J. Braz. Chem. Soc., Vol. 26, No. 6, S1-S2, 2015.
Printed in Brazil - ©2015 Sociedade Brasileira de Química
0103 - 5053 $6.00+0.00

Supplementary Information

Preliminary Investigation of Medicinal Herb Adulteration Using Comprehensive Two-Dimensional Gas Chromatography and Chemometric Analysis

Juliane E. Welke,[a,b] Flaviana C. Damasceno,[b] Karine P. Nicolli,[b] Lilian Mentz,[c] Elina B. Caramão,[b] Fernando H. Pulgati[d] and Cláudia A. Zini*[,b]

[a]Instituto de Ciência e Tecnologia de Alimentos and [b]Instituto de Química, Universidade Federal do Rio Grande do Sul (UFRGS), Av. Bento Gonçalves, 9500, 91501-970 Porto Alegre-RS, Brazil

[c]Faculdade de Farmácia, UFRGS, Av. Ipiranga, 2752, 90610-000 Porto Alegre-RS, Brazil

[d]Instituto de Matemática, UFRGS, Av. Bento Gonçalves, 9500, 91509-900 Porto Alegre-RS, Brazil

Table S1. Validation range, regression equation and determination coefficient (r^2) of some representative compounds of each chemical class identified in fennel and/or anise

Chemical class	Compound	^1t_R / min[a]	^2t_R / s[b]	Validation range / (μg L^{-1})	Regression equation[c]	r^2 [d]
Alcohol	1-Hexanol	12.37	3.33	108-1080	y = 2E+6x + 815108	0.9953
Monoterpene hydrocarbon	α-Pinene	13.30	3.89	55-825	y = 4E+6x + 20968	0.9929
Oxygenated monoterpene	Eucalyptol	19.02	3.93	55-1090	y = 6E+6x + 587803	0.9972
Oxygenated monoterpene	Linalool	21.82	3.95	50-990	y = 780887x + 10909	0.9975
Alcohol	Benzyl alcohol	23.68	3.34	52-1040	y = 229435x – 10684	0.9971
Phenyl propanoid	Anethole	34.30	3.72	55-1090	y = 351561x + 5118.1	0.9956
Sesquiterpene	α-Humulene	37.92	4.59	54-1070	y = 567139x – 27947	0.9969

[a] ^1t_R: retention time in GC×GC/TOFMS first dimension; [b] ^2t_R: retention time in GC×GC/TOFMS second dimension; [c]x designates concentration of volatile compounds (μg L^{-1}) and y designates the peak area; [d]determination coefficient.

*e-mail: claudialcaraz@gmail.com

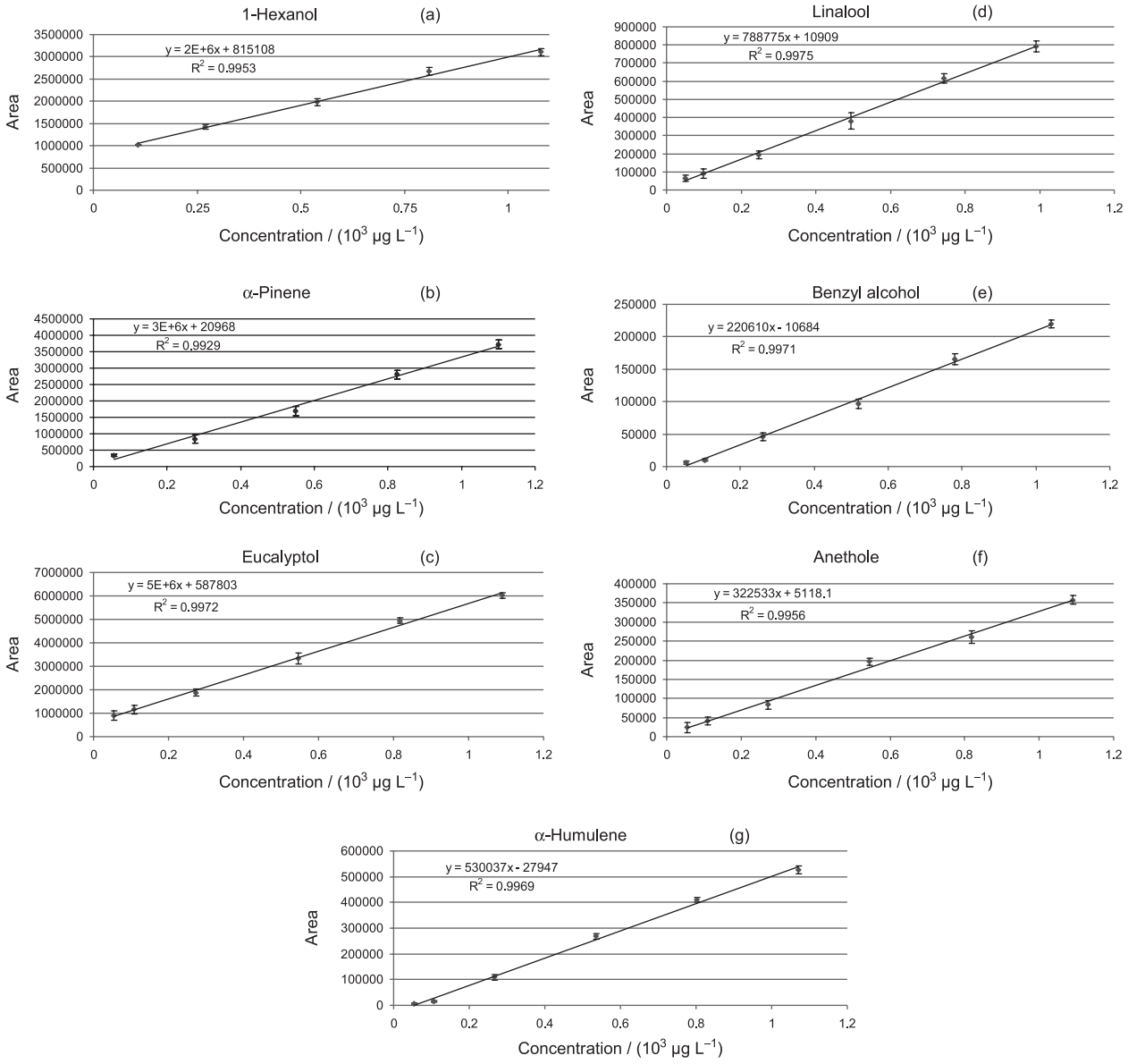

Figure S1. Analytical calibration curve of some representative compounds of each chemical class identified in fennel and/or anise volatile compounds. (a) 1-hexanol, (b) α-pinene, (c) eucalyptol, (d) linalool, (e) benzyl alcohol, (f) anethole, (g) α-humulene. Solutions of different concentrations of each standard compound were injected four times.