Characterisation and Traceability of Calcium Carbonate from the Seaweed *Lithothamnium calcareum*

SUPLEMENTARY INFORMATION

**Quantachrome NovaWin - Data Acquisition and Reduction
for NOVA instruments
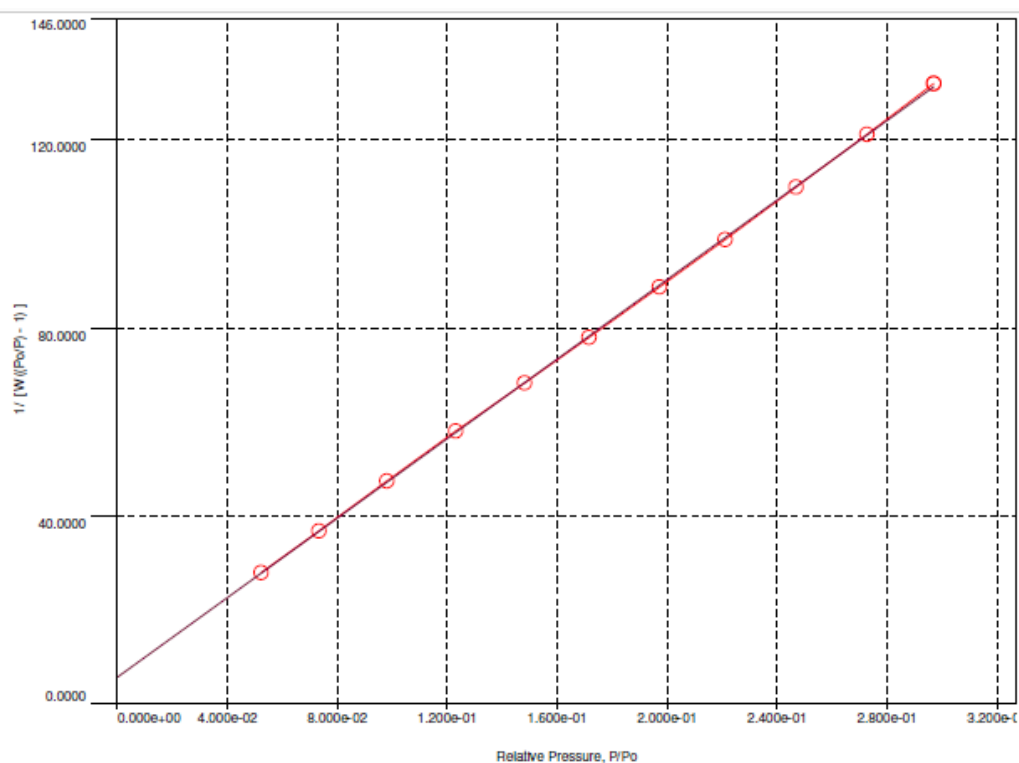©1994-2013, Quantachrome Instruments
version 11.03**

Analysis

			Report			
Operator:	Jefferson	Date:2017/05/11	Operator:	quantachrome	Date:2018/06/13	
Sample ID:	LITHO02	Filename:	LITHO02_B_20170510_1.qps			
Sample Desc:		Comment:				
Sample weight:	1.5134 g	Sample Volume:	0.44381 cc	Sample Density:	3.41 g/cc	
Outgas Time:	0.0 hrs	OutgasTemp:	0.0 C			
Analysis gas:	Nitrogen	Bath Temp:	273.0 K			
Press. Tolerance:	0.100/0.100 (ads/des)	Equil time:	60/60 sec (ads/des)	Equil timeout:	240/240 sec (ads/des)	
Analysis Time:	337.6 min	End of run:	2017/05/11 20:14:10	Instrument:	Nova Station B	
Cell ID:	2					

Multi-Point BET Plot

Data Reduction Parameters

Adsorbate	Nitrogen	**Temperature**	77.350K		
	Molec. Wt.: 28.013	**Cross Section:**	16.200 Å²	**Liquid Density:**	0.808 g/cc

A   BF

BET summary

Slope =	423.270
Intercept =	5.715e+00
Correlation coefficient, r =	0.999952
C constant=	75.065
Surface Area =	8.118 m²/g

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Figure S1. Multi-Point BET graphs of the *Lithothamnium calcareum* calcium carbonate sample and data summaries.

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INSTRUMENTS
Optimizing particle performance

Analysis
Operator:Jefferson   Date:2017/02/02
Sample ID: Carbonato_de_C
Sample Desc: Fabricante
Sample weight: 1.077 g
Outgas Time: 3.0 hrs
Analysis gas: Nitrogen
Press. Tolerance:0.100/0.100 (ads/des)
Analysis Time: 488.4 min
Cell ID: 1

Report
Operator: Date:2/3/2017
Filename: C:\QCdata\Physisorb\Carbonato_de_Calcio_Leve.qps
Comment:
Sample Volume: 1.07229 cc
OutgasTemp: 300.0 C
Bath Temp: 77.3 K
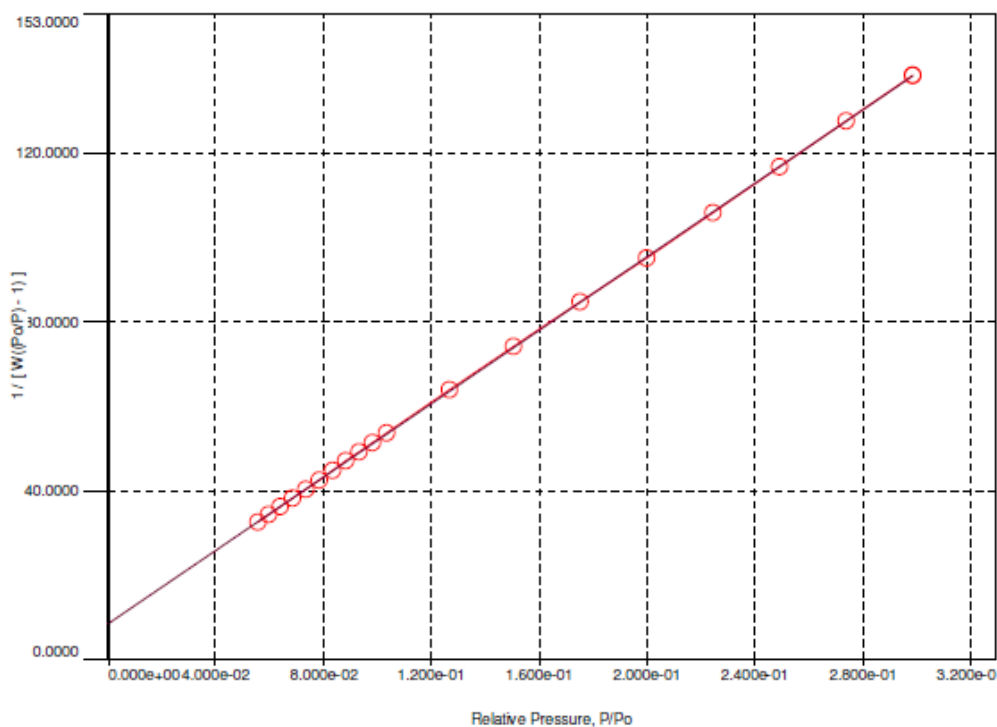Equil time: 60/60 sec (ads/des)   Equil timeout: 240/240 sec (ads/des)
End of run: 2017/02/02 16:01:15   Instrument: Nova Station B

Multi-Point BET Plot

Data Reduction Parameters

Adsorbate   Nitrogen   Temperature   77.350$_K$
                    Molec. Wt.: 28.013 $_g$ Cross Section: 16.200 $_{A^2}$ Liquid Density: 0.808 $_{g/cc}$

A   D   BF

BET summary
Slope =   434.782
Intercept =   8.478e+00
Correlation coefficient, r =   0.999989
C constant=   52.281

Surface Area =   7.857 m²/g

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Figure S2. Multi-Point BET graphs of the inorganic mineral calcium carbonate sample and data summaries.

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Analysis

Operator:	quantachrome	Date:2018/06/08				
Sample ID:	Sarm2005					
Sample Desc:	Lote2116					
Sample weight:	1.462 g					
Outgas Time:	0.0 hrs					
Analysis gas:	Nitrogen					
Press. Tolerance:	0.100/0.100 (ads/des)					
Analysis Time:	132.0 min					
Cell ID:	1					

Report

Operator:	quantachrome	Date:2018/06/13	
Filename:	CaCO3 ostras 080618.qps		
Comment:			
Sample Volume:	0.79336 cc	Sample Density:	1.8428 g/cc
OutgasTemp:	0.0 C		
Bath Temp:	273.0 K		
Equil time:	60/60 sec (ads/des)	Equil timeout:	240/240 sec (ads/des)
End of run:	2018/06/08 15:34:29	Instrument:	Nova Station A

Multi-Point BET Plot

Data Reduction Parameters

Adsorbate	Nitrogen	Temperature	77.350K		
	Molec. Wt.: 28.013	Cross Section:	16.200 Å²	Liquid Density:	0.808 g/cc

A   BF

BET summary
Slope =   1112.187
Intercept =   7.452e+01
Correlation coefficient, r =   0.998042
C constant=   15.925

Surface Area =   2.935 m²/g

Figure S3. Multi-Point BET graphs of the oyster shell calcium carbonate sample and data summaries.

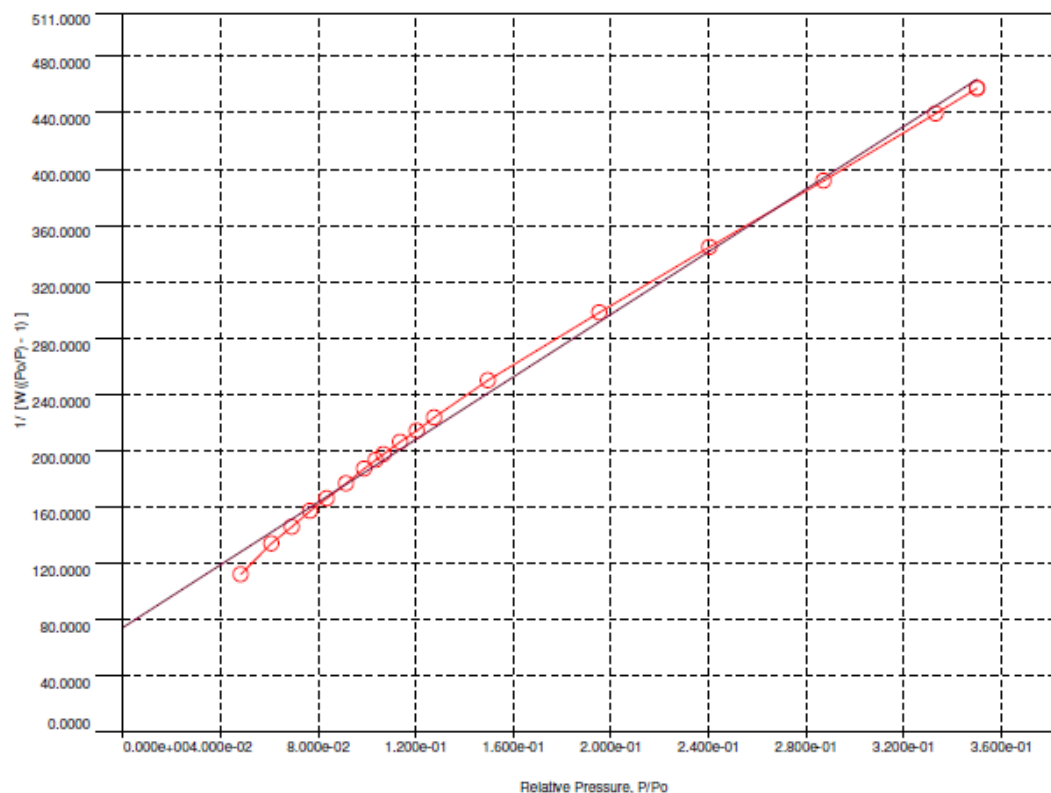# Characterisation and Traceability of Calcium Carbonate from the Seaweed *Lithothamnium calcareum*

Statistical analysis

Tables from the results of the main component graphs for *L. calcareum*, inorganic mineral and oyster shell $CaCO_3$ samples and the two-dimensional graph of the main components. Both factors 1 and 2 correspond to 100% of the information contained in the original variables.

Table S1. Factor coordinates of the variables, based on correlations (Multivariate data).

Variable	Factor 1	Factor 2
Compressibility index (%)	-0.914506	-0.404573
Surface area	0.881762	-0.471695
Pore Volume	-0.988762	-0.149499
Pore size	0.050866	-0.998705
Melting point (°C)	-0.950644	-0.310285
Mass loss (%)	-0.762179	0.647366
Particle microscopy	0.979578	-0.201066
Calcium content (%)	-0.996576	0.082687
Polymorphs	0.872120	0.489293

Table S2. Factor coordinates of cases, based on correlations (Multivariate data).

Case	Factor 1	Factor 2
A	2.62449	0.83953
B	-0.03708	-1.71567
C	-2.58742	0.87614

Table S3. Eigenvalues of correlation matrix, and related statistics (Multivariate data)
Active variables only

Value number	Eigenvalue	% Total	Cumulative	Cumulative
1	6.792031	75.46701	6.792031	75.4670
2	2.207969	24.53299	9.000000	100.0000

Characterisation and Traceability of Calcium Carbonate from the Seaweed *Lithothamnium calcareum*

Table S4. Factor score coefficients, based on correlations (Multivariate data)

Variable	Factor 1	Factor 2
Compressibility index (%)	-0.134644	-0.183233
Surface area	0.129823	-0.213633
Pore Volume	-0.145577	-0.067709
Pore size	0.007489	-0.452319
Melting point (° C)	-0.139965	-0.140529
Mass loss (%)	-0.112217	0.293195
Particle microscopy	0.144225	-0.091064
Calcium contente (%)	-0.146727	0.037449
Polymorphs	0.128403	0.221603

Table S5. Summary statistics (Multivariate data)

Variable	Mean	Std. Dev.
Compressibility index (%)	42.0300	2.853366
Surface area	6.3033	2.919980
Pore Volume	3.4983	1.771302
Pore size	5.7050	3.506611
Melting point (° C)	729.0333	7.710599
Mass loss (%)	41.0000	1.493318
Particle microscopy	2.6667	1.527525
Calcium contente (%)	39.2633	2.501206
Polymorphs	1.6667	1.154701

Table S6. Correlations (multivariate data).

Variable	Compressibility index (%)	Surface area	Pore Volume	Pore size	Melting point (° C)	Mass loss (%)	Particle microscopy	Calcium content (%)	Polymorphs
Compressibility index (%)	1.000000	-0.615541	0.964712	0.357532	0.994902	0.435111	-0.814484	0.877921	-0.995513
Surface area	-0.615541	1.000000	-0.801334	0.515936	-0.691881	-0.977420	0.958596	-0.917745	0.538205
Pore Volume	0.964712	-0.801334	1.000000	0.099011	0.986348	0.656833	-0.938510	0.973014	-0.935468
Pore size	0.357532	0.515936	0.099011	1.000000	0.261528	-0.685297	0.250633	-0.133272	-0.444298
Melting point (° C)	0.994902	-0.691881	0.986348	0.261528	1.000000	0.523693	-0.868842	0.921732	-0.980895
Mass loss (%)	0.435111	-0.977420	0.656833	-0.685297	0.523693	1.000000	-0.876777	0.813098	-0.347960
Particle microscopy	-0.814484	0.958596	-0.938510	0.250633	-0.868842	-0.876777	1.000000	-0.992849	0.755929
Calcium content (%)	0.877921	-0.917745	0.973014	-0.133272	0.921732	0.813098	-0.992849	1.000000	-0.828675
Polymorphs	-0.995513	0.538205	-0.935468	-0.444298	-0.980895	-0.347960	0.755929	-0.828675	1.000000

Characterisation and Traceability of Calcium Carbonate from the Seaweed *Lithothamnium calcareum*

Table S7. Trace element data from samples normalized by carbonaceous chondrite from A (*L. calcareum*), B (Inorganic mineral) and C (oysters shell) $CaCO_3$ samples obtained in ppm values.

Trace elements	A	B	C
Sc	0.09	0.01	0.01
Rb	0.41	0.14	0.05
Sr	424.20	223.00	119.72
Y	1.09	0.43	0.06
Zr	0.30	0.19	0.02
Nb	1.67	0.26	0.37
Cs	0.24	0.05	0.05
Ba	3.01	6.58	0.21
La	6.88	0.64	0.69
Ce	6.04	0.02	0.02
Pr	3.85	0.43	0.28
Nd	2.92	0.36	0.20
Sm	1.73	0.27	0.11
Eu	0.89	0.20	0.18
Gd	1.20	0.27	0.10
Tb	0.90	0.28	0.28
Dy	0.81	0.24	0.05
Ho	0.76	0.28	0.18
Er	0.67	0.26	0.06
Tm	0.65	0.40	0.40
Yb	0.58	0.24	0.06
Lu	0.57	0.40	0.40
Hf	0.33	0.11	0.10
Pb	0.39	0.06	0.01
Th	15.52	1.61	0.44
U	164.30	75.84	3.42