Supporting Information for:

Molecular recognition of *N*-protected dipeptides by pseudopeptidic macrocycles: a comparative study of the supramolecular complexes by ESI-MS and NMR

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Figure S1. Detail of the ESI-TOF spectra for the doubly charged supramolecular complexes formed between **2a** and (a) Z-AA-OH, (b) Z-AF-OH and (c) Z-FF-OH. For every case, the upper and lower traces show the simulated and experimental peaks, respectively.

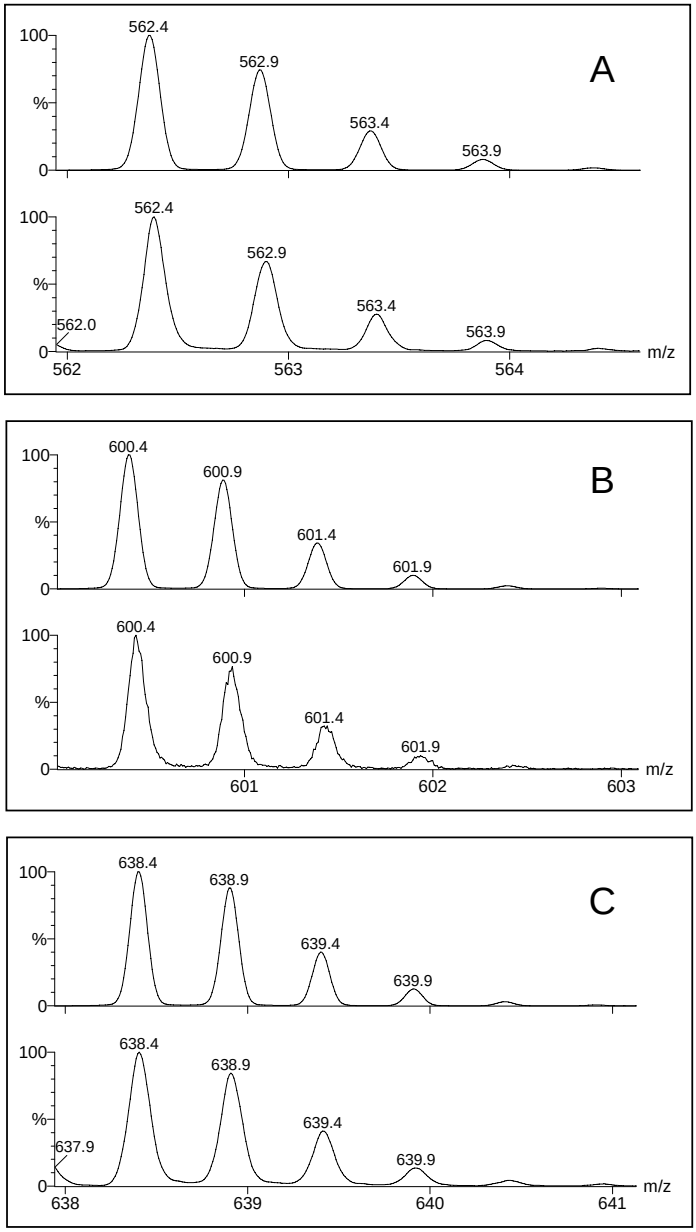


Figure S2. Collision Induced Dissociation (CID) spectra of the mass-selected (A) [**2a** + Z-AA-OH + 2H]$^{2+}$ and (B) [**2a** + Z-AF-OH + 2H]$^{2+}$ supramolecular complexes at increasing collision energies in the $E_{laboratory}$ = 2-12 eV range.

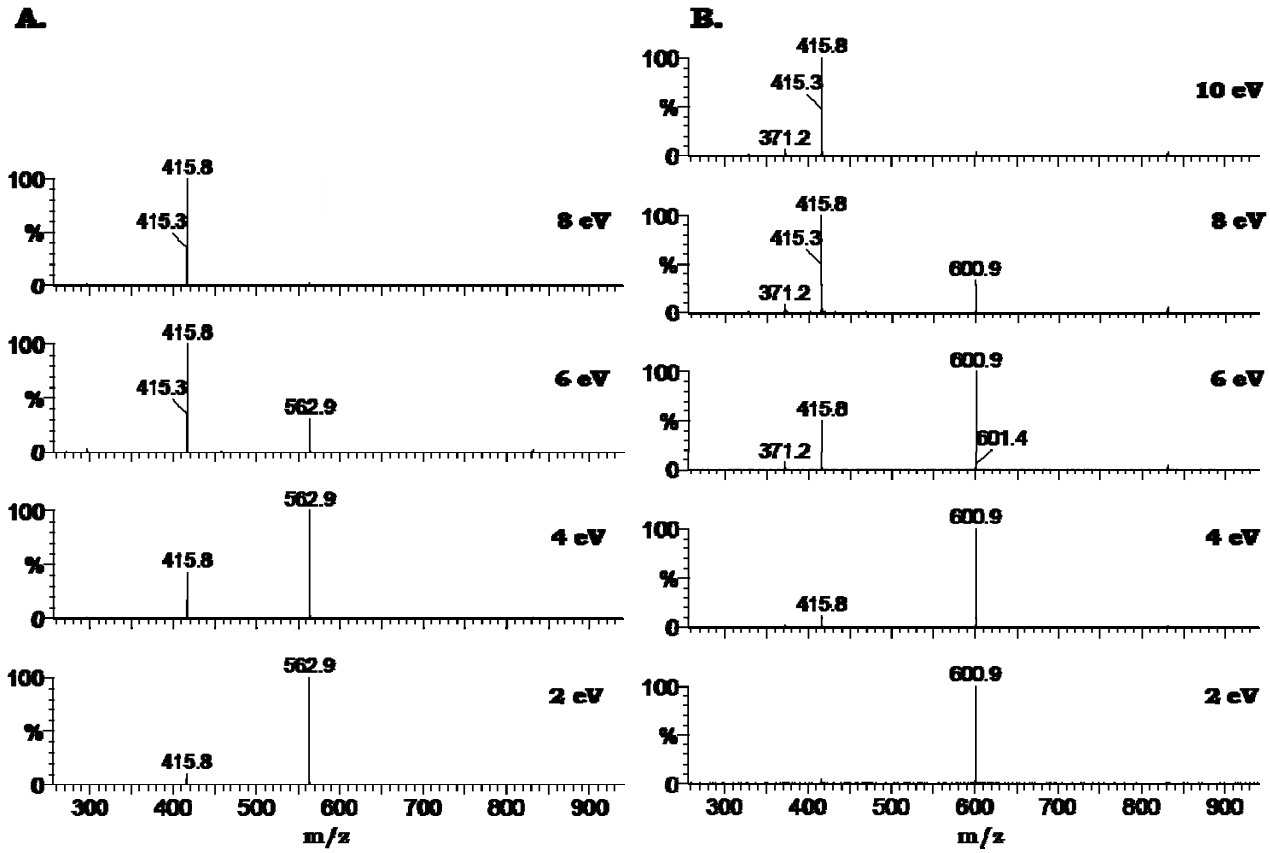


Figure S3. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of Z-AA-OH.

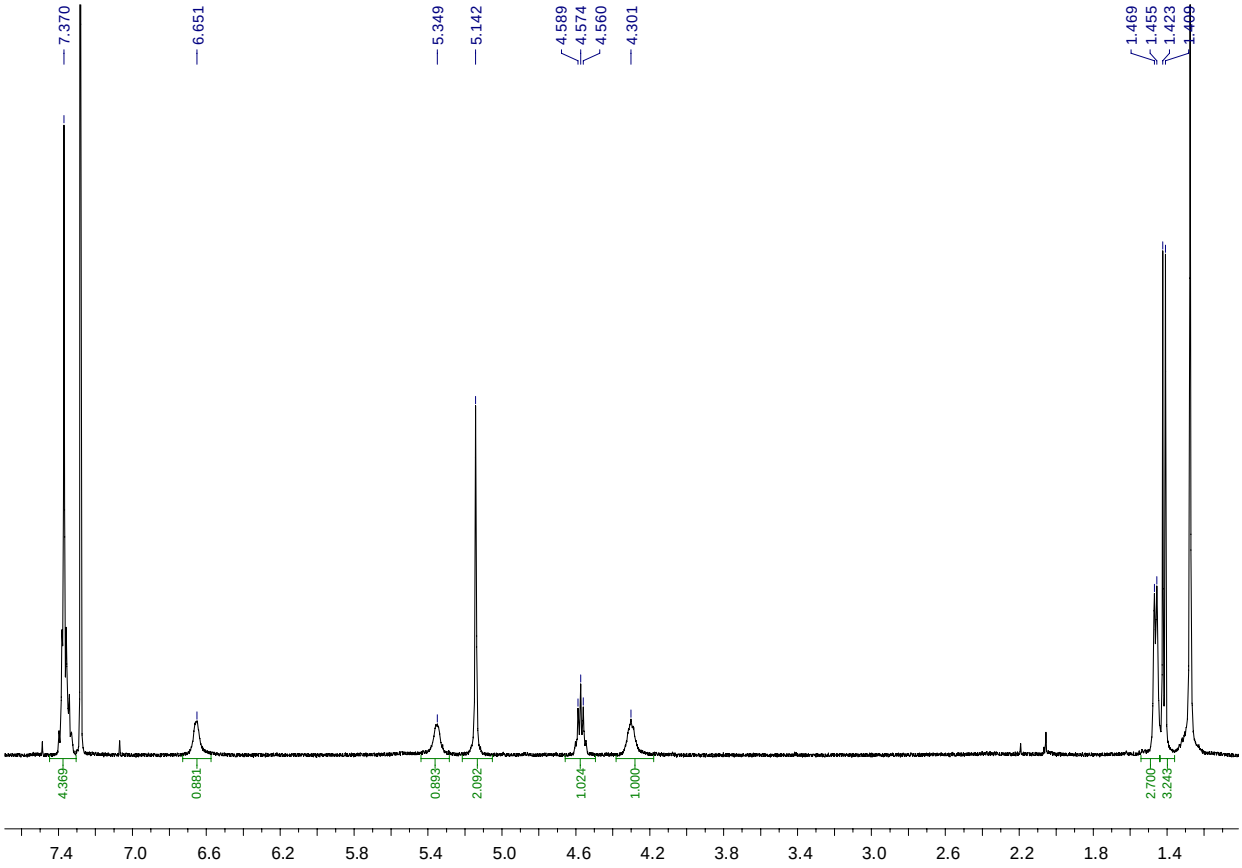


Figure S4. gCOSY NMR spectrum (500 MHz, $CDCl_3$) of Z-AA-OH.

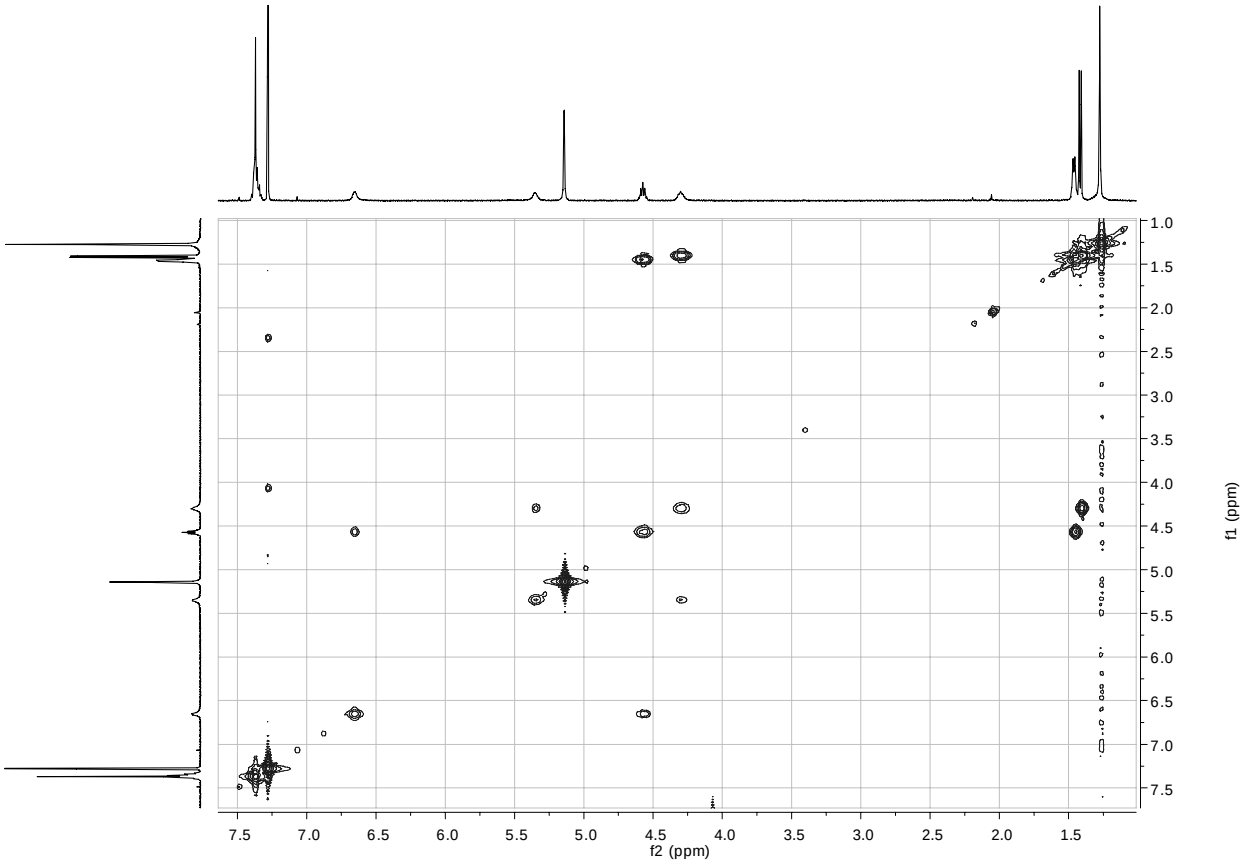


Figure S5. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of Z-AF-OH.

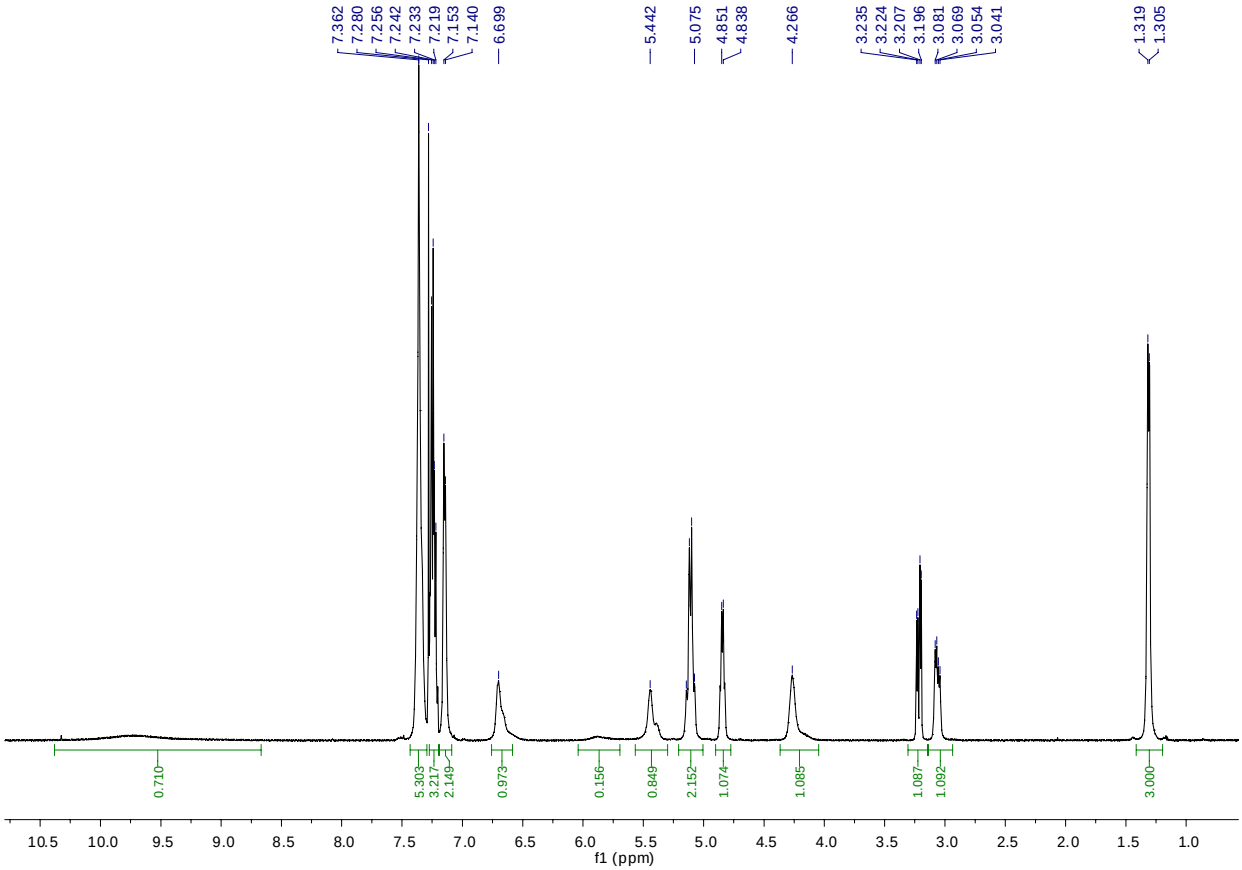


Figure S6. gCOSY NMR spectrum (500 MHz, $CDCl_3$) of Z-AF-OH.

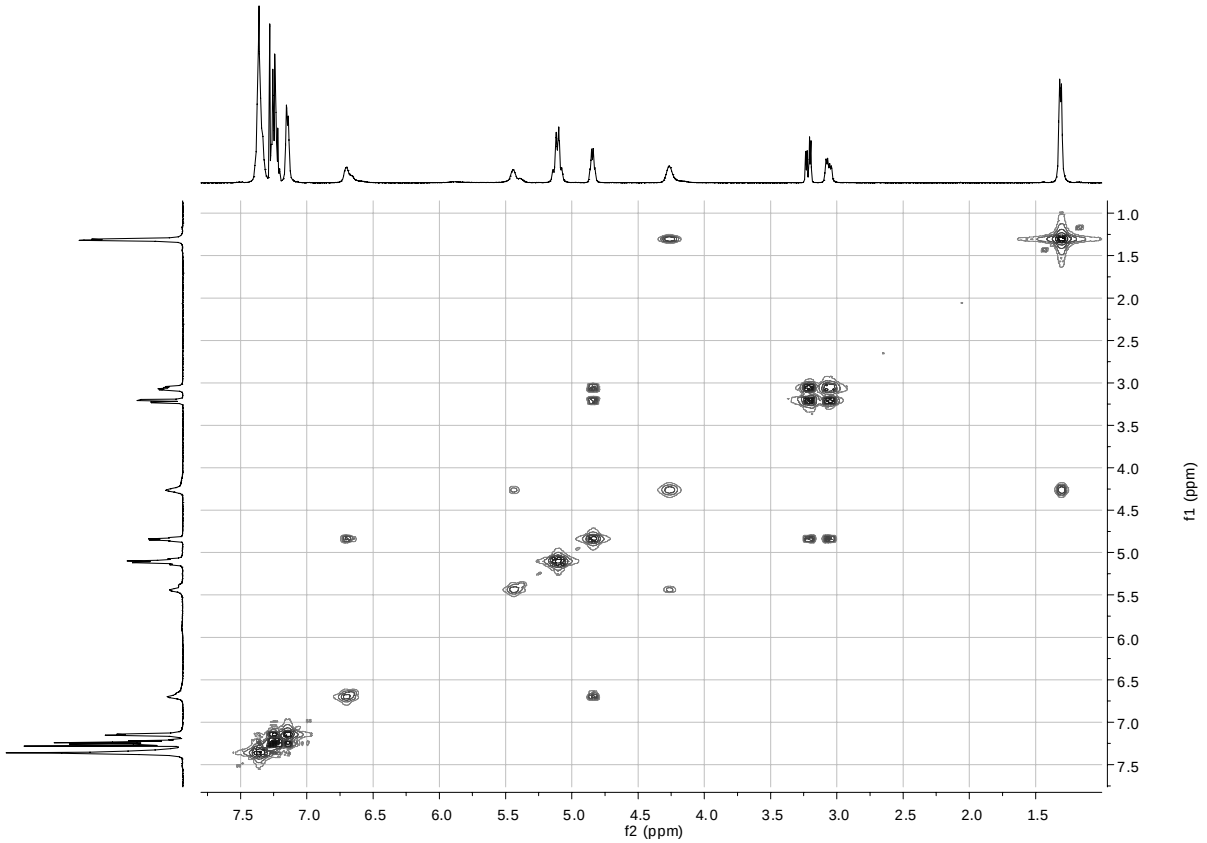
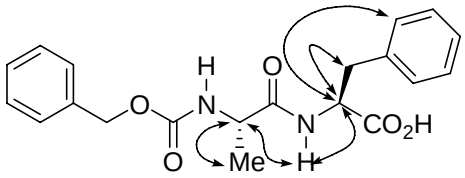


Figure S7. ^{1}H NMR (lower trace) and 1D NOESY spectra (500 MHz, $CDCl_3$) of Z-AF-OH upon irradiation of Ala (upper trace) and Phe (middle trace) Cα protons. The concentration of the sample was 30 mM, and positive nOEs were clearly observed (in antiphase with respect to the corresponding irradiated signal).



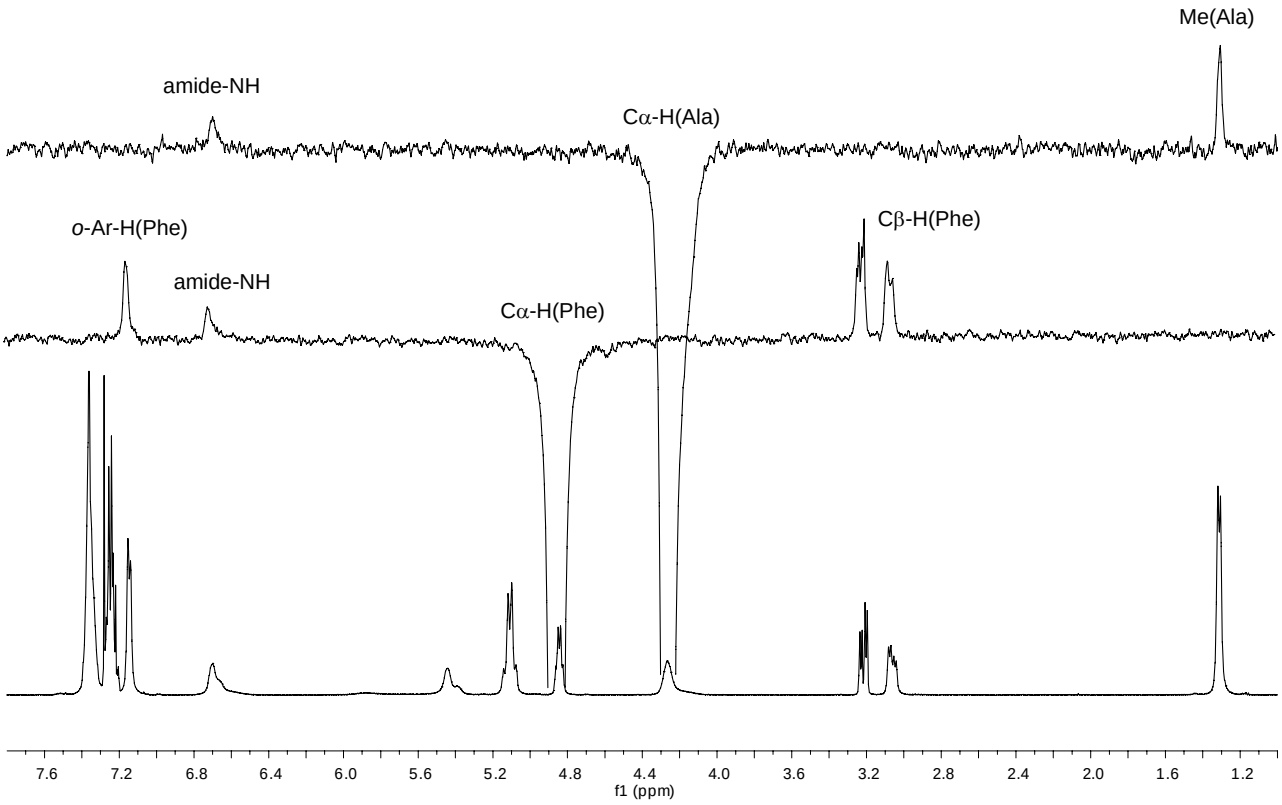


Figure S8. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of Z-FF-OH.

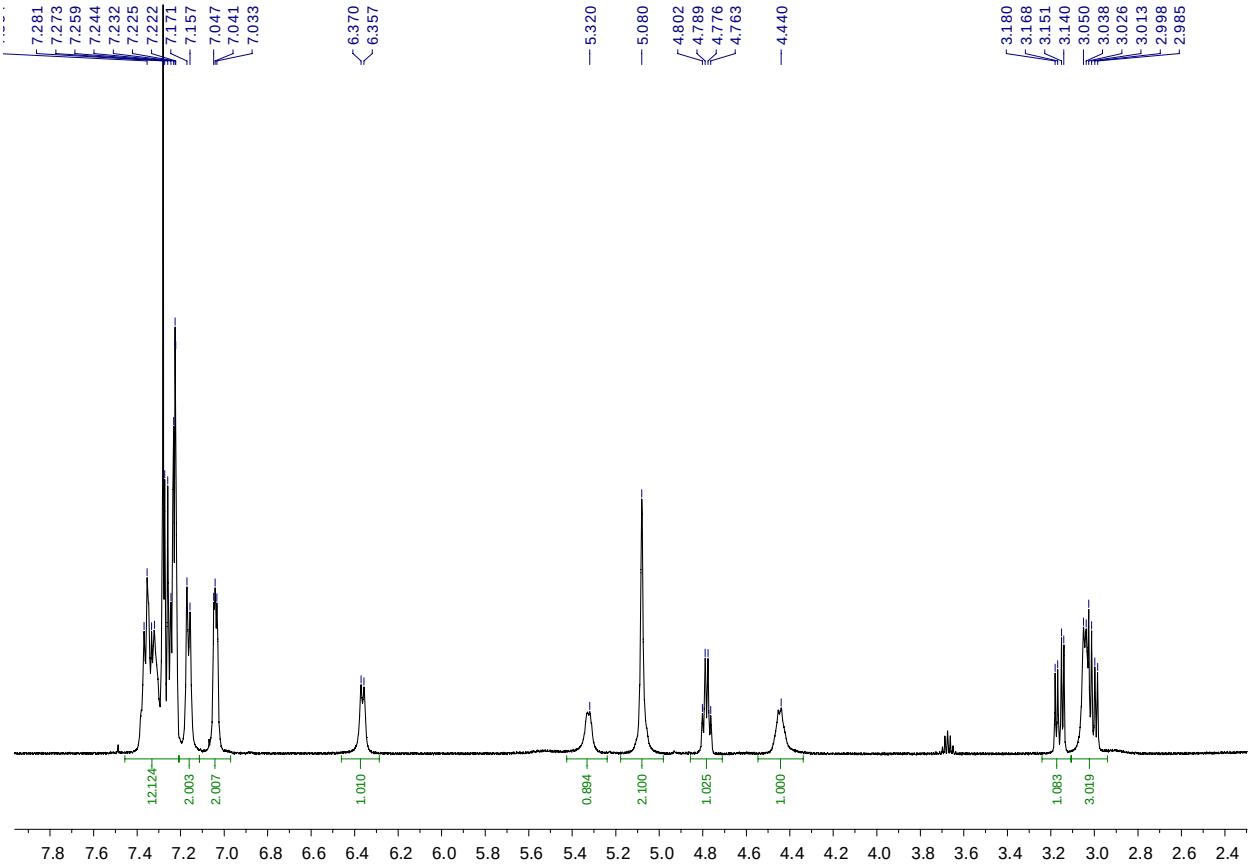


Figure S9. gCOSY NMR spectrum (500 MHz, $CDCl_3$) of Z-FF-OH.

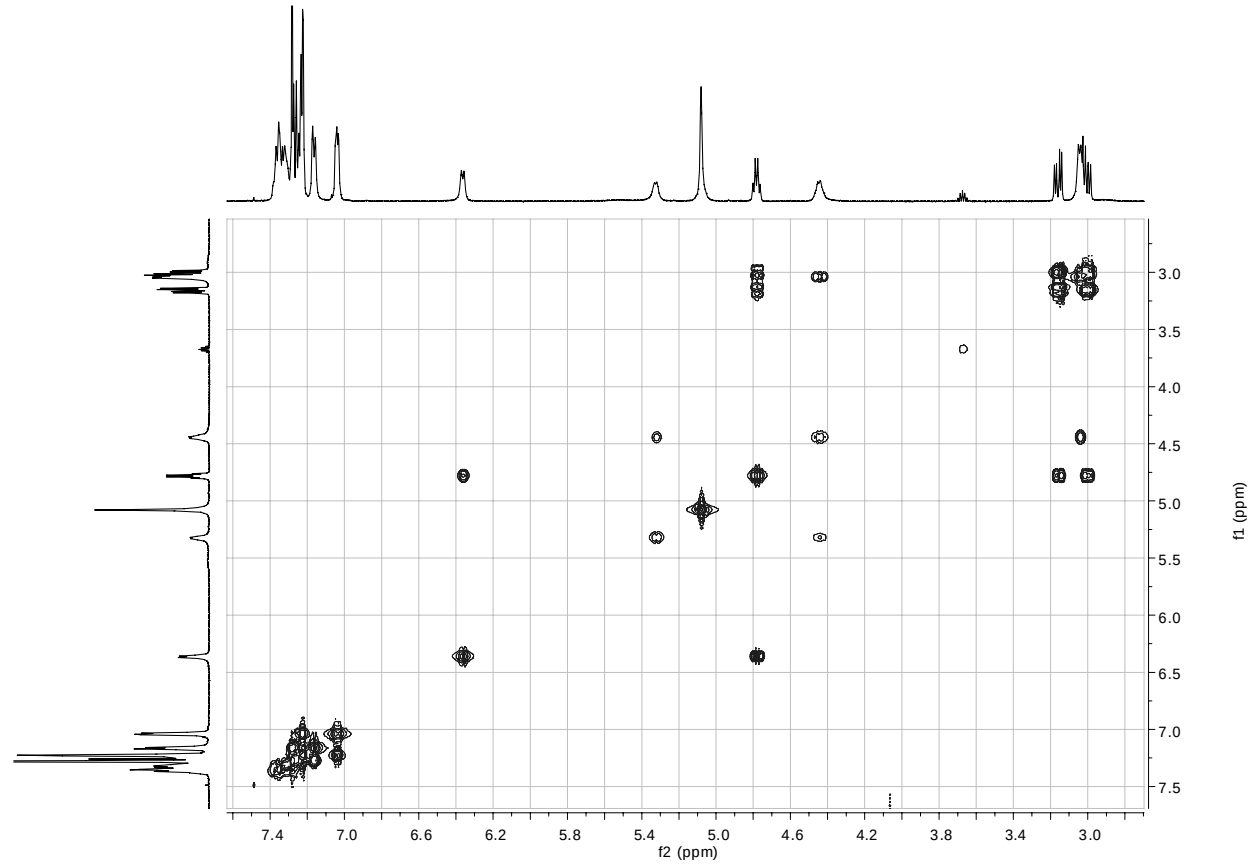


Figure S10. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **2a**.

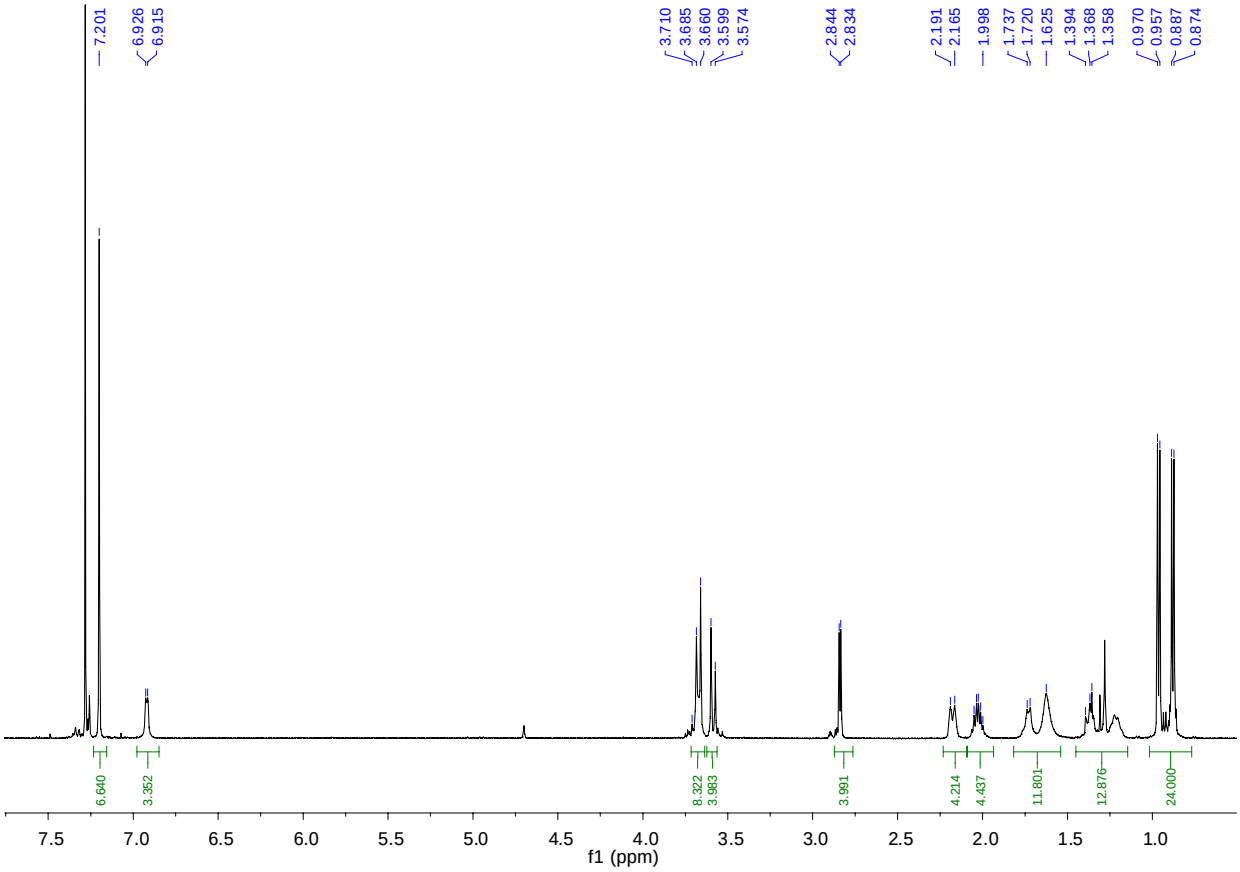


Figure S11. gCOSY NMR spectrum (500 MHz, $CDCl_3$) of **2a**.

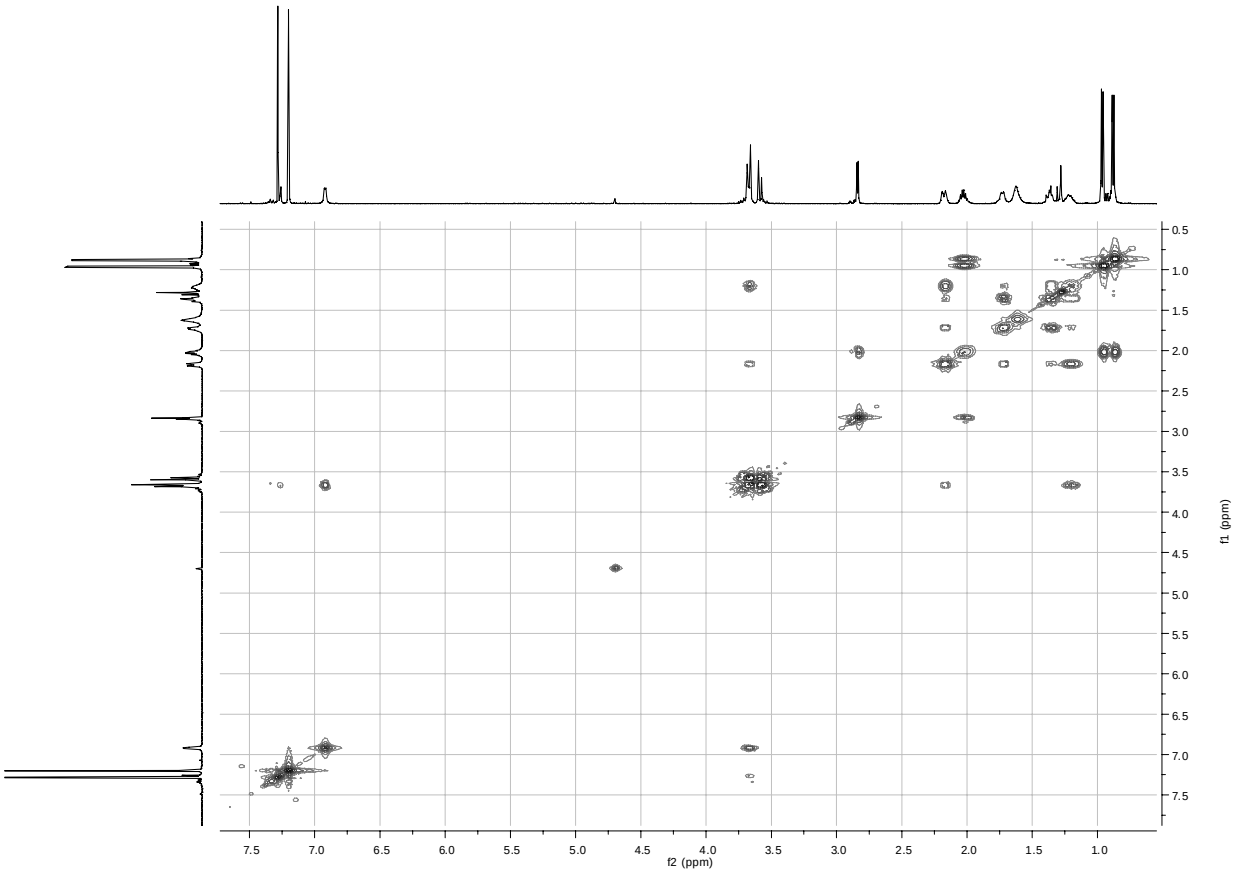


Figure S12. gTOCSY NMR spectrum (500 MHz, $CDCl_3$) of **2a**.

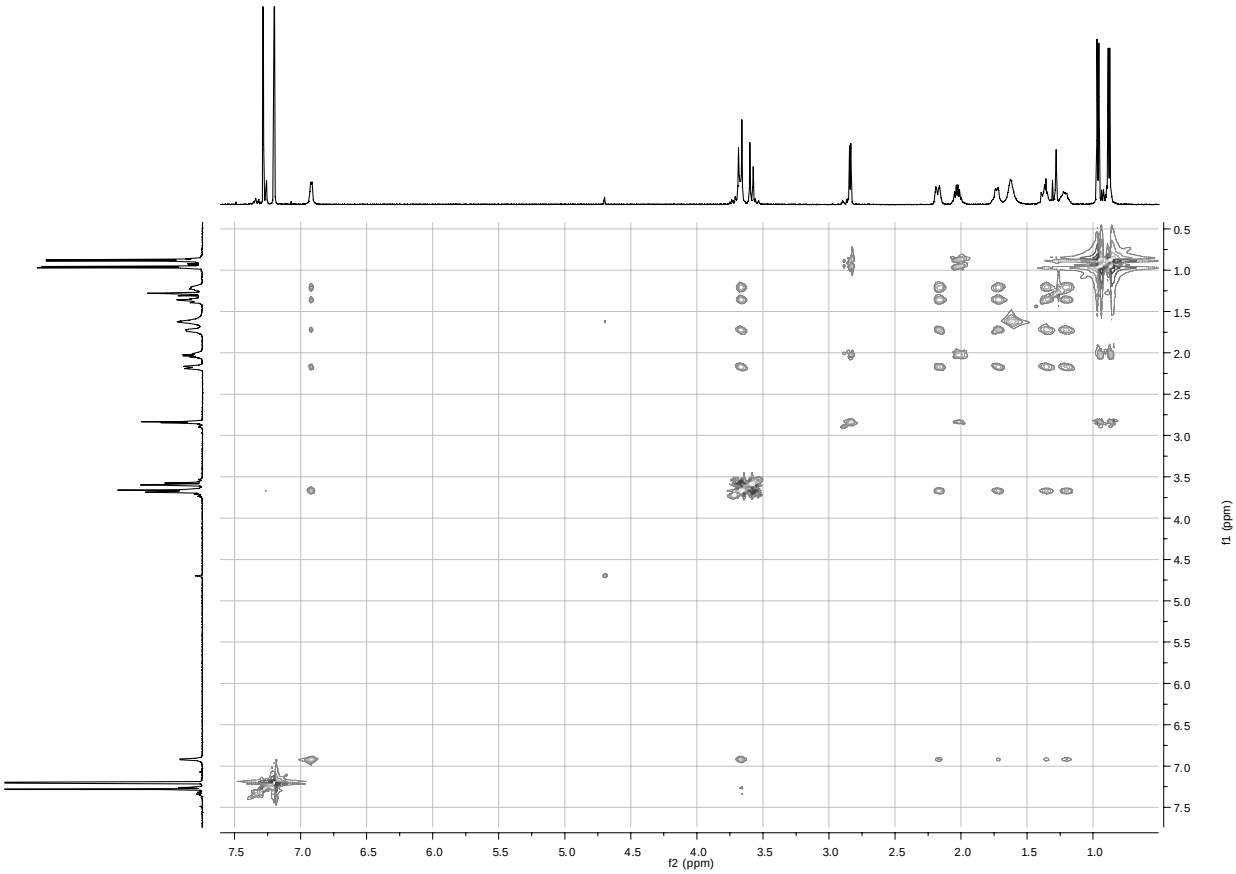


Figure S13. NOESY NMR spectrum (500 MHz, $CDCl_3$) of **2a**.

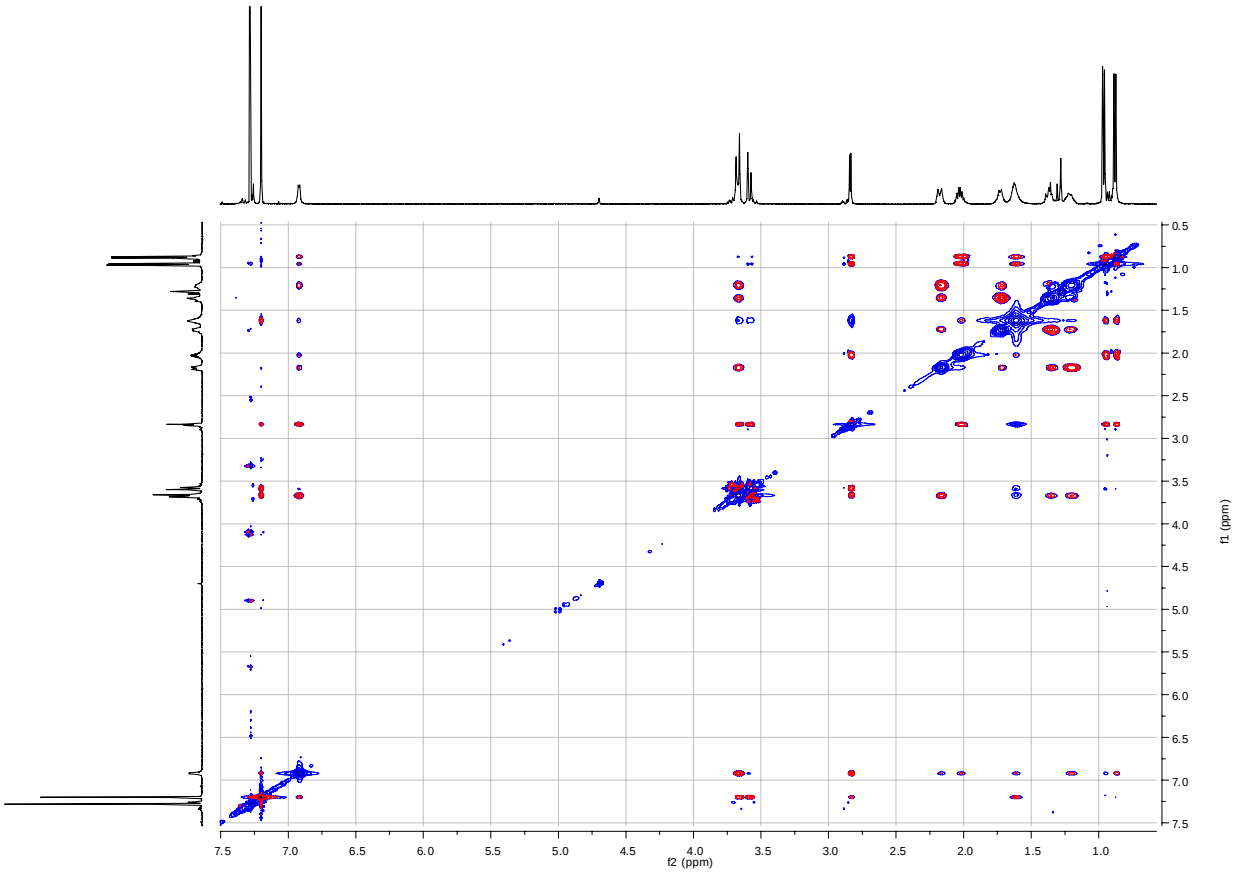


Figure S14. ROESY NMR spectrum (500 MHz, $CDCl_3$) of **2a**.

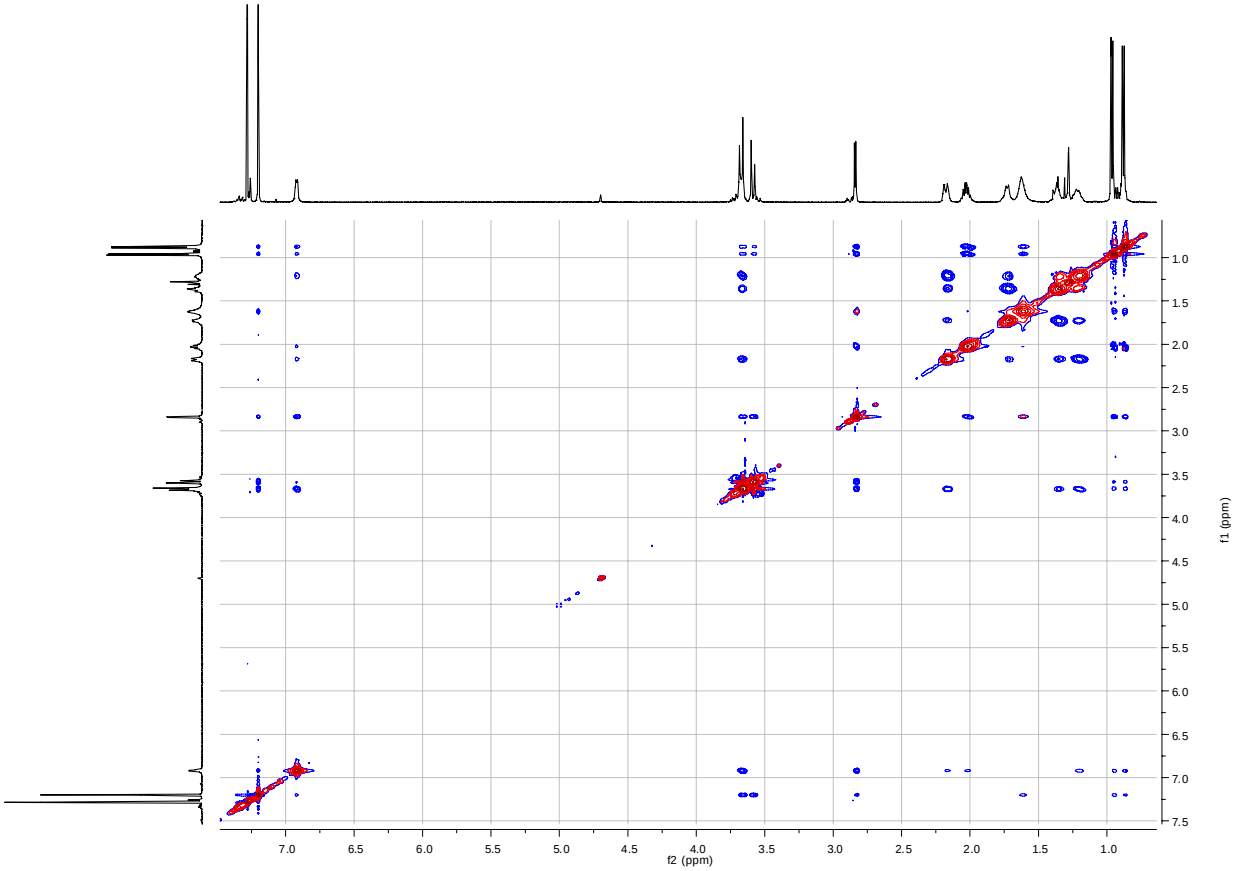


Figure S15. NOESY NMR spectrum (500 MHz, $CDCl_3$) of **2a** saturated with Z-AF-OH

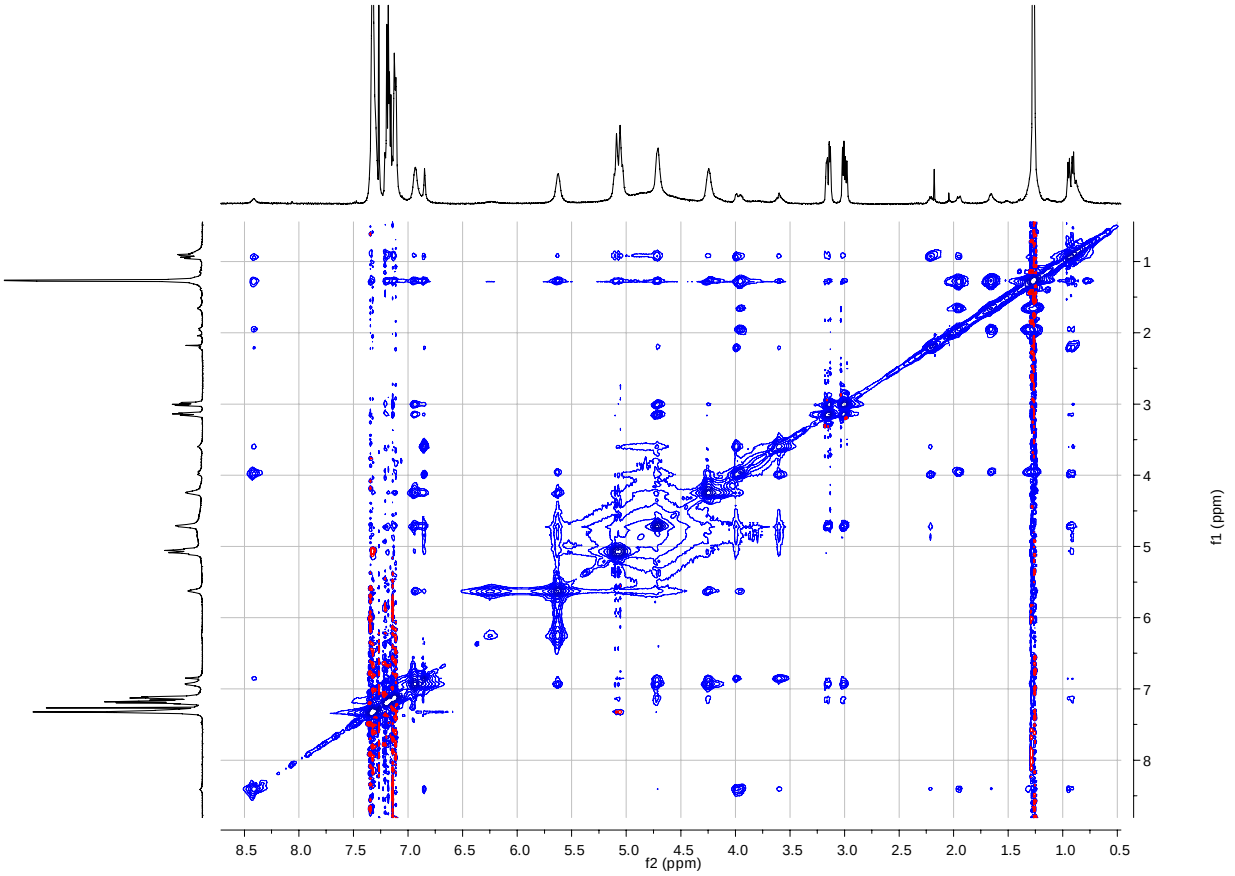


Figure S16. ROESY NMR spectrum (500 MHz, $CDCl_3$) of **2a** saturated with Z-AF-OH

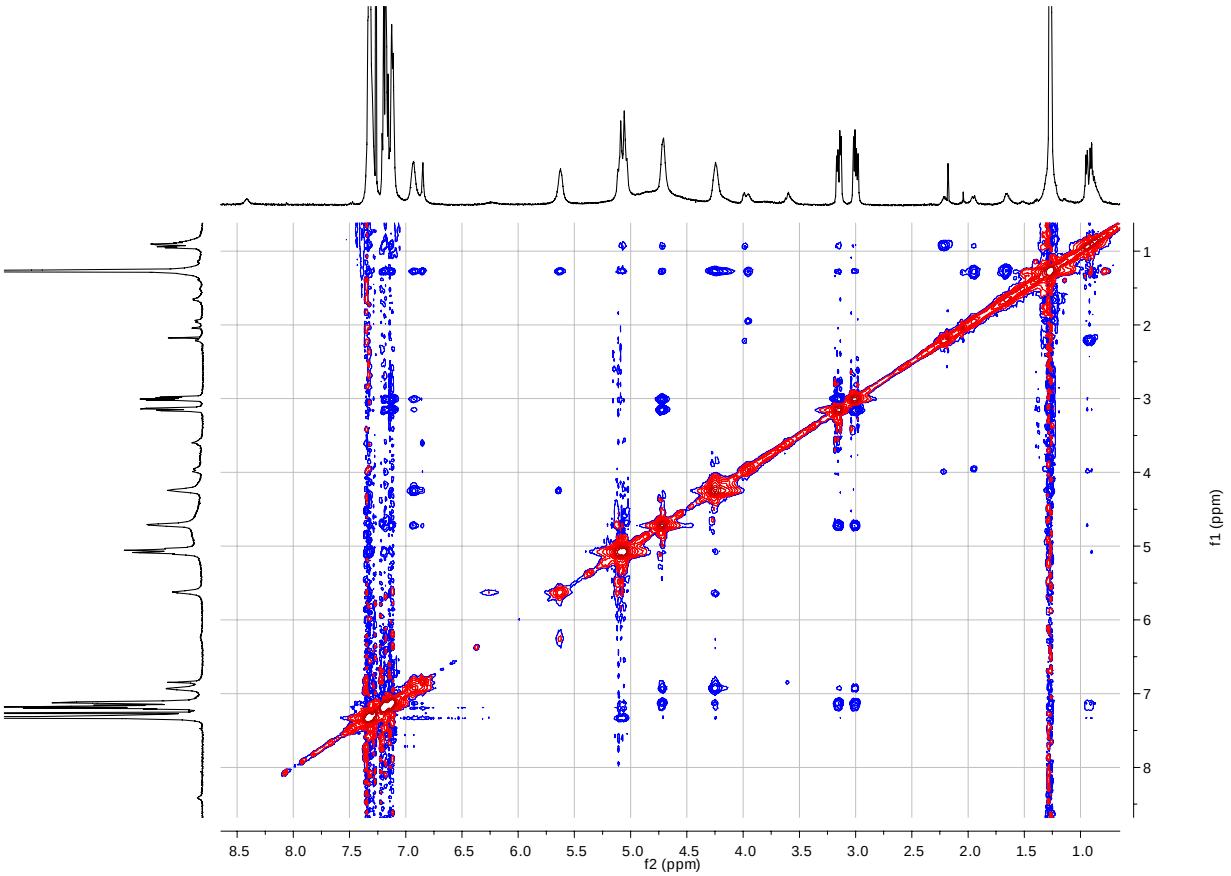
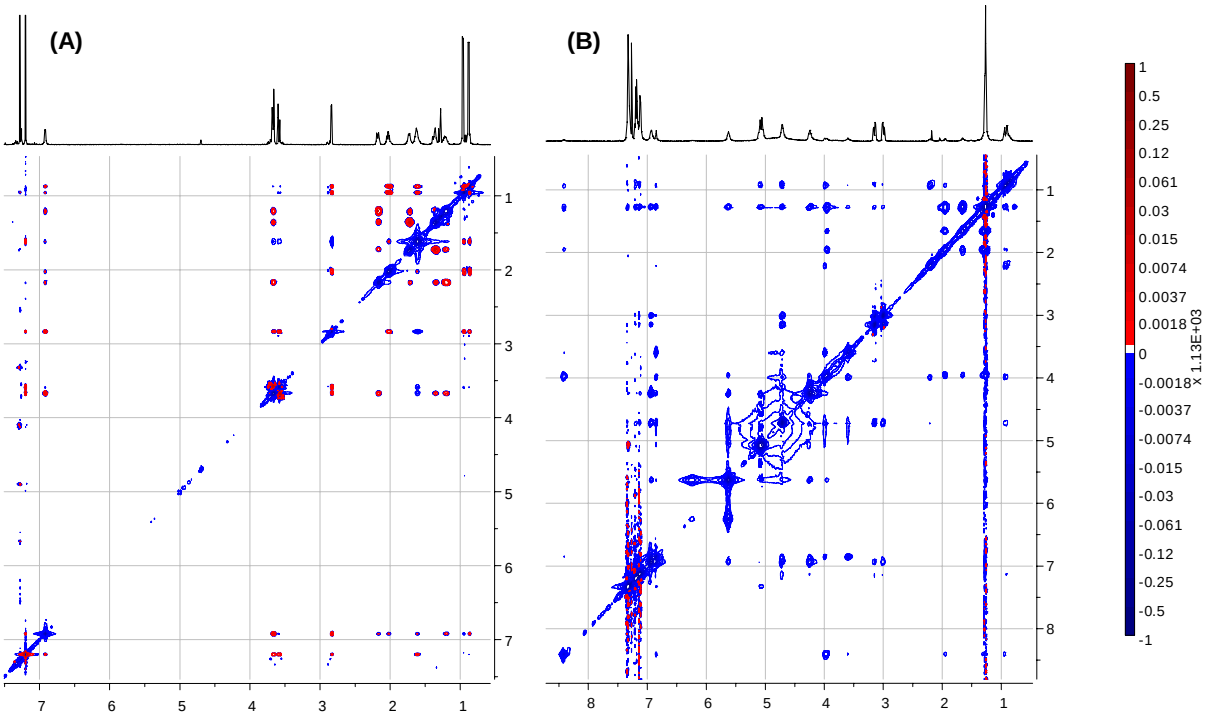


Figure S17. Comparison of the NOESY NMR spectra (500 MHz, $CDCl_3$) of **2a** alone (A) and saturated with Z-AF-OH (B)



^{1}H NMR Titration procedures

All the NMR titrations were performed at 303 K in a Varian INOVA 500 spectrometer operating at 500 MHz for proton. The non-linear least squares fitting calculations were performed with KaleidaGraph versio 4.03 by Synergy Software.

Titration procedure for Z-F-OH: We prepared a 3.3 mM stock solution of **2a** in dry, acid free $CDCl_3$ containing 1% MeOH. For the titrant solutions, weighted amounts of Z-F-OH were dissolved in the stock solution of the receptor (0.5-1.0 M final concentration of Z-F-OH) and thus, the solution of the titrant also contained a 3.3 mM concentration of **2a** in order to keep the concentration of the receptor constant during the titration experiment. Then, 0.5 mL of the stock solution of the receptor was placed in a NMR tube and the ^{1}H NMR spectrum was acquired. Afterwards, the receptor was carefully titrated by addition of small amounts of titrant solutions of the substrate. The ^{1}H NMR spectra were acquired (500 MHz, 303 K) after each addition, using 16-32 scans and a relaxation delay of 5 s. Different ^{1}H NMR signals of **2a** were monitored during the experiment, although the most suitable for quantitative analysis was that corresponding to the receptor amide NH protons.

We used the simplest 1 : 1 binding model to fit the data, using the non-linear least squares fitting of the experimental values to the following equation:[1]

$$\Delta\delta = \frac{\Delta\delta_{max} K_{as} [L]_{tot}}{1 + K_{as} [L]_{tot}}$$

Where: $\Delta\delta$ (y, dependent variable) is the observed variation of the chemical shift ($\delta_{obs} - \delta_o$) being

δ_{obs} the chemical shift at each titration point and δ_o the initial chemical shift (host alone)

$[L]_{tot}$ is the overall concentration of the guest titrant (m0, independent variable)

$\Delta\delta_{max}$ is the maximum variation of the observed chemical shift (m1 in the fitting)

K_{as} is the host-guest binding constant (m2 in the fitting)

[1] Connors, K. A. *Binding Constants: The Measurement of Molecular Complex Stability*, John Wiley & Sons, **1987**.

Figure S18. Titration of Z-F-OH(L) (500 MHz, 303 K, 1% MeOH in $CDCl_3$): the symbols correspond to experimental data and the line to the non-linear least squares fitting. The final values for the best fitting are given in the figure.

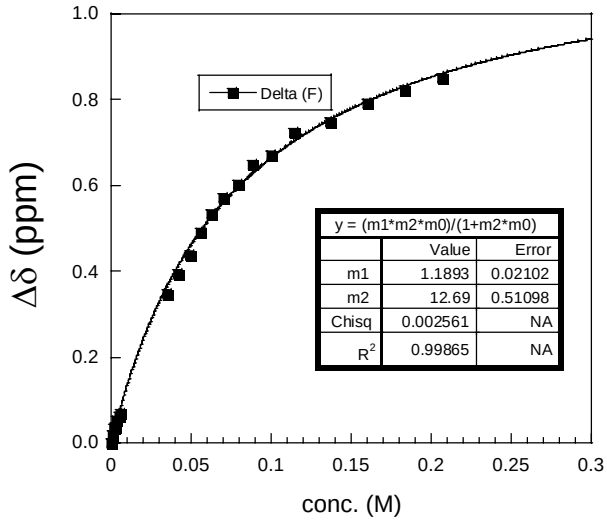
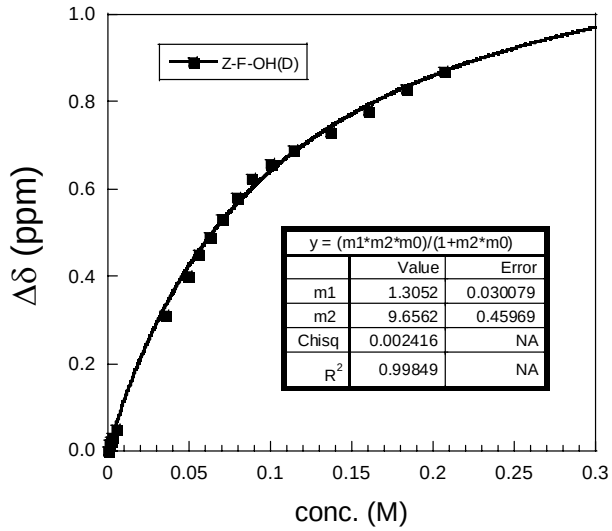


Figure S19. Titration of Z-F-OH(D) (500 MHz, 303 K, 1% MeOH in $CDCl_3$): the symbols correspond to experimental data and the line to the non-linear least squares fitting. The final values for the best fitting are given in the figure.



Self-assembling of dipeptides: Solutions of the dipeptides in $CDCl_3$ containing 1% of MeOH were prepared at different final concentrations (0.1-90 mM, depending on peptide solubility). The ^1H NMR spectra were acquired (500 MHz, 303 K) for every sample, using 32-64 scans and a relaxation delay of 5 s. Different ^1H NMR signals were monitored during the experiment, although the most suitable for quantitative analysis were those corresponding to the amide NH protons.

We used the simplest monomer-dimer equilibrium model to successfully fit the experimental data using the non-linear least squares fitting to the following equation:[2]

$$\delta_{obs} = \delta_m + \frac{1 + 4C_{tot}K_{dim} - \sqrt{1 + 8C_{tot}K_{dim}}}{4C_{tot}K_{dim}} \times (\delta_d - \delta_m)$$

Where: δ_{obs} is the observed chemical shift at each titration point (y, dependent variable)

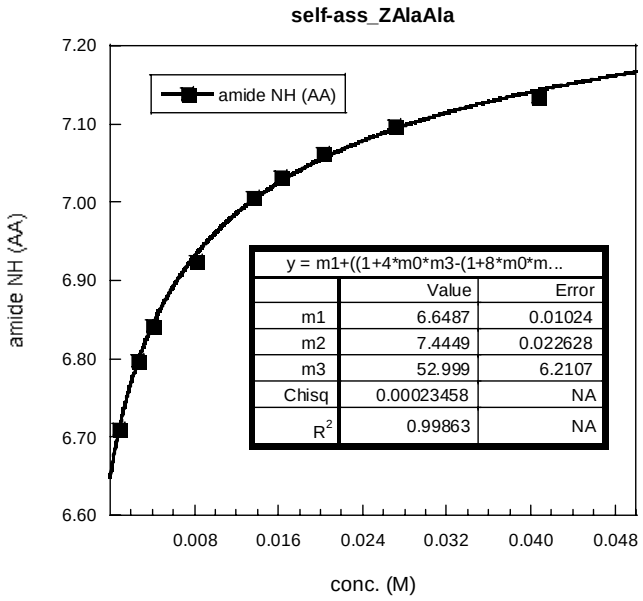
C_{tot} is the overall concentration of the compound (m0, independent variable)

δ_m is the chemical shift of the monomer (m1 in the fitting)

δ_d is the chemical shift of the dimer (m2 in the fitting)

K_{dim} is the dimerization equilibrium constant (m3 in the fitting)

Figure S20. Dilution titration of Z-AA-OH (500 MHz, 303 K, 1% MeOH in $CDCl_3$): the symbols correspond to experimental data and the line to the non-linear least squares fitting. The final values for the best fitting are given in the figure.



[2] (a) Schmuck, C.; Rehm, T.; Geiger, L.; Schäfer, M. *J. Org. Chem.* **2007**, *72*, 6162. (b) Martin, R. B. *Chem. Rev.* **1996**, *96*, 3043. (c) Davis, J. C. Jr.; Deb, K. K. *Adv. Magn. Reson.* **1970**, *4*, 201. (d) Bangerter, B. W.; Chan, S. I. *J. Am. Chem. Soc.* **1969**, *91*, 3910.

Figure S21. Dilution titration of Z-AF-OH (500 MHz, 303 K, 1% MeOH in $CDCl_3$): the symbols correspond to experimental data and the line to the non-linear least squares fitting. The final values for the best fitting are given in the figure.

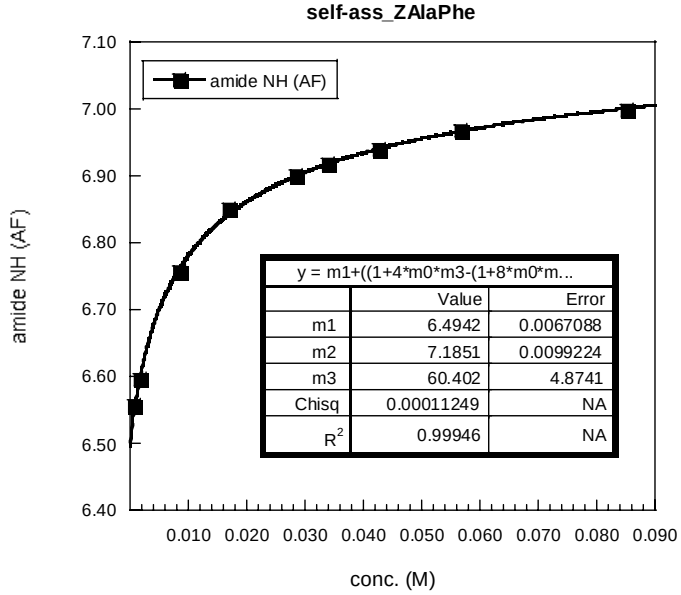
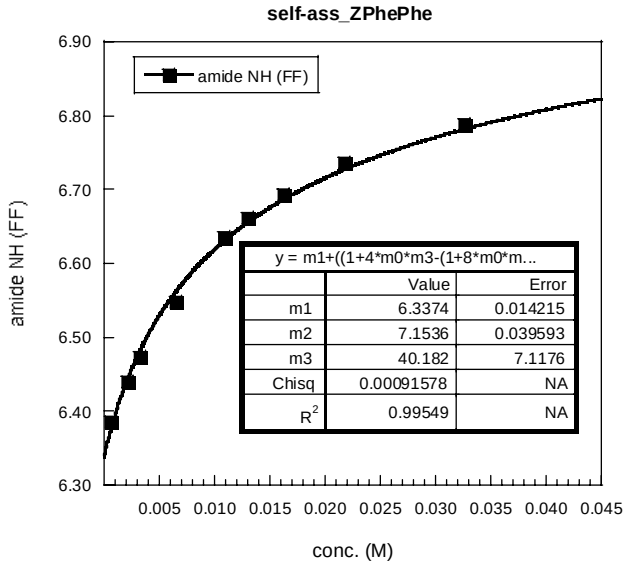


Figure S22. Dilution titration of Z-FF-OH (500 MHz, 303 K, 1% MeOH in $CDCl_3$): the symbols correspond to experimental data and the line to the non-linear least squares fitting. The final values for the best fitting are given in the figure.



Host-guest binding by dilution titration: Samples of exactly equimolecular amounts of **2a** or **1a** and a given substrate were prepared in $CDCl_3$ containing 1% of MeOH and at different final global concentrations (1-20 mM). The ^{1}H NMR spectra were acquired (500 MHz, 303 K) for every sample, using 32-64 scans and a relaxation delay of 5 s. Different ^{1}H NMR signals were monitored during the experiment, although the most suitable for quantitative analysis were those corresponding to the dipeptide amide NH protons.

We used the simplest 1 : 1 binding model to fit the data, using the non-linear least squares fitting of the experimental values to the following equation:[3]

$$\delta_{obs} = \delta_o - \frac{(\delta_o - \delta_c)}{2C_{tot}K_{as}} \times \left(2C_{tot}K_{as} + 1 - \sqrt{4C_{tot}K_{as} + 1} \right)$$

Where: δ_{obs} is the observed chemical shift at each titration point (y, dependent variable)

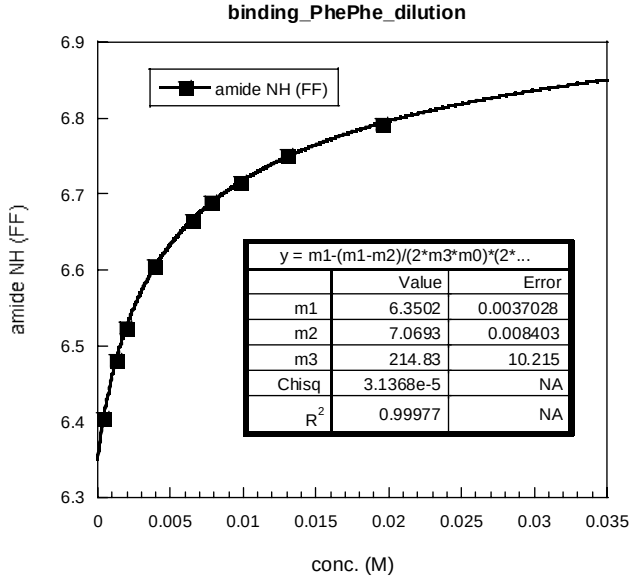
C_{tot} is the overall concentration of both components (m0, independent variable)

δ_o is the chemical shift of the unbound species (m1 in the fitting)

δ_c is the chemical shift of the complex species (m2 in the fitting)

K_{as} is the host-guest binding constant (m3 in the fitting)

Figure S23. Dilution titration of a 1 : 1 mixture of **2a** : Z-FF-OH (500 MHz, 303 K, 1% MeOH in $CDCl_3$) using the dipeptide amide NH proton signal. The symbols correspond to experimental data and the line to the non-linear least squares fitting. The final values for the best fitting are given in the figure.



[3] (a) Peters, L.; Fröhlich, R; Boyd, A. S. F.; Kraft, A. *J. Org. Chem.* **2001**, *66*, 3291. (b) Macomber, R. S. *J. Chem. Educ.* **1992**, *69*, 375. (c) Schneider, H. J.; Kramer, R.; Simova, S.; Schneider, U. *J. Am. Chem. Soc.* **1988**, *110*, 6442.

Figure S24. Dilution titration of a 1 : 1 mixture of **2a** : Z-FF-OH (500 MHz, 303 K, 1% MeOH in $CDCl_3$) using the receptor amide NH proton signal. The symbols correspond to experimental data and the line to the non-linear least squares fitting. The final values for the best fitting are given in the figure.

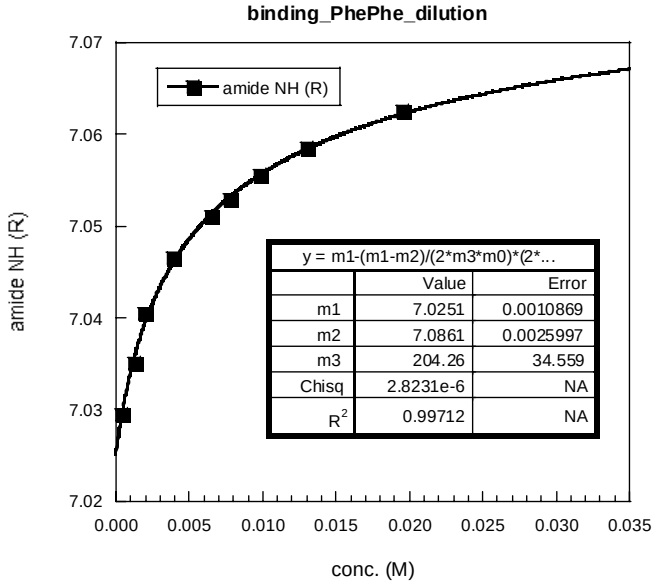


Figure S25. Dilution titration of a 1 : 1 mixture of **2a** : Z-FF-OH (500 MHz, 303 K, 1% MeOH in $CDCl_3$) using the receptor Cα proton signal. The symbols correspond to experimental data and the line to the non-linear squares least fitting. The final values for the best fitting are given in the figure.

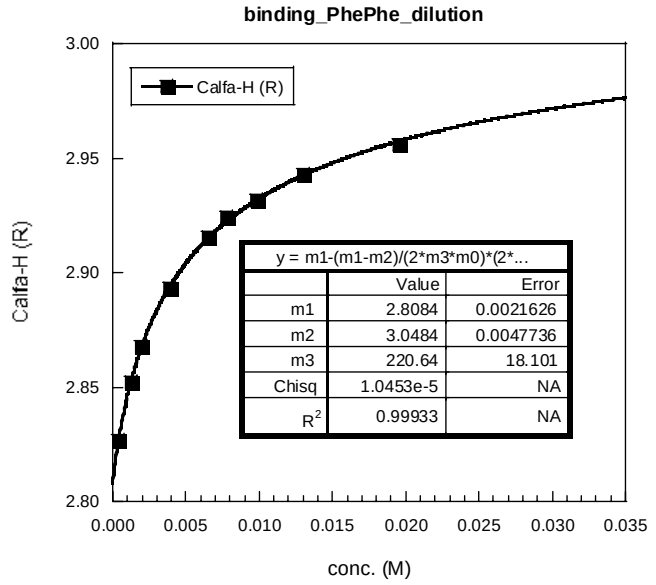


Figure S26. Dilution titration of a 1 : 1 mixture of **2a** : Z-AF-OH (500 MHz, 303 K, 1% MeOH in $CDCl_3$) using the dipeptide amide NH proton signal. The symbols correspond to experimental data and the line to the non-linear least squares fitting. The final values for the best fitting are given in the figure.

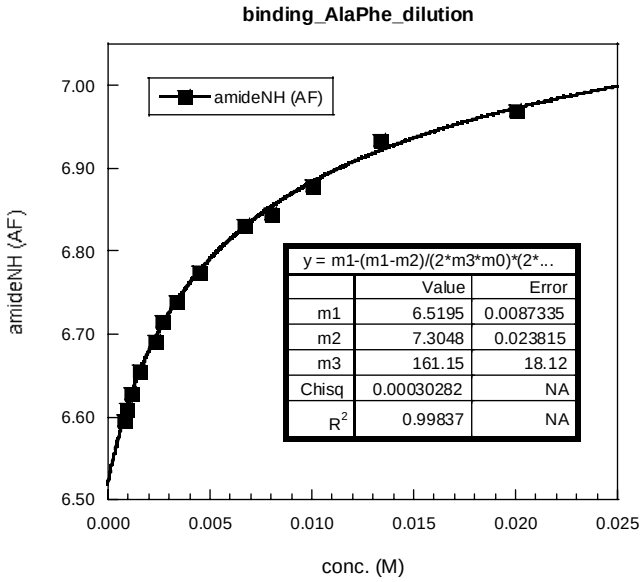


Figure S27. Dilution titration of a 1 : 1 mixture of **2a** : Z-AA-OH (500 MHz, 303 K, 1% MeOH in $CDCl_3$) using the dipeptide amide NH proton signal. The symbols correspond to experimental data and the line to the non-linear least squares fitting. The final values for the best fitting are given in the figure.

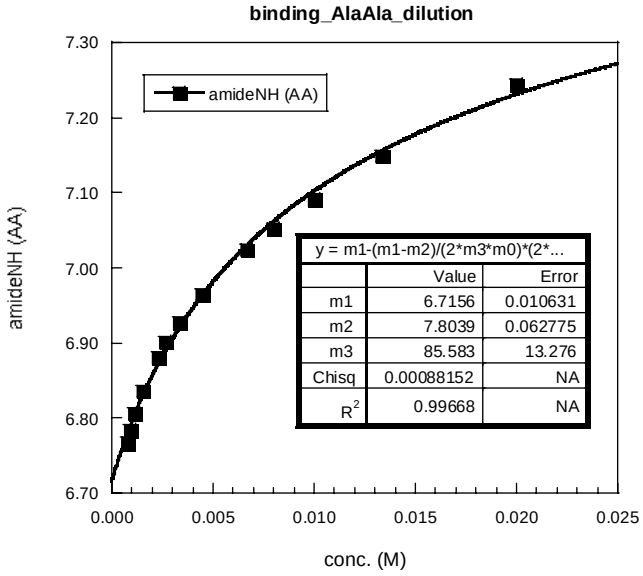


Figure S28. Dilution titration of a 1 : 1 mixture of **1a** : Z-FF-OH (500 MHz, 303 K, 1% MeOH in $CDCl_3$) using the receptor Cα proton signal. The symbols correspond to experimental data and the line to the non-linear squares least fitting. The final values for the best fitting are given in the figure.

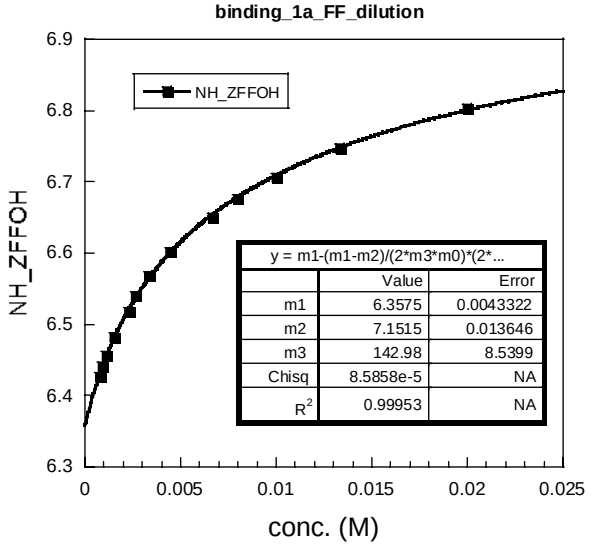
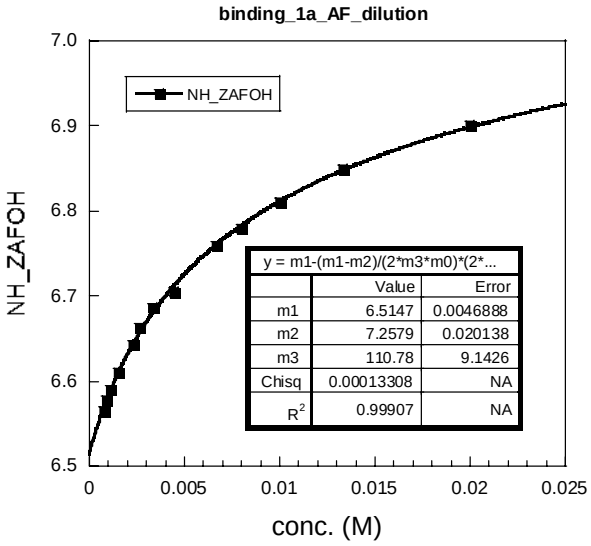


Figure S28. Dilution titration of a 1 : 1 mixture of **1a** : Z-AF-OH (500 MHz, 303 K, 1% MeOH in $CDCl_3$) using the receptor Cα proton signal. The symbols correspond to experimental data and the line to the non-linear squares least fitting. The final values for the best fitting are given in the figure.



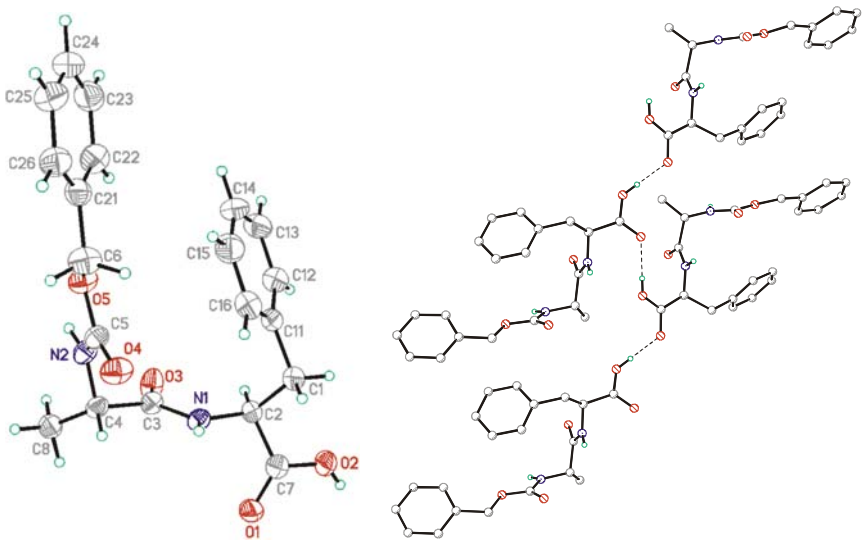


Table S1. Crystal data and structure refinement for Z-AF-OH.

Identification code	nacho1	
Empirical formula	C20 H22 N2 O5	
Formula weight	370.40	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2	
Unit cell dimensions	a = 43.977(3) Å	α= 90°.
	b = 5.0960(3) Å	β= 95.848(6)°.
	c = 8.3187(6) Å	γ = 90°.
Volume	1854.6(2) $Å^3$	
Z	4	
Density (calculated)	1.327 Mg/m^3	
Absorption coefficient	0.096 mm^{-1}	
F(000)	784	
Crystal size	0.19 x 0.17 x 0.14 mm^3	
Theta range for data collection	1.86 to 25.00°.	
Index ranges	-48<=h<=52, -5<=k<=6, -9<=l<=9	
Reflections collected	7601	
Independent reflections	1833 [R(int) = 0.0762]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	None	
Max. and min. transmission	0.9867 and 0.9820	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1833 / 1 / 251	
Goodness-of-fit on F^2	1.151	
Final R indices [I>2sigma(I)]	R1 = 0.0533, wR2 = 0.1587	
R indices (all data)	R1 = 0.0580, wR2 = 0.1607	
Absolute structure parameter	1(3)	
Extinction coefficient	0.014(3)	
Largest diff. peak and hole	0.370 and -0.219 e.$Å^{-3}$	

Cartesian coordinates for the minimum structure of [**2a** · Z-AF-OH]

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	X	Y	Z
C	-2.3200	5.7600	7.3190
C	-1.6110	8.2680	7.0590
C	-3.3090	7.6510	8.7590
C	-2.9310	8.6640	7.6940
C	-3.5330	6.2960	8.1150
C	-1.6000	6.8480	6.4450
H	-0.8350	8.3600	7.8330
H	-2.5240	7.5830	9.5220
H	-3.7140	8.7300	6.9290
H	-4.4120	6.3870	7.4600
H	-2.0650	6.8990	5.4530
H	-1.6120	5.3100	8.0280
H	-1.3480	9.0010	6.2850
H	-4.2250	7.9730	9.2660
H	-2.8380	9.6580	8.1460
H	-3.8120	5.5690	8.8900
N	-2.9130	4.6080	6.4950
H	-3.9410	4.5980	6.4190
C	-2.2310	3.5570	6.0140
C	-2.8970	2.3160	5.3480
H	-3.7420	2.6890	4.7560
O	-0.9760	3.5810	6.1510
C	-2.4910	1.3610	0.6190
C	-1.4480	-1.1830	0.7930
C	-2.6040	0.4860	-0.4780
C	-1.8700	0.9850	1.8340
C	-1.3050	-0.3030	1.8990
C	-2.0890	-0.8090	-0.4090
H	-3.1740	0.8250	-1.3450
H	-0.7860	-0.6780	2.8010
N	-0.1070	6.5650	6.2560
C	2.0010	5.9900	4.9260
C	0.4610	6.0890	5.1340
O	-0.3100	5.6800	4.2170
H	2.3530	5.4550	5.8200
C	2.6980	7.3810	4.9460
H	2.4720	7.8250	5.9270
C	2.1790	8.3870	3.9140
C	4.2260	7.2850	4.8780
H	4.5750	6.9610	3.8930
H	4.6060	6.5820	5.6260
H	4.6790	8.2610	5.0810
H	2.6070	9.3770	4.1070
H	1.0910	8.4940	3.9650
H	2.4470	8.1210	2.8900
C	2.6320	4.3490	1.3180
C	3.0890	2.5110	-0.8510
C	3.1290	3.0530	1.5560
C	2.3740	4.6980	-0.0210
C	2.5910	3.8040	-1.0790
C	3.3350	2.1300	0.4910
H	3.3790	2.7360	2.5710
H	2.0070	5.7000	-0.2660
H	2.3530	4.1580	-2.0830
H	3.6920	1.1130	0.7470
C	3.5620	1.8850	-4.6410
H	2.6260	2.4580	-4.6440
C	-0.8750	-2.4490	-3.6160
C	3.1770	0.4370	-5.1070
C	-0.0760	-1.8060	-4.8050
N	0.6060	-2.4550	-5.7590
H	0.6010	-3.4840	-5.7540
N	2.8440	0.0890	-6.3630
H	2.8540	0.8170	-7.0930
C	2.6930	-1.3430	-6.8940
H	3.2370	-2.0030	-6.2080
C	1.2120	-1.8440	-7.0330
H	0.5650	-1.0050	-7.3190
O	0.0330	-0.5430	-4.7890
O	3.0780	-0.4590	-4.2180
C	1.0410	-2.9700	-8.0830
H	1.3960	-3.9270	-7.6740
C	1.7840	-2.7260	-9.3840
H	1.3720	-1.8470	-9.8940
C	3.2630	-2.5330	-9.1020
H	3.8050	-2.4110	-10.0460
C	3.4640	-1.3040	-8.2360
C	4.5760	2.5630	-5.6110
H	4.1830	2.4720	-6.6320
C	5.9600	1.9050	-5.6040
H	5.8950	0.8300	-5.8000
H	6.4780	2.0490	-4.6510
H	6.5910	2.3410	-6.3870
C	4.7160	4.0690	-5.3560
H	3.7350	4.5510	-5.3110
H	5.2800	4.5400	-6.1690
H	5.2510	4.2840	-4.4260
C	-1.6610	-3.7600	-3.9050
H	-2.4070	-3.9000	-3.1130
C	-0.7610	-4.9960	-3.8000
H	-0.0230	-5.0470	-4.6020
H	-1.3630	-5.9100	-3.8530
H	-0.2310	-5.0050	-2.8360
C	-2.4510	-3.7450	-5.2140
H	-3.1150	-4.6140	-5.2650
H	-1.8010	-3.7880	-6.0930
H	-3.0740	-2.8490	-5.2890
C	-3.4570	1.3700	6.4530
H	-3.9780	1.9890	7.1960
C	-2.3690	0.5930	7.2020
H	-1.6340	1.2720	7.6450
H	-1.8400	-0.1070	6.5480
H	-2.8090	0.0110	8.0190
C	-4.5070	0.3950	5.9050
H	-4.0720	-0.3560	5.2400
H	-4.9940	-0.1400	6.7280
H	-5.2870	0.9320	5.3540
H	-1.1150	-2.2150	0.8910
H	-2.9520	2.3480	0.5170
H	1.6440	-3.5820	-10.0520
H	-0.0260	-3.1110	-8.2990
H	3.6770	-3.4180	-8.6040
H	4.5360	-1.1740	-8.0380
H	3.1580	-0.4280	-8.8260
H	0.5110	6.8880	7.0140
H	-0.1220	-2.6300	-2.8380
C	-2.3470	-1.8380	-1.5000
H	-1.8480	-2.7780	-1.2440
H	-3.4230	-2.0350	-1.5730
C	3.2540	1.5610	-2.0250
H	2.2560	1.3400	-2.4220
H	3.7130	0.6200	-1.7010
C	2.3890	5.4400	2.3620
H	3.1190	6.2320	2.1770
H	1.3750	5.8300	2.2330
C	-1.8490	2.0100	2.9660
H	-0.8960	2.5480	2.9660
H	-2.6480	2.7410	2.7990
N	-2.0620	1.4720	4.3460
H	-2.4970	0.5470	4.2470
H	-1.0980	1.2620	4.7220
N	2.5290	5.0710	3.7990
H	3.5210	4.8700	3.9730
C	1.4990	1.6440	4.7310
O	0.4630	0.9110	4.6910
H	2.0420	4.1490	3.9490
O	1.5470	2.8900	4.4840
C	2.8460	0.9700	5.0230
H	3.5100	1.2280	4.1860
N	2.6630	-0.5110	5.0430
H	2.3540	-0.9250	5.9310
C	2.7750	-1.2600	3.9430
C	2.5040	-2.7480	3.8520
H	1.4250	-2.8590	3.7360
O	3.0670	-0.6810	2.8530
N	3.1860	-3.3270	2.6480
H	4.1940	-3.2210	2.5020
C	2.8420	-3.5240	5.1030
H	3.8470	-3.3100	5.4800
H	2.7420	-4.6050	4.9620
H	2.0940	-3.2090	5.8460
C	3.5080	1.4880	6.2940
H	3.4510	2.5840	6.3100
H	4.5810	1.2550	6.2530
C	2.9330	0.9150	7.5630
C	1.8690	-0.2600	9.8740
C	3.6830	-0.0130	8.3030
C	1.6530	1.2670	8.0130
C	1.1250	0.6780	9.1630
C	3.1490	-0.5990	9.4500
H	4.7110	-0.2660	8.0400
H	1.0620	2.0240	7.5080
H	0.1480	0.9640	9.5480
H	3.7460	-1.2910	10.0480
H	1.4740	-0.6960	10.7940
C	2.5230	-3.7590	1.5780
O	1.2750	-3.5950	1.5500
O	3.2170	-4.0320	0.4260
C	2.4940	-4.9080	-0.4580
H	1.4160	-4.6910	-0.4990
H	2.6500	-5.9370	-0.1140
C	2.9870	-4.7650	-1.8860
C	3.9160	-4.6620	-4.5440
C	3.8000	-3.7070	-2.3190
C	2.6280	-5.7540	-2.8170
C	3.0880	-5.7030	-4.1350
C	4.2710	-3.6650	-3.6370
H	4.1600	-2.9550	-1.6240
H	2.0460	-6.6270	-2.5100
H	2.8780	-6.5330	-4.8140
H	4.9990	-2.9120	-3.9320
H	4.3660	-4.6960	-5.5360
N	-1.8810	-1.4580	-2.9020
H	-2.7430	-1.3750	-3.4730
N	4.0990	2.0640	-3.1700
H	5.0410	1.6470	-3.0790
H	4.2880	3.0680	-3.0070
H	-1.5010	-0.5020	-2.8890

Output file from the HYDRONMR program

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-------------------------------------------------------------
               HYDRONMR Version 7.C
  J. García de la Torre, M.L. Huertas and B. Carrasco,
 "HYDRONMR: prediction of NMR relaxation of globular proteins
 from atomic-level structures and hydrodynamic calculations"
  J. Magnetic Reson. 147, 138-146 (2000).
-------------------------------------------------------------
                         SUMMARY OF DATA AND RESULTS
                            This file:  comp_AF1.res
                                 Case:  comp_AF1
                       Structural file:  comp_AF1.pdb
                           Temperature:  298.0 K
                      Solvent viscosity:  0.00537 poise
             Radius of atomic elements:  2.5 Angs
   Translational diffusion coefficient:  4.543E-06 cm2/s
                Center of diffusion (x):  8.049E-08 cm
                Center of diffusion (y):  9.481E-08 cm
                Center of diffusion (z):  1.295E-07 cm
           Generalized (6x6) diffusion matrix:  (Dtt  Dtr)
                                                (Drt  Drr)
 4.335E-06 -7.138E-09 -1.327E-07     1.299E-01 -1.848E-01 -2.874E-01
-7.023E-09  4.538E-06  1.781E-07    -1.845E-01 -4.769E-01 -1.174E-01
-1.328E-07  1.782E-07  4.754E-06    -2.874E-01 -1.177E-01  4.969E-01
 1.299E-01 -1.845E-01 -2.874E-01     3.232E+08 -2.214E+07 -3.601E+07
-1.848E-01 -4.769E-01 -1.177E-01    -2.214E+07  3.740E+08  8.775E+07
-2.874E-01 -1.174E-01  4.969E-01    -3.601E+07  8.775E+07  4.956E+08
                      ROTATIONAL DIFFUSION TENSOR
                      3.232E+08-2.214E+07-3.601E+07
                     -2.214E+07 3.740E+08 8.775E+07
                     -3.601E+07 8.775E+07 4.956E+08
                Anisotropic rotational diffusion
               Eigenvalue (s^-1)     -- Eigenvector ------------
          1       3.147E+08            0.9612   0.2690   0.0608
          2       3.286E+08           -0.2062   0.8472  -0.4896
          3       5.494E+08           -0.1832   0.4581   0.8698
                Anisotropic rotational diffusion
               Dx,Dy,Dz (s^-1)     -- Eigenvector ------------
        Dz       5.494E+08           -0.1832   0.4581   0.8698
        Dy       3.147E+08            0.9612   0.2690   0.0608
        Dx       3.286E+08           -0.2062   0.8472  -0.4896
     Rotational diffusion coefficient:  3.976E+08 s-1
     Rotational diffusion  anisotropy:  2.281E+08 s-1
                  Relaxation time (1):  5.183E-10 s
                  Relaxation time (2):  4.680E-10 s
                  Relaxation time (3):  4.590E-10 s
                  Relaxation time (4):  3.520E-10 s
                  Relaxation time (5):  3.519E-10 s
   Harm. mean relax.(correlation) time:  4.192E-10 s
            Iflag= 1   N-H bonds, implicit hydrogens (not given in pdb)

          ---------------- Calculation for 11.74 Teslas ----------------
                                NMR DATA AND CONSTANTS
                           Magnetic field:  11.74 Teslas
               Gyromagnetic ratio of 1H :  2.675E+04 rad.s^-1.G^-1
               Gyromagnetic ratio of  X : -2.713E+03 rad.s^-1.G^-1
    Angular resonance frequency of 1H :  3.140E+09 rad.s^-1
              Resonance frequency of 1H :  500. MHz
    Angular resonance frequency of  X :  3.185E+08 rad.s^-1
              Internuclear H-X distance :  1.020E-08 cm
          Chemical shielding anisotropy : -1.600E-04
 Residue-specific T1,T2,RNOE, etc, have been calculated for   0 residues (out
of   1),Mean <T1/T2>= NaN       NO.    IND-CHAIN  AMIN   T1/T2    NABLA
T1       T2     RNOE      TMEAN       TINI   1     1         UNK
                      TABLE OF SPECTRAL DENSITIES

                        0         WX      WH-WX         WH      WH+WX     0.86WH
                  0.000E+00  3.185E+08  2.822E+09  3.140E+09  3.459E+09  2.732E+09
 NO.    IND-CHAIN  AMIN          J(0)      J(WX)   J(WH-WX)      J(WH)
J(WH+WX)  J(0.86WH)   1     1         UNK
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