cosmiq - COmbining Single Masses Into Quantities

David Fischer[‡], Christian Panse[◇], and Endre Laczko[◇]

1 Introduction

cosmiq is a tool for the preprocessing of liquid- or gas-chromatography mass spectrometry (LCMS/GCMS) data with a focus on metabolomics or lipidomics applications. The Bioconductor package [?] has been developed and has shown to be effective using liquid ultra performance capillary chromatography coupled

usually done by the unexported method `xcms:::phenoDataFromPaths`.

```
R> class <- as.data.frame(c(rep("KO",6),
+           rep("WT", 6)))
R> rownames(class) <- basename(my.input.files)
R> xs@phenoData <- class
```

The *xcms* object `xs` will be used as container to keep all the data.

```
R> xs.attr <- attributes(xs)
R> xs.attr$phenoData

         c(rep("KO", 6), rep("WT", 6))
ko15.CDF                            KO
ko16.CDF                            KO
ko18.CDF                            KO
ko19.CDF                            KO
ko21.CDF                            KO
ko22.CDF                            KO
wt15.CDF                            WT
wt16.CDF                            WT
wt18.CDF                            WT
wt19.CDF                            WT
wt21.CDF                            WT
wt22.CDF                            WT
```

2.2 Combination of mass spectra

The first two processing steps search for relevant mass bins in

2.4 Generation and combination of extracted ion chromatograms

Until now only the mz information was considered. In the following processing steps, the chromatographic information will be added. For the comparison of different LCMS datasets, it is important to consider RT shifts.

bined mass spectra or EICs of all samples it is not necessary to align features between different LCMS runs as for a typical raw data processing workflow. Instead, a data matrix with intensity values for every mz/RT feature and every sample can be immediately calculated. An example can bee

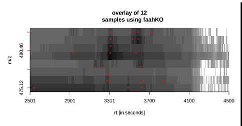

Figure 1: **A "feature map", generated by using *cosmiq*, of the *faahKO* data is shown**

	mz	mzmin	mzmax	rt	rtmin	rtmax	npeaks	ko15.CDF	ko16.CDF	ko18.CDF	ko19.CDF	ko21.CDF	ko22.CDF	wt15.CDF	wt16.CDF	wt18.CDF	wt19.CDF	wt21.CDF	wt22.CDF
13	480.12	479.62	480.62	3308.89	3269.77	3346.45	12.00	50056574.74	49188673.99	42604200.43	32851699.17	32167083.04	28232603.93	50843961.77	53491143.06	44170197.70	31030987.86	33940727.49	26817322.53
16	481.12	480.62	481.62	3308.89	3269.77	3346.45	12.00	13099238.89	12892410.39	11239240.82	8722475.72	8416403.21	7386527.17	13329889.37	13761043.95	11389325.40	8178813.42	8871975.10	7162358.69
20	482.12	481.62	482.62	3587.46	3556.16	3625.01	12.00	9236048.74	9808221.16	9208820.69	5944352.74	6643532.65	4673246.58	6213538.11	9478365.28	8806738.76	7065545.40	6784720.21	5304007.67
1	475.12	474.62	475.62	2543.63	2501.38	2620.32	12.00	5186949.19	487408.49	5335581.42	6752927.55	1041640.40	325511.86	5199329.83	390509.41	4955607.87	7390373.01	1091444.77	332135.57
14	480.12	479.62	480.62	3563.98	3517.03	3599.97	12.00	3793218.13	3609194.92	3262888.26	2278957.11	2281625.97	1919592.19	3233217.08	3710765.24	3778748.06	2791484.26	2661819.89	1700321.22
18	482.12	481.62	482.62	3308.89	3269.77	3346.45	12.00	2436222.04	2411748.96	2178509.21	1850595.04	1760884.74	1513305.56	2430863.62	2558690.87	2246852.34	1680230.77	1852048.69	1488797.21
24	483.12	482.62	483.62	3587.46	3556.16	3625.01	12.00	2453488.79	2644783.20	2465869.41	1600305.36	1788174.64	1259131.65	1710400.41	2486024.63	2350213.82	1842232.12	1838208.47	1479050.87
10	478.12	477.62	478.62	3609.36	3557.72	3659.44	12.00	1781011.37	1530799.56	2339941.43	1746024.01	2002111.10	2306808.53	2315119.37	1184549.17	2596885.26	1610089.96	2152341.25	1936846.77
19	482.12	481.62	482.62	3532.68	3507.64	3556.16	12.00	2894511.13	2223288.19	1837688.94	1028426.47	1058758.71	937052.39	2817059.31	2387335.47	1801587.69	1226877.24	1316071.33	1132986.62
3	475.12	474.62	475.62	3623.45	3582.76	3676.66	12.00	1645767.46	327646.28	2111210.41	3635674.44	313337.16	134904.64	266162.14	264337.89	1828129.46	3371455.60	300460.78	116042.21
2	475.12	474.62	475.62	3488.86	3456.00	3523.29	12.00	1365292.03	207845.48	1974452.50	2501026.19	328727.49	138709.97	1562604.41	130589.92	1736168.07	3149059.84	288418.70	106937.94
12	480.12	479.62	480.62	2931.74	2891.05	2970.86	12.00	320143.15	2244074.91	970810.56	708970.12	453703.41	265494.04	1273170.72	530927.03	1143132.91	681184.49	878490.94	459179.04
5	476.12	475.62	476.62	3632.84	3556.16	3707.96	12.00	1326705.40	223602.11	991497.73	1793404.15	408466.66	219508.80	267728.22	214672.89	953058.81	1552155.54	330294.32	199937.41
4	476.12	475.62	476.62	3277.59	3250.99	3304.20	12.00	1017097.52	566738.36	938016.24	1006652.05	322057.40	277767.96	1014075.61	530283.76	776078.79	957879.55	330335.47	261446.90
23	483.12	482.62	483.62	3532.68	3506.08	3556.16	12.00	824724.45	717630.28	501639.82	300146.18	302852.18	259151.41	789391.93	633351.60	488747.06	340751.93	363169.24	318034.35
6	476.12	475.62	476.62	3837.85	3726.74	3938.01	12.00	75128.82	981658.22	713584.23	696291.39	128107.82	119574.53	61482.87	724052.74	901890.74	621936.43	124351.98	117733.72
9	478.12	477.62	478.62	3224.39	3189.96	3260.38	12.00	593890.64	624494.43	434788.25	274664.24	264986.46	230329.59	620885.22	589401.87	411366.45	300202.21	304203.29	238878.11
8	478.12	477.62	478.62	3157.09	3125.79	3189.96	12.00	496893.92	530543.66	454704.22	300974.64	313026.09	273014.41	569016.99	492274.06	405468.26	313791.05	331575.42	267200.70
22	483.12	482.62	483.62	3307.33	3274.47	3343.32	12.00	338584.18	350909.53	309209.05	294198.03	280731.04	238100.47	354019.82	359693.84	367188.74	254850.40	287734.63	263301.99
25	483.12	482.62	483.62	3725.17	3693.87	3758.04	12.00	106202.28	1157183.66	162057.02	50980.25	50969.98	97685.46	77838.50	449676.22	185229.53	45302.75	45332.99	191087.01

Table 1: **The spreadsheet shows the top 20 most intense rows (`or der(rowSums(peaktable[,8:19]), decreasing=TRUE)`) of the `peakTable` result**

Contact: ° ETHZ|UZH, Functional Genomics Center Zurich, Winterthurerstr. 190, CH-8057 Zurich, SWITZERLAND, Phone: +41 44 635 39 12, Fax: +41 44 635 39 22, EMail: cp@fgcz.ethz.ch, URL: http://bioconductor.org/packages/cosmiq/; ‡ David Fischer, Evolva SA, Basel, SWITZERLAND.