Supporting Information
for

Valine derived poly(acetylenes) as versatile chiral lyotropic liquid crystalline alignment media for RDC based structure elucidations

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1 Experimental procedures and characterization data

1.1 Materials and Instrumentation

Solvents and reagents: Dichloromethane (DCM), chloroform [D_1] ($CDCl_3$) and triethylamine (Et_3N) were distilled from CaH_2 under argon atmosphere. Tetrahydrofuran (THF) was distilled from sodium-benzophenone under argon. Reagents were obtained from commercial sources and used without further purification unless otherwise specified. Moisture and/or air sensitive experiments were conducted under argon atmosphere using typical Schlenk techniques.

NMR-Spectra: ^{1}H-NMR spectra were recorded on Bruker ARX 300 and DRX 500 spectrometers operating at 300 and 500 MHz, respectively at 300 K unless otherwise specified. ^{13}C-NMR spectra were recorded on the same instruments at 75 and 125 MHz, respectively. Chemical shifts (δ) in ^{1}H-NMR and ^{13}C-NMR spectra are reported in ppm. The spectra were referenced against the residual solvent signal as reported in the literature.[1] The fine structure of proton signals was specified as s (singulet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), br (broad).

Thin layer chromatography (TLC): Thin-layer chromatography (TLC) was performed using E. Merck silica gel SilG/UV254 by Macherey Nagel & Co., Düren (thickness of layer 0.2 mm) and visualized by UV fluorescence quenching or oxidizing with $KMnO_4$.

IR-spectra were recorded on a Perkin-Elmer spectrometer Paragon 1000 PC or on a Vector 22 spectrometer from Bruker.

Gel permeation chromatography (GPC): Gel permeation chromatography was performed on two columns (MZ-Gel Sdplus 10^3 Å and 10^5 Å from MZ-Analysentechnik) in an oven at 30°C at a flow rate of 1.0 mL/min and pressure of 35-38 bar (HPLC pump from JASCO). The detector employed was a JASCO UV975-detector operating at 254 nm. Calibration was done using polystyrene standards from Macherey-Nagel GmbH & Co. KG. The chromatograms were analysed using the software package WinGPC from Polymer Standard Service GmbH, Mainz (Germany). Typically 3 mg of the polymer were dissolved in THF (containing 1 drop of toluene per 10 mL of solvent as internal standard; eluting after 25 minutes). 50µL of this solution were injected, the eluent was THF.

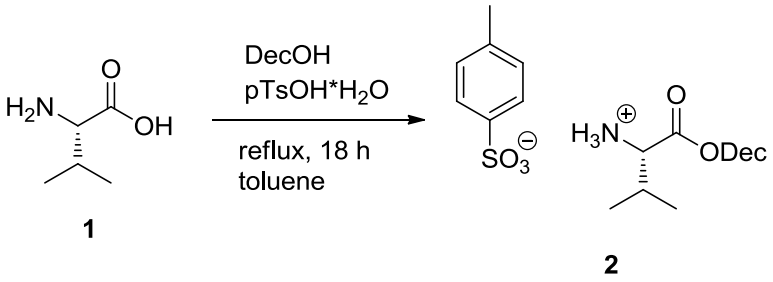
Centrifuge: Centrifugation was performed on a Rotina 46 (Fa. Hettich).

Specific optical rotations were determined on a Perkin Elmer Polarimeter 241 with Haake D8 thermostat or on an Anton Paar MCP 300 polarimeter in 1 dm cuvettes respectively.

CD spectra were recorded on a JASCO J-810 spectrometer equipped with a PTC-423S/15 peltier element as a temperature device.

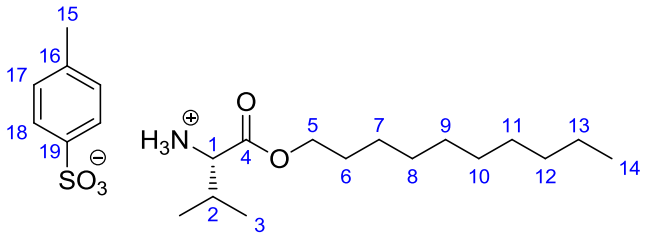
1.2 Monomer synthesis

1.2.1 L-Valine decyl ester hydrotosylate 2



1 **2**

A suspension of L-valine **1** (40.0 g, 341.5 mmol, 1.00 eq.), 1-decanol (61.9 mL, 51.3 g, 324.4 mmol, 0.95 eq.) and *p*-toluenesulfonic acid monohydrate (71.5 g, 375.6 mmol 1.10 eq.) in 1.4 L of toluene was refluxed for 16 h in a Dean-Stark water trap. After this period of time 12.6 mL (700.0 mmol) of water were collected. About 700 mL of toluene were distilled off from the obtained solution under reduced pressure and 700 mL of petroleum ether were added. The resulting mixture was stored at -20°C overnight. The precipitated colorless solid was separated by filtration and dried in vacuo to give 117.4 g (273.2 mmol) of **2**. The enantiomeric compound ***ent*-2** was prepared in the same manner using D-valine ***ent*-1** as reactant. Yield 80 %.



2

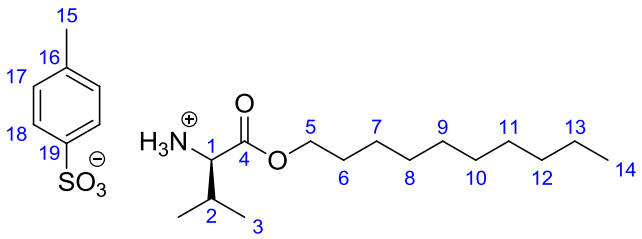
^{1}H-NMR (CDCl$_3$, 300 MHz, 300 K): δ = 8.12 (bd, 3H, ^3J = 3.8 Hz, NH_3), 7.77 (d, 2H, ^3J = 8.1 Hz, 18-H), 7.13 (d, 2H, ^3J = 8.1 Hz, 17-H), 4.07 (dt, 1H, ^2J = 10.7 Hz, ^3J = 7.0 Hz, 5b-H), 3.99 (dt, 1H, ^2J = 10.7 Hz, ^3J = 6.9 Hz, 5a-H), 3.84 („pent“, 1H, 1-H), 2.34 (s, 3H, 15-H), 2.20 (m, 1H, 2-H), 1.54 („quint“, 2H, 6-H), 1.12–1.41 (m, 14H, 7,8,9,10,11,12,13-H), 0.96 (d, 3H, ^3J = 7.1 Hz, 3b-H), 0.93 (d, 3H, ^3J = 7.0 Hz, 3a-H), 0.88 (t, 3H, ^3J = 6.8 Hz, 14-H) ppm.

^{13}C-NMR (CDCl$_3$, 125 MHz, 300 K): δ = 168.9 (4-C), 141.8 (19-C) 140.2 (16-C), 128.9 (17-C), 126.3 (18-C), 66.4 (5-C), 58.5 (1-C), 32.0 (12-C), 29.8 (2-C), 29.7 + 29.6 + 29.4 (9,10,11-C), 29.3 (8-C), 28.5 (6-C), 25.9 (7-C), 22.8 (13-C), 21.4 (15-C), 18.5 (3b-C), 17.6 (3a-C), 14.2 (14-C) ppm.

IR (KBr): $\tilde{\nu}$ = ~3030 (m, -NH_3^+), 2962.0 (m, -CH_3), 2919.7 (s, -C-H), 2872.0 (m, -CH_3), 2850.8 (m, -C-H), 1742.0 (s, -C=O), 1620.1 (m, -N-H) cm^{-1}.

$C_{22}H_{39}NO_5S$ (429.61)	calculated:	C 61.51	H 9.15	N 3.26
	measured:	C 61.65	H 9.29	N 3.27

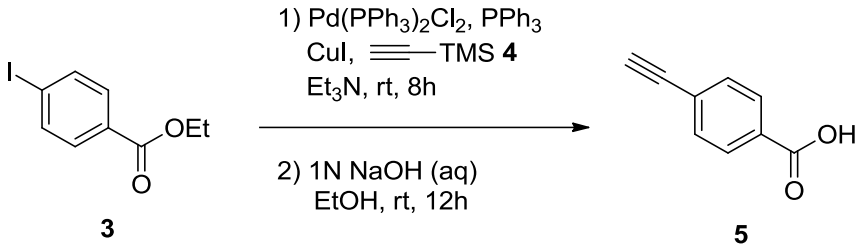
ORD (c = 0.96, MeOH):	$[\alpha]_{589}^{20}$ = 5.54	$[\alpha]_{579}^{20}$ = 4.50	$[\alpha]_{546}^{20}$ = 6.80
	$[\alpha]_{436}^{20}$ = 13.81	$[\alpha]_{405}^{20}$ = 15.38	$[\alpha]_{365}^{20}$ = 25.10



***ent*-2**

ORD (c = 0.91, MeOH):	$[\alpha]_{589}^{20}$ = -6.02	$[\alpha]_{579}^{20}$ = -7.67	$[\alpha]_{546}^{20}$ = -7.34
	$[\alpha]_{436}^{20}$ = -14.02	$[\alpha]_{405}^{20}$ = -20.48	$[\alpha]_{365}^{20}$ = -27.05

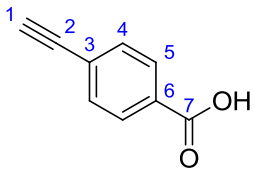
1.2.2 4-Ethynylbenzoic acid 5



3 **5**

4-Ethynylbenzoic acid **5** was prepared similar to the experimental procedure of YASHIMA and OKAMOTO.[2] To a mixture of ethyl 4-iodobenzoate **3** (10.0 mL, 16.5 g, 59.8 mmol, 1.00 eq.), bis(triphenylphosphine)palladium dichloride (0.414 g, 0.59 mmol, 0.01 eq.), triphenylphosphine (0.310 g, 1.18 mmol, 0.02 eq.) and copper(I) iodide (0.224 g, 1.18 mmol 0.02 eq.) in 200 mL of degassed triethylamine under argon atmosphere was slowly added (trimethylsilyl)acetylene **4** (12.8 mL, 8.8 g, 89.7 mmol, 1.50 eq.) at 0°C. The reaction mixture was then slowly warmed to room temperature and stirred for 8 h. The solution was filtered over a silica plug and the filtrate concentrated under reduced pressure.

The resulting ethyl-[4-(trimethylsilyl)ethynyl]benzoate was dissolved in 70 mL of ethanol. Then 90 mL of 1 N NaOH (aq) were added dropwise to the solution at 0°C under stirring. The solution was stirred at 0°C for 2 h and additional 12 h at room temperature. EtOH was removed by rotary evaporation and the aqueous solution washed with 250 mL of diethylether. The aqueous layer was then acidified with 1 N HCl (aq) to pH 1 and the precipitated solid extracted with 500 mL of diethylether. The organic layer was washed twice with 50 mL of water and dried over $MgSO_4$. The solvent was removed *in vacuo* to give 7.7 g (52.7 mmol) of **5** as a brown solid. Yield 88 % over two steps.

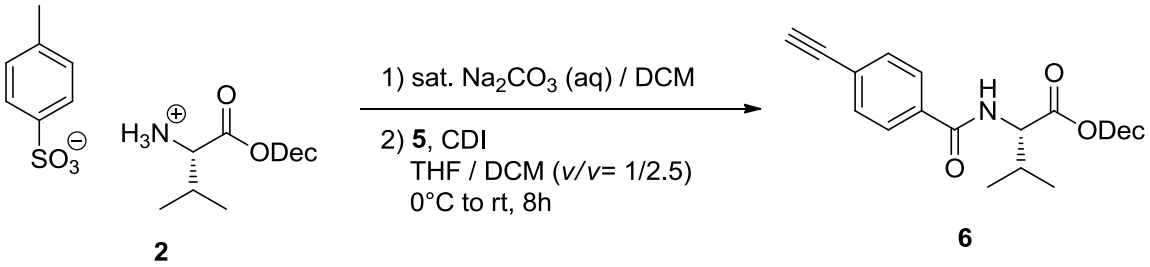


5

^{1}H-NMR (DMSO [D6], 300 MHz; 300 K) δ = 13.12 (bs, 1H, COOH), 7.94 (d, 2H, ^{3}J=8.3 Hz, 5-H), 7.59 (d, 2H, ^{3}J=8.3 Hz, 4-H), 4.42 (s, 1H, 1-H) ppm.

^{13}C-NMR (DMSO [D6], 75.4 MHz, 300 K) δ = 166.6 (7-C), 131.8 (5-C), 130.8 (6-C), 129.4 (4-C), 126.0 (3-C), 83.5 (1-C), 82.7 (2-C) ppm.

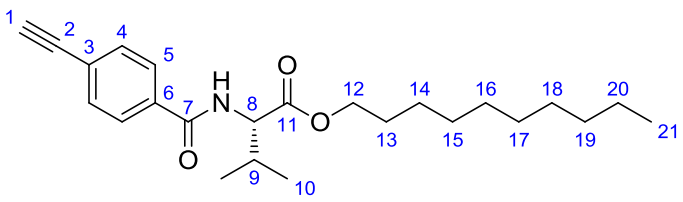
1.2.3 *N*-4-Ethynylbenzoyl-L-valine decyl ester 6



2 **6**

To a solution of 4-Ethynyl-benzoic acid **5** (2.0 g, 13.7 mmol, 1.0 eq.) in 60 mL of dry THF and 150 mL of dry DCM was added carbonyldiimidazole (CDI; 2.4 g, 15.1 mmol, 1.1 eq.) at 0°C in one portion. Gas evolution was observed and the solution was slowly warmed to room temperature. The mixture was stirred for 2 h until the gas evolution ceased.

A solution of L-Valine decyl ester hydrotosylate **2** (5.9 g, 13.7 mmol, 1.0 eq.) in 50 mL dichloromethane was washed with 50 mL saturated aqueous sodium carbonate solution, dried over Na_2SO_4, and evaporated to obtain the free base which was dissolved in 50 mL of dry DCM. The first solution, containing the CDI-activated 4-Ethynyl-benzoic acid **5**, was again cooled to 0°C and the L-Valine decyl ester solution was slowly added. After gas formation receded the solution was slowly warmed to room temperature and stirred for 8 h. The solvents were then evaporated to obtain a yellowish oil, which was dissolved in 140 mL DCM and then washed two times with 100 mL water and once with 100 mL brine. The organic layer was dried over $MgSO_4$ and evaporated to obtain a yellowish oil. This was purified by flash column chromatography (isocratic elution with petroleum ether : ethyl acetate = 10:1 (*v/v*)) to afford a colourless oil of **6**, which solidified after short time. Recrystallization from hexane afforded **6** as colourless needles (4.7 g, 12.2 mmol). The enantiomeric compound ***ent*-6** was prepared in the same manner using D-Valine decyl ester hydrotosylate ***ent*-2** as reactant. Yield 89 %.



6

^{1}H-NMR ($CDCl_3$, 500 MHz, 300 K) δ = 7.77 (d, 2H, ^{3}J = 8.6 Hz, 5-H), 7.56 (d, 2H, ^{3}J = 8.6 Hz, 4-H), 6.64 (d, 1H, ^{3}J = 8.6 Hz, NH), 4.76 (dd, 1H, ^{3}J = 8.6 Hz, ^{3}J = 4.7 Hz, 8-H), 4.16 (m, 2H, 12-H), 3.20 (s, 1H, 1-H), 2.29 (m, 1H, 9-H), 1.65 (m, 2H, 13-H), 1.39-1.21 (m, 14H, 14,15,16,17,18,19, 20-H), 1.01 (d, 3H, ^{3}J = 6.9 Hz, 10b-H), 0.99 (d, 3H, ^{3}J = 6.9 Hz, 10a-H), 0.88 (t, 3H, ^{3}J = 7.0 Hz, 21-H) ppm.

^{13}C-NMR ($CDCl_3$, 125 MHz, 300 K) δ = 172.2 (11-C), 166.4 (7-C), 134.2 (3-C), 132.3 (4-C), 127.0 (5-C), 125.6 (6-C), 82.7 (2-C), 79.6 (1-C), 65.7 (12-C), 57.5 (8-C), 31.9 (19-C), 31.7 (9-C), 29.49 + 29.47 + 29.3 (16-C, 17-C, 18-C), 29.2 (15-C), 28.6 (13-C), 25.9 (14-C), 22.6 (20-C), 19.0 (10b-C), 17.9 (10a-C), 14.1 (21-C) ppm.

EI-MS m/z (%): 385 (14.4, $[M]^+$), 371 (12, $[C_{23}H_{33}NO_3]^+$), 343 (5.6 $[C_{21}H_{29}NO_3]^+$), 200 (100, $[C_{13}H_{14}NO]^+$), 129 (100, $[C_9H_5O]^+$), 101 (60, $[C_8H_5]^+$).

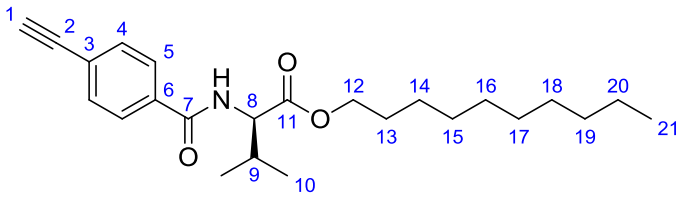
ESI-HRMS ($C_{24}H_{35}NO_3$) Ethyl acetate

negative mode		positive mode	
calculated:	m/z = 384.2533 $[M-H]^-$	calculated:	m/z = 408.2509 $[M+Na]^+$
measured:	m/z = 384.2568 $[M-H]^-$	measured:	m/z = 408.2473 $[M+Na]^+$

IR (KBr) ν = 3366.3 (s, CONH), 3289.4 (s, αC-H), 2926.9 (s, -CH_2/CH_3), 2856.1 (s, -CH_2/CH_3), 2111.8 (w, -C≡C-), 1733.1 (s, COOR), 1642.6 (s, CONH), 1530.9 (s, CH_2/CH_3), 1498.2 (s, CH_2/CH_3), 1194.6 (s, C-O) cm^{-1}.

EA ($C_{24}H_{35}NO_3$)	calculated:	C 74.77	H 9.15	N 3.63
	measured:	C 74.55	H 9.14	N 3.64

ORD (c = 1.00, $CHCl_3$):	$[\alpha]_{589}^{20}$ = 45.1	$[\alpha]_{579}^{20}$ = 49.5	$[\alpha]_{546}^{20}$ = 56.5
	$[\alpha]_{436}^{20}$ = 102.7	$[\alpha]_{405}^{20}$ = 129.1	$[\alpha]_{365}^{20}$ = 181.7

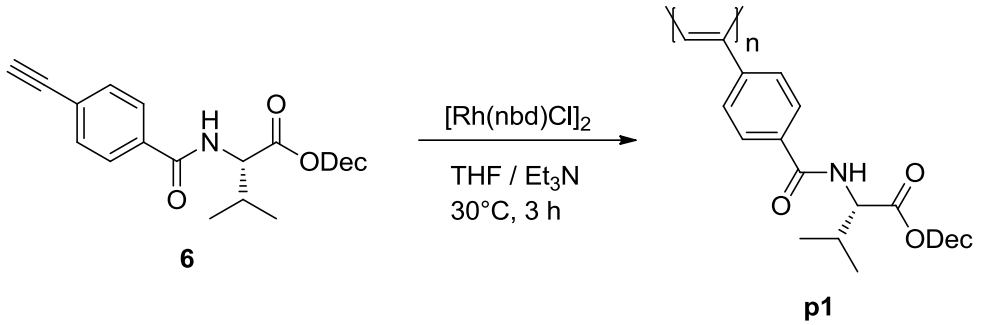


***ent*-6**

ORD (c = 1.04, $CHCl_3$): $[\alpha]_{589}^{20}$ = -45.6 $[\alpha]_{579}^{20}$ = -48.6 $[\alpha]_{546}^{20}$ = -56.0

$[\alpha]_{436}^{20}$ = -102.8 $[\alpha]_{405}^{20}$ = -128.7 $[\alpha]_{365}^{20}$ = -182.1

1.3 Polymerization



6 **p1**

Similar to a published procedure the polymerization was carried out in a flame dried Schlenk tube under dry argon atmosphere with $[Rh(nbd)Cl]_2$ as the catalyst.[3] All solvents were dried, freshly distilled and degassed (by using the freeze, pump and thaw technique) prior to use. A typical polymerization procedure is described below. The analytical data of all synthesized polymers are listed in Table SI 1.

Monomer **6** (2.000 g, 5.2 mmol, 1.000 eq.) was placed in a flame dried Schlenk tube with a magnetic stirring bar, which was then evacuated on a vacuum line and flushed with dry argon (three cycles). A rubber septum was attached to the tube, THF (5.5 mL) and triethylamine (1.8 mL) were added via syringe and the mixture was heated to 30°C. A solution of $[Rh(nbd)Cl]_2$ (2.4 mg, 5.2 µmol, 0.001 eq.) in 0.74 mL THF was added via syringe in one fast shot under rapid stirring. The polymerization proceeded rapidly and an orange-colored highly viscous solution was formed within a few seconds. After 3 h at 30°C, THF was added until the viscosity of the mixture allowed its dropwise transfer into 400 mL of methanol under shaking whereupon precipitation of the polymer occurred. After its isolation by centrifugation the obtained orange solid was dried *in vacuo*, redissolved in about 30 mL THF and then again precipitated in 400 mL methanol. The resulting orange polymer was centrifuged, dried *in vacuo*, taken up in 100 mL of benzene and lyophilized (1.90 g). Yield 95 %.

1.4 Analytical data of the polymers

Table SI 1: Analytical data of the polymers used in the RDC studies.

#	polymer	M_n [a]	M_w [b]	PDI [c]	$[\alpha]^{20}_{589}$	$[\alpha]^{20}_{578}$	$[\alpha]^{20}_{546}$	c [e]	$[\theta]^{T}_{max}$ [10^4*deg*cm^2*dmol^{-1}] [f]							λ_{max} [g]	c [h]
		[10^5 g/mol]	[10^6 g/mol]		[d]	[d]	[d]	[mg/cL]	-10°C	0°C	10°C	20°C	30°C	40°C	50°C	[nm]	[µg/mL]
1	p1-a	9.08	1.99	2.19	581.5	621.4	765.9	0.21	5.23	4.96	4.74	4.46	4.29	3.95	3.35	367.5	17.9
2	p1-b	5.88	1.35	2.29	627.5	670.5	826.7	0.17	5.14	4.87	4.68	4.43	4.23	3.96	3.52	368.0	15.1
3	ent-p1-c	3.25	3.67	11.30	-602,1	-642,8	-791,4	0.18	-4.86	-4.78	-4.59	-4.40	-4.18	-3.85	-3.34	369.0	18.7
4	ent-p1-d	1.46	2.06	14.04	-568,1	-607,9	-749,9	0.20	-5.35	-5.04	-4.79	-4.52	-4.31	-3.96	-3.49	367,5	13.4
5	p1-e	MWC [i]	MWC [i]	MWC [i]	617.9	658.7	812.2	0.18	5.36	5.18	4.97	4.73	4.48	4.12	3.57	368,5	14.3
6	ent-p1-f	1.96	1.15	5.84	-566.8	-605.1	-744,6	0.22	-2.14	-2.08	-1.98	-1.88	-1.76	-1.56	-1.33	369.0	10.7
7	p1-g	1.89	1.34	7.07	503.5	535.5	657.2	0.24	3.87	3.69	3.55	3.37	3.30	3.07	2.63	367.5	9.8
8	p1-h	MWC [i]	MWC [i]	MWC [i]	629.0	673.3	827.1	0.12	4.28	4.13	3.98	3.78	3.57	3.33	2.84	368.0	12.2
9	ent-p1-i	MWC [i]	MWC [i]	MWC [i]	-497.4	-532.0	-653.1	0.19	-3.47	-3.36	-3.19	-3.04	-2.93	-2.72	-2.40	367.5	12.3

a) Number average molecular weight calibrated against polystyrene standard; b) Mass average molecular weight calibrated against polystyrene standard; c) Polydispersity index; d) Optical rotatory dispersion at T=20°C and wavelength λ; e) Concentration of ORD samples in $CHCl_3$; f) Molar ellipticity at Cotton effect and temperature T; g) Wavelength λ of the Cotton effect; h) Concentration of CD spectroscopy samples in $CHCl_3$; i) Molecular weights were not determinable, because the hydrodynamic volume of the analysed polymer exceeded the Molecular Weight Cutoff (MWC) of the SEC column.

1.5 CD spectroscopy

1.5.1 Polymer p1-a

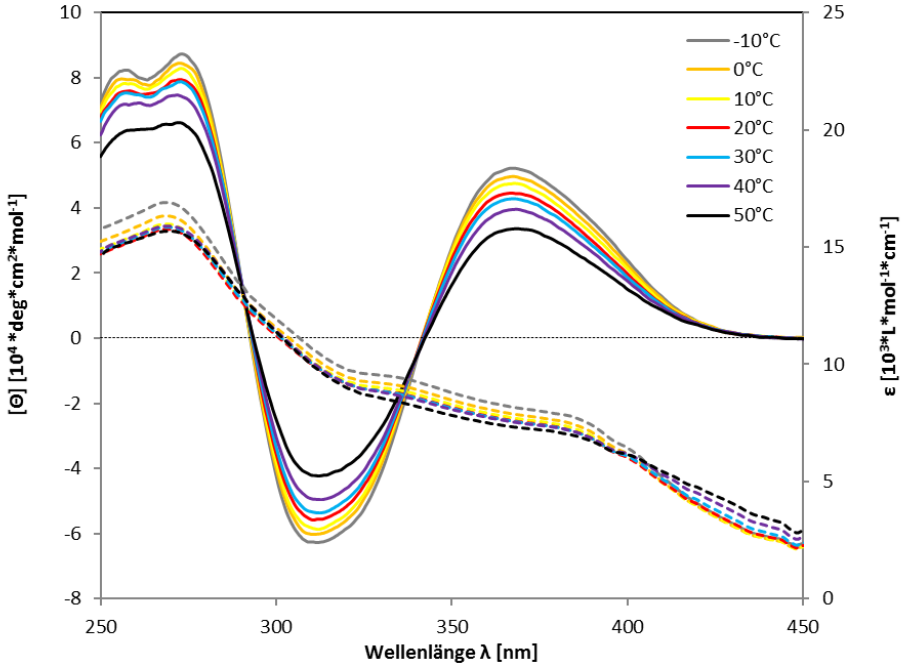


Figure SI 1: Temperature dependent UV and CD spectra of **p1-a**.

1.5.2 Polymer p1-b

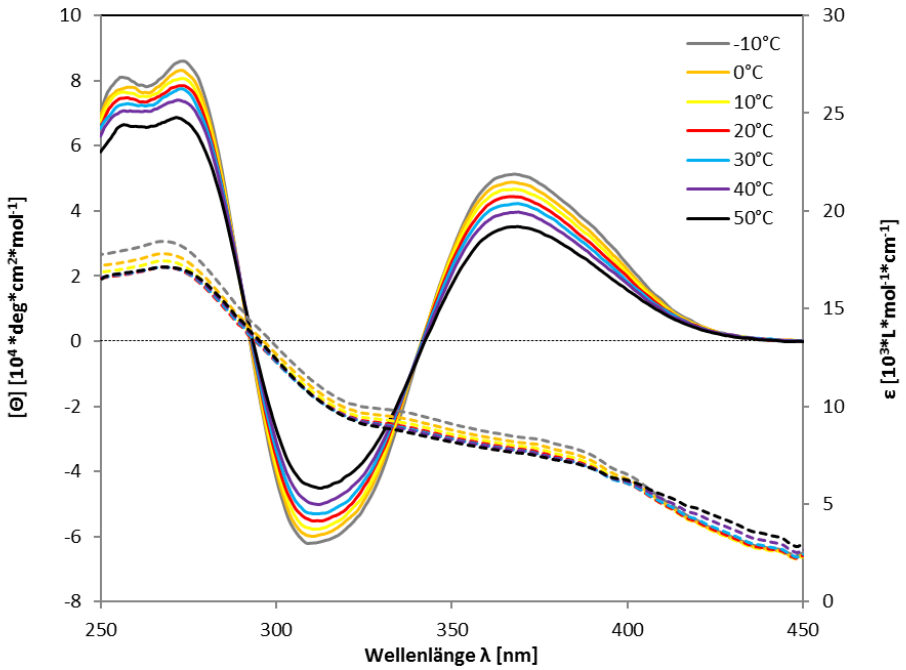


Figure SI 2: Temperature dependent UV and CD spectra of **p1-b**.

1.5.3 Polymer *ent*-p1-c

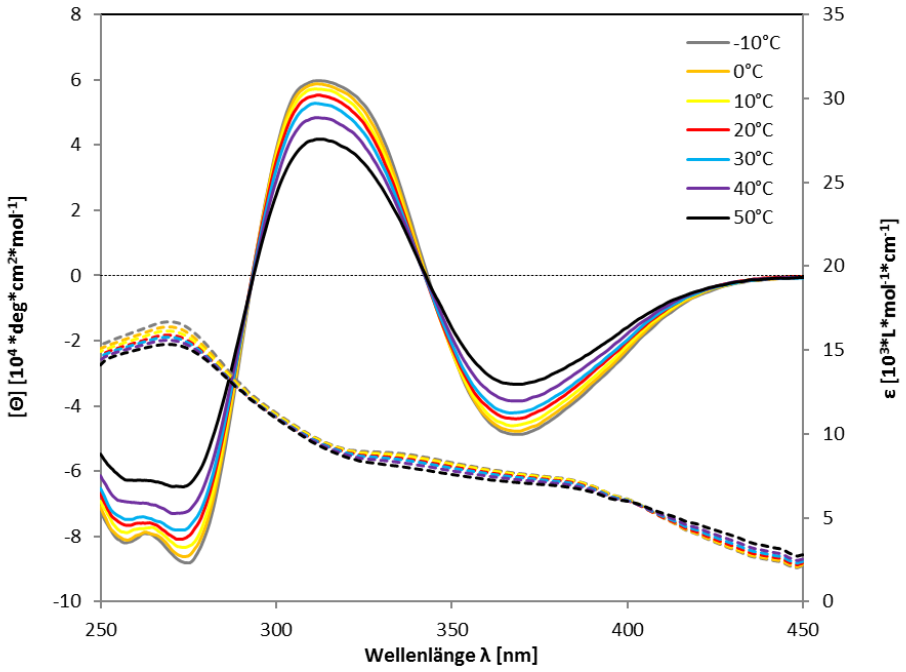


Figure SI 3: Temperature dependent UV and CD spectra of ***ent*-p1-c**.

1.5.4 Polymer *ent*-p1-d

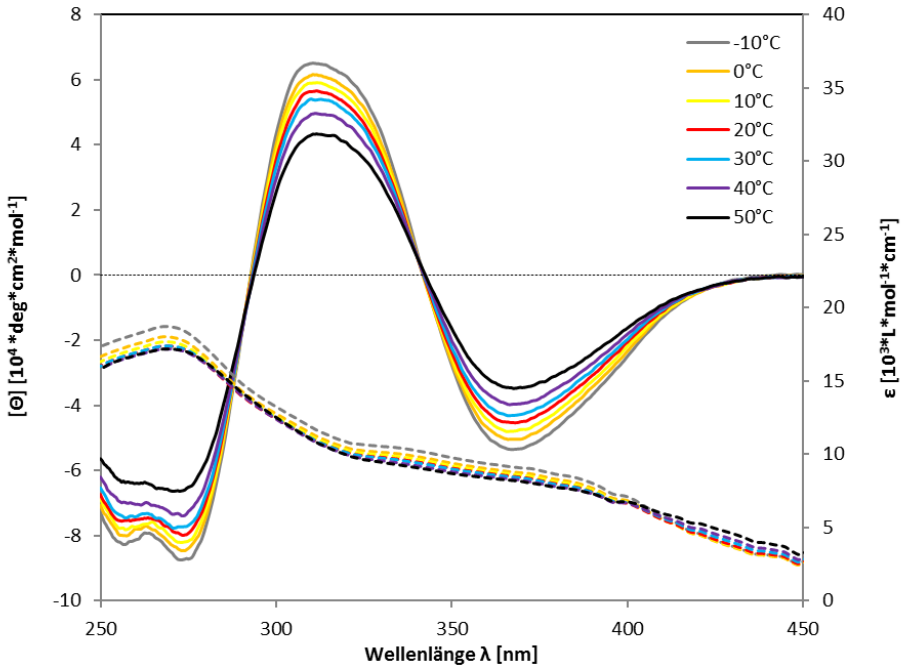


Figure SI 4: Temperature dependent UV and CD spectra of ***ent*-p1-d**.

1.5.5 Polymer p1-e

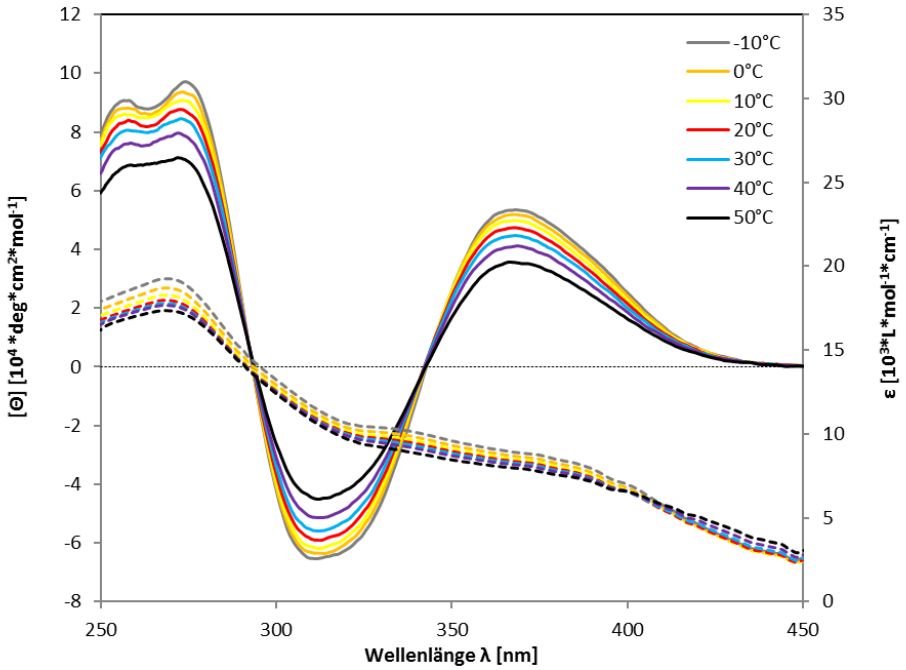


Figure SI 5: Temperature dependent UV and CD spectra of **p1-e**.

1.5.6 Polymer *ent*-p1-f

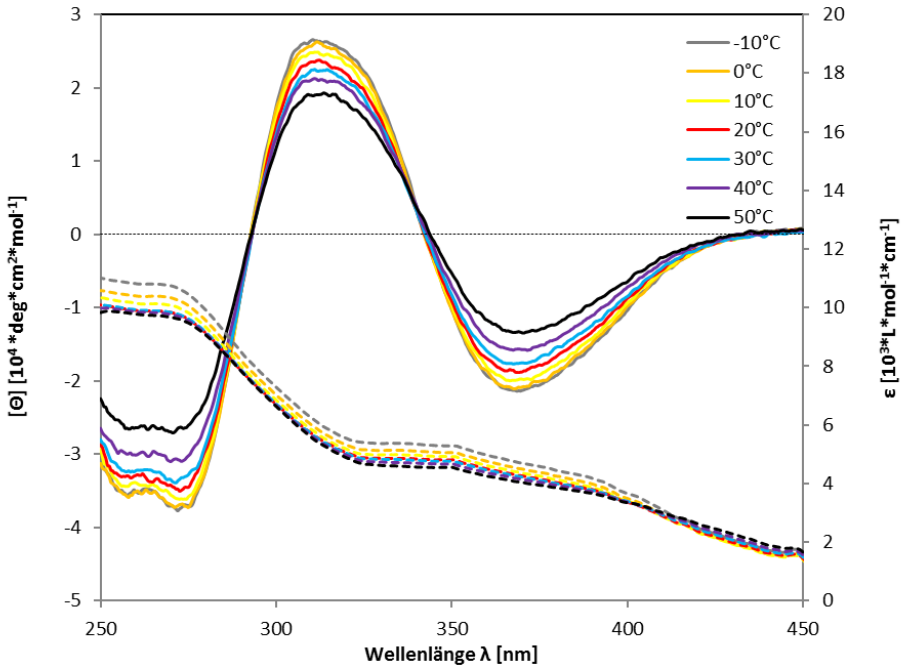


Figure SI 6: Temperature dependent UV and CD spectra of ***ent*-p1-f**.

1.5.7 Polymer p1-g

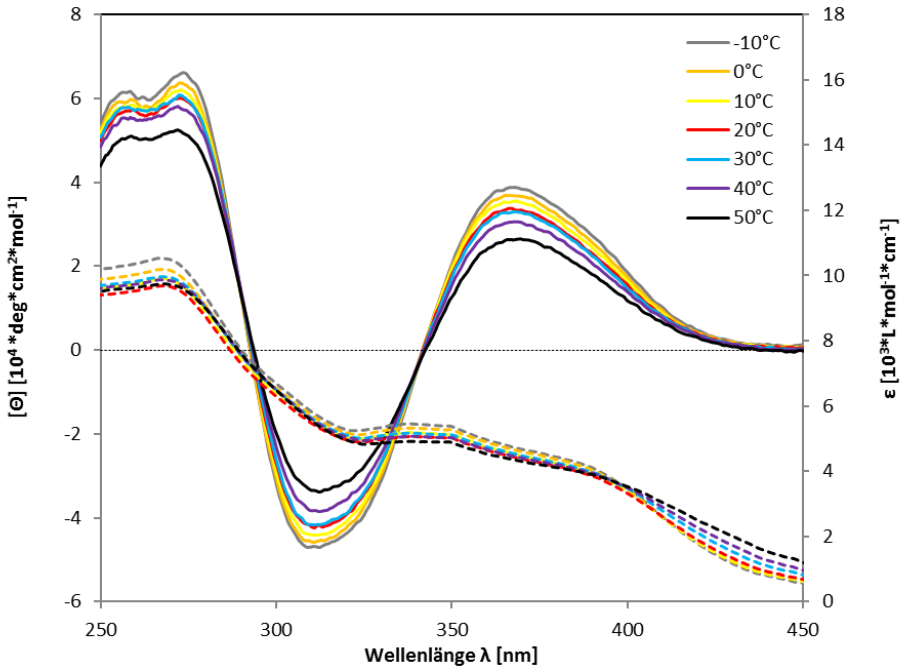


Figure SI 7: Temperature dependent UV and CD spectra of **p1-g**.

1.5.8 Polymer p1-h

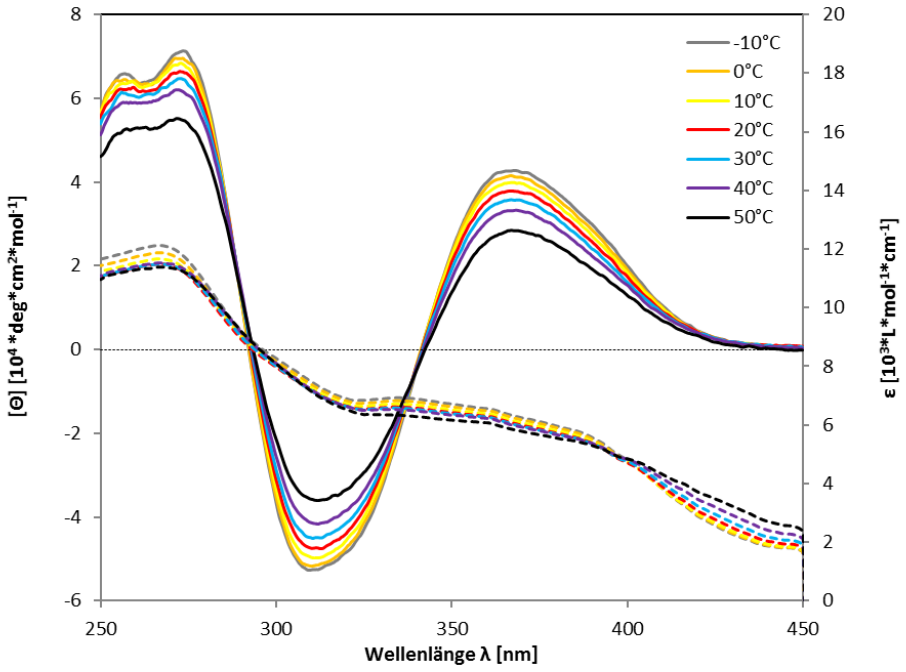


Figure SI 8: Temperature dependent UV and CD spectra of **p1-h**.

1.5.9 Polymer *ent*-p1-i

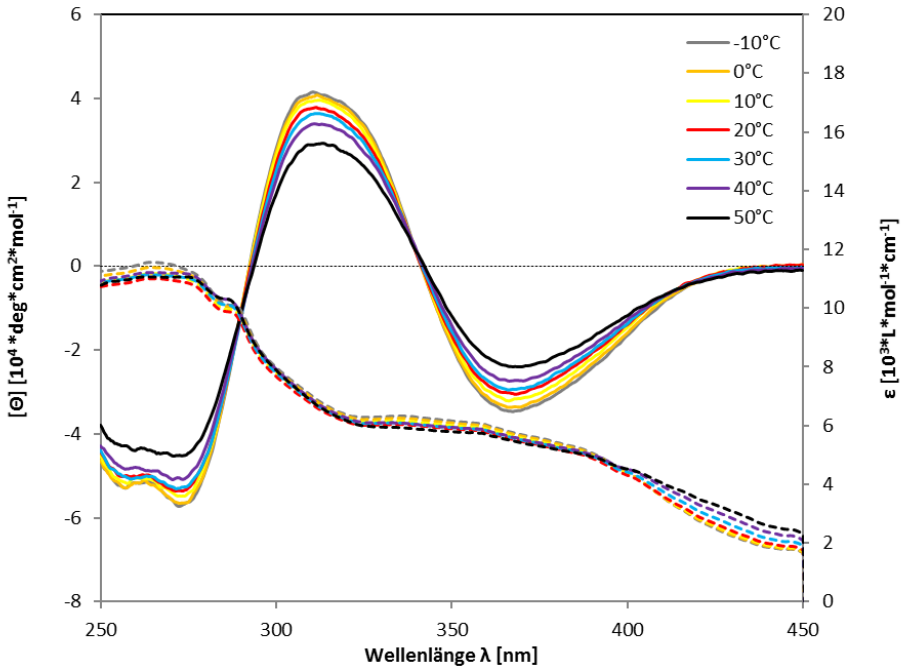


Figure SI 9: Temperature dependent UV and CD spectra of **p1-i**.

2 NMR studies

2.1 Sample preparation

The liquid crystalline phases were prepared directly in the NMR tube (5 mm). A total amount of 100-135 mg of the polymer **p1**/***ent*-p1** (for exact composition see Table SI 2) was weighed directly into the NMR tube. After adding a DMSO-d_6 capillary (for calibration and to provide the lock signal) and a stock solution of the analyte in $CDCl_3$, the NMR-tube was sealed and the polymer was allowed to dissolve overnight. The sample was centrifuged back and forth (1000 rpm) until the ^{2}H-signals of the solvent were sharp and the line widths constant.
For a video see: https://www.youtube.com/watch?v=C8cNWgJViGw

Table SI 2: Sample compositions, quadrupolar splitting of $CDCl_3$, GDO and quality of fit.

#	polymer	T [K]	m ($CDCl_3$) [mg]	analyte	m (analyte) [mg]	m (polymer) [mg]	$\Delta\nu_Q$ [a] [Hz]	GDO [b] [10^{-4}]	RMSD [c] [Hz]
1	**p1-a**	300	491.8	(-)-α-Pinene	25.3	110.9	85	3.99	0.16
2	***ent*-p1-c**	300	473.5	(-)-α-Pinene	29.8	106.9	89	4.55	0.21
3	**p1-e**	300	365.9	β-Caryophyllene	20.5	102.6	110	14.64	0.32
4	***ent*-p1-f**	292	470.0	β-Caryophyllene	23.2	104.1	102	12.41	0.13
5	**p1-g**	300	511.8	(+)-IPC	16.9	119.2	67	9.21	0.26
6	**p1-g**	300	491.0	(-)-IPC	16.2	123.1	75	11.94	0.46
7	**p1-e**	300	530.0	(-)-Menthol	26.5	111.8	62	19.10	0.99
8	***ent*-p1-c**	300	494.8	(-)-Menthol	26.7	105.7	74	17.99	1.26
9	**p1-a**	293	577.0	D-Fructoseacetonide	25.0	105.0	36	11.46	0.36
10	***ent*-p1-c**	295	598.1	D-Fructoseacetonide	27.9	106.1	33	9.76	0.49
11	**p1-b**	300	466.9	(+)-Camphor	23.9	106.4	73	4.94	0.16
12	**p1-b**	300	490.2	(-)-Camphor	23.7	112.9	81	5.20	0.25
13	***ent*-p1-c**	300	472.3	(+)-Carvone	25.0	105.2	63	6.87	0.34
14	***ent*-p1-c**	300	472.3	(-)-Carvone	24.2	105.8	70	8.62	0.48
15	**p1-e**	300	513.9	(-)-Perillaldehyde	27.1	110.7	54	7.14	0.49
16	**ent-p1-d**	300	486.4	(-)-Perillaldehyde	29.0	102.5	34	6.59	0.57
17	**p1-a**	300	473.9	(-)-Nicotine	28.3	106.2	56	10.88	0.11
18	***ent*-p1-c**	300	477.0	(-)-Nicotine	22.2	106.1	57	12.76	0.10
19	**p1-b**	300	422.4	(-)-Sparteine	28.4	106.4	96	13.13	0.50
20	***ent*-p1-d**	300	478.4	(-)-Sparteine	22.4	114.2	95	13.56	0.61
21	**p1-h**	300	491.1	(-)-Strychnine	34.3	115.3	57	13.99	0.78
22	***ent*-p1-i**	293	573.4	(-)-Strychnine	38.8	134.6	54	9.74	0.43
23	**p1-a**	300	487.9	(-)-Cytisine	15.7	106.0	81	11.81	0.88
24	***ent*-p1-d**	300	495.1	(-)-Cytisine	15.5	109.5	80	14.22	1.18

[a] Value of the quadrupolar splitting of the solvent ($CDCl_3$); [b] Generalized degree of order; [c] Root mean square deviation of calculated and experimental RDCs.

2.2 Measurement conditions

All spectra of the analytes in isotropic and oriented samples were recorded on a 500 MHz spectrometer (Bruker DRX-500) with a triple resonance inverse probe equipped with a z-gradient and a BCU extreme. All measurements were carried out without sample spinning. The total coupling constants (^1T) and scalar coupling constants (^1J) were measured by CLIP-HSQC experiments (INEPT delay 145 Hz).[4] A total of 8 k data points were sampled in the direct dimension over an appropriate spectral width. In the indirect dimension 256 data points were acquired over an appropriate spectral width. The spectra were processed using a $\pi/2$ shifted squared sine bell in both dimensions. No zero filling was applied in F2, but by a factor of four in the indirect F1 dimension. For each coupling the corresponding traces of the CLIP-HSQC spectra were extracted, subjected to an inverse Fourier transformation and processed by zero filling to 32 k points. A copy of the trace was overlaid with the original one and shifted until the difference signal reached a minimum. Temperature dependent spectra were measured in steps of two Kelvin (300 K to 250 K; 251 K to 315 K; 316 K to 300 K) with an equilibration time interval of 60 seconds at each temperature.

3 Calculation of orientational properties

The orientational properties were calculated using the program *ConArch*$^+$.[5] For that purpose the coordinates of the analytes (DFT; B3LYP/6-311+G(d,p)[6] as well as the measured RDCs were provided as input. The latter were calculated using $^1T_{CH} = {}^1J_{CH} + 2{}^1D_{CH}$ with $^1T_{CH}$ extracted from the CLIP-HSQC-spectra as described above. For the methyl groups, the measured $^1D_{CH}$ was converted to the corresponding $^1D_{CC}$ according to the literature;[7] only the latter was used for the determination of the order tensor. All uncertainties were calculated using a Monte-Carlo simulation with 10000 steps as described in the literature.[8]

The cosine of the generalized angle between two alignment tensors has been calculated as follows.[9]

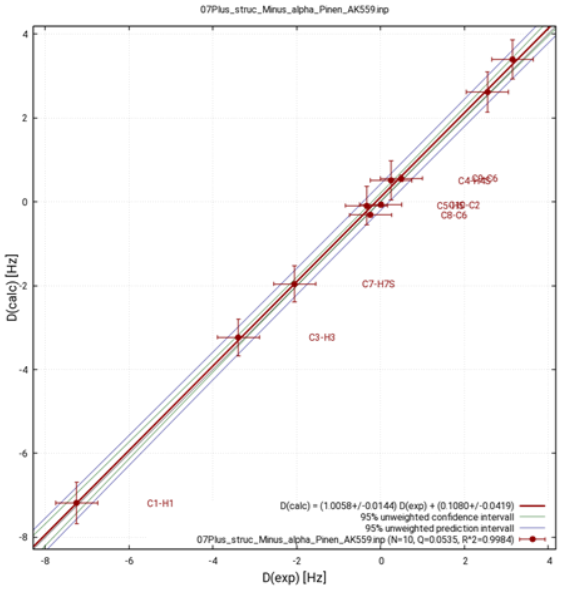
$$GCB = cos\beta = \frac{\langle A^{(1)}|A^{(2)}\rangle}{|A^{(1)}||A^{(2)}|}$$

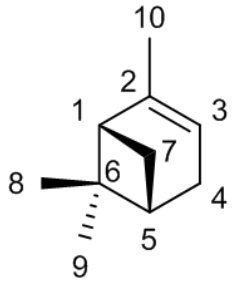
$$\text{with } \langle A^{(1)}|A^{(2)}\rangle = \sum_{i,j} A^{(1)}_{i,j} A^{(2)}_{i,j} \text{ und } |A| = \sqrt{\langle A|A\rangle} = \sqrt{\sum_{i,j} A^2_{i,j}}$$

3.1 Experimental and calculated RDCs –Tensor properties

3.1.1 (-)-α-Pinene in p1-a

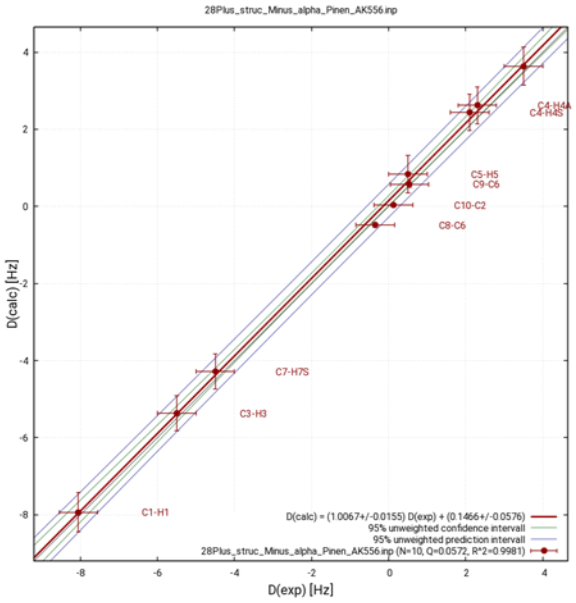
```
------------------------------------------------------------------------------
info : Start Single-Conformer-Single-Tensor (SCST) Fit with 10 RDCs
------------------------------------------------------------------------------

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
 -2.121918e-04  1.496034e-04 -2.152261e-04  8.366512e-05  1.631495e-04
Saupe Tensor (S):                          Alignment Tensor (A):
  1.808976e-04 -2.152261e-04  8.366512e-05    1.205984e-04 -1.434841e-04  5.577675e-05
 -2.152261e-04  3.129422e-05  1.631495e-04   -1.434841e-04  2.086281e-05  1.087663e-04
  8.366512e-05  1.631495e-04 -2.121918e-04    5.577675e-05  1.087663e-04 -1.414612e-04
Trace of Saupe Tensor:       -2.710505e-20 Trace of Alignment Tensor:   -1.807004e-20
Eigenvectors of Saupe Tensor:              Eigenvectors of Alignment Tensor:
  4.988949e-01  8.007749e-01  3.314565e-01    4.988949e-01  8.007749e-01  3.314565e-01
  6.130034e-01 -5.964032e-01  5.181989e-01    6.130034e-01 -5.964032e-01  5.181989e-01
  6.126424e-01 -5.534280e-02 -7.884202e-01    6.126424e-01 -5.534280e-02 -7.884202e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
  1.918506e-05  3.354120e-04 -3.545971e-04    1.279004e-05  2.236080e-04 -2.363981e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
 -3.363942e-04  1.082976e-04  2.111835e-04  9.682459e-05 -2.785924e-04
Tensor Properties:
A(axial)     =  -3.545971e-04        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)   =  -2.108180e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =  5.945282e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =  8.917924e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO          =  3.988387e-04         # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
         D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights    Atom Labels
D[01] =       0.560419      0.082073      0.500000      0.500000      1.000000   r[01] =      -0.060419   w[01] =       0.100000   C9-C6
D[02] =      -0.067952      0.054400      0.010000      0.500000      1.000000   r[02] =       0.077952   w[02] =       0.100000   C10-C2
D[03] =      -0.313836      0.051355     -0.240000      0.500000      1.000000   r[03] =       0.073836   w[03] =       0.100000   C8-C6
D[04] =       0.510004      0.465934      0.250000      0.500000      1.000000   r[04] =      -0.260004   w[04] =       0.100000   C4-H4S
D[05] =       3.395989      0.472049      3.150000      0.500000      1.000000   r[05] =      -0.245989   w[05] =       0.100000   C4-H4A
D[06] =      -1.957683      0.429163     -2.050000      0.500000      1.000000   r[06] =      -0.092317   w[06] =       0.100000   C7-H7S
D[07] =       2.616317      0.479109      2.550000      0.500000      1.000000   r[07] =      -0.066317   w[07] =       0.100000   C7-H7A
D[08] =      -0.089485      0.463169     -0.330000      0.500000      1.000000   r[08] =      -0.240515   w[08] =       0.100000   C5-H5
D[09] =      -7.182067      0.493038     -7.250000      0.500000      1.000000   r[09] =      -0.067933   w[09] =       0.100000   C1-H1
D[10] =      -3.231022      0.437944     -3.390000      0.500000      1.000000   r[10] =      -0.158978   w[10] =       0.100000   C3-H3

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =              5                # rank of cosine matrix (check input if rank < 5)
cond  =   2.232186e+00                # condition number of cosine matrix (check input and singular values if very large)
chisq =       0.024395                # weighted total sum of squared residuals
aic   =      10.975793                # information criterion (AIC) for 5 degrees of freedom
rmsd  =       0.156188                # unweighted root mean square deviation
qfac  =       0.053521                # weighted Q-Factor as defined by Cornilescu
r^2   =       0.996971                # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =       1.992477      1.972000  # mean absolute (calc./exp.) parameter D[i]
|D|min=       0.067952      0.010000  # min. absolute (calc./exp.) parameter D[i]
|D|max=       7.182067      7.250000  # max. absolute (calc./exp.) parameter D[i]
Drange=      -7.250000      3.395989  # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =       0.107984 +/-  0.041924  # linear regression intercept and error
c(m)  =       1.005758 +/-  0.014366  # linear regression slope and error
chisq =       0.013298                # weighted total sum of squared residuals
R     =       0.999185                # weighted Pearson correlation coefficient R
R^2   =       0.998370                # weighted Pearson correlation coefficient R^2
```

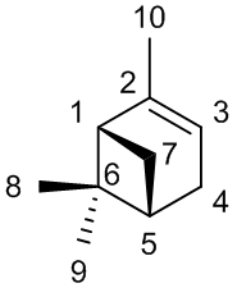




3.1.2 (-)-α-Pinene in *ent*-p1-c

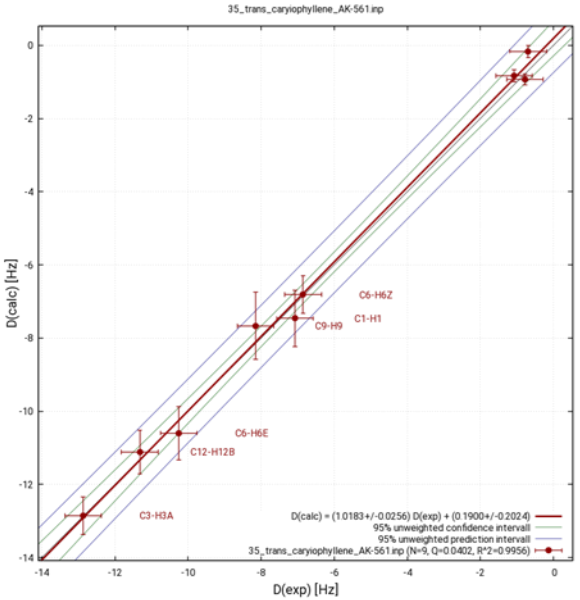
```
------------------------------------------------------------------------------
info : Start Single-Conformer-Single-Tensor (SCST) Fit with 10 RDCs
------------------------------------------------------------------------------

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
 -3.122758e-04  2.608684e-04 -2.185461e-04  1.023960e-04  8.446351e-05
Saupe Tensor (S):                          Alignment Tensor (A):
  2.865721e-04 -2.185461e-04  1.023960e-04    1.910481e-04 -1.456974e-04  6.826402e-05
 -2.185461e-04  2.570366e-05  8.446351e-05   -1.456974e-04  1.713578e-05  5.630901e-05
  1.023960e-04  8.446351e-05 -3.122758e-04    6.826402e-05  5.630901e-05 -2.081838e-04
Trace of Saupe Tensor:       -5.421011e-20 Trace of Alignment Tensor:   -3.614007e-20
Eigenvectors of Saupe Tensor:              Eigenvectors of Alignment Tensor:
  4.122608e-01  2.516856e-01 -8.756114e-01    4.122608e-01  2.516856e-01 -8.756114e-01
  8.131286e-01  3.318439e-01  4.782274e-01    8.131286e-01  3.318439e-01  4.782274e-01
  4.109293e-01 -9.091391e-01 -6.784657e-02    4.109293e-01 -9.091391e-01 -6.784657e-02
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
 -4.241528e-05 -3.714530e-04  4.138682e-04    -2.827685e-05 -2.476353e-04  2.759122e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
 -4.950604e-04  1.325432e-04  1.093310e-04  1.688363e-04 -2.828899e-04
Tensor Properties:
A(axial)      =   4.138682e-04        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =   2.193584e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   5.300200e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   7.950300e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   4.553850e-04        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)      Normalized Weights    Atom Labels
D[01] =       0.572815      0.088384      0.540000      0.500000      1.000000   r[01] =      -0.032815   w[01] =       0.100000   C9-C6
D[02] =       0.035431      0.050851      0.120000      0.500000      1.000000   r[02] =       0.084569   w[02] =       0.100000   C10-C2
D[03] =      -0.485281      0.059208     -0.350000      0.500000      1.000000   r[03] =       0.135281   w[03] =       0.100000   C8-C6
D[04] =       2.437453      0.476888      2.100000      0.500000      1.000000   r[04] =      -0.337453   w[04] =       0.100000   C4-H4S
D[05] =       2.619623      0.479799      2.300000      0.500000      1.000000   r[05] =      -0.319623   w[05] =       0.100000   C4-H4A
D[06] =      -4.283060      0.449236     -4.500000      0.500000      1.000000   r[06] =      -0.216940   w[06] =       0.100000   C7-H7S
D[07] =       3.637614      0.494639      3.500000      0.500000      1.000000   r[07] =      -0.137614   w[07] =       0.100000   C7-H7A
D[08] =       0.836345      0.481732      0.500000      0.500000      1.000000   r[08] =      -0.336345   w[08] =       0.100000   C5-H5
D[09] =      -7.937687      0.506792     -8.050000      0.500000      1.000000   r[09] =      -0.112313   w[09] =       0.100000   C1-H1
D[10] =      -5.369164      0.459017     -5.500000      0.500000      1.000000   r[10] =      -0.130836   w[10] =       0.100000   C3-H3

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =            5                  # rank of cosine matrix (check input if rank < 5)
cond  =   2.232186e+00                # condition number of cosine matrix (check input and singular values if very large)
chisq =       0.045142                # weighted total sum of squared residuals
aic   =      11.805696                # information criterion (AIC) for 5 degrees of freedom
rmsd  =       0.212467                # unweighted root mean square deviation
qfac  =       0.057209                # weighted Q-Factor as defined by Cornilescu
r^2   =       0.996506                # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =       2.821447      2.746000  # mean absolute (calc./exp.) parameter D[i]
|D|min=       0.035431      0.120000  # min. absolute (calc./exp.) parameter D[i]
|D|max=       7.937687      8.050000  # max. absolute (calc./exp.) parameter D[i]
Drange=      -8.050000      3.637614  # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =       0.146625 +/-  0.057591  # linear regression intercept and error
c(m)  =       1.006656 +/-  0.015507  # linear regression slope and error
chisq =       0.024855                # weighted total sum of squared residuals
R     =       0.999052                # weighted Pearson correlation coefficient R
R^2   =       0.998105                # weighted Pearson correlation coefficient R^2
```

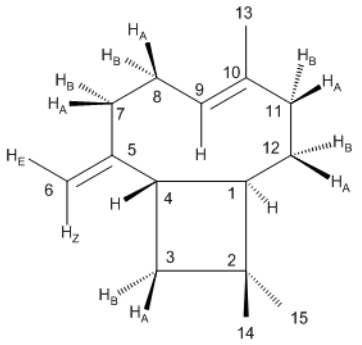




3.1.3 β-Caryophyllene in p1-e

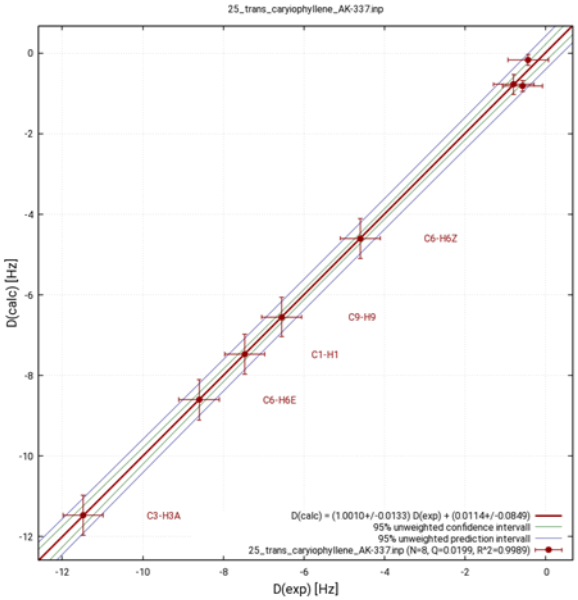
```
------------------------------------------------------------------------------
info : Start Single-Conformer-Single-Tensor (SCST) Fit with 9 RDCs
------------------------------------------------------------------------------

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
 -1.889347e-04 -4.039204e-05 -6.384480e-04 -6.644401e-04 -8.550901e-04
Saupe Tensor (S):                                Alignment Tensor (A):
  7.427131e-05 -6.384480e-04 -6.644401e-04         4.951421e-05 -4.256320e-04 -4.429600e-04
 -6.384480e-04  1.146634e-04 -8.550901e-04        -4.256320e-04  7.644223e-05 -5.700601e-04
 -6.644401e-04 -8.550901e-04 -1.889347e-04        -4.429600e-04 -5.700601e-04 -1.259564e-04
Trace of Saupe Tensor:        0.000000e+00       Trace of Alignment Tensor:    0.000000e+00
Eigenvectors of Saupe Tensor:                    Eigenvectors of Alignment Tensor:
 -8.308891e-01 -2.109688e-01 -5.148937e-01        -8.308891e-01 -2.109688e-01 -5.148937e-01
  1.408019e-01  8.155096e-01 -5.613545e-01         1.408019e-01  8.155096e-01 -5.613545e-01
  5.383290e-01 -5.389213e-01 -6.478933e-01         5.383290e-01 -5.389213e-01 -6.478933e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
  6.129498e-04  8.449047e-04 -1.457855e-03         4.086332e-04  5.632698e-04 -9.719030e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
 -2.995240e-04 -8.600627e-04 -1.106843e-03 -2.614208e-05 -8.264182e-04
Tensor Properties:
A(axial)      =  -1.457855e-03        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =  -1.546366e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   1.060714e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   1.591071e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   1.463993e-03        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights    Atom Labels
D[01] =     -0.927988      0.147688     -0.780000      0.500000      1.000000   r[01] =      0.147988   w[01] =      0.111111   C13-C10
D[02] =     -0.830515      0.164575     -1.080000      0.500000      1.000000   r[02] =     -0.249485   w[02] =      0.111111   C15-C2
D[03] =     -0.162266      0.166274     -0.690000      0.500000      1.000000   r[03] =     -0.527734   w[03] =      0.111111   C14-C2
D[04] =     -7.462388      0.767141     -7.070000      0.500000      1.000000   r[04] =      0.392388   w[04] =      0.111111   C1-H1
D[05] =     -6.811733      0.509168     -6.850000      0.500000      1.000000   r[05] =     -0.038267   w[05] =      0.111111   C6-H6Z
D[06] =    -10.597036      0.729605    -10.250000      0.500000      1.000000   r[06] =      0.347036   w[06] =      0.111111   C6-H6E
D[07] =     -7.669205      0.917295     -8.150000      0.500000      1.000000   r[07] =     -0.480795   w[07] =      0.111111   C9-H9
D[08] =    -12.853262      0.512791    -12.870000      0.500000      1.000000   r[08] =     -0.016738   w[08] =      0.111111   C3-H3A
D[09] =    -11.114219      0.599743    -11.320000      0.500000      1.000000   r[09] =     -0.205781   w[09] =      0.111111   C12-H12B

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =            5                  # rank of cosine matrix (check input if rank < 5)
cond  =   8.361395e+00                # condition number of cosine matrix (check input and singular values if very large)
chisq =      0.101367                 # weighted total sum of squared residuals
aic   =     13.649211                 # information criterion (AIC) for 5 degrees of freedom
rmsd  =      0.318382                 # unweighted root mean square deviation
qfac  =      0.040204                 # weighted Q-Factor as defined by Cornilescu
r^2   =      0.994842                 # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =      6.492068      6.562222  # mean absolute (calc./exp.) parameter D[i]
|D|min=      0.162266      0.690000  # min. absolute (calc./exp.) parameter D[i]
|D|max=     12.853262     12.870000  # max. absolute (calc./exp.) parameter D[i]
Drange=    -12.870000     -0.162266  # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =      0.190039 +/-  0.202437   # linear regression intercept and error
c(m)  =      1.018269 +/-  0.025563   # linear regression slope and error
chisq =      0.089887                 # weighted total sum of squared residuals
R     =      0.997802                 # weighted Pearson correlation coefficient R
R^2   =      0.995608                 # weighted Pearson correlation coefficient R^2
```

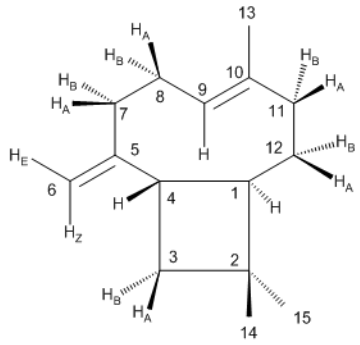




3.1.4 β-Caryophyllene in *ent*-p1-f

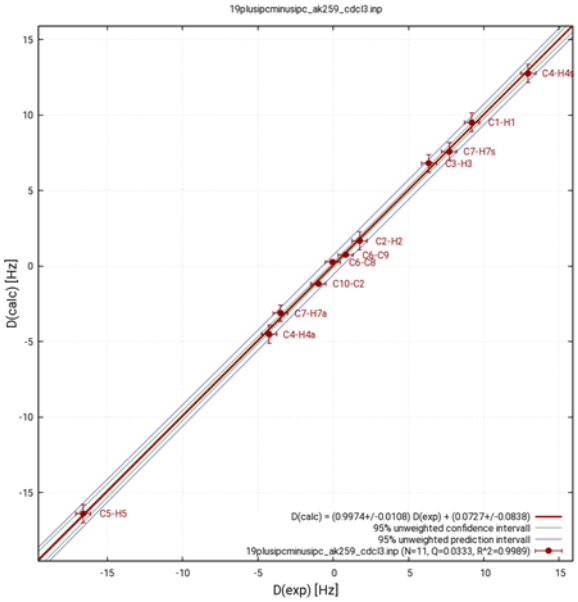
```
------------------------------------------------------------------------------
info : Start Single-Conformer-Single-Tensor (SCST) Fit with 8 RDCs
------------------------------------------------------------------------------

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
 -1.218728e-04  3.507202e-04 -5.230835e-04 -5.830206e-04 -7.062859e-04
Saupe Tensor (S):                                Alignment Tensor (A):
  2.362965e-04 -5.230835e-04 -5.830206e-04         1.575310e-04 -3.487223e-04 -3.886804e-04
 -5.230835e-04 -1.144237e-04 -7.062859e-04        -3.487223e-04 -7.628245e-05 -4.708573e-04
 -5.830206e-04 -7.062859e-04 -1.218728e-04        -3.886804e-04 -4.708573e-04 -8.124854e-05
Trace of Saupe Tensor:       -1.355253e-20       Trace of Alignment Tensor:   -9.035018e-21
Eigenvectors of Saupe Tensor:                    Eigenvectors of Alignment Tensor:
  3.595536e-01  8.069546e-01  4.685569e-01         3.595536e-01  8.069546e-01  4.685569e-01
 -7.879855e-01 -6.380834e-03  6.156608e-01        -7.879855e-01 -6.380834e-03  6.156608e-01
  4.998000e-01 -5.905791e-01  6.335742e-01         4.998000e-01 -5.905791e-01  6.335742e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
  5.722366e-04  6.671231e-04 -1.239360e-03         3.814910e-04  4.447487e-04 -8.262398e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
 -1.932087e-04 -7.546720e-04 -9.142287e-04  2.269891e-04 -6.770883e-04
Tensor Properties:
A(axial)      =  -1.239360e-03        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =  -6.325769e-05        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   5.104063e-02        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   7.656094e-02        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   1.240570e-03        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights    Atom Labels
D[01] =     -0.815430      0.129724     -0.570000      0.500000      1.000000   r[01] =      0.245430   w[01] =      0.125000   C13-C10
D[02] =     -0.772438      0.249476     -0.790000      0.500000      1.000000   r[02] =     -0.017562   w[02] =      0.125000   C15-C2
D[03] =     -0.167577      0.142262     -0.430000      0.500000      1.000000   r[03] =     -0.262423   w[03] =      0.125000   C14-C2
D[04] =     -7.472370      0.494308     -7.470000      0.500000      1.000000   r[04] =      0.002370   w[04] =      0.125000   C1-H1
D[05] =     -4.594832      0.496917     -4.600000      0.500000      1.000000   r[05] =     -0.005168   w[05] =      0.125000   C6-H6Z
D[06] =     -8.600779      0.499888     -8.600000      0.500000      1.000000   r[06] =      0.000779   w[06] =      0.125000   C6-H6E
D[07] =     -6.547640      0.489881     -6.550000      0.500000      1.000000   r[07] =     -0.002360   w[07] =      0.125000   C9-H9
D[08] =    -11.468856      0.501061    -11.480000      0.500000      1.000000   r[08] =     -0.011144   w[08] =      0.125000   C3-H3A

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =           5                  # rank of cosine matrix (check input if rank < 5)
cond  =   1.812882e+01                # condition number of cosine matrix (check input and singular values if very large)
chisq =       0.016197                # weighted total sum of squared residuals
aic   =      10.518290                # information criterion (AIC) for 5 degrees of freedom
rmsd  =       0.127266                # unweighted root mean square deviation
qfac  =       0.019914                # weighted Q-Factor as defined by Cornilescu
r^2   =       0.998936                # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =       5.054990      5.061250  # mean absolute (calc./exp.) parameter D[i]
|D|min=       0.167577      0.430000  # min. absolute (calc./exp.) parameter D[i]
|D|max=      11.468856     11.480000  # max. absolute (calc./exp.) parameter D[i]
Drange=     -11.480000     -0.167577  # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =       0.011406 +/-  0.084947  # linear regression intercept and error
c(m)  =       1.001017 +/-  0.013292  # linear regression slope and error
chisq =       0.016142                # weighted total sum of squared residuals
R     =       0.999471                # weighted Pearson correlation coefficient R
R^2   =       0.998943                # weighted Pearson correlation coefficient R^2
```

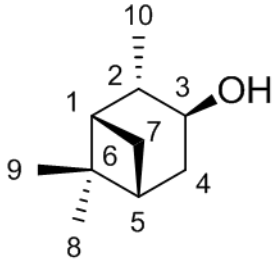




3.1.5 (+)-Isopinocampheol in p1-g

```
------------------------------------------------------------------------------
info : Start Single-Conformer-Single-Tensor (SCST) Fit with 11 RDCs
------------------------------------------------------------------------------

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
 -5.637775e-04 -3.341753e-04 -7.756092e-05  2.473222e-05  6.024143e-04
Saupe Tensor (S):                          Alignment Tensor (A):
  1.148011e-04 -7.756092e-05  2.473222e-05    7.653408e-05 -5.170728e-05  1.648815e-05
 -7.756092e-05  4.489764e-04  6.024143e-04   -5.170728e-05  2.993176e-04  4.016095e-04
  2.473222e-05  6.024143e-04 -5.637775e-04    1.648815e-05  4.016095e-04 -3.758517e-04
Trace of Saupe Tensor:        0.000000e+00 Trace of Alignment Tensor:    0.000000e+00
Eigenvectors of Saupe Tensor:              Eigenvectors of Alignment Tensor:
 -9.936958e-01 -9.632028e-02  5.736748e-02   -9.936958e-01 -9.632028e-02  5.736748e-02
 -6.314660e-02  9.036913e-01  4.235027e-01   -6.314660e-02  9.036913e-01  4.235027e-01
 -9.263439e-02  4.172103e-01 -9.040766e-01   -9.263439e-02  4.172103e-01 -9.040766e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
  1.121779e-04  7.353620e-04 -8.475399e-04    7.478529e-05  4.902413e-04 -5.650266e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
 -8.937740e-04  3.201382e-05  7.797755e-04 -2.162811e-04 -1.003962e-04
Tensor Properties:
A(axial)      =  -8.475399e-04        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =  -4.154560e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   4.901905e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   7.352858e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   9.207479e-04        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights    Atom Labels
D[01] =      9.517343      0.619412      9.200000      0.500000      1.000000   r[01] =     -0.317343   w[01] =      0.090909   C1-H1
D[02] =      1.670296      0.614212      1.750000      0.500000      1.000000   r[02] =      0.079704   w[02] =      0.090909   C2-H2
D[03] =      6.803624      0.571384      6.350000      0.500000      1.000000   r[03] =     -0.453624   w[03] =      0.090909   C3-H3
D[04] =     12.781538      0.597234     12.950000      0.500000      1.000000   r[04] =      0.168462   w[04] =      0.090909   C4-H4s
D[05] =     -4.510415      0.591619     -4.250000      0.500000      1.000000   r[05] =      0.260415   w[05] =      0.090909   C4-H4a
D[06] =    -16.398778      0.591258    -16.600000      0.500000      1.000000   r[06] =     -0.201222   w[06] =      0.090909   C5-H5
D[07] =      7.601800      0.601676      7.700000      0.500000      1.000000   r[07] =      0.098200   w[07] =      0.090909   C7-H7s
D[08] =     -3.118634      0.539534     -3.500000      0.500000      1.000000   r[08] =     -0.381366   w[08] =      0.090909   C7-H7a
D[09] =      0.253879      0.120941     -0.040000      0.500000      1.000000   r[09] =     -0.293879   w[09] =      0.090909   C6-C8
D[10] =      0.737565      0.104848      0.820000      0.500000      1.000000   r[10] =      0.082435   w[10] =      0.090909   C6-C9
D[11] =     -1.173470      0.097333     -0.980000      0.500000      1.000000   r[11] =      0.193470   w[11] =      0.090909   C10-C2

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =              5                # rank of cosine matrix (check input if rank < 5)
cond  =   2.128683e+00                 # condition number of cosine matrix (check input and singular values if very large)
chisq =      0.066836                 # weighted total sum of squared residuals
aic   =     12.940776                 # information criterion (AIC) for 5 degrees of freedom
rmsd  =      0.258526                 # unweighted root mean square deviation
qfac  =      0.033312                 # weighted Q-Factor as defined by Cornilescu
r^2   =      0.998862                 # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =      5.869758      5.830909   # mean absolute (calc./exp.) parameter D[i]
|D|min=      0.253879      0.040000   # min. absolute (calc./exp.) parameter D[i]
|D|max=     16.398778     16.600000   # max. absolute (calc./exp.) parameter D[i]
Drange=    -16.600000     12.950000   # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =      0.072665 +/-  0.083777   # linear regression intercept and error
c(m)  =      0.997421 +/-  0.010795   # linear regression slope and error
chisq =      0.061612                 # weighted total sum of squared residuals
R     =      0.999473                 # weighted Pearson correlation coefficient R
R^2   =      0.998947                 # weighted Pearson correlation coefficient R^2
```





3.1.6 (-)-Isopinocampheol in p1-g

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------------------------------------------------------------------------------
info : Start Single-Conformer-Single-Tensor (SCST) Fit with 11 RDCs
------------------------------------------------------------------------------

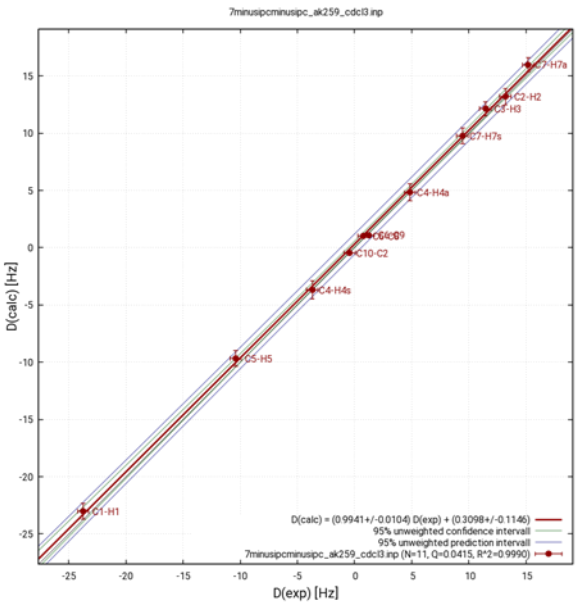
------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
  7.588062e-04 -1.874118e-04 -2.631812e-04 -5.805521e-04  4.719903e-04
Saupe Tensor (S):                                Alignment Tensor (A):
 -4.731090e-04 -2.631812e-04 -5.805521e-04        -3.154060e-04 -1.754541e-04 -3.870347e-04
 -2.631812e-04 -2.856972e-04  4.719903e-04        -1.754541e-04 -1.904648e-04  3.146602e-04
 -5.805521e-04  4.719903e-04  7.588062e-04        -3.870347e-04  3.146602e-04  5.058708e-04
Trace of Saupe Tensor:        0.000000e+00       Trace of Alignment Tensor:    0.000000e+00
Eigenvectors of Saupe Tensor:                    Eigenvectors of Alignment Tensor:
  1.228618e-01  9.254209e-01 -3.584704e-01         1.228618e-01  9.254209e-01 -3.584704e-01
 -9.047030e-01  2.529170e-01  3.428490e-01        -9.047030e-01  2.529170e-01  3.428490e-01
  4.079429e-01  2.821862e-01  8.683050e-01         4.079429e-01  2.821862e-01  8.683050e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
 -4.627832e-04 -7.220625e-04  1.184846e-03        -3.085221e-04 -4.813750e-04  7.898971e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
  1.202959e-03 -7.514767e-04  6.109524e-04 -1.212945e-04 -3.406662e-04
Tensor Properties:
A(axial)      =   1.184846e-03        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =   1.728529e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   1.458864e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   2.188296e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   1.194265e-03        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

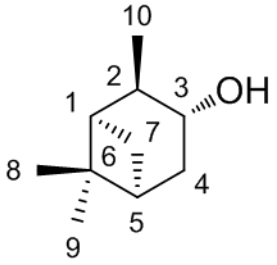
------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights    Atom Labels
D[01] =    -23.019572      0.681917    -23.750000      0.500000      1.000000   r[01] =      -0.730428   w[01] =       0.090909   C1-H1
D[02] =     13.203140      0.719635     13.200000      0.500000      1.000000   r[02] =      -0.003140   w[02] =       0.090909   C2-H2
D[03] =     12.138816      0.616471     11.450000      0.500000      1.000000   r[03] =      -0.688816   w[03] =       0.090909   C3-H3
D[04] =     -3.692849      0.786684     -3.700000      0.500000      1.000000   r[04] =      -0.007151   w[04] =       0.090909   C4-H4s
D[05] =      4.819029      0.745262      4.850000      0.500000      1.000000   r[05] =       0.030971   w[05] =       0.090909   C4-H4a
D[06] =     -9.678841      0.688242    -10.400000      0.500000      1.000000   r[06] =      -0.721159   w[06] =       0.090909   C5-H5
D[07] =      9.764973      0.671359      9.450000      0.500000      1.000000   r[07] =      -0.314973   w[07] =       0.090909   C7-H7s
D[08] =     15.975413      0.612644     15.200000      0.500000      1.000000   r[08] =      -0.775413   w[08] =       0.090909   C7-H7a
D[09] =      1.024157      0.102377      0.780000      0.500000      1.000000   r[09] =      -0.244157   w[09] =       0.090909   C6-C8
D[10] =      1.101685      0.075882      1.240000      0.500000      1.000000   r[10] =       0.138315   w[10] =       0.090909   C6-C9
D[11] =     -0.453223      0.149455     -0.440000      0.500000      1.000000   r[11] =       0.013223   w[11] =       0.090909   C10-C2

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =            5                 # rank of cosine matrix (check input if rank < 5)
cond  =   2.128683e+00                # condition number of cosine matrix (check input and singular values if very large)
chisq =      0.209861                 # weighted total sum of squared residuals
aic   =     19.233904                 # information criterion (AIC) for 5 degrees of freedom
rmsd  =      0.458106                 # unweighted root mean square deviation
qfac  =      0.041545                 # weighted Q-Factor as defined by Cornilescu
r^2   =      0.998236                 # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =      8.624700     8.587273    # mean absolute (calc./exp.) parameter D[i]
|D|min=      0.453223     0.440000    # min. absolute (calc./exp.) parameter D[i]
|D|max=     23.019572    23.750000    # max. absolute (calc./exp.) parameter D[i]
Drange=    -23.750000    15.975413    # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =      0.309785 +/-  0.114594    # linear regression intercept and error
c(m)  =      0.994133 +/-  0.010392    # linear regression slope and error
chisq =      0.115618                 # weighted total sum of squared residuals
R     =      0.999509                 # weighted Pearson correlation coefficient R
R^2   =      0.999017                 # weighted Pearson correlation coefficient R^2
```





3.1.7 (-)-Menthol in p1-e

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------------------------------------------------------------------------------
info : Start Single-Conformer-Single-Tensor (SCST) Fit with 13 RDCs
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SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
 -6.914080e-04  1.832601e-03  9.626395e-04  9.861313e-05 -7.752750e-04
Saupe Tensor (S):                          Alignment Tensor (A):
  1.262004e-03  9.626395e-04  9.861313e-05    8.413362e-04  6.417597e-04  6.574209e-05
  9.626395e-04 -5.705962e-04 -7.752750e-04    6.417597e-04 -3.803975e-04 -5.168500e-04
  9.861313e-05 -7.752750e-04 -6.914080e-04    6.574209e-05 -5.168500e-04 -4.609387e-04
Trace of Saupe Tensor:        0.000000e+00  Trace of Alignment Tensor:    0.000000e+00
Eigenvectors of Saupe Tensor:              Eigenvectors of Alignment Tensor:
  3.376114e-01  2.642008e-01  9.034470e-01    3.376114e-01  2.642008e-01  9.034470e-01
 -5.514033e-01 -7.223668e-01  4.173016e-01   -5.514033e-01 -7.223668e-01  4.173016e-01
  7.628715e-01 -6.390495e-01 -9.819804e-02    7.628715e-01 -6.390495e-01 -9.819804e-02
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
 -8.739786e-05 -1.608530e-03  1.695928e-03    -5.826524e-05 -1.072354e-03  1.130619e-03
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
 -1.096111e-03  1.276465e-04 -1.003529e-03  1.186075e-03  1.246057e-03
Tensor Properties:
A(axial)      =   1.695928e-03        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =   1.014088e-03        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   5.979547e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   8.969321e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   1.909831e-03        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights    Atom Labels
D[01] =      16.225728      0.845979     16.800000      0.500000      1.000000   r[01] =      0.574272   w[01] =      0.076923   C1-H1
D[02] =      14.325458      0.833269     15.950000      0.500000      1.000000   r[02] =      1.624542   w[02] =      0.076923   C2-H2A
D[03] =      -3.604602      1.194636     -4.850000      0.500000      1.000000   r[03] =     -1.245398   w[03] =      0.076923   C2-H2E
D[04] =      17.717579      0.948554     18.700000      0.500000      1.000000   r[04] =      0.982421   w[04] =      0.076923   C3-H3
D[05] =      15.580405      0.892911     13.500000      0.500000      1.000000   r[05] =     -2.080405   w[05] =      0.076923   C4-H4
D[06] =      14.432357      0.952515     13.450000      0.500000      1.000000   r[06] =     -0.982357   w[06] =      0.076923   C5-H5A
D[07] =      -4.198851      1.191006     -3.150000      0.500000      1.000000   r[07] =      1.048851   w[07] =      0.076923   C5-H5E
D[08] =       9.207373      0.755197      8.550000      0.500000      1.000000   r[08] =     -0.657373   w[08] =      0.076923   C6-H6E
D[09] =      18.439988      0.948097     18.300000      0.500000      1.000000   r[09] =     -0.139988   w[09] =      0.076923   C6-H6A
D[10] =      -2.036177      0.225526     -1.990000      0.500000      1.000000   r[10] =      0.046177   w[10] =      0.076923   C7-C1
D[11] =       9.773350      0.719013     10.350000      0.500000      1.000000   r[11] =      0.576650   w[11] =      0.076923   C8-H8
D[12] =      -0.076656      0.300411     -0.140000      0.500000      1.000000   r[12] =     -0.063344   w[12] =      0.076923   C10-C8
D[13] =       1.067446      0.225347      0.690000      0.500000      1.000000   r[13] =     -0.377446   w[13] =      0.076923   C9-C8

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =              5                 # rank of cosine matrix (check input if rank < 5)
cond  =   2.005893e+01                 # condition number of cosine matrix (check input and singular values if very large)
chisq =       0.985474                 # weighted total sum of squared residuals
aic   =      61.244655                 # information criterion (AIC) for 5 degrees of freedom
rmsd  =       0.992710                 # unweighted root mean square deviation
qfac  =       0.084306                 # weighted Q-Factor as defined by Cornilescu
r^2   =       0.986307                 # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =       9.745075      9.724615   # mean absolute (calc./exp.) parameter D[i]
|D|min=       0.076656      0.140000   # min. absolute (calc./exp.) parameter D[i]
|D|max=      18.439988     18.700000   # max. absolute (calc./exp.) parameter D[i]
Drange=      -4.850000     18.700000   # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =       0.214583 +/-  0.408888   # linear regression intercept and error
c(m)  =       0.980254 +/-  0.034725   # linear regression slope and error
chisq =       0.954570                 # weighted total sum of squared residuals
R     =       0.993169                 # weighted Pearson correlation coefficient R
R^2   =       0.986384                 # weighted Pearson correlation coefficient R^2
```
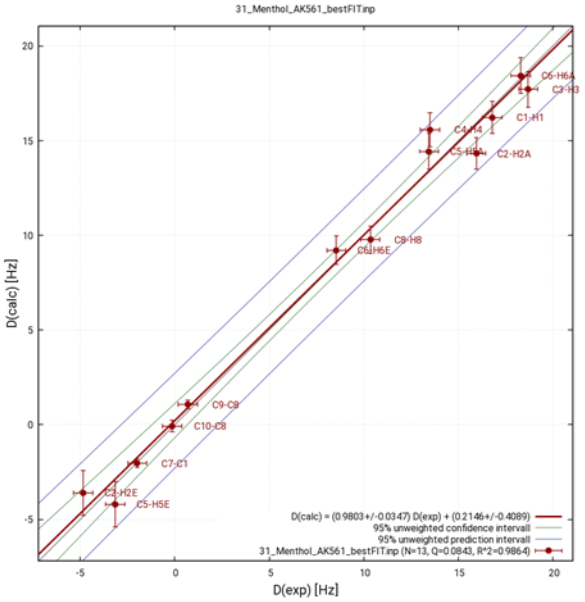
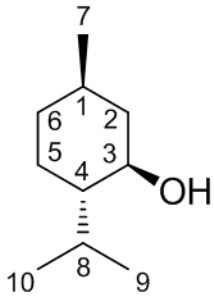
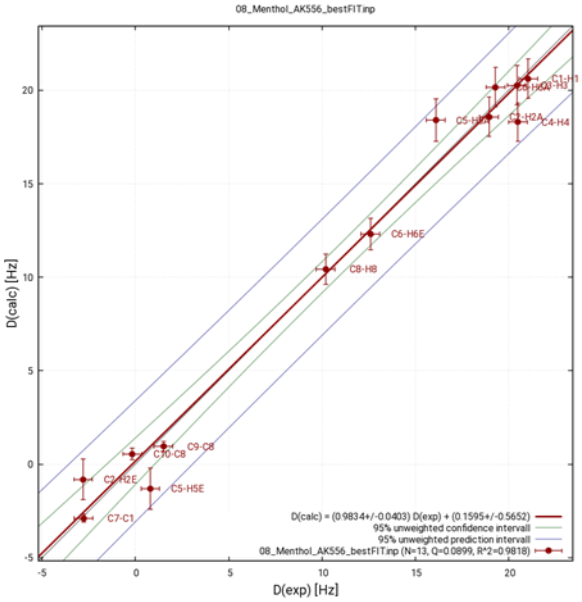
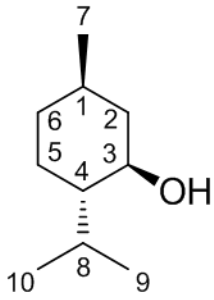





3.1.8 (-)-Menthol in *ent*-p1-c

```
------------------------------------------------------------------------------
info : Start Single-Conformer-Single-Tensor (SCST) Fit with 13 RDCs
------------------------------------------------------------------------------

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
 -1.009006e-03  1.565017e-03  6.734450e-04 -6.705779e-04 -3.854199e-04
Saupe Tensor (S):                                Alignment Tensor (A):
  1.287011e-03  6.734450e-04 -6.705779e-04         8.580076e-04  4.489633e-04 -4.470519e-04
  6.734450e-04 -2.780059e-04 -3.854199e-04         4.489633e-04 -1.853372e-04 -2.569466e-04
 -6.705779e-04 -3.854199e-04 -1.009006e-03        -4.470519e-04 -2.569466e-04 -6.726703e-04
Trace of Saupe Tensor:       -2.168404e-19       Trace of Alignment Tensor:   -1.445603e-19
Eigenvectors of Saupe Tensor:                    Eigenvectors of Alignment Tensor:
 -3.988681e-01 -1.852477e-01 -8.981022e-01        -3.988681e-01 -1.852477e-01 -8.981022e-01
  9.028715e-01 -2.506415e-01 -3.492875e-01         9.028715e-01 -2.506415e-01 -3.492875e-01
 -1.603970e-01 -9.501906e-01  2.672278e-01        -1.603970e-01 -9.501906e-01  2.672278e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
 -5.070479e-04 -1.241406e-03  1.748454e-03        -3.380319e-04 -8.276043e-04  1.165636e-03
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
 -1.599608e-03 -8.680076e-04 -4.988941e-04  1.012893e-03  8.717188e-04
Tensor Properties:
A(axial)      =   1.748454e-03        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =   4.895724e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   2.800030e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   4.200044e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   1.799126e-03        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights    Atom Labels
D[01] =     20.613907      1.052503     21.050000      0.500000      1.000000   r[01] =      0.436093   w[01] =      0.076923   C1-H1
D[02] =     18.574192      1.054229     18.950000      0.500000      1.000000   r[02] =      0.375808   w[02] =      0.076923   C2-H2A
D[03] =     -0.812038      1.097862     -2.800000      0.500000      1.000000   r[03] =     -1.987962   w[03] =      0.076923   C2-H2E
D[04] =     20.264035      1.047854     20.450000      0.500000      1.000000   r[04] =      0.185965   w[04] =      0.076923   C3-H3
D[05] =     18.293943      1.026098     20.500000      0.500000      1.000000   r[05] =      2.206057   w[05] =      0.076923   C4-H4
D[06] =     18.401740      1.124194     16.100000      0.500000      1.000000   r[06] =     -2.301740   w[06] =      0.076923   C5-H5A
D[07] =     -1.304430      1.105651      0.800000      0.500000      1.000000   r[07] =      2.104430   w[07] =      0.076923   C5-H5E
D[08] =     12.309093      0.856020     12.600000      0.500000      1.000000   r[08] =      0.290907   w[08] =      0.076923   C6-H6E
D[09] =     20.171550      1.069841     19.300000      0.500000      1.000000   r[09] =     -0.871550   w[09] =      0.076923   C6-H6A
D[10] =     -2.892009      0.216570     -2.770000      0.500000      1.000000   r[10] =      0.122009   w[10] =      0.076923   C7-C1
D[11] =     10.429934      0.803579     10.200000      0.500000      1.000000   r[11] =     -0.229934   w[11] =      0.076923   C8-H8
D[12] =      0.545495      0.316249     -0.170000      0.500000      1.000000   r[12] =     -0.715495   w[12] =      0.076923   C10-C8
D[13] =      0.949840      0.269897      1.510000      0.500000      1.000000   r[13] =      0.560160   w[13] =      0.076923   C9-C8

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =              5                  # rank of cosine matrix (check input if rank < 5)
cond  =   2.005893e+01                  # condition number of cosine matrix (check input and singular values if very large)
chisq =      1.588384                   # weighted total sum of squared residuals
aic   =     92.595989                   # information criterion (AIC) for 5 degrees of freedom
rmsd  =      1.260311                   # unweighted root mean square deviation
qfac  =      0.089923                   # weighted Q-Factor as defined by Cornilescu
r^2   =      0.981834                   # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =     11.197093     11.323077    # mean absolute (calc./exp.) parameter D[i]
|D|min=      0.545495      0.170000    # min. absolute (calc./exp.) parameter D[i]
|D|max=     20.613907     21.050000    # max. absolute (calc./exp.) parameter D[i]
Drange=     -2.892009     21.050000    # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =      0.159452 +/-  0.565207    # linear regression intercept and error
c(m)  =      0.983439 +/-  0.040327    # linear regression slope and error
chisq =      1.564223                  # weighted total sum of squared residuals
R     =      0.990878                  # weighted Pearson correlation coefficient R
R^2   =      0.981839                  # weighted Pearson correlation coefficient R^2
```





3.1.9 Di-β-D-Fructoseacetonide in p1-a

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------------------------------------------------------------------------------
info : Start Single-Conformer-Single-Tensor (SCST) Fit with 8 RDCs
------------------------------------------------------------------------------

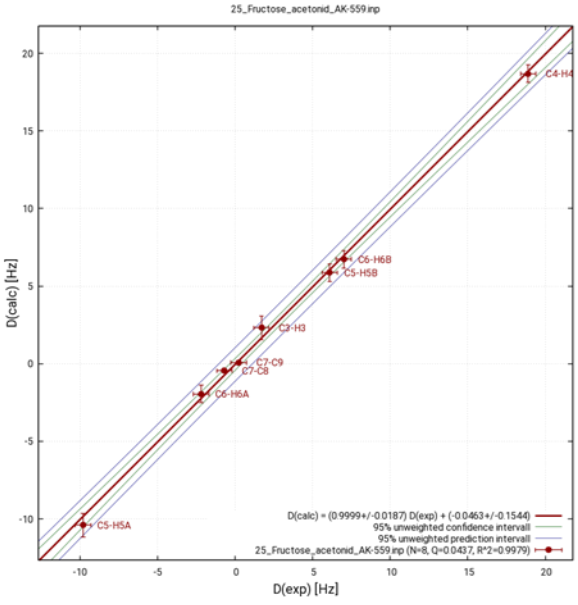
------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
 -5.649274e-04  1.015499e-03 -5.477596e-04  4.185439e-04  1.144942e-04
Saupe Tensor (S):                              Alignment Tensor (A):
  7.902131e-04 -5.477596e-04  4.185439e-04        5.268087e-04 -3.651731e-04  2.790292e-04
 -5.477596e-04 -2.252857e-04  1.144942e-04       -3.651731e-04 -1.501905e-04  7.632947e-05
  4.185439e-04  1.144942e-04 -5.649274e-04        2.790292e-04  7.632947e-05 -3.766183e-04
Trace of Saupe Tensor:        0.000000e+00     Trace of Alignment Tensor:    0.000000e+00
Eigenvectors of Saupe Tensor:                  Eigenvectors of Alignment Tensor:
  1.855778e-01 -3.688451e-01  9.107767e-01        1.855778e-01 -3.688451e-01  9.107767e-01
  7.977250e-01 -4.846505e-01 -3.588157e-01        7.977250e-01 -4.846505e-01 -3.588157e-01
  5.737558e-01  7.931376e-01  2.042966e-01        5.737558e-01  7.931376e-01  2.042966e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
 -2.703643e-04 -8.295316e-04  1.099896e-03       -1.802428e-04 -5.530211e-04  7.332639e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
 -8.955969e-04  5.417704e-04  1.482033e-04  6.572396e-04 -7.090295e-04
Tensor Properties:
A(axial)      =   1.099896e-03        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =   3.727782e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   3.389214e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   5.083821e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   1.146296e-03        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

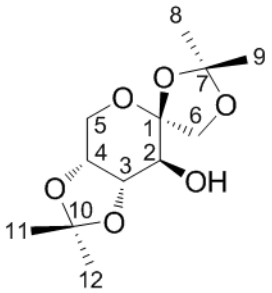
------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights    Atom Labels
D[01] =      0.076039      0.104976      0.230000      0.500000      1.000000   r[01] =      0.153961   w[01] =      0.125000   C7-C9
D[02] =     -0.455187      0.139332     -0.690000      0.500000      1.000000   r[02] =     -0.234813   w[02] =      0.125000   C7-C8
D[03] =      5.864861      0.556478      6.100000      0.500000      1.000000   r[03] =      0.235139   w[03] =      0.125000   C5-H5B
D[04] =    -10.401689      0.764161     -9.800000      0.500000      1.000000   r[04] =      0.601689   w[04] =      0.125000   C5-H5A
D[05] =      6.737808      0.567564      7.000000      0.500000      1.000000   r[05] =      0.262192   w[05] =      0.125000   C6-H6B
D[06] =     -1.956935      0.561520     -2.200000      0.500000      1.000000   r[06] =     -0.243065   w[06] =      0.125000   C6-H6A
D[07] =     18.689364      0.564785     18.900000      0.500000      1.000000   r[07] =      0.210636   w[07] =      0.125000   C4-H4
D[08] =      2.313039      0.759212      1.700000      0.500000      1.000000   r[08] =     -0.613039   w[08] =      0.125000   C3-H3

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =           5                  # rank of cosine matrix (check input if rank < 5)
cond  =   3.631845e+00                # condition number of cosine matrix (check input and singular values if very large)
chisq =      0.130521                 # weighted total sum of squared residuals
aic   =     14.176685                 # information criterion (AIC) for 5 degrees of freedom
rmsd  =      0.361277                 # unweighted root mean square deviation
qfac  =      0.043662                 # weighted Q-Factor as defined by Cornilescu
r^2   =      0.997875                 # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =      5.811865      5.827500   # mean absolute (calc./exp.) parameter D[i]
|D|min=      0.076039      0.230000   # min. absolute (calc./exp.) parameter D[i]
|D|max=     18.689364     18.900000   # max. absolute (calc./exp.) parameter D[i]
Drange=    -10.401689     18.900000   # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =     -0.046292 +/-  0.154425   # linear regression intercept and error
c(m)  =      0.999889 +/-  0.018663   # linear regression slope and error
chisq =      0.128350                 # weighted total sum of squared residuals
R     =      0.998956                 # weighted Pearson correlation coefficient R
R^2   =      0.997914                 # weighted Pearson correlation coefficient R^2
```





3.1.10 Di-β-D-Fructoseacetonide *ent*-p1-c

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------------------------------------------------------------------------------
info : Start Single-Conformer-Single-Tensor (SCST) Fit with 8 RDCs
------------------------------------------------------------------------------

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
 -1.962931e-04  8.582792e-04 -3.537743e-04 -7.633794e-05  6.086511e-04
Saupe Tensor (S):                              Alignment Tensor (A):
  5.272862e-04 -3.537743e-04 -7.633794e-05       3.515241e-04 -2.358495e-04 -5.089196e-05
 -3.537743e-04 -3.309930e-04  6.086511e-04      -2.358495e-04 -2.206620e-04  4.057674e-04
 -7.633794e-05  6.086511e-04 -1.962931e-04      -5.089196e-05  4.057674e-04 -1.308621e-04
Trace of Saupe Tensor:        2.710505e-20     Trace of Alignment Tensor:    1.807004e-20
Eigenvectors of Saupe Tensor:                  Eigenvectors of Alignment Tensor:
 -5.637677e-01  8.115493e-01 -1.534726e-01       -5.637677e-01  8.115493e-01 -1.534726e-01
 -4.580818e-01 -4.618518e-01 -7.595090e-01       -4.580818e-01 -4.618518e-01 -7.595090e-01
 -6.872606e-01 -3.578836e-01  6.321330e-01       -6.872606e-01 -3.578836e-01  6.321330e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
  1.467720e-04  7.622829e-04 -9.090548e-04        9.784797e-05  5.081886e-04 -6.060365e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
 -3.111895e-04 -9.881315e-05  7.878485e-04  5.554857e-04 -4.579315e-04
Tensor Properties:
A(axial)      =  -9.090548e-04        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =  -4.103406e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   4.513926e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   6.770889e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   9.760457e-04        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights    Atom Labels
D[01] =     -0.316018      0.068875     -0.240000      0.500000      1.000000   r[01] =      0.076018   w[01] =      0.125000   C7-C9
D[02] =     -0.545385      0.136498      0.530000      0.500000      1.000000   r[02] =      1.075385   w[02] =      0.125000   C7-C8
D[03] =     -1.929367      0.524068     -1.700000      0.500000      1.000000   r[03] =      0.229367   w[03] =      0.125000   C5-H5B
D[04] =      4.463238      0.611565      5.000000      0.500000      1.000000   r[04] =      0.536762   w[04] =      0.125000   C5-H5A
D[05] =     -9.445699      0.522063     -9.300000      0.500000      1.000000   r[05] =      0.145699   w[05] =      0.125000   C6-H6B
D[06] =     10.995266      0.512265     10.700000      0.500000      1.000000   r[06] =     -0.295266   w[06] =      0.125000   C6-H6A
D[07] =     16.369518      0.527227     16.600000      0.500000      1.000000   r[07] =      0.230482   w[07] =      0.125000   C4-H4
D[08] =      0.995161      0.609917      0.500000      0.500000      1.000000   r[08] =     -0.495161   w[08] =      0.125000   C3-H3

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =           5                  # rank of cosine matrix (check input if rank < 5)
cond  =   3.631845e+00                # condition number of cosine matrix (check input and singular values if very large)
chisq =       0.238709                # weighted total sum of squared residuals
aic   =      17.638681                # information criterion (AIC) for 5 degrees of freedom
rmsd  =       0.488578                # unweighted root mean square deviation
qfac  =       0.061493                # weighted Q-Factor as defined by Cornilescu
r^2   =       0.995699                # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =       5.632456      5.571250  # mean absolute (calc./exp.) parameter D[i]
|D|min=       0.316018      0.240000  # min. absolute (calc./exp.) parameter D[i]
|D|max=      16.369518     16.600000  # max. absolute (calc./exp.) parameter D[i]
Drange=      -9.445699     16.600000  # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =      -0.201849 +/-  0.195674  # linear regression intercept and error
c(m)  =       1.005048 +/-  0.024628  # linear regression slope and error
chisq =       0.201984                # weighted total sum of squared residuals
R     =       0.998203                # weighted Pearson correlation coefficient R
R^2   =       0.996410                # weighted Pearson correlation coefficient R^2
```
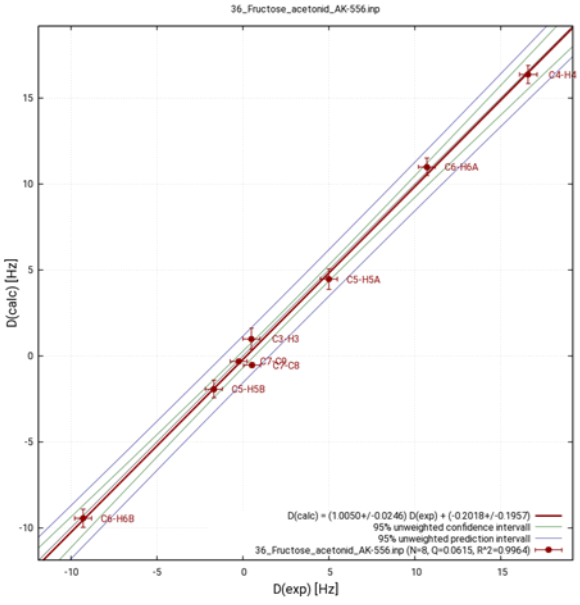
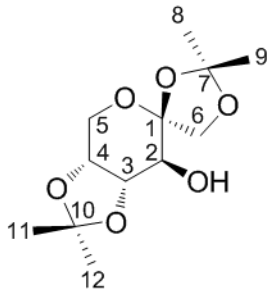
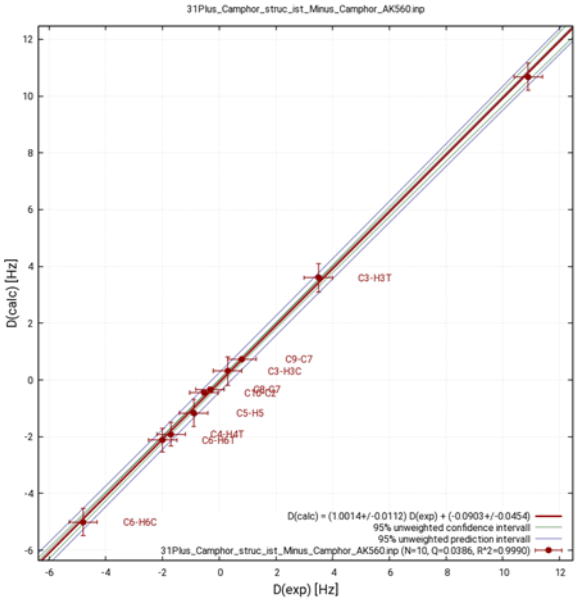
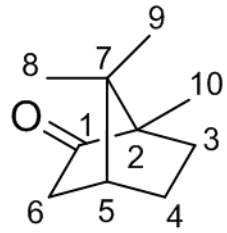





3.1.11 (+)-Camphor in p1-b

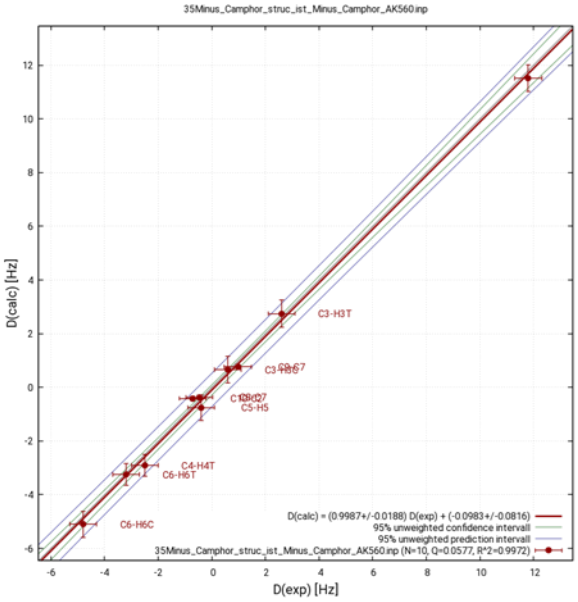
```
------------------------------------------------------------------------------
info : Start Single-Conformer-Single-Tensor (SCST) Fit with 10 RDCs
------------------------------------------------------------------------------

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
  2.800164e-04 -6.165197e-04 -9.616093e-05  1.149754e-04  8.033263e-05
Saupe Tensor (S):                          Alignment Tensor (A):
 -4.482681e-04 -9.616093e-05  1.149754e-04   -2.988454e-04 -6.410729e-05  7.665028e-05
 -9.616093e-05  1.682517e-04  8.033263e-05   -6.410729e-05  1.121678e-04  5.355509e-05
  1.149754e-04  8.033263e-05  2.800164e-04    7.665028e-05  5.355509e-05  1.866776e-04
Trace of Saupe Tensor:        0.000000e+00  Trace of Alignment Tensor:    0.000000e+00
Eigenvectors of Saupe Tensor:              Eigenvectors of Alignment Tensor:
 -2.156519e-01 -8.398864e-02 -9.728516e-01   -2.156519e-01 -8.398864e-02 -9.728516e-01
  8.976073e-01 -4.092971e-01 -1.636369e-01    8.976073e-01 -4.092971e-01 -1.636369e-01
 -3.844416e-01 -9.085273e-01  1.636545e-01   -3.844416e-01 -9.085273e-01  1.636545e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
  1.569484e-04  3.268356e-04 -4.837840e-04    1.046322e-04  2.178904e-04 -3.225227e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
  4.439187e-04  1.488262e-04  1.039839e-04 -3.990169e-04 -1.244724e-04
Tensor Properties:
A(axial)      =  -4.837840e-04        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =  -1.132582e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   2.341090e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   3.511635e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   4.936269e-04        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights    Atom Labels
D[01] =       0.315343      0.495993       0.300000      0.500000      1.000000   r[01] =      -0.015343   w[01] =       0.100000   C3-H3C
D[02] =       3.601078      0.495839       3.500000      0.500000      1.000000   r[02] =      -0.101078   w[02] =       0.100000   C3-H3T
D[03] =      10.684609      0.484633      10.900000      0.500000      1.000000   r[03] =       0.215391   w[03] =       0.100000   C4-H4C
D[04] =      -1.913639      0.411960      -1.700000      0.500000      1.000000   r[04] =       0.213639   w[04] =       0.100000   C4-H4T
D[05] =      -1.164062      0.478903      -0.900000      0.500000      1.000000   r[05] =       0.264062   w[05] =       0.100000   C5-H5
D[06] =      -5.008231      0.482097      -4.800000      0.500000      1.000000   r[06] =       0.208231   w[06] =       0.100000   C6-H6C
D[07] =      -2.121177      0.411512      -2.000000      0.500000      1.000000   r[07] =       0.121177   w[07] =       0.100000   C6-H6T
D[08] =      -0.332821      0.075800      -0.320000      0.500000      1.000000   r[08] =       0.012821   w[08] =       0.100000   C8-C7
D[09] =       0.734661      0.071700       0.800000      0.500000      1.000000   r[09] =       0.065339   w[09] =       0.100000   C9-C7
D[10] =      -0.451804      0.077225      -0.540000      0.500000      1.000000   r[10] =      -0.088196   w[10] =       0.100000   C10-C2

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =              5                 # rank of cosine matrix (check input if rank < 5)
cond  =   3.206053e+00                  # condition number of cosine matrix (check input and singular values if very large)
chisq =       0.024247                  # weighted total sum of squared residuals
aic   =      10.969887                  # information criterion (AIC) for 5 degrees of freedom
rmsd  =       0.155715                  # unweighted root mean square deviation
qfac  =       0.038578                  # weighted Q-Factor as defined by Cornilescu
r^2   =       0.998486                  # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =       2.632742      2.576000    # mean absolute (calc./exp.) parameter D[i]
|D|min=       0.315343      0.300000    # min. absolute (calc./exp.) parameter D[i]
|D|max=      10.684609     10.900000    # max. absolute (calc./exp.) parameter D[i]
Drange=      -5.008231     10.900000    # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =      -0.090347 +/-  0.045365    # linear regression intercept and error
c(m)  =       1.001418 +/-  0.011239    # linear regression slope and error
chisq =       0.016186                  # weighted total sum of squared residuals
R     =       0.999497                  # weighted Pearson correlation coefficient R
R^2   =       0.998993                  # weighted Pearson correlation coefficient R^2
```

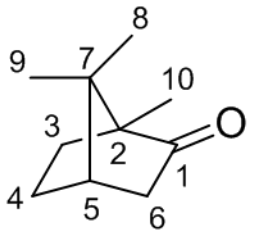




3.1.12 (-)-Camphor in p1-b

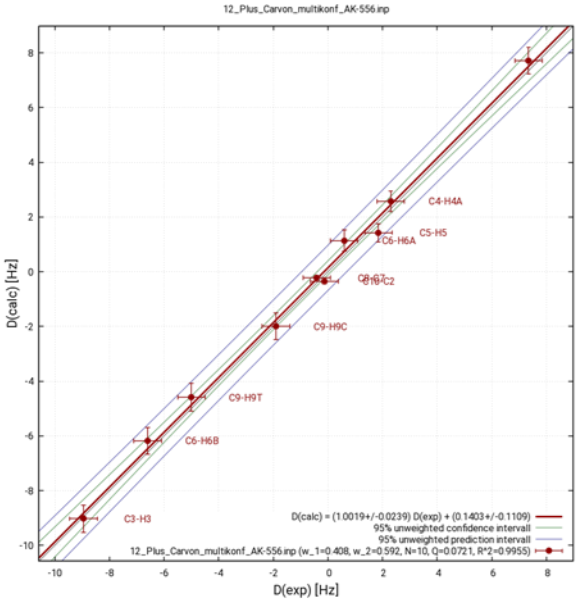
```
------------------------------------------------------------------------------
info : Start Single-Conformer-Single-Tensor (SCST) Fit with 10 RDCs
------------------------------------------------------------------------------

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
  2.844532e-04 -6.300861e-04 -1.379879e-04  1.413922e-04  6.161296e-05
Saupe Tensor (S):                          Alignment Tensor (A):
 -4.572696e-04 -1.379879e-04  1.413922e-04   -3.048464e-04 -9.199193e-05  9.426147e-05
 -1.379879e-04  1.728164e-04  6.161296e-05   -9.199193e-05  1.152109e-04  4.107531e-05
  1.413922e-04  6.161296e-05  2.844532e-04    9.426147e-05  4.107531e-05  1.896355e-04
Trace of Saupe Tensor:        0.000000e+00  Trace of Alignment Tensor:    0.000000e+00
Eigenvectors of Saupe Tensor:              Eigenvectors of Alignment Tensor:
 -2.515250e-01 -1.230478e-01 -9.599971e-01   -2.515250e-01 -1.230478e-01 -9.599971e-01
  9.365281e-01 -2.812419e-01 -2.093277e-01    9.365281e-01 -2.812419e-01 -2.093277e-01
 -2.442341e-01 -9.517154e-01  1.859771e-01   -2.442341e-01 -9.517154e-01  1.859771e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
  1.938082e-04  3.209412e-04 -5.147494e-04    1.292055e-04  2.139608e-04 -3.431663e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
  4.509525e-04  1.830205e-04  7.975288e-05 -4.077971e-04 -1.786139e-04
Tensor Properties:
A(axial)      =  -5.147494e-04        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =  -8.475532e-05        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   1.646535e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   2.469803e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   5.199563e-04        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights    Atom Labels
D[01] =      0.658203      0.499459      0.600000      0.500000      1.000000   r[01] =     -0.058203   w[01] =       0.100000   C3-H3C
D[02] =      2.746786      0.497867      2.600000      0.500000      1.000000   r[02] =     -0.146786   w[02] =       0.100000   C3-H3T
D[03] =     11.517762      0.494581     11.800000      0.500000      1.000000   r[03] =      0.282238   w[03] =       0.100000   C4-H4C
D[04] =     -2.908063      0.411255     -2.500000      0.500000      1.000000   r[04] =      0.408063   w[04] =       0.100000   C4-H4T
D[05] =     -0.752307      0.475324     -0.400000      0.500000      1.000000   r[05] =      0.352307   w[05] =       0.100000   C5-H5
D[06] =     -5.098841      0.485874     -4.800000      0.500000      1.000000   r[06] =      0.298841   w[06] =       0.100000   C6-H6C
D[07] =     -3.246100      0.411683     -3.200000      0.500000      1.000000   r[07] =      0.046100   w[07] =       0.100000   C6-H6T
D[08] =     -0.367806      0.078868     -0.470000      0.500000      1.000000   r[08] =     -0.102194   w[08] =       0.100000   C8-C7
D[09] =      0.766859      0.073594      0.970000      0.500000      1.000000   r[09] =      0.203141   w[09] =       0.100000   C9-C7
D[10] =     -0.414435      0.080010     -0.710000      0.500000      1.000000   r[10] =     -0.295565   w[10] =       0.100000   C10-C2

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =              5                # rank of cosine matrix (check input if rank < 5)
cond  =   3.206053e+00                 # condition number of cosine matrix (check input and singular values if very large)
chisq =      0.062573                 # weighted total sum of squared residuals
aic   =     12.502911                 # information criterion (AIC) for 5 degrees of freedom
rmsd  =      0.250146                 # unweighted root mean square deviation
qfac  =      0.057735                 # weighted Q-Factor as defined by Cornilescu
r^2   =      0.996640                 # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =      2.847716     2.805000    # mean absolute (calc./exp.) parameter D[i]
|D|min=      0.367806     0.400000    # min. absolute (calc./exp.) parameter D[i]
|D|max=     11.517762    11.800000    # max. absolute (calc./exp.) parameter D[i]
Drange=     -5.098841    11.800000    # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =     -0.098290 +/-  0.081555   # linear regression intercept and error
c(m)  =      0.998703 +/-  0.018824   # linear regression slope and error
chisq =      0.052781                 # weighted total sum of squared residuals
R     =      0.998582                 # weighted Pearson correlation coefficient R
R^2   =      0.997166                 # weighted Pearson correlation coefficient R^2
```

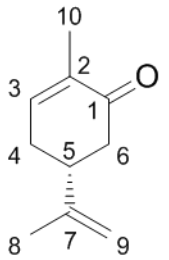




3.1.13 (+)-Carvone in *ent*-p1-c

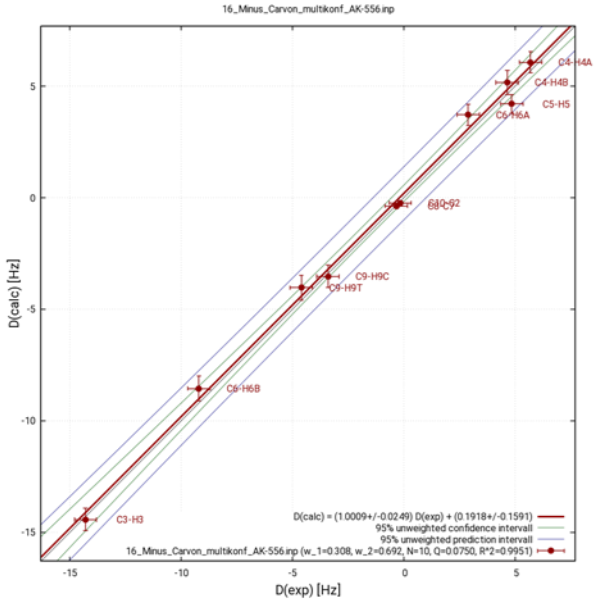
```
------------------------------------------------------------------------------
info : Start Multi-Conformer-Single-Tensor (MCST) Fit with 2 Conformers and 10 RDCs
------------------------------------------------------------------------------
info : relative weight of conformers: w(1) = 0.4080; w(2) = 0.5920

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
 -5.168366e-05  9.180969e-05 -5.176493e-04 -2.847135e-04 -2.645763e-05
Saupe Tensor (S):                          Alignment Tensor (A):
  7.174668e-05 -5.176493e-04 -2.847135e-04    4.783112e-05 -3.450995e-04 -1.898090e-04
 -5.176493e-04 -2.006302e-05 -2.645763e-05   -3.450995e-04 -1.337534e-05 -1.763842e-05
 -2.847135e-04 -2.645763e-05 -5.168366e-05   -1.898090e-04 -1.763842e-05 -3.445577e-05
Trace of Saupe Tensor:       -6.776264e-21 Trace of Alignment Tensor:   -4.517509e-21
Eigenvectors of Saupe Tensor:              Eigenvectors of Alignment Tensor:
 -4.618589e-02 -6.691045e-01  7.417318e-01   -4.618589e-02 -6.691045e-01  7.417318e-01
 -4.878074e-01 -6.328640e-01 -6.012712e-01   -4.878074e-01 -6.328640e-01 -6.012712e-01
  8.717286e-01 -3.895925e-01 -2.971647e-01    8.717286e-01 -3.895925e-01 -2.971647e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
 -2.179366e-05 -5.836425e-04  6.054362e-04    -1.452910e-05 -3.890950e-04  4.036241e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
 -8.193571e-05 -3.685381e-04 -3.424722e-05  5.942003e-05 -6.700542e-04
Tensor Properties:
A(axial)      =   6.054362e-04        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =   3.745659e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   6.186712e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   9.280068e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   6.868607e-04        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights | RDC Conformers  |    Atom
Labels
D[01] =     -9.026499      0.493912     -8.950000      0.500000      1.000000   r[01] =      0.076499   w[01] =      0.100000 |   -8.455  -9.420 |   C3-H3
D[02] =      7.720015      0.492854      7.350000      0.500000      1.000000   r[02] =     -0.370015   w[02] =      0.100000 |    6.287   8.708 |   C4-H4B
D[03] =      2.574083      0.384329      2.300000      0.500000      1.000000   r[03] =     -0.274083   w[03] =      0.100000 |    3.907   1.655 |   C4-H4A
D[04] =      1.427230      0.335119      1.850000      0.500000      1.000000   r[04] =      0.422770   w[04] =      0.100000 |    2.200   0.894 |   C5-H5
D[05] =     -6.179836      0.491471     -6.600000      0.500000      1.000000   r[05] =     -0.420164   w[05] =      0.100000 |   -6.113  -6.226 |   C6-H6B
D[06] =      1.135093      0.385492      0.600000      0.500000      1.000000   r[06] =     -0.535093   w[06] =      0.100000 |    1.713   0.737 |   C6-H6A
D[07] =     -0.222184      0.073728     -0.410000      0.500000      1.000000   r[07] =     -0.187816   w[07] =      0.100000 |    0.550  -0.755 |   C8-C7
D[08] =     -1.993393      0.480657     -1.900000      0.500000      1.000000   r[08] =      0.093393   w[08] =      0.100000 |    5.983  -7.491 |   C9-H9C
D[09] =     -4.589832      0.505089     -5.000000      0.500000      1.000000   r[09] =     -0.410168   w[09] =      0.100000 |   -2.648  -5.928 |   C9-H9T
D[10] =     -0.352049      0.080666     -0.130000      0.500000      1.000000   r[10] =      0.222049   w[10] =      0.100000 |   -0.355  -0.350 |   C10-C2

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =            5                  # rank of cosine matrix (check input if rank < 5)
cond  =   4.998756e+00                # condition number of cosine matrix (check input and singular values if very large)
chisq =      0.112102                 # weighted total sum of squared residuals
aic   =     16.484091                 # information criterion (AIC) for 6 degrees of freedom
rmsd  =      0.334817                 # unweighted root mean square deviation
qfac  =      0.072116                 # weighted Q-Factor as defined by Cornilescu
r^2   =      0.994497                 # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =      3.522021      3.509000   # mean absolute (calc./exp.) parameter D[i]
|D|min=      0.222184      0.130000   # min. absolute (calc./exp.) parameter D[i]
|D|max=      9.026499      8.950000   # max. absolute (calc./exp.) parameter D[i]
Drange=     -9.026499      7.720015   # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =      0.140320 +/-  0.110862   # linear regression intercept and error
c(m)  =      1.001888 +/-  0.023878   # linear regression slope and error
chisq =      0.092913                 # weighted total sum of squared residuals
R     =      0.997736                 # weighted Pearson correlation coefficient R
R^2   =      0.995476                 # weighted Pearson correlation coefficient R^2
```

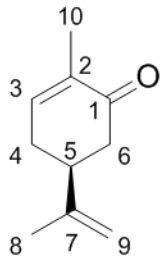




3.1.14 (-)-Carvone in *ent*-p1-c

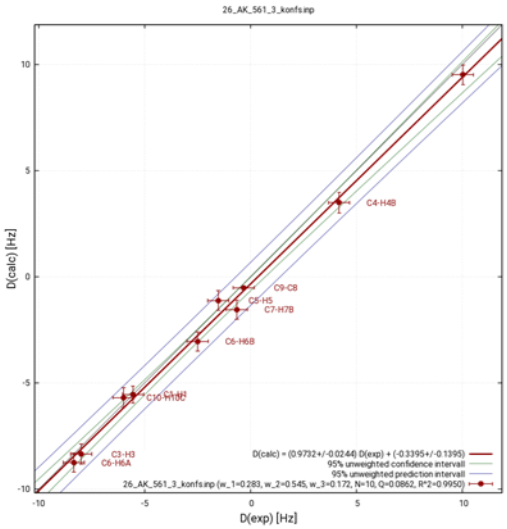
```
--------------------------------------------------------------------------------
info : Start Multi-Conformer-Single-Tensor (MCST) Fit with 2 Conformers and 10 RDCs
--------------------------------------------------------------------------------
info : relative weight of conformers: w(1) = 0.3084; w(2) = 0.6916

--------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
 -2.355796e-04 -2.289737e-04 -6.081266e-04 -3.603997e-04 -4.993432e-05
Saupe Tensor (S):                          Alignment Tensor (A):
  3.302919e-06 -6.081266e-04 -3.603997e-04   2.201946e-06 -4.054178e-04 -2.402665e-04
 -6.081266e-04  2.322766e-04 -4.993432e-05  -4.054178e-04  1.548511e-04 -3.328955e-05
 -3.603997e-04 -4.993432e-05 -2.355796e-04  -2.402665e-04 -3.328955e-05 -1.570530e-04
Trace of Saupe Tensor:       0.000000e+00  Trace of Alignment Tensor:    0.000000e+00
Eigenvectors of Saupe Tensor:              Eigenvectors of Alignment Tensor:
 -3.131489e-01  6.809571e-01 -6.619933e-01  -3.131489e-01  6.809571e-01 -6.619933e-01
 -5.092517e-01  4.679660e-01  7.222677e-01  -5.092517e-01  4.679660e-01  7.222677e-01
  8.016237e-01  5.632985e-01  2.002355e-01   8.016237e-01  5.632985e-01  2.002355e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
 -6.306979e-05 -7.127410e-04  7.758108e-04   -4.204652e-05 -4.751607e-04  5.172072e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
 -3.734716e-04 -4.665076e-04 -6.463584e-05 -1.481938e-04 -7.871696e-04
Tensor Properties:
A(axial)      =   7.758108e-04        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =   4.331141e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   5.582729e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   8.374094e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   8.617269e-04        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

--------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights | RDC Conformers  |   Atom
Labels
D[01] =    -14.438307      0.502905    -14.300000      0.500000      1.000000   r[01] =      0.138307   w[01] =      0.100000 |  -14.591 -14.370 |   C3-H3
D[02] =      5.172849      0.543243      4.650000      0.500000      1.000000   r[02] =     -0.522849   w[02] =      0.100000 |    3.846   5.765 |   C4-H4B
D[03] =      6.076550      0.468135      5.700000      0.500000      1.000000   r[03] =     -0.376550   w[03] =      0.100000 |    8.669   4.920 |   C4-H4A
D[04] =      4.204445      0.411171      4.850000      0.500000      1.000000   r[04] =      0.645555   w[04] =      0.100000 |    6.328   3.257 |   C5-H5
D[05] =     -8.552706      0.554387     -9.200000      0.500000      1.000000   r[05] =     -0.647294   w[05] =      0.100000 |  -10.178  -7.828 |   C6-H6B
D[06] =      3.721370      0.471801      2.900000      0.500000      1.000000   r[06] =     -0.821370   w[06] =      0.100000 |    5.667   2.854 |   C6-H6A
D[07] =     -0.370554      0.092118     -0.330000      0.500000      1.000000   r[07] =      0.040554   w[07] =      0.100000 |    0.464  -0.743 |   C8-C7
D[08] =     -3.531080      0.504601     -3.400000      0.500000      1.000000   r[08] =      0.131080   w[08] =      0.100000 |    4.842  -7.266 |   C9-H9C
D[09] =     -4.031611      0.564246     -4.600000      0.500000      1.000000   r[09] =     -0.568389   w[09] =      0.100000 |   -1.131  -5.325 |   C9-H9T
D[10] =     -0.235181      0.099759     -0.160000      0.500000      1.000000   r[10] =      0.075181   w[10] =      0.100000 |   -0.240  -0.233 |   C10-C2

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =            5                  # rank of cosine matrix (check input if rank < 5)
cond  =   5.269482e+00                # condition number of cosine matrix (check input and singular values if very large)
chisq =      0.229221                 # weighted total sum of squared residuals
aic   =     21.168855                 # information criterion (AIC) for 6 degrees of freedom
rmsd  =      0.478771                 # unweighted root mean square deviation
qfac  =      0.074952                 # weighted Q-Factor as defined by Cornilescu
r^2   =      0.994103                 # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =      5.033465      5.009000   # mean absolute (calc./exp.) parameter D[i]
|D|min=      0.235181      0.160000   # min. absolute (calc./exp.) parameter D[i]
|D|max=     14.438307     14.300000   # max. absolute (calc./exp.) parameter D[i]
Drange=    -14.438307      6.076550   # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =      0.191846 +/-  0.159076   # linear regression intercept and error
c(m)  =      1.000913 +/-  0.024903   # linear regression slope and error
chisq =      0.192869                 # weighted total sum of squared residuals
R     =      0.997533                 # weighted Pearson correlation coefficient R
R^2   =      0.995072                 # weighted Pearson correlation coefficient R^2
```

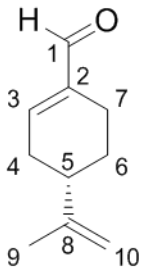




3.1.15 (-)-Perillaldehyde in p1-e

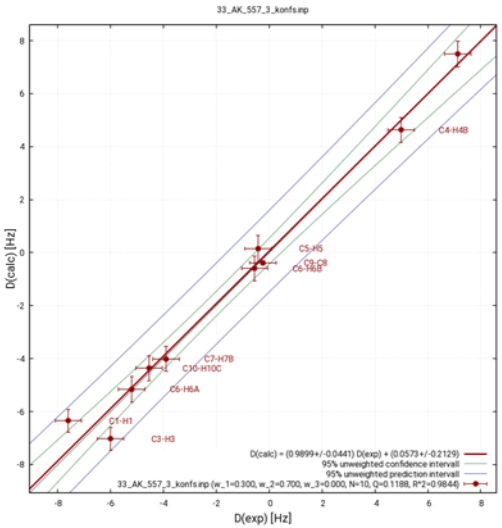
```
------------------------------------------------------------------------------
info : Start Multi-Conformer-Single-Tensor (MCST) Fit with 3 Conformers and 10 RDCs
------------------------------------------------------------------------------
info : relative weight of conformers: w(1) = 0.2827; w(2) = 0.5454; w(3) = 0.1719

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
  2.430942e-04 -3.839639e-04  5.330215e-04  1.287189e-04 -1.447034e-05
Saupe Tensor (S):                          Alignment Tensor (A):
 -3.135290e-04  5.330215e-04  1.287189e-04   -2.090194e-04  3.553477e-04  8.581259e-05
  5.330215e-04  7.043487e-05 -1.447034e-05    3.553477e-04  4.695658e-05 -9.646897e-06
  1.287189e-04 -1.447034e-05  2.430942e-04    8.581259e-05 -9.646897e-06  1.620628e-04
Trace of Saupe Tensor:       2.710505e-20  Trace of Alignment Tensor:    1.807004e-20
Eigenvectors of Saupe Tensor:              Eigenvectors of Alignment Tensor:
 -6.904196e-02 -5.738975e-01  8.160116e-01   -6.904196e-02 -5.738975e-01  8.160116e-01
 -3.011558e-01 -7.678133e-01 -5.654803e-01   -3.011558e-01 -7.678133e-01 -5.654803e-01
  9.510722e-01 -2.847885e-01 -1.198212e-01    9.510722e-01 -2.847885e-01 -1.198212e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
  2.383320e-04  4.634715e-04 -7.018035e-04    1.588880e-04  3.089810e-04 -4.678690e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
  3.853847e-04  1.666160e-04 -1.873066e-05 -2.485048e-04  6.899522e-04
Tensor Properties:
A(axial)      =  -7.018035e-04        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =  -1.500930e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   2.138676e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   3.208013e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   7.137395e-04        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)      Normalized Weights | RDC Conformers          |   Atom Labels
D[01] =     -0.519374      0.058880     -0.340000      0.500000      1.000000   r[01] =      0.179374   w[01] =      0.100000 |  -0.991  -0.315  -0.391 |   C9-C8
D[02] =      3.481298      0.475754      4.180000      0.500000      1.000000   r[02] =      0.698702   w[02] =      0.100000 |   0.446   4.806   4.271 |   C4-H4B
D[03] =     -8.754083      0.448238     -8.350000      0.500000      1.000000   r[03] =      0.404083   w[03] =      0.100000 |  -9.704  -8.357  -8.453 |   C6-H6A
D[04] =     -3.046083      0.449262     -2.500000      0.500000      1.000000   r[04] =      0.546083   w[04] =      0.100000 |  -3.965  -2.574  -3.035 |   C6-H6B
D[05] =     -1.547042      0.451615     -0.650000      0.500000      1.000000   r[05] =      0.897042   w[05] =      0.100000 |   1.989  -2.710  -3.671 |   C7-H7B
D[06] =     -1.128526      0.462063     -1.520000      0.500000      1.000000   r[06] =     -0.391474   w[06] =      0.100000 |  -2.530  -0.484  -0.870 |   C5-H5
D[07] =      9.506551      0.467089     10.030000      0.500000      1.000000   r[07] =      0.523449   w[07] =      0.100000 |   6.288  10.264  12.395 |   C10-H10T
D[08] =     -5.692455      0.456383     -6.000000      0.500000      1.000000   r[08] =     -0.307545   w[08] =      0.100000 | -10.447  -3.612  -4.476 |   C10-H10C
D[09] =     -8.359787      0.479636     -8.000000      0.500000      1.000000   r[09] =      0.359787   w[09] =      0.100000 |  -9.622  -7.978  -7.497 |   C3-H3
D[10] =     -5.544056      0.399825     -5.560000      0.500000      1.000000   r[10] =     -0.015944   w[10] =      0.100000 |  -8.017  -6.949   2.978 |   C1-H1

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =            5                  # rank of cosine matrix (check input if rank < 5)
cond  =   1.060038e+01                # condition number of cosine matrix (check input and singular values if very large)
chisq =      0.243807                 # weighted total sum of squared residuals
aic   =     23.752276                 # information criterion (AIC) for 7 degrees of freedom
rmsd  =      0.493768                 # unweighted root mean square deviation
qfac  =      0.086241                 # weighted Q-Factor as defined by Cornilescu
r^2   =      0.991673                 # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =      4.757925      4.713000  # mean absolute (calc./exp.) parameter D[i]
|D|min=      0.519374      0.340000  # min. absolute (calc./exp.) parameter D[i]
|D|max=      9.506551     10.030000  # max. absolute (calc./exp.) parameter D[i]
Drange=     -8.754083     10.030000  # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =     -0.339529 +/-  0.139484   # linear regression intercept and error
c(m)  =      0.973183 +/-  0.024362   # linear regression slope and error
chisq =      0.139024                 # weighted total sum of squared residuals
R     =      0.997503                 # weighted Pearson correlation coefficient R
R^2   =      0.995012                 # weighted Pearson correlation coefficient R^2
```

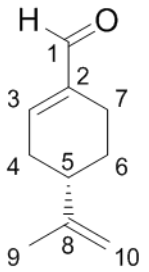




3.1.16 (-)-Perillaldehyde in *ent*-p1-d

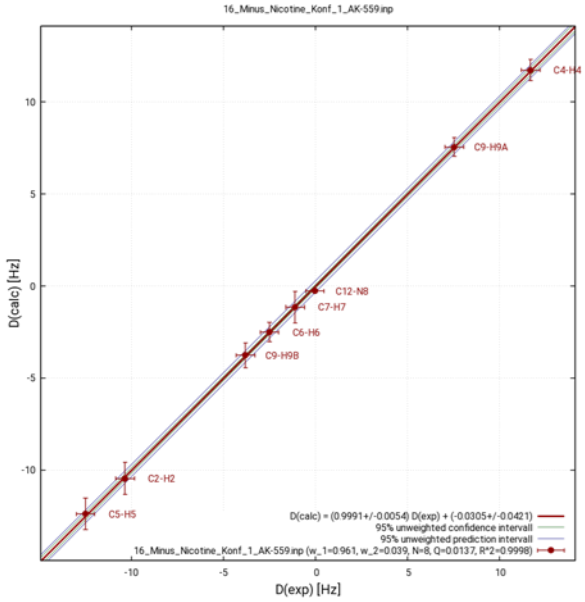
```
------------------------------------------------------------------------------
info : Start Multi-Conformer-Single-Tensor (MCST) Fit with 3 Conformers and 10 RDCs
------------------------------------------------------------------------------
info : relative weight of conformers: w(1) = 0.3000; w(2) = 0.6999; w(3) = 0.0002

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
  4.573731e-04 -1.223936e-04  3.603565e-04  5.332352e-07 -1.877376e-04
Saupe Tensor (S):                          Alignment Tensor (A):
 -2.898834e-04  3.603565e-04  5.332352e-07   -1.932556e-04  2.402377e-04  3.554902e-07
  3.603565e-04 -1.674897e-04 -1.877376e-04    2.402377e-04 -1.116598e-04 -1.251584e-04
  5.332352e-07 -1.877376e-04  4.573731e-04    3.554902e-07 -1.251584e-04  3.049154e-04
Trace of Saupe Tensor:       0.000000e+00  Trace of Alignment Tensor:    0.000000e+00
Eigenvectors of Saupe Tensor:              Eigenvectors of Alignment Tensor:
  6.519261e-01  1.452383e-01 -7.442434e-01    6.519261e-01  1.452383e-01 -7.442434e-01
  6.775105e-01  3.292211e-01  6.577180e-01    6.775105e-01  3.292211e-01  6.577180e-01
  3.405465e-01 -9.330162e-01  1.162273e-01    3.405465e-01 -9.330162e-01  1.162273e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
  8.489370e-05  5.235346e-04 -6.084283e-04    5.659580e-05  3.490231e-04 -4.056189e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
  7.250877e-04  6.902289e-07 -2.430108e-04 -7.921421e-05  4.664517e-04
Tensor Properties:
A(axial)      =  -6.084283e-04        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =  -2.924273e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   4.806273e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   7.209410e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   6.590298e-04        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights | RDC Conformers          |   Atom Labels
D[01] =     -0.382403      0.065988     -0.240000      0.500000      1.000000   r[01] =      0.142403   w[01] =      0.100000 |  -0.125  -0.493  -0.624 |   C9-C8
D[02] =      4.629043      0.474289      4.980000      0.500000      1.000000   r[02] =      0.350957   w[02] =      0.100000 |  -1.097   7.082   7.657 |   C4-H4B
D[03] =     -5.157021      0.481963     -5.200000      0.500000      1.000000   r[03] =     -0.042979   w[03] =      0.100000 |  -2.295  -6.383  -6.900 |   C6-H6A
D[04] =     -0.595566      0.470504     -0.550000      0.500000      1.000000   r[04] =      0.045566   w[04] =      0.100000 |  -5.312   1.425   1.856 |   C6-H6B
D[05] =     -4.016207      0.469994     -3.900000      0.500000      1.000000   r[05] =      0.116207   w[05] =      0.100000 |  -1.924  -4.912  -6.612 |   C7-H7B
D[06] =      0.152380      0.501205     -0.425000      0.500000      1.000000   r[06] =     -0.577380   w[06] =      0.100000 |  -4.922   2.327   2.989 |   C5-H5
D[07] =      7.494226      0.491859      7.130000      0.500000      1.000000   r[07] =     -0.364226   w[07] =      0.100000 |   5.323   8.424  10.335 |   C10-H10T
D[08] =     -4.362107      0.467626     -4.550000      0.500000      1.000000   r[08] =     -0.187893   w[08] =      0.100000 |  -1.082  -5.767  -7.178 |   C10-H10C
D[09] =     -7.029760      0.429712     -6.000000      0.500000      1.000000   r[09] =      1.029760   w[09] =      0.100000 |  -4.318  -8.192  -7.972 |   C3-H3
D[10] =     -6.349707      0.431642     -7.600000      0.500000      1.000000   r[10] =     -1.250293   w[10] =      0.100000 |  -3.250  -7.679   0.014 |   C1-H1

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =              5                 # rank of cosine matrix (check input if rank < 5)
cond  =   1.054727e+01                  # condition number of cosine matrix (check input and singular values if very large)
chisq =      0.328585                   # weighted total sum of squared residuals
aic   =     27.143386                   # information criterion (AIC) for 7 degrees of freedom
rmsd  =      0.573223                   # unweighted root mean square deviation
qfac  =      0.118781                   # weighted Q-Factor as defined by Cornilescu
r^2   =      0.984060                   # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =      4.016842      4.057500    # mean absolute (calc./exp.) parameter D[i]
|D|min=      0.152380      0.240000    # min. absolute (calc./exp.) parameter D[i]
|D|max=      7.494226      7.600000    # max. absolute (calc./exp.) parameter D[i]
Drange=     -7.600000      7.494226    # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =      0.057293 +/-  0.212926    # linear regression intercept and error
c(m)  =      0.989914 +/-  0.044122    # linear regression slope and error
chisq =      0.321043                   # weighted total sum of squared residuals
R     =      0.992147                   # weighted Pearson correlation coefficient R
R^2   =      0.984356                   # weighted Pearson correlation coefficient R^2
```

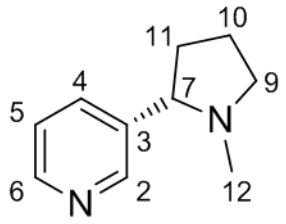




3.1.17 (-)-Nicotine in p1-a

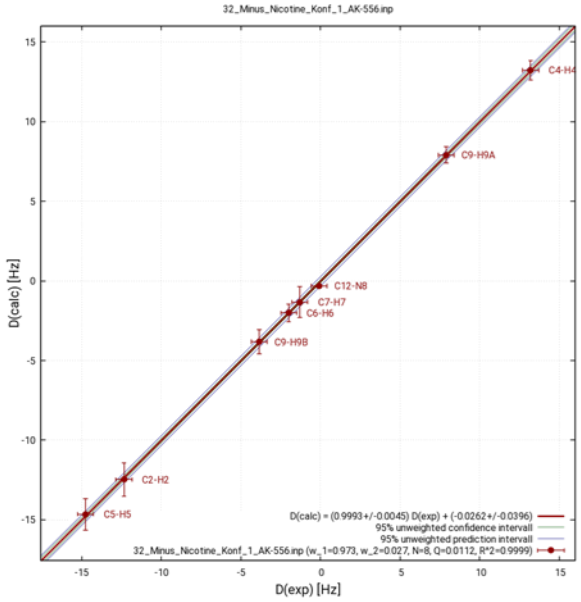
```
------------------------------------------------------------------------------
info : Start Multi-Conformer-Single-Tensor (MCST) Fit with 2 Conformers and 8 RDCs
------------------------------------------------------------------------------
info : relative weight of conformers: w(1) = 0.9606; w(2) = 0.0394

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
 -5.169575e-04 -1.312010e-03  5.039958e-04  4.387902e-05 -1.646253e-05
Saupe Tensor (S):                          Alignment Tensor (A):
 -3.975261e-04  5.039958e-04  4.387902e-05   -2.650174e-04  3.359972e-04  2.925268e-05
  5.039958e-04  9.144837e-04 -1.646253e-05    3.359972e-04  6.096558e-04 -1.097502e-05
  4.387902e-05 -1.646253e-05 -5.169575e-04    2.925268e-05 -1.097502e-05 -3.446384e-04
Trace of Saupe Tensor:        0.000000e+00  Trace of Alignment Tensor:    0.000000e+00
Eigenvectors of Saupe Tensor:              Eigenvectors of Alignment Tensor:
  4.811831e-01  8.154586e-01  3.216988e-01    4.811831e-01  8.154586e-01  3.216988e-01
 -1.626514e-01 -2.775526e-01  9.468416e-01   -1.626514e-01 -2.775526e-01  9.468416e-01
  8.613985e-01 -5.079289e-01 -9.181923e-04    8.613985e-01 -5.079289e-01 -9.181923e-04
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
 -4.893379e-04 -5.963992e-04  1.085737e-03    -3.262253e-04 -3.975995e-04  7.238248e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
 -8.195488e-04  5.679776e-05 -2.130938e-05 -8.491441e-04  6.523809e-04
Tensor Properties:
A(axial)      =   1.085737e-03        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =   7.137422e-05        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   6.573802e-02        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   9.860704e-02        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   1.087495e-03        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights | RDC Conformers  |    Atom
Labels
D[01] =    -10.447563      0.879606    -10.350000      0.500000      1.000000   r[01] =      0.097563   w[01] =      0.125000 | -11.371  12.084 |   C2-H2
D[02] =     11.728329      0.570480     11.700000      0.500000      1.000000   r[02] =     -0.028329   w[02] =      0.125000 |  12.736 -12.840 |   C4-H4
D[03] =    -12.388666      0.854954    -12.500000      0.500000      1.000000   r[03] =     -0.111334   w[03] =      0.125000 | -13.432  13.056 |   C5-H5
D[04] =     -2.511988      0.523642     -2.500000      0.500000      1.000000   r[04] =      0.011988   w[04] =      0.125000 |  -2.395  -5.368 |   C6-H6
D[05] =     -1.144525      0.853931     -1.100000      0.500000      1.000000   r[05] =      0.044525   w[05] =      0.125000 |  -1.092  -2.431 |   C7-H7
D[06] =      7.550103      0.511178      7.550000      0.500000      1.000000   r[06] =     -0.000103   w[06] =      0.125000 |   7.590   6.571 |   C9-H9A
D[07] =     -3.767367      0.678497     -3.800000      0.500000      1.000000   r[07] =     -0.032633   w[07] =      0.125000 |  -3.723  -4.853 |   C9-H9B
D[08] =     -0.272514      0.067893     -0.020000      0.500000      1.000000   r[08] =      0.252514   w[08] =      0.125000 |  -0.272  -0.296 |   C12-N8

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =           5                  # rank of cosine matrix (check input if rank < 5)
cond  =   6.630205e+00                # condition number of cosine matrix (check input and singular values if very large)
chisq =       0.011209                # weighted total sum of squared residuals
aic   =      12.358685                # information criterion (AIC) for 6 degrees of freedom
rmsd  =       0.105872                # unweighted root mean square deviation
qfac  =       0.013680                # weighted Q-Factor as defined by Cornilescu
r^2   =       0.999807                # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =       6.226382      6.190000  # mean absolute (calc./exp.) parameter D[i]
|D|min=       0.272514      0.020000  # min. absolute (calc./exp.) parameter D[i]
|D|max=      12.388666     12.500000  # max. absolute (calc./exp.) parameter D[i]
Drange=     -12.500000     11.728329  # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =      -0.030498 +/-  0.042118  # linear regression intercept and error
c(m)  =       0.999111 +/-  0.005442  # linear regression slope and error
chisq =       0.010306                # weighted total sum of squared residuals
R     =       0.999911                # weighted Pearson correlation coefficient R
R^2   =       0.999822                # weighted Pearson correlation coefficient R^2
```

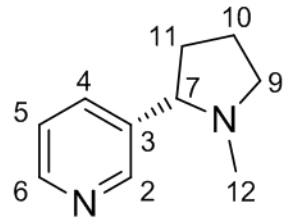




3.1.18 (-)-Nicotine in *ent*-p1-c

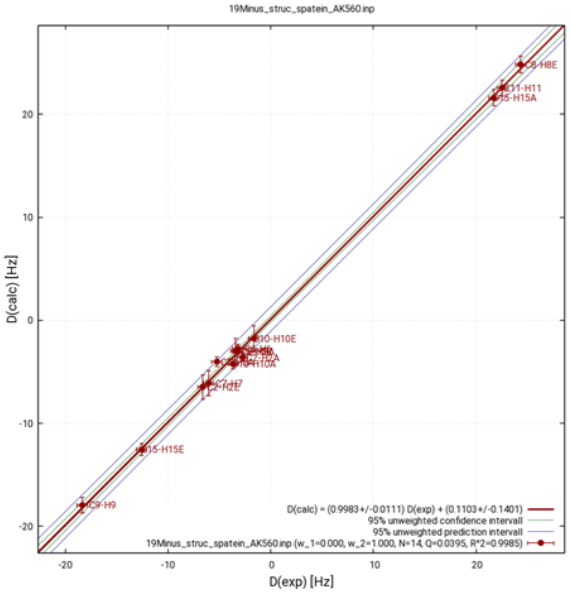
```
------------------------------------------------------------------------------
info : Start Multi-Conformer-Single-Tensor (MCST) Fit with 2 Conformers and 8 RDCs
------------------------------------------------------------------------------
info : relative weight of conformers: w(1) = 0.9728; w(2) = 0.0272

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
 -6.333425e-04 -1.559378e-03  5.562133e-04  2.607832e-05 -4.321078e-05
Saupe Tensor (S):                          Alignment Tensor (A):
 -4.630177e-04  5.562133e-04  2.607832e-05   -3.086785e-04  3.708088e-04  1.738554e-05
  5.562133e-04  1.096360e-03 -4.321078e-05    3.708088e-04  7.309068e-04 -2.880718e-05
  2.607832e-05 -4.321078e-05 -6.333425e-04    1.738554e-05 -2.880718e-05 -4.222284e-04
Trace of Saupe Tensor:        1.084202e-19  Trace of Alignment Tensor:    7.228014e-20
Eigenvectors of Saupe Tensor:              Eigenvectors of Alignment Tensor:
  6.450772e-01  7.008175e-01  3.045162e-01    6.450772e-01  7.008175e-01  3.045162e-01
 -1.927539e-01 -2.363873e-01  9.523482e-01   -1.927539e-01 -2.363873e-01  9.523482e-01
  7.394061e-01 -6.730348e-01 -1.740276e-02    7.394061e-01 -6.730348e-01 -1.740276e-02
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
 -5.993266e-04 -6.756741e-04  1.275001e-03    -3.995511e-04 -4.504494e-04  8.500005e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
 -1.004057e-03  3.375622e-05 -5.593278e-05 -1.009243e-03  7.199720e-04
Tensor Properties:
A(axial)      =   1.275001e-03        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =   5.089832e-05        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   3.992023e-02        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   5.988035e-02        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   1.275762e-03        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights | RDC Conformers  |    Atom
Labels
D[01] =    -12.467096      1.038430    -12.350000      0.500000      1.000000   r[01] =      0.117096   w[01] =      0.125000 |  -13.186  13.215 |   C2-H2
D[02] =     13.222634      0.608563     13.200000      0.500000      1.000000   r[02] =     -0.022634   w[02] =      0.125000 |   14.009 -14.881 |   C4-H4
D[03] =    -14.646327      0.990533    -14.770000      0.500000      1.000000   r[03] =     -0.123673   w[03] =      0.125000 |  -15.460  14.417 |   C5-H5
D[04] =     -2.010123      0.539093     -2.000000      0.500000      1.000000   r[04] =      0.010123   w[04] =      0.125000 |   -1.919  -5.274 |   C6-H6
D[05] =     -1.336370      0.974391     -1.310000      0.500000      1.000000   r[05] =      0.026370   w[05] =      0.125000 |   -1.296  -2.791 |   C7-H7
D[06] =      7.901734      0.516150      7.900000      0.500000      1.000000   r[06] =     -0.001734   w[06] =      0.125000 |    7.935   6.699 |   C9-H9A
D[07] =     -3.827522      0.750880     -3.850000      0.500000      1.000000   r[07] =     -0.022478   w[07] =      0.125000 |   -3.793  -5.047 |   C9-H9B
D[08] =     -0.317361      0.078980     -0.100000      0.500000      1.000000   r[08] =      0.217361   w[08] =      0.125000 |   -0.317  -0.347 |   C12-N8

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =            5                  # rank of cosine matrix (check input if rank < 5)
cond  =   6.617089e+00                # condition number of cosine matrix (check input and singular values if very large)
chisq =        0.009759               # weighted total sum of squared residuals
aic   =       12.312282               # information criterion (AIC) for 6 degrees of freedom
rmsd  =        0.098787               # unweighted root mean square deviation
qfac  =        0.011151               # weighted Q-Factor as defined by Cornilescu
r^2   =        0.999871               # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =        6.966146      6.935000  # mean absolute (calc./exp.) parameter D[i]
|D|min=        0.317361      0.100000  # min. absolute (calc./exp.) parameter D[i]
|D|max=       14.646327     14.770000  # max. absolute (calc./exp.) parameter D[i]
Drange=      -14.770000     13.222634  # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =       -0.026179 +/-  0.039639  # linear regression intercept and error
c(m)  =        0.999322 +/-  0.004474  # linear regression slope and error
chisq =        0.009096               # weighted total sum of squared residuals
R     =        0.999940               # weighted Pearson correlation coefficient R
R^2   =        0.999880               # weighted Pearson correlation coefficient R^2
```

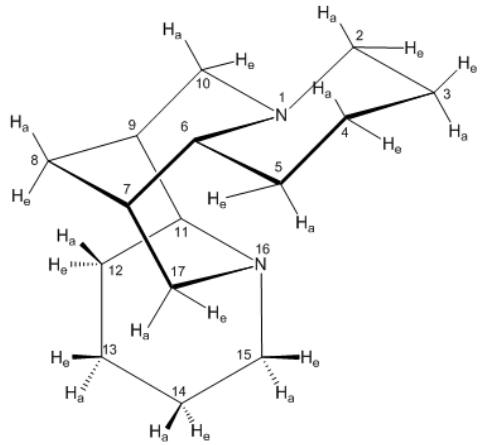




3.1.19 (-)-Sparteine in p1-b

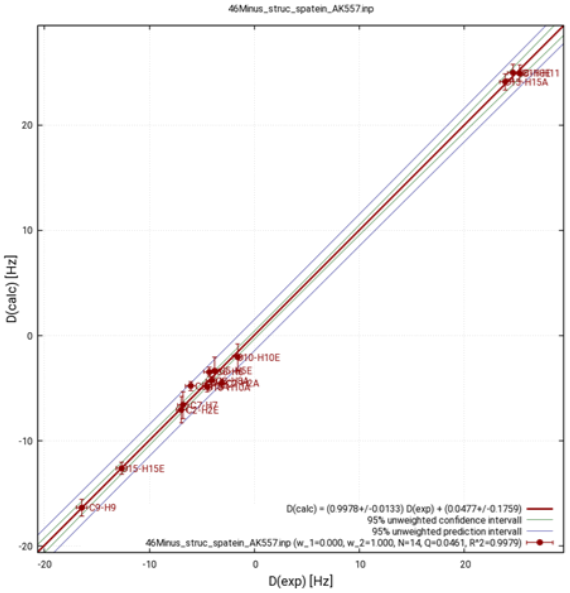
```
------------------------------------------------------------------------------
info : Start Multi-Conformer-Single-Tensor (MCST) Fit with 2 Conformers and 14 RDCs
------------------------------------------------------------------------------
info : relative weight of conformers: w(1) = 0.0002; w(2) = 0.9998

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
 -4.932804e-04 -1.054168e-03 -3.024675e-04  7.886783e-04 -3.452397e-04
Saupe Tensor (S):                              Alignment Tensor (A):
 -2.804436e-04 -3.024675e-04  7.886783e-04      -1.869624e-04 -2.016450e-04  5.257856e-04
 -3.024675e-04  7.737241e-04 -3.452397e-04      -2.016450e-04  5.158160e-04 -2.301598e-04
  7.886783e-04 -3.452397e-04 -4.932804e-04       5.257856e-04 -2.301598e-04 -3.288536e-04
Trace of Saupe Tensor:       1.084202e-19     Trace of Alignment Tensor:    7.228014e-20
Eigenvectors of Saupe Tensor:                  Eigenvectors of Alignment Tensor:
  6.413987e-01 -4.066216e-01 -6.505894e-01       6.413987e-01 -4.066216e-01 -6.505894e-01
  5.589862e-01  8.285094e-01  3.326702e-02       5.589862e-01  8.285094e-01  3.326702e-02
  5.254924e-01 -3.850079e-01  7.587007e-01       5.254924e-01 -3.850079e-01  7.587007e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
  1.021098e-04  1.082604e-03 -1.184714e-03       6.807321e-05  7.217360e-04 -7.898092e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
 -7.820127e-04  1.020879e-03 -4.468842e-04 -6.822664e-04 -3.915192e-04
Tensor Properties:
A(axial)      =  -1.184714e-03        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =  -6.536627e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   5.517474e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   8.276211e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   1.313013e-03        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
          D(calc) [Hz]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights           D(exp)-D(calc)        Normalized Weights | RDC Conformers  |    Atom
Labels
D[01] =      -2.743616      0.415931     -3.200000      0.500000      1.000000    r[01] =      -0.456384    w[01] =       0.071429 |  -2.400  -2.744 |   C6-H6
D[02] =      22.560975      0.773750     22.550000      0.500000      1.000000    r[02] =      -0.010975    w[02] =       0.071429 |   8.671  22.563 |   C11-H11
D[03] =      -1.764285      1.211632     -1.650000      0.500000      1.000000    r[03] =       0.114285    w[03] =       0.071429 |   1.440  -1.765 |   C10-H10E
D[04] =      -4.233572      0.465838     -3.650000      0.500000      1.000000    r[04] =       0.583572    w[04] =       0.071429 |  -4.341  -4.234 |   C10-H10A
D[05] =      -6.470799      1.183423     -6.600000      0.500000      1.000000    r[05] =      -0.129201    w[05] =       0.071429 |  -3.950  -6.471 |   C2-H2E
D[06] =      -3.633004      0.407261     -2.750000      0.500000      1.000000    r[06] =       0.883004    w[06] =       0.071429 |  -2.922  -3.633 |   C2-H2A
D[07] =     -12.550335      0.554273    -12.560000      0.500000      1.000000    r[07] =      -0.009665    w[07] =       0.071429 | -23.716 -12.549 |   C15-H15E
D[08] =      21.611550      0.766206     21.730000      0.500000      1.000000    r[08] =       0.118450    w[08] =       0.071429 |   9.922  21.613 |   C15-H15A
D[09] =     -17.944305      0.749034    -18.350000      0.500000      1.000000    r[09] =      -0.405695    w[09] =       0.071429 | -20.759 -17.944 |   C9-H9
D[10] =      -6.115965      1.219055     -6.050000      0.500000      1.000000    r[10] =       0.065965    w[10] =       0.071429 |  -3.144  -6.116 |   C7-H7
D[11] =      -4.031019      0.455374     -5.250000      0.500000      1.000000    r[11] =      -1.218981    w[11] =       0.071429 |  -2.934  -4.031 |   C5-H5A
D[12] =      -2.976955      1.229464     -3.400000      0.500000      1.000000    r[12] =      -0.423045    w[12] =       0.071429 |  -0.779  -2.977 |   C5-H5E
D[13] =      24.840481      0.785670     24.350000      0.500000      1.000000    r[13] =      -0.490481    w[13] =       0.071429 |  24.830  24.840 |   C8-H8E
D[14] =      -3.037839      0.403236     -3.200000      0.500000      1.000000    r[14] =      -0.162161    w[14] =       0.071429 |  -2.763  -3.038 |   C8-H8A

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =              5                # rank of cosine matrix (check input if rank < 5)
cond  =   5.916492e+00                 # condition number of cosine matrix (check input and singular values if very large)
chisq =       0.248088                 # weighted total sum of squared residuals
aic   =      25.892900                 # information criterion (AIC) for 6 degrees of freedom
rmsd  =       0.498084                 # unweighted root mean square deviation
qfac  =       0.039452                 # weighted Q-Factor as defined by Cornilescu
r^2   =       0.998443                 # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =       9.608193      9.663571   # mean absolute (calc./exp.) parameter D[i]
|D|min=       1.764285      1.650000   # min. absolute (calc./exp.) parameter D[i]
|D|max=      24.840481     24.350000   # max. absolute (calc./exp.) parameter D[i]
Drange=     -18.350000     24.840481   # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =       0.110327 +/-  0.140107   # linear regression intercept and error
c(m)  =       0.998346 +/-  0.011098   # linear regression slope and error
chisq =       0.235531                 # weighted total sum of squared residuals
R     =       0.999259                 # weighted Pearson correlation coefficient R
R^2   =       0.998519                 # weighted Pearson correlation coefficient R^2
```

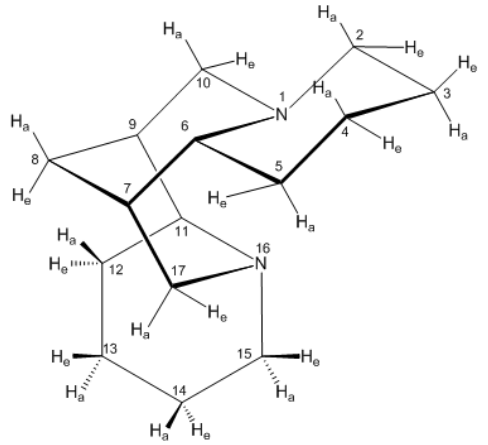




3.1.20 (-)-Sparteine in *ent*-p1-d

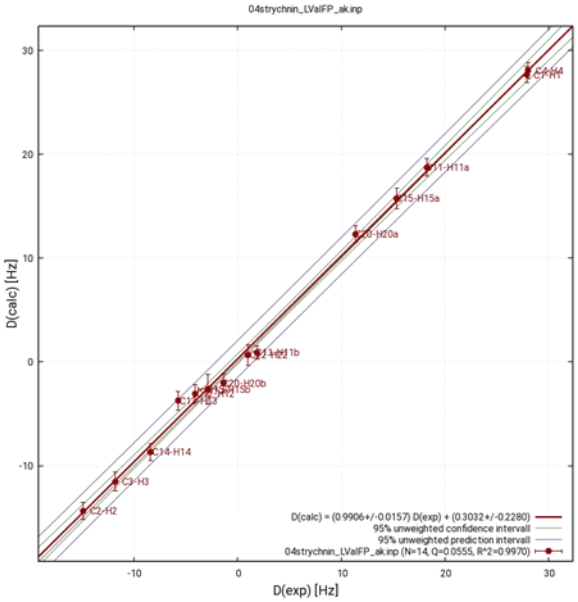
```
------------------------------------------------------------------------------
info : Start Multi-Conformer-Single-Tensor (MCST) Fit with 2 Conformers and 14 RDCs
------------------------------------------------------------------------------
info : relative weight of conformers: w(1) = 0.0002; w(2) = 0.9998

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
 -5.301045e-04 -9.188404e-04 -2.419313e-04  8.628583e-04 -3.928453e-04
Saupe Tensor (S):                                Alignment Tensor (A):
 -1.943679e-04 -2.419313e-04  8.628583e-04        -1.295786e-04 -1.612875e-04  5.752389e-04
 -2.419313e-04  7.244724e-04 -3.928453e-04        -1.612875e-04  4.829816e-04 -2.618969e-04
  8.628583e-04 -3.928453e-04 -5.301045e-04         5.752389e-04 -2.618969e-04 -3.534030e-04
Trace of Saupe Tensor:       0.000000e+00       Trace of Alignment Tensor:    0.000000e+00
Eigenvectors of Saupe Tensor:                    Eigenvectors of Alignment Tensor:
  6.492185e-01 -4.423609e-01 -6.187344e-01         6.492185e-01 -4.423609e-01 -6.187344e-01
  6.119740e-01  7.868660e-01  7.955937e-02         6.119740e-01  7.868660e-01  7.955937e-02
  4.516671e-01 -4.303008e-01  7.815613e-01         4.516671e-01 -4.303008e-01  7.815613e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
  1.778781e-04  1.075311e-03 -1.253189e-03         1.185854e-04  7.168737e-04 -8.354591e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
 -8.403910e-04  1.116899e-03 -5.085057e-04 -5.946814e-04 -3.131600e-04
Tensor Properties:
A(axial)      =  -1.253189e-03        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =  -5.982883e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   4.774128e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   7.161192e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   1.356076e-03        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
         D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights | RDC Conformers  |    Atom
Labels
D[01] =      -3.434569      0.436750     -4.300000      0.500000      1.000000    r[01] =      -0.865431    w[01] =      0.071429 |  -3.526  -3.435 |   C6-H6
D[02] =      24.948906      0.785234     25.300000      0.500000      1.000000    r[02] =       0.351094    w[02] =      0.071429 |   9.232  24.951 |  C11-H11
D[03] =      -2.042710      1.282534     -1.600000      0.500000      1.000000    r[03] =       0.442710    w[03] =      0.071429 |   1.387  -2.043 |  C10-H10E
D[04] =      -4.885372      0.437754     -4.500000      0.500000      1.000000    r[04] =       0.385372    w[04] =      0.071429 |  -5.096  -4.885 |  C10-H10A
D[05] =      -7.043655      1.258087     -6.950000      0.500000      1.000000    r[05] =       0.093655    w[05] =      0.071429 |  -4.237  -7.044 |   C2-H2E
D[06] =      -4.499242      0.379988     -3.100000      0.500000      1.000000    r[06] =       1.399242    w[06] =      0.071429 |  -3.952  -4.499 |   C2-H2A
D[07] =     -12.606122      0.558744    -12.650000      0.500000      1.000000    r[07] =      -0.043878    w[07] =      0.071429 | -22.744 -12.605 |  C15-H15E
D[08] =      24.116355      0.777622     23.900000      0.500000      1.000000    r[08] =      -0.216355    w[08] =      0.071429 |  10.596  24.118 |  C15-H15A
D[09] =     -16.315884      0.795512    -16.450000      0.500000      1.000000    r[09] =      -0.134116    w[09] =      0.071429 | -19.362 -16.315 |   C9-H9
D[10] =      -6.603734      1.296113     -6.800000      0.500000      1.000000    r[10] =      -0.196266    w[10] =      0.071429 |  -3.498  -6.604 |   C7-H7
D[11] =      -4.787088      0.426699     -6.050000      0.500000      1.000000    r[11] =      -1.262912    w[11] =      0.071429 |  -4.050  -4.787 |   C5-H5A
D[12] =      -3.319869      1.301815     -3.800000      0.500000      1.000000    r[12] =      -0.480131    w[12] =      0.071429 |  -0.866  -3.320 |   C5-H5E
D[13] =      24.958466      0.843293     24.650000      0.500000      1.000000    r[13] =      -0.308466    w[13] =      0.071429 |  25.333  24.958 |   C8-H8E
D[14] =      -4.275450      0.388675     -4.100000      0.500000      1.000000    r[14] =       0.175450    w[14] =      0.071429 |  -4.271  -4.275 |   C8-H8A

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =              5                 # rank of cosine matrix (check input if rank < 5)
cond  =   5.916492e+00                  # condition number of cosine matrix (check input and singular values if very large)
chisq =       0.374289                  # weighted total sum of squared residuals
aic   =      32.960161                  # information criterion (AIC) for 6 degrees of freedom
rmsd  =       0.611791                  # unweighted root mean square deviation
qfac  =       0.046126                  # weighted Q-Factor as defined by Cornilescu
r^2   =       0.997872                  # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =      10.274102     10.296429    # mean absolute (calc./exp.) parameter D[i]
|D|min=       2.042710      1.600000    # min. absolute (calc./exp.) parameter D[i]
|D|max=      24.958466     25.300000    # max. absolute (calc./exp.) parameter D[i]
Drange=     -16.450000     25.300000    # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =       0.047702 +/-  0.175915   # linear regression intercept and error
c(m)  =       0.997804 +/-  0.013263   # linear regression slope and error
chisq =       0.371218                 # weighted total sum of squared residuals
R     =       0.998942                 # weighted Pearson correlation coefficient R
R^2   =       0.997884                 # weighted Pearson correlation coefficient R^2
```

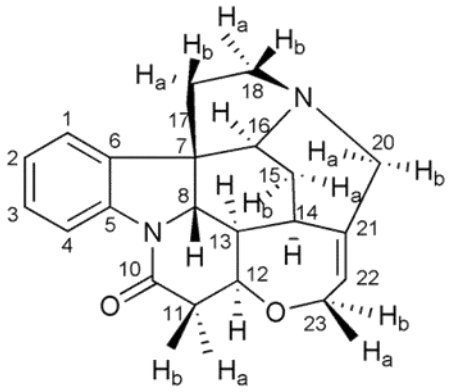




3.1.21 (-)-Strychnine in p1-h

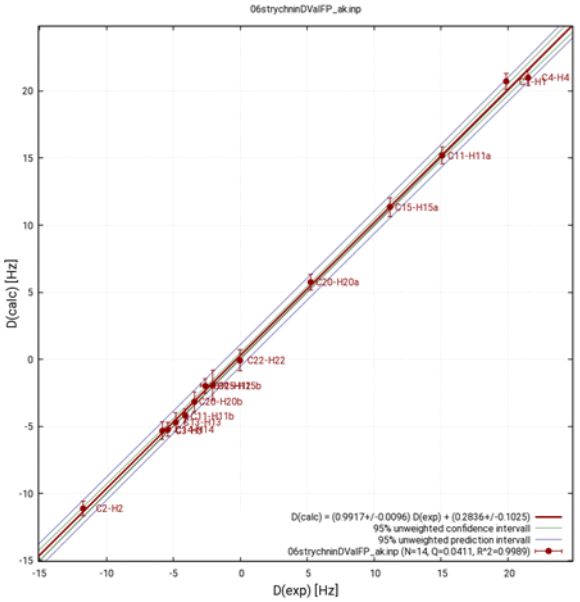
```
------------------------------------------------------------------------------
info : Start Single-Conformer-Single-Tensor (SCST) Fit with 14 RDCs
------------------------------------------------------------------------------

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
  3.007185e-04  7.676416e-04  7.095317e-04 -8.628941e-04  7.025888e-05
Saupe Tensor (S):                          Alignment Tensor (A):
  2.334615e-04  7.095317e-04 -8.628941e-04    1.556410e-04  4.730211e-04 -5.752627e-04
  7.095317e-04 -5.341800e-04  7.025888e-05    4.730211e-04 -3.561200e-04  4.683925e-05
 -8.628941e-04  7.025888e-05  3.007185e-04   -5.752627e-04  4.683925e-05  2.004790e-04
Trace of Saupe Tensor:        0.000000e+00  Trace of Alignment Tensor:    0.000000e+00
Eigenvectors of Saupe Tensor:              Eigenvectors of Alignment Tensor:
  3.507748e-01  5.939906e-01  7.239697e-01    3.507748e-01  5.939906e-01  7.239697e-01
  6.560753e-01 -7.075275e-01  2.626214e-01    6.560753e-01 -7.075275e-01  2.626214e-01
  6.682232e-01  3.828577e-01 -6.378854e-01    6.682232e-01  3.828577e-01 -6.378854e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
 -8.326461e-05 -1.167872e-03  1.251136e-03     -5.550974e-05 -7.785812e-04  8.340909e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
  4.767383e-04 -1.116945e-03  9.094431e-05  4.968243e-04  9.184301e-04
Tensor Properties:
A(axial)      =   1.251136e-03        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =   7.230714e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   5.779318e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   8.668976e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   1.399095e-03        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights    Atom Labels
D[01] =    -11.529070      0.906232    -11.830000      0.100000      1.000000   r[01] =      -0.300930   w[01] =      0.076850   C3-H3
D[02] =      0.678557      0.988726      0.990000      0.100000      1.000000   r[02] =       0.311443   w[02] =      0.076850   C22-H22
D[03] =    -14.331078      0.811508    -14.930000      0.100000      1.000000   r[03] =      -0.598922   w[03] =      0.076850   C2-H2
D[04] =     27.648483      0.755680     27.910000      0.100000      1.000000   r[04] =       0.261517   w[04] =      0.076850   C1-H1
D[05] =     28.075974      0.759713     28.050000      0.100000      1.000000   r[05] =      -0.025974   w[05] =      0.076850   C4-H4
D[06] =     -3.052092      0.840439     -4.110000      0.100000      1.000000   r[06] =      -1.057908   w[06] =      0.076850   C12-H12
D[07] =     12.298067      0.788376     11.390000      0.100000      1.000000   r[07] =      -0.908067   w[07] =      0.076850   C20-H20a
D[08] =     -2.040483      0.898960     -1.380000      0.100000      1.000000   r[08] =       0.660483   w[08] =      0.076850   C20-H20b
D[09] =     -3.742367      0.879256     -5.780000      0.100000      1.000000   r[09] =      -2.037633   w[09] =      0.076850   C13-H13
D[10] =     18.752332      0.832946     18.250000      0.100000      1.000000   r[10] =      -0.502332   w[10] =      0.076850   C11-H11a
D[11] =      0.902376      0.664029      1.830000      0.100000      1.000000   r[11] =       0.927624   w[11] =      0.076850   C11-H11b
D[12] =     -8.683019      0.839536     -8.420000      0.100000      1.000000   r[12] =       0.263019   w[12] =      0.076850   C14-H14
D[13] =     15.766224      0.992583     15.370000      0.100000      1.000000   r[13] =      -0.396224   w[13] =      0.076850   C15-H15a
D[14] =     -2.618557      1.432218     -2.900000      0.900000      1.000000   r[14] =      -0.281443   w[14] =      0.000949   C15-H15b

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =            5                  # rank of cosine matrix (check input if rank < 5)
cond  =   3.277044e+00                # condition number of cosine matrix (check input and singular values if very large)
chisq =      0.652246                 # weighted total sum of squared residuals
aic   =    858.724491                 # information criterion (AIC) for 5 degrees of freedom
rmsd  =      0.782189                 # unweighted root mean square deviation
qfac  =      0.055502                 # weighted Q-Factor as defined by Cornilescu
r^2   =      0.996609                 # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =     10.722763     10.938571   # mean absolute (calc./exp.) parameter D[i]
|D|min=      0.678557      0.990000   # min. absolute (calc./exp.) parameter D[i]
|D|max=     28.075974     28.050000   # max. absolute (calc./exp.) parameter D[i]
Drange=    -14.930000     28.075974   # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =      0.303194 +/-  0.228012   # linear regression intercept and error
c(m)  =      0.990614 +/-  0.015670   # linear regression slope and error
chisq =      0.566730                 # weighted total sum of squared residuals
R     =      0.998502                 # weighted Pearson correlation coefficient R
R^2   =      0.997006                 # weighted Pearson correlation coefficient R^2
```

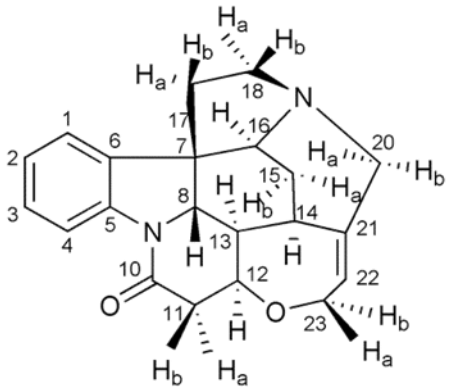




3.1.22 (-)-Strychnine in *ent*-p1-i

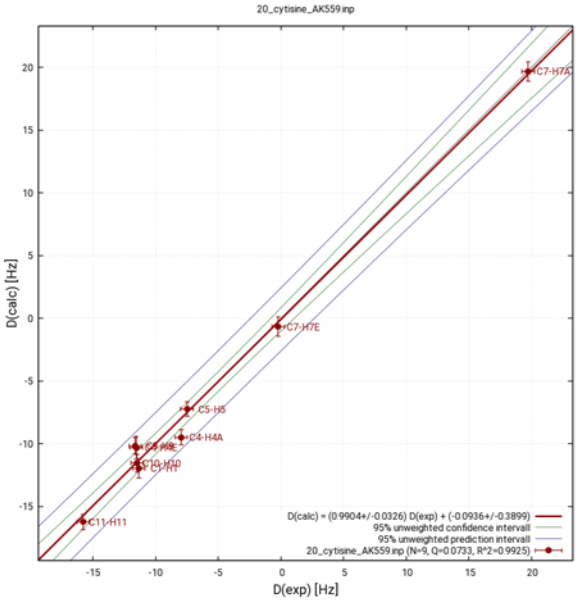
```
------------------------------------------------------------------------------
info : Start Single-Conformer-Single-Tensor (SCST) Fit with 14 RDCs
------------------------------------------------------------------------------

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
  1.377977e-04  2.546161e-04  6.024665e-04 -5.495860e-04  1.271004e-04
Saupe Tensor (S):                                Alignment Tensor (A):
  5.840919e-05  6.024665e-04 -5.495860e-04         3.893946e-05  4.016443e-04 -3.663907e-04
  6.024665e-04 -1.962069e-04  1.271004e-04         4.016443e-04 -1.308046e-04  8.473359e-05
 -5.495860e-04  1.271004e-04  1.377977e-04        -3.663907e-04  8.473359e-05  9.186515e-05
Trace of Saupe Tensor:       2.710505e-20        Trace of Alignment Tensor:    1.807004e-20
Eigenvectors of Saupe Tensor:                    Eigenvectors of Alignment Tensor:
  1.903888e-01  7.390276e-01 -6.462123e-01         1.903888e-01  7.390276e-01 -6.462123e-01
  6.705872e-01  3.828475e-01  6.354059e-01         6.705872e-01  3.828475e-01  6.354059e-01
  7.169832e-01 -5.543158e-01 -4.226926e-01         7.169832e-01 -5.543158e-01 -4.226926e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
  1.107356e-04  7.827354e-04 -8.934710e-04         7.382372e-05  5.218236e-04 -5.956473e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
  2.184550e-04 -7.113936e-04  1.645209e-04  1.647897e-04  7.798431e-04
Tensor Properties:
A(axial)      =  -8.934710e-04        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =  -4.479999e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   5.014151e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   7.521227e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   9.740730e-04        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
         D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)      Normalized Weights    Atom Labels
D[01] =      -5.305804      0.642261     -5.830000      0.100000      1.000000   r[01] =     -0.524196   w[01] =      0.076850   C3-H3
D[02] =      -0.072377      0.784156     -0.030000      0.100000      1.000000   r[02] =      0.042377   w[02] =      0.076850   C22-H22
D[03] =     -11.108532      0.555642    -11.740000      0.100000      1.000000   r[03] =     -0.631468   w[03] =      0.076850   C2-H2
D[04] =      20.704669      0.579739     19.860000      0.100000      1.000000   r[04] =     -0.844669   w[04] =      0.076850   C1-H1
D[05] =      20.999086      0.587726     21.510000      0.100000      1.000000   r[05] =      0.510914   w[05] =      0.076850   C4-H4
D[06] =      -1.967020      0.539382     -2.620000      0.100000      1.000000   r[06] =     -0.652980   w[06] =      0.076850   C12-H12
D[07] =       5.765749      0.582798      5.260000      0.100000      1.000000   r[07] =     -0.505749   w[07] =      0.076850   C20-H20a
D[08] =      -3.142534      0.713479     -3.440000      0.100000      1.000000   r[08] =     -0.297466   w[08] =      0.076850   C20-H20b
D[09] =      -4.676728      0.692274     -4.840000      0.100000      1.000000   r[09] =     -0.163272   w[09] =      0.076850   C13-H13
D[10] =      15.199974      0.625390     15.090000      0.100000      1.000000   r[10] =     -0.109974   w[10] =      0.076850   C11-H11a
D[11] =      -4.195232      0.493020     -4.090000      0.100000      1.000000   r[11] =      0.105232   w[11] =      0.076850   C11-H11b
D[12] =      -5.234514      0.518668     -5.400000      0.100000      1.000000   r[12] =     -0.165486   w[12] =      0.076850   C14-H14
D[13] =      11.353434      0.700035     11.190000      0.100000      1.000000   r[13] =     -0.163434   w[13] =      0.076850   C15-H15a
D[14] =      -1.942732      1.117725     -2.050000      0.900000      1.000000   r[14] =     -0.107268   w[14] =      0.000949   C15-H15b

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =            5                  # rank of cosine matrix (check input if rank < 5)
cond  =   3.277044e+00                # condition number of cosine matrix (check input and singular values if very large)
chisq =      0.194011                 # weighted total sum of squared residuals
aic   =    262.454382                 # information criterion (AIC) for 5 degrees of freedom
rmsd  =      0.425601                 # unweighted root mean square deviation
qfac  =      0.041058                 # weighted Q-Factor as defined by Cornilescu
r^2   =      0.998202                 # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =      7.976313      8.067857  # mean absolute (calc./exp.) parameter D[i]
|D|min=      0.072377      0.030000  # min. absolute (calc./exp.) parameter D[i]
|D|max=     20.999086     21.510000  # max. absolute (calc./exp.) parameter D[i]
Drange=    -11.740000     21.510000  # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =      0.283650 +/-  0.102525   # linear regression intercept and error
c(m)  =      0.991705 +/-  0.009557   # linear regression slope and error
chisq =      0.118255                 # weighted total sum of squared residuals
R     =      0.999443                 # weighted Pearson correlation coefficient R
R^2   =      0.998887                 # weighted Pearson correlation coefficient R^2
```

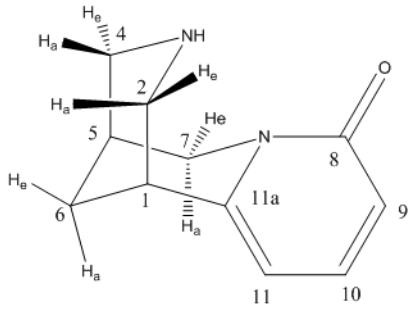




3.1.23 (-)-Cytisine in p1-a

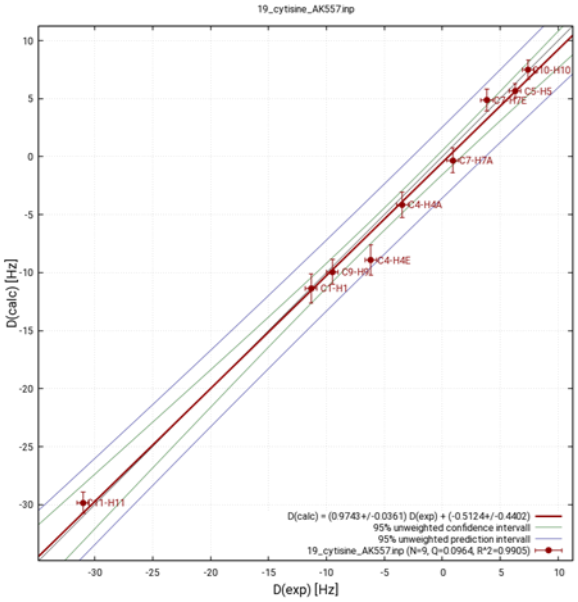
```
------------------------------------------------------------------------------
info : Start Single-Conformer-Single-Tensor (SCST) Fit with 9 RDCs
------------------------------------------------------------------------------

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
  3.703014e-04  1.338914e-03  5.170461e-06 -9.165738e-05 -6.979889e-04
Saupe Tensor (S):                          Alignment Tensor (A):
  4.843061e-04  5.170461e-06 -9.165738e-05    3.228708e-04  3.446974e-06 -6.110492e-05
  5.170461e-06 -8.546075e-04 -6.979889e-04    3.446974e-06 -5.697383e-04 -4.653259e-04
 -9.165738e-05 -6.979889e-04  3.703014e-04   -6.110492e-05 -4.653259e-04  2.468676e-04
Trace of Saupe Tensor:        0.000000e+00  Trace of Alignment Tensor:    0.000000e+00
Eigenvectors of Saupe Tensor:              Eigenvectors of Alignment Tensor:
 -9.384234e-01  3.449058e-01 -2.003897e-02   -9.384234e-01  3.449058e-01 -2.003897e-02
  1.597474e-01  3.817510e-01 -9.103554e-01    1.597474e-01  3.817510e-01 -9.103554e-01
 -3.063370e-01 -8.574999e-01 -4.133419e-01   -3.063370e-01 -8.574999e-01 -4.133419e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
  4.535055e-04  7.179062e-04 -1.171412e-03    3.023370e-04  4.786042e-04 -7.809412e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
  5.870502e-04 -1.186429e-04 -9.034888e-04  8.665565e-04  6.692734e-06
Tensor Properties:
A(axial)      =  -1.171412e-03        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =  -1.762671e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   1.504741e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   2.257112e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   1.181316e-03        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights    Atom Labels
D[01] =     -7.243605      0.582891     -7.480000      0.500000      1.000000   r[01] =      -0.236395   w[01] =       0.111111   C5-H5
D[02] =    -11.968853      0.792485    -11.330000      0.500000      1.000000   r[02] =       0.638853   w[02] =       0.111111   C1-H1
D[03] =     19.686112      0.778690     19.750000      0.500000      1.000000   r[03] =       0.063888   w[03] =       0.111111   C7-H7A
D[04] =     -0.671684      0.769694     -0.200000      0.500000      1.000000   r[04] =       0.471684   w[04] =       0.111111   C7-H7E
D[05] =     -9.485475      0.611173     -7.950000      0.500000      1.000000   r[05] =       1.535475   w[05] =       0.111111   C4-H4A
D[06] =    -10.312346      0.891353    -11.550000      0.500000      1.000000   r[06] =      -1.237654   w[06] =       0.111111   C4-H4E
D[07] =    -16.229500      0.610095    -15.780000      0.500000      1.000000   r[07] =       0.449500   w[07] =       0.111111   C11-H11
D[08] =    -10.167967      0.640771    -11.630000      0.500000      1.000000   r[08] =      -1.462033   w[08] =       0.111111   C9-H9
D[09] =    -11.547206      0.689941    -11.480000      0.500000      1.000000   r[09] =       0.067206   w[09] =       0.111111   C10-H10

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =           5                  # rank of cosine matrix (check input if rank < 5)
cond  =   5.395054e+00                # condition number of cosine matrix (check input and singular values if very large)
chisq =      0.769351                 # weighted total sum of squared residuals
aic   =     37.696647                 # information criterion (AIC) for 5 degrees of freedom
rmsd  =      0.877127                 # unweighted root mean square deviation
qfac  =      0.073347                 # weighted Q-Factor as defined by Cornilescu
r^2   =      0.992456                 # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =     10.812528     10.794444   # mean absolute (calc./exp.) parameter D[i]
|D|min=      0.671684      0.200000   # min. absolute (calc./exp.) parameter D[i]
|D|max=     19.686112     19.750000   # max. absolute (calc./exp.) parameter D[i]
Drange=    -16.229500     19.750000   # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =     -0.093594 +/-  0.389934   # linear regression intercept and error
c(m)  =      0.990428 +/-  0.032607   # linear regression slope and error
chisq =      0.758966                 # weighted total sum of squared residuals
R     =      0.996228                 # weighted Pearson correlation coefficient R
R^2   =      0.992470                 # weighted Pearson correlation coefficient R^2
```

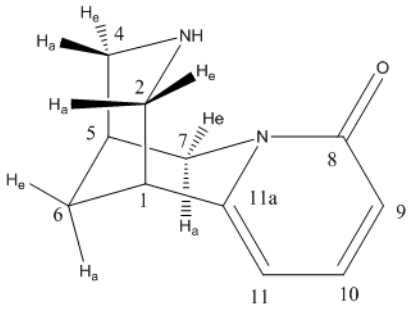




3.1.24 (-)-Cytisine in *ent*-p1-d

```
------------------------------------------------------------------------------
info : Start Single-Conformer-Single-Tensor (SCST) Fit with 9 RDCs
------------------------------------------------------------------------------

------------------------------------------------------------------------------
SVD Best-Fit Saupe Vector S(zz), S(xx-yy), S(xy), S(xz), S(yz):
  1.016693e-03  4.737712e-04 -2.054428e-04 -7.874989e-04 -1.532038e-04
Saupe Tensor (S):                          Alignment Tensor (A):
 -2.714607e-04 -2.054428e-04 -7.874989e-04   -1.809738e-04 -1.369619e-04 -5.249993e-04
 -2.054428e-04 -7.452319e-04 -1.532038e-04   -1.369619e-04 -4.968213e-04 -1.021358e-04
 -7.874989e-04 -1.532038e-04  1.016693e-03   -5.249993e-04 -1.021358e-04  6.777951e-04
Trace of Saupe Tensor:        0.000000e+00 Trace of Alignment Tensor:    0.000000e+00
Eigenvectors of Saupe Tensor:              Eigenvectors of Alignment Tensor:
  7.069446e-01 -5.649467e-01  4.255168e-01    7.069446e-01 -5.649467e-01  4.255168e-01
 -6.328646e-01 -7.738919e-01  2.395332e-02   -6.328646e-01 -7.738919e-01  2.395332e-02
  3.157717e-01 -2.862282e-01 -9.046335e-01    3.157717e-01 -2.862282e-01 -9.046335e-01
Eigenvalues of Saupe Tensor S(xx), S(yy), S(zz):  Eigenvalues of Alignment Tensor A(xx), A(yy), A(zz):
 -4.392990e-04 -9.518699e-04  1.391169e-03   -2.928660e-04 -6.345799e-04  9.274459e-04
Alignment Tensor Irreducible Representation (A0, A1R, A1I, A2R, A2I):
  1.611794e-03 -1.019352e-03 -1.983096e-04  3.066288e-04 -2.659287e-04
Tensor Properties:
A(axial)      =   1.391169e-03        # alignment tensor axial component   = 3/2*A(zz) = S(zz)
A(rhombic)    =   3.417139e-04        # alignment tensor rhombic component = A(xx) - A(yy) = 2/3*(S(xx) - S(yy))
A(rhombicity) =   2.456308e-01        # alignment tensor rhombicity        = A(rhombic) / A(axial)
A(asymmetry)  =   3.684462e-01        # alignment tensor asymmetry         = (A(xx) - A(yy))/A(zz) = (S(xx) - S(yy))/S(zz)
GDO           =   1.422296e-03        # generalized degree of order        = sqrt(3/2)*|A(xx),A(yy),A(zz)| = sqrt(2/3)*|S(xx),S(yy),S(zz)|

------------------------------------------------------------------------------
Results for Multi-Parameter Fit of Calculated and Experimental Data:
        D(calc) [HZ]     +/- Error   D(exp) [Hz]     +/- Error  Rel. Weights          D(exp)-D(calc)       Normalized Weights    Atom Labels
D[01] =      5.662319      0.632274      6.280000      0.500000      1.000000   r[01] =      0.617681   w[01] =      0.111111   C5-H5
D[02] =    -11.354349      1.248633    -11.320000      0.500000      1.000000   r[02] =      0.034349   w[02] =      0.111111   C1-H1
D[03] =     -0.317646      1.062382      0.900000      0.500000      1.000000   r[03] =      1.217646   w[03] =      0.111111   C7-H7A
D[04] =      4.866814      0.934506      3.850000      0.500000      1.000000   r[04] =     -1.016814   w[04] =      0.111111   C7-H7E
D[05] =     -4.134697      1.098422     -3.460000      0.500000      1.000000   r[05] =      0.674697   w[05] =      0.111111   C4-H4A
D[06] =     -8.913899      1.295535     -6.170000      0.500000      1.000000   r[06] =      2.743899   w[06] =      0.111111   C4-H4E
D[07] =    -29.838637      0.896456    -31.000000      0.500000      1.000000   r[07] =     -1.161363   w[07] =      0.111111   C11-H11
D[08] =     -9.946699      1.073310     -9.480000      0.500000      1.000000   r[08] =      0.466699   w[08] =      0.111111   C9-H9
D[09] =      7.491407      0.853609      7.420000      0.500000      1.000000   r[09] =     -0.071407   w[09] =      0.111111   C10-H10

Results for Multi-Parameter Fit of Calculated and Experimental Data:
rank  =           5                  # rank of cosine matrix (check input if rank < 5)
cond  =   5.395054e+00                # condition number of cosine matrix (check input and singular values if very large)
chisq =      1.383906                 # weighted total sum of squared residuals
aic   =     59.820622                 # information criterion (AIC) for 5 degrees of freedom
rmsd  =      1.176395                 # unweighted root mean square deviation
qfac  =      0.096440                 # weighted Q-Factor as defined by Cornilescu
r^2   =      0.989016                 # coefficient of determination r^2 = 1 - chi^2 / (weighted sum of squares)

<|D|> =      9.169608      8.875556  # mean absolute (calc./exp.) parameter D[i]
|D|min=      0.317646      0.900000  # min. absolute (calc./exp.) parameter D[i]
|D|max=     29.838637     31.000000  # max. absolute (calc./exp.) parameter D[i]
Drange=    -31.000000      7.491407  # min. and max. (calc./exp.) parameter D[i]

Results for Linear Regression of Calculated and Experimental Data:
c(b)  =     -0.512444 +/-  0.440229  # linear regression intercept and error
c(m)  =      0.974253 +/-  0.036089  # linear regression slope and error
chisq =      1.148684                # weighted total sum of squared residuals
R     =      0.995232                # weighted Pearson correlation coefficient R
R^2   =      0.990486                # weighted Pearson correlation coefficient R^2
```





Literature

[1] H. E. Gottlieb, V. Kotlyar, A. Nudelman, *J. Org. Chem.* **1997**, *62*, 7512-7515.
[2] E. Yashima, T. Matsushima, Y. Okamoto, *J. Am. Chem. Soc.* **1997**, *119*, 6345-6359.
[3] K. Okoshi, K. Sakajiri, J. Kumaki, E. Yashima, *Macromolecules* **2005**, *38*, 4061-4064.
[4] A. Enthart, J. C. Freudenberger, J. Furrer, H. Kessler, B. Luy, *J. Magn. Reson.* **2008**, *192*, 314-322.
[5] S. Immel, M. Köck, M. Reggelin, *Chem. Eur. J.* **2018**, *24*, 13918-13930.
[6] Gaussian 09, Revision A.01. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, *Wallingford CT* **2009**.
[7] L. Verdier, P. Sakhaii, M. Zweckstetter, C. Griesinger, *J. Magn. Reson.* **2003**, *163*, 353-359.
[8] S. Immel, M. Köck, M. Reggelin, *Chirality* **2019**, *31*, 384-400.
[9] F. Kramer, M. V. Deshmukh, H. Kessler, S. J. Glaser, *Concepts Magn. Reson., Part A* **2004**, *21A*, 10-21.