Comparative Compositions of Metabolites and Dietary Fibre Components in Doughs and Breads Produced from Bread Wheat, Emmer and Spelt and using Yeast and Sourdough Processes

Supporting Material

Table S1. Recipes and conditions used to make the yeast and sourdough breads.
*the energy for mixing and kneading reflects the strength of the doughs.

WHEAT YEAST BREAD

ingredients	**%**	**Weight (g)**
Wheat flour	100	3500
Yeast IDY	0,6	21
Salt (with iodine)	1,5	52,5
Sugar	1	35
Sunflour oil	2	70
Water	80	2870

conditions		**units**
Flour temperature	23	°C
Water temperature / ice water	2	°C
Mixing	3	minutes
Rest 30 minutes, autolyse		
Mixing	3	minutes
Kneading, 2nd speed	circa 10	minutes
Energy for mixing and kneading*	393	KJ
Dough temperature	25	°C
Dough assessment	elastic/ slightly sticky	
Bulk fermentation	45	minutes

Temperature bulk fermentation	27	°C
Scale	870	gram
Modelling	equal/ 28 cm	
Dough assessment	flexible/ liquid	
Final proof	30	°C
Time	70	minutes
Baking program WOW 10	235 / 255	°C
Total baking time	38	minutes
Cooling down	1	hrs

SPELT YEAST BREAD

ingredients	**%**	**Weight (g)**
Spelt flour	100	3500
Yeast IDY	0,6	21
Salt (with iodine)	1,5	52.5
Sugar	1	35
Sunflour oil	2	70
Water	73	2555

conditions		units
Flour temperature	23	°C
Water temperature / ice water	2	°C
Mixing	3	minutes
Rest 30 minutes, autolyse		
Mixing	3	minutes
Kneading, 2nd speed	circa 10	minutes
Energy for mixing and kneading*	393	KJ

Dough temperature	25	°C
Dough assessment	elastic/ sticky	
Bulk fermentation	45	minutes
Temperature bulk fermentation	27	°C
Scale	870	gram
Modelling	equal/ 28 cm	
Dough assessment	flexible/ liquid	
Final proof	30	°C
Time	70	minutes
Baking program WOW 10	235 / 255	°C
Total baking time	38	minutes
Cooling down	1	hrs

EMMER YEAST BREAD

ingredients	**%**	**Weight (g)**
Emmer flour	100	3500
Yeast IDY	0,8	28
Salt (with iodine)	1,5	52,5
Sugar	1	35
Sunflour oil	2	70
Water	70	2450

conditions		**units**
Flour temperature	23	°C
Water temperature / ice water	2	°C
Mixing	3	minutes
Rest 30 minutes, autolyse		

Mixing	3	minutes
Kneading, 2nd speed	circa 10	minutes
Energy for mixing and kneading*	377	KJ
Dough temperature	25	°C
Dough assessment	elastic/ liquid	
Bulk fermentation	45	minutes
Temperature bulk fermentation	27	°C
Scale	900	gram
Modelling	equal/ 28 cm	
Dough assessment	flexible/ very liquid	
Final proof	30	°C
Time	70	minutes
Baking program WOW 10	235 / 255	°C
Total baking time	37	minutes
Cooling down	1	hrs

WHEAT SOURDOUGH BREAD

ingredients	**%**	**Weight (g)**
Wheat flour	100	3500
Wheat sourdough	20	700
Salt (with iodine)	1,5	57,8
Sugar	1	38,5
Sunflour oil	2	77
Water	72,7	2450

Conditions		**units**
Flour temperature	23	°C

Sourdough temperature	25	°C
Water temperature		°C
Mixing	1	minute
Kneading, only slow speed	15	minute
Energy for mixing and kneading*	421,09	KJ
Dough temperature	26	°C
Dough assessment	elastic/ flexible	
Bulk fermentation	15	hrs
Temperature bulk fermentation	5	°C
Controlled Dough Climate	4	hrs
Dough acclimatize until	16	°C
Scale	900	gram
Modelling	equal/ 28 cm	
Dough assessment	flexible/ tension	
Final proof	27	°C
Time	4	hrs
Baking program WOW 11 SD	235 / 255	°C
after 10 minutes	225 / 235	°C
Total baking time	37	minutes
Cooling down	1	hrs

SPELT SOURDOUGH BREAD

ingredients	**%**	**Weight (g)**
Spelt flour	100	3500
Spelt sourdough	20	700
Salt (with iodine)	1,5	57,8
Sugar	1	38,5

Sunflour oil	2	77
Water	72,7	2450

Conditions		**units**
Flour temperature	23	°C
Sourdough temperature	25	°C
Water temperature	6-8	°C
Mixing	1	minute
Kneading, only slow speed	15	minute
Energy for mixing and kneading*	421,09	KJ
Dough temperature	26	°C
Dough assessment	elastic/ flexible	
Bulk fermentation	15	hrs
Temperature bulk fermentation	5	°C
Controlled Dough Climate	4	hrs
Dough acclimatize until	16	°C
Scale	900	gram
Modelling	equal/ 28 cm	
Dough assessment	flexible/ tension	
Final proof	27	°C
Time	4	hrs
Baking program WOW 11 SD	235 / 255	°C
after 10 minutes	225 / 235	°C
Total baking time	37	minutes
Cooling down	1	hrs

EMMER SOURDOUGH BREAD

ingredients	**%**	**Weight (g)**

Emmer flour	100	3500
Emmer sourdough	20	700
Salt (with iodine)	1,5	57,8
Sugar	1	38,5
Sunflour oil	2	77
Water	72,7	2450

Conditions		**units**
Flour temperature	23	°C
Sourdough temperature	25	°C
Water temperature	6-8	°C
Mixing	1	minute
Kneading, only slow speed	15	minute
Energy for mixing and kneading*	419	KJ
Dough temperature	26	°C
Dough assessment	elastic/ flexible	
Bulk fermentation	15	hrs
Temperature bulk fermentation	5	°C
Controlled Dough Climate	4	hrs
Dough acclimatize until	16	°C
Scale	900	gram
Modelling	equal/ 28 cm	
Dough assessment	flexible/ tension	
Final proof	27	°C
Time	4	hrs
Baking program WOW 11 SD	235 / 255	°C

after 10 minutes	225 / 235	°C
Total baking time	37	minutes
Cooling down	1	hrs

Supplementary Table S2. Preparation of sourdough starter.

A	**Start sourdough**	50	gram	Maillander Le Chef starter
		250	gram	Wholemeal flour
		250	gram	Water 25°C
	start up phase		17hours	25°C
B	**sourdough**	500	gram	Sourdough starter (step A)
		500	gram	Wholemeal flour
		500	gram	Water 25°C
	restart phase		4hours	25°C
C	**sourdough**	500	gram	Sourdough starter (step B)
		500	gram	Wholemeal flour
		500	gram	Water 25°C
	restart phase		4hours	25°C

Supplementary Table S3. P values (A) and Tables of means (B) from ANOVA of contents of polar metabolites in flour, dough and bread of the three types of wheat.

Some variables required transformation (square root or $\log_e$) to meet the assumptions of the analysis. Where this is the case it has been indicated in the tables
Further details are given in Statistical Analyses section.

A. P values for individual components

Statistically significant values ($p < 0.05$) are in bold.

	Processed cf flour vs dough or bread	type.processed	processed.dough	type.processed.dough	processed.stage	type.processed.stage	processed.stage.dough	type.processed.stage.dough
Metabolites by NMR								
Adenosine	**0.002**	**0.024**	**<0.001**	**0.015**	0.319	0.117	**0.041**	**0.028**
Trigonelline	0.082	**0.003**	0.912	**0.004**	**0.03**	0.181	**0.003**	**0.019**
Tryptophan	0.234	**0.012**	**<0.001**	**0.048**	**0.002**	0.517	**0.007**	**0.027**
Tyrosine	0.127	**0.041**	**<0.001**	**0.021**	**<0.001**	0.804	0.068	**0.045**
Fumarate	0.681	0.059	**<0.001**	**0.004**	0.28	0.359	**0.014**	0.135
Raffinose	**<0.001**	**<0.001**	**<0.001**	**0.041**	**<0.001**	0.722	0.193	**0.006**
Sucrose	**<0.001**	**<0.001**	**0.003**	**0.015**	**<0.001**	0.456	**<0.001**	**0.016**
log Maltose	**<0.001**	**<0.001**	**<0.001**	**<0.001**	**<0.001**	**0.001**	**<0.001**	0.11
Alpha-Glucose/Maltose	**<0.001**	**<0.001**	**<0.001**	**<0.001**	**0.002**	0.32	**<0.001**	0.242
log beta-Glucose	**<0.001**	0.074	**<0.001**	0.407	**<0.001**	0.139	0.183	**0.02**
log beta-Arabinose	**<0.001**	**0.022**	**<0.001**	**0.009**	**<0.001**	0.396	**0.041**	0.087
Trehalose	**<0.001**	**0.01**	**<0.001**	**0.001**	**<0.001**	0.416	**<0.001**	0.104
sqrt Fructose	**<0.001**	**<0.001**	0.342	**0.002**	**<0.001**	0.151	**<0.001**	**0.03**
sqrt Mannitol	**<0.001**	**<0.001**	**<0.001**	0.064	**<0.001**	0.588	**<0.001**	0.066
Glycerol	**0.01**	**<0.001**	0.17	0.065	**<0.001**	0.445	**<0.001**	0.889
sqrt Lactic acid	**<0.001**	**<0.001**	**<0.001**	**<0.001**	**<0.001**	**0.001**	**<0.001**	**<0.001**
sqrt Succinic acid	**<0.001**	0.08	**<0.001**	**0.001**	**<0.001**	0.413	0.909	0.987
Malic acid	0.11	0.74	0.323	**0.034**	0.97	**0.028**	0.838	**0.006**
Phenylalanine	**<0.001**	**0.002**	**<0.001**	**<0.001**	**0.001**	0.699	**0.066**	**0.016**

log Alanine	**<0.001**	**<0.001**	**<0.001**	**<0.001**	**<0.001**	**0.006**	**<0.001**	**0.039**
sqrt Asparagine	**0.01**	0.644	**<0.001**	**0.03**	**<0.001**	0.837	**0.025**	0.093
sqrt Aspartate	**0.001**	0.055	**<0.001**	**0.002**	**<0.001**	0.755	**0.002**	0.244
sqrt GABA	**<0.001**	**0.038**	**<0.001**	0.165	**<0.001**	0.765	0.075	0.395
Glutamate	**<0.001**	**<0.001**	**<0.001**	**<0.001**	**<0.001**	0.723	0.385	0.805
Glutamine	**<0.001**	0.053	**<0.001**	**0.014**	**<0.001**	0.494	**0.004**	0.145
Methionine	**<0.001**	**0.009**	**<0.001**	**<0.001**	**<0.001**	**0.002**	**<0.001**	0.139
Leucine	**<0.001**	**<0.001**	**<0.001**	**<0.001**	**<0.001**	0.604	**0.048**	0.773
sqrt Isoleucine	**<0.001**	**0.012**	**<0.001**	**0.039**	**<0.001**	0.571	**0.003**	0.642
sqrt Valine	**<0.001**	**0.04**	**<0.001**	**0.05**	**<0.001**	0.135	0.687	0.79
Glycine betaine	**<0.001**	**0.001**	**<0.001**	**<0.001**	0.1	0.687	**<0.001**	0.43
Choline	**<0.001**	0.643	**0.004**	0.581	0.572	0.303	0.152	**0.040**
log Choline sulfate	**0.004**	0.691	0.689	0.204	0.101	0.691	0.25	0.606

B. Table of means for components (mg/g dry wt)

		Total FODMAPs	Total mino acids	Sqrt total organic acids	Log total sugars	Total methyl donors
Emmer	wholemeal	46.22	11.73	1.903	4.105	5.772
	sourdough bread	65.68	18.41	5.454	5.125	8.107
	sourdough dough	64.2	23.40	5.361	5.202	8.741
	Yeast bread	43.89	8.36	1.993	5.194	7.752
	Yeast dough	35.64	12.70	2.195	4.926	7.509
Spelt	wholemeal	45.31	10.97	1.921	3.940	6.529
	sourdough bread	60.19	19.05	5.509	4.797	8.722
	sourdough dough	59.46	25.06	5.569	4.837	9.496
	Yeast bread	41.43	9.71	2.217	4.998	7.960

	Yeastdough	32.06	14.44	2.421	4.633	8.029
Wheat	wholemeal	43.43	9.78	2.048	3.901	5.358
	sourdough bread	57.04	15.00	5.156	4.728	7.045
	sourdough dough	53.59	20.74	5.080	4.724	7.682
	Yeast bread	37.09	7.52	2.248	4.864	7.235
	Yeast dough	30.79	12.14	2.412	4.539	7.038
SEM		0.8592	0.3452	0.02898	0.01848	0.2422

		Adenosine	Trigonelline	Tryptophan	Tyrosine	Fumarate	Raffinose
Emmer	wholemeal	0.4041	0.2008	1.0355	0.2450	0.1475	7.493
	sourdough bread	0.2607	0.1438	0.9808	0.2235	0.0930	3.830
	sourdough dough	0.2964	0.1581	1.0700	0.2886	0.0935	3.847
	yeast bread	0.5258	0.1513	0.7651	0.1661	0.1526	3.483
	yeast dough	0.5053	0.1624	0.8671	0.2026	0.1605	2.408
Spelt	wholemeal	0.3018	0.1275	0.9515	0.1877	0.1372	7.996
	sourdough bread	0.4143	0.2023	1.2492	0.2548	0.1228	4.014
	sourdough dough	0.3369	0.1773	1.2784	0.2773	0.1065	3.680
	yeast bread	0.4676	0.1038	0.8792	0.1437	0.1521	3.013
	Yeast dough	0.4843	0.1586	1.0247	0.2041	0.1631	2.287
Wheat	wholemeal	0.2557	0.1141	0.8851	0.1661	0.1464	6.722
	sourdough bread	0.3431	0.1887	1.0507	0.2178	0.1224	3.926
	sourdough dough	0.2859	0.1523	0.9915	0.2204	0.1060	3.202
	yeast bread	0.4841	0.1399	0.7079	0.1419	0.1834	2.986
	Yeast dough	0.7614	0.3139	1.0973	0.2544	0.2386	2.974

SEM		0.04572	0.02262	0.05112	0.01717	0.01066	0.1612

		Sucrose	Log Maltose	Alpha-glucose and maltose	Log beta-glucose	Log beta-arabinose	Trehalose
Emmer	wholemeal	20.93	2.945	3.87	0.398	-1.2176	0.728
	sourdough bread	8.39	4.435	18.50	2.199	-0.6032	2.347
	sourdough dough	8.33	4.523	22.72	2.261	-0.4502	2.417
	yeast bread	10.25	4.601	17.03	1.063	-1.1522	2.401
	Yeast dough	6.78	4.274	14.66	1.218	-1.0219	1.867
Spelt	wholemeal	18.58	2.655	3.09	0.268	-1.2697	0.576
	sourdough bread	9.31	3.889	12.52	2.182	-0.3613	2.605
	sourdough dough	8.78	3.932	16.19	2.297	-0.3278	2.577
	yeast bread	9.36	4.22	13.24	1.248	-1.0376	2.271
	yeast dough	6.67	3.830	10.35	1.239	-0.9158	1.591
Wheat	wholemeal	17.41	2.650	3.10	0.286	-1.3622	0.615
	sourdough bread	9.66	3.843	11.34	2.059	-0.5562	2.146
	sourdough dough	8.65	3.842	14.55	2.231	-0.5323	2.018
	yeast bread	9.14	4.190	11.31	1.055	-1.0793	1.968
	yeast dough	7.71	3.710	9.06	1.135	-0.7920	1.596
SEM		0.3060	0.01844	0.2558	0.02490	0.04155	0.06753

		Sqrt Fructose	Sqrt Mannitol	Glycerol	Sqrt Lactic acid	Sqrt Succinic acid	Malic acid
Emmer	wholemeal	3.784	5.271	10.91	0.727	0.4442	2.747

	sourdough bread	6.705	6.717	16.72	4.858	0.9953	5.081
	sourdough dough	6.768	6.647	16.17	4.870	1.0433	3.839
	Yeast bread	6.914	4.768	17.67	0.893	0.5048	2.771
	Teast dough	6.239	4.388	13.97	1.197	0.5557	2.915
Spelt	wholemeal	3.652	4.973	12.57	0.714	0.4584	2.835
	sourdough bread	6.188	6.736	10.81	5.092	1.0829	3.121
	sourdough dough	6.075	6.708	10.78	5.112	1.1201	3.527
	yeast bread	6.639	4.946	13.95	0.901	0.5691	3.629
	yeast dough	5.861	4.390	10.50	1.342	0.6049	3.534
Wheat	wholemeal	3.550	4.3967	12.02	0.701	0.4705	3.337
	sourdough bread	5.900	6.501	10.86	4.751	0.9894	2.912
	sourdough dough	5.553	6.292	10.80	4.563	1.0148	3.844
	yeast bread	6.154	4.599	12.96	0.825	0.5827	3.852
	yeast dough	5.554	4.233	9.90	1.213	0.6113	3.736
SEM		0.06004	0.05035	0.3115	0.01855	0.01160	0.2245

		Phenylalanine	Log Alanine	Sqrt Asparagine	Sqrt Aspartate	Sqrt GABA	glutamate
Emmer	wholemeal	0.2991	-1.1292	0.9562	1.047	0.6184	4.380
	sourdough bread	0.3424	-0.6027	1.0156	1.312	1.0568	6.766
	sourdough dough	0.4327	-0.4315	1.2147	1.484	1.1969	8.564
	yeastdough bread	0.2009	-1.1437	0.4391	0.716	0.7255	3.483
	yeastdough dough	0.2339	-0.9308	0.6603	0.838	0.8651	5.245
Spelt	wholemeal	0.2196	-1.1678	0.9987	1.084	0.6323	3.903
	sourdough bread	0.4624	-0.5791	0.9764	1.322	1.0003	7.136

	sourdough dough	0.4859	-0.3740	1.2816	1.569	1.1963	9.073
	yeast bread	0.1790	-1.0839	0.6718	0.951	0.7699	3.800
	yeast dough	0.2482	-0.7825	0.8333	1.029	0.8913	5.657
Wheat	wholemeal	0.2029	-1.2661	0.8219	0.995	0.5791	3.581
	sourdough bread	0.3787	-0.7759	0.7541	1.158	0.8729	5.675
	sourdough dough	0.3609	-0.5766	1.1638	1.420	1.0913	7.583
	yeast bread	0.2109	-1.4249	0.4790	0.725	0.6118	3.103
	yeast dough	0.3833	-1.0381	0.5734	0.815	0.7270	4.774
SEM		0.02551	0.01777	0.04941	0.02768	0.02645	0.1127
		Glutamine	Methinonine	Leucine	Sqrt Isoleucine	Sqrt Valine	Glycine betaine
Emmer	wholemeal	0.5791	0.5340	1.363	0.5569	0.5171	2.612
	sourdough bread	0.8868	1.3411	2.704	0.6262	0.5763	3.726
	sourdough dough	1.2448	1.3392	3.500	0.8060	0.7417	4.062
	yeast bread	0.4118	0.4876	1.041	0.3384	0.3533	3.390
	yeast dough	0.7393	0.8275	1.712	0.5544	0.5340	3.233
Spelt	wholemeal	0.5675	0.4804	1.210	0.5463	0.5134	2.976
	sourdough bread	0.8896	1.2285	2.767	0.6636	0.5866	3.821
	sourdough dough	1.3550	1.4418	3.616	0.8421	0.7767	4.206
	yeast bread	0.5030	0.5304	1.076	0.3878	0.4048	3.759
	yeast dough	0.8281	0.9587	1.786	0.6005	0.5867	3.473
Wheat	wholemeal	0.5483	0.4502	1.140	0.5209	0.5033	2.270
	sourdough bread	0.7147	1.0364	2.191	0.5753	0.5229	2.960
	sourdough dough	1.2067	1.1398	3.012	0.7559	0.7292	3.234
	yeast bread	0.4536	0.4586	0.854	0.3169	0.3406	2.961
	yeast dough	0.7254	0.7859	1.617	0.5559	0.5580	2.736

SEM		0.03154	0.02316	0.04219	0.009942	0.01282	0.05286

		Choline	Log Choline sulphate	Log Acetate
Emmer	wholemeal	0.716	0.841	-2.356
	sourdough bread	1.429	1.063	0.430
	sourdough dough	1.219	1.214	0.483
	yeast bread	1.097	1.183	-1.277
	Yeast dough	1.213	1.122	-1.253
Spelt	wholemeal	0.583	1.088	-2.295
	sourdough bread	1.303	1.276	0.448
	sourdough dough	1.217	1.404	0.514
	Yeast bread	1.184	1.100	-1.245
	yeast dough	1.154	1.224	-1.257
Wheat	wholemeal	0.616	0.893	-2.458
	sourdough bread	1.205	1.036	0.404
	sourdough dough	1.309	1.132	0.413
	yeast bread	1.051	1.170	-1.350
	yeast dough	1.052	1.179	-1.368
SEM		0.05268	0.07239	0.02268

Supplementary Table S4. p values from ANOVA (A) and tables of means (B) of dietary fibre components and arabinoxylan oligosaccharide (AXOS) and gluco-oligosaccharide (GOS) fragments determined by enzyme fingerprinting of flour, dough and bread of the three types of wheat.

Further details are given in Statistical Analyses section.

A. P values

Statistically significant values (p <0.05) are in bold.

	processed	type.processed	processed.dough	type.processed.dough	processed.stage	type.processed.stage	processed.stage.dough	type.processed.stage.dough
DF components								
Klason lignin	0.122	0.410	**<0.001**	0.312	0.279	0.238	**0.018**	0.197
Uronic acid residues	0.231	0.926	0.620	0.498	**0.001**	0.089	0.463	0.438
Log arabinose	**0.002**	0.706	**0.005**	0.572	**0.003**	**0.014**	0.311	0.459
Log xylose	**0.016**	0.540	0.638	0.505	**0.002**	**0.019**	0.540	0.640
Mannose	**0.005**	0.198	**<0.001**	0.439	0.137	0.301	0.931	0.188
Galactose	0.079	0.848	**<0.001**	0.618	0.919	0.929	0.956	0.698
Sqrt glucose	**0.055**	0.916	**<0.001**	0.330	**<0.001**	0.440	0.466	0.398
Log total sugar residues	0.166	0.759	**0.009**	0.501	**<0.001**	**0.023**	0.478	0.560
Dietary fibre without fructans	0.563	0.657	0.616	0.870	**0.002**	0.058	0.469	0.982
Sqrt fructans	**<0.001**	**0.011**	**<0.001**	0.227	**<0.001**	0.117	**0.012**	0.411

Total dietary fibre (with fructans)	**0.006**	0.498	0.659	0.846	**0.009**	**0.046**	0.239	0.939
Log arabinoxylan	**0.019**	0.598	0.228	0.522	**0.002**	**0.015**	0.444	0.570
Log TOT β-glucan	**<0.001**	0.514	**0.002**	0.796	**<0.001**	**0.003**	**0.006**	0.142
AGP								
Galactose mg/g	**<0.001**	**0.002**	**<0.001**	**<0.001**	**<0.001**	0.634	0.151	**0.008**
Galactose nMoles/mg	**<0.001**	**0.002**	**<0.001**	**<0.001**	**<0.001**	0.634	0.151	**0.008**
Arabinose mg/g	**<0.001**	0.536	**0.040**	0.052	0.364	0.330	**0.002**	0.066
Arabinose nMoles/mg	**<0.001**	0.536	**0.040**	0.052	0.364	0.330	**0.002**	0.066
Ara:Gal	**<0.001**	**0.045**	**<0.001**	0.309	**<0.001**	**0.018**	**<0.001**	0.155
AXOS and GOS from fingerprinting								
Log Xylose	**<0.001**	0.484	**<0.001**	0.215	**<0.001**	**0.003**	**0.031**	0.179
Sqrt Xyl2	**<0.001**	0.615	**<0.001**	0.146	**<0.001**	**0.003**	0.052	0.314
Sqrt Xyl3	**<0.001**	0.564	0.651	0.726	**<0.001**	**<0.001**	0.291	0.116
Xyl5	**<0.001**	**<0.001**	**0.008**	0.158	**<0.001**	0.309	0.155	0.176
Log XA3XX	**<0.001**	0.679	**<0.001**	0.499	**<0.001**	**0.002**	0.052	0.188
logXA2 + 3XX	**<0.001**	0.763	**<0.001**	0.689	**0.016**	**0.025**	**0.044**	0.651
Log XA3A3XX	**0.004**	**<0.001**	**<0.001**	**<0.001**	**<0.001**	**<0.001**	**0.003**	0.217
Log XA3XA3XX	0.837	0.731	0.164	0.314	**<0.001**	**0.003**	**0.016**	**0.035**
XA3A23XX	**<0.001**	**0.004**	**0.025**	0.537	**0.003**	**0.049**	**0.013**	0.819
Xa3XA2 + 3XX	**<0.001**	**<0.001**	**0.009**	0.516	**0.004**	**<0.001**	**0.017**	0.574

G3	**<0.001**	**0.017**	0.060	0.711	**<0.001**	**0.002**	**0.024**	0.205
Sqrt G4	**<0.001**	0.127	**<0.001**	0.491	**<0.001**	**0.019**	**0.018**	0.066

B. Table of means

Dietary fibre (DF) fractions (mg/g dry wt)

		Klason lignin	Uronic acid residues	Log arabinose	Log xylose	mannose	galactose
Emmer	wholemeal	0.5911	0.1932	0.1575	0.6087	0.3049	0.2652
	sourdough bread	0.7353	0.1773	0.0298	0.4950	0.2901	0.2704
	sourdough dough	0.8700	0.1849	0.0378	0.5157	0.3006	0.2686
	Yeast bread	0.6139	0.1813	0.0387	0.4649	0.4017	0.2492
	yeast dough	0.5528	0.1770	0.0837	0.5176	0.3957	0.2498
Spelt	wholemeal	0.6554	0.2050	0.3181	0.8672	0.3315	0.3019
	sourdough bread	0.9266	0.1830	0.2311	0.8136	0.2924	0.3104
	sourdough dough	1.0324	0.1957	0.2089	0.8011	0.2979	0.3069
	yeast bread	0.7443	0.1939	0.2701	0.8413	0.3661	0.2852
	yeast dough	0.5722	0.2100	0.2968	0.8711	0.3950	0.2857
Wheat	wholemeal	0.6821	0.2808	0.5902	1.0942	0.3055	0.2717
	sourdough bread	0.7095	0.2687	0.4240	0.9245	0.2880	0.2730
	sourdough dough	0.8092	0.2832	0.5258	1.0561	0.2942	0.2780
	Yeast bread	0.5417	0.2679	0.4524	0.9328	0.3816	0.2503
	Yeast dough	0.6331	0.2801	0.5380	1.0440	0.3787	0.2478

SEM	wholemeal	0.06195	0.005037	0.02331	0.03024	0.009354	0.006267
	Dough/bread	0.05058	0.004113	0.01903	0.02469	0.007638	0.005117

		Sqrt glucose	Log total sugar residues	Dietary fibre without fructan	Sqrt fructan	Total dietary fibre	Log arabinoxylan
Emmer	wholemeal	1.080	1.557	5.531	0.8070	6.182	1.039
	sourdough bread	1.210	1.547	5.609	0.5022	5.861	0.910
	sourdough dough	0.957	1.435	5.256	0.5924	5.608	0.927
	yeast bread	1.245	1.575	5.628	0.3755	5.770	0.900
	yeast dough	1.029	1.497	5.201	0.4467	5.401	0.953
Spelt	wholemeal	1.218	1.770	6.734	0.9813	7.698	1.266
	sourdough bread	1.321	1.769	6.974	0.5872	7.319	1.194
	sourdough dough	1.107	1.666	6.518	0.6602	6.955	1.178
	yeast bread	1.417	1.839	7.227	0.5167	7.494	1.233
	yeast dough	1.198	1.767	6.636	0.5115	6.898	1.264
Wheat	wholemeal	1.367	1.979	8.206	1.1105	9.439	1.482
	sourdough bread	1.475	1.915	7.774	0.7518	8.340	1.351
	sourdough dough	1.261	1.906	7.825	0.8297	8.515	1.476
	yeast bread	1.531	1.959	7.921	0.6397	8.330	1.371
	yeast dough	1.315	1.932	7.829	0.6621	8.267	1.478
SEM	wholemeal	0.01421	0.02278	0.1672	0.01833	0.1675	0.02799
	Dough/bread	0.01160	0.01860	0.1365	0.01497	0.1367	0.02286

Table of means for AGP: galactose equivalents (mg and nMoles/mg dry wt), arabinose equivalents (mg and nMoles/mg dry wt) and ratios.

		Galactose mg/g	Galactose nMoles/mg	Arabinose mg/g	Arabinose nMoles/mg	Ara:Gal
Emmer	wholemeal	1.120	6.22	0.922	6.14	0.988
	sourdough bread	1.985	11.03	1.925	12.82	1.175
	sourdough dough	2.441	13.56	2.387	15.90	1.172
	yeast bread	1.412	7.84	2.229	14.85	1.891
	yeast dough	1.507	8.37	1.806	12.03	1.435
Spelt	wholemeal	1.104	6.13	0.883	5.88	0.959
	sourdough bread	2.753	15.29	2.058	13.71	0.896
	sourdough dough	3.074	17.08	2.472	16.46	0.965
	yeast bread	1.681	9.34	1.885	12.56	1.344
	yeast dough	1.789	9.94	1.848	12.31	1.240
Wheat	wholemeal	0.996	5.53	0.738	4.91	0.888
	sourdough bread	2.268	12.60	1.687	11.24	0.891
	sourdough dough	2.431	13.50	1.703	11.34	0.837
	yeast bread	1.576	8.76	1.801	12.00	1.370
	yeast dough	1.997	11.10	1.715	11.42	1.030
SEM		0.05959	0.3311	0.1057	0.7038	0.04765

Tables of means for oligosaccharide (AXOS) and gluco-oligosaccharide (GOS) fragments determined by enzyme fingerprinting (arbitrary units) and ratios of WE-xylose:TOT-xylose, TOT-arabinoxylan (AX) to β-glucan and ratio of G3:G4 GOS fragments.

		Log Xylose	sqrtXyl2	sqrtXyl3	Xyl5	Log XA3XX	Log XA2 + 3XX	logXA3A3XX
Emmer	wholemeal	1.268	2.210	0.7306	0.24773	0.4706	-0.0003	-0.9869
	sourdough bread	0.911	1.696	0.3053	0.04236	0.1015	-0.2583	-0.6668
	sourdough dough	1.180	1.965	0.4540	0.01771	0.1927	-0.2649	-0.7985
	yeast bread	0.841	1.649	0.3396	0.04131	0.0736	-0.3324	-0.9405
	yeast dough	0.878	1.693	0.4701	0.01806	0.0171	-0.4074	-1.1407
Spelt	wholemeal	1.529	2.454	0.8703	0.31878	0.7490	0.1300	-0.7738
	sourdough bread	1.179	1.949	0.4076	0.06228	0.3570	-0.1864	-0.9056
	sourdough dough	1.578	2.422	0.6993	0.03294	0.6124	0.0145	-0.8869
	yeast bread	0.991	1.801	0.3992	0.05726	0.2816	-0.2476	-0.8800
	yeast dough	1.233	2.059	0.6789	0.02751	0.3959	-0.2147	-1.0044
Wheat	wholemeal	1.733	2.637	0.9817	0.2337	1.0309	0.5023	-0.4127
	sourdough bread	1.303	2.064	0.4371	0.06192	0.5757	0.1995	-0.6859

	sourdough dough	1.726	2.576	0.7361	0.01747	0.8148	0.3608	-0.6572
	yeast bread	1.015	1.753	0.3913	0.04463	0.4715	0.1278	-0.6223
	yeast dough	1.451	2.272	0.8199	0.02171	0.7355	0.2088	-0.6365
SEM		0.04437	0.05809	0.02598	0.004287	0.03525	0.04074	0.01973

		Log XA3XA3XX	XA3A23XX	XA3XA2 + 3XX	G3 GOS	Sqrt G4 GOS	Log Sum AX peaks	Log G3 + G4 GOS
Emmer	wholemeal	-2.431	0.2359	0.4218	2.455	1.0243	2.560	1.2532
	sourdough bread	-2.340	0.1631	0.3845	1.134	0.6433	2.144	0.4349
	sourdough dough	-2.505	0.1699	0.3780	1.384	0.7243	2.342	0.6463
	yeast bread	-2.169	0.1532	0.4288	1.386	0.7434	2.089	0.6618
	yeast dough	-2.638	0.1473	0.3785	1.337	0.7126	2.093	0.6122
Spelt	wholemeal	-2.297	0.2630	0.4974	3.187	1.2080	2.791	1.5358
	sourdough bread	-2.230	0.1606	0.3310	1.484	0.7525	2.355	0.7157
	sourdough dough	-2.368	0.1833	0.3953	2.047	0.8541	2.719	1.0188
	yeast bread	-2.207	0.1663	0.3972	1.711	0.5848	2.235	0.8915

	yeast dough	-2.533	0.1672	0.4090	1.893	0.8778	2.439	0.9774
Wheat	wholemeal	-2.078	0.3555	0.5686	3.128	1.1443	2.995	1.1901
	sourdough bread	-2.009	0.2221	0.3725	1.266	0.6872	2.520	0.5520
	sourdough dough	-2.082	0.2507	0.4440	1.858	0.7890	2.881	0.9064
	yeast bread	-2.103	0.2212	0.3979	1.376	0.7522	2.308	0.6635
	yeast dough	-2.112	0.2335	0.4518	1.973	0.8722	2.692	1.0017
SEM		0.04437	0.005071	0.01194	0.07535	0.01824	0.04321	0.04303

		Log ratio WE-xylose: TOT-xylose	Log (ratio total AX:total β-glucan)	Log ratio G3:G4 GOS	Sqrt Fructan content	Log Fructan DP
Emmer	wholemeal	-2.424	1.307	0.8497	0.8014	3.373
	sourdough bread	-1.120	1.710	1.0068	0.5022	3.291
	sourdough dough	-1.275	1.696	0.9699	0.5934	2.506
	yeast bread	-1.681	1.427	0.9196	0.3755	2.151
	yeast dough	-1.629	1.481	0.9682	0.4467	2.415

Spelt	wholemeal	-2.223	1.255	0.7810	0.9880	3.854
	sourdough bread	-1.150	1.639	0.9621	0.5872	4.000
	sourdough dough	-0.903	1.700	1.0299	0.6602	3.649
	yeast bread	-13.90	1.344	0.8502	0.5167	3.645
	yeast dough	-1.432	1.461	0.8972	0.5115	3.927
Wheat	wholemeal	-2.156	1.505	0.8710	1.1094	4.628
	sourdough bread	-1.302	1.968	0.9858	0.7518	4.704
	sourdough dough	-0.961	1.975	1.0935	0.8297	4.461
	yeast bread	-1.521	1.644	0.8886	0.6397	4.844
	yeast dough	-1.591	1.690	0.9513	0.6621	5.177
SEM		0.1147	0.01351	0.01418	0.01497	0.2424

Figure S1: loaves baked from the emmer, spelt and bread wheat flours using yeast and sourdough (SD) systems

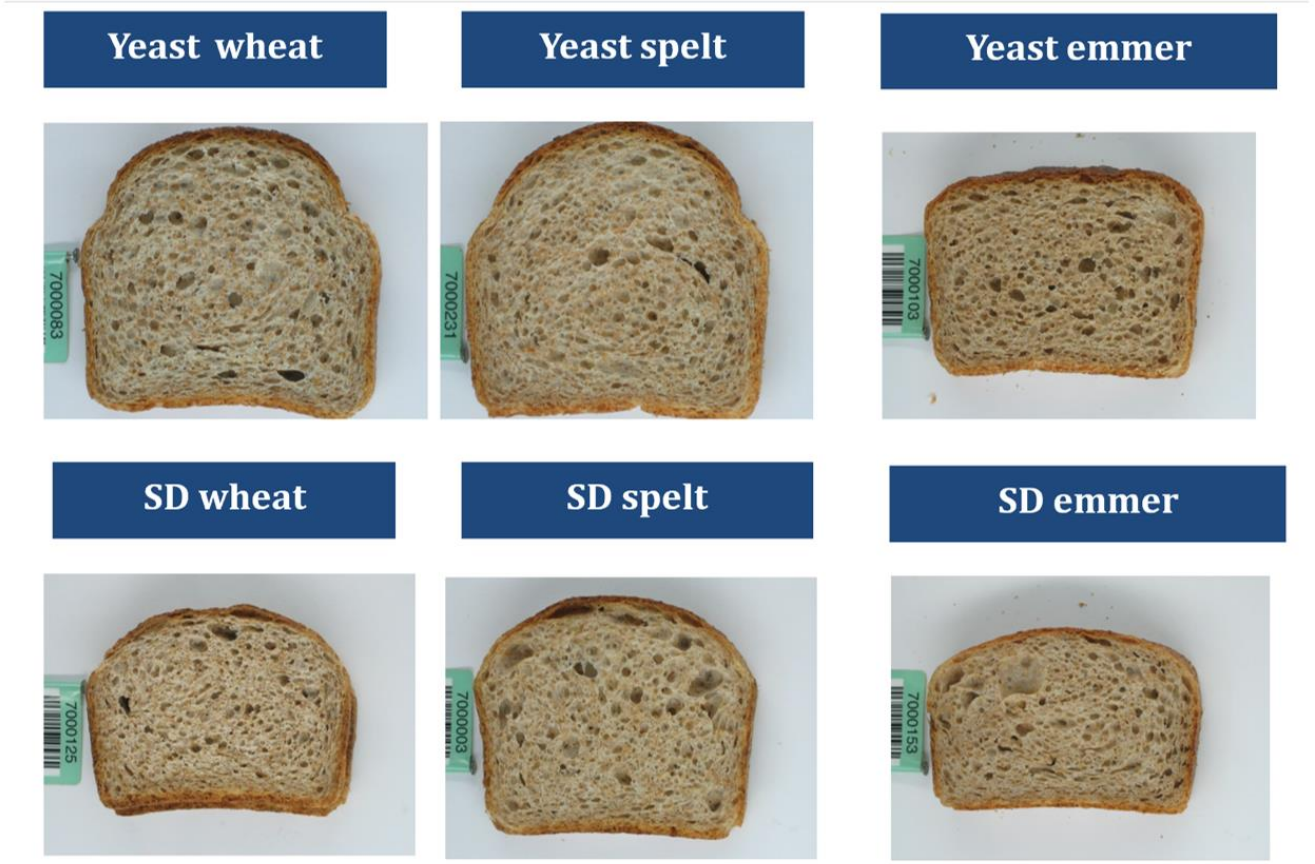

Figure S2. The contents of amino acids in the flour, dough and bread samples determined by ^{1}H NMR spectroscopy. The points are the values from three replicate analyses as described in the text.

AAsummed is combined amounts of all amino acids; Grainmix if the whole meal flours from the blended grains; GABA is γ-amino butyric acid.

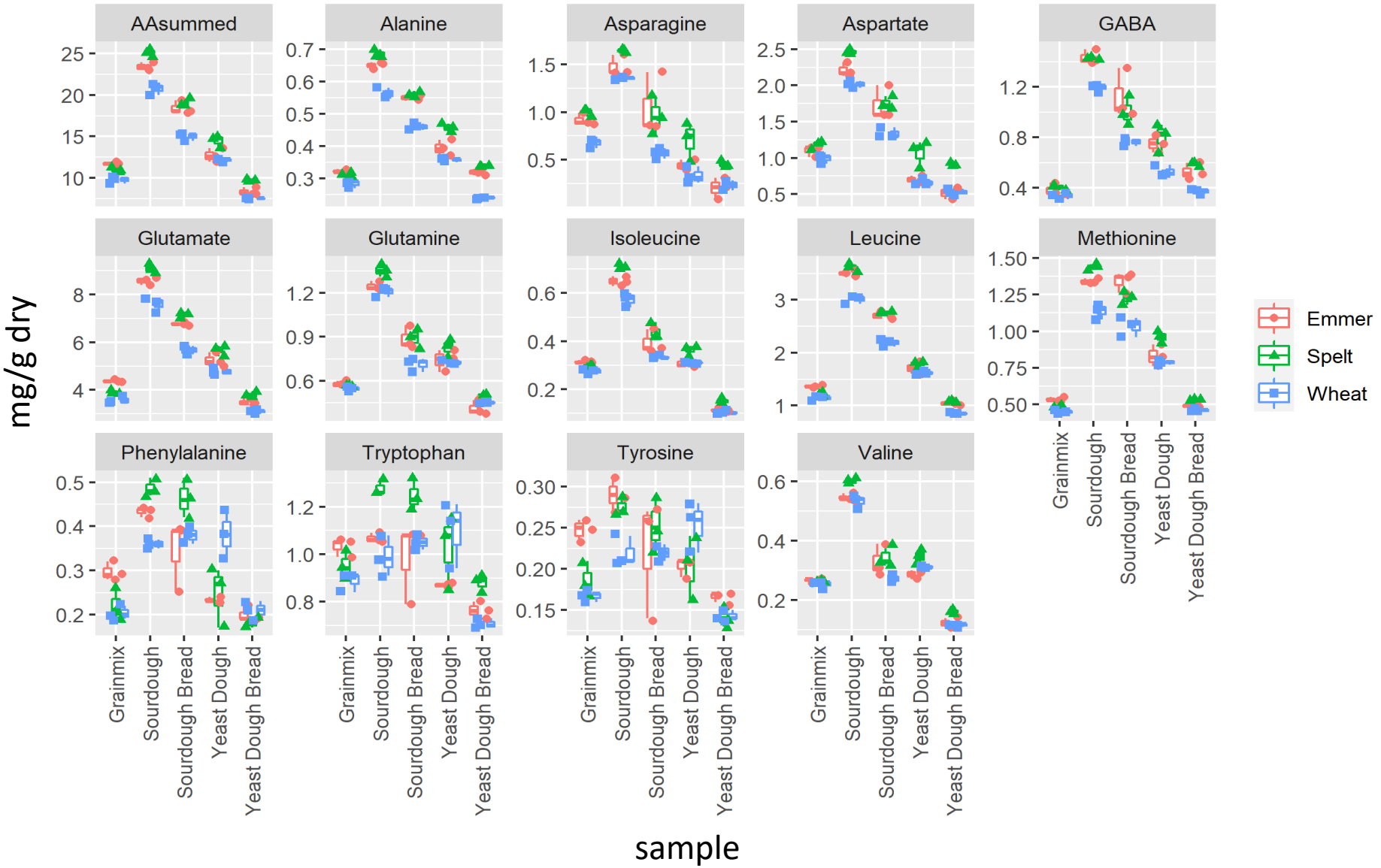

Figure S3. The contents of organic acids in the flour, dough and bread samples determined by ^{1}H NMR spectroscopy (A) and mass spectrometry (B). The points are the values from three replicate analyses as described in the text. AcidsNMR summed is combined amounts of all organic acids; Grainmix if the whole meal flours from the blended grains

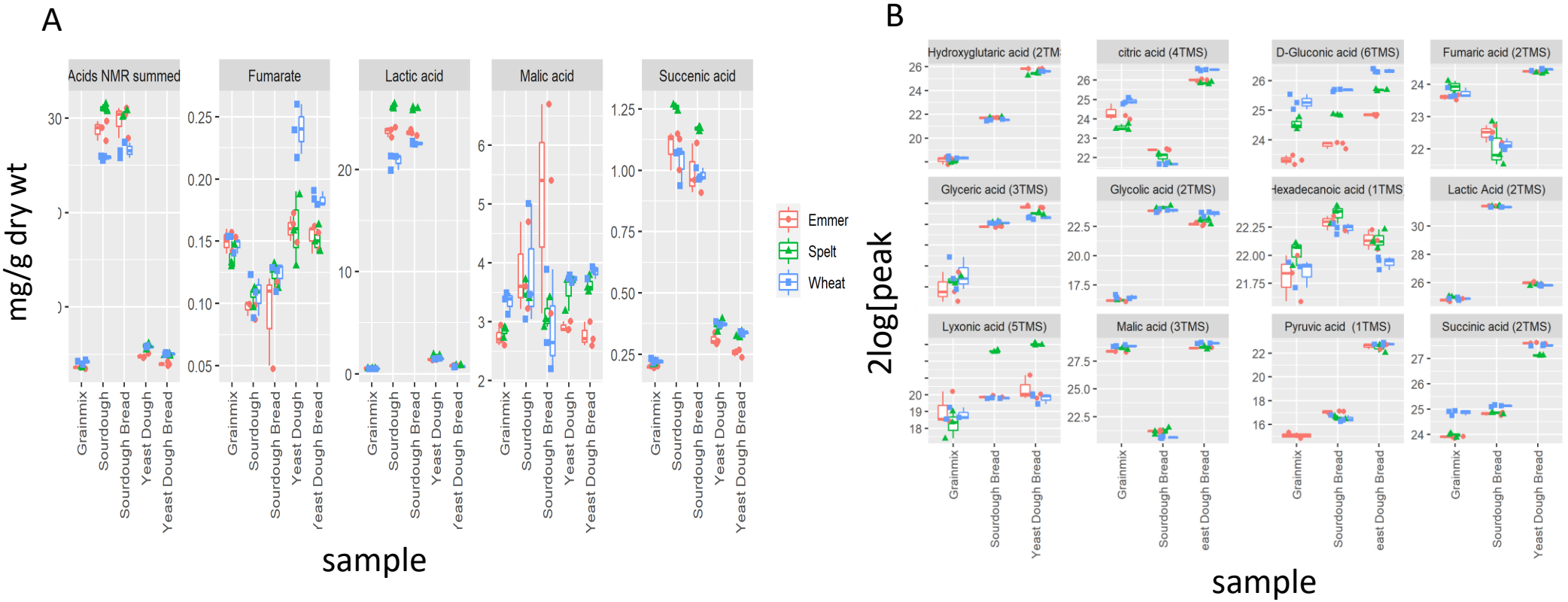

Figure S4. The contents of sugars in the flour, dough and bread samples determined by ^{1}H NMR spectroscopy. The points are the values from three replicate analyses as described in the text.
Sugar summed is combined amounts of all sugars; Grainmix if the whole meal flours from the blended grains

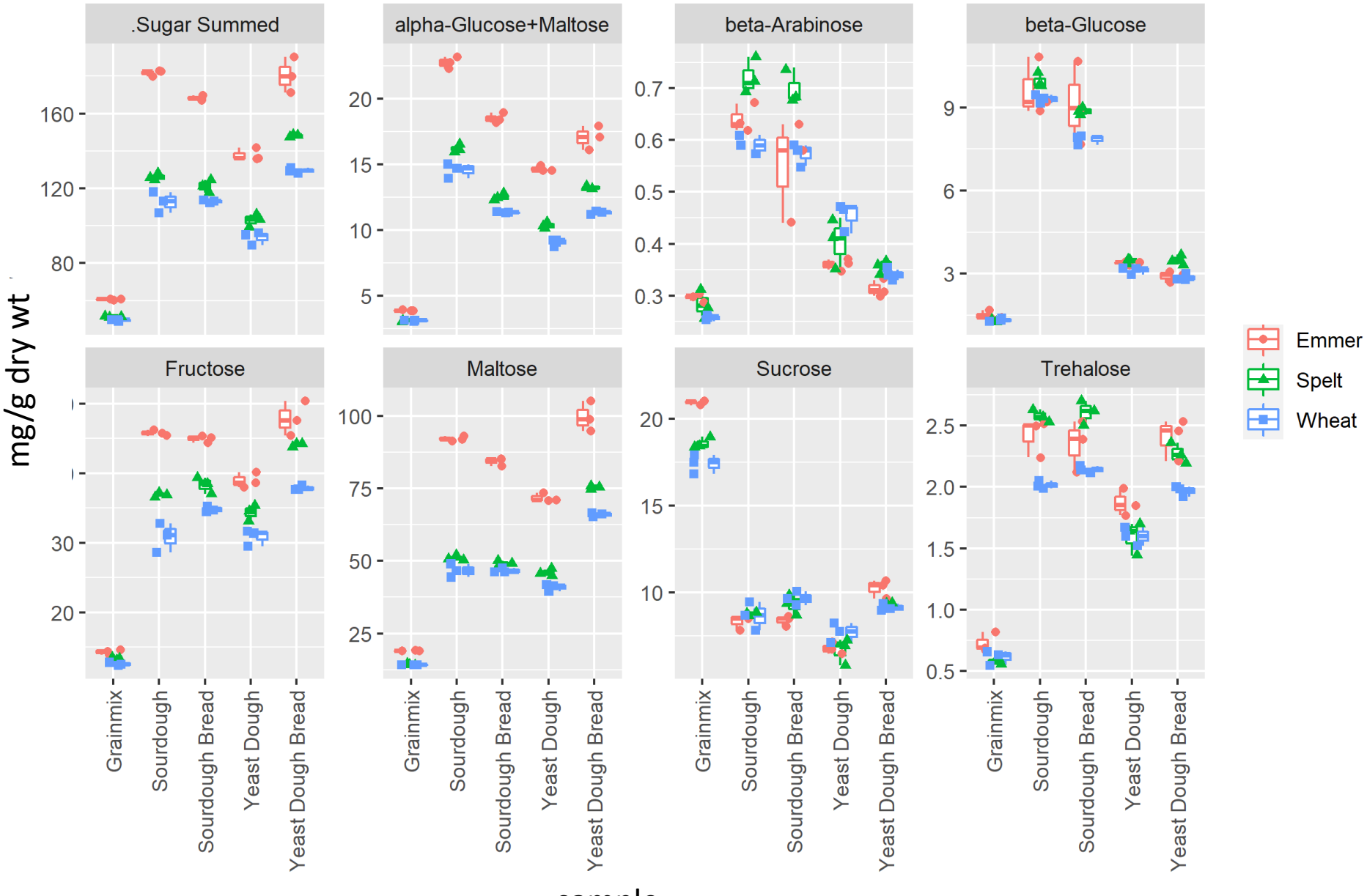

Figure S5. The contents of methyl donors in the flour, dough and bread samples determined by ^{1}H NMR spectroscopy. The points are the values from three replicate analyses as described in the text.
Methyl donors summed is combined amounts of all methyl donors; Grainmix is the whole meal flours from the blended grains.

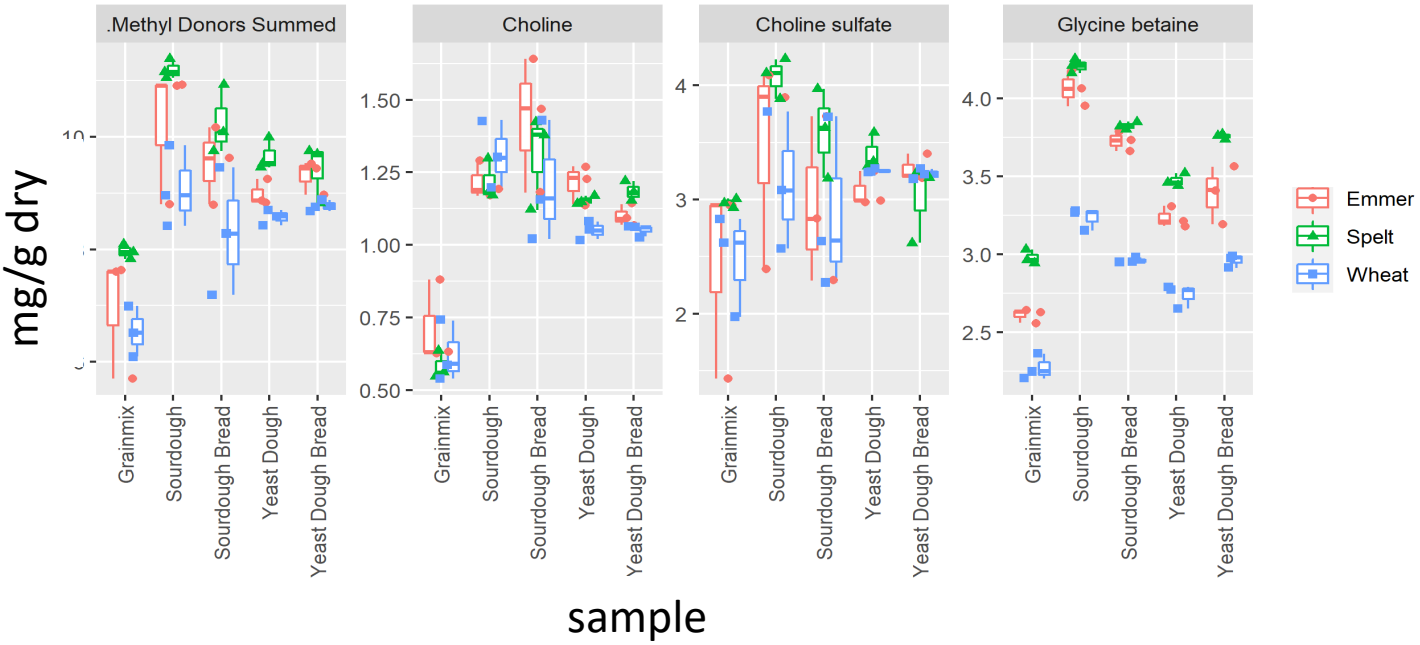

Figure S6. Contents of sugar alcohols in flour, dough and bread samples determined by mass spectrometry.
The points are the values from three replicate analyses as described in the text. Grainmix is the whole meal flours from the blended grains.

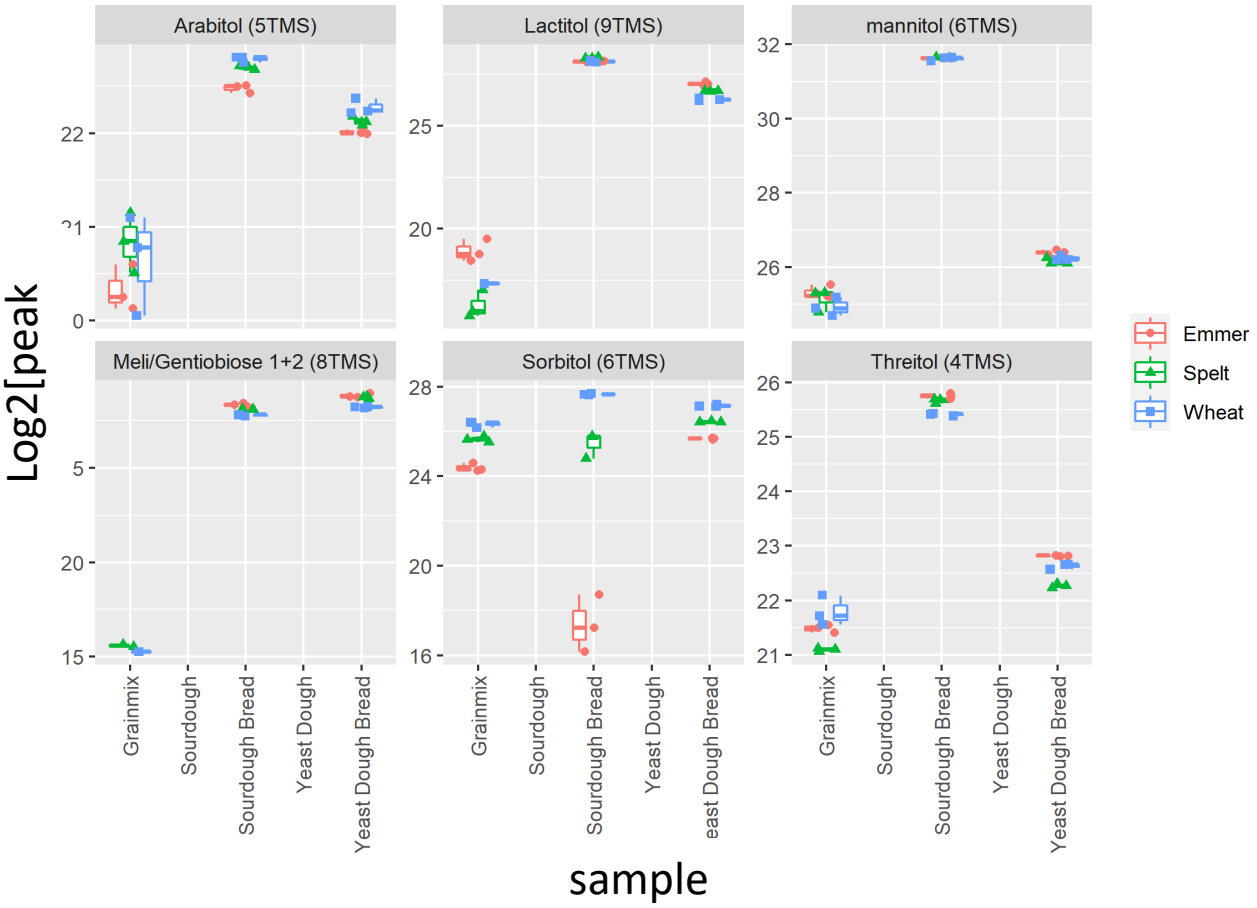

Figure S7. Contents of dietary fibre components in flours, dough and bread samples. Sugar residues and uronic acid were determined after hydrolysis and combined with Klason lignin and fructans to give total dietary fibre (TDF). Arabinoxylan is calculated from arabinose, xylose and galactose residue values assuming that the arabinose to xylose ratio was 0.69 in arabinogalactan.
The points are the values from three replicate analyses as described in the text. Grainmix is the whole meal flours from the blended grains.

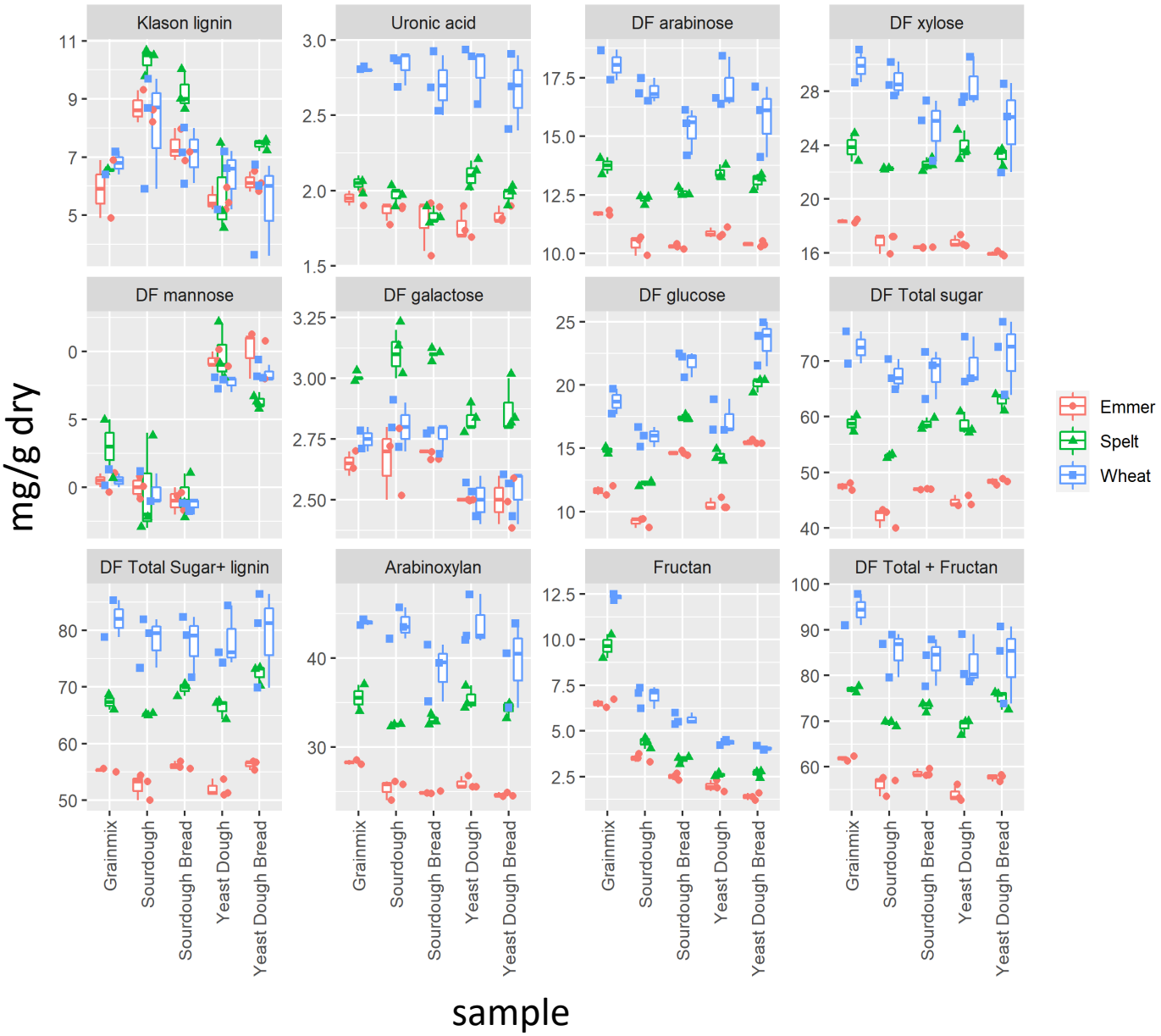

Figure S8. Content of arabinogalactose peptide (AGP) in the flour, dough and bread samples determined by ^{1}H NMR spectroscopy expressed as arabinose (Arab) and galactose (Gal) equivalents and the ratio of these two values.
The points are the values from three replicate analyses as described in the text. Grainmix is the whole meal flours from the blended grains.

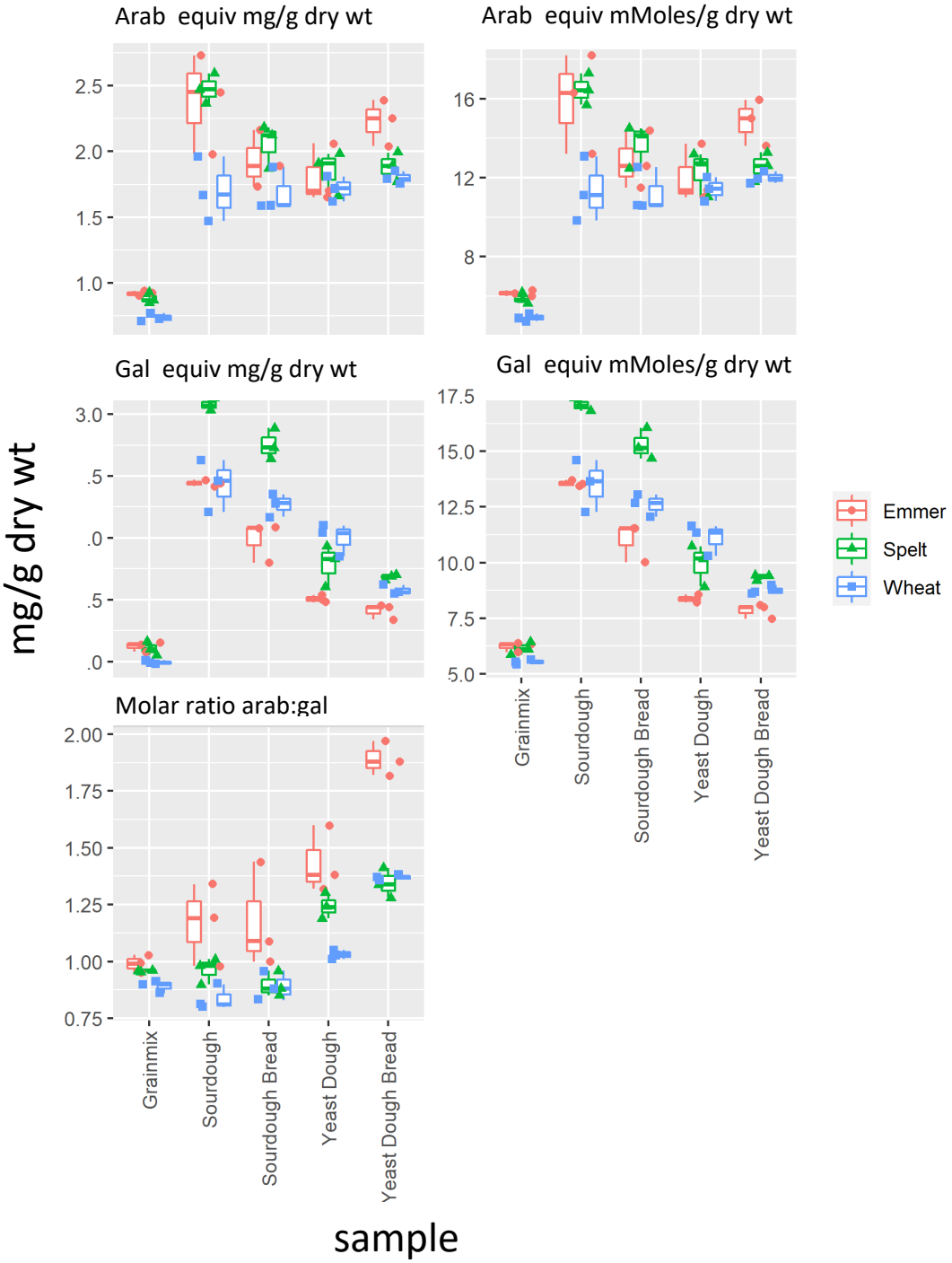

Figure S9. Proportions of oligosaccharides released from enzyme digestion of arabinoxylan (AXOS) and β-glucan (G3 and G4 GOS).
Grainmix is the whole meal flours from the blended grains. Xyl2, Xyl3 and Xyl5 comprise 2, 3 and 5 xylose residues, respectively. X indicates a xylose residue, A3 and A2+3 are xylose residues substituted with arabinose at position 3 and positions 3+4, respectively. G3 and G4 GOS comprise 3 and 4 glucose residues, respectively.