Electronic Supplementary Material (ESI) for Soft Matter.

Supporting Information

Chiral amplification of disodium cromoglycate chromonics induced by a codeine derivative

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X-ray diffraction

Figure S1 X-ray diffraction patterns of a 9 wt% DSCG sample in a 0.3 M NaCl aqueous solution at 290K (left), and the same sample after heating up to 315 K (right).

UV-Vis Spectrum

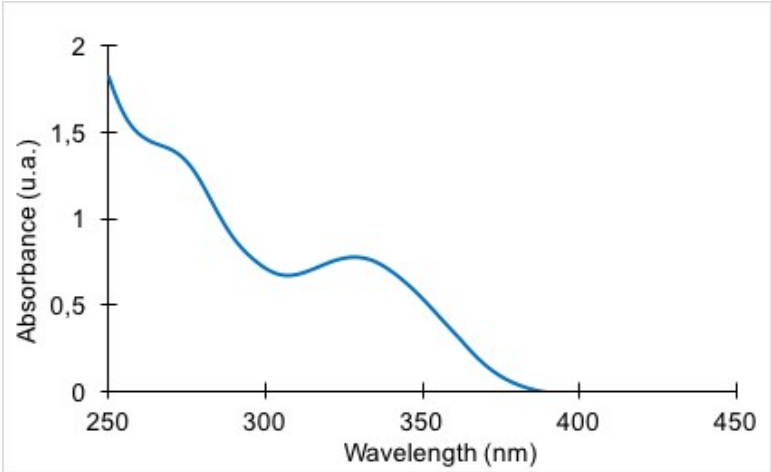

Figure S2 UV-Vis absorption spectrum of a 9 wt% DSCG sample in 0.3M NaCl aqueous solution.

Scheme explaining the meaning of the spins

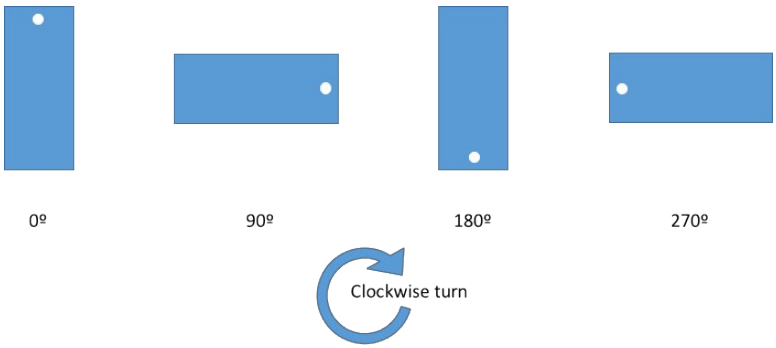

Figure S3 . Simple scheme explaining how the measurements at different spins are made. The blue rectangle represents the cuvette used, and the incident light beam of the CD Spectrometer comes from the direction of the eyes that are reading this.

Circular Dichroism

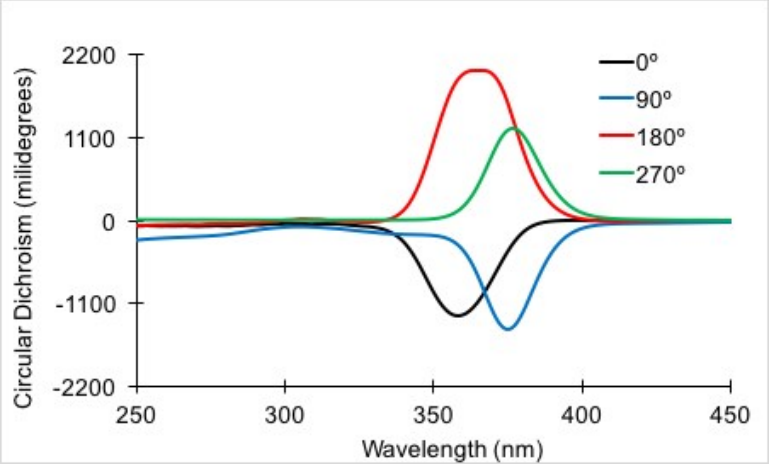

Figure S4 Comparison of Circular Dichroism Spectra of a 9 wt% DSCG sample in a 0.3 M NaCl aqueous solution at 0º, 90º, 180º and 270º with respect to the incident beam.

Diferential Scanning Calorimetry (DSC)

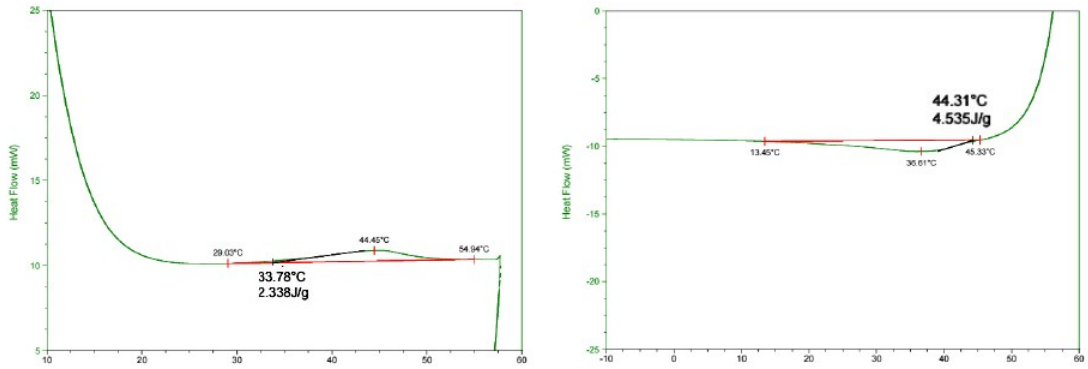

Figure S5 Heating (left) and cooling (right) calorimetry curve for a 9 wt% DSCG + 0.8 wt% NMC sample in aqueous solution.

N-Methyl Codeine Synthesis

To a solution of 98 mg (0.33 mmol) of codeine in 5 mL abs. ethanol was added methyl iodide (0.1 mL, 202 mg, 1.42 mmol). The reaction mixture was refluxed for 1 h and after cooling, the solution was left to crystallize. The solvent was separated and the residue was subsequently crystallized from water. The reaction was followed by TLC. For further identification, mp and NMR were performed. Mp of our product = 243˚(descomposition). ^{1}H and ^{13}C NMR are showed below. The NMR peaks agree with previous results.[1]

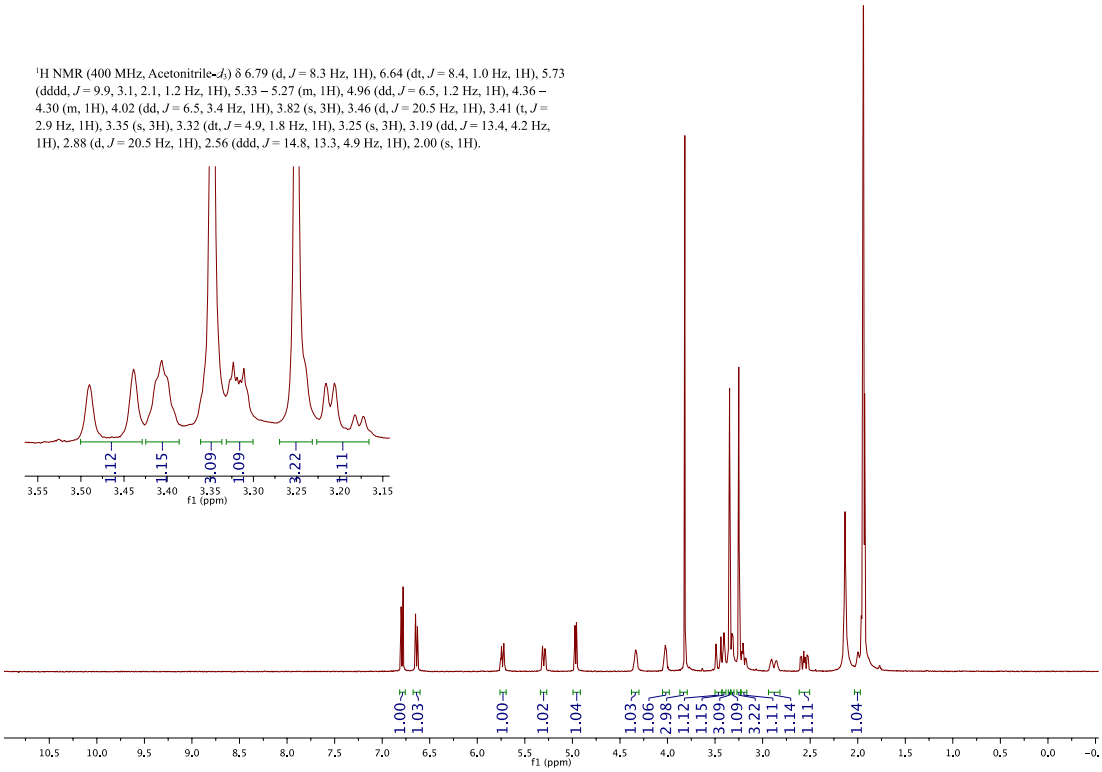

Figure S6 *N*-methyl codeinium iodide ^{1}H-NMR Spectrum

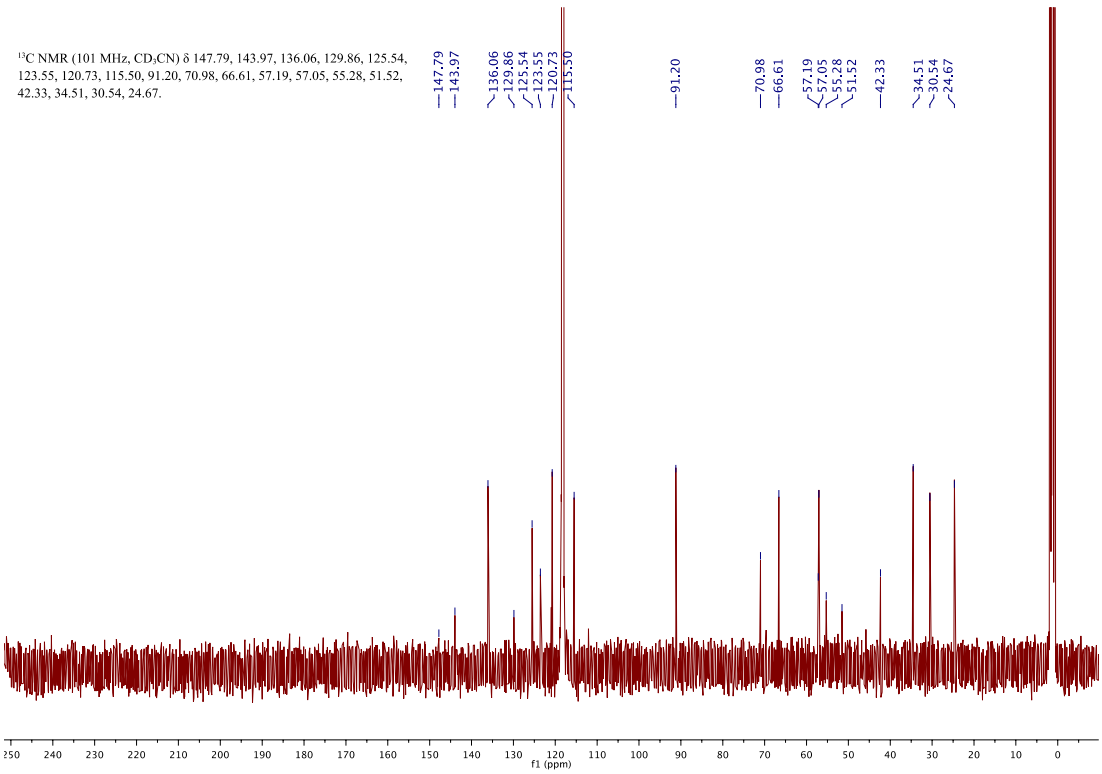

Figure S7 *N*-methyl codeinium iodide ^{13}C-NMR Spectrum

NMR signal attenuation

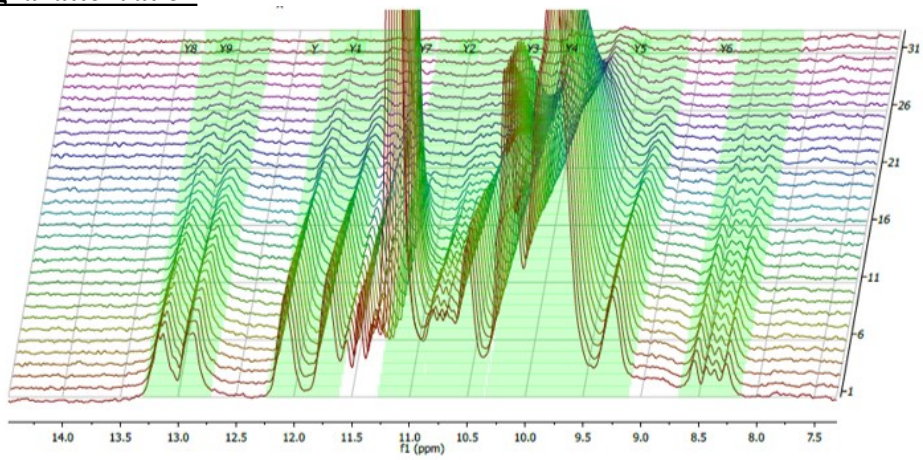

Figure S8 *N*-methyl codeinium iodide signal decay in the liquid crystal sample during the DOSY experiment in the *Z* axis.

$$I = I_0 \exp\left[D\gamma^2 g^2 \delta^2 \left(\Delta - \frac{\delta}{3} \right) \right]$$

$$Z = \gamma^2 g^2 \delta^2 \left(\Delta - \frac{\delta}{3} \right)$$

Equation 1 Diffusion (D) dependence with gradient strength (g) and signal decay (I).

γ is the magnetogyric ratio of the proton (2.675×10^8 rad T^{-1} s^{-1}), δ is the duration of the gradient, and Δ is the time interval during the two gradients.

N-methyl codeinium iodide alignment tensor in the N cromolyn phase[2]

Data obtained by fitting residual dipolar couplings obtained for NMC in the N^d phase, using MSpin.[3]

Alignment tensor
A'x=-2.575e-04
A'y=-1.323e-03
A'z= 1.580e-03

Saupe tensor
S'x=-3.862e-04
S'y=-1.984e-03
S'z= 2.371e-03

Alignment tensor eigenvectors
e[x]=(0.048, 0.994,-0.097)
e[y]=(-0.036, 0.099, 0.994)
e[z]=(0.998,-0.044, 0.041)

Alignment tensor in laboratory coordinates:
[1.572e-03,-7.667e-05,1.132e-04]
[-7.667e-05,-2.644e-04,-1.084e-04]
[1.132e-04,-1.084e-04,-1.308e-03]

SVD condition number is 7.574e+00
Axial component Aa = 2.371e-03
Rhombic component Ar = 1.065e-03
rhombicity R = 4.494e-01
Asimmetry parameter etha =6.742e-01
GDO = 3.032e-03

Euler Angles (degrees)
Set 1 (-47.1,-86.6,-37.3) Set 2 (132.9,266.6,142.7)

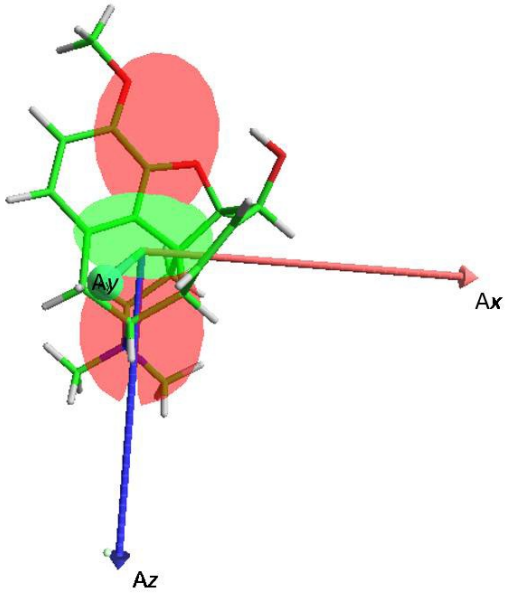

Figure S9 *N*-methyl codeinium iodide and its alignment tensor in the DSCG N^d phase, along with the axis of the alignment tensor.

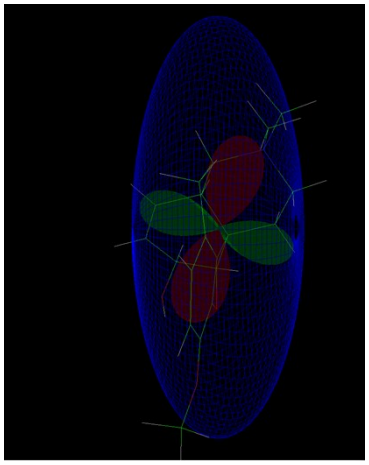

Figure S10 *N*-methyl codeinium iodide molecular elipsoid.

[1] R. W. Seidel, B. R. Bakalska, T. Kolev, D. Vassilev, H. Mayer-Figge, M. Spiteller, W. S. Sheldrick and B. B. Koleva, *Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.*, 2009, **73**, 61–66.

[2] E. Troche-Pesqueira, M. M. Cid and A. Navarro-Vázquez, *Org. Biomol. Chem.*, 2014, **12**, 1957–1964.

[3] A. Navarro-Vázquez, *Magn. Reson. Chem.*, 2012, **50**, S73–S79.