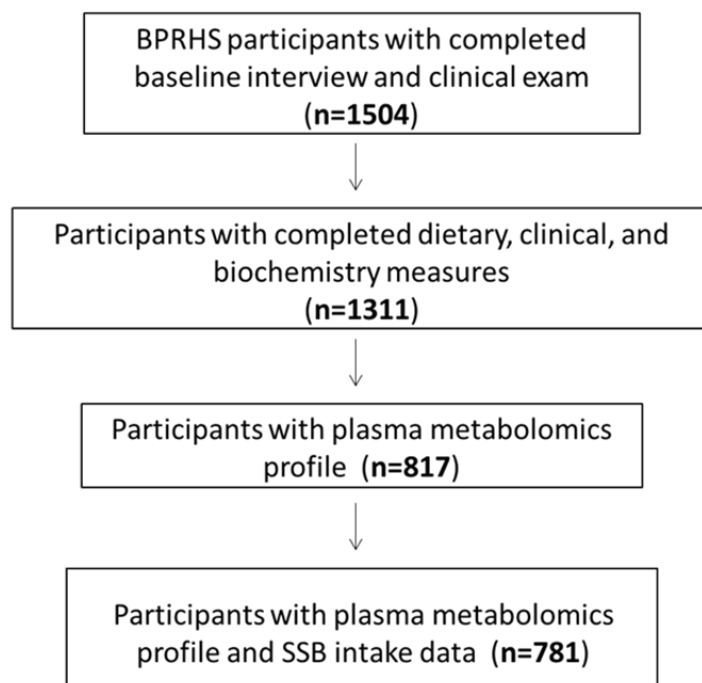


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### **Metabolomic links between sugar-sweetened beverage intake and obesity**

Bingjie Zhou, Reiko Ichikawa, Laurence D. Parnell, Sabrina E. Noel, Xiyuan Zhang, Shilpa N. Bhupathiraju, Caren E. Smith, Katherine L. Tucker, Jose M. Ordovas, Chao-Qiang Lai



**Supplemental Figure 1.** Flowchart of BPRHS sample for metabolomics analysis

**Table S1. Association analysis of metabolites with BMI and/or SSB intake**

[Type here]		BMI			SSB		
CompID	BIOCHEMICAL	Beta*	SE	P value*	Beta*	SE	P value*
54805	3beta-hydroxy-5-cholestenoate	-5.559	0.666	3.15E-16	-0.003	0.018	0.86
48153	mannose	3.756	0.466	2.93E-15	-0.014	0.015	0.321
15506	choline	7.828	1.141	1.40E-11	0.008	0.009	0.373
32418	myristoleate (14:1n5)	2.344	0.352	5.07E-11	0.045	0.026	0.081
33447	palmitoleate (16:1n7)	2.011	0.31	1.53E-10	0.033	0.03	0.274
1604	urate	4.962	0.794	6.85E-10	0.003	0.01	0.741
48258	1-oleoyl-GPC (18:1)	-4.917	0.792	8.80E-10	0.028	0.013	0.03
43829	gamma-glutamylvaline	5.626	0.935	2.80E-09	0.005	0.016	0.732
44526	3-methyl-2-oxobutyrate	3.103	0.527	5.89E-09	-0.017	0.011	0.141
33422	gamma-glutamylphenylalanine	5.604	0.96	7.92E-09	0.012	0.013	0.354
33971	10-heptadecenoate (17:1n7)	2.355	0.426	4.41E-08	0.026	0.024	0.278
34419	1-linoleoyl-GPC (18:2)	-4.159	0.754	4.85E-08	0.019	0.012	0.109
15685	5-hydroxylysine	2.001	0.368	7.01E-08	0.047	0.023	0.041
59	histidine	-8.330	1.555	1.13E-07	0.007	0.007	0.306
512	asparagine	-4.151	0.791	2.00E-07	0.000	0.007	0.986
57	glutamate	8.624	1.669	3.02E-07	0.022	0.018	0.228
1417	kynurenate	2.048	0.397	3.15E-07	-0.008	0.02	0.707
1299	tyrosine	3.907	0.758	3.29E-07	0.014	0.011	0.174
33961	1-stearoyl-GPC (18:0)	-6.249	1.236	5.35E-07	0.013	0.011	0.233
33955	1-palmitoyl-GPC (16:0)	-7.337	1.473	7.84E-07	0.020	0.009	0.03
58	glycine	-4.062	0.825	1.04E-06	0.025	0.013	0.047
34407	isovalerylcarnitine (C5)	1.936	0.412	3.14E-06	-0.020	0.019	0.274
52285	oleate/vaccenate (18:1)	2.532	0.54	3.21E-06	-0.005	0.023	0.825
64	phenylalanine	7.470	1.595	3.33E-06	0.001	0.006	0.9

[Type here]

35136	5-methyluridine (ribothymidine)	-4.663	1.038	8.07E-06	-0.008	0.009	0.407
52603	1,2-dilinoleoyl-GPC (18:2/18:2) lignoceroyl sphingomyelin	-2.976	0.666	9.14E-06	0.039	0.016	0.014
57330	(d18:1/24:0)	-2.243	0.504	9.65E-06	-0.003	0.018	0.85
15749	3-phenylpropionate (hydrocinnamate)	-0.699	0.157	9.97E-06	-0.143	0.061	0.018
1365	myristate (14:0)	2.483	0.562	1.15E-05	0.014	0.019	0.466
1561	alpha-tocopherol linolenate [alpha or gamma;	-2.130	0.495	1.93E-05	0.016	0.026	0.542
34035	(18:3n3 or 6)]	2.185	0.513	2.35E-05	-0.015	0.028	0.576
33972	10-nonadecenoate (19:1n9)	1.904	0.454	3.11E-05	0.012	0.024	0.605
1336	palmitate (16:0)	3.527	0.843	3.20E-05	-0.002	0.016	0.893
1105	linoleate (18:2n6)	2.597	0.653	7.71E-05	-0.006	0.023	0.788
40499	4-hydroxyglutamate	0.979	0.25	0.000101	0.060	0.043	0.165
18369	gamma-glutamylleucine	3.127	0.802	0.000104	-0.006	0.014	0.638
40473	hydantoin-5-propionic acid	0.739	0.191	0.000117	0.001	0.035	0.973
34409	stearoylcarnitine (C18) sphingomyelin (d18:2/16:0,	-2.133	0.551	0.000118	0.020	0.017	0.248
42459	d18:1/16:1)	3.326	0.865	0.000131	0.016	0.01	0.111
32980	adrenate (22:4n6) 1-linoleoyl-2-linolenoyl-GPC	1.516	0.399	0.000155	-0.015	0.025	0.546
53176	(18:2/18:3)	-0.910	0.24	0.000157	0.076	0.03	0.011
47120	9-hydroxystearate gamma-tocopherol/beta-	1.332	0.354	0.000184	0.077	0.027	0.00515
52473	tocopherol	1.566	0.418	0.000195	0.044	0.022	0.044
1301	lysine	4.186	1.131	0.00023	0.003	0.008	0.719
36600	1-linoleoyl-GPE (18:2)	-1.356	0.368	0.000244	0.061	0.019	0.00121
38661	hydroxycotinine 1-(1-enyl-palmitoyl)-2-oleoyl-	-0.773	0.21	0.000253	-0.042	0.042	0.325
52478	GPC (P-16:0/18:1)	-3.578	0.979	0.000274	0.007	0.014	0.619

[Type here]

37506	palmitoyl sphingomyelin (d18:1/16:0)	-5.266	1.443	0.00028	0.001	0.007	0.92
17805	dihomo-linoleate (20:2n6)	1.817	0.504	0.00033	-0.009	0.023	0.705
40008	isoleucylglycine	-7.685	2.132	0.000333	0.053	0.029	0.067
1589	N-acetylmethionine	2.010	0.559	0.000346	0.004	0.015	0.776
37058	succinylcarnitine (C4-DC)	1.996	0.556	0.000355	0.027	0.016	0.094
52710	1-linoleoyl-2-arachidonoyl-GPC (18:2/20:4n6)	-1.913	0.536	0.000381	0.006	0.015	0.685
48351	N1-methylinosine	1.906	0.535	0.000393	0.027	0.016	0.103
36602	1-oleoyl-GPI (18:1)	-1.205	0.339	0.000393	0.053	0.025	0.033
36103	p-cresol sulfate	-0.666	0.192	0.00054	-0.012	0.046	0.801
15720	N-acetylglutamate	1.906	0.569	0.000856	0.022	0.033	0.498
55015	gamma-glutamyl-alpha-lysine	1.898	0.57	0.000921	0.008	0.013	0.54
35628	1-oleoyl-GPE (18:1)	-1.216	0.366	0.000942	0.049	0.021	0.02
52616	1-palmitoyl-2-stearoyl-GPC (16:0/18:0)	-2.571	0.783	0.00108	0.036	0.012	0.00228
52281	2-hydroxybutyrate/2- hydroxyisobutyrate	1.222	0.376	0.00121	-0.068	0.024	0.00443
528	alpha-ketoglutarate	6.231	1.922	0.00124	0.066	0.029	0.021
53242	5-bromotryptophan	-1.580	0.493	0.00142	0.029	0.018	0.105
33968	5-dodecenoate (12:1n7)	1.167	0.367	0.00154	0.021	0.025	0.408
443	aspartate	10.676	3.372	0.00161	-0.002	0.014	0.856
38754	gamma-carboxyglutamate	1.898	0.61	0.00193	0.005	0.015	0.737
32506	2-linoleoylglycerol (18:2)	-0.550	0.179	0.00215	0.024	0.036	0.502
27665	1-methylnicotinamide	-1.219	0.396	0.00219	-0.040	0.022	0.073
33946	N-acetylhistidine	-1.176	0.385	0.00232	0.084	0.027	0.00193
35157	N6-carbamoylthreonyladenosine	1.519	0.498	0.00235	0.024	0.015	0.124
27731	ribonate	1.228	0.412	0.00294	0.027	0.02	0.164
33969	stearidonate (18:4n3)	1.708	0.575	0.00309	-0.011	0.029	0.704
42398	1-stearoyl-GPE (18:0)	-1.876	0.633	0.00314	0.020	0.017	0.249

[Type here]

1898	proline	3.019	1.045	0.00396	0.002	0.009	0.866
52988	adipoylcarnitine (C6-DC)	0.655	0.228	0.00411	0.000	0.025	0.986
43582	5-(galactosylhydroxy)-L-lysine sphingomyelin (d18:1/18:1,	0.934	0.326	0.00432	0.087	0.054	0.104
37529	d18:2/18:0)	2.134	0.747	0.00437	-0.017	0.011	0.131
41220	2-stearoyl-GPE (18:0) 1-(1-enyl-palmitoyl)-GPC (P-	-1.785	0.626	0.0045	0.025	0.021	0.234
52474	16:0)	-3.079	1.088	0.00476	0.022	0.02	0.273
36098	4-vinylphenol sulfate	-0.689	0.243	0.00478	-0.017	0.047	0.723
37752	13-HODE + 9-HODE	106.517	37.656	0.0048	0.050	0.027	0.067
52435	sphingomyelin (d18:2/23:0, d18:1/23:1, d17:1/24:1)	-1.008	0.359	0.00515	-0.007	0.02	0.724
33587	eicosenoate (20:1)	1.341	0.479	0.00529	-0.019	0.025	0.446
553	cotinine	-1.189	0.425	0.00531	-0.011	0.074	0.887
1118	arachidate (20:0)	-3.755	1.346	0.00539	0.015	0.01	0.133
54923	beta-citrylglutamate	1.253	0.452	0.00569	-0.007	0.016	0.654
32412	butyrylcarnitine (C4)	0.369	0.134	0.00583	0.051	0.023	0.025
63	cholesterol	-1.103	0.4	0.00597	0.030	0.014	0.039
47153	sphingomyelin (d18:1/24:1, d18:2/24:0)	-1.605	0.585	0.0062	0.024	0.013	0.079
1868	cysteine	0.561	0.205	0.0063	0.011	0.013	0.382
48492	behenoyl sphingomyelin (d18:1/22:0)	-1.840	0.681	0.00703	-0.003	0.013	0.81
43264	3-hydroxybutyrylcarnitine (1)	0.629	0.234	0.00727	-0.138	0.049	0.00492
42382	S-adenosylhomocysteine (SAH)	2.527	0.942	0.00747	0.035	0.022	0.119
48429	methyl-4-hydroxybenzoate sulfate 1-palmitoyl-2-oleoyl-GPE	-0.189	0.071	0.00784	0.174	0.08	0.03
19263	(16:0/18:1)	0.474	0.178	0.00805	0.032	0.028	0.243
36738	gamma-glutamylglutamate tricosanoyl sphingomyelin	1.986	0.748	0.00808	0.018	0.022	0.411
52436	(d18:1/23:0)	-0.998	0.384	0.01	-0.018	0.017	0.297

[Type here]

36845	o-cresol sulfate	-0.716	0.277	0.01	-0.026	0.055	0.639
60	leucine	2.577	1.037	0.013	-0.008	0.008	0.361
1591	N-acetylvaline	1.974	0.794	0.013	0.008	0.011	0.444
1638	arginine	-3.401	1.373	0.013	0.009	0.01	0.356
2132	citrulline	-2.138	0.864	0.014	-0.001	0.011	0.949
37097	tryptophan betaine	-0.484	0.197	0.014	-0.064	0.063	0.305
39600	3-hydroxyhippurate	0.108	0.044	0.015	-0.001	0.063	0.984
52452	1-stearoyl-2-linoleoyl-GPC (18:0/18:2)	-2.975	1.218	0.015	0.016	0.008	0.033
43231	6-oxopiperidine-2-carboxylate	1.061	0.436	0.015	0.013	0.021	0.522
18477	glycodeoxycholate	-0.547	0.225	0.015	0.046	0.116	0.689
33230	1-palmitoleoyl-GPC (16:1)	-0.893	0.367	0.015	0.071	0.017	4.27E-05
35631	1-palmitoyl-GPE (16:0)	-1.265	0.526	0.016	0.028	0.018	0.115
52975	glycodeoxycholate sulfate	-0.627	0.265	0.018	0.020	0.056	0.727
47154	sphingomyelin (d18:2/14:0, d18:1/14:1)	0.706	0.299	0.018	0.048	0.018	0.00881
52673	1-(1-enyl-palmitoyl)-2- arachidonoyl-GPE (P-16:0/20:4)	1.112	0.47	0.018	-0.014	0.019	0.455
37431	N-methylproline	0.331	0.141	0.019	0.057	0.065	0.386
52464	1-palmitoyl-2-arachidonoyl-GPE (16:0/20:4)	0.684	0.293	0.02	0.002	0.022	0.911
6146	2-aminoadipate	0.762	0.327	0.02	0.002	0.033	0.951
32197	3-(4-hydroxyphenyl)lactate	1.241	0.534	0.021	0.022	0.015	0.15
34389	1-methylxanthine	-0.245	0.106	0.021	0.041	0.053	0.44
1549	3-hydroxyisobutyrate	0.882	0.389	0.024	-0.044	0.021	0.036
35186	1-arachidonoyl-GPE (20:4n6)	-1.263	0.557	0.024	0.015	0.014	0.278
52984	3-hydroxybutyrylcarnitine (2)	0.783	0.348	0.025	-0.063	0.026	0.014
1494	5-oxoproline	-6.076	2.701	0.025	0.001	0.01	0.94
37482	17alpha-hydroxypregnenolone 3- sulfate	-0.660	0.295	0.026	-0.021	0.043	0.631

[Type here]

15677	3-methylhistidine	0.293	0.131	0.026	-0.049	0.052	0.344
1648	serine	-2.852	1.283	0.027	-0.001	0.01	0.909
15443	glucuronate	0.952	0.428	0.027	0.042	0.032	0.193
17945	2-hydroxystearate	-2.398	1.087	0.028	0.000	0.011	0.97
42574	glycohyocholate	-0.273	0.126	0.03	0.053	0.054	0.334
33228	1-arachidonoyl-GPC (20:4n6)	-1.086	0.503	0.031	-0.006	0.017	0.716
39271	1-(1-enyl-stearoyl)-GPE (P-18:0)	-1.751	0.815	0.032	-0.005	0.023	0.824
45095	2-methylbutyrylcarnitine (C5)	0.846	0.394	0.032	-0.021	0.03	0.495
52495	sphingomyelin (d18:1/21:0, d17:1/22:0, d16:1/23:0)	-0.655	0.306	0.033	-0.019	0.018	0.281
53	glutamine	-2.039	0.952	0.033	0.004	0.007	0.524
396	glutarate (C5-DC)	0.893	0.42	0.034	0.041	0.05	0.42
32388	dodecanedioate (C12-DC)	-0.647	0.304	0.034	0.036	0.025	0.146
32504	docosapentaenoate (n3 DPA; 22:5n3)	1.024	0.485	0.035	-0.029	0.024	0.228
1493	ornithine	1.777	0.845	0.036	0.014	0.012	0.246
12261	taurodeoxycholate	-0.181	0.086	0.036	0.035	0.078	0.656
48490	sphingomyelin (d18:1/20:0, d16:1/22:0)	-1.620	0.772	0.036	-0.028	0.011	0.011
20675	1,5-anhydroglucitol (1,5-AG)	-1.086	0.521	0.037	0.090	0.04	0.024
1125	isoleucine	2.163	1.043	0.038	-0.008	0.009	0.36
42449	1-palmitoyl-2-linoleoyl-GPE (16:0/18:2)	0.444	0.216	0.04	0.039	0.026	0.135
53223	palmitoleoylcarnitine (C16:1)	0.573	0.279	0.041	0.028	0.022	0.215
1121	margarate (17:0)	1.409	0.695	0.043	0.002	0.017	0.912
55017	4-hydroxyphenylacetylglutamine	0.168	0.083	0.044	0.071	0.047	0.134
42420	erythronate	1.684	0.838	0.045	0.026	0.012	0.033
36847	2-ethylphenylsulfate	-0.671	0.334	0.045	-0.061	0.032	0.055
35675	2-hydroxypalmitate	-2.347	1.186	0.048	0.002	0.01	0.817

[Type here]

52447	1-stearoyl-2-arachidonoyl-GPE (18:0/20:4)	0.674	0.341	0.049	-0.021	0.019	0.276
52726	1-stearoyl-2-oleoyl-GPI (18:0/18:1)	-0.450	0.23	0.051	0.111	0.034	0.000929
52748	1-(1-enyl-stearoyl)-2-linoleoyl- GPE (P-18:0/18:2)	-0.896	0.466	0.055	0.042	0.018	0.018
52468	1-stearoyl-2-linoleoyl-GPI (18:0/18:2)	-0.897	0.469	0.056	0.066	0.018	0.00032
35305	1-palmitoyl-GPI (16:0)	-0.663	0.349	0.058	0.105	0.027	8.02E-05
45951	1-linolenoyl-GPC (18:3)	-0.496	0.271	0.068	0.060	0.026	0.021
36594	1-linoleoyl-GPI (18:2)	-0.695	0.386	0.072	0.040	0.018	0.024
32346	glycochenodeoxycholate	-0.333	0.186	0.074	0.110	0.049	0.024
52461	1-palmitoyl-2-oleoyl-GPC (16:0/18:1)	-1.477	0.836	0.078	0.037	0.01	0.000311
52615	sphingomyelin (d18:1/17:0, d17:1/18:0, d19:1/16:0)	-1.175	0.668	0.079	-0.034	0.012	0.0057
42374	2-aminobutyrate	0.985	0.573	0.086	-0.060	0.016	0.00014
53260	oleoylcholine	-0.043	0.025	0.089	0.155	0.056	0.00585
32390	N-acetyltyrosine	0.554	0.341	0.105	0.060	0.023	0.00956
52449	1-stearoyl-2-arachidonoyl-GPI (18:0/20:4)	-0.846	0.538	0.116	0.033	0.015	0.024
33950	N-acetylphenylalanine	0.510	0.328	0.12	0.051	0.021	0.013
33364	gamma-glutamylthreonine	1.442	0.935	0.124	0.037	0.016	0.021
52438	1-stearoyl-2-oleoyl-GPC (18:0/18:1)	-0.717	0.479	0.135	0.067	0.015	5.98E-06
31591	androsterone sulfate	-0.674	0.455	0.139	-0.121	0.052	0.02
54967	palmitoleoyl-linoleoyl-glycerol (16:1/18:2) [1]	0.325	0.223	0.145	0.061	0.03	0.043
39379	glycochenodeoxycholate	-0.218	0.151	0.149	0.166	0.058	0.00445
52944	palmitoylcholine	-0.052	0.037	0.162	0.118	0.045	0.0081



[Type here]

18494	taurochenodeoxycholate	-0.060	0.045	0.183	0.137	0.061	0.025
52470	1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)	0.282	0.223	0.206	0.098	0.023	2.37E-05
42446	1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)	-1.575	1.261	0.212	0.015	0.008	0.05
18476	glycocholate	-0.128	0.103	0.215	0.137	0.055	0.012
46115	21-hydroxypregnenolone disulfate	-0.418	0.358	0.244	-0.081	0.03	0.00762
19130	1,2-dipalmitoyl-GPC (16:0/16:0)	-1.128	0.969	0.245	0.037	0.01	0.000101
48434	N-acetylcitrulline	-0.017	0.015	0.248	0.118	0.046	0.011
53261	arachidonoylcholine	-0.034	0.029	0.251	0.096	0.047	0.043
48460	propyl 4-hydroxybenzoate sulfate	-0.042	0.037	0.26	0.159	0.077	0.038
33973	epiandrosterone sulfate	-0.707	0.641	0.27	-0.163	0.052	0.00193
40703	prolylglycine	-1.052	1.035	0.31	0.088	0.043	0.04
15990	glycerophosphorylcholine (GPC)	-0.938	0.99	0.344	0.060	0.024	0.013
22185	N-acetylaspartate (NAA)	0.208	0.245	0.397	0.164	0.05	0.00113
35428	tiglylcarnitine (C5:1-DC)	0.381	0.489	0.436	-0.040	0.018	0.029
33959	N-acetyltryptophan	0.271	0.371	0.465	0.059	0.02	0.00359
47112	etiocolanolone glucuronide palmitoyl-oleoyl-glycerol	-0.269	0.368	0.465	-0.102	0.04	0.011
54942	(16:0/18:1)	0.216	0.299	0.469	0.092	0.044	0.038
35127	pro-hydroxy-pro	-0.165	0.236	0.485	0.079	0.024	0.000861
21127	1-palmitoylglycerol (16:0)	-0.215	0.351	0.539	0.058	0.027	0.034
36808	dimethylarginine (SDMA + ADMA)	0.568	0.992	0.567	0.018	0.008	0.025
37211	androstenediol (3beta,17beta) monosulfate (1)	0.289	0.505	0.568	-0.106	0.041	0.00876
33936	octanoylcarnitine (C8)	0.058	0.107	0.592	-0.068	0.029	0.018
1414	3-phosphoglycerate	-0.197	0.37	0.595	-0.108	0.051	0.033
19503	stearoyl sphingomyelin (d18:1/18:0)	0.387	0.755	0.608	-0.037	0.012	0.00226

[Type here]

48491	sphingomyelin (d18:1/20:1, d18:2/20:0)	-0.347	0.699	0.62	-0.028	0.013	0.027
37186	5alpha-androstan-3alpha,17beta- diol monosulfate (1)	0.170	0.355	0.632	-0.140	0.054	0.01
32425	dehydroisoandrosterone sulfate (DHEA-S)	-0.293	0.691	0.672	-0.091	0.034	0.00795
48885	arabitol/xylitol	-0.109	0.266	0.681	0.046	0.017	0.00645
48408	tyramine O-sulfate	-0.053	0.136	0.695	0.103	0.051	0.044
55001	diacylglycerol (12:0/18:1, 14:0/16:1, 16:0/14:1)	0.035	0.091	0.701	0.156	0.071	0.028
1498	N6,N6,N6-trimethyllysine	-0.101	0.313	0.748	0.046	0.022	0.039
37190	5alpha-androstan-3beta,17beta- diol disulfate	0.180	0.624	0.773	-0.097	0.049	0.046
45970	1-palmitoyl-GPG (16:0)	0.114	0.501	0.819	0.058	0.017	0.000912
22842	cholate	0.012	0.074	0.872	0.219	0.067	0.00116
37192	5alpha-androstan-3beta,17beta- diol monosulfate (2)	-0.063	0.555	0.91	-0.129	0.048	0.00725
52431	1-palmitoleoylglycerol (16:1)	0.017	0.169	0.919	0.108	0.038	0.00523
46957	gulonate	0.022	0.255	0.931	0.124	0.048	0.011
1123	inosine	-0.008	0.278	0.977	0.087	0.032	0.00634
52467	1-palmitoyl-2-arachidonoyl-GPI (16:0/20:4)	-0.004	0.222	0.987	0.114	0.026	8.97E-06

\*All were adjusted for age, sex, alcohol use, smoking, education, physical activity, and total calorie intake.

[Type here]

**Table S2. Metabolic pathways enrichment by SSB intake**

<b>Sub Pathway</b>	<b>Super Pathway</b>	<b>No. of metabolites assigned to the pathway</b>	<b>No. of significant metabolites in each pathway</b>	<b>Total No. of significant metabolites</b>	<b>Z score</b>	<b>P value</b>
Phosphatidylcholine (PC)	Lipid	12	8	86	<b>4.109</b>	<b>3.97E-05</b>
Phosphatidylinositol (PI)	Lipid	4	4	86	<b>4.026</b>	<b>5.68E-05</b>
Lysophospholipid (LPL)	Lipid	19	10	86	<b>3.649</b>	<b>2.63E-04</b>
Fatty Acid Metabolism (Acyl Choline)	Lipid	3	3	86	<b>3.482</b>	<b>4.97E-04</b>
Androgenic Steroids	Lipid	17	8	86	2.857	4.28E-03
Primary Bile Acid Metabolism	Lipid	8	4	86	2.149	3.16E-02
Glutathione Metabolism	Amino Acid	3	2	86	2.033	4.21E-02
Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	Carbohydrate	3	2	86	2.033	4.21E-02
Xanthine Metabolism	Xenobiotics	14	0	86	-1.894	5.82E-02
Long Chain Fatty Acid	Lipid	12	0	86	-1.750	8.02E-02
Polyunsaturated Fatty Acid (n3 and n6)	Lipid	12	0	86	-1.750	8.02E-02
Methionine, Cysteine, SAM and Taurine Metabolism	Amino Acid	11	0	86	-1.673	9.43E-02
Fatty Acid, Dicarboxylate	Lipid	9	0	86	-1.510	1.31E-01
Glutamate Metabolism	Amino Acid	9	0	86	-1.510	1.31E-01
Pyrimidine Metabolism, Uracil containing	Nucleotide	6	0	86	-1.228	2.19E-01
Phosphatidylethanolamine (PE)	Lipid	6	0	86	-1.228	2.19E-01

[Type here]

Leucine, Isoleucine and Valine Metabolism	Amino Acid	20	2	86	-1.135	2.56E-01
Secondary Bile Acid Metabolism	Lipid	12	1	86	-1.017	3.09E-01
Progestin Steroids	Lipid	4	0	86	-1.001	3.17E-01
Fructose, Mannose and Galactose Metabolism	Carbohydrate	4	0	86	-1.001	3.17E-01
Lysoplasmalogen	Lipid	4	0	86	-1.001	3.17E-01
Tryptophan Metabolism	Amino Acid	11	1	86	-0.909	3.63E-01
Nicotinate and Nicotinamide Metabolism	Cofactors and Vitamins	3	0	86	-0.866	3.87E-01
Purine Metabolism, Adenine containing	Nucleotide	3	0	86	-0.866	3.87E-01
Medium Chain Fatty Acid	Lipid	3	0	86	-0.866	3.87E-01
Acetylated Peptides	Peptide	3	0	86	-0.866	3.87E-01
Dihydrosphingomyelins	Lipid	3	0	86	-0.866	3.87E-01
Tobacco Metabolite	Xenobiotics	3	0	86	-0.866	3.87E-01
Sphingomyelins	Lipid	18	5	86	0.853	3.94E-01
Fatty Acid, Monohydroxy	Lipid	10	1	86	-0.793	4.28E-01
Plasmalogen	Lipid	10	1	86	-0.793	4.28E-01
Gamma-glutamyl Amino Acid	Peptide	10	1	86	-0.793	4.28E-01
Histidine Metabolism	Amino Acid	9	1	86	-0.667	5.05E-01
Ascorbate and Aldarate Metabolism	Cofactors and Vitamins	3	1	86	0.584	5.59E-01
Phenylalanine Metabolism	Amino Acid	3	1	86	0.584	5.59E-01
Fatty Acid Metabolism (also BCAA Metabolism)	Lipid	3	1	86	0.584	5.59E-01
Aminosugar Metabolism	Carbohydrate	3	1	86	0.584	5.59E-01

[Type here]

Sterol	Lipid	3	1	86	0.584	5.59E-01
Dipeptide	Peptide	3	1	86	0.584	5.59E-01
Tyrosine Metabolism	Amino Acid	14	2	86	-0.535	5.93E-01
Glycine, Serine and Threonine Metabolism	Amino Acid	8	1	86	-0.529	5.97E-01
Benzoate Metabolism	Xenobiotics	19	3	86	-0.459	6.46E-01
Urea cycle; Arginine and Proline Metabolism	Amino Acid	12	3	86	0.448	6.54E-01
Alanine and Aspartate Metabolism	Amino Acid	4	1	86	0.256	7.98E-01
Pentose Metabolism	Carbohydrate	4	1	86	0.256	7.98E-01
Tocopherol Metabolism	Cofactors and Vitamins	4	1	86	0.256	7.98E-01
Purine Metabolism, (Hypo)Xanthine/Inosine containing	Nucleotide	6	1	86	-0.200	8.42E-01
TCA Cycle	Energy	6	1	86	-0.200	8.42E-01
Monoacylglycerol	Lipid	9	2	86	0.176	8.61E-01
Lysine Metabolism	Amino Acid	9	2	86	0.176	8.61E-01
Fatty Acid Metabolism(Acyl Carnitine)	Lipid	16	3	86	-0.118	9.06E-01
Diacylglycerol	Lipid	15	3	86	0.009	9.93E-01
Pregnenolone Steroids	Lipid	5	1	86	0.005	9.96E-01
Phospholipid Metabolism	Lipid	5	1	86	0.005	9.96E-01

<sup>1</sup>Number of metabolites are the number of detected metabolites assigned to the respective pathway.

[Type here]

**Table S3. Metabolic pathways overpresented by BMI**

<b>Sub Pathway</b>	<b>Super Pathway</b>	<b>No. of metabolites assigned to the pathway</b>	<b>No. of significant metabolites in each pathway</b>	<b>Total No. of significant metabolites</b>	<b>Z score</b>	<b>P value</b>
Long Chain Fatty Acid	Lipid	12	10	148	<b>3.629</b>	<b>2.85E-04</b>
Lysophospholipid	Lipid	19	13	148	3.205	1.35E-03
Sphingomyelins	Lipid	18	11	148	2.449	1.43E-02
Xanthine Metabolism	Xenobiotics	14	1	148	-	2.99E-02
Glutamate Metabolism	Amino Acid	9	6	148	2.068	3.87E-02
Phosphatidylethanolamine (PE)	Lipid	6	4	148	1.682	9.25E-02
Tyrosine Metabolism	Amino Acid	14	2	148	-	1.10E-01
Monoacylglycerol	Lipid	9	1	148	1.477	1.40E-01
Lysine Metabolism	Amino Acid	9	5	148	1.359	1.74E-01
Aminosugar Metabolism	Carbohydrate	3	2	148	1.185	2.36E-01
Glutathione Metabolism	Amino Acid	3	2	148	1.185	2.36E-01
Sterol	Lipid	3	2	148	1.185	2.36E-01
Tobacco Metabolite	Xenobiotics	3	2	148	1.185	2.36E-01
Polyunsaturated Fatty Acid (n3 and n6)	Lipid	12	6	148	1.164	2.44E-01
Gamma-glutamyl Amino Acid	Peptide	10	5	148	1.060	2.89E-01
Plasmalogen	Lipid	10	2	148	-	3.37E-01
Pyrimidine Metabolism, Uracil containing	Nucleotide	6	1	148	0.913	3.61E-01

[Type here]

Fatty Acid, Dicarboxylate	Lipid	9	2	148	-	0.768	4.42E-01
Phospholipid Metabolism	Lipid	5	1	148	-	0.675	5.00E-01
Pregnenolone Steroids	Lipid	5	1	148	-	0.675	5.00E-01
Alanine and Aspartate Metabolism	Amino Acid	4	2	148	0.666	5.06E-01	
Lysoplasmalogen	Lipid	4	2	148	0.666	5.06E-01	
Tocopherol Metabolism	Cofactors and Vitamins	4	2	148	0.666	5.06E-01	
Histidine Metabolism	Amino Acid	9	4	148	0.650	5.16E-01	
Glycine, Serine and Threonine Metabolism	Amino Acid	8	2	148	-	0.556	5.78E-01
Phosphatidylcholine (PC)	Lipid	12	5	148	0.548	5.84E-01	
Urea cycle; Arginine and Proline Metabolism	Amino Acid	12	5	148	0.548	5.84E-01	
Methionine, Cysteine, SAM and Taurine Metabolism	Amino Acid	11	3	148	-	0.494	6.21E-01
Tryptophan Metabolism	Amino Acid	11	3	148	-	0.494	6.21E-01
Fructose, Mannose and Galactose Metabolism	Carbohydrate	4	1	148	-	0.392	6.95E-01
Pentose Metabolism	Carbohydrate	4	1	148	-	0.392	6.95E-01
Fatty Acid, Monohydroxy	Lipid	10	4	148	0.387	6.99E-01	
Fatty Acid Metabolism(Acyl Carnitine)	Lipid	16	5	148	-	0.258	7.96E-01
Benzoate Metabolism	Xenobiotics	19	7	148	0.242	8.09E-01	

[Type here]

Leucine, Isoleucine and Valine Metabolism	Amino Acid	20	7	148	0.071	9.43E-01
Secondary Bile Acid Metabolism	Lipid	12	4	148	-	9.45E-01
Purine Metabolism, (Hypo)Xanthine/Inosine containing	Nucleotide	6	2	148	-	9.62E-01
TCA Cycle	Energy	6	2	148	0.048	9.62E-01
Acetylated Peptides	Peptide	3	1	148	-	9.73E-01
Dipeptide	Peptide	3	1	148	0.034	9.73E-01
Fatty Acid Metabolism (also BCAA Metabolism)	Lipid	3	1	148	-	9.73E-01
Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	Carbohydrate	3	1	148	0.034	9.73E-01
Medium Chain Fatty Acid	Lipid	3	1	148	-	9.73E-01
Nicotinate and Nicotinamide Metabolism	Cofactors and Vitamins	3	1	148	0.034	9.73E-01
Phenylalanine Metabolism	Amino Acid	3	1	148	-	9.73E-01
Purine Metabolism, Adenine containing	Nucleotide	3	1	148	0.034	9.73E-01
Androgenic Steroids	Lipid	17	0	148	-	2.42E-03
Ascorbate and Aldarate Metabolism	Cofactors and Vitamins	3	0	148	3.033	2.10E-01
Diacylglycerol	Lipid	15	0	148	-	4.48E-03



[Type here]

Dihydrosphingomyelins	Lipid	3	0	148	-	1.253	2.10E-01
Fatty Acid Metabolism (Acyl Choline)	Lipid	3	0	148	-	1.253	2.10E-01
Phosphatidylinositol (PI)	Lipid	4	0	148	-	1.449	1.47E-01
Primary Bile Acid Metabolism	Lipid	8	0	148	-	2.059	3.95E-02
Progestin Steroids	Lipid	4	0	148	-	1.449	1.47E-01

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<sup>1</sup>Number of metabolites are the number of detected metabolites assigned to the respective pathway.

[Type here]

**Table S4. Pathway enrichment analysis for common metabolites that are associated with both SSB intake and BMI**

<b>Sub Pathway</b>	<b>Super Pathway</b>	<b>No. of metabolites assigned to the pathway</b>	<b>No. of significant metabolites in each pathway</b>	<b>Total No. of significant metabolites</b>	<b>Z score</b>	<b>P value</b>
Lysophospholipid (LPL)	Lipid	19	6	28	<b>4.539</b>	<b>5.65E-06</b>
Phosphatidylcholine (PC)	Lipid	12	4	28	<b>3.827</b>	<b>1.30E-04</b>
Aminosugar Metabolism	Carbohydrate	3	1	28	1.893	0.0583
Fatty Acid Metabolism (also BCAA Metabolism)	Lipid	3	1	28	1.893	0.0583
Glutathione Metabolism	Amino Acid	3	1	28	1.893	0.0583
Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	Carbohydrate	3	1	28	1.893	0.0583
Sterol	Lipid	3	1	28	1.893	0.0583
Tocopherol Metabolism	Cofactors and Vitamins	4	1	28	1.510	0.1311
Leucine, Isoleucine and Valine Metabolism	Amino Acid	20	0	28	-1.204	0.2285
Benzoate Metabolism	Xenobiotics	19	0	28	-1.172	0.2411
Sphingomyelins	Lipid	18	0	28	-1.140	0.2544
Androgenic Steroids	Lipid	17	0	28	-1.106	0.2686
Fatty Acid Metabolism(Acyl Carnitine)	Lipid	16	0	28	-1.072	0.2838
Diacylglycerol	Lipid	15	0	28	-1.037	0.2999
TCA Cycle	Energy	6	1	28	1.019	0.3081
Tyrosine Metabolism	Amino Acid	14	0	28	-1.000	0.3172
Xanthine Metabolism	Xenobiotics	14	0	28	-1.000	0.3172
Long Chain Fatty Acid	Lipid	12	0	28	-0.924	0.3556

[Type here]

Polyunsaturated Fatty Acid (n3 and n6)	Lipid	12	0	28	-0.924	0.3556
Secondary Bile Acid Metabolism	Lipid	12	0	28	-0.924	0.3556
Urea cycle; Arginine and Proline Metabolism	Amino Acid	12	0	28	-0.924	0.3556
Methionine, Cysteine, SAM and Taurine Metabolism	Amino Acid	11	0	28	-0.883	0.3770
Tryptophan Metabolism	Amino Acid	11	0	28	-0.883	0.3770
Fatty Acid, Monohydroxy	Lipid	10	0	28	-0.841	0.4002
Gamma-glutamyl Amino Acid	Peptide	10	0	28	-0.841	0.4002
Plasmalogen	Lipid	10	0	28	-0.841	0.4002
Fatty Acid, Dicarboxylate	Lipid	9	0	28	-0.797	0.4253
Glutamate Metabolism	Amino Acid	9	0	28	-0.797	0.4253
Histidine Metabolism	Amino Acid	9	0	28	-0.797	0.4253
Lysine Metabolism	Amino Acid	9	0	28	-0.797	0.4253
Monoacylglycerol	Lipid	9	0	28	-0.797	0.4253
Glycine, Serine and Threonine Metabolism	Amino Acid	8	0	28	-0.751	0.4528
Primary Bile Acid Metabolism	Lipid	8	0	28	-0.751	0.4528
Phosphatidylethanolamine (PE)	Lipid	6	0	28	-0.649	0.5166
Purine Metabolism, (Hypo)Xanthine/Inosine containing	Nucleotide	6	0	28	-0.649	0.5166
Pyrimidine Metabolism, Uracil containing	Nucleotide	6	0	28	-0.649	0.5166
Phospholipid Metabolism	Lipid	5	0	28	-0.591	0.5542
Pregnenolone Steroids	Lipid	5	0	28	-0.591	0.5542
Alanine and Aspartate Metabolism	Amino Acid	4	0	28	-0.528	0.5972
Fructose, Mannose and Galactose Metabolism	Carbohydrate	4	0	28	-0.528	0.5972

[Type here]

Lysoplasmalogen	Lipid	4	0	28	-0.528	0.5972
Pentose Metabolism	Carbohydrate	4	0	28	-0.528	0.5972
Phosphatidylinositol (PI)	Lipid	4	0	28	-0.528	0.5972
Progestin Steroids	Lipid	4	0	28	-0.528	0.5972
Acetylated Peptides	Peptide	3	0	28	-0.457	0.6476
Ascorbate and Aldarate Metabolism	Cofactors and Vitamins	3	0	28	-0.457	0.6476
Dihydrosphingomyelins	Lipid	3	0	28	-0.457	0.6476
Dipeptide	Peptide	3	0	28	-0.457	0.6476
Fatty Acid Metabolism (Acyl Choline)	Lipid	3	0	28	-0.457	0.6476
Medium Chain Fatty Acid	Lipid	3	0	28	-0.457	0.6476
Nicotinate and Nicotinamide Metabolism	Cofactors and Vitamins	3	0	28	-0.457	0.6476
Phenylalanine Metabolism	Amino Acid	3	0	28	-0.457	0.6476
Purine Metabolism, Adenine containing	Nucleotide	3	0	28	-0.457	0.6476
Tobacco Metabolite	Xenobiotics	3	0	28	-0.457	0.6476

<sup>1</sup>Number of metabolites are the number of detected metabolites assigned to the respective pathway.