

# Supplementary Materials: Absorption and Excretion of Glucosinolates and Isothiocyanates after Ingestion of Broccoli (*Brassica oleracea* L. var *italica*) Leaf Flour in Mice: A Preliminary Study

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Supplementary Table S1. Chromatographic conditions.

Chromatographic conditions	
Flow	0.3 mL min <sup>-1</sup>
Injection volume	10 µL
Solvent A	13 mM ammonium acetate pH 7
Solvent B	Acetonitrile/formic acid (99.99:0.01, v/v)
Gradient	
Time (min.)	%B
0.20	12.00
0.21	70.00
1.00	30.00
1.01	52.00
2.50	52.00
4.00	100.00
7.00	100.00
80.00	12.00

Supplementary Table S2. Electrospray Ionisation (ESI) conditions.

Electrospray Ionisation (ESI) conditions	
Gas temperature (°C)	225
Gas Flow (L/min)	8
Nebulizer (psi)	30
Seath Gas Heater (°C)	350
Seath Gas Flow (L)	10
Capillary (V)	3500
VCharging (eV)	1250

**Supplementary Table S3.** Retention time and MS2 fragmentation pattern (mass/charge (m/z) ratio) of intact glucosinolates and isothiocyanates.

Compound <sub>z</sub>	Rt (min)	Parent ion (m/z MS [M-H] <sup>-</sup> / m/z MS [M+H] <sup>+</sup> )	Product ion (m/z MS2 [M-H] <sup>-</sup> / m/z MS2 [M+H] <sup>+</sup> )	Dwell	F (eV)	CE (eV)	Cell Acc	Polarity
GR	0.626	438.0 / -	196.0 / -	20	90	4	7	Negative
GE	1.211	420.0 / -	97.1 / -	20	60	20	7	Negative
GB	1.27	447.2 / -	97 / -	20	80	20	7	Negative
GI	0.648	421.9 / -	357.7 / -	20	100	0	7	Negative
SFN	1.644	- / 178.0	- / 114.0	20	75	4	7	Positive
SFN-GSH	1.174	- / 485.0	- / 178.0	20	115	0	7	Positive
SFN-CYS	0.702	- / 299.0	- / 178.0	20	80	0	7	Positive
SFN-NAC	1.108	- / 341.0	- / 178.0	20	80	0	7	Positive
Erucin	0.444	141.1 / -	59.0 / -	20	70	6	7	Negative
I3C	1.284	- / 148.1	- / 77.1	20	70	25	7	Positive
DIM	1.66	- / 247.1	- / 105.0	20	70	25	7	Positive
Iberin	1.542	- / 164.0	- / 105.0	20	90	6	7	Positive

<sup>z</sup>GR, glucoraphanin; GE, glucoerucin; GB, glucobrassicin; GI, glucoiberin; SFN, sulforaphane; SFN-GSH, sulforaphane-glutathione; SFN-CYS, sulforaphane-cysteine; SFN-NAC, sulforaphane-N-acetyl-cysteine; I3C, indole-3-carbinol; DIM, 3,3'-diindolylmethane; Rt, retention time; F, fragmentation energy; CE, collision energy.