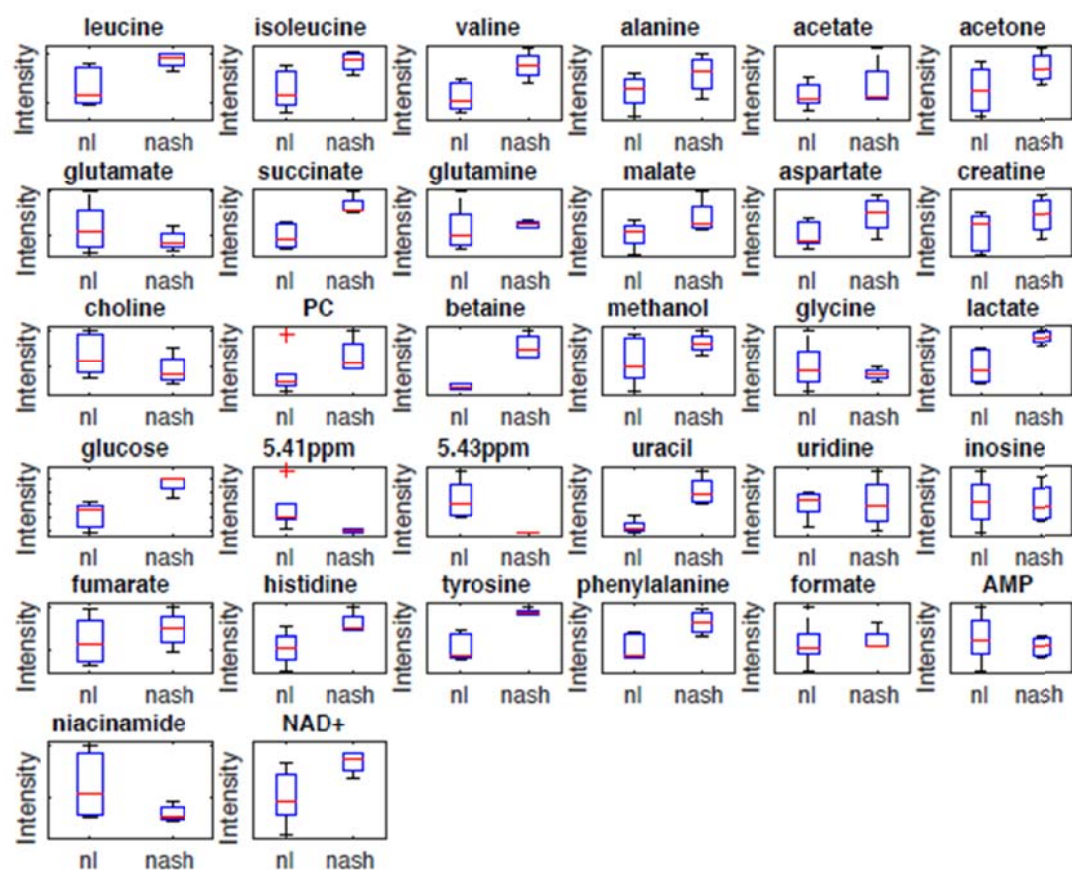


Supplemental Figure 1 Spectral region for an unknown metabolite. Representative traces from ¹H-NMR spectra for the unknown metabolite at 7.685 ppm. Traces shown are for normal (black) NASH (green) and ARLD (ald, blue) livers showing consistency of separation between groups.



Supplemental Figure 2 Reproducibility of ^1H -NMR spectra in repeated analyses. Fraction intensity boxplots for indicated metabolites in normal liver (nl) and NASH (nash) liver samples. Analysis was performed independently to that shown in Figure 3. For each metabolite shown, an unpaired t-test (Welch's t-test) was calculated with a 5% cut-off to test the null hypothesis that the relative peak intensities for pairs of the different classes have the same mean, variances not assumed to be equal. The solid line indicates the median fractional intensity, and the box shows the interquartile range.

Supplemental Table 1 Metabolites significantly altered between patient groups

Comparison of ALD vs NL

Metabolite	p-value	fold_ald_over_nl
Isoleucine	0.011033	1.600684
Valine	0.020093	1.531873
Propyleneglyco	0.079941	4.754069
Succinate	0.011436	1.855135
Aspartate	0.022672	2.40741
Betaine	0.000398	2.005589
Lactate	0.002041	1.709957
Glucose	0.02369	1.641821
5.41ppm	0.016447	0.234659
5.43ppm	0.02369	0.011512
Uracil	0.031881	2.533319
Phenylalanine	0.002042	2.324247

Comparison of NASH vs NL

Metabolite	p-value	fold_nash_over_nl
Leucine	0.085868	1.51735
Isoleucine	0.000269	2.036276
Valine	0.000368	2.050317
Propyleneglyco	0.071982	3.156966
Alanine	0.067683	1.375571
Succinate	0.00731	1.85916
Aspartate	0.058003	1.865317
Betaine	0.000918	1.915848
Lactate	0.000043	1.963971
5.43ppm	0.02835	0.05254
Uracil	0.064848	6.468428
Uridine	0.026855	0.670169
Inosine	0.05583	0.624601
Phenylalanine	0.000065	2.34351
7.68ppm	0.033196	3.234981

Comparison of NASH vs ALD

Metabolite	p-value	fold_nash_over_ald
Leucine	0.003554	1.240478
Isoleucine	0.034248	1.272129
Valine	0.009229	1.338438
Glucose	0.096329	0.760979
5.41ppm	0.093807	3.918674
5.43ppm	0.092352	4.56393
7.68ppm	0.014203	7.690592

For each metabolite shown, an unpaired t-test (Welch's t-test) was calculated with a 5% cut-off to test the null hypothesis that the relative peak intensities

for pairs of the different classes indicated have the same mean, variances not assumed to be equal. Table shows p-values for all those species that were significantly differently expressed.