Electronic Supplementary Material (ESI) for Molecular BioSystems
This journal is © The Royal Society of Chemistry 2011

Supplementary Information

Table of Contents

This journal is © The Royal Society of Chemistry 2011

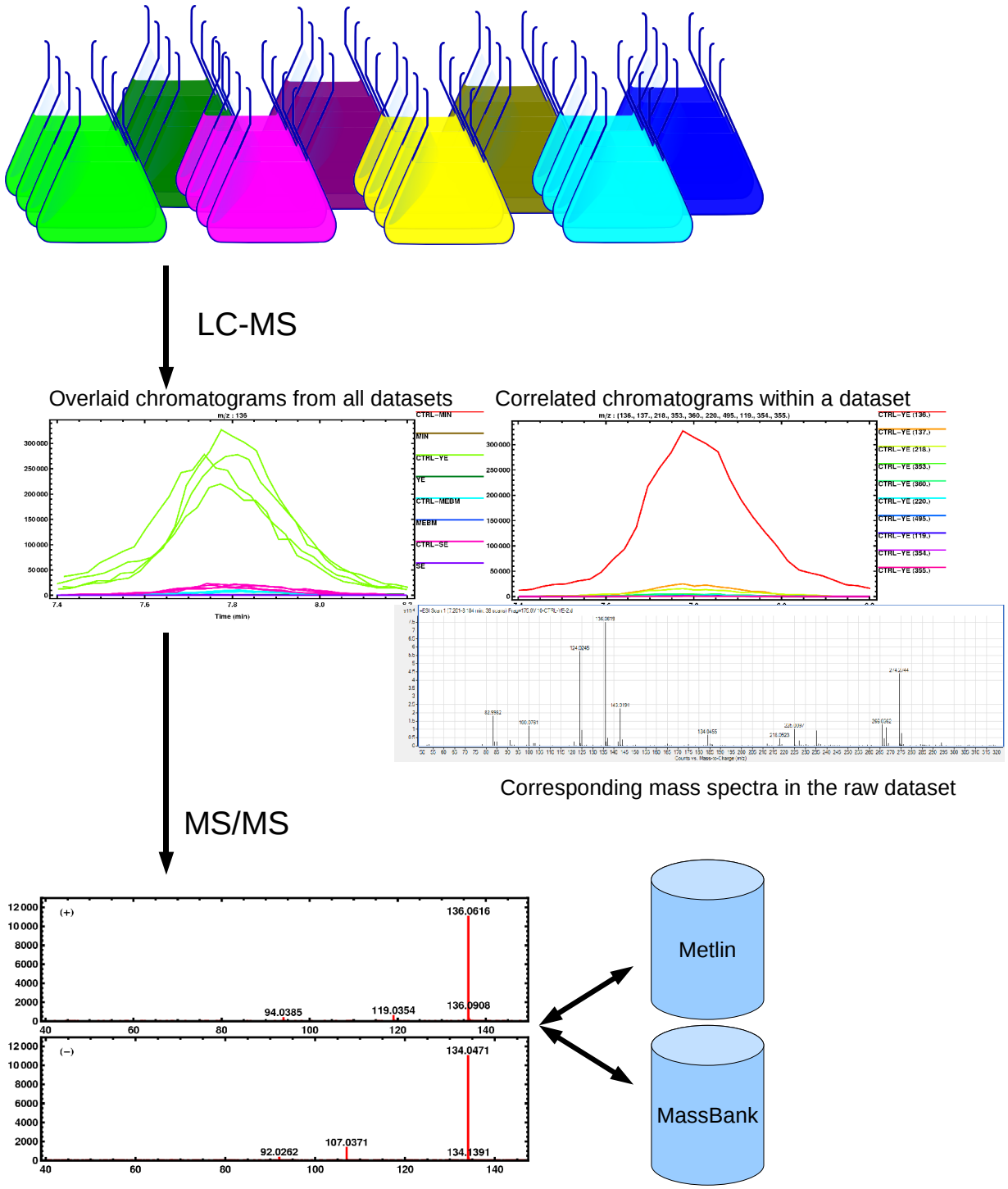
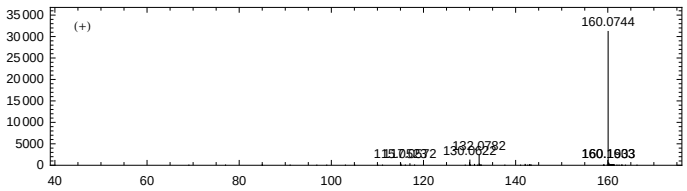


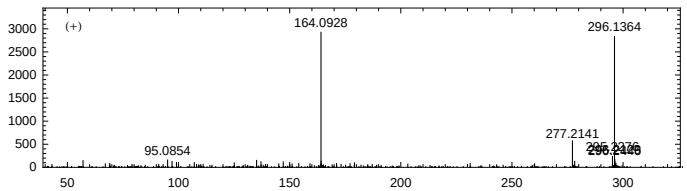
Fig. S1 Data analysis workflow for metabolic footprinting experiment (described in detail in the Materials and Methods section of the main text).

4) (Indole−3−acetaldehyde)



MassBankID: PR100147 MetlinID: 6068

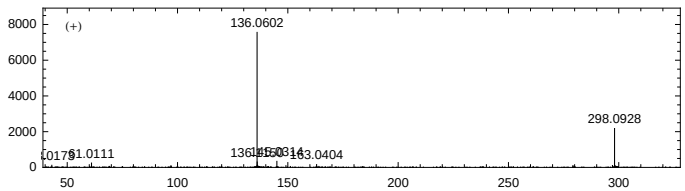
8) (Dimethyladenosine)



MassBankID: PR050718 KOX00004 KOX00787 MetlinID: 86

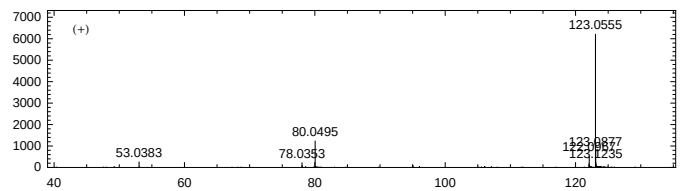
Note: same neutral loss as adenosine or methyladenosine

9) Methylthioadenosine



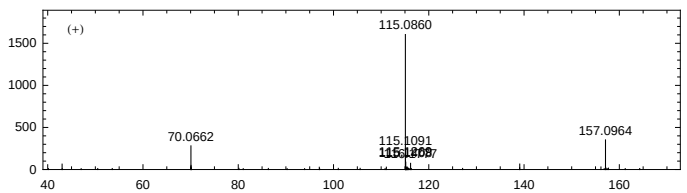
MassBankID: PR050558

11) Nicotinamide



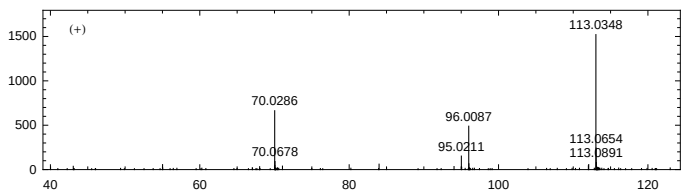
MassBankID: KOX00810

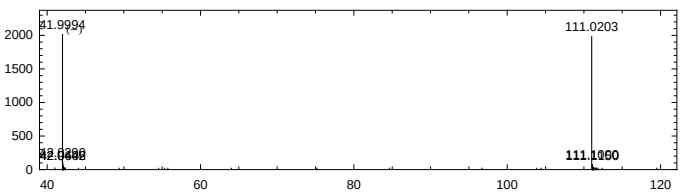
14) (N−acetylornithine −H2O)



MassBankID: KOX00024 MetlinID: 3303

17) Uracil



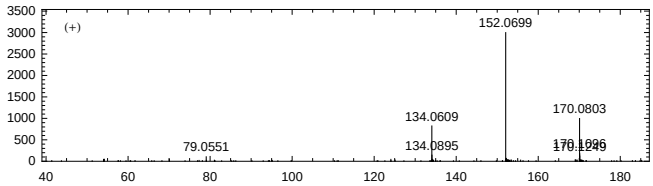


MassBankID: PR050592 PR051166 MetlinID: 258

Fig. S2 continued on the next page..

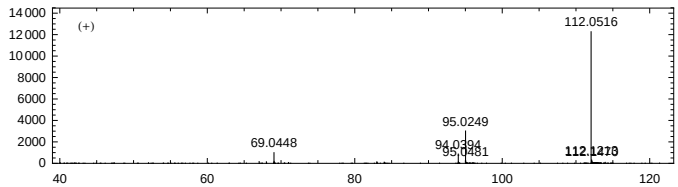
Fig. S2 continued from the previous page..

19) Pyridoxine



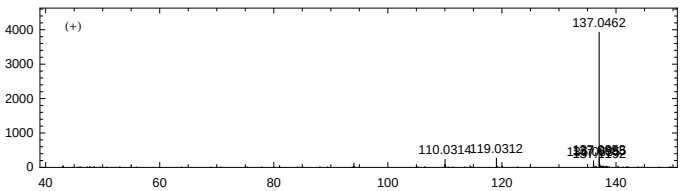
MassBankID: PR051331 MetlinID: 2202

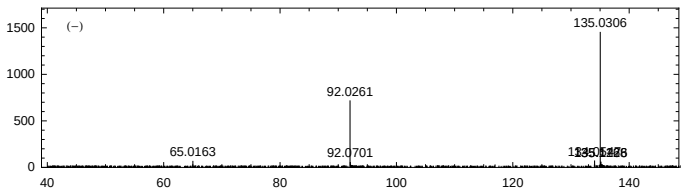
43) Cytosine



MassBankID: PR050083 MetlinID: 283

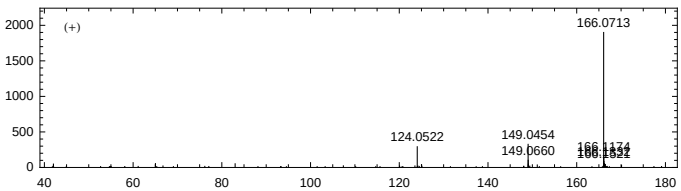
46) Hypoxanthine





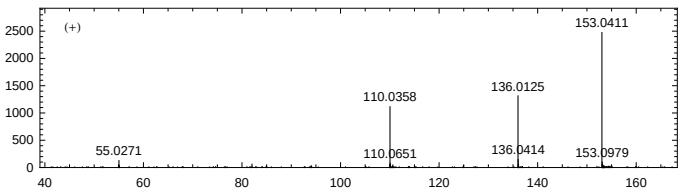
MassBankID: PR050510 KOX00315 MetlinID: 83

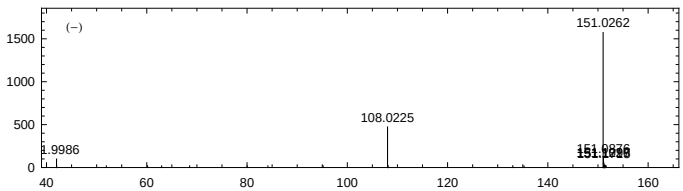
47) Methylguanine



MassBankID: KOX00429 KOX00427

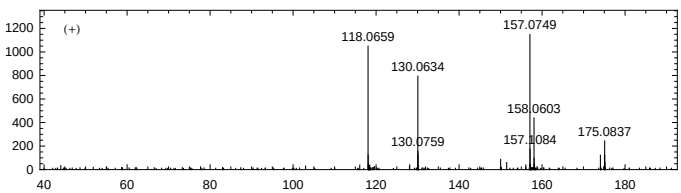
54) Xanthine

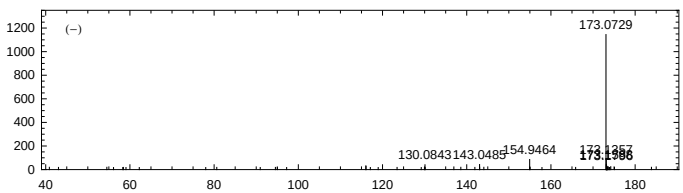




MassBankID: PR051333 MT000100 MetlinID: 82

65) (Indole−3−acetamide)





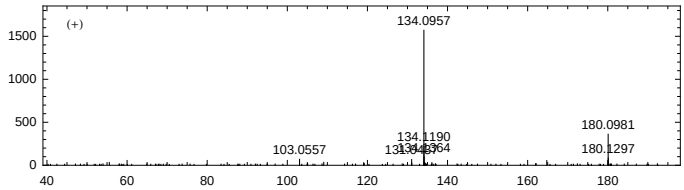
MassBankID: KOX00378 KOX00379

Note: Has 118 peak of tryptophan, amides commonly have NH3 and H2O neutral losses

Fig. S2 continued on the next page..

Fig. S2 continued from the previous page..

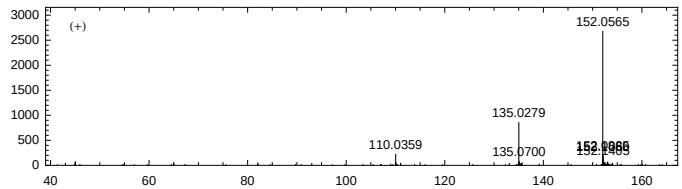
68) ((Methyl or Homo)phenylalanine)



MassBankID: PR050152 PR050524 MetlinID: 28

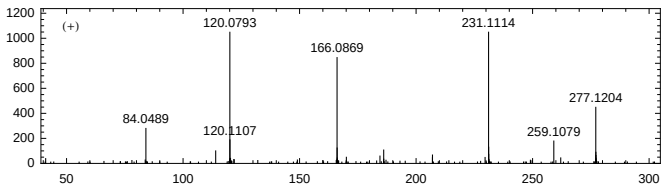
Note: Characteristic neutral loss of CO and H2O

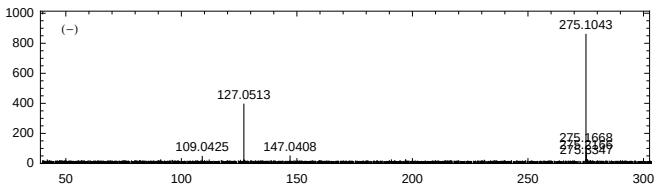
78) Guanine



MassBankID: PR050176 MetlinID: 315

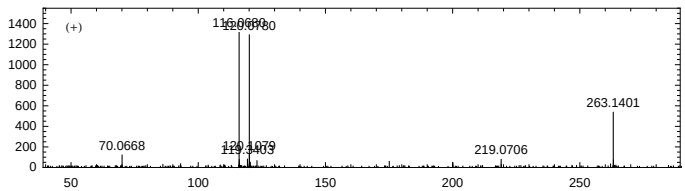
81) (C5H7NO3 + Phe −H2O)





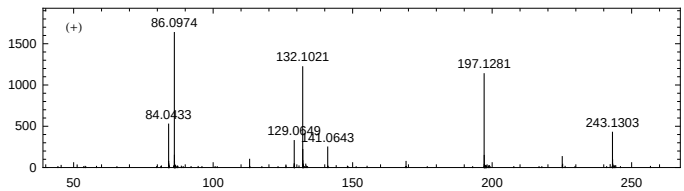
MassBankID: PR050152 PR050524 MetlinID: 28

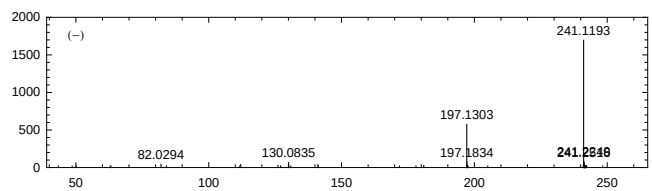
83) (Phe−Pro)



MassBankID: PR050152 PR050581 PR050524 PR050925 MetlinID: 28 29

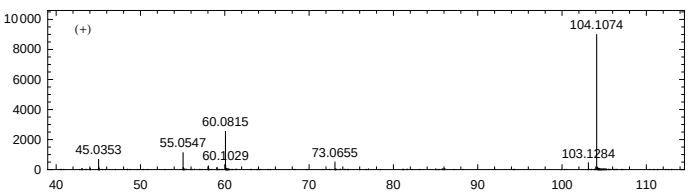
84) (C5H7NO3 + (Leu or Ile) −H2O)





MassBankID: PR050755 PR051168 PR051294 PR050276 MetlinID: 24 23

86) Choline

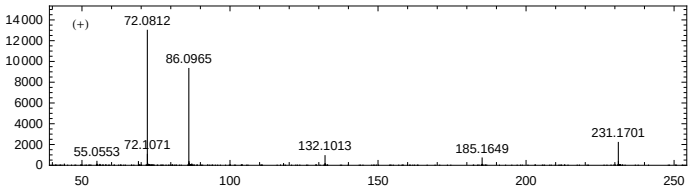


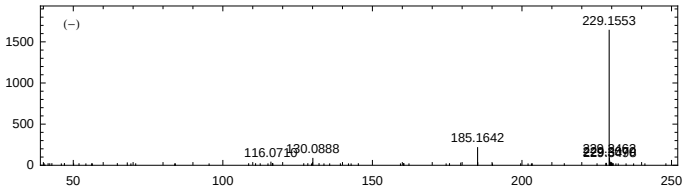
MassBankID: PR100404 MetlinID: 56

Fig. S2 continued on the next page..

Fig. S2 continued from the previous page..

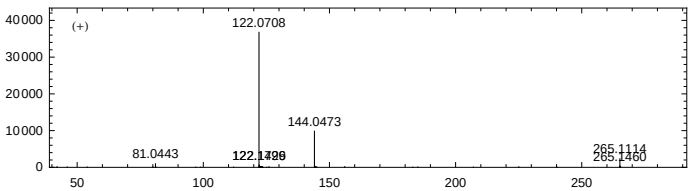
89) (Val–(Leu or Ile))





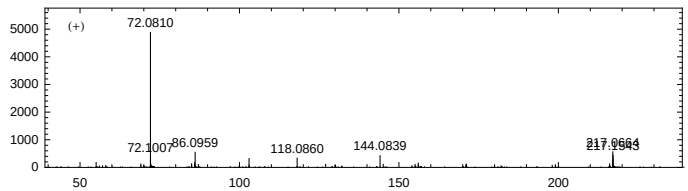
MassBankID: PR050549 PR050755 PR051168 PR051227 PR051294 PR050276 MetlinID: 35 24 23

90) Thiamine



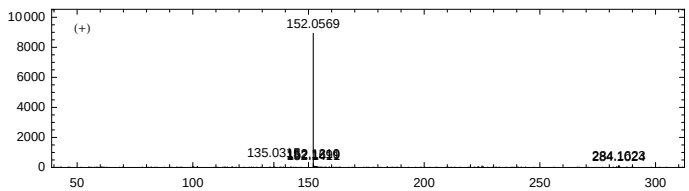
MassBankID: KOX00605 KOX00606 MetlinID: 229

98) (Val–Val)



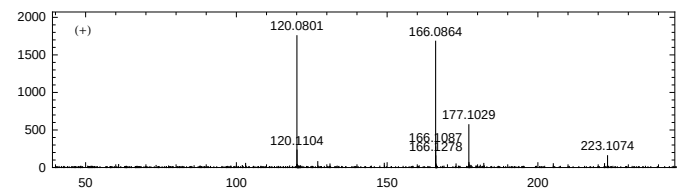
MassBankID: PR050549 PR051227 MetlinID: 35

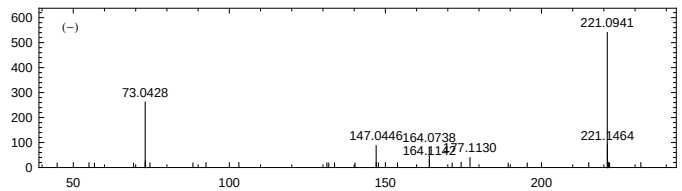
103) Guanosine



MassBankID: KOX00266 MetlinID: 87

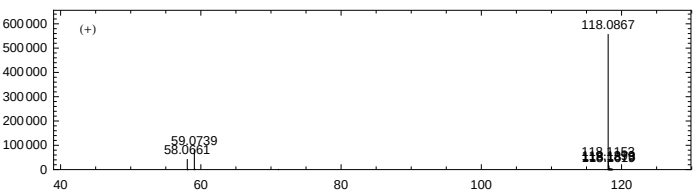
120) Gly–Phe





MassBankID: MT000058 MetlinID: 23966

126) Betaine

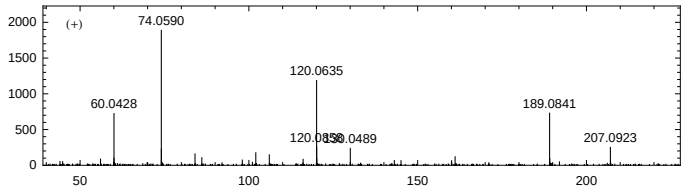


MassBankID: KOX00681 MetlinID: 287

Fig. S2 continued on the next page..

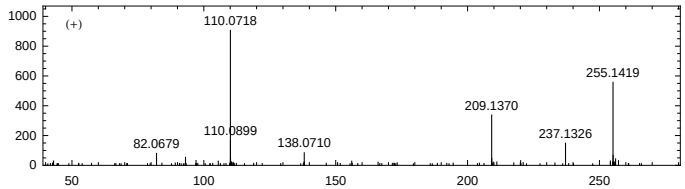
Fig. S2 continued from the previous page..

142) Thr−Ser



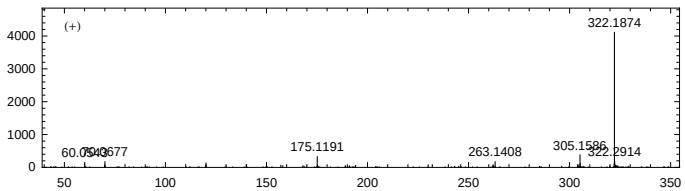
MetlinID: 23808

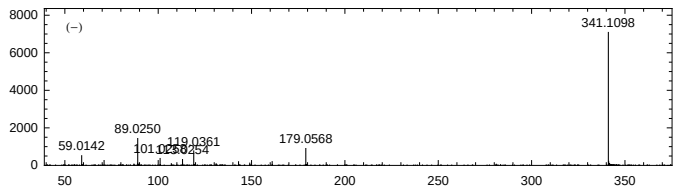
144) His−Val



MetlinID: 23773

147) (Phe−Arg)

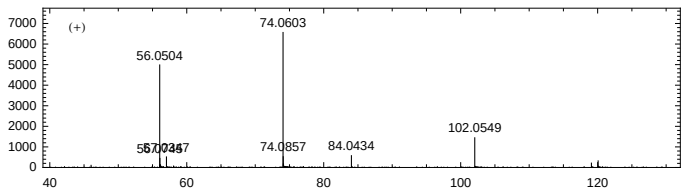




MassBankID: PR050169 PR050046 MetlinID: 13

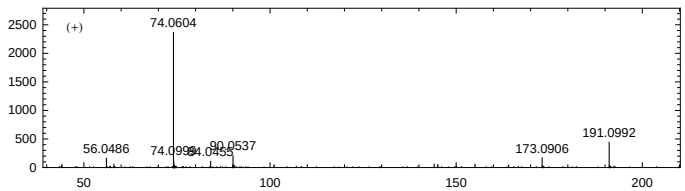
Note: Arginine peaks 60,70,175 in (+)

149) Threonine



MassBankID: PR051013 PR051004 MetlinID: 32

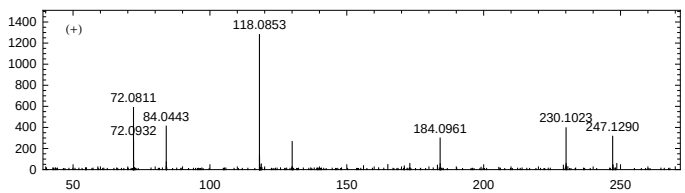
150) Thr−Ala

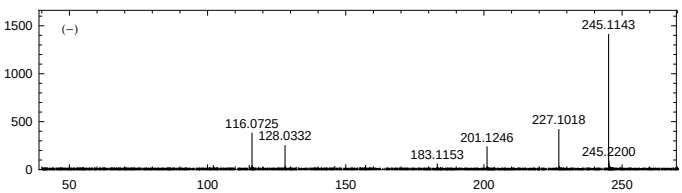


MetlinID: 23982

Note: 56 −C3H5N; 74 −C3H7NO;

158) Val−Glu



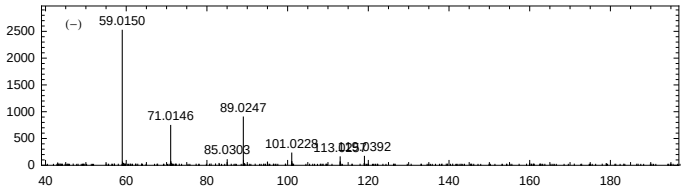


Note: Neutral loss of CO2 indicates Glu on C−terminus (Harrison, 2004)

Fig. S2 continued on the next page..

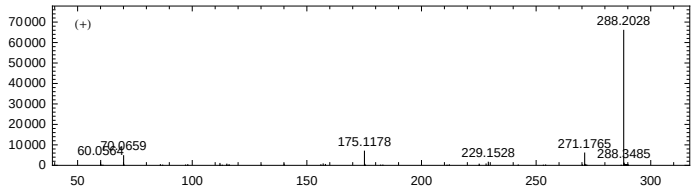
Fig. S2 continued from the previous page..

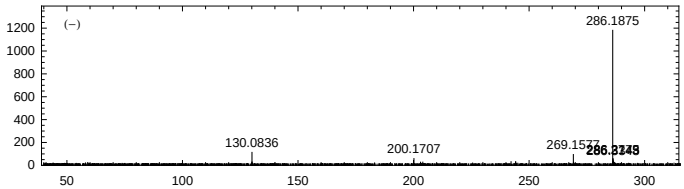
162) Glucose



MassBankID: PR050985 MetlinID: 133

166) ((Leu or Ile)−Arg)

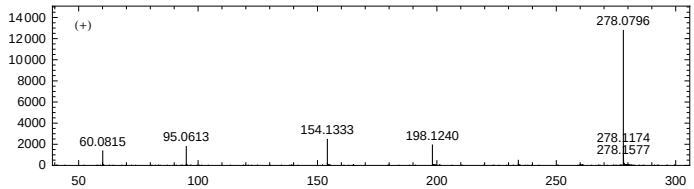




MassBankID: PR100496 KOX00390 PR050169 PR050276 KOX00391 PR050046 MetlinID: 23 24 13

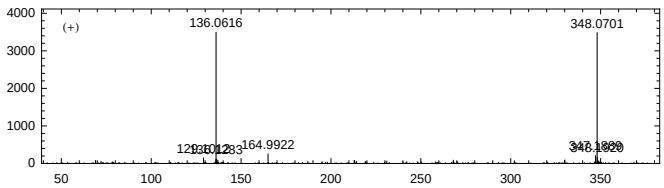
Note: Arginine peaks 60,70,158,175; Leu/Ile fragment 86 in (+) Leu/Ile peak 130 in (−)

169) (Histidine betaine sulfonic acid)



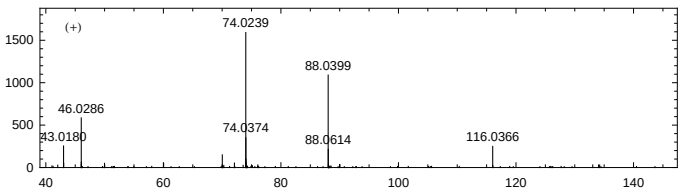
Note: 60 −C3H9N; 95 −C5H6N2; 154 −C8H15N3; 198 −C9H15N3O2;

171) AMP



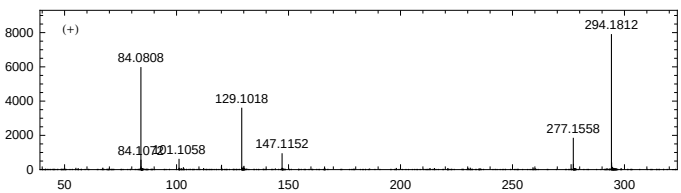
MassBankID: PR100515 PR100064 MetlinID: 34 478

172) Aspartate



MassBankID: PR051379 PR050025 MetlinID: 15

173) (Phe−Lys)

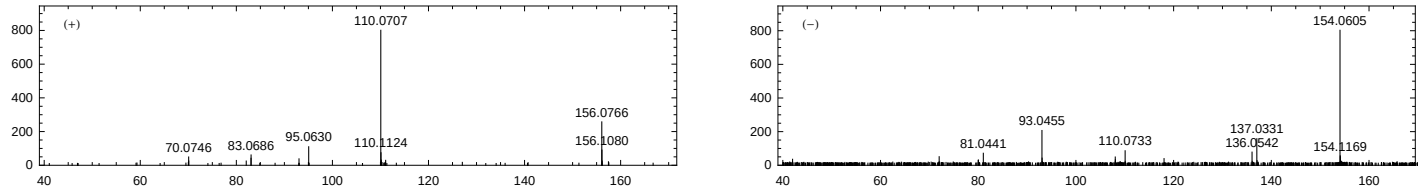


Note: Lysine peaks 84,129(Lys−H2O),147 (+)

Fig. S2 continued on the next page..

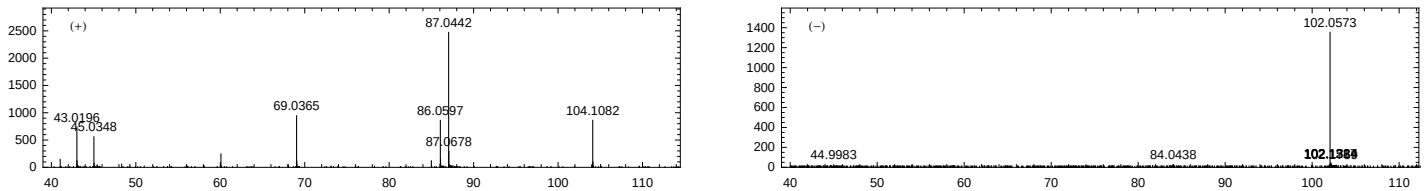
Fig. S2 continued from the previous page..

176) Histidine



MassBankID: PR050393 PR050440 MetlinID: 21

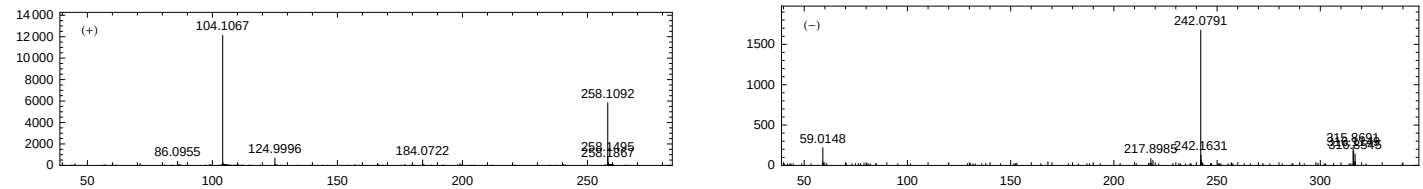
177) (4−aminobutyric acid)



MassBankID: KOX00001 KOX00002 PR100387 PR100331 KOX00039 KOX00113 MetlinID: 279

Note: isomers have different spectra in MassBank

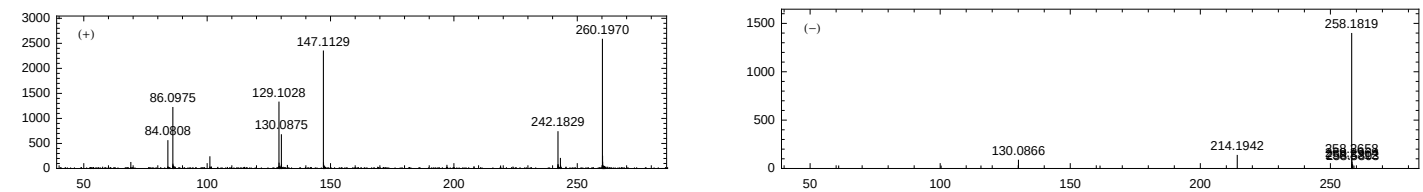
178) Glycerophosphocholine



MassBankID: KOX00741 MetlinID: 370

Note: 316 −acetate adduct in (−)

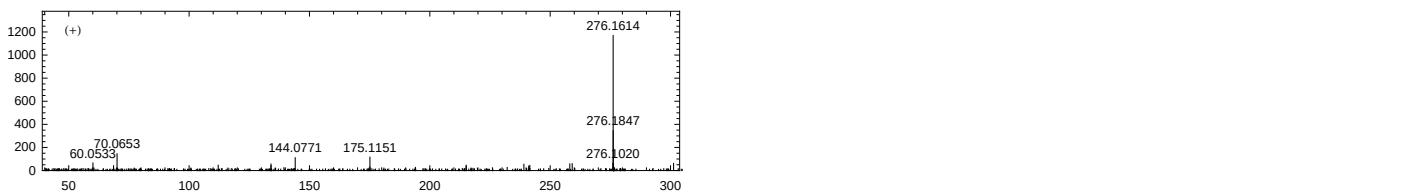
181) ((Leu or Ile)−Lys)



MassBankID: PR100496 KOX00390 PR050420 PR050276 KOX00391 PR050279 MetlinID: 23 24 25

Note: Lysine peaks 84,130,147; Leu/Ile fragment 86 in (+) Leu/Ile peak 130 in (−)

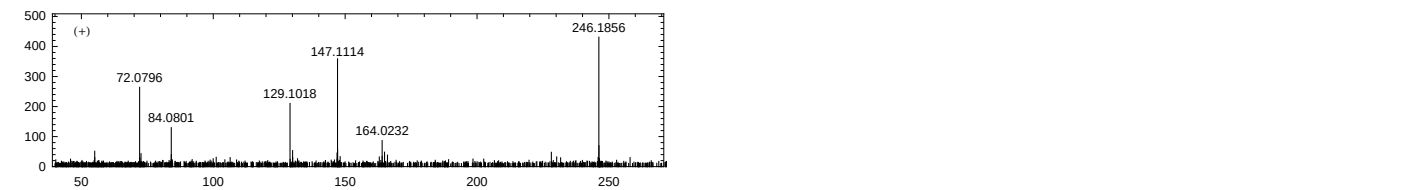
183) (C4H9NO3+Arg−H2O)



MassBankID: PR050169 PR050046 MetlinID: 13

Note: Arginine peaks 60,70,175 in (+)

184) (Val−Lys)



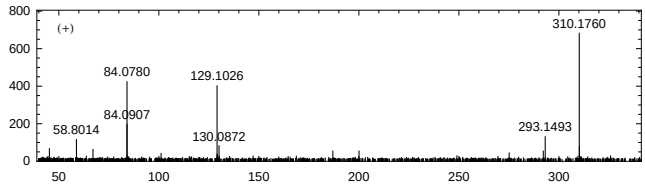
MassBankID: PR051227 PR050279 MetlinID: 35 25

Note: Lysine peaks 84,130,147; Val peak 72 in (+)

Fig. S2 continued on the next page..

Fig. S2 continued from the previous page..

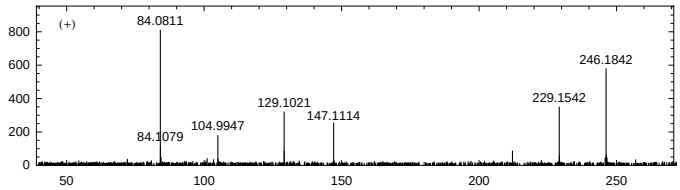
185) (Tyr−Lys)



MassBankID: PR050420 PR050279 MetlinID: 25

Note: Lysine peaks 84,130,147 (+)

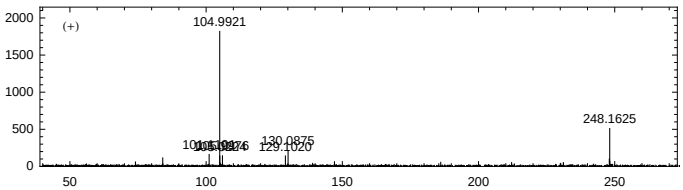
186) (C5H11NO2+Lys−H2O)



MassBankID: PR050420 PR050279 MetlinID: 25

Note: Lysine peaks 84,130,147 (+)

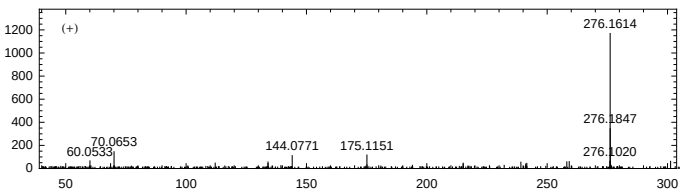
187) (C4H9NO3+Lys−H2O)



MassBankID: PR050420 PR050279 MetlinID: 25

Note: Lysine peaks 84,130,147 (+)

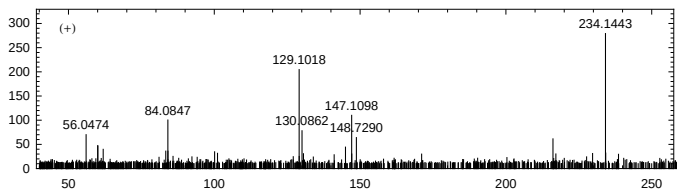
189) (C4H9NO3+Arg−H2O)



MassBankID: PR050169 PR050046 MetlinID: 13

Note: Arginine peaks 60,70,175 in (+)

190) (Ser−Lys)



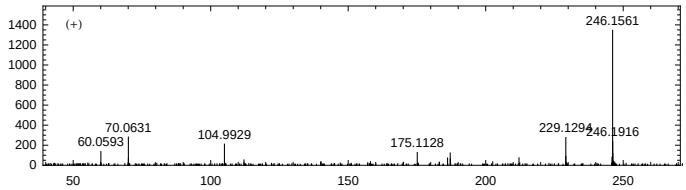
MassBankID: PR050420 PR050279 MetlinID: 25

Note: Lysine peaks 84&130 in (+)

Fig. S2 continued on the next page..

Fig. S2 continued from the previous page..

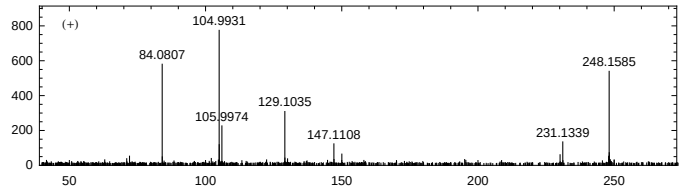
191) ((Ala or beta−Ala or Sarcosine)−Arg)



MassBankID: PR050169 PR050046 MetlinID: 13

Note: Arginine peaks 60,70,175 in (+)

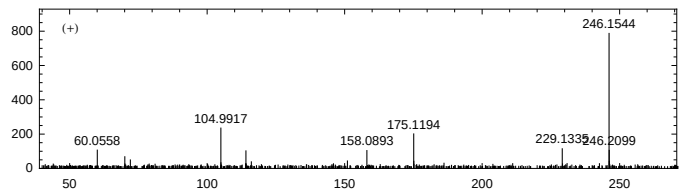
192) (C4H9NO3+Lys−H2O)



MassBankID: PR050420 PR050279 MetlinID: 25

Note: Lysine peaks 84,129(Lys−H2O),147 (+)

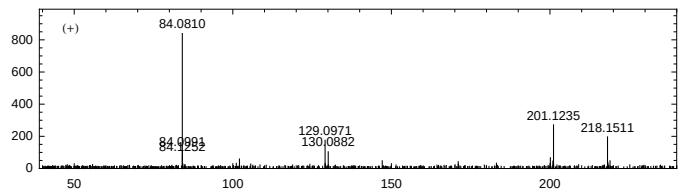
193) ((Ala or beta−Ala or Sarcosine)−Arg)

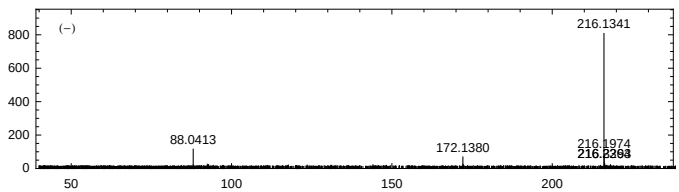


MassBankID: PR050169 PR050046 MetlinID: 13

Note: Arginine peaks 60,70,158,175

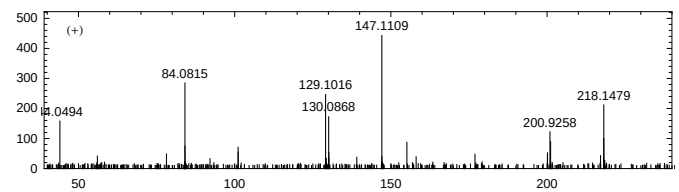
194) (C3H7NO2+Lys−H2O)





Note: Lysine peaks 84&130 in (+) & 145 in (−); no 44 peak of Ala or Sarcosine and no 72 of beta−Ala in (+)

196) ((Ala or Sarcosine)−Lys)



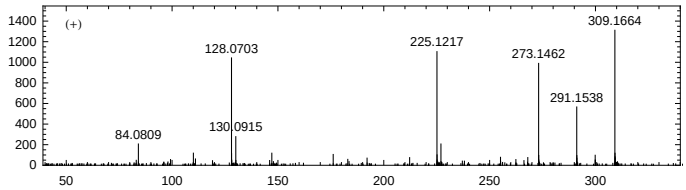
MassBankID: KOX00009 PR050714 PR050420 KOX00010 PR050054 PR050279 MetlinID: 11 51 25

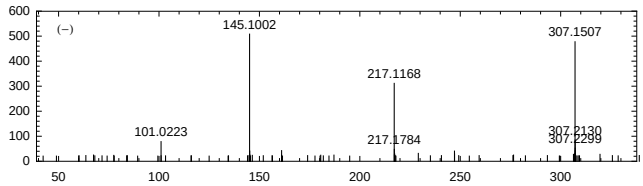
Note: Lysine peaks 84&130 in (+) & 145 in (−); Ala or Sarcosine 44 peak in (+)

Fig. S2 continued on the next page..

Fig. S2 continued from the previous page..

198) (Hexose–Lys)

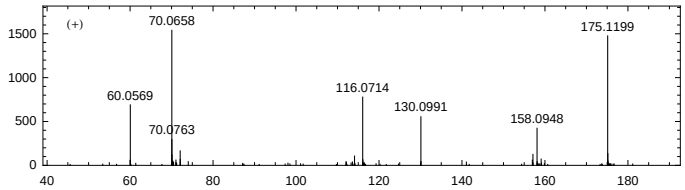


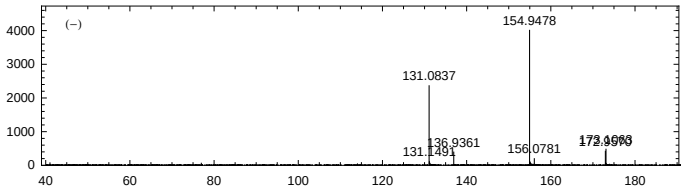


MassBankID: PR050420 PR050279 MetlinID: 25

Note: Lysine peaks 84&130 in (+) & 145 in (–)

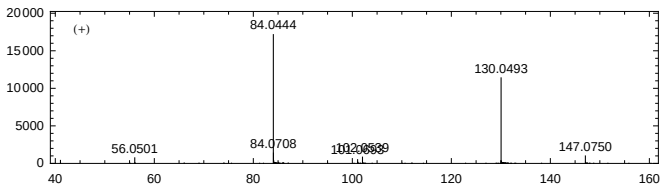
201) Arginine





MassBankID: PR050169 PR050046 MetlinID: 13

202) Lysine



MassBankID: PR050420 PR050279 MetlinID: 25

Fig. S2 Positive mode (+) and negative mode (-) MS/MS spectra (collision energy 10 V) of metabolites identified in this study along with identifiers of corresponding MS/MS spectra of standards or related compounds in mass spectral databases Metlin and MassBank. MS/MS spectra are numbered according to Table S1.

This journal is © The Royal Society of Chemistry 2011

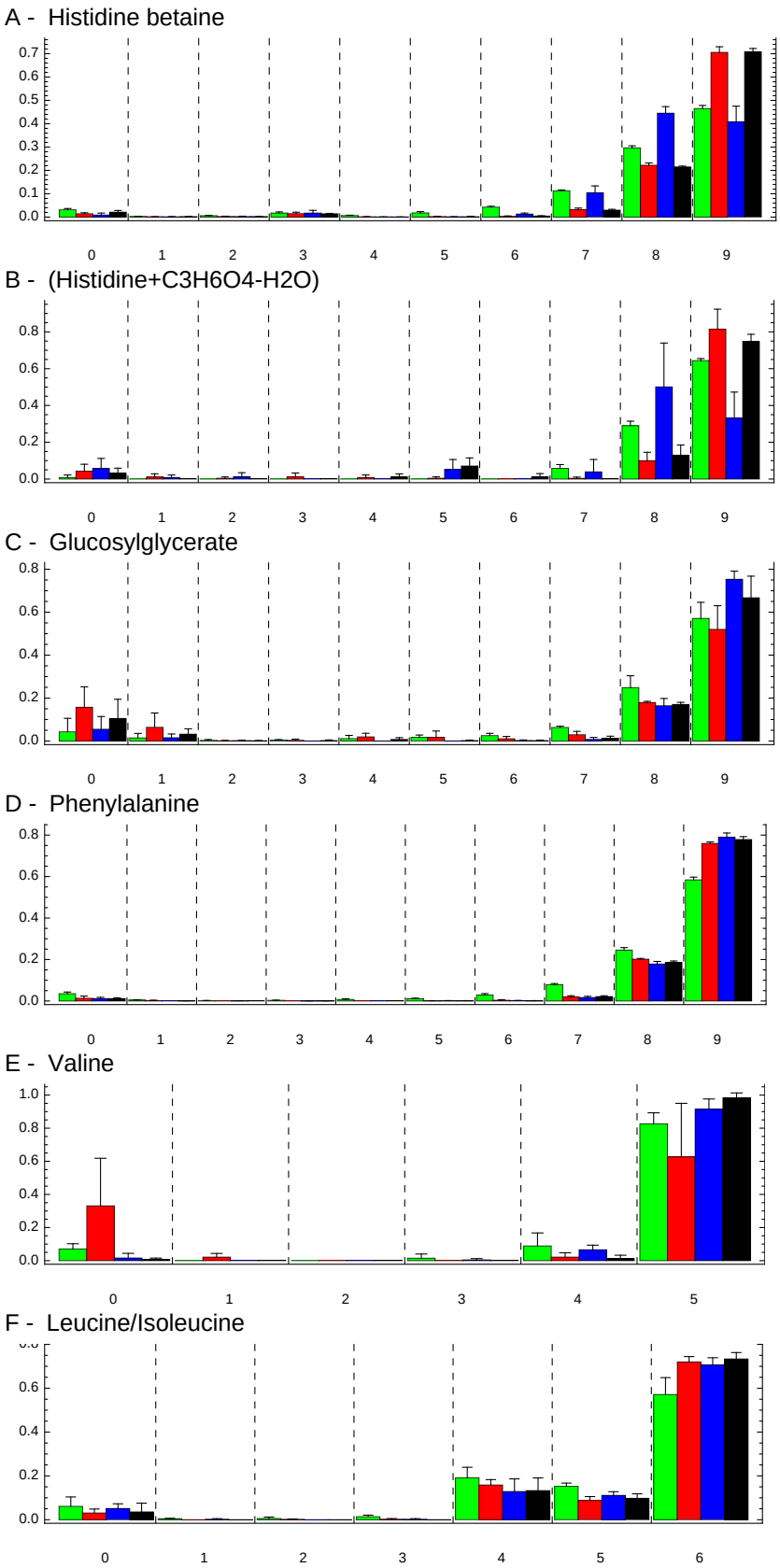


Fig. S3 Relative intensities of mass spectral peaks of selected metabolites containing different numbers of a ^{13}C stable isotope (shown below the abscissa). Intensities were normalized to the sum of intensities of all isotopomers. Intermediate numbers of incorporated ^{13}C isotopes for compounds containing larger number of carbons are not shown for clarity. Cells were grown in media containing [^{13}C]NaHCO3 as the carbon source (black) supplemented with unlabeled [^{12}C]adenine (blue), [^{12}C]glutamate (red), or [^{12}C]SE (green). Shifts towards higher peaks with a smaller number of ^{13}C isotopes show incorporation of carbons from unlabeled metabolites. Figure 4 shows this comparison for additional metabolites.

This journal is © The Royal Society of Chemistry 2011

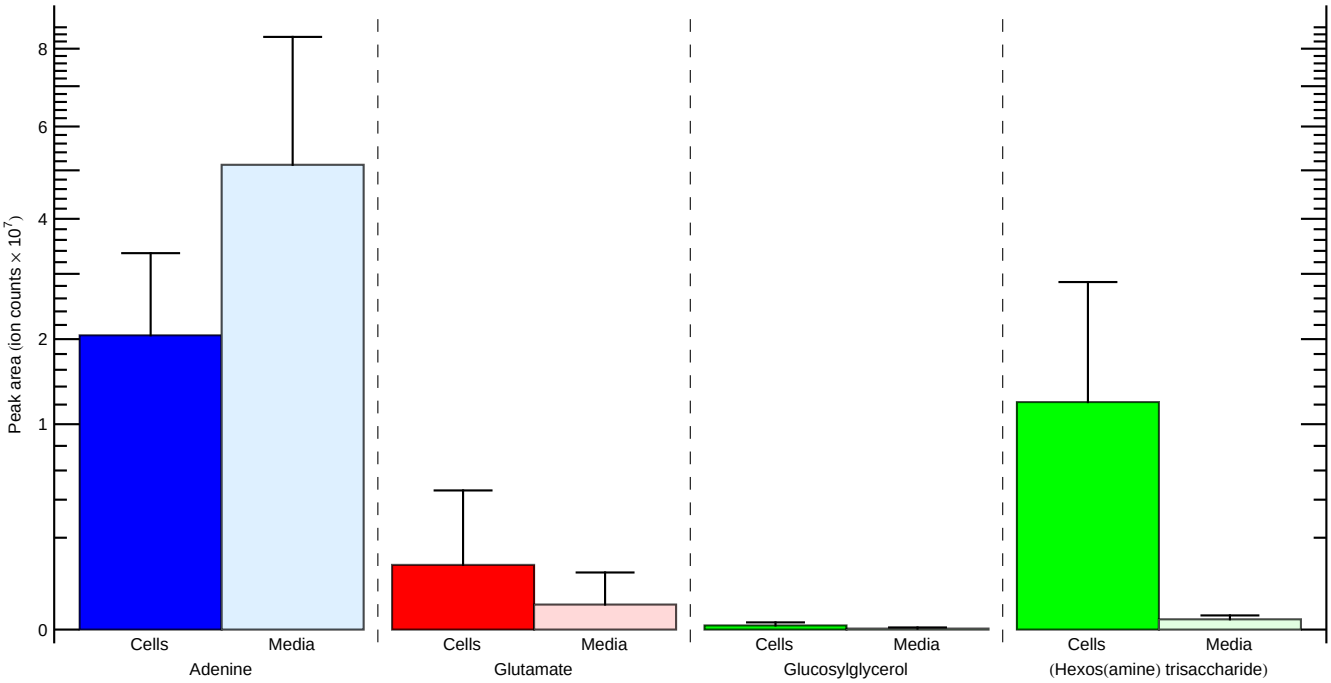


Fig. S4 Peak areas of selected unlabeled (^{12}C) metabolites in cell and media extracts after stable isotope probing experiments. 1.8 ml of media was extracted as opposed to a significantly smaller volume of residual media present in the cell pellet for comparison to show uptake (and turnover) of these metabolites as described in the main text.