



# **Použití GC TOFMS ve speciálních analýzách vzorků potravin**

Pavel Jiroš

# Pegasus BT

- Přístroj s jednotkovým rozlišením
  - TOF (rychlost, plná spektra)
  - Robustnost
  - Citlivost
  - Iontový zdroj bez nutnosti čištění
  - GC nebo GCxGC uspořádání



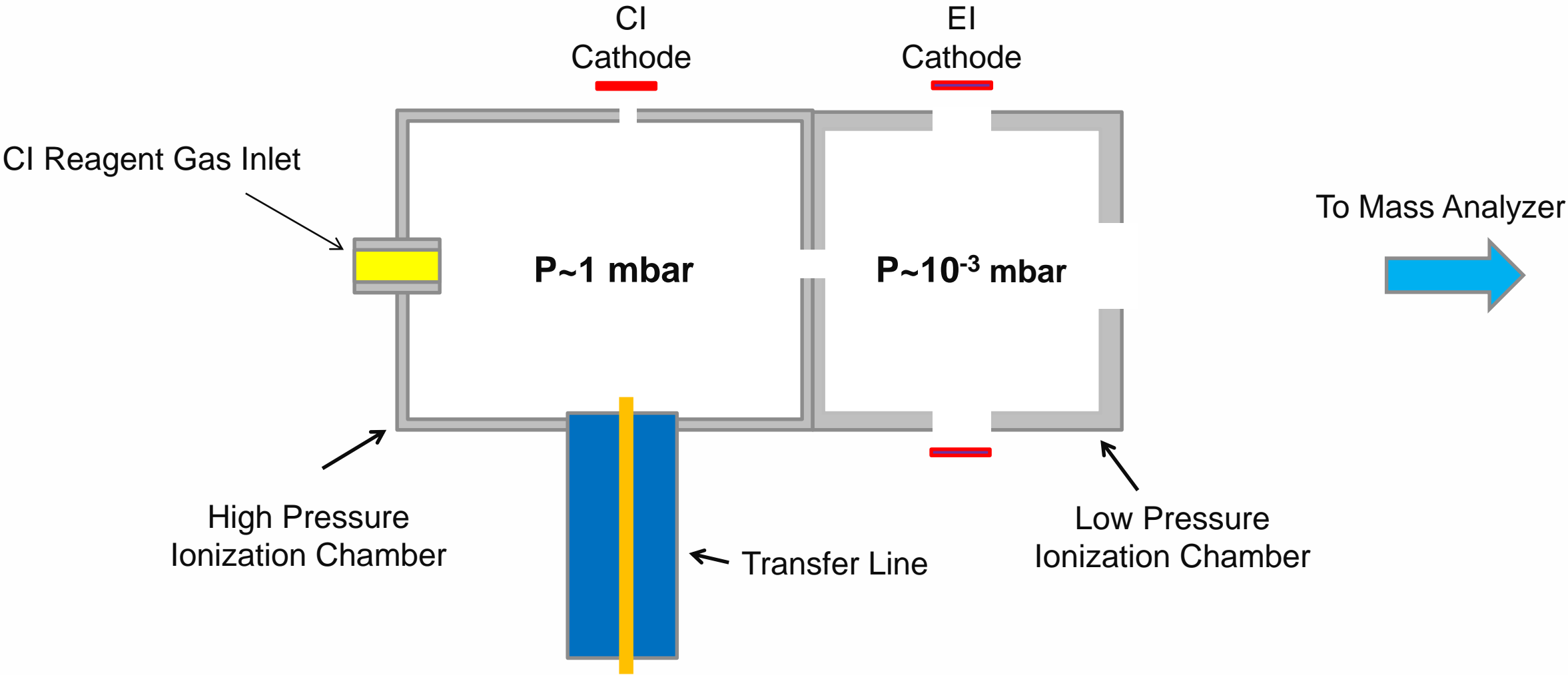
# Pegasus HRT<sup>+</sup>



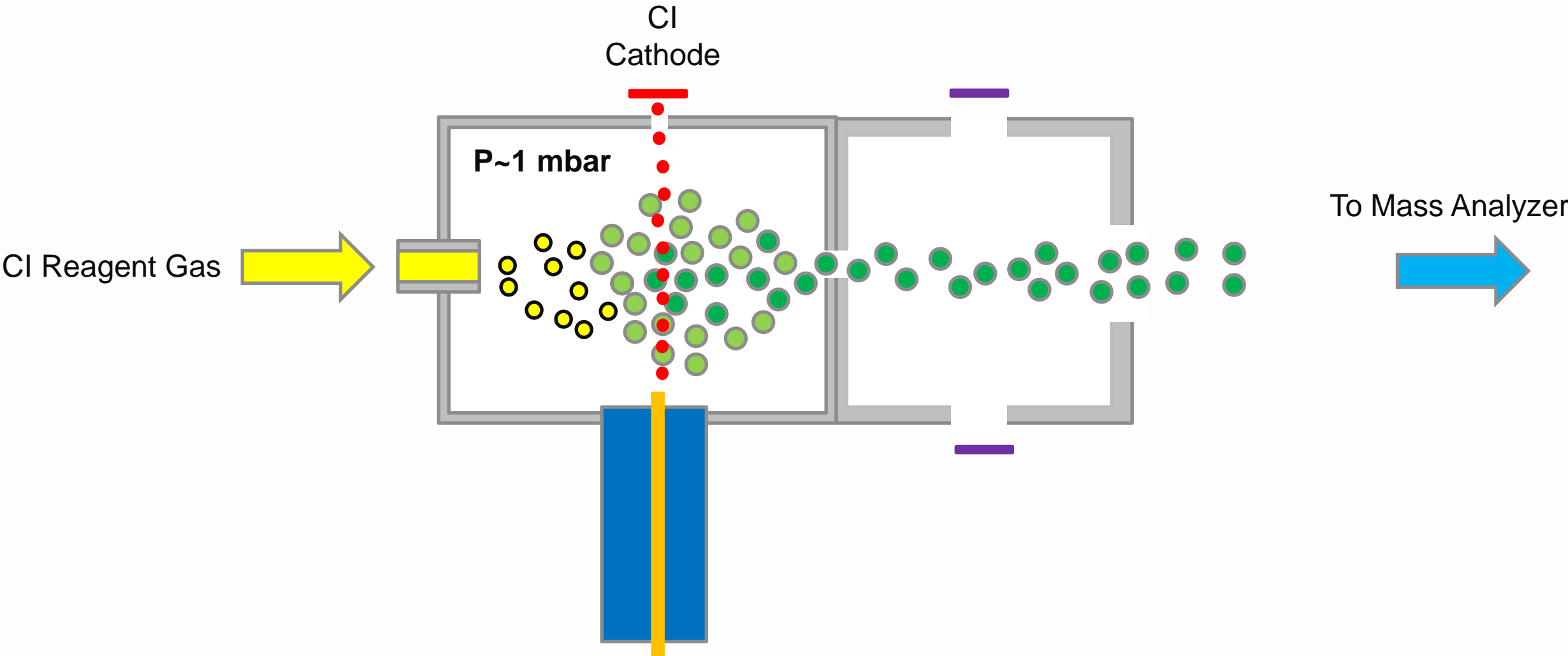
- Příklad s vysokým rozlišením
  - TOF (rychlost, plná spektra)
  - Přesnost do 1 ppm
  - Rozlišení 50 000
  - Iontový zdroj EI a CI
  - GC nebo GCxGC uspořádání

# Dual Chamber Ion Source

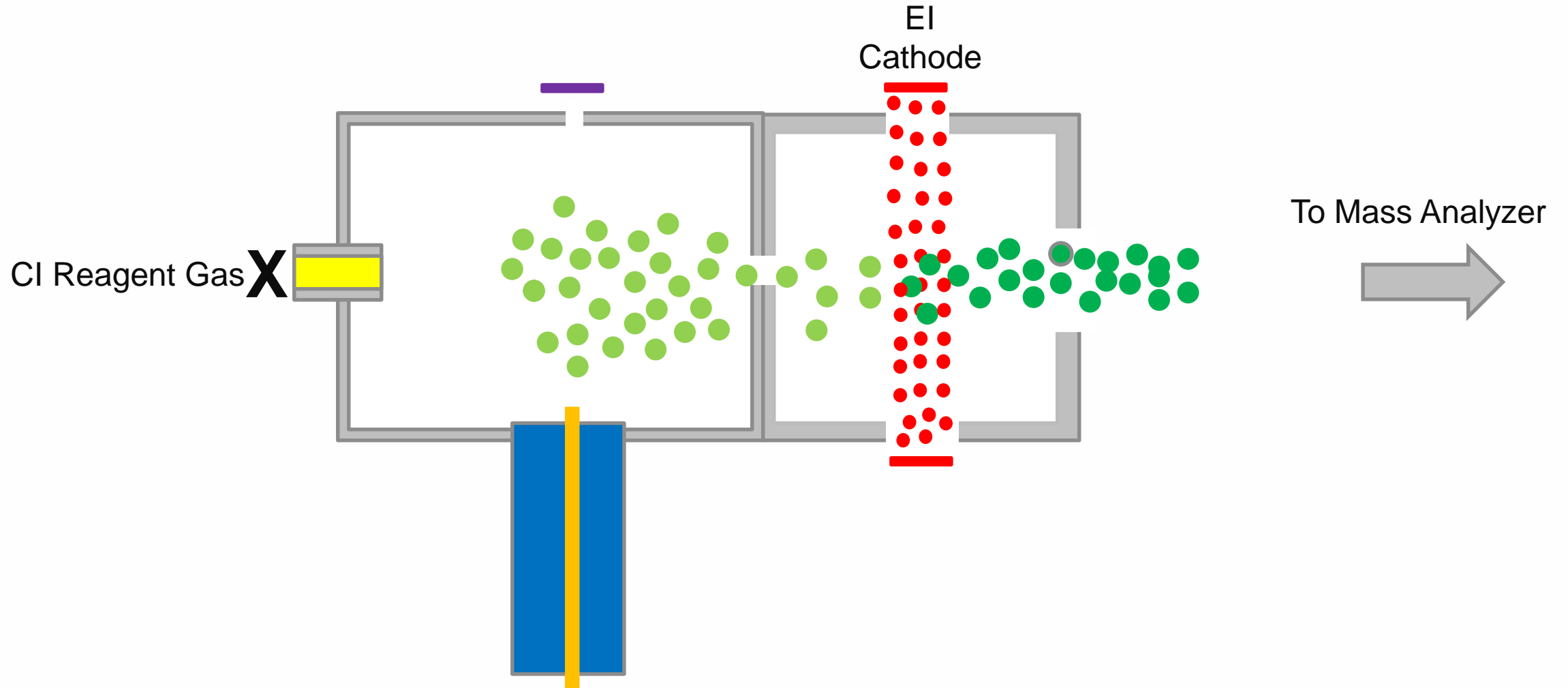
## One Source - Three Ionization Modes



# Dual Chamber Ion Source PCI/NCI



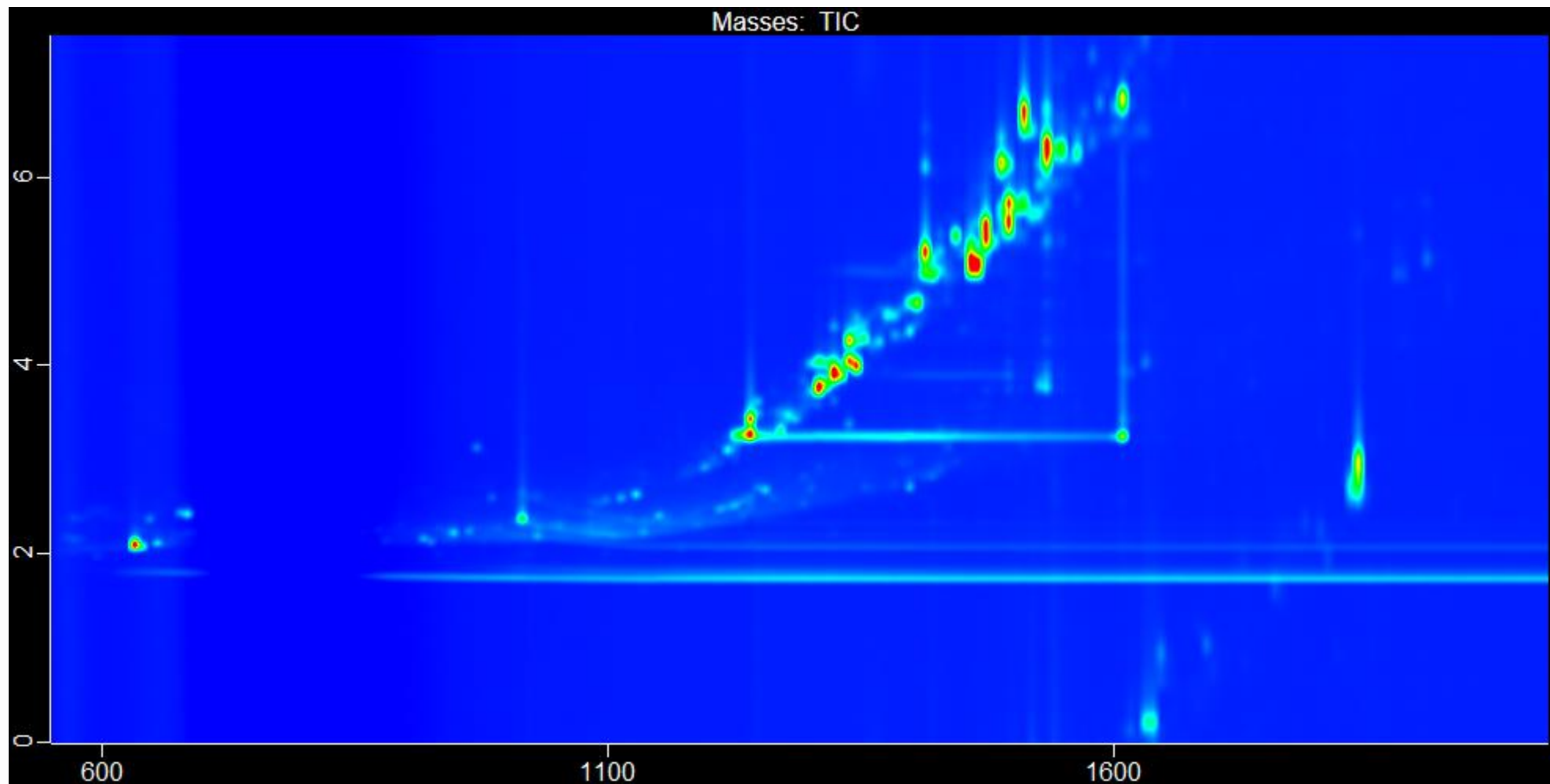
# Dual Chamber Ion Source EI



# Steroidy v potravinových doplňcích

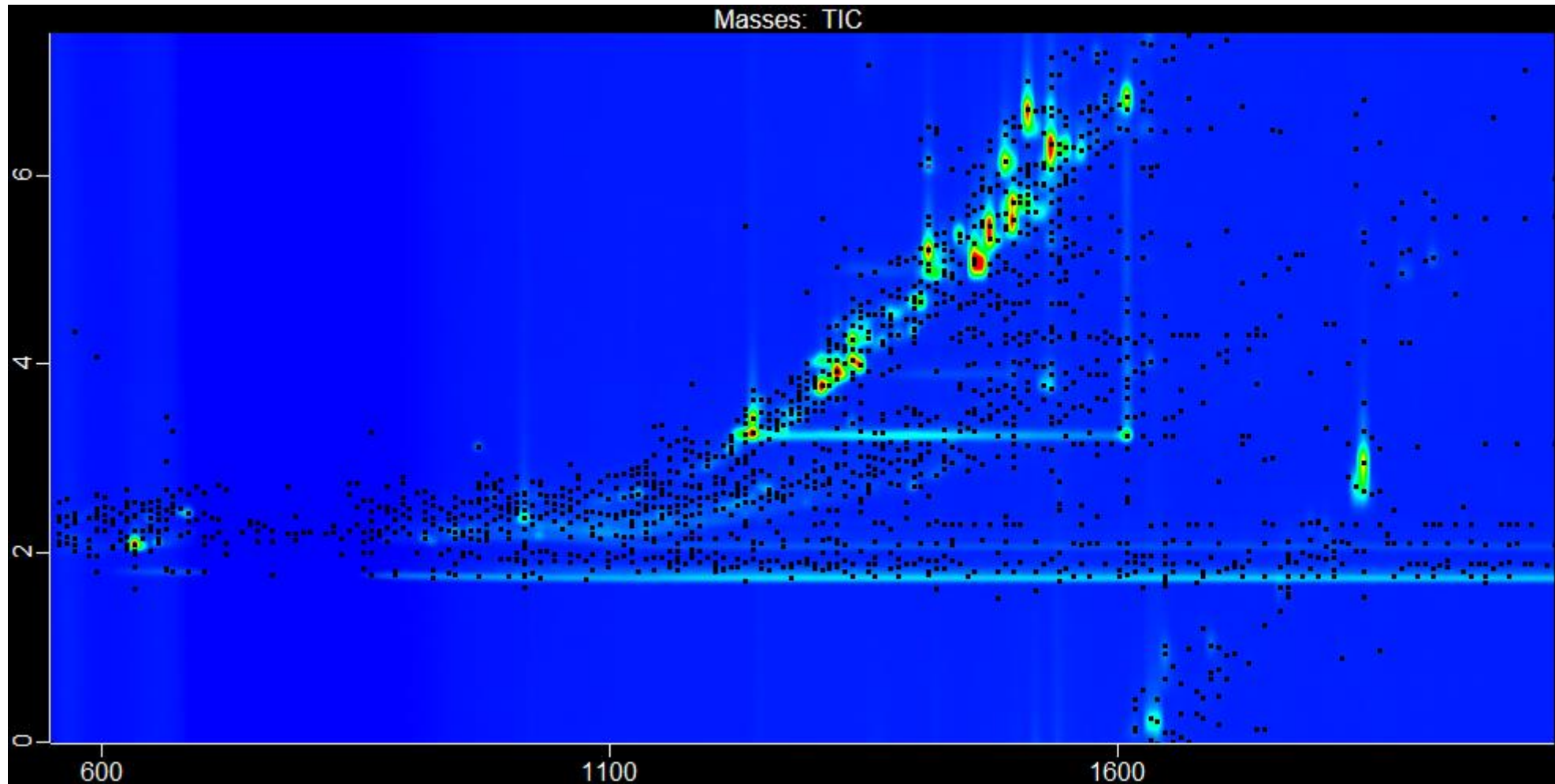
- Vzorke měřeny v minulosti na SZPI technikou GCxGCMS na starším typu Pegasus 4D
- Nyní porovnání na přístroji Pegasus HRT+ 4D s DC iontovým zdrojem

# GCxGC-DC EI

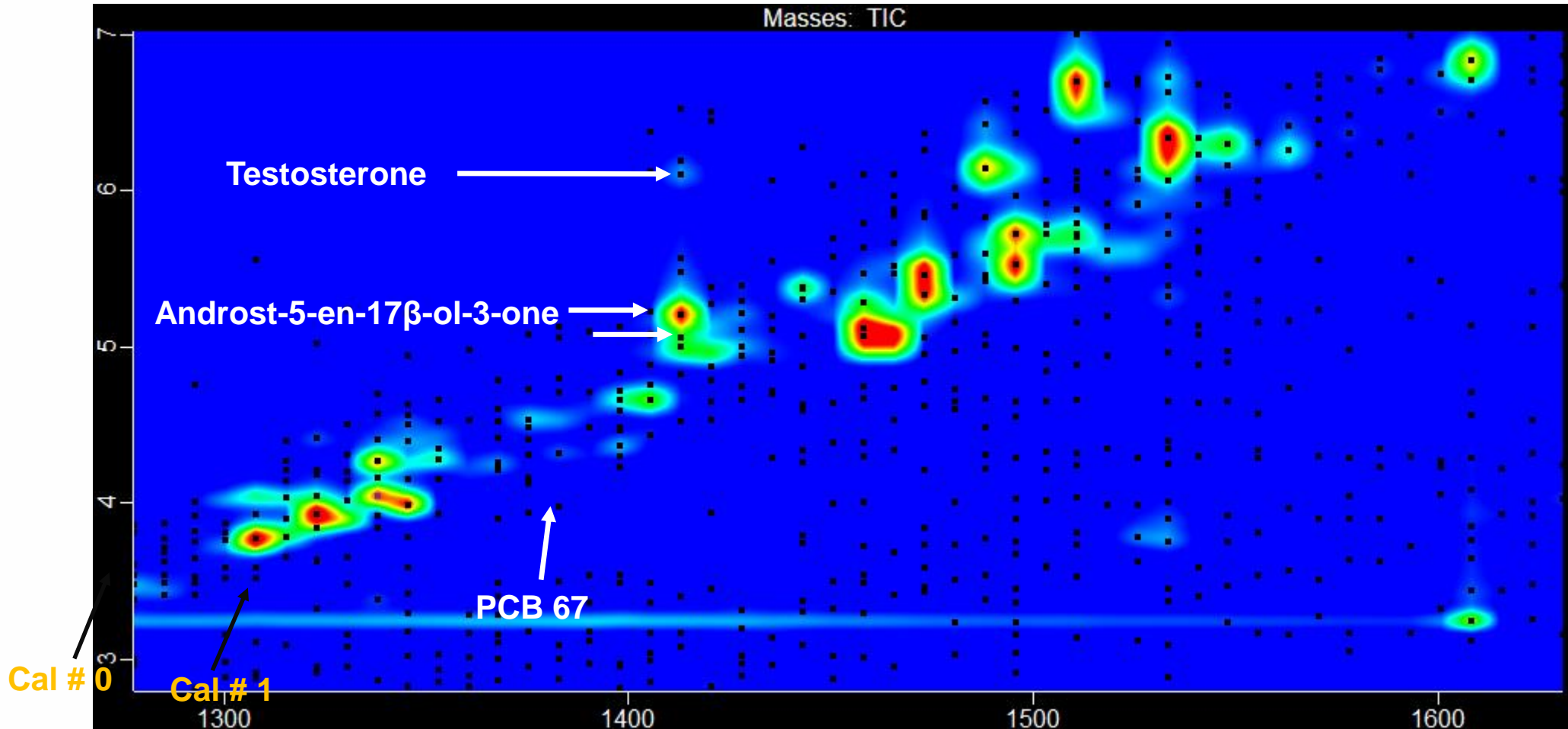




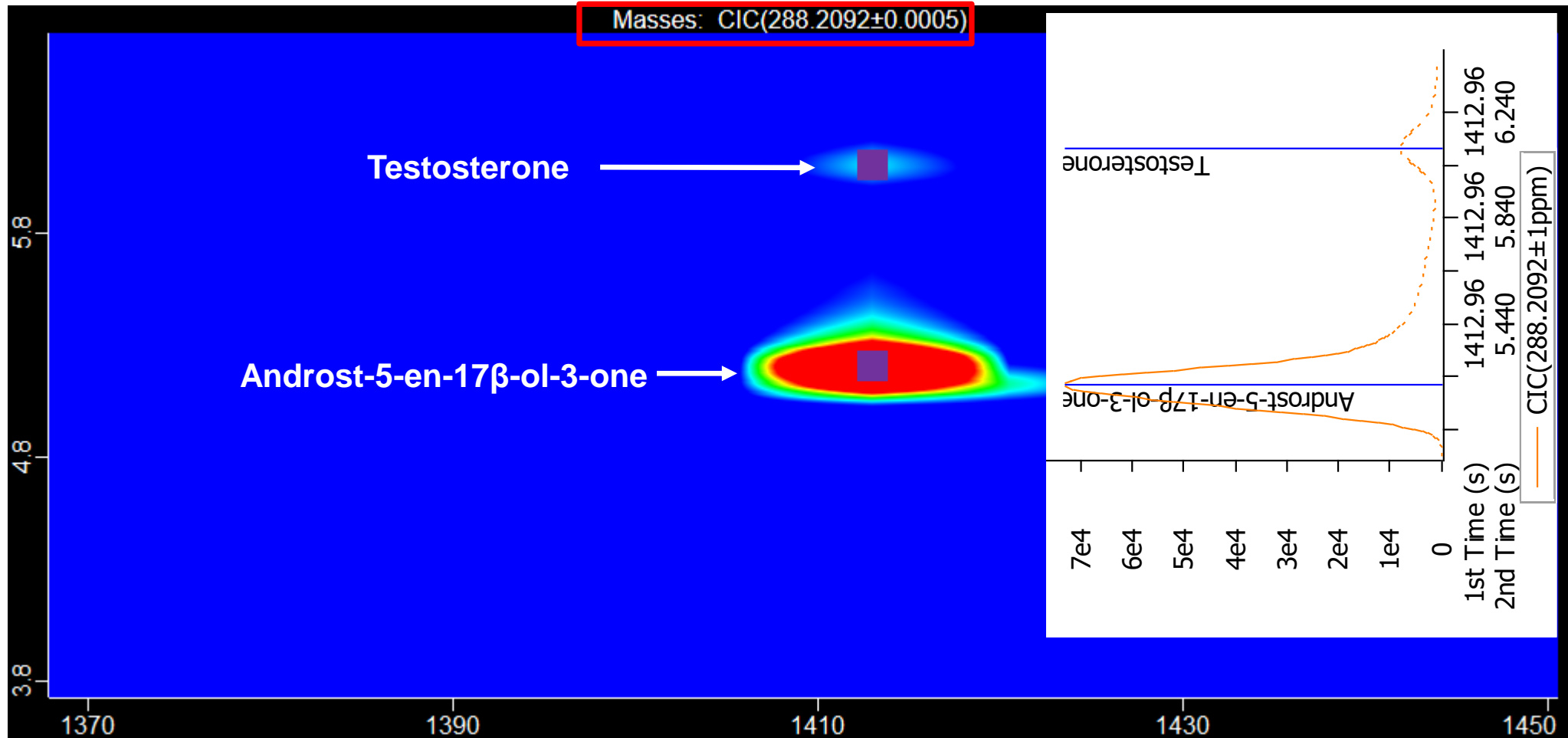
# GCxGC-DC EI po automatickém vyhledávání píků



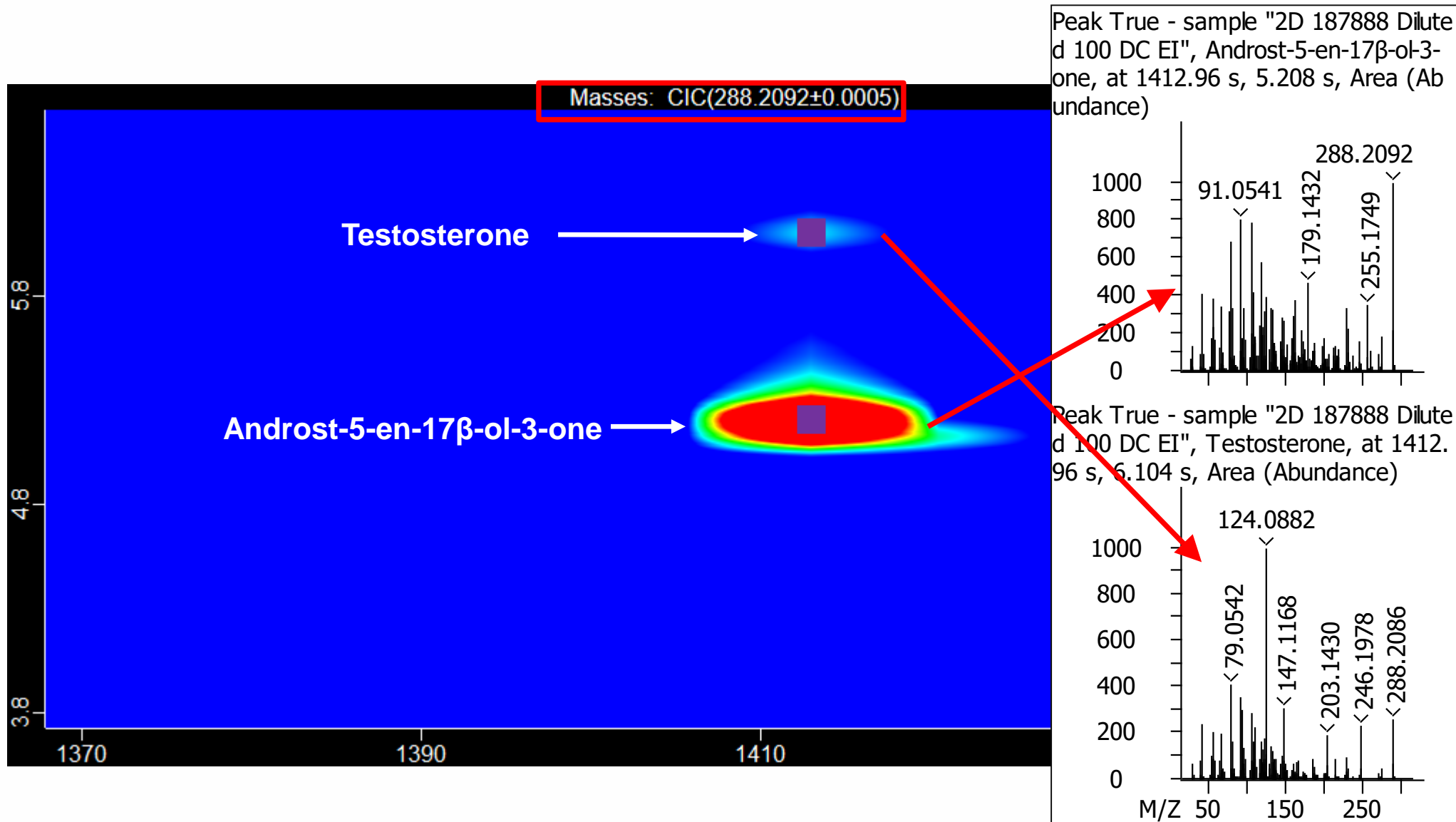
# Testosterone GCxGC-DC EI



# Testosterone GCxGC-DC EI

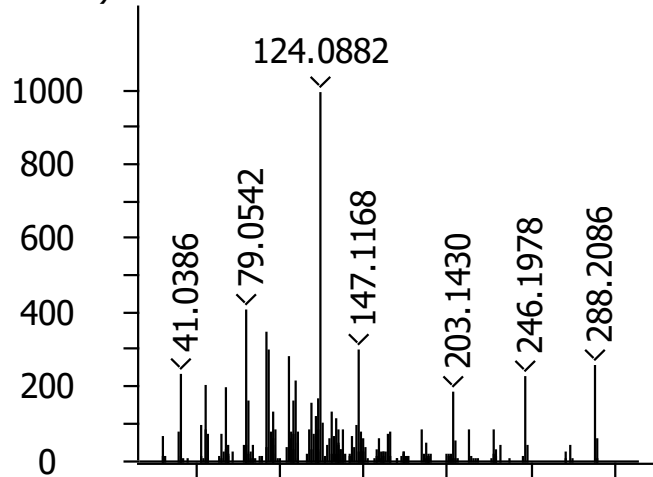


# Testosterone GCxGC-DC EI

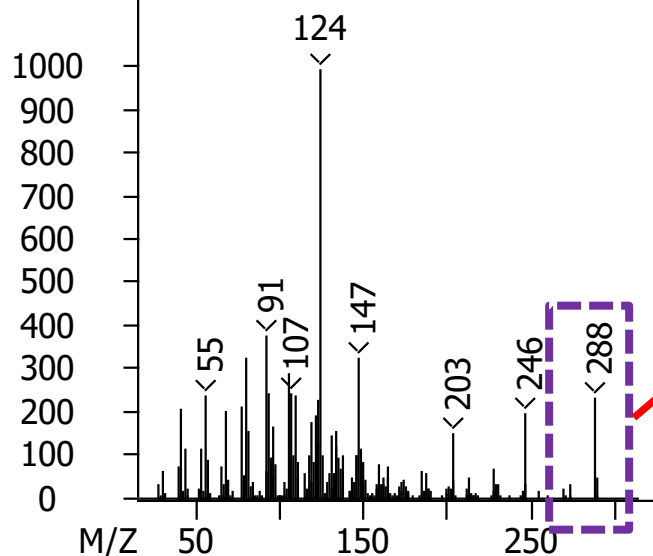


# Testosterone GCxGC-DC EI

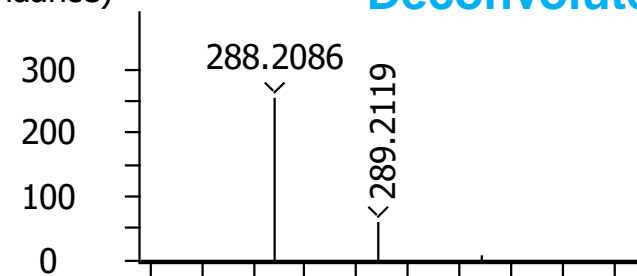
Peak True - sample "2D 187888 Diluted 100 DC EI", Testosterone, at 1412.96 s, 6.104 s, Area (Abundance)



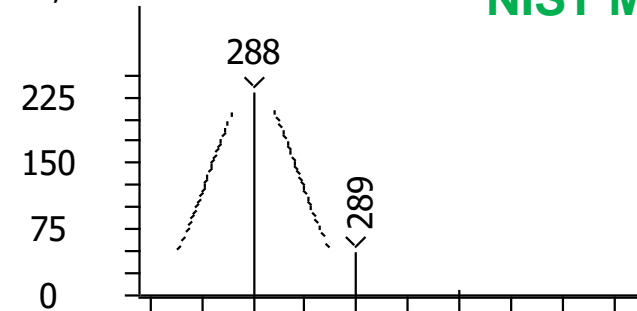
Library Hit - Similarity: 909 - Library: replib - Testosterone, Abundance



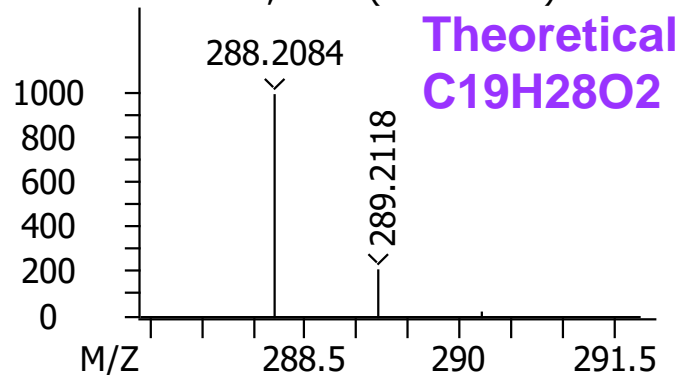
Peak True - sample "2D 187888 Diluted 100 DC EI", Testosterone, at 1412.96 s, 6.104 s, Area (Abundance) **Deconvoluted**

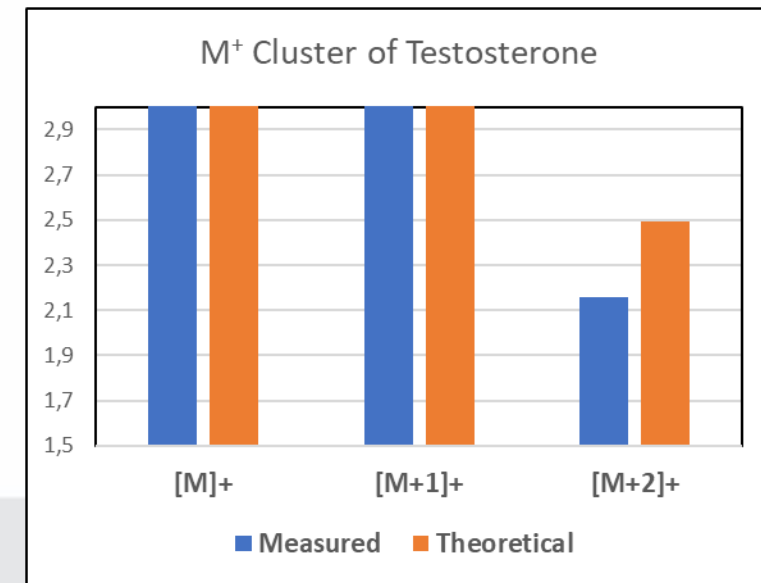
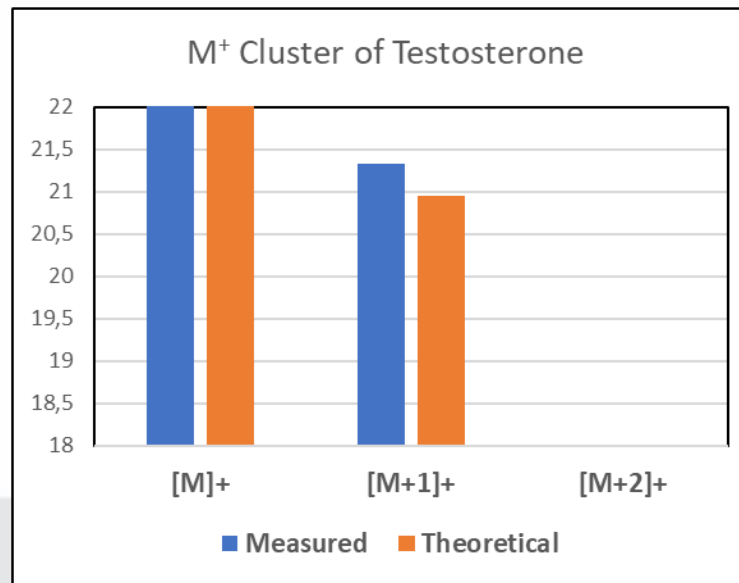
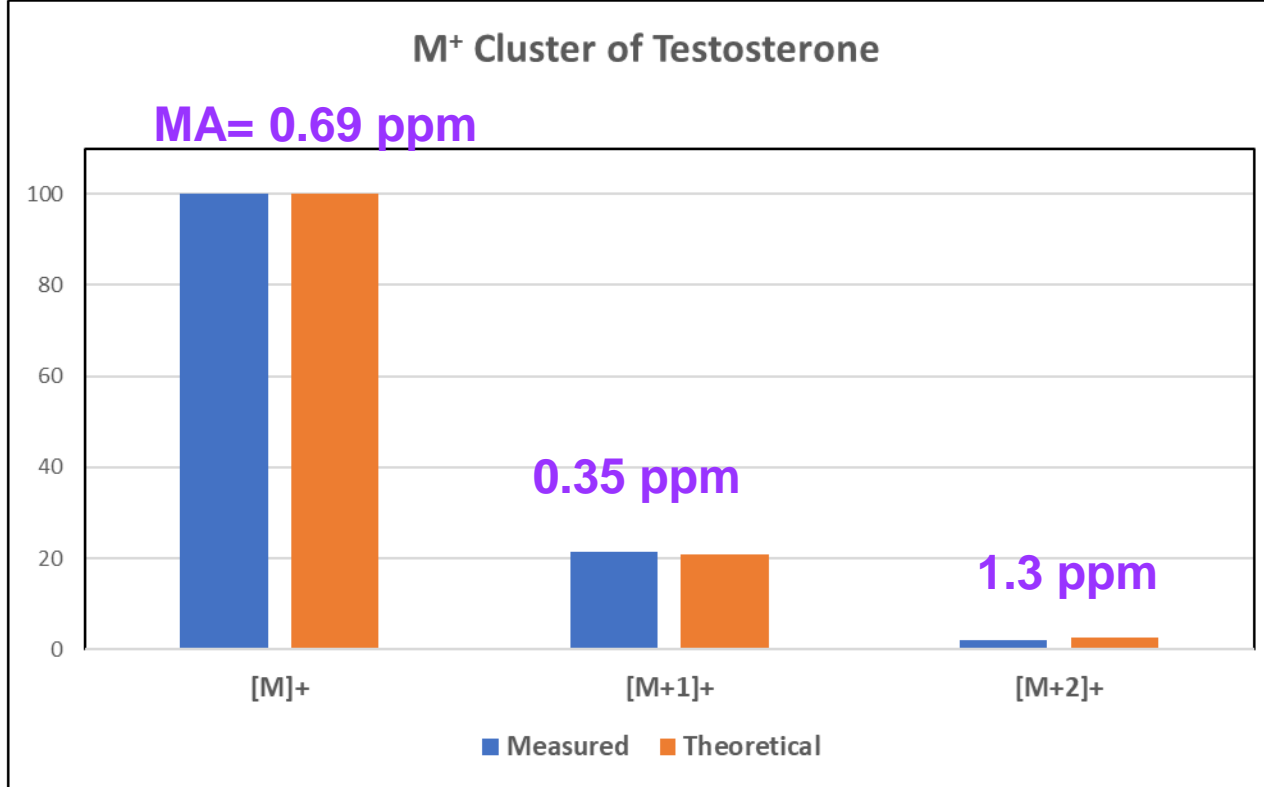


Library Hit - Similarity: 909 - Library: replib - Testosterone, Abundance **NIST MS**



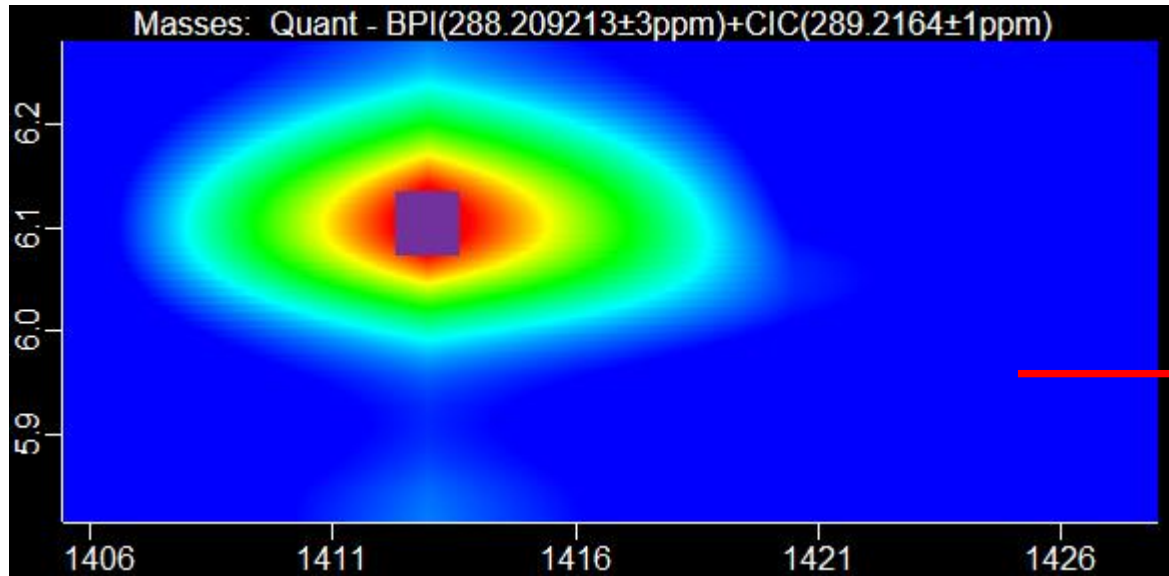
Library Hit - Similarity: 983 - Library: Formula Computation - C19H28O2, Area (Abundance)





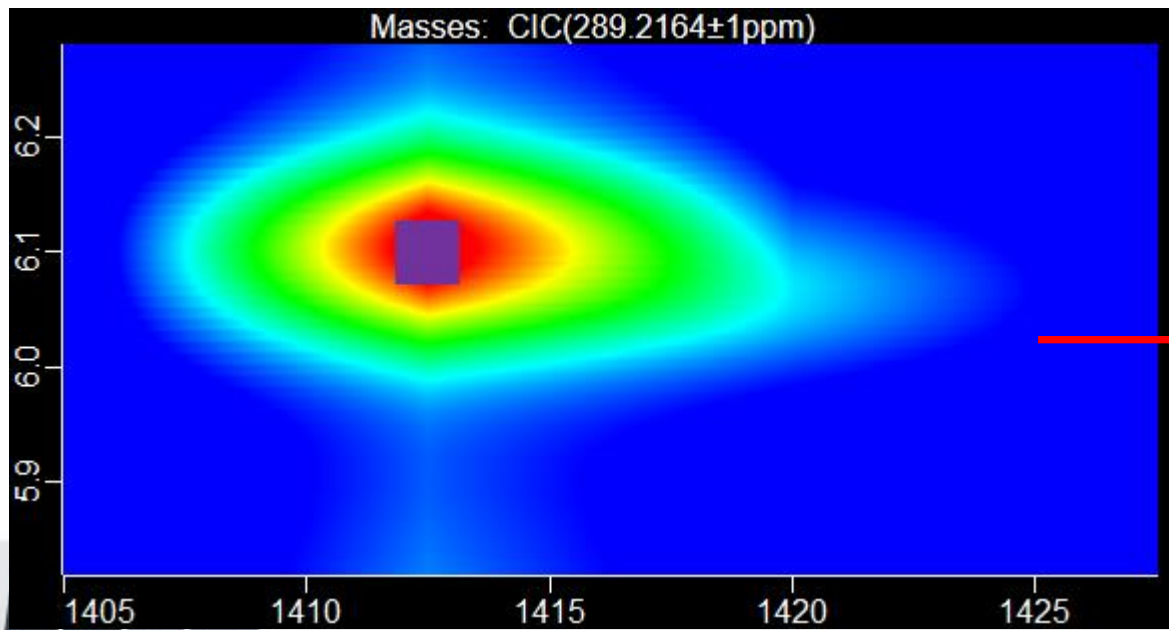
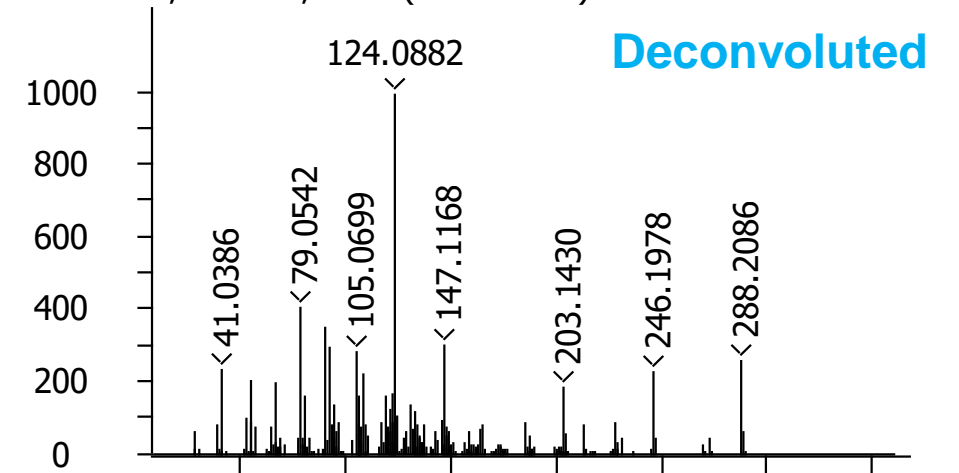


# Testosterone GCxGC-DC PCI



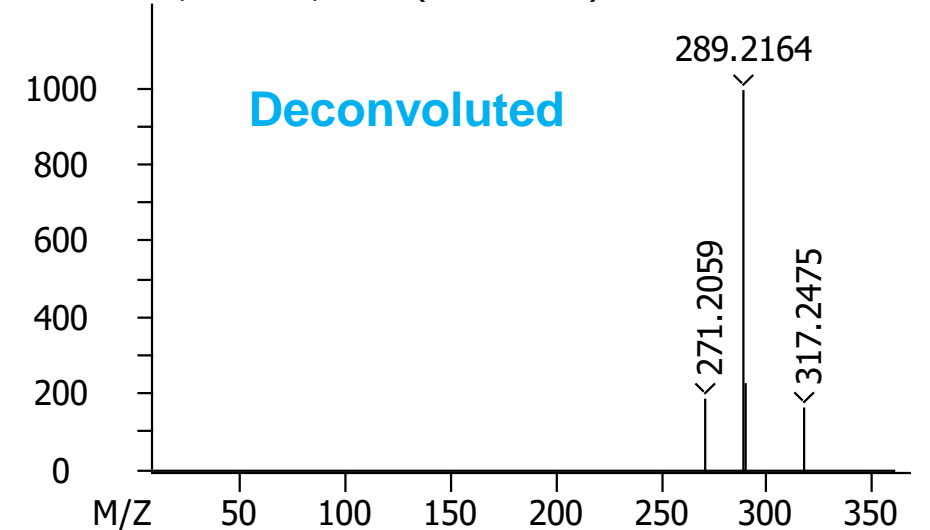
EI

Peak True - sample "2D 187888 Diluted 100 DC EI", Testosterone, at 1412.96 s, 6.104 s, Area (Abundance)

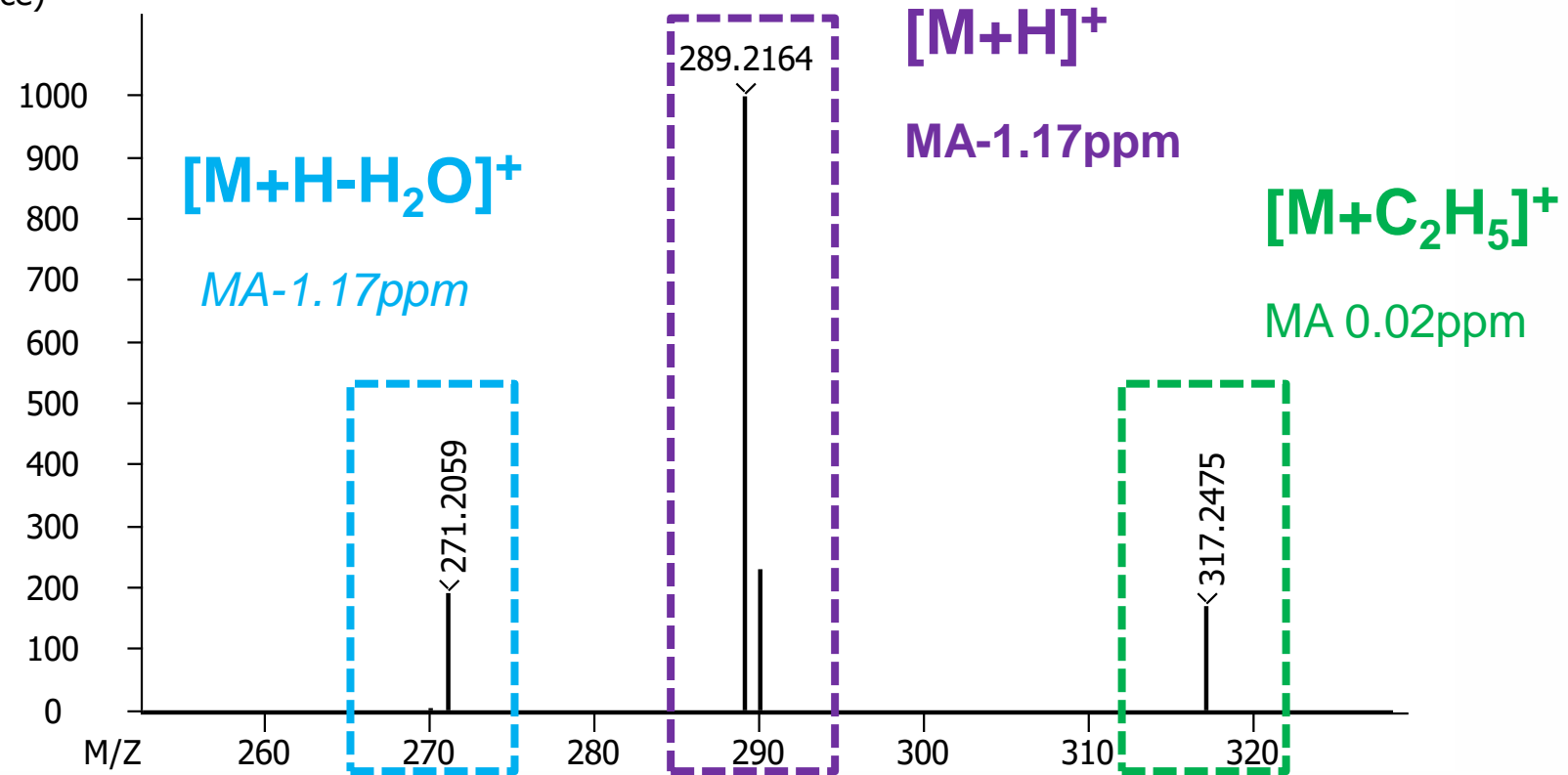


PCI

Peak True - sample "2D 187888 Diluted 100 DC PCI", Testosterone, at 1412.5 s, 6.100 s, Area (Abundance)



Peak True - sample "2D 187888 Diluted 100 DC PCI", Testosterone, at 1412.5 s, 6.100 s, Area (Abundance)

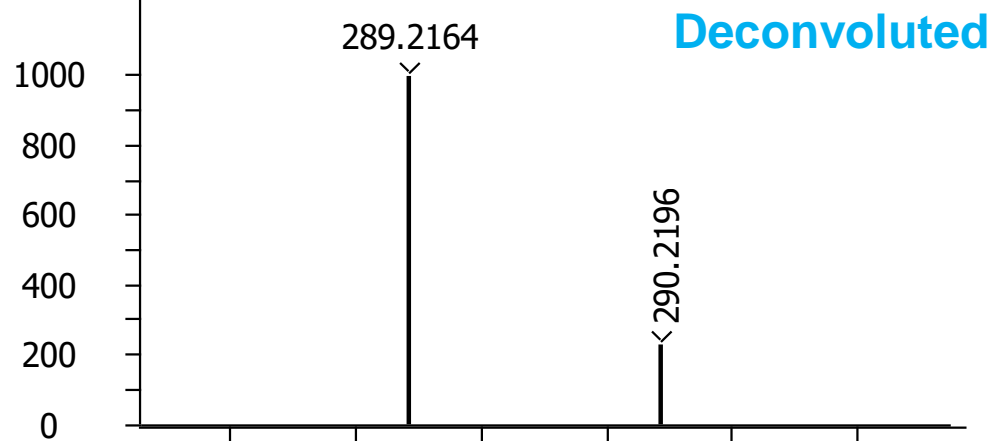


LECO CONFIDENTIAL

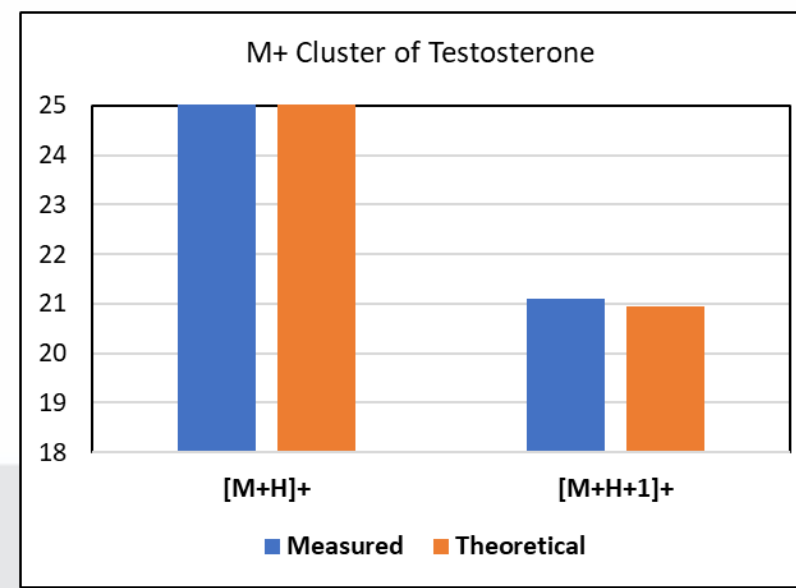
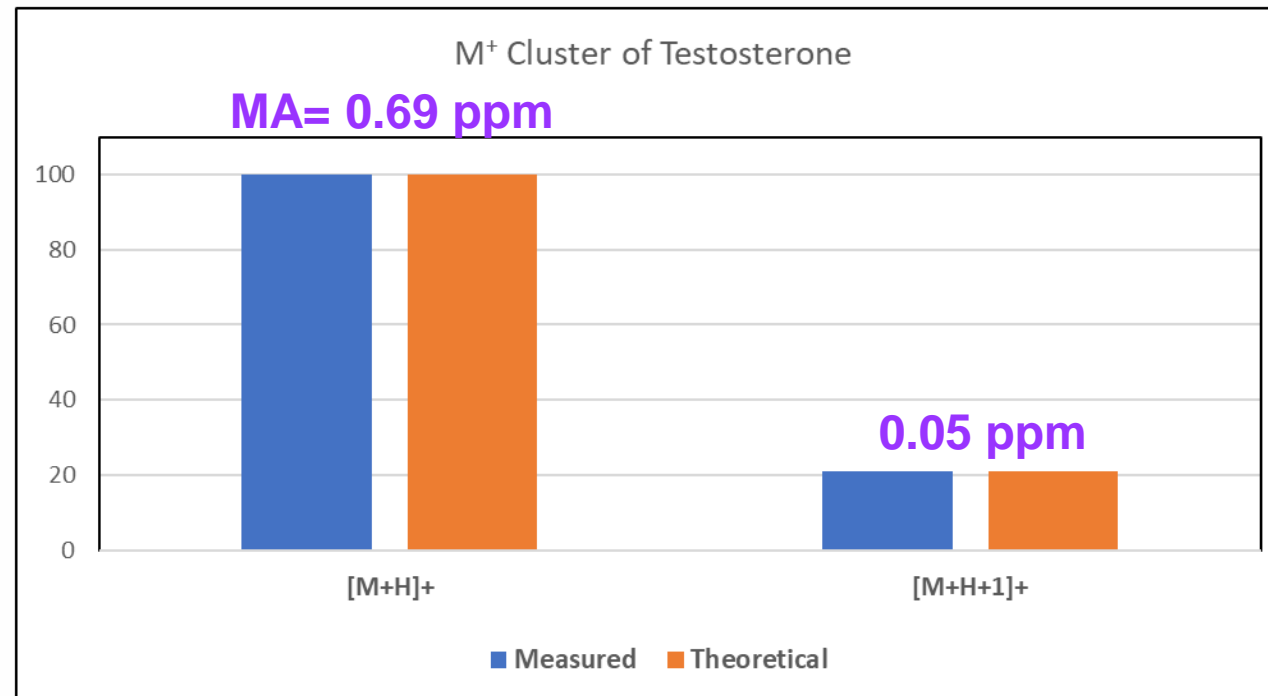
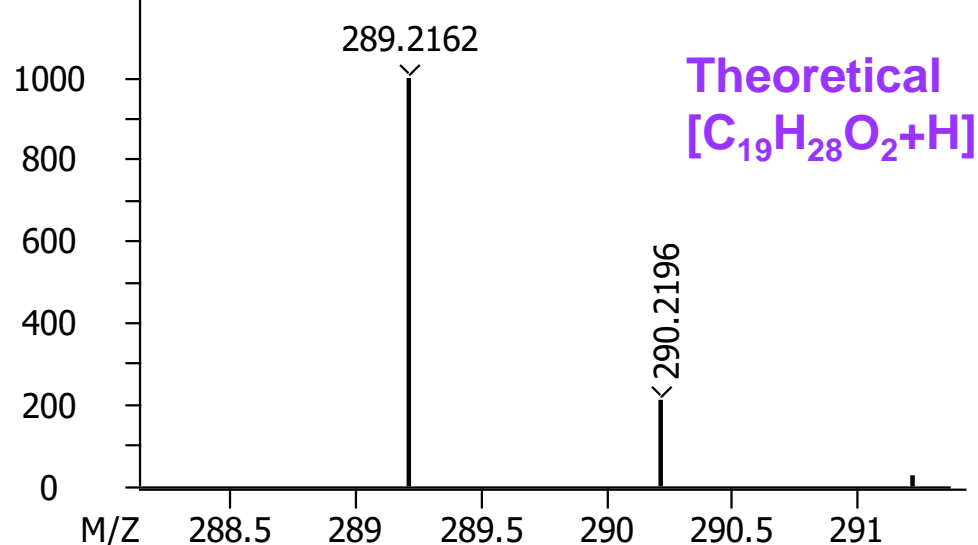


# Testosteron GCxGC-DC PCI

Peak True - sample "2D 187888 Diluted 100 DC PCI", Testosterone, at 1412.5 s, 6.100 s, Area (Abundance)

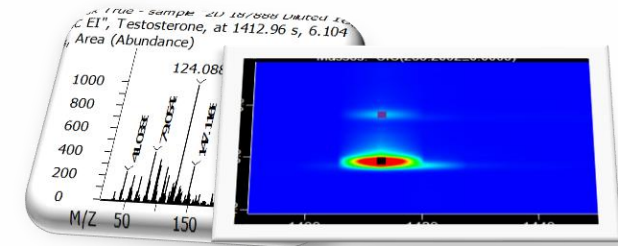


Library Hit - Similarity: 974 - Library: - C<sub>19</sub>H<sub>28</sub>O<sub>2</sub>, Area (Abundance)

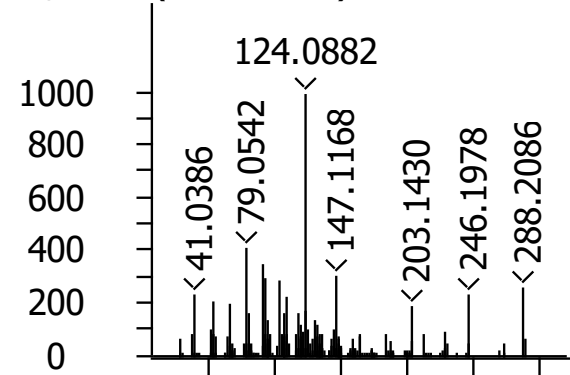


# Identifikace v HR

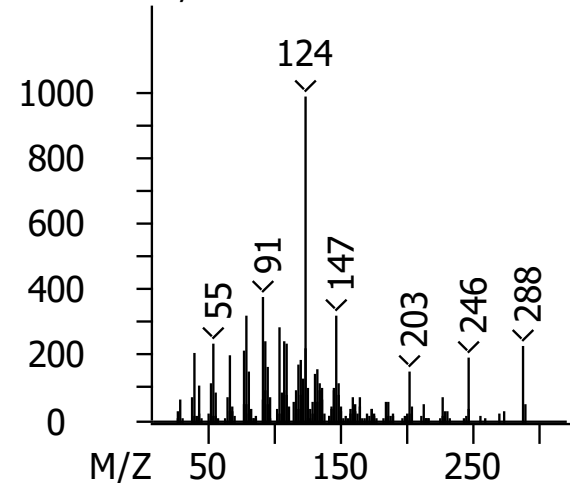
## 1. Porovnání s knihovnami



Peak True - sample "2D 187888 Diluted 10 0 DC EI", Testosterone, at 1412.96 s, 6.104 s, Area (Abundance)

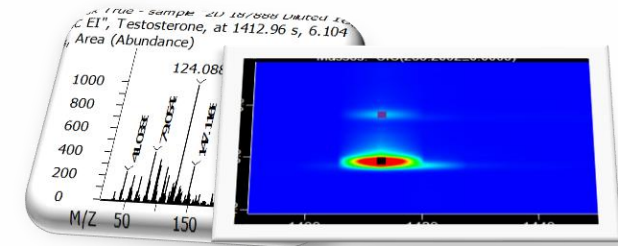


Library Hit - Similarity: 909 - Library: replib - Testosterone, Abundance



# Identifikace v HR

1. Porovnání s knihovnami
2. Porovnání RI



NIST MS Search 2.3 - [Name search]

File Search View Tools Options Window Help

TESTOSTERON Clear a-z mainlib From I

Testosteroid  
Testosteron  
Testosteron-11-ol  
Testosterone  
Testosterone, 10-d  
Testosterone 17-a  
Testosterone 17-a  
Testosterone 17-b  
Testosterone 17- $\beta$ -1  
Testosterone 17- $\beta$ -1  
Testosterone 17- $\beta$ -1  
Testosterone 17- $\beta$ -1  
Testosterone 17- $\beta$ -1  
Testosterone 17- $\beta$ -1  
Testosterone 17- $\beta$ -1  
Testosterone 17-e  
Testosterone, 17-e  
Testosterone 17-h  
Testosterone 17-h  
Testosterone 17-h  
Testosterone, 17-n  
Testosterone, 17-C  
Testosterone 17-pl  
Testosterone-17-pi  
Testosterone, 1-de  
Testosterone, 1-de  
Testosterone, 1-de  
Testosterone, 3-HI  
Testosterone, 3-MI  
Testosterone, 3-MI  
Testosterone, 3-MI

Mass spectrum showing relative abundance (0 to 100) versus m/z (30 to 300). Key peaks are labeled: 29, 41, 55, 67, 79, 91, 105, 124 (base peak), 133, 147, 165, 185, 203, 228, 246, 288. A chemical structure of testosterone is overlaid on the spectrum.

(mainlib) Testosterone

69.component of Mal-O-Fem (Salt/Mix)  
70.component of Intrinsa (Salt/Mix)  
71.component of Tostrex (Salt/Mix)

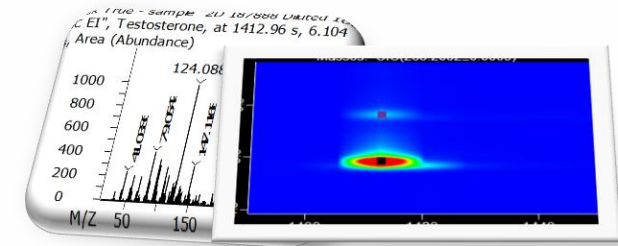
Experimental RI median $\pm$ deviation (#data)  
Standard non-polar: 2620 $\pm$ 11 (5)  
Estimated non-polar retention index (n-alkane scale):  
Value: 2139 iu  
Confidence interval (Low reliability): 174(50%) 752(95%) iu

Retention index.  
1. Value: 2620 iu  
Column Type: Packed  
Column Class: Standard non-polar

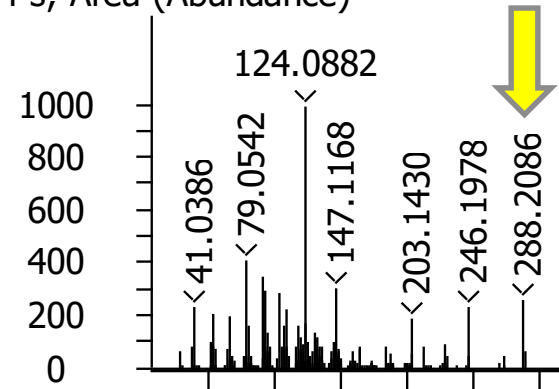
Names Structures Plot/Text Plot

# Identifikace v HR

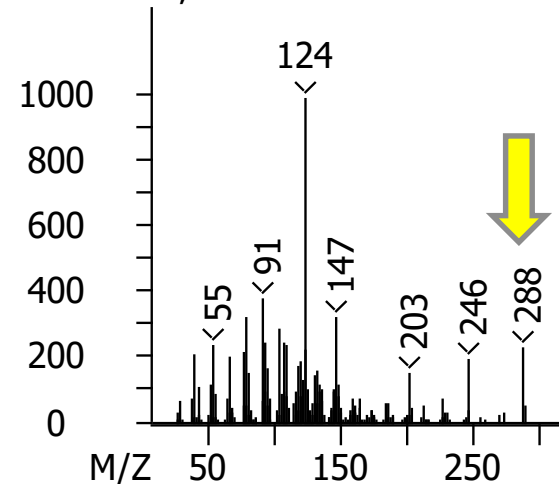
1. Porovnání s knihovnami
2. Porovnání RI
3. Hledání molekulárního píku



Peak True - sample "2D 187888 Diluted 10 0 DC EI", Testosterone, at 1412.96 s, 6.104 s, Area (Abundance)

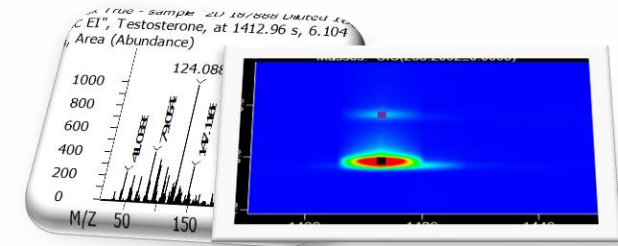


Library Hit - Similarity: 909 - Library: replib - Testosterone, Abundance

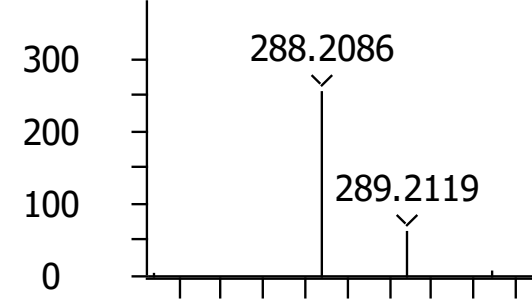


# Identifikace v HR

1. Porovnání s knihovnami
2. Porovnání RI
3. Hledání molekulárního píku
4. Přesnost naměřené hmoty molekulárního píku, pokud je přítomen

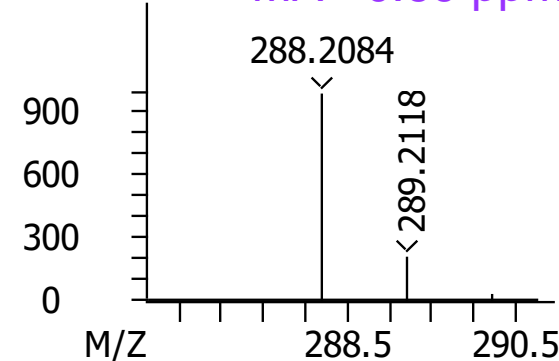


Peak True - sample "2D 187888 Diluted 100 DC EI", Testosterone, at 1412.96 s, 6.104 s, Area (Abundance)



Deconvoluted

Library Hit - Similarity: 983 - Library: Formula Computation - C<sub>19</sub>H<sub>28</sub>O<sub>2</sub>, Area (Abundance)

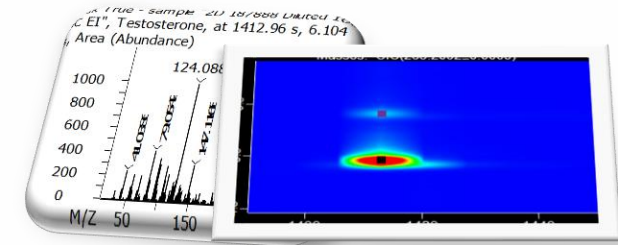


Theoretical  
C<sub>19</sub>H<sub>28</sub>O<sub>2</sub>

# Identifikace v HR

1. Porovnání s knihovnamí
2. Porovnání RI
3. Hledání molekulárního píku
4. Přesnost naměřené hmoty molekulárního píku, pokud je přítomen

Konvenční přístup



Data Processing Method - "Lib + score only"

Auto Select

**Spectral Similarity**  Formula  Reverse Target  Accuracy

Enable Spectral Similarity Library Search

Maximum Results:

Minimum mass to library search:

Maximum mass to library search:

Minimum molecular weight allowed:

Maximum molecular weight allowed:

Relative abundance threshold (0 - 998):

Minimum similarity for matches (0 - 999):

Minimum similarity before hit is assigned (0 - 999):

Add the libraries to use for searching below:

mainlib  
replib

Column Phase:

Retention Index Filtering

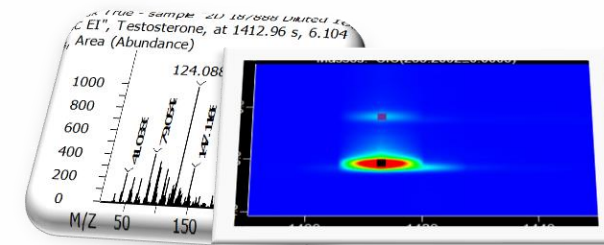
Filter by Retention Index:  
Tolerance

Allow estimated RI substitution for non-polar types

Use other non-polar column type data if selected non-polar type data is absent

# Identifikace v HR

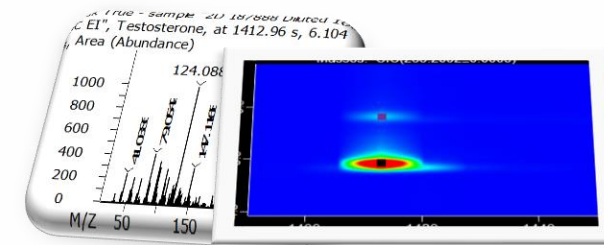
1. Porovnání s knihovnami
2. Porovnání RI
3. Hledání molekulárního píku
4. Přesnost naměřené hmoty molekulárního píku, pokud je přítomen
5. Další možnosti???



# LECO Identification Grading System

1. Porovnání s knihovnami
2. Porovnání RI
3. Hledání molekulárního píku
4. Přesnost naměřené hmoty molekulárního píku, pokud je přítomen
5. Více informací z HRMS dat ~ LECO

**Identification Grading System**





# Identification Grading System

IGS™ Scoring Configuration

Enable Similarity Check  
Minimum Similarity for Pass Rating ( 0 - 999 ):

Minimum Valid Similarity ( 0 - 999 ):

Enable Fragment Ion Check  
Minimum Abundance ( 100 - 998 ):

Required Mass Accuracy:  +/- Mass Window  mDa  ppm

Enable Molecular Ion Check  
Minimum Library Abundance ( 0 - 998 ):

Required Mass Accuracy:  +/- Mass Window  mDa  ppm

Enable Retention Index Check  
Retention Index Window:

Výsledkem je jediná hodnota

# Identification Grading System

Hit Table - 2D 187888 Diluted 100 DC EI

Hit	Name	Lib. RI	Mass Accuracy	Similarity	IGS Score	IGS Concerns
>1*	4-Chlordehydromethyltestosterone	2967 ± 0(1)	0.11	870	3.0	
2	4-Chlordehydromethyltestosterone	2967 ± 0(1)	0.11	844	3.0	
3	Tricyclo[7.4.0.0(3,8)]trideca-5,12-dien-2-one, 4		-0.24	606	-0.5	SS:0 ; Frag:-
4	Turinabol		N/A	580	-0.5	SS:- ; M+:0
5	Turinabol		N/A	571	-0.5	SS:- ; M+:0
6	Cyclopropane, 1-chloro-1-(3,3-diethoxy-1-propyl)		N/A	559	-0.5	SS:- ; M+:0
7	Turinabol		N/A	555	-0.5	SS:- ; M+:0
8	6β-Hydroxymethandienone	2948 ± 0(1)	N/A	681	-1.5	SS:0 ; Frag:- ; M+:0
9	Androsta-1,4-dien-3-one, 6,17-dihydroxy-, (6β,17β)		N/A	675	-1.5	SS:0 ; Frag:- ; M+:0
10	Androsta-1,4-dien-3-one, 17-hydroxy-17-methyl	2794 ± 0(1)	N/A	650	-1.5	SS:0 ; Frag:- ; M+:0

# Identification Grading System

Hit Table - 2D 187888 Diluted 100 DC EI

Hit	Name	Lib. RI	Mass Accuracy	Similarity	IGS Score	IGS Concerns
>1	4-Chlordehydromethyltestosterone	2967 ± 0(1)	0.11	876	3.0	
2	4-Chlordehydromethyltestosterone	2967 ± 0(1)	0.11	844	3.0	
3	Tricyclo[7.4.0.0(3,8)]trideca-5,12-dien-2-one, 4		-0.24	606	-0.5	SS:0 ; Frag:-
4	Turinabol		N/A	580	-0.5	SS:- ; M+:0
5	Turinabol		N/A	571	-0.5	SS:- ; M+:0
6	Cyclopropane, 1-chloro-1-(3,3-diethoxy-1-propyl		N/A	559	-0.5	SS:- ; M+:0
7	Turinabol		N/A	555	-0.5	SS:- ; M+:0
8*	6β-Hydroxymethandienone	2948 ± 0(1)	N/A	681	-1.5	SS:0 ; Frag:- ; M+:0
9	Androsta-1,4-dien-3-one, 6,17-dihydroxy-, (6β,1		N/A	675	-1.5	SS:0 ; Frag:- ; M+:0
10	Androsta-1,4-dien-3-one, 17-hydroxy-17-methyl	2794 ± 0(1)	N/A	656	-1.5	SS:0 ; Frag:- ; M+:0

# Identification Grading System

Hit Table - 2D 187888 Diluted 100 DC EI

Hit	Name	Lib. RI	Mass Accuracy	Similarity	IGS Score	IGS Concerns
>1	4-Chlordehydromethyltestosterone	2967 ± 0(1)	0.11	876	3.0	
2	4-Chlordehydromethyltestosterone	2967 ± 0(1)	0.11	844	3.0	
3	Tricyclo[7.4.0.0(3,8)]trideca-5,12-dien-2-one, 4		-0.24	606	-0.5	SS:0 ; Frag:-
4	Turinabol		N/A	580	-0.5	SS:- ; M+:0
5	Turinabol		N/A	571	-0.5	SS:- ; M+:0
6	Cyclopropane, 1-chloro-1-(3,3-diethoxy-1-propyl)		N/A	559	-0.5	SS:- ; M+:0
7	Turinabol		N/A	555	-0.5	SS:- ; M+:0
8*	6β-Hydroxymethandienone	2948 ± 0(1)	N/A	681	-1.5	SS:0 ; Frag:- ; M+:0
9	Androsta-1,4-dien-3-one, 6,17-dihydroxy-, (6β,1		N/A	675	-1.5	SS:0 ; Frag:- ; M+:0
10	Androsta-1,4-dien-3-one, 17-hydroxy-17-methyl	2794 ± 0(1)	N/A	656	-1.5	SS:0 ; Frag:- ; M+:0

Hit Table

## Hit Concerns:

SS:0

The Forward Similarity is < 700 for current match.

Frag:-

At least one Peak True m/z with an abundance above 300 does not have a mathematically possible formula ±5 PPM based on the matched spectra molecular formula.

M+:0

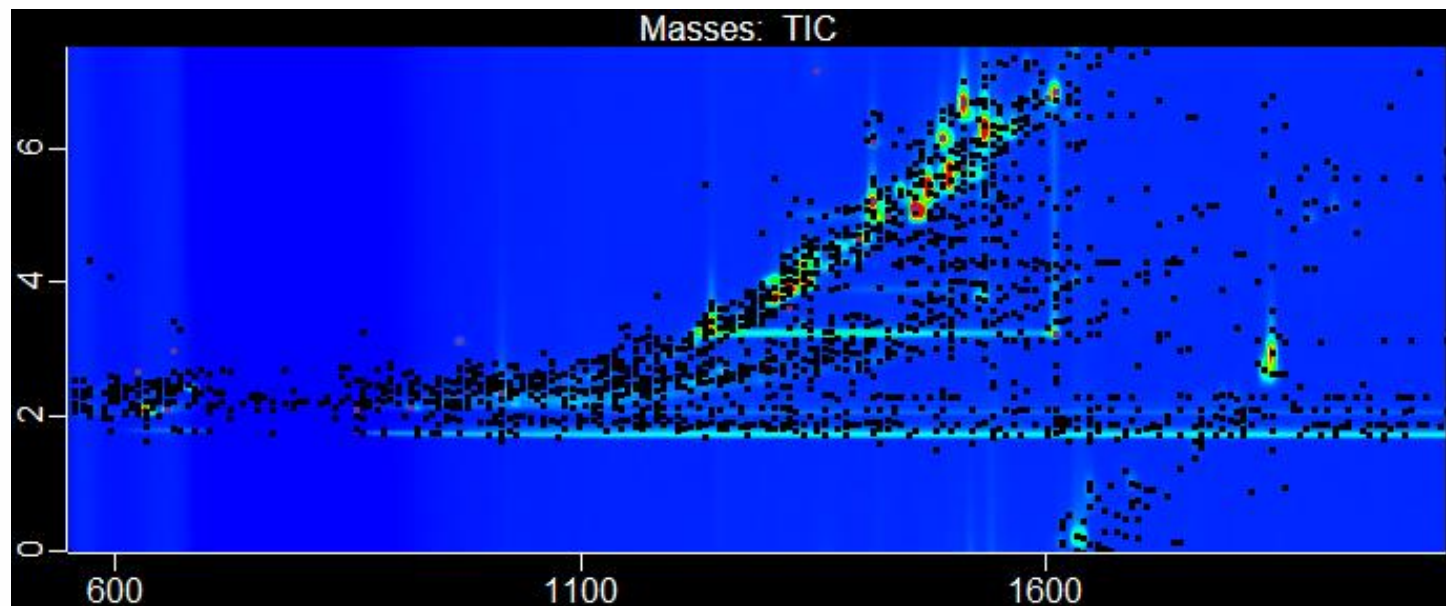
Library match does not contain a molecular ion above the 100 abundance threshold. A molecular ion is not expected.

→ Copy text to clipboard

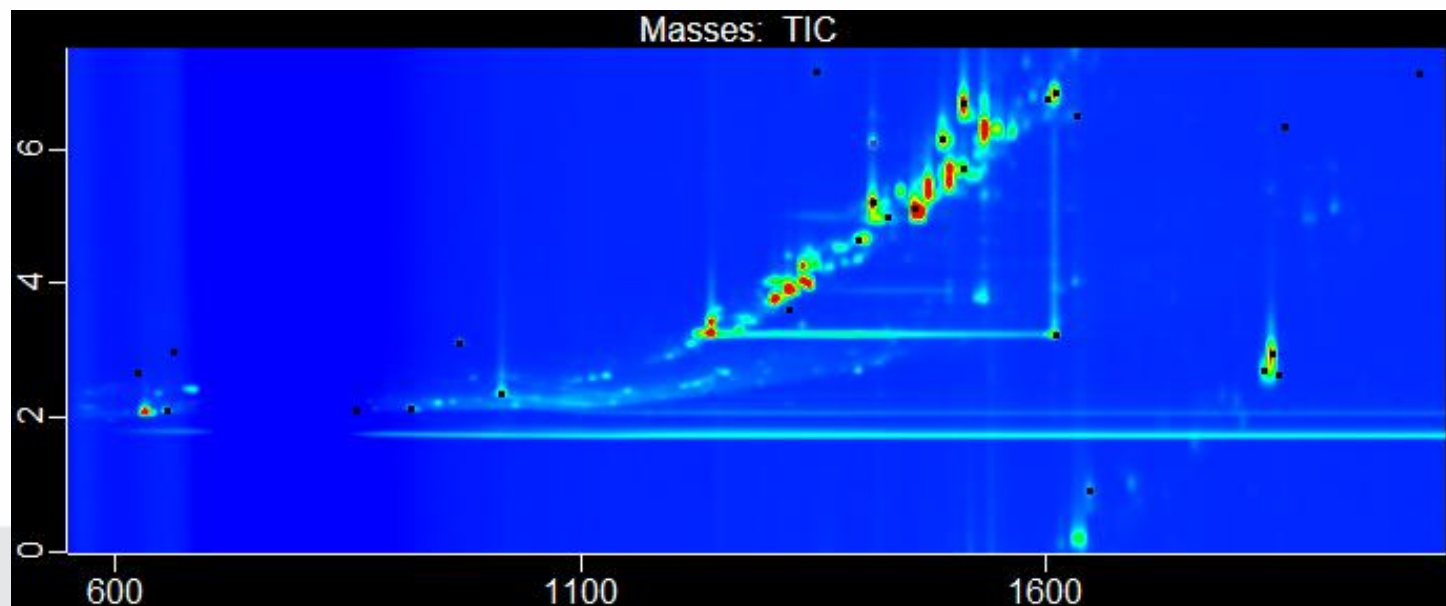
OK

# Identification Grading System

Necílený peak find  
~ 1800 píků

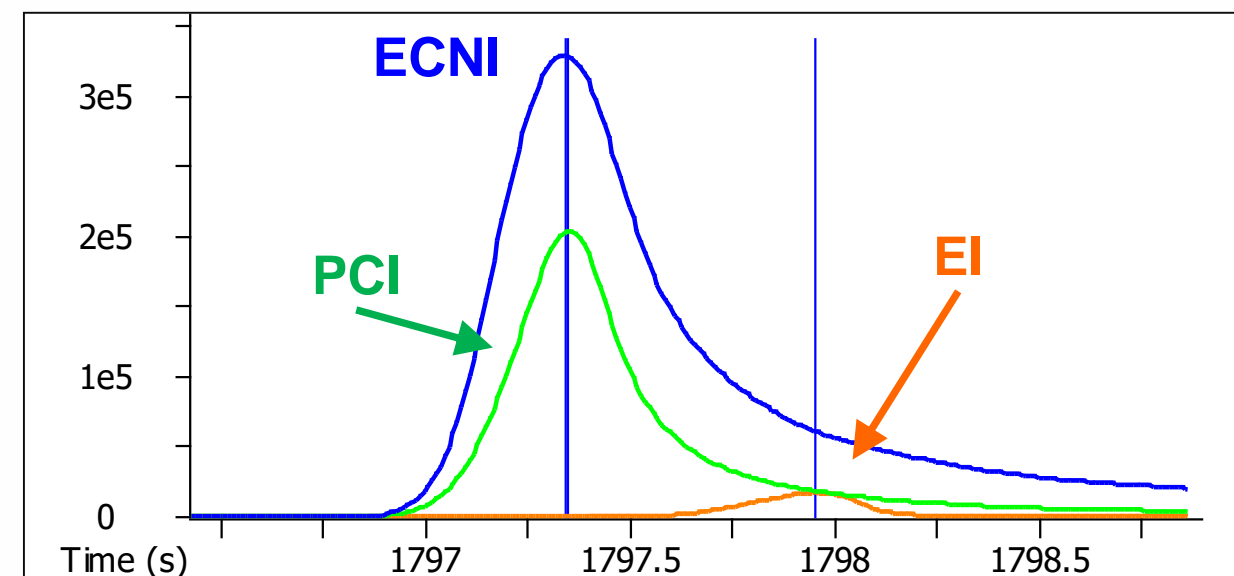
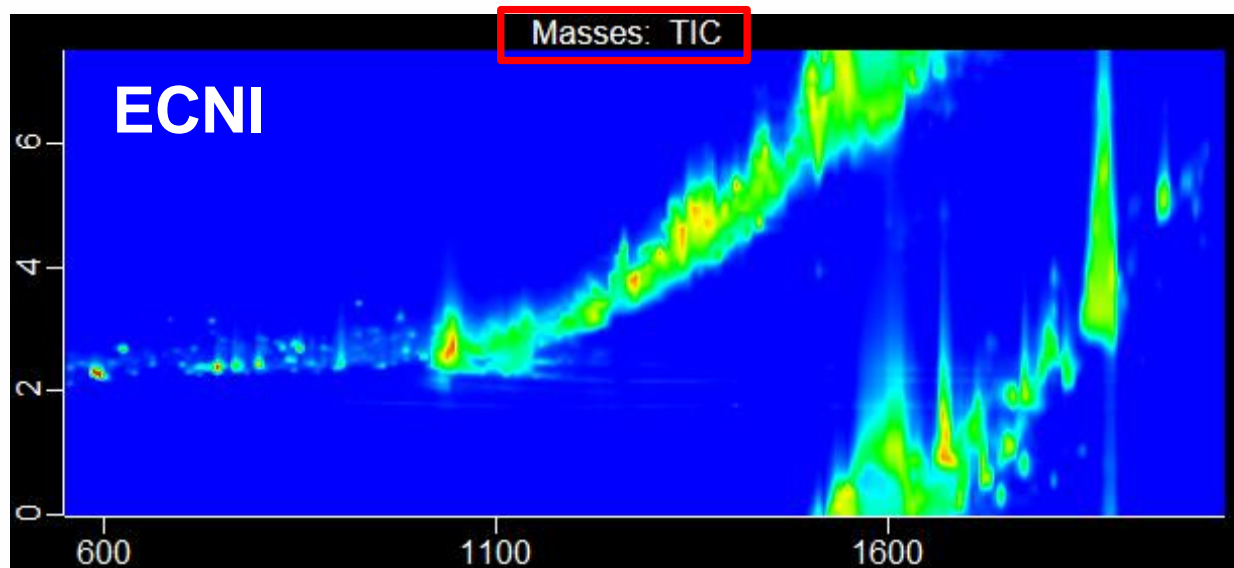
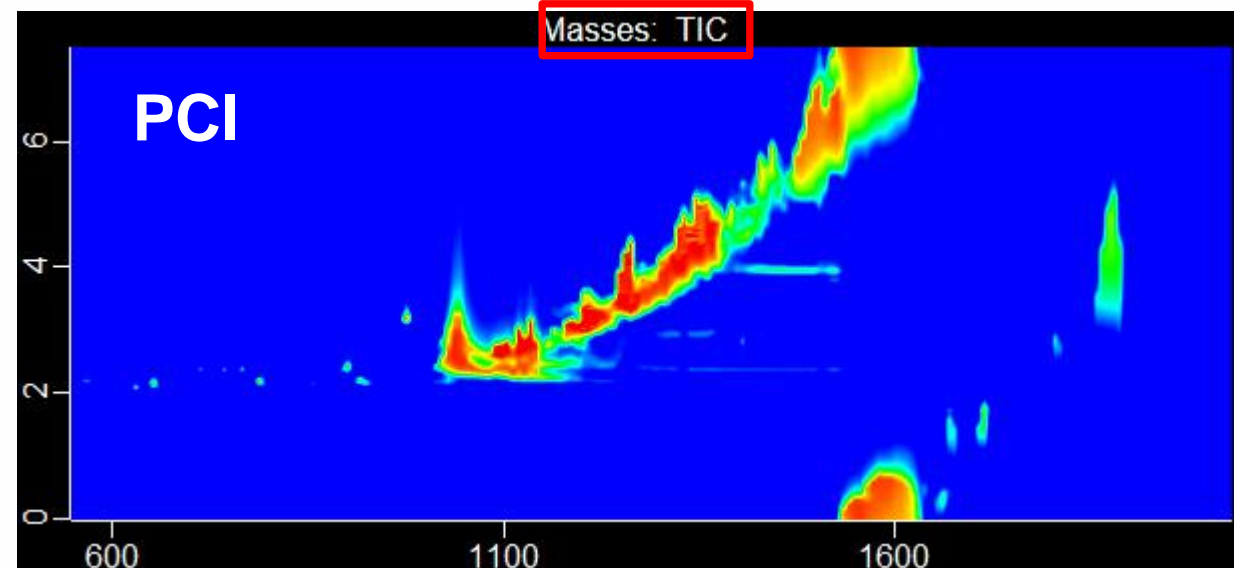
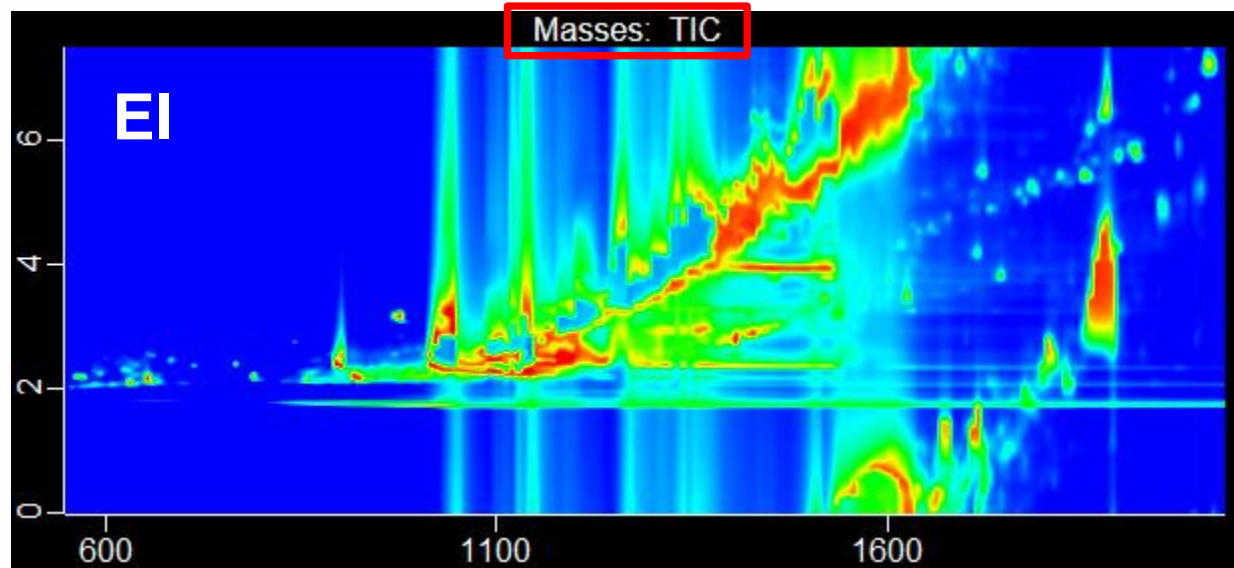


IGS >2  
~ 27 píků

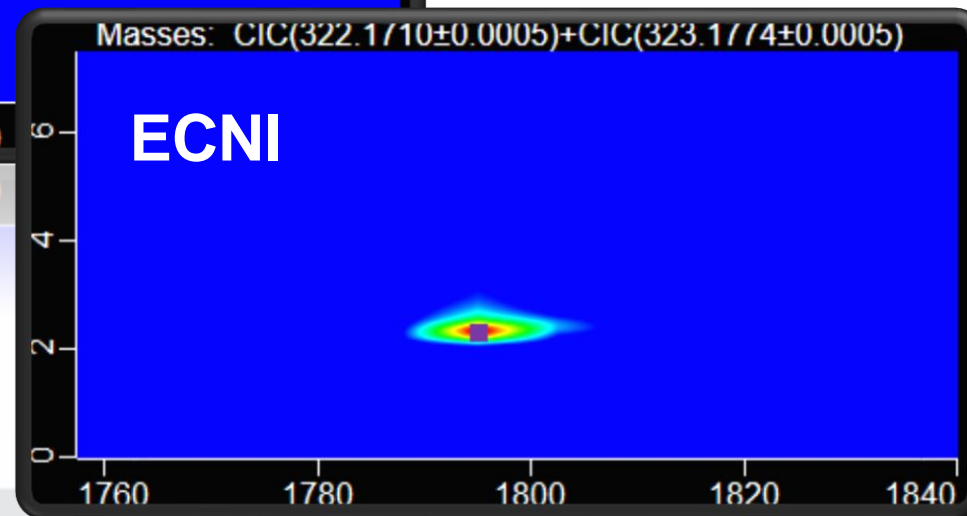
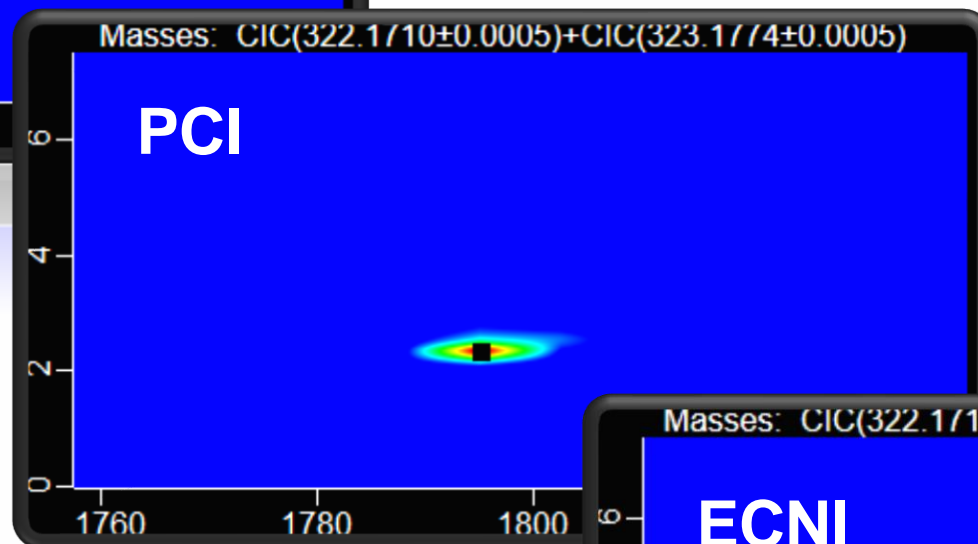
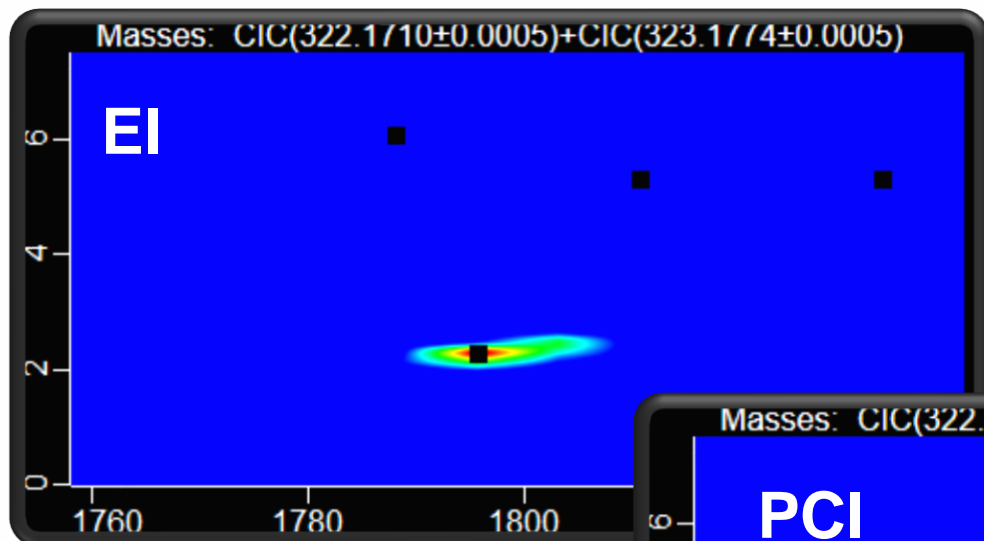




# Clostebol GCxGC-DC ECNI

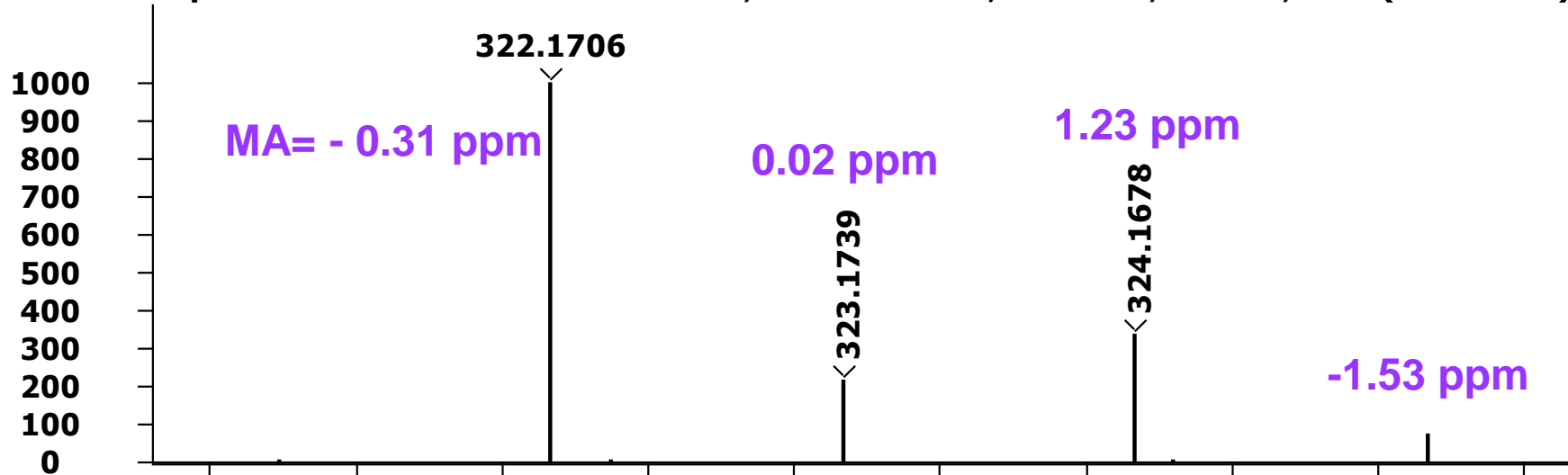


# Clotestbol GCxGC-DC ECNI

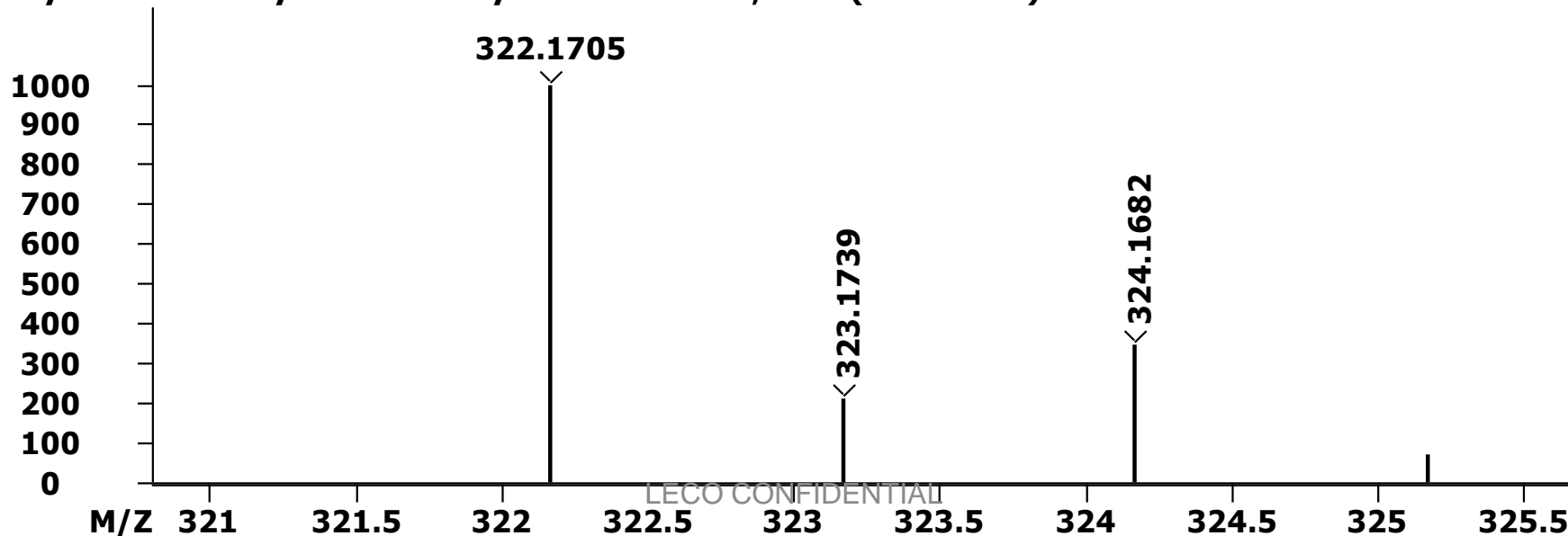


# Clotebol GCxGC-DC ECNI

Peak True - sample "2D 187888 notDiluted DC ECNI", Clotebol ECNI, at 1795 s, 2.340 s, Area (Abundance)



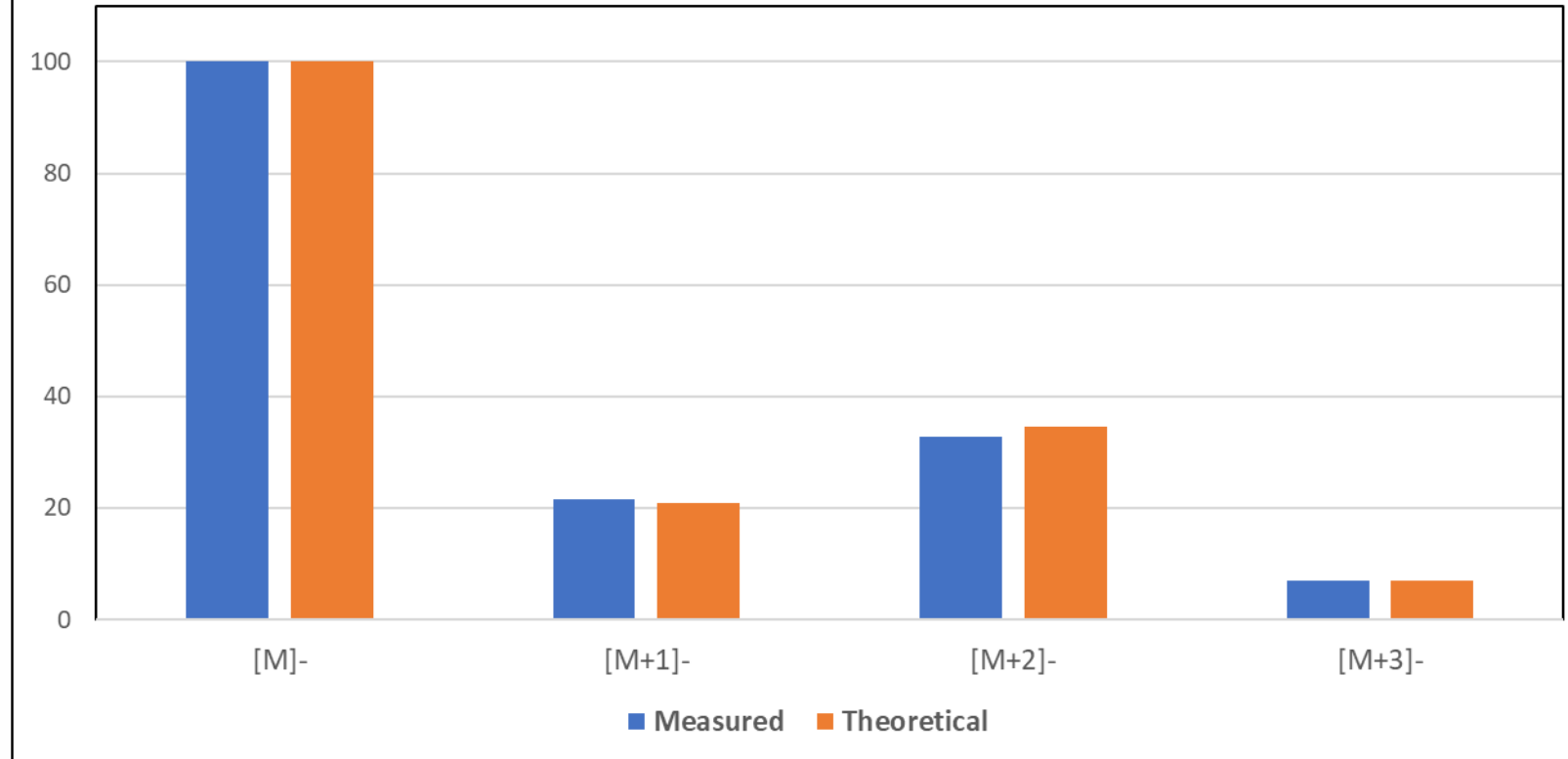
Library Hit - Similarity: 992 - Library: - C<sub>19</sub>H<sub>27</sub>ClO<sub>2</sub>, Area (Abundance)



LECO CONFIDENTIAL



### M<sup>-</sup> Cluster of Clostebol



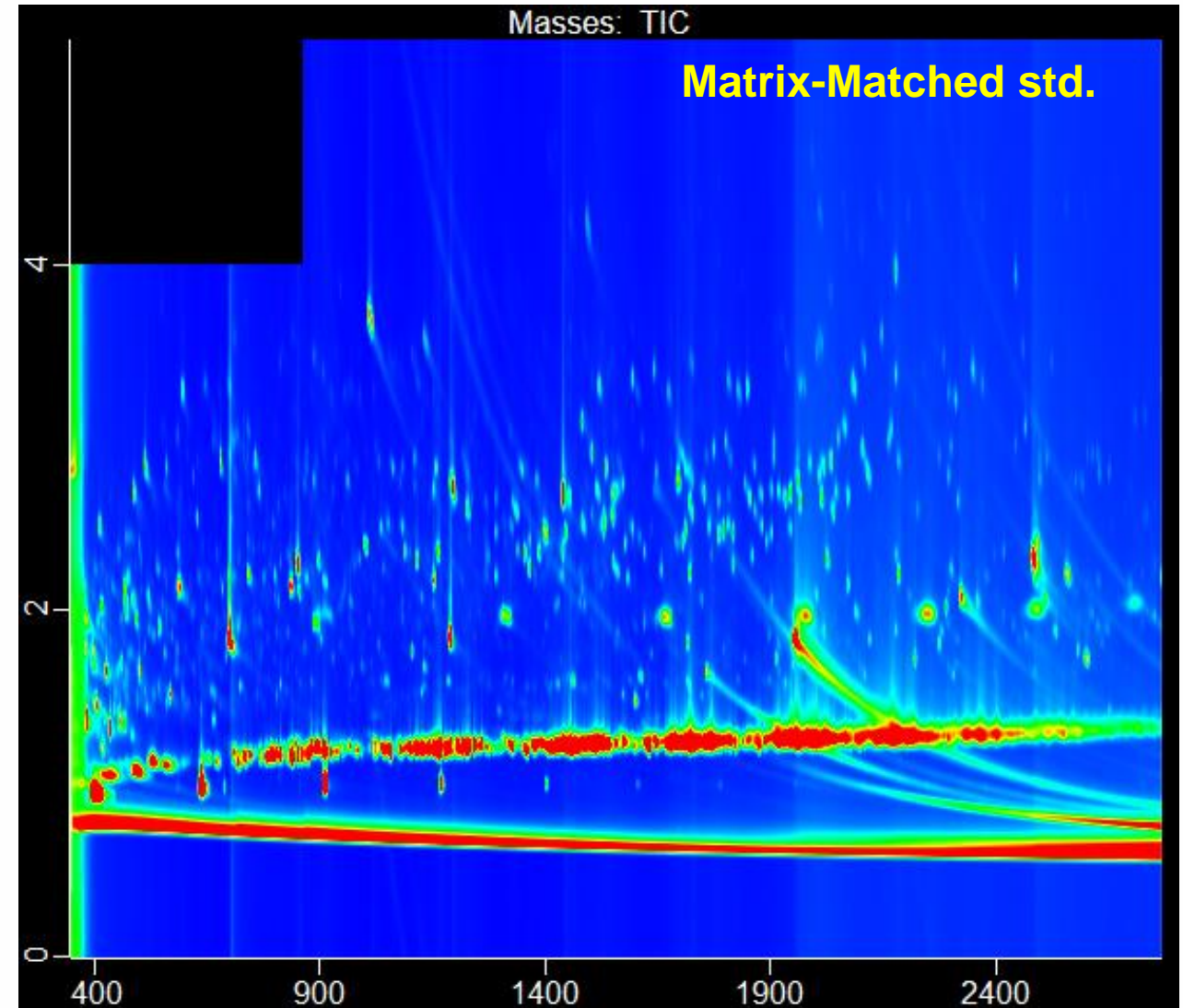
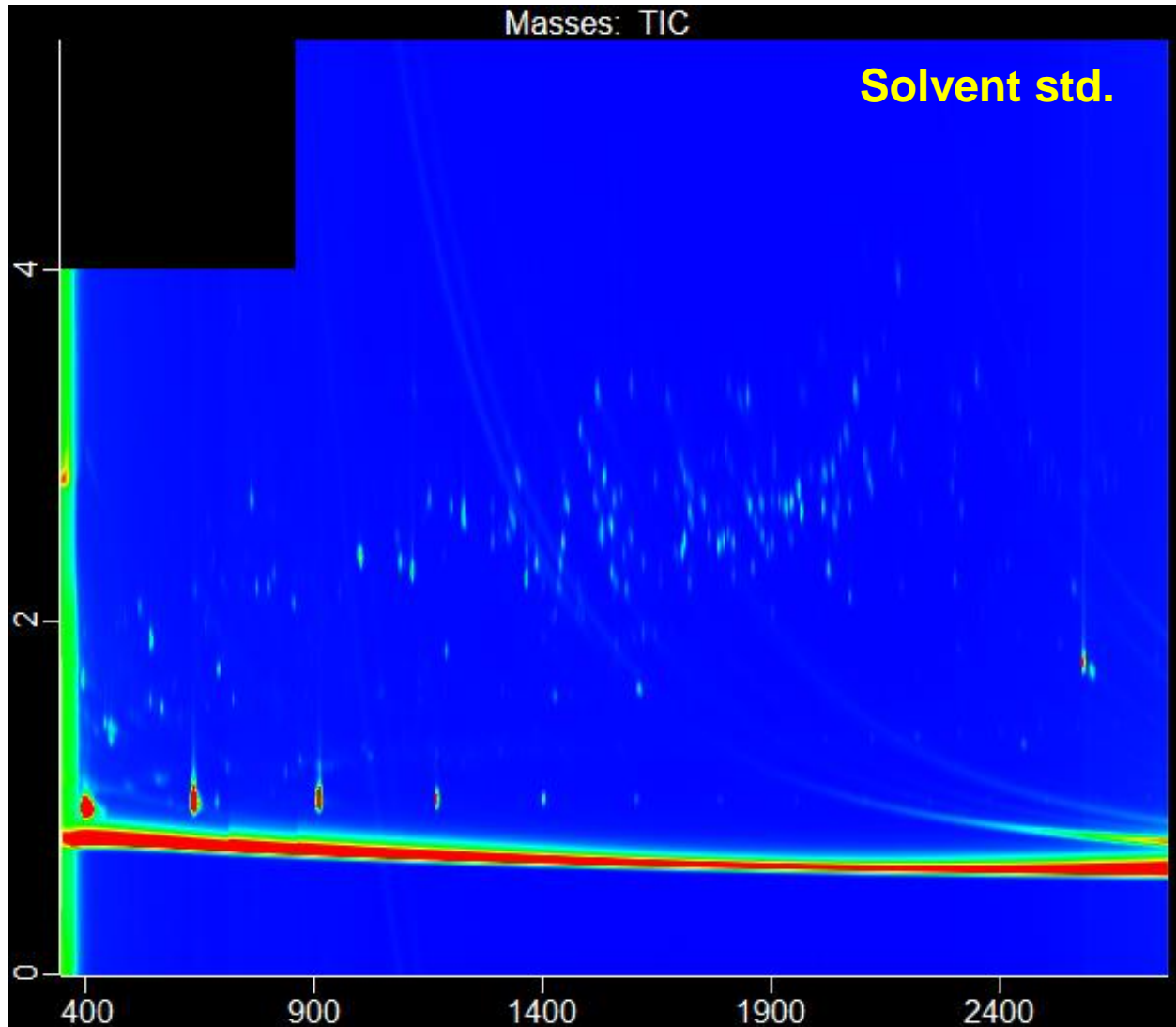
# Pesticidy v rajčatech

- Měřeno na přístroji Pegasus BT 4D
- Standard cca 160 látek
- Kvantifikace pomocí externí kalibrace

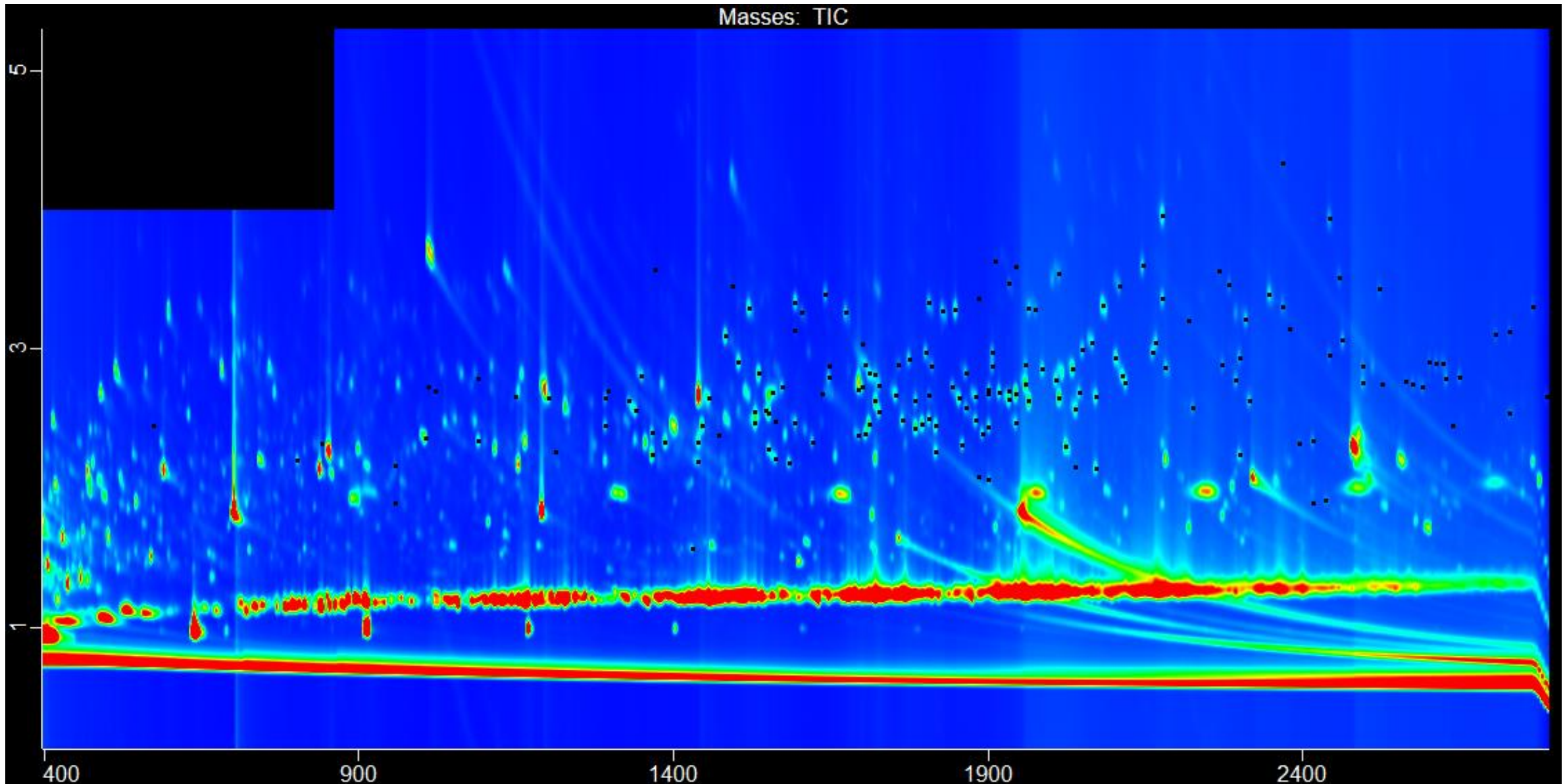
# GC×GC a MS parametry měření

<b>GC</b>	<b>Agilent 7890</b>
<b>Injection</b>	1 µL in Gerstel CIS4 Inlet in cold Splitless mode 40°C (hold 6s), 10°/s to 275°C (hold 28min) SL period: 2 min
<b>Columns</b>	<sup>1</sup> D: HP-5MS UI, 30 m x 0.25 mm i.d. x 0.25 µm coating (Agilent) <sup>2</sup> D: Rxi-17Silms, 1.5 m x 0.15 mm ID x 0.15 µm coating (Restek)
<b>Carrier Gas</b>	He @ 1.2mL/min to 46 min, 5mL/min <sup>2</sup> to 2.5mL (19.8 min)
<b>Oven Program</b>	75°C (hold 2.05 min), ramp 5 °C/min to 320°C (hold 15 min)
<b>Secondary Oven</b>	+5 °C (relative to the main oven temperature)
<b>Modulator</b>	+15 °C (relative to the secondary oven temperature)
<b>Modulation Period</b>	4 sec (0-862 s), 5s (862-end of run)
<b>Transfer line</b>	340°C
<b>MS</b>	<b>LECO Pegasus® BT (BT 4D)</b>
<b>Ion Source Temp</b>	250°C
<b>Mass Range</b>	40-600
<b>Acquisition Rate</b>	250 spectra/s

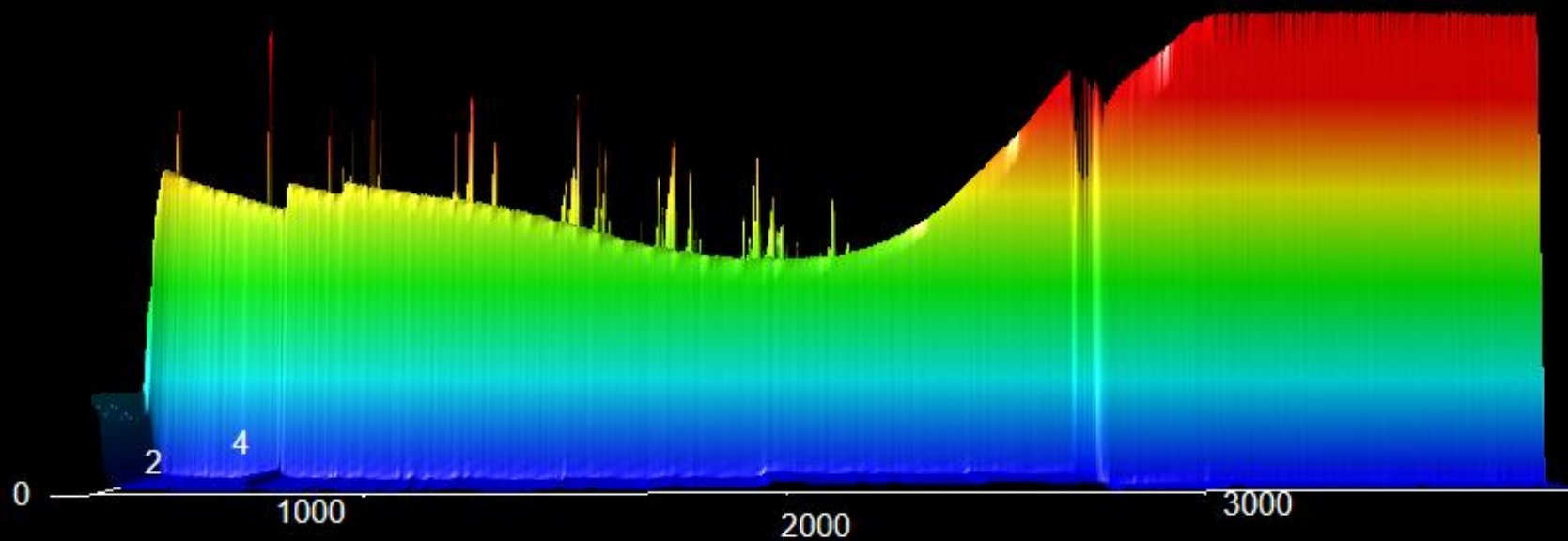
# Porovnání samotného standardu a standardu s maticí



# Lokalizace pesticidů v matrici (50 ng/mL)

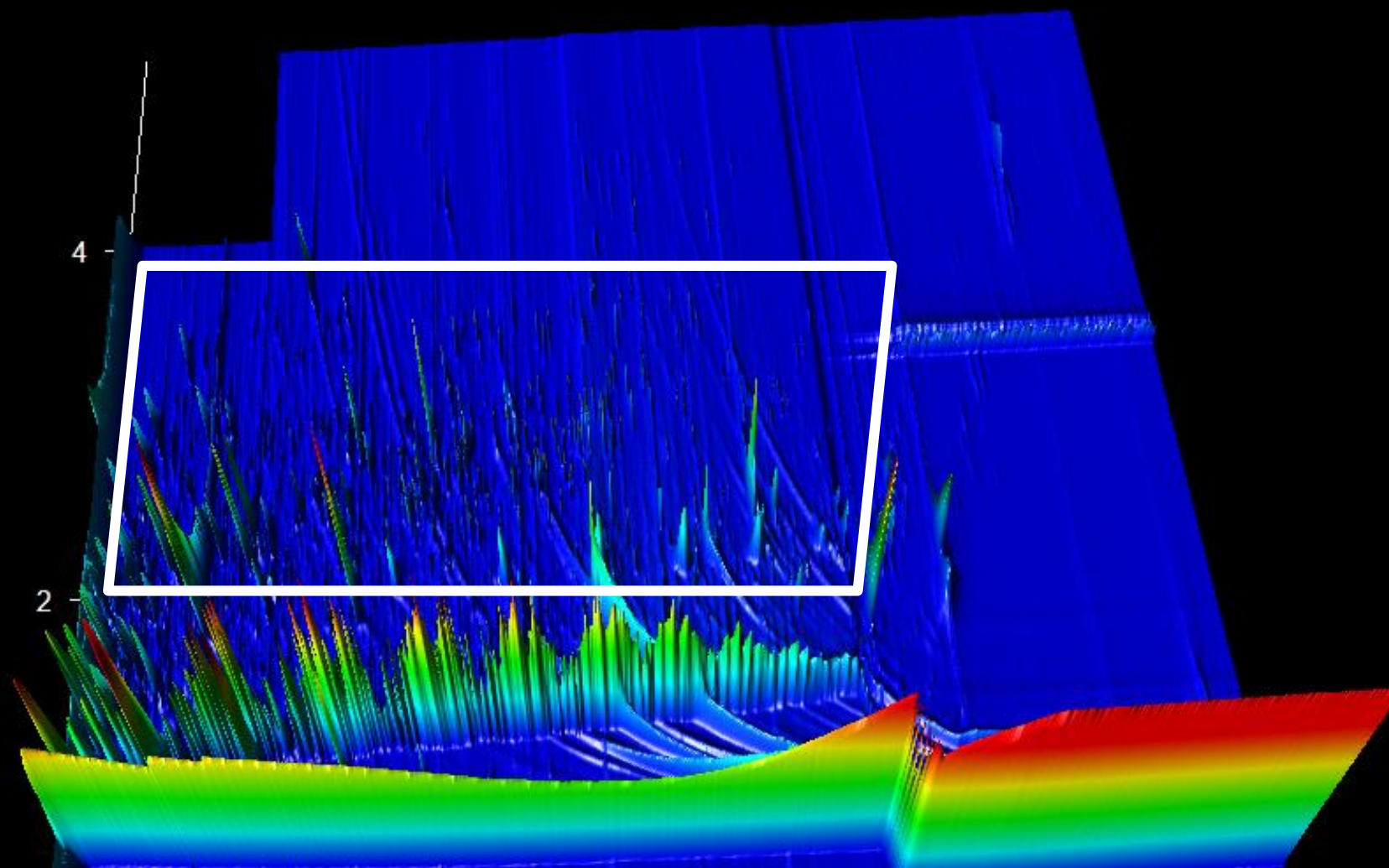


Masses: TIC

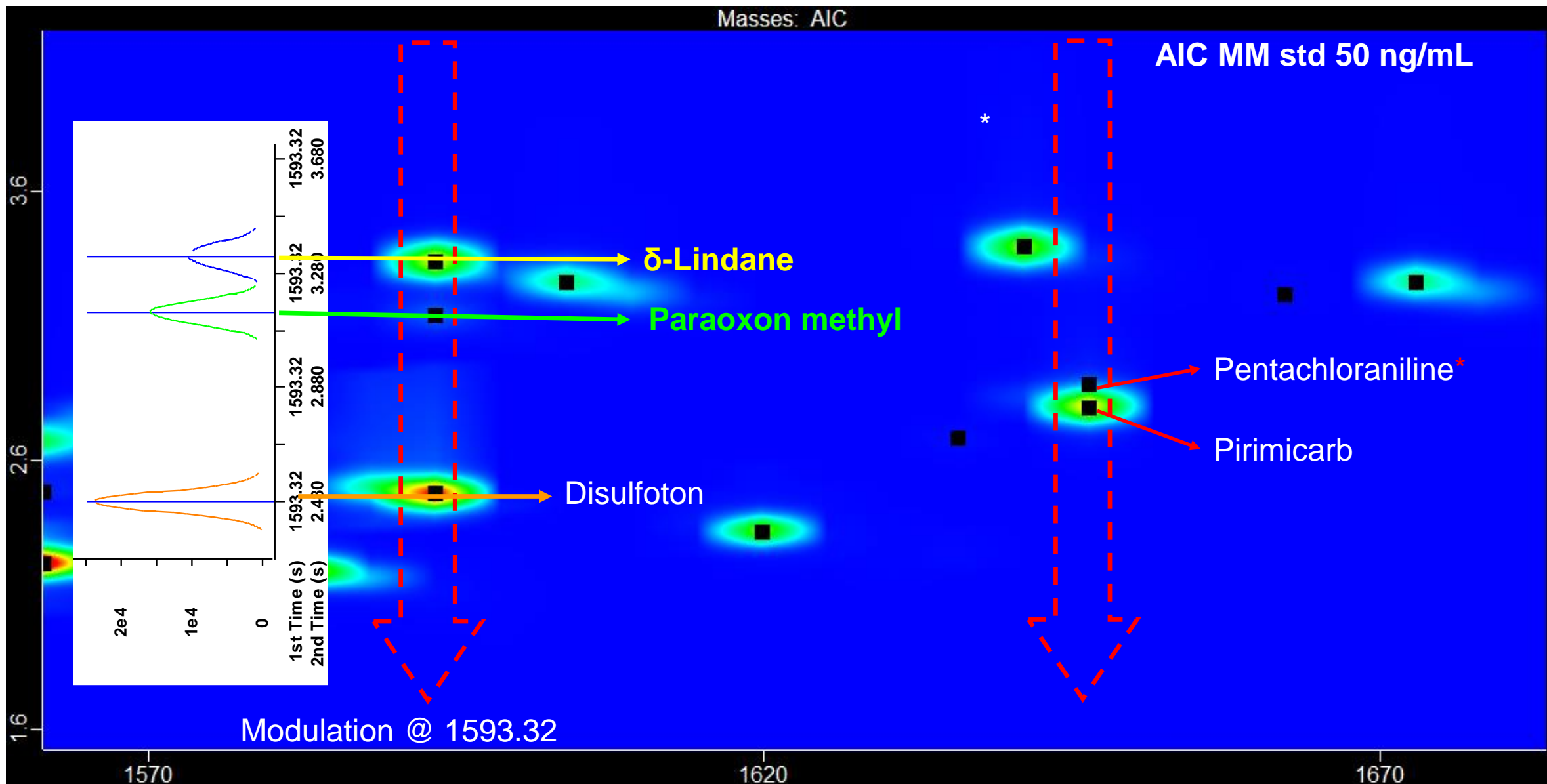




Masses: TIC



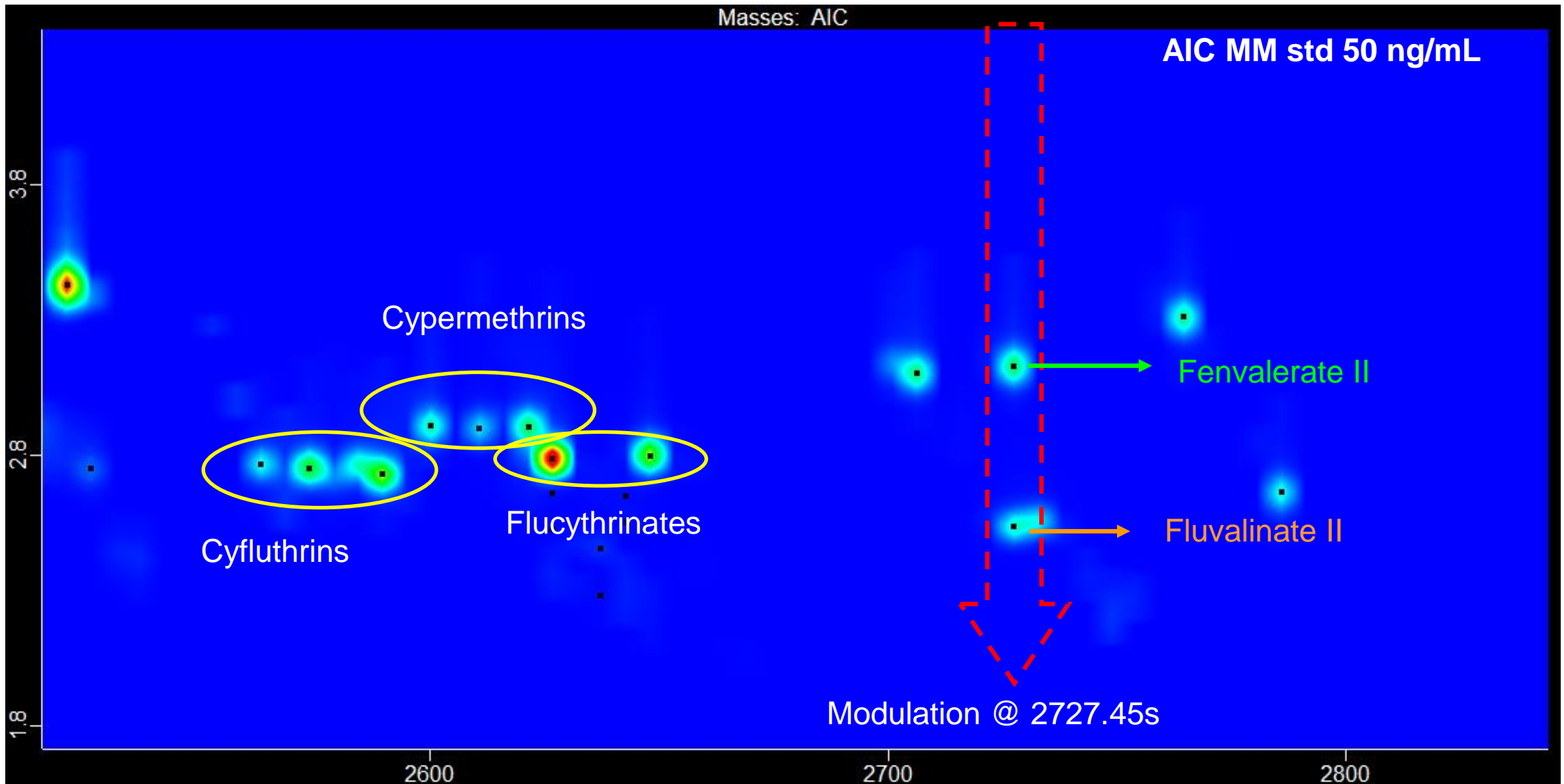
# Výhoda GC×GC-TOF-MS: Vynikající separace



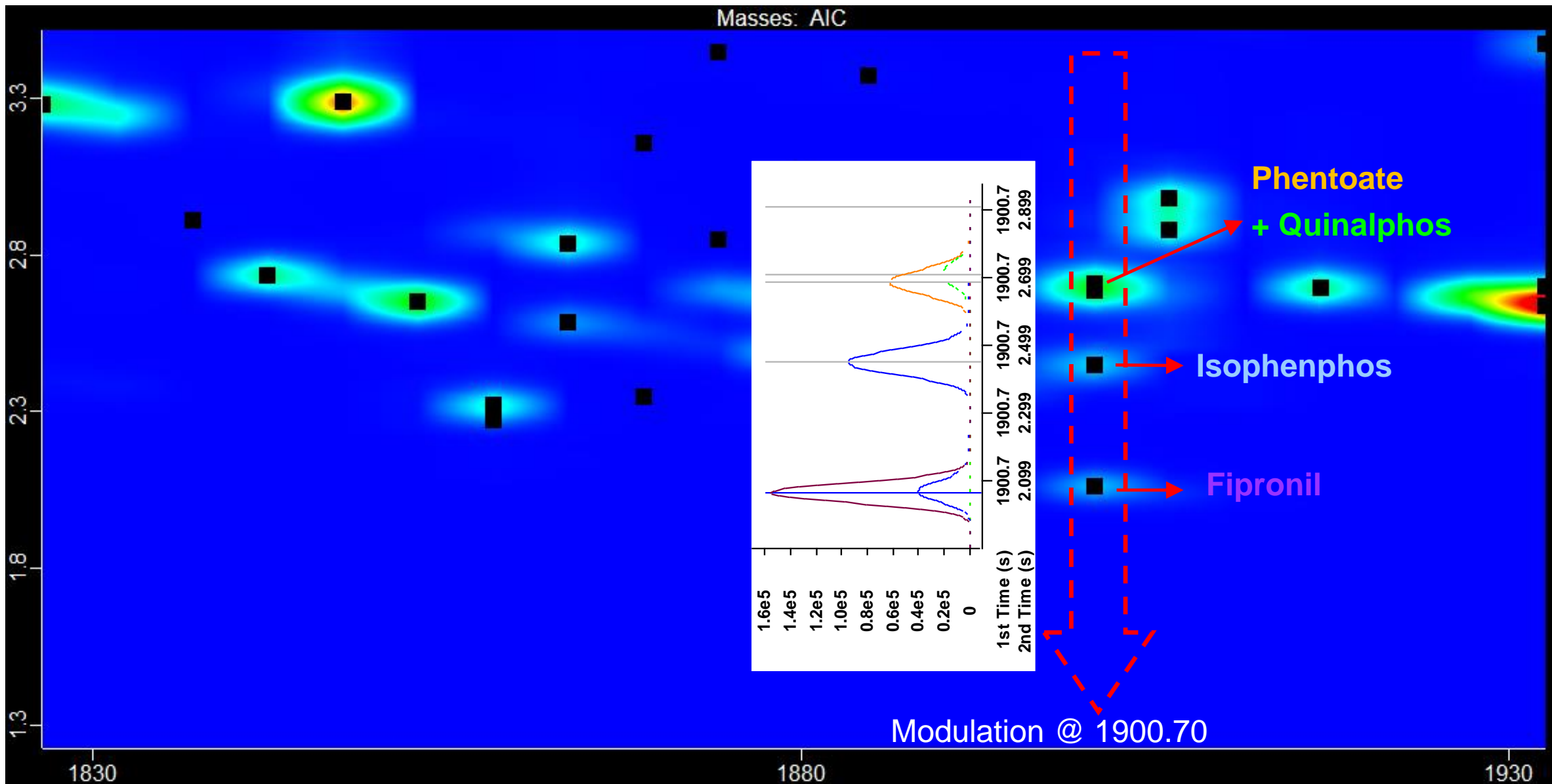
\* - Not in the list of pesticide residues



# Výhoda GC×GC-TOF-MS: Vynikající separace



# Výhoda GC×GC-TOF-MS: Vynikající separace



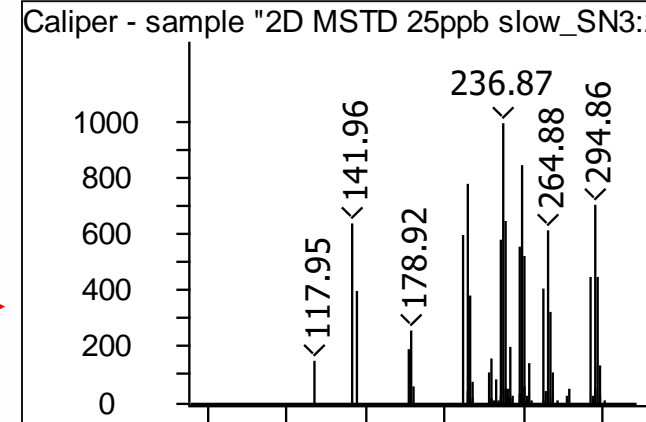
# Kvantifikace

- 1. Lokalizace požadovaných analytů

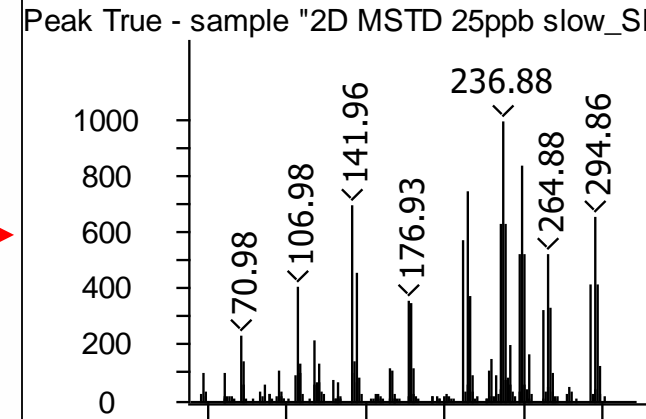
# Kvantifikace

- 1. Lokalizace požadovaných analytů

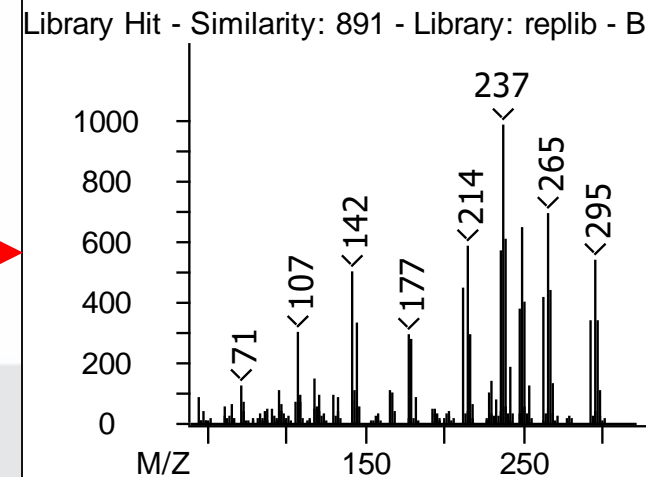
Undeconvoluted



Deconvoluted



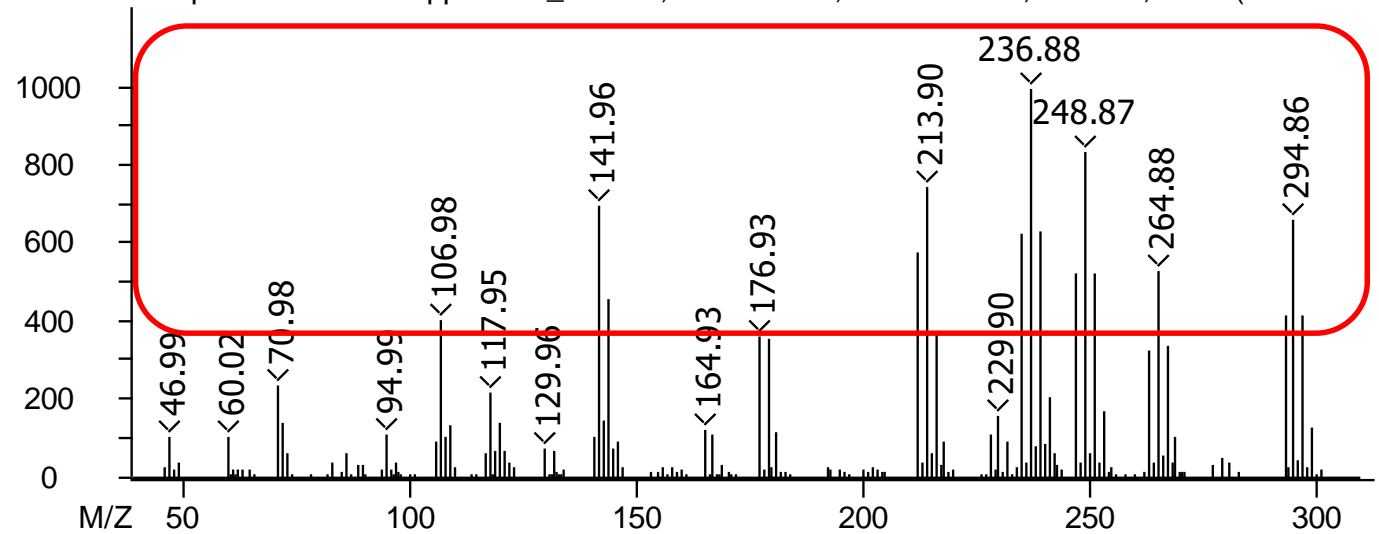
Library hit



# Kvantifikace

- 1. Lokalizace požadovaných analytů
- 2. Výběr charakteristických m/z (dle metodiky SANTE) a nastavení **tresholdu** (např. všechny ionty s intenzitou 40% a více)

Peak True - sample "2D MSTD 25ppb slow\_SN3:2", Quintozene, at 1545.62 s, 2.573 s, Area (Abundance)



Deconvoluted spectrum

# Kvantifikace

- 1. Lokalizace požadovaných analytů
- 2. Výběr charakteristických m/z (dle metodiky SANTE) a nastavení tresholdu (např. všechny ionty s intenzitou 40% a více)
- **3. Výběr iontů, které by měly být pokaždé přítomny a ty použít pro kvantifikace (integrace)**

# MS kritéria dle SANTE

Pro dodržení normy musí platit:

1. Minimálně 3 ionty
2.  $S/N > 3$
3. Překryv vybraných iontů
4.  $\pm 30\%$  v kalibračním rozsahu

Identifikace a kvantifikace vyžaduje překryv minimálně 3 hmot



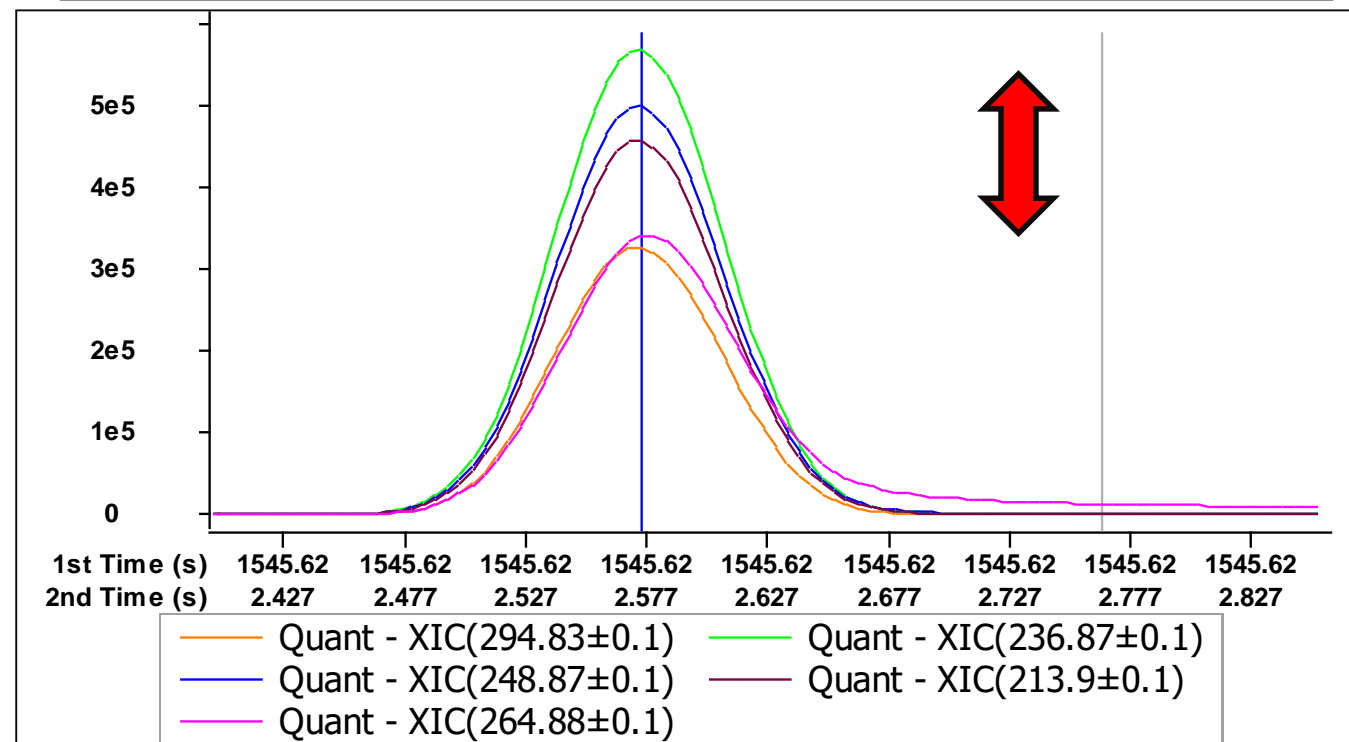
## Target Analyte Finding in ChromaTOF

Input Masses For Target Analyte Finding

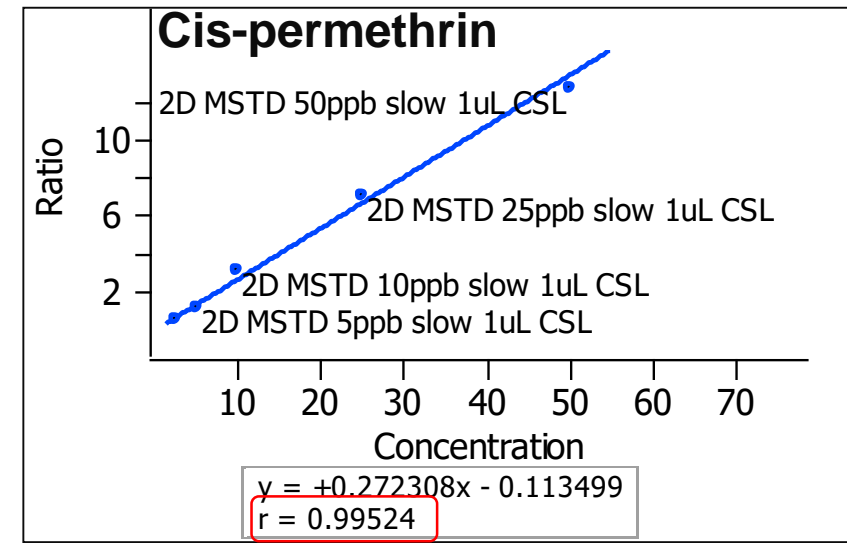
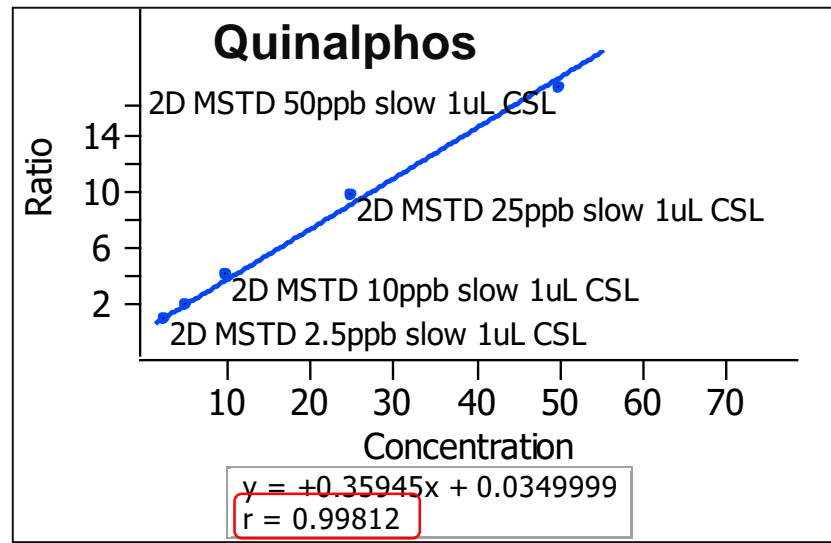
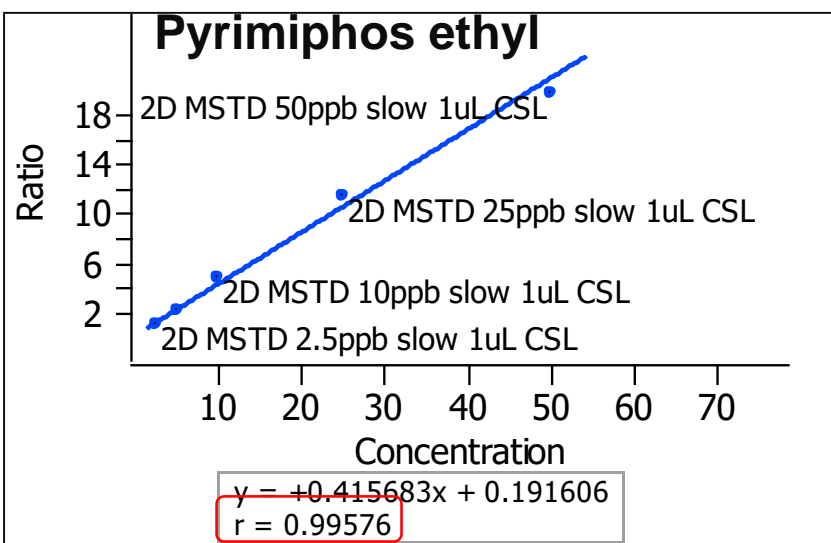
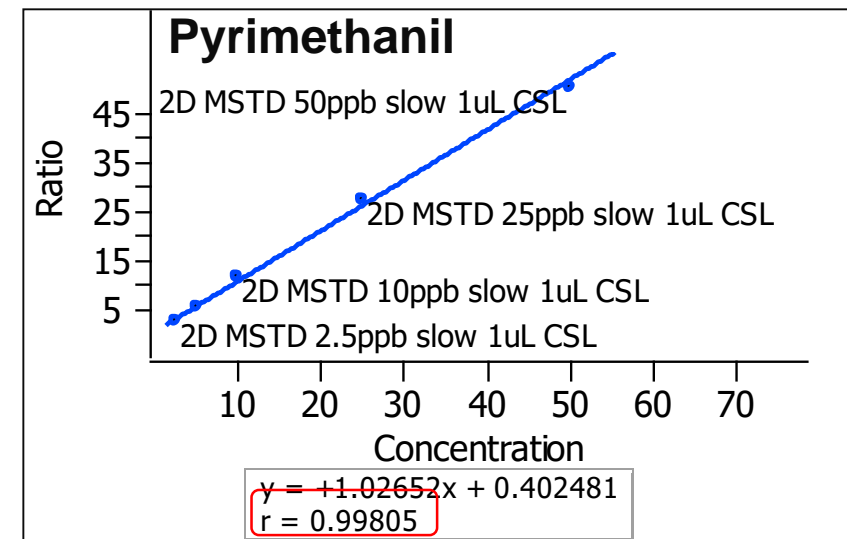
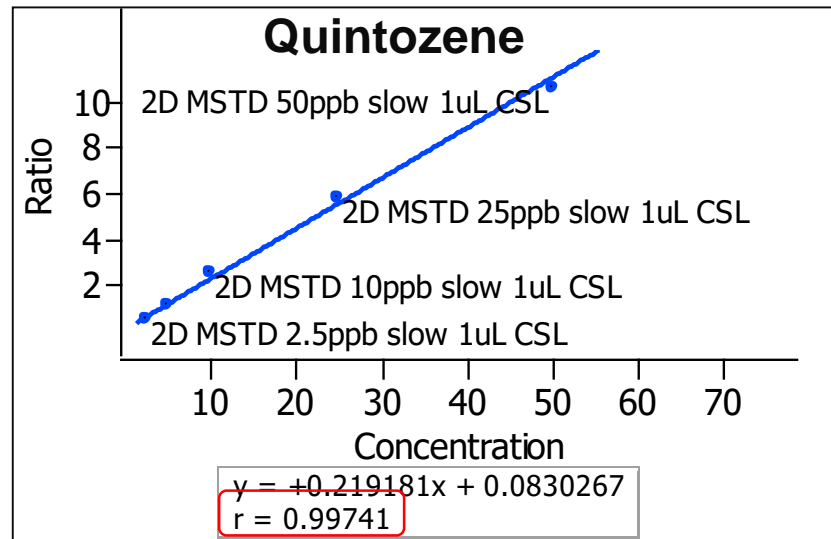
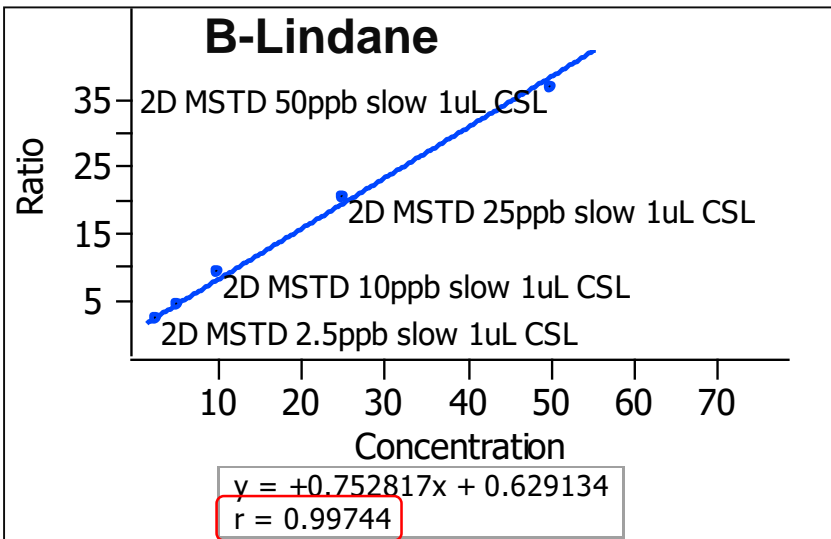
Analyte: Quintozene

#	Formula	Isotope	M/Z	Tolerance	Units	Required
1*	<chem>C6Cl5NO2</chem>	294.83		0.10	Da	<input checked="" type="checkbox"/>
1-2		296.83		0.10	Da	<input type="checkbox"/>
1-3		292.84		0.10	Da	<input type="checkbox"/>
1-4		298.83		0.10	Da	<input type="checkbox"/>
2			236.87	0.10	Da	<input checked="" type="checkbox"/>
3			248.87	0.10	Da	<input checked="" type="checkbox"/>
4			213.90	0.10	Da	<input checked="" type="checkbox"/>
5			264.88	0.10	Da	<input checked="" type="checkbox"/>
6			141.96	0.10	Da	<input type="checkbox"/>

Buttons: Add, Add Isotope, Remove, Promote, Demote



# Příklady kalibračních křivek v GC×GC



Všechny analyty byly kvantifikovány pomocí externích kalibračních křivek a použitého IS hexachlorbenzenu. Kalibrační křivky jsou lineární s výborným korelačním koeficientem ( $R^2$ )



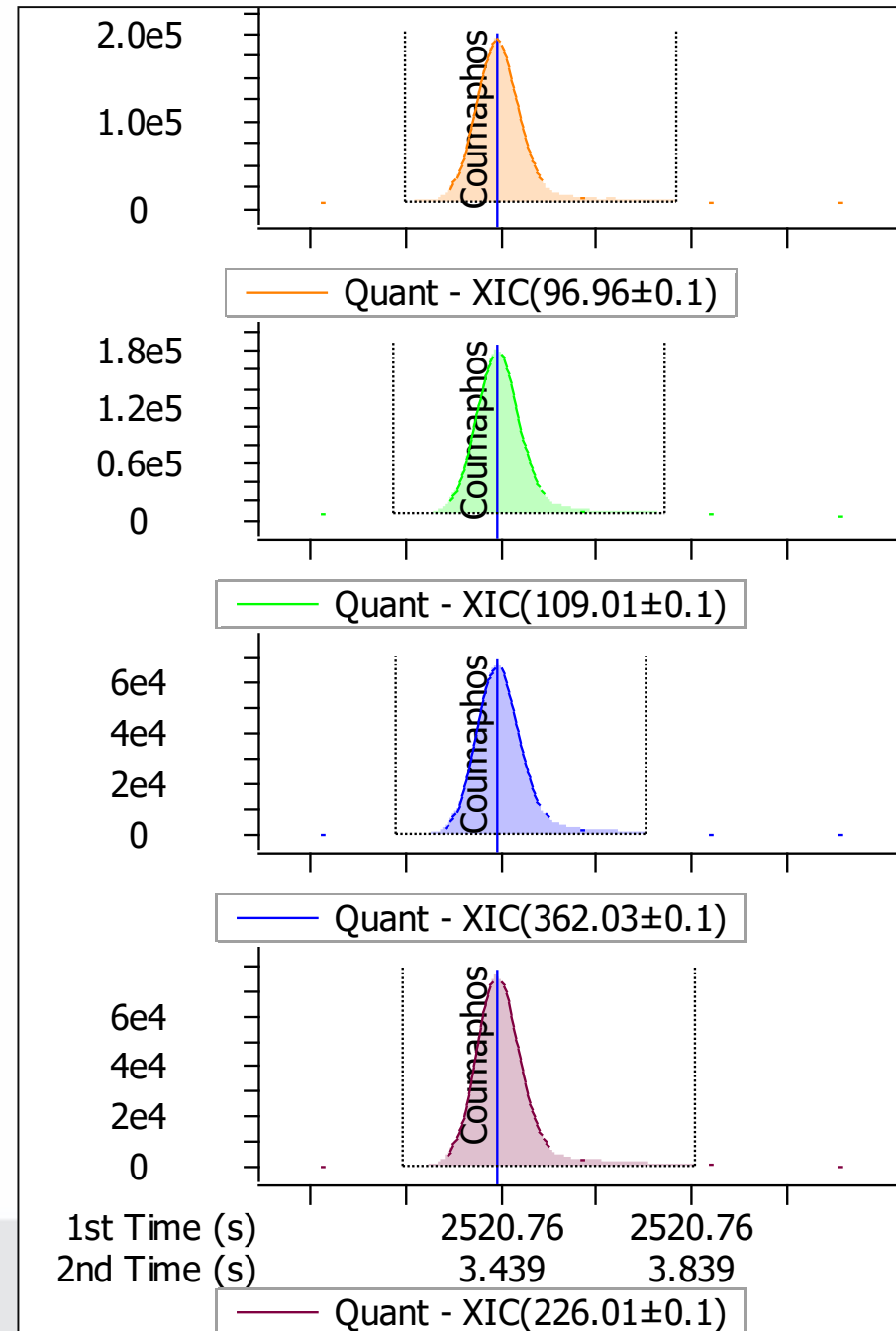
# Tabulka kvantifikace

Quantitation Table - "1uL slow based on cal TAF-3rd trial v428"

Analyte	Name	1st Dimensior	2nd Dimensio	1st Di	2nd D	Type	Mass	Interr	Equation	Correlation Coefficients	Quantitate
40	Beta-Lindane	1519.13	3.310	5	0.2	Analyt	XIC(1	Hexac	$y = +0.752817x + 0.629$	0.99744	Area
41	Propazine	1529.72	2.485	5	0.2	Analyt	XIC(2	Hexac	$y = +0.925693x + 0.582$	0.99622	Area
42	Terbumeton	1529.72	2.550	5	0.2	Analyt	XIC(2	Hexac	$y = +0.879967x + 0.469$	0.99693	Area
43	g-Lindane	1535.02	2.840	5	0.2	Analyt	XIC(1	Hexac	$y = +0.64931x + 0.6134$	0.99539	Area
44	Quintozene	1545.62	2.575	5	0.2	Analyt	XIC(2	Hexac	$y = +0.219181x + 0.083$	0.99741	Area
45	Terbufos	1550.92	2.290	5	0.2	Analyt	XIC(2	Hexac	$y = +0.374253x + 0.323$	0.99632	Area
46	Terbutylazine	1550.92	2.560	5	0.2	Analyt	XIC(2	Hexac	$y = +0.775464x + 0.527$	0.99571	Area
47	Fonofos	1556.22	2.705	5	0.2	Analyt	XIC(2	Hexac	$y = +1.34096x + 2.1595$	0.99788	Area
48	Propyzamide	1561.52	2.230	5	0.2	Analyt	XIC(2	Hexac	$y = +1.19634x + 0.0296$	0.99102	Area
49	Pyrimethanil	1572.12	2.745	5	0.2	Analyt	XIC(1	Hexac	$y = +1.02652x + 0.4024$	0.99805	Area
50	Diazinon	1582.72	2.205	5	0.2	Analyt	XIC(1	Hexac	$y = +0.393387x + 0.665$	0.99849	Area
51	Disulfoton	1593.32	2.485	5	0.2	Analyt	XIC(1	Hexac	$y = +0.25178x + 0.2474$	0.99761	Area
52	Paraoxon methyl	1593.32	3.150	5	0.2	Analyt	XIC(2	Hexac	$y = +0.0639028x + 0.01$	0.98734	Area
53	Delta-Lindane	1593.32	3.350	5	0.2	Analyt	XIC(1	Hexac	$y = +0.477322x + 0.246$	0.99752	Area
54	Chlorothalonil	1603.92	3.275	5	0.2	Analyt	XIC(2	Hexac	$y = +0.239139x - 0.0434$	0.99975	Area

# Integrace jednotlivých látek

Na rozdíl od konvenční 1D chromatografie poskytuje GCxGC daleko užší píky (okolo 0,1s u základní linie). Z tohoto důvodu je pro SW ChromaTOF jednoduchá automatická integrace bez zásahu operátora pro naprostou většinu analytů.



# Neznámý vzorek

Peak Table - 2D spiked sample slow 1uL CSL\_cor method

Peak #	Name	1st Dimension	2nd Dimension Time (s)	Area	Concentration	Conc. Units	Quant Masse	Quant S/N
20	g-Lindane	1535.02	2.830	17578294	19.67	ng/ $\mu$ L	XIC(180.96 $\pm$ 0)	2438
21	Quintozene	1545.62	2.565	6303225	21.51	ng/ $\mu$ L	XIC(294.83 $\pm$ 0)	1431
24	Pyrimethanil	1572.12	2.735	21600626	15.63	ng/ $\mu$ L	XIC(199.11 $\pm$ 0)	3333
26	Delta-Lindane	1593.32	3.340	10145233	15.67	ng/ $\mu$ L	XIC(180.96 $\pm$ 0)	1402
28	Chlorothalonil	1603.92	3.270	872662	2.96	ng/ $\mu$ L	XIC(265.9 $\pm$ 0.1)	163
29	Tefluthrine	1614.52	1.620	37168228	33.27	ng/ $\mu$ L	XIC(177.05 $\pm$ 0)	2250
31	Endosulfan ether	1635.72	2.690	101142	29.23	ng/ $\mu$ L	XIC(341.85 $\pm$ 0)	110
33	Metribuzin	1672.82	3.265	9671074	17.23	ng/ $\mu$ L	XIC(198.09 $\pm$ 0)	1207
34	Vinclozoline	1694.01	2.380	6887693	20.30	ng/ $\mu$ L	XIC(285 $\pm$ 0.1)	1658
36	Heptachlor	1704.61	2.400	13845621	20.08	ng/ $\mu$ L	XIC(100.02 $\pm$ 0)	2586
37	Alachlor	1709.91	2.465	20173241	17.28	ng/ $\mu$ L	XIC(160.13 $\pm$ 0)	2115
39	Metalaxyl	1725.81	2.750	5234327	15.72	ng/ $\mu$ L	XIC(279.15 $\pm$ 0)	694
40	Aldrin	1784.11	2.440	21811309	20.59	ng/ $\mu$ L	XIC(66.06 $\pm$ 0.1)	1435
41	Metolachlor	1794.71	2.470	33957202	16.44	ng/ $\mu$ L	XIC(162.14 $\pm$ 0)	4026
43	Flufenacet	1815.91	2.265	11330371	13.20	ng/ $\mu$ L	XIC(363.07 $\pm$ 0)	1055
44	Chlorthal-dimethyl	1815.91	2.455	23921055	18.10	ng/ $\mu$ L	XIC(300.9 $\pm$ 0.1)	9689

Koncentrace je v uvedeném sloupci chybně, jde o ng/mL!!!

# Shrnutí

- 1. Nový univerzální iontový zdroj DC pro platformu HRT – šikovní pomocník pro analýzu neznámých vzorků**
  - Jednoduché měření vzorku různými ionizačními technikami (CI, PCI, NCI) v jediném iontovém zdroji
  - Možnost využití **Identification Grading System**
  
- 2. Ukázka použitelnosti Pegasu BT4D pro nejsložitější vzorky – GCxGC má smysl**



Děkuji za pozornost

+420 702 008 343

[pavel\\_jiros@leco.com](mailto:pavel_jiros@leco.com)