Supporting Information for

Bowl-in-bowl complex formation with mixed sized calixarenes: Adaptivity towards guest binding

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Materials, Methods and Instruments

C-methylresorcin[4]arene is synthesized following the literature method.[1] Calix[6]arene was purchased from TCI. Calix[8]arene and 4-aminobiphenyl were purchased from Aldrich. DMSO was purchased from Fisher Scientific. DMSO-d_6 and D_2O were purchased from Cambridge Isotope Laboratories. NMR spectra were recorded in a Bruker AV 400 MHz spectrometer,

1. a) L. M. Tunstad, J. A. Tucker, E. Dalcanale, J. Weiser, J. A. Bryant, J. C. Sherman, R. C. Helgeson, C. B. Knobler, D. J. Cram, *J. Org. Chem.* **1989**, *54*, 1305. b) I. Elidrisi, S. Negin, P. V. Bhatt, T. Govender, H. G. Kruger, G. W. Gokel, G. E. M. Maguire, *Org. Biomol. Chem.* **2011**, *9*, 4498.

Note on PMF calculation:

All PMFs were computed with the larger Macrocycle restrained to the center of the simulation box, and the approaching macrocycle restrained to movement in the z direction. This is to ensure convergence within a reasonable amount of time. This choice of reaction coordinate limits the sampling (motions along other directions) but is a reasonable choice on physical grounds. For all the PMF estimates a total of 40 symmetrical windows were used. Histograms necessary for the WHAM were generated using 200 bins of width 0.0125 nm. Each window was simulated for a total of 6 ns with 0.5 ns removed from analysis for equilibration, and the remaining 5.5 ns used for WHAM analysis.

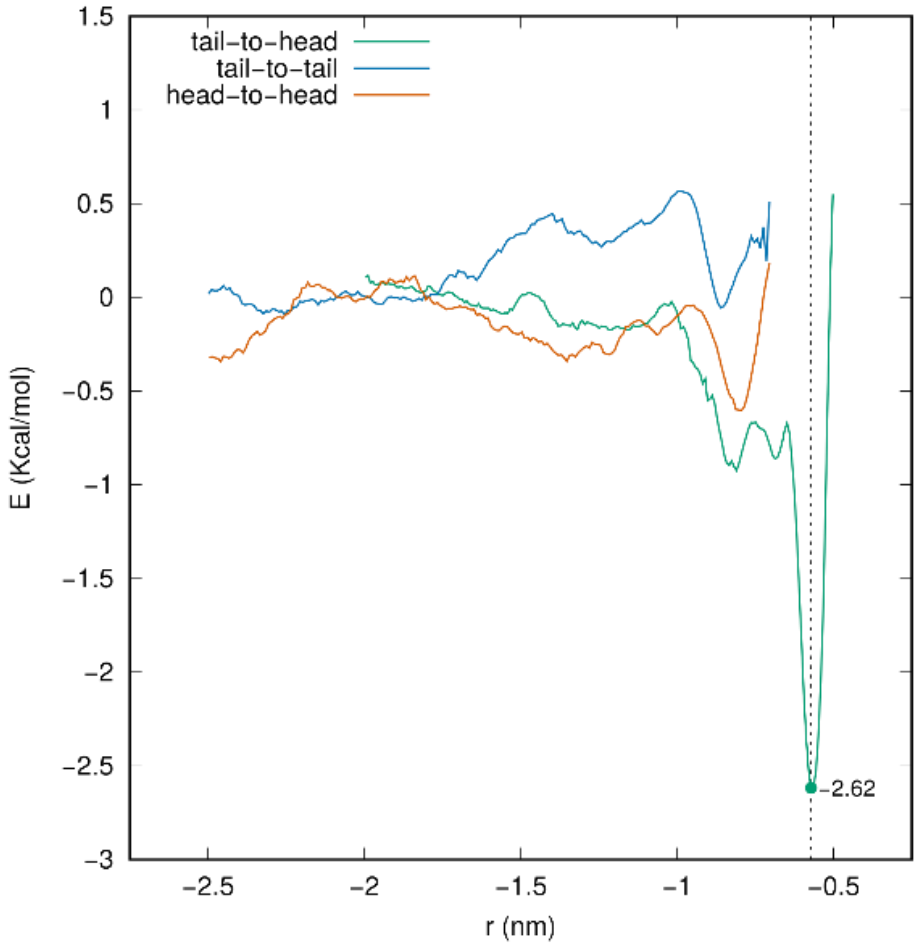


Figure S1. Comparative hypothesized interactions involving various arrangements between RsC1 and Calix6.

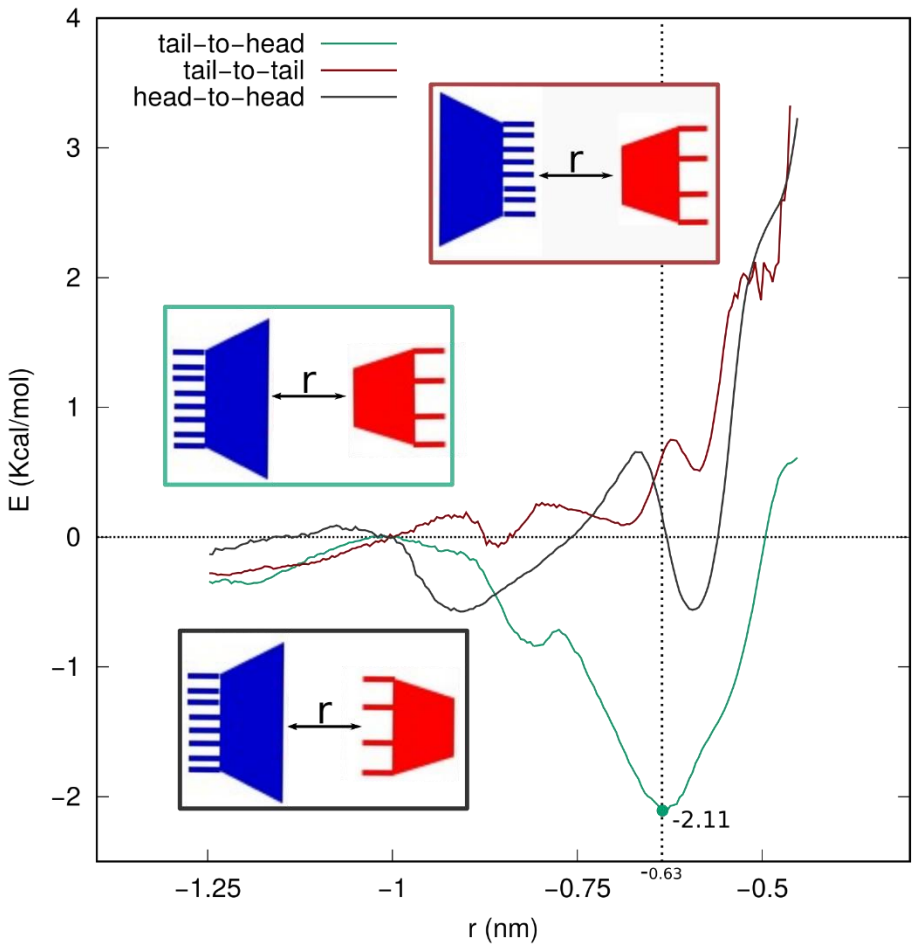


Figure S2. Comparative hypothesized interactions involving various arrangements between RsC1 and Calix8.

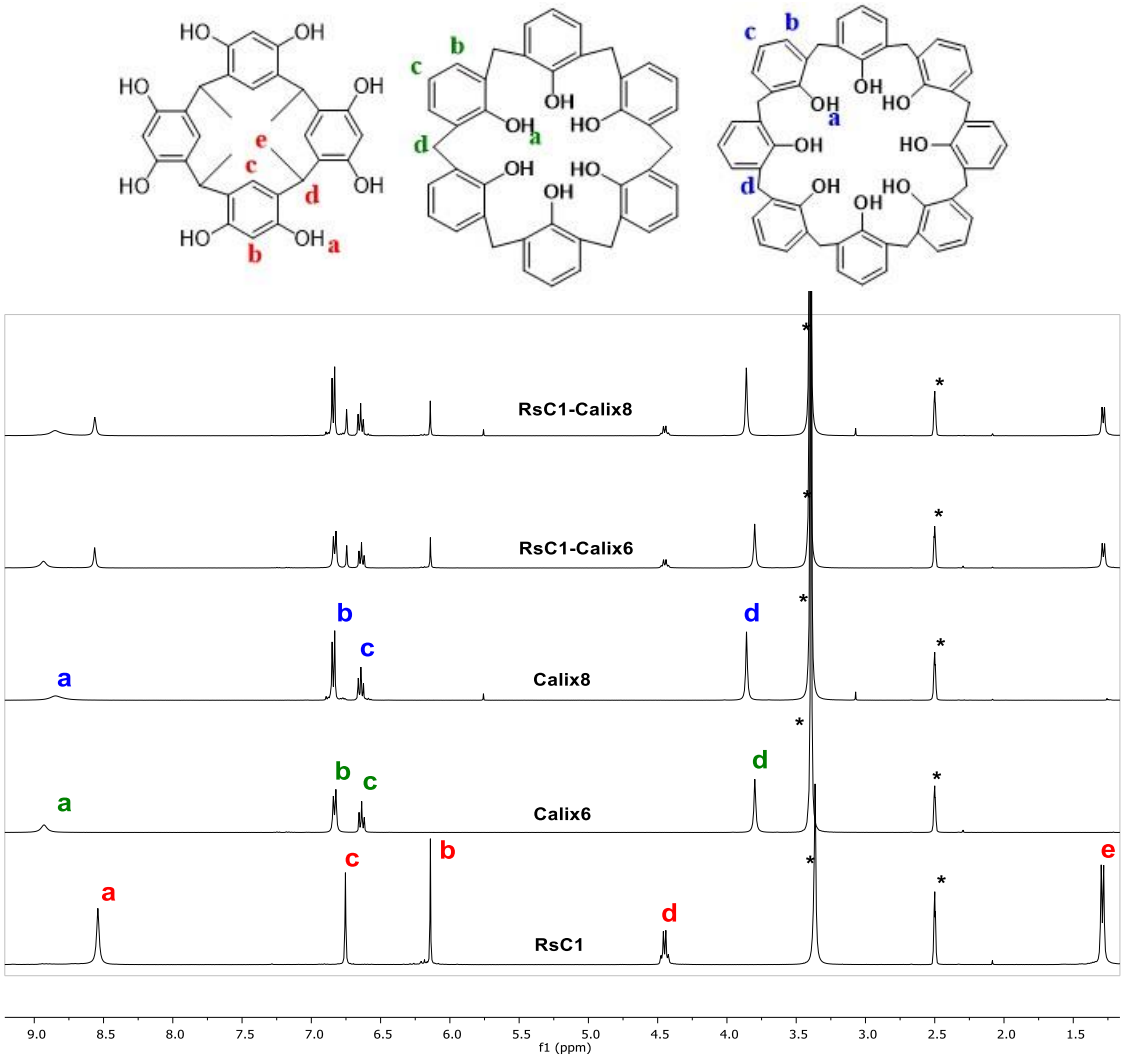


Figure S3. ^{1}H NMR spectra of the samples in DMSO-d_6, prepared at RT.

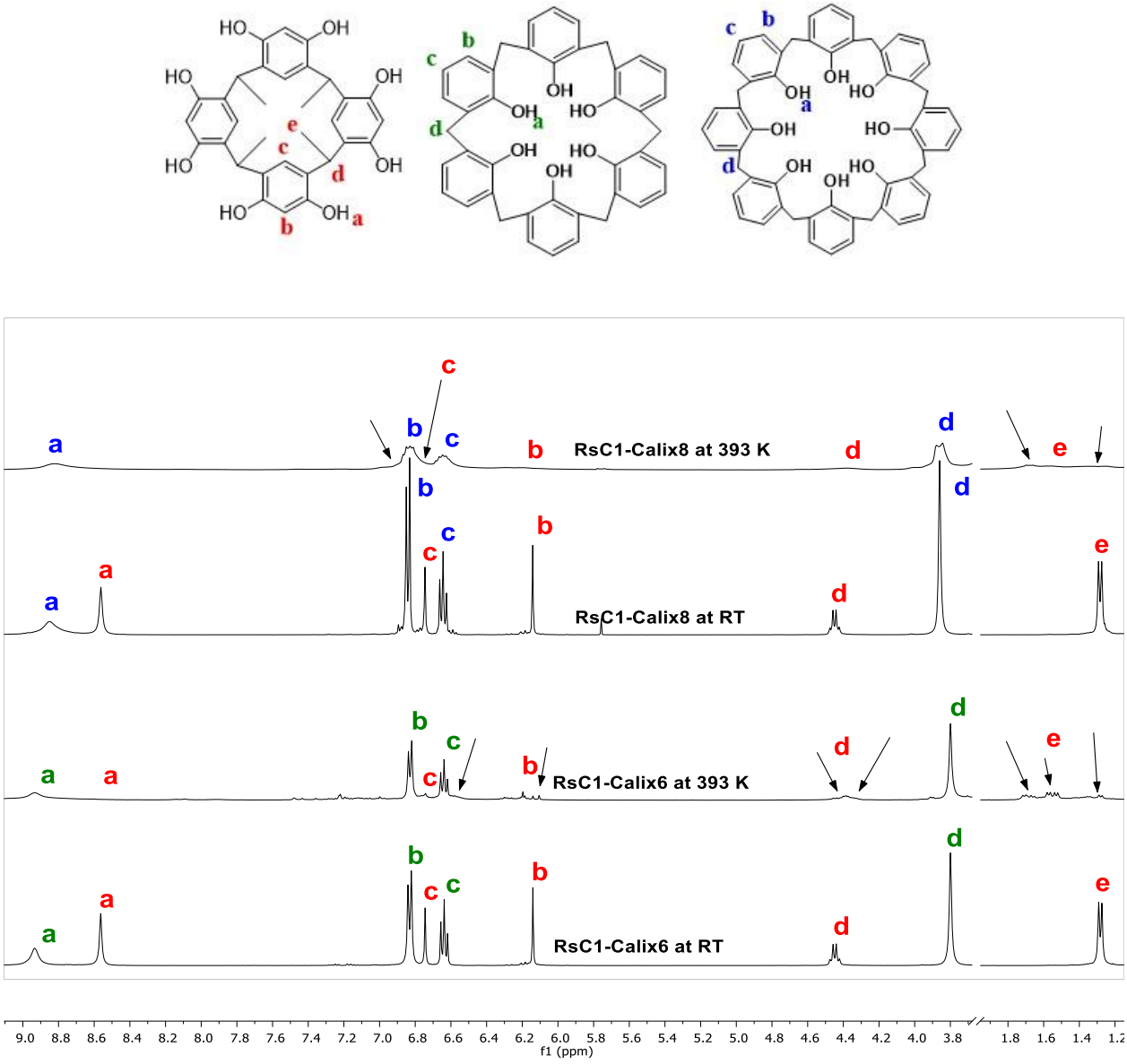


Figure S4. ^{1}H NMR spectra of the samples in DMSO-d_6 containing differently sized macrocycles, prepared at various temperatures.

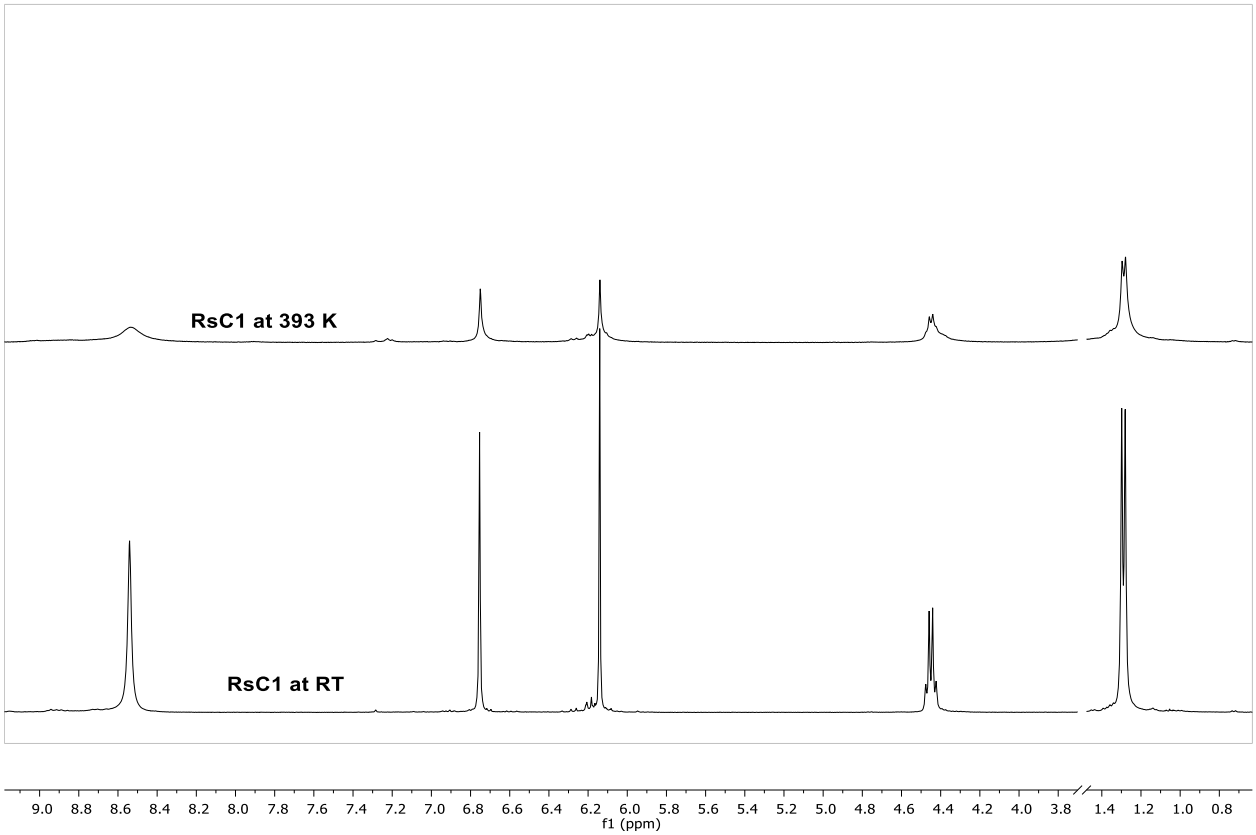


Figure S5. ^{1}H NMR spectra of RsC1in DMSO-d_6, prepared at different temperatures.

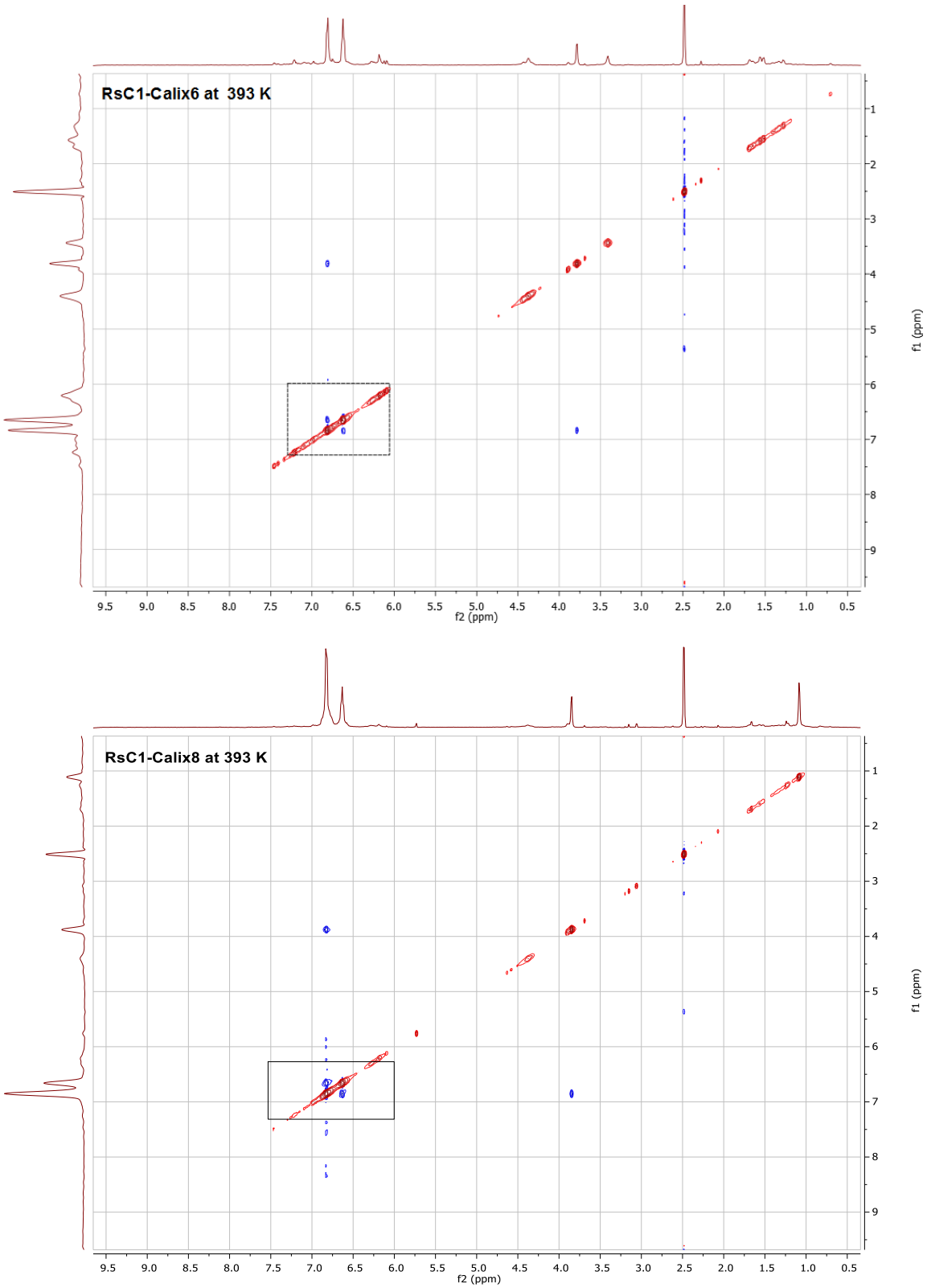


Figure S6. ROESY NMR spectra of RsC1-Calix6 and RSC1-Calix8 in DMSO-d_6, prepared at 393 K. The dotted rectangles indicate the area of the spectra highlighting the interaction between two different macrocycles (presented in Figure 3 of the main text).

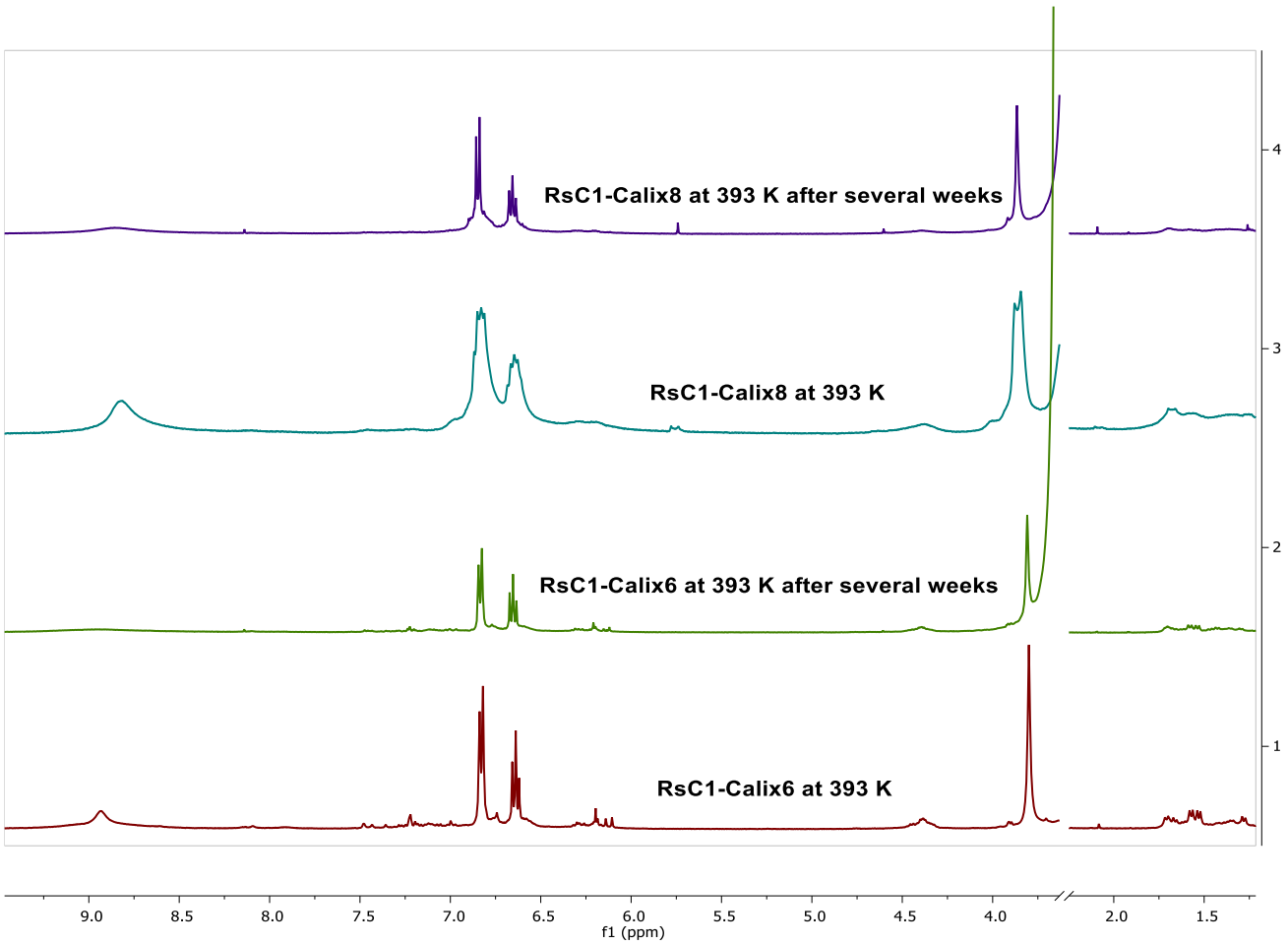


Figure S7. ^{1}H NMR spectra of RsC1-Calix6 and RsC1-Calix8 in DMSO-d_6 prepared at 393 K, with aging time at room tempearture.

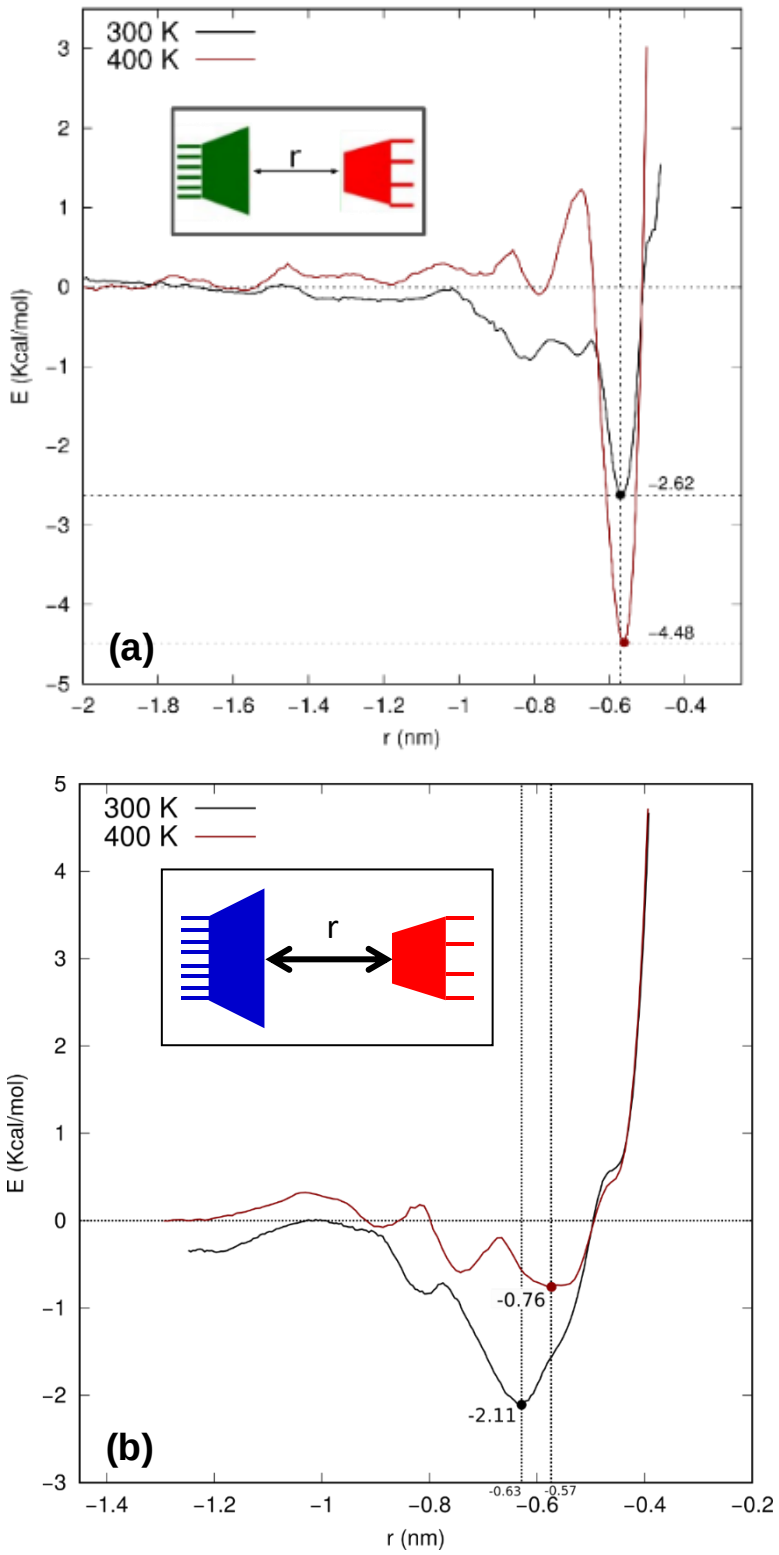


Figure S8. Comparison of PMFs at 300 K and 400 K: (a) RsC1-Calix6 (TH), (b) RsC1-Calix8 (TH).

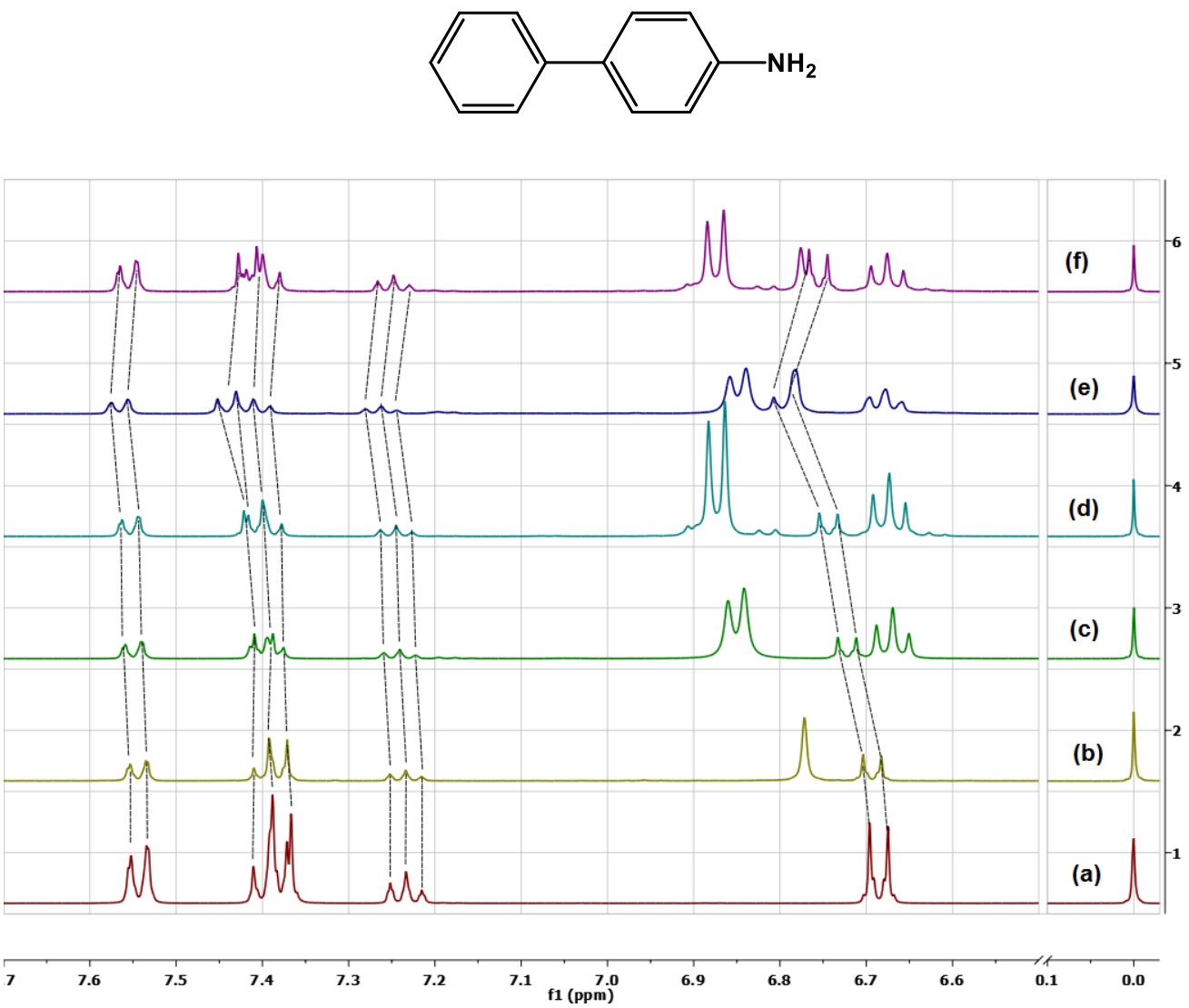


Figure S9. Structure of 4-Aminobiphenyl (ABP) and partial ^{1}H NMR spectra of ABP and various host-guest complexes of ABP in DMSO-d_6 / D_2O (4:1, v/v): (a) ABP, (b) ABP-RsC1 (1:1 by mole), (c) ABP-Calix6 (1:1 by mole), (d) ABP-Calix8 (1:1 by mole), (e) ABP-RsC1-Calix6 (1:0.5:0.5 by mole), (f) ABP-RsC1-Calix8 (1:0.5:0.5 by mole). Shifts of aromatic protons of ABP upon complexation have been marked).

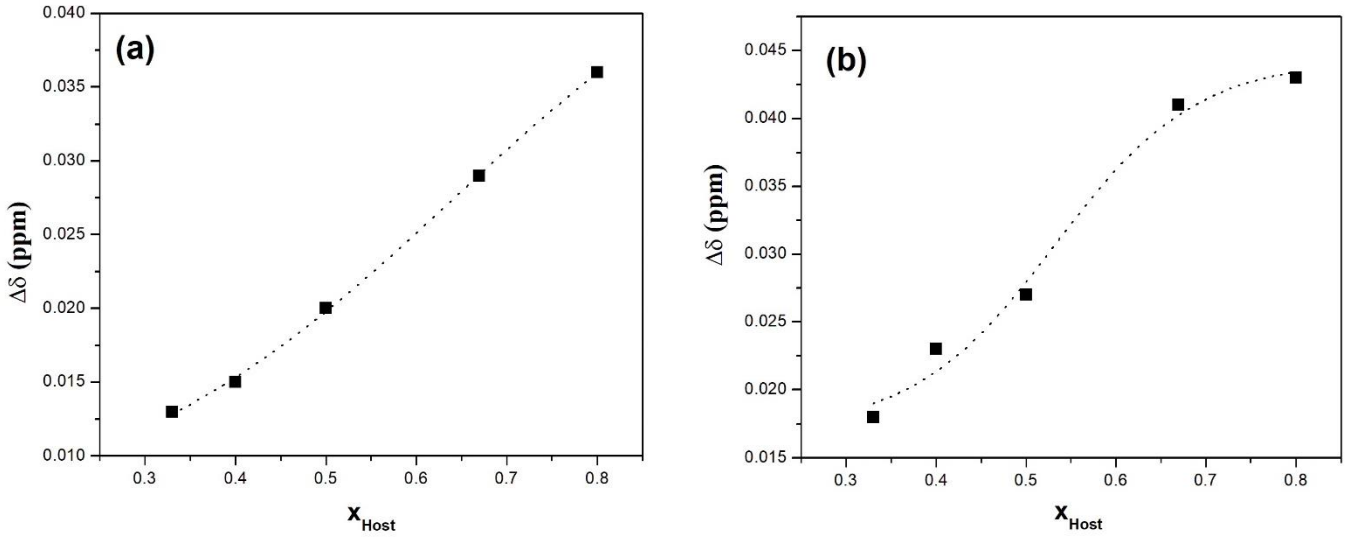


Figure S10. Plot of change in chemical shifts associated with the aromatic proton of ABP with increasing mole fraction of the hosts: (a) RsC1-Calix6 and (b) RsC1-Calix8. The ^{1}H NMR experiments were done in DMSO-d_6 / D_2O (4:1, v/v).

Stoichiometries of the host-guest complexes of RsC1-Calix6 or RsC1-Calix8 with ABP are not clear from the above plots. This is probably because of the multiple equilibria involved in these systems. In bowl-in-bowl systems we can not rule out the presence of an equilibrium between supramolecularly held macrocycles. In presence of a guest, a host-guest equilibrium can be influenced by the host-host equilibrium. In addition, there might be local equilibria between a single bowl with the guest. Therefore, the relation is no longer straightforward. As evident from Fig. S10 such an abnormality is more prominent in case of RsC1-Calix6 system. This is reasonable considering the adaptive nature of RsC1-Calix6 system as discussed in the manuscript. Therefore, further studies on conformational and structural features and associated kinetic and thermodynamic aspects of the bowl-in bowl systems in presence and in absence of the guest molecule, are necessary before we can quantify the association behavior of these unique host-guest systems.

SANS Data for RsC1-Calix6 and RsC1-Calix8 at room temperature and 393 K

Sample Preparation:

The SANS samples RsC1-Calix6 and RsC1-Calix8 were prepared in DMSO-d_6 in the same manner as the ^{1}H-NMR samples. Approximately 0.4 mL of sample was injected into an assembled titanium cell holder with a 1 mm path length and quartz windows. Viton gaskets between the windows and the sides were used to minimize leakage. The filled cell holders were then sealed with a screw wrapped with Teflon tape and another gasket. The holders sat overnight before being placed in the instrument to ensure there was no excessive leakage; any void in the holder that formed during that time was filled by topping off with more sample.

SANS data were collected at 25°C. The scattering data were first corrected for background scattering and sample transmission, and then the reduced data sets were analyzed with Igor Pro analysis macros provided by NIST.[1] Smeared models were used in fitting the data to further correct for the detector resolution and other effects introduced by the instrument geometry. The form factor models tested were Power Law + Sphere, Power Law + Bimodal Schulz Sphere, Power Law + Ellipsoid, and Power Law + Cylinder, with the Power Law model being included in the form factor model to account for the increased low-Q scattering.

The scattering length densities (SLDs) of the solvent and scattering objects were held constant for all fits. The uncertainty for each parameter is +/- one standard deviation; if this value is 0, then that parameter was held constant during the fitting. See below for a short discussion of each model pointing out features that led to their acceptance or dismissal. Fitting to different models suggested that the Power Law + Sphere model is the best fit for all samples (Table S2).

Table S1: Parameters for SLD Calculation

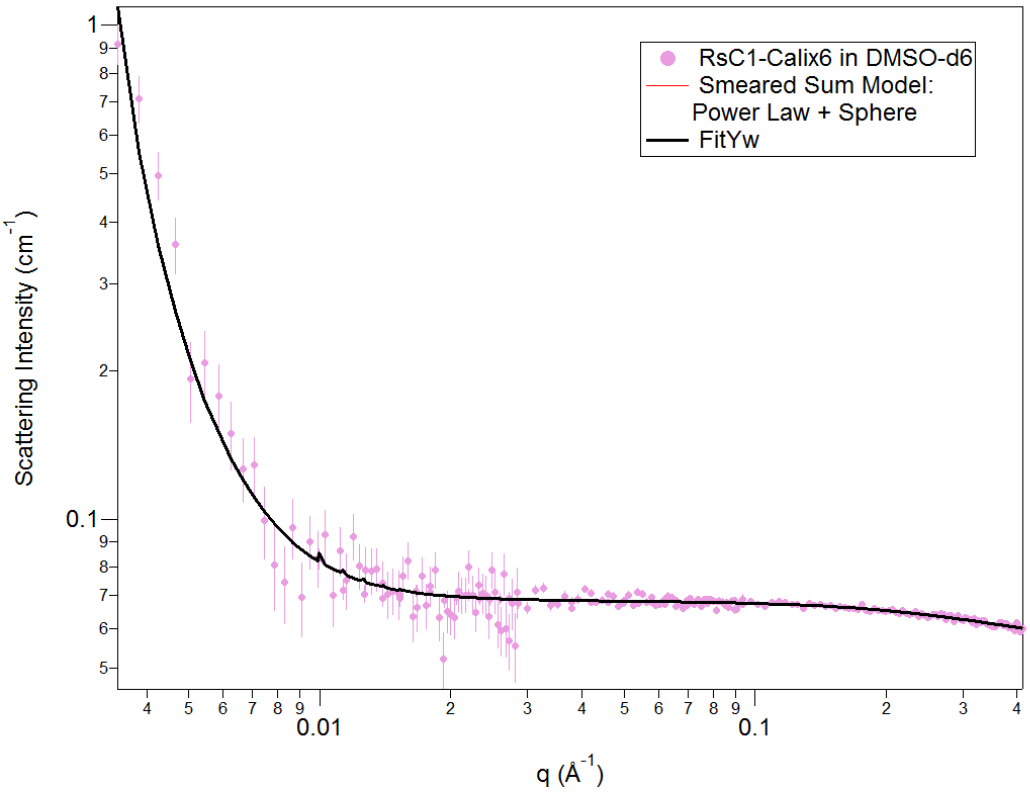
Sample	**Molecular Formula**	**Density (g/mL)**	**Neutron Wavelength (Å)**	**SLD (Å^{-2})**
RsC1	$C_{32}O_8H_{32}$	1.1	6	1.697e-6
Calix[6]arene	$C_{42}O_6H_{36}$	1.3	6	2.206e-6
Calix[8]arene	$C_{56}O_8H_{48}$	1.3	6	2.206e-6
RsC1-Calix6	$C_{74}O_{14}H_{68}$	1.2	6	1.964e-6
RsC1-Calix8	$C_{88}O_{16}H_{80}$	1.2	6	1.998e-6
DMSO	C_2H_6OS	1.1	6	-0.042e-6

[1]S. R. Kline, *J. Appl. Crystallogr.* **2006,** *39*, 895-900.

Table S2. SANS fitting results to Sphere+Power law model for RsC1-Calix6 and RsC1-Calix8 at various temperatures

Sample	Radius (Å)	St. Dev. (± Å)
RsC1-Calix6 at RT	6.504	0.429
RsC1-Calix6 at 393 K	5.910	0.371
RsC1-Calix8	7.473	0.182
RsC1-Calix8 at 393 K	7.525	0.191

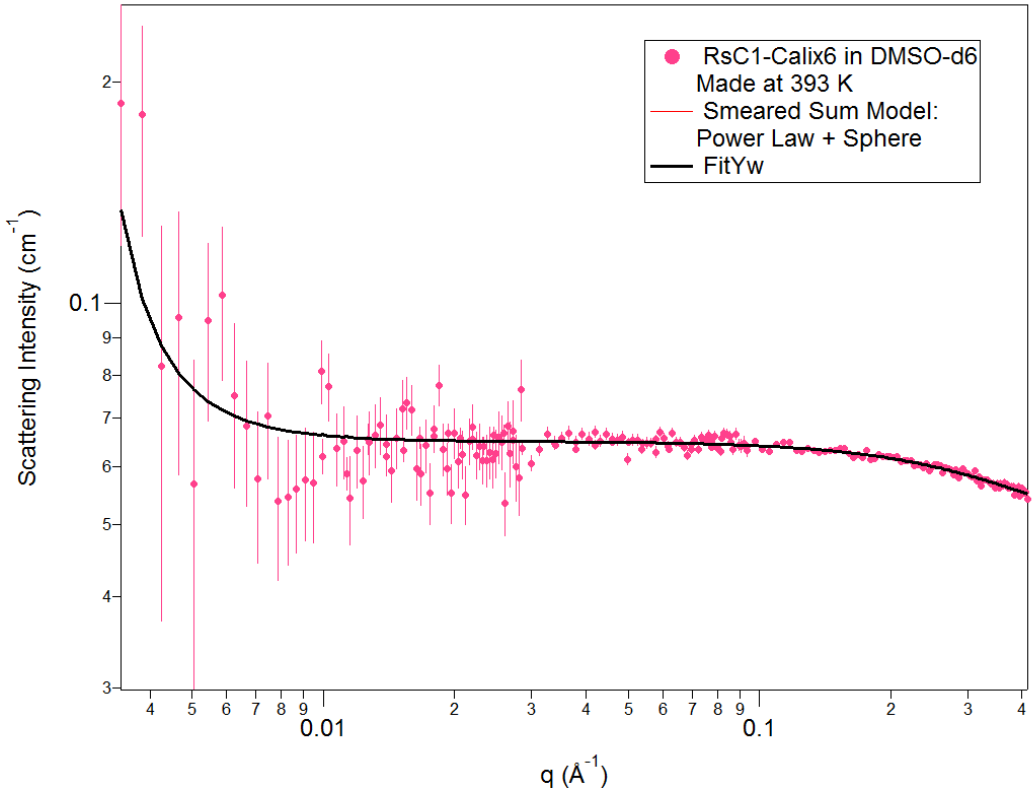
RsC1-Calix6 in DMSO-d_6 (Power Law + Sphere Model)



Coefficient, A =	7.54275e-09	±	3.00229e-09
(-)Power =	3.11039	±	0.0672835
Incoherent Bgd (cm^{-1}) =	0	±	0
scale =	0.0221261	±	0.00591034
Radius (Å) =	6.50427	±	0.429039
SLD sphere ($Å^{-2}$) =	1.964e-06	±	0
SLD solvent ($Å^{-2}$) =	-4.2e-08	±	0
bkgd (cm^{-1}) =	0.0581236	±	0.000800202
Sqrt(χ^2/N) =	1.04636		
Fitted Range =	0.003433	< Q <	0.4054

The returned values are physically reasonable given the size and amounts of the macrocycles used in the sample. The standard deviations for all parameters that were allowed to vary are very small compared to the value returned, and the Sqrt(χ^2/N) of 1.046 is very good. Overall, there was no reason to discount this model.

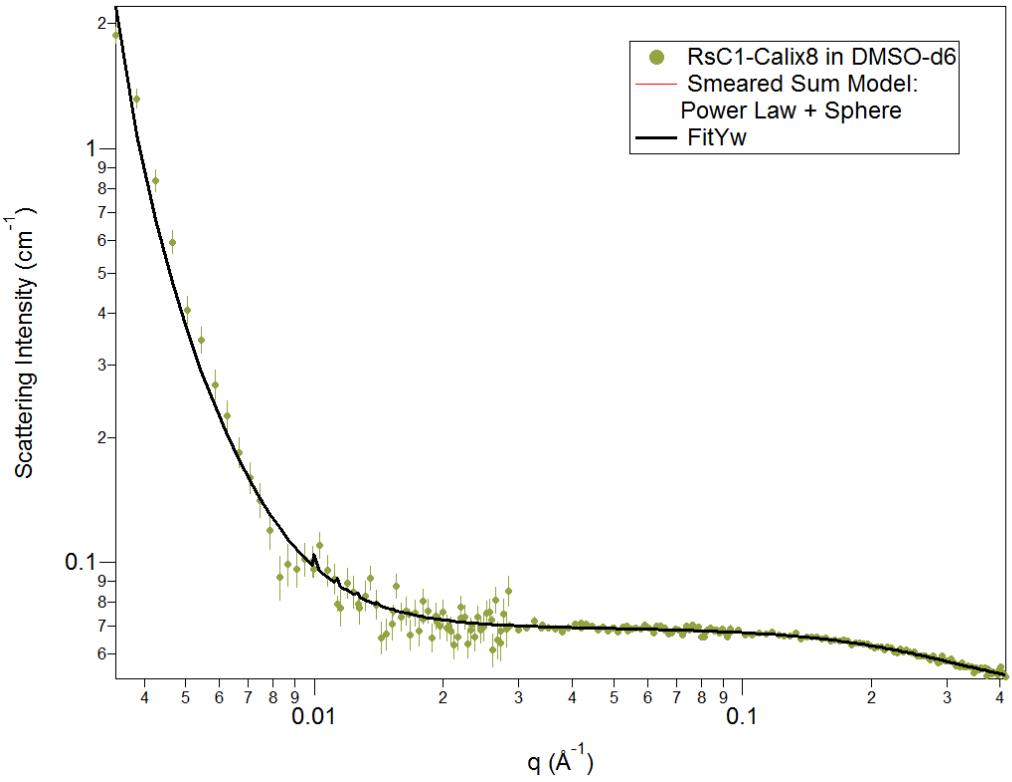
RsC1-Calix6 in DMSO-d_6 Made at 393 K (Power Law + Sphere):



Coefficient, A =	1.176e-09	±	0
(-)Power =	2.99038	±	0.0948936
Incoherent Bgd (cm^{-1}) =	0	±	0
scale =	0.0389846	±	0.0103054
Radius (Å) =	5.90982	±	0.371788
SLD sphere ($Å^{-2}$) =	1.964e-06	±	0
SLD solvent ($Å^{-2}$) =	-4.2e-08	±	0
bkgd (cm^{-1}) =	0.0514216	±	0.00110595
Sqrt(χ^2/N) =	1.02356		
Fitted Range =	0.003433	< Q <	0.4054

The returned values are physically reasonable given the size and amounts of the macrocycles used in the sample. The standard deviations for all parameters that were allowed to vary are small compared to the value returned, and the Sqrt(χ^2/N) of 1.024 is very good. Overall, there was no reason to discount this model.

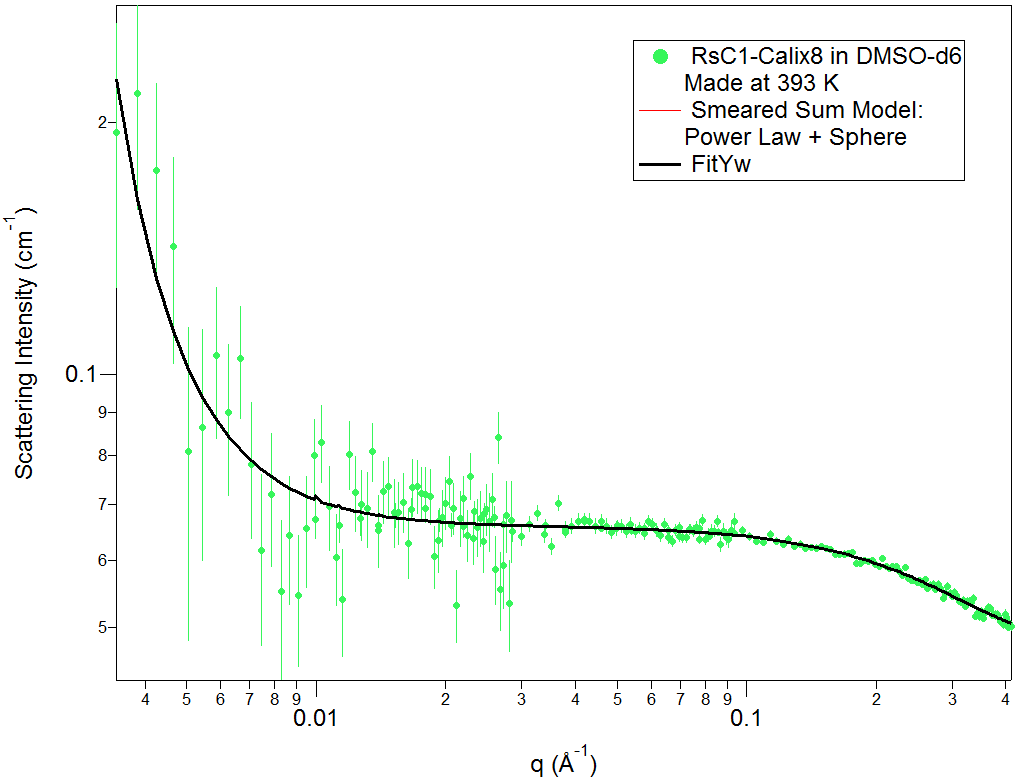
RsC1-Calix8 in DMSO-d6 (Power Law + Sphere):



Coefficient, A =	1.52524e-08	±	2.75068e-09
(-)Power =	3.11502	±	0.0309076
Incoherent Bgd (cm^{-1}) =	0	±	0
scale =	0.0246281	±	0.00228372
Radius (Å) =	7.47369	±	0.181528
SLD sphere ($Å^{-2}$) =	1.998e-06	±	0
SLD solvent ($Å^{-2}$) =	-4.2e-08	±	0
bkgd (cm^{-1}) =	0.0515753	±	0.000442487
Sqrt(χ^2/N) =	1.15554		
Fitted Range =	0.003433	< Q <	0.4121

The returned values are physically reasonable given the size and amounts of the macrocycles used in the sample. The standard deviations for all parameters that were allowed to vary are very small compared to the value returned, and the Sqrt(χ^2/N) of 1.155 is very good. Overall, there was no reason to discount this model.

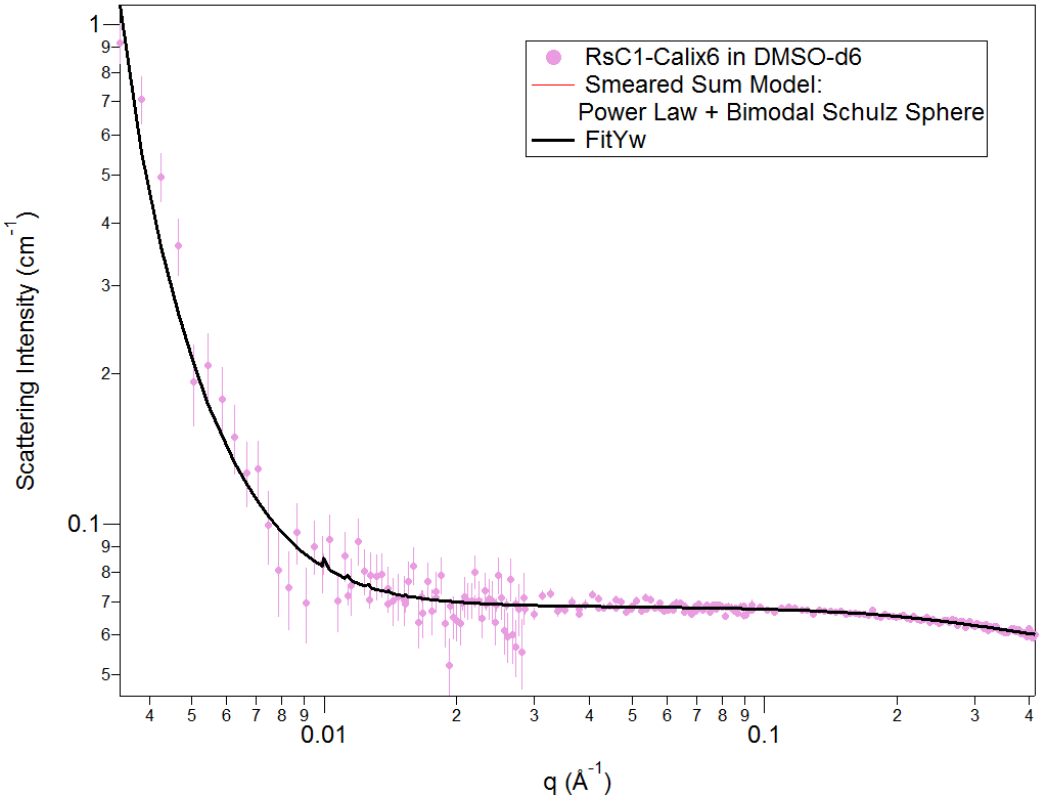
RsC1-Calix8 in DMSO-d6 Made at 393 K (Power Law + Sphere):



Coefficient, A =	2.06805e-08	±	2.771e-08
(-)Power =	2.67455	±	0.249406
Incoherent Bgd (cm^{-1}) =	0	±	0
scale =	0.0232226	±	0.00223561
Radius (Å) =	7.52496	±	0.191412
SLD sphere ($Å^{-2}$) =	1.998e-06	±	0
SLD solvent ($Å^{-2}$) =	-4.2e-08	±	0
bkgd (cm^{-1}) =	0.0487309	±	0.000439704
Sqrt(χ^2/N) =	0.983793		
Fitted Range =	0.003433	< Q <	0.4121

The returned values are physically reasonable given the size and amounts of the macrocycles used in the sample. The standard deviations for all parameters that were allowed to vary are very small compared to the value returned, and the Sqrt(χ^2/N) of 0.9838 is very good. The only exception to this is the standard deviation for the Coefficient A parameter, which is the scaling value for the Power Law model that was used to model the low-Q scattering region. The large standard deviation is most likely due to the poor data statistics of that particular region. Overall, there was no strong reason to discount this model.

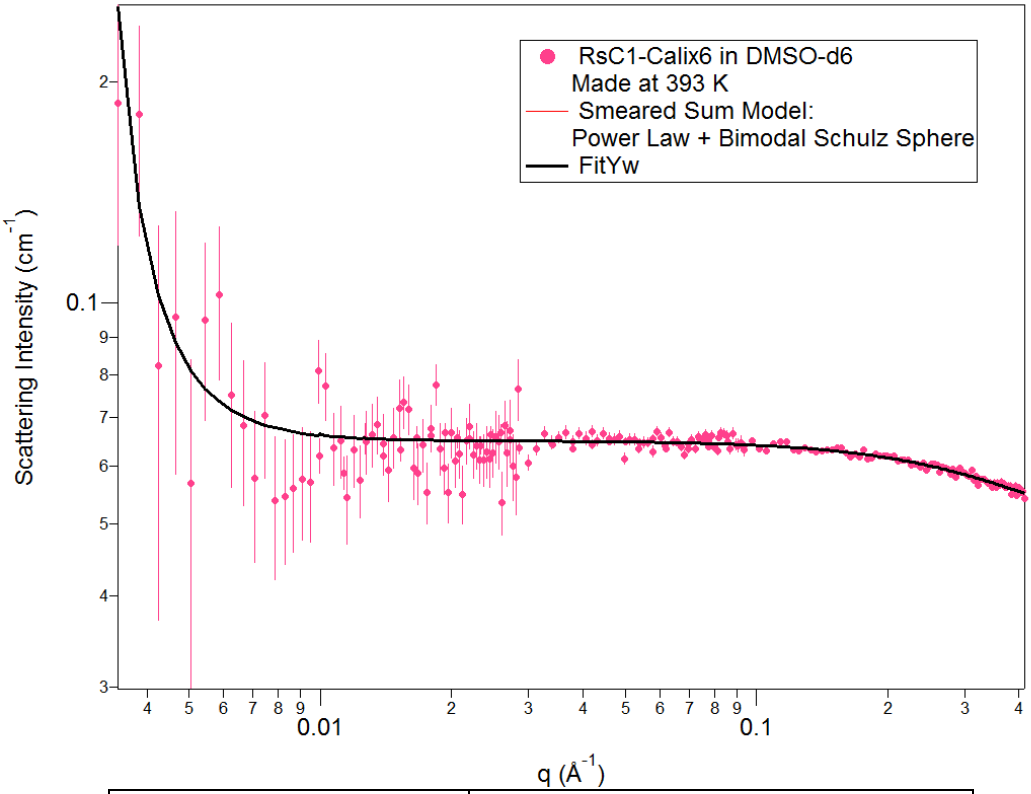
RsC1-Calix6 in DMSO-d6 (Power Law + Bimodal Schulz Sphere Model)



Coefficient, A =	7.477e-09	±	3.04698e-09
(-)Power =	3.11183	±	0.0687749
Incoherent Bgd (cm^{-1}) =	0	±	0
volume fraction(1) =	0.00687569	±	0.0250378
Radius (1) (Å) =	5.29998	±	3.03494e-05
polydispersity(1) =	0.00999994	±	9.34134e-08
SLD(1) ($Å^{-2}$) =	1.697e-06	±	0
volume fraction(2) =	0.0149318	±	0.00599932
Radius (2) =	6.6	±	8.23308e-06
polydispersity(2) =	0.0100001	±	7.70899e-09
SLD(2) =	2.206e-06	±	0
SLD (solvent) =	-4.2e-08	±	0
background (cm^{-1}) =	0.0579843	±	0.00117215
Sqrt(χ^2/N) =	1.04633		
Fitted Range =	0.003433	< Q <	0.4121

For the most part, the standard deviations are quite low compared to their respective parameters in addition to the small Sqrt(χ^2/N) value of 1.046. However, the volume fraction for the first size population (representing RsC1) is unrealistically low considering the actual volume fraction of RsC1 in the sample. This is further supported by its much larger standard deviation. Additionally, the radii for the two size populations did not seem to be fitted—any random entry remained unchanged with low standard deviations after fitting. For these reasons, this model was discounted for this data.

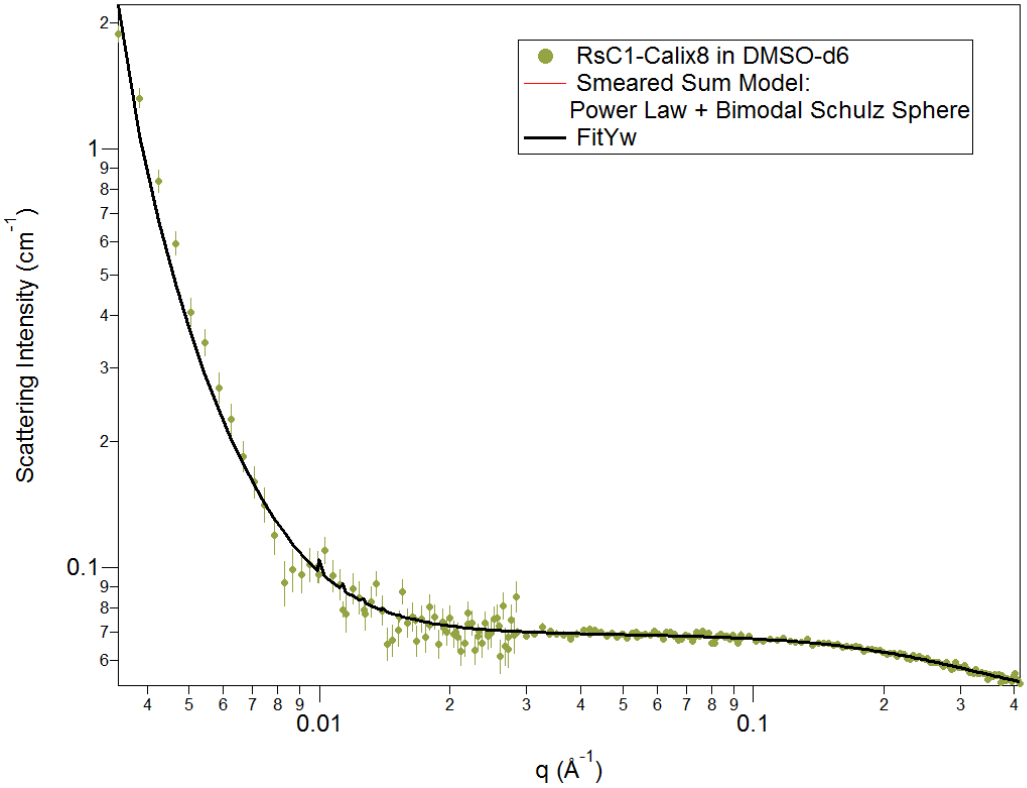
RsC1-Calix6 in DMSO-d6 Made at 393 K (Power Law + Bimodal Schulz Sphere):



Coefficient, A =	3.83067e-11	±	1.81275e-10
(-)Power =	3.57605	±	0.716107
Incoherent Bgd (cm^{-1}) =	0	±	0
volume fraction(1) =	0.0465449	±	0.0234558
Radius (1) (Å) =	5.3	±	6.27033e-06
polydispersity(1) =	0.01	±	8.3231e-09
SLD(1) ($Å^{-2}$) =	1.697e-06	±	0
volume fraction(2) =	0.00858608	±	0.00560504
Radius (2) =	6.60003	±	1.95856e-05
polydispersity(2) =	0.00999997	±	1.26916e-08
SLD(2) =	2.206e-06	±	0
SLD (solvent) =	-4.2e-08	±	0
background (cm^{-1}) =	0.0509707	±	0.00110329
Sqrt(χ^2/N) =	1.01666		
Fitted Range =	0.003433	< Q <	0.4121

For the most part, the standard deviations are quite low compared to their respective parameters in addition to the small Sqrt(χ^2/N) value of 1.017. However, the volume fraction for the first size population (representing RsC1) is unrealistically high considering the actual volume fraction of RsC1 in the sample. Likewise, the volume fraction for the second size population (representing Calix6) is unrealistically low considering the actual volume fraction of Calix6. This is further supported by their relatively large standard deviations. The total volume fraction (the sum of the two) is also larger than the actual total volume fraction of the sample. Additionally, the radii for the two size populations did not seem to be fitted—any random entry remained unchanged with low standard deviations after fitting. For these reasons, this model was discounted for this data.

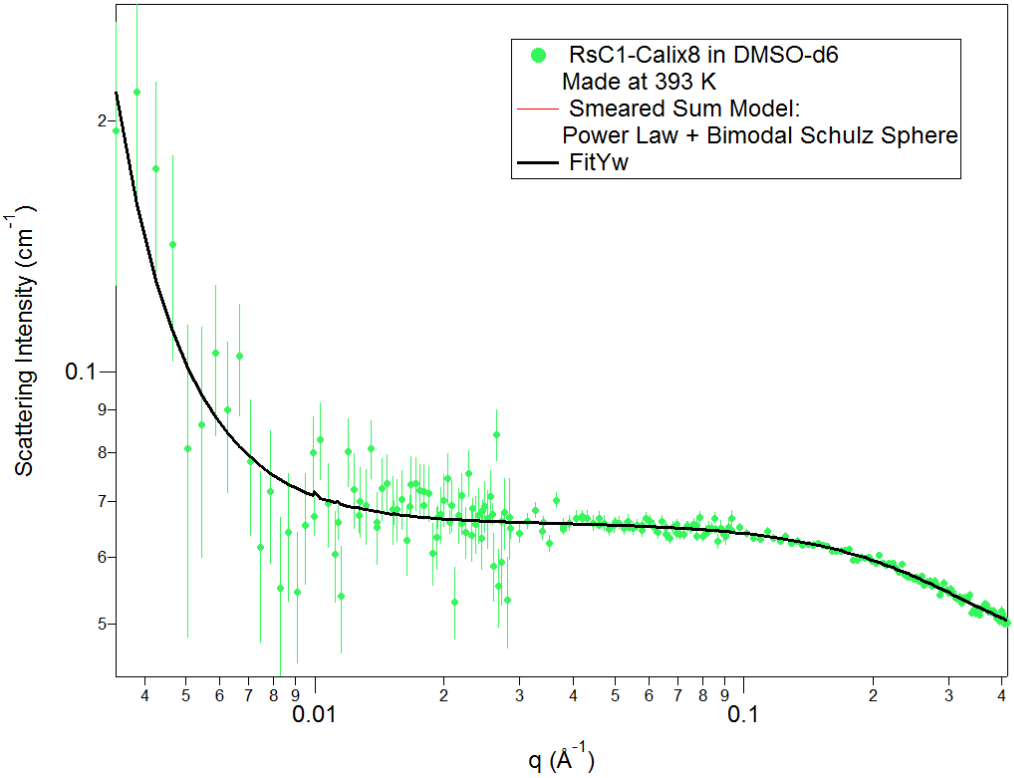
RsC1-Calix8 in DMSO-d6 (Power Law + Bimodal Schulz Sphere):



Coefficient, A =	1.50986e-08	±	2.73017e-09
(-)Power =	3.11666	±	0.0309768
Incoherent Bgd (cm^{-1}) =	0	±	0
volume fraction(1) =	0.0468596	±	0.00881872
Radius (1) (Å) =	5.3	±	3.70312e-06
polydispersity(1) =	0.01	±	6.76207e-09
SLD(1) ($Å^{-2}$) =	1.697e-06	±	0
volume fraction(2) =	0.00872055	±	0.000846037
Radius (2) =	8.4	±	7.44707e-06
polydispersity(2) =	0.01	±	1.08259e-08
SLD(2) =	2.206e-06	±	0
SLD (solvent) =	-4.2e-08	±	0
background (cm^{-1}) =	0.04973	±	0.000698704
Sqrt(χ^2/N) =	1.15828		
Fitted Range =	0.003433	< Q <	0.4121

For the most part, the standard deviations are quite low compared to their respective parameters in addition to the small Sqrt(χ^2/N) value of 1.158. However, the volume fraction for the first size population (representing RsC1) is unrealistically high considering the actual volume fraction of RsC1 in the sample. Likewise, the volume fraction for the second size population (representing Calix8) is unrealistically low considering the actual volume fraction of Calix8. The total volume fraction (the sum of the two) is also larger than the actual total volume fraction of the sample. Additionally, the radii for the two size populations did not seem to be fitted—any random entry remained unchanged with low standard deviations after fitting. For these reasons, this model was discounted for this data.

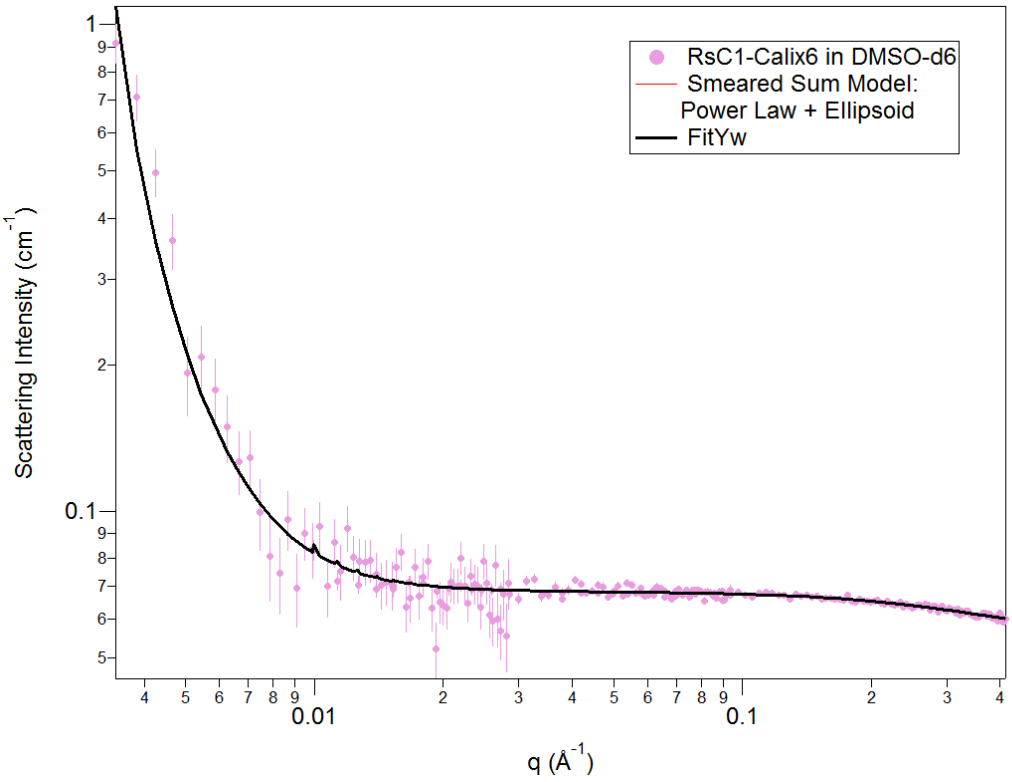
RsC1-Calix8 in DMSO-d6 Made at 393 K (Power Law + Bimodal Schulz Sphere):



Coefficient, A =	2.66086e-08	±	0
(-)Power =	2.62711	±	0.0355613
Incoherent Bgd (cm^{-1}) =	0	±	0
volume fraction(1) =	0.0439945	±	0.00886659
Radius (1) (Å) =	5.3	±	3.45184e-06
polydispersity(1) =	0.00999999	±	9.94917e-09
SLD(1) ($Å^{-2}$) =	1.697e-06	±	0
volume fraction(2) =	0.00856142	±	0.000851121
Radius (2) =	8.39997	±	7.43468e-06
polydispersity(2) =	0.00999999	±	8.87567e-09
SLD(2) =	2.206e-06	±	0
SLD (solvent) =	-4.2e-08	±	0
background (cm^{-1}) =	0.0469367	±	0.000703497
Sqrt(χ^2/N) =	0.983019		
Fitted Range =	0.003433	< Q <	0.4121

For the most part, the standard deviations are quite low compared to their respective parameters in addition to the small Sqrt(χ^2/N) value of 0.9830. However, the volume fraction for the first size population (representing RsC1) is unrealistically high considering the actual volume fraction of RsC1 in the sample. Likewise, the volume fraction for the second size population (representing Calix8) is unrealistically low considering the actual volume fraction of Calix8. The total volume fraction (the sum of the two) is also larger than the actual total volume fraction of the sample. Additionally, the radii for the two size populations did not seem to be fitted—any random entry remained unchanged with low standard deviations after fitting. For these reasons, this model was discounted for this data.

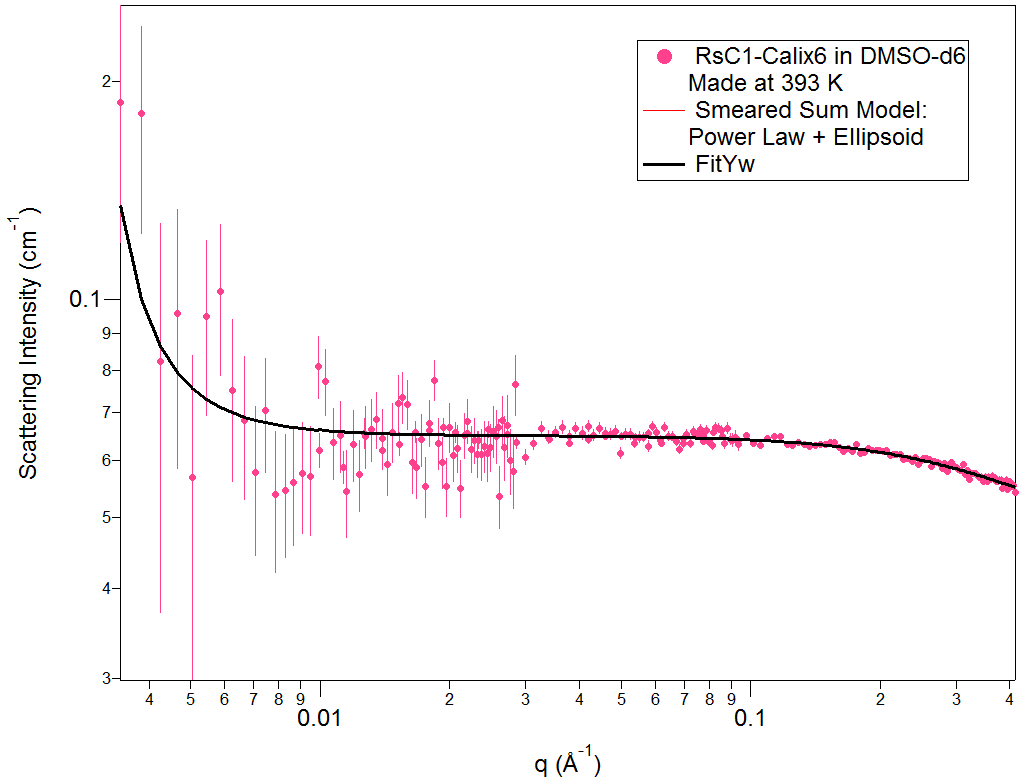
RsC1-Calix6 in DMSO-d6 (Power Law + Ellipsoid Model)



Coefficient, A =	7.5093e-09	±	3.01302e-09
(-)Power =	3.11108	±	0.067824
Incoherent Bgd (cm^{-1}) =	0	±	0
scale =	0.0308847	±	0.14739
R a (rotation axis) (Å) =	8.40392	±	9.06833
R b (Å) =	5	±	12.3345
SLD ellipsoid ($Å^{-2}$) =	1.964e-06	±	0
SLD solvent ($Å^{-2}$) =	-4.2e-08	±	0
incoh. bkg (cm^{-1}) =	0.0574592	±	0.00989414
Sqrt(χ^2/N) =	1.04609		
Fitted Range =	0.003433	< Q <	0.4088

The error bars on the R_a and R_b dimensions and the scale factor are extremely large, especially when compared to their respective parameters. This is indicative of the model containing more information than what the data provides, so this model is not suitable.

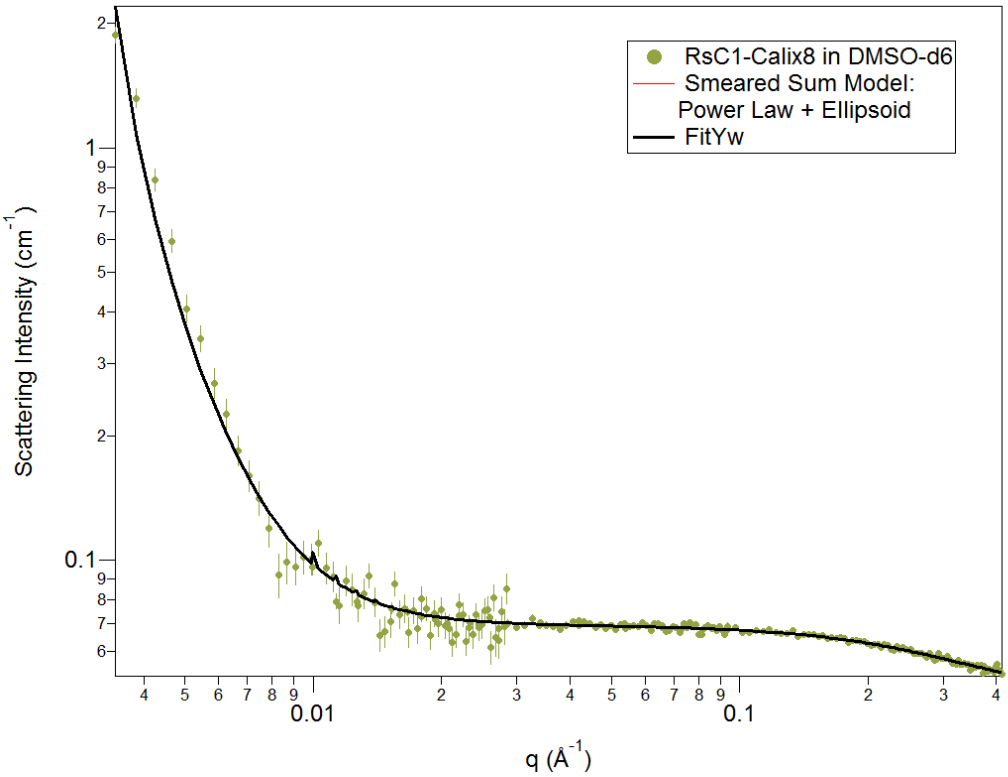
RsC1-Calix6 in DMSO-d6 Made at 393 K (Power Law + Ellipsoid):



Coefficient, A =	7.82088e-10	±	3.47379e-09
(-)Power =	3.05037	±	0.755606
Incoherent Bgd (cm^{-1}) =	0	±	0
scale =	0.0457772	±	0.236546
R a (rotation axis) (Å) =	7.14994	±	15.9562
R b (Å) =	5.03819	±	16.0192
SLD ellipsoid ($Å^{-2}$) =	1.964e-06	±	0
SLD solvent ($Å^{-2}$) =	-4.2e-08	±	0
incoh. bkg (cm^{-1}) =	0.0509858	±	0.0144342
Sqrt(χ^2/N) =	1.02252		
Fitted Range =	0.003433	< Q <	0.4121

The error bars on the R_a and R_b dimensions and the scale factor are extremely large, especially when compared to their respective parameters. This is indicative of the model containing more information than what the data provides, so this model is not suitable.

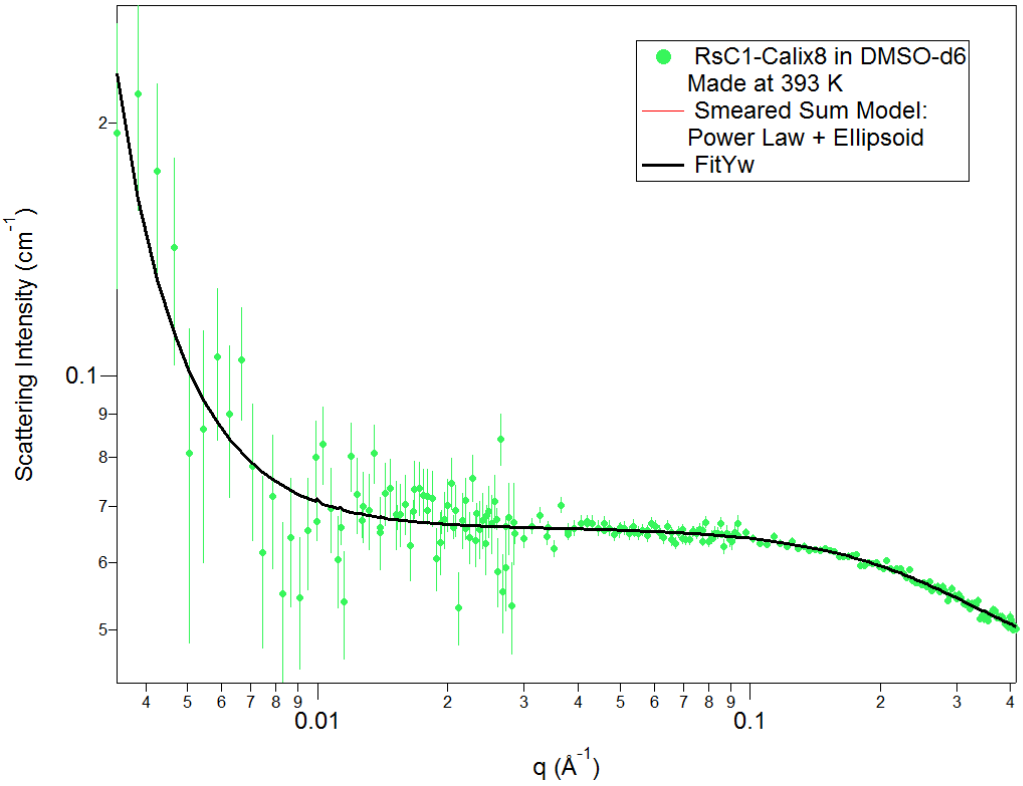
RsC1-Calix8 in DMSO-d6 (Power Law + Ellipsoid):



Coefficient, A =	1.51867e-08	±	2.76361e-09
(-)Power =	3.11571	±	0.0311561
Incoherent Bgd (cm^{-1}) =	0	±	0
scale =	0.0427122	±	0.0644472
R a (rotation axis) (Å) =	10.0848	±	2.2262
R b (Å) =	5.13751	±	3.75021
SLD ellipsoid ($Å^{-2}$) =	1.998e-06	±	0
SLD solvent ($Å^{-2}$) =	-4.2e-08	±	0
incoh. bkg (cm^{-1}) =	0.049696	±	0.00520673
Sqrt(χ^2/N) =	1.15924		
Fitted Range =	0.003433	< Q <	0.4121

The error bars on the R_a and R_b dimensions and the scale factor are extremely large, especially when compared to their respective parameters. This is indicative of the model containing more information than what the data provides, so this model is not suitable.

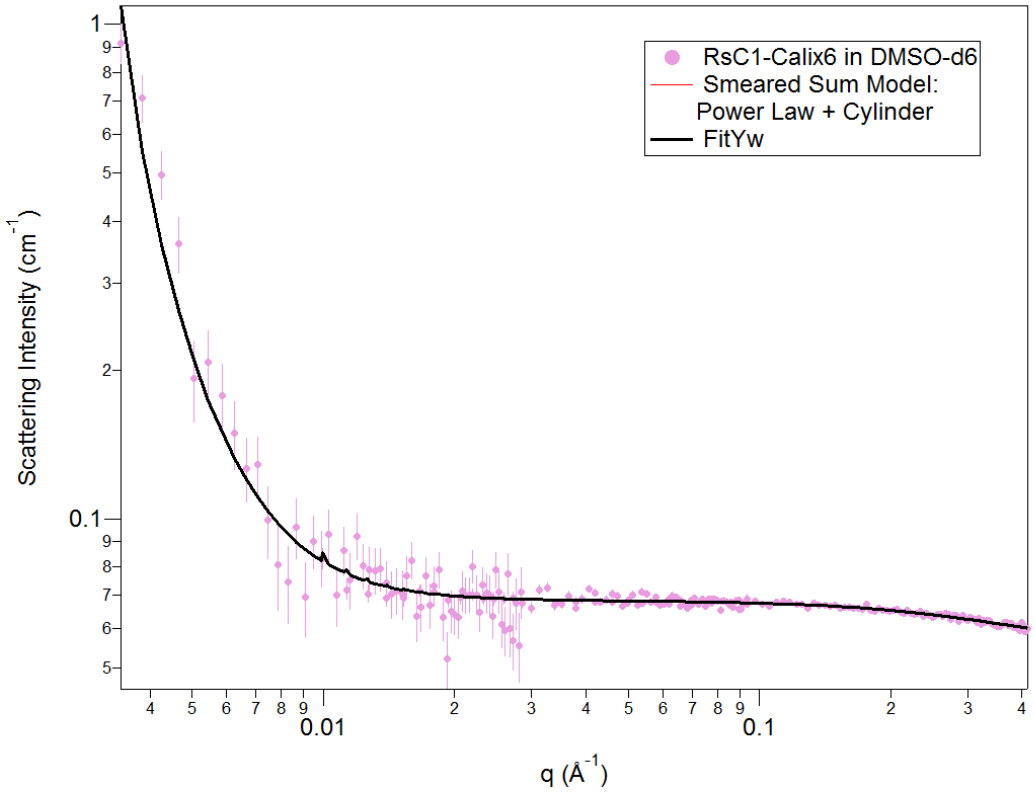
RsC1-Calix8 in DMSO-d6 Made at 393 K (Power Law + Ellipsoid):



Coefficient, A =	1.7383e-08	±	2.39408e-08
(-)Power =	2.70489	±	0.253929
Incoherent Bgd (cm^{-1}) =	0	±	0
scale =	0.044221	±	0.0768797
R a (rotation axis) (Å) =	10.4178	±	1.99875
R b (Å) =	4.91009	±	3.99771
SLD ellipsoid ($Å^{-2}$) =	1.998e-06	±	0
SLD solvent ($Å^{-2}$) =	-4.2e-08	±	0
incoh. bkg (cm^{-1}) =	0.046673	±	0.00569258
Sqrt(χ^2/N) =	0.982524		
Fitted Range =	0.003433	< Q <	0.4121

The error bars on the R_a and R_b dimensions and the scale factor are extremely large, especially when compared to their respective parameters. This is indicative of the model containing more information than what the data provides, so this model is not suitable.

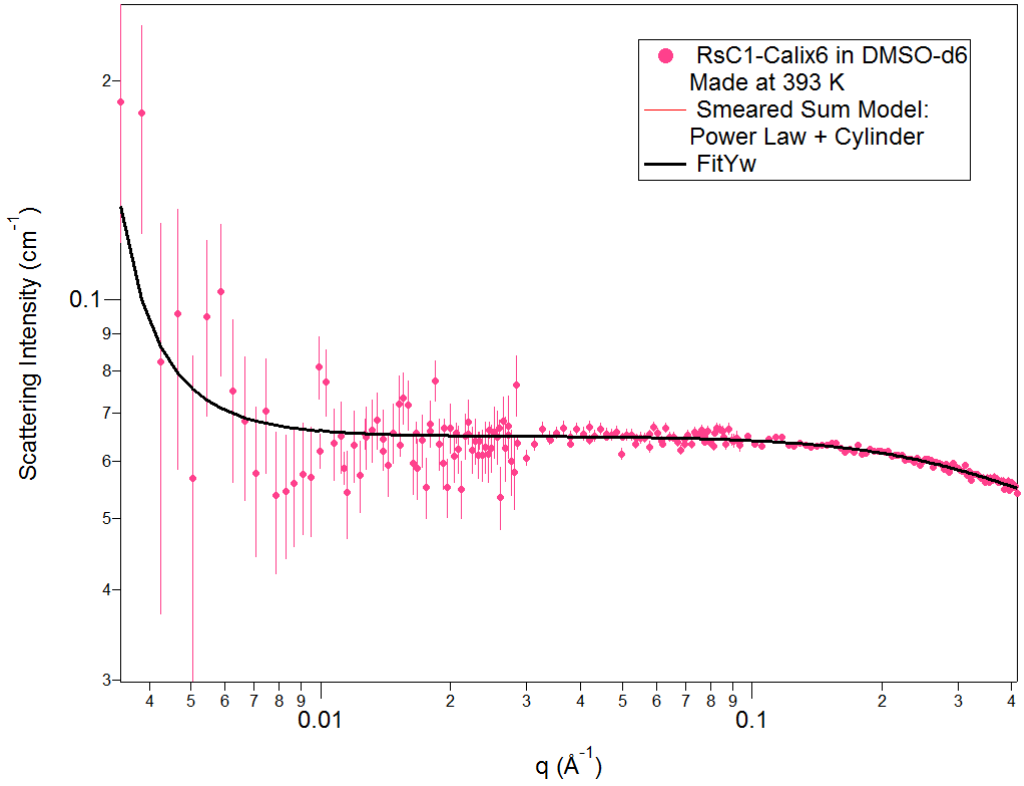
RsC1-Calix6 in DMSO-d6 (Power Law + Cylinder Model)



Coefficient, A =	7.51632e-09	±	3.01423e-09
(-)Power =	3.11094	±	0.0677857
Incoherent Bgd (cm^{-1}) =	0	±	0
scale =	0.0301908	±	0.188237
radius (Å) =	4.74825	±	17.0364
length (Å) =	12.5363	±	26.5084
SLD cylinder ($Å^{-2}$) =	1.964e-06	±	0
SLD solvent ($Å^{-2}$) =	-4.2e-08	±	0
incoh. bkg (cm^{-1}) =	0.0576062	±	0.0125396
Sqrt(χ^2/N) =	1.04622		
Fitted Range =	0.003433	< Q <	0.4121

The error bars on the radius and length dimensions and the scale factor are extremely large, especially when compared to their respective parameters. This is indicative of the model containing more information than what the data provides, so this model is not suitable.

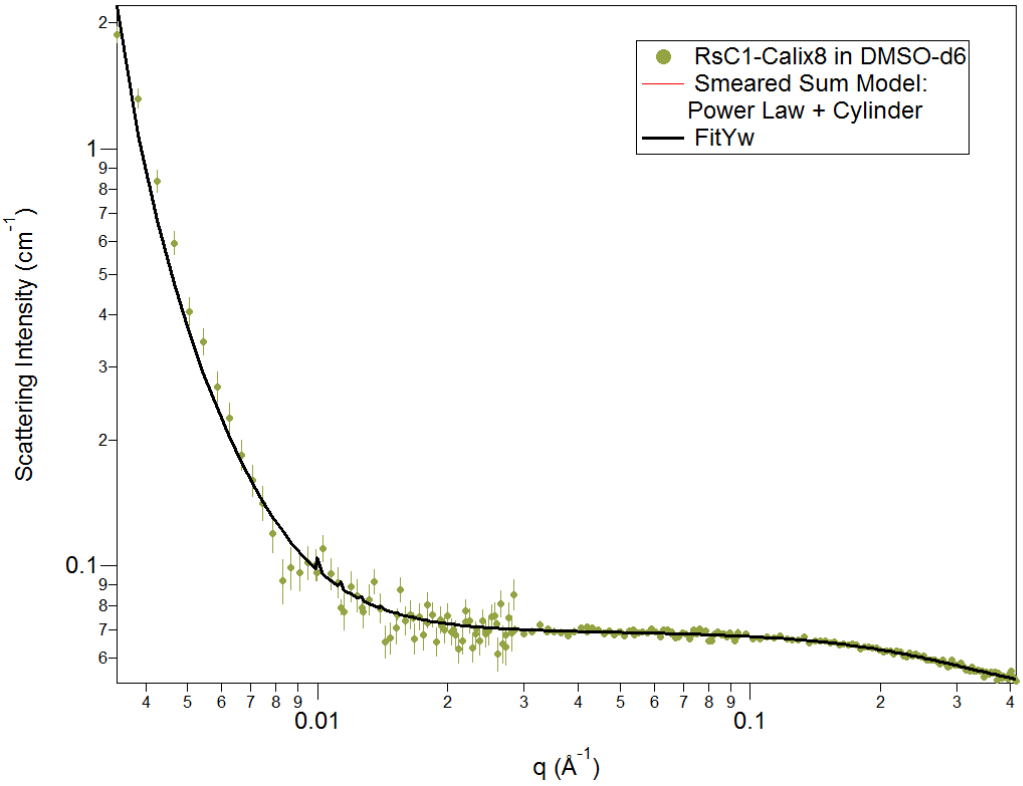
RsC1-Calix6 in DMSO-d6 Made at 393 K (Power Law + Cylinder):



Coefficient, A =	7.79453e-10	±	3.48142e-09
(-)Power =	3.04992	±	0.759938
Incoherent Bgd (cm^{-1}) =	0	±	0
scale =	0.0413	±	0.224911
radius (Å) =	5.13681	±	43.634
length (Å) =	9.82607	±	124.127
SLD cylinder ($Å^{-2}$) =	1.964e-06	±	0
SLD solvent ($Å^{-2}$) =	-4.2e-08	±	0
incoh. bkg (cm^{-1}) =	0.0514643	±	0.0146268
Sqrt(χ^2/N) =	1.02258		
Fitted Range =	0.003433	< Q <	0.4121

The error bars on the radius and length dimensions and the scale factor are extremely large, especially when compared to their respective parameters. This is indicative of the model containing more information than what the data provides, so this model is not suitable.

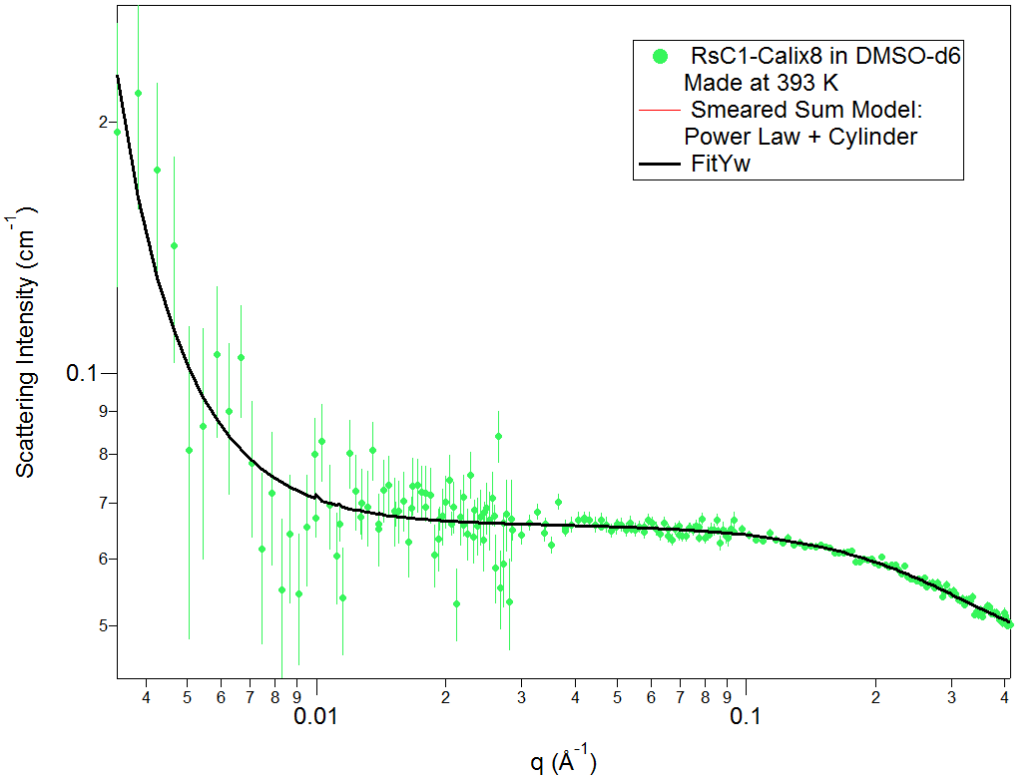
RsC1-Calix8 in DMSO-d6 (Power Law + Cylinder):



Coefficient, A =	1.52223e-08	±	2.76734e-09
(-)Power =	3.11533	±	0.0311306
Incoherent Bgd (cm^{-1}) =	0	±	0
scale =	0.0360595	±	0.0579859
radius (Å) =	5.23727	±	4.68804
length (Å) =	14.7374	±	6.96249
SLD cylinder ($Å^{-2}$) =	1.998e-06	±	0
SLD solvent ($Å^{-2}$) =	-4.2e-08	±	0
incoh. bkg (cm^{-1}) =	0.0504468	±	0.00541752
Sqrt(χ^2/N) =	1.15741		
Fitted Range =	0.003433	< Q <	0.4121

The error bars on the radius and length dimensions and the scale factor are extremely large, especially when compared to their respective parameters. This is indicative of the model containing more information than what the data provides, so this model is not suitable.

RsC1-Calix8 in DMSO-d6 Made at 393 K (Power Law + Cylinder):



Coefficient, A =	1.84219e-08	±	2.52488e-08
(-)Power =	2.69479	±	0.253356
Incoherent Bgd (cm^{-1}) =	0	±	0
scale =	0.0401807	±	0.0813387
radius (Å) =	4.80236	±	4.84242
length (Å) =	15.5755	±	5.37887
SLD cylinder ($Å^{-2}$) =	1.998e-06	±	0
SLD solvent ($Å^{-2}$) =	-4.2e-08	±	0
incoh. bkg (cm^{-1}) =	0.0471394	±	0.00653422
Sqrt(χ^2/N) =	0.98287		
Fitted Range =	0.003433	< Q <	0.4121

The error bars on the radius and length dimensions and the scale factor are extremely large, especially when compared to their respective parameters. This is indicative of the model containing more information than what the data provides, so this model is not suitable.