

Article

# Artificial Intelligence sensing: effective flavor blueprinting of tea infusions for a quality control perspective

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The supplementary material comprises one Supplementary Table ST1:

**Supplementary Table 1 ST1:** Analytes subjected to validation for Ai flavor blueprinting of tea. Analytes are listed together with chromatographic information on retention times ( $t_R$  min), Target/Qualifier Ions  $m/z$  (GC-MS), detection wavelengths nm (LC-UV/DAD), calibration functions and determination coefficients ( $R^2$ ), precision (repeatability and intermediate precision) CV%, and accuracy results from spiked QC infusions at two levels expressed as percent recovery % Rec. Accuracy was tested at +10 and +25  $\mu\text{g/L}$  for aroma compounds and +10 and +25  $\text{mg/L}$  for tastants and quality markers.

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Compound name	$t_R$ (min)	Target Ion (m/z)	Qualifiers (m/z)	Detection wavelength (nm)	Intra-week CV%	Inter-week CV%	Calibration function	Linearity ( $R^2$ )	Accuracy Lv 1	Accuracy Lv 2
(E)-2-Nonenal	20.59	55	70, 83, 96		6.94	15.22	$y=0.097x+0.35$	0.9986	113	116
(E,E)-2,4-Decadienal	27.92	81	41, 55, 67		4.30	16.56	$y=0.44x+1.603$	0.9976	109	112
(E,E)-2,4-Nonadienal	23.22	81	41, 67, 138		9.85	15.87	$y=0.429x+0.533$	0.9967	115	109
(E,Z)-2,6-Nonadienal	20.23	41	70		9.97	12.21	$y=0.191x+0.867$	0.9992	109	106
(Z)-4-Heptenal	8.56	41	55, 68, 84		10.63	17.32	$y=0.059x+0.468$	0.9959	103	100
Beta damascenone	30.49	69	121, 105, 41		7.94	15.40	$y=0.37x+0.256$	0.9968	100	104
Beta ionone	34.68	177	43, 135		10.86	16.93	$y=0.55x+0.14$	0.9959	103	110
Butanal, 2-methyl	2.70	57	41, 71, 86		12.56	22.13	$y=0.57x+0.23$	0.9950	90.0	98.3
Butanal, 3-methyl	2.61	44	58, 71, 86		14.65	24.56	$y=0.008x+1.157$	0.9972	88.3	94.2
Geraniol	24.82	69	41, 123		9.12	14.25	$y=0.14x+5.723$	0.9983	102	105
Hexanal	5.21	56	56, 72, 82		8.02	10.09	$y=0.034x+9.999$	0.9994	114	117
Linalool	17.71	71	93, 121, 55		5.07	14.10	$y=0.121x+15.84$	0.9969	115	119
Phenyl acetaldehyde	14.96	91	120, 65		11.08	13.54	$y=0.127x+50.42$	0.9951	106	109
Epigallocatechin	2.50			280	11.96	14.34	$y=4833.9x$	0.9990	108	107
Catechin	2.85			280	5.91	11.74	$y=15840x$	0.9988	101	100
Epicatechin	3.45			280	7.56	15.76	$y=16605x$	0.9989	104	102
Epigallocatechingallate	4.38			280	2.34	14.68	$y=29412x$	0.9988	108	105
Gallocatechingallate	4.92			280	8.50	11.84	$y=36797x$	0.9987	107	105
Epicatechingallate	5.50			280	11.22	17.55	$y=42214x$	0.9986	101	98.9
Catechingallate	6.14			280	4.16	15.97	$y=43329x$	0.9987	105	104
Theaflavin	7.15			380	2.95	5.10	$y=20085x$	0.9982	110	108
Theaflavin-3-gallate	7.92			380	6.66	4.98	$y=10673x$	0.9978	112	109
Theaflavin-3'-gallate	7.59			380	3.23	6.58	$y=7408.5x$	0.9975	108	106
Theaflavin-3,3'-gallate	8.03			380	2.84	3.99	$y=16271x$	0.9984	109	103
Myricetin-3-o-galactoside	13.12			350	3.22	9.08	$y=31659x$	0.9978	99.4	99
Myricetin-3-o-glucoside	13.37			350	13.60	11.07	$y=29755x$	0.9984	98.6	100
Quercetin-3-o-rutinoside (Rutin)	13.80			350	9.44	14.00	$y=34683x$	0.9978	96.0	98
Quercetin-3-o-galactoside	14.56			350	4.05	9.79	$y=29875x$	0.9993	96.9	99
Quercetin-3-o-glucoside	14.87			350	10.01	11.86	$y=27784x$	0.9968	98.7	102
Kaempferol-3-o-rutinoside	15.40			350	7.08	9.54	$y=40086x$	0.9982	100	100
Kaempferol-3-o-glucoside	15.79			350	5.84	8.94	$y=31976x$	0.9968	101	104
Caffeine	2.66			280	5.86	6.00	$y=87563x$	0.9991	99.0	102

