Electronic Supplementary Information (ESI)

Conformational Preferences of *N*−Acetyl−*N*'−Methylprolineamide in Different Media: A ^{1}H NMR and Theoretical Investigation

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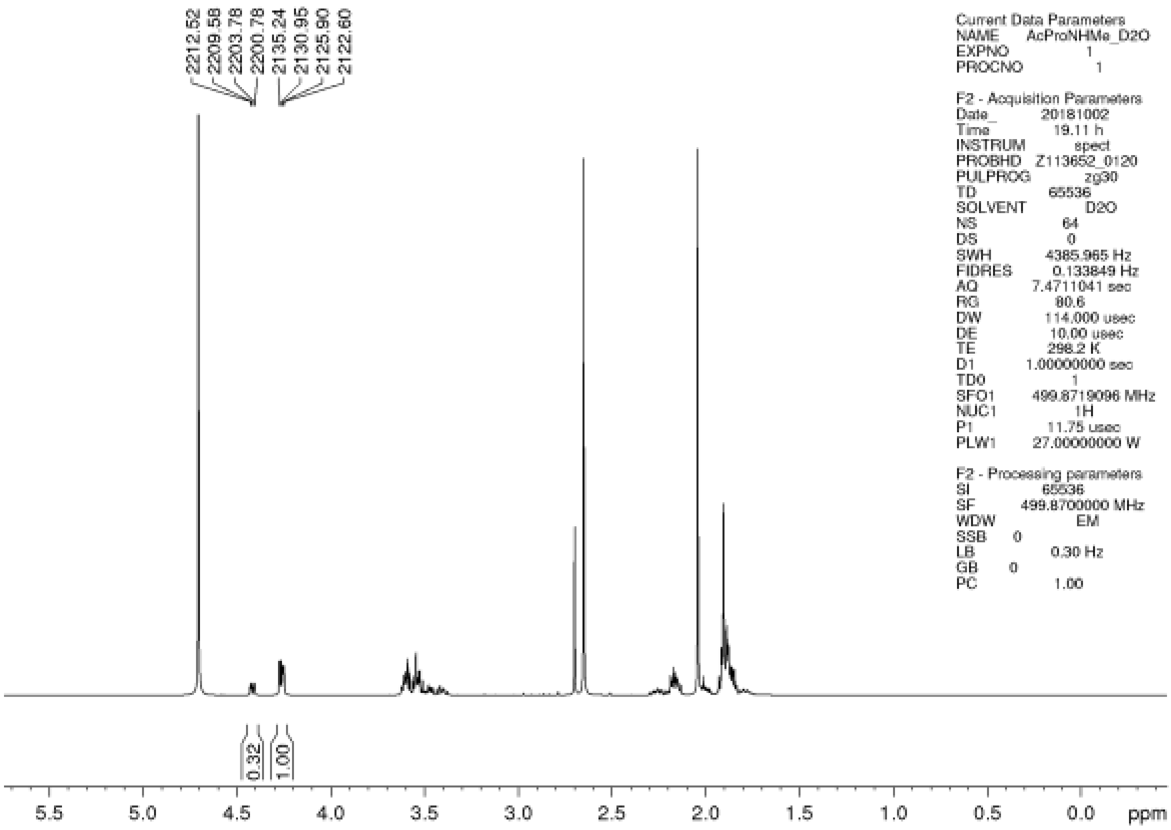

Fig. S1. Ac-Pro-NHMe ^{1}H NMR spectrum in D_2O.

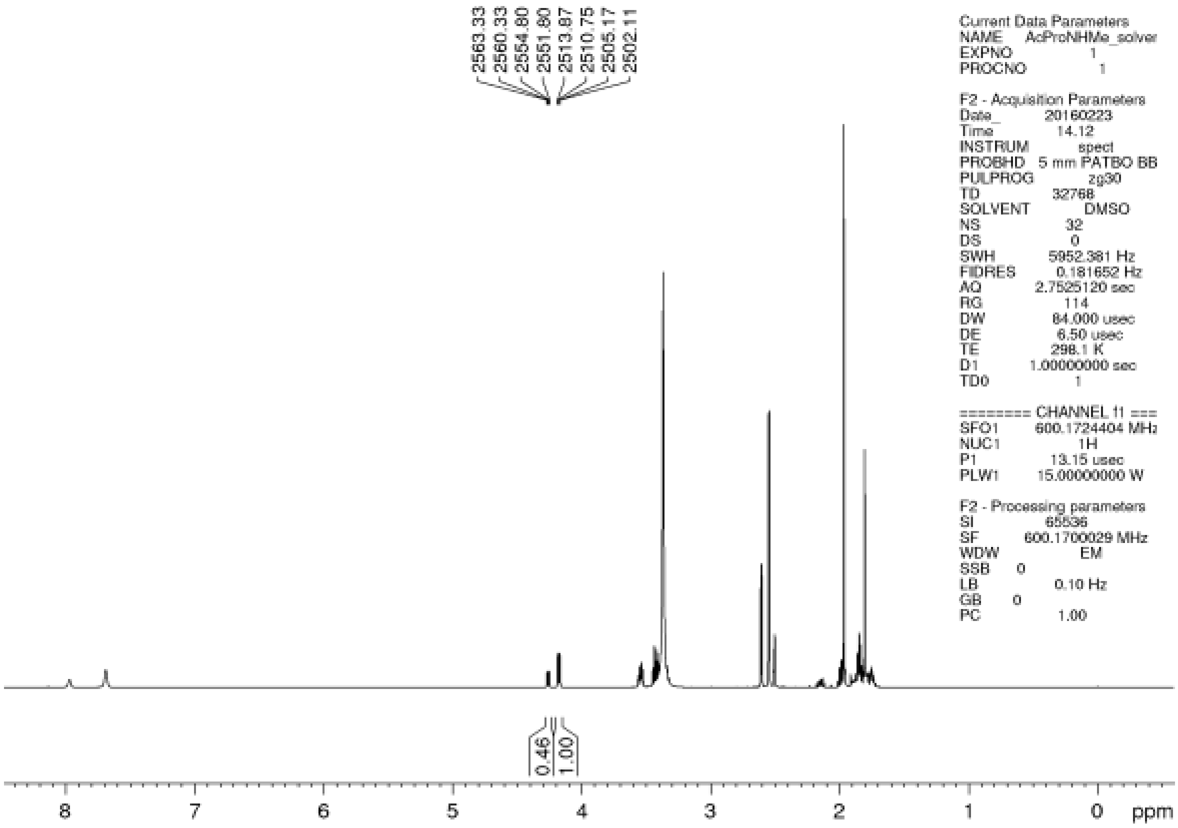

Fig. S2. Ac-Pro-NHMe ^{1}H NMR spectrum in DMSO-d_6.

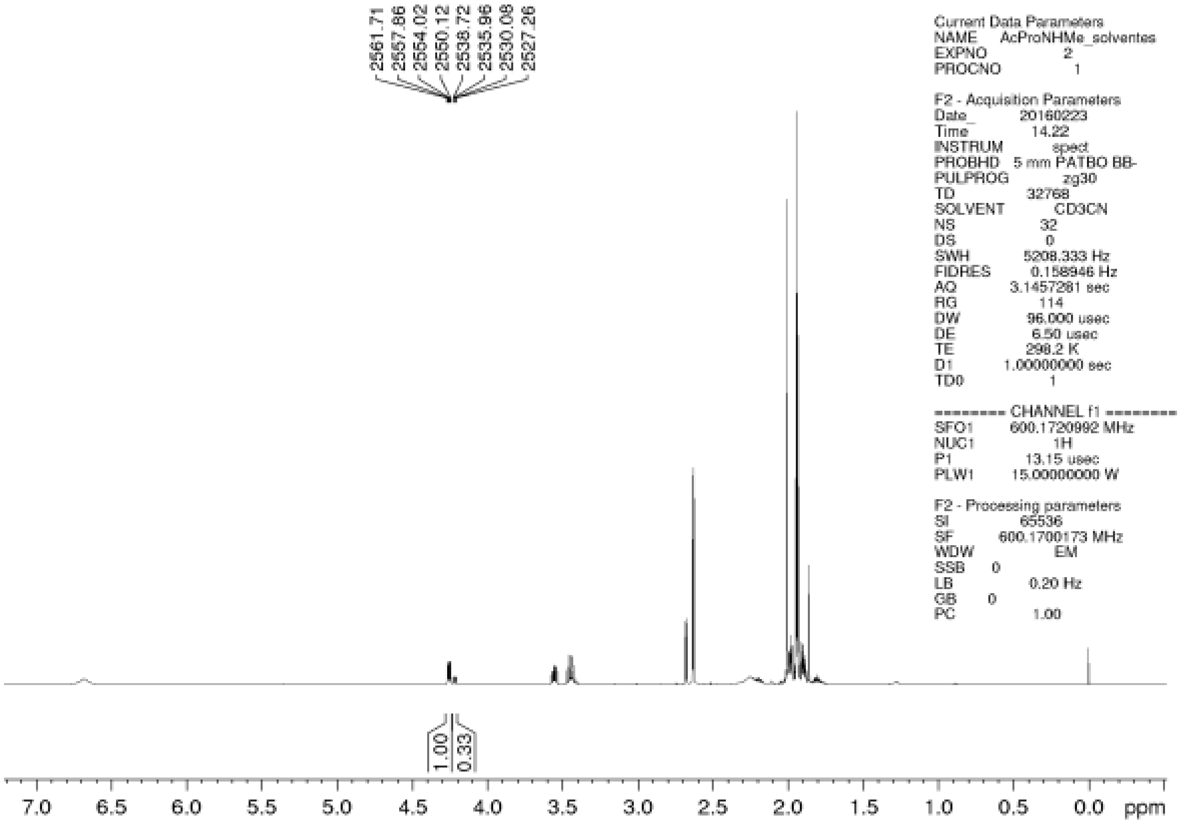

Fig. S3. Ac-Pro-NHMe ^{1}H NMR spectrum in CD_3CN.

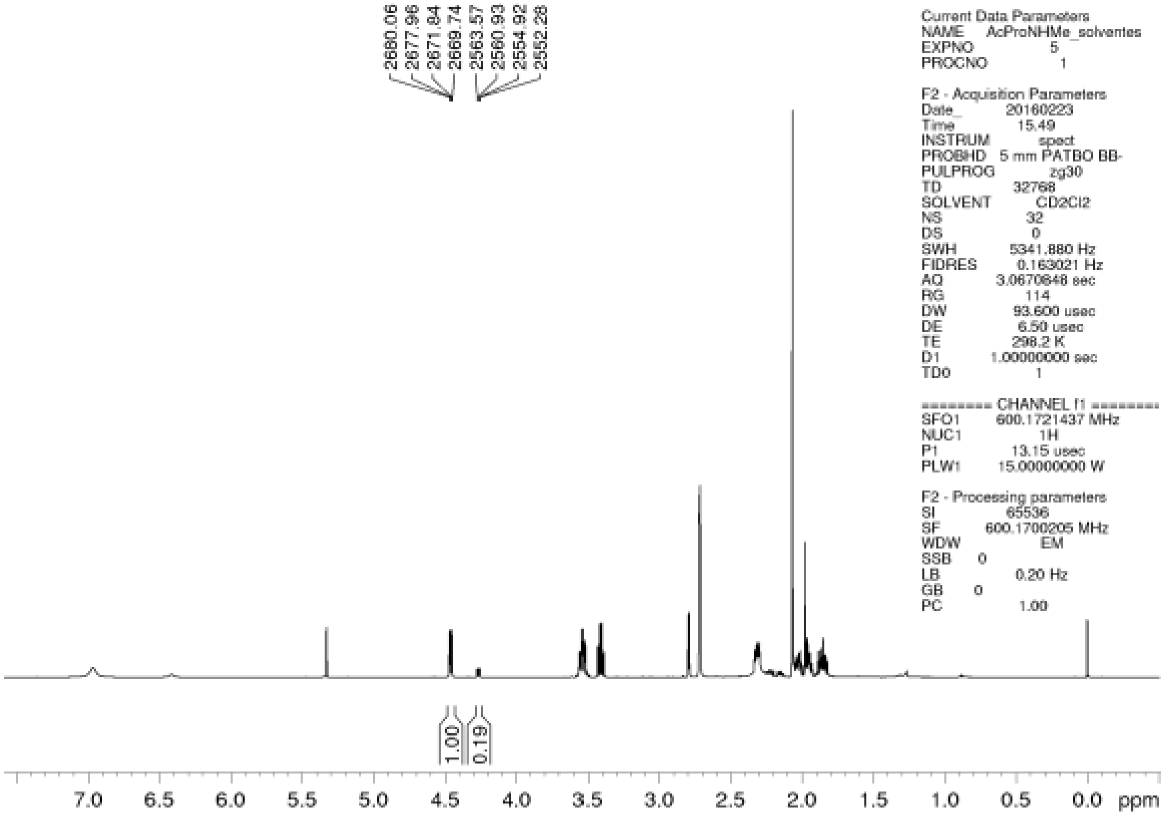

Fig. S4. Ac-Pro-NHMe ^{1}H NMR spectrum in CD_2Cl_2.

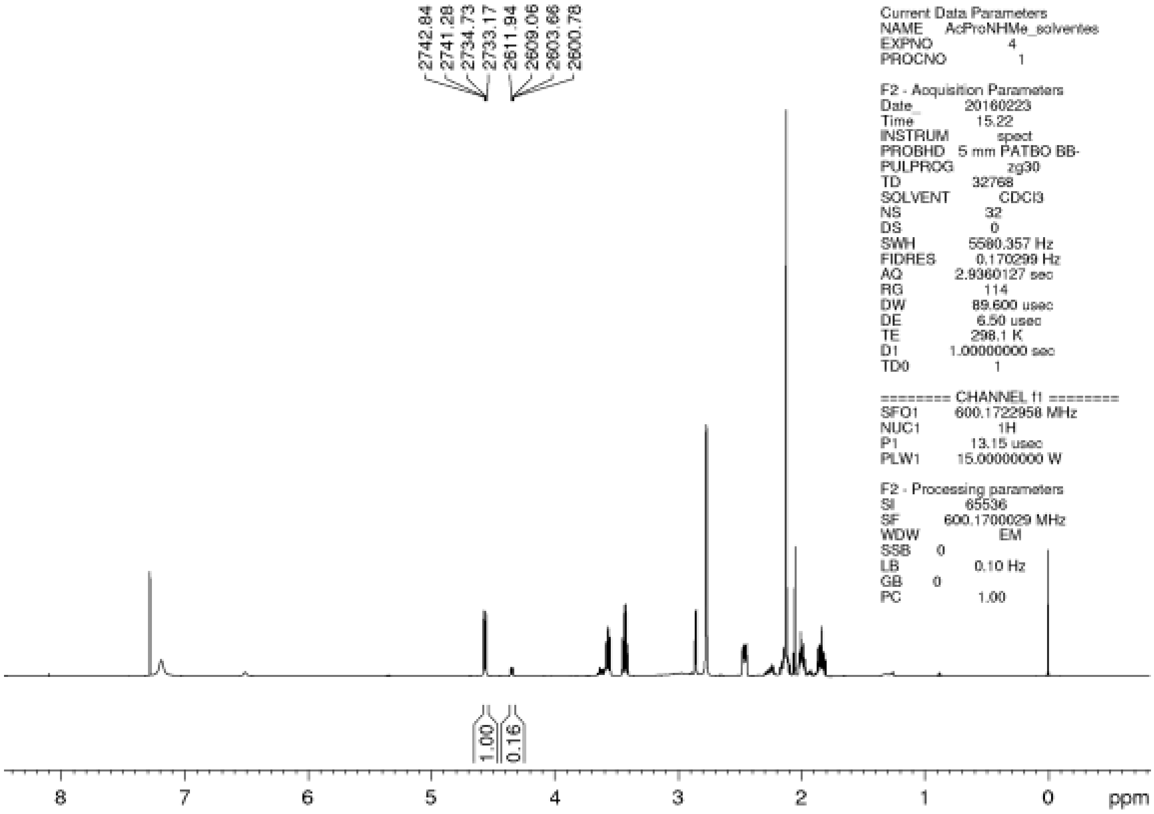

Fig. S5. Ac-Pro-NHMe ^{1}H NMR spectrum in $CDCl_3$.

Table S1. NBO parameters obtained at the M06−2X/aug−cc−pVTZ level for the conformers of Ac−Pro−NHMe. Lewis, hyperconjugative and second order perturbation LP(O)→σ^{*}_{NH} energies are given in kcal mol^{-1}. The threshold for the energy of the hyperconjugative interactions is equal to 0.5 kcal mol^{-1}.

Conformer	**Isolated**		**$CHCl_3$**		**CH_2Cl_2**		**CH_3CN**		**DMSO**		**H_2O**			
	ΔE_{Lewis}	ΔE_{Hyp}	ΔE_{Lewis}	ΔE_{Hyp}	ΔE_{Lewis}	ΔE_{Hyp}	ΔE_{Lewis}	ΔE_{Hyp}	ΔE_{Lewis}	ΔE_{Hyp}	ΔE_{Lewis}	ΔE_{Hyp}	**$LP_1(O)\rightarrow\sigma^*_{NH}$**	**$LP_2(O)\rightarrow\sigma^*_{NH}$**
***trans,trans*−IId**	0.19	2.10	—	—	—	—	—	—	—	—	—	—	2.23	3.38
***trans,trans*−IIu**	0.00	0.00	—	—	—	—	—	—	—	—	—	—	2.35	3.36
***trans,trans*−Id**	—	—	3.63	4.09	3.43	3.66	3.37	3.39	3.43	3.44	3.47	3.45	—	—
***trans,trans*−Iu**	—	—	5.61	5.86	5.60	5.69	5.72	5.66	5.78	5.71	5.81	5.73	—	—
***trans,trans*−IIu**	—	—	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	—	—
***cis,trans*−IIu**	—	—	1.12	1.16	3.34	3.02	3.51	2.76	3.60	2.80	3.60	2.80	—	—
***cis,trans*−Id**	—	—	8.31	7.67	7.94	7.29	7.86	7.17	7.91	7.22	7.91	7.22	—	—
***cis,trans*−Iu**	—	—	11.90	10.95	11.62	10.68	11.45	10.51	11.48	10.54	11.48	10.54	—	—