Table 1. Crystal data and structure refinement for tuberostemonine methanol solvate.

Identification code	041007d
Empirical formula	C22.40 H34.60 N O4.40
Formula weight	388.31
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 9.3605(14) A alpha = 90 deg. b = 9.6806(16) A beta = 90 deg. c = 25.174(4) A gamma = 90 deg.
Volume	2281.2(6) A^3
Z, Calculated density	4, 1.131 Mg/m^3
Absorption coefficient	0.077 mm^-1
F(000)	845
Crystal size	0.56 x 0.46 x 0.43 mm
Theta range for data collection	2.32 to 26.40 deg.
Limiting indices	-11<=h<=7, -10<=k<=12, -26<=l<=31
Reflections collected / unique	13382 / 4672 [R(int) = 0.0483]
Completeness to theta = 26.40	99.7 %
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	4672 / 0 / 252
Goodness-of-fit on F^2	1.010
Final R indices [I>2sigma(I)]	R1 = 0.0685, wR2 = 0.1795
R indices (all data)	R1 = 0.1284, wR2 = 0.2153
Largest diff. peak and hole	0.675 and -0.271 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for tuberostemonine methanol solvate. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	10259(4)	3637(3)	2042(1)	75(1)
O(2)	8502(3)	4547(3)	1565(1)	58(1)
O(3)	8069(3)	12238(3)	603(1)	64(1)
O(4)	8242(4)	14176(4)	155(1)	90(1)
O(5)	8796(10)	17050(10)	-111(3)	90
C(1)	8623(4)	8317(3)	1682(1)	44(1)
C(2)	9569(4)	9568(4)	1562(2)	55(1)
C(3)	8550(4)	10712(4)	1367(2)	50(1)
N(4)	7123(3)	10084(3)	1439(1)	53(1)
C(5)	5853(4)	10768(5)	1231(2)	65(1)
C(6)	4663(5)	10802(5)	1643(2)	76(1)
C(7)	4054(4)	9404(5)	1785(2)	73(1)
C(8)	5134(4)	8340(4)	1973(2)	63(1)
C(9)	6032(4)	7693(4)	1533(2)	50(1)
C(9A)	7301(4)	8611(4)	1357(2)	45(1)
C(10)	6603(4)	6243(4)	1703(2)	52(1)
C(11)	7985(4)	5902(4)	1408(2)	50(1)
C(12)	9212(4)	6874(4)	1552(2)	46(1)

C(13)	9982(4)	6151(4)	1994(1)	49(1)
C(14)	9642(4)	4653(4)	1884(2)	53(1)
C(15)	11561(5)	6435(5)	2054(2)	73(1)
C(16)	5498(5)	5095(4)	1656(2)	74(1)
C(17)	5063(6)	4743(5)	1093(3)	102(2)
C(18)	9011(4)	11134(4)	807(2)	55(1)
C(19)	10480(4)	11763(4)	786(2)	61(1)
C(20)	10400(5)	12841(4)	359(2)	60(1)
C(21)	8828(5)	13198(4)	357(2)	60(1)
C(22)	11305(5)	14096(5)	431(2)	79(1)
C(23)	7504(15)	17102(14)	-292(6)	86(4)

Table 3. Bond lengths [A] and angles [deg] for tuberostemonine methanol solvate.

O(1)-C(14)	1.207(4)
O(2)-C(14)	1.339(5)
O(2)-C(11)	1.453(4)
O(3)-C(21)	1.324(5)
O(3)-C(18)	1.478(5)
O(4)-C(21)	1.207(5)
O(5)-C(23)	1.294(15)
O(5)-H(5D)	0.8200
C(1)-C(9A)	1.510(5)
C(1)-C(2)	1.530(5)
C(1)-C(12)	1.537(5)
C(1)-H(1A)	0.9800
C(2)-C(3)	1.541(5)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-N(4)	1.479(5)
C(3)-C(18)	1.529(5)
C(3)-H(3A)	0.9800
N(4)-C(9A)	1.450(4)
N(4)-C(5)	1.458(5)
C(5)-C(6)	1.522(6)

C(5)-H(5B)	0.9700
C(5)-H(5C)	0.9700
C(6)-C(7)	1.511(6)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(7)-C(8)	1.519(6)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-C(9)	1.525(5)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-C(9A)	1.549(5)
C(9)-C(10)	1.561(5)
C(9)-H(9A)	0.9800
C(9A)-H(9AA)	0.9800
C(10)-C(16)	1.523(5)
C(10)-C(11)	1.528(5)
C(10)-H(10A)	0.9800
C(11)-C(12)	1.528(5)
C(11)-H(11A)	0.9800
C(12)-C(13)	1.500(5)
C(12)-H(12A)	0.9800
C(13)-C(15)	1.511(6)
C(13)-C(14)	1.511(5)
C(13)-H(13A)	0.9800
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-C(17)	1.515(7)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-C(19)	1.505(6)
C(18)-H(18A)	0.9800
C(19)-C(20)	1.498(6)
C(19)-H(19A)	0.9700

C(19)-H(19B)	0.9700
C(20)-C(22)	1.492(6)
C(20)-C(21)	1.512(6)
C(20)-H(20A)	0.9800
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600

C(14)-O(2)-C(11)	111.1(3)
C(21)-O(3)-C(18)	110.5(3)
C(23)-O(5)-H(5D)	109.5
C(9A)-C(1)-C(2)	102.6(3)
C(9A)-C(1)-C(12)	110.4(3)
C(2)-C(1)-C(12)	118.0(3)
C(9A)-C(1)-H(1A)	108.5
C(2)-C(1)-H(1A)	108.5
C(12)-C(1)-H(1A)	108.5
C(1)-C(2)-C(3)	105.9(3)
C(1)-C(2)-H(2A)	110.6
C(3)-C(2)-H(2A)	110.6
C(1)-C(2)-H(2B)	110.6
C(3)-C(2)-H(2B)	110.6
H(2A)-C(2)-H(2B)	108.7
N(4)-C(3)-C(18)	118.5(3)
N(4)-C(3)-C(2)	103.0(3)
C(18)-C(3)-C(2)	108.1(3)
N(4)-C(3)-H(3A)	108.9
C(18)-C(3)-H(3A)	108.9
C(2)-C(3)-H(3A)	108.9
C(9A)-N(4)-C(5)	119.3(3)
C(9A)-N(4)-C(3)	106.4(3)
C(5)-N(4)-C(3)	120.4(3)
N(4)-C(5)-C(6)	111.2(3)
N(4)-C(5)-H(5B)	109.4
C(6)-C(5)-H(5B)	109.4

N(4)-C(5)-H(5C)	109.4
C(6)-C(5)-H(5C)	109.4
H(5B)-C(5)-H(5C)	108.0
C(7)-C(6)-C(5)	114.7(4)
C(7)-C(6)-H(6A)	108.6
C(5)-C(6)-H(6A)	108.6
C(7)-C(6)-H(6B)	108.6
C(5)-C(6)-H(6B)	108.6
H(6A)-C(6)-H(6B)	107.6
C(6)-C(7)-C(8)	115.4(4)
C(6)-C(7)-H(7A)	108.4
C(8)-C(7)-H(7A)	108.4
C(6)-C(7)-H(7B)	108.4
C(8)-C(7)-H(7B)	108.4
H(7A)-C(7)-H(7B)	107.5
C(7)-C(8)-C(9)	114.8(4)
C(7)-C(8)-H(8A)	108.6
C(9)-C(8)-H(8A)	108.6
C(7)-C(8)-H(8B)	108.6
C(9)-C(8)-H(8B)	108.6
H(8A)-C(8)-H(8B)	107.5
C(8)-C(9)-C(9A)	113.2(3)
C(8)-C(9)-C(10)	111.1(3)
C(9A)-C(9)-C(10)	109.4(3)
C(8)-C(9)-H(9A)	107.6
C(9A)-C(9)-H(9A)	107.6
C(10)-C(9)-H(9A)	107.6
N(4)-C(9A)-C(1)	101.7(3)
N(4)-C(9A)-C(9)	115.8(3)
C(1)-C(9A)-C(9)	111.4(3)
N(4)-C(9A)-H(9AA)	109.2
C(1)-C(9A)-H(9AA)	109.2
C(9)-C(9A)-H(9AA)	109.2
C(16)-C(10)-C(11)	112.3(3)
C(16)-C(10)-C(9)	113.7(3)
C(11)-C(10)-C(9)	110.5(3)
C(16)-C(10)-H(10A)	106.6
C(11)-C(10)-H(10A)	106.6

C(9)-C(10)-H(10A)	106.6
O(2)-C(11)-C(10)	110.2(3)
O(2)-C(11)-C(12)	103.9(3)
C(10)-C(11)-C(12)	112.8(3)
O(2)-C(11)-H(11A)	109.9
C(10)-C(11)-H(11A)	109.9
C(12)-C(11)-H(11A)	109.9
C(13)-C(12)-C(11)	104.5(3)
C(13)-C(12)-C(1)	115.9(3)
C(11)-C(12)-C(1)	109.9(3)
C(13)-C(12)-H(12A)	108.7
C(11)-C(12)-H(12A)	108.7
C(1)-C(12)-H(12A)	108.7
C(12)-C(13)-C(15)	117.3(3)
C(12)-C(13)-C(14)	102.1(3)
C(15)-C(13)-C(14)	113.5(3)
C(12)-C(13)-H(13A)	107.8
C(15)-C(13)-H(13A)	107.8
C(14)-C(13)-H(13A)	107.8
O(1)-C(14)-O(2)	121.1(3)
O(1)-C(14)-C(13)	128.3(4)
O(2)-C(14)-C(13)	110.6(3)
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(17)-C(16)-C(10)	114.8(4)
C(17)-C(16)-H(16A)	108.6
C(10)-C(16)-H(16A)	108.6
C(17)-C(16)-H(16B)	108.6
C(10)-C(16)-H(16B)	108.6
H(16A)-C(16)-H(16B)	107.6
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5

H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
O(3)-C(18)-C(19)	103.9(3)
O(3)-C(18)-C(3)	110.2(3)
C(19)-C(18)-C(3)	113.6(3)
O(3)-C(18)-H(18A)	109.7
C(19)-C(18)-H(18A)	109.7
C(3)-C(18)-H(18A)	109.7
C(20)-C(19)-C(18)	105.2(3)
C(20)-C(19)-H(19A)	110.7
C(18)-C(19)-H(19A)	110.7
C(20)-C(19)-H(19B)	110.7
C(18)-C(19)-H(19B)	110.7
H(19A)-C(19)-H(19B)	108.8
C(22)-C(20)-C(19)	116.9(4)
C(22)-C(20)-C(21)	111.5(4)
C(19)-C(20)-C(21)	102.2(3)
C(22)-C(20)-H(20A)	108.6
C(19)-C(20)-H(20A)	108.6
C(21)-C(20)-H(20A)	108.6
O(4)-C(21)-O(3)	120.3(4)
O(4)-C(21)-C(20)	128.6(4)
O(3)-C(21)-C(20)	111.1(3)
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
O(5)-C(23)-H(23A)	109.5
O(5)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
O(5)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for tuberostemonine methanol solvate. 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)	89(2)	48(2)	89(2)	9(1)	-26(2)	10(2)
O(2)	63(2)	36(1)	75(2)	-6(1)	-16(2)	2(1)
O(3)	60(2)	61(2)	70(2)	14(1)	-9(1)	-6(1)
O(4)	98(3)	72(2)	99(2)	34(2)	-8(2)	2(2)
C(1)	49(2)	35(2)	49(2)	-1(2)	-3(2)	-2(2)
C(2)	54(2)	41(2)	70(2)	4(2)	-5(2)	-8(2)
C(3)	52(2)	41(2)	58(2)	-1(2)	-4(2)	-5(2)
N(4)	50(2)	35(2)	74(2)	4(2)	2(2)	-1(1)
C(5)	54(2)	46(2)	94(3)	15(2)	5(2)	10(2)
C(6)	66(3)	55(3)	108(3)	3(2)	19(3)	7(2)
C(7)	52(2)	54(3)	114(4)	3(3)	24(2)	6(2)
C(8)	55(2)	52(2)	82(3)	6(2)	17(2)	-4(2)
C(9)	50(2)	37(2)	65(2)	1(2)	-4(2)	-5(2)
C(9A)	46(2)	33(2)	56(2)	0(2)	0(2)	1(2)
C(10)	43(2)	39(2)	73(2)	6(2)	-2(2)	-4(2)
C(11)	53(2)	33(2)	62(2)	0(2)	-6(2)	1(2)
C(12)	45(2)	42(2)	52(2)	3(2)	-2(2)	1(2)
C(13)	49(2)	41(2)	55(2)	1(2)	-2(2)	-1(2)
C(14)	58(2)	41(2)	60(2)	2(2)	0(2)	3(2)
C(15)	54(3)	69(3)	96(3)	15(2)	-15(2)	2(2)
C(16)	55(2)	47(2)	120(4)	7(2)	-12(3)	-13(2)
C(17)	79(4)	55(3)	171(5)	-6(3)	-46(4)	-12(3)
C(18)	61(3)	40(2)	63(2)	2(2)	-2(2)	-2(2)
C(19)	56(2)	61(3)	67(3)	3(2)	3(2)	-7(2)
C(20)	68(3)	55(3)	58(2)	1(2)	4(2)	-4(2)
C(21)	70(3)	49(2)	60(2)	9(2)	-8(2)	-8(2)
C(22)	81(3)	71(3)	84(3)	2(2)	-3(3)	-22(3)

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

	x	y	z	U(eq)
H(5D)	9305	16634	-323	108
H(1A)	8364	8341	2059	53
H(2A)	10264	9343	1289	66
H(2B)	10074	9862	1878	66
H(3A)	8636	11512	1603	60
H(5B)	5522	10281	917	78
H(5C)	6093	11705	1128	78
H(6A)	5028	11230	1964	92
H(6B)	3896	11380	1510	92
H(7A)	3565	9038	1475	88
H(7B)	3345	9530	2062	88
H(8A)	4628	7610	2158	76
H(8B)	5770	8776	2226	76
H(9A)	5411	7560	1224	61
H(9AA)	7508	8438	981	54
H(10A)	6852	6312	2080	62
H(11A)	7818	5923	1023	60
H(12A)	9856	6948	1246	56
H(13A)	9515	6406	2328	58
H(15A)	11706	7401	2122	109
H(15B)	12047	6180	1733	109
H(15C)	11933	5905	2345	109
H(16A)	5878	4269	1823	89
H(16B)	4652	5365	1853	89
H(17A)	4369	4013	1098	152
H(17B)	5887	4449	896	152
H(17C)	4656	5544	926	152
H(18A)	8968	10331	571	66
H(19A)	10728	12177	1124	74

H(19B)	11190	11069	698	74
H(20A)	10644	12411	19	72
H(22A)	11156	14715	138	118
H(22B)	12293	13831	444	118
H(22C)	11048	14549	756	118
H(23A)	7440	16566	-612	103
H(23B)	7255	18044	-367	103
H(23C)	6859	16734	-32	103

Table 6. Torsion angles [deg] for tuberostemonine methanol solvate.

C(9A)-C(1)-C(2)-C(3)	21.4(4)
C(12)-C(1)-C(2)-C(3)	143.0(3)
C(1)-C(2)-C(3)-N(4)	5.1(4)
C(1)-C(2)-C(3)-C(18)	-121.1(3)
C(18)-C(3)-N(4)-C(9A)	87.6(4)
C(2)-C(3)-N(4)-C(9A)	-31.6(4)
C(18)-C(3)-N(4)-C(5)	-52.2(5)
C(2)-C(3)-N(4)-C(5)	-171.4(4)
C(9A)-N(4)-C(5)-C(6)	91.8(5)
C(3)-N(4)-C(5)-C(6)	-133.4(4)
N(4)-C(5)-C(6)-C(7)	-66.7(5)
C(5)-C(6)-C(7)-C(8)	55.2(6)
C(6)-C(7)-C(8)-C(9)	-76.4(5)
C(7)-C(8)-C(9)-C(9A)	80.8(4)
C(7)-C(8)-C(9)-C(10)	-155.7(3)
C(5)-N(4)-C(9A)-C(1)	-173.7(3)
C(3)-N(4)-C(9A)-C(1)	45.9(3)
C(5)-N(4)-C(9A)-C(9)	-52.8(5)
C(3)-N(4)-C(9A)-C(9)	166.9(3)
C(2)-C(1)-C(9A)-N(4)	-40.5(3)
C(12)-C(1)-C(9A)-N(4)	-167.1(3)
C(2)-C(1)-C(9A)-C(9)	-164.5(3)
C(12)-C(1)-C(9A)-C(9)	68.9(4)
C(8)-C(9)-C(9A)-N(4)	-26.1(5)
C(10)-C(9)-C(9A)-N(4)	-150.6(3)
C(8)-C(9)-C(9A)-C(1)	89.5(4)
C(10)-C(9)-C(9A)-C(1)	-35.0(4)

C(8)-C(9)-C(10)-C(16)	79.0(5)
C(9A)-C(9)-C(10)-C(16)	-155.3(4)
C(8)-C(9)-C(10)-C(11)	-153.6(3)
C(9A)-C(9)-C(10)-C(11)	-27.9(4)
C(14)-O(2)-C(11)-C(10)	-106.0(3)
C(14)-O(2)-C(11)-C(12)	15.0(4)
C(16)-C(10)-C(11)-O(2)	-51.4(4)
C(9)-C(10)-C(11)-O(2)	-179.5(3)
C(16)-C(10)-C(11)-C(12)	-167.0(3)
C(9)-C(10)-C(11)-C(12)	64.8(4)
O(2)-C(11)-C(12)-C(13)	-26.1(4)
C(10)-C(11)-C(12)-C(13)	93.2(3)
O(2)-C(11)-C(12)-C(1)	-151.2(3)
C(10)-C(11)-C(12)-C(1)	-31.9(4)
C(9A)-C(1)-C(12)-C(13)	-150.2(3)
C(2)-C(1)-C(12)-C(13)	92.4(4)
C(9A)-C(1)-C(12)-C(11)	-32.0(4)
C(2)-C(1)-C(12)-C(11)	-149.5(3)
C(11)-C(12)-C(13)-C(15)	151.5(4)
C(1)-C(12)-C(13)-C(15)	-87.3(4)
C(11)-C(12)-C(13)-C(14)	26.7(4)
C(1)-C(12)-C(13)-C(14)	147.9(3)
C(11)-O(2)-C(14)-O(1)	-177.3(4)
C(11)-O(2)-C(14)-C(13)	2.3(4)
C(12)-C(13)-C(14)-O(1)	160.8(4)
C(15)-C(13)-C(14)-O(1)	33.5(6)
C(12)-C(13)-C(14)-O(2)	-18.8(4)
C(15)-C(13)-C(14)-O(2)	-146.1(3)
C(11)-C(10)-C(16)-C(17)	-58.7(5)
C(9)-C(10)-C(16)-C(17)	67.7(5)
C(21)-O(3)-C(18)-C(19)	15.6(4)
C(21)-O(3)-C(18)-C(3)	137.6(3)
N(4)-C(3)-C(18)-O(3)	63.7(4)
C(2)-C(3)-C(18)-O(3)	-179.7(3)
N(4)-C(3)-C(18)-C(19)	179.8(3)
C(2)-C(3)-C(18)-C(19)	-63.6(4)
O(3)-C(18)-C(19)-C(20)	-25.5(4)
C(3)-C(18)-C(19)-C(20)	-145.3(3)

C(18)-C(19)-C(20)-C(22)	147.4(4)
C(18)-C(19)-C(20)-C(21)	25.4(4)
C(18)-O(3)-C(21)-O(4)	178.8(4)
C(18)-O(3)-C(21)-C(20)	0.8(5)
C(22)-C(20)-C(21)-O(4)	39.8(6)
C(19)-C(20)-C(21)-O(4)	165.4(5)
C(22)-C(20)-C(21)-O(3)	-142.4(4)
C(19)-C(20)-C(21)-O(3)	-16.8(5)