Electronic Supplementary Material (ESI) for ChemComm.
This journal is © The Royal Society of Chemistry 2020

Supporting information for

Sensitivity of VCD spectroscopy for small structural and stereochemical changes of macrolide antibiotics

Daniel P. Demarque,[a] Sascha Heinrich,[b] Frank Schulz,[b] Christian Merten[a,*]

[a)] Ruhr Universität Bochum
Lehrstuhl für Organische Chemie II
Universitätsstraße 150
44801 Bochum, Germany
christian.merten@ruhr-uni-bochum.de
www.mertenlab.de

[b)] Ruhr Universität Bochum
Lehrstuhl für Organische Chemie I

Table of Contents

1. Additional spectra

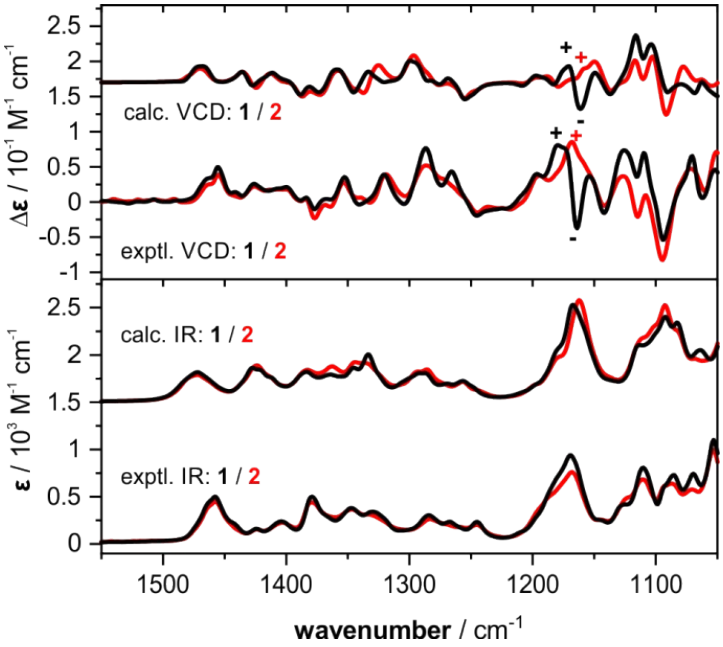


Figure S1. Enlarged view of the spectral IR and VCD spectra of **1** and **2** in the range 1550-1050 cm^{-1}.

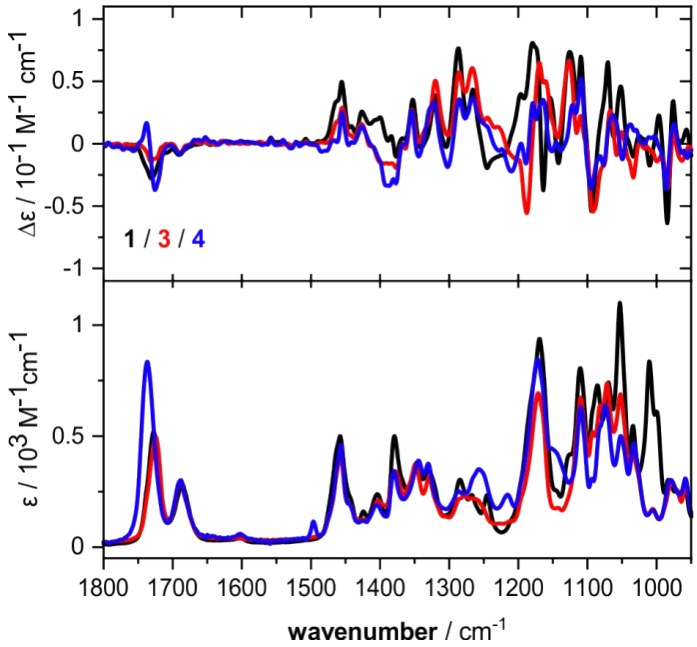


Figure S2. Overlap plot of 1, 3 and 4.

2. Computational data on 1 and 2 and epimers of 1

Table S1. Conformational analysis of 1. Relative zero-point corrected and Gibbs free energies of the 15 lowest energy conformers found for **1.**

Id	ΔE_{ZPC}	ΔG_{298K}	pop(ΔE)	pop(ΔG)
1-c1	0.00[a)]	0.00 [a)]	72.6	50.9
1-c2	1.24	0.61	8.9	18.1
1-c3	1.50	1.33	5.8	5.4
1-c4	1.58	1.79	5.1	2.5
1-c5	2.12	1.10	2.0	8.0
1-c6	2.55	2.18	1.0	1.3
1-c7	2.65	1.64	0.8	3.2
1-c8	2.68	2.44	0.8	0.8
1-c9	2.73	2.56	0.7	0.7
1-c10	3.25	2.92	0.3	0.4
1-c11	3.25	2.92	0.3	0.4
1-c12	3.27	2.01	0.3	1.7
1-c13	3.52	2.08	0.2	1.5
1-c14	3.56	2.42	0.2	0.9
1-c15	3.57	2.28	0.2	1.1
			Σ= 99.1 %	96.8 %

[a] Referenced to E(**1**-c1) = -2521.320521 hartree and G(**1**-c3) = -2521.409763 hartree

Table S2. Conformational analysis of 2. Relative zero-point corrected and Gibbs free energies of the 15 lowest energy conformers found for **2.**

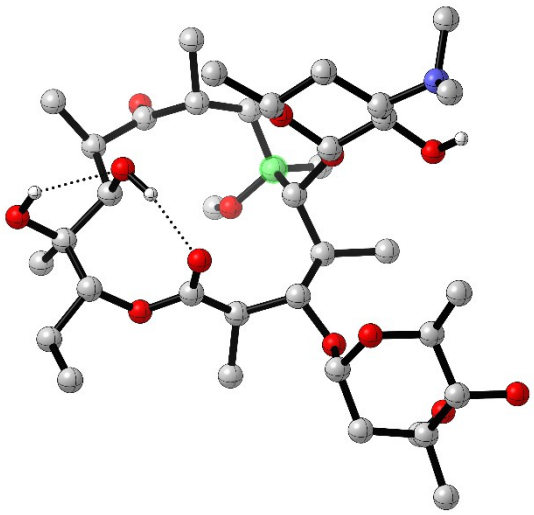
Id	ΔE_{ZPC}	ΔG_{298K}	pop(ΔE)	pop(ΔG)
2-c1	0.00[a]	0.20	28.8	24.3
2-c2	0.19	0.72	20.8	10.0
2-c3	0.40	0.00 [a]	14.7	33.9
2-c4	0.42	0.66	14.2	11.1
2-c5	0.95	1.57	5.8	2.4
2-c6	1.04	1.17	5.0	4.7
2-c7	1.68	2.21	1.7	0.8
2-c8	1.69	2.23	1.7	0.8
2-c9	1.96	2.69	1.0	0.4
2-c10	2.00	2.60	1.0	0.4
2-c11	2.23	1.45	0.7	2.9
2-c12	2.27	2.03	0.6	1.1
2-c13	2.46	1.74	0.5	1.8
2-c14	2.47	1.66	0.4	2.1
2-c15	2.49	3.11	0.4	0.2
			Σ= 97.3 %	96.8 %

[a] Referenced to E(**2**-c1) = -2482.049622 hartree and G(**2**-c3) = -2482.138686 hartree

Table S3. Conformational analysis of (6S)-1. Relative zero-point corrected and Gibbs free energies of the 10 lowest energy conformers found for epimer **(6S)-1.**

Id	ΔE_{ZPC}	ΔG_{298K}	pop(ΔE)	pop(ΔG)
(6S)-1-c1	0.00[a)]	0.00 [a)]	87.0	63.1
(6S)-1-c2	1.59	0.68	6.0	19.9
(6S)-1-c3	1.87	1.84	3.7	2.8
(6S)-1-c4	2.42	1.45	1.5	5.5
(6S)-1-c5	3.32	2.10	0.3	1.8
(6S)-1-c6	3.35	1.62	0.3	4.1
(6S)-1-c7	3.49	3.62	0.2	0.1
(6S)-1-c8	3.53	2.85	0.2	0.5
(6S)-1-c9	3.57	2.48	0.2	1.0
(6S)-1-c10	3.99	2.76	0.1	0.6
			Σ= 99.5 %	99.3 %

[a] Referenced to E(**6S-1**-c1) = -2521. 317981 hartree and G(**6S-1**-c3) = -2521.40742 hartree

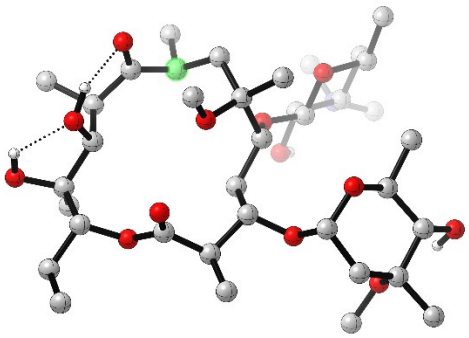


(6S)-1-c1

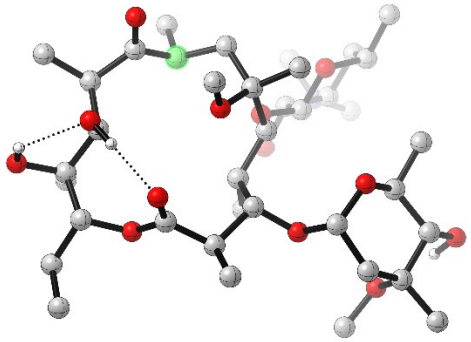
Table S4. Conformational analysis of (8S)-1. Relative zero-point corrected and Gibbs free energies of the 10 lowest energy conformers found for epimer **(8S)-1.**

Id	ΔE_{ZPC}	ΔG_{298K}	pop(ΔE)	pop(ΔG)
(8S)-1-c1	0.00[a)]	0.00 [a)]	46.6	54.8
(8S)-1-c2	0.19	0.50	34.0	23.6
(8S)-1-c3	1.25	1.56	5.6	4.0
(8S)-1-c4	1.47	1.87	3.9	2.3
(8S)-1-c5	1.52	1.20	3.6	7.2
(8S)-1-c6	2.16	2.03	1.2	1.8
(8S)-1-c7	2.17	2.20	1.2	1.3
(8S)-1-c8	2.24	3.04	1.1	0.3
(8S)-1-c9	2.60	2.51	0.6	0.8
(8S)-1-c10	2.71	2.39	0.5	1.0
			Σ= 98.25 %	97.1 %

[a] Referenced to E(8**S-1**-c1) = -2521. 320181 hartree and G(**8S-1**-c3) = -2521.410832 hartree



(8S)-1-c1

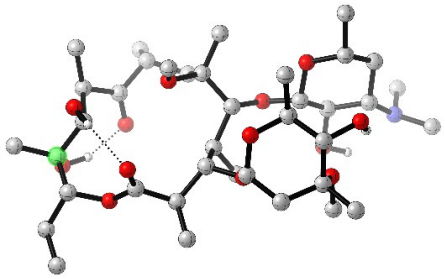


(8S)-1-c2

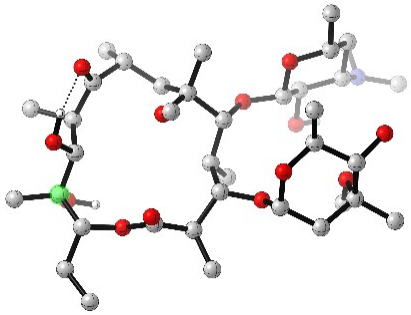
Table S5. Conformational analysis of (12R)-1. Relative zero-point corrected and Gibbs free energies of the 10 lowest energy conformers found for epimer **(12R)-1.**

Id	ΔE_{ZPC}	ΔG_{298K}	pop(ΔE)	pop(ΔG)
(12R)-1-c1	0.00[a)]	0.00 [a)]	57.3	26.1
(12R)-1-c2	1.04	0.01	9.9	25.6
(12R)-1-c3	1.22	1.04	7.3	4.5
(12R)-1-c4	1.44	0.70	5.0	8.1
(12R)-1-c5	1.56	1.29	4.1	3.0
(12R)-1-c6	1.59	0.34	3.9	14.8
(12R)-1-c7	1.74	1.46	3.0	2.2
(12R)-1-c8	2.18	2.20	1.4	0.6
(12R)-1-c9	2.27	2.03	1.3	0.8
(12R)-1-c10	2.35	2.02	1.1	0.9
(12R)-1-c11	2.60	2.41	0.7	0.4
(12R)-1-c12	2.68	1.83	0.6	1.2
(12R)-1-c13	2.70	2.21	0.6	0.6
(12R)-1-c14	2.71	1.51	0.6	2.0
(12R)-1-c15	2.77	1.76	0.5	1.3
(12R)-1-c16	2.87	1.92	0.5	1.0
		Σ=	99.5 %	99.3 %

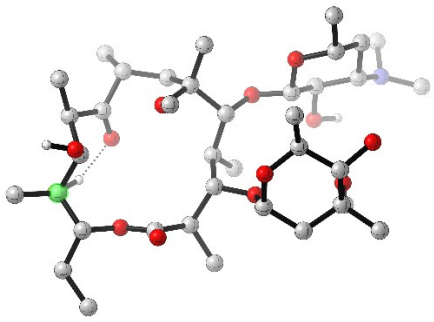
[a] Referenced to E(**12R-1**-c1) = -2521. 316101 hartree and G(**12R-1**-c3) = -2521.404248 hartree



(12R)-1-c1



(12R)-1-c2

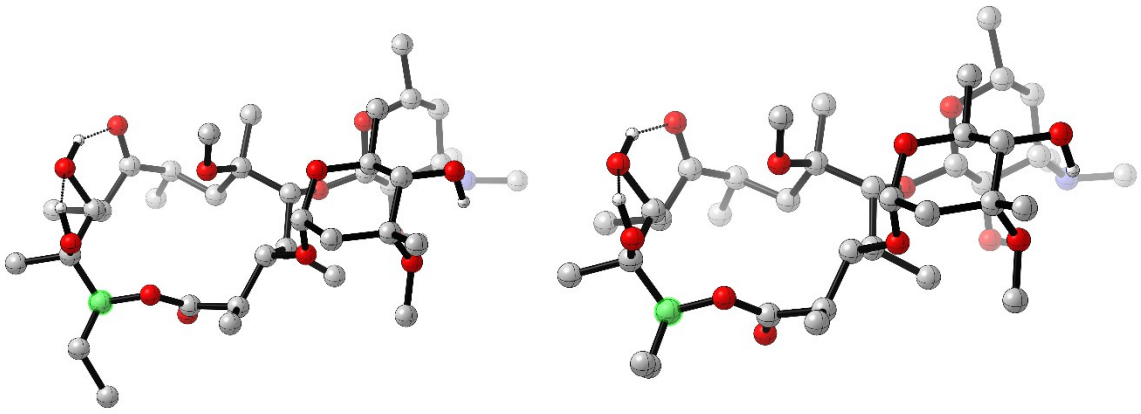


(12R)-1-c3

Table S6. Conformational analysis of (13S)-1. Relative zero-point corrected and Gibbs free energies of the 10 lowest energy conformers found for epimer **(13S)-1.**

Id	ΔE_{ZPC}	ΔG_{298K}	pop(ΔE)	pop(ΔG)
(13S)-1-c1	0.00a)	0.00 a)	62.9	56.4
(13S)-1-c2	0.75	0.46	17.8	26.1
(13S)-1-c3	1.71	2.78	3.5	0.5
(13S)-1-c4	1.81	1.83	3.0	2.6
(13S)-1-c5	1.81	1.83	3.0	2.6
(13S)-1-c6	1.81	1.40	2.9	5.3
(13S)-1-c7	1.93	2.54	2.4	0.8
(13S)-1-c8	2.41	1.99	1.1	2.0
(13S)-1-c9	2.53	2.75	0.9	0.5
(13)-1-c10	2.60	2.15	0.8	1.5
			Σ= 98.3 %	98.4 %

[a] Referenced to E(**13S-1**-c1) = -2521.313382 hartree and G(**13S-1**-c3) = -2521.403650 hartree



(13S)-1-c1 **(13S)-1**-c2

3. Computed NMR data for 1 and the evaluated epimers

Table S7. Experimental and unscaled computed ^{13}C-NMR chemical shifts obtained at the same level the IR and VCD spectra were computed, i.e. B3LYP/6-31G(2d,p)/IEFPCM($CHCl_3$) (unscaled data).

	Exptl.	**1**	**6S**	**8S**	**12R**	**13S**
1	175.9	166.3	170.8	166.1	170.1	164.4
2	45.1	40.5	38.9	40.2	40.5	40.2
2-Me	16.0	11.0	6.6	11.5	10.6	9.2
3	78.5	73.0	69.0	78.2	71.6	75.6
4	39.3	35.0	37.8	37.3	37.0	32.8
4-Me	9.1	5.2	7.7	4.7	5.3	4.6
5	80.8	75.9	69.0	80.0	73.3	71.6
6	78.5	72.9	74.1	75.4	73.0	74.7
6-Me	19.8	13.9	13.1	19.7	16.7	15.4
6-OMe	50.7	43.8	43.2	42.5	45.0	41.7
7	39.4	33.8	32.5	31.2	36.9	34.9
8	45.3	40.1	31.1	38.6	33.4	39.9
8-Me	18.0	11.6	16.7	12.9	13.0	12.4
9	221.1	213.0	208.2	208.5	215.9	213.3
10	37.3	33.4	44.2	41.1	37.6	32.6
10-Me	12.3	8.1	8.3	5.3	6.5	7.0
11	69.1	64.0	61.3	62.7	66.4	66.9
12	74.3	68.3	70.6	69.0	69.2	70.9
12-Me	16.0	10.6	10.8	10.9	13.4	16.1
13	76.7	70.2	71.6	71.2	73.4	69.1
14	21.1	17.2	17.0	17.2	17.4	19.4
15	10.6	5.6	5.6	5.5	4.9	5.0
1'	102.9	97.6	96.6	99.6	96.9	97.2
2'	71.0	63.3	63.3	63.7	63.0	63.7
3'	65.6	59.8	60.0	59.4	60.1	59.0
3'-$N(Me)_2$	40.3	33.1	33.2	33.0	33.1	33.0
4'	28.6	22.0	22.7	21.8	21.9	22.3
5'	68.8	62.9	64.0	63.5	62.8	63.2
6'	21.5	15.0	14.8	15.0	15.1	15.0
1"	96.1	89.3	89.3	92.8	88.9	92.3
2"	34.9	28.6	28.2	29.2	27.8	28.9
3"	72.7	67.6	67.7	67.2	67.5	67.3
3"-OMe	49.5	42.3	42.5	42.4	42.5	42.4
3"-Me	21.5	14.9	14.5	14.5	15.0	14.4
4"	78.0	69.6	70.0	70.1	70.1	70.0
5"	65.8	61.7	59.8	60.1	61.5	60.4
5"-Me	18.7	12.9	10.9	11.9	13.1	11.8

Table S8. Experimental and unscaled computed ^{1}H-NMR chemical shifts obtained at the same level the IR and VCD spectra were computed, i.e. B3LYP/6-31G(2d,p)/IEFPCM($CHCl_3$). (unscaled data).

	Exptl.	**1**	**6S**	**8S**	**12R**	**13S**
2	2.89	3.07	3.59	3.10	3.17	3.05
2-Me	1.20	1.47	1.42	1.42	1.49	1.43
3	3.77	4.23	5.12	4.42	4.32	4.60
4	1.92	2.25	2.38	2.50	2.00	2.97
4-Me	1.10	1.31	1.48	1.41	1.30	1.45
5	3.67	4.24	4.02	4.04	4.20	4.28
6-Me	1.41	1.67	1.31	1.63	1.58	1.58
6-OMe	3.04	3.34	3.21	3.18	3.57	3.42
7ax	1.85	2.15	2.56	2.62	2.66	2.30
7eq	1.72	1.98	1.84	1.98	1.65	1.91
8	2.59	2.80	4.20	3.37	3.46	2.77
8-Me	1.14	1.35	1.18	1.24	1.21	1.39
10	3.00	3.25	2.87	3.32	3.25	3.41
10-Me	1.13	1.37	1.56	1.36	1.55	1.20
11	3.76	4.27	4.03	4.17	3.76	4.49
11-OH	3.98	4.60	3.94	3.69	2.92	4.84
12-Me	1.12	1.34	1.25	1.35	1.19	1.41
12-OH	3.18	3.39	2.46	2.89	4.60	2.87
13-H	5.05	5.67	5.32	5.40	5.36	5.51
14ax	1.48	1.69	1.90	1.78	1.86	2.08
14eq	1.92	2.31	2.28	2.29	2.28	1.95
15	0.85	1.11	1.20	1.13	1.17	1.18
1'	4.44	4.99	5.20	4.67	5.12	4.78
2'	3.19	3.46	3.56	3.57	3.46	3.45
2'-OH	3.45	3.13	3.19	3.10	3.17	3.00
3'	2.41	2.64	2.78	2.65	2.63	2.65
3'-$N(Me)_2$	2.28	2.50	2.50	2.50	2.50	2.50
4'eq	1.66	1.84	1.92	1.87	1.83	1.39
4'ax	1.21	1.34	1.42	1.41	1.33	1.85
5'	3.48	4.02	4.10	3.94	3.95	3.90
5'-Me	1.23	1.38	1.57	1.41	1.38	1.39
1"	4.93	5.26	4.83	5.08	5.27	5.09
2"ax	1.59	1.73	1.63	2.67	1.69	1.69
2"eq	2.37	2.58	2.55	1.72	2.67	2.65
3"-Me	1.25	1.44	1.38	1.39	1.44	1.38
3"-OMe	3.33	3.67	3.61	3.58	3.73	3.58
4"	3.02	3.34	3.21	3.23	3.27	3.23
4"-OH	2.18	2.14	1.74	1.88	2.08	1.89
5"	4.01	4.62	4.53	4.51	4.51	4.53
5"-Me	1.30	1.52	1.48	1.52	1.51	1.59

Summary of NMR analysis

R^2 (x= exptl)	correct structure **1**:	99.93 % (^{13}C)	98.5 % (^{1}H)
(unscaled data)	6S epimer:	99.39 % (^{13}C)	89.8 % (^{1}H)
	8S epimer:	99.59 % (^{13}C)	93.1 % (^{1}H)
	12R epimer:	99.77 % (^{13}C)	91.8 % (^{1}H)
	13S epimer:	99.78 % (^{13}C)	94.3 % (^{1}H)
RMSD	correct structure **1**:	6.01 (^{13}C)	0.34 (^{1}H)
(Unscaled data)	6S epimer:	7.01 (^{13}C)	0.49 (^{1}H)
	8S epimer:	6.06 (^{13}C)	0.40 (^{1}H)
	12R epimer:	5.81 (^{13}C)	0.45 (^{1}H)
	13S epimer:	6.13 (^{13}C)	0.42 (^{1}H)
RMSD	correct structure **1**:	3.78 (^{13}C)	0.26 (^{1}H)
(Scaled data)	6S epimer:	5.09 (^{13}C)	0.41 (^{1}H)
	8S epimer:	4.14 (^{13}C)	0.32 (^{1}H)
	12R epimer:	4.06 (^{13}C)	0.37 (^{1}H)
	13S epimer:	4.08 (^{13}C)	0.32 (^{1}H)
DP4+ analysis[1]	correct structure **1**:	100 %	
(unscaled data)	6S epimer:	0 %	
	8S epimer:	0 %	
	12R epimer:	0 %	
	13S epimer:	0 %	

R^2: coefficient of determination ("R squared")
RMSD: root-mean-square deviation
Unscaled data: chemical shifts obtained at the same level the IR and VCD spectra were computed, i.e. B3LYP/6-31G(2d,p)/IEFPCM($CHCl_3$).
Scaled data: H^1 unscaled data x 0,95 and ^{13}C unscaled data x 1,05

4. Synthesis of 3 and 4

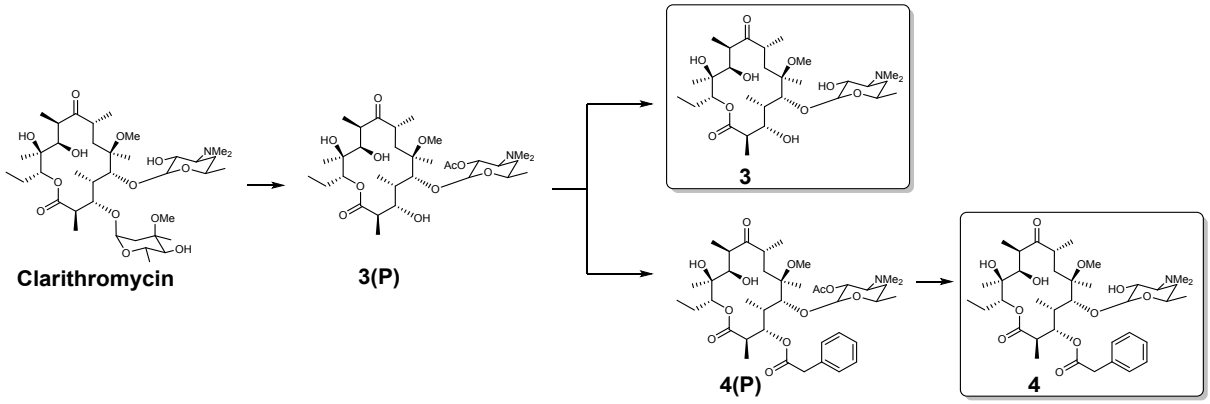


Figure S3. Overview about the synthetic route for compound **3** and **4.**[2]

General

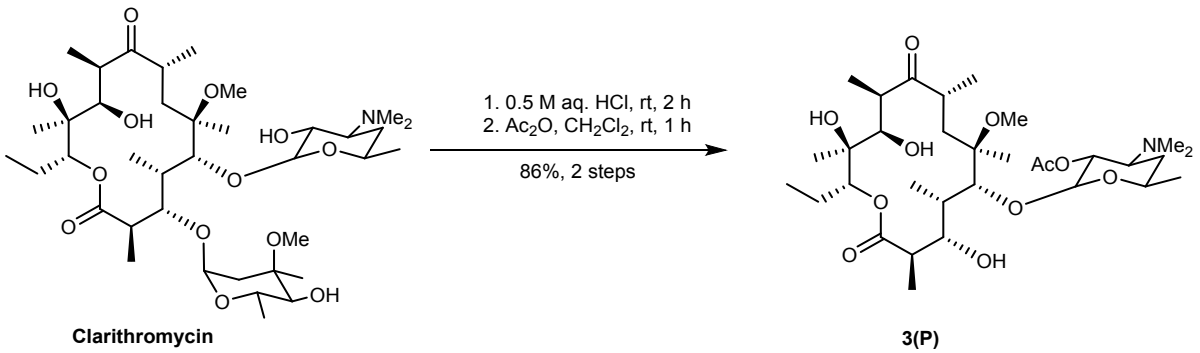
Moisture sensitive reactions were performed in flame dried round bottom flasks under argon atmosphere. Reagents were purchased at highest commercial quality. Solvents of technical commercial quality (MeOH, CH_2Cl_2, EtOAc, Cyclohexane) were distilled using rotational evaporators before use. Dry solvents (Et_2O, CH_2Cl_2 and THF) were taken from a solvent drying system (MBraun, SPS-800). Reactions were monitored by thin layer chromatography using silica gel plates (Merck, 60 F_{254}) and developed using a potassium permanganate solution (9 g $KMnO_4$, 60 g K_2CO_3, 15 mL 5 % aqueous NaOH solution and 900 mL H_2O). Column chromatography was performed on silica gel (Macherey-Nagel, 40-63 µm).

Spectroscopic characterization and miscellaneous analysis

NMR spectra were recorded on Bruker DRX-400 (400 MHz) and DRX-600 (600 MHz) instruments and were calibrated using the residual undeuterated solvent peaks as an internal reference ($CDCl_3$: 7.26 ppm ^{1}H-NMR, 77.2 ppm ^{13}C NMR). As processing software MestReNova 10.0 and ACDLABS 12.0 was used. The following abbreviations were used to explain NMR peak multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sext = sextet, dd = doublet of doublets, dt = doublet of triplets, dq = doublet of quartets, m = multiplet, br = broad. Chemical shifts (δ) are given in ppm (parts per million) and coupling constants (*J*) in Hertz (Hz).

HPLC-HRMS analysis was run on an Ultimate 3000 HPLC System (consisting of a pump, autosampler, column oven and UV detector) coupled to a compact mass spectrometer (BRUKER DALTONIK GmbH, Life Sciences, Bremen, Germany) using the standard electrospray ionization source. All solvents were LC-MS grade (Chromasolv). Direct injection with an isocratic solvent mixture containing 0.1 % formic acid (ACN:H_2O = 75:25, Flow: 0.3 mL/min) was used. For internal calibration a lock mass of 622.028960 (Hexakis(1H,1H,2H-perfluoroethoxy)phosphazene) and sodium formiate clusters were used.

Synthesis of 3(P)



Compound 3(P): To an aqueous 0.5 M aq. HCl (160 mL) Clarithromycin (20 g, 26.74 mmol) was added portion wise. The resulting white suspension was stirred at rt until a clear solution accrues (approx. 2 h). After full consumption of Clarithromycin was observed (TLC control) the pH was set to 9.5 using 33% aq. NH_3 solution whereby white solid precipitates. The precipitate was filtered and dried under high vacuum overnight. The solid was used for the next step without further purification.[2]

Under an argon atmosphere the dried solid from step 1 (14.14 g) was dissolved in dry CH_2Cl_2 (130 mL) at rt and Ac_2O (5.24 mL) was added. After 1 h stirring at rt (TLC-Control) the organic phase was washed with sat. aq. $NaHCO_3$ solution (3 x 100 mL), H_2O (100 mL) and brine (100 mL). Then the organic phase was dried over $MgSO_4$ and the solvent was removed under reduced pressure. After recrystallization of the crude product (*n*-hexane:acetone) **3(P)** was isolated as a colourless solid (14.51 g, 86%, 2 steps).

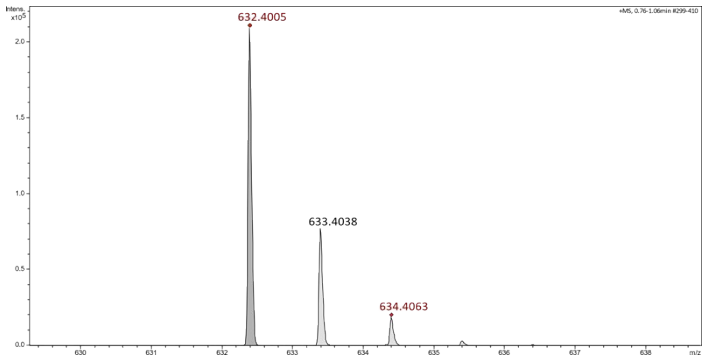
Yield: 86%, 2 steps ≙ 14.51 g (23.00 mmol)

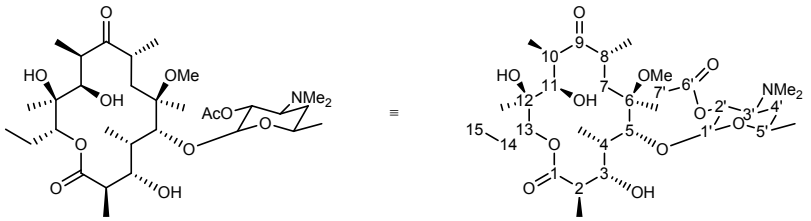
Physical state: colorless amorphous solid.

R_f -value: 0.80 (petrol ether:acetone:NH_3(aq.) = 6:4:0.1)

HRMS (ESI-qTOF):

Ion	Measured m/z	Ion	Sum formula	Calculated m/z	Error [ppm]
$[M+H]^+$	632.4005	$C_{32}H_{58}NO_{11}$	$C_{32}H_{57}NO_{11}$	632.4004	0.0





3(P) ≡ 3(P)

Table S9. ^{1}H and ^{13}C NMR spectra assignments of 3(P).

Position	δ_H ppm (*J* in Hz)	δ_C (ppm)	Position	δ_H ppm (*J* in Hz)	δ_C (ppm)
1	---	174.6	**12-Me**	1.15 (s)	16.2
2	2.63-2.69 (m)	44.0	**13**	5.16 (dd, 11.3, 2.3)	76.8
2-Me	1.24 (d, 5.3)	15.3	**14**	1.46-1.52 (m)	21.3 or 21.5
3	3.45-3.47 (m)	77.7		1.90-2.00 (m)	
4	2.05-2.09 (m)	35.7	**15**	0.83 (t, 7.6)	10.4
4-Me	0.93 (d, 7.6)	7.8	**1'**	4.63 (d, 7.6)	99.6
5	3.72 (d, 2.6)	81.1	**2'**	4.78 (dd, 10.2, 7.6)	71.0
6	---	77.9	**3'**	2.80-2.90 (m)	63.2
6-Me	1.26 (s)	19.2	**3'-NMe$_2$**	2.34 (bm)	40.5
6-OMe	2.94 (s)	49.7	**4'**	1.35 (q, 12.5)	31.1
7	1.43-1.45 (m)	38.4		1.78-1.84 (m)	
	1.73-1.77 (m)		**5'**	3.49-3.53 (m)	68.6
8	2.50-2.56 (m)	45.5	**5'-Me**	1.23 (d, 4.5)	21.3 or 21.5
8-Me	1.11 (d, 3.4)	17.9	**6'**	---	170.6
9	---	220.8	**7'**	2.10 (s)	21.0
10	2.99 (q, 6.8)	37.3		3.95 (bs)	---
10-Me	1.12 (d, 3.0)	12.6	**OH**	3.26 (bs)	---
11	3.81 (s)	69.6		1.90-2.00 (m)	---
12	---	74.1			

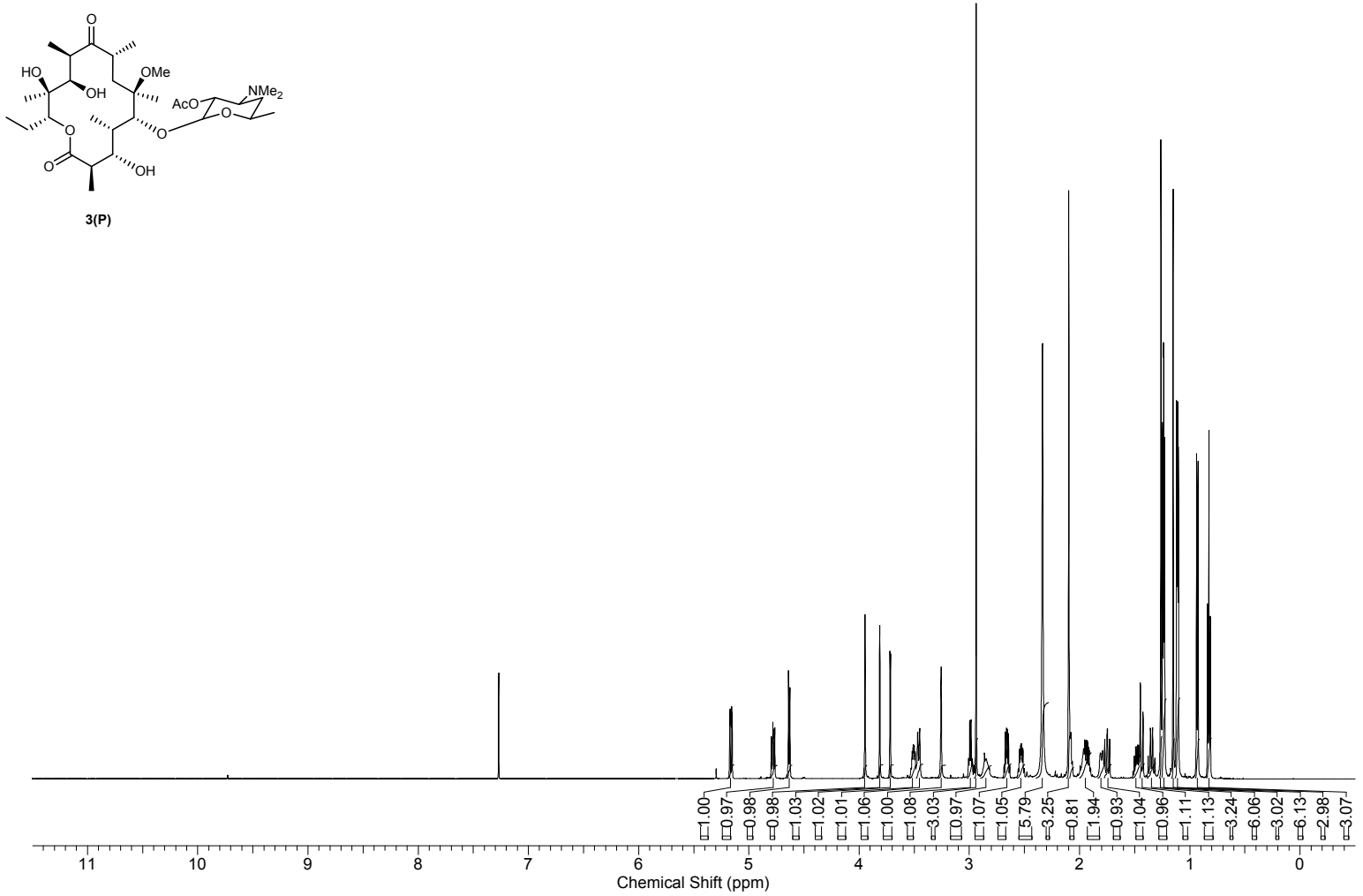


Figure S4. [1]H NMR spectrum of 3(P).

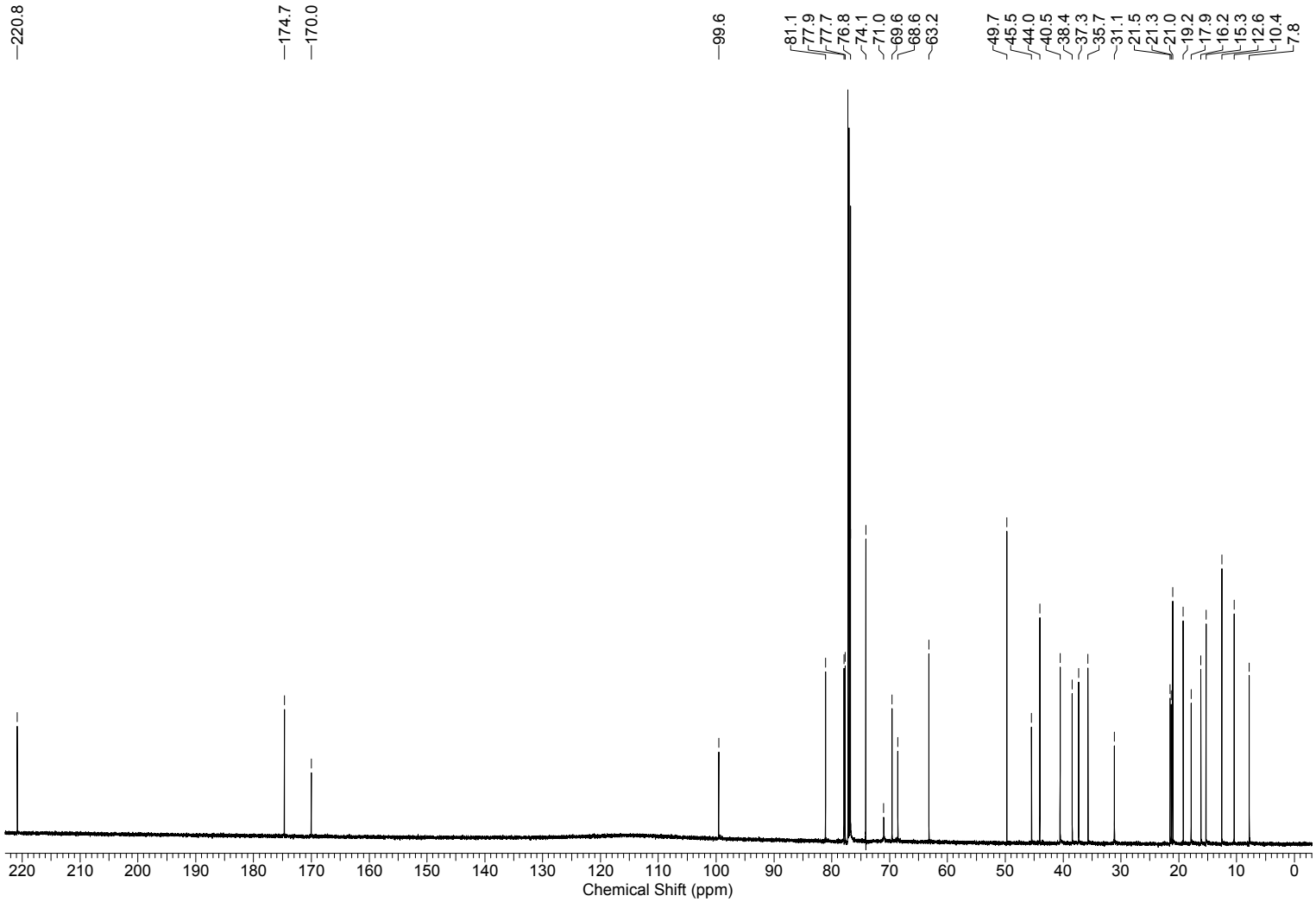


Figure S5. ^{13}C NMR of 3(P).

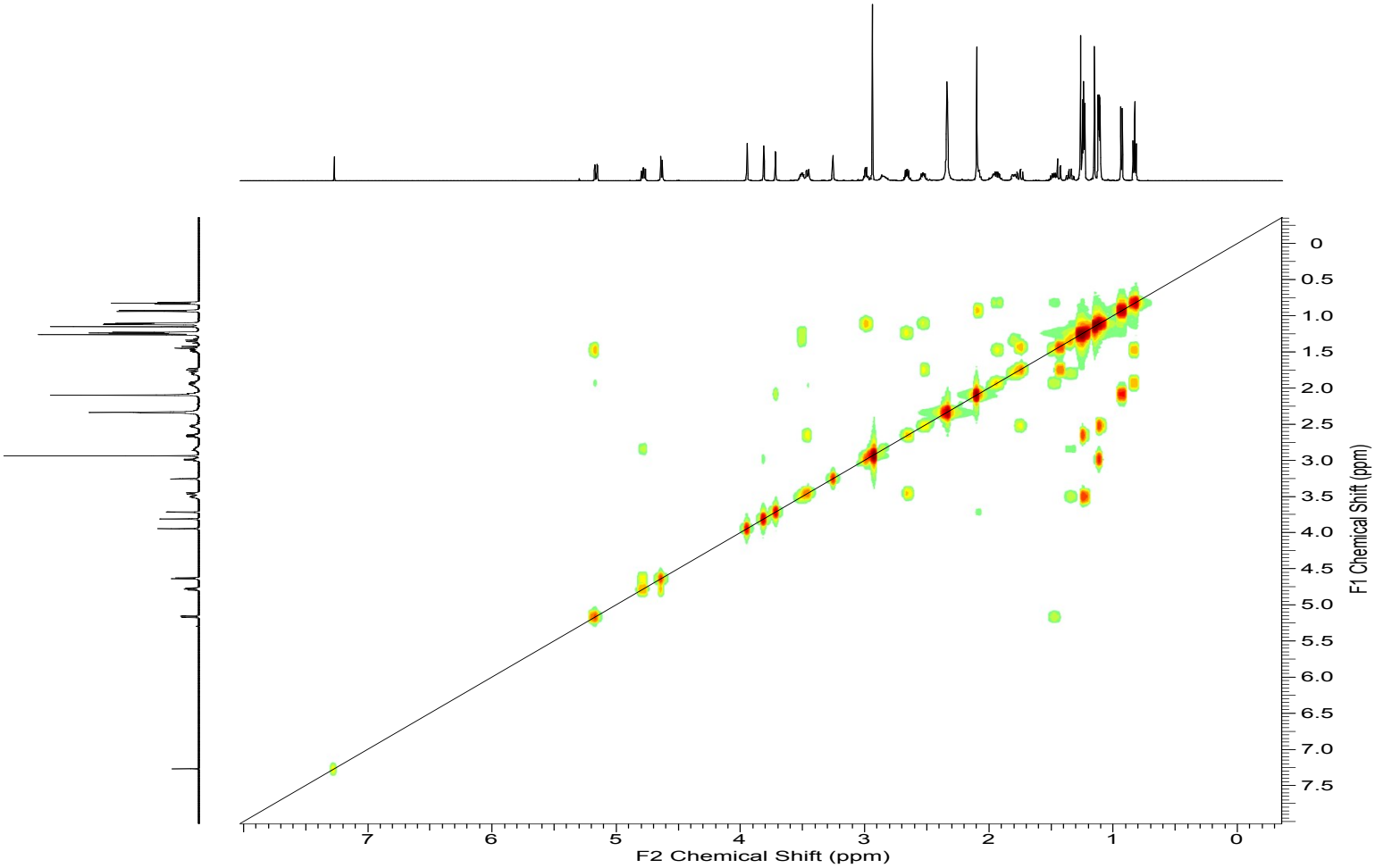


Figure S6. COSY spectrum of 3(P).

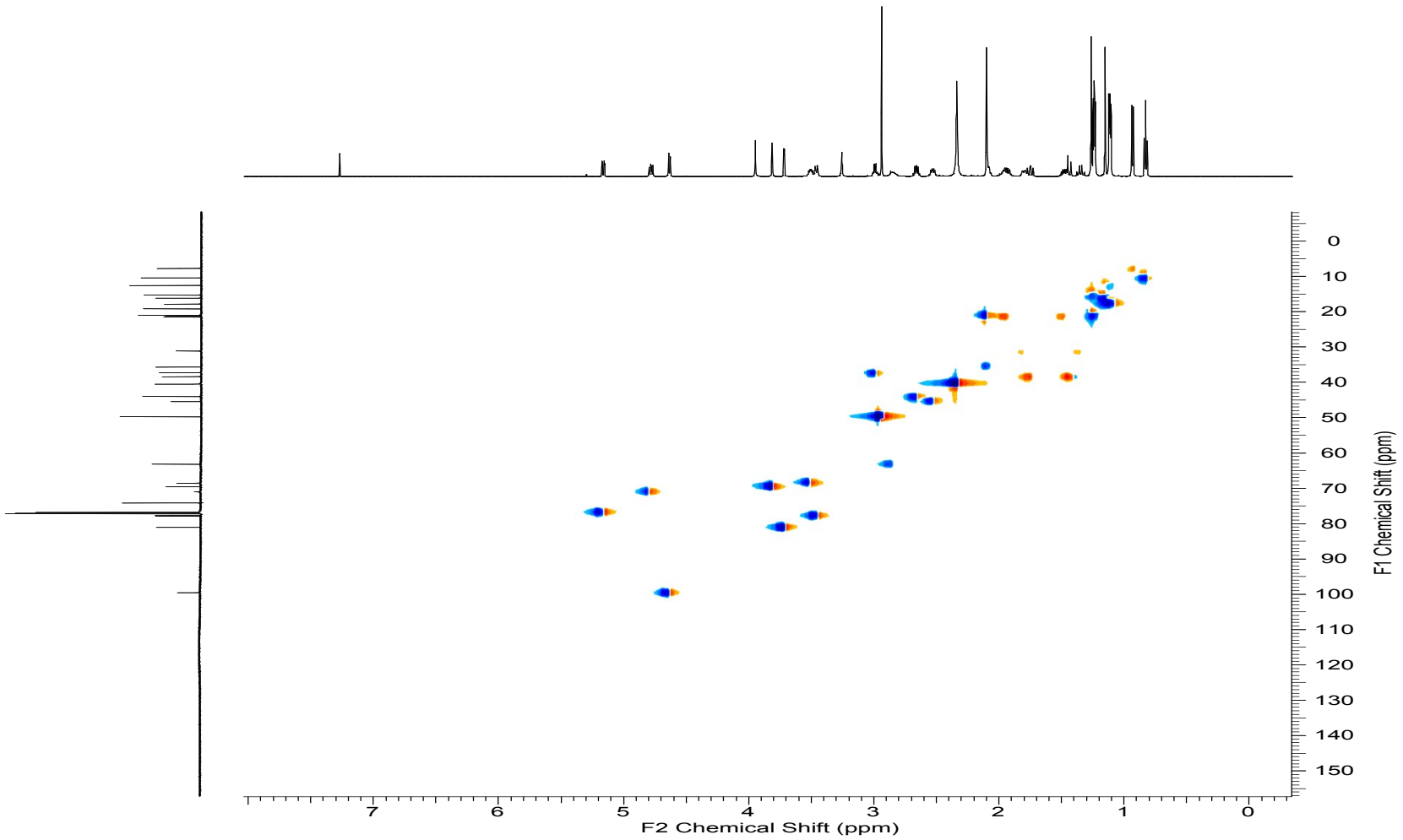


Figure S7. HSQC spectrum of 3(P).

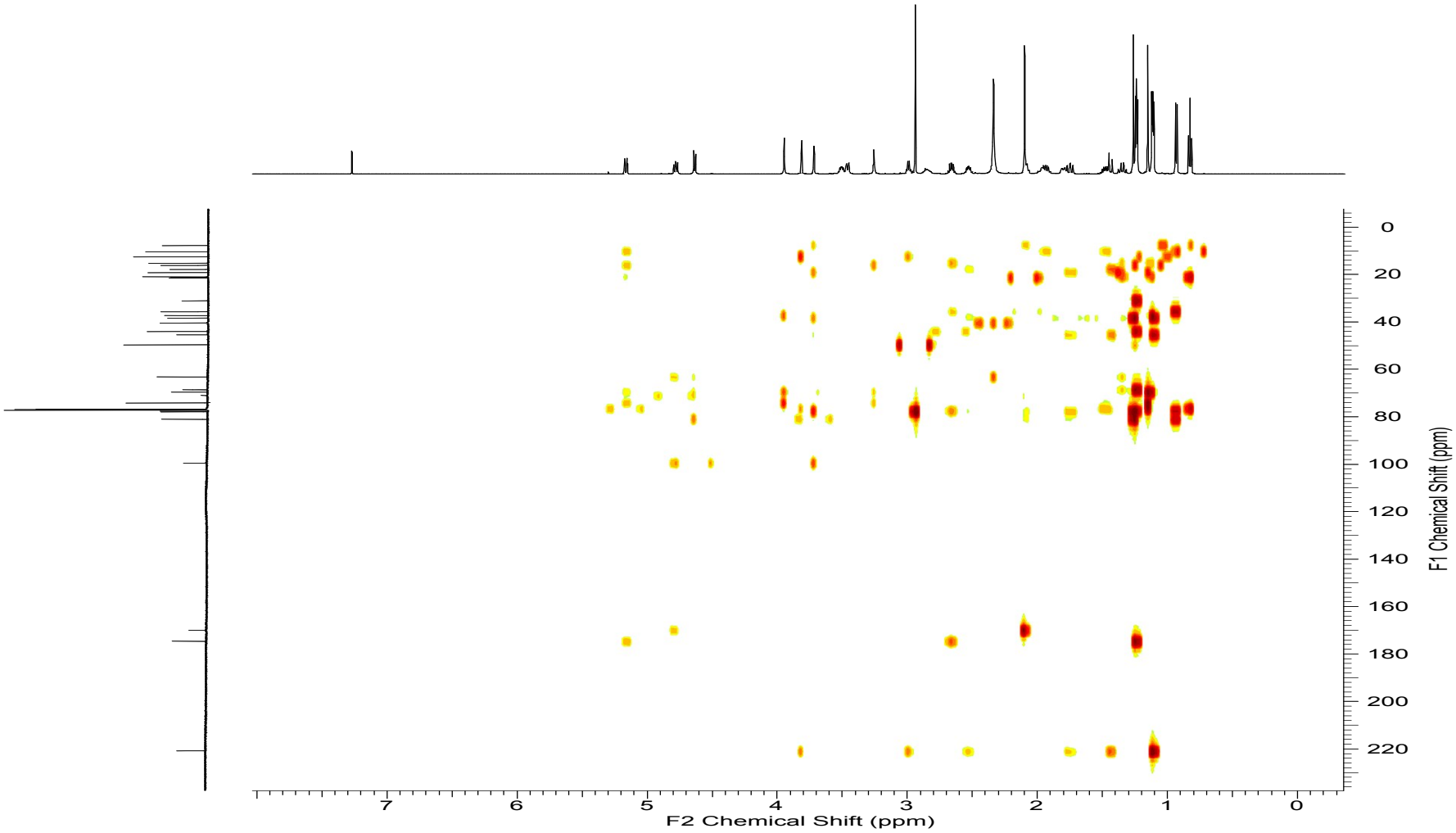
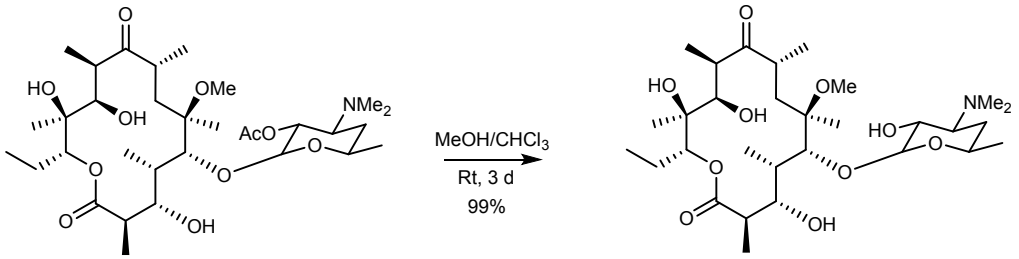


Figure S8. HMBC spectrum of 3(P).

Synthesis of 3



3(P) **3**

Compound 3: **3(P)** (1 g, 1.582 mmol) was dissolved in MeOH (25 mL) and $CHCl_3$ (25 mL) and stirred for 3 d at rt. After removal of the solvent under reduced pressure **3** was isolated as a colourless solid (0.9236 g, 99%).

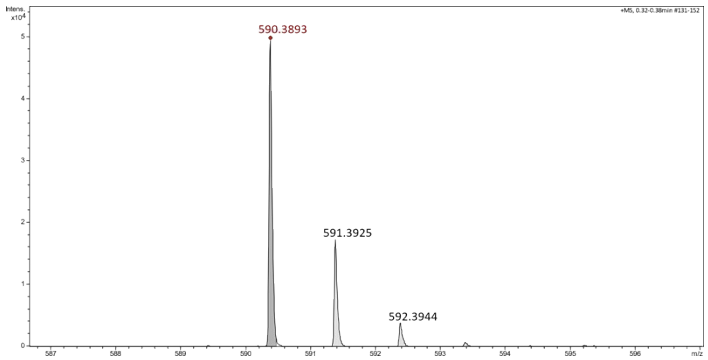
Yield: (99% ≙ 0.9236 g (1.566 mmol)

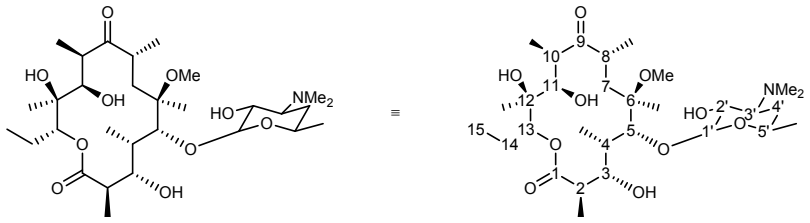
Physical state: colorless amorphous solid.

R_f -value: 0.52 (petrol ether:acetone:NH_3(aq.)) = 6:4:0.1.

HRMS (ESI-qTOF):

Ion	Measured m/z	Ion	Sum formula	Calculated m/z	Error [ppm]
$[M+H]^+$	590.3893	$C_{30}H_{56}NO_{10}$	$C_{30}H_{55}NO_{10}$	590.3899	1.0





3 ≡ 3

Table S10. ^{1}H and ^{13}C NMR spectra assignments of 3.

Position	δ_H ppm (*J* in Hz)	δ_C (ppm)	Position	δ_H ppm (*J* in Hz)	δ_C (ppm)
1	---	175.2	**12-Me**	1.17 (s)	16.4
2	2.70 – 2.60 (m)	44.7	**13**	5.17 (dd, 11.2, 2.5)	76.8
2-Me	1.25 (d, 6.0)	15.4	**14**	1.53 – 1.40 (m) 1.96 – 1.87 (m)	21.6
3	3.59 – 3.45 (m)	79.1			
4	2.16 – 2.05 (m)	36.0	**15**	0.83 (t, 7.3)	10.6
4-Me	1.12 (dd, 6.9, 2.3)	8.4	**1'**	4.38 (d, 7.3)	106.9
5	3.68 (s)	88.7	**2'**	3.23 (dd, 10.2, 7.3)	70.8
6	---	78.2	**3'**	2.47 (ddd, 12.1, 10.2, 3.8)	65.8
6-Me	1.36 (s)	18.9	**3'-NMe$_2$**	2.25 (s)	40.4
6-OMe	2.96 (s)	49.7	**4'**	1.66 (ddd, 12.8, 3.9, 2.1) 1.12 (dd, 6.9, 2.3)	28.2
7	1.96 – 1.87 (m) 1.59 – 1.53 (m)	38.9			
			5'	3.59 – 3.45 (m)	70.4
8	2.56 (dt, 14.0, 7.0)	45.7	**5'-Me**	1.25 (d, 6.0)	21.4
8-Me	1.12 (dd, 6.9, 2.3)	17.9			
9	---	220.8			
10	3.03 – 2.98 (m)	37.7			
10-Me	1.12 (dd, 6.9, 2.3)	12.8			
11	3.85 (s)	69.9			
12	---	74.4			

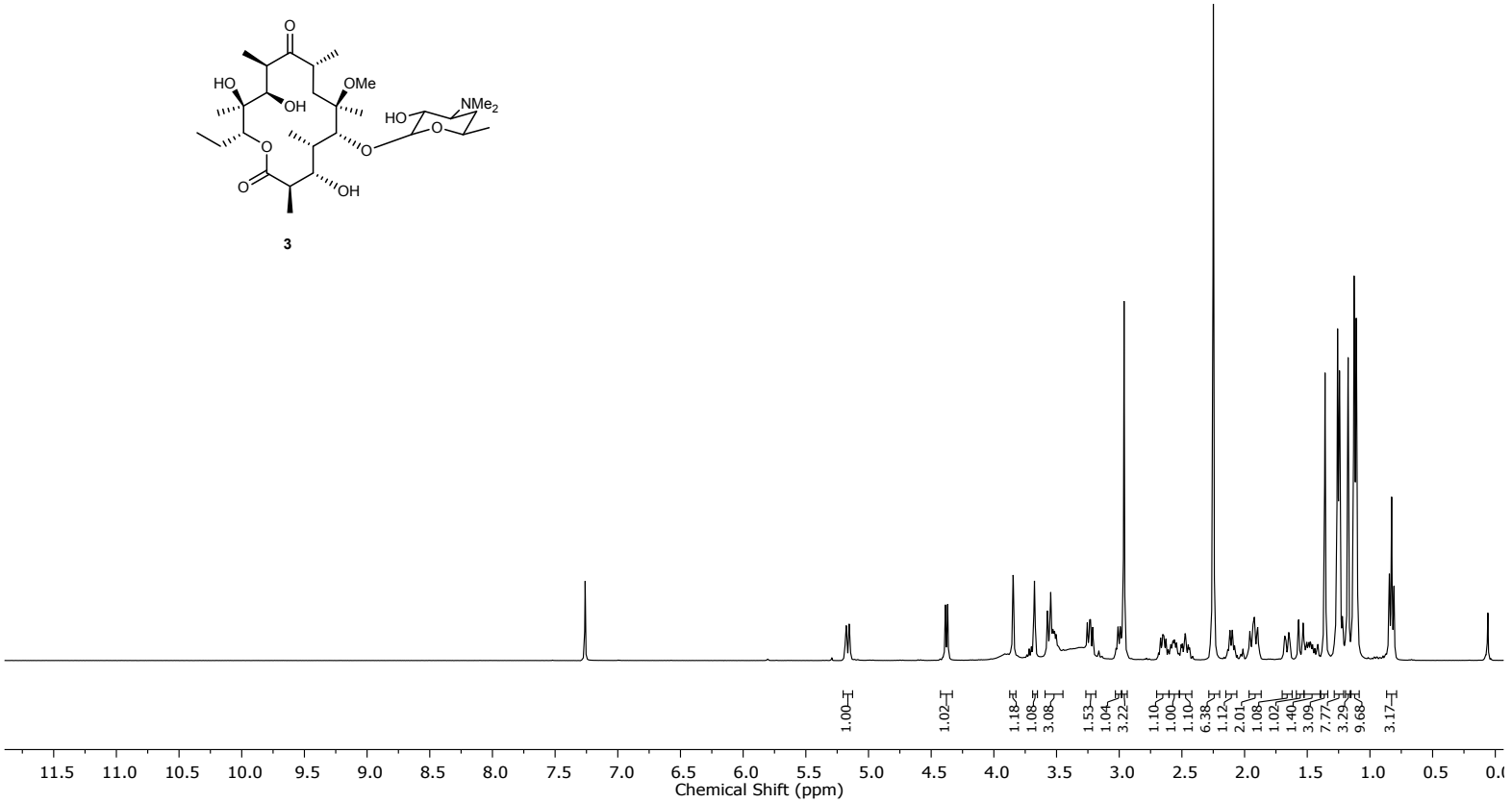


Figure S9. ^{1}H NMR spectrum of 3.

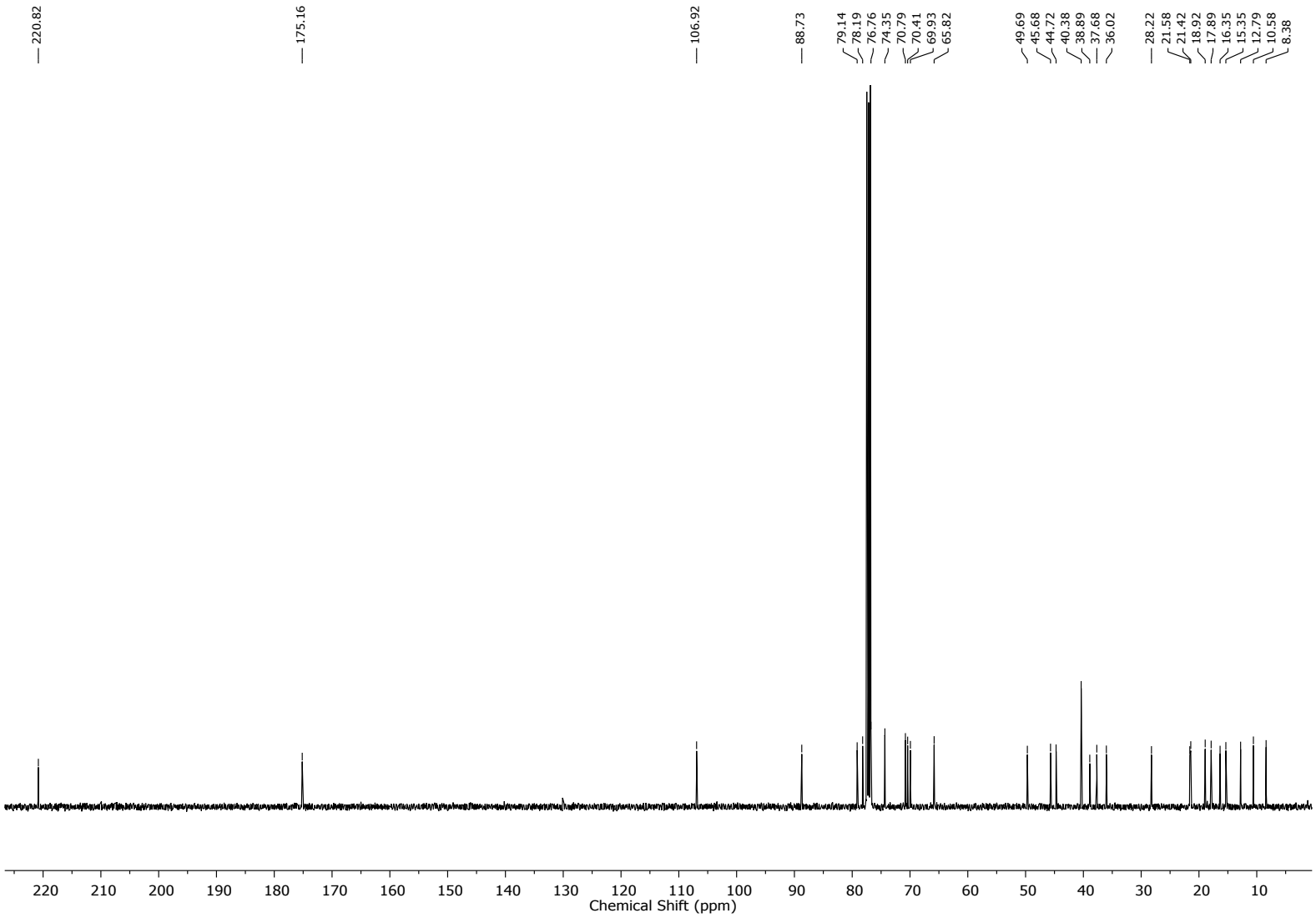


Figure S10. ^{13}C NMR of 3.

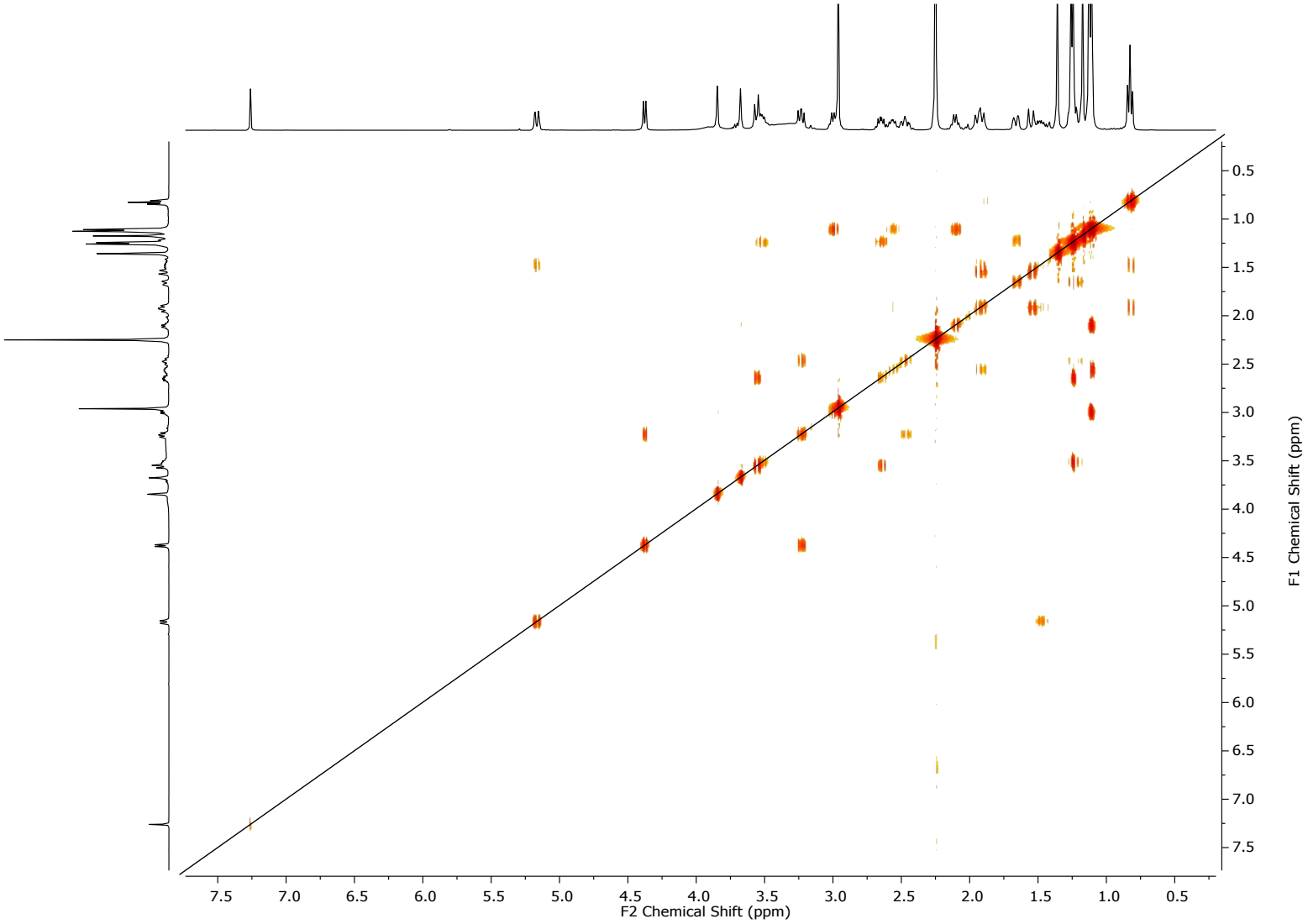


Figure S11. COSY spectrum of 3.

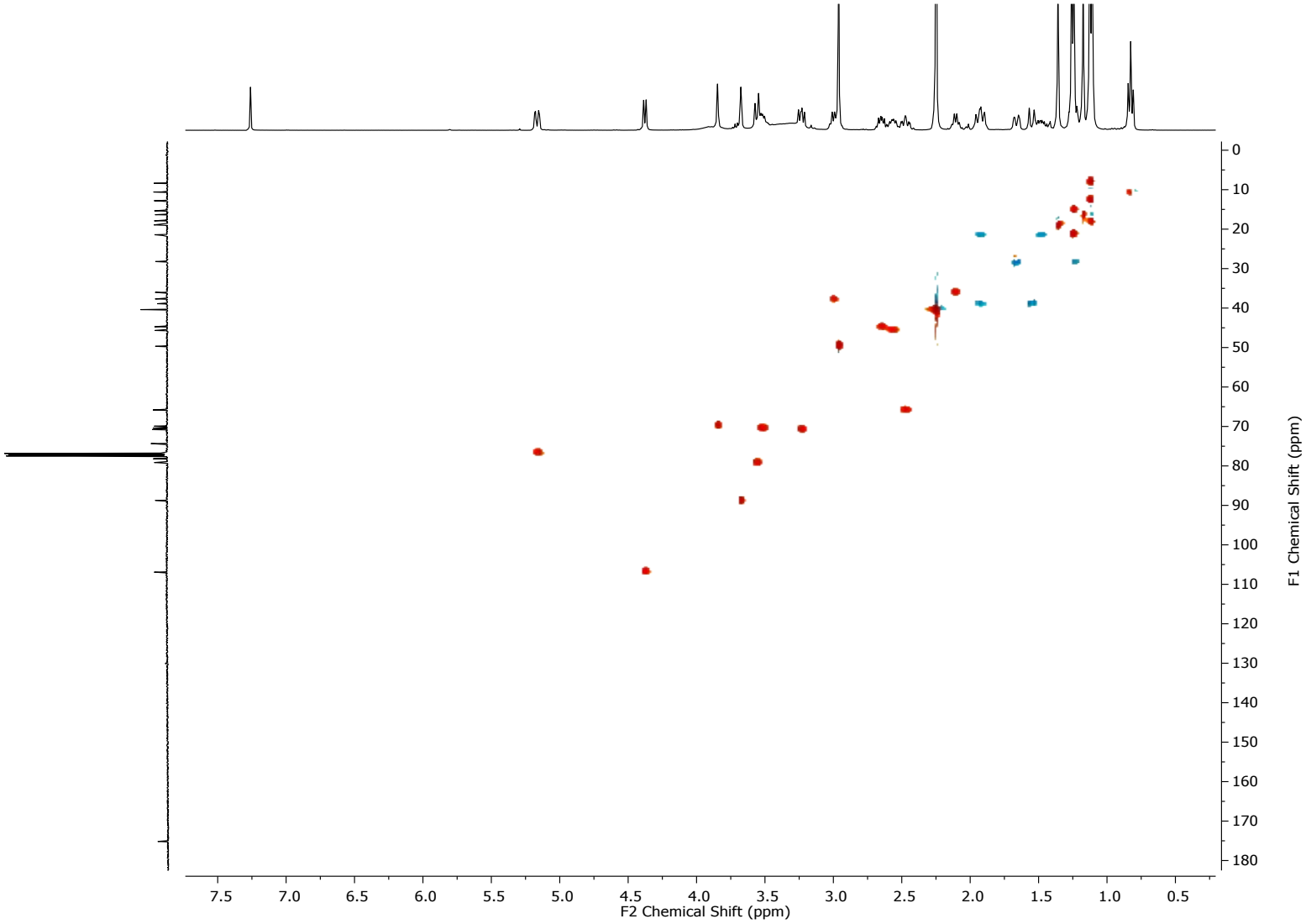


Figure S12. HSQC spectrum of 3.

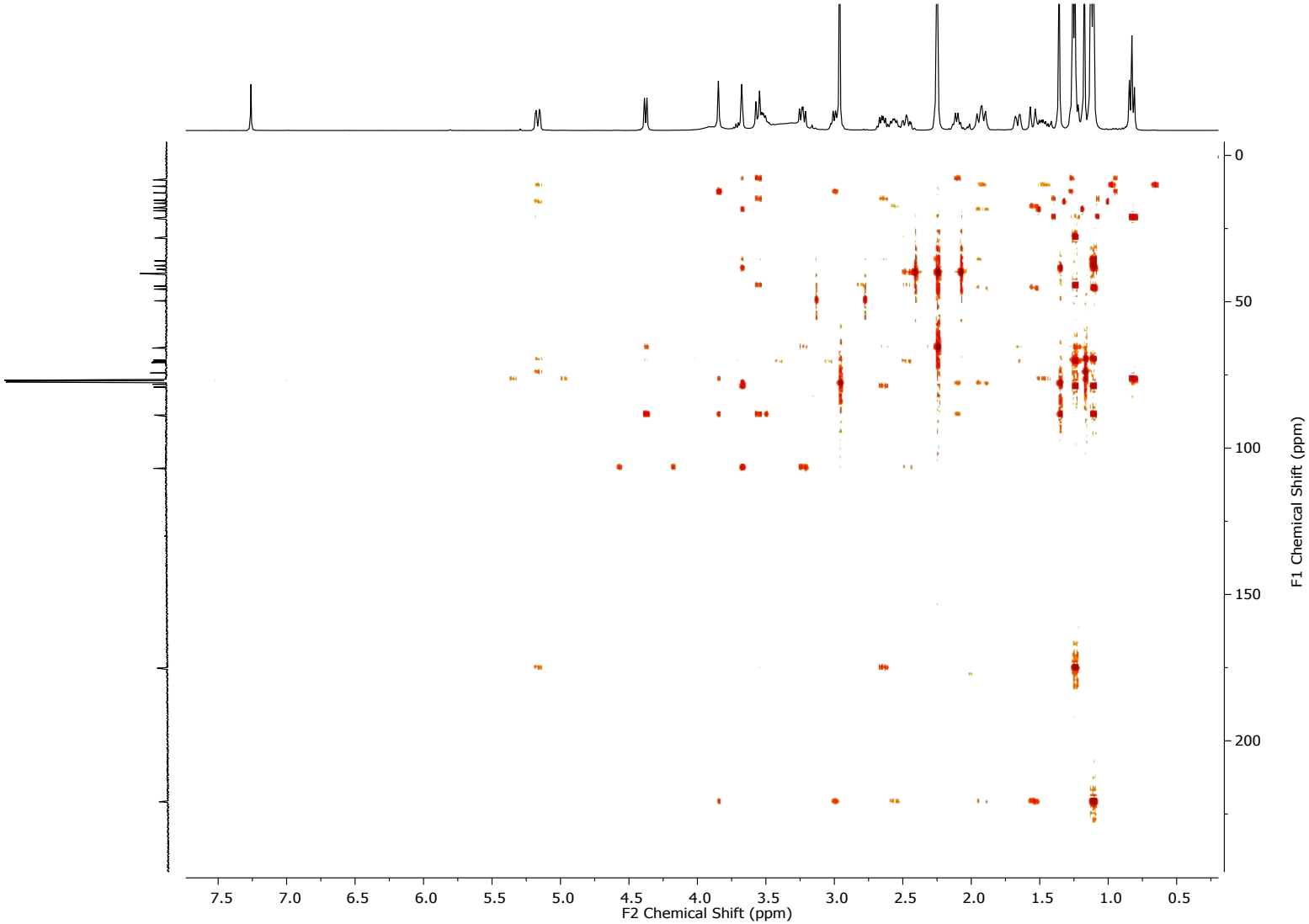
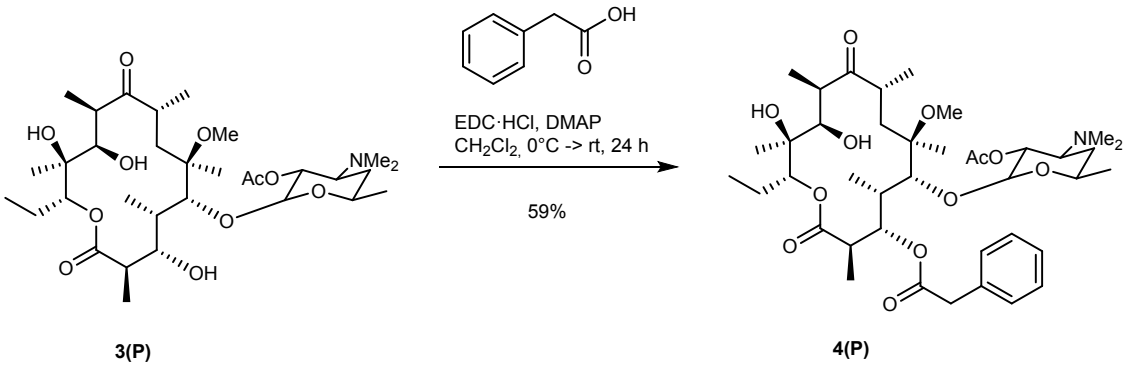


Figure S13. HMBC spectrum of 3.

Synthesis of 4(P)[2]



Compound 4(P): Under an argon atmosphere, compound **3(P)** (500 mg, 0.79 mmol, 1 equiv.) was dissolved in dry CH_2Cl_2 (40 mL / 0.5 mmol of starting material). Phenyl acetic acid (655 mg, 4.81 mmol, 6.08 equiv.), EDC·HCl (912 mg, 4.76 mmol, 6.01 equiv.) and DMAP (99 mg, 0.81 mmol, 1.02 equiv.) were added at 0 °C. After stirring for 45 min, the ice bath was removed, and the reaction mixture was stirred at rt. After completion of the reaction (TLC), the organic phase was washed with sat. aq. $NaHCO_3$ and dried over $MgSO_4$. The solvent was removed under reduced pressure and the corresponding products were purified by flash chromatography (petrol ether:acetone = 99:1 → 78:22). **4(P)** was isolated as a colourless solid (351 mg, 59%).

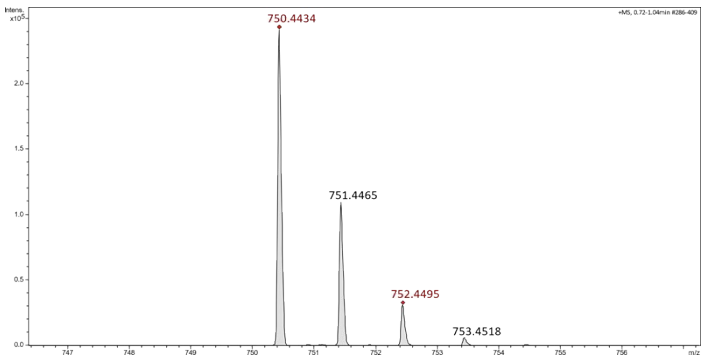
Yield: 59% ≙ 351 mg (0.468 mmol)

Physical state: colorless amorphous solid.

R_f -value: 0.63 (petrol ether:acetone:NH_3(aq.)) = 6:4:0.1.)

HRMS (ESI-qTOF):

Ion	Measured m/z	Ion	Sum formula	Calculated m/z	Error [ppm]
$[M+H]^+$	750.4434	$C_{40}H_{64}NO_{12}$	$C_{40}H_{63}NO_{12}$	750.4423	-1.4



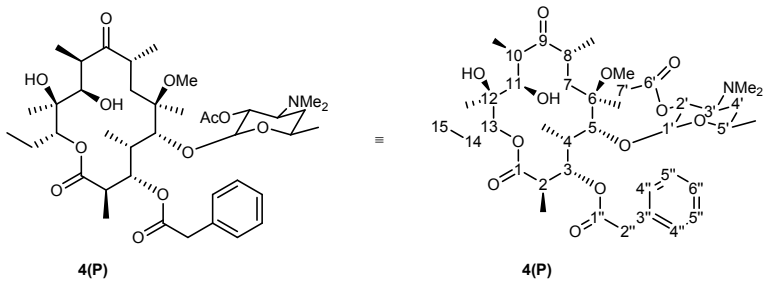


Table S11. ^{1}H and ^{13}C NMR spectra assignments of 4(P).

Position	δ_H ppm (*J* in Hz)	δ_C (ppm)	Position	δ_H ppm (*J* in Hz)	δ_C (ppm)
1	---	173.5	**14**	1.42-1.54 (m) 1.93 (dsext, 7.6, 2.8)	21.2
2	2.78-2.85 (m)	43.0			
2-Me	0.94 (d, 6.8)	15.1	**15**	0.81 (t, 7.3)	10.4
3	5.05 (d, 10.9)	78.5	**1'**	3.90 (d, 7.6)	100.3
4	2.14-2.20 (m)	36.0	**2'**	4.68 (dd, 10.6, 7.3)	71.1
4-Me	0.98 (d, 7.6)	8.8	**3'**	2.49-2.63 (m)	63.2
5	3.68-3.76 (m)	79.7	**3'-NMe$_2$**	2.30 (bs)	40.5
6	---	78.0	**4'**	1.20-1.23 (m) 1.59-1.69 (m)	30.7
6-Me	1.25 (s)	19.3			
6-OMe	3.02 (s)	50.1	**5'**	2.89-2.96 (m)	68.7
7	1.42-1.54 (m) 1.59-1.69 (m)	38.3	**5'-Me**	1.10-1.14 (m)	20.8
			6'	---	169.8
8	2.49-2.63 (m)	45.3	**7'**	2.12 (s)	21.5
8-Me	1.10-1.14 (m)	17.9	**1''**	---	170.9
9	---	220.6	**2''**	3.68-3.76 (m)	41.5
10	2.97-3.00 (m)	37.3	**3''**	---	133.4
10-Me	1.10-1.14 (m)	12.4	**4''**	7.28-7.39 (m)	129.5
11	3.80 (d, 1.3)	69.4	**5''**	7.28-7.39 (m)	128.7
12	---	74.2	**6''**	---	127.4
12-Me	1.10-1.14 (m)	16.1	**OH**	3.95 (bs)	---
13	5.16 (dd, 11.1, 2.3)	77.1		3.23 (bs)	---

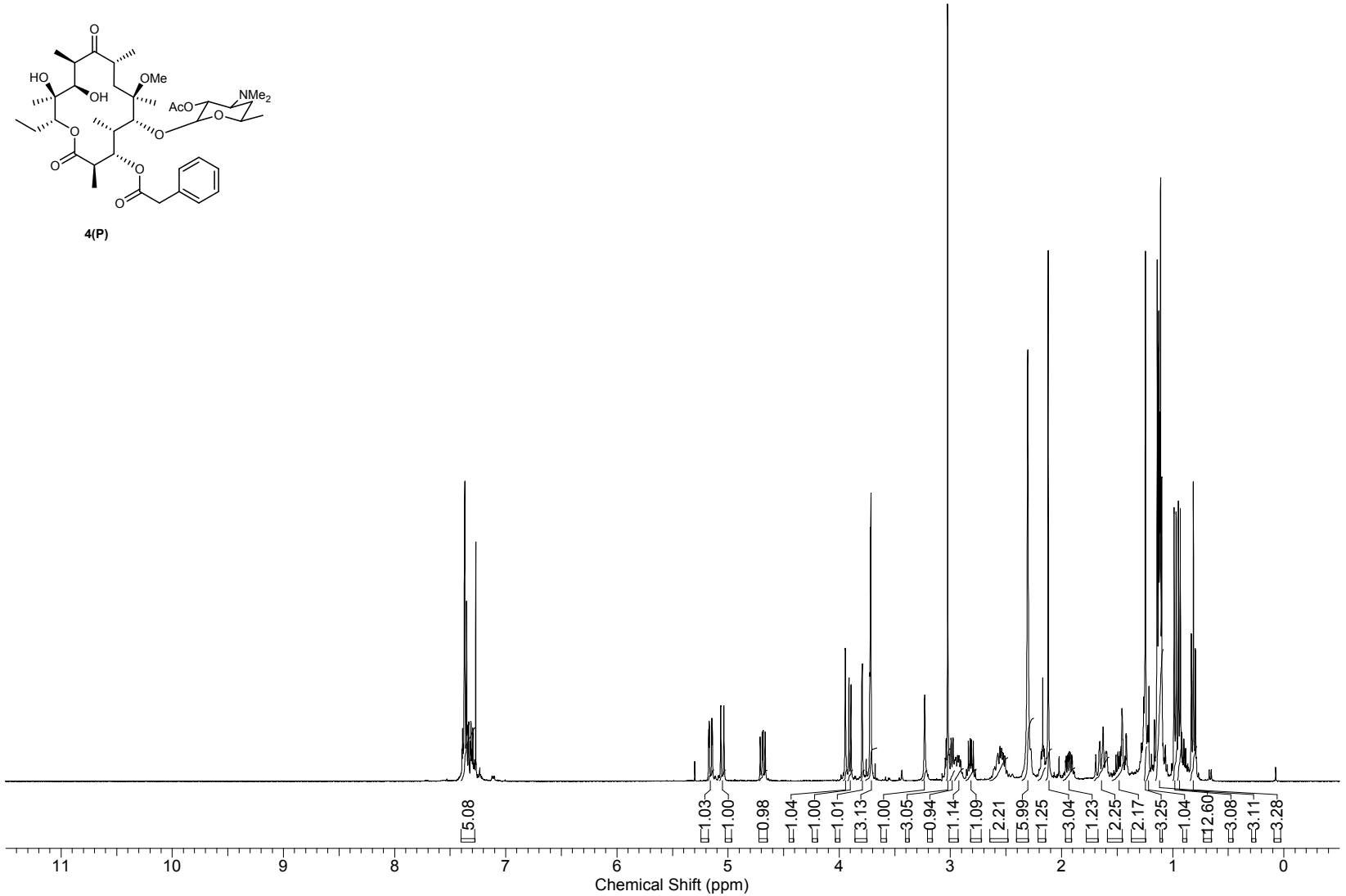


Figure S14. ^{1}H NMR spectrum of 4(P).

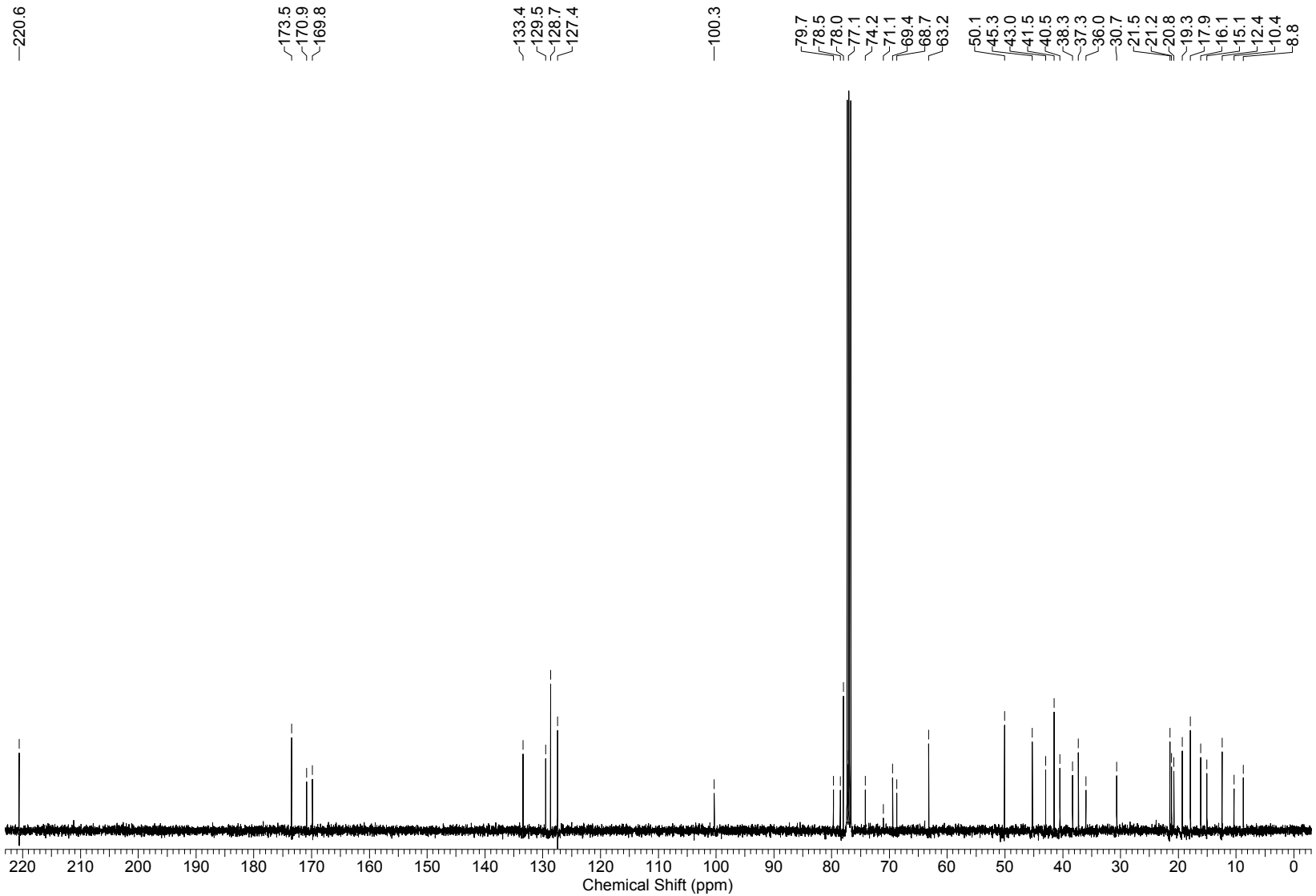


Figure S15. ^{13}C NMR of 4(P).

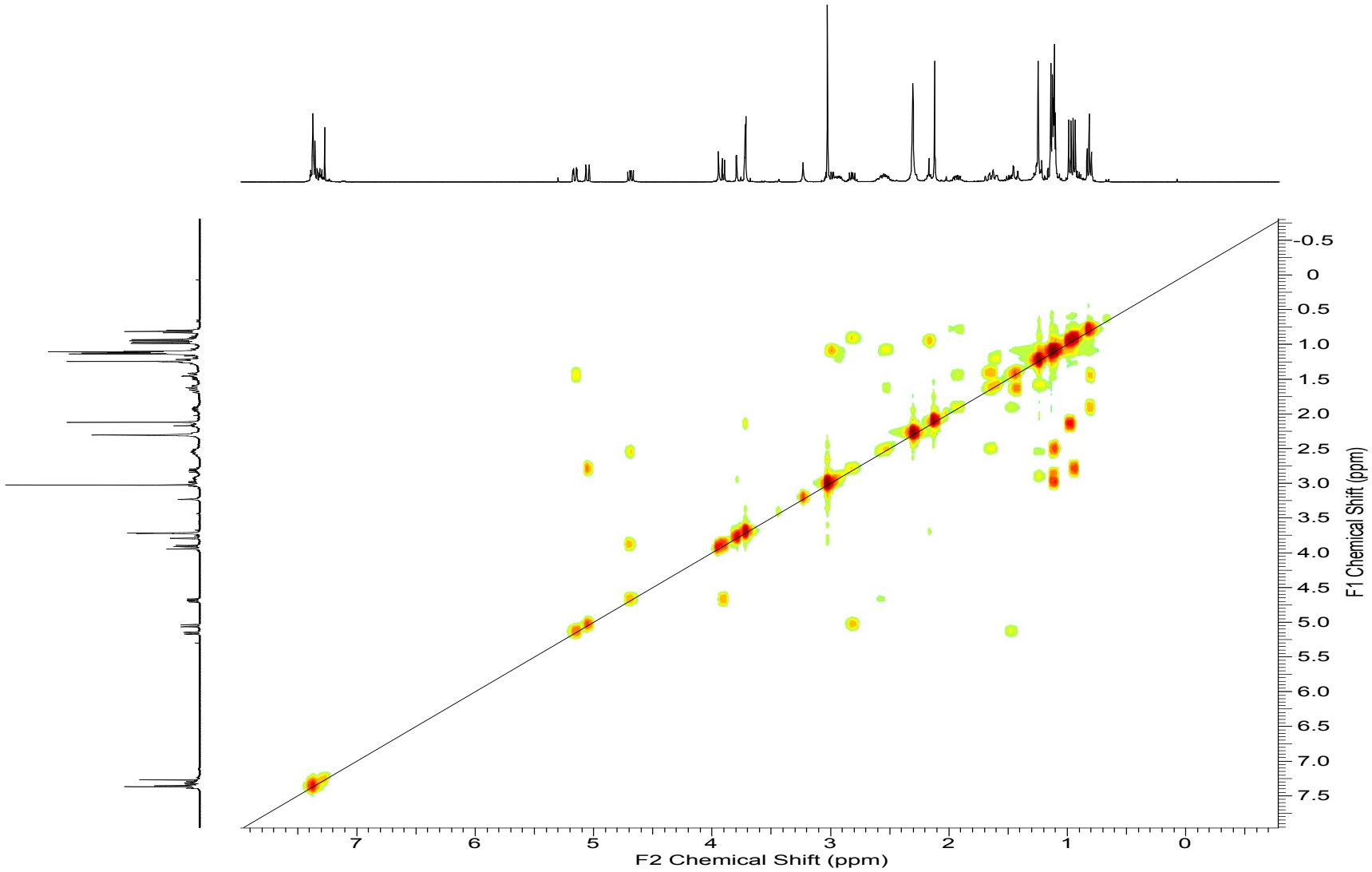


Figure S16. COSY spectrum of 4(P).

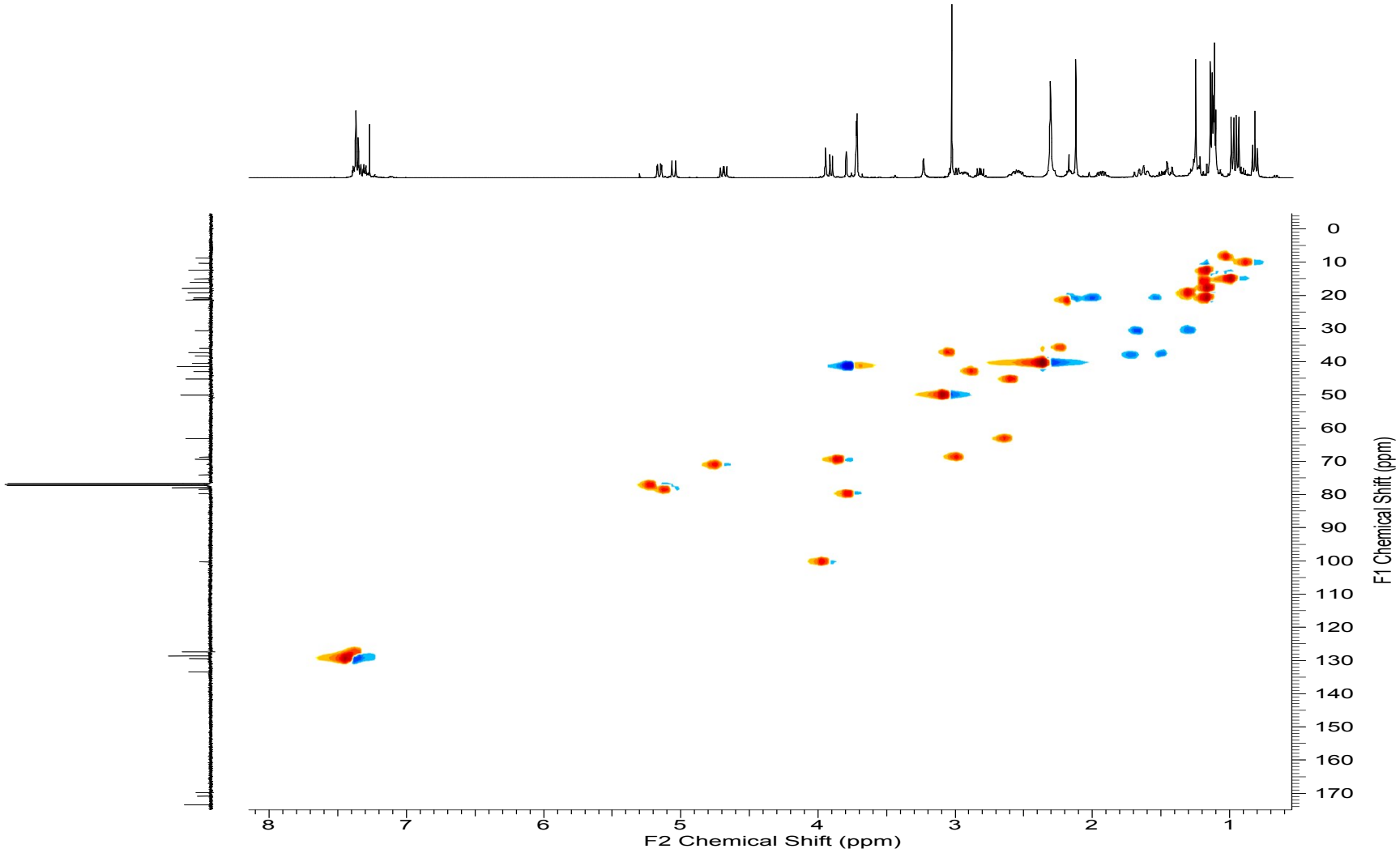


Figure S17. HSQC spectrum of 4(P).

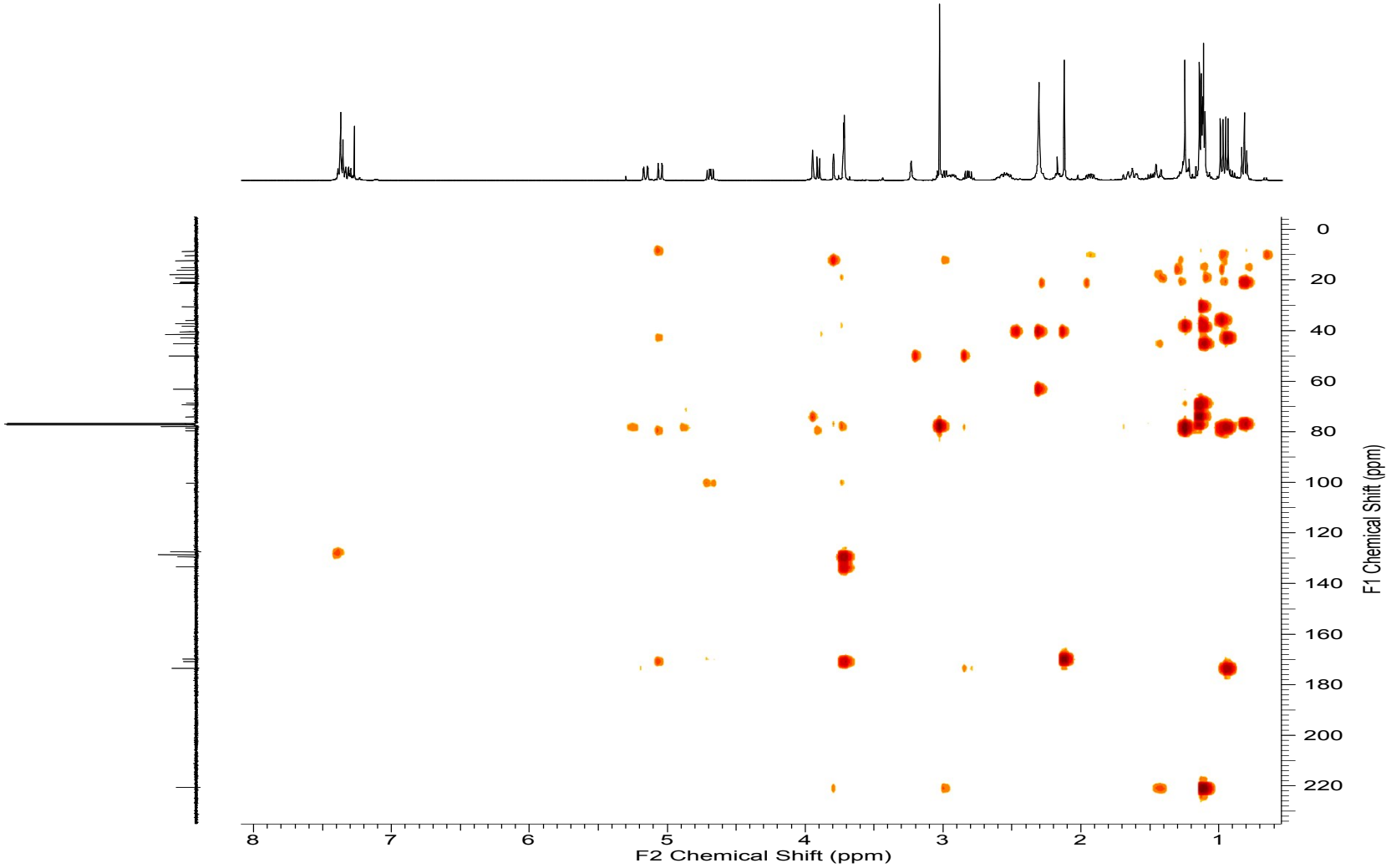
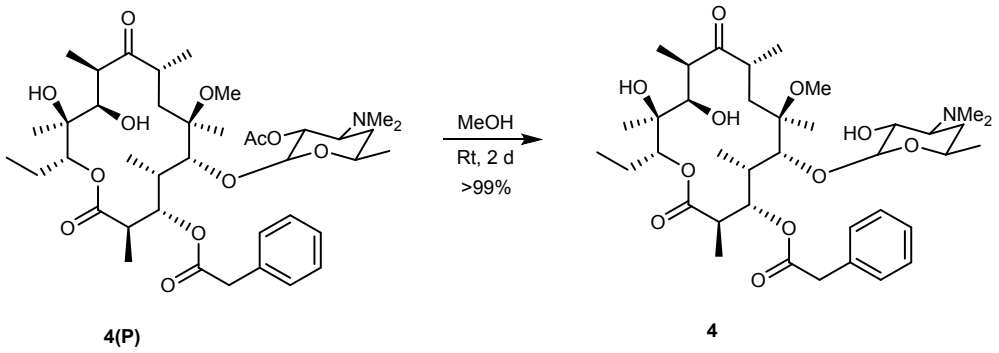


Figure S18. HMBC spectrum of 4(P).

Synthesis of 4[2]



Compound 4: **4(P)** (170 mg, 227 µmol) was dissolved in MeOH (5 mL) and stirred for 2 d at rt. After removal of the solvent under reduced pressure **4** was isolated as a colourless solid (160 mg, 99%).

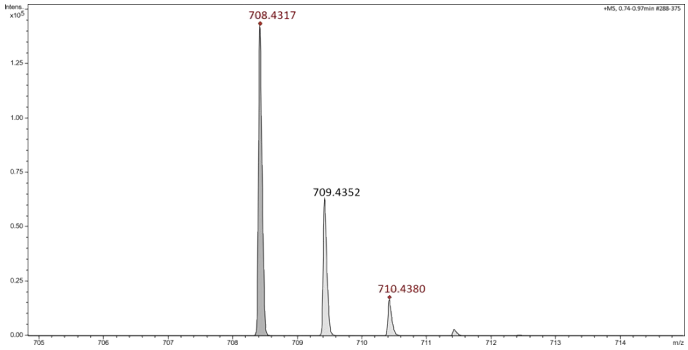
Yield: (99%, 160 mg (0.226 mmol)

Physical state: colorless amorphous solid.

R_f -value: 0.37 (petrol ether:acetone:NH_3(aq.)) = 6:4:0.1.

HRMS (ESI-qTOF):

Ion	Measured m/z	Ion	Sum formula	Calculated m/z	Error [ppm]
$[M+H]^+$	708,4317	$C_{38}H_{62}NO_{11}$	$C_{38}H_{61}NO_{11}$	708,4317	0.1



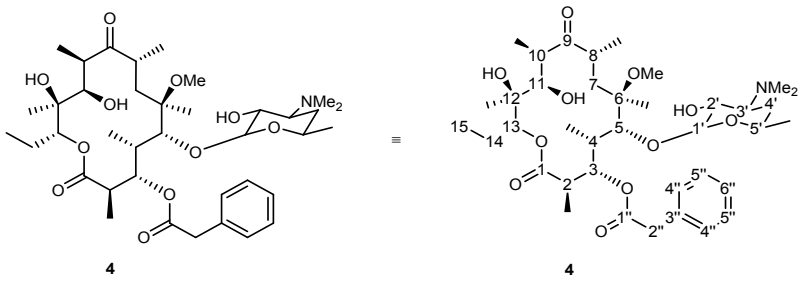


Table S12. ^{1}H and ^{13}C NMR spectra assignments of 4.

Position	δ_H ppm (*J* in Hz)	δ_C (ppm)	Position	δ_H ppm (*J* in Hz)	δ_C (ppm)
1	---	173.6	**13**	5.16 (dd, 11.1, 2.3)	77.2
2	2.78-2.88 (m)	43.0	**14**	1.42-1.51 (m) 1.92 (dsext, 8.1, 2.8)	21.2
2-Me	0.91 (d, 6.8)	15.0			
3	5.07 (d, 10.9)	78.6	**15**	0.81 (t, 7.3)	10.4
4	2.15-2.25 (m)	36.2	**1'**	3.89 (d, 7.1)	102.9
4-Me	1.07-1.15 (m)	9.0	**2'**	3.17-3.23 (m)	70.4
5	3.77 (d, 3.8)	81.1	**3'**	2.43-2.50 (m)	65.9
6	---	78.0	**3'-NMe_2**	2.40 (s)	40.4
6-Me	1.28 (s)	19.4	**4'**	1.18-1.22 (m) 1.60-1.68 (m)	29.2
6-OMe	3.05 (s)	50.2			
7	1.52-1.57 (m) 1.73-1.83 (m)	38.7	**5'**	2.95-3.03 (m)	69.0
			5'-Me	1.07-1.15 (m)	20.9
8	2.51-2.60 (m)	45.3	**1''**	---	171.2
8-Me	1.07-1.15 (m)	18.0	**2''**	3.71 (q, 14.9)	41.5
9	---	220.5	**3''**	---	133.6
10	2.95-3.03 (m)	37.3	**4''**	7.27-7.39 (m)	129.5
10-Me	1.07-1.15 (m)	12.5	**5''**	7.27-7.39 (m)	128.6
11	3.82 (d, 1.5)	69.4	**6''**	---	127.3
12	---	74.2	**OH**	3.94 (bs)	---
12-Me	1.07-1.15 (m)	16.1		3.17-3.23 (m)	---

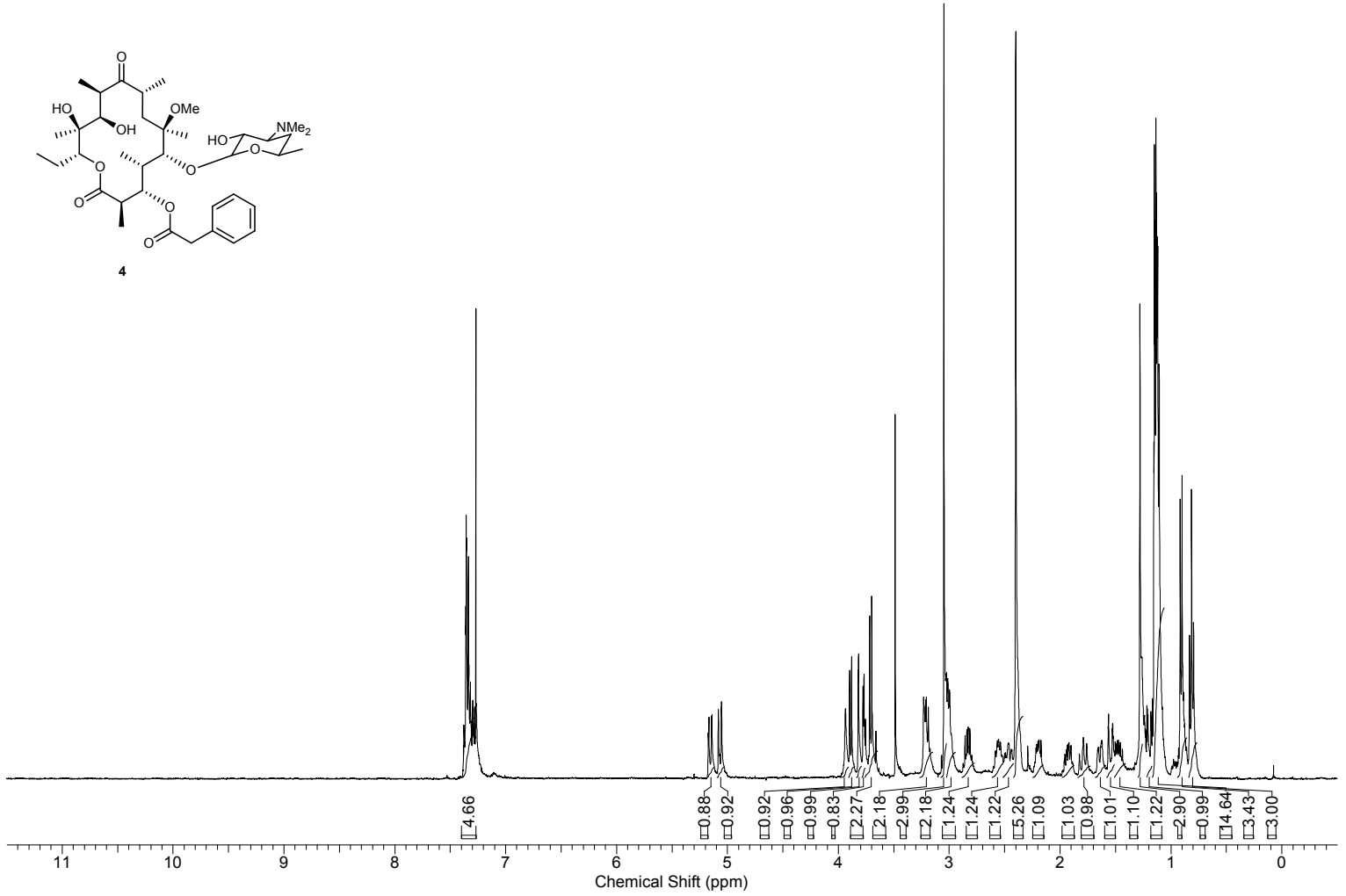


Figure S19. ^{1}H NMR spectrum of 4.

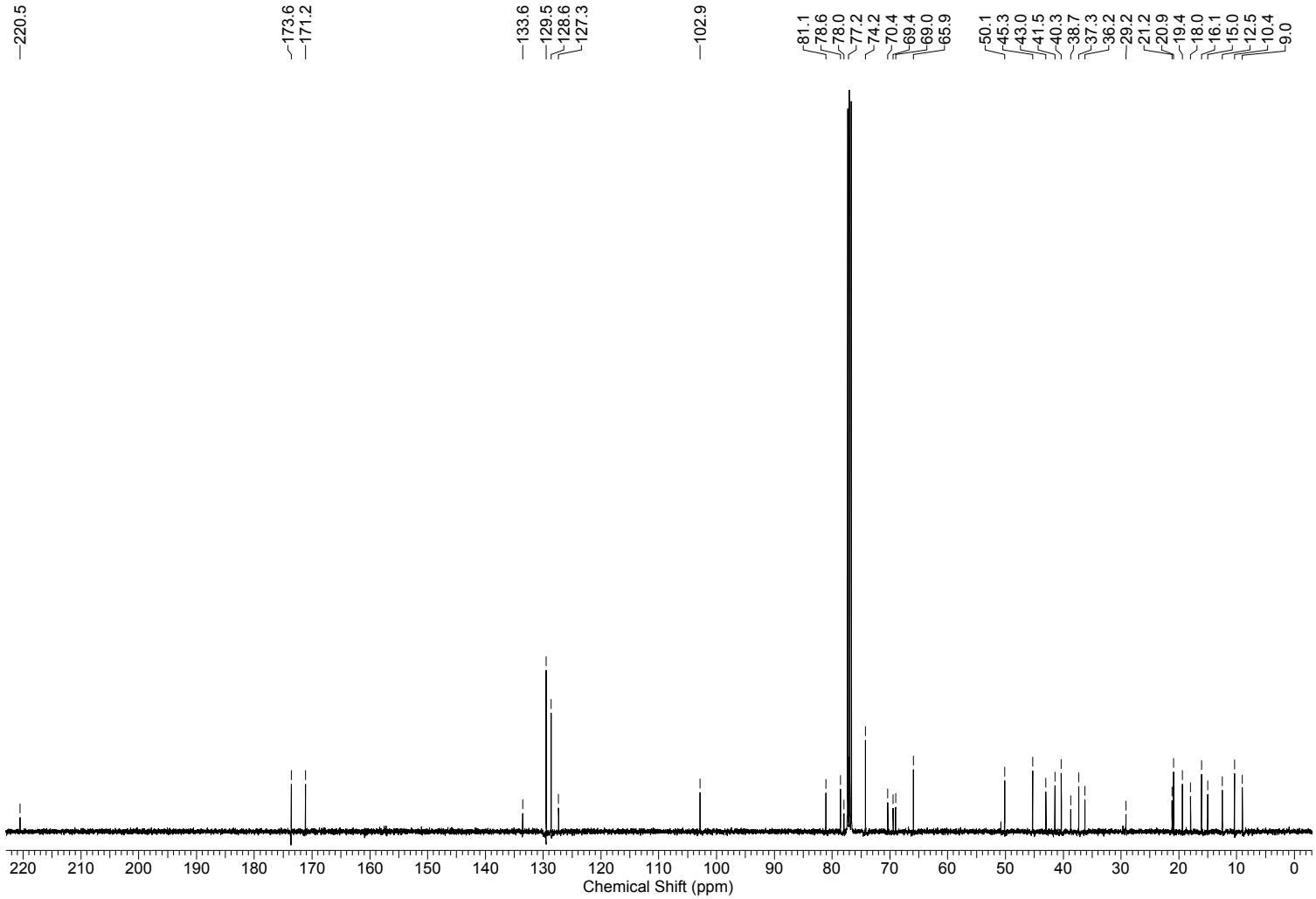


Figure S20. ^{13}C NMR of 4.

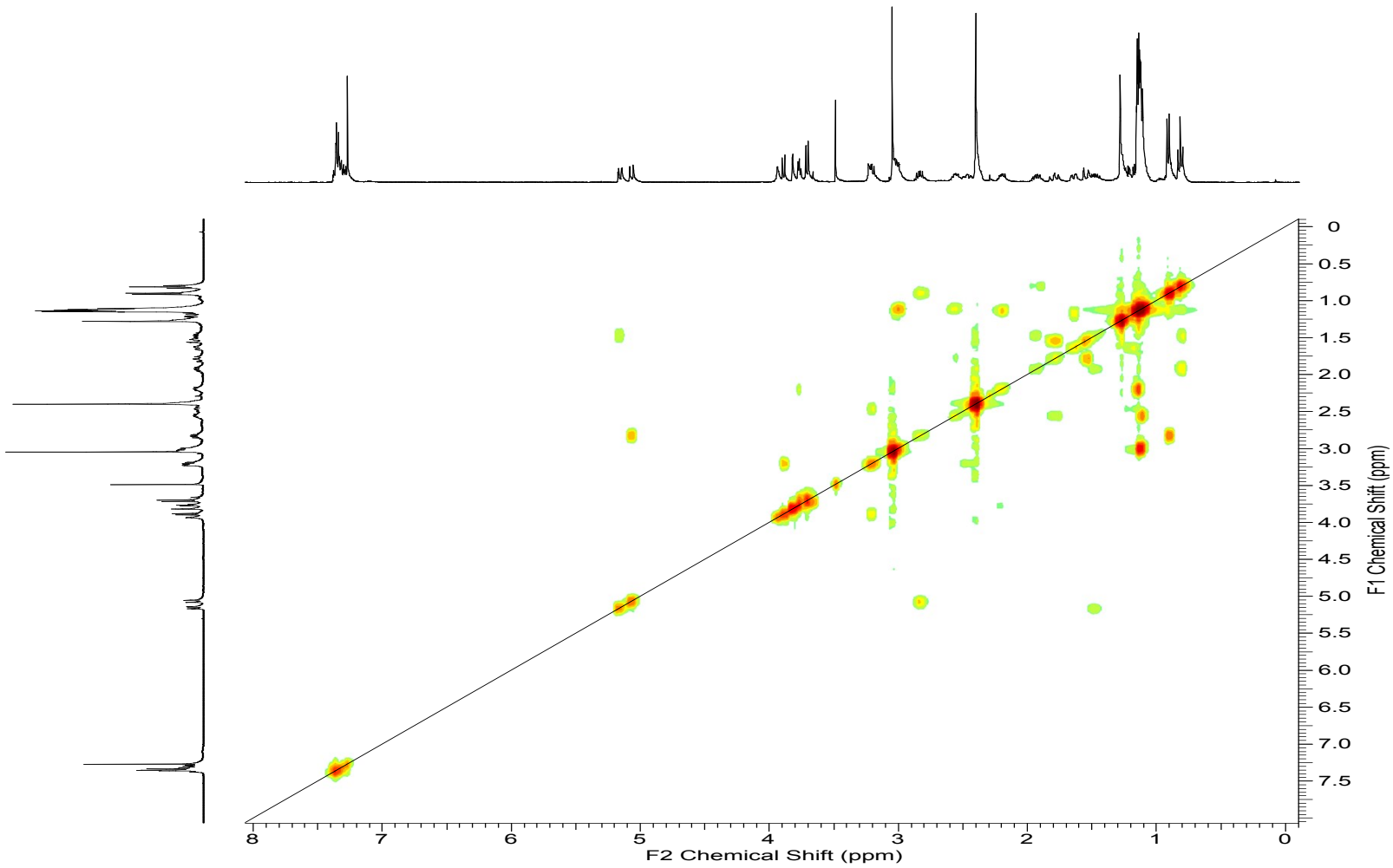


Figure S21. COSY spectrum of 4.

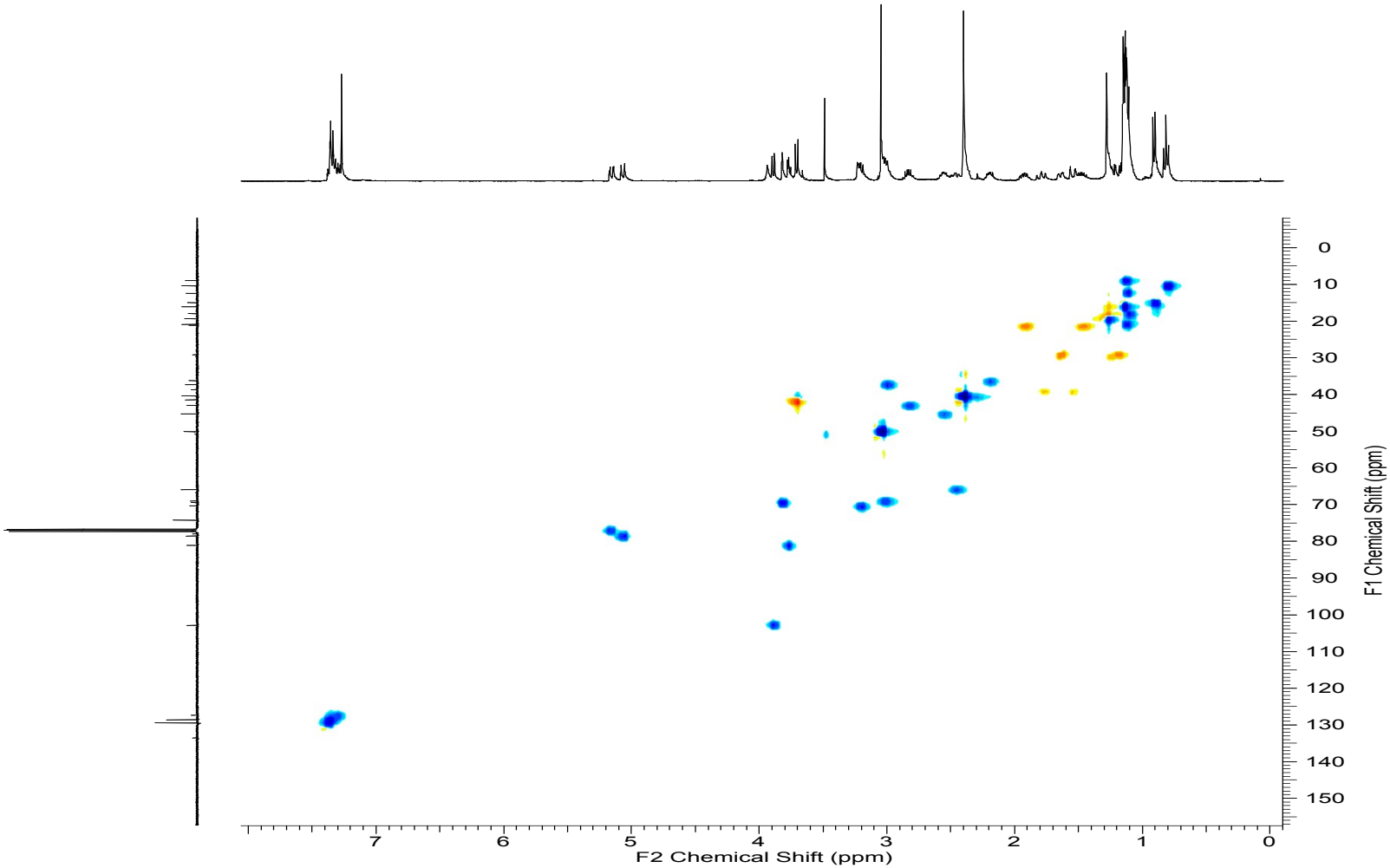


Figure S22. HSQC spectrum of 4.

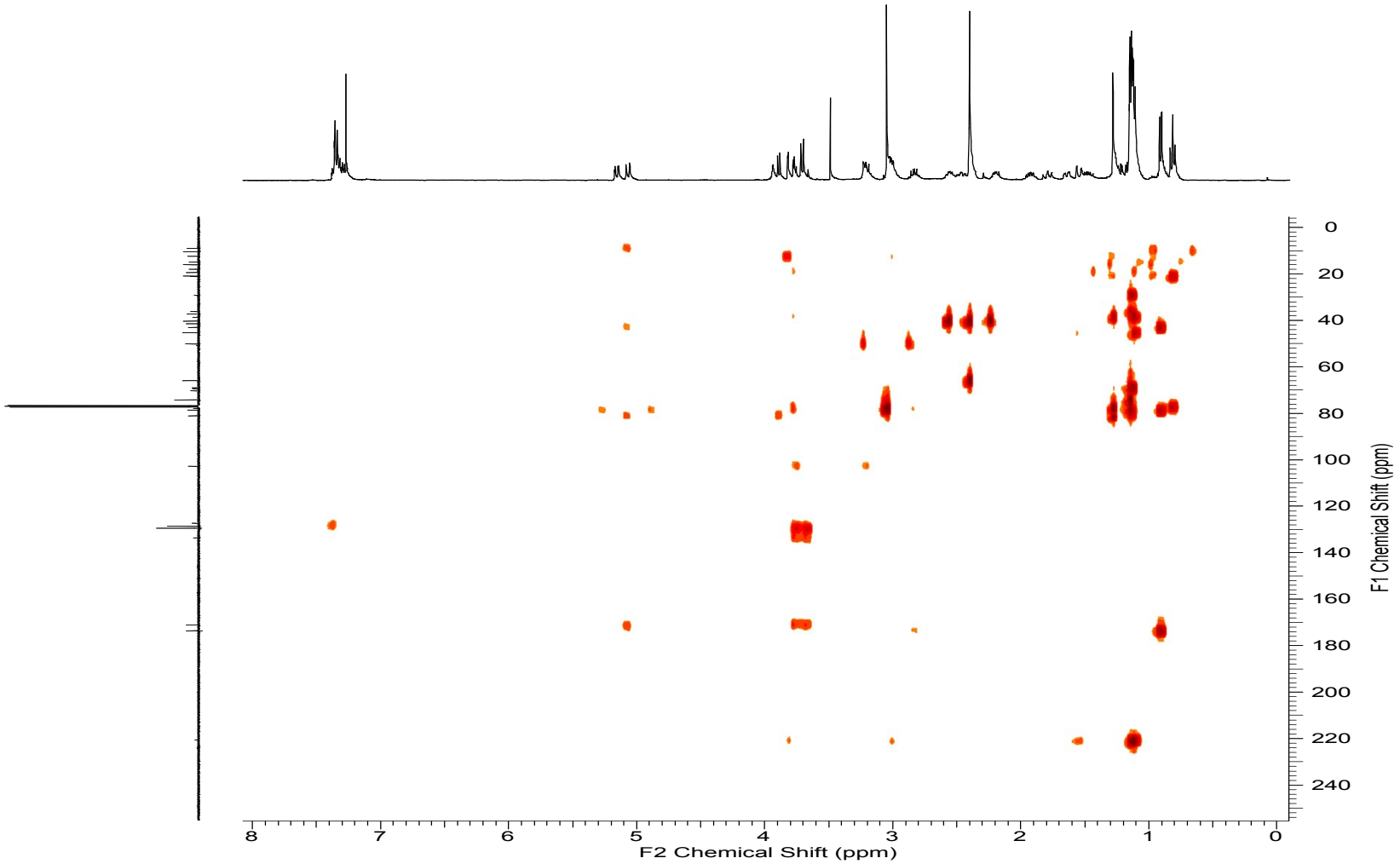


Figure S23. HMBC spectrum of 4.

.

5. Selected Cartesian coordinates

Clarithromycin, lowest energy conformer 1-c1

C	4.56561100	-2.37540200	-0.06572300
C	4.75166700	-0.85435500	0.17108400
C	5.56585700	-0.07308700	-0.90137800
C	5.26347300	1.44701700	-0.69433300
O	3.90502300	1.69798600	-1.16764700
C	1.66019300	2.45849600	-1.01114100
C	0.53386300	1.66240900	-0.26878300
C	0.44803200	0.21736200	-0.81896800
C	-0.28631600	-0.72792400	0.18591300
C	0.69388100	-1.65000000	0.99009200
C	1.31029600	-2.71433900	0.05567200
C	2.36852800	-3.64631300	0.69272900
C	3.66678500	-2.93031700	1.04656000
O	4.03784700	-2.84727700	2.20952600
C	2.98986200	2.19379900	-0.31436500
O	3.19747100	2.43087000	0.85482100
O	-0.75967100	2.26544400	-0.39068200
O	-1.23258000	-1.58629100	-0.47343600
C	5.88138000	-3.18147300	-0.07600800
C	2.64757900	-4.84652300	-0.23488300
C	5.26732200	-0.50868400	-2.33457200
O	5.42330100	-0.60589200	1.40860300
O	6.95633700	-0.28409800	-0.66713300
C	6.20449600	2.39064000	-1.43798300
C	1.46323500	3.98283200	-1.08986100
C	-0.04524700	-2.30845100	2.15985600
O	1.80497100	-0.84564800	1.42284700
C	-2.58550000	-1.31423900	-0.28845900
C	-3.38102100	-1.99389200	-1.40320300
C	-4.88771600	-1.87706600	-1.11072000
C	-5.20892400	-2.44488800	0.27799800
C	-4.34230300	-1.73046900	1.32067500
O	-2.95582700	-1.85431400	0.97766500
N	-5.64029600	-2.39277500	-2.26583600
C	-4.49886600	-2.29626000	2.72351600
O	-3.09902900	-1.38213500	-2.64859600
C	-5.69557700	-3.84887800	-2.37159800
C	-1.10607500	3.18664600	0.62998500
C	-2.26754600	4.04489500	0.13451700
C	-3.64662400	3.37415800	0.22052200
C	-3.82124800	2.80107500	1.64191000
C	-2.63165900	1.91194400	2.04808300
O	-1.37197900	2.58044700	1.87737300
O	-3.76225700	2.19747600	-0.60297600
O	-5.03137000	2.05792100	1.73362900
C	-3.65421400	2.34010800	-2.01080500
C	-6.96755700	-1.80346600	-2.40232700
C	-2.70310200	1.50684400	3.51207900
C	6.01944600	3.86074400	-1.05314700
C	-0.14830900	0.16113200	-2.23295400
C	-4.75700200	4.38046900	-0.10509500
C	1.72684100	-0.15112700	2.65958200
H	4.05757300	-2.49781600	-1.02550300
H	3.74883700	-0.42055900	0.21340000
H	5.28672900	1.65803500	0.37625100
H	1.74374700	2.08651300	-2.03339700
H	0.79768600	1.63244400	0.79083600
H	1.48698500	-0.11841800	-0.88886100
H	-0.82562400	-0.11302700	0.91110600
H	0.49561200	-3.33432200	-0.32652300

H	1.74954600	-2.22011300	-0.81798100
H	1.98952800	-4.03499100	1.64149000
H	6.56998300	-2.79216400	-0.82653300
H	5.68797800	-4.23682100	-0.28955200
H	6.37211200	-3.11824200	0.89776300
H	2.99892800	-4.52976100	-1.22182400
H	3.39503800	-5.52008100	0.19496700
H	1.72582100	-5.41736900	-0.38058600
H	4.21039100	-0.37748200	-2.57566100
H	5.85289900	0.08925500	-3.03736100
H	5.54033100	-1.55419700	-2.48689500
H	5.11225400	-1.28863200	2.03009200
H	7.02722200	-0.38602800	0.29633000
H	6.06252400	2.27168700	-2.51823000
H	7.22404700	2.06587300	-1.21468100
H	0.48185800	4.21505100	-1.50760600
H	1.55724000	4.45430700	-0.10858500
H	2.22173500	4.42266500	-1.74471500
H	-0.82752900	-2.96274000	1.77529400
H	0.63611500	-2.88900500	2.78599700
H	-0.53477400	-1.56286000	2.79087800
H	-2.77834500	-0.23069200	-0.30392000
H	-3.07281300	-3.05144600	-1.41007700
H	-5.10380700	-0.80011900	-1.08756400
H	-6.26797600	-2.30315500	0.52065000
H	-4.99866900	-3.51979000	0.32011400
H	-4.60932300	-0.66163500	1.33483800
H	-5.53659000	-2.20448900	3.05719400
H	-3.85971000	-1.75664100	3.42744300
H	-4.21922200	-3.35431700	2.74345500
H	-3.89712000	-1.56994700	-3.17416000
H	-6.09317800	-4.12024200	-3.35431600
H	-4.69462800	-4.27834000	-2.28611600
H	-6.33818900	-4.31657100	-1.60747800
H	-0.24693400	3.82521400	0.84863000
H	-2.30315100	4.94039500	0.76399200
H	-2.05914600	4.38605500	-0.88283500
H	-3.90258000	3.63494800	2.34889600
H	-2.65753900	1.01768700	1.41814000
H	-5.10564400	1.60360400	0.88131500
H	-3.69600400	1.32685600	-2.41719200
H	-2.69684500	2.78626700	-2.29856300
H	-4.47620300	2.93269800	-2.43040700
H	-6.89285000	-0.71234800	-2.39891300
H	-7.40428900	-2.11196200	-3.35739200
H	-7.66577100	-2.10567600	-1.60269800
H	-1.89300600	0.81617900	3.76223100
H	-3.65857100	1.01897300	3.71661400
H	-2.61296100	2.38831800	4.15567700
H	6.17393000	4.01377200	0.02016800
H	6.73428100	4.49260800	-1.58904600
H	5.01454500	4.21768100	-1.29969700
H	-1.19240400	0.47078500	-2.24938800
H	0.41087600	0.80547000	-2.91793700
H	-0.10874400	-0.85665200	-2.62321200
H	-4.62802700	4.80865000	-1.10300800
H	-5.73565200	3.89824400	-0.05124900
H	-4.74168700	5.20543900	0.61299200
H	0.83684900	0.48668600	2.72842600
H	1.74356000	-0.83731300	3.51342700
H	2.61167500	0.48660600	2.69315600

Erythromycin, lowest energy conformer 2-c1

C	4.57103400	-2.37120700	0.09601500
C	4.79577600	-0.84340900	0.25279800

C	5.54616700	-0.12403600	-0.90420600
C	5.28918800	1.40893900	-0.73695200
O	3.90730600	1.68046200	-1.11789300
C	1.70302000	2.51350500	-0.81935600
C	0.58732100	1.68674300	-0.09885600
C	0.52378200	0.24821300	-0.67374300
C	-0.24895900	-0.70157400	0.29961500
C	0.69667600	-1.59975800	1.15385300
C	1.30652300	-2.72172200	0.27806400
C	2.38859400	-3.60669500	0.94509700
C	3.66742700	-2.83280400	1.24008100
O	3.98625900	-2.58810700	2.39871800
C	3.05609600	2.18415200	-0.20012800
O	3.33747400	2.38508800	0.95885000
O	-0.71317200	2.27311400	-0.24431200
O	-1.15214600	-1.57227700	-0.39983000
C	5.87044400	-3.20359000	0.11357900
C	2.67175000	-4.84935100	0.07893600
C	5.14198500	-0.61087000	-2.29396200
O	5.55786900	-0.55644500	1.42572900
O	6.94597700	-0.35885300	-0.76063800
C	6.19166200	2.30002000	-1.58622200
C	1.53468000	4.04252300	-0.77728800
C	-0.05965400	-2.16217000	2.36015300
O	1.72498500	-0.70207700	1.60725200
C	-2.51504000	-1.31999400	-0.26964000
C	-3.25541300	-1.99471300	-1.42478300
C	-4.77447100	-1.89550900	-1.19471900
C	-5.14929300	-2.48221800	0.17258300
C	-4.33310900	-1.77382700	1.25903800
O	-2.93282700	-1.88306900	0.97181000
N	-5.47265000	-2.40485700	-2.38624500
C	-4.54349000	-2.35762800	2.64735000
O	-2.92792200	-1.36735300	-2.65108000
C	-5.50747700	-3.86004200	-2.51166900
C	-1.10898800	3.18244100	0.76871900
C	-2.25474300	4.03636100	0.22885200
C	-3.63086500	3.35396400	0.24749900
C	-3.86385000	2.76394800	1.65371700
C	-2.68428300	1.88381800	2.10522500
O	-1.42650800	2.56652800	1.99757800
O	-3.70095900	2.18543300	-0.59305000
O	-5.06920000	2.00749300	1.68222300
C	-3.53308100	2.34472100	-1.99302500
C	-6.79950800	-1.82785000	-2.57085700
C	-2.81538200	1.46400000	3.56100600
C	6.06672200	3.78744500	-1.24676700
C	-0.02846600	0.20279300	-2.10577300
C	-4.73431400	4.35492600	-0.11629900
H	4.04879000	-2.53815500	-0.84903600
H	3.80444100	-0.38804300	0.34577500
H	5.39779700	1.65790500	0.32021600
H	1.73967600	2.21702300	-1.86857100
H	0.83434600	1.63035400	0.96499000
H	1.56316300	-0.09113500	-0.71648400
H	-0.82162800	-0.08720000	0.99809700
H	0.49294000	-3.37555300	-0.04703000
H	1.72118600	-2.27910500	-0.63483600
H	2.02907900	-3.94773700	1.92038300
H	6.54698300	-2.86994800	-0.67425800
H	5.65632900	-4.26596200	-0.03275500
H	6.38347600	-3.08741500	1.07087600
H	1.75549400	-5.43818900	-0.02133800
H	3.43414400	-5.48977600	0.53227700
H	3.00334200	-4.58073300	-0.92867800
H	5.39483300	-1.66499000	-2.42236600
H	4.07200400	-0.47630700	-2.46594500
H	5.68276500	-0.04871800	-3.05923900

H	5.20467600	-1.13532600	2.12354300
H	7.09104800	-0.40940700	0.19789300
H	5.96484500	2.14402900	-2.64715200
H	7.21838200	1.95988700	-1.42808500
H	0.55758700	4.32778200	-1.17141800
H	1.64433800	4.43227000	0.23766100
H	2.29861900	4.51792600	-1.40060300
H	-0.43237200	-1.33779100	2.97536000
H	0.59276300	-2.77936900	2.98606300
H	-0.91375900	-2.75981700	2.04046500
H	-2.72067900	-0.23880000	-0.27761100
H	-2.93676400	-3.04921000	-1.42923900
H	-5.00194200	-0.82090500	-1.16874200
H	-6.21877400	-2.35141800	0.37175000
H	-4.93233600	-3.55591600	0.21124800
H	-4.60874400	-0.70723800	1.27465100
H	-3.93872000	-1.82168500	3.38368200
H	-4.25665100	-3.41383000	2.66646600
H	-5.59500600	-2.27782000	2.93821000
H	-3.70211000	-1.55630800	-3.21093200
H	-5.86139300	-4.12323800	-3.51313700
H	-6.17572600	-4.34411200	-1.78044100
H	-4.50619200	-4.27997800	-2.39026200
H	-0.26575600	3.82549200	1.03011900
H	-2.32596200	4.92564700	0.86414700
H	-2.00509600	4.38868400	-0.77537500
H	-3.98666300	3.58962100	2.36438300
H	-2.67226400	0.99450700	1.46761100
H	-5.09874600	1.56164900	0.82276200
H	-3.54878400	1.33584300	-2.41202300
H	-4.34106800	2.93545200	-2.44159300
H	-2.56802200	2.80184700	-2.23395400
H	-7.19288300	-2.12920900	-3.54681300
H	-7.52687800	-2.14714300	-1.80454100
H	-6.73694700	-0.73614700	-2.55147300
H	-2.00183900	0.78929700	3.84111600
H	-3.76851700	0.95441300	3.71790000
H	-2.77345100	2.34126000	4.21532600
H	6.74713400	4.38284000	-1.86318800
H	5.05160800	4.15573900	-1.42554100
H	6.31122300	3.97794200	-0.19635500
H	0.56481100	0.83354100	-2.77409700
H	-1.06513300	0.53359400	-2.15468900
H	0.00174800	-0.81615300	-2.49301500
H	-5.71041400	3.86456100	-0.10979300
H	-4.75693000	5.17265500	0.60987500
H	-4.56566700	4.79430400	-1.10338800
H	2.12493900	-1.06904200	2.40442300

Erythromycin, 2nd lowest energy conformer 2-c2

C	-4.57589600	-2.37616200	-0.02401600
C	-4.80736100	-0.86101300	-0.25893000
C	-5.58183600	-0.08986700	0.85006600
C	-5.30221000	1.43323700	0.62968100
O	-3.93978700	1.70442500	1.07848800
C	-1.70556700	2.48122800	0.88873100
C	-0.56696100	1.68033700	0.17510100
C	-0.48819200	0.24053600	0.74336200
C	0.25379000	-0.70835900	-0.25067400
C	-0.72608300	-1.60122700	-1.08212700
C	-1.32805700	-2.70904000	-0.19380800
C	-2.38943700	-3.62100100	-0.85346400
C	-3.70166300	-2.91015100	-1.16500000
O	-4.10033400	-2.81505500	-2.31725000

C	-3.03252200	2.17635800	0.20244200
O	-3.24562900	2.36827100	-0.97329000
O	0.72397900	2.28335200	0.32214000
O	1.17886800	-1.58103400	0.41809800
C	-5.87341000	-3.20963600	0.03118700
C	-2.65014000	-4.85555500	0.03440900
C	-5.21697700	-0.52208000	2.26914100
O	-5.55128000	-0.63779500	-1.45868500
O	-6.97879800	-0.31836300	0.67848400
C	-6.24024800	2.36905300	1.38670100
C	-1.53484800	4.01040000	0.92043600
C	-0.00868900	-2.17121800	-2.30789400
O	-1.82726400	-0.78148900	-1.50268700
C	2.53692400	-1.32411800	0.25159200
C	3.31056100	-2.01099900	1.37702700
C	4.82218800	-1.90771900	1.10532000
C	5.15766700	-2.47621900	-0.27993800
C	4.31078200	-1.75412500	-1.33357600
O	2.91894200	-1.86900600	-1.00915900
N	5.55393800	-2.43211400	2.26982800
C	4.48292200	-2.31856700	-2.73508300
O	3.01651500	-1.39654900	2.61832600
C	5.59403400	-3.88880700	2.37437000
C	1.09931400	3.20808200	-0.68512500
C	2.25888100	4.05052000	-0.15808300
C	3.63335800	3.36729000	-0.22185700
C	3.83083100	2.79845200	-1.64223300
C	2.63980300	1.92540000	-2.07671400
O	1.38581500	2.60912900	-1.93028700
O	3.72252800	2.18591100	0.59829800
O	5.03415900	2.04201100	-1.71226000
C	3.59685600	2.32420300	2.00500700
C	6.88467800	-1.85554700	2.42555200
C	2.73552900	1.52423900	-3.54043200
C	-6.07011100	3.84071000	1.00119900
C	0.09840700	0.19620600	2.16133100
C	4.74650300	4.36200200	0.12922400
H	-4.03416000	-2.48606900	0.91872400
H	-3.81924000	-0.40350900	-0.35935800
H	-5.34745200	1.63903300	-0.44142400
H	-1.78282700	2.14010500	1.92234400
H	-0.80903600	1.63313500	-0.89045600
H	-1.52707900	-0.09646900	0.80952400
H	0.81066100	-0.09389200	-0.96389000
H	-0.50478900	-3.33993800	0.14960500
H	-1.75461600	-2.25574200	0.70834800
H	-2.01980400	-3.97347800	-1.82000600
H	-6.54528700	-2.82951000	0.80158800
H	-5.65274900	-4.25970900	0.24362700
H	-6.39598400	-3.16008300	-0.92664400
H	-2.99902900	-4.57511700	1.03321200
H	-3.39365300	-5.52128800	-0.41392900
H	-1.72181700	-5.42147800	0.15550200
H	-4.15032500	-0.39194300	2.46259700
H	-5.76947000	0.07769400	2.99683900
H	-5.48441200	-1.56710100	2.43476200
H	-5.22898000	-1.29340100	-2.10287300
H	-7.09080600	-0.43036900	-0.27995800
H	-6.08373300	2.24954100	2.46497000
H	-7.26029700	2.03740900	1.17672100
H	-0.56308700	4.27379800	1.34234700
H	-1.62613900	4.44855000	-0.07650400
H	-2.30817600	4.45749700	1.55270000
H	0.84508000	-2.78137300	-2.01115600
H	-0.68986700	-2.76331500	-2.92324000
H	0.37747000	-1.35304400	-2.92738000
H	2.74138600	-0.24263800	0.26821000
H	2.99282400	-3.06572100	1.37942400

H	5.04854300	-0.83276000	1.08704700
H	6.22099500	-2.34235600	-0.50790300
H	4.93976200	-3.54941000	-0.32640600
H	4.58482300	-0.68696200	-1.34203600
H	5.52567300	-2.23284300	-3.05435300
H	3.85685200	-1.77372000	-3.44669300
H	4.19707500	-3.37487500	-2.76063900
H	3.80476200	-1.59252700	3.15557400
H	5.97534200	-4.16506300	3.36216900
H	4.59040800	-4.30880100	2.27442400
H	6.24283300	-4.36165800	1.61869700
H	0.25186100	3.85721400	-0.91690800
H	2.31575400	4.95117700	-0.77860500
H	2.03323600	4.38455000	0.85799000
H	3.93599300	3.63448000	-2.34352300
H	2.64105100	1.02847700	-1.44972800
H	5.08552200	1.58398800	-0.86021000
H	3.62091500	1.30886000	2.40763000
H	2.64132900	2.78133600	2.28168800
H	4.42016200	2.90498100	2.43829800
H	6.82031300	-0.76376900	2.42279400
H	7.30519300	-2.16948300	3.38610400
H	7.59103500	-2.16324400	1.63521900
H	1.91480400	0.85400900	-3.81078000
H	3.68361800	1.01508400	-3.72620400
H	2.67985800	2.40979300	-4.18239300
H	-6.23911800	3.99358500	-0.07003200
H	-6.78250800	4.46741600	1.54633100
H	-5.06458200	4.20395000	1.23565900
H	1.14180700	0.50751600	2.18284200
H	-0.46651100	0.84518900	2.83727300
H	0.05725900	-0.81887200	2.55832300
H	4.60169000	4.78864200	1.12562300
H	5.72144900	3.87063500	0.09342000
H	4.75335900	5.18908200	-0.58657100
H	-1.59134800	-0.32192900	-2.31641300

Erythromycin, 3rd lowest energy conformer 2-c3

C	-4.46974100	-2.36115000	0.15400600
C	-4.77107800	-0.87524200	-0.16872600
C	-5.49641300	-0.04593300	0.92894700
C	-5.27767200	1.46283700	0.57781400
O	-3.89765200	1.81305700	0.90371400
C	-1.71193400	2.63577600	0.47978200
C	-0.54564400	1.77648600	-0.09876400
C	-0.39461700	0.43708000	0.67092500
C	0.31822600	-0.62819400	-0.21748000
C	-0.68611700	-1.54394100	-1.01122600
C	-1.22757400	-2.65468900	-0.08904400
C	-2.28924800	-3.59982600	-0.69756900
C	-3.62591300	-2.93050000	-0.99244800
O	-4.06642800	-2.89852900	-2.13344800
C	-3.04554700	2.15605400	-0.08138000
O	-3.31331000	2.13738900	-1.26167000
O	0.69567400	2.48999200	-0.03712600
O	1.18035400	-1.42244700	0.60962600
C	-5.73050200	-3.23364700	0.32674900
C	-2.50143500	-4.81533200	0.22952000
C	-5.02823000	-0.35993500	2.34841500
O	-5.59959300	-0.76495700	-1.32860700
O	-6.89438500	-0.32221900	0.86840300
C	-6.18656900	2.42867200	1.33248700
C	-1.59955000	4.13647400	0.15880700
C	-0.01628600	-2.10656900	-2.26880100

O	-1.82000500	-0.75070900	-1.39704200
C	2.40220400	-1.85596000	0.11275300
C	3.47889600	-1.66742800	1.18295900
C	4.80604100	-2.27438400	0.69966400
C	4.60137400	-3.74861900	0.32236400
C	3.46953700	-3.85136200	-0.70692400
O	2.27446800	-3.24095500	-0.19689800
N	5.86876100	-1.93972400	1.66004400
C	3.11240000	-5.28450200	-1.06811100
O	3.65238900	-0.28811000	1.44387800
C	7.19925600	-1.90386700	1.06311700
C	1.15547400	3.06052000	-1.24712000
C	2.00402500	4.29533700	-0.94327300
C	3.42676900	3.99591600	-0.44611700
C	4.07202400	2.96247200	-1.39389200
C	3.15785800	1.74347800	-1.60952300
O	1.84740700	2.13636100	-2.05977000
O	3.45855500	3.31638600	0.82005000
O	5.33165800	2.53980100	-0.88969500
C	2.86294200	3.94440100	1.93992800
C	5.86208300	-2.72279000	2.89314600
C	3.71351500	0.81491700	-2.67777400
C	-6.09383000	3.86956600	0.82450100
C	0.29615900	0.64078300	2.02901100
C	4.26552800	5.27919400	-0.39408200
H	-3.88065500	-2.39047900	1.07401000
H	-3.80889200	-0.39808200	-0.36657200
H	-5.40627100	1.58442500	-0.49948200
H	-1.74310000	2.51834200	1.56513200
H	-0.77985000	1.56895700	-1.14626000
H	-1.41397900	0.08875500	0.86423900
H	0.93877000	-0.09449400	-0.94685300
H	-0.37915700	-3.26304900	0.22957900
H	-1.62878700	-2.19527100	0.82228700
H	-1.93694100	-3.97163300	-1.66374700
H	-6.37735400	-2.82496700	1.10431100
H	-5.46252800	-4.25932100	0.59579500
H	-6.30084900	-3.26453400	-0.60425400
H	-1.55807000	-5.35720700	0.34333700
H	-3.24105800	-5.50867800	-0.18192100
H	-2.83227200	-4.51377800	1.22836600
H	-5.24603300	-1.39814200	2.60528800
H	-3.95699500	-0.18156200	2.46230500
H	-5.55604000	0.27382200	3.06561400
H	-5.27347000	-1.43611300	-1.95456800
H	-7.06437500	-0.51101900	-0.06913200
H	-5.94498900	2.39793600	2.40117500
H	-7.20796000	2.05392100	1.22806900
H	-2.42999600	4.68518700	0.61372000
H	-0.66848200	4.53918600	0.55858300
H	-1.63262900	4.31402500	-0.91946600
H	0.37854900	-1.28776300	-2.88208500
H	-0.73358800	-2.66343100	-2.87712800
H	0.81089300	-2.76844700	-2.00483100
H	2.67815000	-1.29394800	-0.79382800
H	3.12031100	-2.19245800	2.08219200
H	5.06932300	-1.72849800	-0.21685300
H	5.51890000	-4.17293200	-0.09994300
H	4.33356000	-4.34429100	1.20246000
H	3.77464700	-3.31172100	-1.61953100
H	2.77669100	-5.82965500	-0.18046200
H	3.98314200	-5.80023100	-1.48321000
H	2.31070800	-5.30721300	-1.81133000
H	4.57026900	-0.22761900	1.76150600
H	7.91115300	-1.50072300	1.79022700
H	7.56679400	-2.89682700	0.75114200
H	7.19742900	-1.24708900	0.18864700
H	0.29606000	3.35064800	-1.86098600

H	2.09738900	4.85666400	-1.87924400
H	1.47432800	4.94582300	-0.24266900
H	4.26254200	3.44366000	-2.36035300
H	3.07477500	1.21722800	-0.65173500
H	5.17559400	2.37831100	0.05267900
H	3.27942500	4.94067200	2.13303200
H	1.77578300	4.01530100	1.83027200
H	3.08218000	3.30503700	2.79828100
H	6.17749200	-3.76911000	2.74653300
H	6.54953800	-2.26419500	3.61044200
H	4.86540000	-2.72559200	3.34073300
H	3.08222900	-0.07051600	-2.79532800
H	4.72221200	0.49834800	-2.40359500
H	3.75825900	1.32872900	-3.64412100
H	-6.77972800	4.51949800	1.37637500
H	-5.08414200	4.27355500	0.94860300
H	-6.35210000	3.93414900	-0.23798200
H	0.23423200	-0.27018800	2.62709600
H	-0.19253200	1.44319500	2.59058000
H	1.35040200	0.89171700	1.91041300
H	3.81744700	6.02763900	0.26545600
H	5.27303300	5.05148100	-0.03920000
H	4.34303500	5.72332600	-1.39094500
H	-1.67067100	-0.36771300	-2.26831100

Erythromycin, 4th lowest energy conformer 2-c4

C	-4.46992700	-2.36447300	0.03773200
C	-4.74129900	-0.85045400	-0.16746600
C	-5.44127300	-0.09489500	0.99540100
C	-5.24124400	1.43359800	0.73502300
O	-3.84465900	1.77217500	0.98985300
C	-1.70489700	2.65620800	0.45162500
C	-0.56663600	1.77042800	-0.14463800
C	-0.42849000	0.42812200	0.62279500
C	0.31262300	-0.62923900	-0.25492600
C	-0.65048700	-1.53642600	-1.09645000
C	-1.21756500	-2.67090200	-0.21029500
C	-2.29497000	-3.57760200	-0.85413200
C	-3.59758100	-2.83790600	-1.12585100
O	-3.95928600	-2.62905300	-2.27896200
C	-3.06565500	2.17474700	-0.03645300
O	-3.41626200	2.20033100	-1.19380200
O	0.68771000	2.46590300	-0.09374500
O	1.13712500	-1.43790500	0.59466900
C	-5.74629200	-3.22877700	0.10417000
C	-2.53611700	-4.82194100	0.02321700
C	-4.93918600	-0.49888600	2.37911100
O	-5.57464600	-0.63415000	-1.30672400
O	-6.84051100	-0.37226900	0.95128400
C	-6.09980500	2.34324700	1.60949400
C	-1.59113900	4.14352600	0.07593600
C	0.07744900	-2.07820600	-2.33192600
O	-1.70630200	-0.65950300	-1.52679300
C	2.37836000	-1.86632800	0.14209200
C	3.41540100	-1.67904300	1.25106300
C	4.76010100	-2.28359700	0.81531100
C	4.57159800	-3.75686300	0.42632900
C	3.47862100	-3.85747100	-0.64419700
O	2.26473900	-3.25053600	-0.17624000
N	5.78620300	-1.95069800	1.81532400
C	3.13719400	-5.28978800	-1.02340400
O	3.57837200	-0.29996800	1.51982000
C	7.13799900	-1.91325500	1.26852400
C	1.15830900	3.01012500	-1.31157500

C	1.98600000	4.26621500	-1.03441200
C	3.41175500	4.00769000	-0.52332400
C	4.07936100	2.95806800	-1.43622700
C	3.18698400	1.71737400	-1.61471000
O	1.87552000	2.07437900	-2.08925400
O	3.45325000	3.36812900	0.76362800
O	5.34575300	2.57585400	-0.91650300
C	2.82649600	4.01072300	1.85826600
C	5.73393000	-2.73643800	3.04562300
C	3.76729900	0.76135300	-2.64510200
C	-6.04846800	3.81300100	1.18500900
C	0.23650100	0.62165800	1.99562600
C	4.22643100	5.30750400	-0.50670900
H	-3.90534100	-2.48469400	0.96535900
H	-3.76820700	-0.37928100	-0.33381900
H	-5.44097400	1.62267800	-0.32120600
H	-1.69270800	2.57345200	1.54033800
H	-0.81737900	1.55820800	-1.18684500
H	-1.45017300	0.07477100	0.79497400
H	0.95844100	-0.08697700	-0.95377600
H	-0.38415600	-3.30852500	0.09266600
H	-1.61752700	-2.23406600	0.71236100
H	-1.94694900	-3.91659900	-1.83452100
H	-6.39666200	-2.88260800	0.90876600
H	-5.49951200	-4.27969500	0.27859200
H	-6.30246800	-3.15902100	-0.83336800
H	-1.60504800	-5.38868700	0.11310700
H	-3.29083900	-5.48195100	-0.41474900
H	-2.85867200	-4.55403300	1.03400200
H	-5.14745300	-1.55286800	2.57274100
H	-3.86589200	-0.32253800	2.47815300
H	-5.45207400	0.08325600	3.14856900
H	-5.22847700	-1.21767400	-2.00402700
H	-7.04322600	-0.47049200	0.00717600
H	-5.78257000	2.25094000	2.65448500
H	-7.12478600	1.96741000	1.55412400
H	-2.40769400	4.71393900	0.52962000
H	-0.64931700	4.55431900	0.44004400
H	-1.64926100	4.28242600	-1.00682000
H	0.47543300	-1.24642800	-2.92090500
H	-0.60445100	-2.64512300	-2.97465600
H	0.89636800	-2.73958300	-2.04232900
H	2.68596400	-1.30049000	-0.75146600
H	3.02521700	-2.20596600	2.13594100
H	5.05633700	-1.73459100	-0.08918000
H	5.50464500	-4.17860000	0.03673300
H	4.27239800	-4.35564600	1.29413300
H	3.81613900	-3.31417800	-1.54307800
H	2.77011400	-5.83877400	-0.15065000
H	4.02337500	-5.80269900	-1.40821400
H	2.36337800	-5.31085300	-1.79564700
H	4.48393300	-0.23907200	1.87091200
H	7.82200900	-1.51035500	2.02206600
H	7.51774400	-2.90559800	0.96946600
H	7.16835100	-1.25564300	0.39522600
H	0.30370800	3.27037300	-1.94487400
H	2.07503700	4.80421400	-1.98441900
H	1.44246300	4.92666500	-0.35424500
H	4.26270600	3.41127400	-2.41748600
H	3.10266100	1.22410200	-0.63921600
H	5.19302500	2.44958100	0.03173300
H	3.19371800	5.03293000	2.01132600
H	1.73749000	4.02364400	1.74520200
H	3.07552500	3.41808400	2.74173000
H	6.05449600	-3.78249500	2.90845700
H	6.39446600	-2.27952500	3.78881600
H	4.72141400	-2.74006900	3.45613200
H	3.14915300	-0.13568500	-2.74092400

H	4.77693800	0.46793400	-2.34938900
H	3.81632200	1.24373700	-3.62731200
H	-6.69397700	4.42336600	1.82391100
H	-5.03324800	4.21516300	1.26037100
H	-6.38350800	3.94034100	0.14999600
H	0.16012600	-0.29222300	2.58746900
H	-0.25802500	1.42252000	2.55353200
H	1.29435600	0.86626400	1.89770800
H	3.76256300	6.06624900	0.12976700
H	5.23691500	5.10926200	-0.14276700
H	4.29874500	5.72404200	-1.51581100
H	-2.10924300	-1.02660300	-2.32240700

(6S)-1-c1

C	5.05190100	-0.25142400	0.37764900
C	3.94528600	-0.85533400	-0.51130500
C	4.31519100	-2.17273800	-1.26642400
C	3.04556800	-2.71583100	-2.00543900
O	1.97442900	-2.94339500	-1.04253900
C	0.14137700	-2.31279200	0.31056200
C	-1.03027800	-1.28443300	0.47027700
C	-0.84150200	-0.45148500	1.76925100
C	0.31586800	0.59242500	1.56982700
C	1.36592600	0.60856600	2.72427100
C	2.43213800	1.71220500	2.52925000
C	3.36110800	1.61651100	1.30527700
C	4.50836500	0.62891200	1.52224400
O	5.07768800	0.57457400	2.59859900
C	1.02762500	-2.00975500	-0.88378800
O	0.95670600	-0.99868200	-1.56398100
O	-2.29524200	-1.95380900	0.49960800
O	-0.19339900	1.92746700	1.43239800
C	6.15078000	0.50272800	-0.40065000
C	3.99643000	3.00423900	1.04674000
C	4.93296600	-3.23172400	-0.35836500
O	3.55735400	0.11391500	-1.49153700
O	5.26380100	-1.87002100	-2.28992900
C	3.25289700	-4.02056200	-2.76702300
C	-0.27995800	-3.79011700	0.38876800
C	0.69121200	0.83699000	4.08439100
O	1.96604100	-0.70148000	2.61149100
C	-0.43567200	2.37268700	0.13564300
C	-1.33736300	3.60525000	0.19450300
C	-1.51218700	4.17388500	-1.22558100
C	-0.14535100	4.44917700	-1.86748100
C	0.70772300	3.17574200	-1.81094600
O	0.81164700	2.72215400	-0.45318500
N	-2.49624800	5.26700100	-1.18549800
C	2.12041900	3.38195300	-2.33406500
O	-2.60513300	3.26739900	0.72364300
C	-1.99855000	6.53371500	-0.65494000
C	-2.92313600	-2.05853000	-0.76359100
C	-3.99609300	-3.14472900	-0.70804700
C	-5.31098700	-2.72212000	-0.03185800
C	-5.74226200	-1.34618100	-0.58925500
C	-4.58693400	-0.33468200	-0.50738600
O	-3.43637900	-0.82749100	-1.21941100
O	-5.16825400	-2.45348400	1.37567500
O	-6.88142100	-0.86259100	0.10839200
C	-4.68185200	-3.48649800	2.21276700
C	-3.19756900	5.46255500	-2.44939900
C	-4.93679100	1.01284600	-1.11518900
C	2.09977200	-4.34365200	-3.72072000
C	-2.14378200	0.18934300	2.26374600
C	-6.40439300	-3.77088500	-0.27111200
C	2.66148400	-1.21287800	3.74048600
H	5.53652500	-1.06736800	0.91770200

H	3.10353600	-1.07438500	0.15375500
H	2.70946400	-1.94565400	-2.70182000
H	0.82880900	-2.14435900	1.15042800
H	-1.02920100	-0.60826200	-0.38731900
H	-0.50905900	-1.15567800	2.53954800
H	0.86911500	0.34718000	0.65995300
H	1.89620800	2.66305000	2.48373100
H	3.06234500	1.74611200	3.42386300
H	2.80419800	1.35006400	0.40923800
H	6.86768500	0.94230700	0.29828400
H	6.68272100	-0.18821700	-1.05730200
H	5.72854300	1.29899800	-1.01681000
H	3.20557900	3.72317200	0.81944300
H	4.68987700	2.98654400	0.20174700
H	4.54508400	3.34653700	1.93021400
H	5.87507000	-2.87930900	0.06409800
H	5.15029000	-4.14134200	-0.92168400
H	4.25247000	-3.48755200	0.45868100
H	2.62670400	-0.06273500	-1.71215800
H	4.96473100	-1.02848800	-2.66794800
H	3.38262200	-4.84199700	-2.05479100
H	4.18988300	-3.92293800	-3.32313200
H	0.60381100	-4.42967200	0.40401800
H	-0.85374500	-3.96360800	1.30065600
H	-0.90174800	-4.08804300	-0.45943700
H	0.11812900	1.76644200	4.04392700
H	0.01013500	0.02517500	4.34898900
H	1.43127400	0.93646700	4.88239300
H	-0.92023800	1.59175700	-0.47262300
H	-0.82734700	4.33446600	0.84338800
H	-1.99585900	3.37687000	-1.80653000
H	-0.26414900	4.76688900	-2.90933900
H	0.38400800	5.24752300	-1.33493000
H	0.21219800	2.38767300	-2.40243500
H	2.70967000	2.46783500	-2.23000000
H	2.62282800	4.18063200	-1.77941600
H	2.09148200	3.66362100	-3.39104900
H	-3.19716600	3.94002300	0.34266200
H	-1.49023300	6.37713600	0.29942400
H	-2.84566400	7.20316600	-0.47682800
H	-1.30110000	7.04771100	-1.33696800
H	-2.17445900	-2.32388200	-1.52104400
H	-4.23442400	-3.41066300	-1.74334100
H	-3.58587300	-4.04397900	-0.24038600
H	-6.03932500	-1.46567100	-1.63773900
H	-4.32847900	-0.20897600	0.54832000
H	-6.69253000	-1.03255800	1.04293000
H	-5.27266700	-4.40683500	2.13037200
H	-4.76583600	-3.11404500	3.23663200
H	-3.62880500	-3.70717100	2.00781800
H	-4.01476500	6.17591600	-2.30314700
H	-3.62860500	4.51571500	-2.78653600
H	-2.55105200	5.85532400	-3.25323800
H	-4.14763100	1.73974300	-0.90526100
H	-5.87190200	1.37563500	-0.68253600
H	-5.06326700	0.92370500	-2.19968000
H	1.15331300	-4.43959800	-3.17954300
H	1.97738500	-3.56039600	-4.47665400
H	2.28211800	-5.28733400	-4.24312600
H	-2.89389600	-0.58534400	2.42869600
H	-1.97735700	0.71821100	3.20520700
H	-2.54133300	0.91870900	1.55677000
H	-7.32950400	-3.46454900	0.22168400
H	-6.60246800	-3.87407300	-1.34214300
H	-6.11039500	-4.75472100	0.10524000
H	3.09730600	-2.16274300	3.42123100
H	3.47165200	-0.54924700	4.05852700
H	1.98807300	-1.40465500	4.58347300

(8S)-1-c1

C	3.85588100	-2.71352600	-0.09357500
C	4.33761400	-1.24517500	0.07322200
C	5.16340400	-0.62835300	-1.09006700
C	5.16376900	0.92020400	-0.87833100
O	3.81611500	1.41296800	-1.14519800
C	1.81486600	2.60324000	-0.66803300
C	0.61218600	1.91193900	0.04570100
C	0.38002700	0.46836600	-0.48229500
C	-0.45217300	-0.38263300	0.52183300
C	0.31212400	-0.88383500	1.82490400
C	0.50901600	-2.41883500	1.86471500
C	1.40029900	-3.02371000	0.76827400
C	2.88684000	-2.92699500	1.07106600
O	3.32808300	-3.01415100	2.20924100
C	3.13984000	2.04553600	-0.16399400
O	3.55367400	2.20190300	0.96227200
O	-0.57580200	2.69467500	-0.16131500
O	-1.00195500	-1.51937100	-0.16771000
C	4.98459200	-3.75589800	-0.09214700
C	1.08846200	-4.52596900	0.56626300
C	4.63922600	-1.00700300	-2.47253200
O	5.16280500	-1.11527400	1.23369500
O	6.50961000	-1.08890900	-1.00033200
C	6.13143200	1.68346000	-1.77845200
C	1.85264200	4.12487700	-0.44835600
C	-0.52454100	-0.47299800	3.04614100
O	1.59740600	-0.23444900	1.80635400
C	-2.38034200	-1.65659400	-0.20112600
C	-2.73578700	-2.68091900	-1.27997400
C	-4.25010100	-2.95125700	-1.25227100
C	-4.68158000	-3.39485600	0.15284400
C	-4.23240300	-2.34385100	1.17485600
O	-2.81716300	-2.12645300	1.07278500
N	-4.60583300	-3.80929200	-2.39314100
C	-4.51742900	-2.74503700	2.61332200
O	-2.35990200	-2.20095900	-2.55402500
C	-4.26441900	-5.22146700	-2.24092400
C	-1.07626900	3.40369300	0.95272900
C	-1.73428100	4.70778400	0.49702800
C	-3.13392100	4.55419200	-0.11831600
C	-3.98531300	3.65913000	0.80647600
C	-3.24533200	2.35492600	1.15107300
O	-1.96131400	2.62815900	1.73806000
O	-3.13879600	3.81170300	-1.35176500
O	-5.24009700	3.37143500	0.20598200
C	-2.38498300	4.30941200	-2.44235000
C	-5.98627900	-3.64413600	-2.83435200
C	-4.01716500	1.51173800	2.15209600
C	6.27911000	3.15874500	-1.39750400
C	-0.27971800	0.48988900	-1.87137900
C	-3.79663900	5.92432100	-0.30746700
C	2.29762400	-0.09252100	3.03421300
H	3.29107100	-2.77514400	-1.02712700
H	3.44037800	-0.63149000	0.20185800
H	5.38785700	1.11895700	0.17119000
H	1.75579000	2.40508900	-1.74033400
H	0.83529300	1.87681400	1.11364900
H	1.36783900	0.01101900	-0.58467200
H	-1.28407500	0.24318000	0.85499000
H	-0.47746700	-2.88173400	1.81715500
H	0.93820400	-2.68099800	2.83767400
H	1.21387300	-2.52384000	-0.18462600
H	5.50536400	-3.76173000	0.86753600
H	5.71461300	-3.53532600	-0.87264200
H	4.58011500	-4.75829300	-0.26207100

H	1.22240700	-5.07657800	1.50279500
H	0.05191700	-4.64406200	0.23921300
H	1.73563400	-4.98011400	-0.19128000
H	3.60291800	-0.68803000	-2.60393400
H	5.24428500	-0.52851200	-3.24633000
H	4.70303600	-2.08579700	-2.62622700
H	4.79191500	-1.70291500	1.91318000
H	6.67524300	-1.18714700	-0.04902600
H	5.80093100	1.60395000	-2.82024500
H	7.09760900	1.17603500	-1.71146600
H	0.95539300	4.58919500	-0.85705500
H	2.71960400	4.56252300	-0.95298400
H	1.92972200	4.36502000	0.61554200
H	-0.07514700	-0.80964900	3.98393000
H	-0.66421500	0.61104900	3.08198500
H	-1.50969900	-0.93748400	2.95788000
H	-2.86936200	-0.69146800	-0.42066800
H	-2.18169400	-3.59950300	-1.02748600
H	-4.73075200	-1.98579200	-1.46147700
H	-5.76940600	-3.51373900	0.20552000
H	-4.22884200	-4.35806100	0.41464900
H	-4.74748200	-1.39444100	0.95316200
H	-4.19921400	-1.96016200	3.30481700
H	-3.98310800	-3.66617000	2.86609100
H	-5.58870100	-2.91546900	2.75454100
H	-2.96996300	-2.65952800	-3.15813200
H	-4.38090100	-5.72234000	-3.20684200
H	-3.22290100	-5.33340700	-1.93041400
H	-4.90094200	-5.74741100	-1.51025000
H	-0.25273100	3.63234400	1.63757000
H	-1.06729200	5.24416700	-0.18222000
H	-1.84042100	5.33643300	1.38775000
H	-4.19263300	4.20447800	1.73447100
H	-3.10205000	1.79804700	0.21649400
H	-5.03318400	3.18508700	-0.72189400
H	-2.66202000	5.33606200	-2.70981200
H	-2.61021100	3.65855100	-3.29053000
H	-1.30924200	4.25939500	-2.24333600
H	-6.13332100	-4.18660300	-3.77356700
H	-6.72672100	-4.02446600	-2.10952200
H	-6.19517700	-2.58612800	-3.01596900
H	-5.03037300	1.34166800	1.78140400
H	-4.07915400	2.02766500	3.11616300
H	-3.52778900	0.54730100	2.30734500
H	7.00180200	3.65595300	-2.05163600
H	5.32854700	3.69367400	-1.48976800
H	6.62710500	3.27082900	-0.36521800
H	-1.27427700	0.94048500	-1.82669700
H	-0.38585300	-0.51745800	-2.27049800
H	0.31647200	1.07919100	-2.57454900
H	-4.78683500	5.80268700	-0.75190000
H	-3.19789800	6.57794500	-0.94776300
H	-3.91179200	6.42547500	0.65813100
H	3.27089700	0.32144400	2.76862300
H	1.79183300	0.60283400	3.71387000
H	2.44301800	-1.05403000	3.53879300

(8S)-1-c2

C	-4.17606500	-2.51696100	-0.37709000
C	-4.29330400	-0.98729100	-0.13847700
C	-5.00411000	-0.54817300	1.17889500
C	-4.93487700	1.00867200	1.30660600
O	-3.55429600	1.49006900	1.31854900
C	-1.71763600	2.72879900	0.45961300
C	-0.53170700	1.96501400	-0.20276500
C	-0.36972100	0.52472500	0.35580100
C	0.45787600	-0.37853800	-0.60373200

C	-0.26763900	-0.84703700	-1.94177400
C	-0.60492600	-2.35502000	-1.95246500
C	-1.64385700	-2.83545600	-0.92633900
C	-3.08541800	-2.74296300	-1.43338900
O	-3.36306800	-2.92191200	-2.60244700
C	-3.04466000	2.03517300	0.20334300
O	-3.60159000	2.01984100	-0.87944800
O	0.66547200	2.72237300	0.03649000
O	0.89471800	-1.54286700	0.11919500
C	-5.48785900	-3.20028000	-0.77663300
C	-1.40736900	-4.32376600	-0.57584300
C	-4.45573400	-1.24602700	2.41894800
O	-5.00403800	-0.42233100	-1.23893500
O	-6.39537200	-0.85853000	1.08035200
C	-5.60033600	1.57223100	2.55979200
C	-1.84118600	4.17500800	-0.04794200
C	0.68159400	-0.55141900	-3.11336300
O	-1.48521800	-0.08153200	-2.02800000
C	2.25755900	-1.76189400	0.24155200
C	2.48104700	-2.80197400	1.34085700
C	3.97447600	-3.16562600	1.40927600
C	4.46624500	-3.64016200	0.03452800
C	4.14914900	-2.56642800	-1.01281600
O	2.74637900	-2.26233400	-1.00128600
N	4.20279800	-4.04000400	2.57030100
C	4.50011300	-2.98831400	-2.43068900
O	2.05676800	-2.29507500	2.58917800
C	3.78546700	-5.42906500	2.39577000
C	1.26212900	3.35506500	-1.07690300
C	1.93427100	4.65857900	-0.64025900
C	3.28256400	4.48892200	0.07746400
C	4.16115500	3.51959600	-0.74149700
C	3.39869700	2.22549000	-1.07508700
O	2.16790100	2.51313200	-1.76165400
O	3.17444900	3.81030000	1.34220100
O	5.36010300	3.21973500	-0.04154300
C	2.36443100	4.38699200	2.35056600
C	5.55966600	-3.95864600	3.09926700
C	4.20361600	1.30841700	-1.98045600
C	-5.81361000	3.08669000	2.49553300
C	0.23095900	0.54509700	1.77104700
C	3.98124700	5.84364700	0.24659500
C	-2.10707100	0.03679900	-3.29959200
H	-3.79781700	-2.95502200	0.55185300
H	-3.27624300	-0.58697800	-0.11976500
H	-5.41833500	1.42910400	0.42270500
H	-1.55641200	2.74258300	1.53970800
H	-0.72044200	1.91349100	-1.27588900
H	-1.37348900	0.09982500	0.42921400
H	1.34310800	0.19148300	-0.89758300
H	0.32695600	-2.90320100	-1.81021600
H	-0.97676600	-2.61453900	-2.94924100
H	-1.55935900	-2.26615800	0.00294000
H	-5.87227500	-2.77018900	-1.70245100
H	-6.23837500	-3.08391900	0.00628000
H	-5.31962600	-4.26764100	-0.94764400
H	-1.43346700	-4.93879500	-1.48118100
H	-0.42681200	-4.43987600	-0.10628000
H	-2.16179400	-4.71009900	0.11745000
H	-3.38787200	-1.04262900	2.54054100
H	-4.97413600	-0.90074700	3.31576100
H	-4.60425000	-2.32519100	2.35328600
H	-4.67142800	0.48612100	-1.33904600
H	-6.62962400	-0.65680900	0.16064300
H	-4.99336000	1.32314200	3.43648200
H	-6.55962300	1.05920400	2.67250100
H	-0.93198300	4.73198800	0.17912700
H	-2.67819400	4.68544900	0.43811000

H	-2.01574700	4.19630700	-1.12703600
H	0.27249500	-0.88976900	-4.06880700
H	0.90736700	0.51707000	-3.17568300
H	1.61843200	-1.08596600	-2.93936200
H	2.78872100	-0.82702600	0.49222100
H	1.88831100	-3.68555600	1.05413500
H	4.49987500	-2.23103000	1.64897400
H	5.54568900	-3.82663100	0.05135600
H	3.97185800	-4.57395000	-0.25660700
H	4.70659700	-1.64995400	-0.75726800
H	4.27528300	-2.18733700	-3.14016400
H	3.92731400	-3.87553300	-2.71804500
H	5.56572800	-3.22454000	-2.50352700
H	2.59762700	-2.78884000	3.23033300
H	3.80776300	-5.93249100	3.36710700
H	2.76150400	-5.47795800	2.01795800
H	4.43452600	-5.99594800	1.70804800
H	0.49243200	3.57424400	-1.82472200
H	1.24373000	5.24905300	-0.03255800
H	2.12165700	5.23895600	-1.55006900
H	4.45201500	4.01022200	-1.67761100
H	3.17202300	1.71961500	-0.12818300
H	5.08365600	3.08451700	0.87702600
H	2.66323300	5.41406800	2.59193100
H	2.50119600	3.76909800	3.24119600
H	1.30483200	4.36797200	2.07443900
H	5.61249400	-4.50611800	4.04559900
H	6.32027900	-4.38616100	2.42322500
H	5.82135500	-2.91491300	3.29469100
H	5.18199700	1.12092100	-1.53273600
H	4.35069200	1.77456300	-2.96054000
H	3.68902300	0.35542500	-2.12508100
H	-6.29308100	3.44921500	3.40960800
H	-4.86264500	3.61761200	2.38639500
H	-6.45300000	3.36294400	1.65002500
H	1.23115300	0.98567600	1.76766500
H	0.30661100	-0.46188200	2.17795700
H	-0.39089000	1.14289800	2.44411400
H	4.93330400	5.71128800	0.76507300
H	3.36445700	6.54841600	0.81105600
H	4.18103700	6.29136100	-0.73136800
H	-3.02824000	0.59411500	-3.12656400
H	-1.48662000	0.59761500	-4.00807700
H	-2.36271000	-0.93832000	-3.72680800

(12R)-1-c1

C	4.65748800	-2.24847900	0.68759700
C	4.70715000	-0.68194700	0.60493600
C	5.79909200	-0.14860600	-0.37473500
C	5.52492600	1.35821300	-0.66872500
O	4.17084700	1.49056200	-1.21048400
C	1.85868800	1.99046100	-1.15521400
C	0.70106300	1.29638700	-0.34892000
C	0.41290900	-0.11351200	-0.91626300
C	-0.40852600	-0.97833300	0.09651500
C	0.46740100	-2.02692300	0.85215500
C	1.01266400	-3.10824000	-0.12267500
C	2.40200400	-3.66649600	0.25686200
C	3.48596500	-2.69335200	-0.19799700
O	3.43475700	-2.26673200	-1.34688200
C	3.17342500	1.86174800	-0.40035400
O	3.30213600	2.09109100	0.78999200
O	-0.52069900	2.04404900	-0.36078300
O	-1.47093000	-1.69885000	-0.55149900
C	4.67252800	-2.80402600	2.11214700
C	2.65913000	-5.02043500	-0.43842200
C	7.19584300	-0.31311500	0.23481700

O	4.87387700	-0.10387100	1.89324000
O	5.78004000	-0.88085800	-1.59198200
C	6.45919100	1.97083400	-1.70819700
C	1.64016900	3.47869000	-1.49301100
C	-0.33021000	-2.71395900	1.96527000
O	1.62407000	-1.33577400	1.37034000
C	-2.76855600	-1.25277200	-0.31559600
C	-3.68661900	-1.78284900	-1.41712500
C	-5.15293000	-1.47318100	-1.06493400
C	-5.50270200	-2.03116600	0.32058800
C	-4.51315200	-1.46943400	1.34690200
O	-3.16939400	-1.77127800	0.95115700
N	-6.00734700	-1.84922300	-2.20296900
C	-4.69986400	-2.04734700	2.74123500
O	-3.36805000	-1.17171200	-2.65420300
C	-6.26243600	-3.28100700	-2.34174200
C	-0.67188200	2.97897300	0.69117500
C	-1.70796200	4.01990300	0.27453600
C	-3.16776300	3.55456400	0.39110600
C	-3.37804800	2.95683300	1.79767500
C	-2.31447200	1.89450900	2.13169300
O	-0.97831100	2.38460600	1.93657900
O	-3.48289700	2.44026400	-0.46602300
O	-4.67735200	2.38674900	1.90618700
C	-3.41592300	2.62178000	-1.87163000
C	-7.24657200	-1.08360500	-2.27517800
C	-2.39856700	1.45036000	3.58362900
C	6.17680600	3.44759800	-1.99506300
C	-0.23223600	-0.05813300	-2.30905100
C	-4.12805100	4.72420500	0.14361900
C	1.50023500	-0.63624900	2.60329500
H	5.53875700	-2.63400200	0.15886100
H	3.73631100	-0.38002900	0.21805200
H	5.56404900	1.92779800	0.26249500
H	1.99406800	1.46840800	-2.10353600
H	1.03148400	1.20606500	0.68685900
H	1.39589300	-0.58092700	-1.03159600
H	-0.85079700	-0.31586600	0.84506900
H	0.29479900	-3.93158100	-0.15069600
H	1.07870300	-2.72374400	-1.14248800
H	2.46516600	-3.81053900	1.33586500
H	4.70064300	-3.89805200	2.09686300
H	3.79927100	-2.48485800	2.68278100
H	5.56072900	-2.45312200	2.64156400
H	3.65253600	-5.41436200	-0.19957000
H	2.58925900	-4.91372700	-1.52482100
H	1.91768600	-5.75579800	-0.11296900
H	7.34875600	0.36330900	1.07797200
H	7.32974400	-1.33773000	0.59338700
H	7.96198800	-0.12817100	-0.52107900
H	4.43760000	0.76154000	1.84595200
H	4.88319600	-1.25020400	-1.71401100
H	7.48437700	1.86526200	-1.33995800
H	6.39010200	1.37660000	-2.62409300
H	2.41572500	3.82070100	-2.18420100
H	1.68060400	4.11416900	-0.60500900
H	0.66908100	3.61000500	-1.97259900
H	-1.17966900	-3.23740100	1.52827900
H	-0.73226000	-2.00071400	2.68801500
H	0.29987400	-3.43399700	2.49783200
H	-2.81105800	-0.15288100	-0.29812000
H	-3.52497700	-2.87127600	-1.46652400
H	-5.21959700	-0.37793900	-1.00783100
H	-6.52431700	-1.75482100	0.60439500
H	-5.43867500	-3.12533600	0.33047100
H	-4.63136700	-0.37479600	1.39562000
H	-3.97136200	-1.61830100	3.43446500
H	-4.56549900	-3.13356000	2.72683600

H	-5.70438200	-1.82608300	3.11364000
H	-4.20035100	-1.23678000	-3.15538000
H	-6.93601700	-3.68017700	-1.56544100
H	-5.32637200	-3.84310600	-2.30439300
H	-6.72640700	-3.46793400	-3.31502100
H	0.28841100	3.46638900	0.88420700
H	-1.58906200	4.88305700	0.93809400
H	-1.48574600	4.36986900	-0.73672800
H	-3.31979800	3.76605000	2.53496800
H	-2.48660600	1.03693300	1.47406300
H	-4.83962400	1.98124800	1.04129000
H	-4.17233500	3.32888700	-2.23336800
H	-3.60338100	1.63833400	-2.30895800
H	-2.42269000	2.95487700	-2.18962400
H	-7.95202100	-1.31270000	-1.45768600
H	-7.75295100	-1.30262100	-3.22054500
H	-7.02512100	-0.01293800	-2.24783900
H	-3.40974000	1.10372700	3.80759400
H	-2.15652900	2.28411700	4.25117700
H	-1.69493800	0.63715100	3.78176700
H	5.17479900	3.58835000	-2.40950800
H	6.25311400	4.05315200	-1.08489200
H	6.89602200	3.84237200	-2.71899700
H	-1.23595200	0.36418300	-2.27905000
H	0.37329600	0.54309200	-2.99422100
H	-0.31683000	-1.06001800	-2.73213900
H	-5.16465200	4.38911700	0.22400700
H	-3.96388300	5.51149100	0.88516400
H	-3.97435700	5.16452400	-0.84546400
H	2.46339600	-0.14993200	2.75961800
H	1.31121800	-1.31565900	3.44183900
H	0.71408100	0.12813300	2.57944300

(12R)-1-c2

C	4.55826800	-2.32311200	-0.10557400
C	4.87772500	-0.85540400	0.29330700
C	5.67316900	-0.01883800	-0.76126600
C	5.29632900	1.47832000	-0.56262700
O	3.93123100	1.62183900	-1.07632800
C	1.67751100	2.39370900	-1.03939100
C	0.52961800	1.62340900	-0.29834100
C	0.41986600	0.18484500	-0.85551000
C	-0.30311400	-0.76174900	0.15429400
C	0.69093300	-1.69245500	0.92743500
C	1.30800100	-2.72500300	-0.03909200
C	2.37591300	-3.66794900	0.56002400
C	3.65828900	-2.94526700	0.96802500
O	4.00885600	-2.93257700	2.14048300
C	2.98370900	2.17337900	-0.28707100
O	3.16061600	2.48655600	0.86754000
O	-0.75022100	2.25160800	-0.41948200
O	-1.26715800	-1.60891400	-0.49218900
C	5.79175400	-3.23497800	-0.27524600
C	2.67365400	-4.81447400	-0.42733700
C	7.18666000	-0.20711300	-0.62654300
O	5.59079600	-0.77804400	1.52115000
O	5.32510400	-0.41755300	-2.08985200
C	6.17218000	2.47822300	-1.31715000
C	1.46870300	3.91029600	-1.19988600
C	-0.02802800	-2.38747000	2.08831300
O	1.79691900	-0.88363300	1.36936900
C	-2.61329600	-1.32139600	-0.28158900
C	-3.43710500	-1.99568400	-1.37848800
C	-4.93637400	-1.86106500	-1.05787200
C	-5.23703200	-2.41873200	0.33960100
C	-4.34264100	-1.70952200	1.36229100
O	-2.96438900	-1.85132500	0.99384500
N	-5.71659700	-2.37387000	-2.19576600

C	-4.47920000	-2.26693000	2.77053700
O	-3.17146700	-1.38992800	-2.63055700
C	-5.78952200	-3.82980200	-2.29317100
C	-1.07431800	3.18411800	0.59898600
C	-2.23453900	4.04841500	0.11144200
C	-3.61840000	3.39035500	0.22093400
C	-3.77830900	2.82631000	1.64781500
C	-2.59089400	1.92884600	2.04148800
O	-1.32913200	2.58897100	1.85329300
O	-3.75608300	2.21022700	-0.59418800
O	-4.99375200	2.09505900	1.76065600
C	-3.67310700	2.34470400	-2.00442600
C	-7.03996300	-1.77104400	-2.30909500
C	-2.64684200	1.52749000	3.50713700
C	5.71641500	3.93373200	-1.18305100
C	-0.19792700	0.14534200	-2.26043600
C	-4.72408500	4.40500300	-0.09450400
C	1.70970300	-0.21086200	2.61758200
H	4.01699100	-2.28951600	-1.05365700
H	3.89806200	-0.37742600	0.41342000
H	5.27664600	1.70383400	0.50505200
H	1.79641000	1.97343900	-2.03939000
H	0.78940000	1.58481600	0.76172100
H	1.45547400	-0.15718400	-0.94191600
H	-0.82396300	-0.15050900	0.89614200
H	0.49367900	-3.33814600	-0.43357200
H	1.73997600	-2.20435000	-0.90038400
H	1.99494200	-4.11075500	1.48420600
H	5.50037500	-4.28544900	-0.36007800
H	6.45878900	-3.13765500	0.58424500
H	6.33478700	-2.96971600	-1.18386300
H	3.40564700	-5.51683700	-0.01802100
H	3.05198200	-4.44310300	-1.38480300
H	1.75291300	-5.37007400	-0.62892100
H	7.55069900	0.22933700	0.30459300
H	7.45060300	-1.26313700	-0.62233200
H	7.69260800	0.26516800	-1.47061900
H	5.16375600	-1.42590300	2.10866400
H	4.43837000	-0.07388600	-2.26102000
H	7.19006400	2.38923800	-0.92687600
H	6.21060400	2.18686100	-2.37293000
H	2.22789800	4.32455500	-1.86991300
H	1.54720000	4.43315500	-0.24390900
H	0.48811400	4.10737400	-1.63680100
H	-0.79573400	-3.05428900	1.69571300
H	-0.53345200	-1.66502700	2.73319400
H	0.67075300	-2.96254100	2.70008900
H	-2.79447300	-0.23569600	-0.29820800
H	-3.14052300	-3.05648600	-1.38820200
H	-5.13985100	-0.78164100	-1.03607800
H	-6.28957900	-2.26392000	0.60175000
H	-5.03810400	-3.49573600	0.38284600
H	-4.59708700	-0.63753800	1.37614000
H	-3.82146400	-1.73083800	3.45992300
H	-4.21038300	-3.32776600	2.79047700
H	-5.50952600	-2.16248600	3.12289000
H	-3.98037100	-1.57160300	-3.14144500
H	-6.42222800	-4.28679600	-1.51445500
H	-4.79178200	-4.26964000	-2.22476900
H	-6.20888300	-4.10159200	-3.26668000
H	-0.20584100	3.81598900	0.80111200
H	-2.25407800	4.94927800	0.73388700
H	-2.03636000	4.37943800	-0.91130800
H	-3.84167800	3.66448200	2.35154500
H	-2.63053900	1.03373900	1.41339500
H	-5.08421400	1.63621500	0.91235400
H	-4.49899700	2.94011000	-2.41216700
H	-3.72873800	1.32957100	-2.40445300

H	-2.71864400	2.78368600	-2.31254500
H	-7.72557400	-2.06221300	-1.49459700
H	-7.49854200	-2.07909300	-3.25401200
H	-6.95367700	-0.68077300	-2.31216300
H	-3.60391900	1.04862100	3.72492500
H	-2.54073700	2.40952800	4.14750000
H	-1.83990200	0.83005800	3.74865000
H	4.73822600	4.09401600	-1.64483000
H	5.64679900	4.23539300	-0.13289600
H	6.42733300	4.60148900	-1.67862100
H	-1.24182800	0.45567400	-2.25656800
H	0.35019200	0.79892900	-2.94612200
H	-0.16483800	-0.86777400	-2.66346800
H	-5.70613200	3.93171000	-0.02546500
H	-4.69189900	5.23286200	0.61966700
H	-4.60468000	4.82771800	-1.09593300
H	2.58309900	0.44226400	2.66259200
H	1.73941800	-0.91002500	3.46032300
H	0.80981000	0.41150300	2.69811900

(12R)-1-c3

C	4.67509200	-2.33953600	0.58693600
C	4.74073900	-0.76961500	0.73354800
C	5.77934400	-0.09703600	-0.22533800
C	5.37393800	1.39392300	-0.41257500
O	4.09131300	1.36934000	-1.10552700
C	1.79966600	1.84898900	-1.43896900
C	0.69668700	1.16297600	-0.54271300
C	0.35054600	-0.23847700	-1.08417900
C	-0.42896000	-1.07791200	-0.02150100
C	0.47385100	-2.13559000	0.68766100
C	1.02510500	-3.17825600	-0.32562400
C	2.43221300	-3.70788400	0.01401900
C	3.49016900	-2.66188000	-0.33145100
O	3.42025100	-2.09146500	-1.41433700
C	3.05580100	2.07351800	-0.61225700
O	3.11190600	2.78460700	0.36780200
O	-0.50742400	1.92908500	-0.44947100
O	-1.54814100	-1.77161500	-0.59924200
C	4.69633500	-3.08770700	1.92208700
C	2.74915800	-4.98333900	-0.79612800
C	7.19866200	-0.20954700	0.34354200
O	4.92352500	-0.33047400	2.07231100
O	5.80499500	-0.75116400	-1.48465300
C	6.35538500	2.20744400	-1.25496400
C	1.37058100	3.16928400	-2.09924600
C	-0.29020500	-2.86478400	1.79689100
O	1.62958200	-1.43872700	1.20668400
C	-2.81125900	-1.27844900	-0.28125600
C	-3.81880400	-1.76711400	-1.32165500
C	-5.24457200	-1.39504700	-0.87517000
C	-5.52809500	-1.93905500	0.53106900
C	-4.45001500	-1.42150400	1.48933300
O	-3.15073900	-1.78566100	1.00766400
N	-6.18705700	-1.73026900	-1.95487500
C	-4.57221600	-1.98749000	2.89557200
O	-3.55422600	-1.16626500	-2.57638500
C	-6.51160900	-3.14939200	-2.07737700
C	-0.52220200	2.90897900	0.57208200
C	-1.54617000	3.98068300	0.20795000
C	-3.00972700	3.57006600	0.43454600
C	-3.14298200	2.99787800	1.86152500
C	-2.08820400	1.91165800	2.14293800
O	-0.75666200	2.36696100	1.85803500
O	-3.42385800	2.45680700	-0.38201300
O	-4.44794800	2.46646000	2.06322200
C	-3.44297600	2.61709000	-1.79119400
C	-7.39454400	-0.91235100	-1.94438500

C	-2.09521900	1.48600200	3.60291500
C	5.90512700	3.64452000	-1.53072300
C	-0.35149400	-0.18406800	-2.44810900
C	-3.94465300	4.76924400	0.23633900
C	1.51335200	-0.75078900	2.44840900
H	5.55027100	-2.64973000	0.00154900
H	3.75481700	-0.39120000	0.47404600
H	5.21678900	1.85690400	0.56414000
H	2.06998800	1.15379500	-2.23508400
H	1.10078500	1.05115100	0.46556800
H	1.32131300	-0.71823400	-1.23642000
H	-0.80911000	-0.40413100	0.75062200
H	0.32948200	-4.02071800	-0.35973100
H	1.06096500	-2.76687900	-1.33619500
H	2.48869700	-3.94889600	1.07616400
H	4.66687600	-4.16891900	1.75828300
H	3.85770900	-2.80789100	2.56243100
H	5.61905200	-2.87784900	2.47044800
H	3.75289200	-5.36247100	-0.57755800
H	2.69050200	-4.78076600	-1.86963200
H	2.03111900	-5.77162100	-0.55232300
H	7.35827200	0.45526900	1.19688700
H	7.40476500	-1.23951000	0.65374200
H	7.92653300	0.04405200	-0.42939200
H	5.78572300	-0.62442700	2.38776700
H	4.89710900	-1.05522600	-1.68184000
H	7.31306800	2.22994300	-0.72453600
H	6.52589500	1.67351100	-2.19586100
H	2.13699500	3.49887400	-2.80775500
H	1.23018500	3.96495300	-1.36485300
H	0.43523000	3.03328700	-2.64492800
H	-1.13497800	-3.39753100	1.36192600
H	-0.69695800	-2.17663700	2.54066000
H	0.36457200	-3.58204200	2.30279600
H	-2.81061500	-0.17767100	-0.25874700
H	-3.70772900	-2.86129300	-1.38185900
H	-5.25897100	-0.29806400	-0.81409000
H	-6.51627100	-1.61854300	0.87953300
H	-5.51107000	-3.03498300	0.53922700
H	-4.51506200	-0.32227200	1.53965700
H	-3.78497000	-1.58682700	3.53991100
H	-4.48358900	-3.07834000	2.87829700
H	-5.54142500	-1.72402200	3.32908900
H	-4.41894100	-1.19293100	-3.02318800
H	-7.14934200	-3.52220000	-1.25881900
H	-5.59990500	-3.75083500	-2.10156900
H	-7.04576000	-3.31337400	-3.01827300
H	0.47489000	3.35071200	0.66473700
H	-1.35024200	4.84993300	0.84481300
H	-1.38343600	4.30477500	-0.82308300
H	-3.01394300	3.81523600	2.58068400
H	-2.32236500	1.05158300	1.50707700
H	-4.67791800	2.05729700	1.21555300
H	-4.20044000	3.34174600	-2.11444400
H	-3.68625500	1.63409500	-2.20127700
H	-2.46358200	2.91616300	-2.17807900
H	-8.05379300	-1.11468200	-1.08248900
H	-7.97090400	-1.10555500	-2.85467500
H	-7.12626200	0.14781000	-1.93014000
H	-3.10022700	1.17112400	3.89228900
H	-1.78955100	2.31969800	4.24396000
H	-1.40396300	0.65517200	3.76870600
H	4.99055900	3.66929800	-2.13001200
H	5.71161800	4.18952200	-0.60139200
H	6.67762800	4.18558400	-2.08562700
H	-1.34253400	0.26452900	-2.38572600
H	0.24496600	0.39173000	-3.16287100
H	-0.47959300	-1.18892000	-2.85385900

H	-4.98357600	4.47236000	0.39743500
H	-3.69964300	5.56149800	0.94974000
H	-3.84846600	5.18855200	-0.76902700
H	2.48163700	-0.27548300	2.61530600
H	1.31444300	-1.43741400	3.27856100
H	0.73776400	0.02410000	2.42987400

(13S)-1-c1

C	5.64475500	-0.04064000	0.30179900
C	5.17246900	0.39886100	-1.09939800
O	3.90294700	1.10469000	-0.96725700
C	1.73636100	1.77642000	-1.70704700
C	0.64282600	1.34964300	-0.67063000
C	-0.15210100	0.10776400	-1.15805100
C	-0.71684800	-0.75121700	0.01185000
C	0.33173900	-1.64069000	0.77895400
C	1.03360600	-2.59936700	-0.20416300
C	1.97274900	-3.65823500	0.41960900
C	3.15199700	-3.02028800	1.14972400
O	3.22723600	-3.09415000	2.36978400
C	2.86882600	0.74900700	-1.74576600
O	2.84157600	-0.26364200	-2.41582500
O	-0.25313800	2.45223000	-0.45979600
O	-1.68799600	-1.68787000	-0.49728200
C	5.45217500	-3.38767000	0.33268700
C	2.41894000	-4.65580200	-0.66656100
C	7.06719700	-0.62695900	0.23593500
O	5.12714400	-1.15820600	2.32374000
O	5.67777100	1.13998900	1.11375200
C	6.13814400	1.35337800	-1.80982600
C	2.25424100	3.19976400	-1.46935500
C	-0.37120400	-2.41604900	1.90175800
O	1.39529800	-0.81509700	1.29535300
C	-3.03522300	-1.43843100	-0.27216300
C	-3.84448700	-2.33028700	-1.21679600
C	-5.34351100	-2.15918600	-0.91706300
C	-5.62071300	-2.46283700	0.56181300
C	-4.71505500	-1.58950300	1.43950900
O	-3.33966400	-1.77573300	1.07791700
N	-6.12466400	-2.88070000	-1.93382200
C	-4.83305000	-1.91485300	2.92035200
O	-3.58520400	-1.99444100	-2.56420200
C	-6.16456100	-4.33222900	-1.77453600
C	-0.21506300	3.07409500	0.80432000
C	-0.62596400	4.54122400	0.67395300
C	-2.13568300	4.78290800	0.51545800
C	-2.88550000	3.96471800	1.58882200
C	-2.42862000	2.49566800	1.58549600
O	-1.00539400	2.40071600	1.76657100
O	-2.67628200	4.24967800	-0.70751400
O	-4.28936100	4.04558500	1.38782100
C	-2.15031100	4.71471200	-1.93725300
C	-7.46160500	-2.33333500	-2.13389800
C	-3.06778600	1.69396200	2.70621300
C	5.71591300	1.71685100	-3.23561000
C	-1.24196100	0.52441700	-2.16147200
C	-2.46194800	6.27596600	0.64525100
C	1.22080400	-0.18111400	2.55749300
H	3.94205400	-2.18989600	-0.67077800
H	3.68724200	-0.43523500	1.02854400
H	5.00090800	-0.48525000	-1.71682600
H	1.28789300	1.72374100	-2.70417300
H	1.14626400	1.12226000	0.26779000
H	0.55474900	-0.51228100	-1.71314100
H	-1.19817000	-0.09445200	0.74402500
H	0.26048200	-3.12821200	-0.76858800
H	1.60593600	-2.01267600	-0.92756300

H	1.43215300	-4.21767400	1.18750100
H	5.09142600	-4.39061500	0.09236900
H	5.93217000	-3.42689800	1.31267500
H	6.20098100	-3.12596700	-0.41508200
H	2.97435100	-4.16784700	-1.47313400
H	1.53501400	-5.12192200	-1.11212000
H	3.04183100	-5.45309400	-0.25098500
H	7.21162100	-1.30176400	-0.61176600
H	7.78606400	0.18987300	0.15025500
H	7.27910100	-1.17281000	1.15683400
H	4.51909500	-1.78942800	2.74929600
H	5.69054200	0.81431500	2.02520200
H	6.24664600	2.25443100	-1.19791900
H	7.12121600	0.87616200	-1.84750500
H	2.68560500	3.31170800	-0.47169700
H	1.43808400	3.91371600	-1.58305000
H	3.03067800	3.45594200	-2.19513800
H	-0.99263400	-1.75931200	2.51349200
H	0.36315300	-2.90343600	2.54633700
H	-1.03071900	-3.17153100	1.47578300
H	-3.28119500	-0.37778100	-0.44604800
H	-3.52822100	-3.36420200	-1.00469300
H	-5.56520400	-1.09697300	-1.08945500
H	-5.41934100	-3.51637200	0.78709100
H	-6.66951600	-2.26500400	0.80945800
H	-4.98051800	-0.53149000	1.27593500
H	-4.18578700	-1.26442100	3.51420200
H	-4.54332600	-2.95371400	3.10641900
H	-5.86441400	-1.77683100	3.25799300
H	-4.40501300	-2.24722700	-3.02413400
H	-6.58850900	-4.77848200	-2.67929800
H	-6.77745300	-4.66017800	-0.91868100
H	-5.15584000	-4.73178600	-1.64607200
H	0.80003400	3.01327300	1.21212400
H	-0.31270200	5.04221400	1.59612900
H	-0.06736500	5.01067700	-0.13986900
H	-2.67820100	4.39820500	2.57408200
H	-2.69658200	2.06532100	0.61280700
H	-4.40773200	3.95823100	0.43032400
H	-2.19656000	5.80657900	-2.02704900
H	-2.77400200	4.27721500	-2.72045100
H	-1.11940900	4.37674300	-2.08543500
H	-7.92148900	-2.81047500	-3.00506100
H	-8.13376400	-2.49148100	-1.27275700
H	-7.39881300	-1.25884500	-2.32787700
H	-4.15312800	1.80910900	2.66430900
H	-2.71492100	2.05136100	3.67941300
H	-2.82100200	0.63339400	2.61269500
H	5.60801500	0.82372700	-3.86017500
H	4.76462900	2.25564200	-3.25648700
H	6.46695900	2.36223000	-3.70088300
H	-1.75162300	-0.34868000	-2.56707600
H	-1.98279500	1.18262200	-1.70144200
H	-0.79711800	1.07649800	-2.99570400
H	-2.16752500	6.64352800	1.63269000
H	-1.92842300	6.87224000	-0.10011500
H	-3.53553000	6.43597600	0.52472800
H	2.12005500	0.42066200	2.71348700
H	0.34818700	0.48103600	2.57405000
H	1.14887000	-0.90849800	3.37223200

(13S)-1-c2

C	4.25295100	-2.48108900	0.27345800
C	4.61588000	-1.11117700	0.90792200
C	5.61205200	-0.15379800	0.18792300
C	5.09065600	0.25885000	-1.20259600
O	3.84117400	0.99144700	-1.04170200
C	1.70651700	1.73922300	-1.80676900

C	0.63885600	1.33063200	-0.73902800
C	-0.17883600	0.09278600	-1.20020900
C	-0.73397700	-0.75101700	-0.01426800
C	0.31464800	-1.65005000	0.74181000
C	0.98577100	-2.62675000	-0.24564600
C	1.90382900	-3.70958600	0.36991000
C	3.10754300	-3.10338000	1.08673700
O	3.19274600	-3.17156200	2.30617100
C	2.82492100	0.70165500	-1.87237000
O	2.80551600	-0.26705600	-2.60443400
O	-0.24007700	2.44368400	-0.51295100
O	-1.72700500	-1.67707700	-0.49997600
C	5.39897600	-3.51862700	0.25321400
C	2.31350200	-4.71985800	-0.71893000
C	7.03256800	-0.73269000	0.07207500
O	5.15270200	-1.28241700	2.22165300
O	5.66106800	1.01868800	1.01044100
C	6.02119000	1.11880800	-2.07117700
C	2.25767500	3.15406400	-1.59199200
C	-0.38035700	-2.40674000	1.88217700
O	1.39747100	-0.83589300	1.23454100
C	-3.06656900	-1.40909500	-0.25031800
C	-3.90505400	-2.29227300	-1.17745900
C	-5.39570800	-2.10263900	-0.84888600
C	-5.64782200	-2.40057000	0.63561800
C	-4.71556000	-1.53578000	1.49357300
O	-3.34962000	-1.73897500	1.10612100
N	-6.20526500	-2.81595000	-1.84904900
C	-4.80852100	-1.85591500	2.97732200
O	-3.66841100	-1.96116300	-2.53020700
C	-7.53976700	-2.25354600	-2.02213000
C	-0.16895100	3.06921800	0.74791900
C	-0.55732200	4.54266600	0.62001400
C	-2.06539100	4.80980000	0.48822000
C	-2.80980400	4.00670700	1.57674900
C	-2.37766600	2.53021600	1.56901100
O	-0.95333400	2.41237000	1.72628200
O	-2.63704400	4.28354200	-0.72358700
O	-4.21540800	4.11080400	1.40035700
C	-2.12512200	4.73628900	-1.96377600
C	-6.25841300	-4.26685600	-1.68769500
C	-3.01088500	1.74114300	2.70199900
C	6.38589500	2.50397100	-1.52897300
C	-1.28246100	0.51361800	-2.18692100
C	-2.36367600	6.30846800	0.62068800
C	1.24911800	-0.18550500	2.49183100
H	3.89805500	-2.30845800	-0.74627600
H	3.68020600	-0.54797500	0.96964200
H	4.86692600	-0.65110500	-1.76178300
H	1.23182300	1.68980400	-2.79132100
H	1.16509500	1.10343500	0.18706100
H	0.51076900	-0.54057500	-1.76304400
H	-1.19307800	-0.08213200	0.72115800
H	0.19517800	-3.13721600	-0.80279600
H	1.56493600	-2.05453500	-0.97579100
H	1.35561800	-4.25357800	1.14339800
H	5.88713100	-3.55602700	1.22913700
H	6.14506100	-3.27241500	-0.50272200
H	5.02212200	-4.51818100	0.02324200
H	2.87023600	-4.24732300	-1.53375700
H	1.41384200	-5.16677600	-1.15245400
H	2.92306100	-5.53007400	-0.30854300
H	7.13245300	-1.45081900	-0.74577200
H	7.74054500	0.08041000	-0.10023200
H	7.30052600	-1.23006900	1.00608000
H	4.53786900	-1.88997100	2.67038000
H	5.69388000	0.68149800	1.91762800
H	6.92877100	0.53914400	-2.26941400

H	5.52209800	1.22680000	-3.04189700
H	2.70263700	3.26777300	-0.60046300
H	1.45693900	3.88570200	-1.70473800
H	3.03086800	3.38096800	-2.33155800
H	0.35830500	-2.89770700	2.51907700
H	-1.05643100	-3.15727900	1.47380000
H	-0.98335300	-1.73643500	2.49753100
H	-3.30164300	-0.34571400	-0.42252300
H	-3.59714200	-3.32967100	-0.97019800
H	-5.60781100	-1.03807200	-1.01879500
H	-5.45400600	-3.45589100	0.85916700
H	-6.68933300	-2.19037800	0.90302300
H	-4.97177600	-0.47515500	1.33231100
H	-4.14251400	-1.21131200	3.55665400
H	-4.52707400	-2.89751600	3.16073200
H	-5.83152400	-1.70520000	3.33441200
H	-4.50011700	-2.20453500	-2.97357500
H	-8.02294000	-2.72612100	-2.88310200
H	-7.46879800	-1.17998400	-2.21842800
H	-8.19567300	-2.40337100	-1.14709100
H	0.85216700	2.99262900	1.13769200
H	-0.21884900	5.04095800	1.53470400
H	-0.00558600	4.99994400	-0.20533500
H	-2.57777100	4.43878900	2.55709600
H	-2.66887600	2.10247300	0.60185700
H	-4.35215700	4.02332100	0.44532200
H	-1.10338300	4.37931700	-2.12983800
H	-2.15307500	5.82861900	-2.05542900
H	-2.77082100	4.30862300	-2.73448300
H	-5.25189900	-4.67781600	-1.57949500
H	-6.70573600	-4.70878700	-2.58327700
H	-6.85743100	-4.58729600	-0.81927100
H	-4.09479100	1.87356800	2.67785500
H	-2.63623000	2.09478100	3.66841000
H	-2.78259000	0.67655500	2.60684600
H	5.48820800	3.09440000	-1.32862200
H	6.94860300	2.43748600	-0.59649300
H	6.98998500	3.04494900	-2.26436600
H	-1.81113000	-0.35630000	-2.57439400
H	-2.00582800	1.18482200	-1.71786000
H	-0.84763300	1.05285000	-3.03452400
H	-2.04514400	6.67256900	1.60191900
H	-3.43638900	6.48664600	0.51941100
H	-1.83361300	6.89424500	-0.13539800
H	2.15665100	0.40895000	2.62653700
H	0.38385400	0.48590000	2.51436800
H	1.18227200	-0.90268700	3.31611100

6. References

1. Grimblat, N.; Zanardi, M. M.; Sarotti, A. M., Beyond DP4: an Improved Probability for the Stereochemical Assignment of Isomeric Compounds using Quantum Chemical Calculations of NMR Shifts. *J Org Chem* **2015,** *80* (24), 12526-34.

2. Tanikawa, T.; Asaka, T.; Kashimura, M.; Misawa, Y.; Suzuki, K.; Sato, M.; Kameo, K.; Morimoto, S.; Nishida, A., Synthesis and antibacterial activity of acylides (3-O-acyl-erythromycin derivatives): a novel class of macrolide antibiotics. *J Med Chem* **2001,** *44* (24), 4027-30.