Identification of Compounds that Negatively Impact Coffee Quality Using Untargeted LC/MS Analysis

*Sichaya SITTIPOD, Eric SCHWARTZ, Laurianne PARAVISINI, Edisson TELLO, and Devin G. PETERSON**

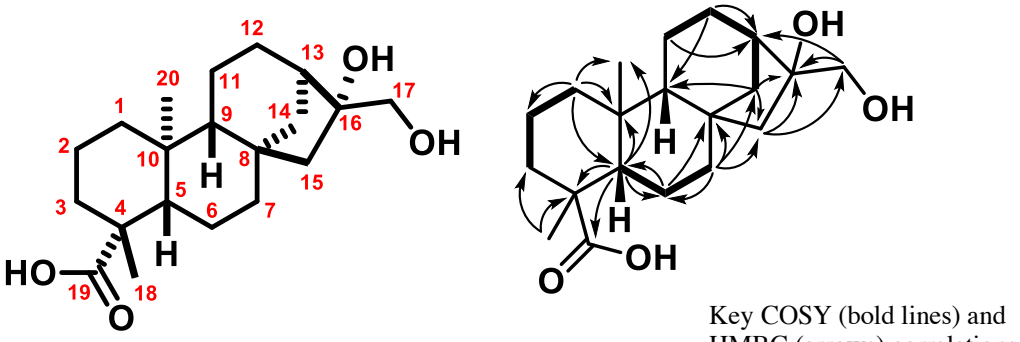
Department of Food Science and Technology, 110 Parker Food Science and Technology Building, The Ohio State University, 2015 Fyffe Rd., Columbus, OH 43210

* Corresponding author: peterson.892@osu.edu

Supplementary Data

Table S1: ^{1}H and ^{13}C NMR Data (MeOD) data of Compound **1**.

	Compound		
position	δ_c, type	δ_H (J in Hz)	HMBC
1a	41.9, CH_2	1.82, m	10, 5
1b		0.79, td (13.3, 4.2)	20, 10, 2
2a	20.2, CH_2	1.87, m	
2b		1.37, m	
3a	39.2, CH_2	2.08, m	
3b		0.97, m	
4	44.6, C		
5	58.1, CH	1.02, dd (8.8, 5.7)	4, 6, 10, 19, 20
6	23.3, CH_2	1.80, m	5, 8, 10,
7a	43.3, CH_2	1.59, m	
7b		1.42, m	5, 6, 8, 14, 15
8	45.7, C		
9	57.3, CH	0.97, m	
10	40.8, C		
11	19.5, CH_2	1.56, m	13
12a	27.2, CH_2	1.64, m	9, 13,
12b		1.44, m	
13	46.2, CH	1.98, m	
14a	38.2, CH_2	1.93, m	12, 13, 9
14b		1.59, m	15, 16, 12
15a	53.7, CH_2	1.49, dd (14.5, 1.8)	9, 13, 14, 17
15b		1.35, d (14.5)	7, 9, 16
16	82.9, C		
17a	66.8, CH_2	3.66, d (11.3)	13, 15
17b		3.55, d (11.3)	13, 15, 16
18	29.5, CH_3	1.14, s	3, 4, 5, 19
19	181.7, C		
20	16.2, CH_3	0.94, s	10



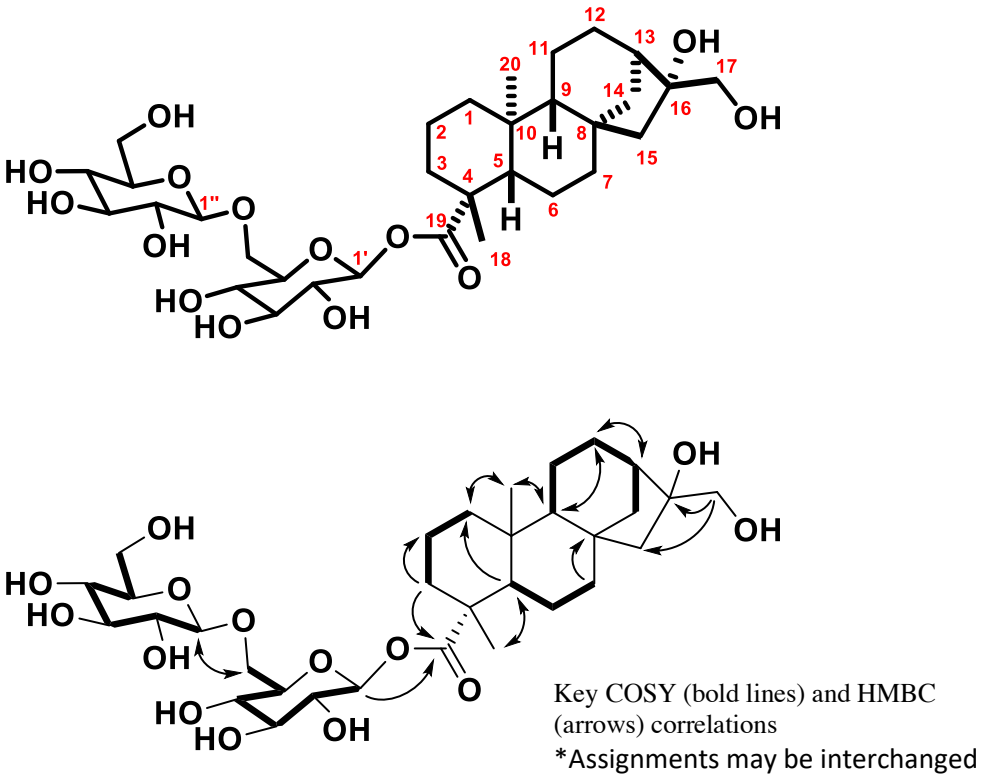
Key COSY (bold lines) and HMBC (arrows) correlations

16α,17-dihydroxy-*ent*-kauran-19-oic acid

Figure S1. Chemical correlations by COSY and HMBC and Structure of compound **1**.

Table S2: ^{1}H and ^{13}C NMR Data (MeOD) data of Compound **2**.

	Compound		
position	δ_c, type	δ_H (J in Hz)	HMBC
1a	41.8, CH_2	1.86, m	
1b		0.83, td (13.0, 3.7)	20
2a	20.1, CH_2	1.92, m	
2b		1.42, m	
3a	39.0, CH_2	2.19, m	
3b		1.05, td (13.4, 4.3)	2
4	45.1, C		
5	58.5, CH	1.10, dd (12.3, 1.9)	4, 6, 10, 18, 19, 20
6a	23.2, CH_2	2.00, m	
6b		1.83, m	
7a	43.3, CH_2	1.61, m	
7b		1.44, m	
8	45.8, C		
9	57.3, CH	1.01, d (7.3)	8, 10, 11, 20
10	40.9, C		
11	19.6, CH_2	1.60, m	
12	27.2, CH_2	1.62, m	
13	46.2, CH	2.0, m	
14a	38.1, CH_2	1.64, m	
14b		1.97, m	12, 15, 16,
15a	53.7, CH_2	1.52, d (14.4)	8, 9, 14, 17
15b		1.38, d (14.4)	7, 9
16	82.9, C		
17a	66.8, CH_2	3.70, d (11.3)	15
17b		3.60, d (11.3)	13
18	29.0, CH_3	1.21, s	3, 4, 5
19	178.2, C		
20	16.4, CH_3	0.97, s	
1’	95.6, CH	5.39, d (8.1)	18
2’	74.0, CH	3.36, m	
3’	77.8, CH	3.40, m	1’
4’	71.0, CH	3.44, m	
5’	*77.9, CH	3.53, ddd (9.5, 5.1, 2.0)	
6’a	69.6, CH_2	4.12, dd (11.7, 2.0)	4’
6’b		3.80, dd (11.7, 5.2)	1”, 5’
1’’	104.7, CH	4.36, d (7.8)	6’
2’’	75.1, CH	3.21, m	1”, 3”
3’’	78.5, CH	3.36, m	
4’’	71.5, CH	3.29, m	
5’’	*78.0, CH	3.24, ddd, (9.5, 5.6, 2.4)	
6’’a	62.7, CH_2	3.85, dd (11.9, 2.3)	4”
6’’b		3.67, dd (11.9, 5.6)	5”



16α,17-dihydroxy-*ent*-kauran-19-diglycoside

Figure S2. ^{1}H and ^{13}C Spectroscopic Data of Compound **2** (MeOD, 700 MHz).

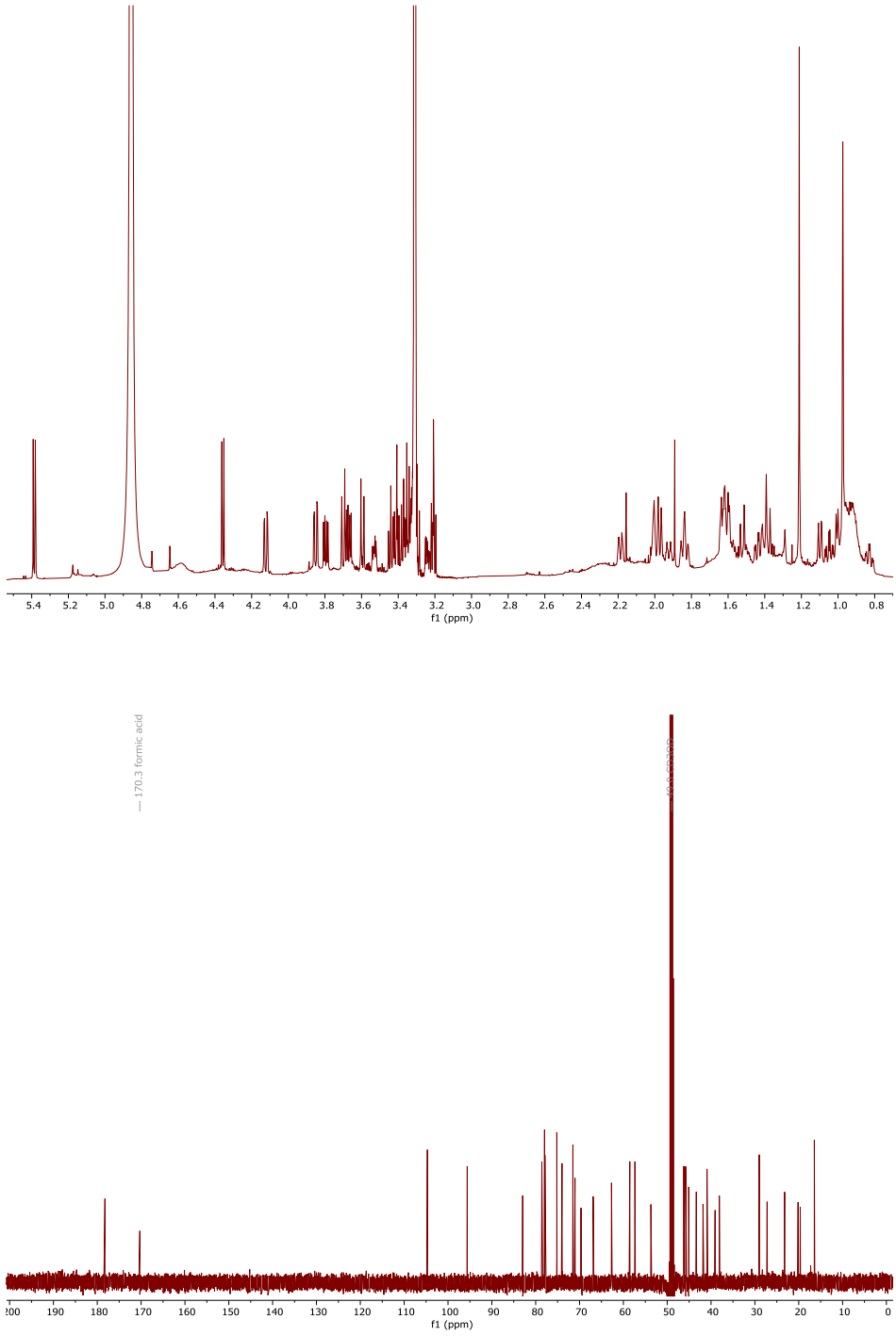
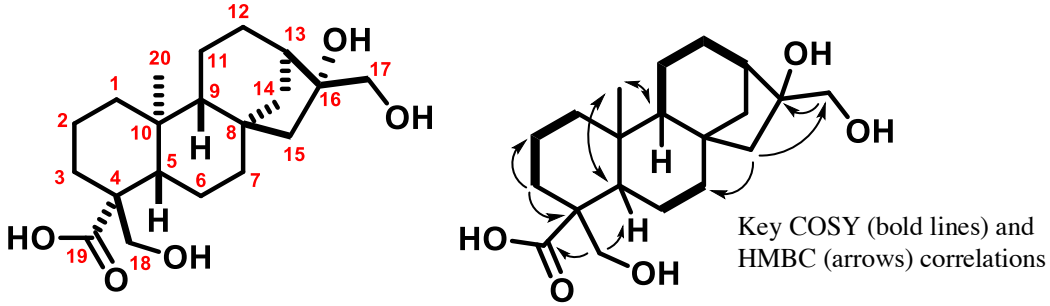


Figure S2b. ^{1}H and ^{13}C Spectra of Compound **2**.

Table S3: ^{1}H and ^{13}C NMR Data (MeOD) data of Compound **5**.

position	Compound		
	δ_c, type	δ_H (J in Hz)	HMBC
1a	41.8, CH_2	1.85, m	
1b		0.79, m	
2a	19.9, CH_2	2.01, m	
2b		1.45, m	
3a	33.3, CH_2	2.16, s	
3b		1.13, m	2, 4
4	51.1, C		
5	52.4, CH	1.26, d (11.4)	1, 4, 20
6	23.2, CH_2	1.78, m	
7a	43.0, CH_2	1.58, m	
7b		1.45, m	
8	45.6, C		
9	57.4, CH	1.01, m	8, 11, 12, 14, 20
10	40.6, C		
11	19.6, CH_2	1.63, m	
12a	27.2, CH_2	1.61, m	
12b		1.48, m	
13	46.2, CH	2.01, m	
14a	38.2, CH_2	1.93, m	12, 15, 16
14b		1.58, m	9
15a	53.8, CH_2	1.52, d (14.7)	9, 14, 17
15b		1.38, d (14.3)	7, 9, 16
16	82.9, C		
17a	66.8, CH_2	3.70, d (11.2)	
17b		3.60, d (11.2)	13, 16
18a	70.9, CH_2	3.68, d (10.6)	3, 5
18b		3.50, d (10.6)	3, 5, 19
19	180.7, C		
20	16.5, CH_3	1.03, s	1, 5, 9

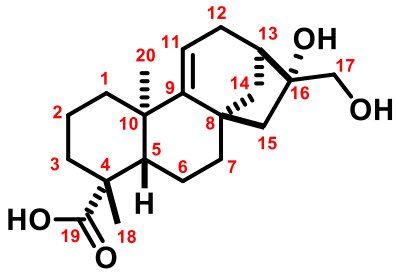


16 ,17,18-trihydroxy-*ent*-kauran-19-oic acid

Figure S3. Chemical correlations by COSY and HMBC and Structure of compound **5**.

Table S4: ^{13}C NMR Data comparation data of Compound **6**.

position	δ_c, type	δ_H (J in Hz)
1a	42.4 CH_2	1.96, m
1b		1.22, m
2a	21.4, CH_2	1.90, m
2b		1.46, m
3a	39.7, CH_2	2.12, m
3b		0.99, m
4	45.6, C	
5	47,7, CH	1.62, t (9.9)
6a	19.6, CH_2	2.58, q (11.3)
6b		1.83, m
7a*	31.3, CH_2	2.20, m
7b*		1.48, m
8	44.0, C	
9	158.9, C	
10	39.9 C	
11	115.0, CH	5.20, d (3.6)
12a*	31.4, CH_2	2.20, m
12b*		1.96, m
13	45.0, CH	2.15, m
14a	44.2, CH_2	2.04, dd (10.7, 5.1)
14b		1.46, t (9.7)
15a	55.7, CH_2	1.96, m
15b		1.53, d (13.2)
16	85.6, C	
17a	68.9, CH_2	3.54, d (11.3)
17b		3.48, d (11.1)
18	28.8, CH_3	1.18, s
19	181.6, C	
20	24.1 CH_3	1.02, s



16α,17-dihydroxy-*ent*-9(11)-kauren-19-oic acid

Figure S4. Chemical structure of compound **6**.