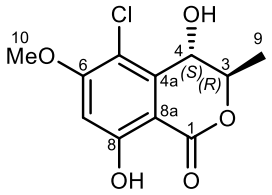
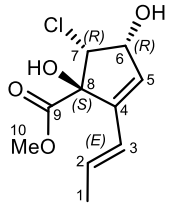
(3*R*,4*S*)-5-chloro-4-hydroxy-6-methoxymellein



solv.	$CDCl_3$
geometry	ωB97X-D/6-31G*
NMR	ωB97X-D/6-31G* + post semiempirical correction (spartan'18)
energy	ωB97X-V/6-311+G(2df,2p)[6-311G*]
parameters	standard deviation: 2.306 ppm, freedom: 11.38
lit.	Inose, K.; Tanaka, K.; Koshino, H.; Hashimoto, M., *Tetrahedron* **2019**, 130470.

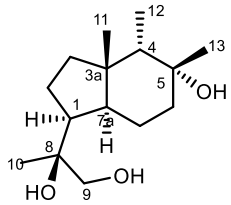
			position	1	8a	8	7	6	5	4a	4	3	9	OMe
			exp.	167.3	100.6	163.1	101.0	161.5	113.2	136.5	65.8	79.8	18.1	56.7
	RMSD (ppm)	$\lvert\Delta\delta\rvert_{max}$ (ppm)	DP4											
(3R,4S)-isomer	**2.3**	**4.7**	**86%**	**169.3**	**102.8**	**164.8**	**100.1**	**160.0**	**108.5**	**140.0**	**67.7**	**78.3**	**17.6**	**55.1**
(3R,4R)-isomer	2.6	4.9	14%	170.7	102.4	164.8	100.0	160.1	108.3	141.3	66.3	77.8	16.6	55.1

cyclopericodiol

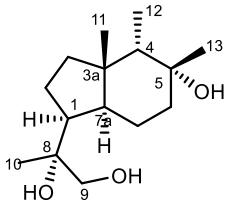


solv.	$CDCl_3$
geometry	ωB97X-D/6-31G*
NMR	ωB97X-D/6-31G* + post semiempirical correction (spartan'18)
energy	ωB97X-V/6-311+G(2df,2p)[6-311G*]
parameters	standard deviation: 2.306 ppm, freedom: 11.38
lit.	Inose, K.; Tanaka, K.; Koshino, H.; Hashimoto, M., *Tetrahedron* **2019**, 130470.

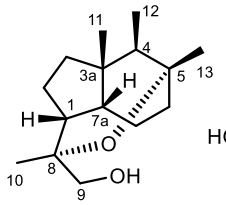
experimental			position	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10
			exp.	19.0	132.3	123.4	144.5	131.2	72.5	68.4	87.9	172.7	54.3
	RMSD (ppm)	$\lvert\Delta\delta\rvert_{max}$ (ppm)	DP4										
(6R,7R,8S)-isomer	**1.5**	**4.1**	**100%**	**19.2**	**133.1**	**124.2**	**144.3**	**132.8**	**72.8**	**69.7**	**88.6**	**176.8**	**54.4**
(6R,7S,8R)-isomer	3.5	7.1	0%	19.1	132.0	124.1	142.9	131.8	79.6	75.3	86.5	176.9	54.0
(6R,7S,8S)-isomer	4.1	8.6	0%	18.9	130.4	125.5	140.9	133.8	81.2	71.8	82.9	178.1	53.9
(6R,7R,8R)-isomer	2.5	4.5	0%	18.9	131.5	125.0	144.0	134.4	75.4	65.7	84.1	177.1	53.8



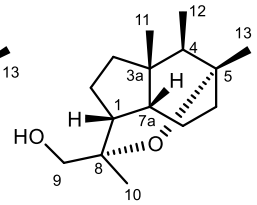
seiricardin B (revised)



seiricardin C (proposed)



seiricardin B by Evidente



seiricardin C by Evidente

solv.	$CDCl_3$
geometry	ωB97X-D/6-31G*
NMR	ωB97X-D/6-31G* + post semiempirical correction (spartan'18)
energy	ωB97X-V/6-311+G(2df,2p)[6-311G*]
parameters	standard deviation: 2.306 ppm, freedom: 11.38
lit.	M. Nishiyama, W. C. Tayone, H. Maeda, K. Tanaka, M. Hashimoto, Bull Chem. Soc. Jpn. *in press*

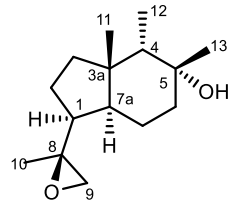
experimental

position	1	2	3	3a	4	5	6	7	7a	8	9	10	11	12	13
seiricardine B	44.1	27.2	36.4	44.1	49.2	73.2	36.3	20.8	40.2	75.7	69.9	22.4	25.6	10.9	32.2
seiricardine B by Evidente	43.9	27.1	36.3	44.0	49.2	73.2	36.2	20.8	40.2	75.7	69.8	22.2	25.6	10.8	32.3
seiricardine C by Evidente	45.1	26.4	36.3	44.0	49.0	73.2	36.1	21.1	39.8	75.1	69.4	25.3	23.8	10.8	32.1
calculated															
seiricardin B	43.3	28.4	36.6	43.8	46.5	72.5	34.9	21.5	39.0	76.0	70.2	23.5	26.1	12.5	31.4
C-8 isomer (seiricardine C)	44.5	28.1	36.7	43.6	46.1	72.6	35.1	22.2	39.4	75.0	70.1	24.3	25.7	12.7	31.5
seiricardine B by Evidente	47.2	25.2	36.6	43.9	46.1	77.3	32.4	20.9	47.8	79.0	66.1	27.5	29.4	11.9	31.7
seiricardine C by Evidente	48.2	23.5	41.8	43.1	45.4	78.2	27.4	19.9	48.7	76.9	70.1	27.8	22.9	14.6	30.4

identical structure

	vs. seiricardin B (revised)			vs. Sericerdin B by Evidente			vs seiricardin C by Evidente		
	$\lvert\Delta\delta\rvert_{max}$ (ppm)	RMSD (ppm)	DP4	$\lvert\Delta\delta\rvert_{max}$ (ppm)	RMSD (ppm)	DP4	$\lvert\Delta\delta\rvert_{max}$ (ppm)	RMSD (ppm)	DP4
seiricardine B	**2.3**	**1.1**	**63.0%**	**2.7**	**1.1**	**67.1%**	2.5	1.4	22.0%
C-8 isomer (seiricardine C)	1.9	1.2	37.0%	3.1	1.3	32.9%	**2.9**	**1.3**	**78.0%**
seiricardine B by Evidente	8.0	3.5	0.0%	7.6	3.5	0.0%	8.0	3.4	0.0%
seiricardine C by Evidente	8.9	4.5	0.0%	8.8	4.5	0.0%	8.9	4.3	0.0%

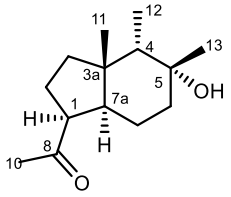
seiricardine B epoxy deriv.



solv.	$CDCl_3$
geometry	ωB97X-D/6-31G*
NMR	ωB97X-D/6-31G* + post semiempirical correction (spartan'18)
energy	ωB97X-V/6-311+G(2df,2p)[6-311G*]
parameters	standard deviation: 2.306 ppm, freedom: 11.38
lit.	M. Nishiyama, W. C. Tayone, H. Maeda, K. Tanaka, M. Hashimoto, Bull Chem. Soc. Jpn. *in press*

	$\lvert\Delta\delta\rvert_{max}$ (ppm)	RMSD (ppm)	DP4	1	2	3	3a	4	5	6	7	7a	8	9	10	11	12	13
			exp.	43.8	26.1	36.1	44.0	49.3	73.4	36.0	20.2	40.5	57.7	52.7	23.2	25.8	10.9	32.2
(1S,8S)-isomer	**1.9**	**0.9**	**98.5%**	**43.9**	**27.4**	**36.3**	**43.7**	**47.9**	**72.6**	**35.6**	**20.4**	**40.0**	**55.8**	**52.1**	**23.0**	**26.6**	**12.5**	**31.7**
(1S,8R)-isomer	3.4	1.5	1.5%	41.4	27.2	36.8	43.6	45.9	72.8	34.8	21.6	39.0	55.6	51.0	23.5	25.7	12.5	31.4

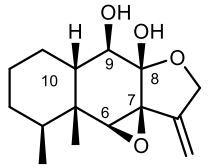
seiricardine ketone



solv.	$CDCl_3$
geometry	ωB97X-D/6-31G*
NMR	ωB97X-D/6-31G* + post semiempirical correction (spartan'18)
energy	ωB97X-V/6-311+G(2df,2p)[6-311G*]
parameters	standard deviation: 2.306 ppm, freedom: 11.38
lit.	M. Nishiyama, W. C. Tayone, H. Maeda, K. Tanaka, M. Hashimoto, Bull Chem. Soc. Jpn. *in press*

	$\lvert\Delta\delta\rvert_{max}$ (ppm)	RMSD (ppm)	DP4	C-1	C-2	C-3	C-3a	C-4	C-5	C-6	C-7	C-7a	C-8	C-9	C-11	C-12	C-13
			exp.	51.3	25.1	36.5	44.7	48.8	73.3	35.5	20.7	41.6	211.9	31.9	23.9	10.9	31.9
seiricardine ketone	**1.0**	**2.2**	**99.1%**	**50.1**	**26.5**	**36.9**	**44.4**	**46.6**	**72.6**	**34.1**	**21.3**	**41.1**	**211.5**	**31.9**	**24.1**	**12.5**	**31.1**
(1R)-isomer	1.9	4.1	0.9%	53.7	26.4	35.9	44.4	47.5	72.5	35.4	23.1	40.9	207.8	28.0	24.3	12.2	31.4

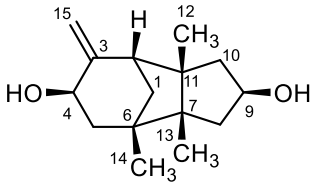
peribysin O



peribysin O

solv.	$CDCl_3$
geometry	ωB97X-D/6-31G*
NMR	ωB97X-D/6-31G* + post semiempirical correction (spartan'18)
energy	ωB97X-V/6-311+G(2df,2p)[6-311G*]
parameters	standard deviation: 2.306 ppm, freedom: 11.38
lit.	newly calculated for this table Inose, K.; Tanaka, K.; Yamada, T.; Koshino, H.; Hashimoto, M., *J. Nat. Prod.* **2019**, *82*, 911.

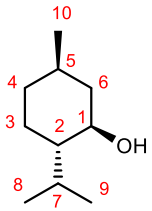
				C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
			exp.	19.9	20	30.7	31.9	38.2	69.6	65.3	98.9	69.6	37.3	142.9	68.1	106.1	16.8	16.9
Label	$\lvert\Delta\delta\rvert_{max}$ (ppm)	RMSD (ppm)	DP4															
peribysin O	**2.9**	**1.3**	**100.0%**	**20.3**	**20.0**	**30.0**	**31.9**	**38.6**	**69.6**	**65.6**	**101.2**	**72.1**	**37.2**	**145.8**	**68.6**	**107.3**	**17.4**	**18.2**
8R-peribysin O	9.9	4.8	0.0%	28.5	22.0	29.8	31.3	39.8	65.1	65.4	104.9	77.7	47.2	144.8	70.7	110.0	17.8	20.8
9S-peribysin O	8.0	3.3	0.0%	27.9	21.5	30.2	31.3	37.3	71.9	66.8	101.9	77.0	35.7	145.0	70.0	109.2	17.5	18.1
10R-peribysin O	8.3	4.5	0.0%	25.8	25.8	29.9	40.2	37.7	75.1	65.9	102.1	74.3	45.5	145.6	69.2	107.5	16.8	12.1
6R7R8R-peribysin O	7.2	2.8	0.0%	21.6	20.1	28.9	30.6	37.8	71.9	66.5	102.8	72.0	44.5	145.2	69.2	105.2	17.8	21.6
6R7R8R10R-peribysin O	6.1	3.5	0.0%	25.7	25.9	29.4	38.0	38.5	72.1	66.3	101.8	75.6	38.7	144.9	69.6	108.8	15.6	13.9
6R7R9S-peribysin O	8.4	3.4	0.0%	21.0	19.3	28.7	38.2	36.7	73.0	63.1	100.7	74.2	39.8	145.8	68.2	106.5	15.3	25.3
6R7R-peribysin O	6.6	3.2	0.0%	21.8	21.6	29.7	33.2	39.1	64.5	69.5	104.6	70.8	43.9	145.4	70.8	108.7	16.9	19.2



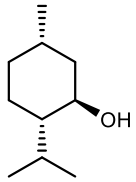
gymnomitran deriv.

solv.	$CDCl_3$
geometry	ωB97X-D/6-31G*
NMR	ωB97X-D/6-31G* + post semiempirical correction (spartan'18)
energy	ωB97X-V/6-311+G(2df,2p)[6-311G*]
parameters	standard deviation: 2.306 ppm, freedom: 11.38
lit.	unpublished results

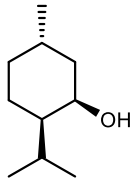
				C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
			exp.	46.1	57.0	153.8	67.9	49.6	46.0	54.6	44.7	77.9	46.5	55.8	29.1	25.0	24.1	107.8
	$\lvert\Delta\delta\rvert_{max}$ (ppm)	RMSD (ppm)	DP4															
4R7R9R11S-isomer	**2.8**	**1.0**	**99.6%**	**46.3**	**55.7**	**153.5**	**67.9**	**50.2**	**44.7**	**55.4**	**44.1**	**78.7**	**45.7**	**55.9**	**29.4**	**25.7**	**25.2**	**110.6**
4R7S9R11R-isomer	8.0	4.4	0.0%	40.7	54.3	152.5	68.6	48.1	44.3	50.6	48.8	69.9	51.8	49.7	22.4	19.5	22.8	110.4
4R7R9S11S-isomer	3.7	1.9	0.4%	45.2	55.7	153.0	68.1	50.3	44.8	51.9	44.1	74.2	45.0	52.5	28.4	24.9	25.0	111.2
4R7S9S11R-isomer	5.9	3.4	0.0%	40.9	55.0	152.8	68.5	48.2	44.7	53.8	48.3	74.5	52.3	52.8	23.2	20.1	23.0	110.2
4S7R9R11S-isomer	6.9	2.7	0.0%	42.2	54.9	154.4	68.1	43.7	44.2	54.2	45.0	77.2	46.5	55.0	28.9	25.8	26.1	114.7
4S7S9R11R-isomer	7.7	5.0	0.0%	39.2	54.6	155.0	68.7	41.9	43.7	50.7	49.5	70.3	51.9	49.9	24.1	20.7	23.7	115.0
4S7R9S11S-isomer	7.1	3.3	0.0%	39.0	53.7	159.3	67.3	44.0	44.4	55.2	45.9	74.5	47.1	56.0	28.3	26.0	26.3	112.3
4S7S9S11R-isomer	7.6	4.2	0.0%	39.4	55.4	155.3	68.7	42.0	44.1	53.9	49.1	74.9	52.2	53.0	25.1	21.3	23.9	114.9



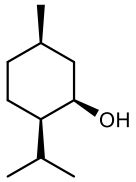
menthol



isomenthol



neomenthol

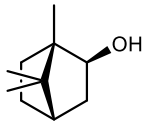


neoisomenthol

solv.	$CDCl_3$
geometry	ωB97X-D/6-31G*
NMR	ωB97X-D/6-31G* + post semiempirical correction (spartan'18)
energy	ωB97X-V/6-311+G(2df,2p)[6-311G*]
parameters	standard deviation: 2.306 ppm, freedom: 11.38
lit.	newly calculated for this table experimental data: :https://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre_index.cgi

		C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10
experimental	(-)-menthol	71.5	50.2	23.3	34.6	31.7	45.1	25.9	16.2	21.0	22.2
	neomenthol	67.8	48.1	24.2	35.2	25.9	42.7	29.2	21.2	20.7	22.4
	(+)-isomenthol	68.0	49.8	19.8	30.7	27.7	40.2	26.3	19.8	20.0	18.3
calculated	menthol	71.1	49.0	24.8	33.3	30.4	44.1	27.2	17.3	20.2	22.3
	isomenthol	67.0	50.0	20.5	30.6	28.2	41.5	27.3	17.5	20.2	18.4
	neomenthol	68.6	46.5	24.5	33.5	25.4	42.3	29.8	20.4	21.0	22.4
	neoisomenthol	69.9	46.7	21.3	30.8	27.2	38.6	29.1	20.7	21.1	20.7

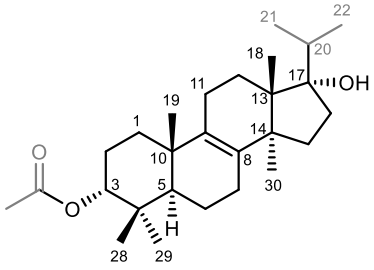
	$\lvert\Delta\delta\rvert_{max}$ (ppm)			RMSD (ppm)			DP4		
	(-)-menthol	neomenthol	(+)-isomenthol	(-)-menthol	neomenthol	(+)-isomenthol	(-)-menthol	neomenthol	(+)-isomenthol
menthol	**1.5**	4.5	5.0	**1.1**	2.4	3.0	**100.0%**	0.1%	0.0%
neomenthol	6.3	**1.7**	4.8	3.3	**0.9**	2.9	0.0%	**99.7%**	0.0%
isomenthol	4.5	4.6	**2.3**	3.0	2.8	**1.0**	0.0%	0.0%	**98.8%**
neoisomenthol	6.5	4.3	3.1	3.6	2.4	1.9	0.0%	0.1%	1.2%



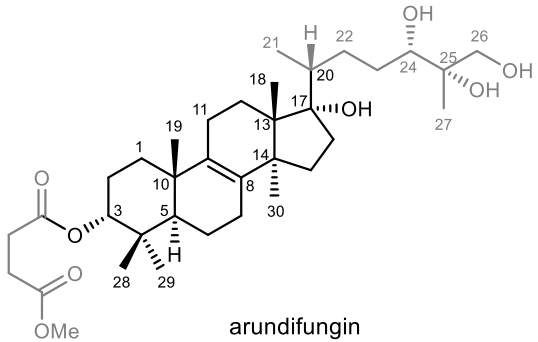
isoborneol

solv.	$CDCl_3$
geometry	ωB97X-D/6-31G*
NMR	ωB97X-D/6-31G* + post semiempirical correction (spartan'18)
energy	ωB97X-V/6-311+G(2df,2p)[6-311G*]
parameters	standard deviation: 2.306 ppm, freedom: 11.38
lit.	newly calculated for this table experimental data: :https://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre_index.cgi

				C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10
			exp.	49.0	79.8	40.5	45.1	27.3	34.0	11.3	46.3	20.5	20.2
	$\lvert\Delta\delta\rvert_{\max}$ (ppm)	RMSD (ppm)	DP4										
isoborneol	**1.5**	**0.7**	**100.0%**	**49.5**	**80.2**	**39.4**	**44.9**	**28.2**	**34.2**	**12.8**	**46.6**	**21.2**	**20.4**
borneol	7.2	2.9	0.0%	50.1	76.9	38.9	44.8	28.8	26.8	15.0	47.8	20.8	19.4



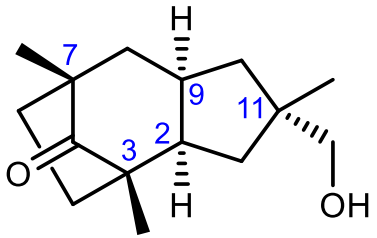
model



arundifungin

solv.	$CDCl_3$
geometry	ωB97X-D/6-31G*
NMR	ωB97X-D/6-31G* + post semiempirical correction (spartan'18)
energy	ωB97X-V/6-311+G(2df,2p)[6-311G*]
parameters	standard deviation: 2.306 ppm, freedom: 11.38
lit.	M. Nishiyama, A. Tonouchi, H. Maeda, H. M.Hashimoto, *Chirality* **2020**, *32*, 17-31.

	$\lvert\Delta\delta\rvert_{max}$ (ppm)	RMSD (ppm)	DP4	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15	C-16	C-17	C-18	C-19	C-28	C-29	C-30
1' (CDCl3)			exp	30.8	23.3	78.5	36.6	45.4	17.9	25.4	135.4	134.0	36.8	20.8	25.2	49.8	50.1	31.4	39.4	85.9	18.6	18.8	21.9	27.3	27.5
model I	**3.5**	**1.3**	**80.1%**	**31.2**	**23.2**	**79.5**	**36.5**	**44.9**	**19.6**	**26.6**	**138.9**	**135.7**	**37.5**	**22.5**	**26.1**	**50.1**	**51.0**	**32.2**	**39.9**	**84.5**	**19.6**	**20.3**	**22.2**	**28.9**	**27.8**
3-isomer	4.0	2.0	0.5%	34.5	23.6	81.0	37.3	49.2	19.7	26.6	138.9	135.6	37.4	22.7	26.1	50.1	50.9	32.3	39.9	84.5	19.7	20.8	17.9	28.3	27.6
5-isomer	10.3	3.6	0.0%	29.1	23.4	77.7	36.9	49.3	24.7	28.0	139.5	134.1	38.5	23.4	26.5	49.5	51.6	31.5	39.7	84.7	19.6	27.6	32.2	27.3	28.0
13-isomer	11.7	3.5	0.0%	30.2	23.2	79.3	36.4	45.3	20.2	29.6	137.1	134.5	38.2	23.0	30.3	49.1	51.6	38.1	39.0	86.9	30.3	20.0	22.4	28.9	23.4
14-isomer	10.9	3.2	0.0%	30.8	22.9	78.9	36.6	46.2	20.1	29.9	136.0	144.9	39.0	24.7	30.1	48.3	51.0	31.4	40.3	87.7	22.6	20.5	22.1	28.8	23.9
17-isomer	4.2	1.7	1.6%	31.1	23.3	79.2	36.5	44.9	19.5	26.5	137.8	136.3	37.5	23.1	29.4	51.1	49.4	31.4	37.9	84.3	20.9	19.9	22.2	28.9	25.0
3,5-isomer	13.7	3.7	0.0%	31.0	24.3	80.7	37.3	44.1	19.1	24.7	140.2	132.3	36.8	24.5	26.3	50.3	51.3	32.0	39.9	84.4	19.4	32.5	28.4	23.8	28.0
3,13-isomer	6.6	2.8	0.0%	33.5	23.6	80.9	37.0	50.1	20.2	29.8	137.4	134.0	38.1	23.0	30.4	49.1	51.5	38.0	38.9	87.1	17.1	20.1	18.4	28.4	23.5
3,14-isomer	9.6	3.4	0.0%	34.0	23.6	80.7	37.3	50.6	20.3	29.9	135.7	143.6	38.9	25.3	29.3	47.8	50.7	31.0	40.3	87.8	22.5	20.8	18.5	28.4	24.9
3,17-isomer	4.1	2.2	0.0%	34.5	23.6	80.7	37.3	49.4	19.7	26.5	137.7	136.0	37.4	23.2	29.3	50.9	49.3	31.6	37.7	84.4	20.9	20.4	18.2	28.3	25.0
5,13-isomer	13.7	5.4	0.0%	34.1	25.3	81.7	38.5	47.7	20.1	25.5	139.6	130.6	37.4	24.1	30.2	49.3	51.7	38.2	39.2	87.0	30.2	32.5	28.2	17.2	23.3
5,14-isomer	14.6	4.8	0.0%	34.0	24.5	81.5	38.6	47.3	20.4	26.1	138.1	138.7	38.4	26.4	29.5	47.8	50.8	31.4	40.6	88.2	22.8	33.4	29.5	18.3	24.7
5,17-isomer	13.4	4.4	0.0%	34.5	25.0	81.0	38.4	48.6	19.2	24.7	139.4	132.3	36.8	24.9	29.7	51.2	49.7	31.2	37.7	84.3	20.7	32.2	28.1	17.5	25.2
13,14-isomer	6.9	2.6	0.0%	30.8	23.3	79.3	36.6	45.3	20.1	27.8	136.8	135.5	37.7	24.3	29.4	50.5	49.5	30.6	37.1	84.5	20.8	21.2	28.8	22.1	25.7
13,17-isomer	7.0	3.0	0.0%	30.2	23.2	79.3	36.4	45.3	20.2	29.6	137.1	134.5	38.2	23.0	30.3	49.1	51.6	38.1	39.0	86.9	17.1	20.0	28.9	22.4	23.4
14,17-isomer	6.9	3.4	0.0%	31.2	23.2	79.2	36.5	45.5	20.0	28.1	133.9	140.6	38.7	23.7	30.0	49.7	50.0	31.0	40.4	85.3	25.2	20.6	28.8	22.1	21.9
3,5,13-isomer	13.7	4.2	0.0%	30.0	24.3	81.3	37.3	43.2	20.0	25.5	139.3	131.0	37.3	24.1	30.3	49.1	51.7	38.2	39.1	87.0	17.1	32.5	28.1	23.7	23.3
3,5,14-isomer	12.8	4.8	0.0%	30.9	24.3	78.4	37.0	47.2	23.4	26.9	135.3	136.5	38.6	26.8	30.7	48.9	51.3	32.1	39.8	87.3	22.9	31.6	27.8	23.3	39.8
3,5,17-isomer	13.5	3.8	0.0%	30.8	24.3	80.6	37.2	43.9	19.1	24.7	139.3	132.8	36.8	25.1	29.7	51.3	49.7	31.2	37.8	84.3	20.7	32.3	28.4	23.6	25.1
3,13,14-isomer	9.2	3.2	0.0%	34.2	23.7	80.7	37.3	50.0	20.1	28.0	137.1	135.1	37.6	24.2	29.3	50.4	49.4	30.6	37.1	84.5	20.7	21.3	28.3	18.1	25.7
3,13-17-isomer	6.6	3.6	0.0%	34.3	23.7	80.5	37.3	50.2	20.5	30.1	138.8	139.9	38.5	24.6	31.8	48.0	50.2	36.2	38.9	88.3	24.4	22.1	18.3	28.3	23.4
3,14,17-isomer	7.5	2.9	0.0%	36.0	23.9	81.0	37.4	48.5	20.2	26.7	137.5	134.8	37.5	21.5	29.9	49.1	51.2	38.9	39.2	86.5	16.8	22.5	17.8	28.2	24.4
5,13,14-isomer	14.6	5.1	0.0%	34.0	24.5	81.5	38.6	47.3	20.4	26.1	138.1	138.8	38.4	26.3	29.5	47.8	50.7	31.4	40.5	88.3	22.7	33.4	29.6	18.3	19.2
5,13,17-isomer	12.8	4.8	0.0%	34.2	24.9	80.6	38.2	48.2	19.1	24.8	136.8	140.7	37.5	25.4	28.7	48.2	50.4	32.2	40.6	87.1	28.7	31.6	28.1	18.5	24.4
5,14,17-isomer	14.8	4.6	0.0%	35.1	24.9	80.9	38.3	48.6	19.5	25.3	138.6	131.4	36.6	22.9	30.3	49.1	51.7	36.4	39.3	86.7	16.8	33.6	27.8	18.0	24.4
13,14,17-isomer	2.9	1.4	17.7%	30.9	23.3	79.4	36.7	45.4	20.2	28.1	138.0	135.0	37.8	23.7	26.5	49.7	51.2	31.3	39.8	84.6	19.5	21.3	22.2	28.9	28.3
3,5,13,14-isomer	14.8	4.0	0.0%	29.9	24.5	81.3	37.4	43.8	19.8	25.0	138.6	132.3	37.1	25.5	29.4	50.3	49.8	30.5	37.3	84.5	21.5	33.6	28.2	24.0	25.7
3,5,13,17-isomer	12.8	4.0	0.0%	30.9	24.3	79.9	37.1	43.6	18.9	24.5	136.7	141.4	37.5	25.7	29.1	48.2	50.5	32.3	40.4	87.2	22.3	31.6	28.3	24.3	24.4
3,5,14,17-isomer	14.0	3.9	0.0%	31.9	24.4	80.3	37.2	44.8	19.8	25.8	138.4	132.1	37.0	23.3	30.3	49.1	51.6	36.5	39.1	86.6	16.9	32.8	28.1	24.5	24.3
3,13,14,17-isomer	4.7	2.1	0.1%	34.3	23.7	80.9	37.3	50.1	20.2	28.1	138.2	134.6	37.6	23.7	26.4	49.6	51.2	31.3	39.7	84.6	19.5	21.4	18.1	28.4	28.2
5,13,14,17-isomer	14.7	4.7	0.0%	34.3	25.4	81.6	38.6	47.9	19.9	25.2	140.0	131.2	37.1	24.9	21.6	51.5	51.4	31.1	38.6	84.5	20.2	33.5	28.7	17.3	31.1
3,5,13,14,17-isomer	14.8	4.0	0.0%	30.0	24.5	81.2	37.3	43.8	19.8	25.3	140.0	131.3	37.0	25.0	26.6	49.7	51.7	31.1	39.7	84.5	20.1	33.6	28.4	24.0	28.5



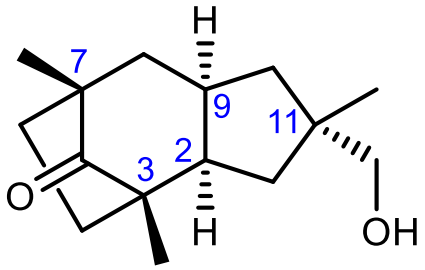
(2*R*,3*S*,7*R*,9*R*,11*S*)
the mirror image of natural product

solv.	$CDCl_3$
geometry	ωB97X-D/6-31G*
NMR	ωB97X-D/6-31G* + post semiempirical correction (spartan'18)
energy	ωB97X-V/6-311+G(2df,2p)[6-311G*]
parameters	standard deviation: 2.306 ppm, freedom: 11.38
lit.	

その1

	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
experimental	36.7	59.3	48.4	32.3	29.0	222.4	46.2	48.6	35.5	40.6	43.8	71.9	27.5	18.4	19.8
repraesentin B[a]	36.8	58.6	48.5	32.5	29.0	222.3	46.2	48.2	35.2	40.6	44.4	72.7	26.7	18.5	19.7
(2R,3S,7R,9R,11S)	37.2	58.5	48.5	32.5	29.2	221.4	46.0	47.3	36.3	39.9	43.5	73.2	27.5	19.8	20.7
(2R,3S,7R,9R,11R)	35.9	57.5	48.2	32.4	29.2	221.5	46.0	46.0	35.9	40.2	44.2	72.1	27.1	19.8	20.6
(2R,3S,7R,9S,11R)	38.5	54.2	47.1	34.6	35.3	220.9	41.6	47.2	38.7	41.6	42.9	72.4	26.5	16.5	22.2
(2R,3S,7R,9S,11S)	39.4	55.0	47.2	34.5	35.3	221.2	41.7	47.2	37.8	40.6	42.8	72.6	26.4	16.5	22.2
(2S,3S,7R,9R,11R)	36.2	55.7	48.7	25.9	31.0	221.4	45.4	43.0	37.4	39.6	43.2	72.4	26.5	18.4	20.9
(2S,3S,7R,9R,11S)	35.0	55.1	48.8	26.0	31.0	221.7	45.5	43.1	38.5	40.8	43.0	72.8	26.4	18.5	21.0
(2S,3S,7R,9S,11S)	38.0	53.0	50.6	25.0	30.4	223.2	45.5	43.6	34.7	41.6	43.4	70.9	25.2	20.4	21.8
(2S,3S,7R,9S,11R)	39.3	54.1	50.2	26.5	30.3	223.0	45.4	43.5	34.7	42.9	43.4	71.1	24.6	20.2	21.6

	vs experimental			repraesentin B[b]			
	RMSD	max deviation	DP4	RMSD	max deviation	DP4	
(2R,3S,7R,9R,11S)	0.8	1.4	66.7%	0.7	1.3	64.3%	proposed diastereomer
(2R,3S,7R,9R,11R)	1.0	2.6	33.3%	0.9	2.2	35.7%	the 11-epimer
(2R,3S,7R,9S,11R)	2.9	6.3	0.0%	2.9	6.3	0.0%	
(2R,3S,7R,9S,11S)	2.8	6.3	0.0%	2.8	6.3	0.0%	
(2S,3S,7R,9R,11R)	2.6	6.4	0.0%	2.6	6.6	0.0%	
(2S,3S,7R,9R,11S)	2.7	6.3	0.0%	2.7	6.5	0.0%	
(2S,3S,7R,9S,11S)	3.1	7.4	0.0%	3.1	7.5	0.0%	
(2S,3S,7R,9S,11R)	2.9	5.9	0.0%	2.8	6.0	0.0%	

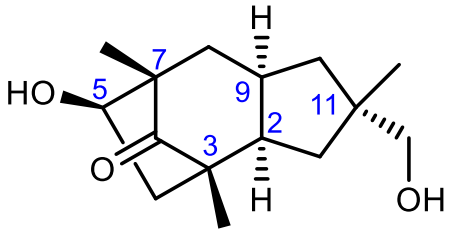


(2*R*,3*S*,7*R*,9*R*,11*S*)
the mirror image of natural product

solv.	$CDCl_3$
geometry	ωB97X-D/6-31G*
NMR	ωB97X-D/6-31G* + post semiempirical correction (spartan'18)
energy	ωB97X-V/6-311+G(2df,2p)[6-311G*]
parameter s	standard deviation: 2.306 ppm, freedom: 11.38
lit.	

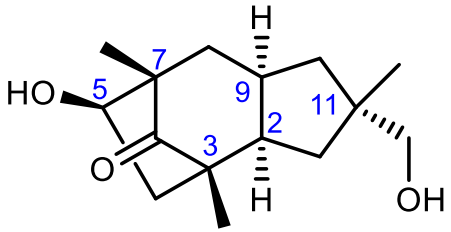
	Hb-1	Ha-1	H-2	Hb-4	Ha-4	Hb-5	Ha-5	Ha-8	Hb-8	H-9	Hb-10	Ha-10	H-12	H-12	H-13	H-14	H-15
experimental	1.67	1.05	2.27	1.98	1.63	1.95	1.58	1.64	1.74	2.52	1.75	1.11	3.24	3.29	1.06	0.95	0.96
repraesentin B[a]	1.32	1.19	2.37	2.01	1.64	1.95	1.59	1.58	1.7	2.55	1.54	1.33	3.34	3.34	0.99	0.97	0.94
(2R,3S,7R,9R,11S)	1.68	1.37	2.33	1.93	1.61	1.90	1.58	1.64	1.74	2.40	1.97	1.18	3.30	3.30	1.00	0.96	0.95
(2R,3S,7R,9R,11R)	1.50	1.30	2.33	1.94	1.63	1.89	1.58	1.50	1.91	2.40	1.52	1.51	3.33	3.35	0.97	0.96	0.93
(2R,3S,7R,9S,11R)	1.59	1.42	2.23	1.78	1.31	1.95	1.84	1.48	1.83	1.60	1.79	0.90	3.34	3.36	1.01	0.99	1.03
(2R,3S,7R,9S,11S)	1.80	1.29	2.30	1.77	1.29	1.97	1.83	1.52	1.84	1.63	1.40	1.32	3.39	3.36	0.97	0.98	1.03
(2S,3S,7R,9R,11R)	1.59	1.14	1.69	1.92	1.39	1.79	1.58	1.61	1.35	2.04	1.39	1.31	3.39	3.37	1.07	0.95	0.97
(2S,3S,7R,9R,11S)	1.69	1.45	2.30	2.06	1.45	1.97	1.68	1.79	1.88	2.24	1.86	1.81	3.44	3.28	1.11	0.89	0.96
(2S,3S,7R,9S,11S)	2.02	1.50	2.35	2.57	1.31	1.95	1.64	1.81	1.91	2.28	2.40	1.20	3.53	3.53	0.93	0.90	0.96
(2S,3S,7R,9S,11R)	1.77	1.45	2.30	2.07	1.46	1.97	1.68	1.79	1.88	2.25	1.83	1.80	3.44	3.31	1.13	0.89	0.96

	vs experimental			vs. repraesentin B			
	RMSD	max deviation	DP4	RMSD	max deviation	DP4	
(2R,3S,7R,9R,11S)	0.10	0.32	99.5%	0.16	0.70	1.5%	proposed diastereomer
(2R,3S,7R,9R,11R)	0.15	0.40	0.5%	0.10	0.70	98.5%	the 11-epimer
(2R,3S,7R,9S,11R)	0.28	0.91	0.0%	0.30	0.71	0.0%	
(2R,3S,7R,9S,11S)	0.28	0.88	0.0%	0.29	0.70	0.0%	
(2S,3S,7R,9R,11R)	0.24	0.58	0.0%	0.25	0.69	0.0%	
(2S,3S,7R,9R,11S)	0.23	0.70	0.0%	0.22	0.68	0.0%	
(2S,3S,7R,9S,11S)	0.30	0.65	0.0%	0.34	0.71	0.0%	
(2S,3S,7R,9S,11R)	0.23	0.69	0.0%	0.22	0.68	0.0%	



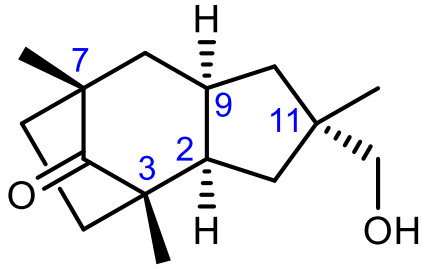
(2*R*,3*S*,5*R*,7*R*,9*R*,11*S*)
the mirror image of natural product

	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
	36.5	59.2	48.5	45.7	71.6	221.0	51.8	47.6	35.2	40.8	44.3	71.9	27.6	18.7	14.3
(2*R*,3*S*,5*R*,7*S*,9*R*,11*S*)	37.0	58.3	48.6	44.5	72.9	220.6	51.8	45.9	35.8	39.9	43.7	73.1	27.5	19.7	15.2
(2*R*,3*S*,5*R*,7*S*,9*R*,11*R*)	35.4	57.5	48.3	44.2	73.0	221.0	51.9	44.0	35.5	40.3	44.5	71.2	27.3	19.8	15.0
(2*R*,3*S*,5*R*,7*S*,9*S*,11*R*)	38.5	55.0	47.7	46.9	78.9	220.4	47.6	46.3	39.1	41.6	43.0	72.6	26.5	16.6	15.6
(2*R*,3*S*,5*R*,7*S*,9*S*,11*S*)	39.4	55.5	47.5	46.7	78.4	219.6	47.4	46.0	38.0	40.2	42.7	72.5	26.3	16.5	15.6
(2*R*,3*S*,5*S*,7*S*,9*R*,11*S*)	37.7	59.7	50.4	44.1	73.5	222.5	52.1	43.6	35.9	40.5	44.0	73.7	27.9	19.8	19.5
(2*S*,3*S*,5*R*,7*S*,9*R*,11*S*)	35.1	54.6	49.1	38.1	74.1	221.0	51.1	41.7	38.0	40.9	43.1	72.7	26.3	18.3	15.5
(2*S*,3*S*,5*R*,7*S*,9*S*,11*S*)	38.0	52.5	50.7	37.1	73.9	222.6	51.8	42.1	34.2	41.6	43.6	70.4	25.4	20.3	15.8
(2*S*,3*S*,5*R*,7*S*,9*R*,11*R*)	36.6	55.4	49.3	38.2	74.6	221.9	51.3	41.7	37.2	39.8	43.6	72.7	26.6	18.4	15.6
(2*S*,3*S*,5*R*,7*S*,9*S*,11*R*)	39.6	53.7	50.4	38.8	74.1	223.1	51.9	42.0	34.2	43.3	43.6	71.4	24.6	20.2	15.7
(2*R*,3*S*,5*S*,7*S*,9*R*,11*R*)	36.1	58.6	49.6	43.6	72.9	221.1	51.8	41.4	35.2	40.4	44.3	71.3	27.2	19.8	19.2
(2*R*,3*S*,5*S*,7*S*,9*S*,11*S*)	39.2	55.2	47.4	46.0	74.1	220.6	48.1	35.5	37.4	40.3	42.9	72.6	26.3	16.5	21.3
(2*R*,3*S*,5*S*,7*S*,9*S*,11*R*)	38.4	54.0	47.3	45.6	74.2	220.5	48.0	35.7	38.5	41.0	43.0	72.5	26.4	16.5	21.3
(2*S*,3*S*,5*S*,7*S*,9*R*,11*S*)	35.2	55.7	50.2	37.5	73.8	221.2	50.9	38.5	37.4	40.6	43.0	72.8	26.3	18.3	19.5
(2*S*,3*S*,5*S*,7*S*,9*S*,11*S*)	38.4	54.3	51.8	35.8	73.4	222.8	51.1	38.6	34.0	40.2	43.7	70.4	25.9	20.4	20.3
(2*S*,3*S*,5*S*,7*S*,9*S*,11*R*)	38.4	54.3	51.8	35.8	73.4	222.8	51.1	38.6	34.0	40.1	43.7	70.4	25.8	20.4	20.3
(2*S*,3*S*,5*S*,7*S*,9*R*,11*R*)	35.2	55.7	50.2	37.5	73.8	221.2	50.9	38.5	37.4	40.6	43.0	72.8	26.3	18.3	19.5



(2*R*,3*S*,5*R*,7*R*,9*R*,11*S*)
the mirror image of natural product

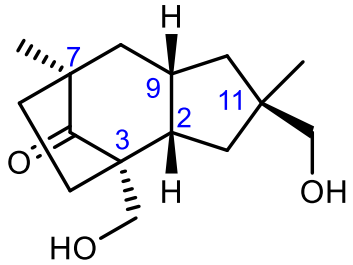
	Hα-1	Hβ-1	H-2	Hα-4	Hβ-4	H-5	Hα-8	Hβ-8	H-9	Hα-10	Hβ-10	H-12	H-12	H-13	H-14	H-15
	1.07	1.67	2.28	1.55	2.62	4.18	1.66	1.85	2.35	1.05	1.75	3.23	3.28	1.06	1.01	0.98
(2*R*,3*S*,5*R*,7*S*,9*R*,11*S*)	1.36	1.68	2.32	1.68	2.45	4.08	1.63	1.70	2.21	1.12	1.96	3.28	3.30	0.98	1.02	0.90
(2*R*,3*S*,5*R*,7*S*,9*R*,11*R*)	1.25	1.55	2.32	1.72	2.45	4.07	1.45	2.03	2.21	1.48	1.61	3.30	3.32	0.92	1.02	0.86
(2*R*,3*S*,5*R*,7*S*,9*S*,11*R*)	1.39	1.57	2.08	1.24	2.47	4.18	1.43	1.85	1.58	0.86	1.77	3.34	3.36	0.99	1.02	0.94
(2*R*,3*S*,5*R*,7*S*,9*S*,11*S*)	1.25	1.78	2.15	1.20	2.45	4.16	1.47	1.84	1.59	1.32	1.34	3.34	3.37	0.95	1.01	0.94
(2*R*,3*S*,5*S*,7*S*,9*R*,11*S*)	1.37	1.75	2.48	2.00	2.03	3.95	1.63	2.07	2.88	1.21	1.92	3.33	3.33	1.03	0.96	0.93
(2*S*,3*S*,5*R*,7*S*,9*R*,11*S*)	1.20	1.66	1.64	1.50	2.52	3.94	1.24	1.59	1.94	0.94	1.76	3.42	3.45	0.96	1.02	0.91
(2*S*,3*S*,5*R*,7*S*,9*S*,11*S*)	1.49	2.04	2.33	1.37	3.23	4.15	1.77	1.89	2.24	1.14	2.32	3.52	3.53	0.90	0.96	0.92
(2*S*,3*S*,5*R*,7*S*,9*R*,11*R*)	1.10	1.59	1.66	1.52	2.44	3.98	1.31	1.60	1.80	1.29	1.35	3.38	3.41	1.05	1.02	0.92
(2*S*,3*S*,5*R*,7*S*,9*S*,11*R*)	1.44	1.77	2.29	1.54	2.66	4.17	1.74	1.86	2.24	1.66	1.78	3.31	3.42	1.12	0.96	0.92
(2*R*,3*S*,5*S*,7*S*,9*R*,11*R*)	1.27	1.57	2.49	2.00	2.04	3.91	1.85	1.92	2.85	1.51	1.61	3.32	3.34	0.94	0.95	0.87
(2*R*,3*S*,5*S*,7*S*,9*S*,11*S*)	1.22	1.79	2.49	1.59	1.77	3.90	1.35	2.30	1.60	1.30	1.39	3.37	3.38	0.97	0.95	1.01
(2*R*,3*S*,5*S*,7*S*,9*S*,11*R*)	1.51	1.38	2.51	1.60	1.83	3.90	1.33	2.25	1.54	1.00	1.73	3.33	3.35	1.02	0.96	0.99
(2*S*,3*S*,5*S*,7*S*,9*R*,11*S*)	1.22	1.70	1.74	1.77	2.05	3.90	1.18	1.99	2.55	0.96	1.73	3.43	3.46	0.99	0.96	0.93
(2*S*,3*S*,5*S*,7*S*,9*S*,11*S*)	1.51	2.26	2.46	1.67	2.80	3.96	1.74	2.26	2.32	1.03	3.01	3.49	3.49	0.89	0.90	0.91
(2*S*,3*S*,5*S*,7*S*,9*S*,11*R*)	1.51	2.26	2.46	1.67	2.79	3.96	1.74	2.26	2.32	1.02	3.00	3.49	3.49	0.89	0.90	0.91
(2*S*,3*S*,5*S*,7*S*,9*R*,11*R*)	1.22	1.70	1.74	1.77	2.05	3.90	1.18	1.99	2.55	0.96	1.73	3.43	3.46	0.99	0.96	0.93



(2*R*,3*S*,7*R*,9*R*,11*S*)
the mirror image of natural product

その3

	^{13}C RMSD (ppm)	max dev (ppm)	DP4	^{1}H RMSD (ppm)	max dev (ppm)	DP4	^{1}H +^{13}C DP4	
(2*R*,3*S*,5*R*,7*S*,9*R*,11*S*)	0.9	1.7	77.3%	0.12	0.29	94.9%	99.7%	proposed diasteromer
(2*R*,3*S*,5*R*,7*S*,9*R*,11*R*)	1.3	3.6	22.2%	0.17	0.43	0.9%	0.3%	11-epimer
(2*R*,3*S*,5*R*,7*S*,9*S*,11*R*)	2.9	7.3	0.0%	0.25	0.77	0.0%	0.0%	
(2*R*,3*S*,5*R*,7*S*,9*S*,11*S*)	2.7	6.8	0.0%	0.26	0.76	0.0%	0.0%	
(2*R*,3*S*,5*S*,7*S*,9*R*,11*S*)	2.0	5.2	0.1%	0.27	0.59	0.0%	0.0%	
(2*S*,3*S*,5*R*,7*S*,9*R*,11*S*)	3.0	7.6	0.0%	0.25	0.64	0.0%	0.0%	
(2*S*,3*S*,5*R*,7*S*,9*S*,11*S*)	3.4	8.6	0.0%	0.28	0.61	0.0%	0.0%	
(2*S*,3*S*,5*R*,7*S*,9*R*,11*R*)	2.9	7.5	0.0%	0.27	0.62	0.0%	0.0%	
(2*S*,3*S*,5*R*,7*S*,9*S*,11*R*)	3.2	6.9	0.0%	0.19	0.61	4.3%	0.0%	
(2*R*,3*S*,5*S*,7*S*,9*R*,11*R*)	2.2	6.2	0.3%	0.28	0.58	0.0%	0.0%	
(2*R*,3*S*,5*S*,7*S*,9*S*,11*S*)	4.1	12.1	0.0%	0.35	0.85	0.0%	0.0%	
(2*R*,3*S*,5*S*,7*S*,9*S*,11*R*)	4.2	11.9	0.0%	0.35	0.81	0.0%	0.0%	
(2*S*,3*S*,5*S*,7*S*,9*R*,11*S*)	3.7	9.1	0.0%	0.27	0.57	0.0%	0.0%	
(2*S*,3*S*,5*S*,7*S*,9*S*,11*S*)	4.3	9.9	0.0%	0.40	1.26	0.0%	0.0%	
(2*S*,3*S*,5*S*,7*S*,9*S*,11*R*)	4.3	9.9	0.0%	0.40	1.25	0.0%	0.0%	
(2*S*,3*S*,5*S*,7*S*,9*R*,11*R*)	3.7	9.1	0.0%	0.27	0.57	0.0%	0.0%	

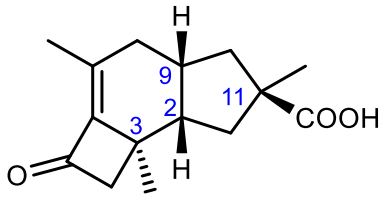


(2*S*,3*R*,7*S*,9*S*,11*R*)
natural enantiomer

	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
	36.5	55.5	54.6	27.7	29.7	220.9	47.3	49.9	36.5	41.1	45.1	71.7	28.4	63.3	19.9
(2*R*,3*R*,7*S*,9*R*,11*R*)	37.0	48.2	55.5	20.1	30.3	229.8	46.3	43.9	34.2	41.5	43.5	70.3	25.2	65.3	21.1
(2*R*,3*R*,7*S*,9*R*,11*S*)	38.6	49.4	55.2	21.9	30.3	229.5	46.2	43.7	34.2	43.3	43.5	71.1	24.5	65.1	21.0
(2*R*,3*R*,7*S*,9*S*,11*R*)	34.1	51.5	54.2	21.4	30.9	227.6	46.4	43.3	37.9	40.5	43.4	72.8	26.2	64.7	20.2
(2*R*,3*R*,7*S*,9*S*,11*S*)	35.9	52.2	53.8	21.4	31.0	227.6	46.5	43.5	37.0	38.7	43.4	72.6	26.3	64.6	20.2
(2*S*,3*R*,7*S*,9*R*,11*R*)	36.7	55.4	52.1	29.4	35.1	228.4	42.8	47.5	38.8	40.3	43.3	72.6	26.4	65.4	21.5
(2*S*,3*R*,7*S*,9*R*,11*S*)	35.5	53.9	53.6	28.7	35.3	228.0	42.8	47.1	40.2	43.9	45.0	75.6	26.1	66.6	21.5
(2*S*,3*R*,7*S*,9*S*,11*R*)	37.8	55.6	54.2	26.7	29.0	226.8	46.7	46.8	36.7	39.0	43.6	73.1	27.7	65.3	20.2
(2*S*,3*R*,7*S*,9*S*,11*S*)	36.0	55.0	53.6	26.8	29.2	227.0	46.7	45.2	36.3	39.2	44.4	71.1	27.1	65.6	20.0

	Hα-1	Hβ-1	H-2	Hα-4	Hβ-H	Hα-5	Hβ-5	H-8	H-8	H-9	Hα-10	Hβ-10	H-12	H-12	H-13	H-14	H-14	H-15
	0.96	1.71	2.52	2.06	1.88	1.56	2.01	1.58	1.75	2.56	1.03	1.78	3.13	3.19	1.03	3.37	3.59	0.87
(2*R*,3*R*,7*S*,9*R*,11*R*)	1.52	2.02	2.98	2.48	1.41	1.63	1.99	1.91	1.85	2.34	1.20	2.54	3.53	3.53	0.92	3.39	3.46	0.94
(2*R*,3*R*,7*S*,9*R*,11*S*)	1.36	1.78	2.93	1.84	1.58	1.67	1.99	1.88	1.82	2.33	1.82	1.87	3.33	3.46	1.11	3.38	3.44	0.94
(2*R*,3*R*,7*S*,9*S*,11*R*)	1.36	1.62	2.14	1.75	1.49	1.55	1.81	1.32	1.62	2.21	1.00	1.80	3.44	3.46	1.00	3.51	3.55	0.94
(2*R*,3*R*,7*S*,9*S*,11*S*)	1.12	1.64	2.26	1.65	1.38	1.57	1.82	1.43	1.65	2.05	1.39	1.56	3.36	3.43	1.02	3.41	3.60	0.95
(2*S*,3*R*,7*S*,9*R*,11*R*)	1.77	2.30	2.36	1.49	1.41	1.81	1.97	1.88	1.58	1.75	1.39	1.40	3.36	3.41	0.98	3.66	3.75	1.02
(2*S*,3*R*,7*S*,9*R*,11*S*)	1.59	2.11	2.33	1.47	1.13	1.80	1.98	1.87	1.40	2.73	1.16	1.85	3.37	3.45	0.88	3.66	3.82	1.03
(2*S*,3*R*,7*S*,9*S*,11*R*)	1.34	1.90	2.30	2.07	1.64	1.56	1.90	1.78	1.66	2.47	1.15	1.97	3.29	3.31	1.00	3.32	3.73	0.94
(2*S*,3*R*,7*S*,9*S*,11*S*)	1.57	2.31	2.31	2.03	1.65	1.56	1.89	2.12	1.50	2.46	1.63	1.47	3.32	3.35	0.92	3.36	3.71	0.92

	^{13}C			^{1}H			^{1}H+^{13}C	
	RMSD	max dev	DP4	RMSD	max dev	DP4	DP4	
(2*R*,3*R*,7*S*,9*R*,11*R*)	4.1	8.9	0.0%	0.34	0.76	0.0%	0.0%	
(2*R*,3*R*,7*S*,9*R*,11*S*)	3.8	8.6	0.0%	0.28	0.79	0.0%	0.0%	
(2*R*,3*R*,7*S*,9*S*,11*R*)	3.3	6.7	0.0%	0.24	0.40	0.0%	0.0%	
(2*R*,3*R*,7*S*,9*S*,11*S*)	3.2	6.7	0.0%	0.25	0.51	0.0%	0.0%	
(2*S*,3*R*,7*S*,9*R*,11*R*)	3.1	7.5	0.0%	0.40	0.81	0.0%	0.0%	
(2*S*,3*R*,7*S*,9*R*,11*S*)	3.3	7.1	0.0%	0.34	0.75	0.0%	0.0%	
(2*S*,3*R*,7*S*,9*S*,11*R*)	2.0	5.9	69.5%	0.16	0.38	100.0%	100.0%	proposed diastereomer
(2*S*,3*R*,7*S*,9*S*,11*S*)	2.2	6.1	30.5%	0.31	0.61	0.0%	0.0%	11-epimer

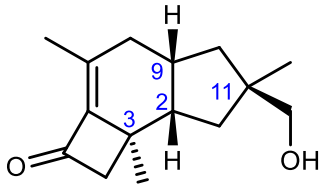


(2*S*,3*R*,9*R*,11*R*)
the natural enantiomer

	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
experimental	37.8	47.2	36.5	60.9	197.0	150.6	143.1	35.4	42.0	45.1	51.0	182.0	24.8	20.4	20.4
(2*R*,3*R*,9*R*11*R*)	38.1	49.9	39.3	47.9	195.0	147.3	138.8	35.5	44.6	41.5	47.5	178.4	26.6	28.6	19.9
(2*R*,3*R*,9*S*,11*R*)	40.1	45.2	35.9	53.1	195.0	143.8	139.0	32.5	37.4	43.2	47.5	178.7	25.3	26.4	19.4
(2*R*,3*R*,9*R*,11*S*)	39.2	50.2	39.0	47.9	195.2	147.5	138.7	35.5	44.1	40.1	47.5	178.4	26.4	28.6	19.9
(2*R*,3*R*,9*S*,11*S*)	42.0	45.1	36.2	54.3	195.2	146.7	139.9	33.3	38.4	45.4	48.7	178.1	24.0	24.2	20.6
(2*S*,3*R*,9*R*,11*R*)	37.7	47.8	36.7	58.6	194.3	150.3	142.0	34.7	41.9	45.9	50.6	178.2	24.2	20.8	19.3
(2*S*,3*R*,9*S*,11*R*)	40.0	49.8	36.4	54.3	195.4	146.8	137.7	37.4	37.3	42.2	47.3	178.9	26.3	21.2	18.5
(2*S*,3*R*,9*R*,11*S*)	38.0	49.0	37.1	58.7	194.3	150.3	141.5	34.7	42.1	45.5	49.2	177.7	23.6	20.7	19.3
(2*S*,3*R*,9*S*,11*S*)	37.0	50.4	36.9	54.4	195.4	147.3	137.5	36.8	37.6	44.7	47.3	179.1	26.1	21.4	18.5

	Hβ-1	Hα-1	H-2	Hβ-4	Hα-4	Hβ-8	Hα-8	H-9	Hα-10	Hβ-10	H-13	H-14	H-15
experimental	1.51	2.37	2.29	2.74	2.68	2.25	1.82	2.45	1.17	2.41	1.40	1.16	2.01
(2*R*,3*R*,9*R*11*R*)	1.8	2.0	1.80	2.66	1.97	1.85	1.77	1.86	1.13	2.26	1.35	1.32	1.86
(2*R*,3*R*,9*S*,11*R*)	1.7	1.8	2.36	2.74	2.31	2.13	2.14	2.41	1.64	2.28	1.33	1.28	1.87
(2*R*,3*R*,9*R*,11*S*)	1.2	2.5	2.02	2.54	1.96	1.86	1.86	1.62	1.58	2.01	1.31	1.32	1.86
(2*R*,3*R*,9*S*,11*S*)	1.2	2.3	2.51	2.85	2.40	2.13	1.80	2.72	1.03	2.51	1.27	1.22	1.94
(2*S*,3*R*,9*R*,11*R*)	1.5	2.4	2.40	2.66	2.47	2.11	1.81	2.49	1.19	2.38	1.37	1.16	1.92
(2*S*,3*R*,9*S*,11*R*)	1.4	2.3	1.85	2.59	2.30	2.29	1.73	1.98	1.76	2.12	1.35	1.16	1.82
(2*S*,3*R*,9*R*,11*S*)	1.7	2.5	2.17	2.59	2.50	2.16	1.93	2.51	1.83	2.07	1.28	1.23	1.93
(2*S*,3*R*,9*S*,11*S*)	1.6	2.3	1.66	2.55	2.32	2.27	1.60	2.24	1.09	2.42	1.34	1.24	1.82

	^{13}C			^{1}H			^{1}H+^{13}C	
	RMSD (ppm)	max dev (ppm)	DP4	RMSD (ppm)	max dev (ppm)	DP4	DP4	
(2*R*,3*R*,9*R*11*R*)	4.7	13.0	0.0%	0.34	0.71	0.0%	0.0%	
(2*R*,3*R*,9*S*,11*R*)	3.9	7.8	0.0%	0.27	0.62	0.0%	0.0%	
(2*R*,3*R*,9*R*,11*S*)	4.8	13.0	0.0%	0.39	0.83	0.0%	0.0%	
(2*R*,3*R*,9*S*,11*S*)	3.1	6.6	0.0%	0.18	0.34	0.1%	0.0%	
(2*S*,3*R*,9*R*,11*R*)	1.5	3.8	87.3%	0.09	0.21	99.9%	100.0%	proposed diastereomer
(2*S*,3*R*,9*S*,11*R*)	3.3	6.6	0.0%	0.29	0.59	0.0%	0.0%	
(2*S*,3*R*,9*R*,11*S*)	1.7	4.3	12.7%	0.24	0.66	0.0%	0.0%	11-epimer
(2*S*,3*R*,9*S*,11*S*)	3.2	6.5	0.0%	0.24	0.63	0.0%	0.0%	

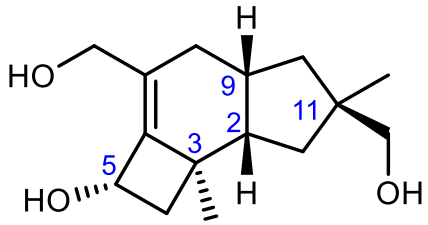


(2*S*,3*R*,9*R*,11*R*)
the natural enantiomer

	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
experiential	36.2	47.4	36.8	60.9	197.2	150.7	143.3	35.8	41.8	43.6	45.5	69.4	24.5	20.4	20.4
(2*R*,3*R*,9*R*,11*R*)	36.3	49.8	39.4	47.8	195.4	147.2	139.1	35.9	44.9	39.9	43.3	72.5	26.5	28.7	19.9
(2*R*,3*R*,9*S*,11*R*)	37.6	45.2	36.0	53.4	195.3	144.8	139.2	33.4	37.5	43.1	43.3	71.4	24.5	26.0	19.8
(2*R*,3*S*,9*R*,11*R*)	35.7	50.1	36.8	54.5	195.7	147.2	137.6	37.5	38.0	43.4	42.7	72.9	26.7	21.5	18.5
(2*R*,3*S*,9*S*,11*R*)	35.2	47.9	36.9	58.8	194.5	150.4	142.2	35.3	42.4	42.6	45.6	71.5	22.4	20.9	19.2
(2*S*,3*R*,9*R*,11*R*)	35.9	48.8	36.9	58.7	194.5	150.3	142.4	35.3	42.5	43.8	45.5	69.9	24.3	20.7	19.3
(2*S*,3*R*,9*S*,11*R*)	37.1	50.6	36.5	54.5	195.7	147.1	137.5	37.4	37.0	42.2	42.6	72.8	26.6	21.5	18.5
(2*S*,3*S*,9*R*,11*R*)	39.0	45.7	36.2	53.6	195.4	145.6	138.6	34.3	38.0	43.6	43.2	71.0	25.6	25.6	20.0
(2*S*,3*S*,9*S*,11*R*)	37.4	50.2	39.3	47.8	195.3	147.3	139.1	35.8	44.0	38.7	43.2	72.6	26.3	28.7	20.0

	Hα-1	Hβ-1	H-2	H-4	H-4	H-8	H-8	H-9	Hα-10	Hβ-10	H-12	H-12	H-13	H-14	H-15
experiential	1.43	1.73	2.18	2.66	2.69	1.43	2.25	2.41	1.06	1.92	3.4	3.43	1.13	1.18	2.01
(2*R*,3*R*,9*R*,11*R*)	1.43	1.73	2.18	2.66	2.69	1.43	2.25	2.41	1.06	1.92	3.4	3.43	1.13	1.18	2.01
(2*R*,3*R*,9*S*,11*R*)	1.54	1.54	1.82	2.62	1.95	1.76	1.83	1.71	1.07	1.79	3.40	3.42	1.05	1.31	1.85
(2*R*,3*S*,9*R*,11*R*)	1.33	1.46	2.45	2.32	2.78	2.07	2.10	2.48	1.53	1.59	3.40	3.41	1.02	1.27	1.89
(2*R*,3*S*,9*S*,11*R*)	1.46	1.79	1.70	2.31	2.56	1.60	2.27	2.07	1.02	2.04	1.04	3.42	3.45	1.20	1.81
(2*S*,3*R*,9*R*,11*R*)	1.44	1.83	2.30	2.48	2.60	1.86	2.12	2.55	1.43	1.53	3.49	3.50	1.05	1.18	1.93
(2*S*,3*R*,9*S*,11*R*)	1.52	1.74	2.18	2.48	2.59	1.83	2.12	2.51	1.13	1.99	3.49	3.52	1.08	1.18	1.92
(2*S*,3*S*,9*R*,11*R*)	1.32	1.81	1.73	2.30	2.56	1.65	2.28	2.02	1.43	1.65	3.44	3.43	1.06	1.19	1.81
(2*S*,3*S*,9*S*,11*R*)	1.17	1.77	2.43	2.34	2.83	1.80	2.17	2.48	1.16	1.93	3.44	3.45	1.01	1.25	1.91
(2*R*,3*R*,9*R*,11*R*)	1.09	1.90	1.86	1.94	2.56	1.84	1.83	1.64	1.37	1.54	3.43	3.45	1.04	1.30	1.86

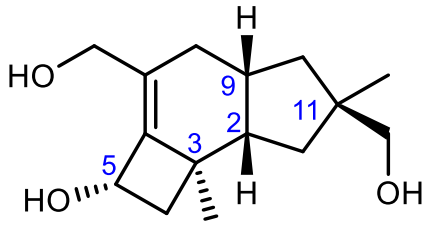
	^{13}C			^{1}H			^{1}H+^{13}C	
	RMSD (ppm)	max dev (ppm)	DP4	RMSD (ppm)	max dev (ppm)	DP4	DP4	
2R3R9R11R	4.7	13.1	0.0%	0.32	0.74	0.0%	0.0%	
(2R3R9S11R)	3.5	7.5	0.0%	0.27	0.64	0.0%	0.0%	
(2R3S9R11R)	3.1	6.4	0.0%	0.88	2.36	0.0%	0.0%	
(2R3S9S11R)	1.3	2.7	12.3%	0.20	0.43	0.2%	0.0%	11-epimer
(2S3R9R11R)	1.1	2.7	87.7%	0.14	0.40	97.2%	100.0%	proposed diastereomer
(2S3R9S11R)	3.2	6.4	0.0%	0.24	0.45	0.0%	0.0%	
(2S3S9R11R)	3.4	7.3	0.0%	0.17	0.37	2.6%	0.0%	
(2S3S9S11R)	4.7	13.1	0.0%	0.37	0.77	0.0%	0.0%	



(2*S*,3*R*,5*S*,9*R*,11*R*)
the natural enantiomer

その1

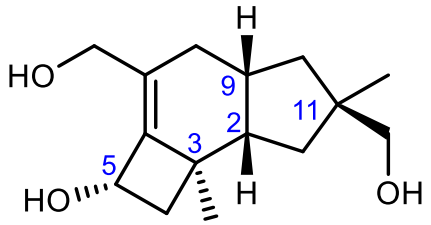
	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
experiential	35.7	47.3	43.1	46.6	69.3	146.1	134.1	29.4	41.6	43.7	45.1	69.4	24.4	21.8	63.7
2S3R5R9S11R	36.1	50.3	37.0	48.0	68.8	143.6	135.6	30.2	40.5	43.1	45.2	69.5	24.4	21.6	64.5
2S3R5S9S11R	35.8	48.0	40.8	44.8	69.3	144.2	137.4	30.1	41.8	43.6	45.1	69.8	24.4	22.1	65.6
2S3S5R9S11R	41.2	45.1	40.9	39.9	69.4	141.6	136.8	27.9	39.0	44.1	43.5	69.6	24.2	25.3	66.7
2R3R5R9R11R	39.6	47.4	39.7	41.5	70.4	146.8	134.2	33.1	37.8	45.3	43.3	71.8	27.7	24.6	64.2
2R3R5R9S11R	35.2	51.1	40.6	38.0	72.9	147.3	131.9	31.8	44.8	39.8	43.2	72.6	26.4	27.0	64.6
2R3R5S9R11R	39.4	45.7	42.9	40.0	69.5	143.7	135.7	28.7	38.7	43.3	43.2	70.9	24.2	24.7	64.4
2R3S5R9R11R	35.2	47.3	40.8	44.8	69.3	144.2	137.5	30.0	41.6	43.1	45.1	72.5	22.2	22.1	65.6
2R3S5R9S11R	35.3	50.1	43.8	42.2	73.2	141.7	134.0	32.2	37.4	43.2	42.5	72.8	26.6	21.9	65.7
2R3S5S9R11R	35.1	49.6	36.8	48.4	69.0	143.2	136.1	30.2	40.4	42.2	45.2	71.6	22.2	21.8	64.4
2S3R5R9R11R	36.3	52.0	37.4	43.9	72.2	143.9	130.2	33.3	37.0	41.9	42.5	72.8	26.5	21.2	64.5
2S3R5S9R11R	36.4	51.1	43.6	42.2	73.2	141.5	134.4	32.0	36.8	42.0	42.4	72.6	26.7	21.7	65.7
2S3S5R9R11R	36.2	52.2	47.3	36.5	74.9	141.8	137.5	30.5	44.7	38.4	43.3	72.6	26.3	28.8	65.4
2S3S5S9R11R	36.2	52.0	40.8	37.8	72.8	148.2	130.9	31.8	43.8	38.5	43.2	72.6	26.3	26.9	64.7
2R3R5S9S11R	34.9	51.5	47.6	36.1	75.2	143.1	137.3	30.8	45.7	40.0	43.2	72.7	26.4	28.6	65.2
2R3S5S9S11R	34.9	51.3	37.8	43.8	72.1	145.0	129.2	33.4	37.8	43.4	42.5	73.0	26.6	21.3	64.5
2S3S5S9S11R	38.0	46.3	37.0	40.4	71.3	140.2	129.0	31.2	35.6	42.1	42.3	73.4	27.8	27.3	64.1



(2*S*,3*R*,5*S*,9*R*,11*R*)
the natural enantiomer

その2

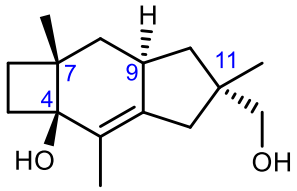
	Hα-1	Hβ-1	H-2	Hα-4	Hβ-4	H-5	Hα-8	Hβ-8	H-9	Hα-10	Hβ-10	H-12A	H-12B	H-13	H-14	H-15A	H-15B
experimental	1.29	1.59	2.09	1.88	2.18	4.97	1.72	2.04	2.35	0.98	1.82	3.37	3.38	1.05	1.25	4.15	4.21
2S3R5R9S11R	1.39	1.58	2.14	1.74	2.38	4.90	1.64	1.72	2.34	0.98	1.96	3.53	3.44	1.06	1.06	4.02	4.17
2S3R5S9S11R	1.38	1.62	2.17	1.86	2.07	4.95	1.74	1.72	2.43	1.04	1.90	3.49	3.45	1.03	1.29	4.14	4.15
2S3S5R9S11R	1.11	1.82	2.22	1.73	2.35	4.89	1.38	2.03	2.46	1.02	1.82	3.45	3.45	1.01	1.31	4.08	4.20
2R3R5R9R11R	1.31	1.82	2.14	1.94	2.07	4.91	2.12	2.35	2.33	1.73	1.90	3.31	3.42	0.91	1.12	3.59	4.43
2R3R5R9S11R	1.36	1.43	1.53	1.59	1.95	4.97	1.57	1.65	1.65	1.01	1.70	3.37	3.39	1.01	1.18	4.05	4.07
2R3R5S9R11R	1.23	1.54	2.26	1.74	2.29	4.87	1.81	2.02	2.51	1.57	1.66	3.40	3.36	0.94	1.35	3.91	4.25
2R3S5R9R11R	1.34	1.53	2.25	1.85	2.08	4.96	1.72	1.76	2.47	1.30	1.52	3.45	3.46	1.04	1.26	4.14	4.16
2R3S5R9S11R	1.31	1.54	1.65	1.83	1.90	5.07	1.41	1.96	1.98	0.92	1.97	3.38	3.39	1.01	1.40	4.00	4.14
2R3S5S9R11R	1.34	1.68	2.27	1.74	2.41	4.91	1.66	1.71	2.37	1.25	1.44	3.45	3.45	1.03	1.05	4.01	4.16
2S3R5R9R11R	1.19	1.65	1.65	1.58	2.25	5.01	1.56	1.94	1.92	1.43	1.54	3.38	3.35	0.99	1.07	3.97	4.07
2S3R5S9R11R	1.23	1.68	1.67	1.82	1.90	5.07	1.47	1.96	1.96	1.42	1.54	3.34	3.38	3.38	1.39	4.00	4.15
2S3S5R9R11R	0.99	1.75	1.56	1.50	1.89	5.12	1.56	1.66	1.54	1.26	1.35	3.34	3.38	0.96	1.61	4.11	4.10
2S3S5S9R11R	1.06	1.79	1.56	1.55	1.95	4.97	1.58	1.69	1.65	1.31	1.34	3.36	3.39	0.99	1.17	4.08	4.08
2R3R5S9S11R	1.35	1.56	1.57	1.56	1.99	5.07	1.58	1.61	1.58	1.02	1.65	3.35	3.39	0.96	1.62	4.10	4.05
2R3S5S9S11R	1.34	1.71	1.65	1.61	2.26	5.01	1.50	1.93	1.97	0.98	1.91	3.40	3.38	1.00	1.10	3.98	4.08
2S3S5S9S11R	1.41	1.61	1.91	1.73	2.11	5.00	1.65	1.95	2.16	1.33	1.86	3.36	3.34	1.07	1.73	4.02	3.99



(2*S*,3*R*,5*S*,9*R*,11*R*)
the natural enantiomer

その3

	^{13}C			^{1}H			^{1}H+^{13}C	
	RMSD (ppm)	max dev (ppm)	DP4	RMSD (ppm)	max dev (ppm)	DP4	DP4	
2S3R5R9S11R	2.0	6.1	3.6%	0.13	0.32	4.1%	0.2%	
2S3R5S9S11R	1.4	3.3	88.5%	0.10	0.32	90.4%	99.5%	proposed diastereomer
2S3S5R9S11R	3.1	6.7	0.0%	0.14	0.34	2.4%	0.0%	
2R3R5R9R11R	2.7	5.1	0.0%	0.28	0.75	0.0%	0.0%	
2R3R5R9S11R	3.6	8.6	0.0%	0.27	0.70	0.0%	0.0%	
2R3R5S9R11R	2.5	6.6	0.0%	0.18	0.59	0.1%	0.0%	
2R3S5R9R11R	1.7	3.4	7.6%	0.14	0.32	2.9%	0.3%	enantiomer of the 11-epimer
2R3S5R9S11R	2.8	4.4	0.0%	0.19	0.44	0.0%	0.0%	
2R3S5S9R11R	2.3	6.3	0.2%	0.17	0.38	0.0%	0.0%	
2S3R5R9R11R	3.2	5.7	0.0%	0.23	0.45	0.0%	0.0%	
2S3R5S9R11R	3.0	4.8	0.0%	0.61	2.33	0.0%	0.0%	
2S3S5R9R11R	4.6	10.1	0.0%	0.34	0.81	0.0%	0.0%	
2S3S5S9R11R	3.8	8.8	0.0%	0.30	0.70	0.0%	0.0%	
2R3R5S9S11R	4.5	10.5	0.0%	0.29	0.77	0.0%	0.0%	
2R3S5S9S11R	3.1	5.3	0.0%	0.18	0.44	0.0%	0.0%	
2S3S5S9S11R	4.1	6.2	3.6%	0.18	0.48	4.1%	0.2%	

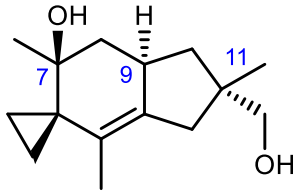


(4*S*,7*R*,9*R*,11*S*)
the mirror image of natural product

	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
experimental	39.9	140.1	126.6	73.4	34.5	22.0	43.8	35.4	37.1	43.0	42.1	70.5	25.4	12.8	23.4
(4*S*,7*R*,9*R*,11*S*)	39.4	140.2	131.1	73.1	34.2	21.6	42.6	35.1	37.5	42.6	42.1	71.3	24.9	14.8	24.0
(4*S*,7*R*,9*S*,11*S*)	39.5	141.8	132.2	78.5	29.6	28.6	40.7	43.7	35.8	41.6	42.5	72.4	24.0	13.2	19.9
(4*S*,7*R*,9*R*,11*R*)	40.1	140.8	130.9	73.0	34.2	21.6	42.5	34.7	37.1	41.6	42.5	72.8	24.5	14.8	23.9
(4*S*,7*R*,9*S*,11*R*)	39.0	141.5	132.4	78.6	29.7	28.6	40.8	44.4	36.0	42.1	42.4	71.0	24.5	13.3	19.9
(4*R*,7*R*,9*R*,11*S*)	37.2	140.0	134.4	79.5	30.0	31.4	43.1	31.6	38.5	44.7	41.4	71.0	25.2	15.0	26.3
(4*R*,7*R*,9*S*,11*S*)	40.4	140.4	132.0	79.1	31.1	32.3	42.4	35.5	39.2	40.6	41.7	76.6	25.4	14.0	24.3
(4*R*,7*R*,9*R*,11*R*)	36.8	139.7	134.7	79.6	30.1	31.4	43.2	31.7	38.4	43.7	41.8	71.8	24.2	15.1	26.2
(4*R*,7*R*,9*S*11*R*)	36.3	139.4	135.9	80.1	31.0	32.3	42.6	33.7	40.0	43.2	41.7	72.3	26.3	14.1	24.3

	Hβ-1	Hα-1	Hβ-5	Hα-5	Hβ-6	Hα-6	Hβ-8	Hα-8	H-9	Hβ-10	Hα-10	H-12	H-12	H-13	H-14	H-15
experimental	2.25	2.07	2.00	2.12	1.48	1.21	1.57	0.84	2.47	1.95	1.05	3.41	3.49	1.09	1.65	1.20
(4*S*,7*R*,9*R*,11*S*)	2.30	2.05	2.01	2.10	1.58	1.28	1.47	0.86	2.68	1.93	1.13	3.43	3.53	1.04	1.64	1.17
(4*S*,7*R*,9*S*,11*S*)	2.33	1.98	1.91	1.99	1.49	1.99	1.80	1.69	2.56	1.51	1.35	3.43	3.44	1.01	1.59	1.07
(4*S*,7*R*,9*R*,11*R*)	2.29	2.10	2.02	2.09	1.60	1.29	1.46	0.99	2.68	1.58	1.40	3.42	3.45	1.07	1.67	1.17
(4*S*,7*R*,9*S*,11*R*)	2.20	2.05	1.92	1.98	1.99	1.48	1.83	1.57	2.55	1.86	1.09	3.38	3.46	1.02	1.58	1.07
(4*R*,7*R*,9*R*,11*S*)	2.27	2.11	2.25	1.83	2.47	1.58	2.29	1.10	2.74	1.88	1.25	3.38	3.47	1.02	1.66	0.89
(4*R*,7*R*,9*S*,11*S*)	2.13	2.01	2.24	1.84	1.48	2.51	2.13	1.55	2.64	1.79	1.71	3.53	3.37	0.91	1.68	1.17
(4*R*,7*R*,9*R*,11*R*)	2.43	1.96	2.27	1.84	1.58	2.47	2.32	1.12	2.77	1.45	1.44	3.40	3.41	1.04	1.65	0.87
(4*R*,7*R*,9*S*11*R*)	2.20	1.87	2.29	1.89	1.51	2.52	1.97	1.48	2.66	1.89	0.89	3.42	3.41	0.96	1.68	1.18

	^{13}C			^{1}H			^{1}H+^{13}C	
	RMSD (ppm)	max dev (ppm)	DP4	RMSD (ppm)	max dev (ppm)	DP4	DP4	
(4*S*,7*R*,9*R*,11*S*)	1.4	4.5	83.5%	0.07	0.21	99.7%	99.9%	proposed diastereomer
(4*S*,7*R*,9*S*,11*S*)	3.9	8.3	0.0%	0.33	0.85	0.0%	0.0%	11-epimer
(4*S*,7*R*,9*R*,11*R*)	1.5	4.3	16.5%	0.15	0.37	0.3%	0.1%	
(4*S*,7*R*,9*S*,11*R*)	4.0	9.0	0.0%	0.25	0.73	0.0%	0.0%	
(4*R*,7*R*,9*R*,11*S*)	4.1	9.4	0.0%	0.36	0.99	0.0%	0.0%	
(4*R*,7*R*,9*S*,11*S*)	3.9	10.3	0.0%	0.45	1.30	0.0%	0.0%	
(4*R*,7*R*,9*R*,11*R*)	4.1	9.4	0.0%	0.44	1.26	0.0%	0.0%	
(4*R*,7*R*,9*S*11*R*)	4.3	10.3	0.0%	0.40	1.31	0.0%	0.0%	

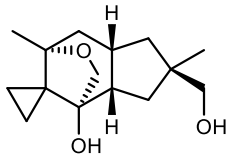


(7*S*,9*R*,11*S*)
the mirror image of natural product

	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
experimental	39.9	135.4	125.2	5.7	7.7	30.2	70.4	43.4	39.1	42.5	42.4	70.6	25.6	13.2	25.8
(7*S*,9*S*,11*S*)	40.7	141.2	125.1	6.7	11.4	31.0	72.0	41.9	36.0	40.8	42.7	72.6	24.4	14.1	26.3
(7S,9*S*,11*R*)	40.2	140.5	125.4	7.0	11.0	30.7	71.8	42.1	36.7	42.1	42.1	71.4	25.3	14.4	26.0
(7*S*,9*R*,11*R*)	39.0	136.7	128.5	7.5	8.9	30.6	70.0	42.7	39.3	42.0	42.5	72.5	25.2	15.2	25.8
(7*S*,9*R*,11*S*)	39.1	136.8	128.5	7.3	9.0	30.6	69.8	43.3	39.8	42.3	42.3	71.7	25.6	15.1	25.8

	Hα-1	Hβ-1	H_S-4	H_R-4	H_S-5	H_R-5	Hβ-8	Hα-8	H-9	Ha-10	Hb10	H-12a	H-12b	H-13	H-14	H-15
experimental	2.05	2.14	0.75	0.69	0.81	0.48	1.37	1.87	2.55	1.02	1.94	3.49	3.40	1.09	1.28	1.20
(7*S*,9*S*,11*S*)	2.07	2.36	0.73	0.68	0.79	0.65	1.33	1.89	3.15	1.44	1.55	3.46	3.43	1.07	1.21	0.80
(7S,9*S*,11*R*)	2.04	2.29	0.64	0.84	0.71	0.66	1.26	1.87	3.05	1.19	1.98	3.57	3.41	1.05	1.20	0.83
(7*S*,9*R*,11*R*)	1.96	2.34	0.85	0.72	0.45	0.82	1.44	1.68	2.76	1.34	1.48	3.44	3.43	1.09	1.24	1.22
(7*S*,9*R*,11*S*)	2.02	2.20	0.84	0.43	0.89	0.73	1.40	1.65	2.73	1.13	1.90	3.51	3.41	1.05	1.24	1.22

	$\delta^{13}C$			$\delta^{1}H$			$^{1}H+^{13}C$	
	RMSD	max dev	DP4	RMSD	max dev	DP4	DP4	
(7*S*,9*S*,11*S*)	2.2	5.8	0.1%	0.24	0.60	0.0%	0.0	
(7S,9*S*,11*R*)	1.8	5.1	2.5%	0.18	0.50	0.6%	0.0	
(7*S*,9*R*,11*R*)	1.3	3.3	30.3%	0.21	0.46	0.0%	0.0	11-epimer
(7*S*,9*R*,11*S*)	1.2	3.3	67.0%	0.12	0.26	99.3%	100.0	proposed diastereomer

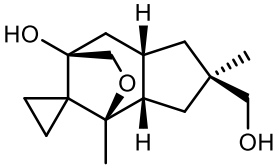


(2*S*,3*R*,7*R*,9*S*,11*R*)
the natural enantiomer

	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
experimental	37.2	46.6	78.0	2.3	3.2	34.3	83.1	39.2	35.4	43.5	43.2	70.3	24.3	71.2	21.7
(2*S*,3*R*,7*R*,9*S*,11*R*)	37.3	47.7	78.2	4.1	4.8	35.3	83.7	39.0	36.7	43.4	42.9	72.2	24.5	73.1	22.7
(2*S*,3*R*,7*R*,9*S*,11*S*)	36.6	46.7	78.4	4.1	4.9	35.4	83.6	39.1	36.5	42.2	43.1	71.0	26.0	72.4	22.8
(2*S*,3*R*,7*R*,9*R*,11*R*)	36.0	51.5	76.8	4.8	4.6	38.1	83.6	41.7	38.6	39.9	42.2	72.5	26.4	72.9	22.2
(2*S*,3*R*,7*R*,9*R*,11*S*)	34.9	50.5	76.7	4.6	4.9	38.0	83.5	41.8	39.6	41.0	42.2	72.6	26.4	73.1	22.1
(2*R*,3*R*,7*R*,9*S*,11*R*)	36.1	51.5	74.5	2.2	4.9	32.5	83.1	41.6	39.1	40.9	42.5	72.6	26.3	78.4	23.3
(2*R*,3*R*,7*R*,9*R*,11*S*)	35.5	51.0	76.3	2.1	6.6	33.1	82.8	43.4	36.6	39.9	43.7	72.2	27.2	78.5	21.9
(2*R*,3*R*,7*R*,9*R*,11*R*)	34.4	50.6	76.4	2.1	6.7	33.1	83.1	41.7	36.8	40.0	44.2	71.6	26.7	78.4	21.9
(2*R*,3*R*,7*R*,9*S*,11*S*)	37.2	52.4	74.4	2.1	4.9	32.4	83.1	41.6	38.0	39.9	42.5	72.5	26.5	78.5	23.4
7,12,14-triol (2*S*,3*R*,7*R*,9*S*,11*R*)	34.7	46.2	73.4	6.4	6.0	29.5	74.7	46.4	33.6	41.8	44.2	69.5	24.5	71.3	27.8

	Hα-1	Hβ-1	H-2	H_R-4	H_S-4	H_R-5	H_S-5	Hα-8	Hβ-8	H-9	Hα-10	Hβ-10	H-12	H-12	H-13	Hβ-14	Hα-14	H-15
experimental	1.53	1.78	2.32	0.52	0.30	0.65	0.68	1.63	1.67	2.45	1.62	1.75	3.31	3.42	1.15	3.48	3.97	1.2
(2*S*,3*R*,7*R*,9*S*,11*R*)	1.80	1.60	2.19	0.33	0.55	0.65	0.74	1.48	1.59	2.45	1.70	2.08	3.35	3.44	1.08	3.53	3.95	0.88
(2*S*,3*R*,7*R*,9*S*,11*S*)	1.50	2.15	2.29	0.59	0.32	0.64	0.73	1.53	1.60	2.50	1.20	2.34	3.50	3.50	0.97	3.39	4.34	0.87
(2*S*,3*R*,7*R*,9*R*,11*R*)	1.18	1.70	1.95	0.75	0.64	0.36	0.54	1.21	1.60	2.24	1.48	1.41	3.42	3.39	1.05	3.48	3.89	0.87
(2*S*,3*R*,7*R*,9*R*,11*S*)	1.31	1.55	1.95	0.59	0.35	0.65	0.79	1.17	1.58	2.21	1.08	1.76	3.43	3.46	1.02	3.48	3.91	0.86
(2*R*,3*R*,7*R*,9*S*,11*R*)	1.41	1.63	2.11	0.58	0.43	0.77	0.51	1.38	1.56	2.37	1.02	1.76	3.38	3.42	1.01	3.39	3.51	0.89
(2*R*,3*R*,7*R*,9*R*,11*S*)	1.95	1.72	2.32	0.61	0.51	0.61	0.86	1.50	1.56	2.56	1.21	1.84	3.28	3.38	1.07	3.65	3.70	0.83
(2*R*,3*R*,7*R*,9*R*,11*R*)	1.22	2.45	2.38	0.54	0.49	0.64	0.85	1.42	1.67	2.58	1.49	1.57	3.39	3.39	0.96	3.63	3.73	0.81
(2*R*,3*R*,7*R*,9*S*,11*S*)	1.24	1.80	2.09	0.58	0.43	0.53	0.79	1.42	1.59	2.38	1.29	1.41	3.39	3.41	1.03	3.48	3.36	0.90
7,12,14-triol (2*S*,3*R*,7*R*,9*S*,11*R*)	1.79	1.28	2.40	0.91	0.18	0.66	0.73	1.65	1.70	2.23	0.86	1.92	3.42	3.48	1.03	3.50	4.10	0.82

	^{13}C			^{1}H			^{1}H+^{13}C	
	RMSD (ppm)	max dev (ppm)	DP4	RMSD (ppm)	max dev (ppm)	DP4	DP4	
(2*S*,3*R*,7*R*,9*S*,11*R*)	1.07	1.9	47.9%	0.16	0.33	98.5%	99.9%	proposed diastereomer
(2*S*,3*R*,7*R*,9*S*,11*S*)	1.01	1.7	52.1%	0.24	0.59	0.1%	0.1%	11-epimer
(2*S*,3*R*,7*R*,9*R*,11*R*)	2.44	4.9	0.0%	0.24	0.42	0.0%	0.0%	
(2S,3R,7*R*,9R,11S)	2.41	4.2	0.0%	0.23	0.54	0.1%	0.0%	
(2*R*,3*R*,7*R*,9*S*,11*R*)	3.01	7.2	0.0%	0.23	0.60	0.1%	0.0%	
(2*R*,3*R*,7*R*,9*R*,11*S*)	3.01	7.3	0.0%	0.20	0.42	1.1%	0.0%	
(2*R*,3*R*,7*R*,9*R*,11*R*)	2.84	7.2	0.0%	0.24	0.67	0.1%	0.0%	
(2*R*,3*R*,7*R*,9*S*,11*S*)	3.11	7.3	0.0%	0.23	0.61	0.1%	0.0%	
7,12,14-triol (2*S*,3*R*,7*R*,9*S*,11*R*)	3.99	8.4	0.0%	0.27	0.76	0.0%	0.0%	

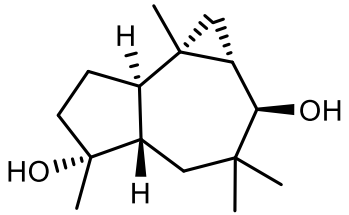


(2*S*,3*R*,7*R*.9*S*,11*R*)
the natural enantiomer

	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
experimental	37.3	53.1	83.7	0.1	4.1	32.2	75.8	41.9	35.9	41.8	44.2	70.9	27.1	20.5	73.7
(2*R*,3*S*,7*S*,9*R*,11*R*)	36.3	53.2	83.7	2.0	6.2	33.3	75.6	40.3	36.7	40.2	44.6	71.3	26.7	21.8	74.9
(2*R*,3*S*,7*S*,9*S*,11*R*)	37.8	55.0	83.3	4.6	1.2	33.0	76.9	41.7	38.0	40.3	42.7	72.6	26.2	19.0	79.7
(2*R*,3*S*,7*S*,9*S*,11*S*)	38.9	55.8	83.1	4.5	1.1	33.0	76.9	41.6	36.8	39.5	42.7	72.4	26.5	18.9	79.7
(2*S*,3*R*,7*R*,9*S*,11*R*)	37.4	53.6	83.8	1.9	6.1	33.5	75.7	41.8	36.7	40.4	44.2	72.2	27.3	21.8	74.9
(2*S*,3*S*,7*S*,9*R*,11*R*)	35.9	53.8	83.2	4.6	4.9	38.0	76.6	39.6	37.8	40.1	42.3	72.7	26.2	19.1	77.1
(2*S*,3*S*,7*S*,9*S*,11*R*)	37.3	46.7	85.5	3.7	4.8	35.0	74.7	38.5	34.5	43.1	43.0	70.0	24.3	20.6	76.1
(2*S*,3*S*,7*S*,9*S*,11*S*)	37.7	49.5	87.9	4.6	5.2	36.2	74.8	37.8	37.2	43.1	43.0	71.4	28.3	19.9	75.7
(2*S*,3*S*,7*S*,9*R*,11*S*)	35.4	52.6	83.2	4.6	4.8	37.9	76.3	39.9	38.8	40.6	42.3	72.6	26.4	19.1	77.3

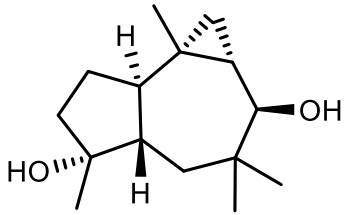
	Hα-1	Hb-1	H-2	H_R-4	H_S-4	H_R-5	H_S-5	Hα-8	Hβ-8	H-9	Hα-10	Hβ-10	H-12	H-12	H-13	H-14	Hα-15	Hβ-15
experimental	1.54	1.51	2.18	0.49	0.58	0.75	0.65	1.7	1.89	2.53	1.19	1.82	3.25	3.35	1.17	0.98	3.57	3.91
(2*R*,3*S*,7*S*,9*R*,11*R*)	1.02	2.19	2.29	0.49	0.66	0.78	0.62	1.91	1.45	2.53	1.52	1.58	3.35	3.37	0.95	0.93	3.57	3.79
(2*R*,3*S*,7*S*,9*S*,11*R*)	1.41	1.35	2.01	0.59	0.75	0.44	0.33	1.68	1.92	2.31	0.98	1.69	3.34	3.39	0.98	0.90	3.67	3.47
(2*R*,3*S*,7*S*,9*S*,11*S*)	1.79	0.90	1.98	0.56	0.77	0.44	0.34	1.72	1.94	2.29	1.26	1.36	3.38	3.37	0.99	0.88	3.47	3.67
(2*S*,3*R*,7*R*,9*S*,11*R*)	1.70	1.56	2.23	0.51	0.58	0.80	0.68	1.74	1.64	2.48	1.19	1.82	3.27	3.37	1.08	0.92	3.51	3.80
(2*S*,3*S*,7*S*,9*R*,11*R*)	1.50	1.31	1.65	0.35	0.56	0.68	0.67	1.45	1.75	2.21	1.34	1.43	3.34	3.37	1.05	0.83	3.59	3.83
(2*S*,3*S*,7*S*,9*S*,11*R*)	1.84	1.47	1.90	0.35	0.57	0.63	0.74	1.69	1.81	2.47	1.65	1.80	3.30	3.47	1.06	0.77	3.63	3.85
(2*S*,3*S*,7*S*,9*S*,11*S*)	2.26	1.41	1.88	0.34	0.66	0.70	0.79	1.72	1.85	2.50	1.39	2.30	3.36	3.41	0.90	0.95	3.62	3.94
(2*S*,3*S*,7*S*,9*R*,11*S*)	1.48	1.15	1.66	0.36	0.63	0.68	0.72	1.48	1.67	2.15	1.03	1.83	3.42	3.42	0.99	0.83	3.60	3.79

	^{13}C			^{1}H			^{1}H+^{13}C	
	RMSD (ppm)	max dev (ppm)	DP4	RMSD (ppm)	max dev (ppm)	DP4		
(2*R*,3*S*,7*S*,9*R*,11*R*)	1.1	2.1	30.4%	0.25	0.65	0.0%	11-epimer	
(2*R*,3*S*,7*S*,9*S*,11*R*)	2.4	6.0	0.0%	0.19	0.44	0.0%		
(2*R*,3*S*,7*S*,9*S*,11*S*)	2.5	6.0	0.0%	0.25	0.64	0.0%		
(2*S*,3*R*,7*R*,9*S*,11*R*)	1.1	2.0	69.6%	0.09	0.25	100.0%	proposed diastereomer	
(2*S*,3*S*,7*S*,9*R*,11*R*)	2.5	5.8	0.0%	0.21	0.53	0.0%		
(2*S*,3*S*,7*S*,9*S*,11*R*)	2.6	6.4	0.0%	0.17	0.46	0.0%		
(2*S*,3*S*,7*S*,9*S*,11*S*)	2.6	4.5	0.0%	0.24	0.72	0.0%		
(2*S*,3*S*,7*S*,9*R*,11*S*)	2.5	5.7	0.0%	0.21	0.52	0.0%		



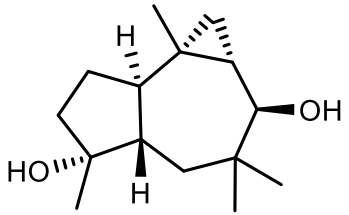
その1

	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15
	42.1	48.2	81.1	41.4	23.2	49.0	19.5	22.6	29.7	81	38	19.1	28.7	25.7	19.4
(2*R*,3*R*,6*R*,7*R*,9*R*,10*R*)	35.2	48.8	82.3	36.5	25.3	44.7	18.6	14.7	28.2	75.9	38.0	24.0	32.1	26.2	30.2
(2*R*,3*R*,6*R*,7*R*,9*S*,10*R*)	41.2	55.4	82.4	38.5	22.4	45.5	17.3	18.9	24.6	76.0	42.2	28.9	28.7	25.8	25.2
(2*R*,3*R*,6*R*,7*S*,9*R*,10*R*)	37.3	52.6	79.3	42.8	25.7	52.2	17.7	21.6	29.2	78.0	41.8	26.0	28.3	25.3	21.0
(2*R*,3*R*,6*R*,7*S*,9*S*,10*R*)	37.4	47.8	79.2	41.4	26.3	45.1	17.4	21.5	27.3	79.1	37.5	23.4	25.1	23.3	24.0
(2*R*,3*R*,6*S*,7*R*,9*R*,10*R*)	36.8	48.2	78.9	42.2	23.8	45.1	21.6	17.0	27.3	76.8	37.7	23.9	31.3	23.3	20.1
(2*R*,3*R*,6*S*,7*R*,9*S*,10*R*)	40.2	52.8	77.0	40.1	21.9	52.8	16.5	20.7	31.7	76.3	41.5	28.5	28.7	25.1	18.7
(2*R*,3*R*,6*S*,7*S*,9*R*,10*R*)	36.0	57.6	75.1	40.1	23.4	48.7	16.8	22.7	24.0	78.5	41.9	27.7	27.4	25.5	30.2
(2*R*,3*R*,6*S*,7*S*,9*S*,10*R*)	37.4	46.9	79.0	40.3	27.1	44.1	23.7	14.5	32.4	78.1	36.3	26.8	27.7	22.4	27.1
(2*R*,3*S*,6*R*,7*R*,9*R*,10*R*)	31.9	46.4	80.1	37.9	25.7	45.7	20.1	13.9	28.7	75.8	37.5	24.0	31.8	29.9	30.3
(2*R*,3*S*,6*R*,7*R*,9*S*,10*R*)	38.8	55.7	79.1	41.3	25.5	45.5	19.3	20.1	23.3	77.6	42.5	25.0	32.7	27.5	25.8
(2*R*,3*S*,6*R*,7*S*,9*R*,10*R*)	35.1	52.1	78.9	42.3	25.8	54.6	17.7	20.7	29.6	78.1	41.2	28.5	26.2	26.9	19.7
(2*R*,3*S*,6*R*,7*S*,9*S*,10*R*)	36.2	47.2	79.8	40.7	26.3	47.4	17.9	20.1	28.3	79.1	37.3	23.5	25.5	26.1	23.2
(2*S*,3*R*,6*R*,7*R*,9*R*,10*R*)	35.5	44.4	80.7	39.3	29.2	45.0	26.0	9.9	30.5	76.9	36.1	28.0	31.4	25.6	27.5
(2*S*,3*R*,6*R*,7*R*,9*S*,10*R*)	37.4	56.4	76.1	40.4	23.6	46.6	17.3	24.1	23.6	77.4	41.1	20.5	29.9	27.2	29.5
(2*S*,3*R*,6*R*,7*S*,9*R*,10*R*)	40.9	53.0	78.1	40.4	23.0	53.8	16.2	19.2	30.8	77.4	41.0	22.9	34.5	27.1	17.9
(2*S*,3*R*,6*R*,7*S*,9*S*,10*R*)*	41.5	47.9	80.1	41.2	24.3	49.3	19.9	21.6	29.8	80.8	37.4	19.9	28.8	25.6	19.8
(2*S*,3*R*,6*S*,7*R*,9*R*,10*R*)	35.5	46.9	79.8	41.1	26.4	44.2	17.7	16.2	27.0	74.4	37.3	24.3	30.5	26.2	24.1
(2*S*,3*R*,6*S*,7*R*,9*S*,10*R*)	37.9	51.4	79.1	42.0	26.2	53.0	18.1	21.3	30.5	76.5	40.8	19.1	30.4	26.9	20.4
(2*S*,3*R*,6*S*,7*S*,9*R*,10*R*)	39.9	53.7	79.2	39.8	22.1	47.0	18.2	17.8	23.5	77.3	41.9	25.1	33.7	29.3	25.4
(2*S*,3*R*,6*S*,7*S*,9*S*,10*R*)	38.8	46.2	80.0	37.3	26.8	45.6	17.0	18.2	30.5	80.2	38.1	19.4	29.2	30.5	29.5
(2*S*,3*S*,6*R*,7*R*,9*R*,10*R*)	37.2	45.3	79.3	40.4	27.7	44.5	25.7	10.2	30.5	76.9	36.4	28.8	30.1	22.2	27.1
(2*S*,3*S*,6*R*,7*R*,9*S*,10*R*)	37.9	57.1	75.2	39.7	23.5	46.7	17.3	23.8	23.5	77.2	41.3	20.5	30.0	25.3	23.5
(2*S*,3*S*,6*R*,7*S*,9*R*,10*R*)	41.6	53.7	76.9	40.6	22.9	53.5	16.4	19.2	30.6	77.3	40.8	22.5	34.2	25.7	17.8
(2*S*,3*S*,6*R*,7*S*,9*S*,10*R*)	46.2	48.7	80.2	42.8	26.2	54.6	18.6	21.3	29.9	81.1	38.0	19.5	28.9	25.9	20.7
(2*S*,3*S*,6*S*,7*R*,9*R*,10*R*)	36.6	47.7	79.3	41.8	26.4	41.7	17.1	17.4	25.8	74.5	37.6	24.1	30.2	22.9	17.4
(2*S*,3*S*,6*S*,7*R*,9*S*,10*R*)	40.0	53.1	79.7	42.4	25.7	50.2	18.1	22.4	29.8	76.4	41.4	18.9	30.4	24.9	21.6
(2*S*,3*S*,6*S*,7*S*,9*R*,10*R*)	43.5	55.3	82.6	38.6	22.3	46.8	16.8	17.5	23.3	76.9	41.6	22.2	34.8	25.5	24.6
(2*S*,3*S*,6*S*,7*S*,9*S*,10*R*)	41.6	48.6	82.0	36.2	27.2	44.2	16.2	18.7	30.4	79.8	38.3	19.6	29.2	25.9	29.3
(2*R*,3*S*,6*S*,7*R*,9*R*,10*R*)	35.5	47.6	80.0	41.5	24.3	45.7	21.6	17.3	27.2	76.8	37.5	24.3	31.3	25.9	19.9
(2*R*,3*S*,6*S*,7*R*,9*S*,10*R*)	39.7	52.9	78.0	40.1	23.5	52.8	16.2	20.7	31.7	76.2	41.6	28.7	28.9	27.4	18.8
(2R,3S,6*S*,7*S*,9*S*,10*R*)	36.8	46.4	80.8	39.0	28.7	45.1	23.5	14.5	32.7	78.2	36.1	26.0	28.4	25.7	14.5
(2R,3S,6*S*,7*S*,9*R*,10*R*)	35.8	57.2	75.8	40.2	23.4	48.5	16.6	22.9	24.5	78.5	41.8	27.5	27.8	27.3	30.3



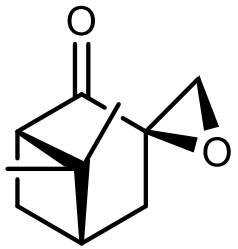
その2

	H-1 1.45	H-1 1.19	H-2 2.61	H-4 1.60	H-4 1.70	H-5 1.80	H-5 1.70	H-6 1.42	H-8 0.45	H-8 0.74	H-9 0.55	H-10 3.14	H-12 0.97	H-13 1.02	H-13 1.27	H-15 0.99
(2*R*,3*R*,6*R*,7*R*,9*R*,10*R*)	1.88	1.07	2.02	1.53	1.67	2.17	1.43	3.12	0.36	0.57	0.72	3.91	1.25	1.09	1.13	1.19
(2*R*,3*R*,6*R*,7*R*,9*S*,10*R*)	1.69	1.15	2.19	1.64	1.75	1.61	0.97	3.12	0.58	0.76	0.86	3.48	1.10	1.15	1.13	1.12
(2*R*,3*R*,6*R*,7*S*,9*R*,10*R*)	2.19	1.19	2.37	1.60	1.79	1.72	1.64	1.96	0.84	0.91	0.42	4.06	1.01	1.03	1.16	1.37
(2*R*,3*R*,6*R*,7*S*,9*S*,10*R*)	1.64	1.45	1.87	1.60	1.63	1.72	1.71	1.74	0.23	0.56	0.77	3.00	1.11	1.08	1.12	0.98
(2*R*,3*R*,6*S*,7*R*,9*R*,10*R*)	1.80	1.36	2.09	1.66	1.52	1.75	1.52	2.05	0.53	0.47	0.62	3.87	1.14	1.12	1.08	1.11
(2*R*,3*R*,6*S*,7*R*,9*S*,10*R*)	1.73	1.35	2.17	1.83	1.75	1.63	1.44	1.30	0.87	0.66	0.60	3.42	1.13	1.11	1.03	1.01
(2*R*,3*R*,6*S*,7*S*,9*R*,10*R*)	2.02	1.32	1.58	1.74	1.73	1.37	1.03	1.90	1.00	1.10	0.53	4.09	1.08	1.02	1.07	1.41
(2*R*,3*R*,6*S*,7*S*,9*S*,10*R*)	1.52	1.33	1.14	1.57	1.54	1.78	1.60	2.04	0.54	0.71	0.89	3.68	1.15	0.96	1.03	1.05
(2*R*,3*S*,6*R*,7*R*,9*R*,10*R*)	1.92	1.37	2.09	1.66	1.55	2.23	1.31	2.26	0.31	0.63	0.78	3.89	1.10	1.23	1.23	1.14
(2*R*,3*S*,6*R*,7*R*,9*S*,10*R*)	1.88	1.60	2.13	1.46	1.42	1.38	1.30	2.31	0.76	0.95	1.21	3.34	1.19	1.15	1.16	1.09
(2*R*,3*S*,6*R*,7*S*,9*R*,10*R*)	2.43	0.89	2.11	1.74	1.57	2.20	1.48	1.78	0.89	0.94	0.38	4.08	1.04	0.99	1.11	1.49
(2*R*,3*S*,6*R*,7*S*,9*S*,10*R*)	1.85	1.16	1.70	1.67	1.48	2.25	1.65	1.67	0.25	0.59	0.77	3.01	1.12	1.06	1.12	1.15
(2*S*,3*R*,6*R*,7*R*,9*R*,10*R*)	1.60	1.39	1.86	1.57	1.52	2.17	1.59	2.72	0.26	0.80	0.93	4.00	1.16	1.12	1.07	0.26
(2*S*,3*R*,6*R*,7*R*,9*S*,10*R*)	1.58	1.52	1.12	1.72	1.71	1.53	0.80	2.42	1.01	1.10	0.40	3.52	1.00	1.18	1.06	1.14
(2*S*,3*R*,6*R*,7*S*,9*R*,10*R*)	1.74	1.20	2.00	1.83	1.82	1.60	1.44	1.86	0.70	0.99	0.56	4.30	1.16	1.16	1.11	1.27
(2*S*,3*R*,6*R*,7*S*,9*S*,10*R*)*	1.33	1.43	1.83	1.56	1.60	1.66	2.01	1.57	0.42	0.69	0.64	3.20	1.14	1.08	1.12	0.97
(2*S*,3*R*,6*S*,7*R*,9*R*,10*R*)	1.97	1.13	1.97	1.63	1.53	2.22	1.63	2.48	0.47	0.50	0.89	3.78	1.04	1.03	1.13	1.22
(2*S*,3*R*,6*S*,7*R*,9*S*,10*R*)	1.83	1.03	2.13	1.71	1.54	2.12	1.52	1.72	0.73	0.94	0.94	3.34	1.02	1.15	1.11	1.13
(2*S*,3*R*,6*S*,7*S*,9*R*,10*R*)	1.90	1.54	2.32	1.60	1.59	1.37	1.07	2.50	0.66	0.84	0.97	4.21	1.16	1.20	1.25	1.43
(2*S*,3*R*,6*S*,7*S*,9*S*,10*R*)	1.55	1.29	2.03	1.67	1.60	1.34	1.40	2.21	0.40	0.57	0.79	3.19	1.22	1.05	1.22	1.11
(2*S*,3*S*,6*R*,7*R*,9*R*,10*R*)	1.75	1.19	1.96	1.59	1.55	1.81	1.63	2.14	0.29	0.92	0.93	3.97	1.11	1.11	1.03	1.06
(2*S*,3*S*,6*R*,7*R*,9*S*,10*R*)	1.61	1.41	1.60	1.73	1.72	1.37	1.02	1.75	0.96	1.11	0.56	3.53	1.07	1.19	1.03	1.73
(2*S*,3*S*,6*R*,7*S*,9*R*,10*R*)	1.59	1.42	2.34	1.76	1.84	1.67	1.43	1.25	0.70	0.91	0.42	4.27	1.17	1.15	1.00	1.32
(2*S*,3*S*,6*R*,7*S*,9*S*,10*R*)	1.67	0.98	2.10	1.51	1.40	2.03	1.43	1.02	0.37	0.70	0.67	3.16	1.18	1.05	1.07	1.07
(2*S*,3*S*,6*S*,7*R*,9*R*,10*R*)	1.73	1.46	2.06	1.62	1.60	1.70	1.68	2.53	0.46	0.57	0.90	3.77	1.04	1.02	1.13	1.04
(2*S*,3*S*,6*S*,7*R*,9*S*,10*R*)	1.59	1.32	2.23	1.65	1.61	1.72	1.61	1.93	0.72	0.89	0.44	3.32	1.03	1.14	1.12	1.00
(2*S*,3*S*,6*S*,7*S*,9*R*,10*R*)	1.50	1.21	2.37	1.68	1.62	1.60	0.89	3.19	0.59	0.78	0.71	4.26	1.23	1.13	1.10	1.46
(2*S*,3*S*,6*S*,7*S*,9*S*,10*R*)	1.36	1.03	1.94	1.61	1.60	1.59	1.59	3.14	0.42	0.60	0.76	3.19	1.24	1.03	1.12	1.15
(2*R*,3*S*,6*S*,7*R*,9*R*,10*R*)	1.96	1.15	1.89	1.64	1.59	1.97	1.61	2.36	0.49	0.59	0.61	3.88	1.11	1.14	1.13	1.03
(2*R*,3*S*,6*S*,7*R*,9*S*,10*R*)	1.66	1.33	1.77	1.86	1.79	1.62	1.36	1.85	0.67	0.94	0.72	3.42	1.14	1.09	1.11	0.94
(2R,3S,6*S*,7*S*,9*S*,10*R*)	1.44	1.32	0.97	1.61	1.51	2.13	1.55	2.57	0.53	0.53	0.88	3.60	1.19	0.98	1.05	1.09
(2R,3S,6*S*,7*S*,9*R*,10*R*)	1.73	1.54	1.09	1.73	1.82	1.53	0.81	2.54	1.01	1.10	0.43	4.08	0.98	1.09	1.07	1.44

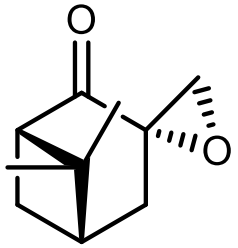


その3

	^{13}C			^{1}H			^{1}H+^{13}C	
	RMSD (ppm)	max dev (ppm)	DP4	RMSD (ppm)	max dev (ppm)	DP4	DP4	
(2*R*,3*R*,6*R*,7*R*,9*R*,10*R*)	4.8	10.8	0.0%	0.54	1.98	0.0%	0.0%	
(2*R*,3*R*,6*R*,7*R*,9*S*,10*R*)	4.4	9.8	0.0%	0.52	1.87	0.0%	0.0%	
(2*R*,3*R*,6*R*,7*S*,9*R*,10*R*)	3.1	6.9	0.0%	0.36	2.01	0.0%	0.0%	
(2*R*,3*R*,6*R*,7*S*,9*S*,10*R*)	2.9	4.7	0.0%	0.25	1.73	3.4%	0.0%	
(2*R*,3*R*,6*S*,7*R*,9*R*,10*R*)	3.1	5.6	0.0%	0.32	1.97	0.0%	0.0%	
(2*R*,3*R*,6*S*,7*R*,9*S*,10*R*)	3.6	9.4	0.0%	0.23	1.85	1.5%	0.0%	
(2*R*,3*R*,6*S*,7*S*,9*R*,10*R*)	5.3	10.8	0.0%	0.49	2.02	0.0%	0.0%	
(2*R*,3*R*,6*S*,7*S*,9*S*,10*R*)	4.5	8.1	0.0%	0.46	1.92	0.0%	0.0%	
(2*R*,3*S*,6*R*,7*R*,9*R*,10*R*)	5.2	10.9	0.0%	0.39	1.97	0.0%	0.0%	
(2*R*,3*S*,6*R*,7*R*,9*S*,10*R*)	4.2	7.5	0.0%	0.41	1.83	0.0%	0.0%	
(2*R*,3*S*,6*R*,7*S*,9*R*,10*R*)	3.9	9.4	0.0%	0.44	2.02	0.0%	0.0%	
(2*R*,3*S*,6*R*,7*S*,9*S*,10*R*)	2.7	5.9	0.0%	0.31	1.73	0.0%	0.0%	
(2*S*,3*R*,6*R*,7*R*,9*R*,10*R*)	5.7	12.7	0.0%	0.48	2.00	0.0%	0.0%	
(2*S*,3*R*,6*R*,7*R*,9*S*,10*R*)	4.4	10.1	0.0%	0.57	1.88	0.0%	0.0%	
(2*S*,3*R*,6*R*,7*S*,9*R*,10*R*)	3.2	5.8	0.0%	0.40	2.07	0.0%	0.0%	
(2*S*,3*R*,6*R*,7*S*,9*S*,10*R*)*	0.6	1.1	99.9%	0.24	1.79	30.7%	100.0%	proposed diastereomer
(2*S*,3*R*,6*S*,7*R*,9*R*,10*R*)	3.9	6.6	0.0%	0.42	1.95	0.0%	0.0%	
(2*S*,3*R*,6*S*,7*R*,9*S*,10*R*)	2.5	4.5	0.0%	0.26	1.83	0.0%	0.0%	
(2*S*,3*R*,6*S*,7*S*,9*R*,10*R*)	4.1	6.2	0.0%	0.49	2.05	0.0%	0.0%	
(2S,3*R*,6*S*,7*S*,9*S*,10*R*)	3.7	10.1	0.0%	0.31	1.79	0.0%	0.0%	
(2*S*,3*S*,6*R*,7*R*,9*R*,10*R*)	5.5	12.4	0.0%	0.37	1.99	0.0%	0.0%	
(2*S*,3*S*,6*R*,7*R*,9*S*,10*R*)	3.9	8.9	0.0%	0.41	1.88	0.0%	0.0%	
(2*S*,3*S*,6*R*,7*S*,9*R*,10*R*)	3.2	5.5	0.0%	0.35	2.07	0.0%	0.0%	
(2*S*,3*S*,6*R*,7*S*,9*S*,10*R*)	2.1	5.6	0.1%	0.24	1.78	1.4%	0.0%	
(2*S*,3*S*,6*S*,7*R*,9*R*,10*R*)	3.9	7.3	0.0%	0.39	1.94	0.0%	0.0%	
(2*S*,3*S*,6*S*,7*R*,9*S*,10*R*)	2.3	4.9	0.0%	0.21	1.82	63.0%	0.0%	
(2*S*,3*S*,6*S*,7*S*,9*R*,10*R*)	4.0	7.1	0.0%	0.59	2.06	0.0%	0.0%	
(2*S*,3*S*,6*S*,7*S*,9*S*,10*R*)	3.6	9.9	0.0%	0.49	1.79	0.0%	0.0%	
(2*R*,3*S*,6*S*,7*R*,9*R*,10*R*)	3.2	6.6	0.0%	0.40	1.97	0.0%	0.0%	
(2*R*,3*S*,6*S*,7*R*,9*S*,10*R*)	3.7	9.6	0.0%	0.31	1.85	0.0%	0.0%	
(2R,3S,6*S*,7*S*,9*S*,10*R*)	4.1	8.1	0.0%	0.56	1.90	0.0%	0.0%	
(2R,3S,6*S*,7*S*,9*R*,10*R*)	5.2	10.9	0.0%	0.64	2.02	0.0%	0.0%	



	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10
実験値A	57.3	207.8	54.3	27.0	40.3	40.8	31.6	25.8	22.3	52.6
実験値B	56.6	208.8	55.3	27.0	40.1	41.8	30.9	25.8	21.2	56.7
β-epoxide	53.9	209.8	54.7	26.6	38.6	39.8	31.7	25.5	20.6	57.0
α-epoxide	54.4	209.6	54.2	26.3	38.8	39.4	31.8	25.4	21.8	52.6



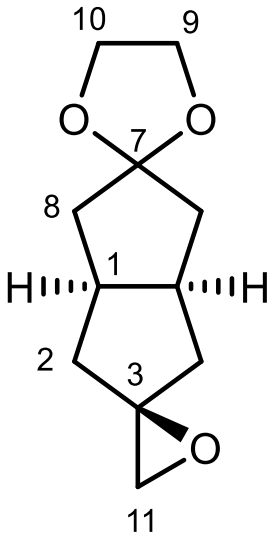
	実験値A	実験値B
β-epoxide	3.5%	91.1%
α-epoxide	96.5%	8.9%

- この系は、SarrotiのDP4+でも基底関数のレベルを上げるかあるいはPCM法で溶媒を考慮する必要がある。
- 残念ながら、サポーティングデータから異性体を特定することが出来なかったが、Spartanの場合、基底関数6-31G*（Sarottiの方法では条件Aに相当）で十分に差がみられる結果になった。
- これら化合物には配座異性体は存在しない。

Ariel M. Sarotti, *J. Org. Chem.* **2015**, *80*, 12526

		B3LYP												mPW1PW91										
		Gas Phase						PCM						Gas Phase						PCM				
	DP4	A	B	C	D	E	F	A	B	C	D	E	F	A	B	C	D	E	F	A	B	C	D	E	F
90a	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
90b	✗	✗	✗	✗	✓	✓	✓	✗	!	!	✓	✓	✓	✗	✗	✗	✓	✓	✓	✗	!	✓	✓	✓	✓

A: 6-31G*; B: 6-31G**; C: 6-31+G**; D: 6-311G*; E: 6-311G**; F: 6-311+G**.



	C-10	C-9	C-7	C-8	C-1	C-2	C-3	C-11	H-8A	H-8B	H-1	H-2A	H-2B	H-11
exp	64.6	63.8	118.2	41.9	38.5	38.9	65.6	49.5	2.05	1.74	2.62	1.56	2.05	2.69
β-epoxide	65.4	64.3	118.9	42.1	39.1	38.2	64.4	44.7	2.13	1.94	2.7	1.22	2.01	2.56
α-epoxide	65.6	64.6	121.1	42.9	39.8	40.1	66.2	47.2	1.62	2.00	2.94	1.59	1.83	2.59

DP4	^{13}C	^{1}H	$^{13}C+^{1}H$
β-epoxide	57.1%	98.2%	98.6%
α-epoxide	42.9%	1.8%	1.4%

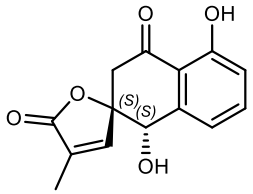
- C-10、C-9については帰属がないため差が小さくなるように配置した。
- ^{1}Hシグナルの帰属がないため、実験値との差が小さくなるように配置した。
- ^{13}Cシグナルでは帰属できないが1Hシグナルを合わせると高い確率で一方を支持した。

		B3LYP												mPW1PW91									
		Gas Phase						PCM						Gas Phase						PCM			
	DP4	A	B	C	D	E	F	A	B	C	D	E	F	A	B	C	D	E	F	A	B	C	D	E	F
89a	✗	✗	✗	✗	✓	✓	✓	✗	✗	!	✓	✓	✓	✗	✗	!	✓	✓	✓	✗	✗	✓	✓	✓	✓

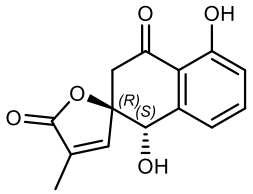
A: 6-31G*; B: 6-31G**; C: 6-31+G**; D: 6-311G*; E: 6-311G**; F: 6-311+G**.

less effective examples

lambertellol A and B



lambertellol A



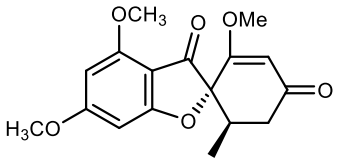
lambertellol B

solv.	$CDCl_3$
geometry	ωB97X-D/6-31G*
NMR	ωB97X-D/6-31G* + post semiempirical correction (spartan'18)
energy	ωB97X-V/6-311+G(2df,2p)[6-311G*]
parameters	standard deviation: 2.306 ppm, freedom: 11.38
lit.	newly calculated for this table experimental data: T. Murakami, Y. Morikawa, M. Hashimoto, T. Okuno, Y. Harada, *Org. Lett.* **2004**, *6*, 157-160.

	C-1	C-2	C-3	C-4	C-4a	C-5	C-6	C-7	C-8	C-8a	C-2'	C-3'	C-4'	C3'-Me
lambertellol A (exp)	198.8	43.6	87.4	70.8	141.4	118.4	137.7	118.7	162.7	115.0	172.4	132.3	147.7	10.8
lambertellol B (exp)	199.2	43.7	86.8	71.9	141.6	118.3	137.8	118.7	162.8	114.7	172.3	132.5	147.5	10.8

	vs. lambertellol A			vs. lambertellol B													
	$\lvert\Delta\delta\rvert_{max}$ (ppm)	RMSD (ppm)	DP4	RMSD (ppm)	$\lvert\Delta\delta\rvert_{max}$ (ppm)	DP4											
lambertellol A	**1.5**	**3.1**	**87.6%**	1.5	2.9	59.7%	199.8	45.3	88.6	70.5	144.5	115.5	137.7	117.8	164.3	115.2	172.2	133.8	147.8	12.1
lambertellol B	1.7	2.9	12.4%	**1.5**	**2.8**	**40.3%**	200.6	46.5	87.7	73.0	142.4	115.7	137.9	117.4	164.2	115.0	171.9	134.7	146.1	12.1

Calculations were not effective!
Reason: RMSD between the isomer in the experimental data (0.25 ppm) << accuracy level of the calculations (ca. 2.0 ppm)



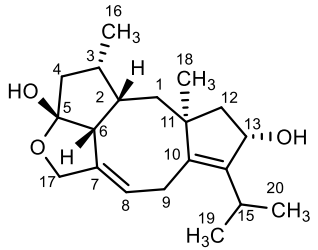
dechlorogriseofluvin

solv.	$CDCl_3$
geometry	ωB97X-D/6-31G*
NMR	ωB97X-D/6-31G* + post semiempirical correction (spartan'18)
energy	ωB97X-V/6-311+G(2df,2p)[6-311G*]
parameters	standard deviation: 2.306 ppm, freedom: 11.38
lit.	newly calculated for this table experimental data: unpublished data.

	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	6-OMe	11-OMe	13-OMe
exp.	14.5	36.8	40.3	197.6	105	171.6	90.2	192.7	104.6	159.4	93.6	170.6	88.8	176.3	56.8	56.3	56.3

Label	$\lvert\Delta\delta\rvert_{max}$ (ppm)	RMSD (ppm)	DP4														
SR-isomer	3.3	1.5	63.7%	14.4	37.1	39.0	194.3	105.1	169.3	92.0	193.3	105.9	158.8	92.8	167.7	88.0	176.6	54.8	54.8	55.2
SS-isomer	3.2	1.6	36.3%	14.3	35.6	40.0	194.6	105.8	169.7	91.9	194.1	106.7	158.6	93.4	167.4	88.3	175.4	54.7	54.8	55.7

bad examples



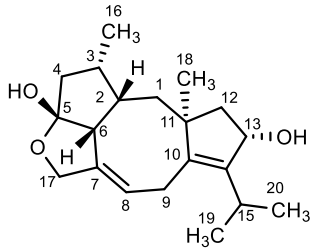
Roussoellol A

solv.	$CDCl_3$
geometry	ωB97X-D/6-31G*
NMR	ωB97X-D/6-31G* + post semiempirical correction (spartan'18)
energy	ωB97X-V/6-311+G(2df,2p)[6-311G*]
parameters	standard deviation: 2.306 ppm, freedom: 11.38
lit.	newly calculated for this table experimental data: H. Takekawa, K. Tanaka, E. Fukushi, K. Matsuo, T. Nehira, M. Hashimoto, M., *J. Nat. Prod*. **2013**, *76*, 1047.

	$\lvert\Delta\delta\rvert_{max}$ (ppm)	RMSD (ppm)	DP4	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15	C-16	C-17	C-18	C-19	C-20
exp.				39.2	42.4	38.3	45.4	119.5	51.5	138.8	116.4	26.3	142.9	49.4	46.4	76.4	143.9	27.0	15.3	72.9	30.7	19.5	23.4
roussoellol A	**3.6**	**1.4**	**12.0%**	**40.5**	**41.7**	**38.9**	**43.9**	**118.5**	**51.4**	**142.4**	**116.9**	**27.1**	**141.9**	**48.6**	**48.4**	**78.6**	**146.2**	**27.8**	**15.9**	**73.4**	**29.3**	**17.7**	**23.9**
2R-isomer	7.8	3.9	0.0%	45.9	46.5	41.6	47.0	117.4	59.3	145.3	117.9	25.5	141.7	45.8	52.5	76.2	147.5	28.2	18.4	75.1	25.3	18.7	22.0
3R-isomer	3.8	2.1	0.0%	42.0	45.5	37.5	45.2	116.1	52.4	142.6	117.2	27.3	142.4	48.9	49.6	78.6	146.2	28.0	18.4	73.0	28.9	17.8	23.9
5S-isomer	7.5	3.7	0.0%	37.9	34.8	40.5	40.1	114.2	57.3	135.5	119.2	26.5	143.0	49.0	49.6	78.6	145.7	27.7	20.6	79.7	28.8	19.6	22.8
11R-isomer	7.4	3.1	0.0%	42.0	41.8	39.2	43.9	117.9	52.9	146.2	119.3	28.6	142.6	46.8	52.8	76.7	143.3	28.2	16.3	71.6	23.6	18.6	24.5
13R-isomer	4.0	1.2	88.0%	38.8	41.7	38.9	44.1	118.8	51.4	142.8	117.7	27.3	144.6	50.6	45.8	77.3	143.5	27.8	16.1	73.4	29.9	20.3	22.5

Investigation of the calculation methods

geometory		ωB97X-D/6-31G*					B3LYP/6-31G*		
chemical shift		ωB97X-D/6-31G*					B3LYP/6-31G*		
Boltzmann dist		ωB97X-D/6-31G* (ΔE)	ωB97X-D/6-31G* (ΔG)	ωB97X-V/6-311+G(2df,2p)[6-311G*]	B3LYP/6-31G*	B3LYP/def2-TZVP (ΔG)	B3LYP/6-31G* (ΔE)	B3LYP/6-31G* (DG)	B3LYP/def2-TZVP (ΔG)
^{13}C	rouissoellol A	4.3%	8.4%	12.0%	4.4%	10.0%	79.2%	81.1%	90.5%
	13R-roussoellol A	95.7%	91.6%	88.0%	95.6%	90.0%	20.8%	18.9%	9.5%
^{1}H	rouissoellol A	100.0%	100%	100%	100%	100%	100%	100%	100.0%
	13R-roussoellol A	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%

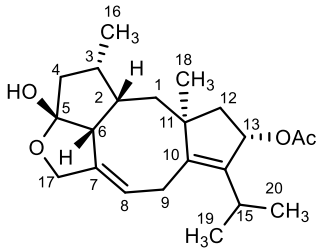


Roussoellol A

solv.	$CDCl_3$
geometry	ωB97X-D/6-31G*
NMR	ωB97X-D/6-31G* + post semiempirical correction (spartan'18)
energy	ωB97X-V/6-311+G(2df,2p)[6-311G*]
parameters	standard deviation: 2.306 ppm, freedom: 11.38
lit.	newly calculated for this table experimental data: H. Takekawa, K. Tanaka, E. Fukushi, K. Matsuo, T. Nehira, M. Hashimoto, M., *J. Nat. Prod*. **2013**, *76*, 1047.

	$\lvert\Delta\delta\rvert_{max}$ (ppm)	RMSD (ppm)	DP4	C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15	C-16	C-17	C-18	C-19	C-20
exp.				39.2	42.4	38.3	45.4	119.5	51.5	138.8	116.4	26.3	142.9	49.4	46.4	76.4	143.9	27.0	15.3	72.9	30.7	19.5	23.4
roussoellol A	**3.6**	**1.4**	**12.0%**	**40.5**	**41.7**	**38.9**	**43.9**	**118.5**	**51.4**	**142.4**	**116.9**	**27.1**	**141.9**	**48.6**	**48.4**	**78.6**	**146.2**	**27.8**	**15.9**	**73.4**	**29.3**	**17.7**	**23.9**
2R-isomer	7.8	3.9	0.0%	45.9	46.5	41.6	47.0	117.4	59.3	145.3	117.9	25.5	141.7	45.8	52.5	76.2	147.5	28.2	18.4	75.1	25.3	18.7	22.0
3R-isomer	3.8	2.1	0.0%	42.0	45.5	37.5	45.2	116.1	52.4	142.6	117.2	27.3	142.4	48.9	49.6	78.6	146.2	28.0	18.4	73.0	28.9	17.8	23.9
5S-isomer	7.5	3.7	0.0%	37.9	34.8	40.5	40.1	114.2	57.3	135.5	119.2	26.5	143.0	49.0	49.6	78.6	145.7	27.7	20.6	79.7	28.8	19.6	22.8
11R-isomer	7.4	3.1	0.0%	42.0	41.8	39.2	43.9	117.9	52.9	146.2	119.3	28.6	142.6	46.8	52.8	76.7	143.3	28.2	16.3	71.6	23.6	18.6	24.5
13R-isomer	4.0	1.2	88.0%	38.8	41.7	38.9	44.1	118.8	51.4	142.8	117.7	27.3	144.6	50.6	45.8	77.3	143.5	27.8	16.1	73.4	29.9	20.3	22.5

derivatization

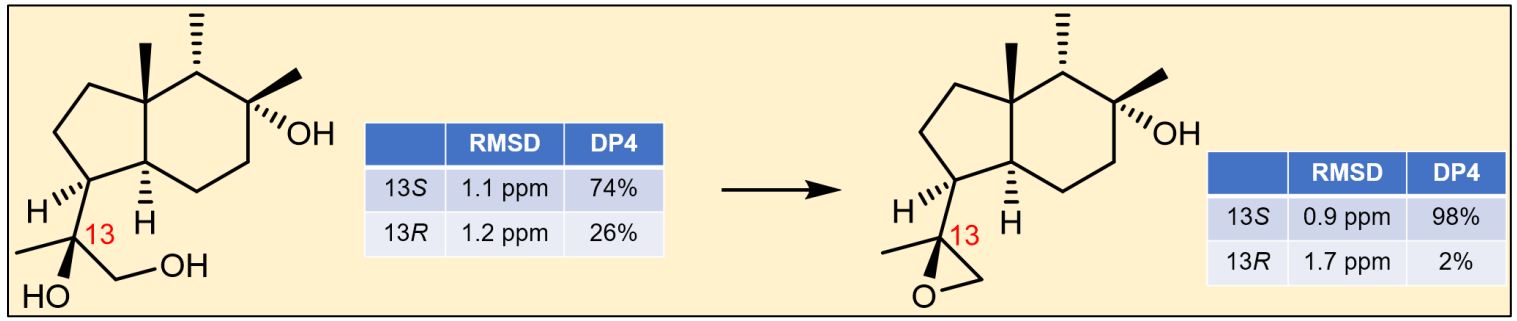


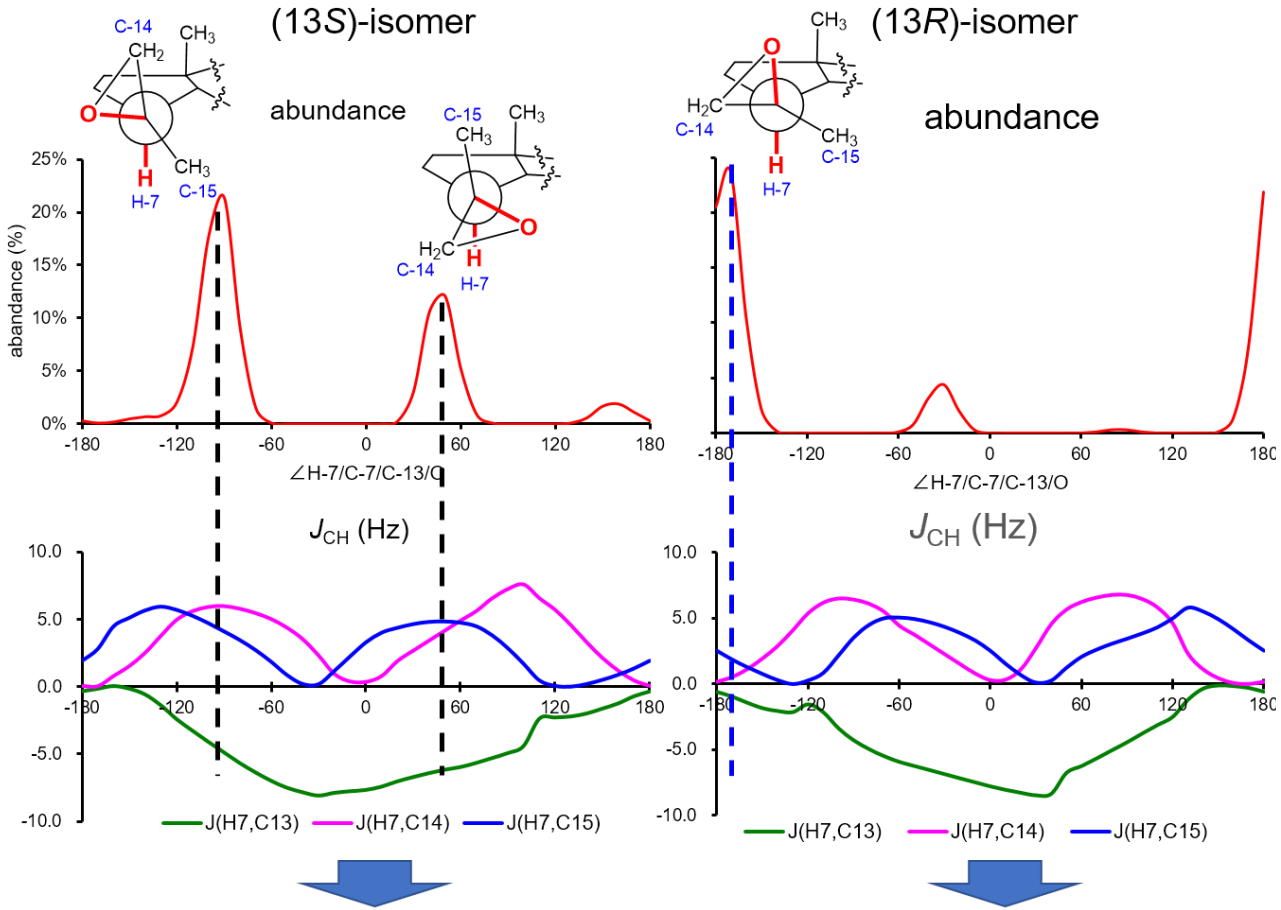
Roussoellol A *O*-acetate

solv.	$CDCl_3$
geometry	ωB97X-D/6-31G*
NMR	ωB97X-D/6-31G* + post semiempirical correction (spartan'18)
energy	ωB97X-V/6-311+G(2df,2p)[6-311G*]
parameters	standard deviation: 2.306 ppm, freedom: 11.38
lit.	newly calculated for this table experimental data: H. Takekawa, K. Tanaka, E. Fukushi, K. Matsuo, T. Nehira, M. Hashimoto, M., *J. Nat. Prod*. **2013**, *76*, 1047.

z				C-1	C-2	C-3	C-4	C-5	C-6	C-7	C-8	C-9	C-10	C-11	C-12	C-13	C-14	C-15	C-16	C-17	C-18	C-19	C-20	CO	COCH3
			exp.	39.2	42.3	38.2	45.3	119.5	51.5	139.1	116.0	26.3	145.5	49.8	43.4	79.3	139.9	26.8	29.8	15.3	72.9	22.5	19.5	171.0	21.6
	$\lvert\Delta\delta\rvert_{max}$ (ppm)	RMSD (ppm)	DP4																						
roussoellol A acetate	**3.7**	**1.3**	**75.4%**	**39.6**	**41.7**	**39.0**	**44.0**	**118.6**	**51.4**	**142.8**	**116.5**	**27.1**	**144.3**	**49.4**	**44.3**	**81.9**	**142.0**	**27.4**	**28.8**	**16.0**	**73.4**	**23.1**	**18.2**	**171.1**	**20.8**
13R-isomer	4.7	1.5	24.6%	37.7	42.6	38.9	45.3	119.3	50.9	143.7	117.6	27.4	148.5	50.6	42.3	81.8	139.7	27.7	29.7	15.9	73.8	21.6	20.7	171.0	21.0

Application of the CH *J* calculations





The HMBC signals can be observed.

The HMBC signals can notbe observed.