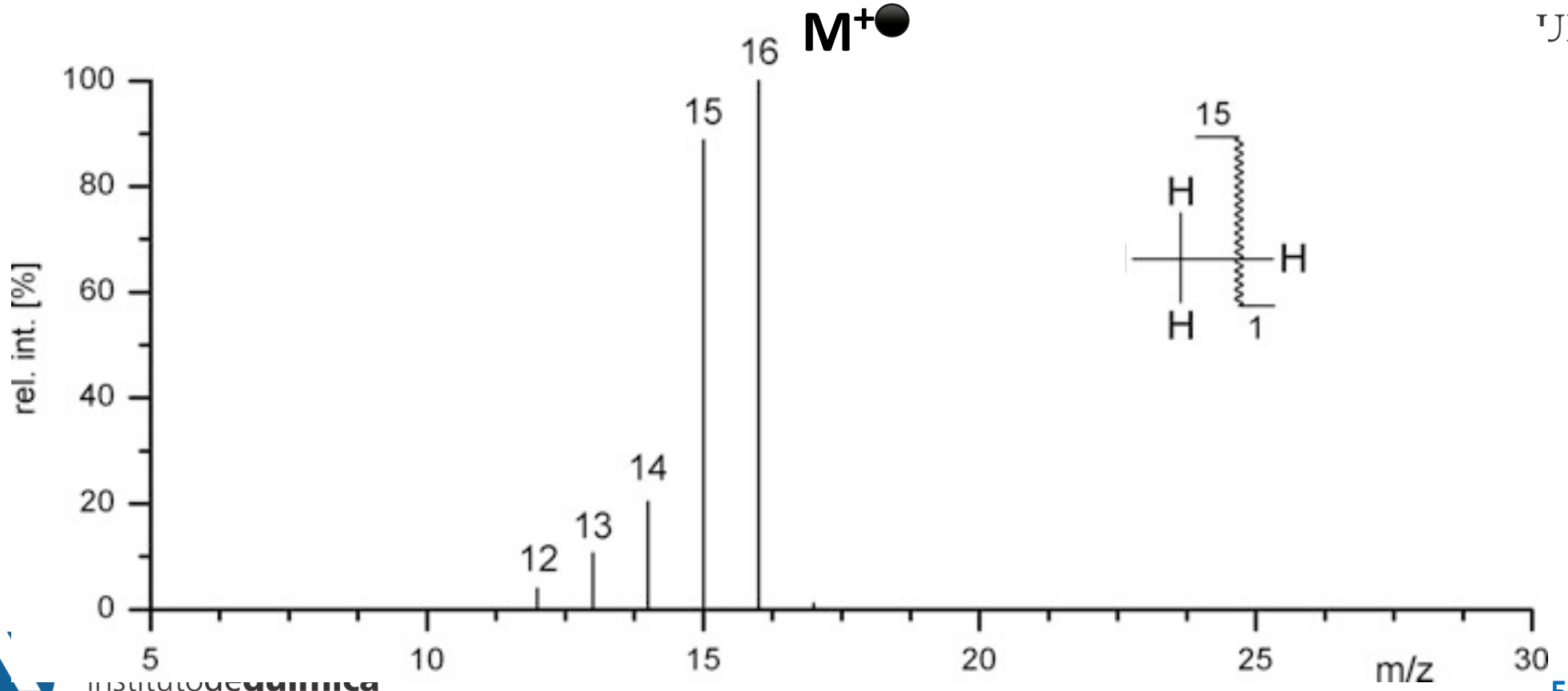
UFRJ

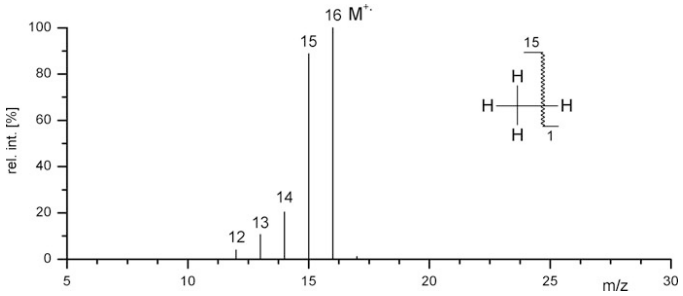
institutodequímica
Universidade Federal do Rio de Janeiro

Exercícios

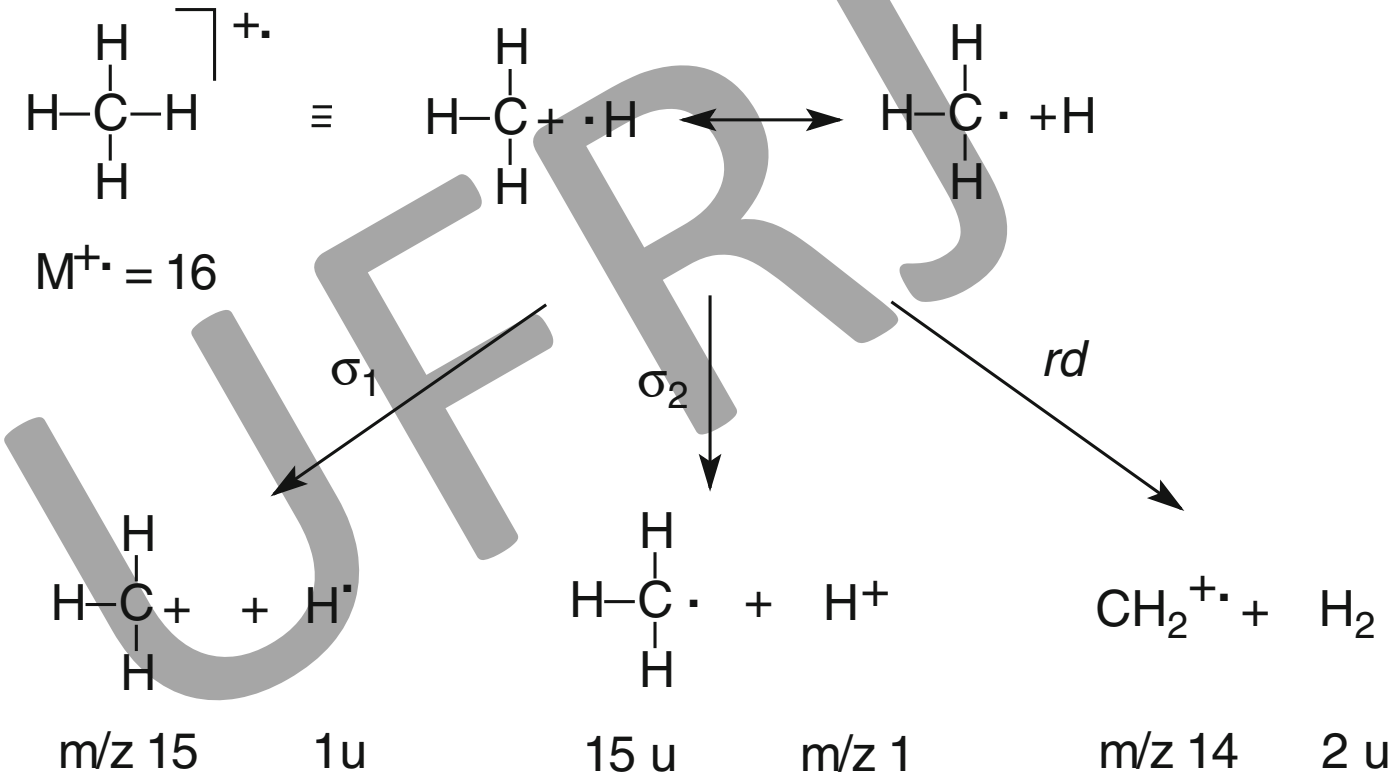


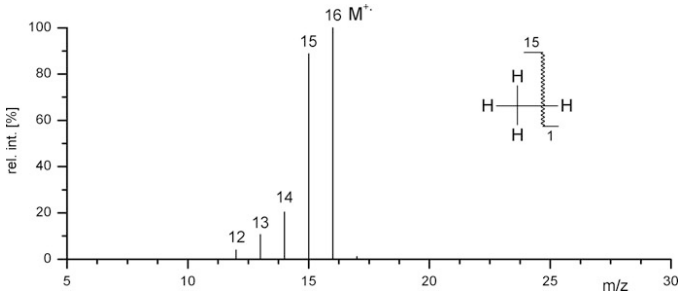
Exercícios





Exercícios





Exercícios

$$CH_4^{+\bullet} \rightarrow CH_3^{+} + H^{\bullet}; m/z\ 16 \rightarrow m/z\ 15$$

$$CH_4^{+\bullet} \rightarrow CH_2^{+\bullet} + H_2;\ m/z\ 16 \rightarrow m/z\ 14$$

$$CH_2^{+\bullet} \rightarrow C^{+\bullet} + H_2;\ m/z\ 14 \rightarrow m/z\ 12$$

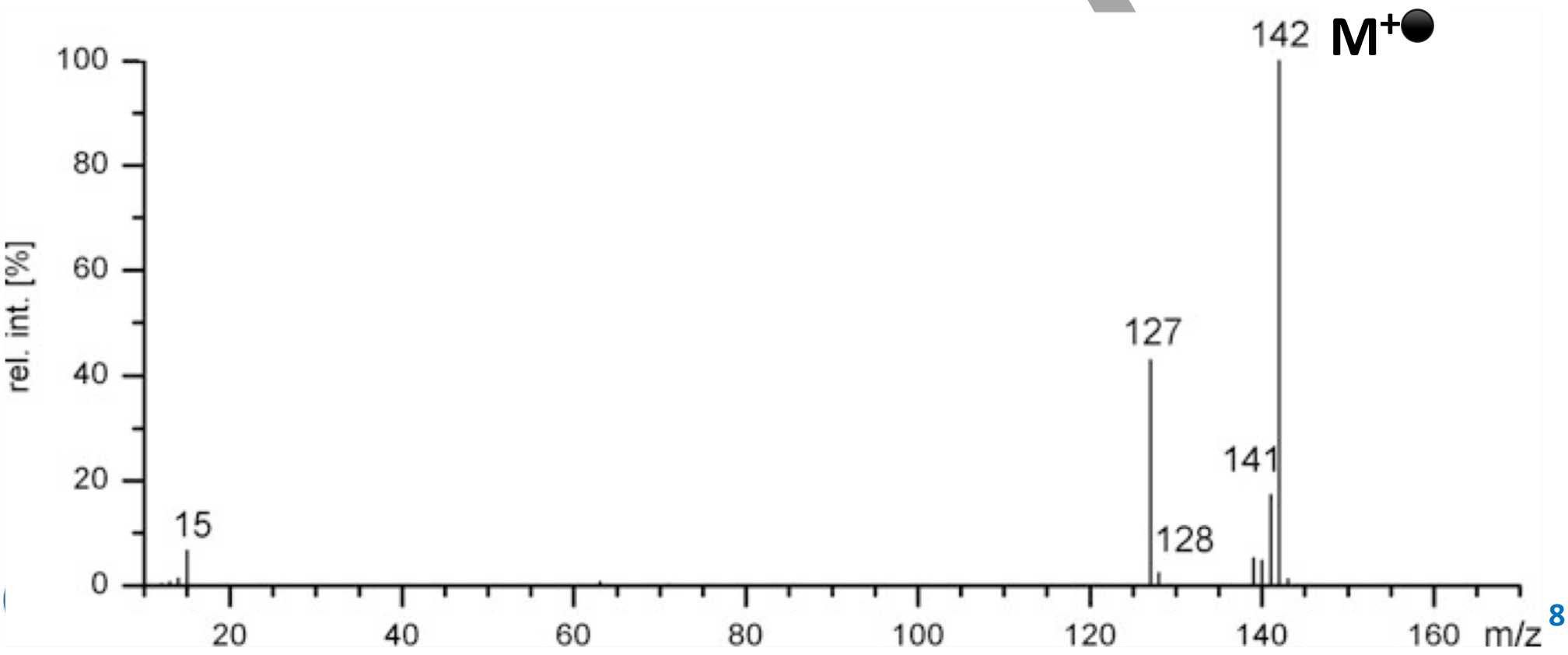
$$CH_2^{+\bullet} \rightarrow CH^{+} + H^{\bullet};\ m/z\ 14 \rightarrow m/z\ 13$$

$$CH_3^{+} \rightarrow CH^{+} + H_2;\ m/z\ 15 \rightarrow m/z\ 13$$

Exercícios

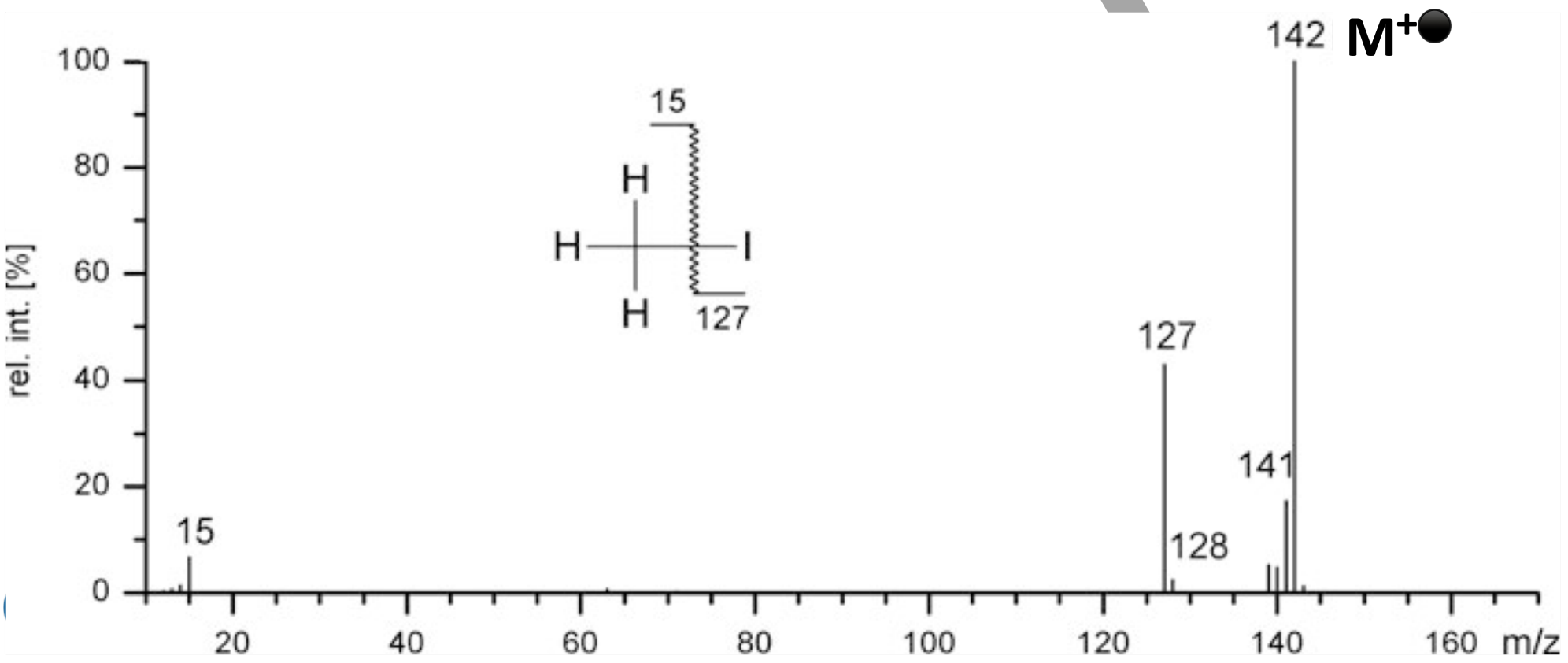
UFRJ

Iodometano



Exercícios

UFRJ



Exercícios

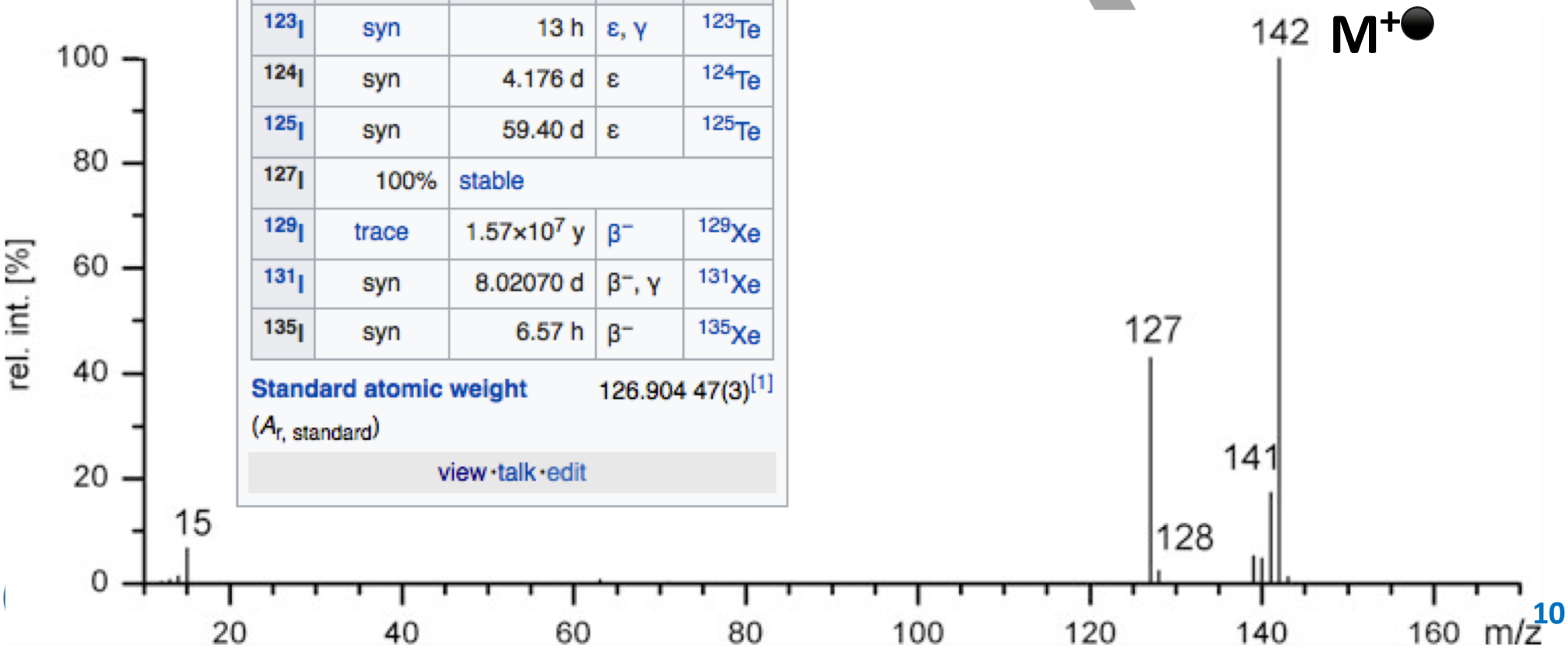
Main isotopes of iodine ($_{53}$I)

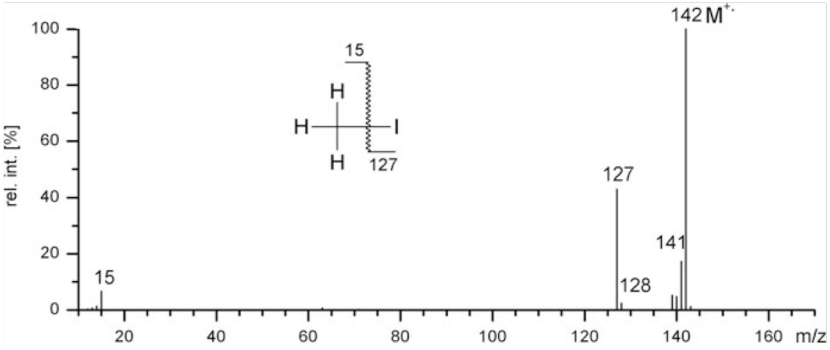
Isotope			Decay	
	abun-dance	half-life ($t_{1/2}$)	mode	pro-duct
^{123}I	syn	13 h	ε, γ	^{123}Te
^{124}I	syn	4.176 d	ε	^{124}Te
^{125}I	syn	59.40 d	ε	^{125}Te
^{127}I	100%	stable		
^{129}I	trace	1.57×10^{7} y	β^-	^{129}Xe
^{131}I	syn	8.02070 d	β^-, γ	^{131}Xe
^{135}I	syn	6.57 h	β^-	^{135}Xe

Standard atomic weight ($A_{r,\,standard}$) 126.904 47(3)[1]

view · talk · edit

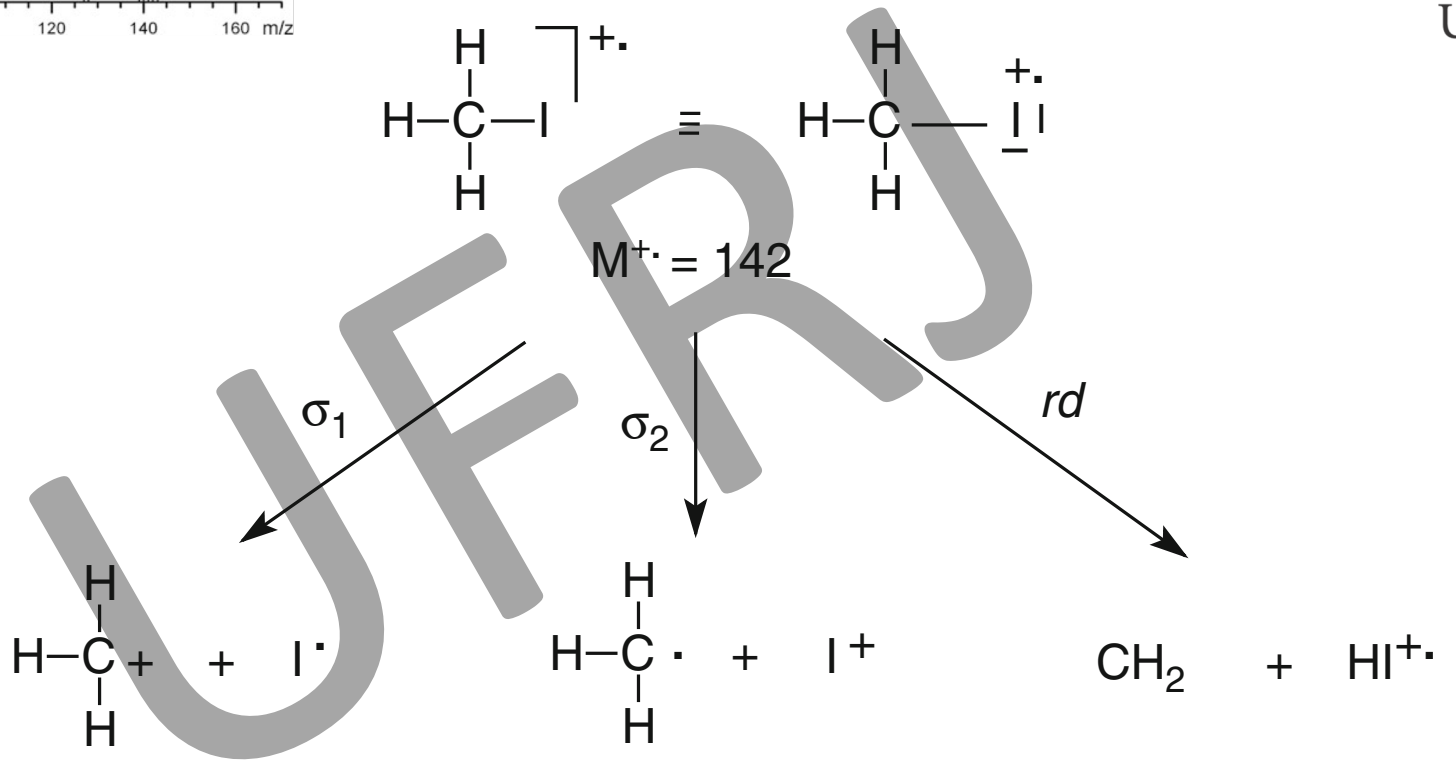
Iodine fission-produced isotopes not discussed above (iodine-128, iodine-130, iodine-132, and iodine-133) have a half lives of a couple of hours or minutes,





Exercícios

UFRJ



Regra de Stevenson

Quando a fragmentação acontece, a carga positiva tende a ficar sobre o fragmento com menor energia de ionização.

UFRJ

É mais fácil manter a carga positiva distribuída em cadeias mais substituídas, mais ramificadas.

Compare para a acetona
Melhor formar $CH_3C{=}O^+$

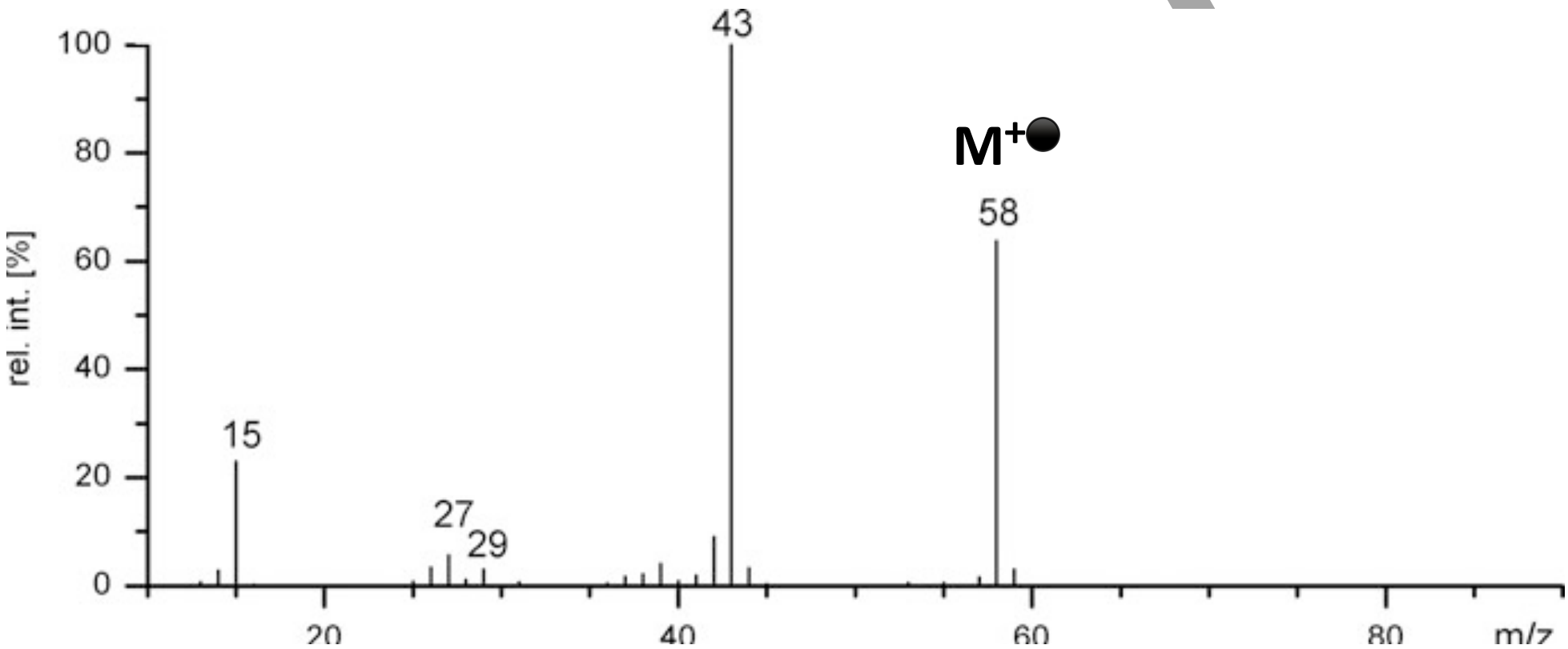
Energias de ionização

Radical	IE^b [eV]	Radical	IE^b [eV]
$H^\bullet$	13.6	$CH_3O^\bullet$	10.7
$^\bullet CH_3$	9.8	$^\bullet CH_2OH$	7.6
$^\bullet C_2H_5$	8.4	$CH_3C^\bullet{=}O$	7.0
n-$^\bullet C_3H_7$	8.2	$C_2H_5C^\bullet{=}O$	5.7
i-$^\bullet C_3H_7$	7.6	$^\bullet CH_2Cl$	8.8
n-$^\bullet C_4H_9$	8.0	$^\bullet CCl_3$	8.1
i-$^\bullet C_4H_9$	7.9	$C_6H_5^\bullet$	8.3
s-$^\bullet C_4H_9$	7.3	$C_6H_5CH_2^\bullet$	7.2
t-$^\bullet C_4H_9$	6.8	$^\bullet CH_2NH_2$	6.3

Exercícios

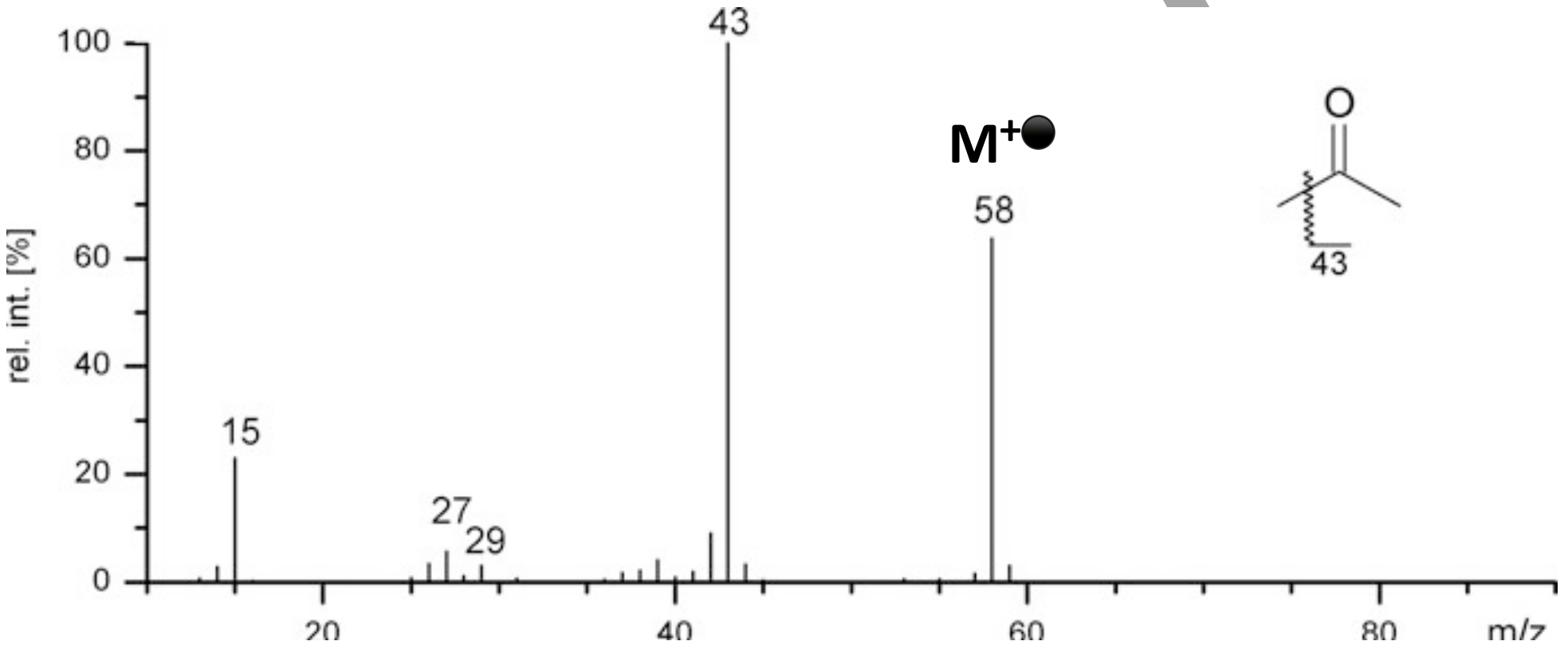
UFRJ

Acetona

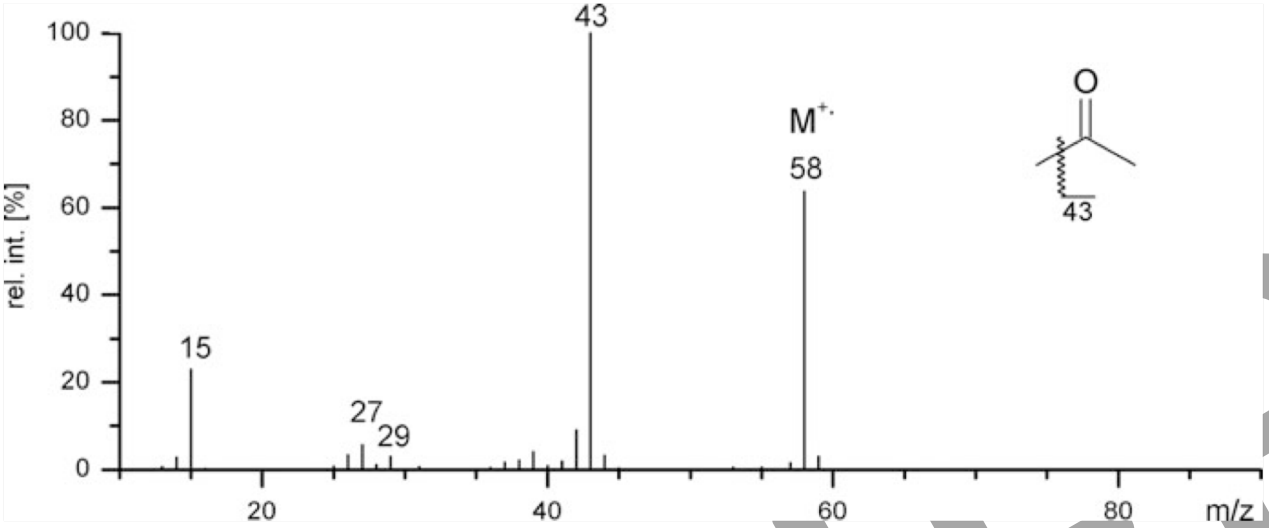


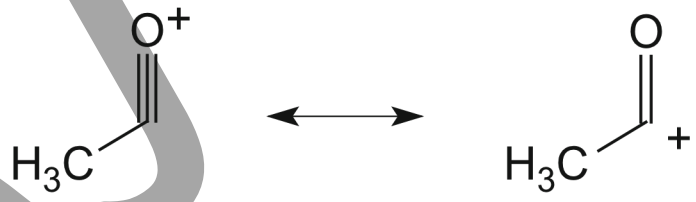
Exercícios

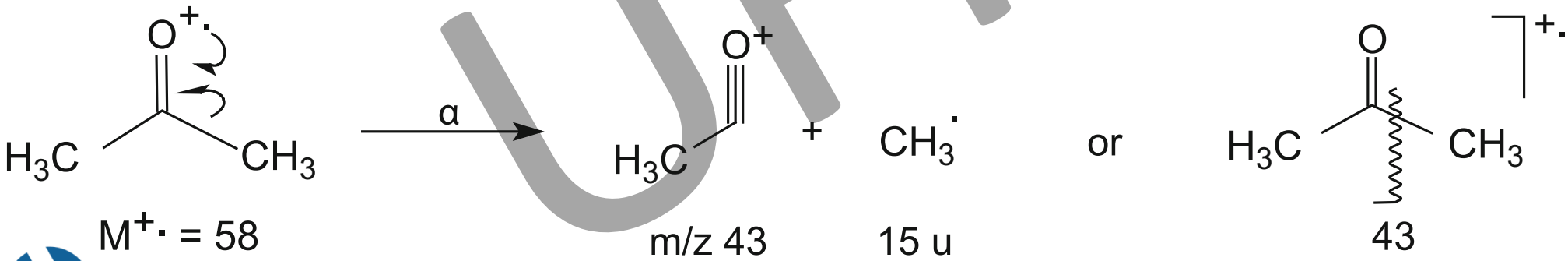
UFRJ



Exercícios (α-clivagem)







$M^{+\cdot}$ = 58

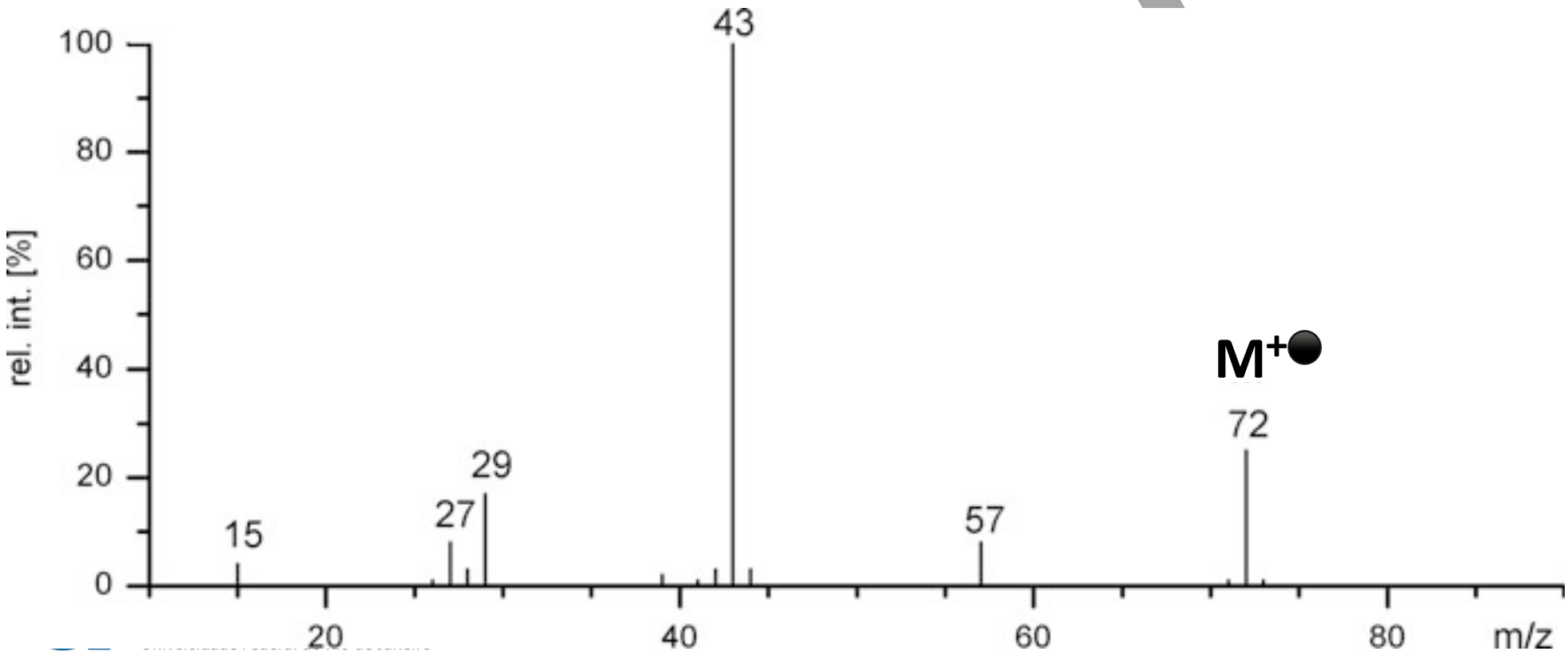
m/z 43

15 u

43

Exercícios

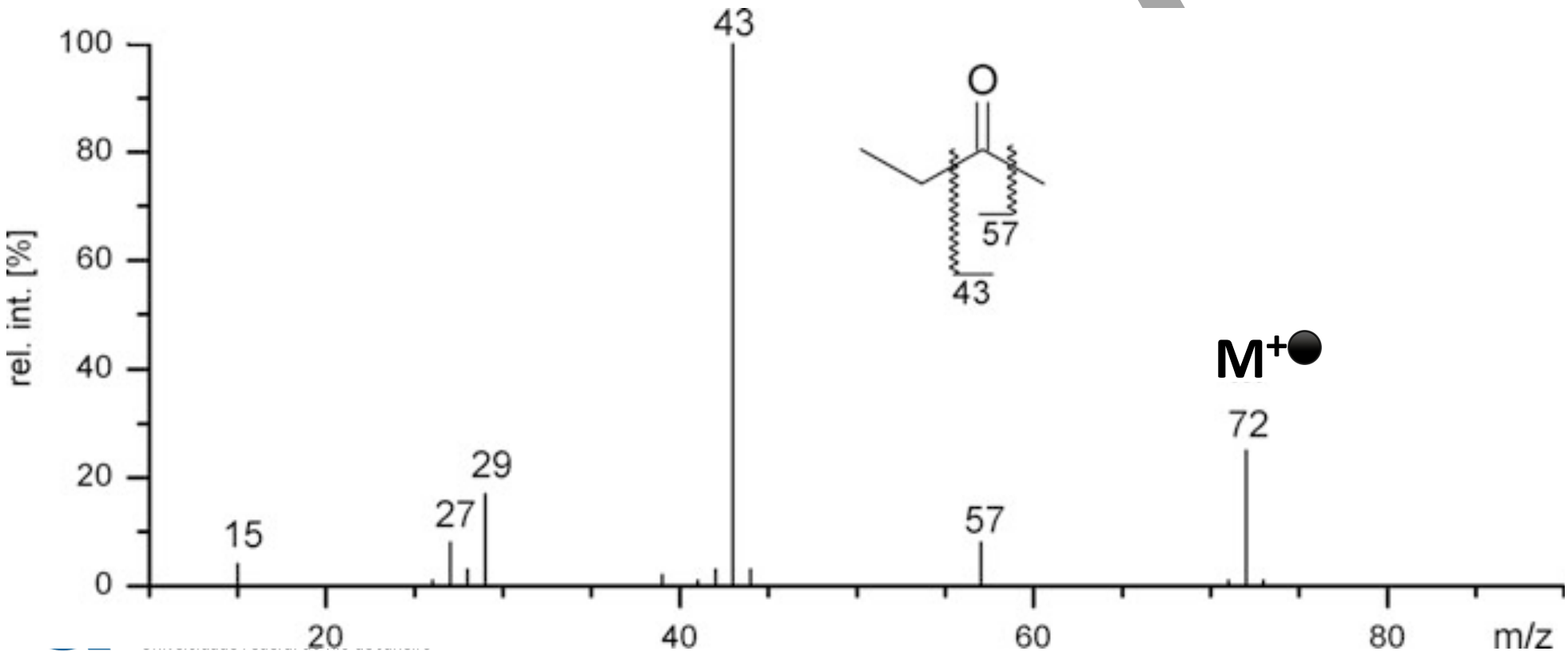
UFRJ



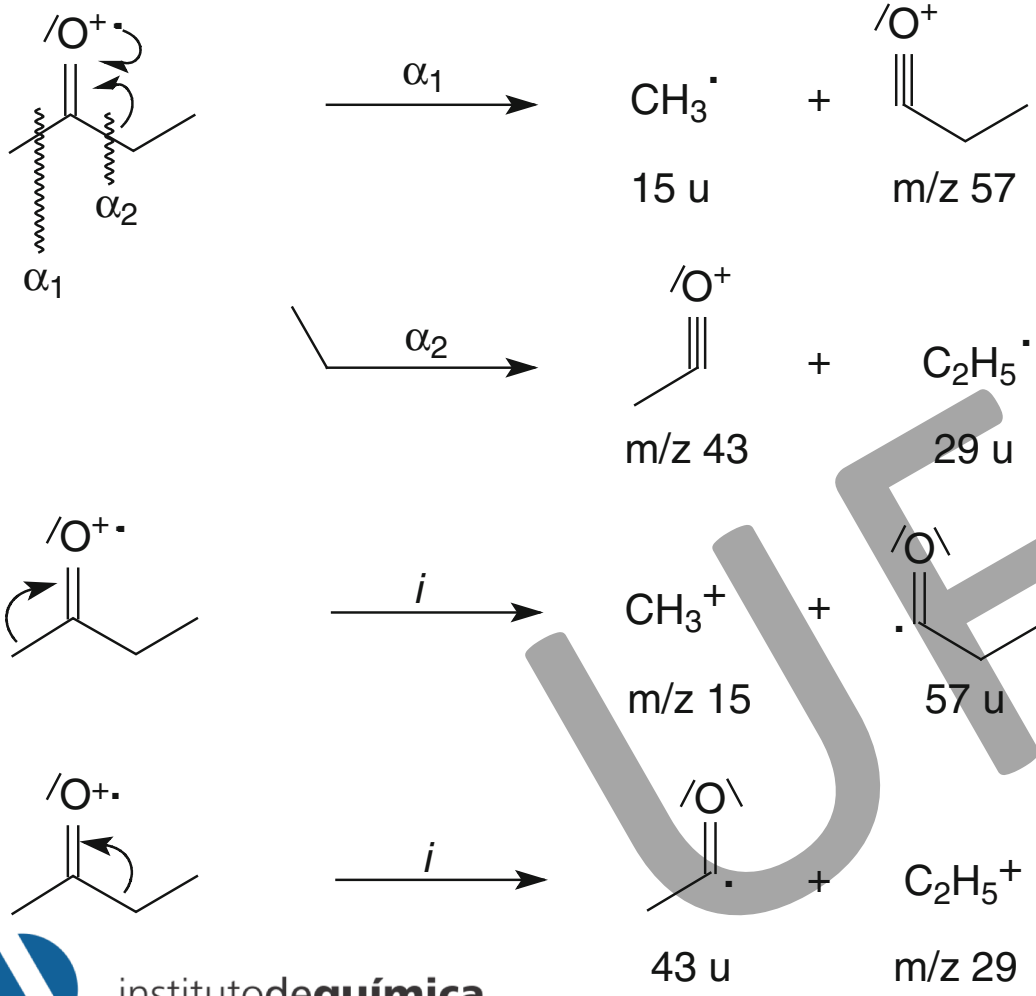
Exercícios

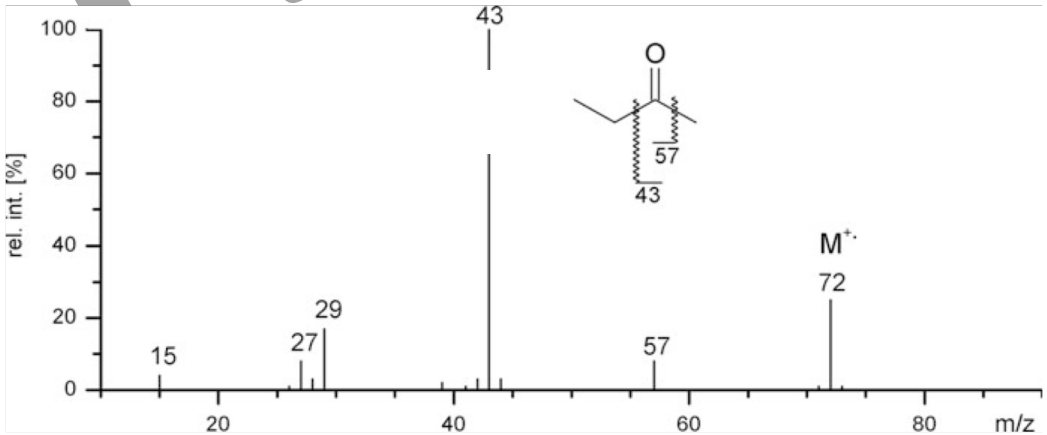
UFRJ

butanona



Exercícios

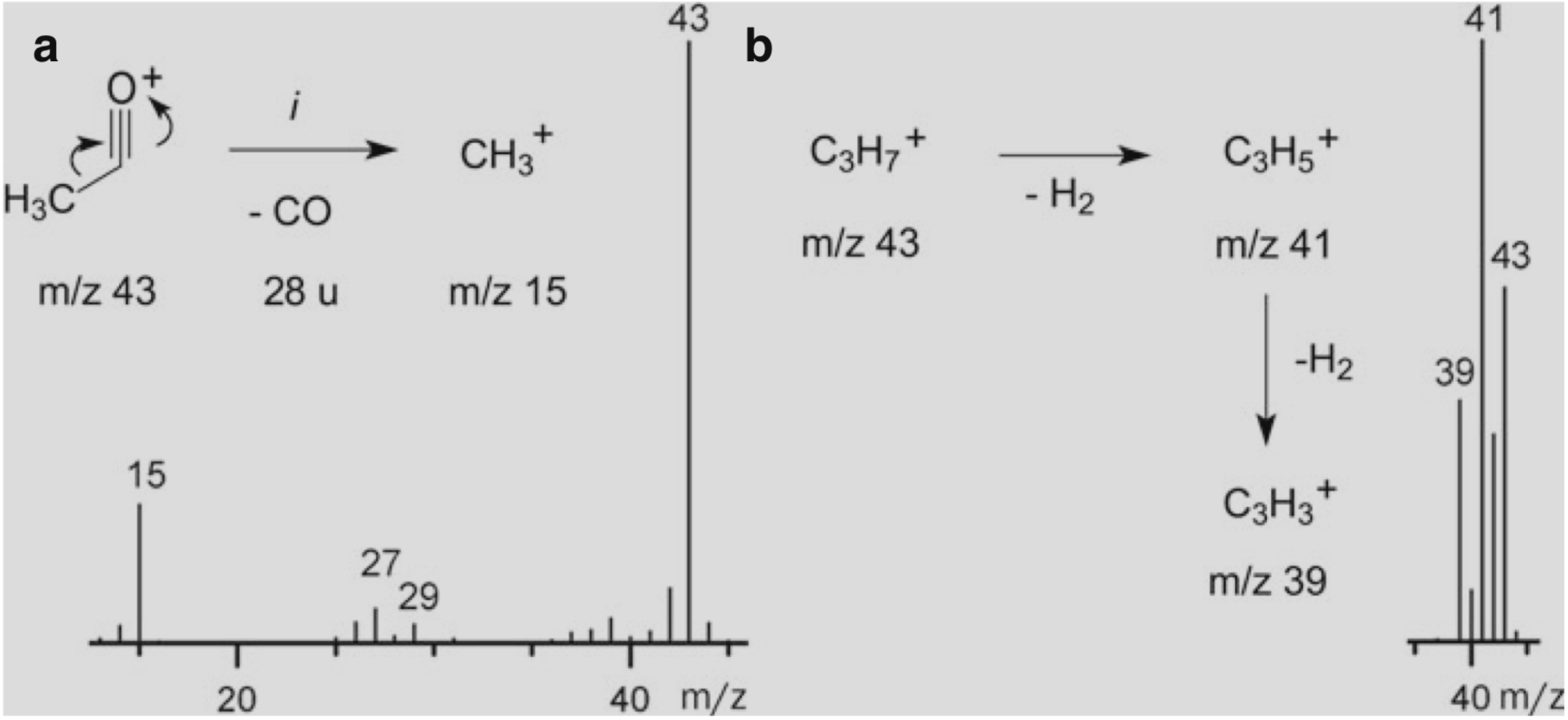




UFRJ

Exercícios

UFRJ



Exercícios – Complete a tabela

Number of nitrogens	Examples	$M^{+\bullet}$ at *m*/*z*
	methane, CH_4	
	acetone, C_3H_6O	
	chloroform, $CHCl_3$	
	[60]fullerene, C_{60}	
	ammonia, NH_3	
	acetonitrile, C_2H_3N	
	pyridine, C_5H_5N	
	N-ethyl-*N*-methyl-propanamine, $C_6H_{15}N$	
	urea, CH_4N_2O	
	pyridazine, $C_4H_4N_2$	
	triazole, $C_2H_3N_3$	
	hexamethylphosphoric triamide, HMPTA, $C_6H_{18}N_3OP$	

UFRJ

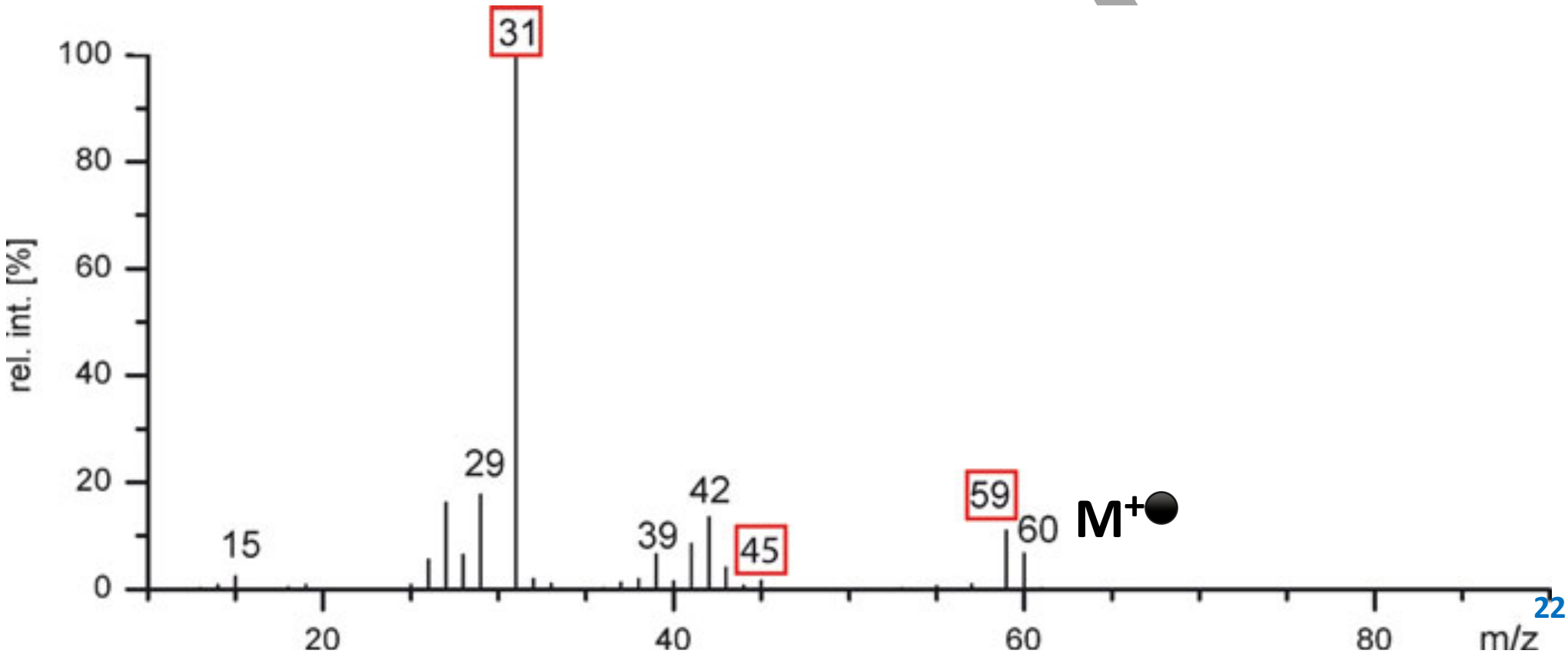
Exercícios – Complete a tabela

Number of nitrogens	Examples	$M^{+\bullet}$ at *m*/*z*
0	methane, CH_4	16
0	acetone, C_3H_6O	58
0	chloroform, $CHCl_3$	118
0	[60]fullerene, C_{60}	720
1	ammonia, NH_3	17
1	acetonitrile, C_2H_3N	41
1	pyridine, C_5H_5N	79
1	*N*-ethyl-*N*-methyl-propanamine, $C_6H_{15}N$	101
2	urea, CH_4N_2O	60
2	pyridazine, $C_4H_4N_2$	80
3	triazole, $C_2H_3N_3$	69
3	hexamethylphosphoric triamide, HMPTA, $C_6H_{18}N_3OP$	179

Exercícios

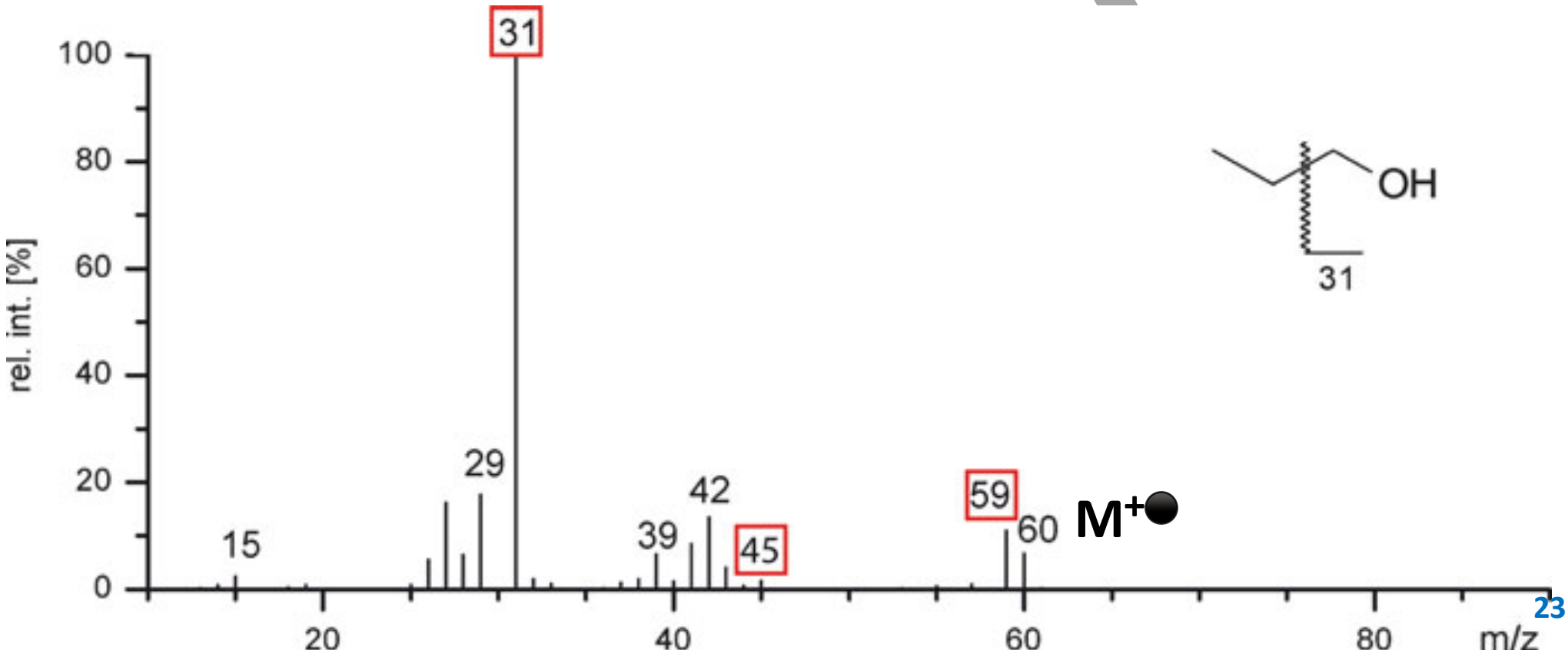
UFRJ

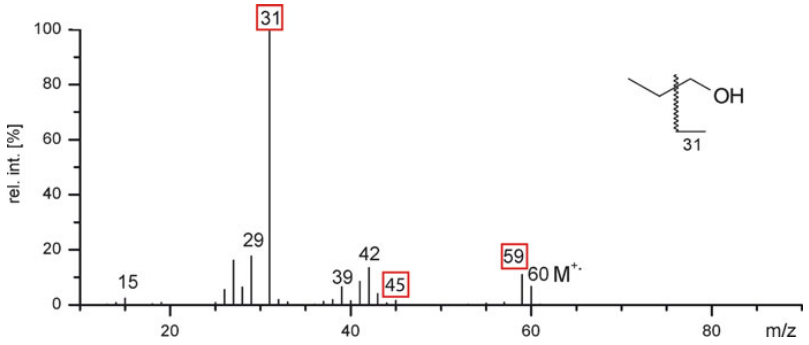
propanol



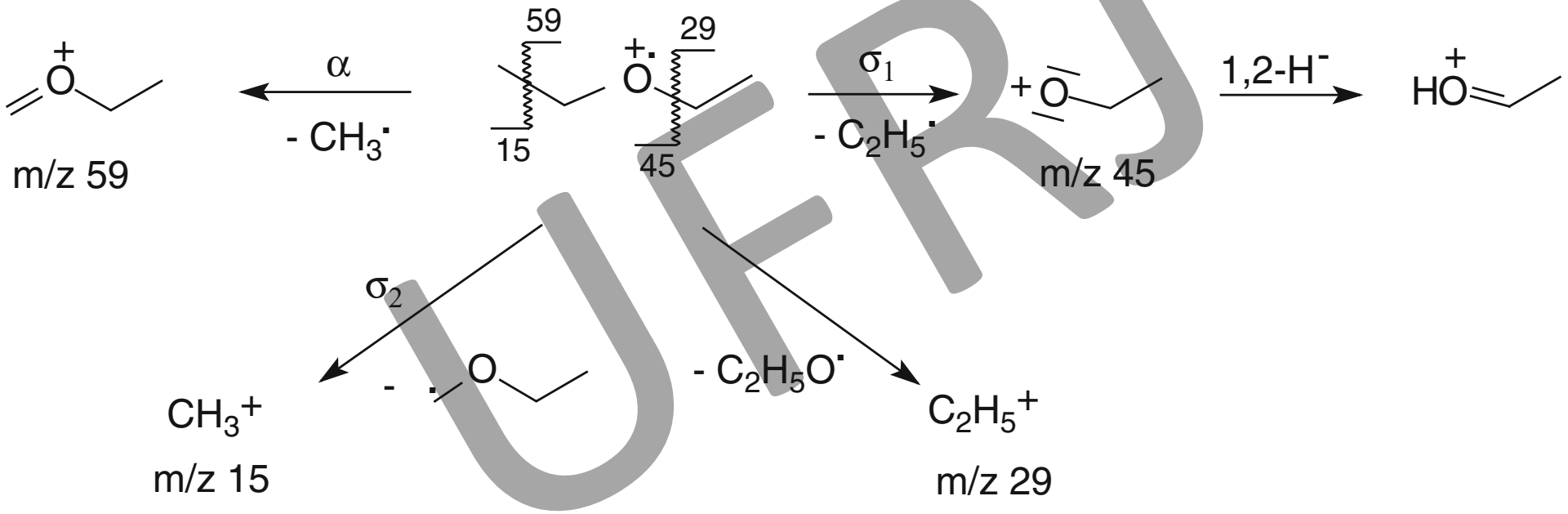
Exercícios

UFRJ





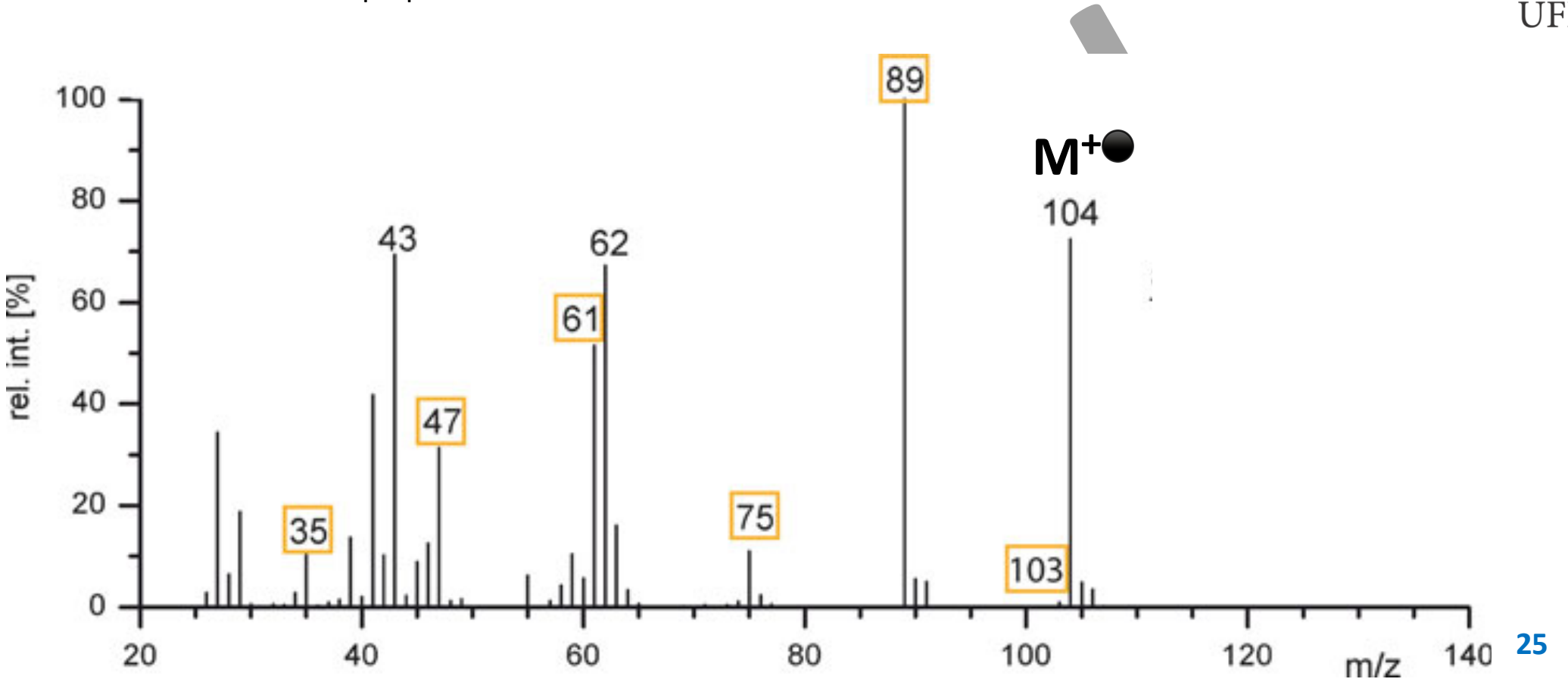
Exercícios



Exercícios

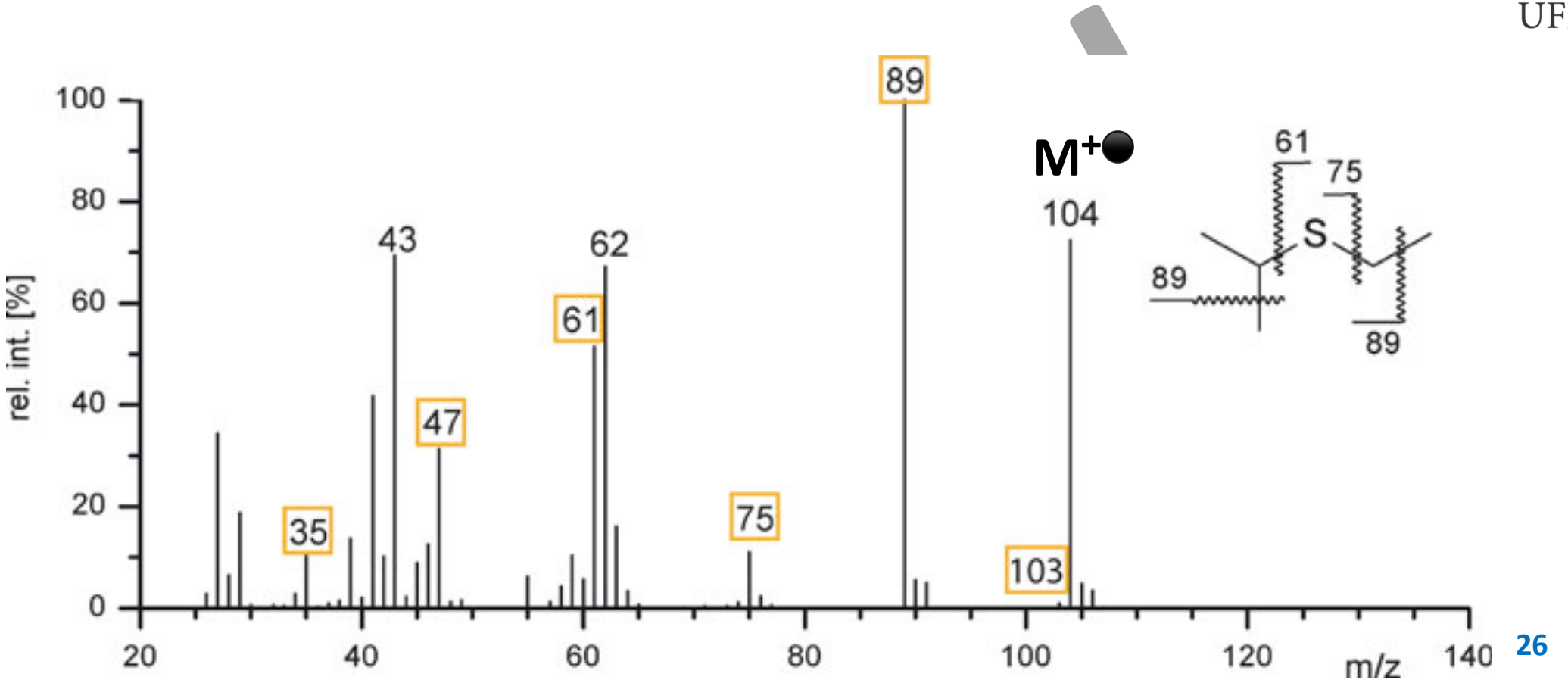
UFRJ

etilisopropileter

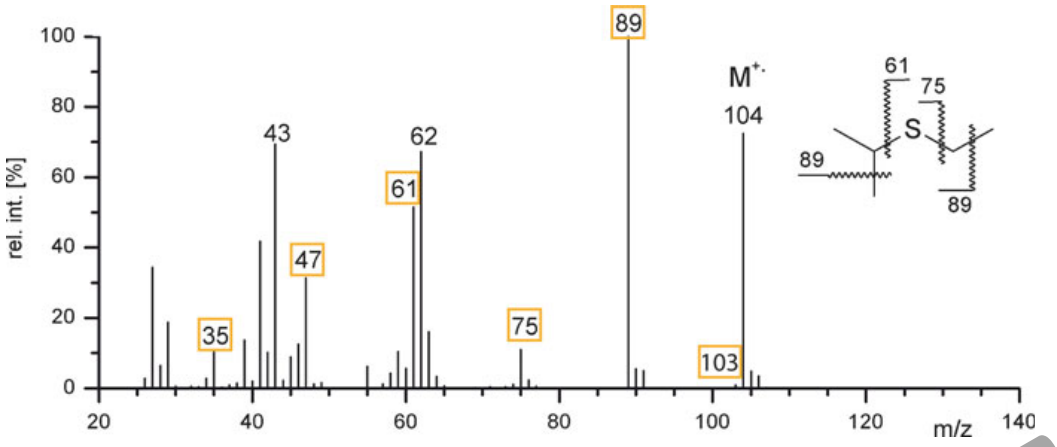


Exercícios

UFRJ



Exercícios

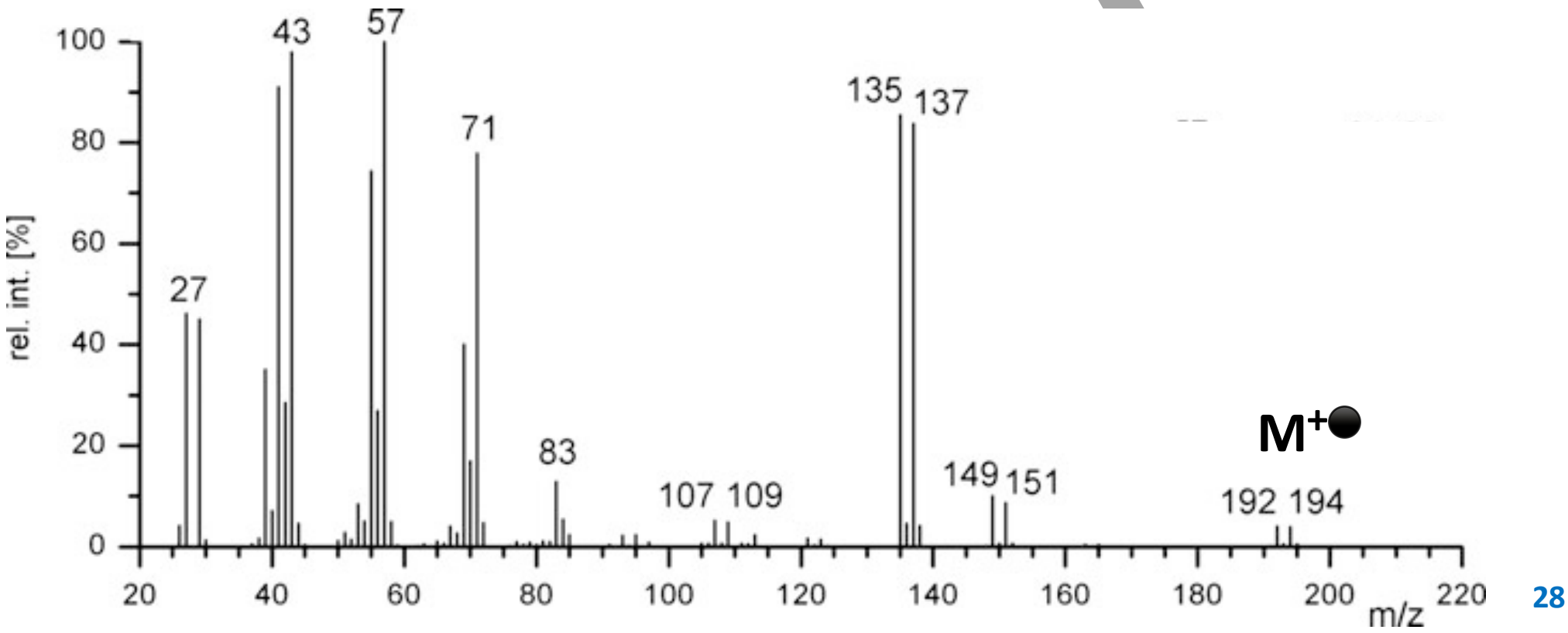


m/*z* (33 + 14*n*)	Sulfonium ions $[C_nH_{2n+1}S]^+$	Accurate mass [u][a]
47	CH_3S^+	46.9950
61	$C_2H_5S^+$	61.0106
75	$C_3H_7S^+$	75.0263
89	$C_4H_9S^+$	89.0419
103	$C_5H_{11}S^+$	103.0576
117	$C_6H_{13}S^+$	117.0732
131	$C_7H_{15}S^+$	131.0889
145	$C_8H_{17}S^+$	145.1045

Exercícios

UFRJ

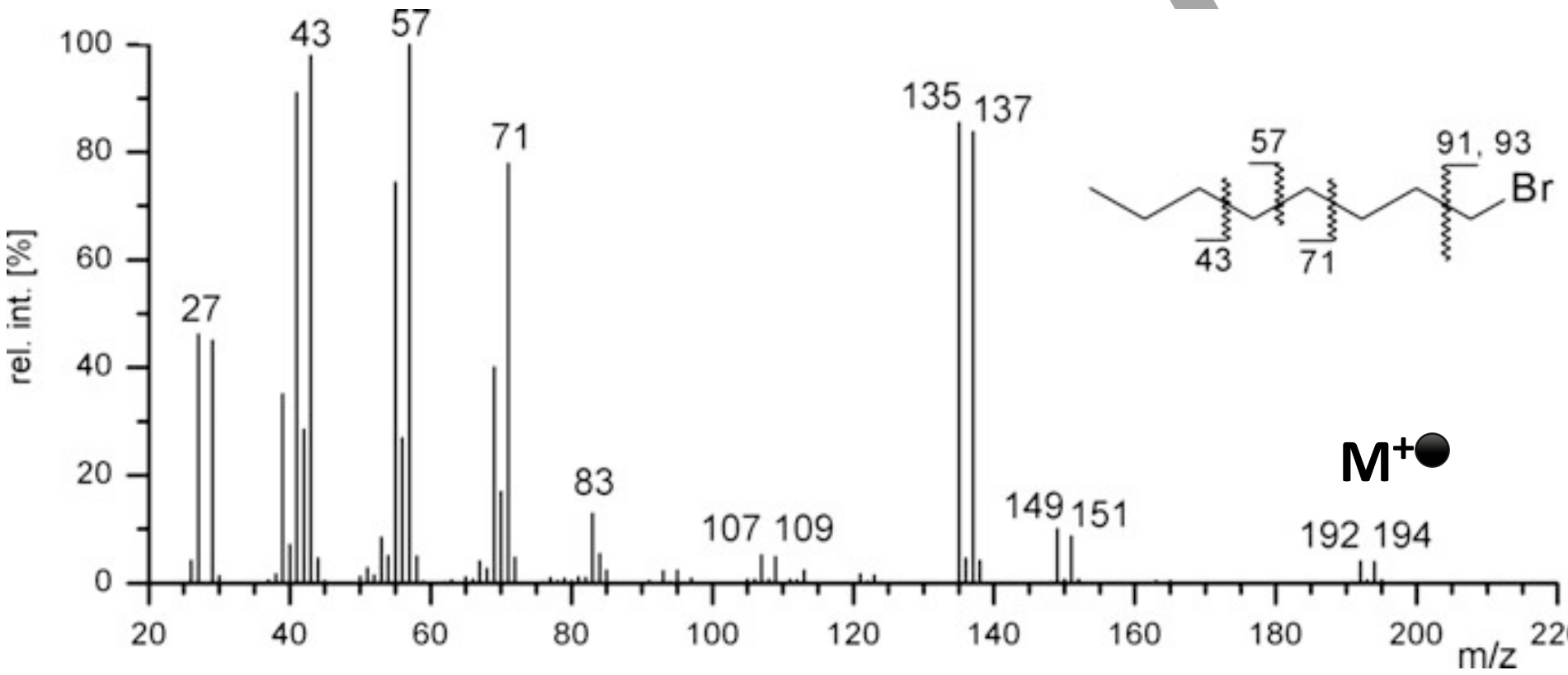
1-bromooctano



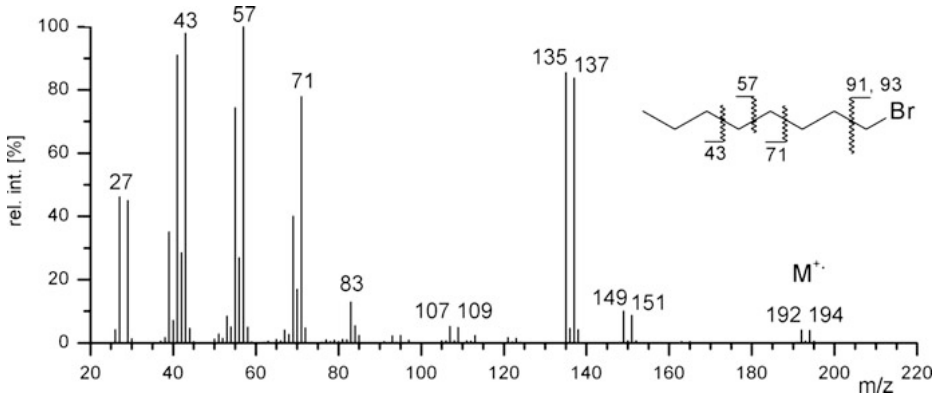
Exercícios

UFRJ

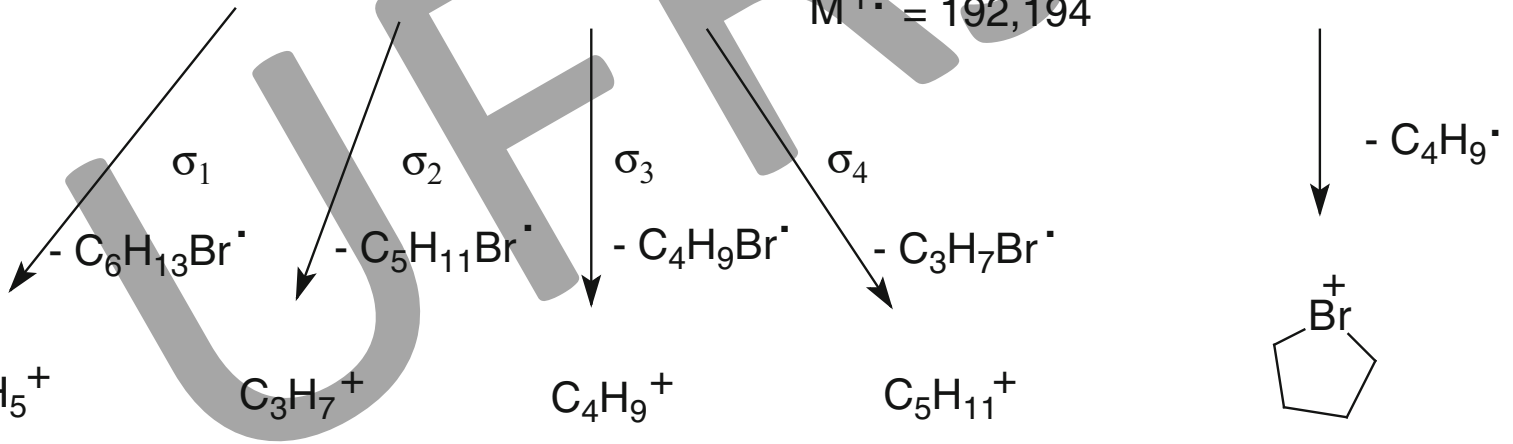
1-bromooctano



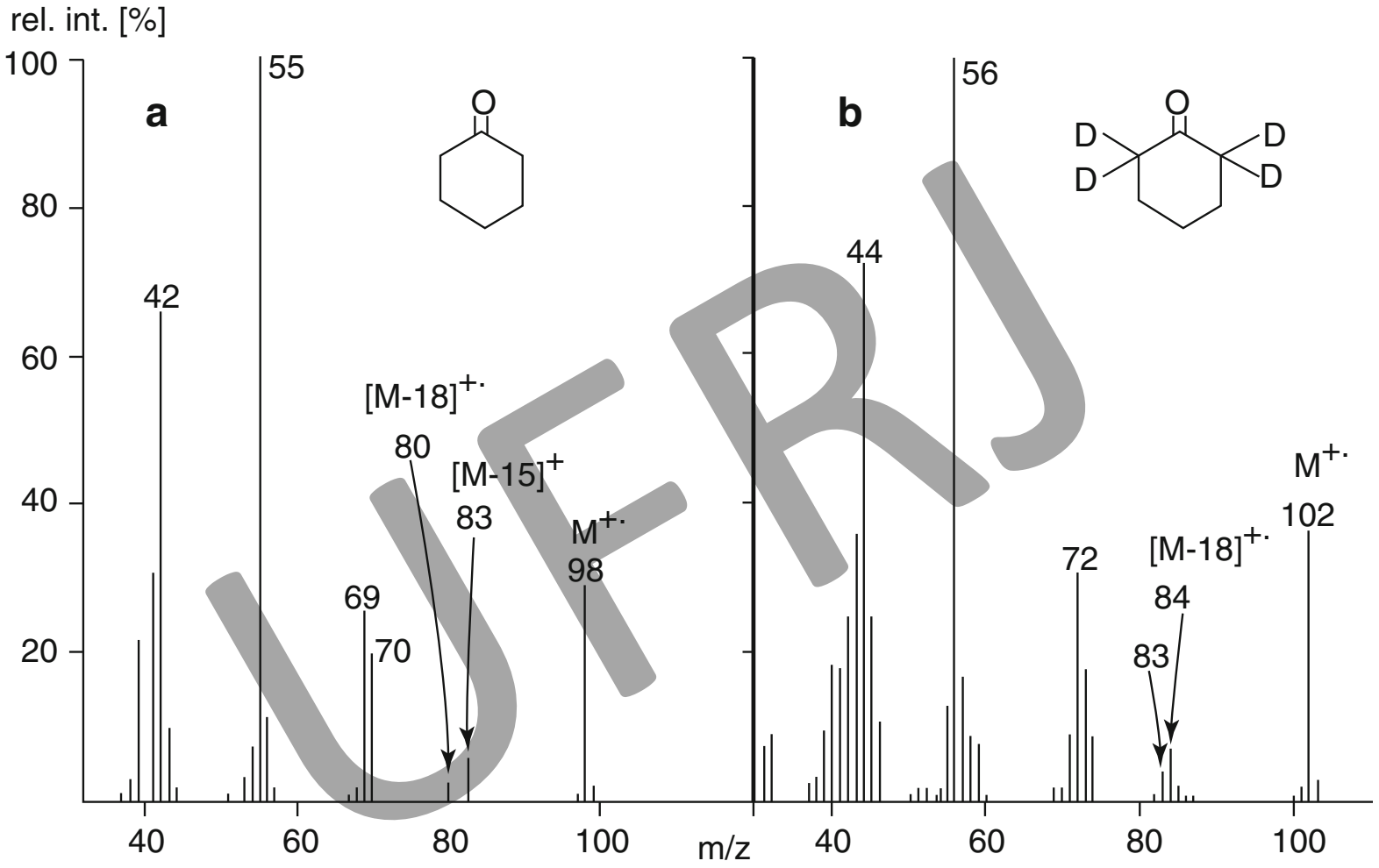
Exercícios



$M^{+\cdot}$ = 192,194

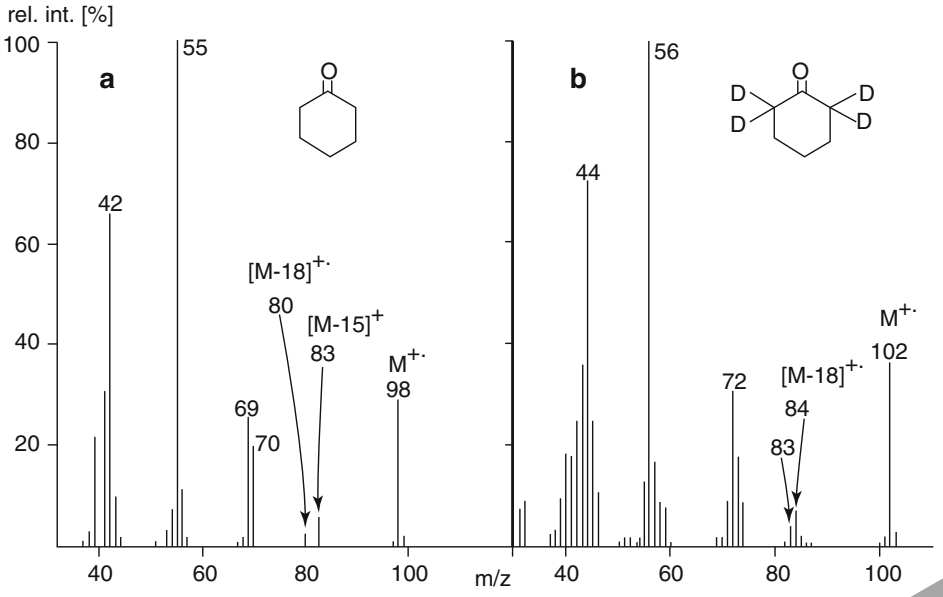


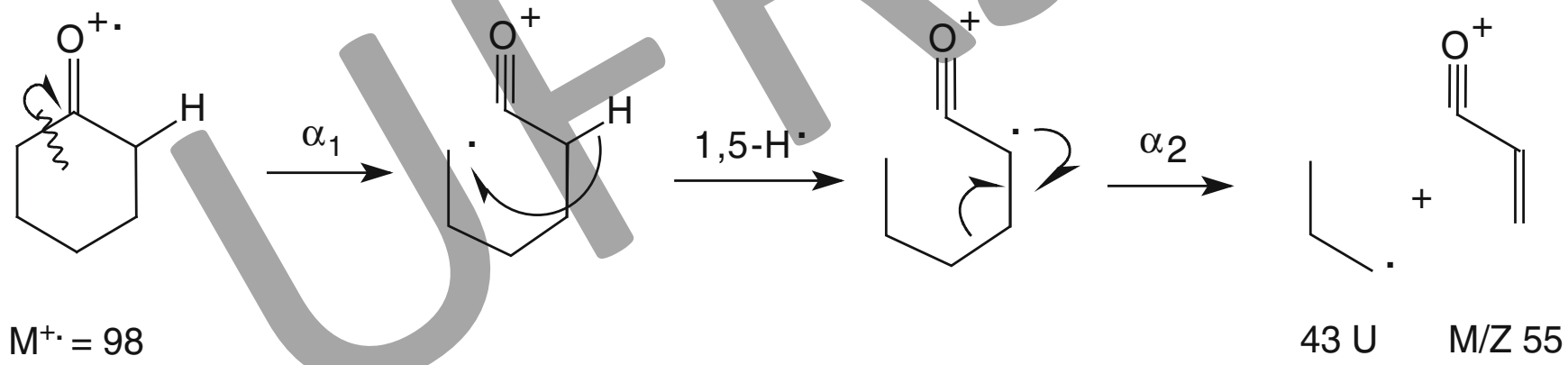
Exercícios



Proponha o mecanismo de fragmentação, explique o pico 56

Exercícios



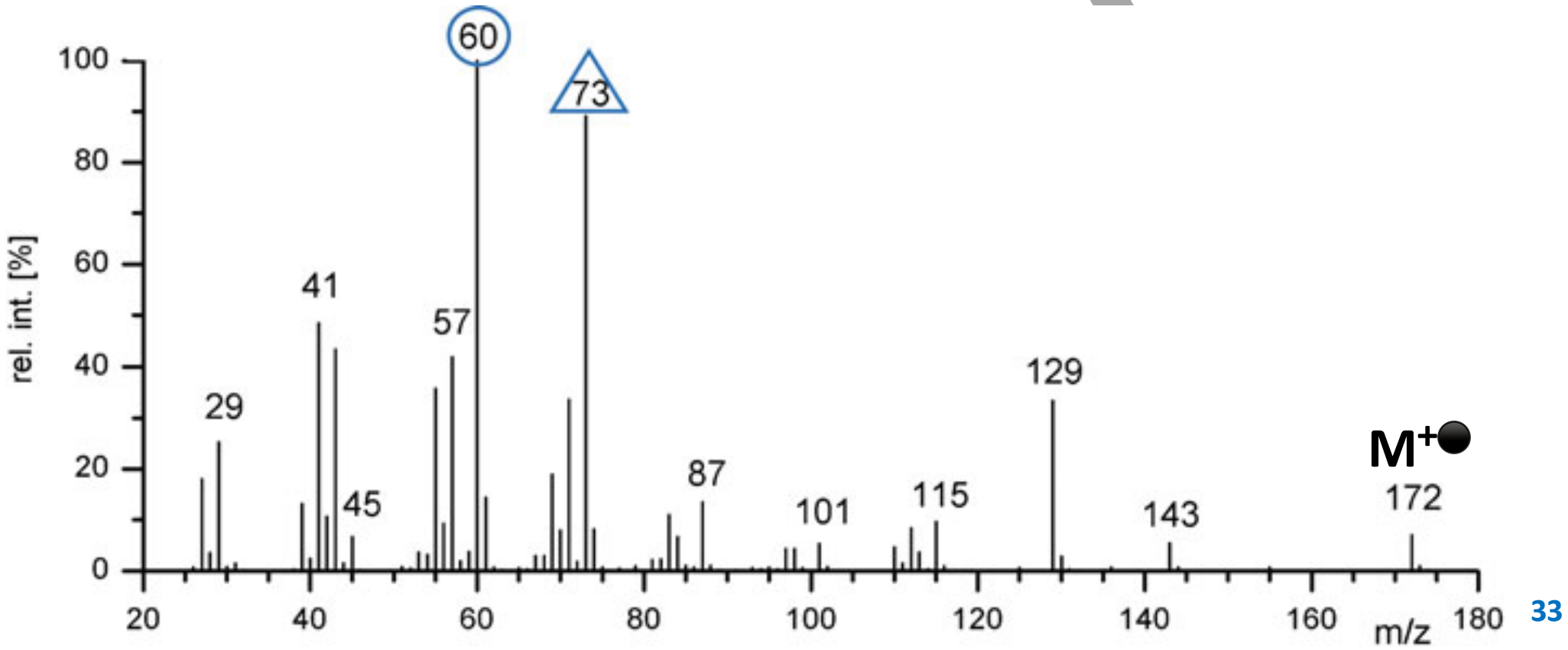


Proponha o mecanismo de fragmentação, explique o pico 56

Exercícios

UFRJ

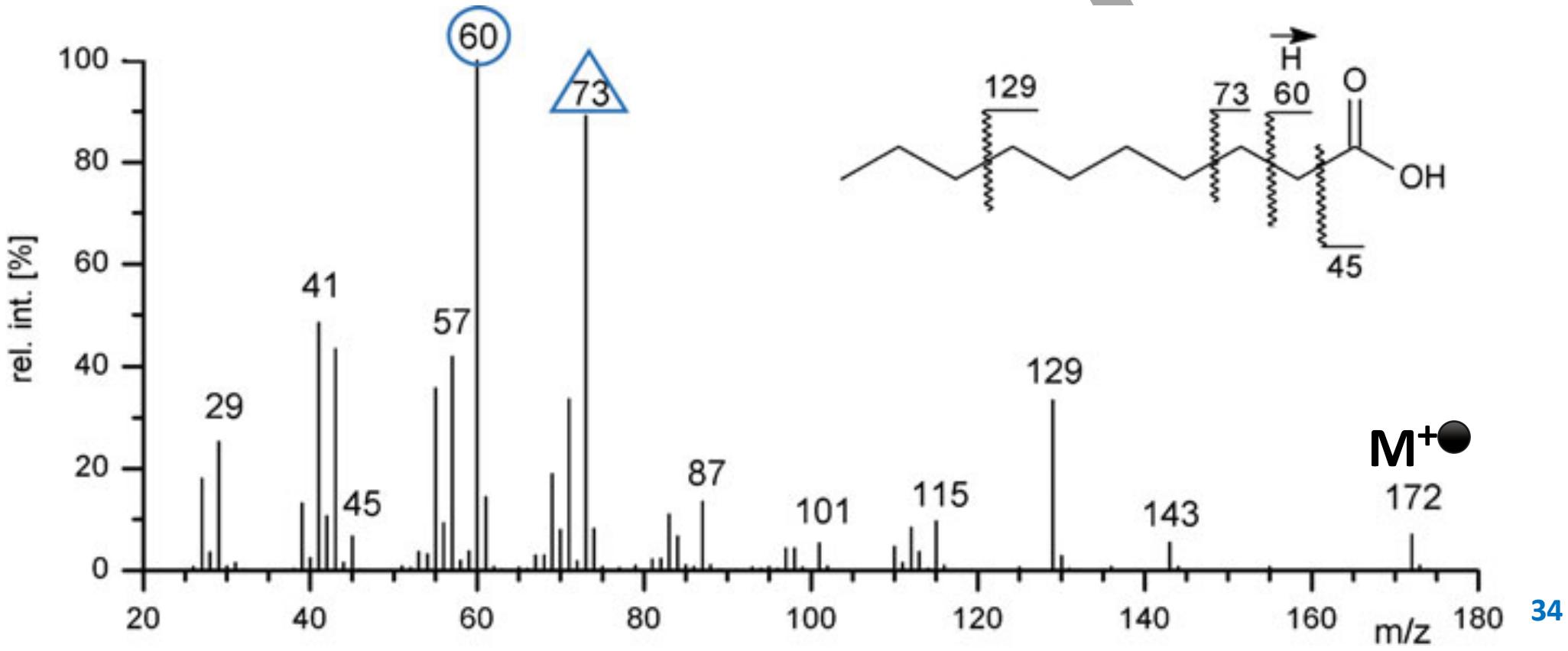
Acido decanóico



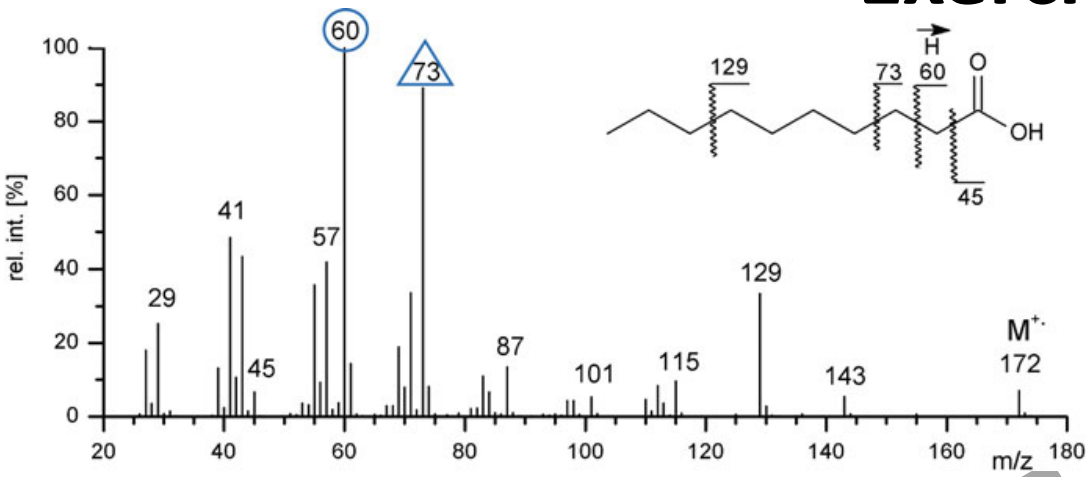
Exercícios

UFRJ

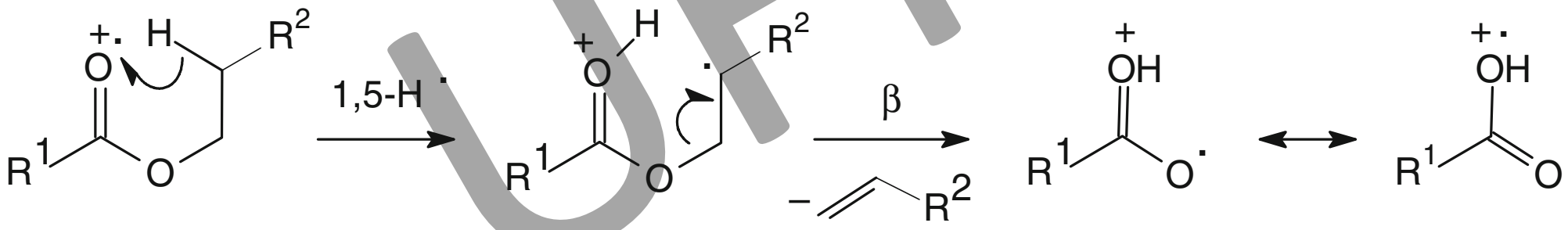
Acido decanóico



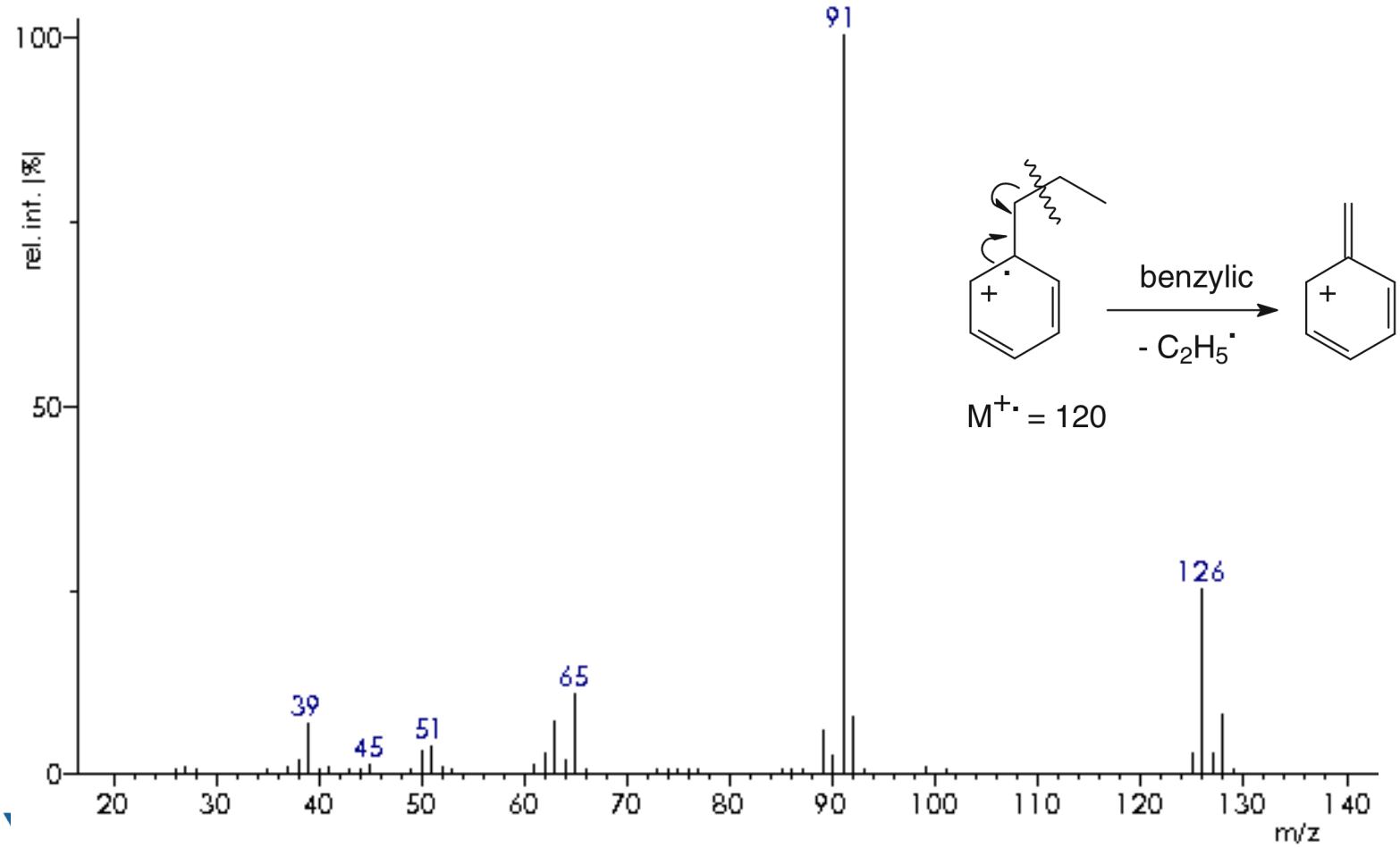
Exercícios

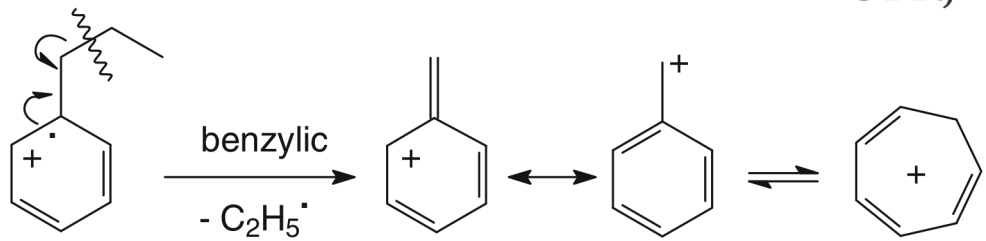


Acido decanóico



Exercícios



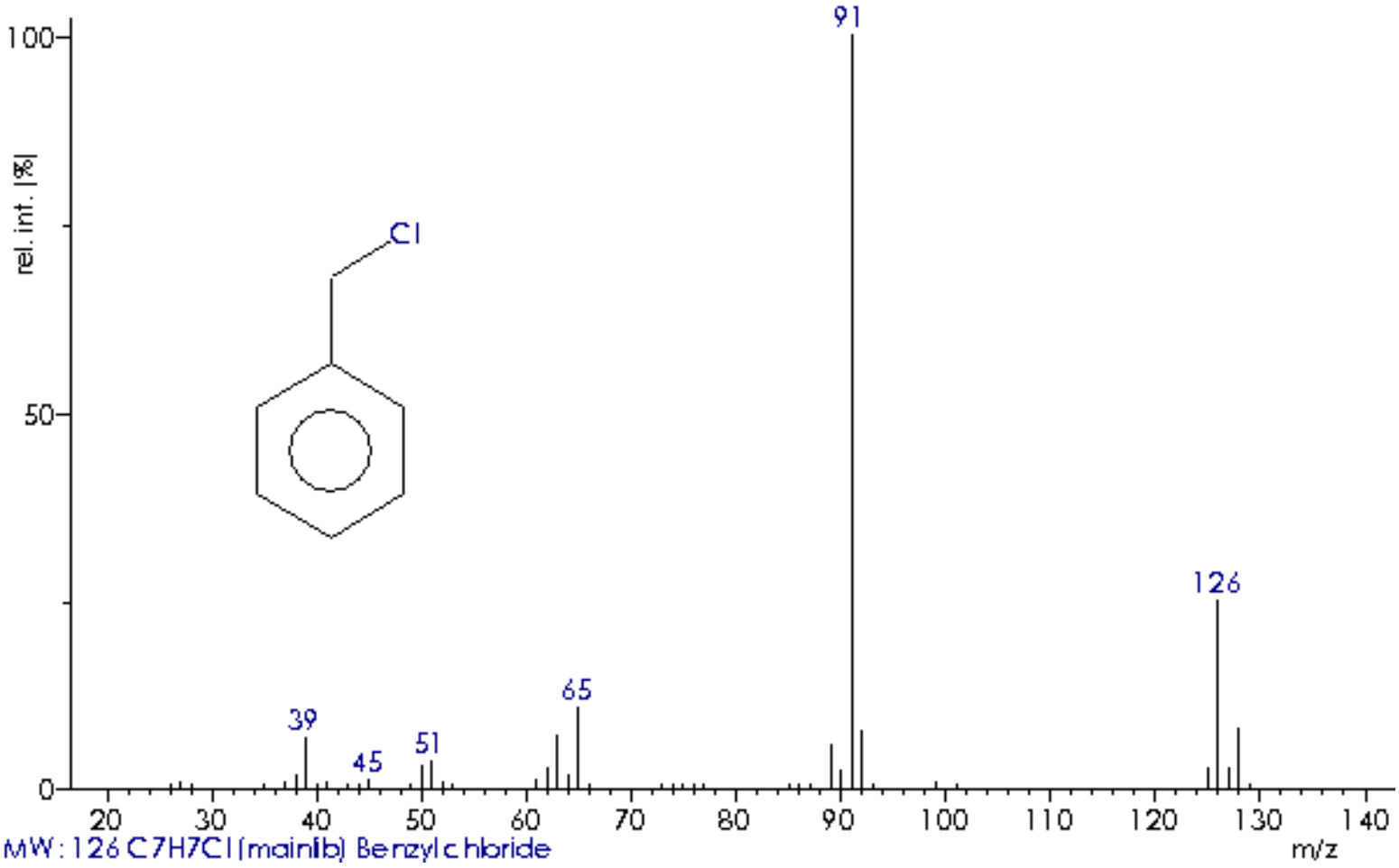


$M^{+\cdot}$ = 120

m/z 91

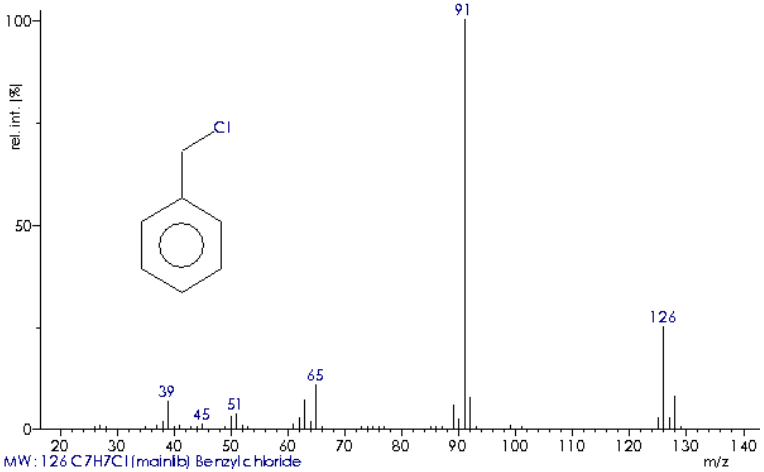
UFRJ

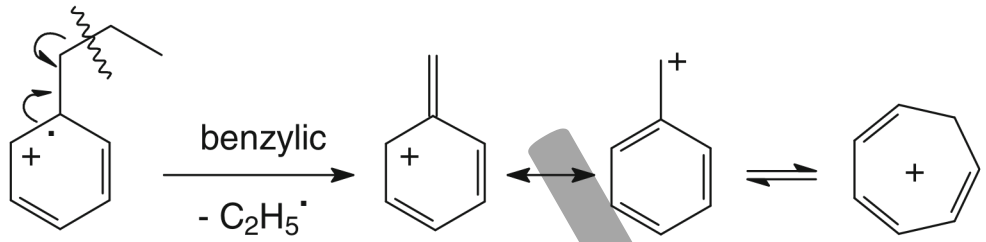
Exercícios



UFRJ

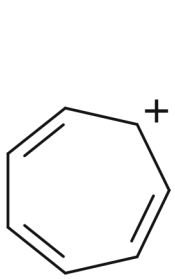
Exercícios

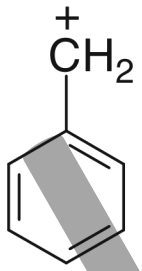


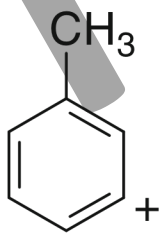


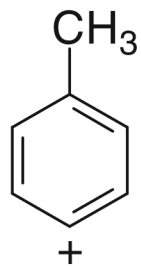
$M^{+\cdot}$ = 120

m/z 91



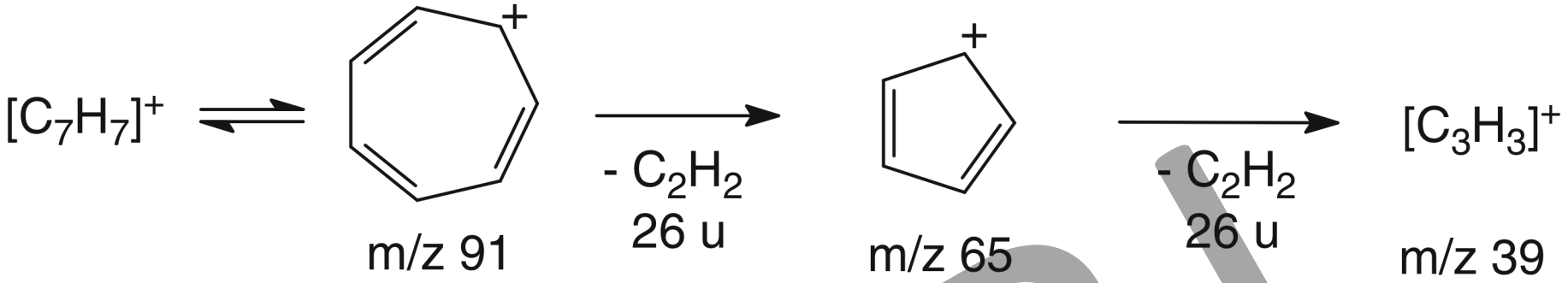


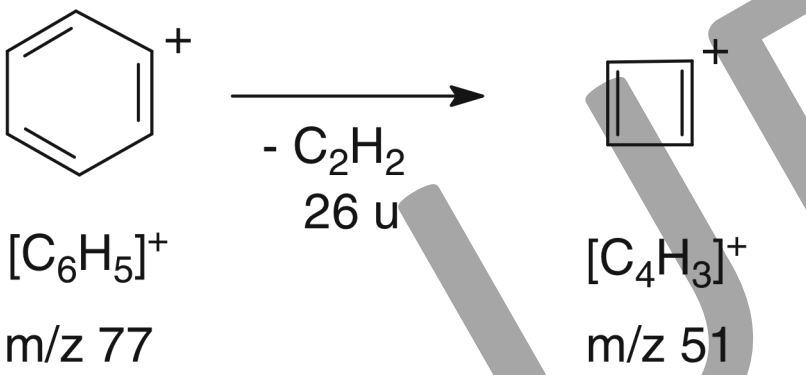


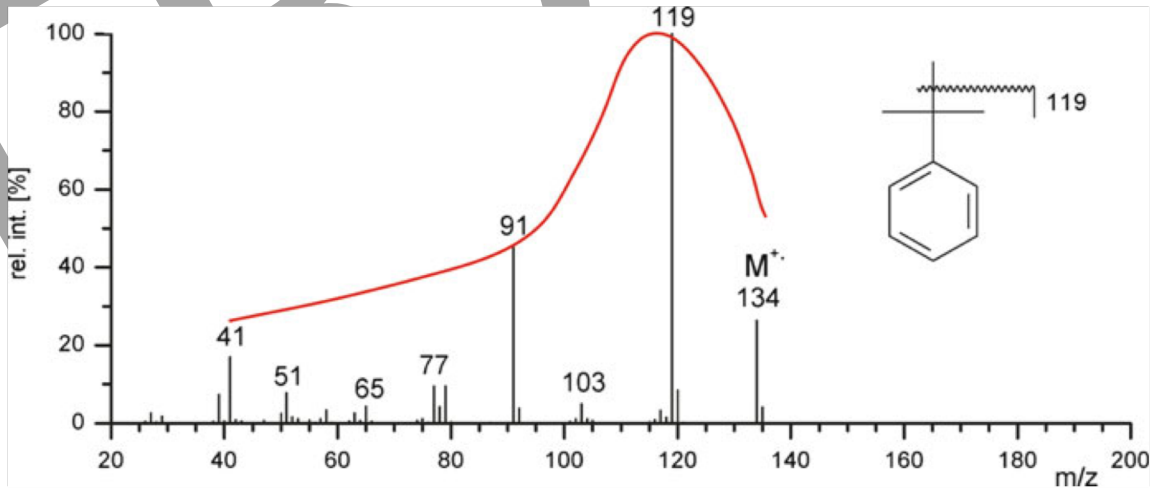


ΔH_f = 866 kJ mol^{-1} 887 kJ mol^{-1} 971 kJ mol^{-1} 987 kJ mol^{-1} 992 kJ mol^{-1}

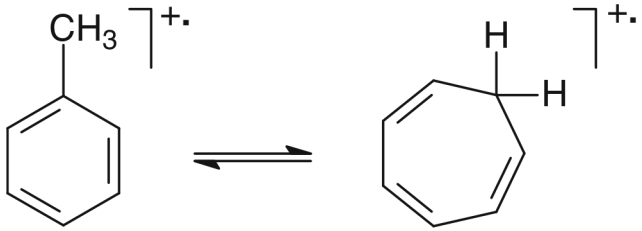
Exercícios



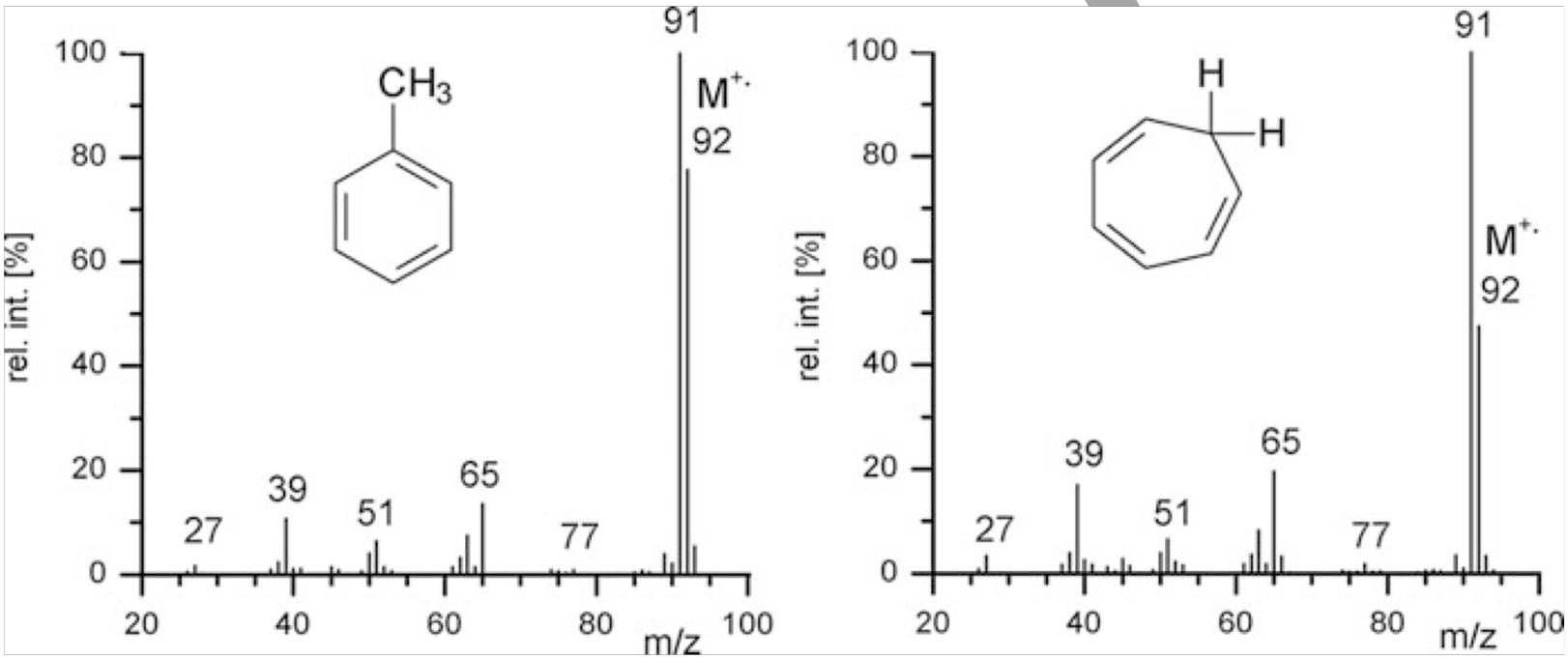




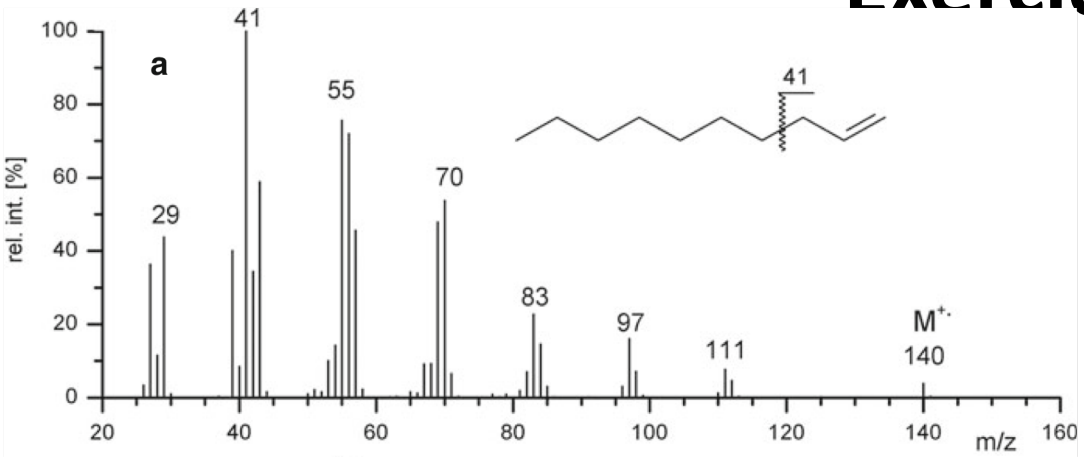
Exercícios

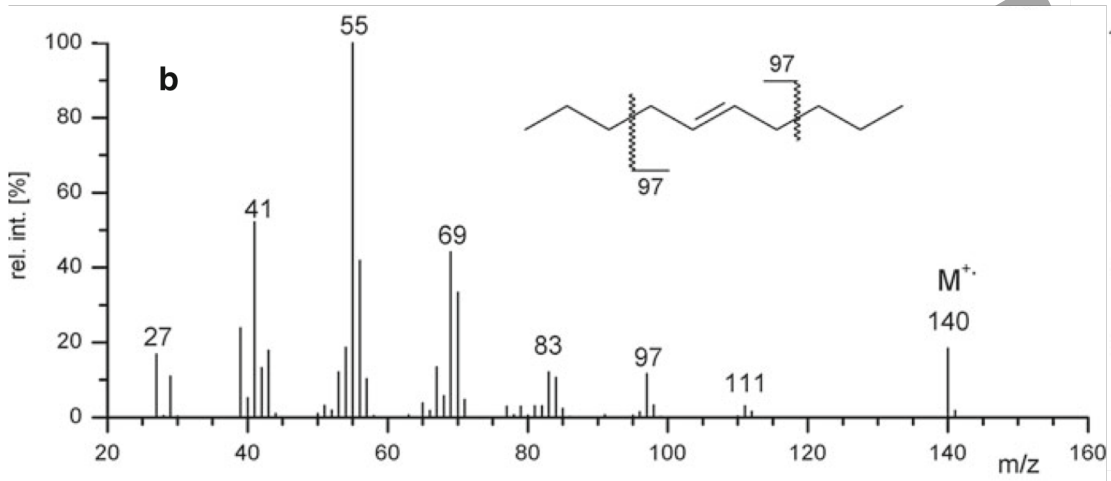


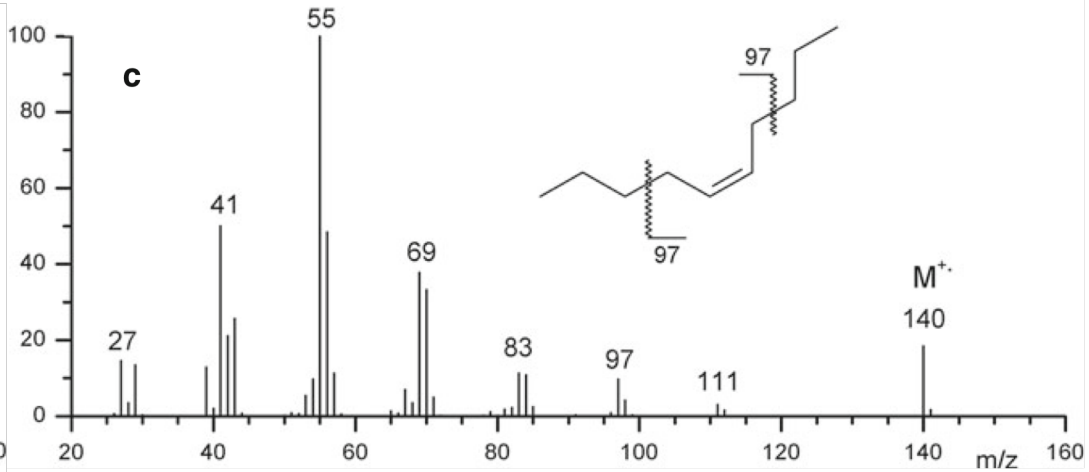
$[C_3H_8]^{+\cdot}$ m/z 92



Exercícios



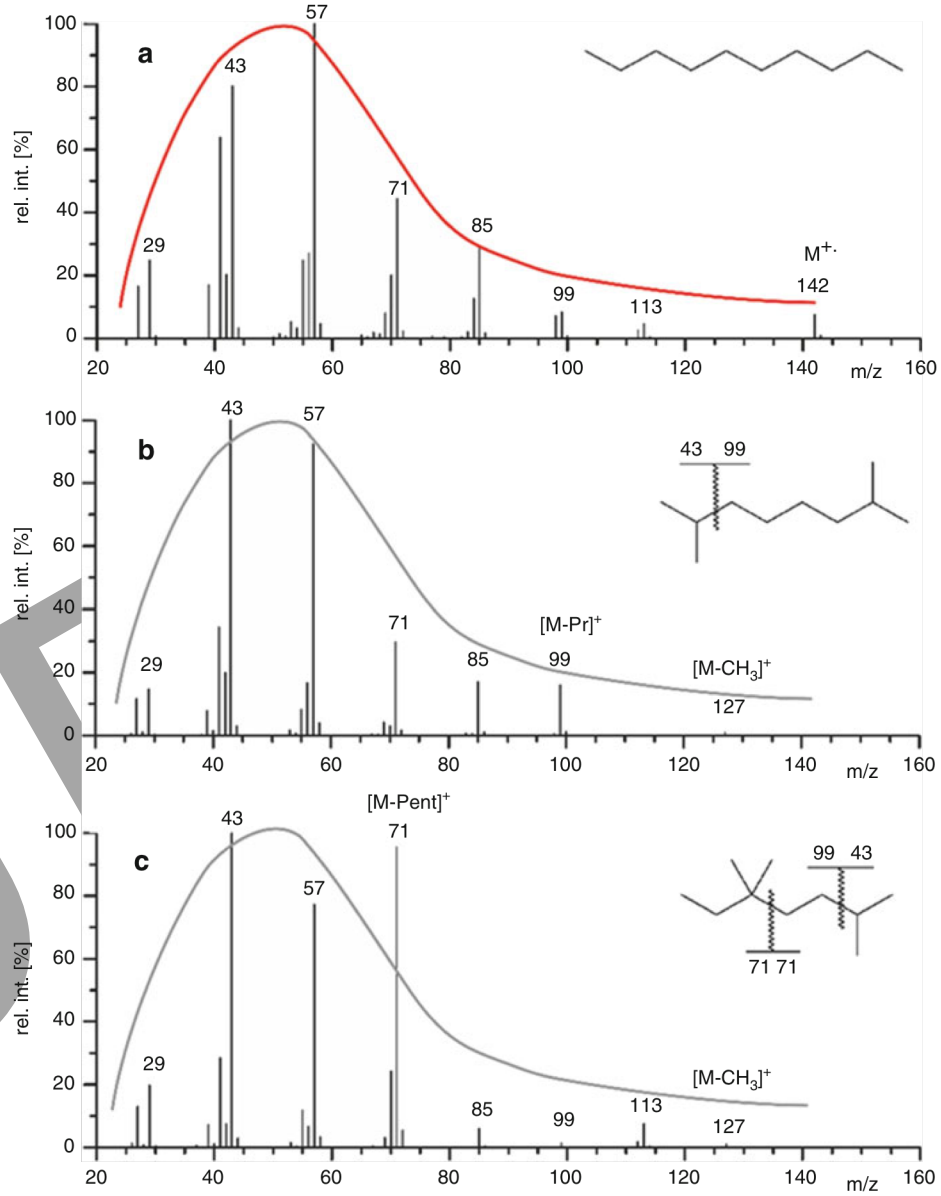




UFRJ

institutodequímica
Universidade Federal do Rio de Janeiro

Exercícios



UFRJ

institutodequímica
Universidade Federal do Rio de Janeiro

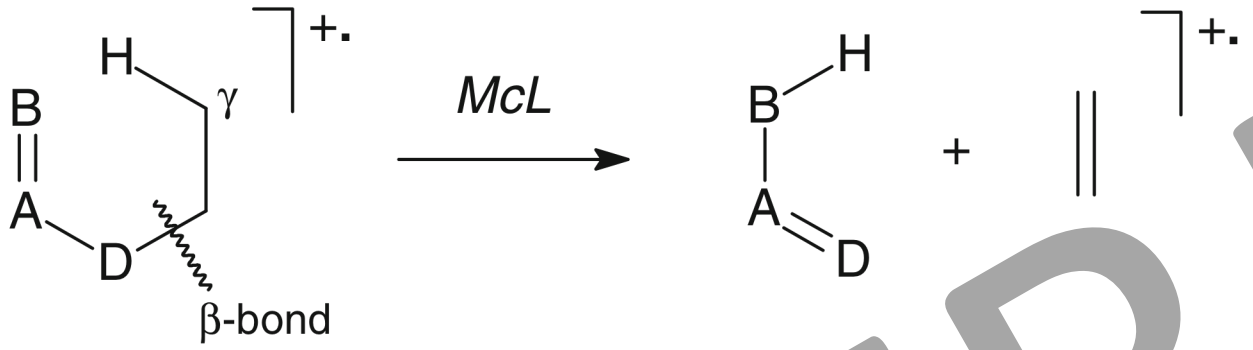
Exercícios

Table 6.11 Commonly observed neutral losses from molecular ions

$[M–X]^+$	Radicals	$[M–XY]^{+\bullet}$	Molecules
−1	$H^\bullet$	−2	H_2
−15	$CH_3^\bullet$	−4	$2 \times H_2$
−16	$NH_2^\bullet$, $O^\bullet$	−17	NH_3
−17	$OH^\bullet$	−18	H_2O
−19	$F^\bullet$	−20	HF
−29	$C_2H_5^\bullet$	−27	HCN
−31	$OCH_3^\bullet$	−28	CO, C_2H_4, (N_2)
−33	$SH^\bullet$	−30	$H_2C{=}O$, NO
−35	$Cl^\bullet$	−32	CH_3OH, H_2S, (O_2)
−43	$C_3H_7^\bullet$, $CH_3CO^\bullet$	−34	H_2S
−45	$OC_2H_5^\bullet$, $COOH^\bullet$	−36	HCl
−57	$C_4H_9^\bullet$	−42	C_3H_6, $H_2C{=}C{=}O$
−79	$Br^\bullet$	−44	CO_2
−91	$C_7H_7^\bullet$	−46	C_2H_5OH, NO_2
−127	$I^\bullet$	−60	CH_3COOH

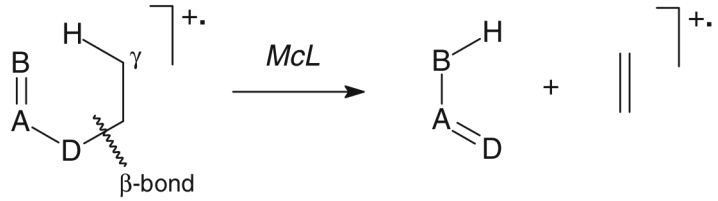
Exercícios

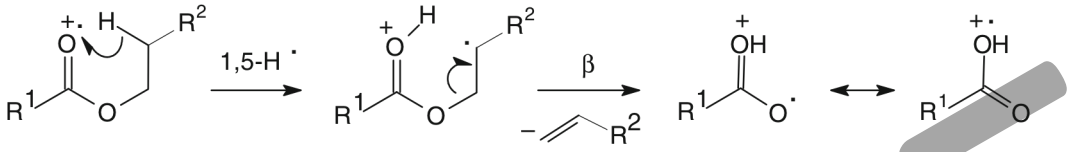
McLafferty rearrangement



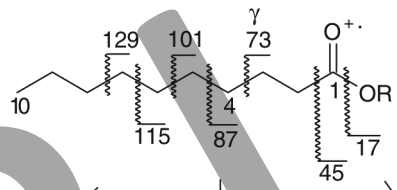
Exercícios

McLafferty rearrangement





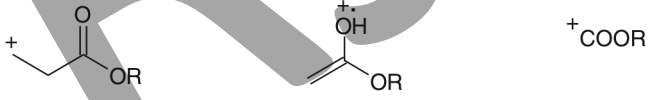
mass labels at structure are for the carboxylic acid only



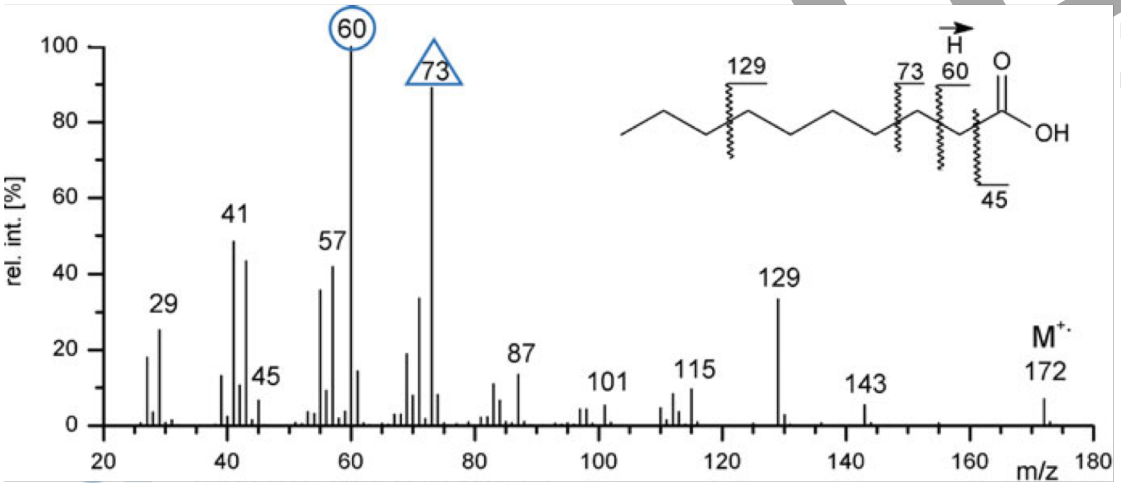
R = H [M-17]$^+$

R = Me [M-31]$^+$

R = Et [M-45]$^+$



H	m/z 73	m/z 60	m/z 45
Me	m/z 87	m/z 74	m/z 59
Et	m/z 101	m/z 88	m/z 73



Exercícios

UFRJ

Find the absorbance and transmittance of a 0.002 40 M solution of a substance with a molar absorptivity of 313 M^{-1} cm^{-1} in a cell with a 2.00-cm pathlength.

Ache a absorbância e a transmitância para uma solução 0,00240M e absortividade molar de 313M^{-1} cm^{-1} em uma célula de caminho ótico de 2cm

Exercícios

UFRJ

17-A. (a) What value of absorbance corresponds to 45.0% T?

(b) If a 0.010 0 M solution exhibits 45.0% T at some wavelength, what will be the percent transmittance for a 0.020 0 M solution of the same substance?

17-B. (a) A 3.96×10^{-4} M solution of compound A exhibited an absorbance of 0.624 at 238 nm in a 1.000-cm cuvet; a blank solution containing only solvent had an absorbance of 0.029 at the same wavelength. Find the molar absorptivity of compound A.

(b) The absorbance of an unknown solution of compound A in the same solvent and cuvet was 0.375 at 238 nm. Find the concentration of A in the unknown.

(c) A concentrated solution of compound A in the same solvent was diluted from an initial volume of 2.00 mL to a final volume of 25.00 mL and then had an absorbance of 0.733. What is the concentration of A in the concentrated solution?

Exercícios

17-1. Fill in the blanks.

(a) If you double the frequency of electromagnetic radiation, you _____ the energy.

(b) If you double the wavelength, you _____ the energy.

(c) If you double the wavenumber, you _____ the energy.

17-2. (a) How much energy (in kilojoules) is carried by one mole of photons of red light with $\lambda = 650$ nm?

(b) How many kilojoules are carried by one mole of photons of violet light with $\lambda = 400$ nm?

17-3. Calculate the frequency (Hz), wavenumber (cm^{-1}), and energy (J/photon and J/[mol of photons]) of visible light with a wavelength of 562 nm.

17-4. Which molecular processes correspond to the energies of microwave, infrared, visible, and ultraviolet photons?

17-5. Characteristic orange light produced by sodium in a flame is due to an intense emission called the sodium D line, which is actually a doublet, with wavelengths (measured in vacuum) of 589.157 88 and 589.755 37 nm. The index of refraction of air at a wavelength near 589 nm is 1.000 292 6. Calculate the frequency, wavelength, and wavenumber of each component of the D line, measured in air.

Exercícios

17-1. Fill in the blanks.

(a) If you double the frequency of electromagnetic radiation, you _____ the energy.

(b) If you double the wavelength, you _____ the energy.

(c) If you double the wavenumber, you _____ the energy.

17-2. (a) How much energy (in kilojoules) is carried by one mole of photons of red light with $\lambda = 650$ nm?

(b) How many kilojoules are carried by one mole of photons of violet light with $\lambda = 400$ nm?

17-3. Calculate the frequency (Hz), wavenumber (cm^{-1}), and energy (J/photon and J/[mol of photons]) of visible light with a wavelength of 562 nm.

17-4. Which molecular processes correspond to the energies of microwave, infrared, visible, and ultraviolet photons?

17-5. Characteristic orange light produced by sodium in a flame is due to an intense emission called the sodium D line, which is actually a doublet, with wavelengths (measured in vacuum) of 589.157 88 and 589.755 37 nm. The index of refraction of air at a wavelength near 589 nm is 1.000 292 6. Calculate the frequency, wavelength, and wavenumber of each component of the D line, measured in air.

Exercícios

UFRJ

17-11. The absorbance of a 2.31×10^{-5} M solution of a compound is 0.822 at a wavelength of 266 nm in a 1.00-cm cell. Calculate the molar absorptivity at 266 nm.

17-12. What color would you expect to observe for a solution of $Fe(ferrozine)_3^{4-}$, which has a visible absorbance maximum at 562 nm?

Exercícios

UFRJ

17-16. A compound with molecular mass 292.16 g/mol was dissolved in a 5-mL volumetric flask. A 1.00-mL aliquot was withdrawn, placed in a 10-mL volumetric flask, and diluted to the mark. The absorbance at 340 nm was 0.427 in a 1.000-cm cuvet. The molar absorptivity at 340 nm is $\varepsilon_{340} = 6\,130\ M^{-1}\,cm^{-1}$.

(a) Calculate the concentration of compound in the cuvet.

(b) What was the concentration of compound in the 5-mL flask?

(c) How many milligrams of compound were used to make the 5-mL solution?