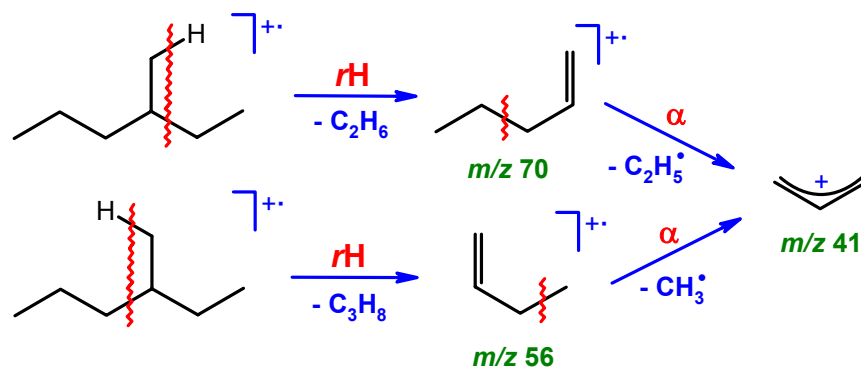
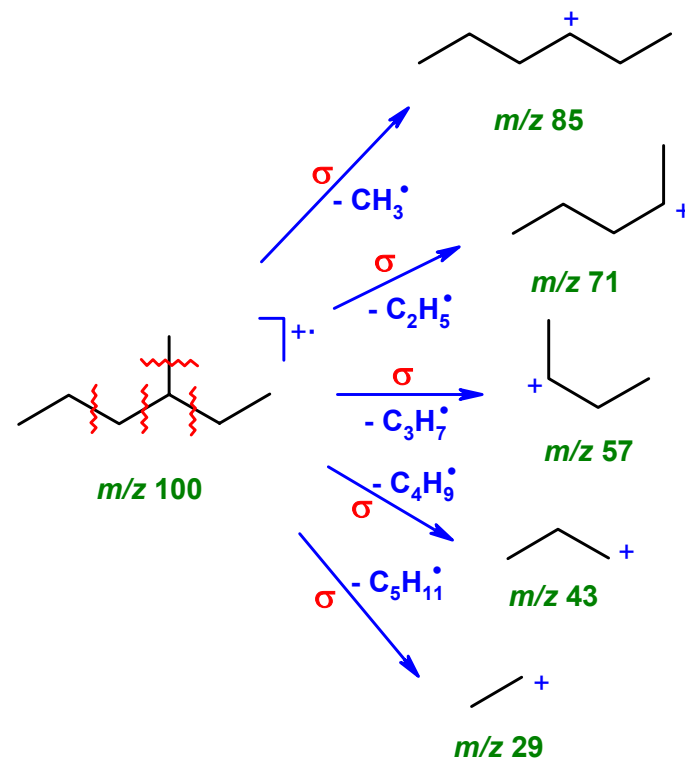
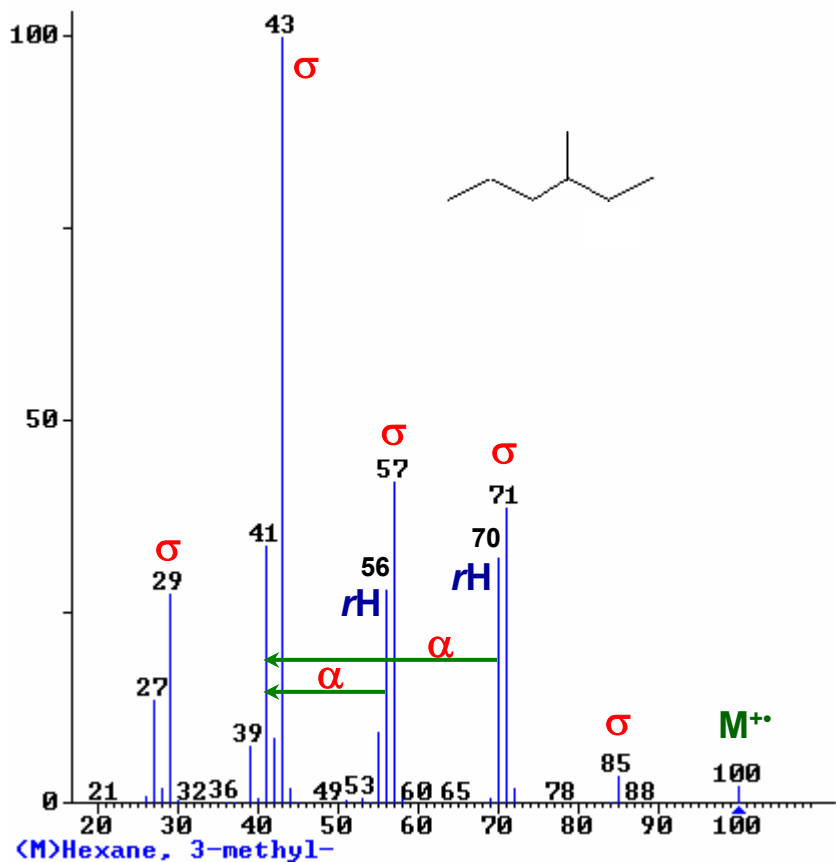
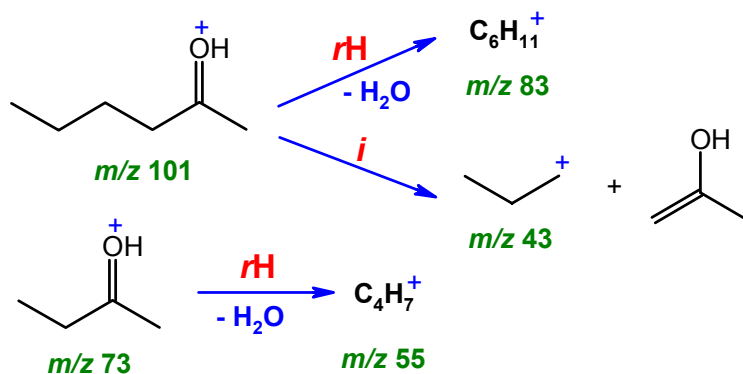
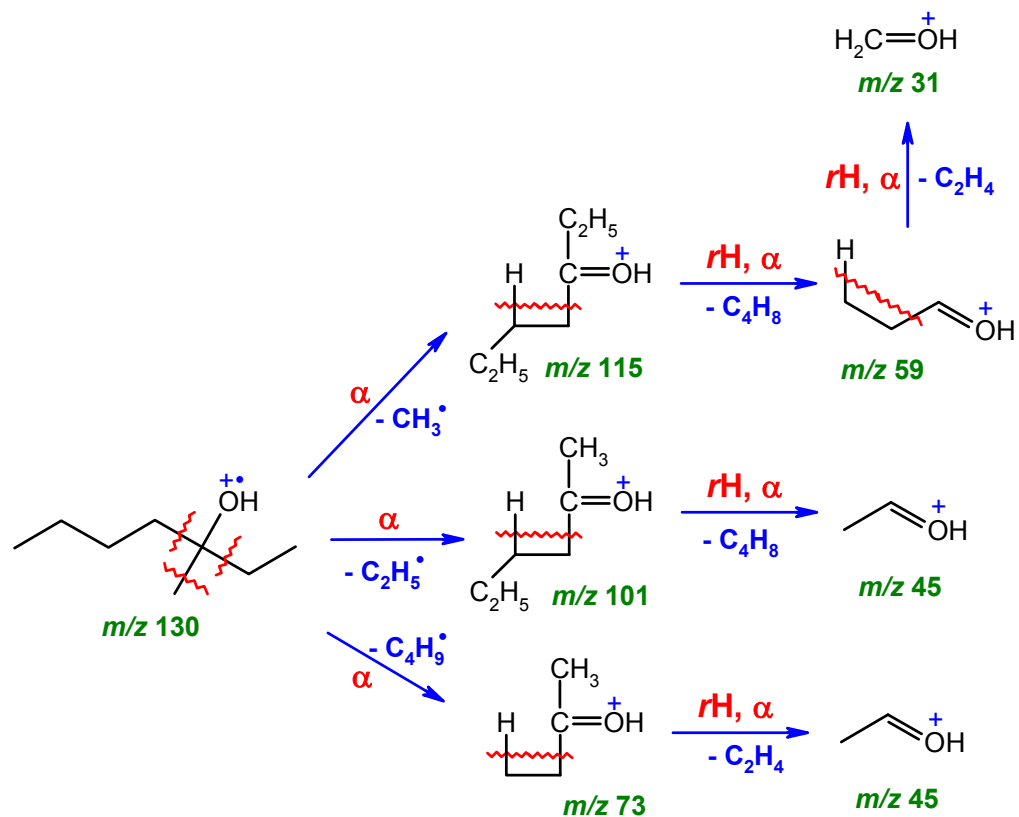
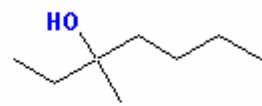
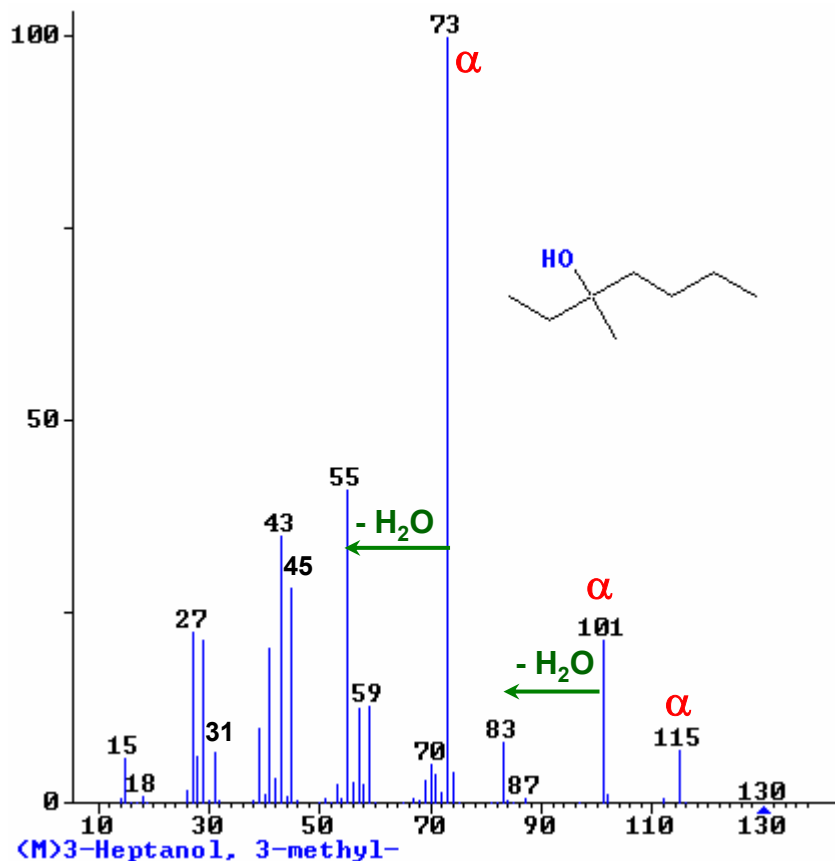


# FRAGMENTACJE WYBRANYCH ZWIĄZKÓW

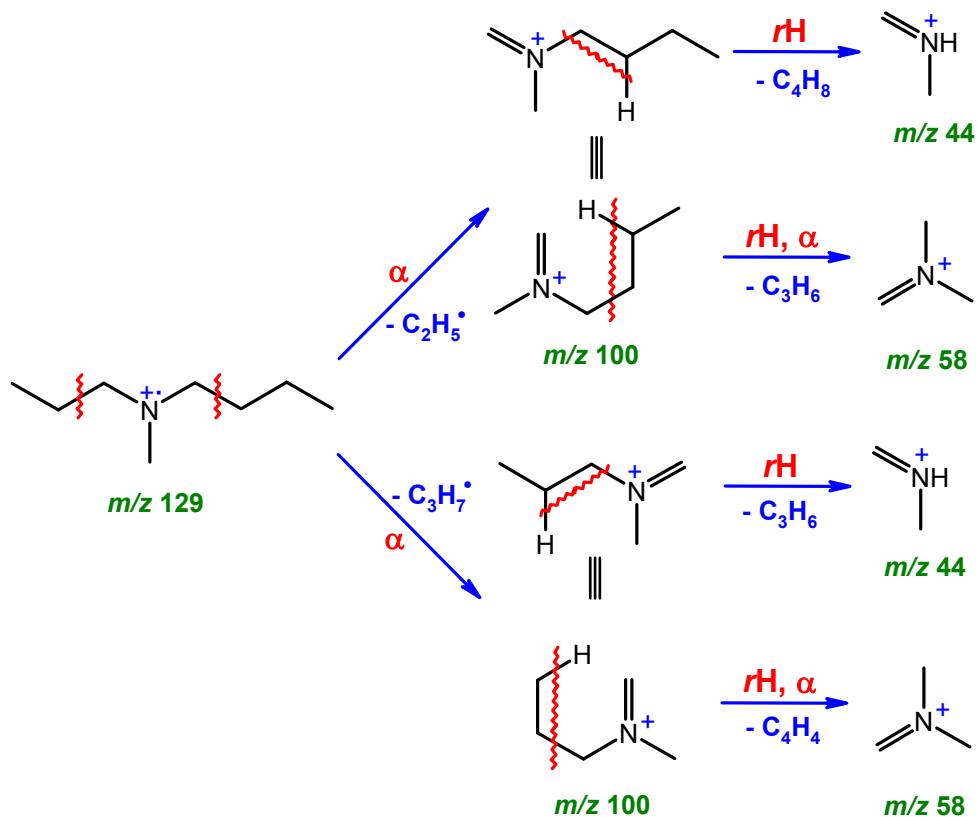
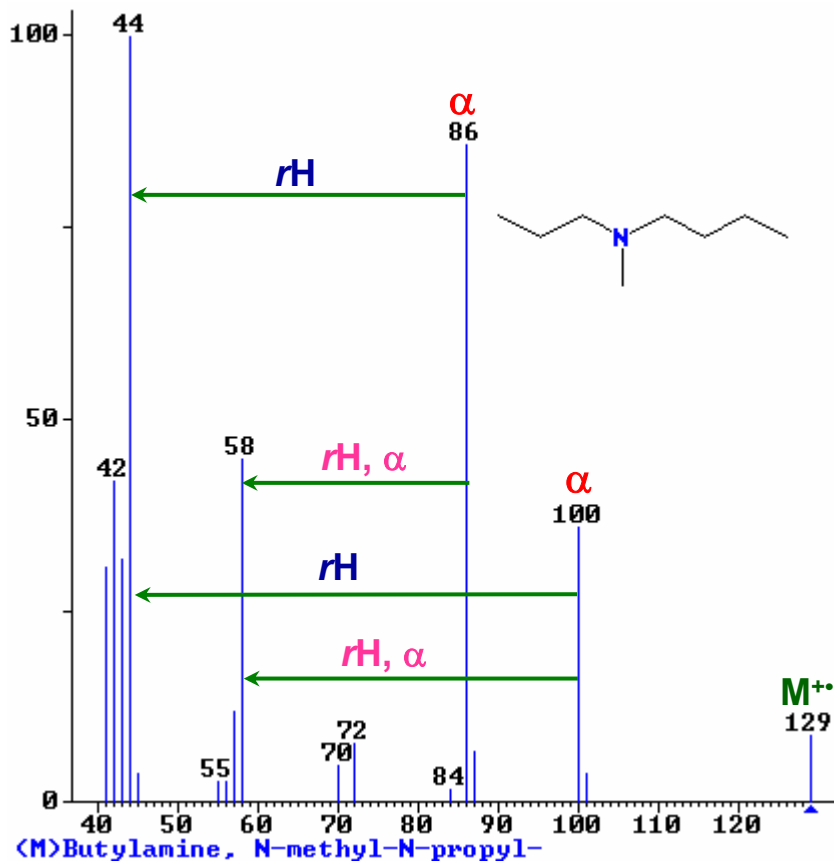
# 3-Metyloheksan



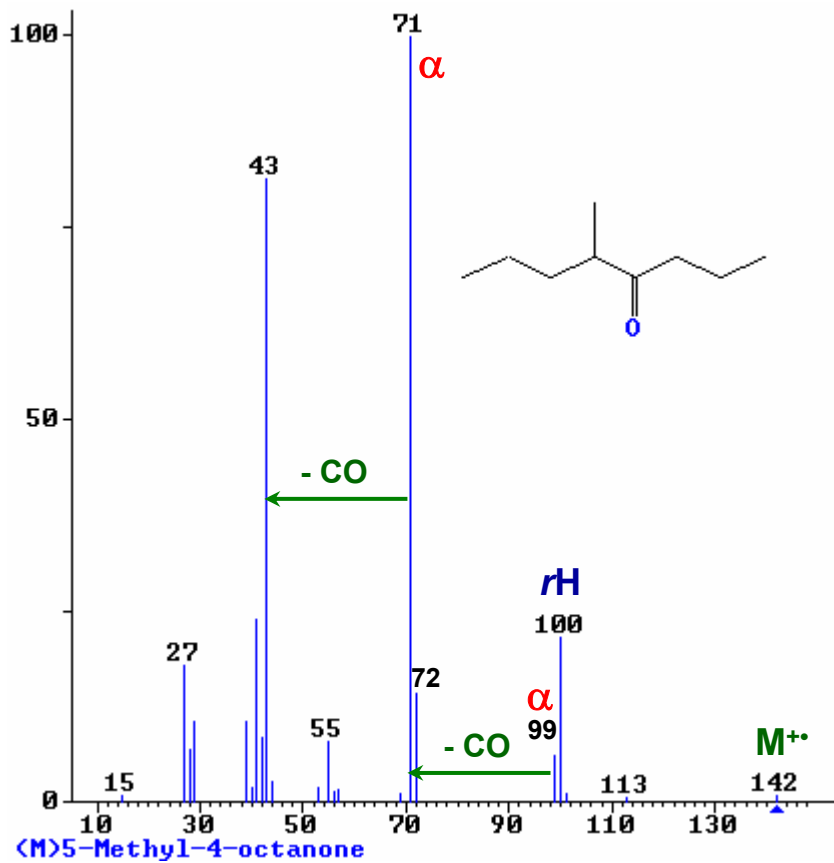
# 3-Metyloheptan-3-ol



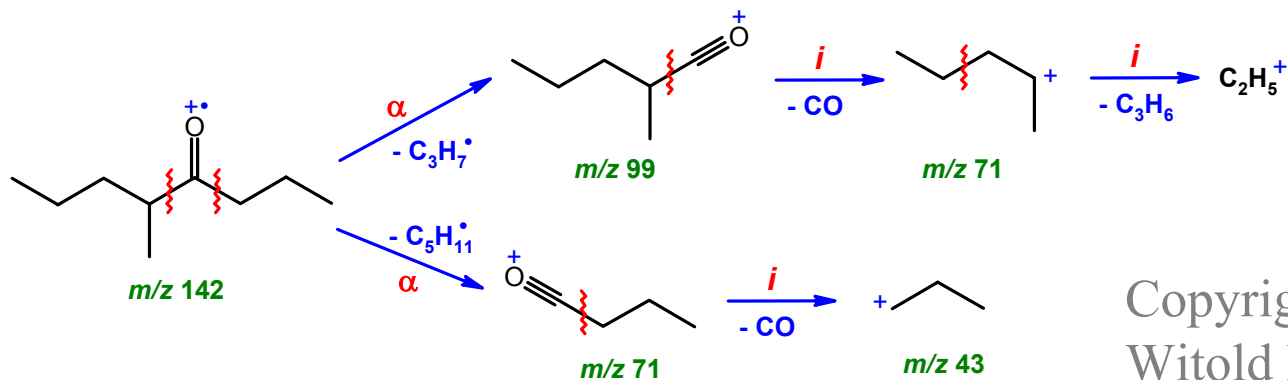
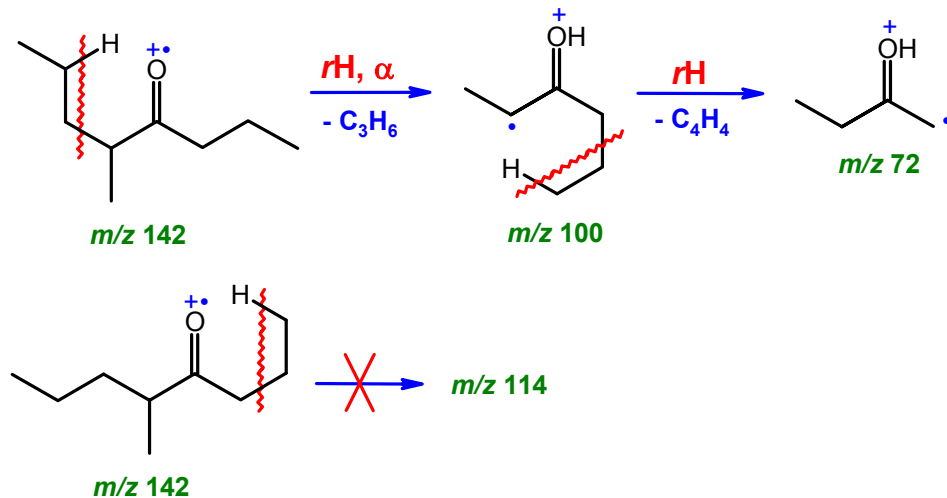
# N-metylo-N-propylobutyloamina



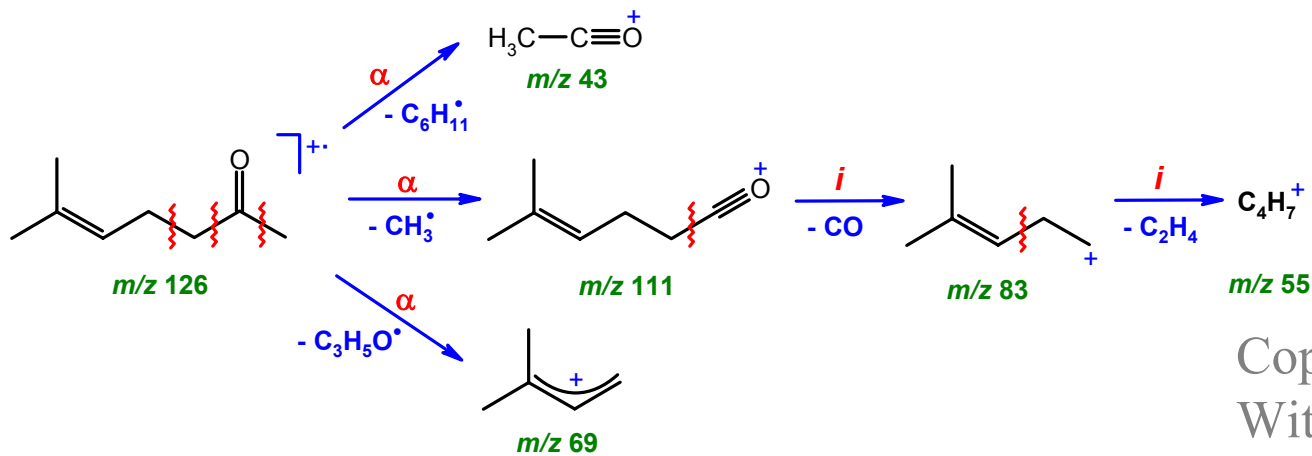
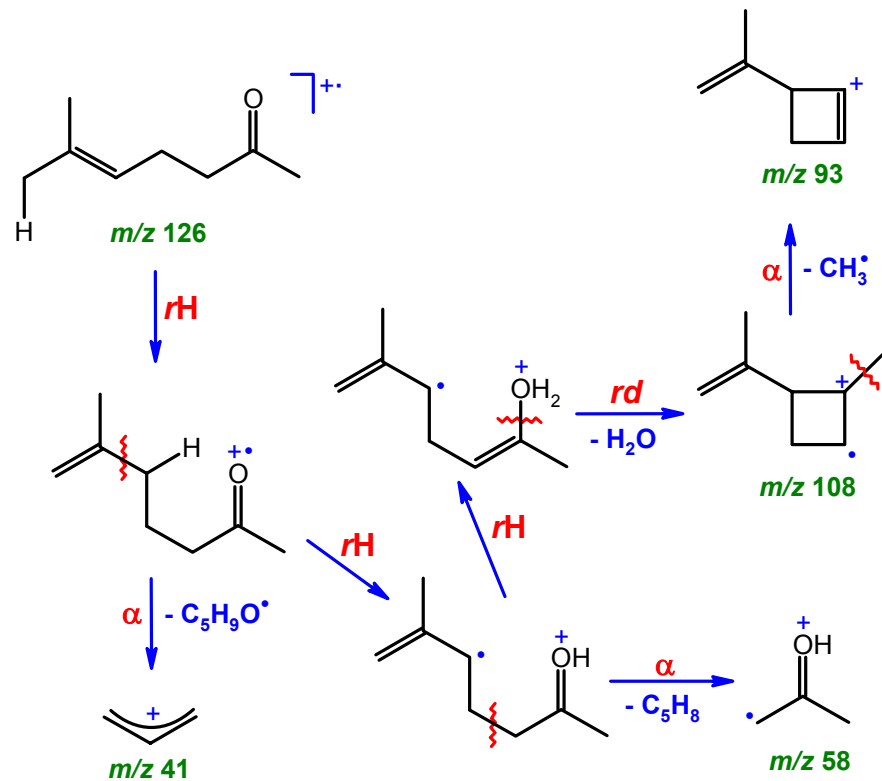
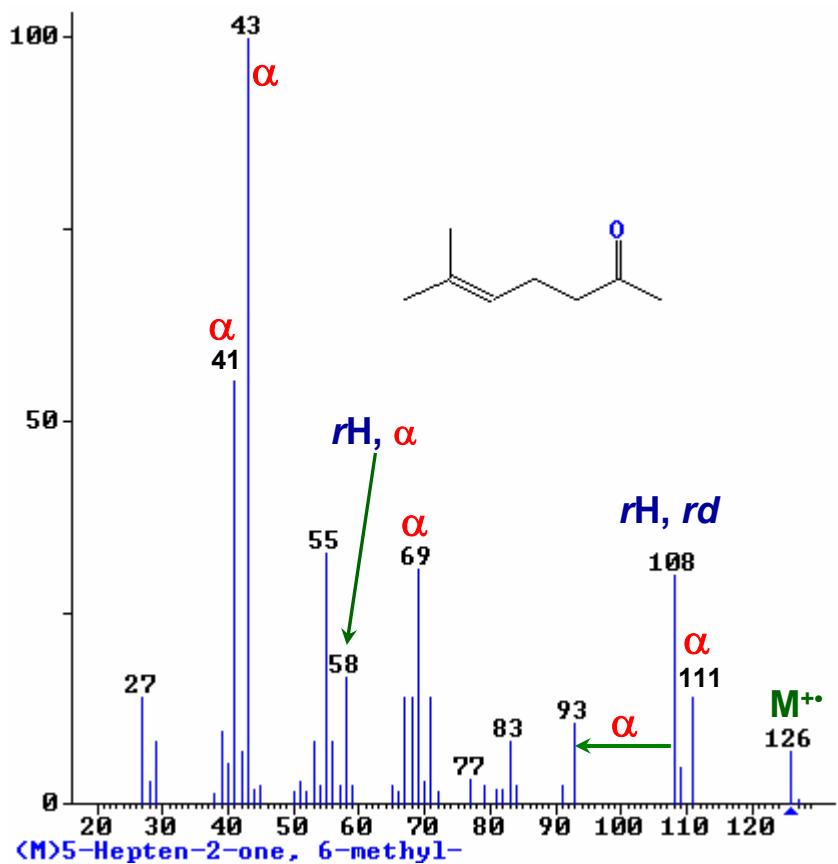
# 5-Metylooktan-2-on



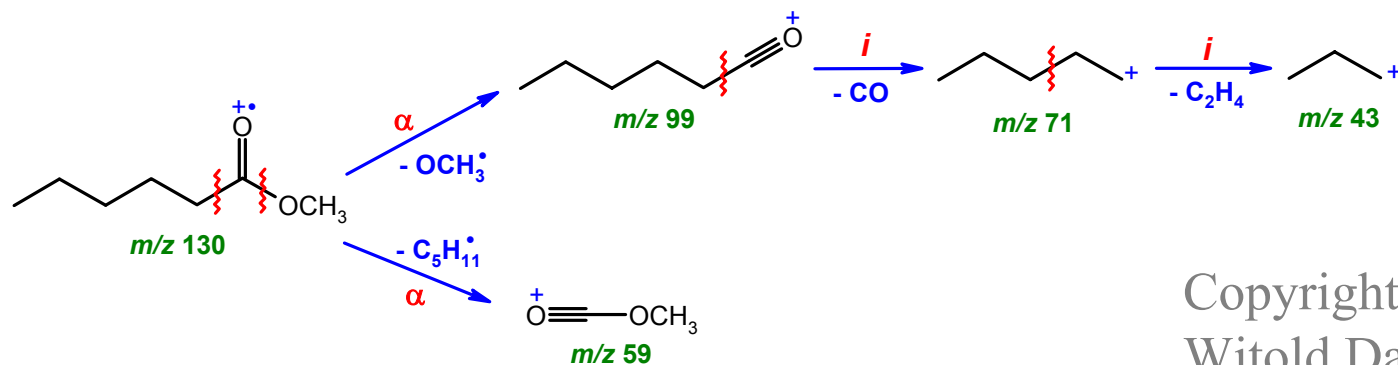
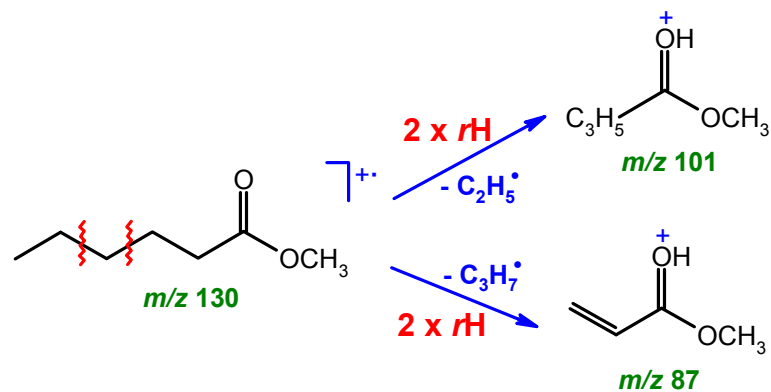
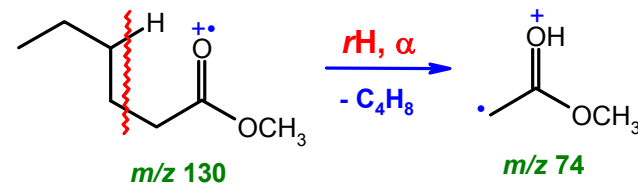
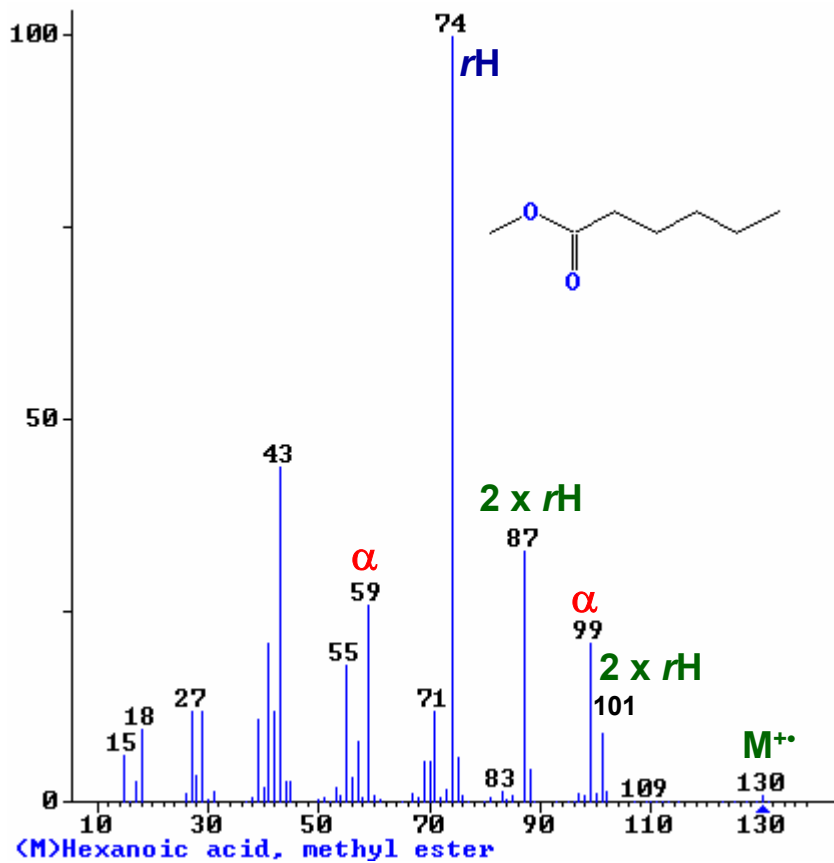
## Przegrupowanie McLafferty'ego



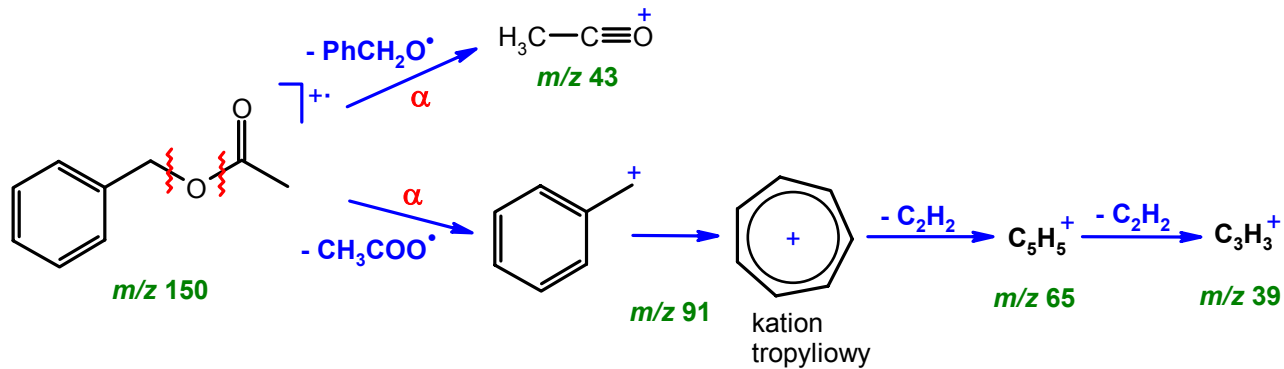
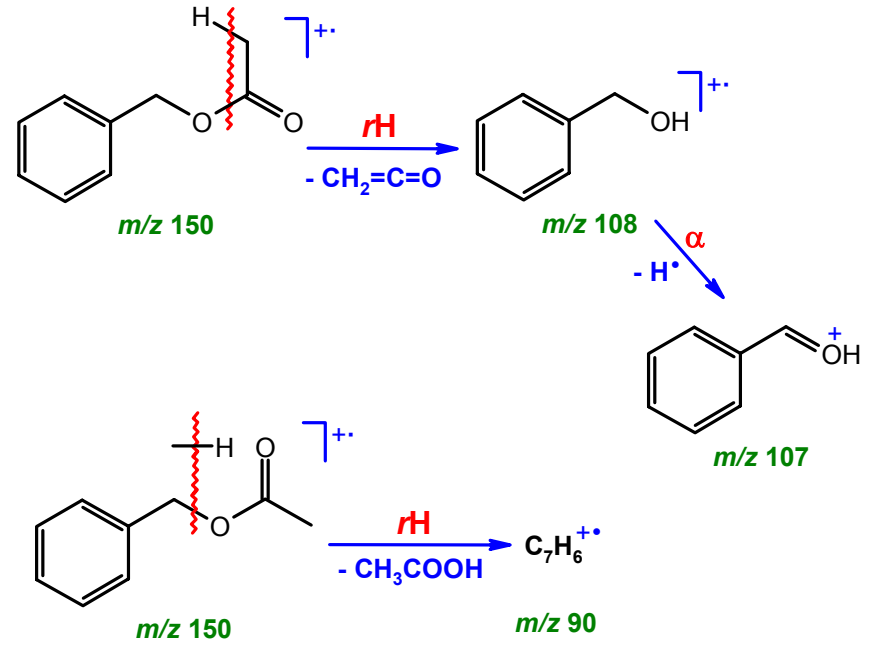
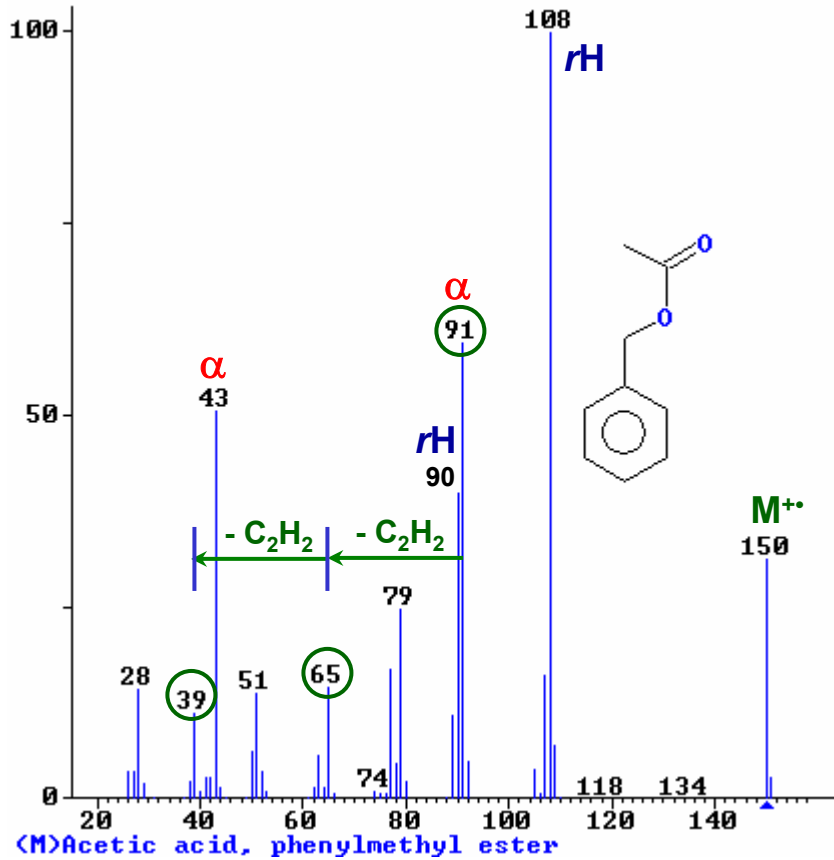
# 6-Metylohept-5-en-2-on



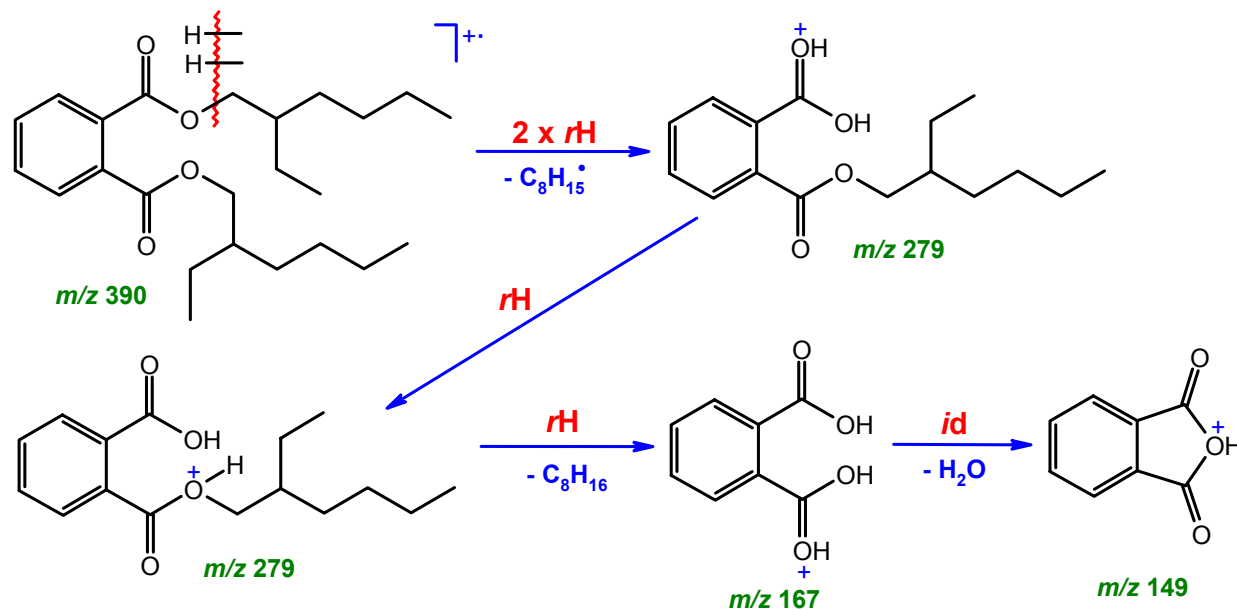
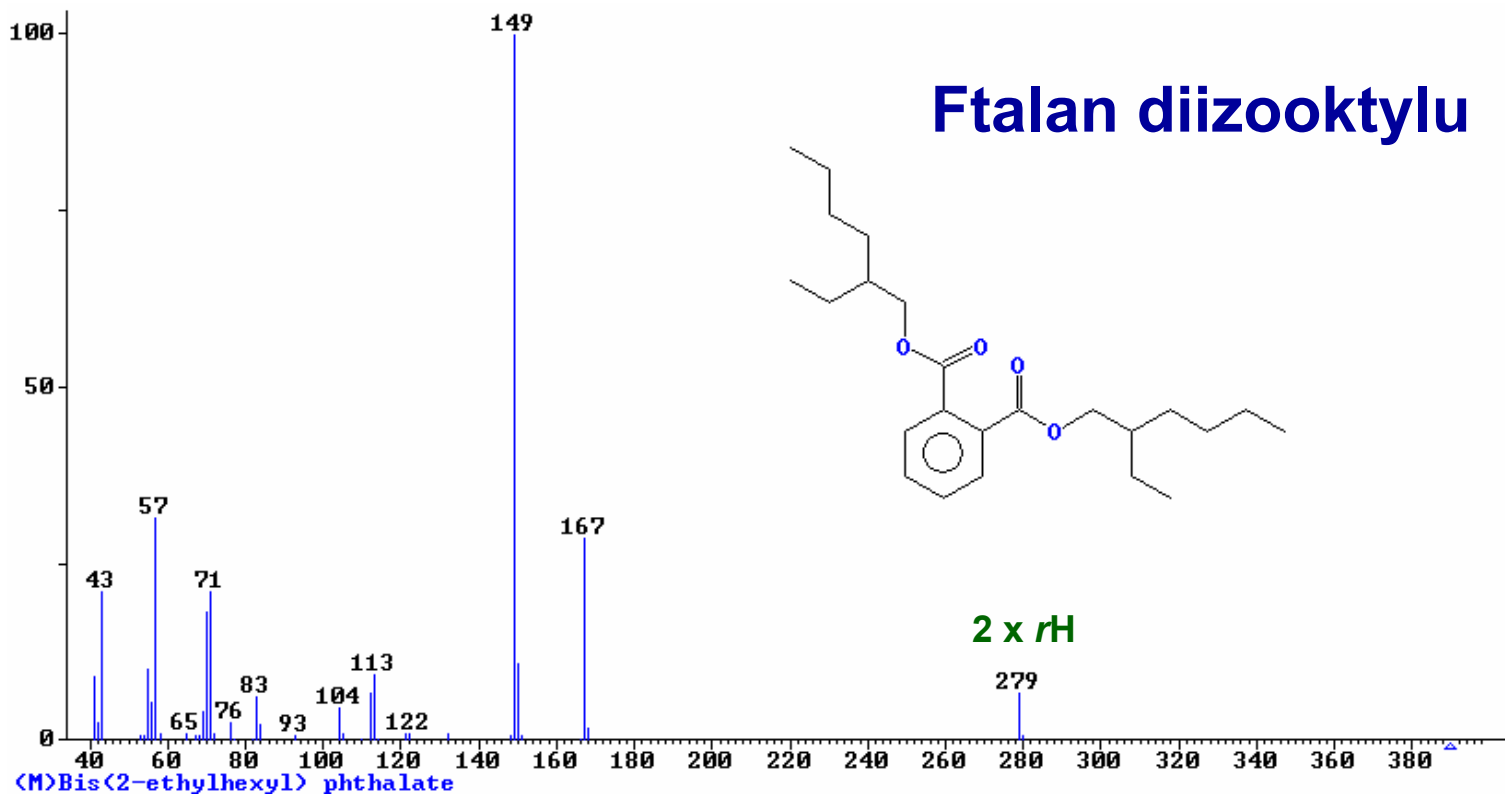
# Ester metylowy kwasu heksanowego



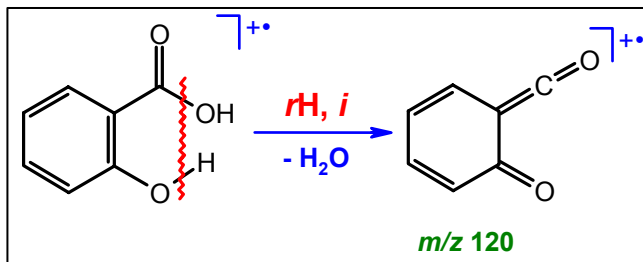
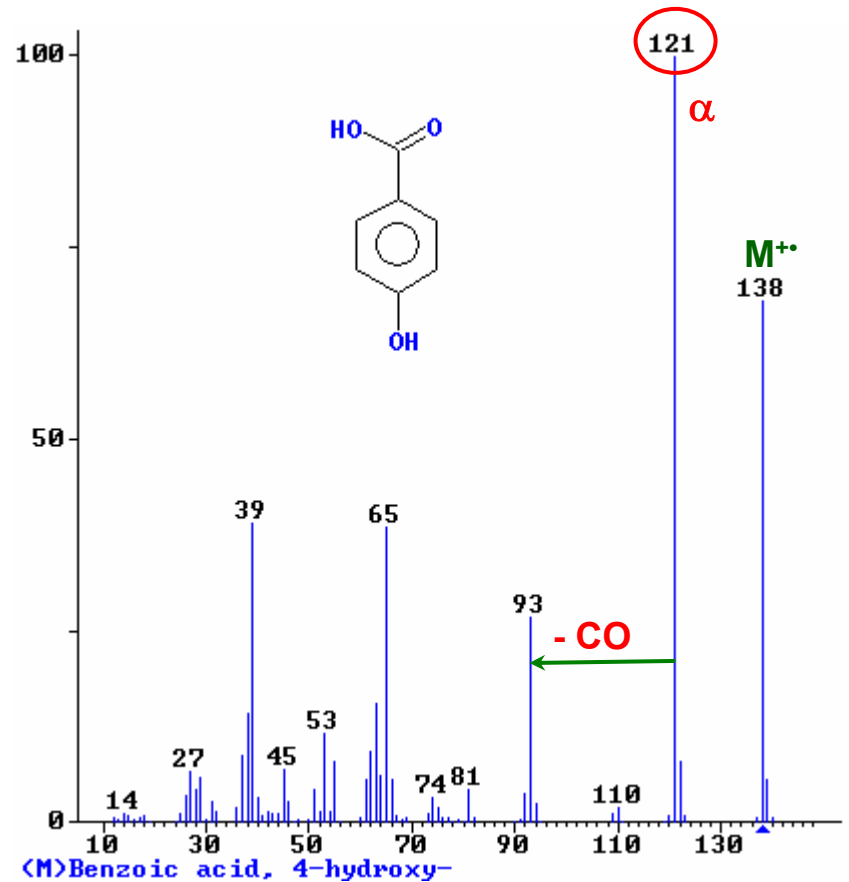
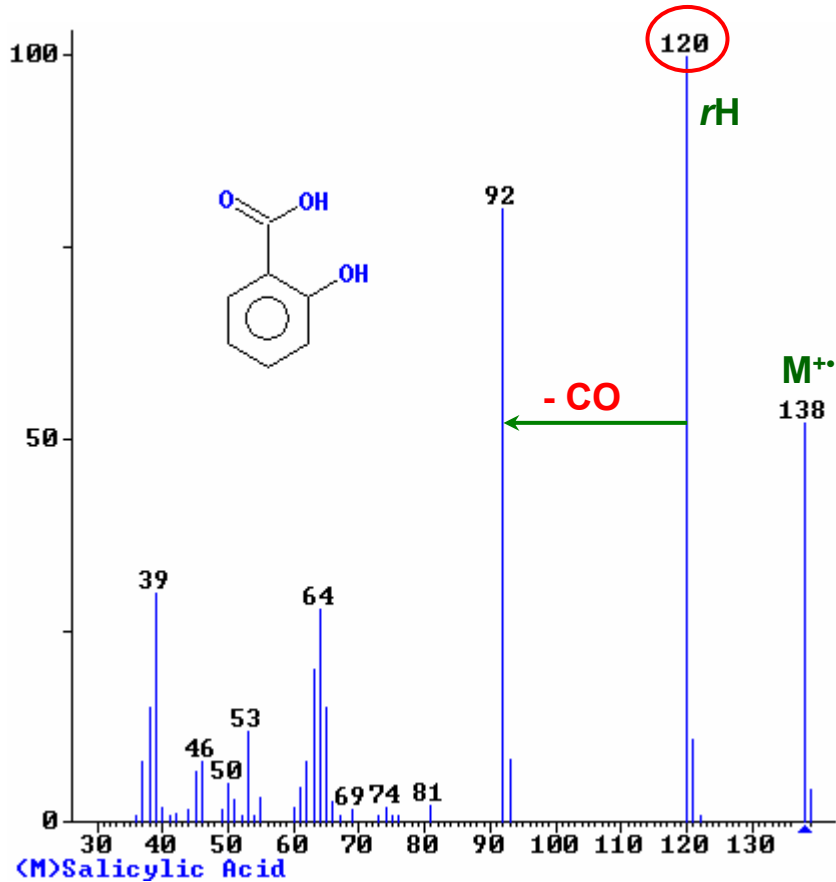
# Octan benzylu



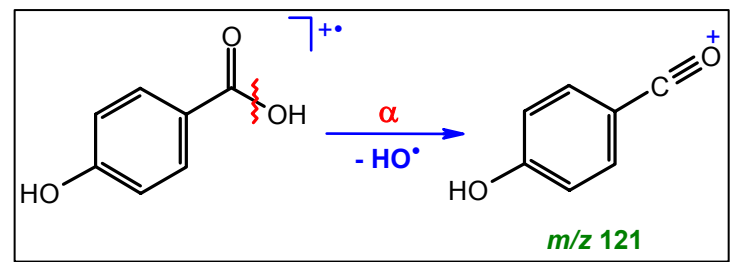
# Ftalan diizooktylu



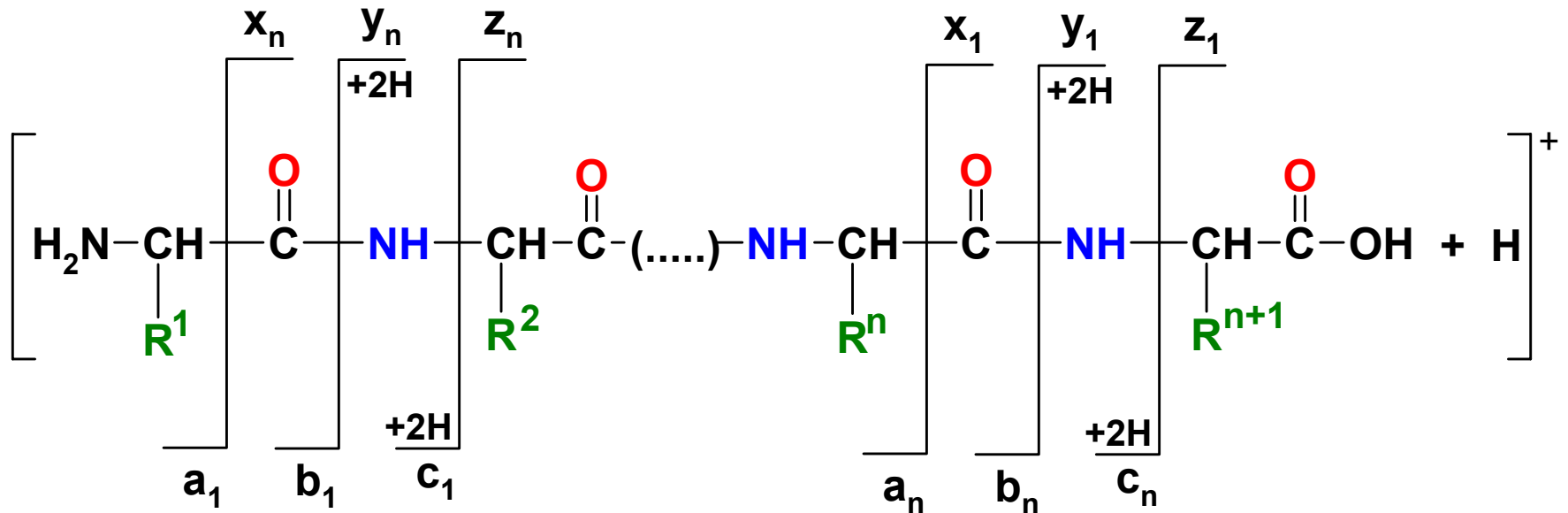
# Kwasy orto- i para-hydroksybenzoesowe



efekt orto

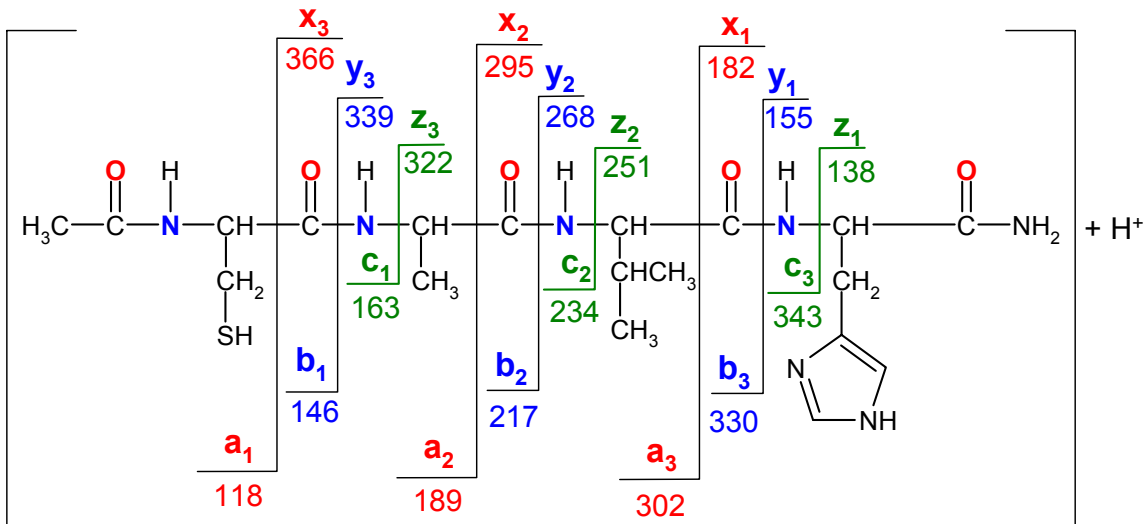


# Klasyfikacja podstawowych typów fragmentacji protonowanego łańcucha peptydowego

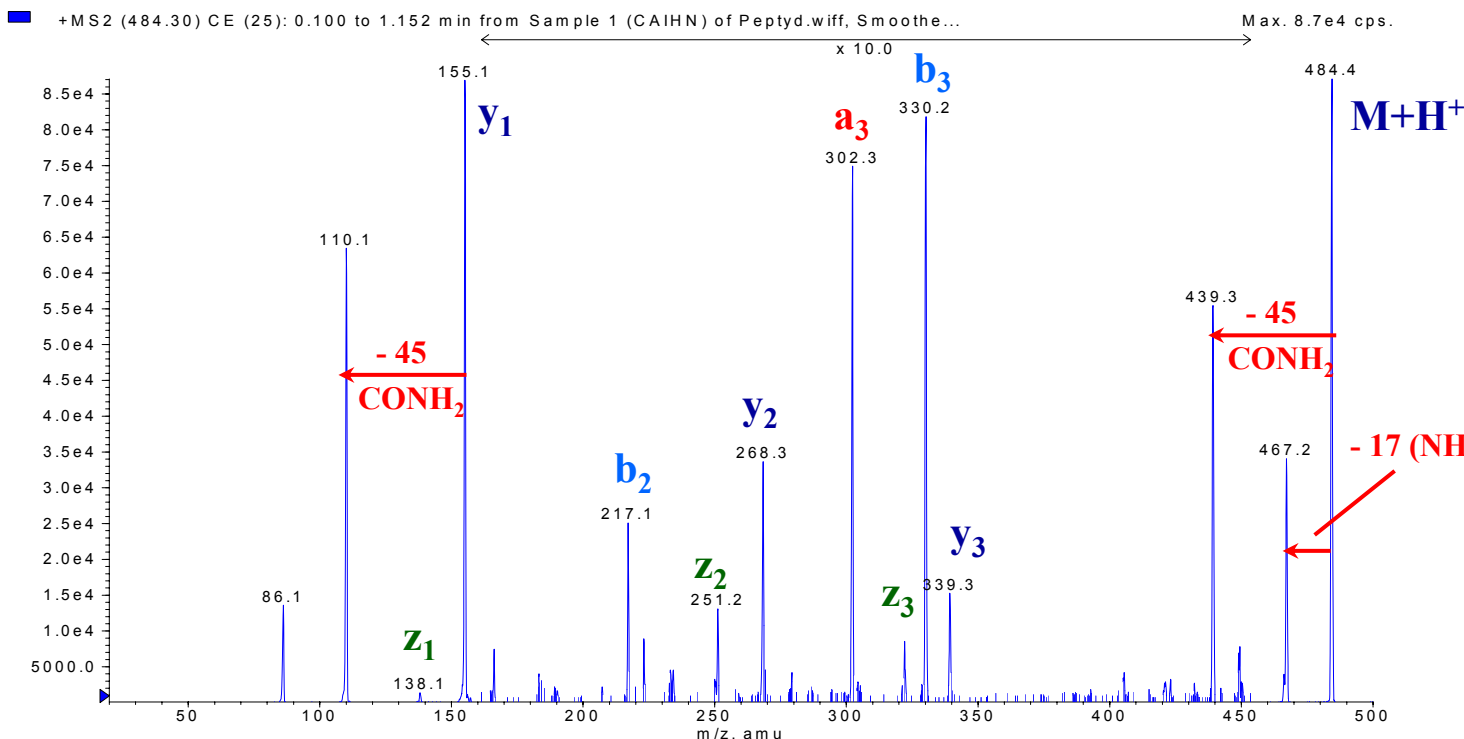


43	103	71	113	137	16
Ac	Cys	Ala	Ile	His	NH <sub>2</sub>

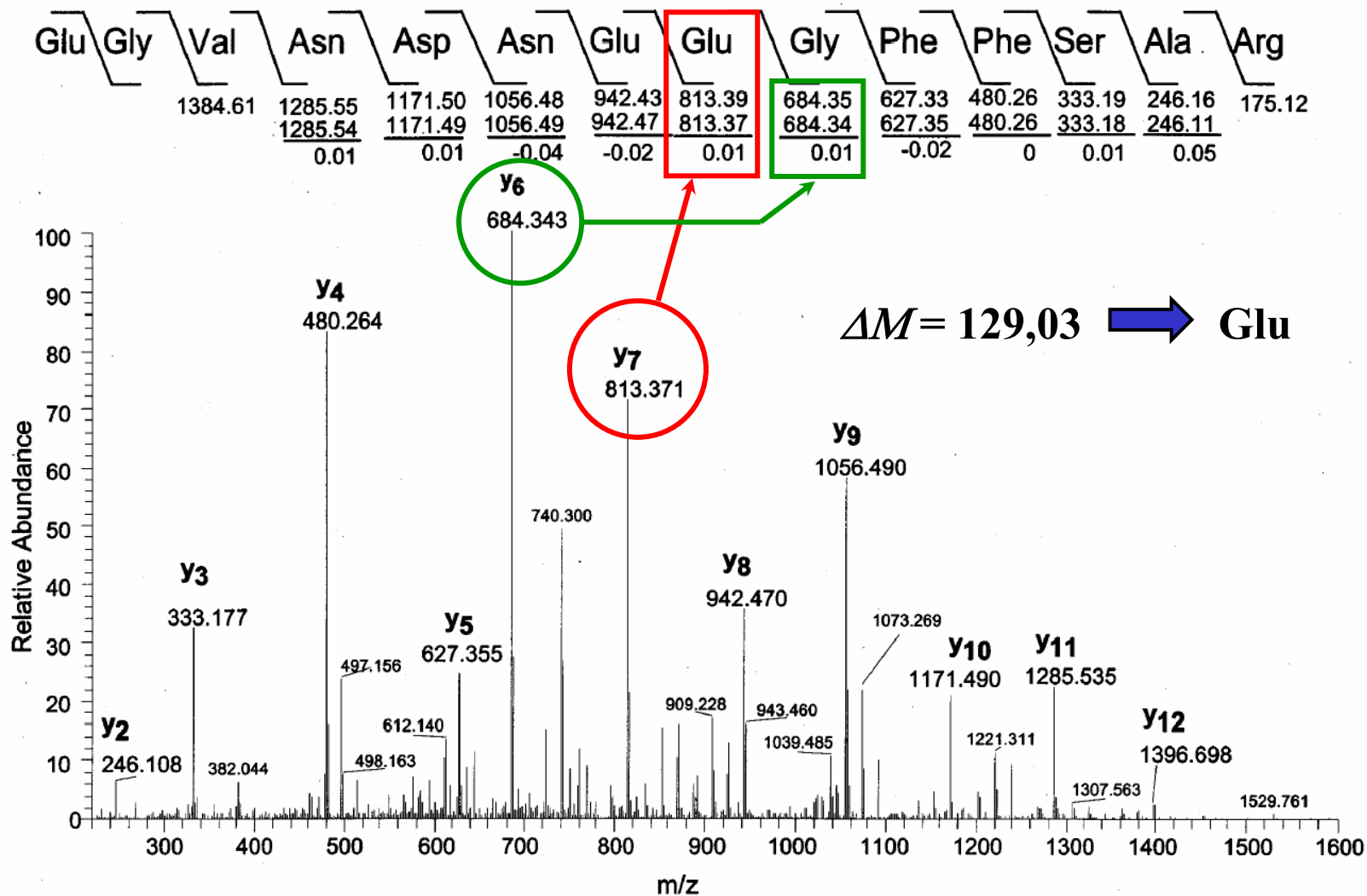
# Ustalanie sekwencji peptydu na podstawie widma ESI-CID-MS/MS



Jony **c** i **y**: +2H<sup>+</sup>



# Ustalenie sekwencji peptydu na podstawie widma ESI-CID-MS/MS

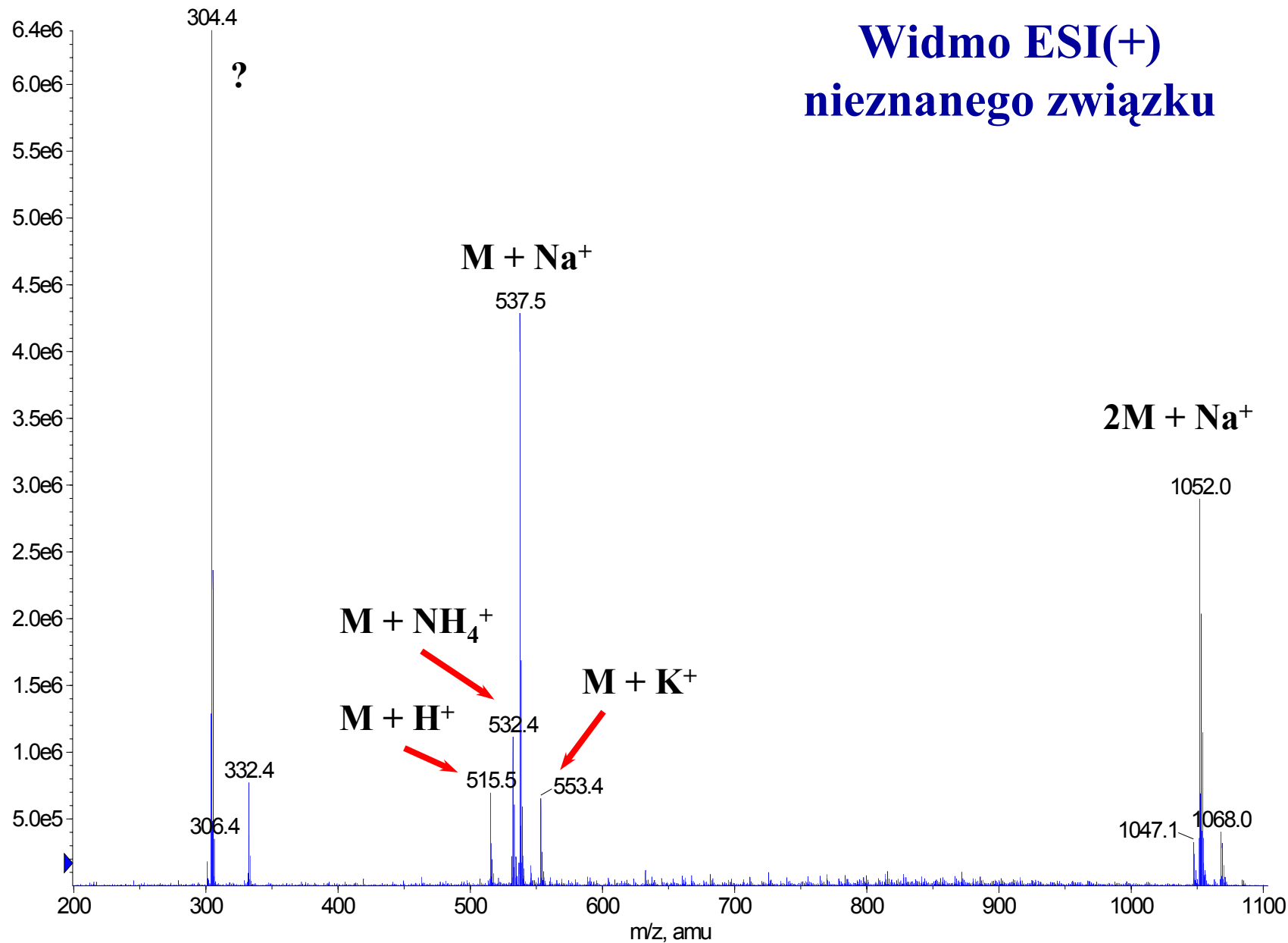


Spektrometr: Finnigan MAT LCQ

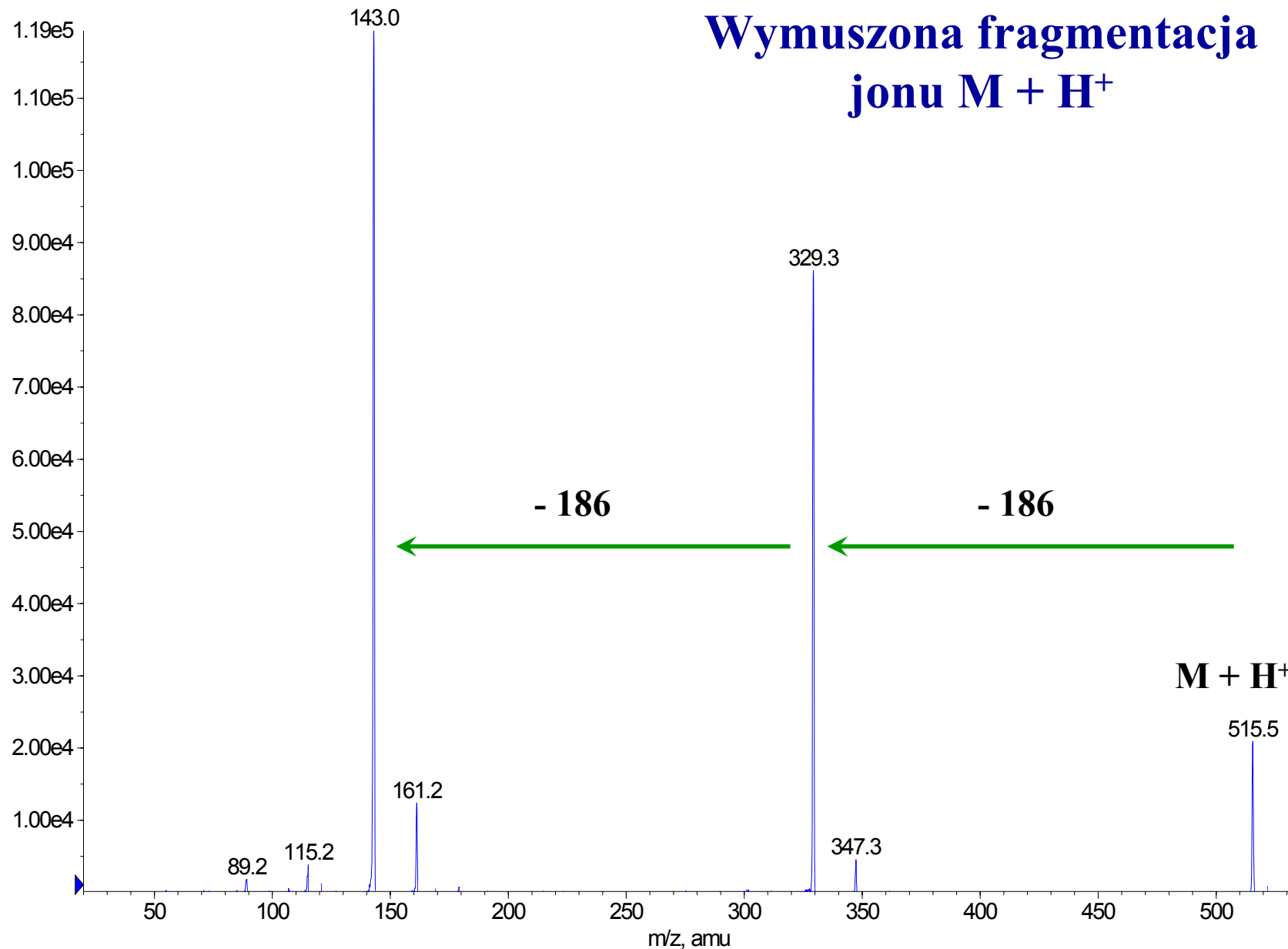
J.R. Yates III, *J. Mass Spectrom.*, 33, 1 (1998)

**Próba ustalenia budowy  
nieznanego związku za pomocą  
ESI-MS i innych technik  
spektrometrii mas**

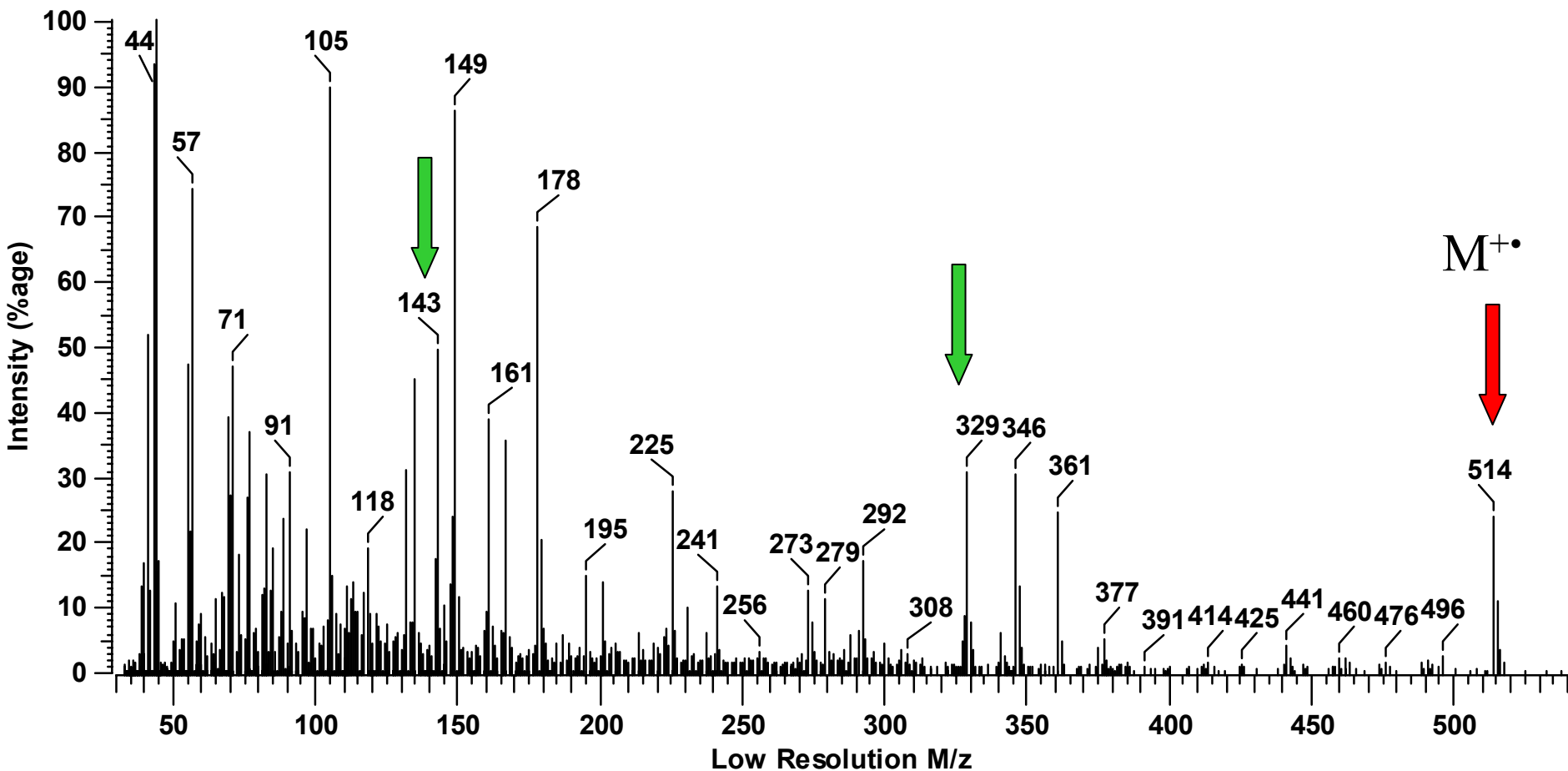
# Widmo ESI(+) nieznanego związku



# Wymuszona fragmentacja jonu $M + H^+$



# Widmo EI nieznanego związku



ATOMIC COMPOSITION REPORT (MANUAL)

Selected isotopes:

Symbol	Min	Max	V'cy	Name
C	0	40	4	Carbon-12
H	0	80	1	Hydrogen-1
O	0	20	2	Oxygen-16
N	0	2	3	Nitrogen-14

Allowable error = minimum of 50.0 ppm, 10.0 mmu.  
 Ring/Double Bond limits = [-0.5 : 100.0]

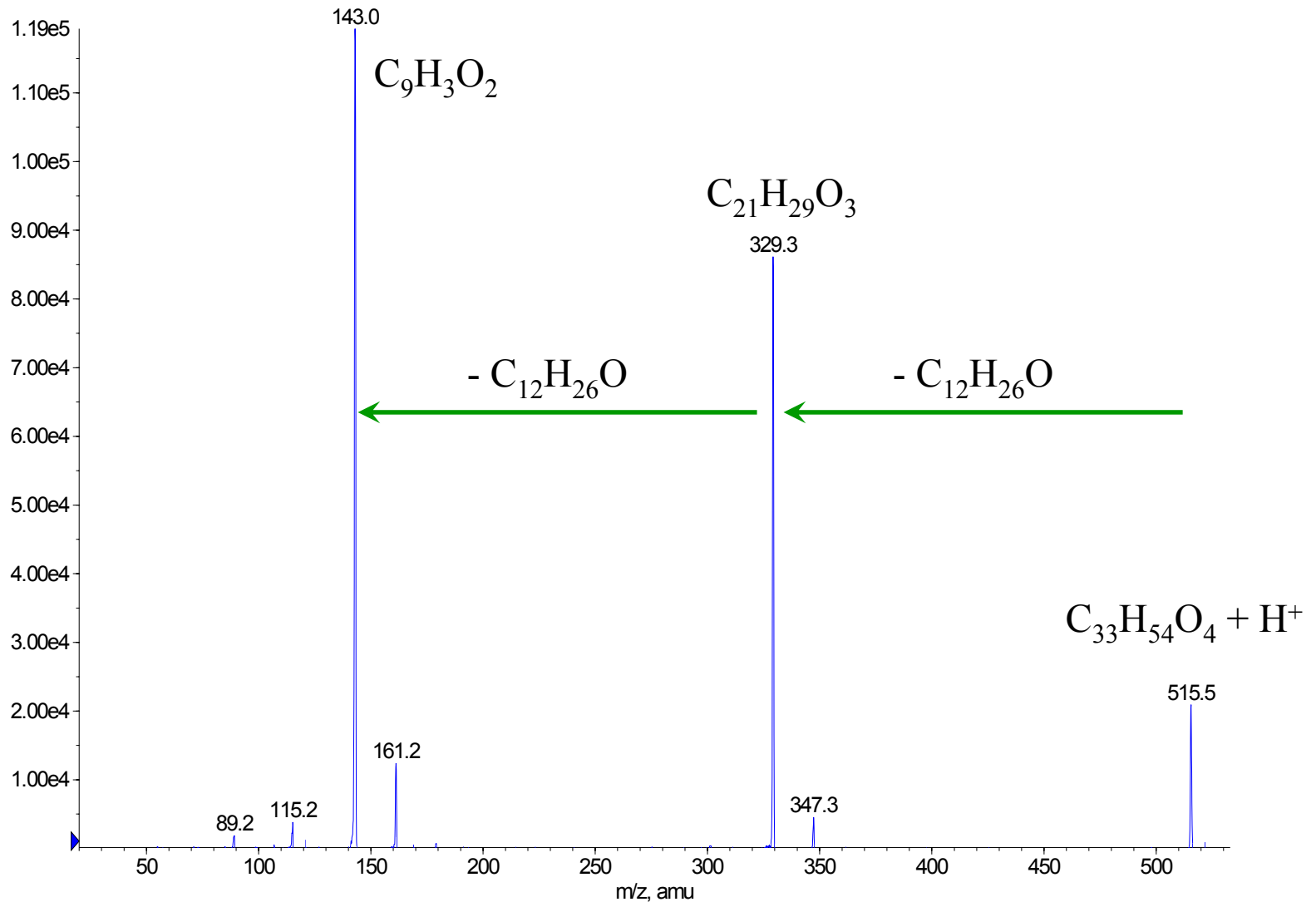
Mass	Calculated	ppm	mmu	R/DB	Formula
514.40617	514.40489	-2.5	-1.3	11.5	C36.H52.O.N
	514.40221	-7.7	-4.0	7.0	C33.H54.O4
	514.41076	8.9	4.6	2.5	C29.H56.O6.N
	514.41344	14.1	7.3	7.0	C32.H54.O3.N2
	514.39819	-15.5	-8.0	3.0	C28.H54.O6.N2
329.21311	329.21435	3.8	1.2	12.0	C24.H27.N
	329.21167	-4.4	-1.4	7.5	C21.H29.O3
	329.20765	-16.6	-5.5	3.5	C16.H29.O5.N2
	329.22022	21.6	7.1	3.0	C17.H31.O5.N
	329.22290	29.7	9.8	7.5	C20.H29.O2.N2
143.01161	143.01330	11.8	1.7	8.5	C9.H3.O2
	143.00928	-16.3	-2.3	4.5	C4.H3.O4.N2
	143.00660	-35.0	-5.0	0.0	C.H5.O7.N

**Wyniki  
dokładnych  
pomiarów  
masy w EI**

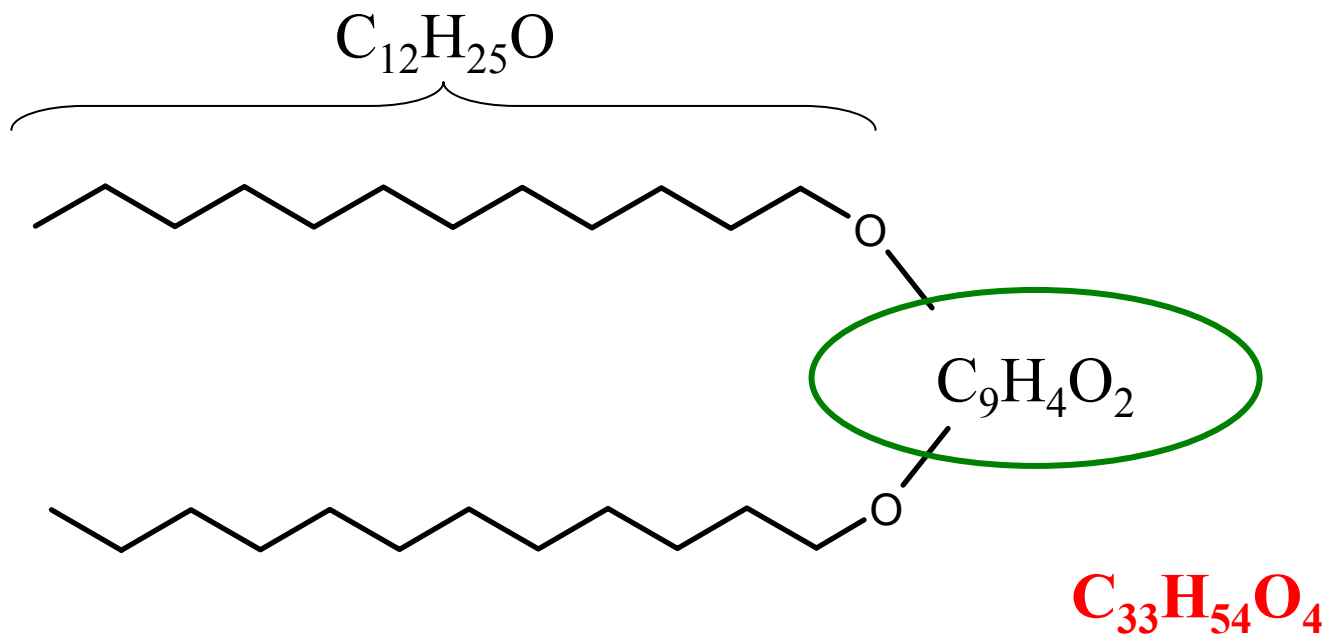
# Składy jonów fragmentacyjnych i obojętnych fragmentów

■ +MS2 (515.40) CE (20): 0.000 to 0.701 min from Sample 2 (1 w MeOH fgr 515 CE 20) of AS0739...

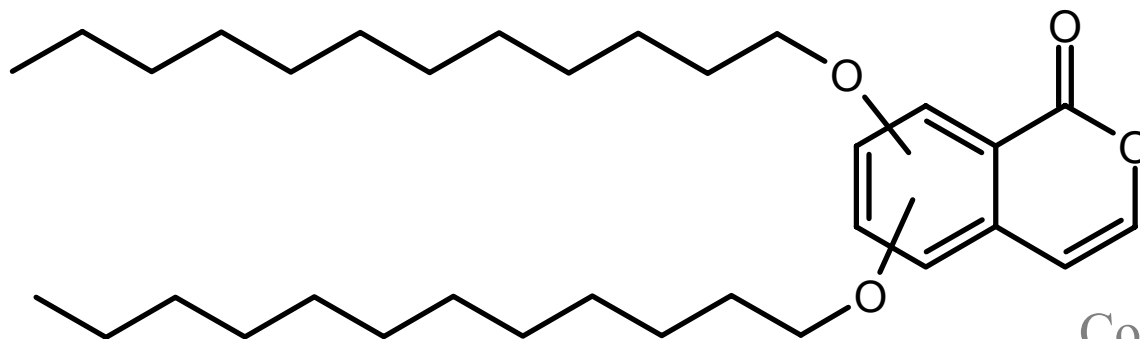
Max. 1.2e5 cps.



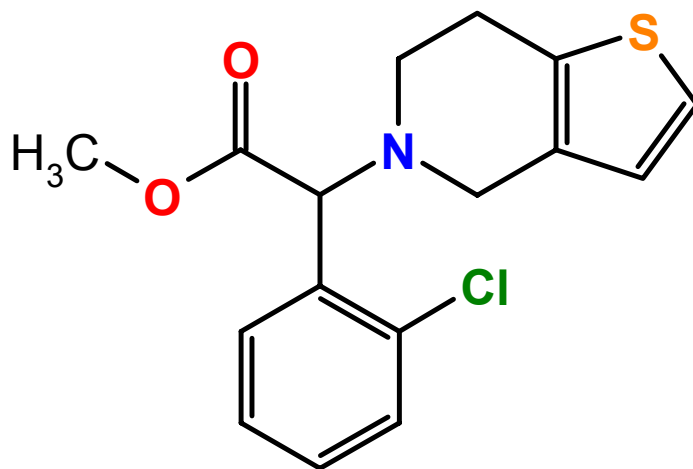
# Proponowany wzór badanego związku



Na przykład:



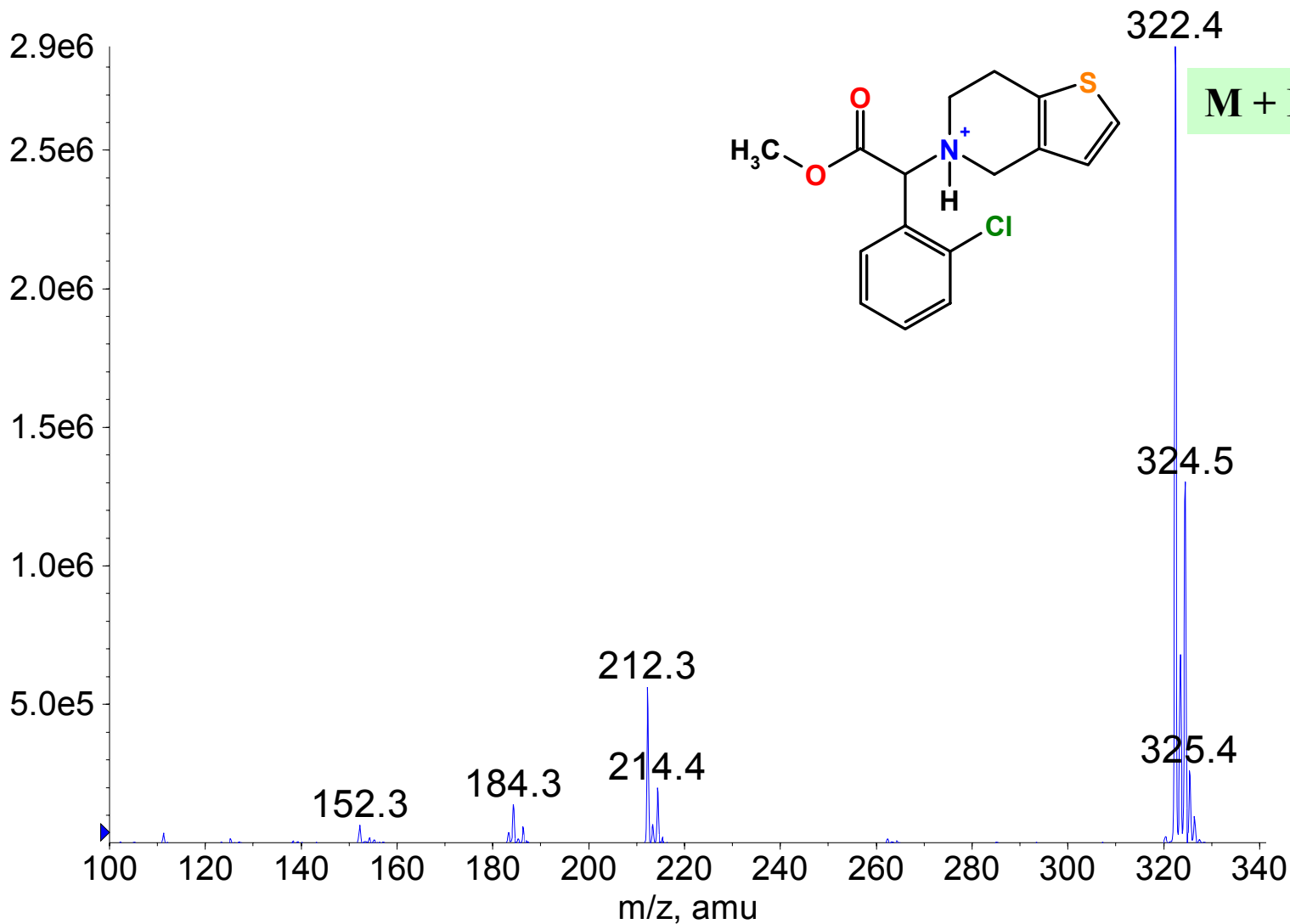
# Fragmentacja Clopidogrelu



# Widmo ESI(+) Clopidogrelu

■ +Q1: 2.172 to 2.406 min from Sample 3 (9/1 ACN H2O AcOH 0.6 ml/min 270 nm) of 050301....

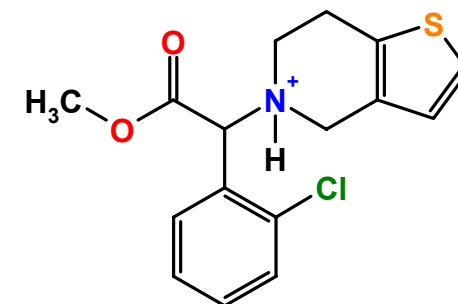
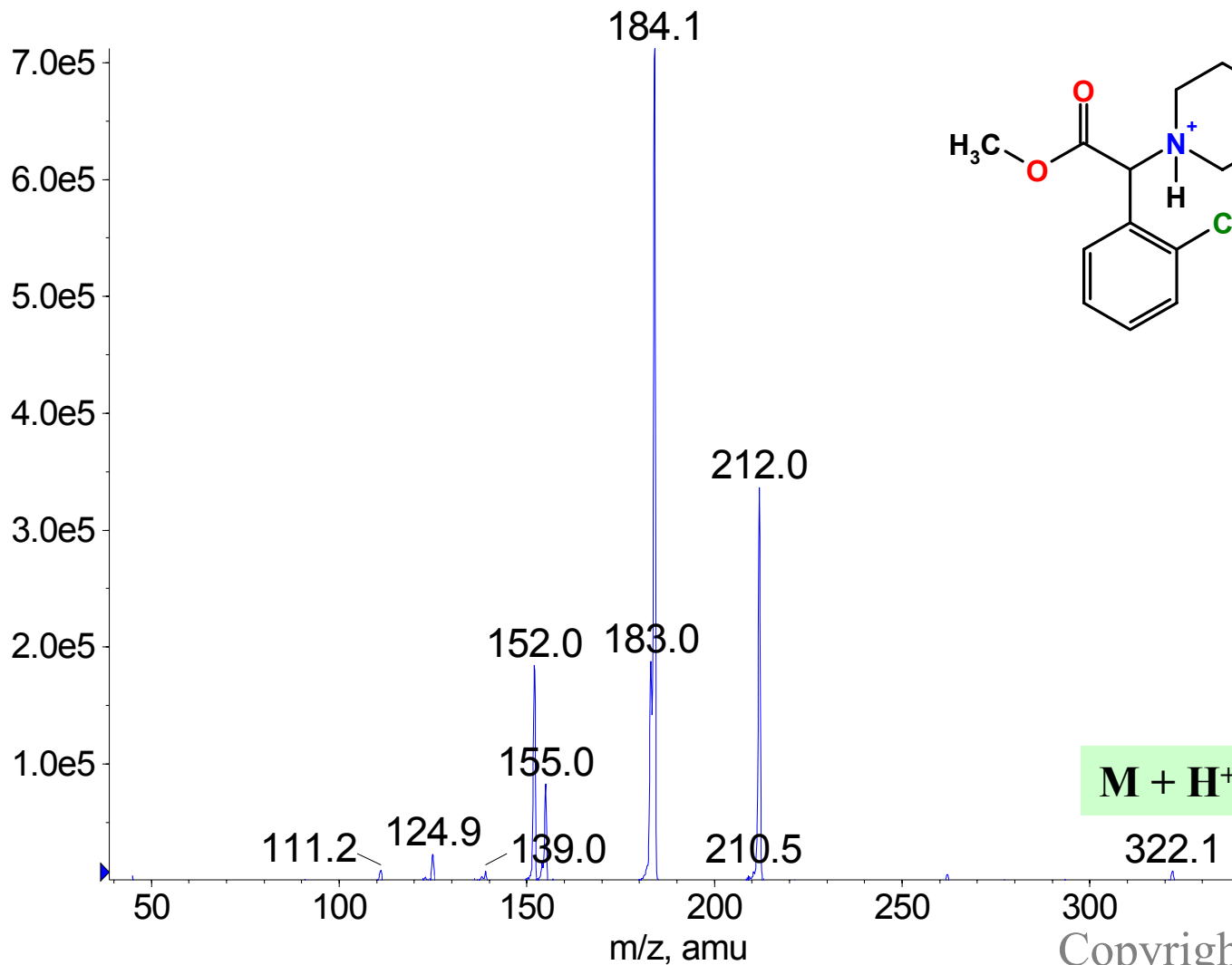
Max. 2.9e6 cps.



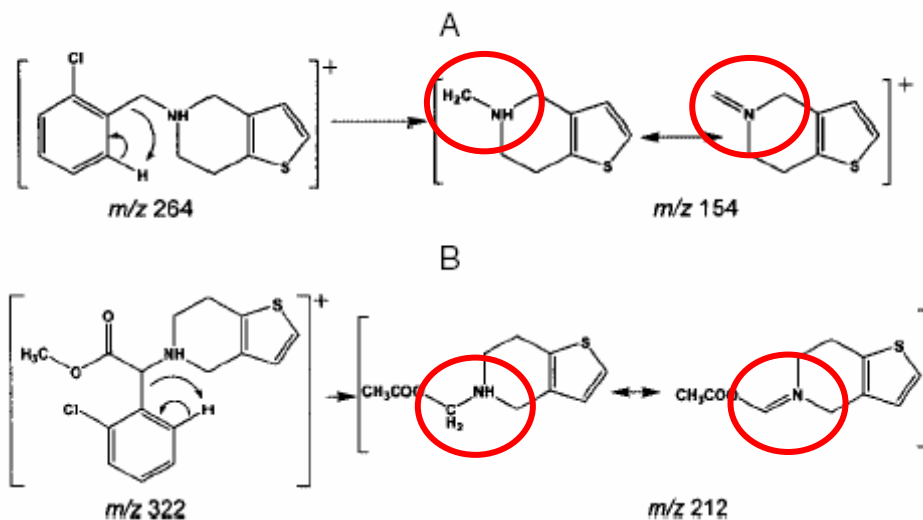
# Fragmentacja Clopidogrelu

■ +MS2 (322.40) CE (30): Period 3, Exp 2, 2.345 to 2.596 min from Sample 4 (frag 9/1 ACN H2...)

Max. 7.1e5 cps.



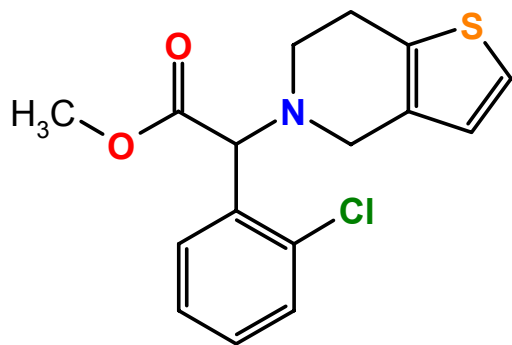
# Fragmentacja Clopidogrelu – dane literaturowe



**Figure 3.** Proposed fragmentation pathways for (A) ticlopidine and (B) clopidogrel.

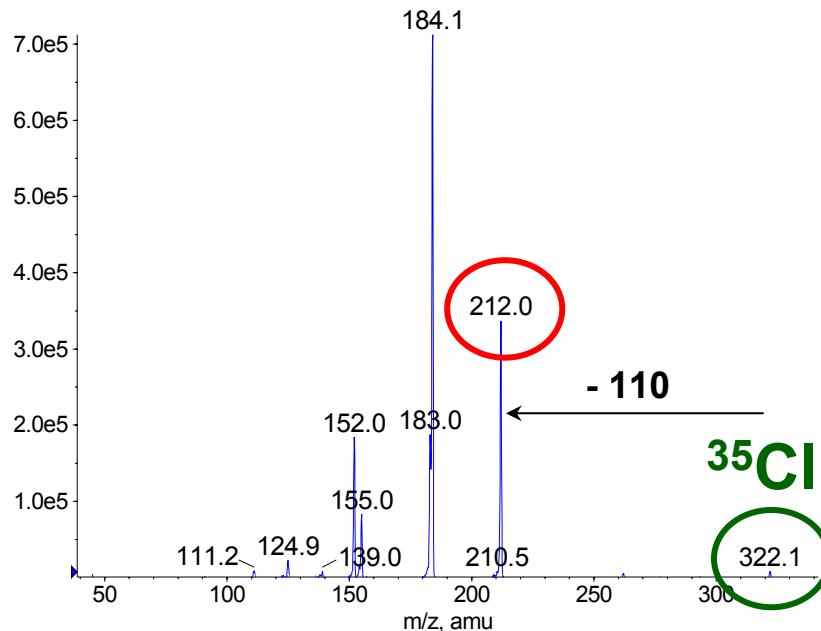
N. C. do Carmo Borges, G. D. Mendes, A. Borges, S. E. de Oliveira, R. E. Barrientos-Astigarraga and G. De Nucci, *J. Mass Spectrom.*, 2004; **39**, 1562-1569

# Fragmentacja Clopidogrelu – fragmentacja jonów zawierających izotop $^{35}\text{Cl}$ i $^{37}\text{Cl}$



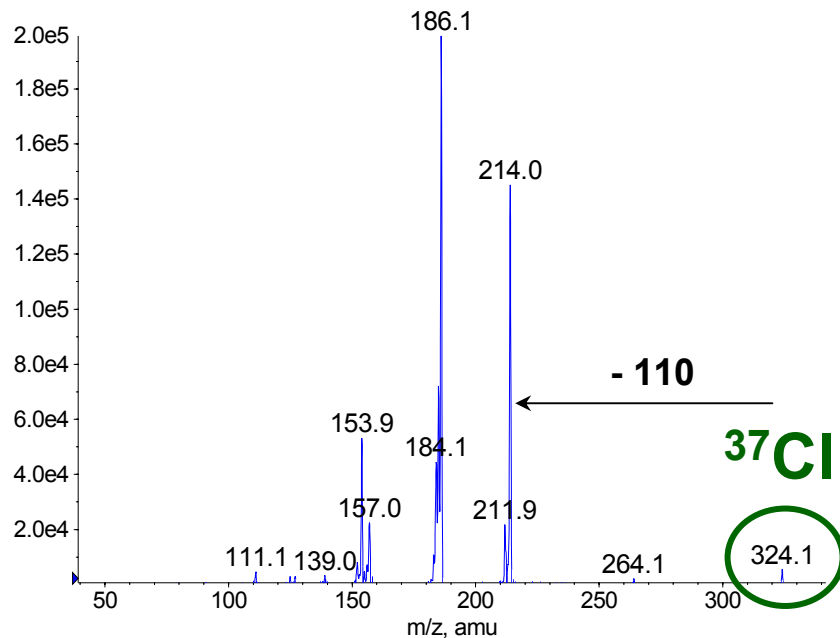
+MS2 (322.40) CE (30): Period 3, Exp 2, 2.345 to 2.596 min from Sample 4 (frag 9/1 ACN H2...

Max. 7.1e5 cps.

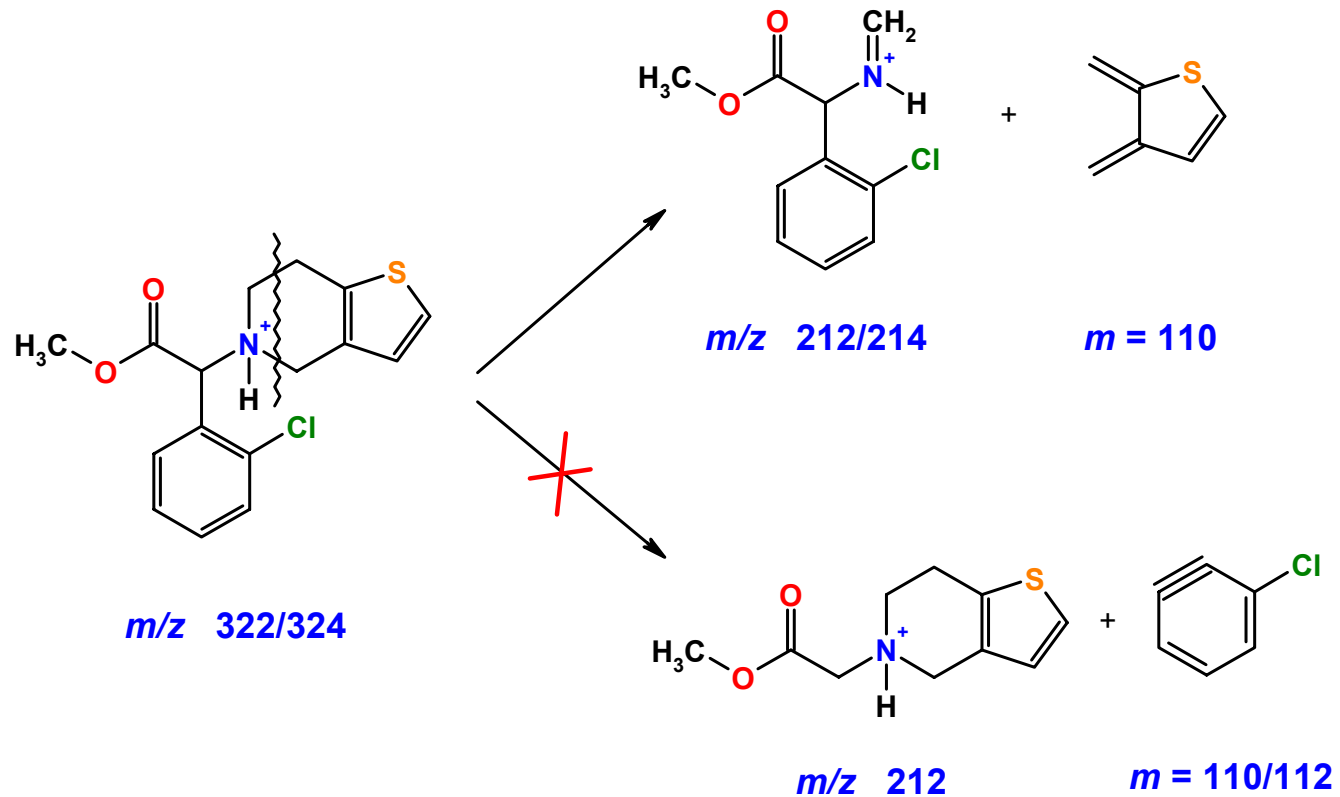


+MS2 (324.40) CE (30): Period 3, Exp 3, 2.362 to 2.613 min from Sample 4 (frag 9/1 ACN H2...

Max. 2.0e5 cps.



# Fragmentacja Clopidogrelu – rzeczywisty przebieg



# Literatura polskojęzyczna z dziedziny spektrometrii mas

