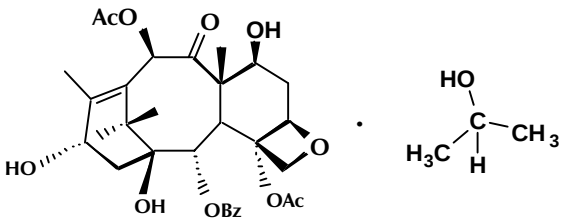
Supplemental Material:

Structure Determination of Baccatin III – iPA Complex
by Single Crystal Analysis



CRYSTAL DATA

Chemical formula: $C_{31}H_{38}O_{11} \cdot C_3H_8O$
Crystal system: Orthorhombic
Space Group: *P2₁2₁2*

a = 9.3975(3) Å α = 90°
b = 41.736(2) Å β = 90°
c = 8.5401(3) Å γ = 90°
Z = 4 d_x = 1.284 g cm^{-3}

V = 3349.6(2) Å^3
No. of reflections for lattice parameters: 25
θ range for lattice parameters (°):22.67-42.17
Absorption coefficient (mm^{-1}): 0.77

EXPERIMENTAL:

Crystallization
Crystal source: CH_2Cl_2/iPA
Crystal description: Unstable colorless plate
Crystal size (mm): 0.20X 0.30 X 0.45
Data Collection
Temperature (K): 295
θ_{max} (°): 75
No. of reflections measured: 3974
No. of independent reflections: 3684
No. of observed reflections ($I \geq 3\sigma$): 3469
Absorption correction (T_{min}-T_{max}): 0.80-1.00
R_{int}: 0.00

REFINEMENT

No. of parameters refined: 415 No. of reflections used: 3469
$R(F)$ = 0.067 $wR(F)$ = 0.087 S = 3.66 Weighting Scheme $w = 1/\sigma^2$ (F)

Treatment of Hydrogen Atoms: Hydrogens of C1 and C13 hydroxyl groups were located from difference Fourier maps while those of C7 and iPA hydroxyl groups were missing. The positions of all the other hydrogen atoms were calculated from an idealized geometry with standard bond lengths and angles. Their positions were calculated from an idealized geometry with standard bond lengths and angles. They

had assigned isotropic temperature factors and were included in structure factor calculations with fixed parameters.

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters U_{eq} ($Å^2$ x 10^3)

	x	y	z	U_{eq}
O(2)	-7916(3)	-636(1)	-8828(3)	44(1)
O(4)	-7807(3)	-610(1)	-12046(3)	48(1)
O(41)	-7752(3)	-988(1)	-13942(3)	55(1)
O(1)	-6451(3)	-1028(1)	-7019(3)	50(1)
O(10)	-9053(4)	-2104(1)	-9514(4)	63(1)
C(2)	-8323(4)	-970(1)	-8936(4)	40(1)
O(21)	-9118(4)	-589(1)	-6549(3)	62(1)
C(4)	-9191(4)	-724(1)	-11512(5)	44(1)
C(21')	-8334(4)	-476(1)	-7528(5)	44(1)
C(3)	-8978(4)	-1035(1)	-10587(4)	39(1)
O(7)	-11988(3)	-1511(1)	-12431(4)	62(1)
O(5)	-11076(4)	-453(1)	-11998(4)	70(1)
O(13)	-4705(3)	-1249(1)	-12087(3)	59(1)
C(11)	-7519(4)	-1651(1)	-9935(4)	44(1)
C(1)	-6945(4)	-1161(1)	-8463(4)	40(1)
O(9)	-11229(4)	-1718(1)	-9279(5)	75(1)
C(19)	-11591(4)	-1084(1)	-9658(6)	59(1)
C(22)	-7753(4)	-147(1)	-7470(5)	48(1)
C(9)	-10239(4)	-1594(1)	-9934(5)	50(1)
C(13)	-5291(4)	-1384(1)	-10694(4)	46(1)
C(14)	-5715(4)	-1103(1)	-9636(5)	47(1)
C(15)	-7254(4)	-1526(1)	-8265(4)	46(1)

C(17)	-8474(5)	-1580(1)	-7093(5)	56(1)
C(12)	-6539(4)	-1600(1)	-11057(5)	46(1)
C(8)	-10385(4)	-1247(1)	-10567(5)	45(1)
C(10)	-8930(4)	-1801(1)	-10315(4)	47(1)
C(23)	-7036(5)	-9(1)	-8723(5)	58(1)
C(7)	-10804(4)	-1298(1)	-12323(5)	50(1)
C(18)	-6634(5)	-1720(1)	-12725(5)	60(1)
C(5)	-10303(4)	-705(1)	-12845(5)	53(1)
C(21)	-7204(4)	-760(1)	-13304(5)	50(1)
C(20)	-9975(5)	-436(1)	-10805(6)	59(1)
C(27)	-7949(6)	23(1)	-6104(5)	65(1)
C(26)	-7371(6)	332(1)	-5990(8)	80(2)
C(25)	-6644(6)	464(1)	-7193(7)	69(1)
C(6)	-11229(5)	-991(1)	-13181(6)	61(1)
C(16)	-5949(5)	-1696(1)	-7536(5)	59(1)
C(24)	-6505(6)	299(1)	-8590(7)	73(1)
O(101)	-9637(10)	-2362(1)	-11654(6)	151(3)
C(42)	-5863(6)	-602(1)	-13772(6)	68(1)
C(101)	-9360(7)	-2364(1)	-10312(7)	76(2)
C(102)	-9310(11)	-2661(1)	-9369(10)	119(3)
O(04)	-11027(9)	-2031(1)	-13946(8)	164(3)
C(03)	-11740(20)	-2471(3)	-15380(20)	305(13)
C(02)	-12662(12)	-1953(3)	-15852(13)	161(4)
C(01)	-11644(11)	-2162(2)	-15214(10)	119(3)
H(1)	-7199	-1019	-6099	80
H(2A)	-9033	-1014	-8156	80
H(3A)	-8292	-1157	-11170	80
H(7A)	-11746	-1675	-12887	80
H(13)	-3777	-1371	-12346	80

H(19A)	-11703	-866	-10003	80
H(19B)	-12458	-1199	-9841	80
H(19C)	-11374	-1086	-8560	80
H(13B)	-4569	-1507	-10173	80
H(14A)	-4896	-1026	-9142	80
H(14B)	-6059	-916	-10432	80
H(17A)	-8647	-1804	-6942	80
H(17B)	-8226	-1483	-6110	80
H(17C)	-9316	-1480	-7500	80
H(10A)	-8933	-1842	-11421	80
H(23A)	-6895	-129	-9667	80
H(7B)	-10006	-1393	-12851	80
H(18A)	-7458	-1854	-12847	80
H(18B)	-6692	-1543	-13439	80
H(18C)	-5793	-1843	-12944	80
H(5A)	-9880	-620	-13781	80
H(20A)	-9427	-243	-10860	80
H(20B)	-10310	-473	-9759	80
H(27A)	-8471	-70	-5254	80
H(26A)	-7480	449	-5029	80
H(25A)	-6238	673	-7069	80
H(6A)	-12192	-938	-12912	80
H(6B)	-11202	-1034	-14285	80
H(16A)	-6138	-1920	-7375	80
H(16B)	-5149	-1672	-8225	80
H(16C)	-5741	-1597	-6549	80
H(24A)	-6046	400	-9464	80
H(42A)	-5465	-713	-14656	80

H(42B)	-6045	-383	-14049	80
H(42C)	-5205	-610	-12914	80
H(10B)	-9541	-2844	-9999	80
H(10C)	-8395	-2692	-8892	80
H(10D)	-10017	-2635	-8569	80
H(04A)	-11491	-1876	-13658	246
H(03A)	-10888	-2573	-15019	80
H(03B)	-12480	-2497	-14610	80
H(03C)	-12038	-2566	-16348	80
H(02A)	-13109	-2045	-16758	80
H(02B)	-13357	-1926	-15038	80
H(02C)	-12261	-1749	-16118	80
H(01A)	-10927	-2153	-16015	80

Table 2. Bond lengths (Å) and angles (°)

O(2)-C(21')	1.354(4)
O(2)-C(2)	1.450(4)
O(4)-C(21)	1.365(5)
O(4)-C(4)	1.458(5)
O(41)-C(21)	1.212(5)
O(1)-C(1)	1.430(4)
O(10)-C(101)	1.313(5)
O(10)-C(10)	1.445(4)
C(2)-C(1)	1.572(5)
C(2)-C(3)	1.562(5)
O(21)-C(21')	1.210(5)
C(4)-C(20)	1.534(5)

C(4)-C(5)	1.547(6)
C(4)-C(3)	1.531(5)
C(21')-C(22)	1.479(5)
C(3)-C(8)	1.590(5)
O(7)-C(7)	1.425(5)
O(5)-C(20)	1.454(5)
O(5)-C(5)	1.469(5)
O(13)-C(13)	1.428(5)
C(11)-C(12)	1.346(5)
C(11)-C(10)	1.502(5)
C(11)-C(15)	1.538(5)
C(1)-C(14)	1.548(5)
C(1)-C(15)	1.562(5)
O(9)-C(9)	1.203(5)
C(19)-C(8)	1.533(5)
C(22)-C(23)	1.390(6)
C(22)-C(27)	1.378(5)
C(9)-C(10)	1.538(6)
C(9)-C(8)	1.553(5)
C(13)-C(12)	1.510(5)
C(13)-C(14)	1.531(5)
C(15)-C(17)	1.538(6)
C(15)-C(16)	1.547(6)
C(12)-C(18)	1.514(5)
C(8)-C(7)	1.566(6)
C(23)-C(24)	1.382(6)
C(7)-C(6)	1.530(6)
C(5)-C(6)	1.507(6)

C(21)-C(42)	1.476(6)
C(27)-C(26)	1.403(7)
C(26)-C(25)	1.351(8)
C(25)-C(24)	1.383(8)
O(101)-C(101)	1.175(7)
C(101)-C(102)	1.478(7)
O(04)-C(01)	1.344(9)
C(03)-C(01)	1.298(14)
C(02)-C(01)	1.404(11)

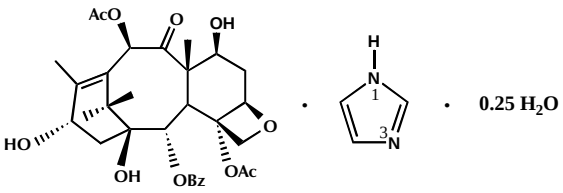
C(21')-O(2)-C(2)	116.7(3)
C(21)-O(4)-C(4)	117.8(3)
C(101)-O(10)-C(10)	119.8(4)
O(2)-C(2)-C(1)	104.7(3)
O(2)-C(2)-C(3)	109.1(3)
C(1)-C(2)-C(3)	118.0(3)
O(4)-C(4)-C(20)	107.2(3)
O(4)-C(4)-C(5)	110.8(3)
C(20)-C(4)-C(5)	85.6(3)
O(4)-C(4)-C(3)	108.7(3)
C(20)-C(4)-C(3)	121.5(3)
C(5)-C(4)-C(3)	120.9(3)
O(21)-C(21')-O(2)	123.5(3)
O(21)-C(21')-C(22)	124.3(3)
O(2)-C(21')-C(22)	112.2(3)
C(4)-C(3)-C(2)	111.8(3)
C(4)-C(3)-C(8)	111.6(3)
C(2)-C(3)-C(8)	114.4(3)
C(20)-O(5)-C(5)	91.5(3)

C(12)-C(11)-C(10)	121.1(3)
C(12)-C(11)-C(15)	119.7(3)
C(10)-C(11)-C(15)	119.0(3)
O(1)-C(1)-C(14)	104.8(3)
O(1)-C(1)-C(2)	107.1(3)
C(14)-C(1)-C(2)	111.7(3)
O(1)-C(1)-C(15)	110.2(3)
C(14)-C(1)-C(15)	111.1(3)
C(2)-C(1)-C(15)	111.7(3)
C(23)-C(22)-C(27)	120.1(4)
C(23)-C(22)-C(21')	122.6(4)
C(27)-C(22)-C(21')	117.3(4)
O(9)-C(9)-C(10)	118.5(4)
O(9)-C(9)-C(8)	119.6(4)
C(10)-C(9)-C(8)	121.4(3)
O(13)-C(13)-C(12)	111.4(3)
O(13)-C(13)-C(14)	106.8(3)
C(12)-C(13)-C(14)	112.0(3)
C(13)-C(14)-C(1)	117.2(3)
C(17)-C(15)-C(16)	105.2(3)
C(17)-C(15)-C(11)	115.7(3)
C(16)-C(15)-C(11)	110.3(3)
C(17)-C(15)-C(1)	110.5(3)
C(16)-C(15)-C(1)	110.2(3)
C(11)-C(15)-C(1)	105.0(3)
C(11)-C(12)-C(13)	118.7(3)
C(11)-C(12)-C(18)	125.2(4)
C(13)-C(12)-C(18)	116.0(4)

C(19)-C(8)-C(9)	107.7(3)
C(19)-C(8)-C(7)	111.1(3)
C(9)-C(8)-C(7)	103.1(3)
C(19)-C(8)-C(3)	111.9(3)
C(9)-C(8)-C(3)	116.7(3)
C(7)-C(8)-C(3)	106.0(3)
O(10)-C(10)-C(11)	109.5(3)
O(10)-C(10)-C(9)	109.2(3)
C(11)-C(10)-C(9)	115.2(3)
C(22)-C(23)-C(24)	119.9(4)
O(7)-C(7)-C(6)	106.7(3)
O(7)-C(7)-C(8)	110.1(3)
C(6)-C(7)-C(8)	114.1(3)
O(5)-C(5)-C(6)	112.1(4)
O(5)-C(5)-C(4)	90.6(3)
C(6)-C(5)-C(4)	119.2(3)
O(41)-C(21)-O(4)	122.4(4)
O(41)-C(21)-C(42)	126.2(4)
O(4)-C(21)-C(42)	111.4(4)
O(5)-C(20)-C(4)	91.7(3)
C(22)-C(27)-C(26)	118.8(5)
C(25)-C(26)-C(27)	121.1(5)
C(26)-C(25)-C(24)	120.1(4)
C(5)-C(6)-C(7)	115.1(3)
C(25)-C(24)-C(23)	119.9(5)
O(101)-C(101)-O(10)	123.2(5)
O(101)-C(101)-C(102)	123.1(5)
O(10)-C(101)-C(102)	113.7(5)

C(03)-C(01)-O(04)	121.3(11)
C(03)-C(01)-C(02)	121.6(12)
O(04)-C(01)-C(02)	110.8(7)

Structure Determination of Baccatin III – Imidazole Complex by Single Crystal Analysis



CRYSTAL DATA

Chemical formula: $C_{31}H_{38}O_{11} \cdot C_3H_4N_2 \cdot 0.25H_2O$
Crystal system: Orthorhombic
Space Group: *P2₁2₁2*

a = 9.2771(4) Å $\alpha = 90°$
b = 41.215(2) Å $\beta = 90°$
c = 8.5788(4) Å $\gamma = 90°$
Z = 4 $d_X = 1.325$ g cm^{-3}

V = 3280.1(2) Å^3
No. of reflections for lattice parameters: 25
θ range for lattice parameters (°):15.93-42.58
Absorption coefficient (mm^{-1}): 0.79

EXPERIMENTAL:

Crystallization
Crystal source: CH_3CN
Crystal description: Colorless thick plate
Crystal size (mm): 0.10X 0.35 X 0.42
Data Collection
Temperature (K): 295
θ_{max} (°): 75
No. of reflections measured: 3894
No. of independent reflections: 3894
No. of observed reflections ($I \geq 3\sigma$): 3266
Absorption correction (T_{min}-T_{max}): 0.88-1.00
R_{int}: 0.00

REFINEMENT

No. of parameters refined: 428 No. of reflections used: 3266
R(F) = 0.039 *wR(F)* = 0.049 *S* = 2.168 Weighting Scheme $w = 1/\sigma^2$ (F)

Treatment of Hydrogen Atoms: The imino and hydroxyl hydrogens, except those for the water were located from difference Fourier maps while the positions of all the other hydrogen atoms were calculated from an idealized geometry with standard bond lengths and angles. Their positions were calculated from an idealized geometry with standard bond lengths and angles. They had assigned isotropic temperature factors and were included in structure factor calculations with fixed parameters.

Table 1. Atomic coordinates and equivalent isotropic displacement parameters U_{eq} ($Å^2$)

	x	y	z	U_{eq}
O1	0.8573(2)	0.10701(4)	-0.3318(2)	3.35(4)
O2	0.7120(2)	0.06572(4)	-0.1530(2)	2.73(3)
O4	0.7250(2)	0.06144(4)	0.1675(2)	3.08(4)
O5	0.3929(2)	0.04544(5)	0.1627(3)	4.27(4)
O7	0.3024(2)	0.15277(5)	0.2128(3)	3.67(4)
O9	0.3717(2)	0.17273(5)	-0.1054(3)	4.25(5)
O10	0.5788(2)	0.21353(4)	-0.0731(3)	3.55(4)
O13	1.0308(2)	0.12628(5)	0.1772(2)	3.65(4)
O21	0.5899(2)	0.06122(5)	-0.3793(2)	4.05(4)
O41	0.7277(2)	0.09865(5)	0.3598(2)	3.65(4)
O101	0.6964(4)	0.23951(5)	0.1140(3)	7.38(7)
C1	0.8071(3)	0.11951(6)	-0.1851(3)	2.57(5)
C2	0.6700(3)	0.09948(5)	-0.1398(3)	2.45(5)
C3	0.6037(3)	0.10490(5)	0.0270(3)	2.29(4)
C4	0.5843(3)	0.07276(6)	0.1168(3)	2.65(5)
C5	0.4707(3)	0.07038(6)	0.2472(3)	3.27(5)
C6	0.3783(3)	0.09963(7)	0.2859(4)	3.84(6)
C7	0.4191(3)	0.13079(6)	0.2013(3)	2.95(5)
C8	0.4606(3)	0.12559(6)	0.0268(3)	2.51(5)
C9	0.4717(3)	0.16124(6)	-0.0359(3)	2.89(5)
C10	0.6009(3)	0.18276(5)	0.0058(3)	2.91(5)
C11	0.7450(3)	0.16815(5)	-0.0327(3)	2.52(5)
C12	0.8421(3)	0.16210(6)	0.0803(3)	2.63(5)
C13	0.9718(3)	0.14090(6)	0.0410(3)	2.78(5)
C14	0.9326(3)	0.11311(6)	-0.0708(4)	2.95(5)
C15	0.7741(3)	0.15639(6)	-0.2003(3)	2.72(5)
C16	0.9052(4)	0.17458(7)	-0.2686(4)	3.91(6)
C17	0.6536(4)	0.16238(7)	-0.3177(3)	3.61(6)
C18	0.8307(3)	0.17223(7)	0.2480(3)	3.41(6)
C19	0.3375(3)	0.10924(7)	-0.0627(4)	3.30(5)
C20	0.5042(3)	0.04404(6)	0.0462(4)	3.42(6)
C21	0.6679(3)	0.04949(6)	-0.2816(3)	2.94(5)
C22	0.7250(3)	0.01596(6)	-0.2868(3)	3.08(5)
C23	0.7966(4)	0.00181(7)	-0.1635(4)	3.90(6)
C24	0.8486(4)	-0.02952(7)	-0.1770(5)	4.87(8)
C25	0.8313(4)	-0.04640(7)	-0.3136(5)	5.10(8)
C26	0.7598(4)	-0.03287(7)	-0.4359(5)	5.28(8)
C27	0.7058(4)	-0.00152(8)	-0.4232(4)	4.28(6)
C41	0.7838(3)	0.07583(6)	0.2948(3)	3.23(5)
C42	0.9205(4)	0.05972(8)	0.3411(4)	4.61(7)
C101	0.6335(4)	0.23996(6)	-0.0076(4)	4.04(7)

C102	0.6101(5)	0.26966(7)	-0.1021(5)	5.91(9)
N01	0.3255(5)	0.22565(9)	0.6280(4)	8.3(1)
N03	0.3622(4)	0.19951(7)	0.4136(4)	6.35(8)
C02	0.3093(5)	0.1981(1)	0.5543(5)	6.8(1)
C04	0.3994(8)	0.2459(1)	0.5328(6)	9.3(2)
C05	0.4174(7)	0.2295(1)	0.4035(5)	8.4(1)
O1'	0.392(1)	0.6266(3)	0.476(2)	8.1(3)
H2	0.594	0.107	-0.208	3.2*
H23	0.810	0.014	-0.071	5.1*
H24	0.891	-0.040	-0.087	6.9*
H25	0.872	-0.068	-0.322	6.8*
H26	0.740	-0.045	-0.531	7.2*
H27	0.654	0.009	-0.509	5.8*
H3	0.674	0.117	0.080	3.1*
H201	0.469	0.048	-0.059	4.7*
H202	0.558	0.024	0.044	4.7*
H5	0.510	0.068	0.351	4.1*
H61	0.385	0.104	0.395	5.2*
H62	0.283	0.095	0.259	5.2*
H421	0.962	0.070	0.430	5.9*
H422	0.903	0.037	0.363	5.9*
H423	0.988	0.061	0.256	5.9*
H7	0.504	0.140	0.250	3.8*
H191	0.327	0.088	-0.029	4.4*
H192	0.251	0.121	-0.047	4.4*
H193	0.361	0.109	-0.172	4.4*
H10	0.605	0.186	0.117	3.7*
H101	0.647	0.288	-0.050	8.1*
H102	0.648	0.268	-0.202	8.1*
H103	0.505	0.273	-0.112	8.1*
H181	0.748	0.185	0.264	4.6*
H182	0.827	0.154	0.314	4.6*
H183	0.915	0.185	0.276	4.6*
H13	1.038	0.155	-0.008	3.6*
H141	1.015	0.108	-0.129	3.8*
H142	0.907	0.095	-0.007	3.8*
H161	0.989	0.172	-0.204	5.2*
H162	0.930	0.166	-0.372	5.2*
H163	0.887	0.197	-0.280	5.2*
H171	0.567	0.152	-0.283	4.7*
H172	0.635	0.185	-0.326	4.7*
H173	0.678	0.154	-0.418	4.7*
H7'	0.300	0.169	0.291	5.0*
H1	0.779	0.107	-0.410	5.0*
H13'	1.117	0.137	0.198	5.5*
H01	0.289	0.231	0.730	10.4*
H02	0.264	0.179	0.600	8.8*
H04	0.434	0.268	0.556	11.6*
H05	0.465	0.238	0.310	10.8*

Table 2. Bond lengths (Å) and angles (°)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
O1	C1	1.437(3)	C4	C20	1.523(4)

O2	C2	1.449(3)	C5	C6	1.516(4)
O2	C21	1.354(3)	C6	C7	1.523(4)
O4	C4	1.453(3)	C7	C8	1.560(4)
O4	C41	1.356(3)	C8	C9	1.568(3)
O5	C5	1.450(3)	C8	C19	1.532(4)
O5	C20	1.438(4)	C9	C10	1.533(4)
O7	C7	1.415(3)	C10	C11	1.503(4)
O9	C9	1.200(3)	C11	C12	1.346(4)
O10	C10	1.452(3)	C11	C15	1.541(4)
O10	C101	1.326(3)	C12	C13	1.525(4)
O13	C13	1.423(3)	C12	C18	1.502(4)
O21	C21	1.208(3)	C13	C14	1.538(4)
O41	C41	1.211(3)	C15	C16	1.544(4)
O101	C101	1.195(5)	C15	C17	1.524(4)
C1	C2	1.565(3)	C21	C22	1.480(4)
C1	C14	1.544(4)	C22	C23	1.379(4)
C1	C15	1.556(3)	C22	C27	1.385(4)
C2	C3	1.573(4)	C23	C24	1.383(4)
C3	C4	1.543(3)	C24	C25	1.373(5)
C3	C8	1.578(3)	C25	C26	1.361(6)
C4	C5	1.540(4)	C26	C27	1.390(5)
C41	C42	1.485(4)	N03	C02	1.304(6)
C101	C102	1.484(5)	N03	C05	1.340(5)
N01	C02	1.309(6)	C04	C05	1.309(7)
N01	C04	1.354(7)			

C2-O2-C21	117.2(2)	O5-C5-C4	91.3(2)
C4-O4-C41	117.5(2)	O5-C5-C6	113.1(2)
C5-O5-C20	91.1(2)	C4-C5-C6	119.7(2)
C10-O10-C101	117.8(2)	C5-C6-C7	115.2(2)
O1-C1-C2	107.0(2)	O7-C7-C6	108.4(2)
O1-C1-C14	104.5(2)	O7-C7-C8	110.1(2)
O1-C1-C15	109.9(2)	C6-C7-C8	113.7(2)
C2-C1-C14	111.4(2)	C3-C8-C7	106.4(2)
C2-C1-C15	112.1(2)	C3-C8-C9	116.8(2)
C14-C1-C15	111.6(2)	C3-C8-C19	113.0(2)
O2-C2-C1	105.6(2)	C7-C8-C9	102.5(2)
O2-C2-C3	108.2(2)	C7-C8-C19	110.9(2)
C1-C2-C3	117.9(2)	C9-C8-C19	106.8(2)
C2-C3-C4	112.2(2)	O9-C9-C8	119.3(2)
C2-C3-C8	113.9(2)	O9-C9-C10	119.5(2)
C4-C3-C8	111.5(2)	C8-C9-C10	120.9(2)
O4-C4-C3	108.7(2)	O10-C10-C9	106.6(2)
O4-C4-C5	112.1(2)	O10-C10-C11	111.9(2)
O4-C4-C20	107.9(2)	C9-C10-C11	114.3(2)
C3-C4-C5	119.8(2)	C10-C11-C12	120.8(2)
C3-C4-C20	121.7(2)	C10-C11-C15	119.1(2)
C5-C4-C20	84.6(2)	C12-C11-C15	119.7(2)
C11-C12-C13	118.4(2)	C21-C22-C27	117.7(3)
C11-C12-C18	126.2(2)	C23-C22-C27	119.3(3)
C13-C12-C18	115.2(2)	C22-C23-C24	119.9(3)
O13-C13-C12	111.4(2)	C23-C24-C25	120.3(3)
O13-C13-C14	106.7(2)	C24-C25-C26	120.5(3)
C12-C13-C14	112.2(2)	C25-C26-C27	119.7(3)
C1-C14-C13	116.6(2)	C22-C27-C26	120.2(3)
C1-C15-C11	105.3(2)	O4-C41-O41	122.5(3)

C1-C15-C16	110.5(2)	O4-C41-C42	111.3(2)
C1-C15-C17	111.0(2)	O41-C41-C42	126.2(3)
C11-C15-C16	109.8(2)	O10-C101-O101	122.9(3)
C11-C15-C17	115.9(2)	O10-C101-C102	113.0(3)
C16-C15-C17	104.4(2)	O101-C101-C102	124.1(3)
O5-C20-C4	92.4(2)	C02-N01-C04	107.5(4)
O2-C21-O21	123.3(2)	C02-N03-C05	104.2(3)
O2-C21-C22	112.2(2)	N01-C02-N03	111.4(4)
O21-C21-C22	124.5(2)	N01-C04-C05	105.0(4)
C21-C22-C23	123.0(3)	N03-C05-C04	111.8(4)