Electronic Supplementary Material (ESI) for RSC Advances.

Supplemental Information

Investigating the effect of a simplified perfume accord and dilution on the formation of mixed-surfactant microemulsion

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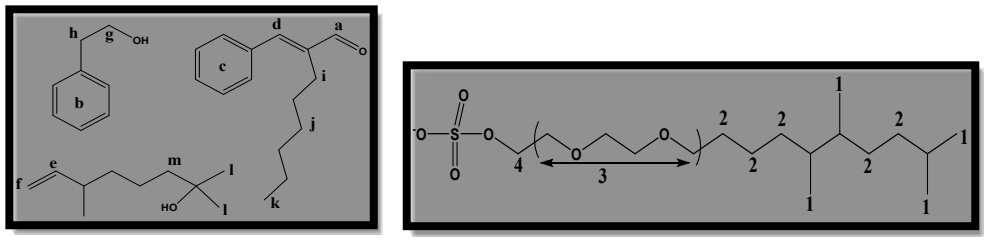


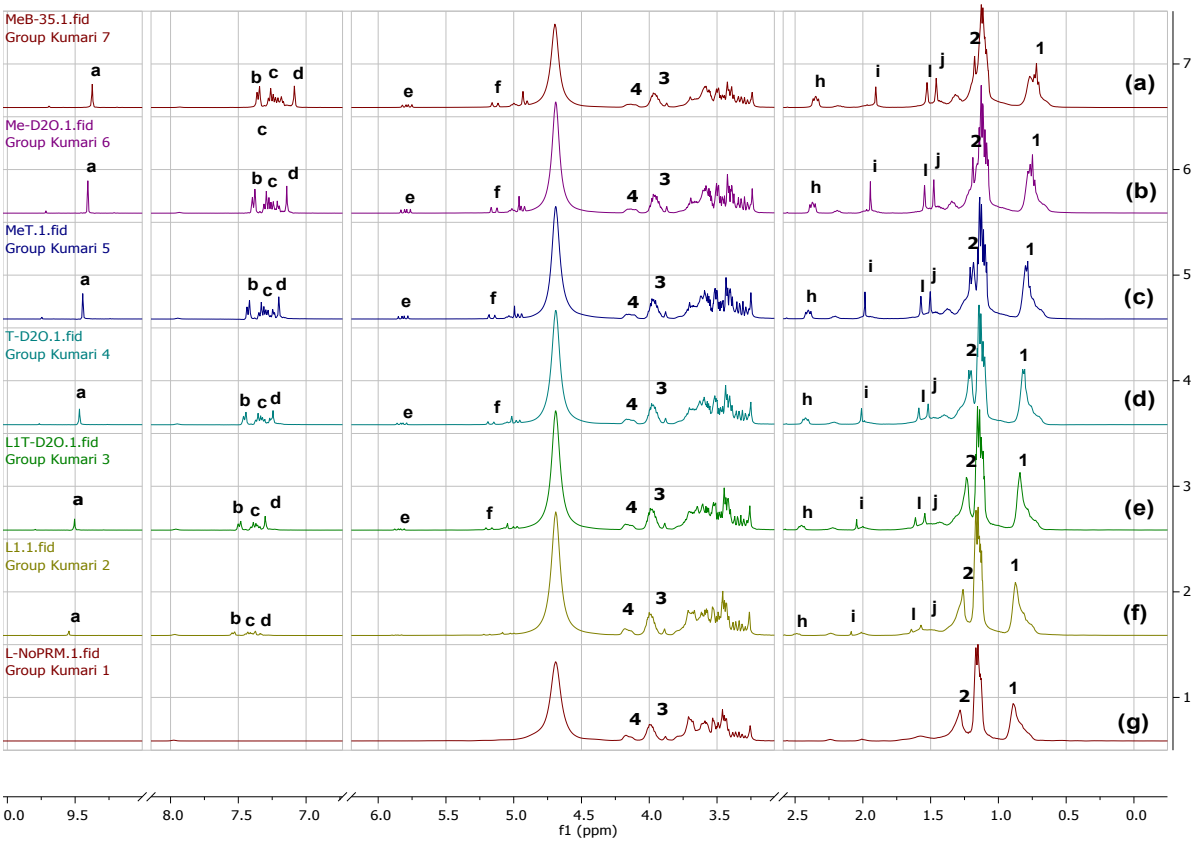


Figure S1. NMR spectra of systems containing varying amounts of 3-PRM perfume mixture at 35 wt% of H_2O/D_2O. In order of decreasing perfume concentration: (a) MeB-35, (b) Me-35 (c) MeT, (d) T-35, (e) L1T-35, (f) L1-35, (g) L1-noPRM-35.

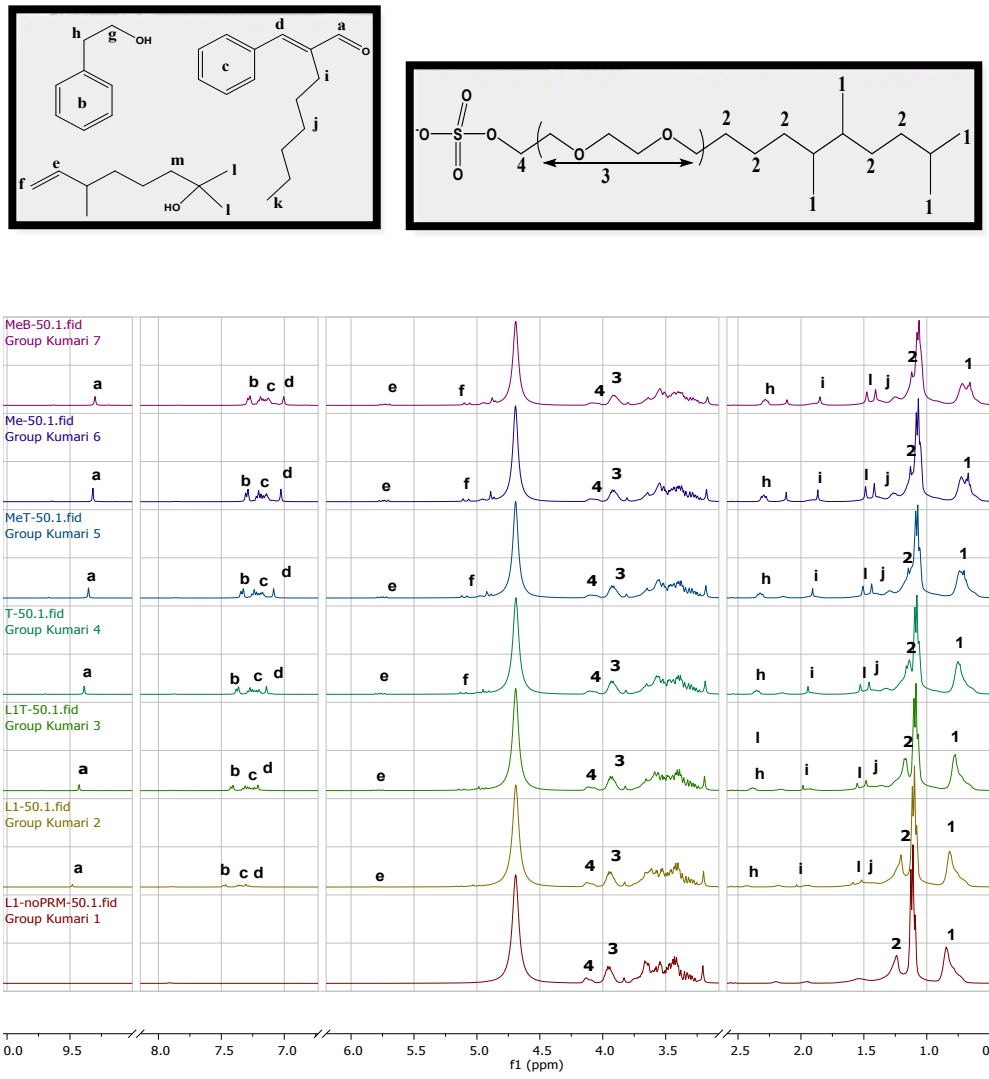
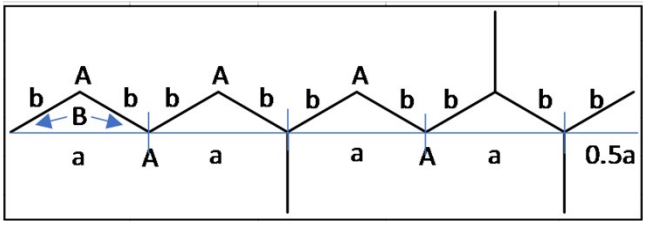


Figure S2. NMR spectra of systems containing varying amounts of 3-PRM perfume mixture at 50% of H_2O/D_2O. In order of decreasing perfume concentration: (a) MeB-50, (b) Me-50, (c) MeT-50, (d) T-50, (e) L1T-50, (f) L1-50, (g) L1-noPRM-50.

Surfactant Tail Length Calculation

The extended lengths of the ST2S tail group with and without the ethoxy groups were calculated to determine the degree of micelle swelling and what portion of the surfactant is contributing to the neutron scattering. The lengths were calculated using geometry and trigonometry (below) and the scattering length densities (SLDs) were calculated using the online NIST neutron activation calculator at https://www.ncnr.nist.gov/resources/activation/. The SLD results showed that the tail group (without ethoxy groups) was the primary contributor to the neutron scattering, as the ethoxy groups and surfactant head group do not contrast enough from the solvent phase.

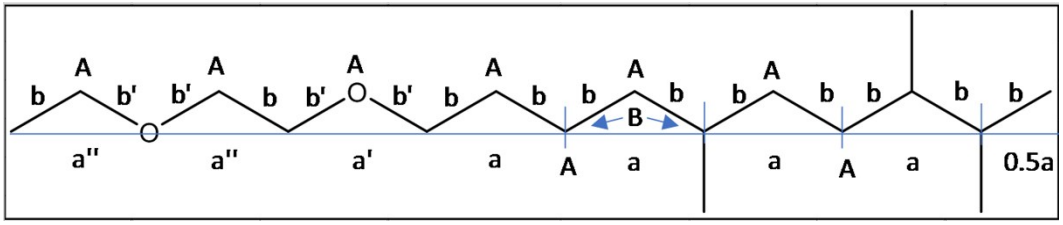
Tail group only (length of C10 group, $C_{10}H_{27}$, d = 0.8 g/cm^3)



$$\frac{a}{\sin A} = \frac{b}{\sin B}$$

Angle A =	109.5	deg
angle B =	35.25	deg
b (C-C bond) =	1.54	Å
a =	2.515256	Å
tail length =	11.32	Å
SLD =	-3.83E-07	Å^{-2}

Tail group with ethoxy groups (length of C10 group + 2 ethoxy groups, $C_{17}H_{35}O_2$, d = 0.9 g/cm^3)



$$a''^2 = b^2 + c^2 - 2bc\cos A$$

$$\frac{a'}{\sin A} = \frac{b'}{\sin B}$$

angle A =	109.5	deg
angle B =	35.25	deg
b (C-C bond) =	1.54	Å
b' (C-O bond) =	1.43	Å
a =	2.515256	Å
a' =	2.335595	Å
a'' =	2.893331	Å
total length =	19.44	Å
SLD =	-1.26E-07	Å^{-2}

Ethoxy groups only (for SLD calculation, $C_4H_8O_2$, d = 0.9 g/cm^3)

SLD = 5.09E-07 Å^{-2}

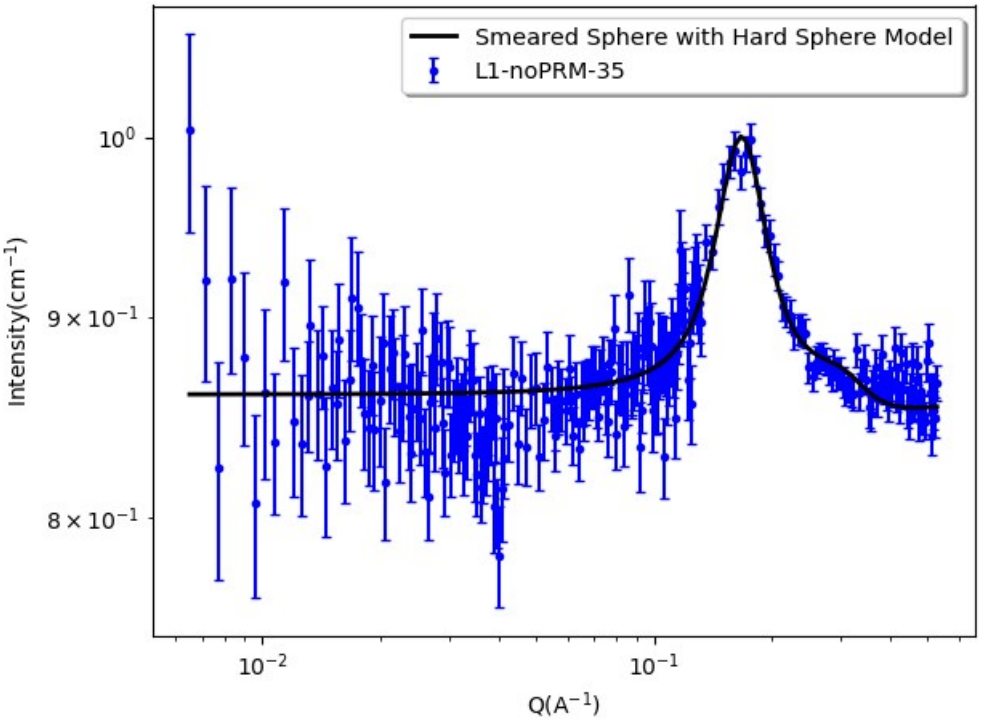
Small-angle Neutron Scattering (SANS) Analysis

Scattering length densities (SLDs) of each surfactant system and its respective solvent system (a mixture consisting of D_2O to improve the SANS signal-to-noise ratio and H_2O from the surfactant) used in modeling the data. The SLDs were calculated using NIST's neutron activation and scattering calculator at https://www.ncnr.nist.gov/resources/activation/. Weighted averages of all components in the surfactant self-assembly (ST2S, CAPB, and the 3 PRMs dihydromyrcenol, hexyl cinnamic aldehyde, and phenylethyl alcohol) and in the solvent phase (D2O, H2O, citric acid, and DPG) were calculated. Those weighted averages, molecular formulae, and each component's density for the scattering phase and the solvent phase were entered into the NIST activation calculator as shown to obtain the reported particle and solvent SLDs. During the fitting process however, it was found that the solvent SLD needed to be fitted for the 35 wt% water samples (sample codes appended with "-35") in order to achieve a good quality fit as the contrast was too low. For those samples, the calculated solvent SLD was not the value used in the final fit.

Code	Entry for Particle SLD	Particle SLD	Entry for Solvent SLD	Solvent SLD
L1-noPRM-35	85.36%wt C17H35NaO6S@1.1 // C19H38N2O3@1.04	3.930E-07	0.71%wt C6H8O7@1.542 // 12.57%wt D2O@1.1 // 48.15%wt C6H14O3@1.023 // H2O@1	6.410E-07
L1-35	77.23%wt C17H35NaO6S@1.1 // 13.25%wt C19H38N2O3@1.04 // 2.38%wt C10H20O@0.784 // 2.38%wt C8H10O@1.02 // C15H20O@0.95	4.180E-07	0.69%wt C6H8O7@1.542 // 14.89%wt D2O@1.1 // 46.87%wt C6H14O3@1.023 // H2O@1	7.830E-07
L1T-35	68.29%wt C17H35NaO6S@1.1 // 11.71%wt C19H38N2O3@1.04 // 5.00%wt C10H20O@0.784 // 5.00%wt C8H10O@1.02 // C15H20O@0.95	4.440E-07	0.66%wt C6H8O7@1.542 // 17.90%wt D2O@1.1 // 45.21%wt C6H14O3@1.023 // H2O@1	9.660E-07
T-35	62.08%wt C17H35NaO6S@1.1 // 10.65%wt C19H38N2O3@1.04 // 6.82%wt C10H20O@0.784 // 6.82%wt C8H10O@1.02 // C15H20O@0.95	4.610E-07	0.64%wt C6H8O7@1.542 // 20.32%wt D2O@1.1 // 43.88%wt C6H14O3@1.023 // H2O@1	1.115E-06
MeT-35	56.91%wt C17H35NaO6S@1.1 // 9.76%wt C19H38N2O3@1.04 // 8.33%wt C10H20O@0.784 // 8.33%wt C8H10O@1.02 // C15H20O@0.95	4.750E-07	0.63%wt C6H8O7@1.542 // 22.60%wt D2O@1.1 // 42.62%wt C6H14O3@1.023 // H2O@1	1.255E-06
Me-35	51.22%wt C17H35NaO6S@1.1 // 8.78%wt C19H38N2O3@1.04 // 10.00%wt C10H20O@0.784 // 10.00%wt C8H10O@1.02 // C15H20O@0.95	4.910E-07	0.60%wt C6H8O7@1.542 // 25.45%wt D2O@1.1 // 41.05%wt C6H14O3@1.023 // H2O@1	1.431E-06

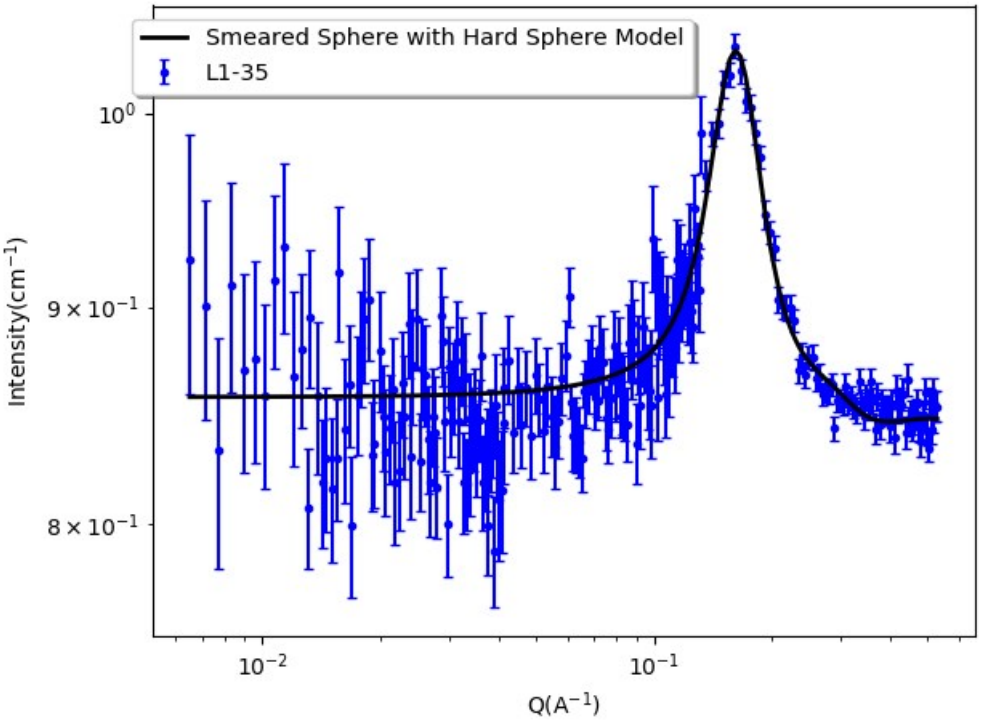
MeB-35	43.97%wt C17H35NaO6S@1.1 // 7.54%wt C19H38N2O3@1.04 // 12.12%wt C10H20O@0.784 // 12.12%wt C8H10O@1.02 // C15H20O@0.95	5.100E-07	0.57%wt C6H8O7@1.542 // 30.92%wt D2O@1.1 // 38.70%wt C6H14O3@1.023 // H2O@1	1.777E-06
L1-noPRM-50	85.36%wt C17H35NaO6S@1.1 // C19H38N2O3@1.04	3.930E-07	0.49%wt C6H8O7@1.542 // 39.47%wt D2O@1.1 // 33.33%wt C6H14O3@1.023 // H2O@1	2.309E-06
L1-50	77.23%wt C17H35NaO6S@1.1 // 13.25%wt C19H38N2O3@1.04 // 2.38%wt C10H20O@0.784 // 2.38%wt C8H10O@1.02 // C15H20O@0.95	4.180E-07	0.47%wt C6H8O7@1.542 // 41.52%wt D2O@1.1 // 32.20%wt C6H14O3@1.023 // H2O@1	2.439E-06
L1T-50	68.29%wt C17H35NaO6S@1.1 // 11.71%wt C19H38N2O3@1.04 // 5.00%wt C10H20O@0.784 // 5.00%wt C8H10O@1.02 // C15H20O@0.95	4.440E-07	0.45%wt C6H8O7@1.542 // 44.13%wt D2O@1.1 // 30.76%wt C6H14O3@1.023 // H2O@1	2.605E-06
T-50	62.08%wt C17H35NaO6S@1.1 // 10.65%wt C19H38N2O3@1.04 // 6.82%wt C10H20O@0.784 // 6.82%wt C8H10O@1.02 // C15H20O@0.95	4.610E-07	0.43%wt C6H8O7@1.542 // 46.20%wt D2O@1.1 // 29.63%wt C6H14O3@1.023 // H2O@1	2.737E-06
MeT-50	56.91%wt C17H35NaO6S@1.1 // 9.76%wt C19H38N2O3@1.04 // 8.33%wt C10H20O@0.784 // 8.33%wt C8H10O@1.02 // C15H20O@0.95	4.750E-07	0.42%wt C6H8O7@1.542 // 48.12%wt D2O@1.1 // 28.57%wt C6H14O3@1.023 // H2O@1	2.861E-06

L1-noPRM-35 (Smeared Sphere with Hard Sphere Model)



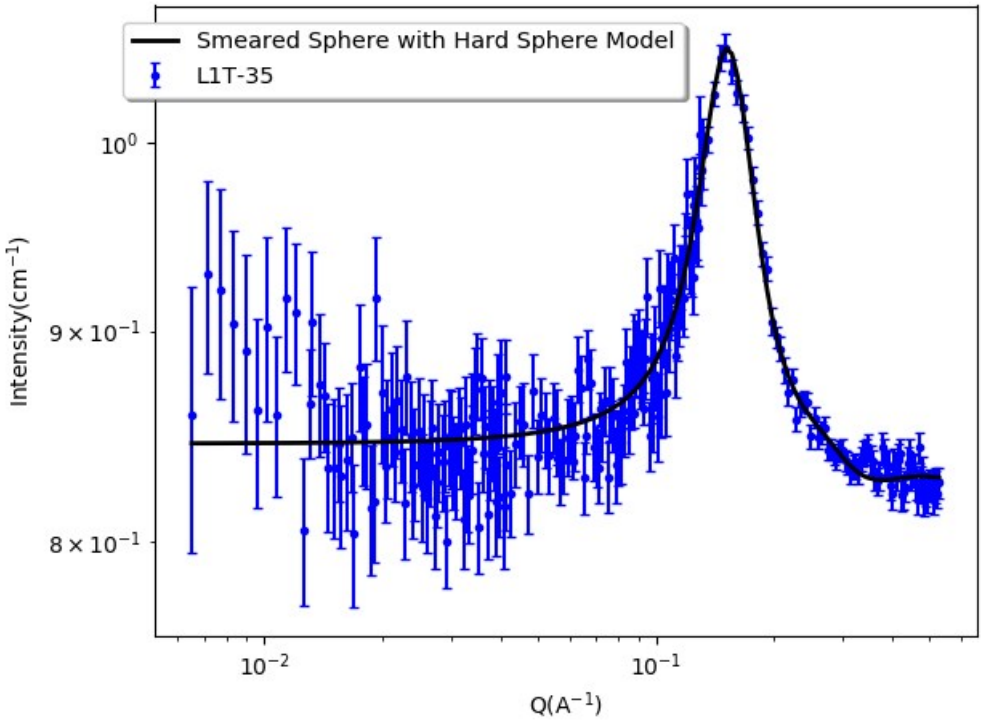
Scale	1	±	0
volume fraction =	0.38364	±	0.00999
Radius (Å) =	9.7735	±	0.26596
Effective Radius	19.395	±	0.17674
SLD ellipsoid (Å^{-2}) =	3.93E-07	±	0
SLD solvent (Å^{-2}) =	1.38E-06	±	3.73E-08
Incoherent Bgd (cm^{-1})	0.85307	±	0.00138
Fitted Range (Å^{-1})	0.006514	< q <	0.5283
Sqrt(χ^2/N)	1.1259		

L1-35 (Smeared Sphere with Hard Sphere Model)



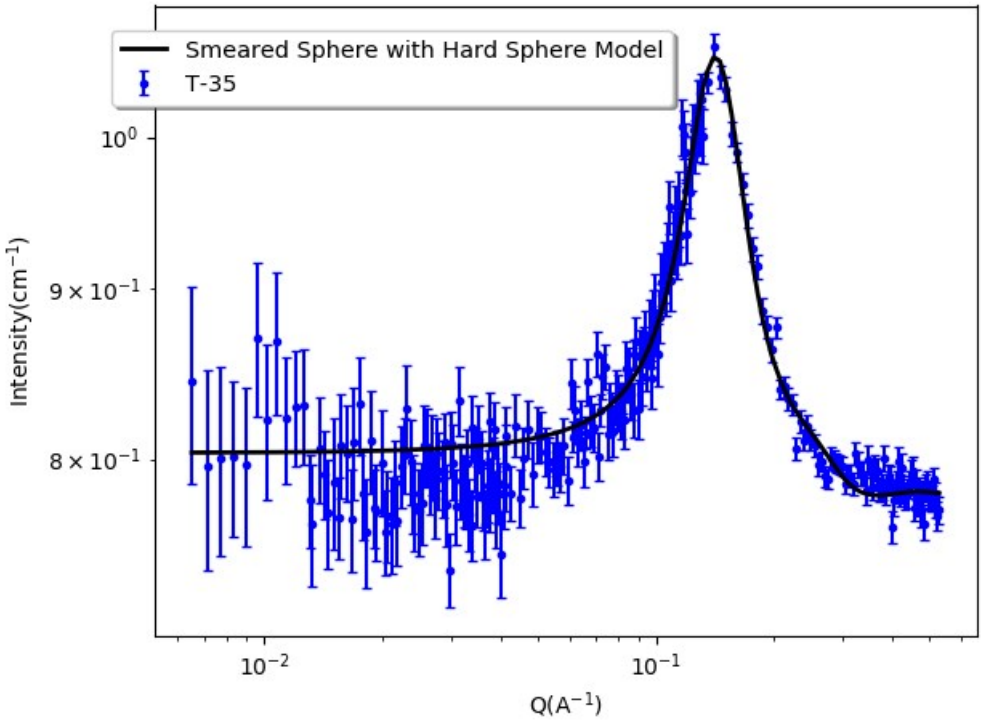
Scale	1	±	0
volume fraction =	0.3733	±	0.00541
Radius (Å) =	11.37	±	0.18436
Effective Radius	19.788	±	0.10985
SLD ellipsoid (Å^{-2}) =	4.18E-07	±	0
SLD solvent (Å^{-2}) =	1.42E-06	±	1.89E-08
Incoherent Bgd (cm^{-1})	0.84533	±	0.00095
Fitted Range (Å^{-1})	0.006514	< q <	0.5283
Sqrt(χ^2/N)	1.1592		

L1T-35 (Smeared Sphere with Hard Sphere Model)



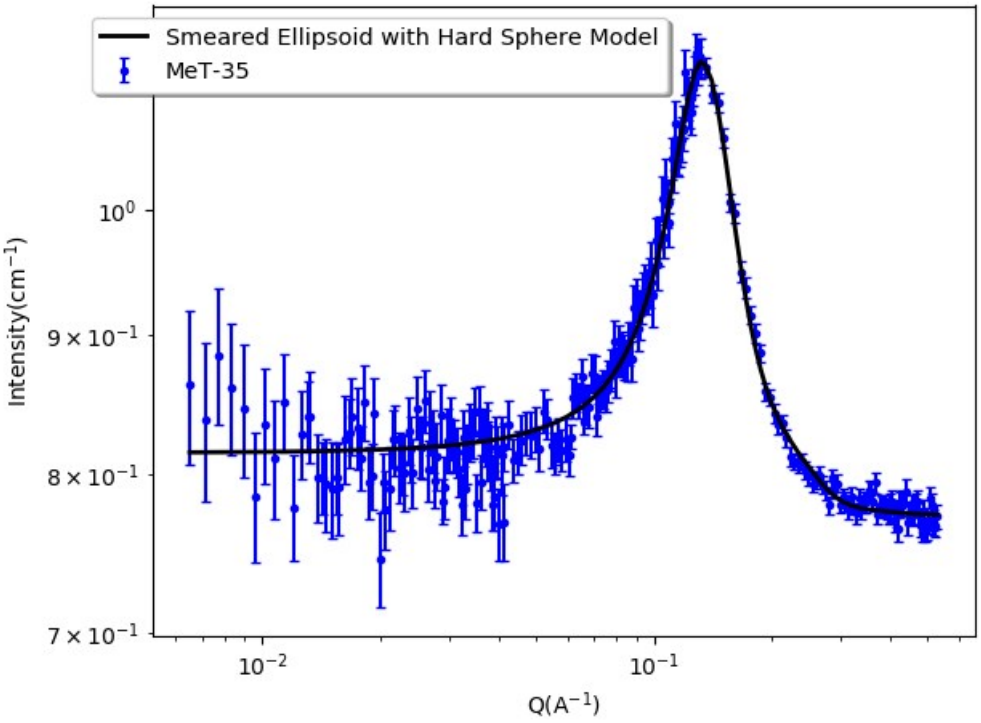
Scale	1	±	0
volume fraction =	0.35268	±	0.00458
Radius (Å) =	12.011	±	0.15464
Effective Radius	20.728	±	0.10356
SLD ellipsoid (Å^{-2}) =	4.44E-07	±	0
SLD solvent (Å^{-2}) =	1.51E-06	±	1.65E-08
Incoherent Bgd (cm^{-1})	0.8276	±	0.00093
Fitted Range (Å^{-1})	0.006514	< q <	0.5283
Sqrt(χ^2/N)	1.0186		

T-35 (Smeared Sphere with Hard Sphere Model)



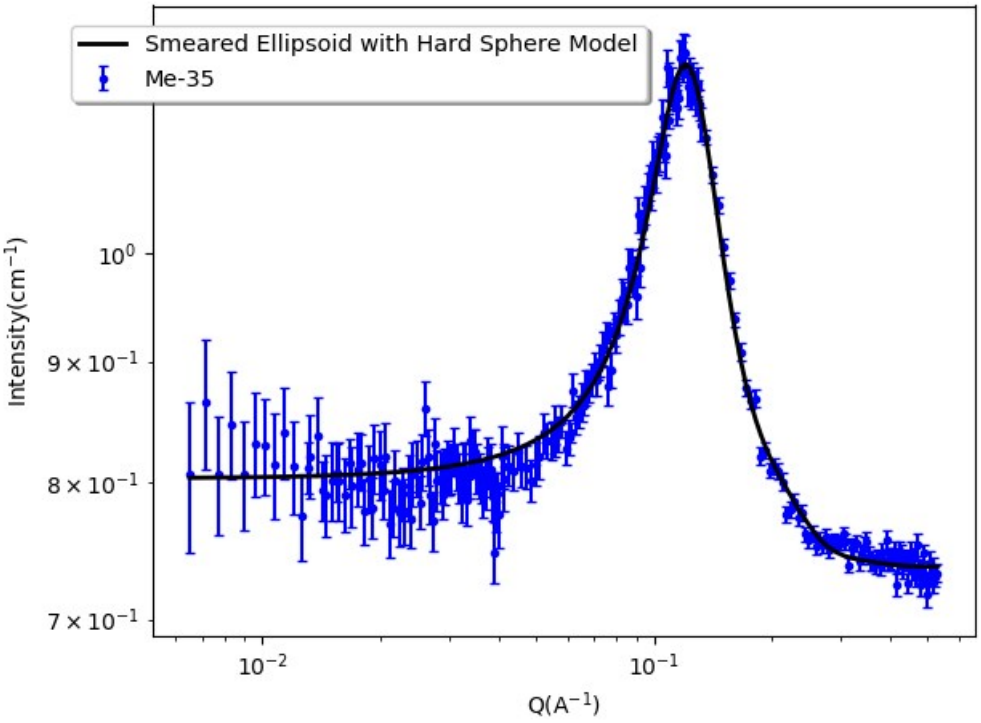
Scale	1	±	0
volume fraction =	0.33673	±	0.00401
Radius (Å) =	12.288	±	0.13577
Effective Radius	22.027	±	0.09939
SLD ellipsoid (Å^{-2}) =	4.61E-07	±	0
SLD solvent (Å^{-2}) =	1.61E-06	±	1.65E-08
Incoherent Bgd (cm^{-1})	0.77979	±	0.00099
Fitted Range (Å^{-1})	0.006514	< q <	0.5283
Sqrt(χ^2/N)	1.2268		

MeT-35 (Smeared Ellipsoid with Hard Sphere Model)



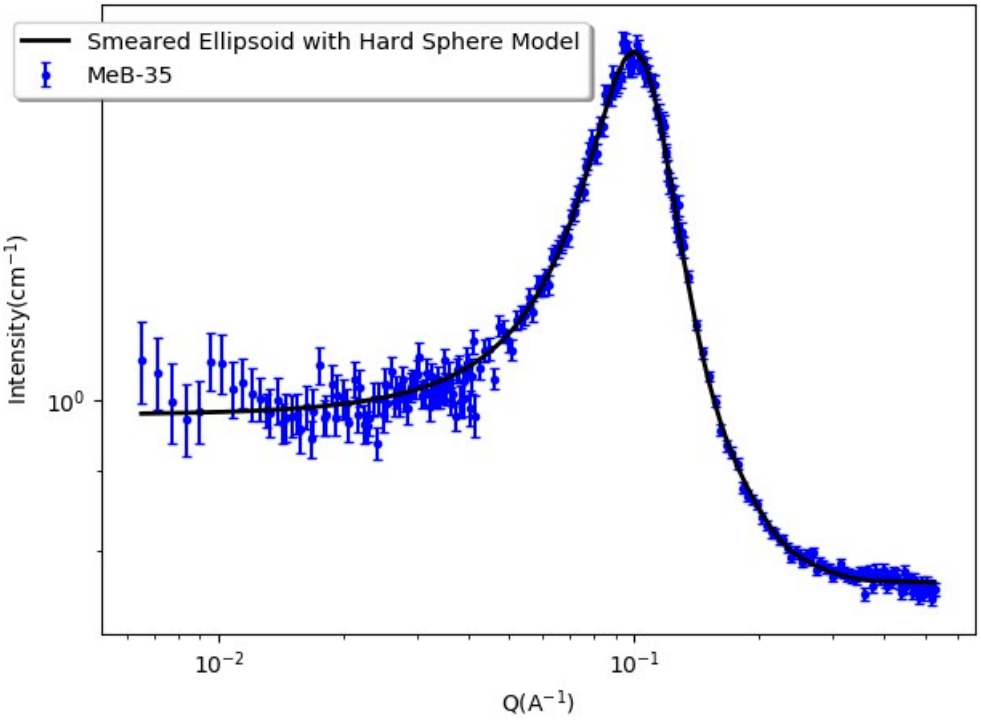
Scale	1	±	0
volume fraction =	0.31862	±	0.00316
R(a) rotation axis (Å) =	9.3386	±	0.59273
R(b) (Å) =	16.284		0.52976
Effective Radius	22.937	±	0.09115
SLD ellipsoid (Å^{-2}) =	4.75E-07	±	0
SLD solvent (Å^{-2}) =	1.74E-06	±	2.24E-08
Incoherent Bgd (cm^{-1})	0.77253	±	0.0012
Fitted Range (Å^{-1})	0.006514	< q <	0.5283
Sqrt(χ^2/N)	0.9837		

Me-35 (Smeared Ellipsoid with Hard Sphere Model)



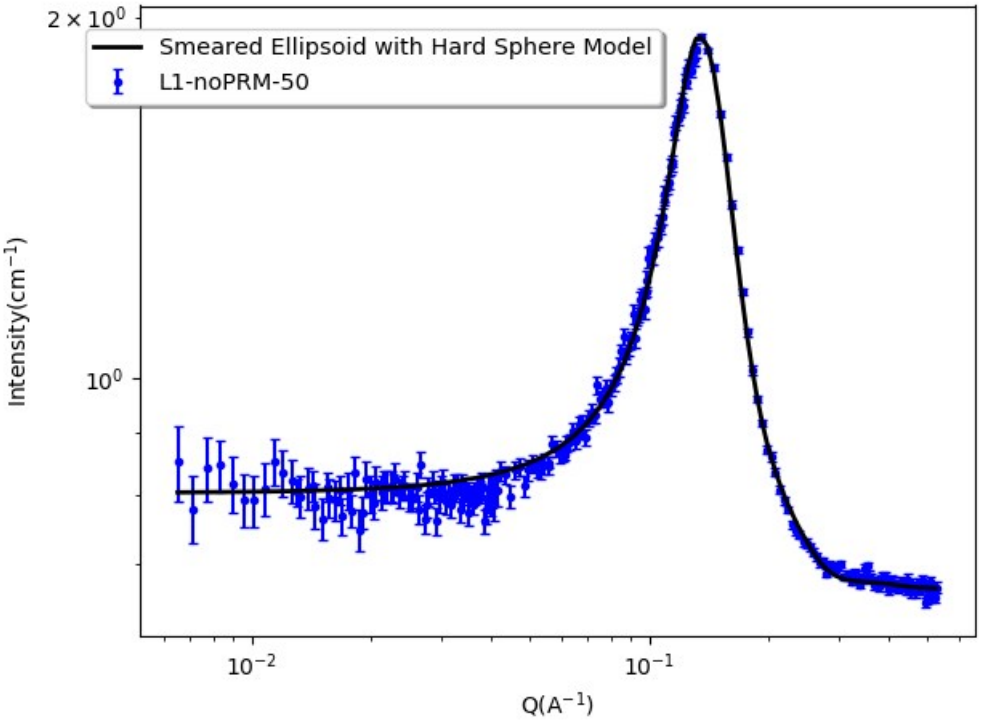
Scale	1	±	0
volume fraction =	0.29366	±	0.00229
R(a) rotation axis (Å) =	9.6221	±	0.45311
R(b) (Å) =	17.495		0.40002
Effective Radius	24.903	±	0.08616
SLD ellipsoid (Å^{-2}) =	4.91E-07	±	0
SLD solvent (Å^{-2}) =	1.86E-06	±	1.90E-08
Incoherent Bgd (cm^{-1})	0.73567	±	0.00116
Fitted Range (Å^{-1})	0.006514	< q <	0.5283
Sqrt(χ^2/N)		1.1200	

MeB-35 (Smeared Ellipsoid with Hard Sphere Model)



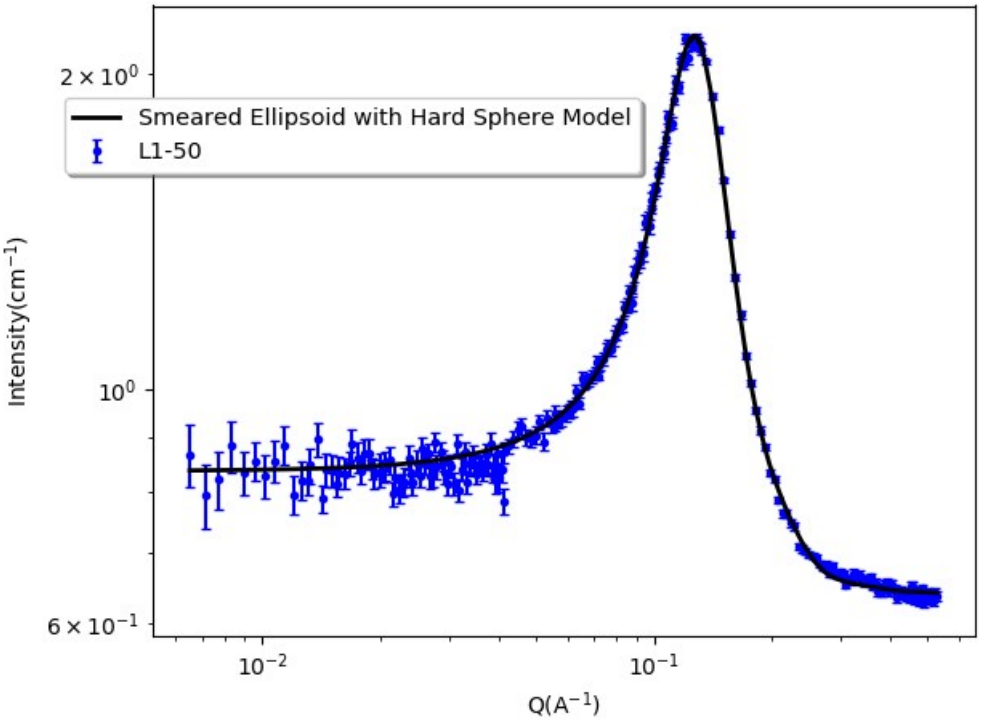
Scale	1	±	0
volume fraction =	0.24981	±	0.0016
R(a) rotation axis (Å) =	10.346	±	0.22918
R(b) (Å) =	22.006		0.26226
Effective Radius	28.58	±	0.06959
SLD ellipsoid (Å^{-2}) =	5.10E-07	±	0
SLD solvent (Å^{-2}) =	2.23E-06	±	1.27E-08
Incoherent Bgd (cm^{-1})	0.76066	±	0.00106
Fitted Range (Å^{-1})	0.006514	< q <	0.5283
Sqrt(χ^2/N)	1.0703		

L1-noPRM-50 (Smeared Ellipsoid with Hard Sphere Model)



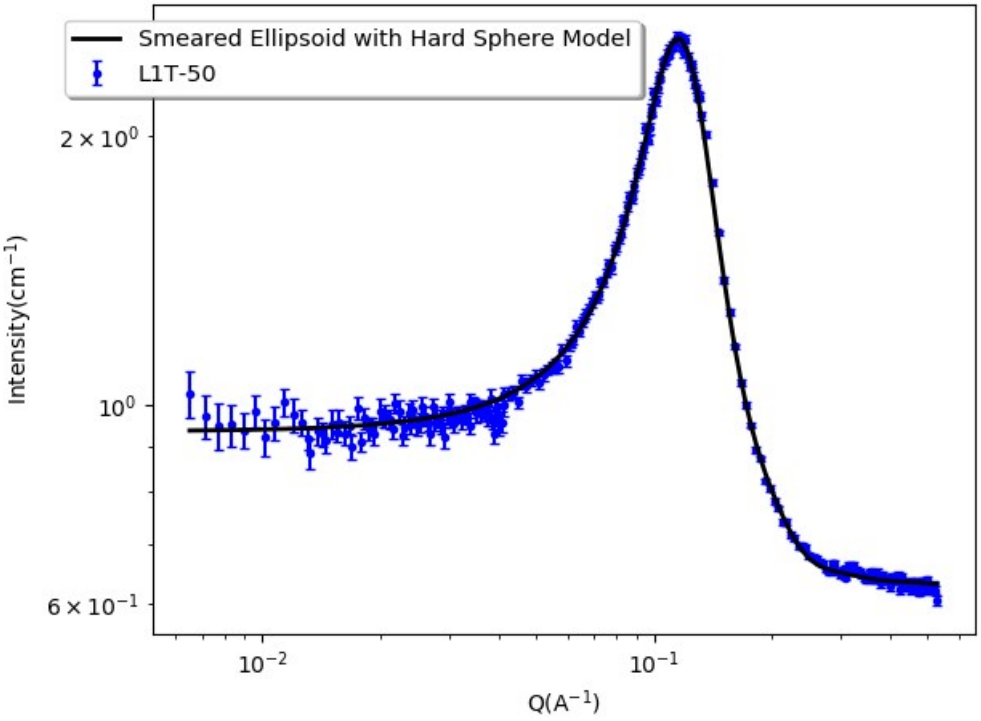
Scale	1.2077	±	0.00951
volume fraction =	0.3431	±	0.00114
R(a) rotation axis (Å) =	10.957	±	0.17708
R(b) (Å) =	17.343		0.1832
Effective Radius	22.86	±	0.02698
SLD ellipsoid (Å^{-2}) =	3.93E-07	±	0
SLD solvent (Å^{-2}) =	2.31E-06	±	0
Incoherent Bgd (cm^{-1})	0.66485	±	0.00102
Fitted Range (Å^{-1})	0.006514	< q <	0.5283
Sqrt(χ^2/N)	1.2808		

L1-50 (Smeared Ellipsoid with Hard Sphere Model)



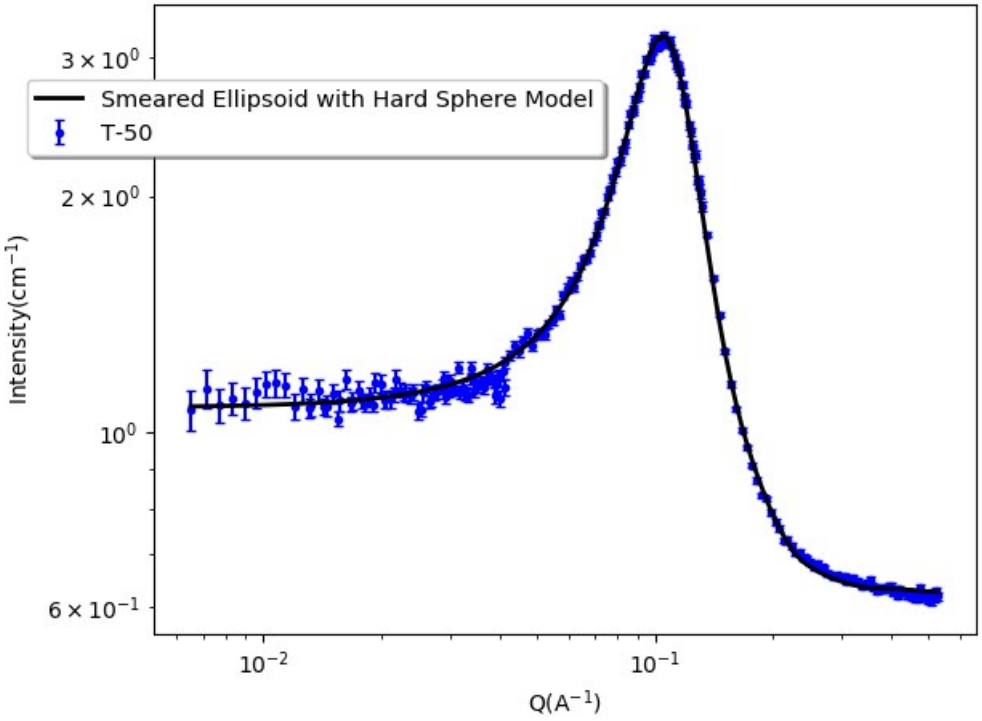
Scale	1.2097	±	0.00774
volume fraction =	0.32731	±	0.00099
R(a) rotation axis (Å) =	11.107	±	0.13259
R(b) (Å) =	18.818		0.15371
Effective Radius	24.026	±	0.02646
SLD ellipsoid (Å^{-2}) =	4.18E-07	±	0
SLD solvent (Å^{-2}) =	2.44E-06	±	0
Incoherent Bgd (cm^{-1})	0.63759	±	0.00095
Fitted Range (Å^{-1})	0.006514	< q <	0.5283
Sqrt(χ^2/N)	1.2961		

L1T-50 (Smeared Ellipsoid with Hard Sphere Model)



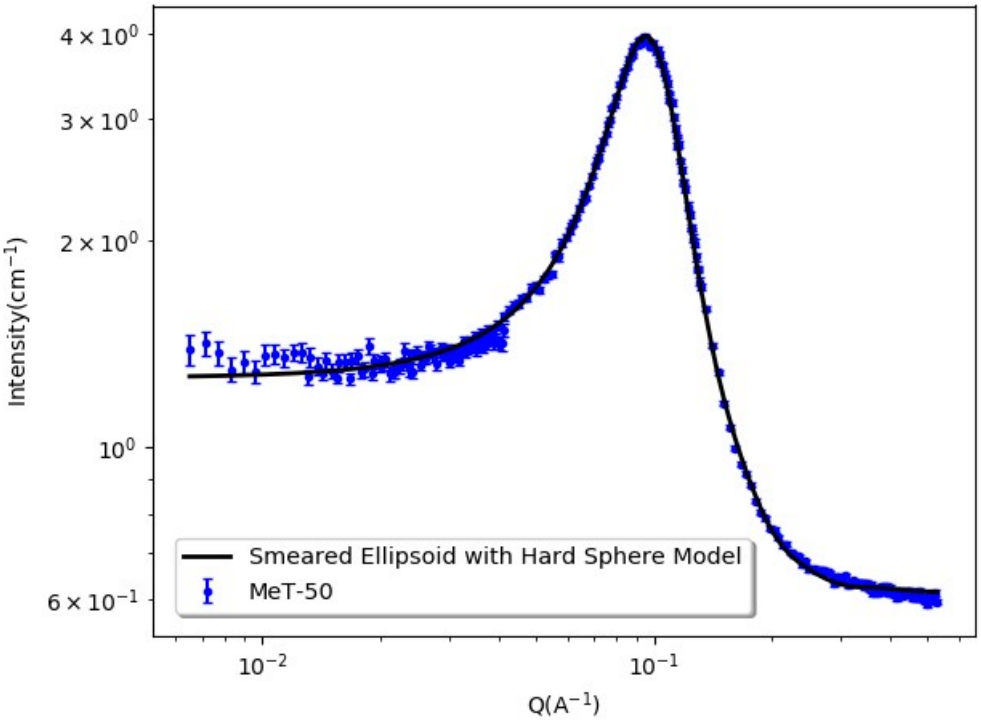
Scale	1.1421	±	0.00573
volume fraction =	0.30802	±	0.00085
R(a) rotation axis (Å) =	12.066	±	0.11273
R(b) (Å) =	20.495		0.13478
Effective Radius	25.915	±	0.02649
SLD ellipsoid (Å^{-2}) =	4.44E-07	±	0
SLD solvent (Å^{-2}) =	2.61E-06	±	0
Incoherent Bgd (cm^{-1})	0.62844	±	0.00087
Fitted Range (Å^{-1})	0.006514	< q <	0.5283
Sqrt(χ^2/N)	1.2480		

T-50 (Smeared Ellipsoid with Hard Sphere Model)



Scale	1.1374	±	0.0048
volume fraction =	0.29687	±	0.00077
R(a) rotation axis (Å) =	12.367	±	0.0862
R(b) (Å) =	22.767		0.11964
Effective Radius	28.273	±	0.02479
SLD ellipsoid (Å^{-2}) =	4.61E-07	±	0
SLD solvent (Å^{-2}) =	2.74E-06	±	0
Incoherent Bgd (cm^{-1})	0.62474	±	0.00082
Fitted Range (Å^{-1})	0.006514	< q <	0.5283
Sqrt(χ^2/N)	1.4004		

MeT-50 (Smeared Ellipsoid with Hard Sphere Model)



Scale	1.1006	±	0.00386
volume fraction =	0.28864	±	0.00069
R(a) rotation axis (Å) =	13.055	±	0.07025
R(b) (Å) =	25.245		0.10843
Effective Radius	30.716	±	0.02404
SLD ellipsoid ($Å^{-2}$) =	4.75E-07	±	0
SLD solvent ($Å^{-2}$) =	2.86E-06	±	0
Incoherent Bgd (cm^{-1})	0.61293	±	0.00079
Fitted Range ($Å^{-1}$)	0.006514	< q <	0.5283
Sqrt(χ^2/N)	1.5934		