Supplemental files belonging to:

An ex vivo fermentation screening platform to study drug metabolism by human gut microbiota

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SUPPLEMENTAL METHODS

Table S1-S7 provide information about the UHPLC gradient conditions used for metabolite profiling.

Table S1. UHPLC gradient conditions used for metabolite profiling of omeprazole, risperidone, sulfinpyrazone, sulindac, sulfasalazine

Column: Phenomenex Kinetix C18; 2.1 x 50 mm, 1.7 µ; 0.4 mL/min; 45°C		
Time (min)	10 mM ammonium acetate in water (%)	Methanol (%)
0	95	5
0.5	95	5
4.0	15	85
4.5	5	95
5.5	5	95
5.6	95	5
6.5	95	5

Table S2. UHPLC gradient conditions used for metabolite profiling of simvastatin

Column: Phenomenex Kinetix C18; 2.1 x 50 mm, 1.7 µ; 0.4 mL/min; 45°C		
Time (min)	10 mM ammonium acetate in water (%)	Methanol (%)
0	95	5
0.5	95	5
4.0	5	95
5.5	5	95
5.6	95	5
6.5	95	5

Table S3. UHPLC gradient conditions used for metabolite profiling of nizatidine

Column: Phenomenex Kinetix C18; 2.1 x 50 mm, 1.7 µ; 0.4 mL/min; 45°C		
Time (min)	10 mM ammonium acetate in water (%)	Methanol (%)
0	95	5
0.5	95	5
4.0	40	40
4.5	5	95
5.5	5	95
5.6	95	5
6.5	95	5

Table S4. UHPLC gradient conditions used for metabolite profiling of metronidazole

Column: Phenomenex Kinetix C18; 2.1 x 50 mm, 1.7 µ; 0.4 mL/min; 45°C		
Time (min)	10 mM ammonium acetate in water (%)	Methanol (%)
0	95	5
0.5	95	5
4.0	70	40
4.5	5	95
5.5	5	95
5.6	95	5
6.5	95	5

Table S5. UHPLC gradient conditions used for metabolite profiling of zonisamide and dapsone

Column: Waters HSS T3; 2.1 x 100 mm, 1.8 µ; 0.3 mL/min; 45°C		
Time (min)	0.1% formic acid water (%)	Acetonitrile (%)
0	95	5
0.5	95	5

5.0	60	40
7.0	5	95
8.0	5	95
8.1	95	5
9.0	95	5

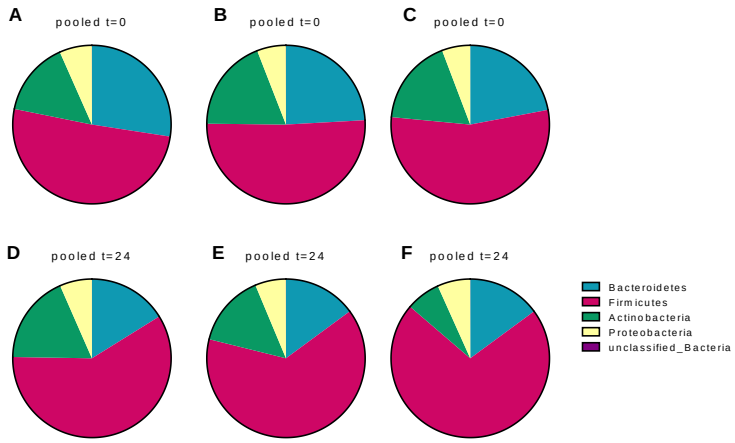
Table S6. UHPLC gradient conditions used for metabolite profiling of levodopa

Column: Waters HSS T3; 2.1 x 100 mm, 1.8 µ; 0.3 mL/min; 45°C		
Time (min)	0.1% formic acid water (%)	Acetonitrile (%)
0	98	2
0.5	95	5
7.0	5	95
8.0	5	95
8.1	98	2
9.0	98	2

Table S7. UHPLC gradient conditions used for metabolite profiling of acetaminophen

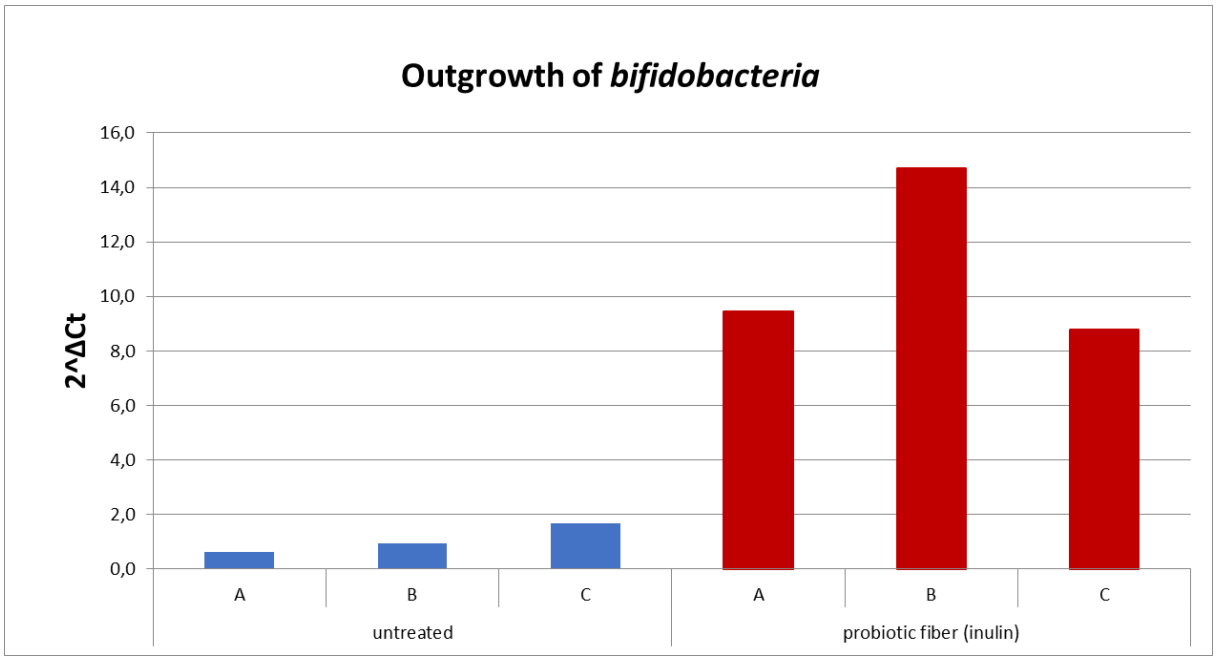
Column: Waters HSS T3; 2.1 x 100 mm, 1.8 µ; 0.3 mL/min; 45°C		
Time (min)	0.1% formic acid water (%)	Acetonitrile (%)
0	98	2
2.5	95	5
5.0	75	25
7.0	5	95
8.0	5	95
8.1	98	2
9.0	98	2

Supplemental Figure 1



Supplemental Figure S1. Microbial composition of pooled human feceal microbiota before (t=0) and after ex vivo fermentation screen for 24 hours (t=24). Intra-experimental variation is shown by presenting A, B and C and D, E and F representing triplicate incubations of one experiment. Data are presented as mean relative abundance of the individual microbial species (n=3).

Supplemental Figure 2



Supplemental Figure S2. Outgrowth of *Bifidobacteria* stimulated by probiotic fiber inulin under anaerobic conditions within the ex vivo fermrnation screen as determined by qPCR. Results are presented as the fold change in the number of bifidobacteria after incubatrion with inulin compared to blanc control incubation of microbiota only (3 individual experiments) applying pooled human feceal microbiota in the ex vivo fermentation screen for 24 hours (t=24).