Table S1 - Final coordinates and equivalent isotropic displacement parameters ($U_{iso} = B_{iso}/8\pi^2$) of all atoms for isotibolone.

Atom	*x/a*	*y/b*	*z/c*	U_{iso} (Å^2)
C(1)	0.5068(4)	0.58923(12)	0.7644(4)	0.0291(6)
C(2)	0.6730(4)	0.63949(11)	0.6736(3)	0.0291(6)
C(3)	0.7128(4)	0.68953(18)	0.7936(5)	0.0291(6)
C(4)	0.5783(4)	0.70880(13)	0.9958(4)	0.0291(6)
C(5)	0.3835(5)	0.67117(15)	1.0631(6)	0.0291(6)
O(6)	0.6331(5)	0.7457(2)	1.1171(5)	0.0291(6)
C(7)	0.7806(5)	0.62724(14)	0.4461(5)	0.0291(6)
C(8)	0.8718(4)	0.55885(12)	0.4089(5)	0.0291(6)
C(9)	0.7033(4)	0.50967(11)	0.4872(4)	0.0291(6)
C(10)	1.0567(6)	0.55263(19)	0.5117(7)	0.0291(6)
C(11)	0.4138(6)	0.60013(13)	1.0063(5)	0.0291(6)
C(12)	0.5990(4)	0.52049(11)	0.7265(4)	0.0291(6)
C(13)	0.4460(5)	0.46904(15)	0.8129(6)	0.0291(6)
C(14)	0.5258(5)	0.39889(14)	0.7647(5)	0.0291(6)
C(15)	0.6150(3)	0.38830(10)	0.5279(3)	0.0291(6)
C(16)	0.7830(4)	0.44046(11)	0.4548(4)	0.0291(6)
C(17)	0.8902(7)	0.41871(14)	0.2296(5)	0.0291(6)
C(18)	0.8645(6)	0.34320(14)	0.2331(5)	0.0291(6)
C(19)	0.7434(3)	0.32565(9)	0.4588(3)	0.0291(6)
C(20)	0.4501(5)	0.3911(2)	0.4005(6)	0.0291(6)
C(21)	0.8760(4)	0.31105(12)	0.6004(4)	0.0291(6)
C(22)	0.9850(7)	0.2981(2)	0.7144(7)	0.0291(6)
O(23)	0.6179(5)	0.27208(15)	0.4506(5)	0.0291(6)
H(24)	0.4018(4)	0.59480(12)	0.6901(4)	0.0349(8)
H(25)	0.8395(4)	0.71163(18)	0.7479(5)	0.0349(8)
H(26)	0.2914(5)	0.68912(15)	0.9854(6)	0.0349(8)
H(27)	0.3235(5)	0.67682(15)	1.2118(6)	0.0349(8)
H(28)	0.8880(5)	0.65826(14)	0.4077(5)	0.0349(8)
H(29)	0.6849(5)	0.63466(14)	0.3598(5)	0.0349(8)
H(30)	0.9185(4)	0.55060(12)	0.2585(5)	0.0349(8)
H(31)	0.6046(4)	0.51594(11)	0.4037(4)	0.0349(8)
H(32)	1.0150(6)	0.55958(19)	0.6641(7)	0.0349(8)
H(33)	1.1530(6)	0.58628(19)	0.4534(7)	0.0349(8)
H(34)	1.1200(6)	0.51148(19)	0.4794(7)	0.0349(8)
H(35)	0.5052(6)	0.58372(13)	1.0870(5)	0.0349(8)
H(36)	0.2870(6)	0.57822(13)	1.0445(5)	0.0349(8)
H(37)	0.7001(4)	0.51708(11)	0.8082(4)	0.0349(8)
H(38)	0.3314(5)	0.47445(15)	0.7521(6)	0.0349(8)
H(39)	0.4049(5)	0.47385(15)	0.9650(6)	0.0349(8)
H(40)	0.4202(5)	0.36795(14)	0.8125(5)	0.0349(8)
H(41)	0.6310(5)	0.39015(14)	0.8370(5)	0.0349(8)
H(42)	0.8807(4)	0.44229(11)	0.5402(4)	0.0349(8)
H(43)	0.3887(5)	0.4334(2)	0.4274(6)	0.0349(8)
H(44)	0.3476(5)	0.3595(2)	0.4541(6)	0.0349(8)
H(45)	0.5077(5)	0.3872(2)	0.2507(6)	0.0349(8)
H(46)	1.0308(7)	0.42987(14)	0.1944(5)	0.0349(8)
H(47)	0.8257(7)	0.43857(14)	0.1279(5)	0.0349(8)
H(48)	0.9935(6)	0.32156(14)	0.1968(5)	0.0349(8)
H(49)	0.7875(6)	0.33126(14)	0.1331(5)	0.0349(8)
H(50)	0.5317(5)	0.26520(15)	0.5960(5)	0.0349(8)
H(51)	1.0689(7)	0.2884(2)	0.8125(7)	0.0349(8)

Table S2 – Some selected bond distances (Angstrom) for isotibolone.

Bonds	Lengths (Å)	Bonds	Lengths (Å)
O(6)-C(4)	1.214(5)	~~C(1)-H(24)~~	~~0.956(4)~~
O(23)-C(19)	1.410(4)	~~C(3)-H(25)~~	~~0.960(4)~~
~~O(23)-H(50)~~	~~0.993(5)~~	~~C(5)-H(26)~~	~~0.964(5)~~
C(1)-C(2)	1.549(4)	~~C(5)-H(27)~~	~~0.957(5)~~
C(1)-C(11)	1.556(4)	~~C(7)-H(28)~~	~~0.962(5)~~
C(1)-C(12)	1.554(3)	~~C(7)-H(29)~~	~~0.963(5)~~
C(2)-C(7)	1.500(4)	~~C(8)-H(30)~~	~~0.963(4)~~
C(2)-C(3)	1.359(4)	~~C(9)-H(31)~~	~~0.963(4)~~
C(3)-C(4)	1.462(4)	~~C(10)-H(32)~~	~~0.968(6)~~
C(4)-C(5)	1.512(4)	~~C(10)-H(33)~~	~~0.971(6)~~
C(5)-C(11)	1.521(4)	~~C(10)-H(34)~~	~~0.957(6)~~
C(7)-C(8)	1.544(4)	~~C(11)-H(35)~~	~~0.962(5)~~

C(8)-C(10)	1.559(5)	C(11)-H(36)	0.955(5)
C(8)-C(9)	1.529(4)	C(12)-H(37)	0.963(4)
C(9)-C(16)	1.531(3)	C(13)-H(38)	0.958(5)
C(9)-C(12)	1.556(4)	C(13)-H(39)	0.960(5)
C(12)-C(13)	1.504(4)	C(14)-H(40)	0.959(5)
C(13)-C(14)	1.559(4)	C(14)-H(41)	0.959(5)
C(14)-C(15)	1.521(4)	C(16)-H(42)	0.959(4)
C(15)-C(16)	1.564(3)	C(17)-H(46)	0.959(7)
C(15)-C(20)	1.540(4)	C(17)-H(47)	0.963(5)
C(15)-C(19)	1.571(3)	C(18)-H(48)	0.965(5)
C(16)-C(17)	1.532(4)	C(18)-H(49)	0.954(5)
C(17)-C(18)	1.575(4)	C(20)-H(43)	0.970(6)
C(18)-C(19)	1.539(4)	C(20)-H(44)	0.961(5)
C(19)-C(21)	1.458(3)	C(20)-H(45)	0.957(5)
C(21)-C(22)	1.191(5)	C(22)-H(51)	0.968(7)

Table S3 – Some selected bond angles (Degrees) for isotibolone.

Bonds	Angles (º)	Bonds	Angles (º)
C(19)-O(23)-H(50)	107.9(3)	C(16)-C(15)-C(20)	112.8(2)
C(2)-C(1)-C(11)	111.8(2)	C(19)-C(15)-C(20)	108.4(2)
C(11)-C(1)-C(12)	110.2(2)	C(16)-C(15)-C(19)	99.29(16)
C(2)-C(1)-C(12)	109.0(2)	C(9)-C(16)-C(15)	113.1(2)
C(1)-C(2)-C(3)	121.6(2)	C(9)-C(16)-C(17)	118.8(2)
C(3)-C(2)-C(7)	124.7(2)	C(15)-C(16)-C(17)	103.5(2)
C(1)-C(2)-C(7)	113.7(2)	C(16)-C(17)-C(18)	104.6(2)
C(2)-C(3)-C(4)	123.3(3)	C(17)-C(18)-C(19)	106.2(2)
O(6)-C(4)-C(3)	121.6(3)	O(23)-C(19)-C(18)	111.2(2)
C(3)-C(4)-C(5)	116.0(3)	O(23)-C(19)-C(21)	108.3(2)
O(6)-C(4)-C(5)	121.5(3)	C(15)-C(19)-C(18)	102.29(17)
C(4)-C(5)-C(11)	111.8(3)	C(15)-C(19)-C(21)	112.37(17)
C(2)-C(7)-C(8)	113.2(2)	C(18)-C(19)-C(21)	111.5(2)
C(7)-C(8)-C(10)	110.2(3)	O(23)-C(19)-C(15)	111.2(2)
C(9)-C(8)-C(10)	115.0(3)	C(19)-C(21)-C(22)	178.0(3)
C(7)-C(8)-C(9)	108.6(2)	C(2)-C(1)-H(24)	107.3(2)
C(8)-C(9)-C(12)	111.3(2)	C(11)-C(1)-H(24)	107.6(3)
C(8)-C(9)-C(16)	111.5(2)	C(12)-C(1)-H(24)	110.3(2)
C(12)-C(9)-C(16)	109.58(19)	C(2)-C(3)-H(25)	118.1(3)
C(1)-C(11)-C(5)	112.5(2)	C(4)-C(3)-H(25)	118.3(3)
C(1)-C(12)-C(9)	111.21(19)	C(4)-C(5)-H(26)	107.5(3)
C(9)-C(12)-C(13)	112.4(2)	C(4)-C(5)-H(27)	110.9(3)
C(1)-C(12)-C(13)	111.9(2)	C(11)-C(5)-H(26)	108.7(3)
C(12)-C(13)-C(14)	114.2(3)	C(11)-C(5)-H(27)	110.5(3)
C(13)-C(14)-C(15)	111.9(2)	H(26)-C(5)-H(27)	107.4(4)
C(14)-C(15)-C(19)	117.95(18)	C(2)-C(7)-H(28)	107.4(3)
C(14)-C(15)-C(20)	111.2(2)	C(2)-C(7)-H(29)	107.8(3)
C(14)-C(15)-C(16)	107.10(19)	C(8)-C(7)-H(28)	108.7(3)
C(8)-C(7)-H(29)	111.0(3)	H(38)-C(13)-H(39)	109.5(4)
H(28)-C(7)-H(29)	108.7(4)	C(13)-C(14)-H(40)	111.2(3)
C(7)-C(8)-H(30)	110.2(3)	C(13)-C(14)-H(41)	110.3(3)
C(9)-C(8)-H(30)	105.0(3)	C(15)-C(14)-H(40)	108.6(3)
C(10)-C(8)-H(30)	107.8(3)	C(15)-C(14)-H(41)	107.0(3)
C(8)-C(9)-H(31)	107.0(3)	H(40)-C(14)-H(41)	107.6(3)
C(12)-C(9)-H(31)	108.6(3)	C(9)-C(16)-H(42)	98.9(2)
C(16)-C(9)-H(31)	108.8(3)	C(15)-C(16)-H(42)	114.2(2)
C(8)-C(10)-H(32)	110.2(4)	C(17)-C(16)-H(42)	108.7(3)
C(8)-C(10)-H(33)	108.4(4)	C(16)-C(17)-H(46)	111.8(3)
C(8)-C(10)-H(34)	110.4(4)	C(16)-C(17)-H(47)	109.0(4)
H(32)-C(10)-H(33)	107.3(5)	C(18)-C(17)-H(46)	109.9(4)
H(32)-C(10)-H(34)	111.3(5)	C(18)-C(17)-H(47)	112.4(4)
H(33)-C(10)-H(34)	109.2(5)	H(46)-C(17)-H(47)	109.2(4)
C(1)-C(11)-H(35)	109.2(4)	C(17)-C(18)-H(48)	112.1(4)
C(1)-C(11)-H(36)	108.7(3)	C(17)-C(18)-H(49)	108.3(3)
C(5)-C(11)-H(35)	106.3(3)	C(19)-C(18)-H(48)	112.3(3)
C(5)-C(11)-H(36)	109.6(4)	C(19)-C(18)-H(49)	108.7(3)
H(35)-C(11)-H(36)	110.6(4)	H(48)-C(18)-H(49)	109.1(4)
C(1)-C(12)-H(37)	107.2(3)	C(15)-C(20)-H(43)	106.0(3)
C(9)-C(12)-H(37)	108.3(3)	C(15)-C(20)-H(44)	109.6(4)
C(13)-C(12)-H(37)	105.5(3)	C(15)-C(20)-H(45)	110.3(3)
C(12)-C(13)-H(38)	109.0(4)	H(43)-C(20)-H(44)	108.8(4)

C(12)-C(13)-H(39)	108.4(3)	H(43)-C(20)-H(45)	108.9(4)
C(14)-C(13)-H(38)	107.9(3)	H(44)-C(20)-H(45)	113.1(5)
C(14)-C(13)-H(39)	107.8(3)	C(21)-C(22)-H(51)	177.7(5)

Table S4 - Torsion angles (Degrees) for isotibolone.

Torsion	Angles (º)
C(11)-C(1)-C(2)-C(3)	-5.6(4)
C(11)-C(1)-C(2)-C(7)	174.6(2)
C(12)-C(1)-C(2)-C(3)	-127.7(3)
C(12)-C(1)-C(2)-C(7)	52.5(3)
C(2)-C(1)-C(11)-C(5)	40.0(4)
C(12)-C(1)-C(11)-C(5)	161.4(3)
C(2)-C(1)-C(12)-C(9)	-54.0(3)
C(2)-C(1)-C(12)-C(13)	179.5(2)
C(11)-C(1)-C(12)-C(9)	-176.9(2)
C(11)-C(1)-C(12)-C(13)	56.5(3)
C(1)-C(2)-C(3)-C(4)	-14.0(4)
C(7)-C(2)-C(3)-C(4)	165.8(3)
C(1)-C(2)-C(7)-C(8)	-54.7(3)
C(3)-C(2)-C(7)-C(8)	125.5(3)
C(2)-C(3)-C(4)-O(6)	166.8(3)
C(2)-C(3)-C(4)-C(5)	-2.4(4)
O(6)-C(4)-C(5)-C(11)	-131.8(4)
C(3)-C(4)-C(5)-C(11)	37.4(4)
C(4)-C(5)-C(11)-C(1)	-56.2(4)
C(2)-C(7)-C(8)-C(9)	55.7(3)
C(2)-C(7)-C(8)-C(10)	-71.1(3)
C(7)-C(8)-C(9)-C(12)	-57.4(3)
C(7)-C(8)-C(9)-C(16)	179.9(2)
C(10)-C(8)-C(9)-C(12)	66.5(3)
C(10)-C(8)-C(9)-C(16)	-56.2(3)
C(8)-C(9)-C(12)-C(1)	59.0(3)
C(16)-C(9)-C(12)-C(1)	-174.7(2)
C(16)-C(9)-C(12)-C(13)	-177.3(2)
C(8)-C(9)-C(16)-C(15)	-50.9(3)
C(8)-C(9)-C(16)-C(17)	-178.7(2)
C(12)-C(9)-C(16)-C(15)	-56.9(4)
C(12)-C(9)-C(16)-C(17)	57.6(3)
C(1)-C(12)-C(13)-C(14)	179.4(3)
C(9)-C(12)-C(13)-C(14)	175.8(2)
C(12)-C(13)-C(14)-C(15)	49.8(4)
C(13)-C(14)-C(15)-C(16)	-53.7(4)
C(13)-C(14)-C(15)-C(19)	55.7(3)
C(13)-C(14)-C(15)-C(20)	167.0(2)
C(14)-C(15)-C(16)-C(9)	-67.8(3)
C(14)-C(15)-C(16)-C(17)	-60.4(3)
C(19)-C(15)-C(16)-C(9)	169.7(2)
C(19)-C(15)-C(16)-C(17)	176.30(19)
C(20)-C(15)-C(16)-C(9)	46.4(2)
C(20)-C(15)-C(16)-C(17)	62.2(3)
C(14)-C(15)-C(19)-O(23)	-67.7(3)
C(14)-C(15)-C(19)-C(18)	81.6(3)
C(14)-C(15)-C(19)-C(21)	-160.8(2)
C(16)-C(15)-C(19)-O(23)	-41.1(3)
C(16)-C(15)-C(19)-C(18)	-163.1(2)
C(16)-C(15)-C(19)-C(21)	-45.5(2)
C(20)-C(15)-C(19)-O(23)	74.3(2)
C(20)-C(15)-C(19)-C(18)	-45.3(3)
C(20)-C(15)-C(19)-C(21)	72.3(3)
C(9) -C(16)-C(17)-C(18)	-168.0(2)
C(15)-C(16)-C(17)-C(18)	-155.8(3)
C(16)-C(17)-C(18)-C(19)	-29.1(3)
C(17)-C(18)-C(19)-O(23)	0.3(4)
C(17)-C(18)-C(19)-C(15)	146.6(3)
C(17)-C(18)-C(19)-C(21)	28.4(3)