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J. Serb. Chem. Soc. 89 (1) S1–S51 (2024) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

Assignment of NMR spectral data of diastereomeric tetrahydrofuranyl acetals directly from their mixture by spectral simulation

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EXPERIMENTAL AND ANALYTICAL DATA

*2-((3,7-Dimethyloct-6-en-1-yl)oxy)tetrahydrofuran (**4**)*. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C (100.6 MHz, $CDCl_3$) for each diastereomer are given in Table S-I; FTIR (neat, cm^{-1}) 2912, 1025; MS (70 eV): *m/z* (%): 226 (0.2), 154 (4.4), 123 (2.5), 95 (4.5), 81 (5.5), 71 (100), 69 (14.1), 67 (5.9), 55 (5.8), 41 (13.8); (+)ESI-HRMS (**m**/**z**): calculated for $[C_{14}H_{26}O_2]^+$ 226.1933, observed 226.1929; Elemental analysis for $C_{14}H_{26}O_2$: Calculated. C 74.28, H 11.58, O 14.14; found C 74.26, H 11.59. RI (DB-5MS) 1553 and 1554 for each diastereomer.

*(Z)-2-(Hex-3-en-1-yloxy)tetrahydrofuran (**5**)*. ^{1}H- (400 MHz, $CDCl_3$) and ^{13}C-NMR (100.6 MHz, $CDCl_3$) are given in Table S-II; FTIR (neat, cm^{-1}) 2911, 1022; MS (70 eV): *m/z* (%): 170 (0.04), 101 (6.2), 87 (6.2), 82 (5.6), 71 (100), 67 (8.9), 55 (12.7), 43 (19.7), 41 (20,1), 39 (9.9); (+)ESI-HRMS (**m**/**z**): calculated for $[C_{10}H_{18}O_2]^+$ 170.1307, observed 170.1310; Elemental analysis for $C_{14}H_{26}O_2$: Calculated. C 70.55, H 10.66, O 18.79; found C 70.57, H 10.65.

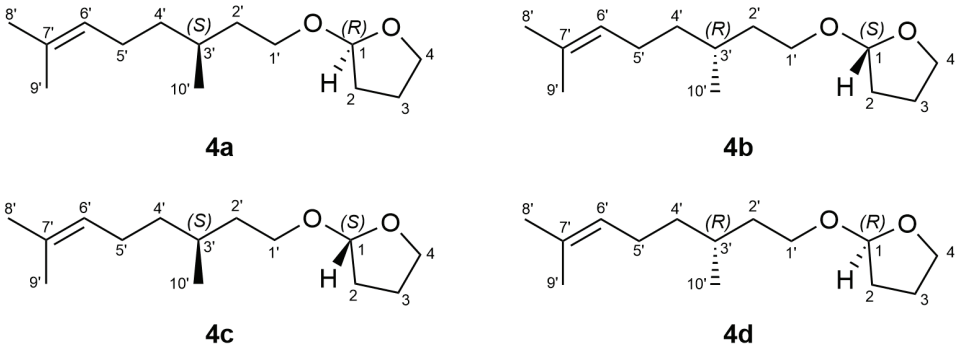

Fig. S-1. Atom numbering scheme of tetrahydrofuranyl acetals of citronellol (**4a**-**4d**).

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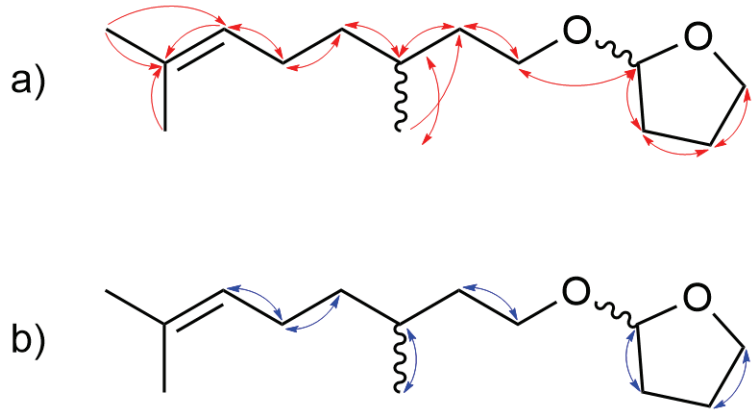

Fig. S-2. Key HMBC (a) and NOESY (b) interactions.

Table S-I. ^{1}H (400 MHz) and ^{13}C (100.6 MHz) NMR data of tetrahydrofuranyl acetals of citronellol ($CDCl_3$, NMR parameters are derived from manual iterative full spin analysis

Position	4c/4d		4a/4b		HMBC[b]	NOESY[c]
	δ_H (m, J (Hz), Integral)[a]	δ_C	δ_H (m, J (Hz), Integral)	δ_C		
1	5.1072 (dd, $^{3}J_{1,2r}$ = 5.3, $^{3}J_{1,2s}$ = 0.9, 1 H)	103.80	5.1032 (dd, $^{3}J_{1,2r}$ = 5.3, $^{3}J_{1,2s}$ = 0.9, 1 H)	103.99	2, 3, 4, 1’	2r, 2s
2r	1.9160 (dddd, $^{2}J_{2r,2s}$ = -11.5, $^{3}J_{2r,3r}$ = 8.3, $^{3}J_{2r,3s}$ = 10.0, $^{3}J_{1,2r}$ = 5.3, 1 H)	23.66	1.9160 (dddd, $^{2}J_{2r,2s}$ = -11.5, $^{3}J_{2r,3r}$ = 8.3, $^{3}J_{2r,3s}$ = 10.0, $^{3}J_{1,2r}$ = 5.3, 1 H)	23.66	1, 3, 4	1
2s	1.8710 (dddd, $^{2}J_{2r,2s}$ = -11.5, $^{3}J_{2s,3r}$ = 8.5, $^{3}J_{2s,3s}$ = 4.0, $^{3}J_{1,2s}$ = 0.9, 1 H)		1.8710 (dddd, $^{2}J_{2r,2s}$ = -11.5, $^{3}J_{2s,3r}$ = 8.5, $^{3}J_{2s,3s}$ = 4.0, $^{3}J_{1,2s}$ = 0.9, 1 H)			
3r	1.9720 (ddddd, $^{2}J_{3r,3s}$ = -11.4, $^{3}J_{2r,3r}$ = 8.3, $^{3}J_{3r,4r}$ = 7.3 $^{3}J_{2s,3r}$ = 8.5, $^{3}J_{3r,4s}$ = 5.6, 1 H)	32.47	1.9720 (ddddd, $^{2}J_{3r,3s}$ = -11.4, $^{3}J_{2r,3r}$ = 8.3, $^{3}J_{3r,4r}$ = 7.3 $^{3}J_{2s,3r}$ = 8.5, $^{3}J_{3r,4s}$ = 5.6, 1 H)	32.46	2, 4	4r, 4s
3s	1.8158 (ddddd, $^{2}J_{3r,3s}$ = -11.4, $^{3}J_{3s,4s}$ = 7.5, $^{3}J_{2r,3s}$ = 10.0, $^{3}J_{3s,4r}$ = 6.2, $^{3}J_{2s,3s}$ = 4.0, 1 H)		1.8158 (ddddd, $^{2}J_{3r,3s}$ = -11.4, $^{3}J_{3s,4s}$ = 7.5, $^{3}J_{2r,3s}$ = 10.0, $^{3}J_{3s,4r}$ = 6.2, $^{3}J_{2s,3s}$ = 4.0, 1 H)			

4r	3.8897 (ddd, $^2J_{4r,4s}$ = -8.1, $^3J_{3r,4r}$ = 7.3, $^3J_{3s,4r}$ = 6.2, 1 H)	66.91	3.8897 (ddd, $^2J_{4r,4s}$ = -8.1, $^3J_{3r,4r}$ = 7.3, $^3J_{3s,4r}$ = 6.2, 1 H)	66.91	1, 3	3r, 3s
4s	3.8570 (ddd, $^2J_{4r,4s}$ = -8.1, $^3J_{3s,4s}$ = 7.5, $^3J_{3r,4s}$ = 5.6, 1 H)		3.8570 (ddd, $^2J_{4r,4s}$ = -8.1, $^3J_{3s,4s}$ = 7.5, $^3J_{3r,4s}$ = 5.6, 1 H)			
1'r	3.3694 (ddd, $^2J_{1'r,1's}$ = -9.6, $^3J_{1'r,2's}$ = 7.9, $^3J_{1'r,2'r}$ = 6.2, 1 H)	65.72	3.4089 (ddd, $^2J_{1'r,1's}$ = -9.7, $^3J_{1'r,2'r}$ = 7.9, $^3J_{1'r,2's}$ = 5.5, 1 H)	65.58	1, 2', 3'	2'r, 2's
1's	3.7168 (ddd, $^2J_{1'r,1's}$ = -9.6, $^3J_{1's,2's}$ = 7.9, $^3J_{1's,2'r}$ = 6.2, 1 H)		3.6801 (ddd, $^2J_{1'r,1's}$ = -9.7, $^3J_{1's,2'r}$ = 7.7, $^3J_{1's,2's}$ = 6.9, 1 H)			
2'r	1.3886 (dddd, $^2J_{2'r,2's}$ = -13.2, $^3J_{2'r,3'}$ = 8.5, $^3J_{1'r,2'r}$ = $^3J_{1's,2'r}$ = 6.2, 1 H)	36.71	1.6008 (dddd, $^2J_{2'r,2's}$ = -13.6, $^3J_{1'r,2'r}$ = 7.9, $^3J_{1's,2'r}$ = 7.7, $^3J_{2'r,3'}$ = 6.5, 1 H)	36.83	1', 3', 4', 10'	1'r, 1's
2's	1.6145 (dddd, $^2J_{2'r,2's}$ = -13.2, $^3J_{1's,2's}$= $J_{1'r,2's}$= 7.9, $^3J_{2's,3'}$ = 6.5, 1 H)		1.3846 (dddd, $^2J_{2'r,2's}$ = -13.6, $^3J_{2's,3'}$ = 8.5, $^3J_{1's,2's}$= 6.9, $J_{1'r,2's}$= 5.5, 1 H)			
3'	1.5332 (ddqdd, $^3J_{3',4'r}$ = 9.2, $^3J_{2'r,3'}$ = 8.5, $^3J_{3',10'}$ = 6.7, $^3J_{2's,3'}$ = 6.5, $^3J_{3',4's}$ = 5.0, 1 H)	29.70	1.5359 (dqddd, $^3J_{2's,3'}$ = 8.5, $^3J_{3',10'}$ = 6.7, $^3J_{2'r,3'}$ = 6.5, $^3J_{3',4's}$ = 6.2, $^3J_{3',4'r}$ = 6.0, 1 H)	29.74	1', 2', 4', 5', 10'	10'
4'r	1.1885 (dddd, $^2J_{4'r,4's}$ = -14.3, $^3J_{3',4'r}$ = 9.2, $^3J_{4'r,5's}$ = 7.6, $^3J_{4'r,5'r}$ = 2.3, 1 H)	37.36	1.3336 (dddd, $^2J_{4'r,4's}$ = -14.3, $^3J_{4'r,5's}$ = 9.8, $^3J_{3',4'r}$ = 6.0, $^3J_{4'r,5'r}$ = 5.9, 1 H)	37.18	2', 3', 5', 6', 10'	5'r, 5's
4's	1.3422 (dddd, $^2J_{4'r,4's}$ = -14.3, $^3J_{4's,5'r}$ = 7.4, $^3J_{4's,5's}$ = 5.6, $^3J_{3',4's}$ = 5.0, 1 H)		1.1448 (dddd, $^2J_{4'r,4's}$ = -14.3, $^3J_{4's,5'r}$ = 8.1, $^3J_{3',4's}$ = 6.2, $^3J_{4's,5's}$ = 4.2, 1 H)			
5'r	1.9617 (dddd, $^2J_{5'r,5's}$ = -14.3, $^3J_{5'r,6'}$ = 7.6, $^3J_{4's,5'r}$ = 7.4, $^3J_{4'r,5'r}$ = 2.3, 1 H)	25.58	2.0006 (dddd, $^2J_{5'r,5's}$ = -14.3, $^3J_{4's,5'r}$ = 8.1, $^3J_{5'r,6'}$ = 7.6, $^3J_{4'r,5'r}$ = 5.9, 1 H)	25.58	3', 4', 6', 7'	4'r, 4's, 6'
5's	2.0107 (dddd, $^2J_{5'r,5's}$ = -14.3, $^3J_{4'r,5's}$ = 7.6, $^3J_{5's,6'}$ = 6.6, $^3J_{4's,5's}$		1.9635 (dddd, $^2J_{5'r,5's}$ = -14.3, $^3J_{4'r,5's}$ = 9.8, $^3J_{5's,6'}$ = 6.6, $^3J_{4's,5's}$ = 4.2, 1 H)			

	= 5.6, 1 H)					
6'	5.0946 (ddqq, $^3J_{5'r,6'}$ = 7.6, $^3J_{5's,6'}$ = 6.6, $^4J_{6',8'}$ = $^4J_{6',9'}$ = -1.4, 1 H)	124.97	5.0946 (ddqq, $^3J_{5'r,6'}$ = 7.6, $^3J_{5's,6'}$ = 6.6, $^4J_{6',8'}$ = $^4J_{6',9'}$ = -1.4, 1 H)	124.97	4', 5', 8', 9'	5'r, 5's
7'	/	131.22	/	131.21	/	/
8'	1.6790 (dq, $^4J_{6',8'}$ = -1.4, $^4J_{8',9'}$ = -0.8, 3 H)	25.85	1.6790 (dq, $^4J_{6',8'}$ = -1.4, $^4J_{8',9'}$ = -0.8, 3 H)	25.85	4', 6', 7', 9'	/
9'	1.5996 (dq, $^4J_{6',9'}$ = -1.4, $^4J_{8',9'}$ = -0.8, 3 H)	17.75	1.5996 (dq, $^4J_{6',9'}$ = -1.4, $^4J_{8',9'}$ = -0.8, 3 H)	17.75	5', 6', 7', 8'	/
10'	0.8898 (d, $^3J_{3',10'}$ = 6.7, 3 H)	19.57	0.8898 (d, $^3J_{3',10'}$ = 6.7, 3 H)	19.72	2', 3', 4'	3'

[a]Coupling constant values were initially inferred from ^{1}H homonuclear selective decoupling NMR experiments and afterward refined through a manual iterative full spin analysis. [b]gHMBC correlations observed between the hydrogen in this row and the carbon in the listed position. [c]Cross-peaks observed in the NOESY spectrum

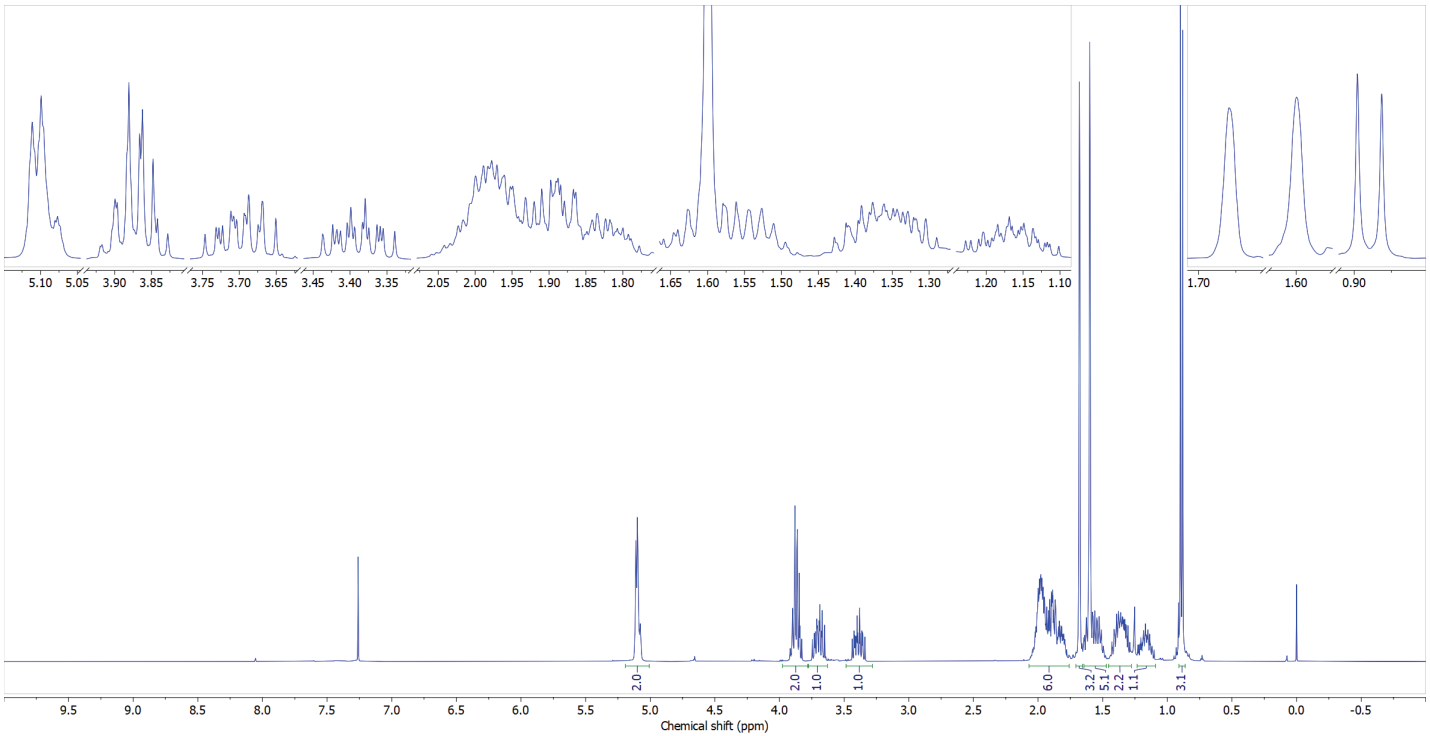

Fig. S-3. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of mixture of tetrahydrofuranyl acetals of citronellol (**4a-4d**) and the corresponding expansions.

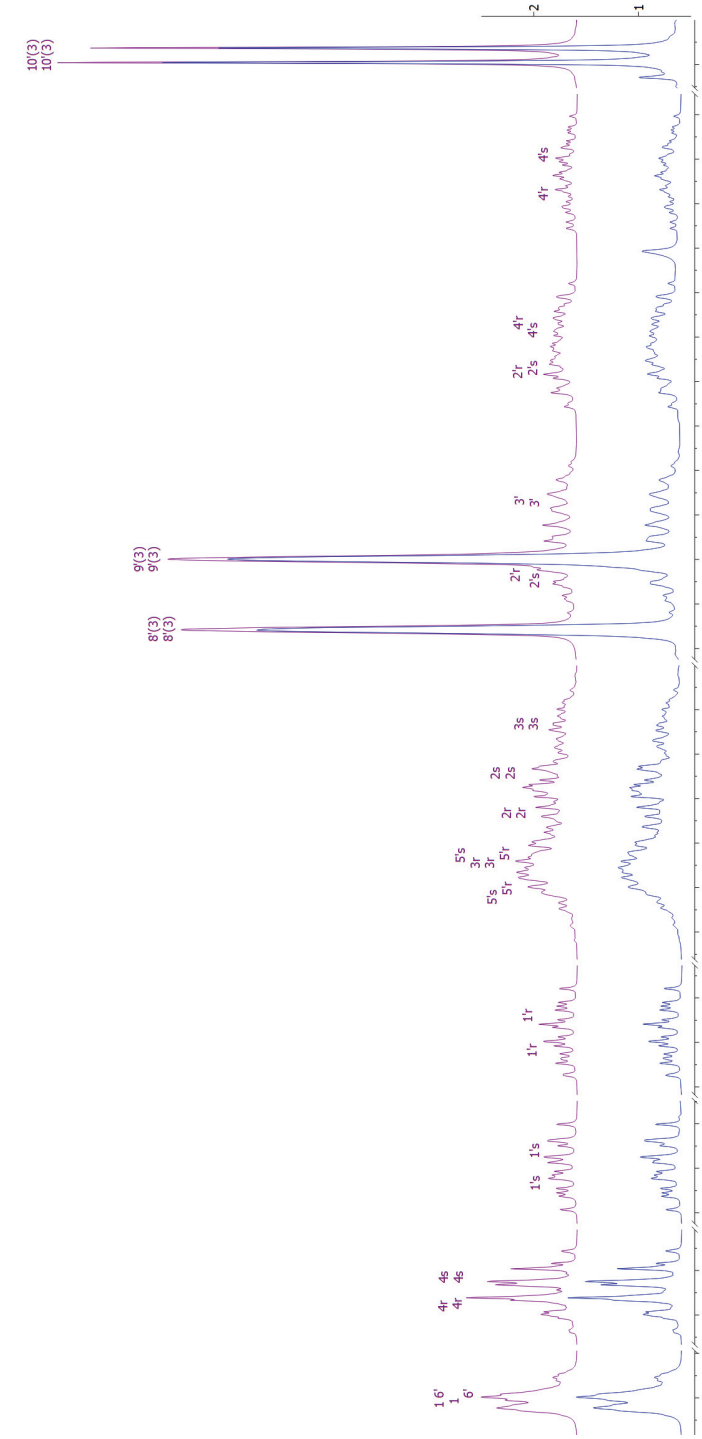

Fig.S-4. Upper trace: simulated ^{1}H NMR (400 MHz) spectrum of equimolar mixture of **4a-4d**; lower trace: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of equimolar mixture of **4a-4d**.

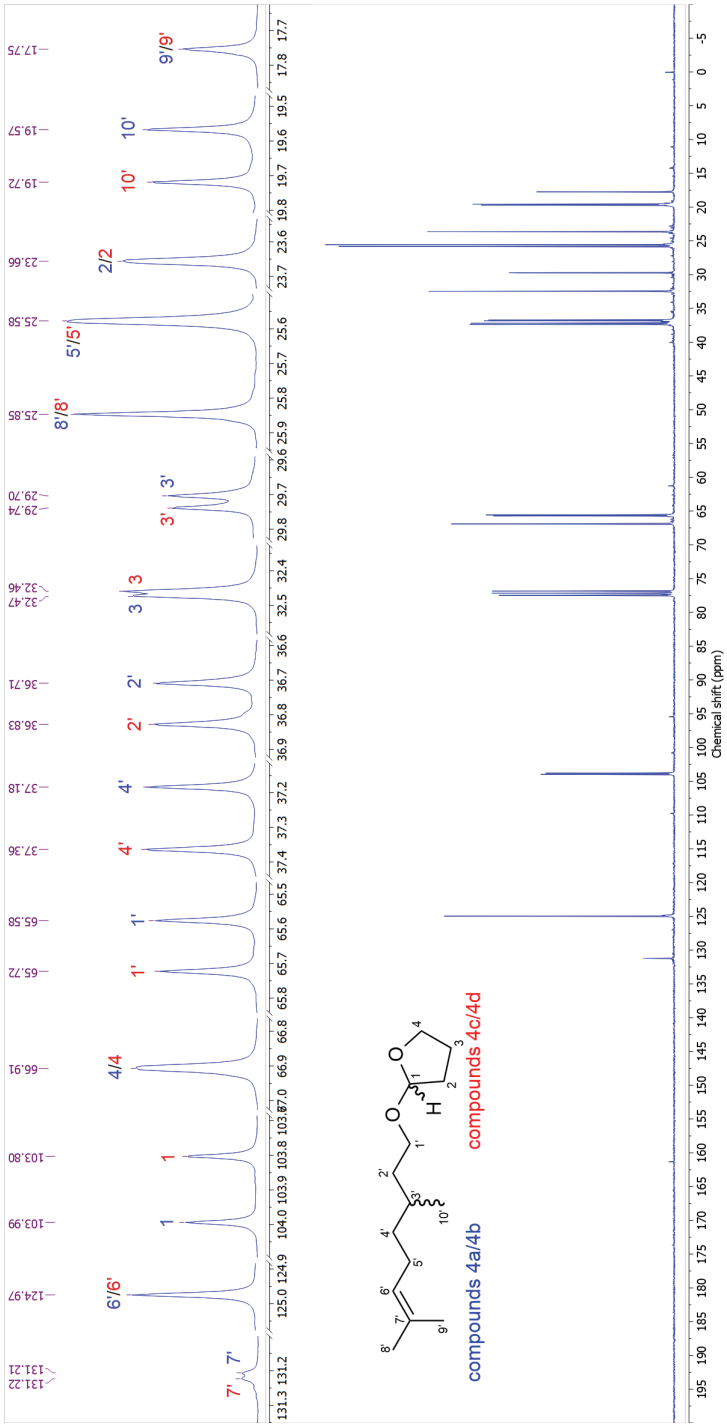

Fig. S.5. ^{13}C NMR (100.6 MHz, $CDCl_3$) spectrum of equimolar mixture of **4a-4d**, and the corresponding expansion.

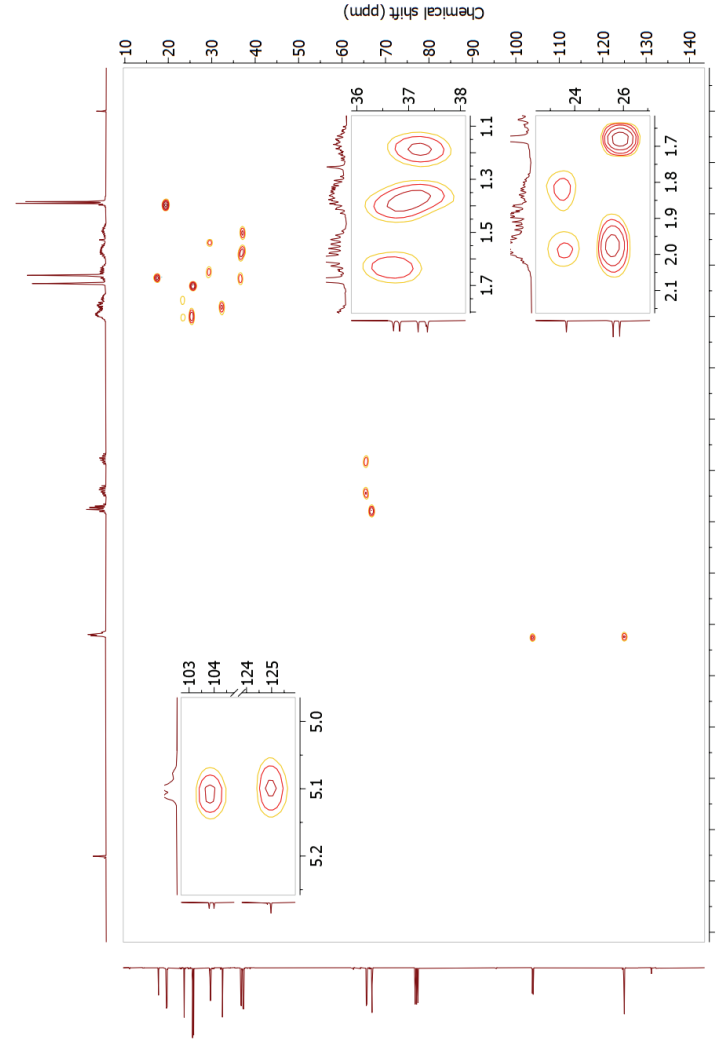

Fig. S-6. grHSQC spectrum of an equimolar mixture of **4a-4d**, and the corresponding expansions.

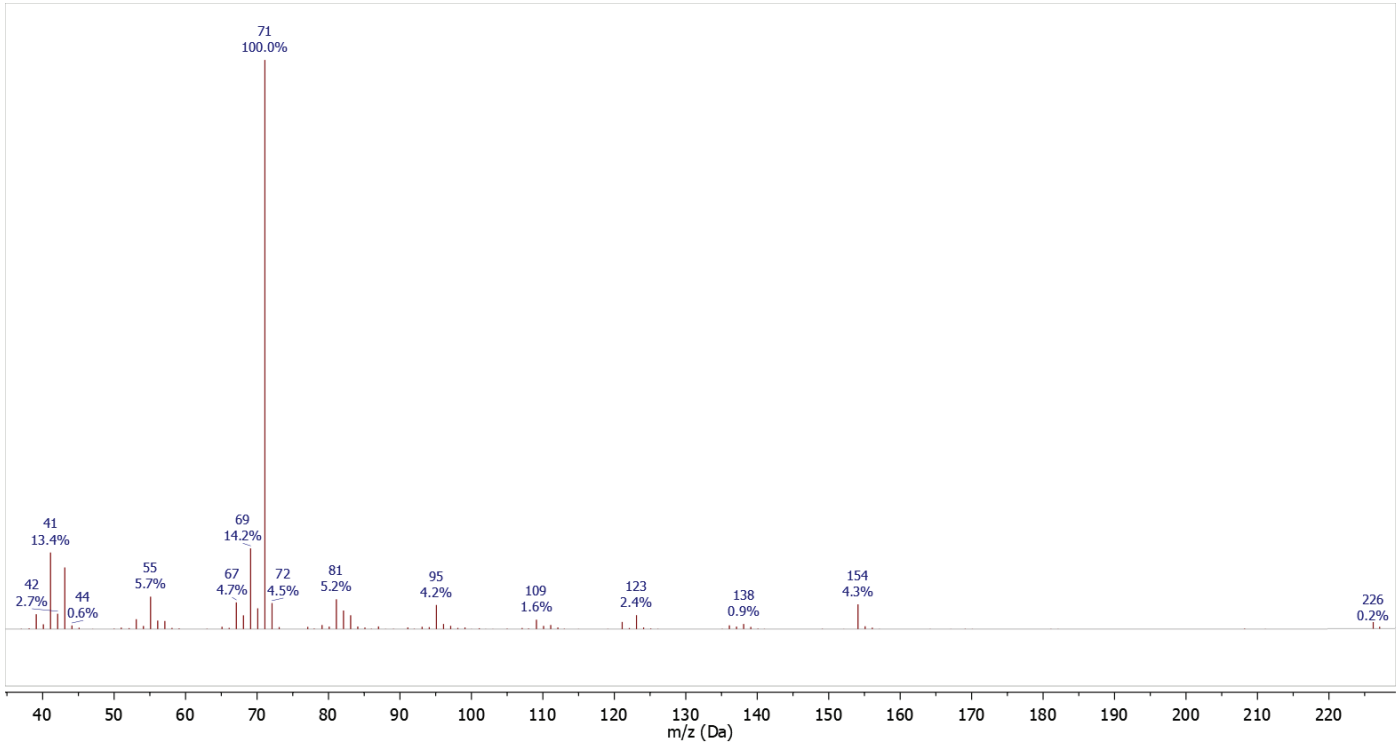

Fig. S-7. EI (70 eV) Mass spectrum of a diastereomer of **4** (RI 1553).

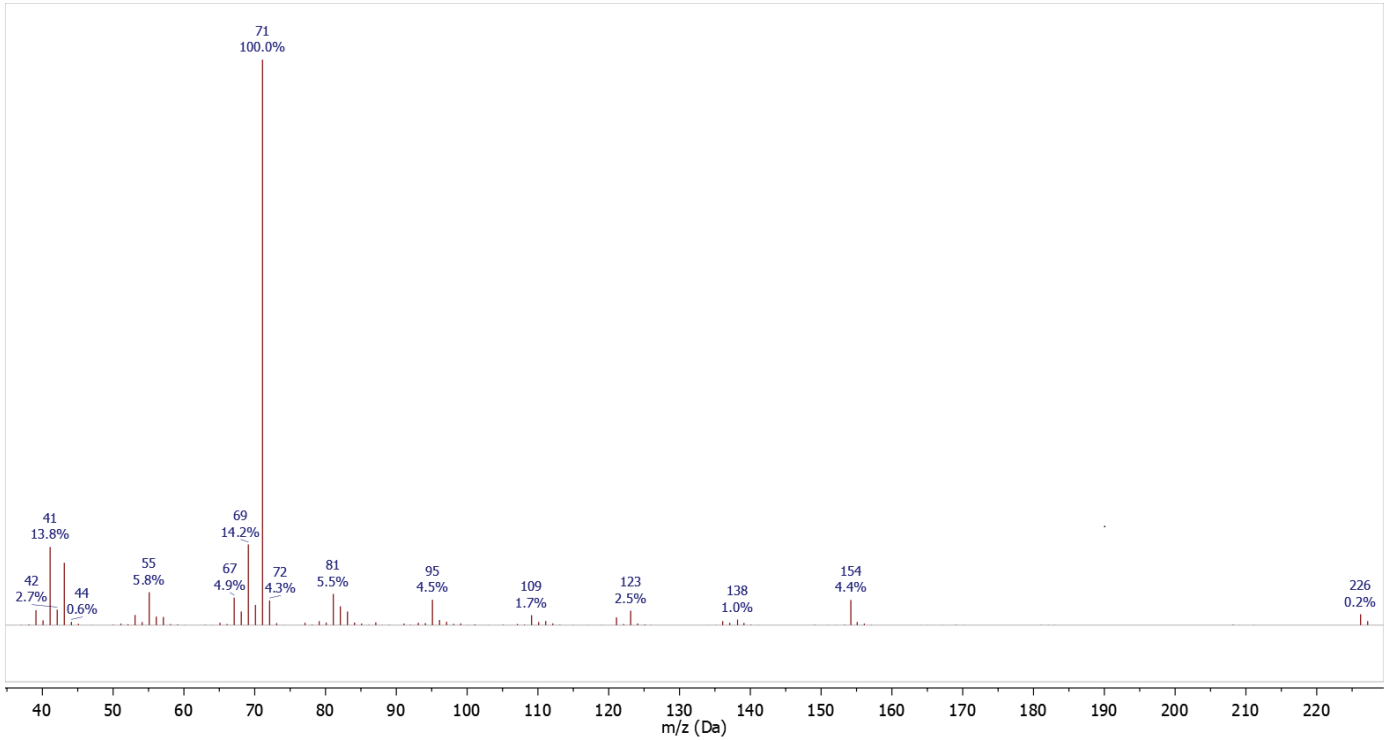

Fig. S-8. EI (70 eV) Mass spectrum of a diastereomer of **4** (RI 1554).

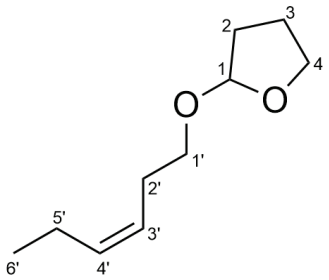

Fig. S-9. Atom numbering scheme of tetrahydrofuranyl acetal of *cis*-3-hexen-1-ol (**5**)

Table S-II. ^{1}H (400 MHz) and ^{13}C (100.6 MHz) NMR data of tetrahydrofuranyl acetal of *cis*-3-hexen-1-ol

Position	**System 1**	
	δ_H (m, *J* (Hz), Integral)[a]	δ_C
1	5.1248 (dd, $^{3}J_{1,2r}$ = 5.0, $^{3}J_{1,2s}$ = 1.5, 1 H)	103.84
2r	1.9170 (dddd, $^{2}J_{2r,2s}$ = -13.1, $^{3}J_{2r,3s}$ = 10.0, $^{3}J_{2r,3r}$ = 8.3, $^{3}J_{1,2r}$ = 5.0, 1 H)	23.58
2s	1.8800 (dddd, $^{2}J_{2r,2s}$ = -13.1, $^{3}J_{2s,3r}$ = 8.5, $^{3}J_{2s,3s}$ = 4.0, $^{3}J_{1,2s}$ = 1.5, 1 H)	
3r	1.9940 (ddddd, $^{2}J_{3r,3s}$ = -13.2, $^{3}J_{2s,3r}$ = 8.5, $^{3}J_{2r,3r}$ = 8.3, $^{3}J_{3r,4r}$ = 7.3, $^{3}J_{3r,4s}$ = 5.6, 1 H)	32.43
3s	1.8165 (ddddd, $^{2}J_{3r,3s}$ = -13.2, $^{3}J_{2s,3s}$ = 4.0, $^{3}J_{3s,4s}$ = 7.5, $^{3}J_{3s,4r}$ = 6.2, $^{3}J_{2r,3s}$ = 10.0, 1 H)	
4r	3.8958 (ddd, $^{2}J_{4r,4s}$ = -8.2, $^{3}J_{3r,4r}$ = 7.3, $^{3}J_{3s,4r}$ = 6.2, 1 H)	66.92
4s	3.8553 (ddd, $^{2}J_{4r,4s}$ = -8.2, $^{3}J_{3s,4s}$ = 7.5, $^{3}J_{3r,4s}$ = 5.6, 1 H)	
1'r	3.3826 (ddd, $^{2}J_{1'r,1's}$ = -9.5, $^{3}J_{1'r,2'r}$ = 7.2, $^{3}J_{1'r,2's}$ = 7.0, 1 H)	66.89
1's	3.6472 (ddd, $^{2}J_{1'r,1's}$ = -9.5, $^{3}J_{1's,2's}$ = 7.2, $^{3}J_{1's,2'r}$ = 7.0, 1 H)	
2'r	2.3170 (dddddd, $^{2}J_{2'r,2's}$ = -21.0, $^{3}J_{2'r,3'}$ = 7.3, $^{3}J_{1'r,2'r}$ = 7.2, $^{3}J_{1's,2'r}$ = 7.0, $^{4}J_{2'r,4'}$ = 1.5, 1 H)	27.96
2's	2.3030 (dddddd, $^{2}J_{2'r,2's}$ = -21.0, $^{3}J_{2's,3'}$ = 7.3, $^{3}J_{1's,2's}$ = 7.2, $J_{1'r,2's}$= 7.0, $^{4}J_{2's,4'}$ = 1.5, 1 H)	

3'	5.3325 (ddddd, $^{3}J_{3',4'} = 10.8$, $^{3}J_{2'r,3'} = {}^{3}J_{2's,3'} = 7.3$, $^{4}J_{3',5'r} = {}^{4}J_{3',5's} = 1.5$, 1 H)	125.03
4'	5.4535 (ddddd, $^{3}J_{3',4'} = 10.8$, $^{3}J_{4',5'r} = {}^{3}J_{4',5's} = 7.3$, $^{4}J_{2'r,4'} = {}^{4}J_{2's,4'} = 1.5$, 1 H)	133.63
5'r	2.0630 (dqdd, $^{2}J_{5'r,5's} = -20.0$, $^{3}J_{5'r,6'} = 7.5$, $^{3}J_{4',5'r} = 7.3$, $^{4}J_{3',5'r} = 1.5$, 1 H)	20.71
5's	2.0490 (dqdd, $^{2}J_{5'r,5's} = -20.0$, $J_{5's,6'} = 7.5$, $^{3}J_{4',5's} = 7.3$, $^{4}J_{3',5's} = 1.5$, 1 H)	
6'	0.9600 (dd, $^{3}J_{5'r,6'} = {}^{3}J_{5's,6'} = 7.5$, 3 H)	14.35

[a]Coupling constant values were initially inferred from ^{1}H homonuclear selective decoupling NMR experiments and afterward refined through a manual iterative full spin analysis.

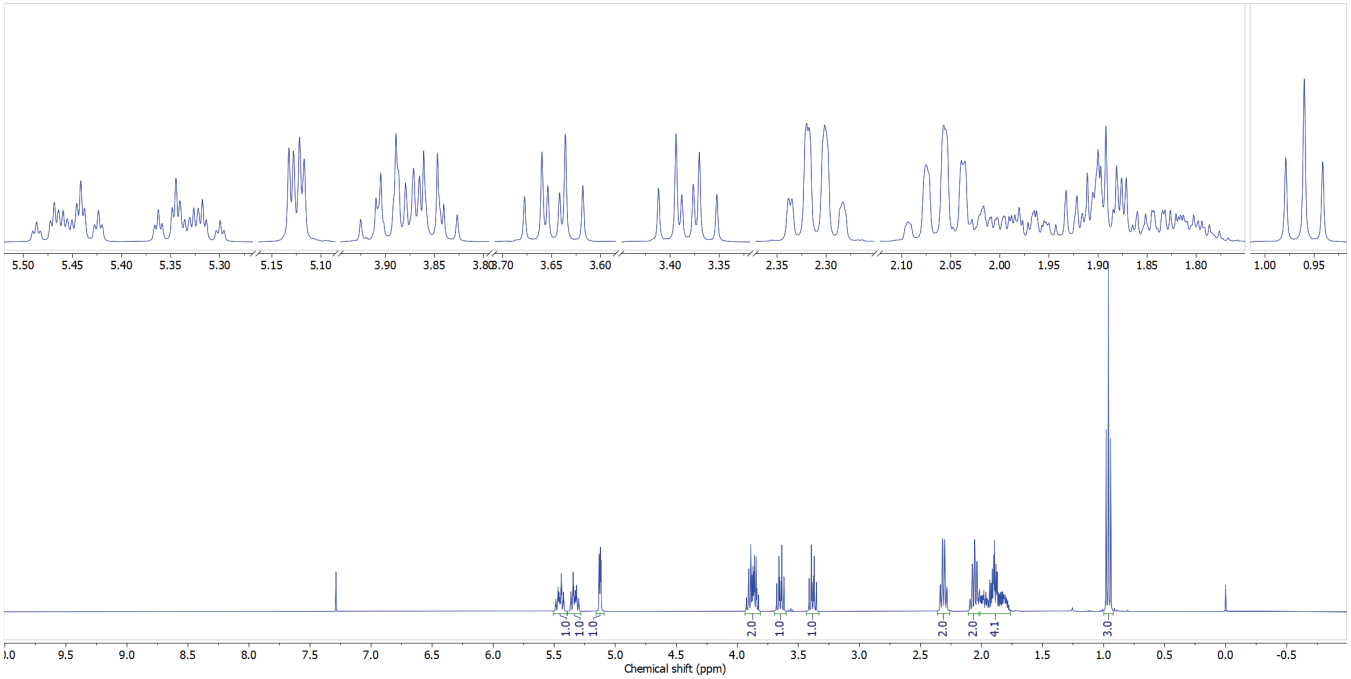

Fig. S-10. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of tetrahydrofuranyl acetal of *cis*-3-hexen-1-ol and the corresponding expansions.

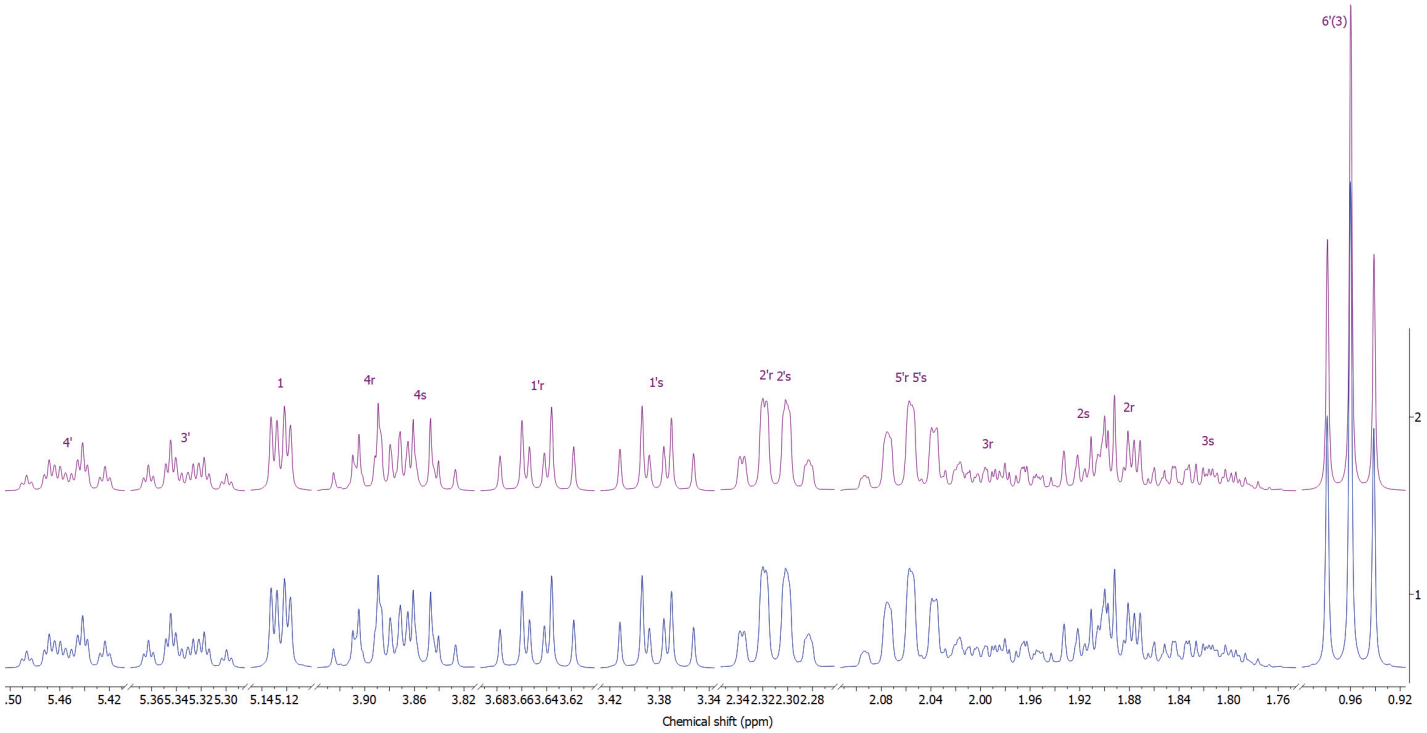

Fig. S-11. Upper trace: simulated ^{1}H NMR (400 MHz) spectrum of **5**; lower trace: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **5**.

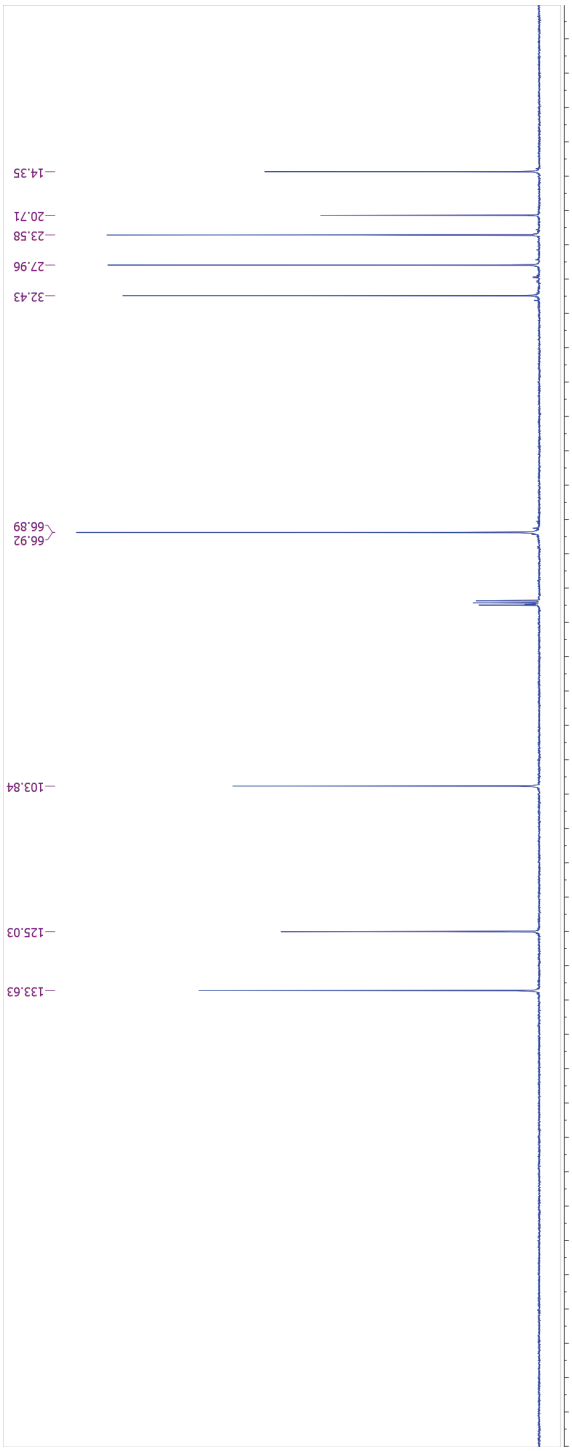

Fig. S-12. ^{13}C-NMR (100.6 MHz, $CDCl_3$) spectrum of **5**.

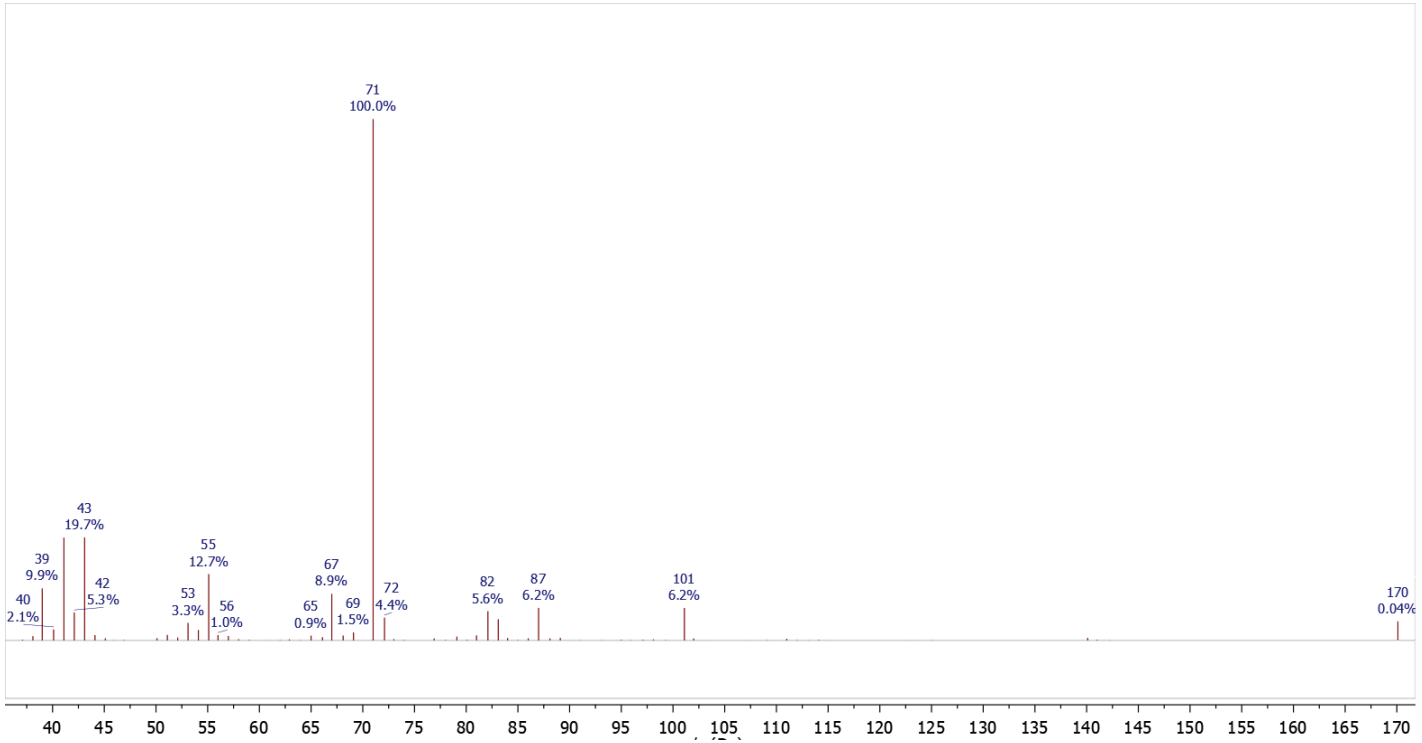

Fig. S-13. EI (70 eV) Mass spectrum of **5**.

Table S-III. Calculated vicinal coupling constants (from H-1 to H-6')

	1 -2r	1 -2s	2r - 3r	2r - 3s	2s - 3r	2s - 3s	3r - 4r	3r - 4s	3s - 4r	3s - 4s	1'r - 2'r	1'r - 2's	1's - 2'r	1's - 2's	2'r-3'	2's-3'	3'-4'r	3'-4's	4'r - 5'r	4'r - 5's	4's - 5'r	4's - 5's	5'r - 6'	5's - 6'
SS new 311	7.73	2.01	11.63	7.38	7.71	2.04	9.61	9.49	2.46	9.40	8.25	7.28	5.28	8.34	11.90	4.75	10.89	4.99	4.15	11.64	11.62	4.26	8.52	8.55
SR new 311	8.87	2.98	8.20	8.41	8.61	4.61	9.08	6.35	5.92	9.16	9.71	4.93	6.09	9.63	8.34	7.49	6.23	7.28	4.09	11.46	11.48	4.59	7.81	8.38
	1 -2r	1 -2s	2r - 3r	2r - 3s	2s - 3r	2s - 3s	3r - 4r	3r - 4s	3s - 4r	3s - 4s	1'r - 2'r	1'r - 2's	1's - 2'r	1's - 2's	2'r-3'	2's-3'	3'-4'r	3'-4's	4'r - 5'r	4'r - 5's	4's - 5'r	4's - 5's	5'r - 6'	5's - 6'
SS new cor	4.95	1.29	11.16	7.09	7.40	1.95	9.22	9.11	2.37	9.02	6.80	5.87	3.94	6.88	11.42	4.56	10.46	4.79	3.98	11.17	11.16	4.09	8.18	8.21
SR new cor	5.68	1.91	7.87	8.08	8.27	4.43	8.71	6.09	5.68	8.80	8.20	3.61	4.73	8.12	8.00	7.19	5.98	6.99	3.93	11.01	11.02	4.41	7.50	8.04

Table S-IV. Dihedral angles between vicinal hydrogens (from H-1 to H-6') for every conformer of **4a**/**4b**

4c/4d (SS/RR)																										
		boltzman	energy	1-2r	1-2s	2r-3r	2r-3s	2s-3r	2s-3s	3r-4r	3r-4s	3s-4r	3s-4s	1'r-2'r	1'r-2's	1's-2'r	1's-2's	2'r-3'	2'p-3'	3'-4'r	3'-4's	4'r-5'r	4'r-5's	4's-5'r	4's-5's	5'r-6'	5's-6'
M0007	-1825209.81	0.206	-695185119.00	-35.85	84.77	159.88	38.54	36.53	-84.80	-23.14	-146.15	98.07	-24.94	58.61	173.40	-59.94	54.84	177.39	61.12	175.75	-68.73	-59.34	-175.11	-174.16	70.06	-161.96	-45.74
M0031	-1825209.01	0.149	-695184813.00	-35.98	84.64	159.78	38.49	36.40	-84.88	-22.65	-145.71	98.56	-24.50	174.29	-70.36	54.54	169.89	179.12	62.54	-179.91	-64.63	-58.22	-174.16	-173.06	71.00	-160.10	-43.77
M0027	-1825208.53	0.123	-695184633.00	-36.00	84.61	158.89	37.70	35.57	-85.62	-21.16	-144.15	99.93	-23.06	172.84	-71.84	53.08	168.39	173.90	56.86	63.58	178.77	-71.63	172.60	173.44	57.67	43.99	160.21
M0009	-1825208.49	0.121	-695184618.00	-36.23	84.45	159.87	38.53	36.48	-84.86	-22.52	-145.56	98.66	-24.38	59.50	174.27	-59.12	55.65	179.54	63.32	179.68	-64.95	-60.68	-176.45	-175.47	68.76	36.50	152.72
M0032	-1825208.43	0.118	-695184593.00	-36.00	84.63	159.86	38.55	36.47	-84.85	-22.70	-145.73	98.49	-24.53	174.52	-70.12	54.78	170.13	177.13	60.54	176.24	-68.32	-61.27	-177.07	-176.29	67.91	44.12	160.34
M0013	-1825206.11	0.046	-695183711.00	-36.08	84.56	159.42	38.13	36.05	-85.24	-22.12	-145.07	99.05	-23.90	58.31	173.04	-60.30	54.42	178.79	62.47	-179.51	-64.19	57.98	-56.96	-56.96	-171.90	64.13	-179.36
M0008	-1825206.00	0.044	-695183668.00	-36.91	83.86	158.92	37.71	35.52	-85.69	-20.36	-143.10	100.74	-22.01	-52.67	62.57	-171.79	-56.55	-60.13	-176.44	-177.58	-61.58	-58.27	-174.06	-173.22	71.00	-170.88	-54.37
M0062	-1825204.27	0.022	-695183008.00	-35.94	84.68	160.22	38.86	36.81	-84.55	-23.45	-146.54	97.84	-25.24	-171.57	-56.53	69.12	-175.84	-57.53	-173.80	-52.35	62.46	-63.87	-179.77	-178.11	65.99	41.72	157.74
M0033	-1825204.22	0.022	-695182990.00	-36.99	83.57	156.71	35.82	33.37	-87.52	-16.27	-139.01	104.43	-18.31	-60.51	53.82	-179.15	-64.82	-154.25	89.17	77.40	-167.06	-63.34	-178.61	-178.45	66.28	44.87	160.84
M0021	-1825204.15	0.021	-695182962.00	-36.28	84.44	160.29	38.89	36.91	-84.49	-23.37	-146.42	97.89	-25.16	58.89	173.72	-59.78	55.05	179.43	63.02	-178.38	-62.74	58.91	-55.67	-56.31	-170.89	-147.84	-32.18
M0024	-1825203.75	0.018	-695182810.00	-35.75	84.92	160.17	38.79	36.85	-84.53	-23.76	-146.79	97.57	-25.47	174.19	-70.35	54.57	170.03	174.41	57.26	60.85	175.89	170.76	55.76	55.71	-59.30	178.45	-65.04
M0029	-1825203.69	0.017	-695182788.00	-36.43	84.24	158.51	37.42	35.11	-85.98	-20.17	-143.03	100.91	-21.96	-76.62	38.01	164.68	-80.69	178.66	62.76	-177.77	-62.46	-58.00	-173.89	-172.68	71.42	-152.44	-36.13
M0028	-1825203.55	0.016	-695182735.00	-36.35	84.34	159.47	38.21	36.00	-85.25	-21.64	-144.69	99.52	-23.53	173.51	-71.13	53.81	169.17	177.69	61.04	179.58	-65.16	57.46	-57.49	-57.60	-172.54	62.84	179.31
M0047	-1825202.93	0.013	-695182499.00	-35.75	84.86	159.62	38.32	36.22	-85.08	-22.59	-145.62	98.62	-24.41	174.87	-69.74	55.26	170.65	-179.93	63.45	-177.65	-62.15	58.80	-55.69	-56.55	-171.04	-147.19	-31.64
M0001	-1825202.43	0.010	-695182307.00	-36.55	84.16	160.12	38.72	36.69	-84.71	-22.88	-145.89	98.33	-24.68	65.53	-179.89	-54.06	60.52	-165.14	77.57	63.89	179.47	166.37	51.87	51.13	-63.37	42.20	157.78
M0015	-1825202.27	0.010	-695182246.00	-36.44	84.38	161.07	39.59	37.61	-83.87	-24.66	-147.59	96.64	-26.29	-53.84	61.01	-172.94	-58.09	-54.22	-170.32	-55.77	59.13	-68.92	175.02	176.53	60.47	43.05	159.13
M0056	-1825201.92	0.009	-695182113.00	-35.93	84.73	160.35	38.95	36.91	-84.49	-23.69	-146.73	97.54	-25.49	-167.38	-52.15	73.02	-171.76	-59.99	-176.44	-174.27	-58.22	58.56	-56.07	-56.64	-171.28	-144.51	-28.79
M0018	-1825201.19	0.006	-695181838.00	-36.68	84.06	159.62	38.35	36.23	-85.04	-22.00	-145.05	99.18	-23.87	77.96	-167.99	-40.86	73.19	-60.20	-175.74	-56.01	59.46	-64.26	178.99	-179.32	63.93	50.91	168.12
M0014	-1825201.06	0.006	-695181787.00	-36.70	83.95	158.91	37.74	35.61	-85.56	-20.57	-143.60	100.50	-22.53	63.70	177.77	-54.65	59.42	-87.06	156.55	174.15	-70.33	57.25	-57.84	-58.52	-173.60	63.23	179.58
M0003	-1825200.48	0.005	-695181566.00	-36.67	83.89	152.22	31.48	29.02	-91.72	-8.74	-131.47	111.86	-10.87	-62.58	52.59	177.70	-67.12	-75.90	167.32	173.16	-70.96	-64.62	179.80	-179.25	65.17	51.21	147.15
M0067	-1825200.04	0.004	-695181399.00	-0.38	118.51	100.46	-21.15	-21.48	-143.09	36.91	-87.33	157.59	33.34	60.38	175.16	-58.30	56.48	-176.62	66.40	-57.85	57.19	-65.00	178.92	-179.61	64.32	-150.98	-34.99
M0058	-1825199.52	0.003	-695181200.00	-36.18	84.48	159.21	37.98	35.83	-85.39	-21.48	-144.50	99.67	-23.35	-178.04	-63.05	61.86	176.84	58.75	-57.47	176.46	-67.59	56.26	-58.68	-58.75	-173.69	63.11	179.71
M0075	-1825197.91	0.002	-695180587.00	-1.59	117.27	101.55	-20.00	-20.35	-141.90	36.40	-87.86	156.99	32.74	173.29	-71.53	53.43	168.62	174.01	57.02	61.11	176.44	170.52	55.99	55.19	-59.34	29.70	145.25
M0054	-1825196.97	0.001	-695180229.00	-37.09	83.58	156.88	35.95	33.49	-87.43	-16.37	-139.49	104.23	-18.69	-59.89	54.46	-178.78	-64.44	-150.86	92.19	71.91	-172.55	174.54	59.85	59.23	-55.47	30.23	145.37
M0012	-1825196.20	0.001	-695179937.00	-35.45	84.96	155.32	34.51	32.18	-88.62	-15.84	-138.76	104.77	-18.16	60.45	175.10	-58.50	56.16	-174.91	68.21	69.77	-174.95	173.38	58.26	58.53	-56.60	-168.81	-52.28
M0006	-1825196.20	0.001	-695179936.00	-38.13	82.62	153.33	32.60	29.90	-90.84	-8.68	-132.09	112.08	-11.33	-63.06	51.80	177.48	-67.65	-76.87	166.65	169.97	-74.37	45.43	-69.47	-69.49	175.60	45.30	160.80
M0037	-1825195.73	0.001	-695179758.00	-0.89	118.08	100.53	-21.13	-21.47	-143.13	37.21	-86.95	157.91	33.75	-55.73	59.14	-174.98	-60.11	-56.92	-173.10	-55.14	59.83	-65.03	178.75	-179.47	64.31	-155.43	-39.01
M0036	-1825195.44	0.001	-695179647.00	-35.88	84.61	158.76	37.51	35.46	-85.78	-20.95	-143.95	100.16	-22.85	73.81	-172.01	-44.26	69.92	-75.53	168.49	175.87	-68.75	57.15	-57.66	-58.45	-173.26	-141.52	-26.06
M0069	-1825195.36	0.001	-695179614.00	-36.70	84.16	160.37	39.00	36.94	-84.43	-23.25	-146.19	98.02	-24.93	-57.26	57.91	-176.46	-61.29	-71.31	172.22	148.38	-95.42	176.42	62.10	61.93	-52.40	35.88	151.61
M0035	-1825195.10	0.001	-695179517.00	-36.18	84.45	157.94	36.84	34.58	-86.52	-19.25	-142.36	101.81	-21.30	-50.37	63.41	-168.94	-55.17	-60.39	-175.36	-53.16	61.55	-63.75	-179.87	-178.19	65.68	-157.14	-40.99
M0042	-1825194.81	0.000	-695179404.00	-36.41	84.26	157.66	36.59	34.31	-86.76	-18.21	-141.21	102.79	-20.20	172.38	-71.64	53.90	169.88	-81.00	162.37	161.30	-82.88	47.25	-68.07	-67.89	176.79	45.86	162.07
M0064	-1825194.62	0.000	-695179334.00	-36.78	83.74	153.18	32.41	29.97	-90.81	-9.76	-133.04	110.80	-12.48	-55.34	59.80	-174.52	-59.38	-64.70	178.82	-176.69	-60.71	55.06	-59.64	-60.04	-174.74	-164.14	-48.19
M0052	-1825194.41	0.000	-695179253.00	-36.65	84.19	160.48	39.04	37.00	-84.44	-22.89	-145.72	98.28	-24.55	-73.61	40.97	167.27	-78.15	55.61	-60.30	176.35	-68.77	-61.91	-177.95	-176.36	67.59	-157.28	-40.92
M0071	-1825194.00	0.000	-695179098.00	-5.59	113.34	104.78	-16.68	-17.17	-138.62	35.19	-89.01	155.70	31.50	-65.21	49.17	176.23	-69.38	-165.20	78.51	-175.07	-59.46	57.81	-56.84	-57.50	-172.15	-145.90	-30.19
M0049	-1825192.91	0.000	-695178682.00	-36.88	83.86	158.39	37.35	35.01	-86.03	-19.50	-142.20	101.53	-21.18	-69.70	44.64	171.49	-74.17	60.67	-55.00	-179.47	-64.60	57.44	-57.38	-57.49	-172.31	65.53	-178.07
M0002	-1825192.46	0.000	-695178512.00	-36.30	84.49	160.98	39.53	37.61	-83.84	-24.16	-147.35	97.02	-26.17	-51.37	63.58	-170.17	-55.22	-51.95	-168.00	-57.12	57.58	-72.74	170.68	172.66	56.08	-160.65	-43.58
M0066	-1825192.29	0.000	-695178446.00	-35.62	85.02	159.50	38.26	36.17	-85.07	-22.73	-145.43	98.46	-24.23	-63.30	51.92	177.37	-67.41	-73.11	170.06	139.84	-104.15	175.49	60.50	61.09	-53.90	-168.60	-51.96
M0034	-1825191.57	0.000	-695178171.00	-36.85	83.85	154.86	34.04	31.54	-89.27	-12.60	-135.59	108.18	-14.80	167.15	-77.51	47.80	163.14	173.01	57.76	58.79	173.96	169.85	54.86	54.66	-60.33	179.46	-64.03
M0004	-1825191.03	0.000	-695177947.00	-35.72	84.90	159.25	38.01	35.88	-85.36	-21.67	-144.88	99.49	-23.72	176.97	-66.81	57.50	173.72	-177.41	65.75	61.98	177.09	167.70	52.76	52.69	-62.26	-179.76	-63.36
M0005	-1825190.29	0.000	-695177685.00	-36.35	84.26	156.78	35.77	33.48	-87.53	-16.86	-140.01	104.06	-19.09	-175.15	-58.91	65.68	-178.08	-57.67	-173.75	-49.83	65.07	-67.35	176.39	178.36	62.11	-161.78	-45.41
M0010	-1825190.02	0.000	-695177582.00	-36.23	84.30	153.95	33.16	30.73	-90.06	-11.53	-134.53	109.23	-13.76	-178.27	-63.33	62.20	177.14	52.87	-63.45	60.03	174.83	175.62	60.31	60.97	-54.33	177.77	-65.69
M0011	-1825189.79	0.000	-695177496.00	-36.84	84.03	160.38	39.09	36.93	-84.35	-22.21	-145.35	99.11	-24.03	52.09	167.72	-66.02	49.61	179.18	62.39	171.24	-73.21	51.63	-63.57	-63.46	-178.66	51.16	167.37
M0068	-1825189.72	0.000	-695177466.00	-36.78	84.04	160.30	38.93	36.83	-84.54	-23.00	-145.85	98.20	-24.65	-56.44	58.60	-175.70	-60.66	-61.16	-177.32	-44.33	69.90	54.41	-59.50	-59.64	-173.55	67.47	-177.12
M0041	-1825189.69	0.000	-695177454.00	-35.48	85.38	162.28	40.82	38.86	-82.60	-27.24	-150.21	94.12	-28.85	60.53	175.80	-57.91	57.36	-170.02	72.51	74.33	-170.45	-175.88	69.46	69.20	-45.46	76.76	-167.30
M0025	-1825187.98	0.000	-695176804.00	-36.50	84.22	159.23	38.00	35.87	-85.35	-20.55	-143.34	100.47	-22.33	70.70	-174.95	-46.99	67.36	-70.58	173.27	-177.62	-62.67	59.08	-55.92	-56.15	-171.16	66.23	-177.34
M0060	-1825182.90	0.000	-695174871.00	-34.99	85.55	159.83	38.62	36.61	-84.60	-23.22	-146.12	97.83	-25.07	66.45	-178.99	-50.98	63.58	-79.08	164.31	176.46	-67.96	57.63	-57.16	-58.39	-173.18	-140.28	-24.72
M0046	-1825182.77	0.000	-695174822.00	-36.75	84.07	160.43	39.01	36.99	-84.43	-23.10	-146.04	98.14	-24.79	-52.03	62.99	-170.87	-55.86	-56.60	-172.88	-62.65	51.54	-179.94	66.24	65.67	-48.16	-164.14	136.07
M0059	-1825182.24	0.000	-695174618.00	-0.01	118.75	100.30	-21.44	-21.58	-143.32	37.66	-86.42	158.43	34.34	54.65	170.19	-63.41	52.12	179.29	62.53	168.90	-75.27	49.39	-65.77	-65.90	178.94	48.58	164.58
M0030	-1825178.91	0.000	-695173851.00	-35.60	85.00	159.34	38.07	36.02	-85.25	-21.86	-144.95	99.34	-23.74	176.24	-67.93	56.87	172.80	-65.23	178.61	-58.58	55.37	-178.00	68.13	68.27	-45.90	168.03	-76.80
M0086	-1825170.56	0.000	-695170171.00	-34.00	86.10	153.59	32.83	30.67	-90.09	-13.38	-136.35	106.76	-16.01	-72.53	40.57	169.46	-77.44	68.48	-45.82	-70.60	43.90	-70.63	173.45	174.99	59.07	-139.40	-22.32

Table S-V. Calculated vicinal coupling constants (from H-1 to H-6') for every conformer of **4a**/**4b**

boltzman	1 -2r	1 -2s	2r - 3r	2r - 3s	2s - 3r	2s - 3s	3r - 4r	3r - 4s	3s - 4r	3s - 4s	1'r - 2'r	1'r - 2's	1's - 2'r	1's - 2's	2'r-3'	2's-3'	3'-4'r	3'-4's	4'r - 5'r	4'r - 5's	4's - 5'r	4's - 5's	5'r - 6'	5's - 6'
0.206	7.76	1.99	11.76	7.34	7.65	1.99	9.54	9.73	2.34	9.32	4.19	12.86	4.01	4.74	12.98	3.85	12.94	2.95	4.09	12.92	12.89	2.82	10.38	6.79
0.149	7.74	1.99	11.74	7.34	7.67	1.99	9.59	9.65	2.37	9.37	12.90	2.79	4.79	12.68	13.00	3.67	13.00	3.41	4.25	12.89	12.85	2.73	10.20	7.08
0.123	7.74	1.99	11.64	7.47	7.80	1.98	9.76	9.38	2.47	9.55	12.84	2.66	5.01	12.57	12.88	4.44	3.53	13.00	2.68	12.83	12.86	4.33	7.05	10.21
0.121	7.70	2.00	11.75	7.34	7.66	1.99	9.61	9.63	2.38	9.39	4.07	12.90	4.12	4.62	13.00	3.57	13.00	3.37	3.91	12.96	12.93	2.95	8.16	9.39
0.118	7.74	1.99	11.75	7.33	7.66	1.99	9.59	9.66	2.37	9.37	12.90	2.82	4.75	12.69	12.97	3.93	12.95	3.00	3.83	12.97	12.96	3.04	7.03	10.23
0.046	7.72	2.00	11.70	7.40	7.73	1.99	9.66	9.54	2.40	9.44	4.23	12.85	3.96	4.80	13.00	3.67	13.00	3.46	4.28	4.43	4.43	12.79	4.24	11.20
0.044	7.59	2.01	11.64	7.47	7.81	1.98	9.85	9.19	2.53	9.67	5.07	3.66	12.79	4.49	3.98	12.96	12.98	3.79	4.24	12.89	12.85	2.73	10.98	5.52
0.022	7.75	1.99	11.80	7.28	7.61	2.00	9.50	9.79	2.32	9.28	12.77	4.49	2.91	12.94	4.35	12.88	5.12	3.68	3.50	13.00	12.99	3.25	7.39	9.97
0.022	7.58	2.01	11.36	7.76	8.14	1.98	10.26	8.45	2.87	10.06	3.93	4.89	13.00	3.38	11.01	1.99	2.26	12.47	3.56	12.99	12.99	3.22	6.92	10.27
0.021	7.69	2.00	11.80	7.28	7.59	2.00	9.51	9.77	2.33	9.29	4.15	12.87	4.03	4.71	13.00	3.60	12.99	3.64	4.15	4.62	4.52	12.74	8.76	8.76
0.018	7.77	1.99	11.79	7.30	7.60	2.00	9.46	9.84	2.31	9.25	12.89	2.79	4.78	12.69	12.90	4.38	3.89	12.95	12.73	4.60	4.61	4.10	11.19	4.13
0.017	7.67	2.00	11.59	7.51	7.87	1.98	9.87	9.18	2.55	9.67	2.30	7.42	12.27	2.10	12.99	3.64	12.98	3.68	4.28	12.88	12.83	2.70	9.36	8.21
0.016	7.68	2.00	11.71	7.39	7.74	1.99	9.71	9.48	2.44	9.49	12.87	2.72	4.90	12.63	12.98	3.86	13.00	3.34	4.36	4.35	4.34	12.82	4.39	11.20
0.013	7.77	1.99	11.72	7.37	7.70	1.99	9.60	9.64	2.37	9.38	12.92	2.85	4.68	12.72	13.00	3.55	12.98	3.72	4.17	4.61	4.49	12.75	8.67	8.83
0.010	7.65	2.00	11.78	7.31	7.63	1.99	9.57	9.68	2.35	9.35	3.30	13.00	4.86	3.93	12.31	2.25	3.50	13.00	12.42	5.19	5.31	3.56	7.32	9.97
0.010	7.67	2.00	11.89	7.17	7.48	2.01	9.35	9.97	2.25	9.14	4.89	3.86	12.84	4.27	4.83	12.70	4.60	4.12	2.93	12.92	12.96	3.94	7.19	10.11
0.009	7.75	1.99	11.81	7.27	7.59	2.00	9.47	9.83	2.30	9.25	12.50	5.13	2.56	12.78	4.00	12.96	12.90	4.25	4.20	4.56	4.47	12.76	8.30	9.21
0.006	7.63	2.00	11.72	7.37	7.70	1.99	9.67	9.54	2.41	9.45	2.23	12.53	6.96	2.55	3.97	12.94	4.57	4.07	3.45	13.00	13.00	3.49	6.02	10.84
0.006	7.63	2.01	11.64	7.46	7.80	1.98	9.83	9.28	2.51	9.61	3.52	12.98	4.77	4.08	1.98	11.33	12.89	2.80	4.39	4.30	4.20	12.87	4.34	11.20
0.005	7.63	2.01	10.71	8.42	8.77	2.04	10.78	7.05	3.76	10.66	3.66	5.08	12.98	3.12	2.33	12.49	12.85	2.74	3.41	13.00	13.00	3.34	8.89	8.67
0.004	11.00	4.76	2.51	9.77	9.73	9.19	7.59	1.98	11.47	8.14	3.95	12.93	4.24	4.50	12.96	3.20	4.30	4.39	3.36	13.00	13.00	3.44	9.18	8.37
0.003	7.71	2.00	11.68	7.42	7.76	1.98	9.73	9.44	2.45	9.51	12.99	3.60	3.75	12.97	4.17	4.35	12.96	3.07	4.53	4.18	4.17	12.87	4.36	11.20
0.002	10.99	4.56	2.60	9.89	9.85	8.98	7.67	1.98	11.39	8.23	12.86	2.69	4.95	12.59	12.89	4.42	3.85	12.96	12.72	4.57	4.69	4.09	9.09	8.41
0.001	7.57	2.01	11.38	7.74	8.12	1.98	10.23	8.54	2.85	10.03	4.01	4.80	13.00	3.43	10.50	2.05	2.65	12.82	12.90	4.02	4.11	4.65	9.02	8.45
0.001	7.82	1.99	11.17	7.97	8.32	1.98	10.29	8.41	2.90	10.08	3.94	12.92	4.21	4.54	12.92	3.01	2.85	12.92	12.86	4.24	4.20	4.48	10.88	5.82
0.001	7.40	2.04	10.88	8.25	8.65	2.02	10.78	7.16	3.79	10.63	3.60	5.21	12.98	3.07	2.29	12.44	12.68	2.46	6.22	2.88	2.88	12.94	6.85	10.27
0.001	11.00	4.69	2.52	9.77	9.73	9.20	7.55	1.98	11.51	8.08	4.61	4.12	12.92	3.99	4.43	12.85	4.70	4.02	3.36	13.00	13.00	3.45	9.71	7.79
0.001	7.75	1.99	11.62	7.50	7.82	1.98	9.79	9.35	2.49	9.57	2.50	12.80	6.41	2.84	2.37	12.58	12.95	2.95	4.40	4.33	4.21	12.86	7.87	9.54
0.001	7.63	2.00	11.81	7.26	7.59	2.00	9.52	9.73	2.33	9.32	4.38	4.29	12.96	3.83	2.71	12.81	10.10	2.18	12.96	3.72	3.74	5.11	8.25	9.26
0.001	7.71	2.00	11.52	7.60	7.96	1.98	9.97	9.06	2.62	9.75	5.43	3.56	12.61	4.69	3.95	12.93	5.00	3.79	3.51	13.00	12.99	3.28	9.90	7.50
0.000	7.67	2.00	11.48	7.64	8.00	1.98	10.07	8.85	2.71	9.87	12.82	2.68	4.88	12.68	2.09	12.04	11.92	2.03	5.93	3.02	3.04	12.97	6.77	10.38
0.000	7.61	2.01	10.86	8.28	8.64	2.02	10.73	7.34	3.62	10.56	4.67	4.03	12.90	4.08	3.40	13.00	12.96	3.90	4.71	4.05	3.99	12.91	10.56	6.42
0.000	7.63	2.00	11.83	7.26	7.58	2.00	9.57	9.65	2.35	9.36	2.51	6.95	12.48	2.22	4.63	3.96	12.96	2.95	3.75	12.99	12.96	3.07	9.92	7.51
0.000	10.91	3.97	2.91	10.22	10.17	8.38	7.86	1.99	11.22	8.42	3.34	5.62	12.95	2.89	12.31	2.20	12.92	4.07	4.31	4.44	4.35	12.80	8.50	9.03
0.000	7.60	2.01	11.57	7.52	7.89	1.98	9.94	9.03	2.60	9.76	2.86	6.35	12.77	2.47	3.91	4.72	13.00	3.41	4.36	4.37	4.35	12.81	4.08	11.19
0.000	7.69	2.00	11.88	7.18	7.48	2.01	9.41	9.93	2.27	9.16	5.27	3.53	12.69	4.68	5.18	12.55	4.40	4.34	2.58	12.72	12.83	4.56	10.26	7.11
0.000	7.80	1.99	11.71	7.38	7.71	1.99	9.58	9.60	2.36	9.40	3.57	5.19	12.98	3.09	2.55	12.69	8.60	2.84	12.94	3.93	3.85	4.88	10.86	5.87
0.000	7.60	2.01	11.10	8.04	8.41	1.99	10.55	7.82	3.29	10.38	12.48	2.25	5.84	12.12	12.92	4.31	4.17	12.88	12.67	4.74	4.77	3.96	11.20	4.25
0.000	7.78	1.99	11.68	7.42	7.75	1.98	9.71	9.51	2.44	9.47	12.97	3.16	4.35	12.87	12.98	3.28	3.74	12.97	12.52	5.06	5.07	3.70	11.20	4.33
0.000	7.68	2.00	11.36	7.77	8.12	1.98	10.20	8.64	2.83	9.99	12.92	4.15	3.28	12.99	4.33	12.88	5.52	3.36	3.10	12.96	12.99	3.72	10.36	6.84
0.000	7.70	2.00	10.97	8.17	8.53	2.00	10.62	7.62	3.41	10.46	12.99	3.57	3.71	12.97	5.04	3.55	4.00	12.91	12.94	3.96	3.87	4.82	11.19	4.06
0.000	7.60	2.00	11.81	7.25	7.59	2.00	9.65	9.59	2.41	9.43	5.16	12.52	3.25	5.55	13.00	3.68	12.76	2.55	5.23	3.54	3.55	12.99	5.98	10.80
0.000	7.61	2.00	11.81	7.27	7.61	2.00	9.55	9.68	2.35	9.35	4.50	4.19	12.94	3.91	3.84	12.98	6.40	2.84	4.81	4.07	4.05	12.87	3.86	11.18
0.000	7.82	1.98	12.03	6.97	7.28	2.04	9.02	10.40	2.12	8.80	3.93	12.94	4.29	4.37	12.68	2.60	2.46	12.71	12.95	2.88	2.91	6.22	3.05	10.78
0.000	7.66	2.00	11.68	7.42	7.76	1.98	9.83	9.24	2.51	9.63	2.76	12.92	5.97	3.10	2.77	12.86	12.98	3.65	4.13	4.58	4.55	12.75	4.00	11.18
0.000	7.89	1.98	11.75	7.32	7.64	1.99	9.53	9.72	2.32	9.30	3.20	13.00	5.33	3.53	2.17	12.23	12.96	3.03	4.33	4.40	4.22	12.85	7.69	9.70
0.000	7.62	2.00	11.82	7.26	7.58	2.00	9.54	9.71	2.34	9.33	5.17	3.61	12.74	4.59	4.48	12.84	3.65	5.25	13.00	3.22	3.29	5.78	10.94	7.06
0.000	11.00	4.79	2.50	9.73	9.72	9.23	7.48	1.98	11.58	7.99	4.77	12.70	3.56	5.16	13.00	3.67	12.61	2.39	5.59	3.27	3.26	13.00	6.36	10.59
0.000	7.80	1.99	11.69	7.41	7.73	1.99	9.69	9.52	2.43	9.46	12.95	3.04	4.43	12.84	3.34	12.99	4.20	4.66	12.99	3.02	3.00	6.20	10.83	3.05
0.000	8.04	1.98	10.92	8.22	8.54	2.00	10.48	7.96	3.12	10.28	2.60	7.01	12.65	2.26	2.98	6.16	2.77	6.47	2.77	12.86	12.92	4.13	7.56	9.96

Table S-VI. The product of multiplying the Boltzman weights and Calculated vicinal coupling constants (from H-1 to H-6') for every conformer of **4a**/**4b**

1 -2r	1 -2s	2r - 3r	2r - 3s	2s - 3r	2s - 3s	3r - 4r	3r - 4s	3s - 4r	3s - 4s	1'r - 2'r	1'r - 2's	1's - 2'r	1's - 2's	2'r-3'	2's-3'	3'-4'r	3'-4's	4'r - 5'r	4'r - 5's	4's - 5'r	4's - 5's	5'r - 6'	5's - 6'
1.60	0.41	2.42	1.51	1.58	0.41	1.96	2.00	0.48	1.92	0.86	2.65	0.83	0.98	2.67	0.79	2.67	0.61	0.84	2.66	2.66	0.58	2.14	1.40
1.15	0.30	1.75	1.09	1.14	0.30	1.43	1.44	0.35	1.40	1.92	0.42	0.71	1.89	1.94	0.55	1.94	0.51	0.63	1.92	1.91	0.41	1.52	1.06
0.95	0.25	1.43	0.92	0.96	0.24	1.20	1.15	0.30	1.17	1.58	0.33	0.62	1.55	1.58	0.55	0.43	1.60	0.33	1.58	1.58	0.53	0.87	1.26
0.93	0.24	1.42	0.89	0.93	0.24	1.16	1.16	0.29	1.14	0.49	1.56	0.50	0.56	1.57	0.43	1.57	0.41	0.47	1.57	1.57	0.36	0.99	1.14
0.91	0.24	1.39	0.87	0.90	0.23	1.13	1.14	0.28	1.11	1.52	0.33	0.56	1.50	1.53	0.46	1.53	0.35	0.45	1.53	1.53	0.36	0.83	1.21
0.36	0.09	0.54	0.34	0.36	0.09	0.44	0.44	0.11	0.43	0.19	0.59	0.18	0.22	0.60	0.17	0.60	0.16	0.20	0.20	0.20	0.59	0.19	0.52
0.33	0.09	0.51	0.33	0.34	0.09	0.43	0.40	0.11	0.43	0.22	0.16	0.56	0.20	0.18	0.57	0.57	0.17	0.19	0.57	0.57	0.12	0.48	0.24
0.17	0.04	0.26	0.16	0.17	0.04	0.21	0.22	0.05	0.20	0.28	0.10	0.06	0.28	0.10	0.28	0.11	0.08	0.08	0.29	0.29	0.07	0.16	0.22
0.17	0.04	0.25	0.17	0.18	0.04	0.23	0.19	0.06	0.22	0.09	0.11	0.29	0.07	0.24	0.04	0.05	0.27	0.08	0.29	0.29	0.07	0.15	0.23
0.16	0.04	0.25	0.15	0.16	0.04	0.20	0.21	0.05	0.20	0.09	0.27	0.08	0.10	0.27	0.08	0.27	0.08	0.09	0.10	0.09	0.27	0.18	0.18
0.14	0.04	0.21	0.13	0.14	0.04	0.17	0.18	0.04	0.17	0.23	0.05	0.09	0.23	0.23	0.08	0.07	0.23	0.23	0.08	0.08	0.07	0.20	0.07
0.13	0.03	0.20	0.13	0.13	0.03	0.17	0.16	0.04	0.16	0.04	0.13	0.21	0.04	0.22	0.06	0.22	0.06	0.07	0.22	0.22	0.05	0.16	0.14
0.12	0.03	0.19	0.12	0.12	0.03	0.16	0.15	0.04	0.15	0.21	0.04	0.08	0.20	0.21	0.06	0.21	0.05	0.07	0.07	0.07	0.21	0.07	0.18
0.10	0.03	0.15	0.10	0.10	0.03	0.12	0.13	0.03	0.12	0.17	0.04	0.06	0.17	0.17	0.05	0.17	0.05	0.05	0.06	0.06	0.17	0.11	0.11
0.08	0.02	0.12	0.07	0.08	0.02	0.10	0.10	0.02	0.09	0.03	0.13	0.05	0.04	0.12	0.02	0.03	0.13	0.12	0.05	0.05	0.04	0.07	0.10
0.08	0.02	0.12	0.07	0.07	0.02	0.09	0.10	0.02	0.09	0.05	0.04	0.13	0.04	0.05	0.13	0.05	0.04	0.03	0.13	0.13	0.04	0.07	0.10
0.07	0.02	0.11	0.07	0.07	0.02	0.09	0.09	0.02	0.08	0.11	0.05	0.02	0.12	0.04	0.12	0.12	0.04	0.04	0.04	0.04	0.11	0.07	0.08
0.05	0.01	0.07	0.04	0.05	0.01	0.06	0.06	0.01	0.06	0.01	0.08	0.04	0.02	0.02	0.08	0.03	0.02	0.02	0.08	0.08	0.02	0.04	0.07
0.05	0.01	0.07	0.04	0.05	0.01	0.06	0.06	0.02	0.06	0.02	0.08	0.03	0.02	0.01	0.07	0.08	0.02	0.03	0.03	0.03	0.08	0.03	0.07
0.04	0.01	0.05	0.04	0.04	0.01	0.05	0.04	0.02	0.05	0.02	0.03	0.06	0.02	0.01	0.06	0.06	0.01	0.02	0.06	0.06	0.02	0.04	0.04
0.04	0.02	0.01	0.04	0.04	0.04	0.03	0.01	0.05	0.03	0.02	0.05	0.02	0.02	0.05	0.01	0.02	0.02	0.01	0.05	0.05	0.01	0.04	0.03
0.02	0.01	0.04	0.02	0.02	0.01	0.03	0.03	0.01	0.03	0.04	0.01	0.01	0.04	0.01	0.01	0.04	0.01	0.01	0.01	0.01	0.04	0.01	0.03
0.02	0.01	0.01	0.02	0.02	0.02	0.02	0.00	0.02	0.02	0.03	0.01	0.01	0.03	0.03	0.01	0.01	0.03	0.03	0.01	0.01	0.01	0.02	0.02
0.01	0.00	0.01	0.01	0.01	0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.01	0.00	0.01	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.01	0.01
0.01	0.00	0.01	0.01	0.01	0.00	0.01	0.01	0.00	0.01	0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.01	0.01
0.01	0.00	0.01	0.01	0.01	0.00	0.01	0.01	0.00	0.01	0.00	0.01	0.01	0.00	0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.01	0.01	0.01
0.01	0.00	0.00	0.01	0.01	0.01	0.01	0.00	0.01	0.01	0.00	0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.01	0.00	0.01	0.01
0.01	0.00	0.01	0.01	0.01	0.00	0.01	0.01	0.00	0.01	0.00	0.01	0.01	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01
0.01	0.00	0.01	0.01	0.01	0.00	0.01	0.01	0.00	0.01	0.00	0.01	0.01	0.00	0.00	0.01	0.01	0.00	0.00	0.01	0.01	0.00	0.01	0.01
0.01	0.00	0.01	0.01	0.01	0.00	0.01	0.01	0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.01	0.00	0.01	0.01
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table S-VII. Dihedral angles between vicinal hydrogens (from H-1 to H-6') for every conformer of **4c**/**4d**

4a/4b (SR/RS)																											
Label	E (kJ/mol)	energy	boltzman	1 -2r	1 -2s	2r - 3r	2r - 3s	2s - 3r	2s - 3s	3r - 4r	3r - 4s	3s - 4r	3s - 4s	1'r - 2'r	1'r - 2's	1's - 2'r	1's - 2's	2'r-3'	2's-3'	3'-4'r	3'-4's	4'r - 5'r	4'r - 5's	4's - 5'r	4's - 5's	5'r - 6'	5's - 6'
M0082	-1825218.06	-695188263.00	0.145	34001.00	122.01	97.12	-24.50	-24.74	-146.36	38.18	-85.55	159.06	35.33	-56.63	58.28	-175.41	-60.50	-63.63	-179.95	66.49	-178.14	-70.23	173.56	174.90	58.70	53.59	169.99
M0018	-1825217.79	-695188158.00	0.130	-37.48	83.52	159.27	38.01	35.82	-85.43	-21.08	-143.47	99.97	-22.41	178.12	-67.32	58.38	172.94	177.44	61.22	-59.90	54.54	-63.68	179.77	-177.91	65.54	-171.68	-55.33
M0027	-1825217.38	-695188001.00	0.110	-37.48	83.53	159.29	38.04	35.84	-85.41	-21.04	-143.37	100.03	-22.30	178.50	-66.92	58.80	173.38	177.71	61.48	-61.36	53.10	-66.82	176.68	178.96	62.46	53.89	170.12
M0015	-1825216.90	-695187818.00	0.090	-5.26	113.89	104.29	-16.97	-17.54	-138.81	35.01	-88.70	155.49	31.77	59.75	174.31	-58.93	55.63	-178.83	65.20	63.35	179.30	-70.46	173.33	174.61	58.40	55.85	172.31
M0017	-1825214.95	-695187077.00	0.041	-37.66	83.37	157.99	36.87	34.64	-86.48	-18.56	-140.96	102.42	-19.99	-52.57	61.70	-170.96	-56.69	-60.94	-176.69	178.30	-66.60	-58.63	-174.91	-173.42	70.30	-172.06	-55.64
M0021	-1825214.58	-695186938.00	0.036	-37.72	83.33	157.53	36.49	34.12	-86.91	-17.75	-140.14	103.18	-19.20	-172.52	-57.40	67.88	-177.00	-64.79	178.59	176.12	-68.79	-59.58	-175.84	-174.47	69.27	-172.04	-55.60
M0020	-1825214.55	-695186926.00	0.035	-37.74	83.31	157.91	36.79	34.49	-86.63	-18.24	-140.64	102.74	-19.66	-172.40	-57.30	67.97	-176.93	-63.99	179.40	177.03	-67.90	-59.17	-175.44	-174.05	69.68	-172.03	-55.58
M0072	-1825214.19	-695186786.00	0.030	-37.49	83.53	158.76	37.37	35.34	-85.85	-20.18	-142.54	100.85	-21.51	-175.64	-61.58	64.13	178.19	61.08	-54.45	-177.74	-63.10	53.43	-61.60	-60.80	-175.83	68.59	-175.14
M0030	-1825214.02	-695186723.00	0.028	-37.86	83.22	158.60	37.43	35.17	-86.00	-19.23	-141.64	101.78	-20.63	177.21	-67.88	57.53	172.43	-176.05	68.18	63.74	179.45	-70.54	173.24	174.70	58.47	55.32	171.79
M0025	-1825213.94	-695186692.00	0.027	-37.74	83.30	157.76	36.69	34.35	-86.72	-18.02	-140.39	102.92	-19.45	-172.95	-57.88	67.47	-177.46	-66.40	177.01	174.10	-70.73	-62.52	-178.79	-177.44	66.29	56.96	173.40
M0081	-1825213.91	-695186680.00	0.027	-37.40	83.58	158.90	37.70	35.48	-85.72	-20.51	-142.85	100.51	-21.82	-176.37	-62.29	63.43	177.52	60.70	-54.81	-177.72	-63.08	53.40	-61.63	-60.81	-175.85	68.80	-174.94
M0086	-1825213.84	-695186656.00	0.026	-7.00	112.14	105.97	-15.20	-15.85	-137.02	34.03	-89.68	154.45	30.75	60.90	175.30	-57.81	56.59	176.27	60.36	-59.74	54.54	-63.58	179.91	-177.89	65.60	-172.63	-56.43
M0003	-1825213.83	-695186649.00	0.026	-37.32	83.65	159.28	38.00	35.89	-85.39	-21.24	-143.65	99.84	-22.57	178.26	-67.01	58.26	173.00	178.04	61.95	149.08	-95.56	-65.79	178.36	179.89	64.04	-171.56	-55.30
M0078	-1825213.34	-695186465.00	0.022	-4.52	114.66	103.56	-17.71	-18.28	-139.55	35.36	-88.31	155.87	32.21	-171.31	-56.56	68.82	-176.43	-64.08	179.40	68.54	-176.44	176.04	61.10	61.42	-53.52	177.64	-66.24
M0089	-1825213.05	-695186354.00	0.019	-0.79	118.29	100.26	-21.18	-21.55	-142.99	36.87	-86.83	157.55	33.86	-58.32	56.58	-177.05	-62.16	-68.52	174.43	-56.92	57.77	-63.62	179.82	-178.27	65.17	-172.12	-55.80
M0070	-1825212.83	-695186270.00	0.018	-7.76	111.40	106.78	-14.38	-15.06	-136.22	33.56	-90.10	153.96	30.30	178.65	-66.69	58.71	173.37	-174.25	69.34	67.10	-177.52	175.08	60.10	60.70	-54.29	176.20	-67.58
M0042	-1825212.20	-695186031.00	0.014	-36.52	84.45	160.31	38.94	36.90	-84.47	-23.33	-145.81	97.80	-24.68	-176.86	-62.03	63.86	178.69	179.19	62.71	-62.79	51.64	-64.92	178.48	-179.15	64.25	57.37	173.84
M0060	-1825211.94	-695185929.00	0.012	-37.72	83.33	157.42	36.34	34.04	-87.04	-17.52	-139.90	103.40	-18.98	-174.02	-58.87	66.41	-178.44	-67.81	175.99	66.79	-178.16	174.95	60.00	60.29	-54.65	176.00	-67.77
M0031	-1825211.86	-695185899.00	0.012	-4.62	114.54	103.86	-17.43	-17.93	-139.22	34.95	-88.70	155.48	31.83	-68.17	45.94	173.93	-71.96	-166.93	77.18	70.63	-173.87	-66.80	176.84	177.82	61.45	-174.47	-58.10
M0050	-1825211.75	-695185858.00	0.011	-37.67	83.35	157.52	36.46	34.14	-86.92	-17.61	-139.97	103.32	-19.04	-172.94	-57.83	67.46	-177.44	-65.58	177.80	175.52	-69.61	54.11	-60.86	-60.45	-173.42	66.52	-177.36
M0034	-1825211.67	-695185827.00	0.011	-37.75	83.29	157.91	36.78	34.53	-86.59	-18.26	-140.63	102.70	-19.67	-173.29	-58.24	67.14	-177.81	-66.28	177.09	174.95	-70.17	53.58	-61.39	-60.98	-175.95	65.60	-178.29
M0046	-1825211.58	-695185794.00	0.011	-37.75	83.30	157.76	36.68	34.37	-86.71	-18.01	-140.40	102.94	-19.45	177.47	-67.67	57.83	172.70	-174.88	69.29	65.66	-178.92	174.51	59.56	60.13	-54.82	175.50	-68.26
M0066	-1825211.53	-695185774.00	0.010	-37.70	83.34	157.91	36.80	34.53	-86.57	-18.34	-140.75	102.62	-19.80	-56.71	57.68	-175.09	-60.69	-70.03	173.91	-56.73	57.96	-63.62	179.81	-178.23	65.19	-172.36	-55.98
M0051	-1825211.41	-695185729.00	0.010	-37.56	83.46	158.84	37.64	35.41	-85.78	-20.24	-142.61	100.78	-21.59	179.21	-66.12	59.18	173.85	178.89	62.74	146.21	-98.59	47.83	-67.69	-66.22	178.26	64.15	-179.60
M0062	-1825211.31	-695185692.00	0.010	-37.79	83.28	157.71	36.61	34.30	-86.80	-17.81	-140.23	103.12	-19.30	-176.46	-61.24	64.13	179.34	-71.92	171.26	-58.64	56.16	-66.06	177.36	179.15	62.57	55.32	171.75
M0033	-1825211.29	-695185684.00	0.009	-19.46	100.00	120.66	0.07	-1.37	-121.96	23.79	-99.50	143.80	20.50	-54.03	60.38	-172.39	-57.98	-63.50	-178.81	69.24	-175.36	-67.07	176.72	178.06	61.85	-173.44	-56.96
M0035	-1825211.27	-695185675.00	0.009	-10.15	108.98	108.40	-11.63	-12.38	-133.41	31.92	-91.65	152.21	28.64	67.82	-178.74	-50.28	63.16	53.74	-61.14	-178.08	-62.45	-57.88	-174.26	-178.57	70.05	179.99	-63.10
M0069	-1825211.05	-695185592.00	0.009	-37.71	83.35	158.41	37.26	35.00	-86.15	-19.16	-141.54	101.84	-20.54	177.48	-67.74	58.05	172.83	177.76	62.11	-60.08	54.32	-64.02	179.44	-178.21	65.24	-171.96	-55.64
M0040	-1825210.94	-695185548.00	0.008	-37.73	83.34	157.92	36.82	34.51	-86.60	-18.29	-140.69	102.66	-19.73	178.54	-66.64	59.14	173.96	178.51	62.83	-61.12	53.29	-66.43	177.05	179.37	62.85	56.61	172.91
M0016	-1825210.43	-695185357.00	0.007	-9.25	110.00	108.42	-12.63	-13.44	-134.49	32.60	-91.08	152.93	29.25	-53.09	61.20	-171.48	-57.18	-60.86	-176.61	178.21	-66.69	-58.73	-175.02	-179.51	70.20	-172.35	-55.93
M0058	-1825209.90	-695185156.00	0.005	-37.37	83.68	158.90	37.73	35.58	-85.60	-20.42	-142.83	100.63	-21.78	65.70	-179.61	-53.16	61.53	-177.52	66.14	127.74	-116.66	46.67	-69.04	-67.30	176.99	60.40	177.13
M0004	-1825209.66	-695185062.00	0.005	-37.68	83.35	157.32	36.30	33.90	-87.13	-17.30	-139.69	103.62	-18.78	-177.06	-62.67	63.02	177.41	61.03	-54.21	-177.89	-62.91	-61.22	-177.40	-175.87	67.95	55.64	172.09
M0006	-1825209.64	-695185056.00	0.005	-37.70	83.36	158.18	37.04	34.75	-86.39	-18.72	-141.11	102.26	-20.13	-176.84	-62.46	63.25	177.63	61.20	-54.00	-177.82	-62.84	-61.36	-177.54	-176.01	67.80	56.19	172.68
M0028	-1825209.21	-695184889.00	0.004	-37.56	120.22	99.00	-22.52	-22.84	-144.36	37.46	-86.31	158.17	34.40	-175.74	-60.47	64.92	-179.81	-67.17	175.93	67.39	-177.29	-67.29	176.41	177.66	61.36	-173.33	-56.85
M0012	-1825209.06	-695184836.00	0.004	-37.66	83.42	158.24	37.11	34.80	-86.32	-18.83	-141.23	102.15	-20.25	-177.53	-62.80	62.48	177.22	57.86	-57.60	70.57	-173.49	-68.40	175.32	176.68	60.59	55.56	172.08
M0029	-1825208.76	-695184719.00	0.003	-1.77	117.32	101.55	-19.84	-20.27	-141.66	36.26	-87.49	156.84	33.10	173.92	-70.95	54.58	169.71	-178.04	65.28	63.13	178.77	-71.39	172.41	173.88	57.67	54.66	171.08
M0009	-1825208.50	-695184619.00	0.003	-37.73	120.71	98.63	-22.93	-23.22	-144.77	37.63	-86.14	158.36	34.59	-174.01	-58.77	66.66	-178.10	-63.31	179.33	177.70	-67.22	-58.65	-174.86	-178.54	70.25	-171.21	-54.83
M0023	-1825208.39	-695184580.00	0.003	-0.18	118.91	100.08	-21.39	-21.75	-143.22	36.99	-86.77	157.64	33.88	174.70	-70.21	55.32	170.41	-176.76	66.54	64.87	-179.47	-68.86	174.87	176.37	60.10	-173.70	-57.17
M0022	-1825208.35	-695184562.00	0.003	0.32	119.42	99.62	-21.86	-22.22	-143.70	37.20	-86.57	157.89	34.12	174.68	-70.23	55.30	170.39	-177.08	66.22	64.36	-179.98	-69.01	174.72	176.22	59.95	-173.90	-57.37
M0013	-1825208.10	-695184468.00	0.003	-1.24	117.83	101.13	-20.31	-20.69	-142.13	36.52	-87.25	157.14	33.37	-178.61	-63.45	62.29	177.45	-74.12	168.55	169.23	-75.41	-65.51	178.44	179.52	63.47	54.32	170.66
M0005	-1825206.91	-695184013.00	0.002	-37.03	121.38	97.94	-23.62	-23.90	-145.46	37.87	-85.96	158.61	34.78	-176.85	-62.02	63.88	178.71	179.28	62.78	-62.75	51.68	-64.97	178.45	-179.18	64.23	57.10	173.56
M0039	-1825206.32	-695183791.00	0.001	-37.72	83.31	157.66	36.58	34.26	-86.82	-17.76	-140.15	103.18	-19.22	-176.59	-62.07	63.46	177.97	61.11	-53.97	-177.32	-62.67	54.23	-60.66	-60.01	-174.89	70.64	-173.14
M0064	-1825206.24	-695183758.00	0.001	-7.19	111.95	106.33	-14.83	-15.52	-136.68	33.94	-89.80	154.36	30.62	-56.98	57.47	-175.36,	-60.64,	-69.88,	175.84,	57.56	57.12,	-65.62,	177.60,	179.55,	63.88,	56.21,	171.66,
M0026	-1825206.13	-695183719.00	0.001	0.66	119.73	99.50	-22.00	-22.32	-143.83	37.25	-86.54	157.93	34.14	-176.94	-61.94	63.95	178.95	-76.19	166.55	168.92	-75.85	48.71	-66.52	-66.14	178.63	57.87	173.76
M0068	-1825206.08	-695183698.00	0.001	0.70	119.81	99.38	-22.11	-22.46	-143.95	37.25	-86.53	157.93	34.15	178.95	-66.13	59.74	174.66	178.16	61.59	-61.43	52.98	-64.62	178.78	-178.80	64.60	-170.89	-54.50
M0067	-1825205.59	-695183512.00	0.001	1.00	120.10	99.13	-22.38	-22.72	-144.23	37.35	-86.43	158.04	34.27	179.46	-65.65	60.22	175.11	178.35	61.79	-61.42	52.98	-64.67	178.73	-178.86	64.54	-171.02	-54.65
M0057	-1825205.07	-695183313.00	0.001	-37.03	83.98	158.59	37.39	35.15	-86.04	-20.08	-142.59	100.91	-21.39	-176.86	-61.45	63.37	178.79	62.74	-52.44	-173.30	-58.77	55.71	-59.16	-58.55	-173.42	70.19	-173.60
M0002	-1825205.00	-695183285.00	0.001	-37.03	83.97	158.89	37.66	35.49	-85.74	-20.64	-143.13	100.36	-22.13	-176.44	-61.01	63.81	179.25	62.95	-52.26	-173.27	-58.74	55.66	-59.20	-58.60	-173.46	70.06	-173.74
M0036	-1825201.07	-695181791.00	0.000	-0.66	118.41	100.71	-20.72	-20.96	-142.39	36.59	-87.15	157.23	33.48	63.30	178.19	-54.75	60.13	-179.48	64.17	137.42	-107.22	44.61	-71.34	-69.44	174.61	59.49	176.10
M0079	-1825197.90	-695180582.00	0.000	-37.46	83.54	157.74	36.64	34.39	-86.71	-18.13	-140.51	102.81	-19.57	-179.69	-64.52	60.37	175.54	56.95	-58.59	176.04	-69.79	-172.74	73.15	73.43	-60.69	163.64	-60.67
M0061	-1825196.99	-695180237.00	0.000	-37.25	83.77	157.70	36.59	34.34	-86.77	-18.21	-140.68	102.73	-19.74	173.57	-72.04	53.68	168.07	38.04	-76.77	-58.26	55.69	-67.99	174.93	177.73	60.65	60.85	177.40

Table S-VIII. Calculated vicinal coupling constants (from H-1 to H-6') for every conformer of **4c**/**4d**

bolatzman	1 -2r	1 -2s	2r - 3r	2r - 3s	2s - 3r	2s - 3s	3r - 4r	3r - 4s	3s - 4r	3s - 4s	1'r - 2'r	1'r - 2's	1's - 2'r	1's - 2's	2'r-3'	2's-3'	3'-4'r	3'-4's	4'r - 5'r	4'r - 5's	4's - 5'r	4's - 5's	5'r - 6'	5's - 6'
0.145	11.89	5.34	2.28	9.37	9.34	9.76	7.39	1.98	11.66	7.84	4.48	4.24	12.93	3.93	3.53	13.00	3.19	12.99	2.81	12.87	12.92	4.18	5.63	10.94
0.130	7.50	2.01	11.68	7.42	7.76	1.98	9.77	9.26	2.47	9.62	12.99	3.10	4.22	12.84	12.98	3.84	4.01	4.79	3.52	13.00	12.99	3.30	11.02	5.38
0.110	7.50	2.01	11.68	7.42	7.76	1.98	9.78	9.24	2.48	9.63	12.99	3.14	4.17	12.86	12.98	3.80	3.82	5.00	3.16	12.96	13.00	3.68	5.39	10.95
0.090	10.92	4.05	2.86	10.19	10.14	8.42	7.89	1.98	11.19	8.38	4.03	12.90	4.15	4.62	13.00	3.34	3.56	13.00	2.78	12.86	12.91	4.22	5.31	11.05
0.041	7.48	2.02	11.52	7.60	7.95	1.98	10.04	8.81	2.68	9.89	5.09	3.77	12.74	4.47	3.87	12.96	12.99	3.18	4.19	12.92	12.86	2.80	11.04	5.34
0.036	7.47	2.02	11.46	7.66	8.03	1.98	10.12	8.66	2.75	9.97	12.82	4.36	3.04	12.97	3.39	12.99	12.95	2.95	4.06	12.94	12.90	2.90	11.04	5.35
0.035	7.46	2.02	11.51	7.61	7.97	1.98	10.07	8.75	2.71	9.93	12.82	4.38	3.03	12.97	3.48	13.00	12.97	3.04	4.11	12.93	12.89	2.86	11.03	5.35
0.030	7.50	2.01	11.62	7.49	7.84	1.98	9.87	9.09	2.54	9.73	12.94	3.79	3.47	12.99	3.85	4.80	12.98	3.59	4.95	3.79	3.89	12.94	3.75	11.14
0.028	7.44	2.02	11.60	7.51	7.86	1.98	9.97	8.93	2.62	9.82	12.98	3.04	4.35	12.82	12.95	3.01	3.52	13.00	2.78	12.85	12.91	4.21	5.38	11.02
0.027	7.46	2.02	11.49	7.63	7.99	1.98	10.09	8.71	2.72	9.95	12.84	4.30	3.09	12.98	3.20	12.97	12.89	2.76	3.67	13.00	12.98	3.21	5.16	11.09
0.027	7.52	2.01	11.64	7.47	7.82	1.98	9.84	9.15	2.52	9.69	12.96	3.70	3.55	12.98	3.91	4.74	12.98	3.60	4.96	3.78	3.89	12.95	3.72	11.13
0.026	10.86	3.80	3.03	10.35	10.29	8.08	8.04	1.99	11.04	8.53	3.88	12.93	4.31	4.48	12.96	3.95	4.04	4.79	3.53	13.00	12.99	3.29	11.06	5.23
0.026	7.53	2.01	11.68	7.42	7.75	1.98	9.76	9.29	2.46	9.60	12.99	3.13	4.24	12.84	12.99	3.74	10.22	2.19	3.27	12.99	13.00	3.48	11.01	5.39
0.022	10.94	4.16	2.78	10.12	10.07	8.55	7.84	1.98	11.24	8.31	12.76	4.49	2.94	12.96	3.47	13.00	2.97	12.96	12.95	3.85	3.81	4.94	11.19	4.00
0.019	11.00	4.72	2.50	9.76	9.72	9.18	7.60	1.98	11.47	8.07	4.23	4.48	12.97	3.71	2.97	12.90	4.43	4.31	3.53	13.00	12.99	3.34	11.04	5.32
0.018	10.83	3.70	3.12	10.41	10.36	7.93	8.11	2.00	10.97	8.59	12.99	3.17	4.18	12.86	12.89	2.89	3.13	12.98	12.92	3.99	3.91	4.82	11.16	3.85
0.014	7.65	2.00	11.81	7.27	7.60	2.00	9.51	9.67	2.32	9.35	12.97	3.73	3.50	12.99	13.00	3.64	3.63	5.23	3.37	12.99	13.00	3.45	5.10	11.10
0.012	7.47	2.02	11.45	7.68	8.04	1.98	10.14	8.62	2.77	10.00	12.89	4.16	3.20	12.99	3.05	12.95	3.16	12.99	12.92	4.00	3.96	4.77	11.16	3.83
0.012	10.94	4.14	2.81	10.15	10.10	8.49	7.90	1.98	11.19	8.37	3.01	6.14	12.88	2.65	12.46	2.27	2.77	12.88	3.16	12.97	12.98	3.81	11.12	5.00
0.011	7.47	2.02	11.46	7.66	8.02	1.98	10.13	8.63	2.76	9.99	12.84	4.30	3.09	12.98	3.30	12.98	12.94	2.87	4.85	3.88	3.94	12.93	3.97	11.18
0.011	7.46	2.02	11.51	7.61	7.96	1.98	10.07	8.75	2.70	9.93	12.86	4.24	3.12	12.98	3.22	12.97	12.92	2.81	4.93	3.81	3.87	12.95	4.07	11.19
0.011	7.46	2.02	11.49	7.63	7.99	1.98	10.09	8.71	2.73	9.95	12.98	3.06	4.30	12.83	12.92	2.90	3.29	13.00	12.90	4.06	3.98	4.74	11.15	3.78
0.010	7.47	2.02	11.51	7.61	7.96	1.98	10.06	8.77	2.70	9.91	4.46	4.32	12.92	3.91	2.82	12.88	4.46	4.28	3.53	13.00	12.99	3.34	11.05	5.29
0.010	7.49	2.02	11.63	7.48	7.83	1.98	9.86	9.11	2.54	9.72	13.00	3.23	4.11	12.88	13.00	3.64	9.74	2.37	5.84	3.06	3.22	12.99	4.23	11.20
0.010	7.45	2.02	11.49	7.64	8.00	1.98	10.11	8.68	2.74	9.96	12.96	3.83	3.47	13.00	2.65	12.76	4.19	4.54	3.24	12.98	13.00	3.66	5.38	11.02
0.009	9.95	2.48	5.11	11.00	10.99	5.33	9.46	2.44	9.32	9.84	4.86	3.95	12.82	4.28	3.54	13.00	2.90	12.93	3.13	12.97	12.99	3.75	11.09	5.16
0.009	10.71	3.38	3.44	10.61	10.56	7.41	8.36	2.04	10.71	8.83	3.05	12.99	5.44	3.59	4.91	3.85	12.99	3.68	4.30	12.89	12.87	2.82	11.20	4.36
0.009	7.47	2.02	11.58	7.54	7.89	1.98	9.98	8.91	2.63	9.83	12.98	3.06	4.27	12.84	12.98	3.72	3.99	4.82	3.48	13.00	12.99	3.34	11.03	5.34
0.008	7.46	2.02	11.51	7.61	7.97	1.98	10.07	8.76	2.70	9.92	12.99	3.18	4.12	12.88	12.99	3.63	3.85	4.98	3.20	12.97	13.00	3.63	5.20	11.07
0.007	10.75	3.51	3.31	10.55	10.49	7.61	8.25	2.02	10.82	8.74	5.01	3.84	12.77	4.40	3.88	12.96	12.99	3.17	4.18	12.92	12.87	2.81	11.05	5.30
0.005	7.52	2.01	11.64	7.46	7.80	1.98	9.85	9.15	2.52	9.69	3.28	13.00	5.00	3.80	12.98	3.23	6.36	4.46	6.02	2.92	3.10	12.97	4.70	11.18
0.005	7.47	2.02	11.44	7.69	8.06	1.98	10.16	8.58	2.79	10.02	12.97	3.65	3.60	12.98	3.86	4.84	12.99	3.62	3.84	12.98	12.95	3.03	5.34	11.04
0.005	7.47	2.02	11.55	7.57	7.93	1.98	10.02	8.84	2.66	9.88	12.97	3.68	3.58	12.98	3.84	4.87	12.98	3.63	3.82	12.98	12.95	3.05	5.26	11.06
0.004	2.40	5.04	2.40	9.61	9.57	9.42	7.51	1.98	11.55	7.98	12.94	3.94	3.37	13.00	3.12	12.95	3.09	12.98	3.10	12.96	12.98	3.82	11.08	5.17
0.004	7.48	2.02	11.55	7.56	7.92	1.98	10.01	8.86	2.65	9.86	12.98	3.63	3.67	12.98	4.30	4.34	2.77	12.87	2.99	12.94	12.96	3.92	5.35	11.04
0.003	10.99	4.57	2.60	9.91	9.86	8.94	7.70	1.98	11.37	8.18	12.88	2.74	4.78	12.66	12.99	3.33	3.59	13.00	2.70	12.82	12.88	4.33	5.48	10.99
0.003	9.35	5.12	2.38	9.56	9.53	9.49	7.48	1.98	11.57	7.95	12.89	4.17	3.17	12.99	3.57	13.00	12.98	3.11	4.19	12.92	12.87	2.80	11.00	5.45
0.003	11.00	4.82	2.48	9.74	9.70	9.22	7.58	1.98	11.48	8.06	12.91	2.81	4.67	12.71	12.97	3.19	3.38	13.00	2.94	12.92	12.96	3.98	11.10	5.13
0.003	11.00	4.90	2.45	9.69	9.64	9.30	7.55	1.98	11.51	8.03	12.91	2.81	4.67	12.71	12.97	3.22	3.44	13.00	2.92	12.91	12.95	4.01	11.10	5.10
0.003	11.00	4.65	2.57	9.86	9.82	9.02	7.65	1.98	11.41	8.14	12.99	3.55	3.70	12.98	2.48	12.59	12.63	2.38	3.30	12.99	13.00	3.55	5.53	10.97
0.002	2.34	5.27	2.33	9.48	9.44	9.61	7.44	1.98	11.60	7.92	12.97	3.73	3.50	12.99	13.00	3.63	3.64	5.22	3.37	12.99	13.00	3.46	5.14	11.09
0.001	7.47	2.02	11.48	7.65	8.00	1.98	10.12	8.66	2.75	9.97	12.96	3.73	3.55	12.99	3.85	4.87	12.98	3.65	4.83	3.91	4.00	12.92	3.55	11.08
0.001	10.85	3.77	3.07	10.38	10.32	8.02	8.05	2.00	11.03	8.55	4.42	4.35	12.93	3.88	2.83	12.88	4.34	4.40	3.27	12.98	13.00	3.61	5.25	11.06
0.001	11.00	4.96	2.44	9.67	9.63	9.32	7.54	1.98	11.51	8.02	12.97	3.74	3.48	13.00	2.33	12.43	12.61	2.35	5.69	3.19	3.23	12.99	5.03	11.10
0.001	11.00	4.97	2.43	9.66	9.62	9.35	7.54	1.98	11.51	8.02	13.00	3.23	4.04	12.91	12.99	3.79	3.81	5.02	3.41	13.00	13.00	3.41	10.98	5.50
0.001	11.00	5.02	2.41	9.63	9.59	9.39	7.52	1.98	11.53	8.00	13.00	3.29	3.97	12.92	12.99	3.76	3.81	5.02	3.40	12.99	13.00	3.42	10.99	5.48
0.001	7.37	2.01	11.60	7.52	7.87	1.98	9.88	9.10	2.55	9.72	12.97	3.81	3.56	13.00	3.64	5.11	12.86	4.17	4.61	4.12	4.20	12.86	3.59	11.09
0.001	7.37	2.01	11.64	7.48	7.82	1.98	9.82	9.20	2.50	9.65	12.96	3.86	3.51	13.00	3.61	5.13	12.86	4.17	4.62	4.11	4.19	12.86	3.60	11.10
0.000	11.00	4.74	2.53	9.81	9.79	9.07	7.64	1.98	11.42	8.12	3.57	12.99	4.75	3.98	13.00	3.46	8.16	3.17	6.36	2.70	2.88	12.91	4.82	11.16
0.000	7.51	2.01	11.49	7.64	7.98	1.98	10.08	8.73	2.71	9.94	13.00	3.42	3.95	12.94	4.43	4.19	12.95	2.85	12.83	2.55	2.53	6.99	10.52	2.83
0.000	7.54	2.01	11.49	7.64	7.99	1.98	10.07	8.76	2.71	9.92	12.87	2.64	4.92	12.55	7.42	2.29	4.24	4.61	3.03	12.92	12.98	3.91	4.64	11.18

Table S-IX. The product of multiplying the Boltzman weights and Calculated vicinal coupling constants (from H-1 to H-6') for every conformer of **4c**/**4d**

1-2r	1-2s	2r-3r	2r-3s	2s-3r	2s-3s	3r-4r	3r-4s	3s-4r	3s-4s	1'r-2'r	1'r-2's	1's-2'r	1's-2's	2'r-3'	2's-3'	3'-4'r	3'-4's	4'r-5'r	4'r-5's	4's-5'r	4's-5's	5'r-6'	5's-6'
1.72	0.77	0.33	1.36	1.35	1.42	1.07	0.29	1.69	1.14	0.65	0.61	1.88	0.57	0.51	1.88	0.46	1.88	0.41	1.87	1.87	0.61	0.82	1.59
0.98	0.26	1.52	0.96	1.01	0.26	1.27	1.20	0.32	1.25	1.69	0.40	0.55	1.67	1.69	0.50	0.52	0.62	0.46	1.69	1.69	0.43	1.43	0.70
0.83	0.22	1.29	0.82	0.85	0.22	1.08	1.02	0.27	1.06	1.43	0.35	0.46	1.41	1.43	0.42	0.42	0.55	0.35	1.43	1.43	0.40	0.61	1.20
0.98	0.36	0.26	0.92	0.91	0.76	0.71	0.18	1.01	0.75	0.36	1.16	0.37	0.42	1.17	0.30	0.32	1.17	0.25	1.16	1.16	0.38	0.48	0.99
0.31	0.08	0.47	0.31	0.33	0.08	0.41	0.36	0.11	0.41	0.21	0.15	0.52	0.18	0.16	0.53	0.53	0.13	0.17	0.53	0.53	0.11	0.45	0.22
0.27	0.07	0.41	0.28	0.29	0.07	0.36	0.31	0.10	0.36	0.46	0.16	0.11	0.47	0.12	0.47	0.47	0.11	0.15	0.47	0.46	0.10	0.40	0.19
0.26	0.07	0.40	0.27	0.28	0.07	0.35	0.31	0.09	0.35	0.45	0.15	0.11	0.45	0.12	0.45	0.45	0.11	0.14	0.45	0.45	0.10	0.39	0.19
0.23	0.06	0.35	0.22	0.24	0.06	0.30	0.27	0.08	0.29	0.39	0.11	0.10	0.39	0.12	0.14	0.39	0.11	0.15	0.11	0.12	0.39	0.11	0.33
0.21	0.06	0.32	0.21	0.22	0.06	0.28	0.25	0.07	0.28	0.36	0.09	0.12	0.36	0.36	0.08	0.10	0.36	0.08	0.36	0.36	0.12	0.15	0.31
0.20	0.05	0.31	0.21	0.22	0.05	0.27	0.24	0.07	0.27	0.35	0.12	0.08	0.35	0.09	0.35	0.35	0.07	0.10	0.35	0.35	0.09	0.14	0.30
0.20	0.05	0.31	0.20	0.21	0.05	0.27	0.25	0.07	0.26	0.35	0.10	0.10	0.35	0.11	0.13	0.35	0.10	0.13	0.10	0.11	0.35	0.10	0.30
0.28	0.10	0.08	0.27	0.27	0.21	0.21	0.05	0.29	0.22	0.10	0.34	0.11	0.12	0.34	0.10	0.10	0.12	0.09	0.34	0.34	0.09	0.29	0.14
0.20	0.05	0.30	0.19	0.20	0.05	0.25	0.24	0.06	0.25	0.34	0.08	0.11	0.33	0.34	0.10	0.27	0.06	0.09	0.34	0.34	0.09	0.29	0.14
0.24	0.09	0.06	0.22	0.22	0.19	0.17	0.04	0.25	0.18	0.28	0.10	0.06	0.29	0.08	0.29	0.07	0.29	0.28	0.08	0.08	0.11	0.25	0.09
0.21	0.09	0.05	0.19	0.18	0.17	0.14	0.04	0.22	0.15	0.08	0.09	0.25	0.07	0.06	0.25	0.08	0.08	0.07	0.25	0.25	0.06	0.21	0.10
0.19	0.07	0.06	0.19	0.19	0.14	0.15	0.04	0.20	0.15	0.23	0.06	0.08	0.23	0.23	0.05	0.06	0.23	0.23	0.07	0.07	0.09	0.20	0.07
0.11	0.03	0.17	0.10	0.11	0.03	0.13	0.14	0.03	0.13	0.18	0.05	0.05	0.18	0.18	0.05	0.05	0.07	0.05	0.18	0.18	0.05	0.07	0.16
0.09	0.02	0.14	0.09	0.10	0.02	0.12	0.10	0.03	0.12	0.15	0.05	0.04	0.16	0.04	0.16	0.04	0.16	0.16	0.05	0.05	0.06	0.13	0.05
0.13	0.05	0.03	0.12	0.12	0.10	0.09	0.02	0.13	0.10	0.04	0.07	0.15	0.03	0.15	0.03	0.03	0.15	0.04	0.16	0.16	0.05	0.13	0.06
0.08	0.02	0.13	0.08	0.09	0.02	0.11	0.09	0.03	0.11	0.14	0.05	0.03	0.14	0.04	0.14	0.14	0.03	0.05	0.04	0.04	0.14	0.04	0.12
0.08	0.02	0.13	0.08	0.09	0.02	0.11	0.10	0.03	0.11	0.14	0.05	0.03	0.14	0.04	0.14	0.14	0.03	0.05	0.04	0.04	0.14	0.04	0.12
0.08	0.02	0.13	0.08	0.09	0.02	0.11	0.10	0.03	0.11	0.14	0.03	0.05	0.14	0.14	0.03	0.04	0.14	0.14	0.04	0.04	0.05	0.12	0.04
0.07	0.02	0.12	0.08	0.08	0.02	0.10	0.09	0.03	0.10	0.04	0.04	0.13	0.04	0.03	0.13	0.04	0.04	0.04	0.13	0.13	0.03	0.11	0.05
0.07	0.02	0.12	0.07	0.08	0.02	0.10	0.09	0.03	0.10	0.13	0.03	0.04	0.13	0.13	0.04	0.10	0.02	0.06	0.03	0.03	0.13	0.04	0.11
0.07	0.02	0.11	0.08	0.08	0.02	0.10	0.09	0.03	0.10	0.13	0.04	0.03	0.13	0.03	0.13	0.04	0.05	0.03	0.13	0.13	0.04	0.05	0.11
0.09	0.02	0.05	0.10	0.10	0.05	0.09	0.02	0.08	0.09	0.04	0.04	0.12	0.04	0.03	0.12	0.03	0.12	0.03	0.12	0.12	0.03	0.10	0.05
0.10	0.03	0.03	0.10	0.10	0.07	0.08	0.02	0.10	0.08	0.03	0.12	0.05	0.03	0.04	0.03	0.12	0.03	0.04	0.12	0.12	0.03	0.10	0.04
0.07	0.02	0.10	0.07	0.07	0.02	0.09	0.08	0.02	0.09	0.12	0.03	0.04	0.12	0.12	0.03	0.04	0.04	0.03	0.12	0.12	0.03	0.10	0.05
0.06	0.02	0.09	0.06	0.06	0.02	0.08	0.07	0.02	0.08	0.10	0.03	0.03	0.10	0.10	0.03	0.03	0.04	0.03	0.10	0.10	0.03	0.04	0.09
0.08	0.02	0.02	0.07	0.07	0.05	0.06	0.01	0.08	0.06	0.04	0.03	0.09	0.03	0.03	0.09	0.09	0.02	0.03	0.09	0.09	0.02	0.08	0.04
0.04	0.01	0.06	0.04	0.04	0.01	0.05	0.05	0.01	0.05	0.02	0.06	0.02	0.02	0.06	0.02	0.03	0.02	0.03	0.01	0.02	0.06	0.02	0.06
0.04	0.01	0.06	0.04	0.04	0.01	0.05	0.04	0.01	0.05	0.06	0.02	0.02	0.06	0.02	0.02	0.06	0.02	0.02	0.06	0.06	0.02	0.03	0.06
0.04	0.01	0.06	0.04	0.04	0.01	0.05	0.04	0.01	0.05	0.06	0.02	0.02	0.06	0.02	0.02	0.06	0.02	0.02	0.06	0.06	0.02	0.03	0.06
0.01	0.02	0.01	0.04	0.04	0.04	0.03	0.01	0.05	0.03	0.05	0.02	0.01	0.05	0.01	0.05	0.01	0.05	0.01	0.05	0.05	0.02	0.04	0.02
0.03	0.01	0.05	0.03	0.03	0.01	0.04	0.04	0.01	0.04	0.05	0.01	0.01	0.05	0.02	0.02	0.01	0.05	0.01	0.05	0.05	0.02	0.02	0.04
0.03	0.01	0.01	0.03	0.03	0.03	0.02	0.01	0.03	0.02	0.04	0.01	0.01	0.04	0.04	0.01	0.01	0.04	0.01	0.04	0.04	0.01	0.02	0.03
0.03	0.02	0.01	0.03	0.03	0.03	0.02	0.01	0.03	0.02	0.04	0.01	0.01	0.04	0.01	0.04	0.04	0.01	0.01	0.04	0.04	0.01	0.03	0.02
0.03	0.01	0.01	0.03	0.03	0.03	0.02	0.01	0.03	0.02	0.04	0.01	0.01	0.04	0.04	0.01	0.01	0.04	0.01	0.04	0.04	0.01	0.03	0.02
0.03	0.01	0.01	0.03	0.03	0.03	0.02	0.01	0.03	0.02	0.04	0.01	0.01	0.04	0.04	0.01	0.01	0.04	0.01	0.04	0.04	0.01	0.03	0.02
0.03	0.01	0.01	0.03	0.03	0.03	0.02	0.01	0.03	0.02	0.04	0.01	0.01	0.04	0.01	0.04	0.04	0.01	0.01	0.04	0.04	0.01	0.02	0.03
0.00	0.01	0.00	0.02	0.02	0.02	0.01	0.00	0.02	0.02	0.03	0.01	0.01	0.03	0.03	0.01	0.01	0.01	0.01	0.03	0.03	0.01	0.01	0.02
0.01	0.00	0.01	0.01	0.01	0.00	0.01	0.01	0.00	0.01	0.01	0.00	0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.01	0.00	0.01
0.01	0.00	0.00	0.01	0.01	0.01	0.01	0.00	0.01	0.01	0.00	0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.01	0.00	0.01	0.01
0.01	0.00	0.00	0.01	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.00	0.00	0.01	0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.01	0.01	0.01
0.01	0.00	0.00	0.01	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.00	0.00	0.01	0.01	0.00	0.00	0.01	0.00	0.01	0.01	0.00	0.01	0.01
0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.00	0.00	0.01	0.01	0.00	0.00	0.01	0.00	0.01	0.01	0.00	0.01	0.01
0.01	0.00	0.01	0.01	0.01	0.00	0.01	0.01	0.00	0.01	0.01	0.00	0.00	0.01	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.00	0.01
0.01	0.00	0.01	0.01	0.01	0.00	0.01	0.01	0.00	0.01	0.01	0.00	0.00	0.01	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.00	0.01
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Cartesian coordinates for the lowest energy conformers obtained by a multi-step conformation method (see experimental section)

Lowest energy conformer of **4a/4b** (SR/RS):
Standard Nuclear Orientation (Angstroms)

I	Atom	X	Y	Z
1	C	1.900180	1.776441	0.012429
2	C	0.404426	1.785415	0.270323
3	C	-0.342783	0.525443	-0.172133
4	C	-1.811199	0.599260	0.303967
5	C	-2.609839	-0.695017	0.103342
6	C	-3.954355	-0.638983	0.758318
7	C	-5.137235	-0.467420	0.184730
8	C	-6.395640	-0.398179	1.012305
9	C	-5.353279	-0.322984	-1.306240
10	O	2.470374	0.675706	0.699009
11	C	3.839248	0.471682	0.436503
12	C	4.311877	-0.678443	1.312698
13	C	4.850922	-1.736201	0.331789
14	C	4.126351	-1.333658	-0.957073
15	O	4.095987	0.087835	-0.914732
16	H	2.124051	1.692997	-1.053048
17	H	2.351096	2.711913	0.380671
18	H	-0.003748	2.637795	-0.211858
19	H	0.249555	1.923985	1.310942

20	H	-1.834478	0.860673	1.382795
21	H	-2.331617	1.425853	-0.218674
22	H	-2.043329	-1.519729	0.526931
23	H	-2.706778	-0.907004	-0.952020
24	H	-3.931814	-0.718667	1.842518
25	H	-6.205213	-0.511513	2.087324
26	H	-6.909854	0.558506	0.862931
27	H	-7.087861	-1.180720	0.709783
28	H	-5.993940	-1.123242	-1.692691
29	H	-5.870387	0.617320	-1.523060
30	H	-4.433292	-0.336135	-1.888084
31	H	4.374412	1.396682	0.588779
32	H	5.062969	-0.357210	2.023766
33	H	3.415549	-1.043038	1.882922
34	H	4.643670	-2.752583	0.650036
35	H	5.943139	-1.642322	0.197619
36	H	4.644446	-1.622107	-1.870245
37	H	3.100420	-1.714602	-0.995099
38	C	-0.249769	0.298096	-1.687588
39	H	-0.757067	-0.651379	-1.982976
40	H	0.781819	0.222543	-2.023776
41	H	-0.725324	1.131509	-2.251815
42	H	0.139254	-0.320569	0.321884

Lowest energy conformer of 4c/4d (SS/RR):

Standard Nuclear Orientation (Angstroms)

I	Atom	X	Y	Z
1	C	-1.870172	-1.062509	-0.885732
2	C	-0.439810	-0.666472	-1.211667
3	C	0.488120	-0.483261	-0.000017
4	C	0.559279	-1.746720	0.861329
5	C	1.876871	-0.035473	-0.481909
6	C	2.827598	0.431014	0.631959
7	C	4.093289	1.031661	0.083986
8	C	5.311702	0.478235	0.024798
9	C	6.477007	1.224105	-0.572988
10	C	5.651873	-0.899824	0.529673
11	O	-2.429901	-0.094725	-0.013855
12	C	-3.701012	-0.428564	0.480235
13	C	-4.172283	0.699272	1.386018
14	C	-4.776868	1.677670	0.372058
15	C	-5.353279	0.732018	-0.689045
16	O	-4.666681	-0.522552	-0.540733
17	H	-2.464509	-1.123894	-1.805748
18	H	-1.909460	-2.054439	-0.408094
19	H	-0.463867	0.267193	-1.788701
20	H	-0.026043	-1.437484	-1.879580
21	H	0.068357	0.323286	0.615807
22	H	1.239732	-1.620003	1.710261

23	H	-0.419421	-2.005738	1.279366
24	H	0.913401	-2.605890	0.274112
25	H	2.356527	-0.853531	-1.039687
26	H	1.754287	0.788785	-1.198523
27	H	3.053808	-0.399108	1.307560
28	H	2.310931	1.186104	1.240480
29	H	3.975366	2.031422	-0.337235
30	H	7.288841	1.335781	0.159265
31	H	6.898555	0.678309	-1.428273
32	H	6.193670	2.224544	-0.916530
33	H	6.369185	-0.844002	1.360153
34	H	6.136367	-1.487215	-0.261923
35	H	4.783065	-1.466149	0.874305
36	H	-3.655257	-1.416941	0.956583
37	H	-4.939673	0.315401	2.068360
38	H	-3.354822	1.120064	1.975313
39	H	-3.994556	2.312112	-0.054611
40	H	-5.544588	2.324564	0.808204
41	H	-6.422031	0.539862	-0.535941
42	H	-5.209104	1.098267	-1.710405

NMR data calculations obtained using the "Spartan-NMR" calculation method for 4c/4d (SS/RR):

Table S-X. Geminal and vicinal coupling constants obtained using the "Spartan-NMR" calculation method for compounds **4c/4d** (SS/RR):

H\H	1's	1'r	2's	2'r	3'	10'			4'r	4's	5'r	5's	6'	1	2r	2s	3r	3s	4s	4r
1's		-8.7	3.8	13.1																
1'r	-8.7		1.1	6.1																
2's	3.8	1.1		-13.2	11.4															
2'r	13.1	6.1	-13.2		4.1															
3'			11.4	4.1		6.9	6.9	6.9	12.0	4.0										
10'					6.9		-12.8	-12.8												
					6.9	-12.8		-12.8												
					6.9	-12.8	-12.8													
4'r					12.0					-12.9	3.5	4.4								
4's					4.0				-12.9		4.6	13.5								
5'r									3.5	4.6		-14.3	11.6							

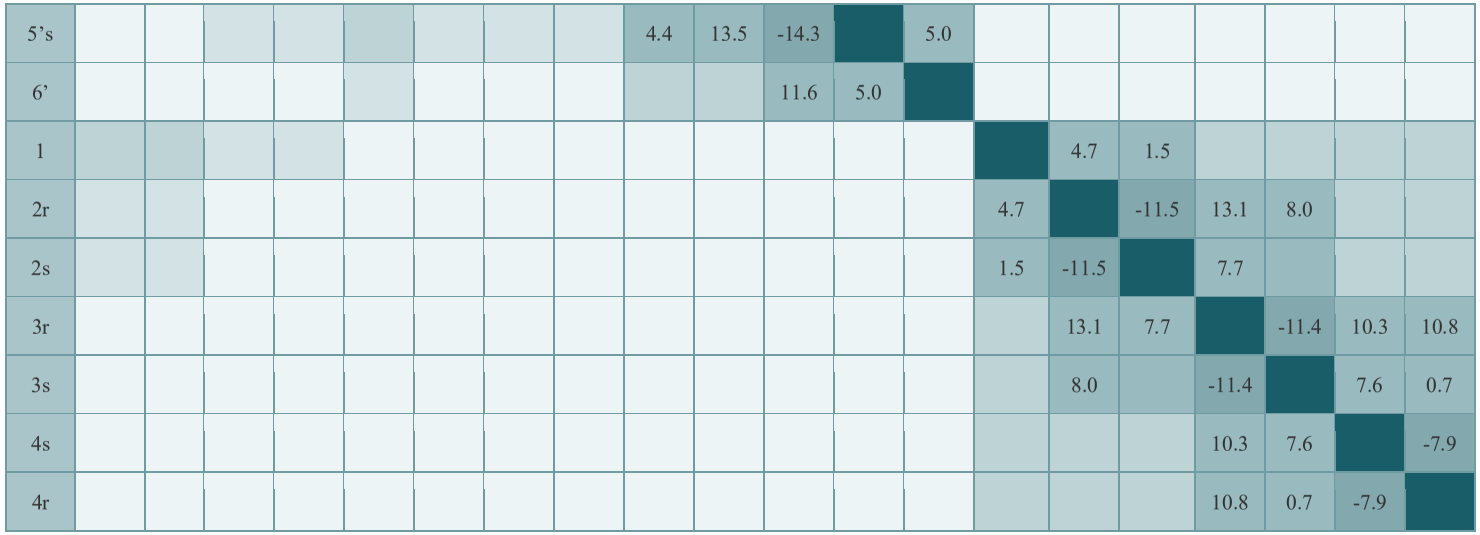

Table S-XI. Chemical shifts, coupling constants, and HMBC interactions obtained using the "Spartan-NMR" calculation method for **4c/4d** (SS/RR):

position	δ_C	mult	δ_H		(J in Hz)	HMBC(H→C)
1'	59.9	CH_2	4.08	m	(13.1,-8.7,3.8)	1, 2, 3, 4, 10, 11
.			3.29	m	(-8.7,6.1,1.1)	1, 2, 3, 11
2'	36.4	CH_2	1.04	m	(-13.2,11.4,3.8,1.1)	2, 3, 4, 10
.			1.94	m	(-13.2,13.1,6.1,4.1)	2, 3, 4, 5, 10
3'	24.2	CH	2.51	m	$(12.0,11.4,6.9_{x3},4.1,4.0)$	1, 3, 4, 5

10’	19.2	CH_3	1.00	m	(6.9)	1, 2, 4, 5
4’	31.8	CH_2	0.96	m	(-12.9,12.0,4.4,3.5)	1, 2, 3, 5, 6, 8
.			2.09	m	(-12.9,4.6,4.0,1.3)	1, 2, 3, 5, 6, 13
5’	24.7	CH_2	2.32	m	(-14.3,11.6,4.6,3.5)	2, 4, 6, 7, 8
.			2.15	m	(-14.3,13.5,5.0,4.4)	1, 2, 4, 6, 7, 8, 9
6’	126.1	CH	5.91	m	$(11.6,5.0,-2.4_{x3},-1.8_{x3})$	2, 4, 5, 7, 8, 9
7’	130.3	C				...
8’	26.5	CH_3	1.65	ddd	(1.9,-1.8,0.5)	4, 5, 6, 7, 9
9’	17.9	CH_3	1.56	ddd	(-2.4,1.6,0.9)	4, 5, 6, 7, 8, 13
1	102.1	CH	5.06	m	(4.7,1.5)	1, 11, 12, 13
2	33.2	CH_2	1.63	m	(13.1,-11.5,8.0,4.7)	10, 12, 13
.			1.91	m	(-11.5,7.7,1.5)	10, 12, 13
3	24.5	CH_2	2.37	m	(13.1,-11.4,10.8,10.3,7.7)	6, 7, 8, 10, 11, 13
.			1.59	m	(-11.4,8.0,7.6,0.7)	8, 10, 11, 13
4	68.4	CH_2	3.82	m	(10.3,-7.9,7.6)	10, 12
.			4.12	m	(10.8,-7.9,0.7)	4, 6, 7, 9, 10, 11, 12
Label	δ				..	
O	260.1					...
O1	260.4					...

NMR data calculation short output for 4c/4d (SR/RS):

Job type: Geometry optimization.
Method: RHF
Basis set: 3-21G(*)
Number of basis functions: 196
Number of electrons: 126
Parallel Job: 8 threads

SCF model:
A restricted Hartree-Fock SCF calculation will be
performed using Pulay DIIS + Geometric Direct Minimization

Optimization:

Step	Energy	Max Grad.	Max Dist.
1	-691.149054	0.020450	0.091146
2	-691.157759	0.006403	0.116146
3	-691.158450	0.001931	0.027906
4	-691.158524	0.001273	0.065197
5	-691.158586	0.000353	0.018503

Reason for exit: Successful completion
Quantum Calculation CPU Time : 59.77

Quantum Calculation Wall Time: 11.33

SPARTAN'20 Quantum Mechanics Driver: (Win/64b) Release 1.1.4
Job type: Reading previous wavefunction

Job type: Single point.
Method: RWB97X-D
Basis set: 6-31G(D)
Number of basis functions: 292
Number of electrons: 126
Parallel Job: 8 threads

SCF model:
A restricted hybrid HF-DFT SCF calculation will be
performed using Pulay DIIS + Geometric Direct Minimization

SCF total energy: -699.3749650 hartrees

Reason for exit: Successful completion
Quantum Calculation CPU Time : 8:10.89
Quantum Calculation Wall Time: 1:41.83

SPARTAN'20 Quantum Mechanics Driver: (Win/64b) Release 1.1.4
Job type: Geometry optimization.
Method: RWB97X-D
Basis set: 6-31G(D)
Number of basis functions: 292
Number of electrons: 126
Parallel Job: 8 threads

SCF model:
A restricted hybrid HF-DFT SCF calculation will be
performed using Pulay DIIS + Geometric Direct Minimization

Optimization:

Step	Energy	Max Grad.	Max Dist.
1	-699.374965	0.017139	0.070020
2	-699.380637	0.014433	0.146120
3	-699.381405	0.012991	0.104132
4	-699.382234	0.005476	0.081789
5	-699.382901	0.006009	0.104781
6	-699.383352	0.004750	0.094658
7	-699.383672	0.004757	0.104896

8	-699.383559	0.004977	0.058298
9	-699.383858	0.001669	0.043910
10	-699.383829	0.003051	0.030386
11	-699.383889	0.001130	0.024249
12	-699.383886	0.001770	0.009998
13	-699.383893	0.000127	0.002339

Reason for exit: Successful completion
Quantum Calculation CPU Time : 1:37:52.11
Quantum Calculation Wall Time: 19:47.30

SPARTAN'20 Quantum Mechanics Driver: (Win/64b) Release 1.1.4

forcing reuse of RIC despite likely change in input file.

Job type: Geometry optimization.
Method: RWB97X-D
Basis set: 6-31G(D)
Number of basis functions: 292
Number of electrons: 126
Parallel Job: 8 threads

SCF model:

A restricted hybrid HF-DFT SCF calculation will be
performed using Pulay DIIS + Geometric Direct Minimization

2 -699.383893 0.000127 0.000718 Restart with RIC

Reason for exit: Successful completion
Quantum Calculation CPU Time : 3:39.55
Quantum Calculation Wall Time: 37.55

SPARTAN'20 Quantum Mechanics Driver: (Win/64b) Release 1.1.4

Job type: Single point.
Method: RWB97XRV
Basis set: 6-311+G(2DF,2P) [6-311G*]
Number of basis functions: 366 (small basis)
Number of electrons: 126
Parallel Job: 8 threads

SCF model:
A restricted hybrid HF-DFT SCF calculation will be
performed using Pulay DIIS + Geometric Direct Minimization

Number of basis functions: 778 (large basis)

SCF total energy: -699.6155507 hartrees

Reason for exit: Successful completion
Quantum Calculation CPU Time : 29:53.44
Quantum Calculation Wall Time: 4:51.29

SPARTAN'20 Quantum Mechanics Driver: (Win/64b) Release 1.1.4

Job type: Single point.
Method: RWB97X-D
Basis set: 6-31G(D)
Number of basis functions: 292
Number of electrons: 126

SCF model:
A restricted hybrid HF-DFT SCF calculation will be
performed using Pulay DIIS + Geometric Direct Minimization

SCF total energy: -699.3838930 hartrees
NMR shifts (ppm)

Atom		Isotropic	Rel. Shift
1	C	136.9696	

2	C1	158.2735
3	C2	170.0882
4	C3	174.8911
5	C4	162.7652
6	C5	169.5927
7	C6	72.4178
8	C7	68.3592
9	C8	167.8103
10	C9	176.1559
11	O	260.1396
12	C10	96.7206
13	C11	161.3298
14	C12	169.7624
15	C13	129.2388
16	O1	260.4384
17	H-1's	28.3270
18	H-1'r	29.0942
19	H-2's	31.2776
20	H-2'r	30.4056
21	H-3'	29.8903
22	H-10'	30.7571

23	H-10’	31.3329
24	H-10’	31.6444
25	H-4’r	31.3543
26	H-4’s	30.2540
27	H-5’r	30.0305
28	H-5’s	30.1978
29	H-6’	26.4766
30	H-8’	30.6248
31	H-8’	30.5789
32	H-8’	30.6769
33	H-9’	30.1806
34	H-9’	31.0668
35	H-9’	30.8953
36	H-1	27.4167
37	H-2r	30.7050
38	H-2s	30.4343
39	H-3r	29.9799
40	H-3s	30.7428
41	H-4s	28.5762
42	H-4r	28.2813

<step 2>
Job type: NMR coupling constants.

Method: RB3LYP
Basis set: PCJ-0

Reason for exit: Successful completion
Quantum Calculation CPU Time : 3:11:35.02
Quantum Calculation Wall Time: 3:14:23.84

NMR data calculations obtained using the "Spartan-NMR" calculation method for 4a/4b (SR/RS):

Table S-XII. Vicinal coupling constants obtained using the "Spartan-NMR" calculation method for compounds **4a/4b** (SR/RS):

H\H	10'	1	2r	2s	3r	3s	4r	4s	3'	6'	1'r	2'r	4'r	5'r	1's	2's	4's	5's
10'									6.4									
1			5.3	0.7														
2r		5.3			12.6	7.3												
2s		0.7			7.7	0.5												
3r			12.6	7.7			9.4	9.4										
3s			7.3	0.5			1.1	7.8										
4r					9.4	1.1												

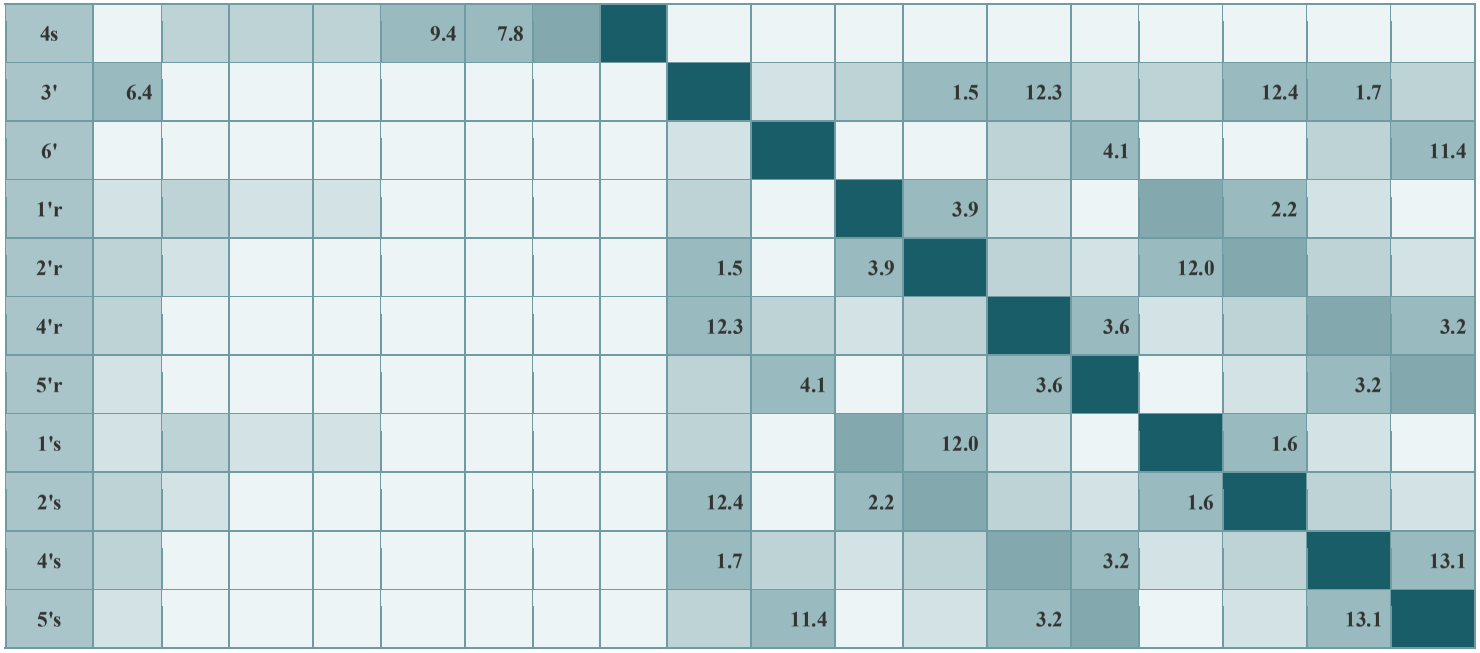

Table S-XIII. Chemical shifts, coupling constants, and HMBC interactions obtained using the "Spartan-NMR" calculation method for **4a/4b** (SR/RS):

position	δ_C	mult	δ_H		(J in Hz)	HMBC(H→C)
-1	98.2	CH	5.1	dd	(5.3,0.7)	-3, -4, -1'
-2	34.0	CH_2	1.74	ddd	(12.6,7.3,5.3)	
.			2.06	ddd	(7.7,0.7,0.5)	-4
-3	25.2	CH_2	2.52	m	(12.6,9.4,9.4,7.7)	
.			1.77	m	(7.8,7.3,1.1,0.5)	-1
-4	65.3	CH_2	4.14	dd	(9.4,1.1)	-1, -2
.			3.93	dd	(9.4,7.8)	-1
-7	129.8	C				...
10'	20.6	CH_3	1.70	d	(6.4)	-2', -4'
-1'	58.5	CH_2	4.05	dd	(3.9,2.2)	-1, -3'
.			3.64	dd	(12.0,1.6)	-1, -3'
-2'	34.0	CH_2	0.86	ddd	(12.0,3.9,1.5)	14, -4'
.			2.37	ddd	(12.4,2.2,1.6)	14, -4'
-3'	24.8	CH	2.32	m	(12.4,12.3,6.4$_{x3}$,1.7,1.5)	-1', -5'
-4'	35.8	CH_2	1.49	ddd	(12.3,3.6,3.2)	14, -2', -6'
.			1.65	ddd	(13.1,3.2,1.7)	14, -2', -6'
-5'	26.4	CH_2	2.04	ddd	(4.1,3.6,3.2)	-7, -3'
.			2.55	ddd	(13.1,11.4,3.2)	-7, -3'
-6'	122.1	CH	5.55	dd	(11.4,4.1)	-4', -8', -9'
-8'	27.6	CH_3	1.88	s		-6', -9'
-9'	19.4	CH_3	1.97	s		-6', -8'

Label	δ	..	
O-C	257.3		...
O-T	256.9		...

NMR data calculation short output for 4a/4b (SR/RS):

Job type: Geometry optimization.
Method: RHF
Basis set: 3-21G(*)
Number of basis functions: 196
Number of electrons: 126
Parallel Job: 8 threads

SCF model:
A restricted Hartree-Fock SCF calculation will be
performed using Pulay DIIS + Geometric Direct Minimization

Optimization:

Step	Energy	Max Grad.	Max Dist.
1	-691.149968	0.018721	0.067863
2	-691.158411	0.009051	0.140266
3	-691.159240	0.005097	0.180275
4	-691.159702	0.004813	0.187081

5	-691.160212	0.006340	0.179353
6	-691.160770	0.005444	0.178209
7	-691.161066	0.003618	0.065290
8	-691.161139	0.006370	0.189339
9	-691.161352	0.003556	0.040822
10	-691.161428	0.002491	0.026574
11	-691.161485	0.000910	0.020079
12	-691.161512	0.000561	0.010548

Reason for exit: Successful completion
Quantum Calculation CPU Time : 2:31.70
Quantum Calculation Wall Time: 22.05

SPARTAN'20 Quantum Mechanics Driver: (Win/64b) Release 1.1.4
Job type: Reading previous wavefunction

Job type: Single point.
Method: RWB97X-D
Basis set: 6-31G(D)
Number of basis functions: 292
Number of electrons: 126
Parallel Job: 8 threads

SCF model:
A restricted hybrid HF-DFT SCF calculation will be
performed using Pulay DIIS + Geometric Direct Minimization

SCF total energy: -699.3766056 hartrees
Reason for exit: Successful completion
Quantum Calculation CPU Time : 8:24.58
Quantum Calculation Wall Time: 1:43.71
SPARTAN'20 Quantum Mechanics Driver: (Win/64b) Release 1.1.4
Job type: Geometry optimization.
Method: RWB97X-D
Basis set: 6-31G(D)
Number of basis functions: 292
Number of electrons: 126
Parallel Job: 8 threads
SCF model:
A restricted hybrid HF-DFT SCF calculation will be
performed using Pulay DIIS + Geometric Direct Minimization

Optimization:

Step	Energy	Max Grad.	Max Dist.
1	-699.376605	0.016169	0.230909
2	-699.372802	0.053463	0.120018

3	-699.377720	0.028155	0.131144
4	-699.378924	0.016620	0.079836
5	-699.378457	0.030392	0.112922
6	-699.381414	0.011629	0.086629
7	-699.379762	0.014341	0.072367
8	-699.382541	0.006247	0.068542
9	-699.381977	0.010908	0.050659
10	-699.383286	0.003823	0.143375
11	-699.383135	0.007341	0.062972
12	-699.383580	0.003543	0.076927
13	-699.383786	0.005418	0.087621
14	-699.384172	0.005457	0.081487
15	-699.384657	0.005887	0.062677
16	-699.385040	0.002453	0.080985
17	-699.385125	0.003419	0.056921
18	-699.385165	0.003178	0.030648
19	-699.385247	0.003205	0.028567
20	-699.385270	0.003504	0.022221
21	-699.385279	0.001668	0.039333
22	-699.385304	0.001997	0.025995
23	-699.385318	0.001070	0.014798
24	-699.385331	0.000494	0.012480

Reason for exit: Successful completion
Quantum Calculation CPU Time : 2:25:36.17
Quantum Calculation Wall Time: 40:38.27

SPARTAN'20 Quantum Mechanics Driver: (Win/64b) Release 1.1.4

forcing reuse of RIC despite likely change in input file.

Job type: Geometry optimization.
Method: RWB97X-D
Basis set: 6-31G(D)
Number of basis functions: 292
Number of electrons: 126
Parallel Job: 8 threads

SCF model:
A restricted hybrid HF-DFT SCF calculation will be
performed using Pulay DIIS + Geometric Direct Minimization

2 -699.385331 0.000493 0.001781 Restart with RIC

Reason for exit: Successful completion
Quantum Calculation CPU Time : 3:29.08

Quantum Calculation Wall Time: 42.45

SPARTAN'20 Quantum Mechanics Driver: (Win/64b) Release 1.1.4

Job type: Single point.
Method: RWB97XRV
Basis set: 6-311+G(2DF,2P) [6-311G*]
Number of basis functions: 366 (small basis)
Number of electrons: 126
Parallel Job: 8 threads

SCF model:
A restricted hybrid HF-DFT SCF calculation will be
performed using Pulay DIIS + Geometric Direct Minimization

Number of basis functions: 778 (large basis)
SCF total energy: -699.6161237 hartrees

Reason for exit: Successful completion
Quantum Calculation CPU Time : 31:47.42
Quantum Calculation Wall Time: 5:43.83

SPARTAN'20 Quantum Mechanics Driver: (Win/64b) Release 1.1.4

Job type: Single point.
Method: RWB97X-D
Basis set: 6-31G(D)
Number of basis functions: 292
Number of electrons: 126

SCF model:
A restricted hybrid HF-DFT SCF calculation will be
performed using Pulay DIIS + Geometric Direct Minimization

SCF total energy: -699.3853308 hartrees

NMR shifts (ppm)

	Atom	Isotropic	Rel. Shift
1	C-1'	136.5505	
2	C-2'	160.9610	
3	C-3'	170.1754	
4	C-4'	159.1862	
5	C-5'	168.5623	
6	C-6'	72.8738	
7	C-7	65.2432	

8	C-8'	167.4099
9	C-9'	175.6451
10	O-C	257.3006
11	C-1	96.7993
12	C-2	161.0552
13	C-3	169.7674
14	C-4	129.7580
15	O-T	256.8932
16	H-1's	28.3934
17	H-1'r	28.7983
18	H-2's	31.5794
19	H-2'r	30.0736
20	H-4'r	30.9513
21	H-4's	30.7931
22	H-5'r	30.4028
23	H-5's	29.8890
24	H-6'	26.8868
25	H-8'a	30.5102
26	H-8'c	30.4960
27	H-8'b	30.6781
28	H-9'b	31.0755
29	H-9'a	29.9914
30	H-9'c	30.3373

31	H-1	27.3399
32	H-2r	30.7011
33	H-2s	30.3806
34	H-3r	29.9200
35	H-3s	30.6741
36	H-4s	28.5102
37	H-4r	28.2994
38	C14	174.4288
39	H-10'a	31.4821
40	H-10'b	30.3953
41	H-10'c	31.6973
42	H-3'	30.1206

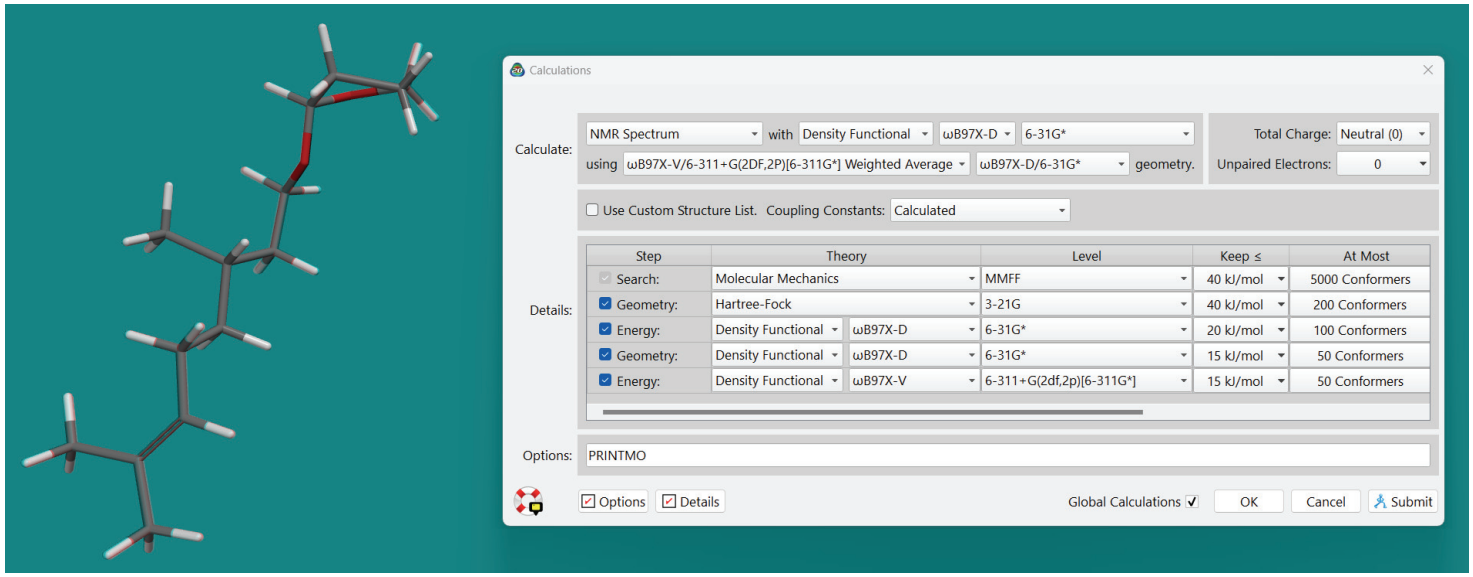

Fig. S-17. NMR data calculation parameters window for “Spartan-NMR” calculation method.