Supporting Information

Configurational Assignment of Rhizopodin, an Actin-Binding Macrolide from the Myxobacterium *Myxococcus stipitatus*

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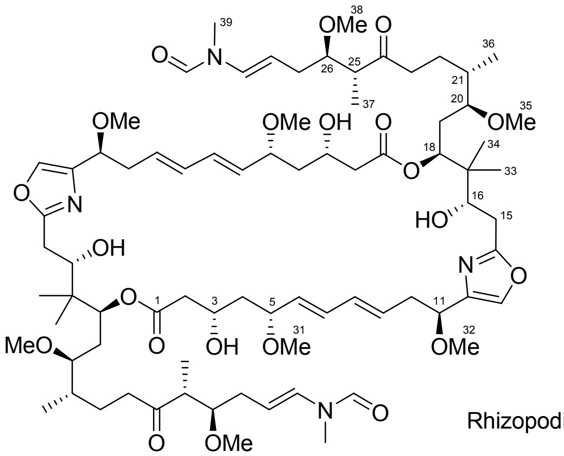
General experimental

Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker AM 600 spectrometer operating at a proton frequency of 600.13. Proton spectra were referenced to 3.34 for residual CHD_2OD. The ROESY experiments were acquired with mixing times of 500ms.

Table 1. ^{1}H-NMR data and ROESY Correlations for rhizopodin (600 MHz, CD_3OD)



Rhizopodin (**1**)

#-H	δ (ppm)	M	*J* (Hz)	ROESY Correlations[a]
2a-H	2.61	dd	14.69 / 5.04	4b-H (m), 4a-H, 3-H (s), 5-H (m), 16-H (vw), 20-H (w)
2b-H	2.54	dd	14.67 / 8.44	4a-H (m), 4b-H (w), 3-H (m), 5-H (w), 16-H (w), 20-H (vw)
3-H	4.11	dddd	4.40 / 4.40 / 8.44 / 8.44	2a-H (s), 2b-H (m), 4a-H (m), 4b-H (s), 33/34-Me (w), 20-H (m), 31-Me (w), 5-H (s), 18-H (w), 6-H (s), 8-H (w), 7-H (m)
4a-H	1.87	ddd	14.04 / 9.54 / 6.41	2a-H, 2b-H (m), 3-H (m), 4b-H (s), 5-H (s), 6-H (m)
4b-H	1.69	ddd	14.03 / 7.89 / 3.95	2a-H (m), 2b-H (w), 3-H (s), 4a-H (s), 5-H (m), 6-H (s)
5-H	3.86	ddd	6.97 / 6.97 / 6.97	31-Me (s), 2a-H (m), 2b-H (w), 3-H (s), 7-H (s), 6-H (s), 4a/b-H (s), 10-H_2 (w)
6-H	5.44	dd	15.22 / 8.25	4b-H (s), 4a-H (m), 31-Me (s), 3-H (s), 9-H (w), 8-H (s), 7-H (m)
7-H	6.24	dd	15.04 / 10.64	10-H_2 (m), 31-Me (m), 5-H (s), 3-H (m), 6-H (m), 9-H (s), 8-H (s)
8-H	6.14	dd	15.04 / 10.64	10-H_2 (s), 31-Me (m), 3-H (vw), 11-H (m), 6-H (s), 9-H (s), 7-H (s)
9-H	5.68	ddd	14.67 / 6.97 / 6.97	10-H_2 (s), 11-H (s), 7-H (s), 13-H (vw), 8-H (m), 32-Me (vw)
10-H_2	2.66	m		32-Me (w), 8-H (s), 7-H (m), 11-H (s), 9-H (s), 13-H (w), 5-H (w)
11-H	4.26	t	6.60 / 6.60	32-Me (s), 9-H (s), 8-H (m), 13-H(s), 10-H_2 (s)
13-H	7.74	s		11-H (s), 16-H (w), 32-Me (s), 15a-H (vw), 15b-H (w), 10-H_2 (w), 8-H (w), 9-H (m)
15-Ha	3.00	dd	15.41 / 2.57	33/34-Me (s), 16-H (s), 18-H (s), 15b-H (s)
15-Hb	2.88	dd	15.22 / 10.45	33/34-Me (s), 16-H (m), 18-H (w), 15a-H (s)
16-H	3.98	dd	10.27 / 2.57	2b-H (w), 33/34-Me (s), 15a-H (s), 15b-H (m), 18-H (s), 19-H_2 (m)
18-H	5.34	dd	9.54 / 2.20	33/34-Me (s), 19-H (s), 15b-H (m), 15a-H (s), 20-H (s), 35-Me (s), 16-H (s), 3-H (vw), 21/22a-H (w)
19-H_2	1.65	m		36-Me (m), 33/34-Me (s), 22b-H (m), 21/22a-H (m), 20-H (s), 18-H (s), 16-H (s)
20-H	3.09	ddd	9.17 / 2.93 / 2.93	36-Me (s), 22b-H (w), 19-H_2 (s), 23-H (s), 35-Me (s), 3-H (m), 18-H (s) 21/22a-H (s)
21/22a-H	1.82	m		36-Me (m), 22b-H (s), 19-H_2 (m), 23-H (s), 25-H (w), 20-H (s), 35-Me (s), 18-H (w)
22-Hb	1.29	m		36-Me (m), 19-H_2 (m), 20-H (w), 35-Me (w), 21/22a-H (s), 23-H (s)
23-H_2	2.61	m		36-Me (s), 33/34-Me (w), 37-Me (s), 21/22a-H (s), 22b-H (s), 25-H (m), 20-H (m), 26-H (m)
25-H	2.85	d	8.54	28-H (m), 38-Me (m), 23-H (s), 27a-H (w), 27b-H (m), 21/22a-H (w), 37-Me (s), 26-H (s)

[a]definitions: (s) = strong, (m) = medium, (w) = weak

[b]19a/19b are resolved in $CDCl_3$: crucial ROESY data 19a-H: 16-H (w), 18-H (m), 20-H (s), 21-H (m), 22a-H (w), 22b-H (m), 33/34-Me (s), 36-Me (m), 19b-H: 16-H (w), 18-H (s), 20-H (m), 21-H (m), 22a-H (w), 22b-H (m), 33/34-Me (s), 36-Me (m)

#-H	δ (ppm)	M	*J* (Hz)	ROESY Correlations[a]
26-H	3.52	ddd	8.34 / 8.34 / 4.22	37-Me (s), 38-Me (s), 28-H (m), 27b-H (s), 27a-H (s), 23-H (s), 25-H (s)
27-Ha	2.54	ddd	15.10 / 4.70 / 4.70	37-Me (m), 27a-H (s), 25-H (m), 38-Me (s), 26-H (s), 28-H (m), 29-H (w)
27-Hb	2.24	ddd	14.20 / 7.90 / 5.20	37-Me (s), 25-H (m), 27a-H (s), 28-H (m), 29-H (m), 26-H (s)
28-H	5.23	ddd	14.31 / 7.70 / 6.60	25-H (m), 39-Me (s), 38-Me (m), 26-H (m), 27a-H (s), 27b-H (s), 29-H (s),
29-H	6.77 / 7.17*	d	13.94 / 14.31*	37-Me (w), 27b-H (s), 27a-H (m), 39-Me (w), 38-Me (vw), 30-H (s), 28-H (s)
30-H	8.36 / 8.12*	s		39-Me (w), 29-H (s)
31-H_3	3.26	s		4b-H (w), 4a-H (s), 5-H (s), 3-H (w), 6-H (m), 9-H (w), 8-H (w), 7-H (m)
32-H_3	3.31	s		10-H_2 (m), 9-H (m), 8-H (m), 13-H (s), 11-H (s)
33-H_3	0.97	s		19-H_2 (s), 15b-H (s), 15a-H (s), 16-H (s), 3-H (w), 18-H (s)
35-H_3	3.37	s		36-Me (m), 33/34-Me (m), 37-Me (w), 22b-H (m), 19-H (m), 23-H (m), 20-H (s), 3-H (w), 18-H (s), 21/22a-H (s)
36-H_3	0.89	d	6.97	22b-H (s), 19-H (s), 23-H (s), 20-H (s), 35-Me (s), 21/22a-H (m)
37-H_3	1.04 / 1.04*	d	6.97 / 6.60*	21/22a-H (w), 27b-H (s), 27a-H (m), 23-H (m), 38-Me (w), 26-H (s), 25-H (s), 28-H (w)
38-H_3	3.35	s		33/34-Me (w), 37-Me (w), 21/22a-H (w), 27b-H (w), 27a-H (m), 26-H (s), 28-H (m), 29-H (w)
39-H_3	3.06 / 3.15*	s		28-H (s), 29-H (m), 30-H (w)

[a]definitions: (s) = strong, (m) = medium, (w) = weak *minor isomer

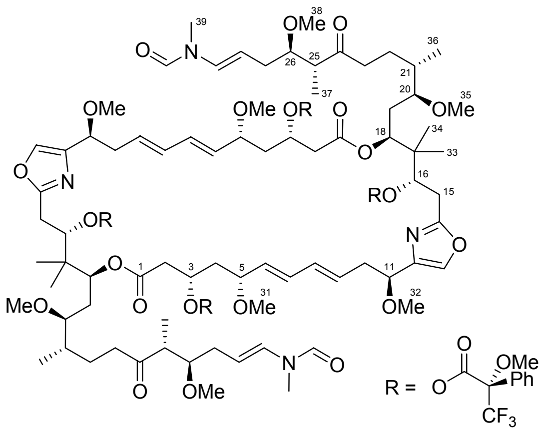
Table 2. ^{1}H-NMR data for rhizopodin (600 MHz, $CDCl_3$)

#-H	δ (ppm)	M	*J* (Hz)
2a-H	2.49	m	
2b-H	2.47	m	
3-H	4.28	m	
4a-H	1.86	ddd	14.31 / 8.44 / 8.44
4b-H	1.63	ddd	14.31 / 3.67 / 3.67
5-H	3.79	ddd	8.80 / 8.80 / 5.14
6-H	5.38	dd	15.04 / 8.07
7-H	6.18	dd	14.67 / 10.27
8-H	6.12	dd	
9-H	5.76	ddd	14.67 / 7.24 / 6.97
10a-H	2.62	ddd	15.22 / 7.89 / 7.70
10b-H	2.50	m	
11-H	4.12	s	
13-H	7.43	s	
15-H_2	2.80	m	
16-OH	3.76	d	5.14
16-H	4.09	ddd	8.70 / 4.50 / 4.50
18-H	5.29	dd	9.17 / 1.80
19-Ha	1.57		
19-Hb	1.55		
20-H	3.01	m	

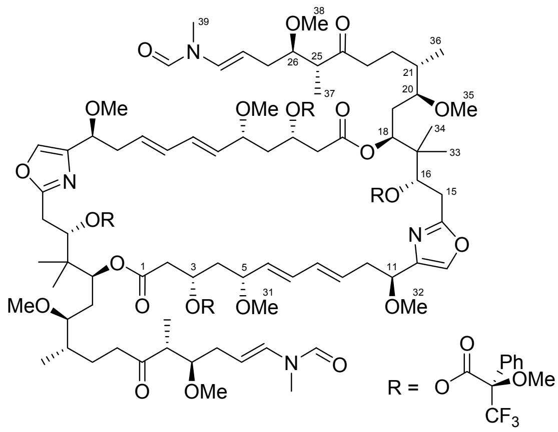
*minor isomer

#-H	δ (ppm)	M	*J* (Hz)
21-H	1.73	m	
22-Ha	1.77	m	
22-Hb	1.28	m	
23-Ha	2.52	m	
23-Hb	"	"	
25-H	2.69	dq	
26-H	3.44	ddd	8.80 / 8.80 / 4.03
27-Ha	2.44	m	
27-Hb	2.13	ddd	13.94 / 7.70 / 5.14
28-H	5.07	ddd	14.67 / 8.06 / 6.97
29-H	6.50 / 7.17*	d	13.94
30-H	8.27 / 8.05*	s	
31-H	3.21	s	
32-H	3.28	s	
33/34-H_3	0.90	s	
35-H_3	3.35	s	
36-H_3	0.83	d	6.97
37-H_3	0.98 / 0.96*	d	7.34
38-H_3	3.28	s	
39-H_3	3.02 / 3.05*	s	

Table 3. ^{1}H-NMR data for the tetra-Mosher esters of rhizopodin (selected signals) (600 MHz, CD_3OD)



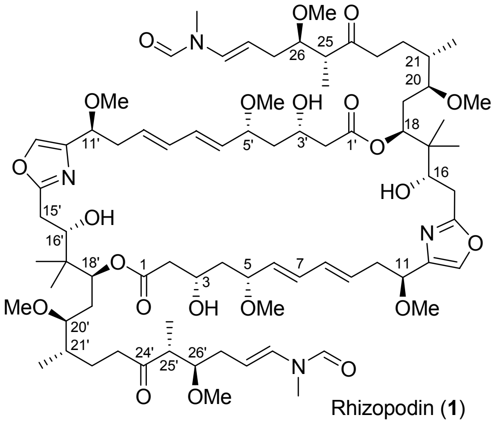
Tetra- (*S*)-Mosher ester of rhizopodin

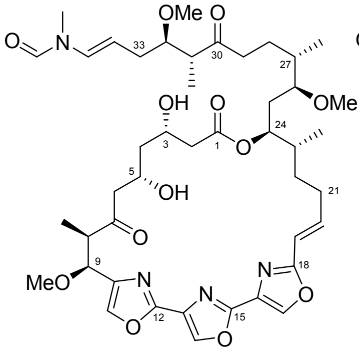


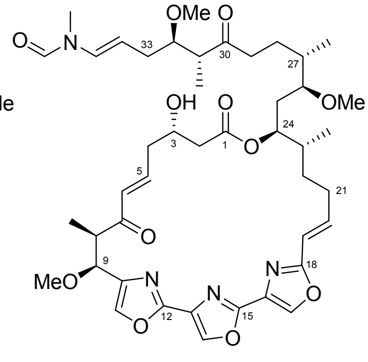
Tetra- (*R*)-Mosher ester of rhizopodin

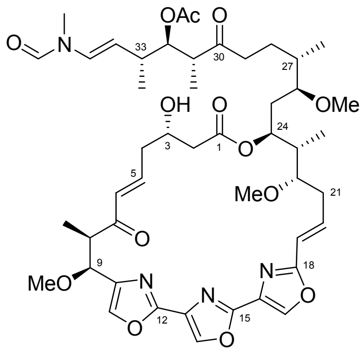
#-H	*S*-Mosher ester of rhizopodin δ (ppm)	*R*-Mosher ester of rhizopodin δ (ppm)	Δ *δ* (S-R)
2a-H	2.88	2.79	0.09
2b-H	2.88	2.72	0.16
3-H	5.48	5.52	-0.04
4a-H	2.00	2.12	-0.12
4b-H	1.77	1.93	-0.16
5-H	3.44	3.71	-0.27
6-H	5.27	5.40	-0.13
7-H	5.99	6.09	-0.15
8-H	6.02	6.14	-0.07
9-H	5.62	5.64	-0.02
11-H	4.22	4.23	-0.01
13-H	7.69	7.74	-0.05
15-Ha	3.30	3.30	0
15-Hb	3.07	3.21	-0.14
16-H	5.62	5.51	0.11
18-H	5.22	5.07	0.15
19-H_2	1.64	1.55	0.09
20-H	3.03	2.93	0.1
21-H	1.82	1.76	0.06
22-Ha	1.81	1.76	0.05
22-Hb	1.25	1.22	0.03
26-H	3.51	3.52	-0.01
27-Ha	2.54	2.55	-0.01
27-Hb	2.23	2.24	-0.01
28-H	5.27	5.23	0.04
31-H_3	3.09	3.20	-0.11
32-H_3	3.22	3.28	-0.06
33/34-H_3	0.90	0.89	0.01
35-H_3	3.33	3.24	0.09

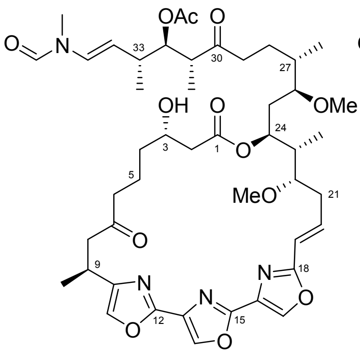
Table 4. ^{13}C NMR data: comparison of the rhizopodin side chain with structurally related polyketides

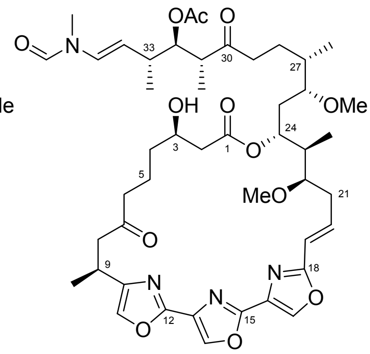

Rhizopodin (**1**)


Jaspisamide A (**6**)


Halichondramid (**7**)


Mycalolide A (**8**)


Ulapualide A (**9**)


Ulapualide A -Isomer (**10**)

Only the data of the major isomer is compared

#-C	**1**[1] **δ (ppm)**	**6** [2] **δ (ppm)**	**7**[3] **δ (ppm)**	**8** [4] **δ (ppm)**	**9** [5] **δ (ppm)** natural: 20,21 syn	**10** [5] **δ (ppm)** synthetic: 20,21 anti
C-18 / 24	75.7	74.60	74.0	73.2	73.0	72.8
C-19 / 25	31.0	33.14	32.0	32.0	32.1	32.0
C-20 / 26	81.9	81.88	81.6	81.8	81.8	81.0
C-21 / 27	34.6	34.68	34.5	34.4	40.4	40.3
C-22 / 28	24.9	24.93	24.8	25.0	27.6	26.6
C-23 / 29	41.6	42.37	41.1	39.5	39.8	39.9
C-24 / 30	213.6	214.12	213.5	211.6	211.8	211.5
C-25 / 31	49.0	49.10	48.6	48.9	48.6	48.6
C-26 / 32	82.5	87.38	82.1	77.5	77.3	77.6
C-27 / 33	30.9	29.72	30.1	36.9	37.0	36.9
C-28 / 34	105.4	111.38	105.1	110.5	110.5	110.5
C-29 / 35	130.4	130.07	130.1	129.5	129.6	130.1
C-30 / NCHO	162.1	162.18	162.1	162.1	162.2	162.2
C-35 / 26OMe	58.1	58.18	57.8	58.2	58.1	57.8
C-36 / 27Me	15.6	15.47	15.4	15.5	15.5	14.2
C-37 / 31Me	12.8	13.52	12.7	13.3	13.4	13.4
C-38 / 32OMe	57.8	56.82	57.4	---	---	---
C-39 / NMe	26.7	27.65	27.5	27.6	33.1	32.8

[1] $CDCl_3$, 125 MHz, [2] $CDCl_3$, 100 MHz, J. Kobayashi, O. Murata, H. Shigemori, *J. Nat. Prod.* **1993**, *56 (5)*, 787-791. [3] $CDCl_3$, 90 MHz, M.R. Kernan, T.F. Molinski, D.J. Faulkner, *J. Org. Chem.* **1988**, *53*, 5014-5020. [4] $CDCl_3$, 125 MHz, N. Fusetani, K. Yasumuro, S. Matsunaga, K. Hashimoto, *THL* **1989**, *30(21)*, 2809-2812. [5] $CDCl_3$, 125 MHz, S.K. Chattopadhyay, G. Pattenden, *J. Chem. Soc. Perkin Trans. 1*, **2000**, 2429-2454.

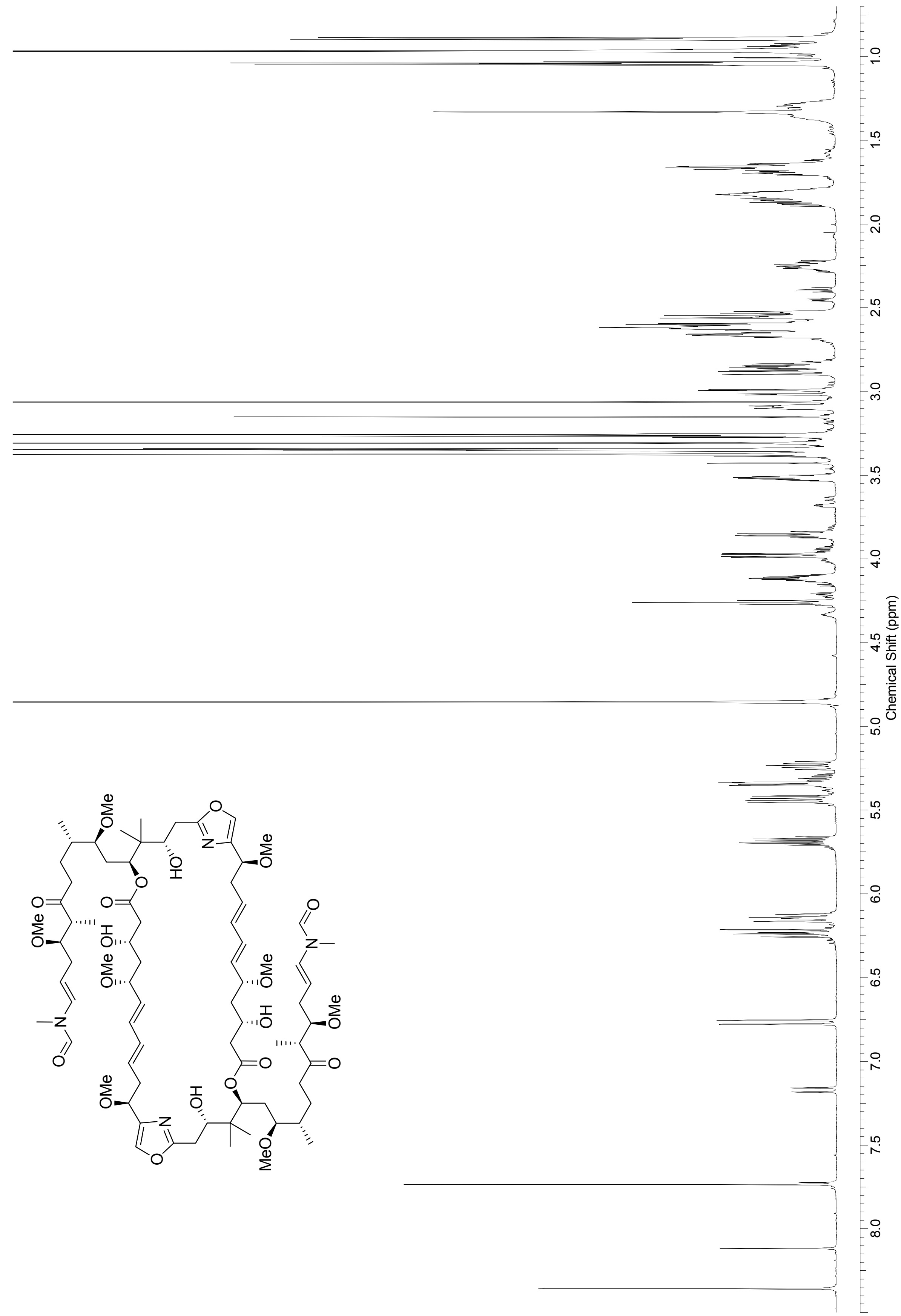
Table 5. ^{1}H NMR data: comparison of the rhizopodin side chain with structurally related polyketides

#-C	1[1)] δ (ppm)	6 [2)] δ (ppm)	7[3)] δ (ppm)
18/24-H	5.29	5.17	5.10
19a/25-H	1.57	1.58	1.60
19b/25'-H	1.55	1.58	1.60
20/26-H	3.01	2.98	2.97
21/27-H	1.73	1.70	1.75
22a/28-H	1.77	1.70	1.74
22b/28'-H	1.28	1.36	1.36
23a/29-H	2.52	2.53	2.53
23b/29'-H	2.52	2.50	2.53
25/31-H	2.69	2.74	2.74
26/32-H	3.44	3.44	3.48
27a/33-H	2.44	2.50	2.46
27b/33'-H	2.13	2.15	2.13
28/34-H	5.07	5.10	5.10
29/35-H	6.50	6.52	6.52
30-H/NCHO	8.27	8.28	8.29
35-H_3/26OMe	3.35	3.33	3.32
36-H_3/27Me	0.83	0.84	0.85
37-H_3/31Me	0.98	0.99	0.98
38-H_3/32OMe	3.28	3.29	3.30
39-H_3/NMe	3.02	3.03	3.04

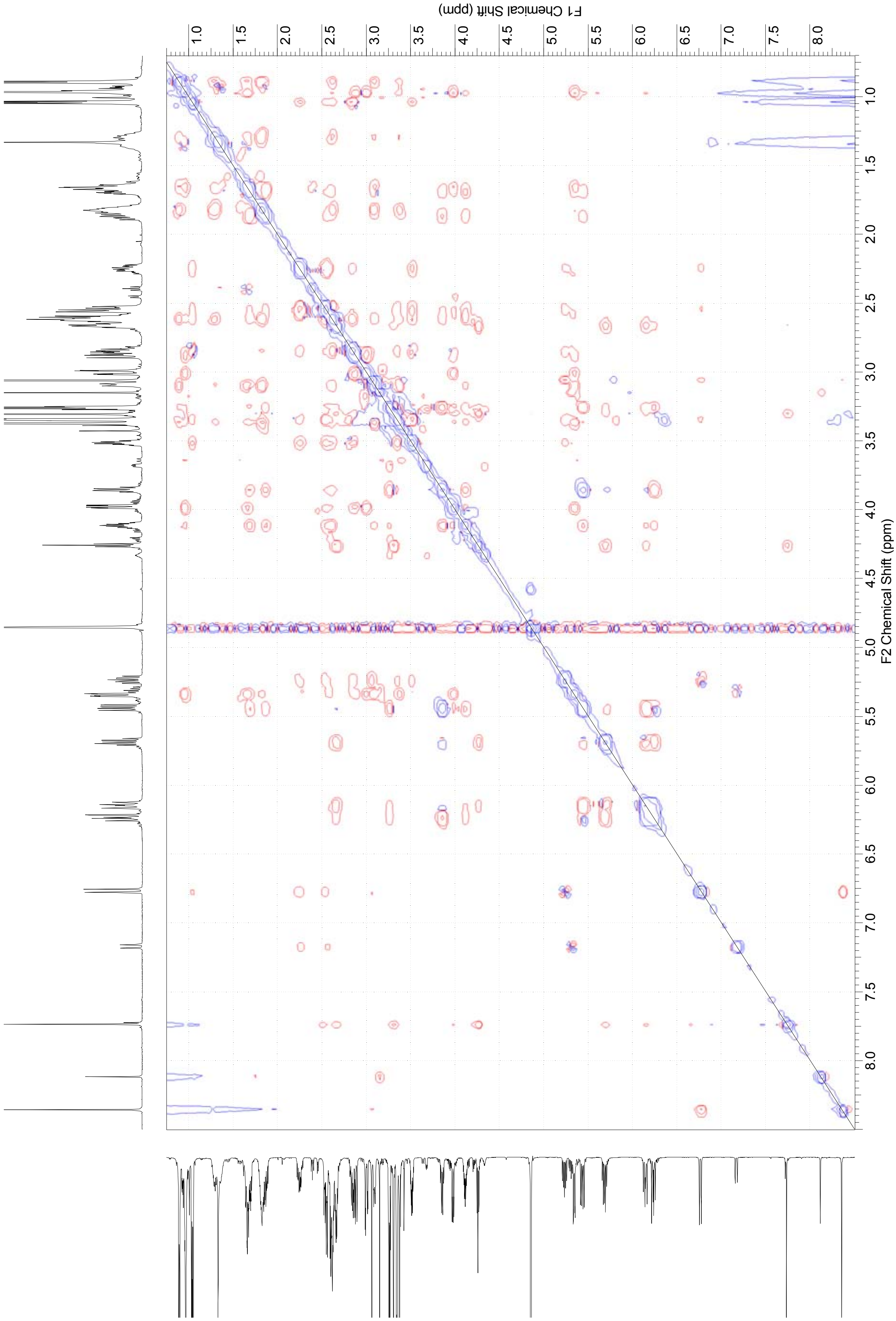
[1)] $CDCl_3$, 600 MHz, [2)] $CDCl_3$, 400 MHz, J. Kobayashi, O. Murata, H. Shigemori, *J. Nat. Prod.* **1993**, *56 (5)*, 787-791. [3)] $CDCl_3$, 360 MHz, M.R. Kernan, T.F. Molinski, D.J. Faulkner, *J. Org. Chem.* **1988**, *53*, 5014-5020.

II. Copies of 1D and 2D NMR spectra

[1]H NMR Spectrum of rhizopodin (1) in CD_3OD (600 MHz)



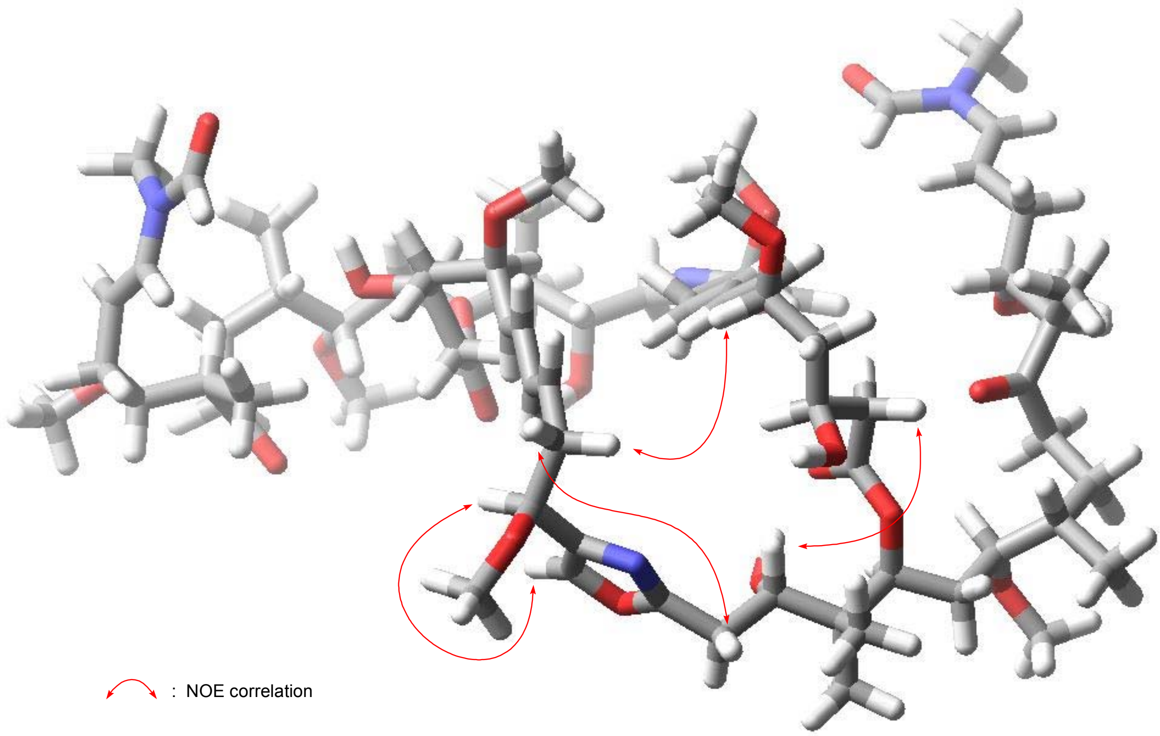
ROESY Spectrum of rhizopodin (1) in CD_3OD (600 MHz)



III. Molecular Modeling

Molecular modeling studies were performed on potential diastereomers of archazolid using Macromodel (version 8.5)[1] and the MMFFs force field, together with the generalized Born/Surface area (GB/SA) chloroform solvent model. Files with constrained torsion angles were generated on the basis of spectral analysis (see Figure 2 of the manuscript). Structures were subjected to a minimization procedure to the nearest local minimum prior to the generation of new local energy conformers by Monte Carlo searching (20,000 steps). All conformations within 50 KJ mol^{-1} were recorded. The normal set-up protocol was employed, with experiments sampling batches of 1000 to 2000 structures.

Perspective drawing of the lowest energy conformation of rhizopodin generated by Macromodel V 8.5



[1] Mohamadi, F.; Richards, N. G. J.; Guida, W. C.; Liskamp, R.; Lipton, M.; Caufield, C.; Chang, G.; Hendrickson, T.; Still, W. C. *J. Comp. Chem.* **1990**, *11*, 440.

Output-file for the lowest energy conformation of rhizopodin

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228
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