

Supplementary Materials: Using NMR-Based Metabolomics to Evaluate Postprandial Urinary Responses Following Consumption of Minimally Processed Wheat Bran or Wheat Aleurone by Men and Women

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Table S1. VIPs, mean concentrations and differences in concentrations from ¹H NMR spectra of postprandial urine samples of aleurone *vs.* control at one hour for all chemical shifts having VIP value (for the first component) greater than 1 with 95% confidence (Jack-knifing (JK)).

Chemical Shift (ppm)	VIP Component 1	Aleurone		Control		Difference	%Difference
		Mean	S D	Mean	S D		
1.32	4.16249	14.27098	3.062182	7.251501	3.532878	-7.0194747	96.8
3.24	4.02001	8.238791	2.588537	15.48616	5.210814	7.24736637	-46.8
1.56	2.76565	6.473607	1.496637	3.359924	1.474532	-3.1136826	92.7
1.28	2.64036	8.245262	2.292278	5.049026	1.458486	-3.1962359	63.3
2.20	2.57021	6.966328	1.482933	4.224484	1.237119	-2.7418449	64.9
3.04	2.52177	131.2192	21.17296	140.6509	25.05072	9.43164082	-6.7
2.16	2.40019	9.034263	2.01052	6.329951	1.294214	-2.7043116	42.7
3.68	2.04940	24.73493	2.915893	21.96961	2.613812	-2.765314	12.6
3.56	2.04011	21.48823	12.23908	16.69236	4.407347	-4.7958611	28.7
2.64	1.91181	17.03774	4.481938	13.79421	4.72138	-3.2435321	23.5
3.20	1.82369	10.11876	2.830314	12.41903	2.017475	2.30026418	-18.5
2.56	1.82318	17.86715	4.32289	14.81978	4.639181	-3.0473721	20.6
0.88	1.80630	6.056719	1.614553	4.274602	1.145499	-1.7821171	41.7
2.68	1.77217	11.47222	2.989625	9.088912	2.670513	-2.3833079	26.2
7.12	1.72949	7.563787	2.595824	10.1234	4.151092	2.55960879	-25.3
7.56	1.67562	8.993662	5.203298	6.364859	2.274758	-2.6288023	41.3
2.52	1.60445	12.81225	2.705371	10.60473	3.280017	-2.2075179	20.8
1.36	1.44145	6.628033	1.925712	5.156502	1.243227	-1.4715309	28.5
1.48	1.42126	7.383495	2.577708	5.792986	1.149702	-1.5905089	27.5
1.52	1.38900	4.552364	1.597154	3.174042	1.449549	-1.3783217	43.4
3.72	1.32316	24.77209	6.872864	27.50995	7.370964	2.73785758	-9.9
8.20	1.27111	1.62975	0.745981	2.541526	0.74379	0.91177571	-35.9
6.20	1.23316	2.059606	1.095524	3.157927	1.341406	1.09832099	-34.8
3.88	1.21410	12.07729	3.242255	10.51419	2.078541	-1.5631039	14.9
3.28	1.20412	39.61967	14.88219	36.19298	12.36631	-3.4266905	9.5
7.84	1.18946	9.148038	5.364928	7.251094	2.732067	-1.8969441	26.2
6.04	1.15493	2.670983	1.364873	3.718709	1.2259	1.04772621	-28.2
3.36	1.14254	5.396922	0.836671	4.497122	1.047115	-0.8997994	20.0
1.40	1.10427	3.597015	1.390195	2.679131	0.671401	-0.9178847	34.3
0.80	1.09112	1.663855	0.736458	2.486962	0.98416	0.82310676	-33.1
8.12	1.08660	1.564265	0.772817	2.418736	1.103402	0.85447033	-35.3
8.16	1.05923	1.594912	0.741849	2.304637	0.604794	0.70972484	-30.8
8.08	1.03982	1.746189	0.660921	2.435821	0.663232	0.68963148	-28.3
7.88	1.02049	1.514524	0.793137	2.213375	0.634138	0.69885115	-31.6
6.40	1.01839	1.843823	0.809777	2.560051	0.70907	0.71622764	-27.9
8.24	1.00073	1.807235	0.983574	2.607875	1.033628	0.80064038	-30.7

Table S2. VIPs, mean concentrations and differences in concentrations from ¹H NMR spectra of postprandial urine samples of aleurone *vs.* control at two hours for all chemical shifts having VIP value (for the first component) greater than 1 with 95% confidence (Jack-knifing (JK)).

Chemical Shift (ppm)	VIP Component	Aleurone		Control		Difference	%Difference
		Mean	S D	Mean	S D		
1.32	4.12820	10.58116	2.690213	5.068215	1.417053	-5.51294	108.8
3.24	3.99567	8.889558	1.857856	15.48453	5.350281	6.594973	-42.6
3.92	3.25484	17.91443	7.870071	11.68593	4.777831	-6.2285	53.3
3.68	2.96992	26.68105	3.804554	21.92234	4.805783	-4.75872	21.7
3.04	2.76697	130.0666	32.05445	140.5462	22.52962	10.47969	-7.5
2.16	2.56255	8.651467	2.097343	5.860334	1.571695	-2.79113	47.6
1.56	2.55878	6.246367	1.034049	3.741607	1.60901	-2.50476	66.9
2.20	2.52924	6.39849	1.257234	4.019585	1.22371	-2.37891	59.2
1.28	2.19122	7.336893	1.969555	5.08087	1.476247	-2.25602	44.4
3.88	1.86983	12.26883	2.369351	10.08988	2.421863	-2.17895	21.6
7.56	1.73913	8.931182	3.697961	6.627128	2.713853	-2.30405	34.8
3.56	1.68759	19.68856	15.695	15.62201	4.22624	-4.06655	26.0
3.72	1.64661	23.5168	6.926321	26.75966	7.677015	3.242852	-12.1
2.72	1.59706	7.308311	0.809606	8.84356	2.070914	1.535249	-17.4
7.84	1.56286	9.005062	4.298748	6.874986	2.494041	-2.13008	30.9
0.88	1.56004	5.225581	1.31502	3.971861	0.842471	-1.25372	31.6
3.20	1.52903	10.38416	2.419885	12.26833	3.067967	1.884173	-15.4
1.36	1.50424	5.875327	1.241649	4.617884	1.165326	-1.25744	27.2
1.52	1.47182	4.091221	1.372411	2.931726	0.679603	-1.15949	39.5
3.64	1.36743	21.24291	2.927706	19.63015	2.230882	-1.61277	8.2
8.04	1.36031	4.114875	1.798802	5.746628	3.225487	1.631754	-28.4
6.32	1.32868	2.181474	0.946195	3.196211	1.063185	1.014737	-31.7
7.12	1.31352	7.523299	1.810512	9.192125	3.744832	1.668826	-18.2
7.28	1.29916	5.603135	0.951467	4.506218	1.485876	-1.09692	24.3
3.60	1.26684	10.0813	1.418628	8.709099	2.642426	-1.3722	15.8
3.80	1.25362	20.62982	4.68134	18.93676	1.794172	-1.69305	8.9
8.00	1.22489	5.299584	2.180769	4.147602	0.891356	-1.15198	27.8
2.24	1.20716	6.914553	1.201491	5.928257	1.193245	-0.9863	16.6
5.84	1.19703	4.675383	1.565235	5.880151	2.092716	1.204768	-20.5
7.36	1.15432	14.89945	6.204194	12.83476	6.039477	-2.06468	16.1
3.96	1.14727	26.08123	4.571917	24.46342	2.922645	-1.61781	6.6
6.12	1.09125	2.506214	0.708541	3.264201	0.962606	0.757987	-23.2
8.72	1.05726	1.520031	0.43754	2.235113	1.027241	0.715082	-31.9
6.72	1.05630	1.820275	0.604988	2.612203	1.262673	0.791928	-30.3
6.36	1.05137	2.220641	0.665685	2.995081	1.179953	0.77444	-25.9
8.60	1.04735	1.592131	0.508814	2.290507	0.9637	0.698376	-30.5
5.92	1.04555	2.294618	0.941447	3.097444	1.16875	0.802826	-25.9
6.56	1.04503	2.288887	0.798836	3.082522	1.216018	0.793634	-25.7
6.44	1.03204	2.343104	0.811768	3.14314	1.286103	0.800036	-25.5
3.52	1.01803	7.737351	1.810099	6.713265	1.962173	-1.02409	15.3
2.28	1.01244	9.226281	2.920357	7.950052	3.090526	-1.27623	16.1

Table S3. VIPs, mean concentrations and differences in concentrations from ¹H NMR spectra of postprandial urine samples of bran *vs.* control at one hour for all chemical shifts having VIP value (for the first component) greater than 1 with 95% confidence (Jack-knifing (JK)).

Chemical Shift (ppm)	VIP Component 1	Bran		Control		Difference	%Difference
		Mean	S D	Mean	S D		
1.32	3.22976	14.03238	4.202006	7.251501	3.532878	-6.78088	93.5
3.04	2.86864	125.8705	35.36431	140.6509	25.05072	14.78038	-10.5
1.56	2.82864	7.656341	1.730762	3.359924	1.474532	-4.29642	127.9
2.16	2.80171	10.41921	1.486837	6.329951	1.294214	-4.08926	64.6
2.20	2.48770	7.529601	1.17753	4.224484	1.237119	-3.30512	78.2
1.28	2.47481	8.523068	1.529586	5.049026	1.458486	-3.47404	68.8
3.28	2.13642	45.76975	31.2463	36.19298	12.36631	-9.57677	26.5
3.68	2.08969	25.92788	4.657039	21.96961	2.613812	-3.95827	18.0
3.24	2.06281	11.24925	3.377741	15.48616	5.210814	4.236908	-27.4
3.52	1.83286	8.874555	1.622894	6.551043	1.325381	-2.32351	35.5
3.88	1.69588	13.0864	2.655948	10.51419	2.078541	-2.57221	24.5
3.48	1.58521	4.57805	1.62778	2.756616	0.771308	-1.82143	66.1
7.12	1.57914	7.181518	3.319688	10.1234	4.151092	2.941877	-29.1
1.52	1.46920	4.807517	0.784111	3.174042	1.449549	-1.63347	51.5
3.60	1.44529	10.71369	1.677407	8.904177	1.517849	-1.80951	20.3
0.88	1.41586	5.807304	1.119021	4.274602	1.145499	-1.5327	35.9
1.36	1.40303	6.642524	0.846141	5.156502	1.243227	-1.48602	28.8
2.32	1.35996	4.124396	1.445991	2.725516	0.363736	-1.39888	51.3
6.12	1.33917	1.743012	1.062808	3.099028	0.915711	1.356016	-43.8
2.40	1.29894	4.226376	1.454959	2.883284	0.493987	-1.34309	46.6
6.52	1.24760	1.495537	0.799044	2.609847	0.696087	1.11431	-42.7
2.08	1.23366	7.955319	1.700262	6.469628	1.358598	-1.48569	22.9
6.04	1.19758	2.352536	1.502606	3.718709	1.2259	1.366173	-36.7
3.92	1.17109	18.50879	10.04208	15.17661	8.72161	-3.33218	21.9
8.36	1.14194	1.499548	0.588641	2.481909	0.800473	0.982361	-39.6
6.48	1.13920	1.469445	0.684679	2.361819	0.423019	0.892374	-37.8
8.08	1.13438	1.495018	0.634877	2.435821	0.663232	0.940803	-38.6
8.24	1.12107	1.528618	0.815723	2.607875	1.033628	1.079257	-41.4
8.44	1.11464	1.341518	0.829322	2.313624	0.660986	0.972105	-42.0
5.92	1.10277	1.801126	0.931051	2.838936	0.864324	1.03781	-36.6
6.00	1.10246	1.740932	0.977829	2.822414	0.9943	1.081482	-38.3
3.56	1.09193	19.41944	9.454625	16.69236	4.407347	-2.72707	16.3
6.20	1.09136	1.958378	1.205285	3.157927	1.341406	1.199549	-37.9
3.72	1.08381	24.72037	7.960002	27.50995	7.370964	2.789585	-10.1
7.88	1.07787	1.312408	0.730276	2.213375	0.634138	0.900967	-40.7
1.72	1.07724	4.090233	1.499458	2.916696	1.008155	-1.17354	40.2
6.56	1.07070	1.556704	0.930317	2.533062	0.754844	0.976358	-38.5
6.72	1.06493	1.401119	0.806436	2.313751	0.650196	0.912632	-39.4
6.64	1.06436	1.524363	0.777374	2.459477	0.765956	0.935114	-38.0
6.16	1.06166	1.754865	0.930114	2.761349	0.91607	1.006483	-36.4
1.68	1.04916	4.06487	1.339947	2.958195	1.020548	-1.10668	37.4
2.28	1.03384	9.272414	3.194829	7.628114	2.517126	-1.6443	21.6
6.60	1.03281	1.473845	0.80967	2.363446	0.683028	0.889601	-37.6
8.88	1.03014	1.163835	0.73215	2.050069	0.751731	0.886234	-43.2
8.52	1.02924	1.173862	0.709709	2.007899	0.580988	0.834037	-41.5
8.40	1.02075	1.41175	0.931872	2.291947	0.546338	0.880197	-38.4
8.76	1.01721	1.22601	0.750698	2.130143	0.849487	0.904133	-42.4
6.28	1.01390	1.604322	0.888807	2.541234	0.876	0.936912	-36.9
1.76	1.01269	3.556252	1.249734	2.577541	0.658803	-0.97871	37.9
5.96	1.01143	1.715038	0.890254	2.686527	1.022677	0.971489	-36.2
9.04	1.01010	1.138126	0.694567	1.967909	0.648979	0.829783	-42.2
8.04	1.01004	3.864529	2.350451	5.503831	3.426292	1.639301	-29.8
9.16	1.00815	1.209	0.783377	2.046918	0.598297	0.837918	-40.9
8.32	1.00750	1.358208	0.787128	2.266683	0.874335	0.908475	-40.1
2.12	1.00287	7.279841	1.525802	6.139425	1.288506	-1.14042	18.6

Table S4. VIPs, mean concentrations and differences in concentrations from ^1H NMR spectra of postprandial urine samples of bran *vs.* control at two hours for all chemical shifts having VIP value (for the first component) greater than 1 with 95% confidence (Jack-knifing (JK)).

Chemical Shift (ppm)	VIP Component 1	Bran		Control		Difference	%Difference
		Mean	S D	Mean	S D		
1.32	4.99671	14.56618	3.347656	5.068215	1.417053	-1.87403	187.4
3.04	3.69807	121.4823	32.31417	140.5462	22.52962	0.135642	-13.6
2.16	3.31868	10.37552	2.252464	5.860334	1.571695	-0.77047	77.0
1.56	3.27916	8.147486	2.46779	3.741607	1.60901	-1.17754	117.8
2.20	3.27164	8.422423	1.947318	4.019585	1.22371	-1.09535	109.5
1.28	2.69190	8.623663	1.701308	5.08087	1.476247	-0.69728	69.7
3.68	2.58043	29.29499	7.445593	21.92234	4.805783	-0.33631	33.6
3.28	2.24345	36.65182	15.80437	30.98786	6.875153	-0.18278	18.3
3.88	2.20662	14.18108	2.052555	10.08988	2.421863	-0.40548	40.5
3.24	2.13798	11.38725	4.252732	15.48453	5.350281	0.264605	-26.5
3.92	2.10417	16.14767	6.609428	11.68593	4.777831	-0.38181	38.2
1.52	2.02322	4.72478	1.480755	2.931726	0.679603	-0.6116	61.2
3.56	1.94370	21.46209	10.54476	15.62201	4.22624	-0.37384	37.4
1.24	1.89483	8.553053	5.04785	9.375028	2.237279	0.087677	-8.8
1.36	1.48712	5.867329	1.252633	4.617884	1.165326	-0.27057	27.1
0.88	1.43091	5.089939	1.164659	3.971861	0.842471	-0.2815	28.2
6.32	1.36127	1.884843	0.753703	3.196211	1.063185	0.410288	-41.0
3.80	1.35580	22.12046	4.073146	18.93676	1.794172	-0.16812	16.8
6.44	1.31358	1.859738	0.848478	3.14314	1.286103	0.408319	-40.8
3.60	1.27876	11.1747	2.525064	8.709099	2.642426	-0.28311	28.3
3.52	1.21077	8.992438	1.828222	6.713265	1.962173	-0.3395	33.9
6.12	1.16552	2.135908	0.932849	3.264201	0.962606	0.345657	-34.6
8.04	1.15442	4.053297	2.156819	5.746628	3.225487	0.294665	-29.5
2.64	1.13131	13.44189	3.893371	15.5738	5.368122	0.136891	-13.7
7.84	1.02218	5.449178	1.936268	6.874986	2.494041	0.207391	-20.7
3.40	1.01008	5.408643	2.069119	4.36044	1.906471	-0.24039	24.0