Toward Global Metabolomics Analysis with Hydrophilic Interaction Liquid Chromatography-Mass Spectrometry

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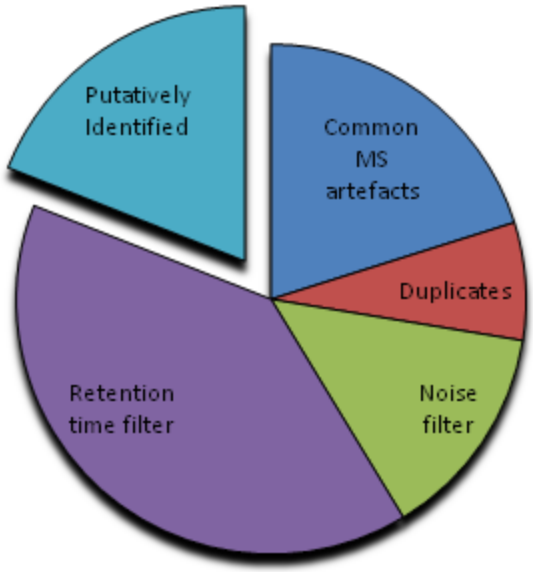
Supporting information 4: (A) Distribution of 3,133 putatively identified peaks from the mixtures of metabolite standards. 627 peaks were putatively identified; 1,314 peaks rejected based on predicted retention time; 455 were classified as noise if they had very small peaks (< 10,000) or were present in blank samples; 247 were annotated as duplicate or shoulder peaks based on mass and retention time; 667 were common MS artefacts such as isotopes, adducts and fragments (B). (B) Common related peaks observed on HILIC-Orbitrap platform for automated removal in data processing by matching the mass difference (within 3 ppm) and retention time (within 9 seconds) if the peak has a lower intensity than the base peak.

A



B

Related peak	Mass difference
^{13}C isotopes	+1.003355
^{15}N isotopes	+0.997035
^{18}O isotopes	+2.004245
^{34}S isotopes	+1.995796
^{37}Cl isotopes	+1.997050
Double charge	Mass/2
Triple charge	Mass/3
Sodium adduct	+21.98194
Potassium adduct	+37.95588
Sodium–potassium exchange	+15.97394
Sodium–ammonium exchange	–4.95540
Sodium formate adduct	+67.98740
Acetonitrile adduct	+41.02655
Acetonitrile and sodium adduct	+63.00849
Ammonium adduct	+17.02655
Water loss	–18.01057
CO_2 loss	–43.98983
Formic acid loss	–46.00548
Ammonium loss	–17.02655
Centroid/ apodisation artefact	+/– <0.9 [a]

a) Only if peak intensity >50-fold lower than the base peak