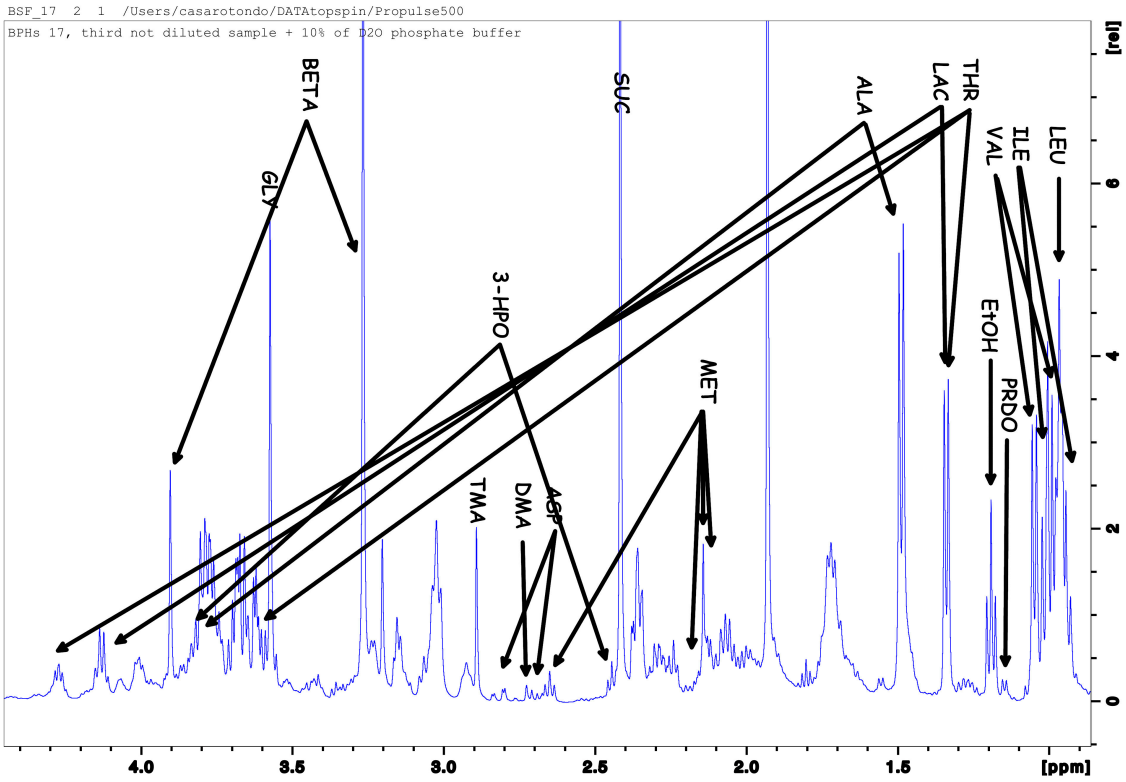
Figure S1. ^{1}H-NMR spectrum run with NOESY presaturation of the water signal (noesypresat).



This region (1–4 ppm) shows the main assignment of the crucial peaks. The subsequent integration allowed the quantification of the described 31 metabolites. The ^{1}H-NMR spectrum for with the assignment pointing to specific metabolites along with other data concerning the assignment and overlapped assignments was later resolved through the MARA-NMR algorithm.

Table S1. Specific assignments allowing quantification after MARA-NMR procedure.

Extended names	Assignment code	Number	Integration limits		Integration values
	TSP reference	int_1	0.048	-0.042	10.000
leucine	9/4*LEU	int_2	0.949	0.902	88.571
isoleucine	3/4*LEU+6*ILE	int_3	0.983	0.949	236.679
valine	3*VAL+3/2*LEU	int_4	1.015	0.983	170.178
	3/2*LEU	int_5	1.031	1.015	45.817

valine	3*VAL	int_6	1.072	1.031	131.241
	propylenglycol	int_7	1.162	1.132	10.499
ethanol	3*EtOH	int_8	1.218	1.162	84.766
	1*ILE	int_9	1.317	1.218	35.898
lactate + threonine	3*LAC+3*THR	int_10	1.362	1.317	135.917
alanine	3*ALA+1*ILE	int_11	1.522	1.422	277.710
	butyrrate	int_12	1.580	1.523	22.841
	1*LEU	int_13	1.676	1.588	60.305
	2*LEU+ macrostructures	int_14	1.772	1.676	234.713
propandiol	PRDO	int_15	1.838	1.772	35.573
4-aminobutyrrate	2*GABA	int_16	1.913	1.858	57.901
acetate	3*AcO	int_17	1.954	1.913	277.032
proline + glutamate	3*PRO+1*GLU+1*ILE	int_18	2.109	1.954	203.081
methionine	1*GLU+5*MET	int_19	2.210	2.109	98.692
	1*VAL+2*4-HBU+3*ACO+2*GABA	int_20	2.330	2.210	109.181
	2*GLU+1*PRO	int_21	2.388	2.330	123.570
succinate	4*SUC	int_22	2.430	2.388	223.131
3-hydroxypropionate	3-HPRO	int_23	2.470	2.430	23.670
	2*MET	int_24	2.672	2.617	9.437
aspartate	2*ASP+6*DMA	int_25	2.741	2.672	3.911
dimethyl-amine	6*DMA	int_26	2.777	2.750	-1.366
	2*ASP	int_27	2.849	2.778	1.509
trimethyl amine	9*TMA	int_28	2.901	2.863	35.449
macromolecular tyramine		int_29	2.963	2.901	30.591
macromolecular system		int_30	3.058	2.963	155.646
	unknown	int_31	3.095	3.058	21.668

	2*ETN+1*PHE+2gaba?	int_32	3.175	3.095	67.802
	9*CHO	int_33	3.215	3.175	50.039
	2*TYM macro	int_34	3.248	3.215	45.902
betaine	9*BETA	int_35	3.288	3.248	223.646
	1*PHE+1*PRO+1*TRP	int_36	3.379	3.288	35.039
	1*PRO	int_37	3.446	3.379	21.689
	unknown	int_38	3.492	3.446	11.625
	2*TRP	int_39	3.536	3.492	17.329
	2*GLY+2*0.71*GLYOH	int_40	3.584	3.543	121.686
	2*0.29*GLYOH+2*4-HBU+1*THR	int_41	3.615	3.584	48.560
	1*VAL	int_42	3.637	3.615	53.728
	2*GLYOH+2*EtOH+1*ILE	int_43	3.693	3.637	149.765
	2*3-HPRO	int_44	3.721	3.693	40.847
	1*ALA+1*GLU+1*GLYOH+LEU+2*PRDO	int_45	3.813	3.721	264.094
	2*ETN+1*MET+1*SER	int_46	3.879	3.813	78.949
	2*BETA+1*ASP	int_47	3.933	3.879	75.667
	unknown	int_48	3.983	3.933	23.577
	1*PHE+unknown	int_49	4.042	3.983	44.252
	2*CHO+1*TRP	int_50	4.092	4.042	19.854
	1*LAC+1*PRO	int_51	4.162	4.092	53.595
	1*THR	int_52	4.216	4.162	8.731
		int_53	4.324	4.224	33.728
		int_54	5.839	5.753	-3.059
uracyl	1*URA	int_55	6.456	6.355	4.244
	2*TYM+2*TYR	int_56	6.965	6.815	56.014
		int_57	7.130	7.083	1.877
	2*TYM+2*TYR+1*TRP	int_58	7.250	7.130	71.203
	1*TRP	int_59	7.299	7.251	11.665
	1*TRP+1*PHE	int_60	7.354	7.300	40.250
	1*PHE	int_61	7.403	7.354	21.238
	2*PHE	int_62	7.467	7.403	34.346

	1*TRP+1*URA	int_63	7.577	7.489	8.069
	1*TRP	int_64	7.762	7.684	5.313
		int_65	7.877	7.843	0.649
		int_66	7.949	7.877	2.607
		int_67	8.244	8.172	3.722
	1*FOR	int_68	8.507	8.428	27.793

Assignment inferred by a) comparison of the spectral profile with databases fitting both chemical shifts and fine structures and b) 1D TOCSY confirming the specific spin system.