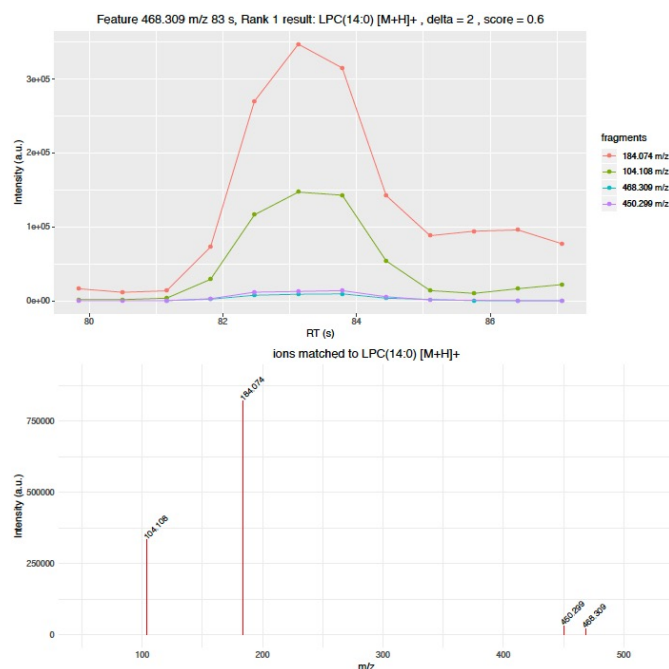# Gonçalo Graça

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Section of Bioinformatics, Department of Metabolism, Digestion and Reproduction
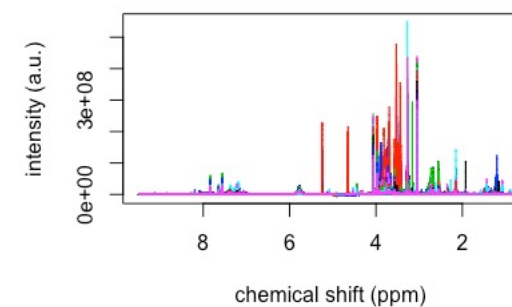
Imperial College London

## LC-MS All-ion fragmentation (AIF) annotation

MetaboAnnotatoR

1D ^{1}H-NMR automated annotation

Urine spectra
(N =132 aligned)

hmdb_name	hmdb_id	spectrum_id	matches	reference_peaks	score	rank
Hippuric acid	HMDB0000714	1494	10	21	0.45454545	1
Hippuric acid	HMDB0062583	1494	10	21	0.45454545	1
Benzoic acid	HMDB0001870	5095	5	8	0.35714286	2
m-Chlorobenzoic acid	HMDB0001544	1728	3	4	0.25000000	3
Urocanic acid	HMDB0000301	1322	2	6	0.13333333	4
Urocanic acid	HMDB0034174	1322	2	6	0.13333333	4

All-ion fragmentation (AIF, MS^E, MS/MS^{ALL}, bbCID)
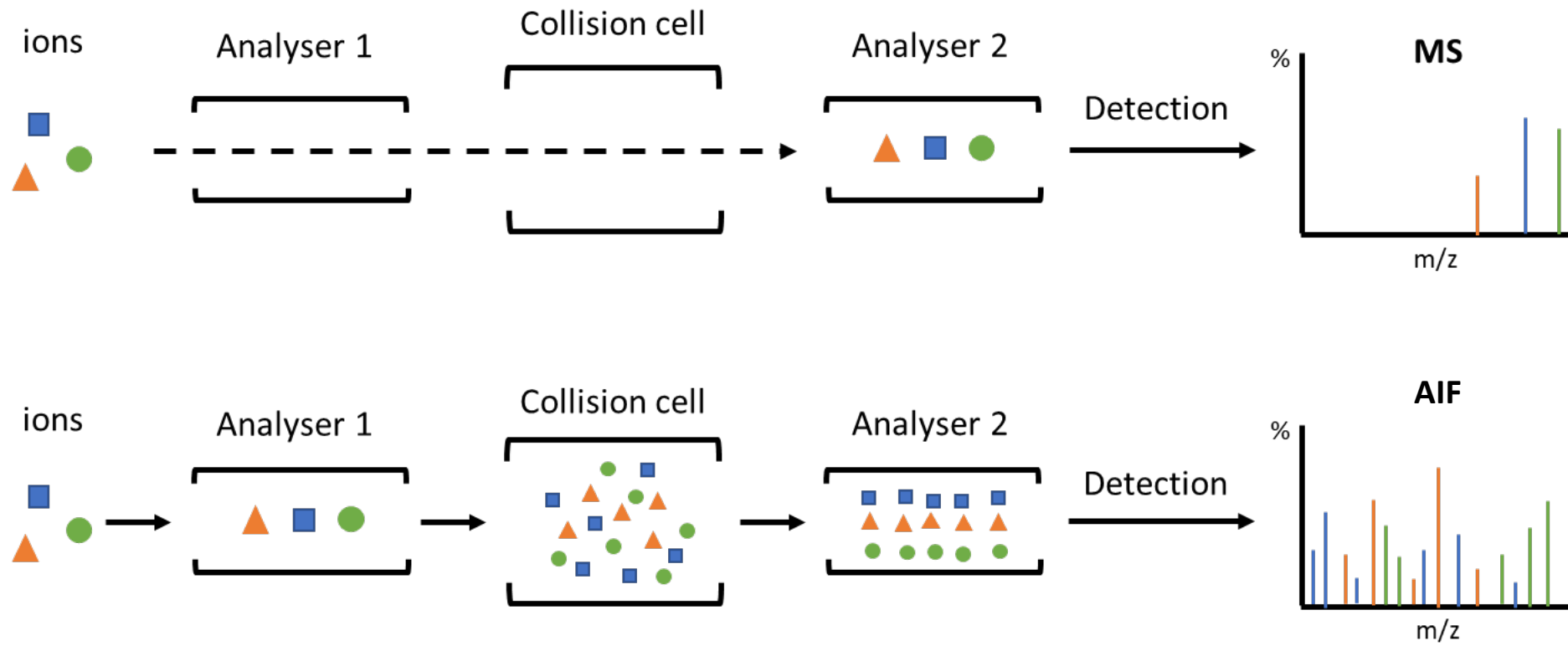
MetaboAnnotatoR
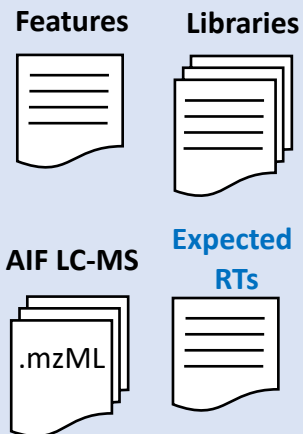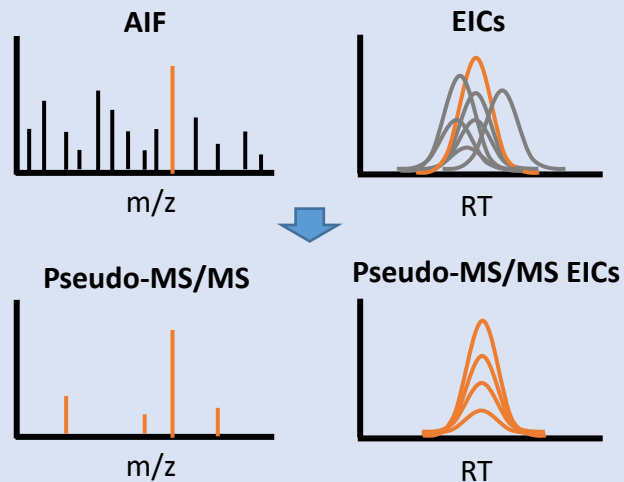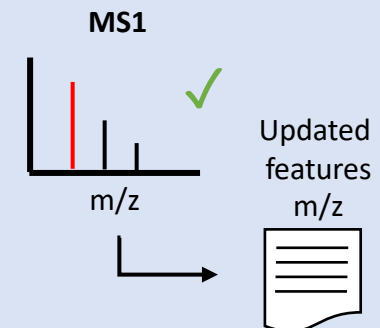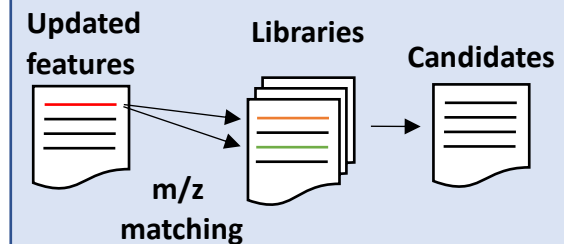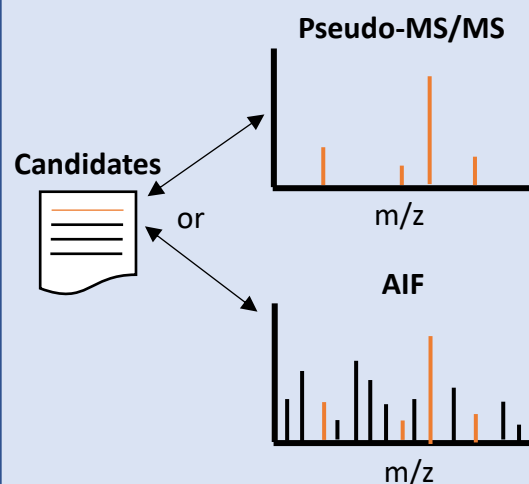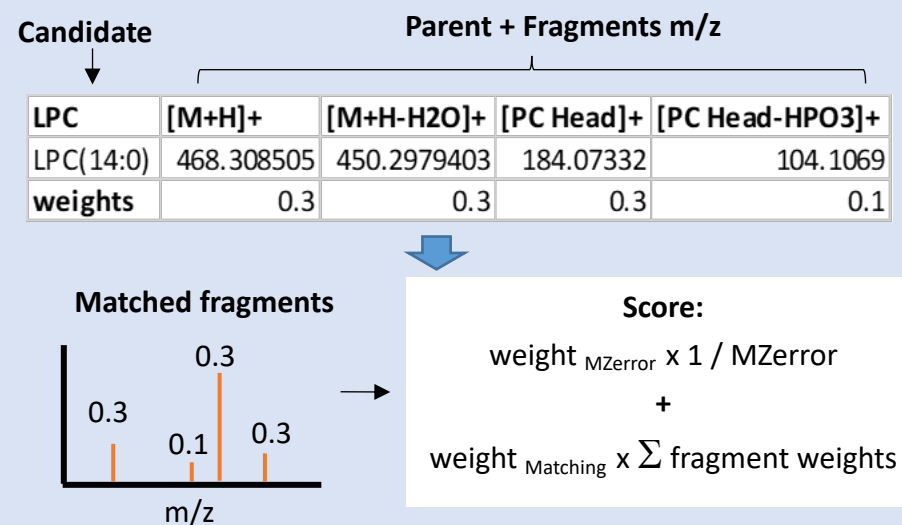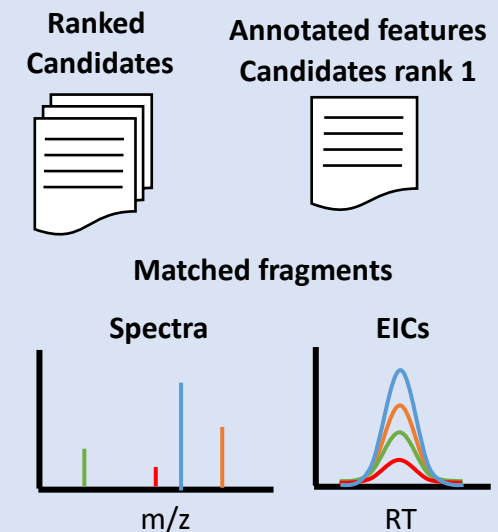
Outputs

Global result (for a list of features – rank 1 results)

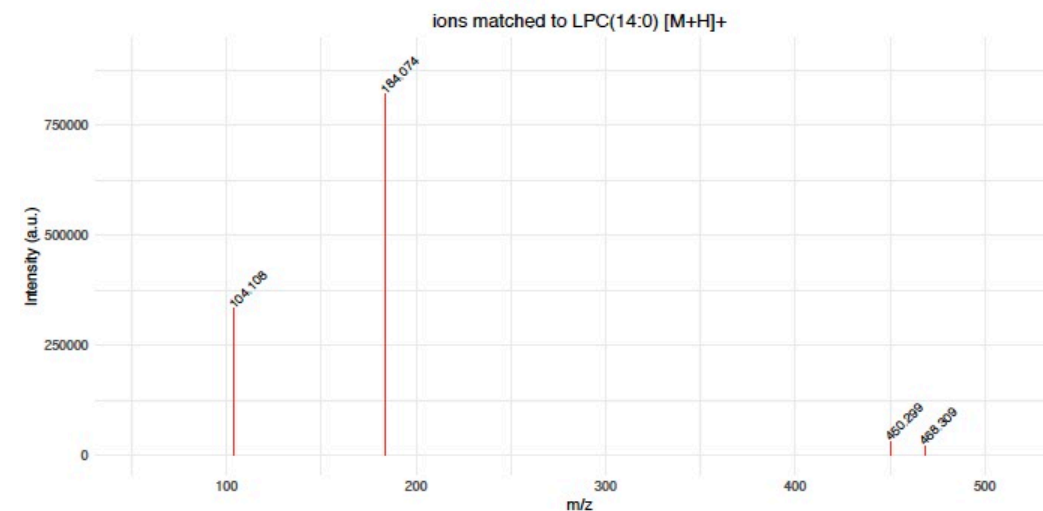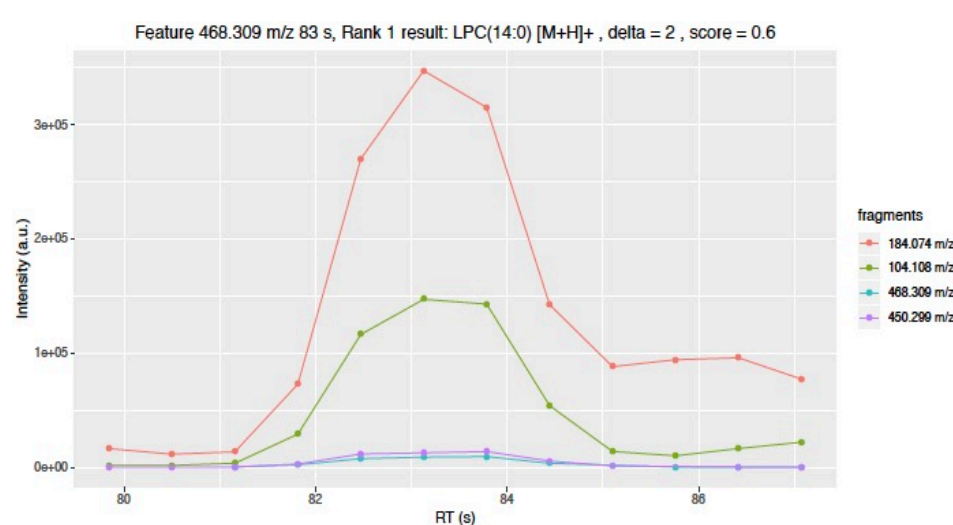| feature.mz	feature.rt	Sample.name	metabolite.annotation	feature.type	ion.type	isotope	mz.metabolite	matched.mz	mz.error	pseudoMSMS	fraction	score
490.291076	82.4720005	MESA_COMBI_BIO_P2_LP_iQC1	LPC(14:0)	parent	[M+Na]+	M+0	490.289885	490.289885	2.42957716	TRUE	2 of 6	0.43079713
468.309454	82.9200861	MESA_COMBI_BIO_P2_LP_iQC1	LPC(14:0)	parent	[M+H]+	M+0	468.308505	468.308505	2.02686491	TRUE	4 of 4	0.5966864
542.324749	82.9815002	MESA_COMBI_BIO_P2_LP_iQC1	LPC(20:5)	parent	[M+H]+	M+0	542.324155	542.324155	1.0952847	TRUE	4 of 4	0.85650231
518.32476	84.6522849	MESA_COMBI_BIO_P2_LP_iQC1	LPC(18:3)	parent	[M+H]+	M+0	518.324155	518.324155	1.16760774	TRUE	3 of 4	0.70322601
518.32476	84.6522849	MESA_COMBI_BIO_P2_LP_iQC1	LPC(18:3)	parent	[M+H]+	M+0	518.324155	518.324155	1.16760774	TRUE	3 of 4	0.70322601
568.340376	96.6959011	MESA_COMBI_BIO_P2_LP_iQC1	LPC(22:6)	parent	[M+H]+	M+0	568.339805	568.339805	1.00538344	TRUE	3 of 4	0.7223227
483.328152	97.2724273	MESA_COMBI_BIO_P2_LP_iQC1	LPC(15:0)	parent	[M+H]+	M+1	482.324155	482.324155	1.23754793	TRUE	3 of 4	0.77902475
544.340591	100.311502	MESA_COMBI_BIO_P2_LP_iQC1	LPC(20:4)	parent	[M+H]+	M+0	544.339805	544.339805	1.44358149	TRUE	4 of 4	0.59636077
502.329894	100.427526	MESA_COMBI_BIO_P2_LP_iQC1	NA	NA	NA	M+0	NA	NA	NA	TRUE	NA	NA
542.322298	100.614234	MESA_COMBI_BIO_P2_LP_iQC1	LPC(18:2)	parent	[M+Na]+	M+0	542.321185	542.321185	2.05265394	TRUE	5 of 6	0.48108709

Individual feature result

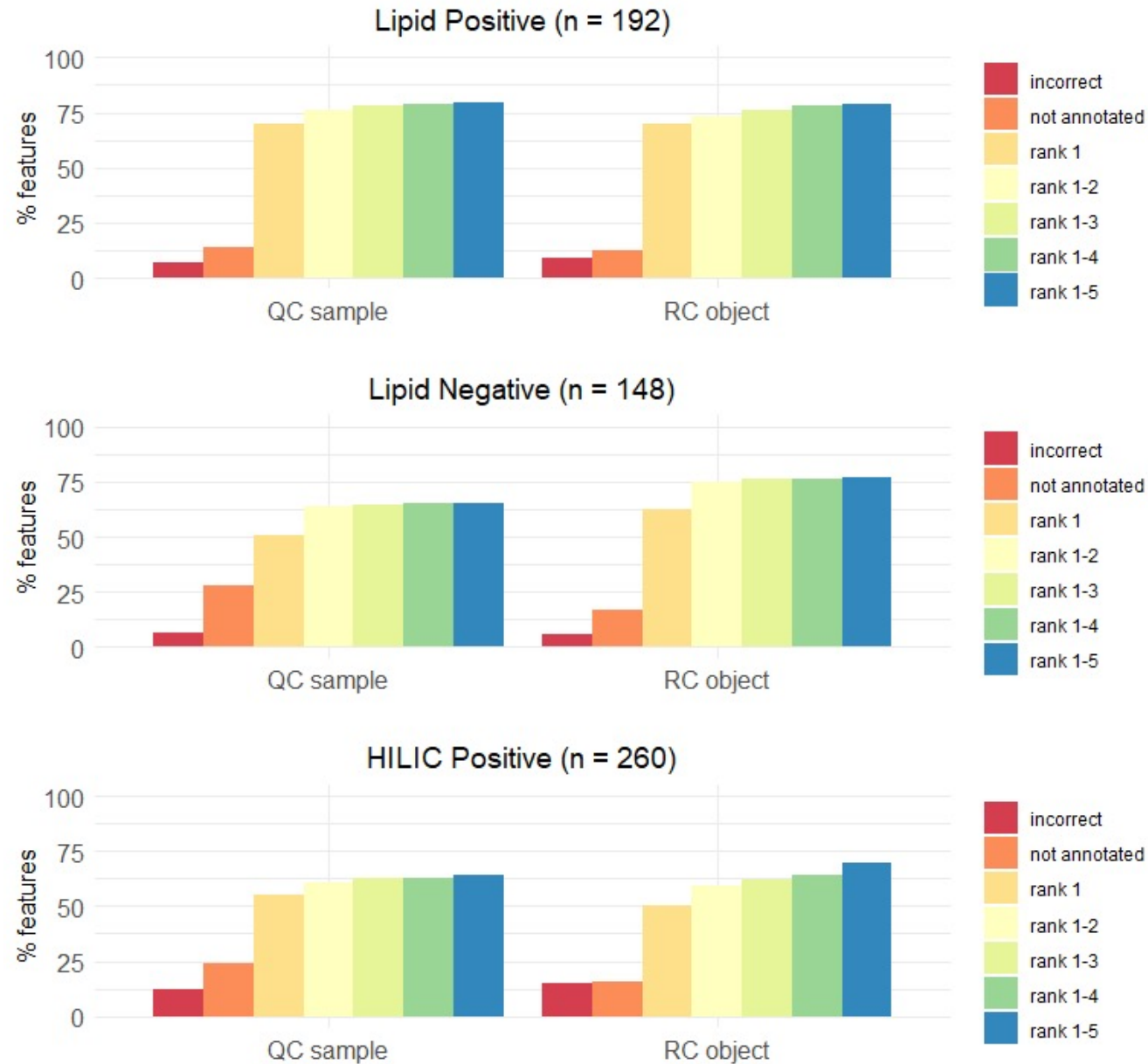| feature.mz	feature.rt	metabolite	feature.type	ion.type	isotope	mz.metabolite	matched.mz	mz.error	pseudoMSMS	fraction	score	rank
468.309454	82.9200861	LPC(14:0)	parent	[M+H]+	M+0	468.308505	468.308505	2.02686491	TRUE	4 of 4	0.5966864	1
468.309454	82.9200861	LPE(17:0)	parent	[M+H]+	M+0	468.308485	468.308485	2.06957171	TRUE	2 of 5	0.25409588	2
468.309454	82.9200861	LPE(17:0)	fragment	[M+H-H2O]+	M+0	490.289325	468.308485	2.06957171	TRUE	1 of 8	0.24576255	3

Feature 468.309 m/z 83 s, Rank 1 result: LPC(14:0) [M+H]+ , delta = 2 , score = 0.6

fragments
- 184.074 m/z
- 104.108 m/z
- 468.309 m/z
- 450.299 m/z

ions matched to LPC(14:0) [M+H]+

Results – annotation of MESA cohort dataset features
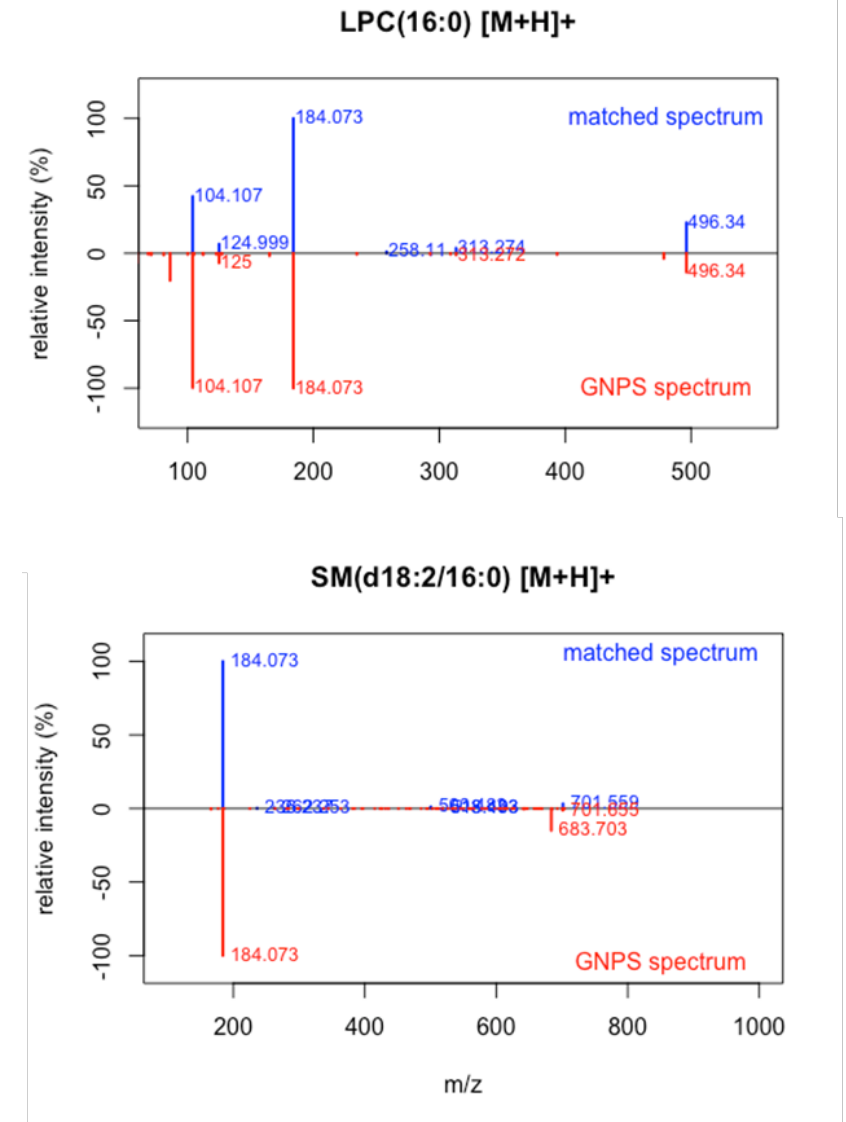
Results – annotation of MESA features from a QC sample: comparison with MS-DIAL
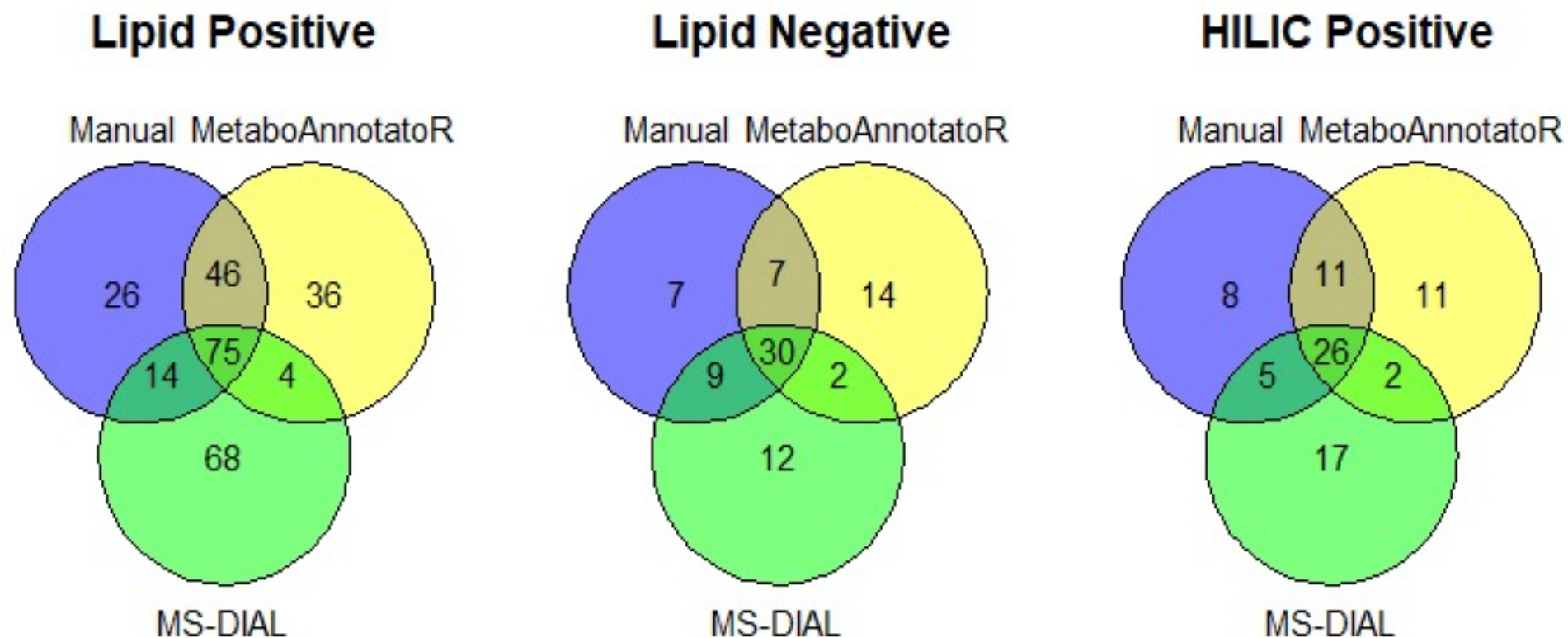
Slightly better agreement with manual annotation than MS-DIAL 4.38 (using MS2Dec).

Summary

- Workflow for "targeted" annotation of features from all-ion fragmentation LC-MS

- Based on fragment libraries rather than spectra

- Designed to assist annotation process of all types of features

- Works with mzML, netCDF or pseudo-MS/MS (RAMClustR)

- Results depend on dataset / libraries:

  - 70-75% agreement with manual annotations on human serum data (MESA) (rank 1-5)

  - HILIC adipose tissue extract: 81-91% agreement (rank 1-3)

  - Human urine data (MTBLS816) 30% agreement (rank 1-3)

- Package and libraries:

  https://github.com/gggraca/MetaboAnnotatoR (coming soon)

Imperial College London

- Timothy Ebbels
- Elizabeth Want
- Yuheng Cai
- Chung-Ho Lau
- Panos Vorkas

Wake Forest® School of Medicine

- David Herrington