

Bridging the gap between non-targeted stable isotope labeling and metabolic flux analysis

Supplemental Information

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Table S1: All compounds which have been detected as isotopically enriched along with their corrected MIDs of the largest detected fragment after [1,2-¹³C₂]glucose.

Metabolite	RI	Ions (M0)	M	21% O ₂	15% O ₂	10% O ₂	5% O ₂	1% O ₂
RI 981	980.688	184 0 0 0 0	0	0.990	NA	NA	NA	NA
			1	-0.018	NA	NA	NA	NA
			2	0.030	NA	NA	NA	NA
Lactic acid 2TMS	1061.92	219 0 219 219 219	0	0.795	NA	0.794	0.798	0.802
			1	0.024	NA	0.025	0.022	0.020
			2	0.194	NA	0.195	0.195	0.202
Alanine 2TMS	1105.03	190 190 190 190 190	0	0.851	0.850	0.832	0.819	0.849
			1	0.023	0.013	0.010	0.019	0.015
			2	0.144	0.148	0.150	0.179	0.143
			3	NA	NA	0.011	NA	NA
Proline 1TMS	1172.79	172 0 0 0 0	0	0.895	NA	NA	NA	NA
			1	0.030	NA	NA	NA	NA
			2	0.079	NA	NA	NA	NA
Serine 2TMS	1257.33	132 132 132 0 0	0	0.904	0.928	0.944	NA	NA
			1	0.050	0.048	0.028	NA	NA
			2	0.043	0.022	0.041	NA	NA
Glycerol 3TMS	1277.11	218 218 0 0 218	0	0.936	0.931	NA	NA	0.916
			1	0.015	0.012	NA	NA	0.015
			2	0.051	0.063	NA	NA	0.080
Proline 2TMS	1296.26	0 244 0 0 0	0	NA	0.909	NA	NA	NA
			1	NA	0.022	NA	NA	NA
			2	NA	0.070	NA	NA	NA
Glycine 3TMS	1305.68	0 0 0 158 0	0	NA	NA	NA	0.946	NA
			1	NA	NA	NA	0.031	NA
			2	NA	NA	NA	0.025	NA
			3	NA	NA	NA	-0.011	NA

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Metabolite	RI	Ions (M0)	M	21% O ₂	15% O ₂	10% O ₂	5% O ₂	1% O ₂
RI 1313	1312.95	0 173 0 0 0	4	NA	NA	NA	0.014	NA
			0	NA	0.803	NA	NA	NA
			1	NA	0.010	NA	NA	NA
			2	NA	0.194	NA	NA	NA
Serine 3TMS	1360.03	278 278 278 278 0	0	0.938	0.941	0.963	0.938	NA
			1	0.038	0.032	0.010	0.035	NA
			2	0.024	0.028	0.038	0.037	NA
Aspartic acid 2TMS	1419.6	160 160 0 0 0	0	0.884	0.883	NA	NA	NA
			1	0.063	0.057	NA	NA	NA
			2	0.043	0.055	NA	NA	NA
			3	0.012	NA	NA	NA	NA
Malic acid 3TMS	1487.79	335 335 335 335 0	0	0.882	0.889	0.894	0.997	NA
			1	0.026	0.034	0.047	-0.021	NA
			2	0.078	0.068	0.060	0.013	NA
			3	0.004	0.000	0.011	0.017	NA
			4	0.017	0.015	NA	NA	NA
Pyroglutamic acid 2TMS	1516.67	0 0 0 214 0	0	NA	NA	NA	0.940	NA
			1	NA	NA	NA	0.006	NA
			2	NA	NA	NA	0.063	NA
Aspartic acid 3TMS	1519.17	334 334 334 0 0	0	0.892	0.879	0.924	NA	NA
			1	0.039	0.017	0.013	NA	NA
			2	0.062	0.083	0.059	NA	NA
			3	NA	0.023	NA	NA	NA
RI 1530	1529.69	216 216 216 0 0	0	0.789	0.787	0.793	NA	NA
			1	0.016	0.018	0.018	NA	NA
			2	0.205	0.203	0.201	NA	NA
Glutamic acid 2TMS	1531.47	276 276 276 276 0	0	0.894	0.892	0.910	0.963	NA
			1	0.011	0.021	0.022	0.001	NA

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Metabolite	RI	Ions (M0)	M	21% O ₂	15% O ₂	10% O ₂	5% O ₂	1% O ₂
2-Hydroxypent-2-endioic acid 3TMS	1604.44	347 347 0 0 0	2	0.093	0.074	0.073	0.034	NA
			3	NA	-0.003	NA	NA	NA
			4	NA	0.012	NA	NA	NA
			0	0.864	0.890	NA	NA	NA
Glutamic acid 3TMS	1617.07	348 348 348 0 0	1	0.037	0.010	NA	NA	NA
			2	0.081	0.086	NA	NA	NA
			3	0.012	0.004	NA	NA	NA
			4	0.013	0.019	NA	NA	NA
RI 1627	1627.07	124 124 124 0 0	0	0.901	0.899	0.936	NA	NA
			1	0.022	0.023	0.010	NA	NA
			2	0.085	0.085	0.060	NA	NA
			0	0.877	0.917	0.918	NA	NA
RI 1634	1633.9	0 0 0 0 247	1	0.035	0.031	0.025	NA	NA
			2	0.080	0.069	0.062	NA	NA
			3	0.010	NA	NA	NA	NA
			4	0.005	NA	NA	NA	NA
			5	0.015	NA	NA	NA	NA
N-acetylaspartic acid 2TMS	1651.79	245 245 245 245 0	0	NA	NA	NA	NA	0.486
			1	NA	NA	NA	NA	0.449
			2	NA	NA	NA	NA	0.061
RI 1701	1701.11	218 218 0 218 218	0	0.917	0.927	0.995	1.014	NA
			1	0.040	0.021	-0.034	0.006	NA
			2	0.051	0.056	0.058	0.016	NA
RI 1716	1715.91	307 307 307 307 307	0	0.795	0.795	NA	0.772	0.808
			1	0.014	0.022	NA	0.017	0.014
			2	0.193	0.190	NA	0.183	0.195
			3	NA	NA	NA	0.032	NA
			0	0.790	0.830	0.833	0.795	0.844

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Metabolite	RI	Ions (M0)	M	21% O ₂	15% O ₂	10% O ₂	5% O ₂	1% O ₂
Xylitol 5TMS	1720.45	319 319 319 319 319	1	0.086	0.055	0.053	0.114	0.066
			2	0.115	0.108	0.138	0.111	0.087
			3	NA	-0.002	NA	NA	0.016
			4	NA	0.014	NA	NA	NA
			0	0.646	0.674	0.654	0.631	0.614
			1	0.229	0.205	0.213	0.224	0.225
			2	0.110	0.105	0.109	0.119	0.129
RI 1734	1734.44	217 217 217 217 0	3	0.014	0.014	0.020	0.022	0.025
			4	NA	NA	0.013	0.014	NA
			0	0.646	0.648	0.645	0.648	NA
			1	0.328	0.322	0.330	0.324	NA
Glycerol-3-phosphate 4TMS	1757.53	357 357 0 357 0	2	0.032	0.035	0.030	0.031	NA
			0	0.816	0.828	NA	0.831	NA
			1	0.021	0.030	NA	0.013	NA
			2	0.133	0.148	NA	0.140	NA
			3	0.017	NA	NA	0.025	NA
RI 1763	1763.39	217 217 0 0 0	4	0.025	NA	NA	NA	NA
			0	0.616	0.606	NA	NA	NA
			1	0.051	0.058	NA	NA	NA
			2	0.382	0.376	NA	NA	NA
RI 1774	1774.3	292 292 0 0 0	0	0.569	0.601	NA	NA	NA
			1	0.420	0.382	NA	NA	NA
			2	0.007	0.030	NA	NA	NA
Fructose 5TMS MP	1796.75	319 319 319 319 319	3	0.017	NA	NA	NA	NA
			0	0.938	0.959	0.962	0.936	0.963
			1	0.039	0.021	0.017	0.027	0.002
			2	0.024	0.022	0.025	0.031	0.001
			3	NA	NA	NA	0.017	0.052

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Metabolite	RI	Ions (M0)	M	21% O ₂	15% O ₂	10% O ₂	5% O ₂	1% O ₂
Fructose 5TMS BP	1805.14	277 277 0 277 277	0	0.972	0.997	NA	0.946	0.949
			1	-0.006	-0.009	NA	0.028	0.000
			2	-0.034	-0.018	NA	-0.034	0.001
			3	0.025	0.013	NA	0.019	0.017
			4	0.041	0.029	NA	0.042	0.016
			5	NA	NA	NA	0.011	0.024
Citric acid 4TMS	1812.45	375 375 375 375 0	0	0.748	0.765	0.804	0.912	NA
			1	0.039	0.040	0.022	0.010	NA
			2	0.192	0.174	0.161	0.082	NA
			3	0.010	0.011	0.005	NA	NA
			4	0.014	0.013	0.012	NA	NA
RI 1823	1823.07	329 329 0 0 329	0	0.453	0.485	NA	NA	0.546
			1	0.051	0.029	NA	NA	-0.002
			2	0.393	0.400	NA	NA	0.409
			3	0.031	0.014	NA	NA	0.029
			4	0.070	0.068	NA	NA	0.030
			5	0.013	NA	NA	NA	NA
RI 1834	1833.51	217 217 0 0 0	0	0.921	0.930	NA	NA	NA
			1	0.038	0.017	NA	NA	NA
			2	0.036	0.050	NA	NA	NA
			3	-0.001	NA	NA	NA	NA
			4	0.011	NA	NA	NA	NA
Mannose [-H ₂ O] 4TMS MP	1838.31	217 217 0 0 0	0	0.559	0.564	NA	NA	NA
			1	0.418	0.421	NA	NA	NA
			2	0.023	0.022	NA	NA	NA
RI 1883	1882.7	103 0 0 0 0	0	0.934	NA	NA	NA	NA
			1	0.064	NA	NA	NA	NA
Glucose 5TMS BP	1887.02	435 435 435 435 435	0	0.553	0.552	0.560	0.558	0.558

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Metabolite	RI	Ions (M0)	M	21% O ₂	15% O ₂	10% O ₂	5% O ₂	1% O ₂
			1	0.002	0.003	-0.005	0.002	0.003
			2	0.538	0.541	0.533	0.530	0.525
RI 1897	1896.72	0 0 0 0 204	0	NA	NA	NA	NA	0.662
			1	NA	NA	NA	NA	0.374
RI 1897	1896.9	204 0 0 204 0	0	0.629	NA	NA	0.647	NA
			1	0.351	NA	NA	0.334	NA
			2	-0.009	NA	NA	-0.003	NA
			3	0.018	NA	NA	0.012	NA
			4	0.000	NA	NA	-0.007	NA
			5	0.013	NA	NA	0.019	NA
Glucose 1MEOX 5TMS	1908.55	217 217 160 0 0	0	0.865	0.955	0.550	NA	NA
			1	0.130	0.078	0.045	NA	NA
			2	-0.004	NA	0.453	NA	NA
			3	0.024	NA	NA	NA	NA
Lysine 4TMS	1916.85	0 0 0 0 186	0	NA	NA	NA	NA	0.949
			1	NA	NA	NA	NA	-0.005
			2	NA	NA	NA	NA	0.013
			3	NA	NA	NA	NA	0.015
			4	NA	NA	NA	NA	0.030
			5	NA	NA	NA	NA	0.030
RI 1922	1922.17	319 319 0 319 0	0	0.912	0.936	NA	0.927	NA
			1	0.027	0.014	NA	0.014	NA
			2	0.058	0.048	NA	0.034	NA
			3	NA	-0.010	NA	0.022	NA
			4	NA	0.017	NA	NA	NA
RI 1929	1929.02	345 345 345 345 345	0	0.581	0.614	0.597	0.596	0.616
			1	0.012	0.010	0.009	0.014	0.005
			2	0.470	0.434	0.452	0.451	0.447

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Metabolite	RI	Ions (M0)	M	21% O ₂	15% O ₂	10% O ₂	5% O ₂	1% O ₂
RI 1955	1954.81	333 333 0 0 0	0	0.926	0.969	NA	NA	NA
			1	0.014	0.004	NA	NA	NA
			2	0.030	0.085	NA	NA	NA
			3	0.037	-0.069	NA	NA	NA
			4	NA	0.011	NA	NA	NA
Glucose 5TMS MP	1974.11	435 435 435 435 435	0	0.565	0.567	0.554	0.563	0.574
			1	-0.001	0.000	-0.001	-0.001	-0.009
			2	0.525	0.516	0.533	0.523	0.530
RI 1986	1986.25	217 217 217 217 217	0	0.857	0.872	0.863	0.877	0.825
			1	0.136	0.126	0.123	0.111	0.148
			2	NA	NA	NA	NA	0.010
RI 1990	1989.96	333 0 0 0 292	0	0.550	NA	NA	NA	0.589
			1	0.013	NA	NA	NA	0.003
			2	0.437	NA	NA	NA	0.460
			3	0.003	NA	NA	NA	NA
RI 2012	2012.02	243 243 243 243 0	0	0.537	0.531	0.541	0.537	NA
			1	0.282	0.293	0.287	0.302	NA
			2	0.112	0.106	0.111	0.112	NA
			3	0.056	0.046	0.055	0.061	NA
			4	0.024	0.021	0.017	NA	NA
RI 2023	2023.22	0 346 0 0 0	0	NA	0.895	NA	NA	NA
			1	NA	0.021	NA	NA	NA
			2	NA	0.073	NA	NA	NA
			3	NA	0.022	NA	NA	NA
Hexadecanoic acid 1TMS	2042.73	313 313 0 0 0	0	0.762	0.779	NA	NA	NA
			1	0.021	0.008	NA	NA	NA

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Metabolite	RI	Ions (M0)	M	21% O ₂	15% O ₂	10% O ₂	5% O ₂	1% O ₂
RI 2070	2069.62	103 103 0 0 0	2	0.094	0.102	NA	NA	NA
			3	0.031	0.020	NA	NA	NA
			4	0.083	0.070	NA	NA	NA
			5	-0.010	0.003	NA	NA	NA
			6	0.024	0.024	NA	NA	NA
			0	0.889	0.870	NA	NA	NA
RI 2075	2075.49	0 103 103 0 0	1	0.120	0.115	NA	NA	NA
			2	-0.023	0.004	NA	NA	NA
			3	0.015	0.010	NA	NA	NA
			0	NA	0.889	0.870	NA	NA
RI 2158	2157.62	282 0 0 0 0	1	NA	0.124	0.101	NA	NA
			2	NA	-0.024	0.008	NA	NA
			3	NA	0.011	0.022	NA	NA
RI 2163	2163.02	0 217 0 217 0	0	0.920	NA	NA	NA	NA
			1	0.032	NA	NA	NA	NA
			2	0.049	NA	NA	NA	NA
			0	NA	0.938	NA	0.891	NA
RI 2249	2248.81	0 217 217 0 0	1	NA	0.032	NA	0.039	NA
			2	NA	0.029	NA	0.062	NA
			3	NA	0.000	NA	0.028	NA
			4	NA	0.012	NA	NA	NA
RI 2268	2268.1	0 232 232 0 232	0	NA	0.902	0.926	NA	NA
			1	NA	0.054	0.033	NA	NA
			2	NA	0.042	0.051	NA	NA
RI 2473	2472.66	287 287 287 287 287	0	NA	0.525	0.515	NA	0.528
			1	NA	0.472	0.478	NA	0.479
			2	NA	NA	0.011	NA	NA
0	0.500	0.534	0.541	0.515	0.550			

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Metabolite	RI	Ions (M0)	M	21% O ₂	15% O ₂	10% O ₂	5% O ₂	1% O ₂
RI 2578	2578.32	363 363 363 363 0	1	0.470	0.445	0.523	0.458	0.470
			2	0.032	0.019	NA	0.028	NA
			3	NA	NA	NA	0.017	NA
			0	0.821	0.832	0.869	0.939	NA
			1	0.052	0.033	0.003	0.006	NA
			2	0.113	0.131	0.113	0.067	NA
RI 2865	2864.58	315 315 315 315 315	3	0.004	-0.002	-0.005	NA	NA
			4	0.007	0.011	0.004	NA	NA
			5	0.016	NA	0.038	NA	NA
			0	0.995	0.991	1.007	1.007	0.946
			1	NA	NA	NA	NA	-0.007
			2	NA	NA	NA	NA	0.057
RI 3037	3037.3	258 258 258 258 258	3	NA	NA	NA	NA	-0.007
			4	NA	NA	NA	NA	0.012
			0	0.529	0.548	0.534	0.571	0.599
			1	0.299	0.274	0.270	0.251	0.185
			2	0.113	0.123	0.122	0.125	0.114
			3	0.044	0.046	0.057	0.054	0.046
AMP 5TMS	3050.94	169 169 169 0 169	4	0.019	0.020	0.018	0.007	0.026
			5	NA	NA	0.012	0.014	0.012
			6	NA	NA	NA	NA	0.035
			0	0.517	0.537	0.533	NA	0.633
			1	0.306	0.278	0.279	NA	0.198
			2	0.122	0.131	0.126	NA	0.094
			3	0.045	0.046	0.045	NA	0.060
			4	NA	0.011	0.020	NA	0.017

Table S2: All compounds which have been detected as isotopically enriched along with their corrected MIDs of the largest detected fragment after [U-¹³C]glutamine.

Metabolite	RI	Ions (M0)	M	21% O ₂	15% O ₂	10% O ₂	5% O ₂	1% O ₂
RI 965	964.562	0 0 131 131 0	0	NA	NA	0.950	0.940	NA
			1	NA	NA	0.007	-0.001	NA
			2	NA	NA	0.004	0.003	NA
			3	NA	NA	0.003	0.008	NA
			4	NA	NA	0.021	0.040	NA
			5	NA	NA	-0.001	-0.005	NA
			6	NA	NA	0.021	-0.001	NA
Proline 1TMS	1173.02	0 103 103 103 0	0	NA	0.665	0.654	0.663	NA
			1	NA	0.313	0.350	0.322	NA
			2	NA	0.013	NA	0.016	NA
			3	NA	0.010	NA	NA	NA
Proline 2TMS	1296.65	216 216 216 216 216	0	0.731	0.736	0.721	0.718	0.774
			1	0.034	0.035	0.016	0.020	0.006
			2	-0.007	-0.007	-0.003	-0.004	-0.001
			3	0.001	0.001	0.001	0.001	0.000
			4	0.234	0.223	0.253	0.265	0.219
			5	-0.012	-0.003	-0.006	-0.014	-0.012
Aspartic acid 2TMS	1419.9	160 160 160 0 0	0	0.629	0.644	0.621	NA	NA
			1	0.085	0.081	0.063	NA	NA
			2	0.081	0.086	0.098	NA	NA
			3	0.210	0.189	0.221	NA	NA
Malic acid 3TMS	1487.87	245 245 245 245 245	0	0.643	0.656	0.649	0.668	0.652
			1	0.042	0.042	0.021	0.004	0.008
			2	0.091	0.086	0.071	0.038	0.023

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Table S2 – *continued from previous page*

Metabolite	RI	Ions (M0)	M	21% O ₂	15% O ₂	10% O ₂	5% O ₂	1% O ₂
Pyroglutamic acid 2TMS	1516.53	258 258 258 258 258	3	0.059	0.064	0.103	0.186	0.290
			4	0.191	0.175	0.179	0.120	0.030
			0	0.568	0.578	0.565	0.579	0.574
			1	0.012	0.011	0.005	0.001	0.000
			2	0.015	0.013	0.015	0.010	0.003
			3	0.040	0.035	0.033	0.023	0.005
Aspartic acid 3TMS	1519.22	306 306 306 306 306	4	0.013	0.013	0.013	0.014	0.016
			5	0.384	0.380	0.403	0.408	0.437
			0	0.621	0.635	0.615	0.648	0.633
			1	0.074	0.069	0.058	0.022	0.019
			2	0.072	0.075	0.090	0.121	0.156
			3	0.234	0.223	0.235	0.209	0.178
Glutamic acid 2TMS	1531.48	276 276 276 276 276	4	NA	NA	NA	NA	0.010
			5	NA	NA	NA	NA	0.010
			0	0.595	0.594	0.574	0.583	0.584
			1	0.028	0.041	0.030	0.009	0.007
			2	0.019	0.041	0.030	0.031	0.022
			3	0.097	0.084	0.077	0.048	0.015
2-Hydroxypent-2-endioic acid 3TMS	1604.4	0 347 0 0 0	4	0.018	0.013	0.016	0.019	0.022
			5	0.264	0.251	0.296	0.337	0.374
			6	NA	NA	NA	NA	0.010
			0	NA	0.592	NA	NA	NA
			1	NA	0.033	NA	NA	NA
			2	NA	0.035	NA	NA	NA
Glutamic acid 3TMS	1616.94	348 348 348 348 348	3	NA	0.087	NA	NA	NA
			4	NA	0.029	NA	NA	NA
			5	NA	0.261	NA	NA	NA
			0	0.582	0.599	0.580	0.596	0.596

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Table S2 – continued from previous page

Metabolite	RI	Ions (M0)	M	21% O ₂	15% O ₂	10% O ₂	5% O ₂	1% O ₂
			1	0.032	0.030	0.018	0.001	0.005
			2	0.035	0.037	0.032	0.022	0.006
			3	0.093	0.092	0.078	0.044	0.008
			4	0.011	0.009	0.011	0.013	0.016
			5	0.283	0.270	0.324	0.373	0.425
RI 1627	1627.07	172 172 172 0 0	0	0.619	0.597	0.599	NA	NA
			1	0.059	0.053	0.048	NA	NA
			2	0.350	0.347	0.355	NA	NA
			3	NA	-0.017	NA	NA	NA
			4	NA	0.020	NA	NA	NA
			5	0.635	0.667	0.638	0.700	0.666
N-acetylaspartic acid 2TMS	1651.78	245 245 245 245 245	0	0.038	0.019	0.010	0.002	0.009
			1	0.066	0.073	0.060	0.030	0.023
			2	0.083	0.079	0.107	0.154	0.266
			3	0.183	0.170	0.183	0.122	0.041
			4	NA	NA	NA	0.014	NA
			5	0.949	NA	NA	NA	1.010
Xylitol 5TMS	1718.27	319 0 0 0 319	0	0.052	NA	NA	NA	NA
			1	0.519	0.530	0.514	0.499	0.513
			1	0.012	0.006	0.008	0.023	0.013
			2	0.044	0.052	0.052	0.067	0.056
			3	0.004	-0.011	0.004	0.011	0.014
			4	0.019	0.010	0.021	0.013	0.023
			5	0.453	0.460	0.457	0.438	0.438
			6	NA	0.018	NA	NA	NA
			0	0.616	0.645	0.623	0.665	NA
			1	0.048	0.043	0.022	0.024	NA
			2	0.091	0.081	0.068	0.028	NA
Citric acid 4TMS	1812.45	375 375 375 375 0	0	0.616	0.645	0.623	0.665	NA
			1	0.048	0.043	0.022	0.024	NA
			2	0.091	0.081	0.068	0.028	NA

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Table S2 – continued from previous page

Metabolite	RI	Ions (M0)	M	21% O ₂	15% O ₂	10% O ₂	5% O ₂	1% O ₂
RI 1823	1823.07	0 404 0 0 0	3	0.061	0.060	0.076	0.072	NA
			4	0.150	0.133	0.134	0.077	NA
			5	0.042	0.048	0.092	0.163	NA
			0	NA	0.928	NA	NA	NA
			1	NA	0.035	NA	NA	NA
RI 1920	1920.26	0 0 362 0 0	2	NA	0.035	NA	NA	NA
			0	NA	NA	0.593	NA	NA
			1	NA	NA	0.022	NA	NA
			2	NA	NA	0.094	NA	NA
Pantothenic acid 3TMS	1983.3	0 0 0 291 0	3	NA	NA	0.017	NA	NA
			4	NA	NA	0.313	NA	NA
			0	NA	NA	NA	0.941	NA
			1	NA	NA	NA	0.000	NA
RI 2024	2023.57	346 0 0 0 0	2	NA	NA	NA	0.078	NA
			0	0.535	NA	NA	NA	NA
			1	0.032	NA	NA	NA	NA
			2	0.105	NA	NA	NA	NA
			3	0.032	NA	NA	NA	NA
			4	0.264	NA	NA	NA	NA
RI 2075	2075.48	0 132 0 132 0	5	-0.002	NA	NA	NA	NA
			6	0.031	NA	NA	NA	NA
			0	NA	0.916	NA	0.878	NA
			1	NA	0.047	NA	0.059	NA
			2	NA	0.012	NA	0.071	NA
			3	NA	0.036	NA	NA	NA
RI 2158	2157.57	282 282 282 0 0	0	0.618	0.625	0.609	NA	NA
			1	0.025	0.022	0.013	NA	NA
			2	0.088	0.081	0.071	NA	NA

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Table S2 – continued from previous page

Metabolite	RI	Ions (M0)	M	21% O ₂	15% O ₂	10% O ₂	5% O ₂	1% O ₂
Octadecanoic acid 1TMS	2239.24	0 341 0 0 0	3	0.011	0.010	0.011	NA	NA
			4	0.273	0.264	0.291	NA	NA
			0	NA	0.883	NA	NA	NA
			1	NA	-0.006	NA	NA	NA
			2	NA	0.048	NA	NA	NA
			3	NA	0.031	NA	NA	NA
			4	NA	0.040	NA	NA	NA
			5	NA	0.011	NA	NA	NA
RI 2473	2472.66	0 0 0 287 0	0	NA	NA	NA	0.517	NA
			1	NA	NA	NA	0.020	NA
			2	NA	NA	NA	0.022	NA
			3	NA	NA	NA	0.012	NA
			4	NA	NA	NA	0.020	NA
			5	NA	NA	NA	0.395	NA
			6	NA	NA	NA	0.007	NA
			7	NA	NA	NA	0.000	NA
RI 2578	2578.32	363 363 363 363 0	8	NA	NA	NA	0.028	NA
			0	0.681	0.705	0.686	0.710	NA
			1	0.028	0.013	-0.001	0.028	NA
			2	0.070	0.079	0.067	0.049	NA
			3	0.157	0.152	0.148	0.093	NA
			4	0.015	0.007	0.012	0.021	NA
			5	0.061	0.062	0.116	0.124	NA

Table S3: Metabolites, derivatives and ions in Figure 3 (MID variation).

[1,2-¹³C₂]glucose		
Metabolite	Derivative	M₀ m/z
Malate	Malic acid 3TMS	335
<i>N</i> -acetylaspartic acid	<i>N</i> -acetylaspartic acid 2TMS	245
Citrate	Citric acid 4TMS	375
<i>Unidentified</i>	RI 2578	363
AMP	5TMS	169

[U-¹³C]glutamine		
Metabolite	Derivative	M₀ m/z
Citrate	Citric acid 4TMS	375
Malate	Malic acid 3TMS	245
Glutamate	Glutamic acid 2TMS	276
Glutamate (not shown)	Glutamic acid 3TMS	348
<i>N</i> -acetylaspartic acid	<i>N</i> -acetylaspartic acid 2TMS	245

Table S4: Metabolites, derivatives and ions in Figure 4 (MID similarity).

<i>N</i>-acetylaspartic acid ([U-¹³C]glutamine)		
Metabolite	Derivative	M₀ m/z
Malate	Malic acid 3TMS	335
Aspartate	Aspartic acid 3TMS	334
<i>N</i> -acetylaspartic acid	<i>N</i> -acetylaspartic acid 2TMS	304
Proline	Proline 1TMS	172

<i>N</i>-acetylaspartic acid ([1,2-¹³C₂]glucose)		
Metabolite	Derivative	M₀ m/z
<i>N</i> -acetylaspartic acid	<i>N</i> -acetylaspartic acid 2TMS	245
Citrate	Citric acid 4TMS	375
Alanine	Alanine 2TMS	218

RI 2578 ([U-¹³C]glutamine)		
Metabolite	Derivative	M₀ m/z
RI 2578	?	363
Citrate	Citric acid 4TMS	375

RI 2578 ([1,2-¹³C₂]glucose)		
Metabolite	Derivative	M₀ m/z
RI 2578	?	363
Glycerol-3-phosphate	G3P 4TMS	357
Pyroglutamate	Pyroglutamic acid 2TMS	214

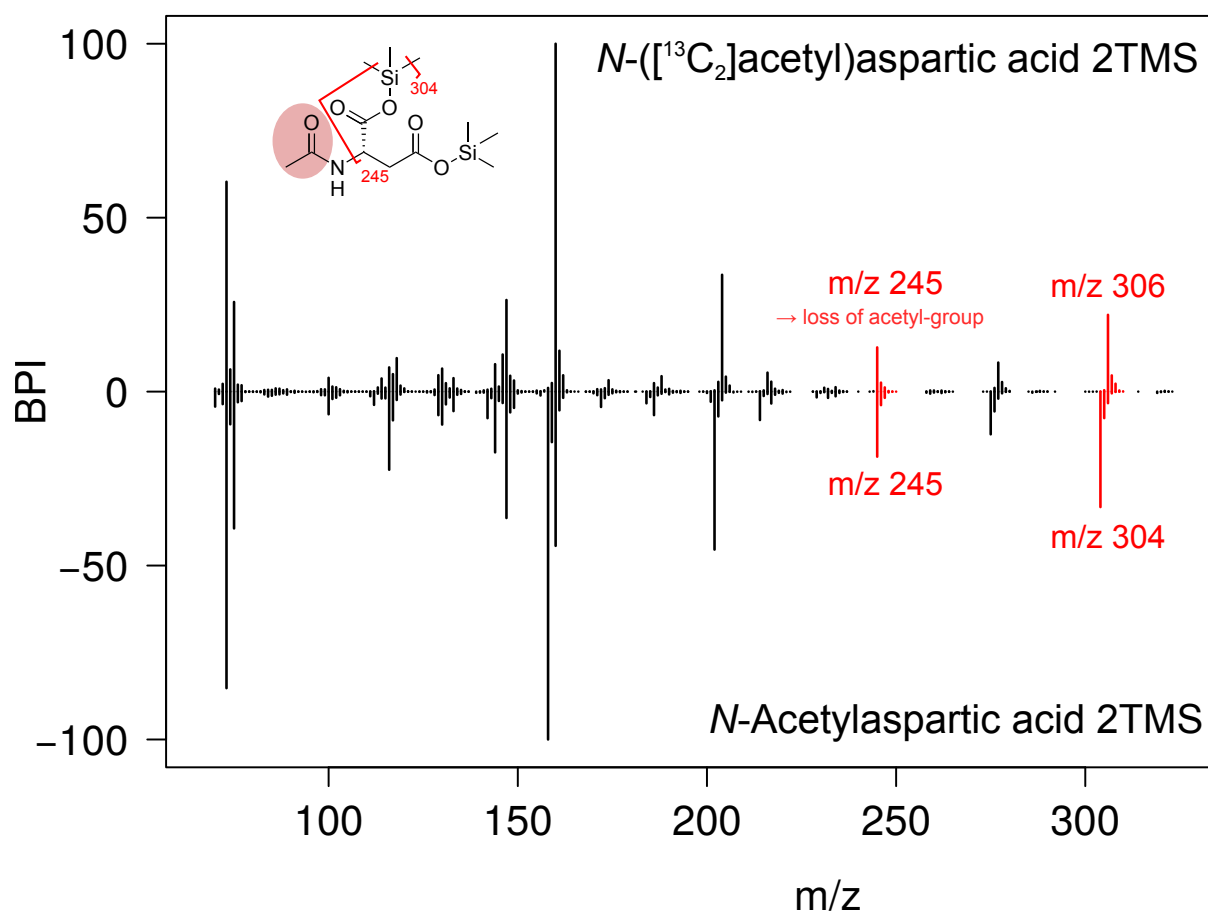


Figure S5: EI-MS spectrum of labeled and unlabeled *N*-acetylaspartic acid 2TMS confirming the loss of the acetyl-group in fragment m/z 245.

Table S6: siRNA target sequences for gene silencing as part of ON-TARGETplus smart pools (Dharmacon/GEHealthcare).

Gene symbol	Target sequence
<i>non-targeting</i>	5'-UGGUUUACAUGUCGACUAA-3'
	5'-UGGUUUACAUGUUGUGUGA-3'
	5'-UGGUUUACAUGUUUUCUGA-3'
	5'-UGGUUUACAUGUUUUCUA-3'
NAT8L	5'-CUUAAUUCUUGGGACAAA-3'
	5'-CGGACAUCGAGCAGUACUA-3'
	5'-GUUUGUACCCUAAGACACA-3'
	5'-AGUUCGCCGUGGUGCACAA-3'

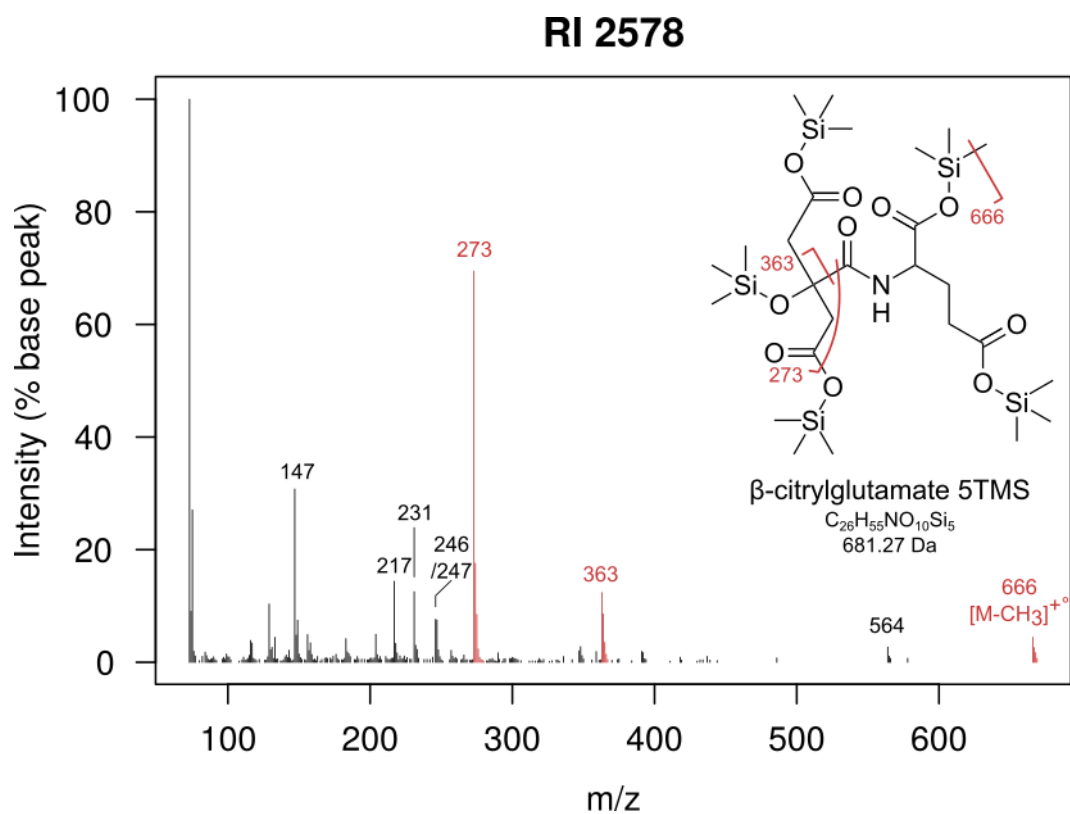


Figure S7: EI-MS spectrum with putative structure of β -citrylglutamate 5TMS and fragmentation of RI 2578.