Effect of the solvent on the conformation of monocrotaline as determined by isotropic and anisotropic NMR parameters.

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*1.NMR Experiments of monocrotaline (**1**) in D_2O*

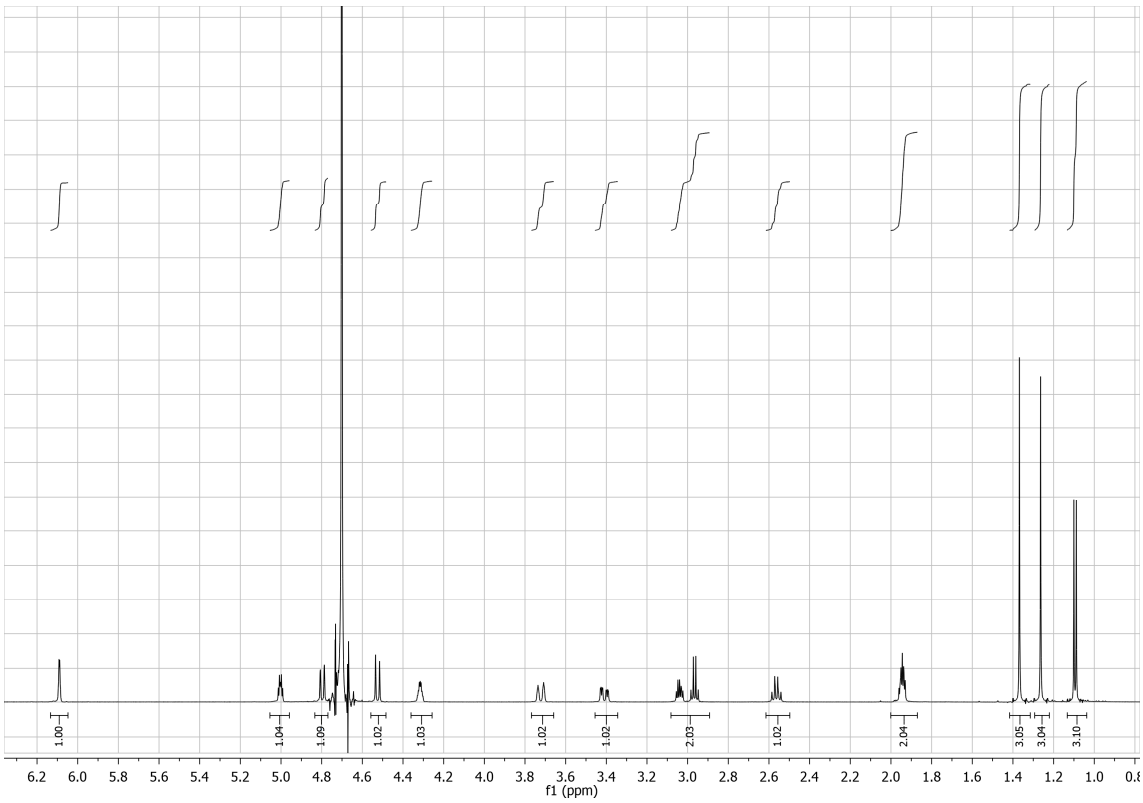

Figure S2. ^{1}H NMR spectrum of monocrotaline (**1**) in D_2O (600 MHz).

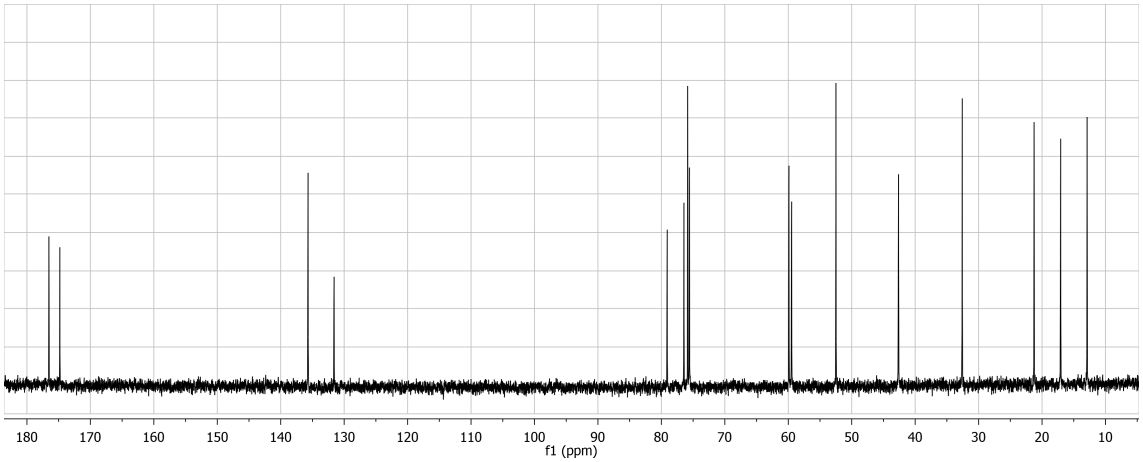

Figure S3. ^{13}C NMR spectrum of monocrotaline (**1**) in D_2O (150 MHz).

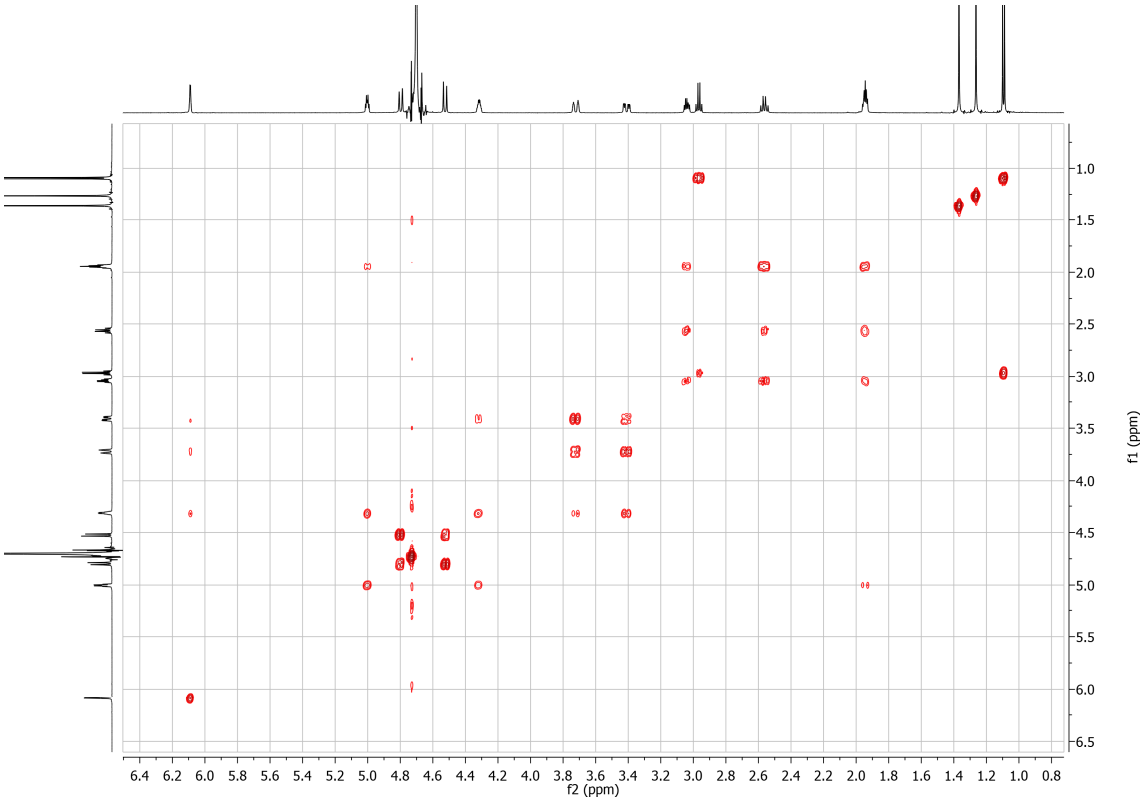

Figure S4. COSY spectrum of monocrotaline (**1**) in D_2O (600 MHz)

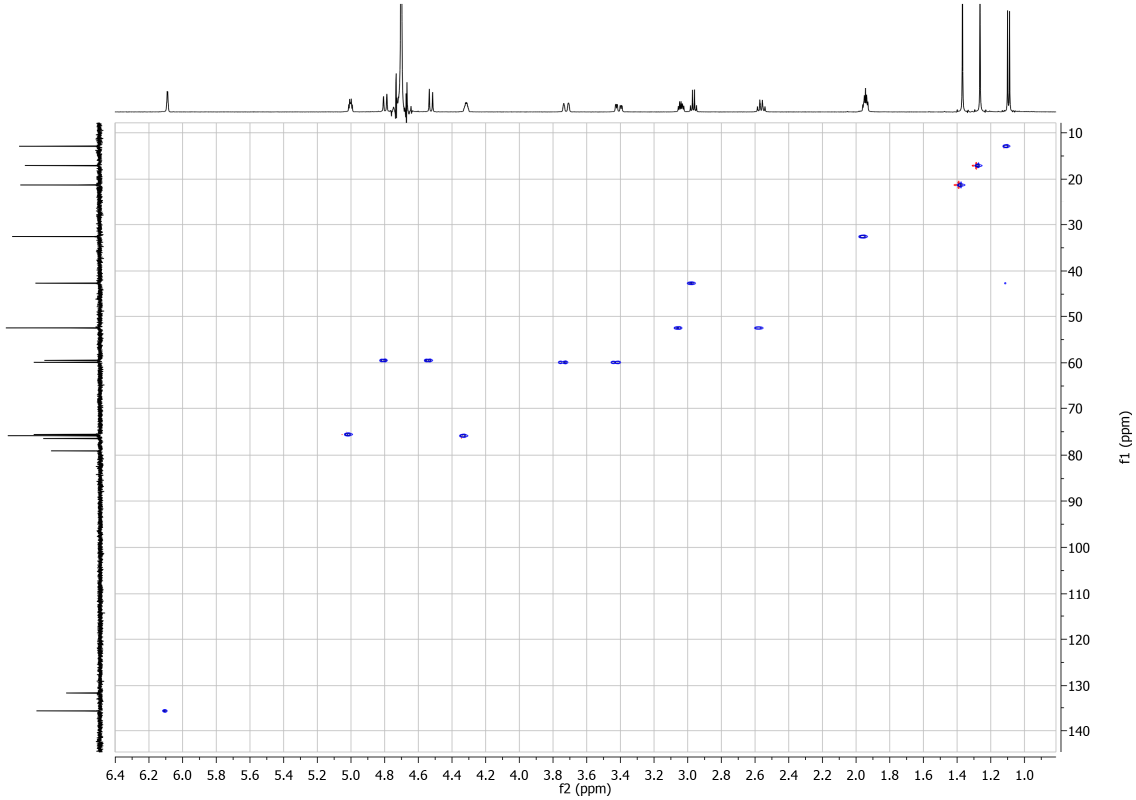

Figure S5. ^{1}H-^{13}C HSQC spectrum of monocrotaline (**1**) in D_2O (^{1}H = 600 MHz and ^{13}C = 150 MHz).

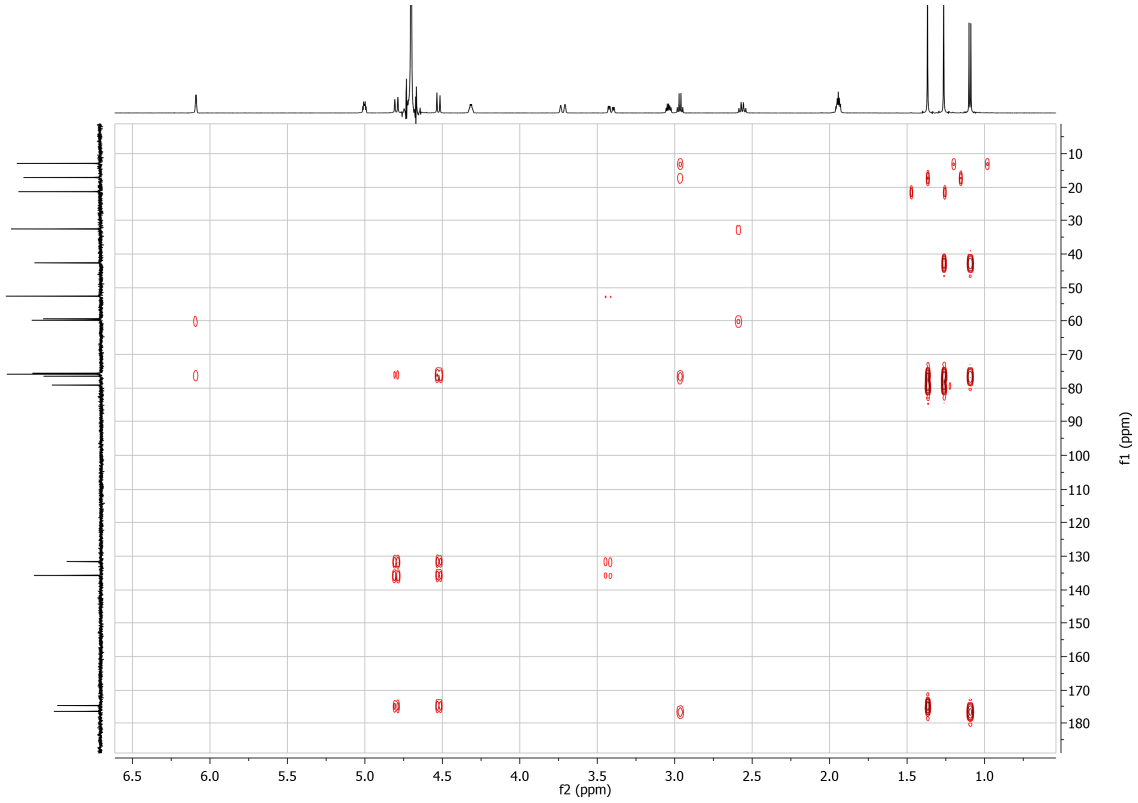

Figure S6. ^{1}H-^{13}C HMBC spectrum of monocrotaline (**1**) in D_2O (^{1}H = 600 MHz and ^{13}C = 150 MHz)

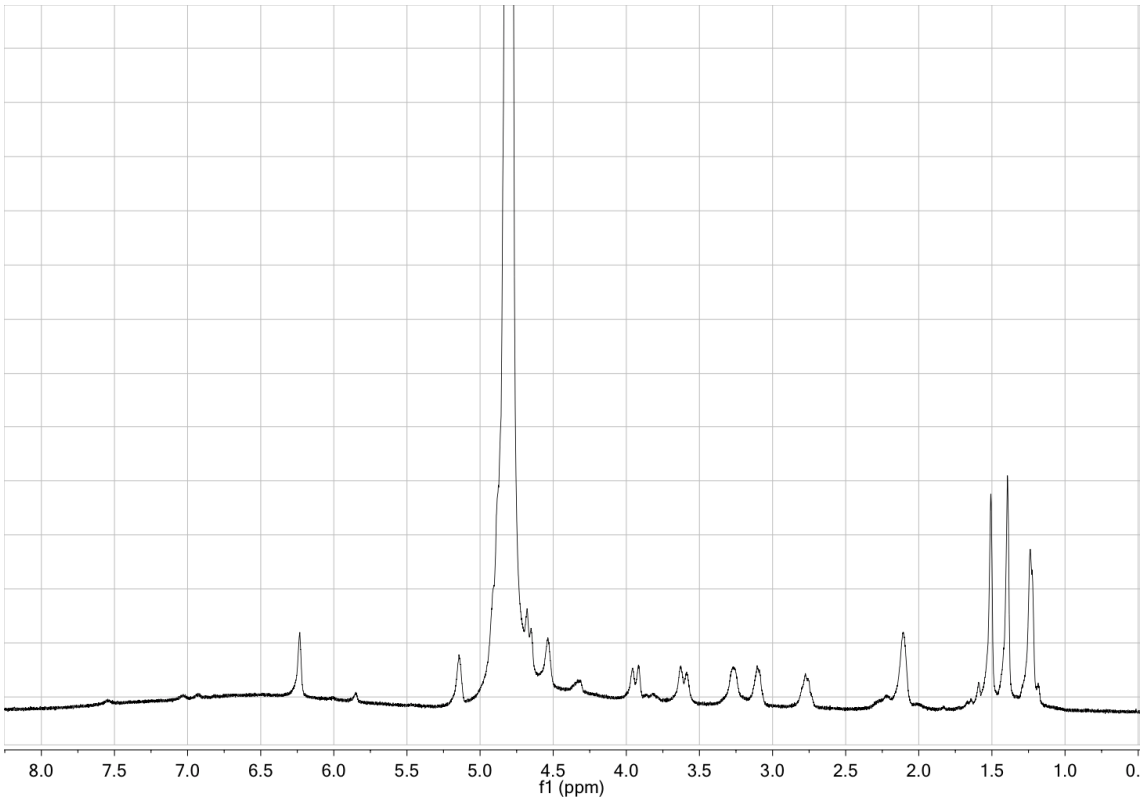

Figure S7. ^{1}H NMR spectrum of monocrotaline (**1**) in DSCG/NaCl/D_2O (399.7 MHz).

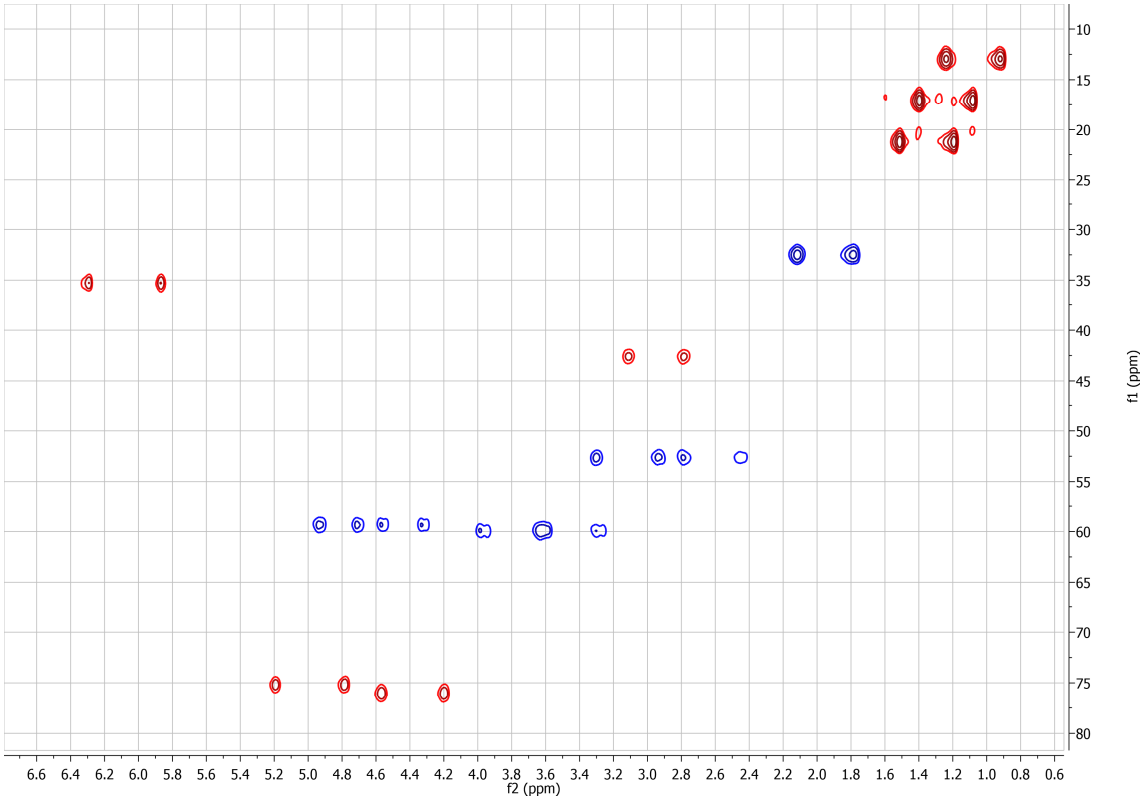

Figure S7. ^{1}H-^{13}C HSQC NMR spectrum coupled in F2 of monocrotaline (**1**) in DSCG/NaCl/D_2O at 28°C (isotropic condition) (^{1}H = 399.7 MHz and ^{13}C = 100.52 MHz)

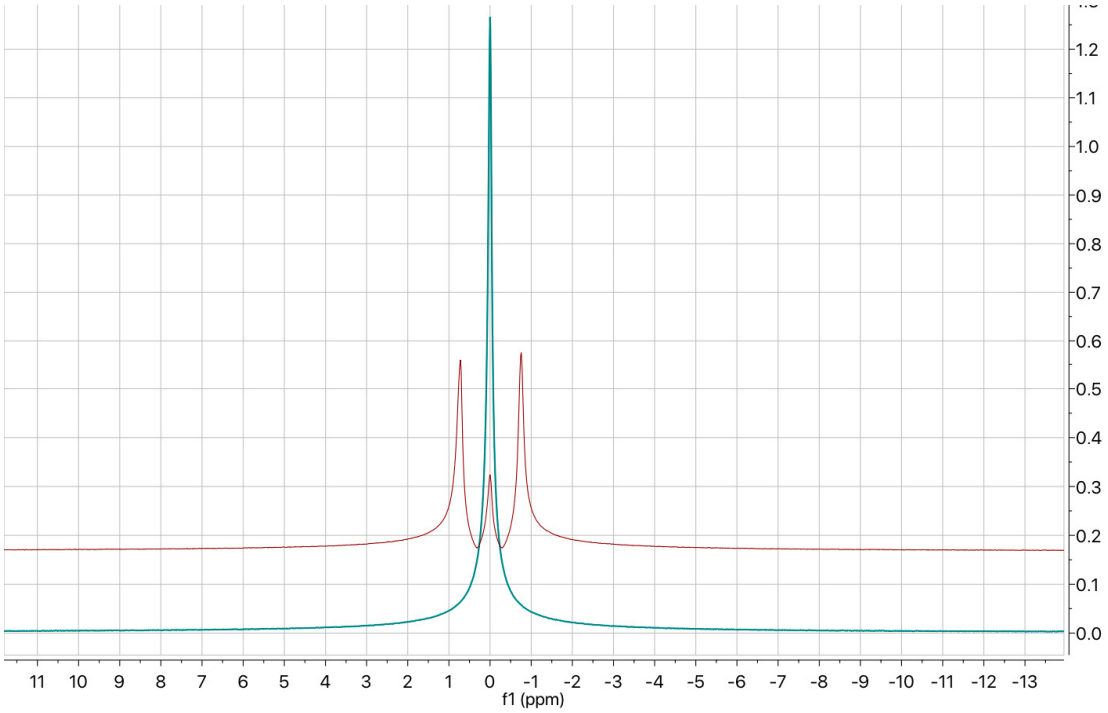

Figure S8. ^{2}H NMR spectra of monocrotaline (**1**) in DSCG/NaCl/D_2O: green spectrum corresponds to the isotropic signal and red the anisotropic signal (61.3 MHz).

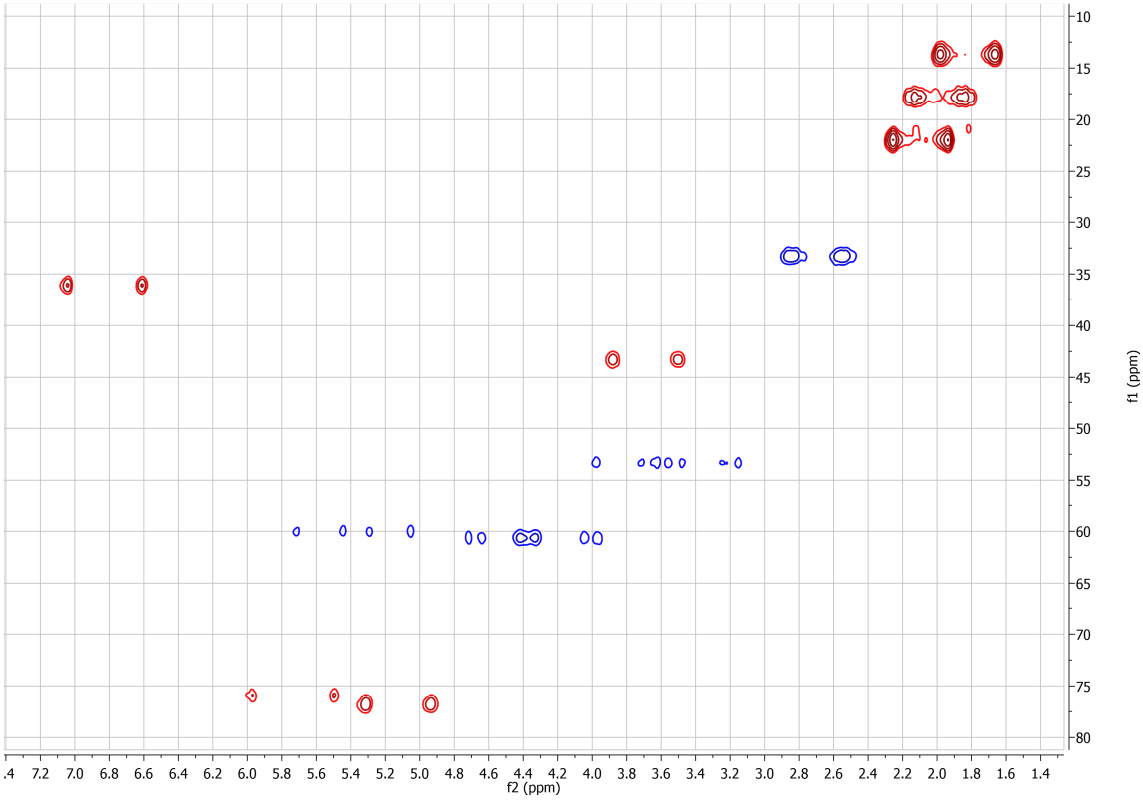

Figure S9. ^{1}H-^{13}C HSQC NMR spectrum coupled in F2 of monocrotaline in DSCG/NaCl/D_2O at 23°C (anisotropic condition) (^{1}H = 399.7 MHz and ^{13}C = 100.52 MHz)

*2.NMR Experiments of monocrotaline (**1**) in DMSO-d_6*

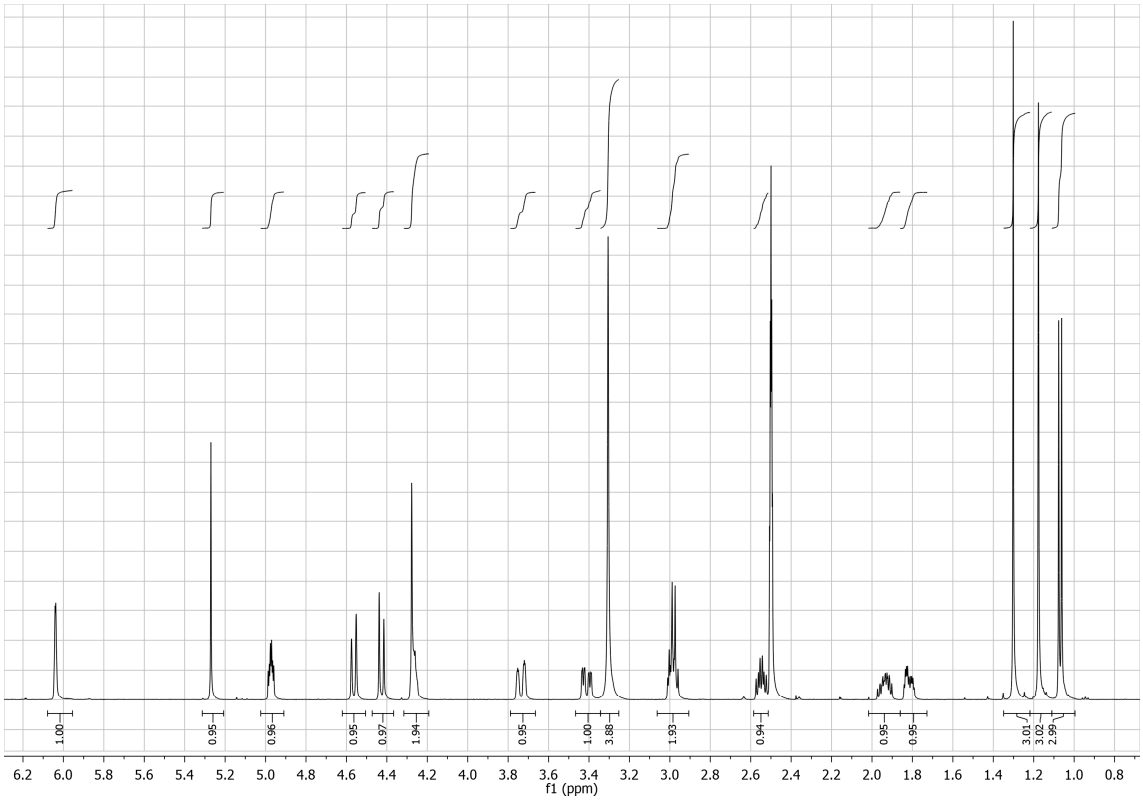

Figure S10. ^{1}H NMR spectrum of monocrotaline (**1**) in DMSO-d_6 (500.13 MHz)

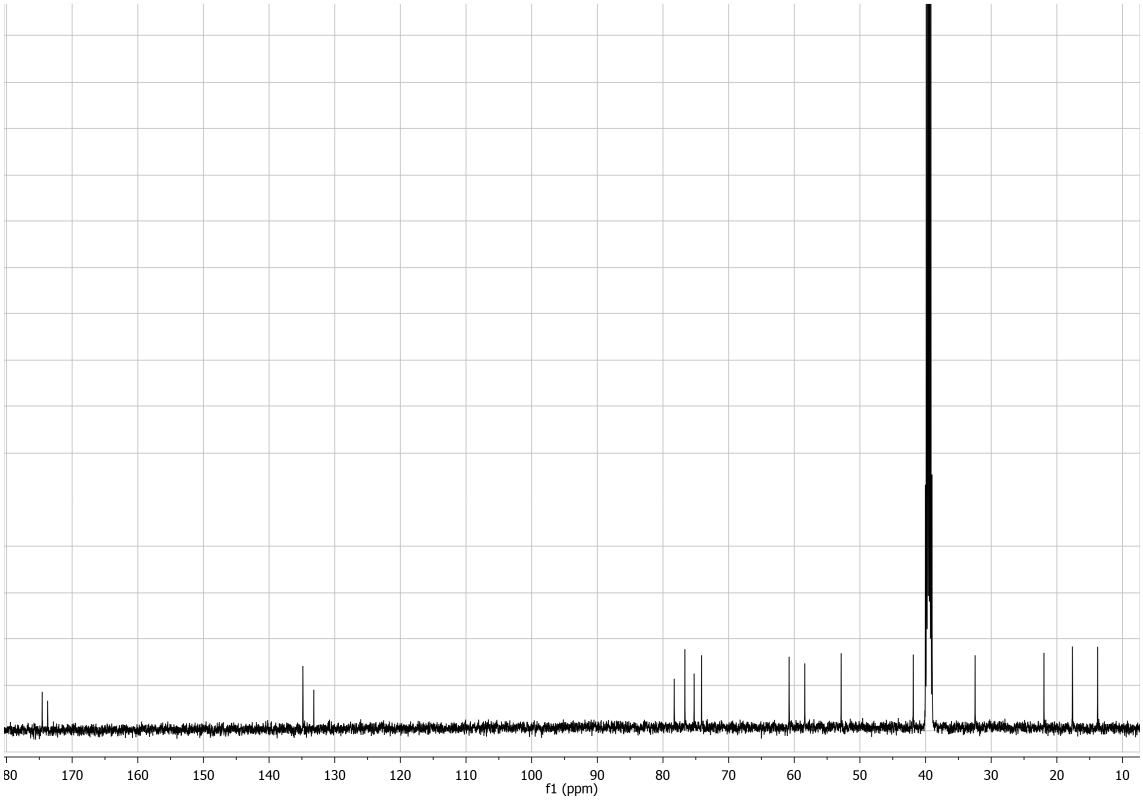

Figure S8. ^{13}C NMR spectrum of monocrotaline (**1**) in DMSO-d_6 (125.77 MHz)

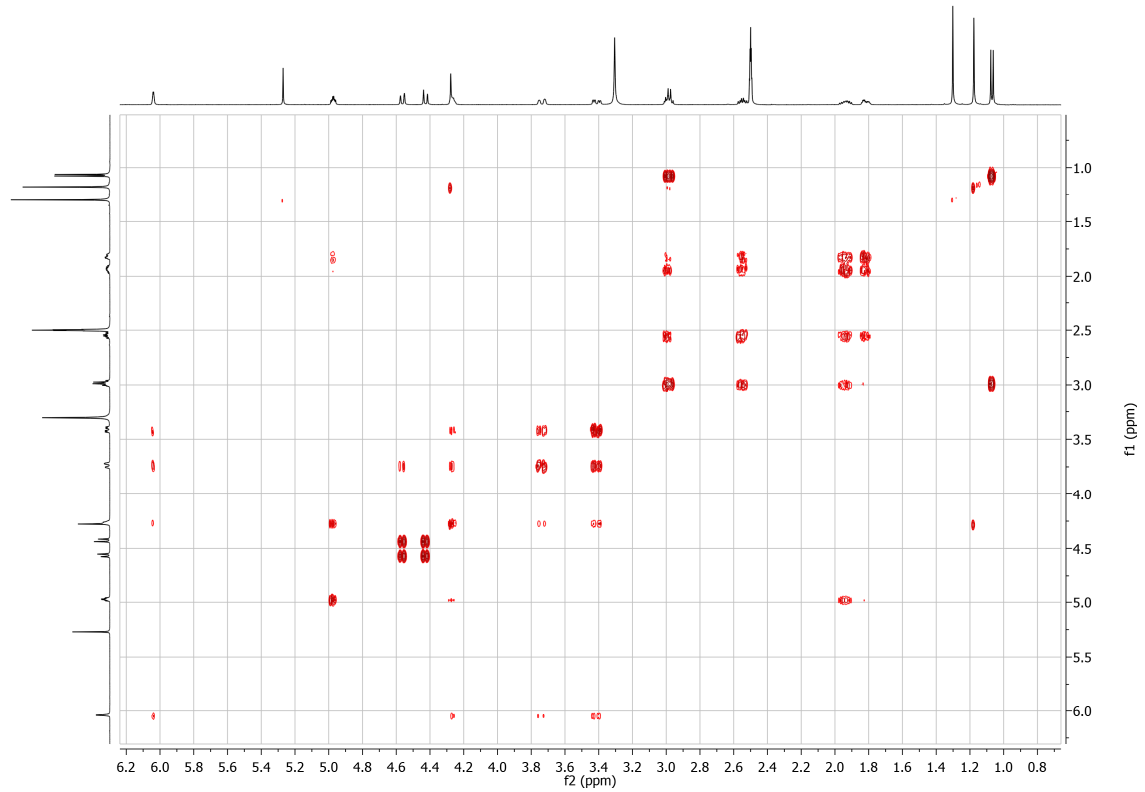

Figure S9. COSY NMR spectrum of monocrotaline (**1**) in DMSO-d_6 (125.77 MHz)

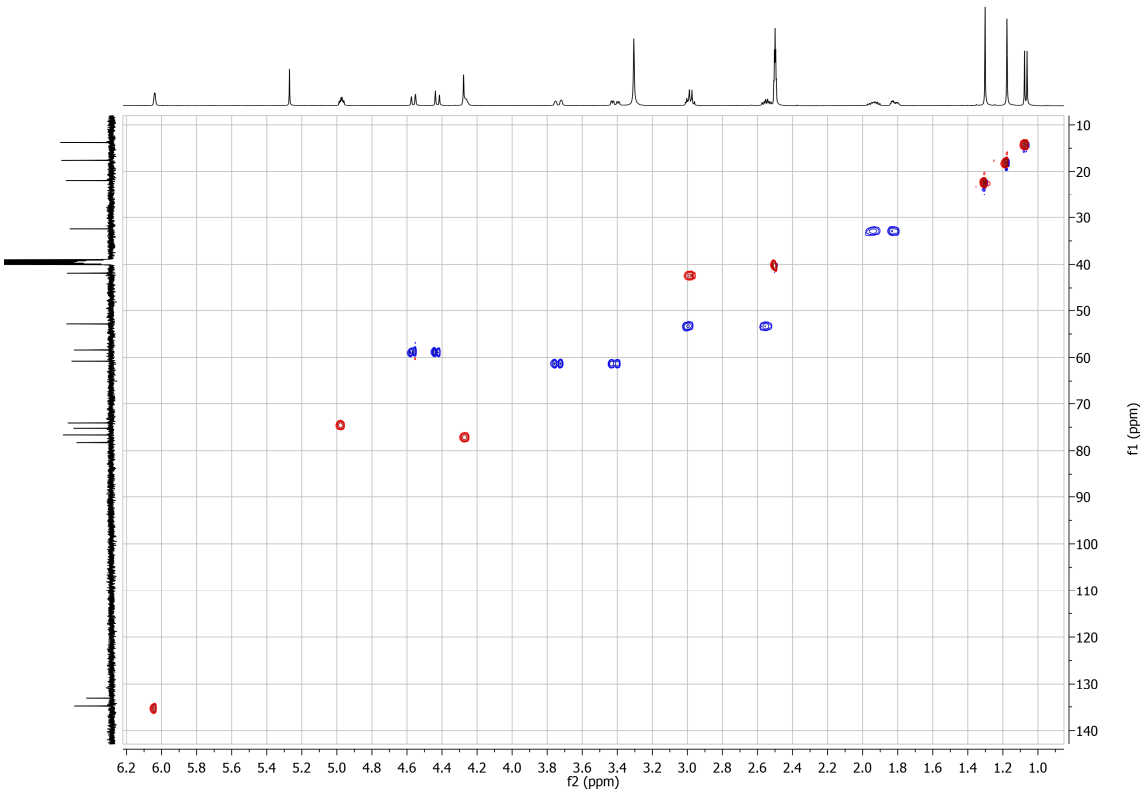

Figure S10. ^{1}H-^{13}C HSQC NMR spectrum of monocrotaline (**1**) in DMSO-d_6 (^{1}H = 500.13 MHz and ^{13}C = 125.77 MHz)

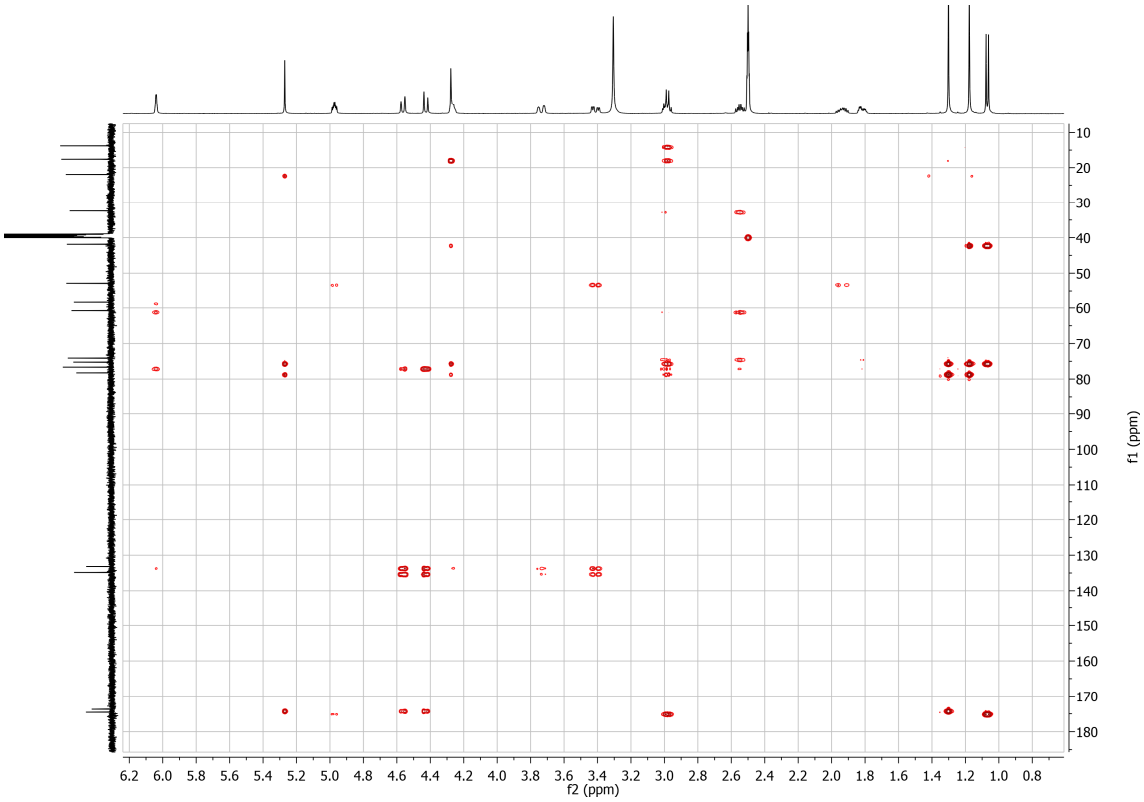

Figure S11. ^{1}H-^{13}C HMBC NMR spectrum of monocrotaline (**1**) in DMSO-d_6 (^{1}H = 500.13 MHz and ^{13}C = 125.77 MHz)

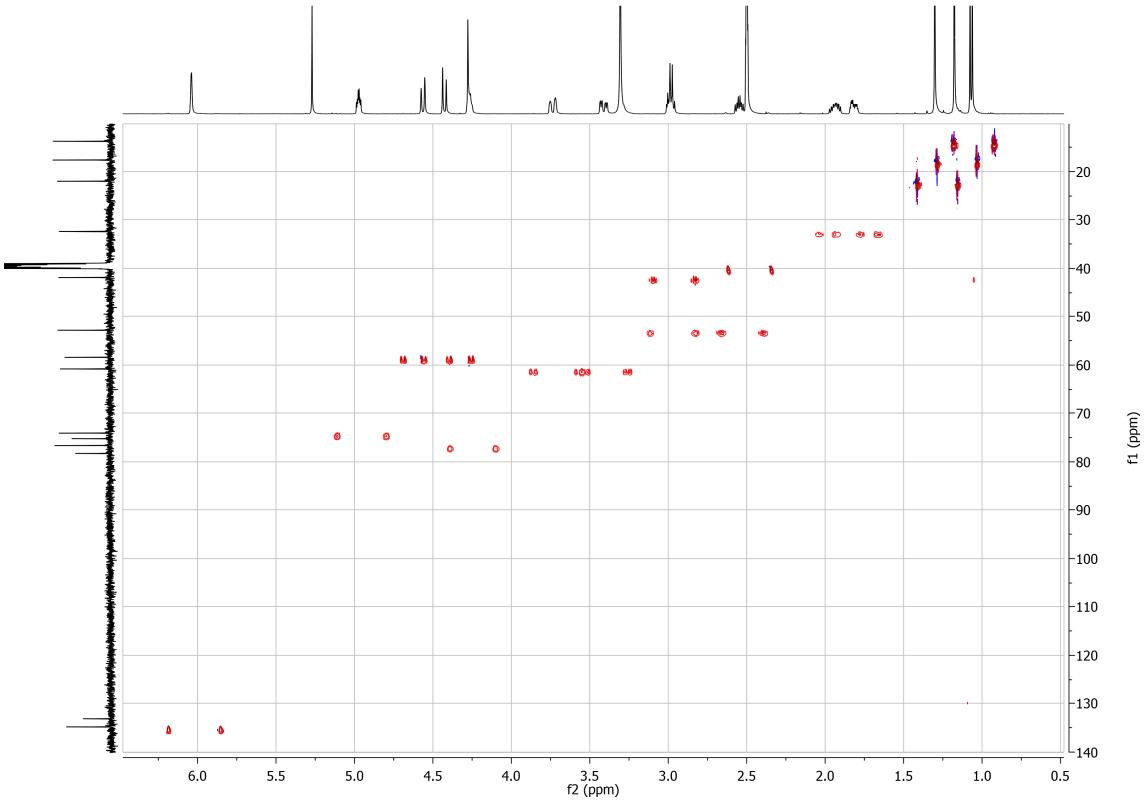

Figure S12. ^{1}H-^{13}C HSQC coupled in F2 NMR spectrum of monocrotaline (**1**) in DMSO-d_6 (^{1}H = 500.13 MHz and ^{13}C = 125.77 MHz)

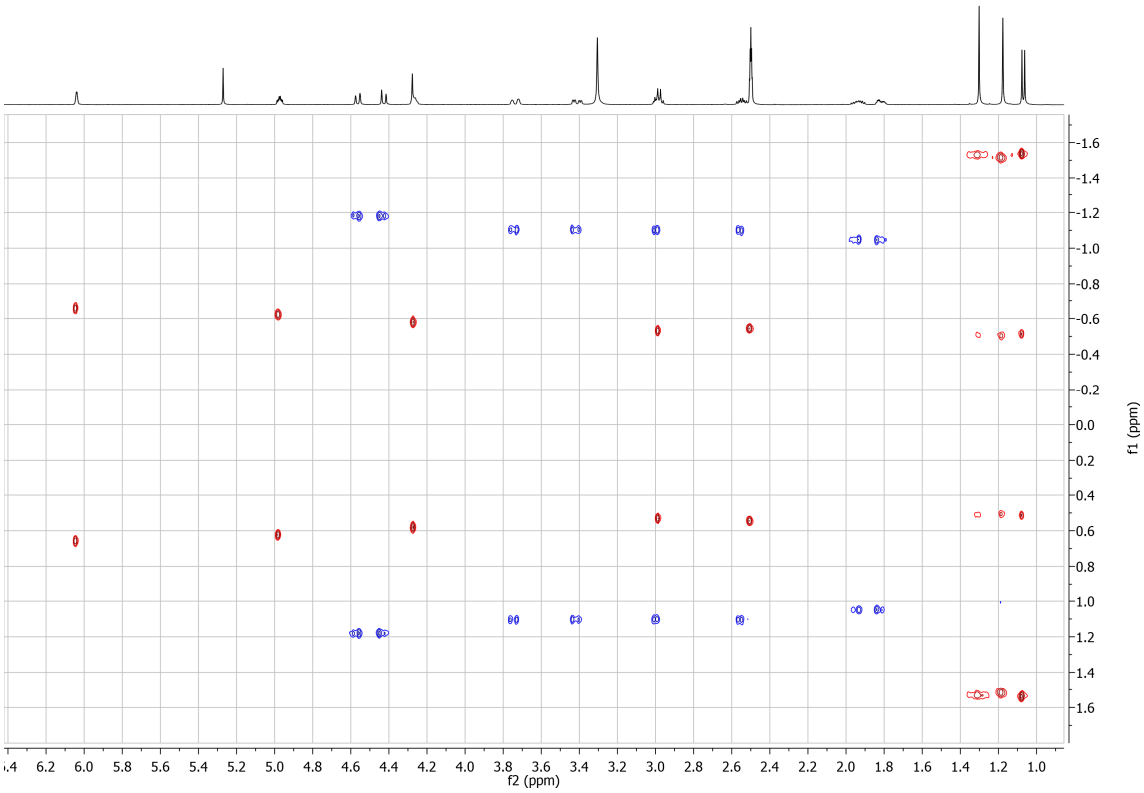

Figure S13. ^{1}H-^{13}C J-Resolved HSQC NMR spectrum of monocrotaline (**1**) in DMSO-d_6 (^{1}H = 500.13 MHz and ^{13}C = 125.77 MHz)

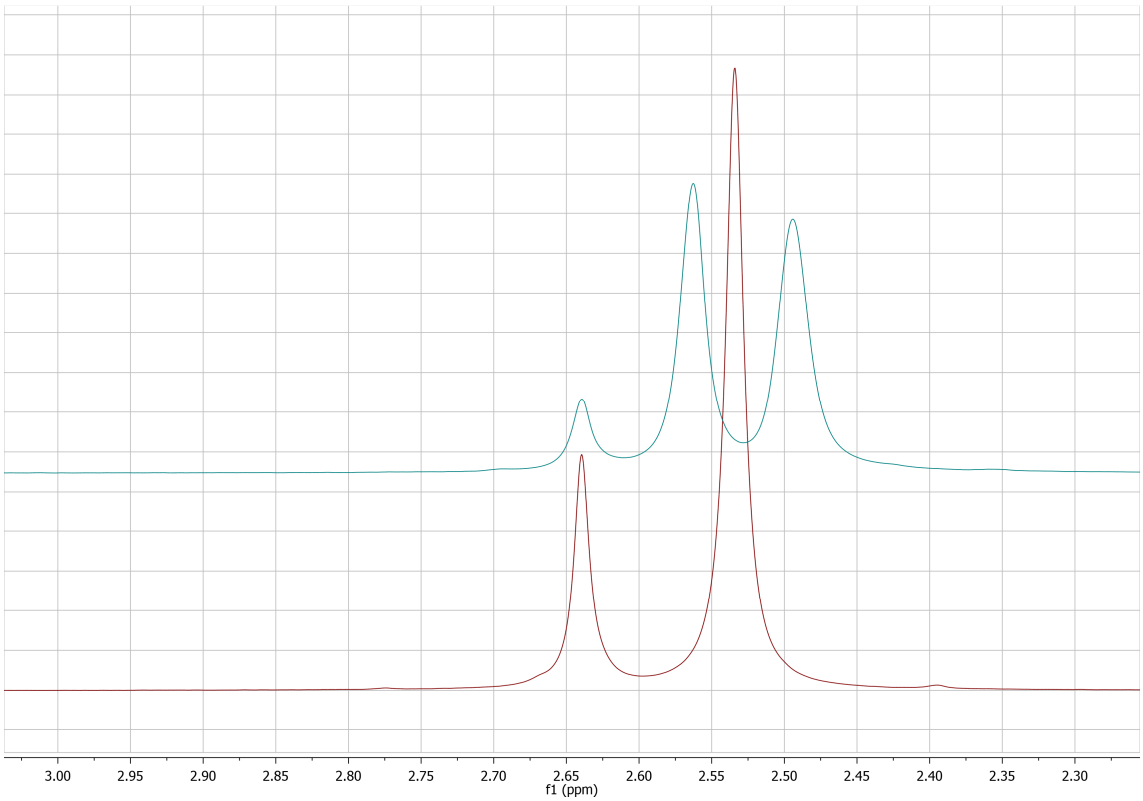

Figure S17. ^{2}H NMR spectra of monocrotaline (**1**) in polyHEMA gel and DMSO-d_6: red spectrum corresponds to the relaxed gel and green spectrum to the compressed gel (76.77 MHz)

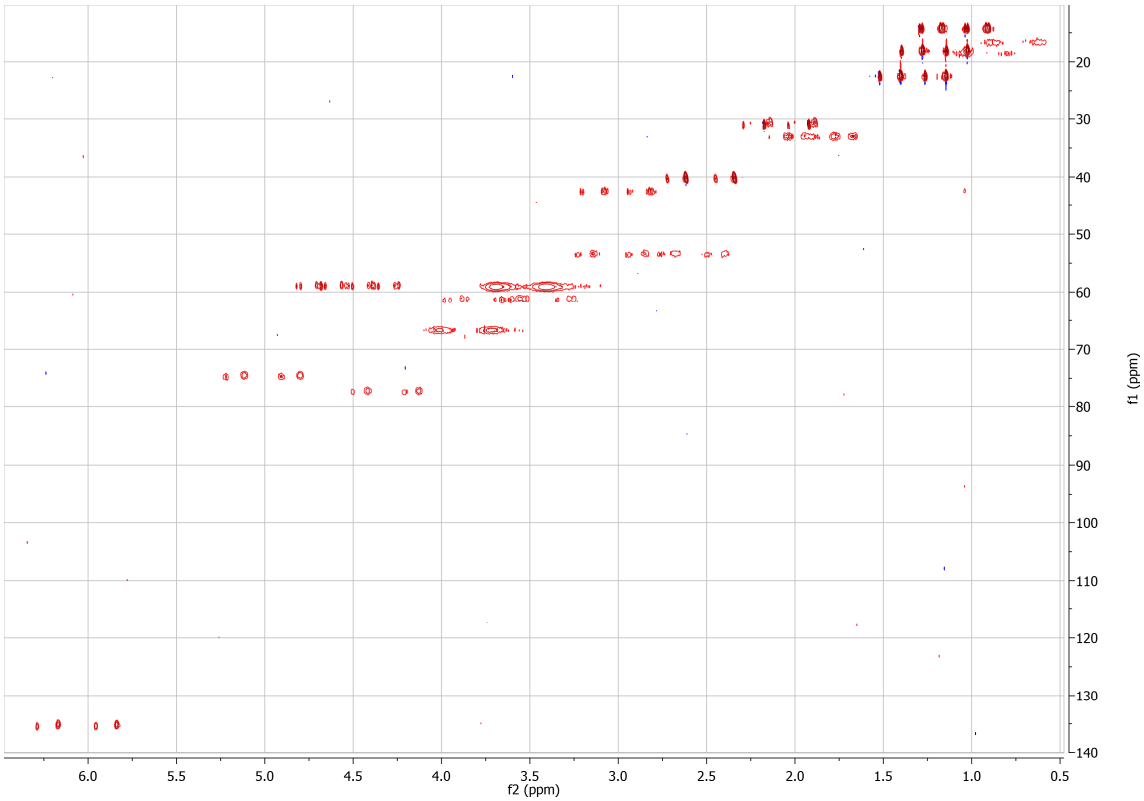

Figure S18. ^{1}H-^{13}C HSQC coupled in F2 NMR spectrum of monocrotaline (**1**) in polyHEMA gel at the relaxed condition (^{1}H = 500.13 MHz and ^{13}C = 125.77 MHz)

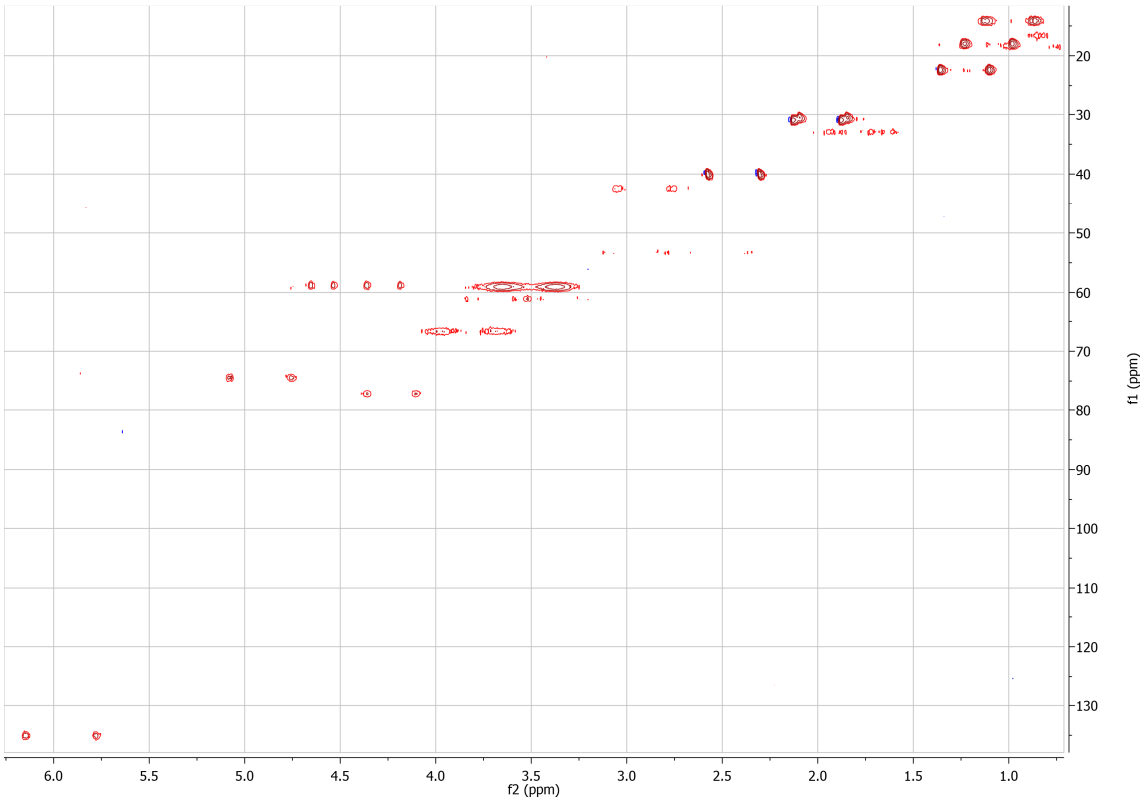

Figure S19. ^{1}H-^{13}C HSQC coupled in F2 NMR spectrum of monocrotaline (**1**) in polyHEMA gel at the compressed condition (^{1}H = 500.13 MHz and ^{13}C = 125.77 MHz)

*3.NMR Experiments of monocrotaline (**1**) in $CDCl_3$*

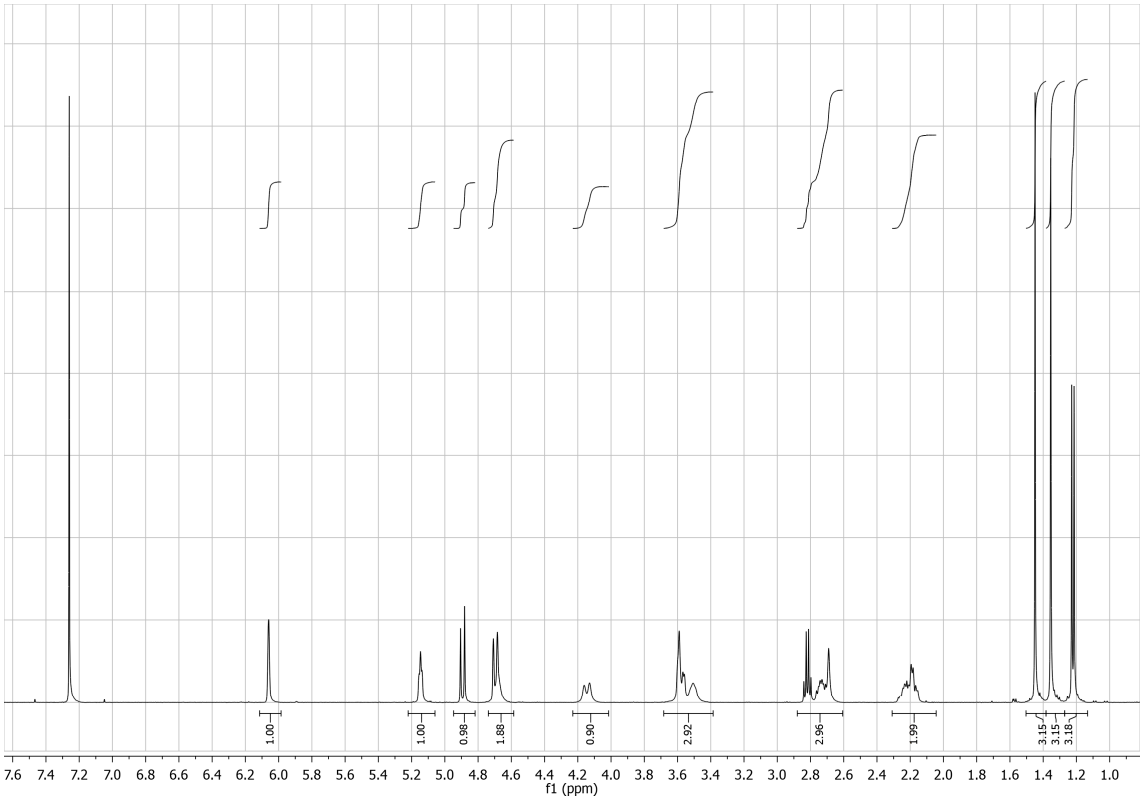

Figure S20. ^{1}H NMR spectrum of monocrotaline (**1**) in $CDCl_3$ (500.13 MHz)

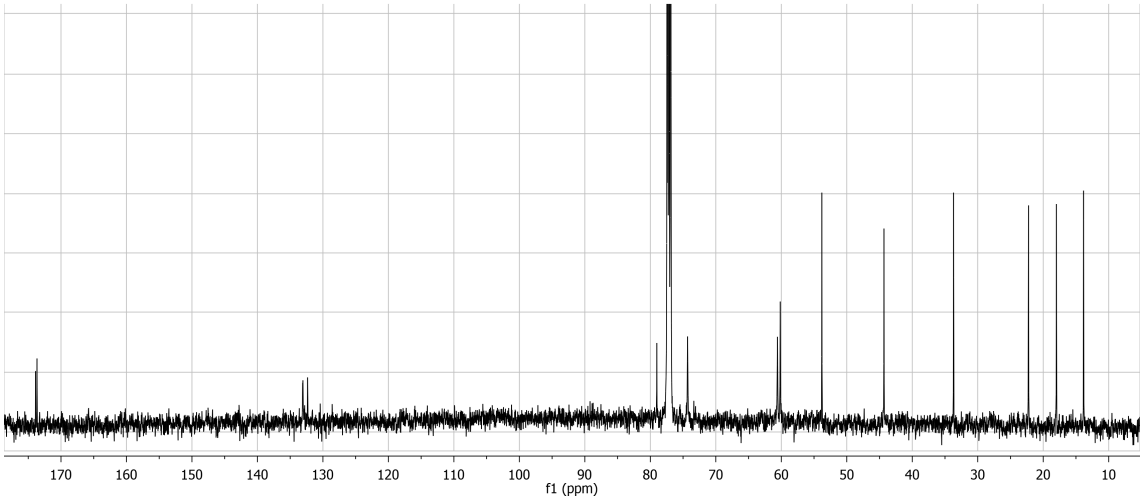

Figure S14. ^{13}C NMR spectrum of monocrotaline (**1**) in $CDCl_3$ (125.77 MHz)

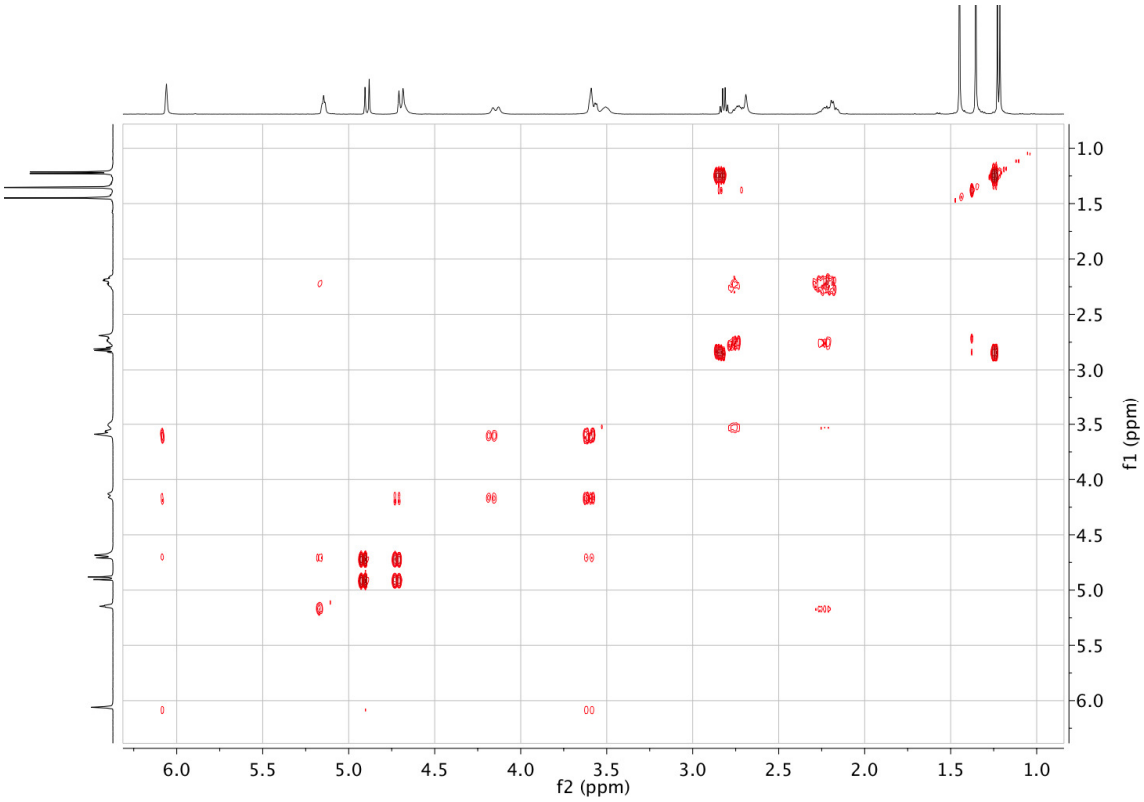

Figure S22. COSY NMR spectrum of monocrotaline (**1**) in $CDCl_3$ (500.13 MHz)

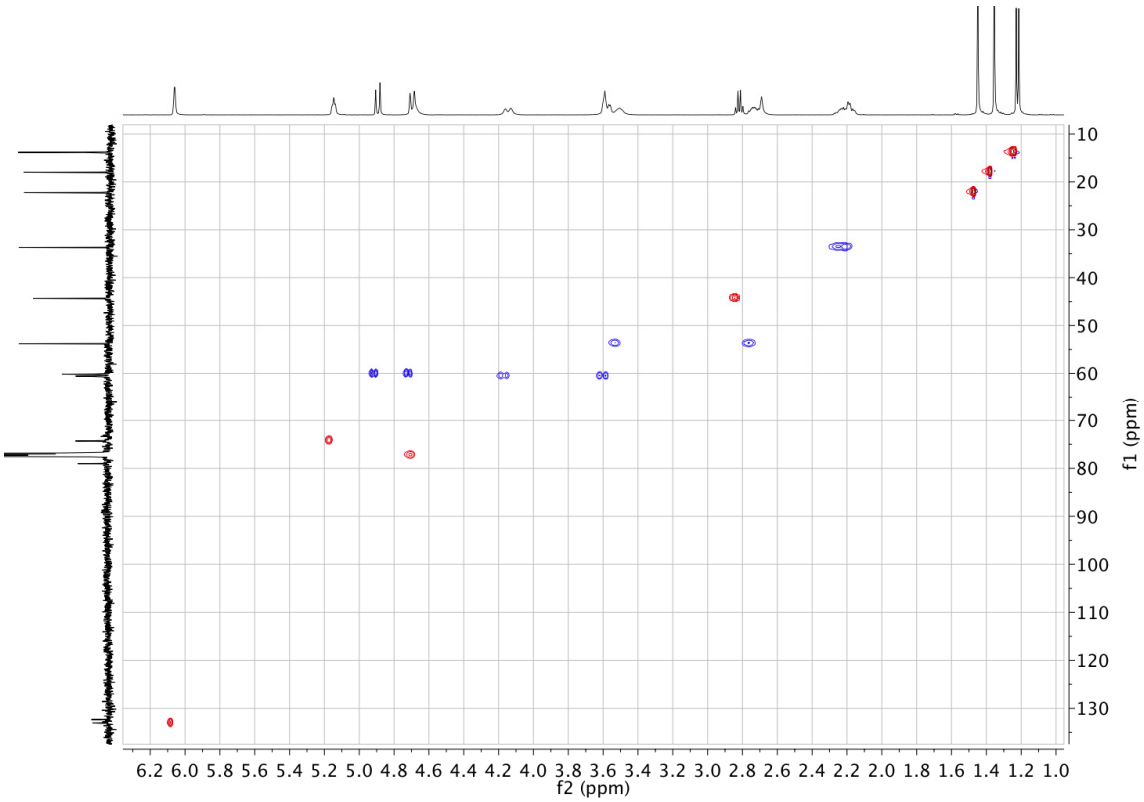

Figure S23. ^{1}H-^{13}C HSQC NMR spectrum of monocrotaline (**1**) in $CDCl_3$ (^{1}H = 500.13 MHz and ^{13}C = 125.77 MHz)

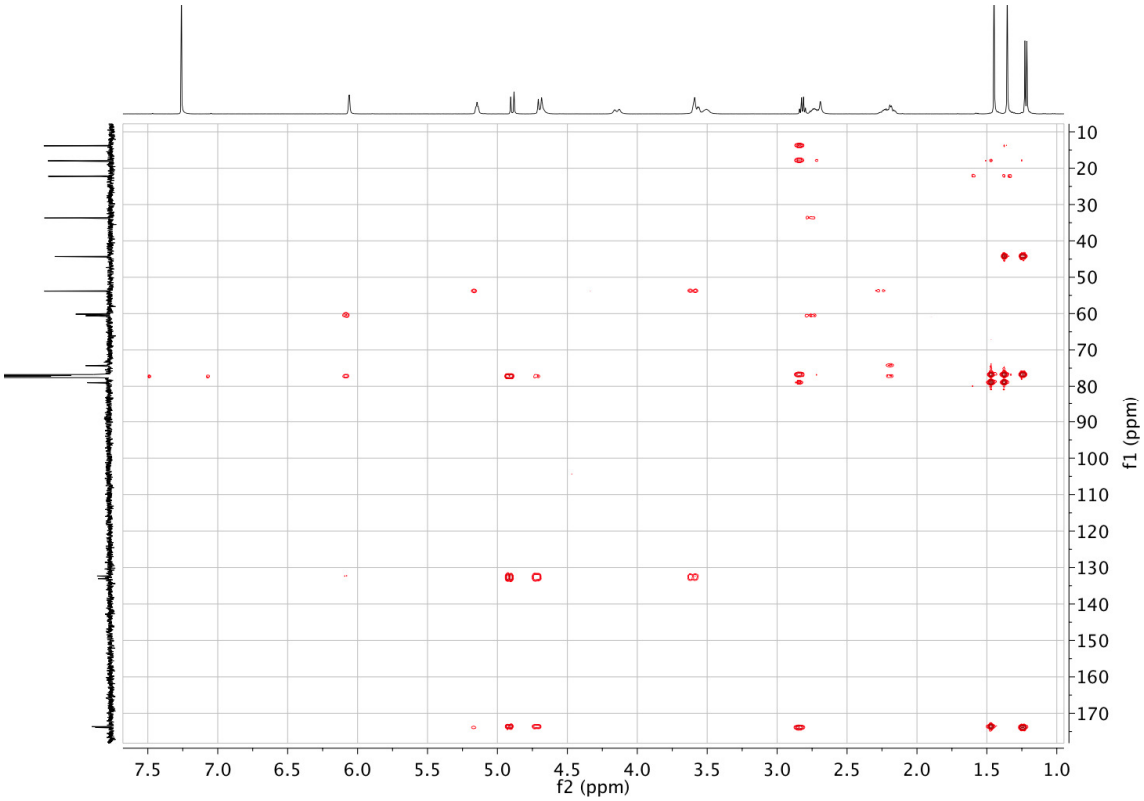

Figure S24. ^{1}H-^{13}C HMBC NMR spectrum of monocrotaline (**1**) in $CDCl_3$ (^{1}H = 500.13 MHz and ^{13}C = 125.77 MHz)

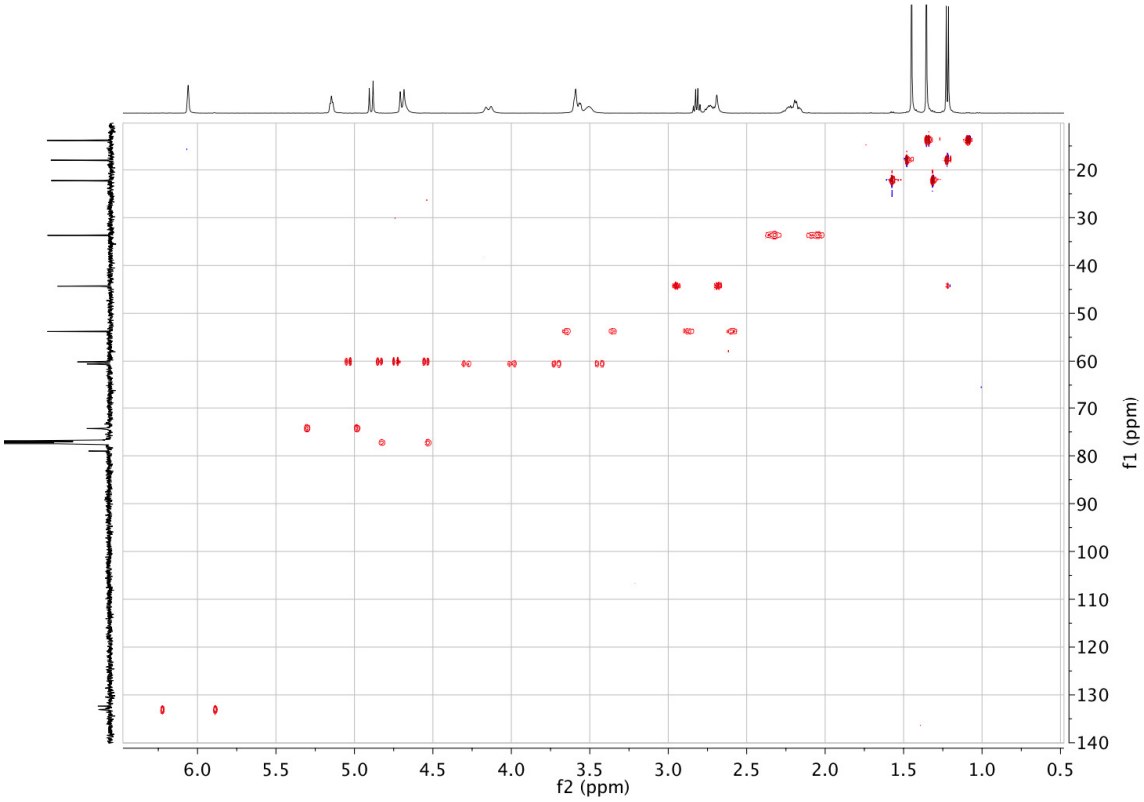

Figure S25.^{1}H-^{13}C HSQC coupled in F2 NMR spectrum of monocrotaline (**1**) in $CDCl_3$ (^{1}H = 500.13 MHz and ^{13}C = 125.77 MHz)

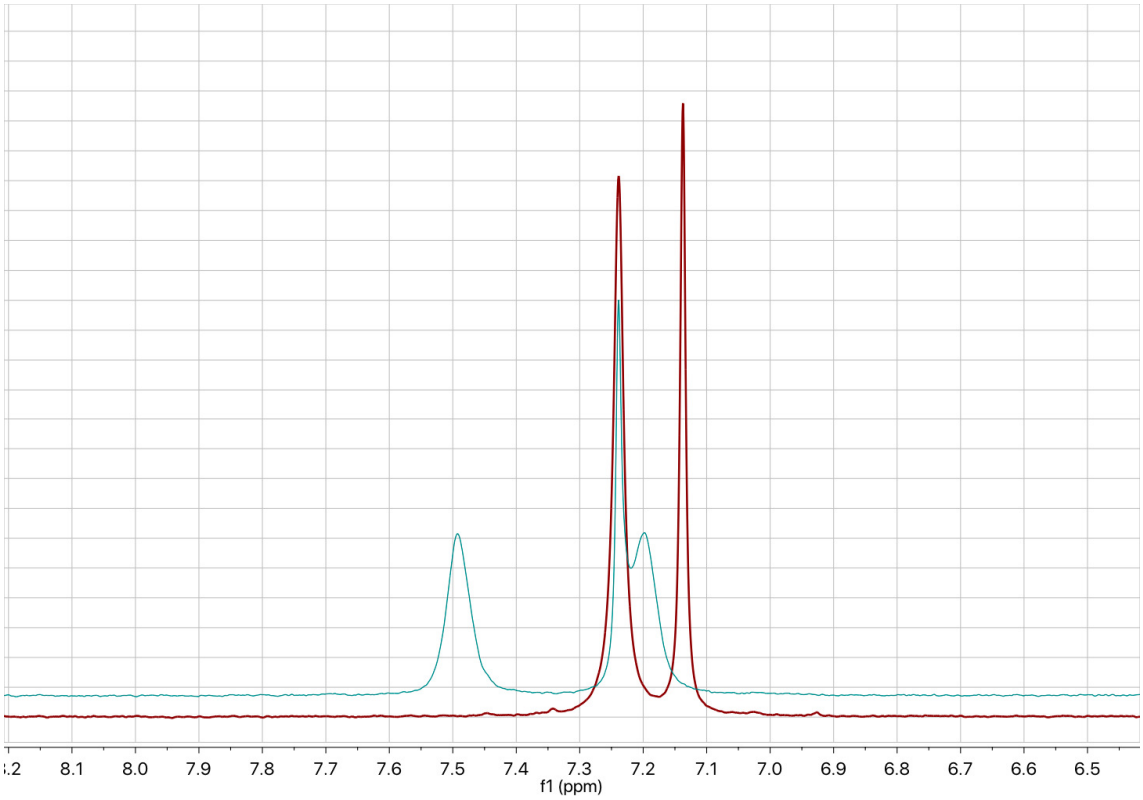

Figure S26. ^{2}H NMR spectra of monocrotaline (**1**) in PMMA gel and $CDCl_3$: red spectrum corresponds to the relaxed gel and green spectrum to the compressed gel (76.77 MHz)

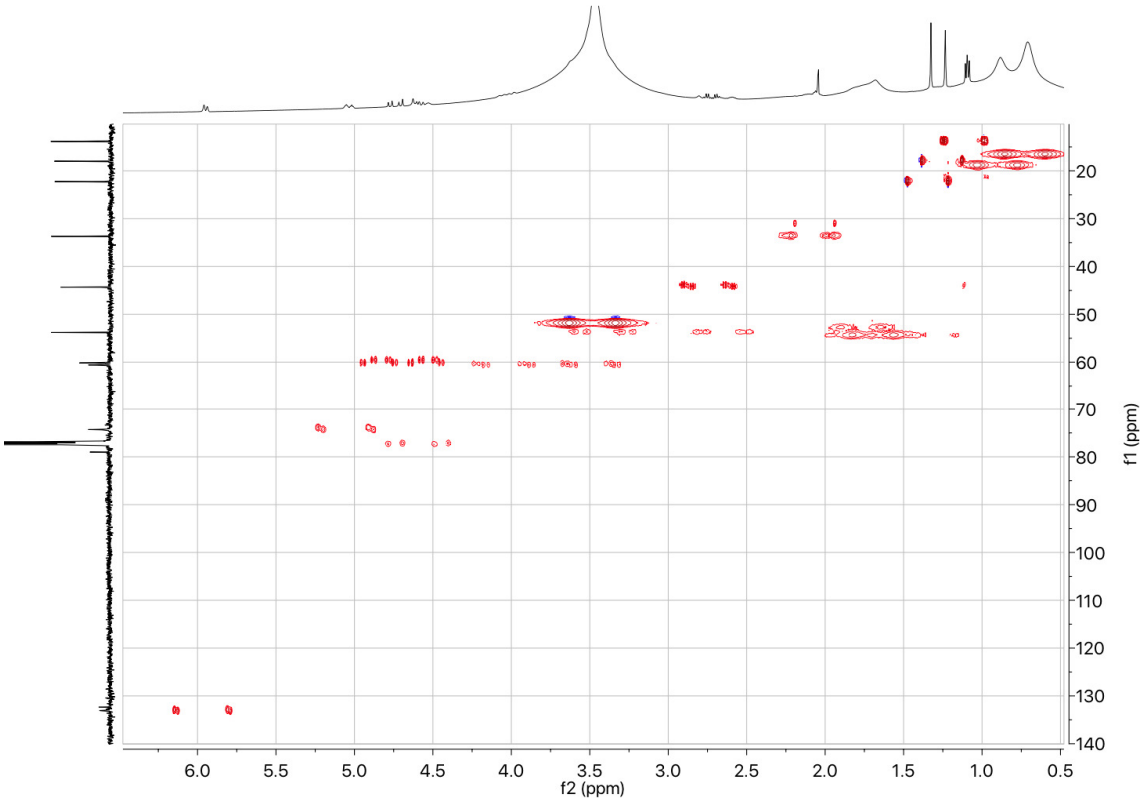

Figure S27. ^{1}H-^{13}C HSQC coupled in F2 NMR spectrum of monocrotaline (**1**) in PMMA gel at the relaxed condition (^{1}H = 500.13 MHz and ^{13}C = 125.77 MHz)

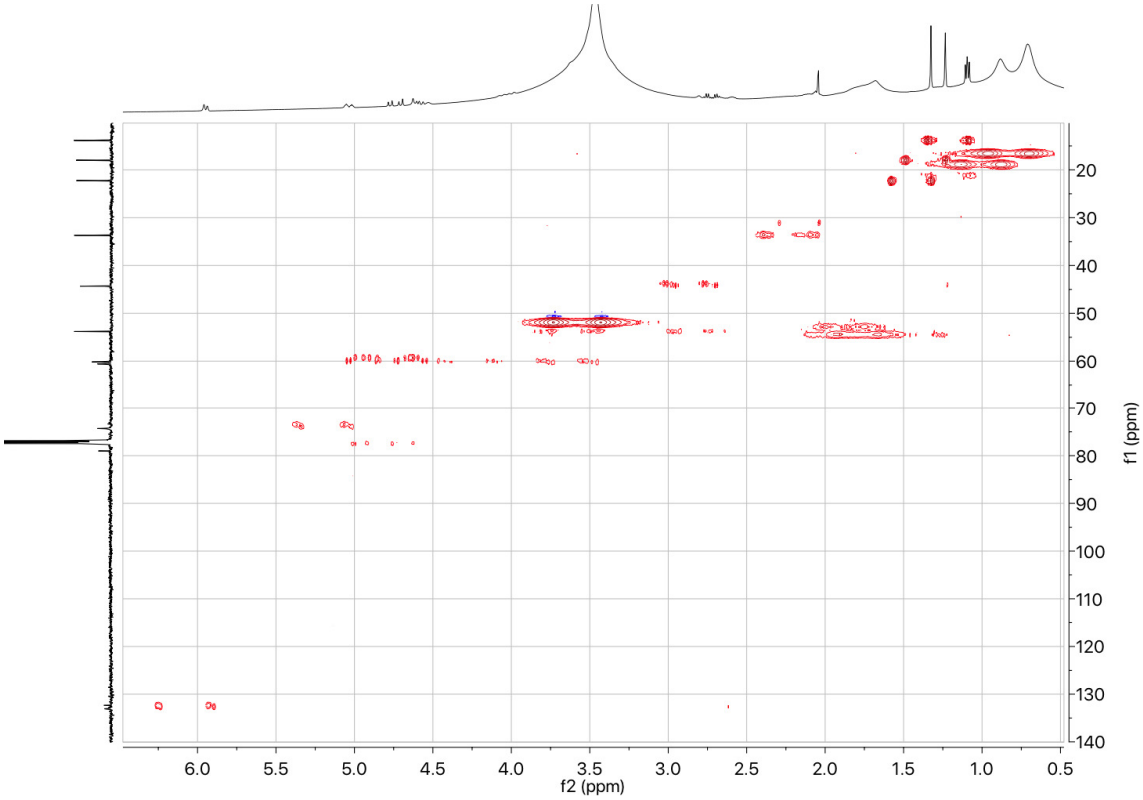

Figure S28. ^{1}H-^{13}C HSQC coupled in F2 NMR spectrum of monocrotaline (**1**) in PMMA gel at the compressed condition (^{1}H = 500.13 MHz and ^{13}C = 125.77 MHz)

*4.NMR Experiments of monocrotaline (**1**) in C_6D_6*

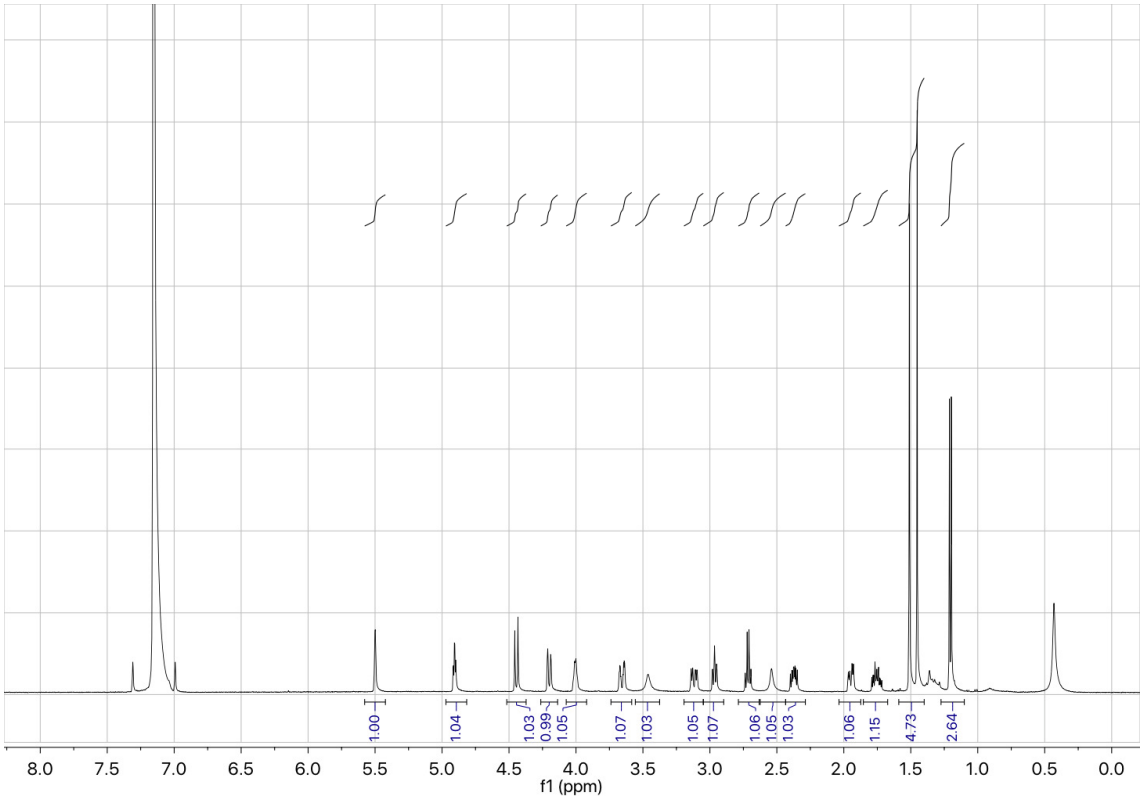

Figure S29. ^{1}H NMR spectrum of monocrotaline (**1**) in C_6D_6 (500.13 MHz).

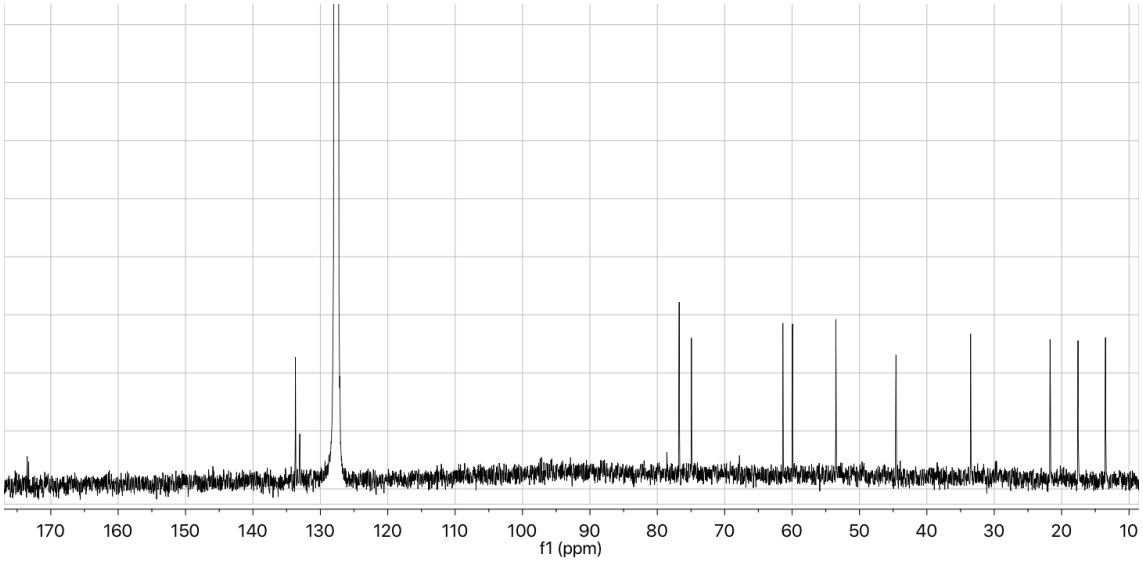

Figure S30. ^{13}C NMR spectrum of monocrotaline (**1**) in C_6D_6 (125.77 MHz)

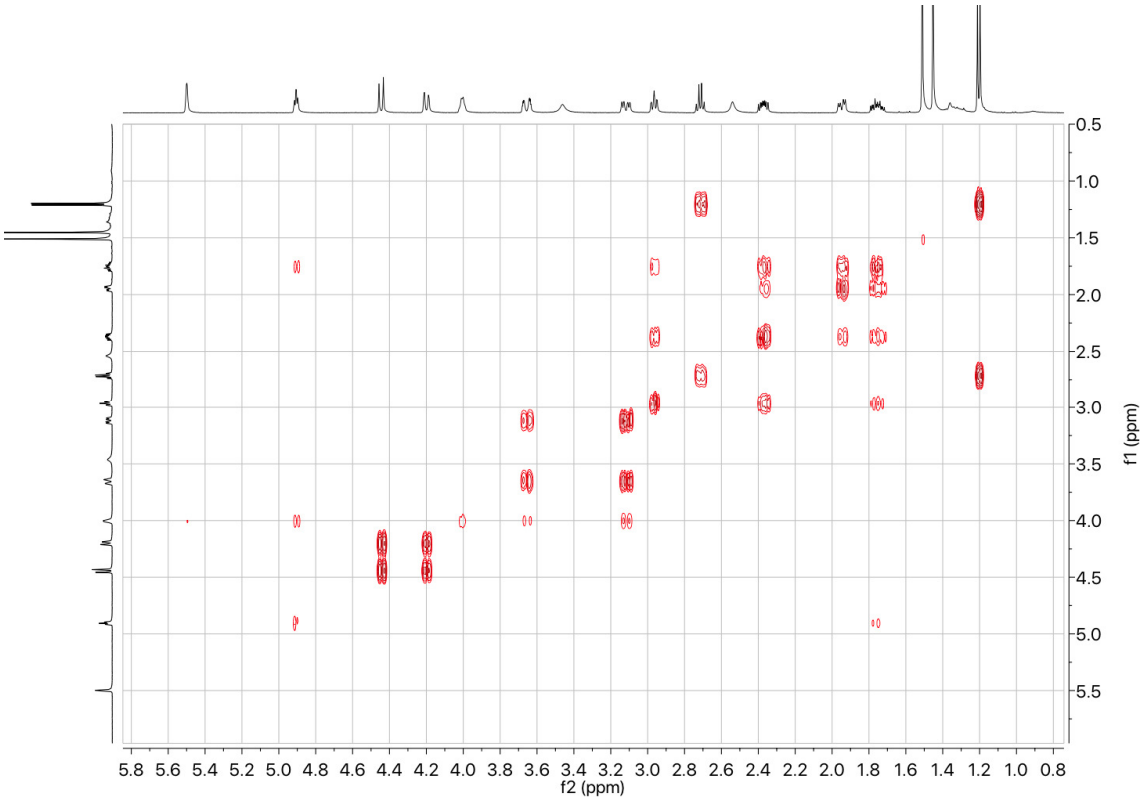

Figure S31. COSY NMR spectrum of monocrotaline (**1**) in C_6D_6 (500.13 MHz)

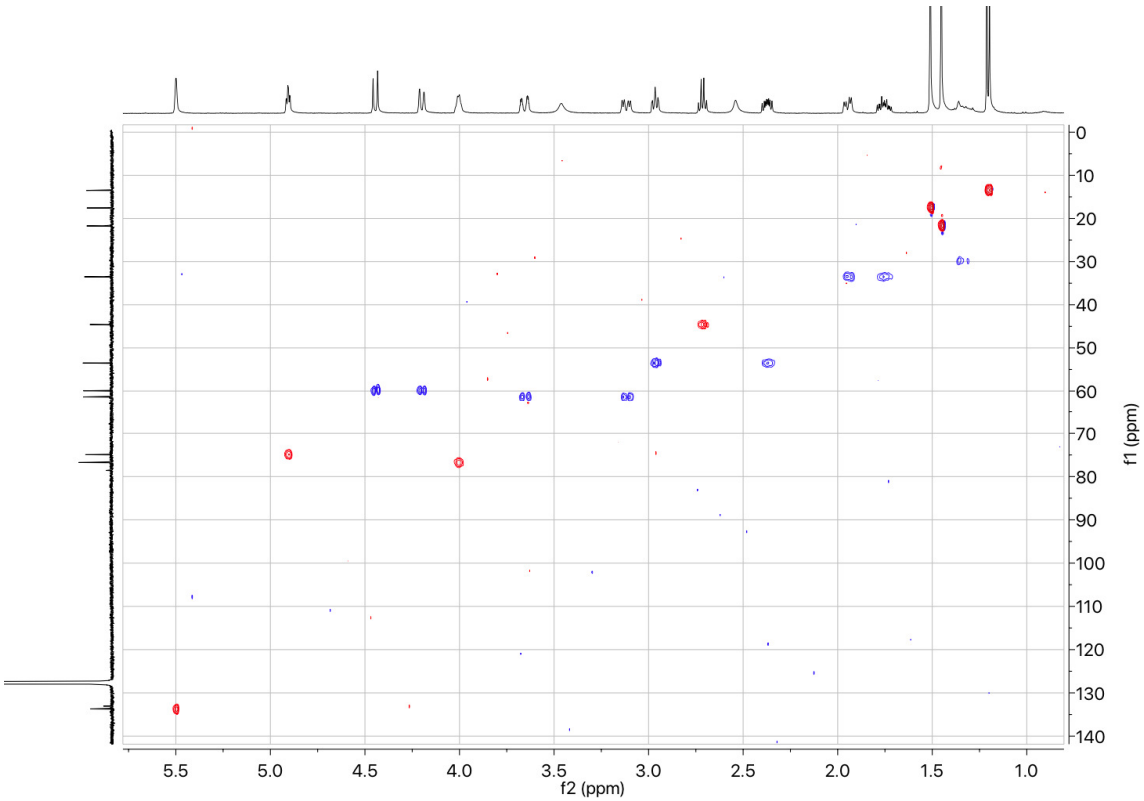

Figure S32. ^{1}H-^{13}C HSQC NMR spectrum of monocrotaline (**1**) in C_6D_6 (^{1}H = 500.13 MHz and ^{13}C = 125.77 MHz)

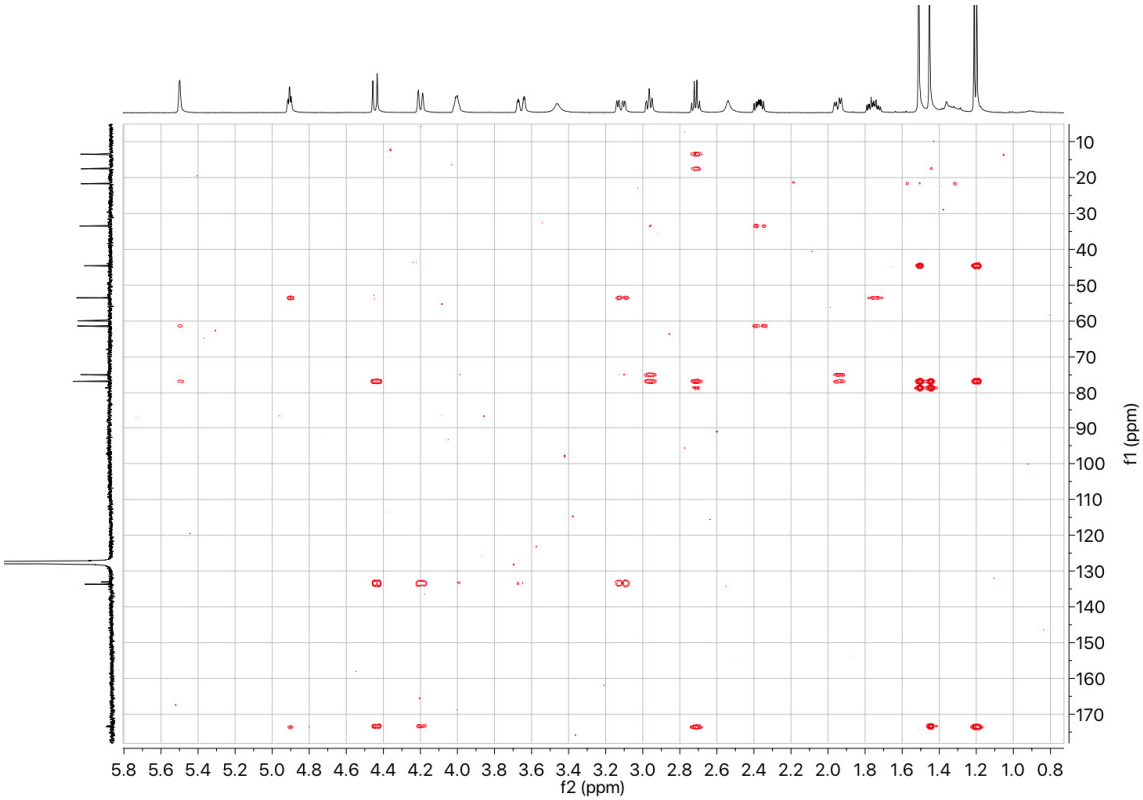

Figure S33. ^{1}H-^{13}C HMBC NMR spectrum of monocrotaline (**1**) in C_6D_6 (^{1}H = 500.13 MHz and ^{13}C = 125.77 MHz)

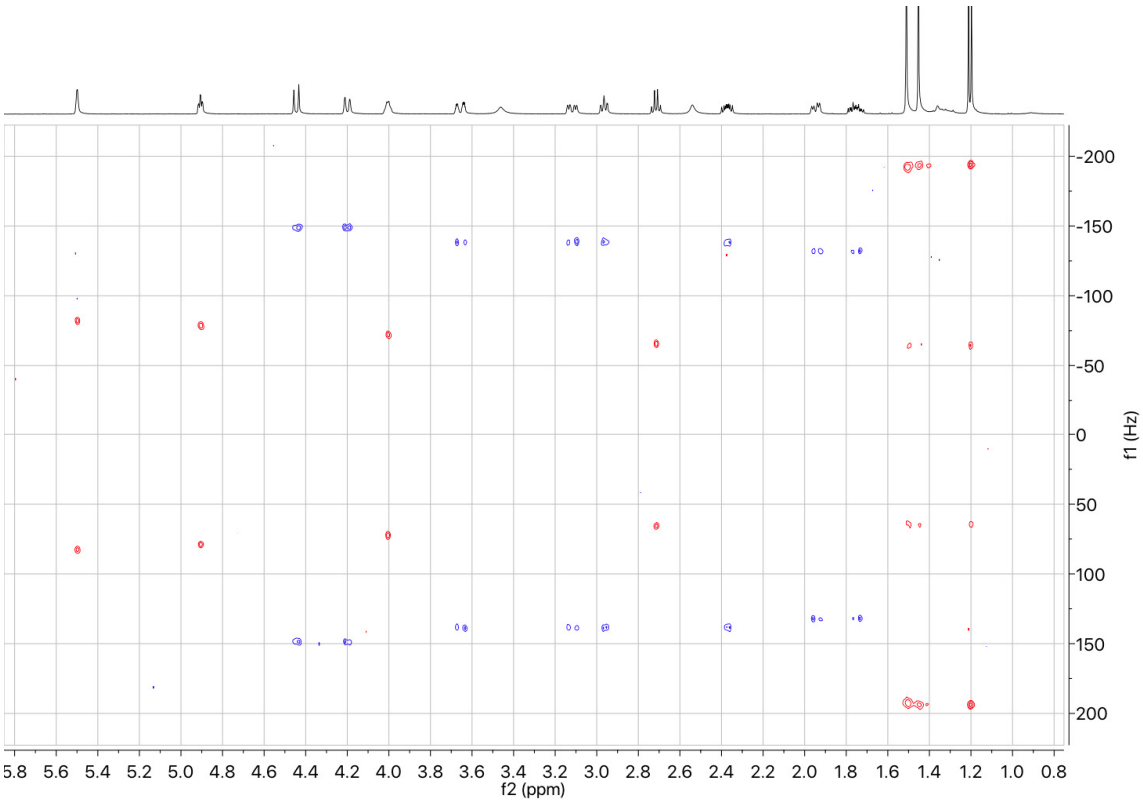

Figure S34. ^{1}H-^{13}C HSQC *J*-Resolved NMR spectrum of monocrotaline (**1**) in C_6D_6 (^{1}H = 500.13 MHz and ^{13}C = 125.77 MHz)

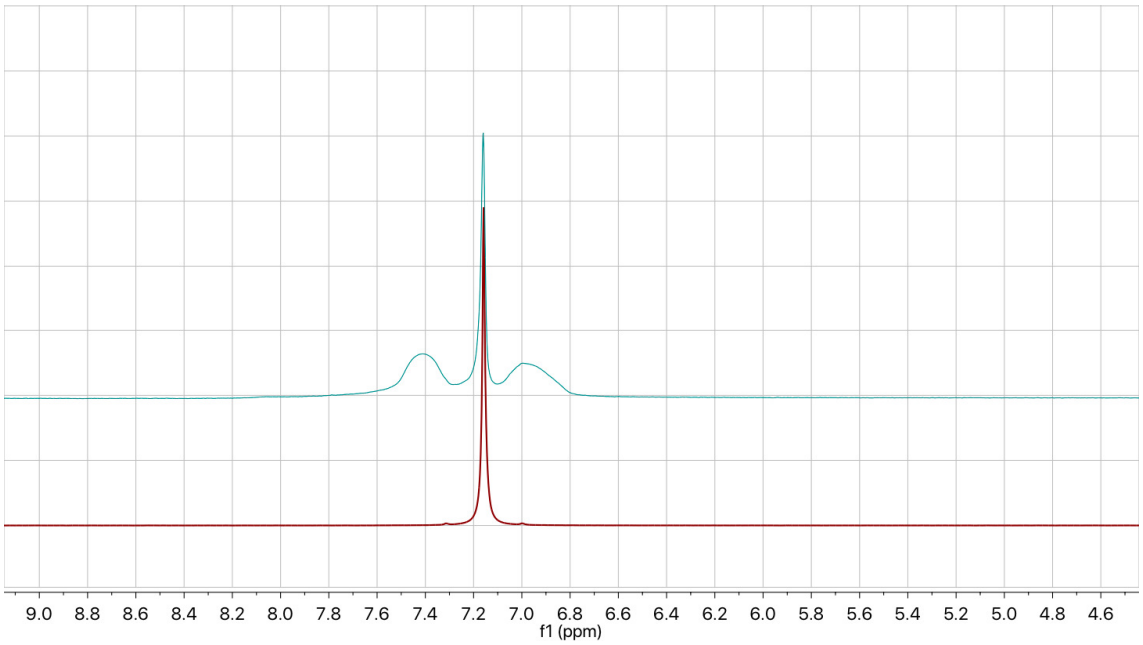

Figure S35. ^{2}H NMR spectra of monocrotaline (**1**) in PMMA gel and C_6D_6 : red spectrum corresponds to the relaxed gel and green spectrum to the compressed gel (76.77 MHz)

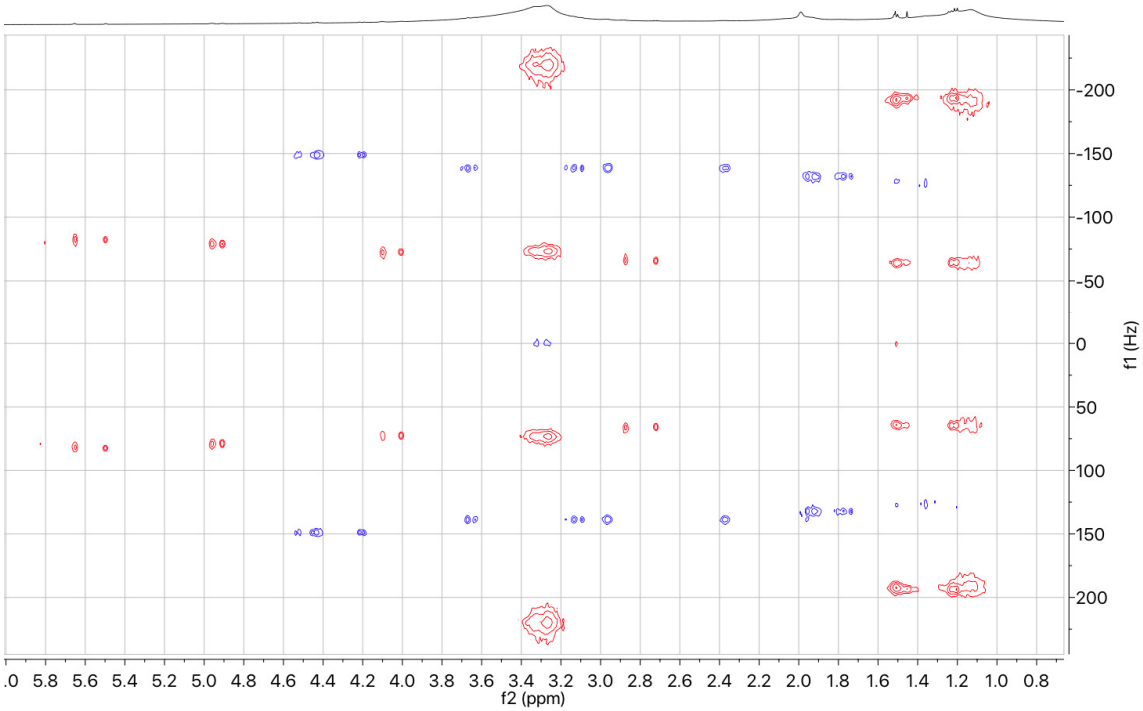

Figure S36. ^{1}H-^{13}C HSQC *J*-Resolved NMR spectrum of monocrotaline (**1**) in PMMA gel at the relaxed condition (^{1}H = 500.13 MHz and ^{13}C = 125.77 MHz)

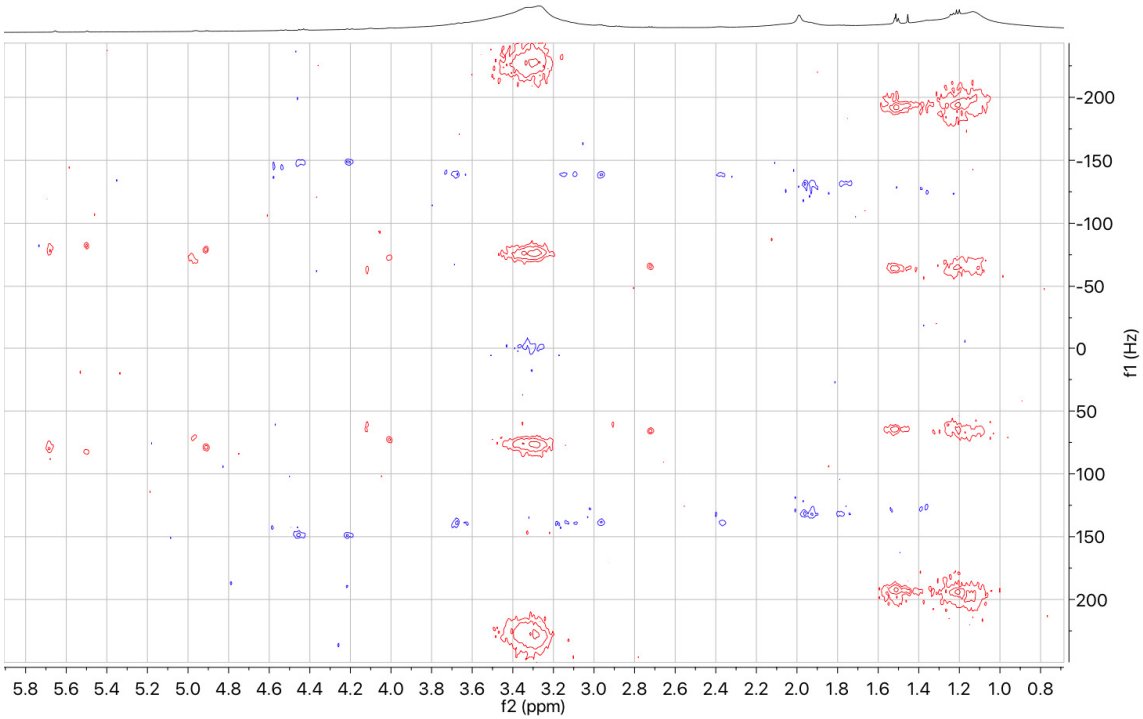

Figure S37. ^{1}H-^{13}C HSQC *J*-Resolved NMR spectrum of monocrotaline (**1**) in PMMA gel at the compressed condition (^{1}H = 500.13 MHz and ^{13}C = 125.77 MHz)

5. Anisotropic NMR data Analyses

Table S1. Experimental and back-calculated RDCs values for monocrotaline (**1**) in DSCG/NaCl/D_2O. AIC values and the conformational population of each permutation.

Permutation	1		2		3		4	
AIC	12.607		20.933		60.298		63.114	
Populations	69% conf 1; 31% conf 4;		58% conf 1; 42% conf 4		21% conf 1; 21% conf 6; 8% conf 10; 29% conf 13; 22% conf 18		41% conf 2; 21% conf 10; 23% conf 13; 15% conf 17	
	RDC exp	RDC cal	RDC exp	RDC calc	RDC exp	RDC calc	RDC exp	RDC calc
C2-H2	4.70	3.35	4.70	3.39	4.70	5.55	4.70	3.01
C3-H3a	**-19.30**	**-20.25**	**-19.30**	**-21.82**	**-19.30**	**-20.18**	**-19.30**	**-22.11**
C3-H3b	**16.98**	**15.09**	**16.98**	**14.74**	**16.98**	**17.53**	**16.98**	**18.81**
C6-H6a	**-12.80**	**-13.61**	-	-	**-12.80**	**-13.39**	-	-
C6-H6b	-	-	**-12.80**	**-10.49**	-	-	**-12.80**	**-10.64**
C7-H7	26.00	25.00	26.00	25.53	26.00	22.05	26.00	22.66
C8-H8	-0.11	1.77	-0.11	0.67	-0.11	-1.10	-0.11	-0.25
C9-H9a	**20.49**	**20.95**	**20.49**	**20.70**	**3.69**	**6.59**	**3.69**	**7.75**
C9-H9b	**3.69**	**4.43**	**3.69**	**2.94**	**20.49**	**17.37**	**20.49**	**16.70**
C12'-H12'	-0.70	-1.02	-0.70	-1.38	-0.70	-3.60	-0.70	-3.41
C13'-H13'	-6.11	-7.15	-6.11	-7.31	-6.11	-6.11	-6.11	-3.92
C14-H14	17.11	17.37	17.11	17.87	17.11	19.03	17.11	18.51
C14'-H14'	-1.94	-0.61	-1.94	0.19	-1.94	-7.01	-1.94	-4.63

conf= conformation

Permutations	5		6		7		8	
AIC	110.326		71.754		19.828		47.671	
Populations	45% conf 8; 55% conf 18;		5% conf 2; 58% conf 5; 25% conf 15; 12% conf 17		45% conf 9; 55% conf 13;		17% conf 8; 3% conf 17; 80% conf 18;	
	RDC exp	RDC cal	RDC exp	RDC calc	RDC exp	RDC calc	RDC exp	RDC calc
C2-H2	4.70	7.80	4.70	6.97	4.70	7.36	4.70	3.21
C3-H3a	**16.98**	**16.36**	**16.98**	**18.11**	**16.98**	**17.75**	**16.98**	**15.09**
C3-H3b	**-19.30**	**-14.36**	**-19.30**	**-22.20**	**-19.30**	**-19.13**	**-19.30**	**-17.88**
C6-H6a	**-**	**-**	**-12.80**	**-13.36**	**-12.80**	**-13.92**	**-**	**-**
C6-H6b	**-12.80**	**-12.67**	**-**	**-**	**-**	**-**	**-12.80**	**-11.47**
C7-H7	26.00	24.88	26.00	20.21	26.00	24.02	26.00	26.59
C8-H8	-0.11	-8.44	-0.11	2.65	-0.11	0.61	-0.11	-4.92
C9-H9a	**3.69**	**5.17**	**3.69**	**5.48**	**20.49**	**19.90**	**20.49**	**19.20**
C9-H9b	**20.49**	**15.28**	**20.49**	**16.29**	**3.69**	**4.36**	**3.69**	**2.37**
C12'-H12'	-0.70	1.01	-0.70	-4.22	-0.70	0.15	-0.70	3.46
C13'-H13'	-6.11	-5.50	-6.11	-6.42	-6.11	-3.09	-6.11	-7.38
C14-H14	17.11	21.11	17.11	19.35	17.11	18.22	17.11	18.67
C14'-H14'	-1.94	-3.44	-1.94	-1.86	-1.94	-1.26	-1.94	-4.19

Table S2. Experimental and back-calculated RDCs values for monocrotaline (**1**) in DMSO-d_6 and poly-HEMA gel as alignment medium. AIC values and the conformational population of each permutation.

Permutation	1		2		3		4	
AIC	7.118		14.61		144.59		208.211	
Populations	61% conf 1; 39% conf 2;		35% conf 1; 58% conf 2; 8% conf 9		100% conf 2		100% conf 2	
	RDC exp	RDC calc	RDC exp	RDC calc	RDC exp	RDC calc	RDC exp	RDC calc
C2-H2	17.4	17.68	17.4	17.98	17.4	18.34	17.4	21.43
C3-H3b	**-15.6**	**-14.94**	**-**	**-**	**-15.6**	**-18.52**	**-**	**-**
C3-H3a	**-**	**-**	**-15.6**	**-14.02**	**-**	**-**	**-15.6**	**-11.25**
C5-H5*	-12.8	-12.22	-12.8	-11.88	-12.8	-8.06	-12.8	-5.19
C6-H6*	-7.0	-8.31	-7.0	-5.49	-7.0	-4.54	-7.0	-8.32
C7-H7	3.8	3.23	3.8	3.32	3.8	10.08	3.8	11.19
C8-H8	-18.5	-17.55	-18.5	-20.54	-18.5	-16.23	-18.5	-15.50
C9-H9a	**0.5**	**0.63**	**0.5**	**0.28**	**24.5**	**15.92**	**24.5**	**15.61**
C9-H9b	**24.5**	**24.96**	**24.5**	**23.51**	**0.5**	**4.42**	**0.5**	**6.13**
C12'-H12'	-0.1	-1.06	-0.1	0.64	-0.1	2.27	-0.1	-0.38
C13'-H13'	-1.0	-2.37	-1.0	-2.27	-1.0	-3.88	-1.0	-3.93
C14-H14	9.5	9.54	9.5	9.91	9.5	13.76	9.5	13.36
C14'-H14'	-4.2	-4.93	-4.2	-5.44	-4.2	-2.06	-4.2	-1.53

*values extracted from the HSQC experiment coupled in F1.

Table S3. Experimental and back-calculated RDCs values for monocrotaline (**1**) in $CDCl_3$, using PMMA as alignment medium. AIC values and the conformational population of each permutation.

Permutation	1		2		3		4	
AIC	27.932		109.371		7.031		3.678	
Populations	25% Conf. 1; 42 % Conf. 12; 34 % Conf. 17		21% conf 12; 79 % Conf 17		65% Conf 1; 22% Conf. 10; 13% Conf. 11		25 % Conf. 4 75% Conf. 9	
	RDC exp.	RDC calc	RDC exp	RDC calc	RDC exp	RDC calc	RDC exp	RDC calc
C2-H2	-6.26	-5.93	-6.26	-0.30	-6.26	-6.76	-6.26	-6.40
C5-H5a	**4.78**	**3.41**	**-**	**-**	**-**	**-**	**4.78**	**4.74**
C5-H5b	**-**	**-**	**4.78**	**4.13**	**4.78**	**4.97**	**-**	**-**
C6-H6*	-6.69	-7.80	-6.69	-4.28	-6.69	-6.55	-6.69	-5.55
C7-H7	-7.57	-7.51	-7.57	-7.68	-7.57	-8.03	-7.57	-7.42
C8-H8	-18.67	-17.14	-18.67	-17.59	-18.67	-19.25	-18.67	-19.43
C9-H9b	**5.96**	**5.47**	**5.96**	**2.48**	**-18.74**	**-17.66**	**-18.74**	**-18.54**
C9-H9a	**-18.74**	**-19.08**	**-18.74**	**-16.27**	**5.96**	**6.25**	**5.96**	**5.45**
C12'-H12'	-2.45	1.50	-2.45	4.10	-2.45	-2.36	-2.45	-2.79
C13'-H13'	2.14	5.66	2.14	2.06	2.14	3.49	2.14	2.02
C14-H14	-7.15	-6.42	-7.15	-12.05	-7.15	-6.69	-7.15	-6.92
C14'-H14'	-5.91	-5.87	-5.91	-0.75	-5.91	-5.43	-5.91	-5.80

*values extracted from the HSQC experiment coupled in F1.

Table S4. Experimental and back-calculated RDCs values for monocrotaline (**1**) in C_6D_6, using PMMA as alignment medium. AIC values and the conformational population.

AIC	8.033	
Population	21% conf 9; 22% conf 10; 11% conf 12; 37% conf 13; 9% conf 17	
	RDC exp	RDC calc
C2-H2	-7.25	-7.22
C3-H3	0.29	0.30
C5-H5	0.07	0.14
C6-H6	-2.07	-2.17
C7-H7	-15.07	-15.07
C8-H8	-19.55	-19.56
C9-H9	-4.07	-4.02
C12'H12'	-0.34	-0.44
C13'-H13'	-0.08	-0.18
C14-H14	-6.51	-6.55
C14'-H14'	3.40	3.32

6. MagNes-CASE-3D Input file:

For D_2O

```
rdc_data {
#C2-H2
4 27 4.7
#C3-H3
3 26 -19.3
3 25 16.98
#C6-H6
7 29 -12.8
#C7-H7
6 28 26
#C8-H8
1 24 -0.11
#C9-H9
10 33 20.49
#C9-H9
10 34 3.69
#C12-H12 (CH3)
(21,40) (21,41) (21,42) -0.7
#C13-H13 (CH3)
(22,43) (22,44) (22,45) -6.11
#C14-H14
15 35 17.11
#C14-H14 (CH3)
(19,36) (19,37) (19,38) -1.94
}

least_squares_method {
nnls
}

rdc_standard_error {
1.2
}
```

For DMSO-d_6

```
rdc_data {
#C2-H2
4 27 17.4
#C3-H3
3 26  -15.6
#C5-H5
(8,31) (8,32) -12.8
#C6-H6
```

(7,29) (7,30) -7
#C7-H7
6 28 3.8
#C8-H8
1 24 -18.5
#C9-H9 (4.6)
10 34 24.5
#C9-H9 (4.4)
10 33 0.5
#C12-H12 (CH3)
(21,40) (21,41) (21,42) -0.1
#C13-H13 (CH3)
(22,43) (22,44) (22,45) -1.0
#C14-H14
15 35 9.5
#C14-H14 (CH3)
(19,36) (19,37) (19,38) -4.2
}

least_squares_method {
nnls
}

rdc_standard_error {
1.2
}

For $CDCl_3$

rdc_data {
#C2-H2
4 27 -6.26
#C5-H5
8 32 4.78
#C6-H6
(7,29) (7,30) -6.69
#C7-H7
6 28 -7.57
#C8-H8
1 24 -18.67
#C9-H9
10 33 5.96
#C9-H9
10 34 -18.74
#C12-H12 (CH3)
(21,40) (21,41) (21,42) -2.45
#C13-H13 (CH3)
(22,43) (22,44) (22,45) 2.14
#C14-H14
15 35 -7.15
#C14-H14 (CH3)

(19,36) (19,37) (19,38) -5.91
}

least_squares_method {
nnls
}

rdc_standard_error {
1.2
}

For C_6D_6

rdc_data {
#C2-H2
4 27 -7.25
#C3-H3
(3,26) (3,25) 0.29
#C5-H5
(8,31) (8,32) 0.07
#C6-H6
(7,29) (7,30) -2.07
#C7-H7
6 28 -15.07
#C8-H8
1 24 -19.55
#C9-H9
(10,33) (10,34) -4.07
#C12-H12 (CH3)
(21,40) (21,41) (21,42) -0.34
#C13-H13 (CH3)
(22,43) (22,44) (22,45) -0.08
#C14-H14
15 35 -6.51
#C14-H14 (CH3)
(19,36) (19,37) (19,38) 3.4
}

least_squares_method {
nnls
}

rdc_standard_error {
1.2
}

XYZ Coordinates in water

XYZ coordinates for structures computed at the M062X/6-31+G** level of theory using IEFPCM water parameters
Gaussian09 route
#M062x/6-31+G** scrf=(pcm,solvent=water) opt integral=(grid=ultrafine)

46
#1

C	2.727208	-0.312038	0.754378
N	3.813377	0.217131	-0.111033
C	3.996914	-0.683149	-1.260055
C	2.957920	-1.752956	-1.068414
C	2.234262	-1.544751	0.032485
C	1.751540	0.853514	0.974093
C	2.633271	2.075732	0.726403
C	3.503632	1.614234	-0.440688
O	0.714904	0.775486	-0.026797
C	1.142755	-2.438515	0.536448
C	-0.983038	-1.329030	0.650087
O	-0.787319	-0.939572	1.780233
C	-2.286791	-1.089454	-0.121122
C	-2.664490	0.432807	-0.213821
C	-1.476350	1.260695	-0.814018
C	-0.379587	1.519606	0.201251
O	-0.132648	-2.076822	-0.051448
O	-0.460387	2.317293	1.110577
C	-1.934007	2.613887	-1.371197
O	-3.756622	0.506690	-1.118303
C	-3.371389	-1.910924	0.585226
C	-3.181844	0.998305	1.101996
O	-2.181357	-1.519960	-1.470259
H	3.120363	-0.592279	1.743188
H	3.854666	-0.147179	-2.209856
H	5.007271	-1.111090	-1.283630
H	2.841622	-2.594458	-1.744782
H	1.275039	0.833008	1.955343
H	3.246587	2.255390	1.615273
H	2.051186	2.973845	0.513913
H	4.416153	2.207221	-0.548044
H	2.936481	1.686617	-1.383462
H	1.048263	-2.400976	1.623397
H	1.305404	-3.466471	0.213281
H	-1.045848	0.664511	-1.625122
H	-1.079074	3.151079	-1.790808
H	-2.673522	2.469149	-2.158360
H	-2.371086	3.235242	-0.586144
H	-3.504588	0.033689	-1.925998
H	-3.140775	-2.974130	0.476149
H	-3.427107	-1.668855	1.648020
H	-4.334409	-1.707191	0.112249
H	-4.131020	0.518399	1.348409
H	-2.472834	0.836825	1.913592
H	-3.359355	2.070834	0.998343
H	-1.449682	-2.145800	-1.558054

46
#2

C	2.861370	-0.303786	0.776474
N	3.988992	-0.141655	-0.180207
C	3.965726	-1.267353	-1.130106
C	2.686903	-1.998346	-0.824183
C	2.059158	-1.462793	0.223196
C	2.179134	1.079951	0.875066
C	3.237264	2.023205	0.311229
C	3.862487	1.185115	-0.798151
O	1.030899	1.167058	0.005019

C	0.776866	-1.948362	0.825206
C	-1.537678	-1.494388	0.508318
O	-1.804547	-1.928283	1.603426
C	-2.544516	-0.860565	-0.457079
C	-2.636913	0.702186	-0.247537
C	-1.262352	1.405175	-0.465639
C	-0.188606	1.099722	0.558397
O	-0.307020	-1.484153	-0.017083
O	-0.377910	0.889675	1.738871
C	-1.392140	2.940774	-0.507792
O	-3.501352	1.172690	-1.273601
C	-3.896781	-1.537394	-0.271246
C	-3.308108	1.060147	1.071939
O	-2.152854	-1.092538	-1.806062
H	3.239034	-0.558419	1.777619
H	3.999952	-0.905667	-2.166129
H	4.832926	-1.926009	-0.992586
H	2.351354	-2.869468	-1.378755
H	1.862041	1.317418	1.889502
H	3.977371	2.234960	1.088889
H	2.802894	2.963669	-0.033321
H	4.837830	1.558831	-1.120926
H	3.193852	1.162164	-1.675477
H	0.618511	-1.551071	1.831411
H	0.727231	-3.039338	0.857633
H	-0.877973	1.084864	-1.440455
H	-1.621178	3.348603	0.480173
H	-0.452681	3.381846	-0.848957
H	-2.186357	3.224976	-1.198691
H	-3.193094	0.790283	-2.110172
H	-4.641242	-1.044810	-0.898781
H	-3.810808	-2.584302	-0.571009
H	-4.214050	-1.498629	0.770644
H	-2.808235	0.582014	1.914707
H	-3.289227	2.141474	1.223427
H	-4.352694	0.744805	1.038289
H	-1.187022	-1.101936	-1.868712

46
#3

C	2.701712	-0.197737	0.778541
N	4.101083	-0.239422	0.285050
C	4.147944	-1.128917	-0.894830
C	2.876801	-1.917145	-0.795048
C	2.058558	-1.402119	0.124401
C	2.149945	1.220464	0.399588
C	3.213206	1.811894	-0.519251
C	4.487794	1.148180	0.003971
O	0.896956	1.223969	-0.299950
C	0.772308	-2.011054	0.582230
C	-1.540919	-1.532074	0.396665
O	-1.753502	-2.041170	1.471675
C	-2.608543	-0.855516	-0.466126
C	-2.746951	0.672858	-0.100585
C	-1.436706	1.461293	-0.394484
C	-0.218120	1.105102	0.432171
O	-0.334649	-1.468902	-0.180045
O	-0.206476	0.835204	1.616162
C	-1.624162	2.982826	-0.226049
O	-3.734794	1.190696	-0.982763
C	-3.923984	-1.605124	-0.286330
C	-3.279252	0.884064	1.309396
O	-2.275702	-0.944301	-1.846428
H	2.675171	-0.293950	1.871189
H	4.189095	-0.569196	-1.843662
H	5.034540	-1.772091	-0.861209
H	2.680296	-2.809464	-1.380985
H	2.024885	1.817043	1.307176
H	3.233497	2.903273	-0.494162
H	3.009879	1.487447	-1.546526

```
H       4.815116    1.627556    0.934139
H       5.321618    1.179445   -0.700503
H       0.589476   -1.800108    1.638318
H       0.772909   -3.092273    0.425442
H      -1.176578    1.280471   -1.442626
H      -0.760177    3.510339   -0.637002
H      -2.518896    3.304221   -0.760482
H      -1.722900    3.257087    0.827305
H      -3.493391    0.920157   -1.882452
H      -4.713618   -1.096010   -0.840536
H      -3.806870   -2.618214   -0.677705
H      -4.199124   -1.669119    0.765954
H      -4.275358    0.445839    1.393820
H      -2.618850    0.437345    2.053484
H      -3.366457    1.953000    1.515123
H      -1.314306   -0.912787   -1.954221

46
#4
C       2.864197   -0.283823    0.778880
N       4.008194   -0.133566   -0.161154
C       4.014828   -1.286673   -1.078049
C       2.727123   -2.009920   -0.790858
C       2.072727   -1.453085    0.228751
C       2.180991    1.102472    0.848837
C       3.234148    2.035873    0.259021
C       3.867225    1.169979   -0.823416
O       1.025943    1.173707   -0.012461
C       0.778786   -1.932651    0.812008
C      -1.519408   -1.502678    0.465994
O      -1.788068   -1.977030    1.547538
C      -2.554316   -0.853595   -0.467743
C      -2.646072    0.698185   -0.214593
C      -1.273894    1.397704   -0.459510
C      -0.188173    1.097654    0.553416
O      -0.288460   -1.463577   -0.044433
O      -0.359623    0.889338    1.737243
C      -1.401724    2.932786   -0.508149
O      -3.547570    1.200390   -1.192517
C      -3.899485   -1.544447   -0.262876
C      -3.274481    1.012580    1.136808
O      -2.140911   -0.954303   -1.822207
H       3.226303   -0.526613    1.788668
H       4.083942   -0.954576   -2.121992
H       4.877189   -1.940045   -0.892590
H       2.406040   -2.893613   -1.334040
H       1.871917    1.361616    1.860436
H       3.972150    2.275676    1.030521
H       2.793230    2.962616   -0.113308
H       4.838775    1.542008   -1.159307
H       3.197921    1.111115   -1.698854
H       0.613318   -1.537716    1.818329
H       0.728406   -3.023955    0.845293
H      -0.905978    1.055582   -1.431893
H      -1.652567    3.344941    0.472953
H      -0.454225    3.371906   -0.829530
H      -2.179385    3.218165   -1.216840
H      -3.265517    0.853146   -2.052962
H      -4.664183   -1.033695   -0.850063
H      -3.829359   -2.586038   -0.592227
H      -4.183964   -1.547786    0.789221
H      -2.761701    0.493439    1.946394
H      -3.231522    2.086388    1.330490
H      -4.325037    0.715538    1.117636
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46
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46
#6

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46
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46
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46
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46
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46
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46
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46
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C      3.093463    1.698814   -0.791887
C      4.307247    1.240388    0.026237
O      0.707800    1.266539   -0.527830
C      0.945295   -1.611166   -0.951143
C     -1.362989   -1.575537   -0.421161
O     -1.649835   -2.025948   -1.510894
C     -2.397214   -1.018290    0.562050
C     -2.809287    0.404850   -0.017311
C     -1.638570    1.218195   -0.645232
C     -0.404682    1.400681    0.213997
O     -0.114030   -1.395551    0.004954
O     -0.399158    1.695786    1.388727
C     -2.089542    2.619593   -1.094884
O     -3.725982    0.152935   -1.087358
C     -1.888890   -1.023705    1.999583
C     -3.597433    1.181424    1.026179
O     -3.534205   -1.851983    0.550854
H      1.900886   -0.281735    1.624423
H      5.390330   -1.054758   -0.123931
H      4.703927   -1.830212    1.301016
H      3.540067   -2.810649   -0.947309
H      1.891790    2.027997    0.981051
H      3.114052    2.763729   -1.030643
H      3.000944    1.124086   -1.719671
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H      4.631542    2.042739    0.697828
H      5.157821    0.974809   -0.606300
H      0.944649   -2.657471   -1.265494
H      0.740572   -0.979109   -1.822254
H     -1.311174    0.673712   -1.539622
H     -2.282027    3.263172   -0.233111
H     -1.310243    3.082301   -1.704738
H     -3.000413    2.543048   -1.691666
H     -3.252534   -0.240950   -1.837376
H     -2.694105   -0.694783    2.658169
H     -1.621590   -2.048524    2.269923
H     -1.022218   -0.382641    2.142291
H     -2.935241    1.550963    1.811513
H     -4.095842    2.027897    0.550434
H     -4.360850    0.535701    1.467770
H     -4.056841   -1.628550   -0.234783

46
#14
C      2.401250   -0.041396    0.674619
N      3.870490    0.055791    0.842477
C      4.425805   -1.258553    0.472109
C      3.345092   -1.919420   -0.347835
C      2.206362   -1.231729   -0.262469
C      2.001649    1.337182    0.126782
C      3.134986    1.665194   -0.825235
C      4.341720    1.184766   -0.008708
O      0.741785    1.308296   -0.549024
C      0.923119   -1.585822   -0.942767
C     -1.386621   -1.591107   -0.422108
O     -1.650336   -2.229510   -1.418607
C     -2.449271   -0.997838    0.499711
C     -2.797146    0.473789   -0.009528
C     -1.605056    1.244369   -0.637678
C     -0.362990    1.371917    0.215367
O     -0.153247   -1.287710   -0.027801
O     -0.337172    1.578629    1.409045
C     -1.998533    2.669914   -1.069039
O     -3.667034    0.326610   -1.126513
C     -2.022004   -1.084635    1.961839
C     -3.512464    1.247979    1.094288
O     -3.617210   -1.787947    0.368899
H      1.895449   -0.238559    1.628915
H      5.372407   -1.141403   -0.063928
H      4.638199   -1.857357    1.368352
H      3.480676   -2.855342   -0.880568
H      1.949058    2.059148    0.946470
H      3.185552    2.724888   -1.082074
H      3.019383    1.079037   -1.743208
H      4.705739    1.992384    0.635476
H      5.172276    0.869870   -0.645538
H      0.888180   -2.643491   -1.212536
H      0.763968   -0.983012   -1.844094
H     -1.322722    0.692380   -1.541595
H     -1.204362    3.103717   -1.681131
H     -2.916750    2.637304   -1.657258
H     -2.154284    3.314979   -0.200583
H     -4.472207   -0.107961   -0.812417
H     -1.717997   -2.110151    2.185115
H     -1.199227   -0.407544    2.185768
H     -2.875130   -0.834727    2.594926
H     -4.331018    0.644171    1.499501
H     -2.829696    1.512503    1.904059
H     -3.939960    2.160992    0.675260
H     -3.610636   -2.176953   -0.520348

46
#15
C      2.567918   -0.283693    0.887696
N      3.909823   -0.081892    0.295335
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C      3.940954   -0.794105   -0.999384
C      2.820115   -1.784373   -0.878452
C      2.052138   -1.514567    0.177909
C      1.771972    1.042647    0.651436
C      2.721616    1.934700   -0.155543
C      4.100563    1.367786    0.196723
O      0.549666    0.765758   -0.057096
C      0.966250   -2.397494    0.703534
C     -1.006015   -1.580751   -0.290714
O     -0.602591   -1.879831   -1.396613
C     -2.425986   -1.047554   -0.072321
C     -2.494176    0.475433    0.304239
C     -1.656047    1.335008   -0.728603
C     -0.341920    1.765631   -0.107645
O     -0.324084   -1.755398    0.831475
O     -0.114499    2.873753    0.328661
C     -2.406702    2.573376   -1.213849
O     -3.865287    0.823207    0.219049
C     -3.139059   -1.928794    0.953760
C     -2.099369    0.765468    1.747456
O     -3.111530   -1.166945   -1.310420
H      2.650317   -0.447603    1.969295
H      3.775052   -0.121522   -1.857613
H      4.912217   -1.277821   -1.150653
H      2.679266   -2.616805   -1.560344
H      1.500138    1.506767    1.603464
H      2.604875    2.993374    0.079170
H      2.509207    1.789581   -1.221443
H      4.433216    1.750401    1.168744
H      4.872543    1.606177   -0.538505
H      1.193579   -2.710697    1.724820
H      0.854210   -3.277507    0.066857
H     -1.411333    0.705432   -1.591542
H     -1.756576    3.170252   -1.857780
H     -3.289946    2.288663   -1.786788
H     -2.724110    3.193608   -0.372771
H     -4.197936    0.495487   -0.630516
H     -3.177903   -2.954022    0.577143
H     -2.619816   -1.926261    1.912564
H     -4.158639   -1.563182    1.090875
H     -1.093796    0.401227    1.972967
H     -2.136402    1.844557    1.922431
H     -2.807143    0.285712    2.425353
H     -2.466683   -1.419235   -1.990985

46
#16
C      2.740889    0.508387   -0.796182
N      3.932362    0.148658    0.016039
C      3.953391    0.979104    1.231338
C      2.703108    1.810074    1.142612
C      2.022001    1.554506    0.024941
C      1.994059   -0.813582   -1.044065
C      3.098947   -1.854771   -0.919877
C      3.924850   -1.304564    0.243112
O      1.056161   -0.971664    0.035382
C      0.796334    2.281427   -0.422239
C     -1.491560    1.655108   -0.118225
O     -1.733405    2.640670    0.547470
C     -2.574621    0.633699   -0.488974
C     -2.536385   -0.624016    0.481042
C     -1.122326   -1.113681    0.886895
C     -0.174946   -1.403791   -0.256132
O     -0.302883    1.353222   -0.630311
O     -0.457184   -1.988407   -1.281168
C     -1.175998   -2.371689    1.772461
O     -3.067980   -0.190865    1.728994
C     -2.495664    0.310874   -1.980849
C     -3.418976   -1.730838   -0.093170
O     -3.827083    1.268496   -0.277083
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H      3.038109    0.919024   -1.772666
H      3.959591    0.354566    2.136234
H      4.849012    1.612010    1.274739
H      2.421129    2.540119    1.895144
H      1.451955   -0.839196   -1.989929
H      3.688025   -1.863369   -1.842390
H      2.705135   -2.857482   -0.740925
H      4.941523   -1.706505    0.265603
H      3.436795   -1.555438    1.198641
H      0.954947    2.766086   -1.390630
H      0.497295    3.027404    0.313517
H     -0.673240   -0.306193    1.474242
H     -1.482700   -3.247586    1.195134
H     -0.187354   -2.568575    2.194694
H     -1.881593   -2.220177    2.590993
H     -3.956378    0.151160    1.554222
H     -2.489352    1.248174   -2.543404
H     -1.609820   -0.267452   -2.234660
H     -3.385284   -0.252126   -2.268151
H     -2.951498   -2.204230   -0.959026
H     -3.592127   -2.486272    0.675666
H     -4.388094   -1.317070   -0.389168
H     -3.672243    2.043416    0.287448

46
#17
C      2.269891    0.008455    0.727031
N      3.692333    0.379909    0.871910
C      4.440036   -0.888037    0.800938
C      3.536456   -1.816028    0.019070
C      2.307993   -1.301393   -0.056468
C      1.661039    1.234796    0.048865
C      2.697043    1.588014   -1.005149
C      4.010403    1.318729   -0.249574
O      0.356899    0.938533   -0.469969
C      1.164954   -1.866990   -0.826920
C     -1.152373   -1.529111   -0.748992
O     -1.213722   -1.568415   -1.962565
C     -2.386330   -1.212908    0.095730
C     -2.377348    0.264713    0.648334
C     -1.997814    1.290629   -0.506929
C     -0.608576    1.858371   -0.278424
O     -0.049518   -1.748403   -0.048229
O     -0.375886    2.993488    0.071161
C     -2.993873    2.441161   -0.632436
O     -3.698795    0.507512    1.093509
C     -2.554796   -2.245893    1.206182
C     -1.510044    0.435078    1.891599
O     -3.512033   -1.300720   -0.765433
H      1.807660   -0.165601    1.708258
H      5.420185   -0.733570    0.341774
H      4.613843   -1.285546    1.809978
H      3.849401   -2.773803   -0.383996
H      1.565795    2.038874    0.782705
H      2.609723    2.616732   -1.359522
H      2.585088    0.909691   -1.857673
H      4.415044    2.244992    0.168488
H      4.769349    0.892468   -0.912933
H      1.319206   -2.921639   -1.067690
H      1.019775   -1.310628   -1.756297
H     -1.962772    0.753222   -1.461383
H     -2.650451    3.142557   -1.396090
H     -3.976312    2.068641   -0.925836
H     -3.095081    2.979127    0.312436
H     -4.300943    0.205256    0.396017
H     -1.680442   -2.276587    1.857361
H     -3.438222   -1.994987    1.797302
H     -2.696894   -3.232383    0.758575
H     -1.484084    1.490701    2.179003
H     -1.947711   -0.128777    2.716748
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H     -0.490535    0.081832    1.726950
H     -3.193475   -1.313402   -1.682475

46
#18
C      2.679304   -0.101757    0.783421
N      4.091933   -0.146716    0.322778
C      4.201707   -1.161853   -0.746229
C      2.941995   -1.961452   -0.610698
C      2.082237   -1.376155    0.224753
C      2.110869    1.270040    0.279370
C      3.150809    1.771758   -0.713357
C      4.439855    1.212279   -0.111334
O      0.834516    1.228515   -0.377183
C      0.787622   -1.967337    0.681508
C     -1.525545   -1.568201    0.339912
O     -1.800027   -2.122361    1.378773
C     -2.535510   -0.862626   -0.570897
C     -2.759332    0.623166   -0.073534
C     -1.508450    1.499915   -0.348228
C     -0.246494    1.128264    0.406923
O     -0.285023   -1.464802   -0.148601
O     -0.175528    0.873786    1.592542
C     -1.749924    2.988707   -0.029238
O     -3.748406    1.188592   -0.927409
C     -3.832680   -1.664786   -0.571285
C     -3.232686    0.688490    1.376780
O     -2.073592   -0.854001   -1.910072
H      2.628998   -0.107972    1.879347
H      4.273408   -0.709679   -1.748856
H      5.096659   -1.778996   -0.606715
H      2.781453   -2.911082   -1.111312
H      2.016873    1.950078    1.131160
H      3.140535    2.858136   -0.822521
H      2.957218    1.316290   -1.691948
H      4.743578    1.805422    0.759439
H      5.279387    1.188554   -0.809082
H      0.567562   -1.697873    1.717722
H      0.797321   -3.055574    0.585201
H     -1.295680    1.421050   -1.417466
H     -0.910543    3.585850   -0.394764
H     -2.661184    3.325633   -0.524070
H     -1.843880    3.154984    1.046685
H     -4.623759    1.020581   -0.556383
H     -3.625076   -2.672113   -0.939127
H     -4.260846   -1.744689    0.427828
H     -4.549251   -1.192952   -1.245865
H     -4.157881    0.118959    1.502881
H     -2.485938    0.297437    2.067101
H     -3.441589    1.727857    1.640473
H     -1.109077   -0.781436   -1.920781
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XYZ Coordinates in $CHCl_3$

XYZ coordinates for structures computed at the M062X/6-31+G** level of theory using IEFPCM chloroform parameters
Gaussian09 route
#M062x/6-31+G** scrf=(pcm,solvent=chloroform) opt integral=(grid=ultrafine)

M062X/6-31+G** structures for monocrotaline
46
#1

C	-2.723710	-0.314402	-0.754010
N	-3.809921	0.219178	0.106030
C	-4.001760	-0.675882	1.255480
C	-2.964620	-1.749312	1.071560
C	-2.235340	-1.545341	-0.026190
C	-1.744781	0.847979	-0.974240
C	-2.626971	2.072179	-0.737100
C	-3.504361	1.617858	0.427780
O	-0.714711	0.770219	0.032160
C	-1.142880	-2.441311	-0.523350
C	0.983870	-1.334531	-0.649160
O	0.782410	-0.952761	-1.779150
C	2.288750	-1.089310	0.116370
C	2.662699	0.435180	0.210590
C	1.477159	1.259640	0.819960
C	0.377789	1.522809	-0.191420
O	0.132810	-2.079631	0.061210
O	0.453609	2.326839	-1.093310
C	1.938509	2.610800	1.378650
O	3.758469	0.505430	1.109320
C	3.375090	-1.900910	-0.597550
C	3.169209	1.006980	-1.106880
O	2.199800	-1.541360	1.461290
H	-3.115540	-0.598382	-1.742680
H	-3.860921	-0.137592	2.204610
H	-5.014000	-1.100032	1.275800
H	-2.852910	-2.589122	1.751070
H	-1.262331	0.824289	-1.952730
H	-3.236111	2.247268	-1.629730
H	-2.043941	2.970569	-0.529240
H	-4.418791	2.210068	0.524260
H	-2.943381	1.697758	1.374030
H	-1.047440	-2.408671	-1.610660
H	-1.307050	-3.468121	-0.196060
H	1.049449	0.661239	1.631510
H	1.089269	3.140629	1.819050
H	2.696839	2.464880	2.147440
H	2.354069	3.239610	0.588150
H	3.515109	0.009850	1.905990
H	3.149750	-2.965450	-0.492500
H	3.425080	-1.650560	-1.658560
H	4.338130	-1.694530	-0.125810
H	4.121629	0.535470	-1.356470
H	2.457569	0.842330	-1.915820
H	3.338539	2.080560	-1.002760
H	1.365430	-2.010760	1.593730

46
#2

C	2.859560	-0.299090	0.775560
N	3.986310	-0.142661	-0.180980
C	3.965950	-1.272811	-1.123230
C	2.687369	-2.003420	-0.813500
C	2.057349	-1.461300	0.229010
C	2.178820	1.085870	0.867630
C	3.241200	2.024440	0.303200

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C      3.867000    1.181539   -0.802490
O      1.032460    1.174200   -0.002850
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C     -1.540061   -1.497169    0.505220
O     -1.806451   -1.935579    1.596680
C     -2.543990   -0.859479   -0.460060
C     -2.638130    0.701701   -0.244910
C     -1.265200    1.408331   -0.462940
C     -0.187250    1.099001    0.555110
O     -0.305811   -1.485599   -0.020020
O     -0.370320    0.882101    1.733970
C     -1.400799    2.943751   -0.492450
O     -3.503690    1.174852   -1.268410
C     -3.896401   -1.537668   -0.280090
C     -3.305430    1.053881    1.077850
O     -2.147120   -1.084839   -1.809590
H      3.237870   -0.549480    1.777890
H      3.999590   -0.916991   -2.161690
H      4.834989   -1.928291   -0.981230
H      2.352579   -2.878860   -1.362000
H      1.860960    1.326510    1.881360
H      3.981171    2.235909    1.081110
H      2.810041    2.965120   -0.045040
H      4.845260    1.551029   -1.121760
H      3.200550    1.160130   -1.681920
H      0.608779   -1.537290    1.832950
H      0.724189   -3.033230    0.873330
H     -0.884060    1.095581   -1.441570
H     -1.611259    3.342741    0.503250
H     -0.470059    3.391191   -0.849240
H     -2.211459    3.229221   -1.163590
H     -3.209560    0.775851   -2.102040
H     -4.643080   -1.035618   -0.897410
H     -3.811481   -2.579968   -0.595470
H     -4.207661   -1.514198    0.764090
H     -2.796270    0.581661    1.918600
H     -3.296640    2.135631    1.226910
H     -4.347370    0.729952    1.048240
H     -1.181130   -1.100659   -1.863080

46
#3
C      2.700231   -0.186809    0.777470
N      4.099531   -0.230728    0.286680
C      4.155501   -1.138898   -0.876250
C      2.882801   -1.924849   -0.773700
C      2.059381   -1.397749    0.133890
C      2.147210    1.227481    0.385840
C      3.209440    1.809481   -0.540340
C      4.485030    1.152272   -0.010390
O      0.893250    1.228821   -0.309630
C      0.770191   -1.999689    0.593190
C     -1.541819   -1.536550    0.389650
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46
#4
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#5
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46
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#7

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46
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#10

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46
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O      -0.109130    2.873179    0.327041
C      -2.405620    2.577939   -1.207139
O      -3.865029    0.820079    0.212741
C      -3.140669   -1.928461    0.945681
C      -2.104129    0.766549    1.745311
O      -3.099199   -1.164931   -1.318579
H       2.662021   -0.446401    1.969821
H       3.760131   -0.121181   -1.864409
H       4.902591   -1.276311   -1.161069
H       2.662051   -2.611921   -1.563239
H       1.498480    1.505469    1.607931
H       2.596720    2.994499    0.086561
H       2.496830    1.795219   -1.217169
H       4.437500    1.748919    1.160471
H       4.864940    1.608349   -0.549009
H       1.195921   -2.706521    1.734661
H       0.855871   -3.277711    0.077971
H      -1.409969    0.709129   -1.592429
H      -1.753940    3.182449   -1.842209
H      -3.286570    2.295999   -1.785139
H      -2.727740    3.190079   -0.362179
H      -4.194939    0.490739   -0.636959
H      -3.182239   -2.952541    0.566021
H      -2.624159   -1.929241    1.906121
H      -4.159359   -1.559461    1.079661
H      -1.099609    0.401199    1.973851
H      -2.140800    1.845819    1.918551
H      -2.816239    0.288919    2.420081
H      -2.453239   -1.438361   -1.989649

46
#12
C      -2.596821    0.454730    0.765651
N      -4.035491    0.373779    0.431201
C      -4.208461    0.868849   -0.950059
C      -2.949241    1.643590   -1.209279
C      -2.050941    1.437490   -0.245659
C      -2.030000   -1.008280    0.654121
C      -3.210850   -1.843840    0.157721
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C     -4.420570   -1.027311    0.624701
O     -0.950830   -1.052890   -0.286219
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C      1.537789    1.685531    0.088121
O      1.842929    2.736201   -0.435429
C      2.572569    0.677161    0.591921
C      2.662410   -0.588058   -0.361589
C      1.312990   -1.128299   -0.905009
C      0.262100   -1.435559    0.138291
O      0.288439    1.296771    0.320341
O      0.461640   -2.004559    1.190091
C      1.504420   -2.397849   -1.754409
O      3.306460   -0.149228   -1.552159
C      2.301219    0.374401    2.067241
C      3.513320   -1.662008    0.316131
O      3.840019    1.313132    0.523461
H     -2.461461    0.808040    1.795761
H     -4.319741    0.050959   -1.681549
H     -5.105141    1.494379   -1.024969
H     -2.817881    2.299320   -2.063949
H     -1.660650   -1.357240    1.619371
H     -3.192990   -2.867880    0.536861
H     -3.173530   -1.877570   -0.936969
H     -4.612250   -1.199881    1.690361
H     -5.339930   -1.252961    0.079571
H     -0.852801    2.964150    0.663101
H     -0.483051    2.659290   -1.048139
H      0.904820   -0.348569   -1.554089
H      1.775551   -3.253509   -1.130839
H      0.574290   -2.635549   -2.276809
H      2.288680   -2.232149   -2.495059
H      4.134539    0.272432   -1.280719
H      1.379060   -0.183309    2.217141
H      3.136450   -0.200958    2.469761
H      2.247659    1.320551    2.612951
H      2.967570   -2.150038    1.126461
H      3.798270   -2.411948   -0.424249
H      4.428060   -1.212788    0.715281
H      3.721449    2.156632    0.056721

46
#13
C      2.401200   -0.059991    0.670880
N      3.867340    0.076329    0.833380
C      4.464810   -1.203701    0.416810
C      3.395220   -1.883701   -0.401910
C      2.235110   -1.237491   -0.287440
C      1.957520    1.318129    0.153010
C      3.083770    1.707999   -0.784520
C      4.299670    1.252939    0.032570
O      0.701240    1.256580   -0.527610
C      0.950390   -1.621820   -0.947680
C     -1.355280   -1.571770   -0.418150
O     -1.643520   -1.992380   -1.519440
C     -2.387010   -1.019660    0.570580
C     -2.812140    0.393750   -0.020500
C     -1.646970    1.216030   -0.649250
C     -0.414420    1.408550    0.209800
O     -0.104280   -1.416400    0.013670
O     -0.410970    1.724110    1.378000
C     -2.110960    2.612760   -1.098800
O     -3.718830    0.125450   -1.094680
C     -1.871350   -1.008410    2.005110
C     -3.612180    1.169320    1.014270
O     -3.516080   -1.862460    0.575270
H      1.905160   -0.289561    1.623380
H      5.395600   -1.035011   -0.133870
H      4.718670   -1.817761    1.291710
H      3.553570   -2.805101   -0.953540
H      1.875350    2.018249    0.988520
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H      2.995800    1.137599   -1.715550
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H      5.153670    0.998429   -0.600510
H      0.954580   -2.667250   -1.265740
H      0.737050   -0.989600   -1.816610
H     -1.317040    0.672980   -1.543280
H     -2.304840    3.255160   -0.236440
H     -1.338290    3.082240   -1.712330
H     -3.024220    2.526990   -1.690860
H     -3.240310   -0.315480   -1.815150
H     -2.676970   -0.679970    2.663300
H     -1.598110   -2.029570    2.282640
H     -1.008540   -0.360790    2.140770
H     -2.954670    1.559300    1.793940
H     -4.126100    2.000800    0.528550
H     -4.363950    0.515380    1.463420
H     -4.047010   -1.654860   -0.208470

46
#14
C      2.401010   -0.044991    0.673349
N      3.869900    0.047728    0.839919
C      4.423370   -1.264052    0.464229
C      3.339750   -1.922112   -0.354951
C      2.202130   -1.233041   -0.265831
C      2.003421    1.336139    0.129619
C      3.141071    1.669078   -0.815901
C      4.344361    1.182728    0.002449
O      0.747311    1.311399   -0.551681
C      0.915920   -1.585351   -0.941801
C     -1.391040   -1.593990   -0.416681
O     -1.652370   -2.250420   -1.400971
C     -2.454230   -0.993210    0.499079
C     -2.794949    0.480750   -0.009581
C     -1.600379    1.243100   -0.642101
C     -0.360039    1.371699    0.212789
O     -0.157080   -1.280301   -0.027501
O     -0.334509    1.575049    1.405999
C     -1.990759    2.665930   -1.084681
O     -3.670390    0.340781   -1.121271
C     -2.031340   -1.082230    1.962709
C     -3.500689    1.259941    1.097669
O     -3.626140   -1.776939    0.360229
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H      4.639040   -1.865302    1.358129
H      3.471869   -2.858422   -0.888121
H      1.947411    2.052559    0.954039
H      3.192471    2.730128   -1.067701
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H      4.705541    1.984698    0.655549
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H      0.876049   -2.643671   -1.209121
H      0.757620   -0.985431   -1.845421
H     -1.320259    0.683870   -1.542201
H     -1.195219    3.093230   -1.699741
H     -2.908729    2.629270   -1.673101
H     -2.145028    3.317970   -0.221071
H     -4.447960   -0.144859   -0.812701
H     -1.730830   -2.108840    2.185859
H     -1.208240   -0.406470    2.190349
H     -2.886700   -0.832900    2.592869
H     -4.323199    0.661691    1.503329
H     -2.814549    1.519960    1.906099
H     -3.923139    2.175251    0.678499
H     -3.585990   -2.210159   -0.507671

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#15
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C      2.570530   -0.282962    0.888350
N      3.907130   -0.079953    0.287870
C      3.932619   -0.792933   -1.005120
C      2.812079   -1.782832   -0.878940
C      2.051439   -1.514182    0.182510
C      1.769590    1.041208    0.655090
C      2.715761    1.936738   -0.152890
C      4.096791    1.368897    0.190290
O      0.548060    0.761329   -0.050700
C      0.966749   -2.395851    0.712110
C     -1.001571   -1.582000   -0.287450
O     -0.593961   -1.888410   -1.388910
C     -2.421641   -1.046879   -0.076250
C     -2.494240    0.475341    0.301180
C     -1.654959    1.337160   -0.728020
C     -0.341059    1.766200   -0.105710
O     -0.323321   -1.755810    0.839470
O     -0.109249    2.873479    0.326650
C     -2.406149    2.577721   -1.207030
O     -3.865000    0.819961    0.213290
C     -3.140671   -1.928689    0.945670
C     -2.103960    0.766311    1.745520
O     -3.099461   -1.164789   -1.318480
H      2.661330   -0.446222    1.969870
H      3.761990   -0.121623   -1.863910
H      4.903509   -1.276873   -1.159280
H      2.662938   -2.611982   -1.562950
H      1.498781    1.506159    1.607440
H      2.596551    2.994468    0.084790
H      2.497321    1.794008   -1.217930
H      4.436771    1.749507    1.160750
H      4.865331    1.608417   -0.548410
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H      0.855998   -3.277481    0.077090
H     -1.410170    0.709140   -1.592310
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H     -3.287179    2.295571   -1.784830
H     -2.728208    3.189971   -0.362140
H     -4.195040    0.490802   -0.636420
H     -3.182152   -2.952749    0.565970
H     -2.624171   -1.929449    1.906110
H     -4.159411   -1.559808    1.079630
H     -1.099400    0.401020    1.973950
H     -2.140729    1.845561    1.918820
H     -2.815990    0.288611    2.420350
H     -2.453601   -1.438279   -1.989630

46
#16
C      2.739900    0.519139   -0.792179
N      3.926910    0.163599    0.025121
C      3.932820    0.980579    1.247821
C      2.682260    1.810409    1.152271
C      2.011210    1.558960    0.027891
C      2.001980   -0.806410   -1.047549
C      3.117349   -1.838001   -0.935589
C      3.941440   -1.291541    0.231101
O      1.070780   -0.980410    0.033241
C      0.782371    2.278600   -0.421889
C     -1.504600    1.653541   -0.125069
O     -1.750679    2.654731    0.513411
C     -2.583630    0.623331   -0.481149
C     -2.528640   -0.636339    0.486031
C     -1.108870   -1.114230    0.884451
C     -0.166490   -1.397970   -0.263719
O     -0.310520    1.343710   -0.625279
O     -0.453411   -1.963680   -1.296789
C     -1.149551   -2.370300    1.773421
O     -3.058310   -0.212519    1.736451
C     -2.517040    0.304721   -1.975199
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H      3.926130    0.346739    2.146781
H      4.828100    1.612709    1.309111
H      2.389921    2.533779    1.907361
H      1.457040   -0.831940   -1.991979
H      3.704850   -1.832181   -1.859229
H      2.732469   -2.845851   -0.766499
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H      0.938861    2.762660   -1.391419
H      0.478821    3.025490    0.311351
H     -0.663160   -0.302910    1.468861
H     -1.451931   -3.250079    1.199531
H     -0.157521   -2.558450    2.191831
H     -1.852911   -2.220119    2.594211
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H     -2.523820    1.243941   -2.534869
H     -1.631170   -0.268989   -2.239379
H     -3.407070   -0.261279   -2.254749
H     -2.934021   -2.217719   -0.956729
H     -3.567291   -2.507429    0.680311
H     -4.377000   -1.343669   -0.379499
H     -3.674509    2.048921    0.272751

46
#17
C      2.270981    0.003830    0.725891
N      3.693341    0.372260    0.870891
C      4.441271   -0.893210    0.790121
C      3.534231   -1.819770    0.009731
C      2.305531   -1.304940   -0.059699
C      1.661421    1.231540    0.050101
C      2.701191    1.591530   -0.998209
C      4.010911    1.326510   -0.235329
O      0.360891    0.934560   -0.473989
C      1.157971   -1.869410   -0.824389
C     -1.157539   -1.534020   -0.743119
O     -1.219839   -1.587710   -1.955629
C     -2.389659   -1.208420    0.099781
C     -2.375229    0.270230    0.648031
C     -1.994069    1.289690   -0.512329
C     -0.605009    1.858120   -0.285109
O     -0.052399   -1.748150   -0.041869
O     -0.370719    2.992290    0.061351
C     -2.989039    2.440570   -0.642449
O     -3.693739    0.518140    1.095691
C     -2.564129   -2.237370    1.213261
C     -1.505369    0.443000    1.889411
O     -3.514729   -1.291320   -0.762569
H      1.808571   -0.171860    1.706811
H      5.418711   -0.735589    0.325691
H      4.622651   -1.294250    1.796541
H      3.844581   -2.777840   -0.395119
H      1.562811    2.033820    0.785651
H      2.609491    2.620580   -1.350589
H      2.596361    0.914150   -1.852589
H      4.402091    2.252010    0.197411
H      4.780751    0.916410   -0.896809
H      1.309881   -2.924540   -1.065829
H      1.009611   -1.314130   -1.754009
H     -1.958679    0.746180   -1.463479
H     -2.642819    3.141840   -1.405009
H     -3.971219    2.068000   -0.937399
H     -3.092089    2.979370    0.301411
H     -4.298669    0.215170    0.401451
H     -1.688199   -2.273830    1.862221
H     -3.444409   -1.976400    1.804621
H     -2.716919   -3.223410    0.768081
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H     -1.477539    1.499750    2.171991
H     -1.945479   -0.115260    2.717041
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H     -3.192249   -1.341910   -1.676739

46
#18
C      2.671149   -0.072420    0.780810
N      4.087289   -0.117110    0.332000
C      4.224719   -1.176290   -0.687560
C      2.964119   -1.974030   -0.549000
C      2.087479   -1.365070    0.250840
C      2.099129    1.283640    0.239830
C      3.131119    1.751900   -0.776460
C      4.424599    1.225590   -0.154250
O      0.815309    1.234210   -0.398960
C      0.787179   -1.947790    0.702410
C     -1.521721   -1.582250    0.315670
O     -1.808201   -2.164230    1.334500
C     -2.518981   -0.860840   -0.596040
C     -2.762301    0.607990   -0.058240
C     -1.529391    1.511380   -0.325180
C     -0.253221    1.139190    0.405970
O     -0.271751   -1.454610   -0.147430
O     -0.159291    0.891310    1.590370
C     -1.791750    2.986150    0.037290
O     -3.769391    1.182971   -0.883430
C     -3.810341   -1.671169   -0.642540
C     -3.216271    0.629181    1.400040
O     -2.034391   -0.814120   -1.924870
H      2.610809   -0.053350    1.875990
H      4.320699   -0.767200   -1.706880
H      5.117139   -1.784640   -0.499230
H      2.814959   -2.940590   -1.020080
H      2.019719    1.987970    1.073910
H      3.111980    2.832900   -0.930740
H      2.936969    1.254800   -1.734560
H      4.725619    1.854690    0.692220
H      5.264649    1.181320   -0.850590
H      0.554759   -1.662360    1.732020
H      0.797149   -3.037720    0.624640
H     -1.331421    1.463150   -1.398750
H     -0.964310    3.606900   -0.316760
H     -2.711130    3.321860   -0.443170
H     -1.880020    3.119250    1.118320
H     -4.637511    0.955081   -0.528640
H     -3.586021   -2.672259   -1.017070
H     -4.265321   -1.768179    0.343380
H     -4.507081   -1.195339   -1.334740
H     -4.111341    0.014391    1.531970
H     -2.443151    0.263750    2.075360
H     -3.468161    1.654581    1.680840
H     -1.071421   -0.724480   -1.914420
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Table S5. M062X/6-31+G** relative SCF Energies (kcal/mol)

Conformer	Chloroform	Water
1	1.37	1.03
2	2.00	1.70
3	3.07	2.65
4	3.50	2.62
5	3.47	3.43
6	1.48	1.26
7	3.16	3.16
8	3.17	2.77
9	3.48	3.19
10	0.00	0.00
11	2.44	2.09
12	4.79	4.68
13	3.90	3.74
14	3.47	3.43
15	2.44	2.09
16	3.16	3.16
17	5.62	5.57
18	6.01	5.13