Breath volatile metabolome reveals the impact of dietary fibres on the gut microbiota: proof of concept in healthy volunteers

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Supplementary Materials

Table S1. Baseline characteristics of participants [1]

Women/men N (%)	8/7 (53/47)
Age (years old)	21 ± 2
Body weight (kg)	67.3 ± 10.5
BMI (kg/m2)	22.3 ± 2.0
SBP, mm Hg	123.1 ± 11.3
DBP, mm Hg	76.9 ± 6.1

[1]Values are means ± SD. BMI, body mass index; DBP, diastolic blood pressure; SBP, systolic blood pressure
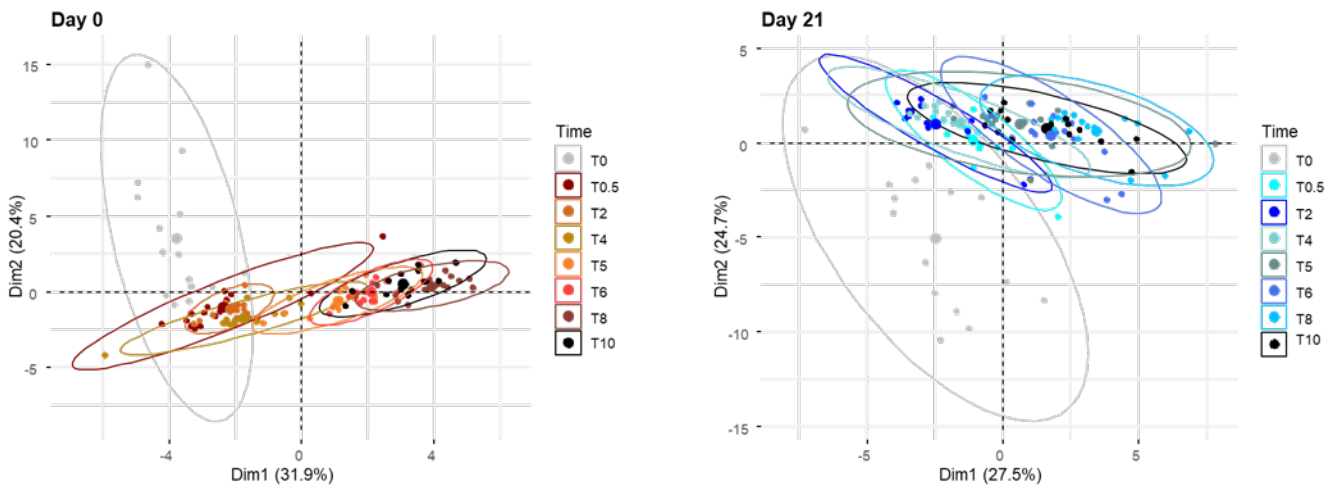
Figure S1. Untargeted analysis of breath from 15 healthy subjects prior (day 0) and after (day 21) chitin-glucan intake during 3 weeks. Principal component analysis (PCA) score plots obtained from the MS-fragment spectra (H_3O+, NO+ and O_2+ ionizations using SIFT-MS) at different times after the breakfast rich in dietary fibre.
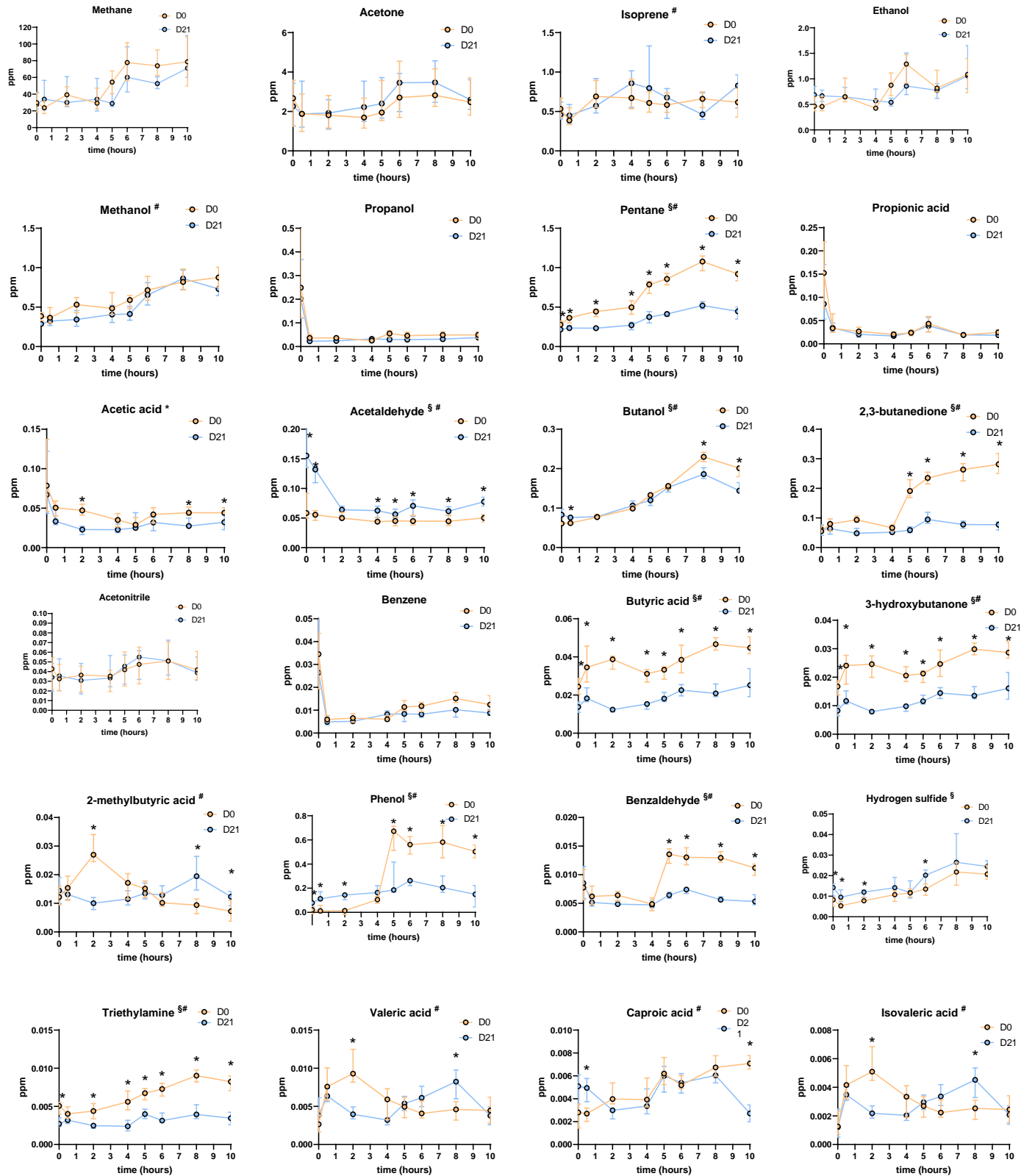
Figure S2. Targeted BVM concentrations presented in absolute values (ppm) exhaled in the breath of healthy subjects (n=15) prior (day 0) and after (day 21) chitin-glucan intake. Data are medians ± interquartile ranges (mixed model: §significant effect of treatment, #significant interaction between treatment and time, *Šídák post test: p<0.05).
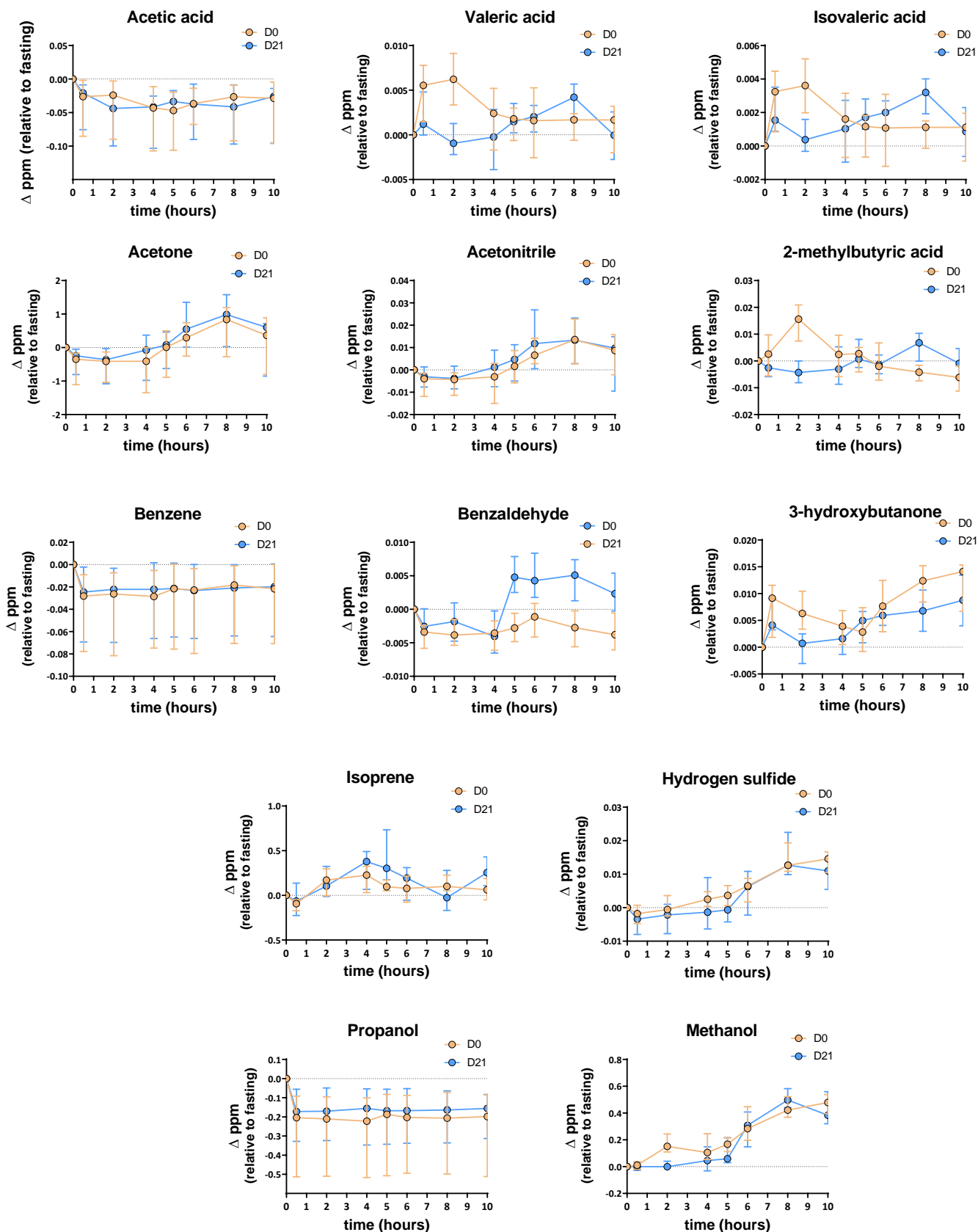
Figure S3. Targeted BVM concentrations (changes from baseline) exhaled in breath of healthy subjects (n=15) in response to a standardized breakfast intake prior (day 0) and after (day 21) chitin‑glucan intake (and not significantly affected by the chitin‑glucan intake during 3 weeks). Data are medians ± interquartile ranges (p>0.05; matched‑pairs Wilcoxon signed‑rank test on net area under the curve).

Table S2. Power calculation and effect size on targeted BVM significantly affected by the chitin-glucan treatment[1]

	D0	D21	D21-D0	Power	Cohen's d
Butyric acid					
Mean	0,078	0,041	-0,036	62%	0,63
SD	0,042	0,032	0,057		
Butanol					
Mean	0,421	0,256	-0,165	90%	0,91
SD	0,128	0,119	0,182		
Caproic acid					
Mean	0,016	-0,004	-0,020	85%	0,83
SD	0,010	0,019	0,024		
Ethanol					
Mean	2,059	0,390	-1,669	90%	0,89
SD	2,134	1,721	1,864		
Methane					
Mean	163,700	96,260	-67,420	77%	0,75
SD	77,950	60,550	89,820		
Pentane					
Mean	2,451	0,969	-1,482	100%	2,07
SD	0,459	0,428	0,715		
Phenol					
Mean	2,151	0,806	-1,345	100%	3,20
SD	0,361	0,319	0,421		
Triethylamine					
Mean	0,009	0,004	-0,005	62%	0,66
SD	0,007	0,005	0,008		
3-hydroxubutanone					
Mean	0,048	0,030	-0,018	41%	0,48
SD	0,028	0,021	0,037		
2,3 butanedione					
Mean	0,682	0,007	-0,675	100%	3,82
SD	0,146	0,182	0,177		

[1]Power computation was carried out on net AUC of BVM using the PASS 14.0.7 software with a significance level of 0,05 (Wilcoxon test) taking into account the difference (change after 21 days from day 0), the standard deviation (SD) and the sample size (n=15). Effect size was calculated with Cohen's d i.e. by dividing the mean difference by the SD of the difference (*Cohen, 1998. Statistical Power Analysis for the Behavioral Sciences. 2nd ed. Hillsdale, NJ: Lawrence Erlbaum Associates*).
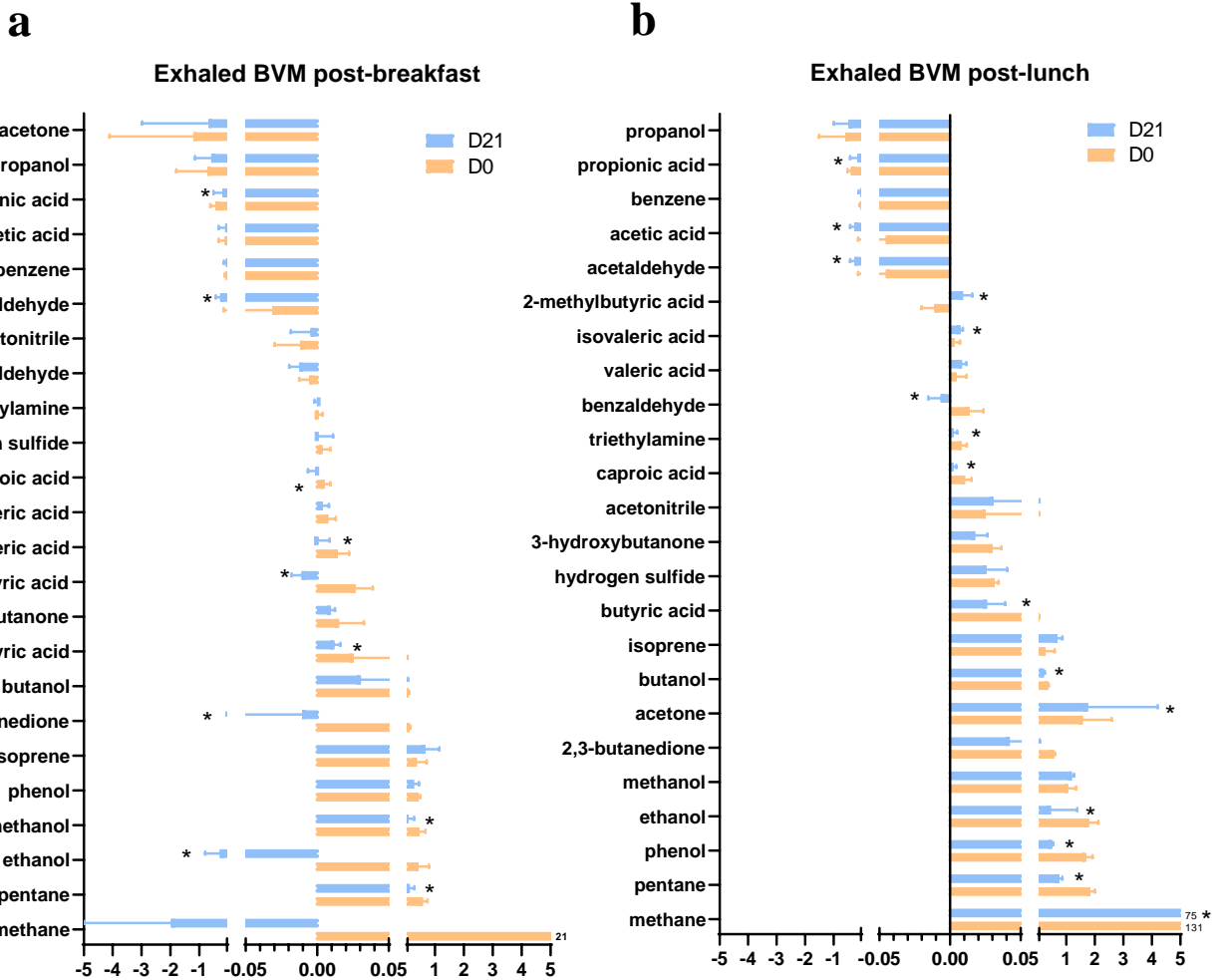
Figure S4. Net area under the curves of targeted BVM concentrations exhaled in breath after the breakfast intake (a) and after the lunch intake (b) of healthy subjects (n=15) prior (day 0) and after (day 21) chitin-glucan. Data are medians ± interquartile ranges (*p<0.05; matched-pairs Wilcoxon signed-rank test on net area under the curve).

Table S3. Baseline score of gastrointestinal symptoms of the participants at fasting state[1]

	Day 0			Day 21		
Nausea	0.3	±	1.0 (0[0-0])	0.0	±	0.0 (0[0-0])
Flatulence	2.7	±	5.2 (0[0-3])	2.5	±	5.4 (0[0-1])
Bloating	2.6	±	4.9 (0[0-6])	4.1	±	6.6 (0[0-9])
Cramp	1.5	±	4.2 (0[0-0])	0.0	±	0.0 (0[0-0])
Rumbling	6.3	±	13.4 (0[0-14])	2.9	±	7.9 (0[0-0])
Reflux	0.2	±	0.8 (0[0-0])	0.1	±	0.5 (0[0-0])
Discomfort	2.4	±	4.7 (0[0-2])	2.1	±	3.7 (0[0-4])
Burp	0.6	±	1.8 (0[0-0])	0.1	±	0.5 (0[0-0])

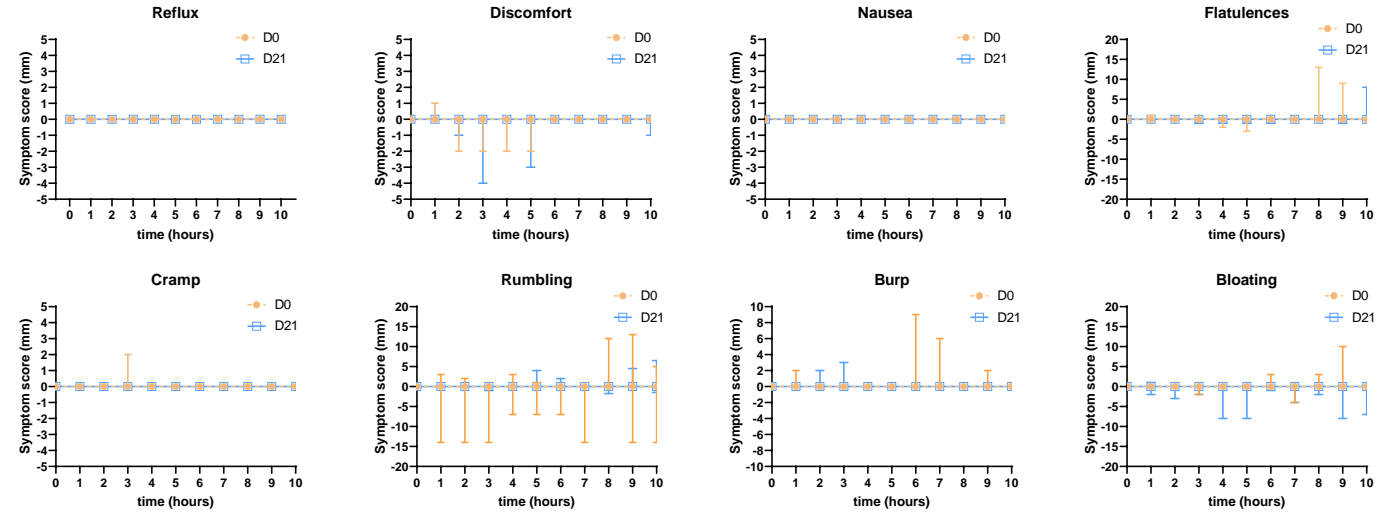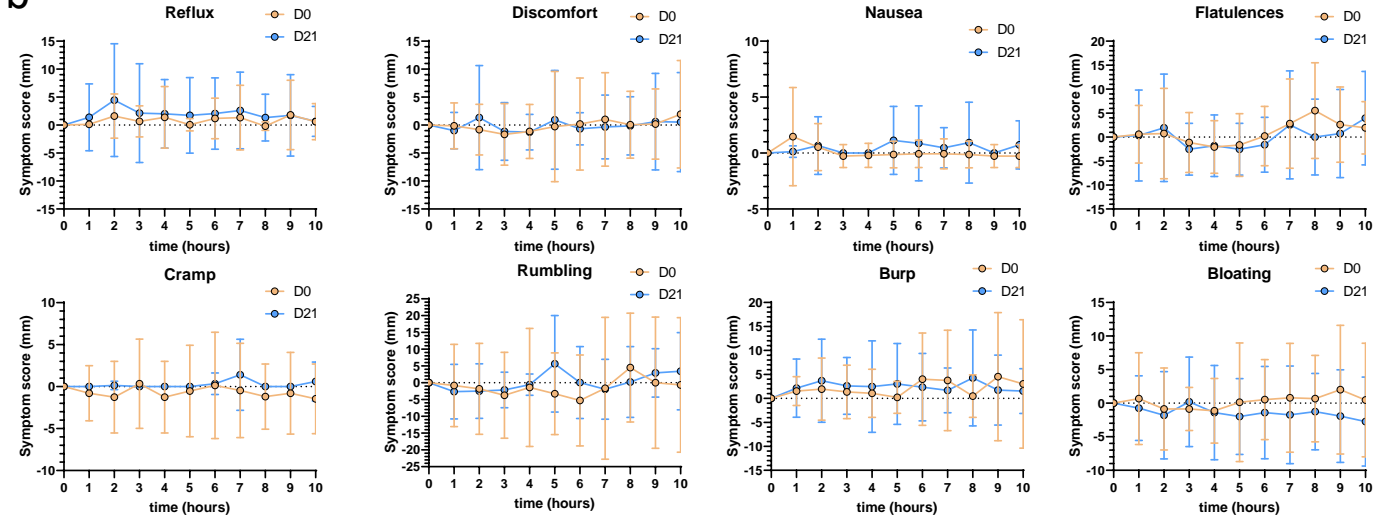[1]Values are means ± SD (medians [interquartile ranges]) (n=15, $p > 0.05$, matched-pairs Wilcoxon signed-rank test).

Figure S5. Gastrointestinal tolerance of healthy subjects (n=15) about 8 symptoms assessed by visual analog scale (changes from baseline) in response to a standardized breakfast intake prior (day 0) and after (day 21) chitin-glucan intake during 3 weeks. Data are medians ± interquartile ranges (a). Data are means ± SD (b); p > 0.05; matched-pairs Wilcoxon signed-rank test on net AUC.