Supporting Information

Self-consistent metabolic mixture analysis by heteronuclear NMR - Application to a human cancer cell line

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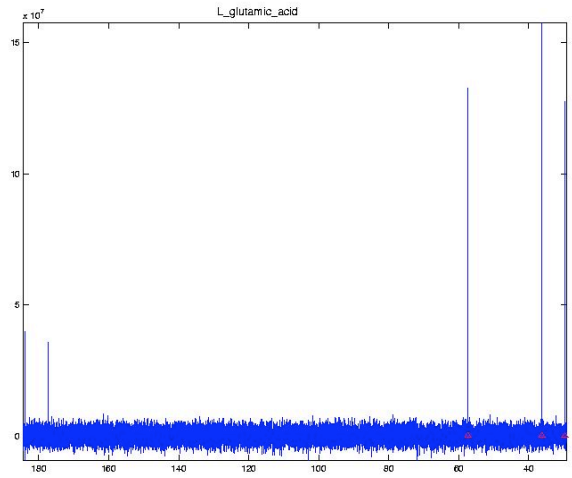

Figure S1a. Top returns for ^{13}C trace number 5:

L_glutamic_acid	1	1	1	1	0.056	5
L_arginine_L_glutamate	2	2	2	2	0.1	11
S_Adenosyl_L_homocysteine	3	3	3	3	0.61	11
L_cystathionine	5	4	5	5	0.8	5
N_acetyl_L_glutamine	6	5	6	6	0.84	7

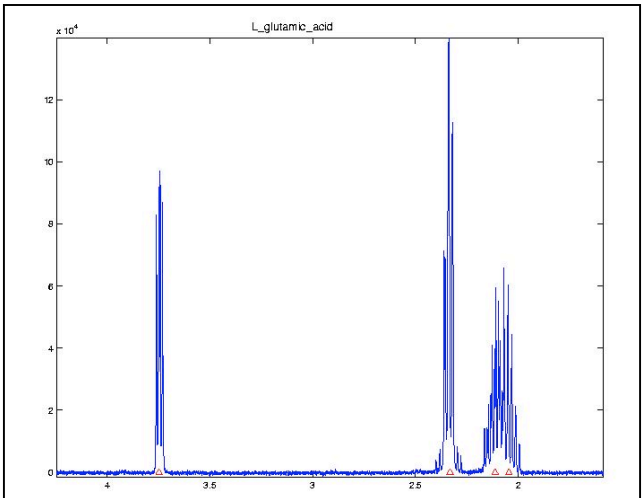

Figure S1b. Top returns for ^{1}H trace number 8:

L_glutamic_acid	1	1	1	1	0.018	3
L_arginine_L_glutamate	2	2	2	2	0.033	6
L_glutamine	5	3	4	4	0.046	3
N_acetylneuraminic_acid	6	5	7	6	0.079	9
L_homoserine	9	4	6	6	0.07	3

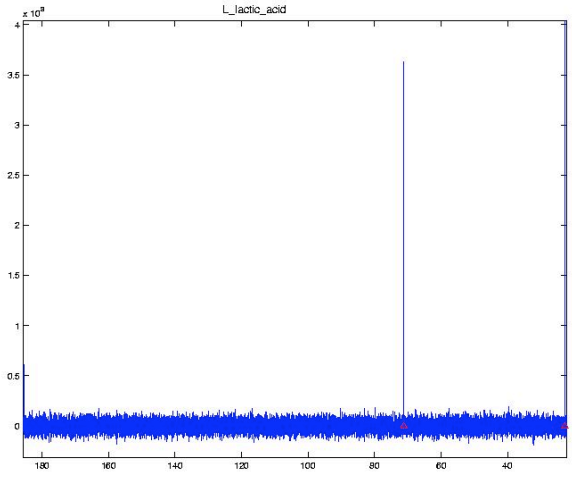

Figure S1c. Top returns for ^{13}C trace number 6:

L_lactic_acid	1	1	1	1	0.024	3
R_Lactate	2	2	2	2	0.031	3
1_2_Propanediol	3	3	3	3	0.26	4
Pantothenate	4	4	4	4	0.34	9
acetylcarnitine	5	5	5	5	0.49	11

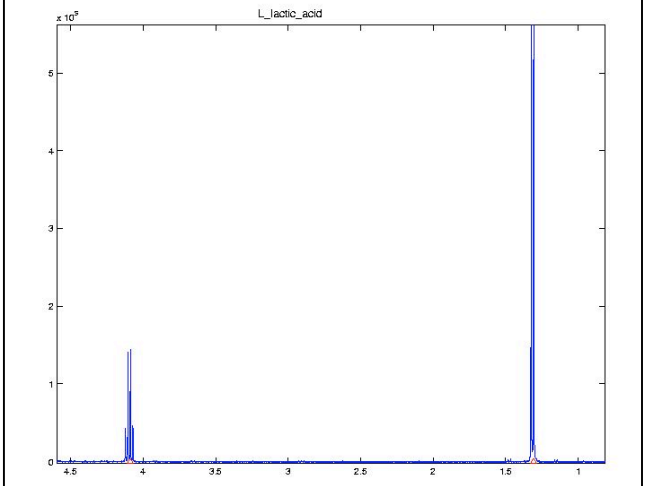

Figure S1d. Top returns for ^{1}H trace number 9:

L_lactic_acid	1	1	1	1	0.0069	2
R_Lactate	2	2	2	2	0.0081	2
N_acetyl_L_alanine	3	3	3	3	0.024	3
D_fructose_6_phosphate	7	12	7	9	0.1	8
6_phosphogluconic_acid	10	8	10	9	0.09	7

Figure S1. ^{13}C and ^{1}H COLMAR query results for the DemixC traces representing glutamic acid and lactic acid of the cancer cell line extract. The spectra are the top returns for each input trace, copied directly from the COLMAR query website result. The tables under each figure show the top 5 compounds that are returned for each input trace taken directly from COLMAR query website. The table entries are (from left to right): compound name, forward assignment index, reverse assignment index, matching index, consensus matching index, average score, and number of reference peaks.