

## Appendix IV - Cited in Chapter 7

**Appendix IV.I.** Comparison of means of the activity of *Phlomis purpurea* root extract (PRE) HPLC fractions on *Phytophthora cinnamomi* mycelial growth and respective control using T-test for independent samples.

**Estadísticas de grupo**

Fraction	N	Média	Desvio Padrão	Erro padrão da média
Co_diameter Control F1	3	45,67	,577	,333
Fraction 1	3	45,67	,577	,333

**Teste de amostras independentes**

		Teste de Levene para igualdade de variâncias		teste-t para igualdade de Médias						
		Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	95% Intervalo de Confiança da Diferença	
									Inferior	Superior
Co_diameter	Variâncias iguais assumidas	,000	1,000	,000	4	1,000	,000	,471	-1,309	1,309
	Variâncias iguais não assumidas			,000	4,000	1,000	,000	,471	-1,309	1,309

**Estadísticas de grupo**

Fraction	N	Média	Desvio Padrão	Erro padrão da média
Co_diameter Control F2	3	45,67	,577	,333
Fraction 2	3	46,33	,577	,333

**Teste de amostras independentes**

		Teste de Levene para igualdade de variâncias		teste-t para igualdade de Médias						
		Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	95% Intervalo de Confiança da Diferença	
									Inferior	Superior
Co_diameter	Variâncias iguais assumidas	,000	1,000	-1,414	4	,230	-,667	,471	-1,975	,642
	Variâncias iguais não assumidas			-1,414	4,000	,230	-,667	,471	-1,975	,642

**Estadísticas de grupo**

Fraction	N	Média	Desvio Padrão	Erro padrão da média
Co_diameter Control F3	3	46,00	,000	,000
Fraction 3	3	44,33	,577	,333

**Teste de amostras independentes**

		Teste de Levene para igualdade de variâncias		teste-t para igualdade de Médias						
		Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	95% Intervalo de Confiança da Diferença	
									Inferior	Superior
Co_diameter	Variâncias iguais assumidas	16,000	,016	5,000	4	,007	1,667	,333	,741	2,592
	Variâncias iguais não assumidas			5,000	2,000	,038	1,667	,333	,232	3,101

**Estadísticas de grupo**

Fraction	N	Média	Desvio Padrão	Erro padrão da média
Co_diameter Control F4	3	46,33	,577	,333
Fraction F4	3	14,00	2,000	1,155

**Teste de amostras independentes**

		Teste de Levene para igualdade de variâncias		teste-t para igualdade de Médias						
		Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	95% Intervalo de Confiança da Diferença	
									Inferior	Superior
Co_diameter	Variâncias iguais assumidas	1,730	,259	26,903	4	,000	32,333	1,202	28,996	35,670
	Variâncias iguais não assumidas			26,903	2,331	,001	32,333	1,202	27,806	36,861

**Estadísticas de grupo**

Fraction	N	Média	Desvio Padrão	Erro padrão da média
Co_diameter Control F5	3	46,33	,577	,333
Fraction F5	3	,00	,000	,000

**Teste de amostras independentes**

		Teste de Levene para igualdade de variâncias		teste-t para igualdade de Médias						
		Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão de diferença	95% Intervalo de Confiança da Diferença	
									Inferior	Superior
Co_diameter	Variâncias iguais assumidas	16,000	,016	139,000	4	,000	46,333	,333	46,408	47,259
	Variâncias iguais não assumidas			139,000	2,000	,000	46,333	,333	44,899	47,768

Estadísticas de grupo

Fraction	N	Média	Desvio Padrão	Erro padrão da média
CoL_diameter Control F6	3	46,33	,577	,333
Fraction 6	3	13,00	1,000	,577

Teste de amostras independentes

	Teste de Levene para igualdade de variâncias		teste-t para igualdade de Médias						
	Z	Sig.	t	df	Sig. (2 extremidades)	Diferença média	Erro padrão da diferença	95% Intervalo de Confiança da Diferença	
								inferior	superior
CoL_diameter	400	,561	50,000	4	,000	33,333	,867	31,482	35,184
			50,000	3,200	,000	33,333	,867	31,285	35,382

**Appendix IV.II.** Analysis of variance of the mean of activity of commercially supplied natural compounds on *Phytophthora cinnamomi* mycelial growth.

Comparações múltiplas

Variável dependente: CoL\_diameter

DMS

(i) Fraction	(j) Fraction	Diferença média (i-j)	Erro Padrão	Sig.	Intervalo de Confiança 95%	
					Limite inferior	Limite superior
Control	Caffeic acid	,43333 <sup>*</sup>	,09124	,000	,2481	,6186
	Vanillic acid	1,35833 <sup>*</sup>	,09124	,000	1,1731	1,5436
	Chlorogenic acid	-,05000	,09124	,587	-,2352	,1352
	Rosmarinic acid	,01667	,09124	,856	-,1686	,2019
	Hederagenin	,01667	,09124	,856	-,1686	,2019
	Rutin	-,01667	,09124	,856	-,2019	,1686
	Caffeic acid	Control	-,43333 <sup>*</sup>	,09124	,000	-,6186
Vanillic acid		,92500 <sup>*</sup>	,09124	,000	,7398	1,1102
Chlorogenic acid		-,48333 <sup>*</sup>	,09124	,000	-,6686	-,2981
Rosmarinic acid		-,41667 <sup>*</sup>	,09124	,000	-,6019	-,2314
Hederagenin		-,41667 <sup>*</sup>	,09124	,000	-,6019	-,2314
Rutin		-,45000 <sup>*</sup>	,09124	,000	-,6352	-,2648
Vanillic acid		Control	-,135833 <sup>*</sup>	,09124	,000	-,15436
	Caffeic acid	-,92500 <sup>*</sup>	,09124	,000	-,11102	-,7398
	Chlorogenic acid	-,140833 <sup>*</sup>	,09124	,000	-,15936	-,12231
	Rosmarinic acid	-,134167 <sup>*</sup>	,09124	,000	-,15269	-,11564
	Hederagenin	-,134167 <sup>*</sup>	,09124	,000	-,15269	-,11564
	Rutin	-,137500 <sup>*</sup>	,09124	,000	-,15602	-,11898
	Chlorogenic acid	Control	,05000	,09124	,587	-,1352
Caffeic acid		,48333 <sup>*</sup>	,09124	,000	,2981	,6686
Vanillic acid		1,40833 <sup>*</sup>	,09124	,000	1,2231	1,5936
Rosmarinic acid		,06667	,09124	,470	-,1186	,2519
Hederagenin		,06667	,09124	,470	-,1186	,2519
Rutin		,03333	,09124	,717	-,1519	,2186
Rosmarinic acid		Control	-,01667	,09124	,856	-,2019
	Caffeic acid	,41667 <sup>*</sup>	,09124	,000	,2314	,6019
	Vanillic acid	1,34167 <sup>*</sup>	,09124	,000	1,1564	1,5269
	Chlorogenic acid	-,06667	,09124	,470	-,2519	,1186
	Hederagenin	,00000	,09124	1,000	-,1852	,1852
	Rutin	-,03333	,09124	,717	-,2186	,1519
	Hederagenin	Control	-,01667	,09124	,856	-,2019
Caffeic acid		,41667 <sup>*</sup>	,09124	,000	,2314	,6019
Vanillic acid		1,34167 <sup>*</sup>	,09124	,000	1,1564	1,5269
Chlorogenic acid		-,06667	,09124	,470	-,2519	,1186
Rosmarinic acid		,00000	,09124	1,000	-,1852	,1852
Rutin		-,03333	,09124	,717	-,2186	,1519
Rutin		Control	,01667	,09124	,856	-,1686
	Caffeic acid	,45000 <sup>*</sup>	,09124	,000	,2648	,6352
	Vanillic acid	1,37500 <sup>*</sup>	,09124	,000	1,1898	1,5602
	Chlorogenic acid	-,03333	,09124	,717	-,2186	,1519
	Rosmarinic acid	,03333	,09124	,717	-,1519	,2186
	Hederagenin	,03333	,09124	,717	-,1519	,2186

\*. A diferença média é significativa no nível 0.05.

Comparações múltiplas

Variável dependente: Col\_diameter  
DMS

(I) Fraction	(J) Fraction	Diferença média (I-J)	Erro Padrão	Sig.	Intervalo de Confiança 95%	
					Limite inferior	Limite superior
Control 2 Synergies	Caffeic+Vanillic	1,48333	,07876	,000	1,3235	1,6432
	Caffeic+Chlorogenic	,75833 <sup>*</sup>	,07876	,000	,5985	,9182
	Caffeic+Rosmarinic	,65833 <sup>*</sup>	,07876	,000	,4985	,8182
	Vanillic+Chlorogenic	1,32500 <sup>*</sup>	,07876	,000	1,1651	1,4849
	Vanillic+Rosmarinic	1,14167 <sup>*</sup>	,07876	,000	,9818	1,3015
	Chlorogenic+Rosmarinic	,23333 <sup>*</sup>	,07876	,005	,0735	,3932
Caffeic+Vanillic	Control 2 Synergies	-1,48333 <sup>*</sup>	,07876	,000	-1,6432	-1,3235
	Caffeic+Chlorogenic	-,72500 <sup>*</sup>	,07876	,000	-,8849	-,5651
	Caffeic+Rosmarinic	-,82500 <sup>*</sup>	,07876	,000	-,9849	-,6651
	Vanillic+Chlorogenic	-,15833	,07876	,052	-,3182	,0015
	Vanillic+Rosmarinic	-,34167 <sup>*</sup>	,07876	,000	-,5015	-,1818
	Chlorogenic+Rosmarinic	-1,25000 <sup>*</sup>	,07876	,000	-1,4099	-1,0901
Caffeic+Chlorogenic	Control 2 Synergies	-,75833 <sup>*</sup>	,07876	,000	-,9182	-,5985
	Caffeic+Vanillic	,72500 <sup>*</sup>	,07876	,000	,5651	,8849
	Caffeic+Rosmarinic	-,10000	,07876	,213	-,2599	,0599
	Vanillic+Chlorogenic	,56667 <sup>*</sup>	,07876	,000	,4068	,7265
	Vanillic+Rosmarinic	,38333 <sup>*</sup>	,07876	,000	,2235	,5432
	Chlorogenic+Rosmarinic	-,52500 <sup>*</sup>	,07876	,000	-,6849	-,3651
Caffeic+Rosmarinic	Control 2 Synergies	-,65833 <sup>*</sup>	,07876	,000	-,8182	-,4985
	Caffeic+Vanillic	,82500 <sup>*</sup>	,07876	,000	,6651	,9849
	Caffeic+Chlorogenic	-,10000	,07876	,213	-,0599	,2599
	Vanillic+Chlorogenic	,66667 <sup>*</sup>	,07876	,000	,5068	,8265
	Vanillic+Rosmarinic	,48333 <sup>*</sup>	,07876	,000	,3235	,6432
	Chlorogenic+Rosmarinic	-,42500 <sup>*</sup>	,07876	,000	-,5849	-,2651
Vanillic+Chlorogenic	Control 2 Synergies	-1,32500 <sup>*</sup>	,07876	,000	-1,4849	-1,1651
	Caffeic+Vanillic	,15833	,07876	,052	-,0015	,3182
	Caffeic+Chlorogenic	-,56667 <sup>*</sup>	,07876	,000	-,7265	-,4068
	Caffeic+Rosmarinic	-,66667 <sup>*</sup>	,07876	,000	-,8265	-,5068
	Vanillic+Rosmarinic	-,18333 <sup>*</sup>	,07876	,026	-,3432	-,0235
	Chlorogenic+Rosmarinic	-1,09167 <sup>*</sup>	,07876	,000	-1,2515	-,9318
Vanillic+Rosmarinic	Control 2 Synergies	-1,14167 <sup>*</sup>	,07876	,000	-1,3015	-,9818
	Caffeic+Vanillic	,34167 <sup>*</sup>	,07876	,000	,1818	,5015
	Caffeic+Chlorogenic	-,38333 <sup>*</sup>	,07876	,000	-,5432	-,2235
	Caffeic+Rosmarinic	-,48333 <sup>*</sup>	,07876	,000	-,6432	-,3235
	Vanillic+Chlorogenic	,18333	,07876	,026	,0235	,3432
	Chlorogenic+Rosmarinic	-,90833 <sup>*</sup>	,07876	,000	-1,0682	-,7485
Chlorogenic+Rosmarinic	Control 2 Synergies	-,23333 <sup>*</sup>	,07876	,005	-,3932	-,0735
	Caffeic+Vanillic	1,25000 <sup>*</sup>	,07876	,000	1,0901	1,4099
	Caffeic+Chlorogenic	,52500 <sup>*</sup>	,07876	,000	,3651	,6849
	Caffeic+Rosmarinic	,42500 <sup>*</sup>	,07876	,000	,2651	,5849
	Vanillic+Chlorogenic	1,09167 <sup>*</sup>	,07876	,000	,9318	1,2515
	Vanillic+Rosmarinic	,90833 <sup>*</sup>	,07876	,000	,7485	1,0682

\*. A diferença média é significativa no nível 0.05.

Multiple Comparisons

Dependent Variable: Col\_diameter  
LSD

(I) Fraction	(J) Fraction	Mean Difference (I-J)	Std. Error	Sig.	95% Confidence Interval	
					Lower Bound	Upper Bound
Control 3 Synergies	Caffeic+Vanillic+Chlorogenic	1,25833	,06948	,000	1,1152	1,4014
	Caffeic+Vanillic+Rosmarinic	1,23333 <sup>*</sup>	,06948	,000	1,0902	1,3764
	Caffeic+Chlorogenic+Rosmarinic	,41667 <sup>*</sup>	,06948	,000	-,2736	,5598
	Vanillic+Chlorogenic+Rosmarinic	1,03333 <sup>*</sup>	,06948	,000	,8902	1,1764
	Control 3 Synergies	-1,25833	,06948	,000	-1,4014	-1,1152
Caffeic+Vanillic+Chlorogenic	Caffeic+Vanillic+Rosmarinic	-,02500	,06948	,722	-,1681	,1181
	Caffeic+Chlorogenic+Rosmarinic	-,84167 <sup>*</sup>	,06948	,000	-,9848	-,6986
	Vanillic+Chlorogenic+Rosmarinic	-,22500 <sup>*</sup>	,06948	,003	-,3651	-,0819
	Control 3 Synergies	1,25833	,06948	,000	1,1152	1,4014
	Control 3 Synergies	-1,25833	,06948	,000	-1,3764	-1,0902
Caffeic+Vanillic+Rosmarinic	Caffeic+Vanillic+Chlorogenic	-,02500	,06948	,722	-,1181	,1681
	Caffeic+Chlorogenic+Rosmarinic	-,81667 <sup>*</sup>	,06948	,000	-,9598	-,6736
	Vanillic+Chlorogenic+Rosmarinic	-,20000 <sup>*</sup>	,06948	,008	-,3431	-,0569
	Control 3 Synergies	1,25833	,06948	,000	1,1152	1,4014
	Control 3 Synergies	-1,25833	,06948	,000	-1,3764	-1,0902
Caffeic+Chlorogenic+Rosmarinic	Caffeic+Vanillic+Chlorogenic	-,41667 <sup>*</sup>	,06948	,000	-,5598	-,2736
	Caffeic+Vanillic+Rosmarinic	,84167 <sup>*</sup>	,06948	,000	,6986	,9848
	Caffeic+Vanillic+Rosmarinic	,81667 <sup>*</sup>	,06948	,000	,6736	,9598
	Vanillic+Chlorogenic+Rosmarinic	,61667 <sup>*</sup>	,06948	,000	,4736	,7598
	Control 3 Synergies	1,25833	,06948	,000	1,1152	1,4014
Vanillic+Chlorogenic+Rosmarinic	Control 3 Synergies	-1,03333	,06948	,000	-1,1764	-,8902
	Caffeic+Vanillic+Chlorogenic	-,22500 <sup>*</sup>	,06948	,003	-,3651	-,0819
	Caffeic+Vanillic+Rosmarinic	-,20000 <sup>*</sup>	,06948	,008	-,3431	-,0569
	Caffeic+Chlorogenic+Rosmarinic	-,81667 <sup>*</sup>	,06948	,000	-,9598	-,6736
	Control 3 Synergies	1,25833	,06948	,000	1,1152	1,4014

\*. The mean difference is significant at the 0.05 level.

**Appendix IV.III.** Comparison of means of the activity of commercially supplied natural compounds on *Phytophthora cinnamomi* mycelial growth.

Descriptives								
Col_diameter	N	Mean	Std. Deviation	Std. Error	95% Confidence Interval for Mean		Minimum	Maximum
					Lower Bound	Upper Bound		
Control	6	4,0750	,19429	,07932	3,8711	4,2789	3,80	4,30
Caffeic acid	6	3,6417	,14289	,05833	3,4917	3,7916	3,50	3,90
Vanillic acid	6	2,7167	,15055	,06146	2,5597	2,8747	2,60	3,00
Chlorogenic acid	6	4,1250	,15411	,06292	3,9633	4,2867	3,90	4,30
Rosmarinic acid	6	4,0583	,21311	,08700	3,8347	4,2820	3,80	4,35
Hederagenin	6	4,0583	,13934	,05689	3,9121	4,2046	3,90	4,25
Rutin	6	4,0917	,07360	,03005	4,0144	4,1689	4,00	4,20
Control 2 Synergies	6	4,0417	,12007	,04902	3,9157	4,1677	3,90	4,20
Caffeic+Vanillic	6	2,5583	,08010	,03270	2,4743	2,6424	2,50	2,70
Caffeic+Chlorogenic	6	3,2833	,05164	,02108	3,2291	3,3375	3,20	3,35
Caffeic+Rosmarinic	6	3,3833	,13292	,05426	3,2438	3,5228	3,20	3,60
Vanillic+Chlorogenic	6	2,7167	,07528	,03073	2,6377	2,7967	2,60	2,80
Vanillic+Rosmarinic	6	2,9000	,18708	,07638	2,7037	3,0963	2,65	3,10
Chlorogenic+Rosmarinic	6	3,8083	,22004	,08983	3,5774	4,0392	3,50	4,10
Control 3 Synergies	6	3,9500	,13784	,05627	3,8053	4,0947	3,80	4,20
Caffeic+Vanillic+Chlorogenic	6	2,6917	,14289	,05833	2,5417	2,8416	2,50	2,90
Caffeic+Vanillic+Rosmarinic	6	2,7167	,06831	,02789	2,6450	2,7884	2,60	2,80
Caffeic+Chlorogenic+Rosmarinic	6	3,5333	,15055	,06146	3,3753	3,6913	3,40	3,80
Vanillic+Chlorogenic+Rosmarinic	6	2,9167	,07528	,03073	2,8377	2,9957	2,80	3,00
Total	114	3,4351	,59570	,05579	3,3246	3,5456	2,50	4,35

**Appendix IV.IV.** Experimental details of x-ray-diffraction

Crystal data

Chemical formula	4(C <sub>29</sub> H <sub>46</sub> O <sub>6</sub> ) Na CH <sub>4</sub> O 5(O)
$M_r$	1100.83
Crystal system, space group	Monoclinic, C2
Temperature (K)	100
a, b, c (Å)	51.762 (10), 8.7460 (17), 26.208 (5)
$\beta$ (°)	96.91 (3)
$V$ (Å <sup>3</sup> )	11778 (4)
Z	8
Radiation type	Synchrotron monochrome, $\lambda = 0.97625$ Å
$\mu$ (mm <sup>-1</sup> )	0.20
Crystal size (mm)	0.4 × 0.05 × 0.05

Data collection

Diffractometer	MD2 (MAATEL) diffractometer
Absorption correction	Multi-scan
$T_{min}$ , $T_{max}$	0.897, 0.992
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	32427, 9594, 8160
$R_{int}$	0.097
$\theta_{max}$ (°)	27.7
$(\sin \theta/\lambda)_{max}$ (Å <sup>-1</sup> )	0.476

Refinement

$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ , $S$	0.092, 0.264, 1.14
N <sup>o</sup> . of reflections	9594
N <sup>o</sup> . of parameters	1632
N <sup>o</sup> . of restraints	1755
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$ , $\Delta\rho_{min}$ (e Å <sup>-3</sup> )	0.49, .0.47
Absolute structure	Flack x determined using 3119 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	0.11 (17)

Computer programs: ESRF ID23-1 Beamline, XDS (Kabsch, 2010), AutoPROC (Bricogne et al., 2011), SHELXD (Sheldrick, 2008), SHELXL2014 (Sheldrick, 2014), ORTEP-3 for Windows (Farrugia, 2012), WinGX publication routines (Farrugia, 2012).



**Appendix IV.VI.** Structure of four molecules of the cristal structure of phlomispurpentaolone.

