Supporting Information

for

Programmable alignment media from self-assembled oligopeptide amphiphiles for the measurement of independent sets of residual dipolar couplings in organic solvents

Yuexiao Lin,‡[a] Jiaqian Li,‡[a] Si-Yong Qin,‡[b] Han Sun,[c] Yan-Ling Yang,[a] Armando Navarro-Vázquez [d] and Xinxiang Lei *[ab]

‡ These authors contributed equally to this work.

[a] School of Pharmaceutical Sciences, South-Central University for Nationalities, Wuhan, 430074, China. E-mail: xxlei@mail.scuec.edu.cn.

[b] Key Laboratory of Analytical Chemistry of the State Ethnic Affairs Commission, South-Central University for Nationalities, Wuhan, 430074, China.

[c] Group of Structural Chemistry and Computational Biology, Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP) 13125 Berlin (Germany).

[d] Departamento de Química Fundamental, Universidade Federal de Pernambuco Cidade Universitária, CEP: 50740-540 Recife, PE, Brazil.

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Experimental Procedures

Materials

N-9-Fluorenylmethoxycarbonyl (Fmoc) protected L-amino acids (Fmoc-Lys (Boc)-OH, Fmoc-Val-OH, Fmoc-Ala-OH, Fmoc-Glu(otBu)-OH and Fmoc-Phe-OH), rink amide-AM resin (100-200 mesh, loading: 0.55 mmol/g, 1% DVB), coupling reagents including 2-(1H-Benzotriazole-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate (HBTU) and 1-hydroxybenzotriazole (HOBT) were provided by GL Biochem. Ltd (Shanghai, China). *N*, *N*-dimethylformamide (DMF), dichloromethane (CH_2Cl_2), methanol (MeOH), ether, and Triisopropylsilane (TIS) were purchased from Sinopharm Chemical Reagent Co. Ltd (Shanghai, China). Palmitic acid (AR), trifluoroacetic acid (TFA), artemether, gibberellin, and α-santonin were bought from Aladdin Reagent Co.Ltd (Shanghai, China).

Methods

Synthesis of OPAs. Take OPA-**1** as an example, the peptide amphiphile of $C_{15}H_{31}$-CONH-VVAAEEKK-$CONH_2$ was synthesized by standard 9-fluorenylmethoxycarbonyl (Fmoc) solid-phase method on a rink amide-AM resin. The protective group and resin were removed with a cocktail of trifluoroacetic acid, triisopropylsilane and water (TFA/TIS/H_2O=95/2.5/2.5(v/v)). The obtained crude peptide was purified by high-pressure liquid chromatography (HPLC) to a purity of more than 98%.

Structural characterization of OPAs. Liquid chromatography high resolution mass spectrometry was used to record the molecular weight of OPAs. The purity of OPAs was measured by high-pressure liquid chromatography (HPLC, LC-20AR, Shimadzu, Japan) equipped with a C18 column (SinoChrom ODS-BP, 4.6*250 mm, 5 μm). The mobile phase of HPLC was acetonitrile (MeCN)/water (v/v, both containing 0.1% TFA), and gradient elution was performed at a flow rate of 1.0 ml/min (95: 5-0: 100, 30 min). The product was then freeze-dried, and a white solid was obtained as purified OPAs.

Preparation of the self-assembled alignment media. For the preparation of the alignment medium, a certain amount of the lyophilized peptide was directly dissolved with methanol. The concentration of all aligned media used in this experiment is 5 %(w/v) by default unless otherwise specified.

Characterization of the secondary conformation of the self-assembly. The secondary conformation of self-assembled OPA was characterized by Fourier transform infrared spectroscopy (FT-IR). The infrared spectrum was obtained by the instrument IRTracer-100 Fourier infrared spectrometer. The spectrum was recorded in the range of 500-4000 cm^{-1} and a total of 300 scans were performed with a resolution of 0.25 cm^{-1}.

NMR experiments. All NMR spectra were measured using a Bruker Ascend IIITM 600 MHz NMR spectrometer equipped with a 5 mm CPPBBO forward broadband liquid nitrogen cryogenic probe. All the experiments were conducted at 293 K.The 1D ^{2}H NMR spectra were collected using locking channel records at eight scans. To collect the 2D [^{1}H, ^{13}C]-CLIP-HSQC spectra, the acquisition time (AQ), and the relaxation delay (RD) were 0.378s and 2.00 s, respectively. The spectral width (SW) of these spectra was 10.0 ppm (^{1}H) and 170 ppm (^{13}C). At the spectral width of 10 ppm, a total of 0.3 k data points were sampled in a direct dimension. The one-bond coupling constant was 145.0 Hz. Prior to Fourier transform, 1 Hz LB was used for F2 and 0.3 Hz LB for F1. The NMR data were read and processed by Bruker Topspin 3.5 pl 6 and M-spin software.

The recovery of analytes. All samples were recovered by HPLC. The key to high recovery is to ensure that the viscous OPA solution can be completely transferred from the NMR tube and washing the NMR tube with methanol many times can appropriately improve the recovery.

Results and Discussion

1. Characterization of the self-assembly media

1.1. HPLC and Ms of OPAs

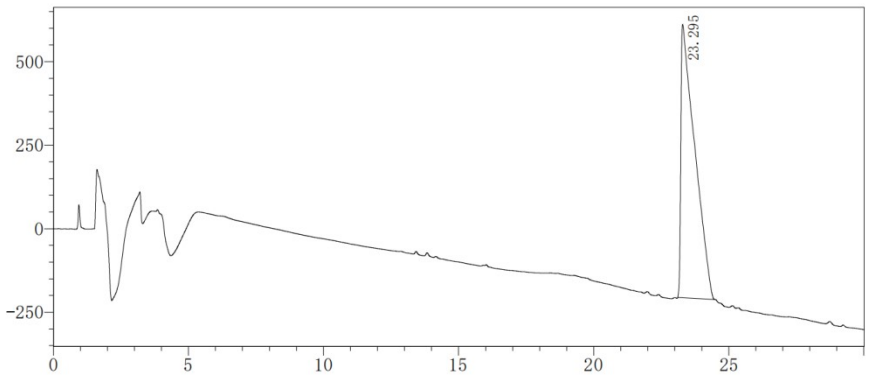


Figure S1. HPLC profile of $C_{15}H_{31}$-CONH-VVAAEEKK-$CONH_2$ (OPA-**1,** purity 98.0%).

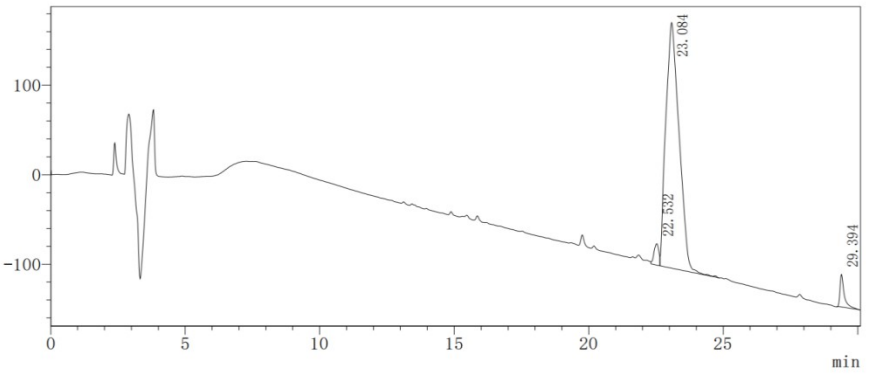


Figure S2. HPLC profile of D-OPA-**1** (synthesis of D-type amino acids, purity 95.0%).

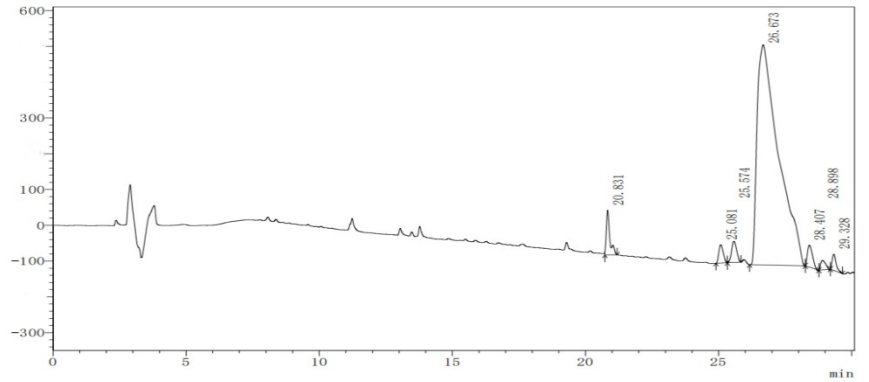


Figure S3. HPLC profile of $C_{15}H_{31}$-CONH-FFVVAAEEKK-$CONH_2$ (OPA-**2**, purity 91.2%).

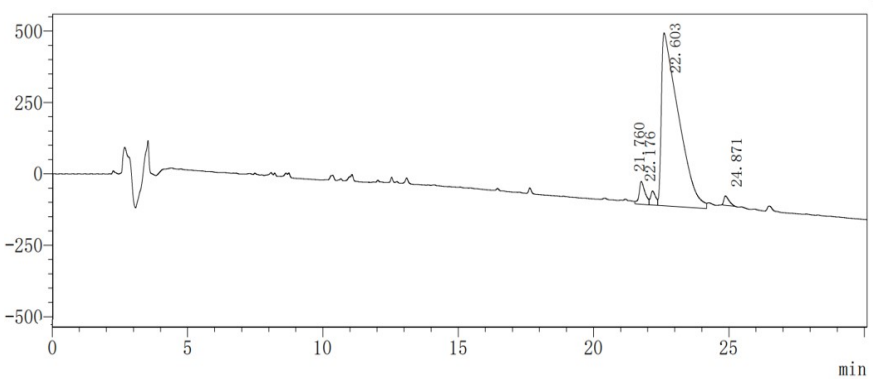


Figure S4. HPLC profile of $C_{15}H_{31}$-CONH-FFVVVVKKK-$CONH_2$ (OPA-**4**, purity 92.1%).

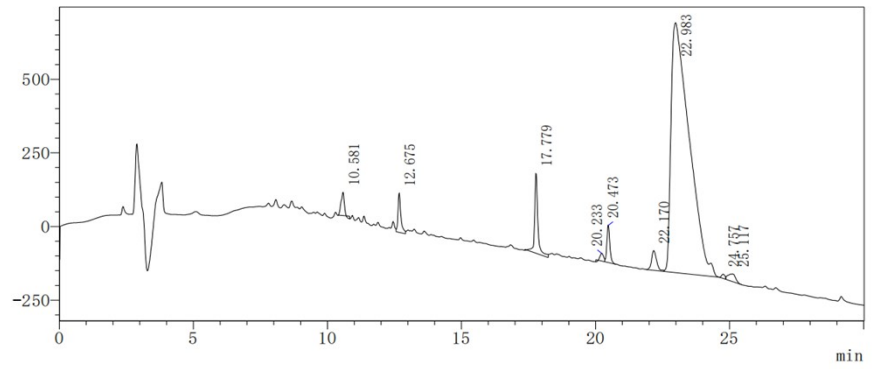
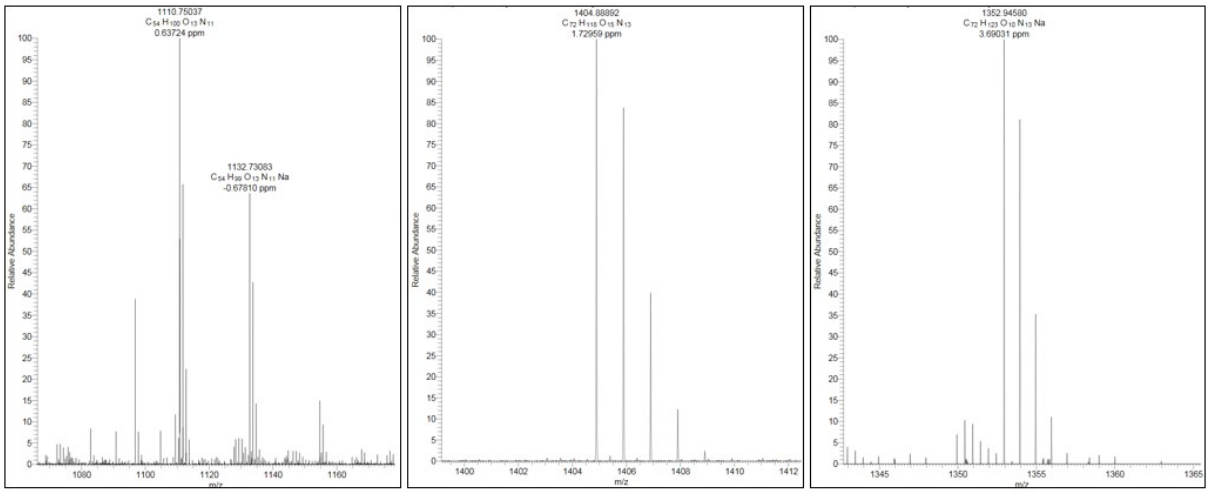


Figure S5. HPLC profile of crude OPA-**1** (purity 85.7%).



OPA-**1** OPA-**2** OPA-**4**

Figure S6. Mass spectra of OPAs.

1.2. FT-IR and CD of self-assembly OPAs

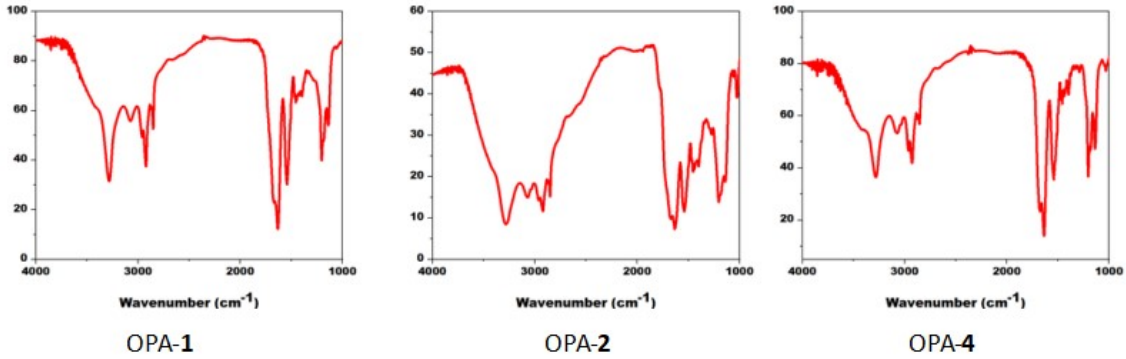


Figure S7. FT-IR spectra of freeze-dried OPAs nanofibers.

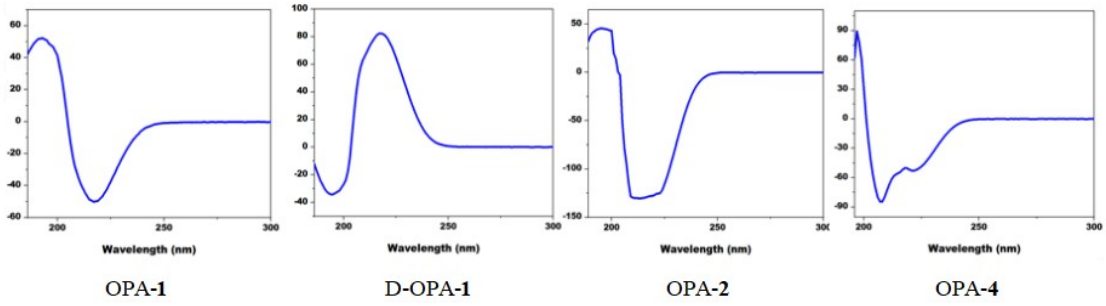


Figure S8. CD spectra of self-assembly OPAs.

1.3. ^{2}H NMR spectra of CD_3OD in self-assembly media.

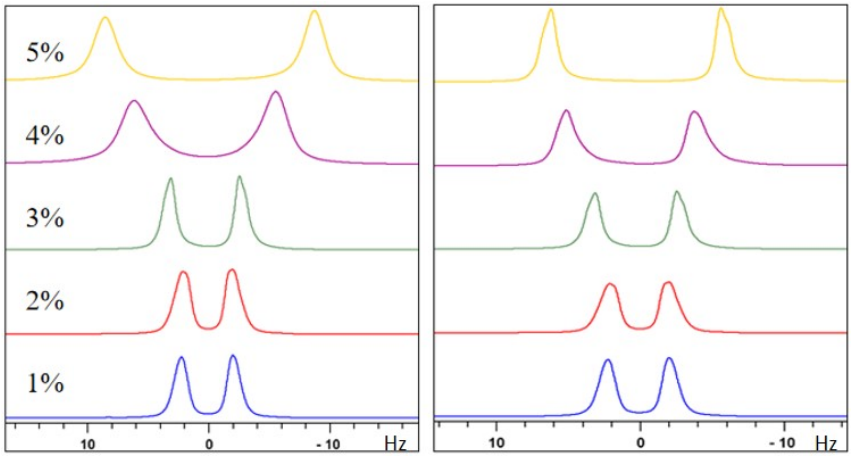
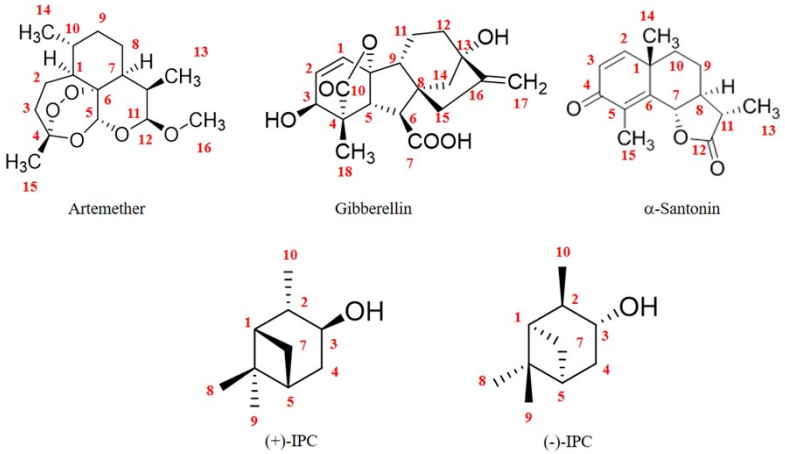


Figure S9. 1D ^{2}H NMR spectra (-CD_3) of the OPA-**1** (left) and OPA-**2** (right) phase at different concentrations.

2. NMR assignment of compounds

2.1. The atom numbers of compounds



2.2. ^{1}H NMR spectra of analytes in isotropic and anisotropic media

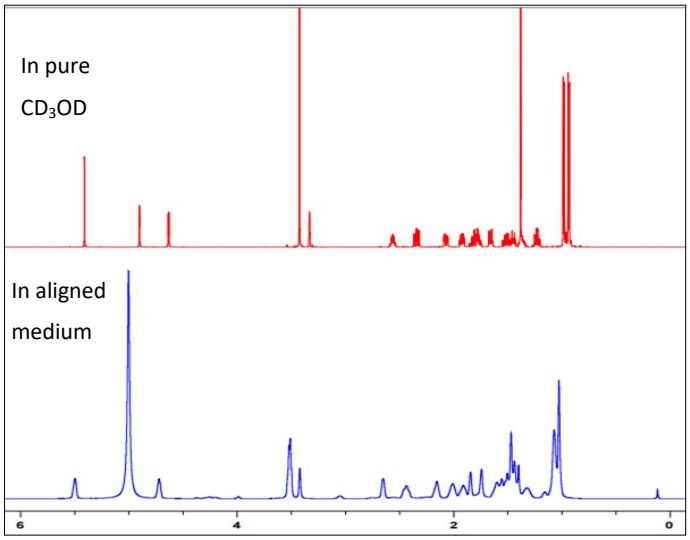


Figure S10. ^{1}H NMR spectra of 10 mg artemether under pure CD_3OD and aligned OPA-**1** medium (5%).

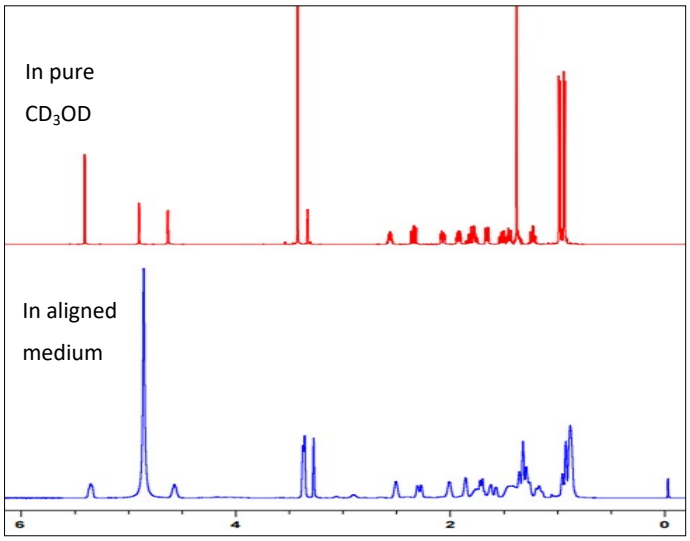


Figure S11. ^{1}H NMR spectra of 10mg artemether under pure CD_3OD and aligned OPA-**2** medium (5%).

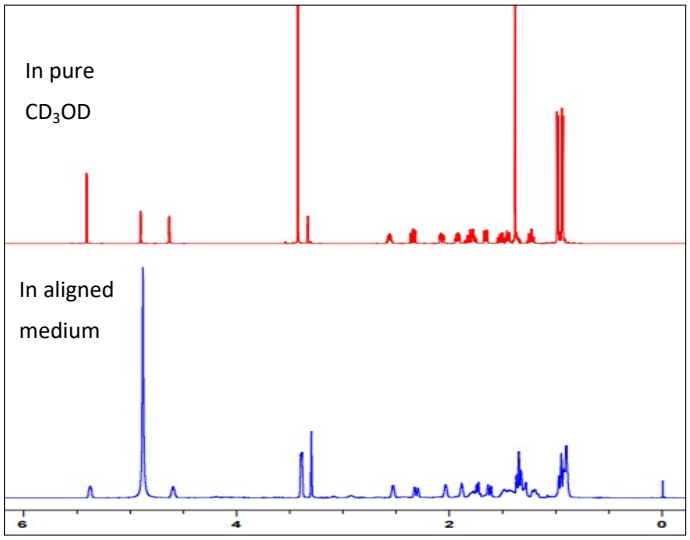


Figure S12. ^{1}H NMR spectra of 10mg artemether under pure CD_3OD and aligned OPA-**2** medium (2%).

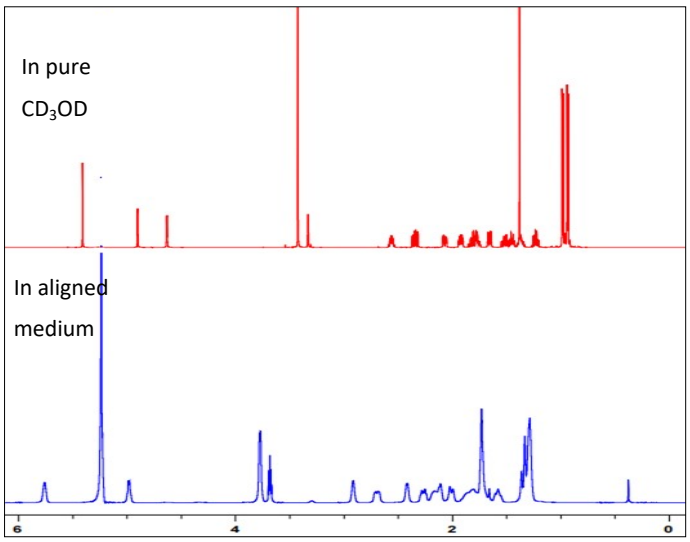


Figure S13. ^{1}H NMR spectra of 10mg artemether under pure CD_3OD and aligned OPA-**3** medium (5%).

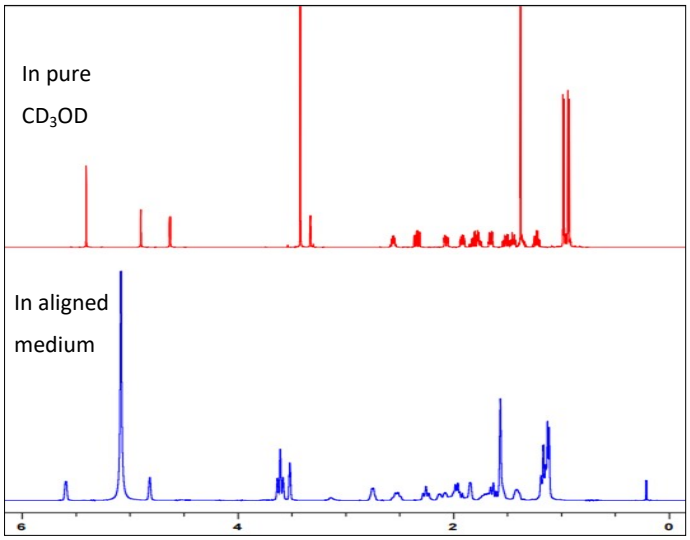


Figure S14. ^{1}H NMR spectra of 10 mg artemether under pure CD_3OD and aligned OPA-**4** medium (5%).

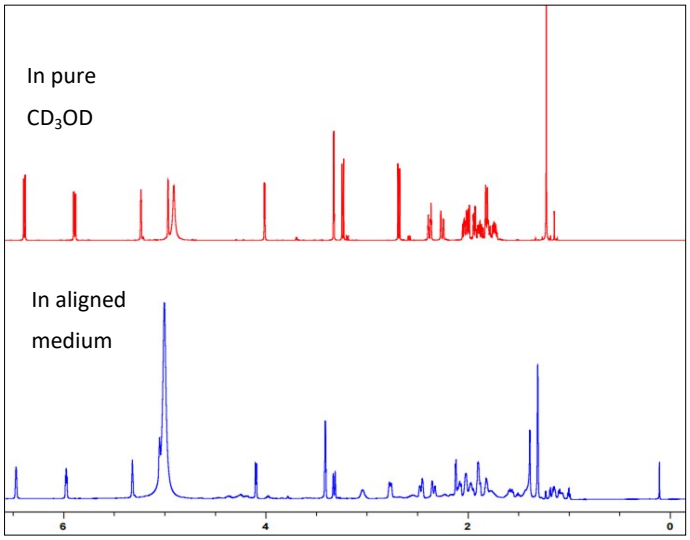


Figure S15. ^{1}H NMR spectra of 10 mg gibberellin under pure CD_3OD and aligned OPA-**1** medium (5%).

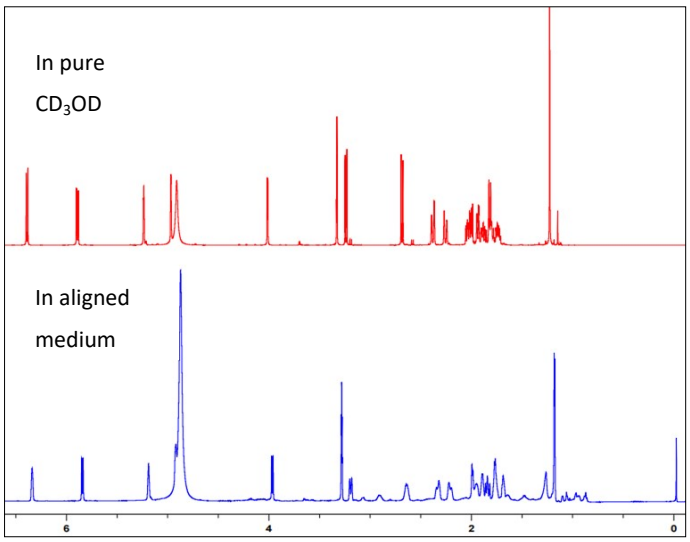


Figure S16. ^{1}H NMR spectra of 10 mg gibberellin under pure CD_3OD and aligned OPA-**2** medium (5%).

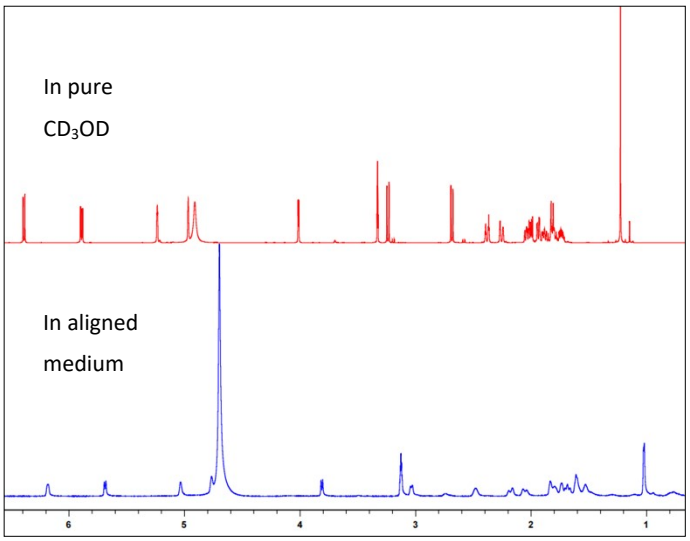


Figure S17. ^{1}H NMR spectra of 10 mg gibberellin under pure CD_3OD and aligned OPA-**3** medium (5%).

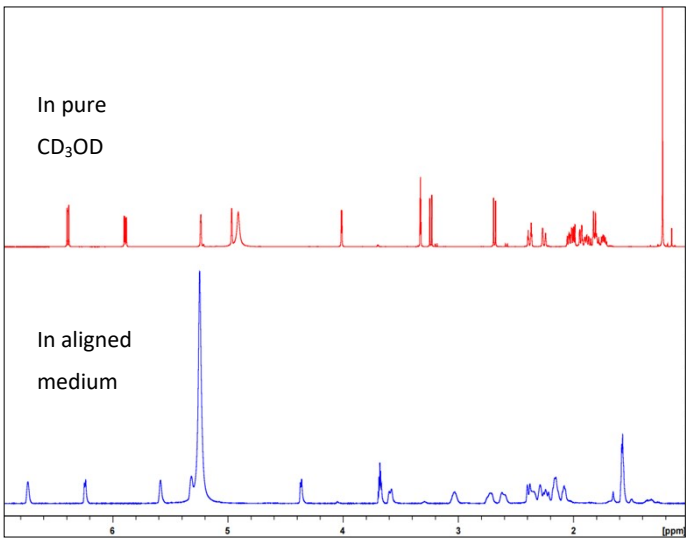


Figure S18. ^{1}H NMR spectra of 10 mg gibberellin under pure CD_3OD and aligned OPA-**4** medium (5%).

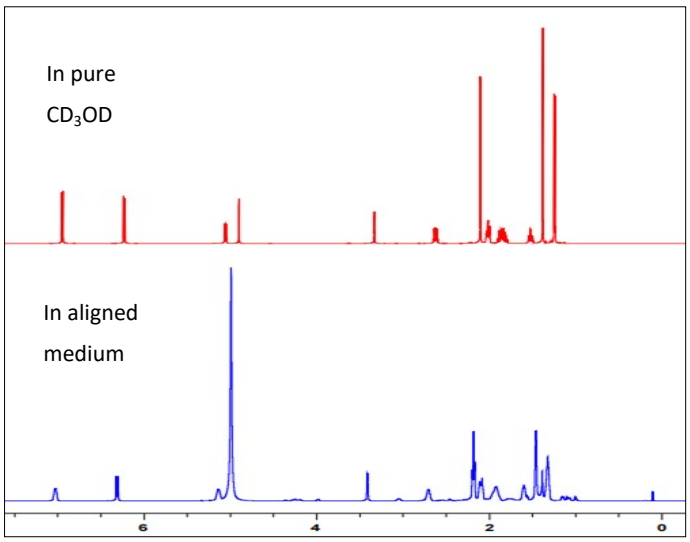


Figure S19. ^{1}H NMR spectra of 10 mg α-santonin under pure CD_3OD and aligned OPA-**1** medium (5%).

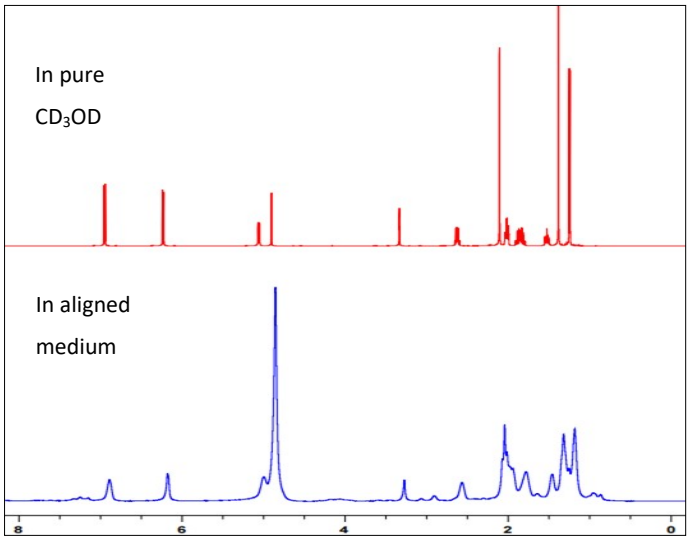


Figure S20. ^{1}H NMR spectra of 10 mg α-santonin under pure CD_3OD and aligned OPA-**2** medium (5%).

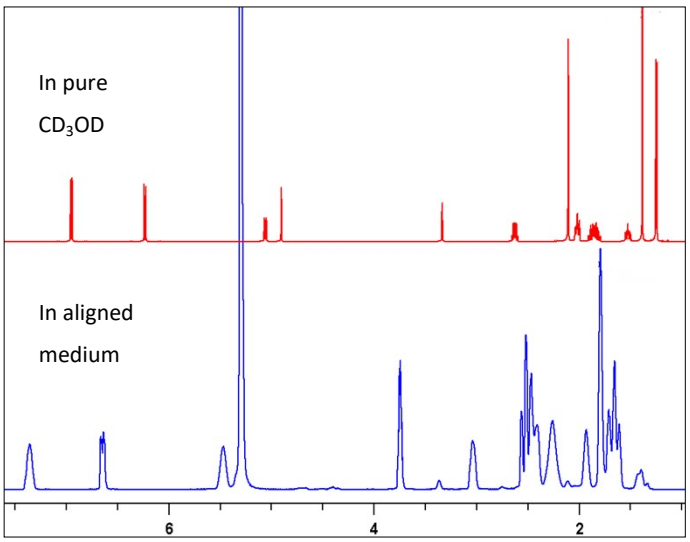


Figure S21. ^{1}H NMR spectra of 10 mg α-santonin under pure CD_3OD and aligned OPA-**3** medium (5%).

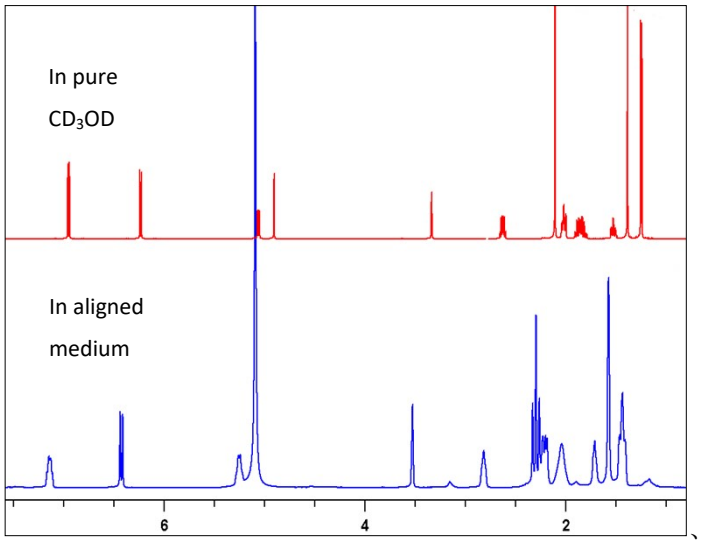


Figure S22. ^{1}H NMR spectra of 10 mg α-santonin under pure CD_3OD and aligned OPA-**4** medium (5%).

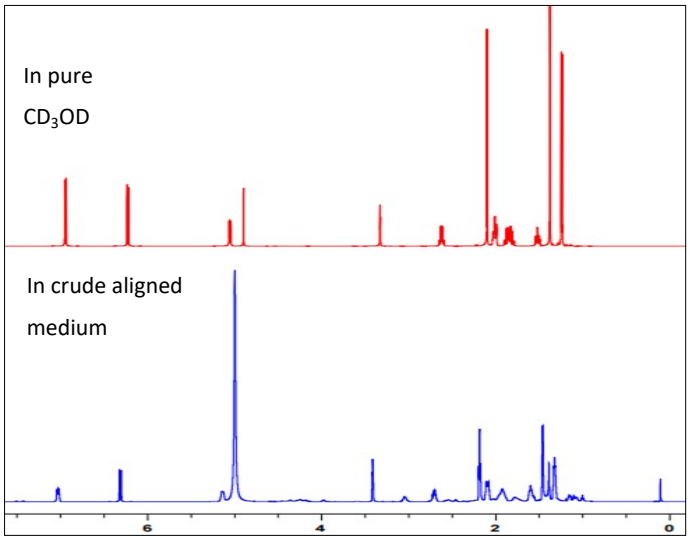


Figure S23. ^{1}H NMR spectra of 10 mg α-santonin under pure CD_3OD and crude aligned OPA-**1** medium (5%).

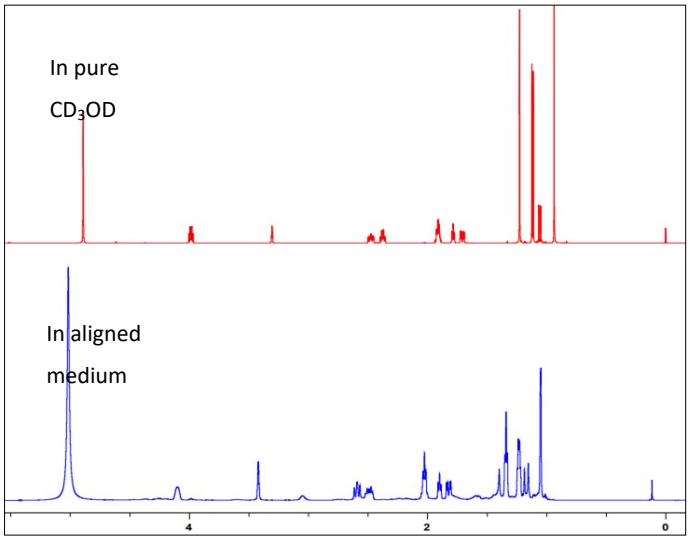


Figure S24. ^{1}H NMR spectra of 10 mg (+)-IPC under pure CD_3OD and aligned OPA-**1** medium (5%).

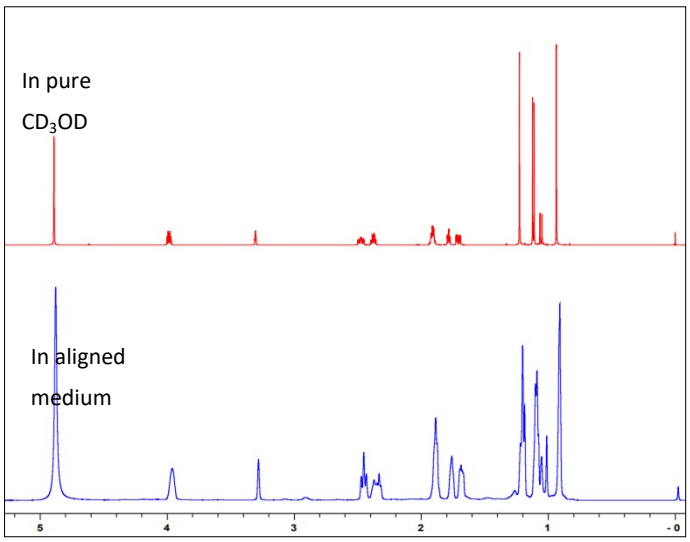


Figure S25. ^{1}H NMR spectra of 10 mg (+)-IPC under pure CD_3OD and aligned OPA-**2** medium (5%).

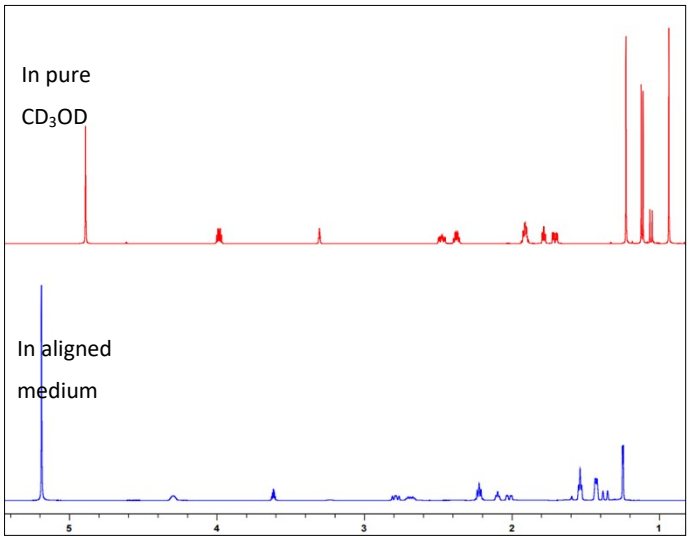


Figure S26. ^{1}H NMR spectra of 10 mg (+)-IPC under pure CD_3OD and aligned OPA-**3** medium (5%).

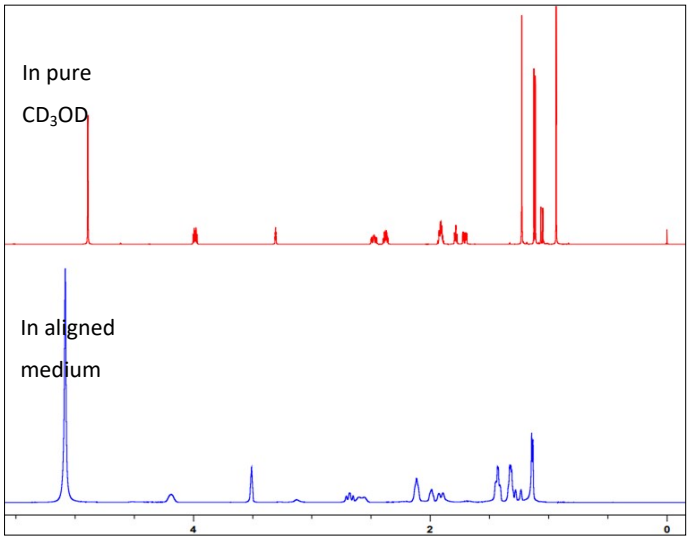


Figure S27. ^{1}H NMR spectra of 10 mg (+)-IPC under pure CD_3OD and aligned OPA-**4** medium (5%).

2.3. ^{2}H NMR spectra of CD_3OD in aligned media with different analytes.

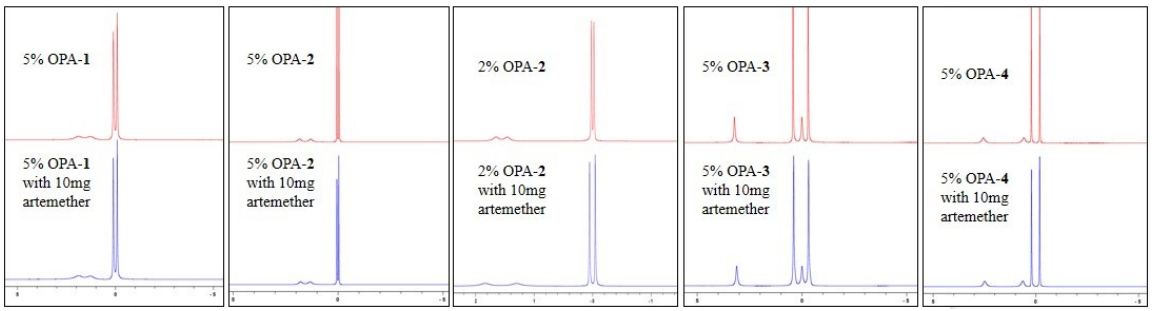


Figure S28. ^{2}H NMR spectra of CD_3OD in aligned media with 10 mg artemether.

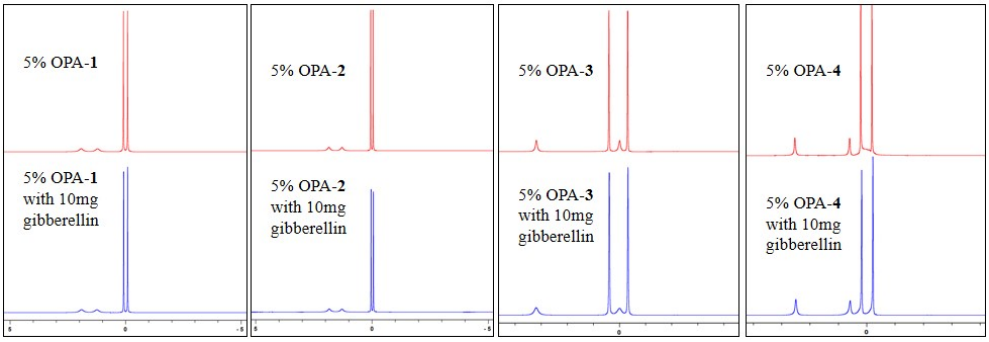


Figure S29. ^{2}H NMR spectra of CD_3OD in aligned media with 10 mg gibberellin.

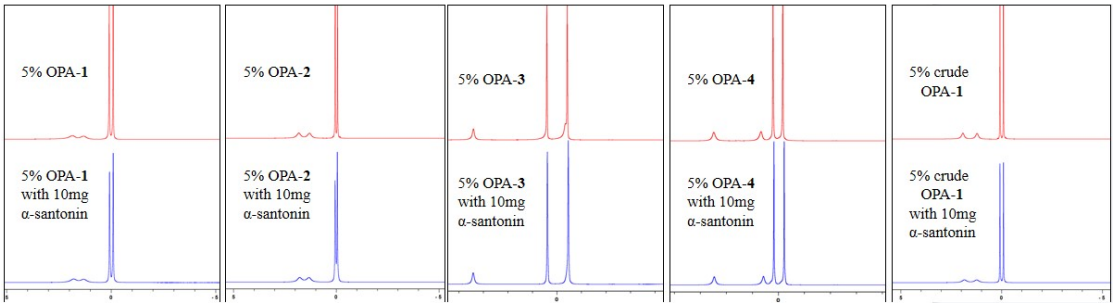


Figure S30. ^{2}H NMR spectra of CD_3OD in aligned media with 10 mg α-santonin.

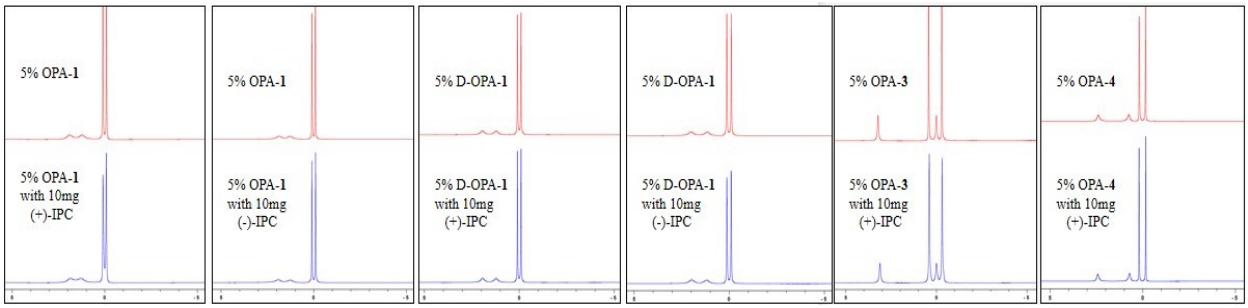


Figure S31. ^{2}H NMR spectra of CD_3OD in aligned media with 10 mg IPC.

3. Alignment of compounds in aligned media and RDC analysis

3.1. Data analysis of artemether

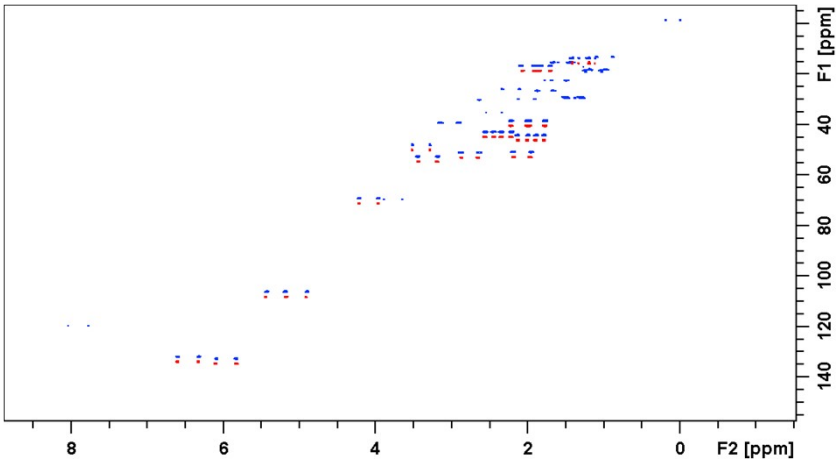


Figure S32. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10 mg artemether in the isotropic phase (red contours) and 5% aligned OPA-**1** /CD_3OD medium (anisotropic, blue contours).

Table S1. The one bond scalar ($^{1}J_{CH}$), total couplings ($^{1}T_{CH}$), residual dipolar couplings ($^{1}D_{CH}$) values and calculated ones of 10 mg artemether in 5% OPA-**1** aligned medium.

Atom number	$^{1}J_{CH}$	$^{1}T_{CH}$	$^{1}D_{CH}$	$^{1}D_{CH}$ Calculation
C1H1	126.0	146.7	20.7	21.0
C3H3a	126.6	130.2	3.6	3.9
C3H3b	128.5	148.7	20.2	21.9
C5H5	168.0	170.0	2.0	0.8
C7H7	128.2	150.6	22.4	20.7
C9H9a	128.1	113.1	-15.0	-14.0
C9H9b	123.3	143.0	19.7	20.2
C11H11	127.2	121.4	-5.8	-6.0
C12H12	165.0	153.4	-11.6	-11.2
C13H13(Me)	126.3	126.7	0.4	0.5

C14H14(Me)	125.1	127.3	2.2	2.3
C15H15(Me)	128.9	136.3	7.4	6.4

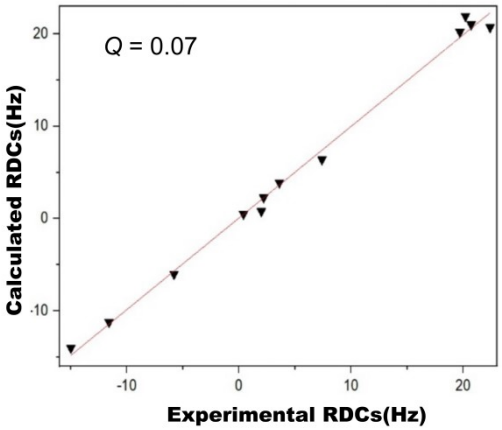


Figure S33. Correlations between the experimental and calculated $^{1}D_{CH}$ values of 10 mg artemether in 5% OPA-**1** aligned medium.

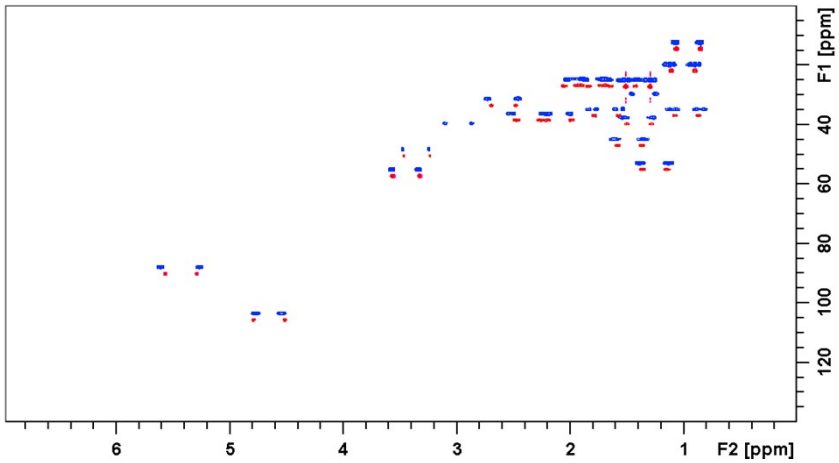


Figure S34. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10mg artemether in the isotropic phase (red contours) and 5% aligned OPA-**2** /CD_3OD medium (anisotropic, blue contours).

Table S2. The one bond scalar ($^{1}J_{CH}$), total couplings ($^{1}T_{CH}$), residual dipolar couplings ($^{1}D_{CH}$) values and calculated ones of 10mg artemether in 5% OPA-**2** aligned medium.

Atom number	$^{1}J_{CH}$	$^{1}T_{CH}$	$^{1}D_{CH}$	$^{1}D_{CH}$ Calculation
C1H1	126.0	150.2	24.2	23.2
C3H3a	126.6	124.7	-1.9	-2.4
C3H3b	128.5	168.4	39.9	40.6
C5H5	168.0	200.0	32.0	32.4
C7H7	128.2	150.2	22.0	21.9
C9H9a	128.1	135.7	7.6	9.6
C9H9b	123.3	143.0	19.7	20.2

C11H11	127.2	154.1	26.9	24.1
C12H12	165.0	139.3	-25.7	-26.2
C13H13(Me)	126.3	130.2	3.9	2.3
C14H14(Me)	125.1	132.3	7.2	8.4
C15H15(Me)	128.9	135.7	6.8	9.9

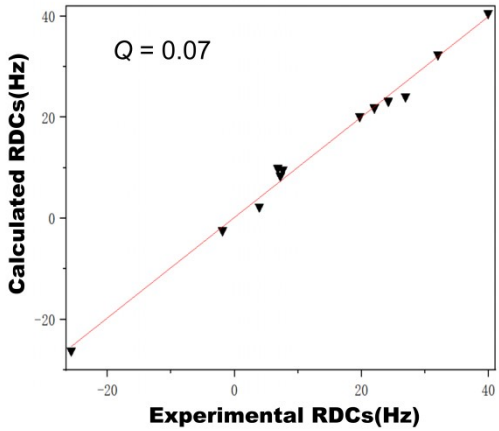


Figure S35. Correlations between the experimental and calculated $^{1}D_{CH}$ values of 10 mg artemether in 5% OPA-**2** aligned medium.

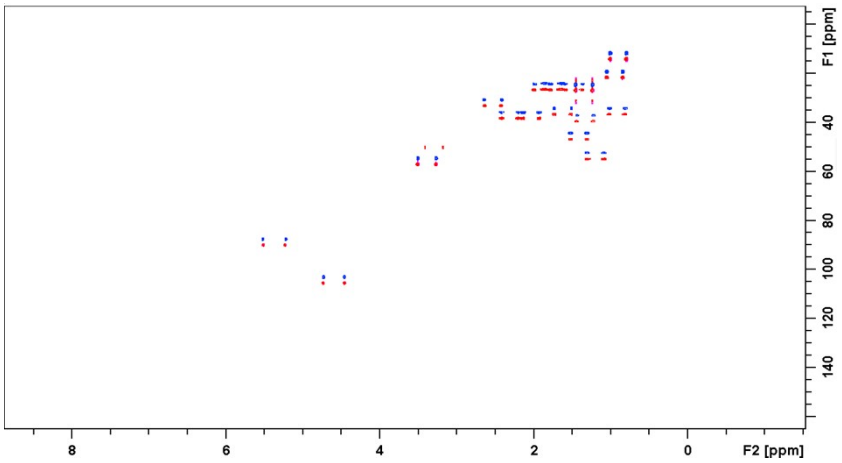


Figure S36. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10 mg artemether in the isotropic phase (red contours) and 2% aligned OPA-**2** /CD_3OD medium (anisotropic, blue contours).

Table S3. The one bond scalar ($^{1}J_{CH}$), total couplings ($^{1}T_{CH}$), residual dipolar couplings ($^{1}D_{CH}$) values and calculated ones of 10 mg artemether in 2% OPA-**2** aligned medium.

Atom number	$^{1}J_{CH}$	$^{1}T_{CH}$	$^{1}D_{CH}$	$^{1}D_{CH}$ Calculation
C1H1	126.0	148.3	22.3	19.7
C3H3a	126.6	117.9	-8.7	-8.4
C3H3b	128.5	157.5	29.0	30.6
C5H5	168.0	191.8	23.8	22.8
C7H7	128.2	146.4	18.2	18.8

C9H9a	128.1	134.2	6.1	7.5
C9H9b	123.3	139.9	16.6	17.8
C11H11	127.2	145.5	18.3	17.6
C12H12	165.0	147.5	-17.5	-17.3
C13H13(Me)	126.3	129.2	2.9	3.4
C14H14(Me)	125.1	130.8	5.7	5.4
C15H15(Me)	128.9	134.8	5.9	6.6

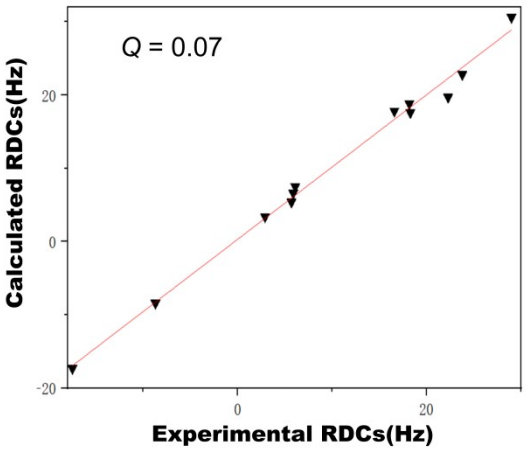


Figure S37. Correlations between the experimental and calculated $^{1}D_{CH}$ values of 10 mg artemether in 2% OPA-**2** aligned medium.

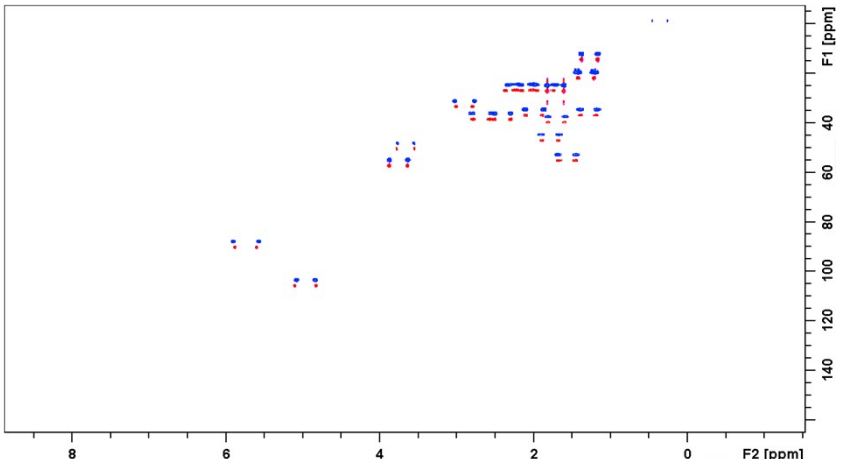


Figure S38. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10 mg artemether in the isotropic phase (red contours) and 5% aligned OPA-**3** /CD_3OD medium (anisotropic, blue contours).

Table S4. The one bond scalar ($^{1}J_{CH}$), total couplings ($^{1}T_{CH}$), residual dipolar couplings ($^{1}D_{CH}$) values and calculated ones of 10 mg artemether in 5% OPA-**3** aligned medium.

Atom number	$^{1}J_{CH}$	$^{1}T_{CH}$	$^{1}D_{CH}$	$^{1}D_{CH}$ Calculation
C1H1	126.0	115.2	-10.8	-11.5
C3H3a	126.6	124.9	-1.7	-1.0

C3H3b	128.5	134.9	6.4	6.3
C5H5	168.0	198.0	30.0	29.1
C7H7	128.2	116.4	-11.8	-12.5
C9H9a	128.1	154.2	26.1	25.8
C9H9b	123.3	107.5	-15.8	-13.7
C11H11	127.2	155.3	28.1	29.9
C12H12	165.0	154.6	-10.4	-9.8
C13H13(Me)	126.3	125.6	-0.7	-0.6
C14H14(Me)	125.1	130.6	5.5	4.4
C15H15(Me)	128.9	131.5	2.6	2.9

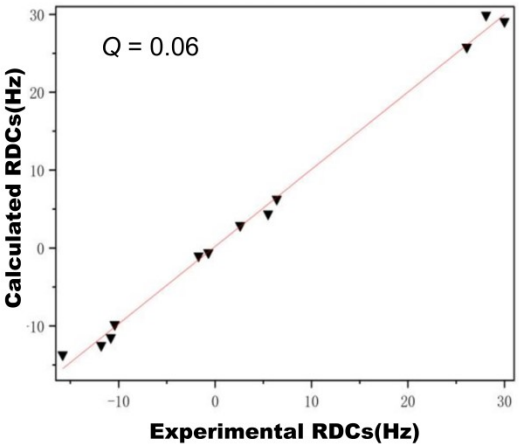


Figure S39. Correlations between the experimental and calculated $^{1}D_{CH}$ values of 10 mg artemether in 5% OPA-**3** aligned medium.

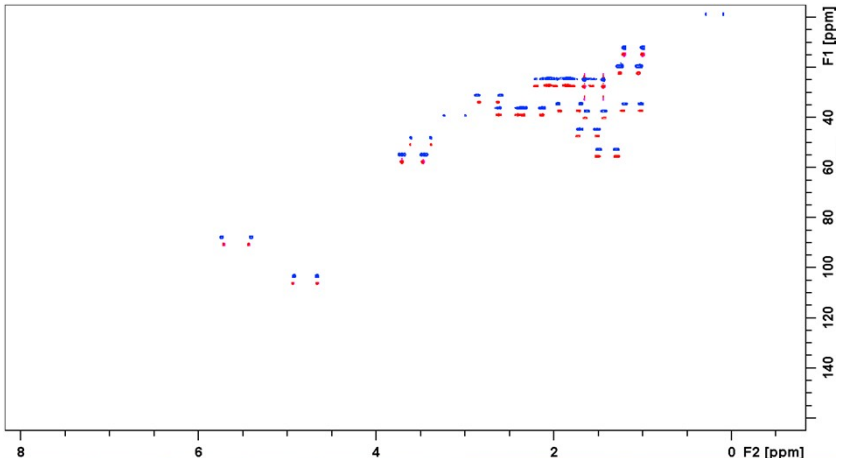


Figure S40. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10 mg artemether in the isotropic phase (red contours) and 5% aligned OPA-**4** /CD_3OD medium (anisotropic, blue contours).

Table S5. The one bond scalar ($^{1}J_{CH}$), total couplings ($^{1}T_{CH}$), residual dipolar couplings ($^{1}D_{CH}$) values and calculated ones of 10 mg artemether in 5% OPA-**4** aligned medium.

Atom number	$^1J_{CH}$	$^1T_{CH}$	$^1D_{CH}$	$^1D_{CH}$ Calculation
C1H1	126.0	144.3	18.3	15.9
C3H3a	126.6	123.0	-3.6	-3.6
C3H3b	128.5	154.3	25.8	27.6
C5H5	168.0	199.2	31.2	30.5
C7H7	128.2	142.7	14.5	15.1
C9H9a	128.1	144.7	16.6	18.0
C9H9b	123.3	136.6	13.3	13.8
C11H11	127.2	152.8	25.6	24.3
C12H12	165.0	146.7	-18.3	-18.3
C13H13(Me)	126.3	128.9	2.6	3.1
C14H14(Me)	125.1	133.3	8.2	8.3
C15H15(Me)	128.9	130.9	2.0	1.9

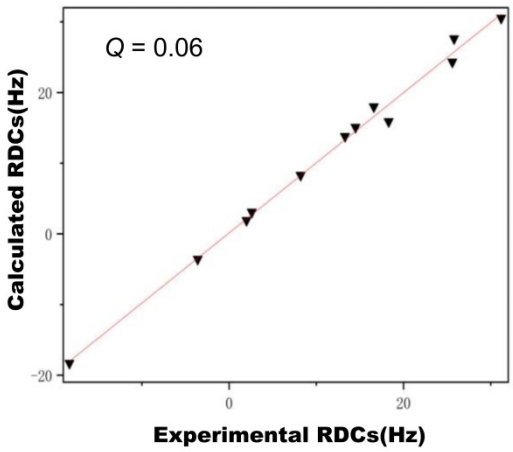


Figure S41. Correlations between the experimental and calculated $^1D_{CH}$ values of 10 mg artemether in 5% OPA-**4** aligned medium.

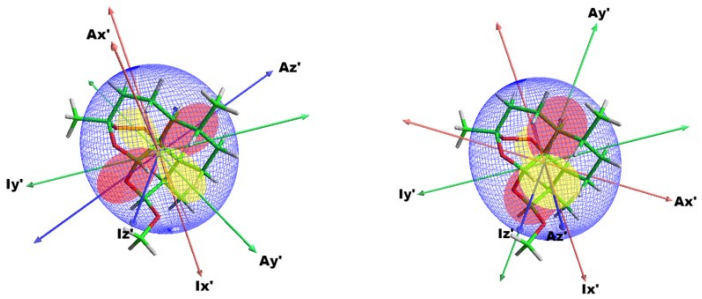


Figure S42. Inertia tensor (I) and alignment tensor (A) of artemether in OPA-**3** (left) and OPA-**4** (right).

3.2. Data analysis of gibberellin

Figure S43. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10 mg gibberellin in the isotropic phase (red contours) and 5% aligned OPA-**1** /CD_3OD medium (anisotropic, blue contours).

Table S6. The one bond scalar ($^{1}J_{CH}$), total couplings ($^{1}T_{CH}$), residual dipolar couplings ($^{1}D_{CH}$) values and calculated ones of 10 mg gibberellin in 5% OPA-**1** aligned medium.

Atom number	$^{1}J_{CH}$	$^{1}T_{CH}$	$^{1}D_{CH}$	$^{1}D_{CH}$ Calculation
C2H2	164.5	157.0	-7.5	-6.3
C3H3	147.1	150.6	3.5	2.9
C5H5	142.3	158.0	15.7	14.7
C6H6	129.8	145.4	15.6	16.3
C9H9	127.6	142.1	14.5	15.0
C12H12a	127.4	136.6	9.2	9.2
C12H12b	127.3	131.9	4.6	4.1
C14H14a	134.7	149.8	15.1	15.6
C14H14b	130.9	128.5	-2.4	-2.5
C15H15a	128.0	126.7	-1.3	-1.4
C15H15b	139.4	145.3	5.9	4.9
C17H17a	158.7	144.9	-13.8	-12.8
C17H17b	158.8	172.5	13.7	14.9
C18H18(Me)	128.2	129.6	1.4	1.4

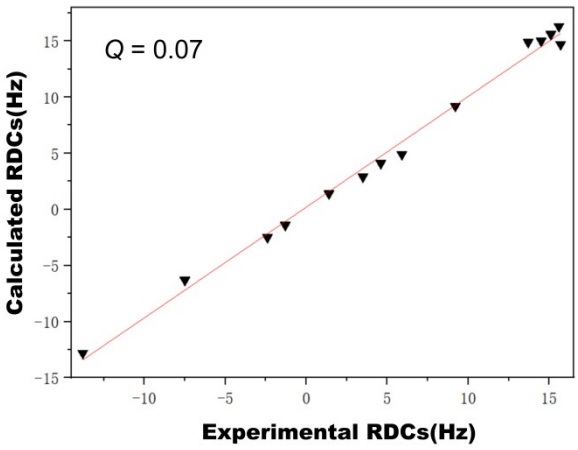


Figure S44. Correlations between the experimental and calculated $^{1}D_{CH}$ values of 10 mg gibberellin in 5% OPA-**1** aligned medium.

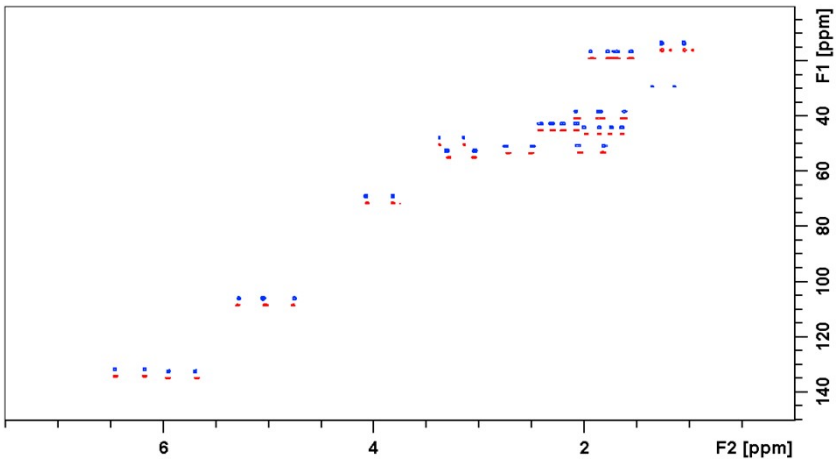


Figure S45. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10 mg gibberellin in the isotropic phase (red contours) and 5% aligned OPA-**2** /CD_3OD medium (anisotropic, blue contours).

Table S7. The one bond scalar ($^{1}J_{CH}$), total couplings ($^{1}T_{CH}$), residual dipolar couplings ($^{1}D_{CH}$) values and calculated ones of gibberellin in OPA-**2** aligned medium.

Atom number	$^{1}J_{CH}$	$^{1}T_{CH}$	$^{1}D_{CH}$	$^{1}D_{CH}$ Calculation
C2H2	164.5	153.0	-11.5	-11.5
C3H3	147.1	152.8	5.7	4.3
C5H5	142.3	160.7	18.4	18.7
C6H6	129.8	154.1	24.3	22.3
C9H9	127.6	147.7	20.1	21.1
C12H12a	127.4	142.9	15.5	15.5
C12H12b	127.3	130.1	2.8	2.2
C14H14a	134.7	156.6	21.9	23.6
C14H14b	130.9	131.9	1.0	1.1
C15H15a	128.0	133.1	5.1	4.1

C15H15b	139.4	141.2	1.8	1.8
C17H17a	158.7	136.9	-21.8	-21.9
C17H17b	158.8	180.0	21.2	20.6
C18H18(Me)	128.2	128.4	0.2	0.1

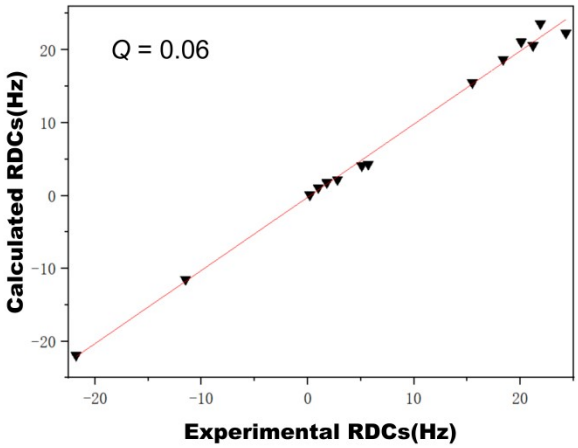


Figure S46. Correlations between the experimental and calculated $^{1}D_{CH}$ values of 10 mg gibberellin in 5% OPA-**2** aligned medium.

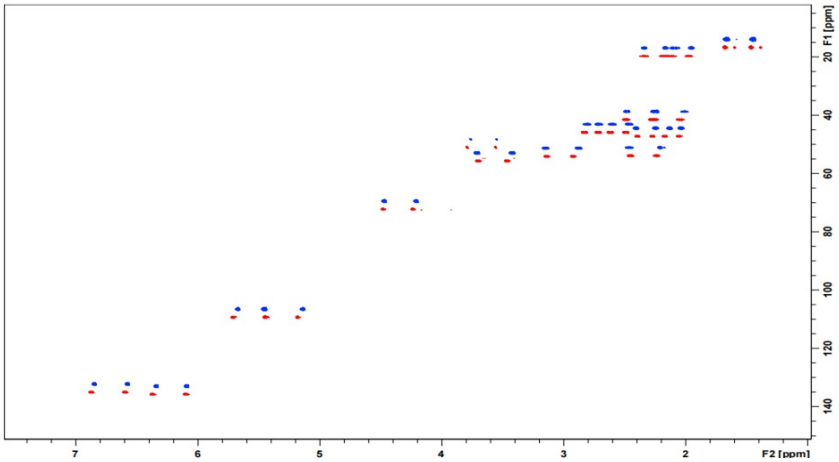


Figure S47. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10 mg gibberellin in the isotropic phase (red contours) and 5% aligned OPA-**3** /CD_3OD medium (anisotropic, blue contours).

Table S8. The one bond scalar ($^{1}J_{CH}$), total couplings ($^{1}T_{CH}$), residual dipolar couplings ($^{1}D_{CH}$) values and calculated ones of gibberellin in OPA-**3** aligned medium.

Atom number	$^{1}J_{CH}$	$^{1}T_{CH}$	$^{1}D_{CH}$	$^{1}D_{CH}$ Calculation
C2H2	164.5	151.2	-13.3	-11.8
C3H3	147.1	154.3	7.2	6.6
C5H5	142.3	172.6	30.3	29.4
C6H6	129.8	162.5	32.7	29.7
C9H9	127.6	152.1	24.5	26.2
C12H12a	127.4	138.8	11.4	12.6

C12H12b	127.3	138.4	11.1	11.2
C14H14a	134.7	164.9	30.2	31.2
C14H14b	130.9	124.7	-6.2	-6.9
C15H15a	128.0	123.0	-5.0	-5.0
C15H15b	139.4	150.0	10.6	10.1
C17H17a	158.7	136.2	-22.5	-22.1
C17H17b	158.8	187.8	29.0	30.7
C18H18(Me)	128.2	131.0	2.8	4.1

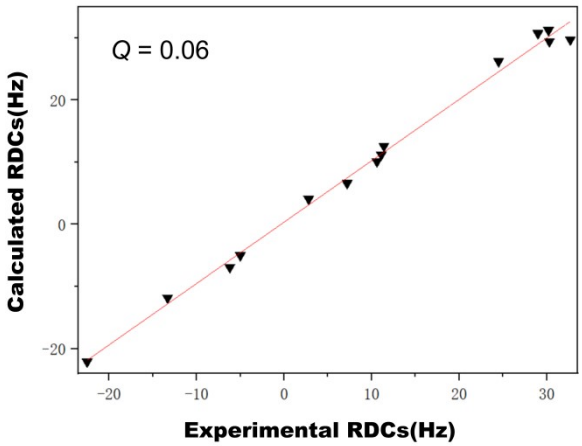


Figure S48. Correlations between the experimental and calculated $^{1}D_{CH}$ values of 10 mg gibberellin in 5% OPA-**3** aligned medium.

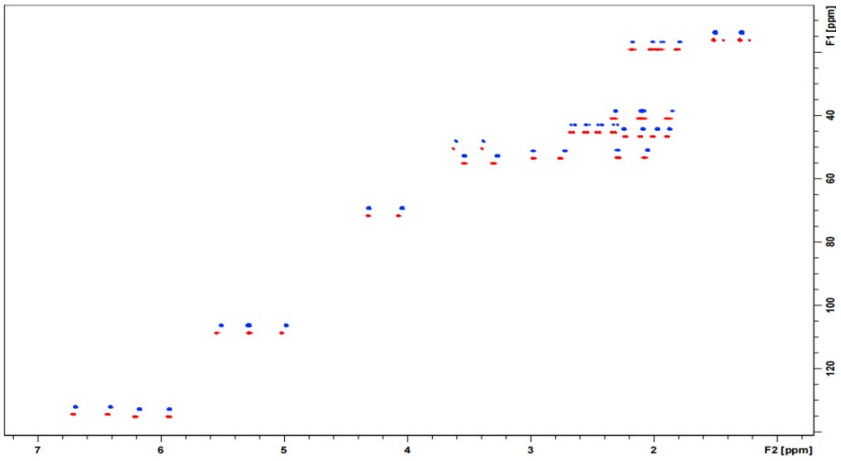


Figure S49. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10 mg gibberellin in the isotropic phase (red contours) and 5% aligned OPA-**4** /CD_3OD medium (anisotropic, blue contours).

Table S9. The one bond scalar ($^{1}J_{CH}$), total couplings ($^{1}T_{CH}$), residual dipolar couplings ($^{1}D_{CH}$) values and calculated ones of gibberellin in OPA-**4** aligned medium.

Atom number	$^{1}J_{CH}$	$^{1}T_{CH}$	$^{1}D_{CH}$	$^{1}D_{CH}$ Calculation
C2H2	164.5	146.2	-18.3	-17.9
C3H3	147.1	159.4	12.3	10.7

C5H5	142.3	160.3	18.0	18.3
C6H6	129.8	155.1	25.3	26.4
C9H9	127.6	151.9	24.3	26.0
C12H12a	127.4	153.5	26.1	24.2
C12H12b	127.3	124.4	-2.9	-3.5
C14H14a	134.7	162.0	27.3	28.2
C14H14b	130.9	129.8	-1.1	-0.8
C15H15a	128.0	132.5	4.5	3.3
C15H15b	139.4	138.0	-1.4	-3.4
C17H17a	158.7	132.4	-26.3	-25.9
C17H17b	158.8	180.8	22.0	20.6
C18H18(Me)	128.2	127.2	-1.0	-1.1

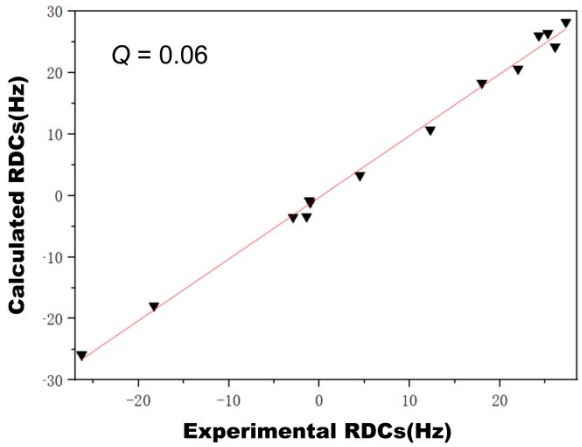


Figure S50. Correlations between the experimental and calculated $^{1}D_{CH}$ values of 10 mg gibberellin in 5% OPA-**4** aligned medium.

Table S10. The β angle and ratio of GDO between four kinds of aligned media for gibberellin

Ratio of GDO / β-angle	OPA-**1**	OPA-**2**	OPA-**3**	OPA-**4**
OPA-**1**	_	G**2** /G**1** = 1.62	G**3** /G**1** = 1.82	G**4** /G**1** = 2.01
OPA-**2**	15.0	_	G**3** /G**2** = 1.21	G**4** /G**2** = 1.24
OPA-**3**	9.7	22.3	_	G**4** /G**3** = 1.11
OPA-**4**	23.7	13.6	31.2	_

3.3. Data analysis of α-santonin

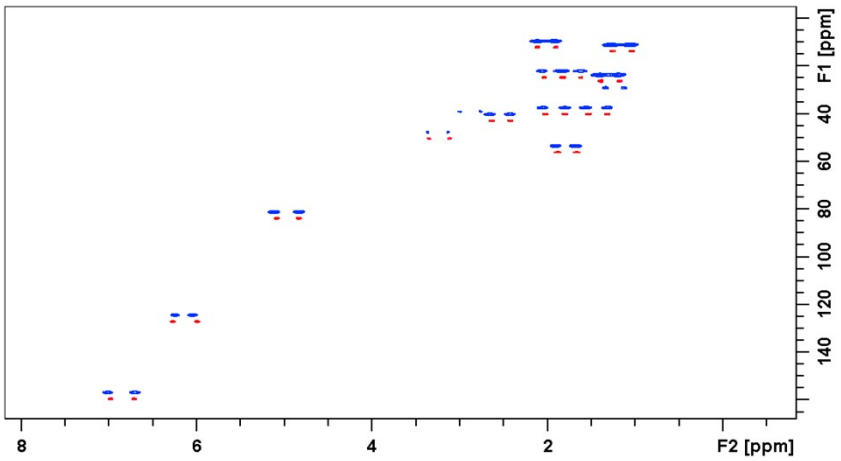


Figure S51. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10 mg α-santonin in the isotropic phase (red contours) and 5% aligned OPA-**1** /CD_3OD medium (anisotropic, blue contours).

Table S11. The one bond scalar ($^{1}J_{CH}$), total couplings ($^{1}T_{CH}$), residual dipolar couplings ($^{1}D_{CH}$) values and calculated ones of 10 mg α-santonin in 5% OPA-**1** aligned medium.

Atom number	$^{1}J_{CH}$	$^{1}T_{CH}$	$^{1}D_{CH}$	$^{1}D_{CH}$ Calculation
C2H2	161.3	173.3	12.0	12.0
C3H3	165.3	145.5	-19.8	-19.8
C7H7	149.1	155.6	6.5	6.6
C8H8	130.1	137.5	7.4	7.9
C10H10a	131.9	141.2	9.3	9.0
C10H10b	129.3	138.8	9.5	9.5
C11H11	127.5	134.7	7.2	6.9
C13H13(Me)	128.3	133.2	4.9	5.4
C14H14(Me)	129.6	128.4	-1.2	-1.2
C15H15(Me)	129.4	124.8	-4.6	-4.6

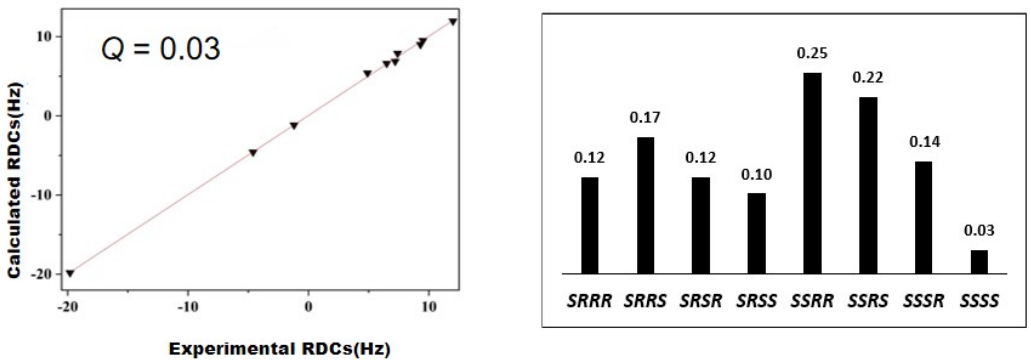


Figure S52. Correlations between the experimental and calculated $^{1}D_{CH}$ values of a-santonin and *Q* factors of the RDCs for the eight possible diastereomeric configurations of a-santonin in OPA-**1** aligned medium.

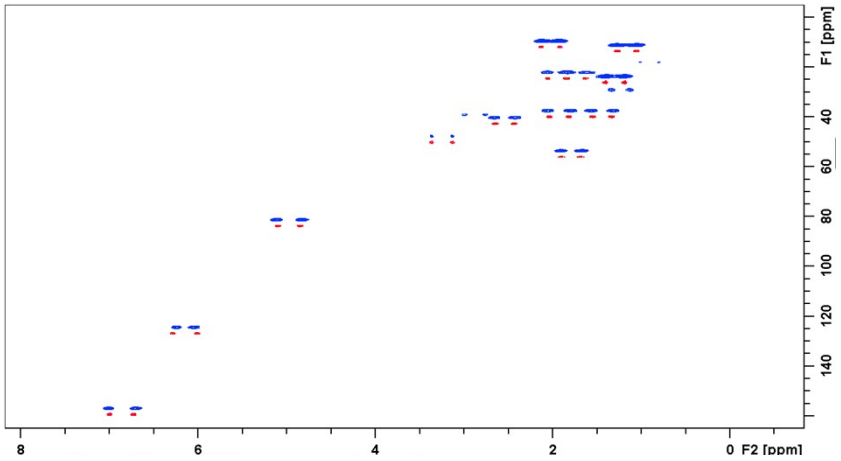


Figure S53. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10mg a-santonin in the isotropic phase (red contours) and 5% aligned OPA-**2** /CD_3OD medium (anisotropic, blue contours).

Table S12. The one bond scalar ($^{1}J_{CH}$), total couplings ($^{1}T_{CH}$), residual dipolar couplings ($^{1}D_{CH}$) values and calculated ones of a-santonin in OPA-**2** aligned medium.

Atom number	$^{1}J_{CH}$	$^{1}T_{CH}$	$^{1}D_{CH}$	$^{1}D_{CH}$ Calculation
C2H2	161.3	177.8	16.5	16.0
C3H3	165.3	122.4	-42.9	-42.9
C7H7	149.1	167.3	18.2	18.1
C8H8	130.1	145.4	15.3	14.8
C10H10a	131.9	144.4	12.5	13.1
C10H10b	129.3	150.5	21.2	21.7
C11H11	127.5	144.0	16.5	16.5
C13H13(Me)	128.3	131.9	3.6	4.5
C14H1a(Me)	129.6	124.5	-5.1	-5.0
C15H15(Me)	129.4	121.6	-7.8	-7.7

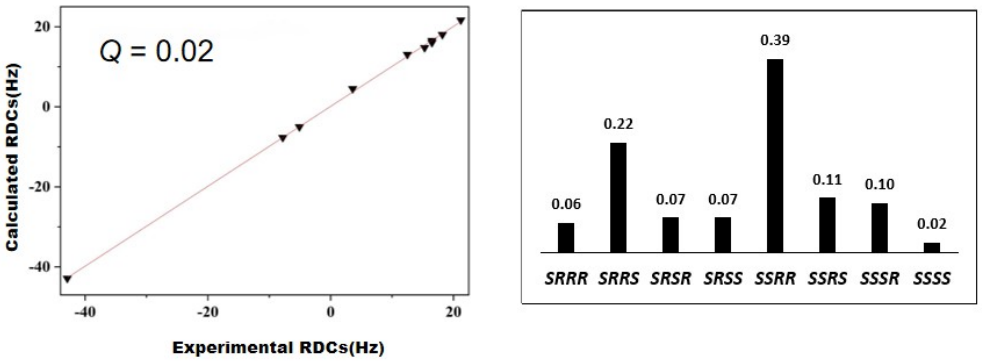


Figure S54. Correlations between the experimental and calculated $^{1}D_{CH}$ values of a-santonin and *Q* factors of the RDCs for the eight possible diastereomeric configurations of a-santonin in OPA-**2** aligned medium.

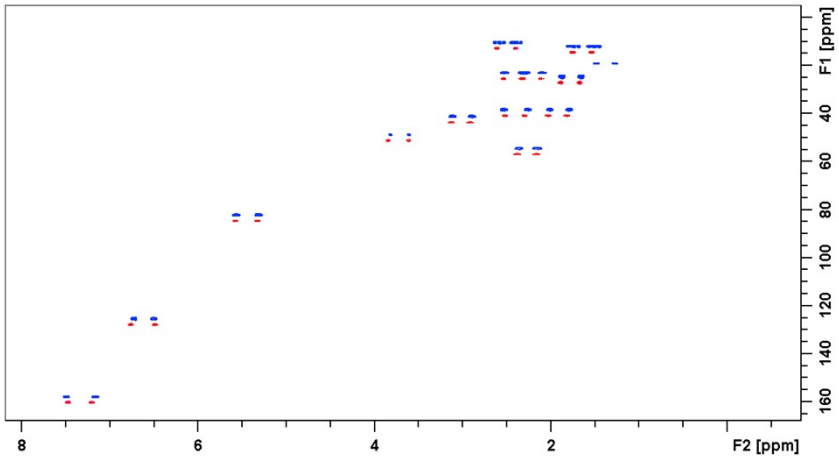


Figure S55. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10mg a-santonin in the isotropic phase (red contours) and 5% aligned OPA-**3** /CD_3OD medium (anisotropic, blue contours).

Table S13. The one bond scalar ($^{1}J_{CH}$), total couplings ($^{1}T_{CH}$), residual dipolar couplings ($^{1}D_{CH}$) values and calculated ones of a-santonin in OPA-**3** aligned medium.

Atom number	$^{1}J_{CH}$	$^{1}T_{CH}$	$^{1}D_{CH}$	$^{1}D_{CH}$ Calculation
C2H2	161.3	187.6	26.3	26.6
C3H3	165.3	134.5	-30.8	-30.8
C7H7	149.1	154.8	5.7	6.2
C8H8	130.1	136.8	6.7	6.3
C10H10a	131.9	139.3	7.4	7.3
C10H10b	129.3	153.4	24.1	23.8
C11H11	127.5	132.9	5.4	5.5
C13H13(Me)	128.3	135.7	7.4	7.9
C14H1a(Me)	129.6	128.8	-0.8	-1.1
C15H15(Me)	129.4	119.8	-9.6	-9.5

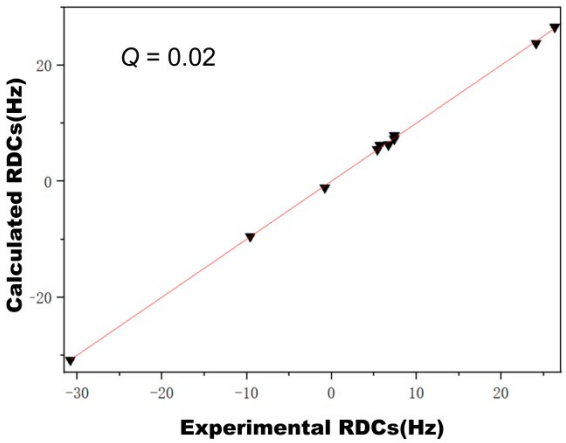


Figure S56. Correlations between the experimental and calculated $^{1}D_{CH}$ values of 10 mg a-santonin in 5% OPA-**3** aligned medium.

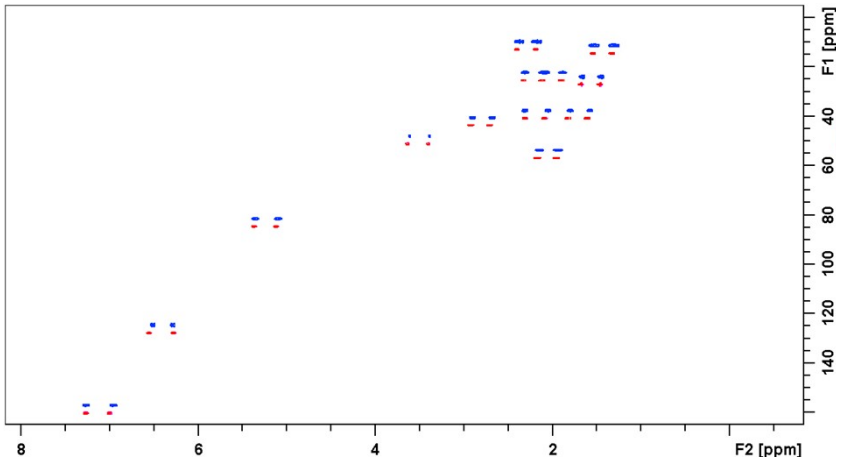


Figure S57. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10mg a-santonin in the isotropic phase (red contours) and 5% aligned OPA-**4** /CD_3OD medium (anisotropic, blue contours).

Table S14. The one bond scalar ($^{1}J_{CH}$), total couplings ($^{1}T_{CH}$), residual dipolar couplings ($^{1}D_{CH}$) values and calculated ones of a-santonin in OPA-**4** aligned medium.

Atom number	$^{1}J_{CH}$	$^{1}T_{CH}$	$^{1}D_{CH}$	$^{1}D_{CH}$ Calculation
C2H2	161.3	196.7	35.4	34.4
C3H3	165.3	136.1	-29.2	-29.2
C7H7	149.1	145.1	-4.0	-4.5
C8H8	130.1	126.7	-3.4	-1.9
C10H10a	131.9	125.9	-6.0	-6.1
C10H10b	129.3	159.8	30.5	31.5
C11H11	127.5	132.9	5.4	4.4
C13H13(Me)	128.3	140.6	12.3	13.6
C14H1a(Me)	129.6	133.1	3.5	4.5
C15H15(Me)	129.4	117.3	-12.1	-12.7

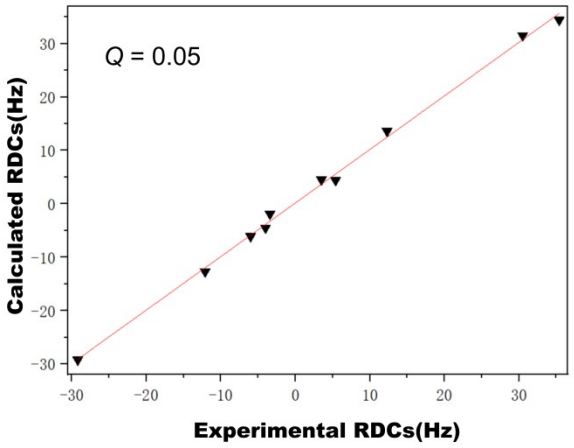


Figure S58. Correlations between the experimental and calculated $^{1}D_{CH}$ values of 10 mg a-santonin in 5% OPA-**4** aligned medium.

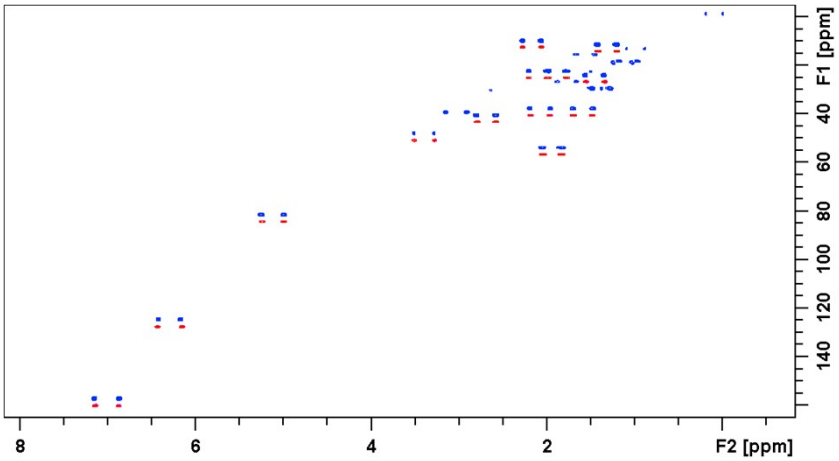


Figure S59. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10mg a-santonin in the isotropic phase (red contours) and 5% aligned crude OPA-**1** /CD_3OD medium (anisotropic, blue contours).

Table S15. The one bond scalar ($^{1}J_{CH}$), total couplings ($^{1}T_{CH}$), residual dipolar couplings ($^{1}D_{CH}$) values and calculated ones of a-santonin in crude OPA-**1** aligned medium.

Atom number	$^{1}J_{CH}$	$^{1}T_{CH}$	$^{1}D_{CH}$	$^{1}D_{CH}$ Calculation
C2H2	161.3	169.2	7.9	7.7
C3H3	165.3	150.8	-14.5	-14.5
C7H7	149.1	154.9	5.8	5.7
C8H8	130.1	135.7	5.6	5.7
C10H10a	131.9	139.5	7.6	7.9
C10H10b	129.3	134.7	5.4	5.5
C11H11	127.5	133.6	6.1	6.0
C13H13(Me)	128.3	130.8	2.5	3.2
C14H1a(Me)	129.6	128.4	-1.2	-1.2
C15H15(Me)	129.4	125.3	-4.1	-3.2

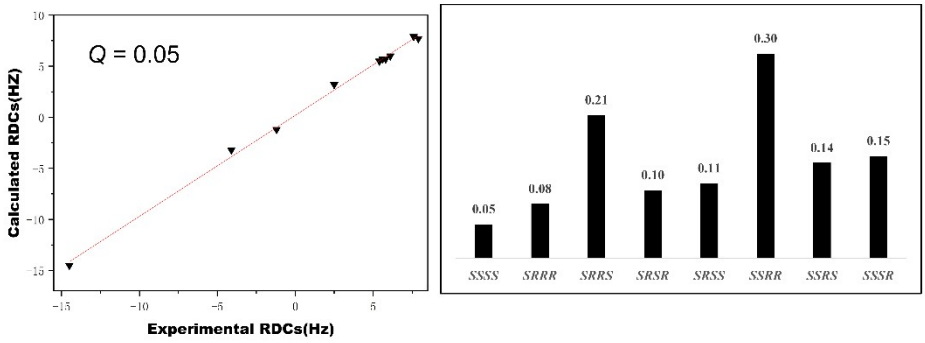


Figure S60. Correlations between the experimental and calculated $^{1}D_{CH}$ values of a-santonin and *Q* factors of the RDCs for the eight possible diastereomeric configurations of a-santonin in crude OPA-**1** aligned medium.

Table S16. The β angle and ratio of GDO between four kinds of aligned media for a-santonin

Ratio of GDO / β-angle	OPA-**1**	OPA-**2**	OPA-**3**	OPA-**4**
OPA-**1**	_	G**2** /G**1** = 1.39	G**3** /G**1** = 1.42	G**4** /G**1** = 1.94
OPA-**2**	36.4	_	G**3** /G**2** = 1.02	G**4** /G**2** = 1.40
OPA-**3**	13.1	32.7	_	G**4** /G**3** = 1.37
OPA-**4**	28.2	38.0	26.0	_

3.4. Data analysis of IPC

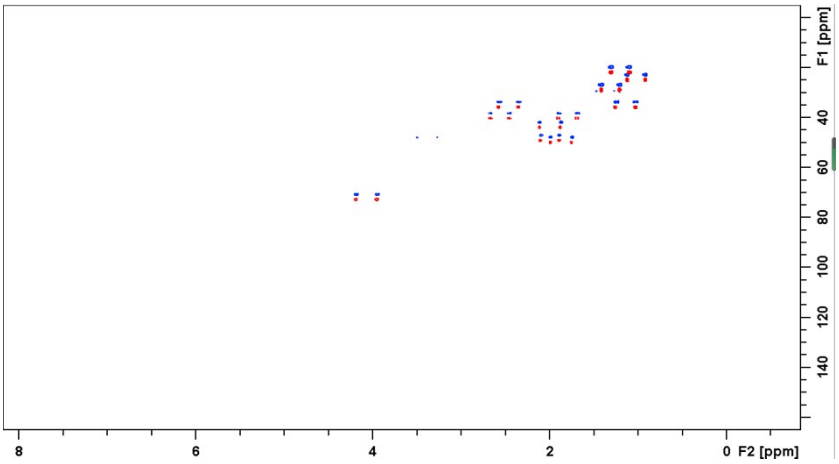


Figure S61. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10mg (+)-IPC in the isotropic phase (red contours) and 5% aligned OPA-**1** /CD_3OD medium (anisotropic, blue contours).

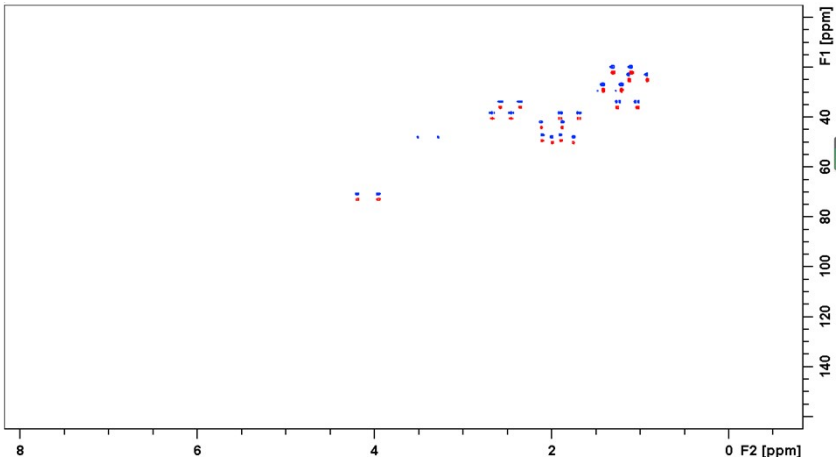


Figure 62. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10mg (-)-IPC in the isotropic phase (red contours) and 5% aligned OPA-**1** /CD_3OD medium (anisotropic, blue contours).

Table S17. The one bond scalar ($^{1}J_{CH}$), total couplings ($^{1}T_{CH}$), residual dipolar couplings ($^{1}D_{CH}$) values and calculated ones of 10mg (±)-IPC in 5% L-OPA-**1** aligned medium.

Atom number	(-)-IPC in L-OPA-**1**				(+)-IPC in L-OPA-**1**		
	$^{1}J_{CH}$	$^{1}T_{CH}$	$^{1}D_{CH}$	$^{1}D_{CH}$ Calculation	$^{1}T_{CH}$	$^{1}D_{CH}$	$^{1}D_{CH}$ Calculation
C1H1	140.2	146.5	6.3	6.6	149.0	8.8	8.7

C2H2	126.9	122.3	-4.6	-4.2	122.1	-4.8	-5.2
C3H3	141.6	143.7	2.1	2.2	141.1	-0.5	-0.4
C4H4a	125.5	129.9	4.4	4.1	129.8	4.3	4.4
C4H4b	127.6	126.6	-1.0	-1.1	125.2	-2.4	-2.6
C5H5	141.1	144.8	3.7	3.8	144.5	3.4	3.4
C7H7a	135.5	131.4	-4.1	-4.0	132.5	-3.0	-3.2
C7H7b	137.2	127.4	-9.8	-9.9	127.2	-10.0	-9.7
C8H8(Me)	123.6	126.4	2.8	3.0	126.0	2.4	2.4
C9H9(Me)	123.6	122.8	-0.8	-0.7	124.1	0.5	0.1
C10H10(Me)	124.6	122.5	-2.1	-2.2	123.0	-1.6	-1.5

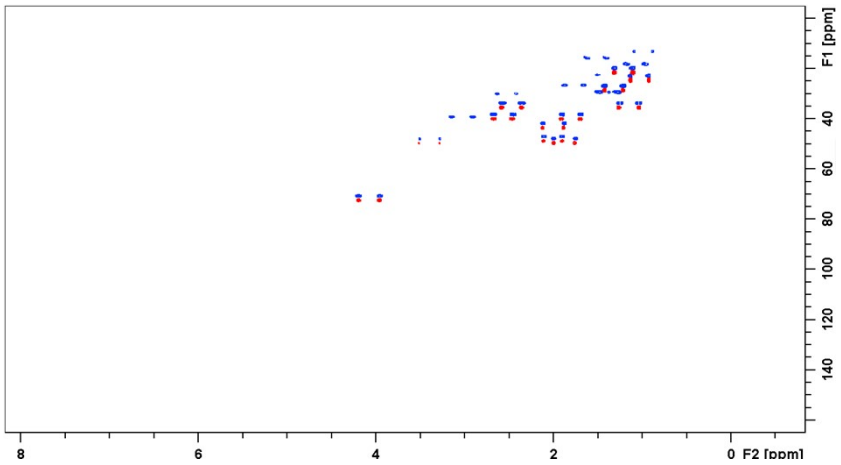


Figure S63. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10 mg (+)-IPC in the isotropic phase (red contours) and 5% aligned D-OPA-**1** /CD_3OD medium (anisotropic, blue contours).

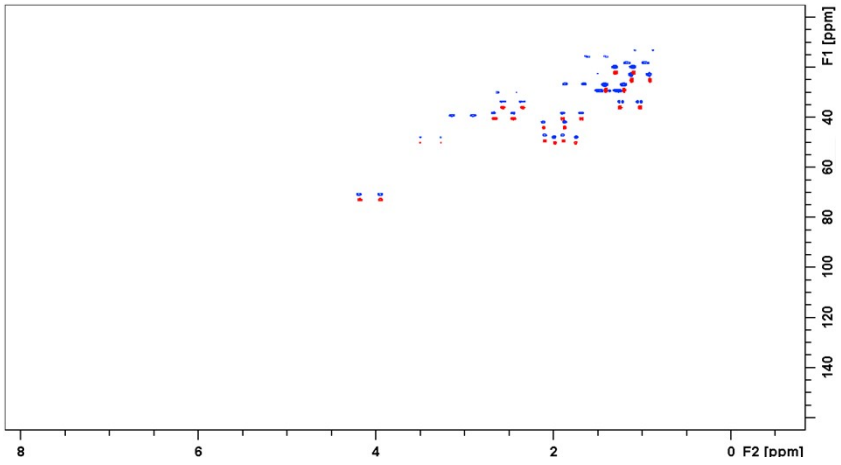


Figure S64. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10 mg (-)-IPC in the isotropic phase (red contours) and 5% aligned D-OPA-**1** /CD_3OD medium (anisotropic, blue contours).

Table S18. The one bond scalar ($^1J_{CH}$), total couplings ($^1T_{CH}$), residual dipolar couplings ($^1D_{CH}$) values and calculated ones of 10 mg (±)-IPC in 5% D-OPA-**1** aligned medium.

Atom number	(-)-IPC in D-OPA-**1**				(+)-IPC in D-OPA-**1**		
	$^1J_{CH}$	$^1T_{CH}$	$^1D_{CH}$	$^1D_{CH}$ Calculation	$^1T_{CH}$	$^1D_{CH}$	$^1D_{CH}$ Calculation
C1H1	140.2	148.7	8.5	8.7	147.2	7.0	6.8
C2H2	126.9	121.3	-5.6	-5.7	123.2	-3.7	-4.2
C3H3	141.6	140.9	-0.7	-0.4	143.7	2.1	2.1
C4H4a	125.5	129.9	4.4	4.3	129.5	4.0	4.4
C4H4b	127.6	125.0	-2.6	-2.8	126.3	-1.3	-1.2
C5H5	141.1	144.8	3.7	3.8	144.7	3.6	3.6
C7H7a	135.5	132.6	-2.9	-3.0	131.7	-3.8	-3.9
C7H7b	137.2	126.7	-10.5	-10.3	127.2	-10.0	-9.8
C8H8(Me)	123.6	126.2	2.6	2.4	126.4	2.8	2.9
C9H9(Me)	123.6	123.7	0.1	0.1	123.0	-0.6	-0.6
C10H10(Me)	124.6	123.0	-1.6	-1.6	122.6	-2.0	-2.1

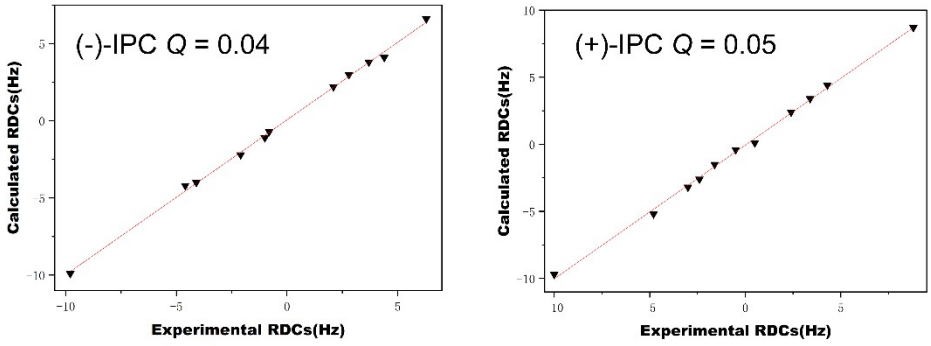


Figure S65. Correlation between experimental $^1D_{CH}$ and the calculated ones for (±)-IPCin the L-OPA-**1** medium.

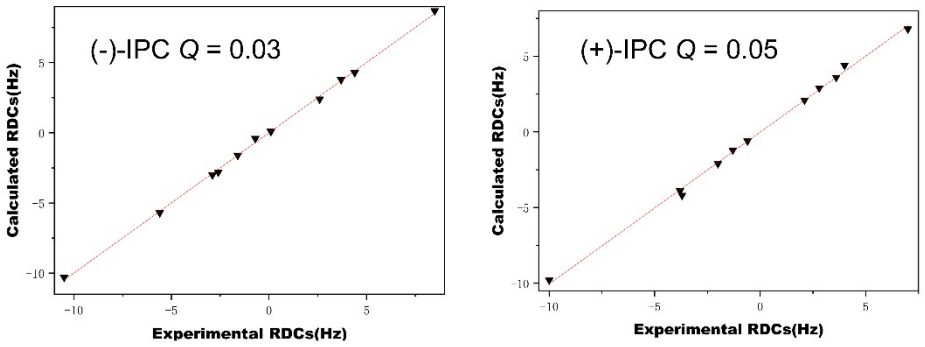


Figure S66. Correlation between experimental $^1D_{CH}$ and the calculated ones for (±)-IPCin the D-OPA-**1** medium.

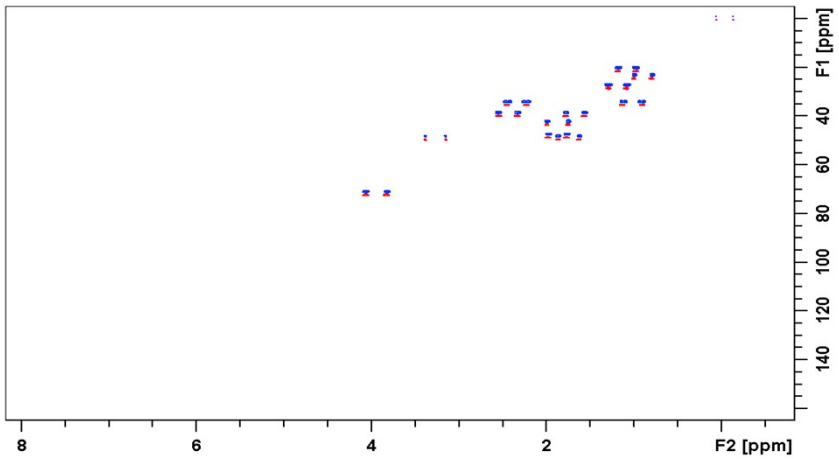


Figure S67. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10 mg (+)-IPC in the isotropic phase (red contours) and 5% aligned OPA-**2** /CD_3OD medium (anisotropic, blue contours).

Table S19. The one bond scalar ($^{1}J_{CH}$), total couplings ($^{1}T_{CH}$), residual dipolar couplings ($^{1}D_{CH}$) values and calculated ones of 10 mg (+)-IPC in 5% OPA-**2** aligned medium.

Atom number	$^{1}J_{CH}$	$^{1}T_{CH}$	$^{1}D_{CH}$	$^{1}D_{CH}$ Calculation
C1H1	140.2	147.9	7.7	8.2
C2H2	126.9	123.9	-3.0	-2.6
C3H3	141.6	146.9	5.3	5.5
C4H4a	125.5	132.2	6.7	6.5
C4H4b	127.6	129.4	1.8	1.8
C5H5	141.1	142.3	1.2	1.5
C7H7a	135.5	128.4	-7.1	-6.8
C7H7b	137.2	126.8	-10.4	-10.3
C8H8(Me)	123.6	128.1	4.5	4.3
C9H9(Me)	123.6	121.8	-1.8	-1.7
C10H10(Me)	124.6	122.2	-2.4	-2.6

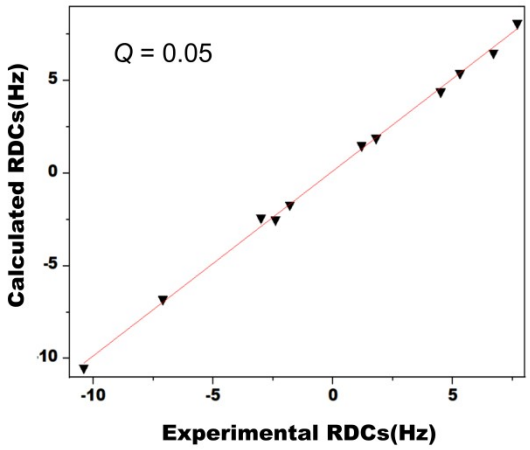


Figure S68. Correlation between experimental $^{1}D_{CH}$ and the calculated ones for (+)-IPC in the OPA-**2** medium.

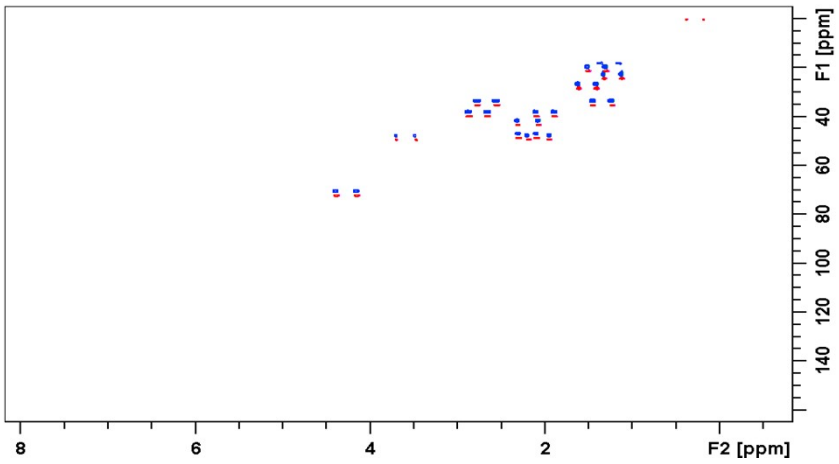


Figure S69. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10 mg (+)-IPC in the isotropic phase (red contours) and 5% aligned OPA-**3** /CD_3OD medium (anisotropic, blue contours).

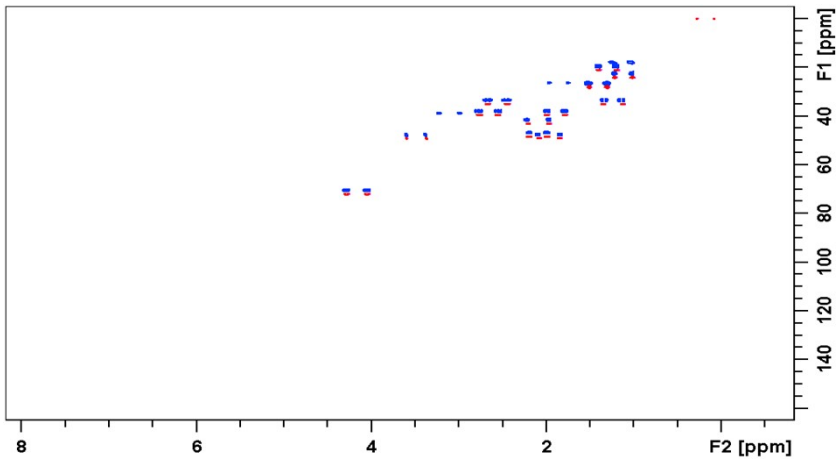


Figure S70. Overlaid [^{1}H, ^{13}C]-CLIP-HSQC spectra of 10mg (+)-IPC in the isotropic phase (red contours) and 5% aligned OPA-**4** /CD_3OD medium (anisotropic, blue contours).

Table S20. The one bond scalar ($^{1}J_{CH}$), total couplings ($^{1}T_{CH}$), residual dipolar couplings ($^{1}D_{CH}$) values and calculated ones of 10 mg (+)-IPC in 5% OPA-**3** and OPA-**4** aligned media.

Atom number	OPA-**3**				OPA-**4**		
	$^{1}J_{CH}$	$^{1}T_{CH}$	$^{1}D_{CH}$	$^{1}D_{CH}$ Calculation	$^{1}T_{CH}$	$^{1}D_{CH}$	$^{1}D_{CH}$ Calculation
C1H1	140.2	150.5	10.3	10.5	155.3	15.1	14.7
C2H2	126.9	123.3	-3.6	-3.8	115.7	-11.2	-10.7
C3H3	141.6	140.3	-1.3	-1.0	140.6	-1.0	-1.4
C4H4a	125.5	131.3	5.8	6.1	134.3	8.8	8.3
C4H4b	127.6	125.5	-2.1	-1.9	120.5	-7.1	-7.4
C5H5	141.1	142.3	1.2	1.7	153.5	12.4	11.6
C7H7a	135.5	130.3	-5.2	-5.0	129.3	-6.2	-6.7
C7H7b	137.2	128.3	-8.9	-8.5	117.2	-20.0	-20.9
C8H8(Me)	123.6	126.6	3.0	2.6	128.7	5.1	5.0

C9H9(Me)	123.6	123.0	-0.6	0.2	123.2	-0.4	0.3
C10H10(Me)	124.6	123.2	-1.4	-0.8	121.4	-3.2	-3.6

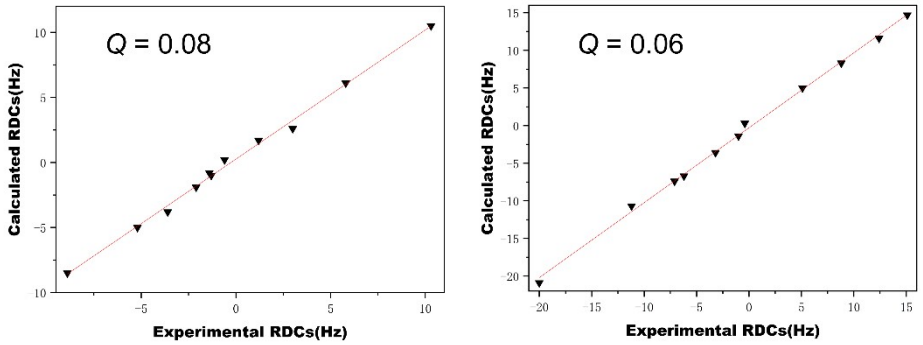


Figure S71. Correlation between experimental $^1D_{CH}$ and the calculated ones for (+)-IPC in the OPA-**3** (left) and OPA-**4** (right) media.

Table S21. The β angle and ratio of GDO between four kinds of aligned media for (+)-IPC

Ratio of GDO / β-angle	OPA-**1**	OPA-**2**	OPA-**3**	OPA-**4**
OPA-**1**	_	G**2** /G**1** = 1.30	G**3** /G**1** = 1.05	G**4** /G**1** = 2.05
OPA-**2**	24.4	_	G**3** /G**2** = 0.81	G**4** /G**2** = 1.58
OPA-**3**	14.0	27.3	_	G**4** /G**3** = 1.95
OPA-**4**	12.1	29.0	23.6	_

4. The recovery of analytes

Table S22. The recovery of three analytes in OPA-**1**

Compound	Initial (mg)	Recovered (mg)	Recovery
α-santonin	10	8.9	89%
artemether	10	8.4	84%
gibberellin	10	8.1	81%

5. Output files of MSpin for the RDCs analysis

Table S23. The XYZ coordinates of artemether

	X	Y	Z
C(1)	-2.672	0.769	0.393
C(2)	-3.140	-0.578	-0.173
C(3)	-2.087	-1.700	-0.062
O(4)	-1.204	-1.430	1.047
C(5)	-0.054	-0.706	0.692

C(6)	-0.294	0.253	-0.493
C(7)	-1.368	1.348	-0.199
C(8)	1.044	0.854	-1.001
C(9)	1.528	2.022	-0.118
C(10)	0.452	3.096	0.039
C(11)	-0.836	2.532	0.652
O(12)	0.957	-1.678	0.423
C(13)	2.221	-1.181	0.006
C(14)	2.082	-0.274	-1.222
C(15)	-2.679	-3.084	0.156
H(16)	-1.600	1.751	-1.197
C(17)	-1.883	3.644	0.821
H(18)	0.816	1.276	-1.992
O(19)	2.893	-0.503	1.043
C(20)	3.441	0.219	-1.731
C(21)	3.269	-1.345	2.130
O(22)	-1.314	-1.821	-1.242
O(23)	-0.811	-0.503	-1.634
H(24)	-2.554	0.662	1.478
H(25)	-3.478	1.494	0.240
H(26)	-4.032	-0.888	0.383
H(27)	-3.434	-0.495	-1.225
H(28)	0.231	-0.123	1.576
H(29)	1.832	1.651	0.866
H(30)	2.424	2.459	-0.572
H(31)	0.831	3.911	0.669
H(32)	0.222	3.540	-0.942
H(33)	-0.592	2.148	1.655
H(34)	2.781	-2.090	-0.257
H(35)	1.654	-0.929	-1.989
H(36)	-3.443	-3.296	-0.598
H(37)	-1.893	-3.842	0.101
H(38)	-3.139	-3.123	1.147
H(39)	-2.761	3.310	1.383
H(40)	-1.449	4.493	1.361
H(41)	-2.226	4.010	-0.156
H(42)	3.316	0.839	-2.626
H(43)	4.078	-0.632	-2.002
H(44)	3.973	0.805	-0.977
H(45)	3.826	-0.723	2.833
H(46)	2.392	-1.769	2.633
H(47)	3.912	-2.168	1.785

Table S24. The XYZ coordinates of gibberellin

	X	Y	Z
C(1)	-1.601	-2.002	-1.250
C(2)	-2.899	-1.727	-1.389
C(3)	-3.563	-0.557	-0.696
C(4)	-2.617	0.159	0.305
C(5)	-1.261	0.314	-0.379
C(6)	-0.166	1.050	0.390
C(7)	-0.105	2.518	0.081
C(8)	1.158	0.317	0.020
C(9)	0.717	-1.100	-0.500
C(10)	-0.788	-1.136	-0.331
C(11)	1.483	-2.245	0.157
C(12)	2.992	-1.985	0.175
C(13)	3.333	-0.496	0.417
C(14)	2.167	0.176	1.163
C(15)	2.030	0.993	-1.056
C(16)	3.352	0.286	-0.900
C(17)	4.403	0.342	-1.714
C(18)	-3.253	1.411	0.876
C(19)	-2.255	-0.853	1.405
O(20)	-3.961	0.424	-1.647
O(21)	-0.531	3.052	-0.914
O(22)	0.549	3.197	1.049
O(23)	-1.128	-1.522	1.047
O(24)	4.576	-0.480	1.089
O(25)	-2.827	-1.047	2.441
H(26)	-1.132	-2.851	-1.747
H(27)	-3.535	-2.342	-2.030
H(28)	-4.441	-0.915	-0.130
H(29)	-1.345	0.700	-1.400
H(30)	-0.309	0.941	1.472
H(31)	0.898	-1.132	-1.584
H(32)	1.263	-3.189	-0.358
H(33)	1.109	-2.369	1.179
H(34)	3.468	-2.305	-0.760
H(35)	3.459	-2.554	0.988
H(36)	1.802	-0.407	2.015
H(37)	2.458	1.170	1.532
H(38)	2.167	2.060	-0.821
H(39)	1.606	0.940	-2.066
H(40)	5.319	-0.196	-1.469
H(41)	4.385	0.920	-2.639

H(42)	-3.467	2.121	0.073
H(43)	-4.185	1.157	1.394
H(44)	-2.590	1.886	1.609
H(45)	-4.578	0.016	-2.270
H(46)	0.586	4.128	0.762
H(47)	4.892	0.435	1.090

Table S25. The XYZ coordinates of α-santonin

	X	Y	Z
C(1)	3.463	-0.260	-0.540
C(2)	2.895	1.089	-0.426
C(3)	1.472	1.220	0.007
C(4)	0.758	0.107	0.305
C(5)	1.345	-1.313	0.290
C(6)	2.756	-1.349	-0.218
C(7)	-0.708	0.049	0.649
C(8)	-1.482	-0.771	-0.401
C(9)	-1.022	-2.222	-0.367
C(10)	0.494	-2.258	-0.635
O(11)	-1.437	1.299	0.719
C(12)	-2.737	1.079	0.361
C(13)	-2.926	-0.376	-0.072
O(14)	3.583	2.079	-0.697
O(15)	-3.557	1.966	0.402
H(16)	-1.236	-0.348	-1.387
C(17)	-3.966	-0.540	-1.178
C(18)	1.395	-1.895	1.738
C(19)	0.951	2.641	0.050
H(20)	4.490	-0.321	-0.890
H(21)	3.203	-2.339	-0.296
H(22)	-0.827	-0.425	1.632
H(23)	-1.265	-2.675	0.603
H(24)	-1.535	-2.815	-1.132
H(25)	0.670	-1.960	-1.676
H(26)	0.877	-3.279	-0.527
H(27)	-3.255	-0.925	0.826
H(28)	-4.108	-1.598	-1.418
H(29)	-3.654	-0.019	-2.090
H(30)	-4.929	-0.128	-0.862
H(31)	0.398	-2.055	2.157
H(32)	1.907	-2.863	1.728
H(33)	1.944	-1.222	2.403
H(34)	1.797	3.326	-0.029
H(35)	0.273	2.847	-0.787

H(36)	0.401	2.848	0.969

Table S26. The XYZ coordinates of IPC

	X	Y	Z
C(1)	-0.465	0.464	-0.996
C(2)	-0.612	-1.022	-1.428
C(3)	-0.822	-1.334	0.076
C(4)	0.563	-1.493	0.725
C(5)	1.503	-0.272	0.484
C(6)	1.020	0.696	-0.642
C(7)	-1.393	0.121	0.233
C(8)	-2.880	0.197	-0.163
C(9)	-1.254	0.849	1.576
C(10)	1.370	2.155	-0.319
O(11)	2.865	-0.676	0.284
H(12)	-0.825	1.241	-1.683
H(13)	-1.493	-1.217	-2.044
H(14)	0.258	-1.481	-1.912
H(15)	-1.485	-2.165	0.349
H(16)	0.474	-1.671	1.804
H(17)	1.041	-2.389	0.306
H(18)	1.564	0.301	1.413
H(19)	1.589	0.425	-1.545
H(20)	-3.197	1.244	-0.247
H(21)	-3.103	-0.291	-1.116
H(22)	-3.504	-0.277	0.605
H(23)	-1.914	0.385	2.320
H(24)	-0.245	0.844	1.991
H(25)	-1.564	1.897	1.479
H(26)	1.144	2.810	-1.169
H(27)	2.440	2.250	-0.096
H(28)	0.811	2.526	0.547
H(29)	2.895	-1.193	-0.538

Output files of MSpin for the RDCs analysis of artemether in 5% OPA-**1** aligned medium:

Cornilescu Quality factor: 0.0672947

Alignment tensor information:

A'x= 4.488e-06

A'y= 3.546e-04

A'z=-3.591e-04

Saupe tensor

S'x= 6.732e-06

S'y= 5.319e-04

S'z=-5.386e-04

Alignment tensor eigenvectors

e[x]=(0.964,-0.264,-0.004)

e[y]=(0.262, 0.954, 0.148)

e[z]=(-0.035,-0.144, 0.989)

Alignment tensor in laboratory coordinates:

[2.807e-05,8.565e-05,2.620e-05]

[8.565e-05,3.154e-04,1.009e-04]

[2.620e-05,1.009e-04,-3.435e-04]

SVD condition number is 6.495e+00

Axial component Aa = -5.386e-04

Rhombic component Ar = -3.501e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.650

Asimmetry parameter etha =9.750e-01

GDO = 7.554e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(-103.8,8.5,88.4)

Set 2

(76.2,-8.5,-91.6)

Output files of MSpin for the RDCs analysis of artemether in 5% OPA-**2** aligned medium:

Cornilescu Quality factor: 0.0703049

Alignment tensor information:

A'x= 9.030e-05

A'y= 5.771e-04

A'z=-6.674e-04

Saupe tensor

S'x= 1.354e-04

S'y= 8.656e-04

S'z=-1.001e-03

Alignment tensor eigenvectors

e[x]=(0.976, 0.125,-0.177)

e[y]=(-0.150, 0.980,-0.134)

e[z]=(0.156, 0.158, 0.975)

Alignment tensor in laboratory coordinates:

[8.264e-05,-8.997e-05,-1.058e-04]

[-8.997e-05,5.386e-04,-1.805e-04]

[-1.058e-04,-1.805e-04,-6.213e-04]

SVD condition number is 6.495e+00

Axial component Aa = -1.001e-03

Rhombic component Ar = -4.868e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.486

Asimmetry parameter etha =7.294e-01

GDO = 1.301e-03

ZY'Z'' Euler Angles (degrees)

Set 1

(45.2,12.8,-37.2)

Set 2

(-134.8,-12.8,142.8)

Output files of MSpin for the RDCs analysis of artemether in 2% OPA-**2** aligned medium:

Cornilescu Quality factor: 0.0683022

Alignment tensor information:

A'x= 1.398e-04

A'y= 3.356e-04

A'z=-4.755e-04

Saupe tensor

S'x= 2.097e-04

S'y= 5.035e-04

S'z=-7.132e-04

Alignment tensor eigenvectors

e[x]=(0.958, 0.047,-0.282)

e[y]=(-0.079, 0.991,-0.105)

e[z]=(0.275, 0.123, 0.954)

Alignment tensor in laboratory coordinates:

[9.466e-05,-3.620e-05,-1.595e-04]

[-3.620e-05,3.229e-04,-9.275e-05]

[-1.595e-04,-9.275e-05,-4.176e-04]

SVD condition number is 6.495e+00

Axial component Aa = -7.132e-04

Rhombic component Ar = -1.958e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.275

Asimmetry parameter etha =4.119e-01

GDO = 8.577e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(24.2,17.5,-20.5)

Set 2

(-155.8,-17.5,159.5)

Output files of MSpin for the RDCs analysis of artemether in 5% OPA-**3** aligned medium:

Cornilescu Quality factor: 0.0626097

Alignment tensor information:

A'x=-2.446e-05

A'y=-4.414e-04

A'z= 4.658e-04

Saupe tensor

S'x=-3.670e-05

S'y=-6.620e-04

S'z= 6.987e-04

Alignment tensor eigenvectors

e[x]=(-0.865, 0.079, 0.496)

e[y]=(0.456, 0.535, 0.711)

e[z]=(-0.210, 0.841,-0.499)

Alignment tensor in laboratory coordinates:

[-8.971e-05,-1.882e-04,-8.398e-05]

[-1.882e-04,2.029e-04,-3.643e-04]

[-8.398e-05,-3.643e-04,-1.132e-04]

SVD condition number is 6.495e+00

Axial component Aa = 6.987e-04

Rhombic component Ar = 4.169e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.597

Asimmetry parameter etha =8.950e-01

GDO = 9.548e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(104.0,119.9,124.9)

Set 2

(-76.0,-119.9,-55.1)

Output files of MSpin for the RDCs analysis of artemether in 5% OPA-**4** aligned medium:

Cornilescu Quality factor: 0.0623512

Alignment tensor information:

A'x= 7.097e-05

A'y= 4.694e-04

A'z=-5.403e-04

Saupe tensor

S'x= 1.064e-04

S'y= 7.041e-04

S'z=-8.105e-04

Alignment tensor eigenvectors

e[x]=(0.585, 0.784,-0.209)

e[y]=(-0.811, 0.576,-0.106)

e[z]=(0.037, 0.231, 0.972)

Alignment tensor in laboratory coordinates:

[3.318e-04,-1.913e-04,1.196e-05]

[-1.913e-04,1.706e-04,-1.615e-04]

[1.196e-05,-1.615e-04,-5.025e-04]

SVD condition number is 6.495e+00

Axial component Aa = -8.105e-04

Rhombic component Ar = -3.984e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.492

Asimmetry parameter etha =7.373e-01

GDO = 1.055e-03

ZY'Z'' Euler Angles (degrees)

Set 1

(80.8,13.5,-26.9)

Set 2

(-99.2,-13.5,153.1)

Output files of MSpin for the RDCs analysis of gibberellin in OPA-**1** aligned medium:

Cornilescu Quality factor: 0.0703663

Alignment tensor information:

A'x= 2.429e-05

A'y= 2.285e-04

A'z=-2.528e-04

Saupe tensor

S'x= 3.643e-05

S'y= 3.428e-04

S'z=-3.792e-04

Alignment tensor eigenvectors

e[x]=(0.018, 0.947, 0.320)

e[y]=(-0.977, 0.084,-0.196)

e[z]=(-0.212,-0.309, 0.927)

Alignment tensor in laboratory coordinates:

[2.067e-04,-3.502e-05,9.363e-05]

[-3.502e-05,-7.521e-07,7.605e-05]

[9.363e-05,7.605e-05,-2.060e-04]

SVD condition number is 2.289e+00

Axial component Aa = -3.792e-04

Rhombic component Ar = -2.042e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.539

Asimmetry parameter etha =8.079e-01

GDO = 5.043e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(-124.5,22.0,-148.5)

Set 2

(55.5,-22.0,31.5)

Output files of MSpin for the RDCs analysis of gibberellin in OPA-**2** aligned medium:

Cornilescu Quality factor: 0.0602742

Alignment tensor information:

A'x=-6.080e-05

A'y=-3.616e-04

A'z= 4.224e-04

Saupe tensor

S'x=-9.120e-05

S'y=-5.424e-04

S'z= 6.336e-04

Alignment tensor eigenvectors

e[x]=(-0.061, 0.937, 0.345)

e[y]=(-0.266,-0.348, 0.899)

e[z]=(0.962,-0.037, 0.270)

Alignment tensor in laboratory coordinates:

[3.651e-04,-4.497e-05,1.977e-04]

[-4.497e-05,-9.659e-05,8.931e-05]

[1.977e-04,8.931e-05,-2.685e-04]

SVD condition number is 2.289e+00

Axial component Aa = 6.336e-04

Rhombic component Ar = 3.008e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.475

Asimmetry parameter etha =7.121e-01

GDO = 8.191e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(-2.2,74.3,111.0)

Set 2

(177.8,-74.3,-69.0)

Output files of MSpin for the RDCs analysis of gibberellin in OPA-**3** aligned medium:

Cornilescu Quality factor: 0.0642791

Alignment tensor information:

A'x= 9.954e-05

A'y= 3.895e-04

A'z=-4.890e-04

Saupe tensor

S'x= 1.493e-04

S'y= 5.842e-04

S'z=-7.335e-04

Alignment tensor eigenvectors

e[x]=(0.080, 0.908, 0.412)

e[y]=(-0.978, 0.151,-0.141)

e[z]=(-0.190,-0.392, 0.900)

Alignment tensor in laboratory coordinates:

[3.558e-04,-8.663e-05,1.408e-04]

[-8.663e-05,1.567e-05,2.015e-04]

[1.408e-04,2.015e-04,-3.715e-04]

SVD condition number is 2.289e+00

Axial component Aa = -7.335e-04

Rhombic component Ar = -2.899e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.395

Asimmetry parameter etha =5.929e-01

GDO = 9.184e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(-115.9,25.8,-161.1)

Set 2

(64.1,-25.8,18.9)

Output files of MSpin for the RDCs analysis of gibberellin in OPA-**4** aligned medium:

Cornilescu Quality factor: 0.0639454

Alignment tensor information:

A'x=-6.956e-05

A'y=-4.513e-04

A'z= 5.209e-04

Saupe tensor

S'x=-1.043e-04

S'y=-6.770e-04

S'z= 7.813e-04

Alignment tensor eigenvectors

e[x]=(-0.081, 0.976, 0.202)

e[y]=(-0.370,-0.218, 0.903)

e[z]=(0.925,-0.002, 0.379)

Alignment tensor in laboratory coordinates:

[3.839e-04,-3.183e-05,3.346e-04]

[-3.183e-05,-8.766e-05,7.464e-05]

[3.346e-04,7.464e-05,-2.962e-04]

SVD condition number is 2.289e+00

Axial component Aa = 7.813e-04

Rhombic component Ar = 3.818e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.489

Asimmetry parameter etha =7.329e-01

GDO = 1.016e-03

ZY'Z'' Euler Angles (degrees)

Set 1

(-0.1,67.7,102.6)

Set 2

(179.9,-67.7,-77.4)

Output files of MSpin for the RDCs analysis of SSSS for α-santonin in OPA-**1** aligned medium:

Cornilescu Quality factor: 0.0274889

Alignment tensor information:

A'x=-9.857e-05

A'y=-3.907e-04

A'z= 4.893e-04

Saupe tensor

S'x=-1.478e-04

S'y=-5.861e-04

S'z= 7.339e-04

Alignment tensor eigenvectors

e[x]=(0.246, 0.599,-0.762)

e[y]=(-0.093, 0.797, 0.597)

e[z]=(0.965,-0.076, 0.252)

Alignment tensor in laboratory coordinates:

[4.460e-04,-2.163e-05,1.590e-04]

[-2.163e-05,-2.807e-04,-1.503e-04]

[1.590e-04,-1.503e-04,-1.654e-04]

SVD condition number is 9.006e+00

Axial component Aa = 7.339e-04

Rhombic component Ar = 2.921e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.398

Asimmetry parameter etha =5.971e-01

GDO = 9.199e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(-4.5,75.4,38.1)

Set 2

(175.5,-75.4,-141.9)

Output files of MSpin for the RDCs analysis of SSSS for α-santonin in OPA-**2** aligned medium:

Cornilescu Quality factor: 0.0228648

Alignment tensor information:

A'x=-1.371e-04

A'y=-5.448e-04

A'z= 6.819e-04

Saupe tensor

S'x=-2.057e-04

S'y=-8.172e-04

S'z= 1.023e-03

Alignment tensor eigenvectors

e[x]=(0.042, 0.151, 0.988)

e[y]=(-0.088,-0.984, 0.154)

e[z]=(0.995,-0.094,-0.028)

Alignment tensor in laboratory coordinates:

[6.709e-04,-1.119e-04,-1.689e-05]

[-1.119e-04,-5.248e-04,6.381e-05]

[-1.689e-05,6.381e-05,-1.461e-04]

SVD condition number is 9.006e+00

Axial component Aa = 1.023e-03

Rhombic component Ar = 4.077e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.399

Asimmetry parameter etha =5.978e-01

GDO = 1.282e-03

ZY'Z'' Euler Angles (degrees)

Set 1

(-5.4,91.6,171.2)

Set 2

(174.6,-91.6,-8.8)

Output files of MSpin for the RDCs analysis of SSSS for α-santonin in OPA-**3** aligned medium:

Cornilescu Quality factor: 0.019653

Alignment tensor information:

A'x=-9.303e-05

A'y=-5.801e-04

A'z= 6.732e-04

Saupe tensor

S'x=-1.395e-04

S'y=-8.702e-04

S'z= 1.010e-03

Alignment tensor eigenvectors

e[x]=(0.170, 0.427,-0.888)

e[y]=(-0.104, 0.904, 0.414)

e[z]=(0.980, 0.022, 0.198)

Alignment tensor in laboratory coordinates:

[6.374e-04,6.209e-05,1.700e-04]

[6.209e-05,-4.908e-04,-1.792e-04]

[1.700e-04,-1.792e-04,-1.465e-04]

SVD condition number is 9.006e+00

Axial component Aa = 1.010e-03

Rhombic component Ar = 4.871e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.482

Asimmetry parameter etha =7.236e-01

GDO = 1.310e-03

ZY'Z'' Euler Angles (degrees)

Set 1

(1.3,78.6,25.0)

Set 2

(-178.7,-78.6,-155.0)

Output files of MSpin for the RDCs analysis of SSSS for α-santonin in OPA-**4** aligned medium:

Cornilescu Quality factor: 0.0504156

Alignment tensor information:

A'x= 1.117e-05

A'y= 8.396e-04

A'z=-8.507e-04

Saupe tensor

S'x= 1.675e-05

S'y= 1.259e-03

S'z=-1.276e-03

Alignment tensor eigenvectors

e[x]=(-0.463,-0.156, 0.872)

e[y]=(0.885,-0.136, 0.445)

e[z]=(0.049, 0.978, 0.201)

Alignment tensor in laboratory coordinates:

[6.578e-04,-1.413e-04,3.180e-04]

[-1.413e-04,-7.985e-04,-2.198e-04]

[3.180e-04,-2.198e-04,1.406e-04]

SVD condition number is 9.006e+00

Axial component Aa = -1.276e-03

Rhombic component Ar = -8.284e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.649

Asimmetry parameter etha =9.738e-01

GDO = 1.789e-03

ZY'Z'' Euler Angles (degrees)

Set 1

(87.1,78.4,153.0)

Set 2

(-92.9,-78.4,-27.0)

Output files of MSpin for the RDCs analysis of SSSS for α-santonin in crude OPA-**1** aligned medium:

Cornilescu Quality factor: 0.0539493

Alignment tensor information:

A'x=-8.040e-05

A'y=-2.174e-04

A'z= 2.978e-04

Saupe tensor

S'x=-1.206e-04

S'y=-3.261e-04

S'z= 4.467e-04

Alignment tensor eigenvectors

e[x]=(0.195, 0.233,-0.953)

e[y]=(0.027, 0.970, 0.243)

e[z]=(0.980,-0.074, 0.183)

Alignment tensor in laboratory coordinates:

[2.830e-04,-3.090e-05,6.689e-05]

[-3.090e-05,-2.072e-04,-3.738e-05]

[6.689e-05,-3.738e-05,-7.584e-05]

SVD condition number is 9.006e+00

Axial component Aa = 4.467e-04

Rhombic component Ar = 1.370e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.307

Asimmetry parameter etha =4.601e-01

GDO = 5.424e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(-4.3,79.5,14.3)

Set 2

(175.7,-79.5,-165.7)

Output files of MSpin for the RDCs analysis of (-)-IPC in L-OPA-**1** aligned medium:

Cornilescu Quality factor: 0.042663

Alignment tensor information:

A'x=-3.708e-05

A'y=-1.435e-04

A'z= 1.806e-04

Saupe tensor

S'x=-5.561e-05

S'y=-2.153e-04

S'z= 2.709e-04

Alignment tensor eigenvectors

e[x]=(0.225, 0.394, 0.891)

e[y]=(-0.076,-0.905, 0.420)

e[z]=(0.971,-0.162,-0.174)

Alignment tensor in laboratory coordinates:

[1.677e-04,-4.168e-05,-3.331e-05]

[-4.168e-05,-1.184e-04,4.654e-05]

[-3.331e-05,4.654e-05,-4.926e-05]

SVD condition number is 2.156e+00

Axial component Aa = 2.709e-04

Rhombic component Ar = 1.065e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.393

Asimmetry parameter etha =5.894e-01

GDO = 3.389e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(-9.5,100.0,154.8)

Set 2

(170.5,-100.0,-25.2)

Output files of MSpin for the RDCs analysis of (+)-IPC in L-OPA-**1** aligned medium:

Cornilescu Quality factor: 0.047674

Alignment tensor information:

A'x=-5.405e-06

A'y=-1.559e-04

A'z= 1.613e-04

Saupe tensor

S'x=-8.107e-06

S'y=-2.338e-04

S'z= 2.419e-04

Alignment tensor eigenvectors

e[x]=(0.318, 0.556, 0.768)

e[y]=(0.009,-0.812, 0.583)

e[z]=(0.948,-0.178,-0.264)

Alignment tensor in laboratory coordinates:

[1.444e-04,-2.705e-05,-4.247e-05]

[-2.705e-05,-9.933e-05,7.914e-05]

[-4.247e-05,7.914e-05,-4.506e-05]

SVD condition number is 2.156e+00

Axial component Aa = 2.419e-04

Rhombic component Ar = 1.505e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.622

Asimmetry parameter etha =9.330e-01

GDO = 3.347e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(-10.7,105.3,142.8)

Set 2

(169.3,-105.3,-37.2)

Output files of MSpin for the RDCs analysis of (-)-IPC in D-OPA-**1** aligned medium:

Cornilescu Quality factor: 0.0332272

Alignment tensor information:

A'x=-8.563e-06

A'y=-1.583e-04

A'z= 1.669e-04

Saupe tensor

S'x=-1.285e-05

S'y=-2.375e-04

S'z= 2.504e-04

Alignment tensor eigenvectors

e[x]=(0.344, 0.532, 0.774)

e[y]=(-0.004,-0.823, 0.567)

e[z]=(0.939,-0.199,-0.281)

Alignment tensor in laboratory coordinates:

[1.461e-04,-3.323e-05,-4.599e-05]

[-3.323e-05,-1.032e-04,7.978e-05]

[-4.599e-05,7.978e-05,-4.290e-05]

SVD condition number is 2.156e+00

Axial component Aa = 2.504e-04

Rhombic component Ar = 1.498e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.598

Asimmetry parameter etha =8.974e-01

GDO = 3.424e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(-11.9,106.3,143.8)

Set 2

(168.1,-106.3,-36.2)

Output files of MSpin for the RDCs analysis of (+)-IPC in D-OPA-**1** aligned medium:

Cornilescu Quality factor: 0.0454214

Alignment tensor information:

A'x=-3.622e-05

A'y=-1.423e-04

A'z= 1.785e-04

Saupe tensor

S'x=-5.433e-05

S'y=-2.134e-04

S'z= 2.678e-04

Alignment tensor eigenvectors

e[x]=(0.231, 0.435, 0.870)

e[y]=(-0.062,-0.886, 0.459)

e[z]=(0.971,-0.160,-0.178)

Alignment tensor in laboratory coordinates:

[1.658e-04,-3.914e-05,-3.407e-05]

[-3.914e-05,-1.141e-04,4.925e-05]

[-3.407e-05,4.925e-05,-5.178e-05]

SVD condition number is 2.156e+00

Axial component Aa = 2.678e-04

Rhombic component Ar = 1.061e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.396

Asimmetry parameter etha =5.942e-01

GDO = 3.354e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(-9.3,100.2,152.2)

Set 2

(170.7,-100.2,-27.8)

Output files of MSpin for the RDCs analysis of (+)-IPC in OPA-**2** aligned medium:

Cornilescu Quality factor: 0.0473956

Alignment tensor information:

A'x=-7.826e-05

A'y=-1.651e-04

A'z= 2.434e-04

Saupe tensor

S'x=-1.174e-04

S'y=-2.477e-04

S'z= 3.651e-04

Alignment tensor eigenvectors

e[x]=(0.105, 0.392, 0.914)

e[y]=(-0.005,-0.919, 0.395)

e[z]=(0.994,-0.046,-0.094)

Alignment tensor in laboratory coordinates:

[2.399e-04,-1.519e-05,-3.003e-05]

[-1.519e-05,-1.509e-04,3.290e-05]

[-3.003e-05,3.290e-05,-8.892e-05]

SVD condition number is 2.156e+00

Axial component Aa = 3.651e-04

Rhombic component Ar = 8.689e-05

Field=11.74 Teslas[3.63]

rhombicity R = 0.238

Asimmetry parameter etha =3.570e-01

GDO = 4.348e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(-2.7,95.4,156.7)

Set 2

(177.3,-95.4,-23.3)

Output files of MSpin for the RDCs analysis of (+)-IPC in OPA-**3** aligned medium:

Cornilescu Quality factor: 0.0828676

Alignment tensor information:

A'x= 1.804e-05

A'y= 1.590e-04

A'z=-1.770e-04

Saupe tensor

S'x= 2.707e-05

S'y= 2.385e-04

S'z=-2.655e-04

Alignment tensor eigenvectors

e[x]=(0.143, 0.661, 0.737)

e[y]=(0.987,-0.045,-0.151)

e[z]=(-0.067, 0.749,-0.659)

Alignment tensor in laboratory coordinates:

[1.546e-04,3.530e-06,-2.962e-05]

[3.530e-06,-9.117e-05,9.725e-05]

[-2.962e-05,9.725e-05,-6.343e-05]

SVD condition number is 2.156e+00

Axial component Aa = -2.655e-04

Rhombic component Ar = -1.409e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.531

Asimmetry parameter etha =7.961e-01

GDO = 3.518e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(95.1,131.2,-168.4)

Set 2

(-84.9,-131.2,11.6)

Output files of MSpin for the RDCs analysis of (+)-IPC in OPA-**4** aligned medium:

Cornilescu Quality factor: 0.0550789

Alignment tensor information:

A'x=-1.070e-05

A'y=-3.198e-04

A'z= 3.305e-04

Saupe tensor

S'x=-1.605e-05

S'y=-4.797e-04

S'z= 4.957e-04

Alignment tensor eigenvectors

e[x]=(0.353, 0.459, 0.815)

e[y]=(-0.111,-0.844, 0.524)

e[z]=(0.929,-0.276,-0.247)

Alignment tensor in laboratory coordinates:

[2.798e-04,-1.165e-04,-6.025e-05]

[-1.165e-04,-2.050e-04,1.600e-04]

[-6.025e-05,1.600e-04,-7.478e-05]

SVD condition number is 2.156e+00

Axial component Aa = 4.957e-04

Rhombic component Ar = 3.091e-04

Field=11.74 Teslas[3.63]

rhombicity R = 0.624

Asimmetry parameter etha =9.353e-01

GDO = 6.862e-04

ZY'Z'' Euler Angles (degrees)

Set 1

(-16.5,104.3,147.3)

Set 2

(163.5,-104.3,-32.7)