Supplementary information

Comparative analysis of four hop cultivars grown in Brazil and the USA by GC-MS-based metabolomics

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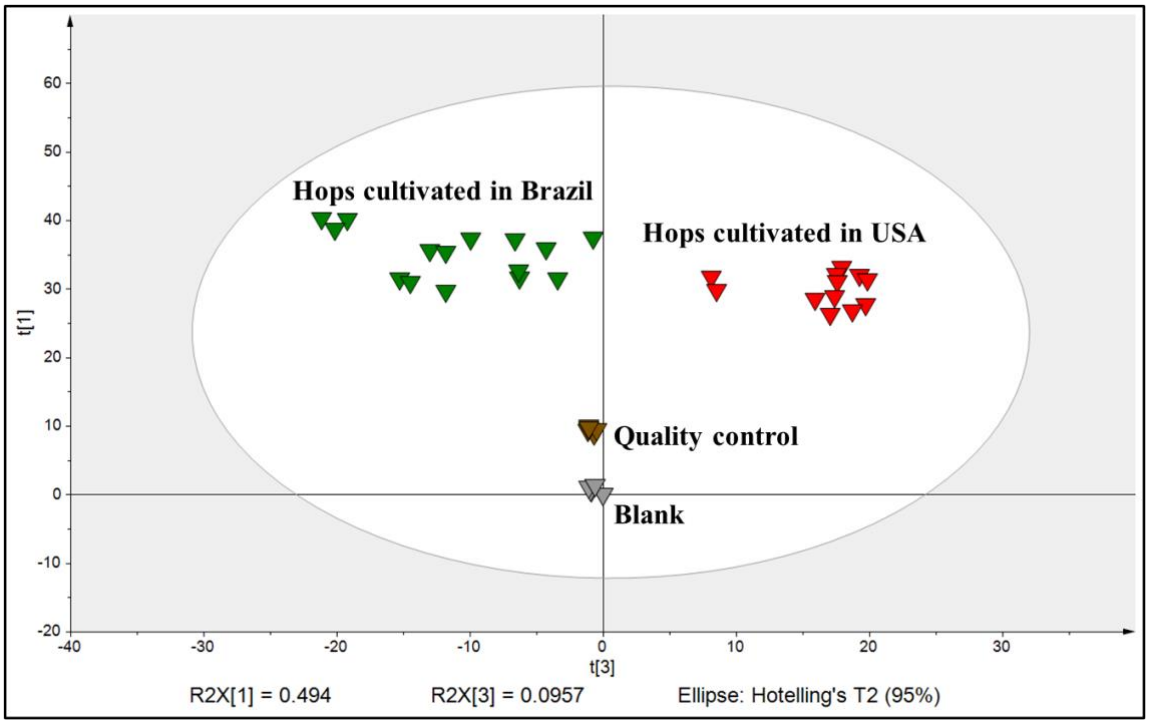

Figure S1. PCA score plot as a function of the first and third components. The first and third components explain 49,4% and 9,57% of the variation, respectively (R_2X = 0.783; Q^2 = 0.629). Samples were represented as coloured triangles (green, Brazil; red, United States; brown, quality control samples; grey, blank).

Table S1. Discriminating metabolites for the samples of Chinook, Columbus, Nugget, and Centennial grown in Brazil and the USA. **ID**, peak identification number; **Rt**, retention time in minutes; **Ri calc**, calculated retention index; **Ri lit**, literature retention index; **Match score (%)**, percentage match in spectral similarity with NIST (National Institute of Standards and Technology - 2011), Wiley e FFNSC (Flavors and Fragrances of Natural and Synthetic Compounds) data libraries.

ID	Rt	Ri	Ri lit	Match score (%)	Compound Name
1	5.5	990	990	97	*β*-myrcene
2	6.2	1015	1013	95	isopentyl isobutyrate
3	6.6	1030	1027	90	limonene
4	7.0	1045	1045	87	*trans*-*β*-ocimene
5	8.2	1093	1095	80	myrcenol
6	8.8	1109	1107	95	isoamyl isovalerate
7	11.4	1194	1192	85	2-decanone
8	13.4	1253	1254	93	geraniol
9	15.1	1295	1303	87	2-undecanol
10	15.6	1277	1283	90	methyl nerolate
11	17.3	1374	1375	93	*α*-coapene
12	18.0	1395	1388	91	2-dodecanone
13	19.0	1428	1428	93	*β*-copaene
14	19.1	1431	1433	95	*trans*- *α*-bergamotene
15	19.8	1453	1452	95	*α*-humulene
16	20.8	1487	1487	94	*β*-selinene
17	20.9	1490	1490	90	germacrene D
18	21.0	1494	1494	92	*α*-selinene
19	21.6	1511	1511	92	*γ*-cadinene
20	21.7	1516	1515	95	*δ*-cadinene
21	21.7	1517	1518	80	*ι*-gurjunene
22	21.8	1520	1520	87	*trans*-calamenene
23	22.1	1531	1525	85	cadina-1,4-diene
24	22.3	1535	1536	88	*α*-cadinene
25	22.4	1540	1541	94	calacorene
26	23.0	1560	1567	81	*trans*-nerolidol
27	24.4	1608	1606	88	humulene epoxide II
28	24.7	1617	1609	81	viridiflorol
29	25.1	1632	1629	84	humuladienone
30	25.4	1642	1642	89	*τ*-cadinol
31	26.2	1672	1678	86	aromadendrene oxide II