Electronic Supplementary Information

Zinc(II) and cadmium(II) complexes of N-terminally free peptides containing two separate cysteinyl binding sites

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Fig. S1. ^{1}H NMR and ^{1}H-^{1}H COSY spectra of CSSACS-NH_2 recorded in D_2O at pD=2.85.

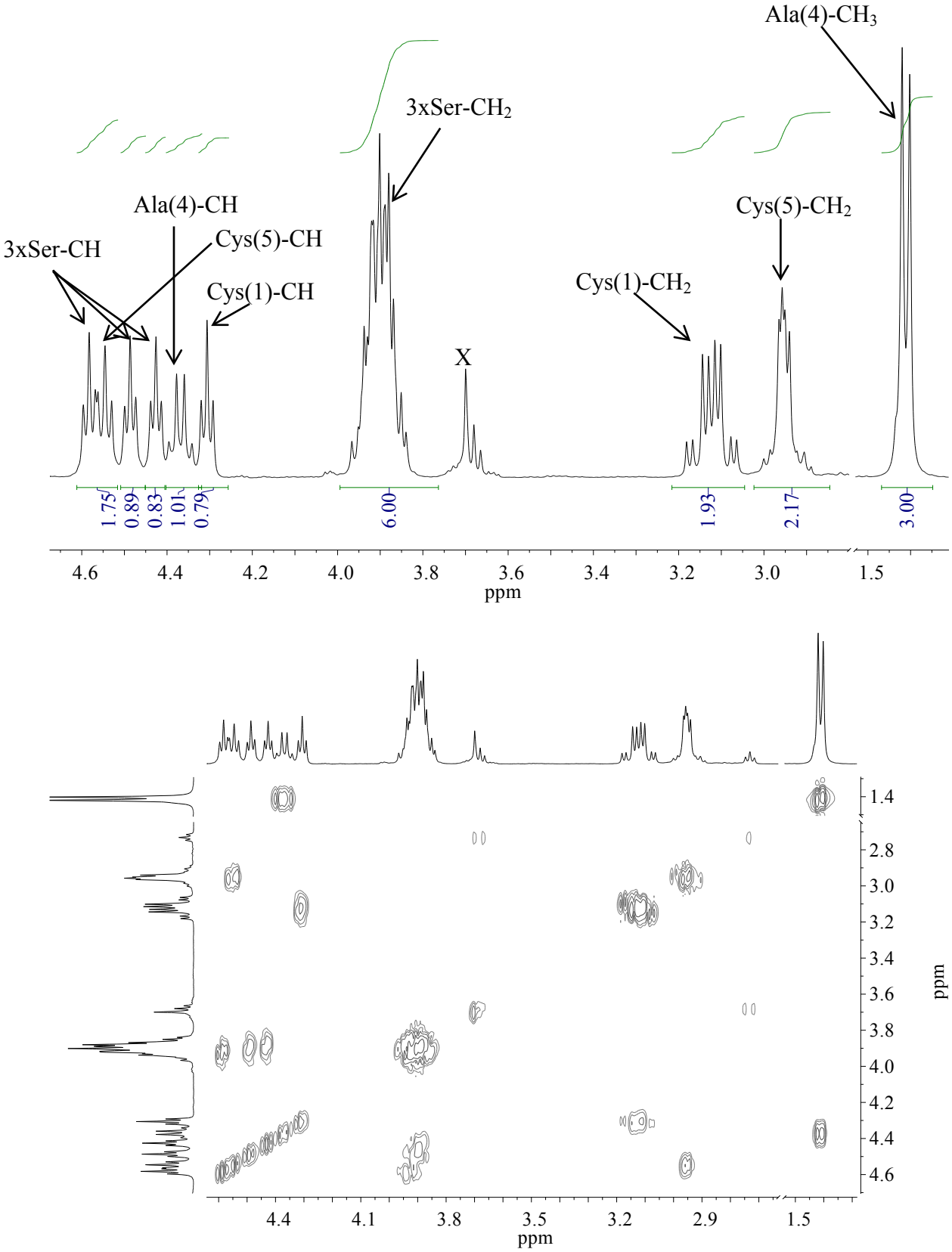


Fig. S2. ^{1}H NMR and ^{1}H-^{1}H COSY spectra of ACSSACS-NH_2 recorded in D_2O at pD=2.88.

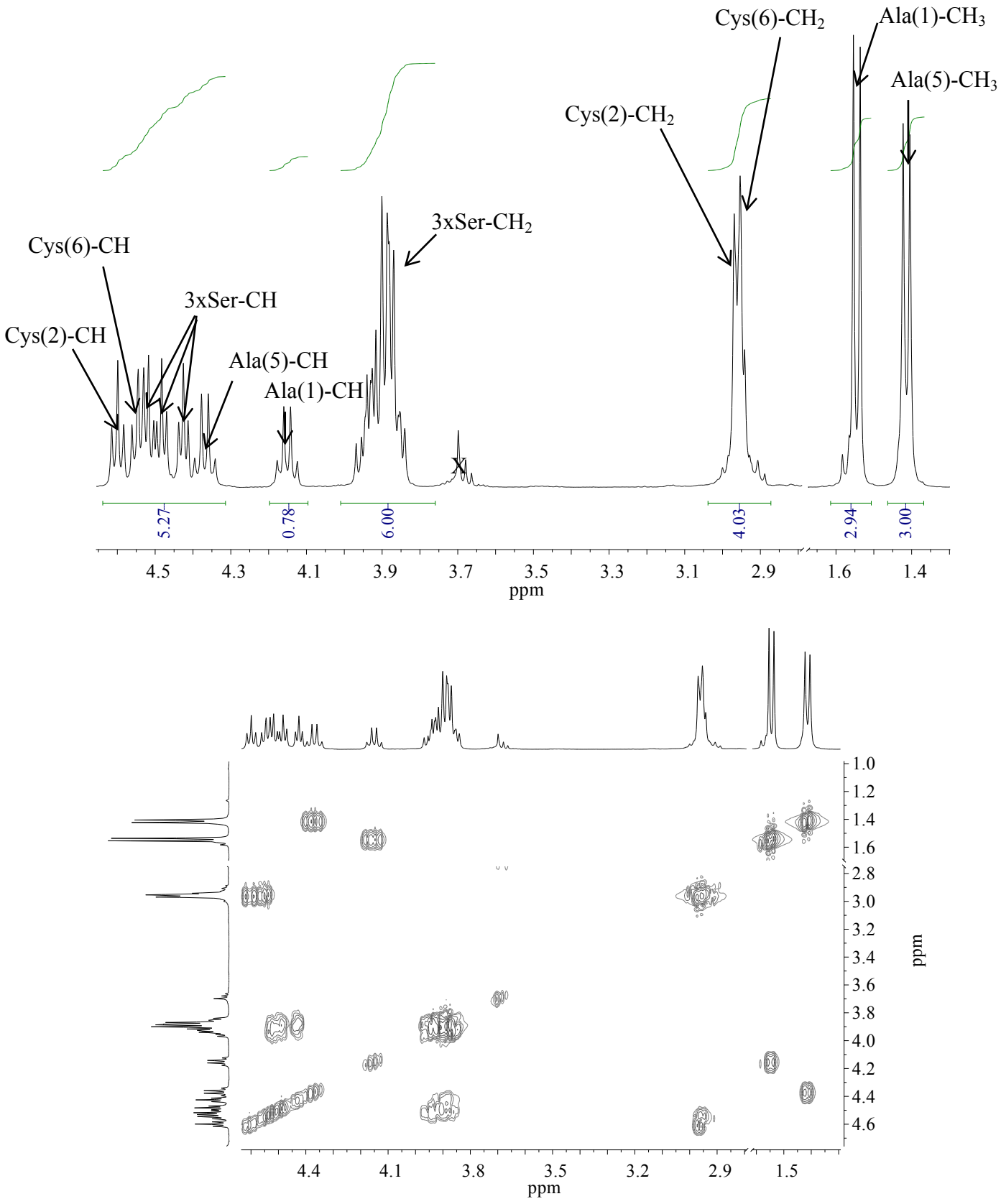


Fig. S3. pH dependent ^{1}H NMR spectra of the hexapeptide CSSACS-NH_2 recorded in D_2O, c_L = 10 mM.

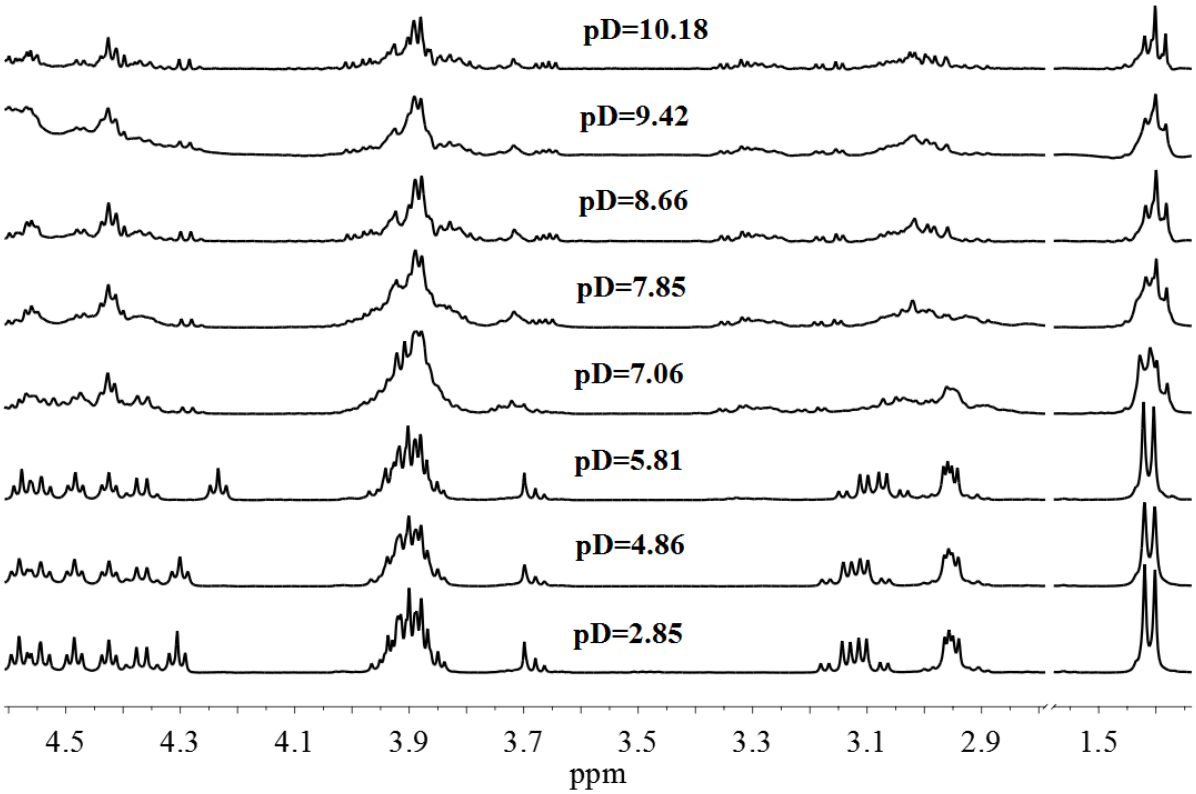


Fig. S4. pH dependent ^{1}H NMR spectra of the heptapeptide ACSSACS-NH_2 recorded in D_2O, c_L = 10 mM.

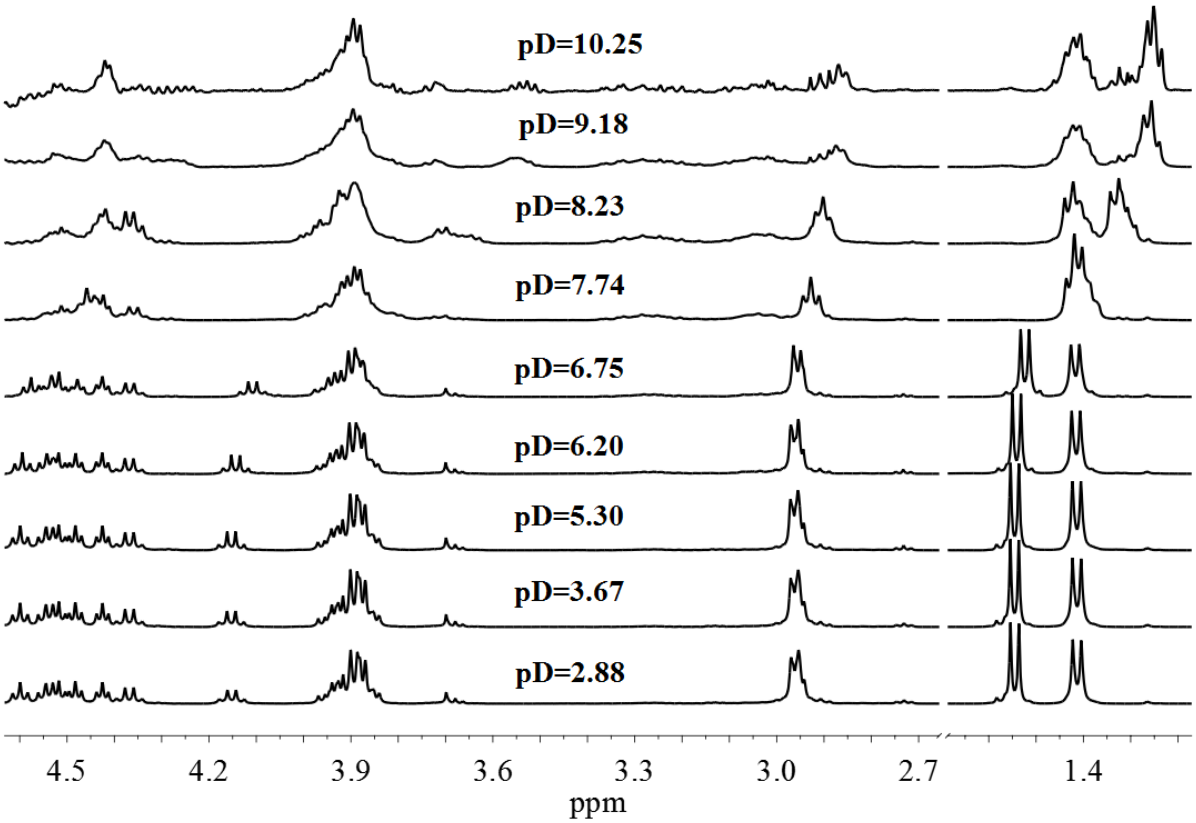


Fig. S5. ESI MS spectra recorded in the zinc(II) –CSSACS-NH_2 system at pH 7.6 (a) and calculated spectra for the species $[ZnLCl]^-$=$[Zn(C_{18}H_{31}N_7O_9S_2)Cl^-]$ (b).

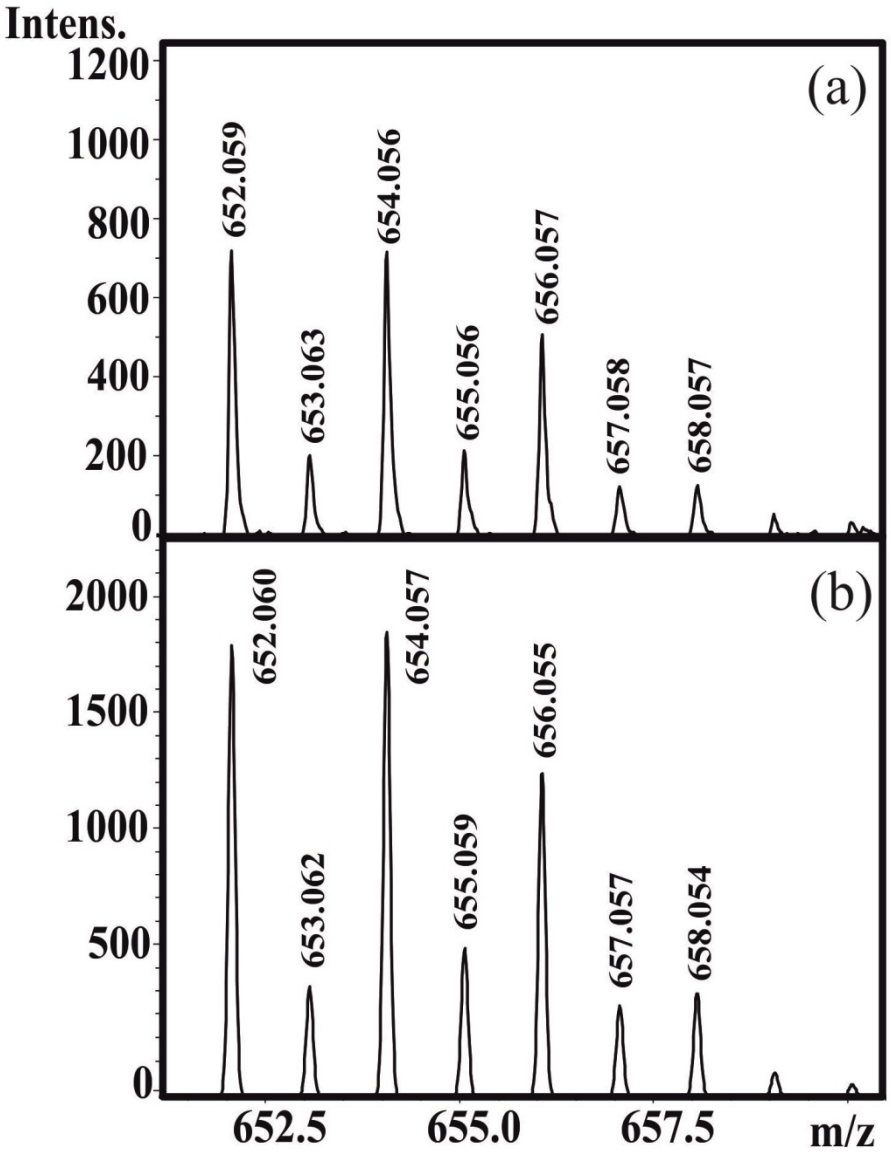


Fig. S6. ESI MS spectra recorded in the cadmium(II) –ACSSACS-NH_2 system at pH 9.84 (a) and calculated spectra for the species $[CdH_{-1}L]^-$ = $[Cd(C_{21}H_{35}N_8O_{10}S_2)^-]$ containing deprotonated amide nitrogen (b).

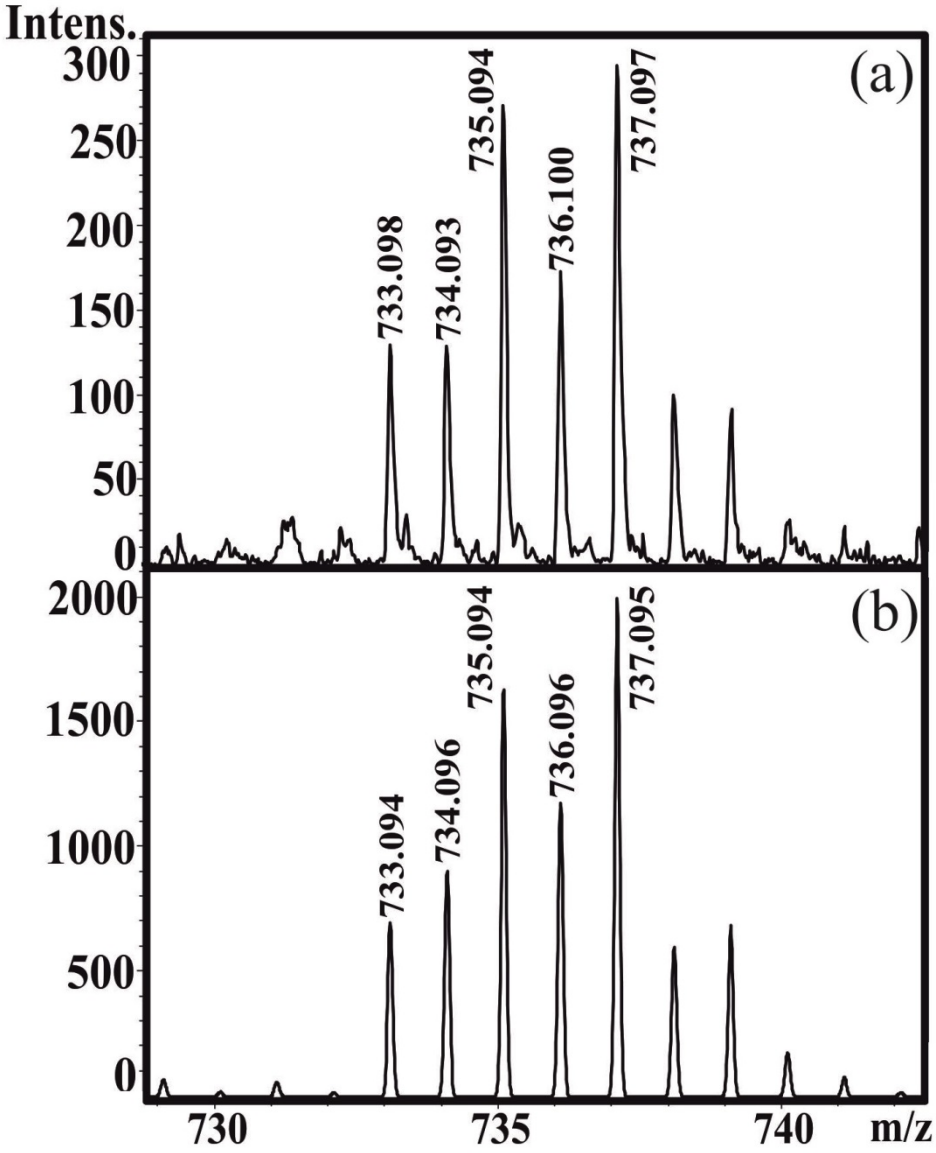
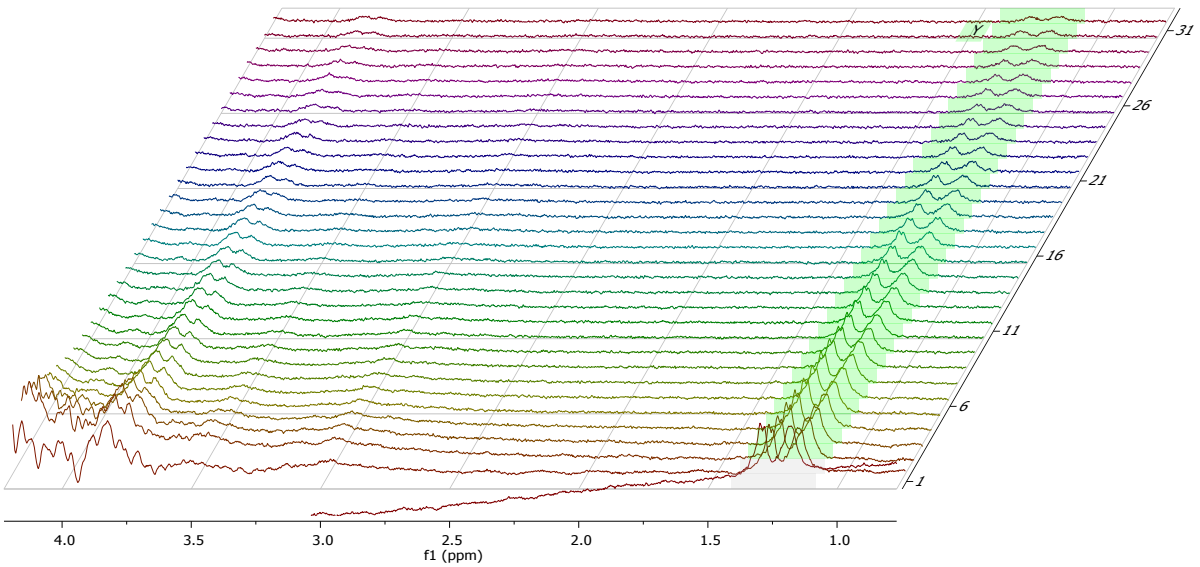
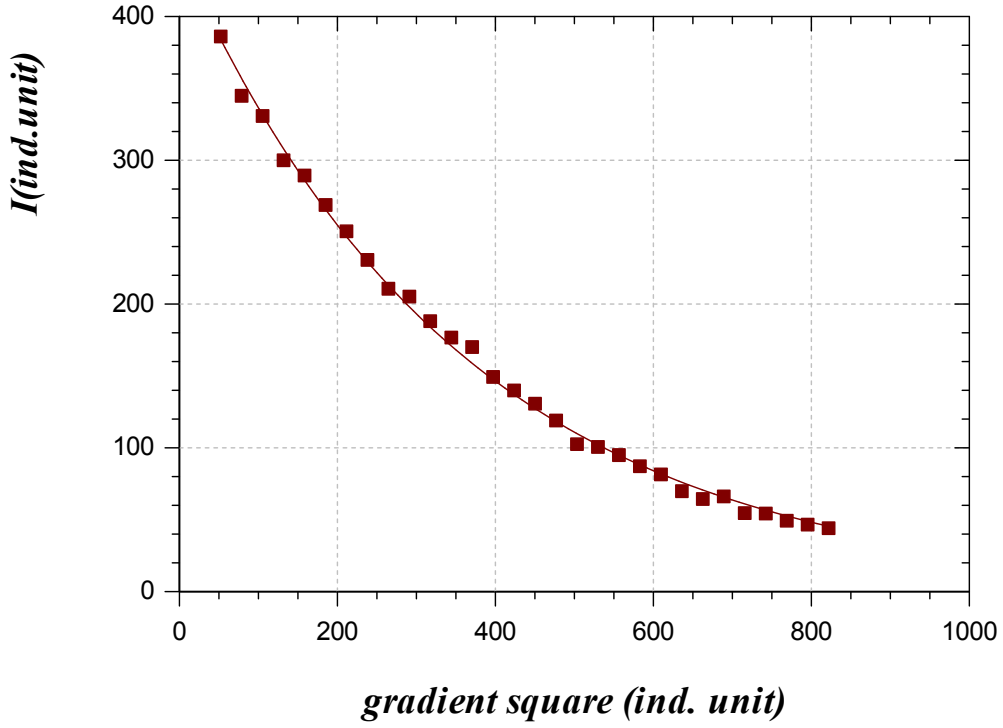


Fig. S7. Diffusion rate and data evaluation for $[CdH_{-1}L]^-$ complex



Typical series of ^1H NMR spectra as a function of gradient square. The first spectrum is distorted by the large water peak, however the remaining peaks of methyl protons at 1.0-1.5 ppm could be integrated. The other peaks of the Cd-complex were too noisy for evaluation.

The goodness of parameter fitting by Scientist (© Micromath) software



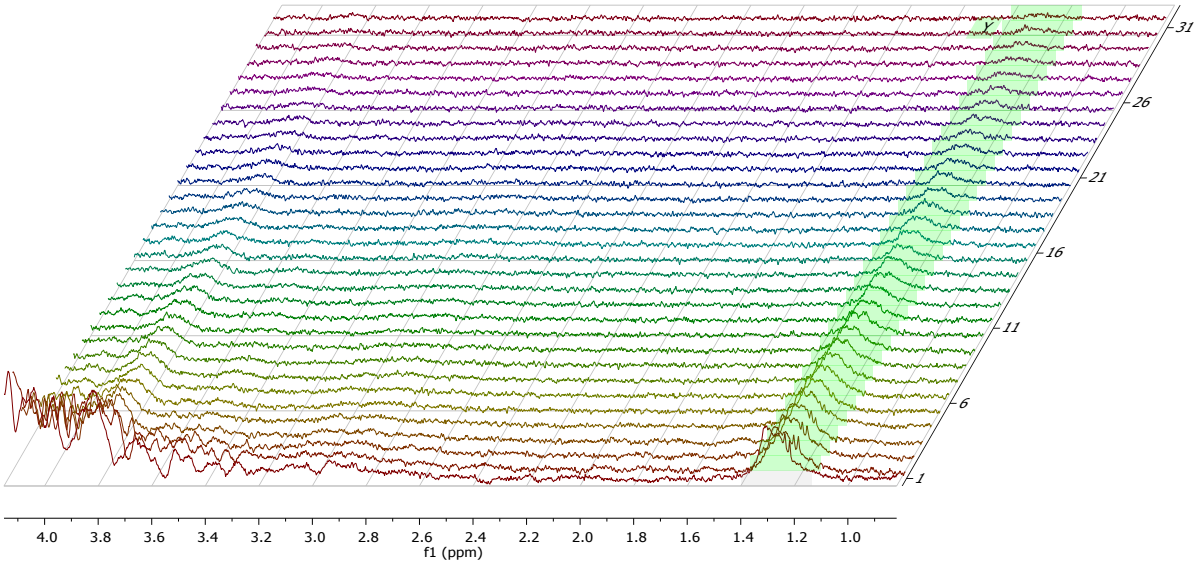
Statistical parameters:

Confidence Intervals:

Parameter Name :	I_0		
Estimate Value =	**443.983753**		
Standard Deviation =	**3.66183740**		
95% Range (Univar) =	436.482819	451.484687	
95% Range (S-Plane) =	434.518933	453.448573	

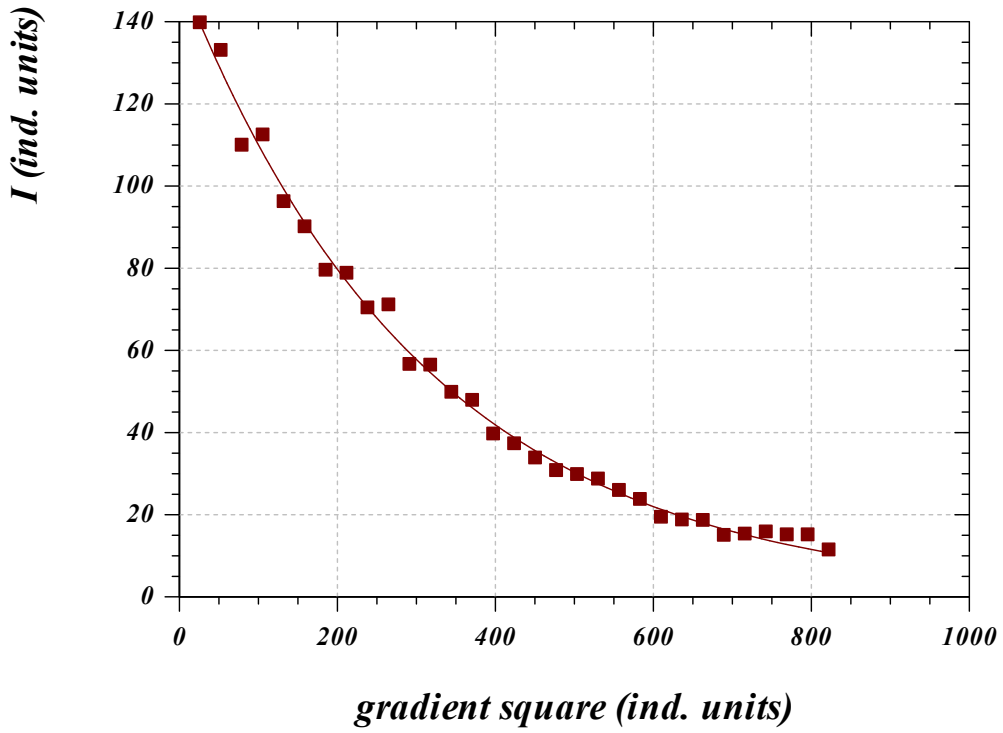
Parameter Name :	D	
Estimate Value =	**2.77415080E-6**	**2.77 (± 0.06)x10^{-6} cm^2 s^{-1}**
Standard Deviation =	**3.13916350E-8**	
95% Range (Univar) =	2.70984795E-6	2.83845365E-6
95% Range (S-Plane) =	2.69301225E-6	2.85528935E-6

Fig. S8. Diffusion rate and data evaluation for $[ZnH_{-1}L]^-$ complex



Typical series of ^1H NMR spectra as a function of gradient square. The first spectrum is distorted by the large water peak, however the remaining peaks of methyl protons at 1.0-1.5 ppm could be integrated. The other peaks of the Zn-complex were too noisy for evaluation.

The goodness of parameter fitting by Scientist (© Micromath) software



Confidence Intervals:

Parameter Name :	I_0		
Estimate Value =	**151.871678**		
Standard Deviation =	**1.87617040**		
95% Range (Univar) =	148.034479	155.708877	
95% Range (S-Plane) =	147.031555	156.711801	

Parameter Name :	D	
Estimate Value =	**3.22272979E-6**	**3.2 ($\pm$ 0.1)x10^{-6} cm^2 s^{-1}**
Standard Deviation =	**5.65128336E-8**	
95% Range (Univar) =	3.10714807E-6	3.33831151E-6
95% Range (S-Plane) =	3.07693863E-6	3.36852095E-6