Ethyl 7-acetyl-8a-methyl-3-(1-phenyl-1*H*-tetrazol-5-yl)-1,4,4a,5,6,8a-hexahydro-7*H*-pyrano[2,3-c]pyridazine-1-carboxylate

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Supplementary Material

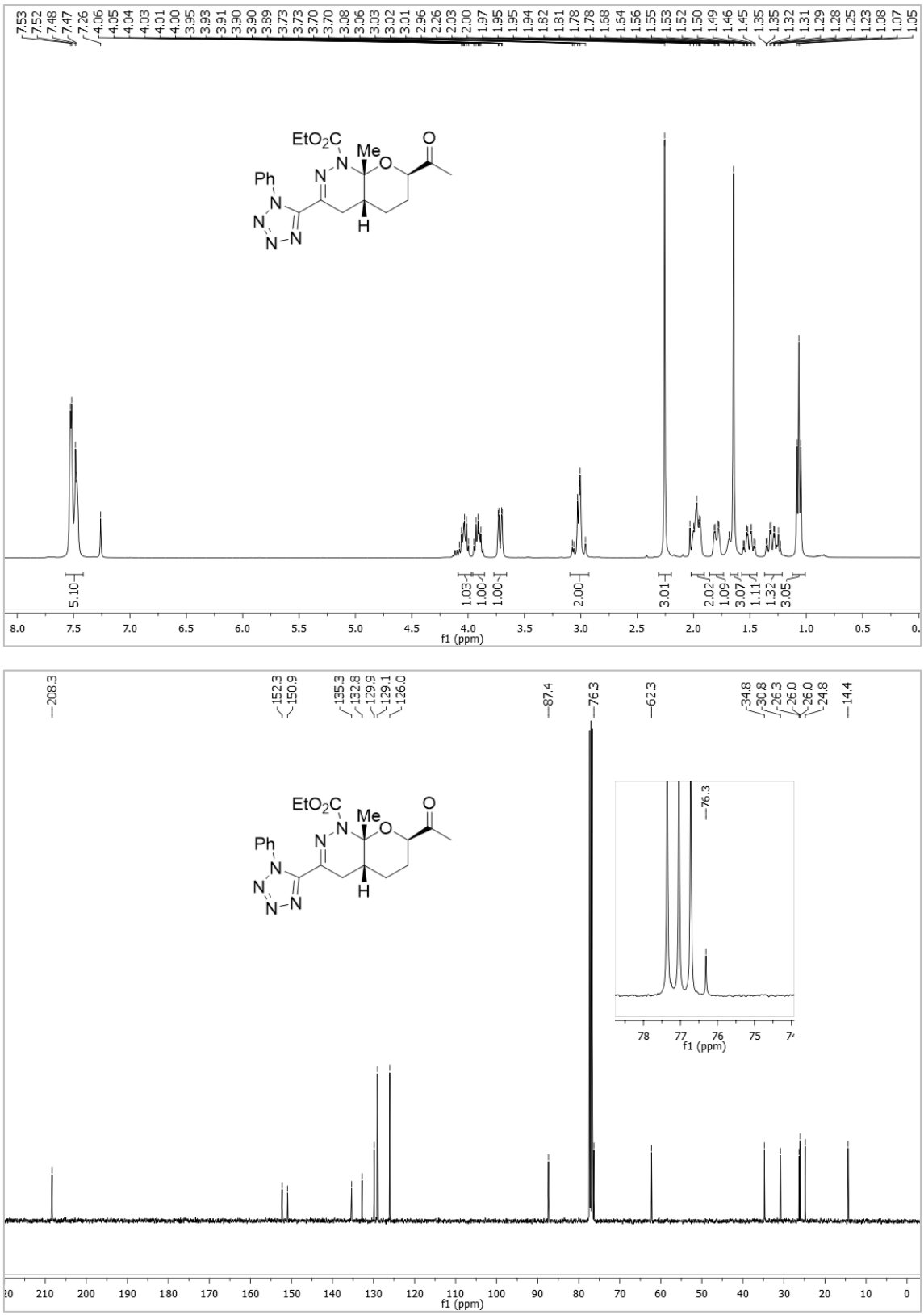


Figure S1. ^{1}H and ^{13}C NMR spectra of compound **7** ($CDCl_3$, 400 MHz).

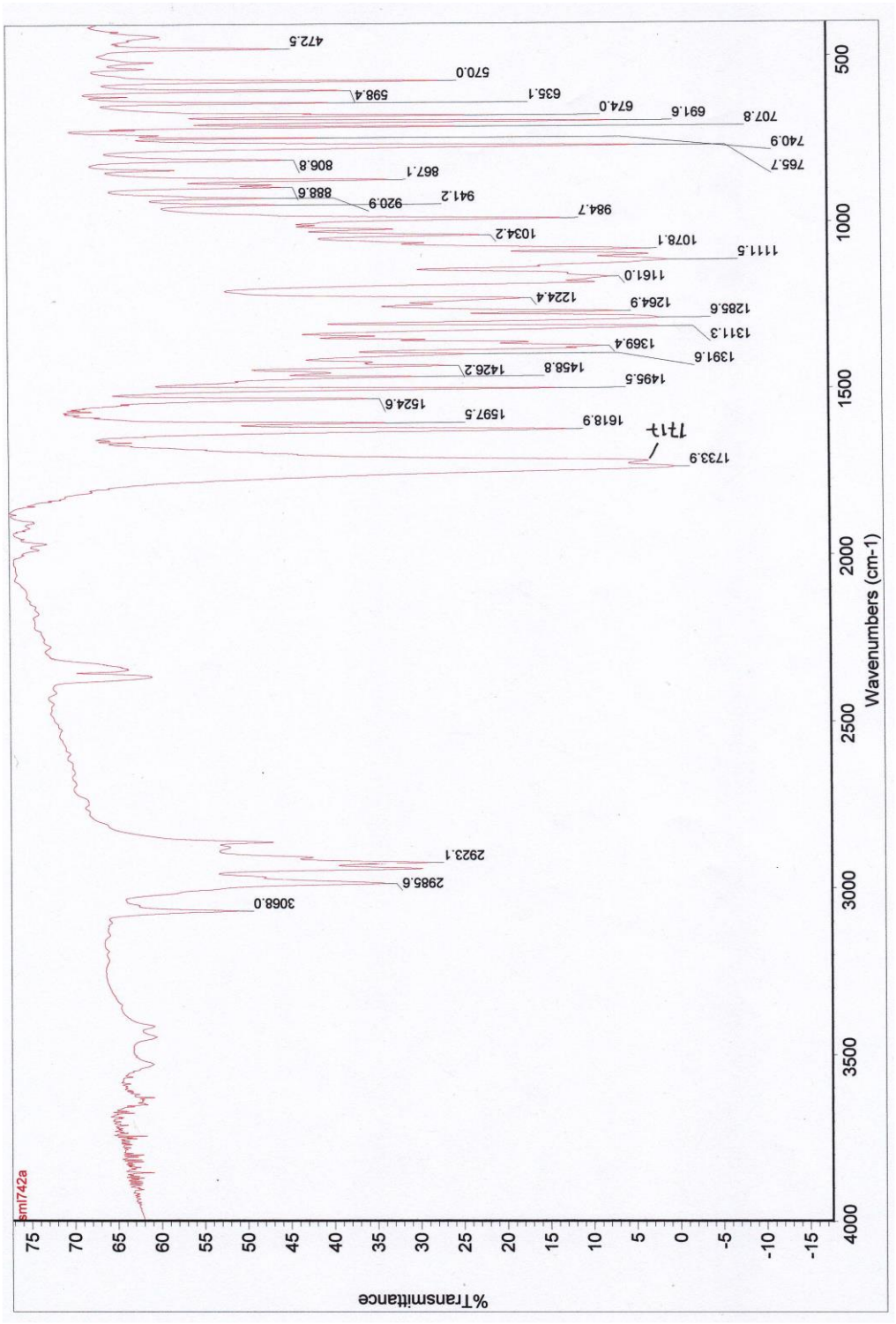
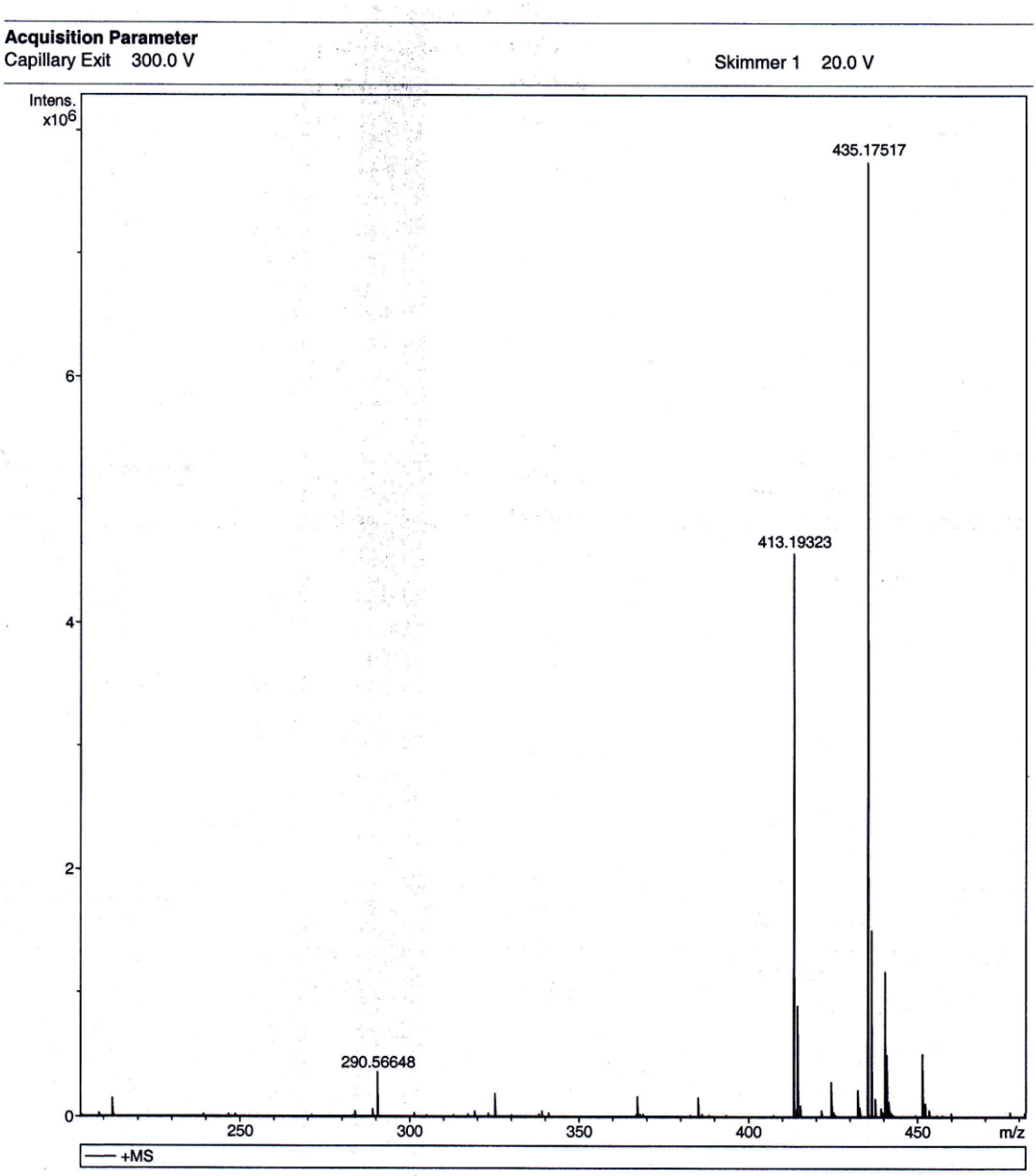


Figure S2. IR spectra of compound **7** (KBr).



Mass Spectrum Molecular Formula Report

Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
413.19323	1	C 20 H 25 N 6 O 4	100.00	413.19318	-0.1	-0.1	30.8	11.5	even	ok
	2	C 23 H 26 N 4 Na O 2	31.87	413.19480	1.6	3.8	43.4	12.5	even	ok
435.17517	1	C 20 H 24 N 6 Na O 4	100.00	435.17512	-0.0	-0.1	31.9	11.5	even	ok

Figure S3. HRMS of compound **7**.

Crystallographic data for Ethyl 7-acetyl-8a-methyl-3-(1-phenyl-1*H*-tetrazol-5-yl)-1,4,4a,5,6,8a-hexahydro-7*H*-pyrano[2,3-*c*]pyridazine-1-carboxylate (7).

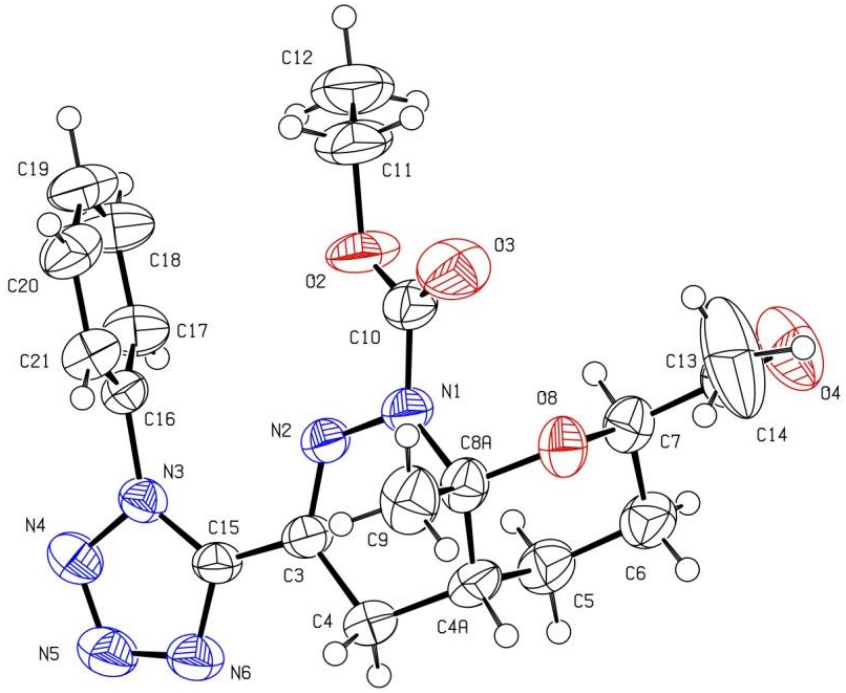


Figure S4. ORTEP-3 diagram of compound **7** with anisotropic displacement ellipsoids drawn at the 50% probability level. The methyl groups at C12 and C14 are disordered over two alternate positions; for clarity, only one of these positions is shown.

Table S1 - Crystal Data and Details of the Structure Determination

Crystal Data			
Formula			C20 H24 N6 O4
Formula Weight			412.45
Crystal System			triclinic
Space group		P-1	(No. 2)
a, b, c [Angstrom]	9.6243(3)	9.8590(2)	12.5952(3)
alpha, beta, gamma [deg]	68.645(2)	72.467(2)	75.230(2)
V [Ang**3]			1047.06(5)
Z			2
D(calc) [g/cm**3]			1.308
Mu(MoKa) [/mm]			0.094
F(000)			436
Crystal Size [mm]		0.13 x 0.17 x	0.18

Data Collection

Temperature (K)		293
Radiation [Angstrom]	MoKa	0.71073
Theta Min-Max [Deg]		1.8, 25.0
Dataset		-11: 11 ; -11: 11 ; -14: 14
Tot., Uniq. Data, R(int)		31073, 3684, 0.042
Observed Data [I > 2.0 sigma(I)]		2287

Refinement

Nref, Npar	3684, 296
R, wR2, S	0.0465, 0.1359, 1.00
w = ^2^(FO^2^)+(0.0641P)^2^+0.2961P] WHERE P=(FO^2^+2FC^2^)/3'	
Max. and Av. Shift/Error	0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-0.19, 0.21

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms

Atom	x	y	z	U(eq) [Ang^2]
O2	0.63708(18)	-0.0239(2)	0.21692(17)	0.0706(7)
O3	0.5633(2)	0.2144(2)	0.13135(18)	0.0816(8)
O4	0.8328(3)	0.3131(3)	-0.26002(19)	0.1008(10)
O8	0.80056(17)	0.35267(16)	0.01041(12)	0.0504(6)
N1	0.79049(19)	0.13472(19)	0.17513(15)	0.0452(6)
N2	0.85231(19)	0.02734(19)	0.26130(15)	0.0414(6)
N3	0.96181(18)	-0.18754(19)	0.45586(15)	0.0397(6)
N4	1.0540(2)	-0.2666(2)	0.52746(16)	0.0507(7)
N5	1.1661(2)	-0.1992(2)	0.49300(18)	0.0572(8)
N6	1.1506(2)	-0.0773(2)	0.40038(17)	0.0510(7)
C3	0.9681(2)	0.0444(2)	0.28196(18)	0.0419(8)
C4	1.0505(3)	0.1715(3)	0.2172(2)	0.0525(8)
C4A	1.0053(3)	0.2558(3)	0.1023(2)	0.0509(8)
C5	1.0806(3)	0.1761(3)	0.0103(2)	0.0574(9)
C6	1.0289(3)	0.2531(3)	-0.1020(2)	0.0590(9)
C7	0.8617(3)	0.2767(3)	-0.07430(19)	0.0508(8)
C8A	0.8385(3)	0.2825(2)	0.11948(19)	0.0479(8)
C9	0.7579(3)	0.3828(3)	0.1933(2)	0.0680(10)
C10	0.6522(3)	0.1158(3)	0.1724(2)	0.0515(9)
C11	0.4944(3)	-0.0572(4)	0.2272(3)	0.0889(15)
*C12A	0.5183(8)	-0.2097(13)	0.2153(10)	0.097(3)
*C12B	0.4854(13)	-0.090(3)	0.139(2)	0.127(9)
C13	0.8012(3)	0.3638(3)	-0.1817(2)	0.0608(10)
*C14A	0.735(4)	0.516(2)	-0.202(2)	0.088(7)

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued)

Atom	x	y	z	U(eq) [Ang^2]
*C14B	0.686(4)	0.500(2)	-0.175(2)	0.142(7)
C15	1.0242(2)	-0.0717(2)	0.37743(18)	0.0395(7)
C16	0.8234(2)	-0.2336(2)	0.47598(18)	0.0396(7)
C17	0.8245(3)	-0.3582(3)	0.4525(2)	0.0580(9)
C18	0.6916(3)	-0.4041(3)	0.4762(3)	0.0761(11)
C19	0.5618(3)	-0.3261(3)	0.5221(2)	0.0691(11)
C20	0.5644(3)	-0.2030(3)	0.5459(2)	0.0611(9)
C21	0.6957(3)	-0.1558(3)	0.5239(2)	0.0518(8)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites are disordered

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters

Atom	x	y	z	U(iso) [Ang^2]
H4A	1.03756	0.35218	0.07277	0.0610
H4B	1.15593	0.13540	0.20222	0.0630
H4C	1.02891	0.23642	0.26439	0.0630
H5A	1.18666	0.17089	-0.00640	0.0690
H5B	1.05974	0.07592	0.04180	0.0690
H6A	1.06933	0.19350	-0.15431	0.0710
H6B	1.06324	0.34738	-0.14075	0.0710
H7	0.82980	0.17998	-0.04177	0.0610
H9A	0.79092	0.47677	0.15682	0.1020
H9B	0.77805	0.33907	0.26987	0.1020
H9C	0.65363	0.39636	0.19993	0.1020
H11A	0.44858	0.01550	0.16615	0.1060
H11B	0.42987	-0.05504	0.30259	0.1060
*H12A	0.42468	-0.23567	0.22496	0.1450
*H12B	0.56678	-0.28038	0.27436	0.1450
*H12C	0.57869	-0.20964	0.13916	0.1450
*H12D	0.50865	-0.01004	0.06791	0.1910
*H12E	0.38686	-0.10584	0.14993	0.1910
*H12F	0.55393	-0.17800	0.13240	0.1910
*H14A	0.80974	0.57550	-0.22272	0.1310
*H14B	0.66501	0.52802	-0.13137	0.1310
*H14C	0.68439	0.54710	-0.26389	0.1310
*H14D	0.67673	0.56084	-0.25222	0.2130
*H14E	0.71615	0.55448	-0.13828	0.2130
*H14F	0.59287	0.47037	-0.12909	0.2130

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters (continued)

Atom	x	y	z	U(iso) [Ang^2]
H17	0.91247	-0.41091	0.42132	0.0700
H18	0.68972	-0.48900	0.46089	0.0910
H19	0.47253	-0.35725	0.53674	0.0830
H20	0.47658	-0.15039	0.57743	0.0730
H21	0.69786	-0.07250	0.54122	0.0620

==========

The Temperature Factor has the Form of Exp(-T) where

T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - Bond Distances (Angstrom)

O2	-C10	1.313(3)	C13	-C14A	1.43(2)
O2	-C11	1.450(4)	C16	-C17	1.361(4)
O3	-C10	1.192(4)	C16	-C21	1.369(4)
O4	-C13	1.190(4)	C17	-C18	1.377(4)
O8	-C7	1.423(3)	C18	-C19	1.373(4)
O8	-C8A	1.407(3)	C19	-C20	1.360(4)
N1	-N2	1.373(3)	C20	-C21	1.373(4)
N1	-C8A	1.494(3)	C4	-H4B	0.9700
N1	-C10	1.402(4)	C4	-H4C	0.9700
N2	-C3	1.281(3)	C4A	-H4A	0.9800
N3	-N4	1.351(3)	C5	-H5A	0.9700
N3	-C15	1.346(3)	C5	-H5B	0.9700
N3	-C16	1.437(3)	C6	-H6A	0.9700
N4	-N5	1.291(3)	C6	-H6B	0.9700
N5	-N6	1.349(3)	C7	-H7	0.9800
N6	-C15	1.316(3)	C9	-H9A	0.9600
C3	-C4	1.496(4)	C9	-H9B	0.9600
C3	-C15	1.457(3)	C9	-H9C	0.9600
C4	-C4A	1.514(4)	C11	-H11A	0.9700
C4A	-C5	1.534(4)	C11	-H11B	0.9700
C4A	-C8A	1.520(4)	C12A	-H12A	0.9600
C5	-C6	1.508(4)	C12A	-H12B	0.9600
C6	-C7	1.515(4)	C12A	-H12C	0.9600
C7	-C13	1.510(4)	C12B	-H12F	0.9600
C8A	-C9	1.513(3)	C12B	-H12D	0.9600
C11	-C12A	1.518(13)	C12B	-H12E	0.9600
C11	-C12B	1.30(2)	C14A	-H14C	0.9600
C13	-C14B	1.52(3)	C14A	-H14A	0.9600

Table S5 - Bond Distances (Angstrom) (continued)

C14A	-H14B	0.9700	C18	-H18	0.9300
C14B	-H14D	0.9600	C19	-H19	0.9300
C14B	-H14E	0.9600	C20	-H20	0.9300
C14B	-H14F	0.9600	C21	-H21	0.9300
C17	-H17	0.9300			

Table S5 - Bond Angles (Degrees)

C10	-O2	-C11	116.5(2)	N1	-C8A	-C9	110.6(2)
C7	-O8	-C8A	116.26(18)	C4A	-C8A	-C9	113.5(2)
N2	-N1	-C8A	121.14(19)	O2	-C10	-O3	125.3(3)
N2	-N1	-C10	114.65(18)	O2	-C10	-N1	111.1(2)
C8A	-N1	-C10	120.8(2)	O3	-C10	-N1	123.6(3)
N1	-N2	-C3	119.64(19)	O2	-C11	-C12A	108.1(4)
N4	-N3	-C15	107.76(18)	O2	-C11	-C12B	114.4(8)
N4	-N3	-C16	119.38(17)	O4	-C13	-C7	118.4(3)
C15	-N3	-C16	132.83(18)	O4	-C13	-C14B	123.9(10)
N3	-N4	-N5	106.73(18)	O4	-C13	-C14A	118.8(10)
N4	-N5	-N6	110.76(19)	C7	-C13	-C14B	117.1(10)
N5	-N6	-C15	106.38(19)	C7	-C13	-C14A	121.4(11)
N2	-C3	-C4	126.1(2)	N3	-C15	-N6	108.36(18)
N2	-C3	-C15	116.47(19)	N3	-C15	-C3	128.50(19)
C4	-C3	-C15	117.40(19)	N6	-C15	-C3	123.14(19)
C3	-C4	-C4A	109.6(2)	N3	-C16	-C17	118.7(2)
C4	-C4A	-C5	111.4(2)	N3	-C16	-C21	119.2(2)
C4	-C4A	-C8A	111.2(2)	C17	-C16	-C21	122.0(2)
C5	-C4A	-C8A	110.5(2)	C16	-C17	-C18	118.1(3)
C4A	-C5	-C6	112.1(2)	C17	-C18	-C19	120.8(3)
C5	-C6	-C7	109.2(2)	C18	-C19	-C20	119.7(3)
O8	-C7	-C6	110.6(2)	C19	-C20	-C21	120.5(3)
O8	-C7	-C13	108.5(2)	C16	-C21	-C20	118.8(3)
C6	-C7	-C13	112.3(2)	C3	-C4	-H4B	110.00
O8	-C8A	-N1	110.3(2)	C3	-C4	-H4C	110.00
O8	-C8A	-C4A	109.87(19)	C4A	-C4	-H4B	110.00
O8	-C8A	-C9	105.83(19)	C4A	-C4	-H4C	110.00
N1	-C8A	-C4A	106.86(19)	H4B	-C4	-H4C	108.00

Table S5 - Bond Angles (Degrees) (continued)

C4	-C4A	-H4A	108.00	H11A	-C11	-H11B	108.00
C5	-C4A	-H4A	108.00	C11	-C12A	-H12A	110.00
C8A	-C4A	-H4A	108.00	C11	-C12A	-H12B	109.00
C4A	-C5	-H5A	109.00	C11	-C12A	-H12C	109.00
C4A	-C5	-H5B	109.00	H12A	-C12A	-H12B	109.00
C6	-C5	-H5A	109.00	H12A	-C12A	-H12C	110.00
C6	-C5	-H5B	109.00	H12B	-C12A	-H12C	109.00
H5A	-C5	-H5B	108.00	C11	-C12B	-H12F	110.00
C5	-C6	-H6A	110.00	C11	-C12B	-H12D	110.00
C5	-C6	-H6B	110.00	C11	-C12B	-H12E	110.00
C7	-C6	-H6A	110.00	H12E	-C12B	-H12F	109.00
C7	-C6	-H6B	110.00	H12D	-C12B	-H12E	109.00
H6A	-C6	-H6B	108.00	H12D	-C12B	-H12F	109.00
O8	-C7	-H7	108.00	C13	-C14A	-H14A	110.00
C6	-C7	-H7	108.00	H14A	-C14A	-H14B	109.00
C13	-C7	-H7	108.00	C13	-C14A	-H14B	109.00
C8A	-C9	-H9A	109.00	C13	-C14A	-H14C	110.00
C8A	-C9	-H9B	109.00	H14A	-C14A	-H14C	110.00
C8A	-C9	-H9C	109.00	H14B	-C14A	-H14C	109.00
H9A	-C9	-H9B	109.00	C13	-C14B	-H14D	110.00
H9A	-C9	-H9C	109.00	H14E	-C14B	-H14F	109.00
H9B	-C9	-H9C	110.00	C13	-C14B	-H14F	109.00
O2	-C11	-H11A	110.00	H14D	-C14B	-H14E	110.00
O2	-C11	-H11B	110.00	C13	-C14B	-H14E	109.00
C12A	-C11	-H11A	110.00	H14D	-C14B	-H14F	110.00
C12A	-C11	-H11B	110.00	C16	-C17	-H17	121.00
C12B	-C11	-H11A	59.00	C18	-C17	-H17	121.00
C12B	-C11	-H11B	135.00	C17	-C18	-H18	120.00

Table S5 - Bond Angles (Degrees) (continued)

C19	-C18	-H18	120.00	C21	-C20	-H20	120.00
C18	-C19	-H19	120.00	C20	-C21	-H21	121.00
C20	-C19	-H19	120.00	C16	-C21	-H21	121.00
C19	-C20	-H20	120.00				

Table S6 - Torsion Angles (Degrees)

C11	-O2	-C10	-O3	-6.6(4)
C11	-O2	-C10	-N1	175.6(2)
C10	-O2	-C11	-C12A	149.9(5)
C8A	-O8	-C7	-C6	-60.0(3)
C8A	-O8	-C7	-C13	176.5(2)
C7	-O8	-C8A	-N1	-59.2(3)
C7	-O8	-C8A	-C4A	58.3(3)
C7	-O8	-C8A	-C9	-178.8(2)
C8A	-N1	-N2	-C3	-11.1(3)
C10	-N1	-N2	-C3	-170.5(2)
N2	-N1	-C8A	-O8	159.62(18)
N2	-N1	-C8A	-C4A	40.3(2)
N2	-N1	-C8A	-C9	-83.7(3)
C10	-N1	-C8A	-O8	-42.3(3)
C10	-N1	-C8A	-C4A	-161.6(2)
C10	-N1	-C8A	-C9	74.4(3)
N2	-N1	-C10	-O2	-26.1(3)
N2	-N1	-C10	-O3	156.1(2)
C8A	-N1	-C10	-O2	174.49(19)
C8A	-N1	-C10	-O3	-3.4(4)
N1	-N2	-C3	-C4	-2.3(3)
N1	-N2	-C3	-C15	177.87(18)
C15	-N3	-N4	-N5	0.4(2)
C16	-N3	-N4	-N5	-177.76(18)
N4	-N3	-C15	-N6	-0.8(2)
N4	-N3	-C15	-C3	179.6(2)
C16	-N3	-C15	-N6	177.1(2)
C16	-N3	-C15	-C3	-2.6(4)

Table S6 - Torsion Angles (Degrees) (continued)

N4	-N3	-C16	-C17	-71.0(3)
N4	-N3	-C16	-C21	105.5(2)
C15	-N3	-C16	-C17	111.4(3)
C15	-N3	-C16	-C21	-72.2(3)
N3	-N4	-N5	-N6	0.1(2)
N4	-N5	-N6	-C15	-0.5(2)
N5	-N6	-C15	-N3	0.8(2)
N5	-N6	-C15	-C3	-179.51(19)
N2	-C3	-C4	-C4A	-16.1(3)
C15	-C3	-C4	-C4A	163.7(2)
N2	-C3	-C15	-N3	-8.0(3)
N2	-C3	-C15	-N6	172.4(2)
C4	-C3	-C15	-N3	172.2(2)
C4	-C3	-C15	-N6	-7.5(3)
C3	-C4	-C4A	-C5	-77.9(3)
C3	-C4	-C4A	-C8A	45.9(3)
C4	-C4A	-C5	-C6	176.1(2)
C8A	-C4A	-C5	-C6	51.9(3)
C4	-C4A	-C8A	-O8	-176.3(2)
C4	-C4A	-C8A	-N1	-56.7(3)
C4	-C4A	-C8A	-C9	65.4(3)
C5	-C4A	-C8A	-O8	-52.0(3)
C5	-C4A	-C8A	-N1	67.6(2)
C5	-C4A	-C8A	-C9	-170.3(2)
C4A	-C5	-C6	-C7	-52.5(3)
C5	-C6	-C7	-O8	54.4(3)
C5	-C6	-C7	-C13	175.6(2)
O8	-C7	-C13	-O4	-175.5(3)

Table S6 - Torsion Angles (Degrees) (continued)

O8	-C7	-C13	-C14B	-4.2(15)
C6	-C7	-C13	-O4	62.0(4)
C6	-C7	-C13	-C14B	-126.7(15)
N3	-C16	-C17	-C18	177.7(2)
C21	-C16	-C17	-C18	1.3(4)
N3	-C16	-C21	-C20	-178.2(2)
C17	-C16	-C21	-C20	-1.8(4)
C16	-C17	-C18	-C19	0.1(4)
C17	-C18	-C19	-C20	-0.8(4)
C18	-C19	-C20	-C21	0.3(4)
C19	-C20	-C21	-C16	1.0(4)

Table S7 – Potential Hydrogen Bonds/Short Contacts (Angstrom, Deg)

C4	-- H4C	.. N4	0.9700	2.6000	3.464(3)	148.00	2_756
C7	-- H7	.. N1	0.9800	2.5300	2.879(3)	101.00	.
C11	-- H11A	.. O3	0.9700	2.3300	2.671(4)	100.00	.
C11	-- H11B	.. N6	0.9700	2.6300	3.379(4)	135.00	1_455