The Unexpected isolation of CTP-431, a Novel Thiopyrone from the Sponge *Cacospongia mycofijiensis.*

Tyler A. Johnson,[†‡] Taro Amagata,[†] Allen G. Oliver,[†] Karen Tenney,[†] Frederick A. Valeriote,[§] and Phillip Crews.[*†‡]

[†]*Department of Chemistry and Biochemistry and* [‡]*Department of Ocean Sciences, University of California, Santa Cruz, California 95064,* [§] *Josephine Ford Cancer Center, Henry Ford Health System, Detroit, Michigan 48202.*

[Supporting Information]

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Experimental Procedures:

General Experimental Procedures. Optical rotations were obtained on a digital polarimeter. The NMR spectra were recorded in $CDCl_3$ and C_6D_6 on 500 and 600 spectrometers operating at 500 and 600 MHz for ^1H and 125.6 and 150.0 MHz for ^{13}C, respectively. Semi preparative HPLC was performed using a 5 μm C_{18} ODS column by means of a single wavelength (λ = 230nm) for compound detection. High resolution mass measurements were obtained from a ESI-TOF mass spectrometer.

Assembling the substructures (see scheme S1)

The first of these, substructure **A,** was constructed using $CDCl_3$ data starting from the vinyl proton H-19 (δ_H 8.41), which showed $^{2\text{-}3}J_{H,C}$ correlations to C-17 (δ_C 172.1) and to an olefinic carbon C-18 (δ_C 133.4). An NH proton (δ_H 8.35) also exhibited $^{2\text{-}3}J_{H,C}$ connectivity to C-17, C-18, and C-19. This NH proton, along with a methoxyl group (δ_H 3.78), displayed $^{2\text{-}3}J_{H,C}$ correlations to C-20 (δ_C 154.5), assigned as a carbamate group, whose ^{13}C δ was consistent with that expected for this residue.[1-3]

A similar analysis as above was used to define substructures **B** and **C** while a slightly different rationale was used to propose **D**. The ^1H-^1H gCOSY correlations (in C_6D_6) from H-4 through to H-14 allowed assembly of the twelve contiguous carbons of **B**, which was supported by HMBC data. (Table 1). The *E* stereochemistry at $\Delta^{6,7}$ was straightforwardly assigned from the large vicinal $^3J_{6,7}$ = 15.2 Hz. Substructure **C** was envisioned as possessing an α,β-unsaturated carboxylate analogous to that present in latrunculeic acid,[4] C-1 (δ_C 170), C-2 (δ_C 116), and C-3 (δ_C 163) because of their parallel NMR shifts. This proposition was further verified from the $CDCl_3$ data as H_3-21 (δ_H 1.87) showed a $^{2\text{-}3}J_{H,C}$ correlation to C-2 (δ_C 115.9), C-3 (δ_C 163.1); and H-2 (δ_H 5.67) exhibited $^{2\text{-}3}J_{H,C}$ correlations to C-1 (δ_C 170.6) and C-3. In addition, H-2 exhibited (in C_6D_6 & $CDCl_3$) a $^4J_{H,H}$ = 1.2 Hz to H_3-21. The geometry of the trisubstituted double bond $\Delta^{2,3}$ was determined as *Z* based on the characteristic downfield C-21 δ_C 25 versus that of the comparable methyl in latrunculeic acid[1] with δ_C at 26. This information set completed the description of **B** and **C**. Finally, the remaining two unassigned sp^2 quaternary carbons (C-15 and C-16) were joined to form substructure **D**.

The fragments **A** – **D** were eventually merged into a near final substructure **E**, which based on the analysis of unassigned unsaturation elements had to contain three rings. A total of ten gHMBC correlations obtained from $CDCl_3$ spectra provided the basis to join these fragments. The initial step in the process was to use the correlations from (a) H-19 to C-15 (δ_C 149.3); (b) from H-8 (δ_H 3.96) to C-15, to C-16 (δ_C 136.5), and to C-17; and (c) from H-14a (δ_H 2.50) to C-15 and C-16. Overall, these data allowed substructures **A** and **B** to be interconnected through **D**. The proposal of a cyclopentane ring within **B** was substantiated based on the gHMBC correlation from H-14a to C-12 (δ_C 29.4). Lastly, the gHMBC

correlations from H-4a (δ_H 2.65) to C-2 and C-3, and H_3-21 to C-4 (δ_C 33.0) steered the addition of **C** completing the assembly of **E**.

X-ray crystallography of 1. The sample crystallizes as colorless columnar crystals. There are four crystallographically independent molecules of the compound in the unit cell of the primitive, acentric triclinic space group P1. The correct enantiomorph of the space group and handedness of the molecule were determined by comparison of Friedel pairs of reflections and by the known stereochemistry at C10 and C13. Both techniques were in agreement. Flack parameter = 0.02 (6); value of 0 indicates the correct enantiomorph, value of +1 the inverted absolute stereochemistry.

The compound consists of three fused-rings (a thiopyranone, a cyclohexene and a cyclopentane ring). Ancillary functionalities consist of a methyl group (on the cyclopentane ring), a carbamate group bonded to the thiopyranone and a 3-methyl, 2,6-hepta-diene-oic acid functionality bonded to the cyclohexene ring (see Figures).

The four independent molecules are chemically identical. They differ primarily in the torsion angles within the fused ring system and the seven-carbon carboxylic acid chain (see Figures and Table of Torsion Angles). The molecules stack in a head-to-tail fashion with the orientation of the thiopyranone ring alternating between each molecule. The molecules are not stacked evenly within the lattice; as evidenced by the angle formed by the mean planes of the fused ring systems (inter-planar angles with respect to the previous molecules' plane): 12.68(5); 23.93(6); 31.01(5); 20.71(5) (for molecule 4 to the translation-related molecule 1).

The amide hydrogen atoms were located from a difference Fourier map and included in their observed positions with thermal parameters tied to that of the nitrogen to which they are boned. Two of the four carboxylic acid hydrogen's were observed in a difference Fourier map. All four were included with a riding model on the oxygen to which they are bonded. The carboxylic acid moieties form good hydrogen-bonds to the pyranone oxygen of a molecule two removed from the molecule in question (see packing diagrams and Table of Hydrogen-bonds).

The bond distances and angles within the molecule are unexceptional and do confirm the expected geometry about the molecules.

Data Collection

A fragment of a colorless columnar-like crystal of $C_{23}H_{29}NO_5S$ having approximate dimensions of 0.38 × 0.16 × 0.10 mm was mounted on a Kapton loop using Paratone N hydrocarbon oil. All measurements were made on a Bruker APEX-II[5] CCD area detector with graphite monochromated Mo-Kα radiation.

Cell constants and an orientation matrix, obtained from a least-squares refinement using the measured positions of 6217 centered reflections with $I > 10\sigma(I)$ in the range $2.69 < \theta < 25.98°$ corresponded to a triclinic cell with dimensions:

a = 10.2207(13) Å	α = 72.802(2)°
b = 15.0552(19) Å	β = 72.958(2)°
c = 16.326(2) Å	γ = 73.405(1)°
V = 2239.4(5) Å^3	

For Z = 4 and F.W. = 431.53, the calculated density is 1.280 g/cm^3.

Analysis of the systematic absences allowed the space group to be uniquely determined to be:

P1

The data were collected at a temperature of 153(2) K. Frames corresponding to an arbitrary sphere of data were collected using ω-scans of 0.3° counted for a total of 30 seconds per frame.

Data Reduction

Data were integrated by the program SAINT[6] to a maximum θ-value of 26.83°. The data were corrected for Lorentz and polarization effects. Data were analyzed for agreement and possible absorption using XPREP.[7] An empirical absorption correction based on comparison of redundant and equivalent reflections was applied using SADABS.[8] (Tmax = 0.9824, Tmin = 0.9354). Of the 20214 reflections that were collected, 16235 were unique (R_{int} = 0.0312); equivalent reflections were merged. No decay correction was applied.

Structure Solution and Refinement

The structure was solved by direct methods[9] and expanded using Fourier techniques.[10] Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in calculated positions but were not refined. The final cycle of full-matrix least-squares refinement[11] was based on 16235 reflections (all data) and 1106 variable parameters and converged (largest parameter shift was 0.004 times its esd) with conventional unweighted and weighted agreement factors of:

$$R_1 = \Sigma||Fo| - |Fc|| / \Sigma|Fo| = 0.0580 \text{ for 12120 data with } I > 2\sigma(I)$$

$$wR_2 = [(\Sigma w (|Fo|^2 - |Fc|^2)^2 / \Sigma w |Fo|^2)]^{1/2} = 0.1288$$

The standard deviation of an observation of unit weight[12] was 1.070. The weighting scheme was based on counting statistics and included a factor to downweight the intense reflections. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.266 and -0.498 e$^-$.Å^3, respectively.

Neutral atom scattering factors were taken from Cromer and Waber.[13] Anomalous dispersion effects were

included in Fcalc;[6] the values for Δf' and Δf'' were those of Creagh and McAuley.[14] The values for the mass attenuation coefficients are those of Creagh and Hubbel.[15] All calculations were performed using the SHELXTL[5-10] crystallographic software package of Bruker Analytical X-ray Systems Inc.

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(3) Hassfeld, J.; Fares, C.; Steinmetz, H.; Carlomagno, T.; Menche, D. *Org. Lett.* **2006***,8,* 4751-4754.

(4) Vilozny, B.; Amagata, T.; Mooberry, S. L.; Crews, P. *J. Nat. Prod.* **2004** 67, 1055-1057.

(5) APEX-II: Area-Detector Software Package v2.1, Bruker Analytical X-ray Systems, Inc.: Madison, WI, (2006)

(6) SAINT: SAX Area-Dectector Integration Program, 7.34A; Siemens Industrial Automation, Inc.: Madison, WI, (2006)

(7) XPREP:(v 6.14) Part of the SHELXTL Crystal Structure Determination Package,
Siemens Industrial Automation, Inc.: Madison, WI, (1995)

(8) SADABS: Siemens Area Detector ABSorption correction program v.2.10, George Sheldrick, (2005).

(9) XS: Program for the Solution of X-ray Crystal Structures, Part of the SHELXTL Crystal Structure Determination Package, Bruker Analytical X-ray Systems Inc.: Madison, WI, (1995-99)

(10) XL: Program for the Refinement of X-ray Crystal Structure Part of the SHELXTL Crystal Structure Determination Package, Bruker Analytical X-ray Systems Inc.: Madison, WI, (1995-99)

(11) Least-Squares:

Function minimized: $\Sigma w\,(|Fo|^2 - |Fc|^2)^2$

(12) Standard deviation of an observation of unit weight:

$[\Sigma w(|Fo|^2 - |Fc|^2)^2/(N_o - N_v)]^{1/2}$
where: N_o = number of observations
N_v = number of variables

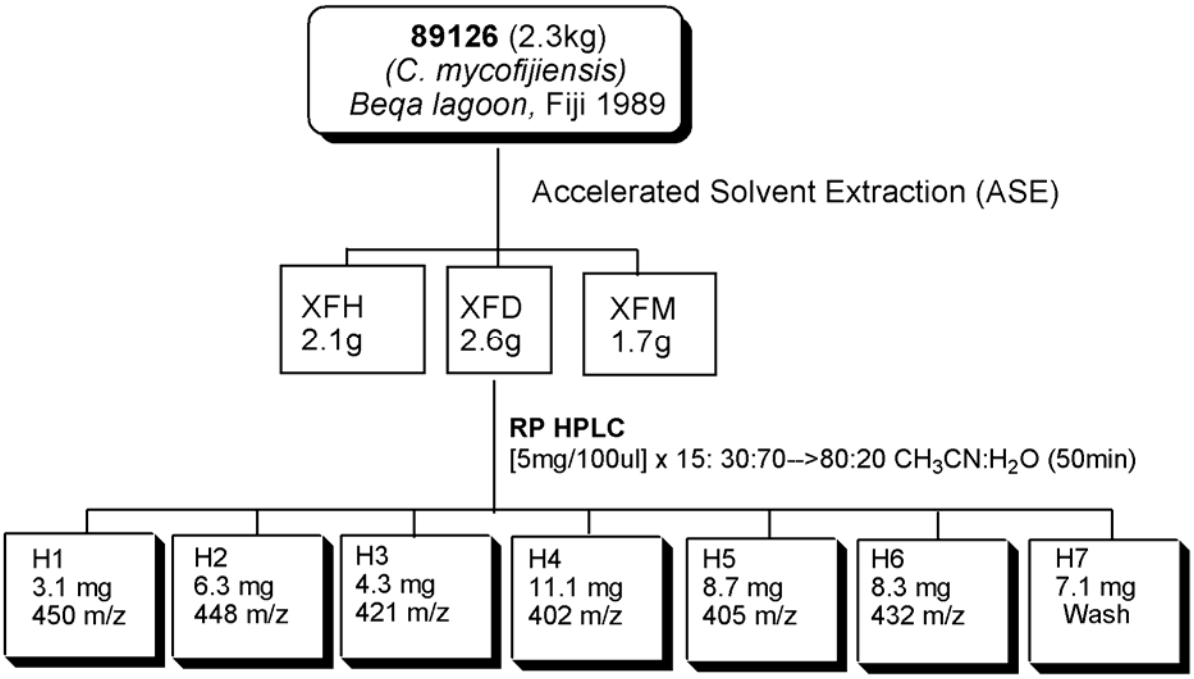
(13) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(14) Creagh, D. C. & McAuley, W. J.; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(15) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

Crystal data for $C_{23}H_{29}NO_5S$; M = 431.53; triclinic; space group P1; *a* = 10.2207(13) Å; *b* = 15.0552(19) Å; *c* = 16.326(2) Å; α = 72.802(2)°; β = 72.958(2)°; γ = 73.4050(10)°; V = 2239.4(5) $Å^3$; Z = 4; T = 153(2) K; λ(Mo-Kα) = 0.71073 Å; μ(Mo-Kα) = 0.178 mm^{-1}; d_{calc} = 1.280; 20214 reflections collected; 16235 unique (R_{int} = 0.0312); giving R_1 = 0.0580, wR_2 = 0.1288 for 12120 data with [I>2σ(I)] and R_1 = 0.0780, wR_2 = 0.1385 for all 16235 data. Residual electron density ($e^-.Å^{-3}$) max/min: 0.266/-0.498. An arbitrary sphere of data were collected on a colorless columnar-like crystal, having approximate dimensions of 0.38 × 0.16 × 0.10 mm, on a single crystal X-ray diffractometer using a combination of ω- and φ-scans of 0.3°. Data were corrected for absorption and polarization effects and analyzed for space group determination. The structure was solved by direct methods and expanded routinely. The model was refined by full-matrix least-squares analysis of F^2 against all reflections. All non-hydrogen atoms were refined with anisotropic thermal displacement parameters. Unless otherwise noted, hydrogen atoms were included in calculated positions. Thermal parameters for the hydrogens were tied to the isotropic thermal parameter of the atom to which they are bonded (1.5 X for methyl, 1.2 for all others).

Chart S1. Accelerated solvent extraction scheme and ELSD analysis of Coll. No. 89126 XFD fraction with annotations including *m/z* ions.



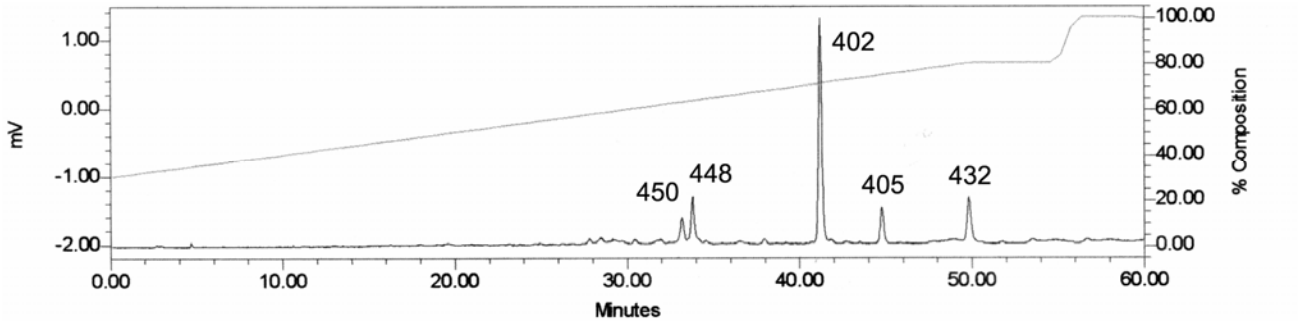
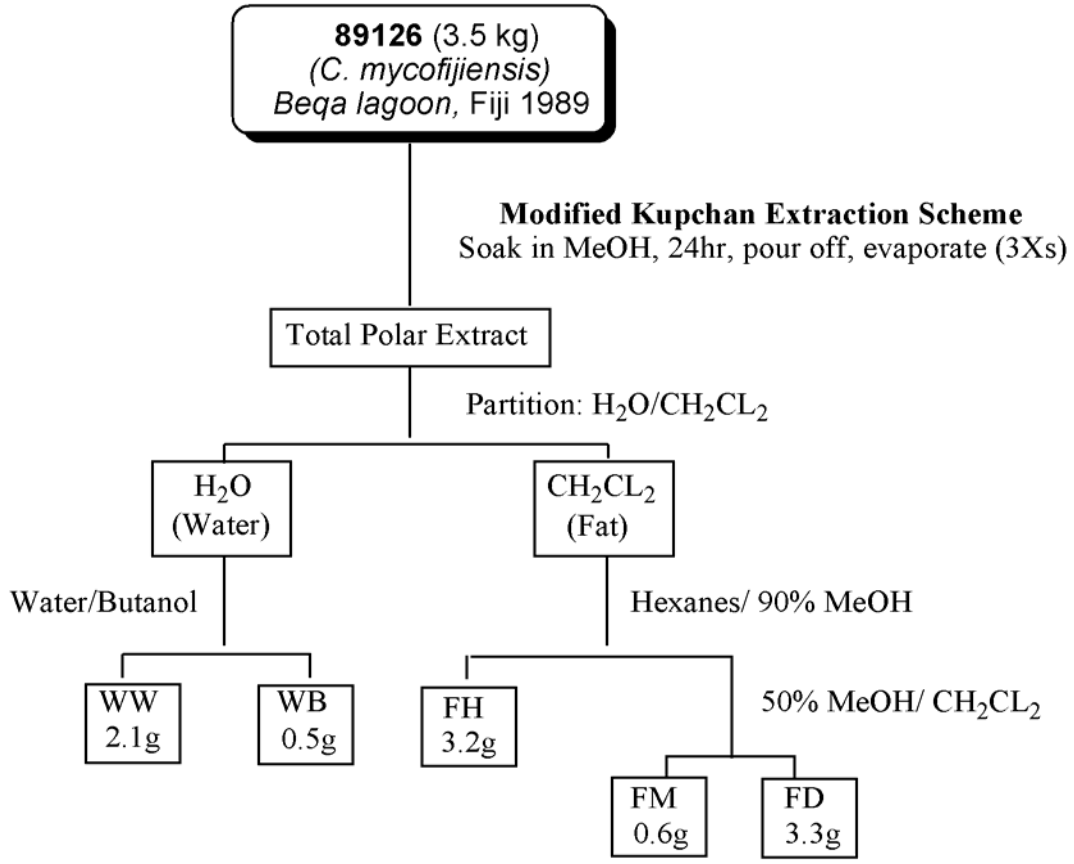
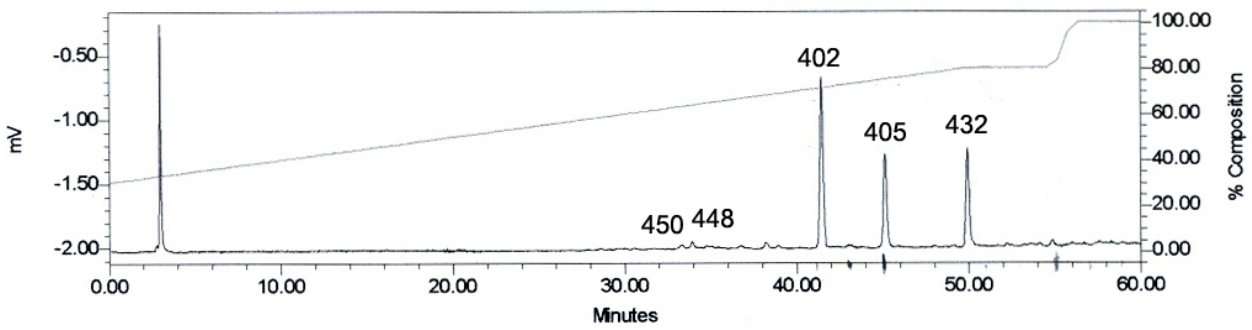
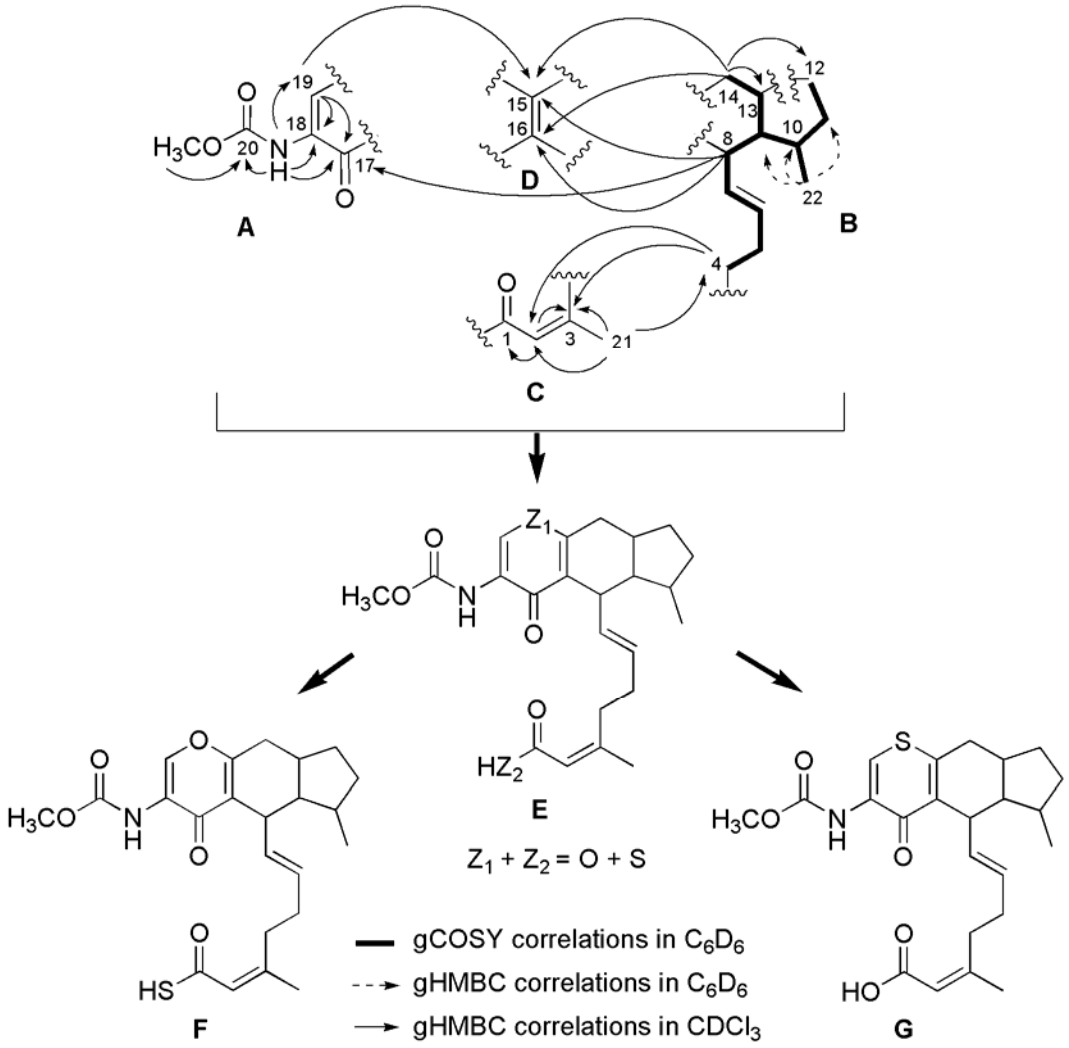


Chart S2. Modified Kupchan extraction scheme and ELSD analysis of Coll. No. 89126 FD fraction with annotations including *m/z* ions.

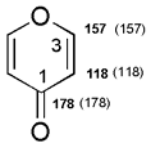




Scheme S1. Substructures and significant 2D NMR correlations for CTP-431 (**1**)

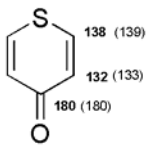


Scheme S2. Experimental δ_C values (in bold) and DFT calculation results (in parenthesis) for γ-pyrone and γ-thiopyrone.



γ – pyrone

MAE = 0.1, % Score = 100



γ – thiopyrone

MAE = 1.0, % Score = 100

Table S1. ^{1}H and ^{13}C NMR[a] data of **mycothiazole** in $CDCl_3$

position	δ_H (J in Hz)[b]	δ_C	Type[b]
1		157.3	C
2	3.48 (dddd, 13.8, 7.2, 6.6, 6.0)	39.5	CH_2
2'	3.11 (dddd, 13.8, 8.4, 6.0, 4.8)		
3	2.30 (dddd, 13.8, 8.4, 6.0, 0.6)	37.3	CH_2
3'	2.02 (dddd, 13.8, 6.6, 4.8, 1.2)		
4		142.6	C
5	5.78 (ddd, 11.4, 1.8, 0.6)	131.0	CH
6	5.67 (ddd, 11.4, 9.0, 3.6)	130.7	CH
7	2.56 (dddd, 14.4, 10.2, 9.0, 0.6)	30.7	CH_2
7'	2.50 (dddd, 14.4, 3.6, 2.4, 1.8)		
8	3.79 (dd, 10.5, 2.1)	78.3	CH
9		44.7	C
10		179.6	C
11	6.31 (s)	111.9	CH
12		155.1	C
13	3.33 (d, 7.2)	29.5	CH_2
14	5.62 (dtt, 10.8, 7.8, 1.2)	126.9	CH
15	5.53 (dtt, 10.7, 7.5, 1.5)	129.0	CH
16	2.69 (ddd, 7.8, 6.6, 1.2)	31.6	CH_2
17	5.72 (ddt, 16.9, 10.6, 6.4)	136.5	CH
18	5.02 (dq, 17.4, 1.8)	115.2	CH_2
18'	4.97 (dq, 10.2, 1.8)		
19	4.95 (bs)	116.0	CH_2
19'	4.89 (bs)		
20	1.34 (s)	26.8	CH_3
21	1.28 (s)	23.9	CH_3
O-Me	3.48 (s)	52.3	CH_3
NH	5.36 (bs)		

[a] measured at 600 MHz (^{1}H) and 125 MHz (^{13}C). [b] Carbon type determined by DEPT and HMQC experiments

Table S2. Crystal data and structure refinement for **1**.

Identification code	xsc07087
Empirical formula	$C_{23}H_{29}NO_5S$
Formula weight	431.53
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	triclinic
Space group	P1
Unit cell dimensions	a = 10.2207(13) Å α = 72.802(2)°
	b = 15.0552(19) Å β = 72.958(2)°
	c = 16.326(2) Å γ = 73.4050(10)°
Volume	2239.4(5) $Å^3$
Z	4
Density (calculated)	1.280 g/cm^3
Absorption coefficient (μ)	0.178 mm^{-1}
F(000)	920
Crystal size	0.38 × 0.16 × 0.10 mm^3
ω range for data collection	2.14 to 26.83°
Index ranges	$-12 \le h \le 2$, $-18 \le k \le 18$, $-20 \le l \le 18$
Reflections collected	20214
Independent reflections	16235 [R_{int} = 0.0312]
Completeness to θ = 26.83°	96.5 %
Absorption correction	Empirical
Max. and min. transmission	0.9824 and 0.9354
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	16235 / 3 / 1106
Goodness-of-fit on F^2	1.070
Final R indices [I>2σ(I)]	R_1 = 0.0580, wR_2 = 0.1288
R indices (all data)	R_1 = 0.0780, wR_2 = 0.1385
Absolute structure parameter	0.02(6)
Largest diff. peak and hole	0.266 and -0.498 $e^-.Å^{-3}$

Table S3. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
S11	0.57221(11)	0.35171(7)	0.89193(8)	0.038(1)
O11	0.0434(3)	0.75539(18)	0.42397(19)	0.035(1)
O21	0.1682(3)	0.69563(19)	0.5272(2)	0.044(1)
O31	0.1893(3)	0.57580(18)	0.8842(2)	0.037(1)
O41	-0.0322(3)	0.3429(2)	0.9604(2)	0.046(1)
O51	0.1740(3)	0.2451(2)	0.9825(2)	0.044(1)
N11	0.1544(4)	0.4047(2)	0.9239(3)	0.039(1)
C11	0.0838(4)	0.7600(3)	0.4934(3)	0.033(1)
C21	0.0164(4)	0.8511(3)	0.5190(3)	0.031(1)
C31	0.0218(4)	0.8721(3)	0.5918(3)	0.033(1)
C41	0.0950(4)	0.8061(3)	0.6618(3)	0.033(1)
C51	0.2472(4)	0.8128(3)	0.6451(3)	0.035(1)
C61	0.2983(4)	0.7680(3)	0.7277(3)	0.033(1)
C71	0.3944(4)	0.6877(3)	0.7437(3)	0.033(1)
C81	0.4352(4)	0.6465(3)	0.8310(3)	0.030(1)
C91	0.5767(4)	0.6637(3)	0.8286(3)	0.030(1)
C101	0.6081(4)	0.7615(3)	0.7801(3)	0.037(1)
C111	0.7674(4)	0.7441(3)	0.7705(3)	0.046(1)
C121	0.8283(4)	0.6373(3)	0.7731(3)	0.041(1)
C131	0.7001(4)	0.5961(3)	0.7844(3)	0.033(1)
C141	0.7040(4)	0.4953(3)	0.8380(3)	0.040(1)
C151	0.5601(4)	0.4720(3)	0.8615(3)	0.032(1)
C161	0.4374(4)	0.5398(3)	0.8595(3)	0.028(1)
C171	0.3021(4)	0.5143(3)	0.8841(3)	0.029(1)
C181	0.2926(4)	0.4147(3)	0.9073(3)	0.034(1)
C191	0.4039(4)	0.3405(3)	0.9132(3)	0.034(1)
C201	0.1048(4)	0.3238(3)	0.9577(3)	0.034(1)
C211	0.5197(5)	0.8423(3)	0.8236(4)	0.058(1)
C221	-0.0475(4)	0.9709(3)	0.6078(3)	0.040(1)
C231	-0.0984(5)	0.2630(3)	1.0011(3)	0.048(1)
S12	0.22150(11)	0.48555(7)	0.61254(8)	0.038(1)

O12	0.6694(3)	0.09530(19)	0.24409(18)	0.036(1)
O22	0.5414(3)	0.15525(19)	0.35913(19)	0.042(1)
O32	0.5845(3)	0.29034(17)	0.70607(18)	0.033(1)
O42	0.8012(3)	0.52292(18)	0.58747(18)	0.031(1)
O52	0.6032(3)	0.61076(19)	0.54328(18)	0.036(1)
N12	0.6153(3)	0.4591(2)	0.6289(2)	0.033(1)
C12	0.6199(4)	0.0883(3)	0.3298(3)	0.031(1)
C22	0.6664(4)	-0.0073(3)	0.3825(3)	0.029(1)
C32	0.6155(4)	-0.0378(3)	0.4678(3)	0.031(1)
C42	0.5101(4)	0.0242(3)	0.5264(3)	0.034(1)
C52	0.5846(4)	0.0819(3)	0.5534(3)	0.040(1)
C62	0.4848(4)	0.1539(3)	0.6025(3)	0.036(1)
C72	0.4551(4)	0.1403(3)	0.6890(3)	0.030(1)
C82	0.3565(4)	0.2077(3)	0.7443(3)	0.028(1)
C92	0.2084(4)	0.1875(3)	0.7772(3)	0.031(1)
C102	0.1952(4)	0.0839(3)	0.8095(3)	0.037(1)
C112	0.0394(4)	0.0925(3)	0.8147(3)	0.047(1)
C122	-0.0051(5)	0.1850(3)	0.7463(3)	0.051(1)
C132	0.1254(4)	0.2278(3)	0.7066(3)	0.036(1)
C142	0.0995(4)	0.3363(3)	0.6842(3)	0.038(1)
C152	0.2353(4)	0.3687(3)	0.6677(3)	0.030(1)
C162	0.3509(4)	0.3111(3)	0.6962(3)	0.027(1)
C172	0.4777(4)	0.3436(3)	0.6810(3)	0.029(1)
C182	0.4865(4)	0.4425(3)	0.6350(3)	0.030(1)
C192	0.3790(4)	0.5071(3)	0.6042(3)	0.037(1)
C202	0.6676(4)	0.5378(3)	0.5827(3)	0.028(1)
C212	0.2411(5)	0.0338(3)	0.8963(3)	0.046(1)
C222	0.6661(4)	-0.1386(3)	0.5144(3)	0.039(1)
C232	0.8663(4)	0.6040(3)	0.5402(3)	0.038(1)
S13	0.52633(11)	0.35493(7)	0.35607(8)	0.041(1)
O13	0.0571(3)	0.74755(19)	-0.0783(2)	0.040(1)
O23	0.1722(3)	0.7015(2)	0.0293(2)	0.051(1)
O33	0.1537(3)	0.58715(18)	0.37636(19)	0.035(1)
O43	-0.0874(3)	0.3627(2)	0.4654(2)	0.045(1)
O53	0.1191(3)	0.2628(2)	0.4840(2)	0.049(1)
N13	0.1052(4)	0.4197(3)	0.4126(3)	0.039(1)

C13	0.0900(4)	0.7614(3)	-0.0101(3)	0.034(1)
C23	0.0209(4)	0.8557(3)	0.0071(3)	0.033(1)
C33	0.0136(4)	0.8842(3)	0.0790(3)	0.032(1)
C43	0.0744(4)	0.8228(3)	0.1552(3)	0.038(1)
C53	0.2263(4)	0.8309(3)	0.1432(3)	0.038(1)
C63	0.2738(4)	0.7809(3)	0.2263(3)	0.032(1)
C73	0.3691(4)	0.7002(3)	0.2375(3)	0.030(1)
C83	0.4067(4)	0.6486(3)	0.3255(3)	0.029(1)
C93	0.5496(4)	0.6566(3)	0.3297(3)	0.030(1)
C103	0.5847(4)	0.7555(3)	0.2958(3)	0.037(1)
C113	0.7430(4)	0.7324(3)	0.2878(4)	0.051(1)
C123	0.8000(4)	0.6293(3)	0.2763(3)	0.047(1)
C133	0.6701(4)	0.5959(3)	0.2766(3)	0.037(1)
C143	0.6691(4)	0.4915(3)	0.3152(3)	0.043(1)
C153	0.5215(4)	0.4737(3)	0.3385(3)	0.032(1)
C163	0.4014(4)	0.5430(3)	0.3451(3)	0.029(1)
C173	0.2640(4)	0.5229(3)	0.3709(3)	0.031(1)
C183	0.2465(4)	0.4253(3)	0.3892(3)	0.033(1)
C193	0.3547(4)	0.3489(3)	0.3849(3)	0.037(1)
C203	0.0520(5)	0.3404(3)	0.4570(3)	0.038(1)
C213	0.4985(5)	0.8237(3)	0.3547(4)	0.051(1)
C223	-0.0529(4)	0.9860(3)	0.0863(3)	0.040(1)
C233	-0.1588(5)	0.2857(3)	0.5143(3)	0.056(1)
S14	0.18633(10)	0.49842(7)	0.12779(7)	0.038(1)
O14	0.7028(3)	0.10409(19)	-0.22435(19)	0.038(1)
O24	0.6057(3)	0.1409(2)	-0.0940(2)	0.053(1)
O34	0.5605(3)	0.27192(18)	0.15702(18)	0.032(1)
O44	0.7917(3)	0.49950(18)	0.0696(2)	0.036(1)
O54	0.5852(3)	0.60282(18)	0.05589(19)	0.035(1)
N14	0.6027(3)	0.4413(2)	0.1019(2)	0.032(1)
C14	0.6645(4)	0.0810(3)	-0.1364(3)	0.033(1)
C24	0.6978(4)	-0.0221(3)	-0.1017(3)	0.033(1)
C34	0.6757(4)	-0.0664(3)	-0.0161(3)	0.033(1)
C44	0.6266(4)	-0.0155(3)	0.0581(3)	0.033(1)
C54	0.4672(4)	0.0067(3)	0.0891(3)	0.035(1)
C64	0.4245(4)	0.0627(3)	0.1589(3)	0.034(1)

C74	0.3525(4)	0.1516(3)	0.1502(3)	0.031(1)
C84	0.3086(4)	0.2074(3)	0.2202(3)	0.026(1)
C94	0.1608(4)	0.1999(3)	0.2763(3)	0.032(1)
C104	0.1300(4)	0.1006(3)	0.3163(3)	0.037(1)
C114	-0.0322(4)	0.1199(3)	0.3384(3)	0.050(1)
C124	-0.0838(4)	0.2215(3)	0.2845(3)	0.047(1)
C134	0.0497(4)	0.2527(3)	0.2246(3)	0.034(1)
C144	0.0466(4)	0.3589(3)	0.2016(3)	0.038(1)
C154	0.1932(4)	0.3792(3)	0.1716(3)	0.032(1)
C164	0.3122(4)	0.3125(3)	0.1807(3)	0.028(1)
C174	0.4488(4)	0.3347(3)	0.1529(3)	0.028(1)
C184	0.4640(4)	0.4336(3)	0.1194(3)	0.028(1)
C194	0.3540(4)	0.5083(3)	0.1056(3)	0.032(1)
C204	0.6520(4)	0.5222(3)	0.0740(3)	0.029(1)
C214	0.1971(5)	0.0462(3)	0.3944(3)	0.054(1)
C224	0.6970(4)	-0.1730(3)	0.0132(3)	0.038(1)
C234	0.8587(4)	0.5802(3)	0.0347(3)	0.036(1)
H1O1	0.0937	0.7075	0.4051	0.042
H1N1	0.089(5)	0.457(3)	0.912(3)	0.047
H2A1	-0.0354	0.8990	0.4806	0.037
H4A1	0.0925	0.7398	0.6654	0.040
H4B1	0.0433	0.8211	0.7194	0.040
H5C1	0.3060	0.7797	0.5982	0.042
H5D1	0.2541	0.8804	0.6252	0.042
H6B1	0.2580	0.8002	0.7742	0.039
H7B1	0.4393	0.6550	0.6978	0.039
H8C1	0.3621	0.6781	0.8757	0.036
H9C1	0.5836	0.6522	0.8909	0.036
H10B1	0.5906	0.7765	0.7198	0.044
H11C1	0.7865	0.7612	0.8193	0.055
H11D1	0.8103	0.7833	0.7141	0.055
H12A1	0.8742	0.6062	0.8231	0.050
H12B1	0.8977	0.6284	0.7177	0.050
H13A1	0.6878	0.6001	0.7248	0.040
H14A1	0.7341	0.4873	0.8926	0.048
H14B1	0.7731	0.4506	0.8039	0.048

H19C1	0.3870	0.2780	0.9304	0.041
H21B1	0.4215	0.8518	0.8220	0.087
H21E1	0.5530	0.9009	0.7919	0.087
H21F1	0.5277	0.8263	0.8849	0.087
H22A1	-0.0839	1.0114	0.5566	0.060
H22B1	0.0215	0.9986	0.6170	0.060
H22C1	-0.1249	0.9665	0.6601	0.060
H23A1	-0.1985	0.2837	1.0013	0.072
H23B1	-0.0869	0.2376	1.0618	0.072
H23C1	-0.0549	0.2133	0.9679	0.072
H1O2	0.6360	0.1499	0.2166	0.055
H1N2	0.679(4)	0.417(3)	0.652(3)	0.039
H2D2	0.7386	-0.0507	0.3531	0.034
H4G2	0.4615	-0.0163	0.5796	0.041
H4H2	0.4389	0.0679	0.4945	0.041
H5G2	0.6477	0.0378	0.5910	0.048
H5H2	0.6432	0.1153	0.4999	0.048
H6D2	0.4408	0.2124	0.5695	0.043
H7D2	0.5009	0.0812	0.7201	0.036
H8D2	0.3941	0.1968	0.7974	0.033
H9D2	0.1582	0.2197	0.8267	0.037
H10D2	0.2537	0.0485	0.7633	0.045
H11G2	-0.0174	0.0967	0.8746	0.056
H11H2	0.0266	0.0365	0.8004	0.056
H12G2	-0.0345	0.1702	0.7000	0.061
H12H2	-0.0838	0.2298	0.7751	0.061
H13D2	0.1803	0.2040	0.6528	0.043
H14G2	0.0605	0.3627	0.6310	0.046
H14H2	0.0299	0.3611	0.7334	0.046
H19D2	0.3931	0.5696	0.5757	0.044
H21J2	0.3419	0.0287	0.8870	0.069
H21K2	0.2212	-0.0301	0.9168	0.069
H21L2	0.1895	0.0708	0.9407	0.069
H22J2	0.7409	-0.1715	0.4733	0.058
H22K2	0.5881	-0.1714	0.5366	0.058
H22L2	0.7022	-0.1388	0.5638	0.058

H23J2	0.9657	0.5863	0.5419	0.056
H23K2	0.8191	0.6577	0.5681	0.056
H23L2	0.8579	0.6225	0.4788	0.056
H1O3	0.1003	0.6934	-0.0868	0.048
H1N3	0.039(5)	0.473(3)	0.413(3)	0.047
H2C3	-0.0228	0.9010	-0.0367	0.040
H4E3	0.0730	0.7556	0.1614	0.045
H4F3	0.0159	0.8420	0.2100	0.045
H5E3	0.2885	0.8020	0.0943	0.045
H5F3	0.2308	0.8988	0.1282	0.045
H6C3	0.2323	0.8092	0.2753	0.039
H7C3	0.4163	0.6733	0.1880	0.036
H8B3	0.3343	0.6775	0.3722	0.035
H9B3	0.5567	0.6333	0.3926	0.036
H10C3	0.5661	0.7834	0.2356	0.044
H11E3	0.7633	0.7383	0.3414	0.061
H11F3	0.7877	0.7769	0.2364	0.061
H12E3	0.8437	0.5885	0.3253	0.056
H12F3	0.8705	0.6273	0.2200	0.056
H13C3	0.6580	0.6128	0.2148	0.044
H14E3	0.7070	0.4695	0.3688	0.052
H14F3	0.7307	0.4541	0.2721	0.052
H19B3	0.3334	0.2880	0.3989	0.044
H21C3	0.5336	0.8825	0.3346	0.077
H21D3	0.5067	0.7938	0.4156	0.077
H21I3	0.4000	0.8386	0.3517	0.077
H22G3	-0.0891	1.0216	0.0337	0.059
H22H3	0.0174	1.0157	0.0910	0.059
H22I3	-0.1302	0.9865	0.1387	0.059
H23G3	-0.2574	0.3060	0.5107	0.084
H23H3	-0.1531	0.2693	0.5761	0.084
H23I3	-0.1140	0.2298	0.4891	0.084
H1O4	0.6648	0.1611	-0.2430	0.057
H1N4	0.662(4)	0.386(3)	0.116(3)	0.039
H2B4	0.7385	-0.0609	-0.1432	0.040
H4C4	0.6600	0.0447	0.0381	0.039

H4D4	0.6683	-0.0558	0.1081	0.039
H5A4	0.4245	0.0440	0.0388	0.042
H5B4	0.4335	-0.0533	0.1133	0.042
H6A4	0.4513	0.0318	0.2131	0.041
H7A4	0.3264	0.1828	0.0958	0.037
H8A4	0.3758	0.1801	0.2598	0.032
H9A4	0.1432	0.2310	0.3259	0.038
H10A4	0.1674	0.0632	0.2698	0.044
H11A4	-0.0702	0.1162	0.4022	0.059
H11B4	-0.0635	0.0724	0.3220	0.059
H12C4	-0.1469	0.2205	0.2491	0.057
H12D4	-0.1346	0.2653	0.3240	0.057
H13B4	0.0737	0.2304	0.1690	0.040
H14C4	-0.0046	0.3916	0.1542	0.045
H14D4	-0.0050	0.3852	0.2539	0.045
H19A4	0.3731	0.5701	0.0819	0.038
H21A4	0.2993	0.0371	0.3748	0.080
H21G4	0.1718	-0.0160	0.4184	0.080
H21H4	0.1633	0.0827	0.4401	0.080
H22D4	0.7410	-0.2011	-0.0380	0.058
H22E4	0.6062	-0.1903	0.0416	0.058
H22F4	0.7578	-0.1970	0.0551	0.058
H23D4	0.9606	0.5573	0.0262	0.053
H23E4	0.8253	0.6217	0.0763	0.053
H23F4	0.8355	0.6161	-0.0218	0.053

Table S4. Bond lengths [Å] for **1**.

atom-atom	distance	atom-atom	distance	
S11-C191	1.700(4)	S11-C151	1.708(4)	O11-
C11	1.341(5)	O11-H1O1	0.8400	O21-
C11	1.214(4)	O31-C171	1.256(4)	O41-
C201	1.336(5)	O41-C231	1.441(5)	O51-
C201	1.214(5)	N11-C201	1.355(5)	N11-
C181	1.401(5)	N11-H1N1	0.89(4)	C11-
C21	1.469(5)	C21-C31	1.337(6)	C21-
H2A1	0.9500	C31-C41	1.503(5)	C31-
C221	1.517(6)	C41-C51	1.526(5)	C41-
H4A1	0.9900	C41-H4B1	0.9900	C51-
C61	1.491(5)	C51-H5C1	0.9900	C51-
H5D1	0.9900	C61-C71	1.334(5)	C61-
H6B1	0.9500	C71-C81	1.506(6)	C71-
H7B1	0.9500	C81-C91	1.529(5)	C81-
C161	1.530(5)	C81-H8C1	1.0000	C91-
C131	1.522(5)	C91-C101	1.527(5)	C91-
H9C1	1.0000	C101-C211	1.518(6)	C101-
C111	1.541(6)	C101-H10B1	1.0000	C111-
C121	1.541(6)	C111-H11C1	0.9900	C111-
H11D1	0.9900	C121-C131	1.546(6)	C121-
H12A1	0.9900	C121-H12B1	0.9900	C131-
C141	1.507(6)	C131-H13A1	1.0000	C141-
C151	1.522(6)	C141-H14A1	0.9900	C141-
H14B1	0.9900	C151-C161	1.375(5)	C161-
C171	1.451(5)	C171-C181	1.459(5)	C181-
C191	1.352(5)	C191-H19C1	0.9500	C211-
H21B1	0.9800	C211-H21E1	0.9800	C211-
H21F1	0.9800	C221-H22A1	0.9800	C221-
H22B1	0.9800	C221-H22C1	0.9800	C231-
H23A1	0.9800	C231-H23B1	0.9800	C231-
H23C1	0.9800	S12-C192	1.691(4)	S12-
C152	1.709(4)	O12-C12	1.325(5)	O12-
H1O2	0.8400	O22-C12	1.219(4)	O32-
C172	1.253(4)	O42-C202	1.341(4)	O42-
C232	1.461(4)	O52-C202	1.213(4)	N12-
C202	1.362(5)	N12-C182	1.379(5)	N12-
H1N2	0.85(4)	C12-C22	1.467(5)	C22-
C32	1.325(5)	C22-H2D2	0.9500	C32-
C222	1.500(5)	C32-C42	1.517(5)	C42-
C52	1.525(6)	C42-H4G2	0.9900	C42-
H4H2	0.9900	C52-C62	1.505(6)	C52-
H5G2	0.9900	C52-H5H2	0.9900	C62-

C72	1.319(6)	C62-H6D2	0.9500	C72-
C82	1.512(5)	C72-H7D2	0.9500	C82-
C162	1.516(5)	C82-C92	1.537(5)	C82-
H8D2	1.0000	C92-C132	1.510(6)	C92-
C102	1.524(5)	C92-H9D2	1.0000	C102-
C212	1.535(6)	C102-C112	1.538(6)	C102-
H10D2	1.0000	C112-C122	1.552(6)	C112-
H11G2	0.9900	C112-H11H2	0.9900	C122-
C132	1.534(6)	C122-H12G2	0.9900	C122-
H12H2	0.9900	C132-C142	1.526(6)	C132-
H13D2	1.0000	C142-C152	1.526(6)	C142-
H14G2	0.9900	C142-H14H2	0.9900	C152-
C162	1.365(5)	C162-C172	1.442(5)	C172-
C182	1.472(5)	C182-C192	1.353(5)	C192-
H19D2	0.9500	C212-H21J2	0.9800	C212-
H21K2	0.9800	C212-H21L2	0.9800	C222-
H22J2	0.9800	C222-H22K2	0.9800	C222-
H22L2	0.9800	C232-H23J2	0.9800	C232-
H23K2	0.9800	C232-H23L2	0.9800	S13-
C193	1.700(4)	S13-C153	1.714(4)	O13-
C13	1.338(5)	O13-H1O3	0.8400	O23-
C13	1.214(5)	O33-C173	1.259(4)	O43-
C203	1.341(5)	O43-C233	1.452(5)	O53-
C203	1.203(5)	N13-C203	1.370(5)	N13-
C183	1.402(5)	N13-H1N3	0.89(4)	C13-
C23	1.464(5)	C23-C33	1.340(6)	C23-
H2C3	0.9500	C33-C43	1.494(6)	C33-
C223	1.513(5)	C43-C53	1.542(5)	C43-
H4E3	0.9900	C43-H4F3	0.9900	C53-
C63	1.489(6)	C53-H5E3	0.9900	C53-
H5F3	0.9900	C63-C73	1.324(5)	C63-
H6C3	0.9500	C73-C83	1.519(5)	C73-
H7C3	0.9500	C83-C93	1.522(5)	C83-
C163	1.540(5)	C83-H8B3	1.0000	C93-
C133	1.518(5)	C93-C103	1.534(5)	C93-
H9B3	1.0000	C103-C213	1.525(6)	C103-
C113	1.529(6)	C103-H10C3	1.0000	C113-
C123	1.541(6)	C113-H11E3	0.9900	C113-
H11F3	0.9900	C123-C133	1.546(6)	C123-
H12E3	0.9900	C123-H12F3	0.9900	C133-
C143	1.513(6)	C133-H13C3	1.0000	C143-
C153	1.525(6)	C143-H14E3	0.9900	C143-
H14F3	0.9900	C153-C163	1.365(5)	C163-
C173	1.436(5)	C173-C183	1.462(5)	C183-
C193	1.351(5)	C193-H19B3	0.9500	C213-
H21C3	0.9800	C213-H21D3	0.9800	C213-

H21I3	0.9800	C223-H22G3	0.9800	C223-
H22H3	0.9800	C223-H22I3	0.9800	C233-
H23G3	0.9800	C233-H23H3	0.9800	C233-
H23I3	0.9800	S14-C194	1.685(4)	S14-
C154	1.714(4)	O14-C14	1.337(5)	O14-
H1O4	0.8400	O24-C14	1.212(5)	O34-
C174	1.262(4)	O44-C204	1.355(4)	O44-
C234	1.452(4)	O54-C204	1.208(4)	N14-
C204	1.354(5)	N14-C184	1.394(5)	N14-
H1N4	0.89(4)	C14-C24	1.462(5)	C24-
C34	1.341(6)	C24-H2B4	0.9500	C34-
C224	1.503(5)	C34-C44	1.510(6)	C44-
C54	1.526(5)	C44-H4C4	0.9900	C44-
H4D4	0.9900	C54-C64	1.504(6)	C54-
H5A4	0.9900	C54-H5B4	0.9900	C64-
C74	1.319(5)	C64-H6A4	0.9500	C74-
C84	1.504(5)	C74-H7A4	0.9500	C84-
C164	1.529(5)	C84-C94	1.535(5)	C84-
H8A4	1.0000	C94-C134	1.510(5)	C94-
C104	1.528(5)	C94-H9A4	1.0000	C104-
C214	1.531(6)	C104-C114	1.549(6)	C104-
H10A4	1.0000	C114-C124	1.551(6)	C114-
H11A4	0.9900	C114-H11B4	0.9900	C124-
C134	1.533(6)	C124-H12C4	0.9900	C124-
H12D4	0.9900	C134-C144	1.524(5)	C134-
H13B4	1.0000	C144-C154	1.523(5)	C144-
H14C4	0.9900	C144-H14D4	0.9900	C154-
C164	1.353(5)	C164-C174	1.440(5)	C174-
C184	1.462(5)	C184-C194	1.362(5)	C194-
H19A4	0.9500	C214-H21A4	0.9800	C214-
H21G4	0.9800	C214-H21H4	0.9800	C224-
H22D4	0.9800	C224-H22E4	0.9800	C224-
H22F4	0.9800	C234-H23D4	0.9800	C234-
H23E4	0.9800	C234-H23F4	0.9800	

Symmetry transformations used to generate equivalent atoms:

Table S5. Bond angles [°] for **1**.

atom-atom-atom	angle	atom-atom-atom	angle	
C191-S11-C151	103.97(19)	C11-O11-H1O1	109.5	C201-
O41-C231	115.0(3)	C201-N11-C181	128.1(4)	C201-
N11-H1N1	114(3)	C181-N11-H1N1	118(3)	O21-
C11-O11	121.8(4)	O21-C11-C21	126.7(4)	O11-
C11-C21	111.5(3)	C31-C21-C11	125.5(4)	C31-
C21-H2A1	117.3	C11-C21-H2A1	117.3	C21-
C31-C41	125.8(4)	C21-C31-C221	119.8(4)	C41-
C31-C221	114.5(4)	C31-C41-C51	113.3(3)	C31-
C41-H4A1	108.9	C51-C41-H4A1	108.9	C31-
C41-H4B1	108.9	C51-C41-H4B1	108.9	
H4A1-C41-H4B1	107.7	C61-C51-C41	109.5(3)	C61-
C51-H5C1	109.8	C41-C51-H5C1	109.8	C61-
C51-H5D1	109.8	C41-C51-H5D1	109.8	H5C1-
C51-H5D1	108.2	C71-C61-C51	127.3(4)	C71-
C61-H6B1	116.4	C51-C61-H6B1	116.4	C61-
C71-C81	123.1(4)	C61-C71-H7B1	118.5	C81-
C71-H7B1	118.5	C71-C81-C91	112.4(3)	C71-
C81-C161	109.7(3)	C91-C81-C161	110.4(3)	C71-
C81-H8C1	108.1	C91-C81-H8C1	108.1	C161-
C81-H8C1	108.1	C131-C91-C101	103.0(3)	C131-
C91-C81	112.7(3)	C101-C91-C81	117.9(3)	C131-
C91-H9C1	107.6	C101-C91-H9C1	107.6	C81-
C91-H9C1	107.6	C211-C101-C91	114.7(4)	C211-
C101-C111	115.3(4)	C91-C101-C111	102.8(3)	C211-
C101-H10B1	107.9	C91-C101-H10B1	107.9	C111-
C101-H10B1	107.9	C101-C111-C121	107.1(3)	C101-
C111-H11C1	110.3	C121-C111-H11C1	110.3	C101-
C111-H11D1	110.3	C121-C111-H11D1	110.3	
H11C1-C111-H11D1	108.6	C111-C121-C131	104.6(3)	C111-
C121-H12A1	110.8	C131-C121-H12A1	110.8	C111-
C121-H12B1	110.8	C131-C121-H12B1	110.8	
H12A1-C121-H12B1	108.9	C141-C131-C91	109.9(3)	C141-
C131-C121	116.4(3)	C91-C131-C121	104.1(3)	C141-
C131-H13A1	108.7	C91-C131-H13A1	108.7	C121-
C131-H13A1	108.7	C131-C141-C151	110.6(3)	C131-
C141-H14A1	109.5	C151-C141-H14A1	109.5	C131-
C141-H14B1	109.5	C151-C141-H14B1	109.5	
H14A1-C141-H14B1	108.1	C161-C151-C141	123.8(4)	C161-
C151-S11	125.1(3)	C141-C151-S11	111.1(3)	C151-
C161-C171	121.9(4)	C151-C161-C81	122.1(3)	C171-
C161-C81	116.0(3)	O31-C171-C161	122.3(3)	O31-
C171-C181	117.0(3)	C161-C171-C181	120.6(3)	C191-

C181-N11	123.8(4)	C191-C181-C171	123.9(4)	N11-
C181-C171	112.2(3)	C181-C191-S11	124.3(3)	C181-
C191-H19C1	117.9	S11-C191-H19C1	117.9	O51-
C201-O41	124.5(4)	O51-C201-N11	125.2(4)	O41-
C201-N11	110.2(3)	C101-C211-H21B1	109.5	C101-
C211-H21E1	109.5	H21B1-C211-H21E1	109.5	C101-
C211-H21F1	109.5	H21B1-C211-H21F1	109.5	
H21E1-C211-H21F1	109.5	C31-C221-H22A1	109.5	C31-
C221-H22B1	109.5	H22A1-C221-H22B1	109.5	C31-
C221-H22C1	109.5	H22A1-C221-H22C1	109.5	
H22B1-C221-H22C1	109.5	O41-C231-H23A1	109.5	O41-
C231-H23B1	109.5	H23A1-C231-H23B1	109.5	O41-
C231-H23C1	109.5	H23A1-C231-H23C1	109.5	
H23B1-C231-H23C1	109.5	C192-S12-C152	103.7(2)	C12-
O12-H1O2	109.5	C202-O42-C232	113.9(3)	C202-
N12-C182	128.2(3)	C202-N12-H1N2	109(3)	C182-
N12-H1N2	123(3)	O22-C12-O12	121.7(3)	O22-
C12-C22	125.4(4)	O12-C12-C22	112.8(3)	C32-
C22-C12	125.0(4)	C32-C22-H2D2	117.5	C12-
C22-H2D2	117.5	C22-C32-C222	120.6(4)	C22-
C32-C42	124.5(4)	C222-C32-C42	114.8(4)	C32-
C42-C52	109.9(3)	C32-C42-H4G2	109.7	C52-
C42-H4G2	109.7	C32-C42-H4H2	109.7	C52-
C42-H4H2	109.7	H4G2-C42-H4H2	108.2	C62-
C52-C42	113.0(3)	C62-C52-H5G2	109.0	C42-
C52-H5G2	109.0	C62-C52-H5H2	109.0	C42-
C52-H5H2	109.0	H5G2-C52-H5H2	107.8	C72-
C62-C52	123.5(4)	C72-C62-H6D2	118.2	C52-
C62-H6D2	118.2	C62-C72-C82	127.6(4)	C62-
C72-H7D2	116.2	C82-C72-H7D2	116.2	C72-
C82-C162	112.0(3)	C72-C82-C92	112.0(3)	C162-
C82-C92	110.6(3)	C72-C82-H8D2	107.3	C162-
C82-H8D2	107.3	C92-C82-H8D2	107.3	C132-
C92-C102	103.7(3)	C132-C92-C82	112.0(3)	C102-
C92-C82	118.0(3)	C132-C92-H9D2	107.5	C102-
C92-H9D2	107.5	C82-C92-H9D2	107.5	C92-
C102-C212	113.3(4)	C92-C102-C112	102.2(3)	C212-
C102-C112	114.5(4)	C92-C102-H10D2	108.9	C212-
C102-H10D2	108.9	C112-C102-H10D2	108.9	C102-
C112-C122	106.1(3)	C102-C112-H11G2	110.5	C122-
C112-H11G2	110.5	C102-C112-H11H2	110.5	C122-
C112-H11H2	110.5	H11G2-C112-H11H2	108.7	C132-
C122-C112	105.4(3)	C132-C122-H12G2	110.7	C112-
C122-H12G2	110.7	C132-C122-H12H2	110.7	C112-
C122-H12H2	110.7	H12G2-C122-H12H2	108.8	C92-
C132-C142	109.1(3)	C92-C132-C122	103.6(3)	C142-

C132-C122	116.3(3)	C92-C132-H13D2	109.2	C142-
C132-H13D2	109.2	C122-C132-H13D2	109.2	C152-
C142-C132	110.8(3)	C152-C142-H14G2	109.5	C132-
C142-H14G2	109.5	C152-C142-H14H2	109.5	C132-
C142-H14H2	109.5	H14G2-C142-H14H2	108.1	C162-
C152-C142	123.4(4)	C162-C152-S12	125.1(3)	C142-
C152-S12	111.5(3)	C152-C162-C172	122.5(4)	C152-
C162-C82	122.4(4)	C172-C162-C82	115.1(3)	O32-
C172-C162	122.5(3)	O32-C172-C182	116.7(3)	C162-
C172-C182	120.8(3)	C192-C182-N12	125.9(4)	C192-
C182-C172	122.7(4)	N12-C182-C172	111.4(3)	C182-
C192-S12	125.3(3)	C182-C192-H19D2	117.4	S12-
C192-H19D2	117.4	O52-C202-O42	124.9(4)	O52-
C202-N12	125.3(4)	O42-C202-N12	109.9(3)	C102-
C212-H21J2	109.5	C102-C212-H21K2	109.5	
H21J2-C212-H21K2	109.5	C102-C212-H21L2	109.5	
H21J2-C212-H21L2	109.5	H21K2-C212-H21L2	109.5	C32-
C222-H22J2	109.5	C32-C222-H22K2	109.5	
H22J2-C222-H22K2	109.5	C32-C222-H22L2	109.5	
H22J2-C222-H22L2	109.5	H22K2-C222-H22L2	109.5	O42-
C232-H23J2	109.5	O42-C232-H23K2	109.5	
H23J2-C232-H23K2	109.5	O42-C232-H23L2	109.5	
H23J2-C232-H23L2	109.5	H23K2-C232-H23L2	109.5	C193-
S13-C153	104.0(2)	C13-O13-H1O3	109.5	C203-
O43-C233	115.2(4)	C203-N13-C183	126.7(4)	C203-
N13-H1N3	112(3)	C183-N13-H1N3	119(3)	O23-
C13-O13	121.8(4)	O23-C13-C23	125.7(4)	O13-
C13-C23	112.4(3)	C33-C23-C13	126.1(4)	C33-
C23-H2C3	117.0	C13-C23-H2C3	117.0	C23-
C33-C43	124.6(4)	C23-C33-C223	120.9(4)	C43-
C33-C223	114.4(4)	C33-C43-C53	111.6(3)	C33-
C43-H4E3	109.3	C53-C43-H4E3	109.3	C33-
C43-H4F3	109.3	C53-C43-H4F3	109.3	H4E3-
C43-H4F3	108.0	C63-C53-C43	109.3(3)	C63-
C53-H5E3	109.8	C43-C53-H5E3	109.8	C63-
C53-H5F3	109.8	C43-C53-H5F3	109.8	H5E3-
C53-H5F3	108.3	C73-C63-C53	125.5(4)	C73-
C63-H6C3	117.3	C53-C63-H6C3	117.3	C63-
C73-C83	123.3(4)	C63-C73-H7C3	118.4	C83-
C73-H7C3	118.4	C73-C83-C93	113.3(3)	C73-
C83-C163	109.4(3)	C93-C83-C163	109.9(3)	C73-
C83-H8B3	108.0	C93-C83-H8B3	108.0	C163-
C83-H8B3	108.0	C133-C93-C83	112.8(3)	C133-
C93-C103	103.2(3)	C83-C93-C103	117.6(3)	C133-
C93-H9B3	107.6	C83-C93-H9B3	107.6	C103-
C93-H9B3	107.6	C213-C103-C113	115.3(4)	C213-

C103-C93	112.9(4)	C113-C103-C93	102.6(3)	C213-
C103-H10C3	108.6	C113-C103-H10C3	108.6	C93-
C103-H10C3	108.6	C103-C113-C123	107.3(3)	C103-
C113-H11E3	110.3	C123-C113-H11E3	110.3	C103-
C113-H11F3	110.3	C123-C113-H11F3	110.3	
H11E3-C113-H11F3	108.5	C113-C123-C133	104.9(3)	C113-
C123-H12E3	110.8	C133-C123-H12E3	110.8	C113-
C123-H12F3	110.8	C133-C123-H12F3	110.8	
H12E3-C123-H12F3	108.8	C143-C133-C93	110.1(3)	C143-
C133-C123	117.1(3)	C93-C133-C123	103.4(3)	C143-
C133-H13C3	108.6	C93-C133-H13C3	108.6	C123-
C133-H13C3	108.6	C133-C143-C153	111.6(3)	C133-
C143-H14E3	109.3	C153-C143-H14E3	109.3	C133-
C143-H14F3	109.3	C153-C143-H14F3	109.3	
H14E3-C143-H14F3	108.0	C163-C153-C143	124.6(4)	C163-
C153-S13	124.5(3)	C143-C153-S13	110.9(3)	C153-
C163-C173	122.9(4)	C153-C163-C83	121.1(4)	C173-
C163-C83	116.0(3)	O33-C173-C163	122.6(3)	O33-
C173-C183	116.7(4)	C163-C173-C183	120.7(3)	C193-
C183-N13	123.8(4)	C193-C183-C173	123.6(4)	N13-
C183-C173	112.6(3)	C183-C193-S13	124.2(3)	C183-
C193-H19B3	117.9	S13-C193-H19B3	117.9	O53-
C203-O43	125.1(4)	O53-C203-N13	125.6(4)	O43-
C203-N13	109.2(4)	C103-C213-H21C3	109.5	C103-
C213-H21D3	109.5	H21C3-C213-H21D3	109.5	C103-
C213-H21I3	109.5	H21C3-C213-H21I3	109.5	
H21D3-C213-H21I3	109.5	C33-C223-H22G3	109.5	C33-
C223-H22H3	109.5	H22G3-C223-H22H3	109.5	C33-
C223-H22I3	109.5	H22G3-C223-H22I3	109.5	
H22H3-C223-H22I3	109.5	O43-C233-H23G3	109.5	O43-
C233-H23H3	109.5	H23G3-C233-H23H3	109.5	O43-
C233-H23I3	109.5	H23G3-C233-H23I3	109.5	
H23H3-C233-H23I3	109.5	C194-S14-C154	104.15(19)	C14-
O14-H1O4	109.5	C204-O44-C234	114.4(3)	C204-
N14-C184	127.4(3)	C204-N14-H1N4	118(3)	C184-
N14-H1N4	114(3)	O24-C14-O14	121.8(4)	O24-
C14-C24	126.6(4)	O14-C14-C24	111.6(3)	C34-
C24-C14	125.3(4)	C34-C24-H2B4	117.3	C14-
C24-H2B4	117.3	C24-C34-C224	121.5(4)	C24-
C34-C44	124.1(4)	C224-C34-C44	114.5(4)	C34-
C44-C54	112.0(3)	C34-C44-H4C4	109.2	C54-
C44-H4C4	109.2	C34-C44-H4D4	109.2	C54-
C44-H4D4	109.2	H4C4-C44-H4D4	107.9	C64-
C54-C44	109.5(3)	C64-C54-H5A4	109.8	C44-
C54-H5A4	109.8	C64-C54-H5B4	109.8	C44-
C54-H5B4	109.8	H5A4-C54-H5B4	108.2	C74-

C64-C54	124.8(4)	C74-C64-H6A4	117.6	C54-
C64-H6A4	117.6	C64-C74-C84	124.8(4)	C64-
C74-H7A4	117.6	C84-C74-H7A4	117.6	C74-
C84-C164	111.7(3)	C74-C84-C94	111.5(3)	C164-
C84-C94	108.9(3)	C74-C84-H8A4	108.2	C164-
C84-H8A4	108.2	C94-C84-H8A4	108.2	C134-
C94-C104	104.6(3)	C134-C94-C84	111.8(3)	C104-
C94-C84	117.9(3)	C134-C94-H9A4	107.4	C104-
C94-H9A4	107.4	C84-C94-H9A4	107.4	C94-
C104-C214	113.0(4)	C94-C104-C114	103.5(3)	C214-
C104-C114	114.8(4)	C94-C104-H10A4	108.4	C214-
C104-H10A4	108.4	C114-C104-H10A4	108.4	C104-
C114-C124	106.7(3)	C104-C114-H11A4	110.4	C124-
C114-H11A4	110.4	C104-C114-H11B4	110.4	C124-
C114-H11B4	110.4	H11A4-C114-H11B4	108.6	C134-
C124-C114	105.1(3)	C134-C124-H12C4	110.7	C114-
C124-H12C4	110.7	C134-C124-H12D4	110.7	C114-
C124-H12D4	110.7	H12C4-C124-H12D4	108.8	C94-
C134-C144	108.9(3)	C94-C134-C124	103.8(3)	C144-
C134-C124	116.4(3)	C94-C134-H13B4	109.2	C144-
C134-H13B4	109.2	C124-C134-H13B4	109.2	C154-
C144-C134	112.3(3)	C154-C144-H14C4	109.1	C134-
C144-H14C4	109.1	C154-C144-H14D4	109.1	C134-
C144-H14D4	109.1	H14C4-C144-H14D4	107.9	C164-
C154-C144	124.5(4)	C164-C154-S14	124.6(3)	C144-
C154-S14	110.8(3)	C154-C164-C174	122.9(4)	C154-
C164-C84	121.1(3)	C174-C164-C84	116.0(3)	O34-
C174-C164	122.9(3)	O34-C174-C184	116.4(3)	C164-
C174-C184	120.6(3)	C194-C184-N14	124.8(4)	C194-
C184-C174	123.0(3)	N14-C184-C174	112.3(3)	C184-
C194-S14	124.5(3)	C184-C194-H19A4	117.8	S14-
C194-H19A4	117.8	O54-C204-N14	127.0(4)	O54-
C204-O44	123.9(4)	N14-C204-O44	109.2(3)	C104-
C214-H21A4	109.5	C104-C214-H21G4	109.5	
H21A4-C214-H21G4	109.5	C104-C214-H21H4	109.5	
H21A4-C214-H21H4	109.5	H21G4-C214-H21H4	109.5	C34-
C224-H22D4	109.5	C34-C224-H22E4	109.5	
H22D4-C224-H22E4	109.5	C34-C224-H22F4	109.5	
H22D4-C224-H22F4	109.5	H22E4-C224-H22F4	109.5	O44-
C234-H23D4	109.5	O44-C234-H23E4	109.5	
H23D4-C234-H23E4	109.5	O44-C234-H23F4	109.5	
H23D4-C234-H23F4	109.5	H23E4-C234-H23F4	109.5	

Symmetry transformations used to generate equivalent atoms:

Table S6. Torsion angles [°] for **1**.

atom-atom-atom-atom	angle	atom-atom-atom-atom	angle	
O21-C11-C21-C31	-10.3(7)	O11-C11-C21-C31	171.2(4)	C11-
C21-C31-C41	-1.5(6)	C11-C21-C31-C221	177.2(4)	C21-
C31-C41-C51	90.5(5)	C221-C31-C41-C51	-88.2(4)	C31-
C41-C51-C61	163.7(4)	C41-C51-C61-C71	111.5(5)	C51-
C61-C71-C81	-177.7(4)	C61-C71-C81-C91	-103.9(4)	C61-
C71-C81-C161	132.9(4)	C71-C81-C91-C131	-77.8(4)	C161-
C81-C91-C131	44.9(4)	C71-C81-C91-C101	41.9(5)	C161-
C81-C91-C101	164.7(3)	C131-C91-C101-C211	-166.9(4)	C81-
C91-C101-C211	68.4(5)	C131-C91-C101-C111	-41.0(4)	C81-
C91-C101-C111	-165.7(4)	C211-C101-C111-C121	150.8(4)	C91-
C101-C111-C121	25.2(5)	C101-C111-C121-C131	-0.1(5)	C101-
C91-C131-C141	166.8(3)	C81-C91-C131-C141	-65.1(4)	C101-
C91-C131-C121	41.5(4)	C81-C91-C131-C121	169.6(3)	C111-
C121-C131-C141	-146.4(4)	C111-C121-C131-C91	-25.3(4)	C91-
C131-C141-C151	48.9(5)	C121-C131-C141-C151	166.9(3)	C131-
C141-C151-C161	-19.3(6)	C131-C141-C151-S11	161.7(3)	C191-
S11-C151-C161	2.1(4)	C191-S11-C151-C141	-178.9(3)	C141-
C151-C161-C171	-178.8(4)	S11-C151-C161-C171	0.2(6)	C141-
C151-C161-C81	1.3(6)	S11-C151-C161-C81	-179.8(3)	C71-
C81-C161-C151	110.6(4)	C91-C81-C161-C151	-13.8(5)	C71-
C81-C161-C171	-69.3(4)	C91-C81-C161-C171	166.3(3)	C151-
C161-C171-O31	178.4(4)	C81-C161-C171-O31	-1.7(6)	C151-
C161-C171-C181	-3.5(6)	C81-C161-C171-C181	176.4(4)	C201-
N11-C181-C191	8.4(7)	C201-N11-C181-C171	-170.8(4)	O31-
C171-C181-C191	-177.5(4)	C161-C171-C181-C191	4.4(6)	O31-
C171-C181-N11	1.7(5)	C161-C171-C181-N11	-176.4(4)	N11-
C181-C191-S11	179.2(3)	C171-C181-C191-S11	-1.7(6)	C151-
S11-C191-C181	-1.3(4)	C231-O41-C201-O51	3.8(6)	C231-
O41-C201-N11	-175.7(4)	C181-N11-C201-O51	2.9(7)	C181-
N11-C201-O41	-177.6(4)	O22-C12-C22-C32	9.4(7)	O12-
C12-C22-C32	-168.8(4)	C12-C22-C32-C222	177.1(4)	C12-
C22-C32-C42	-5.9(6)	C22-C32-C42-C52	-80.4(5)	C222-
C32-C42-C52	96.7(4)	C32-C42-C52-C62	173.0(4)	C42-
C52-C62-C72	100.0(5)	C52-C62-C72-C82	-179.8(4)	C62-
C72-C82-C162	-31.1(6)	C62-C72-C82-C92	93.8(5)	C72-
C82-C92-C132	-78.9(4)	C162-C82-C92-C132	46.8(4)	C72-
C82-C92-C102	41.4(5)	C162-C82-C92-C102	167.1(4)	C132-
C92-C102-C212	-166.1(3)	C82-C92-C102-C212	69.3(5)	C132-
C92-C102-C112	-42.5(4)	C82-C92-C102-C112	-167.0(4)	C92-
C102-C112-C122	26.9(5)	C212-C102-C112-C122	149.7(4)	C102-
C112-C122-C132	-1.9(5)	C102-C92-C132-C142	166.2(3)	C82-
C92-C132-C142	-65.5(4)	C102-C92-C132-C122	41.7(4)	C82-

C92-C132-C122	170.0(3)	C112-C122-C132-C92	-24.1(5)	C112-
C122-C132-C142	-143.8(4)	C92-C132-C142-C152	49.0(5)	C122-
C132-C142-C152	165.7(4)	C132-C142-C152-C162	-19.3(6)	C132-
C142-C152-S12	162.4(3)	C192-S12-C152-C162	0.0(4)	C192-
S12-C152-C142	178.3(3)	C142-C152-C162-C172	-179.1(4)	S12-
C152-C162-C172	-1.0(6)	C142-C152-C162-C82	2.3(6)	S12-
C152-C162-C82	-179.6(3)	C72-C82-C162-C152	110.3(4)	C92-
C82-C162-C152	-15.4(5)	C72-C82-C162-C172	-68.4(4)	C92-
C82-C162-C172	165.9(3)	C152-C162-C172-O32	-179.0(4)	C82-
C162-C172-O32	-0.3(5)	C152-C162-C172-C182	1.3(6)	C82-
C162-C172-C182	-180.0(3)	C202-N12-C182-C192	-8.8(7)	C202-
N12-C182-C172	171.9(4)	O32-C172-C182-C192	179.7(4)	C162-
C172-C182-C192	-0.6(6)	O32-C172-C182-N12	-0.9(5)	C162-
C172-C182-N12	178.8(4)	N12-C182-C192-S12	-179.8(3)	C172-
C182-C192-S12	-0.5(6)	C152-S12-C192-C182	0.7(4)	C232-
O42-C202-O52	0.2(6)	C232-O42-C202-N12	-179.6(3)	C182-
N12-C202-O52	5.6(7)	C182-N12-C202-O42	-174.5(4)	O23-
C13-C23-C33	-14.7(7)	O13-C13-C23-C33	167.7(4)	C13-
C23-C33-C43	-0.8(6)	C13-C23-C33-C223	176.0(4)	C23-
C33-C43-C53	90.6(5)	C223-C33-C43-C53	-86.3(4)	C33-
C43-C53-C63	171.2(4)	C43-C53-C63-C73	109.9(5)	C53-
C63-C73-C83	-175.7(4)	C63-C73-C83-C93	-107.2(4)	C63-
C73-C83-C163	129.8(4)	C73-C83-C93-C133	-73.4(4)	C163-
C83-C93-C133	49.2(4)	C73-C83-C93-C103	46.5(5)	C163-
C83-C93-C103	169.1(3)	C133-C93-C103-C213	-165.8(4)	C83-
C93-C103-C213	69.3(5)	C133-C93-C103-C113	-41.1(4)	C83-
C93-C103-C113	-166.0(4)	C213-C103-C113-C123	147.6(4)	C93-
C103-C113-C123	24.5(5)	C103-C113-C123-C133	0.8(5)	C83-
C93-C133-C143	-64.3(4)	C103-C93-C133-C143	167.8(3)	C83-
C93-C133-C123	169.9(3)	C103-C93-C133-C123	42.0(4)	C113-
C123-C133-C143	-147.5(4)	C113-C123-C133-C93	-26.2(5)	C93-
C133-C143-C153	44.1(5)	C123-C133-C143-C153	161.7(4)	C133-
C143-C153-C163	-15.2(6)	C133-C143-C153-S13	165.1(3)	C193-
S13-C153-C163	-1.9(4)	C193-S13-C153-C143	177.8(3)	C143-
C153-C163-C173	-177.3(4)	S13-C153-C163-C173	2.4(6)	C143-
C153-C163-C83	2.1(6)	S13-C153-C163-C83	-178.2(3)	C73-
C83-C163-C153	106.4(4)	C93-C83-C163-C153	-18.5(5)	C73-
C83-C163-C173	-74.1(4)	C93-C83-C163-C173	161.0(3)	C153-
C163-C173-O33	-179.6(4)	C83-C163-C173-O33	0.9(6)	C153-
C163-C173-C183	-1.9(6)	C83-C163-C173-C183	178.6(4)	C203-
N13-C183-C193	19.5(7)	C203-N13-C183-C173	-159.8(4)	O33-
C173-C183-C193	179.1(4)	C163-C173-C183-C193	1.2(6)	O33-
C173-C183-N13	-1.5(5)	C163-C173-C183-N13	-179.4(4)	N13-
C183-C193-S13	179.6(3)	C173-C183-C193-S13	-1.1(6)	C153-
S13-C193-C183	1.3(5)	C233-O43-C203-O53	2.5(6)	C233-
O43-C203-N13	-177.9(4)	C183-N13-C203-O53	0.9(7)	C183-

N13-C203-O43	-178.7(4)	O24-C14-C24-C34	-4.3(7)	O14-
C14-C24-C34	177.9(4)	C14-C24-C34-C224	172.5(4)	C14-
C24-C34-C44	-6.8(6)	C24-C34-C44-C54	91.8(5)	C224-
C34-C44-C54	-87.5(4)	C34-C44-C54-C64	-176.4(3)	C44-
C54-C64-C74	114.4(4)	C54-C64-C74-C84	179.4(4)	C64-
C74-C84-C164	144.6(4)	C64-C74-C84-C94	-93.3(5)	C74-
C84-C94-C134	-69.7(4)	C164-C84-C94-C134	54.0(4)	C74-
C84-C94-C104	51.5(5)	C164-C84-C94-C104	175.2(3)	C134-
C94-C104-C214	-160.9(3)	C84-C94-C104-C214	74.2(5)	C134-
C94-C104-C114	-36.1(4)	C84-C94-C104-C114	-161.0(4)	C94-
C104-C114-C124	17.7(5)	C214-C104-C114-C124	141.3(4)	C104-
C114-C124-C134	6.8(5)	C104-C94-C134-C144	165.5(3)	C84-
C94-C134-C144	-65.9(4)	C104-C94-C134-C124	40.9(4)	C84-
C94-C134-C124	169.5(3)	C114-C124-C134-C94	-29.0(5)	C114-
C124-C134-C144	-148.6(4)	C94-C134-C144-C154	42.5(5)	C124-
C134-C144-C154	159.4(4)	C134-C144-C154-C164	-12.7(6)	C134-
C144-C154-S14	169.1(3)	C194-S14-C154-C164	-2.2(4)	C194-
S14-C154-C144	175.9(3)	C144-C154-C164-C174	-178.8(4)	S14-
C154-C164-C174	-0.8(6)	C144-C154-C164-C84	2.3(6)	S14-
C154-C164-C84	-179.8(3)	C74-C84-C164-C154	101.6(4)	C94-
C84-C164-C154	-22.0(5)	C74-C84-C164-C174	-77.4(4)	C94-
C84-C164-C174	159.0(3)	C154-C164-C174-O34	-176.1(4)	C84-
C164-C174-O34	2.9(6)	C154-C164-C174-C184	5.0(6)	C84-
C164-C174-C184	-176.1(3)	C204-N14-C184-C194	4.3(7)	C204-
N14-C184-C174	-176.9(4)	O34-C174-C184-C194	175.4(4)	C164-
C174-C184-C194	-5.6(6)	O34-C174-C184-N14	-3.3(5)	C164-
C174-C184-N14	175.6(3)	N14-C184-C194-S14	-179.4(3)	C174-
C184-C194-S14	2.0(6)	C154-S14-C194-C184	1.6(4)	C184-
N14-C204-O54	-3.0(7)	C184-N14-C204-O44	176.6(4)	C234-
O44-C204-O54	-4.3(6)	C234-O44-C204-N14	176.1(3)	

Symmetry transformations used to generate equivalent atoms:

Table S7. Anisotropic displacement parameters $(Å)^2$ for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S11	0.0363(6)	0.0273(6)	0.0492(7)	-0.0126(5)	-0.0125(5)	0.0008(4)
O11	0.0345(15)	0.0273(15)	0.0434(18)	-0.0126(13)	-0.0079(13)	-0.0042(12)
O21	0.0447(18)	0.0271(16)	0.058(2)	-0.0062(14)	-0.0219(15)	0.0008(13)
O31	0.0285(15)	0.0244(15)	0.057(2)	-0.0138(13)	-0.0091(13)	0.0004(12)
O41	0.0338(17)	0.0327(17)	0.073(2)	-0.0123(16)	-0.0133(15)	-0.0092(13)
O51	0.0439(18)	0.0323(17)	0.055(2)	0.0009(15)	-0.0219(15)	-0.0100(14)
N11	0.031(2)	0.0221(19)	0.065(3)	-0.0095(18)	-0.0132(18)	-0.0072(15)
C11	0.032(2)	0.028(2)	0.041(3)	-0.0057(19)	-0.0070(19)	-0.0112(18)
C21	0.0230(19)	0.025(2)	0.039(2)	-0.0031(17)	-0.0049(17)	-0.0049(15)
C31	0.024(2)	0.032(2)	0.039(3)	-0.0067(19)	-0.0049(17)	-0.0054(17)
C41	0.029(2)	0.037(2)	0.035(2)	-0.0005(19)	-0.0105(17)	-0.0109(17)
C51	0.029(2)	0.038(2)	0.036(2)	-0.0007(19)	-0.0097(18)	-0.0096(17)
C61	0.032(2)	0.037(2)	0.032(2)	-0.0060(18)	-0.0106(18)	-0.0119(18)
C71	0.028(2)	0.031(2)	0.041(3)	-0.0108(19)	-0.0058(18)	-0.0082(17)
C81	0.026(2)	0.027(2)	0.036(2)	-0.0086(18)	-0.0061(17)	-0.0047(16)
C91	0.033(2)	0.030(2)	0.028(2)	-0.0074(17)	-0.0081(17)	-0.0075(17)
C101	0.037(2)	0.035(2)	0.042(3)	-0.001(2)	-0.0156(19)	-0.0154(19)
C111	0.040(3)	0.043(3)	0.059(3)	-0.006(2)	-0.013(2)	-0.019(2)
C121	0.036(2)	0.056(3)	0.040(3)	-0.018(2)	-0.006(2)	-0.017(2)
C131	0.031(2)	0.043(3)	0.029(2)	-0.0115(19)	-0.0053(18)	-0.0115(18)
C141	0.034(2)	0.040(3)	0.045(3)	-0.016(2)	-0.010(2)	-0.0010(19)
C151	0.032(2)	0.028(2)	0.036(3)	-0.0101(18)	-0.0086(18)	-0.0040(17)
C161	0.031(2)	0.029(2)	0.027(2)	-0.0106(17)	-0.0095(17)	-0.0014(17)
C171	0.031(2)	0.025(2)	0.035(2)	-0.0088(17)	-0.0096(17)	-0.0069(17)
C181	0.040(2)	0.025(2)	0.039(3)	-0.0111(18)	-0.0118(19)	-0.0040(18)
C191	0.034(2)	0.027(2)	0.043(3)	-0.0150(19)	-0.0073(19)	-0.0032(17)
C201	0.038(2)	0.034(2)	0.038(3)	-0.014(2)	-0.0111(19)	-0.0096(19)
C211	0.055(3)	0.032(3)	0.095(4)	-0.015(3)	-0.028(3)	-0.010(2)
C221	0.039(2)	0.042(3)	0.040(3)	-0.014(2)	-0.010(2)	-0.0043(19)
C231	0.041(3)	0.040(3)	0.067(4)	-0.012(2)	-0.008(2)	-0.020(2)
S12	0.0357(6)	0.0286(6)	0.0488(7)	-0.0023(5)	-0.0172(5)	-0.0041(4)

O12	0.0420(17)	0.0280(15)	0.0340(17)	-0.0046(12)	-0.0084(13)	-0.0026(12)
O22	0.0569(19)	0.0242(15)	0.0418(18)	-0.0131(13)	-0.0112(14)	0.0032(13)
O32	0.0334(15)	0.0238(14)	0.0397(17)	-0.0017(12)	-0.0112(13)	-0.0064(12)
O42	0.0283(14)	0.0263(14)	0.0390(17)	-0.0059(12)	-0.0065(12)	-0.0088(11)
O52	0.0365(16)	0.0307(16)	0.0395(18)	0.0009(13)	-0.0147(13)	-0.0084(12)
N12	0.0265(18)	0.0206(17)	0.049(2)	-0.0006(16)	-0.0125(16)	-0.0062(14)
C12	0.035(2)	0.023(2)	0.037(3)	-0.0087(18)	-0.0125(19)	-0.0037(17)
C22	0.033(2)	0.023(2)	0.032(2)	-0.0097(17)	-0.0080(18)	-0.0055(17)
C32	0.033(2)	0.024(2)	0.041(3)	-0.0095(18)	-0.0117(18)	-0.0081(16)
C42	0.037(2)	0.036(2)	0.037(3)	-0.0155(19)	-0.0072(18)	-0.0105(18)
C52	0.039(2)	0.049(3)	0.042(3)	-0.024(2)	-0.007(2)	-0.010(2)
C62	0.034(2)	0.035(2)	0.041(3)	-0.016(2)	-0.0098(19)	-0.0020(18)
C72	0.031(2)	0.025(2)	0.035(3)	-0.0057(17)	-0.0118(18)	-0.0059(16)
C82	0.032(2)	0.024(2)	0.028(2)	-0.0053(17)	-0.0058(17)	-0.0087(16)
C92	0.030(2)	0.029(2)	0.037(2)	-0.0110(18)	-0.0073(18)	-0.0072(17)
C102	0.037(2)	0.027(2)	0.045(3)	-0.0034(19)	-0.0035(19)	-0.0150(18)
C112	0.042(3)	0.045(3)	0.055(3)	0.000(2)	-0.011(2)	-0.024(2)
C122	0.042(3)	0.045(3)	0.067(4)	0.000(3)	-0.017(2)	-0.019(2)
C132	0.036(2)	0.035(2)	0.039(3)	-0.0056(19)	-0.0096(19)	-0.0157(18)
C142	0.035(2)	0.036(2)	0.044(3)	-0.004(2)	-0.010(2)	-0.0133(19)
C152	0.034(2)	0.030(2)	0.024(2)	-0.0055(17)	-0.0097(17)	-0.0029(17)
C162	0.035(2)	0.023(2)	0.027(2)	-0.0066(16)	-0.0083(17)	-0.0083(16)
C172	0.030(2)	0.026(2)	0.030(2)	-0.0074(17)	-0.0101(17)	-0.0025(17)
C182	0.032(2)	0.025(2)	0.034(2)	-0.0059(17)	-0.0076(17)	-0.0098(16)
C192	0.040(2)	0.028(2)	0.043(3)	-0.0066(19)	-0.018(2)	-0.0046(18)
C202	0.028(2)	0.031(2)	0.027(2)	-0.0118(18)	-0.0049(17)	-0.0057(17)
C212	0.044(3)	0.034(2)	0.055(3)	-0.003(2)	-0.009(2)	-0.012(2)
C222	0.048(3)	0.028(2)	0.041(3)	-0.0029(19)	-0.019(2)	-0.0059(19)
C232	0.039(2)	0.034(2)	0.040(3)	-0.0027(19)	-0.0041(19)	-0.0185(19)
S13	0.0373(6)	0.0276(6)	0.0555(8)	-0.0147(5)	-0.0115(5)	0.0016(4)
O13	0.0383(16)	0.0298(16)	0.051(2)	-0.0139(14)	-0.0134(14)	0.0023(13)
O23	0.0518(19)	0.0297(17)	0.066(2)	-0.0054(16)	-0.0289(17)	0.0077(14)
O33	0.0306(15)	0.0248(15)	0.0498(19)	-0.0128(13)	-0.0082(13)	-0.0020(12)
O43	0.0393(17)	0.0441(18)	0.055(2)	-0.0154(15)	0.0000(15)	-0.0204(14)
O53	0.058(2)	0.0339(18)	0.050(2)	-0.0038(15)	-0.0097(16)	-0.0131(15)
N13	0.031(2)	0.0246(19)	0.060(3)	-0.0114(18)	-0.0051(17)	-0.0085(15)

C13	0.034(2)	0.024(2)	0.041(3)	-0.0036(18)	-0.0072(19)	-0.0090(17)
C23	0.027(2)	0.028(2)	0.042(3)	-0.0037(19)	-0.0104(18)	-0.0026(16)
C33	0.025(2)	0.025(2)	0.043(3)	-0.0038(18)	-0.0083(18)	-0.0068(16)
C43	0.029(2)	0.038(2)	0.043(3)	0.001(2)	-0.0120(18)	-0.0119(18)
C53	0.035(2)	0.043(3)	0.034(2)	0.0030(19)	-0.0128(19)	-0.0140(19)
C63	0.029(2)	0.034(2)	0.038(2)	-0.0077(19)	-0.0110(18)	-0.0109(17)
C73	0.027(2)	0.036(2)	0.030(2)	-0.0099(18)	-0.0078(17)	-0.0085(17)
C83	0.028(2)	0.029(2)	0.030(2)	-0.0076(17)	-0.0075(17)	-0.0041(16)
C93	0.028(2)	0.032(2)	0.035(2)	-0.0089(18)	-0.0120(17)	-0.0056(16)
C103	0.042(2)	0.034(2)	0.041(3)	-0.0047(19)	-0.016(2)	-0.0151(19)
C113	0.036(2)	0.050(3)	0.071(4)	-0.010(3)	-0.013(2)	-0.020(2)
C123	0.030(2)	0.055(3)	0.061(3)	-0.020(2)	-0.012(2)	-0.010(2)
C133	0.031(2)	0.041(3)	0.039(3)	-0.012(2)	-0.0099(18)	-0.0057(18)
C143	0.027(2)	0.042(3)	0.064(3)	-0.024(2)	-0.012(2)	0.0005(19)
C153	0.032(2)	0.028(2)	0.040(3)	-0.0134(18)	-0.0079(18)	-0.0029(17)
C163	0.031(2)	0.029(2)	0.029(2)	-0.0116(18)	-0.0053(17)	-0.0046(17)
C173	0.036(2)	0.022(2)	0.035(2)	-0.0119(17)	-0.0048(18)	-0.0068(17)
C183	0.034(2)	0.028(2)	0.038(3)	-0.0128(19)	-0.0062(19)	-0.0064(18)
C193	0.042(3)	0.026(2)	0.044(3)	-0.0140(19)	-0.006(2)	-0.0077(18)
C203	0.044(3)	0.038(3)	0.035(3)	-0.018(2)	-0.002(2)	-0.013(2)
C213	0.049(3)	0.043(3)	0.072(4)	-0.019(3)	-0.022(2)	-0.014(2)
C223	0.033(2)	0.039(3)	0.052(3)	-0.018(2)	-0.017(2)	-0.0007(18)
C233	0.065(3)	0.050(3)	0.055(3)	-0.014(2)	0.004(3)	-0.033(3)
S14	0.0296(6)	0.0266(6)	0.0522(8)	-0.0019(5)	-0.0130(5)	-0.0016(4)
O14	0.0443(17)	0.0262(15)	0.0409(19)	-0.0020(13)	-0.0141(14)	-0.0044(12)
O24	0.078(2)	0.0235(16)	0.050(2)	-0.0140(15)	-0.0078(17)	-0.0022(15)
O34	0.0277(14)	0.0249(14)	0.0377(17)	-0.0014(12)	-0.0082(12)	-0.0040(11)
O44	0.0307(15)	0.0240(15)	0.054(2)	-0.0043(13)	-0.0121(13)	-0.0079(12)
O54	0.0331(15)	0.0228(15)	0.0476(19)	-0.0041(13)	-0.0130(13)	-0.0024(12)
N14	0.0291(19)	0.0210(18)	0.045(2)	-0.0046(16)	-0.0097(16)	-0.0050(14)
C14	0.035(2)	0.024(2)	0.041(3)	-0.0045(19)	-0.0130(19)	-0.0048(17)
C24	0.037(2)	0.017(2)	0.044(3)	-0.0096(18)	-0.010(2)	-0.0006(17)
C34	0.030(2)	0.023(2)	0.045(3)	-0.0072(18)	-0.0119(18)	-0.0020(16)
C44	0.028(2)	0.029(2)	0.045(3)	-0.0138(19)	-0.0099(18)	-0.0036(16)
C54	0.033(2)	0.032(2)	0.043(3)	-0.0106(19)	-0.0075(19)	-0.0101(17)
C64	0.037(2)	0.028(2)	0.038(3)	-0.0091(18)	-0.0085(18)	-0.0072(17)

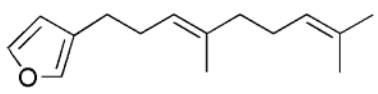
C74	0.029(2)	0.031(2)	0.030(2)	-0.0077(17)	-0.0051(17)	-0.0051(16)
C84	0.026(2)	0.024(2)	0.026(2)	-0.0039(16)	-0.0069(16)	-0.0033(16)
C94	0.031(2)	0.031(2)	0.030(2)	-0.0087(18)	-0.0009(17)	-0.0068(17)
C104	0.034(2)	0.032(2)	0.041(3)	-0.0080(19)	0.0012(19)	-0.0125(18)
C114	0.037(2)	0.039(3)	0.064(3)	-0.005(2)	0.001(2)	-0.016(2)
C124	0.037(3)	0.050(3)	0.054(3)	-0.008(2)	-0.007(2)	-0.017(2)
C134	0.029(2)	0.036(2)	0.034(2)	-0.0095(19)	-0.0024(18)	-0.0083(17)
C144	0.025(2)	0.033(2)	0.051(3)	-0.007(2)	-0.0120(19)	-0.0006(17)
C154	0.035(2)	0.028(2)	0.032(2)	-0.0053(18)	-0.0088(18)	-0.0047(17)
C164	0.031(2)	0.028(2)	0.026(2)	-0.0064(17)	-0.0063(16)	-0.0089(17)
C174	0.030(2)	0.024(2)	0.030(2)	-0.0058(17)	-0.0061(17)	-0.0039(17)
C184	0.026(2)	0.027(2)	0.030(2)	-0.0079(17)	-0.0044(17)	-0.0062(16)
C194	0.035(2)	0.027(2)	0.033(2)	-0.0043(18)	-0.0101(18)	-0.0061(17)
C204	0.031(2)	0.030(2)	0.025(2)	-0.0077(17)	-0.0049(17)	-0.0053(17)
C214	0.046(3)	0.046(3)	0.054(3)	0.007(2)	-0.004(2)	-0.014(2)
C224	0.046(3)	0.022(2)	0.045(3)	-0.0043(19)	-0.010(2)	-0.0066(18)
C234	0.035(2)	0.029(2)	0.046(3)	-0.0077(19)	-0.0074(19)	-0.0134(18)

Table S8. Hydrogen bonds for **1** [Å and °].

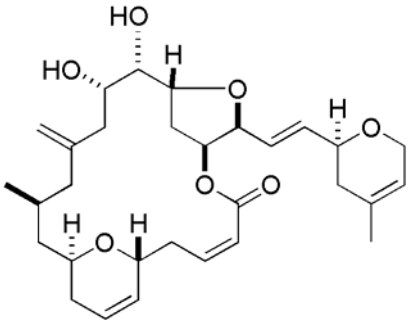
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O11-H1O1...O33	0.84	1.89	2.704(4)	162.1
O12-H1O2...O34	0.84	1.87	2.708(4)	179.1
O13-H1O3...O31#1	0.84	1.87	2.710(4)	174.3
O14-H1O4...O32#1	0.84	1.92	2.757(4)	176.0

Symmetry transformations used to generate equivalent atoms:
#1 x,y,z-1

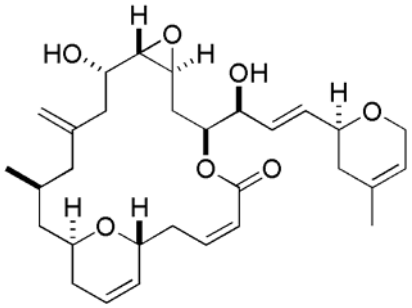
Figure S1. Structures of dendrolasen, fijianolide A, B, latrunculin A, B, latrunculeic acid and mycothiazole.



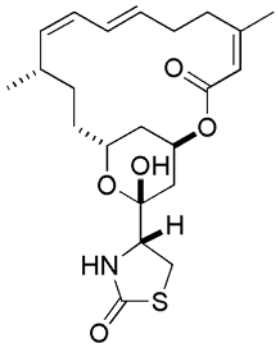
dendrolasen



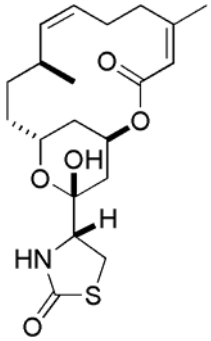
fijianolide A



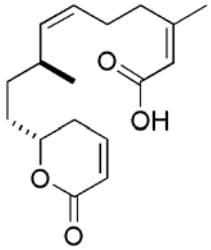
fijianolide B



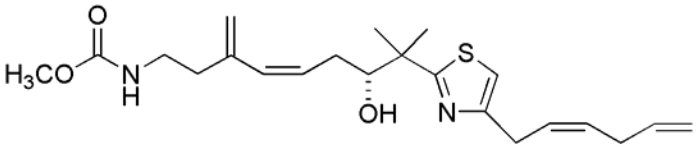
latrunculin A



latrunculin B



latrunculeic acid



mycothiazole

Figure S2. ^{1}H NMR spectrum of mycothiazole, (500 MHz, $CDCl_3$)

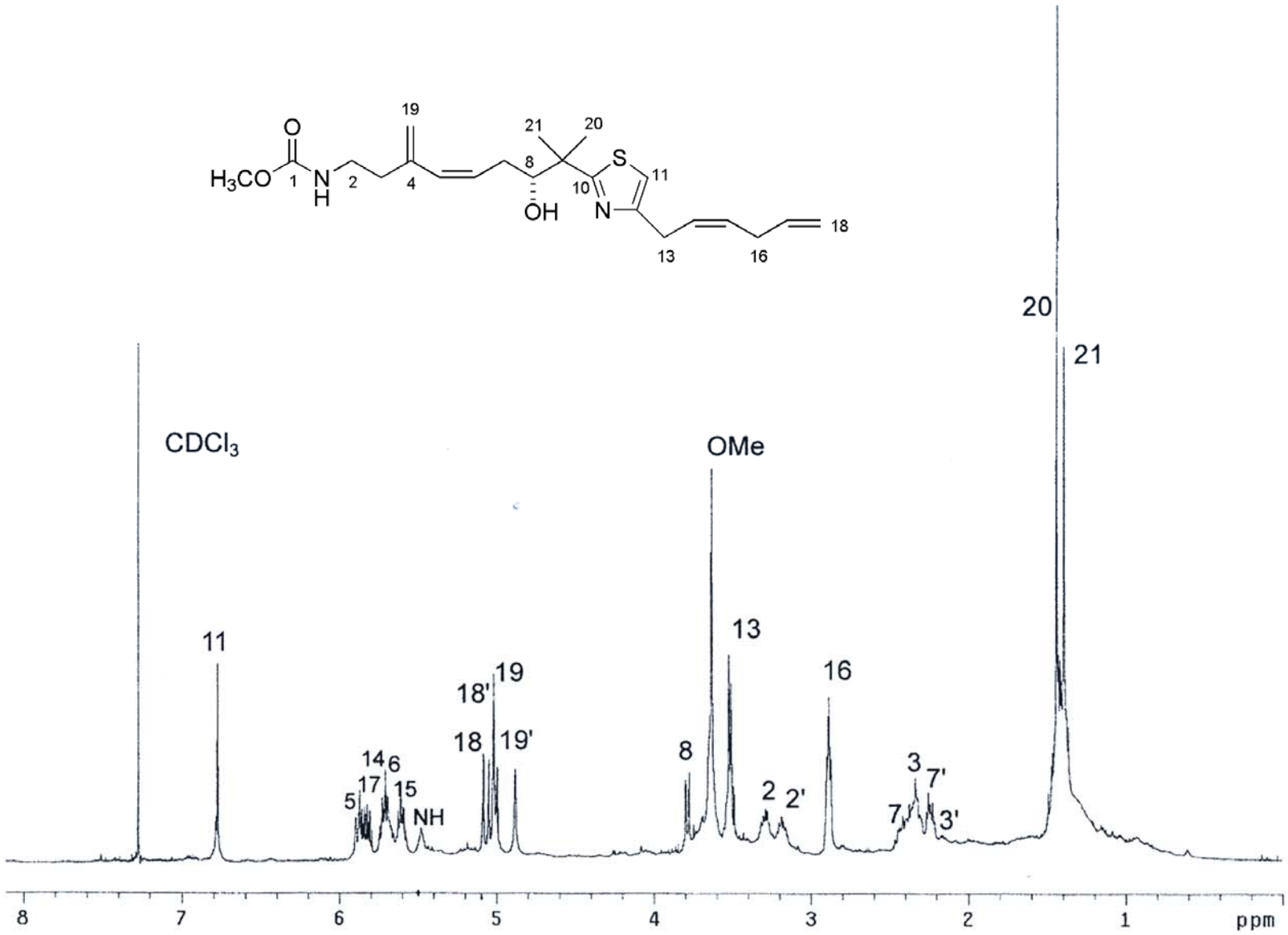


Figure S3. ^{13}C NMR spectrum of mycothiazole, (125 MHz, $CDCl_3$)

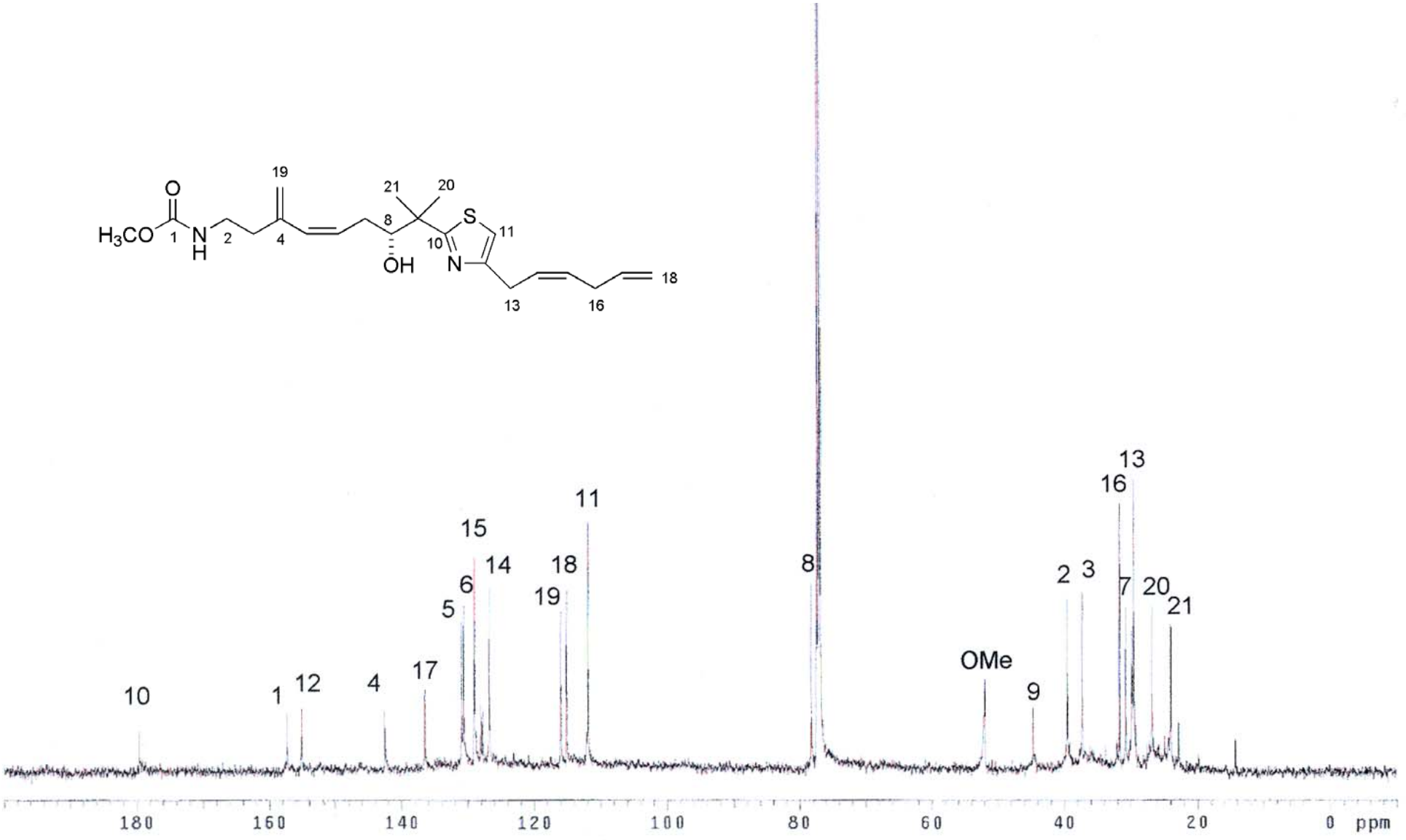


Figure S4. ^{1}H NMR spectrum of CTP-431 (**1**), (600 MHz, C_6D_6)

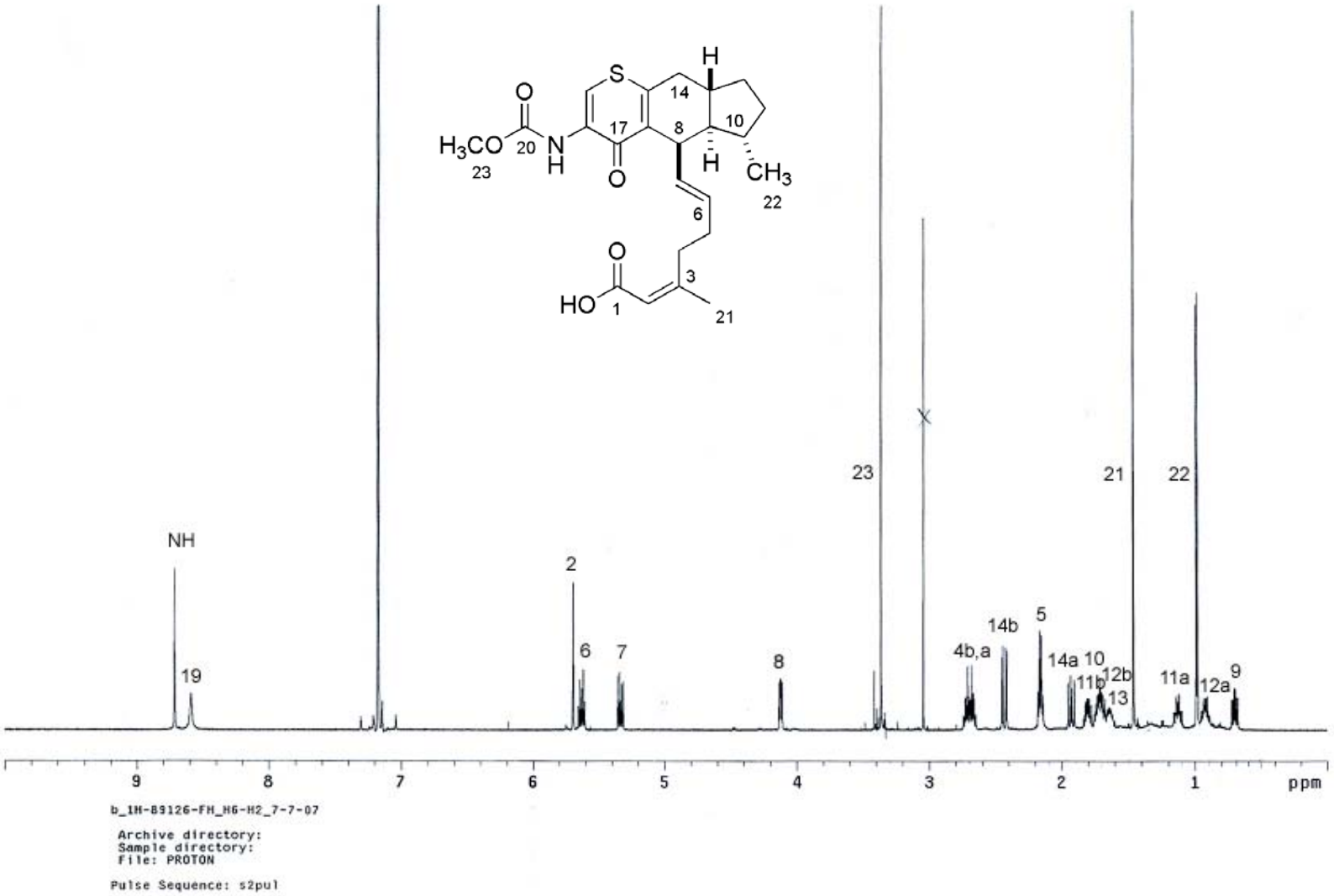


Figure S5. ^{13}C NMR spectrum of CTP-431 (**1**), (125 MHz, C_6D_6)

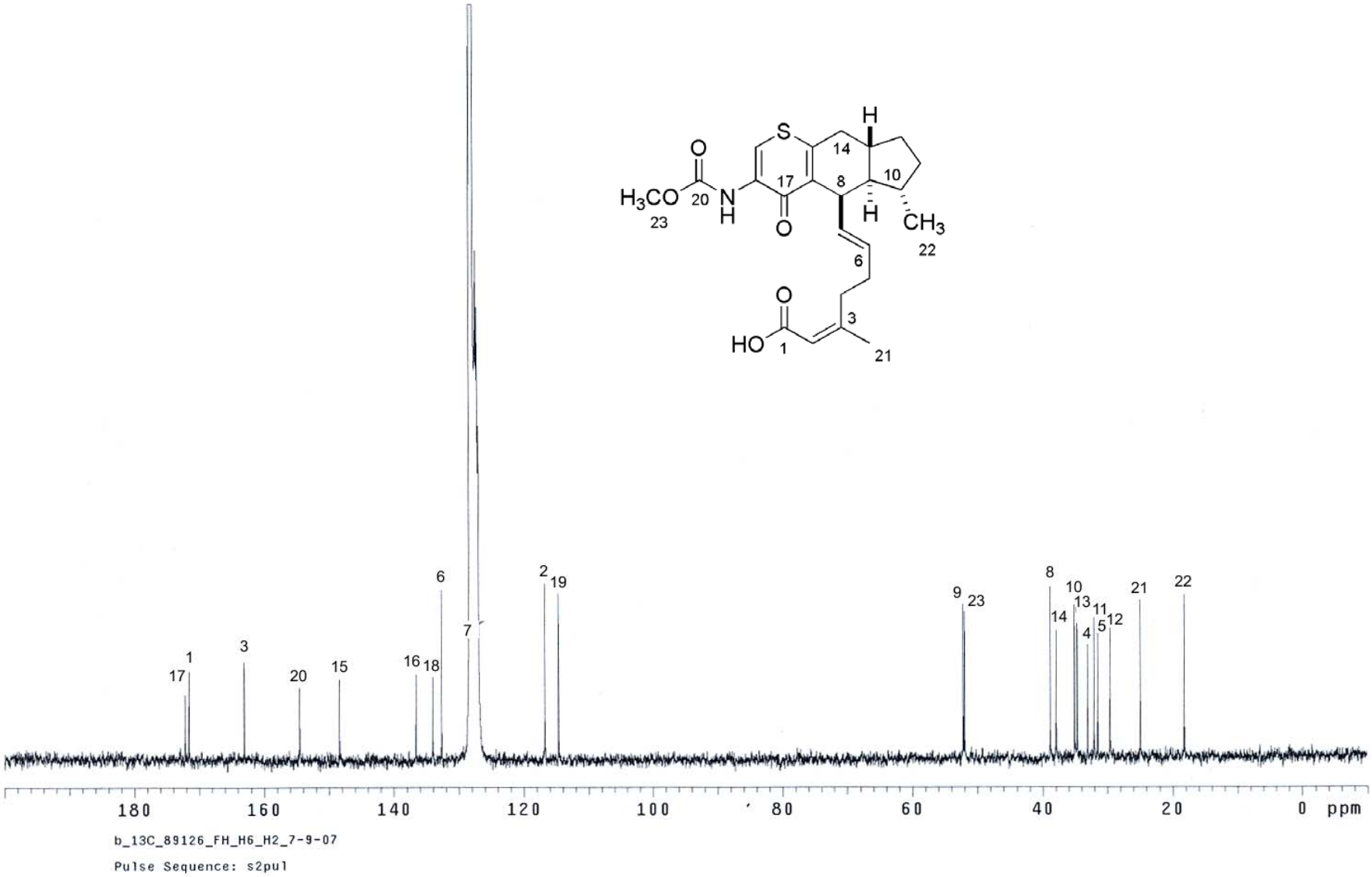


Figure S6. COSY spectrum of CTP-431 (**1**), (600 MHz, C_6D_6)

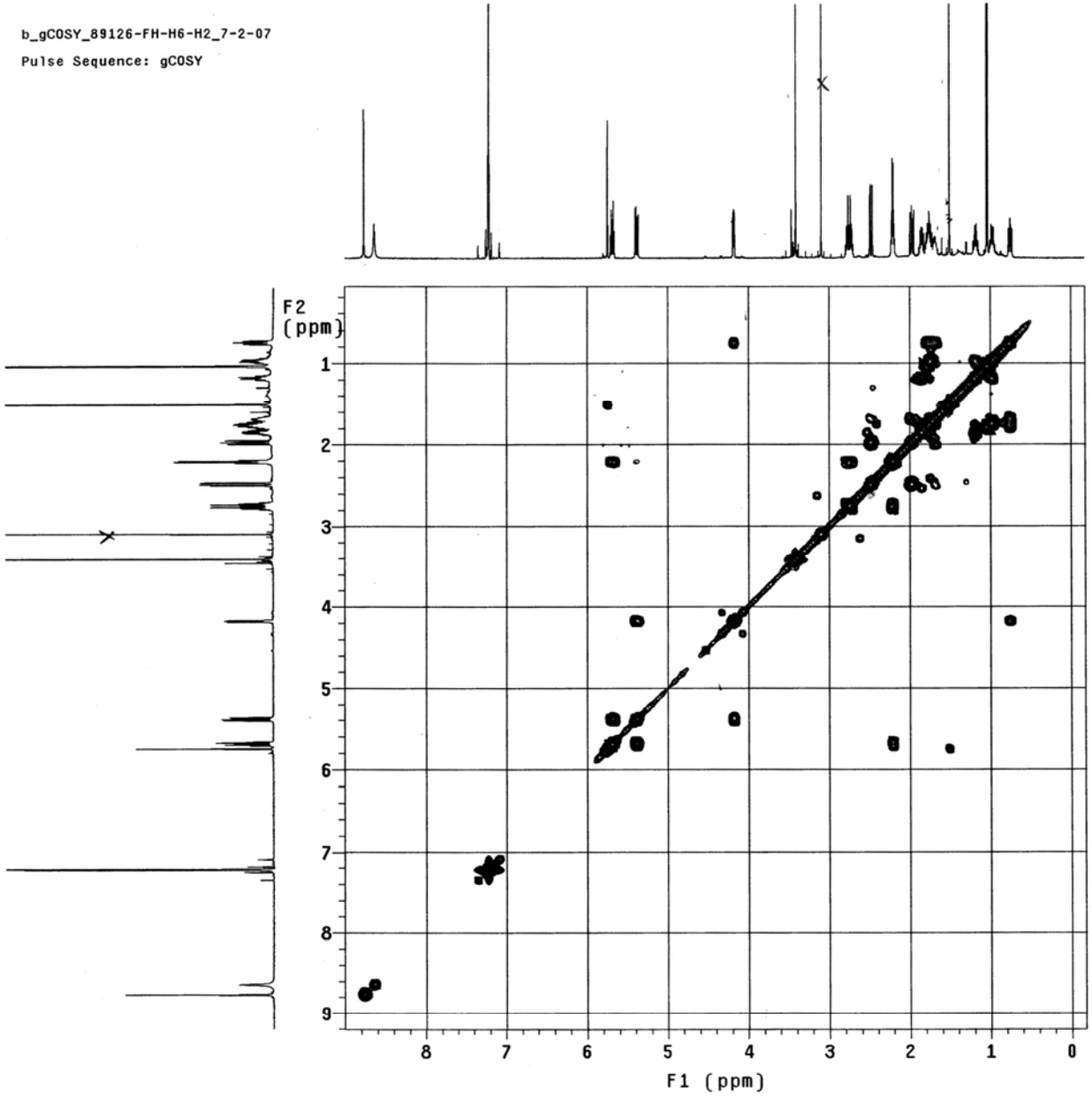


Figure S7. HMQC spectrum of CTP-431 (**1**), (600 MHz, C_6D_6)

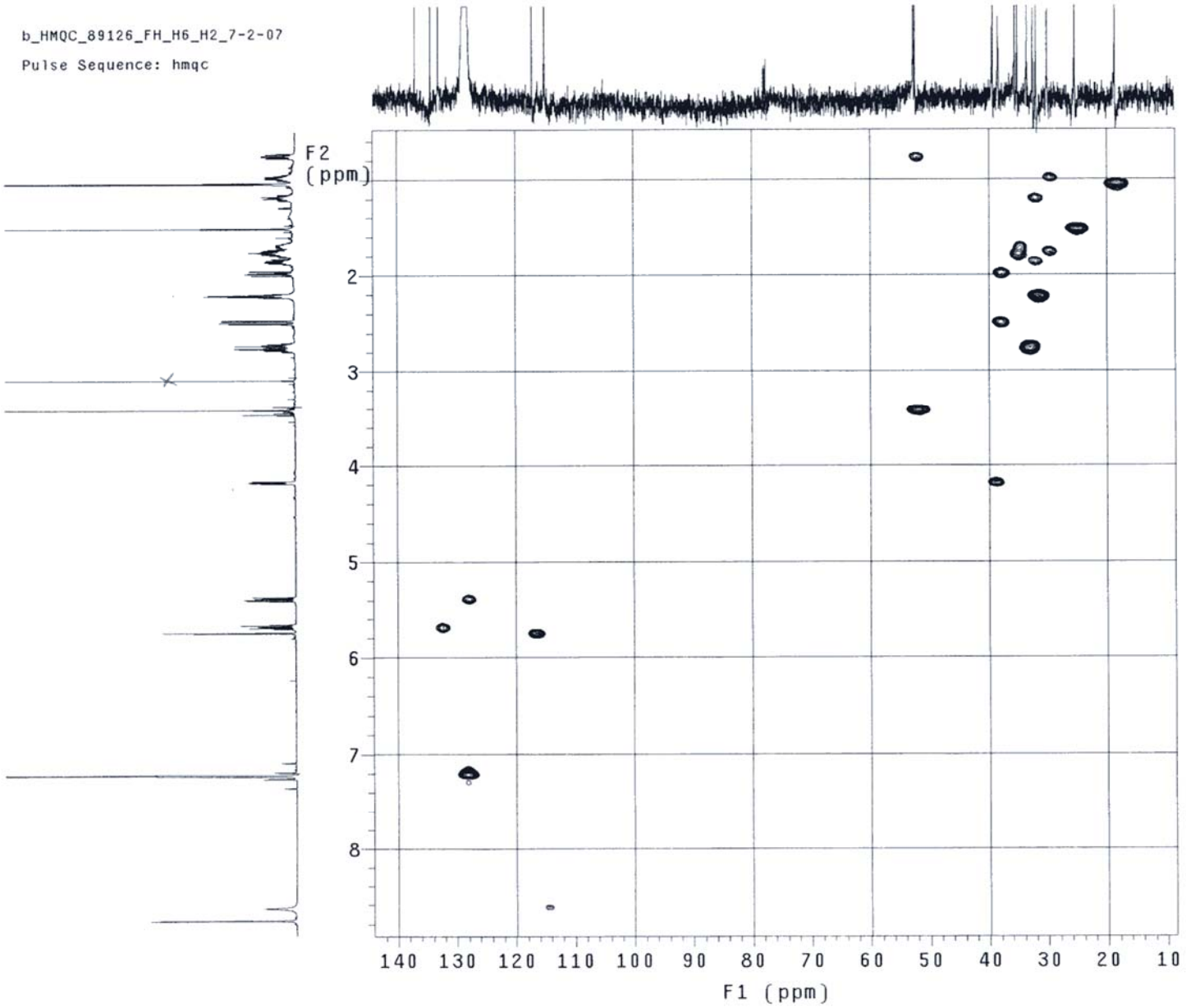


Figure S8. HMBC spectrum of CTP-431 (**1**), (600 MHz, C_6D_6)

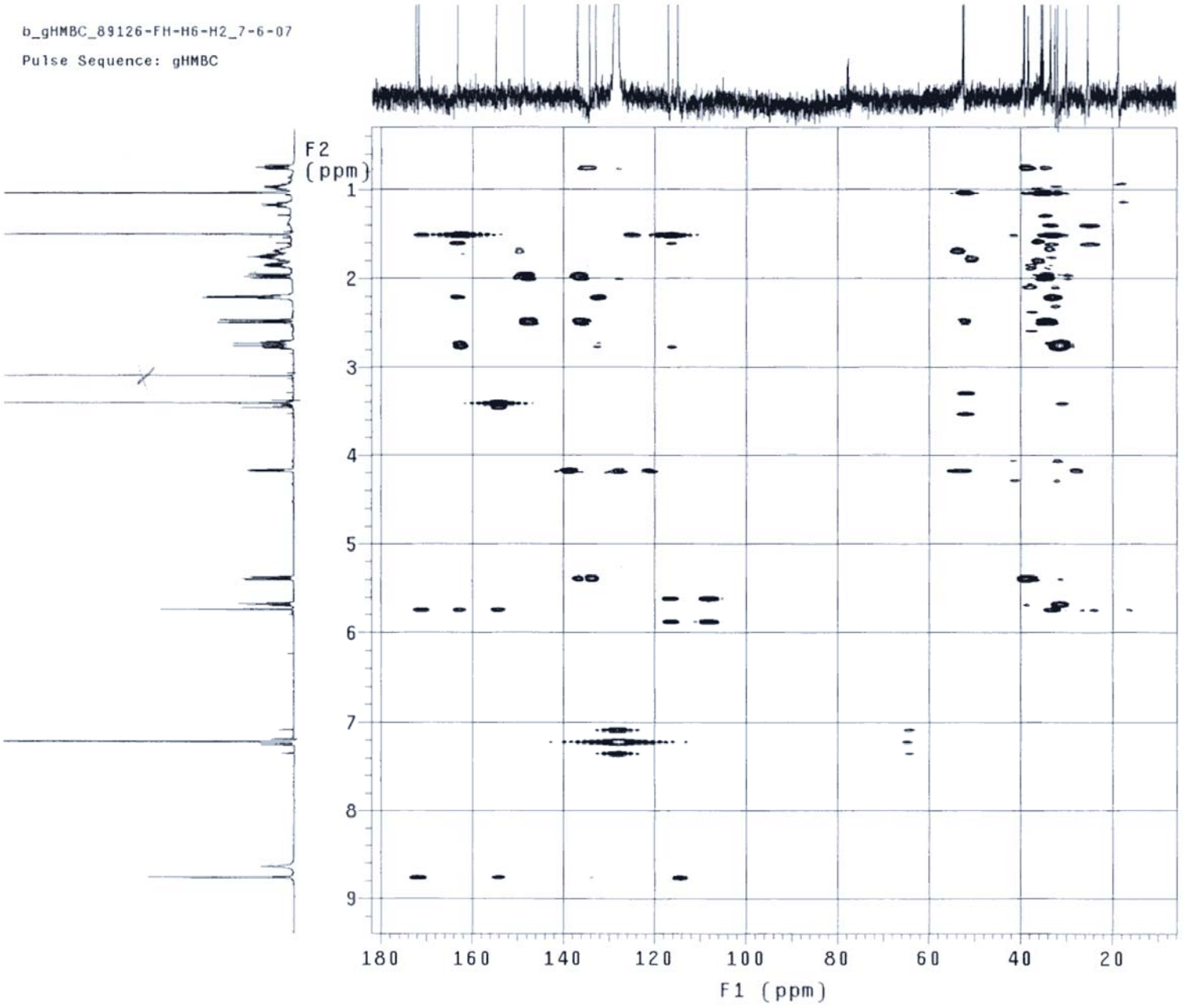


Figure S9. NOE enhancement of H-9 of **1** in C_6D_6 at 600 MHz

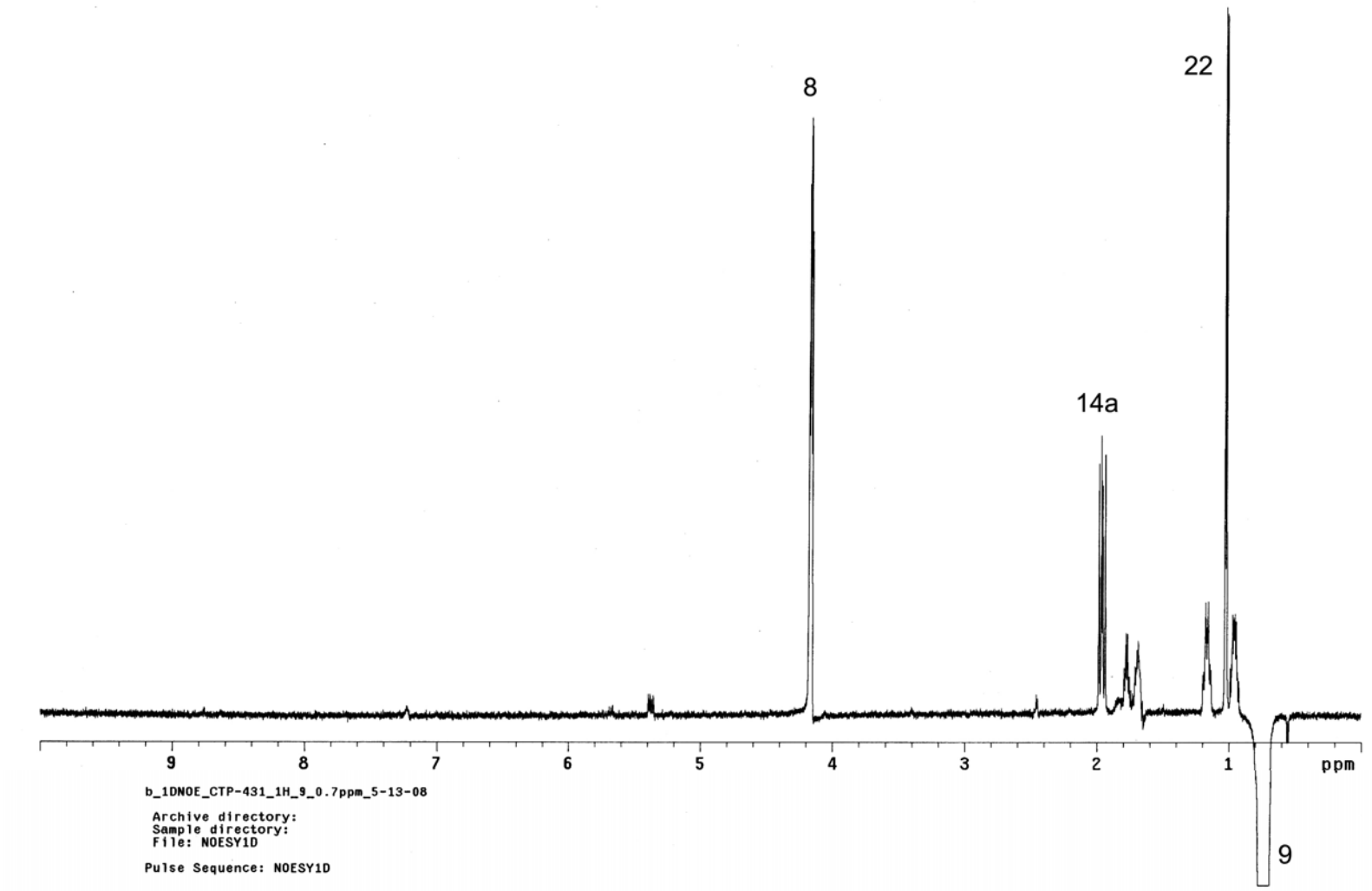


Figure S10. ^{1}H NMR spectrum of CTP-431 (**1**), (600 MHz, $CDCl_3$)

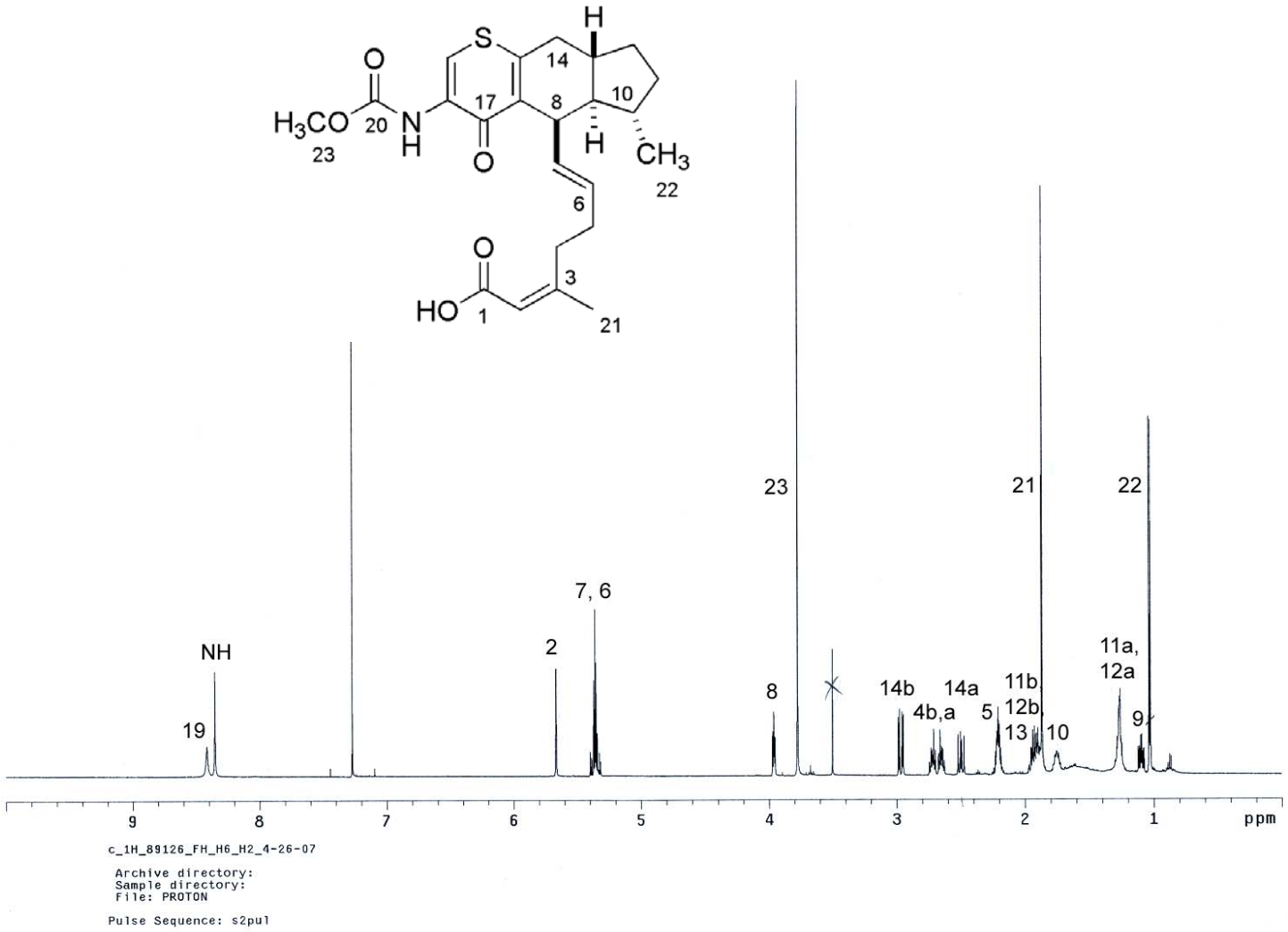


Figure S11. ^{13}C NMR spectrum of CTP-431 (**1**), (125 MHz, $CDCl_3$)

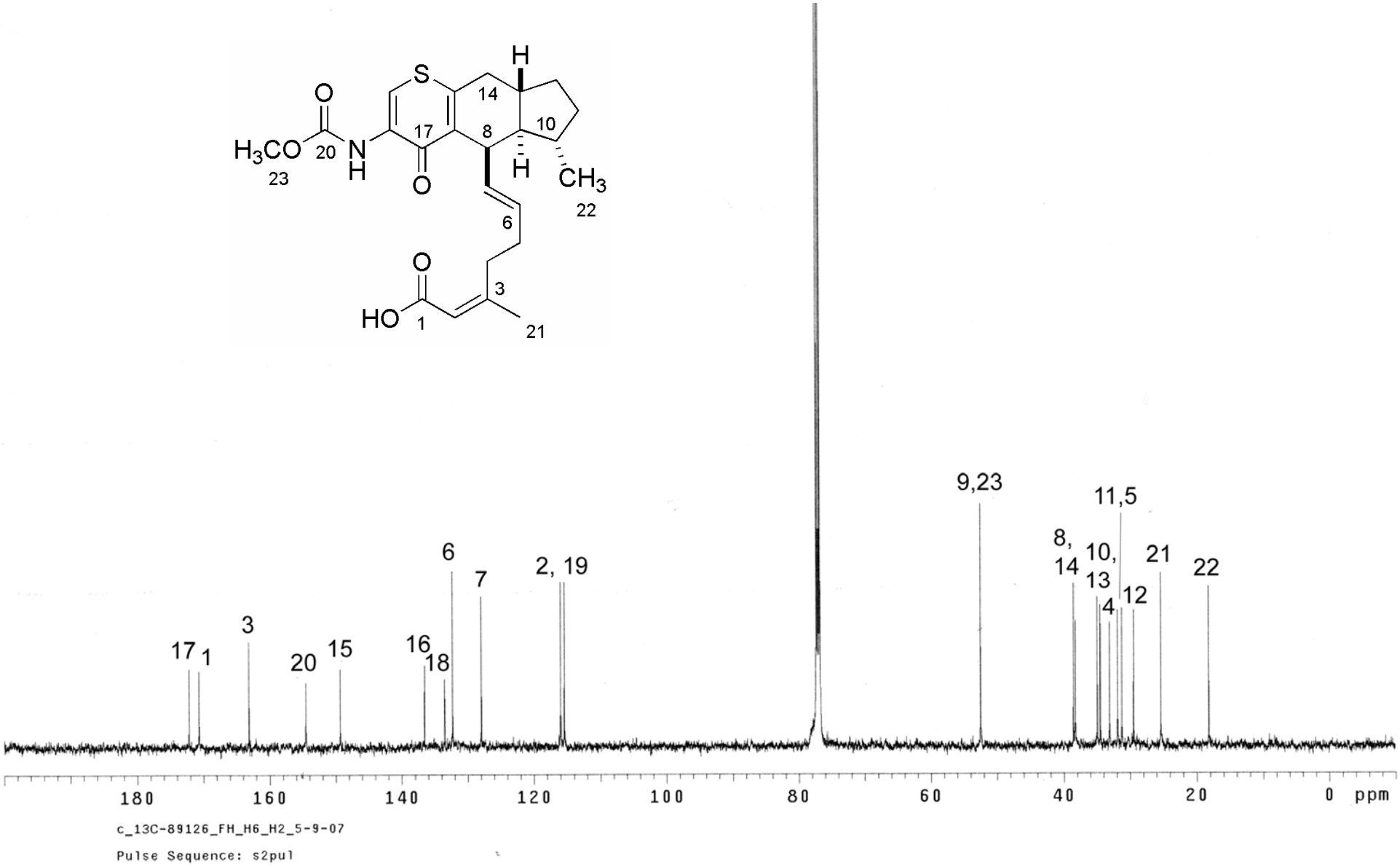


Figure S12. COSY spectrum of CTP-431 (**1**), (600 MHz, $CDCl_3$)

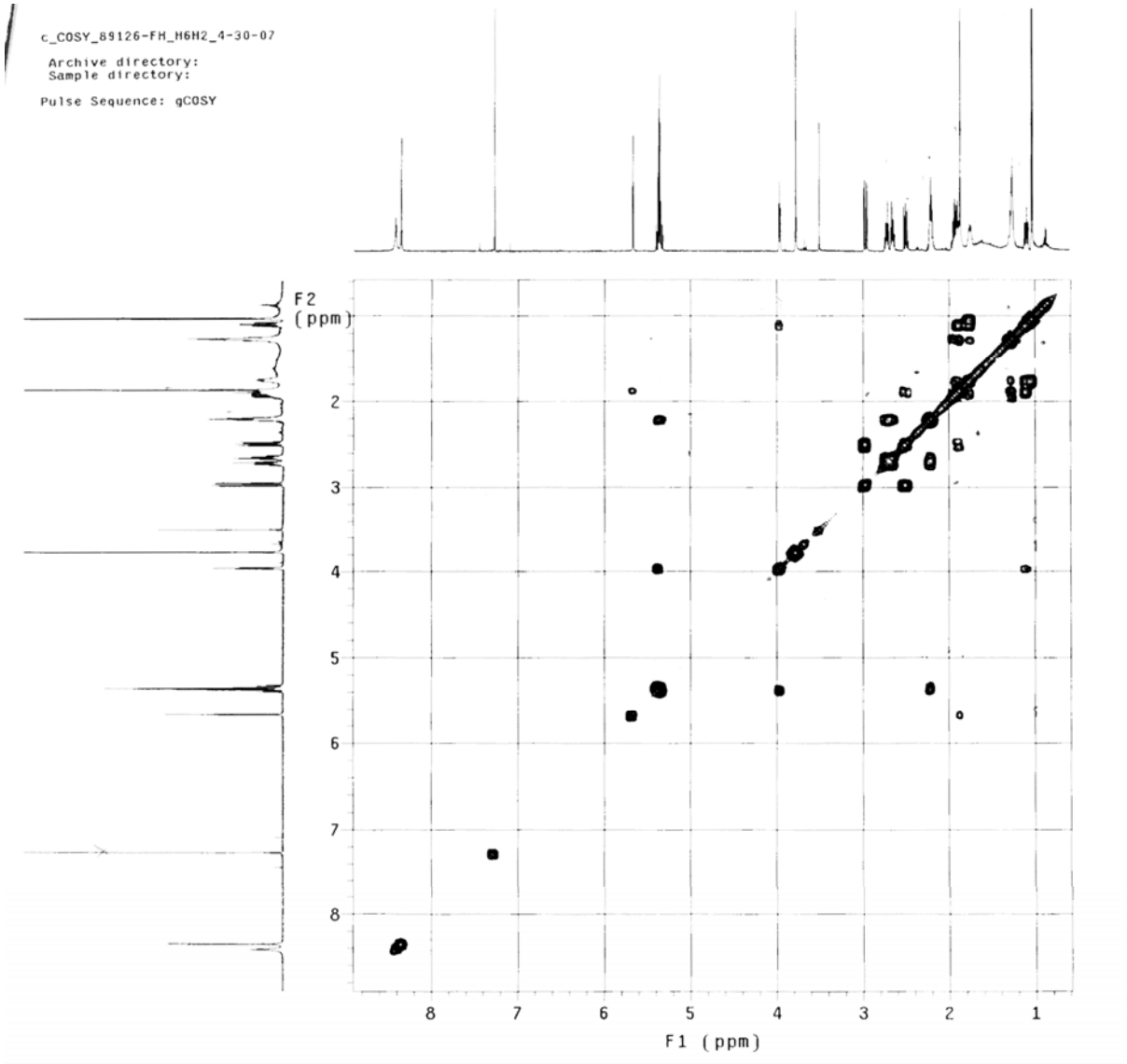


Figure S13. HMQC spectrum of CTP-431 (**1**), (600 MHz, $CDCl_3$)

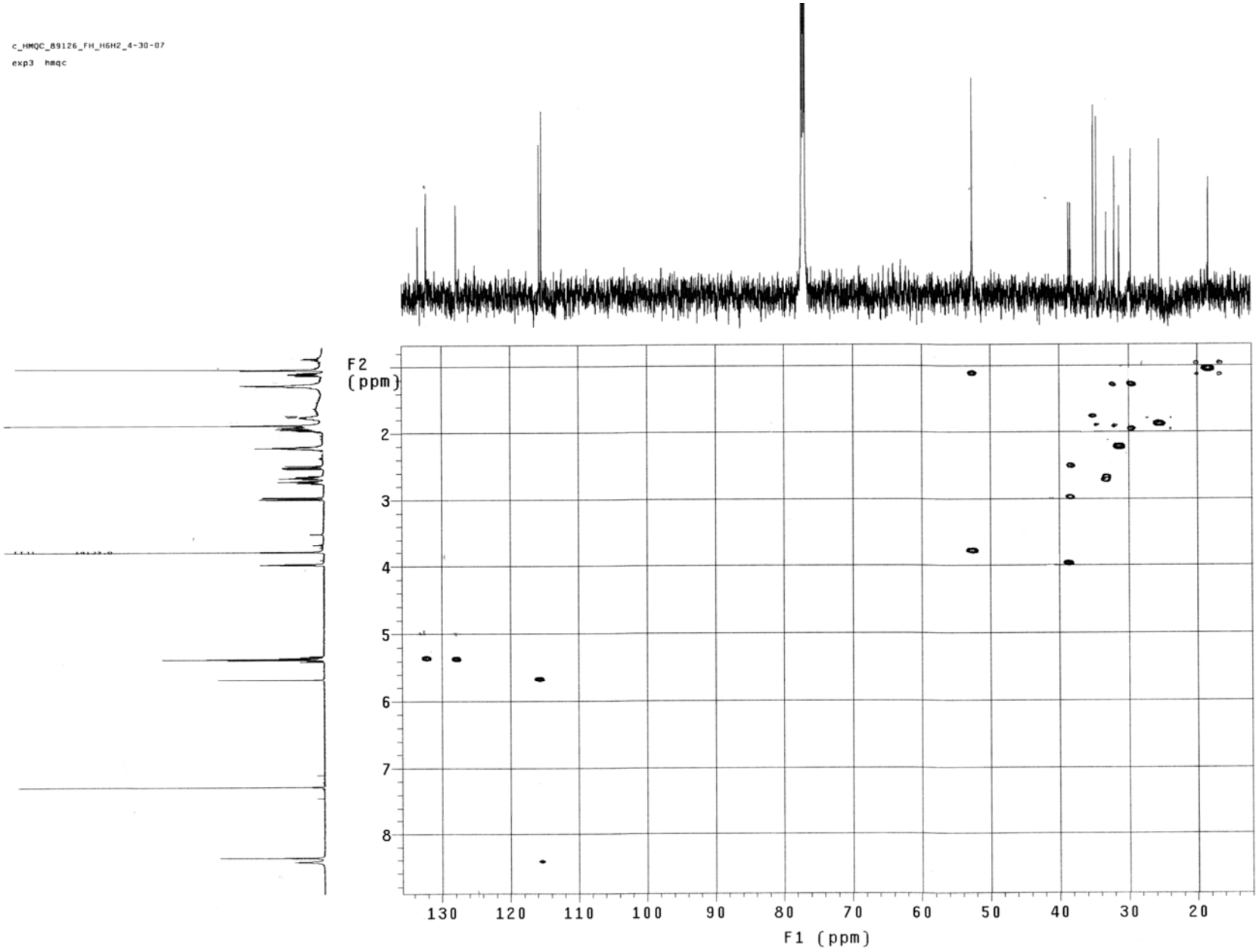


Figure S14. HMBC spectrum of CTP-431 (**1**), (600 MHz, $CDCl_3$)

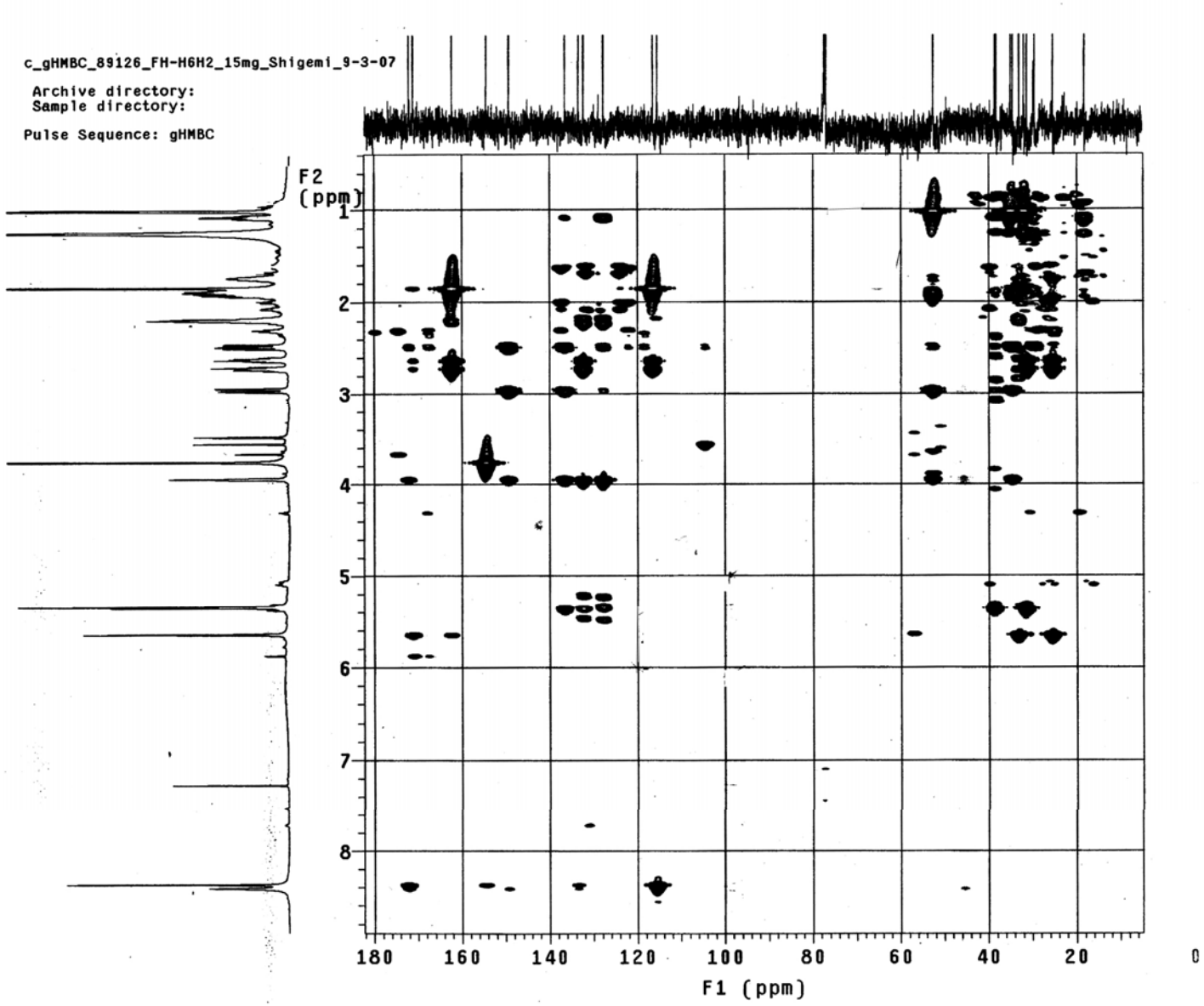


Figure S15. NOE enhancement of H-7 of **1** in $CDCl_3$ at 600 MHz

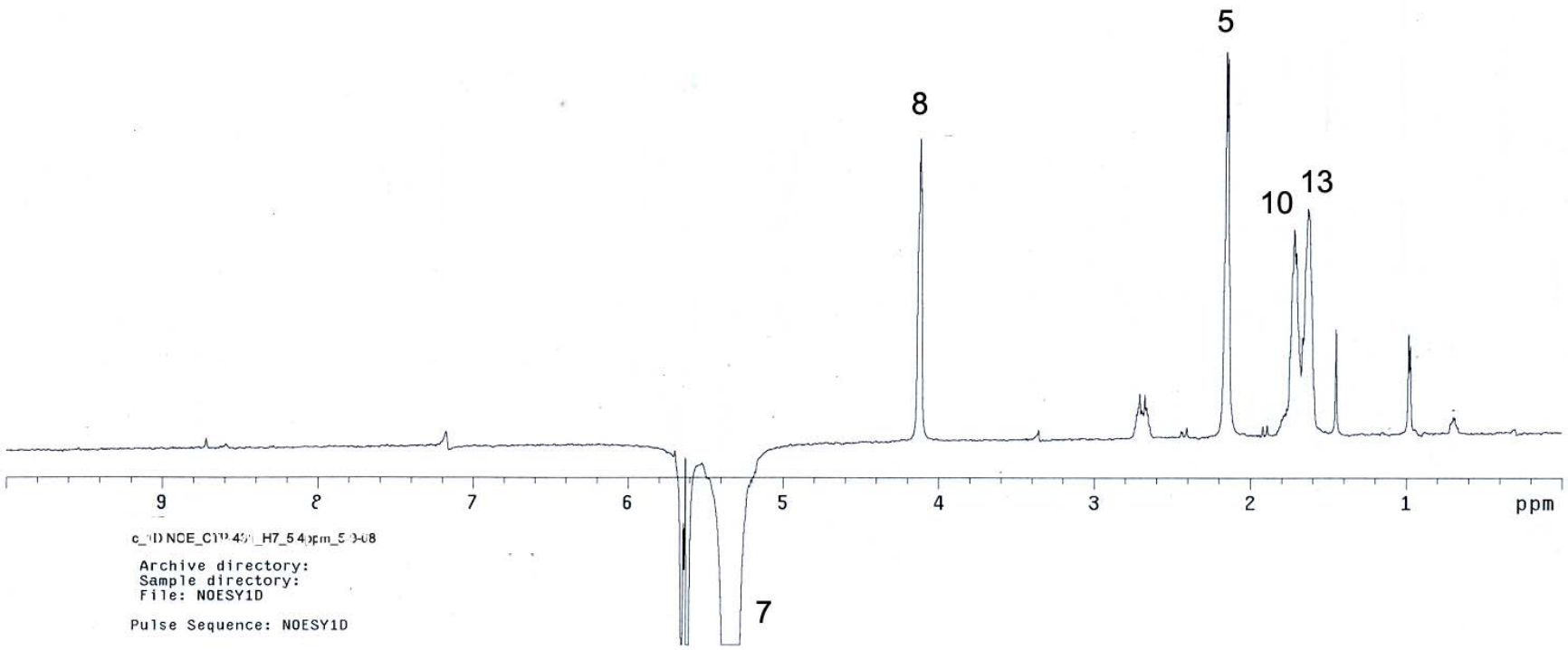


Figure S16. NOE enhancement of H_3-22 of **1** in $CDCl_3$ at 600 MHz