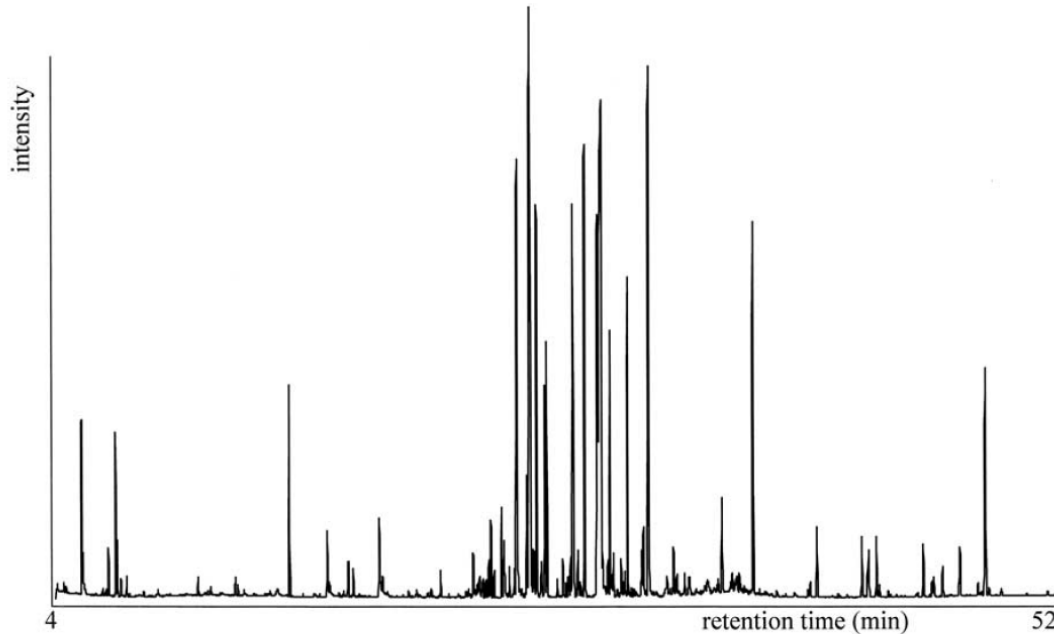


Rhizosphere 2018 – Metabolite profiling



Home: Current Biology | GMD - MS Analysis Input | AMDIS Download Page

Suchen

BinVestigate | SciFinder | Evernote | BLAST | NEB Calc | LEO | Amazon | Outlook | VirusTotal | Lucum | GCMs | GMD | Thesaurus.com

COLM METABOLOME DATABASE

CH & PREDICTION OF FUNCTIONAL GROUPS

of metabolites within the GMD by means of user submitted GC-MS spectra consisting of retention index intensities ratios. In addition, a functional group prediction will help to characterise those metabolites without included in the GMD so far. Instead, the unknown metabolite is characterised by predicted presence or absence users this functionality presented here is exposed as [soap based web services](#).

g. J., Walther, D. and Kopka, J. (2010) Decision tree supported substructure prediction of metabolites from GC-MS profiles, *Metabolomics*. <http://dx.doi.org/10.1007/s11306-010-0198-7>

Query

Enter the **GC-column type** the alkane retention index is based on! VARS

Enter the **alkane retention index** here (if neither an alkane RI for VARS nor MDN35 is available in your setup please select 'none' in the input field above)

Paste the **spectrum** under investigation into the textbox below!

(197	1)	(199	2)	(203	22)	(204	1000)	(206	76)
(213	2)	(215	4)	(217	260)	(218	84)	(219	33)
(220	5)	(231	33)	(233	17)	(242	2)	(243	14)
(244	2)	(245	5)	(247	8)	(248	3)	(249	2)
(255	3)	(257	3)	(259	3)	(261	3)	(265	2)
(271	5)	(272	1)	(273	3)	(287	5)	(288	2)
(289	3)	(290	9)	(303	4)	(317	6)	(331	4)
(332	4)	(333	4)	(334	2)	(335	3)	(345	6)
(346	1)	(347	2)	(348	1)	(361	3)	(362	1)
(363	1)	(377	13)	(378	4)	(379	3)	(380	1)
(435	2)	(436	1)						

If you want us to get back to you in case of errors, please leave your email address:

Advanced Query Parameters (Show Details...)

submit

You can directly hyperlink your spectra for a [automatic search](#) in the GMD!

service last updated 17/02/2017 © 2009-2014 GoIM Metabolome Database - All rights reserved

Franz Hadacek



Plant Molecular Biology **48**: 155–171, 2002.

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Metabolomics – the link between genotypes and phenotypes

Oliver Fiehn

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(e-mail fiehn@mpimp-golm.mpg.de)

Key words: functional genomics, mass spectrometry, metabolism, metabolite profiling

“Finally, if metabolomics profiling is to be used to its fullest, it is imperative that publicly available metabolomic databases be created.”

Instrumentation

CHROMATOGRAPHY

Gas chromatography (GC)

Liquid chromatography (LC)

Capillary chromatography (CC)

DETECTORS

Ion trap (Orbitrap)

Quadrupol

Time-of-flight (TOF)

Fourier transform ion cyclotron resonance (FT-ICR)

Conditions

Ions

A^+ or A^-

Electron impact ionization (EI)

Chemical ionization (CI)

Mass accuracy

e^-

0.0005 Dalton (Da)

Chromatogram

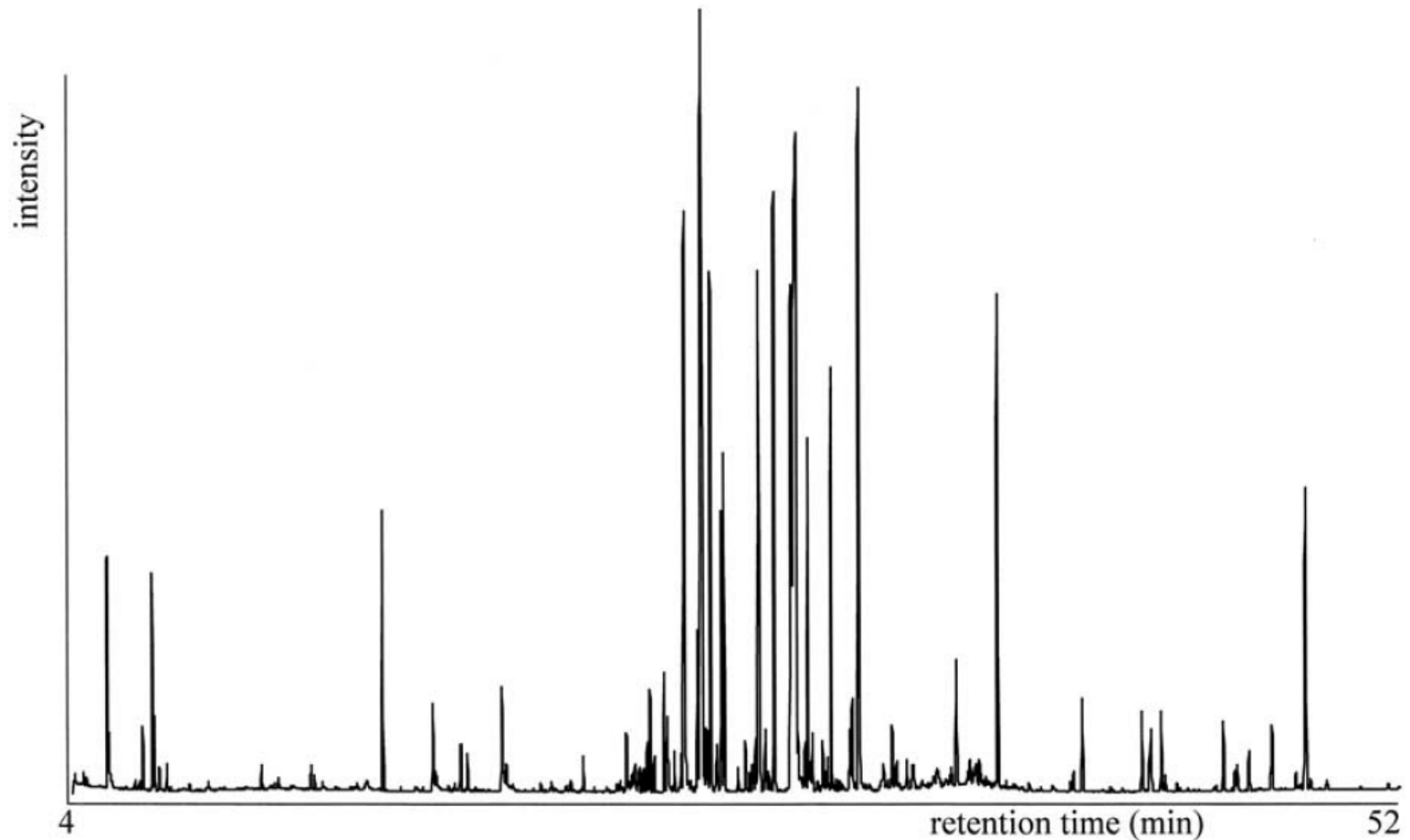
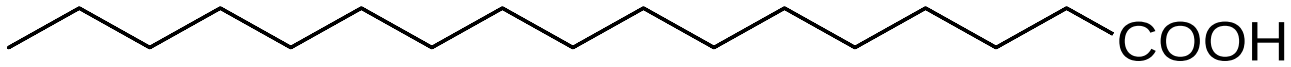


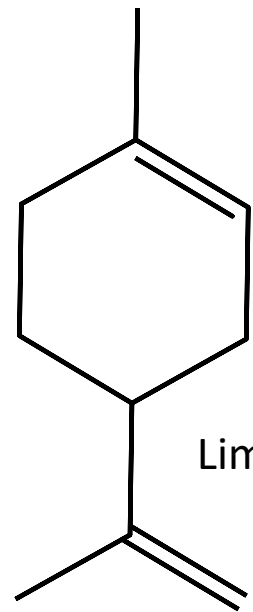
Figure 1. Lipophilic phase of *Arabidopsis thaliana* leaves analysed by GC/quadrupole MS (unpublished results). Inspection of peaks apparent in the base peak chromatogram results in 160 distinct metabolites. Abundant peaks in the middle of the chromatogram are methylated fatty acids. At the end of the chromatogram, trimethylsilylated sterols are eluted.



Lipophilic



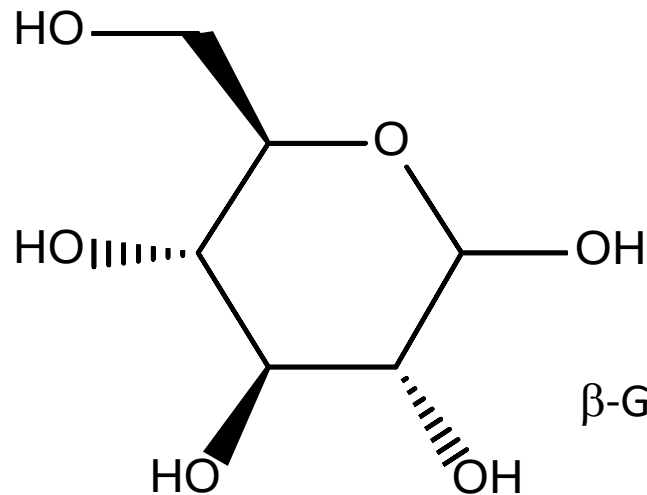
Palmitic acid



Limonene

Hexane, cyclohexane, diethylether, chloroform, ethyl acetate, ...

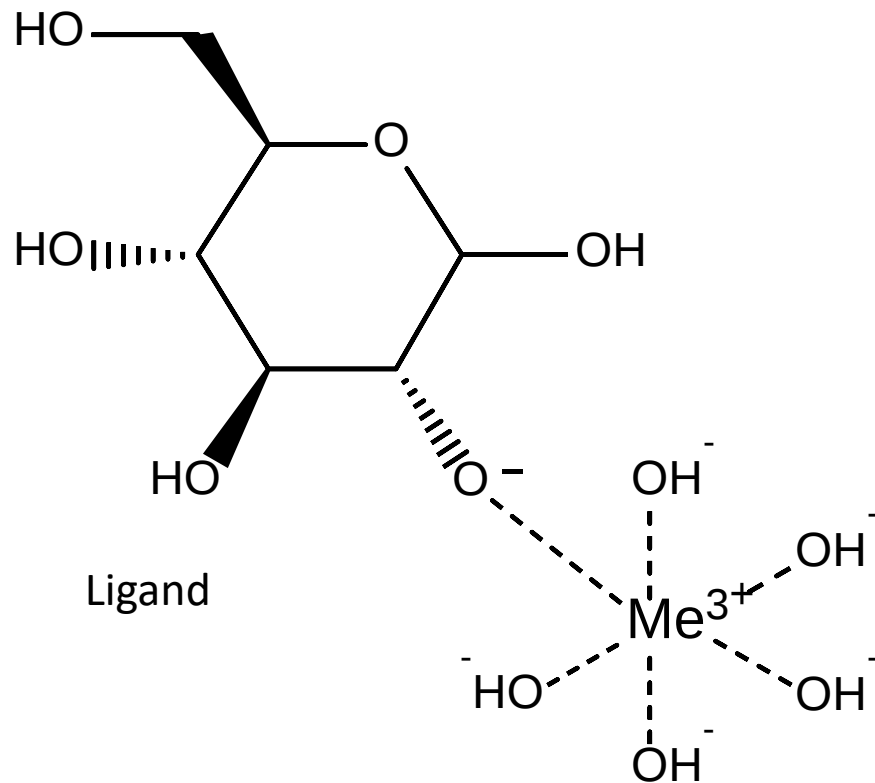
Hydrophilic



β -Glucose

Water, methanol, ethanol, ...

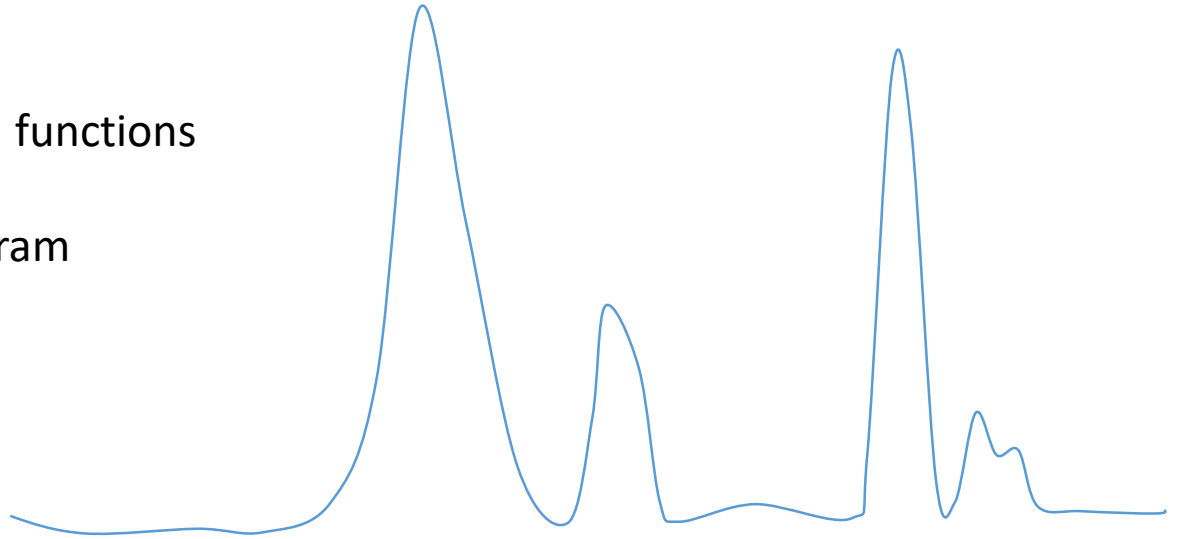
Coordination complex



Me, metal, central atom

Consequences for chromatography

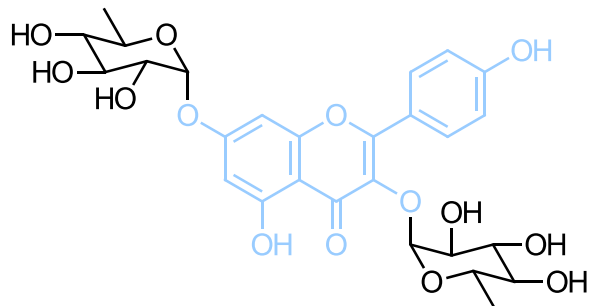
Low pH,
No dissociation of O, S and N functions
No coordination complexes
Slim peaks in the chromatogram



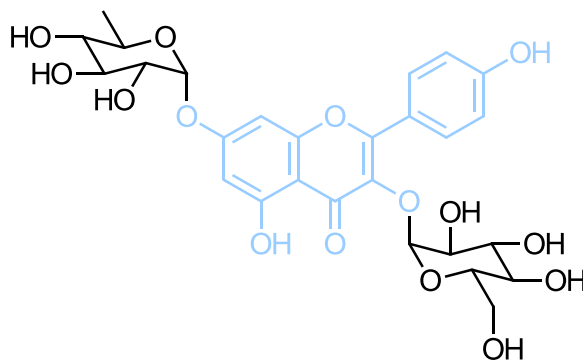
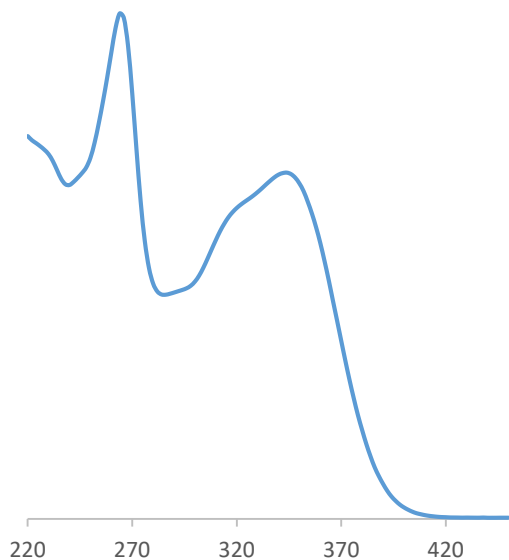
High pH,
Dissociation of O, S and N functions
Plethora of coordination complexes
Polymerization of analytes



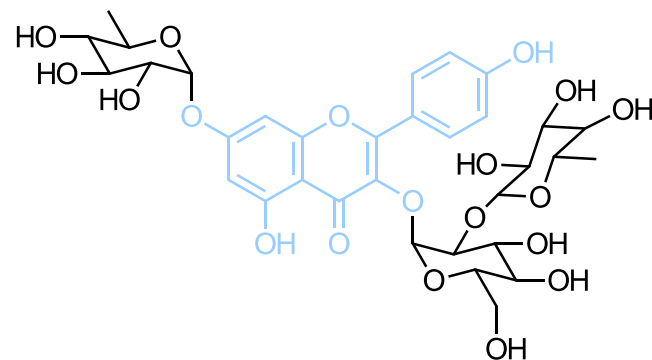
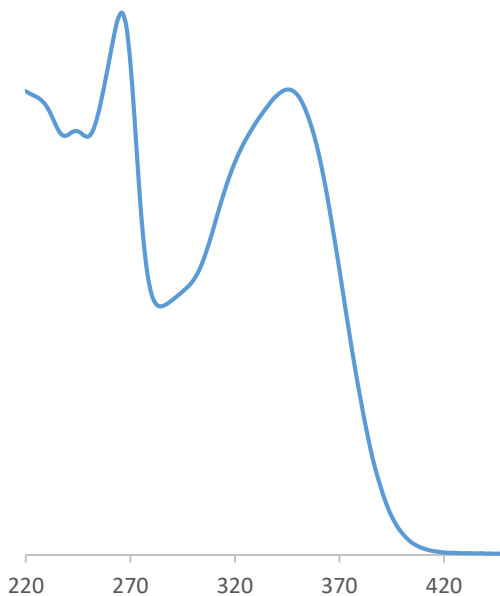
Flavonoids - UV spectra



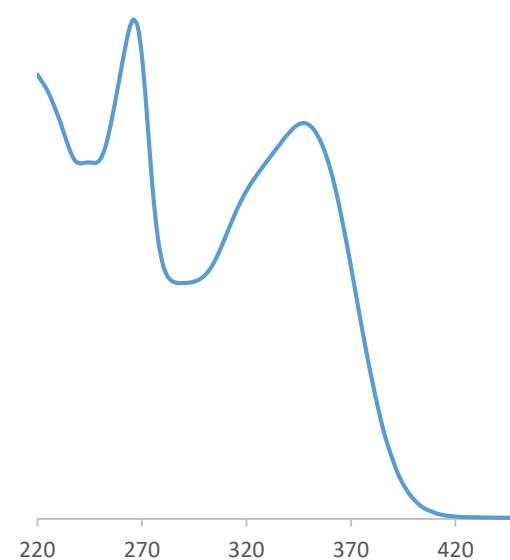
Kaempferol-3,7-dirhamnopyranoside
(19.6 min)



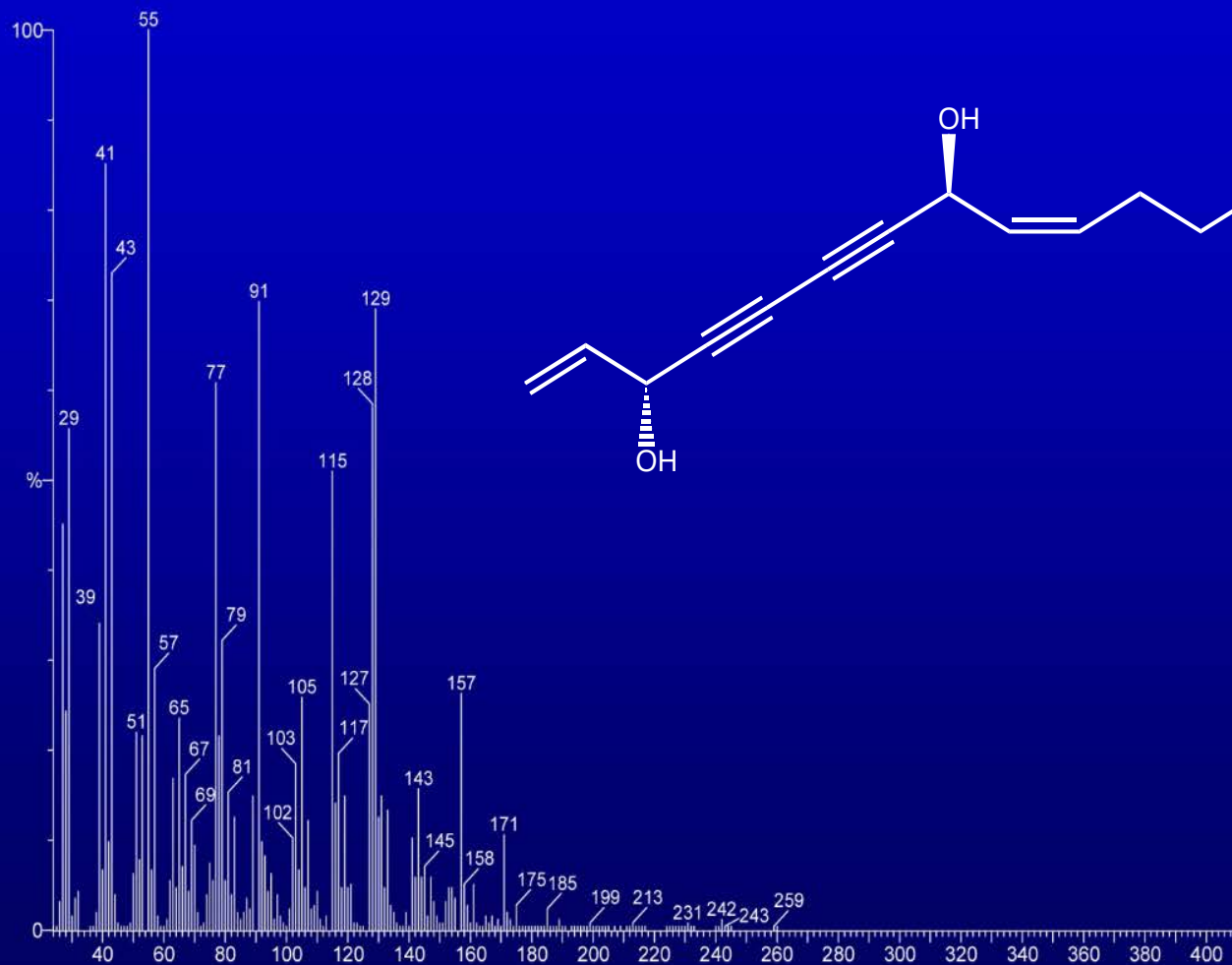
Kaempferol-3-glucopyranosyl-7-rhamnopyranoside (18.3 min)



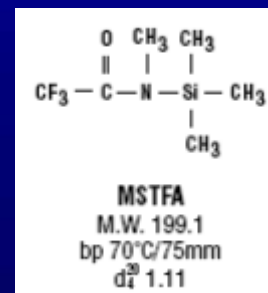
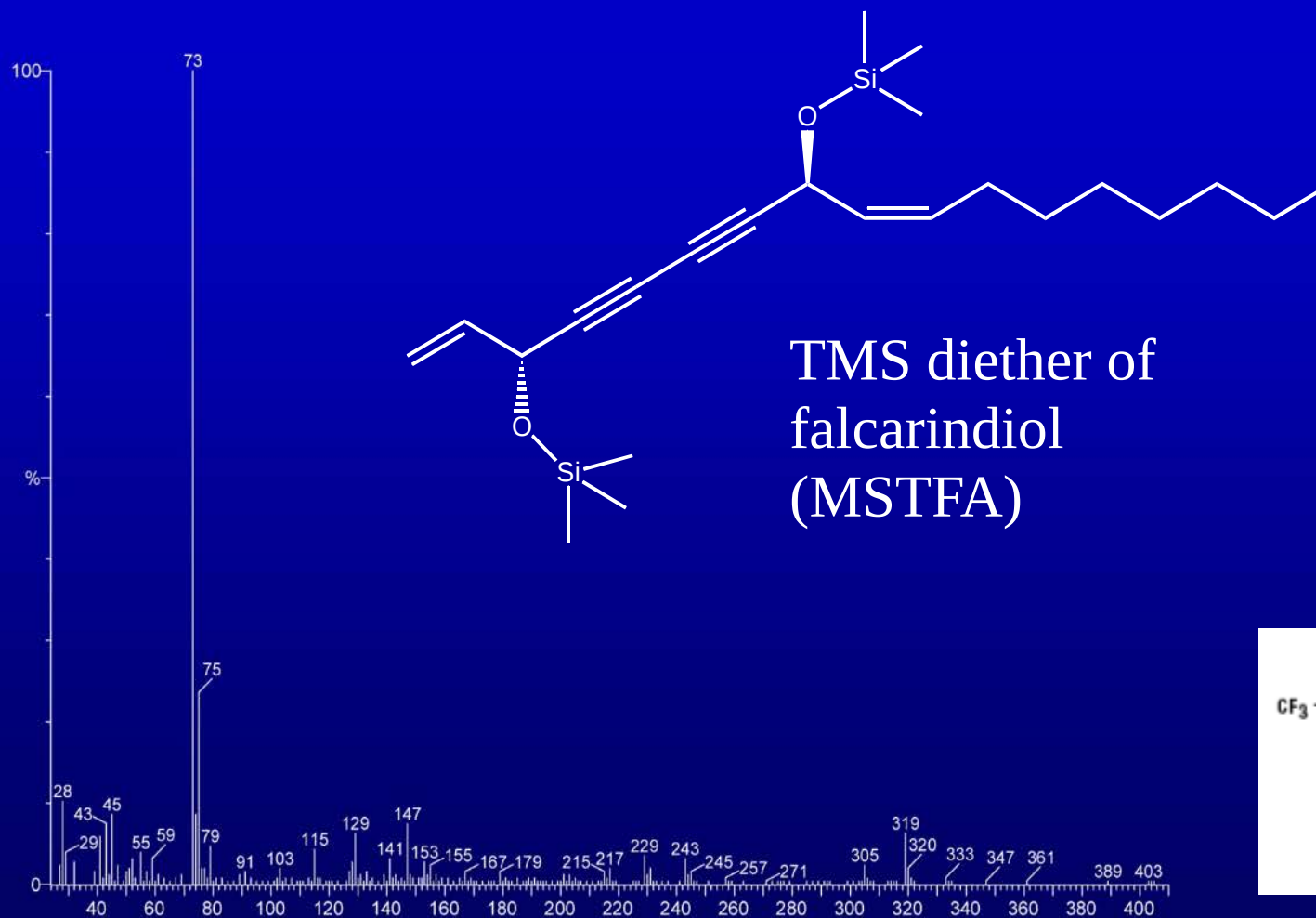
Kaempferol-3-glucopyranosyl-(1→2) rhamnopyranosyl-7-rhamnopyranoside (16.9 min)



EI spectrum of falcarindiol



EI spectrum of derivatized falcarindiol



Chromatogram

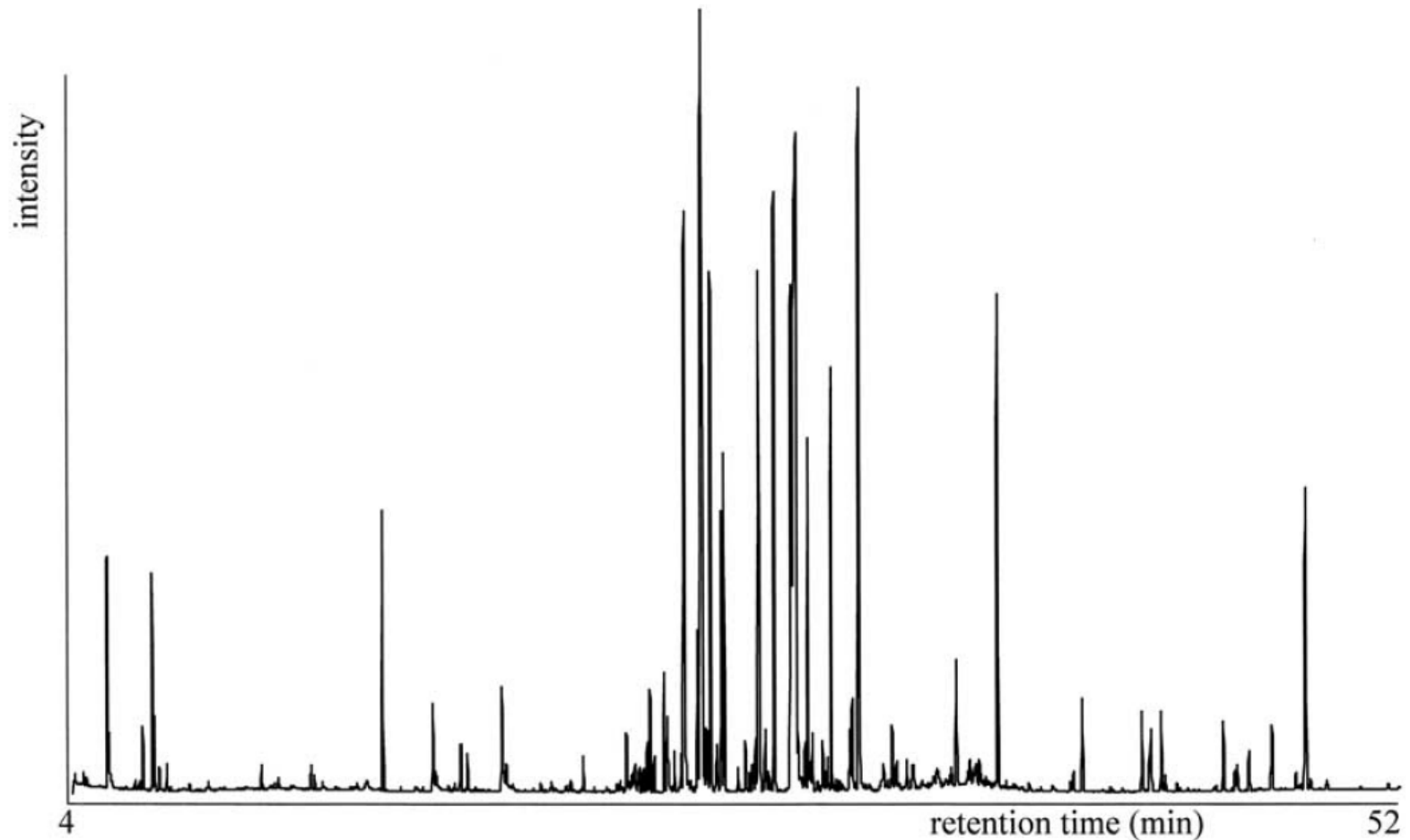


Figure 1. Lipophilic phase of *Arabidopsis thaliana* leaves analysed by GC/quadrupole MS (unpublished results). Inspection of peaks apparent in the base peak chromatogram results in 160 distinct metabolites. Abundant peaks in the middle of the chromatogram are methylated fatty acids. At the end of the chromatogram, trimethylsilylated sterols are eluted.

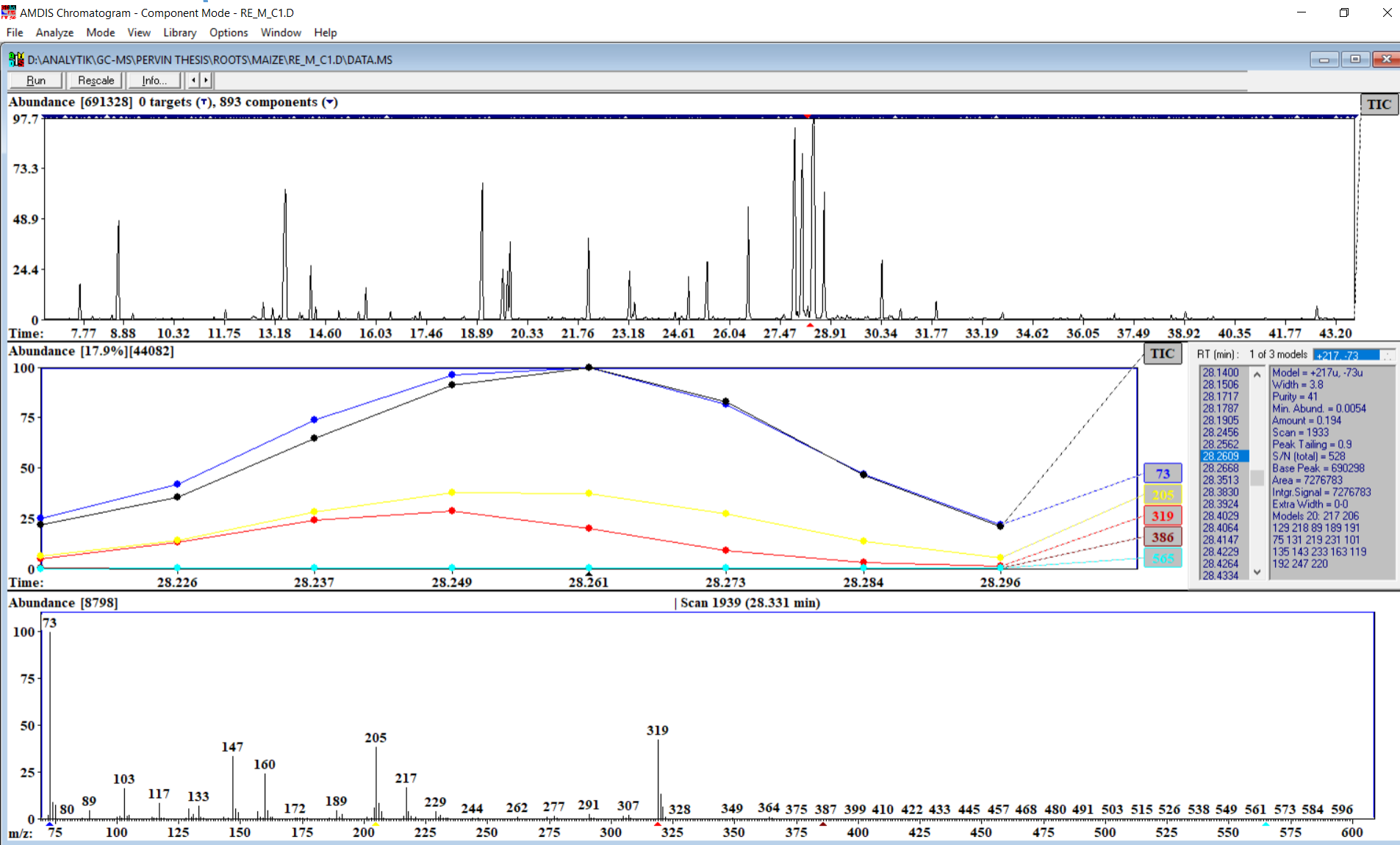


Gas chromatography

Electron impact mass spectrometry

Analysis of central (primary) metabolites

Deconvolution and peak integration (GC-EIMS)



<https://chemdata.nist.gov/mass-spc/amdis/downloads/>

Exported spectrum (EI-MS)

NAME: 28.2609 min RE_M_C1

COMMENT: 28.2609 min RE_M_C1

RT: 28.261

SOURCE: D:\Temp\test.msp

NUM PEAKS: 107

(71 9) (75 36) (76 3) (77 3) (78 1)
(81 5) (85 7) (87 8) (89 81) (90 8)
(91 5) (94 1) (97 2) (99 7) (101 18)
(109 2) (111 4) (113 7) (116 23) (119 10)
(120 2) (125 1) (129 88) (131 51) (132 5)
(133 289) (134 33) (135 17) (137 1) (143 14)
(144 2) (146 28) (151 2) (153 1) (155 6)
(159 18) (163 9) (164 2) (165 2) (169 14)
(170 3) (171 4) (174 4) (175 8) (176 1)
(179 1) (181 1) (183 3) (185 4) (187 4)
(189 45) (191 58) (192 11) (193 6) (194 1)
(197 1) (199 2) (203 22) (204 1000) (206 76)
(213 2) (215 4) (217 260) (218 84) (219 33)
(220 8) (231 33) (233 17) (242 2) (243 14)
(244 2) (245 5) (247 8) (248 3) (249 2)
(255 3) (257 3) (259 3) (261 3) (265 2)
(271 5) (272 1) (273 3) (287 5) (288 2)
(289 3) (290 9) (303 4) (317 6) (331 4)
(332 4) (333 4) (334 2) (335 3) (345 6)
(346 1) (347 2) (348 1) (361 3) (362 1)
(363 1) (377 13) (378 4) (379 3) (380 1)
(435 2) (436 1)

Database search (GC-EIMS)

GMD - MS Analysis Input

gmd.mpimp-golm.mpg.de/analysisinput.aspx

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SPECTRUM LIBRARY SEARCH & PREDICTION OF FUNCTIONAL GROUPS

This page facilitates the search of metabolites within the GMD by means of user submitted GC-MS spectra consisting of retention index (n-alkanes, if available) and mass intensities ratios. In addition, a functional group prediction will help to characterise those metabolites without available reference mass spectra included in the GMD so far. Instead, the unknown metabolite is characterised by predicted presence or absence of functional groups. For power users this functionality presented here is exposed as [soap based web services](#).

We kindly ask users to cite the following paper when publishing results derived from this service:

Hummel, J., Strehmel, N., Selbig, J., Walther, D. and Kopka, J. (2010) Decision tree supported substructure prediction of metabolites from GC-MS profiles, *Metabolomics*. <http://dx.doi.org/10.1007/s11306-010-0198-7>

Query

Enter the **GC-column type** the alkane retention index is based on!

VAR5

Enter the **alkane retention index** here (if neither an alkane RIs for VAR5 nor MDN35 is available in your setup please select 'none' in the input field above!)

1898

Paste the **spectrum** under investigation into the textbox below!

```
70 3 71 3 72 16 73 999 74 87 75 78 76 4 77 5 81 1 82 6 83 13 84 4 85 3 86 4 87 5 88 4 89 52 90 4 91 2 97 2 98 1 99 4
100 12 101 16 102 9 103 116 104 11 105 26 106 2 107 1 111 1 112 1 113 4 114 11 115 7 116 5 117 93 118 9 119 8 126 1
127 3 128 3 129 101 130 19 131 25 132 4 133 60 134 8 135 4 140 1 141 1 142 4 143 13 144 2 145 6 146 1 147 276 148 44
149 27 150 3 151 1 156 1 157 70 158 12 159 5 160 148 161 26 162 7 163 8 164 1 168 1 169 2 170 1 172 3 173 4 174 1 175
4 177 4 186 2 187 1 189 28 190 7 191 13 192 2 193 1 201 5 202 1 203 3 204 23 205 162 206 31 207 16 208 2 210 2 214 1
215 2 216 8 217 88 218 18 219 8 220 1 221 6 222 1 229 23 230 6 231 11 232 3 233 4 234 3 235 1 243 1 244 2 245 1 246 2
247 1 256 1 262 3 263 1 269 2 270 1 274 4 275 1 277 4 278 1 291 7 292 2 293 1 300 1 305 4 306 1 307 4 308 1 318 1 319
122 320 37 321 17 322 3 323 1 343 1 364 2 365 1
```

feedback

Top

Golm Metabolome Database

help

Results per page: 10 ▾

Search results (GC-EIMS)

csv export of library search result set

msp export of spectra hits

jcamp-dx export of spectra hits

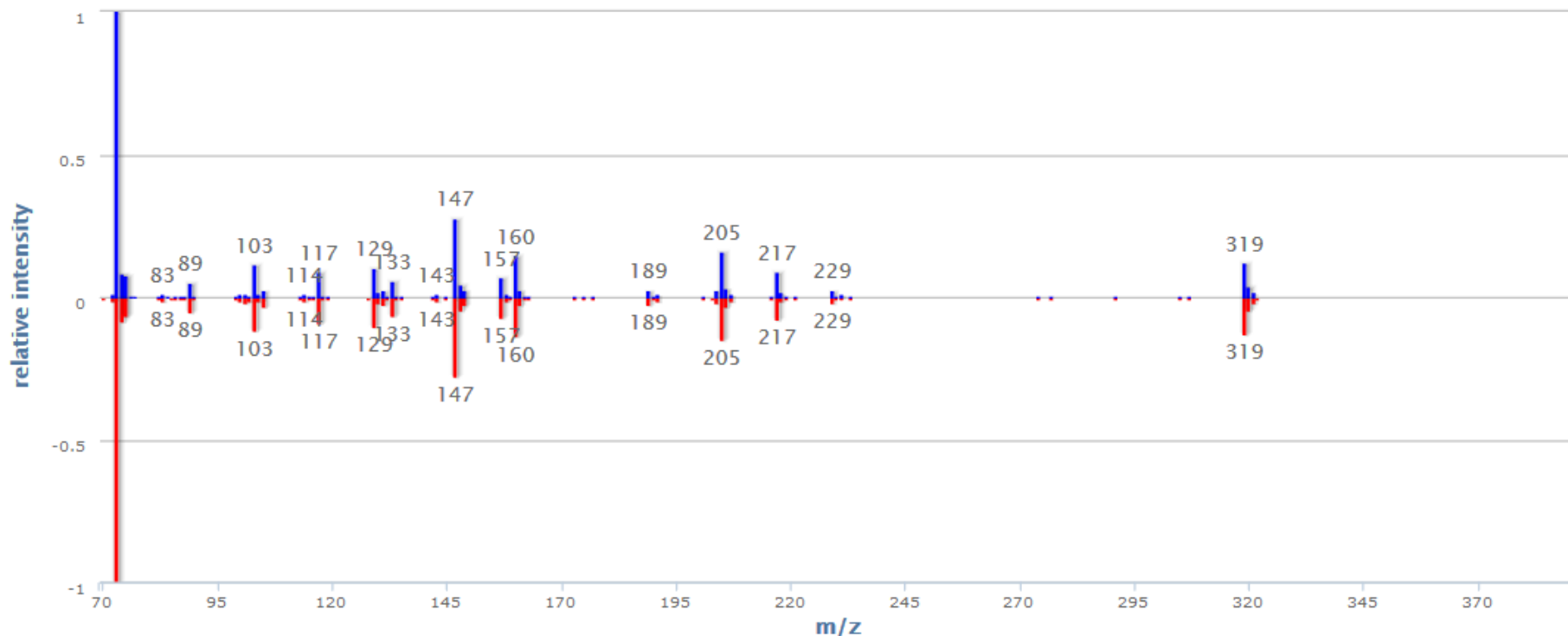
analyze details

metabolite details

spectral north-south-plot matching

spectral match with Glucose (1MEOX) (5TMS) MP

Reset zoom



north: user spectrum; south: library spectrum;

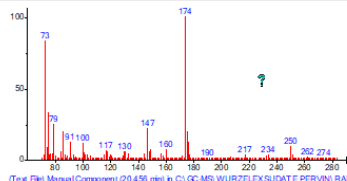
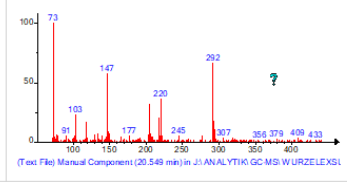
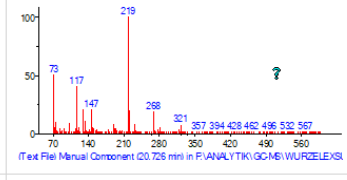
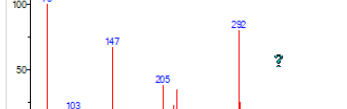
Search results (GC-EIMS)

Auswertung 2.xlsx - Excel Franz Hadacek

Datei Start Einfügen Seitenlayout Formeln Daten Überprüfen Ansicht Add-Ins ChemOffice16 ACROBAT Suchen Freigeben

Normal Umbruchvorschau Benutzerdef. Ansichten Seitenlayout Lineal Bearbeitungsleiste Gitternetzlinien Überschriften Arbeitsmappenansichten Anzeigen Zoom 100% Auswahl vergrößern Neues Fenster Alle anordnen Fenster fixieren Teilen Ausblenden Einblenden Fenster wechseln Makros Makros

R79

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1															
2			t	RI	RI rep		TMS	Ox							
81		?	20.45	1559	1573	Phenethylamine	2	1559	1573	Phenethylamine	2				
83		?	20.53	1563	1528	Erythronic acid	4	1563	1528	Erythronic acid	4	1268505	2085900	1315493	5125073
84		?	20.71	1571	1577	A155004 (GMD Standard)		1571	1577	A155004 (GMD Standard)		516047	2415403	44499582	624839
85		?	20.95	1581	1562	Threonic acid	4	1581	1562	Threonic acid	4	2356735	39531516	7793295	41561205

RAW Data Data_konsolidiert Data_korr ...

Bereit 70 %

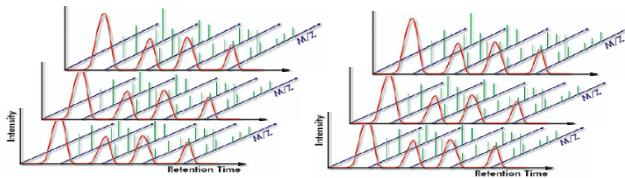
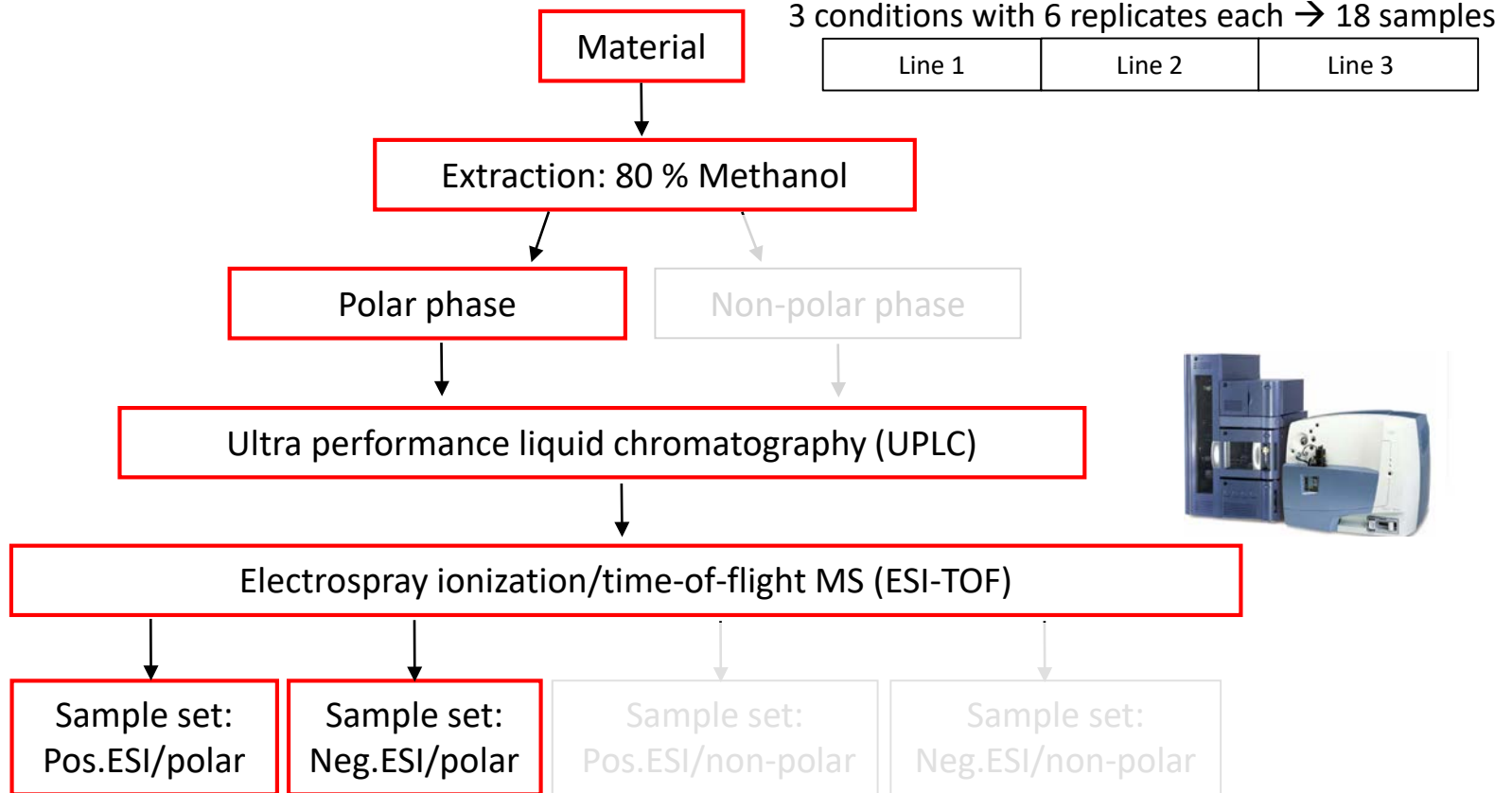
Liquid chromatography

Electrospray interface

Time-of-flight mass spectrometry

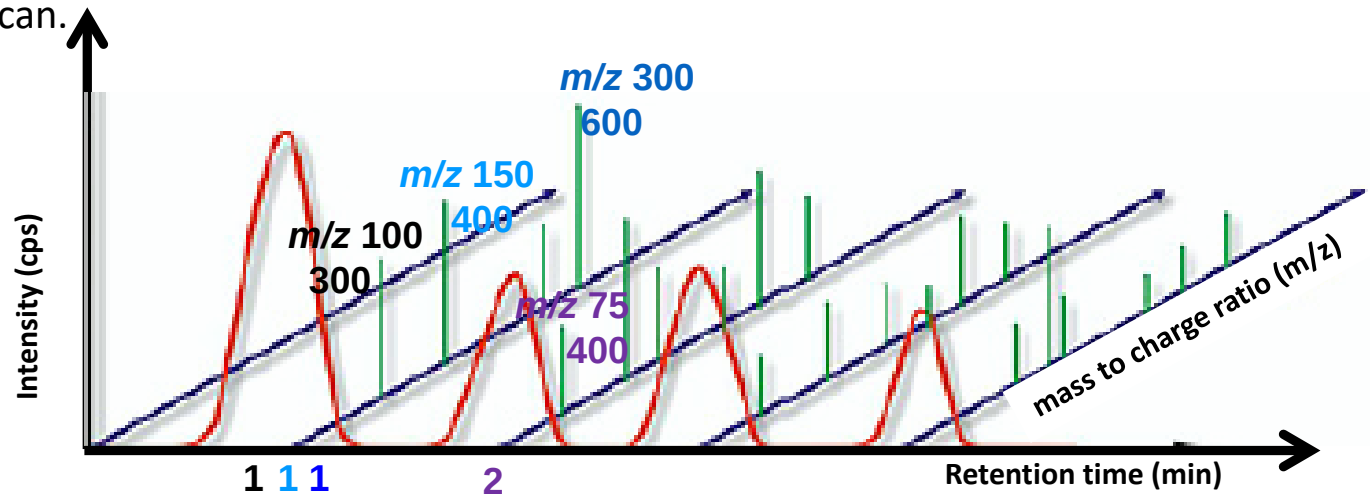
Analysis of specialized (secondary) metabolites

Metabolite fingerprinting



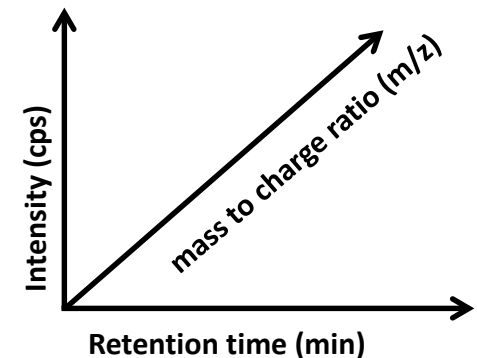
A MS signal is characterized by m/z , R_t and the signal intensity

A TIC (Total Ion Chromatogram) is a chromatogram created by summing up all intensities of all m/z peaks belonging to the same scan.



Total ion chromatogram (TIC)

A MS signal is characterized by the three parameters:
 m/z (300), R_t (1min) and signal intensity (600 cps)



Retention time	m/z	Intensity
1	100	300
1	150	400
1	300	600
2	75	400



Open and inspect TICs

MassLynx - Wound - KF123_master_practical_course_150511.SPL

File View Run Help

Shortcut Queue Status

Queue Is Empty

Spectrum Chromatogram Map Edit Samples

	File Name	File	MS File	Inlet File	Bottle	Inject Volume
1						0.000
2	KF122_masterprak_eg_p_pos_150424_02c		Wpos_DRE_10min_85_1200Da	Polar_HSST3_column1_14min	1:1	2.000
3	KF122_masterprak_wt1_c01_p_pos_150424_01		Wpos_DRE_10min_85_1200Da	Polar_HSST3_column1_14min	1:3	1.000
4	KF122_masterprak_wt2_c01_p_pos_150424_01		Wpos_DRE_10min_85_1200Da	Polar_HSST3_column1_14min	1:4	1.000
5	KF122_masterprak_wt3_c011_p_pos_150424_01		Wpos_DRE_10min_85_1200Da	Polar_HSST3_column1_14min	1:5	1.000

Open a total ion chromatogram (TIC):
Left click on the number (3) of the selected run (→ black)
Left click on chromatogram

Chromatogram - [KF122_masterprak_wt1_c01_p_pos_150424_01]

File Edit Display Process Window Tools Help

TIC

KF122_masterprak_wt1_c01_p_pos_150424_01

1: TOF MS ES+
TIC
4.78e5

100 0.42 8.97

4.52 4.76 8.53

4.05 1.95 2.67 3.27 7.70

%

Time

1.00 2.00 3.00 4.00 5.00 6.00 7.00 8.00 9.00

Open and inspect TICs

MassLynx - Wound - KF123_master_practical_course_150511.SPL

File View Run Help

Shortcut Queue Status

Queue Is Empty

Spectrum Chromatogram Map Edit Samples

	File Name	File	MS File	Inlet File	Bottle	Inject Volume
1						0.000
2	KF122_masterprak_eg_p_pos_150424_02c		Wpos_DRE_10min_85_1200Da	Polar_HSST3_column1_14min	1:1	2.000
3	KF122_masterprak_wt1_c01_p_pos_150424_01		Wpos_DRE_10min_85_1200Da	Polar_HSST3_column1_14min	1:3	1.000
4	KF122_masterprak_wt2_c01_p_pos_150424_01					1.000
5	KF122_masterprak_wt3_c01_p_pos_150424_01					1.000
6						0.000
7	KF122_masterprak_eg_p_pos_150424_01					1.000
8	KF122_masterprak_wt1_c01_p_pos_150424_01					
9	KF122_masterprak_wt2_c01_p_pos_150424_01					
10	KF122_masterprak_wt3_c01_p_pos_150424_01					
11						
12	KF123_masterprak_wt1_c01_p_pos_150424_01					
13	KF123_masterprak_wt2_c01_p_pos_150424_01					
14	KF123_masterprak_wt3_c01_p_pos_150424_01					
15	KF123_masterprak_wt4_c01_p_pos_150424_01					
16	KF123_masterprak_wt5_c01_p_pos_150424_01					
17	KF123_masterprak_wt6_c01_p_pos_150424_01					
18	KF123_masterprak_wt7_c01_p_pos_150424_01					
19	KF123_masterprak_wt8_c01_p_pos_150424_01					
20	KF123_masterprak_wt9_c01_p_pos_150424_01					
21	KF123_masterprak_wt10_c01_p_pos_150424_01					
22	KF123_masterprak_wt11_c01_p_pos_150424_01					
23	KF123_masterprak_wt12_c01_p_pos_150424_01					
24	KF123_masterprak_wt13_c01_p_pos_150424_01					
25	KF123_masterprak_wt14_c01_p_pos_150424_01					
26	KF123_masterprak_wt15_c01_p_pos_150424_01					
27	KF123_masterprak_wt16_c01_p_pos_150424_01					
28	KF123_masterprak_wt17_c01_p_pos_150424_01					
29	KF123_masterprak_wt18_c01_p_pos_150424_01					
30	KF123_masterprak_wt19_c01_p_pos_150424_01					
31	KF123_masterprak_wt20_c01_p_pos_150424_01					
32	KF123_masterprak_wt21_c01_p_pos_150424_01					
33	KF123_masterprak_wt22_c01_p_pos_150424_01					
34	KF123_masterprak_wt23_c01_p_pos_150424_01					
35	KF123_masterprak_wt24_c01_p_pos_150424_01					
36	KF123_masterprak_wt25_c01_p_pos_150424_01					
37	KF123_masterprak_wt26_c01_p_pos_150424_01					

Tools

- Optimize
- Colors and Fonts
- Print Desktop
- Strip
- Accurate Mass Measure
- Accurate Mass Filter
- Extended Statistics
- Combine Functions
- Combine All Files
- Molecular Weight Calculator

Chromatogram - [KF122_masterprak_wt1_c01_p_pos_150424_01,KF122_masterprak...

File Edit Display Process Window Tools Help

TIC

KF122_masterprak_wt1_c01_p_neg_150424_01

1: TOF MS ES-
TIC
1.95e5

Line1, neg.ESI

0.84 2.48 2.66 3.15 3.30 4.04 4.51 4.75 7.13 7.71 8.89

KF122_masterprak_wt1_c01_p_pos_150424_01

1: TOF MS ES+
TIC
4.78e5

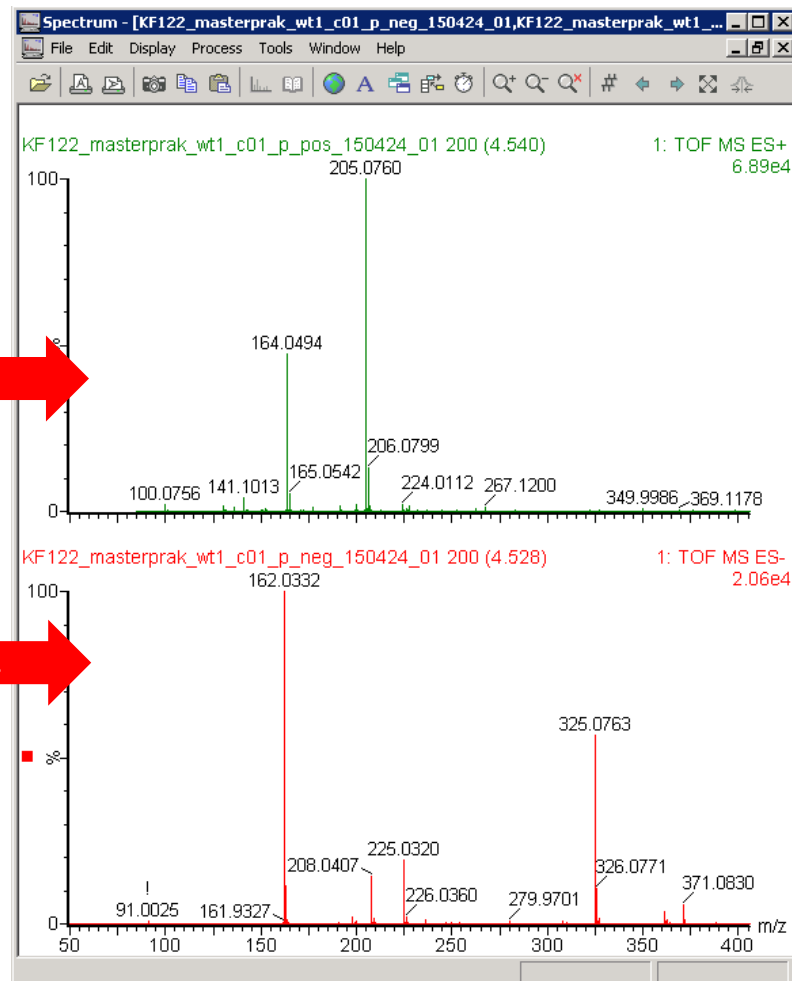
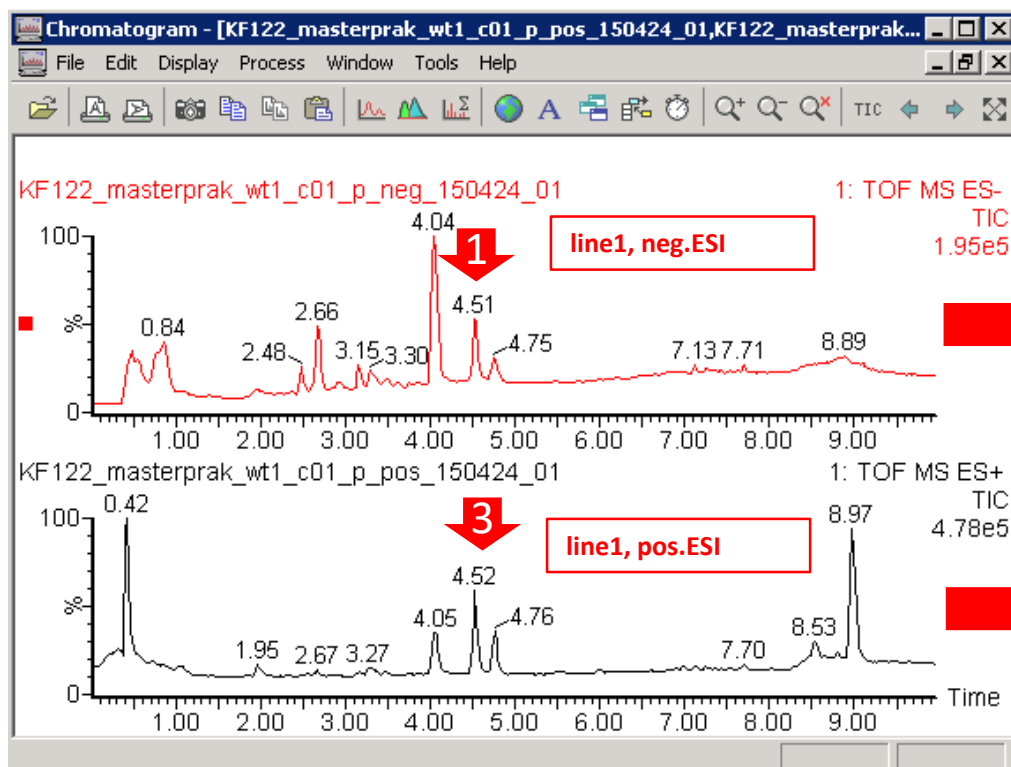
line1, pos.ESI

0.42 1.95 2.67 3.27 4.05 4.52 4.76 7.70 8.53 8.97

Time

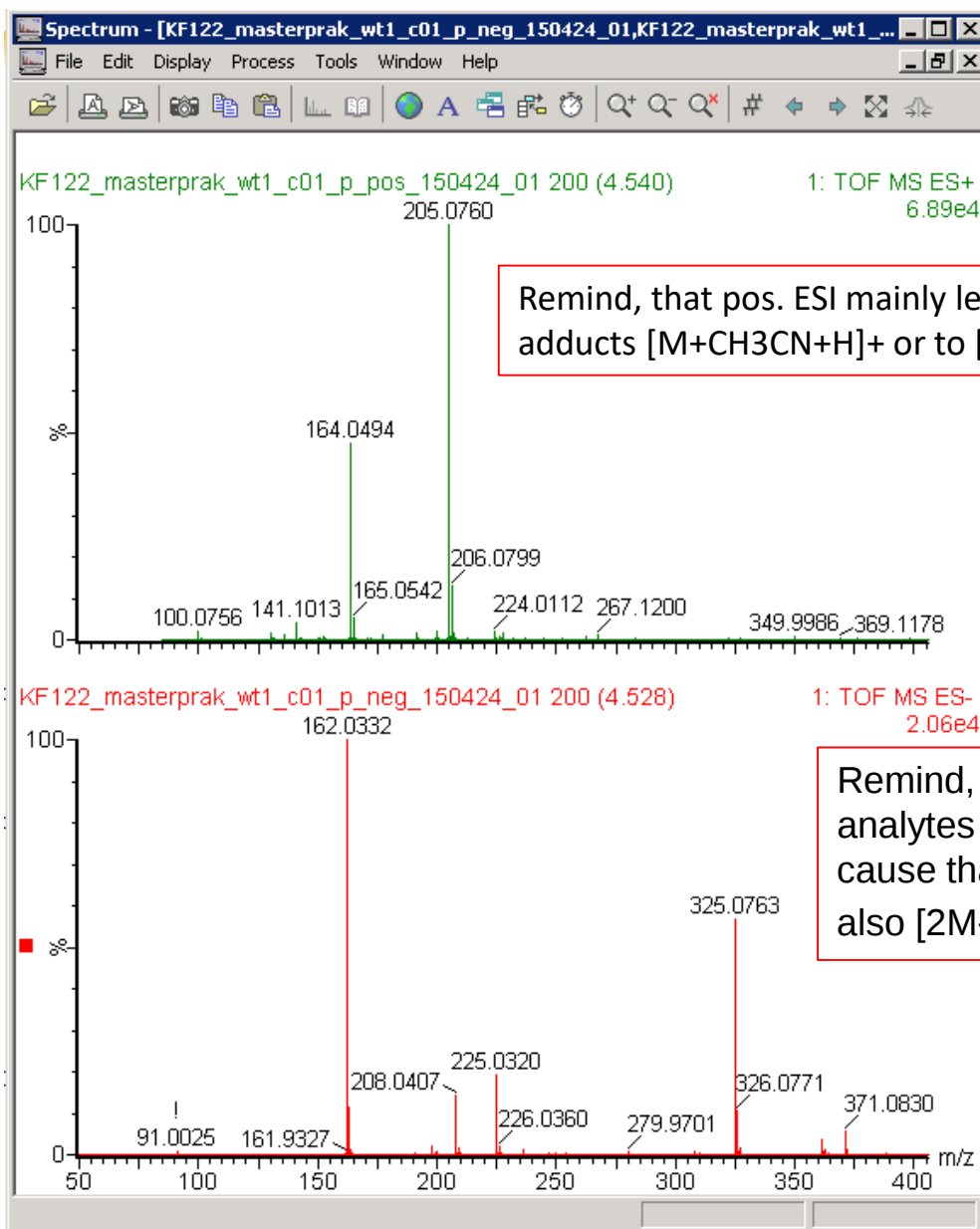
Open and inspect the mass spectra

Open the mass spectra at 4.52 min for both analysis by left double click or right click into the chromatogram.



Walk through the chromatogram and search different scans (mass spectra) by moving the right/left key on the key board or moving the cursor.

Search for a mass signal of a compound, that occurs in pos. and neg. mode and describe their corresponding adducts in both modi (for adduct rules see next slide)



Remind, that pos. ESI mainly leads to protonated analytes $[M+H]^+$ and solvent adducts $[M+CH_3CN+H]^+$ or to $[M+Na]^+$ and $[M+NH_4]^+$ adducts

Remind, that neg. ESI mainly leads to deprotonated analytes $[M-H]^-$ and the formic acid $[M+HCOO]^-$ adduct. In case that the concentration of a compound is very high, also $[2M-H]^-$ adducts are built in the source.

How to identify adducts?

Adducts are built during ionisation in the source. Because of that, they have the identical RT as its protonated or deprotonated ion and are characterized by a very exact mass shift to that corresponding ion (see below).

Mass differences (neg. ESI mode):

$[M-H]^-$ to $[M+HCOO]^- \rightarrow 46.0055$

$[M-H]^-$ to $[2M-H]^- \rightarrow [2M-1.0073]^-$

Mass differences (pos. ESI mode):

$[M+H]^+$ to $[M+Na]^+ \rightarrow 21.9825$ } 4.956

$[M+H]^+$ to $[M+NH_4]^+ \rightarrow 17.0265$ }

$[M+H]^+$ to $[2M-H]^- \rightarrow [2M+1.0073]^+$

$[M+H]^+$ to $[M+CH_3CN+H]^+ \rightarrow 41.0265$

Exact masses for common element of organic compounds:

H: 1.0078 Da, but H^+ : 1.0073

C: 12.0000 Da

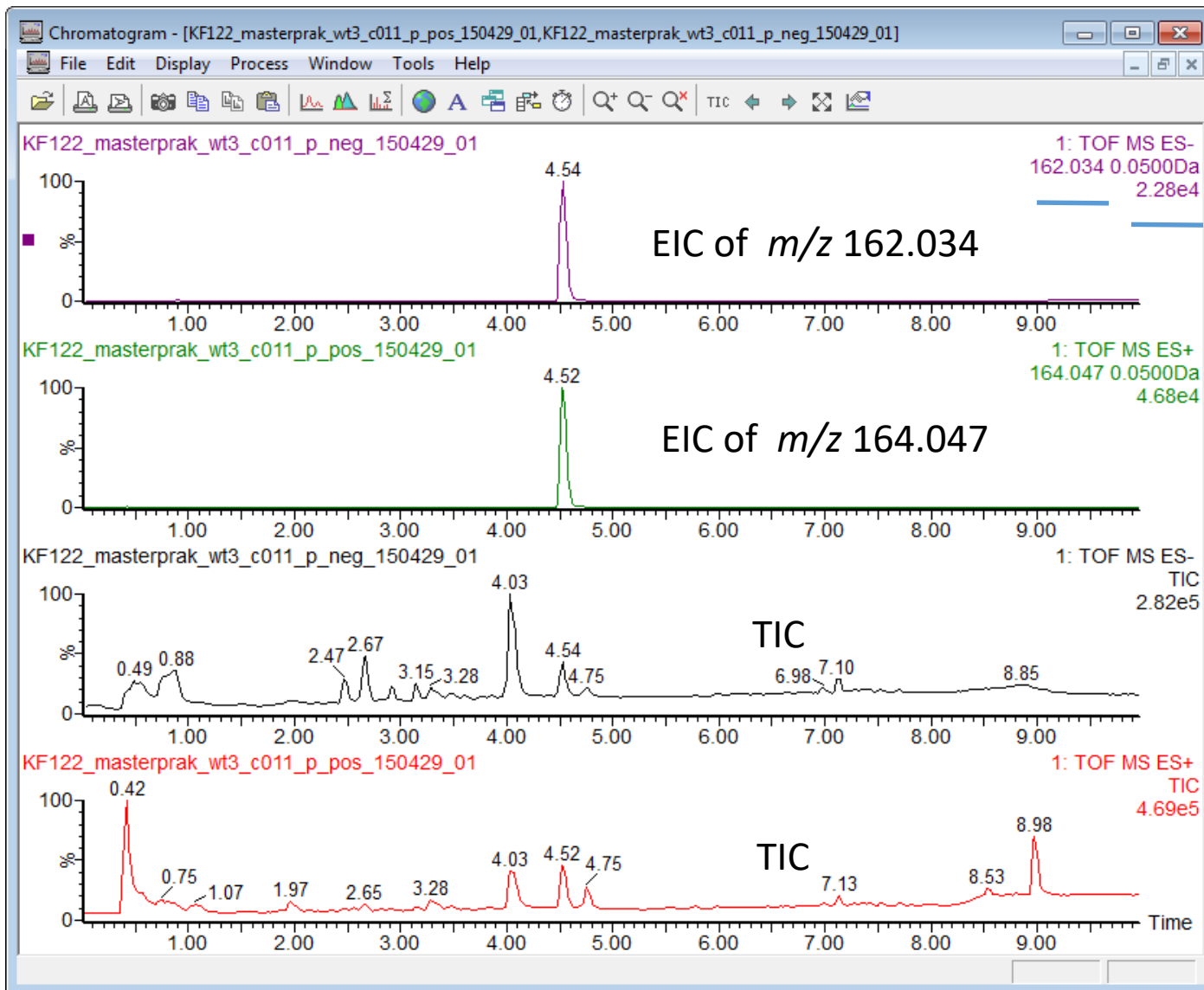
O: 15.9949 Da

N: 14.0031 Da

P: 30.9738 Da

S: 31.9721 Da

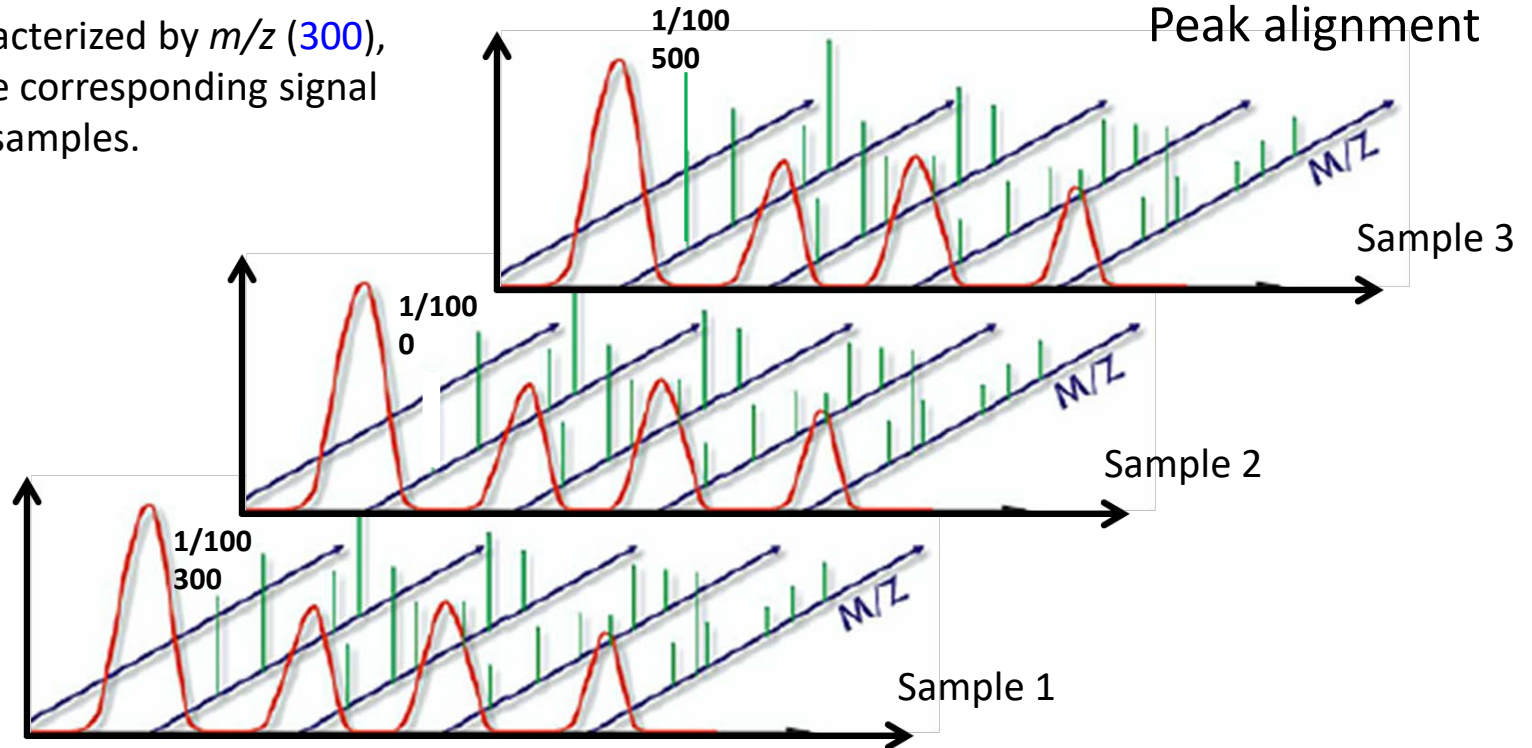
Extracted mass chromatogram (EIC, XIC)



Intensity of
the extracted mass
signal (cps)

MarkerLynx performs peak picking and peak alignment

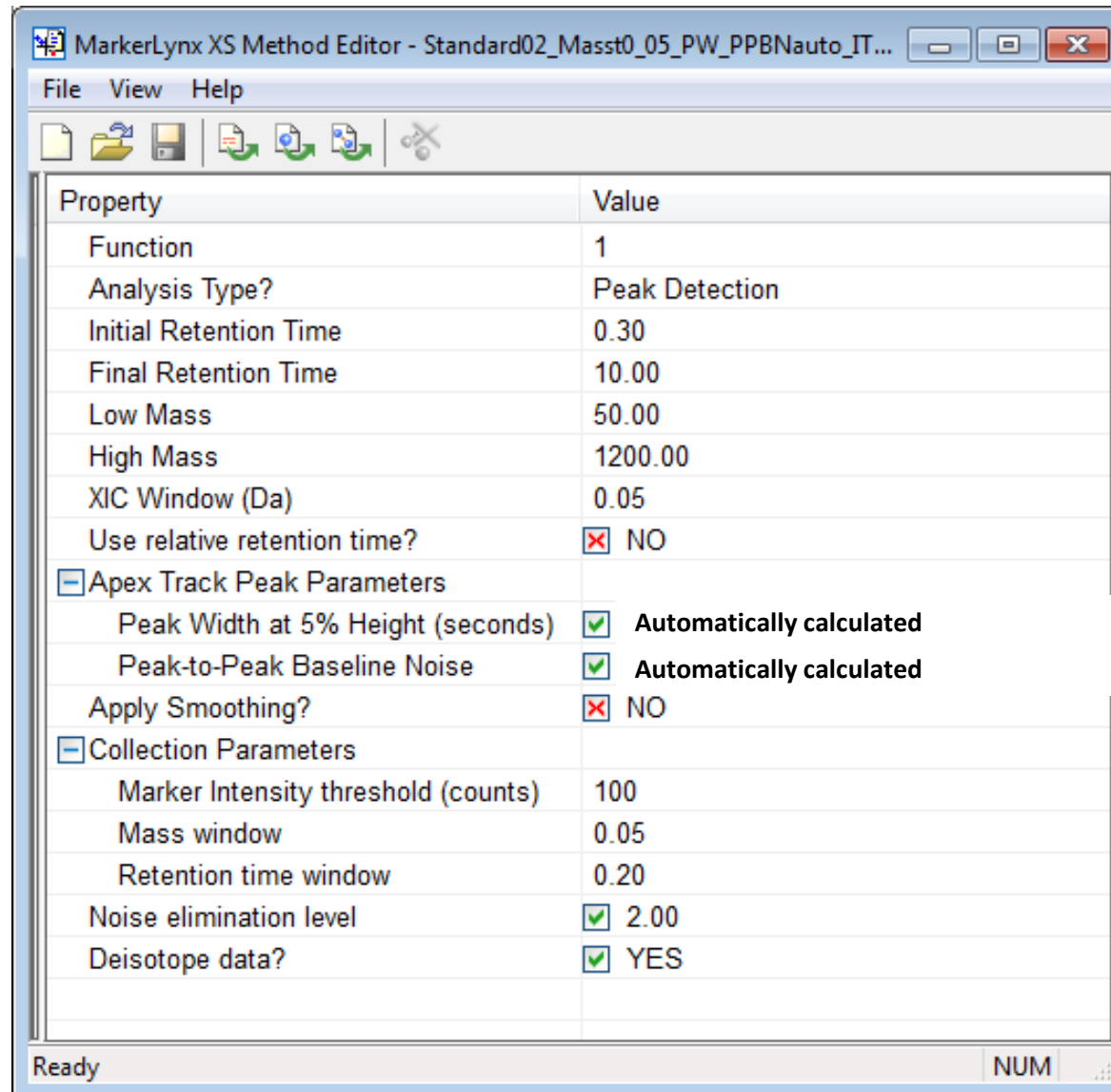
A **feature** is characterized by m/z (300), Rt (1min) and the corresponding signal intensities of all samples.



➔ Data matrix

	one feature				
	Rt / m/z				
	1/100	1/150	1/300		2/75
Sample 1	300	400	600		400
Sample 2	0	0	30		10
Sample 3	500	21	16		8
.....					
Sample n	0	0	35		12

MarkerLynx performs peak picking and peak alignment



MarkerLynx creates a data matrix

					group 1			group 2			group 3			group 4			group 5			group 6			
					line 1	line 2	line 3	line 1	line 2	line 3	line 1	line 2	line 3	line 1	line 2	line 3	line 1	line 2	line 3	line 1	line 2	line 3	
Ret. Time	m/z	Biotransf	Included	Saturated	KF123_ma	KF123_ma	KF123_ma	KF123_ma	KF123_ma	KF123_ma	KF123_ma	KF123_ma	KF123_ma	KF123_ma	KF123_ma	KF123_ma	KF123_ma	KF123_ma	KF123_ma	KF123_ma	KF123_ma	KF123_ma	
9.0716	101.0715		Yes	No	882.0952	262.7163	0	283.7944	619.7363	1162.66	0	0	0	0	921.9146	0	0	801.4941	0	383.4438	1087.562	299.6514	
9.7887	101.0714		Yes	No	0	354.0166	681.0884	363.5645	314.2451	202.9902	499.5205	0	0	482.127	0	253.7441	361.6699	0	0	328.0645	216.165	0	
8.8178	101.0713		Yes	No	1154.428	1172.914	1158.673	1245.879	1248.584	1008.378	1238.956	1429.4	1311.273	1327.131	1690.79	1403.039	1557.743	1960.483	1759.028	1362.172	1524.441	1408.715	
9.2701	101.0713		Yes	No	417.085	714.499	0	0	473.7627	0	0	0	0	682.2817	304.2061	508.9824	778.376	545.9521	850.8374	0	256.4126	360.4023	
9.5318	101.0712		Yes	No	314.1738	0	0	0	447.7827	693.7471	0	0	0	0	0	0	0	0	424.7026	0	0	413.5869	
8.4987	101.0712		Yes	No	548.4849	636.7832	223.2461	463.8796	521.9688	390.8638	0	0	647.071	651.9302	251.147	156.0684	250.6074	0	261.2695	276.168	127.3477	221.7402	
0.3576	100.0767		Yes	No	0	0	0	236.6903	226.496	211.6368	377.2024	0	347.4537	0	218.1116	0	0	323.2346	0	293.1354	0	383.3393	
8.5524	100.0766		Yes	No	125.2697	153.4164	0	228.1321	139.4534	27.0656	150.2716	0	0	145.2825	103.2449	270.1361	201.2876	464.4622	0	0	179.0063	43.4053	
8.7742	100.0763		Yes	No	268.8967	303.024	468.2544	362.1595	321.9352	379.1399	254.5883	390.9028	415.6243	504.0273	574.6771	0	437.8279	551.9454	315.3832	353.0796	394.2798	376.2729	
0.7735	100.0763		Yes	No	603.622	578.1069	635.5267	382.7745	231.8239	189.2976	663.0088	552.723	298.9272	546.4854	393.7505	307.7651	292.7864	567.5922	461.8815	305.2363	612.438	0	
1.3838	100.0762		Yes	No	108.6471	204.8467	38.823	221.4904	102.9684	96.4639	215.2853	0	53.2627	152.3521	83.523	103.0213	73.1382	0	39.1654	112.6183	0	45.0715	
0.5772	100.0761		Yes	No	0	0	455.5798	0	381.0845	0	0	0	344.5036	0	0	0	0	0	0	0	0	178.1351	
2.6759	100.0761		Yes	No	306.1294	0	0	0	54.8224	0	0	0	0	0	0	294.9215	273.5017	0	264.5965	328.3875	0	0	
0.4104	94.0451		Yes	No	627.6673	420.7847	676.8804	819.5258	431.9557	862.4532	698.5081	451.0273	849.0703	686.172	623.0878	780.2838	897.8263	501.6707	921.1264	562.8005	506.076	847.6222	
0.4222	86.5821		Yes	No	136.6347	274.6291	16.2025	545.1334	449.8309	101.7945	212.3313	268.7368	37.4729	212.9345	385.7653	121.7012	124.103	431.5797	0	210.127	314.9386	167.5492	
0.485	112.8968		Yes	No	427.4036	184.74	50.6329	273.551	155.7257	254.4329	519.8291	130.277	472.7988	111.3924	275.4526	145.3938	460.104	126.7795	115.4288	351.1493	218.7673	117.5218	
0.4103	111.0385		Yes	No	2360.795	1730.289	1715.175	2063.221	1918.056	1697.267	2445.888	2288.683	1937.034	2810.959	1928.101	2150.84	2126.823	2512.878	1816.645	1864.936	2291.697	2160.416	
0.441	108.5756		Yes	No	19.2405	86.4135	15.4193	156.5653	202.4172	37.8059	73.8115	71.5436	17.7742	35.6593	245.0024	105.3164	20.2532	184.5401	67.091	92.1519	115.5671	70.981	
0.4407	106.0508		Yes	No	614.1013	565.6454	388.3525	1021.834	603.9758	402.7023	763.0594	709.3617	481.9627	738.2966	553.6714	657.8618	626.3096	649.9551	0	658.2168	710.1682	549.9656	
0.4217	105.0432		Yes	No	430.1598	408.2475	464.5026	696.9055	406.4919	287.3443	390.4571	401.6479	386.7248	379.6534	0	373.3494	518.8275	383.9574	585.6287	443.0052	316.6424	431.1303	
9.5114	105.043		Yes	No	0	0	1145.032	520.9121	755.4917	601.7397	1252.806	1579.861	924.3716	1710.675	684.7075	545.186	954.1631	2101.408	1324.661	0	0	949.459	
9.0919	105.0429		Yes	No	0	0	828.9619	0	0	635.6992	0	0	0	0	247.8135	0	0	0	0	0	0	656.3809	
8.5284	105.0428		Yes	No	3464	3095.705	1413.669	569.6016	2465.163	1451.181	3116.457	3733.392	1849.939	3727.597	3773.33	866.1016	3771.936	3568.118	563.5547	3591.108	4474.91	1528.078	
9.3275	105.0427		Yes	No	1141.644	0	1145.032	1422.371	562.8584	167.0898	381.3472	230.2793	523.7207	1894.398	0	0	1009.84	0	892.3164	0	235.793	327.168	
9.7608	105.0426		Yes	No	0	0	0	724.4727	498.8281	0	1140.785	0	883.5762	1217.606	1163.224	775.8818	1098.387	497.2559	1081.367	1026.18	0	1261.216	
7.8748	105.0425		Yes	No	0	0	0	0	0	0	0	239.3794	0	276.6528	0	0	86.2819	0	0	215.8767	0	0	
8.7202	105.0425		Yes	No	1864.55	2134.779	1290.898	3061.77	1349.021	1799.292	4059.114	1684.168	1783.396	2054.786	708.9268	2114.42	1864.489	5123.484	2594.85	1208.708	2851.748	1119.277	
8.187	105.0424		Yes	No	0	0	0	236.4973	0	0	210.1033	0	0	200.2227	256.824	172.2122	201.0728	0	0	227.3059	0	233.2175	
0.4948	104.1069		Yes	No	3651.015	3748.58	2051.784	3689.213	3614.463	3814.795	3808.646	3797.738	3832.834	3531.703	3904.681	3584.891	3871.593	3979.554	3301.108	3887.903	3691.648	3330.798	



Department of Bioinformatics

Metabolomics Project

MarVis

MarVis-Graph

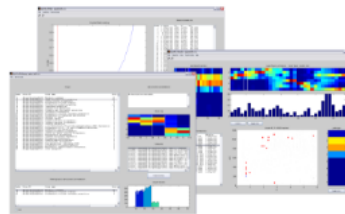
MarVis

The MarVis-Suite: Marker Visualization, Filtering, Clustering, and Functional Analysis

Rechteckiges Ausschneiden

The **MarVis-Suite** (**Marker Visualization**) is a toolbox for interactive ranking, filtering, combination, clustering, visualization, and functional analysis of data sets containing intensity-based profile vectors (data set features or marker candidates), as obtained e.g. from mass spectrometry (MS), microarray, or RNA-seq experiments. The clustering algorithm is based on a realization of one-dimensional self-organizing maps (1D-SOMs). Additionally, the MarVis-Suite includes specialized functions for analysis of MS data in the context of non-targeted metabolomics studies, such as adduct and isotope correction, molecular formula calculation, and pathway reconstruction based on accurate masses.

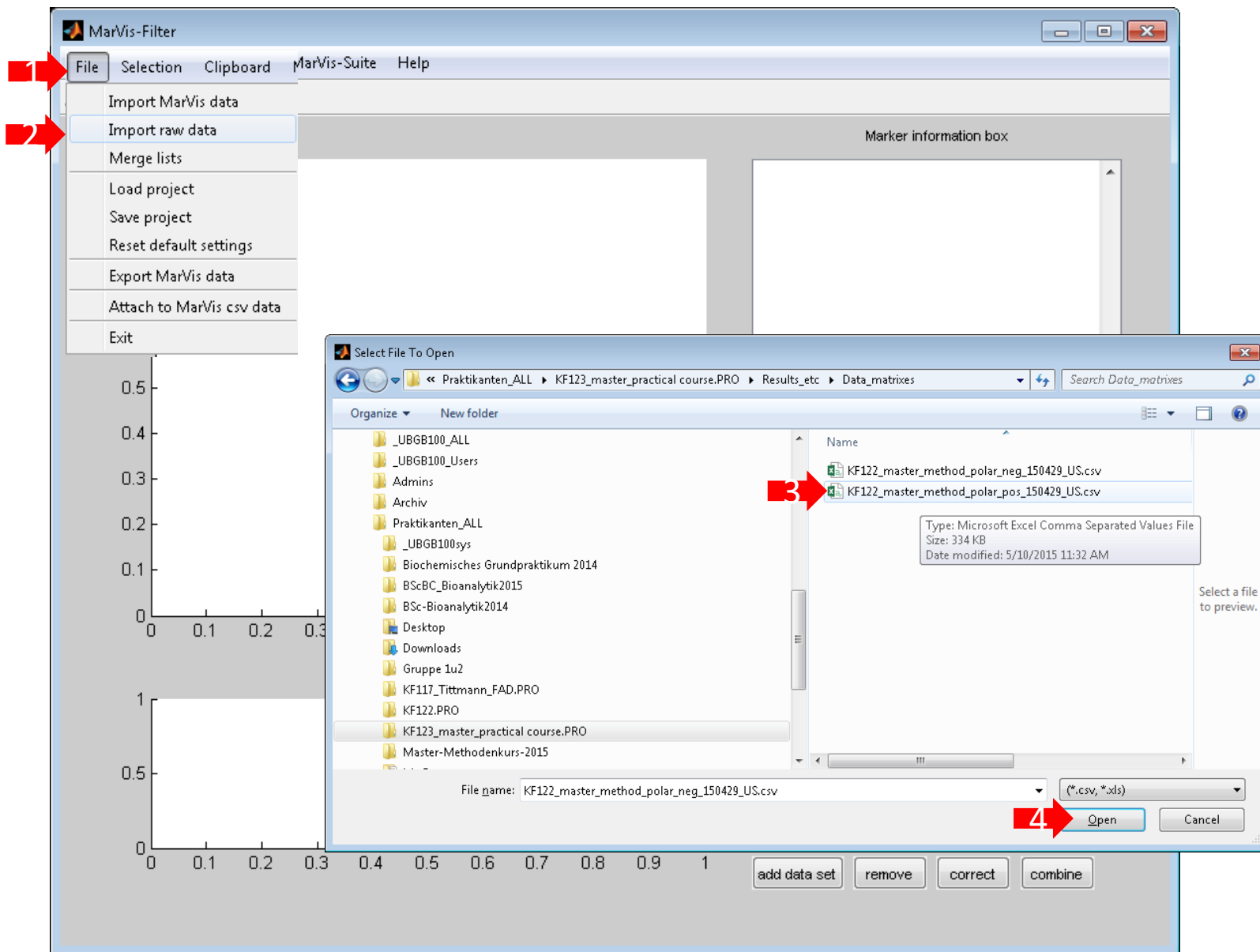
Within the MarVis-Suite framework, the MarVis-Filter interface provides functions for import, preprocessing, filtering, and combination of raw data files, while the MarVis-Cluster interface was designed for high-level visualization and cluster analysis. The MarVis-Pathway interface is used for functional annotation of filtered/combined (cross-omics) data sets or selected clusters in the context of reference or organism-specific pathway maps. For statistical analysis of combined data sets from different omics platforms, MarVis-Pathway provides an extensive framework for (Gene/Metabolite) Set Enrichment Analysis and meta-analysis. Within the MarVis-Suite, selected data can be easily exchanged between the different interfaces. Nonetheless, the interfaces can also be used as independent tools.



Open MarVis Filter 2.6

Import data matrix1 (pos. ESI)

W:\Praktikanten_ALL\KF123_master_practical course.PRO\Results_etc\Data_matrixes



Import data matrix (pos. ESI)

Import dialog

Delimiter:
Start row:
Start column:

ID column:
☒ Generate IDs
ID label:
x column: x label:
y column: y label:
Condition identifiers (separated by delimiter):

Additional columns:
Additional labels:

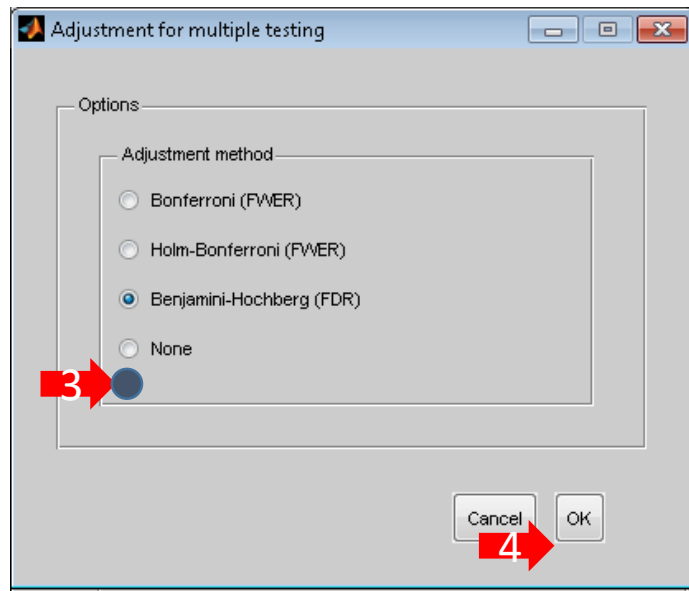
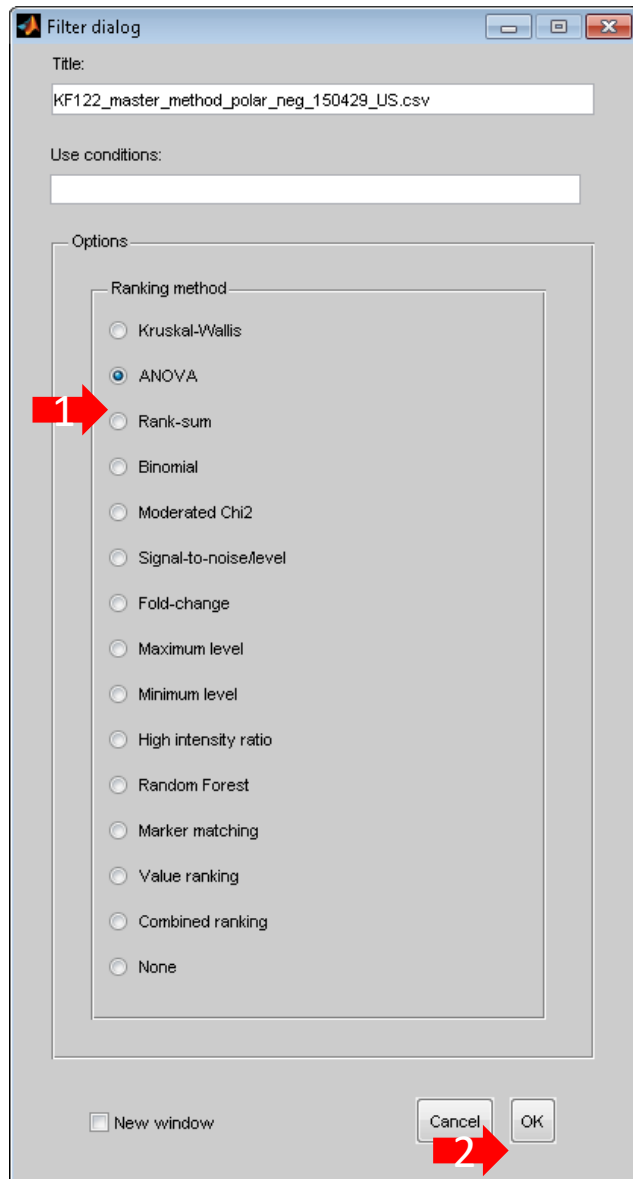
? 27 sample columns found (9 9 9 samples per condition). Continue?

Log-scale transformation

? Perform log-scale transformation of intensities?

Select type of sample-based normalization

Rank the data by ANOVA



Filter the data set

Correct the adducts

The screenshot displays the MarVis-Filter software interface with several windows and a main data plot. The main window shows a plot of FDR (False Discovery Rate) versus marker, with a blue curve rising from left to right. Below this plot is a histogram of sample intensities, with the x-axis labeled 'sample' (ranging from 0 to 25) and the y-axis labeled 'intensity' (ranging from 0 to 300). The histogram bars are colored blue for samples 1-10 and green for samples 11-25.

Numbered red arrows indicate the following steps:

1. Click on the 'Selection' menu in the top-left corner.
2. Click on 'Adduct and isotope correction' in the Selection menu.
3. Click on the 'Isotope correction' dialog box.
4. Click on the 'OK' button in the Isotope correction dialog box.
5. Click on the 'Cosine ...' dialog box.
6. Click on the 'OK' button in the Cosine ... dialog box.
7. Click on the 'Select input file for adduct rules' dialog box.
8. Click on the 'adduct_pos.txt' file in the file list.
9. Click on the 'Open' button in the Select input file for adduct rules dialog box.
10. Click on the 'Tolerances' dialog box.
11. Click on the 'rt tolerance' input field.
12. Click on the 'm/z tolerance' input field.
13. Click on the 'OK' button in the Tolerances dialog box.

The 'Isotope correction' dialog box has a text field for 'Maximal number of C13 isotopes per marker candidate' with the value '0'.

The 'Cosine ...' dialog box has a text field for 'Minimal cosine similarity (0-1)' with the value '0.75'.

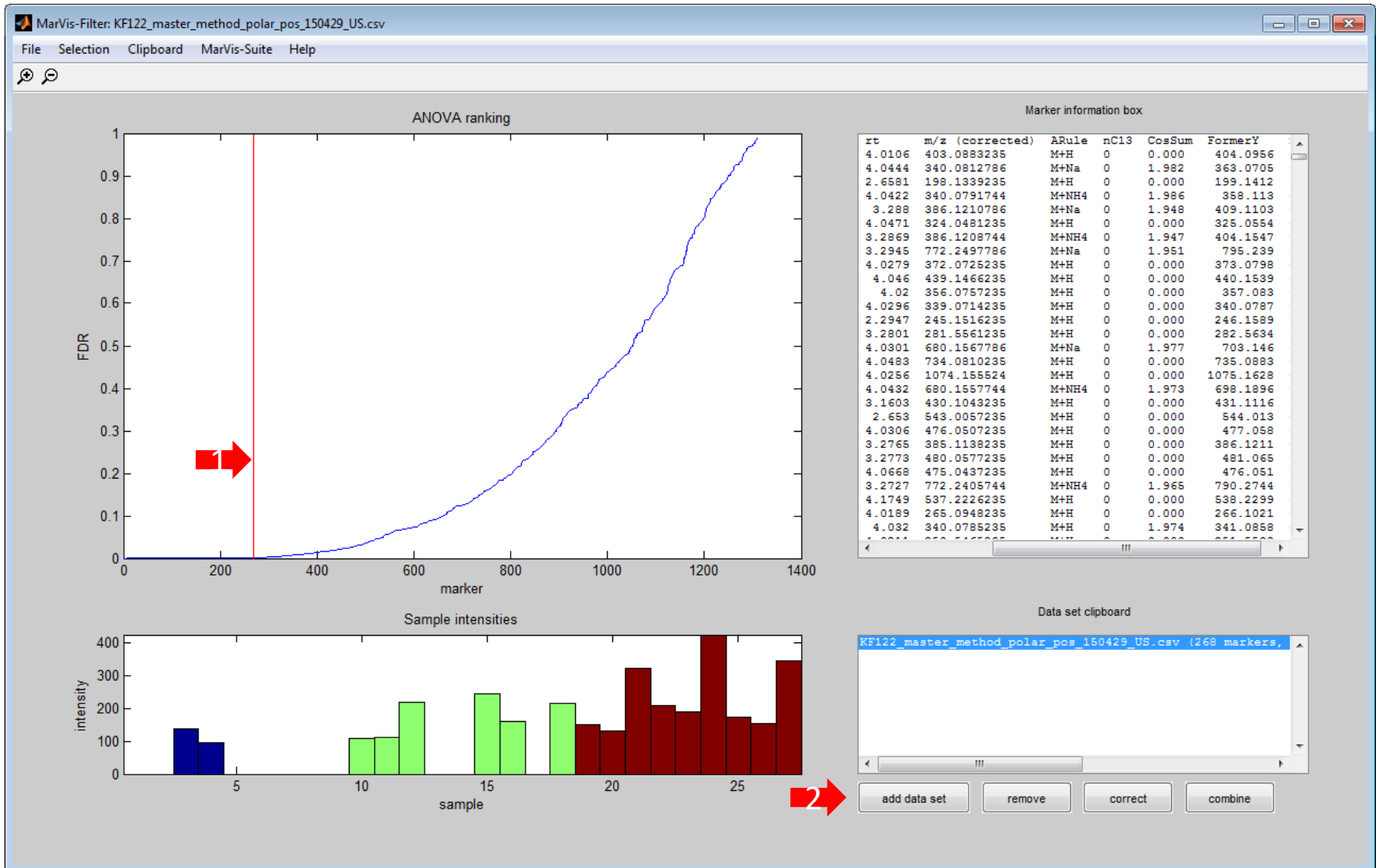
The 'Select input file for adduct rules' dialog box shows a file list with 'adduct_neg.txt' and 'adduct_pos.txt' selected.

The 'Tolerances' dialog box has input fields for 'rt tolerance' (0.08) and 'm/z tolerance' (0.01).

At the bottom of the main window, there are buttons for 'add data set', 'remove', and 'OK'.

Filter the data set

Transfer the filtered data to the data set clipboard



Open MarVis Filter 2.6

Import data matrix2 (neg. ESI)

W:\Praktikanten_ALL\KF123_master_practical course.PRO\Results_etc\Data_matrixes

The screenshot shows the MarVis-Filter application window. The 'File' menu is open, with 'Import raw data' highlighted. A 'Select File To Open' dialog box is overlaid, showing the file 'KF122_master_method_polar_neg_150429_US.csv' selected. The dialog box also shows the file 'KF122_master_method_polar_pos_150429_US.csv'. The 'File name' field at the bottom of the dialog box contains 'KF122_master_method_polar_neg_150429_US.csv'. The 'Open' button is highlighted. The background shows a plot with a y-axis from 0 to 0.5 and an x-axis from 0 to 0.4.

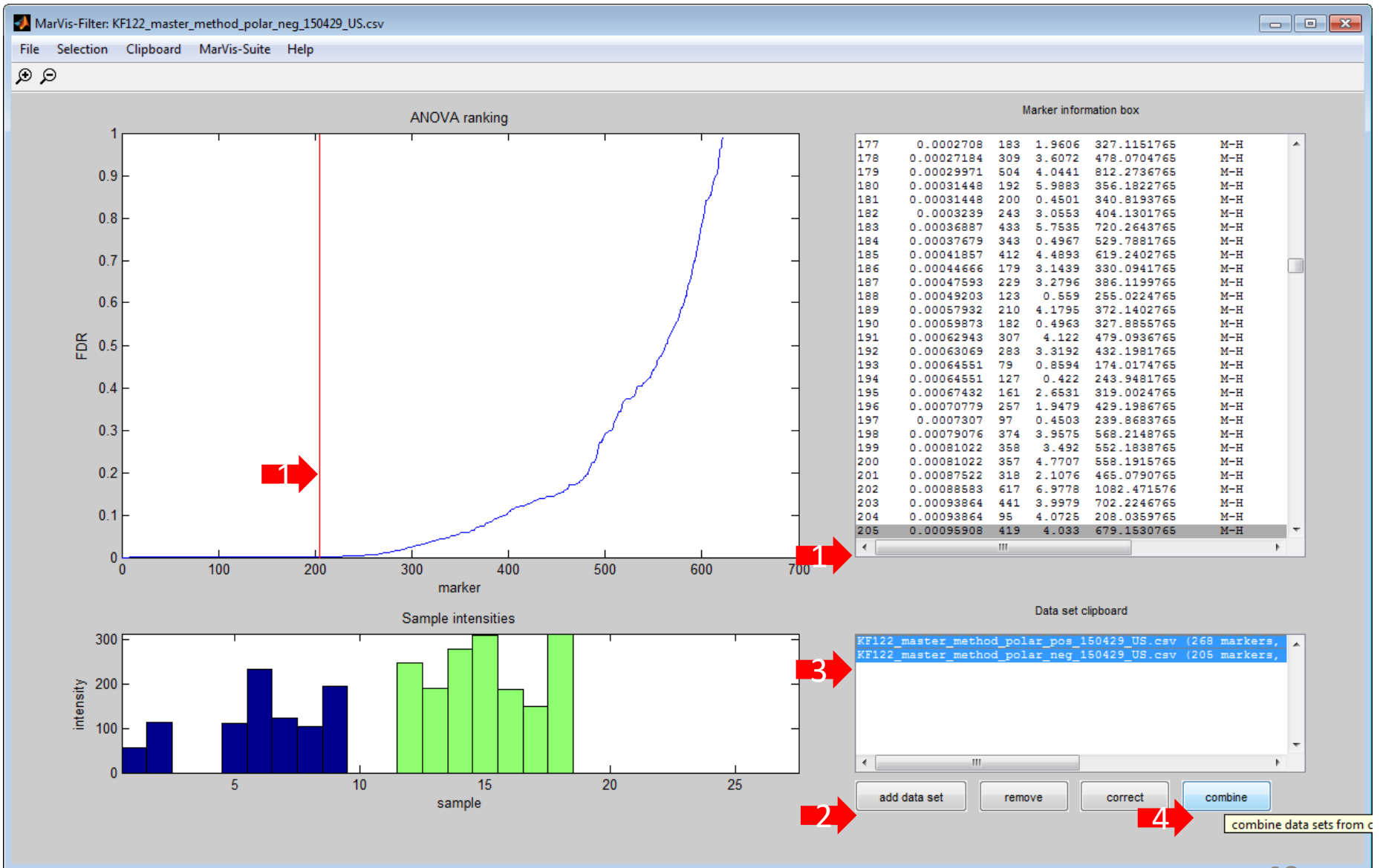
3

4

5

Repeat the steps from slide 2-4 for the second data matrix)

Combine the filtered and adduct corrected data sets



Rearrange the combine data by mass

The image shows a sequence of four software dialog boxes with numbered red arrows indicating a workflow:

- Condition handling**: A dialog box with a question mark icon and the text "Interlace conditions and replicate samples over all data sets?". A red arrow labeled "1" points to the "Yes" button.
- Filter dialog**: A large dialog box with a "Title" field containing "Combined data set" and a "Use conditions" field. Under the "Options" section, the "Ranking method" list has "Value ranking" selected. A red arrow labeled "2" points to this selection.
- Label selec...**: A dialog box with a list of labels. "m/z (corrected)" is selected. A red arrow labeled "3" points to this selection. Below the list, a red arrow labeled "4" points to the "OK" button.
- Order**: A dialog box with a question mark icon and the text "Sort values in ascending order?". A red arrow labeled "5" points to the "Yes" button.

Start MarVis Compound for db search

The screenshot displays the MarVis-Filter software interface. The main window is titled "MarVis-Filter: Combined data set". The menu bar includes "File", "Selection", "Clipboard", "MarVis-Suite", and "Help". The "MarVis-Suite" menu is open, showing options: "Goto MarVis-Cluster", "Goto MarVis-Compound", "Goto MarVis-Pathway", "Hide cursors", "Show cursors", "Export graphics", "Errorplot", "Boxplot", "Plot x/y values", "Mass2Formula", "Open shell", and "View log". A red arrow labeled "2" points to the "MarVis-Suite" menu, and a red arrow labeled "3" points to the "Goto MarVis-Compound" option.

The main plot area shows a line graph of "value" (y-axis, 0 to 1200) versus "marker" (x-axis, 0 to 500). A blue line represents the data, and a vertical red line is positioned at marker 450. A red arrow labeled "1" points to this vertical line. Below the main plot is a histogram titled "Sample intensities" showing "intensity" (y-axis, 0 to 400) versus "sample" (x-axis, 0 to 25). The histogram bars are colored blue and green.

On the right side, there is a "Marker information box" displaying a table of marker data. A red arrow labeled "4" points to the "Import dialog" window, which is open in the bottom right corner. The "Import dialog" has fields for "m/z (corrected) correction:" (set to 0) and "m/z (corrected) tolerance:" (set to 0.005). It also has "add", "Cancel", and "OK" buttons.

Marker	Value	Sample	Intensity	
902.20578	572	3.2899	902.2057765	KF1:
911.35148	570	6.7958	911.3514765	KF1:
918.24002	1293	4.066	918.2400235	KF1:
918.24208	565	4.0509	918.2420765	KF1:
920.47452	1292	6.9784	920.4745235	KF1:
933.21428	589	2.6636	933.2142765	KF1:
934.08028	587	2.6573	934.0802765	KF1:
947.22718	584	3.1426	947.2271765	KF1:
974.22885	596	4.03	974.2288521	KF1:
974.2307	603	4.018	974.2306971	KF1:
990.25998	576	4.0563	990.2599765	KF1:
990.50058	607	6.486	990.5005765	KF1:
1004.2029	1282	4.0289	1004.202924	KF1:
1020.2354	1307	4.03	1020.235374	KF1:
1020.236	1309	4.019	1020.236024	KF1:
1042.2067	1306	4.0663	1042.206724	KF1:
1058.1839	1304	4.0206	1058.183924	KF1:
1058.1913	594	4.0281	1058.191276	KF1:
1058.3487	593	4.0887	1058.348676	KF1:
1066.277	622	3.4827	1066.276976	KF1:
1074.1522	621	4.0288	1074.152176	KF1:
1074.1555	1303	4.0256	1074.155524	KF1:
1080.2892	618	4.0272	1080.289176	KF1:
1082.4716	617	6.9778	1082.471576	KF1:
1084.3	616	4.0769	1084.299976	KF1:
1156.3191	611	4.0892	1156.319076	KF1:
1156.3304	1299	4.0797	1156.330424	KF1:
1158.3596	610	3.286	1158.359576	KF1:

Inspect the putativ identities of compounds

MarVis-Compound: Combined data set

File MarVis-Suite Help

Results

acycCount	keggCount	internalName
8		Alanin (RT 0.45) (89.0477; 0.0012445; 0)
2		
2		
2		
2		
10		
4		
4		
4		Indole-3-acetaldehyde (159.0684; -0.00019046; 0) / 1H-4-oxoqui
4		Indole-3-acetaldehyde (159.0684; -0.00019046; 0) / 1H-4-oxoqui
4		Indole-3-acetaldehyde (159.0684; -0.00019046; 0) / 1H-4-oxoqui
1		
19		
0		
0		
6		Phenylalanin (RT 1.87) (165.079; -0.00045546; 0)
6		Phenylalanin (RT 1.87) (165.079; -0.00020254; 0)
6		Phenylalanin (RT 1.87) (165.079; 0.0004181; 0)
1		
4		
5		N-Methyltryptamine; N-Methylindoleethylamine (174.1157; -0.004
11		
11		
6		1,3,8-Trihydroxynaphthalene (176.0473; -0.00032146; 0)
5		
3		
5		Tyrosin (RT 0.96) (181.0739; -0.00047046; 0)
8		
2		
1		
3		5-Hydroxyindoleacetate (191.0582; -0.0045205; 0)
3		
11		1,3,6,8-Tetrahydroxynaphthalene (192.0423; -3.6457e-05; 0)
10		Ferulate (194.0579; -0.00018646; 0) / 6-Hydroxymellein (194.05
10		Ferulate (194.0579; -0.00018646; 0) / 6-Hydroxymellein (194.05
3		
1		
0		
3		

Names

internal: Ferulate (194.0579; -0.00018646; 0) / 6
aracyc: 5-hydroxy-coniferaldehyde (194.0579; -0.0
knaps: 4-Hydroxymellein (194.0579; -0.00018646; 0
lipidm: 2E,4E,6Z,8Z-Decatetraenedioic acid (194.0
metacyc: 5-hydroxy-coniferaldehyde (194.0579; -0.
kegg: Scytalone;3,4-Dihydroxy-3,6,8-trihydroxy-1(2

1

2

Goto

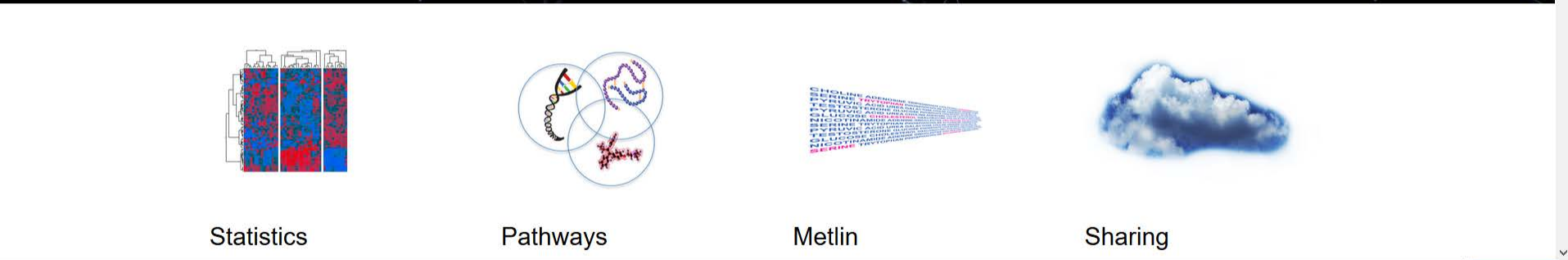
KEGG

Column plot

Additional information

total number: 473
found in databases: 281 (59%)

internal: 8% total, 24% relative
aracyc: 20% total, 24% relative
knaps: 46% total, 38% relative
lipidm: 20% total, 35% relative
metacyc: 35% total, 32% relative
kegg: 45% total, 38% relative





Apps



Outlook Web App



mysms



Biochemie



Petr Karlovsky



Funding



Weitere Lesezeichen

LIGAND Relational Database

The primary database of KEGG LIGAND is a relational database with the [KegDraw](#) interface, which is used to generate the secondary (flat file) database for DBGET. A read-only copy of the LIGAND relational database is made publicly accessible.

Search COMPOUND

Exact Mass ▼

example) 100 - 200

Go

Clear

Rechteckiges Ausschneiden

Search GLYCAN

Glycan ID ▼

example) G10596

Go

Clear

Search REACTION

Reaction ID ▼

example) R00259

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Chemical Structure Search

Search similar compound structures

SIMCOMP: maximal common subgraph search -- a portion of the query compound is optimally matched to a portion of the database compound [[references](#)]

SUBCOMP: isomorphic subgraph search -- the query compound is fully matched to a portion of the database compound (substructure match) or a portion of the query compound is fully matched to the database compound (superstructure match)

Search similar glycan structures

KCaM: local or global search for matching tree structures [[reference](#)]

Download chemical structure drawing tool

Tentative structure elucidation

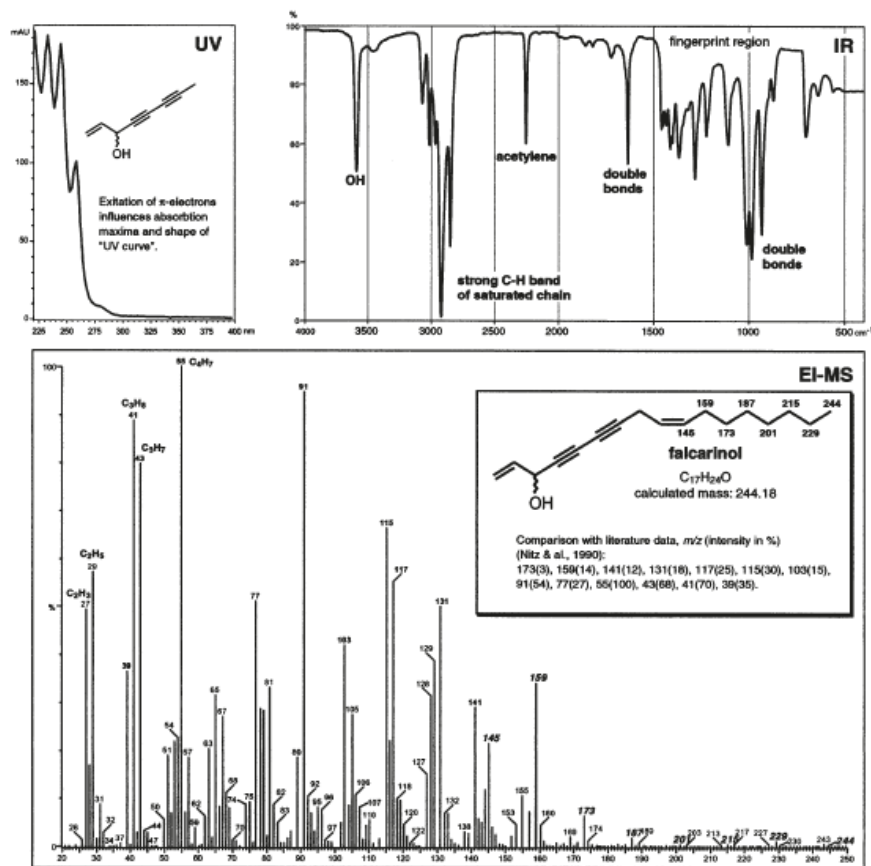


FIGURE 2. UV, IR, and EI-MS spectrum of the polyacetylene falcariol, a characteristic secondary metabolite found in *Apiaceae* and *Araliaceae*. The UV spectrum was obtained on-line from a HPLC run by a diode-array system (Hewlett Packard 1090), the mobile phase was a gradient of MeOH and aqueous buffer; 2 mg of a pure sample dissolved in CCl₄ was used for IR (Perkin Elmer 1600 PC FTIR); the MS was obtained from a GC-MS run at standard 70 eV, carrier gas helium (Perkin Elmer Autosystem with Turbomass).

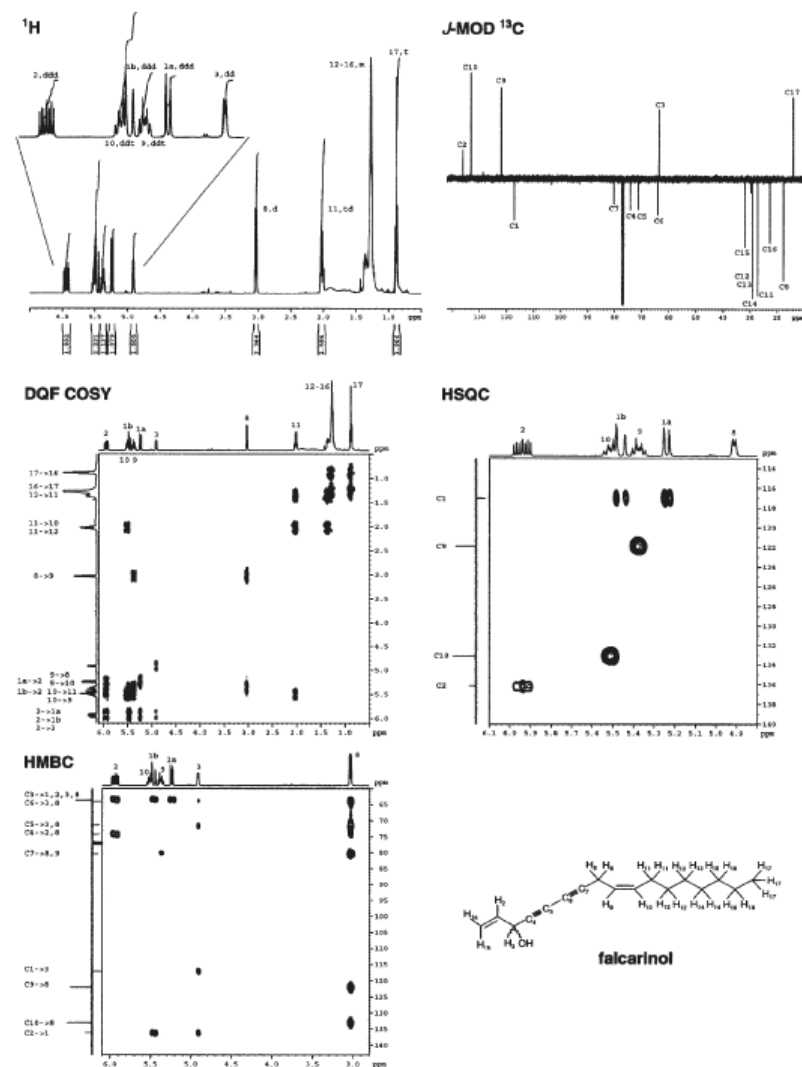


FIGURE 3. One- and two-dimensional NMR spectra of the polyacetylene falcarinol: one-dimensional technologies: ^1H -NMR (proton NMR), J -mod ^{13}C (carbon NMR); two-dimensional technologies: DQF-COSY (double quantum filtered correlation spectrum), HMQC (heteronuclear single quantum coherence), HMBC (heteronuclear multiple bond correlation). Measurements were carried out with 10 mg falcarinol dissolved in CDCl_3 at 300K on a Bruker DRX400.

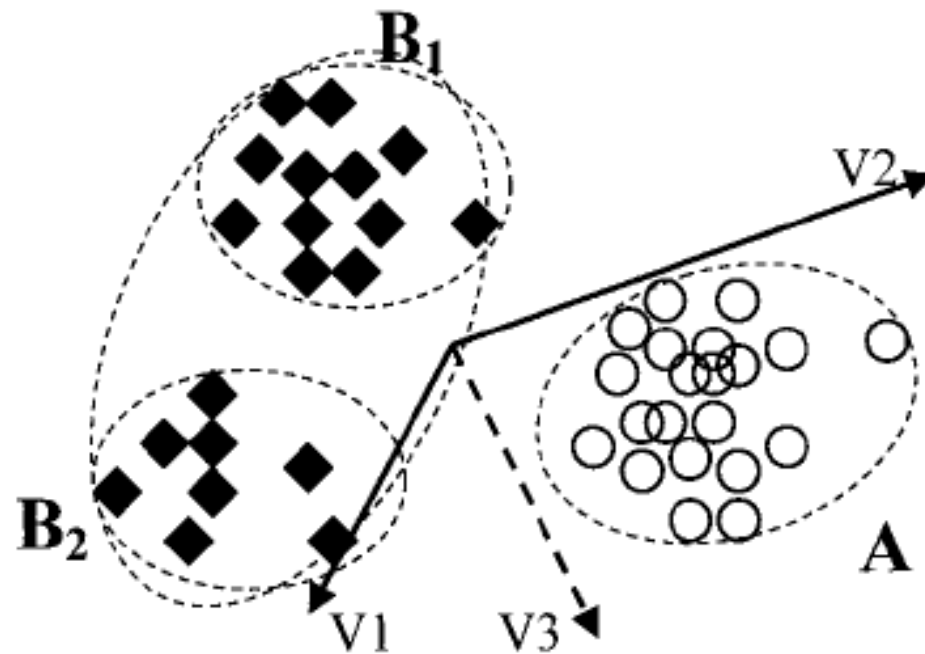
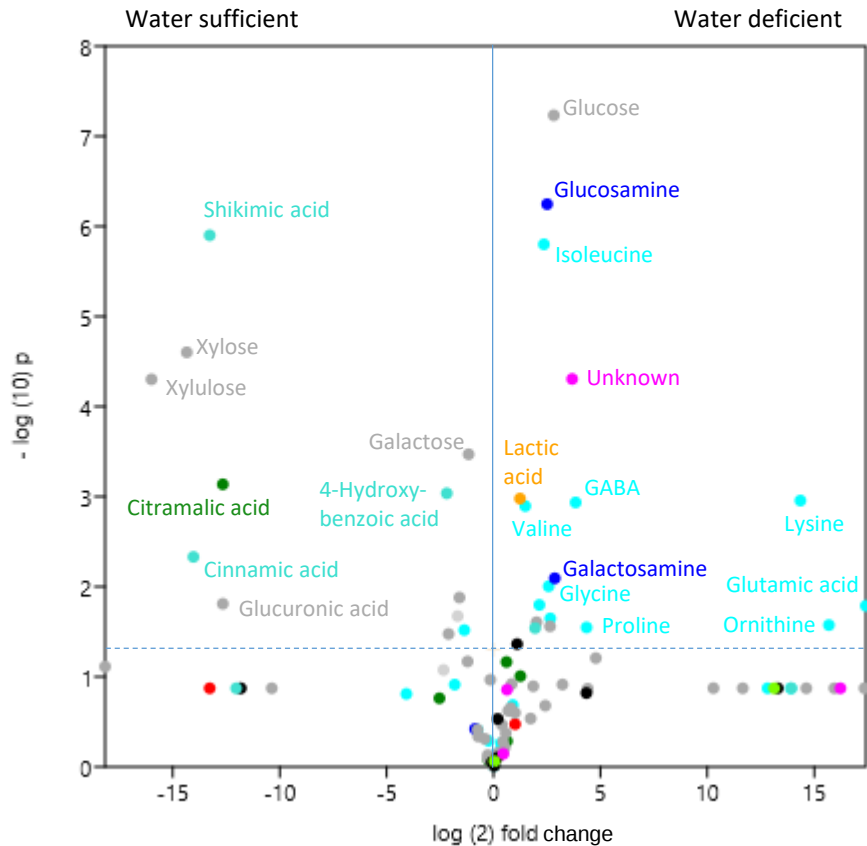


Figure 2. Cluster analysis of a hypothetical experiment. Clustering of the samples by principal-component analysis might result in the expected separation of samples from origin A (such as wild-type samples) and from origin B (such as mutant samples). In this example, B samples fall into two sub-groups, B₁ and B₂, as indicated by covers (dotted lines).

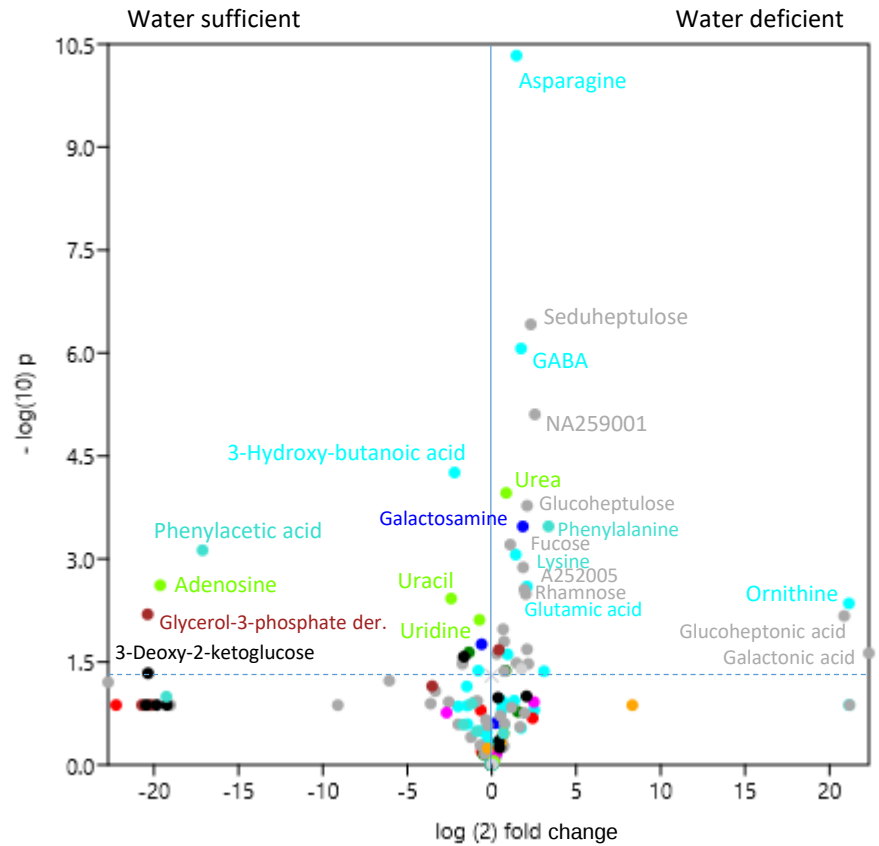


Volcano plot

Root exudate



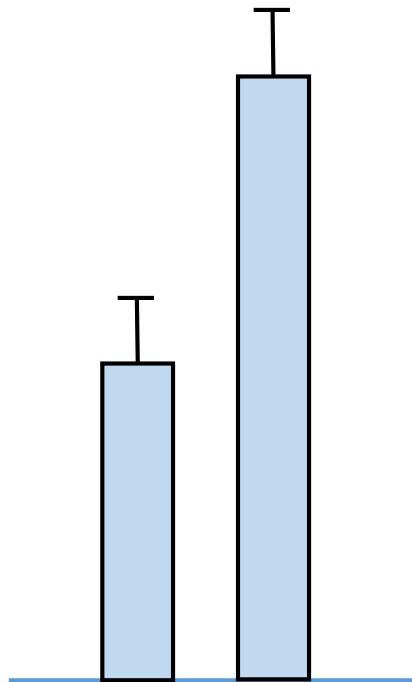
Root



Arabidopsis

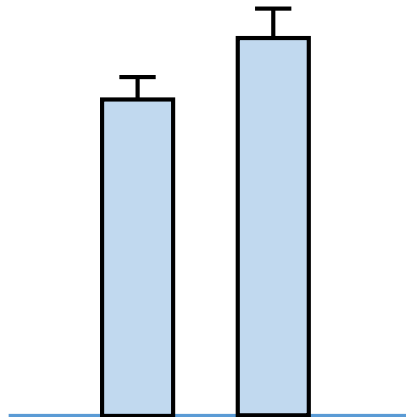
Relevance and significance

1)



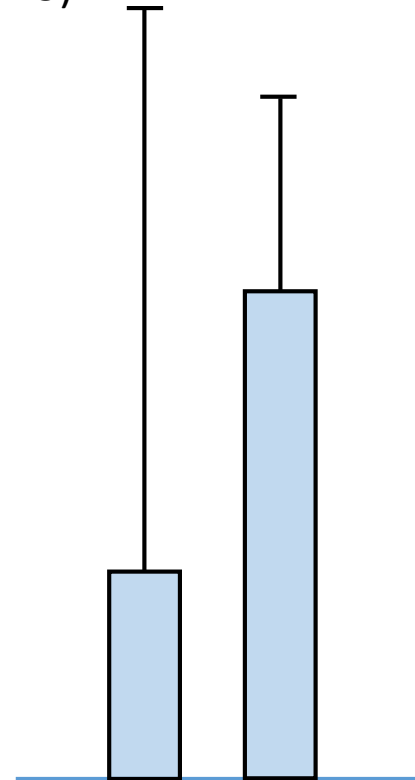
$p < 0.05$

2)



$p < 0.05$

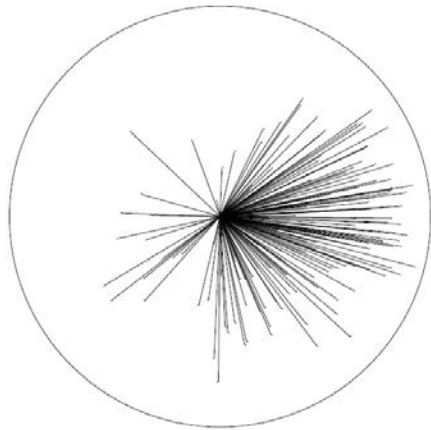
3)



$p > 0.05$

log (2) fold change, Gower quantitative similarity, multidimensional scaling

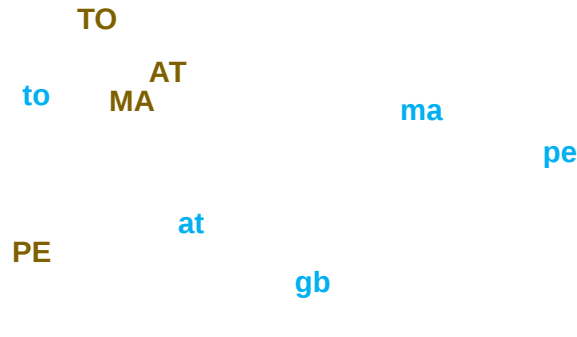
2D Stress: 0.09



All 175 metabolites

RS

rs



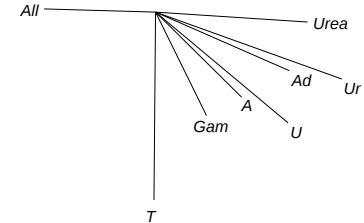
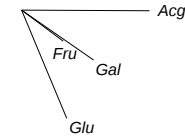
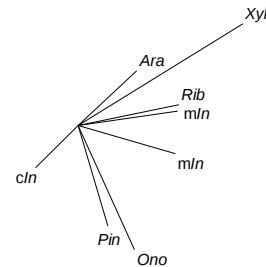
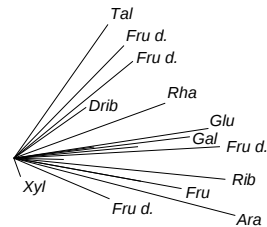
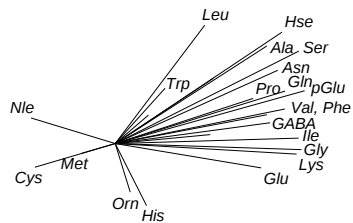
Amino acids

Monosaccharides

Sugar alcohols

Aminosugars

Nucleotide biosynthesis



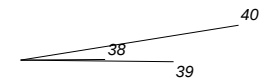
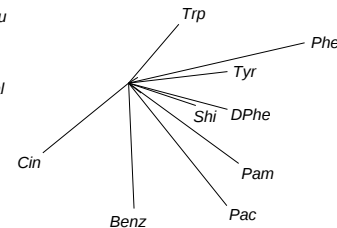
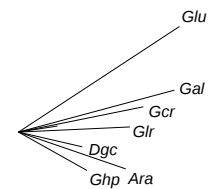
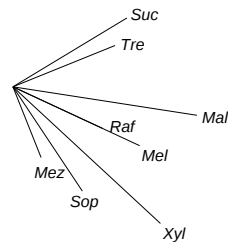
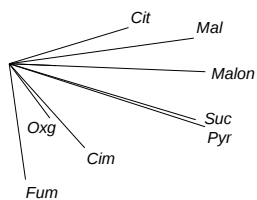
Organic acids

Di- and trisaccharides

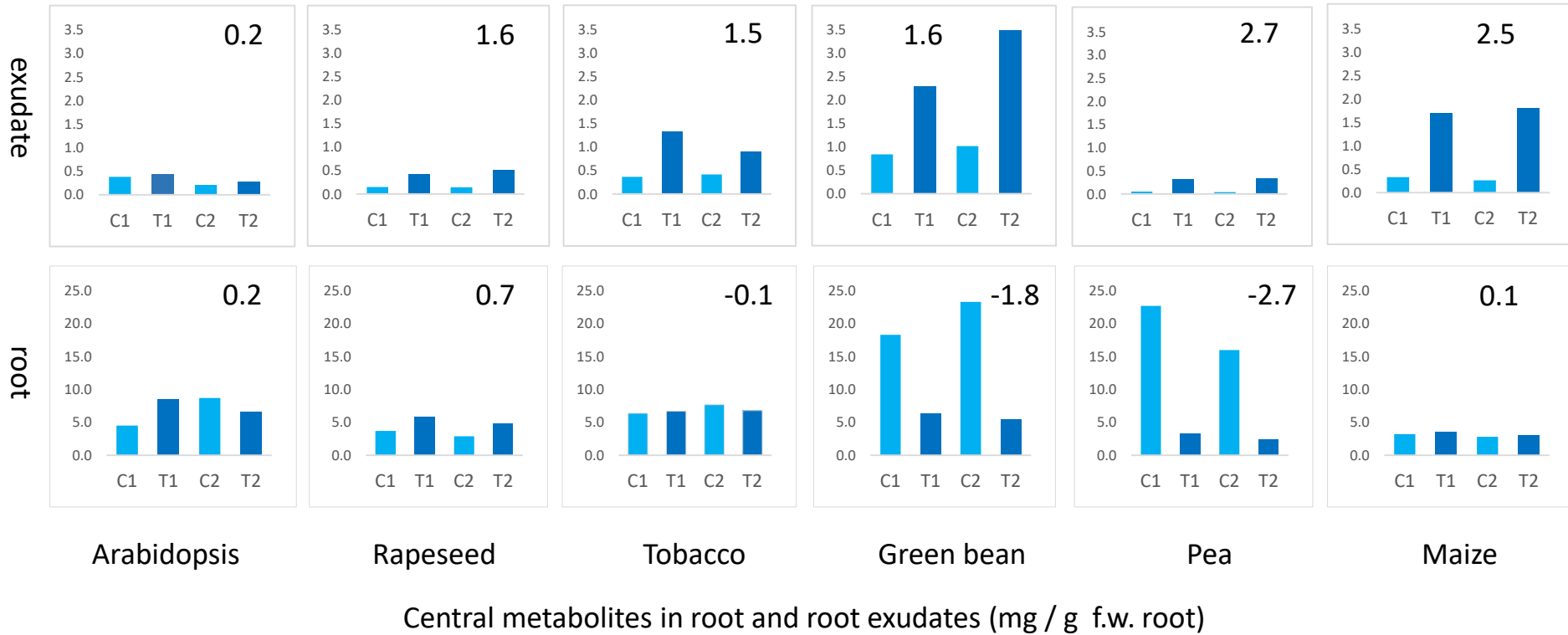
Sugar acids

Shikimic acid pathway

Ascorbate metabolism



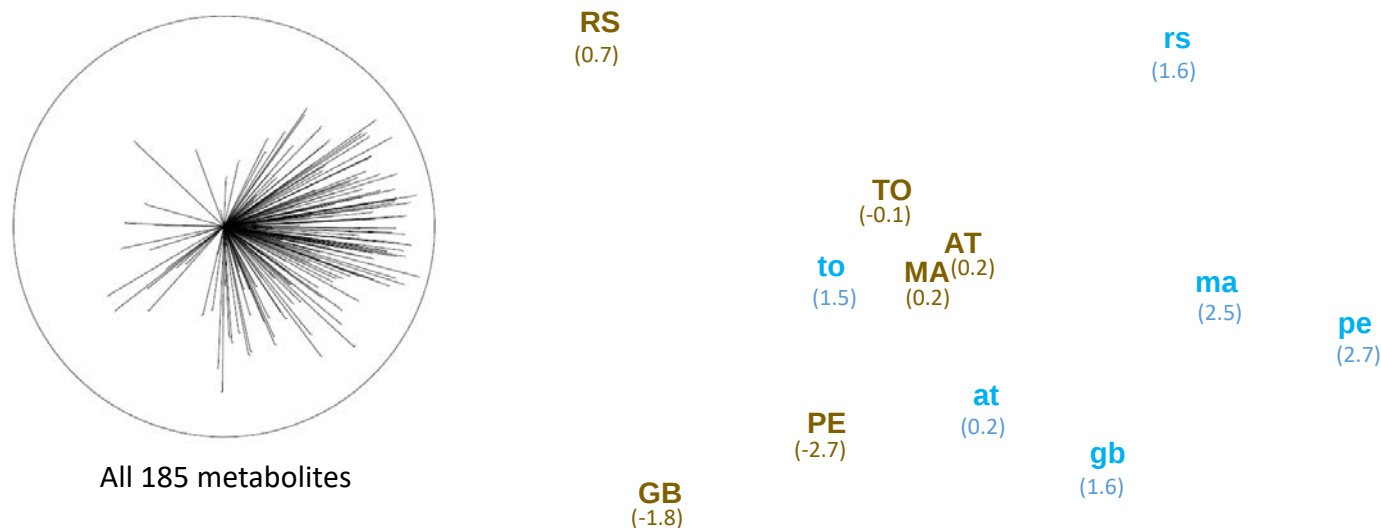
Fold change



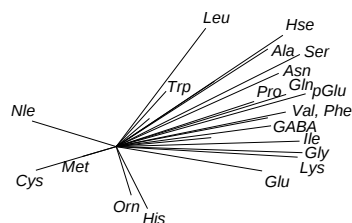
log (2) fold change, Gower quantitative similarity; multidimensional scaling;

at, Arabidopsis; gb, Green Bean; ma, Maize; pe, Pea; rs, Rapeseed; to, Tobacco; small letter: root exudates; capital letters, roots;
fold change calculated on determined amounts (mg / g FW).

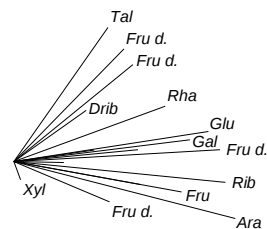
2D Stress: 0.09



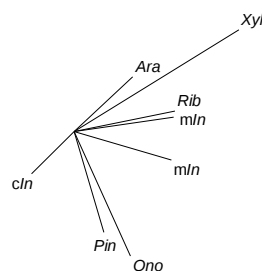
Amino acids



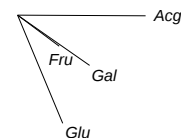
Monosaccharides



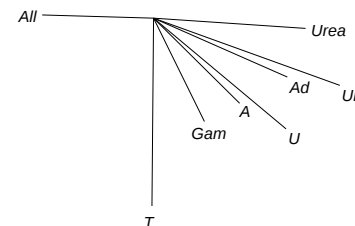
Sugar alcohols



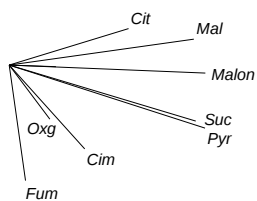
Aminosugars



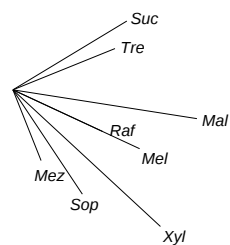
Nucleotide biosynthesis



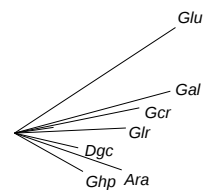
Organic acids



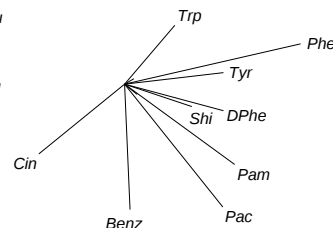
Di- and trisaccharides



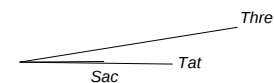
Sugar acids



Shikimic acid pathway



Ascorbate metabolism



Systemic

Chaotic

Non-linear