Supplementary Material 1.

Table 1. Crystal data and structure refinement for shelx_a.

Identification code	shelx_a
Empirical formula	$C_{48}\ H_{55}\ F_2\ N_6\ O_{15.50}$
Formula weight	1001.98
Temperature	173(2) K
Wavelength	1.54186 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 13.4283(3) Å
	b = 7.01490(10) Å β= 95.1830(10)°.
	c = 49.9625(9) Å
Volume	4687.13(15) Å^3
Z	4
Density (calculated)	1.420 Mg/m^3
Absorption coefficient	0.947 mm^{-1}
F(000)	2108
Crystal size	0.089 x 0.046 x 0.034 mm^3
Theta range for data collection	3.344 to 68.241°.
Index ranges	-16<=h<=15, -8<=k<=8, -59<=l<=60
Reflections collected	33571
Independent reflections	8551 [R(int) = 0.0815]
Completeness to theta = 67.686°	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.969 and 0.646
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8551 / 44 / 673

Goodness-of-fit on F^2	0.956
Final R indices [I>2sigma(I)]	R_1 = 0.0903, wR_2 = 0.2247
R indices (all data)	R_1 = 0.1513, wR_2 = 0.2797
Extinction coefficient	n/a
Largest diff. peak and hole	0.731 and -0.636 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for shelx_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1)	4942(2)	-361(4)	4656(1)	65(1)
N(1)	3199(3)	2057(5)	3675(1)	46(1)
O(1)	4970(3)	3446(5)	3062(1)	70(1)
C(1)	5374(4)	3038(7)	3286(1)	56(1)
N(2)	2840(3)	-26(5)	4591(1)	50(1)
O(2)	6363(2)	3097(5)	3339(1)	63(1)
F(2)	4441(2)	8453(4)	3169(1)	65(1)
C(2)	3793(4)	2501(6)	3483(1)	52(1)
O(3)	6262(2)	1961(5)	3816(1)	60(1)
N(3)	1547(3)	-624(6)	5011(1)	55(1)
C(3)	4812(3)	2480(7)	3516(1)	49(1)
C(4)	5308(4)	1973(6)	3769(1)	49(1)
O(4)	3392(2)	5011(5)	4732(1)	70(1)
N(4)	5541(3)	5864(5)	4196(1)	46(1)
C(5)	4675(3)	1465(6)	3976(1)	45(1)
O(5)	2166(2)	5335(5)	4406(1)	64(1)
N(5)	6467(3)	8138(5)	3333(1)	52(1)
O(6)	2557(2)	6382(5)	3944(1)	58(1)
N(6)	7955(3)	9297(6)	2990(1)	60(1)
C(6)	3632(3)	1549(6)	3931(1)	46(1)
C(7)	3027(3)	1145(6)	4138(1)	48(1)
O(7)	-761(2)	3373(5)	4666(1)	63(1)

C(8)	3437(3)	520(6)	4390(1)	46(1)
O(8)	-1151(3)	890(6)	4401(1)	86(1)
C(9)	4487(4)	383(6)	4422(1)	50(1)
O(9)	-1128(3)	1139(6)	3892(1)	83(1)
C(11)	3118(4)	591(7)	4870(1)	56(1)
O(11)	10164(3)	7725(6)	3133(1)	79(1)
C(10)	5088(3)	870(6)	4229(1)	50(1)
O(10)	9093(3)	6332(5)	2832(1)	67(1)
C(14)	1223(3)	-1143(7)	4726(1)	55(1)
O(14)	6143(3)	3768(6)	2626(1)	82(1)
C(13)	1754(3)	47(7)	4528(1)	54(1)
O(13)	8088(3)	2932(6)	2805(1)	85(1)
C(12)	2650(4)	-717(7)	5064(1)	55(1)
O(12)	12007(3)	7009(7)	3155(1)	95(1)
C(16)	1619(4)	1485(8)	3366(1)	62(1)
O(16)	850(3)	3114(5)	5047(1)	70(1)
C(15)	2108(3)	2245(7)	3624(1)	50(1)
O(15)	5239(8)	3592(15)	4940(2)	159(4)
C(17)	1476(3)	477(7)	3625(1)	54(1)
C(18)	3129(4)	5318(7)	4494(1)	57(1)
C(19)	4836(3)	5509(6)	4364(1)	49(1)
C(20)	3834(3)	5714(6)	4290(1)	46(1)
C(21)	3484(3)	6257(6)	4021(1)	49(1)
C(22)	4246(3)	6676(6)	3844(1)	46(1)
C(23)	5262(3)	6496(6)	3930(1)	45(1)
C(24)	6005(3)	6896(6)	3760(1)	50(1)
C(25)	5754(3)	7547(7)	3499(1)	48(1)

C(26)	4724(4)	7719(7)	3419(1)	50(1)
C(27)	3994(3)	7281(6)	3579(1)	52(1)
C(28)	6420(4)	7489(7)	3051(1)	60(1)
C(29)	6897(3)	8970(7)	2884(1)	60(1)
C(30)	7520(3)	8306(7)	3445(1)	55(1)
C(31)	8061(3)	9718(7)	3284(1)	59(1)
C(32)	6591(3)	5489(7)	4280(1)	51(1)
C(33)	6982(4)	5952(8)	4563(1)	68(2)
C(34)	7285(4)	7138(8)	4338(1)	61(1)
C(35)	-853(4)	2593(8)	4431(1)	58(1)
C(36)	-618(3)	3700(7)	4194(1)	49(1)
C(37)	-770(4)	2923(8)	3936(1)	62(1)
C(38)	-554(4)	4007(9)	3714(1)	68(2)
C(39)	-172(4)	5824(9)	3749(1)	71(2)
C(40)	-15(4)	6599(8)	4006(1)	70(2)
C(41)	-234(3)	5541(7)	4220(1)	59(1)
C(42)	9974(4)	6538(8)	2943(1)	59(1)
C(43)	10804(4)	5425(9)	2854(1)	83(1)
C(44)	11790(4)	5723(8)	2959(1)	63(1)
C(45)	12573(4)	4630(9)	2868(1)	70(2)
C(46)	12366(5)	3288(10)	2677(1)	94(2)
C(47)	11399(5)	2954(10)	2576(1)	86(1)
C(48)	10616(4)	4018(10)	2660(1)	93(2)

Table 3. Bond lengths [Å] and angles [°] for shelx_a.

F(1)-C(9)	1.371(5)
N(1)-C(2)	1.340(5)
N(1)-C(6)	1.402(5)
N(1)-C(15)	1.470(5)
O(1)-C(1)	1.233(6)
C(1)-O(2)	1.331(5)
C(1)-C(3)	1.483(6)
N(2)-C(8)	1.390(5)
N(2)-C(13)	1.465(5)
N(2)-C(11)	1.476(5)
F(2)-C(26)	1.374(5)
C(2)-C(3)	1.364(6)
O(3)-C(4)	1.281(5)
N(3)-C(12)	1.482(5)
N(3)-C(14)	1.496(5)
C(3)-C(4)	1.422(6)
C(4)-C(5)	1.440(6)
O(4)-C(18)	1.230(5)
N(4)-C(19)	1.342(5)
N(4)-C(23)	1.422(5)
N(4)-C(32)	1.458(5)
C(5)-C(10)	1.396(6)
C(5)-C(6)	1.401(6)
O(5)-C(18)	1.329(5)
N(5)-C(25)	1.385(5)

N(5)-C(28)	1.478(5)
N(5)-C(30)	1.478(5)
O(6)-C(21)	1.273(5)
N(6)-C(29)	1.489(6)
N(6)-C(31)	1.495(5)
C(6)-C(7)	1.400(6)
C(7)-C(8)	1.401(6)
O(7)-C(35)	1.290(5)
C(8)-C(9)	1.408(6)
O(8)-C(35)	1.265(6)
C(9)-C(10)	1.357(6)
O(9)-C(37)	1.352(6)
C(11)-C(12)	1.513(6)
O(11)-C(42)	1.272(6)
O(10)-C(42)	1.270(5)
C(14)-C(13)	1.521(6)
O(12)-C(44)	1.341(6)
C(16)-C(15)	1.492(6)
C(16)-C(17)	1.501(6)
C(15)-C(17)	1.503(6)
C(18)-C(20)	1.479(6)
C(19)-C(20)	1.370(6)
C(20)-C(21)	1.432(6)
C(21)-C(22)	1.443(6)
C(22)-C(23)	1.399(6)
C(22)-C(27)	1.403(6)
C(23)-C(24)	1.395(6)

C(24)-C(25)	1.395(6)
C(25)-C(26)	1.408(6)
C(26)-C(27)	1.353(6)
C(28)-C(29)	1.510(7)
C(30)-C(31)	1.502(6)
C(32)-C(33)	1.494(6)
C(32)-C(34)	1.497(6)
C(33)-C(34)	1.483(7)
C(35)-C(36)	1.475(6)
C(36)-C(41)	1.393(6)
C(36)-C(37)	1.396(6)
C(37)-C(38)	1.397(7)
C(38)-C(39)	1.380(7)
C(39)-C(40)	1.392(7)
C(40)-C(41)	1.356(6)
C(42)-C(43)	1.463(7)
C(43)-C(48)	1.390(8)
C(43)-C(44)	1.395(7)
C(44)-C(45)	1.411(7)
C(45)-C(46)	1.350(7)
C(46)-C(47)	1.370(8)
C(47)-C(48)	1.385(7)

C(2)-N(1)-C(6)	119.2(4)
C(2)-N(1)-C(15)	120.3(4)
C(6)-N(1)-C(15)	120.4(3)
O(1)-C(1)-O(2)	121.5(4)

O(1)-C(1)-C(3)	123.4(5)
O(2)-C(1)-C(3)	115.0(5)
C(8)-N(2)-C(13)	117.7(4)
C(8)-N(2)-C(11)	119.1(4)
C(13)-N(2)-C(11)	110.7(3)
N(1)-C(2)-C(3)	124.6(5)
C(12)-N(3)-C(14)	111.1(3)
C(2)-C(3)-C(4)	119.6(4)
C(2)-C(3)-C(1)	118.6(4)
C(4)-C(3)-C(1)	121.8(5)
O(3)-C(4)-C(3)	122.9(4)
O(3)-C(4)-C(5)	120.9(4)
C(3)-C(4)-C(5)	116.2(4)
C(19)-N(4)-C(23)	120.1(4)
C(19)-N(4)-C(32)	120.3(4)
C(23)-N(4)-C(32)	119.5(3)
C(10)-C(5)-C(6)	117.9(4)
C(10)-C(5)-C(4)	120.7(4)
C(6)-C(5)-C(4)	121.4(4)
C(25)-N(5)-C(28)	120.4(4)
C(25)-N(5)-C(30)	119.1(4)
C(28)-N(5)-C(30)	110.0(3)
C(29)-N(6)-C(31)	112.5(3)
C(7)-C(6)-C(5)	120.8(4)
C(7)-C(6)-N(1)	120.3(4)
C(5)-C(6)-N(1)	119.0(4)
C(6)-C(7)-C(8)	121.4(4)

N(2)-C(8)-C(7)	122.0(4)
N(2)-C(8)-C(9)	122.5(4)
C(7)-C(8)-C(9)	115.5(4)
C(10)-C(9)-F(1)	117.0(4)
C(10)-C(9)-C(8)	123.9(4)
F(1)-C(9)-C(8)	119.1(4)
N(2)-C(11)-C(12)	110.1(4)
C(9)-C(10)-C(5)	120.4(4)
N(3)-C(14)-C(13)	111.8(4)
N(2)-C(13)-C(14)	111.0(4)
N(3)-C(12)-C(11)	108.9(4)
C(15)-C(16)-C(17)	60.3(3)
N(1)-C(15)-C(16)	118.1(4)
N(1)-C(15)-C(17)	118.7(4)
C(16)-C(15)-C(17)	60.2(3)
C(16)-C(17)-C(15)	59.6(3)
O(4)-C(18)-O(5)	120.5(4)
O(4)-C(18)-C(20)	123.7(5)
O(5)-C(18)-C(20)	115.8(5)
N(4)-C(19)-C(20)	122.8(4)
C(19)-C(20)-C(21)	120.8(4)
C(19)-C(20)-C(18)	117.8(4)
C(21)-C(20)-C(18)	121.3(4)
O(6)-C(21)-C(20)	122.2(4)
O(6)-C(21)-C(22)	121.8(4)
C(20)-C(21)-C(22)	116.0(4)
C(23)-C(22)-C(27)	117.6(4)

C(23)-C(22)-C(21)	121.2(4)
C(27)-C(22)-C(21)	121.2(4)
C(24)-C(23)-C(22)	121.8(4)
C(24)-C(23)-N(4)	119.4(4)
C(22)-C(23)-N(4)	118.9(4)
C(23)-C(24)-C(25)	120.6(4)
N(5)-C(25)-C(24)	122.4(4)
N(5)-C(25)-C(26)	121.3(4)
C(24)-C(25)-C(26)	116.1(4)
C(27)-C(26)-F(2)	117.7(4)
C(27)-C(26)-C(25)	124.0(4)
F(2)-C(26)-C(25)	118.2(4)
C(26)-C(27)-C(22)	119.9(4)
N(5)-C(28)-C(29)	109.3(4)
N(6)-C(29)-C(28)	110.4(4)
N(5)-C(30)-C(31)	110.0(4)
N(6)-C(31)-C(30)	112.8(4)
N(4)-C(32)-C(33)	118.7(4)
N(4)-C(32)-C(34)	119.0(4)
C(33)-C(32)-C(34)	59.4(3)
C(34)-C(33)-C(32)	60.4(3)
C(33)-C(34)-C(32)	60.2(3)
O(8)-C(35)-O(7)	120.8(5)
O(8)-C(35)-C(36)	119.4(5)
O(7)-C(35)-C(36)	119.9(5)
C(41)-C(36)-C(37)	118.1(5)
C(41)-C(36)-C(35)	121.1(4)

C(37)-C(36)-C(35)	120.8(5)
O(9)-C(37)-C(36)	122.1(5)
O(9)-C(37)-C(38)	118.1(5)
C(36)-C(37)-C(38)	119.8(5)
C(39)-C(38)-C(37)	120.2(5)
C(38)-C(39)-C(40)	120.1(5)
C(41)-C(40)-C(39)	119.3(5)
C(40)-C(41)-C(36)	122.5(5)
O(10)-C(42)-O(11)	121.2(5)
O(10)-C(42)-C(43)	120.8(5)
O(11)-C(42)-C(43)	118.1(5)
C(48)-C(43)-C(44)	118.5(5)
C(48)-C(43)-C(42)	119.7(5)
C(44)-C(43)-C(42)	121.8(5)
O(12)-C(44)-C(43)	120.8(5)
O(12)-C(44)-C(45)	118.8(5)
C(43)-C(44)-C(45)	120.3(6)
C(46)-C(45)-C(44)	119.7(6)
C(45)-C(46)-C(47)	120.4(6)
C(46)-C(47)-C(48)	121.2(6)
C(47)-C(48)-C(43)	119.8(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for shelx_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(1)	59(2)	68(2)	67(2)	8(1)	4(1)	5(1)
N(1)	44(2)	46(2)	49(2)	1(2)	12(2)	-1(2)
O(1)	70(2)	82(3)	62(2)	4(2)	27(2)	-3(2)
C(1)	55(3)	42(3)	75(4)	-3(3)	27(3)	1(2)
N(2)	53(2)	53(2)	46(2)	-1(2)	10(2)	-5(2)
O(2)	55(2)	61(2)	77(2)	-2(2)	29(2)	1(2)
F(2)	60(2)	70(2)	64(2)	3(1)	9(1)	3(1)
C(2)	57(3)	47(3)	54(3)	0(2)	17(2)	-6(2)
O(3)	46(2)	58(2)	76(2)	-2(2)	15(2)	2(2)
N(3)	59(3)	51(3)	58(3)	-1(2)	20(2)	-2(2)
C(3)	49(3)	49(3)	52(3)	-3(2)	17(2)	3(2)
C(4)	50(3)	41(3)	58(3)	-6(2)	15(2)	0(2)
O(4)	68(2)	74(3)	74(3)	10(2)	31(2)	5(2)
N(4)	41(2)	46(2)	53(2)	-6(2)	9(2)	-2(2)
C(5)	42(3)	39(3)	54(3)	-5(2)	10(2)	2(2)
O(5)	53(2)	64(2)	77(2)	-11(2)	20(2)	-5(2)
N(5)	49(2)	58(3)	52(2)	-6(2)	17(2)	-4(2)
O(6)	44(2)	58(2)	72(2)	-7(2)	8(2)	0(2)
N(6)	59(3)	55(3)	69(3)	0(2)	24(2)	2(2)
C(6)	53(3)	42(3)	43(2)	-3(2)	9(2)	-4(2)
C(7)	45(3)	47(3)	52(3)	-3(2)	12(2)	-4(2)
O(7)	63(2)	69(2)	58(2)	-3(2)	12(2)	-4(2)

C(8)	44(3)	48(3)	48(3)	0(2)	7(2)	0(2)
O(8)	132(4)	61(3)	69(2)	-5(2)	28(2)	-30(2)
C(9)	52(3)	43(3)	52(3)	0(2)	-1(2)	-1(2)
O(9)	121(3)	65(3)	66(2)	-11(2)	20(2)	-21(2)
C(11)	57(3)	60(3)	53(3)	0(2)	7(2)	-5(2)
O(11)	71(3)	87(3)	81(3)	-17(2)	13(2)	0(2)
C(10)	45(3)	45(3)	60(3)	-7(2)	6(2)	-3(2)
O(10)	48(2)	69(2)	85(2)	-9(2)	4(2)	3(2)
C(14)	54(3)	57(3)	58(3)	-6(2)	16(2)	-6(2)
O(14)	83(3)	100(3)	66(2)	-14(2)	24(2)	-19(2)
C(13)	49(3)	59(3)	53(3)	-1(2)	10(2)	-7(2)
O(13)	82(3)	69(3)	106(3)	12(2)	23(2)	-9(2)
C(12)	59(3)	58(3)	50(3)	1(2)	8(2)	0(2)
O(12)	60(3)	118(4)	105(3)	-32(3)	0(2)	0(2)
C(16)	56(3)	77(4)	54(3)	5(3)	6(2)	-7(3)
O(16)	67(2)	63(2)	80(3)	-11(2)	-1(2)	8(2)
C(15)	44(3)	50(3)	58(3)	-1(2)	9(2)	2(2)
O(15)	144(7)	141(7)	188(8)	7(7)	-1(6)	0(6)
C(17)	49(3)	50(3)	65(3)	3(2)	10(2)	-6(2)
C(18)	47(3)	43(3)	82(4)	-1(3)	20(3)	-3(2)
C(19)	51(3)	40(3)	57(3)	-4(2)	13(2)	-2(2)
C(20)	43(3)	41(3)	56(3)	-4(2)	13(2)	-1(2)
C(21)	44(3)	38(3)	66(3)	-9(2)	14(2)	-1(2)
C(22)	45(3)	39(3)	55(3)	-3(2)	14(2)	-3(2)
C(23)	46(3)	37(3)	55(3)	-5(2)	11(2)	-4(2)
C(24)	48(3)	46(3)	55(3)	-5(2)	10(2)	1(2)
C(25)	43(3)	49(3)	54(3)	-8(2)	13(2)	-7(2)

C(26)	57(3)	44(3)	50(3)	1(2)	8(2)	6(2)
C(27)	42(3)	48(3)	66(3)	-6(2)	9(2)	1(2)
C(28)	61(3)	62(3)	60(3)	-8(3)	17(2)	-3(3)
C(29)	49(3)	67(4)	66(3)	3(3)	13(2)	-2(3)
C(30)	48(3)	62(3)	55(3)	1(2)	11(2)	0(2)
C(31)	52(3)	64(3)	62(3)	-9(3)	17(2)	-2(3)
C(32)	37(3)	56(3)	60(3)	-6(2)	7(2)	2(2)
C(33)	54(3)	81(4)	68(3)	-3(3)	7(3)	-1(3)
C(34)	45(3)	62(4)	77(4)	-5(3)	8(2)	0(3)
C(35)	52(3)	55(3)	67(3)	-3(3)	13(2)	-1(3)
C(36)	40(3)	50(3)	59(3)	-3(2)	9(2)	-4(2)
C(37)	62(3)	58(4)	68(3)	1(3)	17(3)	2(3)
C(38)	69(4)	77(4)	61(3)	6(3)	15(3)	7(3)
C(39)	56(3)	77(4)	83(4)	22(3)	20(3)	4(3)
C(40)	65(4)	64(4)	84(4)	10(3)	14(3)	-14(3)
C(41)	47(3)	60(3)	71(3)	-2(3)	11(2)	-5(3)
C(42)	60(3)	61(3)	57(3)	1(3)	11(2)	0(3)
C(43)	64(3)	99(4)	86(3)	-24(3)	9(2)	15(3)
C(44)	66(3)	61(3)	63(3)	5(3)	12(3)	-3(3)
C(45)	55(3)	89(5)	69(4)	21(3)	16(3)	11(3)
C(46)	68(4)	108(5)	108(5)	-19(4)	14(3)	27(4)
C(47)	68(3)	101(4)	90(3)	-26(3)	9(2)	16(3)
C(48)	56(4)	105(5)	117(5)	-43(4)	1(3)	23(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for shelx_a.

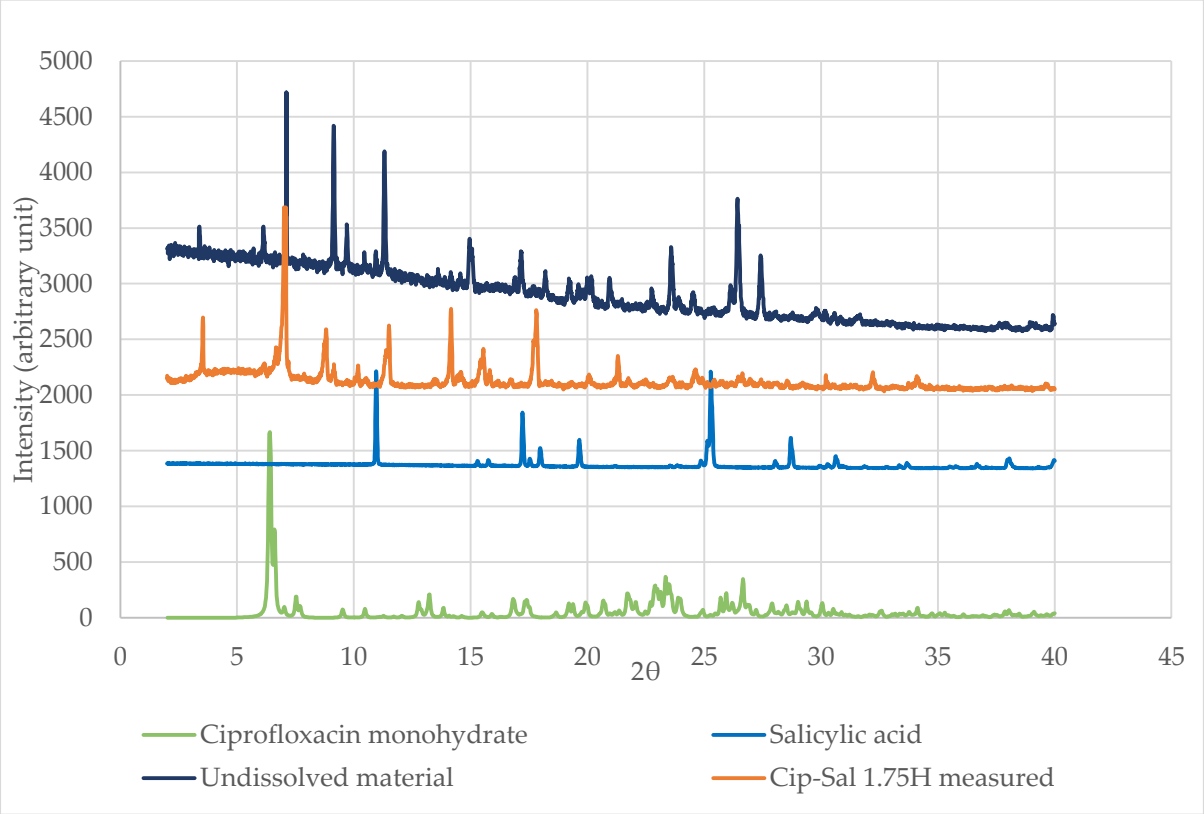
	x	y	z	U(eq)
H(2A)	6514	2804	3500	95
H(2)	3483	2855	3312	62
H(3A)	1335	577	5045	66
H(3AB)	1261	-1437	5124	66
H(5A)	2104	5583	4241	96
H(6A)	8206	10291	2900	72
H(6AB)	8322	8243	2958	72
H(7)	2323	1298	4106	57
H(9)	-1229	630	4039	125
H(11A)	2887	1915	4894	68
H(11B)	3855	569	4907	68
H(10)	5794	806	4266	60
H(14A)	492	-951	4692	67
H(14B)	1364	-2509	4698	67
HA14	5700(20)	3780(100)	2748(6)	123
HB14	6019(18)	2940(40)	2492(5)	123
H(13A)	1580	-438	4344	64
H(13B)	1524	1386	4535	64
HA13	7465(15)	3120(90)	2733(10)	127
HB13	8410(30)	4030(30)	2793(13)	127
H(12A)	2883	-2041	5041	67

H(12B)	2852	-317	5251	67
H(12)	11478	7536	3194	142
H(16A)	2051	868	3241	74
H(16B)	1045	2203	3278	74
HA16	410(30)	3320(80)	4906(5)	105
HB16	990(40)	4130(40)	5150(7)	105
H(15)	1808	3429	3694	60
HA15	4704(14)	3970(50)	4836(7)	238
HB15	5710(20)	4480(40)	4968(4)	238
H(17A)	1821	-758	3659	65
H(17B)	814	578	3696	65
H(19)	5040	5097	4542	58
H(24)	6688	6724	3823	59
H(27)	3312	7382	3511	62
H(28A)	5714	7294	2980	73
H(28B)	6777	6260	3040	73
H(29A)	6873	8535	2695	72
H(29B)	6519	10180	2888	72
H(30A)	7851	7047	3440	66
H(30B)	7546	8729	3635	66
H(31A)	7796	11010	3314	71
H(31B)	8779	9714	3350	71
H(32)	6886	4339	4200	61
H(33A)	6510	6516	4682	81
H(33B)	7488	5086	4653	81
H(34A)	7980	7008	4289	73
H(34B)	7002	8439	4318	73

H(38)	-672	3491	3538	82
H(39)	-15	6548	3598	85
H(40)	242	7854	4031	85
H(41)	-122	6077	4395	71
H(45)	13243	4838	2940	84
H(46)	12895	2571	2613	113
H(47)	11264	1976	2447	103
H(48)	9951	3786	2585	112

Supplementary Material 2

Diffractogram of undissolved material in media pH 1.2 consisted of the starting materials (ciprofloxacin monohydrate and salicylic acid) and ciprofloxacin salicylate 1.75 hydrate peaks.



Supplementary Material 3

Diffractogram of potassium bromide, cocrystal, and the mixture; pressed to make a pellet for FTIR.