Optimization of diffusion-filtered NMR experiments for selective suppression of residual non-deuterated solvent and water signals from ^{1}H NMR spectra of organic compounds

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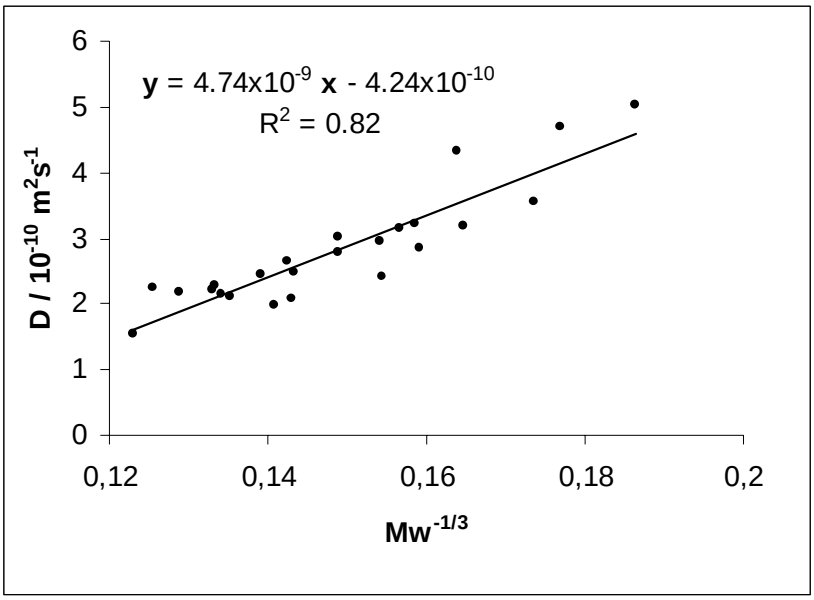
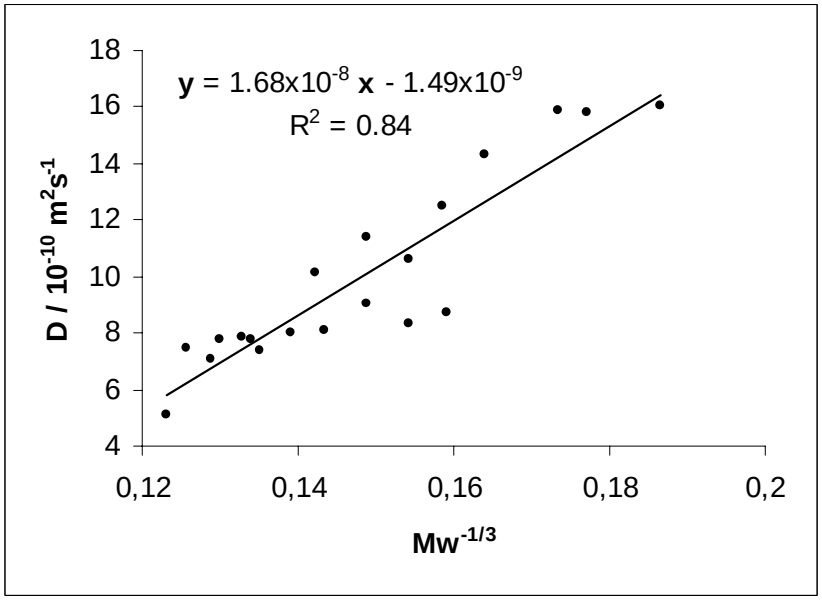
Linear relationship between the self-diffusion coefficient, *D*, and the reciprocal of the cube-root of molecular weight for the training set of organic compounds in DMSO-d_6.



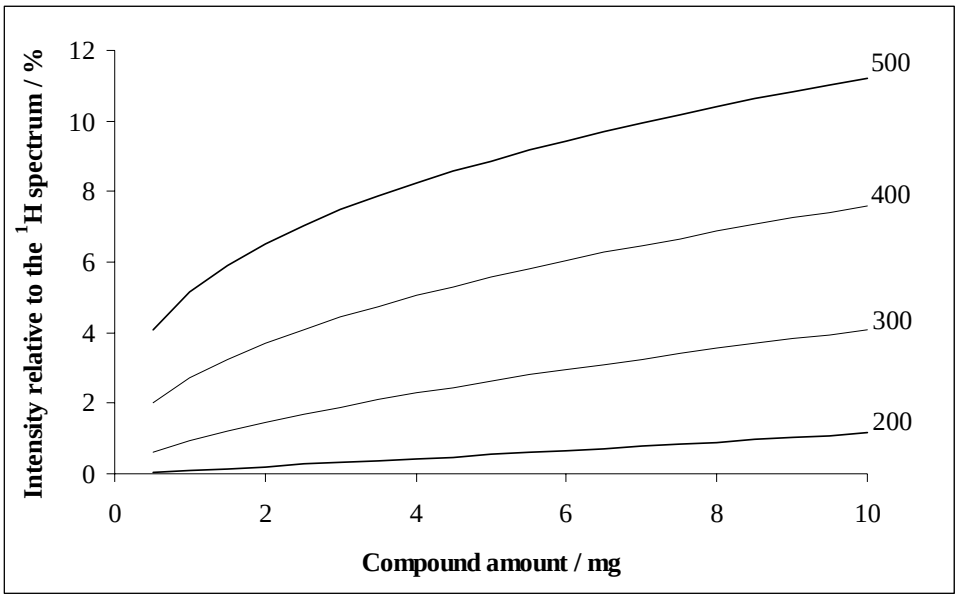
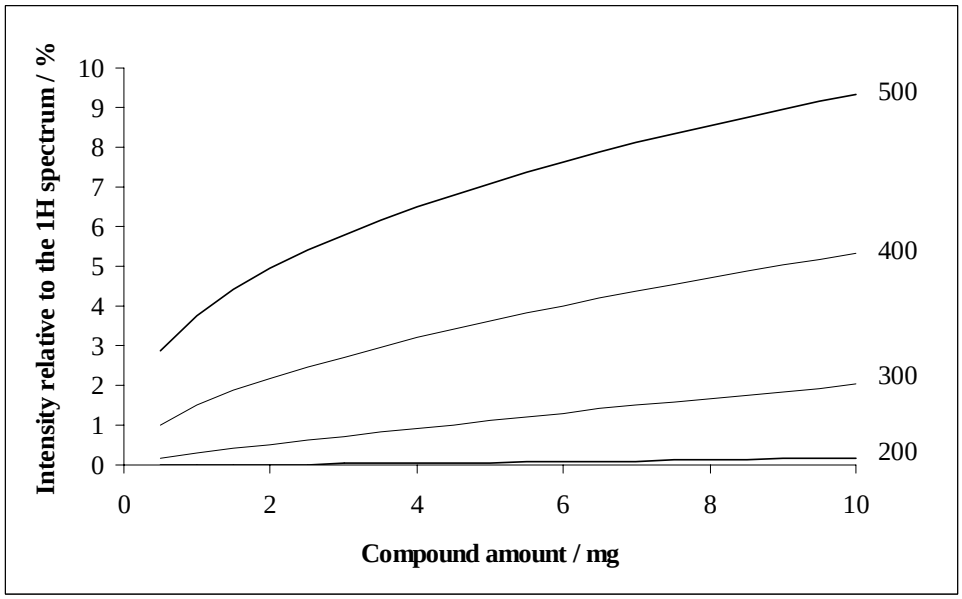
Linear relationship between the self-diffusion coefficient, *D*, and the reciprocal of the cube-root of molecular weight for the training set of organic compounds in CD_3OD.



List of compounds used to build the calibration curves

NAME OF THE COMPOUND	*Mw*	DIFFUSION COEFICIENT $D / 10^{-10}\ m^2\ s^{-1}$		
		$CDCl_3$	DMSO-d_6	CD_3OD
4-TERT-BUTYLCYCLOHEXANONE	154.3	14.29 ± 0.07	5.04 ± 0.02	16.00± 0.11
9-FLUORENONE	180.2	15.37 ± 0.13	4.69 ± 0.01	15.78 ± 0.12
4-BENZYL-4-HYDROXIPIPERIDINE	191.3	12.89± 0.15	3.56 ± 0.02	15.89 ± 0.08
9-FLUORENONE-1-CARBOXYLIC ACID	224.2	12.91± 0.05	3.19 ± 0.01	
4-(TERT-BUTYL)BEZYL BROMIDE	227.1	13.9 ± 0.04	4.33 ± 0.05	14.29± 0.13
PINDOLOL	248.3		2.86 ± 0.02	8.75 ± 0.03
D-(+)-10-CAMPHORSULFONYL CHLORIDE	250.7	12.47 ± 0.15	3.20 ± 0.01	12.51± 0.06
TRIPHENYLMETHANOL	260.3	11.89 ± 0.05	3.15 ± 0.02	
PROCAINAMIDE HYDROCHLORIDE	271.8		2.41± 0.01	8.31± 0.04
BOC-GLY-OSU	272.3	10.13 ± 0.15	2.97 ± 0.01	10.63 ± 0.01
3,3,3-TRIPHENYLPROPIONIC ACID	302.4	8.65 ± 0.11	2.77 ± 0.01	9.06 ± 0.02
2,4,6-TRIISOPROPYLBENZENSULFONYL CHLORIDE	302.9	11.72 ± 0.08	3.01± 0.01	11.40 ± 0.03
9-FLUORENYLMETHYL SUCCINIMIDYL CARBONATE	337.3	9.92 ± 0.09		
FMOC-L-VALINE	339.4	7.37 ± 0.03	2.48 ± 0.01	8.12 ± 0.06
BETA-D-LACTOSE	342.3		2.07 ± 0.02	
NIFEDIPINE	346.4	9.29 ± 0.07	2.64 ± 0.01	10.16 ± 0.15
LACTOBIONIC ACID	358.3		1.97 ± 0.04	
Z-D-GLU-OBZL	371.4	7.22 ± 0.05	2.44 ± 0.01	7.99 ± 0.05
FLUNARIZINE	404.5	6.89 ± 0.06	2.10 ± 0.01	7.38 ± 0.01
DILTIAZEM	414.5	7.36 ± 0.04	2.14 ± 0.01	7.80 ± 0.02
n-BENZYLCINCHONINIUM CHLORIDE	421.0		2.27 ± 0.01	
FMOC-GLU(OTBU)-OH	425.5	6.77 ± 0.08	2.21 ± 0.01	7.82± 0.03
(+/-)VERAPAMIL	454.6	6.66 ± 0.07		7.79± 0.04
FMOC-LYS(BOC)-OH	468.5	5.74 ± 0.03	2.18 ± 0.01	7.09± 0.01
LIDOFLAZINE	491.6			
DIPYRIDAMOLE	504.6	7.05 ± 0.05	2.26 ± 0.03	7.45 ± 0.04
ERIOCHROME CYANINE R	536.4		1.55 ± 0.04	5.10 ± 0.06

Intensities of the optimized diffusion filtered spectra relative to that of the ^{1}H spectra in DMSO-d_6 as a function of the amount of compound for different molecular weights.



Intensities of the optimized diffusion filtered spectra relative to that of the ^{1}H spectra in CD_3OD as a function of the amount of compound for different molecular weights.