

Supplementary Table S2

Supplementary Table S2. Chromatographic and electrospray ionization conditions.

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

^zSFN-NAC, Sulforaphane-*N*-acetyl-cysteine; SFN-CYS, Sulforaphane-cysteine; DIM, 3,3'-Diindolylmethane; SFN, Sulforaphane; I3C, indole-3-carbinol; SFN-GSH, Sulforaphane-glutathione; GB, Glucobrassicin; GR, Glucoraphanin; GI, Glucoiberin; GE, Glucoerucin; F, fragmentation energy; CE, collision energy.