A Novel Integrative Methodology for Research on Pot-honey Variations During Post-harvest

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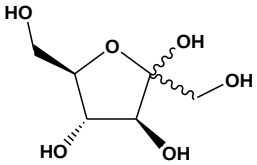
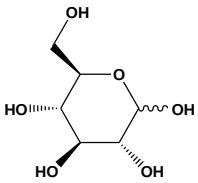
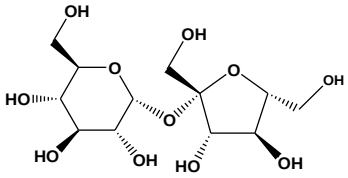
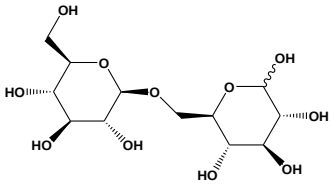
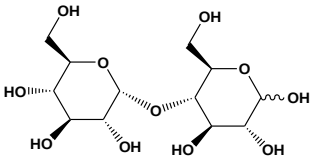
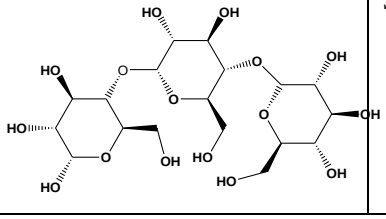
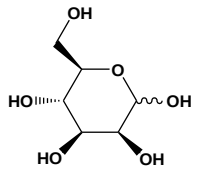
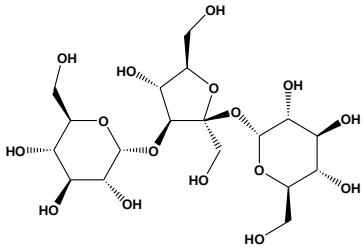
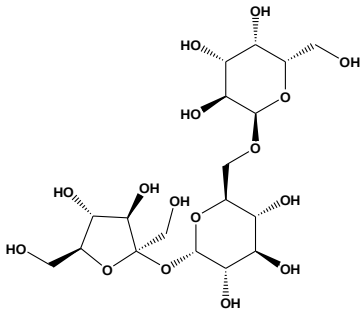
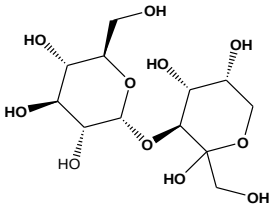
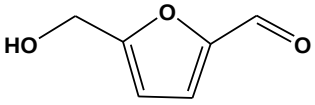
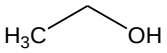
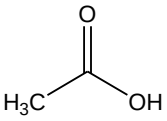
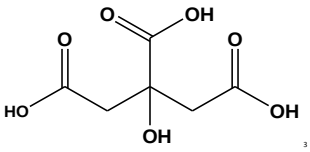
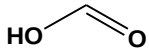
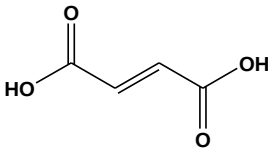
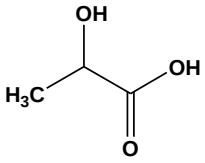
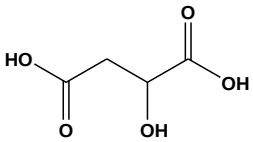
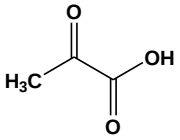
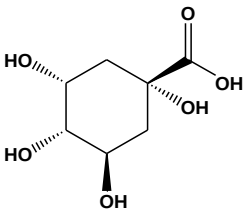
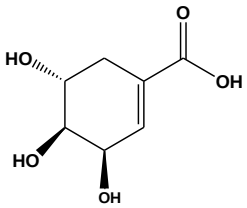
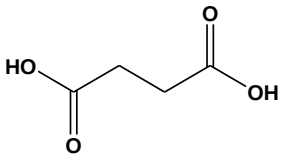
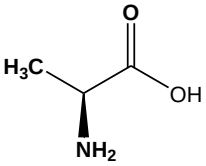
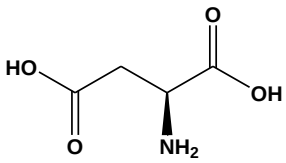
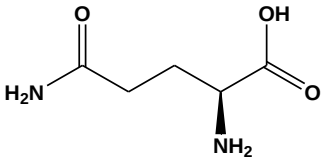
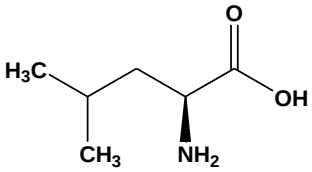
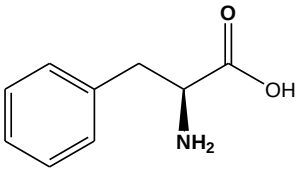
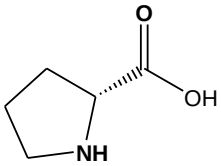
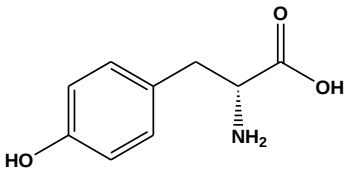
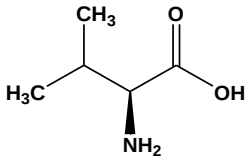
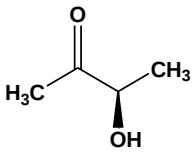
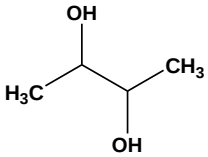
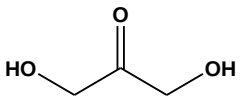
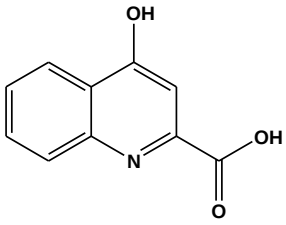
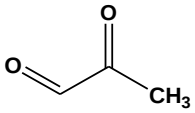
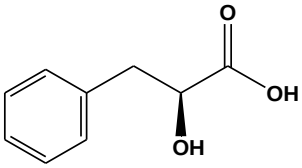
Table S1. Targeted 36 organic metabolites, Limit of Quatitation LoQ, molecular formula, chemical structure, regions of the ^{1}H-NMR spectra (ppm), and signal type

No.	LoQ[1]	Organic metabolite Molecular formula	Chemical structure	^{1}H-NMR range (ppm)	Signal type
	g/100g	**Sugars**			
1	10	**Fructose** $C_6H_{12}O_6$ Monosaccharide		4.075–4.115	doublet
2	10	**Glucose** $C_6H_{12}O_6$ Monosaccharide		4.615–4.650	singlet
3	0.5	**Sucrose** $C_{12}H_{22}O_{11}$ Disaccharide		4.185–4.215	doublet
4	0.3	**Gentiobiose** $C_{12}H_{22}O_{11}$ Disaccharide		4.483–4.507	doublet
5	0.5	**Maltose** $C_{12}H_{22}O_{11}$ Disaccharide		5.377–5.394	doublet
6	1	**Maltotriose** $C_{18}H_{32}O_{16}$ Trisaccharide		3.260–3.290	doublet

7	0.01	**Mannose** $C_6H_{12}O_6$ Monosaccharide		5.162–5.178	doublet
8	1	**Melezitose** $C_{18}H_{32}O_{16}$ Trisaccharide		5.420–5.445 4.273–4.290	doublet
9	0.1	**Raffinose** $C_{18}H_{32}O_{16}$ Trisaccharide		4.972–4.990	doublet
10	0.2	**Turanose** $C_{12}H_{22}O_{11}$ Disaccharide		5.270–5.300	doublet
	mg/kg	**Indicator of quality**			
11	5	**5-Hydroxymethylfurfural** (HMF) $C_6H_6O_3$		9.430–9.460	singlet
	mg/kg	**Alcohol**			
12	5	**Ethanol** C_2H_6O		1.145–1.195	triplet
	mg/kg	**Aliphatic Organic Acids (AOA)**			
13	10	**Acetic Acid** $C_2H_4O_2$ Monocarboxylic acid		2.090–2.080	singlet
14	50	**Citric Acid** $C_6H_8O_7$ Tricarboxylic acid		2.920–2.988 2.770–2.838	doublet of doublets

15	5	**Formic Acid** CH_2O_2 Monocarboxylic acid		8.230–8.310	singlet
16	5	**Fumaric Acid** $C_4H_4O_4$ Dicarboxylic acid		6.720–6.750	singlet
17	10	**Lactic Acid** $C_3H_6O_3$ Monocarboxylic acid		1.375–1.415	doublet
18	100	**Malic Acid** $C_4H_6O_5$ Dicarboxylic acid		2.740–2.820 2.850–2.930	double doublet
19	10	**Pyruvic Acid** $C_3H_4O_3$ Monocarboxylic acid		2.365–2.372	singlet
20	300	**Quinic Acid** $C_7H_{12}O_6$ Monocarboxylic acid		1.850–1.950	doublet
21	80	**Shikimic Acid** $C_7H_{10}O_5$ Cyclitol and cyclohexanecarboxylic acid		6.780–6.815	multiplet
22	5	**Succinic Acid** $C_4H_6O_4$ Dicarboxylic acid		2.640–2.675	singlet
	mg/kg	**Amino Acids**			
23	5	**Alanine** $C_3H_7NO_2$		1.470–1.498	doublet

24	150	**Aspartic acid** $C_4H_7NO_4$		2.910–2.945	doublet
25	200	**Glutamine** $C_5H_{10}N_2O_3$		2.420–2.482	multiplet
26	40	**Leucine** $C_6H_{13}NO_2$		0.932–0.945 0.950–0.963	multiplet
27	100	**Phenylalanine** $C_9H_{11}NO_2$		7.395–7.450	multiplet
28	150	**Proline** $C_5H_9NO_2$		2.070–2.110 2.285–2.400	multiplet
29	50	**Tyrosine** $C_9H_{11}NO_3$		6.860–6.915	multiplet
30	10	**Valine** $C_5H_{11}NO_2$		0.974–0.997 1.015–1.046	doublet
	mg/kg	**Botanical markers**			
31	20	**Acetoin** $C_4H_8O_2$		2.230–2.220 1.350–1.376	doublet singlet
32	20	**2,3-Butanediol** $C_4H_{10}O_2$		1.115–1.138	doublet

33	5	**Dihydroxyacetone** (DHA) $C_3H_6O_3$		4.405–4.41	singlet
34	30	**Kynurenic acid** $C_{10}H_7NO_3$		6.980–7.080	singlet
35	30	**Methylglyoxal** (MGO) $C_3H_4O_2$		1.355–1.365 Methylglyoxal monohydrate 2.285 – 2.295 Methylglyoxal dihydrate	singlet singlet
36	300	**3-Phenyllactic acid** $C_9H_{10}O_3$		2.935–3.000	doublet

[1]**LoQ** Limit of Quantitation