Electronic supplementary materials for the paper

Crystal engineering of molecules with through-space α-effect hydrogen bonds: 3a,6:7,9a-diepoxybenzo[*de*]isoquinolines possessing a free amino group

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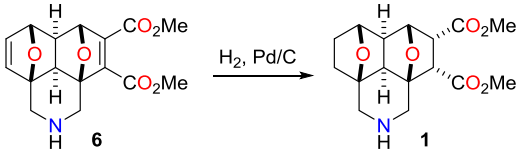
Table of contents:

Synthetic details

All commercially available reagents and solvents were used without further purification. Values of the melting point were measured on a capillary point apparatus equipped with a digital thermometer (SMP 30) and were left unchanged. ^{1}H NMR, ^{13}C NMR spectra were recorded on 400, 600, 700 (for ^{1}H), 100, 150, 176 (for ^{13}C) MHz spectrometers with TMS as the internal standard, using $CDCl_3$ and DMSO-d_6 as solvents. Data for ^{1}H NMR spectra are reported as follows: chemical shift δ (ppm), referenced to TMS; multiplicities are indicated as the following: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; dd, doublet of doublets; coupling constants (Hz) and integration. Data for ^{13}C NMR spectra are reported in terms of chemical shift δ (ppm) relative to residual solvent peaks. IR spectra were obtained in KBr pellets or in thin films using an Infralum FT-801 IR-Fourier spectrometer. High-resolution MALDI mass spectra were obtained using a Bruker autoflex speed mass spectrometer equipped with a solid body UV-laser (λ = 355 nm) and operated in positive reflectron mode. Solutions of the analytes in CH_2Cl_2 (2 mg/mL) were mixed with a solution of 2,5-dihydrobeznoic acid in THF (2 mg/mL) and 1 μl of the mixtures were spotted on a steel target plate and air-dried. Analytical TLC was performed on silica plates Sorbfil (visualization by I_2 vapours or 0.1 % $KMnO_4$ solution).

General procedure for the synthesis of compounds 1−5. (see Reference 8 of the main text for the synthesis of the precursors 6-9)

Dimethyl (3a*SR*,4*SR*,5*RS*,6*RS*,6a*SR*,7*RS*,9a*SR*,9b*RS*)-octahydro-1*H*,4*H*,7*H*-3a,6:7,9a-diepoxybenzo[*de*]isoquinoline-4,5 dicarboxylate (1)



Scheme S1. Synthesis of **1**

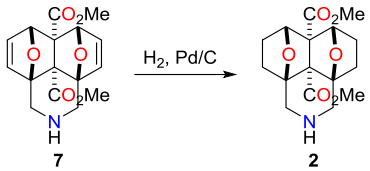
A 0.025 M solution of the corresponding adduct **6** (2.5 mmol, 0.81 g) in EtOH was introduced into the continuous-flow hydrogenation H-Cube Pro™ device under the following condition: 7 cm steel cartridge charged with 10% Pd/C, 100% of H_2 production (full mode), 80 °C, 80 atm., flow rate of 1 mL·min^{-1}. Evaporation of the obtained solution and recrystallization of the residue from EtOH affords pure product **1**.

Colorless needles (0.65 g, 2.0 mmol, 80%). m.p. 135.0−138.5 °C (from EtOH).

^{1}H NMR ($CDCl_3$, 400.1 MHz) δ = 4.68 (1H, d, J = 5.3 Hz, H-6), 4.48 (1H, d, J = 5.3 Hz, H-7), 3.68 (3H, s, CO_2Me), 3.67 (3H, s, CO_2Me), 3.39 (1H, dd, J = 5.3 and J = 12.0 Hz, H-5), 3.25 (1H, d, J = 14.7 Hz, H-1A), 3.16 (1H, d, J = 14.7 Hz, H-3A), 3.08 (1H, d, J = 14.7 Hz, H-3B), 2.94 (1H, d, J = 14.7 Hz, H-1B), 2.76 (1H, d, J = 12.0 Hz, H-4), 2.52 (1H, d, J = 6.9 Hz, H- 9b), 2.49 (1H, d, J = 6.9 Hz, H-6a), 2.34 (1H, br s, NH), 1.83−1.75 (1H, m, H-8A), 1.56−1.50 (1H, m, H-8B), 1.44−1.40 (1H, m, H-9A), 1.39−1.31 (1H, m, H-9B) ppm. ^{13}C NMR ($CDCl_3$, 100.6 MHz) δ = 170.5, 84.6, 81.7, 81.1, 79.6, 77.5, 77.1, 76.8, 51.7, 51.6, 50.1, 50.0, 49.9, 47.7, 47.1, 45.1, 32.1, 30.7 ppm. IR ν_{max}/cm^{-1} (tablet KBr): 3313, 2956, 2886, 1747, 1432, 1195. MALDI-HRMS: found, *m/z*: 324.1452 $[M+H]^+$. $C_{16}H_{22}NO_6$. Calculated, 324.1447.

The sample for the XRD experiment was obtained form an ethyl acetate/heptane solution at r.t.

Dimethyl (3a*RS*,6*SR*,7*RS*,9a*SR*)-hexahydro-1*H*,4*H*,7*H*-3a,6:7,9adiepoxybenzo[*de*]isoquinoline-6a,9b-dicarboxylate (2)



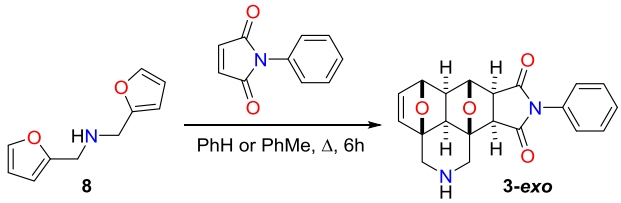
Scheme S2. Synthesis of **2**

A 0.025 M solution of adduct **7** (2.5 mmol, 0.81 g) in EtOH was introduced into a continuous-flow hydrogenation H-Cube Pro^{TM} device under the following conditions: 7 cm steel cartridge charged with 10% Pd/C, 100% of H_2 production (full mode), 80 °C, 40 atm, flow rate of 1 mL·min^{-1}. Evaporation of the obtained solution and recrystallization of the residue from EtOH affords pure product **2** as colorless needles (0.58 g, 1.8 mmol, 72%), m.p. 108.4−110.1 °C (from EtOH).

^{1}H NMR ($CDCl_3$, 600.2 MHz) δ = 4.64 (2H, d, J = 5.5 Hz, H-6 and H-7), 3.75 (3H, s, CO_2Me), 3.72 (3H, s, CO_2Me), 3.22 (2H, d, J = 14.8 Hz, H-1A and H-3A), 3.11 (2H, d, J = 14.8 Hz, H-1B and H-3B), 2.15 (1H, br s, NH), 1.96−1.91, 1.84−1.77 and 1.34−1.29 (8H, m, H-4, H-5, H-8 and H-9) ppm. ^{13}C NMR ($CDCl_3$, 100.6 MHz) δ = 169.4, 86.2, 82.7, 68.9, 62.7, 51.6, 51.5, 47.3, 30.6, 29.0 ppm. IR ν_{max}/cm^{-1} (tablet KBr): 3331, 2955, 1746, 1719, 1430, 1247. MALDI-HRMS: found, m/z: 324.1440 $[M+H]^+$. $C_{16}H_{22}NO_6$ Calculated, 324.1447.

The sample for RSA experiment was obtained from ethyl acetate/heptane solution at r.t.

(3a*SR*,3a1*RS*,6*RS*,6a*SR*,7*RS*,10b*SR*)-9-Phenyl-2,3,6a,7,7a,10a-hexahydro-1*H*,6*H*-3a,6:7,10b-diepoxybenzo[*de*]pyrrolo[3,4-*h*]isoquinoline-8,10(3a1*H*,9*H*)-dione (3)



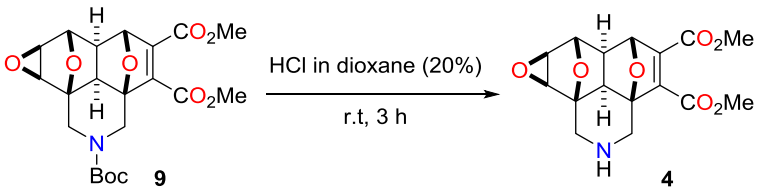
Scheme S3. Synthesis of **3**

Method A. N-Phenylmaleimide (0.01 mol, 0.90 g) was added to a solution of difurfurylamine **8** (0.01 mol, 0.92 g) in benzene (30 mL). The reaction mixture was refluxed for 6 h and then cooled to r.t. Next day, product **3** was filtered off and washed with benzene (2 x 5 mL). This method affords a mixture of *exo*/*endo* diastereoisomers in the ratio of 80/20 (yield 90%).

Method B. N-Phenylmaleimide (0.01 mol, 0.90 g) was added to a solution of difurfurylamine **8** (0.01 mol, 0.92 g) in toluene (30 mL). The reaction mixture was heated at reflux for 6 h. After cooling to r.t, the pure *exo*-isomer **3** was filtered off and washed with toluene (2 x 5 mL). White powder (1.69 g, 4.8 mmol, 93%), m.p. 252−255 ˚C (dec.). The NMR data are given for a mixture of the both isomers.

^{1}H NMR (DMSO-d_6, 700 MHz): δ = 7.61–7.47 (m, 5H, H-Ph, *maj*), 7.33–7.16 (m, 5H, *min*), 7.26 (d, 2H, J = 7.9 Hz,), 7.19 (d, 2H, J = 7.6 Hz,), 6.44 (s, 1H, H-5, *maj*+*min*), 6.34 (s, 1H, H-4), 6.28 (d, 1H, J = 5.5 Hz, H-4 *min*), 4.95 (s, 1H, H-6, *min*), 4.92 (s, 1H, H-6, *maj*), 4.74 (s, 1H, H-7, *min*), 4.72 (s, 1H, H-7, *maj*), 4.26 (dd, 1H, J = 9.1, 4.7 Hz, H-3A, *maj*+*min*), 3.50 (d, 1H, J = 12.5 Hz, H-3B, *maj*+*min*), 3.29 (d, 1H, J = 7.2 Hz, H-10a, *maj*), 3.21 (d, 2H, J = 14.5 Hz, H-1A and 1B, *min*), 3.15 (d, 1H, J = 7.0 Hz, H-7a, *maj*), 2.17 (d, 1H, J = 6.5 Hz, H-6a, *maj*), 2.16 (d, 1H, J = 6.4 Hz, H-6a, *min*), 1.88 (d, 1H, J = 6.4 Hz, H-10c, *min*), 1.86 (d, 1H, J = 6.4 Hz, H-10c, *maj*) ppm. ^{13}C NMR (DMSO-d_6, 176 MHz): δ = 176.90, 176.23, 174.99, 174.92, 138.59, 138.51, 138.34, 138.20, 132.70, 132.64, 129.46, 129.43, 128.95, 128.89, 128.84, 127.63, 127.39, 127.30, 85.12, 84.55, 83.26, 83.00, 81.15, 80.82, 80.76, 62.45, 52.10, 51.99, 51.73, 51.61, 50.51, 49.70, 49.48, 47.79, 47.44, 46.75, 45.87, 45.46, 32.29, 25.97 ppm. IR ν_{max}/cm^{-1} (tablet KBr): 2878, 2944, 1745, 1686, 1475, 1365. MALDI-HRMS: found, m/z: 351.1300 $[M+H]^+$. $C_{20}H_{18}N_2O_4$ Calculated, 351.1312.
The sample for the XRD experiment was obtained from a methanol/DMF solution at r.t.

Dimethyl (3a*SR*,6*RS*,7*SR*,8b*SR*)-2,3,3a1,6a,7a,8a-hexahydro-1*H*,6*H*,7*H*-3a,6:7,8b-diepoxybenzo[*de*]oxireno[2,3-*h*]isoquinoline-4,5-dicarboxylate (4)

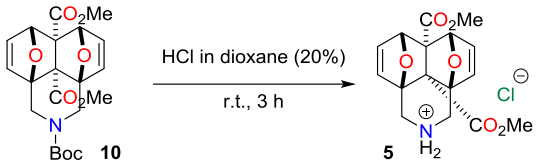


Scheme S4. Synthesis of **4**

HCl (20%) in dioxane (10 mL) was slowly added to a solution of **9** (2 mmol, 0.1 g) in abs. dioxane (10 mL) at r.t. The reaction mixture was stirred at r.t for 3 h and then was poured into cold water (25 mL). The obtained solution was gently treated with NH_4OH (25%) until pH ~ 12. After extraction with DCM (3 × 25 mL) the organic layers were combined and dried under anhydrous Na_2SO_4. Solvent was evaporated to give product **4** as white solid.
White powder (0.76 g, 0.23 mmol, 98%), m.p. 270−272 °C (dec.) ^{1}H NMR (DMSO-d_6, 700 MHz): δ = 5.16 (s, 1H, H-6), 4.48 (s, 1H, H-1A), 3.80 (s, 3H, CO_2Me), 3.69 (s, 3H, CO_2Me), 3.44–3.35 (m, 2H, H-3a), 3.30 (d, 1H, *J* = 3.3 Hz, H-7a), 3.22 (d, 1H, *J* = 14.9 Hz, H-8a), 3.12 (d, 1H, *J* = 3.3 Hz, H-7), 3.03 (d, 1H, J = 15.0 Hz, H-6a), 2.25–2.20 (m, 1H, NH), 1.99 (d, 1H, *J* = 6.4 Hz, H-8c) ppm. ^{13}C NMR (DMSO-d_6, 176.1 MHz) δ = 169.7, 169.2, 141.3, 137.8, 85.9, 83.7, 71.4, 67.1, 53.00, 52.6, 42.2 ppm. IR ν_{max}/cm^{-1} (tablet KBr): 3222, 2965, 1731, 1684, 1435, 1313. MALDI-HRMS: found, m/z: 335.1010 $[M+H]^+$. $C_{16}H_{17}NO_7$. Calculated, 335.1005.
The sample for the XRD experiment was obtained by slow crystallization from a mixture of ethyl acetate/heptane at r.t.

Dimethyl (3a*SR*,6*RS*,6a*SR*,7*RS*,9a*SR*,9b*RS*)-2,3,6a,9b-tetrahydro-1*H*,6*H*,7*H*-3a,6:7,9a-diepoxybenzo[*de*]isoquinoline-4,5-dicarboxylate (5)

HCl in dioxane (20%, 10 mL) was added dropwise to a solution of the initial adduct **10** (0.5 g, 0.0012 mol) in Et_2O (abs., 20 mL) at −10 °C − 0 °C. The mixture was stirred for 2 h at r.t, until crystals of the hydrochloride were completely formed. The obtained crystals of **5** were filtered off and washed with dioxane (2 □ 5 mL).



Scheme S5. Synthesis of **5**

White powder (0.33 g, 1.1 mmol, 87%). R_f 0.20 (EtOAc, Sorbfil); m.p. 193.8–195.2 °C. ^{1}H NMR (400.2 MHz, $CDCl_3$) δ 6.51 (1H, dd, J = 1.7 and J = 5.6 Hz, H-8), 6.33 (1H, d, J = 5.6 Hz, H-9), 5.18 (1H, s, H-6), 4.98 (1H, d, J = 1.7 Hz, H-7), 3.82 (3H, s, CO_2Me), 3.78 (3H, s, CO_2Me), 3.48 (1H, d, J = 14.8 Hz, H-1A), 3.46 (1H, d, J = 14.8 Hz, H-3A), 3.31 (1H, d, J = 14.8 Hz, H-1B), 3.18 (1H, d, J = 14.8 Hz, H-3B), 2.27 (1H, d, J = 6.2 Hz, H-6a), 2.18 (1H, br s, NH), 2.07 (1H, d, J = 6.2 Hz, H-9b). ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 163.9, 162.6, 148.5, 145.4, 139.1, 138.9, 87.3, 84.1, 81.7, 80.7, 52.3, 51.0, 49.2, 46.0, 44.4. MALDI-HRMS: found, m/z: 320.1136 $[M+H]^+$. $C_{16}H_{18}NO_6$. Calculated, 320.1134. The sample for the XRD experiment was obtained from chloroform solution at r.t.

X-ray Data and refinement

Table S1 Crystal data and structure refinement for 1.	
Identification code	FZ1163
Empirical formula	$C_{16}H_{21}NO_6$
Formula weight	323.34
Temperature/K	296(2)
Crystal system	orthorhombic
Space group	Pbca
a/Å	8.2376(5)
b/Å	18.9540(12)
c/Å	19.6823(12)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3073.1(3)
Z	8
ρ_{calc}g/cm^3	1.398
μ/mm^{-1}	0.107
F(000)	1376.0
Crystal size/mm^3	0.5 × 0.3 × 0.2

Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	8.228 to 54.992
Index ranges	-10 ≤ h ≤ 10, -24 ≤ k ≤ 24, -25 ≤ l ≤ 25
Reflections collected	44252
Independent reflections	3516 [R_{int} = 0.0600, R_{sigma} = 0.0280]
Data/restraints/parameters	3516/0/212
Goodness-of-fit on F^2	1.012
Final R indexes [I>=2σ (I)]	R_1 = 0.0428, wR_2 = 0.0953
Final R indexes [all data]	R_1 = 0.0718, wR_2 = 0.1095
Largest diff. peak/hole / e $Å^{-3}$	0.25/-0.18

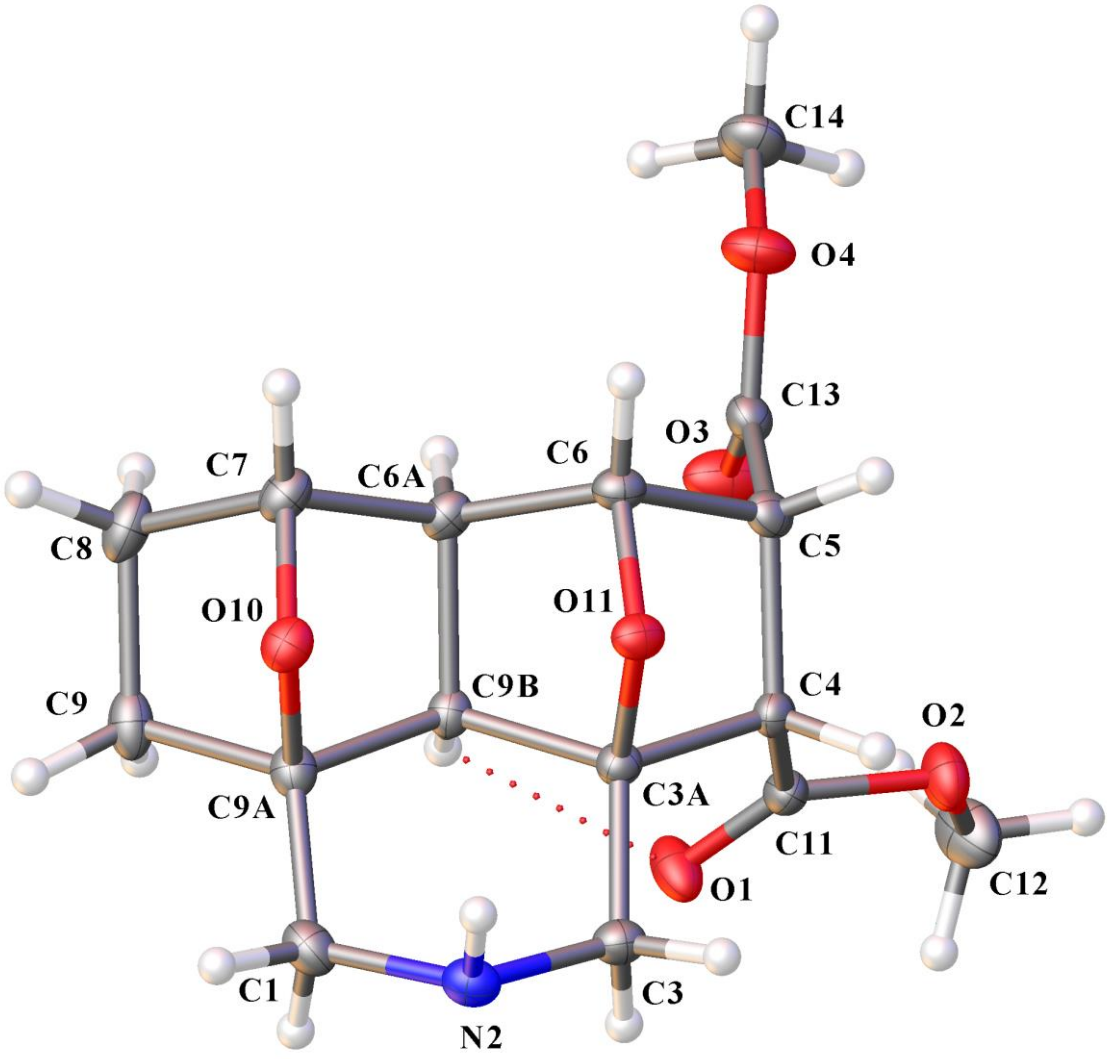


Figure S1. Molecule of compound **1**. A weak C-H···O bond is depicted in the picture

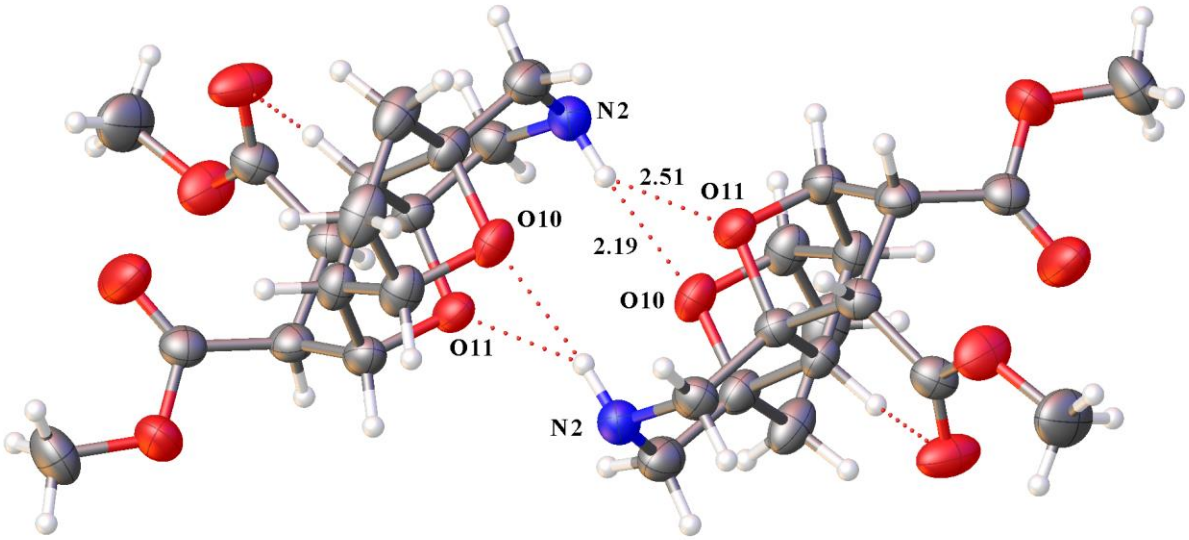


Figure S2. Dimer of two molecules in the crystal packing of compound **1**

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 1. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	1411.1(17)	6643.4(7)	6938.6(7)	58.1(4)
O2	325.8(17)	7453.7(7)	6259.9(7)	55.4(4)
O3	3633(2)	7911.6(8)	6585.0(7)	70.3(5)
O4	5271.6(18)	8237.4(6)	5750.6(7)	56.9(4)
O10	6430.3(14)	5269.0(6)	5811.7(5)	39.8(3)
O11	4185.5(14)	6105.5(5)	5165.7(5)	36.6(3)
N2	3031.9(19)	4697.6(7)	5696.8(8)	43.2(4)
C1	4130(2)	4628.6(9)	6274.1(9)	46.3(4)
C3A	3191.9(19)	6012.4(8)	5768.2(8)	32.5(3)
C3	2143(2)	5362.5(8)	5703.3(9)	40.6(4)
C4	2308(2)	6731.9(8)	5771.2(8)	34.8(4)
C5	3704(2)	7239.8(8)	5543.3(8)	37.2(4)
C6	5091(2)	6700.8(8)	5403.2(8)	37.5(4)
C6A	5839(2)	6447.6(8)	6070.6(8)	36.7(4)
C7	7233(2)	5909.0(9)	6018.5(9)	42.9(4)
C8	7816(2)	5716.9(11)	6732.4(9)	52.5(5)
C9B	4455.5(19)	5967.4(8)	6339.2(7)	32.2(3)
C9A	5278(2)	5239.1(8)	6370.4(8)	37.4(4)
C9	6436(2)	5229.9(10)	6981.9(9)	49.2(5)
C11	1367(2)	6928.5(9)	6397.8(9)	37.8(4)
C12	-541(3)	7731.2(11)	6836.0(12)	69.4(7)
C13	4153(2)	7821.0(8)	6026.7(9)	38.9(4)

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 1. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C14	5756(3)	8847.0(10)	6140.5(12)	62.9(6)

Table S3 Anisotropic Displacement Parameters (Å^2×10^3) for 1. The Anisotropic displacement factor exponent takes the form: -2π^2[h^{2}a*^{2}U$_{11}$+2hka*b*U$_{12}$+…].

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	60.3(9)	62.9(8)	51.0(8)	22.1(6)	20.2(7)	23.8(7)
O2	56.9(8)	55.2(8)	54.2(8)	8.5(6)	4.4(6)	24.4(7)
O3	85.4(11)	80.6(10)	45.0(8)	-13.8(7)	15.3(8)	-32.4(9)
O4	65.8(9)	44.5(7)	60.4(8)	-4.9(6)	16.8(7)	-17.9(7)
O10	38.0(6)	47.2(7)	34.1(6)	-9.3(5)	4.4(5)	6.1(5)
O11	39.5(6)	42.4(6)	27.8(5)	-2.8(5)	2.7(5)	-5.9(5)
N2	48.3(9)	38.3(7)	43.1(8)	-3.6(6)	7.7(7)	-4.2(7)
C1	55.7(11)	40.3(9)	42.9(10)	4.1(7)	8.0(9)	6.3(8)
C3A	30.7(8)	36.9(8)	29.8(8)	1.1(6)	2.0(6)	-0.7(6)
C3	37.7(9)	42.2(9)	41.8(9)	0.0(7)	2.7(7)	-6.4(8)
C4	32.1(8)	39.2(8)	33.1(8)	4.7(6)	-4.4(7)	0.2(7)
C5	42.3(9)	38.4(8)	30.9(8)	5.9(7)	-0.1(7)	-1.6(7)
C6	37.8(9)	39.9(8)	35.0(9)	-0.9(7)	4.8(7)	-6.9(7)
C6A	32.8(8)	41.2(8)	35.9(8)	-8.4(7)	-0.5(7)	0.0(7)
C7	32.6(9)	52.6(10)	43.4(10)	-9.6(8)	0.7(8)	2.5(8)
C8	40.1(10)	68.4(13)	49.0(11)	-14.3(9)	-9.8(9)	16.6(9)
C9B	32.9(8)	36.5(8)	27.4(8)	-3.2(6)	0.9(6)	5.2(7)
C9A	40.4(9)	41.3(9)	30.6(8)	-2.2(7)	3.4(7)	9.7(7)
C9	56.2(12)	55.7(11)	35.7(9)	-3.7(8)	-4.0(9)	24.6(9)
C11	31.0(8)	37.4(8)	45.1(10)	5.7(7)	0.4(7)	1.5(7)
C12	70.6(15)	56.7(12)	80.8(16)	0.8(11)	26.2(12)	24.1(11)
C13	41.2(9)	37.4(8)	38.1(9)	7.4(7)	-0.4(8)	1.7(7)
C14	67.9(14)	40.3(10)	80.3(15)	-4.4(10)	-2.9(12)	-12.1(10)

Table S4 Bond Lengths for 1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C11	1.1942(19)	C3A	C4	1.546(2)
O2	C11	1.3414(19)	C3A	C9B	1.534(2)
O2	C12	1.439(2)	C4	C5	1.565(2)

Table S4 Bond Lengths for 1.					
Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
O3	C13	1.192(2)	C4	C11	1.504(2)
O4	C13	1.329(2)	C5	C6	1.557(2)
O4	C14	1.443(2)	C5	C13	1.502(2)
O10	C7	1.440(2)	C6	C6A	1.528(2)
O10	C9A	1.4537(19)	C6A	C7	1.539(2)
O11	C3A	1.4517(18)	C6A	C9B	1.552(2)
O11	C6	1.4311(18)	C7	C8	1.529(2)
N2	C1	1.458(2)	C8	C9	1.544(3)
N2	C3	1.457(2)	C9B	C9A	1.539(2)
C1	C9A	1.506(2)	C9A	C9	1.536(2)
C3A	C3	1.510(2)			

Table S5 Bond Angles for 1.							
Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C11	O2	C12	115.39(14)	C6	C6A	C9B	100.41(12)
C13	O4	C14	116.71(15)	C7	C6A	C9B	100.46(12)
C7	O10	C9A	96.83(11)	O10	C7	C6A	103.61(13)
C6	O11	C3A	97.05(11)	O10	C7	C8	101.73(14)
C3	N2	C1	112.49(13)	C8	C7	C6A	109.33(14)
N2	C1	C9A	114.73(13)	C7	C8	C9	101.72(14)
O11	C3A	C3	110.64(12)	C3A	C9B	C6A	102.49(12)
O11	C3A	C4	99.29(11)	C3A	C9B	C9A	112.19(12)
O11	C3A	C9B	102.86(12)	C9A	C9B	C6A	102.49(12)
C3	C3A	C4	116.78(13)	O10	C9A	C1	110.17(13)
C3	C3A	C9B	113.88(13)	O10	C9A	C9B	102.85(12)
C9B	C3A	C4	111.45(12)	O10	C9A	C9	100.80(13)
N2	C3	C3A	114.75(14)	C1	C9A	C9B	114.07(14)
C3A	C4	C5	101.29(12)	C1	C9A	C9	118.66(14)
C11	C4	C3A	117.69(13)	C9	C9A	C9B	108.36(13)
C11	C4	C5	117.49(13)	C9A	C9	C8	101.62(14)
C6	C5	C4	100.72(12)	O1	C11	O2	122.38(16)
C13	C5	C4	116.78(14)	O1	C11	C4	127.08(15)
C13	C5	C6	114.37(14)	O2	C11	C4	110.35(14)
O11	C6	C5	101.12(12)	O3	C13	O4	122.71(16)
O11	C6	C6A	104.08(12)	O3	C13	C5	126.95(16)
C6A	C6	C5	110.47(13)	O4	C13	C5	110.32(14)
C6	C6A	C7	116.86(14)				

Table S6 Hydrogen Bonds for 1.						
D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
N2	H2	O10[1]	0.92(2)	2.19(2)	3.0028(19)	146.4(17)
N2	H2	O11[1]	0.92(2)	2.52(2)	3.2331(19)	135.0(15)
C4	H4A	O4[2]	0.98	2.48	3.434(2)	163.1
C8	H8A	O1[3]	0.97	2.59	3.356(2)	136.1
C9B	H9BA	O1	0.98	2.39	3.0533(19)	124.1

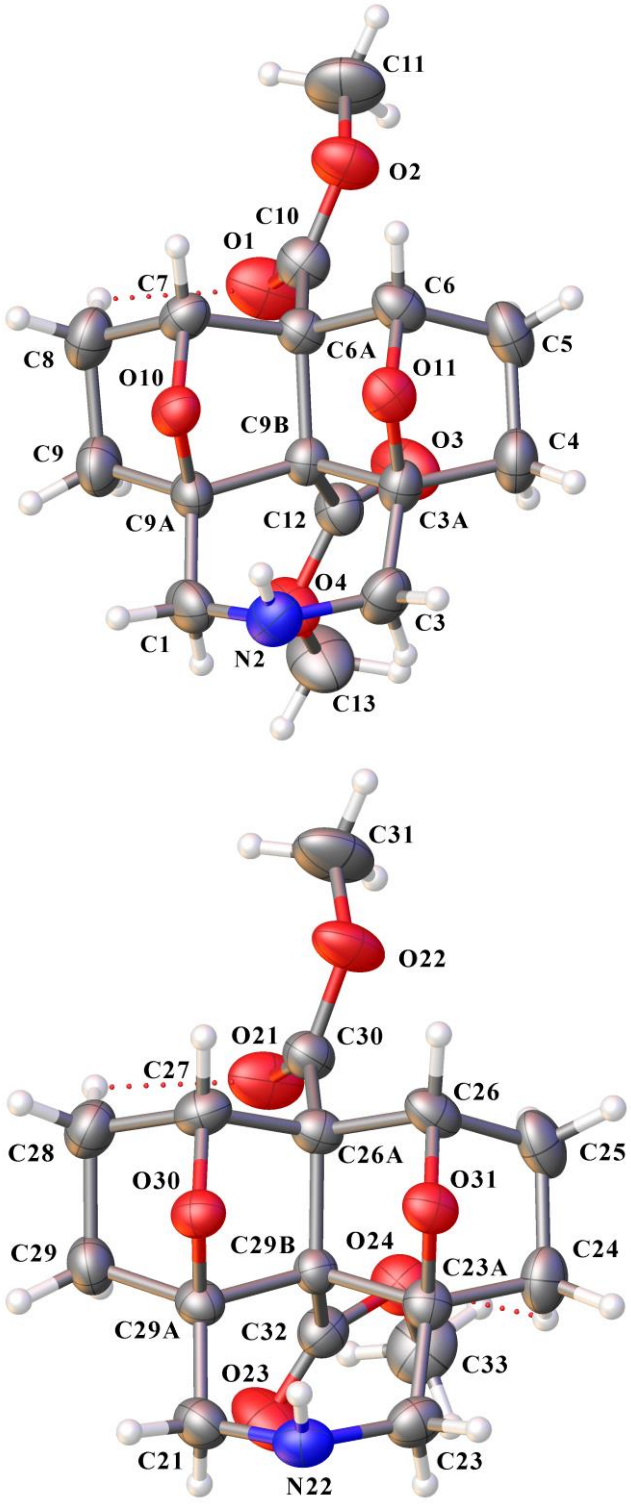
[1]1-X,1-Y,1-Z; [2]-1/2+X,3/2-Y,1-Z; [3]1/2+X,+Y,3/2-Z

Table S7 Torsion Angles for 1.									
A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
O10	C7	C8	C9	-34.22(16)	C5	C6	C6A	C7	179.91(13)
O10	C9A	C9	C8	35.63(15)	C5	C6	C6A	C9B	72.46(14)
O11	C3A	C3	N2	66.94(17)	C6	O11	C3A	C3	-175.43(13)
O11	C3A	C4	C5	-38.77(13)	C6	O11	C3A	C4	61.23(13)
O11	C3A	C4	C11	-168.28(13)	C6	O11	C3A	C9B	-53.44(13)
O11	C3A	C9B	C6A	31.45(14)	C6	C5	C13	O3	-112.1(2)
O11	C3A	C9B	C9A	-77.80(14)	C6	C5	C13	O4	66.94(17)
O11	C6	C6A	C7	72.09(17)	C6	C6A	C7	O10	-71.87(17)
O11	C6	C6A	C9B	-35.36(14)	C6	C6A	C7	C8	-179.73(15)
N2	C1	C9A	O10	-67.09(18)	C6	C6A	C9B	C3A	1.80(14)
N2	C1	C9A	C9B	47.96(19)	C6	C6A	C9B	C9A	118.25(12)
N2	C1	C9A	C9	177.55(14)	C6A	C7	C8	C9	74.90(16)
C1	N2	C3	C3A	52.76(19)	C6A	C9B	C9A	O10	-31.86(14)
C1	C9A	C9	C8	155.91(15)	C6A	C9B	C9A	C1	-151.14(13)
C3A	O11	C6	C5	-58.95(13)	C6A	C9B	C9A	C9	74.29(15)
C3A	O11	C6	C6A	55.69(14)	C7	O10	C9A	C1	175.98(13)
C3A	C4	C5	C6	3.90(14)	C7	O10	C9A	C9B	54.02(14)
C3A	C4	C5	C13	-120.57(14)	C7	O10	C9A	C9	-57.84(14)
C3A	C4	C11	O1	12.3(3)	C7	C6A	C9B	C3A	-118.26(12)
C3A	C4	C11	O2	-162.83(14)	C7	C6A	C9B	C9A	-1.82(14)
C3A	C9B	C9A	O10	77.39(15)	C7	C8	C9	C9A	-1.11(16)
C3A	C9B	C9A	C1	-41.90(17)	C9B	C3A	C3	N2	-48.34(19)
C3A	C9B	C9A	C9	-176.46(13)	C9B	C3A	C4	C5	69.09(15)
C3	N2	C1	C9A	-52.6(2)	C9B	C3A	C4	C11	-60.42(18)
C3	C3A	C4	C5	-157.63(13)	C9B	C6A	C7	O10	35.54(15)

Table S7 Torsion Angles for 1.									
A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
C3	C3A	C4	C11	72.86(18)	C9B	C6A	C7	C8	-72.31(16)
C3	C3A	C9B	C6A	151.22(13)	C9B	C9A	C9	C8	-71.94(16)
C3	C3A	C9B	C9A	41.97(18)	C9A	O10	C7	C6A	-56.02(14)
C4	C3A	C3	N2	179.48(13)	C9A	O10	C7	C8	57.44(14)
C4	C3A	C9B	C6A	-74.08(14)	C11	C4	C5	C6	133.54(14)
C4	C3A	C9B	C9A	176.68(13)	C11	C4	C5	C13	9.1(2)
C4	C5	C6	O11	32.84(14)	C12	O2	C11	O1	10.1(3)
C4	C5	C6	C6A	-76.93(15)	C12	O2	C11	C4	-174.59(16)
C4	C5	C13	O3	5.2(3)	C13	C5	C6	O11	158.94(12)
C4	C5	C13	O4	-175.84(14)	C13	C5	C6	C6A	49.18(17)
C5	C4	C11	O1	-109.2(2)	C14	O4	C13	O3	-4.6(3)
C5	C4	C11	O2	75.70(18)	C14	O4	C13	C5	176.39(16)

Table S8 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 1.				
Atom	***x***	***y***	***z***	**U(eq)**
H2	3630(30)	4684(10)	5301(10)	60(6)
H1A	4763.4	4201.14	6217.28	56
H1B	3487.65	4574.81	6683.87	56
H3A	1380.5	5354.57	6078.72	49
H3B	1518.81	5397.77	5286.77	49
H4A	1525.33	6718.35	5396.61	42
H5A	3390.66	7454.69	5109.83	45
H6A	5895.4	6871.05	5075.09	45
H6AA	6089.74	6837.03	6380.89	44
H7A	8107.61	6055.24	5711.97	51
H8A	7918.59	6132.16	7017.28	63
H8B	8847.53	5470.41	6719.16	63
H9BA	4030.31	6121.53	6779.9	39
H9A	6830.07	4757.3	7074.57	59
H9B	5918.78	5417.06	7386.19	59
H12A	-1251.91	8102.3	6689.18	104
H12B	-1167.4	7361.83	7042.27	104
H12C	219.67	7914.58	7160.75	104
H14A	6562.84	9107.21	5893.43	94
H14B	4828.44	9142.57	6219.48	94
H14C	6198.3	8696.75	6567.87	94

Table S9 Crystal data and structure refinement for 2.	
Identification code	FZ1170_RT
Empirical formula	$C_{16}H_{21}NO_6$
Formula weight	323.34
Temperature/K	296(2)
Crystal system	triclinic
Space group	P-1
a/Å	8.1315(6)
b/Å	13.2200(10)
c/Å	14.3234(9)
α/°	84.858(3)
β/°	89.157(3)
γ/°	89.327(3)
Volume/Å^3	1533.30(19)
Z	4
ρ_{calc}g/cm^3	1.401
μ/mm^{-1}	0.107
F(000)	688.0
Crystal size/mm^3	0.36 × 0.28 × 0.18
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	7.548 to 54.998
Index ranges	$-10 \leq h \leq 10$, $-17 \leq k \leq 16$, $-18 \leq l \leq 15$
Reflections collected	23542
Independent reflections	6992 [R_{int} = 0.0623, R_{sigma} = 0.0822]
Data/restraints/parameters	6992/0/424
Goodness-of-fit on F^2	1.002
Final R indexes [I>=2σ (I)]	R_1 = 0.0558, wR_2 = 0.1171
Final R indexes [all data]	R_1 = 0.1167, wR_2 = 0.1409
Largest diff. peak/hole / e Å^{-3}	0.22/-0.19



2A **2B**

Figure S3. Two independent molecules **2A** and **2B** in the crystal packing of **2**

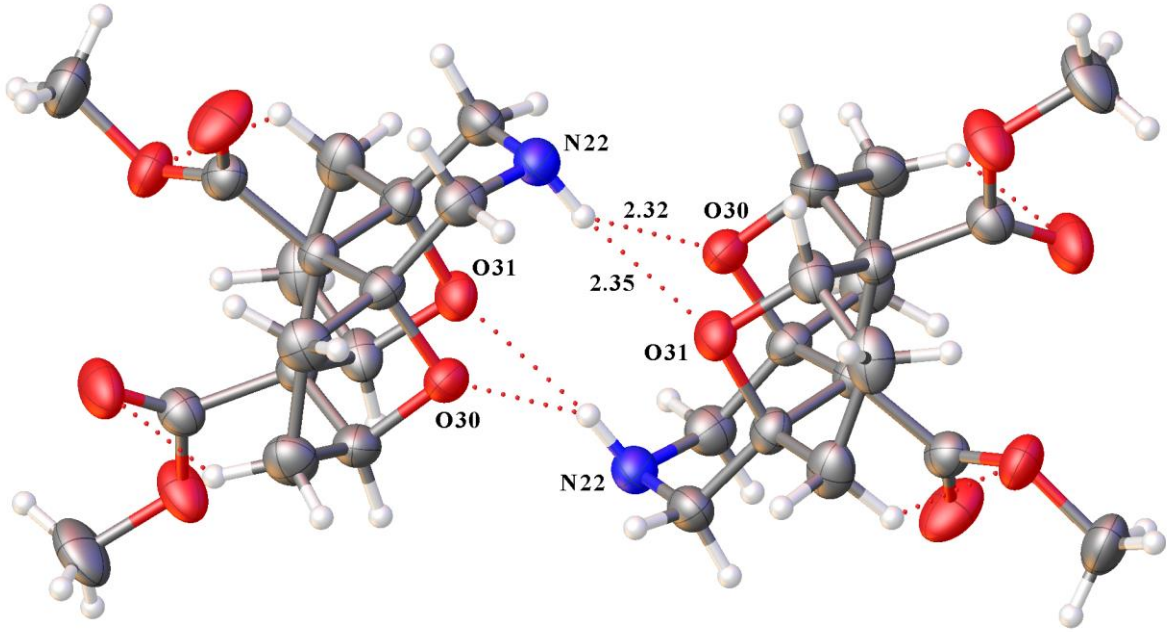


Figure S4. Dimer of two molecules **2A** and **2B** in the crystal packing of compound **2**

Table S10 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 2. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	1795(2)	6225.3(13)	5471.7(13)	63.8(6)
O2	-669(2)	6917.2(13)	5200.3(12)	53.5(5)
O3	3045(2)	5988.5(13)	3695.8(13)	61.3(5)
O4	5495(2)	6708.1(12)	3723.5(12)	51.6(5)
O10	3116.2(19)	9282.3(11)	4627.4(10)	38.8(4)
O11	1292.9(19)	8972.4(11)	3196.7(10)	41.6(4)
N2	4894(3)	9559.4(17)	2887.7(15)	48.1(6)
C1	5570(3)	9036.3(18)	3739.4(17)	45.5(6)
C3	3924(3)	8873.3(19)	2375.8(16)	46.7(6)
C3A	2585(3)	8293.4(17)	2927.3(15)	37.1(6)
C4	1562(3)	7566(2)	2405.1(17)	51.4(7)
C5	36(3)	7434(2)	3049.0(18)	52.9(7)
C6	330(3)	8227.1(17)	3747.3(16)	40.8(6)
C6A	1553(3)	7815.1(16)	4505.0(15)	33.7(5)
C7	2047(3)	8626.0(17)	5186.2(15)	38.7(6)
C8	3232(3)	8188(2)	5948.7(16)	51.0(7)
C9	4813(3)	8053(2)	5355.9(16)	50.0(7)
C9A	4295(3)	8517.7(17)	4383.3(15)	34.9(5)
C9B	3177(3)	7775.9(16)	3904.4(14)	32.3(5)
C10	958(3)	6877.0(18)	5086.2(16)	40.8(6)
C11	-1396(4)	6095(2)	5802(2)	71.2(9)

Table S10 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 2. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C12	3860(3)	6721.8(18)	3786.6(16)	39.5(6)
C13	6229(4)	5726(2)	3587(2)	67.7(9)
O21	7403(2)	9262.6(12)	9505.0(11)	53.8(5)
O22	8084(2)	8556.0(12)	10921.2(11)	52.1(5)
O23	6544(2)	7803.4(15)	7345.3(11)	61.1(5)
O24	8750(2)	8134.3(12)	8145.0(10)	43.9(4)
O30	4474.7(18)	6539.1(11)	9888.6(9)	35.4(4)
O31	7424.7(18)	5729.1(10)	10038.2(10)	36.2(4)
N22	5176(3)	5141.4(15)	8502.7(15)	40.0(5)
C21	4297(3)	6099.2(17)	8308.7(16)	40.3(6)
C23	6949(3)	5261.3(17)	8461.7(16)	39.0(6)
C23A	7645(3)	6033.9(16)	9050.7(15)	32.8(5)
C24	9510(3)	6174.2(18)	9021.3(17)	43.7(6)
C25	9783(3)	6704.4(18)	9919.8(17)	46.8(7)
C26	8065(3)	6624.9(16)	10383.3(16)	37.7(6)
C26A	6919(3)	7470.3(15)	9940.4(14)	31.7(5)
C27	5105(3)	7387.6(17)	10312.5(15)	38.6(6)
C28	4017(3)	8247.0(18)	9871.4(16)	45.2(6)
C29A	4810(3)	6909.5(16)	8925.2(14)	32.5(5)
C29B	6691(3)	7093.6(15)	8936.2(14)	28.0(5)
C29	3864(3)	7930.2(18)	8860.9(16)	42.4(6)
C30	7514(3)	8528.6(17)	10048.6(16)	36.6(6)
C31	8522(4)	9542.3(19)	11208.2(19)	66.1(9)
C32	7287(3)	7723.4(16)	8067.7(16)	35.7(5)
C33	9456(3)	8637(2)	7305.2(18)	57.5(7)

Table S11 Anisotropic Displacement Parameters (Å^2×10^3) for 2. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	59.5(13)	47.0(11)	79.7(14)	22.0(10)	2.9(11)	5.4(10)
O2	46.4(12)	47.4(11)	63.9(12)	9.9(9)	7.6(9)	-8.2(9)
O3	57.1(12)	35.0(10)	93.1(15)	-13.7(10)	6.0(10)	-7.8(9)
O4	42.0(11)	40.9(10)	74.0(12)	-16.4(9)	-5.5(9)	5.9(8)
O10	44.5(10)	33.9(9)	38.7(9)	-7.9(7)	2.0(8)	-3.9(7)
O11	44.7(10)	35.1(9)	43.4(9)	6.2(7)	-5.5(8)	2.0(8)

Table S11 Anisotropic Displacement Parameters ($Å^2×10^3$) for 2. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.						
Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
N2	55.3(15)	40.8(13)	48.7(14)	-5.6(11)	6.0(12)	-11.2(12)
C1	41.0(15)	43.5(15)	54.3(16)	-14.8(13)	-1.6(13)	-10.4(12)
C3	60.5(18)	45.9(15)	33.3(13)	-1.5(11)	2.4(12)	-7.0(13)
C3A	45.3(15)	35.0(13)	31.3(12)	-3.4(10)	-4.5(11)	-3.4(11)
C4	60.1(19)	54.4(16)	41.2(14)	-8.8(12)	-12.7(13)	-9.6(14)
C5	49.5(17)	52.2(16)	56.8(16)	-0.2(13)	-19.3(14)	-11.7(13)
C6	34.1(14)	38.7(13)	48.1(14)	5.7(11)	-4.3(11)	-2.3(11)
C6A	33.8(13)	31.1(12)	35.4(12)	1.2(10)	-0.8(10)	-0.3(10)
C7	45.3(15)	36.2(13)	34.6(13)	-3.1(10)	5.9(11)	-3.3(11)
C8	64.6(19)	53.9(16)	34.8(14)	-4.6(12)	-7.4(13)	-4.8(14)
C9	51.9(17)	58.7(17)	40.3(14)	-7.1(12)	-14.2(13)	2.6(13)
C9A	33.6(13)	36.6(13)	35.7(13)	-8.5(10)	-3.5(10)	-2.4(10)
C9B	36.6(13)	29.1(12)	31.2(12)	-1.6(10)	-3.2(10)	-0.6(10)
C10	45.7(16)	32.2(13)	43.8(14)	0.0(11)	-0.4(12)	-0.9(12)
C11	70(2)	60.2(19)	79(2)	13.6(16)	23.8(17)	-18.1(16)
C12	41.8(16)	34.1(13)	43.0(14)	-5.3(11)	-3.4(12)	-0.5(11)
C13	57.3(19)	52.1(17)	96(2)	-23.0(16)	-8.7(17)	19.7(15)
O21	85.1(14)	30.6(9)	44.8(10)	3.5(8)	-10.9(9)	-4.9(9)
O22	74.6(13)	36.7(10)	46.3(10)	-5.9(8)	-24.3(9)	-7.0(9)
O23	59.2(13)	86.6(15)	34.5(10)	14.7(9)	-7.8(9)	-13.8(10)
O24	44.5(11)	43.3(10)	42.0(10)	6.9(8)	5.0(8)	-11.0(8)
O30	37.4(9)	36.6(9)	32.1(9)	-3.4(7)	3.6(7)	-5.6(7)
O31	45.2(10)	29.0(8)	33.3(9)	3.4(7)	-4.4(7)	-1.6(7)
N22	47.8(14)	37.4(12)	35.6(12)	-5.7(10)	0.6(10)	-7.7(10)
C21	37.0(14)	46.4(14)	37.9(13)	-4.9(11)	-4.4(11)	-4.0(11)
C23	48.0(16)	31.4(12)	37.7(13)	-4.7(10)	2.7(11)	1.7(11)
C23A	35.3(13)	29.6(12)	32.2(12)	3.9(10)	0.4(10)	0.3(10)
C24	37.1(15)	34.8(13)	57.4(16)	4.3(12)	1.8(12)	7.4(11)
C25	38.0(15)	38.0(14)	62.7(17)	7.2(12)	-16.4(13)	1.6(11)
C26	45.1(15)	33.0(13)	34.8(12)	1.2(10)	-13.8(11)	-3.0(11)
C26A	37.0(13)	28.7(11)	29.5(12)	-1.5(9)	-3.5(10)	-3.3(10)
C27	44.4(15)	38.5(13)	33.7(13)	-7.7(10)	4.1(11)	-3.3(11)
C28	40.6(15)	44.4(14)	51.3(15)	-8.9(12)	3.5(12)	6.2(12)
C29A	33.0(13)	36.9(12)	27.1(12)	-0.1(10)	-0.3(10)	-1.5(10)
C29B	28.1(12)	27.2(11)	28.2(11)	0.2(9)	-1.6(9)	0.9(9)
C29	34.6(14)	45.4(14)	46.7(14)	-2.1(11)	-4.7(11)	6.4(11)
C30	39.2(14)	34.9(13)	36.2(13)	-4.4(11)	-6.2(11)	0.9(11)

Table S11 Anisotropic Displacement Parameters ($Å^2×10^3$) for 2. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.						
Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
C31	92(2)	44.1(16)	65.7(18)	-18.9(14)	-27.2(17)	-10.5(15)
C32	40.1(15)	32.5(12)	33.6(13)	1.0(10)	1.2(11)	2.8(11)
C33	62.4(19)	47.7(16)	59.6(17)	8.4(13)	16.3(14)	-11.9(14)

Table S12 Bond Lengths for 2.					
Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
O1	C10	1.193(3)	O21	C30	1.192(3)
O2	C10	1.332(3)	O22	C30	1.343(3)
O2	C11	1.451(3)	O22	C31	1.452(3)
O3	C12	1.198(3)	O23	C32	1.201(2)
O4	C12	1.331(3)	O24	C32	1.324(3)
O4	C13	1.450(3)	O24	C33	1.436(3)
O10	C7	1.422(3)	O30	C27	1.426(2)
O10	C9A	1.447(3)	O30	C29A	1.445(2)
O11	C3A	1.444(3)	O31	C23A	1.445(2)
O11	C6	1.438(3)	O31	C26	1.430(2)
N2	C1	1.459(3)	N22	C21	1.454(3)
N2	C3	1.462(3)	N22	C23	1.452(3)
C1	C9A	1.507(3)	C21	C29A	1.514(3)
C3	C3A	1.511(3)	C23	C23A	1.503(3)
C3A	C4	1.530(3)	C23A	C24	1.529(3)
C3A	C9B	1.581(3)	C23A	C29B	1.590(3)
C4	C5	1.537(4)	C24	C25	1.540(3)
C5	C6	1.535(3)	C25	C26	1.539(3)
C6	C6A	1.542(3)	C26	C26A	1.545(3)
C6A	C7	1.572(3)	C26A	C27	1.562(3)
C6A	C9B	1.568(3)	C26A	C29B	1.578(3)
C6A	C10	1.511(3)	C26A	C30	1.508(3)
C7	C8	1.537(3)	C27	C28	1.529(3)
C8	C9	1.547(4)	C28	C29	1.550(3)
C9	C9A	1.534(3)	C29A	C29B	1.552(3)
C9A	C9B	1.555(3)	C29A	C29	1.542(3)
C9B	C12	1.517(3)	C29B	C32	1.511(3)

Table S13 Bond Angles for 2.							
Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C10	O2	C11	116.1(2)	C30	O22	C31	117.16(18)
C12	O4	C13	115.1(2)	C32	O24	C33	116.58(19)
C7	O10	C9A	97.41(16)	C27	O30	C29A	97.31(16)
C6	O11	C3A	97.16(16)	C26	O31	C23A	97.38(15)
C1	N2	C3	111.29(19)	C23	N22	C21	112.56(19)
N2	C1	C9A	113.9(2)	N22	C21	C29A	113.34(17)
N2	C3	C3A	116.42(19)	N22	C23	C23A	116.42(18)
O11	C3A	C3	110.86(18)	O31	C23A	C23	111.16(18)
O11	C3A	C4	99.43(18)	O31	C23A	C24	99.31(16)
O11	C3A	C9B	102.56(16)	O31	C23A	C29B	102.28(15)
C3	C3A	C4	117.20(19)	C23	C23A	C24	117.48(19)
C3	C3A	C9B	113.40(19)	C23	C23A	C29B	112.98(17)
C4	C3A	C9B	111.46(19)	C24	C23A	C29B	111.68(18)
C3A	C4	C5	101.27(19)	C23A	C24	C25	101.58(18)
C6	C5	C4	101.82(19)	C26	C25	C24	101.30(18)
O11	C6	C5	102.20(19)	O31	C26	C25	102.67(18)
O11	C6	C6A	102.29(17)	O31	C26	C26A	102.80(16)
C5	C6	C6A	110.63(19)	C25	C26	C26A	110.24(18)
C6	C6A	C7	113.38(18)	C26	C26A	C27	113.49(18)
C6	C6A	C9B	100.59(17)	C26	C26A	C29B	100.34(16)
C9B	C6A	C7	99.85(17)	C27	C26A	C29B	99.57(16)
C10	C6A	C6	113.49(19)	C30	C26A	C26	113.66(18)
C10	C6A	C7	108.51(18)	C30	C26A	C27	108.40(18)
C10	C6A	C9B	120.33(18)	C30	C26A	C29B	120.66(18)
O10	C7	C6A	103.45(16)	O30	C27	C26A	103.94(16)
O10	C7	C8	100.71(19)	O30	C27	C28	101.04(17)
C8	C7	C6A	112.27(18)	C28	C27	C26A	111.95(19)
C7	C8	C9	100.63(18)	C27	C28	C29	100.89(17)
C9A	C9	C8	102.10(18)	O30	C29A	C21	107.92(18)
O10	C9A	C1	107.69(18)	O30	C29A	C29B	101.93(15)
O10	C9A	C9	101.31(17)	O30	C29A	C29	100.92(16)
O10	C9A	C9B	101.45(16)	C21	C29A	C29B	114.49(18)
C1	C9A	C9	119.0(2)	C21	C29A	C29	118.88(18)
C1	C9A	C9B	114.21(18)	C29	C29A	C29B	110.29(18)
C9	C9A	C9B	110.68(19)	C26A	C29B	C23A	100.86(15)
C6A	C9B	C3A	101.08(17)	C29A	C29B	C23A	109.69(17)
C9A	C9B	C3A	109.72(17)	C29A	C29B	C26A	101.82(16)
C9A	C9B	C6A	101.77(16)	C32	C29B	C23A	110.44(17)

Table S13 Bond Angles for 2.							
Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C12	C9B	C3A	109.96(17)	C32	C29B	C26A	120.83(18)
C12	C9B	C6A	115.57(19)	C32	C29B	C29A	112.23(17)
C12	C9B	C9A	117.32(18)	C29A	C29	C28	101.82(17)
O1	C10	O2	122.9(2)	O21	C30	O22	123.2(2)
O1	C10	C6A	126.5(2)	O21	C30	C26A	128.0(2)
O2	C10	C6A	110.3(2)	O22	C30	C26A	108.54(18)
O3	C12	O4	122.6(2)	O23	C32	O24	122.1(2)
O3	C12	C9B	125.0(2)	O23	C32	C29B	123.1(2)
O4	C12	C9B	112.3(2)	O24	C32	C29B	114.61(18)

Table S14 Hydrogen Bonds for 2.						
D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
C1	H1A	O10[1]	0.97	2.62	3.552(3)	161.0
C1	H1B	O4	0.97	2.51	3.081(3)	117.4
C4	H4A	O3	0.97	2.32	2.922(3)	119.7
C8	H8A	O1	0.97	2.33	2.996(3)	125.3
C9	H9B	O4	0.97	2.55	3.102(3)	115.8
C11	H11B	O3[2]	0.96	2.62	3.099(3)	111.5
C13	H13C	N22[3]	0.96	2.55	3.511(3)	179.1
N22	H22	O30[4]	0.90(3)	2.32(3)	3.068(3)	140(2)
N22	H22	O31[4]	0.90(3)	2.35(3)	3.108(3)	141(2)
C21	H21B	O23	0.97	2.57	3.128(3)	116.4
C24	H24A	O24	0.97	2.23	2.841(3)	120.3
C28	H28A	O21	0.97	2.42	3.095(3)	126.0
C29	H29B	O23	0.97	2.49	3.067(3)	117.8
C33	H33C	O11[1]	0.96	2.44	3.231(3)	140.0

[1]1-X,2-Y,1-Z; [2]-X,1-Y,1-Z; [3]1-X,1-Y,1-Z; [4]1-X,1-Y,2-Z

Table S15 Torsion Angles for 2.									
A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
O10	C7	C8	C9	-39.0(2)	O30	C27	C28	C29	-38.1(2)
O10	C9A	C9B	C3A	70.2(2)	O30	C29A	C29B	C23A	70.84(18)
O10	C9A	C9B	C6A	-36.27(19)	O30	C29A	C29B	C26A	-35.38(18)
O10	C9A	C9B	C12	-163.43(18)	O30	C29A	C29B	C32	-166.01(16)
O11	C3A	C4	C5	-41.5(2)	O30	C29A	C29	C28	31.9(2)

Table S15 Torsion Angles for 2.									
A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
O11	C3A	C9B	C6A	29.10(19)	O31	C23A	C24	C25	-41.5(2)
O11	C3A	C9B	C9A	-77.8(2)	O31	C23A	C29B	C26A	29.65(19)
O11	C3A	C9B	C12	151.72(18)	O31	C23A	C29B	C29A	-77.21(18)
O11	C6	C6A	C7	66.0(2)	O31	C23A	C29B	C32	158.58(17)
O11	C6	C6A	C9B	-39.7(2)	O31	C26	C26A	C27	66.2(2)
O11	C6	C6A	C10	-169.56(18)	O31	C26	C26A	C29B	-39.1(2)
N2	C1	C9A	O10	-58.2(2)	O31	C26	C26A	C30	-169.33(18)
N2	C1	C9A	C9	-172.5(2)	N22	C21	C29A	O30	-60.3(2)
N2	C1	C9A	C9B	53.7(3)	N22	C21	C29A	C29B	52.4(3)
N2	C3	C3A	O11	67.2(3)	N22	C21	C29A	C29	-174.3(2)
N2	C3	C3A	C4	-179.6(2)	N22	C23	C23A	O31	66.5(2)
N2	C3	C3A	C9B	-47.5(3)	N22	C23	C23A	C24	179.92(19)
C1	N2	C3	C3A	52.9(3)	N22	C23	C23A	C29B	-47.8(3)
C1	C9A	C9B	C3A	-45.4(2)	C21	N22	C23	C23A	53.0(3)
C1	C9A	C9B	C6A	-151.80(18)	C21	C29A	C29B	C23A	-45.4(2)
C1	C9A	C9B	C12	81.0(3)	C21	C29A	C29B	C26A	-151.59(18)
C3	N2	C1	C9A	-55.0(3)	C21	C29A	C29B	C32	77.8(2)
C3	C3A	C4	C5	-160.9(2)	C21	C29A	C29	C28	149.5(2)
C3	C3A	C9B	C6A	148.70(18)	C23	N22	C21	C29A	-53.9(3)
C3	C3A	C9B	C9A	41.8(2)	C23	C23A	C24	C25	-161.32(19)
C3	C3A	C9B	C12	-88.7(2)	C23	C23A	C29B	C26A	149.23(19)
C3A	O11	C6	C5	-55.21(19)	C23	C23A	C29B	C29A	42.4(2)
C3A	O11	C6	C6A	59.38(19)	C23	C23A	C29B	C32	-81.8(2)
C3A	C4	C5	C6	8.0(2)	C23A	O31	C26	C25	-55.00(17)
C3A	C9B	C12	O3	-76.7(3)	C23A	O31	C26	C26A	59.51(19)
C3A	C9B	C12	O4	98.6(2)	C23A	C24	C25	C26	8.4(2)
C4	C3A	C9B	C6A	-76.4(2)	C23A	C29B	C32	O23	101.3(2)
C4	C3A	C9B	C9A	176.64(19)	C23A	C29B	C32	O24	-74.8(2)
C4	C3A	C9B	C12	46.2(3)	C24	C23A	C29B	C26A	-75.7(2)
C4	C5	C6	O11	28.2(2)	C24	C23A	C29B	C29A	177.44(17)
C4	C5	C6	C6A	-80.1(2)	C24	C23A	C29B	C32	53.2(2)
C5	C6	C6A	C7	174.28(19)	C24	C25	C26	O31	27.8(2)
C5	C6	C6A	C9B	68.6(2)	C24	C25	C26	C26A	-81.2(2)
C5	C6	C6A	C10	-61.3(3)	C25	C26	C26A	C27	175.06(17)
C6	O11	C3A	C3	-175.77(17)	C25	C26	C26A	C29B	69.8(2)
C6	O11	C3A	C4	60.23(19)	C25	C26	C26A	C30	-60.4(2)
C6	O11	C3A	C9B	-54.41(18)	C26	O31	C23A	C23	-175.60(18)
C6	C6A	C7	O10	-73.7(2)	C26	O31	C23A	C24	60.00(17)

Table S15 Torsion Angles for 2.									
A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
C6	C6A	C7	C8	178.6(2)	C26	O31	C23A	C29B	-54.76(18)
C6	C6A	C9B	C3A	5.88(19)	C26	C26A	C27	O30	-72.8(2)
C6	C6A	C9B	C9A	118.96(17)	C26	C26A	C27	C28	178.99(17)
C6	C6A	C9B	C12	-112.76(19)	C26	C26A	C29B	C23A	5.0(2)
C6	C6A	C10	O1	152.6(2)	C26	C26A	C29B	C29A	118.02(18)
C6	C6A	C10	O2	-34.0(3)	C26	C26A	C29B	C32	-116.9(2)
C6A	C7	C8	C9	70.4(2)	C26	C26A	C30	O21	144.0(2)
C6A	C9B	C12	O3	36.9(3)	C26	C26A	C30	O22	-41.9(3)
C6A	C9B	C12	O4	-147.81(19)	C26A	C27	C28	C29	72.0(2)
C7	O10	C9A	C1	177.92(17)	C26A	C29B	C32	O23	-141.6(2)
C7	O10	C9A	C9	-56.41(19)	C26A	C29B	C32	O24	42.4(3)
C7	O10	C9A	C9B	57.67(18)	C27	O30	C29A	C21	177.73(18)
C7	C6A	C9B	C3A	-110.37(17)	C27	O30	C29A	C29B	56.83(17)
C7	C6A	C9B	C9A	2.71(19)	C27	O30	C29A	C29	-56.86(18)
C7	C6A	C9B	C12	130.99(18)	C27	C26A	C29B	C23A	-111.18(17)
C7	C6A	C10	O1	-80.4(3)	C27	C26A	C29B	C29A	1.81(19)
C7	C6A	C10	O2	93.0(2)	C27	C26A	C29B	C32	126.9(2)
C7	C8	C9	C9A	4.5(2)	C27	C26A	C30	O21	-88.8(3)
C8	C9	C9A	O10	30.6(2)	C27	C26A	C30	O22	85.3(2)
C8	C9	C9A	C1	148.4(2)	C27	C28	C29	C29A	3.3(2)
C8	C9	C9A	C9B	-76.4(2)	C29A	O30	C27	C26A	-56.49(18)
C9	C9A	C9B	C3A	177.06(19)	C29A	O30	C27	C28	59.67(19)
C9	C9A	C9B	C6A	70.6(2)	C29A	C29B	C32	O23	-21.5(3)
C9	C9A	C9B	C12	-56.5(3)	C29A	C29B	C32	O24	162.49(18)
C9A	O10	C7	C6A	-56.50(18)	C29B	C23A	C24	C25	65.8(2)
C9A	O10	C7	C8	59.72(18)	C29B	C26A	C27	O30	32.98(19)
C9A	C9B	C12	O3	157.1(2)	C29B	C26A	C27	C28	-75.2(2)
C9A	C9B	C12	O4	-27.7(3)	C29B	C26A	C30	O21	24.8(4)
C9B	C3A	C4	C5	66.1(2)	C29B	C26A	C30	O22	-161.04(19)
C9B	C6A	C7	O10	32.43(19)	C29B	C29A	C29	C28	-75.3(2)
C9B	C6A	C7	C8	-75.3(2)	C29	C29A	C29B	C23A	177.37(16)
C9B	C6A	C10	O1	33.5(3)	C29	C29A	C29B	C26A	71.16(19)
C9B	C6A	C10	O2	-153.10(18)	C29	C29A	C29B	C32	-59.5(2)
C10	C6A	C7	O10	159.21(18)	C30	C26A	C27	O30	159.93(16)
C10	C6A	C7	C8	51.5(3)	C30	C26A	C27	C28	51.7(2)
C10	C6A	C9B	C3A	131.3(2)	C30	C26A	C29B	C23A	130.6(2)
C10	C6A	C9B	C9A	-115.6(2)	C30	C26A	C29B	C29A	-116.4(2)
C10	C6A	C9B	C12	12.6(3)	C30	C26A	C29B	C32	8.7(3)

Table S15 Torsion Angles for 2.									
A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
C11	O2	C10	O1	-2.1(3)	C31	O22	C30	O21	2.2(4)
C11	O2	C10	C6A	-175.8(2)	C31	O22	C30	C26A	-172.3(2)
C13	O4	C12	O3	-3.2(3)	C33	O24	C32	O23	-3.3(3)
C13	O4	C12	C9B	-178.57(19)	C33	O24	C32	C29B	172.74(18)

Table S16 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 2.				
Atom	***x***	***y***	***z***	**U(eq)**
H2	4290(30)	10010(20)	3041(19)	61(10)
H1A	6146.35	9524.53	4077.69	55
H1B	6368.02	8532.85	3565.34	55
H3A	4668.55	8385.61	2122.08	56
H3B	3421.34	9267.51	1849.24	56
H4A	2134.61	6924.86	2354.25	62
H4B	1276.63	7862.24	1783.81	62
H5A	-968.58	7578.12	2703.17	63
H5B	-12.75	6753.47	3362.9	63
H6A	-686.65	8503.74	4003.89	49
H7A	1097.97	8981.31	5438.09	46
H8A	2850.72	7544.06	6247.7	61
H8B	3394.11	8657.47	6421.22	61
H9A	5727.32	8416.77	5590.21	60
H9B	5112.74	7342.14	5345.89	60
H11A	-2565.7	6196.02	5836.68	107
H11B	-1158.36	5460.54	5548.24	107
H11C	-945.25	6084.61	6418.26	107
H13A	7403.54	5787.05	3549.19	102
H13B	5934.82	5248.07	4104.74	102
H13C	5833.24	5494.02	3015.79	102
H22	4890(30)	4860(20)	9078(19)	70(9)
H21A	3127.23	5982.09	8396.76	48
H21B	4483.84	6345.17	7657.68	48
H23A	7270.59	5443.55	7814.14	47
H23B	7454.53	4608.06	8650.84	47
H24A	9856.67	6597.27	8466.71	52
H24B	10087.57	5526.74	9040.61	52
H25A	10608.88	6352.66	10312.47	56

Table S16 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 2.				
Atom	***x***	***y***	***z***	**U(eq)**
H25B	10101.34	7406.66	9776.74	56
H26A	8088.74	6592.99	11069.2	45
H27A	5024.09	7309.83	10998.45	46
H28A	4540.34	8901.86	9877.49	54
H28B	2953.46	8266.91	10185.46	54
H29A	2723.48	7844.91	8697.93	51
H29B	4370.38	8422.98	8405.93	51
H31A	8910.75	9464.91	11840.55	99
H31B	9373	9832.13	10799.72	99
H31C	7573.32	9982.13	11174.09	99
H33A	10508.86	8904.31	7442.05	86
H33B	9587.67	8159.99	6841.38	86
H33C	8741.56	9181.88	7070.89	86

Table S17 Crystal data and structure refinement for 3.	
Identification code	3_FM_LT
Empirical formula	$C_{20}H_{18}N_2O_4$
Formula weight	350.36
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.4849(10)
b/Å	8.8446(9)
c/Å	19.102(2)
α/°	90
β/°	95.807(4)
γ/°	90
Volume/Å^3	1594.2(3)
Z	4
ρ_{calc}g/cm^3	1.460
μ/mm^{-1}	0.103
F(000)	736.0
Crystal size/mm^3	0.14 × 0.12 × 0.04
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.808 to 54.99
Index ranges	-12 ≤ h ≤ 12, -11 ≤ k ≤ 11, -24 ≤ l ≤ 24
Reflections collected	44419

Independent reflections	3653 [R_{int} = 0.1114, R_{sigma} = 0.0609]
Data/restraints/parameters	3653/0/239
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0530, wR_2 = 0.1082
Final R indexes [all data]	R_1 = 0.1071, wR_2 = 0.1296
Largest diff. peak/hole / e $Å^{-3}$	0.47/-0.23

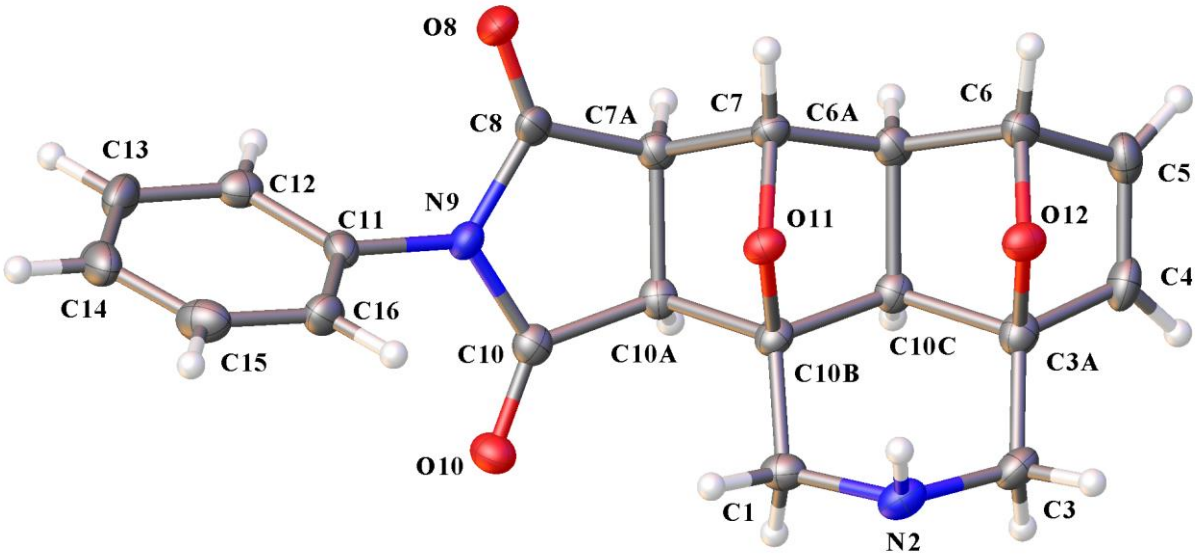


Figure S5. Molecule of **3**

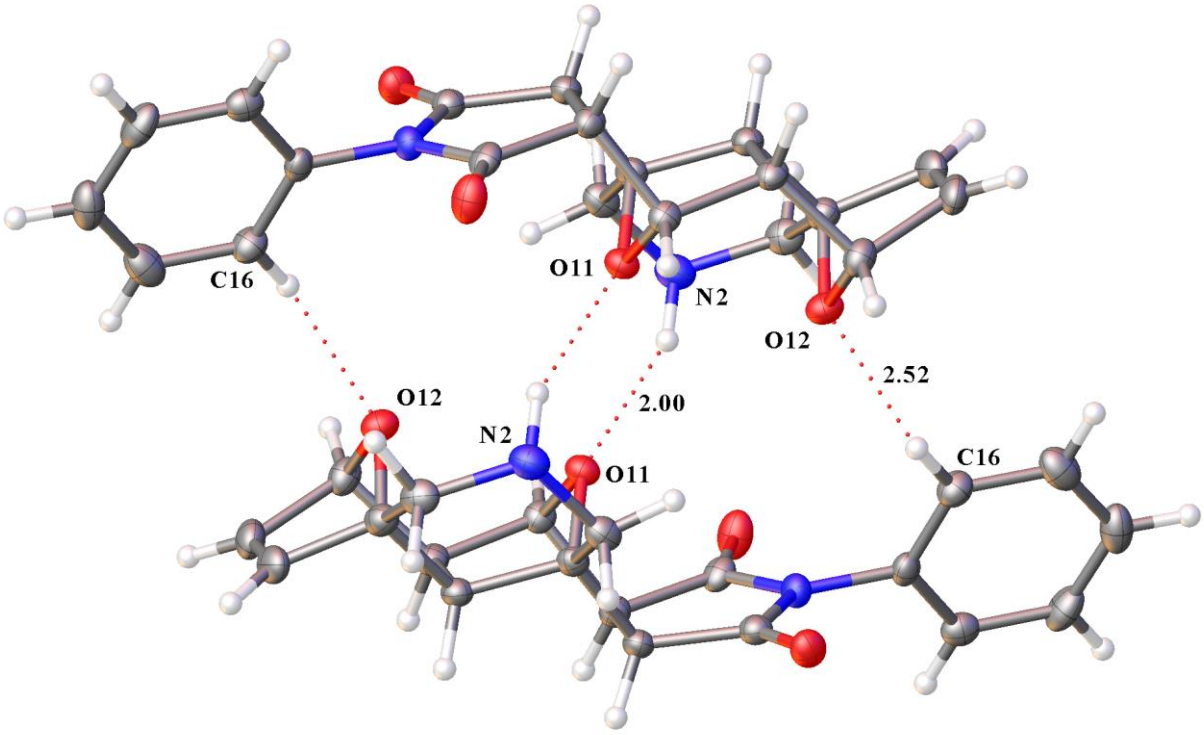


Figure S6. Dimer in the crystal packing of compound **3**

Table S18 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 3. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.				
Atom	***x***	***y***	***z***	**U(eq)**
O8	5535.5(16)	5321(2)	7587.2(8)	28.0(4)
O10	2721.3(16)	8438.3(18)	6146.9(8)	23.9(4)
O11	5853.8(15)	5959.0(17)	5707.4(8)	17.9(3)
O12	7910.8(16)	5992.5(17)	4806.9(8)	20.7(4)
N2	5060(2)	7148(2)	4235.4(10)	23.3(5)
N9	3867.5(18)	6798(2)	6950.7(9)	17.9(4)
C1	4559(2)	7701(3)	4888.5(11)	21.3(5)
C3	6425(2)	7782(3)	4086.8(12)	23.1(5)
C3A	7575(2)	7581(3)	4680.4(12)	21.2(5)
C4	9043(2)	8246(3)	4662.7(12)	25.7(5)
C5	9897(3)	7436(3)	5104.9(12)	25.7(6)
C6	8960(2)	6230(3)	5395.6(11)	21.8(5)
C6A	8099(2)	7086(3)	5925.3(11)	19.2(5)
C7	6988(2)	6158(3)	6266.0(11)	17.8(5)
C7A	6263(2)	7207(3)	6770.7(11)	18.3(5)
C8	5245(2)	6312(3)	7164.4(11)	19.8(5)
C10	3806(2)	7877(2)	6417.5(12)	19.1(5)
C10A	5299(2)	8199(3)	6248.3(11)	18.1(5)
C10B	5636(2)	7538(2)	5530.6(11)	17.5(5)
C10C	7129(2)	8077(3)	5411.3(11)	17.9(5)
C11	2640(2)	6236(2)	7254.2(11)	18.2(5)
C12	2497(2)	6554(3)	7960.0(12)	21.9(5)
C13	1329(3)	6013(3)	8248.4(13)	28.5(6)
C14	298(3)	5155(3)	7847.9(13)	30.0(6)
C15	479(3)	4832(3)	7150.7(13)	29.6(6)
C16	1643(2)	5374(3)	6850.7(12)	22.3(5)

Table S19 Anisotropic Displacement Parameters (Å^2×10^3) for 3_FM_LT. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.						
Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O8	25.4(9)	37.2(10)	22.1(9)	11.1(8)	5.4(7)	6.0(8)
O10	20.9(8)	22.2(9)	28.3(9)	3.6(7)	1.8(7)	2.9(7)
O11	20.6(8)	16.0(8)	16.5(8)	1.1(6)	-0.6(6)	-1.8(6)
O12	24.8(8)	19.2(8)	17.9(8)	-1.1(7)	0.7(6)	2.8(7)
N2	29.4(11)	21.4(11)	18.3(10)	2.0(9)	-1.0(8)	-2.1(9)

Table S19 Anisotropic Displacement Parameters ($Å^2×10^3$) for 3_FM_LT. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.						
Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
N9	19.3(9)	20.1(10)	14.7(9)	2.4(8)	3.3(7)	-0.9(8)
C1	21.2(12)	19.7(12)	22.0(12)	2.8(10)	-1.9(9)	-0.2(10)
C3	31.3(13)	22.4(13)	16.0(11)	3.0(10)	3.4(9)	0.2(10)
C3A	24.9(12)	19.1(12)	20.2(12)	-0.2(10)	5.2(9)	0.1(10)
C4	29.7(13)	25.9(13)	23.4(13)	0.6(11)	12.9(10)	-4.4(11)
C5	20.8(12)	32.5(14)	25.1(13)	-3.3(11)	8.9(10)	-2.1(11)
C6	19.5(11)	28.6(13)	17.5(12)	-0.6(10)	2.3(9)	3.1(10)
C6A	19.5(11)	21.4(12)	16.5(11)	-3.6(10)	1.3(9)	-0.1(9)
C7	18.0(11)	20.2(12)	14.9(11)	0.0(9)	-0.2(8)	0.8(9)
C7A	17.1(11)	19.8(12)	17.8(11)	-2.0(9)	1.0(9)	0.2(9)
C8	20.0(11)	26.7(13)	12.7(11)	-3.0(10)	2.1(9)	2.4(10)
C10	21.5(12)	17.4(11)	18.6(11)	-1.8(10)	2.6(9)	-0.5(9)
C10A	19.3(11)	15.2(11)	20.2(11)	-1.6(9)	3.7(9)	-1.5(9)
C10B	21.3(11)	14.3(11)	16.9(11)	1.7(9)	2.8(9)	-0.3(9)
C10C	20.2(11)	16.3(12)	17.5(11)	-1.9(9)	2.7(9)	-1.0(9)
C11	16.1(11)	18.2(12)	20.8(11)	2.5(9)	4.8(9)	3.2(9)
C12	23.9(12)	20.0(12)	21.0(12)	0.1(10)	-0.9(9)	3.8(10)
C13	33.1(14)	34.6(14)	19.5(12)	5.0(11)	10.7(10)	10.7(12)
C14	22.8(13)	35.1(15)	33.3(14)	12.7(12)	8.1(11)	3.2(11)
C15	24.5(13)	28.9(14)	33.9(14)	6.2(12)	-4.2(11)	-3.8(11)
C16	23.7(12)	26.1(13)	17.3(11)	-1.4(10)	2.2(9)	2.2(10)

Table S20 Bond Lengths for 3.					
Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
O8	C8	1.205(3)	C5	C6	1.528(3)
O10	C10	1.210(3)	C6	C6A	1.559(3)
O11	C7	1.447(2)	C6A	C7	1.532(3)
O11	C10B	1.447(3)	C6A	C10C	1.548(3)
O12	C3A	1.455(3)	C7	C7A	1.548(3)
O12	C6	1.440(3)	C7A	C8	1.507(3)
N2	C1	1.463(3)	C7A	C10A	1.555(3)
N2	C3	1.465(3)	C10	C10A	1.511(3)
N9	C8	1.396(3)	C10A	C10B	1.553(3)
N9	C10	1.392(3)	C10B	C10C	1.533(3)
N9	C11	1.441(3)	C11	C12	1.397(3)
C1	C10B	1.522(3)	C11	C16	1.386(3)

Table S20 Bond Lengths for 3.					
Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
C3	C3A	1.502(3)	C12	C13	1.372(3)
C3A	C4	1.515(3)	C13	C14	1.402(4)
C3A	C10C	1.562(3)	C14	C15	1.390(4)
C4	C5	1.321(3)	C15	C16	1.380(3)

Table S21 Bond Angles for 3.							
Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C10B	O11	C7	97.62(15)	C8	C7A	C10A	104.55(17)
C6	O12	C3A	96.38(16)	O8	C8	N9	124.3(2)
C1	N2	C3	114.03(18)	O8	C8	C7A	127.0(2)
C8	N9	C11	123.14(18)	N9	C8	C7A	108.71(18)
C10	N9	C8	113.15(18)	O10	C10	N9	124.4(2)
C10	N9	C11	123.71(18)	O10	C10	C10A	127.3(2)
N2	C1	C10B	113.95(18)	N9	C10	C10A	108.34(18)
N2	C3	C3A	113.38(19)	C10	C10A	C7A	105.05(17)
O12	C3A	C3	111.70(19)	C10	C10A	C10B	113.51(18)
O12	C3A	C4	101.09(18)	C10B	C10A	C7A	101.18(16)
O12	C3A	C10C	101.38(17)	O11	C10B	C1	110.38(17)
C3	C3A	C4	122.4(2)	O11	C10B	C10A	101.20(16)
C3	C3A	C10C	113.58(18)	O11	C10B	C10C	102.88(17)
C4	C3A	C10C	104.07(18)	C1	C10B	C10A	119.63(18)
C5	C4	C3A	106.3(2)	C1	C10B	C10C	113.93(18)
C4	C5	C6	105.6(2)	C10C	C10B	C10A	106.85(17)
O12	C6	C5	101.51(18)	C6A	C10C	C3A	102.16(17)
O12	C6	C6A	102.23(16)	C10B	C10C	C3A	112.52(18)
C5	C6	C6A	105.02(19)	C10B	C10C	C6A	103.18(17)
C7	C6A	C6	116.36(19)	C12	C11	N9	118.7(2)
C7	C6A	C10C	100.53(17)	C16	C11	N9	119.98(19)
C10C	C6A	C6	100.36(17)	C16	C11	C12	121.3(2)
O11	C7	C6A	104.11(17)	C13	C12	C11	118.6(2)
O11	C7	C7A	100.86(16)	C12	C13	C14	121.1(2)
C6A	C7	C7A	108.16(18)	C15	C14	C13	119.2(2)
C7	C7A	C10A	101.99(17)	C16	C15	C14	120.5(2)
C8	C7A	C7	110.11(18)	C15	C16	C11	119.3(2)

Table S22 Hydrogen Bonds for 3.						
D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
N2	H2	O11[1]	0.98(3)	2.00(3)	2.887(3)	151(2)
C3	H3A	O10[2]	0.99	2.57	3.479(3)	152.3
C5	H5A	O10[3]	0.95	2.48	3.293(3)	144.1
C12	H12A	N2[4]	0.95	2.55	3.459(3)	159.9
C16	H16A	O12[1]	0.95	2.52	3.455(3)	167.7

[1]1-X,1-Y,1-Z; [2]1-X,2-Y,1-Z; [3]1+X,+Y,+Z; [4]+X,3/2-Y,1/2+Z

Table S23 Torsion Angles for 3.									
A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
O10	C10	C10A	C7A	178.1(2)	C6A	C7	C7A	C10A	74.1(2)
O10	C10	C10A	C10B	-72.3(3)	C7	O11	C10B	C1	174.54(17)
O11	C7	C7A	C8	75.8(2)	C7	O11	C10B	C10A	-57.78(18)
O11	C7	C7A	C10A	-34.81(19)	C7	O11	C10B	C10C	52.61(18)
O11	C10B	C10C	C3A	77.6(2)	C7	C6A	C10C	C3A	-117.98(18)
O11	C10B	C10C	C6A	-31.7(2)	C7	C6A	C10C	C10B	-1.0(2)
O12	C3A	C4	C5	-32.6(2)	C7	C7A	C8	O8	65.5(3)
O12	C3A	C10C	C6A	33.4(2)	C7	C7A	C8	N9	-113.4(2)
O12	C3A	C10C	C10B	-76.6(2)	C7	C7A	C10A	C10	118.53(18)
O12	C6	C6A	C7	70.6(2)	C7	C7A	C10A	C10B	0.2(2)
O12	C6	C6A	C10C	-36.8(2)	C7A	C10A	C10B	O11	34.49(19)
N2	C1	C10B	O11	-68.4(2)	C7A	C10A	C10B	C1	155.90(19)
N2	C1	C10B	C10A	174.90(19)	C7A	C10A	C10B	C10C	-72.8(2)
N2	C1	C10B	C10C	46.8(3)	C8	N9	C10	O10	179.0(2)
N2	C3	C3A	O12	64.6(2)	C8	N9	C10	C10A	-1.0(2)
N2	C3	C3A	C4	-175.5(2)	C8	N9	C11	C12	65.6(3)
N2	C3	C3A	C10C	-49.3(3)	C8	N9	C11	C16	-113.2(2)
N9	C10	C10A	C7A	-1.9(2)	C8	C7A	C10A	C10	3.8(2)
N9	C10	C10A	C10B	107.7(2)	C8	C7A	C10A	C10B	-114.51(18)
N9	C11	C12	C13	-179.8(2)	C10	N9	C8	O8	-175.3(2)
N9	C11	C16	C15	179.4(2)	C10	N9	C8	C7A	3.6(2)
C1	N2	C3	C3A	54.1(3)	C10	N9	C11	C12	-114.3(2)
C1	C10B	C10C	C3A	-41.9(3)	C10	N9	C11	C16	66.9(3)
C1	C10B	C10C	C6A	-151.22(18)	C10	C10A	C10B	O11	-77.5(2)
C3	N2	C1	C10B	-52.6(3)	C10	C10A	C10B	C1	43.9(3)
C3	C3A	C4	C5	-157.4(2)	C10	C10A	C10B	C10C	175.20(18)
C3	C3A	C10C	C6A	153.39(19)	C10A	C7A	C8	O8	174.4(2)

Table S23 Torsion Angles for 3.									
A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
C3	C3A	C10C	C10B	43.4(3)	C10A	C7A	C8	N9	-4.5(2)
C3A	O12	C6	C5	-49.64(19)	C10A	C10B	C10C	C3A	-176.26(17)
C3A	O12	C6	C6A	58.70(18)	C10A	C10B	C10C	C6A	74.4(2)
C3A	C4	C5	C6	0.9(2)	C10B	O11	C7	C6A	-54.32(18)
C4	C3A	C10C	C6A	-71.2(2)	C10B	O11	C7	C7A	57.73(17)
C4	C3A	C10C	C10B	178.80(19)	C10C	C3A	C4	C5	72.3(2)
C4	C5	C6	O12	31.5(2)	C10C	C6A	C7	O11	33.7(2)
C4	C5	C6	C6A	-74.7(2)	C10C	C6A	C7	C7A	-72.94(19)
C5	C6	C6A	C7	176.22(18)	C11	N9	C8	O8	4.7(3)
C5	C6	C6A	C10C	68.9(2)	C11	N9	C8	C7A	-176.33(18)
C6	O12	C3A	C3	-178.12(18)	C11	N9	C10	O10	-1.1(3)
C6	O12	C3A	C4	50.15(18)	C11	N9	C10	C10A	178.93(19)
C6	O12	C3A	C10C	-56.83(18)	C11	C12	C13	C14	0.2(3)
C6	C6A	C7	O11	-73.5(2)	C12	C11	C16	C15	0.6(3)
C6	C6A	C7	C7A	179.82(18)	C12	C13	C14	C15	0.9(4)
C6	C6A	C10C	C3A	1.6(2)	C13	C14	C15	C16	-1.3(4)
C6	C6A	C10C	C10B	118.49(17)	C14	C15	C16	C11	0.6(4)
C6A	C7	C7A	C8	-175.32(17)	C16	C11	C12	C13	-1.0(3)

Table S24 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3.				
Atom	***x***	***y***	***z***	**U(eq)**
H2	5110(30)	6050(40)	4273(15)	47(8)
H1A	3689.55	7140.58	4974.33	26
H1B	4302.39	8781.73	4828.88	26
H3A	6303.78	8874.75	3985.77	28
H3B	6723.24	7291.44	3659.84	28
H4A	9297.62	9079.93	4388.35	31
H5A	10886.78	7574.57	5218.52	31
H6A	9465.41	5301.07	5583.89	26
H6B	8714.69	7697.23	6274.6	23
H7A	7357.97	5192.27	6486.13	21
H7B	6953.38	7811.55	7087.16	22
H10A	5541.85	9296.74	6294.17	22
H10B	7267.53	9183.56	5501.3	22
H12A	3193.34	7131.32	8234.45	26
H13A	1216.32	6224.55	8727.19	34

Table S24 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3.				
Atom	***x***	***y***	***z***	**U(eq)**
H14A	-513.74	4798.72	8050.61	36
H15A	-203.47	4233.12	6878.35	36
H16A	1758.96	5159.59	6372.68	27

Table S25 Crystal data and structure refinement for 4.	
Identification code	Liza_LT
Empirical formula	$C_{16}H_{17}NO_7$
Formula weight	335.30
Temperature/K	100(2)
Crystal system	triclinic
Space group	P1
a/Å	7.7282(7)
b/Å	9.9974(10)
c/Å	19.2246(17)
α/°	83.079(4)
β/°	81.948(3)
γ/°	89.975(4)
Volume/Å^3	1459.8(2)
Z	4
ρ_{calc}g/cm^3	1.526
μ/mm^{-1}	0.121
F(000)	704.0
Crystal size/mm^3	0.4 × 0.16 × 0.14
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	8.214 to 59.998
Index ranges	-10 ≤ h ≤ 10, -13 ≤ k ≤ 14, -27 ≤ l ≤ 27
Reflections collected	24899
Independent reflections	14009 [R_{int} = 0.0425, R_{sigma} = 0.0907]
Data/restraints/parameters	14009/3/877
Goodness-of-fit on F^2	1.022
Final R indexes [I>=2σ (I)]	R_1 = 0.0573, wR_2 = 0.1110
Final R indexes [all data]	R_1 = 0.0861, wR_2 = 0.1242
Largest diff. peak/hole / e Å^{-3}	0.36/-0.36
Flack parameter	0.2(6)

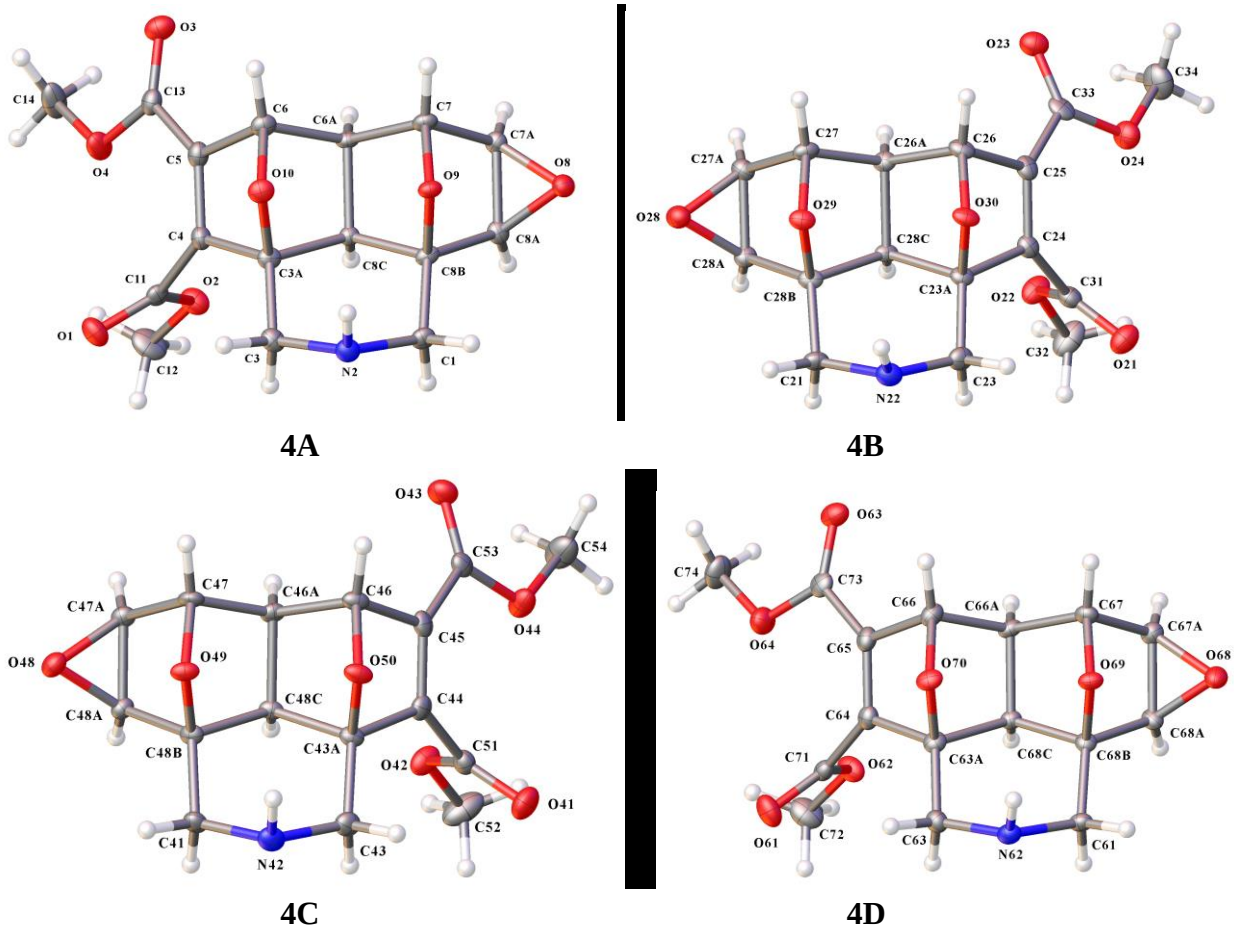


Figure S7. Four independent molecules **4A**, **4B**, **4C**, **4D** in the crystal packing of compound **4**

Table S26 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 4. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	6772(4)	7591(3)	1001.3(16)	20.6(6)
O2	6225(4)	9397(3)	1586.2(16)	19.0(6)
O3	391(4)	8220(3)	1928.6(16)	20.6(6)
O4	2826(4)	8674(3)	1139.9(15)	20.8(7)
O8	4157(4)	7950(3)	5194.7(14)	14.9(6)
O9	4093(3)	6208(3)	4351.7(14)	11.8(5)
O10	3957(4)	5693(3)	2988.7(15)	14.8(6)
N2	7429(5)	5429(3)	3526.2(18)	14.5(7)
C1	7250(5)	6455(4)	4012(2)	14.3(8)
C3	7132(5)	5953(4)	2807(2)	15.3(8)
C3A	5386(5)	6641(4)	2784(2)	13.0(8)
C4	4885(5)	7375(4)	2100(2)	13.9(8)
C5	3119(5)	7381(4)	2206(2)	14.8(8)
C6	2562(5)	6648(4)	2945(2)	14.5(8)

Table S26 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 4. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C6A	2957(5)	7638(4)	3465(2)	11.3(7)
C7	2665(5)	7107(4)	4256(2)	12.8(8)
C7A	3168(5)	8312(4)	4621(2)	13.2(8)
C8A	5079(5)	8337(4)	4491(2)	13.1(8)
C8B	5499(5)	7146(4)	4057(2)	11.4(7)
C8C	5000(5)	7681(4)	3323(2)	10.5(7)
C11	6054(5)	8103(4)	1503(2)	13.8(8)
C12	7086(6)	10242(5)	977(3)	26.8(10)
C13	1949(5)	8121(4)	1759(2)	15.3(8)
C14	1815(6)	9496(5)	679(2)	27.2(10)
O21	299(4)	2793(3)	825.4(16)	22.6(7)
O22	1019(4)	4513(3)	1392.3(16)	20.8(7)
O23	6306(4)	3397(3)	1729.5(16)	21.2(7)
O24	4760(4)	3531(3)	815.8(16)	21.8(7)
O28	913(4)	2885(3)	4913.8(15)	17.8(6)
O29	1362(3)	1128(3)	4065.2(15)	14.0(6)
O30	2152(3)	615(3)	2667.2(15)	14.2(6)
N22	-1615(5)	463(4)	3289(2)	17.1(7)
C21	-1627(5)	1441(4)	3806(2)	15.6(8)
C23	-929(5)	1032(4)	2566(2)	17.3(8)
C23A	885(5)	1636(4)	2509(2)	12.9(8)
C24	1853(5)	2374(4)	1817(2)	14.2(8)
C25	3551(5)	2301(4)	1888(2)	15.1(8)
C26A	3046(5)	2512(4)	3145(2)	12.8(8)
C26	3636(5)	1505(4)	2609(2)	15.1(8)
C27A	2239(5)	3222(4)	4308(2)	14.6(8)
C27	2889(5)	1993(4)	3939(2)	14.3(8)
C28B	143(5)	2089(4)	3805(2)	12.6(8)
C28A	373(5)	3268(4)	4226(2)	13.6(8)
C28C	1072(5)	2623(4)	3054(2)	11.8(7)
C31	977(5)	3223(4)	1278(2)	15.8(8)
C32	148(7)	5458(4)	918(3)	28.5(11)
C33	5025(5)	3122(4)	1484(2)	17.0(8)
C34	6091(7)	4461(5)	420(3)	30.5(11)
O41	9555(4)	5771(3)	9183.0(16)	24.4(7)
O42	9145(4)	7783(3)	8571.6(16)	20.9(7)

Table S26 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 4. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O43	3658(4)	6829(3)	8319.4(17)	21.9(7)
O44	5494(4)	6730(3)	9137.5(16)	22.9(7)
O48	9092(4)	7868(3)	5063.5(15)	17.3(6)
O49	8628(3)	5710(3)	5900.6(15)	13.7(6)
O50	7822(3)	4533(3)	7301.0(15)	14.8(6)
N42	11607(5)	4648(3)	6668.5(19)	17.4(7)
C41	11618(5)	5872(4)	6165(2)	15.8(8)
C43	10911(5)	4875(4)	7399(2)	17.1(8)
C43A	9098(5)	5458(4)	7462(2)	12.9(7)
C44	8150(5)	5888(4)	8154(2)	13.9(8)
C45	6450(5)	5869(4)	8089(2)	14.6(8)
C46	6337(5)	5418(4)	7367(2)	14.7(8)
C46A	6963(5)	6664(4)	6828(2)	12.7(8)
C47	7106(5)	6524(4)	6036(2)	13.5(8)
C47A	7769(5)	7914(4)	5669(2)	13.7(8)
C48A	9627(5)	7923(4)	5747(2)	12.9(8)
C48B	9843(5)	6537(4)	6168(2)	12.4(7)
C48C	8935(5)	6720(4)	6914(2)	11.9(7)
C51	9017(5)	6441(4)	8700(2)	15.6(8)
C52	9908(7)	8453(5)	9087(3)	32.9(12)
C53	5033(5)	6516(4)	8510(2)	15.3(8)
C54	4243(7)	7447(5)	9583(3)	30.9(11)
O61	3098(4)	705(3)	8955.8(17)	24.7(7)
O62	3912(4)	2811(3)	8473.7(16)	19.9(6)
O63	9627(4)	1776(3)	8033.4(17)	21.6(6)
O64	7297(4)	1652(3)	8885.8(16)	23.1(7)
O68	5821(4)	3030(3)	4801.8(15)	16.7(6)
O69	5877(3)	900(3)	5642.6(15)	13.0(6)
O70	6004(3)	-251(3)	7005.8(15)	15.2(6)
N62	2541(4)	-246(3)	6476.0(19)	15.3(7)
C61	2724(5)	999(4)	5985(2)	14.2(8)
C63	2837(5)	-47(4)	7199(2)	15.6(8)
C63A	4577(5)	624(4)	7212(2)	14.1(8)
C64	5128(5)	1030(4)	7898(2)	15.1(8)
C65	6876(5)	1058(4)	7791(2)	15.7(8)
C66	7412(5)	665(4)	7043(2)	15.2(8)

Table S26 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 4. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.				
Atom	***x***	***y***	***z***	**U(eq)**
C66A	7024(5)	1910(4)	6530(2)	12.7(8)
C67	7318(5)	1749(4)	5730(2)	13.9(8)
C67A	6825(5)	3124(4)	5372(2)	14.9(8)
C68A	4907(5)	3092(4)	5501(2)	14.0(8)
C68B	4476(5)	1712(4)	5936(2)	12.3(8)
C68C	4992(5)	1906(4)	6667(2)	11.9(7)
C71	3946(5)	1471(4)	8496(2)	13.8(8)
C72	2924(6)	3334(5)	9075(3)	27.8(10)
C73	8087(5)	1534(4)	8231(2)	16.4(8)
C74	8373(6)	2194(5)	9342(2)	27.6(11)

Table S27 Anisotropic Displacement Parameters (Å^2×10^3) for 4. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.						
Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	24.5(17)	17.8(15)	18.1(16)	-3.2(12)	2.6(13)	4.5(12)
O2	21.4(16)	11.8(14)	22.2(17)	-0.6(12)	1.5(13)	0.6(11)
O3	18.0(16)	16.6(15)	27.9(17)	-1.7(12)	-6.3(13)	2.4(11)
O4	23.3(16)	23.7(16)	14.8(15)	2.5(12)	-4.6(12)	9.4(12)
O8	15.0(14)	15.8(14)	13.4(14)	-0.5(11)	-1.3(11)	-0.2(10)
O9	9.1(13)	9.8(13)	16.0(14)	0.6(10)	-2.5(11)	0.2(10)
O10	16.4(14)	8.4(13)	19.4(15)	0.5(11)	-3.6(12)	1.9(10)
N2	15.8(17)	10.9(16)	16.5(18)	0.7(13)	-2.8(14)	2.4(12)
C1	13.6(19)	12.5(19)	17(2)	0.3(15)	-4.7(16)	3.0(14)
C3	17(2)	12.3(19)	15(2)	0.4(15)	-0.4(16)	1.6(15)
C3A	14.3(19)	9.4(18)	14.3(19)	2.4(14)	-2.1(15)	0.6(14)
C4	17(2)	12.8(18)	11.4(19)	-1.5(14)	-1.7(15)	0.2(14)
C5	20(2)	12.3(19)	13.2(19)	-1.7(15)	-4.2(16)	2.0(15)
C6	14.3(19)	11.3(18)	18(2)	1.0(15)	-3.8(16)	2.1(14)
C6A	8.5(17)	9.1(17)	16(2)	0.2(14)	-1.7(15)	-0.6(13)
C7	10.0(18)	10.1(18)	19(2)	-0.5(15)	-3.5(15)	2.1(13)
C7A	14.6(19)	10.1(18)	15(2)	-2.1(14)	-2.4(16)	1.8(14)
C8A	16.3(19)	9.3(18)	13.0(19)	0.5(14)	-1.6(16)	1.3(14)
C8B	11.3(18)	6.8(17)	16.0(19)	1.7(14)	-4.1(15)	-0.2(13)
C8C	11.1(18)	8.5(17)	11.6(18)	0.1(13)	-1.8(15)	0.1(13)
C11	13.3(19)	14.3(19)	14(2)	0.4(15)	-5.1(16)	3.6(14)

Table S27 Anisotropic Displacement Parameters ($Å^2×10^3$) for 4. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.						
Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
C12	30(3)	19(2)	26(3)	7.4(18)	7(2)	-3.4(18)
C13	21(2)	12.1(19)	14(2)	-2.7(15)	-5.3(16)	0.7(15)
C14	38(3)	28(2)	16(2)	-1.2(18)	-7(2)	19(2)
O21	29.9(18)	15.3(15)	24.6(17)	-1.7(12)	-11.2(14)	0.1(12)
O22	28.1(17)	11.6(14)	25.1(17)	-2.6(12)	-11.3(14)	4.9(12)
O23	18.5(16)	17.8(16)	26.8(18)	-1.6(13)	-2.6(13)	-0.2(11)
O24	24.7(17)	19.6(16)	19.3(16)	3.4(12)	-1.5(13)	-1.5(12)
O28	16.1(15)	19.4(15)	17.2(15)	0.5(12)	-2.3(12)	-0.9(11)
O29	13.1(14)	7.6(13)	20.6(15)	1.7(10)	-2.6(11)	0.4(10)
O30	10.6(13)	7.6(13)	23.5(16)	-0.2(11)	-1.1(11)	1.9(10)
N22	16.9(18)	11.5(17)	22(2)	-0.5(14)	-2.5(15)	-0.7(13)
C21	11.8(19)	13.4(19)	22(2)	-2.6(16)	-3.4(16)	-2.0(14)
C23	18(2)	13(2)	22(2)	-5.7(16)	-4.1(17)	-0.5(15)
C23A	11.9(18)	9.0(17)	18(2)	-1.2(14)	-2.2(15)	3.0(14)
C24	16(2)	9.9(18)	16(2)	-1.5(14)	-0.1(16)	0.6(14)
C25	18(2)	10.9(18)	16(2)	-1.2(15)	0.1(16)	4.7(14)
C26A	13.7(19)	8.9(18)	15(2)	2.7(14)	-3.4(15)	0.9(14)
C26	11.3(19)	10.6(18)	22(2)	0.6(15)	-0.8(16)	2.8(14)
C27A	14.6(19)	11.9(19)	16(2)	1.4(15)	-0.4(16)	0.5(14)
C27	12.7(19)	9.3(18)	22(2)	-1.2(15)	-5.9(16)	-1.0(14)
C28B	13.0(18)	5.9(17)	18(2)	3.0(14)	-3.2(15)	0.4(13)
C28A	15.3(19)	9.8(18)	16(2)	0.2(14)	-3.1(16)	1.9(14)
C28C	10.7(18)	6.7(17)	18(2)	-1.8(14)	-3.2(15)	0.8(13)
C31	14(2)	14(2)	18(2)	-0.3(15)	-0.2(17)	2.0(15)
C32	46(3)	13(2)	29(3)	2.4(18)	-19(2)	4.1(19)
C33	15(2)	11.0(19)	23(2)	-0.9(16)	1.8(17)	6.7(15)
C34	38(3)	24(2)	26(3)	4.9(19)	4(2)	-6(2)
O41	33.0(19)	19.2(16)	21.9(17)	1.1(13)	-9.9(14)	4.7(13)
O42	27.8(17)	11.4(14)	25.3(17)	-1.3(12)	-11.1(13)	0.7(12)
O43	17.5(15)	23.3(16)	25.0(17)	-5.2(13)	-0.9(13)	5.6(12)
O44	24.7(16)	28.2(18)	16.6(16)	-6.2(13)	-2.4(13)	13.4(13)
O48	19.2(15)	18.5(15)	15.4(15)	-3.2(12)	-5.5(12)	4.3(11)
O49	11.1(13)	9.9(13)	22.0(16)	-7.0(11)	-4.9(11)	2.9(10)
O50	10.4(13)	9.5(13)	24.7(16)	-4.3(11)	-1.1(12)	1.4(10)
N42	16.4(17)	12.3(17)	23(2)	-1.2(14)	-1.8(15)	3.9(13)
C41	11.9(19)	16(2)	18(2)	-0.5(16)	0.6(16)	3.6(14)
C43	17(2)	12.4(19)	21(2)	0.5(16)	-2.9(17)	2.6(15)

Table S27 Anisotropic Displacement Parameters ($Å^2×10^3$) for 4. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.						
Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
C43A	11.5(18)	9.0(17)	18(2)	-2.9(14)	-1.4(15)	-0.5(13)
C44	19(2)	9.0(18)	14(2)	1.1(14)	-3.3(16)	1.0(14)
C45	19(2)	9.6(18)	13(2)	0.4(14)	1.0(16)	-2.2(14)
C46	10.5(18)	10.0(18)	23(2)	-2.4(15)	-2.2(16)	1.3(13)
C46A	11.8(18)	8.9(18)	18(2)	-2.7(14)	-4.4(15)	2.8(13)
C47	7.9(17)	15.2(19)	19(2)	-5.6(15)	-2.9(15)	3.3(14)
C47A	13.4(19)	12.8(19)	16(2)	-4.1(15)	-2.8(16)	3.4(14)
C48A	14.6(19)	10.8(18)	14.2(19)	-2.0(14)	-4.4(15)	1.8(14)
C48B	11.9(18)	12.3(18)	14.0(19)	-5.8(14)	-1.4(15)	2.3(14)
C48C	10.2(18)	8.9(17)	17(2)	-4.5(14)	-1.5(15)	1.5(13)
C51	16(2)	15(2)	15(2)	-1.8(15)	0.7(16)	1.6(15)
C52	42(3)	21(2)	44(3)	-11(2)	-27(3)	4(2)
C53	16(2)	10.7(18)	17(2)	1.6(15)	1.0(16)	0.1(14)
C54	32(3)	39(3)	24(3)	-11(2)	-4(2)	18(2)
O61	33.4(18)	18.2(16)	19.7(16)	1.0(12)	2.8(14)	-4.2(13)
O62	21.6(16)	10.3(14)	25.4(17)	0.7(12)	2.2(13)	1.4(11)
O63	18.6(16)	16.8(15)	29.5(18)	0.2(12)	-6.8(13)	-0.7(11)
O64	23.9(16)	28.6(17)	17.7(16)	-5.0(13)	-4.5(13)	-1.1(13)
O68	15.4(14)	18.3(15)	16.2(15)	-2.9(11)	-1.2(12)	3.7(11)
O69	10.3(13)	9.6(13)	19.8(15)	-4.8(11)	-2.4(11)	0.3(10)
O70	14.2(14)	8.4(13)	23.9(16)	-3.8(11)	-4.3(12)	2.9(10)
N62	13.5(17)	12.8(17)	19.9(19)	-2.0(13)	-3.5(14)	-1.3(13)
C61	11.1(18)	12.1(18)	19(2)	-2.0(15)	-2.8(16)	-0.6(14)
C63	17(2)	13.4(19)	16(2)	-0.5(15)	-0.7(16)	-0.2(15)
C63A	14.9(19)	11.2(18)	17(2)	-3.7(15)	-2.5(16)	3.3(14)
C64	19(2)	11.4(19)	15(2)	-0.1(15)	-3.8(16)	-0.3(15)
C65	20(2)	13.3(19)	14(2)	-1.2(15)	-4.0(16)	4.3(15)
C66	17(2)	13.2(19)	17(2)	-4.3(15)	-5.7(16)	3.0(15)
C66A	10.6(18)	9.7(18)	19(2)	-4.3(15)	-4.9(15)	1.8(13)
C67	11.7(18)	10.7(18)	19(2)	-1.7(15)	-1.5(16)	-1.8(14)
C67A	16(2)	12.1(19)	17(2)	-3.4(15)	-3.0(16)	0.8(14)
C68A	14.5(19)	10.6(18)	16(2)	-1.3(15)	0.3(16)	2.1(14)
C68B	12.4(19)	10.4(18)	14.3(19)	-3.5(14)	-0.7(15)	2.8(14)
C68C	11.9(18)	9.4(17)	14.9(19)	-3.1(14)	-2.4(15)	0.7(13)
C71	14.2(19)	11.6(18)	16(2)	0.8(15)	-5.1(16)	-0.8(14)
C72	31(3)	20(2)	31(3)	-9.6(19)	6(2)	2.4(18)
C73	20(2)	8.7(18)	21(2)	1.3(15)	-5.8(17)	2.5(15)

Table S27 Anisotropic Displacement Parameters ($Å^2×10^3$) for 4. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.						
Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
C74	36(3)	26(2)	24(3)	-4.3(19)	-14(2)	-6(2)

Table S28 Bond Lengths for 4.					
Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
O1	C11	1.212(5)	O41	C51	1.202(5)
O2	C11	1.331(5)	O42	C51	1.336(5)
O2	C12	1.439(5)	O42	C52	1.450(5)
O3	C13	1.209(5)	O43	C53	1.201(5)
O4	C13	1.341(5)	O44	C53	1.345(5)
O4	C14	1.446(5)	O44	C54	1.448(5)
O8	C7A	1.440(5)	O48	C47A	1.443(5)
O8	C8A	1.447(5)	O48	C48A	1.439(5)
O9	C7	1.441(4)	O49	C47	1.442(4)
O9	C8B	1.443(4)	O49	C48B	1.438(4)
O10	C3A	1.436(5)	O50	C43A	1.442(4)
O10	C6	1.445(4)	O50	C46	1.450(5)
N2	C1	1.462(5)	N42	C41	1.465(5)
N2	C3	1.468(5)	N42	C43	1.477(5)
C1	C8B	1.516(5)	C41	C48B	1.524(5)
C3	C3A	1.518(5)	C43	C43A	1.512(5)
C3A	C4	1.526(5)	C43A	C44	1.535(5)
C3A	C8C	1.554(5)	C43A	C48C	1.559(5)
C4	C5	1.352(6)	C44	C45	1.338(6)
C4	C11	1.473(6)	C44	C51	1.480(6)
C5	C6	1.522(6)	C45	C46	1.524(6)
C5	C13	1.472(6)	C45	C53	1.467(6)
C6	C6A	1.547(5)	C46	C46A	1.551(6)
C6A	C7	1.536(5)	C46A	C47	1.535(6)
C6A	C8C	1.564(5)	C46A	C48C	1.558(5)
C7	C7A	1.540(5)	C47	C47A	1.535(6)
C7A	C8A	1.463(5)	C47A	C48A	1.465(5)
C8A	C8B	1.543(5)	C48A	C48B	1.539(5)
C8B	C8C	1.548(5)	C48B	C48C	1.539(5)
O21	C31	1.198(5)	O61	C71	1.214(5)
O22	C31	1.336(5)	O62	C71	1.336(5)
O22	C32	1.463(5)	O62	C72	1.446(5)

Table S28 Bond Lengths for 4.					
Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
O23	C33	1.201(5)	O63	C73	1.213(5)
O24	C33	1.343(5)	O64	C73	1.339(5)
O24	C34	1.453(5)	O64	C74	1.440(5)
O28	C27A	1.446(5)	O68	C67A	1.441(5)
O28	C28A	1.449(5)	O68	C68A	1.437(5)
O29	C27	1.438(5)	O69	C67	1.441(4)
O29	C28B	1.441(4)	O69	C68B	1.445(4)
O30	C23A	1.449(4)	O70	C63A	1.449(5)
O30	C26	1.436(5)	O70	C66	1.437(5)
N22	C21	1.475(5)	N62	C61	1.462(5)
N22	C23	1.462(5)	N62	C63	1.477(5)
C21	C28B	1.513(5)	C61	C68B	1.516(5)
C23	C23A	1.512(5)	C63	C63A	1.507(5)
C23A	C24	1.536(6)	C63A	C64	1.540(6)
C23A	C28C	1.543(5)	C63A	C68C	1.557(5)
C24	C25	1.339(5)	C64	C65	1.337(6)
C24	C31	1.495(6)	C64	C71	1.476(6)
C25	C26	1.522(6)	C65	C66	1.538(6)
C25	C33	1.475(6)	C65	C73	1.462(6)
C26A	C26	1.549(5)	C66	C66A	1.549(5)
C26A	C27	1.542(6)	C66A	C67	1.549(5)
C26A	C28C	1.562(5)	C66A	C68C	1.555(5)
C27A	C27	1.541(5)	C67	C67A	1.535(5)
C27A	C28A	1.473(5)	C67A	C68A	1.468(5)
C28B	C28A	1.532(5)	C68A	C68B	1.536(5)
C28B	C28C	1.552(6)	C68B	C68C	1.547(5)

Table S29 Bond Angles for 4.							
Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C11	O2	C12	115.4(3)	C51	O42	C52	115.9(3)
C13	O4	C14	116.0(3)	C53	O44	C54	115.8(3)
C7A	O8	C8A	60.9(2)	C48A	O48	C47A	61.1(2)
C7	O9	C8B	97.6(3)	C48B	O49	C47	97.6(3)
C3A	O10	C6	97.2(3)	C43A	O50	C46	97.1(3)
C1	N2	C3	113.0(3)	C41	N42	C43	112.6(3)
N2	C1	C8B	113.5(3)	N42	C41	C48B	114.0(3)
N2	C3	C3A	113.1(3)	N42	C43	C43A	113.0(3)

Table S29 Bond Angles for 4.							
Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O10	C3A	C3	111.3(3)	O50	C43A	C43	111.9(3)
O10	C3A	C4	101.0(3)	O50	C43A	C44	100.5(3)
O10	C3A	C8C	102.8(3)	O50	C43A	C48C	102.7(3)
C3	C3A	C4	121.8(3)	C43	C43A	C44	123.0(3)
C3	C3A	C8C	114.0(3)	C43	C43A	C48C	113.3(3)
C4	C3A	C8C	103.6(3)	C44	C43A	C48C	102.9(3)
C5	C4	C3A	104.6(3)	C45	C44	C43A	105.4(3)
C5	C4	C11	127.1(4)	C45	C44	C51	128.7(4)
C11	C4	C3A	127.6(3)	C51	C44	C43A	125.0(3)
C4	C5	C6	106.2(3)	C44	C45	C46	106.1(3)
C4	C5	C13	127.7(4)	C44	C45	C53	127.1(4)
C13	C5	C6	125.4(4)	C53	C45	C46	124.6(4)
O10	C6	C5	100.3(3)	O50	C46	C45	100.6(3)
O10	C6	C6A	102.5(3)	O50	C46	C46A	102.8(3)
C5	C6	C6A	105.9(3)	C45	C46	C46A	104.7(3)
C6	C6A	C8C	100.3(3)	C46	C46A	C48C	100.6(3)
C7	C6A	C6	117.0(3)	C47	C46A	C46	118.2(3)
C7	C6A	C8C	100.2(3)	C47	C46A	C48C	100.3(3)
O9	C7	C6A	104.6(3)	O49	C47	C46A	104.1(3)
O9	C7	C7A	101.8(3)	O49	C47	C47A	101.8(3)
C6A	C7	C7A	104.1(3)	C47A	C47	C46A	104.1(3)
O8	C7A	C7	113.9(3)	O48	C47A	C47	114.1(3)
O8	C7A	C8A	59.8(2)	O48	C47A	C48A	59.3(2)
C8A	C7A	C7	103.6(3)	C48A	C47A	C47	103.8(3)
O8	C8A	C7A	59.3(2)	O48	C48A	C47A	59.6(2)
O8	C8A	C8B	114.1(3)	O48	C48A	C48B	114.5(3)
C7A	C8A	C8B	103.0(3)	C47A	C48A	C48B	102.6(3)
O9	C8B	C1	111.1(3)	O49	C48B	C41	111.2(3)
O9	C8B	C8A	101.8(3)	O49	C48B	C48A	102.0(3)
O9	C8B	C8C	103.0(3)	O49	C48B	C48C	103.6(3)
C1	C8B	C8A	122.4(3)	C41	C48B	C48A	121.8(3)
C1	C8B	C8C	113.1(3)	C41	C48B	C48C	113.3(3)
C8A	C8B	C8C	103.2(3)	C48C	C48B	C48A	102.8(3)
C3A	C8C	C6A	101.8(3)	C46A	C48C	C43A	102.0(3)
C8B	C8C	C3A	111.9(3)	C48B	C48C	C43A	112.5(3)
C8B	C8C	C6A	102.5(3)	C48B	C48C	C46A	102.5(3)
O1	C11	O2	124.2(4)	O41	C51	O42	124.9(4)
O1	C11	C4	124.5(4)	O41	C51	C44	124.6(4)

Table S29 Bond Angles for 4.							
Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O2	C11	C4	111.3(3)	O42	C51	C44	110.6(3)
O3	C13	O4	124.1(4)	O43	C53	O44	124.6(4)
O3	C13	C5	124.3(4)	O43	C53	C45	124.8(4)
O4	C13	C5	111.6(4)	O44	C53	C45	110.6(3)
C31	O22	C32	116.0(3)	C71	O62	C72	116.3(3)
C33	O24	C34	114.2(3)	C73	O64	C74	115.4(4)
C27A	O28	C28A	61.2(2)	C68A	O68	C67A	61.3(2)
C27	O29	C28B	98.1(3)	C67	O69	C68B	97.9(3)
C26	O30	C23A	97.2(3)	C66	O70	C63A	97.5(3)
C23	N22	C21	113.2(3)	C61	N62	C63	113.2(3)
N22	C21	C28B	113.5(3)	N62	C61	C68B	113.7(3)
N22	C23	C23A	112.6(3)	N62	C63	C63A	112.5(3)
O30	C23A	C23	111.5(3)	O70	C63A	C63	111.0(3)
O30	C23A	C24	99.9(3)	O70	C63A	C64	100.0(3)
O30	C23A	C28C	102.7(3)	O70	C63A	C68C	102.3(3)
C23	C23A	C24	122.9(3)	C63	C63A	C64	122.1(3)
C23	C23A	C28C	114.0(3)	C63	C63A	C68C	114.9(3)
C24	C23A	C28C	103.2(3)	C64	C63A	C68C	103.8(3)
C25	C24	C23A	105.2(3)	C65	C64	C63A	105.4(3)
C25	C24	C31	129.4(4)	C65	C64	C71	128.2(4)
C31	C24	C23A	124.1(3)	C71	C64	C63A	125.9(3)
C24	C25	C26	106.1(3)	C64	C65	C66	105.9(3)
C24	C25	C33	128.4(4)	C64	C65	C73	129.0(4)
C33	C25	C26	123.3(4)	C73	C65	C66	124.6(4)
C26	C26A	C28C	99.8(3)	O70	C66	C65	100.1(3)
C27	C26A	C26	117.7(3)	O70	C66	C66A	102.8(3)
C27	C26A	C28C	100.3(3)	C65	C66	C66A	105.6(3)
O30	C26	C25	100.7(3)	C66	C66A	C67	116.5(3)
O30	C26	C26A	103.7(3)	C66	C66A	C68C	100.8(3)
C25	C26	C26A	104.4(3)	C67	C66A	C68C	100.1(3)
O28	C27A	C27	113.4(3)	O69	C67	C66A	103.9(3)
O28	C27A	C28A	59.5(2)	O69	C67	C67A	102.2(3)
C28A	C27A	C27	103.2(3)	C67A	C67	C66A	103.9(3)
O29	C27	C26A	103.9(3)	O68	C67A	C67	113.5(3)
O29	C27	C27A	102.3(3)	O68	C67A	C68A	59.2(2)
C27A	C27	C26A	103.9(3)	C68A	C67A	C67	103.4(3)
O29	C28B	C21	111.5(3)	O68	C68A	C67A	59.4(2)
O29	C28B	C28A	102.1(3)	O68	C68A	C68B	114.4(3)

Table S29 Bond Angles for 4.							
Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O29	C28B	C28C	102.9(3)	C67A	C68A	C68B	103.3(3)
C21	C28B	C28A	121.9(3)	O69	C68B	C61	110.8(3)
C21	C28B	C28C	113.6(3)	O69	C68B	C68A	101.8(3)
C28A	C28B	C28C	102.6(3)	O69	C68B	C68C	102.6(3)
O28	C28A	C27A	59.3(2)	C61	C68B	C68A	122.9(3)
O28	C28A	C28B	114.6(3)	C61	C68B	C68C	113.3(3)
C27A	C28A	C28B	103.2(3)	C68A	C68B	C68C	103.2(3)
C23A	C28C	C26A	102.6(3)	C66A	C68C	C63A	102.0(3)
C23A	C28C	C28B	112.3(3)	C68B	C68C	C63A	111.9(3)
C28B	C28C	C26A	102.5(3)	C68B	C68C	C66A	103.1(3)
O21	C31	O22	125.5(4)	O61	C71	O62	123.7(4)
O21	C31	C24	124.5(4)	O61	C71	C64	123.9(4)
O22	C31	C24	110.0(3)	O62	C71	C64	112.4(3)
O23	C33	O24	124.2(4)	O63	C73	O64	123.8(4)
O23	C33	C25	123.4(4)	O63	C73	C65	124.5(4)
O24	C33	C25	112.4(4)	O64	C73	C65	111.8(4)

Table S30 Hydrogen Bonds for 4.						
D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
N2	H2	O68	0.86(5)	2.62(5)	3.322(5)	140(4)
C3	H3B	$O3^{1}$	0.99	2.51	3.496(5)	173.7
C6A	H6AA	$O30^{2}$	1.00	2.35	3.280(5)	153.9
C7	H7A	$O48^{3}$	1.00	2.43	3.113(5)	125.0
C7A	H7AA	$O29^{2}$	1.00	2.32	3.271(5)	157.8
C14	H14A	$O61^{4}$	0.98	2.50	3.395(6)	152.4
C21	H21B	$O68^{3}$	0.99	2.58	3.123(5)	114.5
C23	H23A	$O23^{3}$	0.99	2.60	3.576(5)	168.7
C23	H23B	$O3^{5}$	0.99	2.43	3.306(5)	147.0
C26A	H26A	O10	1.00	2.30	3.226(5)	154.3
C27A	H27A	O9	1.00	2.35	3.327(5)	165.0
C28A	H28B	$N2^{3}$	1.00	2.55	3.436(5)	147.8
C34	H34A	$O44^{6}$	0.98	2.42	3.227(6)	139.0
C34	H34B	O1	0.98	2.55	3.511(6)	165.4
C41	H41B	$O8^{1}$	0.99	2.57	3.113(5)	114.6
C43	H43B	O63	0.99	2.41	3.290(5)	148.0
C46A	H46A	$O70^{2}$	1.00	2.28	3.219(5)	156.6
C47A	H47A	$O69^{2}$	1.00	2.34	3.321(5)	166.2

Table S30 Hydrogen Bonds for 4.						
D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
C48A	H48B	N62[7]	1.00	2.56	3.448(5)	148.0
C54	H54B	O61[2]	0.98	2.53	3.493(6)	167.0
N62	H62	O8[5]	0.89(5)	2.57(5)	3.330(5)	143(4)
C63	H63B	O63[3]	0.99	2.42	3.410(5)	174.4
C66A	H66A	O50	1.00	2.33	3.263(5)	154.5
C67	H67B	O28[1]	1.00	2.45	3.134(5)	124.8
C67A	H67A	O49	1.00	2.32	3.270(5)	158.8

[1]1+X,+Y,+Z; [2]+X,1+Y,+Z; [3]-1+X,+Y,+Z; [4]+X,1+Y,-1+Z; [5]+X,-1+Y,+Z; [6]+X,+Y,-1+Z; [7]1+X,1+Y,+Z

Table S31 Torsion Angles for 4.									
A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
O8	C7A	C8A	C8B	110.5(3)	O48	C47A	C48A	C48B	-111.2(3)
O8	C8A	C8B	O9	28.6(4)	O48	C48A	C48B	O49	-28.1(4)
O8	C8A	C8B	C1	-96.1(4)	O48	C48A	C48B	C41	96.5(4)
O8	C8A	C8B	C8C	135.2(3)	O48	C48A	C48B	C48C	-135.3(3)
O9	C7	C7A	O8	-30.1(4)	O49	C47	C47A	O48	30.3(4)
O9	C7	C7A	C8A	32.6(4)	O49	C47	C47A	C48A	-31.9(4)
O9	C8B	C8C	C3A	-76.3(4)	O49	C48B	C48C	C43A	78.1(4)
O9	C8B	C8C	C6A	32.0(3)	O49	C48B	C48C	C46A	-30.6(3)
O10	C3A	C4	C5	33.0(4)	O50	C43A	C44	C45	-32.9(4)
O10	C3A	C4	C11	-155.8(4)	O50	C43A	C44	C51	157.2(3)
O10	C3A	C8C	C6A	-31.3(3)	O50	C43A	C48C	C46A	31.9(3)
O10	C3A	C8C	C8B	77.4(3)	O50	C43A	C48C	C48B	-77.2(4)
O10	C6	C6A	C7	-70.2(4)	O50	C46	C46A	C47	71.9(4)
O10	C6	C6A	C8C	36.9(3)	O50	C46	C46A	C48C	-36.0(4)
N2	C1	C8B	O9	64.5(4)	N42	C41	C48B	O49	-67.5(4)
N2	C1	C8B	C8A	-175.1(3)	N42	C41	C48B	C48A	172.2(3)
N2	C1	C8B	C8C	-50.7(4)	N42	C41	C48B	C48C	48.8(4)
N2	C3	C3A	O10	-67.1(4)	N42	C43	C43A	O50	65.3(4)
N2	C3	C3A	C4	174.0(3)	N42	C43	C43A	C44	-175.1(3)
N2	C3	C3A	C8C	48.6(5)	N42	C43	C43A	C48C	-50.4(4)
C1	N2	C3	C3A	-54.6(4)	C41	N42	C43	C43A	55.9(4)
C1	C8B	C8C	C3A	43.7(4)	C41	C48B	C48C	C43A	-42.5(4)
C1	C8B	C8C	C6A	152.1(3)	C41	C48B	C48C	C46A	-151.3(3)
C3	N2	C1	C8B	56.0(4)	C43	N42	C41	C48B	-55.0(4)

Table S31 Torsion Angles for 4.									
A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
C3	C3A	C4	C5	156.8(4)	C43	C43A	C44	C45	-157.8(4)
C3	C3A	C4	C11	-32.0(6)	C43	C43A	C44	C51	32.2(6)
C3	C3A	C8C	C6A	-151.9(3)	C43	C43A	C48C	C46A	152.9(3)
C3	C3A	C8C	C8B	-43.1(4)	C43	C43A	C48C	C48B	43.8(4)
C3A	O10	C6	C5	51.2(3)	C43A	O50	C46	C45	-50.9(3)
C3A	O10	C6	C6A	-57.8(3)	C43A	O50	C46	C46A	57.0(3)
C3A	C4	C5	C6	-0.4(4)	C43A	C44	C45	C46	0.5(4)
C3A	C4	C5	C13	170.6(4)	C43A	C44	C45	C53	-162.9(4)
C3A	C4	C11	O1	89.3(5)	C43A	C44	C51	O41	-88.5(5)
C3A	C4	C11	O2	-90.5(5)	C43A	C44	C51	O42	90.4(4)
C4	C3A	C8C	C6A	73.6(3)	C44	C43A	C48C	C46A	-72.2(3)
C4	C3A	C8C	C8B	-177.7(3)	C44	C43A	C48C	C48B	178.7(3)
C4	C5	C6	O10	-32.0(4)	C44	C45	C46	O50	31.8(4)
C4	C5	C6	C6A	74.3(4)	C44	C45	C46	C46A	-74.6(4)
C4	C5	C13	O3	-170.2(4)	C44	C45	C53	O43	156.5(4)
C4	C5	C13	O4	9.8(6)	C44	C45	C53	O44	-22.6(6)
C5	C4	C11	O1	-101.3(5)	C45	C44	C51	O41	104.0(5)
C5	C4	C11	O2	78.9(5)	C45	C44	C51	O42	-77.2(5)
C5	C6	C6A	C7	-174.8(3)	C45	C46	C46A	C47	176.7(3)
C5	C6	C6A	C8C	-67.7(3)	C45	C46	C46A	C48C	68.8(3)
C6	O10	C3A	C3	177.4(3)	C46	O50	C43A	C43	-176.7(3)
C6	O10	C3A	C4	-51.9(3)	C46	O50	C43A	C44	51.2(3)
C6	O10	C3A	C8C	55.0(3)	C46	O50	C43A	C48C	-54.8(3)
C6	C5	C13	O3	-0.7(6)	C46	C45	C53	O43	-4.1(6)
C6	C5	C13	O4	179.2(3)	C46	C45	C53	O44	176.8(3)
C6	C6A	C7	O9	73.4(4)	C46	C46A	C47	O49	-73.0(4)
C6	C6A	C7	C7A	179.9(3)	C46	C46A	C47	C47A	-179.3(3)
C6	C6A	C8C	C3A	-3.3(3)	C46	C46A	C48C	C43A	2.4(4)
C6	C6A	C8C	C8B	-119.2(3)	C46	C46A	C48C	C48B	119.1(3)
C6A	C7	C7A	O8	-138.7(3)	C46A	C47	C47A	O48	138.3(3)
C6A	C7	C7A	C8A	-76.0(3)	C46A	C47	C47A	C48A	76.0(3)
C7	O9	C8B	C1	-174.5(3)	C47	O49	C48B	C41	174.6(3)
C7	O9	C8B	C8A	53.7(3)	C47	O49	C48B	C48A	-54.0(3)
C7	O9	C8B	C8C	-53.1(3)	C47	O49	C48B	C48C	52.5(3)
C7	C6A	C8C	C3A	116.7(3)	C47	C46A	C48C	C43A	-119.1(3)
C7	C6A	C8C	C8B	0.8(3)	C47	C46A	C48C	C48B	-2.5(3)
C7	C7A	C8A	O8	-110.0(3)	C47	C47A	C48A	O48	110.1(3)
C7	C7A	C8A	C8B	0.5(4)	C47	C47A	C48A	C48B	-1.1(4)

Table S31 Torsion Angles for 4.									
A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
C7A	O8	C8A	C8B	-91.2(3)	C47A	O48	C48A	C48B	90.5(4)
C7A	C8A	C8B	O9	-33.3(3)	C47A	C48A	C48B	O49	34.0(4)
C7A	C8A	C8B	C1	-158.0(3)	C47A	C48A	C48B	C41	158.5(3)
C7A	C8A	C8B	C8C	73.3(3)	C47A	C48A	C48B	C48C	-73.2(3)
C8A	O8	C7A	C7	92.2(3)	C48A	O48	C47A	C47	-92.2(3)
C8A	C8B	C8C	C3A	178.0(3)	C48A	C48B	C48C	C43A	-175.9(3)
C8A	C8B	C8C	C6A	-73.7(3)	C48A	C48B	C48C	C46A	75.3(3)
C8B	O9	C7	C6A	54.9(3)	C48B	O49	C47	C46A	-55.0(3)
C8B	O9	C7	C7A	-53.3(3)	C48B	O49	C47	C47A	53.0(3)
C8C	C3A	C4	C5	-73.3(4)	C48C	C43A	C44	C45	72.9(4)
C8C	C3A	C4	C11	98.0(4)	C48C	C43A	C44	C51	-97.0(4)
C8C	C6A	C7	O9	-33.8(3)	C48C	C46A	C47	O49	35.0(3)
C8C	C6A	C7	C7A	72.7(3)	C48C	C46A	C47	C47A	-71.3(3)
C11	C4	C5	C6	-171.7(4)	C51	C44	C45	C46	169.9(4)
C11	C4	C5	C13	-0.7(7)	C51	C44	C45	C53	6.5(7)
C12	O2	C11	O1	10.7(6)	C52	O42	C51	O41	-3.7(6)
C12	O2	C11	C4	-169.5(3)	C52	O42	C51	C44	177.5(4)
C13	C5	C6	O10	156.7(4)	C53	C45	C46	O50	-164.2(3)
C13	C5	C6	C6A	-97.0(4)	C53	C45	C46	C46A	89.4(4)
C14	O4	C13	O3	3.7(6)	C54	O44	C53	O43	-3.0(6)
C14	O4	C13	C5	-176.2(3)	C54	O44	C53	C45	176.1(4)
O28	C27A	C27	O29	30.9(4)	O68	C67A	C68A	C68B	110.7(3)
O28	C27A	C27	C26A	138.7(3)	O68	C68A	C68B	O69	28.7(4)
O28	C27A	C28A	C28B	-110.9(3)	O68	C68A	C68B	C61	-95.8(4)
O29	C28B	C28A	O28	-28.5(4)	O68	C68A	C68B	C68C	134.8(3)
O29	C28B	C28A	C27A	33.5(4)	O69	C67	C67A	O68	-30.3(4)
O29	C28B	C28C	C23A	78.8(3)	O69	C67	C67A	C68A	31.7(4)
O29	C28B	C28C	C26A	-30.7(3)	O69	C68B	C68C	C63A	-77.2(4)
O30	C23A	C24	C25	-33.3(4)	O69	C68B	C68C	C66A	31.7(3)
O30	C23A	C24	C31	158.6(3)	O70	C63A	C64	C65	32.6(4)
O30	C23A	C28C	C26A	31.8(4)	O70	C63A	C64	C71	-154.9(4)
O30	C23A	C28C	C28B	-77.5(4)	O70	C63A	C68C	C66A	-31.6(3)
N22	C21	C28B	O29	-67.8(4)	O70	C63A	C68C	C68B	77.9(4)
N22	C21	C28B	C28A	171.5(3)	O70	C66	C66A	C67	-71.1(4)
N22	C21	C28B	C28C	48.0(4)	O70	C66	C66A	C68C	36.0(3)
N22	C23	C23A	O30	65.4(4)	N62	C61	C68B	O69	64.7(4)
N22	C23	C23A	C24	-176.2(3)	N62	C61	C68B	C68A	-174.9(3)
N22	C23	C23A	C28C	-50.4(4)	N62	C61	C68B	C68C	-49.9(4)

Table S31 Torsion Angles for 4.									
A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
C21	N22	C23	C23A	55.8(4)	N62	C63	C63A	O70	-67.1(4)
C21	C28B	C28A	O28	96.6(4)	N62	C63	C63A	C64	175.6(3)
C21	C28B	C28A	C27A	158.6(3)	N62	C63	C63A	C68C	48.4(4)
C21	C28B	C28C	C23A	-41.9(4)	C61	N62	C63	C63A	-54.6(4)
C21	C28B	C28C	C26A	-151.4(3)	C61	C68B	C68C	C63A	42.3(4)
C23	N22	C21	C28B	-55.1(5)	C61	C68B	C68C	C66A	151.2(3)
C23	C23A	C24	C25	-157.1(3)	C63	N62	C61	C68B	56.0(4)
C23	C23A	C24	C31	34.8(6)	C63	C63A	C64	C65	155.3(4)
C23	C23A	C28C	C26A	152.6(3)	C63	C63A	C64	C71	-32.3(6)
C23	C23A	C28C	C28B	43.2(4)	C63	C63A	C68C	C66A	-152.0(3)
C23A	O30	C26	C25	-51.4(3)	C63	C63A	C68C	C68B	-42.5(4)
C23A	O30	C26	C26A	56.4(3)	C63A	O70	C66	C65	51.7(3)
C23A	C24	C25	C26	1.0(4)	C63A	O70	C66	C66A	-56.9(3)
C23A	C24	C25	C33	-162.1(4)	C63A	C64	C65	C66	-0.3(4)
C23A	C24	C31	O21	-83.8(5)	C63A	C64	C65	C73	171.9(4)
C23A	C24	C31	O22	94.4(4)	C63A	C64	C71	O61	81.6(5)
C24	C23A	C28C	C26A	-71.7(3)	C63A	C64	C71	O62	-98.2(4)
C24	C23A	C28C	C28B	178.9(3)	C64	C63A	C68C	C66A	72.0(3)
C24	C25	C26	O30	31.9(4)	C64	C63A	C68C	C68B	-178.4(3)
C24	C25	C26	C26A	-75.4(4)	C64	C65	C66	O70	-32.5(4)
C24	C25	C33	O23	148.8(4)	C64	C65	C66	C66A	73.9(4)
C24	C25	C33	O24	-30.6(6)	C64	C65	C73	O63	-164.6(4)
C25	C24	C31	O21	111.1(5)	C64	C65	C73	O64	16.5(6)
C25	C24	C31	O22	-70.8(5)	C65	C64	C71	O61	-107.6(5)
C26	O30	C23A	C23	-176.8(3)	C65	C64	C71	O62	72.5(5)
C26	O30	C23A	C24	51.8(3)	C65	C66	C66A	C67	-175.5(3)
C26	O30	C23A	C28C	-54.3(3)	C65	C66	C66A	C68C	-68.5(3)
C26	C25	C33	O23	-11.7(6)	C66	O70	C63A	C63	177.9(3)
C26	C25	C33	O24	168.8(3)	C66	O70	C63A	C64	-51.9(3)
C26	C26A	C27	O29	-71.9(4)	C66	O70	C63A	C68C	54.8(3)
C26	C26A	C27	C27A	-178.5(3)	C66	C65	C73	O63	6.3(6)
C26	C26A	C28C	C23A	1.8(4)	C66	C65	C73	O64	-172.7(3)
C26	C26A	C28C	C28B	118.4(3)	C66	C66A	C67	O69	73.3(4)
C27A	O28	C28A	C28B	91.2(4)	C66	C66A	C67	C67A	179.8(3)
C27	O29	C28B	C21	175.0(3)	C66	C66A	C68C	C63A	-2.3(3)
C27	O29	C28B	C28A	-53.2(3)	C66	C66A	C68C	C68B	-118.4(3)
C27	O29	C28B	C28C	52.9(3)	C66A	C67	C67A	O68	-138.1(3)
C27	C26A	C26	O30	71.7(4)	C66A	C67	C67A	C68A	-76.2(3)

Table S31 Torsion Angles for 4.									
A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
C27	C26A	C26	C25	176.8(3)	C67	O69	C68B	C61	-174.5(3)
C27	C26A	C28C	C23A	-119.0(3)	C67	O69	C68B	C68A	53.3(3)
C27	C26A	C28C	C28B	-2.3(3)	C67	O69	C68B	C68C	-53.3(3)
C27	C27A	C28A	O28	109.6(3)	C67	C66A	C68C	C63A	117.4(3)
C27	C27A	C28A	C28B	-1.3(4)	C67	C66A	C68C	C68B	1.3(3)
C28B	O29	C27	C26A	-55.5(3)	C67	C67A	C68A	O68	-109.6(3)
C28B	O29	C27	C27A	52.3(3)	C67	C67A	C68A	C68B	1.2(4)
C28A	O28	C27A	C27	-91.9(4)	C67A	O68	C68A	C68B	-91.4(3)
C28A	C27A	C27	O29	-31.3(4)	C67A	C68A	C68B	O69	-33.5(4)
C28A	C27A	C27	C26A	76.5(4)	C67A	C68A	C68B	C61	-158.0(3)
C28A	C28B	C28C	C23A	-175.5(3)	C67A	C68A	C68B	C68C	72.6(3)
C28A	C28B	C28C	C26A	75.1(3)	C68A	O68	C67A	C67	92.0(4)
C28C	C23A	C24	C25	72.4(4)	C68A	C68B	C68C	C63A	177.4(3)
C28C	C23A	C24	C31	-95.8(4)	C68A	C68B	C68C	C66A	-73.8(3)
C28C	C26A	C26	O30	-35.5(3)	C68B	O69	C67	C66A	55.2(3)
C28C	C26A	C26	C25	69.6(3)	C68B	O69	C67	C67A	-52.6(3)
C28C	C26A	C27	O29	35.0(3)	C68C	C63A	C64	C65	-72.8(4)
C28C	C26A	C27	C27A	-71.6(3)	C68C	C63A	C64	C71	99.6(4)
C28C	C28B	C28A	O28	-134.9(3)	C68C	C66A	C67	O69	-34.2(3)
C28C	C28B	C28A	C27A	-72.9(3)	C68C	C66A	C67	C67A	72.4(3)
C31	C24	C25	C26	168.4(4)	C71	C64	C65	C66	-172.5(4)
C31	C24	C25	C33	5.2(7)	C71	C64	C65	C73	-0.3(7)
C32	O22	C31	O21	0.3(6)	C72	O62	C71	O61	6.0(6)
C32	O22	C31	C24	-177.9(4)	C72	O62	C71	C64	-174.1(3)
C33	C25	C26	O30	-163.9(3)	C73	C65	C66	O70	154.9(4)
C33	C25	C26	C26A	88.8(4)	C73	C65	C66	C66A	-98.7(4)
C34	O24	C33	O23	-5.7(6)	C74	O64	C73	O63	4.6(6)
C34	O24	C33	C25	173.8(3)	C74	O64	C73	C65	-176.4(3)

Table S32 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 4.				
Atom	***x***	***y***	***z***	**U(eq)**
H2	6640(60)	4820(50)	3690(20)	17
H1A	8189.38	7143.57	3856.07	17
H1B	7412.25	6028.65	4489.97	17
H3A	7187.13	5198.71	2514.71	18
H3B	8080.36	6604.23	2595.22	18

Table S32 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 4.				
Atom	***x***	***y***	***z***	**U(eq)**
H6A	1353.16	6248.8	3032.29	17
H6AA	2435.46	8543.53	3361.63	14
H7A	1477.12	6708.38	4437.52	15
H7AA	2493.21	9165.59	4590.33	16
H8AA	5753.39	9207.13	4369.74	16
H8CA	5495.65	8599.11	3137.59	13
H12A	7150.73	11170.24	1088.8	40
H12B	8269.84	9915.52	848.83	40
H12C	6423.9	10216.11	580.08	40
H14A	2574.5	9849.16	243.32	41
H14B	870.5	8948.43	560.85	41
H14C	1315.92	10247.72	918.68	41
H22	-1090(60)	-150(50)	3470(30)	20
H21A	-2034.42	976.13	4285.29	19
H21B	-2471.9	2155.31	3699.98	19
H23A	-1727.36	1737.65	2400.98	21
H23B	-899.95	314.87	2252.03	21
H26A	3683.91	3397.83	3022.93	15
H26B	4772.25	1054.72	2665.83	18
H27A	2967.5	4064.04	4255.2	18
H27B	3965.43	1570.46	4095.57	17
H28B	-209.88	4147.11	4118.54	16
H28A	733.15	3562.48	2891.71	14
H32A	253.7	6371.57	1045.79	43
H32B	697.74	5432.31	428.7	43
H32C	-1090.5	5203.71	962.3	43
H34A	5809.92	4712.88	-58.98	46
H34B	6129.74	5270.69	659.45	46
H34C	7231.81	4027.03	394.42	46
H42	10800(60)	4030(50)	6540(30)	21
H41A	12027.68	5644.49	5683.25	19
H41B	12465.74	6528.18	6278.02	19
H43A	11711.21	5497.46	7568.2	21
H43B	10878.88	4008.23	7710.29	21
H46B	5190.61	5009.97	7310.76	18
H46A	6342.78	7500.62	6949.71	15
H47B	6021.68	6184.49	5880.6	16

Table S32 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 4.				
Atom	***x***	***y***	***z***	**U(eq)**
H47A	7045.77	8734.23	5724.15	16
H48B	10209.97	8748.3	5858.92	16
H48A	9285.48	7578.22	7079.39	14
H52A	9941.8	9428.22	8945.11	49
H52B	9199.09	8250.28	9552.46	49
H52C	11098.68	8132.01	9112.32	49
H54A	4698.88	7550.64	10024.92	46
H54B	4048.17	8337.72	9336.03	46
H54C	3136.41	6936.12	9690.82	46
H62	3320(60)	-790(50)	6280(20)	18
H61A	1785.48	1618.94	6137.12	17
H61B	2562.79	785.37	5508.31	17
H63A	2781.16	-932.29	7494.46	19
H63B	1892.66	513.33	7408.67	19
H66B	8613.73	294.45	6950.17	18
H66A	7558.37	2760.36	6635.19	15
H67B	8501.53	1426.35	5548.06	17
H67A	7506.45	3960.6	5401.29	18
H68B	4238.26	3909.93	5621.18	17
H68A	4512.16	2745.72	6849.84	14
H72A	2986.08	4320.79	9004.46	42
H72B	1701.83	3033.12	9123.75	42
H72C	3415.8	3001.46	9505.56	42
H74A	7685.33	2241.73	9807.01	41
H74B	9375.68	1609.59	9395.86	41
H74C	8788.96	3099.79	9134.07	41

Table S33 Crystal data and structure refinement for 5.	
Identification code	FZ1
Empirical formula	$C_{16}H_{18}ClNO_6$
Formula weight	355.76
Temperature/K	295(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	7.8932(10)
b/Å	26.076(3)
c/Å	8.2119(10)

α/°	90
β/°	107.482(14)
γ/°	90
Volume/Å^3	1612.1(4)
Z	4
ρ_{calc}g/cm^3	1.466
μ/mm^{-1}	0.270
F(000)	744.0
Crystal size/mm^3	0.42 × 0.31 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	7.002 to 59.968
Index ranges	-10 ≤ h ≤ 10, -36 ≤ k ≤ 36, -10 ≤ l ≤ 11
Reflections collected	14665
Independent reflections	4364 [R_{int} = 0.0670, R_{sigma} = 0.0649]
Data/restraints/parameters	4364/0/224
Goodness-of-fit on F^2	1.082
Final R indexes [I>=2σ (I)]	R_1 = 0.0691, wR_2 = 0.1751
Final R indexes [all data]	R_1 = 0.0959, wR_2 = 0.2043
Largest diff. peak/hole / e Å^{-3}	0.61/-0.40

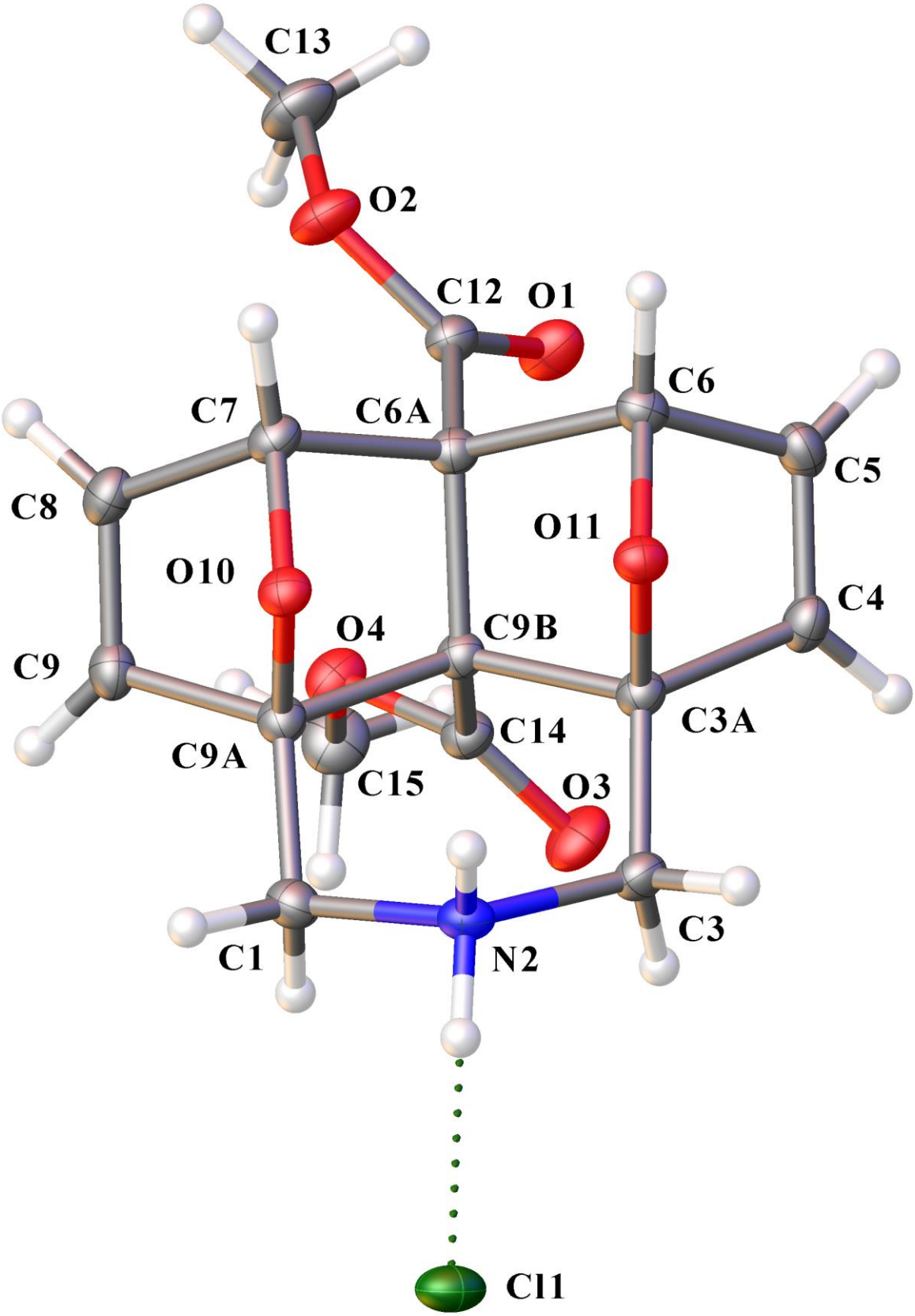


Figure S8. View of one molecule in the crystal of compound **5**

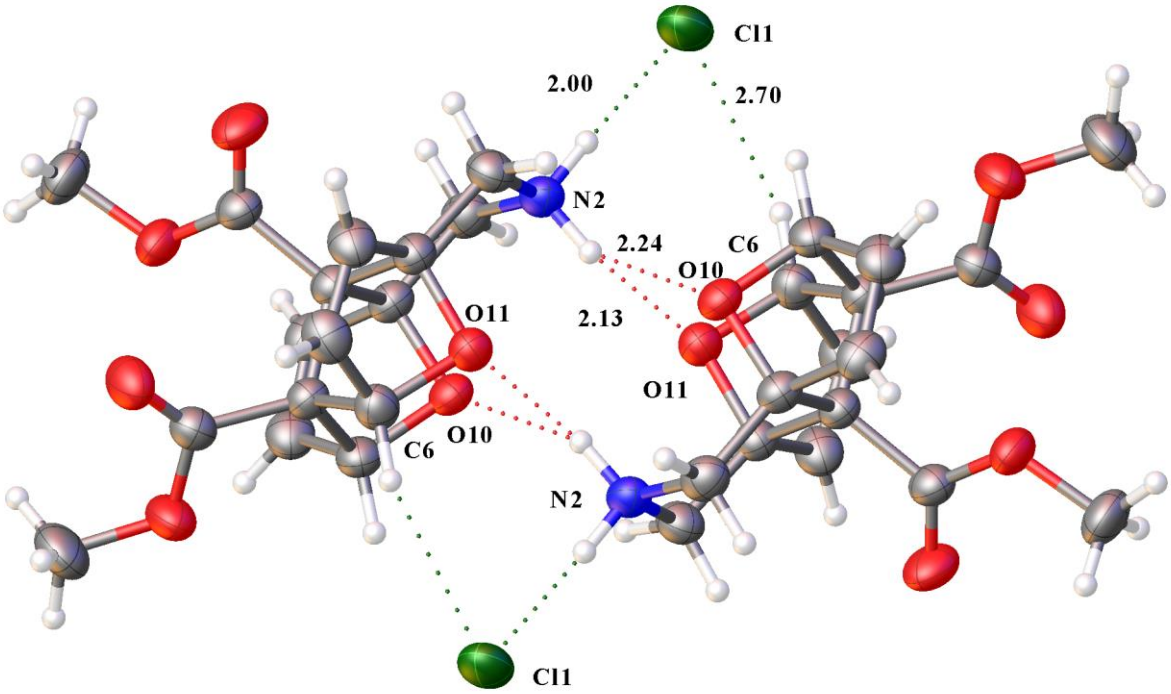


Figure S9. The H-bonds in the crystal of compound **5**. Non-bonded hydrogens are omitted for clarity.

Table S34 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 5. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cl1	10159.1(9)	5746.8(3)	7676.4(10)	52.0(3)
O1	4628(3)	2797.2(7)	6434(3)	51.8(6)
O2	2284(3)	3160.7(7)	6774(3)	53.1(6)
O3	8788(3)	3480.4(8)	8108(3)	54.1(6)
O4	6787(3)	3329.8(7)	9435(3)	43.7(5)
O10	4170(2)	4587.2(6)	6772(2)	34.9(4)
O11	5099(2)	4246.9(6)	4145(2)	35.6(4)
N2	7470(3)	4931.8(8)	6693(3)	36.3(5)
C1	7096(4)	4799.8(10)	8368(3)	39.2(6)
C3	8007(3)	4494.0(9)	5782(4)	38.6(6)
C3A	6684(3)	4076.1(9)	5387(3)	33.0(5)
C4	6979(4)	3587.0(9)	4467(4)	40.7(6)
C5	5451(4)	3396.7(10)	3724(4)	42.4(6)
C6	4192(4)	3771.0(9)	4084(3)	36.6(5)
C6A	4250(3)	3715.1(9)	6115(3)	32.7(5)
C7	3176(3)	4131.2(9)	6752(3)	36.8(5)
C8	3474(4)	4058.9(10)	8732(4)	41.8(6)
C9	5047(4)	4223.9(9)	9532(4)	40.1(6)
C9A	5706(3)	4401.9(9)	8028(3)	33.8(5)

Table S34 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 5. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C9B	6095(3)	3912.3(8)	7029(3)	31.4(5)
C12	3802(3)	3173.2(9)	6469(3)	37.1(5)
C13	1760(5)	2672.8(12)	7262(6)	65.1(10)
C14	7383(3)	3550.4(9)	8231(3)	36.2(5)
C15	7900(5)	2966.1(11)	10591(4)	53.8(8)

Table S35 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 5. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	38.0(4)	58.3(5)	51.6(5)	1.7(3)	1.5(3)	-12.6(3)
O1	49.0(12)	34.9(10)	75.9(16)	1.6(9)	25.5(11)	0.8(8)
O2	35.6(10)	45.4(11)	81.6(16)	9.3(10)	22.7(11)	-2.3(8)
O3	36.2(11)	62.5(13)	65.8(14)	15.2(10)	18.7(10)	17.8(9)
O4	37.6(10)	45.5(10)	47.4(11)	15.0(8)	12.0(9)	9.2(7)
O10	29.7(8)	33.4(9)	39.7(9)	3.1(7)	7.6(7)	6.2(6)
O11	33.2(9)	35.2(9)	36.2(9)	3.2(7)	7.4(7)	-0.7(6)
N2	29.5(10)	34.5(11)	40.5(12)	1.0(8)	3.6(9)	-1.9(8)
C1	36.8(13)	37.8(13)	40.0(14)	-3.8(10)	6.7(11)	1.1(10)
C3	31.7(12)	40.5(13)	45.4(14)	0.1(11)	14.3(11)	-2.5(9)
C3A	29.9(11)	32.0(12)	37.1(12)	0.8(9)	10.1(9)	2.4(8)
C4	42.0(14)	38.2(13)	48.3(15)	-1.6(11)	23.1(12)	3.7(10)
C5	51.1(16)	38.9(13)	40.2(14)	-7.6(11)	18.3(13)	-4.0(11)
C6	37.4(13)	35.6(12)	35.2(13)	0.1(9)	8.4(10)	-2.7(9)
C6A	30.2(11)	32.2(12)	34.0(12)	2.1(9)	7.4(9)	2.1(8)
C7	29.1(11)	37.3(13)	44.6(14)	3.1(10)	12.1(10)	3.1(9)
C8	40.7(14)	41.8(14)	48.9(15)	2.1(11)	22.7(12)	5.3(10)
C9	43.4(14)	43.0(14)	36.4(13)	0.1(10)	15.8(11)	8.9(10)
C9A	30.9(11)	35.4(12)	33.9(12)	0.9(9)	8.1(10)	5.2(9)
C9B	29.0(11)	29.7(11)	35.4(12)	0.7(9)	9.6(9)	3.6(8)
C12	33.0(12)	38.3(13)	40.0(14)	-0.1(10)	11.0(11)	-2.5(9)
C13	53.8(19)	56.7(19)	93(3)	10.4(17)	34(2)	-12.5(14)
C14	30.3(12)	35.1(12)	42.4(14)	0.7(10)	9.8(10)	3.9(9)
C15	53.0(17)	50.6(17)	54.1(18)	18.7(13)	10.3(15)	16.4(13)

Table S36 Bond Lengths for 5.					
Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
O1	C12	1.182(3)	C3A	C4	1.535(3)
O2	C12	1.297(3)	C3A	C9B	1.611(3)
O2	C13	1.431(4)	C4	C5	1.277(4)
O3	C14	1.158(3)	C5	C6	1.485(4)
O4	C14	1.345(3)	C6	C6A	1.662(3)
O4	C15	1.439(3)	C6A	C7	1.560(3)
O10	C7	1.422(3)	C6A	C9B	1.514(3)
O10	C9A	1.420(3)	C6A	C12	1.506(3)
O11	C3A	1.427(3)	C7	C8	1.583(4)
O11	C6	1.426(3)	C8	C9	1.291(4)
N2	C1	1.530(3)	C9	C9A	1.548(4)
N2	C3	1.494(3)	C9A	C9B	1.597(3)
C1	C9A	1.475(4)	C9B	C14	1.515(3)
C3	C3A	1.476(3)			

Table S37 Bond Angles for 5.							
Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C12	O2	C13	116.0(2)	O10	C7	C6A	103.42(18)
C14	O4	C15	119.2(2)	O10	C7	C8	100.2(2)
C9A	O10	C7	94.10(17)	C6A	C7	C8	109.5(2)
C6	O11	C3A	94.40(17)	C9	C8	C7	107.8(2)
C3	N2	C1	116.0(2)	C8	C9	C9A	101.3(2)
C9A	C1	N2	108.8(2)	O10	C9A	C1	108.8(2)
C3A	C3	N2	112.71(19)	O10	C9A	C9	105.27(19)
O11	C3A	C3	109.69(19)	O10	C9A	C9B	98.81(18)
O11	C3A	C4	97.9(2)	C1	C9A	C9	118.0(2)
O11	C3A	C9B	105.62(17)	C1	C9A	C9B	114.4(2)
C3	C3A	C4	121.3(2)	C9	C9A	C9B	109.44(19)
C3	C3A	C9B	112.0(2)	C6A	C9B	C3A	98.73(19)
C4	C3A	C9B	108.42(18)	C6A	C9B	C9A	102.77(17)
C5	C4	C3A	107.3(2)	C6A	C9B	C14	117.9(2)
C4	C5	C6	104.0(2)	C9A	C9B	C3A	111.52(17)
O11	C6	C5	102.7(2)	C14	C9B	C3A	113.88(18)
O11	C6	C6A	100.29(18)	C14	C9B	C9A	111.0(2)
C5	C6	C6A	108.9(2)	O1	C12	O2	122.1(2)
C7	C6A	C6	114.93(19)	O1	C12	C6A	127.7(2)
C9B	C6A	C6	101.53(18)	O2	C12	C6A	110.2(2)

Table S37 Bond Angles for 5.							
Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C9B	C6A	C7	97.83(18)	O3	C14	O4	123.5(2)
C12	C6A	C6	109.78(19)	O3	C14	C9B	121.0(2)
C12	C6A	C7	113.93(19)	O4	C14	C9B	115.5(2)
C12	C6A	C9B	118.0(2)				

Table S38 Hydrogen Bonds for 5.						
D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
N2	H2A	O10[1]	0.93(3)	2.24(3)	3.022(3)	141(2)
N2	H2A	O11[1]	0.93(3)	2.14(3)	2.887(3)	137(3)
N2	H2B	Cl1	0.94(3)	2.00(3)	2.940(2)	178(3)
C1	H1A	Cl1[2]	0.97	2.74	3.612(3)	149.8
C3	H3A	Cl1[3]	0.97	2.85	3.609(3)	136.2
C6	H6A	Cl1[1]	0.98	2.70	3.533(3)	143.4
C13	H13A	O3[4]	0.96	2.64	3.377(4)	134.2

[1]1-X,1-Y,1-Z; [2]2-X,1-Y,2-Z; [3]2-X,1-Y,1-Z; [4]-1+X,+Y,+Z

Table S39 Torsion Angles for 5.									
A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
O10	C7	C8	C9	-33.5(2)	C6	C6A	C7	C8	-175.43(19)
O10	C9A	C9B	C3A	67.2(2)	C6	C6A	C9B	C3A	3.56(19)
O10	C9A	C9B	C6A	-37.7(2)	C6	C6A	C9B	C9A	118.10(18)
O10	C9A	C9B	C14	-164.68(18)	C6	C6A	C9B	C14	-119.5(2)
O11	C3A	C4	C5	-36.5(3)	C6	C6A	C12	O1	65.5(4)
O11	C3A	C9B	C6A	33.3(2)	C6	C6A	C12	O2	-112.1(2)
O11	C3A	C9B	C9A	-74.2(2)	C6A	C7	C8	C9	74.8(3)
O11	C3A	C9B	C14	159.23(19)	C6A	C9B	C14	O3	128.0(3)
O11	C6	C6A	C7	65.1(2)	C6A	C9B	C14	O4	-53.0(3)
O11	C6	C6A	C9B	-39.2(2)	C7	O10	C9A	C1	179.5(2)
O11	C6	C6A	C12	-164.87(19)	C7	O10	C9A	C9	-53.2(2)
N2	C1	C9A	O10	-57.6(2)	C7	O10	C9A	C9B	59.86(18)
N2	C1	C9A	C9	-177.3(2)	C7	C6A	C9B	C3A	-113.97(18)
N2	C1	C9A	C9B	51.8(3)	C7	C6A	C9B	C9A	0.6(2)
N2	C3	C3A	O11	67.6(3)	C7	C6A	C9B	C14	123.0(2)
N2	C3	C3A	C4	-179.4(2)	C7	C6A	C12	O1	-164.0(3)
N2	C3	C3A	C9B	-49.3(3)	C7	C6A	C12	O2	18.5(3)

Table S39 Torsion Angles for 5.									
A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
C1	N2	C3	C3A	56.9(3)	C7	C8	C9	C9A	0.4(2)
C1	C9A	C9B	C3A	-48.2(3)	C8	C9	C9A	O10	33.6(2)
C1	C9A	C9B	C6A	-153.1(2)	C8	C9	C9A	C1	155.1(2)
C1	C9A	C9B	C14	80.0(3)	C8	C9	C9A	C9B	-71.8(2)
C3	N2	C1	C9A	-56.7(3)	C9	C9A	C9B	C3A	176.9(2)
C3	C3A	C4	C5	-155.3(3)	C9	C9A	C9B	C6A	72.0(2)
C3	C3A	C9B	C6A	152.69(19)	C9	C9A	C9B	C14	-55.0(3)
C3	C3A	C9B	C9A	45.2(3)	C9A	O10	C7	C6A	-63.0(2)
C3	C3A	C9B	C14	-81.4(2)	C9A	O10	C7	C8	50.04(19)
C3A	O11	C6	C5	-53.7(2)	C9A	C9B	C14	O3	-113.8(3)
C3A	O11	C6	C6A	58.55(19)	C9A	C9B	C14	O4	65.1(3)
C3A	C4	C5	C6	2.8(3)	C9B	C3A	C4	C5	73.0(3)
C3A	C9B	C14	O3	13.0(4)	C9B	C6A	C7	O10	37.3(2)
C3A	C9B	C14	O4	-168.0(2)	C9B	C6A	C7	C8	-68.8(2)
C4	C3A	C9B	C6A	-70.8(2)	C9B	C6A	C12	O1	-50.1(4)
C4	C3A	C9B	C9A	-178.3(2)	C9B	C6A	C12	O2	132.3(2)
C4	C3A	C9B	C14	55.1(3)	C12	C6A	C7	O10	162.7(2)
C4	C5	C6	O11	32.3(3)	C12	C6A	C7	C8	56.6(3)
C4	C5	C6	C6A	-73.4(3)	C12	C6A	C9B	C3A	123.6(2)
C5	C6	C6A	C7	172.5(2)	C12	C6A	C9B	C9A	-121.9(2)
C5	C6	C6A	C9B	68.2(2)	C12	C6A	C9B	C14	0.5(3)
C5	C6	C6A	C12	-57.5(3)	C13	O2	C12	O1	6.9(5)
C6	O11	C3A	C3	179.79(19)	C13	O2	C12	C6A	-175.3(3)
C6	O11	C3A	C4	52.39(19)	C15	O4	C14	O3	-3.3(4)
C6	O11	C3A	C9B	-59.33(19)	C15	O4	C14	C9B	177.7(2)
C6	C6A	C7	O10	-69.4(2)					

Table S40 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 5.				
Atom	***x***	***y***	***z***	**U(eq)**
H2A	6550(40)	5102(11)	5890(40)	44
H2B	8340(40)	5189(11)	7030(40)	44
H1A	8170.88	4675.04	9195.66	47
H1B	6702.53	5103.62	8832.73	47
H3A	8171.82	4618.36	4726.39	46
H3B	9135.66	4359.5	6483.81	46
H4A	8067.59	3453.95	4454.27	49

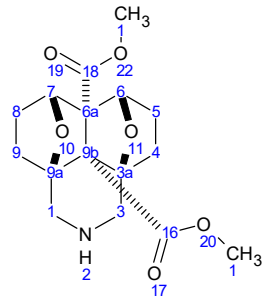
Table S40 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 5.				
Atom	***x***	***y***	***z***	**U(eq)**
H5A	5187.99	3093.71	3100.83	51
H6A	2995.84	3762.55	3268.44	44
H7A	1925.76	4155.97	6069.23	44
H8A	2661.57	3921.88	9230.97	50
H9A	5627.89	4233.28	10698.44	48
H13A	625.51	2704.28	7458.45	98
H13B	1677.65	2428.85	6366.18	98
H13C	2626.43	2558.16	8289.13	98
H15A	7296.67	2843.12	11370.08	81
H15B	8154.01	2683.12	9953.77	81
H15C	8989.95	3129.29	11219.73	81

Table S31. Hydrogen bonds with H···A < r(A) + 2.000 Å and ∠DHA > 110° between molecules of compound 5

D-H	d(D-H)	d(H..A)	∠DHA	d(D..A)	A
N1-H2A	0.96(4)	1.96(4)	176(3)	2.939(3)	Cl1
N1-H2B	0.95(3)	2.14(3)	133(3)	2.885(3)	O6 [1-x, 1-y, 1-z]
N1-H2B	0.95(3)	2.20(3)	143(3)	3.024(3)	O5 [1-x, 1-y, 1-z]
C3-H3B	1.07(4)	2.75(3)	137(3)	3.605(3)	Cl1 [2-x, 1-y, 1-z]
C5-H6	1.01(3)	2.70(3)	140(3)	3.532(3)	Cl1 [1-x, 1-y, 1-z]
C1-H1A	1.04(3)	2.67(3)	150(3)	3.613(4)	Cl1 [2-x, 1-y, 2-z]

Formula $C_{16}H_{21}NO_6$	***FW***	323.3410	

Acquisition Time (sec)	1.4549	***Comment***	single_pulse	***Date***	15 Jan 2014 09:32:20	***Date Stamp***	15 Jan 2014 08:41:42
File Name	H:\DOWNLOADS\FZ3515-1.JDF			***Frequency (MHz)***	600.17	***Nucleus***	1H	***Number of Transients***	8
Origin	ECA 600	***Original Points Count***	16384	***Owner***	delta	***Points Count***	16384	***Pulse Sequence***	single_pulse.ex2
Receiver Gain	26.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	3019.2939	***Sweep Width (Hz)***	11261.26
Temperature (degree C)	24.100								



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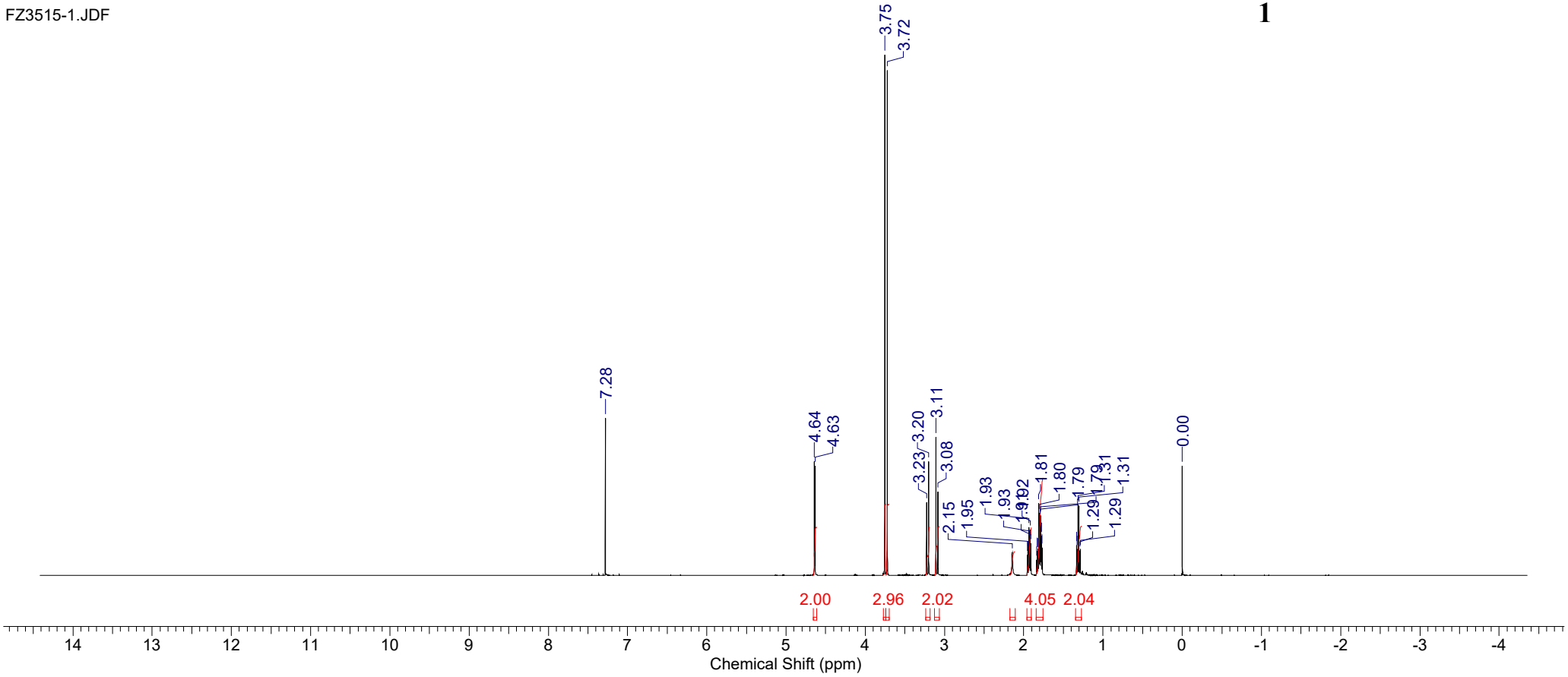
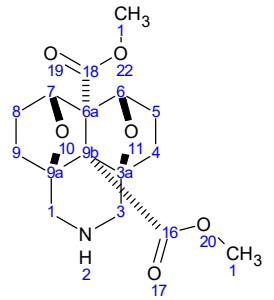
FZ3515-1.JDF



Formula $C_{16}H_{21}NO_6$	***FW***	323.3410	

Acquisition Time (sec)	1.4549	***Comment***	single_pulse	***Date***	15 Jan 2014 09:32:20		***Date Stamp***	15 Jan 2014 08:41:42
File Name	H:\DOWNLOADS\FZ3515-1.JDF			***Frequency (MHz)***	600.17	***Nucleus*** 1H	***Number of Transients***	8
Origin	ECA 600	***Original Points Count***	16384	***Owner***	delta	***Points Count*** 16384	***Pulse Sequence***	single_pulse.ex2
Receiver Gain	26.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)*** 3019.2939	***Sweep Width (Hz)***	11261.26
Temperature (degree C)	24.100							



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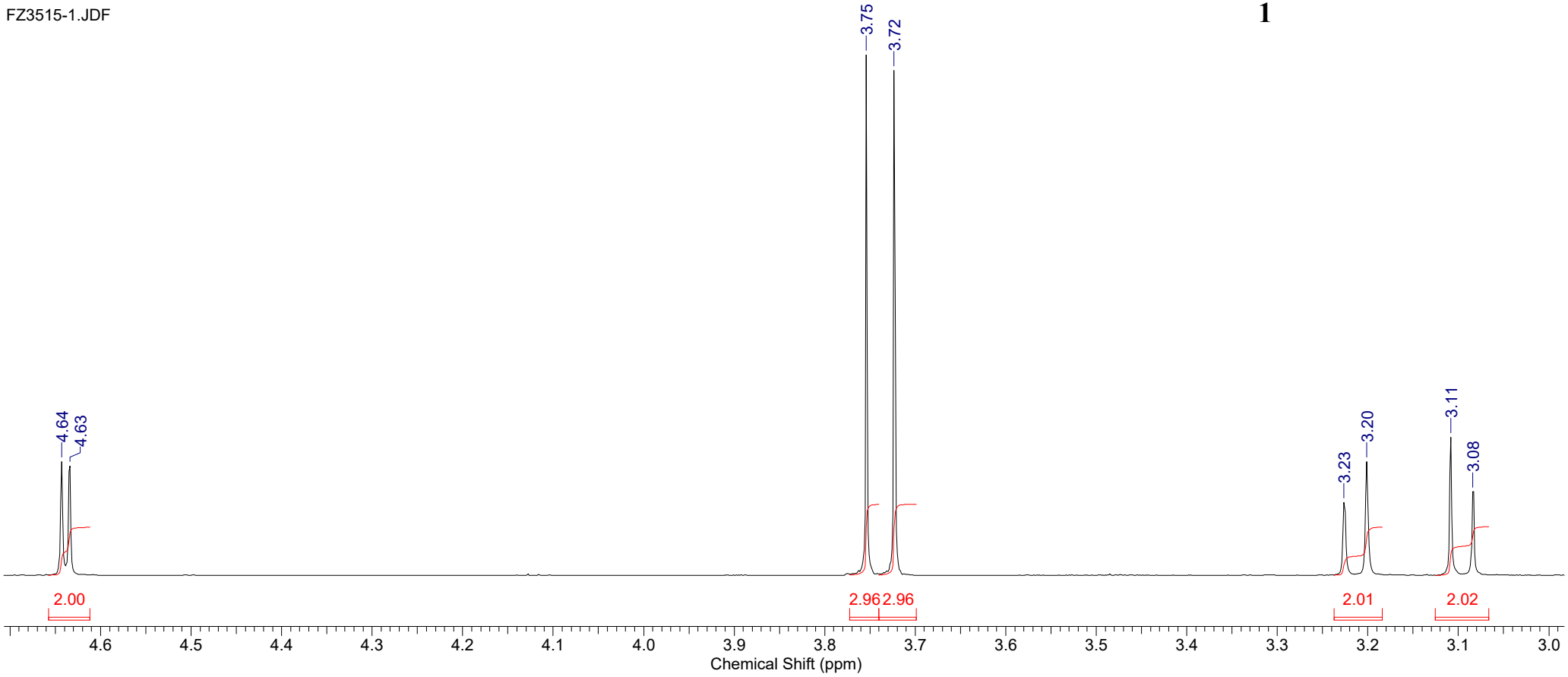
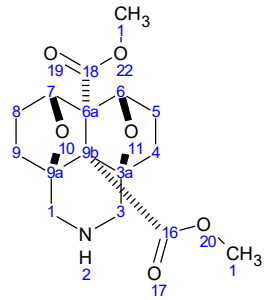
FZ3515-1.JDF



Formula $C_{16}H_{21}NO_6$	***FW***	323.3410							
Acquisition Time (sec)	1.4549	***Comment***	single_pulse	***Date***	15 Jan 2014 09:32:20			***Date Stamp***	15 Jan 2014 08:41:42
File Name	H:\DOWNLOADS\FZ3515-1.JDF			***Frequency (MHz)***	600.17	***Nucleus***	1H	***Number of Transients***	8
Origin	ECA 600	***Original Points Count***	16384	***Owner***	delta	***Points Count***	16384	***Pulse Sequence***	single_pulse.ex2
Receiver Gain	26.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	3019.2939	***Sweep Width (Hz)***	11261.26
Temperature (degree C)	24.100								



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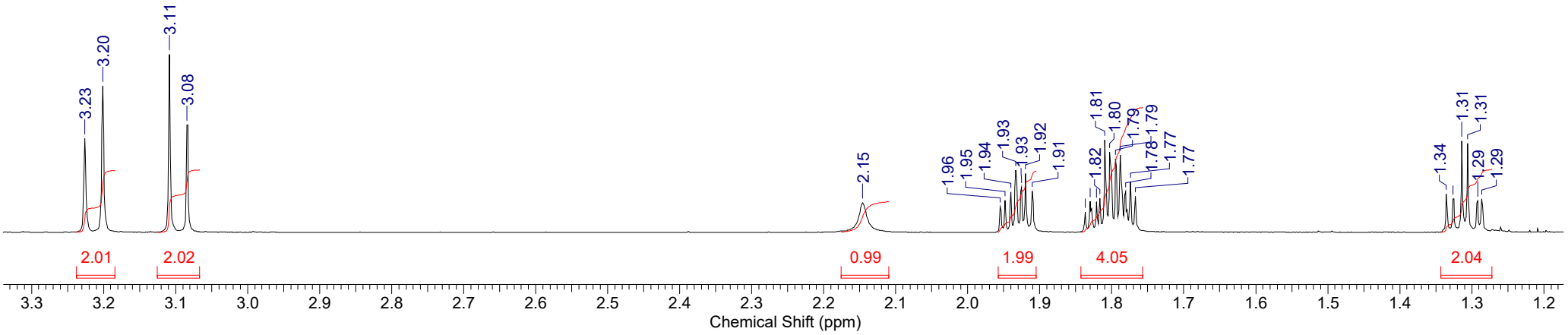
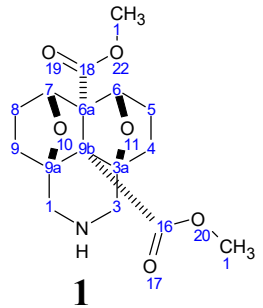
FZ3515-1.JDF



Formula $C_{16}H_{21}NO_6$	FW	323.3410

Acquisition Time (sec)	0.5571	**Comment**	5 mm QNP 1H/15N/13C/31P Z3379/0400			**Date**	20 May 2014 10:25:04
Date Stamp	20 May 2014 10:25:04			**File Name**	H:\DESKTOP\FZ-0414-N22-1170-C13DEC-1_001001r		
Frequency (MHz)	100.61	**Nucleus**	13C	**Number of Transients**	214	**Origin**	spect
Original Points Count	16384	**Owner**	root	**Points Count**	65536	**Pulse Sequence**	zgpg
Receiver Gain	32768.00	**SW(cyclical) (Hz)**	29411.77	**Solvent**	CHLOROFORM-d		
Spectrum Offset (Hz)	9621.1436	**Sweep Width (Hz)**	29411.32	**Temperature (degree C)**	27.000		



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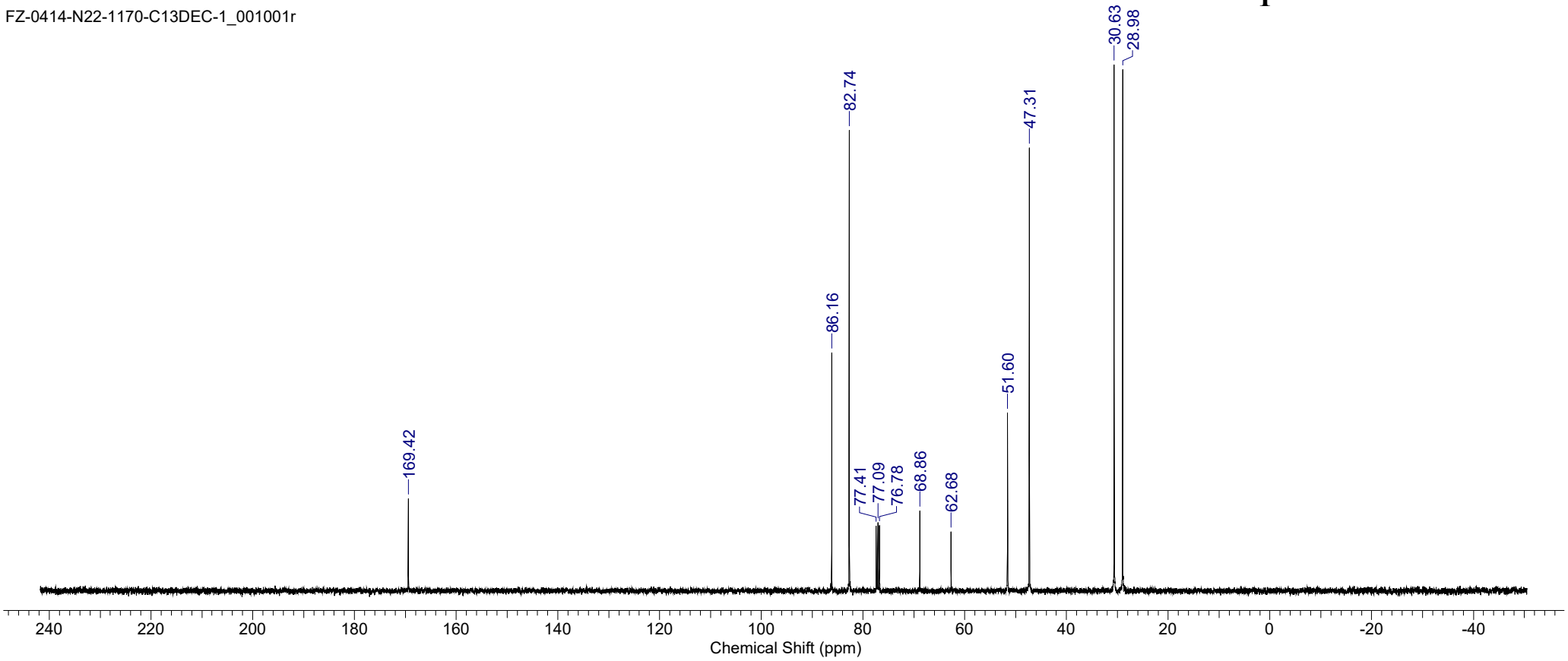
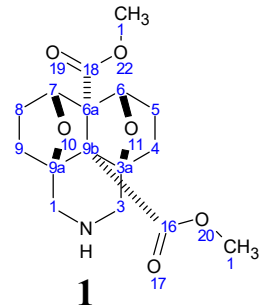
FZ-0414-N22-1170-C13DEC-1_001001r



Formula $C_{16}H_{21}NO_6$	FW	323.3410

Acquisition Time (sec)	0.5571	**Comment**	5 mm QNP 1H/15N/13C/31P Z3379/0400			**Date**	20 May 2014 10:25:04
Date Stamp	20 May 2014 10:25:04			**File Name**	H:\DESKTOP\FZ-0414-N22-1170-C13DEC-1_001001r		
Frequency (MHz)	100.61	**Nucleus**	13C	**Number of Transients**	214	**Origin**	spect
Original Points Count	16384	**Owner**	root	**Points Count**	65536	**Pulse Sequence**	zgpg
Receiver Gain	32768.00	**SW(cyclical) (Hz)**	29411.77	**Solvent**	CHLOROFORM-d		
Spectrum Offset (Hz)	9621.1436	**Sweep Width (Hz)**	29411.32	**Temperature (degree C)**	27.000		



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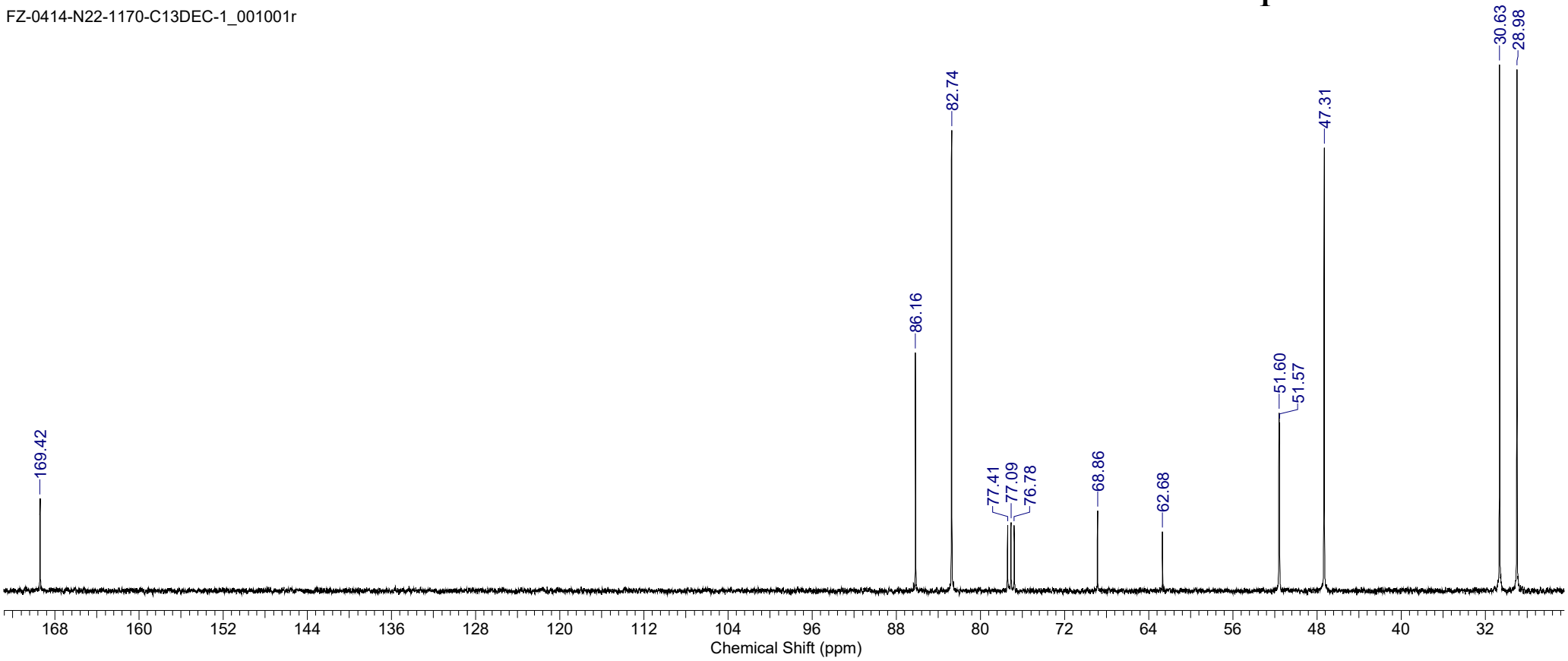
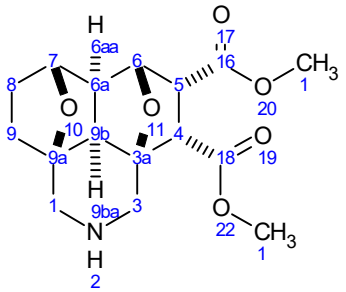
FZ-0414-N22-1170-C13DEC-1_001001r



Formula $C_{16}H_{21}NO_6$	***FW***	323.3410	

Acquisition Time (sec)	1.6056	***Comment***	5 mm QNP 1H/15N/13C/31P Z3379/0400			***Date***	26 Dec 2013 13:05:04
Date Stamp	26 Dec 2013 13:05:04			***File Name***	H:\DESKTOP\от РОМЫ домино NH восстановленный\FZ-251213-N11-1163_001001r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	16384	***Owner***	root	***Points Count***	65536	***Pulse Sequence***	zg
Receiver Gain	64.00	***SW(cyclical) (Hz)***	10204.08	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	2651.9934	***Sweep Width (Hz)***	10203.93	***Temperature (degree C)***	27.000		



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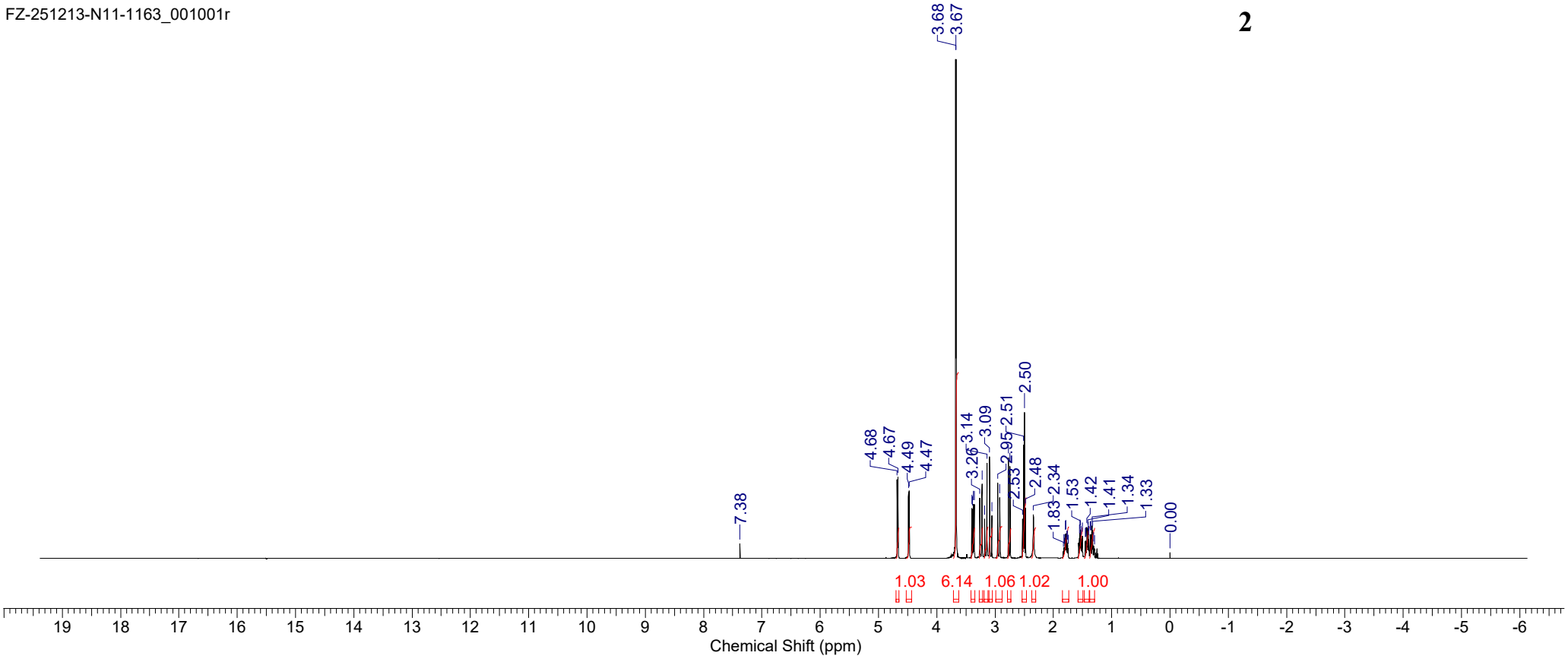
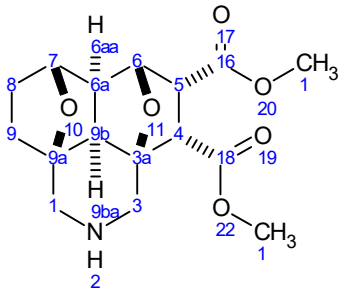
FZ-251213-N11-1163_001001r



Formula $C_{16}H_{21}NO_6$	FW	323.3410

Acquisition Time (sec)	1.6056	**Comment**	5 mm QNP 1H/15N/13C/31P Z3379/0400			**Date**	26 Dec 2013 13:05:04
Date Stamp	26 Dec 2013 13:05:04			**File Name**	H:\DESKTOP\от РОМЫ домино NH восстановленный\FZ-251213-N11-1163_001001r		
Frequency (MHz)	400.13	**Nucleus**	1H	**Number of Transients**	16	**Origin**	spect
Original Points Count	16384	**Owner**	root	**Points Count**	65536	**Pulse Sequence**	zg
Receiver Gain	64.00	**SW(cyclical) (Hz)**	10204.08	**Solvent**	CHLOROFORM-d		
Spectrum Offset (Hz)	2651.9934	**Sweep Width (Hz)**	10203.93	**Temperature (degree C)**	27.000		



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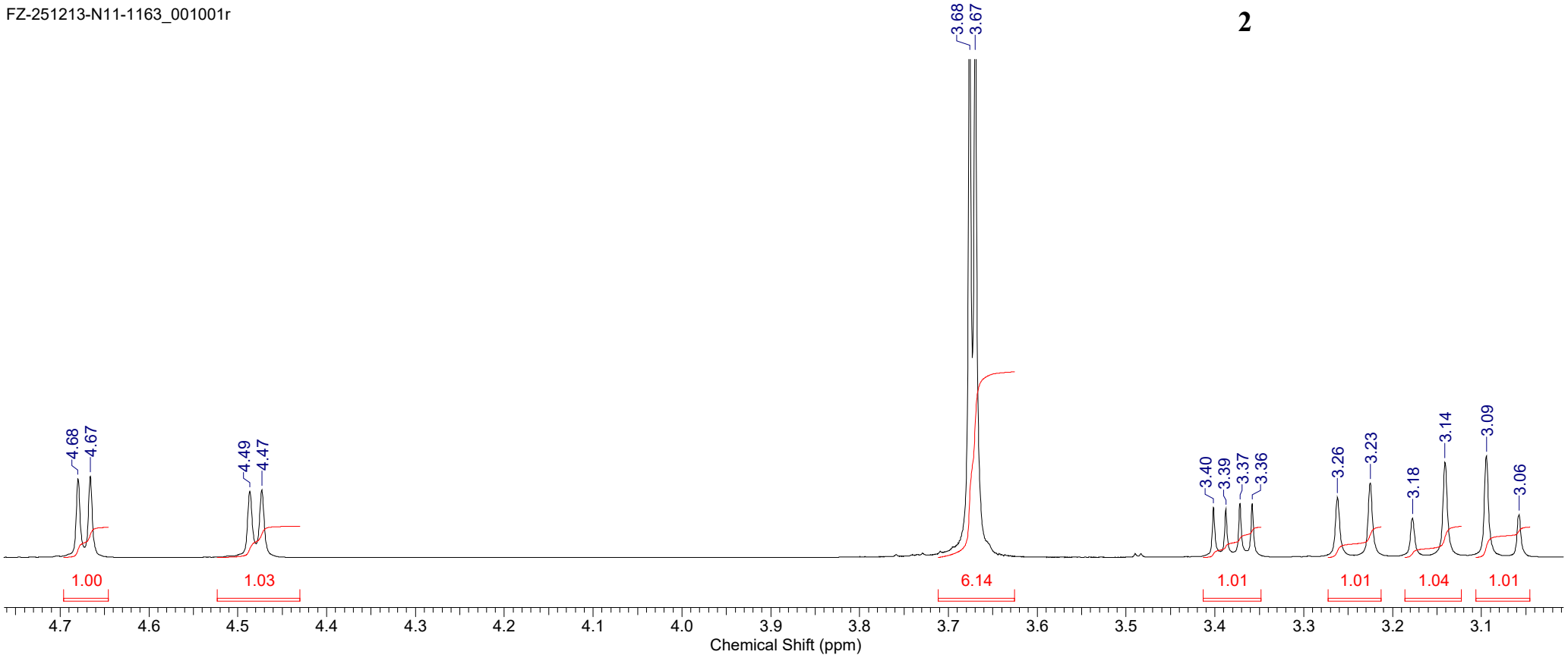
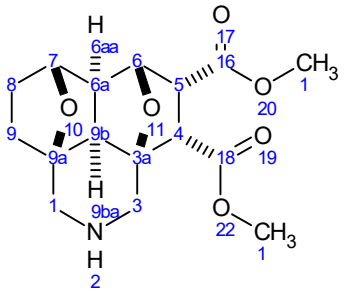
FZ-251213-N11-1163_001001r



Formula $C_{16}H_{21}NO_6$	***FW***	323.3410	

Acquisition Time (sec)	1.6056	***Comment***	5 mm QNP 1H/15N/13C/31P Z3379/0400			***Date***	26 Dec 2013 13:05:04
Date Stamp	26 Dec 2013 13:05:04			***File Name***	H:\DESKTOP\от РОМЫ домино NH восстановленный\FZ-251213-N11-1163_001001r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	16384	***Owner***	root	***Points Count***	65536	***Pulse Sequence***	zg
Receiver Gain	64.00	***SW(cyclical) (Hz)***	10204.08	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	2651.9934	***Sweep Width (Hz)***	10203.93	***Temperature (degree C)***	27.000		



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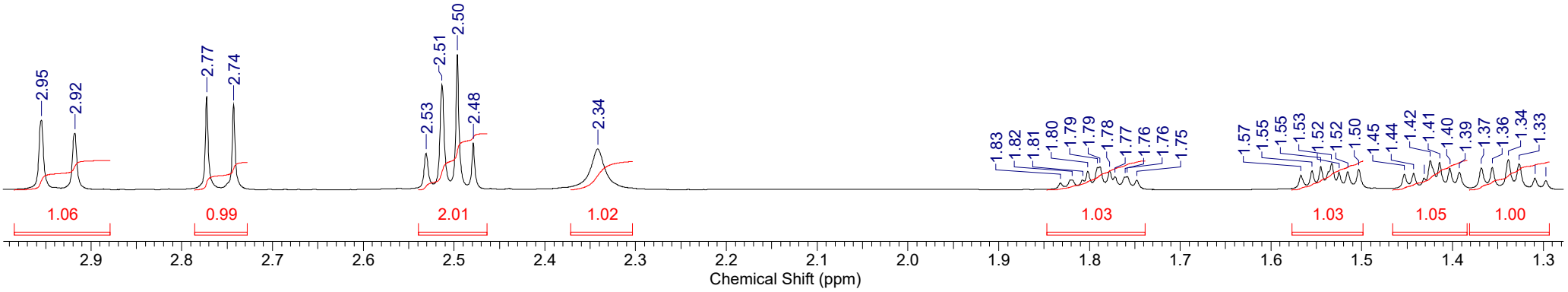
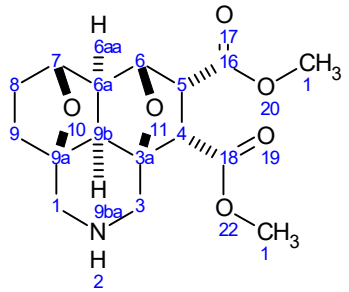
FZ-251213-N11-1163_001001r



Formula $C_{16}H_{21}NO_6$	***FW***	323.3410	

Acquisition Time (sec)	0.5571	***Comment***	5 mm QNP 1H/15N/13C/31P Z3379/0400			***Date***	26 Dec 2013 13:07:12
Date Stamp	26 Dec 2013 13:07:12			***File Name***	H:\DESKTOP\от РОМЫ домино NH восстановленный\FZ-251213-N11-1163-C13DEC_001001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	298	***Origin***	spect
Original Points Count	16384	***Owner***	root	***Points Count***	65536	***Pulse Sequence***	zgpg
Receiver Gain	32768.00	***SW(cyclical) (Hz)***	29411.77	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	9620.7012
Sweep Width (Hz)	29411.32	***Temperature (degree C)***	27.000				



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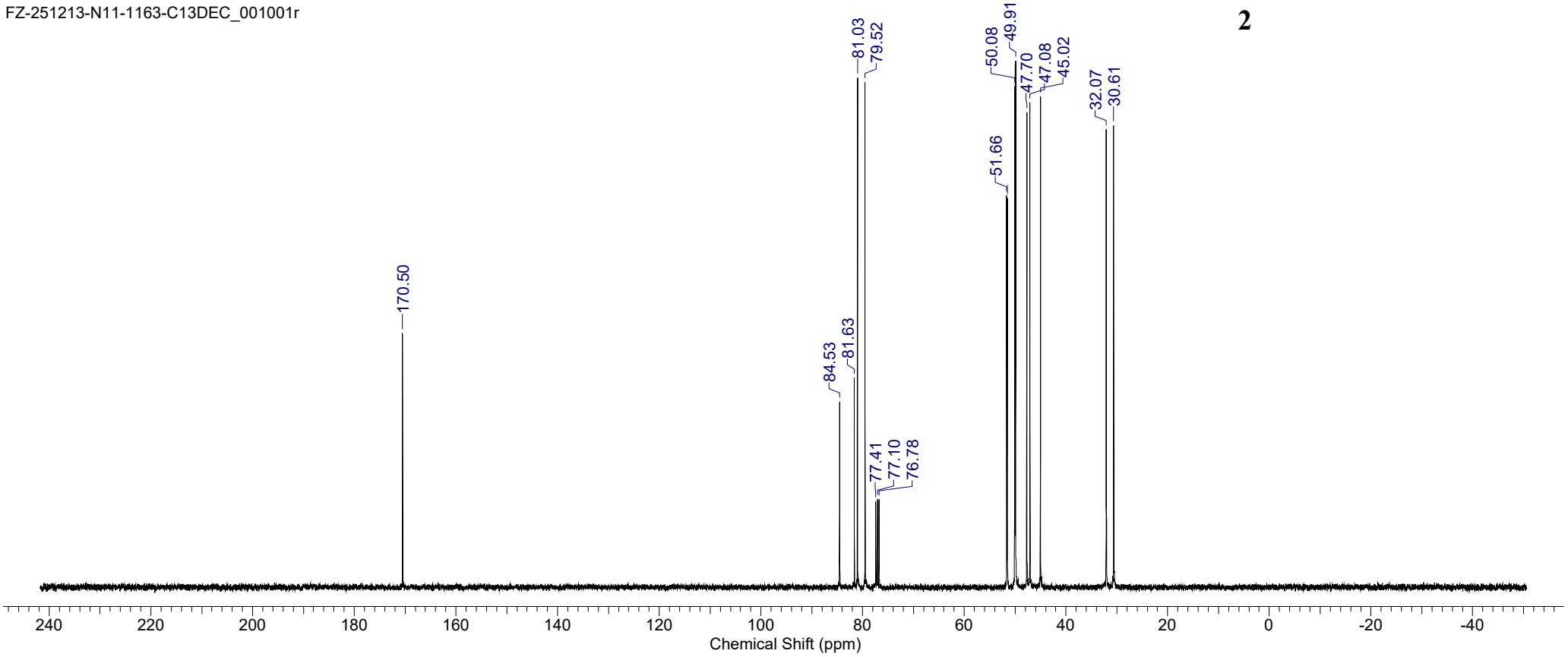
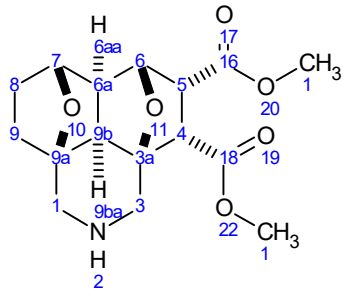
FZ-251213-N11-1163-C13DEC_001001r



Formula $C_{16}H_{21}NO_6$	***FW***	323.3410	

Acquisition Time (sec)	0.5571	***Comment***	5 mm QNP 1H/15N/13C/31P Z3379/0400			***Date***	26 Dec 2013 13:07:12
Date Stamp	26 Dec 2013 13:07:12			***File Name***	H:\DESKTOP\от РОМЫ домино NH восстановленный\FZ-251213-N11-1163-C13DEC_001001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	298	***Origin***	spect
Original Points Count	16384	***Owner***	root	***Points Count***	65536	***Pulse Sequence***	zgpg
Receiver Gain	32768.00	***SW(cyclical) (Hz)***	29411.77	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	9620.7012
Sweep Width (Hz)	29411.32	***Temperature (degree C)***	27.000				



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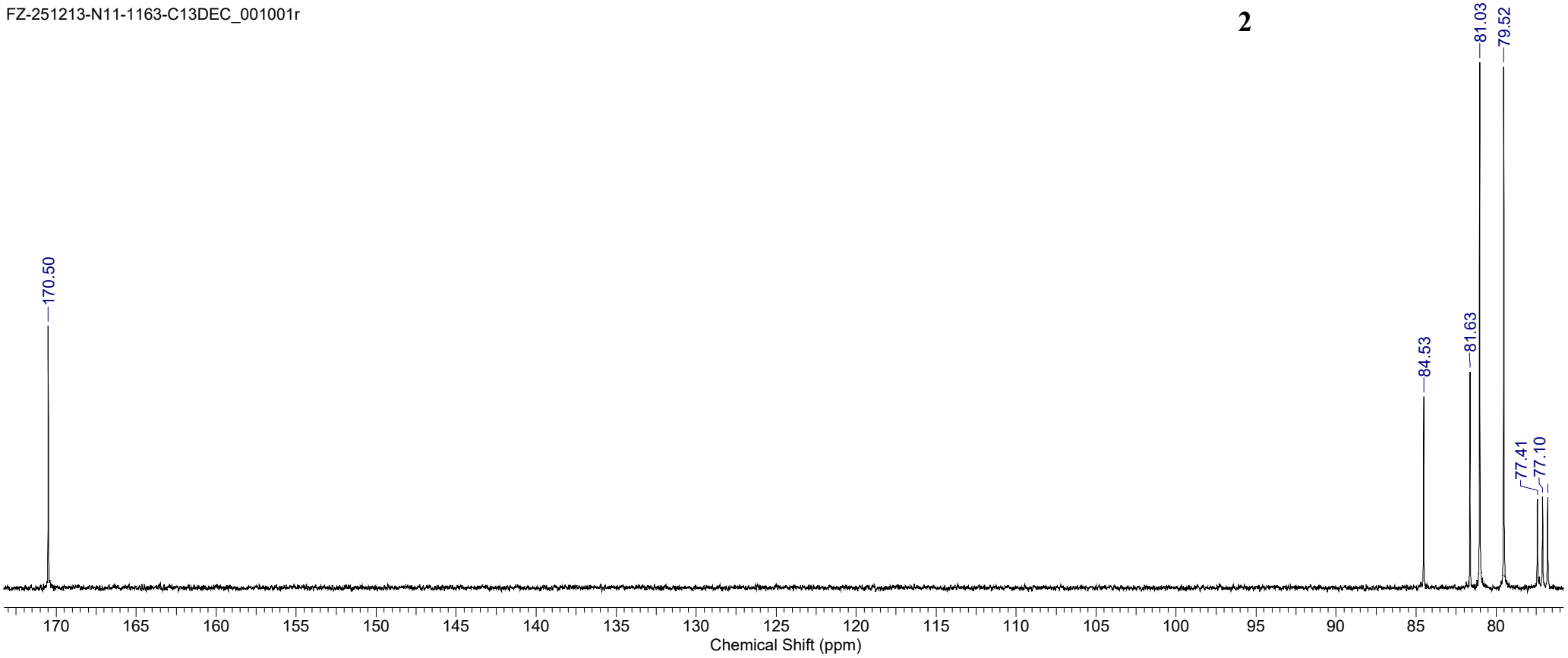
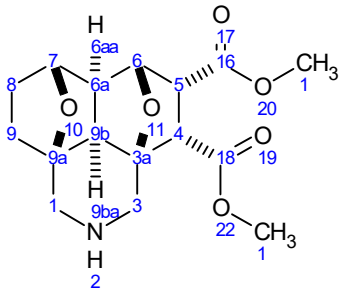
FZ-251213-N11-1163-C13DEC_001001r



Formula $C_{16}H_{21}NO_6$	***FW***	323.3410	

Acquisition Time (sec)	0.5571	***Comment***	5 mm QNP 1H/15N/13C/31P Z3379/0400			***Date***	26 Dec 2013 13:07:12
Date Stamp	26 Dec 2013 13:07:12			***File Name***	H:\DESKTOP\от РОМЫ домино NH восстановленный\FZ-251213-N11-1163-C13DEC_001001r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	298	***Origin***	spect
Original Points Count	16384	***Owner***	root	***Points Count***	65536	***Pulse Sequence***	zgpg
Receiver Gain	32768.00	***SW(cyclical) (Hz)***	29411.77	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	9620.7012
Sweep Width (Hz)	29411.32	***Temperature (degree C)***	27.000				



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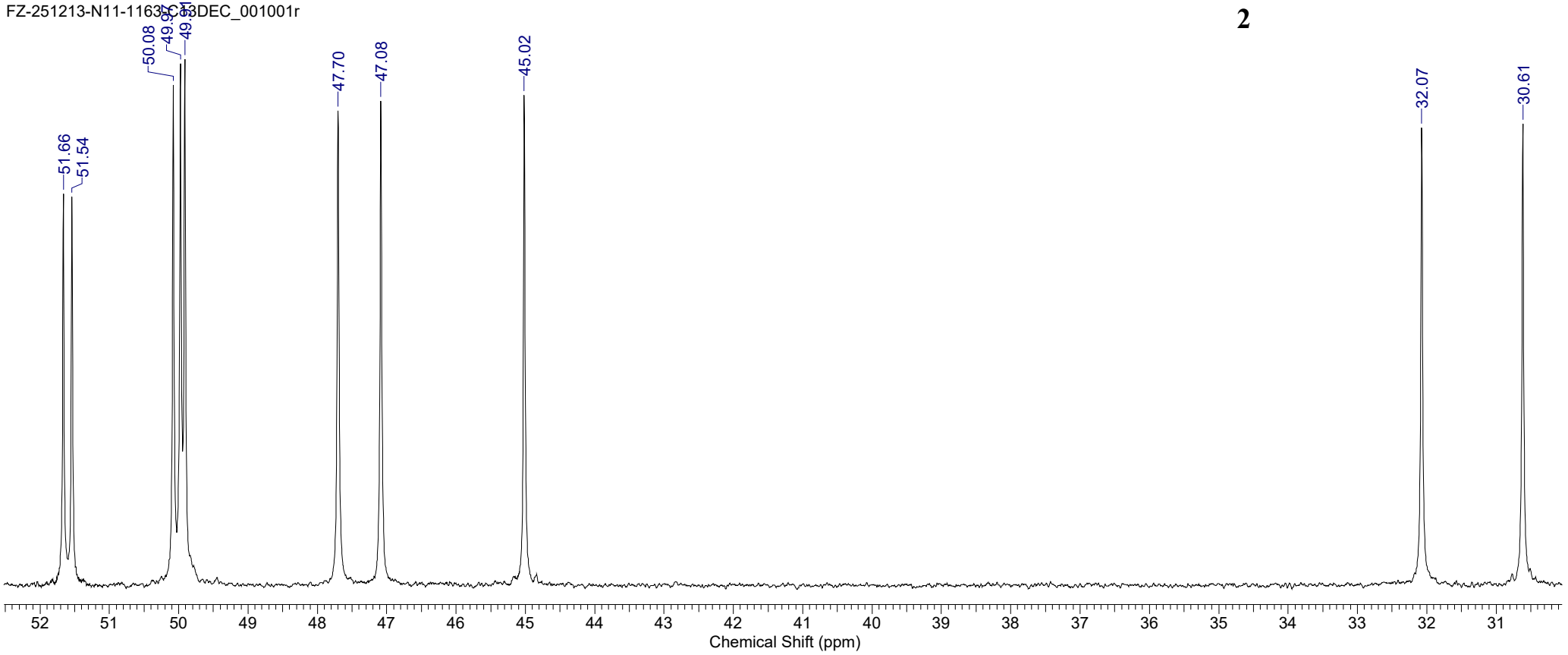
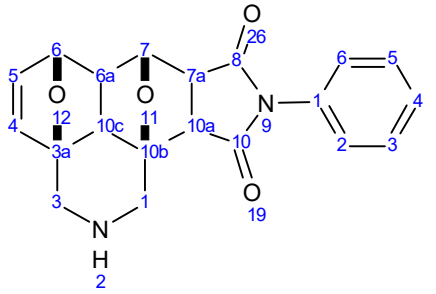


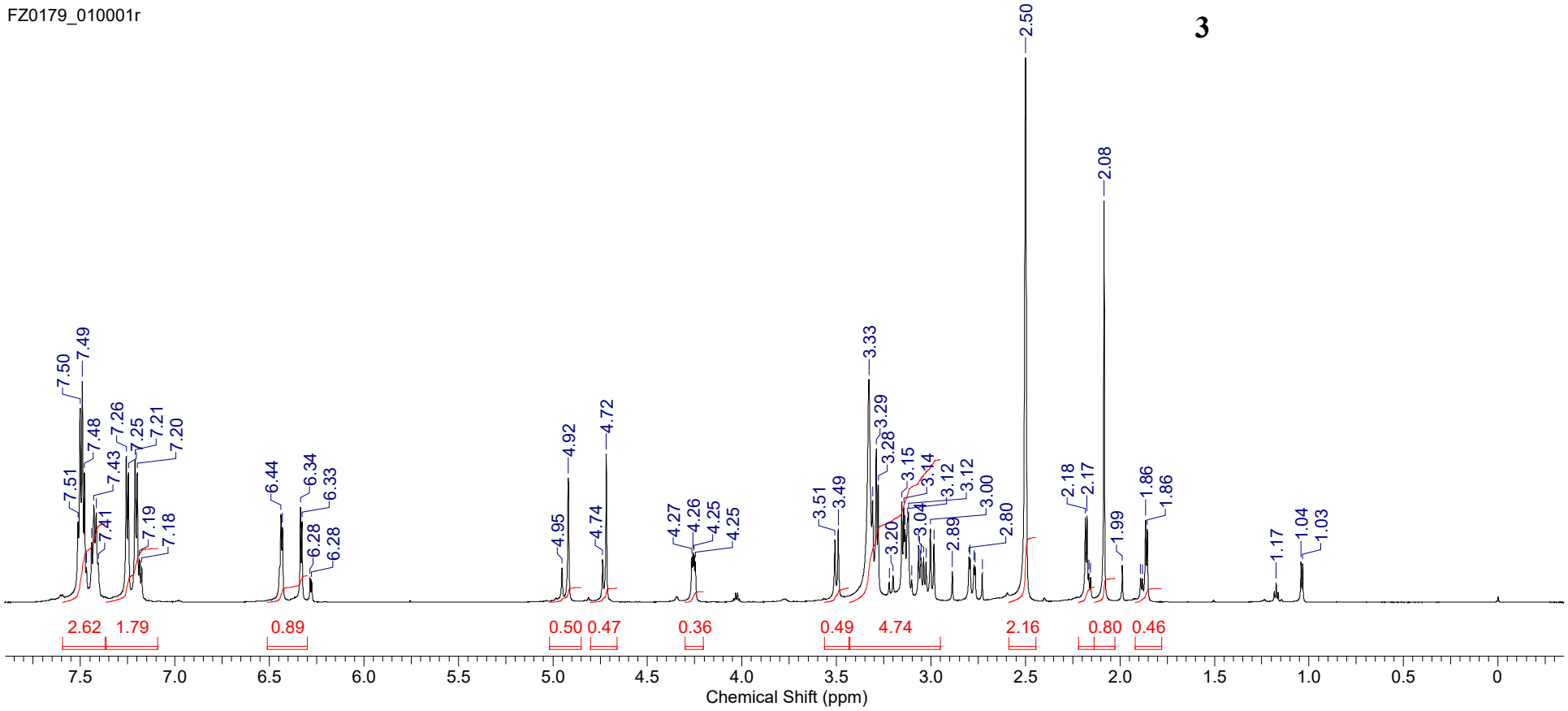
Formula $C_{20}H_{18}N_2O_4$	FW	350.3679

Acquisition Time (sec)	2.0972	**Date**	11 Aug 2021 09:57:20			**Date Stamp**	11 Aug 2021 09:57:20
File Name	C:\USERS\ALEXA\DOWNLOADS\NMR11082021\FZ0179_010001r					**Frequency (MHz)**	700.17
Nucleus	1H	**Number of Transients**	8	**Origin**	Avance	**Original Points Count**	32768
Owner	nmr	**Points Count**	65536	**Pulse Sequence**	zg30	**Receiver Gain**	59.43
SW(cyclical) (Hz)	15625.00	**Solvent**	DMSO-d6	**Spectrum Offset (Hz)**	6295.9395	**Sweep Width (Hz)**	15624.76
Temperature (degree C)	24.988						



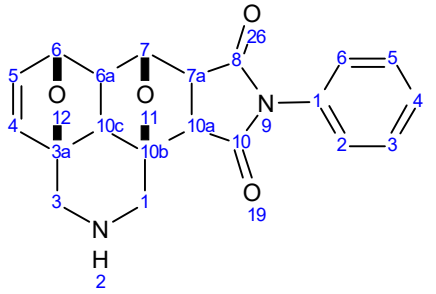
3

FZ0179_010001r



Formula $C_{20}H_{18}N_2O_4$	***FW*** 350.3679

Acquisition Time (sec)	2.0972	***Date***	11 Aug 2021 09:57:20			***Date Stamp***	11 Aug 2021 09:57:20
File Name	C:\USERS\ALEXA\DOWNLOADS\NMR11082021\FZ0179_010001r					***Frequency (MHz)***	700.17
Nucleus	1H	***Number of Transients***	8	***Origin***	Avance	***Original Points Count***	32768
Owner	nmr	***Points Count***	65536	***Pulse Sequence***	zg30	***Receiver Gain***	59.43
SW(cyclical) (Hz)	15625.00	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	6295.9395	***Sweep Width (Hz)***	15624.76
Temperature (degree C)	24.988						



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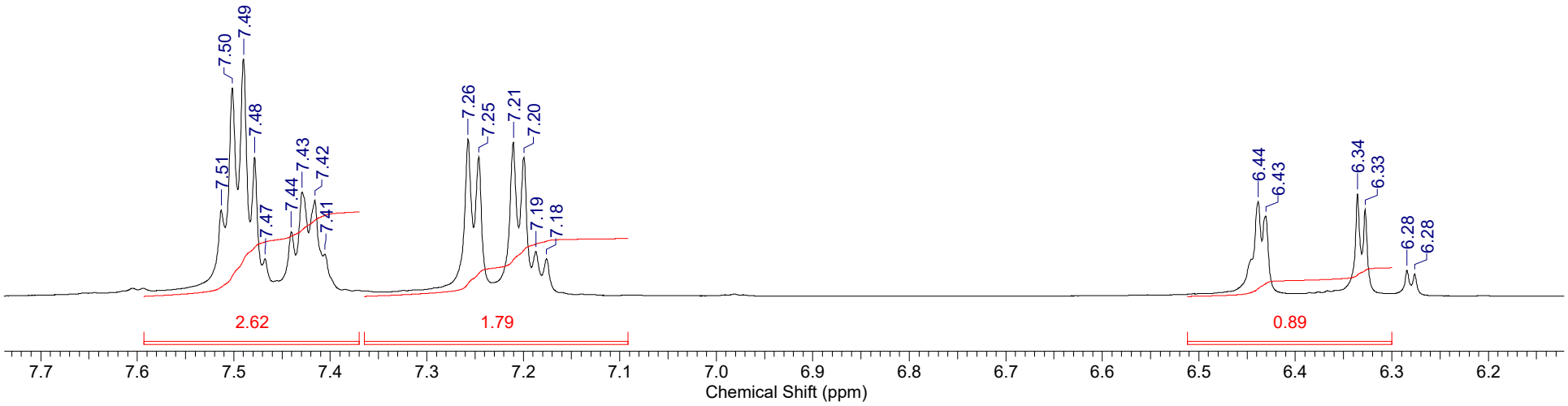
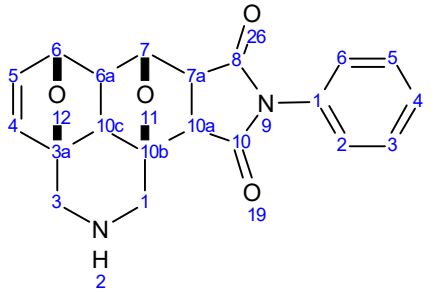
FZ0179_010001r



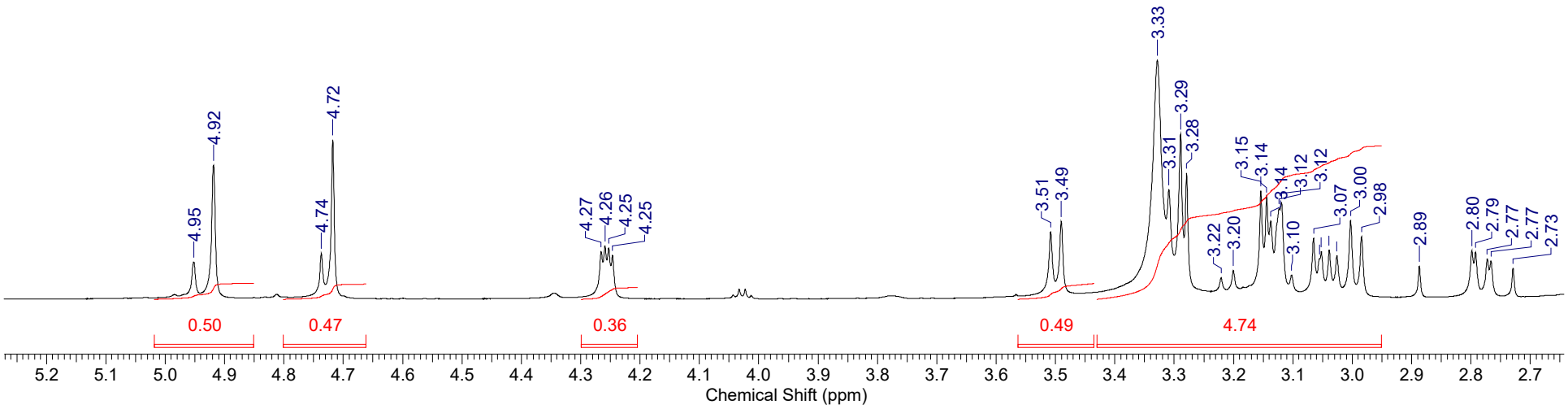
Formula $C_{20}H_{18}N_2O_4$	***FW*** 350.3679

Acquisition Time (sec)	2.0972	***Date***	11 Aug 2021 09:57:20			***Date Stamp***	11 Aug 2021 09:57:20
File Name	C:\USERS\ALEXA\DOWNLOADS\NMR11082021\FZ0179_010001r					***Frequency (MHz)***	700.17
Nucleus	1H	***Number of Transients***	8	***Origin***	Avance	***Original Points Count***	32768
Owner	nmr	***Points Count***	65536	***Pulse Sequence***	zg30	***Receiver Gain***	59.43
SW(cyclical) (Hz)	15625.00	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	6295.9395	***Sweep Width (Hz)***	15624.76
Temperature (degree C)	24.988						



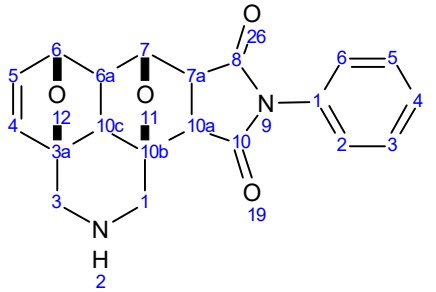
3

FZ0179_010001r



Formula $C_{20}H_{18}N_2O_4$	***FW*** 350.3679

Acquisition Time (sec)	2.0972	***Date***	11 Aug 2021 09:57:20			***Date Stamp***	11 Aug 2021 09:57:20
File Name	C:\USERS\ALEXA\DOWNLOADS\NMR11082021\FZ0179_010001r					***Frequency (MHz)***	700.17
Nucleus	1H	***Number of Transients***	8	***Origin***	Avance	***Original Points Count***	32768
Owner	nmr	***Points Count***	65536	***Pulse Sequence***	zg30	***Receiver Gain***	59.43
SW(cyclical) (Hz)	15625.00	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	6295.9395	***Sweep Width (Hz)***	15624.76
Temperature (degree C)	24.988						



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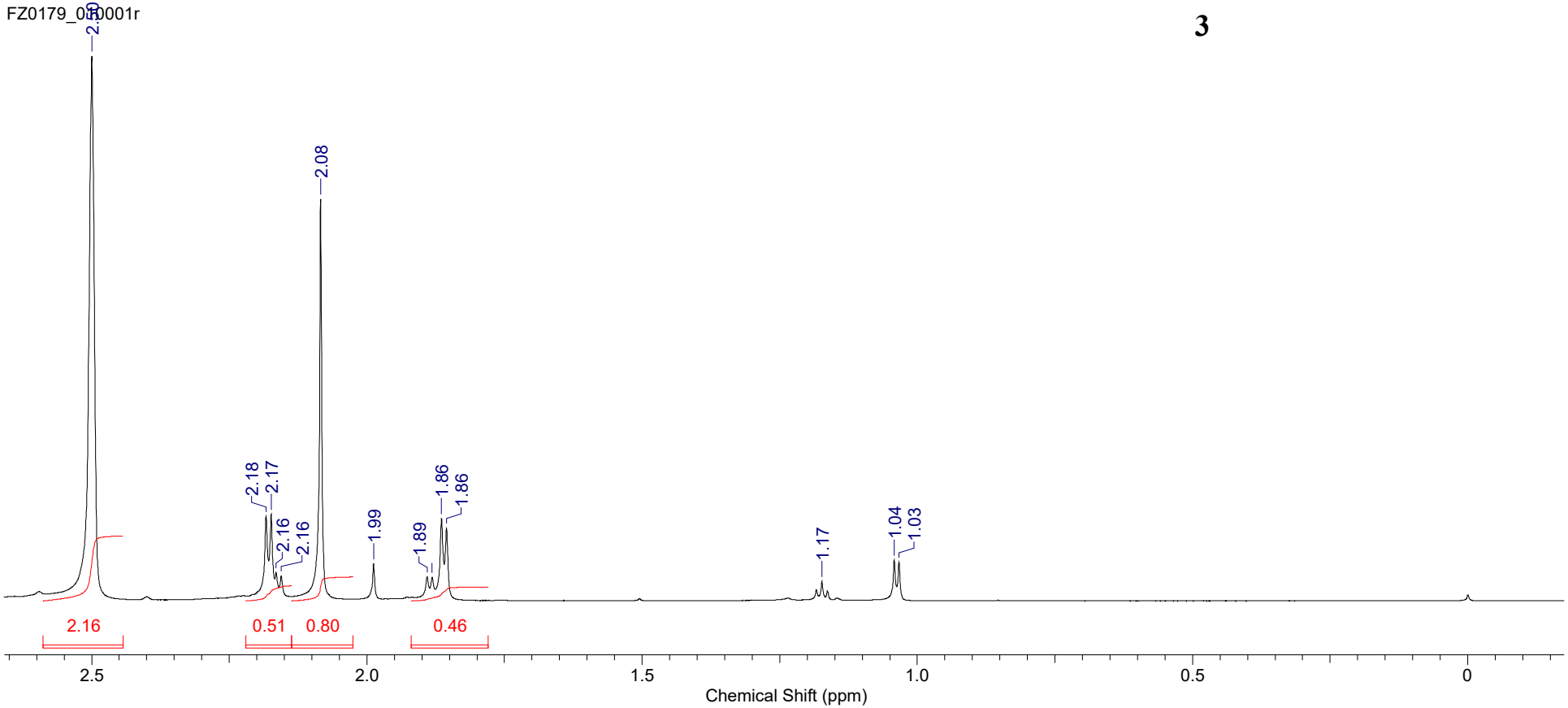
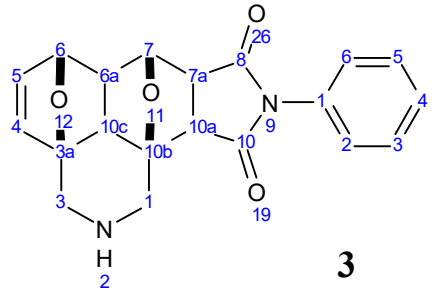


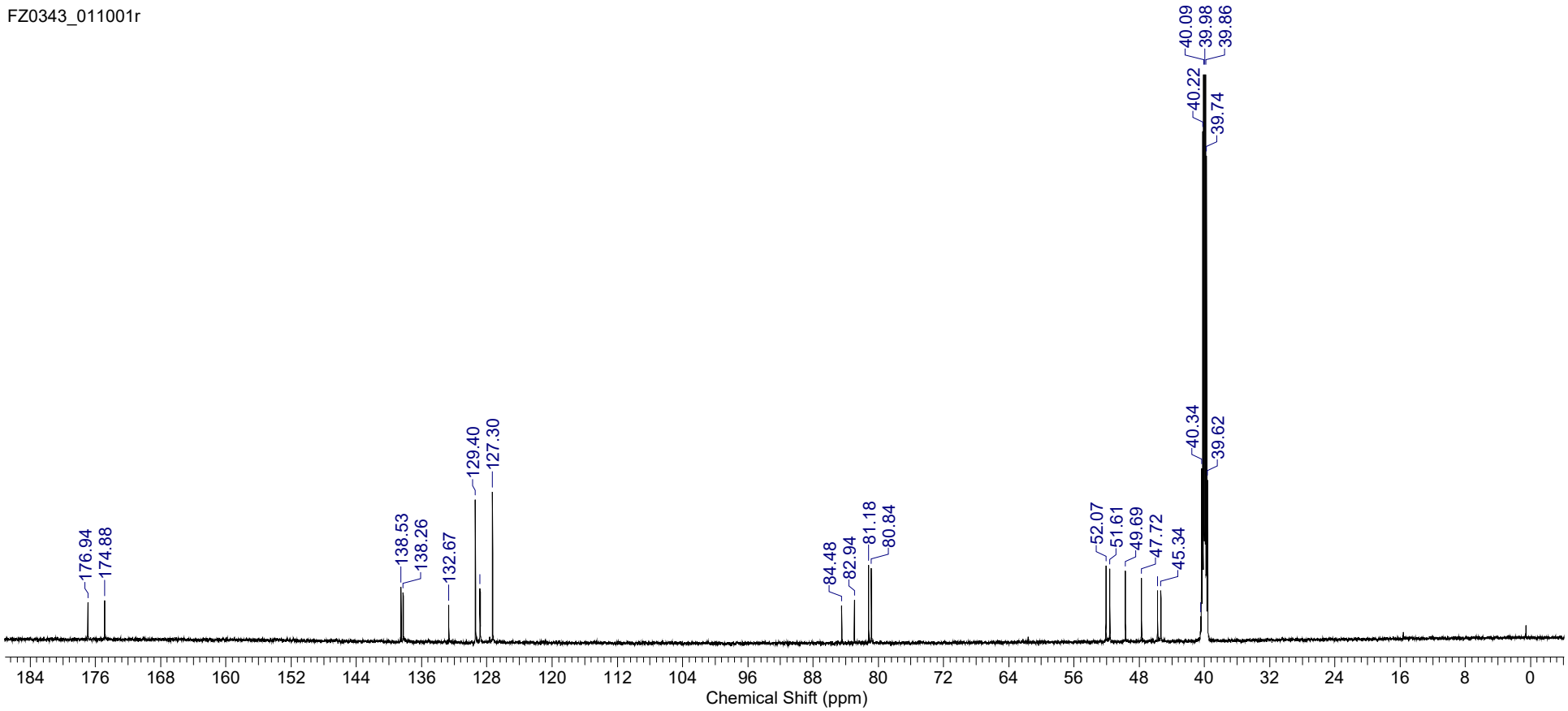
Formula $C_{20}H_{18}N_2O_4$	***FW*** 350.3679

Acquisition Time (sec)	0.7406	***Date***	04 Oct 2021 13:32:48			***Date Stamp***	04 Oct 2021 13:32:48
File Name	C:\USERS\ALEXA\DOWNLOADS\NMR04102021\FZ0343_011001r					***Frequency (MHz)***	176.06
Nucleus	13C	***Number of Transients***	400	***Origin***	Avance	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	101.00
SW(cyclical) (Hz)	44247.79	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	19366.3652	***Sweep Width (Hz)***	44246.44
Temperature (degree C)	25.004						



3

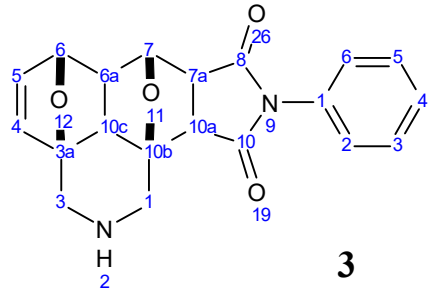
FZ0343_011001r



05.10.2021 17:35:30

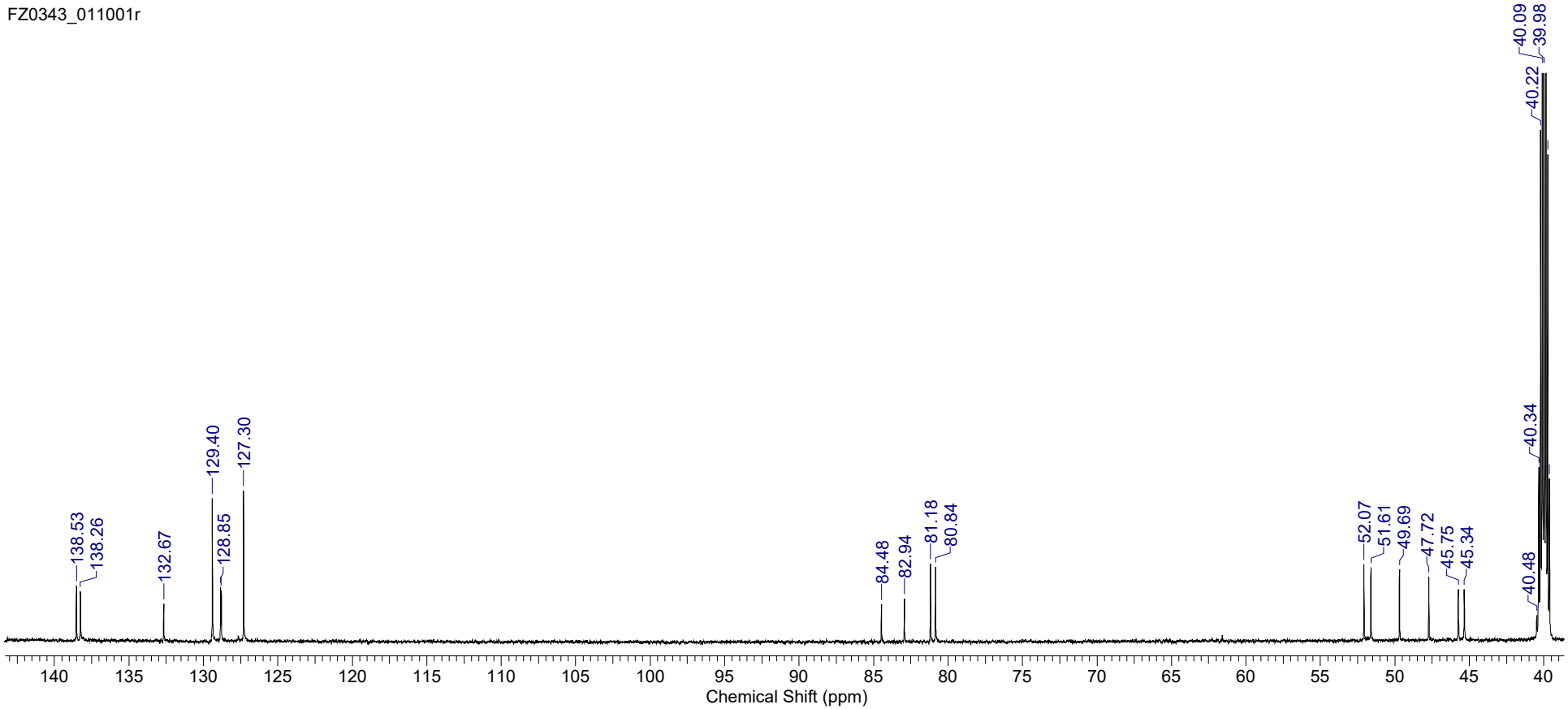
Formula $C_{20}H_{18}N_2O_4$	***FW***	350.3679	

Acquisition Time (sec)	0.7406	***Date***	04 Oct 2021 13:32:48			***Date Stamp***	04 Oct 2021 13:32:48
File Name	C:\USERS\ALEXA\DOWNLOADS\NMR04102021\FZ0343_011001r					***Frequency (MHz)***	176.06
Nucleus	13C	***Number of Transients***	400	***Origin***	Avance	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	101.00
SW(cyclical) (Hz)	44247.79	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	19366.3652	***Sweep Width (Hz)***	44246.44
Temperature (degree C)	25.004						



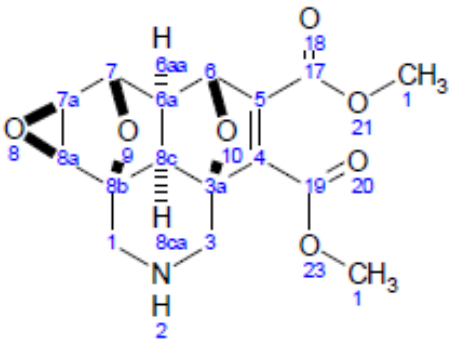
3

FZ0343_011001r

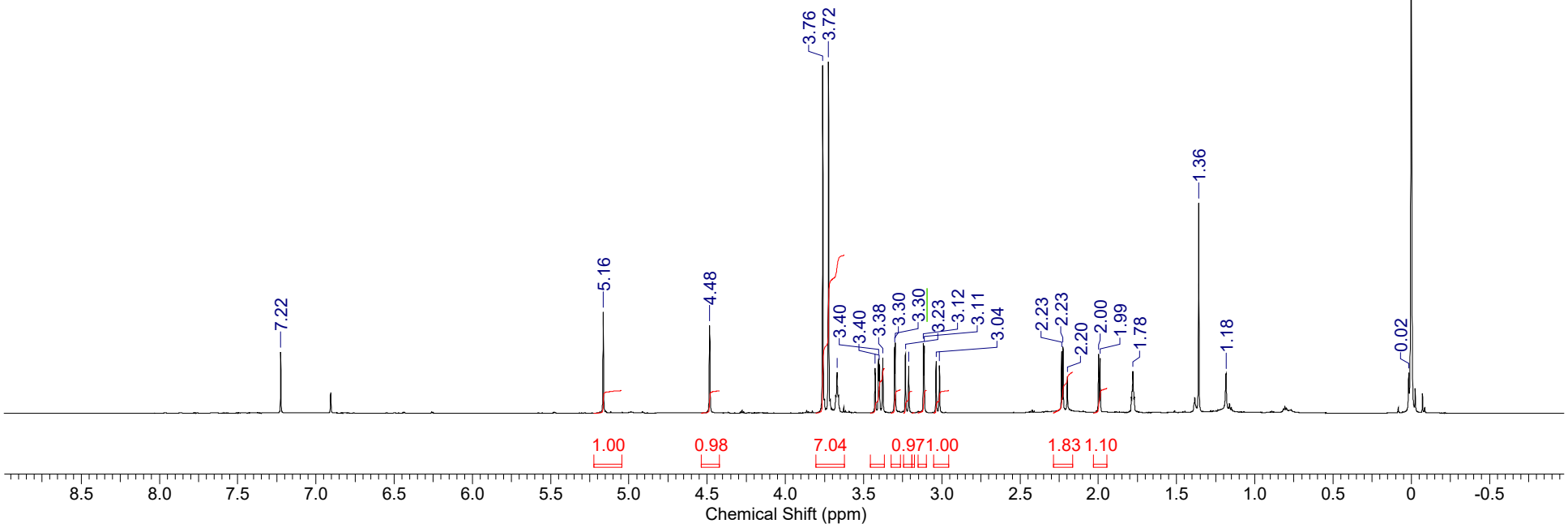


Acquisition Time (sec)	2.0972	***Date***	11 Mar 2022 12:52:16			***Date Stamp***	11 Mar 2022 12:52:16		
File Name	F:\FZ0725_010001r			***Frequency (MHz)***	700.17	***Nucleus***	1H	***Number of Transients***	8
Origin	Avance	***Original Points Count***	32768	***Owner***	nmr	***Points Count***	65536	***Pulse Sequence***	zg30
Receiver Gain	11.30	***SW(cyclical) (Hz)***	15625.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	6261.3374
Sweep Width (Hz)	15624.76	***Temperature (degree C)***	25.006						

FZ0725_010001r



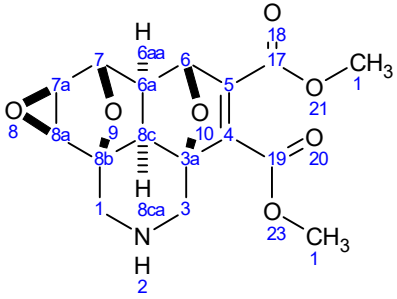
4



07.10.2021 16:02:31

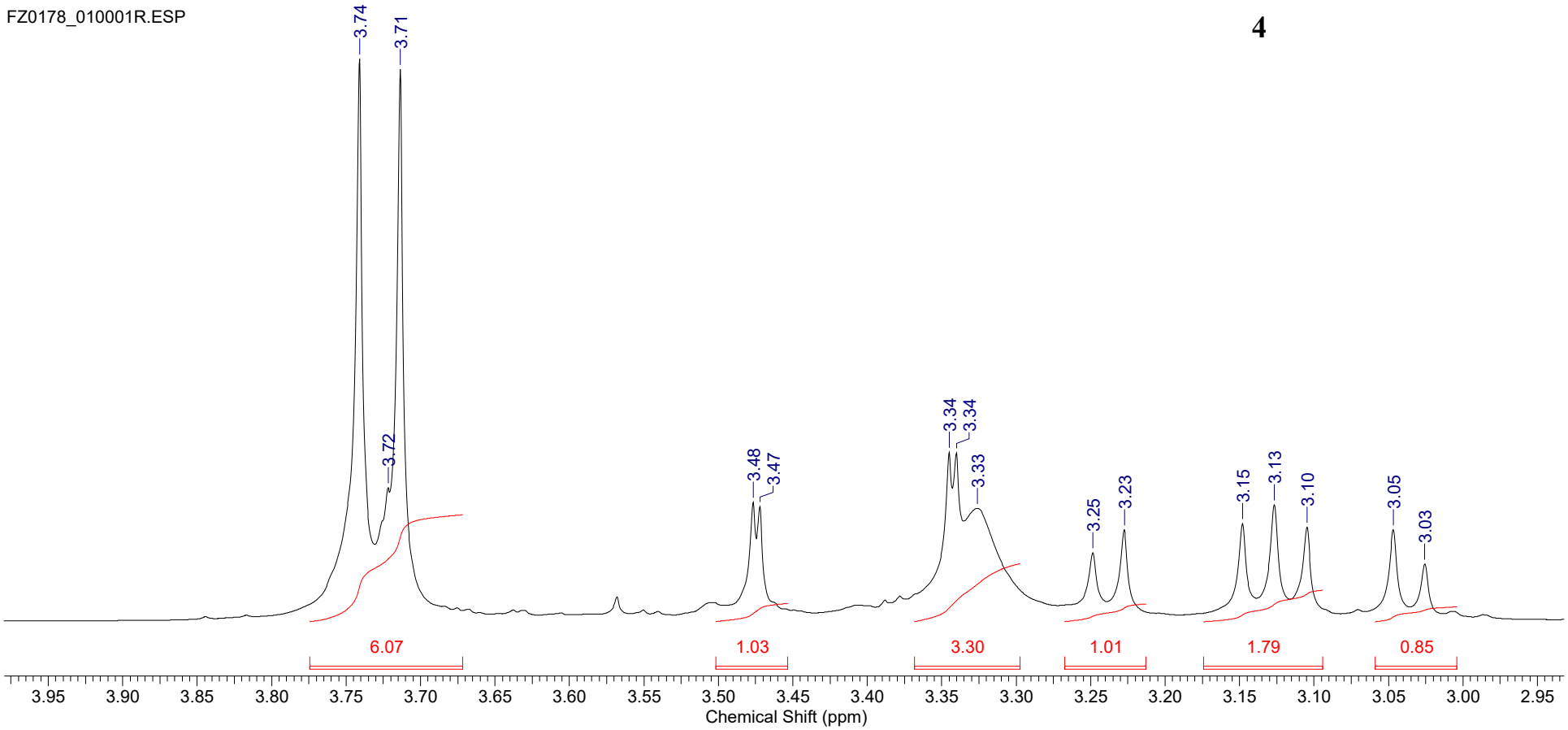
Formula $C_{16}H_{17}NO_7$	FW	335.3087

Acquisition Time (sec)	2.0972	**Date**	11 Aug 2021 09:53:04			**Date Stamp**	11 Aug 2021 09:53:04
File Name	C:\USERS\LIZA \DESKTOP\FZ0178_010001r			**Frequency (MHz)**	700.17	**Nucleus**	1H
Number of Transients	8	**Origin**	Avance	**Original Points Count**	32768	**Owner**	nmr
Points Count	65536	**Pulse Sequence**	zg30	**Receiver Gain**	78.83	**SW(cyclical) (Hz)**	15625.00
Solvent	DMSO-d6	**Spectrum Offset (Hz)**	6297.7075	**Sweep Width (Hz)**	15624.76	**Temperature (degree C)**	24.989



4

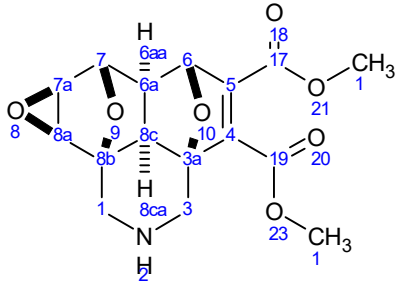
FZ0178_010001R.ESP



07.10.2021 16:02:42

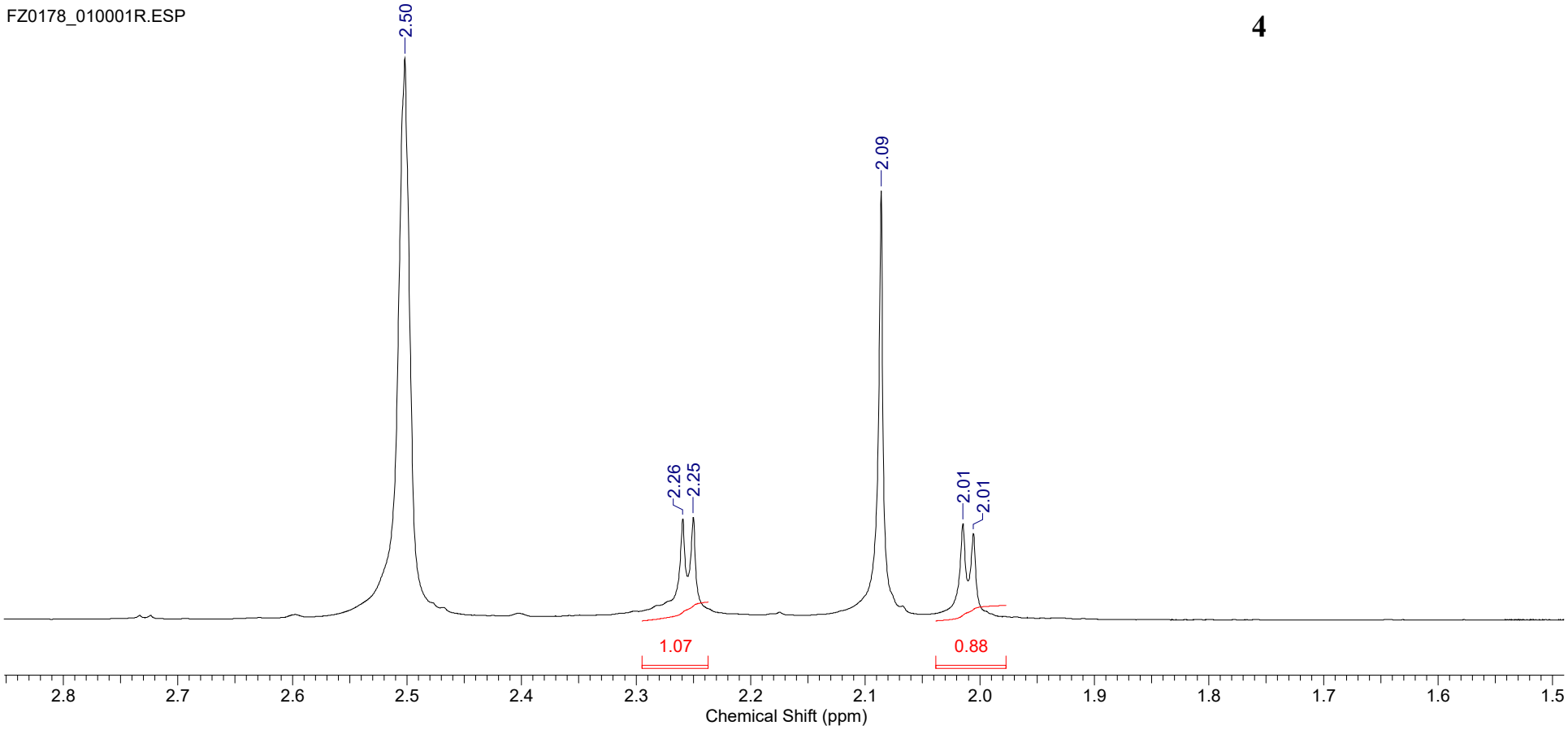
Formula $C_{16}H_{17}NO_7$	FW	335.3087

Acquisition Time (sec)	2.0972	**Date**	11 Aug 2021 09:53:04			**Date Stamp**	11 Aug 2021 09:53:04
File Name	C:\USERS\LIZA \DESKTOP\FZ0178_010001r			**Frequency (MHz)**	700.17	**Nucleus**	1H
Number of Transients	8	**Origin**	Avance	**Original Points Count**	32768	**Owner**	nmr
Points Count	65536	**Pulse Sequence**	zg30	**Receiver Gain**	78.83	**SW(cyclical) (Hz)**	15625.00
Solvent	DMSO-d6	**Spectrum Offset (Hz)**	6297.7075	**Sweep Width (Hz)**	15624.76	**Temperature (degree C)**	24.989



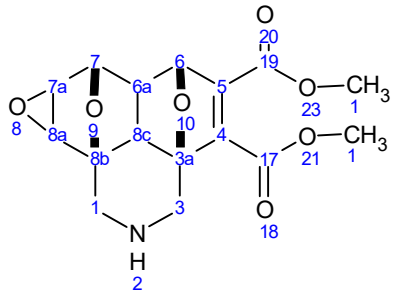
4

FZ0178_010001R.ESP



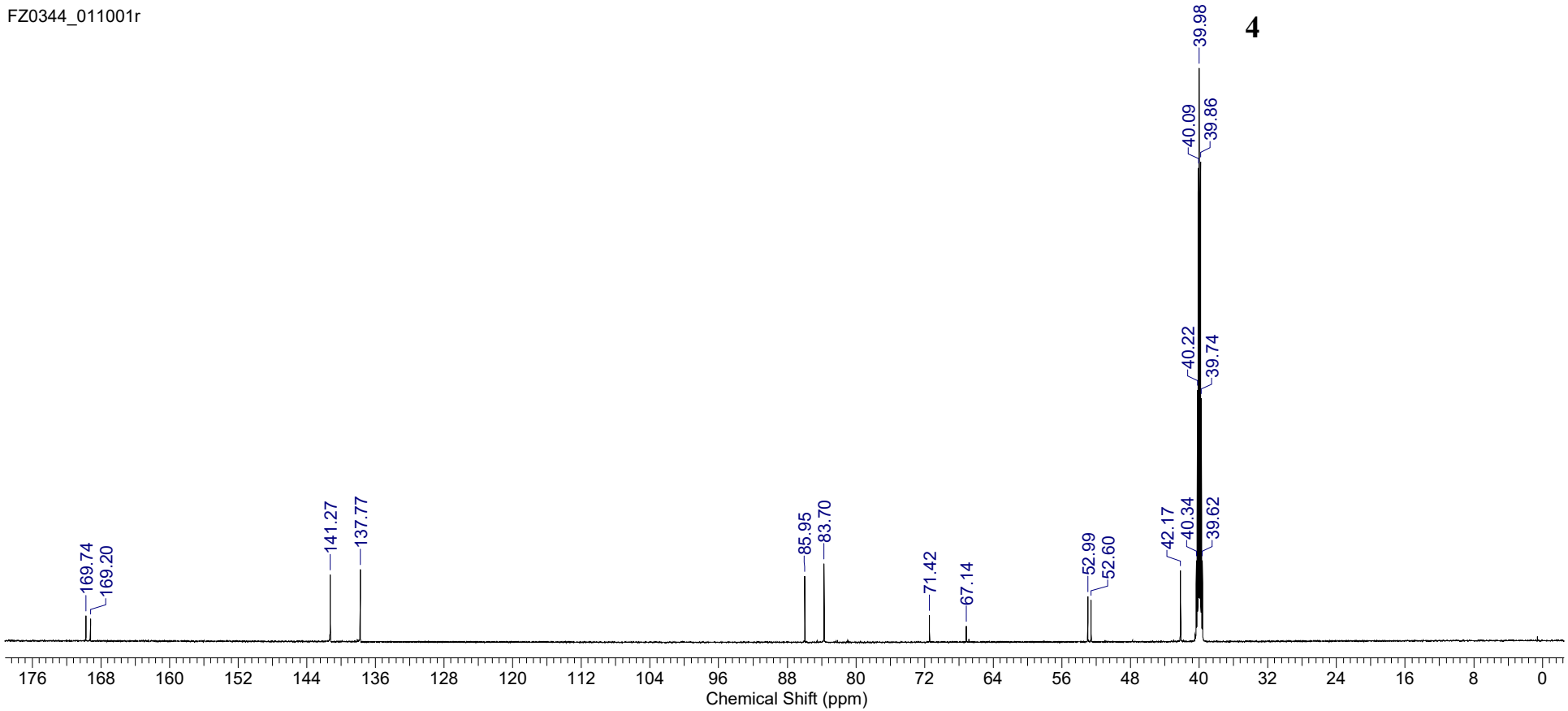
Formula $C_{16}H_{17}NO_7$	***FW***	335.3087	

Acquisition Time (sec)	0.7406	***Date***	04 Oct 2021 13:17:52			***Date Stamp***	04 Oct 2021 13:17:52
File Name	C:\USERS\ALEXA\DOWNLOADS\NMR04102021\FZ0344_011001r					***Frequency (MHz)***	176.06
Nucleus	13C	***Number of Transients***	400	***Origin***	Avance	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	101.00
SW(cyclical) (Hz)	44247.79	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	19366.3652	***Sweep Width (Hz)***	44246.44
Temperature (degree C)	25.005						



4

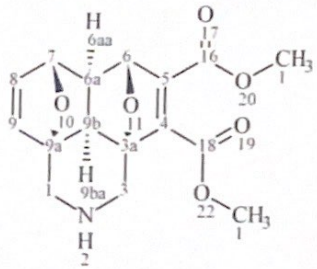
FZ0344_011001r



22.10.2014 19:50:01

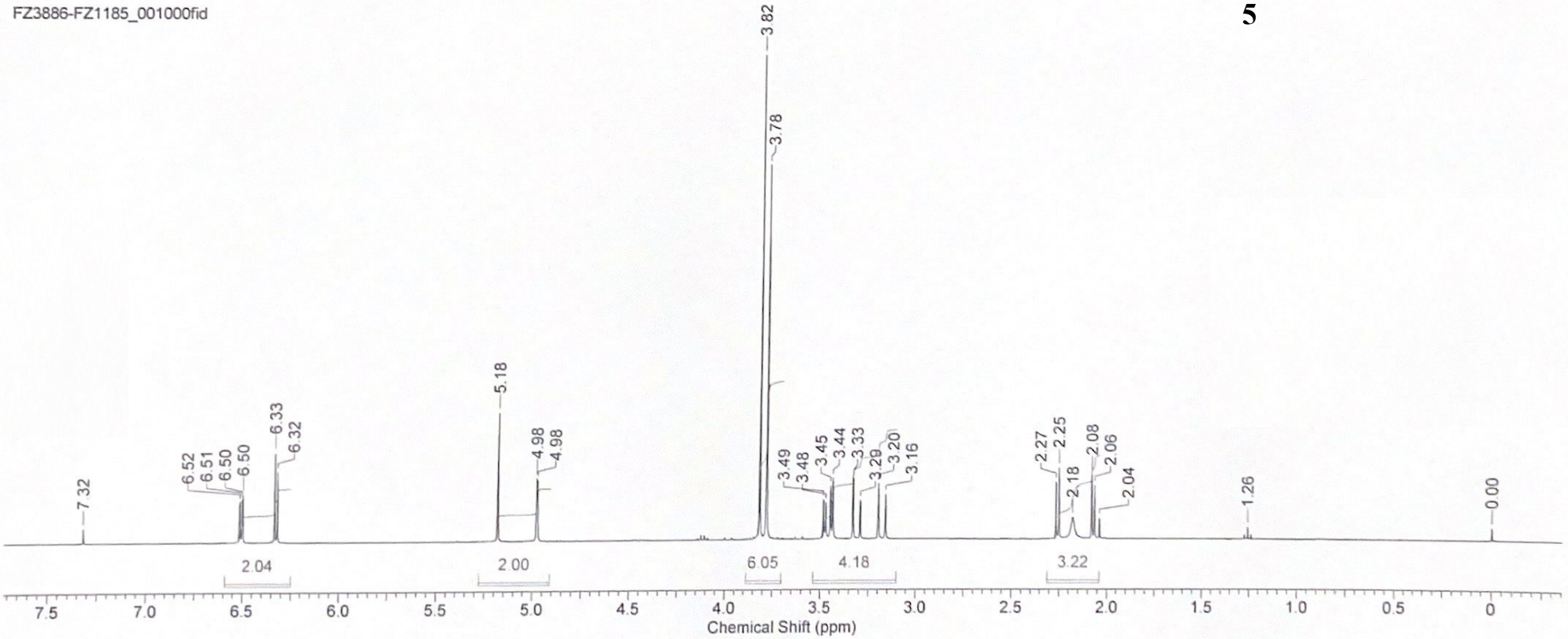
Formula $C_{16}H_{17}NO_6$	FW 319.3093

Acquisition Time (sec)	1.6056	*Comment*	5 mm QNP 1H/15N/13C/31P Z3379/0400			*Date*	22 Oct 2014 14:56:00
Date Stamp	22 Oct 2014 14:56:00			*File Name*	C:\Users\Fedor\Desktop\17.10.14\FZ3886-FZ1185\FZ3886-FZ1185_001000fid		
Frequency (MHz)	400.14	*Nucleus*	1H	*Number of Transients*	6	*Origin*	spect
Original Points Count	16384	*Owner*	root	*Points Count*	16384	*Pulse Sequence*	zg
Receiver Gain	128.00	*SW(cyclical) (Hz)*	10204.08	*Solvent*	CHLOROFORM-d		
Spectrum Offset (Hz)	2629.7024	*Sweep Width (Hz)*	10203.46	*Temperature (degree C)*	27.000		



5

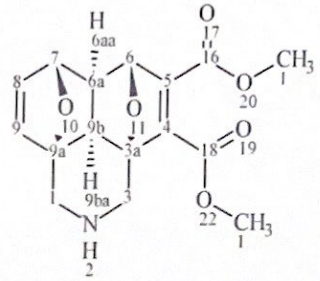
FZ3886-FZ1185_001000fid



22.10.2014 19:50:07

Formula $C_{16}H_{17}NO_6$	FW 319.3093

Acquisition Time (sec)	1.6056	*Comment*	5 mm QNP 1H/15N/13C/31P Z3379/0400			*Date*	22 Oct 2014 14:56:00
Date Stamp	22 Oct 2014 14:56:00			*File Name*	C:\Users\Fedor\Desktop\17.10.14\FZ3886-FZ1185\FZ3886-FZ1185_001000fid		
Frequency (MHz)	400.14	*Nucleus*	1H	*Number of Transients*	6	*Origin*	spect
Original Points Count	16384	*Owner*	root	*Points Count*	16384	*Pulse Sequence*	zg
Receiver Gain	128.00	*SW(cyclical) (Hz)*	10204.08	*Solvent*	CHLOROFORM-d		
Spectrum Offset (Hz)	2629.7024	*Sweep Width (Hz)*	10203.46	*Temperature (degree C)*	27.000		



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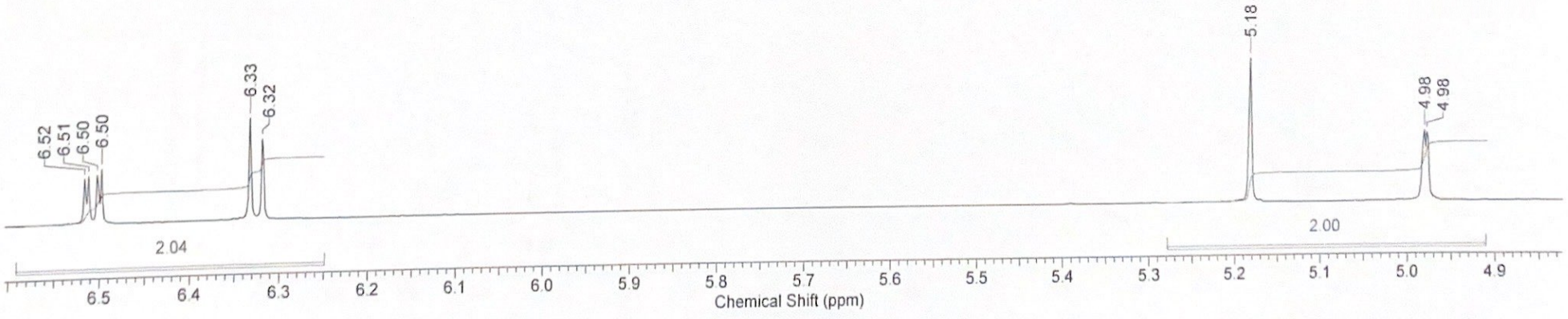
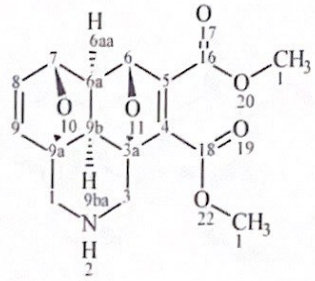
FZ3886-FZ1185_001000fid



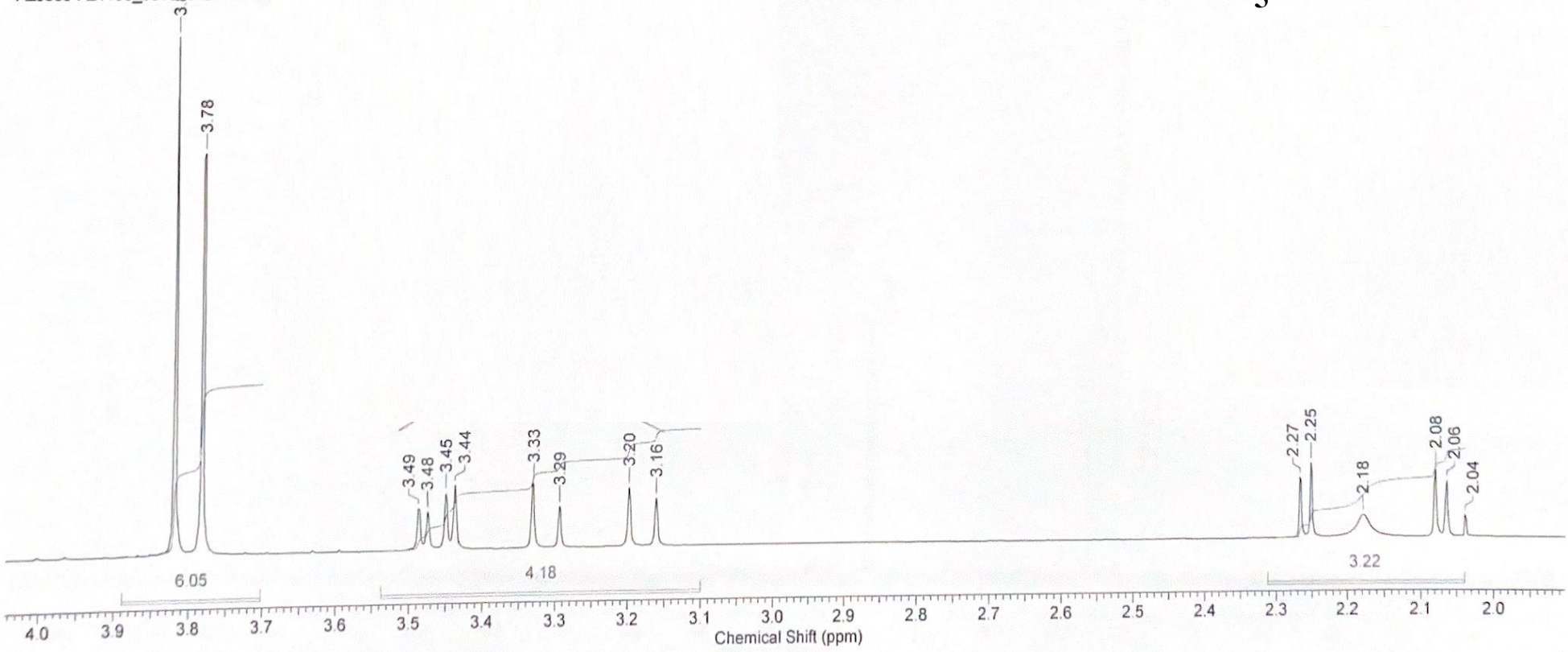
Formula $C_{16}H_{17}NO_6$	FW 319.3093

Acquisition Time (sec)	1.6056	*Comment*	5 mm QNP 1H/15N/13C/31P Z3379/0400			*Date*	22 Oct 2014 14:56:00
Date Stamp	22 Oct 2014 14:56:00			*File Name*	C:\Users\Fedor\Desktop\17.10.14\FZ3886-FZ1185\FZ3886-FZ1185_001000fid		
Frequency (MHz)	400.14	*Nucleus*	1H	*Number of Transients*	6	*Origin*	spect
Original Points Count	16384	*Owner*	root	*Points Count*	16384	*Pulse Sequence*	zg
Receiver Gain	128.00	*SW(cyclical) (Hz)*	10204.08	*Solvent*	CHLOROFORM-d		
Spectrum Offset (Hz)	2629.7024	*Sweep Width (Hz)*	10203.46	*Temperature (degree C)*	27.000		



5

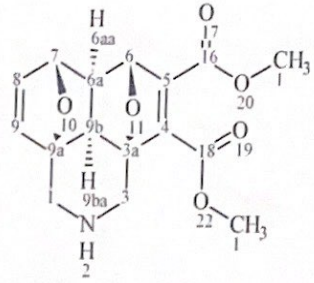
FZ3886-FZ1185_001000fid



22.10.2014 19:55:17

Formula $C_{16}H_{17}NO_6$	FW 319.3093

Acquisition Time (sec)	0.5571	*Comment*	5 mm QNP 1H/15N/13C/31P Z3379/0400			*Date*	22 Oct 2014 14:56:00
Date Stamp	22 Oct 2014 14:56:00			*File Name*	C:\Users\Fedor\Desktop\17.10.14\FZ3886-FZ1185-c13dec\FZ3886-FZ1185-c13dec_001000fid		
Frequency (MHz)	100.62	*Nucleus*	13C	*Number of Transients*	156	*Origin*	spect
Original Points Count	16384	*Owner*	root	*Points Count*	16384	*Pulse Sequence*	zgpg
Receiver Gain	32768.00	*SW(cyclical) (Hz)*	29411.77	*Solvent*	CHLOROFORM-d		
Spectrum Offset (Hz)	9628.4102	*Sweep Width (Hz)*	29409.97	*Temperature (degree C)*	27.000		



5

FZ3886-FZ1185-c13dec_001000fid