SUPPLEMENTARY MATERIAL

Table 1. Crystal data and structure refinement for 1.

Identification code	1
Empirical formula	$C_{48}\ N_4\ O_4\ H_{36}$
Formula weight	796.81
Temperature	173(2) K
Wavelength	0.71070 A
Crystal system, space group	monoclinic, P $2_1/n$
Unit cell dimensions	a = 10.168(2) A b = 33.916(7) A β = 98.58(3) deg. c = 11.277(2) A
Volume	3845.1(13) A^3
Z, Calculated density	8, 1.376 Mg/m^3
Absorption coefficient	0.095 mm^{-1}
F(000)	1600
Crystal size	0.30 x 0.30 x 42 mm
Theta range for data collection	2.98 to 22.50 deg.
Index ranges	-11<=h<=12, -40<=k<=40, -13<=l<=13
Reflections collected / unique	16717 / 4946 [R(int) = 0.0897]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4702 / 0 / 577
Goodness-of-fit on F^2	1.007
Final R indices [I>2sigma(I)]	R1 = 0.0579, wR2 = 0.1447
R indices (all data)	R1 = 0.0761, wR2 = 0.1612
Largest diff. peak and hole	0.470 and -0.243 $e.A^{-3}$

After anisotropic refinement of all non-hydrogen atoms, aromatic and hydroxyl hydrogen atoms were placed in idealized positions and allowed to ride on the atom to which they are attached. The C=C based on C30/C31 was found to lie disordered across two positions. Atoms C30A/C31A and C30B/C31B were therefore refined with fixed site occupancies of 0.65 and 0.25, respectively. Carbon atoms of the corresponding pyridyl units, C27 and C32, were found to lie disordered across two sites. C27A/C32A and C27B/C32B were therefore refined with fixed site occupancies of 0.72 and 0.28, respectively. Electron density corresponding to a cyclobutane ring was found to lie between the two bipyridines. Carbon atoms of the ring, C30C, C31C, C42B, and C43B, were therefore refined with fix site occupancies of 0.10. Additionally, carbon atoms of the C=C based on C42/C43, C42A and C43A, were refined with fix site occupancies of 0.90. All crystallographic calculations were conducted using SHELXL-93 locally implemented on an IBM compatible pentium-based PC.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	5602(2)	-691(1)	8121(2)	48(1)
O(2)	5888(2)	-827(1)	6235(2)	53(1)
O(3)	7742(3)	-98(1)	9537(2)	55(1)
O(4)	8028(2)	-259(1)	7678(2)	51(1)
O(5)	-4678(2)	1680(1)	5407(2)	39(1)
O(6)	-4432(2)	2245(1)	4448(2)	51(1)
O(7)	-2927(2)	2129(1)	7168(2)	43(1)
O(8)	-2792(2)	1511(1)	7860(2)	55(1)
N(1)	3640(3)	-238(1)	7089(2)	50(1)
N(2)	-2993(3)	1329(1)	4194(2)	44(1)
N(3)	6161(3)	430(1)	8551(2)	49(1)
N(4)	-827(3)	1933(1)	6243(2)	47(1)
C(1)	7214(3)	-1164(1)	7830(3)	40(1)
C(2)	6971(4)	-1540(1)	7372(3)	52(1)
C(3)	7727(4)	-1861(1)	7803(3)	59(1)
C(4)	8766(4)	-1806(1)	8675(3)	52(1)
C(5)	9098(3)	-1428(1)	9176(3)	47(1)
C(6)	10177(4)	-1377(1)	10081(3)	57(1)
C(7)	10506(3)	-1021(1)	10566(3)	54(1)
C(8)	9750(3)	-685(1)	10150(3)	53(1)
C(9)	8691(3)	-715(1)	9244(3)	41(1)
C(10)	8306(3)	-1092(1)	8739(3)	39(1)
C(11)	6193(3)	-868(1)	7309(3)	41(1)
C(12)	8093(3)	-334(1)	8736(3)	41(1)
C(13)	-5741(3)	2236(1)	6025(2)	30(1)
C(14)	-6689(3)	2496(1)	5485(3)	38(1)
C(15)	-7721(3)	2633(1)	6072(3)	44(1)
C(16)	-7832(3)	2494(1)	7177(3)	42(1)
C(17)	-6889(3)	2227(1)	7777(3)	35(1)
C(18)	-7064(3)	2071(1)	8902(3)	42(1)
C(19)	-6165(3)	1813(1)	9488(3)	46(1)
C(20)	-5011(3)	1725(1)	9007(3)	41(1)
C(21)	-4778(3)	1877(1)	7932(2)	32(1)
C(22)	-5773(3)	2113(1)	7231(2)	30(1)
C(23)	-4852(3)	2062(1)	5230(3)	34(1)
C(24)	-3414(3)	1813(1)	7628(3)	39(1)
C(25)	3674(4)	-149(1)	5942(3)	57(1)
C(26)	2781(5)	81(1)	5267(4)	64(1)
C(28)	1665(4)	141(1)	6973(4)	65(1)
C(29)	2632(4)	-96(1)	7584(3)	57(1)
C(33)	-2083(4)	1099(1)	4797(3)	52(1)
C(34)	-2984(4)	1378(1)	3029(3)	51(1)
C(35)	-2055(4)	1201(1)	2441(4)	68(1)
C(36)	-1120(4)	964(1)	3075(6)	72(1)
C(37)	6160(4)	536(1)	7411(3)	53(1)
C(38)	5204(4)	758(1)	6785(3)	56(1)

C(40)	4146(4)	776(1)	8521(4)	66(1)
C(41)	5162(4)	548(1)	9099(3)	57(1)
C(45)	109(3)	1693(1)	6778(3)	44(1)
C(46)	-802(3)	2028(1)	5105(3)	53(1)
C(47)	168(4)	1898(1)	4483(3)	58(1)
C(48)	1133(3)	1650(1)	5045(3)	51(1)
C(27A)	1829(7)	234(1)	5673(5)	44(1)
C(30A)	823(5)	481(1)	4884(5)	42(1)
C(31A)	-218(5)	660(2)	5177(6)	40(1)
C(32A)	-1143(6)	907(2)	4415(7)	47(2)
C(39)	4158(4)	885(1)	7315(3)	54(1)
C(42A)	3160(4)	1129(1)	6610(4)	53(1)
C(43A)	2136(4)	1279(1)	6971(4)	55(1)
C(44)	1112(3)	1542(1)	6224(3)	43(1)
C(27B)	1449(14)	239(4)	6065(15)	24(4)
C(30B)	319(16)	496(4)	5568(13)	36(3)
C(31B)	33(13)	646(3)	4449(13)	27(3)
C(32B)	-994(15)	907(4)	3966(16)	19(4)
C(42B)	2398(35)	976(9)	6063(28)	41(7)
C(43B)	1201(35)	1137(9)	6562(29)	44(8)
C(30C)	1642(38)	643(10)	5470(33)	53(9)
C(31C)	316(29)	805(8)	5856(27)	27(6)

Table 3. Bond lengths [A] and angles [deg] for 1.

Distances

O(1)-C(11)	1.314(4)
O(2)-C(11)	1.213(4)
O(3)-C(12)	1.295(4)
O(4)-C(12)	1.212(4)
O(5)-C(23)	1.319(3)
O(6)-C(23)	1.209(3)
O(7)-C(24)	1.320(4)
O(8)-C(24)	1.211(4)
N(1)-C(29)	1.329(4)
N(1)-C(25)	1.334(4)
N(2)-C(33)	1.319(4)
N(2)-C(34)	1.326(4)
N(3)-C(41)	1.327(5)
N(3)-C(37)	1.335(4)
N(4)-C(46)	1.327(4)
N(4)-C(45)	1.328(4)
C(1)-C(2)	1.385(4)
C(1)-C(10)	1.415(4)
C(1)-C(11)	1.498(4)
C(2)-C(3)	1.378(5)
C(3)-C(4)	1.344(5)
C(4)-C(5)	1.421(5)
C(5)-C(6)	1.393(5)
C(5)-C(10)	1.440(4)
C(6)-C(7)	1.346(5)
C(7)-C(8)	1.416(5)
C(8)-C(9)	1.373(5)
C(9)-C(10)	1.428(4)
C(9)-C(12)	1.506(4)
C(13)-C(14)	1.378(4)
C(13)-C(22)	1.427(4)
C(13)-C(23)	1.488(4)
C(14)-C(15)	1.401(4)
C(15)-C(16)	1.351(4)
C(16)-C(17)	1.416(4)
C(17)-C(18)	1.410(4)
C(17)-C(22)	1.423(4)
C(18)-C(19)	1.364(5)
C(19)-C(20)	1.396(5)
C(20)-C(21)	1.368(4)
C(21)-C(22)	1.434(4)
C(21)-C(24)	1.493(4)
C(25)-C(26)	1.345(5)
C(26)-C(27A)	1.243(8)
C(26)-C(27B)	1.815(13)
C(28)-C(27B)	1.067(15)
C(28)-C(29)	1.373(5)
C(28)-C(27A)	1.533(7)
C(33)-C(32A)	1.284(7)
C(33)-C(32B)	1.69(2)
C(34)-C(35)	1.371(5)

C(35)-C(36)	1.362(6)
C(36)-C(32B)	1.012(14)
C(36)-C(32A)	1.528(8)
C(37)-C(38)	1.344(5)
C(38)-C(39)	1.365(5)
C(40)-C(41)	1.375(5)
C(40)-C(39)	1.410(5)
C(45)-C(44)	1.371(5)
C(46)-C(47)	1.367(5)
C(47)-C(48)	1.372(5)
C(48)-C(44)	1.383(5)
C(27A)-C(30A)	1.507(8)
C(30A)-C(31A)	1.304(8)
C(31A)-C(32A)	1.444(9)
C(39)-C(42A)	1.452(5)
C(42A)-C(43A)	1.279(5)
C(43A)-C(44)	1.525(5)
C(27B)-C(30B)	1.48(2)
C(30B)-C(31B)	1.35(2)
C(31B)-C(32B)	1.41(2)
C(42B)-C(30C)	1.47(5)
C(42B)-C(43B)	1.52(5)
C(43B)-C(31C)	1.58(5)
C(30C)-C(31C)	1.58(5)

Angles

C(29)-N(1)-C(25)	117.3(3)
C(33)-N(2)-C(34)	118.5(3)
C(41)-N(3)-C(37)	118.4(3)
C(46)-N(4)-C(45)	118.2(3)
C(2)-C(1)-C(10)	120.4(3)
C(2)-C(1)-C(11)	113.3(3)
C(10)-C(1)-C(11)	126.2(3)
C(3)-C(2)-C(1)	122.5(4)
C(4)-C(3)-C(2)	118.9(3)
C(3)-C(4)-C(5)	122.1(3)
C(6)-C(5)-C(4)	121.2(3)
C(6)-C(5)-C(10)	119.4(3)
C(4)-C(5)-C(10)	119.4(3)
C(7)-C(6)-C(5)	122.0(3)
C(6)-C(7)-C(8)	119.8(3)
C(9)-C(8)-C(7)	120.9(3)
C(8)-C(9)-C(10)	120.1(3)
C(8)-C(9)-C(12)	116.5(3)
C(10)-C(9)-C(12)	123.1(3)
C(1)-C(10)-C(9)	125.6(3)
C(1)-C(10)-C(5)	116.6(3)
C(9)-C(10)-C(5)	117.7(3)
O(2)-C(11)-O(1)	124.6(3)
O(2)-C(11)-C(1)	121.8(3)
O(1)-C(11)-C(1)	113.3(3)
O(4)-C(12)-O(3)	125.3(3)
O(4)-C(12)-C(9)	120.9(3)
O(3)-C(12)-C(9)	113.8(3)
C(14)-C(13)-C(22)	119.6(3)
C(14)-C(13)-C(23)	115.8(2)

C(22)-C(13)-C(23)	124.1(2)
C(13)-C(14)-C(15)	121.8(3)
C(16)-C(15)-C(14)	119.4(3)
C(15)-C(16)-C(17)	121.3(3)
C(18)-C(17)-C(16)	120.2(3)
C(18)-C(17)-C(22)	120.2(3)
C(16)-C(17)-C(22)	119.5(3)
C(19)-C(18)-C(17)	120.8(3)
C(18)-C(19)-C(20)	119.3(3)
C(21)-C(20)-C(19)	122.1(3)
C(20)-C(21)-C(22)	119.8(3)
C(20)-C(21)-C(24)	116.0(3)
C(22)-C(21)-C(24)	123.9(3)
C(17)-C(22)-C(13)	117.8(2)
C(17)-C(22)-C(21)	117.1(3)
C(13)-C(22)-C(21)	125.1(3)
O(6)-C(23)-O(5)	124.2(3)
O(6)-C(23)-C(13)	123.2(3)
O(5)-C(23)-C(13)	112.3(2)
O(8)-C(24)-O(7)	123.9(3)
O(8)-C(24)-C(21)	123.1(3)
O(7)-C(24)-C(21)	112.8(3)
N(1)-C(25)-C(26)	124.6(4)
C(27A)-C(26)-C(25)	122.0(4)
C(25)-C(26)-C(27B)	112.4(6)
C(27B)-C(28)-C(29)	133.9(8)
C(29)-C(28)-C(27A)	115.4(4)
N(1)-C(29)-C(28)	122.8(4)
C(32A)-C(33)-N(2)	128.8(4)
N(2)-C(33)-C(32B)	114.2(6)
N(2)-C(34)-C(35)	122.1(4)
C(36)-C(35)-C(34)	118.8(4)
C(32B)-C(36)-C(35)	127.5(9)
C(35)-C(36)-C(32A)	118.8(4)
N(3)-C(37)-C(38)	123.6(4)
C(37)-C(38)-C(39)	119.8(4)
C(41)-C(40)-C(39)	119.3(4)
N(3)-C(41)-C(40)	121.5(4)
N(4)-C(45)-C(44)	123.6(3)
N(4)-C(46)-C(47)	122.5(3)
C(46)-C(47)-C(48)	118.8(3)
C(47)-C(48)-C(44)	119.6(3)
C(26)-C(27A)-C(30A)	120.7(5)
C(26)-C(27A)-C(28)	117.9(5)
C(30A)-C(27A)-C(28)	121.2(6)
C(31A)-C(30A)-C(27A)	127.9(6)
C(30A)-C(31A)-C(32A)	126.9(6)
C(33)-C(32A)-C(31A)	123.1(6)
C(33)-C(32A)-C(36)	113.0(5)
C(31A)-C(32A)-C(36)	123.9(6)
C(38)-C(39)-C(40)	117.4(3)
C(38)-C(39)-C(42A)	117.8(4)
C(40)-C(39)-C(42A)	124.8(4)
C(43A)-C(42A)-C(39)	126.1(4)
C(42A)-C(43A)-C(44)	125.4(4)
C(45)-C(44)-C(48)	117.3(3)
C(45)-C(44)-C(43A)	117.3(3)

C(48)-C(44)-C(43A)	125.3(3)
C(28)-C(27B)-C(30B)	125.6(14)
C(28)-C(27B)-C(26)	108.8(10)
C(30B)-C(27B)-C(26)	125.3(12)
C(31B)-C(30B)-C(27B)	128.3(16)
C(30B)-C(31B)-C(32B)	129.7(17)
C(36)-C(32B)-C(31B)	118.6(15)
C(36)-C(32B)-C(33)	118.8(12)
C(31B)-C(32B)-C(33)	122.4(14)
C(30C)-C(42B)-C(43B)	93(3)
C(31C)-C(43B)-C(42B)	89(2)
C(42B)-C(30C)-C(31C)	91(3)
C(43B)-C(31C)-C(30C)	87(2)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 1.

The anisotropic displacement factor exponent takes the form:
$-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
O(1)	45(1)	59(1)	41(1)	-1(1)	6(1)	14(1)
O(2)	60(2)	64(2)	35(1)	-1(1)	3(1)	5(1)
O(3)	70(2)	47(1)	45(1)	-1(1)	-2(1)	15(1)
O(4)	68(2)	43(1)	41(1)	10(1)	9(1)	9(1)
O(5)	45(1)	32(1)	43(1)	-3(1)	17(1)	3(1)
O(6)	58(2)	50(1)	50(1)	12(1)	24(1)	3(1)
O(7)	31(1)	40(1)	61(1)	4(1)	10(1)	-2(1)
O(8)	40(1)	50(1)	73(2)	19(1)	7(1)	13(1)
N(1)	49(2)	52(2)	46(2)	-1(1)	2(1)	4(1)
N(2)	42(2)	37(2)	55(2)	-1(1)	14(1)	2(1)
N(3)	57(2)	39(2)	49(2)	-5(1)	5(1)	3(1)
N(4)	32(2)	55(2)	55(2)	12(1)	10(1)	1(1)
C(1)	52(2)	35(2)	36(2)	3(1)	16(2)	5(2)
C(2)	70(3)	44(2)	45(2)	-2(2)	20(2)	1(2)
C(3)	82(3)	43(2)	57(2)	-1(2)	28(2)	9(2)
C(4)	69(3)	36(2)	59(2)	15(2)	34(2)	21(2)
C(5)	49(2)	53(2)	44(2)	17(2)	19(2)	13(2)
C(6)	55(2)	59(2)	59(2)	21(2)	20(2)	18(2)
C(7)	41(2)	74(3)	47(2)	19(2)	0(2)	11(2)
C(8)	50(2)	59(2)	48(2)	9(2)	4(2)	-2(2)
C(9)	38(2)	49(2)	36(2)	10(2)	7(1)	7(2)
C(10)	44(2)	38(2)	36(2)	11(1)	14(2)	8(1)
C(11)	42(2)	41(2)	41(2)	-3(2)	9(2)	-4(2)
C(12)	42(2)	43(2)	37(2)	-1(2)	2(1)	-1(2)
C(13)	30(2)	25(1)	35(2)	-1(1)	5(1)	-5(1)
C(14)	39(2)	34(2)	40(2)	5(1)	6(1)	-2(1)
C(15)	39(2)	36(2)	57(2)	3(2)	8(2)	10(1)
C(16)	37(2)	38(2)	53(2)	-10(2)	14(2)	6(1)
C(17)	36(2)	30(2)	39(2)	-7(1)	8(1)	-2(1)
C(18)	46(2)	40(2)	43(2)	-6(2)	17(2)	0(2)
C(19)	58(2)	48(2)	36(2)	0(2)	16(2)	-7(2)
C(20)	44(2)	35(2)	40(2)	2(1)	-1(2)	0(1)
C(21)	35(2)	29(2)	30(2)	-4(1)	3(1)	-3(1)
C(22)	30(2)	23(1)	36(2)	-4(1)	4(1)	-4(1)
C(23)	32(2)	38(2)	34(2)	0(1)	7(1)	-3(1)
C(24)	36(2)	38(2)	41(2)	2(1)	0(1)	0(2)
C(25)	61(3)	59(2)	51(2)	3(2)	6(2)	-8(2)
C(26)	82(3)	53(2)	55(2)	6(2)	-1(2)	-14(2)
C(28)	55(3)	47(2)	88(3)	-21(2)	-4(2)	13(2)
C(29)	59(2)	59(2)	52(2)	-9(2)	8(2)	11(2)
C(33)	54(2)	40(2)	64(2)	6(2)	10(2)	-6(2)
C(34)	49(2)	51(2)	56(2)	2(2)	16(2)	2(2)
C(35)	70(3)	74(3)	68(3)	-4(2)	35(2)	-3(2)
C(36)	54(3)	57(3)	112(4)	-21(3)	39(3)	-1(2)
C(37)	60(2)	41(2)	56(2)	1(2)	8(2)	-2(2)
C(38)	70(3)	39(2)	61(2)	1(2)	11(2)	0(2)
C(40)	67(3)	42(2)	92(3)	-16(2)	25(2)	3(2)

C(41)	69(3)	42(2)	58(2)	-2(2)	8(2)	10(2)
C(45)	39(2)	42(2)	47(2)	8(2)	-2(2)	-6(2)
C(46)	43(2)	55(2)	60(2)	19(2)	8(2)	7(2)
C(47)	50(2)	76(3)	50(2)	15(2)	16(2)	-5(2)
C(48)	38(2)	51(2)	68(2)	-10(2)	16(2)	-8(2)
C(27A)	65(4)	30(3)	39(3)	4(2)	17(3)	-8(3)
C(30A)	47(3)	36(3)	43(3)	0(2)	4(3)	-2(3)
C(31A)	45(3)	39(3)	36(3)	-3(3)	4(3)	0(3)
C(32A)	56(4)	40(3)	54(4)	7(3)	34(3)	-2(2)
C(39)	66(3)	25(2)	67(2)	9(2)	-9(2)	-2(2)
C(42A)	51(3)	48(2)	60(3)	-1(2)	14(2)	-6(2)
C(43A)	46(3)	46(2)	73(3)	-15(2)	11(2)	-11(2)
C(44)	44(2)	29(2)	55(2)	1(2)	3(2)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1.

	x	y	z	U(eq)
H(1O)	4952(21)	-560(8)	7780(2)	58
H(3O)	7160(27)	59(7)	9208(6)	66
H(5O)	-4145(25)	1594(2)	4966(21)	47
H(7O)	-2207(17)	2071(2)	6929(27)	52
H(2)	6257(4)	-1579(1)	6737(3)	62
H(3)	7518(4)	-2117(1)	7488(3)	71
H(4)	9294(4)	-2026(1)	8965(3)	62
H(6)	10697(4)	-1600(1)	10364(3)	68
H(7)	11245(3)	-996(1)	11186(3)	65
H(8)	9977(3)	-435(1)	10504(3)	63
H(14)	-6641(3)	2585(1)	4694(3)	45
H(15)	-8338(3)	2822(1)	5697(3)	53
H(16)	-8556(3)	2578(1)	7558(3)	50
H(18)	-7818(3)	2146(1)	9255(3)	51
H(19)	-6322(3)	1694(1)	10216(3)	55
H(20)	-4367(3)	1556(1)	9439(3)	49
H(25)	4379(4)	-256(1)	5576(3)	69
H(26)	2880(5)	129(1)	4455(4)	77
H(28)	945(4)	240(1)	7332(4)	78
H(29)	2577(4)	-162(1)	8394(3)	68
H(33)	-2131(4)	1072(1)	5628(3)	63
H(34)	-3642(4)	1541(1)	2587(3)	61
H(35)	-2063(4)	1242(1)	1607(4)	82
H(36)	-466(4)	837(1)	2690(6)	86
H(37)	6875(4)	450(1)	7021(3)	63
H(38)	5255(4)	826(1)	5976(3)	68
H(40)	3443(4)	860(1)	8930(4)	79
H(41)	5149(4)	473(1)	9908(3)	68
H(45)	82(3)	1621(1)	7588(3)	52
H(46)	-1484(3)	2194(1)	4708(3)	63
H(47)	175(4)	1977(1)	3676(3)	70
H(48)	1812(3)	1554(1)	4627(3)	62
H(30A)	963(5)	510(1)	4074(5)	51
H(31A)	-384(5)	623(2)	5977(6)	49
H(42A)	3278(4)	1182(1)	5806(4)	63
H(43A)	2001(4)	1222(1)	7769(4)	66
H(30B)	-281(16)	564(4)	6106(13)	43
H(31B)	608(13)	564(3)	3905(13)	32

Table S6. Crystal data and structure refinement for 1 (SCSC).

Identification code	1 (SCSC)
Empirical formula	C_{48} N_4 O_8 H_{36}
Formula weight	796.81
Temperature	173(2) K
Wavelength	0.71070 A
Crystal system, space group	monoclinic, P $2_1/n$
Unit cell dimensions	a = 10.169(2) A b = 34.357(7) A β = 100.32(3) deg. c = 11.181(2) A
Volume	3842.9(13) A^3
Z, Calculated density	4, 1.377 Mg/m^3
Absorption coefficient	0.095 mm^{-1}
F(000)	1664
Crystal size	0.20 x 0.25 x 0.30 mm
Theta range for data collection	2.99 to 22.50 deg.
Index ranges	-12<=h<=12, -40<=k<=40, -12<=l<=13
Reflections collected / unique	18767 / 4994 [R(int) = 0.0596]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4656 / 0 / 540
Goodness-of-fit on F^2	1.028
Final R indices [I>2sigma(I)]	R1 = 0.0557, wR2 = 0.1299
R indices (all data)	R1 = 0.0804, wR2 = 0.1471
Largest diff. peak and hole	0.389 and -0.336 $e.A^{-3}$

After anisotropic refinement of all non-hydrogen atoms, aromatic, methine, and hydroxyl hydrogen atoms were placed in idealized positions and allowed to ride on the atom to which they are attached. All crystallographic calculations were conducted using SHELXL-93 locally implemented on an IBM compatible pentium-based PC.

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1 (SCSC).

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	10461(2)	-727(1)	13325(2)	46(1)
O(2)	10882(3)	-900(1)	11499(2)	59(1)
O(3)	12265(3)	23(1)	14533(2)	57(1)
O(4)	12643(2)	-216(1)	12762(2)	56(1)
O(5)	354(2)	1716(1)	10034(2)	45(1)
O(6)	645(3)	2285(1)	9140(2)	61(1)
O(7)	2008(2)	2170(1)	12002(2)	48(1)
O(8)	2256(2)	1547(1)	12594(2)	62(1)
N(1)	8437(3)	-349(1)	11973(3)	49(1)
N(2)	2159(3)	1340(1)	8938(3)	44(1)
N(3)	10772(3)	548(1)	13297(3)	50(1)
N(4)	4167(3)	2055(1)	11124(3)	48(1)
C(1)	12343(4)	-1118(1)	13252(3)	48(1)
C(2)	12375(4)	-1502(1)	12939(4)	66(1)
C(3)	13382(6)	-1759(1)	13582(5)	84(2)
C(4)	14301(5)	-1611(2)	14491(5)	85(2)
C(5)	14330(4)	-1221(1)	14830(4)	70(1)
C(6)	15342(4)	-1073(2)	15790(4)	78(2)
C(7)	15360(4)	-698(2)	16144(4)	83(2)
C(8)	14416(4)	-444(1)	15525(3)	65(1)
C(9)	13462(3)	-561(1)	14560(3)	51(1)
C(10)	13344(3)	-962(1)	14192(3)	52(1)
C(11)	11169(3)	-898(1)	12597(3)	44(1)
C(12)	12720(3)	-236(1)	13871(3)	48(1)
C(13)	-706(3)	2263(1)	10677(3)	36(1)
C(14)	-1570(3)	2550(1)	10171(3)	45(1)
C(15)	-2584(3)	2688(1)	10762(3)	51(1)
C(16)	-2786(3)	2516(1)	11800(3)	48(1)
C(17)	-1947(3)	2218(1)	12354(3)	41(1)
C(18)	-2204(3)	2022(1)	13397(3)	48(1)
C(19)	-1358(4)	1747(1)	13957(3)	51(1)
C(20)	-140(4)	1679(1)	13560(3)	48(1)
C(21)	158(3)	1863(1)	12560(3)	38(1)
C(22)	-804(3)	2111(1)	11849(3)	35(1)
C(23)	197(3)	2096(1)	9885(3)	41(1)
C(24)	1566(3)	1835(1)	12363(3)	44(1)
C(25)	8678(4)	-245(1)	10901(4)	57(1)
C(26)	7982(4)	47(1)	10210(3)	56(1)
C(27)	6983(3)	248(1)	10658(3)	43(1)
C(28)	6676(4)	106(1)	11726(3)	49(1)
C(29)	7418(4)	-185(1)	12355(3)	52(1)
C(30)	6547(3)	632(1)	10095(3)	48(1)
C(31)	5266(3)	821(1)	10391(3)	47(1)
C(32)	4215(3)	977(1)	9368(3)	42(1)
C(33)	3093(3)	1148(1)	9695(3)	44(1)
C(34)	2277(3)	1355(1)	7776(3)	47(1)

C(35)	3322(3)	1186(1)	7344(3)	52(1)
C(36)	4306(3)	997(1)	8155(3)	49(1)
C(37)	10856(3)	669(1)	12180(3)	58(1)
C(38)	9833(3)	837(1)	11393(3)	51(1)
C(39)	8598(3)	878(1)	11719(3)	44(1)
C(40)	8512(4)	777(1)	12884(4)	52(1)
C(41)	9600(4)	613(1)	13654(3)	54(1)
C(42)	7410(3)	990(1)	10751(3)	46(1)
C(43)	6158(3)	1155(1)	11148(3)	46(1)
C(44)	5713(3)	1560(1)	10795(3)	41(1)
C(45)	4876(3)	1737(1)	11469(3)	44(1)
C(46)	4293(4)	2220(1)	10075(4)	56(1)
C(47)	5147(4)	2077(1)	9360(4)	56(1)
C(48)	5872(3)	1742(1)	9720(3)	48(1)

Table S8. Bond lengths [A] and angles [deg] for 1 (SCSC).

Distances

O(1)-C(11)	1.317(4)
O(2)-C(11)	1.210(4)
O(3)-C(12)	1.295(4)
O(4)-C(12)	1.230(4)
O(5)-C(23)	1.321(4)
O(6)-C(23)	1.206(4)
O(7)-C(24)	1.324(4)
O(8)-C(24)	1.214(4)
N(1)-C(25)	1.316(4)
N(1)-C(29)	1.317(4)
N(2)-C(34)	1.327(4)
N(2)-C(33)	1.329(4)
N(3)-C(37)	1.334(4)
N(3)-C(41)	1.341(4)
N(4)-C(46)	1.328(5)
N(4)-C(45)	1.329(4)
C(1)-C(2)	1.366(5)
C(1)-C(10)	1.431(5)
C(1)-C(11)	1.491(5)
C(2)-C(3)	1.442(6)
C(3)-C(4)	1.350(7)
C(4)-C(5)	1.392(7)
C(5)-C(10)	1.431(5)
C(5)-C(6)	1.439(7)
C(6)-C(7)	1.348(7)
C(7)-C(8)	1.388(6)
C(8)-C(9)	1.376(5)
C(9)-C(10)	1.436(5)
C(9)-C(12)	1.484(5)
C(13)-C(14)	1.373(4)
C(13)-C(22)	1.430(4)
C(13)-C(23)	1.500(4)
C(14)-C(15)	1.403(5)
C(15)-C(16)	1.350(5)
C(16)-C(17)	1.405(5)
C(17)-C(18)	1.410(5)
C(17)-C(22)	1.428(4)
C(18)-C(19)	1.353(5)
C(19)-C(20)	1.409(5)
C(20)-C(21)	1.364(4)
C(21)-C(22)	1.428(4)
C(21)-C(24)	1.490(5)
C(25)-C(26)	1.382(5)
C(26)-C(27)	1.393(5)
C(27)-C(28)	1.376(5)
C(27)-C(30)	1.496(4)
C(28)-C(29)	1.370(5)
C(30)-C(31)	1.543(5)
C(30)-C(42)	1.608(5)
C(31)-C(32)	1.517(5)
C(31)-C(43)	1.604(5)

C(32)-C(36)	1.378(5)
C(32)-C(33)	1.389(5)
C(34)-C(35)	1.372(5)
C(35)-C(36)	1.385(5)
C(37)-C(38)	1.364(5)
C(38)-C(39)	1.375(5)
C(39)-C(40)	1.367(5)
C(39)-C(42)	1.520(5)
C(40)-C(41)	1.393(5)
C(42)-C(43)	1.531(5)
C(43)-C(44)	1.495(4)
C(44)-C(45)	1.375(5)
C(44)-C(48)	1.390(5)
C(46)-C(47)	1.372(5)
C(47)-C(48)	1.386(5)

Angles

C(25)-N(1)-C(29)	117.7(3)
C(34)-N(2)-C(33)	117.5(3)
C(37)-N(3)-C(41)	115.8(3)
C(46)-N(4)-C(45)	118.2(3)
C(2)-C(1)-C(10)	120.3(3)
C(2)-C(1)-C(11)	114.8(4)
C(10)-C(1)-C(11)	124.8(3)
C(1)-C(2)-C(3)	120.6(5)
C(4)-C(3)-C(2)	118.7(5)
C(3)-C(4)-C(5)	123.0(4)
C(4)-C(5)-C(10)	118.9(5)
C(4)-C(5)-C(6)	121.3(4)
C(10)-C(5)-C(6)	119.8(5)
C(7)-C(6)-C(5)	121.7(4)
C(6)-C(7)-C(8)	119.0(5)
C(9)-C(8)-C(7)	122.3(5)
C(8)-C(9)-C(10)	121.0(3)
C(8)-C(9)-C(12)	114.1(4)
C(10)-C(9)-C(12)	124.4(3)
C(1)-C(10)-C(5)	118.4(4)
C(1)-C(10)-C(9)	125.6(3)
C(5)-C(10)-C(9)	116.0(4)
O(2)-C(11)-O(1)	124.8(3)
O(2)-C(11)-C(1)	121.4(3)
O(1)-C(11)-C(1)	113.6(3)
O(4)-C(12)-O(3)	125.0(3)
O(4)-C(12)-C(9)	120.0(4)
O(3)-C(12)-C(9)	114.9(3)
C(14)-C(13)-C(22)	119.7(3)
C(14)-C(13)-C(23)	116.5(3)
C(22)-C(13)-C(23)	123.5(3)
C(13)-C(14)-C(15)	121.2(3)
C(16)-C(15)-C(14)	119.7(3)
C(15)-C(16)-C(17)	121.6(3)
C(16)-C(17)-C(18)	121.6(3)
C(16)-C(17)-C(22)	119.1(3)
C(18)-C(17)-C(22)	119.3(3)
C(19)-C(18)-C(17)	121.3(3)
C(18)-C(19)-C(20)	119.5(3)

C(21)-C(20)-C(19)	121.2(3)
C(20)-C(21)-C(22)	120.2(3)
C(20)-C(21)-C(24)	116.8(3)
C(22)-C(21)-C(24)	122.4(3)
C(17)-C(22)-C(21)	117.2(3)
C(17)-C(22)-C(13)	117.6(3)
C(21)-C(22)-C(13)	125.1(3)
O(6)-C(23)-O(5)	124.4(3)
O(6)-C(23)-C(13)	123.3(3)
O(5)-C(23)-C(13)	112.1(3)
O(8)-C(24)-O(7)	124.0(3)
O(8)-C(24)-C(21)	123.7(3)
O(7)-C(24)-C(21)	112.1(3)
N(1)-C(25)-C(26)	123.1(3)
C(25)-C(26)-C(27)	119.5(3)
C(28)-C(27)-C(26)	115.5(3)
C(28)-C(27)-C(30)	125.5(3)
C(26)-C(27)-C(30)	117.8(3)
C(29)-C(28)-C(27)	121.0(3)
N(1)-C(29)-C(28)	122.6(3)
C(27)-C(30)-C(31)	118.7(3)
C(27)-C(30)-C(42)	112.7(3)
C(31)-C(30)-C(42)	89.6(2)
C(32)-C(31)-C(30)	119.6(3)
C(32)-C(31)-C(43)	113.7(3)
C(30)-C(31)-C(43)	89.7(2)
C(36)-C(32)-C(33)	116.2(3)
C(36)-C(32)-C(31)	126.7(3)
C(33)-C(32)-C(31)	116.8(3)
N(2)-C(33)-C(32)	124.7(3)
N(2)-C(34)-C(35)	122.7(3)
C(34)-C(35)-C(36)	118.8(3)
C(32)-C(36)-C(35)	120.0(3)
N(3)-C(37)-C(38)	124.5(3)
C(37)-C(38)-C(39)	120.0(3)
C(40)-C(39)-C(38)	116.3(3)
C(40)-C(39)-C(42)	124.4(3)
C(38)-C(39)-C(42)	119.0(3)
C(39)-C(40)-C(41)	120.8(3)
N(3)-C(41)-C(40)	122.2(3)
C(39)-C(42)-C(43)	118.9(3)
C(39)-C(42)-C(30)	115.5(3)
C(43)-C(42)-C(30)	90.0(2)
C(44)-C(43)-C(42)	119.7(3)
C(44)-C(43)-C(31)	114.2(3)
C(42)-C(43)-C(31)	90.2(2)
C(45)-C(44)-C(48)	117.0(3)
C(45)-C(44)-C(43)	117.0(3)
C(48)-C(44)-C(43)	124.9(3)
N(4)-C(45)-C(44)	124.2(3)
N(4)-C(46)-C(47)	122.2(3)
C(46)-C(47)-C(48)	119.1(3)
C(47)-C(48)-C(44)	119.1(3)

Table S9. Anisotropic displacement parameters (A^2 x 10^3) for 1 (SCSC).

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
O(1)	37(1)	58(2)	45(1)	5(1)	7(1)	14(1)
O(2)	66(2)	70(2)	38(2)	-3(1)	3(1)	12(1)
O(3)	57(2)	71(2)	40(1)	7(1)	-2(1)	1(1)
O(5)	44(1)	49(2)	46(1)	-6(1)	15(1)	4(1)
O(6)	61(2)	67(2)	63(2)	18(1)	34(2)	8(1)
O(7)	31(1)	53(2)	60(2)	-4(1)	10(1)	-2(1)
O(8)	42(2)	68(2)	74(2)	23(1)	7(1)	11(1)
N(1)	44(2)	48(2)	55(2)	1(2)	5(2)	4(1)
N(2)	36(2)	47(2)	49(2)	-2(1)	9(1)	1(1)
N(3)	42(2)	63(2)	43(2)	4(2)	1(1)	-3(1)
N(4)	34(2)	43(2)	66(2)	3(2)	8(2)	1(1)
C(1)	47(2)	54(2)	48(2)	14(2)	23(2)	14(2)
C(2)	78(3)	61(3)	71(3)	15(2)	43(2)	17(2)
C(3)	101(4)	58(3)	112(4)	31(3)	72(4)	37(3)
C(4)	70(3)	103(4)	94(4)	54(3)	49(3)	43(3)
C(5)	51(3)	92(4)	76(3)	53(3)	35(2)	31(2)
C(6)	30(2)	143(5)	64(3)	65(3)	14(2)	34(3)
C(7)	45(3)	135(5)	71(3)	44(3)	12(2)	4(3)
C(8)	41(2)	107(3)	45(2)	32(2)	1(2)	-4(2)
C(9)	28(2)	84(3)	39(2)	29(2)	3(2)	2(2)
C(10)	35(2)	75(3)	49(2)	33(2)	21(2)	21(2)
C(11)	42(2)	44(2)	44(2)	0(2)	8(2)	1(2)
C(12)	36(2)	78(3)	29(2)	14(2)	4(2)	-12(2)
C(13)	26(2)	41(2)	42(2)	-3(2)	6(2)	-5(2)
C(14)	37(2)	46(2)	50(2)	4(2)	5(2)	-2(2)
C(15)	37(2)	55(2)	60(3)	-3(2)	6(2)	9(2)
C(16)	33(2)	56(2)	54(2)	-12(2)	11(2)	2(2)
C(17)	35(2)	47(2)	40(2)	-12(2)	6(2)	-7(2)
C(18)	42(2)	57(2)	49(2)	-13(2)	17(2)	-10(2)
C(19)	59(2)	57(2)	41(2)	-5(2)	21(2)	-15(2)
C(20)	55(2)	45(2)	43(2)	2(2)	9(2)	-4(2)
C(21)	34(2)	42(2)	37(2)	-5(2)	7(2)	-4(2)
C(22)	32(2)	36(2)	37(2)	-7(2)	8(2)	-6(1)
C(23)	30(2)	47(2)	45(2)	2(2)	6(2)	-1(2)
C(24)	42(2)	50(2)	37(2)	4(2)	-1(2)	0(2)
C(25)	53(2)	63(3)	59(3)	1(2)	20(2)	24(2)
C(26)	64(3)	63(2)	44(2)	5(2)	18(2)	13(2)
C(27)	40(2)	38(2)	49(2)	2(2)	-2(2)	5(2)
C(28)	53(2)	47(2)	52(2)	-1(2)	19(2)	10(2)
C(29)	58(2)	53(2)	46(2)	4(2)	11(2)	6(2)
C(30)	42(2)	54(2)	47(2)	-1(2)	9(2)	4(2)
C(31)	44(2)	45(2)	54(2)	4(2)	12(2)	5(2)
C(32)	38(2)	41(2)	48(2)	0(2)	7(2)	0(2)
C(33)	42(2)	42(2)	49(2)	1(2)	8(2)	1(2)
C(34)	32(2)	57(2)	51(2)	5(2)	1(2)	1(2)
C(35)	45(2)	67(2)	46(2)	5(2)	13(2)	-3(2)
C(36)	35(2)	52(2)	60(3)	-2(2)	13(2)	6(2)

C(37)	33(2)	86(3)	53(3)	11(2)	6(2)	7(2)
C(38)	41(2)	68(2)	41(2)	6(2)	4(2)	4(2)
C(39)	42(2)	40(2)	48(2)	-2(2)	4(2)	-4(2)
C(40)	41(2)	53(2)	64(3)	-3(2)	14(2)	10(2)
C(41)	60(3)	59(2)	45(2)	-2(2)	13(2)	-6(2)
C(42)	38(2)	51(2)	49(2)	6(2)	9(2)	2(2)
C(43)	42(2)	49(2)	47(2)	-3(2)	9(2)	4(2)
C(44)	39(2)	39(2)	42(2)	0(2)	-1(2)	-1(2)
C(45)	41(2)	43(2)	46(2)	0(2)	4(2)	-7(2)
C(46)	46(2)	45(2)	73(3)	12(2)	5(2)	8(2)
C(47)	55(2)	55(2)	59(2)	19(2)	13(2)	4(2)
C(48)	38(2)	53(2)	54(2)	-5(2)	9(2)	-2(2)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1 (SCSC).

	x	y	z	U(eq)
H(1O)	9811(19)	-610(8)	12909(2)	56
H(3O)	11858(33)	197(6)	14082(3)	68
H(5O)	889(28)	1635(2)	9599(25)	54
H(7O)	2758(16)	2135(2)	11803(31)	57
H(2)	11727(4)	-1601(1)	12291(4)	80
H(3)	13400(6)	-2026(1)	13369(5)	101
H(4)	14957(5)	-1781(2)	14919(5)	102
H(6)	16015(4)	-1245(2)	16184(4)	94
H(7)	16009(4)	-609(2)	16807(4)	100
H(8)	14429(4)	-179(1)	15776(3)	78
H(14)	-1480(3)	2657(1)	9406(3)	54
H(15)	-3126(3)	2901(1)	10433(3)	61
H(16)	-3513(3)	2599(1)	12165(3)	57
H(18)	-2985(3)	2085(1)	13712(3)	58
H(19)	-1584(4)	1602(1)	14614(3)	61
H(20)	486(4)	1501(1)	13995(3)	57
H(25)	9363(4)	-378(1)	10586(4)	69
H(26)	8184(4)	110(1)	9436(3)	67
H(28)	5940(4)	212(1)	12032(3)	59
H(29)	7187(4)	-272(1)	13098(3)	63
H(30)	6542(3)	631(1)	9200(3)	57
H(31)	4849(3)	651(1)	10945(3)	57
H(33)	2985(3)	1126(1)	10519(3)	53
H(34)	1611(3)	1488(1)	7220(3)	57
H(35)	3369(3)	1198(1)	6503(3)	62
H(36)	5045(3)	882(1)	7875(3)	58
H(37)	11685(3)	636(1)	11913(3)	69
H(38)	9973(3)	926(1)	10621(3)	61
H(40)	7700(4)	818(1)	13173(4)	63
H(41)	9509(4)	545(1)	14458(3)	65
H(42)	7703(3)	1164(1)	10131(3)	55
H(43)	6201(3)	1115(1)	12041(3)	55
H(45)	4800(3)	1624(1)	12229(3)	53
H(46)	3774(4)	2444(1)	9811(4)	67
H(47)	5240(4)	2206(1)	8628(4)	68
H(48)	6471(3)	1639(1)	9238(3)	58

Figure S1. ^{1}H NMR spectrum of **1** (prior to reaction).

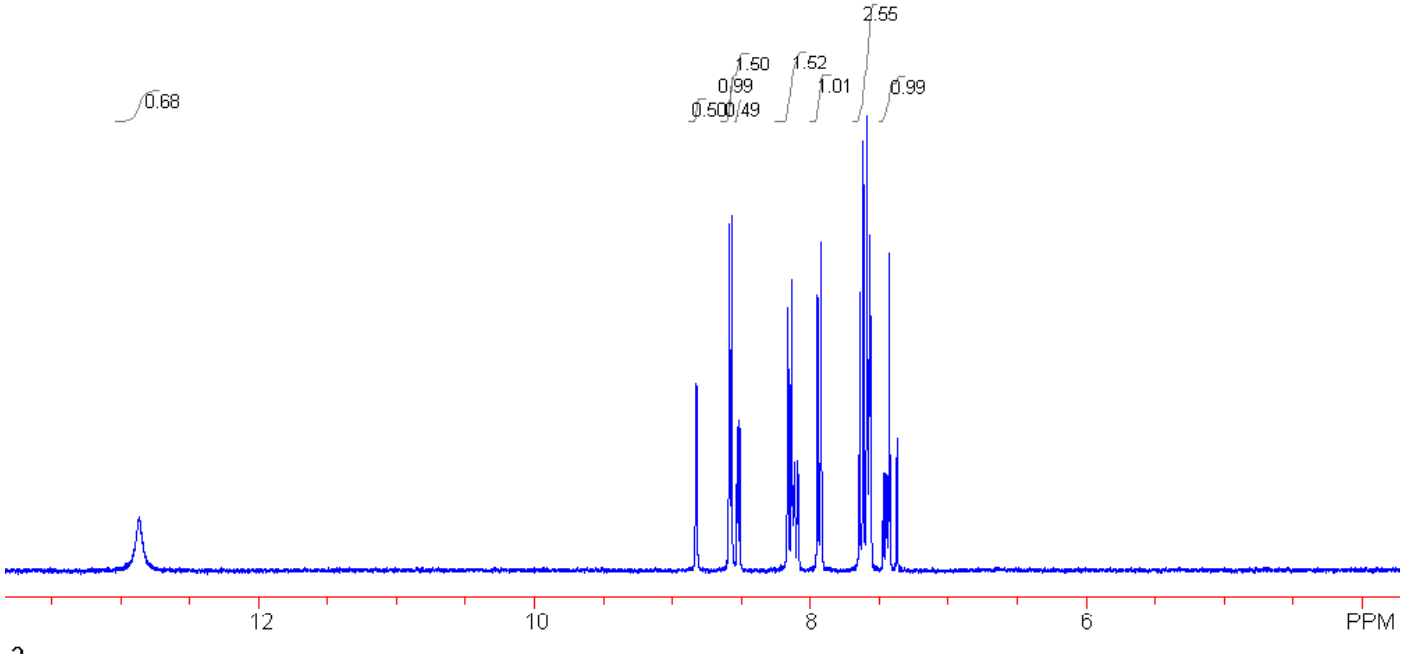


Figure S2. ^{1}H NMR spectrum of **1** (ambient UV light).

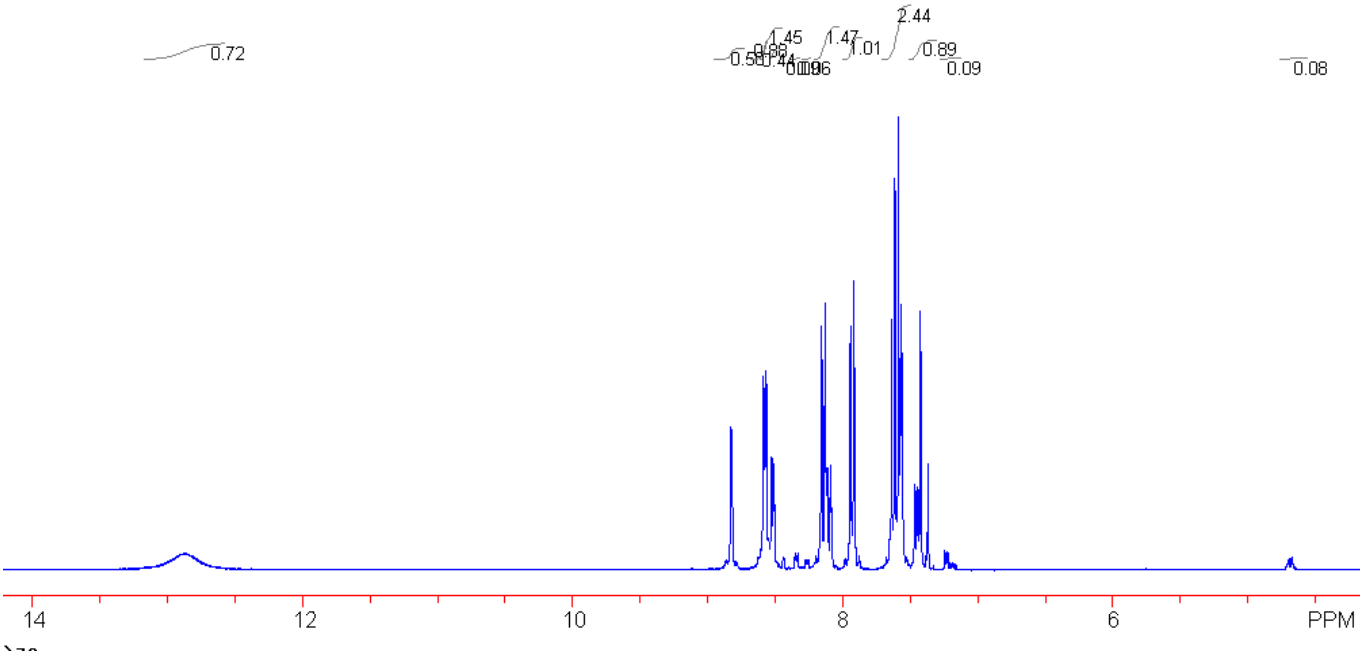


Figure S3. ^{1}H NMR spectrum of **1** (following exposure to broadband Hg lamp).

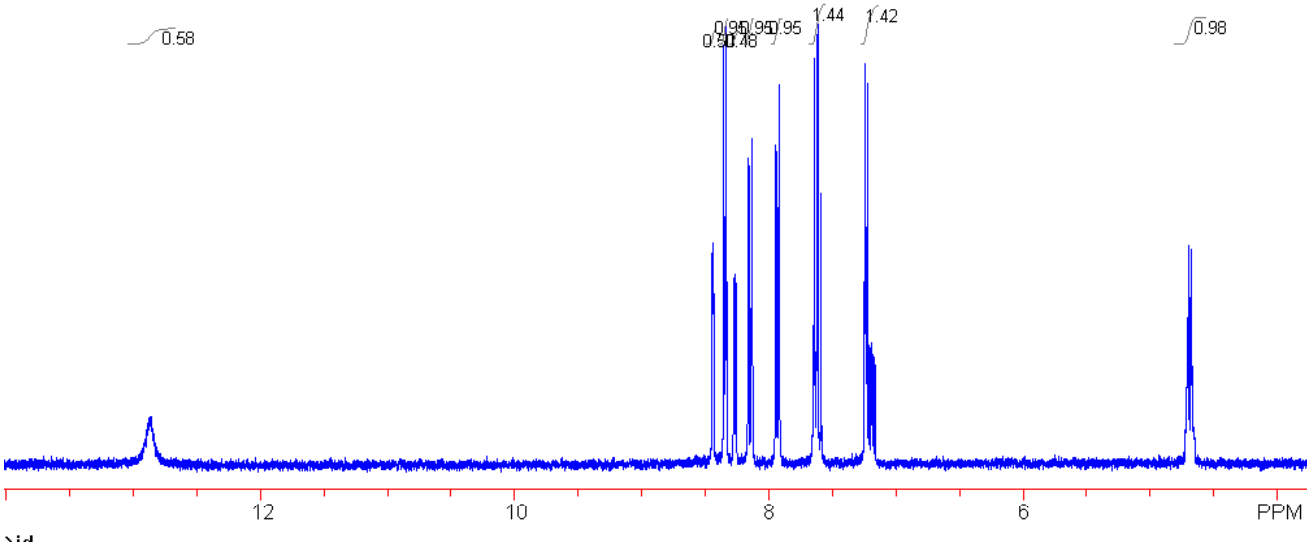


Figure S4. ^{1}H NMR spectrum of **1** (following exposure to 400 nm UV source).

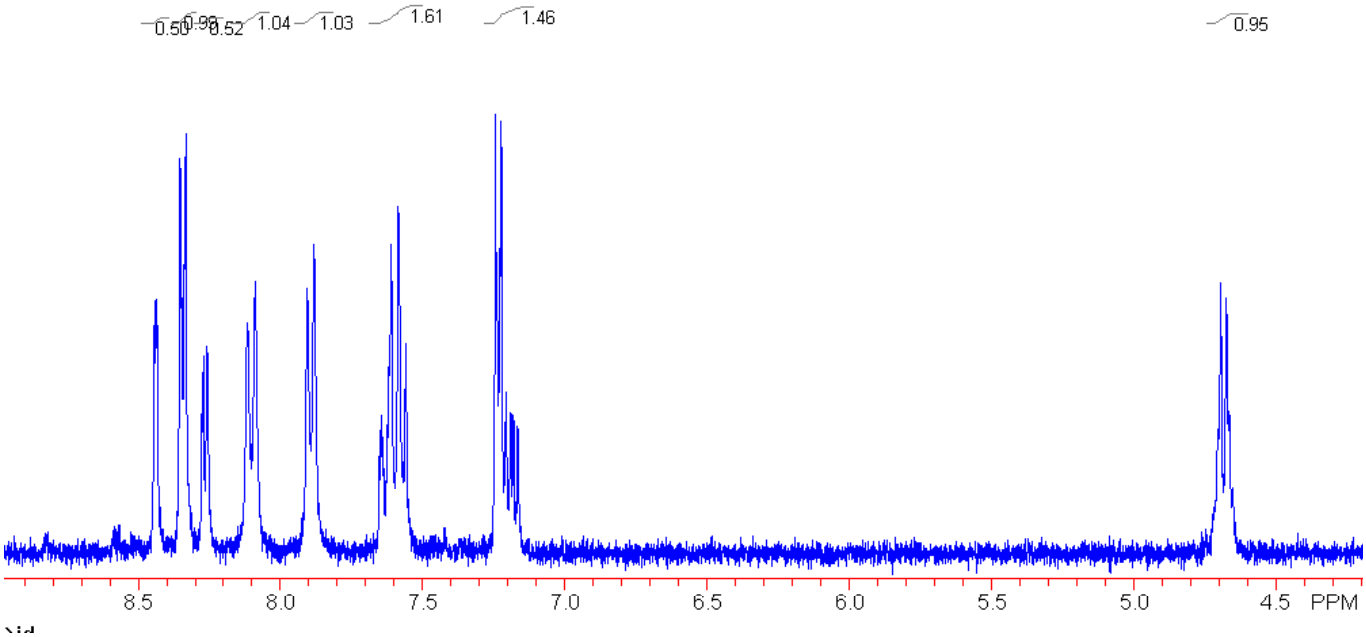


Figure S5. Simulated X-ray powder pattern for **1** (before reaction).

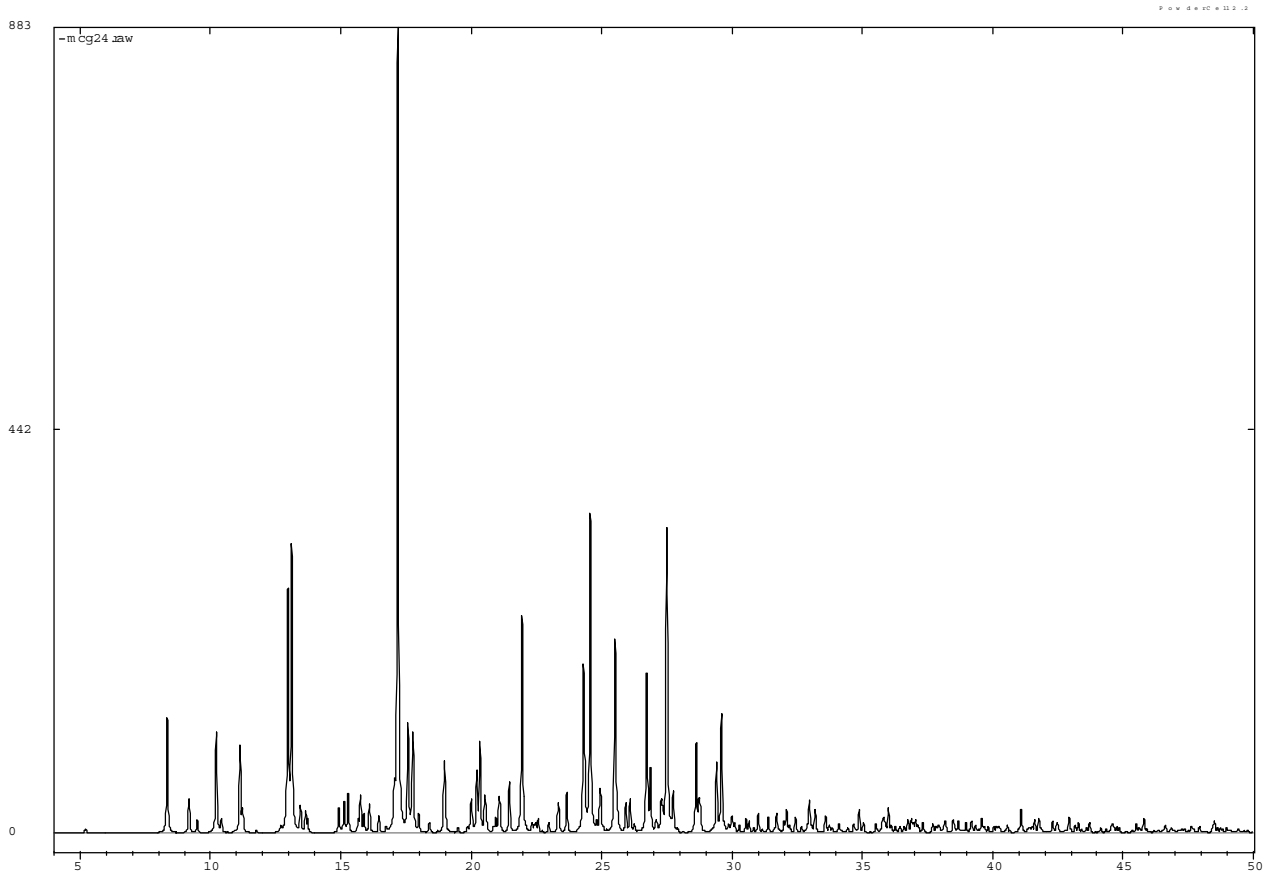


Figure S6. Experimental X-ray powder pattern of **1** (before reaction).

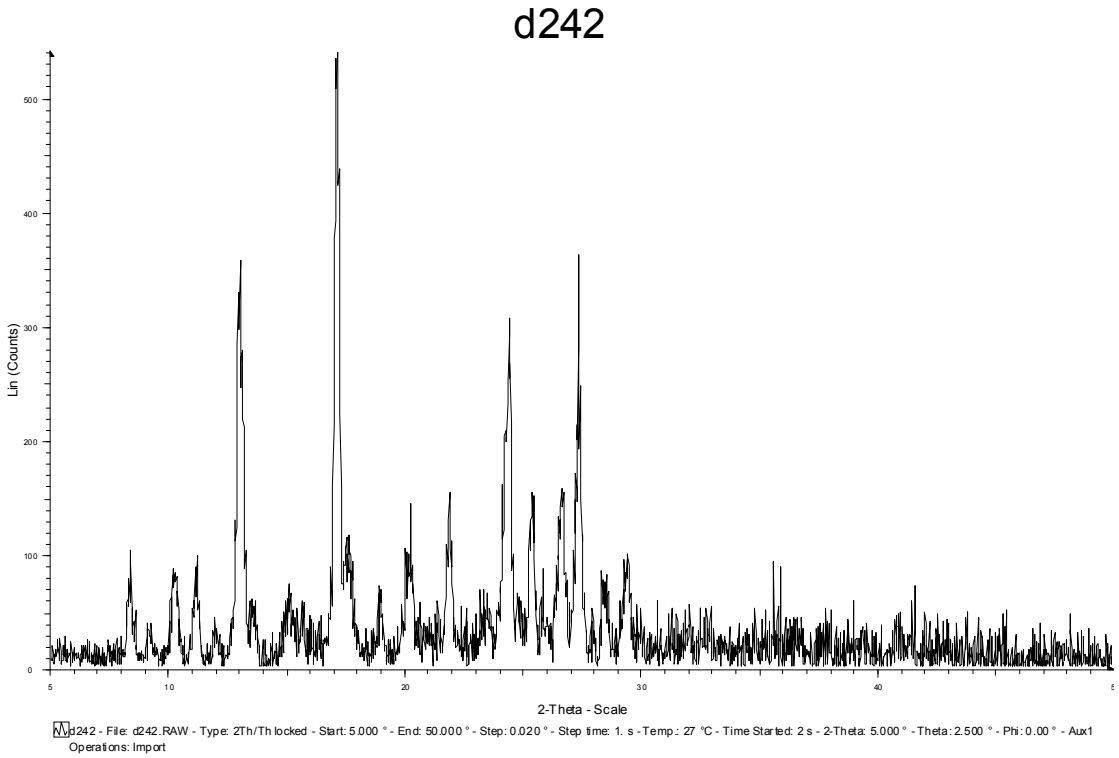


Figure S7. Experimental X-ray powder pattern of **1** (after reaction).

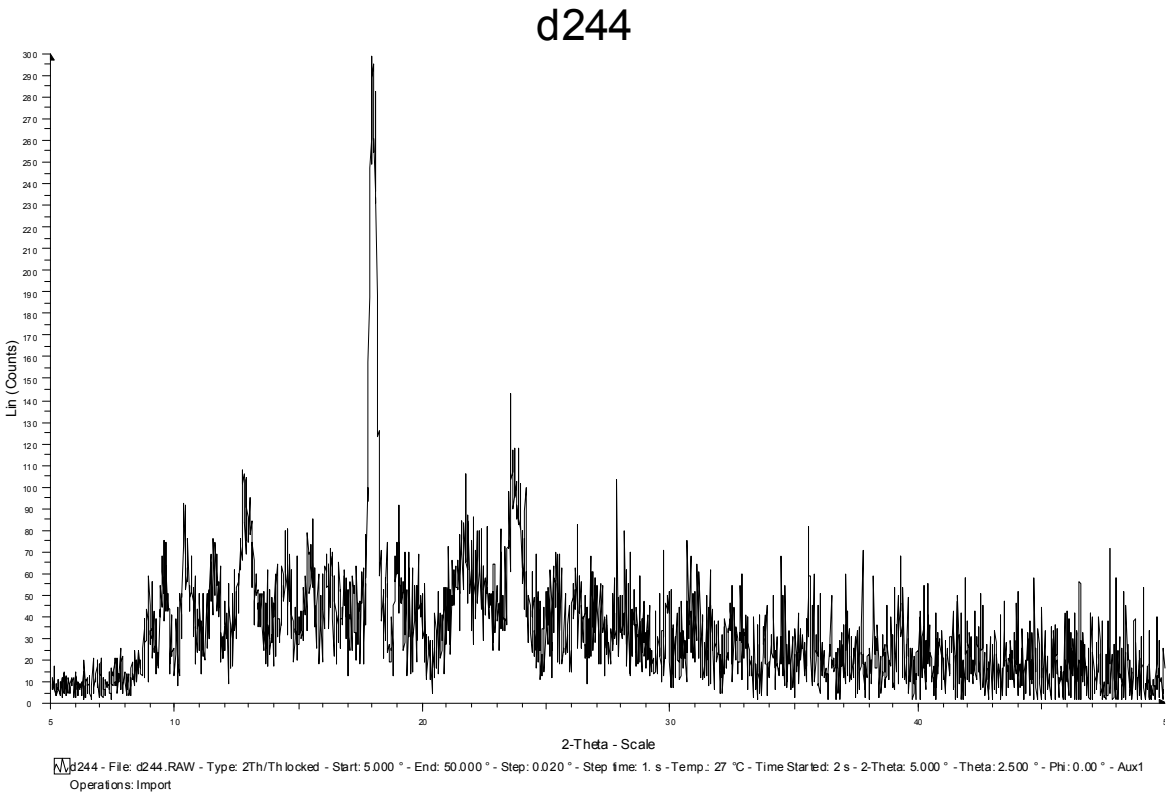
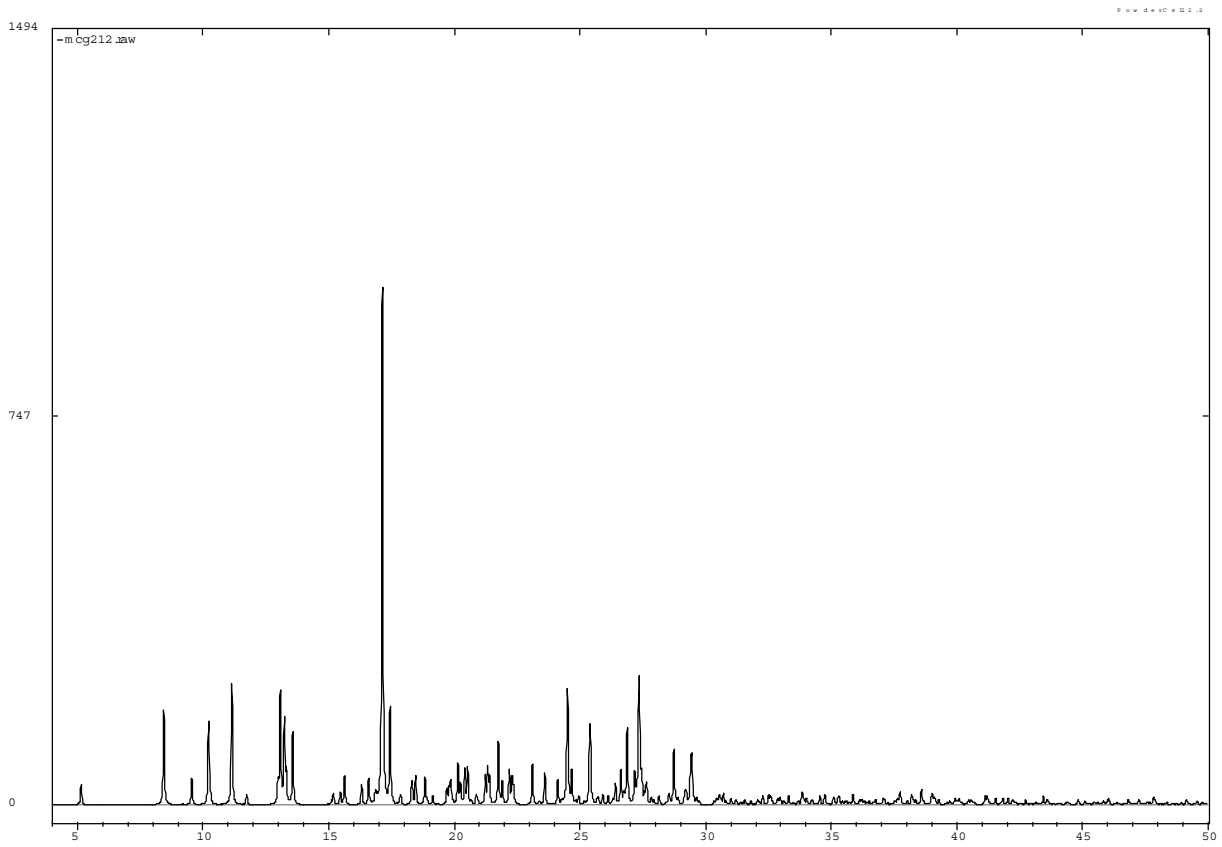


Figure S8. Simulated X-ray powder pattern for **1 (SCSC)**.



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