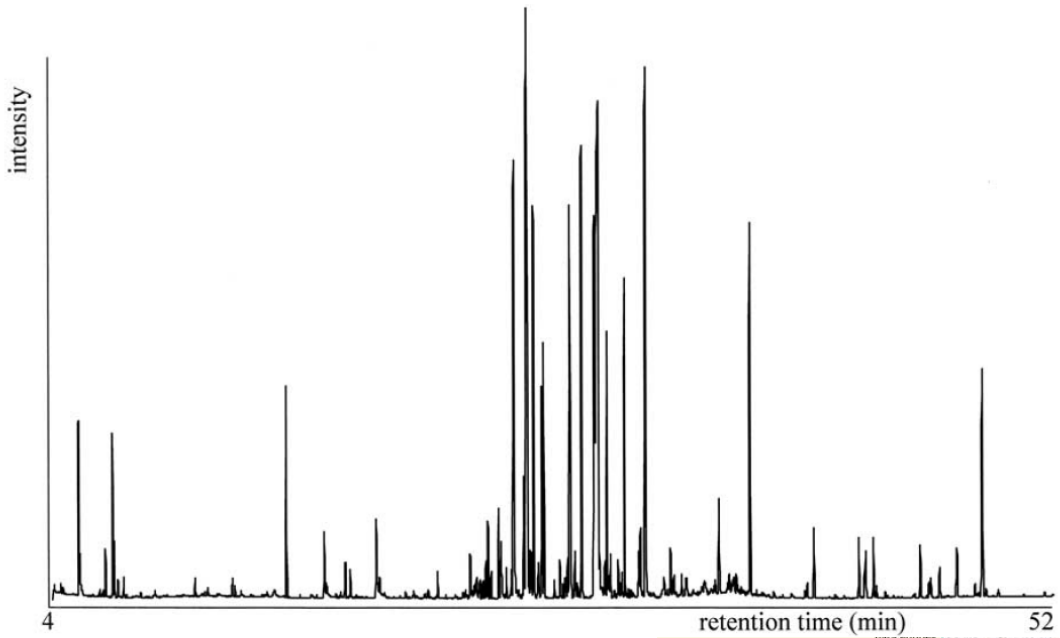
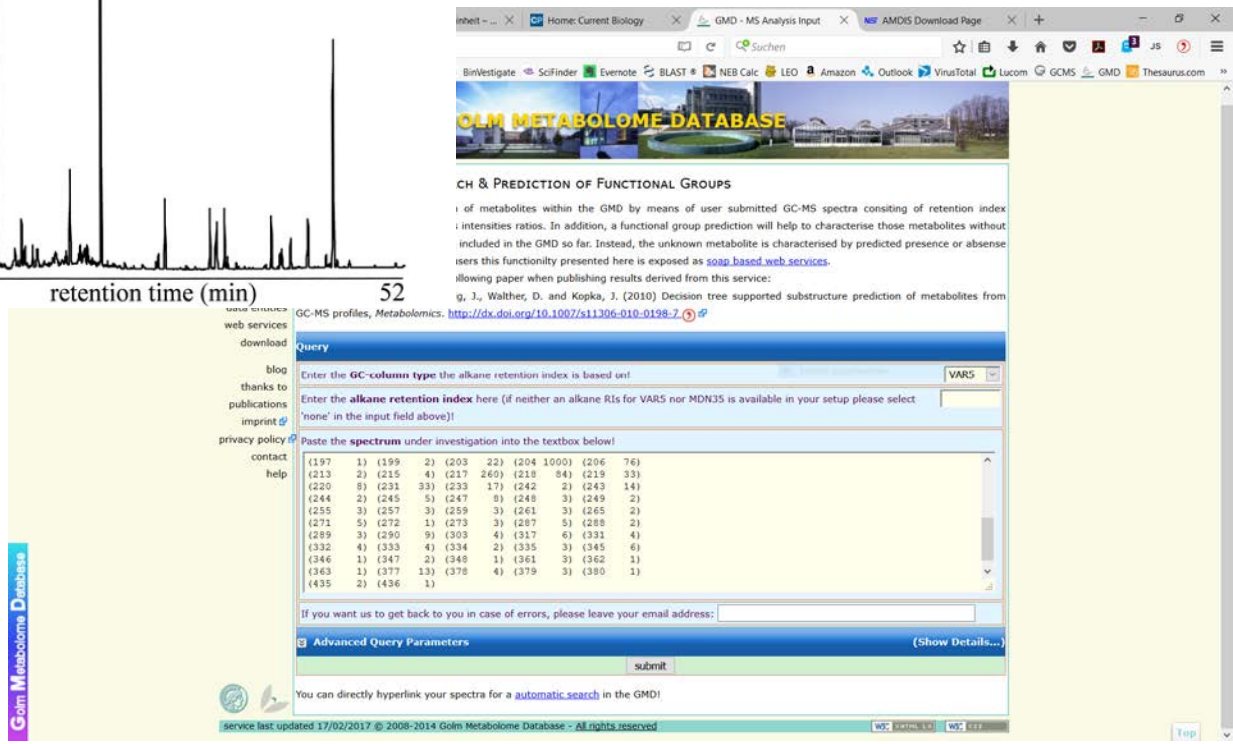
Rhizosphere 2018 – Metabolite profiling



Franz Hadacek



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

Metabolomics – the link between genotypes and phenotypes

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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

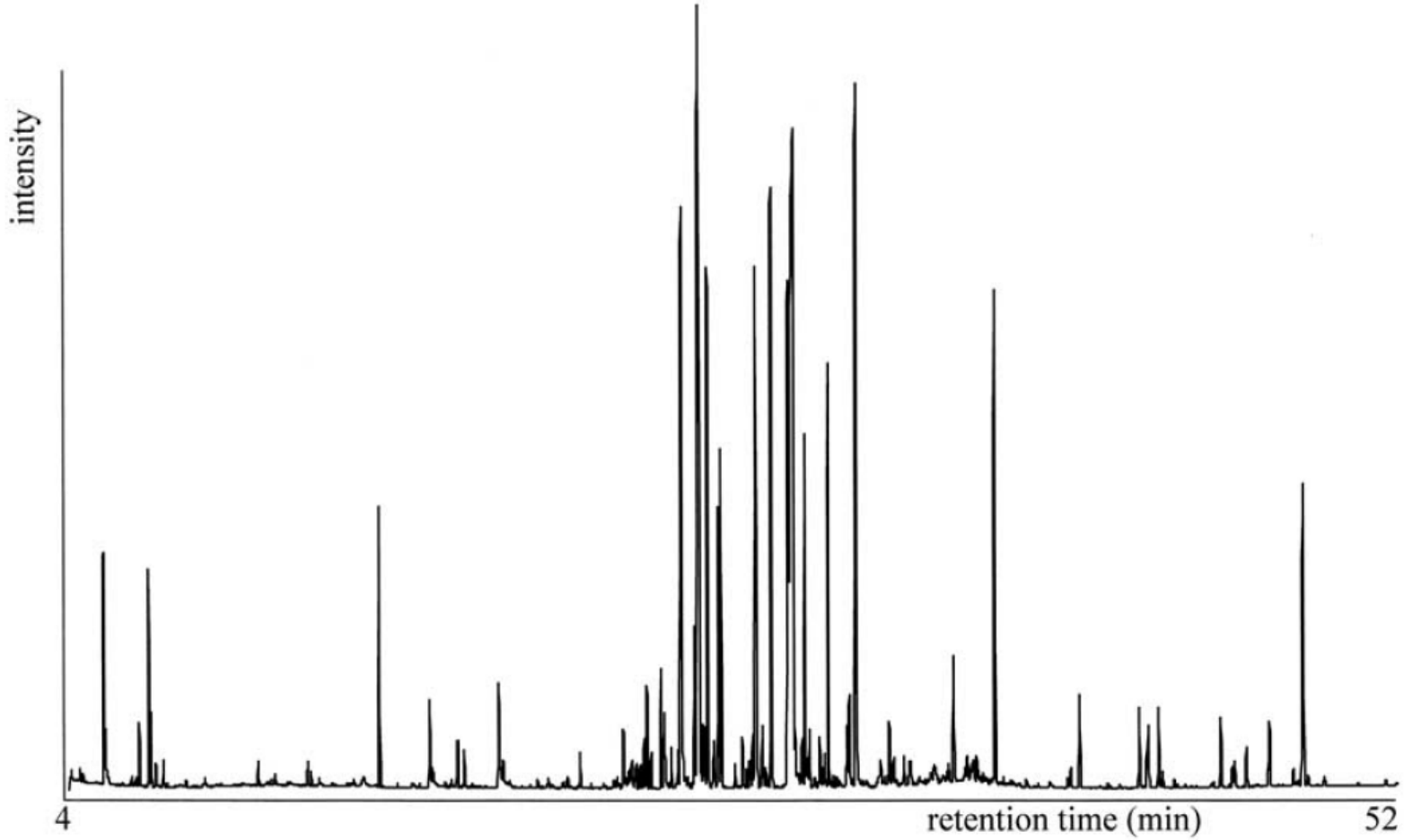

Figure 1. Lipophilic phase of *Arabidopsis thaliana* leaves analysed by GC/quadrupole MS (unpublished results). Inspection of peaks apparent in the base peak chromatogram results in 160 distinct metabolites. Abundant peaks in the middle of the chromatogram are methylated fatty acids. At the end of the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

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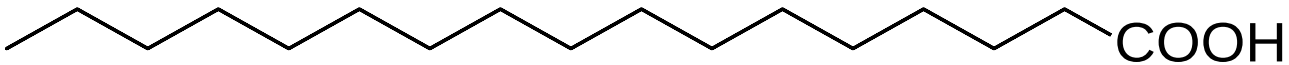
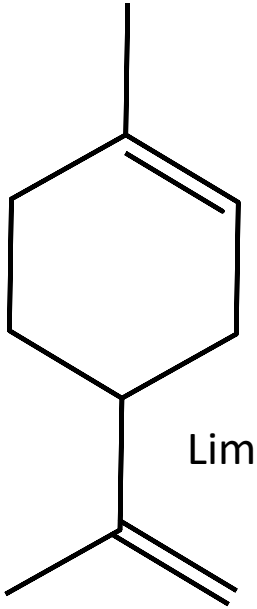
Lipophilic



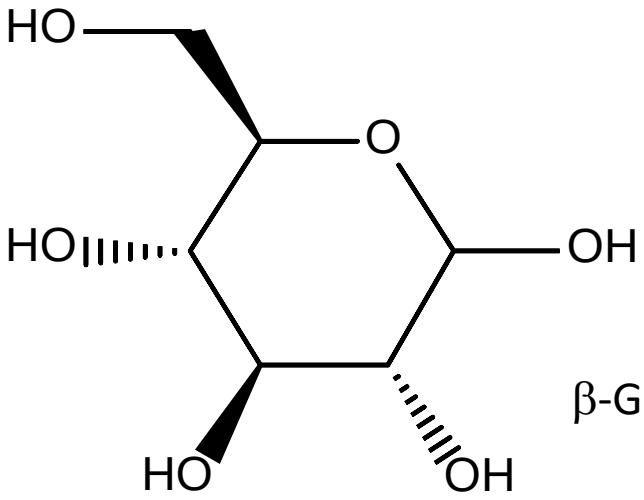
Palmitic acid



Limonene

Hexane, cyclohexane, diethylether, chloroform, ethyl acetate, …

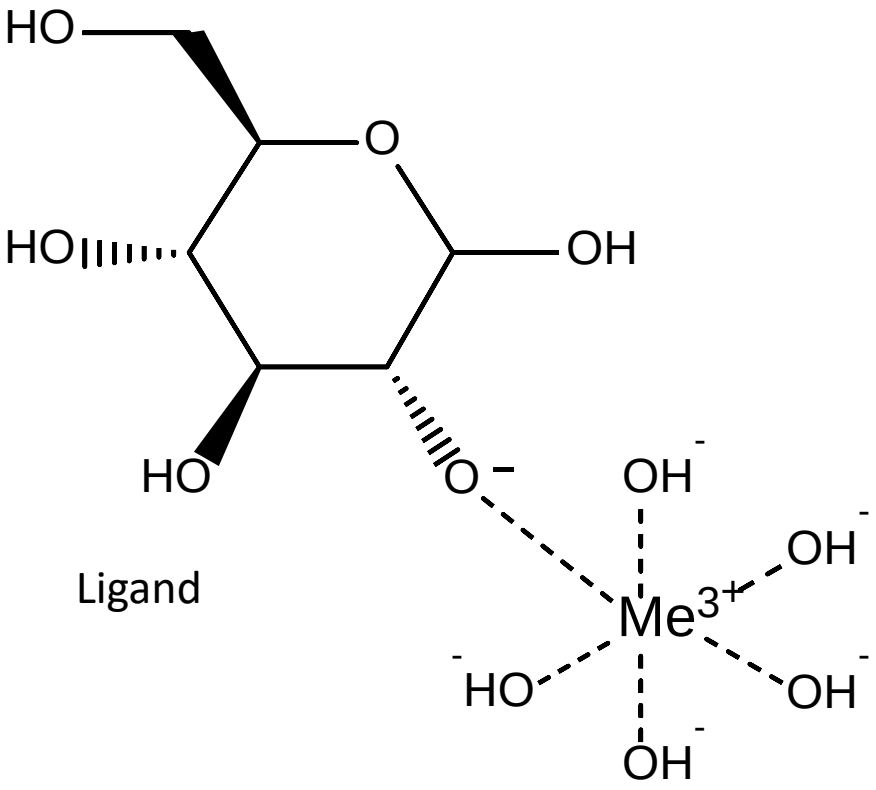
Hydrophilic



β-Glucose

Watert, methanol, ethanol, …

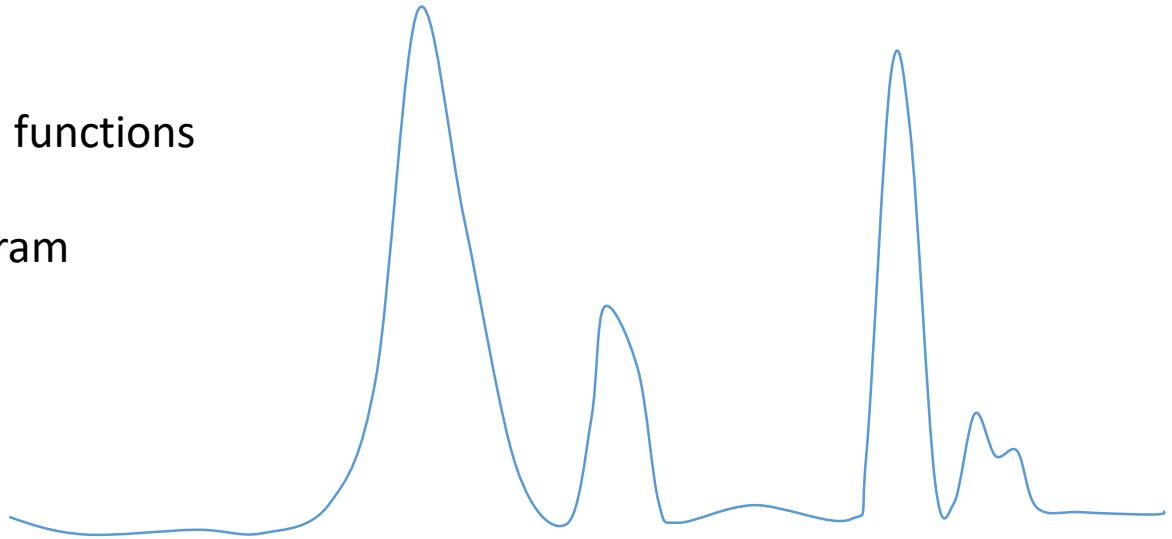
Coordination complex



Me, metal, central atom

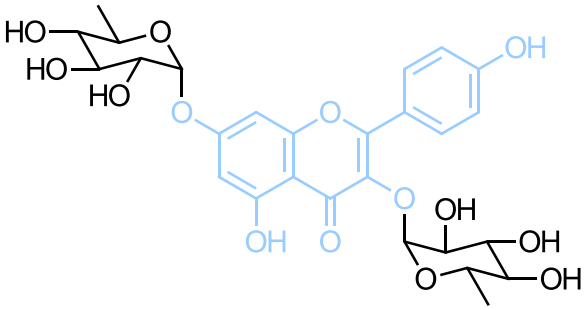
Consequences for chromatography

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

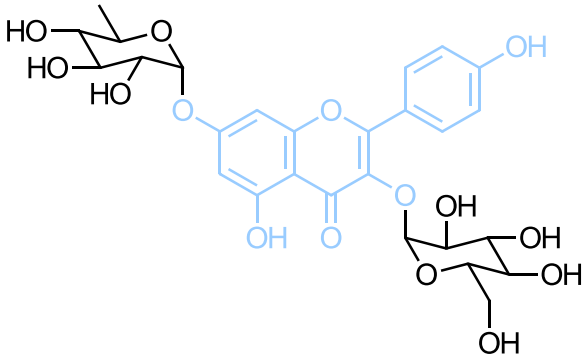


High pH,
Dissociation of O, S and N functions
Plethora of coordination complexes
Polymerization of analytes

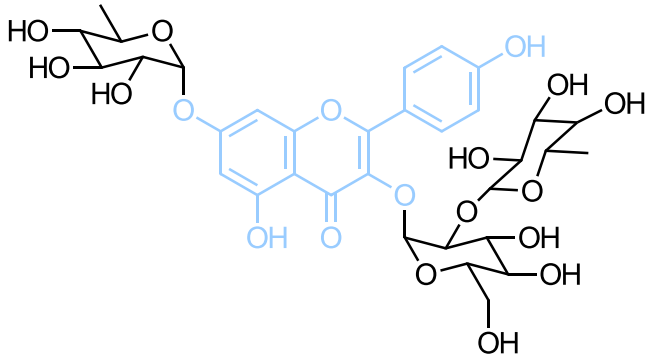
Flavonoids - UV spectra



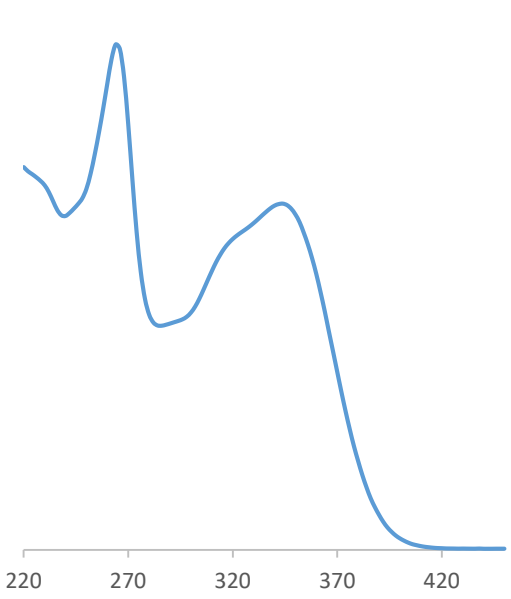
Kaempferol-3,7-dirhamnopyranoside (19.6 min)

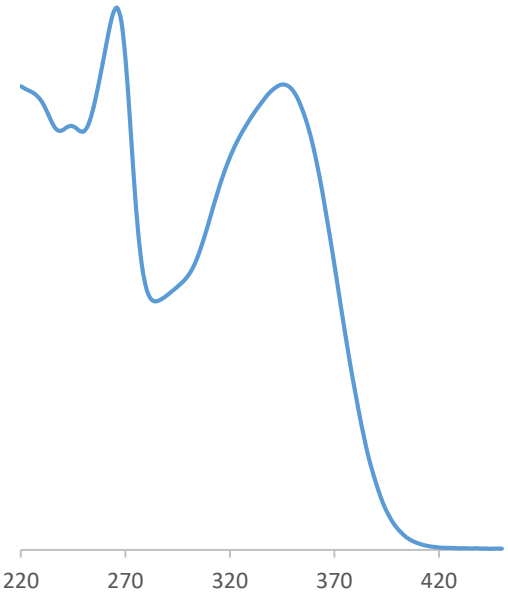


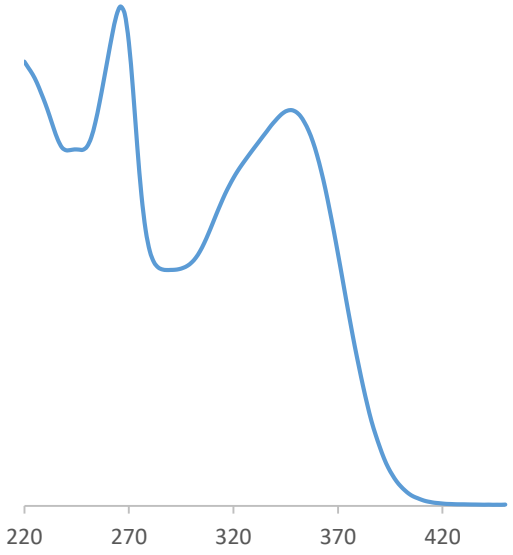
Kaempferol-3-glucopyranosyl-7-rhamnopyranoside (18.3 min)



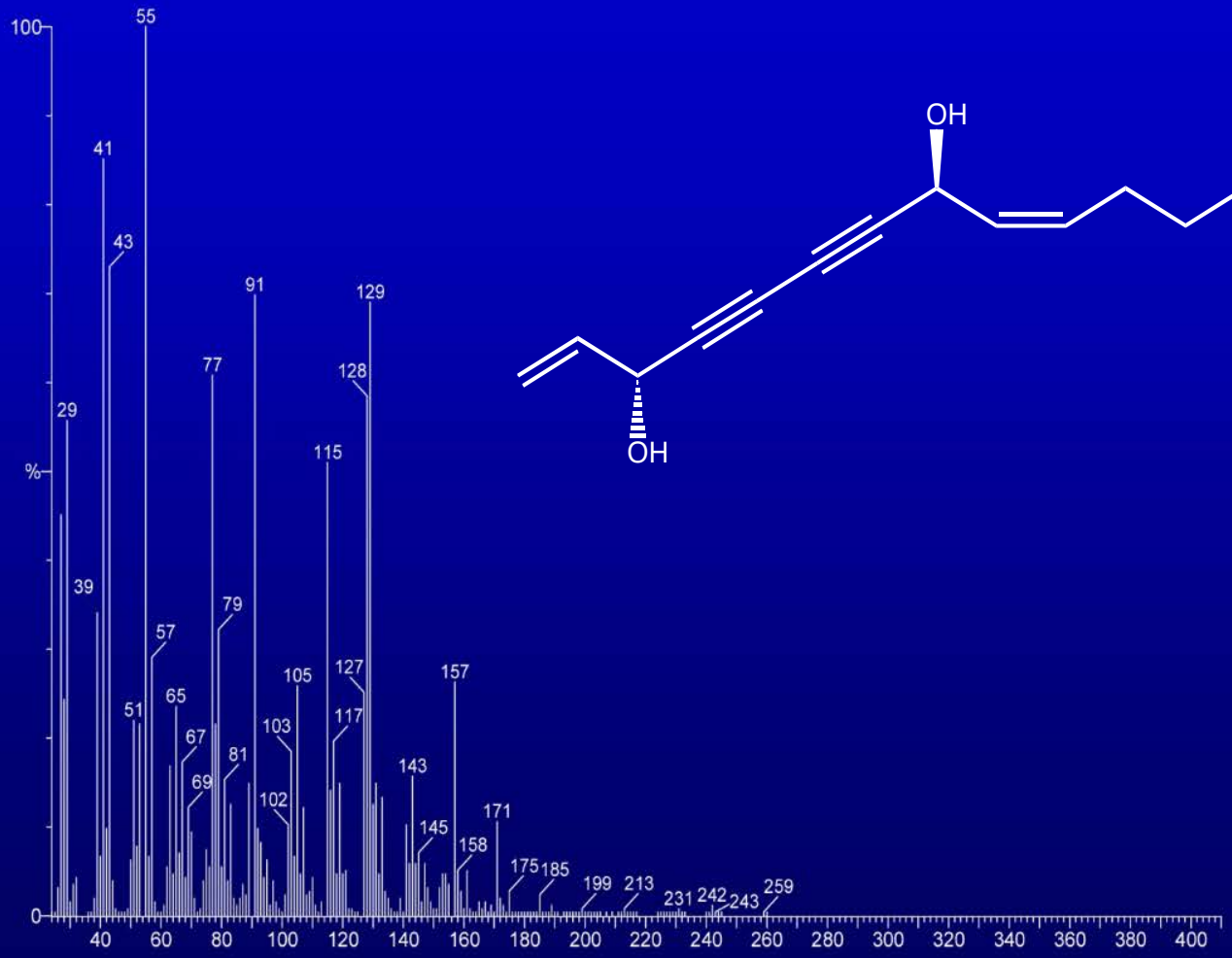
Kaempferol-3-glucopyranosyl-(1→2) rhamno-pyranosyl-7-rhamnopyranoside (16.9 min)



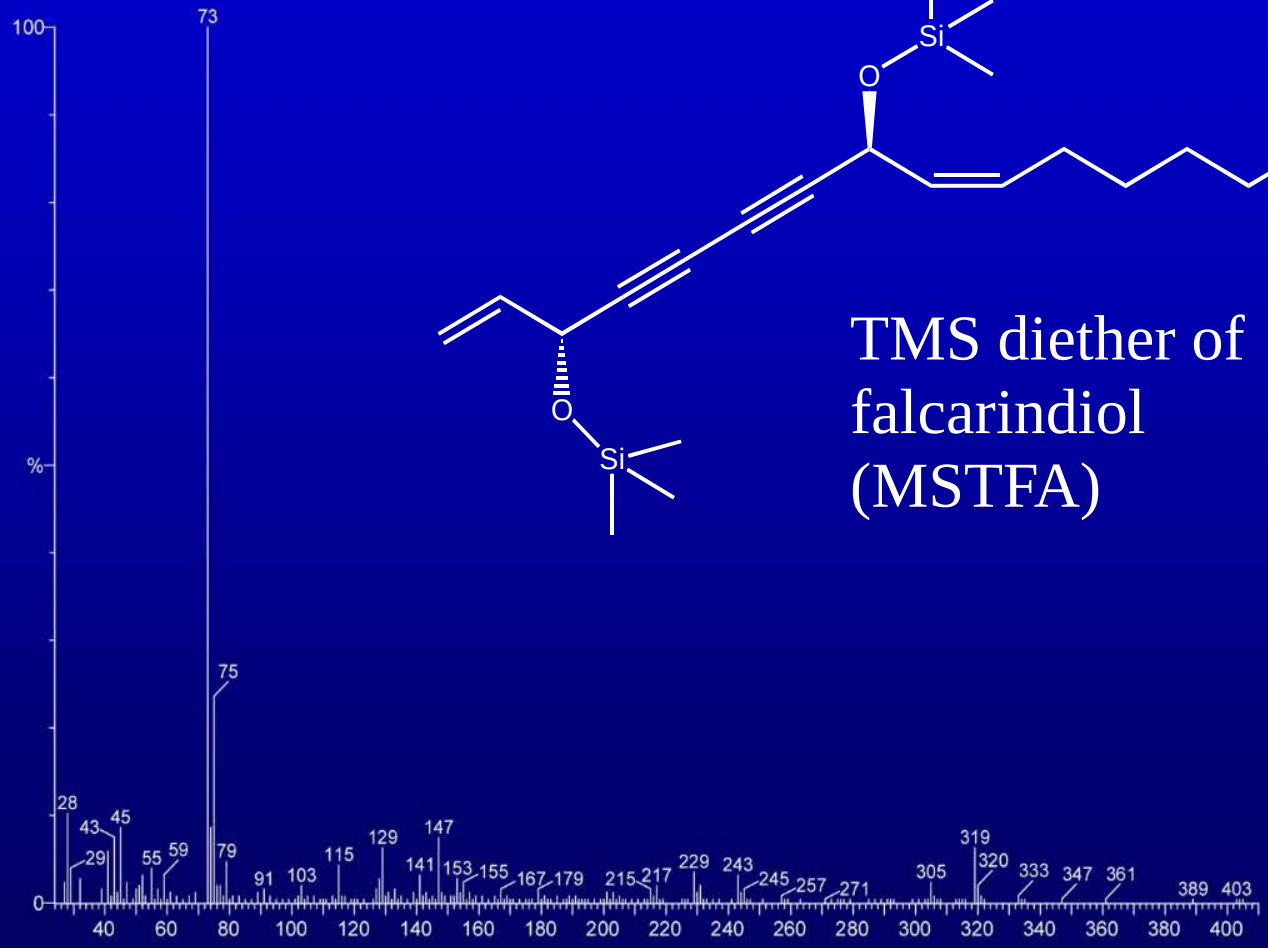




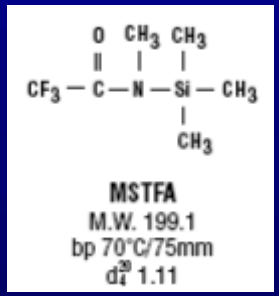
EI spectrum of falcarindiol



EI spectrum of derivatized falcarindiol



TMS diether of falcarindiol (MSTFA)



Chromatogram

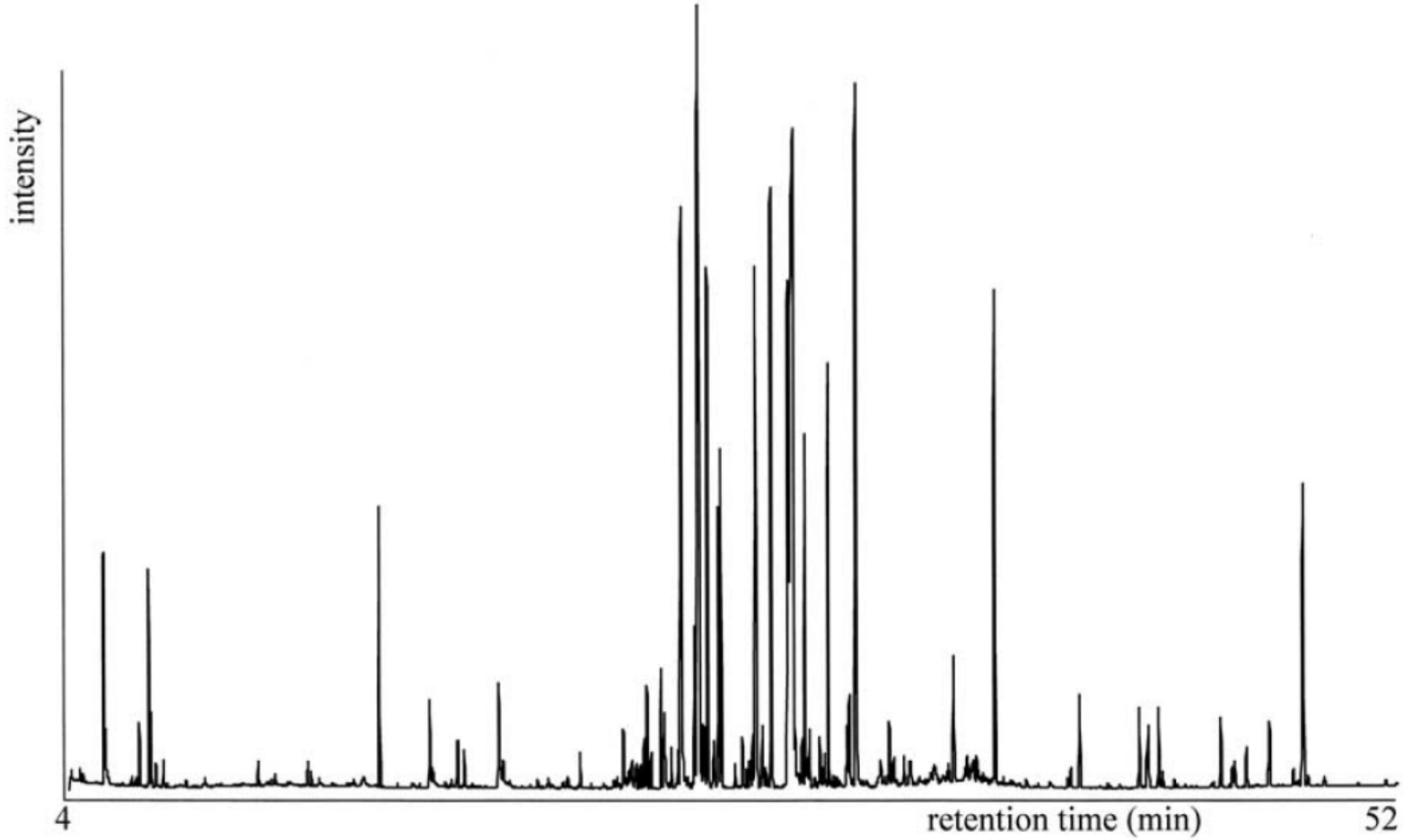


Figure 1. Lipophilic phase of *Arabidopsis thaliana* leaves analysed by GC/quadrupole MS (unpublished results). Inspection of peaks apparent in the base peak chromatogram results in 160 distinct metabolites. Abundant peaks in the middle of the chromatogram are methylated fatty acids. At the end of the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

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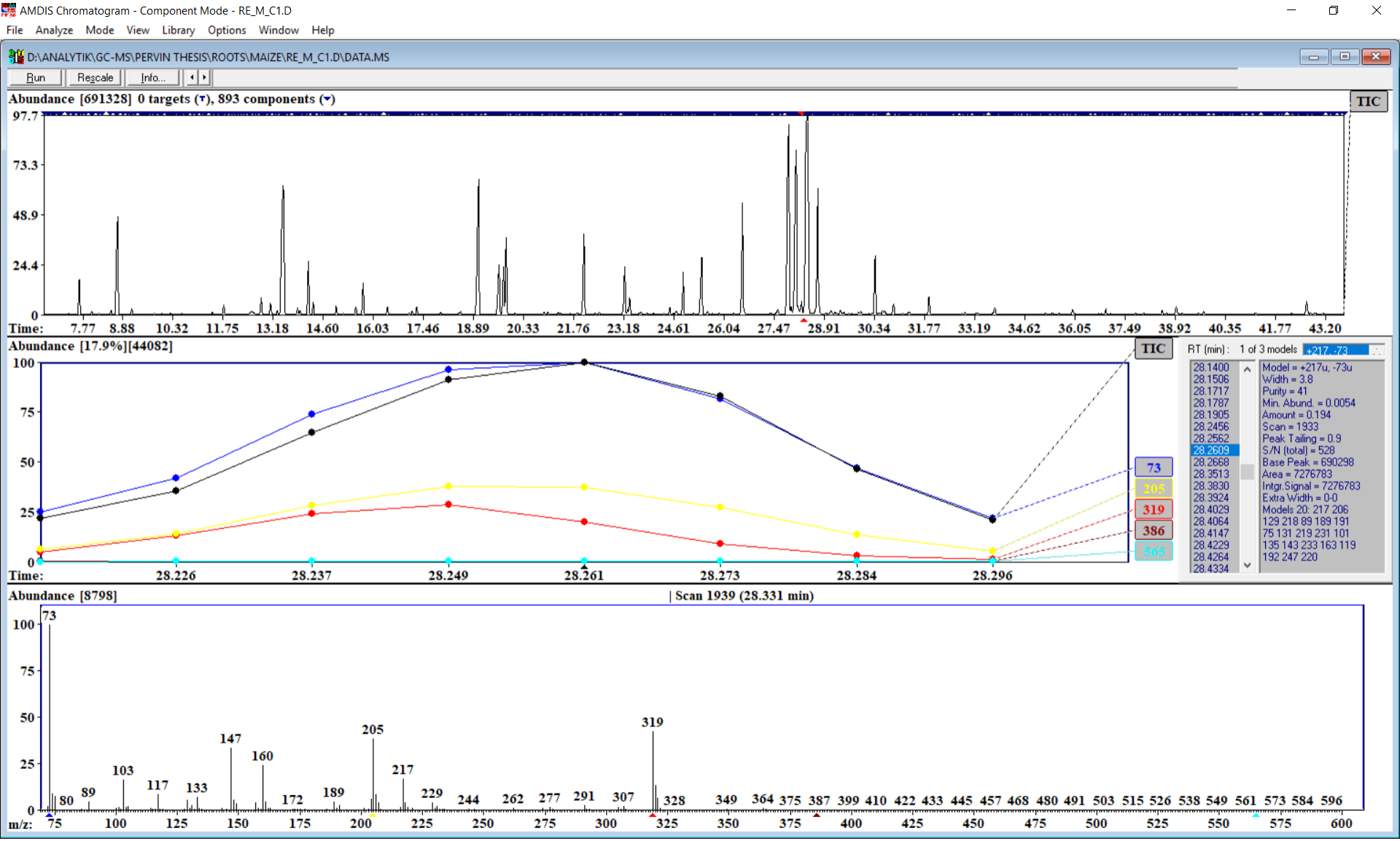
Gas chromatography

Electron impact mass spectrometry

Analysis of central (primary) metabolites

Deconvolution and peak integtration (GC–EIMS)

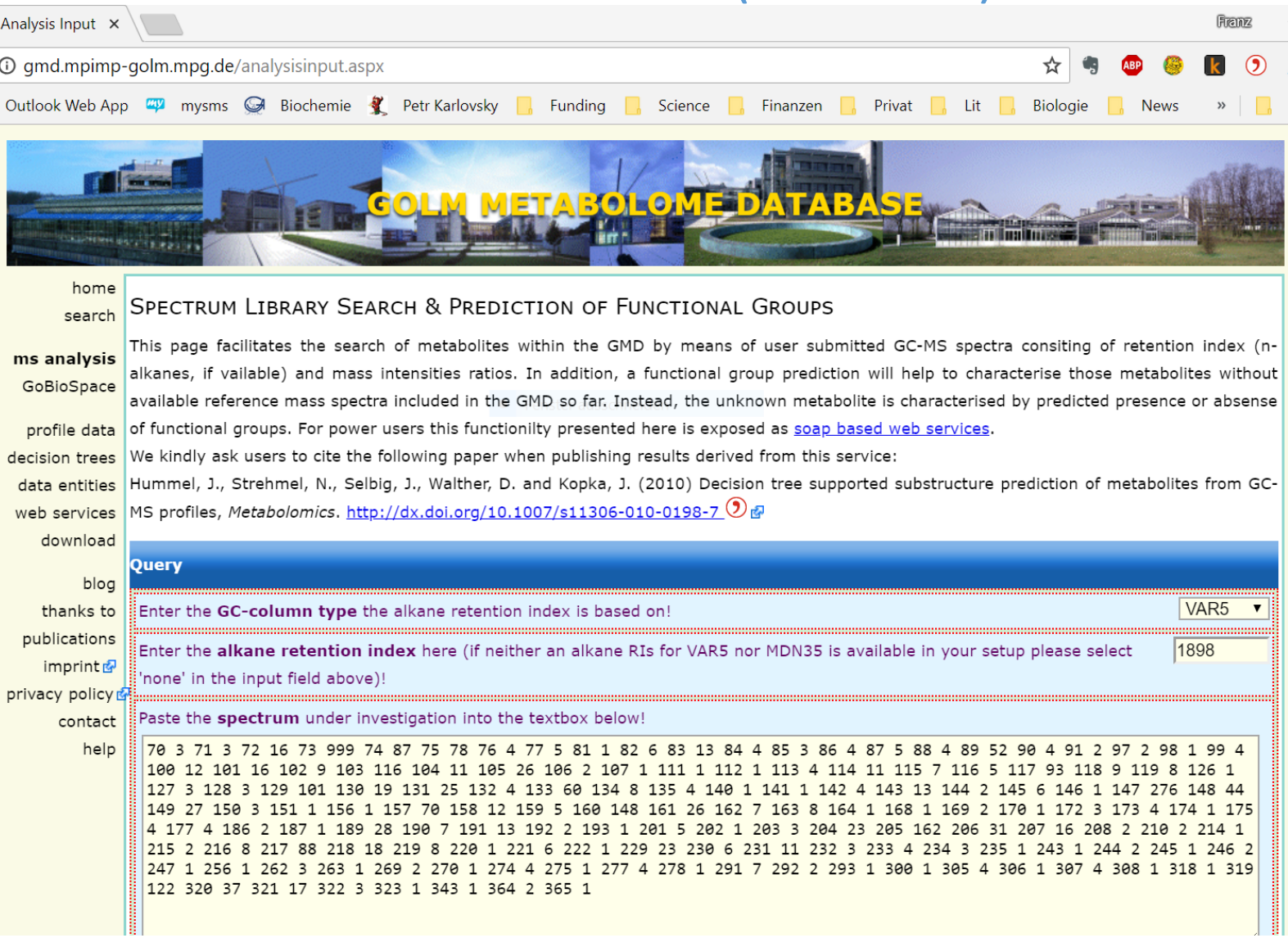


https://chemdata.nist.gov/mass-spc/amdis/downloads/

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)



Search results (GC–EIMS)

home
search

ms analysis
- library search
- prediction

GoBioSpace

profile data
decision trees
data entities
web services
download

blog
thanks to
publications
imprint
privacy policy
contact
help

Library Search Results

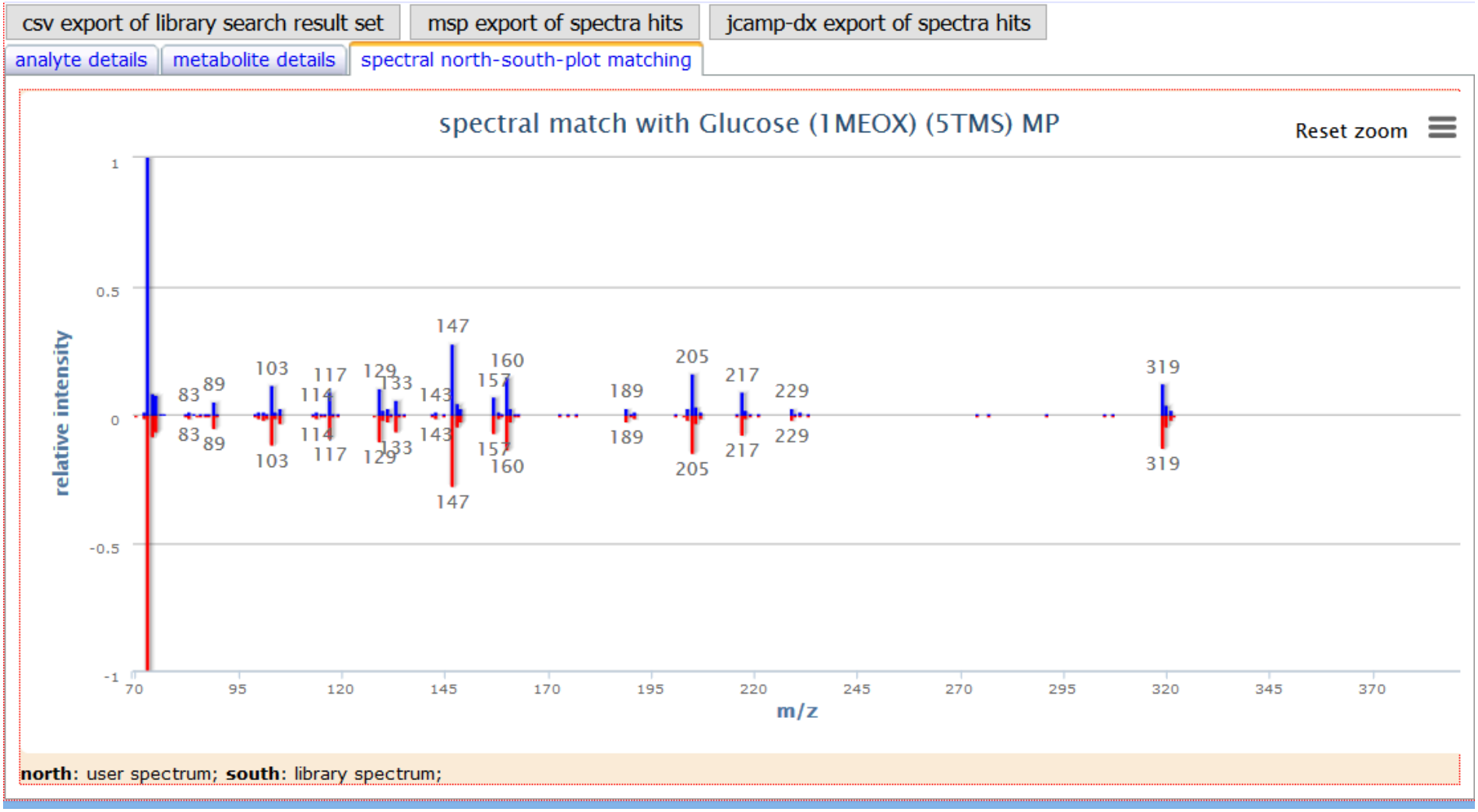
spectrum linked to analyte	RI of spectrum	RI difference	(1-dotprod) distance	euclidean distance	hamming distance	jaccard distance	s12gowleg distance
Glucose (1MEOX) (5TMS) MP	1,880.50	1,880.50	0.0005	0.00	41	0.23	0.35
Talose (1MEOX) (5TMS) MP	1,872.62	1,872.62	0.0017	0.00	44	0.25	0.37
Idose (1MEOX) (5TMS) MP	1,871.46	1,871.46	0.0017	0.00	37	0.22	0.35
Mannose (1MEOX) (5TMS) MP	1,868.46	1,868.46	0.0019	0.00	46	0.26	0.38
Gulose (1MEOX) (5TMS) MP	1,868.11	1,868.11	0.0019	0.00	44	0.25	0.37
Galactose (1MEOX) (5TMS) MP	1,876.07	1,876.07	0.0022	0.00	59	0.31	0.42
Altrose (1MEOX) (5TMS) MP	1,880.27	1,880.27	0.0024	0.01	43	0.25	0.37
Allose (1MEOX) (5TMS) MP	1,861.72	1,861.72	0.0030	0.01	36	0.22	0.35
Gulose (1MEOX) (5TMS) BP	1,891.97	1,891.97	0.0035	0.01	47	0.30	0.42
Mannose (1MEOX) (5TMS) BP	1,885.22	1,885.22	0.0037	0.01	121	0.48	0.54

36 library search hit(s).

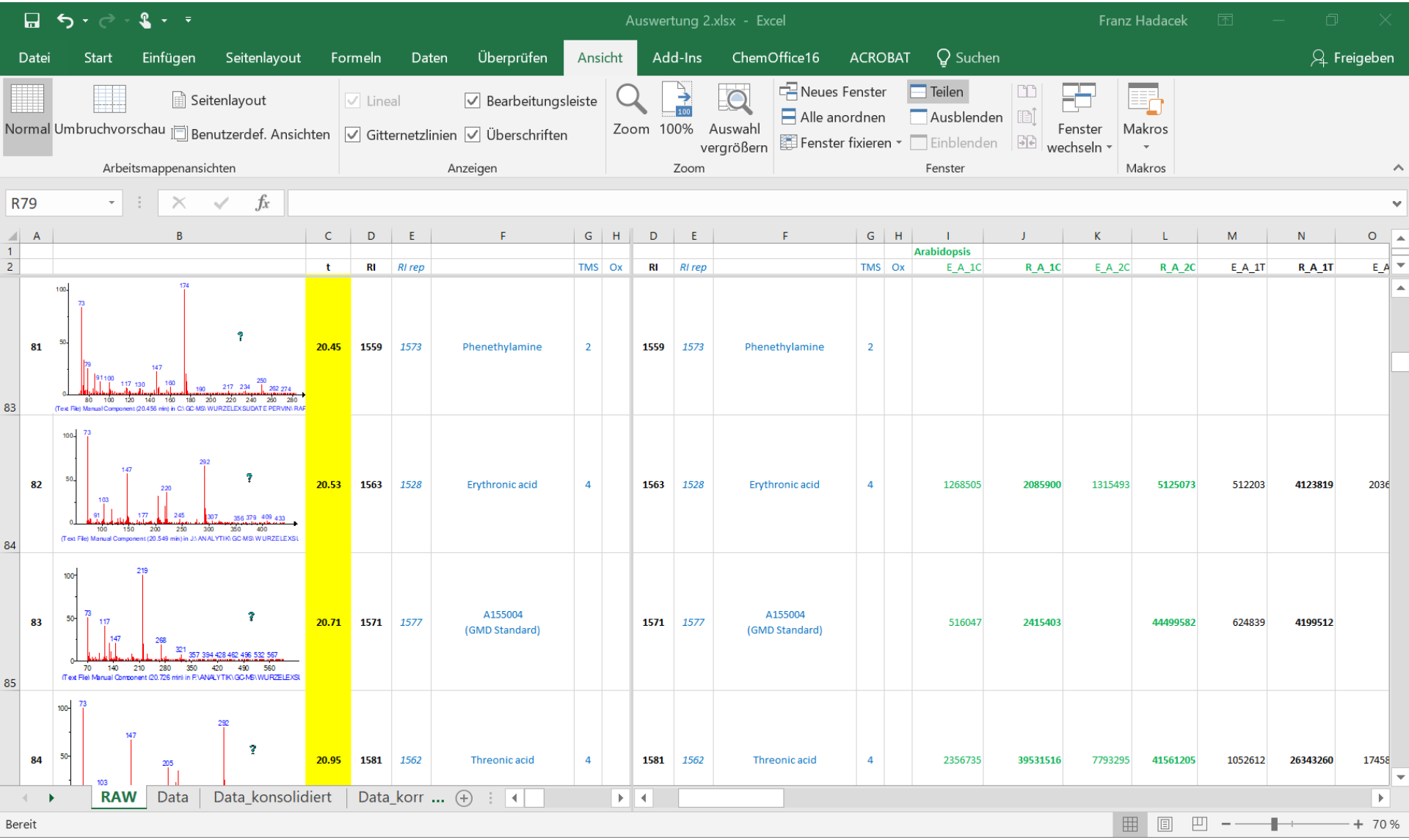
Page 1 of 4

Results per page: 10

Search results (GC–EIMS)



Search results (GC–EIMS)



		t	RI	RI rep		TMS	Ox	RI	RI rep		TMS	Ox	E_A_1C	R_A_1C	E_A_2C	R_A_2C	E_A_1T	R_A_1T	E_A
81		20.45	1559	1573	Phenethylamine	2		1559	1573	Phenethylamine	2								
82		20.53	1563	1528	Erythronic acid	4		1563	1528	Erythronic acid	4		1268505	2085900	1315493	5125073	512203	4123819	2036
83		20.71	1571	1577	A155004 (GMD Standard)			1571	1577	A155004 (GMD Standard)			516047	2415403		44499582	624839	4199512	
84		20.95	1581	1562	Threonic acid	4		1581	1562	Threonic acid	4		2356735	39531516	7793295	41561205	1052612	26343260	17458

Liquid chromatography

Electrospray interface

Time-of-flight mass spectrometry

Analysis of specialized (secondary) metabolites

Metabolite fingerprinting

3 conditions with 6 replicates each → 18 samples

Line 1	Line 2	Line 3

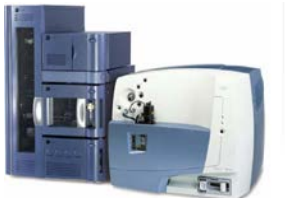
Material

Extraction: 80 % Methanol

Polar phase

Non-polar phase

Ultra performance liquid chromatography (UPLC)



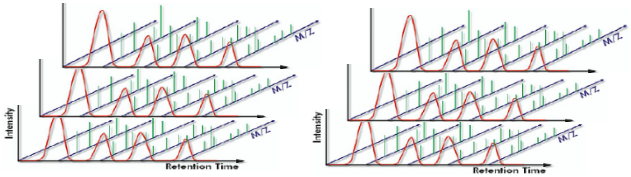
Electrospray ionization/time-of-flight MS (ESI-TOF)

Sample set: Pos.ESI/polar

Sample set: Neg.ESI/polar

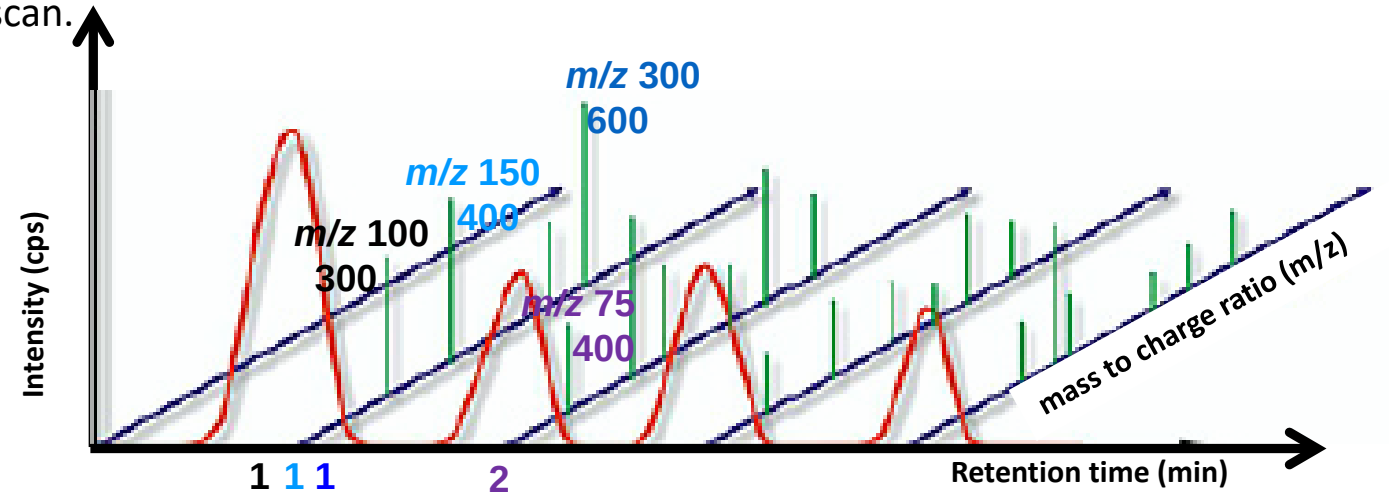
Sample set: Pos.ESI/non-polar

Sample set: Neg.ESI/non-polar

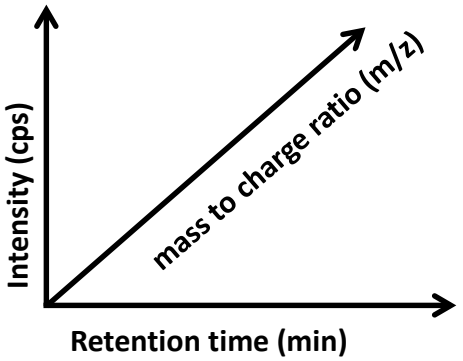


A MS signal is characterized by m/z, Rt and the signal intensity

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



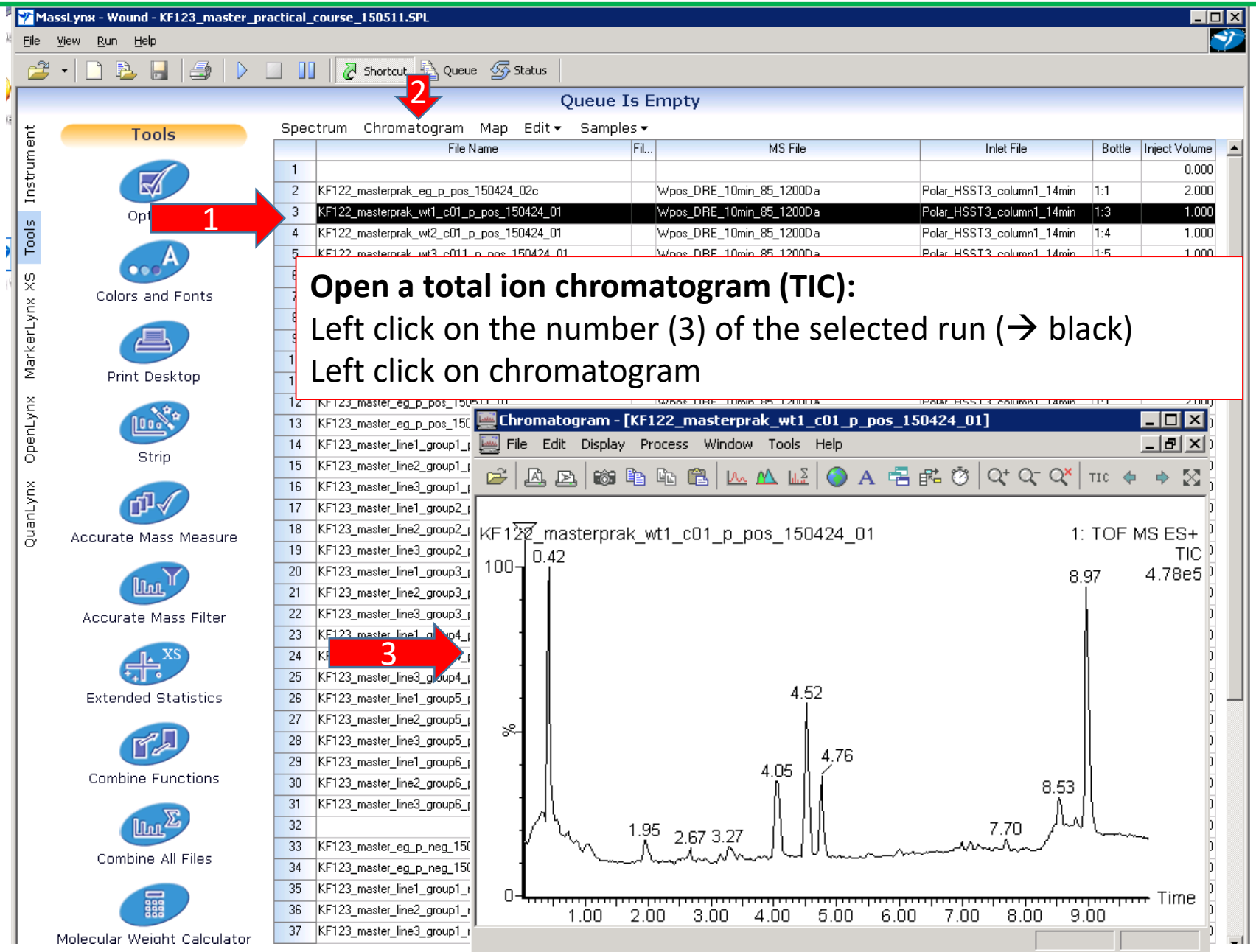
Total ion chromatogram (TIC)



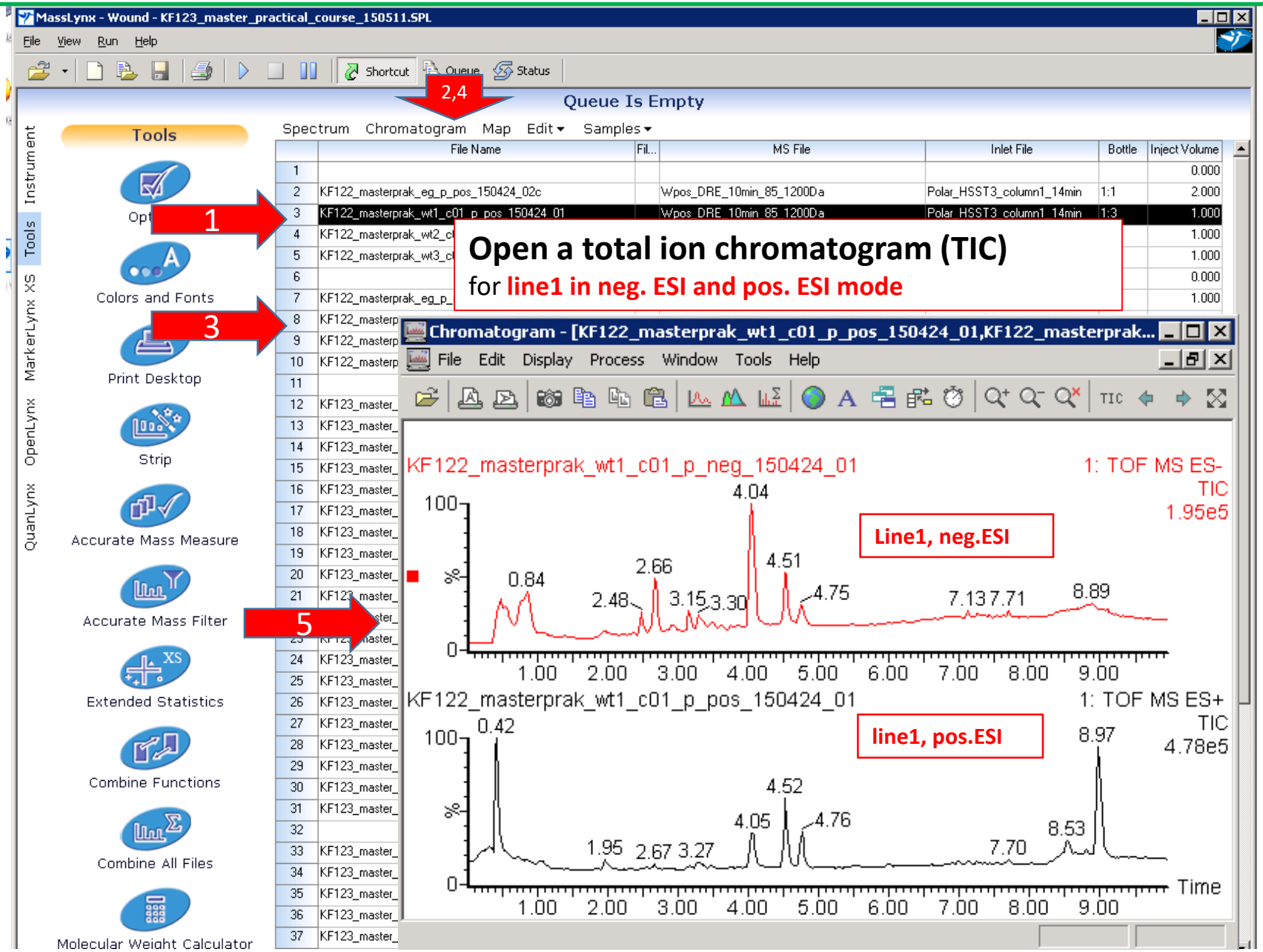
A MS signal is characterized by the three parameters:
m/z (300), Rt (1min) and signal intensity (600 cps)

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

Open and inspect TICs

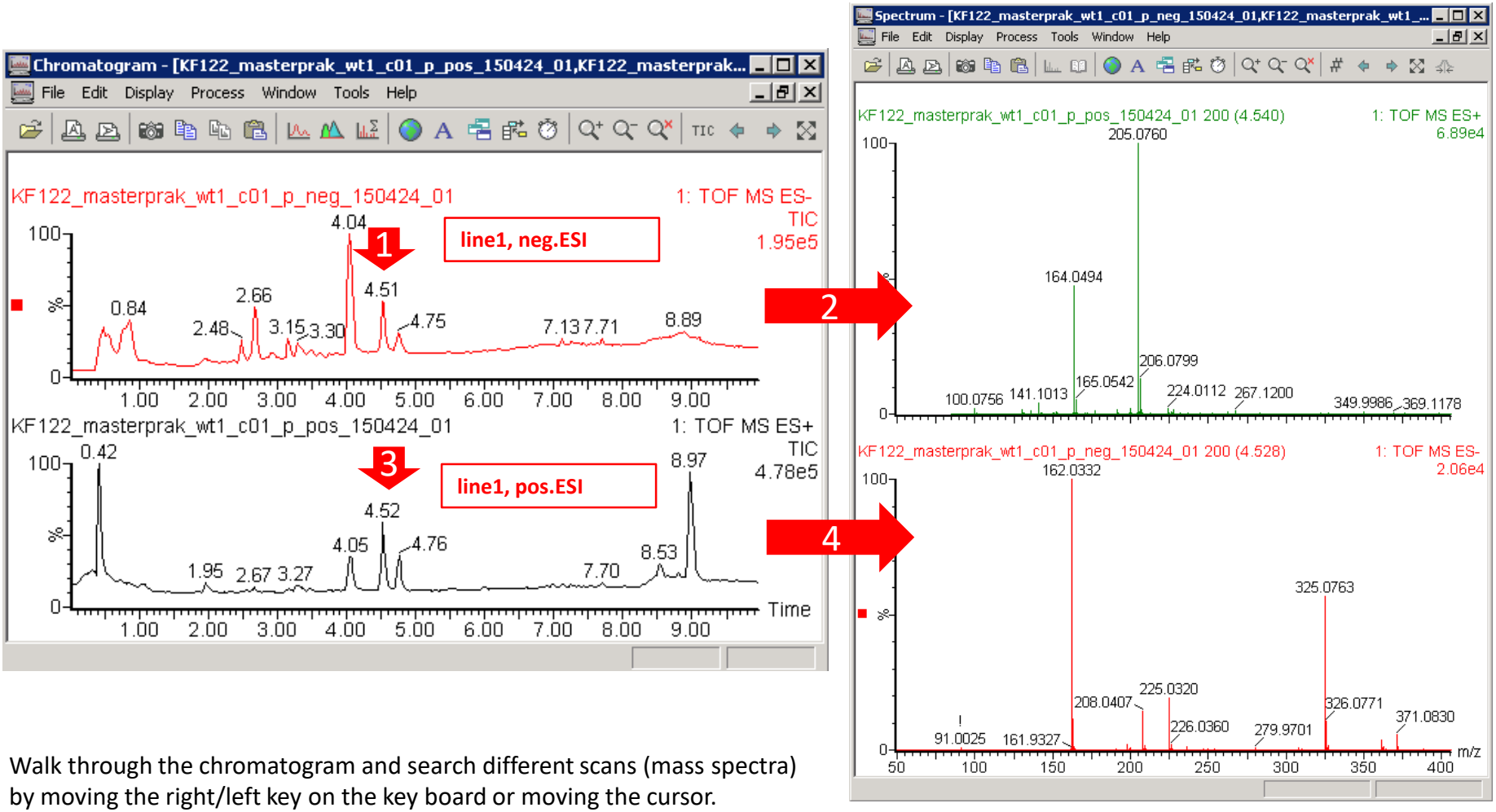


Open and inspect TICs



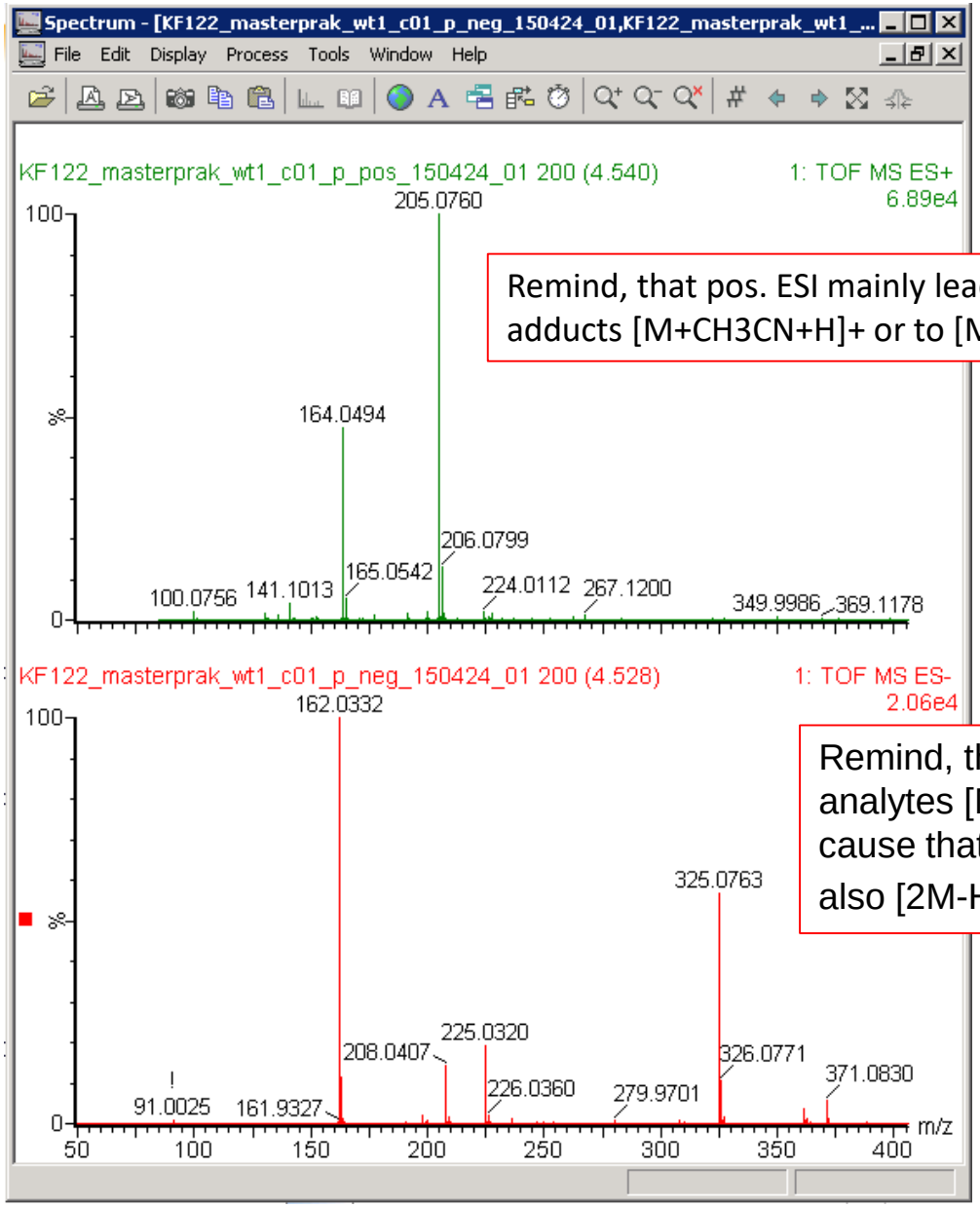
Open and inspect the mass spectra

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+CH3CN+H]+ or to [M+Na]+ and [M+NH4]+ adducts

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

How to identify adducts?

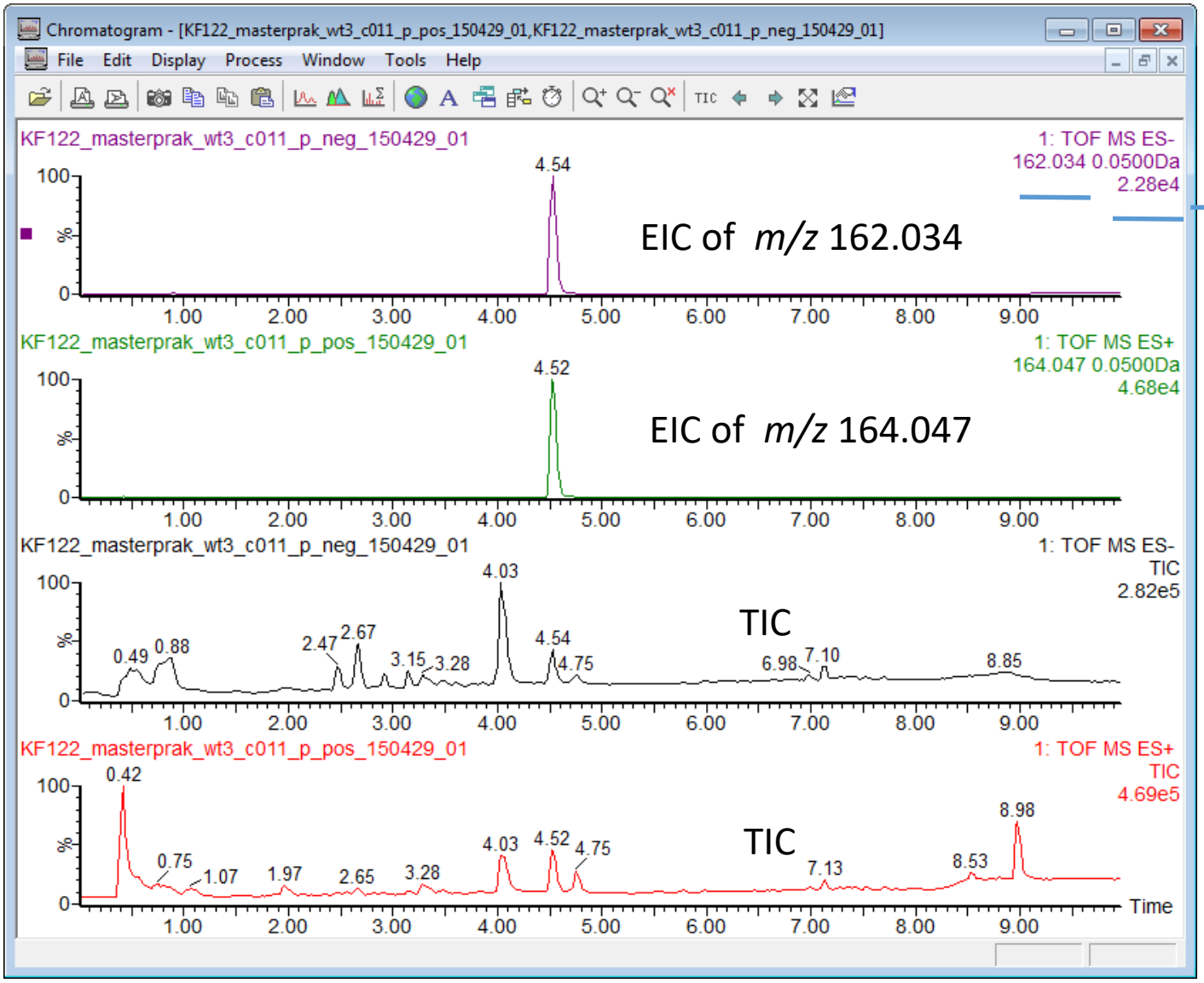
Adducts are built during ionisation in the source. Because of that, they have the identical RT as its protonated or deprotonated ion and are characterized by a very exact mass shift to that corresponding ion (see below).

Mass differences (neg. ESI mode):
[M-H+]- to [M+HCOO-]- → 46.0055
[M-H+]- to [2M-H+]- → [2M-1.0073]-

Mass differences (pos. ESI mode):
[M+H+]+ to [M+Na+]+ → 21.9825
[M+H+]+ to [M+NH4+]+ → 17.0265
} 4.956
[M+H+]+ to [2M-H+]- → [2M+1.0073]+
[M+H+]+ to [M+CH3CN+H+]+ → 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

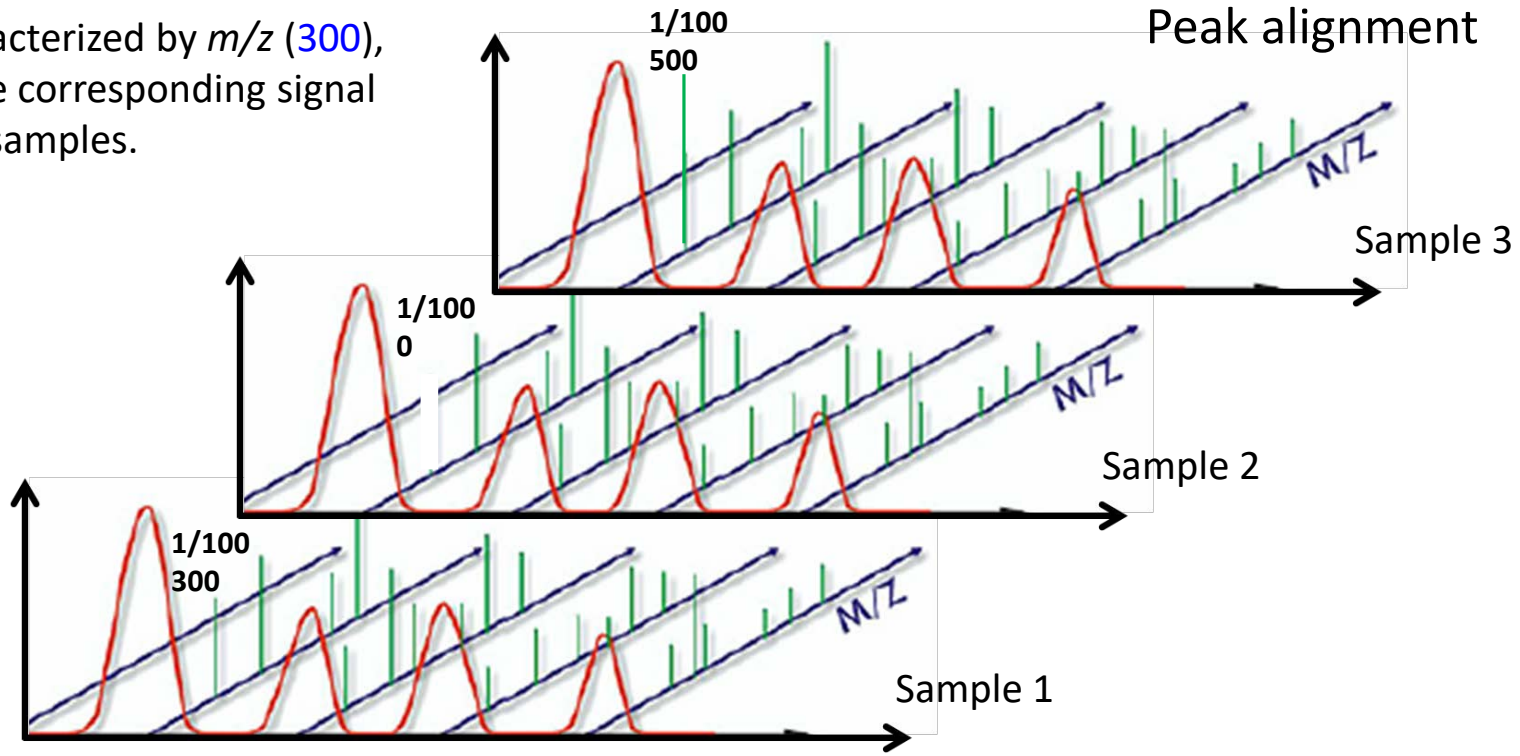
Extracted mass chromatogram (EIC, XIC)



Intensity of the extracted mass signal (cps)

MarkerLynx performs peak picking and peak alignment

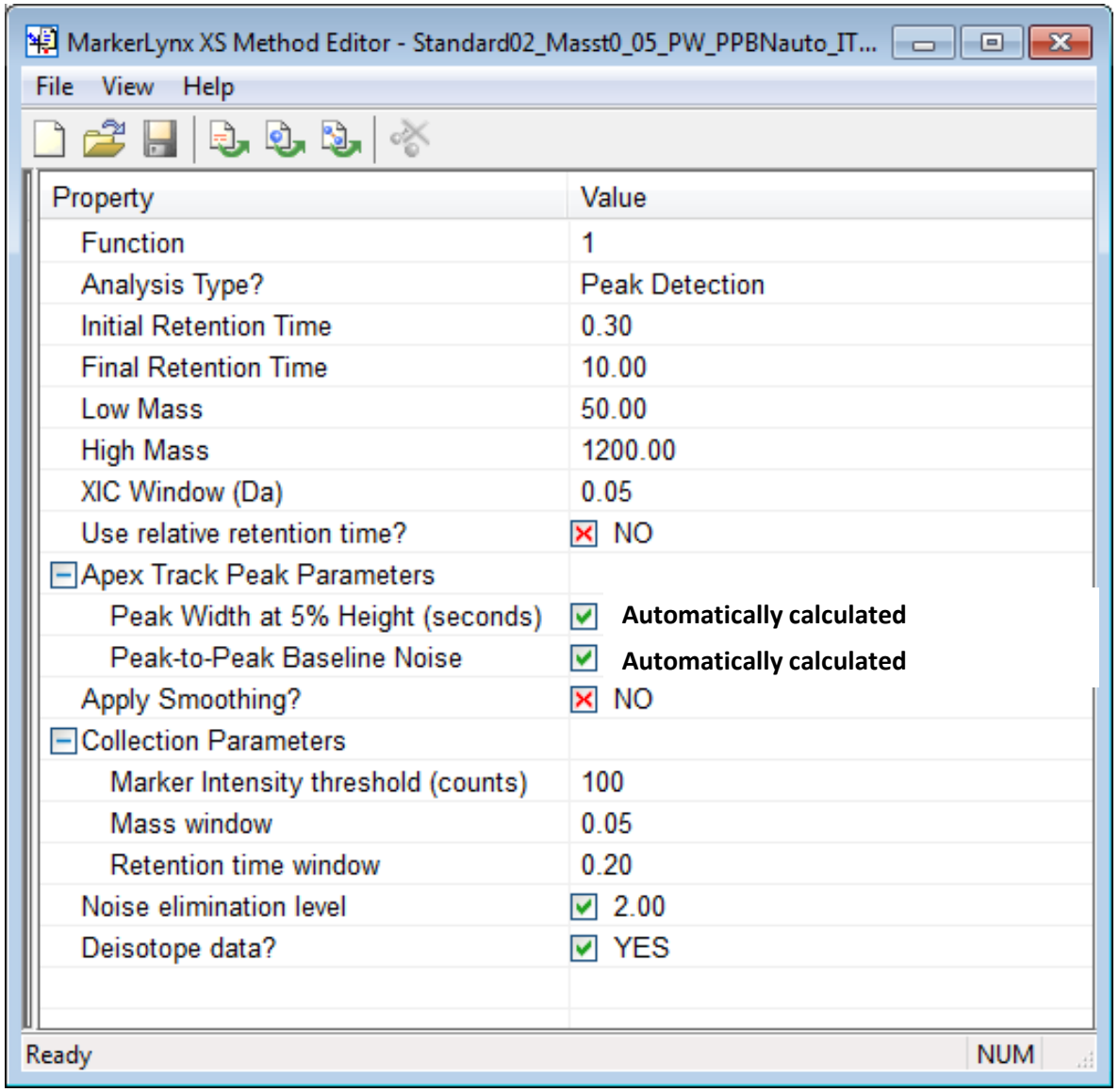
A **feature** is characterized by *m/z* (300), Rt (1min) and the corresponding signal intensities of all samples.



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	Biotransfc	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_mast
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	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	0	447.7827	693.7471	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

MarVis Homepage

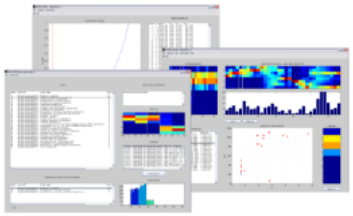
marvis.gobics.de

Apps | Outlook Web App | mysms | Biochemie | Petr Karlovsky | Funding | » | Weitere Lesezeichen

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

The **MarVis-Suite** (**Mar**ker **Vis**ualization) 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.

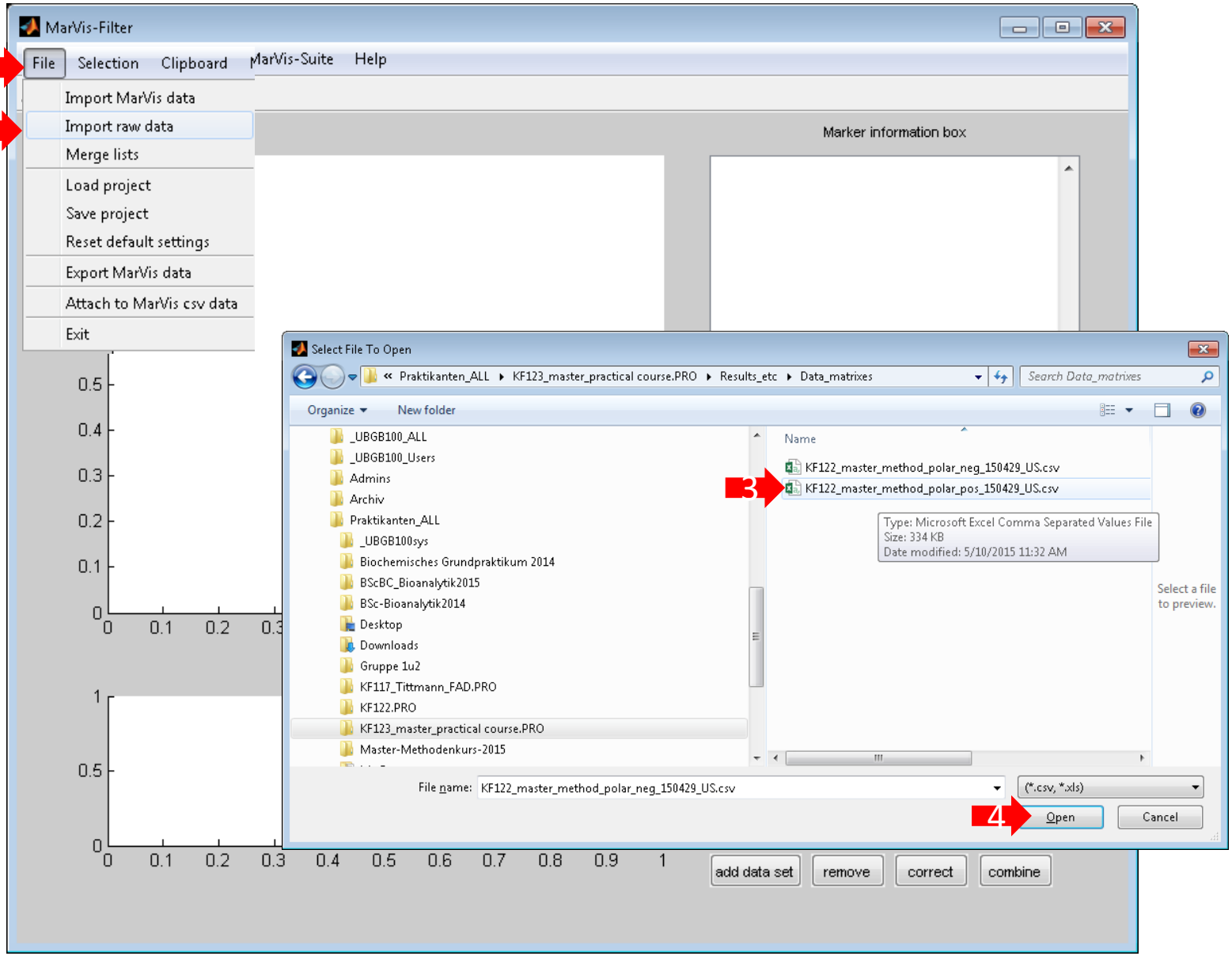
Within the MarVis-Suite framework, the MarVis-Filter interface provides functions for import, preprocessing, filtering, and combination of raw data files, while the MarVis-Cluster interface was designed for high-level visualization and cluster analysis. The MarVis-Pathway interface is used for functional 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.



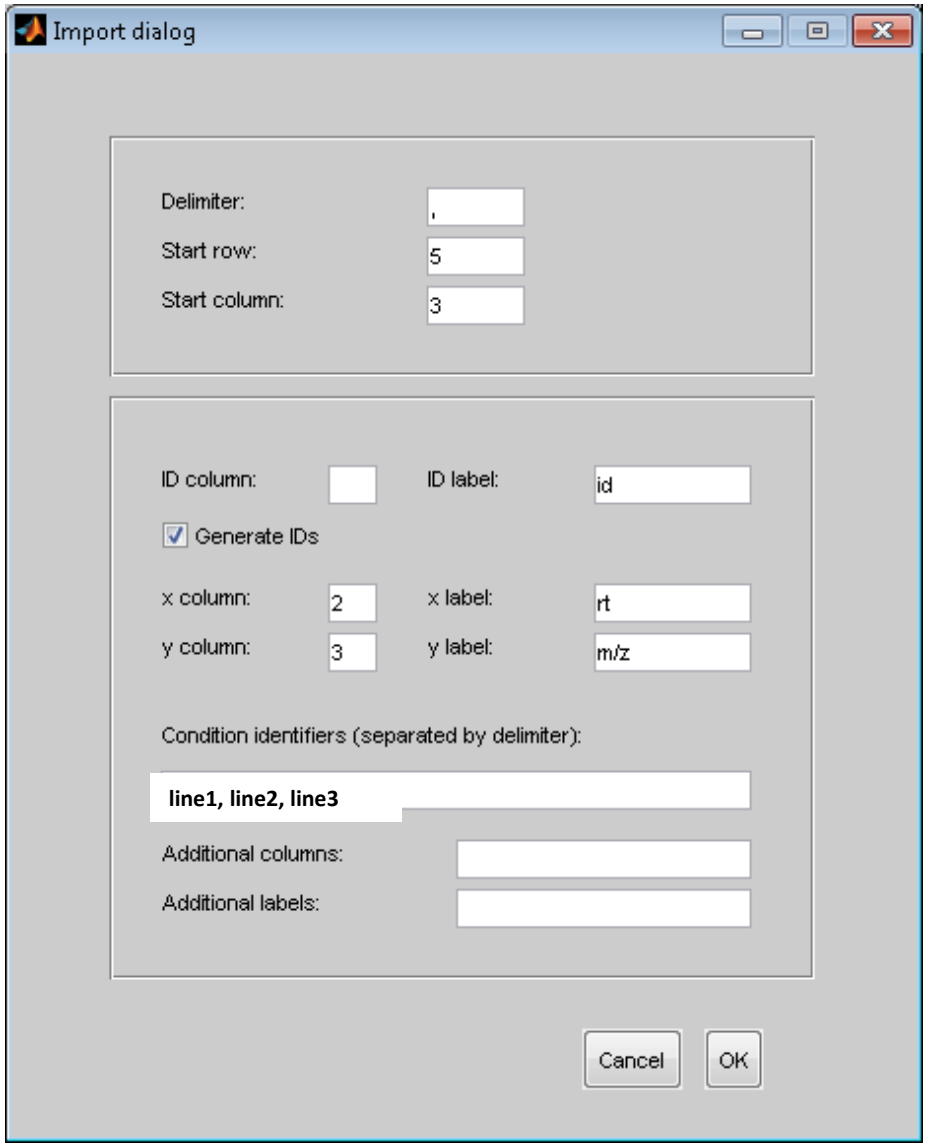
The MarVis-Suite software is free for academic use. It comes with no guarantee or warranty at all. Use it at your own risk. Please send questions, bug reports and feature requests to marvis(AT)gobics(DOT)de.

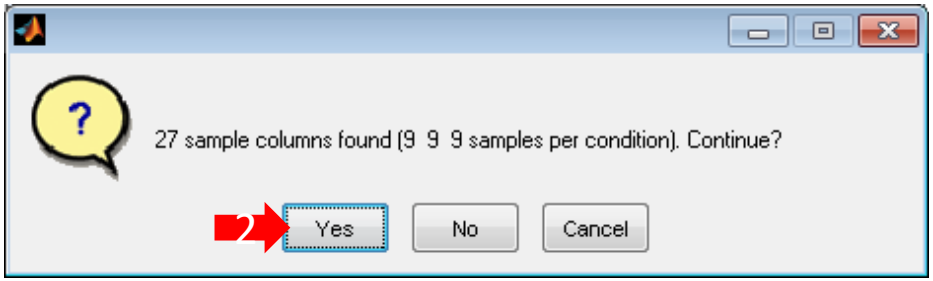
Open MarVis Filter 2.6
Import data matrix1 (pos. ESI)

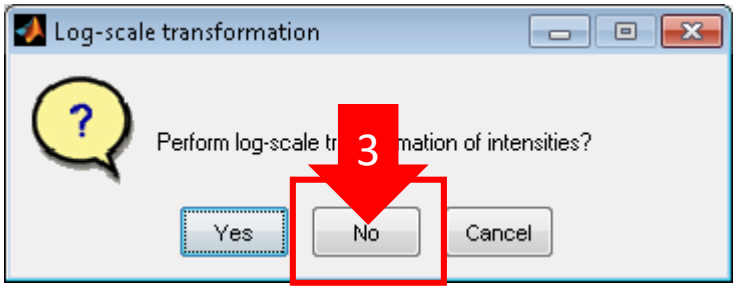
W:\Praktikanten_ALL\KF123_master_practical course.PRO\Results_etc\Data_matrixes

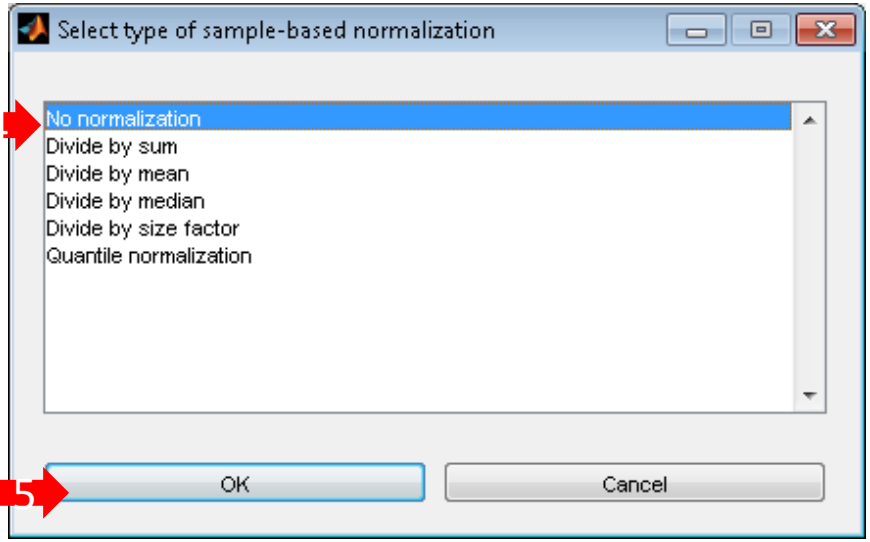


Import data matrix (pos. ESI)

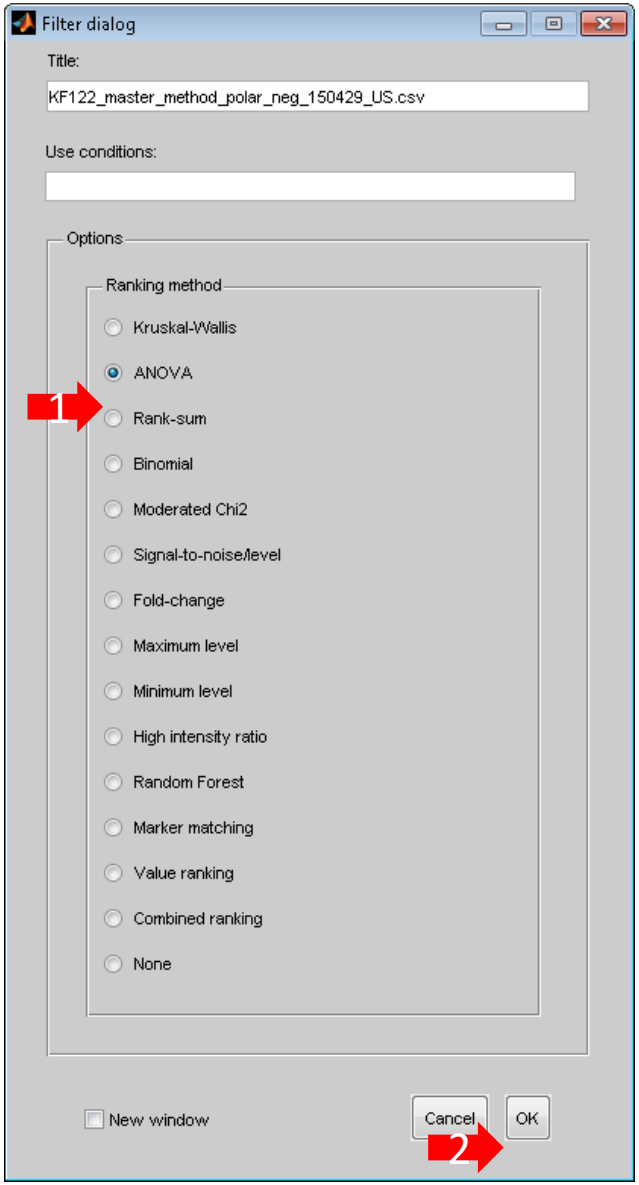


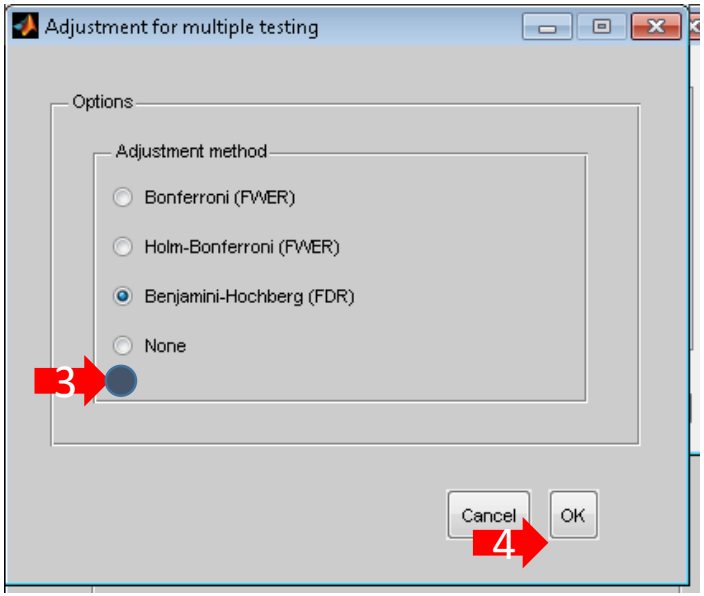




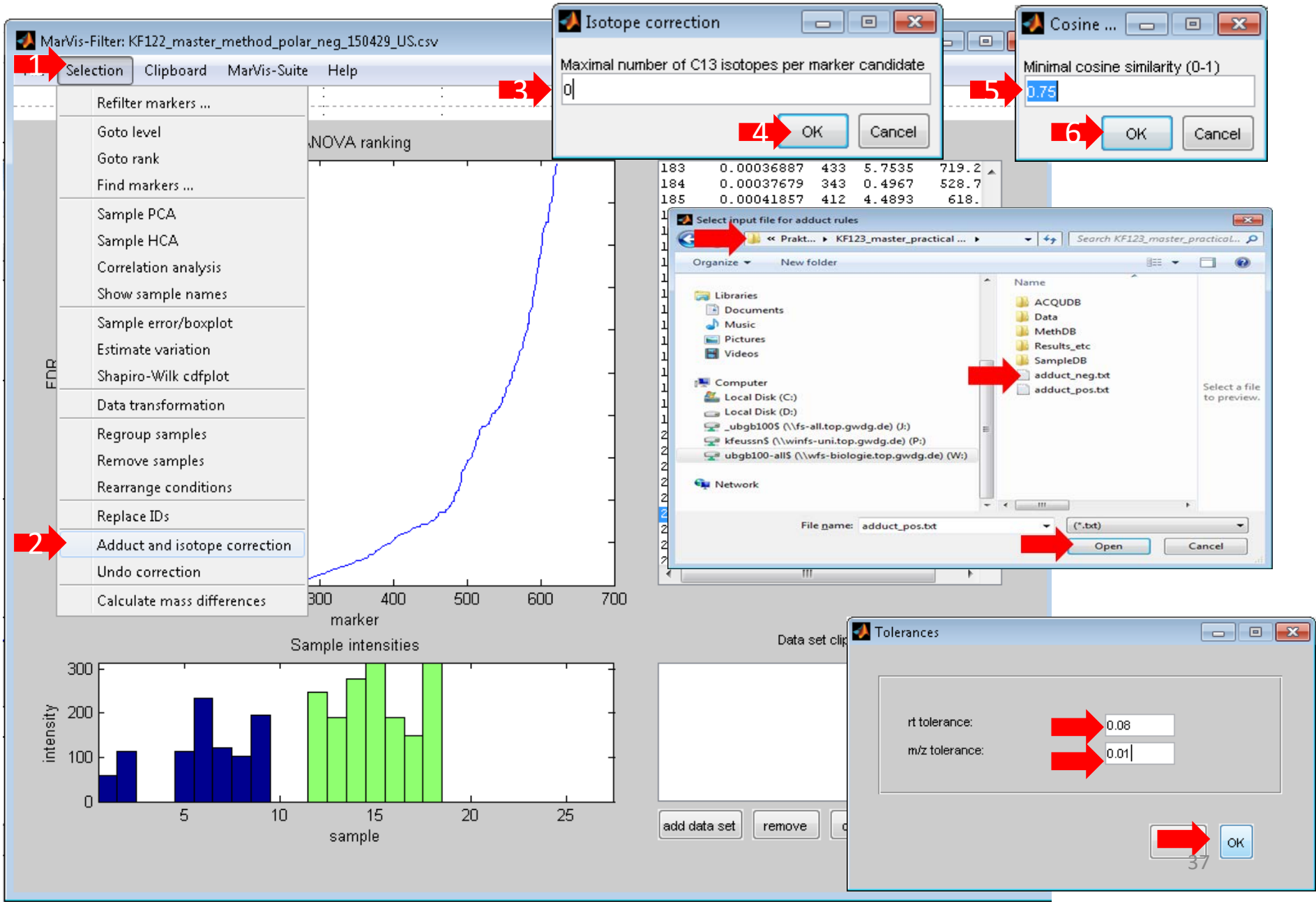


Rank the data by ANOVA

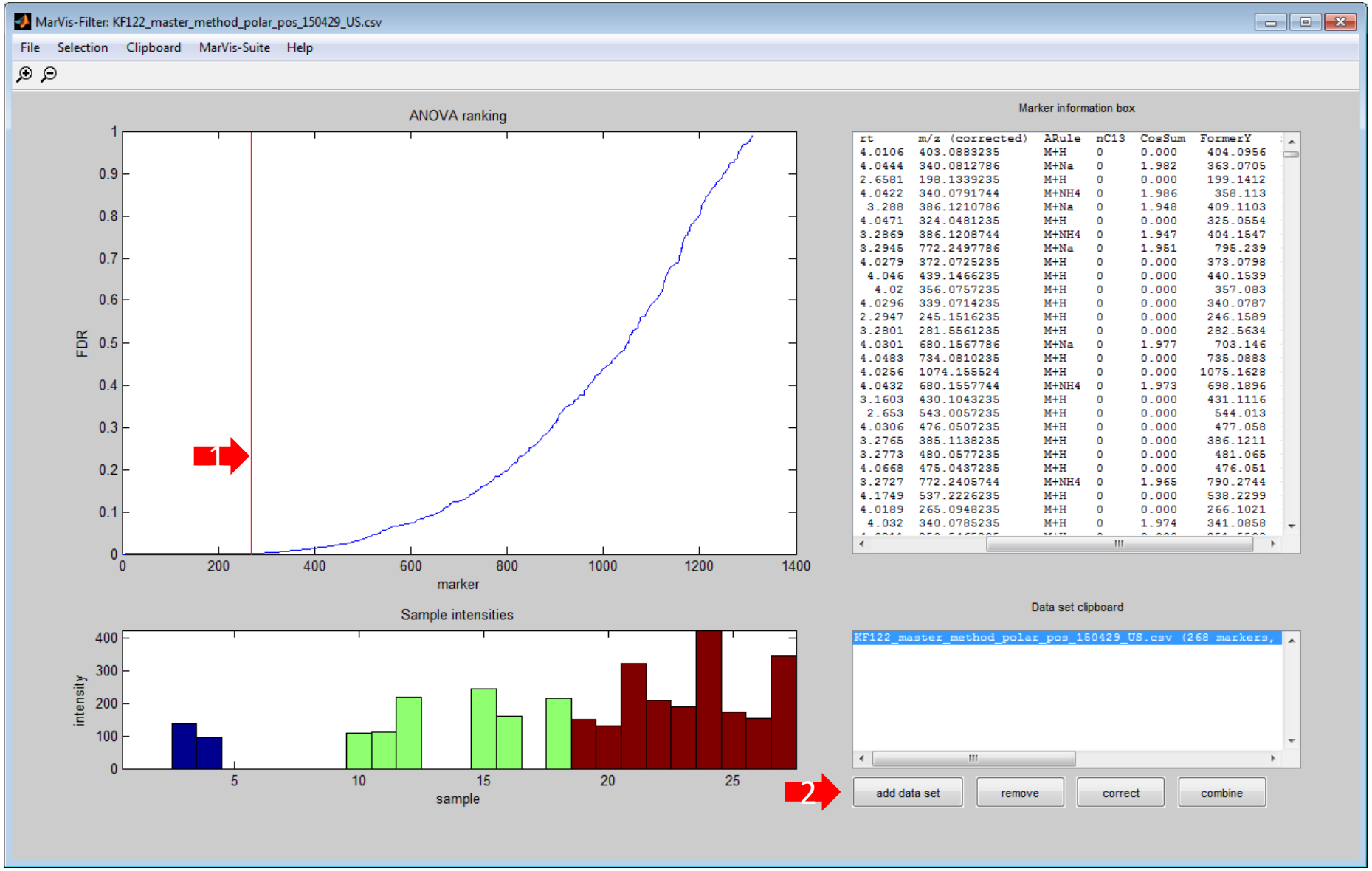




Filter the data set
Correct the adducts

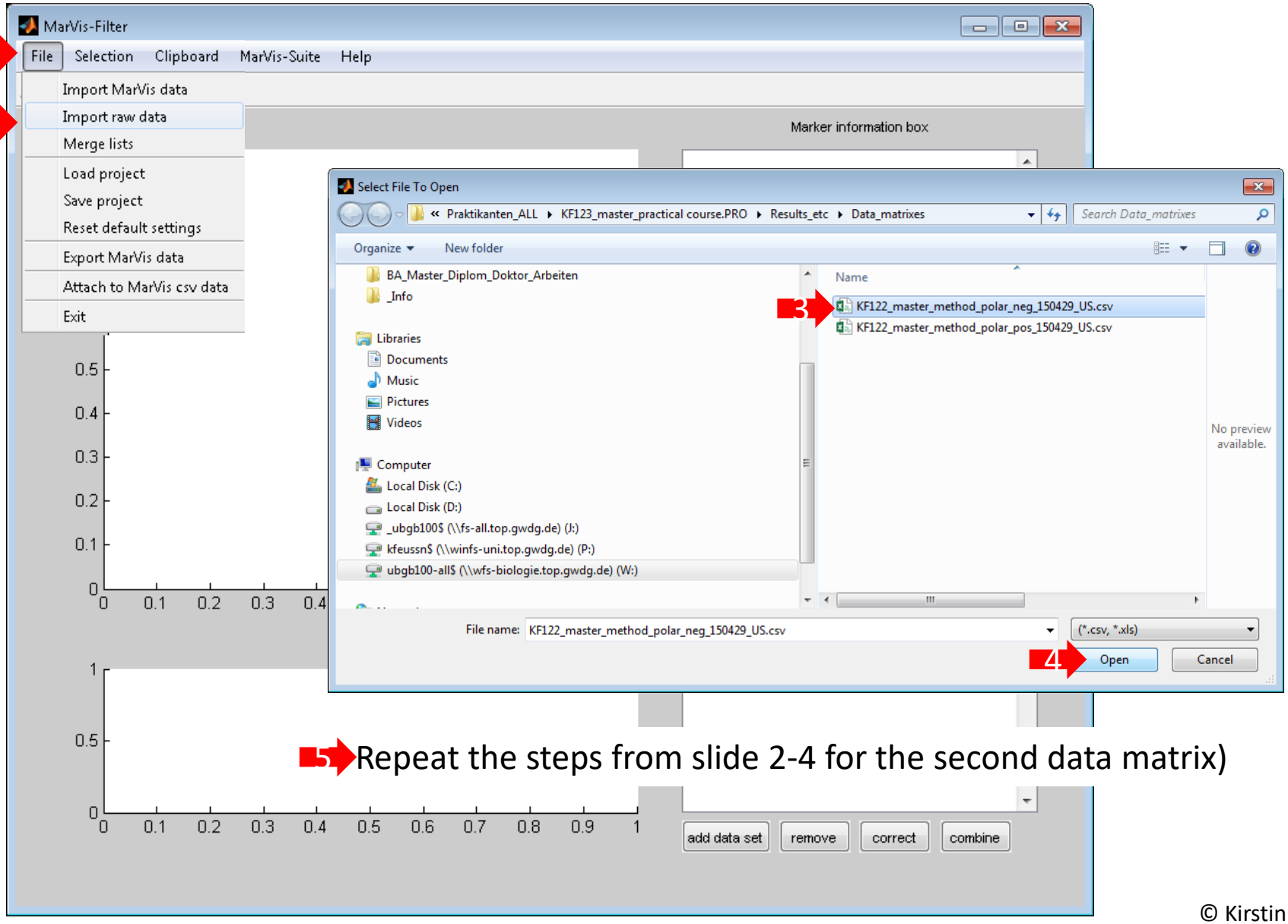


Filter the data set
Transfer the filtered data to the data set clipboard



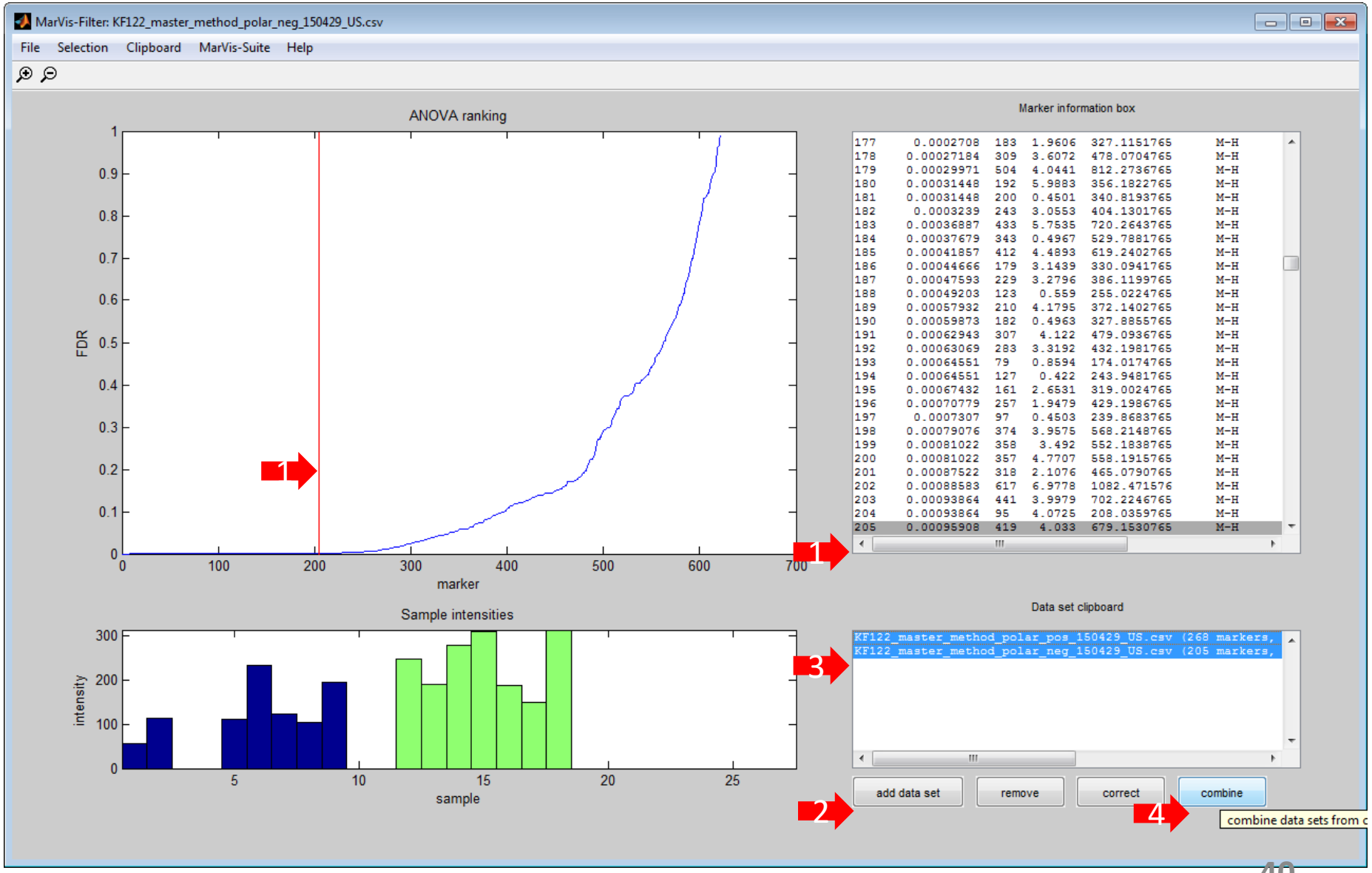
Open MarVis Filter 2.6
Import data matrix2 (neg. ESI)

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

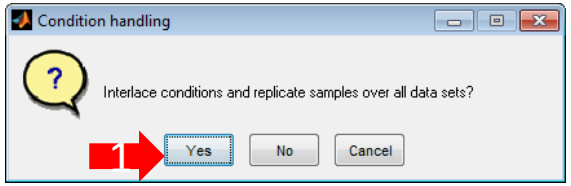


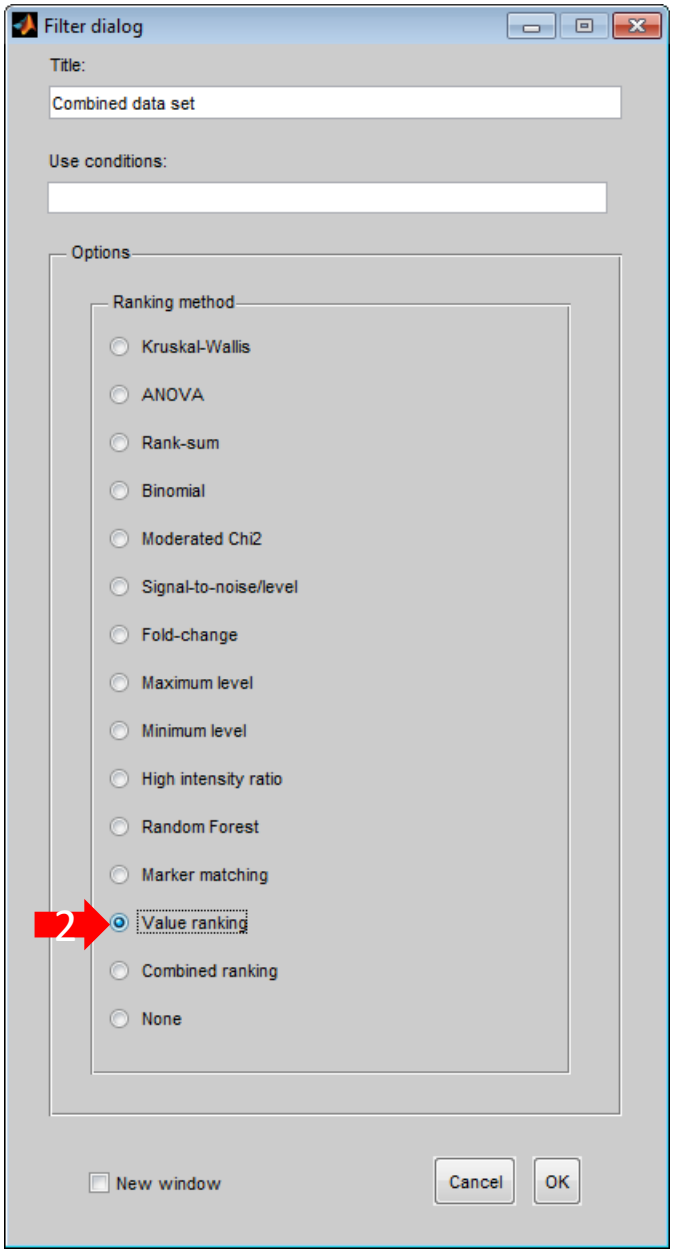
5 Repeat the steps from slide 2-4 for the second data matrix)

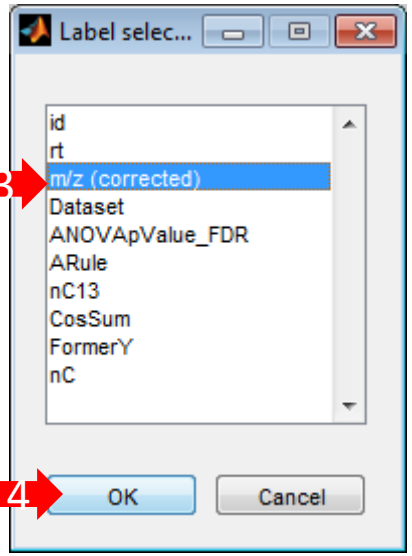
Combine the filtered and adduct corrected data sets

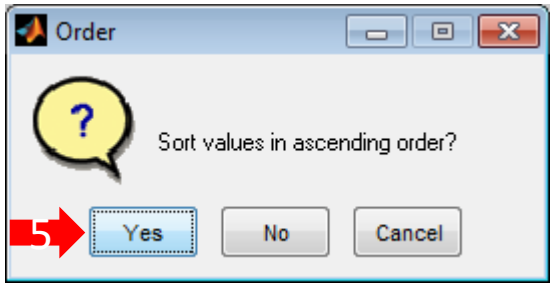


Rearrange the combine data by mass

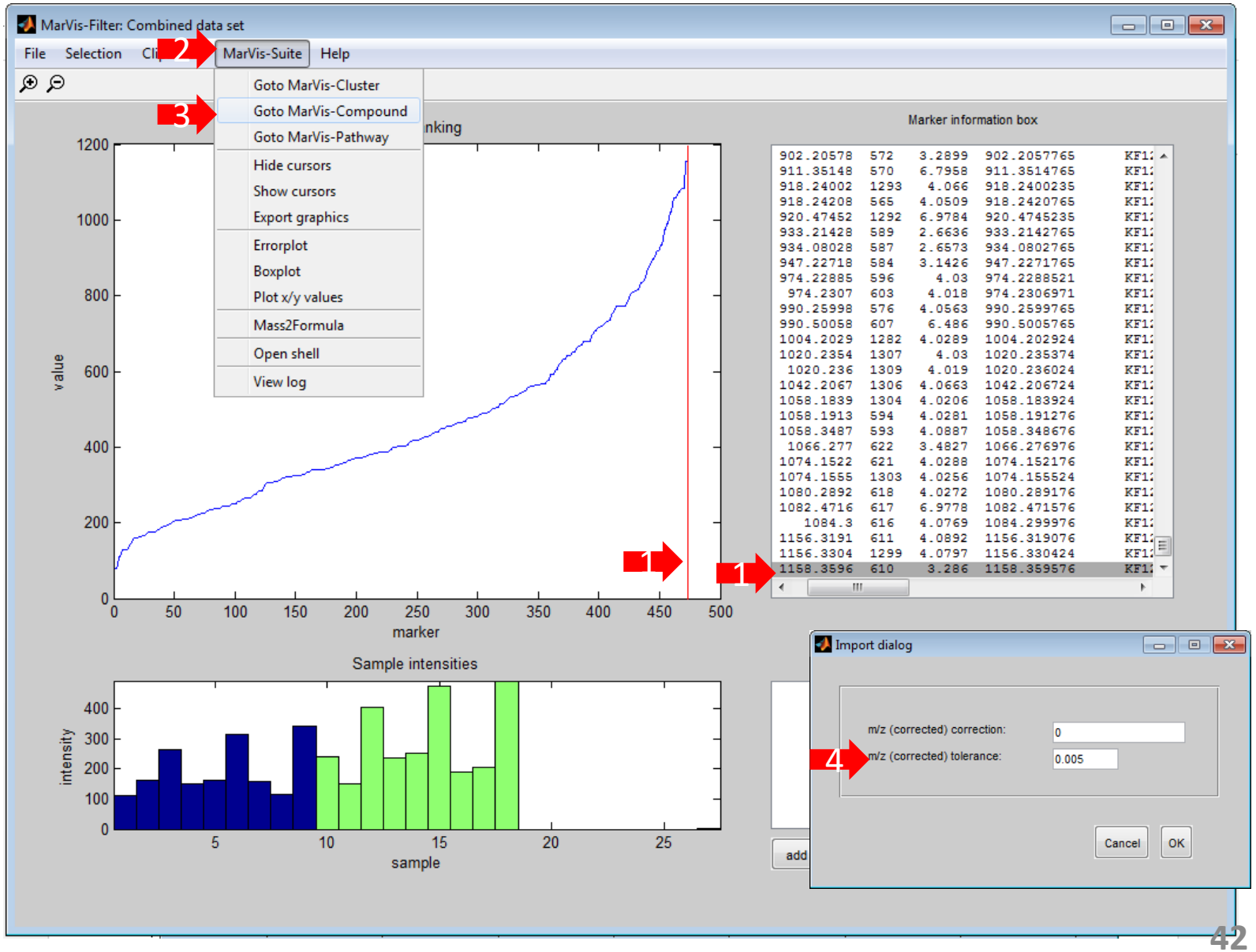




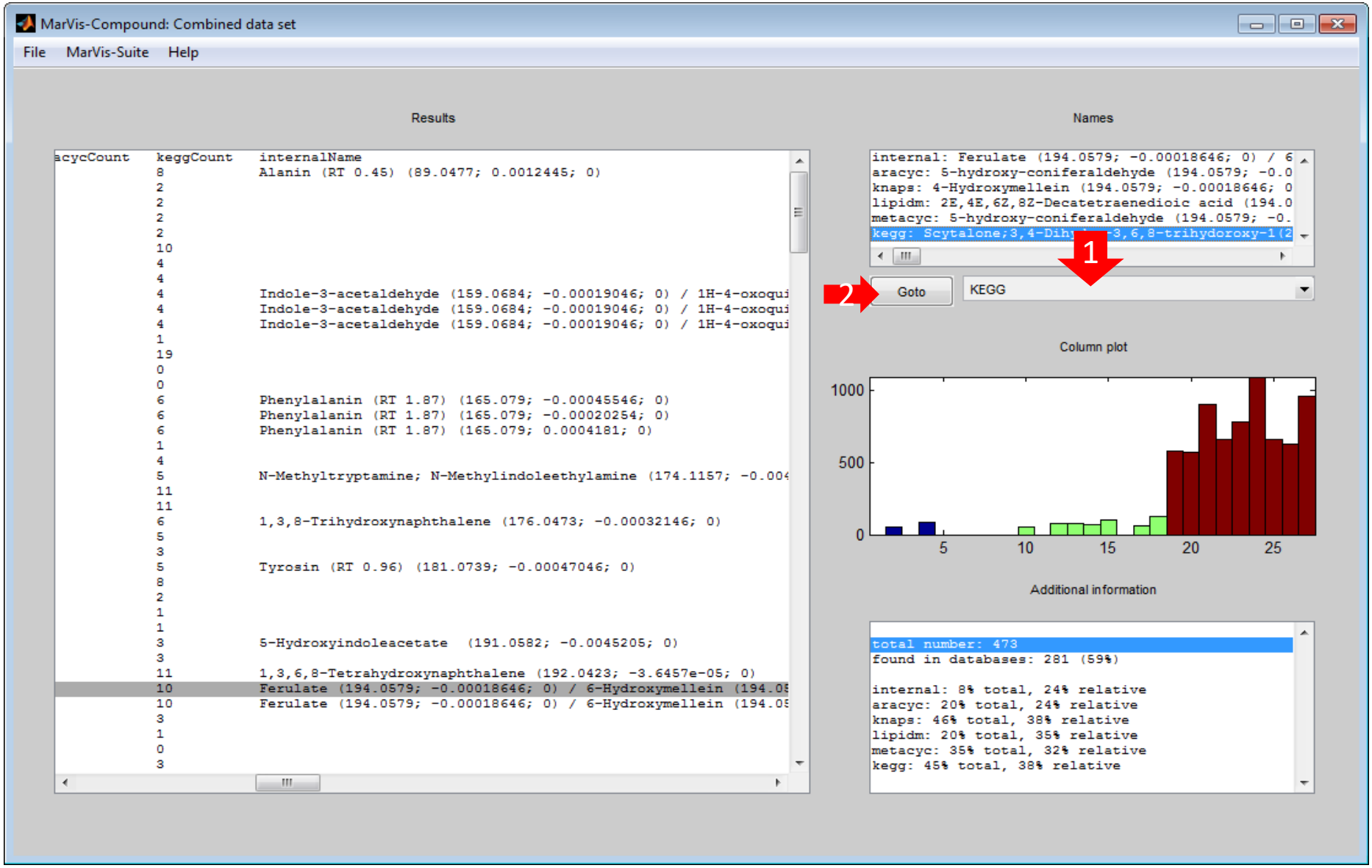


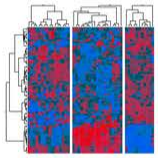


Start MarVis Compound for db search

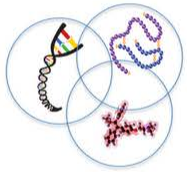


Inspect the putativ identities of compounds





Statistics



Pathways

Metlin

Sharing

LIGAND Relational Database

The primary database of KEGG LIGAND is a relational database with the KegDraw interface, which is used to generated 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

Search GLYCAN

Glycan ID ▼ example) G10596 Go Clear

Search REACTION

Reaction ID ▼ example) R00259 Go Clear

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

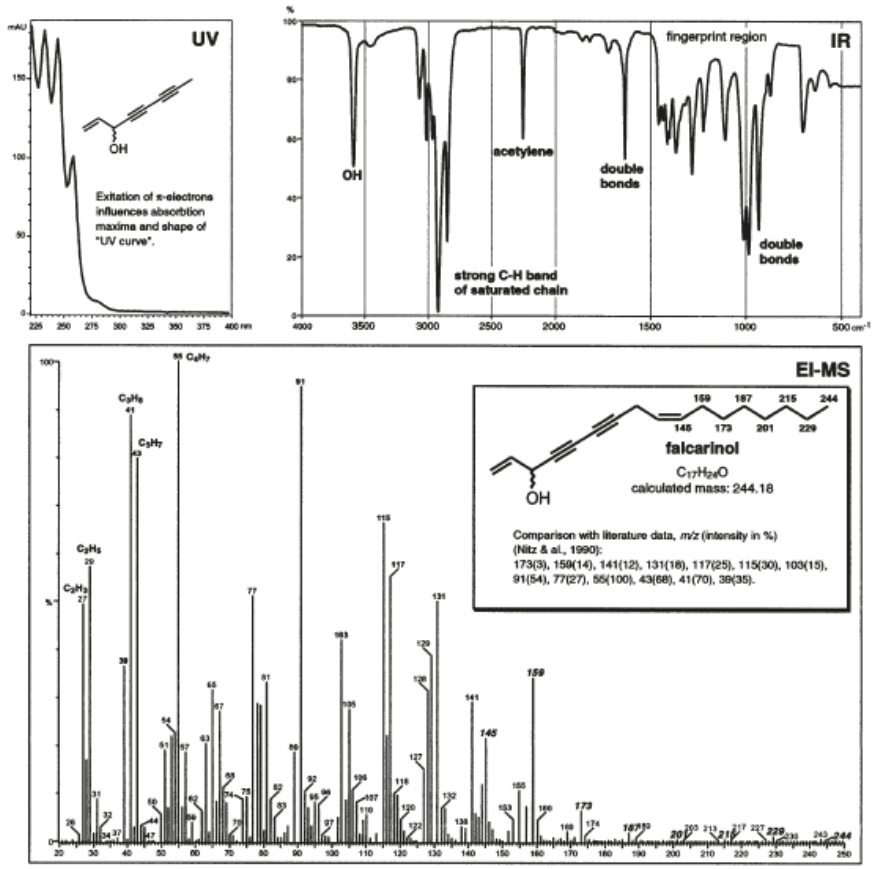


FIGURE 2. UV, IR, and EI–MS spectrum of the polyacetylene falcarinol, a characteristic secondary metabolite found in *Apiaceae* and *Araliaceae*. The UV spectrum was obtained on-line from a HPLC run by a diode-array system (Hewlett Packard 1090), the mobile phase was a gradient of MeOH and aqueous buffer; 2 mg of a pure sample dissolved in CCl_4 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).

Critical Reviews in Plant Sciences, 21(4):273–322 (2002)

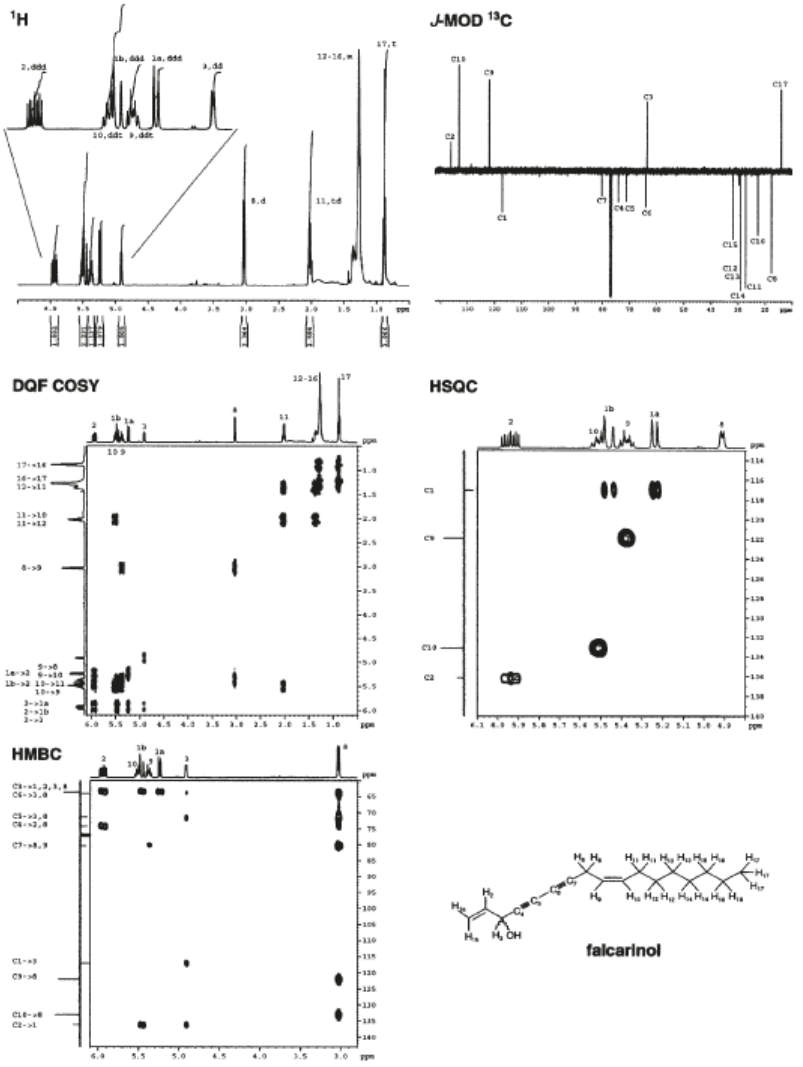


FIGURE 3. One- and two-dimensional NMR spectra of the polyacetylene falcarinol: one-dimensional technologies: ^{1}H-NMR (proton NMR), *J*-mod ^{13}C (carbon NMR); two-dimensional technologies: DQF-COSY (double quantum filtered correlation spectrum), HSQC (heteronuclear single quantum coherence), HMBC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

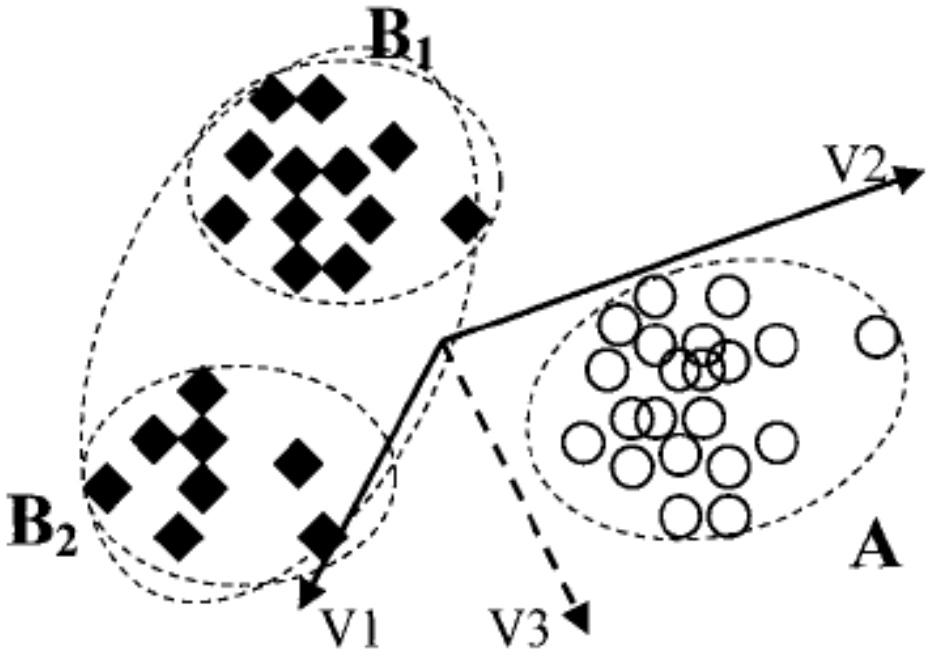
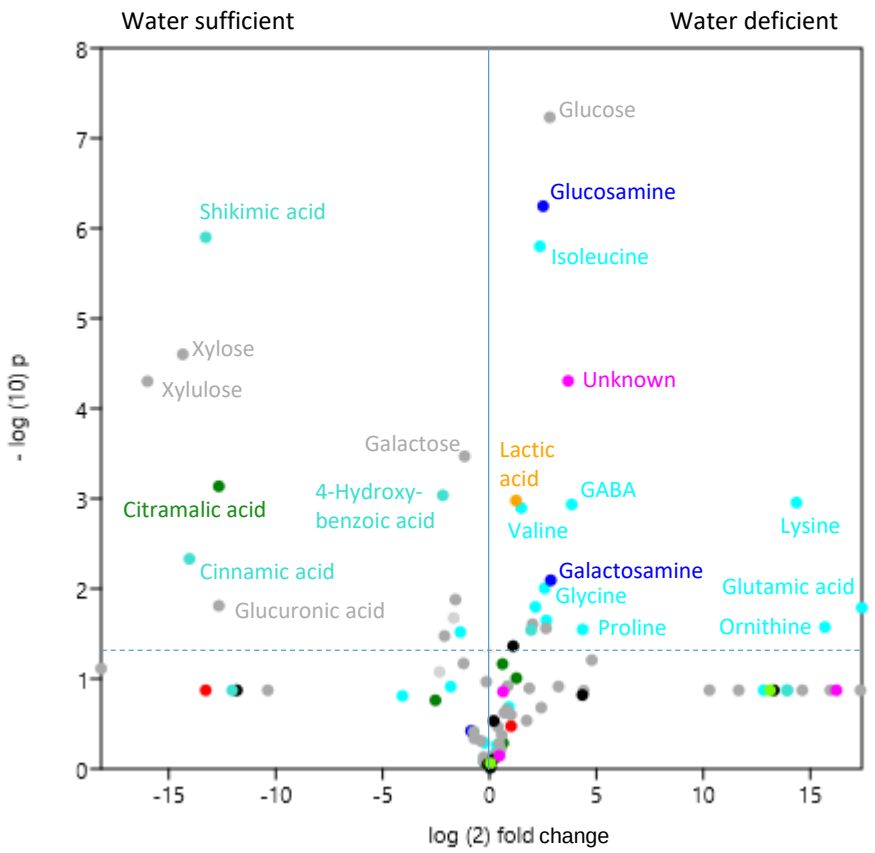


Figure 2. Cluster analysis of a hypothetical experiment. Clustering of the samples by principal-component analysis might result in the expected separation of samples from origin A (such as wild-type samples) and from origin B (such as mutant samples). In this example, B samples fall into two sub-groups, B_1 and B_2, as indicated by covers (dotted lines).

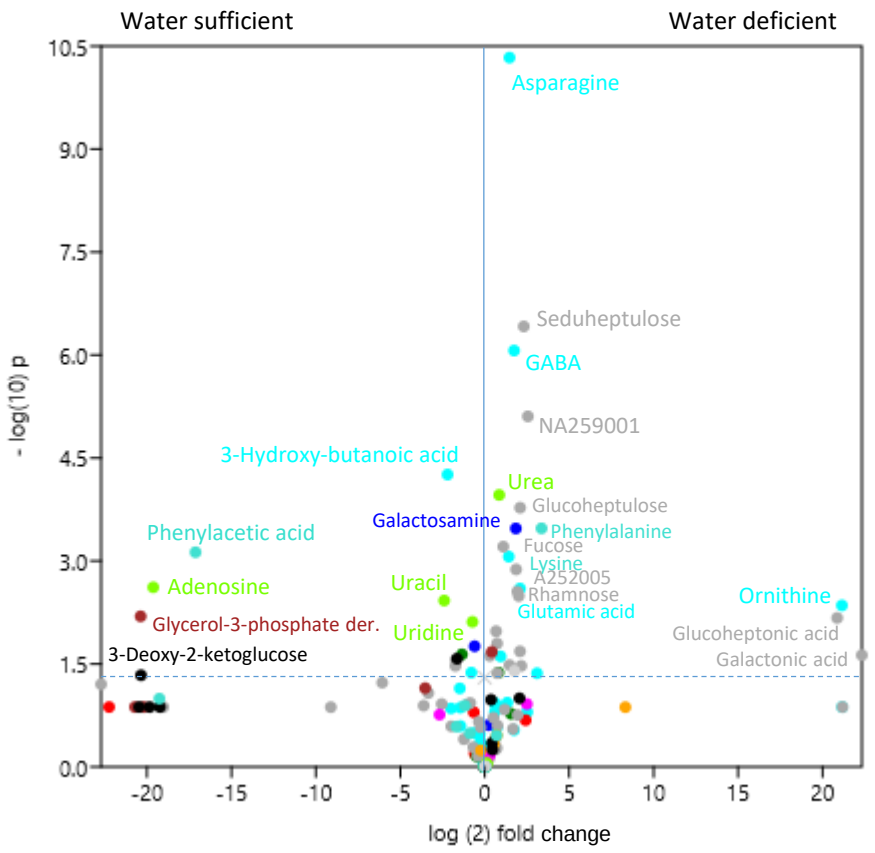
Plant Molecular Biology **48:** 155–171, 2002.

Volcano plot

Root exudate

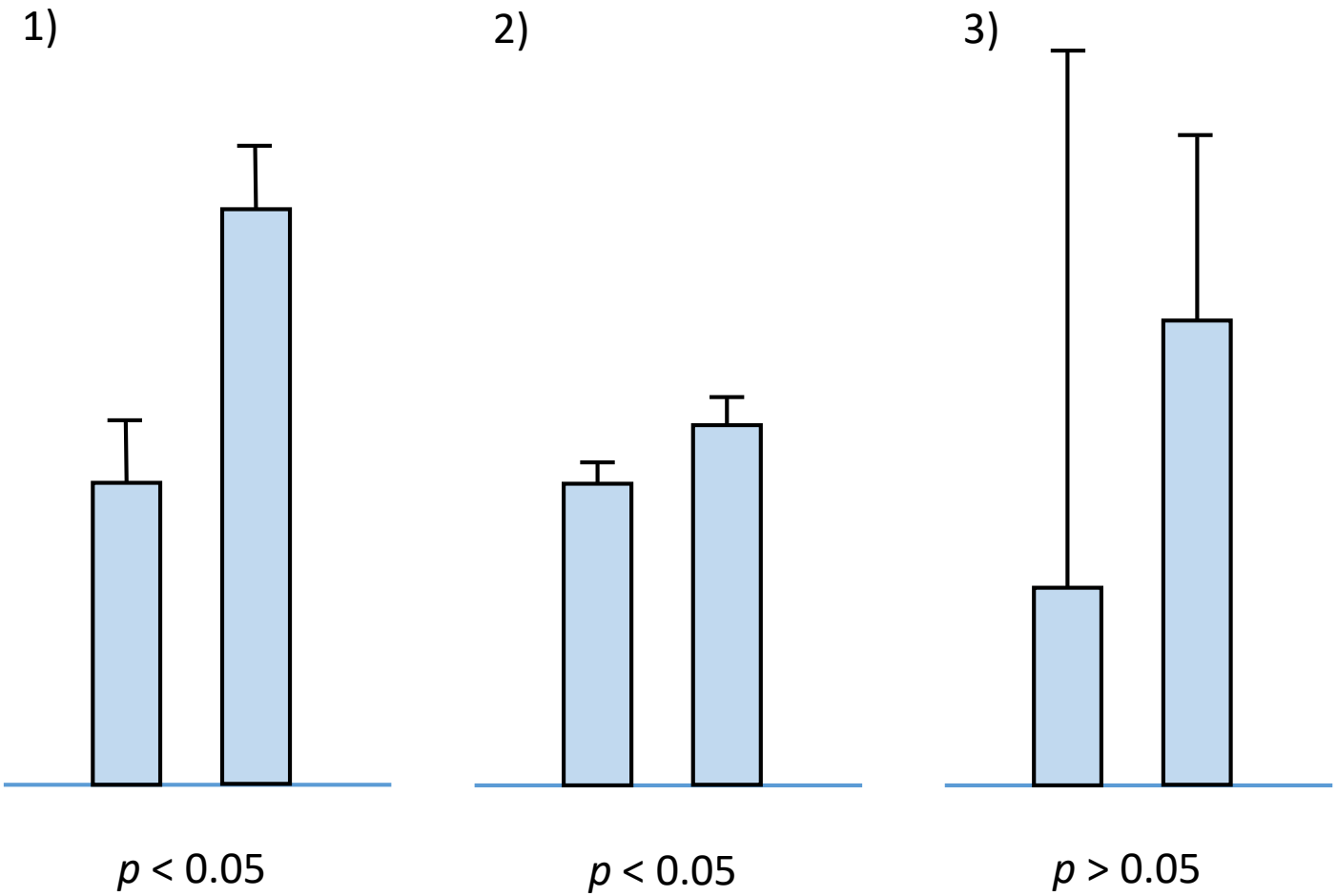


Root

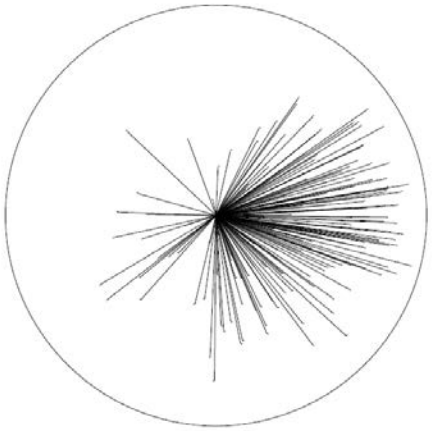


Arabidopsis

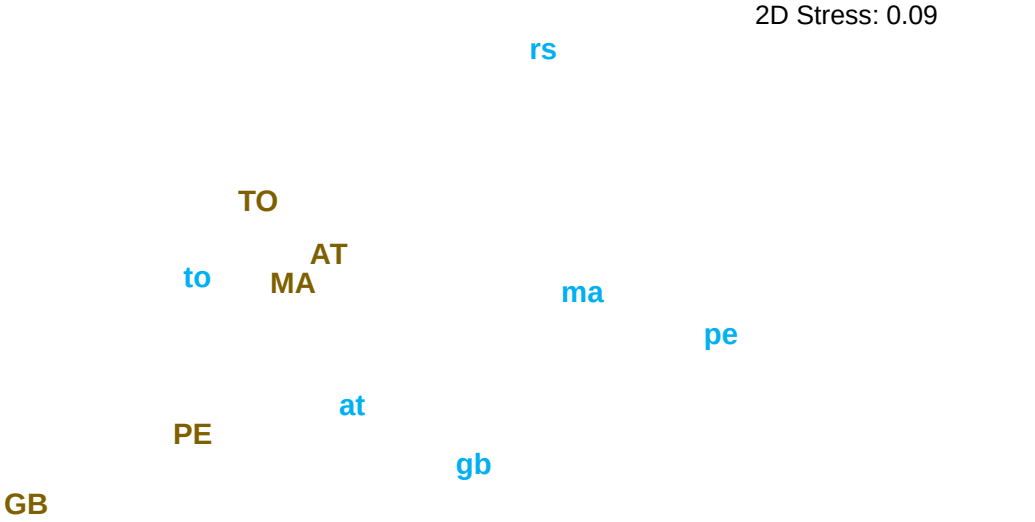
Relevance and significance



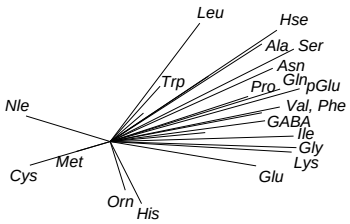
log (2) fold change, Gower quantitative similarity, multidimensional scaling



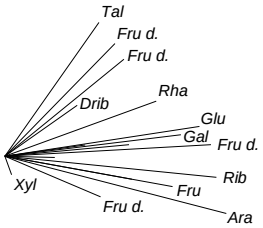
All 175 metabolites



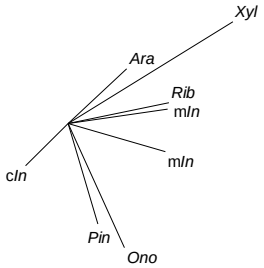
Amino acids



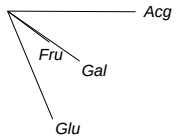
Monosaccharides



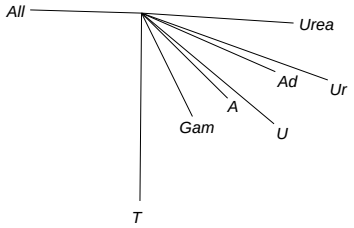
Sugar alcohols



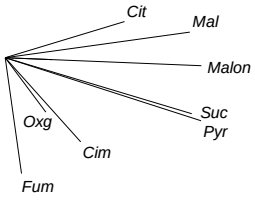
Aminosugars



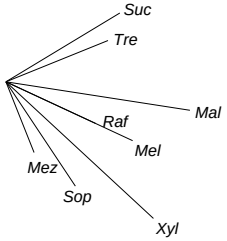
Nucleotide biosynthesis



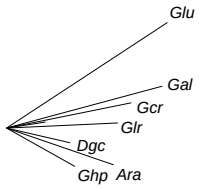
Organic acids



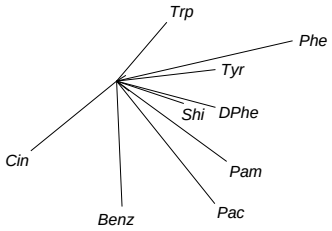
Di- and trisaccharides



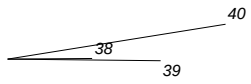
Sugar acids



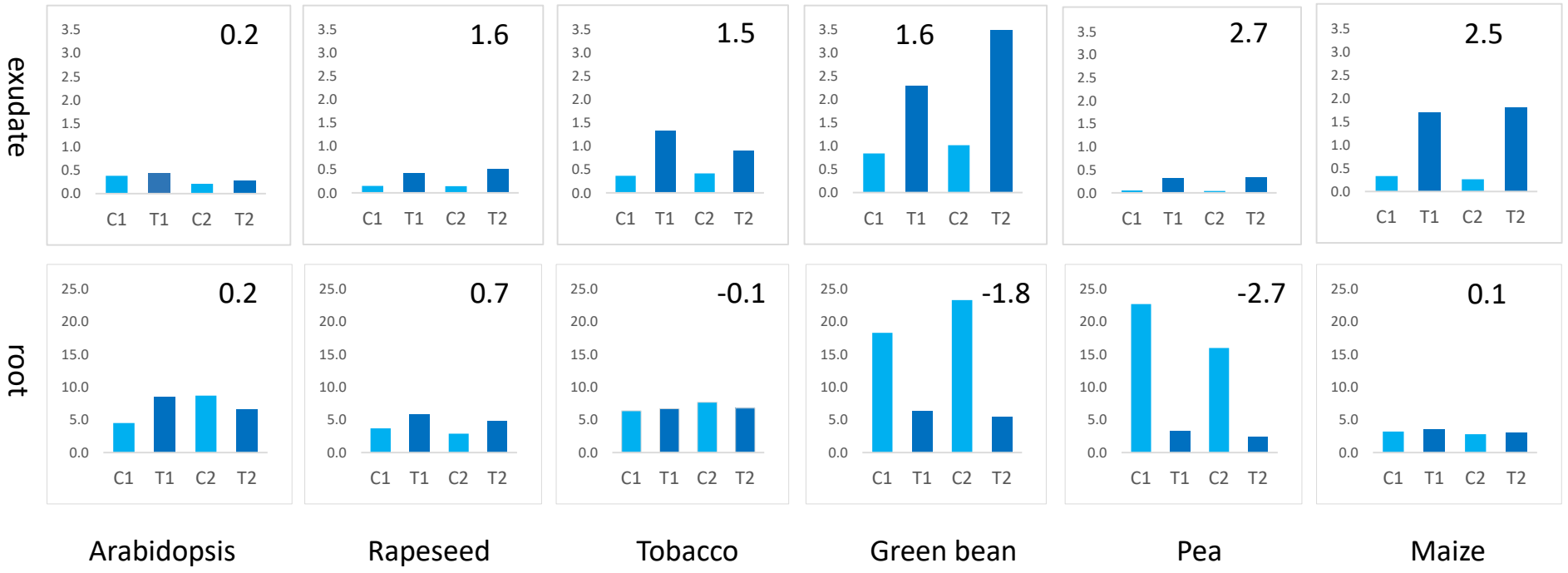
Shikimic acid pathway



Ascorbate metabolism



Fold change

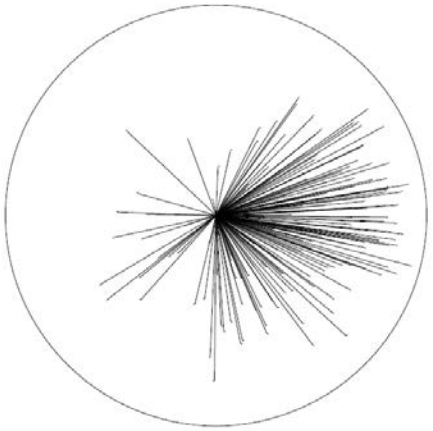


Central metabolites in root and root exudates (mg / g f.w. root)

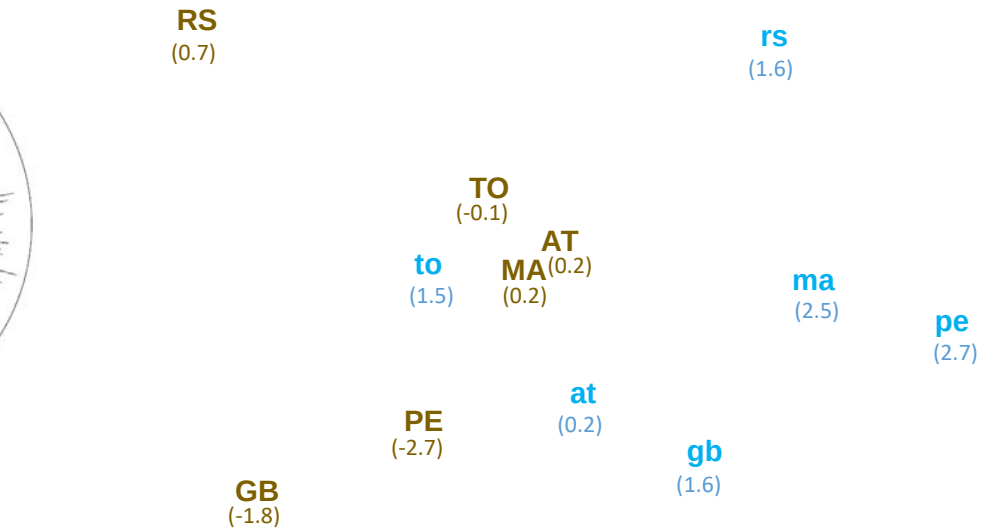
log (2) fold change, Gower quantitative similarity; multidimensional scaling;

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

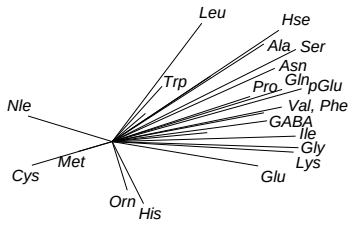
2D Stress: 0.09



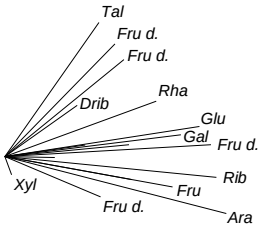
All 185 metabolites



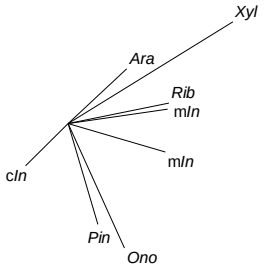
Amino acids



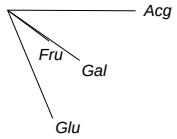
Monosaccharides



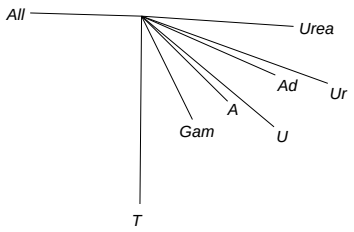
Sugar alcohols



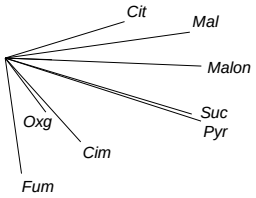
Aminosugars



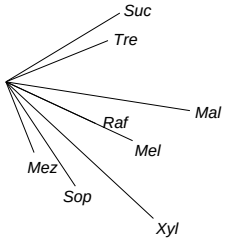
Nucleotide biosynthesis



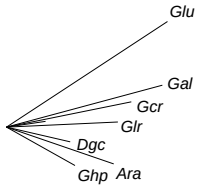
Organic acids



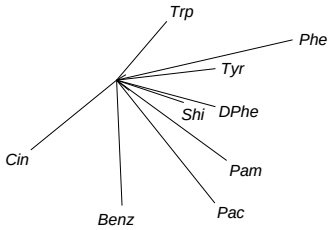
Di- and trisaccharides



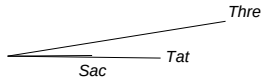
Sugar acids



Shikimic acid pathway



Ascorbate metabolism



Systemic

Chaotic

Non-linear