Ch. No	Description	Method	RT	ESI Mode	Collision energy (eV)
1	Identified in Boraginaceae	B	11.4	Positive	25
2	A semisynthetic analog of Ch. 1	B	10.5	Positive	30
3	Plant-derived	A	11.7	Positive	25
4	Common in foods such as wine, chocolate, peanuts, fruits	A	5.0	Positive	6-50 ramp
5	Plant-derived	A	11.3	Positive	25
6	From licorice	A	21.4	Positive	6-50 ramp
7	Common in Leguminosae	A	14.7	Negative	25
8	Common in Leguminosae	Infusion	-	Positive	25
9	Rare plant-derived compound	A	8.7	Positive	15
10	Common in Leguminosae	A	15.4	Positive	25
11	Identified in licorice	A	21.3	Positive	6-50 ramp
12	Plant derived	A	14.4	Positive	25
13	Plant-derived	Legacy	N/A	Positive	N/A
14	Unreported compound identified in licorice	A	19.9	Positive	25
15	Unreported compound identified in Ranunculaceae	6-36%B 30 min	9.8	Positive	15
16	A semisynthetic analog of a common plant compound	A	5.0	Positive	15
17	A compound from mangosteen fruit	50-90%B 15min	12.4	Negative	30
18	Endogenous	A	2.0	Negative	15
19	Common in foods such as wine, chocolate, fruits	A	8.9	Negative	15
20	Plant derived	A	12.6	Positive	6-50 ramp

Chromatographic conditions: Method A: YMC AQ 2.0x100 mm, 3µm; 10-95%MeCN/0.1%formic acid over 30 min

Method B: YMC AQ 2.0x100 mm, 3µm; 5-40%MeCN/0.1%formic acid over 30 min

Challenge Data

- The MS and MSMS files (zip of text files)
- The MS and MSMS files (mgf files) thanks Ming
- The MS and MSMS files (metabolomics resolver page) thanks Ming
- An example tsv file
- An example txt file