Electronic Supplementary Material (ESI) for Chemical Communications

Supporting information

Weakly Ordered Chiral Alignment Medium Derived from 5´-GMP: Guanosine

Lokesh and N. Suryaprakash*

NMR Research Centre, Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore-560012, India.

Fax: +91 80 23601550;

Tel: +91 80 22933300;

E-mail:nsp@sif.iisc.ernet.in

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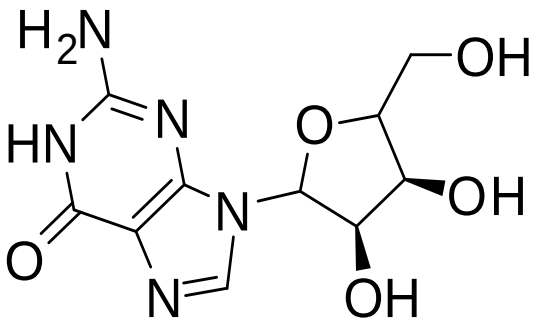
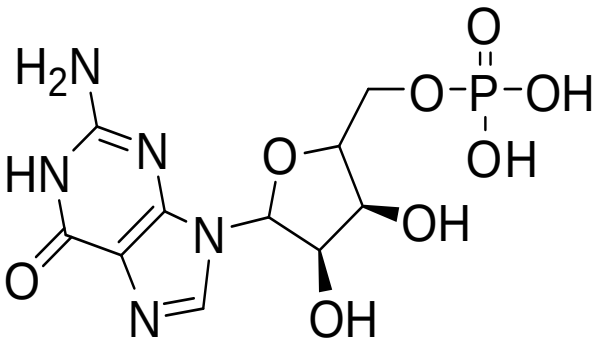
1. **The structures of Guanosine and 5´-GMP**



Guanosine



5´-GMP

2. Sample preparation and experimental details

All the chemicals were purchased from Sigma-Aldrich, used directly without further purification.

For RDC Measurement

5´-GMPNa$_2$ and guanosine were taken in of D_2O (0.1 molar NaCl solution). The mixture was heated to 343-353 K for 5 to 10 minutes till it becomes a clear solution, and then cooled to room temperature. After nearly an hour the deuterium spectrum was recorded for homogenized sample to confirm the anisotropic phase (quadrupole doublet splitting of solvent D_2O). sample (tripeptide or L-proline) was added to the mesophase in an NMR tube, centrifuged back and forth, slightly warmed to solublize the solute molecules.

A). Tripeptide sample

26 mg of 5´-GMPNa$_2$ and 13.5 mg of guanosine were taken in 0.5 ml of D_2O + 6 mg of tripeptide (Gly-Glu-Cys)

B). L-Proline sample

26.5 mg of 5´-GMPNa$_2$ and 13 mg of guanosine were taken in 0.5 ml of D_2O + 5 mg of L-proline

For Enantiomeric (Enantiotopic) Discrimination

5´-GMPNa$_2$ and guanosine were taken in H_2O (0.1 molar NaCl solution). The mixture was heated to 343-353 K for 5 to 10 minutes till it becomes a clear solution, cooled to room temperature and allowed for an 1hr. sample (alanine) was added to the mesophase in an NMR tube, centrifuged back and forth, slightly warmed to solublize the solute molecules

Composition

A). For DL-alanine-d$_3$ sample

64.2 mg of 5´-GMPNa$_2$ and 36 mg of guanosine in 0.5 ml of H_2O + 8 mg of DL-alanine-d$_3$

B). Scalemic mixture with excess of L-alanine-d$_3$

64.2mg of 5´-GMPNa$_2$ and 36 mg of guanosine in 0.5 ml of H_2O + 4mg of D-alanine-d$_3$ + 5.95 mg of L-alanine-d$_3$

C). For glycine-d$_3$ sample

65.5 mg of 5´-GMPNa$_2$ and 36 mg of guanosine in 0.5 ml of H_2O + 9.5 mg of glycine-d$_2$

All NMR experiments were carried out using Bruker DRX-500 NMR spectrometer equipped with a TXI probe and a BVT-3000 temperature controller.

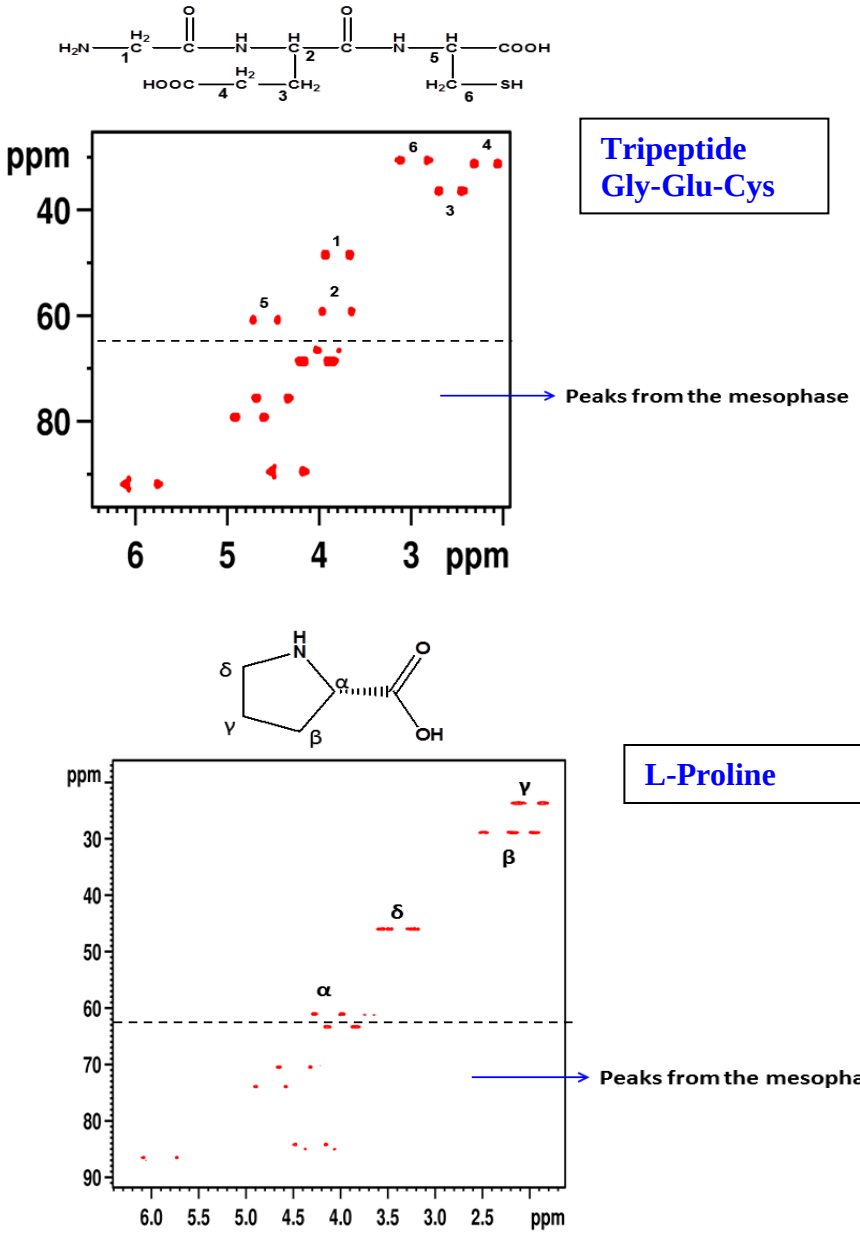
3. Table S1: The variation of $\Delta\nu_Q$ as a function of the molar ratio of 5´-GMP and guanosine in the solvent D_2O. The molar ratios were also altered by varying the quantity of guanosine keeping the quantity of 5´-GMP fixed. Notice the enhanced separation with the increased quantity of guanosine.

Molar ratio [5´-GMP/Guanosine]	5´-GMP$Na_2 \cdot H_2O$ [mg in 1ml]*	Guanosine [mg in 1ml]*	Quadrupolar splitting [Hz]*
1.16	20±1	12±1	3.5±2
1.39	40±1	20±1	11.2±2
1.113	40±1	25±1	15.0±2
1.739	50±1	20±1	13.9±2
1.242	50±1	28±1	23.8±2
2.434	70±1	20±1	15.0±2
1.6314	70±1	30±1	22.8±2

***The large errors are intentionaly reported as there may be slight evaporation of water during heating and the concentration may not be very precise.**

4. The complete F_2- coupled ^{13}C-^{1}H HSQC spectra of tripeptide and L-proline in 5´-GMP:guanosine mesophase

The complete spectrum contains peaks both from the solute and the aligning medium. Nevertheless they are clearly separated and distinguishable. This demarcation is indicated by a horizontal dotted line. The aliphatic region of the spectrum is completely free from the signals of the liquid crystal background [upto 65 ppm in ^{13}C spectrum and up to 3.8 ppm in ^{1}H spectrum].

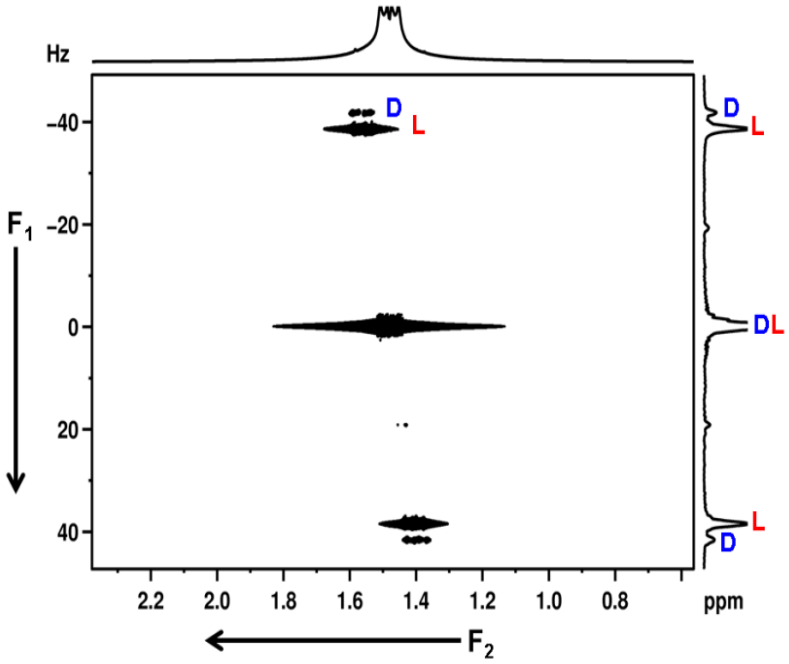


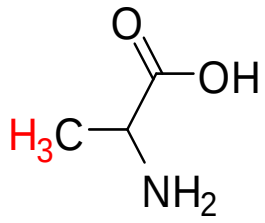
5. Table S2: The RDCs calculated from F2 coupled 13C-1H HSQC spectrum of L-proline. The large errors are reported for two couplings, because the measurement of frequency separation is likely to be imprecise due to severe overlap of transitions.

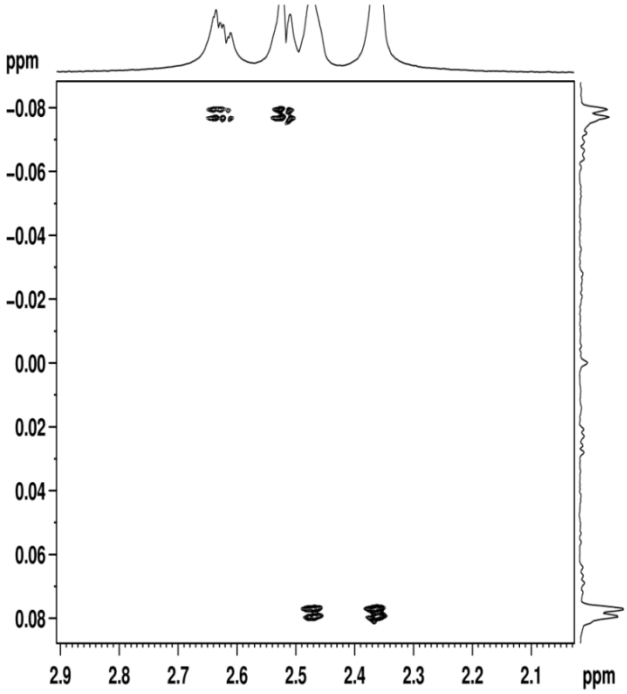
	$2^1D_{CH}+^2J_{CH}$	$^1J_{CH}{}^*$	$^1D_{CH}$
C_α-H_α	145.5±0.2	148.7±0.4	-1.6±0.3
C_β-H_β	159.3±4.0	141.0±2.0	9.2±3.0
C_β-H_β'	115.2±4.0	136.1±2.0	-10.1±3.0
C_γ-H_γ	133.2±0.5	135.7±0.2	-1.3±0.3
C_δ-H_δ	140.1±0.3	147.3±0.3	-3.6±0.3
C_δ-H_δ'	149.0±0.5	147.5±1.0	0.8±0.7

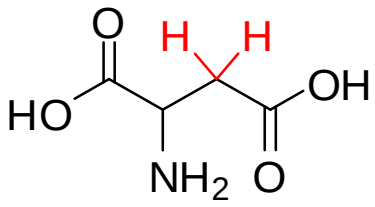
***The values were calculated from the isotropic phase in the solvent D_2O.**

6. 2D Proton SERF NMR spectra of (D/L)-alanine and (D/L)-aspartic acid with selective excitation of CH_3 and CH_2 groups respectively.









7. Table S3: The comparison of experimental parameters of different mesophases

Aligning media	Minimum quadrupolar coupling attainble	Applicability	Preparation time of the mesophase	Preparation steps
5´-GMP:Guanosine	< 5Hz	Measurement of RDCs and Enantiodiscrimination	1 Hr	Mixing solutes and solvent
Xanthane[1]	45Hz	Measurement of RDCs and Enantiodiscrimination	Minimum of one day	Sonification, lyophilization, mixing solute and solvent
Folic acid[2]	70Hz	Enantiodiscrimination	Minimum of two days	Mixing solute and solvent
DNA[3]	45Hz	Enantiodiscrimination	Minimum of one day	Sonification, lyophilization, mixing solute and solvent
Beta-Peptide[4]	<15Hz	Measurement of RDCs and Enantiodiscrimination	-	Invloves multi-step synthesis

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4. (a). C. M. Thiele, W C. Pomerantz, N. L. Abbott and S. H. Gellman., *Chem. Commun.*, 2011, **47,** 502. **(**b) W. C. Pomerantz, N. L. Abbott and S. H. Gellman, *J. Am. Chem. Soc*., 2006, **128**, 8730;

8. Table S4. Experimentally measured quadrupolar splittings of D_2O solvent at 298K and the corresponding line width.

Quadrupolar splittings [Hz]	Line width [Hz]
8.2	1.2
17.5	2.2
38.1	4.2
52.5	7.5
75.4	11.1
90.5	13.7
112.5	16.4