Electronic supplementary information

for

Weakly aligned Ti$_3$C$_2$T$_x$ MXene liquid crystal: Measuring residual dipolar couplings in multiple co-solvent systems

You Zhao,‡[a,b] Huan Qin,‡[a,b] Yan-Ling Yang,‡[c] Jia-Qian Li,[c] Si-Yong Qin,*[a,b] Ai-Qing Zhang,*[a,b] & Xinxiang Lei*[c]

[a]Hubei Engineering Technology Research Centre of Energy Polymer Materials, School of Chemistry and Materials Science, South-Central Minzu University, Wuhan 430074, China

[b]Key Laboratory of Catalysis and Energy Materials Chemistry of Ministry of Education and Hubei Key Laboratory of Catalysis and Materials Science, South-Central Minzu University, Wuhan, China

[c]School of Pharmaceutical Sciences, South-Central Minzu University, Wuhan, China

Corresponding Author: sy-qin@mail.scuec.edu.cn; aizhang@scuec.edu.cn;

xxlei@mail.scuec.edu.cn

Supplementary Information

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Materials

Hydrochloric acid (HCl, 36%) was purchased from Shanghai Runjie Chemical Reagent Co., Ltd. Lithium fluoride (LiF, 99%) was purchased from Aladdin Reagent (Shanghai) Co., Ltd. Ti_3AlC_2 (99%, 400 mesh) was brought from Shandong Xiyan New Material Technology Co., Ltd. L-camphor, artemether, estrone and gibberellin were purchased from Aladdin Reagent Co. Ltd (Shanghai, China). L-Proline, (+)-IPC and Boc-D-tryptophan were provided from Aladdin Reagent Co. Ltd (Shanghai, China). Methanol-d_4 (CD$_3$OD), Dimethyl-d_6 sulphoxide + 0.03% TMS (v/v) (DMSO-d_6), Deuterium oxide (D$_2$O), N,N-Dimethylformamide-d_7 (DMF-d_7) and Acetone-d_6 (CD$_3$COCD$_3$) were purchased from Cambridge Isotope Laboratories, Inc. All materials are reagent grade and used as received without further purification.

Characterization

A D8 diffractometer with a Cu Kα radiation source was used for X-ray diffraction with a scanning step size of 0.02° and a time step of 0.5 s, within the 2θ range of 3.5-80°. The surface electronic states of MXA (Ti_3AlT_x powder) and MXene ($Ti_3C_2T_x$ powder) were analyzed by X-ray photoelectron spectroscopy (MULT1LAB2000, America). Dynamic light scattering (DLS) and ζ-potential measurements were read on a Zeta-sizer Nano ZS (Malvern Instruments). Scanning electron microscopy (SEM) images were performed on a field-emission microscope (SU8010, Japan). The NMR spectra were obtained by the Bruker Ascend IIITM 600 MHz NMR spectrometer. The morphology of MXene was further imaged by scanning transmission electron microscopy (TALOS F200X, Thermo Fisher Scientific Co., Ltd.).

Synthesis of $Ti_3C_2T_x$ MXene

14 mL of HCl (12 M) and 1.4 g of LiF were stirred continuously at 35°C for 5 min. Subsequently, 0.7 g of MAX (Ti_3AlC_2 powder) was added slowly to the mixture, and the etching reaction was carried out for three days at 45°C. After the reaction was completed, the mixture was centrifuged and washed three times with 1 M HCl to remove unreacted LiF. After that, the $Ti_3C_2T_x$ precipitate was repeatedly washed with deionized water and centrifuged at 12000 r/min for 1 min, until the pH value of $Ti_3C_2T_x$ dispersion exceeded 5. The precipitate was further redispersed in 30 mL deionized water by shaking. The obtained dispersion was then subjected to the sonication in an ice bath for 30 min under nitrogen protection. The upper layer solution was collected by centrifuging at 3500 r/min for 30 min. The collected solution was lyophilized to obtain the $Ti_3C_2T_x$ solid.

Preparation of samples for NMR experiments

^{2}H NMR spectra of the anisotropic LC samples with different $Ti_3C_2T_x$ MXene concentrations in water phase

25 mg of $Ti_3C_2T_x$ solid were added into 500 μL of H_2O (containing 10% D_2O) in a 5 mm NMR tube, which was subjected to the sonication with a high-power NC ultrasonic cleaner (KQ-400 KDE, 40 kHz, 400 W) to generate 50 mg/mL MXene dispersion. The stock solution was diluted with H_2O (containing 10% D_2O) to generate the needed concentrations for the ^{2}H NMR experiments.

^{2}H quadrupolar splitting of different co-solvent systems in $Ti_3C_2T_x$ MXene LCs

1) DMSO-d_6/D_2O phase: Taking the 80% DMSO-d_6 co-solvent phase as an example, 10 mg of $Ti_3C_2T_x$ was dispersed with 100 μL D_2O in the a 5 mm NMR tube by a high-power NC ultrasonic cleaner (KQ-400 KDE, 40 kHz, 400 W) for a few seconds. Then 400 μL of DMSO-d_6 was further added to create the co-solvent system with the help of a sonication for 4 h. The other samples, such

as 20%, 40% and 60% (v/v) of DMSO-d_6, were prepared according to the above method through adjusting the solvent ratio.

2) CD$_3$OD/D$_2$O phase: 600 µL of D$_2$O and 60 mg of lyophilized Ti$_3$C$_2$T$_x$ were added into a 10 mL EP tube and subjected to the sonication treatment for a few seconds, then 2400 µL of CD$_3$OD was added to the above system. Sonication was applied by ultrasonic homogenizer JY92-IIN for 15 min under a pulse setting (5 s on and 5 s off at 50% amplitude), providing 20 mg/mL Ti$_3$C$_2$T$_x$ MXene solution in co-solvent. 450 µL of the above solution was added into a 5 mm NMR tube for the NMR experiment.

3) DMF-d_7/D$_2$O phase: The sample preparation method is the same as that for the co-solvent of DMSO-d_6/D$_2$O.

4) acetone-d_6/D$_2$O: 250 µL of D$_2$O and 10 mg of Ti$_3$C$_2$T$_x$ were added into a 5 mm NMR tube, followed by the sonication treatment for about 2 min, then 250 µL of acetone-d_6 was used to accomplish the co-solvent system after the sonication by a high-power NC ultrasonic cleaner (KQ-400 KDE, 40 kHz, 400 W) for 4 h.

NMR experiments

Without the special instruction, NMR spectra were obtained at 295 K by a Bruker Ascend IIITM 600 MHz NMR spectrometer. The spectrometer was equipped with a 5 mm CPPBBO forward broadband liquid nitrogen cryogenic probe. One-dimensional ^{1}H NMR spectra were collected in eight scans using locked channel recording. To obtain two-dimensional [^{1}H, ^{13}C]-CLIP-HSQC spectra, the acquisition time (AQ) was 0.327 seconds and the relaxation delay (RD) was 2.00 seconds. The spectral width (SW) was 10.0 ppm (^{1}H) or 140 ppm (^{13}C) during each spectrum. When the spectral width was 10 ppm, a total of 4k indirect dimensional data points were collected.

Chemical shift (δ) values were given in parts per million (ppm), while coupling constants and RDCs were expressed in hertz (Hz). The ^{13}C-^{1}H one-bond coupling constant was 145.0 Hz. F1 was set to 0.3 Hz and F2 to 1 Hz before the Fourier transform was performed. NMR data were obtained and processed by Bruker Topspin 3.5 pl 6 and MSpin software (Mestrelab Research). The published methods were used to estimate the errors of experimental C-H couplings.[1,2]

Note about the computation of 3D conformations and anisotropic NMR data analysis by MSpin

The single-tensor ensemble fitting approach is adopted to the large-amplitude conformational jumping between different energy minima. Therefore, when more than one conformation with the lowest-energy for organic molecules such as L-proline and Boc-D-tryptophan is present, the single-tensor SVD (Singular Value Decomposition) approach is used to analyze RDCs for flexible systems in MSpin and the molecules were rotated to maximize the superimposition of atom coordinates for defining a common frame. At the same time, the SVD approach provides the best minimum squares solution according to the experimental data.[3]

After drawing the chemical structure in ChemDraw, the file was imported in ChemDraw 3D. Then select the 'Calculations/MM2/Minimize Energy command' to optimize the molecular mechanics of the MM2 configuration in ChemDraw 3D, and the optimised structures were saved in mol2 file. These files were imported in Sybyl (Trepos) for conformer research, performed a minimization with MMFF and saved the coordinates in a.sdf file. Then the redundant structures from the Sybyl output were removed when the energy was positive. The geometry optimization and free-energy calculation were performed in Gaussian View 06 (at B3LYP/6 31 G(d) basis group level, IEFPCM solventised model, 'solvent'). The self-consistent field DFT energies was retrieved

from the Gaussian View 06 files in MSpin, so the calculation of Boltzmann populations can be computed.[4] The NVT ensemble (number of particles, volume, and temperature) was selected to calculate Boltzmann populations. Furthermore, we obtained the retention of the lowest energy set that can be formed from one to several tens of conformers, due to the cut-off value of 2 kcal/mol. These preserved conformations were imported into MSpin, and their corresponding Boltzmann constants were pasted into the corresponding positions. After loading the RDC input file, the Q values were calculated with performing a single-tensor SVD in MSpin. The good data quality means that a Q value is typically lower than 0.2 for the right structure.

Characterization of $Ti_3C_2T_x$ MXene

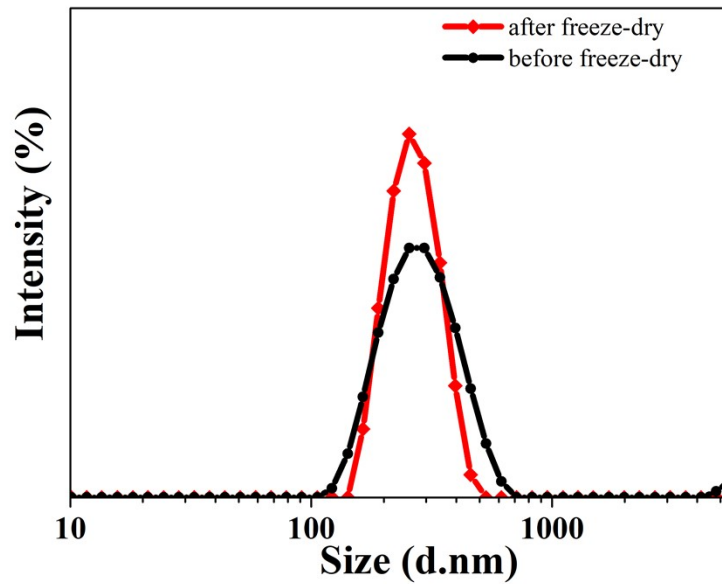**Fig. S1.** The XPS spectra of $Ti_3C_2T_x$ MXene. (a) The O 1s spectra, (b) The Ti 2p spectra and (c) C 1s spectra.

Fig. S2. The size of $Ti_3C_2T_x$ nanosheet before (black) and after (red) the freeze dry.
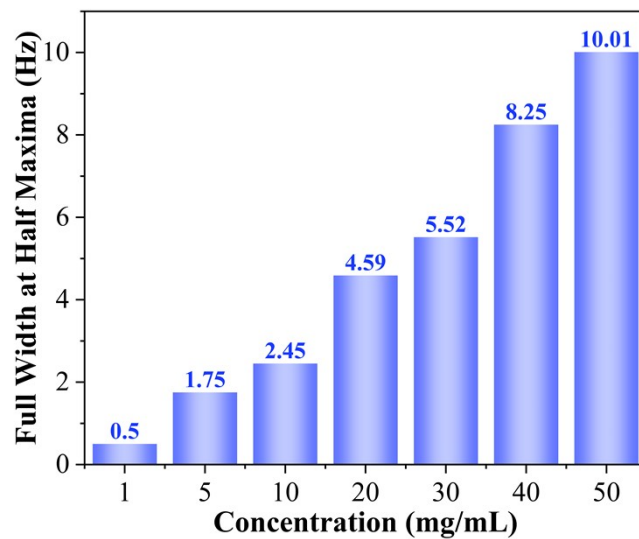
NMR Data

Fig. S3. The full width at half maxima of ^2H quadrupolar splittings with different $Ti_3C_2T_x$ concentrations in D_2O.
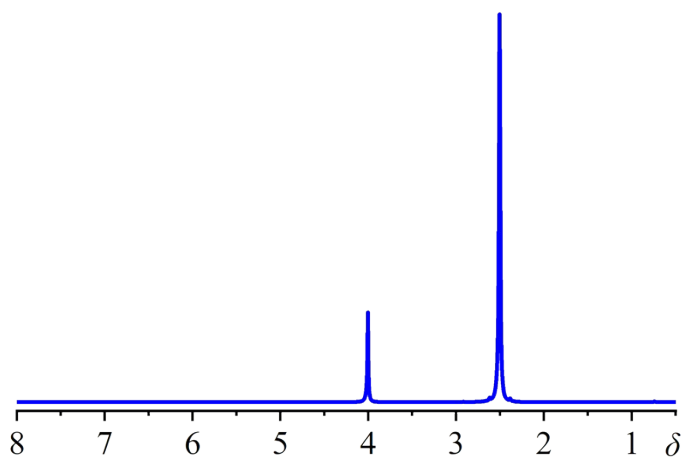
Fig. S4. ^1H NMR of $Ti_3C_2T_x$ (2 wt%) in DMSO-d_6/D_2O (DMSO-d_6 : D_2O=4:1).

Fig. S5. 1D ^2H NMR spectra of $Ti_3C_2T_x$ LC (2 wt%) in DMSO-d_6/D_2O (DMSO-d_6 : D_2O=4:1) with increased temperature from 295 K to 315 K.
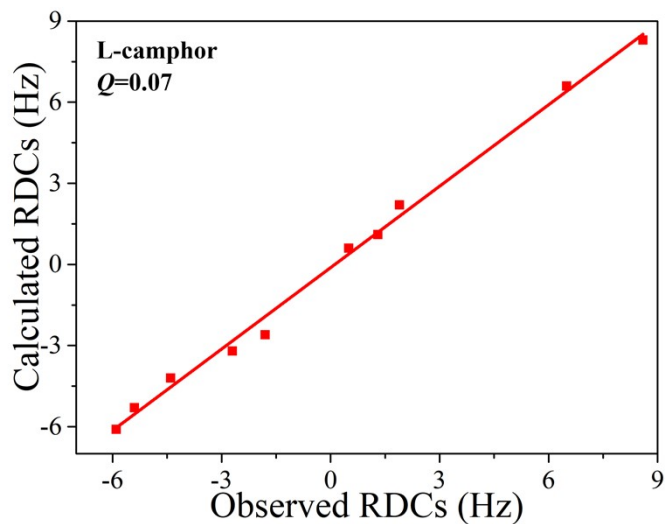
Fig. S6. Correlation between the experimental RDC values and calculated ones of L-camphor in the DMSO-d_6/D$_2$O bearing Ti$_3$C$_2$T$_x$ MXene LC (2 wt%, DMSO-d_6 : D$_2$O=4:1).

Table S1. The scalar coupling value, compound coupling value, experimental RDCs and theoretical RDCs of L-camphor in DMSO-d_6/D$_2$O bearing Ti$_3$C$_2$T$_x$ LC phase (2 wt%, DMSO-d_6 : D$_2$O=4:1).

Atom number	$^1J_{CH}$	$^1T_{CH}$	$^1D_{CH}$	$^1D_{CH}$ Calculation
C3H3a	128.8±0.4	130.1±0.2	1.3±0.6	1.1
C3H3b	133.6±0.5	128.2±0.1	-5.4±0.6	-5.3
C4H4	137.9±0.4	146.5±0.1	8.6±0.5	8.3
C5H5a	134.2±0.3	128.3±0.3	-5.9±0.6	-6.1
C5H5b	133.9±0.2	131.2±0	-2.7±0.2	-3.2
C6H6a	131.4±0.2	137.9±0.3	6.5±0.5	6.6
C6H6b	135.1±0.5	130.7±0.2	-4.4±0.7	-4.2

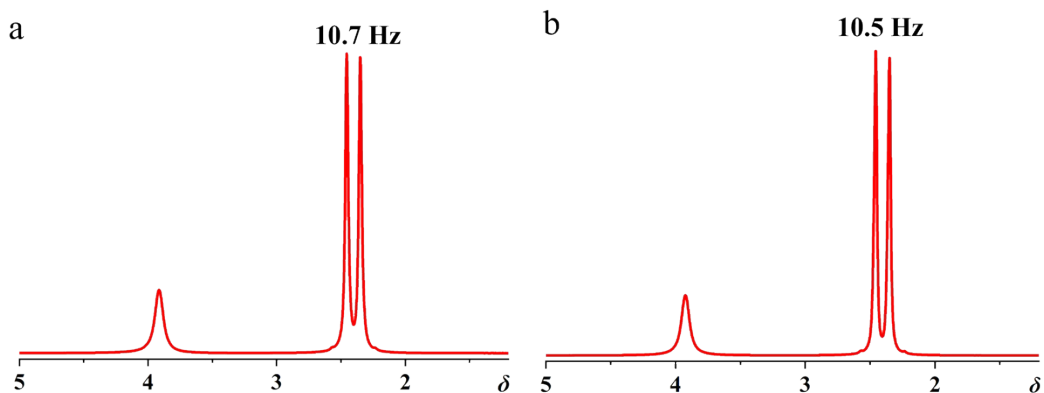|				
C8H8(Me)	124.8±0	126.7±0.3	1.9±0.3	2.2
C9H9(Me)	125.9±0.2	126.4±0.0	0.5±0.2	0.6
C10H10(Me)	125.0±0.8	123.2±0.1	-1.8±0.9	-2.6

Fig. S7. The quadrupolar DMSO-d_6 and D_2O splittings before (a) and after (b) adding artemether in the anisotropic sample of DMSO-d_6/D_2O bearing $Ti_3C_2T_x$ LC phase (2 wt%, DMSO-d_6 : D_2O=4:1).
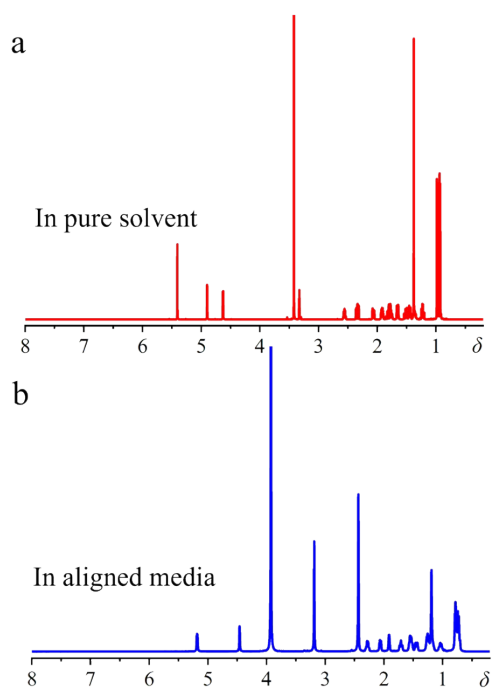
Fig. S8. [1]H spectra of artemether in (a) pure solvent (DMSO-d_6/D$_2$O=4:1) and (b) DMSO-d_6/D$_2$O bearing Ti$_3$C$_2$T$_x$ LC medium (2 wt%, DMSO-d_6/D$_2$O=4:1).
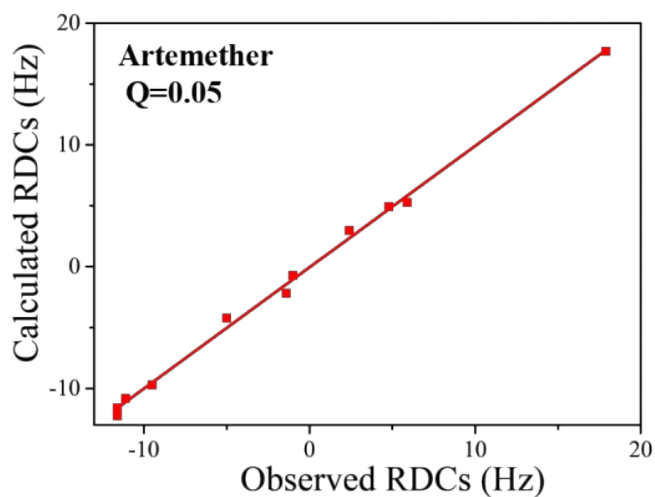

Fig. S9. Correlation between the experimental RDC values and calculated ones of artemether in the DMSO-d_6/D$_2$O bearing Ti$_3$C$_2$T$_x$ MXene LC (2 wt%, DMSO-d_6 : D$_2$O=4:1).

Table S2. The scalar coupling value, compound coupling value, experimental RDCs and theoretical RDCs of artemether in DMSO-d_6/D_2O bearing $Ti_3C_2T_x$ LC phase (2 wt%, DMSO-d_6 : D_2O=4:1).

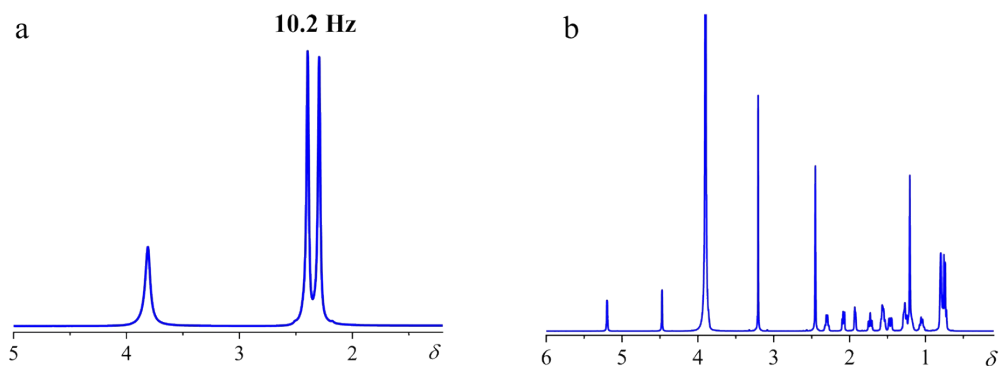| Atom number	$^1J_{CH}$	$^1T_{CH}$	$^1D_{CH}$	$^1D_{CH}$ Calculation
C1H1	126.0±0.0	130.8±0.1	4.8±0.1	4.9
C3H3a	126.6±0.7	144.5±0.1	17.9±0.8	17.7
C3H3b	128.5±0.3	127.5±0.1	-1.0±0.4	-0.7
C5H5	168.0±0.2	156.9±0.3	-11.1±0.5	-10.8
C9H9a	128.1±0.7	116.5±0.4	-11.6±1.1	-11.6
C9H9b	123.3±0.4	129.2±0.2	5.9±0.6	5.3
C11H11	127.2±0.3	115.6±0.2	-11.6±0.5	-12.3
C12H12	165.0±0.3	155.5±0.2	-9.5±0.5	-9.7
C13H13(Me)	126.3±0.2	121.3±0.3	-5.0±0.5	-4.2
C14H14(Me)	125.1±0.2	127.5±0.5	2.4±0.7	3.0
C15H15(Me)	129.5±0.3	128.1±0.4	-1.4±0.7	-2.2

Fig. S10. (a)The quadrupolar DMSO-d_6 and D_2O splittings after adding artemether and (b) ^1H spectra of artemether in the anisotropic sample of DMSO-d_6/D_2O bearing $Ti_3C_2T_x$ LC phase (2 wt%, DMSO-d_6 : D_2O=4:1, at 305 K).
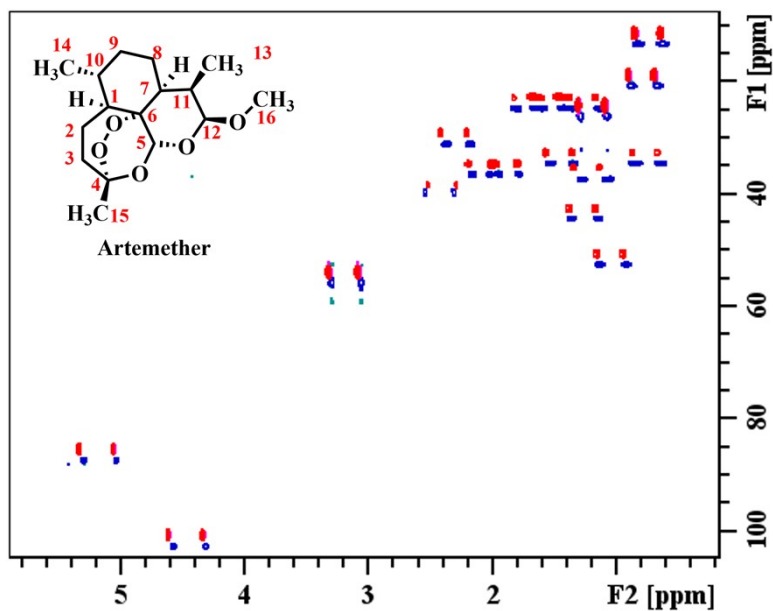

Fig. S11. Overlaid [^1H, ^{13}C]-CLIP-HSQC spectra of artemether (5 mg) in the isotropic phase (DMSO-d_6/D_2O=4:1, red contours) and 2% alignment $Ti_3C_2T_x$ LC medium (anisotropic, blue contours) at 305 K.

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Table S3. The scalar coupling value, compound coupling value, experimental RDCs and theoretical RDCs of artemether in DMSO-d_6/D_2O bearing $Ti_3C_2T_x$ LC phase (2 wt%, DMSO-d_6/D_2O=4:1) at 305 K.

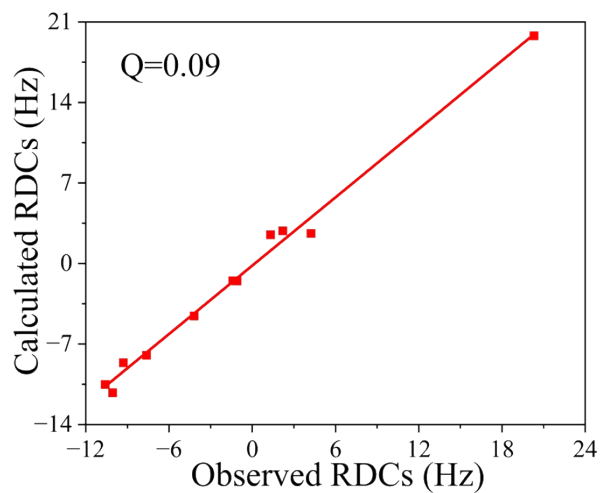| Atom number	$^1J_{CH}$	$^1T_{CH}$	$^1D_{CH}$	$^1D_{CH}$ Calculation
C1H1	126.0±0.0	127.3±0.2	1.3±0.2	2.5
C3H3a	126.6±0.7	146.9±3.1	20.3±3.8	19.8
C3H3b	128.5±0.3	127.1±0.1	-1.4±0.4	-1.5
C5H5	168.0±0.2	158.7±0.5	-9.3±0.7	-8.6
C9H9a	128.1±0.7	117.5±0.3	-10.6±1.0	-10.5
C9H9b	123.3±0.4	127.5±0.5	4.2±0.9	2.6
C11H11	127.2±0.3	117.1±0.5	-10.1±0.8	-11.2
C12H12	165.0±0.3	157.4±0.1	-7.6±0.4	-8.0
C13H13(Me)	126.3±0.2	122.1±0.1	-4.2±0.3	-4.6
C14H14(Me)	125.1±0.2	127.3±0.1	2.2±0.3	2.9
C15H15(Me)	129.5±0.3	128.4±0.0	-1.1±0.3	-1.5

Fig. S12. Correlation between the experimental RDC values and calculated RDC values of artemether in the DMSO-d_6/D$_2$O bearing Ti$_3$C$_2$T$_x$ MXene LC (2 wt%, DMSO-d_6 : D$_2$O=4:1) at 305 K.
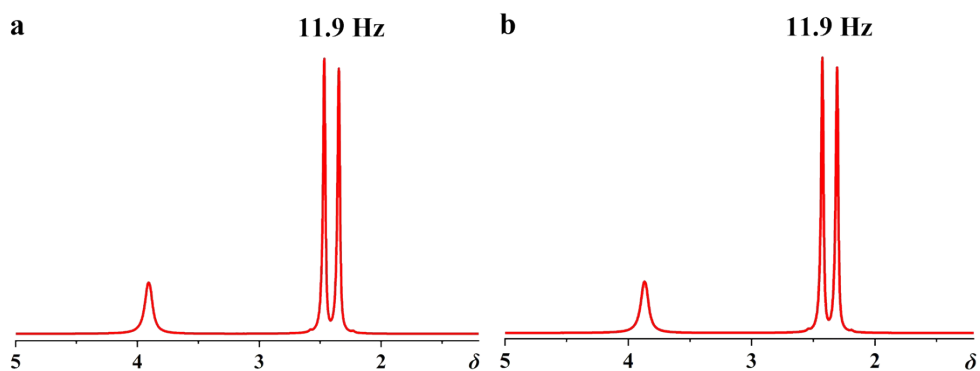

Fig. S13. The quadrupolar splitting of DMSO-d_6/D$_2$O before (a) and after (b) adding α-santonin in the anisotropic sample (2 wt%, DMSO-d_6 : D$_2$O=4:1).
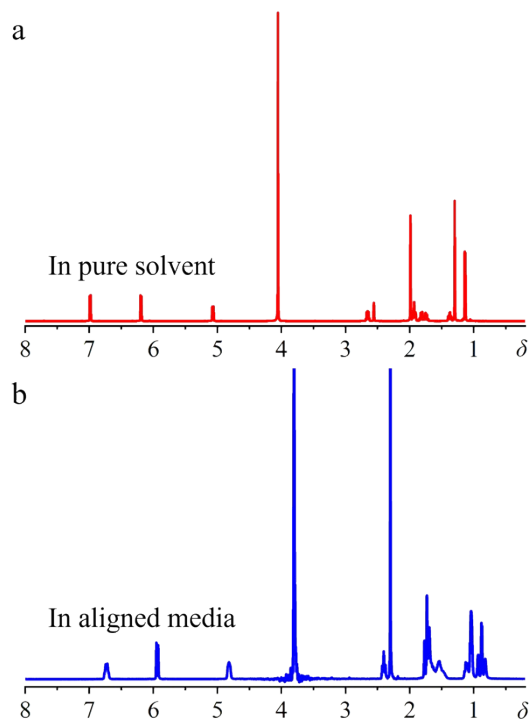
Fig. S14. ¹H spectra of α-santonin in (a) pure solvent (DMSO-d_6/D$_2$O=4:1) and (b) DMSO-d_6/D$_2$O
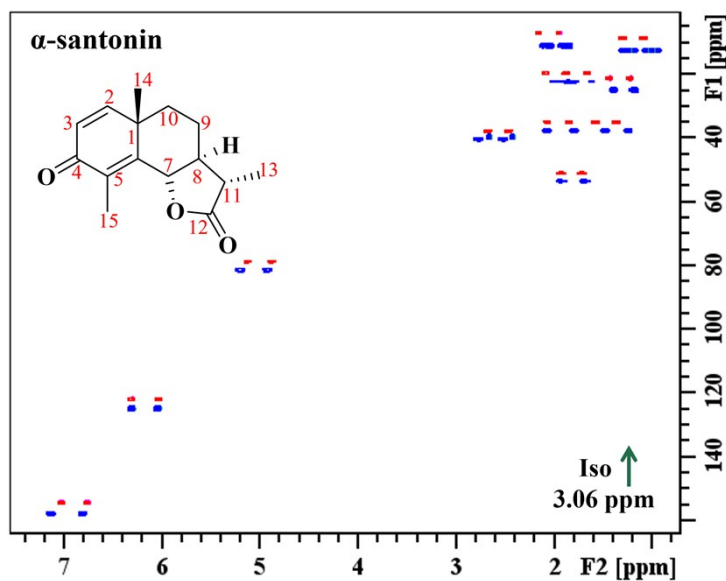
bearing Ti$_3$C$_2$T$_x$ LC medium (2 wt%, DMSO-d_6/D$_2$O=4:1).

Fig. S15. Overlaid [¹H, ¹³C]-CLIP-HSQC spectra of α-santonin (5 mg) in the isotropic phase (DMSO-d_6/D$_2$O=4:1, red contours) and 2% alignment Ti$_3$C$_2$T$_x$ LC medium (anisotropic, blue contours).

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Table S4. The scalar coupling value, compound coupling value, experimental RDCs and theoretical RDCs of α-santonin in DMSO-d_6/D_2O bearing $Ti_3C_2T_x$ LC phase (2 wt%, DMSO-d_6/D_2O=4:1).

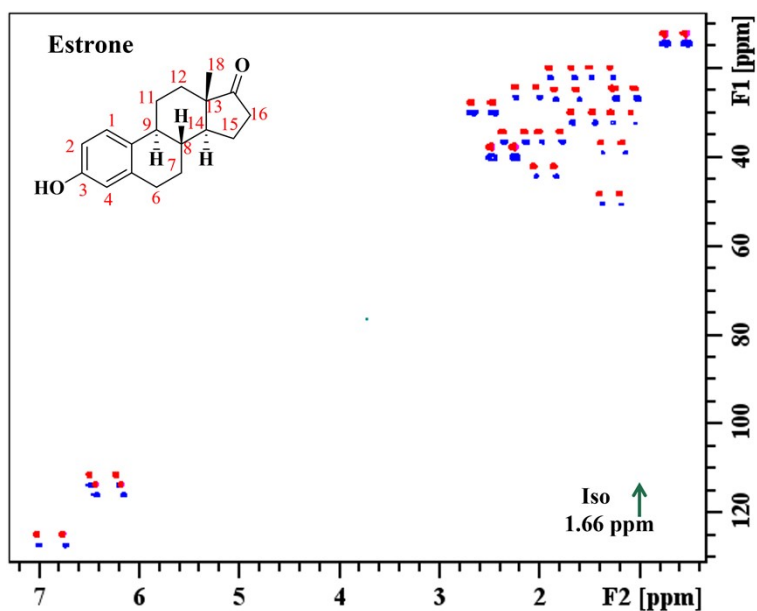| Atom number	$^1J_{CH}$	$^1T_{CH}$	$^1D_{CH}$	$^1D_{CH}$ Calculation
C2H2	161.3±0.1	195.4±0.7	34.1±0.8	33.8
C3H3	165.3±0.2	158.7±0.4	-6.6±0.6	-6.7
C7H7	149.1±0.2	165.9±0.4	16.8±0.6	16.0
C8H8	130.1±0.2	150.4±2.5	20.3±2.7	23.1
C10H10a	131.9±0.1	165.4±0.6	33.5±0.8	32.4
C10H10b	129.3±0.4	145.2±1.2	15.9±1.6	16.3
C11H11	128.3±0.0	140.4±0.3	12.5±0.3	11.3
C13H13(Me)	128.2±0.0	143.1±0.5	14.8±0.5	15.2
C14H14(Me)	129.6±0.1	126.5±0	-3.1±0.1	-3.9
C15H15(Me)	129.4±0.6	120.0±0.2	-9.4±0.8	-8.2

Fig. S16. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of estrone (2 mg) in the isotropic phase (red contours) and DMSO-d_6/D$_2$O bearing aligned Ti$_3$C$_2$T$_x$ medium (2%, blue contours).

Table S5. The scalar coupling value, compound coupling value, experimental RDCs and theoretical RDCs of estrone in DMSO-d_6/D$_2$O bearing Ti$_3$C$_2$T$_x$ LC phase (2 wt%, DMSO-d_6 : D$_2$O=4:1)

Atom number	$^1J_{CH}$	$^1T_{CH}$	$^1D_{CH}$
C1H1	154.1±0.3	163.5±0.4	9.4±0.7
C2H2	158.1±0.0	169.5±0.7	11.4±0.7
C4H4	154.2±0.1	164.6±0.4	10.4±0.5
C7H7a	128.2±0.6	139.1±0.3	10.9±0.9
C7H7b	124.5±0.1	125.2±0.1	0.7±0.2
C8H8	124.6±0.0	124.8±0.0	0.2±0.0

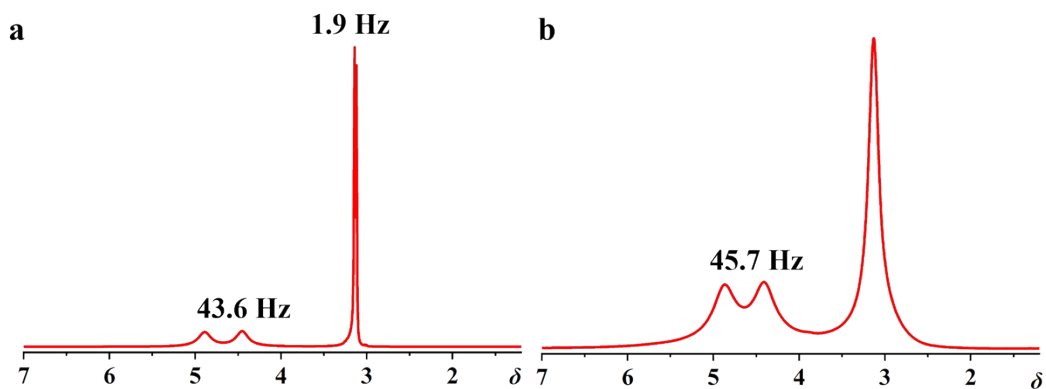|			
C9H9	122.8±0.2	124.7±0.2	1.9±0.4
C11H11a	127.6±0.5	141.4±0.3	13.8±0.8
C11H11b	126.0±0.1	123.7±0.0	-2.3±0.1
C12H12a	128.7±0.1	134.7±0.2	6.0±0.3
C12H12b	126.5±0.0	125.9±0.0	-0.6±0.0
C14H14	115.0±0.3	116.1±0.2	1.1±0.5
C15H15a	138.9±0.4	147.4±0.1	8.5±0.5
C15H15b	117.3±0.2	126.2±0.1	8.9±0.3
C16H16a	134.4±0.0	133.1±0.0	-1.3±0.0
C16H16b	125.6±0.7	125.1±0	-0.5±0.7
C18H18(Me)	127.8±0.0	126.3±0.0	-1.5±0.0

Fig. S17. The quadrupolar splittings of CD_3OD/D_2O before (a) and after (b) adding (+)-IPC in the anisotropic $Ti_3C_2T_x$ LC medium (2 wt%, $CD_3OD : D_2O=4:1$).
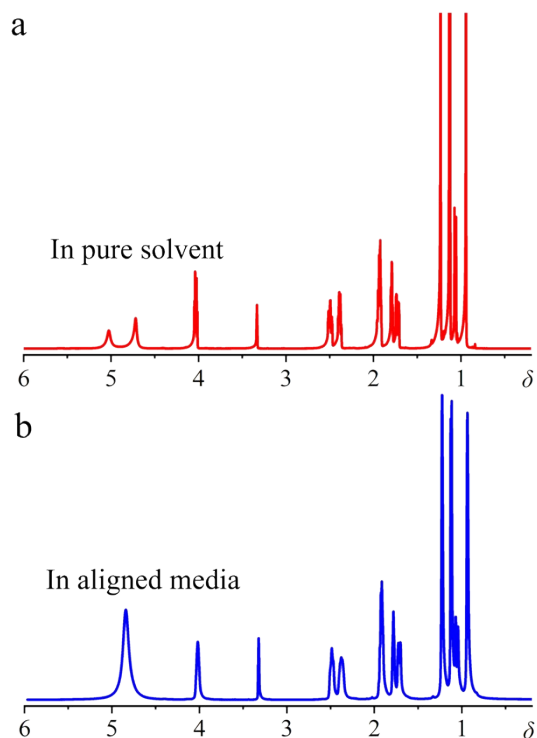
Fig. S18. ^1H spectra of (+)-IPC in (a) pure solvent (CD_3OD/D_2O=4:1) and (b) CD_3OD/D_2O bearing $Ti_3C_2T_x$ LC mediun (2 wt%, $CD_3OD : D_2O$=4:1).

Table S6. The scalar coupling value, compound coupling value, experimental RDCs and theoretical RDCs of (+)-IPC in CD_3OD/D_2O bearing $Ti_3C_2T_x$ LC phase (2 wt%, $CD_3OD : D_2O$=4:1).

Atom number	$^1J_{CH}$	$^1T_{CH}$	$1D_{CH}$	$^1D_{CH}$ Calculation
C1H1	140.4±0.2	145.6±0.5	5.2±0.7	4.7
C2H2	126.9±0.2	125.4±0.2	-1.5±0.4	-1.5
C3H3	142.1±0.3	143.4±0.0	1.3±0.3	0.9
C4H4a	126.8±0.2	134.6±0.0	7.8±0.2	7.8

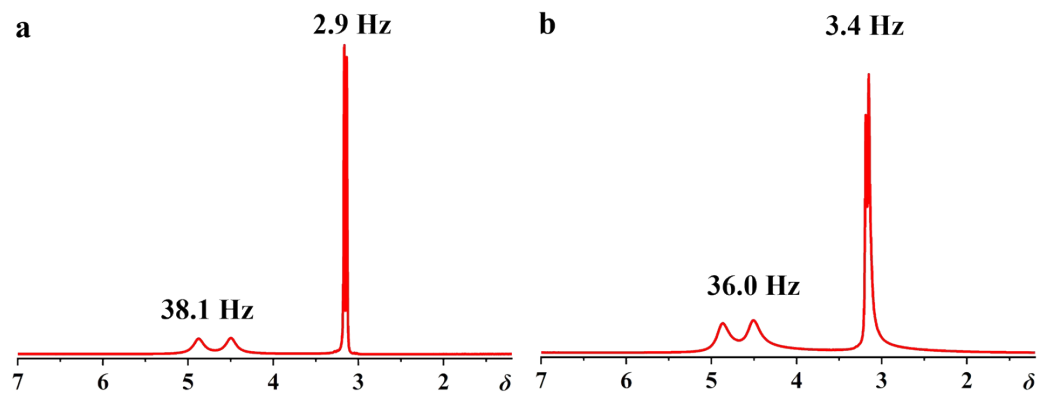|				
C4H4b	128.1±0.1	119.9±0.4	-8.2±0.5	-8.2
C5H5	141.4±0.3	144.8±0.4	3.4±0.7	2.9
C7H7a	135.4±0.2	136.6±0.1	1.2±0.3	0.9
C7H7b	137.2±0.3	129.4±0.8	-7.8±1.1	-8.5
C8H8(Me)	123.7±0.1	125.2±0.1	1.5±0.2	1.2
C9H9(Me)	123.6±0.4	122.7±0.1	-0.9±0.5	-0.3
C10H10(Me)	125.1±0.0	125.3±0.0	0.2±0.0	0.5

Fig. S19. The quadrupolar splittings of CD_3OD/D_2O before (a) and after (b) adding gibberellin in the anisotropic sample (2 wt%, $CD_3OD : D_2O=4:1$).
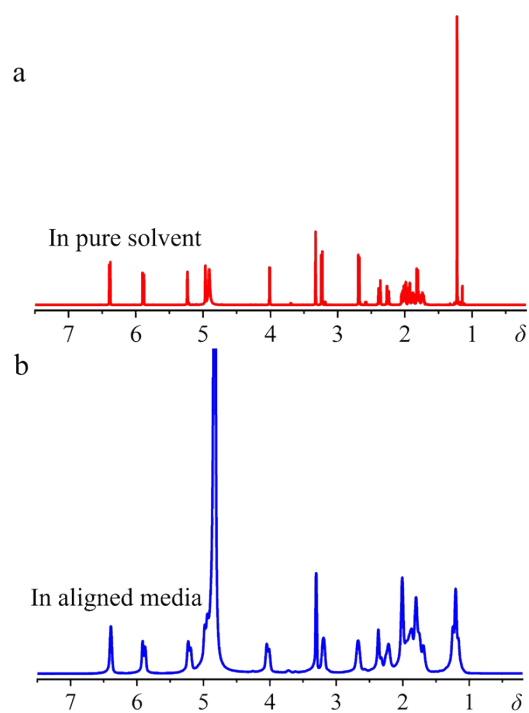
Fig. S20. [1]H spectra of gibberellin in (a) pure solvent (CD_3OD/D_2O=4:1) and (b) CD_3OD/D_2O bearing $Ti_3C_2T_x$ LC medium (2 wt%, $CD_3OD : D_2O$=4:1).
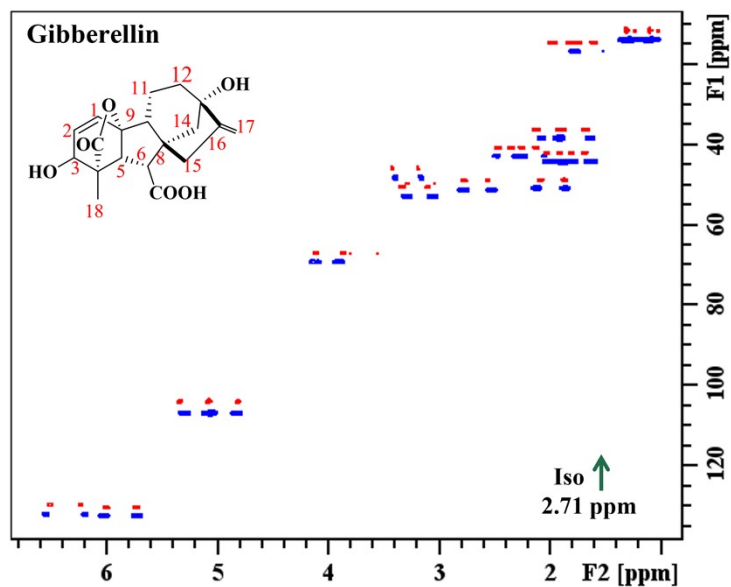

Fig. S21. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of gibberellin (10 mg) in the isotropic phase (red contours) and CD_3OD/D_2O bearing $Ti_3C_2T_x$ medium (2 wt%, $CD_3OD : D_2O$=4:1, blue contours).

Table S7. The scalar coupling value, compound coupling value, experimental RDCs and theoretical RDCs of gibberellin in CD_3OD/D_2O bearing $Ti_3C_2T_x$ LC phase (2 wt%; CD_3OD : D_2O=4:1).

Atom number	$^1J_{CH}$	$^1T_{CH}$	$^1D_{CH}$	$^1D_{CH}$ Calculation
C1H1	166.4±0.1	200.1±1.3	33.7±1.4	32.3
C3H3	147.1±0.2	127.2±0.8	-19.9±1.0	-18.4
C5H5	142.3±0.0	134.9±0.0	-7.4±0.0	-7.4
C6H6	129.8±0.1	151.4±0.6	21.6±0.7	22.6
C9H9	127.6±1.3	151.6±1.5	24.0±2.8	23.0
C12H12b	127.4±1.4	106.4±1.1	-21.0±2.5	-17.8
C12H12b	137.3±0.2	156.3±2.3	29.0±2.5	32.2
C17H17a	158.7±0.2	142.1±2.3	-16.6±2.5	-17.8
C17H17b	158.8±0.0	153.3±1.5	-5.5±1.5	-6.1
C18H18(Me)	128.2±0.0	117.9±0.9	-10.3±0.9	-11.0

Fig. S22. A quadrupolar D_2O splitting before (a) and after (b) adding L-proline in the anisotropic sample (2 wt% MXene $Ti_3C_2T_x$ LC phase).

Fig. S23. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of L-proline (5 mg) in the isotropic phase (red contours) and D_2O-bearing $Ti_3C_2T_x$ LC medium (2 wt% $Ti_3C_2T_x$, blue contours).

Table S8. The scalar coupling value, compound coupling value, experimental RDCs and theoretical RDCs of L-proline in D_2O bearing $Ti_3C_2T_x$ LC phase (2 wt%).

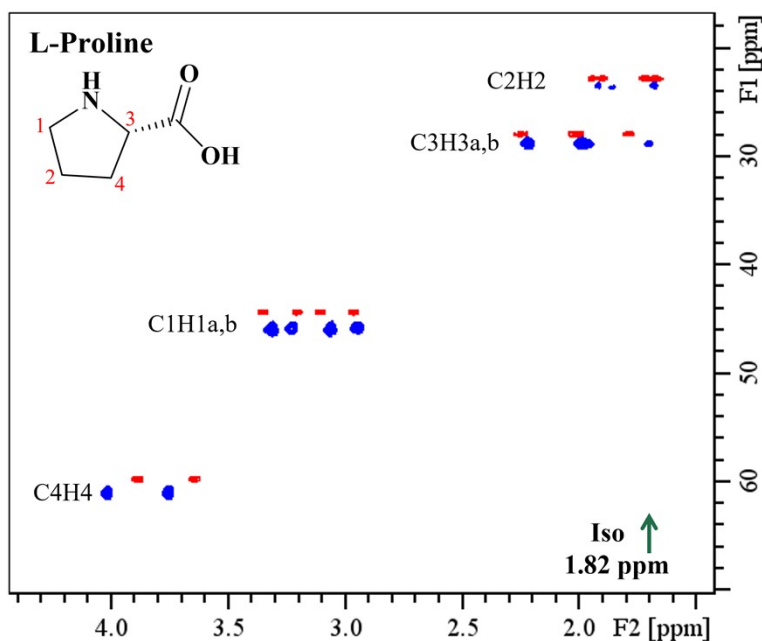| Atom number	$^1J_{CH}$	$^1T_{CH}$	$^1D_{CH}$	$^1D_{CH}$ Calculation
C1H1a	146.8±0.1	150.7±0.5	3.9±0.6	3.5
C1H1b	147.4±0.0	169.9±0.7	22.5±0.7	22.9
C2H2a	135.2±0.1	144.0±0.2	8.8±0.3	8.4
C3H3a	137.3±0.2	135.5±0.5	-1.8±0.7	-2.4
C3H3b	135.5±1.1	173.4±0.4	37.9±1.5	37.8
C4H4	148.4±0.1	157.8±0.3	9.4±0.4	9.1

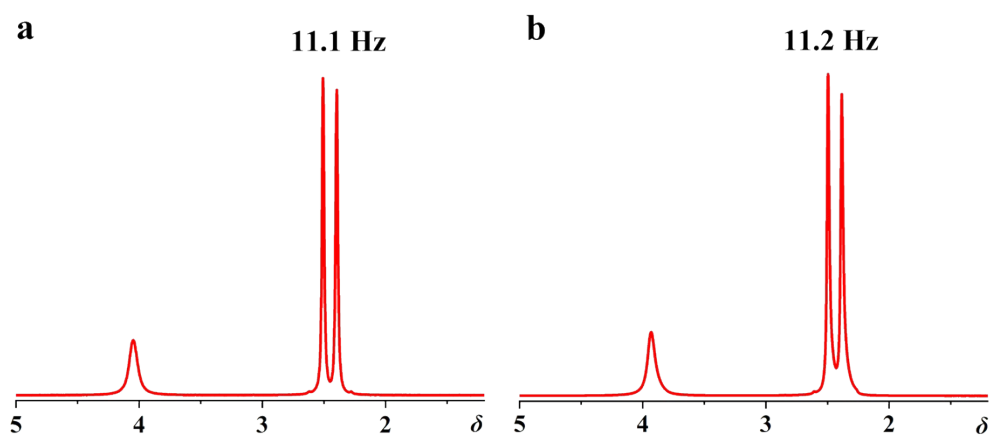**Fig. S24.** The quadrupolar splittings of DMSO-d_6/D_2O before (a) and after (b) adding L-proline in the anisotropic sample (2 wt% MXene $Ti_3C_2T_x$ LC phase, DMSO-d_6 : D_2O=4:1).

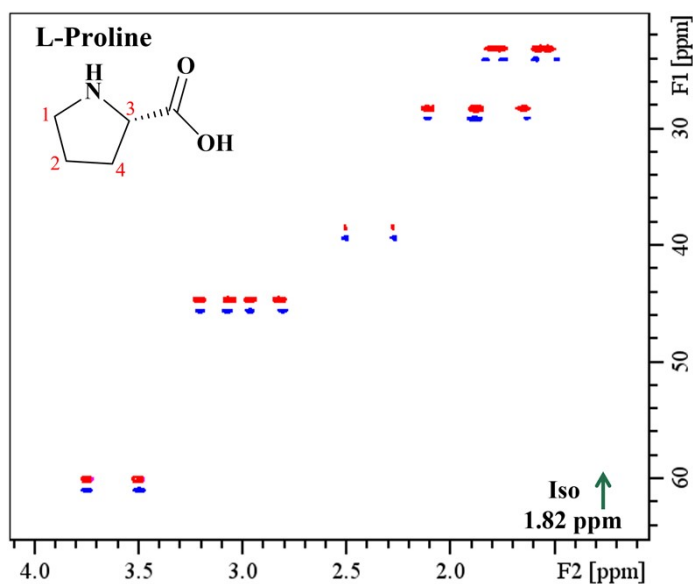**Fig. S25.** Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of L-proline (5 mg) in the isotropic phase (DMSO-d_6/D$_2$O=4 : 1, red contours) and DMSO-d_6/D$_2$O bearing Ti$_3$C$_2$T$_x$ medium (2%, DMSO-d_6/D$_2$O=4 : 1, blue contours).

Table S9. The scalar coupling value, compound coupling value, experimental RDCs and theoretical RDCs of L-proline in DMSO-d_6/D$_2$O bearing Ti$_3$C$_2$T$_x$ LC phase (2 wt%, DMSO-d_6 : D$_2$O=4:1).

Atom number	$^1J_{CH}$	$^1T_{CH}$	$^1D_{CH}$	$^1D_{CH}$ Calculation
C1H1a	146.6±0.3	144.2±0.3	-2.4±0.6	-1.8
C1H1b	145.8±0.1	160.7±0.4	14.9±0.5	14.3
C2H2a	134.1±0.7	147.9±0.5	13.8±1.2	14.4
C3H3a	141.6±0.2	138.1±0.2	-3.4±0.4	-2.7
C3H3b	133.6±0.0	147.4±0.3	13.8±0.3	13.9
C4H4	146.5±0.0	151.2±0.3	4.7±0.3	5.0

Fig. S26. The ^{2}H NMR spectra of $Ti_3C_2T_x$ media in the DMSO-d_6/D_2O (a) and CD_3OD/D_2O with adding Boc-D-tryptophan in the anisotropic sample (2 wt% MXene $Ti_3C_2T_x$ LC phase, DMSO-d_6 : D_2O=4:1)

Fig. S27. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of Boc-D-tryptophan (5 mg) in the isotropic phase (red contours) and DMSO-d_6/D_2O bearing $Ti_3C_2T_x$ medium (2 wt%, blue contours).

Table S10. The scalar coupling value, compound coupling value, experimental RDCs and theoretical RDCs of Boc-D-tryptophan in DMSO-d_6/D$_2$O bearing Ti$_3$C$_2$T$_x$ LC phase (2 wt%, DMSO-d_6 : D$_2$O=4:1).

Atom number	$^1J_{CH}$	$^1T_{CH}$	$^1D_{CH}$	$^1D_{CH}$ Calculation
C1H1	159.2±0.3	160.4±0.5	1.2±0.8	1.0
C2H2	157.4±0.0	158.2±0.2	0.8±0.2	0.8
C3H3	158.8±0.0	156.0±0.1	1.2±0.1	1.4
C4H4	158.7±0.0	158.4±0.0	-0.3±0.0	-0.3
C8H8	180.7±0.0	181.9±0.1	1.2±0.1	1.0
C10H10a	128.3±0.1	126.7±0.0	-1.6±0.1	-1.5
C10H10b	129.9±0.0	125.3±0.5	-4.6±0.5	-4.6
C11H11	141.2±0.1	138.6±0.2	-2.6±0.3	-2.8

Fig. S28. Correlation between the experimental and calculated RDC values of Boc-D-tryptophan in the DMSO-d_6/D$_2$O bearing Ti$_3$C$_2$T$_x$ LC phase (2 wt%, DMSO-d_6 : D$_2$O=4:1).
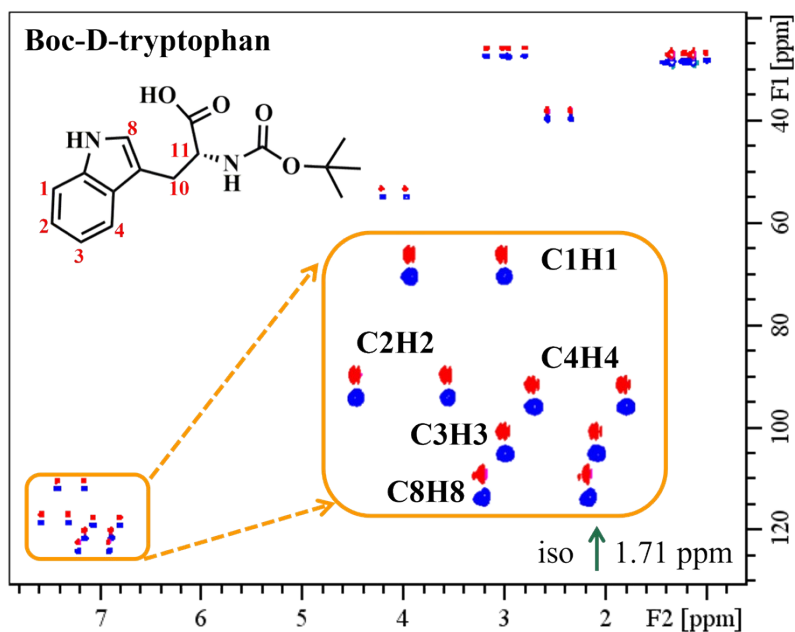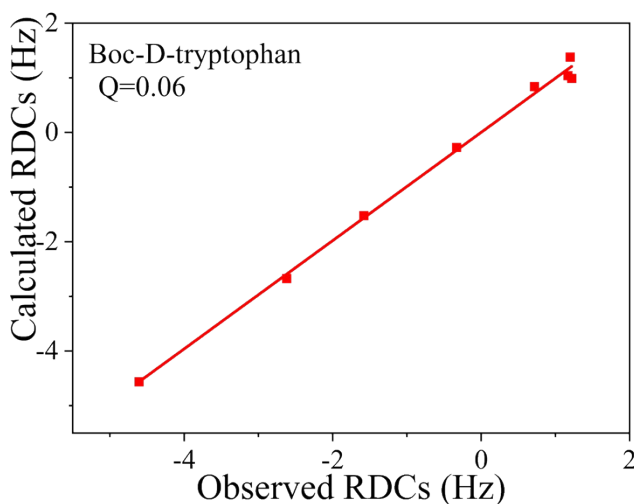
Fig. S29. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of Boc-D-tryptophan (5 mg) in the isotropic phase (red contours) and CD$_3$OD/D$_2$O bearing Ti$_3$C$_2$T$_x$ medium (2%, CD$_3$OD : D$_2$O=4:1, blue contours).

Table S11. The scalar coupling value, compound coupling value, experimental RDCs and theoretical RDCs of Boc-D-tryptophan in CD$_3$OD/D$_2$O bearing Ti$_3$C$_2$T$_x$ LC phase (2 wt%, CD$_3$OD : D$_2$O=4:1).

Atom number	$^1J_{CH}$	$^1T_{CH}$	$^1D_{CH}$	$^1D_{CH}$ Calculation
C1H1	159.2±0.3	160.3±0.4	1.1±0.7	1.4
C2H2	157.5±0.0	161.8±0.0	4.3±0.0	4.2
C3H3	158.6±0.1	160.4±0.1	1.8±0.2	1.8
C4H4	158.5±0.0	159.7±0.1	1.3±0.1	1.0
C8H8	180.4±0.0	182.2±0.1	1.8±0.1	1.9
C10H10a	129.6±0.0	126.4±0.1	-3.2±0.1	-3.0

C10H10b	129.2±0.0	125.0±0.2	-4.1±0.2	-4.2
C11H11	142.4±0.3	140.9±0.2	-1.5±0.5	-1.9

Fig. S30. Correlation between the experimental and calculated RDC values of Boc-D-tryptophan in the CD_3OD/D_2O bearing $Ti_3C_2T_x$ medium (2%, $CD_3OD : D_2O=4:1$).

References

1   G. Kummerlöwe, S. Schmitt and B. Luy, *Open Spectrosc. J.*, 2010, **4**, 16–27.

2   P. Trigo-Mouriño, A. Navarro-Vázquez, J. Ying, R. R. Gil and A. Bax, *Angew. Chemie Int. Ed.*, 2011, **50**, 7576–7580.

3   J. A. Losonczi, M. Andrec, M. W. F. Fischer and J. H. Prestegard, *J. Magn. Reson.*, 1999, **138**, 334–342.

4   Y. Liu, A. Navarro-Vázquez, R. R. Gil, C. Griesinger, G. E. Martin and R. T. Williamson, *Nat. Protoc.*, 2019, **14**, 217–247.

MSpin output Data

Calculated Corresponding alignment tensor for L-camphor in $Ti_3C_2T_x$ MXene with DMSO-d_6/D_2O.

Cornilescu Quality factor: 0.0738825

Alignment tensor information:

A'x= 6.870e-05

A'y= 1.546e-04

A'z=-2.233e-04

Saupe tensor

S'x= 1.031e-04

S'y= 2.319e-04

S'z=-3.350e-04

Alignment tensor eigenvectors

e[x]=(0.982,-0.169, 0.080)

e[y]=(0.182, 0.776,-0.603)

e[z]=(0.040, 0.607, 0.793)

Alignment tensor in laboratory coordinates:

[7.109e-05,5.060e-06,-1.874e-05]

[5.060e-06,1.276e-05,-1.810e-04]

[-1.874e-05,-1.810e-04,-8.385e-05]

SVD condition number is 2.426e+00

Axial component Aa = -3.350e-04

Rhombic component Ar = -8.591e-05

Field=11.74 Teslas[3.63]

rhombicity R = 0.256

Asimmetry parameter etha =3.847e-01

GDO = 4.009e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(86.2,37.5,-97.5)

Set 2

(-93.8,-37.5,82.5)

Calculated Corresponding alignment tensor for artemether in $Ti_3C_2T_x$ MXene with DMSO-d_6/D_2O.

Cornilescu Quality factor: 0.0544837

Alignment tensor information:

A'x= 1.442e-04

A'y= 1.824e-04

A'z=-3.266e-04

Saupe tensor

S'x= 2.163e-04

S'y= 2.736e-04

S'z=-4.899e-04

Alignment tensor eigenvectors

e[x]=(-0.575, 0.815, 0.078)

e[y]=(0.619, 0.371, 0.692)

e[z]=(0.535, 0.446,-0.718)

Alignment tensor in laboratory coordinates:

[2.411e-05,-1.035e-04,1.971e-04]

[-1.035e-04,5.588e-05,1.604e-04]

[1.971e-04,1.604e-04,-7.999e-05]

SVD condition number is 6.542e+00

Axial component Aa = -4.899e-04

Rhombic component Ar = -3.819e-05

Field=11.74 Teslas[3.63]

rhombicity R = 0.078

Asimmetry parameter etha =1.169e-01

GDO = 5.676e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(39.8,135.9,96.4)

Set 2

(-140.2,-135.9,-83.6)

Calculated Corresponding alignment tensor for artemether in $Ti_3C_2T_x$ MXene with DMSO-d_6/D_2O at

305 K.

Cornilescu Quality factor: 0.0915959

Alignment tensor information:

A'x= 1.239e-04

A'y= 2.300e-04

A'z=-3.540e-04

Saupe tensor

S'x= 1.859e-04

S'y= 3.451e-04

S'z=-5.310e-04

Alignment tensor eigenvectors

e[x]=(-0.099, 0.942, 0.322)

e[y]=(0.810,-0.112, 0.576)

e[z]=(0.578, 0.318,-0.751)

Alignment tensor in laboratory coordinates:

[3.384e-05,-9.743e-05,2.571e-04]

[-9.743e-05,7.694e-05,1.074e-04]

[2.571e-04,1.074e-04,-1.108e-04]

SVD condition number is 6.542e+00

Axial component Aa = -5.310e-04

Rhombic component Ar = -1.061e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.200

Asimmetry parameter etha =2.998e-01

GDO = 6.267e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(28.8,138.7,119.2)

Set 2

(-151.2,-138.7,-60.8)

Calculated Corresponding alignment tensor for α-santonin in $Ti_3C_2T_x$ MXene with DMSO-d_6/D_2O.

Output files of MSpin for the RDCs analysis of SSSS for α-santonine:

Cornilescu Quality factor: 0.0598082

Alignment tensor information:

A'x= 1.533e-04

A'y= 1.123e-03

A'z=-1.276e-03

Saupe tensor

S'x= 2.299e-04

S'y= 1.684e-03

S'z=-1.914e-03

Alignment tensor eigenvectors

e[x]=(0.100,-0.813, 0.574)

e[y]=(0.911, 0.307, 0.275)

e[z]=(-0.400, 0.495, 0.771)

Alignment tensor in laboratory coordinates:

[7.294e-04,5.540e-04,6.844e-04]

[5.540e-04,-1.056e-04,-4.638e-04]

[6.844e-04,-4.638e-04,-6.238e-04]

SVD condition number is 9.006e+00

Axial component Aa = -1.914e-03

Rhombic component Ar = -9.696e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.507

Asimmetry parameter etha =7.598e-01

GDO = 2.509e-03

ZY'Z'' Euler Angles (degrees)

Set 1

(128.9,39.5,154.3)

Set 2

(-51.1,-39.5,-25.7)

Output files of MSpin for the RDCs analysis of SRRR for α-santonine:

Cornilescu Quality factor: 0.20601

Alignment tensor information:

A'x= 2.338e-04

A'y= 1.155e-03

A'z=-1.389e-03

Saupe tensor

S'x= 3.508e-04

S'y= 1.733e-03

S'z=-2.084e-03

Alignment tensor eigenvectors

e[x]=(0.117,-0.744, 0.658)

e[y]=(0.861, 0.406, 0.306)

e[z]=(-0.494, 0.531, 0.688)

Alignment tensor in laboratory coordinates:

[5.209e-04,7.482e-04,7.947e-04]

[7.482e-04,-7.281e-05,-4.790e-04]

[7.947e-04,-4.790e-04,-4.481e-04]

SVD condition number is 8.634e+00

Axial component Aa = -2.084e-03

Rhombic component Ar = -9.214e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.442

Asimmetry parameter etha =6.633e-01

GDO = 2.658e-03

ZY'Z'' Euler Angles (degrees)

Set 1

(132.9,46.5,155.1)

Set 2

(-47.1,-46.5,-24.9)

Output files of MSpin for the RDCs analysis of SRSR for α-santonine:

Cornilescu Quality factor: 0.165632

Alignment tensor information:

A'x=-1.649e-04

A'y=-8.933e-04

A'z= 1.058e-03

Saupe tensor

S'x=-2.473e-04

S'y=-1.340e-03

S'z= 1.587e-03

Alignment tensor eigenvectors

e[x]=(0.231, 0.759, 0.608)

e[y]=(0.498,-0.629, 0.596)

e[z]=(0.836, 0.165,-0.524)

Alignment tensor in laboratory coordinates:

[5.080e-04,3.973e-04,-7.521e-04]

[3.973e-04,-4.200e-04,1.675e-04]

[-7.521e-04,1.675e-04,-8.800e-05]

SVD condition number is 6.838e+00

Axial component Aa = 1.587e-03

Rhombic component Ar = 7.285e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.459

Asimmetry parameter etha =6.884e-01

GDO = 2.038e-03

ZY'Z'' Euler Angles (degrees)

Set 1

(11.2,121.6,135.6)

Set 2

(-168.8,-121.6,-44.4)

Output files of MSpin for the RDCs analysis of SSRR for α-santonine:

Cornilescu Quality factor: 0.295325

Alignment tensor information:

A'x=-1.263e-04

A'y=-8.455e-04

A'z= 9.717e-04

Saupe tensor

S'x=-1.894e-04

S'y=-1.268e-03

S'z= 1.458e-03

Alignment tensor eigenvectors

e[x]=(-0.419, 0.547, 0.725)

e[y]=(-0.128,-0.826, 0.549)

e[z]=(0.899, 0.137, 0.416)

Alignment tensor in laboratory coordinates:

[7.495e-04,5.875e-05,4.612e-04]

[5.875e-05,-5.966e-04,3.885e-04]

[4.612e-04,3.885e-04,-1.529e-04]

SVD condition number is 6.851e+00

Axial component Aa = 1.458e-03

Rhombic component Ar = 7.192e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.493

Asimmetry parameter etha =7.402e-01

GDO = 1.900e-03

ZY'Z'' Euler Angles (degrees)

Set 1

(8.6,65.4,142.9)

Set 2

(-171.4,-65.4,-37.1)

Output files of MSpin for the RDCs analysis of SRRS for α-santonine:

Cornilescu Quality factor: 0.203519

Alignment tensor information:

A'x= 2.267e-04

A'y= 1.167e-03

A'z=-1.394e-03

Saupe tensor

S'x= 3.400e-04

S'y= 1.750e-03

S'z=-2.090e-03

Alignment tensor eigenvectors

e[x]=(0.144,-0.765, 0.628)

e[y]=(0.880, 0.389, 0.272)

e[z]=(-0.453, 0.513, 0.729)

Alignment tensor in laboratory coordinates:

[6.227e-04,6.985e-04,7.600e-04]

[6.985e-04,-5.776e-05,-5.068e-04]

[7.600e-04,-5.068e-04,-5.650e-04]

SVD condition number is 8.038e+00

Axial component Aa = -2.090e-03

Rhombic component Ar = -9.402e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.450

Asimmetry parameter etha =6.747e-01

GDO = 2.674e-03

ZY'Z'' Euler Angles (degrees)

Set 1

(131.4,43.2,156.6)

Set 2

(-48.6,-43.2,-23.4)

Output files of MSpin for the RDCs analysis of SSRS for α-santonine:

Cornilescu Quality factor: 0.251565

Alignment tensor information:

A'x=-2.705e-04

A'y=-5.167e-04

A'z= 7.872e-04

Saupe tensor

S'x=-4.058e-04

S'y=-7.750e-04

S'z= 1.181e-03

Alignment tensor eigenvectors

e[x]=(0.093, 0.425,-0.900)

e[y]=(-0.454, 0.823, 0.342)

e[z]=(0.886, 0.377, 0.270)

Alignment tensor in laboratory coordinates:

[5.092e-04,4.453e-04,2.910e-04]

[4.453e-04,-2.869e-04,3.837e-05]

[2.910e-04,3.837e-05,-2.223e-04]

SVD condition number is 6.104e+00

Axial component Aa = 1.181e-03

Rhombic component Ar = 2.461e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.208

Asimmetry parameter etha =3.127e-01

GDO = 1.396e-03

ZY'Z'' Euler Angles (degrees)

Set 1

(23.0,74.4,20.8)

Set 2

(-157.0,-74.4,-159.2)

Output files of MSpin for the RDCs analysis of SSSR for α-santonine:

Cornilescu Quality factor: 0.144216

Alignment tensor information:

A'x=-1.948e-04

A'y=-1.271e-03

A'z= 1.466e-03

Saupe tensor

S'x=-2.923e-04

S'y=-1.907e-03

S'z= 2.199e-03

Alignment tensor eigenvectors

e[x]=(-0.453, 0.620,-0.641)

e[y]=(-0.450, 0.461, 0.764)

e[z]=(0.770, 0.635, 0.070)

Alignment tensor in laboratory coordinates:

[5.707e-04,1.035e-03,4.605e-04]

[1.035e-03,2.449e-04,-3.053e-04]

[4.605e-04,-3.053e-04,-8.156e-04]

SVD condition number is 7.165e+00

Axial component Aa = 2.199e-03

Rhombic component Ar = 1.076e-03

Field=11.74 Teslas[3.63]

rhombicity R = 0.489

Asimmetry parameter etha =7.342e-01

GDO = 2.861e-03

ZY'Z'' Euler Angles (degrees)

Set 1

(39.5,86.0,50.0)

Set 2

(-140.5,-86.0,-130.0)

Output files of MSpin for the RDCs analysis of SRSS for α-santonine:

Cornilescu Quality factor: 0.29817

Alignment tensor information:

A'x=-4.111e-04

A'y=-8.645e-04

A'z= 1.276e-03

Saupe tensor

S'x=-6.167e-04

S'y=-1.297e-03

S'z= 1.913e-03

Alignment tensor eigenvectors

e[x]=(0.104, 0.993,-0.052)

e[y]=(-0.662, 0.108, 0.742)

e[z]=(0.742,-0.043, 0.669)

Alignment tensor in laboratory coordinates:

[3.201e-04,-2.169e-05,1.060e-03]

[-2.169e-05,-4.133e-04,-8.508e-05]

[1.060e-03,-8.508e-05,9.323e-05]

SVD condition number is 5.131e+00

Axial component Aa = 1.913e-03

Rhombic component Ar = 4.534e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.237

Asimmetry parameter etha =3.554e-01

GDO = 2.278e-03

ZY'Z'' Euler Angles (degrees)

Set 1

(-3.3,48.0,86.0)

Set 2

(176.7,-48.0,-94.0)

Calculated Corresponding alignment tensor for (+)-IPC in $Ti_3C_2T_x$ MXene with CD_3OD/D_2O.

Cornilescu Quality factor: 0.0823784

Alignment tensor information:

A'x=-1.899e-06

A'y=-1.375e-04

A'z= 1.394e-04

Saupe tensor

S'x=-2.848e-06

S'y=-2.062e-04

S'z= 2.091e-04

Alignment tensor eigenvectors

e[x]=(-0.661, 0.680, 0.319)

e[y]=(0.007,-0.420, 0.908)

e[z]=(0.751, 0.602, 0.273)

Alignment tensor in laboratory coordinates:

[7.768e-05,6.420e-05,2.810e-05]

[6.420e-05,2.542e-05,7.481e-05]

[2.810e-05,7.481e-05,-1.031e-04]

SVD condition number is 2.051e+00

Axial component Aa = 2.091e-04

Rhombic component Ar = 1.356e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.649

Asimmetry parameter etha =9.728e-01

GDO = 2.930e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(38.7,74.2,109.4)

Set 2

(-141.3,-74.2,-70.6)

Calculated Corresponding alignment tensor for gibberellin in $Ti_3C_2T_x$ MXene with CD_3OD/D_2O.

Cornilescu Quality factor: 0.0822114

Alignment tensor information:

A'x= 8.581e-05

A'y= 4.514e-04

A'z=-5.372e-04

Saupe tensor

S'x= 1.287e-04

S'y= 6.771e-04

S'z=-8.058e-04

Alignment tensor eigenvectors

e[x]=(0.865,-0.275, 0.421)

e[y]=(0.262, 0.961, 0.089)

e[z]=(-0.429, 0.033, 0.903)

Alignment tensor in laboratory coordinates:

[-3.629e-06,1.008e-04,2.497e-04]

[1.008e-04,4.227e-04,1.292e-05]

[2.497e-04,1.292e-05,-4.191e-04]

SVD condition number is 3.327e+00

Axial component Aa = -8.058e-04

Rhombic component Ar = -3.656e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.454

Asimmetry parameter etha =6.805e-01

GDO = 1.033e-03

ZY'Z'' Euler Angles (degrees)

Set 1

(175.6,25.5,168.0)

Set 2

(-4.4,-25.5,-12.0)

Calculated Corresponding alignment tensor for L-proline in $Ti_3C_2T_x$ MXene with D_2O

(Conformer 1: 35.1%, Conformer 2: 3.6%, Conformer 3: 52.8%, Conformer 4: 1.1%, Conformer 5: 7.4%)

Cornilescu Quality factor: 0.0202586

Alignment tensor information:

A'x=-5.925e-05

A'y=-9.820e-04

A'z= 1.041e-03

Saupe tensor

S'x=-8.888e-05

S'y=-1.473e-03

S'z= 1.562e-03

Alignment tensor eigenvectors

e[x]=(-0.114, 0.443, 0.889)

e[y]=(0.385,-0.805, 0.451)

e[z]=(0.916, 0.394,-0.079)

Alignment tensor in laboratory coordinates:

[7.274e-04,6.826e-04,-2.392e-04]

[6.826e-04,-4.875e-04,3.010e-04]

[-2.392e-04,3.010e-04,-2.400e-04]

SVD condition number is 3.156e+00

Axial component Aa = 1.562e-03

Rhombic component Ar = 9.227e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.591

Asimmetry parameter etha =8.862e-01

GDO = 2.128e-03

ZY'Z" Euler Angles (degrees)

Set 1

(23.3,94.5,153.1)

Set 2

(-156.7,-94.5,-26.9)

Calculated Corresponding alignment tensor for L-proline in $Ti_3C_2T_x$ MXene with DMSO-d_6/D_2O

(Conformer 1: 35.1%, Conformer 2: 3.6%, Conformer 3: 52.8%, Conformer 4: 1.1%, Conformer 5: 7.4%)

Cornilescu Quality factor: 0.0515514

Alignment tensor information:

A'x=-1.047e-04

A'y=-5.069e-04

A'z= 6.116e-04

Saupe tensor

S'x=-1.571e-04

S'y=-7.603e-04

S'z= 9.174e-04

Alignment tensor eigenvectors

e[x]=(-0.146, 0.249, 0.957)

e[y]=(0.641,-0.714, 0.283)

e[z]=(0.754, 0.655,-0.055)

Alignment tensor in laboratory coordinates:

[1.372e-04,5.374e-04,-1.028e-04]

[5.374e-04,-2.388e-06,5.546e-05]

[-1.028e-04,5.546e-05,-1.348e-04]

SVD condition number is 3.156e+00

Axial component Aa = 9.174e-04

Rhombic component Ar = 4.021e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.438

Asimmetry parameter etha =6.576e-01

GDO = 1.168e-03

ZY'Z" Euler Angles (degrees)

Set 1

(41.0,93.2,163.5)

Set 2

(-139.0,-93.2,-16.5)

Calculated Corresponding alignment tensor for Boc-D-Trypophan in $Ti_3C_2T_x$ MXene with DMSO-d_6/D_2O (Conformer 1: 9.9%, Conformer 2: 73.2%, Conformer 3: 16.9%)

Cornilescu Quality factor: 0.0598416

Alignment tensor information:

A'x= 5.120e-04

A'y= 7.490e-04

A'z=-1.261e-03

Saupe tensor

S'x= 7.680e-04

S'y= 1.124e-03

S'z=-1.891e-03

Alignment tensor eigenvectors

e[x]=(0.093, 0.895,-0.437)

e[y]=(-0.527, 0.417, 0.741)

e[z]=(0.845, 0.162, 0.510)

Alignment tensor in laboratory coordinates:

[-6.870e-04,-2.945e-04,-8.567e-04]

[-2.945e-04,5.067e-04,-7.333e-05]

[-8.567e-04,-7.333e-05,1.803e-04]

SVD condition number is 4.594e+01

Axial component Aa = -1.891e-03

Rhombic component Ar = -2.370e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.125

Asimmetry parameter etha =1.880e-01

GDO = 2.203e-03

ZY'Z'' Euler Angles (degrees)

Set 1

(10.8,59.3,59.4)

Set 2

(-169.2,-59.3,-120.6)

Calculated Corresponding alignment tensor for Boc-D-Trypophan in $Ti_3C_2T_x$ MXene with CD_3OD/D_2O (Conformer 1: 9.9%, Conformer 2: 73.2%, Conformer 3: 16.9%)

Cornilescu Quality factor: 0.0850145

Alignment tensor information:

A'x=-5.401e-07

A'y=-6.143e-04

A'z= 6.148e-04

Saupe tensor

S'x=-8.102e-07

S'y=-9.214e-04

S'z= 9.222e-04

Alignment tensor eigenvectors

e[x]=(-0.201,-0.564, 0.801)

e[y]=(0.934, 0.136, 0.331)

e[z]=(-0.296, 0.814, 0.500)

Alignment tensor in laboratory coordinates:

[-4.819e-04,-2.264e-04,-2.804e-04]

[-2.264e-04,3.959e-04,2.227e-04]

[-2.804e-04,2.227e-04,8.606e-05]

SVD condition number is 1.289e+01

Axial component Aa = 9.222e-04

Rhombic component Ar = 6.137e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.665

Asimmetry parameter etha =9.982e-01

GDO = 1.303e-03

ZY'Z" Euler Angles (degrees)

Set 1

(110.0,60.0,157.6)

Set 2

(-70.0,-60.0,-22.4)