SUPPLEMENTARY TABLE

Table 1S. List of putative polyphenolic compounds, sulforaphane, and indoles identified in the optimised lactofermented beverage made from broccoli leaves.

Tentative identification	Molecular formula	Precursor ion [m/z]	Product ion [m/z]	Polarity
Phenolic acid				
3-O-Caffeoylquinic acid	C16H18O9	353	191	–
5-O-Caffeoylquinic acid	C16H18O9	353	191	–
4-O-Caffeoylquinic acid	C16H18O9	353	191	–
1-O-Feruloylquinic acid	C17H20O9	367	191	–
5-O-Feruloylquinic acid	C17H20O9	367	191	–
1,2-Disinapoylgentiobioside	C34H42O19	753	205	–
Sinapic acid	C11H12O5	223	208	–
Ferulic acid	C10H10O4	193	178	–
Deacylated flavonoids				
K-3,7-O-diGlu	C27H30O16	609	284	–
K-3-O-Soph-7-O-D-Glu	C33H40O21	771	284	–
K-3-O-sophoroside	C27H30O16	609	284	–
Q-diGlu	C27H30O17	625	300	–
Acylated flavonoids				
K 3-O-hFer-Soph-7-O-Glu	C45H56O23	963	284	–
K 3-O-Caf-Soph-7-O-Glu	C42H46O24	933	284	–
K-3-O-Sin-Soph-7-O-Glu	C44H50O25	977	284	–
K-3-O-FerSoph-7-O-Glu	C43H48O24	947	284	–
K-3HFerSoph	C37H38O20	801	284	–
K-3FeSoph	C37H38O19	785	284	–
K-3-O-Caf-Soph-7-O-Sin-Glu	C53H56O28	1140	284	–
K-3CafSoph-7dGlu	C48H56O29	1095	284	–
Sulforaphane and indoles				
Sulforaphane	C6H11NOS2	178	114	+
Ascorbigen	C15H15NO6	306	130	+
Indole-3-carbinol	C9H9NO	130	77	+
Diindolylmethane	C17H14N2	247	130	+

Kaempferol (K); Quercetin (Q); Glucoside (Glu); diglucoside (dGlu); Sophoroside (Soph); Sinapoyl (Sin); Feruloyl (Fer); Hydroxyferuloyl (hFe); Caffeoyl (Caf).