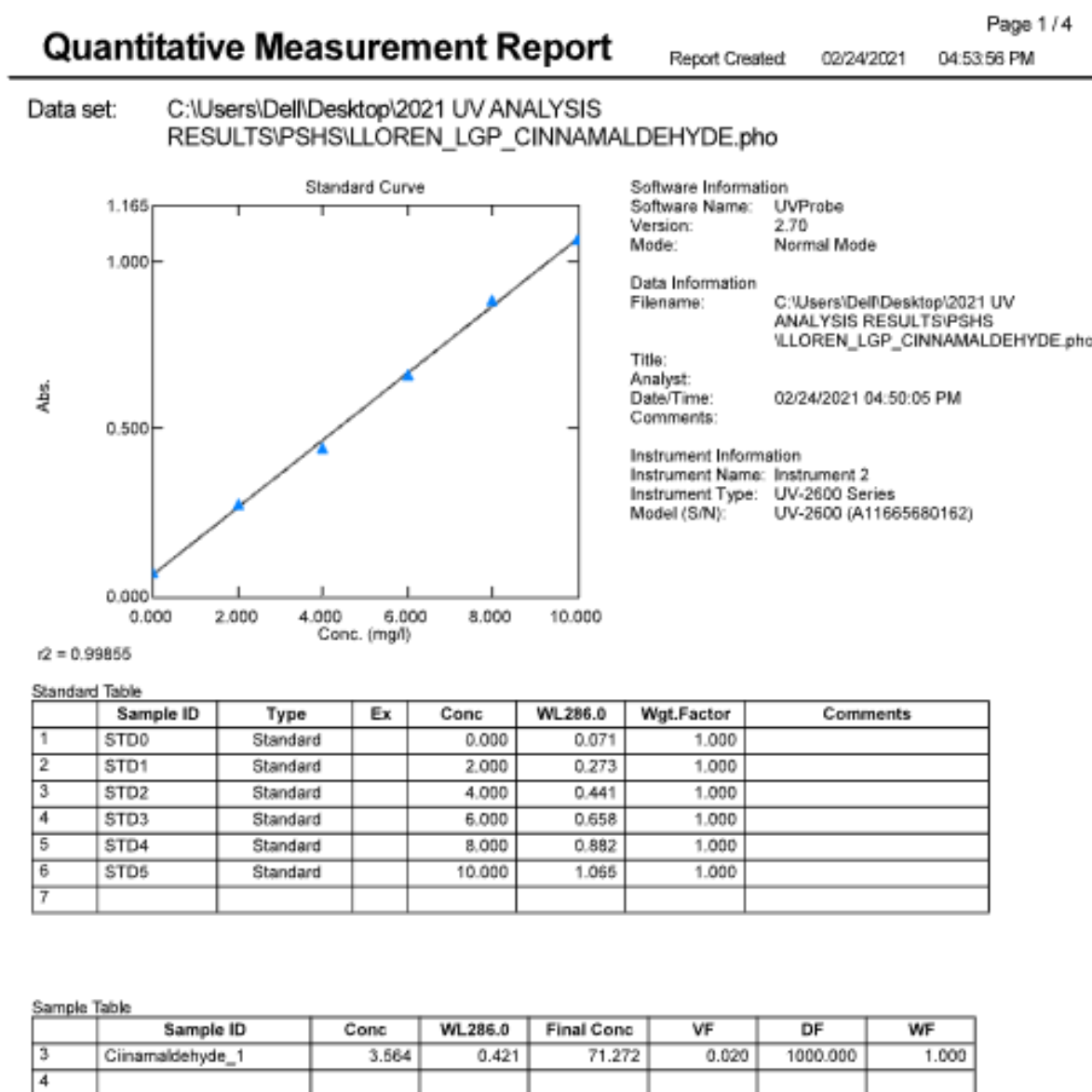


APPENDIX A

DLSU UV SPECTROSCOPY RESULTS AND EE CALCULATION



Appendix A1. First page of the analysis report provided by DLSU for UV spectroscopy.

Quantitative Measurement Report

Page 2 / 4

Report Created 02/24/2021 04:53:56 PM

Data set: C:\Users\Dell\Desktop\2021 UV ANALYSIS
RESULTS\PSHS\LLOREN_LGP_CINNAMALDEHYDE.pho

[Wavelengths]

Wavelength Name: WL286.0
Wavelength: 286.00 nm

[Calibration Curve]

Column for Cal. Curve: WL286.0
Cal. Curve Type: Multi Point
Cal. Curve Unit: mg/l
Selected Wavelength: WL286.0
Calibration Equation: Abs = K1*(Conc) + K0
Zero Interception: Not Selected

[Measurement Parameters(Standard)]

Data Acquired by: Instrument
Delay sample read: Disabled
Repeat: Disabled

[Measurement Parameters(Sample)]

Data Acquired by: Instrument
Delay sample read: Disabled
Repeat: Disabled

[Equations]

Equation Name: Final Conc
Equation: (Conc*VF*DF)/WF
Units: 1

[Pass Fail]

[Method Summary]

Title:
Date/Time: 02/23/2021 03:19:10 PM
Comments:
Sample Preparations:

[Instrument Properties]

Instrument Type: UV-2600 Series
Measuring Mode: Absorbance
Slit Width: 1.0
Accumulation time: 0.1 sec.
Light Source Change Wavelength: 323.0 nm
Detector Unit: Direct
S/R Exchange: Normal
Slair Correction: OFF

[Attachment Properties]

Attachment: None

Appendix A2. Second page of the analysis report provided by DLSU for UV spectroscopy.

$$EE = \frac{\text{mass of complexed compound}}{\text{initial mass of compound}} \times 100\%$$

$$EE = \frac{\frac{71.272 \times 10^{-3} \text{ g cinnamaldehyde}}{\text{g inclusion complex}} \times 16 \text{ g inclusion complexes}}{1.864 \text{ g cinnamaldehyde}} \times 100\%$$

$$EE = 61.18\%$$

APPENDIX B

DOST DIFFERENTIAL SCANNING CALORIMETRY RESULTS



Republic of the Philippines
Department of Science and Technology
INDUSTRIAL TECHNOLOGY DEVELOPMENT INSTITUTE
ADVANCED DEVICE AND MATERIALS TESTING LABORATORY
DOST Cpd., General Santos Ave., Bicutan, Taguig City
Tel.: (02) 837-0461 Email: services@admatel.com
http://www.admatel.com/



AB
PMS Accredited
Testing Laboratory
PMS 5031:IC 17025:2017
LA-2015-271B

REPORT OF ANALYSIS

Reference No. : ADMATEL 2102-2343

Customer : Clarissa Beatriz P. Laurito
Philippine Science High School
B21.clarissa.laurito@pshs.edu.ph

Sample Label : One (1) Beta-cyclodextrin and Cinnamon Oil Inclusion Complexes

Analysis Requested : Differential Scanning Calorimetry (DSC)

Date Received : February 19, 2021

Date Tested : February 22, 2021

I. Test Description

Measuring Cell : Perkin Elmer DSC 4000

Sample Holder : Standard aluminum pan, crimped

Temperature Program : Isothermal at 30°C for 2 min
Heat from 30°C to 430°C at 10°C/min
Isothermal at 430°C for 2 min

Atmosphere : Nitrogen at 20 mL/min

II. Summary

The photo and the Differential Scanning Calorimetry (DSC) curves of the Beta-cyclodextrin and Cinnamon Oil Inclusion Complexes sample is presented in **Figures 1 and 2**, respectively. The corresponding DSC profile is summarized in **Table 1**.

III. Results

Table 1. Summary of DSC profile

Sample ID	Endothermic Peak Temperature (T_p), °C
Beta-cyclodextrin and Cinnamon Oil Inclusion Complexes	$T_{p1} = 55.88$
	$T_{p2} = 80.69$
	$T_{p3} = 103.12$
	$T_{p4} = 137.55$
	$T_{p5} = 173.49$
	$T_{p6} = 231.45$
	$T_{p7} = 322.16$
	$T_{p8} = 336.12$
	$T_{p9} = 344.65$



Appendix B1. First page of the analysis report provided by DOST for differential scanning calorimetry.



IV. Remarks

The sample was tested as-received.



Figure 1. Photograph of the Beta-cyclodextrin and Cinnamon Oil Inclusion Complexes sample

VALIDITY OF THE REPORT: The test results are those obtained at the time of the test and pertain only to the sample/s received by ADMATEL.


LYNNE JERISA V. ALFECHE
Analyst
Date: 02/23/2021


ANGELENE J. ALCAIN
Laboratory Head
Date: 03/04/2021

Issued under the authority of:


ARACELI M. MONSADA, Dr. -Eng'g.
Laboratory Manager
Date: 03/04/2021

Form: AL-F25c
Issue: December 14, 2020
Revision: 02



Appendix B2. Second page of the analysis report provided by DOST for differential scanning calorimetry.

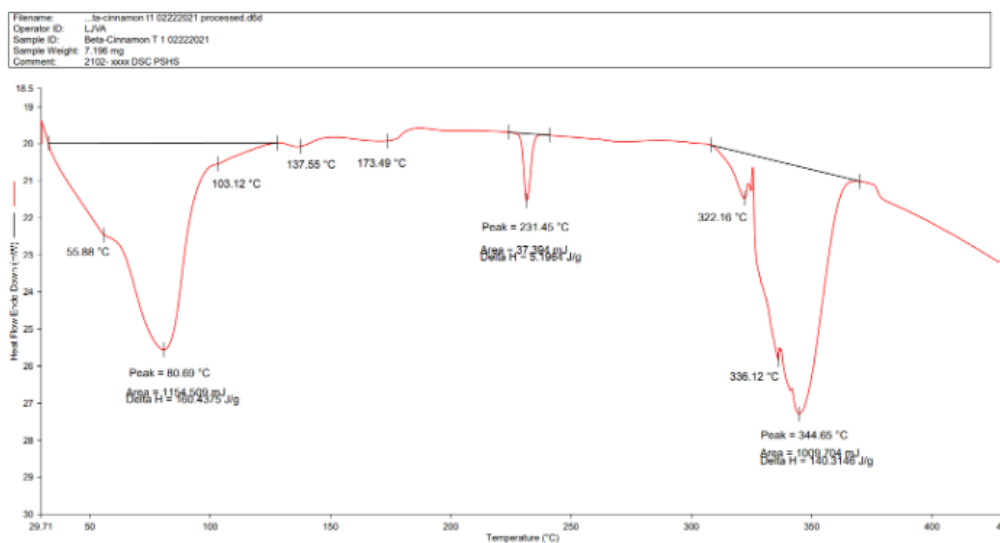


Figure 1. DSC thermogram of the Beta-cyclodextrin and Cinnamon Oil Inclusion Complexes

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Appendix B3. Third page of the analysis report provided by DOST for differential scanning calorimetry.

APPENDIX C

DOST PARTICLE SIZE ANALYSIS RESULTS



REPORT OF ANALYSIS

Reference No. : ADMATEL 2102-2342
Customer : Philippine Science High School
Sample Label : Beta-cyclodextrin and cinnamon oil inclusion complexes
Analysis Requested : Optical Microscopy w/ Particle Size Analysis
Date Received : February 23, 2021
Date Tested : February 26, 2021

I. Test Description

A *beta-cyclodextrin and cinnamon oil inclusion complexes* sample was submitted for particle size analysis as shown in **Figure 1**. The particles of the sample were imaged using Carl Zeiss Stereo Microscope at 10x magnification while the particle size analysis was performed via Feret's Method using the *IMAGEJ* software.



Figure 1. Image of the as-received *beta-cyclodextrin and cinnamon oil inclusion complexes* sample.

Page 1 of 3

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Appendix C1. First page of the analysis report provided by DOST for differential scanning calorimetry.

II. Results

Images containing the photomicrographs and particle outlines of the submitted sample are shown, together with a histogram of particle distribution. Each histogram is followed by a table to summarize the analysis results.

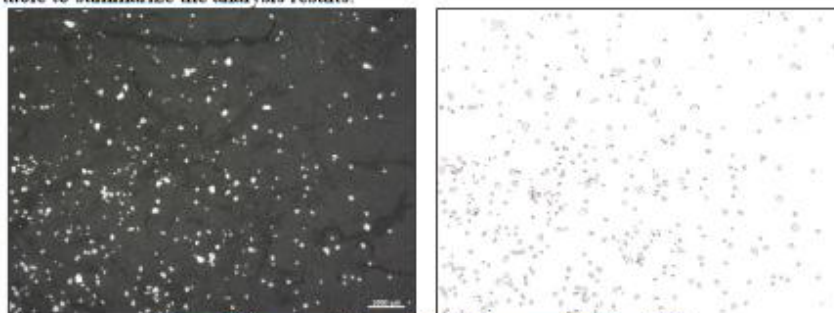


Figure 2. Images of the sample at 10x magnification (left) and particle outlines (right).

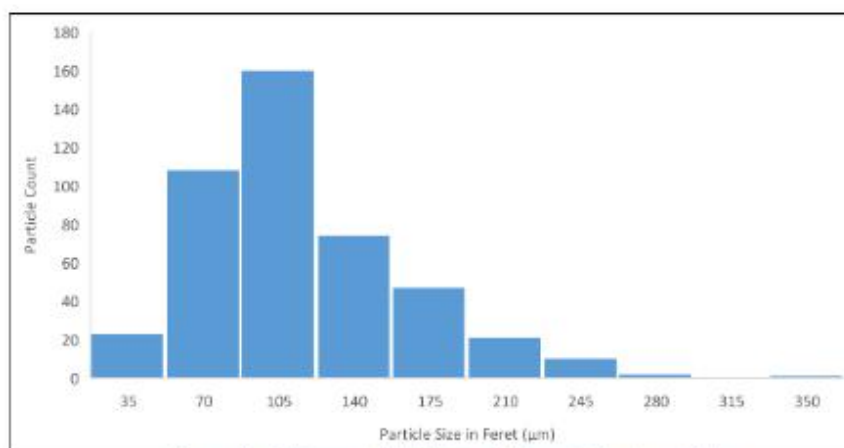


Figure 3. Histogram/ distribution of the particle size analysis.

Table I. Summary of particle size analysis results.

Count	Average Particle Area (µm ²)	Average Particle Size (Feret) (µm)	Minimum Feret (µm)
446	5630.235	98.269	68.929

Appendix C2. Second page of the analysis report provided by DOST for differential scanning calorimetry.



VALIDITY OF THE REPORT: The test results are those obtained at the time of the test and pertain only to the sample/s received by ADMATEL.


Aldrin Jan E. Tabuso

Analyst

Date: 03/01/2021


Bee Jay T. Salon

Laboratory Head

Date: 03/01/2021

Issued under the authority of:


Araceli M. Monsada, Dr.-Engg

Laboratory Manager

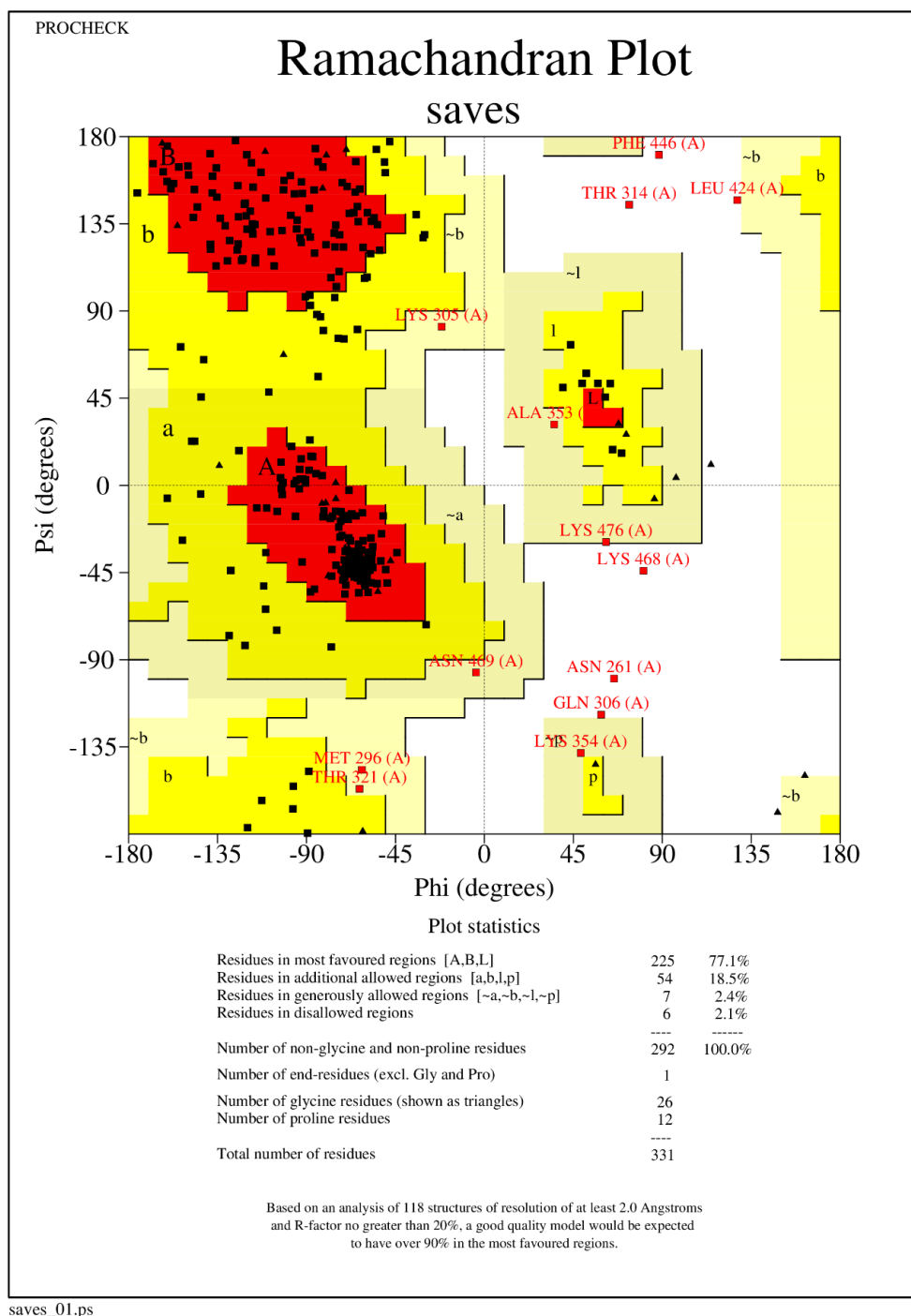
Date: 03/01/2021

Form: AL-21-F25
Issue: December 14, 2020
Revision: 02

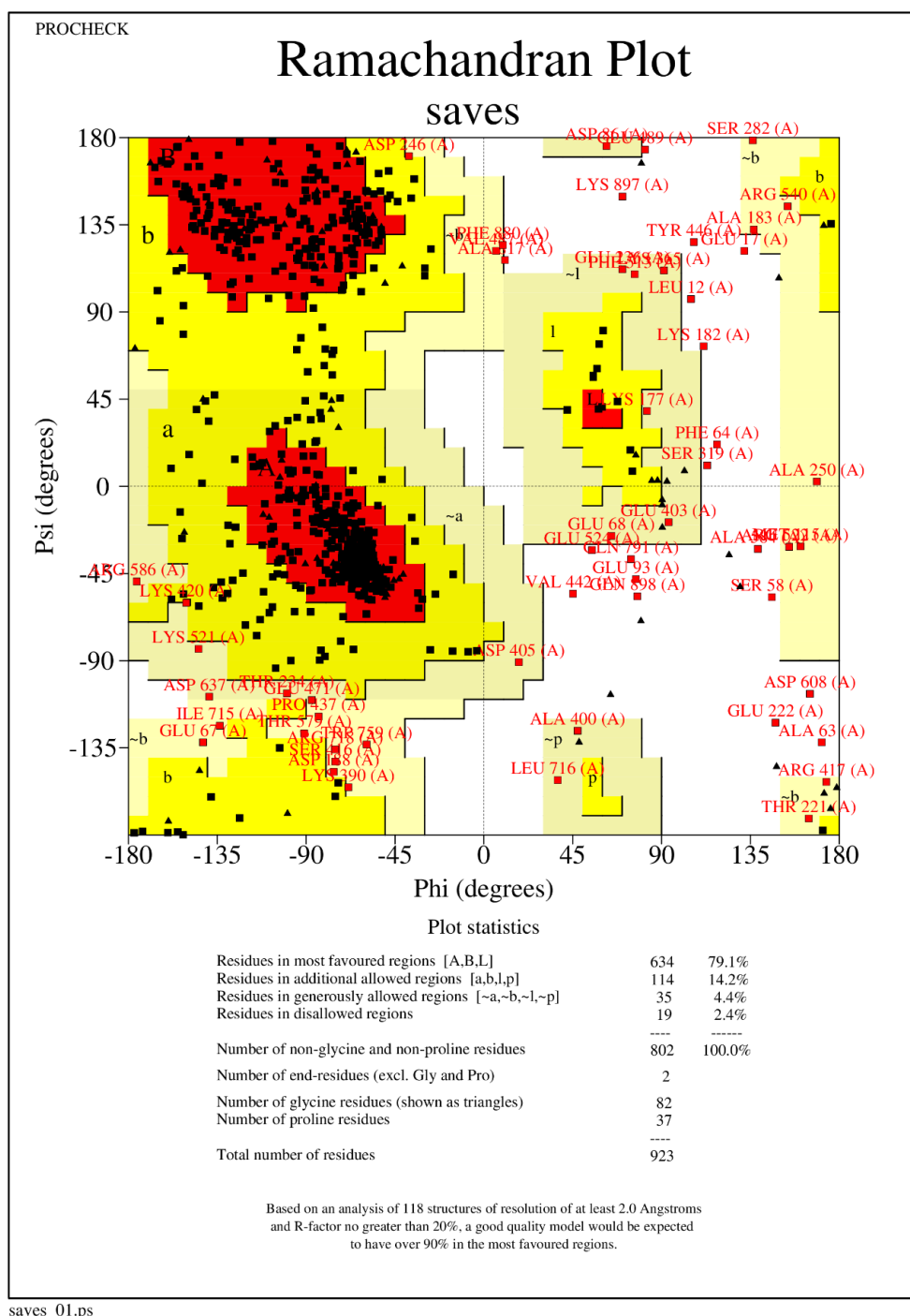
Appendix C3. Third page of the analysis report provided by DOST for differential scanning calorimetry.

APPENDIX D

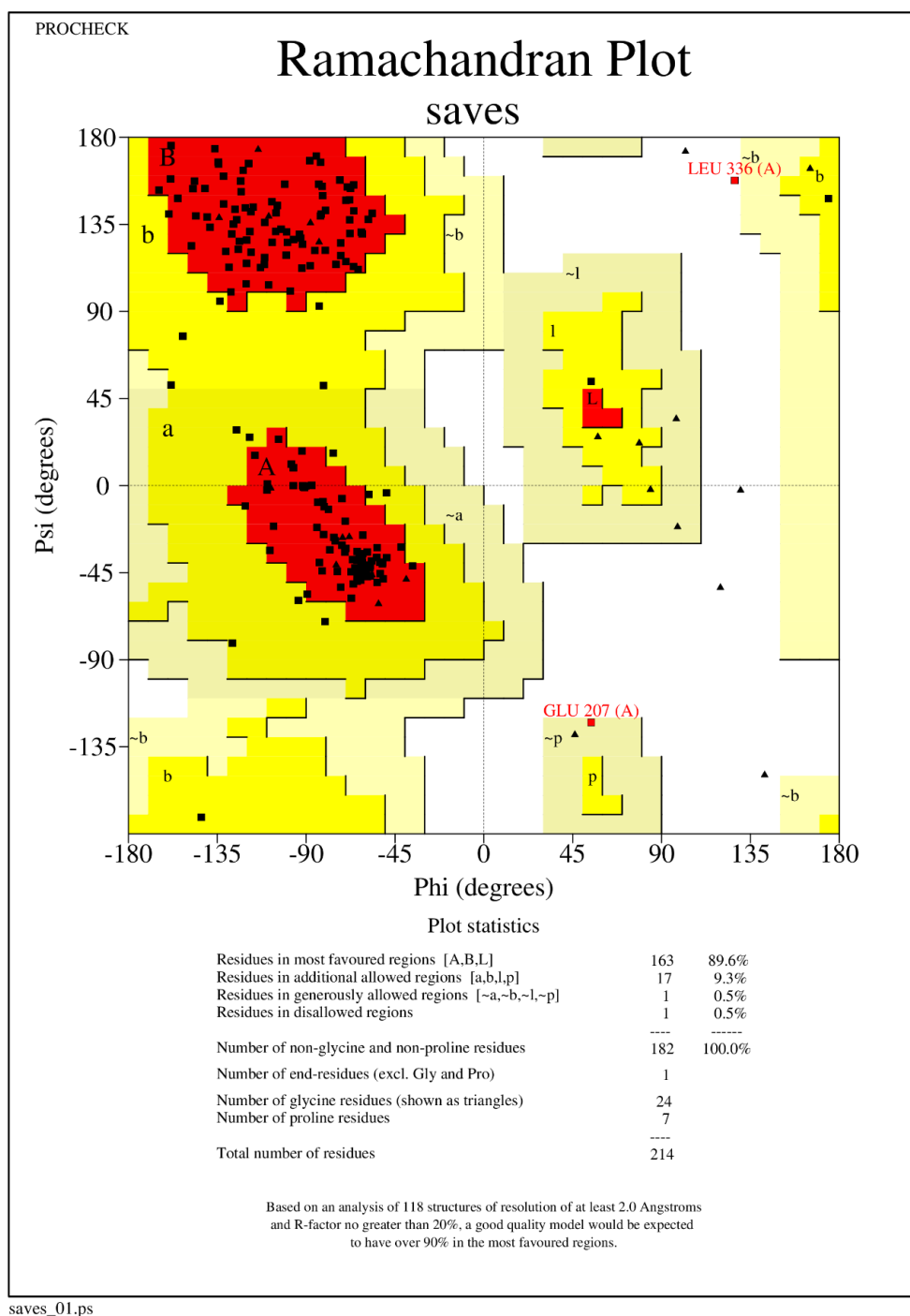
PROCHECK RAMACHANDRAN PLOTS AND STATISTICS



Appendix D1. Ramachandran plot and statistics for chitin synthase model generated by PROCHECK.



Appendix D2. Ramachandran plot and statistics for plasma membrane ATPase model generated by PROCHECK.

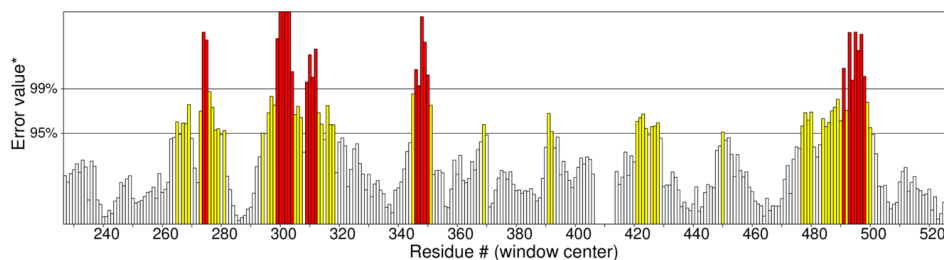


Appendix D3. Ramachandran plot and statistics for sterol 24-C-methyltransferase model generated by PROCHECK.

APPENDIX E

ERRAT OVERALL QUALITY GRAPHS

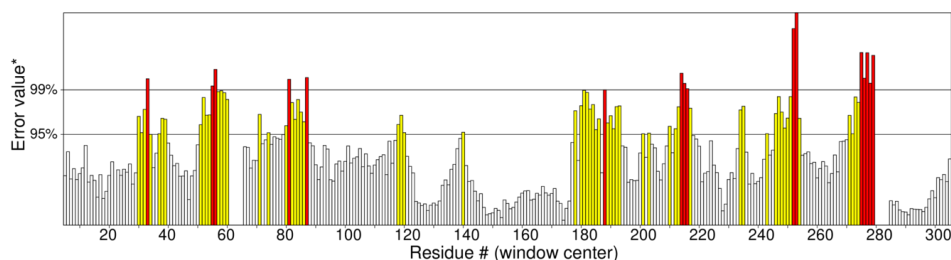
Program: ERRAT2
File: chitin.pdb
Chain#:A
Overall quality factor**: 76.899



*On the error axis, two lines are drawn to indicate the confidence with which it is possible to reject regions that exceed that error value.
**Expressed as the percentage of the protein for which the calculated error value falls below the 95% rejection limit. Good high resolution structures generally produce values around 95% or higher. For lower resolutions (2.5 to 3Å) the average overall quality factor is around 91%.

Appendix E1. Overall quality graph for chitin synthase model generated by ERRAT.

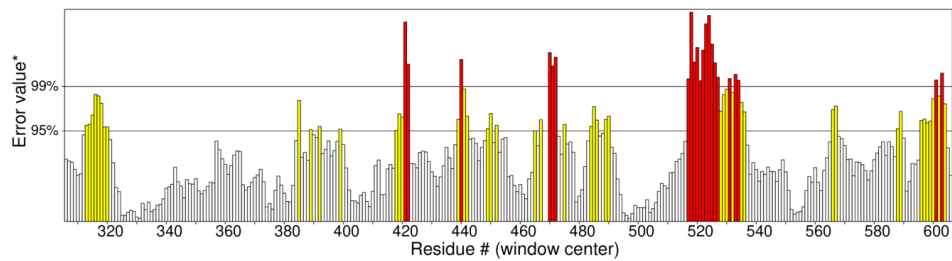
Program: ERRAT2
File: plasma.pdb
Chain#:A
Overall quality factor**: 77.283



*On the error axis, two lines are drawn to indicate the confidence with which it is possible to reject regions that exceed that error value.
**Expressed as the percentage of the protein for which the calculated error value falls below the 95% rejection limit. Good high resolution structures generally produce values around 95% or higher. For lower resolutions (2.5 to 3Å) the average overall quality factor is around 91%.

Appendix E2. Overall quality graph for the first section of plasma membrane ATPase model generated by ERRAT.

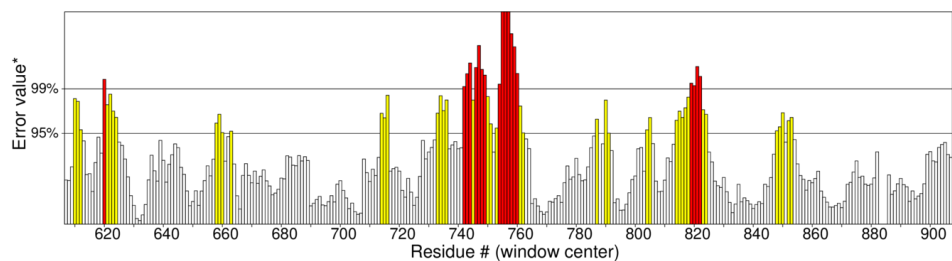
Program: ERRAT2
 File: plasma.pdb
 Chain#:A
 Overall quality factor**: 77.283



*On the error axis, two lines are drawn to indicate the confidence with which it is possible to reject regions that exceed that error value.
 **Expressed as the percentage of the protein for which the calculated error value falls below the 95% rejection limit. Good high resolution structures generally produce values around 95% or higher. For lower resolutions (2.5 to 3Å) the average overall quality factor is around 91%.

Appendix E3. Overall quality graph for the second section of plasma membrane ATPase model generated by ERRAT.

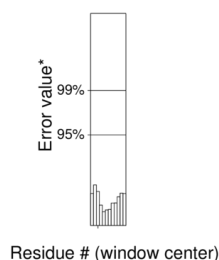
Program: ERRAT2
 File: plasma.pdb
 Chain#:A
 Overall quality factor**: 77.283



*On the error axis, two lines are drawn to indicate the confidence with which it is possible to reject regions that exceed that error value.
 **Expressed as the percentage of the protein for which the calculated error value falls below the 95% rejection limit. Good high resolution structures generally produce values around 95% or higher. For lower resolutions (2.5 to 3Å) the average overall quality factor is around 91%.

Appendix E4. Overall quality graph for the third section of plasma membrane ATPase model generated by ERRAT.

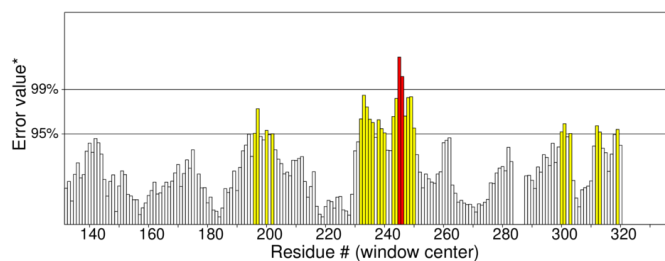
Program: ERRAT2
 File: plasma.pdb
 Chain#:A
 Overall quality factor**: 77.283



*On the error axis, two lines are drawn to indicate the confidence with which it is possible to reject regions that exceed that error value.
 **Expressed as the percentage of the protein for which the calculated error value falls below the 95% rejection limit. Good high resolution structures generally produce values around 95% or higher. For lower resolutions (2.5 to 3Å) the average overall quality factor is around 91%.

Appendix E5. Overall quality graph for the last section of plasma membrane ATPase model generated by ERRAT.

Program: ERRAT2
 File: sterol.pdb
 Chain#:A
 Overall quality factor**: 85.870

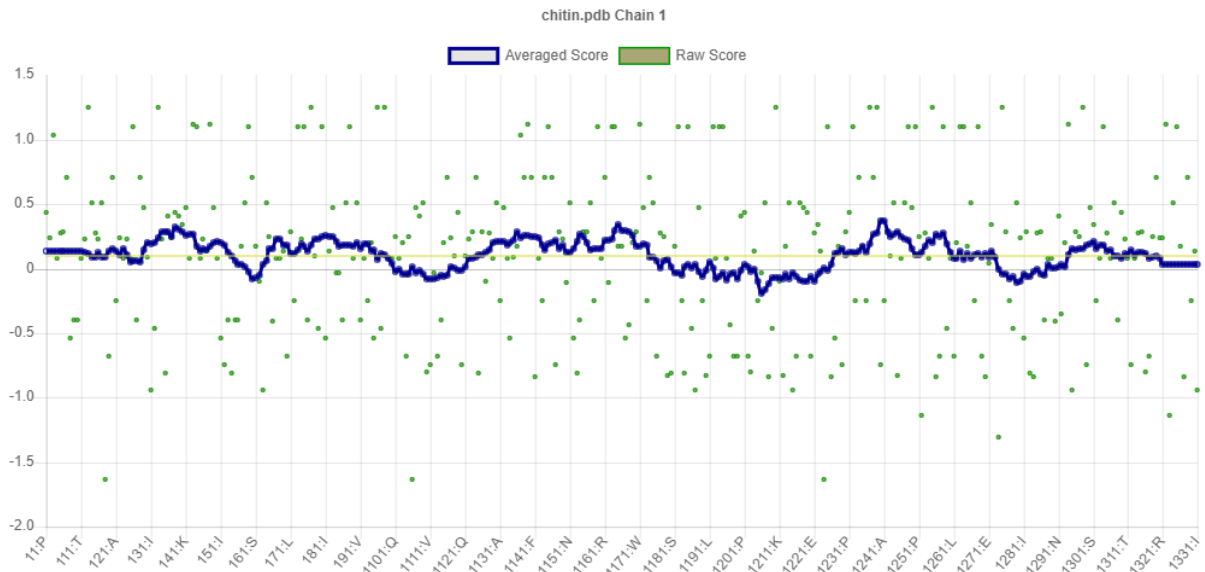


*On the error axis, two lines are drawn to indicate the confidence with which it is possible to reject regions that exceed that error value.
 **Expressed as the percentage of the protein for which the calculated error value falls below the 95% rejection limit. Good high resolution structures generally produce values around 95% or higher. For lower resolutions (2.5 to 3Å) the average overall quality factor is around 91%.

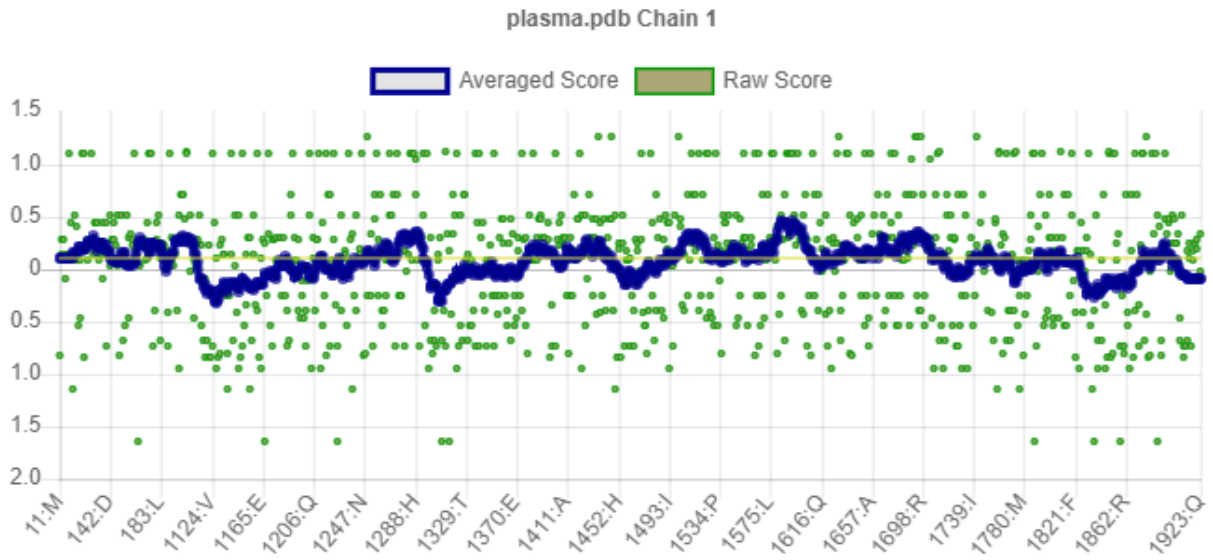
Appendix E6. Overall quality graph for sterol 24-C-methyltransferase model generated by ERRAT.

APPENDIX F

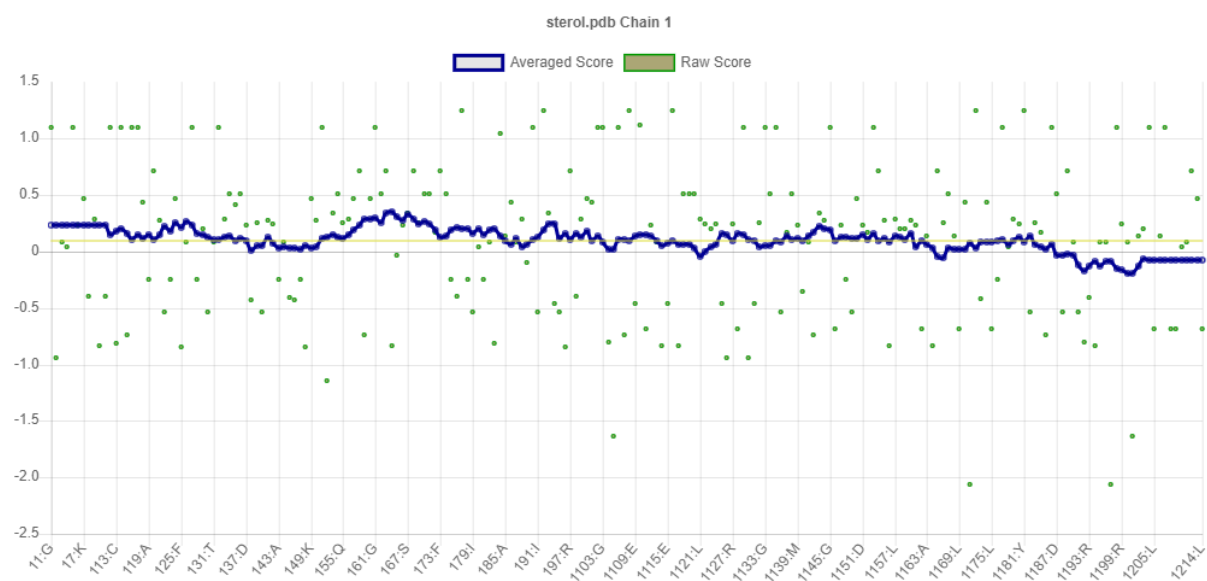
VERIFY3D 3D-1D AVERAGED SCORE PLOTS



Appendix F1. 3D-1-D averaged score plot for chitin synthase model generated by VERIFY3D.



Appendix F2. 3D-1-D averaged score plot for plasma membrane ATPase model generated by VERIFY3D.



Appendix F3. 3D-1-D averaged score plot for sterol 24-C-methyltransferase model generated by VERIFY3D.

APPENDIX G

NON-BONDED INTERACTIONS WITH CHITIN SYNTHASE AMINO ACIDS

Appendix G1. Hydrophobic interactions of cinnamaldehyde with the amino acids of chitin synthase.

Index	Residue	Amino Acid	Distance	Ligand Atom	Protein Atom
1	392A	LEU	3.59	2641	1367
2	392A	LEU	3.69	2635	1366
3	392A	LEU	3.76	2638	1365
4	405A	ALA	3.76	2637	1468
5	521A	VAL	3.68	2640	2376

APPENDIX H

NON-BONDED INTERACTIONS WITH PLASMA MEMBRANE ATPASE

Appendix H1. Hydrophobic interactions of cinnamaldehyde with the amino acids of plasma membrane ATPase.

Index	Residue	Amino Acid	Distance	Ligand Atom	Protein Atom
1	558A	LYS	3.70	7038	4208
2	558A	LYS	3.93	7040	4207
3	560A	LEU	3.60	7040	4225
4	560A	LEU	3.94	7037	4227
5	604A	VAL	3.63	7039	4542
6	610A	PHE	3.72	7038	4578
7	610A	PHE	3.86	7040	4581
8	621A	VAL	3.67	7039	4676
9	621A	VAL	3.85	7035	4678

APPENDIX I

NON-BONDED INTERACTIONS WITH STEROL 24-C-METHYLTRANSFERASE

Appendix I1. Hydrophobic interactions of cinnamaldehyde with the amino acids of sterol 24-C-methyltransferase.

Index	Residue	Amino Acid	Distance	Ligand Atom	Protein Atom
1	216A	LYS	3.64	2048	822
2	278A	ASP	3.70	2051	1428

Appendix I2. Hydrogen bonding interactions of cinnamaldehyde with the amino acids of sterol 24-C-methyltransferase.

Index	Residue	AA	Dist. (H-A)	Dist. (D-A)	Protein Donor?	Side Chain	Donor Atom	Acceptor Atom
1	217A	GLY	1.94	2.92	/	X	830 [Nam]	2049 [O2]
2	219A	TYR	2.76	3.32	/	X	844 [Nam]	2049 [O2]
3	220A	SER	2.10	2.97	/	X	858 [Nam]	2049 [O2]

APPENDIX J

THIRD DAY RAW DATA AND STATISTICAL ANALYSIS

Appendix J1. Colony diameter of Foc-TR4 set-ups with different treatments based on the spread plate method on the third day of bioassay reading.

Treatment	Colony Diameters (cm)			Mean (cm)	SDev
Negative Control	3.00	2.50	2.50	2.67	0.236
Positive Control	0.70	0.70	0.70	0.70	0.00
Cinnamon Oil (0.10 mL/mL)	0.70	0.70	0.70	0.70	0.00
Cinnamon Oil (0.010 mL/mL)	2.60	2.80	2.50	2.63	0.125
Beta-cyclodextrin (0.025 g/mL)	2.00	2.50	2.75	2.42	0.312
Inclusion Complexes (0.44 g/mL)	2.50	2.50	2.40	2.47	0.0470
Inclusion Complexes (0.025 g/mL)	2.50	2.50	2.50	2.50	0.000

Appendix J2. Pairwise Dunn Test results for the colony diameters of Foc-TR4 set-ups with different treatments on the third day of bioassay reading.

Comparison	Z-Value	P-Value
BCD - CO (0.10 mL/mL)	1.9773081	0.048006816
BCD - CO (0.010 mL/mL)	-0.8325508	0.405098130
CO (0.10 mL/mL) - CO (0.010 mL/mL)	-2.8098589	0.004956323
BCD - IC (0.44 g/mL)	0.3468962	0.728669334
CO (0.10 mL/mL) - IC (0.44 g/mL)	-1.6304119	0.103014464
CO (0.010 mL/mL) - IC (0.44 g/mL)	1.1794469	0.238220256
BCD - IC (0.025 g/mL)	0.0000000	1.000000000
CO (0.10 mL/mL) - IC (0.025 g/mL)	1.9773081	0.048006816
CO (0.010 mL/mL) - IC (0.025 g/mL)	0.8325508	0.405098130
IC (0.44 g/mL) - IC (0.025 g/mL)	-0.3468962	0.728669334
BCD - Negative CTRL	-0.5550339	0.578871507
CO (0.10 mL/mL) - Negative CTRL	-2.5323419	0.011330344
CO (0.010 mL/mL) - Negative CTRL	0.2775169	0.781383212
IC (0.44 g/mL) - Negative CTRL	-0.9019300	0.367094050
IC (0.025 g/mL) - Negative CTRL	-0.5550339	0.578871507
BCD - Positive CTRL	1.9773081	0.048006816
CO (0.10 mL/mL) - Positive CTRL	0.0000000	1.000000000
CO (0.010 mL/mL) - Positive CTRL	2.8098589	0.004956323
IC (0.44 g/mL) - Positive CTRL	1.6304119	0.103014464
IC (0.025 g/mL) - Positive CTRL	1.9773081	0.048006816
Negative CTRL - Positive CTRL	2.5323419	0.011330344

APPENDIX K

SEVENTH DAY RAW DATA AND STATISTICAL ANALYSIS

Appendix K1. Colony diameter of Foc-TR4 set-ups with different treatments based on the spread plate method on the seventh day of bioassay reading.

Treatment	Colony Diameter (cm)			Mean (cm)	SDev
Negative Control	6.10	6.20	7.60	6.63	0.685
Positive Control	0.90	1.00	0.90	0.93	0.0471
Cinnamon Oil (0.10 mL/mL)	0.70	0.70	0.70	0.70	0.00
Cinnamon Oil (0.010 mL/mL)	3.70	4.20	3.80	3.90	0.216
Beta-cyclodextrin (0.025 g/mL)	4.10	6.50	5.80	5.47	1.01
Inclusion Complexes (0.44 g/mL)	3.90	3.80	3.80	3.83	0.0471
Inclusion Complexes (0.025 g/mL)	6.50	5.00	5.00	5.50	0.707

Appendix K2. Pairwise Dunn Test results for the colony diameters of Foc-TR4 set-ups with different treatments on the seventh day of bioassay reading.

Comparison	Z-Value	P-Value
BCD - CO (0.10 mL/mL)	2.01725930	0.0436684606
BCD - CO (0.010 mL/mL)	-0.06613965	0.9472666445
CO (0.10 mL/mL) - CO (0.010 mL/mL)	-2.08339895	0.0372148740
BCD - IC (0.44 g/mL)	0.00000000	1.0000000000
CO (0.10 mL/mL) - IC (0.44 g/mL)	-2.01725930	0.0436684606
CO (0.010 mL/mL) - IC (0.44 g/mL)	0.06613965	0.9472666445
BCD - IC (0.025 g/mL)	-0.29762842	0.7659867800
CO (0.10 mL/mL) - IC (0.025 g/mL)	-2.31488772	0.0206190775
CO (0.010 mL/mL) - IC (0.025 g/mL)	-0.23148877	0.8169351071
IC (0.44 g/mL) - IC (0.025 g/mL)	-0.29762842	0.7659867800
BCD - Negative CTRL	-1.45507228	0.1456492518
CO (0.10 mL/mL) - Negative CTRL	-3.47233158	0.0005159586
CO (0.010 mL/mL) - Negative CTRL	-1.38893263	0.1648532363
IC (0.44 g/mL) - Negative CTRL	-1.45507228	0.1456492518
IC (0.025 g/mL) - Negative CTRL	-1.15744386	0.2470910631
BCD - Positive CTRL	1.42200246	0.1550255376
CO (0.10 mL/mL) - Positive CTRL	-0.59525684	0.5516717994
CO (0.010 mL/mL) - Positive CTRL	1.48814211	0.1367134211
IC (0.44 g/mL) - Positive CTRL	1.42200246	0.1550255376
IC (0.025 g/mL) - Positive CTRL	1.71963088	0.0854995595
Negative CTRL - Positive CTRL	2.87707474	0.0040138052

APPENDIX L

FOURTEENTH DAY RAW DATA AND STATISTICAL ANALYSIS

Appendix L1. Colony diameter of Foc-TR4 set-ups with different treatments based on the spread plate method on the fourteenth day of bioassay reading.

Treatment	Colony Diameter (cm)			Mean (cm)	SDev
Negative Control	9.00	9.00	9.00	9.00	0.000
Positive Control	1.20	1.50	1.20	1.30	0.141
Cinnamon Oil (0.10 mL/mL)	0.70	0.70	0.70	0.70	0.00
Cinnamon Oil (0.010 mL/mL)	5.00	7.70	7.00	6.57	1.14
Beta-cyclodextrin (0.025 g/mL)	4.90	9.00	6.50	6.80	1.69
Inclusion Complexes (0.44 g/mL)	7.00	7.10	6.20	6.77	0.403
Inclusion Complexes (0.025 g/mL)	7.00	7.00	7.50	7.17	0.236

Appendix L2. Pairwise Dunn Test results for the colony diameters of Foc-TR4 set-ups with different treatments on the fourteenth day of bioassay reading.

Comparison	Z-Value	P-Value
BCDCD - CO (0.10 mL/mL)	2.02324229	0.0430481739
BCDCD - CO (0.010 mL/mL)	-0.06633581	0.9471104716
CO (0.10 mL/mL) - CO (0.010 mL/mL)	-2.08957810	0.0366557156
BCD - IC (0.44 g/mL)	0.00000000	1.0000000000
CO (0.10 mL/mL) - IC (0.44 g/mL)	-2.02324229	0.0430481739
CO (0.010 mL/mL) - IC (0.44 g/mL)	0.06633581	0.9471104716
BCD - IC (0.025 g/mL)	-0.29851116	0.7653130620
CO (0.10 mL/mL) - IC (0.025 g/mL)	-2.32175344	0.0202462154
CO (0.010 mL/mL) - IC (0.025 g/mL)	-0.23217534	0.8164018269
IC (0.44 g/mL) - IC (0.025 g/mL)	-0.29851116	0.7653130620
BCD - Negative CTRL	-1.45938788	0.1444583802
CO (0.10 mL/mL) - Negative CTRL	-3.48263017	0.0004965138
CO (0.010 mL/mL) - Negative CTRL	-1.39305207	0.1636040466
IC (0.44 g/mL) - Negative CTRL	-1.45938788	0.1444583802
IC (0.025 g/mL) - Negative CTRL	-1.16087672	0.2456920366
BCD - Positive CTRL	1.42621997	0.1538048562

CO (0.10 mL/mL) - Positive CTRL	-0.59702231	0.5504924827
CO (0.010 mL/mL) - Positive CTRL	1.49255579	0.1355535044
IC (0.44 g/mL) - Positive CTRL	1.42621997	0.1538048562
IC (0.025 g/mL) - Positive CTRL	1.72473113	0.0845759383
Negative CTRL - Positive CTRL	2.88560785	0.0039065858