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Supporting information for article:

Implementation of a Self-Consistent Slab Model of Bilayer Structure in the SasView Suite

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This supporting information document contains supplementary discussion, the code of the fitting function described in this work, along with supporting data figures.

S1. Internal inconsistency of the fit with existing model – 'lamellar_hg'.

The DPPC in D_2O at 50 °C was fit using the existing lamellar slab model within SasView (lamellar_hg) demonstrates the internal inconsistency of the fit results. This is the same dataset discussed in the main text.

Here, we will focus on the breakdown of a simple estimation of the head group water content. We will even constrain the model with fixed SLD in the solvent and acyl core since these values are known. This illustrates how such inconsistencies emerge even for one unconstrained slab. In this fit we have fixed the SLD of the central tail region at -0.036 fm/Å^3, the sld of the solvent at 0.636 fm/Å^3, as these are known. The other parameters of the fit (scale, background, length_tail, length_head, sld_head) were allowed to float. The resulting fit converged, reproduced the data closely and showed no strong covariance between variables (fit not shown). The resulting values were length_tail = 14.2 +/- 1.4 Å, length_head = 10.4 +/- 1.3 Å, and sld_head = 0.365 fm/Å^3, error of the fit reported for this example. From here there are two routes one might use to compute the water content – each resulting in a different value. This demonstrates the internal inconsistency of the fit result since the fit is unconstrained by the molecular volumes and

Estimating water content from the head thickness. - We can take the area per lipid to be 63.4 Å^2 from the quotient of molecular volume of DPPC tails and the reported tail thickness. One can then estimate the volume per lipid of the head group slab geometrically as the product of the area per lipid and the head group thickness, 659 Å^3. Subtracting the known lipid portion of this volume, 331 Å^3, reveals the amount of volume occupied by water in the head group region, 328 Å^3. Taking the volume of water to be 30.4 Å^3 per molecule, we obtain an estimate of 10.8 water molecules per lipid.

Estimating water content from the head SLD. – The SLD of the head group region is defined as the quotient of the sum of bound coherent scattering lengths of all atoms within the headgroup region and the volume of the headgroup region, or $\mathrm{SLD_H} = \frac{n_w * b_W + b_H}{APL * D_H}$. Rearranging this to solve for n_w gives, $n_w = (\mathrm{SLD_H} * APL * D_H - b_H)/b_W$ which we can used to compute a value of 9.4 water molecules per lipid. Here we use the volume and scattering length values found in Table 1 of the main text and the thickness values of the lamellar_hg fit.

S2. Fitting Function Code.

Below can be found the code used for fitting using the self-consistent slab model for lamellar structures. This code is also included as the file "lamellar_slab_APL_nW.py".

Begin Code

```
# Note: model title and parameter table are inserted automatically
r"""
This model provides the scattering intensity, $I(q)$, for a
lyotropic lamellar
phase where a random distribution in solution are assumed. The SLD
of the outer,
solvent-exposed region is taken to be different from the SLD of the
inner region.

This model is intended to be used with input parameters including
the molecualr
volumes and  bound coherrent scattering length of the inner portion
of the
amphiphile (solvent not exposed), the outer portion of the
amphiphile (outer
solvent exposed), and solvent molecule.

The variable parameters are intended to be the APL, the average area
per
amphiphile (lipid) molecules at the inner/outer interface and n_W,
the number
of solvent (water) molecules residing in the outer region of the
bilayer.

This model is adapted from the lipid bilayer model of Nagle and
Wiener(1988) and fitting function lamellar_hg.

Note that the model can be applied with other combinations of input
parameters/
assumptions; and is ideally applied as a simultaneous fit to
datasets with
multiple independent measurments; such as neutron contrast variation
strategies.


Definition
----------


The scattering intensity $I(q)$ is


.. math::


   I(q) = 2\pi\frac{\text{scale}}{2(\delta_H + \delta_T)}  P(q)
\frac{1}{q^2}
```

```
The form factor $P(q)$ is


.. math::


    P(q) = \frac{4}{q^2}
        \left\lbrace
            \Delta \rho_H
            \left[\sin[q(\delta_H + \delta_T)\ -
\sin(q\delta_T)\right]
            + \Delta\rho_T\sin(q\delta_T)
        \right\rbrace^2


where $\delta_T$ is *length_tail*, $\delta_H$ is *length_head*,
$\Delta\rho_H$ is the head contrast (*sld_head* $-$ *sld_solvent*),
and $\Delta\rho_T$ is tail contrast (*sld_tail* $-$ *sld_solvent*),
$\length_tail$ equals (*Volume_tail*$/$*APL*),
$\length_head$ equals
((*Volume_head*$+$*n_H*$*$*Volume_water*)$/$*APL*),
$\sld_head$ equals
(*B_head*$+$*n_H*$*$*B_water*)$/$(*Volume_head*$+$*n_H*$*$*Volume_wa
ter*),
$\sld_tails equals (*B_tail*$/$*Volume_tail*).


The total thickness of the lamellar sheet is $\delta_H + \delta_T +
\delta_T + \delta_H$.
Note that in a non aqueous solvent the chemical "head" group may be
the
"Tail region" and vice-versa.


The 2D scattering intensity is calculated in the same way as 1D,
where
the $q$ vector is defined as


.. math:: q = \sqrt{q_x^2 + q_y^2}



References
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.. [#] F Nallet, R Laversanne, and D Roux, *J. Phys. II France*, 3,
(1993) 487-502
.. [#] J Berghausen, J Zipfel, P Lindner, W Richtering, *J. Phys.
Chem. B*, 105, (2001) 11081-11088
.. [#] Nagle, J., & Wiener, M. (1988). Structure of fully hydrated
bilayer dispersions. Biochimica et Biophysica Acta (BBA)-
Biomembranes, 942(1), 1-10
```

```
.. [#] Tan, L., Elkins J.G., Davison, B.H., Kelly, E.G., Nickels,
J.D. Implementation of Slab Model of Bilayer Structure in SASview.
Submitted (2020)

Authorship and Verification
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G. Kelly and Jonathan D. Nickels
"""


import numpy as np
from numpy import inf


name = "lamellar_Slab_APL_nW"
title = "Random lamellar phase with Head and Tail Groups"
description = """\
    [Random lamellar phase with Head and Tail Groups]
        I(q)= 2*pi*P(q)/(2(H+T)*q^(2)), where
        P(q)= see manual
        layer thickness =(H+T+T+H) = 2(Head+Tail)
        SLD_c = Tail scattering length density
        SLD_h = Head scattering length density
        SLD_w = solvent scattering length density
        background = incoherent background
        scale = scale factor
        B_h = Bound coherrent scattering length of lipid headgroup
        B_c = Bound coherrent scattering length of lipid tails
        B_w = Bound coherrent scattering length of water
        APL = Average area per lipid
        V_w = Molecualar volume of water
        V_h = Molecular volume of lipid headgroup
        V_c = Molecualr volume of lipid tails
        N_w = Number molecules of water molecule permeating into
bilayer region
        Dc = Average length of lipid tail
        Dh = Average length of lipid headgroup
"""
category = "shape:lamellae"


# pylint: disable=bad-whitespace, line-too-long
#             ["name", "units", default, [lower, upper],
"type","description"],
parameters = [["B_h", "1e-6*Ang",       58,   [-inf, inf],
"volume",  "Bound coherrent scattering length of lipid headgroup"],
              ["B_c", "1e-6*Ang",       -9.05984,   [-inf, inf],
"volume",  "Bound coherrent scattering length of lipid tails"],
              ["B_w", "1e-6*Ang", 19.145, [-inf,inf], "volume",
"Bound coherrent scattering length of water"],
              ["APL", "Ang^2", 60,   [0,inf], "volume",    "Area"],
    ["V_w", "Ang^3", 30.4,   [0,inf], "volume",    "Molecualar
volume of water"],
```

```
    ["V_h", "Ang^3", 211,   [0,inf], "volume",    "Molecular volume
of lipid headgroup"],
    ["V_c", "Ang^3", 896.608,   [0,inf], "volume",    "Molecualr
volume of lipid tails"],
          ["N_w", "None", 20,   [0,inf], "sld",    "Number molecules
of water molecule permeating into bilayer region"]
   ]
# pylint: enable=bad-whitespace, line-too-long


# No volume normalization despite having a volume parameter
# This should perhaps be volume normalized?



def Iq(q,
       B_h=58,
       B_c=-9.05984,
       B_w=19.145,
       APL=60,
       V_w=30.4,
       V_h=211,
       V_c=896.608,
       N_w=20):
    SLD_h = (B_h + N_w*B_w)/(V_h +N_w*V_w) #the calculation of sld
of headgroup
    SLD_c = (B_c/V_c) #the calculation of sld of tail
    SLD_w = (B_w/V_w) #the calculation of sld of solvent
    Dc = (V_c)/(APL) #the calculation of length of lipid hydrocarbon
chains
    Dh = (V_h + N_w*V_w)/APL #the calculation of length of lipid
headgroup
    qsq = q*q # q square
    drh = (SLD_h - SLD_w) #delta rho_H (the head contrast)
    drt = (SLD_c - SLD_w) #delat rho_T  (the tail contrast)
    qT = q*Dc
    Pq = drh*(np.sin(q*(Dh + Dc))-np.sin(qT)) + drt*np.sin(qT)
    Pq *= Pq
    Pq *=4.0/(qsq)
    inten = 2*np.pi*Pq/qsq
    inten /=2.0*(Dc +Dh)
    return inten


def random(): #the random function which can generate random number
for the vriable parameters
    """Return a random parameter set for the model."""
    APL = np.random.uniform(1, 500)
    N_w = np.random.uniform(0, 100)
    pars = dict(
        APL = APL,
        N_w = N_w
    )
    return pars
```

End Code

S2.1. Import to SasView

Be sure you have installed SasView from https://www.sasview.org/download/.

Prior to inclusion in a SasView release it is necessary to import this algorithm as a plugin model. This is a straightforward process as follows:

Open SasView

Select the drop down menu labelled 'Fitting' and select 'Manage Custom Models'.

Select 'Add File' from the interface which pops up and select the model to be added from the location where you have saved it.

S2.2. Using Plugin Model

Once you have added the file, the model will now appear as an option in the Plugin category of the fitting tab.

Load your dataset in the Data Explorer and select the curve(s) you wish to fit, and select "Fitting" from the drop down menu next to the button to "Send Data to". Then press the button.

Your data is now loaded and ready for fitting.

The model can now be found in the Plugin Models category. Select this category and then select lamellar_slab_APL_nW. (If an error appears "couldn't find the model name", close the SasView Program and reopen it again. If it still does not work, select the drop down menu labelled 'Fitting; and select 'Edit Custom Models'. Then select the import file and change the name as same as it shown in the category.)

You can now enter the appropriate parameters for your system. We suggest ensuring an appropriate data range has been set in the fit options tab, and be sure that your input parameters are held constant before selecting the "Fit" button.

The choice of fit algorithm can be selected in the "Fitting" menu; along with options for simultaneous and constrained fitting.

Further details can be found in the associated documentation of SasView.

S3. Supporting Data Figures.

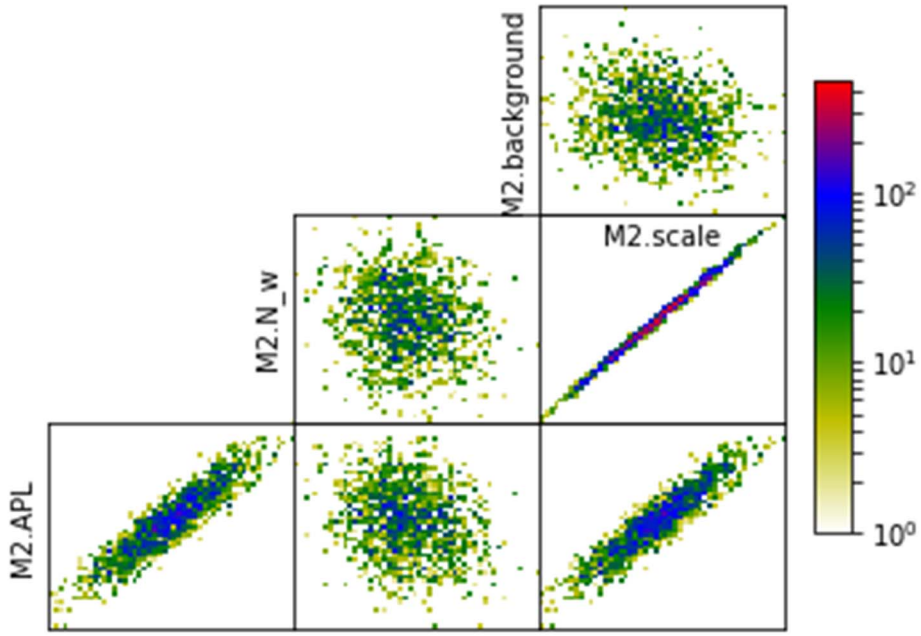

Figure S1 Covariance matrix for fitting of DPPC in D2O at 50C. A moderate covariance is seen between the scale factor and APL, the scale factor and n_W, and n_W and APL.

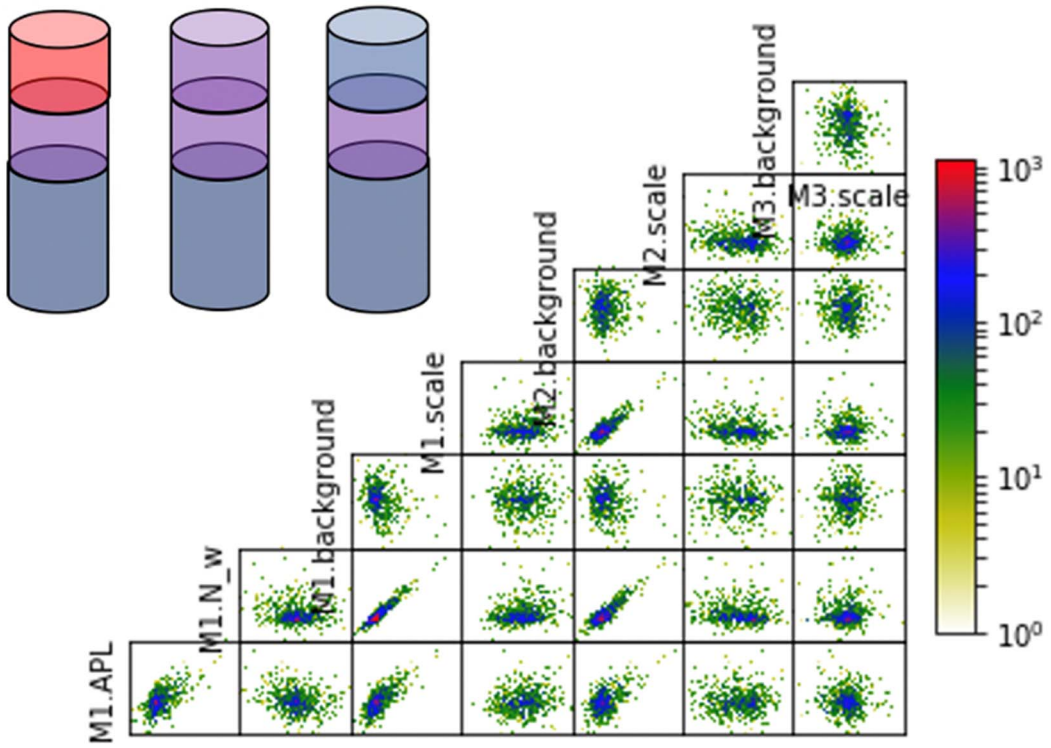

Figure S2 Contrast scheme and covariance matrix for DMPC simultaneous fit of the 90/10 D/H lipid bilayers in 0%, 35%, and 100% D2O. The samples are referred to by M4, M5 and M6 respectively in this figure obtained from SasView.

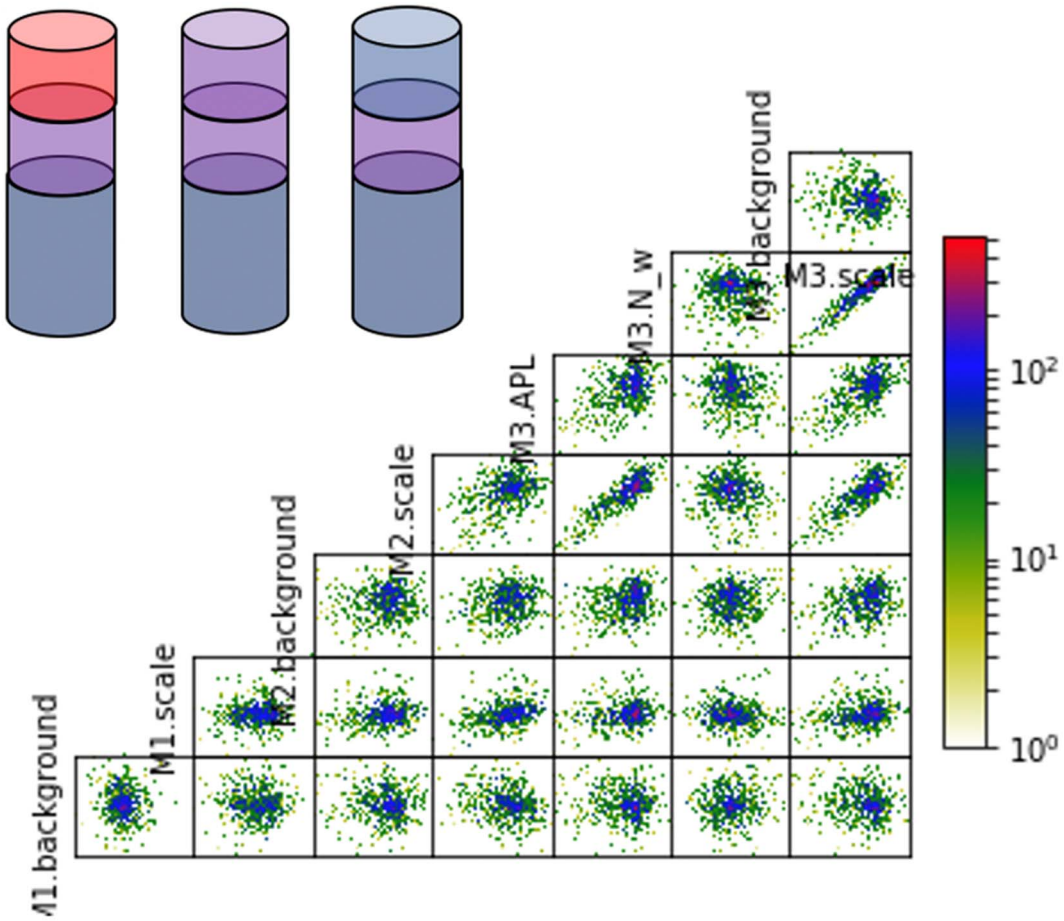

Figure S3 Contrast scheme and covariance matrix for DSPC simultaneous fit of the 90/10 D/H lipid bilayers in 0%, 35%, and 100% D2O. The samples are referred to by M7, M8 and M9 respectively in this figure obtained from SasView.

Table S1 Results of data fitting using our self-consistent lamellar model for tail matched DMPC at 35C individually, as simultaneously fit pairs, and simultaneously fit for all three contrast conditions. Errors represent the 95% confidence interval.

Sample	Solvent(s)	APL (Å^2)	n_W	$2D_C$ (Å)
H/D DMPC	35% D_2O	62.1 +/- 0.5	0.3 +/- 12.2	24.7 +/- 0.4
H/D DMPC	100% D_2O	78.0 +/- 1.1	26.3 +/- 1.2	19.7 +/- 0.5
H/D DMPC	0% D_2O	64.1 +/- 0.5	18.9 +/- 1.6	24.0 +/- 0.2
H/D DMPC	35% and 100% D_2O	64.5 +/- 0.3	11.3 +/- 0.4	23.8 +/- 0.2
H/D DMPC	0% and 35% D_2O	62.7+/- 0.2	14.7 +/- 0.8	24.5 +/- 0.2
H/D DMPC	0% and 100% D_2O	63.5 +/- 0.3	10.8 +/- 0.4	24.2 +/- 0.2
H/D DMPC	0%, 35%, and 100% D_2O	62.9 +/- 0.3	9.9 +/- 0.4	24.4+/- 0.2

Table S2 Results of data fitting using our self-consistent lamellar model for tail matched DSPC at 35C individually, as simultaneously fit pairs, and simultaneously fit for all three contrast conditions. Errors represent the 95% confidence interval.

Sample	Solvent(s)	APL (Å^2)	n_W	$2D_C$ (Å)
H/D DSPC	35% D_2O	63.6 +/- 0.5	3.8 +/- 2.3	32.0 +/- 0.5
H/D DSPC	100% D_2O	68.7 +/- 0.3	104.6 +/- 19.2	29.6 +/- 0.3
H/D DSPC	0% D_2O	71.2 +/- 2.4	19.5 +/- 3.4	28.6 +/- 2.0
H/D DSPC	35% and 100% D_2O	67.2 +/- 0.2	19.9 +/- 1.0	30.3 +/- 0.2
H/D DSPC	0% and 35% D_2O	65.4+/- 0.2	11.6 +/- 0.4	31.1 +/- 0.2
H/D DSPC	0% and 100% D_2O	69.0 +/- 0.3	16.4 +/- 0.4	29.5 +/- 0.2
H/D DSPC	0%, 35%, and 100% D_2O	66.9 +/- 0.2	14.1 +/- 0.4	30.4 +/- 0.2

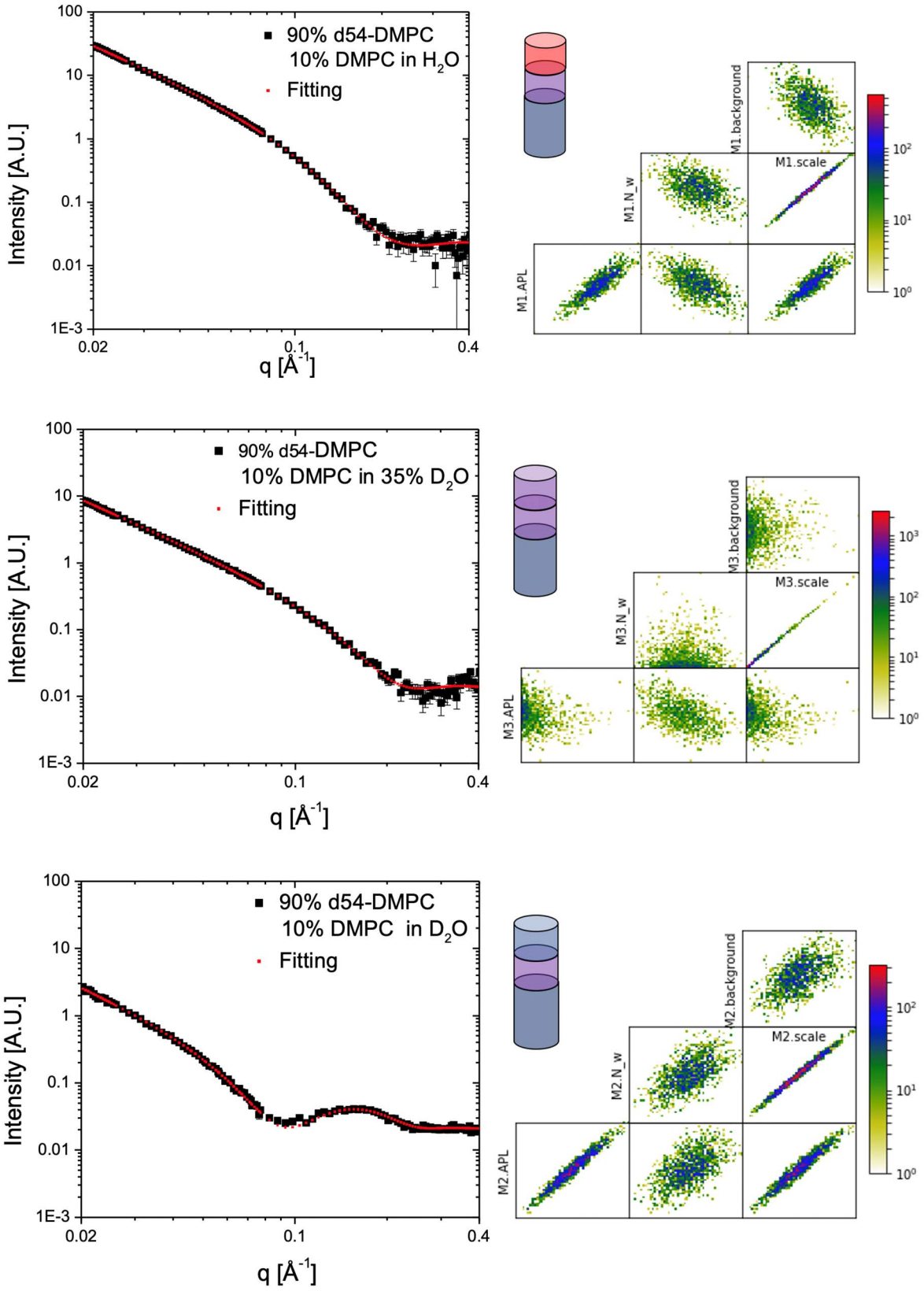

Figure S4 Single data set fitting for DMPC contrast variants.

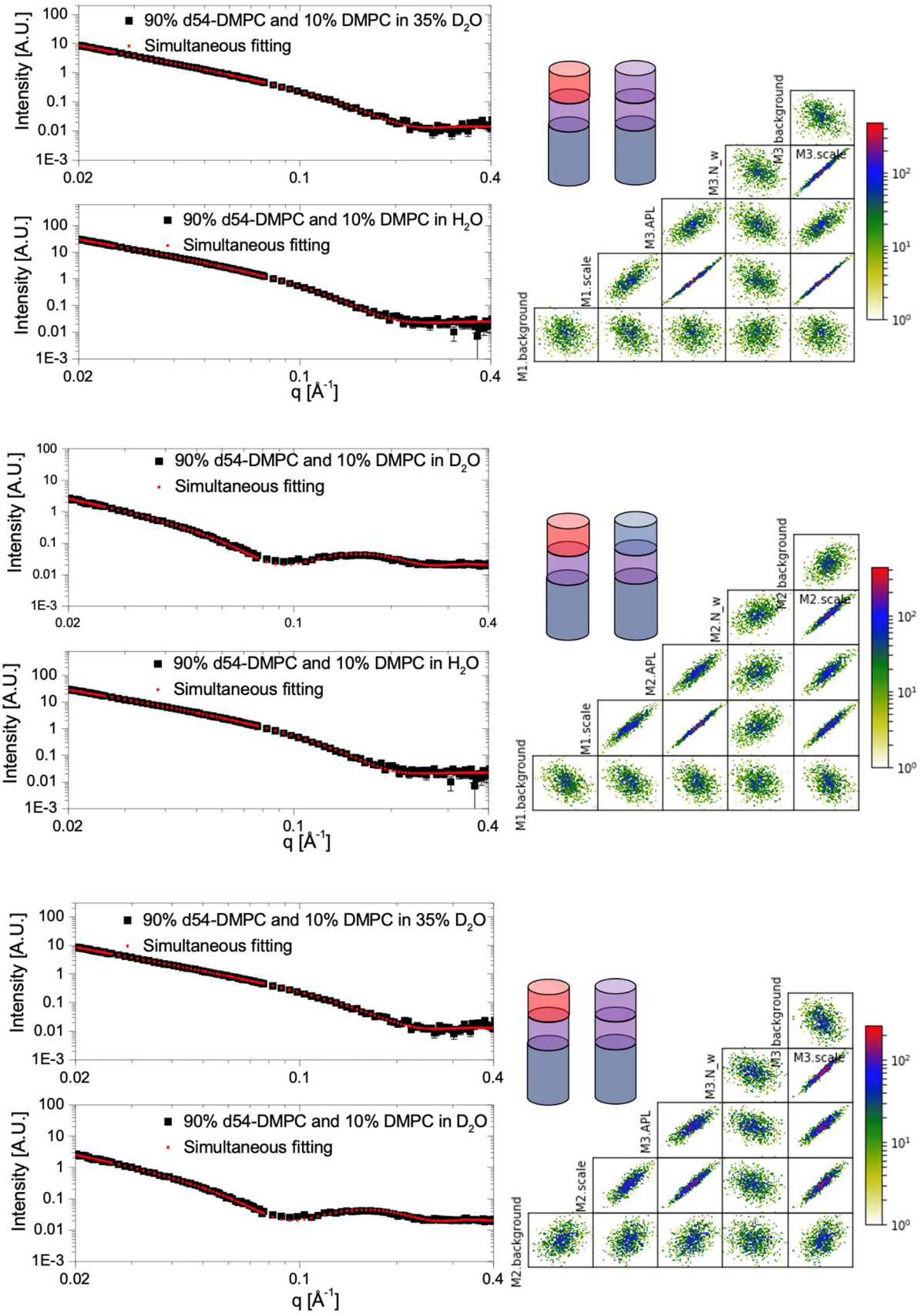

Figure S5 Two-way simultaneous fits of DMPC scattering data.

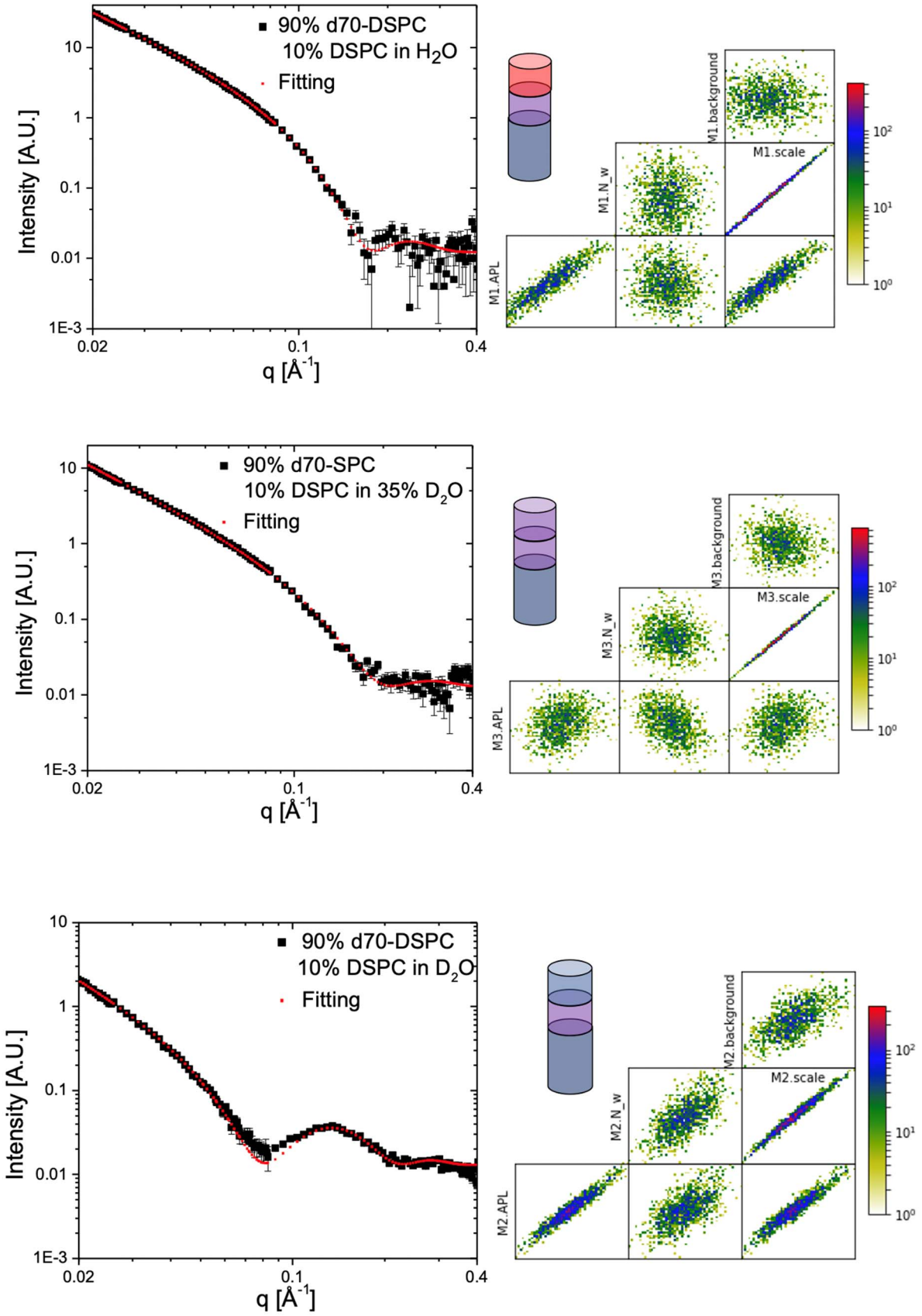

Figure S6 Single data set fitting for DSPC contrast variants.

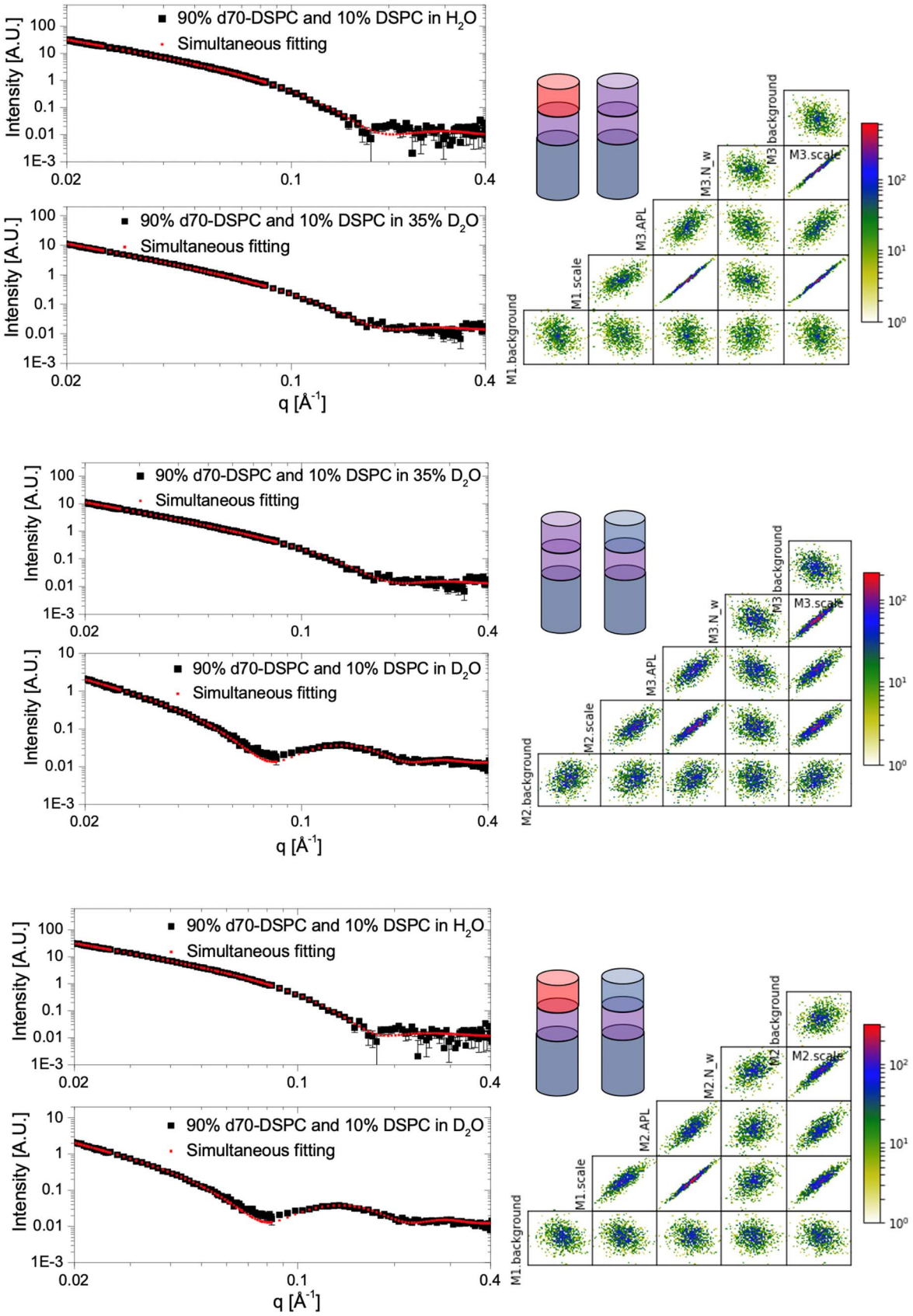

Figure S7 Two-way simultaneous fits of DSPC scattering data.