CASE STUDY
Molecular Weight Comparison of Polycarbonate Water Bottles Subjected to Thermal Treatments

OBJECTIVE

The objective of this work was to determine if any change in molecular weight occurred in a Polycarbonate Water Bottle that was exposed to various thermal treatments which simulate typical washing processes. Gel permeation chromatography (GPC) is an excellent method for molecular weight analysis.

ANALYTICAL STRATEGY

Samples were collected from a reusable polycarbonate water bottle in the as-received state, after three dishwashing cycles, and after heating in an oven at 130°C for 2 days. GPC analysis was then performed on each of the three samples to determine the molecular weight of each sample.

CONCLUSIONS

No statistically significant difference was observed in the molecular weights for the samples under any of the thermal treatments studied. It was therefore concluded that the bottles did not degrade.

Read the following report to see the full analysis.

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JORDI

December 15, 2010

Client Name
Company Name
Address

Dear Valued Client:

Please find enclosed the test results for your samples described as:

1. *Polycarbonate Water Bottle*

The following test was performed:

1. Gel Permeation Chromatography (GPC)

Objective

The objective of this work was to determine if any change in molecular weight occurred in a *Polycarbonate Water Bottle* that was exposed to various thermal treatments which simulate typical washing processes. Gel permeation chromatography (GPC) is an excellent method for molecular weight analysis.

Summary of Results

Samples were collected from a reusable polycarbonate water bottle in the as-received state, after three dishwashing cycles, and after heating in an oven at 130°C for 2 days. GPC analysis was then performed on each of the three samples to determine the molecular weight of each sample. The average molecular weights for each sample are provided in **Table I**. No statistically significant difference was observed in the molecular weights for the samples under any of the thermal treatments studied. It was therefore concluded that the bottles did not degrade.

Individual Test Results

A summary of the individual test results is provided below. All accompanying data, including spectra, has been included in the data section of this report.

Definitions
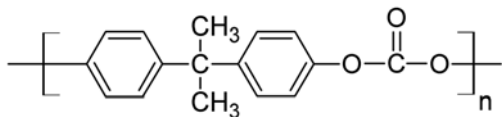
Polycarbonate (PC)

GPC – <u>GPC Background:</u> A polymer is a large molecule which is formed using a repeating subunit. A polymeric sample does not have a single molecular weight but rather a range of values and thus an average value is used to indicate its molecular weight.

Three different molecular weight averages are commonly used to provide information about polymers. These are the number average molecular weight (Mn), the weight average molecular weight (Mw), and the Z average molecular weight (Mz).

Mn provides information about the lowest molecular weight portion of the sample. Mw is the average closest to the center of the peak and Mz represents the highest molecular weight portion of the sample. The different molecular weight averages can each be related to specific polymer properties such as material toughness, tensile strength, and total elongation.

By comparing the different averages, it is possible to define a fourth parameter called the polydispersity index (PDI). This parameter gives an indication of how broad a range of molecular weights are in the sample.

<u>**Results:**</u> A *Polycarbonate Water Bottle* was exposed to two different thermal treatments in order to determine if any change in the molecular weight of the polycarbonate (PC) would be observed. The first treatment consisted of running the bottle through three normal dishwasher cycles to simulate normal product use. The second treatment consisted of placing the bottle into a 130°C oven for 2 days. Samples were collected after each of the treatments and were compared to a control sample from the bottle prior to any thermal treatment.

Analysis by GPC requires that a suitable solvent be found to dissolve the sample. Samples were found to dissolve in Tetrahydrofuran (THF). Enclosed are refractive index chromatograms for each sample, as well as cumulative weight fraction curves, molecular weight distribution curves and summary reports. A second individual summary report is included to show the reproducibility of the data. A calibration curve and chromatographic overlay of the standards are included. Also please find an overlay of the different samples with standards. The average molecular weights are summarized in **Table I**. **Figure I** shows an overlay of the chromatograms for the three samples.

Table I:

Avg. Molecular Wt.

Sample ID	Run #	Mn	Avg.	Mw	Avg.	Mz	Avg.	Mw/Mn	Avg.
Control Bottle	1	19,927	20,047	56,855	56,881	97,111	97,340	2.85	2.84
	2	20,166		56,907		97,569		2.82	
Dishwasher Bottle	1	19,164	19,129	56,892	56,986	97,860	97,639	2.97	2.98
	2	19,093		57,080		97,417		2.99	
Oven Bottle	1	19,463	19,409	56,170	56,029	95,753	95,718	2.89	2.89
	2	19,354		55,888		95,682		2.89	

Relative to polystyrene standards
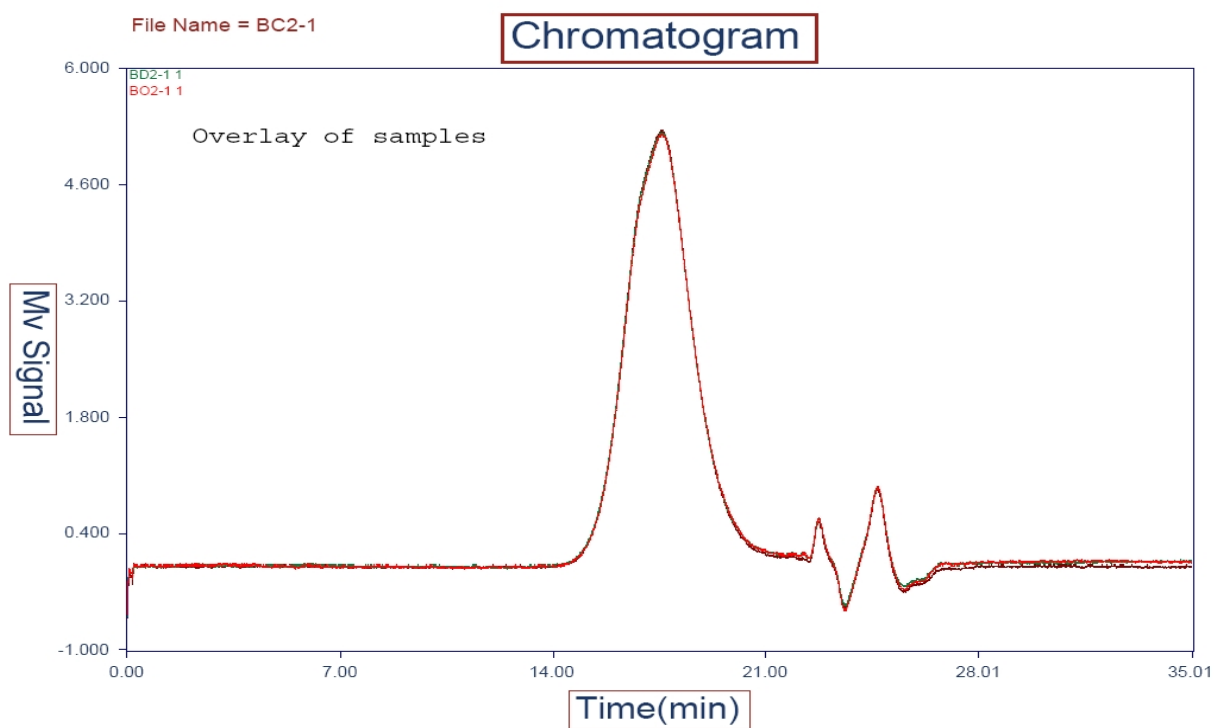
Figure I: Overlay of the chromatogram for all three polycarbonate samples. Note the consistency of peak shape indicating a lack of degradation.

Analysis Conditions

GPC

This section of a Jordi report provides information on the methods used including instrument type, temperatures, solvents, sample preparation, etc. The specific conditions have been removed for this case study.

Closing Comments

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Jordi Labs specializes in polymer testing and has 25 years experience doing complete polymer deformulations. We are one of the few labs in the country specialized in this type of testing. We will work closely with you to help explain your test results and solve your problem. We appreciate your business and are looking forward to speaking with you concerning these results.

Sincerely,

Mark Jordi   *Lars Qvicklund*
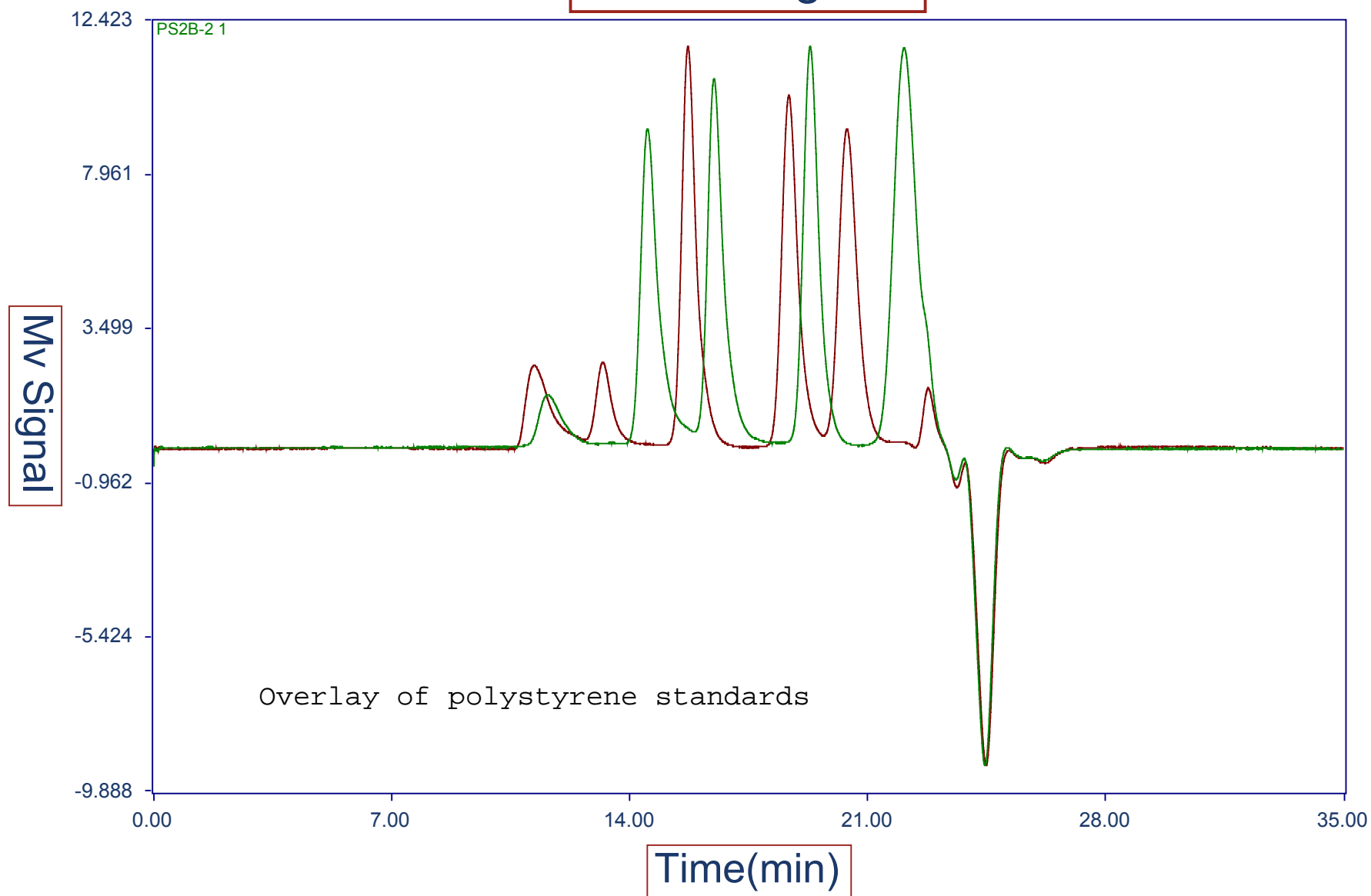
Mark Jordi, Ph. D.   Lars Qvicklund
President   Laboratory Technician
Jordi Labs LLC   Jordi Labs LLC

GPC RESULTS

File Name = JordiCal110910.ASC

Calibration
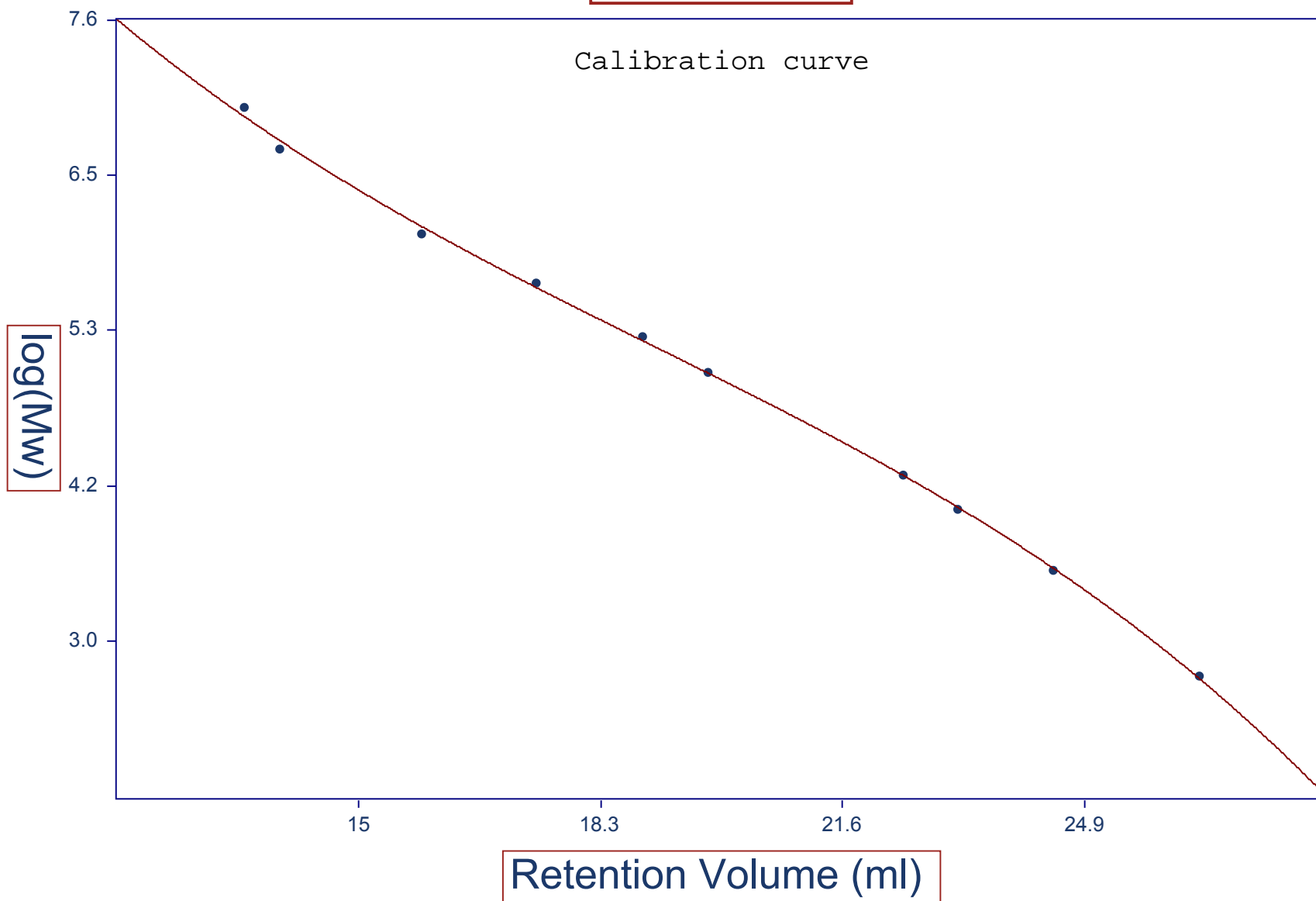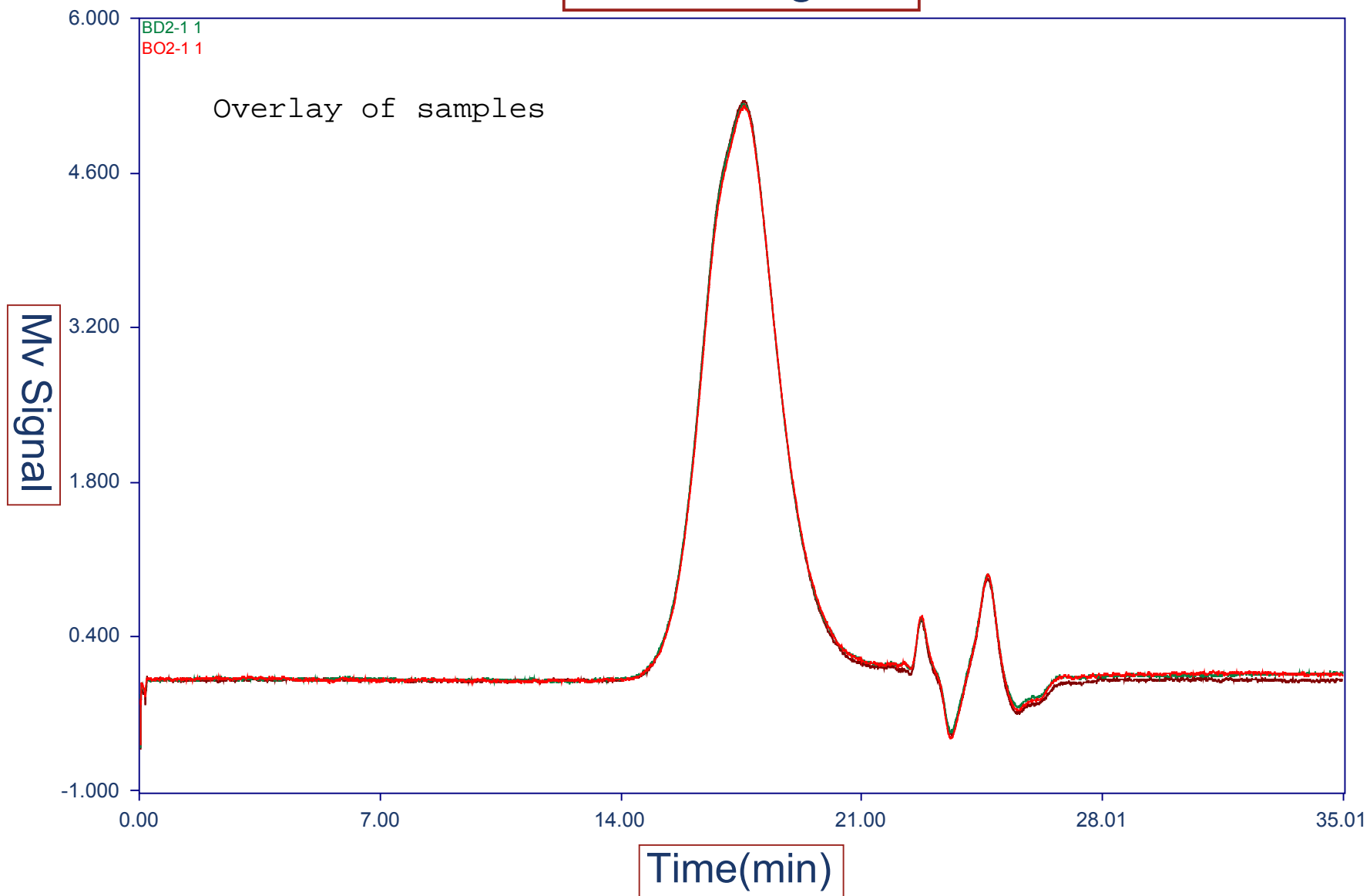
Calibration curve

log(Mw)

Retention Volume (ml)

Chromatogram

File Name = BC2-1

BD2-1 1
BO2-1 1

Overlay of samples

Mv Signal

Time(min)

Chromatogram

File Name = BC2-1

BD2-1 1
BO2-1 1

Enlarged overlay of samples

Mv Signal

Time(min)

Chromatogram

File Name = BC2-1

BD2-1 1
BO2-1 1
PS1C-1 1
PS2B-2 1

Overlay of samples
and standards
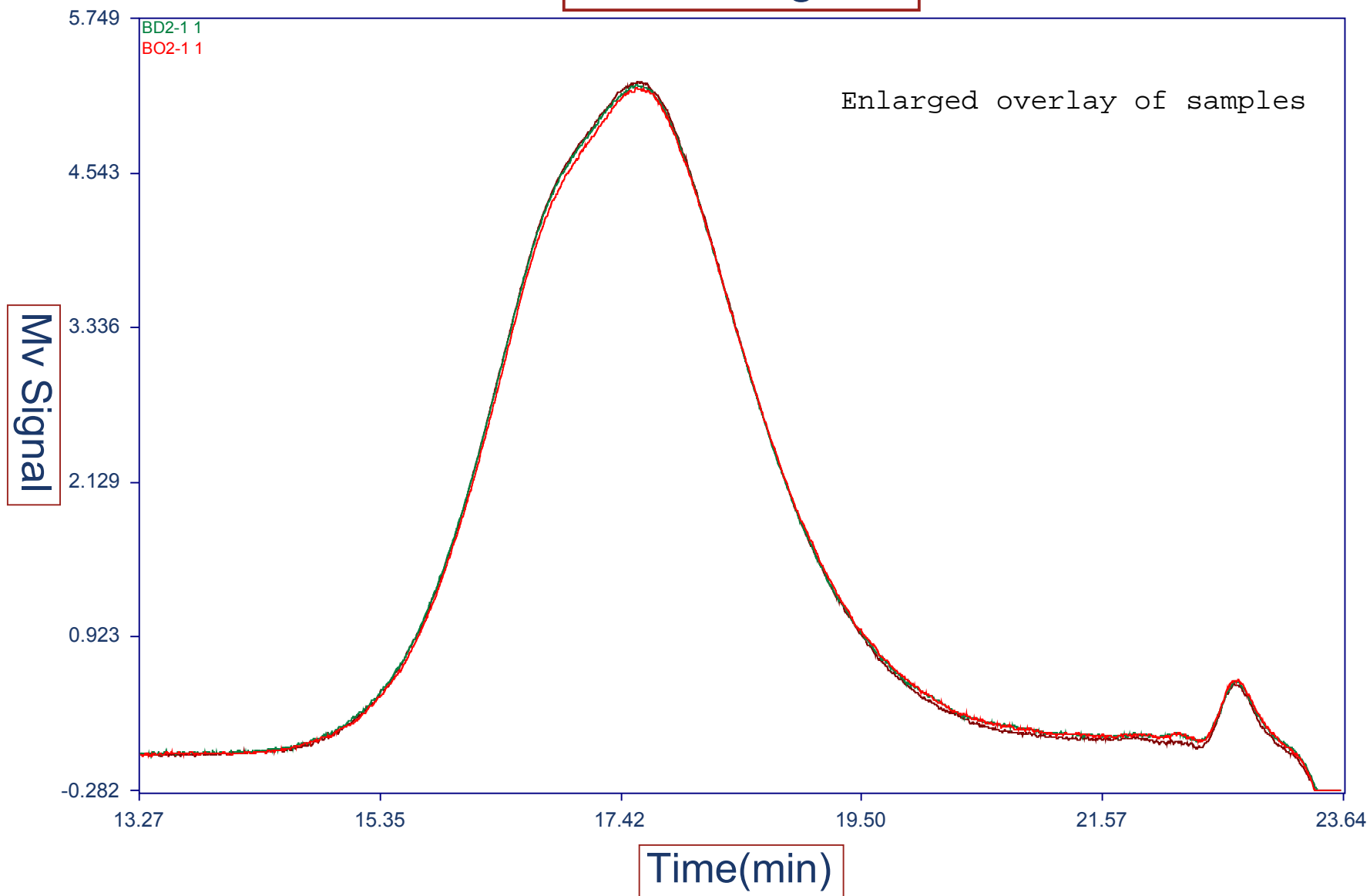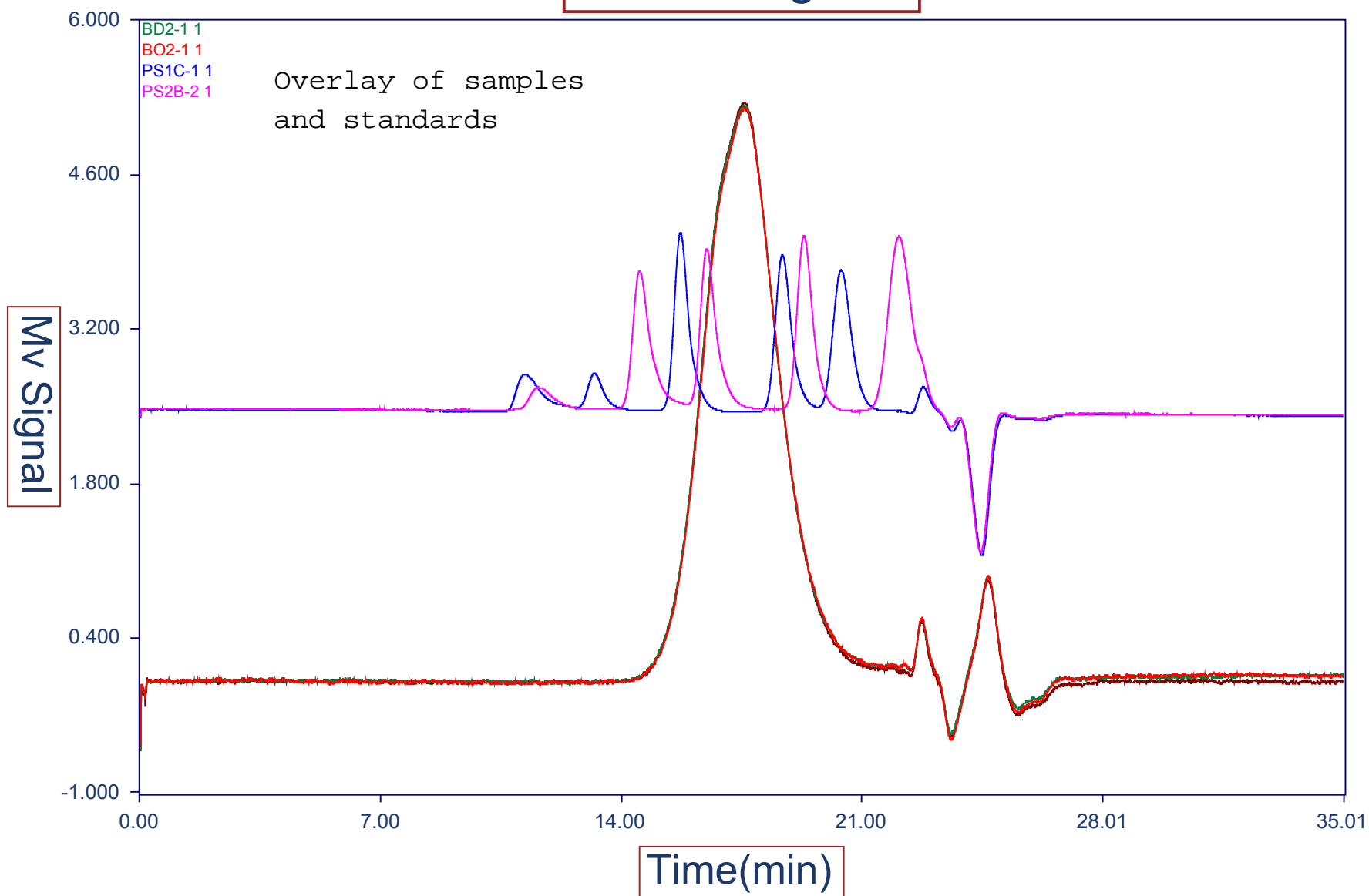
Chromatogram
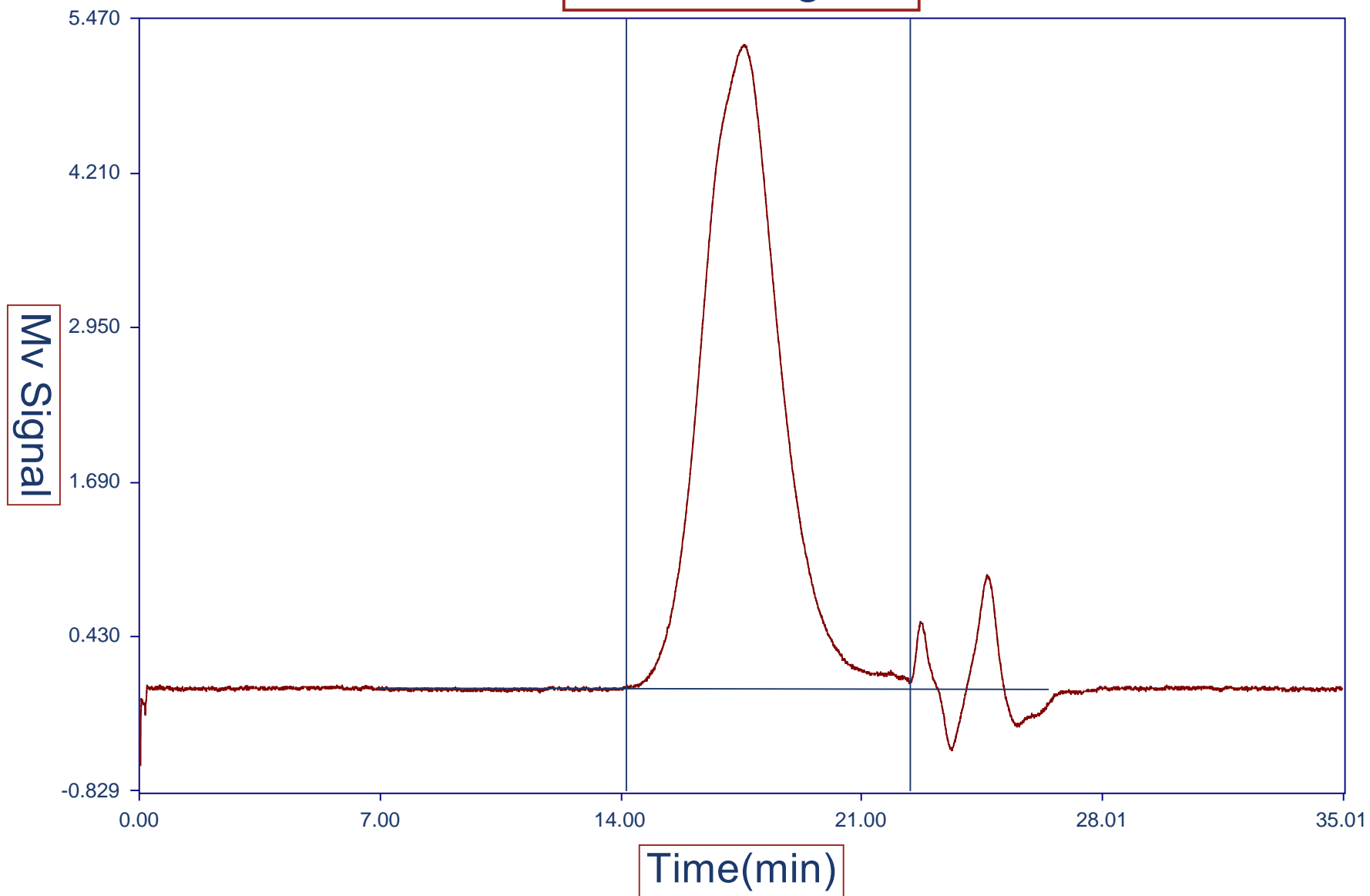
File Name = BC2-1

Molecular Weight Distribution Curve

File Name = BC2-1

- - - - Mn = 19927
- ● - ● Mp = 42710
——— Mw = 56855
•••••• Mz = 97111

Y-axis: 10*Wf/d[logMW]

X-axis: log(Molecular Weight)

Cumulative Wf Distribution Curve
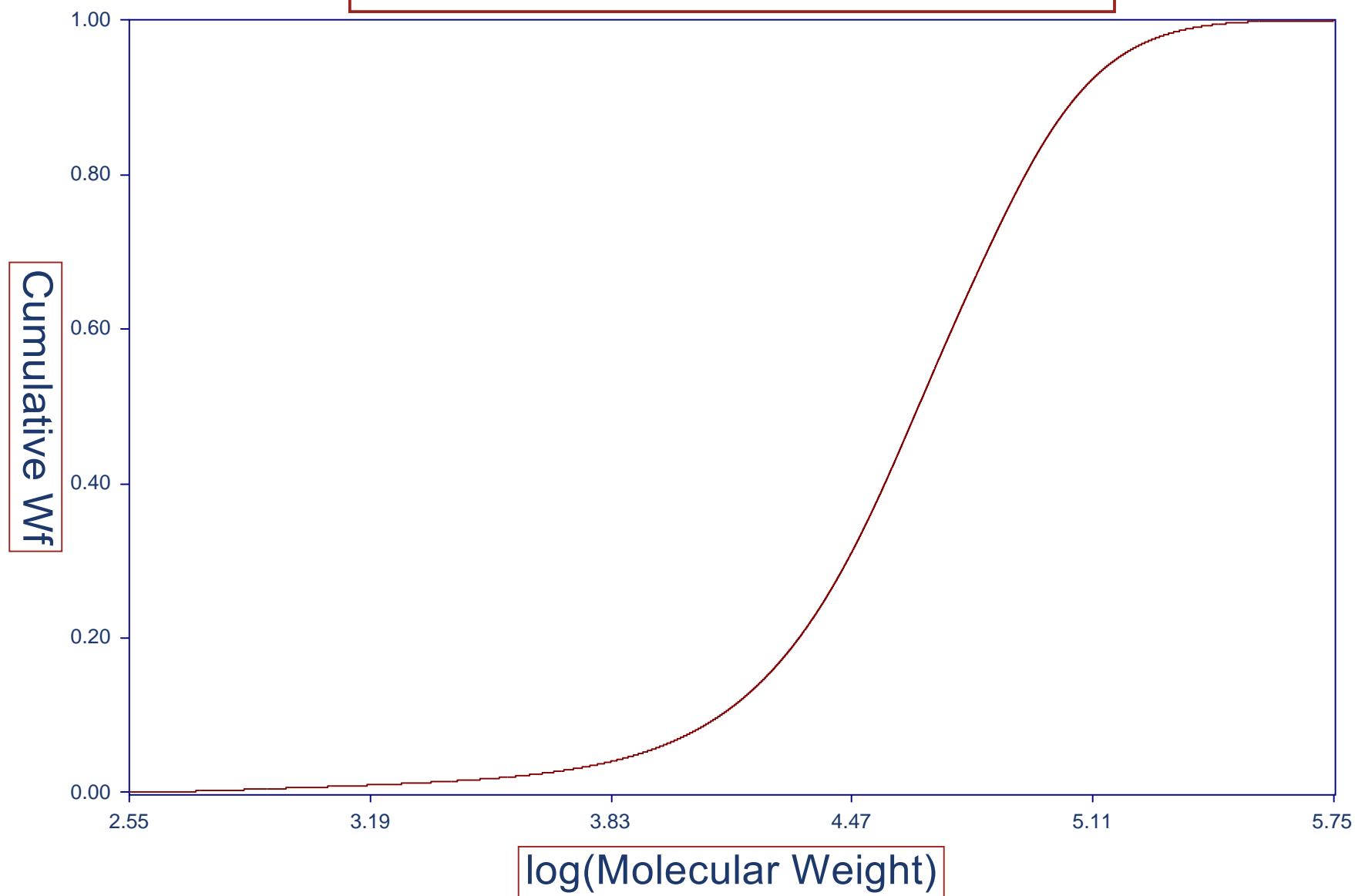
File Name = BC2-1

Summary of Molecular Weights

File Name = BC2-1

Sample Name = Bottle Control

Calibration File Name = JordiCal110910.ASC

Number Average Molecular Weight (Mn) = 19927   Integration Limits =

Weight Average Molecular Weight (Mw) = 56855   Left = 16.98

Z Average Molecular Weight (Mz) = 97111   Right = 26.90

Peak Maximum Molecular Weight (Mp) = 42710

Polydispersity = 2.85

Peak Area = 8229

Mobile Phase = Tetrahydrofuran   Temperature = 45 ^{0} C

Detector = Refractive Index   Inj. Volume = 50 µl

Concentration = 2.5 mg/ml   Flow Rate = 1.2 ml/min

Run Date = 11/4/2010 4:00:38 AM

Column = Jordi Gel DVB Mixed Bed 500 x 10 mm

Comments = None

Summary of Molecular Weights

File Name = BC2-2

Sample Name = Bottle Control

Calibration File Name = JordiCal110910.ASC

Number Average Molecular Weight (Mn) = 20166   Integration Limits =

Weight Average Molecular Weight (Mw) = 56907   Left = 16.98

Z Average Molecular Weight (Mz) = 97569   Right = 26.90

Peak Maximum Molecular Weight (Mp) = 43925

Polydispersity = 2.82

Peak Area = 8206

Mobile Phase = Tetrahydrofuran   Temperature = 45 º C

Detector = Refractive Index   Inj. Volume = 50 μl

Concentration = 2.5 mg/ml   Flow Rate = 1.2 ml/min

Run Date = 11/4/2010 4:41:34 AM

Column = Jordi Gel DVB Mixed Bed 500 x 10 mm

Comments = None

File Name = BD2-1

Chromatogram
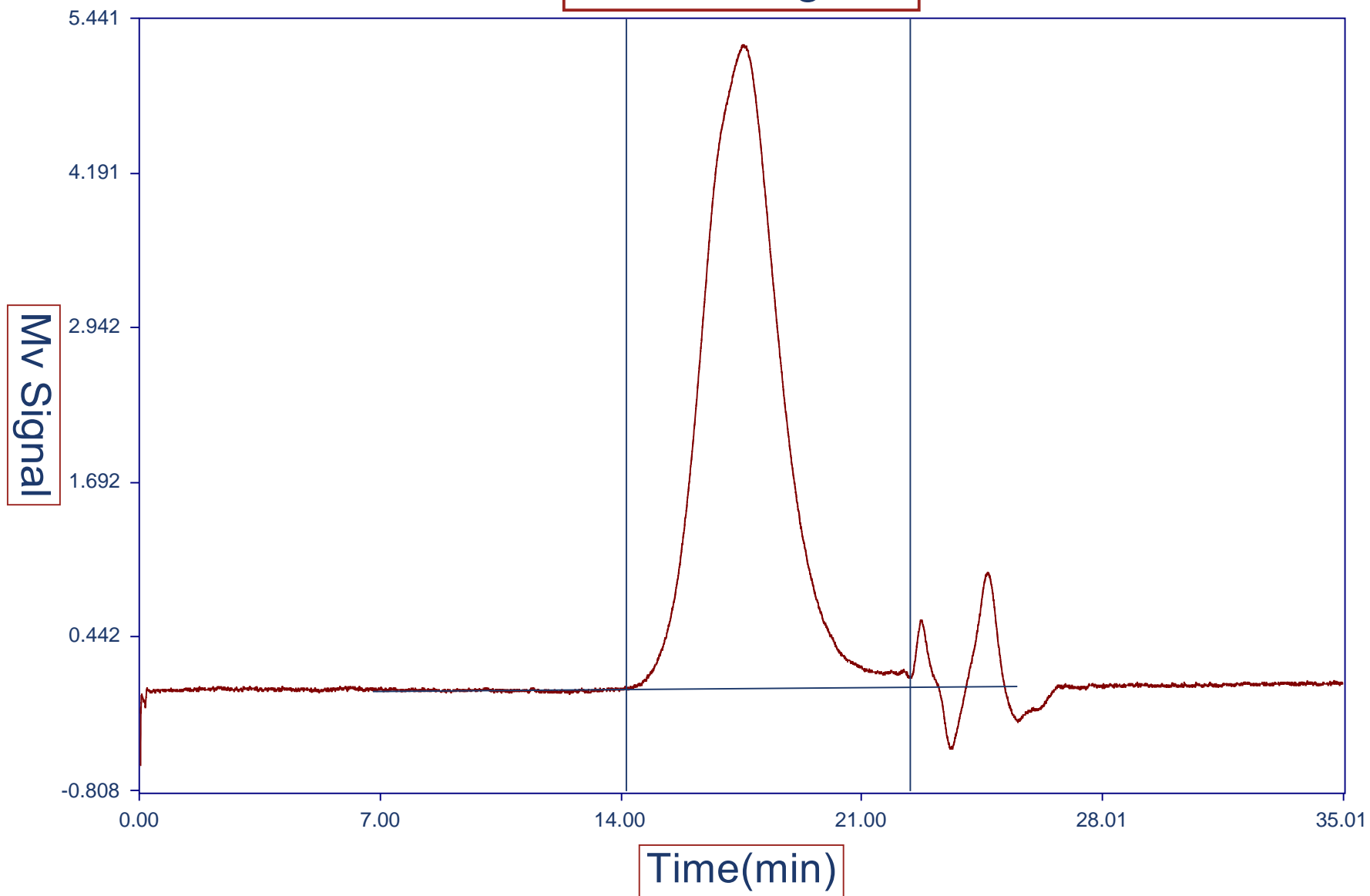
Molecular Weight Distribution Curve

File Name = BD2-1

- - - - Mn = 19164
- - - Mp = 43043
——— Mw = 56892
······ Mz = 97860

10*Wf/d[logMW]
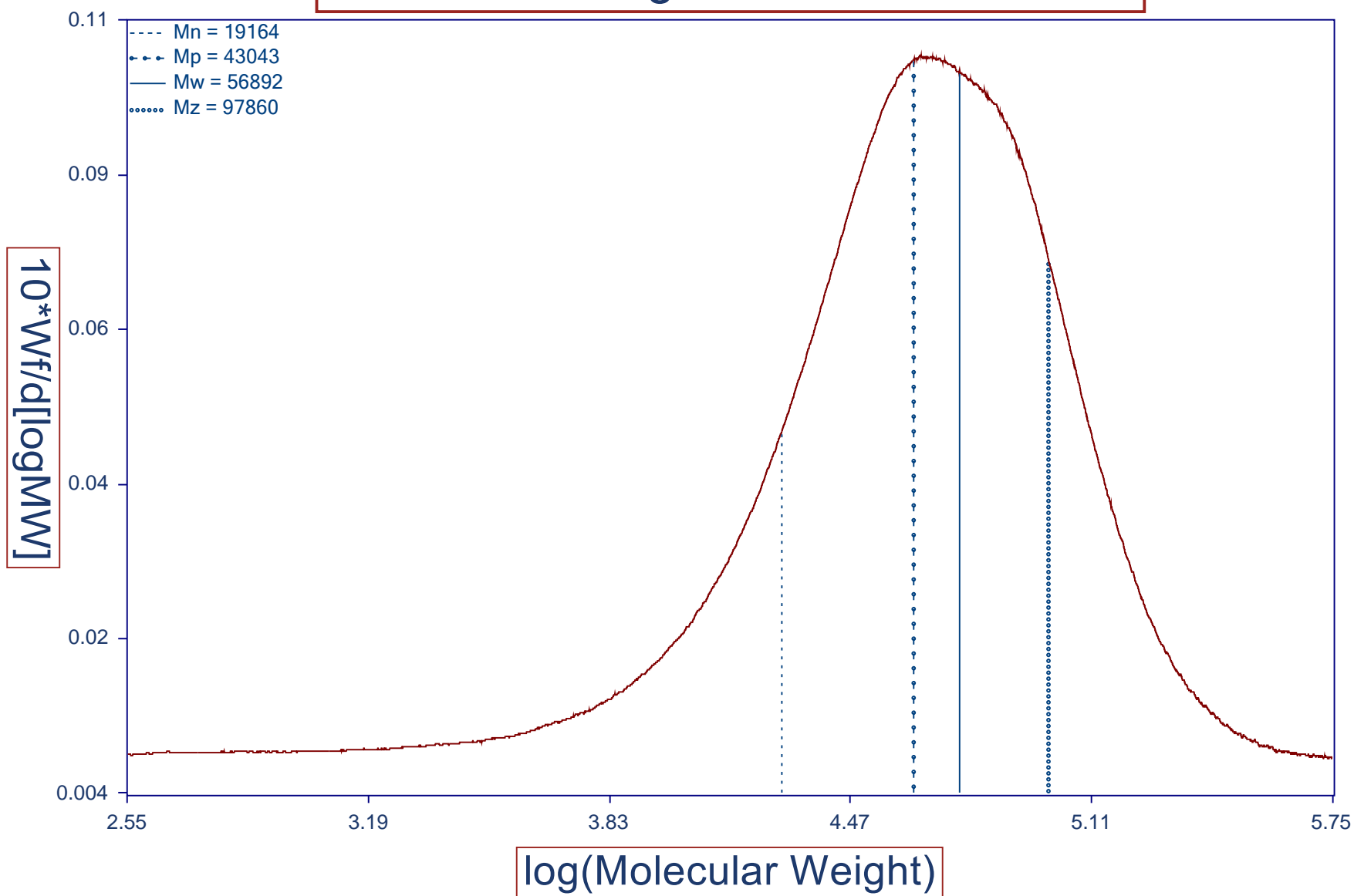
log(Molecular Weight)

Cumulative Wf Distribution Curve
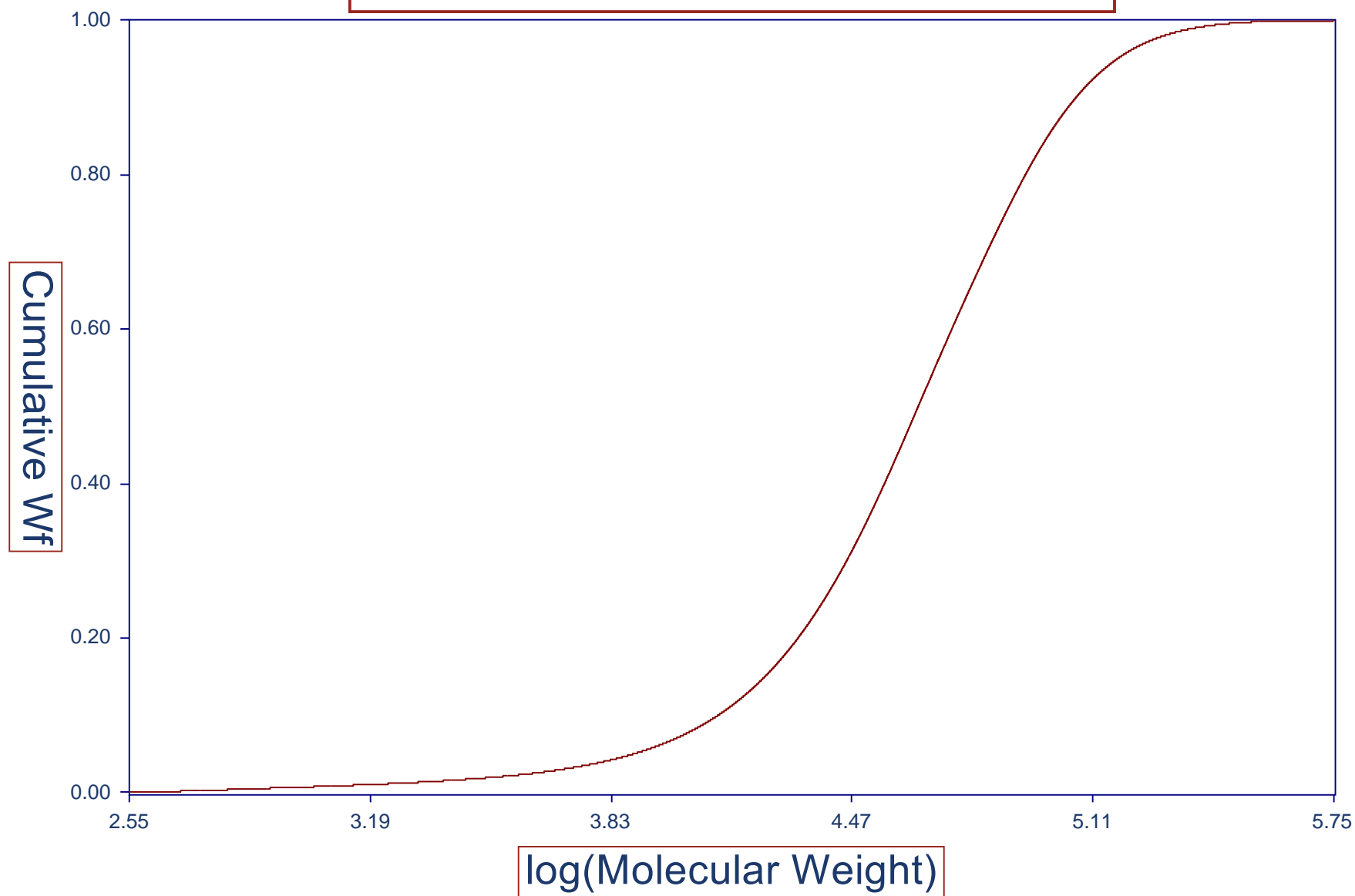
Summary of Molecular Weights

File Name = BD2-1

Sample Name = Bottle Dishwasher

Calibration File Name = JordiCal110910.ASC

Number Average Molecular Weight (Mn) = 19164   Integration Limits =

Weight Average Molecular Weight (Mw) = 56892   Left = 16.98

Z Average Molecular Weight (Mz) = 97860   Right = 26.90

Peak Maximum Molecular Weight (Mp) = 43043

Polydispersity = 2.97

Peak Area = 8186

Mobile Phase = Tetrahydrofuran   Temperature = 45 ^{0} C

Detector = Refractive Index   Inj. Volume = 50 µl

Concentration = 2.5 mg/ml   Flow Rate = 1.2 ml/min

Run Date = 11/4/2010 6:03:33 AM

Column = Jordi Gel DVB Mixed Bed 500 x 10 mm

Comments = None

Summary of Molecular Weights

File Name = BD2-3

Sample Name = Bottle Dishwasher

Calibration File Name = JordiCal110910.ASC

Number Average Molecular Weight (Mn) = 19093   Integration Limits =

Weight Average Molecular Weight (Mw) = 57080   Left = 16.98

Z Average Molecular Weight (Mz) = 97417   Right = 26.90

Peak Maximum Molecular Weight (Mp) = 43250

Polydispersity = 2.99

Peak Area = 8190

Mobile Phase = Tetrahydrofuran   Temperature = 45 ^{0} C

Detector = Refractive Index   Inj. Volume = 50 µl

Concentration = 2.5 mg/ml   Flow Rate = 1.2 ml/min

Run Date = 11/4/2010 7:25:27 AM

Column = Jordi Gel DVB Mixed Bed 500 x 10 mm

Comments = None

Chromatogram

File Name = BO2-1

Mv Signal

Time(min)

Molecular Weight Distribution Curve

File Name = BO2-1

Mn = 19463
Mp = 43150
Mw = 56170
Mz = 95753
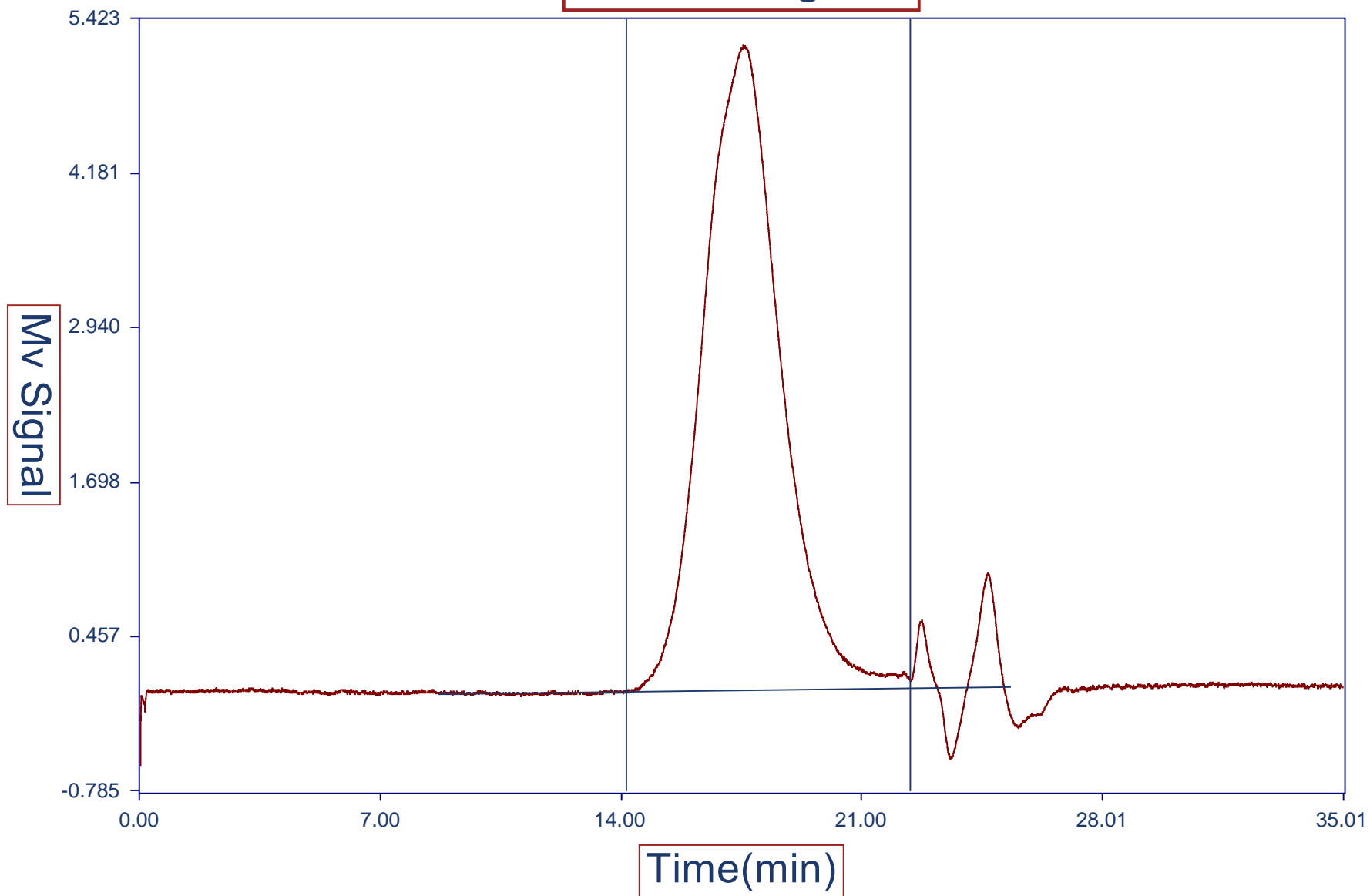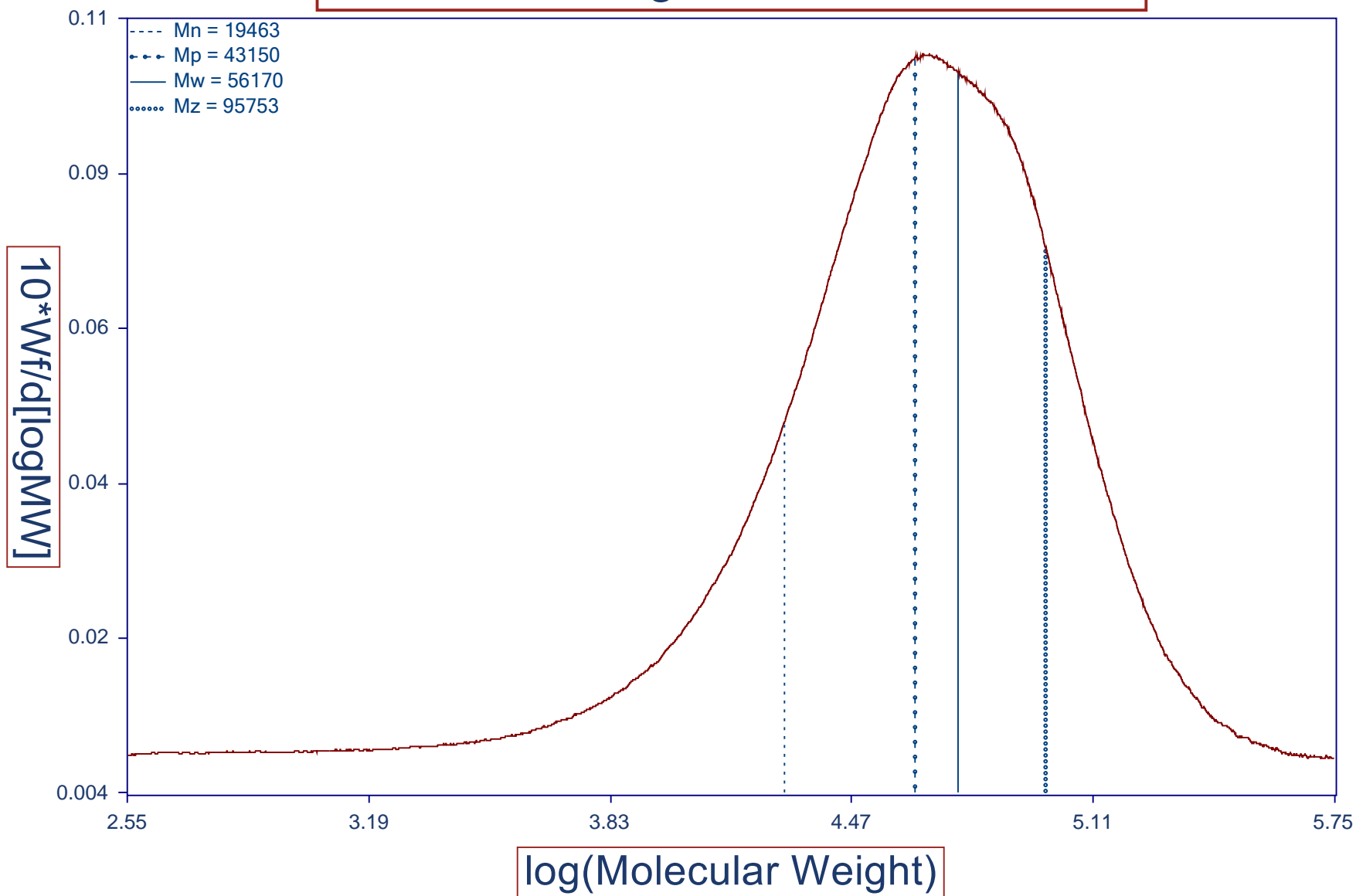
File Name = BO2 -1

Cumulative Wf Distribution Curve

Cumulative Wf

log(Molecular Weight)
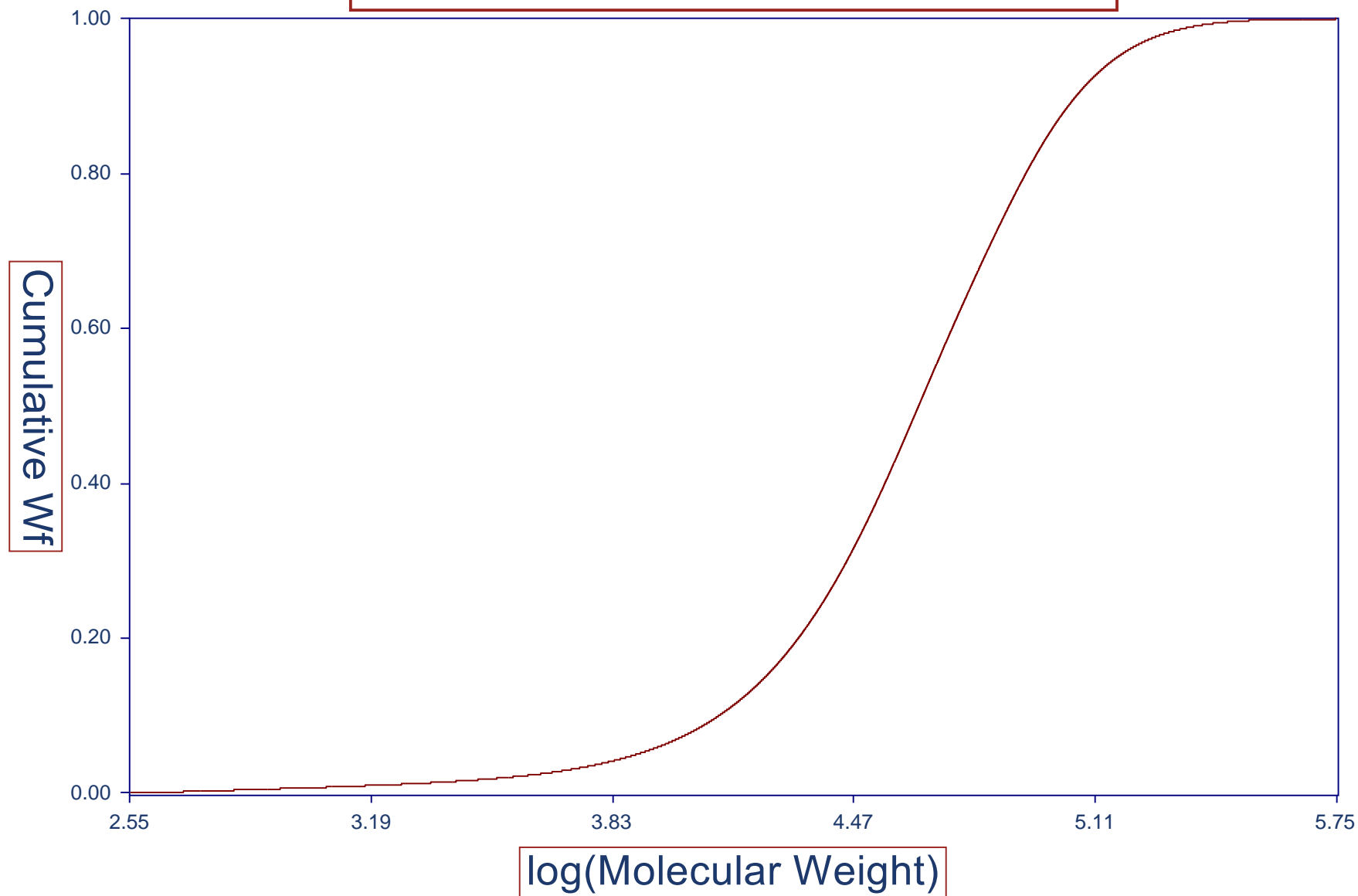
Summary of Molecular Weights

File Name = BO2-1

Sample Name = Bottle Oven

Calibration File Name = JordiCal110910.ASC

Number Average Molecular Weight (Mn) = 19463   Integration Limits =

Weight Average Molecular Weight (Mw) = 56170   Left = 16.98

Z Average Molecular Weight (Mz) = 95753   Right = 26.90

Peak Maximum Molecular Weight (Mp) = 43150

Polydispersity = 2.89

Peak Area = 8099

Mobile Phase = Tetrahydrofuran   Temperature = 45 º C

Detector = Refractive Index   Inj. Volume = 50 µl

Concentration = 2.5 mg/ml   Flow Rate = 1.2 ml/min

Run Date = 11/4/2010 8:06:27 AM

Column = Jordi Gel DVB Mixed Bed 500 x 10 mm

Comments = None

Summary of Molecular Weights

File Name = BO2-3

Sample Name = Bottle Oven

Calibration File Name = JordiCal110910.ASC

Number Average Molecular Weight (Mn) = 19354   Integration Limits =

Weight Average Molecular Weight (Mw) = 55888   Left = 16.98

Z Average Molecular Weight (Mz) = 95682   Right = 26.90

Peak Maximum Molecular Weight (Mp) = 43712

Polydispersity = 2.89

Peak Area = 8151

Mobile Phase = Tetrahydrofuran   Temperature = 45 ^{0} C

Detector = Refractive Index   Inj. Volume = 50 µl

Concentration = 2.5 mg/ml   Flow Rate = 1.2 ml/min

Run Date = 11/4/2010 9:28:24 AM

Column = Jordi Gel DVB Mixed Bed 500 x 10 mm

Comments = None