α acid fraction from Hop extract exerts an endothelium-derived hyperpolarization vasorelaxant effect through TRPV4 employing a feedforward mechanism of PKCα

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Table S1: Qualitative characterization of different Hop fractions by UHPLC-MS/MS

Peak	r_t (min)	Compound	$[M-H]^-$	[MS/MS]	Error (ppm)	PDA λ_{max} (nm)	Molecular Formula
Hop Fraction A (HOP A)							
Hydroxycinnamic acid							
1	1.83	3'- caffeolquinic acid (Chlorogenic acid) *	353.0850	191.0625, 179.0385	0.85	320	$C_{16}H_{18}O_9$
2	2.65	3'- coumaroylquinic acid	337.0922	163.0407, 119.0394	-2.67	304	$C_{16}H_{18}O_8$
3	3.52	3' - feruloylquinic acid	367.1040	193.0516, 134.0216	1.36	322	$C_{17}H_{20}O_9$
Flavonols							
4	6.50	Quercetin 3-O-(2-rhamnosyl) - hexoside	755.2036	301.0333, 255.0535 271.0211	-0.53	256, 299	$C_{33}H_{40}O_{20}$
5	6.99	Quercetin 3-O-galactoside*	463.0855	301.0346, 271.0255 255.0290	-3.89	255	$C_{21}H_{20}O_{12}$
6	7.48	Rutin*	609.1445	301.0362, 255.0306 271.0269	-4.43	353	$C_{27}H_{30}O_{16}$
7	7.78	Quercetin 3-O-glucoside*	463.0855	301.0346, 271.0255 255.0290	-4.53	255	$C_{21}H_{20}O_{12}$
8	8.33	Quercetin 3-O-(acetyl) -hexoside	505.0972	301.0381, 271.0204 255.0288	-3.17	311	$C_{23}H_{22}O_{13}$
9	863	Kaempferol 3-O-hexoside	635.1601	285.0384, 593.1373 255.0300 227.0416	0.63	262, 345	$C_{29}H_{32}O_{16}$
10	8.88	Kaempferol 3-O-di-hexoside	593.1413	285.0393, 255.0279 227.0656	-2.42	265, 344	$C_{27}H_{30}O_{15}$
11	8.94	Kaempferol 3-O-–(malonyl-hexoside)-O-rhamnoside	447.0949	285.0433, 255.0302 227.0741	4.03	264, 345	$C_{21}H_{20}O_{11}$
12	2.30	Epicatechin dimer	577.1247	407.0662, 289.0448	-4.97	279	$C_{30}H_{26}O_{12}$
13	3.10	Epicatechin dimer isomer II	577.1288	407.0729, 289.0619	1.73	279	$C_{30}H_{26}O_{12}$
Hop Fraction B (HOP B)							
α- and β- acids derivatives							
14	13.50	Oxy-humulinone	393.1912	349.2050, 263.1292 395.1898	-4.42	255, 323	$C_{21}H_{30}O_7$
15	14.00	Humulinone isomer	377.1928	263.1259, 221.0969	-5.04	285, 323	$C_{21}H_{30}O_6$
16	15.15	Oxidized humulinone derivative	409.1879	263.1285, 295.1130	0.98	285, 323	$C_{21}H_{30}O_8$
17	16.6	Oxidized humulinone derivative	409.1879	263.1285,	0.98	285,	$C_{21}H_{30}O$

	0	isomer		295.1130		323	$_{8}$
18	17.69	Cohumulone	347.1862	278.1176, 235.0624	-0.58	285, 323	$C_{20}H_{28}O_{5}$
19	18.65	Cohumulinone	363.1814	278.1176, 235.0624	-1.38	275, 310	$C_{20}H_{28}O_{6}$
20	19.15	Humulinone	377.1968	292.1315, 249.0765	-5.04	285, 323	$C_{21}H_{30}O_{6}$
21	20.84	Cohumulone isomer	347.1862	235.0624,278.1176	-0.58	285, 323	$C_{20}H_{28}O_{5}$
22	21.40	Iso-α-ad/n-humulone	361.2015	265.1428, 363.1836	2.21	285, 323	$C_{21}H_{30}O_{5}$
23	21.70	Deoxycohumulone	331.1920	262.1292, 194.0621	1.51	290, 335	$C_{20}H_{28}O_{4}$
24	24.30	Prehumulone	375.1818	306.1319	2.40	285, 325	$C_{22}H_{32}O_{5}$
25	18.10	Cohulupone	317.1765	248.0959, 135.3119	2.21	280, 335	$C_{19}H_{26}O_{4}$
Hop Fraction C (HOP C)							
β- acids and derivatives							
26	21.70	Lupulone E	415.2489	259.1037, 303.1277	-0.24	235, 360	$C_{25}H_{36}O_{5}$
27	22.56	Postlupulone	385.1228	273.0903, 248.9524	-3.63	280, 335	$C_{24}H_{34}O_{4}$
28	24.10	Colupulone	399.2541	287.1253, 219.0712	-0.25	280, 335	$C_{25}H_{36}O_{4}$
29	26.10	Deoxyhumulone/deoxyadlupulone	345.2064	346.2135, 301.2297 221.0866	-2.03	290, 335	$C_{21}H_{30}O_{4}$
30	26.80	Lupulone	413.2698	301.1446, 344.1991, 233.0808	2.83	235, 360	$C_{26}H_{38}O_{4}$
31	26.95	Adlupolone	413.2698	301.1446, 344.1991, 233.0808	2.83	235, 360	$C_{26}H_{38}O_{4}$
Prenylflavonoids							
32	18.25	Oxy-Xanthohumol	369.1336	249.0772	-5.40	255, 307	$C_{21}H_{22}O_{6}$
33	18.32	Isoxanthohumol	353.1405	233.0921, 189.0277 175.0147	-0.85	370	$C_{21}H_{22}O_{5}$
34	20.10	Xanthohumol*	353.1405	233.0921, 189.0277 175.0147	-0.85	370	$C_{21}H_{22}O_{5}$
35	25.10	Prenyl-naringenin	339.1229	219.0672, 245.0805	-1.75	294, 337	$C_{20}H_{20}O_{5}$

* Identified according to standard retention times.