Integrating two-dimensional gas and liquid chromatography-mass spectrometry for untargeted colorectal cancer metabolomics: a proof-of-principle study

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Supplemental Data

Table S1. Mass spectrometer parameters for 2DLC-MS analysis

General and full MS parameters		dd-MS^2 parameters	
Runtime	0 to 20 min	Microscans	2
Polarity	negative/positive	Resolution	15,000
In-source CID	0.0 eV	ACG target	5e4
Microscans	2	Maximum IT	100 ms
Resolution	30,000	Loop count	6
ACG target	1e6	MSX count	1
Maximum IT	50 ms	Isolation window	0.4 m/z
Number of scan ranges	1	Isolation offset	0.0 m/z
Scan ranges	60 to 900 m/z	(N)CE/stepped (N)CE	nce:10/20/40/60
Spectrum data type	Centroid	Spectrum data type	Centroid
		Minimum ACG target	8.00e3
		Exclude isotopes	on
		Dynamic exclusion	1.2 s

Table S2. ChromaTOF software parameters for GC×GC-MS analysis

Parameters	Setting values
Baseline offset	1.0 (just above the noise)
Number of data points averaged for smoothing	Auto
First dimension peak width	12 s
Second dimension peak width	0.1 s
Match required to combine	600
Minimum S/N	10
Mass to use for area/height calculation	Unique mass
Integration approach	Traditional
Minimum/maximum molecular weight allowed	29/800
Mass threshold (relative abundance of base ion)	5
Libraries to use for searching	NIST-14
Minimum similarity match before name is assigned	0
Maximum number of unknown peaks to find	5000
Number of library hits to returned	10
Exported information	Name, CAS, 1^{st} dimension time (s), 2^{nd} dimension time (s), similarity, quant masses, area, S/N