

Supplementary Information for
Detection of Biomolecular Interactions Using Polyfluorine
Tracers in Diffusion Ordered Spectroscopy

Tasneem S. Habib,^a Abdulrahman M. Alazemi,^{a,*} Laila A. Alhaddad,^a Abdul-Hamid M. Emwas,^b Mohamed K. Emira,^a Fouzi Mouffouk,^{a,*}

^a Chemistry Department, Faculty of Science, Kuwait University, P.O. Box 5969, Safat 13060, Kuwait

^b Core Labs, King Abdullah University of Science and Technology (KAUST), Thuwal, 23955-6900, Saudi Arabia.

*Corresponding authors: Abdulrahman M. Alazemi, fax: +965 24816482, E-mail: a.alazmi@ku.edu.kw. Fouzi Mouffouk, fax: +965 24816482, E-mail: fmouffouk@ku.edu.kw

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a. Original (used in manuscript) DOSY data of the diffusion coefficient for biotin-pentadecafluorooctanoyl.

SIMFIT RESULTS

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Dataset :

/opt/topspin3.5pl7/abdelhamid/data/Mariusz_Fouzi_DOSY_D6_1H_31jan24/31/pdata/1/c
t1t2.txt

AREA fit : Diffusion : Variable Gradient :

$$I=I[0]*\exp(-D*\text{SQR}(2*\text{PI}*\text{gamma}*\text{Gi}*\text{LD})*(BD-LD/3)*1e4)$$

31 points for Integral 1, Integral Region from 4.665 to 3.567 ppm

Converged after 57 iterations!

Results Comp. 1

$$I[0] \quad = \quad 9.219\text{e-}01$$

$$\text{Diff Con.} \quad = \quad 1.889\text{e-}08 \text{ m}^2/\text{s}$$

$$\text{Gamma} \quad = \quad 1.071\text{e+}03 \text{ Hz/G}$$

$$\text{Little Delta} \quad = \quad 2.000\text{m}$$

$$\text{Big Delta} \quad = \quad 197.130\text{m}$$

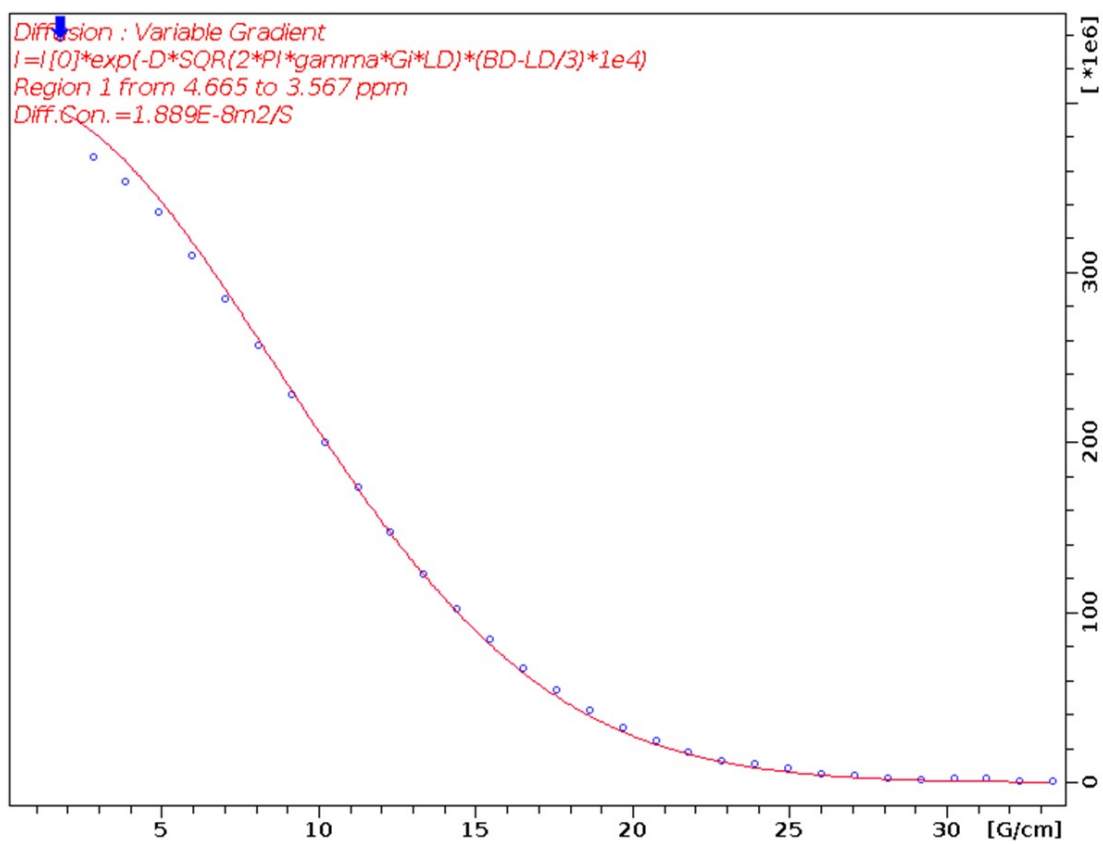
$$\text{RSS} \quad = \quad 1.252\text{e-}02$$

$$\text{SD} \quad = \quad 2.010\text{e-}02$$

Point	Gradient	Expt	Calc	Difference
1	1.736e+00	1.000e+00	9.034e-01	-9.659e-02
2	2.790e+00	8.407e-01	8.749e-01	3.427e-02
3	3.845e+00	8.077e-01	8.347e-01	2.706e-02
4	4.900e+00	7.681e-01	7.846e-01	1.647e-02
5	5.954e+00	7.080e-01	7.266e-01	1.857e-02
6	7.009e+00	6.497e-01	6.628e-01	1.310e-02

7	8.064e+00	5.884e-01	5.957e-01	7.307e-03
8	9.118e+00	5.227e-01	5.275e-01	4.809e-03
9	1.017e+01	4.580e-01	4.601e-01	2.055e-03
10	1.123e+01	3.978e-01	3.954e-01	-2.413e-03
11	1.228e+01	3.376e-01	3.347e-01	-2.896e-03
12	1.334e+01	2.809e-01	2.792e-01	-1.749e-03
13	1.439e+01	2.344e-01	2.294e-01	-5.014e-03
14	1.545e+01	1.923e-01	1.857e-01	-6.579e-03
15	1.650e+01	1.544e-01	1.481e-01	-6.294e-03
16	1.756e+01	1.239e-01	1.163e-01	-7.524e-03
17	1.861e+01	9.764e-02	9.007e-02	-7.573e-03
18	1.967e+01	7.356e-02	6.868e-02	-4.886e-03
19	2.072e+01	5.653e-02	5.160e-02	-4.932e-03
20	2.177e+01	4.033e-02	3.819e-02	-2.147e-03
21	2.283e+01	2.909e-02	2.784e-02	-1.255e-03
22	2.388e+01	2.539e-02	2.000e-02	-5.389e-03
23	2.494e+01	1.932e-02	1.415e-02	-5.163e-03
24	2.599e+01	1.220e-02	9.866e-03	-2.339e-03
25	2.705e+01	1.067e-02	6.778e-03	-3.888e-03
26	2.810e+01	6.683e-03	4.586e-03	-2.097e-03
27	2.916e+01	3.864e-03	3.056e-03	-8.076e-04
28	3.021e+01	5.745e-03	2.008e-03	-3.737e-03
29	3.127e+01	6.037e-03	1.299e-03	-4.738e-03
30	3.232e+01	2.560e-03	8.277e-04	-1.732e-03
31	3.338e+01	2.430e-03	5.199e-04	-1.910e-03

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b. Original (second run) DOSY data of the diffusion coefficient for biotin-pentadecafluorooctanoyl.

SIMFIT RESULTS

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Dataset :

/opt/topspin3.5pl7/abdelhamid/data/Mariusz_Fouzi_DOSY_Ref_1H_15Sep25/33/pdata/1/ct1t2.txt

AREA fit : Diffusion : Variable Gradient :

$$I=I[0]*\exp(-D*\text{SQR}(2*PI*\gamma*Gi*LD)*(BD-LD/3)*1e4)$$

31 points for Integral 1, Integral Region from 7.447 to 7.110 ppm

Converged after 59 iterations!

Results Comp. 1

$$I[0] \quad = \quad 1.001e+00$$

$$\text{Diff Con.} \quad = \quad 3.474e-08 \text{ m}^2/\text{s}$$

$$\text{Gamma} \quad = \quad 1.071e+03 \text{ Hz/G}$$

$$\text{Little Delta} \quad = \quad 2.000\text{m}$$

$$\text{Big Delta} \quad = \quad 197.130\text{m}$$

$$\text{RSS} \quad = \quad 2.489e-04$$

$$\text{SD} \quad = \quad 2.834e-03$$

Point	Gradient	Expt	Calc	Difference
1	6.810e-01	1.000e+00	9.953e-01	-4.682e-03
2	2.790e+00	9.047e-01	9.093e-01	4.581e-03
3	3.845e+00	8.336e-01	8.339e-01	3.276e-04
4	4.900e+00	7.437e-01	7.441e-01	4.430e-04
5	5.954e+00	6.491e-01	6.460e-01	-3.082e-03

6	7.009e+00	5.435e-01	5.456e-01	2.154e-03
7	8.064e+00	4.435e-01	4.483e-01	4.827e-03
8	9.118e+00	3.614e-01	3.584e-01	-2.913e-03
9	1.017e+01	2.770e-01	2.788e-01	1.757e-03
10	1.123e+01	2.131e-01	2.109e-01	-2.179e-03
11	1.228e+01	1.560e-01	1.553e-01	-6.757e-04
12	1.334e+01	1.143e-01	1.112e-01	-3.046e-03
13	1.439e+01	7.426e-02	7.748e-02	3.221e-03
14	1.545e+01	5.555e-02	5.254e-02	-3.012e-03
15	1.650e+01	3.426e-02	3.465e-02	3.919e-04
16	1.756e+01	2.379e-02	2.223e-02	-1.557e-03
17	1.861e+01	1.307e-02	1.388e-02	8.098e-04
18	1.967e+01	1.017e-02	8.429e-03	-1.738e-03
19	2.072e+01	5.515e-03	4.982e-03	-5.333e-04
20	2.177e+01	2.675e-03	2.863e-03	1.886e-04
21	2.283e+01	4.074e-03	1.601e-03	-2.473e-03
22	2.388e+01	1.324e-03	8.716e-04	-4.524e-04
23	2.494e+01	1.201e-03	4.613e-04	-7.392e-04
24	2.599e+01	1.081e-03	2.375e-04	-8.432e-04
25	2.705e+01	-9.510e-04	1.191e-04	1.070e-03
26	2.810e+01	-4.904e-03	5.803e-05	4.962e-03
27	2.916e+01	-1.096e-03	2.751e-05	1.124e-03
28	3.021e+01	2.501e-03	1.270e-05	-2.488e-03
29	3.127e+01	8.395e-03	5.700e-06	-8.389e-03
30	3.232e+01	-1.823e-03	2.489e-06	1.826e-03
31	3.338e+01	1.299e-03	1.058e-06	-1.298e-03

