Supporting Information

Reversible Single-Chain Selective Point Folding via Cyclodextrin Driven Host/Guest Chemistry in Water

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Materials

2-Bromoisobutyric acid (Sigma Aldrich, 98 %), carbon disulfide (Acros, 99.9 %), copper(I) iodide (CuI, Sigma Aldrich, purum, > 99.5 %), deuterium oxide (D_2O; Eurisotop, 99.9 %), *N*,*N*'-dicyclohexylcarbodiimide (DCC; ABCR, 99 %), *N*,*N*-diisopropylethylamine (DIPEA; Acros, 99.5+ %), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (EDC; TCI, > 98 %), *N*,*N*-dimethylaminopyridine (DMAP; Sigma Aldrich, 99 %), 3,3'-disulfanediyldipropanoic acid (ABCR, 99 %), dithiothreitol (DTT; ABCR), ethylenediaminetetraacetic acid disodium salt (EDTA; ABCR, 99 %), potassium phosphate monohydrate (Sigma-Aldrich, puriss.), propargylalcohol (Alfa Aesar, 99 %), silica gel

(Merck, Geduran SI60. 0.063−0.200 mm), and triethylamine (Acros, 99 %) were used as received. *N*,*N*-dimethylacrylamide (DMAa; TCI, 99 %) was passed over a short column of basic alumina prior to use. 2,2'-Azobis(2-methylpropionitrile) (AIBN; Fluka, 99 %) was recrystallized twice from methanol. Anhydrous dichloromethane (DCM) and tetrahydrofuran (THF) were purchased from Acros (extra dry over molecular sieves) and used as received. All other solvents were of analytical grade and used as received.

Characterization Methods

Nuclear magnetic resonance (NMR) measurements were carried out on a Bruker Avance 400 spectrometer (^{1}H, 400 MHz; ^{13}C, 100 MHz) for structure confirmation. Samples were dissolved in $CDCl_3$. The δ-scale was referenced with tetramethylsilane (δ = 0.00) as internal standard. Abbreviations used in the description of the materials synthesis include singlet (s), broad singlet (bs), doublet (d), triplet (t), quartet (q), quintet (quin), and multiplet (m).

NOESY experiments were performed on a 600 MHz Bruker Avance III spectrometer equipped with a ^{1}H, ^{13}C, ^{15}N-TCI inversely detecting cryoprobe at a temperature of 295 K or 320 K. The mixing time was set to 200 µs. The 90° pulse was determined to be 8.7 µs. Spectra were recorded with 4k × 1k complex data points using 16 or 20 scans per t_1 increment and 16 dummy scans at 25 °C and 50 °C. The spectral width was set to 8 × 8 ppm which leads to a total experiment time of 5 h, 33 min and 43 s and 6 h, 57 min and 4 s, respectively. After zero filling to 4k × 2k points and apodization, using a 90°-phase shifted squared sine function, the spectra were Fourier transformed.

DOSY experiments were performed on a 400 MHz Bruker Avance III spectrometer equipped with a broadband ^{1}H decoupling probe (PABBO) using an Eddy current compensated bipolar gradient pulse sequence (BPLED)[1] at a temperature of 298 K. Proton pulse lengths were determined to be 11.15 µs and bipolar gradients of δ = 4.8 – 6.4 ms (depending on the diffusion behavior of the measured sample) length were incremented from G = 1 G/cm to 49 G/cm in 32

steps. 8 scans with 12k complex data points were recorded for each increment with 8 dummy scans per experiment, leading to an overall experiment time of 20 minutes and 31 seconds per sample. The diffusion delay Δ was set to 100 ms. Processing was achieved using Topspin 3.1 with the Dynamics Center 2.0.4. After zero filling to 24k points and apodization using an exponential window function with an additional linewidth of 0.1 Hz, 1D increment spectra were Fourier transformed and the signal decay due to gradients was fitted using

$$f(G) = I_0 \cdot e^{\left(-\gamma_H{}^2 \cdot G^2 \cdot \delta^2 \cdot \left(\Delta - \frac{\delta}{3}\right)\right) \cdot D}$$

with the proton gyromagnetic ratio γ_H and the full signal intensity I_0. Corresponding diffusion coefficients D of the polymer signals and the solvent are the result of the fitting procedure (see the Appendix to the Supporting Information section) and are plotted against chemical shifts in Figure S11.

Size exclusion chromatography (SEC) was performed on a Polymer Laboratories PL-GPC 50 Plus Integrated System, comprising an autosampler, a PLgel 5 μm bead-size guard column (50 × 7.5 mm) followed by three PLgel 5 μm MixedC columns (300 × 7.5 mm) and a differential refractive index detector using *N*,*N*-dimethylacetamide (DMAc) containing 0.03 wt% LiBr as eluent at 50 °C with a flow rate of 1.0 mL min^{-1}. The SEC system was calibrated against linear polystyrene standards with molecular weights ranging from 474 to $2.5 \cdot 10^6$ g mol^{-1}. All SEC calculations were carried out relative to polystyrene calibration (Mark-Houwink-Parameters $K = 14.1 \cdot 10^{-5}$ dL g^{-1}; $\alpha = 0.7$).[2]

Electrospray ionization-mass spectrometry (ESI-MS) spectra were recorded on a LXQmass spectrometer (ThermoFisher Scientific, San Jose, CA) equipped with an atmospheric pressure ionization source operating in the nebulizer-assisted electrospray mode. The instrument was calibrated in the *m*/*z* range 195-1822 Da using a standard containing caffeine, Met-Arg-Phe-Ala acetate (MRFA), and a mixture of fluorinated phosphazenes (Ultramark 1621) (all from Aldrich). A constant spray voltage of 4.5 kV was used, and nitrogen at a

dimensionless sweep gas flow rate of 2 (~ 3 L min^{-1}) and a dimensionless sheath gas flow rate of 12 (~ 1 L min^{-1}) were applied. The capillary voltage, the tube lens offset voltage, and the capillary temperature were set to 60 V, 110 V, and 300 °C, respectively. The samples were dissolved with a concentration of 0.1 mg mL^{-1} in a mixture of THF and MeOH (3:2) containing 100 μmol of sodium triflate and infused with a flow of 10 μL min^{-1}.

Dynamic light scattering (DLS) was performed on a NICOMP 380 DLS spectrometer (Particle Sizing Systems, Santa Barbara, USA) with a 90 mW laser diode operating at 658 nm equipped with an avalanche photodiode detector. The measurements were performed in automatic mode and evaluated with a standard Gaussian and an advanced evaluation method, the latter using an inverse Laplace algorithm to analyze for multimodal distributions. Numbers given in text are the number-weighted average values as calculated by the NICOMP evaluation. All measurements were determined at 90° to the incident beam.

UV/Vis spectra were recorded on a Varian Cary 300 Bio spectrophotometer featuring a thermostatted sample cell holder at 25 °C in acetonitrile from 200 nm to 800 nm with a resolution of 1 nm and slit width of 2 nm.

Experimental Procedures

Synthesis of di(prop-2-yn-1-yl) 3,3'-disulfanediyldipropanoate

In a 500 mL Schlenk flask 3,3'-disulfanediyldipropanoic acid (6.00 g, 28.53 mmol, 1.0 eq.), propargyl alcohol (5.1 mL, 88.25 mmol, 3.1 eq.), and DMAP (1.40 g, 11.42 mmol, 0.4 eq.) were dissolved in anhydrous THF (240 mL). The mixture was cooled to 0 °C and a solution of DCC (17.67 g, 85.64 mmol, 3.0 eq.) in anhydrous DCM (90 mL) was added. After one hour the solution was warmed to ambient temperature, stirred overnight, filtered, and concentrated under reduced pressure. The residual oil was purified by column chromatography on silicagel with a 6:1 mixture of *n*-hexane/ethyl acetate as the eluent that was changed gradually to 5:1. The product-containing fractions were concentrated and di(prop-2-yn-1-yl) 3,3'-disulfanediyldipropanoate was obtained as a viscous oil (6.12 g, 21.37 mmol, 75 %).

^{1}H-NMR (400 MHz, $CDCl_3$): [δ, ppm] = 2.49 (t, 2H, C***H***-C-CH_2), 2.79 (t, 4H, O=C-C***H***$_2$), 2.93 (t, 4H, S-C***H***$_2$), 4.71 (d, 4H, C-C***H***$_2$-O). ^{13}C-NMR (100 MHz, $CDCl_3$): [δ, ppm] = 32.9 (S-CH_2-***C***H_2), 34.0 (S-***C***H_2-CH_2), 52.4 (O-***C***H_2-C-CH), 75.3 (CH_2-C-***C***H), 77.5 (CH_2-***C***-CH), 171.0 (***C***=O). ESI-MS: $[M + Na^+]_{exp}$ = 309.08 and $[M + Na^+]_{calc}$ = 309.02.

Synthesis of 2-methyl-2-((((3-oxo-3-(prop-2-yn-1-yloxy)propyl)thio)carbonothioyl)thio) propanoic acid (CTA1)

In a 250 mL round-bottom flask di(prop-2-yn-1-yl) 3,3'-disulfanediyldipropanoate (6.12 g, 21.37 mmol, 1.0 eq.) and triethylamine (4.1 mL, 29.58 mmol, 1.4 eq.) were dissolved in DCM (70 mL). The mixture was purged with argon for 30 min and DTT (4.85 g, 31.44 mmol, 1.5 eq.) was added subsequently. The mixture was stirred at ambient temperature overnight. 1N HCl (120 mL) was added, the organic phase was separated, washed with brine (120 mL), dried over Na_2SO_4, and filtered. After evaporation of the solvent the yellow oil was purified by column chromatography on silica gel with *n*-hexane/ethyl acetate 10:1 as eluent to give prop-2-yn-1-yl

3-mercaptopropanoate as colorless oil (3.91 g, 27.12 mmol, 64 %), which was used directly in the subsequent reaction.

Based on a literature procedure,[3, 4] in a 250 mL round-bottom flask prop-2-yn-1-yl 3-mercaptopropanoate (3.90 g, 27.04 mmol, 1.1 eq.) was dissolved in a suspension of K_3PO_4 (7.42 g, 35.00 mmol, 1.4 eq.) in acetone (100 mL) at ambient temperature. After stirring for 20 min at ambient temperature carbon disulfide (4.5 mL, 74.47 mmol, 3.0 eq.) was added and the solution turned yellow. 2-Bromoisobutyric acid (4.29 g, 25.15 mmol, 1.0 eq.) was added after 20 min and the mixture was stirred at ambient temperature overnight. 1N HCl (300 mL) was added and the aqueous phase was extracted with DCM (2 × 200 mL). The combined organic extracts were washed with deionized H_2O (200 mL), brine (200 mL), dried over Na_2SO_4, and filtered. After evaporation of the solvent the yellow oil was purified via column chromatography on silica gel with *n*-hexane/ethyl acetate as eluent that was gradually changed from 5:1 to 3:1 to give **CTA1** as a yellow solid (3.59 g, 11.72 mmol, 47 %).

^{1}H-NMR (400 MHz, $CDCl_3$): [δ, ppm] = 1.72 (s, 6H, 2x C-C***H***$_3$), 2.49 (t, 1H, C***H***-C-CH_2), 2.80 (t, 2H, O=C-C***H***$_2$), 3.56 (t, 2H, S-C***H***$_2$), 4.70 (d, 2H, C-C***H***$_2$-O). ^{13}C-NMR (100 MHz, $CDCl_3$): [δ, ppm] = 25.3 (2x ***C***H_3-C), 31.1 (S-CH_2-***C***H_2), 33.0 (S-***C***H_2-CH_2), 52.5 (***C***$(CH_3)_2$), 56.0 (O-***C***H_2-C-CH), 75.4 (CH_2-C-***C***H), 77.4 (CH_2-***C***-CH), 170.8 (***C***=O), 178.7 (***C***=O), 220.2 (***C***=S). ESI-MS: $[M + Na^+]_{exp}$ = 329.33 and $[M + Na^+]_{calc}$ = 328.99.

Synthesis of 6-(((3s,5s,7s)-adamantan-1-yl)amino)-6-oxohexyl 2-methyl-2-((((3-oxo-3-(prop-2-yn-1-yloxy)propyl)thio)carbonothioyl)thio)propanoate (CTA2)

CTA1 (1 g, 3.26 mmol, 1 eq.), *N*-(adamantan-1-yl)-6-hydroxyhexanamide[5, 6] (1.3 g, 4.89 mmol, 1.5 eq.), and DMAP (40 mg, 0.33 mmol, 0.1 eq.) were dissolved in dry DCM (20 mL) in a flame-dried Schlenk flask and cooled to 0 °C. EDC (937 mg, 4.89 mmol, 1.5 eq.) was added and the mixture was stirred over night at ambient temperature. Subsequently, the reaction mixture was washed with $NaHCO_3$ solution (100 mL). The aqueous phase was extracted with

DCM (2 × 50 mL). The combined organic layers were successively washed with 1N HCl, deionized H_2O, and brine (100 mL each) and dried over Na_2SO_4. **CTA2** was isolated as a yellow oil (638 mg, 1.15 mmol, 35 %) by column chromatography on silica gel with *n*-hexane/ethyl acetate (4:1) as the eluent.

^{1}H-NMR (400 MHz, $CDCl_3$): [δ, ppm] = 1.34 (quin, 2H, H_h), 1.54 – 1.75 (m, 16H, $H_{e,g,i,m}$), 1.99 (s, 6H, H_k), 2.00 – 2.14 (m, 5H, $H_{j,l}$), 2.49 (s, 1H, H_a), 2.78 (t, 2H, H_c), 3.54 (t, 2H, H_d), 4.08 (t, 2H, H_f), 4.70 (s, 2H, H_b), 5.14 (bs, 1H, NH). ^{13}C-NMR (100 MHz, $CDCl_3$): [δ, ppm] = 25.3, 25.6, 28.2, 29.5, 30.9, 32.9, 36.4, 37.5, 41.7, 51.9, 52.4, 56.4, 66.0, 75.3, 77.3, 170.6, 172.0, 172.8, 220.6. ESI-MS: $[M + Na^+]_{exp} = 576.19$ and $[M + Na^+]_{calc} = 576.16$.

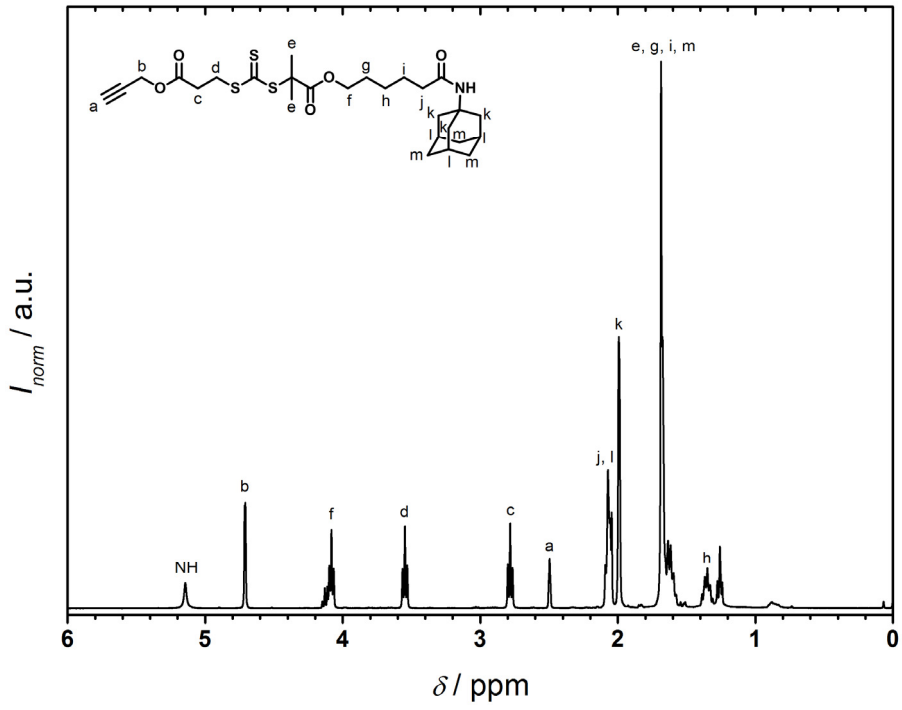

Figure S1. ^{1}H NMR spectrum (400 MHz) of **CTA2** at 25 °C in $CDCl_3$.

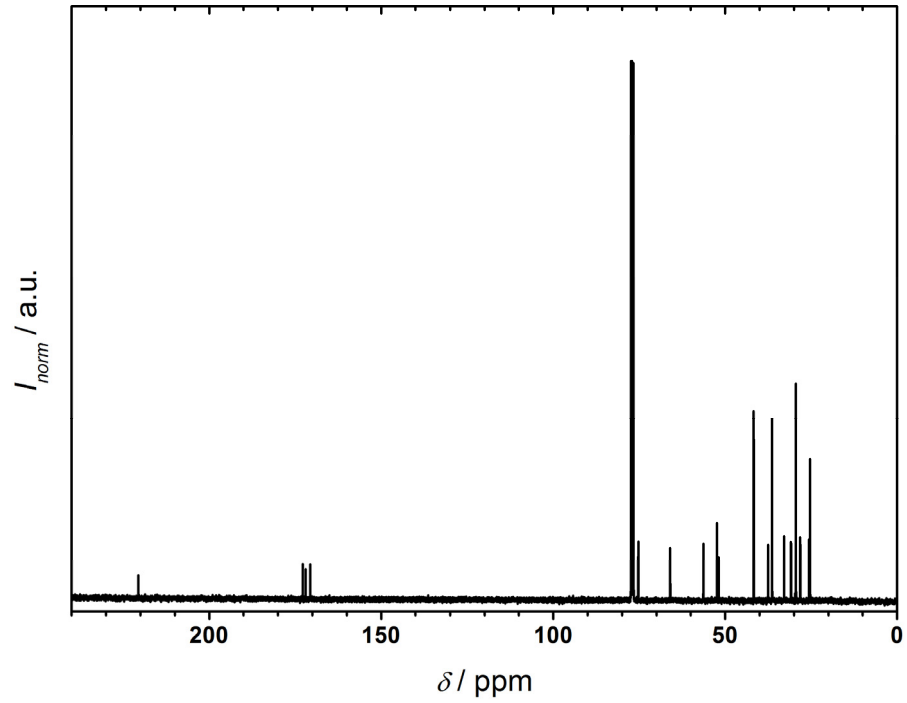

Figure S2. ^{13}C NMR spectrum (100 MHz) of **CTA2** at 25 °C in $CDCl_3$.

RAFT Polymerization of DMAa with CTA2 for ^1H NMR and ESI-MS Analysis

CTA2 (38.77 mg, 0.07 mmol, 1 eq.), AIBN (2.13 mg, 0.013 mmol, 0.2 eq.), DMAa (200 mg, 2 mmol, 30 eq.) and DMF (2 mL) were added into a Schlenk tube. After three freeze-pump-thaw cycles, the tube was backfilled with argon and placed into an oil bath pre-heated to 60 °C for 4 h. The polymerization was stopped by cooling the reaction mixture in liquid nitrogen and opening the tube to the atmosphere. The mixture was dialyzed against deionized water with a SpectraPor3 membrane (MWCO = 1000 Da) for three days at ambient temperature. The solvent was removed in vacuo at a freeze-drier to yield the polymer Alkyne-PDMAa-Ada as a yellow solid (29 mg, 0.006 mmol). SEC (DMAC, RI): $M_{n,SEC}$ = 5000 g mol^{-1}, $M_{m,SEC}$ = 5250 g mol^{-1}, $Đ$ = 1.06. The NMR number-average molar mass ($M_{n,NMR}$) was calculated from the integrals of the resonances at 2.27 – 2.75 ppm and 4.67 - 4.74 ppm. $M_{n,NMR}$ = 4000 g mol^{-1}.

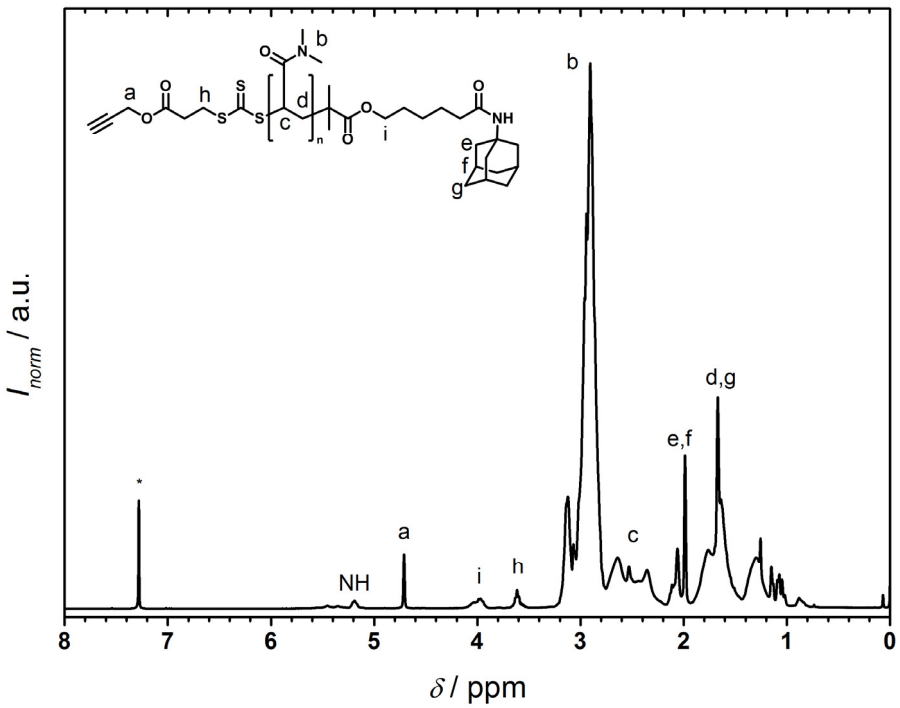

Figure S3. ^{1}H NMR spectrum (400 MHz) of Alkyne-PDMAa-Ada at 25 °C in $CDCl_3$.

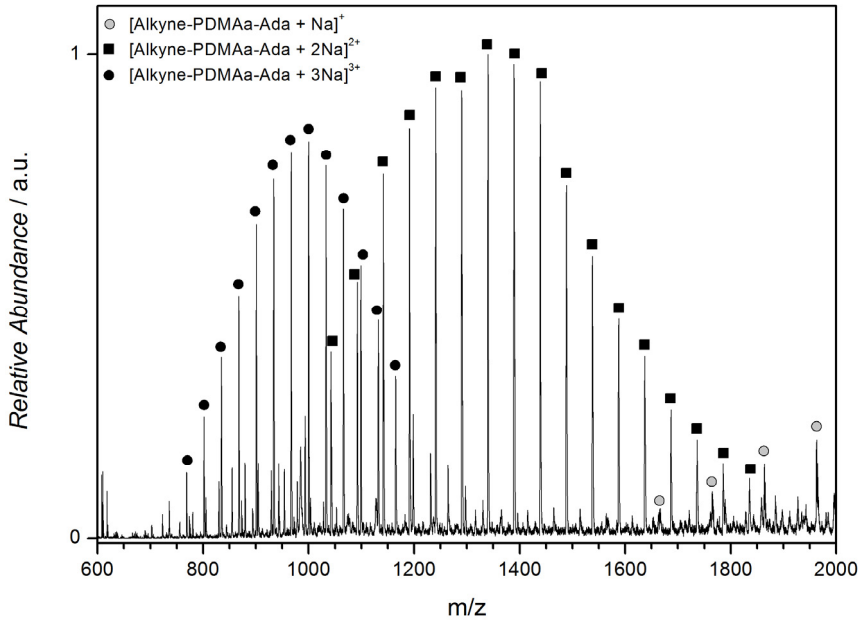

Figure S4. ESI-MS spectrum of Alkyne-PDMAa-Ada ($M_{n,SEC}$ = 5000 g mol^{-1}, $M_{m,SEC}$ = 5250 g mol^{-1}, $Đ$ = 1.06).

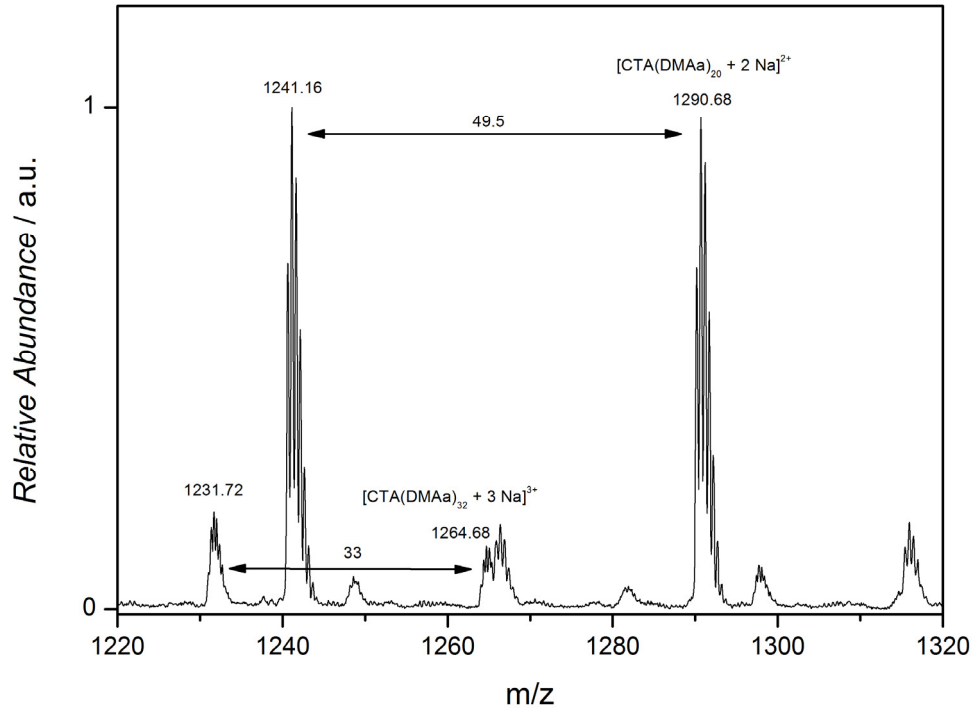

Figure S5. Section of the ESI-MS spectrum of Alkyne-PDMAa-Ada ($M_{n,SEC}$ = 5000 g mol^{-1}, $M_{m,SEC}$ = 5250 g mol^{-1}, $Đ$ = 1.06).

Table S1. Theoretical and experimental m/z of poly(DMAa) polymerized with CTA2.

Species	m/z_{theo}	m/z_{exp}	$\Delta m/z$
■ **[CTA(DMAa)$_{19}$ + 2 Na]$^{2+}$**	1240.74	1240.64	0.10
● **[CTA(DMAa)$_{31}$ + 3 Na]$^{3+}$**	1231.10	1231.04	0.06

RAFT Polymerization of DMAa with CTA2

CTA2 (124.2 mg, 0.22 mmol, 1 eq.), AIBN (7.4 mg, 0.045 mmol, 0.2 eq.), DMAa (2 g, 20.18 mmol, 90 eq.), and DMF (20 mL) were added into a Schlenk tube. After three freeze-pump-thaw cycles, the tube was backfilled with argon and placed into an oil bath pre-heated to 60 °C for 4 h. The polymerization was stopped by cooling the reaction mixture in liquid nitrogen and opening the tube to the atmosphere. The solution was dialyzed against deionized water with a SpectraPor3 membrane (MWCO = 1000 Da) for three days at ambient temperature. The

solvent was removed in vacuo at a freeze-drier to yield the polymer Alkyne-PDMAa-Ada as a yellow solid (806.5 mg, 73.3 x 10^{-3} mmol). SEC (DMAC, RI): $M_{n,SEC}$ = 11000 g mol^{-1}, $M_{m,SEC}$ = 13100 g mol^{-1}, $Đ$ = 1.19. The NMR number-average molar mass ($M_{n,NMR}$) was calculated from the integrals of the resonances at 2.27 – 2.75 ppm and 4.67 - 4.74 ppm. $M_{n,NMR}$ = 16900 g mol^{-1}.

Synthesis of the β-CD-PDMAa-Ada α,ω-functional Polymer

In a flame-dried Schlenk tube, Alkyne-PDMAa-Ada (50 mg, 4.55 x 10^{-3} mmol, 1 eq.), β-CD-N_3[7] (26.34 mg, 0.023 mmol, 5 eq.) and DIPEA (0.8 µL, 4.55 x 10^{-3} mmol, 1 eq.) were dissolved in DMF (2 mL). The mixture was degassed by three consecutive freeze-pump-thaw cycles, before copper(I) iodide (0.87 mg, 4.55 × 10^{-3} mmol, 1 eq.) was added. Subsequently, two freeze-pump-thaw cycles were performed, the tube backfilled with argon and the mixtures stirred at ambient temperature for 24 h. EDTA-solution (5 wt.%, 1 mL) was added and the residue was dialyzed against deionized water with a SpectraPor3 membrane (MWCO = 2000 Da) for 3 days at ambient temperature. The solvent was removed under vacuo at a freeze-drier to yield the polymer β-CD-PDMAa-Ada as a white solid (26.4 mg, 2.28 x 10^{-3} mmol). SEC (DMAC, RI): $M_{n,SEC}$ = 11600 g mol^{-1}, $M_{m,SEC}$ = 14000 g mol^{-1}, $Đ$ = 1.20.

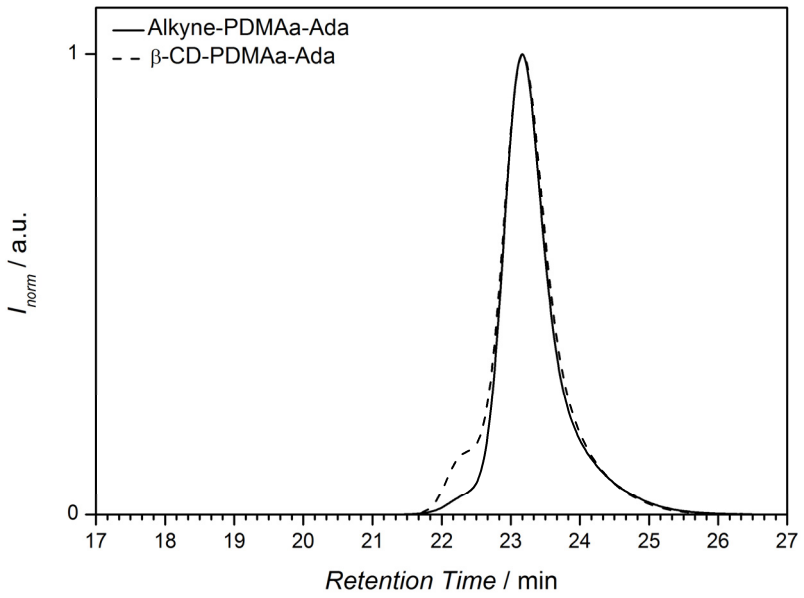

Figure S6. Normalized SEC traces of Alkyne-PDMAa-Ada (solid line) and β-CD-PDMAa-Ada (dashed line).

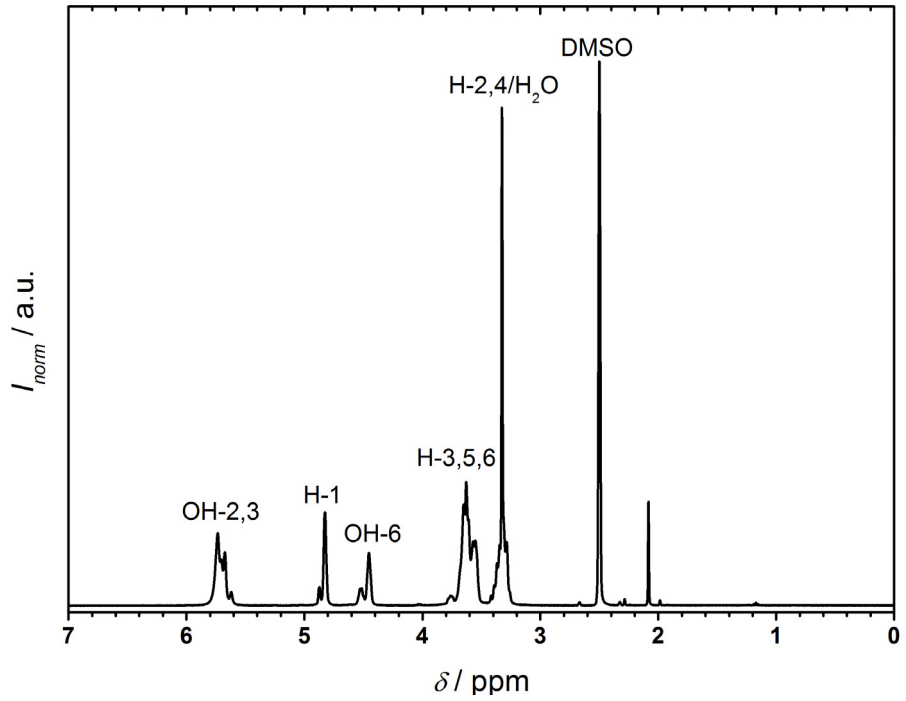

Figure S7. Normalized ^{1}H NMR spectrum (400 MHz, DMSO-d6) of the employed β-CD-azide.

ESI-MS: $[M + Na^+]_{exp} = 1182.42$ and $[M + Na^+]_{calc} = 1182.37$.

Additional Characterization Data

To investigate the stability of the trithiocarbonate moiety against aminolysis in the presence of adamantylamine hydrochloride, a solution of Alkyne-PDMAa-Ada in water was stirred with an excess of sAda at ambient temperature for 24 h. A comparison of the NMR and UV/Vis spectra (Fig. S7 and Fig. S8, respectively) before and after the treatment shows that the integral ratio of two end group resonances remains constant (1.02 vs. 1.04) and the characteristic UV absorption of the trithiocarbonate at around 307 nm is unchanged. These observations lead to the conclusion that the trithiocarbonate remains intact.

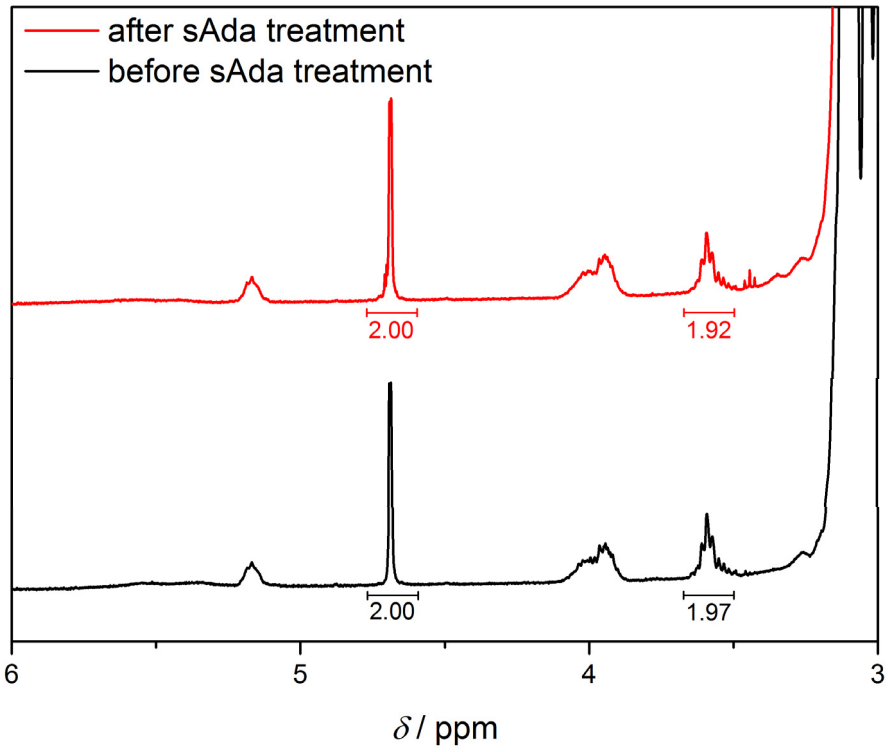

Figure S8. ^{1}H NMR spectra (400 MHz) of Alkyne-PDMAa-Ada before (black) and after (red) the treatment with 1-adamantylamine hydrochloride.

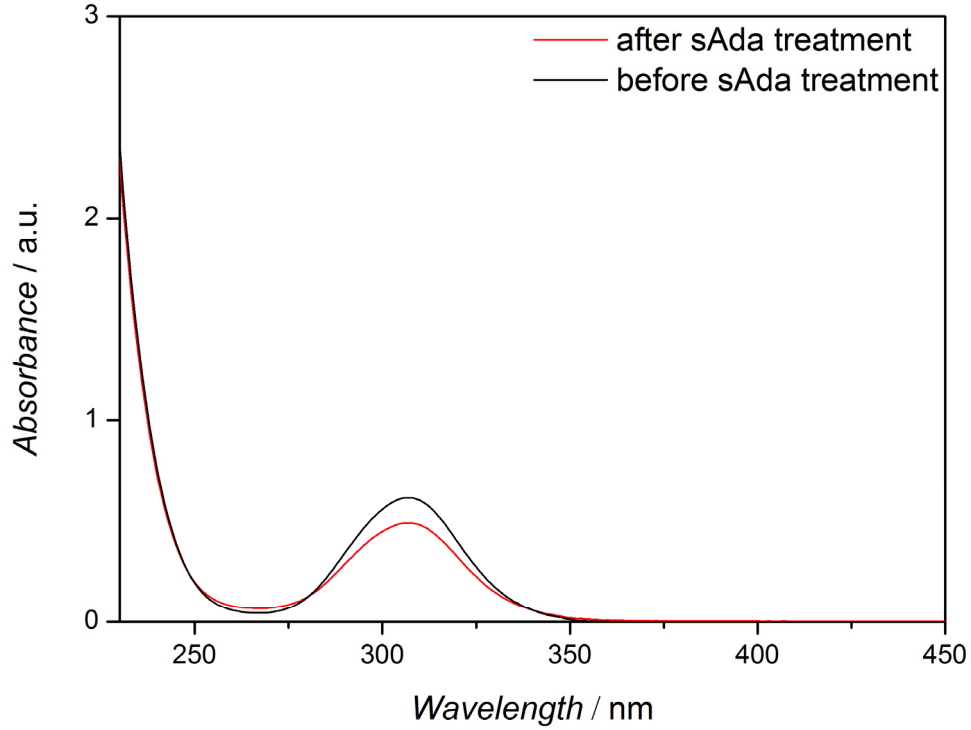

Figure S9. UV/Vis spectra of Alkyne-PDMAa-Ada before (black) and after (red) the treatment with 1-adamantylamine hydrochloride.

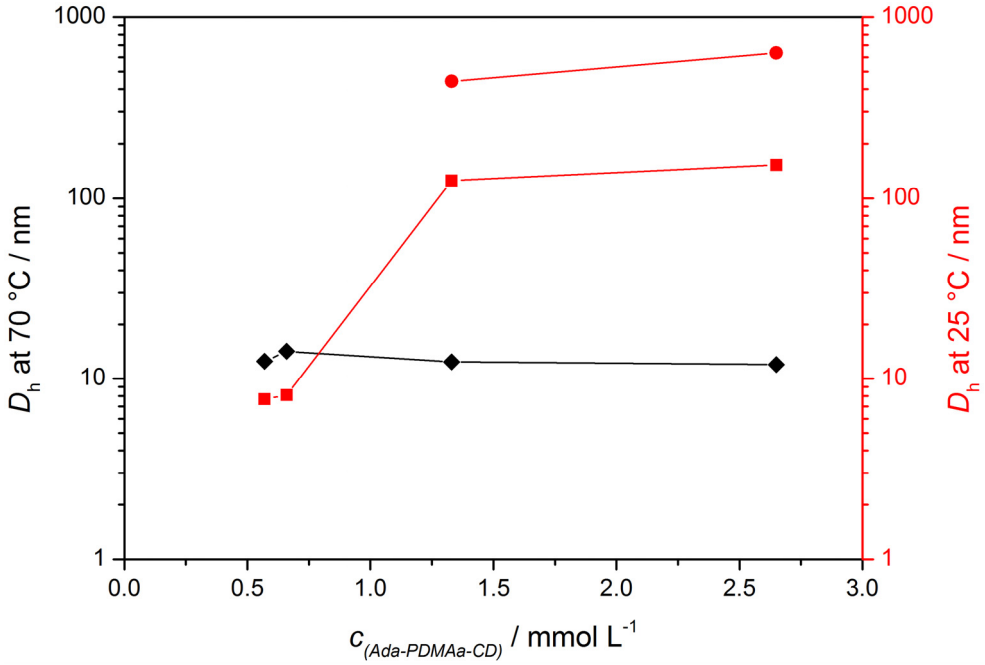

Figure S10. Number-weighted mean hydrodynamic diameter of β-CD-PDMAa-Ada at variable concentrations in water at 25 °C (red) and 70 °C (black). The red dots represent the mean hydrodynamic diameter of a second population. The lines are drawn to guide the eye.

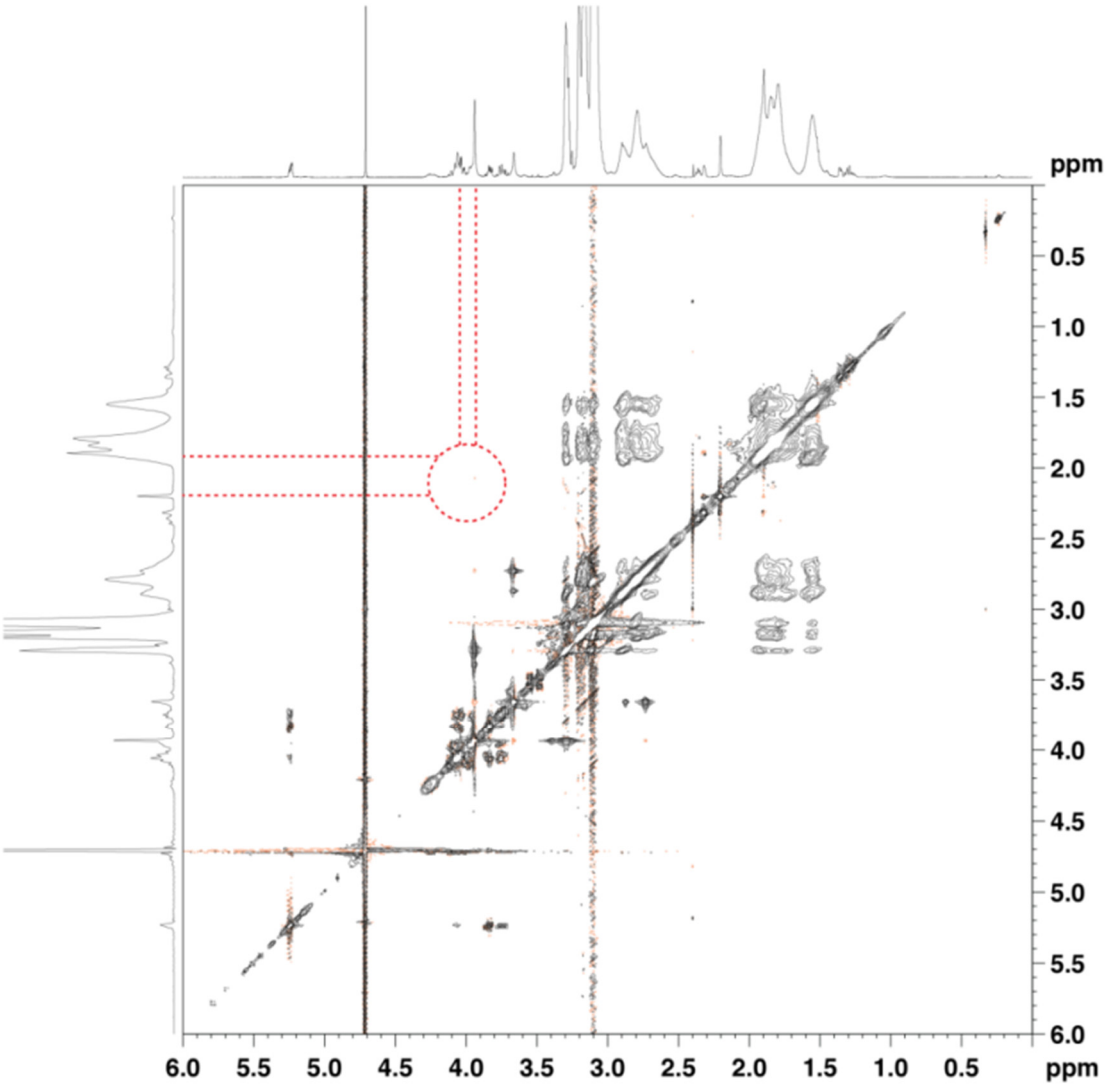

Figure S11. NOESY NMR spectrum of β-CD-PDMAa-Ada in D_2O at 50 °C. The marked area shows the absence of cross-correlation peaks.

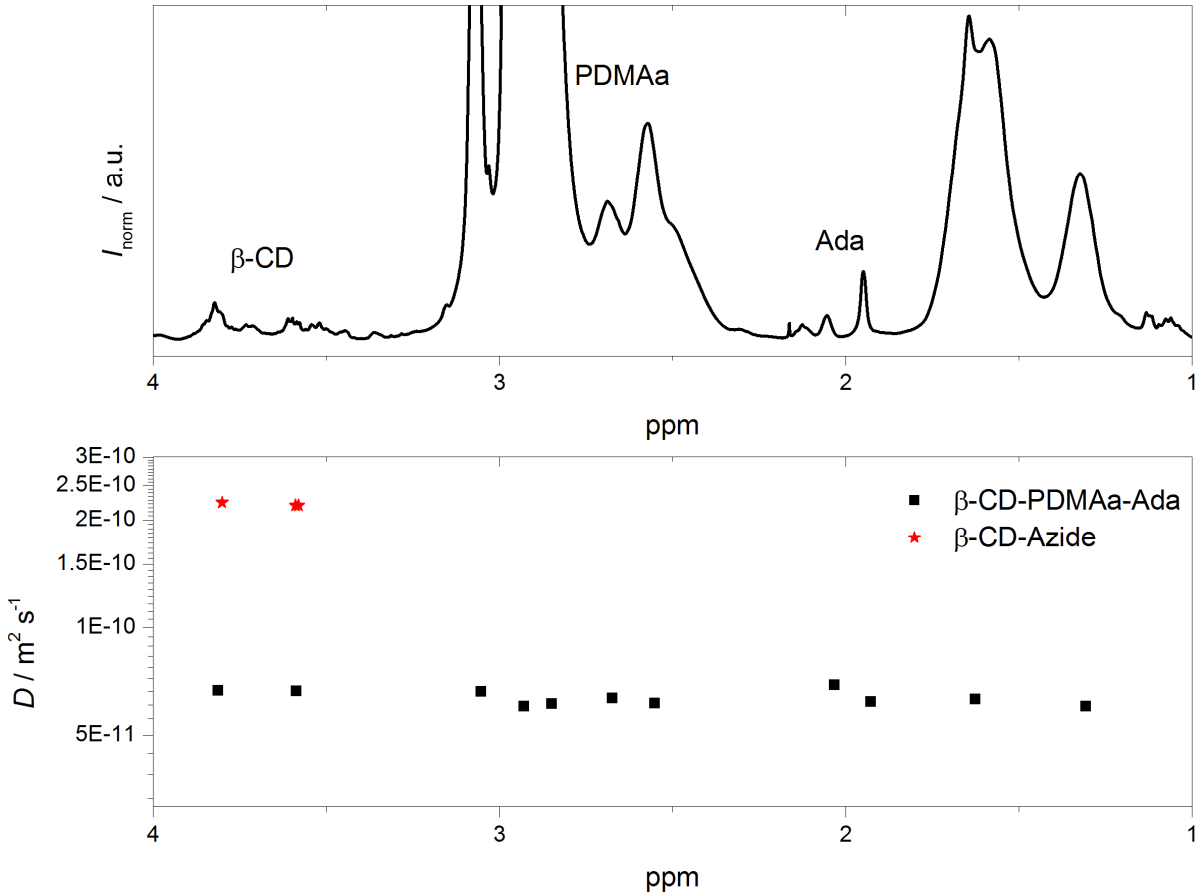

Figure S12. Top: Partial ^{1}H NMR spectrum (400 MHz, D_2O) of β-CD-PDMAa-Ada. Bottom: Diffusion coefficients corresponding to various resonances of the ^{1}H NMR spectrum at varying concentration of β-CD-PDMAa-Ada. For comparison the diffusion coefficients of β-CD-azide are plotted.

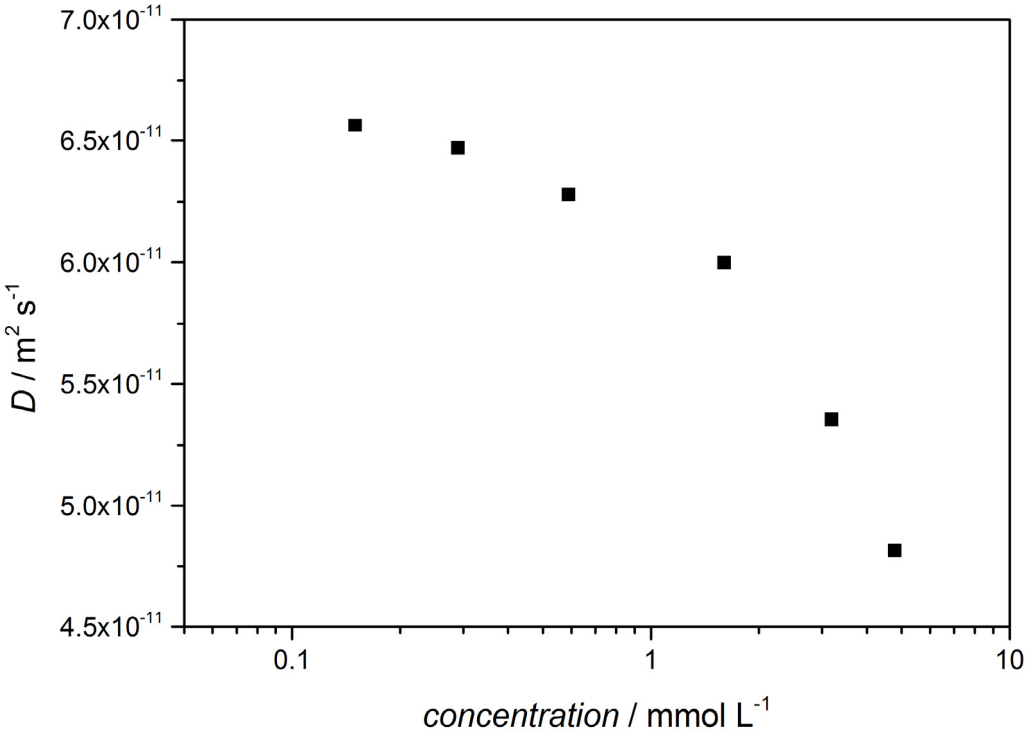

Figure S13. Averaged diffusion coefficient *D* plotted against the concentration of β-CD-PDMAa-Ada in D_2O. Taking into account the 5 % change in the diffusion coefficient of D_2O from the sample with the lowest to the sample with the highest concentration (see attached raw data below, Appendix to the SI section), the averaged diffusion coefficient at the highest concentration can be corrected to prevent an error potentially occurring due to changes in the solvent viscosity. With the corrected value of the averaged diffusion coefficient at the highest concentration, an averaged relative hydrodynamic radius between the lowest and highest concentration was estimated. With a value of 1.28 for the averaged relative hydrodynamic radius, the DOSY data leads to the assumption that oligomers are formed at higher concentrations.

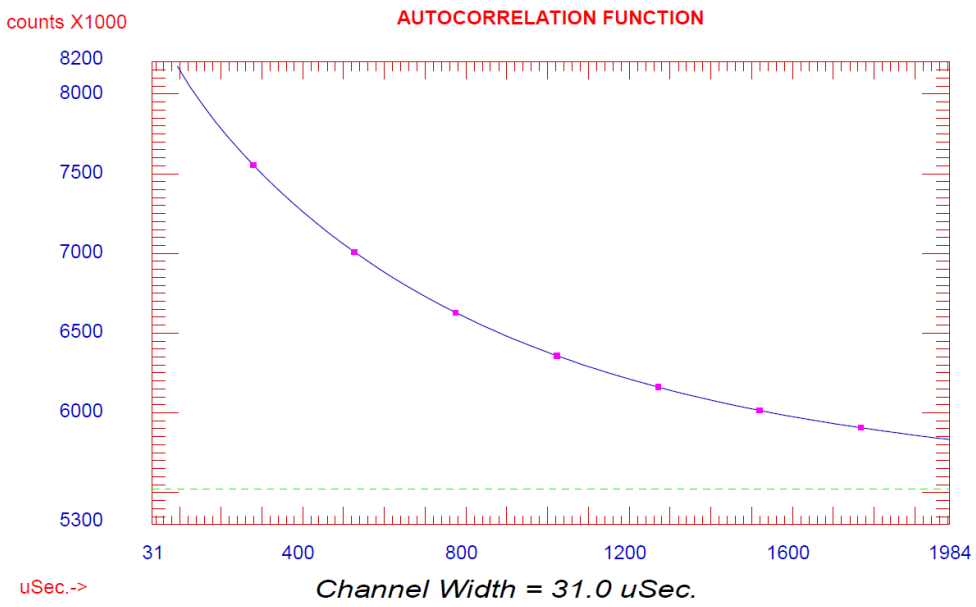

Figure S14. Autocorrelation function for the DLS measurement of β-CD-PDMAa-Ada in MilliQ water at 25 °C ($c_{polymer}$ = 0.57 mmol L^{-1}).

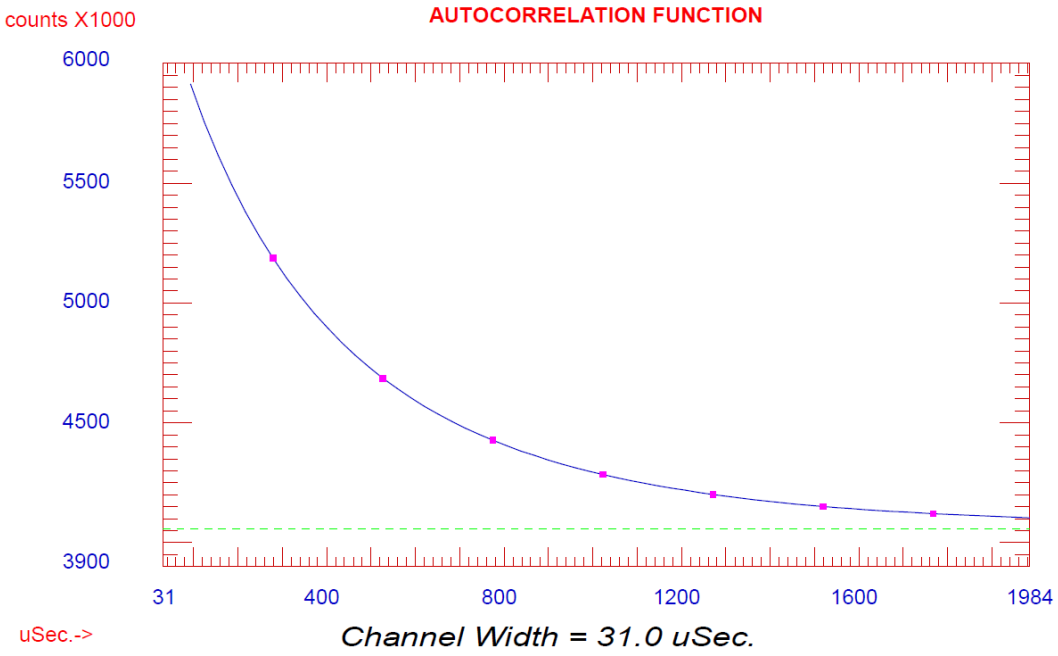

Figure S15. Autocorrelation function for the DLS measurement of β-CD-PDMAa-Ada in MilliQ water at 70 °C ($c_{polymer}$ = 0.57 mmol L^{-1}).

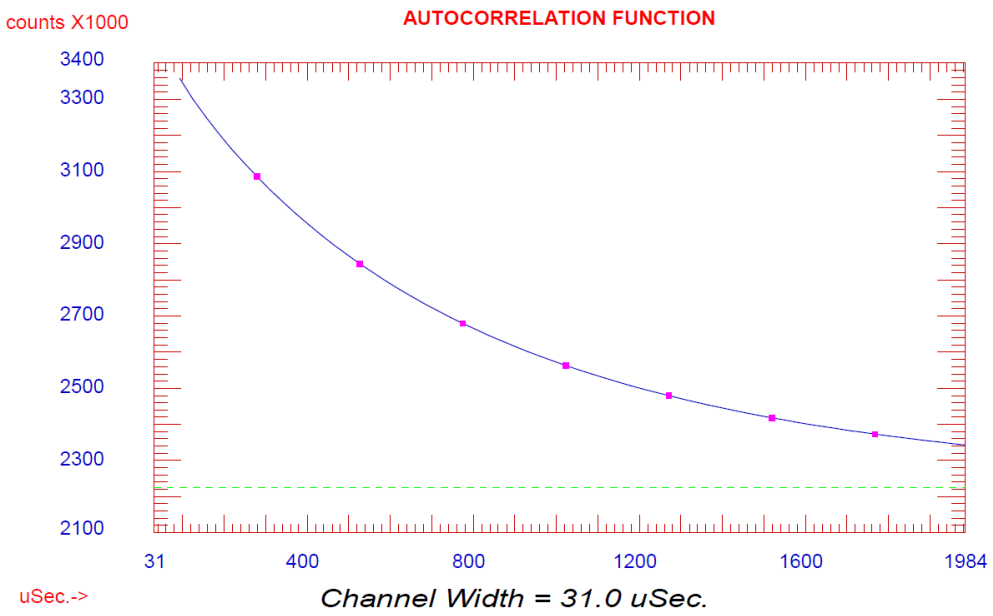

Figure S16. Autocorrelation function for the DLS measurement of β-CD-PDMAa-Ada in MilliQ water at 25 °C after cooling from 70 °C and 24 h of equilibration time ($c_{polymer}$ 0.57 mmol L^{-1}).

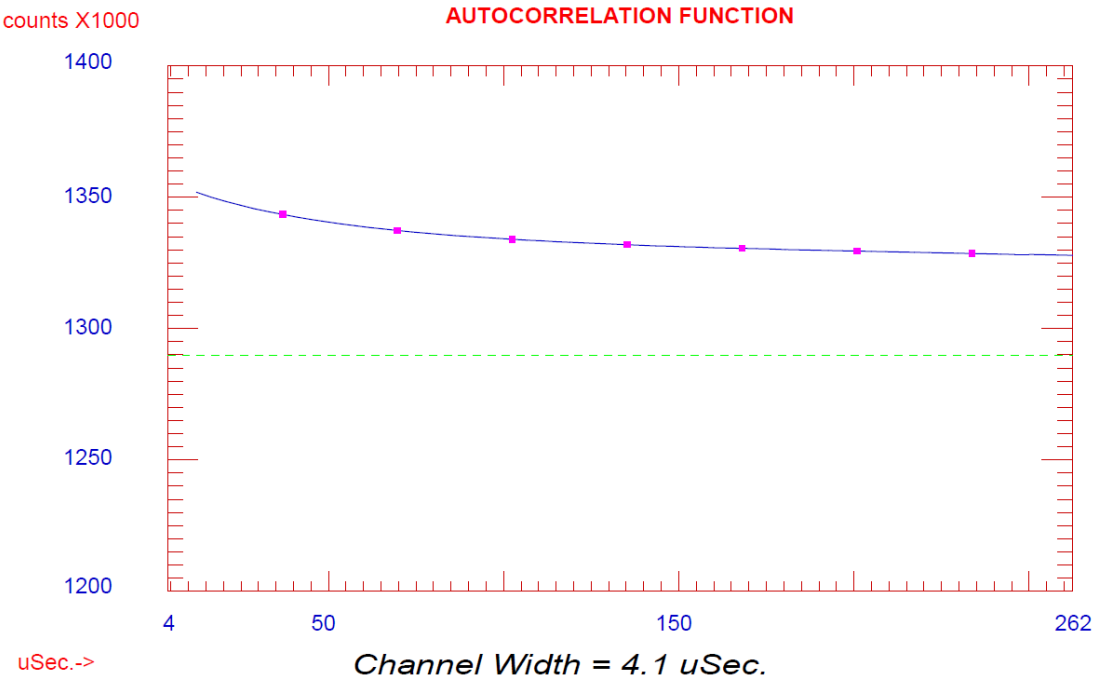

Figure S17. Autocorrelation function for the DLS measurement of β-CD-PDMAa-Ada with an excess of adamanthylamine hydrochloride in MilliQ water at 25 °C ($c_{polymer}$ = 0.57 mmol L^{-1}).

REFERENCES

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2. C. Strazielle, H. Benoit and O. Vogl, *Eur. Polym. J.*, 1978, **14**, 331-334.
3. B. V. K. J. Schmidt, M. Hetzer, H. Ritter and C. Barner-Kowollik, *Macromolecules*, 2011, **44**, 7220-7232.
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5. Z. Yu, A. R. Sawkar, L. J. Whalen, C.-H. Wong and J. W. Kelly, *J. Med. Chem.*, 2006, **50**, 94-100.
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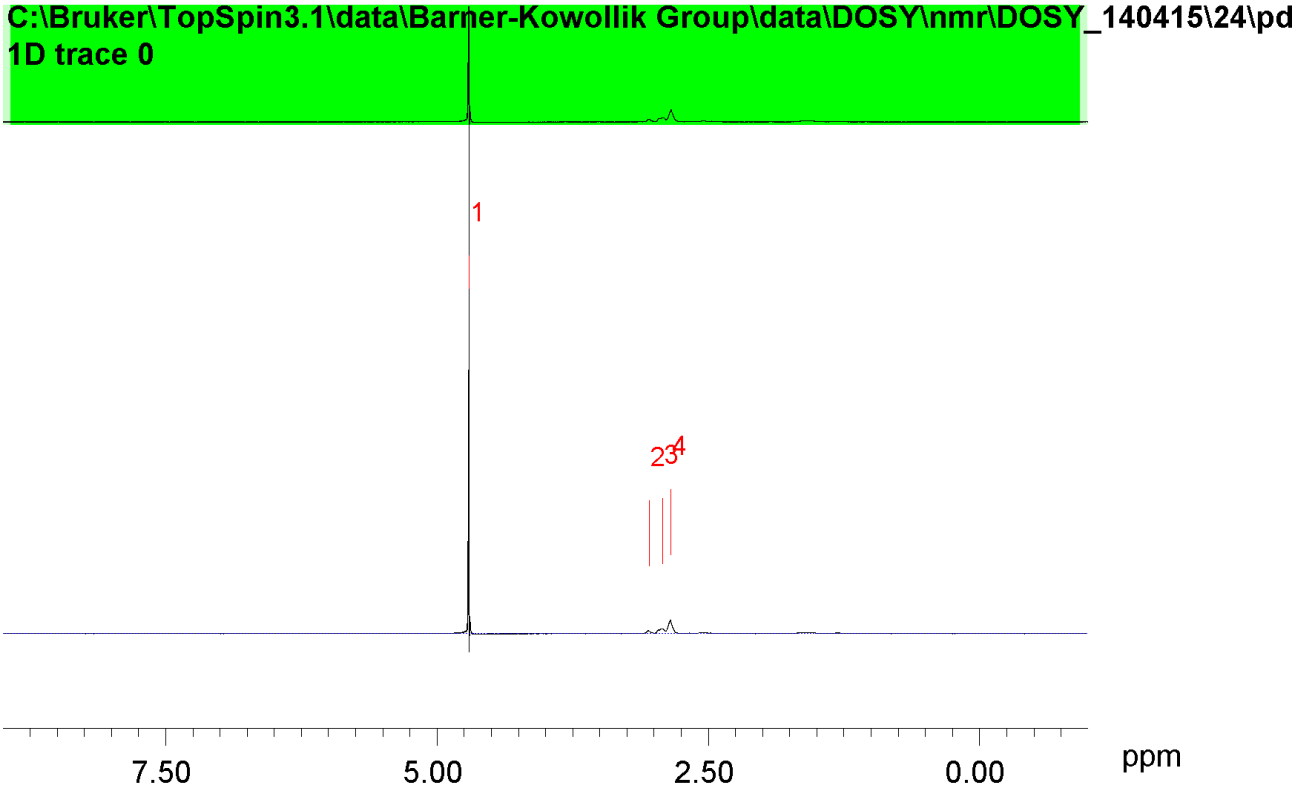
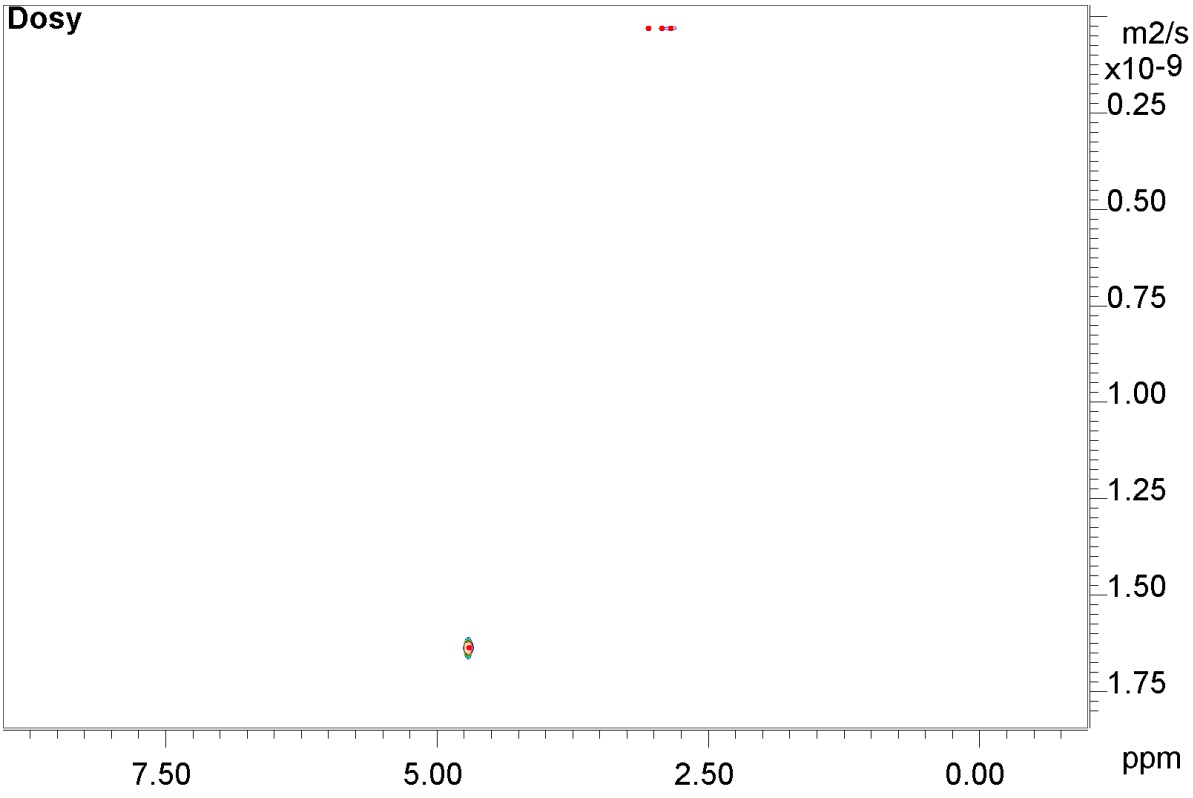
Primary DOSY Data - Appendix

Diffusion Analysis

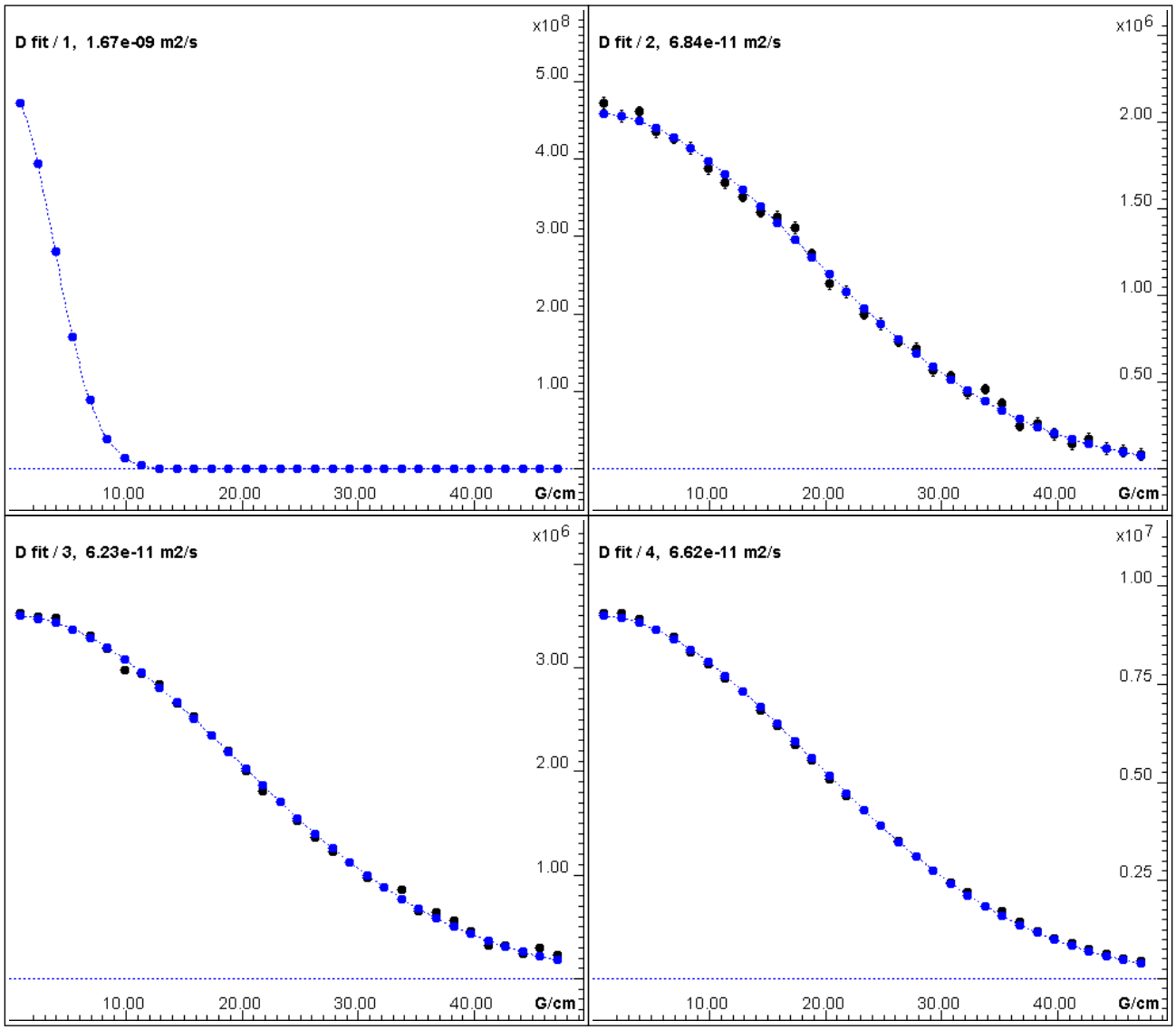
sample name:	JW183 1.7 mg/mL
Description/Title:	standard demo sample
Origin:	in-house
Date of preparation:	04 / 2014
Temperature (K):	298.0
Weight (Daltons):	11600


C:\Bruker\TopSpin3.1\data\Barner-Kowollik Group\data\DOSY\nmr\DOSY_140415\24\pd
1D trace 0
1
2
3
4
7.50
5.00
2.50
0.00
ppm


Dosy
m2/s
x10-9
0.25
0.50
0.75
1.00
1.25
1.50
1.75
7.50
5.00
2.50
0.00
ppm

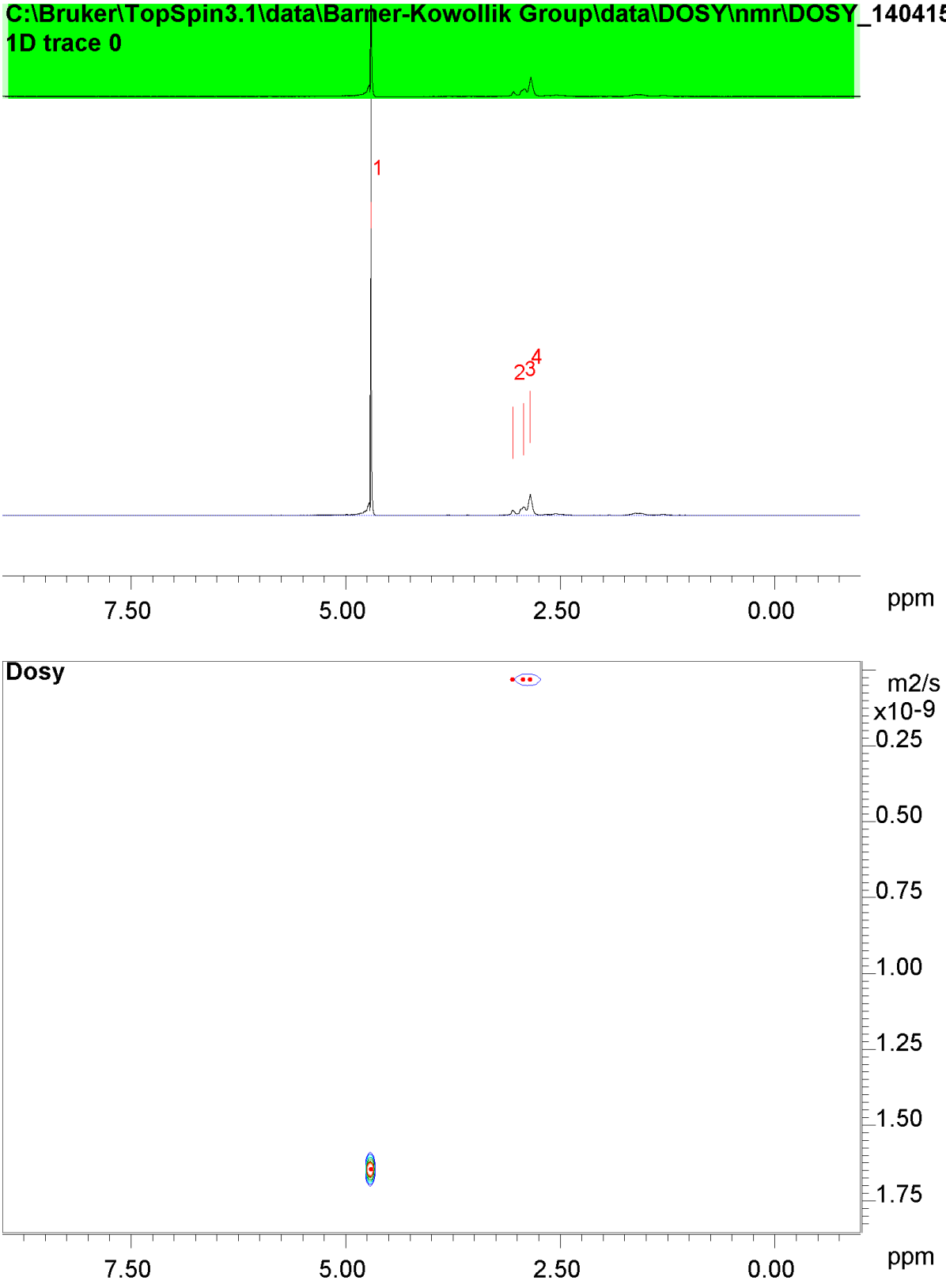
Fitted function:	f (x) = A * exp (-D * x^2 * gamma^2 * littleDelta^2 (bigDelta-littleDelta/3)* 10^4
used gamma:	26752 rad/(s*Gauss)
used little delta:	0.0055000 s
used big delta:	0.099900 s
used gradient strength:	variable
Random error estimation of data:	RMS per spectrum (or trace/plane)
Systematic error estimation of data:	worst case per peak scenario
Fit parameter Error estimation method:	from fit using arbitray y uncertainties
Confidence level:	95%
Used peaks:	peaks from C:\Bruker\TopSpin3.1\data\Barner-Kowollik Group\data\DOSY\nmr\DOSY_140415\21\pdata\1\peaklist.xml
Used integrals:	peak intensities
Used Gradient strength:	all values (including replicates) used

Peak name	F2 [ppm]	D [m2/s]	error
1	4.701	1.67e-09	1.884e-12
2	3.045	6.84e-11	2.073e-12
3	2.922	6.23e-11	1.264e-12
4	2.843	6.62e-11	7.925e-13


D fit / 1, 1.67e-09 m2/s
x10^8
5.00
4.00
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm
D fit / 2, 6.84e-11 m2/s
x10^6
2.00
1.50
1.00
0.50
10.00
20.00
30.00
40.00
G/cm
D fit / 3, 6.23e-11 m2/s
x10^6
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm
D fit / 4, 6.62e-11 m2/s
x10^7
1.00
0.75
0.50
0.25
10.00
20.00
30.00
40.00
G/cm

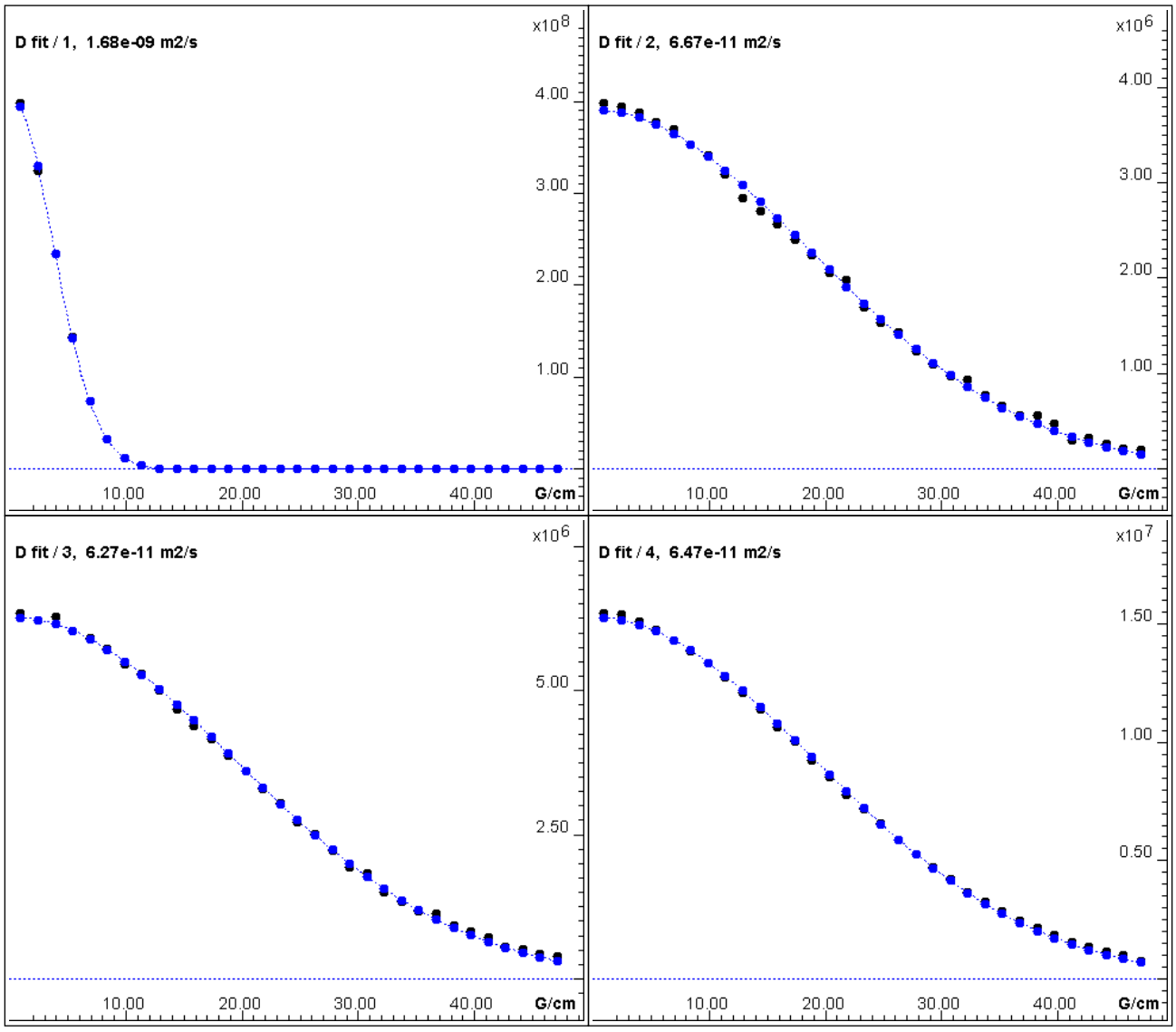
Diffusion Analysis

sample name:	JW183 3.4 mg/mL
Description/Title:	standard demo sample
Origin:	in-house
Date of preparation:	04 / 2014
Temperature (K):	298.0
Weight (Daltons):	11600


C:\Bruker\TopSpin3.1\data\Barner-Kowollik Group\data\DOSY\nmr\DOSY_140415\14\pd
1D trace 0
1
2
3
4
7.50
5.00
2.50
0.00
ppm
Dosy
m2/s
x10-9
0.25
0.50
0.75
1.00
1.25
1.50
1.75
7.50
5.00
2.50
0.00
ppm

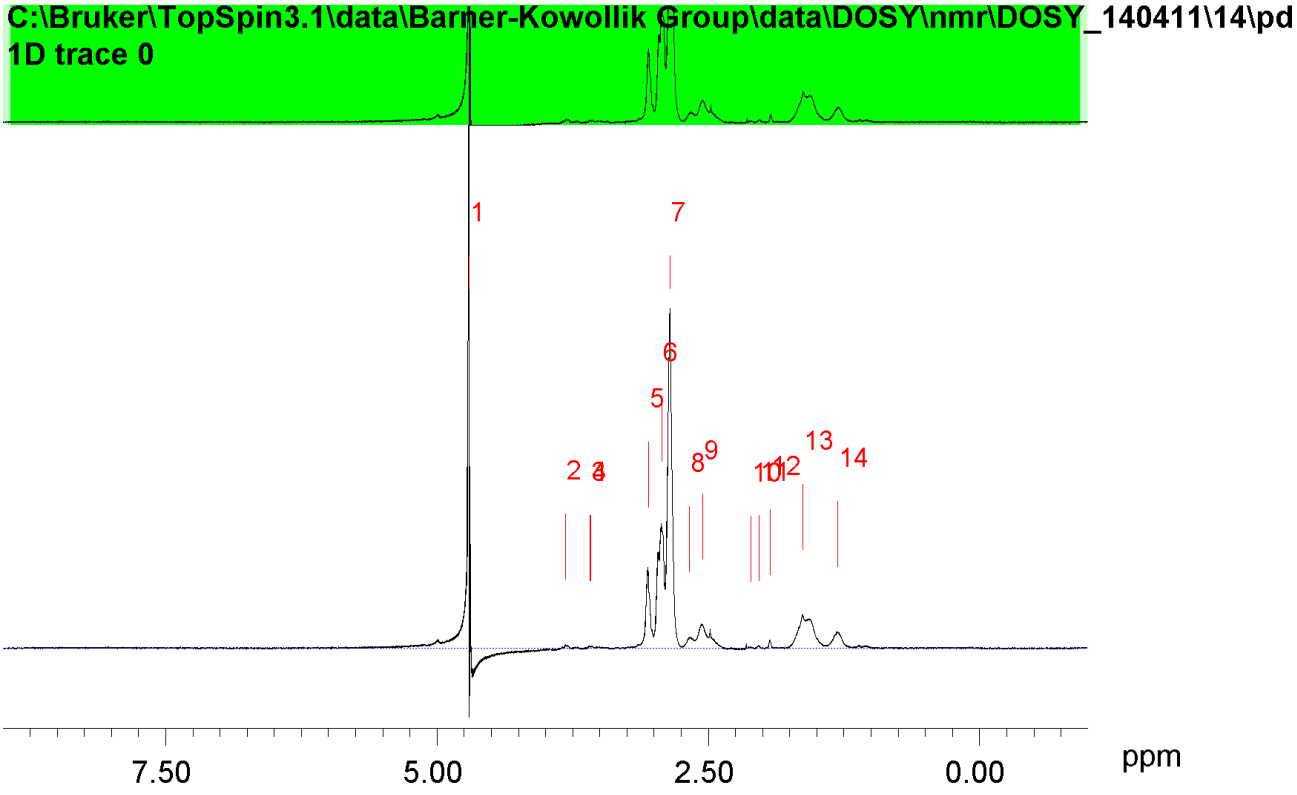
Fitted function:	f (x) = A * exp (-D * x^2 * gamma^2 * littleDelta^2 (bigDelta-littleDelta/3)* 10^4
used gamma:	26752 rad/(s*Gauss)
used little delta:	0.0055000 s
used big delta:	0.099900 s
used gradient strength:	variable
Random error estimation of data:	RMS per spectrum (or trace/plane)
Systematic error estimation of data:	worst case per peak scenario
Fit parameter Error estimation method:	from fit using arbitray y uncertainties
Confidence level:	95%
Used peaks:	peaks from C:\Bruker\TopSpin3.1\data\Barner-Kowollik Group\data\DOSY\nmr\DOSY_140415\11\pdata\1\peaklist.xml
Used integrals:	peak intensities
Used Gradient strength:	all values (including replicates) used

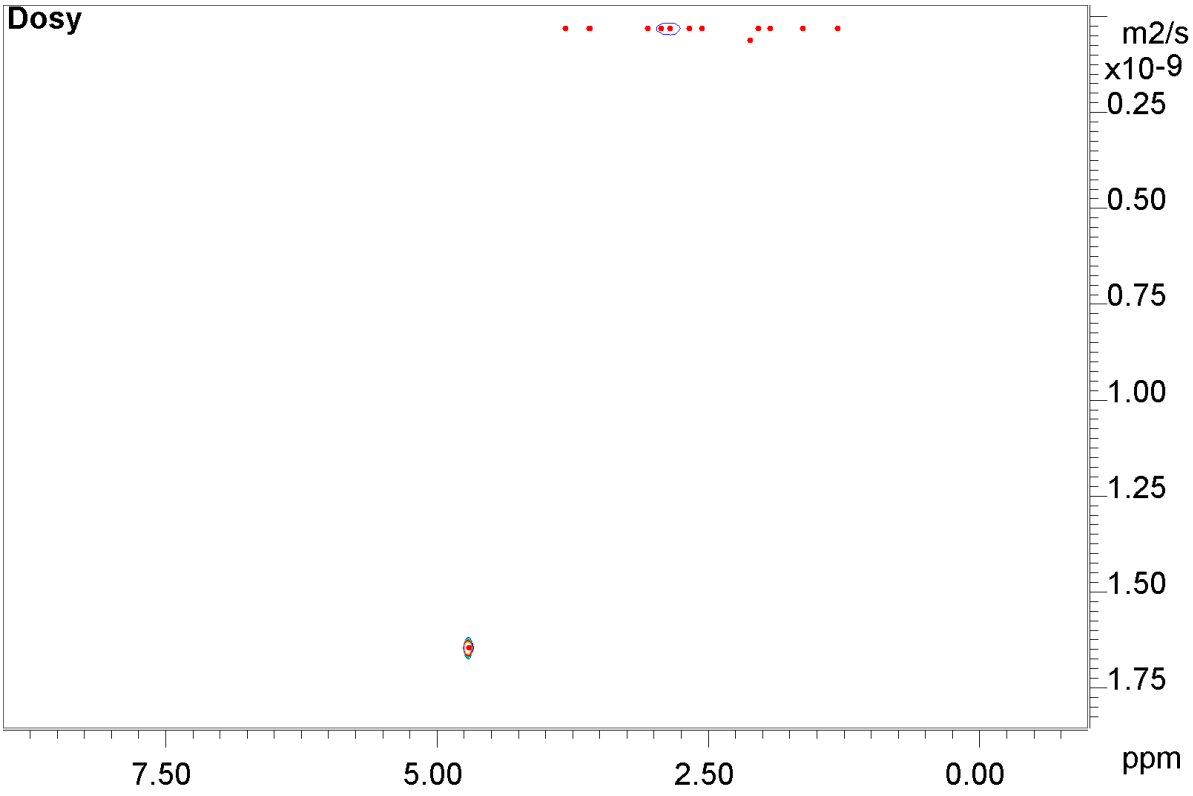
Peak name	F2 [ppm]	D [m2/s]	error
1	4.701	1.68e-09	1.918e-11
2	3.051	6.67e-11	1.741e-12
3	2.928	6.27e-11	9.683e-13
4	2.849	6.47e-11	8.070e-13


D fit / 1, 1.68e-09 m2/s
x10^8
4.00
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm
D fit / 2, 6.67e-11 m2/s
x10^6
4.00
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm
D fit / 3, 6.27e-11 m2/s
x10^6
5.00
2.50
10.00
20.00
30.00
40.00
G/cm
D fit / 4, 6.47e-11 m2/s
x10^7
1.50
1.00
0.50
10.00
20.00
30.00
40.00
G/cm

Diffusion Analysis

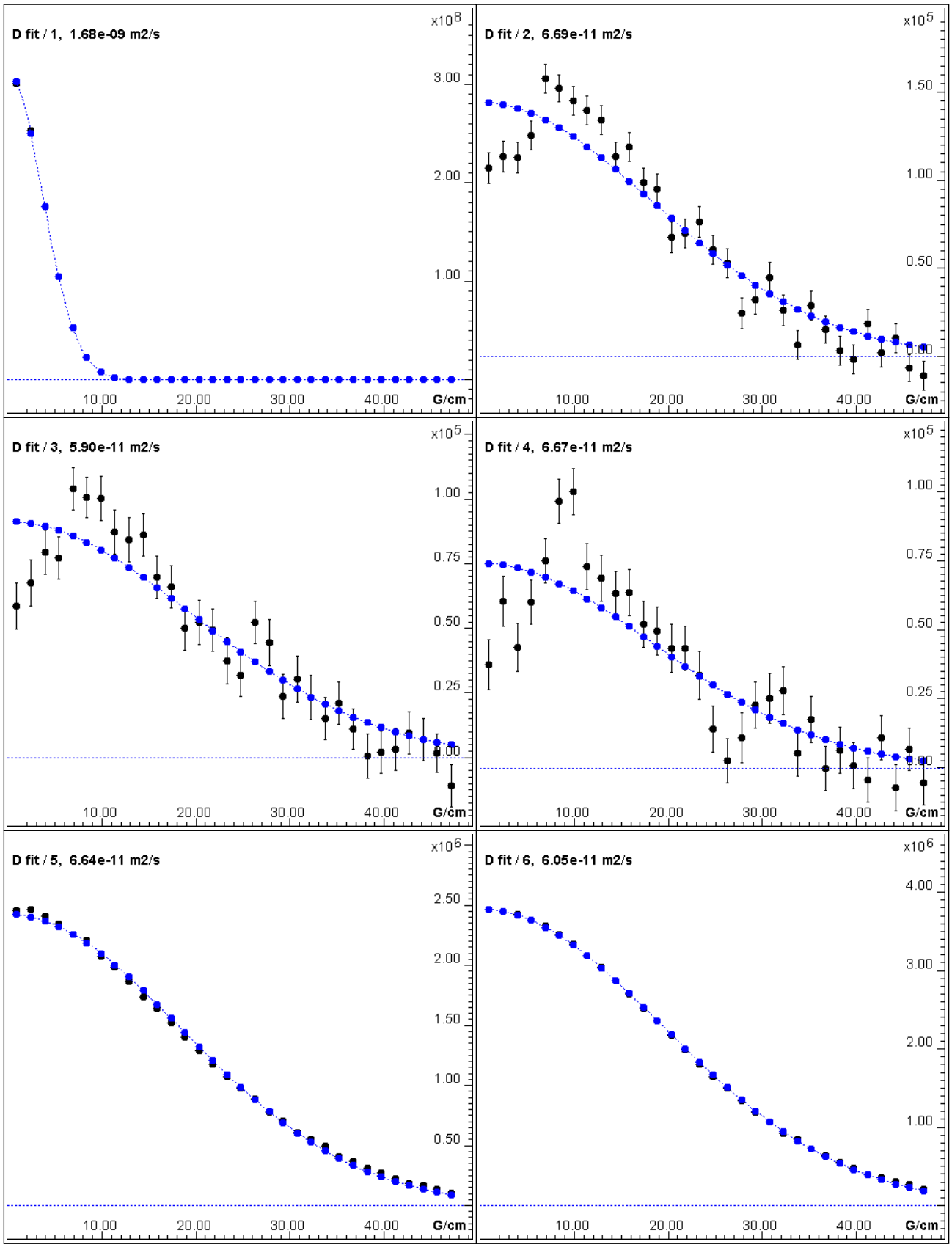
sample name:	JW183 6.8 mg/mL
Description/Title:	standard demo sample
Origin:	in-house
Date of preparation:	04 / 2014
Temperature (K):	298.0
Weight (Daltons):	11600


C:\Bruker\TopSpin3.1\data\Barner-Kowollik Group\data\DOSY\nmr\DOSY_140411\14\pd
1D trace 0
1
7
6
5
2
3
8
9
10
11
12
13
14
7.50
5.00
2.50
0.00
ppm


Dosy
m2/s
x10-9
0.25
0.50
0.75
1.00
1.25
1.50
1.75
7.50
5.00
2.50
0.00
ppm

Fitted function:	f (x) = A * exp (-D * x^2 * gamma^2 * littleDelta^2 (bigDelta-littleDelta/3)* 10^4
used gamma:	26752 rad/(s*Gauss)
used little delta:	0.0056000 s
used big delta:	0.099900 s
used gradient strength:	variable
Random error estimation of data:	RMS per spectrum (or trace/plane)
Systematic error estimation of data:	worst case per peak scenario
Fit parameter Error estimation method:	from fit using arbitray y uncertainties
Confidence level:	95%
Used peaks:	peaks from C:\Bruker\TopSpin3.1\data\Barner-Kowollik Group\data\DOSY\nmr\DOSY_140411\11\pdata\1\peaklist.xml
Used integrals:	peak intensities
Used Gradient strength:	all values (including replicates) used

Peak name	F2 [ppm]	D [m2/s]	error
1	4.701	1.68e-09	1.057e-11
2	3.813	6.69e-11	1.374e-11
3	3.593	5.90e-11	1.388e-11
4	3.586	6.67e-11	2.438e-11
5	3.052	6.64e-11	1.526e-12
6	2.929	6.05e-11	4.760e-13
7	2.849	6.15e-11	2.663e-13
8	2.673	6.36e-11	3.983e-12
9	2.551	6.16e-11	1.800e-12
10	2.109	1.01e-10	3.802e-11
11	2.032	6.92e-11	1.425e-11
12	1.927	6.23e-11	4.365e-12
13	1.626	6.32e-11	1.018e-12
14	1.307	6.05e-11	2.015e-12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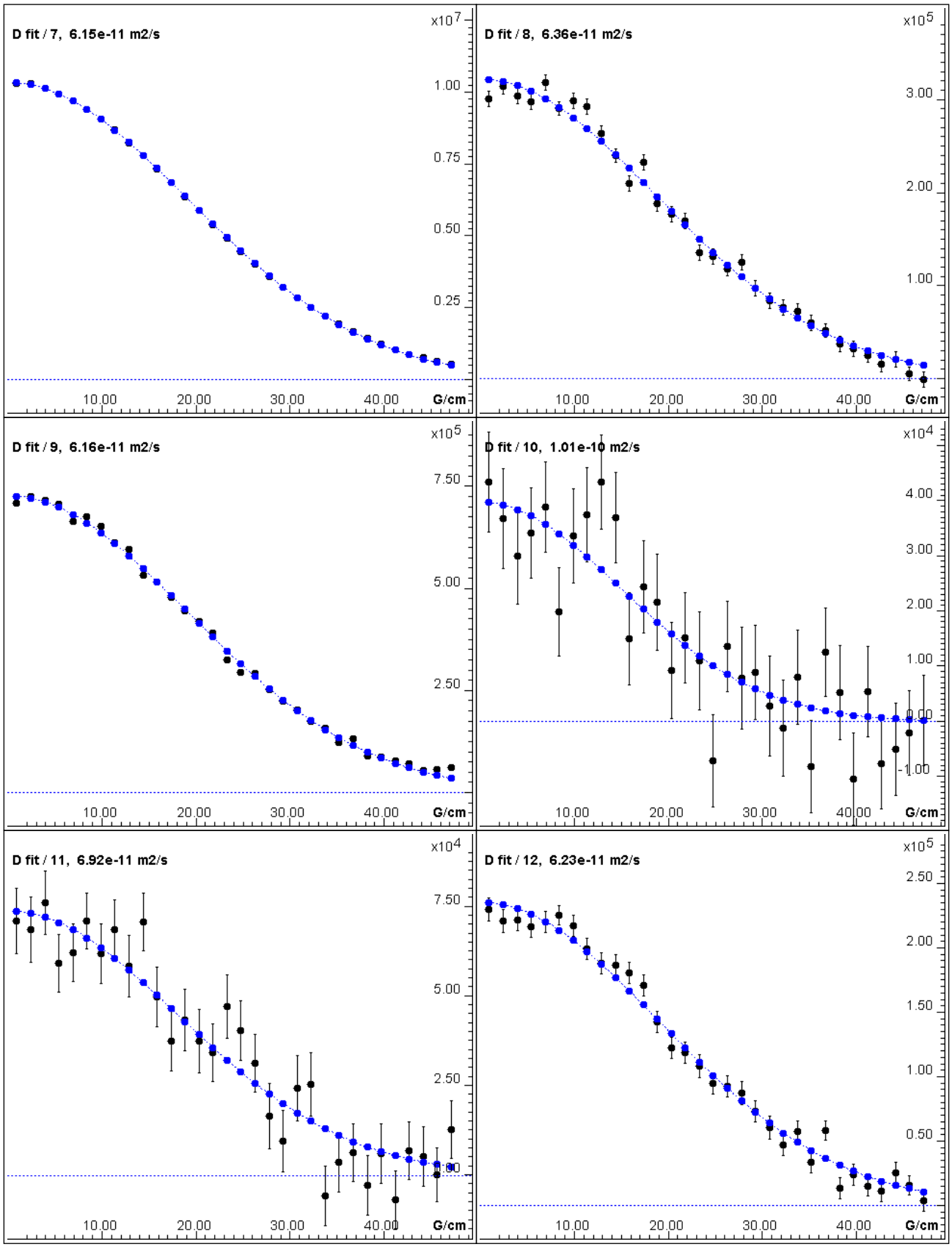
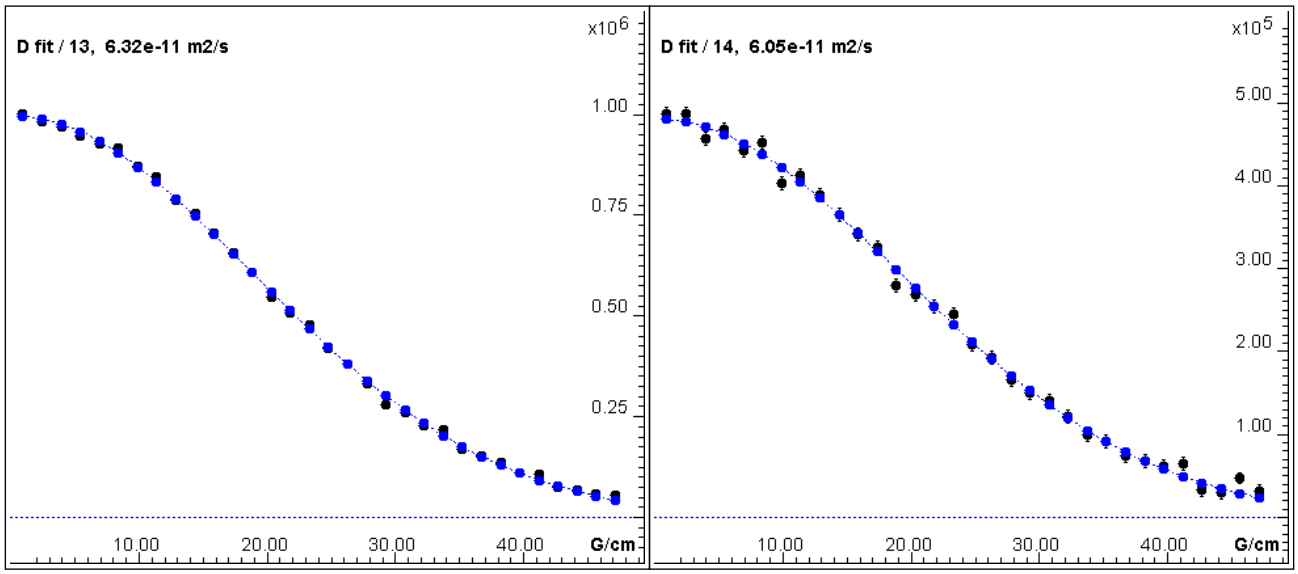
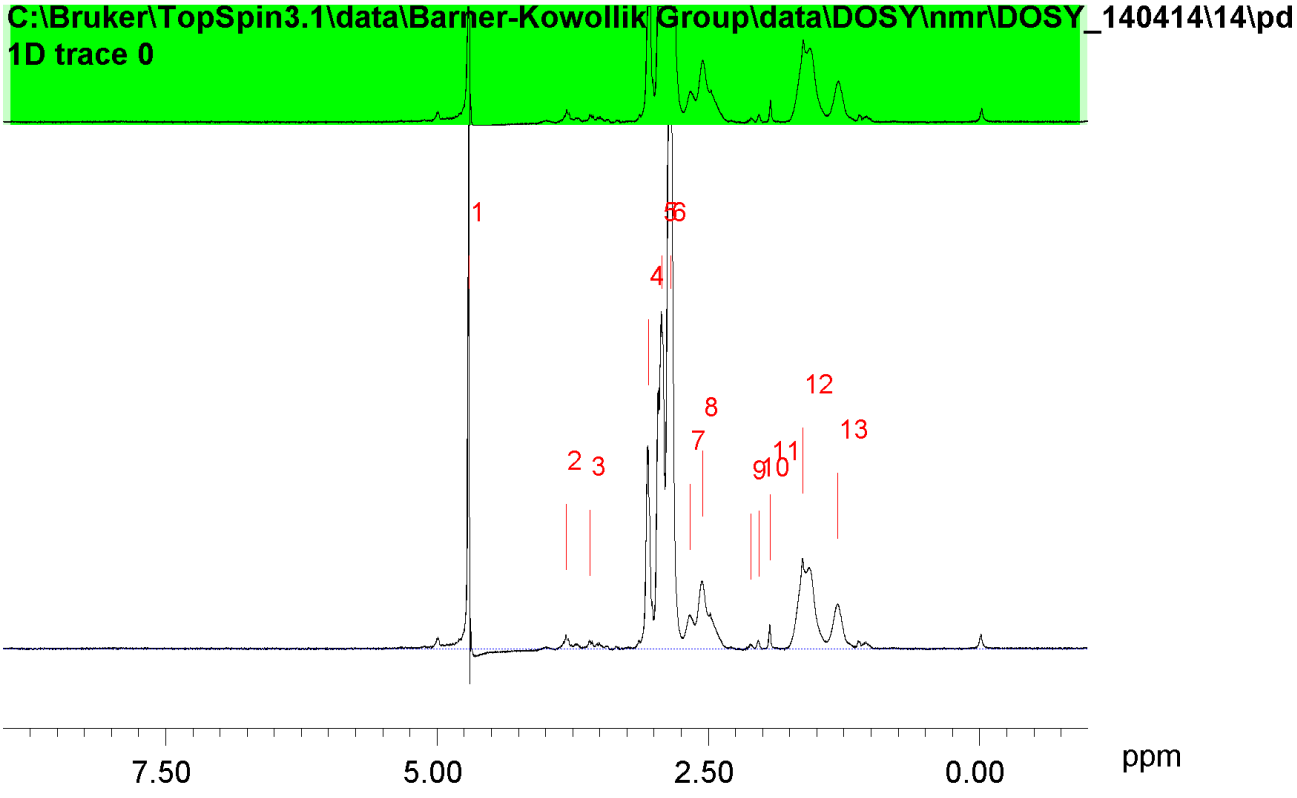
x10^8
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm
D fit / 2, 6.69e-11 m2/s
x10^5
1.50
1.00
0.50
D fit / 3, 5.90e-11 m2/s
x10^5
1.00
0.75
0.50
0.25
D fit / 4, 6.67e-11 m2/s
x10^5
1.00
0.75
0.50
0.25
D fit / 5, 6.64e-11 m2/s
x10^6
2.50
2.00
1.50
1.00
0.50
D fit / 6, 6.05e-11 m2/s
x10^6
4.00
3.00
2.00
1.00


D fit / 7, 6.15e-11 m2/s
x10^7
1.00
0.75
0.50
0.25
10.00
20.00
30.00
40.00
G/cm
D fit / 8, 6.36e-11 m2/s
x10^5
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm
D fit / 9, 6.16e-11 m2/s
x10^5
7.50
5.00
2.50
10.00
20.00
30.00
40.00
G/cm
D fit / 10, 1.01e-10 m2/s
x10^4
4.00
3.00
2.00
1.00
0.00
-1.00
10.00
20.00
30.00
40.00
G/cm
D fit / 11, 6.92e-11 m2/s
x10^4
7.50
5.00
2.50
10.00
20.00
30.00
40.00
G/cm
D fit / 12, 6.23e-11 m2/s
x10^5
2.50
2.00
1.50
1.00
0.50
10.00
20.00
30.00
40.00
G/cm


D fit / 13, 6.32e-11 m2/s
x10^6
1.00
0.75
0.50
0.25
10.00
20.00
30.00
40.00
G/cm
D fit / 14, 6.05e-11 m2/s
x10^5
5.00
4.00
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm

Diffusion Analysis

sample name:	JW183 18.6 mg/mL
Description/Title:	standard demo sample
Origin:	in-house
Date of preparation:	04 / 2014
Temperature (K):	298.0
Weight (Daltons):	11600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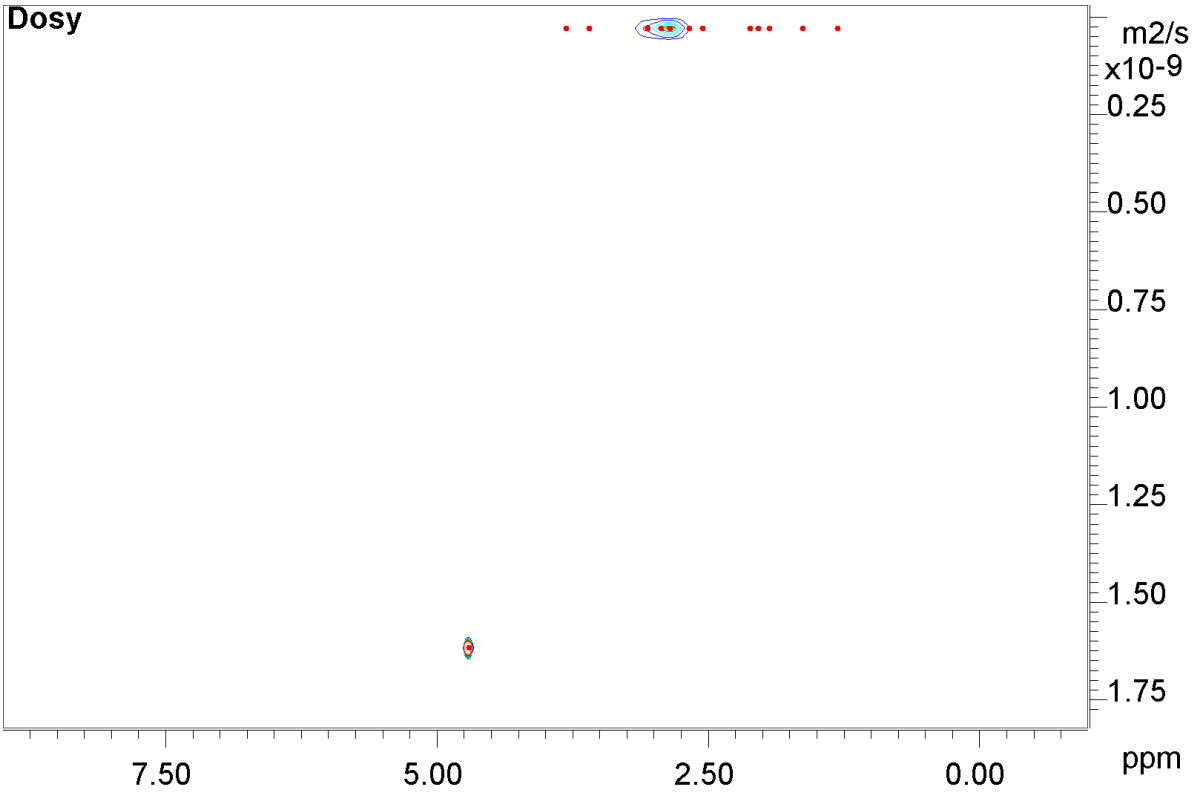
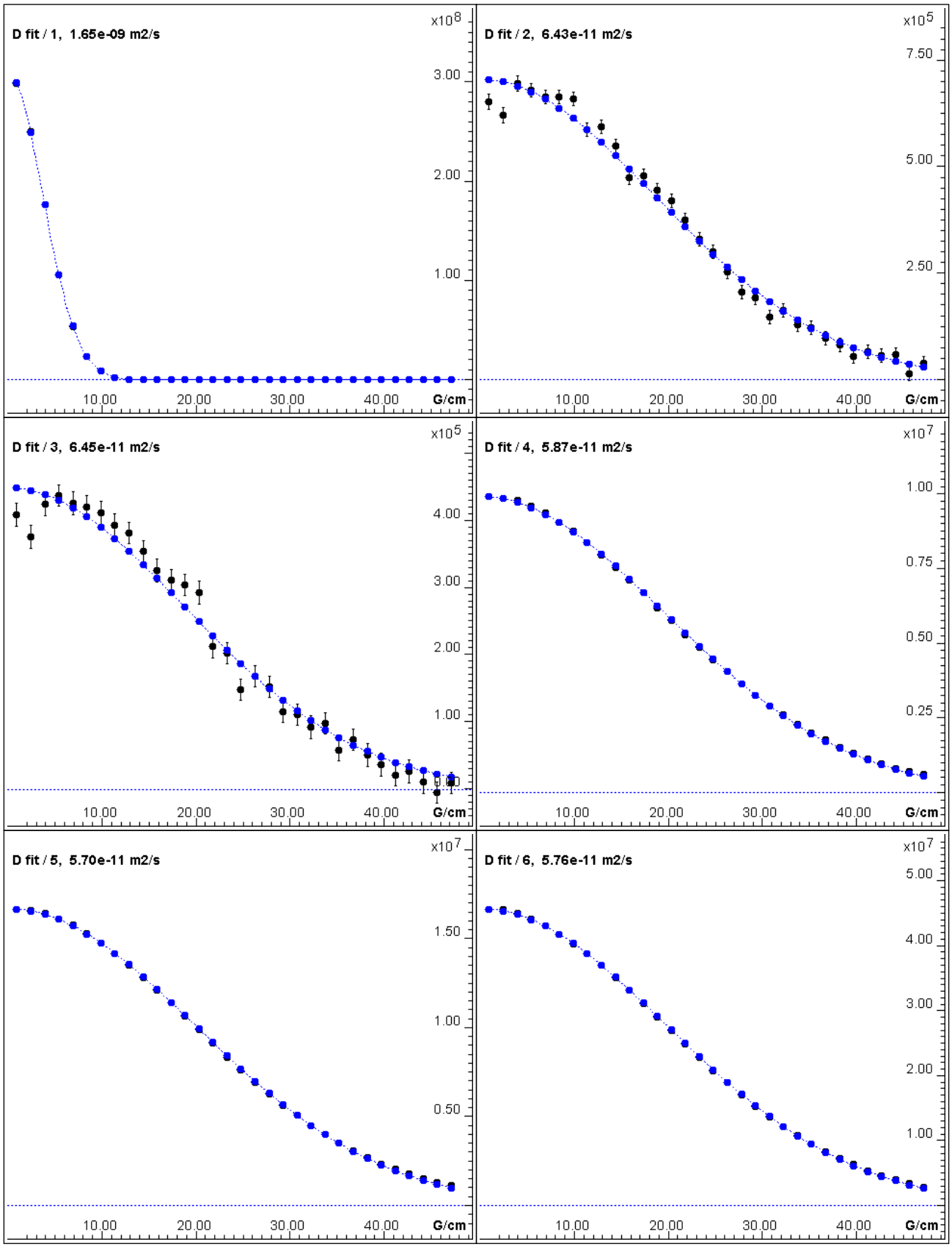
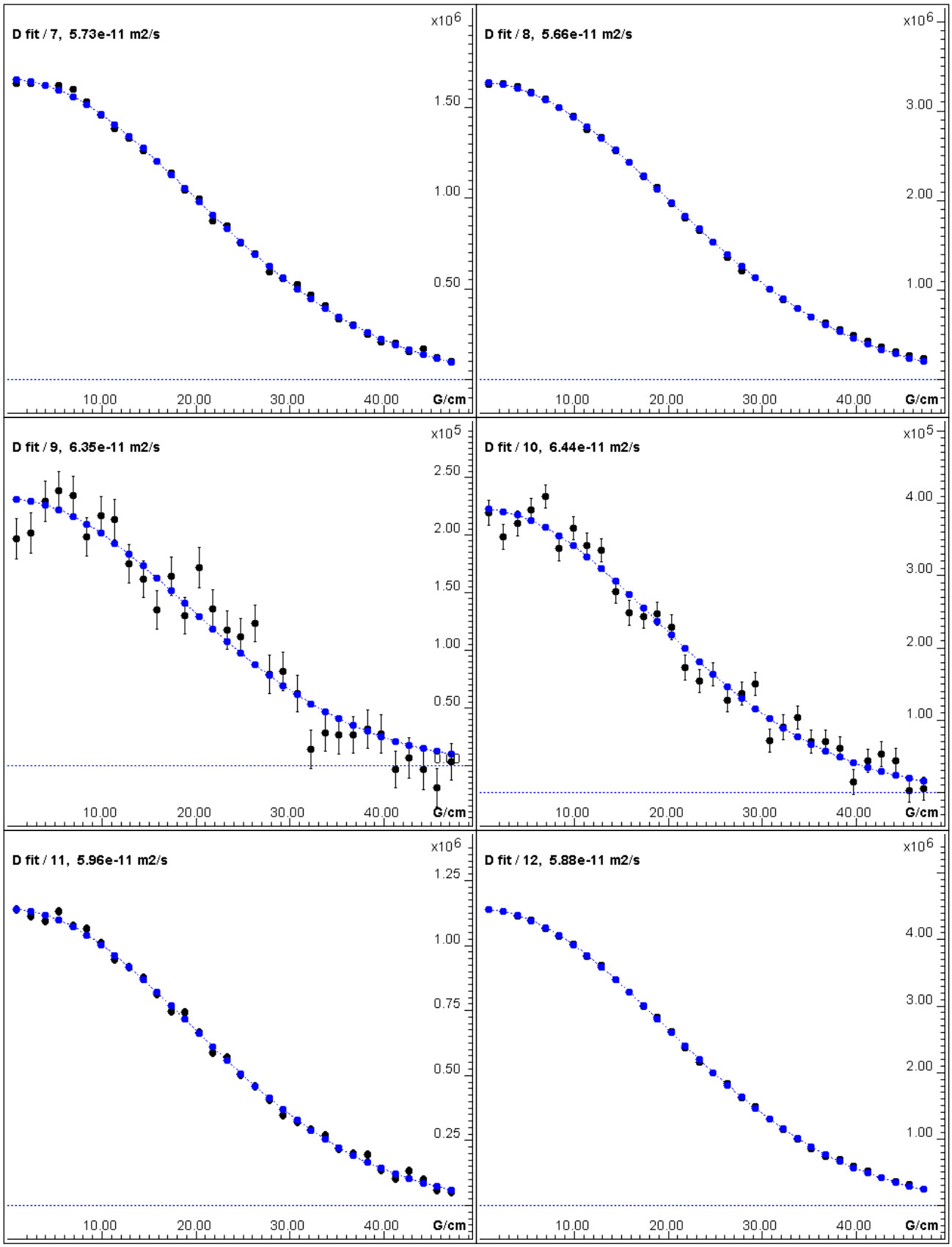
1D trace 0
1
2
3
4
5
6
7
8
9
10
11
12
13
7.50
5.00
2.50
0.00
ppm

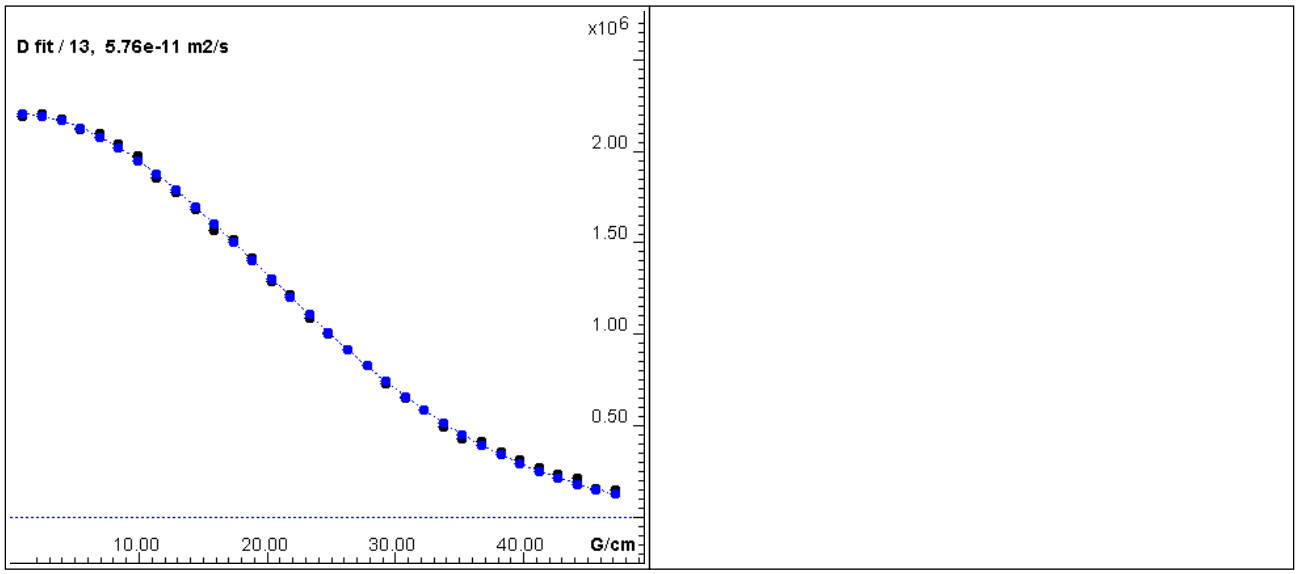

Dosy
m2/s
x10-9
0.25
0.50
0.75
1.00
1.25
1.50
1.75
7.50
5.00
2.50
0.00
ppm

Fitted function:	f (x) = A * exp (-D * x^2 * gamma^2 * littleDelta^2 (bigDelta-littleDelta/3)* 10^4
used gamma:	26752 rad/(s*Gauss)
used little delta:	0.0056000 s
used big delta:	0.099900 s
used gradient strength:	variable
Random error estimation of data:	RMS per spectrum (or trace/plane)
Systematic error estimation of data:	worst case per peak scenario
Fit parameter Error estimation method:	from fit using arbitray y uncertainties
Confidence level:	95%
Used peaks:	peaks from C:\Bruker\TopSpin3.1\data\Barner-Kowollik Group\data\DOSY\nmr\DOSY_140414\11\pdata\1\peaklist.xml
Used integrals:	peak intensities
Used Gradient strength:	all values (including replicates) used

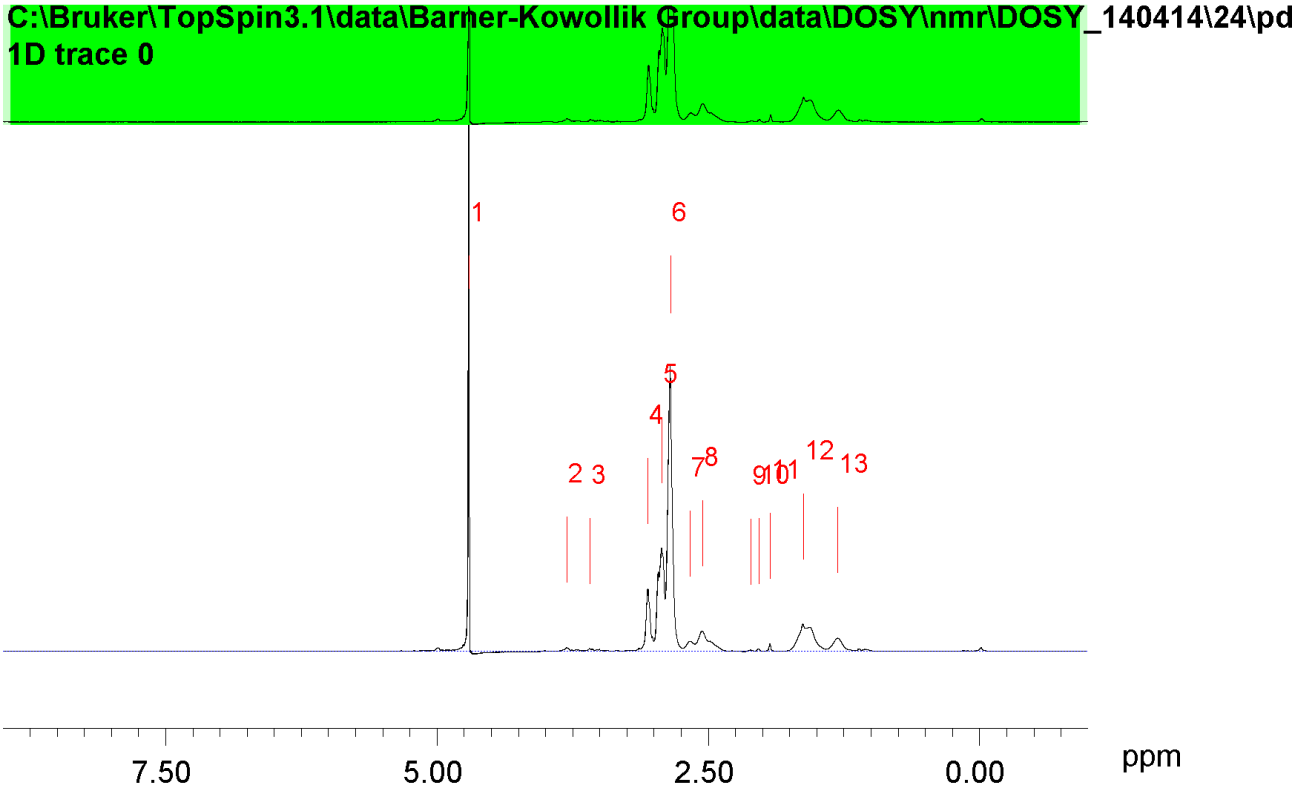
Peak name	F2 [ppm]	D [m2/s]	error
1	4.701	1.65e-09	7.080e-12
2	3.807	6.43e-11	4.141e-12
3	3.592	6.45e-11	6.003e-12
4	3.051	5.87e-11	4.327e-13
5	2.928	5.70e-11	3.556e-13
6	2.848	5.76e-11	2.515e-13
7	2.670	5.73e-11	1.076e-12
8	2.549	5.66e-11	6.410e-13
9	2.108	6.35e-11	9.877e-12
10	2.033	6.44e-11	6.144e-12
11	1.929	5.96e-11	1.546e-12
12	1.627	5.88e-11	4.675e-13
13	1.305	5.76e-11	8.305e-13

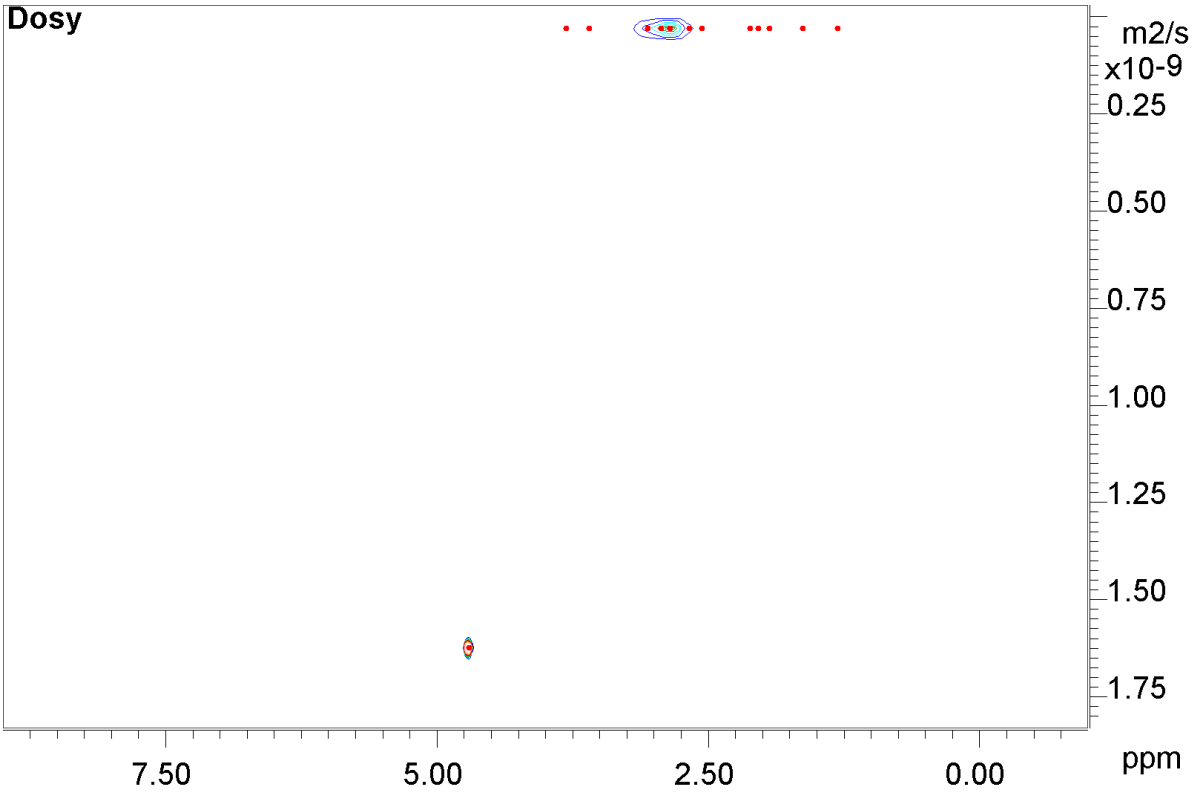

D fit / 1, 1.65e-09 m2/s
x10^8
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm
D fit / 2, 6.43e-11 m2/s
x10^5
7.50
5.00
2.50
D fit / 3, 6.45e-11 m2/s
x10^5
4.00
3.00
2.00
1.00
D fit / 4, 5.87e-11 m2/s
x10^7
1.00
0.75
0.50
0.25
D fit / 5, 5.70e-11 m2/s
x10^7
1.50
1.00
0.50
D fit / 6, 5.76e-11 m2/s
x10^7
5.00
4.00
3.00
2.00
1.00


D fit / 7, 5.73e-11 m2/s
x10^6
1.50
1.00
0.50
10.00
20.00
30.00
40.00
G/cm
D fit / 8, 5.66e-11 m2/s
x10^6
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm
D fit / 9, 6.35e-11 m2/s
x10^5
2.50
2.00
1.50
1.00
0.50
10.00
20.00
30.00
40.00
G/cm
D fit / 10, 6.44e-11 m2/s
x10^5
4.00
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm
D fit / 11, 5.96e-11 m2/s
x10^6
1.25
1.00
0.75
0.50
0.25
10.00
20.00
30.00
40.00
G/cm
D fit / 12, 5.88e-11 m2/s
x10^6
4.00
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm


D fit / 13, 5.76e-11 m2/s
x10^6
2.00
1.50
1.00
0.50
10.00
20.00
30.00
40.00
G/cm

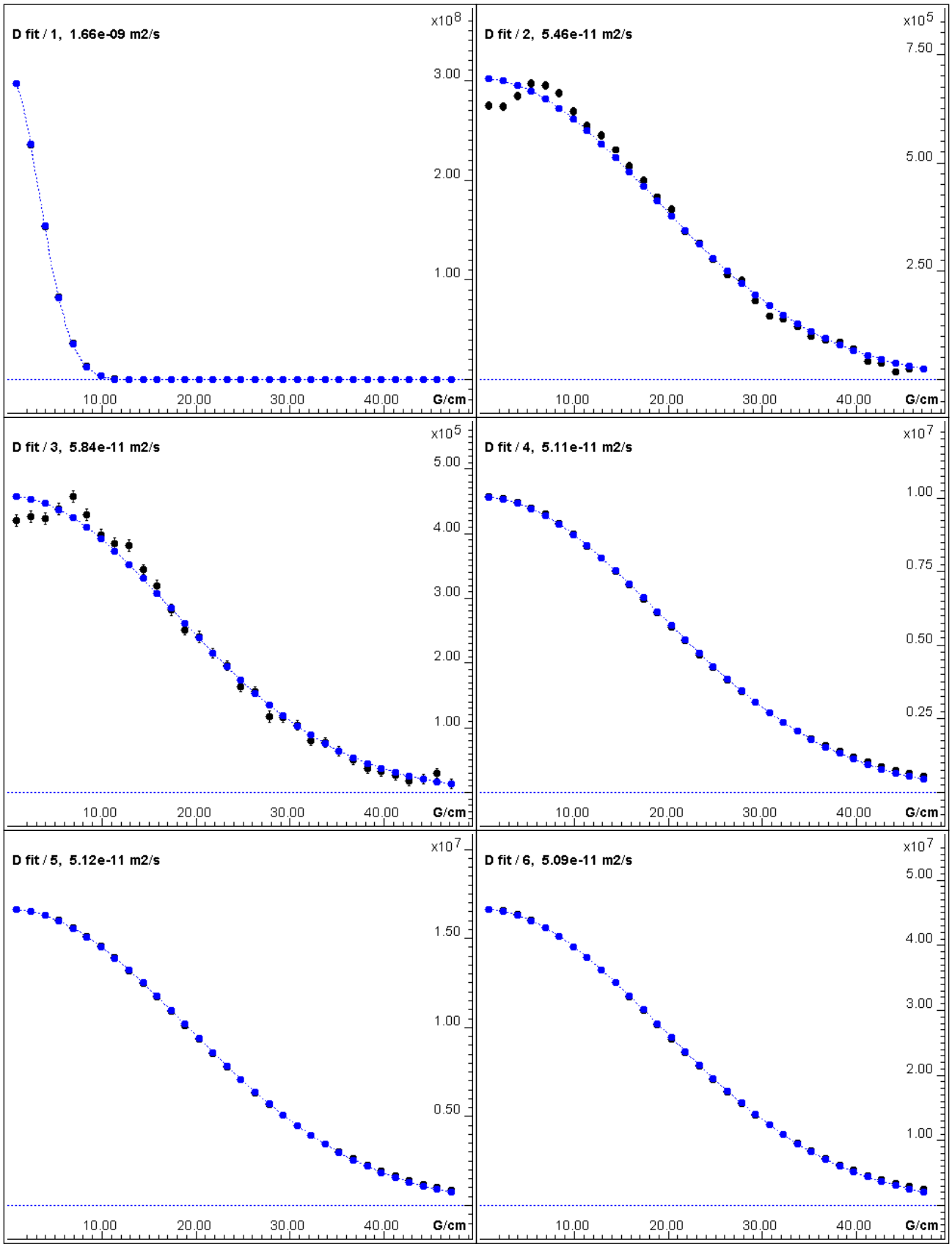
sample name:	JW183 37 mg/mL
Description/Title:	standard demo sample
Origin:	in-house
Date of preparation:	04 / 2014
Temperature (K):	298.0
Weight (Daltons):	11600

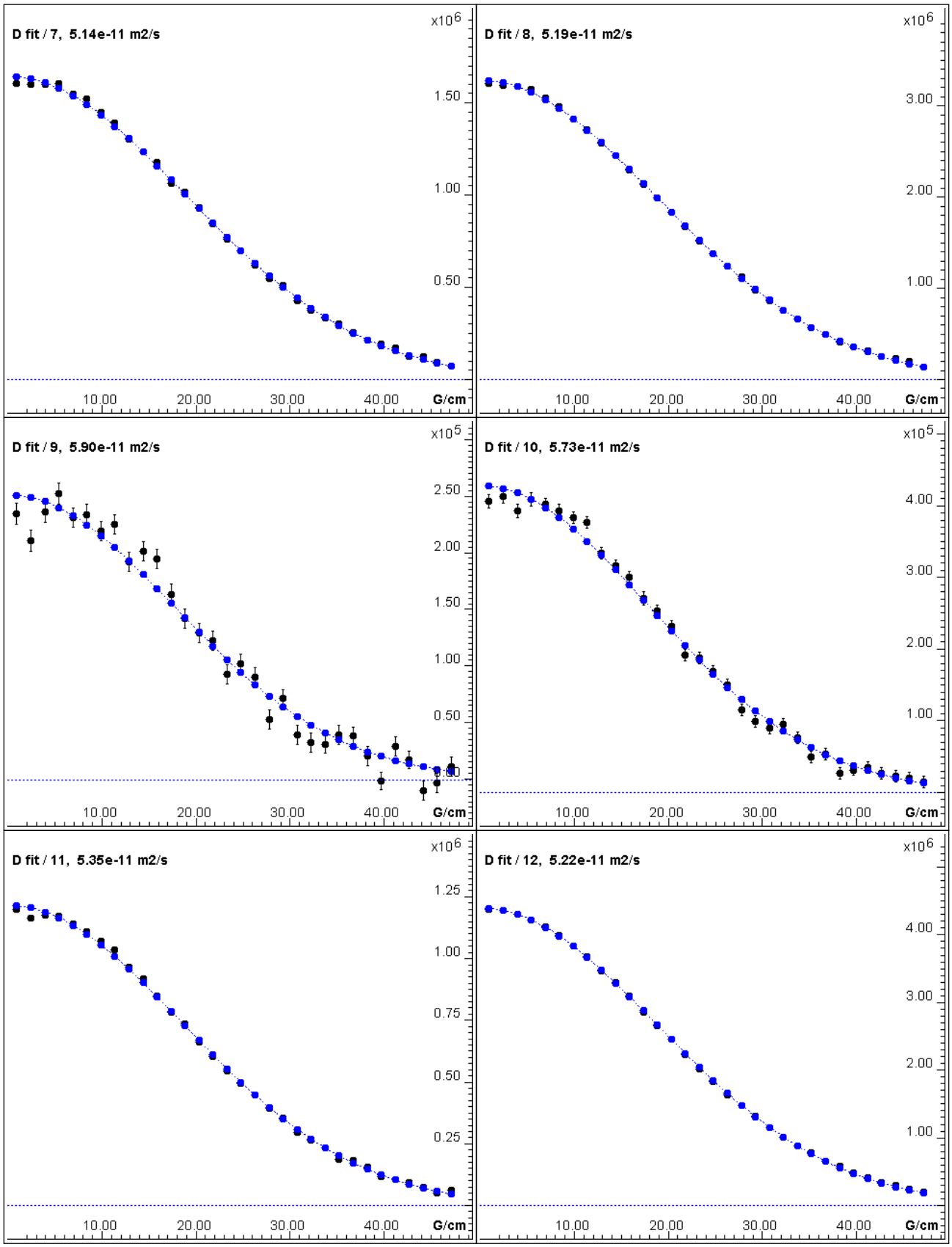

C:\Bruker\TopSpin3.1\data\Barner-Kowollik Group\data\DOSY\nmr\DOSY_140414\24\pd
1D trace 0
1
6
5
4
2 3
7
8
9
10
11
12
13
7.50
5.00
2.50
0.00
ppm

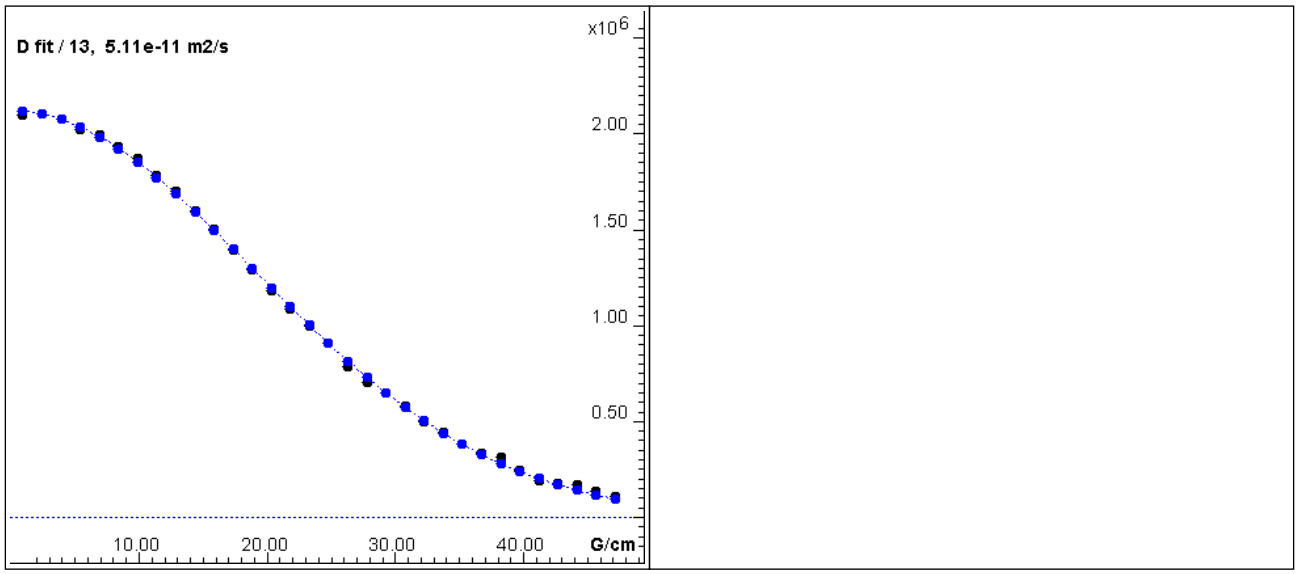

Dosy
m2/s
x10-9
0.25
0.50
0.75
1.00
1.25
1.50
1.75
7.50
5.00
2.50
0.00
ppm

Fitted function:	f (x) = A * exp (-D * x^2 * gamma^2 * littleDelta^2 (bigDelta-littleDelta/3)* 10^4
used gamma:	26752 rad/(s*Gauss)
used little delta:	0.0062000 s
used big delta:	0.099900 s
used gradient strength:	variable
Random error estimation of data:	RMS per spectrum (or trace/plane)
Systematic error estimation of data:	worst case per peak scenario
Fit parameter Error estimation method:	from fit using arbitray y uncertainties
Confidence level:	95%
Used peaks:	peaks from C:\Bruker\TopSpin3.1\data\Barner-Kowollik Group\data\DOSY\nmr\DOSY_140414\21\pdata\1\peaklist.xml
Used integrals:	peak intensities
Used Gradient strength:	all values (including replicates) used

Peak name	F2 [ppm]	D [m2/s]	error
1	4.701	1.66e-09	8.303e-12
2	3.804	5.46e-11	3.006e-12
3	3.591	5.84e-11	3.374e-12
4	3.054	5.11e-11	4.836e-13
5	2.927	5.12e-11	3.270e-13
6	2.847	5.09e-11	3.523e-13
7	2.667	5.14e-11	8.754e-13
8	2.551	5.19e-11	3.934e-13
9	2.107	5.90e-11	6.178e-12
10	2.032	5.73e-11	2.700e-12
11	1.929	5.35e-11	1.013e-12
12	1.624	5.22e-11	2.771e-13
13	1.305	5.11e-11	6.058e-13

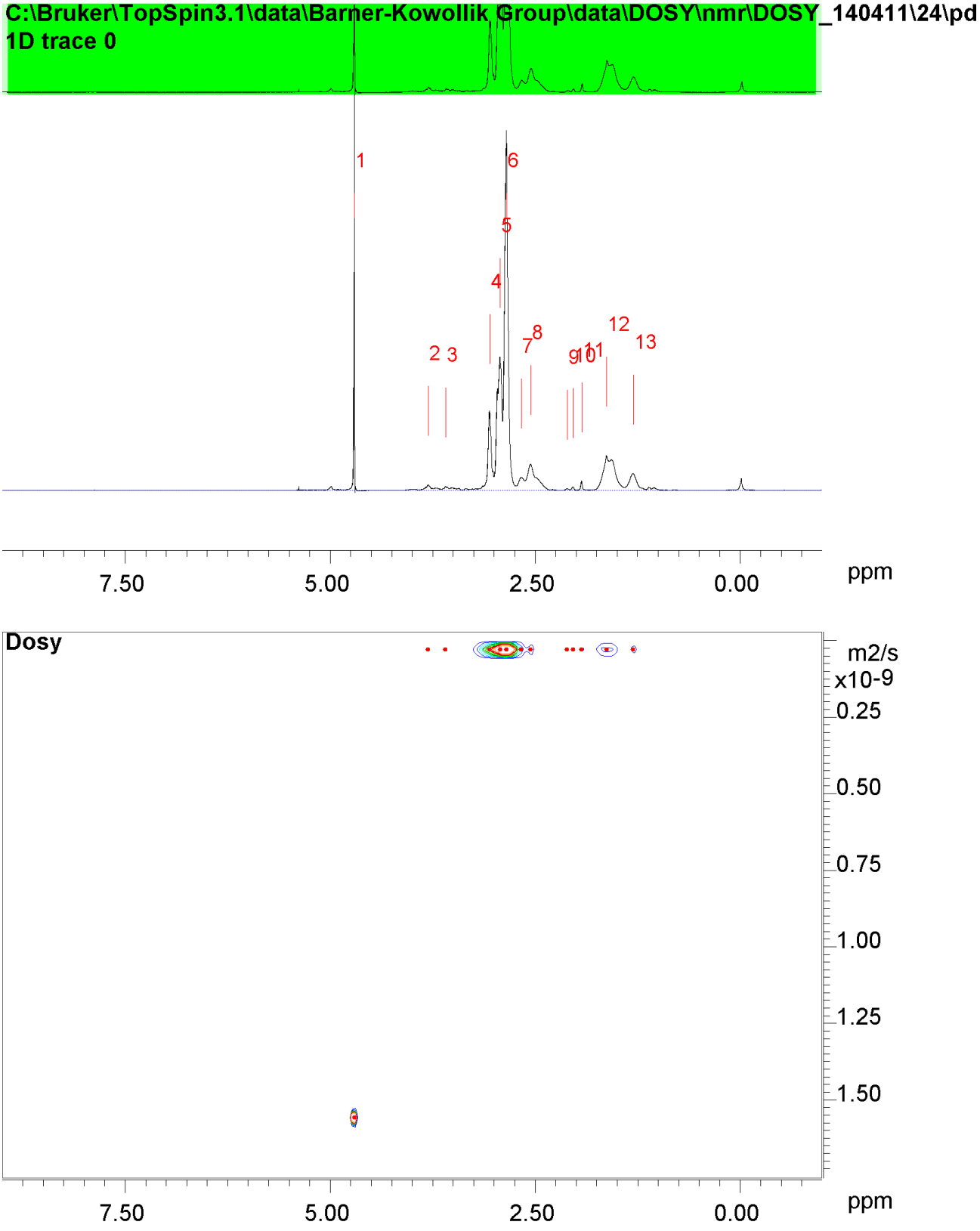

D fit / 1, 1.66e-09 m2/s
x10^8
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm
D fit / 2, 5.46e-11 m2/s
x10^5
7.50
5.00
2.50
10.00
20.00
30.00
40.00
G/cm
D fit / 3, 5.84e-11 m2/s
x10^5
5.00
4.00
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm
D fit / 4, 5.11e-11 m2/s
x10^7
1.00
0.75
0.50
0.25
10.00
20.00
30.00
40.00
G/cm
D fit / 5, 5.12e-11 m2/s
x10^7
1.50
1.00
0.50
10.00
20.00
30.00
40.00
G/cm
D fit / 6, 5.09e-11 m2/s
x10^7
5.00
4.00
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm


D fit / 7, 5.14e-11 m2/s
x10^6
1.50
1.00
0.50
10.00
20.00
30.00
40.00
G/cm
D fit / 8, 5.19e-11 m2/s
x10^6
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm
D fit / 9, 5.90e-11 m2/s
x10^5
2.50
2.00
1.50
1.00
0.50
10.00
20.00
30.00
40.00
G/cm
D fit / 10, 5.73e-11 m2/s
x10^5
4.00
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm
D fit / 11, 5.35e-11 m2/s
x10^6
1.25
1.00
0.75
0.50
0.25
10.00
20.00
30.00
40.00
G/cm
D fit / 12, 5.22e-11 m2/s
x10^6
4.00
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm


D fit / 13, 5.11e-11 m2/s
x10^6
2.00
1.50
1.00
0.50
10.00
20.00
30.00
40.00
G/cm

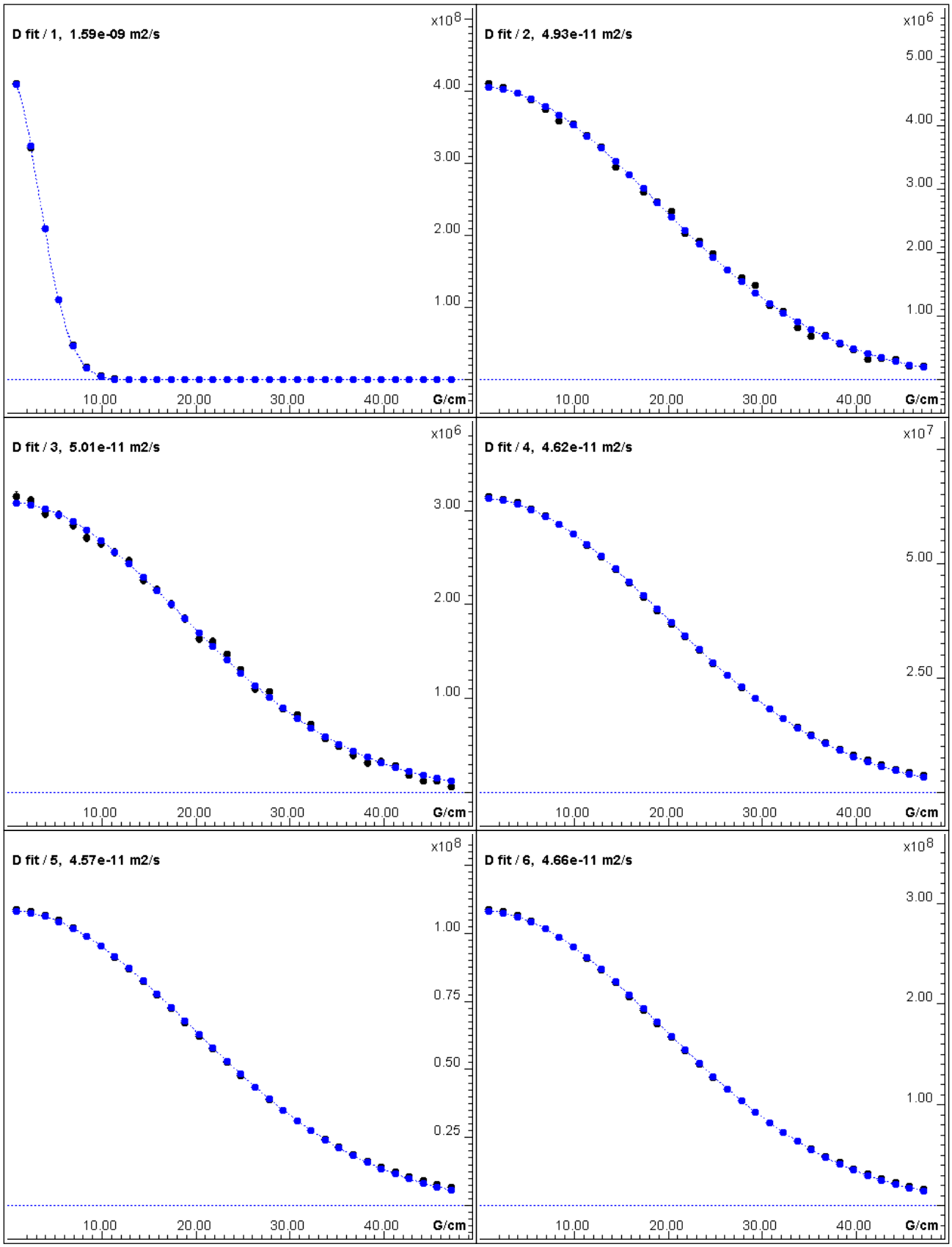
Diffusion Analysis

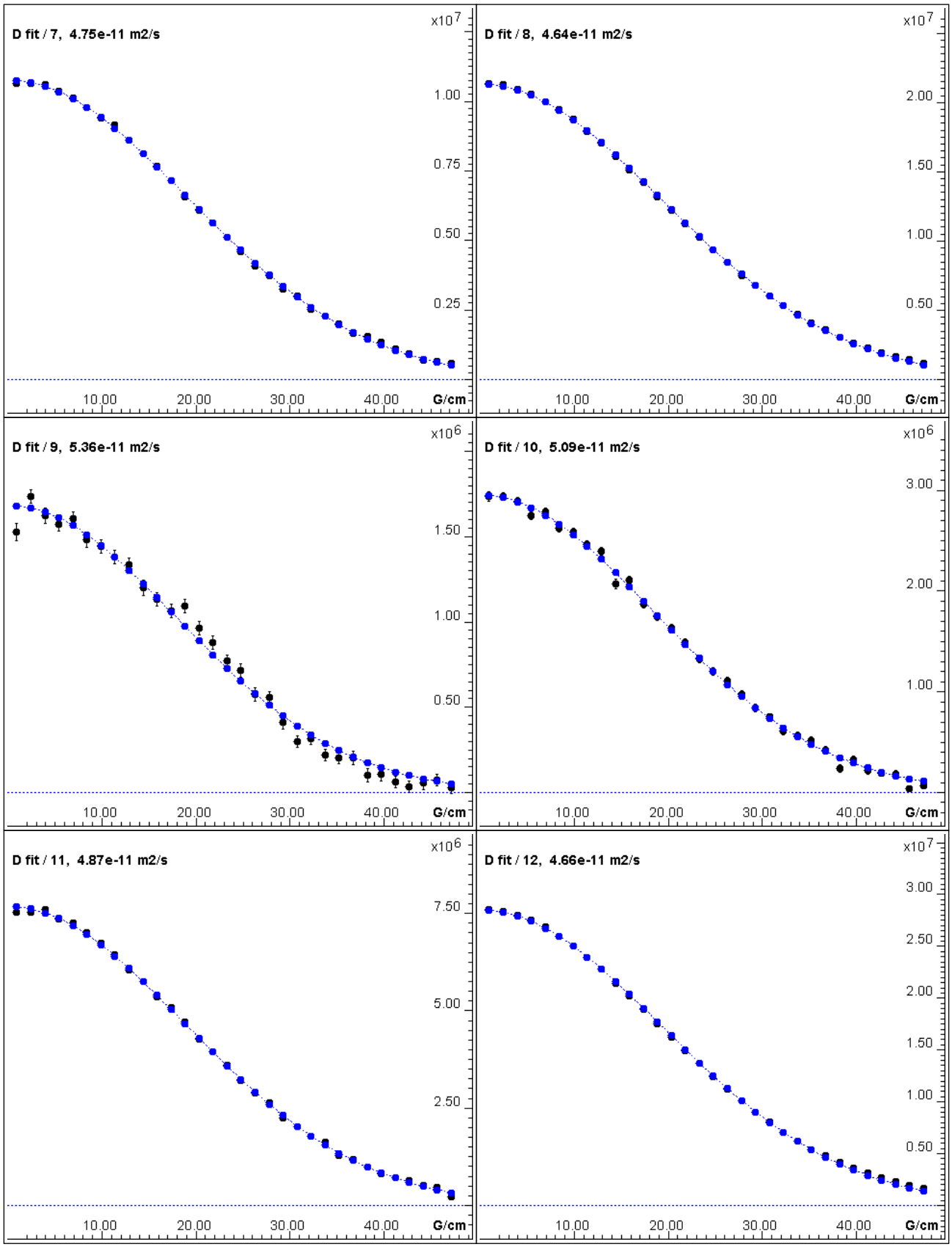
sample name:	JW183 55.6 mg/mL
Description/Title:	standard demo sample
Origin:	in-house
Date of preparation:	04 / 2014
Temperature (K):	298.0
Weight (Daltons):	11600

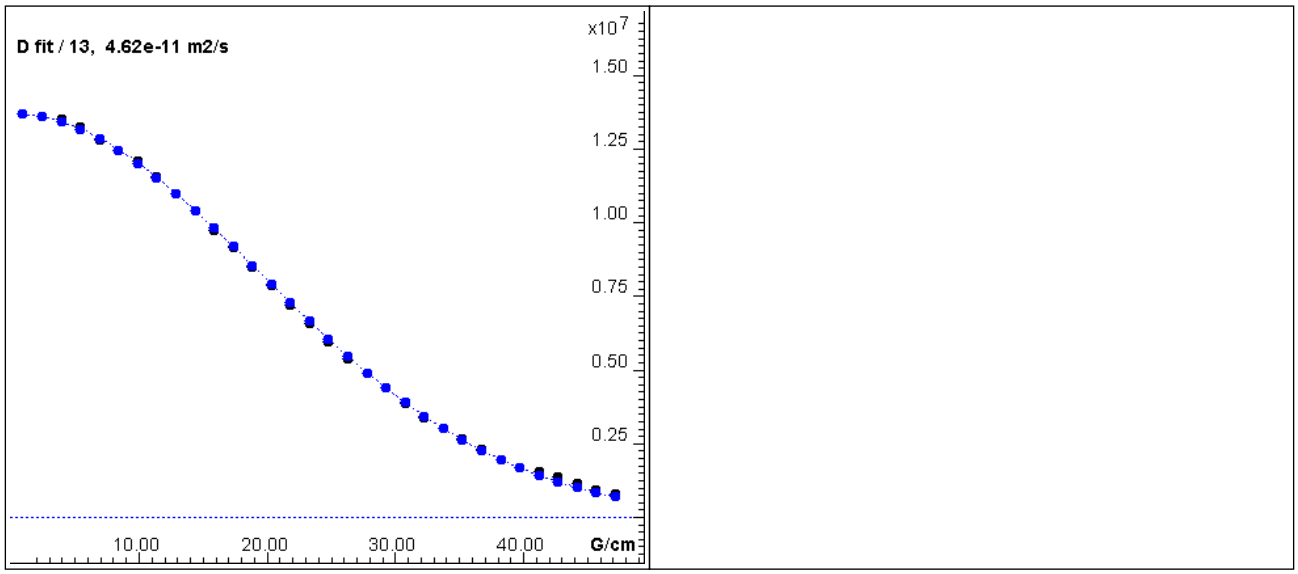

C:\Bruker\TopSpin3.1\data\Barner-Kowollik Group\data\DOSY\nmr\DOSY_140411\24\pd
1D trace 0
1
6
5
4
2 3
7
8
9
10
11
12
13
7.50
5.00
2.50
0.00
ppm
Dosy
m2/s
x10-9
0.25
0.50
0.75
1.00
1.25
1.50
7.50
5.00
2.50
0.00
ppm

Fitted function:	f (x) = A * exp (-D * x^2 * gamma^2 * littleDelta^2 (bigDelta-littleDelta/3)* 10^4
used gamma:	26752 rad/(s*Gauss)
used little delta:	0.0064000 s
used big delta:	0.099900 s
used gradient strength:	variable
Random error estimation of data:	RMS per spectrum (or trace/plane)
Systematic error estimation of data:	worst case per peak scenario
Fit parameter Error estimation method:	from fit using arbitray y uncertainties
Confidence level:	95%
Used peaks:	peaks from C:\Bruker\TopSpin3.1\data\Barner-Kowollik Group\data\DOSY\nmr\DOSY_140411\21\pdata\1\peaklist.xml
Used integrals:	peak intensities
Used Gradient strength:	all values (including replicates) used

Peak name	F2 [ppm]	D [m2/s]	error
1	4.701	1.59e-09	1.166e-11
2	3.803	4.93e-11	1.091e-12
3	3.590	5.01e-11	1.251e-12
4	3.053	4.62e-11	3.700e-13
5	2.926	4.57e-11	4.168e-13
6	2.847	4.66e-11	3.556e-13
7	2.668	4.75e-11	4.669e-13
8	2.551	4.64e-11	2.973e-13
9	2.109	5.36e-11	3.281e-12
10	2.036	5.09e-11	1.439e-12
11	1.930	4.87e-11	6.274e-13
12	1.626	4.66e-11	4.024e-13
13	1.302	4.62e-11	4.214e-13


D fit / 1, 1.59e-09 m2/s
x10^8
4.00
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm
D fit / 2, 4.93e-11 m2/s
x10^6
5.00
4.00
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm
D fit / 3, 5.01e-11 m2/s
x10^6
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm
D fit / 4, 4.62e-11 m2/s
x10^7
5.00
2.50
10.00
20.00
30.00
40.00
G/cm
D fit / 5, 4.57e-11 m2/s
x10^8
1.00
0.75
0.50
0.25
10.00
20.00
30.00
40.00
G/cm
D fit / 6, 4.66e-11 m2/s
x10^8
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm


D fit / 7, 4.75e-11 m2/s
x10^7
1.00
0.75
0.50
0.25
10.00
20.00
30.00
40.00
G/cm
D fit / 8, 4.64e-11 m2/s
x10^7
2.00
1.50
1.00
0.50
10.00
20.00
30.00
40.00
G/cm
D fit / 9, 5.36e-11 m2/s
x10^6
1.50
1.00
0.50
10.00
20.00
30.00
40.00
G/cm
D fit / 10, 5.09e-11 m2/s
x10^6
3.00
2.00
1.00
10.00
20.00
30.00
40.00
G/cm
D fit / 11, 4.87e-11 m2/s
x10^6
7.50
5.00
2.50
10.00
20.00
30.00
40.00
G/cm
D fit / 12, 4.66e-11 m2/s
x10^7
3.00
2.50
2.00
1.50
1.00
0.50
10.00
20.00
30.00
40.00
G/cm


D fit / 13, 4.62e-11 m2/s
x10 7
1.50
1.25
1.00
0.75
0.50
0.25
10.00
20.00
30.00
40.00
G/cm