

## Supplementary Material

### Figure S1: Representative data and the fitting parameters

Since we obtained 4 apparent diffusion constants from the four peaks of the NaDS the averaged value was used for further analysis. We had 24 diffusion experiments for Figure 2 of the manuscript therefore almost one hundred data were fitted with the MestreNova software. In order to illustrate the quality of the data we show below randomly selected spectra from each concentration

This are the comment of Mnova software about the fitting results:

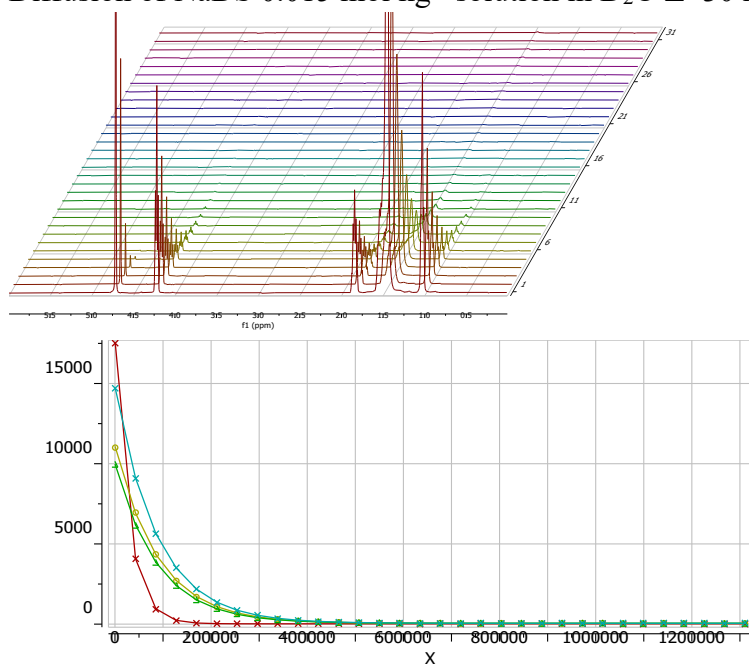
NOTE: The **Probnomono** value is important to assess whether or not the model for the fit we are assuming, in this case, a three parameter-exponential model satisfies. For instance, if you assume a mono-exponential model but the experimental data follows a bi or multi-exponential behavior, then the analysis will not be fully correct. On the other hand, if we assume that the model is mono-exponential, the '**rError**' value gives the [absolute] probable error in the value of 'r', where 'r' is:  
 $y = a \cdot \exp(-r \cdot x) + b$

We applied the above equation in the following form

$B + F \cdot \exp(-x \cdot G)$  therefore the rError is for  $G$ , the apparent diffusion coefficient.

We always checked the  $B/F \cdot 100$  values (offset %). It was not more than 1% in either cases.

Diffusion of NaDS 0.015 mol kg<sup>-1</sup> solution in D<sub>2</sub>O  $\Delta=30$  ms,  $\delta=8$  ms



Water peak (4.71 ppm)

B= 13.5723, F= 17857.2, G= 3.46422e-05

rError = 2.81893e-08, probnotmono = 0.983053

CH<sub>2</sub> 4.22 ppm

B= 34.7125, F= 11074.3, G= 1.11381e-05

rError = 1.89289e-08, probnotmono = 0.92135

CH<sub>2</sub> 1.84 ppm

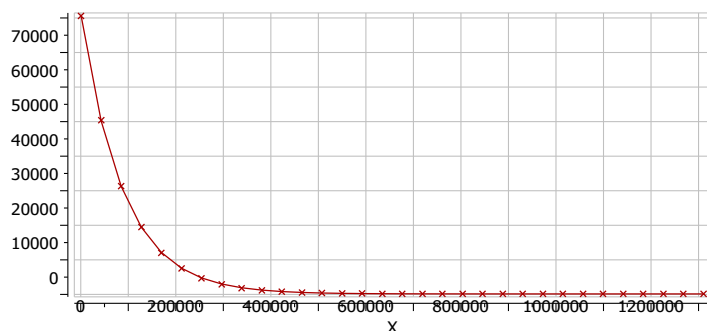
B= 39.9349, F= 9954.4, G= 1.13319e-05

rError = 1.68905e-08, probnotmono = 0.96145

CH<sub>3</sub> 1.03 ppm

B= -77.8792, F= 15200.9, G= 9.92067e-06

rError = 1.06481e-07, probnotmono = 0.993336

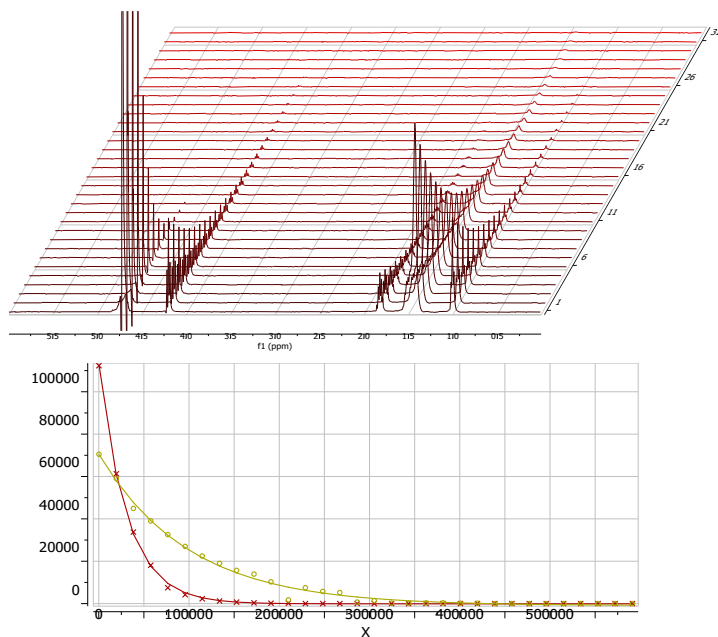


CH<sub>2</sub> peak (1.45-1.55 ppm)

B= -3475.41, F= 490054, G= 1.05753e-05

rError = 4.97833e-08, probnotmono = 1

Diffusion of NaDs 0.005 mol kg<sup>-1</sup> solution in D<sub>2</sub>O  $\Delta=15$  ms,  $\delta=8$  ms



Water peak (4.71 ppm)

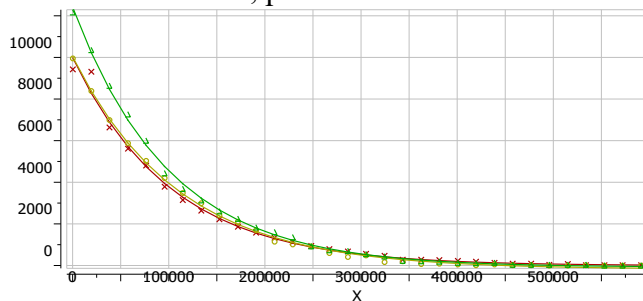
B= -104.773, F= 113720, G= 3.32785e-05

rError = 1.7288e-07, probnotmono = 0.999998

CH<sub>2</sub> 1.42-1.53 ppm

B= -927.287, F= 71540.7, G= 1.00499e-05

rError = 2.32229e-07, probnotmono = 0.999796



CH<sub>2</sub> 4.22 ppm

B= -6.47894, F= 10001.7, G= 9.7169e-06

rError = 2.34496e-07, probnotmono = 0.92135

CH<sub>2</sub> 1.84 ppm

B= -172.298, F= 10207.8, G= 9.06488e-06

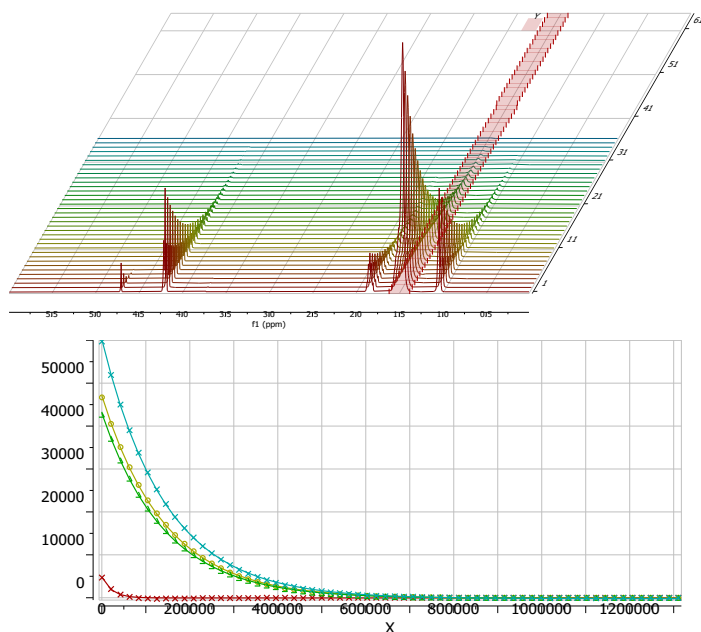
rError = 9.56075e-08, probnotmono = 0.999269

CH<sub>3</sub> 1.03 ppm

B= -77.8792, F= 15200.9, G= 9.92067e-06

rError = 1.06481e-07, probnotmono = 0.993336

Diffusion of NaDs  $0.074 \text{ mol kg}^{-1}$  solution in  $\text{D}_2\text{O}$   $\Delta=30 \text{ ms}$ ,  $\delta=8 \text{ ms}$



Water peak 4.71 ppm

B= -36.605, F= 4903.88, G= 3.36471e-05

rError = 8.87396e-07, probnotmono = 1

CH<sub>2</sub> 4.22 ppm

B= -124.228, F= 47283, G= 7.01776e-06

rError = 1.30441e-08, probnotmono = 1

CH<sub>2</sub> 1.84 ppm

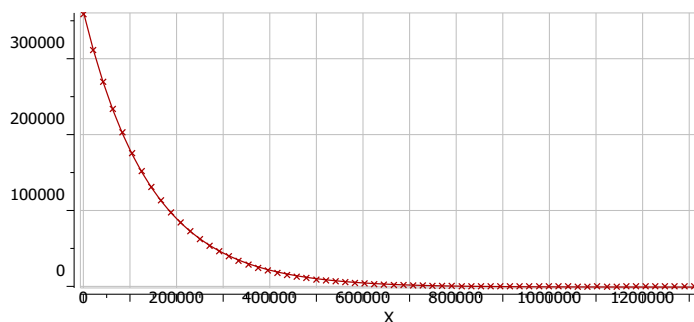
B= -121.582, F= 43192.5, G= 7.0181e-06

rError = 1.23635e-08, probnotmono = 1

CH<sub>3</sub> 1.03 ppm

B= -163.557, F= 60490.6, G= 6.96134e-06

rError = 1.22043e-08, probnotmono = 1

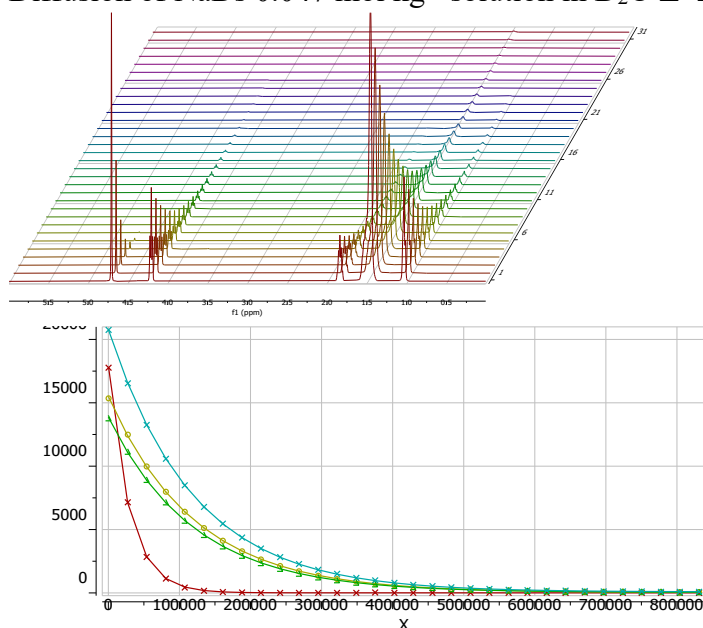


CH<sub>2</sub> peak 1.43-1.53 ppm

B= -999.561, F= 362961, G= 6.96679e-06

rError = 1.22093e-08, probnotmono = 1

Diffusion of NaDs 0.047 mol kg<sup>-1</sup> solution in D<sub>2</sub>O  $\Delta=20$  ms,  $\delta=8$  ms



Water peak 4.71 ppm

B= 11.6092, F= 17995.2, G= 3.4249e-05

rError = 3.98459e-08, probnotmono = 0.855578

CH<sub>2</sub> 4.22 ppm

B= 45.0069, F= 15466.4, G= 8.2649e-06

rError = 1.68678e-08, probnotmono = 0.997661

CH<sub>2</sub> 1.84 ppm

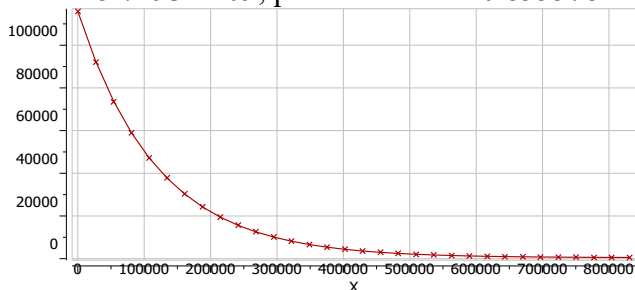
B= 53.8717, F= 13825.4, G= 8.29809e-06

rError = 1.00387e-08, probnotmono = 0.92135

CH<sub>3</sub> 1.03 ppm

B= 94.9812, F= 20698.5, G= 8.38078e-06

rError = 5.72934e-09, probnotmono = 0.855578

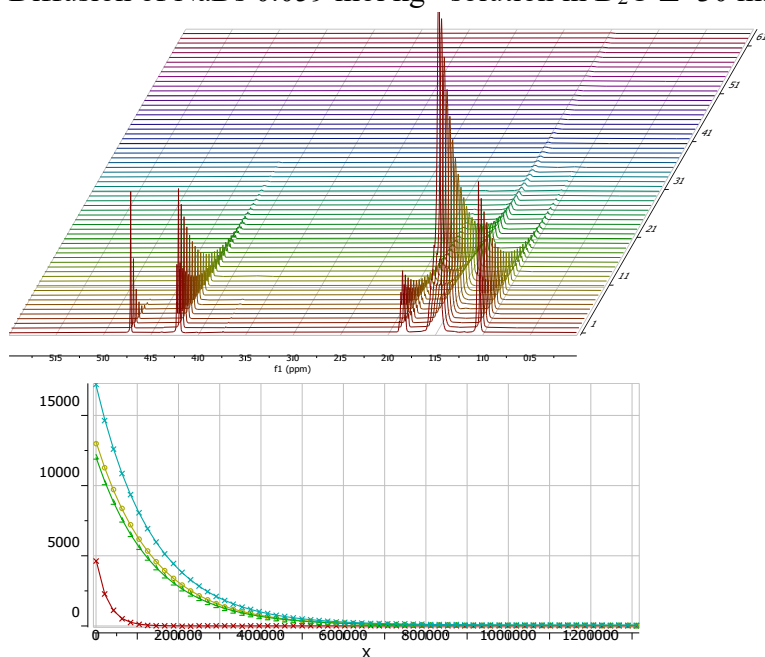


CH<sub>2</sub> peak 1.43-1.53 ppm

B= 455.465, F= 115408, G= 8.40559e-06

rError = 8.11708e-09, probnotmono = 0.99995

Diffusion of NaDs 0.059 mol kg<sup>-1</sup> solution in D<sub>2</sub>O  $\Delta=30$  ms,  $\delta=8$  ms



Water peak 4.71 ppm

B= 0.388892, F= 4737.32, G= 3.47174e-05  
rError = 5.7734e-08, probnotmono = 0.97725

CH<sub>2</sub> 4.22 ppm

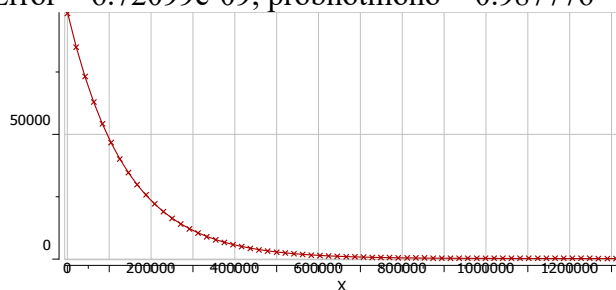
B= 22.1, F= 13105, G= 7.24064e-06  
rError = 7.68164e-09, probnotmono = 1

CH<sub>2</sub> 1.84 ppm

B= 28.7228, F= 11992.2, G= 7.32302e-06  
rError = 6.8353e-09, probnotmono = 0.99702

CH<sub>3</sub> 1.03 ppm

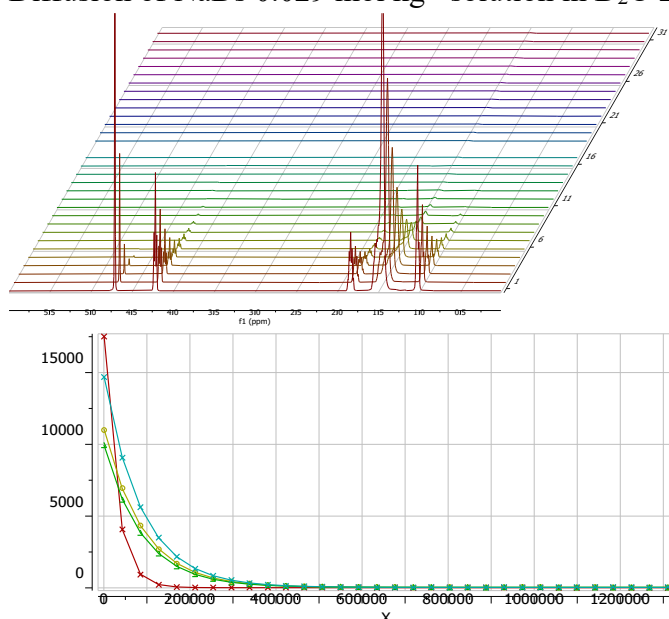
B= 48.8479, F= 17119.7, G= 7.28536e-06  
rError = 6.72099e-09, probnotmono = 0.987776



CH<sub>2</sub> peak 1.43-1.53 ppm

B= 213.327, F= 98876.2, G= 7.2341e-06  
rError = 4.61981e-09, probnotmono = 1

Diffusion of NaDs 0.029 mol kg<sup>-1</sup> solution in D<sub>2</sub>O  $\Delta=30$  ms,  $\delta=8$  ms



Water peak 4.71 ppm

B= 13.5723, F= 17857.2, G= 3.46422e-05  
rError = 2.81893e-08, probnotmono = 0.983053

CH<sub>2</sub> 4.22 ppm

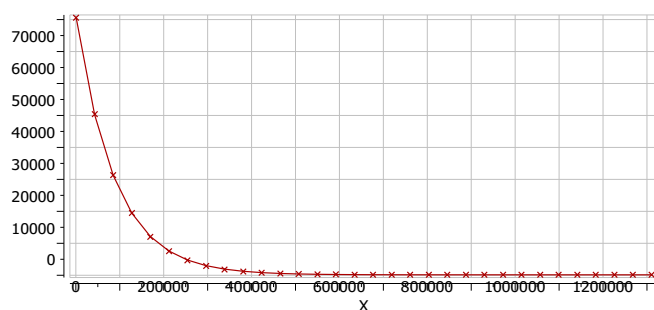
B= 34.7125, F= 11074.3, G= 1.11381e-05  
rError = 1.89289e-08, probnotmono = 0.92135

CH<sub>2</sub> 1.84 ppm

B= 39.9349, F= 9954.4, G= 1.13319e-05  
rError = 1.68905e-08, probnotmono = 0.96145

CH<sub>3</sub> 1.03 ppm

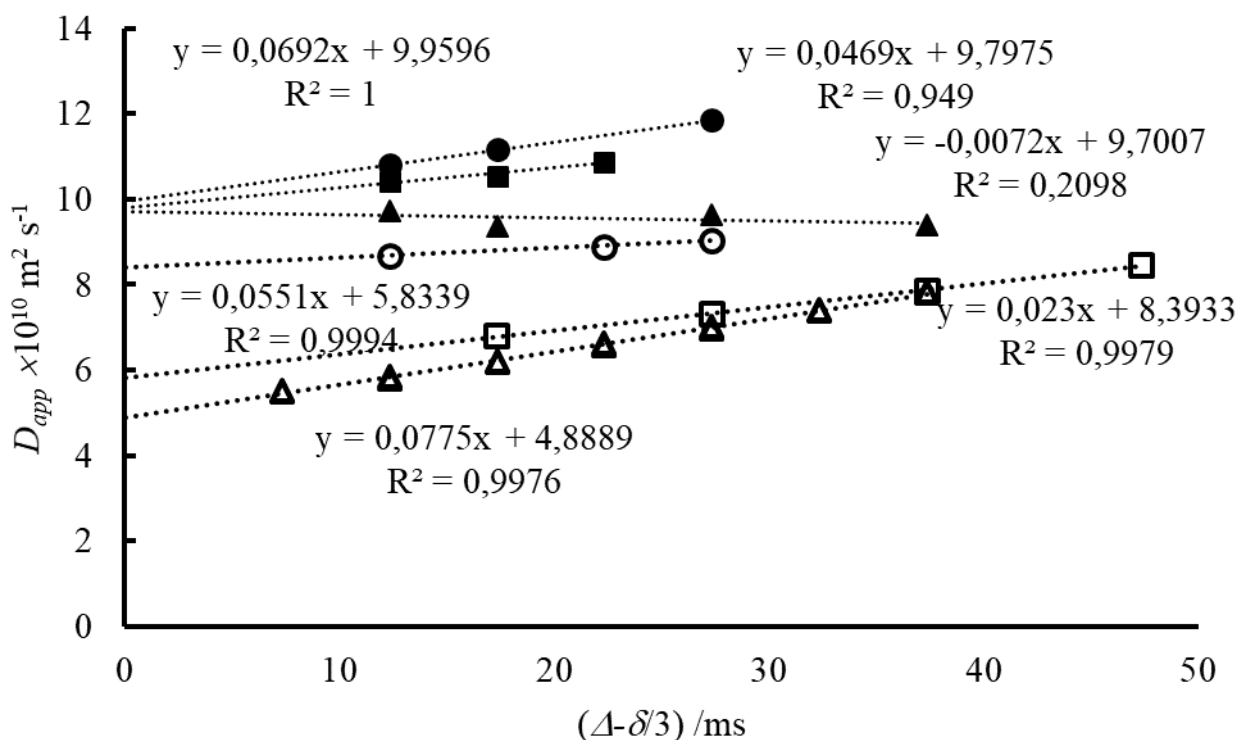
B= 34.2499, F= 14751.2, G= 1.14127e-05  
rError = 9.54809e-09, probnotmono = 0.92135



CH<sub>2</sub> peak 1.43-1.53 ppm

B= 136.632, F= 81115.2, G= 1.12706e-05  
rError = 1.23238e-08, probnotmono = 0.999998

Illustration of the determination of real diffusion coefficients.



**Figure S2.** The apparent self-diffusion coefficients measured at different concentrations as a function of the diffusion time ( $\Delta$ ) at 319 K. Concentrations: ▲ 0,005 mol kg<sup>-1</sup>, ● 0.015 mol kg<sup>-1</sup>, ■ 0.029 mol kg<sup>-1</sup>, ○ 0.047 mol kg<sup>-1</sup>, □ 0.059 mol kg<sup>-1</sup>, Δ 0.074 mol kg<sup>-1</sup>. The extrapolation of apparent diffusion coefficients to zero diffusion time. The values are written in the Figure in that order as the lines are drawn except the value of 0.047 mol kg<sup>-1</sup> which is at the most right position.