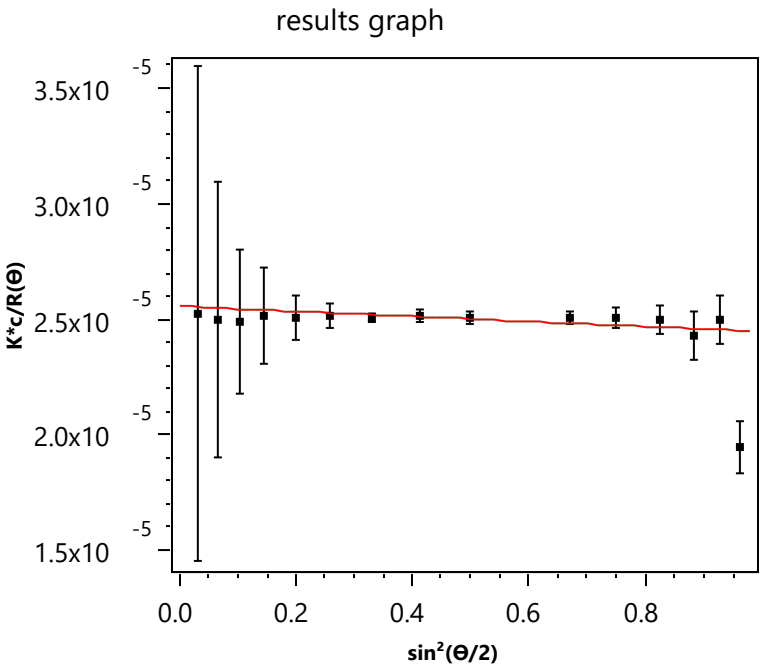
ASTRA Report Covid_poly3[072420_Covid2]

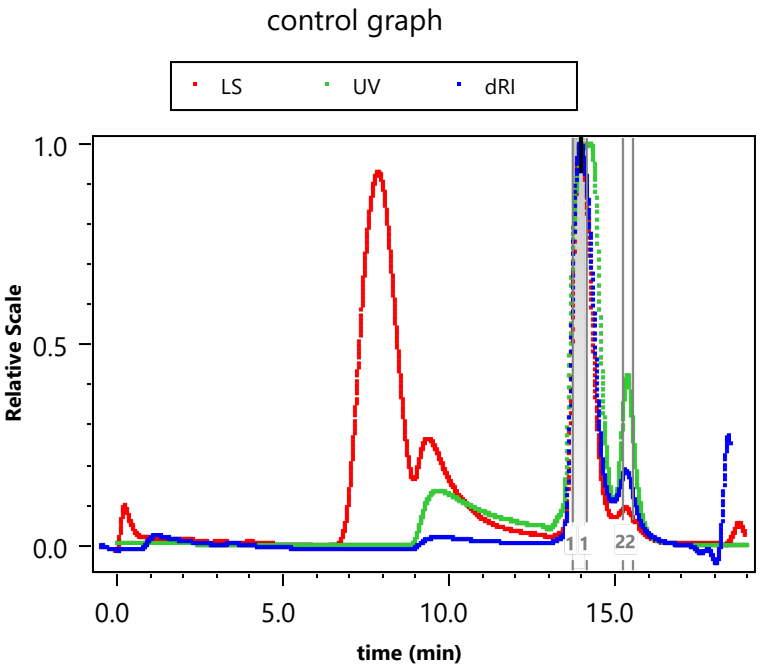
File Properties

File Name: D:\GoogleDrive\LBNL\SIBYLS_Group\MALS and DLS Data\Sequences\Covid_poly3[072420_Covid2].afe7
Created: July 26, 2020 17:49:59.704

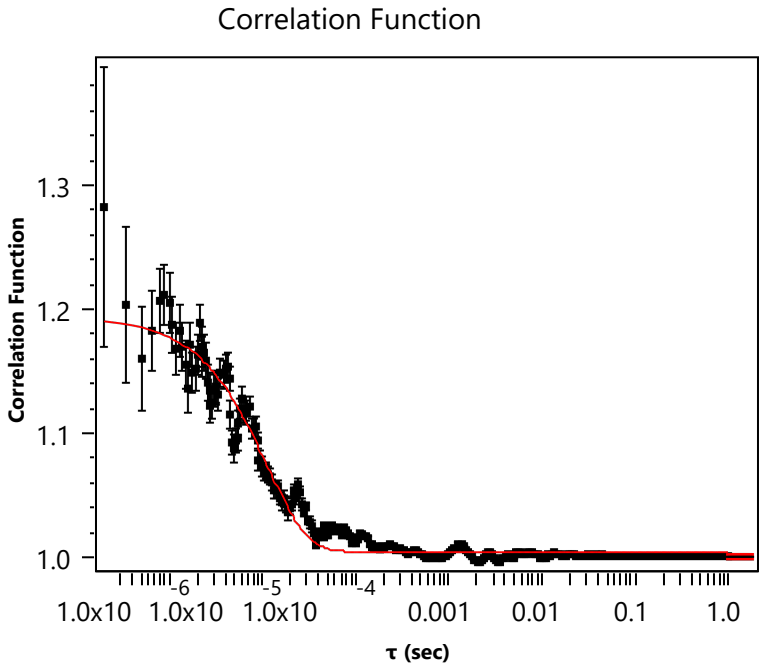
Sample: Covid_poly3
dn/dc: 0.1750 mL/g
Concentration: 2.000 mg/mL



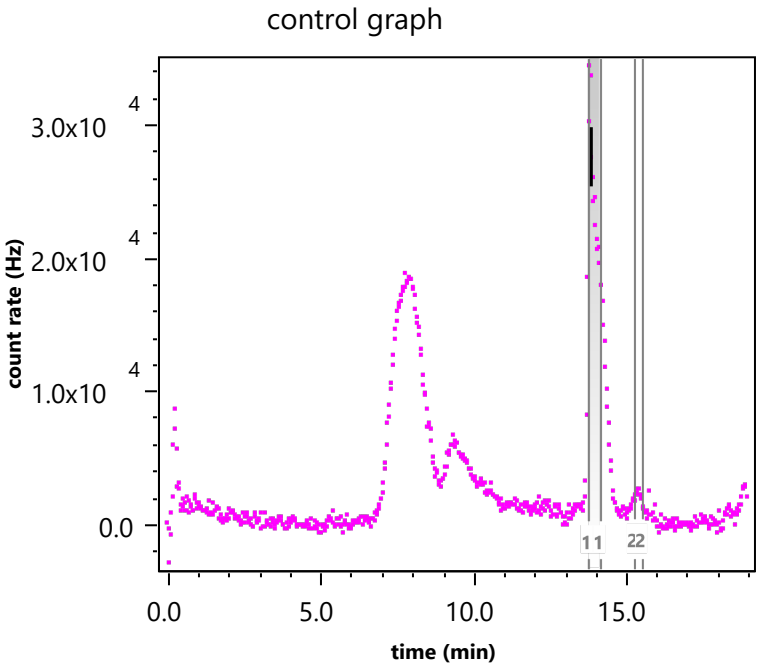
Fit R^2=0.1507



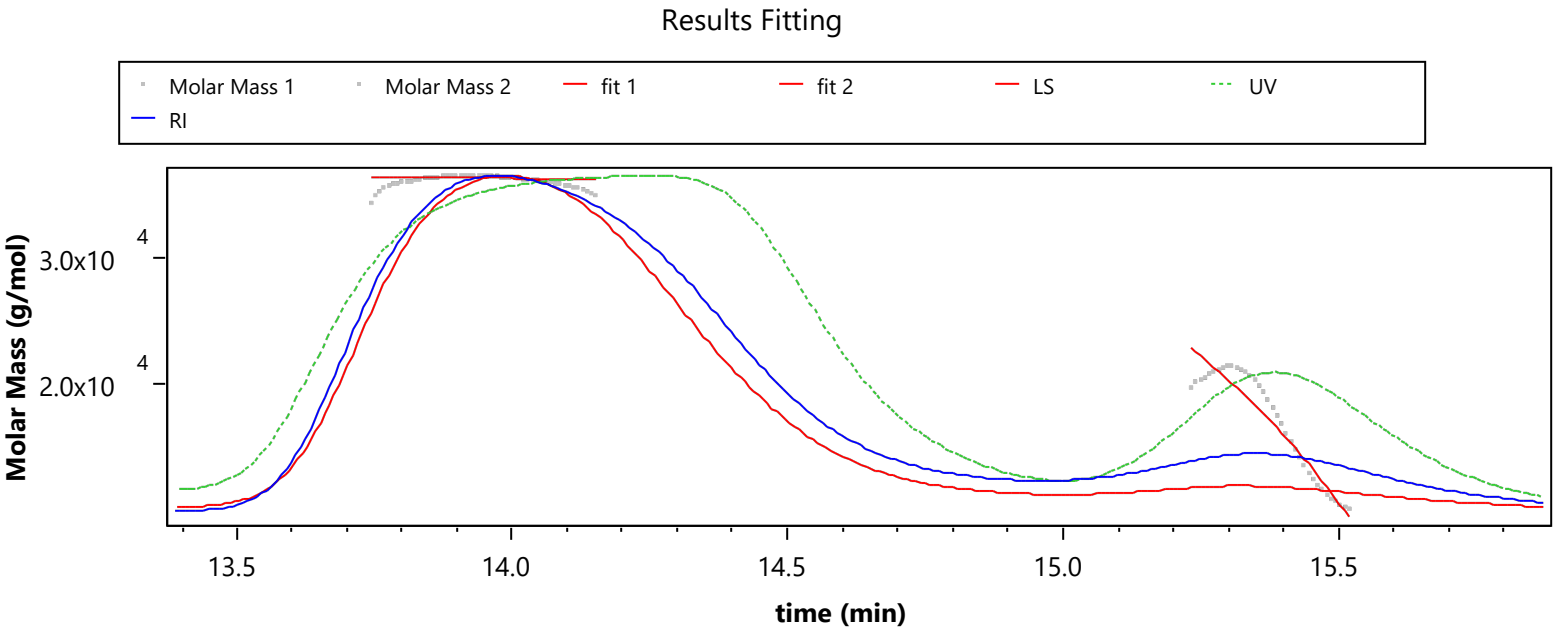
Index = 13.972 min



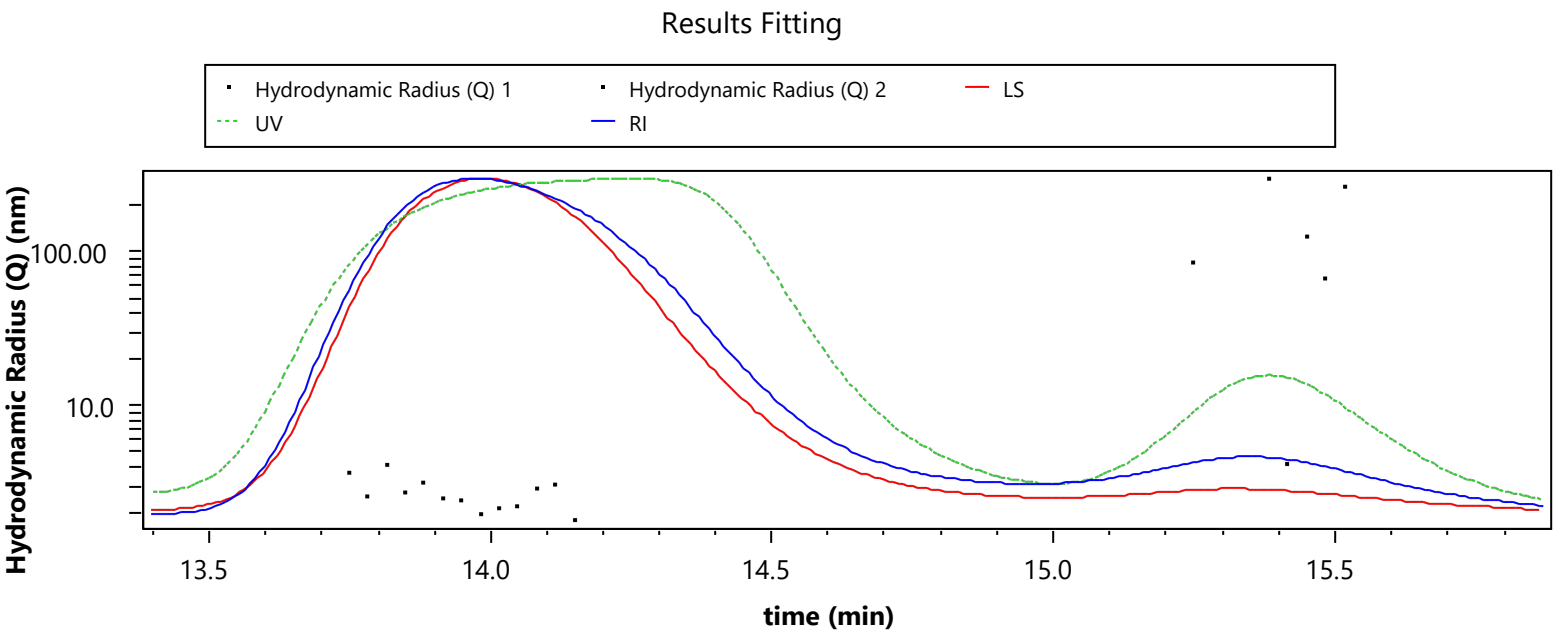
Fit R^2=0.8711

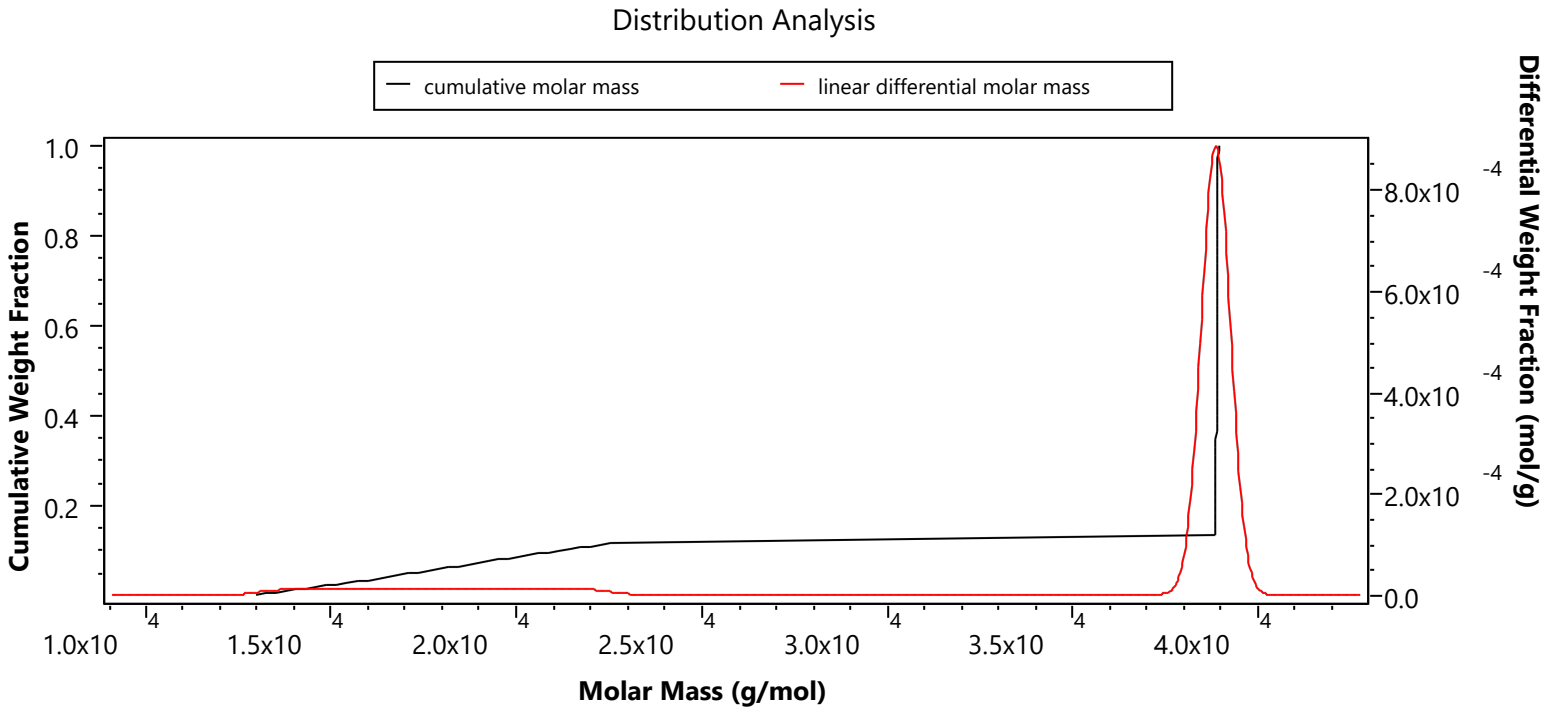


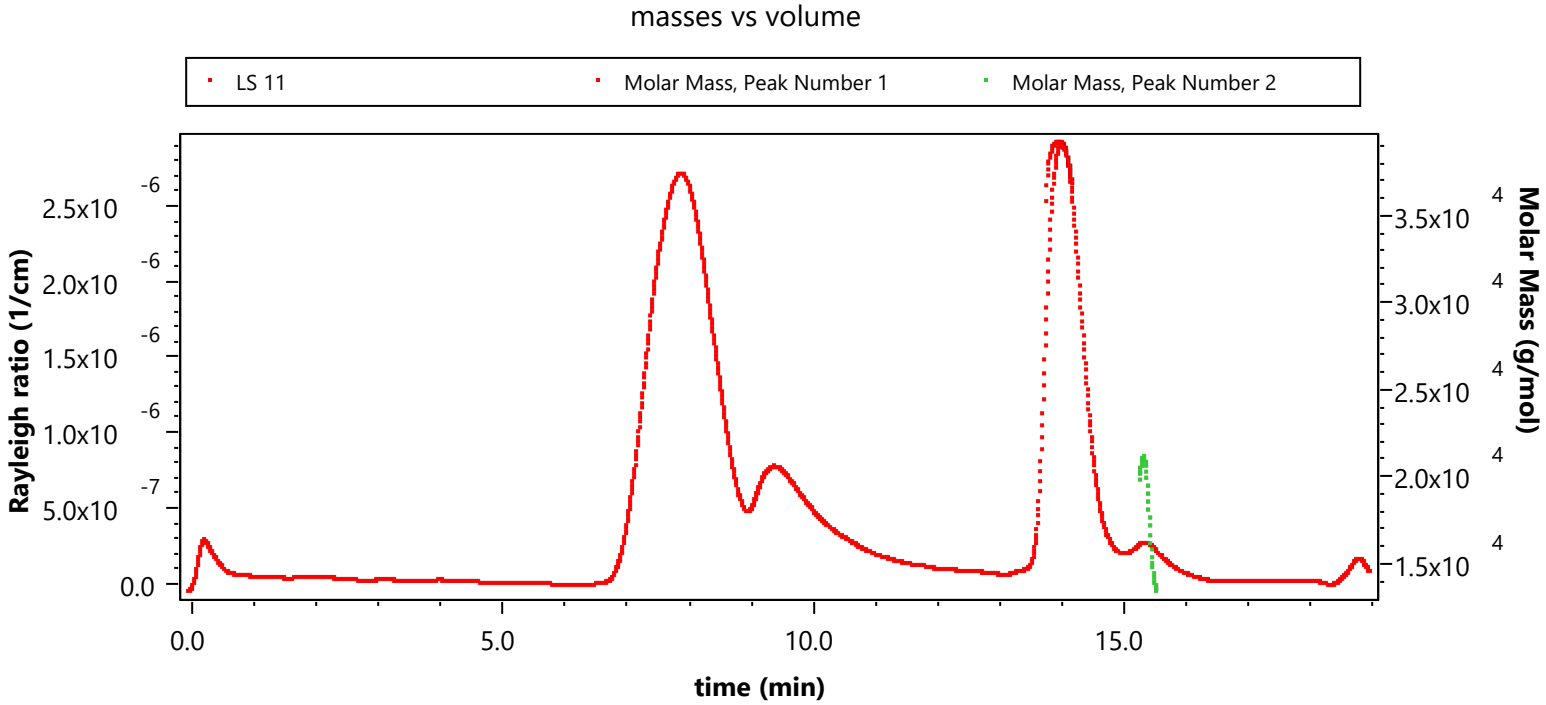
Index = 13.849 min



Peak 1 Fit Adjusted R^2=n/a; Peak 2 Fit Adjusted R^2=0.9225







Configuration

Abscissa Units: min
Concentration Source: RI
Flow Rate: 0.500 mL/min
Pulse Correction Enabled: yes

Light Scattering Instrument: DAWN HELEOS
Cell Type: Fused Silica
Wavelength: 660.0 nm
Calibration Constant: 3.3316×10^{-5} 1/(V cm)

RI Instrument: Optilab T-rEX
Wavelength: 658.0 nm

UV Instrument: Generic UV

Solvent: PBS, Aqueous

Refractive Index: 1.331

Fluid Connections

Source Instrument	Destination Instrument	Delay Volume (mL)
Generic Pump	Injector	0.000
Injector	Generic UV Instrument	0.000
Generic UV Instrument	DAWN HELEOS	0.026
DAWN HELEOS	Optilab rEX	0.222

Aux Connections

Source Instrument	Destination Instrument	Source Aux Channel	Destination Aux Channel	Calibration Constant
Generic UV Instrument	DAWN HELEOS		2	1.000
Generic UV Instrument	DAWN HELEOS	2	3	1.000

Autoinject Connections

Source Instrument	Destination Instrument
autoinject	DAWN HELEOS

Processing

Collection Operator: MICHAELFARADAY\Michael Faraday (MICHAELFARADAY\Michael Faraday (Michael Faraday))
Collection Time: Sunday, July 26, 2020 17:31:19 PM
Collection Version: 7.1.4.8
Processing Operator: ALAN-TURING\Alan Turing (Alan Turing)
Processing Time: Monday, July 27, 2020 10:12:03 AM
Despiking Level: Heavy

Peak settings:

Peak Name	Peak 1	Peak 2
Peak Limits (min)	13.738 - 14.155	15.231 - 15.528
Light Scattering Model	Zimm	Zimm
Fit Degree	1	1
dn/dc (mL/g)	0.1700	0.1700
dn/dc Ref. Temp. (°C)	25.000	25.000
Modifier dn/dc (mL/g)	0.0000	0.0000
Modifier dn/dc Ref. Temp. (°C)	25.000	25.000
A2 (mol mL/g²)	0.000	0.000
UV Ext. Coef. (mL/(mg cm))	0.667	0.667
UV Ext. Coef. Ref. Temp. (°C)	25.000	25.000
Modifier UV Ext. Coef. (mL/(mg cm))	0.000	0.000
Modifier UV Ext. Coef. Ref. Temp. (°C)	25.000	25.000
Real Refractive Index	0	0
Imaginary Refractive Index	0	0
Shell Thickness (nm)	0.000	0.000
Shell Real Refractive Index	0	0
Shell Imaginary Refractive Index	0	0
Rod radius (nm)	0.000	0.000
Molecular Standard	n/a	n/a
Concentration (mg/mL)	2.000	2.000
Concentration Ref. Temp. (°C)	25.000	25.000
Mn (g/mol)	0.000	0.000
Mw (g/mol)	0.000	0.000
Mp (g/mol)	0.000	0.000
Intrinsic Viscosity (mL/g)	0.000	0.000
Intrinsic Viscosity Ref. Temp. (°C)	25.000	25.000
Mark-Houwink-Sakurada K (mL/g)	0.000	0.000
Mark-Houwink-Sakurada a	0	0
Flory-Fox Equation Phi Parameter	0	0
Ptitsyn-Eizner Equation Epsilon Parameter	0	0
Viscometry Model	Huggins	Huggins
Huggins Equation Parameter	0	0
Kraemers Equation Parameter	0	0
radius (nm)	3.480	3.480
Radius Type	rms	rms

Molar Mass & Radius from LS:

Peak Name: Peak 1
Molar Mass: (3.913 ± 0.069) e+4 g/mol
rms radius: 0.0 ± 0.0 nm
Light Scattering Model: Zimm
Fit Degree: 1
Concentration: (4.100 ± 0.004) e-1 mg/mL
dn/dc: 0.171 mL/g
Slice Index: 1713
Abscissa Position: 13.972 min

Fit R^2: 0.1507
Enabled Detectors: 3 4 5 6 7 8 9 10 11 13 14 15 16 17 18

rh from QELS:
Use Disabled Slices: no
Prefilter Correlation Function before Averaging: yes
Minimum Delay for Fit: 2.000×10^{-7} sec
Maximum Delay for Fit: 1.0 sec
Minimum Radius Threshold: 1.00 nm
Maximum Radius Threshold: 300.00 nm
Suppress Distribution Peaks Below: 0.50 nm
Suppress Distribution Peaks Above: 10000.000 nm

Results Fitting Procedure:

Data	Fit Model	Degree	R^2	Extrapolation
Molar Mass	Polynomial	1	n/a	none

Results

Peak Results

	Peak 1	Peak 2
Hydrodynamic radius (Q) moments (nm)		
rh(Q)n	2.665 (±7.897%)	146.497 (±30.836%)
Std Dev rh(Q)n	0.642	118.060
rh(Q)w	2.665 (±7.898%)	142.495 (±30.704%)
Std Dev rh(Q)w	0.642	117.154
rh(Q)z	2.665 (±7.899%)	138.509 (±30.744%)
Std Dev rh(Q)z	0.642	117.222
rh(Q)(avg)	2.332 (±2.009%)	4.538 (±29.685%)
General (mL/(mg cm))		
UV Ext. Coef. (mL/(mg cm))	2.246	5.094
Masses		
Injected Mass (µg)	100.00	100.00
Calculated Mass (µg)	79.88	10.29
Mass Recovery (%)	79.9	10.3
Mass Fraction (%)	88.6	11.4
Concentration (mg/mL)		
Average concentration	0.379 (±0.000%)	0.071 (±0.000%)
Molar mass moments (g/mol)		
Mn	3.886×10^{4} (±0.463%)	1.742×10^{4} (±2.956%)
Mp	3.886×10^{4} (±0.337%)	1.870×10^{4} (±2.690%)
Mv	n/a	n/a
Mw	3.886×10^{4} (±0.463%)	1.786×10^{4} (±3.022%)
Mz	3.886×10^{4} (±1.035%)	1.828×10^{4} (±6.846%)
Mz+1	3.886×10^{4} (±1.668%)	1.868×10^{4} (±10.972%)
M(avg)	3.886×10^{4} (±0.056%)	1.673×10^{4} (±0.473%)
Polydispersity		
Mw/Mn	1.000 (±0.654%)	1.025 (±4.227%)
Mz/Mn	1.000 (±1.133%)	1.049 (±7.456%)
rms radius moments (nm)		
rn	n/a	n/a
Std Dev rn	n/a	n/a
rw	n/a	n/a
Std Dev rw	n/a	n/a
rz	n/a	n/a
Std Dev rz	n/a	n/a
r(avg)	6.0 (±57.3%)	18.2 (±62.6%)
Light scattering peak statistics		
Peak Area (1/cm min)	1.073×10^{-6}	3.246×10^{-7}
Peak Height (1/cm)	2.860×10^{-6}	2.831×10^{-7}
Retention Time (min)	13.962	15.317
Peak Width at Half-Height (min)	0.000	0.283
Peak Width at Quarter-Height (min)	0.000	0.000
Peak Width at Tenth-Height (min)	0.000	0.000
Peak Width at User-Specified-Height (4.4%, min)	0.000	0.000
Asymmetry Factor	0.000	0.000
Tailing Factor	0.000	0.000
Column Plate Count	0.000	16303.693
Mean (min)	13.955	15.361
Standard Deviation (min)	0.115	0.080
Skew	-4.529	83.549
Peak Area (%)	76.782	23.218

	Peak 1	Peak 2
Refractive index peak statistics		
Peak Area (RIU min)	2.716×10^{-5}	3.498×10^{-6}
Peak Height (RIU)	6.990×10^{-5}	1.294×10^{-5}
Retention Time (min)	13.974	15.350
Peak Width at Half-Height (min)	0.000	0.000
Peak Width at Quarter-Height (min)	0.000	0.000
Peak Width at Tenth-Height (min)	0.000	0.000
Peak Width at User-Specified-Height (4.4%, min)	0.000	0.000
Asymmetry Factor	0.000	0.000
Tailing Factor	0.000	0.000
Column Plate Count	0.000	0.000
Mean (min)	13.954	15.376
Standard Deviation (min)	0.117	0.081
Skew	-1.121	2.576
Peak Area (%)	88.588	11.412
UV peak statistics		
Peak Area (channel 1) (AU min)	3.588×10^{-1}	1.048×10^{-1}
Peak Area (channel 2) (AU min)	-0.000	-0.000
Peak Height (channel 1) (AU)	9.317×10^{-1}	3.951×10^{-1}
Peak Height (channel 2) (AU)	-0.000	-0.000
Retention Time (channel 1) (min)	14.268	15.383
Retention Time (channel 2) (min)	13.633	15.424
Peak Width at Half-Height (channel 1) (min)	0.000	0.000
Peak Width at Half-Height (channel 2) (min)	0.000	0.000
Peak Width at Quarter-Height (channel 1) (min)	0.000	0.000
Peak Width at Quarter-Height (channel 2) (min)	0.000	0.000
Peak Width at Tenth-Height (channel 1) (min)	0.000	0.000
Peak Width at Tenth-Height (channel 2) (min)	0.000	0.000
Peak Width at User-Specified-Height (channel 1) (4.4%, min)	0.000	0.000
Peak Width at User-Specified-Height (channel 2) (4.4%, min)	0.000	0.000
Asymmetry Factor (channel 1)	0.000	0.000
Asymmetry Factor (channel 2)	0.000	0.000
Column Plate Count (channel 1)	0.000	0.000
Column Plate Count (channel 2)	0.000	0.000
Tailing Factor (channel 1)	0.000	0.000
Tailing Factor (channel 2)	0.000	0.000
Mean (channel 1) (min)	13.952	15.382
Mean (channel 2) (min)	13.941	15.376
Standard Deviation (channel 1) (min)	0.119	0.081
Standard Deviation (channel 2) (min)	0.120	0.085
Skew (channel 1)	-0.012	-0.004
Skew (channel 2)	0.000	0.000
Peak Area % (channel 1) (%)	77.389	22.611
Peak Area % (channel 2) (%)	71.353	28.647
Translational diffusion coefficient moments (cm²/sec)		
Dt(n)	1.27×10^{-6} (±7.34%)	1.87×10^{-7} (±33.60%)
Dt(w)	1.27×10^{-6} (±7.34%)	1.89×10^{-7} (±33.67%)
Dt(z)	1.27×10^{-6} (±7.34%)	1.86×10^{-7} (±33.77%)
Dt(avg)	1.19×10^{-6} (±2.02%)	1.23×10^{-8} (±17.45%)

laser monitor average: 0.999 V
Forward Monitor Average: 0.942 V
laser current average: 0.156 amps
laser voltage average: -225644.235 V
rh(Q) conformation plot slope: -4.013 (±4.257%) log(nm)/log(g/mol)
rh(Q) Conformation Plot y-intercept: 18.815 (±4.162%) log(nm)
rms radius vs. rh(Q) plot slope: 0.032 (±8.226%) rms radius vs. rh(Q) plot slope
rms radius vs. rh(Q) Plot y-intercept: 4.001 (±6.484%) log(nm)