Supporting Information

Nonactic acid derivatives isolated from *Streptomyces werraensis* IFM12104 in a screening program for BMI1 promoter inhibitory activity

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Table S1. X-ray analysis data for compound 1

A. Crystal Data

Empirical Formula	$C_{11}H_{20}O_4$
Formula Weight	216.28
Crystal Color, Habit	colorless, block
Crystal Dimensions	0.200 X 0.200 X 0.100 mm
Crystal System	monoclinic
Lattice Type	C-centered
Lattice Parameters	a = 17.5569(12) Å
	b = 7.0031(5) Å
	c = 19.4677(13) Å
	b = 98.386(5) ^{o}
	V = 2368.0(3) Å^3
Space Group	C2/c (#15)
Z value	8
D_{calc}	1.213 g/cm^3
F_{000}	944.00
m(CuKa)	7.515 cm^{-1}

B. Intensity Measurements

Diffractometer	R-AXIS RAPID
Radiation	CuKa (l = 1.54187 Å)
Voltage, Current	40kV, 30mA
Temperature	-180.0°C
Detector Aperture	460.0 x 256.0 mm
Data Images	30 exposures
w oscillation Range (c=54.0, f=0.0)	80.0 - 260.0°
Exposure Rate	4.0 sec./°
w oscillation Range (c=54.0, f=90.0)	80.0 - 260.0°
Exposure Rate	4.0 sec./°
w oscillation Range (c=54.0, f=180.0)	80.0 - 260.0°
Exposure Rate	4.0 sec./°
w oscillation Range (c=54.0, f=270.0)	80.0 - 260.0°
Exposure Rate	4.0 sec./°
w oscillation Range (c=0.0, f=0.0)	80.0 - 260.0°
Exposure Rate	4.0 sec./°
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2q_{max}$	136.4°
No. of Reflections Measured	Total: 11976
	Unique: 2156 (R_{int} = 0.0808)
Corrections	Lorentz-polarization
	Absorption
	(trans. factors: 0.361 - 0.928)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR2008)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$S\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\ s^2(Fo^2) + (0.0906 \cdot P)^2 + 2.0188 \cdot P\ ]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2q_{max}$ cutoff	136.4^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	2156
No. Variables	136
Reflection/Parameter Ratio	15.85
Residuals: R1 (I>2.00s(I))	0.0629
Residuals: R (All reflections)	0.0863
Residuals: wR2 (All reflections)	0.1970
Goodness of Fit Indicator	1.138
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	$0.60\ e^-/Å^3$
Minimum peak in Final Diff. Map	$-0.60\ e^-/Å^3$

Table S2. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
O1	0.70712(12)	0.0337(3)	0.18138(10)	2.61(4)
O2	0.58008(12)	0.0725(3)	0.17309(10)	2.64(4)
O3	0.69800(11)	0.0523(3)	0.39867(9)	2.20(4)
O4	0.70062(11)	0.1633(3)	0.56771(9)	1.93(4)
C1	0.64309(17)	0.0860(4)	0.20618(13)	2.06(5)
C2	0.66092(18)	0.1598(4)	0.28012(13)	2.15(5)
C3	0.59689(18)	0.2857(4)	0.29957(14)	2.44(6)
C4	0.67916(17)	-0.0145(4)	0.32758(13)	2.01(5)
C5	0.61487(18)	-0.1596(4)	0.32987(14)	2.31(6)
C6	0.63637(17)	-0.2471(4)	0.40219(13)	2.16(5)
C7	0.66664(17)	-0.0747(4)	0.44638(13)	1.98(5)
C8	0.60637(17)	0.0292(4)	0.48003(14)	2.00(5)
C9	0.63510(15)	0.2129(4)	0.51709(13)	1.89(5)
C10	0.57295(17)	0.3095(4)	0.55189(14)	2.20(5)
C11	0.60085(19)	0.4910(4)	0.59187(16)	2.91(6)

B_{eq} = 8/3 $p^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos g + 2U_{13}(aa^*cc^*)\cos b + 2U_{23}(bb^*cc^*)\cos a)$

Table S3. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H1	0.74558	0.05397	0.21156	3.135
H2	0.70864	0.23923	0.28338	2.576
H3A	0.61395	0.34633	0.34456	2.929
H3B	0.55119	0.20764	0.30265	2.929
H3C	0.58424	0.38444	0.26406	2.929
H4	0.72500	-0.08179	0.31410	2.417
H4A	0.73451	0.11175	0.54760	2.310
H5A	0.61460	-0.25714	0.29304	2.773
H5B	0.56386	-0.09667	0.32502	2.773
H6A	0.67662	-0.34614	0.40227	2.598
H6B	0.59086	-0.30397	0.41899	2.598
H7	0.70904	-0.11727	0.48316	2.372
H8A	0.58730	-0.05727	0.51397	2.394
H8B	0.56236	0.06019	0.44392	2.394
H9	0.65218	0.30294	0.48248	2.262
H10A	0.55416	0.21802	0.58438	2.645
H10B	0.52902	0.34245	0.51596	2.645
H11A	0.63919	0.45713	0.63178	3.495
H11B	0.55709	0.55455	0.60819	3.495
H11C	0.62412	0.57741	0.56120	3.495

Table S4. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O1	0.0301(12)	0.0397(12)	0.0282(11)	0.0012(10)	0.0000(9)	-0.0063(9)
O2	0.0277(12)	0.0400(13)	0.0316(11)	0.0014(10)	0.0003(9)	-0.0072(9)
O3	0.0317(12)	0.0325(11)	0.0193(9)	-0.0092(9)	0.0038(8)	-0.0027(8)
O4	0.0227(11)	0.0277(10)	0.0228(10)	0.0020(8)	0.0034(8)	0.0010(7)
C1	0.0324(18)	0.0225(14)	0.0237(14)	-0.0004(12)	0.0048(13)	0.0024(11)
C2	0.0306(17)	0.0254(15)	0.0253(14)	-0.0036(12)	0.0029(12)	-0.0032(11)
C3	0.0400(19)	0.0251(15)	0.0275(14)	0.0011(13)	0.0045(13)	-0.0057(12)
C4	0.0277(16)	0.0291(15)	0.0196(13)	-0.0015(13)	0.0030(11)	-0.0052(11)
C5	0.0355(18)	0.0251(14)	0.0261(15)	-0.0026(13)	0.0007(13)	-0.0034(11)
C6	0.0315(17)	0.0223(13)	0.0280(14)	-0.0032(12)	0.0027(12)	-0.0011(11)
C7	0.0288(16)	0.0249(14)	0.0207(13)	-0.0023(12)	0.0012(12)	0.0012(11)
C8	0.0284(16)	0.0250(14)	0.0218(13)	-0.0008(12)	0.0016(12)	-0.0009(11)
C9	0.0257(16)	0.0239(14)	0.0205(13)	0.0003(12)	-0.0015(11)	0.0009(11)
C10	0.0277(17)	0.0268(15)	0.0285(14)	0.0029(13)	0.0016(13)	-0.0016(11)
C11	0.0388(19)	0.0309(16)	0.0403(17)	0.0038(14)	0.0037(14)	-0.0094(13)

The general temperature factor expression: $\exp(-2p^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S5. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
O1	C1	1.338(4)	O2	C1	1.200(3)
O3	C4	1.453(3)	O3	C7	1.451(3)
O4	C9	1.444(3)	C1	C2	1.518(4)
C2	C3	1.520(4)	C2	C4	1.536(4)
C4	C5	1.524(4)	C5	C6	1.531(4)
C6	C7	1.532(4)	C7	C8	1.510(4)
C8	C9	1.525(4)	C9	C10	1.524(4)
C10	C11	1.533(4)			

Table S6. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
O1	H1	0.840	O4	H4A	0.840
C2	H2	1.000	C3	H3A	0.980
C3	H3B	0.980	C3	H3C	0.980
C4	H4	1.000	C5	H5A	0.990
C5	H5B	0.990	C6	H6A	0.990
C6	H6B	0.990	C7	H7	1.000
C8	H8A	0.990	C8	H8B	0.990
C9	H9	1.000	C10	H10A	0.990
C10	H10B	0.990	C11	H11A	0.980
C11	H11B	0.980	C11	H11C	0.980

Table S7. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C4	O3	C7	110.94(19)	O1	C1	O2	122.8(2)
O1	C1	C2	111.6(2)	O2	C1	C2	125.6(3)
C1	C2	C3	112.1(2)	C1	C2	C4	107.2(2)
C3	C2	C4	114.1(2)	O3	C4	C2	108.4(2)
O3	C4	C5	104.7(2)	C2	C4	C5	117.2(2)
C4	C5	C6	102.1(2)	C5	C6	C7	102.7(2)
O3	C7	C6	104.9(2)	O3	C7	C8	109.7(2)
C6	C7	C8	114.6(2)	C7	C8	C9	114.1(2)
O4	C9	C8	107.2(2)	O4	C9	C10	110.7(2)
C8	C9	C10	112.1(2)	C9	C10	C11	113.4(2)

Table S8. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
C1	O1	H1	109.5	C9	O4	H4A	109.5
C1	C2	H2	107.7	C3	C2	H2	107.7
C4	C2	H2	107.7	C2	C3	H3A	109.5
C2	C3	H3B	109.5	C2	C3	H3C	109.5
H3A	C3	H3B	109.5	H3A	C3	H3C	109.5
H3B	C3	H3C	109.5	O3	C4	H4	108.8
C2	C4	H4	108.8	C5	C4	H4	108.8
C4	C5	H5A	111.4	C4	C5	H5B	111.4
C6	C5	H5A	111.4	C6	C5	H5B	111.3
H5A	C5	H5B	109.2	C5	C6	H6A	111.2
C5	C6	H6B	111.2	C7	C6	H6A	111.2
C7	C6	H6B	111.2	H6A	C6	H6B	109.1
O3	C7	H7	109.2	C6	C7	H7	109.2
C8	C7	H7	109.2	C7	C8	H8A	108.7
C7	C8	H8B	108.7	C9	C8	H8A	108.7
C9	C8	H8B	108.7	H8A	C8	H8B	107.6
O4	C9	H9	108.9	C8	C9	H9	108.9
C10	C9	H9	108.9	C9	C10	H10A	108.9
C9	C10	H10B	108.9	C11	C10	H10A	108.9
C11	C10	H10B	108.9	H10A	C10	H10B	107.7
C10	C11	H11A	109.5	C10	C11	H11B	109.5
C10	C11	H11C	109.5	H11A	C11	H11B	109.5
H11A	C11	H11C	109.5	H11B	C11	H11C	109.5

Table S9. Torsion Angles(°)

(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C4	O3	C7	C6	8.5(3)	C4	O3	C7	C8	-115.0(2)
C7	O3	C4	C2	141.5(2)	C7	O3	C4	C5	15.7(3)
O1	C1	C2	C3	158.5(2)	O1	C1	C2	C4	-75.5(3)
O2	C1	C2	C3	-22.3(4)	O2	C1	C2	C4	103.6(3)
C1	C2	C4	O3	178.9(2)	C1	C2	C4	C5	-63.0(3)
C3	C2	C4	O3	-56.4(3)	C3	C2	C4	C5	61.7(3)
O3	C4	C5	C6	-33.2(2)	C2	C4	C5	C6	-153.3(2)
C4	C5	C6	C7	37.9(3)	C5	C6	C7	O3	-29.0(3)
C5	C6	C7	C8	91.3(2)	O3	C7	C8	C9	-55.9(3)
C6	C7	C8	C9	-173.49(18)	C7	C8	C9	O4	-56.7(3)
C7	C8	C9	C10	-178.38(18)	O4	C9	C10	C11	58.3(3)
C8	C9	C10	C11	177.92(18)					

Table S10. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O1	C4	2.977(3)	O2	C3	2.858(3)
O2	C4	3.304(3)	O2	C5	3.433(3)
O3	O4	3.375(3)	O3	C3	2.924(3)
O3	C9	2.923(3)	O4	C7	2.881(3)
O4	C11	2.966(4)	C1	C5	3.058(4)
C3	C5	3.181(4)	C4	C8	3.412(4)
C5	C8	3.232(4)			

Table S11. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
O1	H2	2.450	O1	H4	2.682
O1	H5A	3.541	O2	H1	2.896
O2	H2	3.107	O2	H3B	2.809
O2	H3C	2.807	O2	H5A	3.277
O2	H5B	3.237	O3	H2	2.628
O3	H3A	2.660	O3	H3B	3.149
O3	H4A	2.907	O3	H5A	3.192
O3	H5B	2.776	O3	H6A	2.818
O3	H6B	3.184	O3	H8A	3.268
O3	H8B	2.657	O3	H9	2.603
O4	H7	2.581	O4	H8A	2.614
O4	H8B	3.243	O4	H10A	2.666
O4	H10B	3.283	O4	H11A	2.710
O4	H11C	3.191	C1	H3A	3.353
C1	H3B	2.782	C1	H3C	2.654
C1	H4	2.642	C1	H5A	3.022
C1	H5B	3.141	C2	H1	2.262
C2	H5A	3.051	C2	H5B	2.707
C3	H4	3.403	C3	H5B	2.799
C3	H8B	3.355	C3	H9	3.554
C4	H1	2.731	C4	H3A	2.814
C4	H3B	2.718	C4	H3C	3.393
C4	H6A	2.744	C4	H6B	3.238
C4	H7	3.083	C4	H8B	3.311
C5	H2	3.430	C5	H3A	3.555
C5	H3B	2.823	C5	H7	3.207
C5	H8B	2.957	C6	H4	2.735
C6	H8A	2.791	C6	H8B	2.699
C7	H3A	3.598	C7	H4	2.907
C7	H4A	2.515	C7	H5A	3.253
C7	H5B	2.760	C7	H9	2.758
C8	H3A	3.465	C8	H4A	2.503
C8	H5B	3.128	C8	H6A	3.357
C8	H6B	2.615	C8	H10A	2.694

C8	H10B	2.724	C9	H3A	3.454
C9	H7	2.778	C9	H11A	2.805
C9	H11B	3.384	C9	H11C	2.709

Table S11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C10	H4A	3.169	C10	H8A	2.694
C10	H8B	2.718	C11	H9	2.764
H1	H2	2.079	H1	H4	2.287
H2	H3A	2.307	H2	H3B	2.852
H2	H3C	2.389	H2	H4	2.333
H3A	H5B	3.232	H3A	H8B	3.015
H3A	H9	2.688	H3B	H5A	3.454
H3B	H5B	2.180	H3B	H8B	2.917
H4	H5A	2.281	H4	H5B	2.870
H4	H6A	2.742	H4	H7	3.353
H4A	H7	2.045	H4A	H8A	2.831
H4A	H8B	3.400	H4A	H9	2.226
H4A	H10A	3.428	H4A	H11A	3.484
H5A	H6A	2.328	H5A	H6B	2.567
H5B	H6A	2.892	H5B	H6B	2.329
H5B	H8B	2.566	H6A	H7	2.261
H6A	H8A	3.504	H6B	H7	2.611
H6B	H8A	2.538	H6B	H8B	2.657
H7	H8A	2.341	H7	H8B	2.861
H7	H9	3.107	H8A	H9	2.871
H8A	H10A	2.483	H8A	H10B	2.983
H8B	H9	2.365	H8B	H10A	2.972
H8B	H10B	2.541	H9	H10A	2.872
H9	H10B	2.364	H9	H11A	3.140
H9	H11C	2.551	H10A	H11A	2.341
H10A	H11B	2.401	H10A	H11C	2.865
H10B	H11A	2.863	H10B	H11B	2.327
H10B	H11C	2.417			

Table S12. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O1	O4[1]	2.596(3)	O1	C2[2]	3.504(4)
O2	O4[1]	3.561(3)	O2	C3[3]	3.557(4)
O2	C10[1]	3.557(3)	O2	C11[4]	3.485(4)
O3	O4[5]	2.688(3)	O3	C9[5]	3.546(3)
O3	C11[5]	3.523(4)	O4	O1[6]	2.596(3)
O4	O2[6]	3.561(3)	O4	O3[5]	2.688(3)
O4	O4[5]	3.573(3)	O4	C1[6]	3.483(3)
C1	O4[1]	3.483(3)	C2	O1[7]	3.504(4)
C3	O2[3]	3.557(4)	C9	O3[5]	3.546(3)
C10	O2[6]	3.557(3)	C11	O2[8]	3.485(4)
C11	O3[5]	3.523(4)			

Symmetry Operators:

(1) X,-Y,Z
(2) -X+1/2+1,Y+1/2-1,-Z+1/2
(3) -X+1,Y,-Z+1/2
(4) X,-Y+1,Z
(5) -X+2,-Y+1,-Z+1
(6) X,-Y,Z+1
(7) -X+1/2+1,Y+1/2,-Z+1/2
(8) X,-Y+1,Z+1

Table S13. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
O1	H2[1]	2.572	O1	H3A[1]	3.508
O1	H4[2]	2.941	O1	H4A[3]	2.901
O1	H5A[2]	3.426	O1	H6A[2]	2.915
O1	H10A[3]	3.522	O2	H3B[4]	2.598
O2	H5B[4]	2.796	O2	H8A[3]	3.121
O2	H8B[4]	3.129	O2	H10A[3]	2.664
O2	H11A[5]	3.580	O2	H11B[5]	2.904
O2	H11C[5]	3.442	O3	H4A[6]	2.770
O3	H9[6]	3.395	O3	H11A[6]	3.003
O3	H11C[6]	3.237	O4	H1[7]	3.184
O4	H2[6]	3.172	O4	H3A[6]	3.449
O4	H4A[6]	3.093	O4	H6A[8]	3.091
O4	H9[6]	2.903	C1	H2[1]	3.544
C1	H3B[4]	3.496	C1	H4[2]	3.346
C1	H10A[3]	3.393	C1	H11A[5]	3.509
C1	H11B[5]	3.379	C2	H1[2]	3.204
C2	H4[2]	3.424	C3	H1[2]	3.376
C3	H3B[4]	3.084	C3	H3C[4]	3.313
C3	H5A[9]	3.221	C3	H6A[9]	3.433
C4	H1[1]	3.428	C4	H2[1]	3.572
C4	H11A[6]	3.197	C5	H1[1]	3.355
C5	H3A[10]	3.472	C5	H3C[10]	3.453
C6	H1[1]	3.533	C6	H3A[10]	3.065
C6	H4A[8]	3.460	C6	H7[8]	3.389
C6	H9[10]	3.510	C6	H10A[11]	3.399
C6	H10B[11]	3.573	C6	H11C[10]	3.366
C7	H7[8]	3.229	C7	H11C[10]	3.460
C8	H8A[11]	3.425	C8	H8B[11]	3.555
C8	H10A[11]	3.389	C8	H10B[11]	3.533
C8	H11C[10]	3.530	C9	H4A[6]	3.029
C10	H6B[11]	3.012	C10	H8A[11]	3.410
C10	H8B[11]	3.523	C10	H10B[12]	3.194
C11	H3C[13]	3.517	C11	H4[6]	3.387
C11	H6B[11]	3.589	C11	H8A[9]	3.501

C11	H10B^{12}	3.093	H1	O4^{3}	3.184
H1	C2^{1}	3.204	H1	C3^{1}	3.376
H1	C4^{2}	3.428	H1	C5^{2}	3.355

Table S13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H1	C6^{2}	3.533	H1	H2^{1}	2.343
H1	H3A^{1}	3.190	H1	H3C^{1}	3.186
H1	H4^{2}	2.664	H1	H4A^{3}	3.375
H1	H5A^{2}	2.801	H1	H6A^{2}	2.855
H1	H11A^{6}	3.406	H2	O1^{2}	2.572
H2	O4^{6}	3.172	H2	C1^{2}	3.544
H2	C4^{2}	3.572	H2	H1^{2}	2.343
H2	H4^{2}	2.679	H2	H4A^{6}	3.458
H2	H11A^{6}	3.236	H3A	O1^{2}	3.508
H3A	O4^{6}	3.449	H3A	C5^{9}	3.472
H3A	C6^{9}	3.065	H3A	H1^{2}	3.190
H3A	H4A^{6}	3.153	H3A	H5A^{9}	2.953
H3A	H6A^{9}	2.598	H3A	H6B^{9}	2.904
H3A	H11B^{12}	3.339	H3B	O2^{4}	2.598
H3B	C1^{4}	3.496	H3B	C3^{4}	3.084
H3B	H3B^{4}	2.522	H3B	H3C^{4}	2.824
H3B	H11B^{12}	3.219	H3C	C3^{4}	3.313
H3C	C5^{9}	3.453	H3C	C11^{5}	3.517
H3C	H1^{2}	3.186	H3C	H3B^{4}	2.824
H3C	H3C^{4}	2.929	H3C	H5A^{9}	2.611
H3C	H6A^{9}	3.487	H3C	H11A^{5}	3.085
H3C	H11B^{5}	3.032	H4	O1^{1}	2.941
H4	C1^{1}	3.346	H4	C2^{1}	3.424
H4	C11^{6}	3.387	H4	H1^{1}	2.664
H4	H2^{1}	2.679	H4	H11A^{6}	2.612
H4	H11C^{6}	3.322	H4A	O1^{7}	2.901
H4A	O3^{6}	2.770	H4A	O4^{6}	3.093
H4A	C6^{8}	3.460	H4A	C9^{6}	3.029
H4A	H1^{7}	3.375	H4A	H2^{6}	3.458
H4A	H3A^{6}	3.153	H4A	H4A^{6}	2.788
H4A	H6A^{8}	2.530	H4A	H9^{6}	2.235
H5A	O1^{1}	3.426	H5A	C3^{10}	3.221
H5A	H1^{1}	2.801	H5A	H3A^{10}	2.953
H5A	H3C^{10}	2.611	H5A	H11A^{3}	3.521

H5B	O2[4]	2.796	H5B	H5B[4]	3.413
H5B	H10A[11]	3.032	H6A	O1[1]	2.915
H6A	O4[8]	3.091	H6A	C3[10]	3.433

Table S13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H6A	H1^{1}	2.855	H6A	H3A^{10}	2.598
H6A	H3C^{10}	3.487	H6A	H4A^{8}	2.530
H6A	H7^{8}	2.786	H6A	H9^{10}	2.976
H6A	H11C^{10}	3.397	H6B	C10^{11}	3.012
H6B	C11^{11}	3.589	H6B	H3A^{10}	2.904
H6B	H9^{10}	3.143	H6B	H10A^{11}	2.608
H6B	H10B^{10}	3.387	H6B	H10B^{11}	2.624
H6B	H11B^{11}	3.115	H6B	H11C^{10}	2.868
H7	C6^{8}	3.389	H7	C7^{8}	3.229
H7	H6A^{8}	2.786	H7	H7^{8}	2.383
H7	H9^{6}	3.279	H7	H11C^{10}	3.125
H7	H11C^{6}	3.185	H8A	O2^{7}	3.121
H8A	C8^{11}	3.425	H8A	C10^{11}	3.410
H8A	C11^{10}	3.501	H8A	H8A^{11}	3.138
H8A	H8B^{11}	2.864	H8A	H10A^{11}	3.117
H8A	H10B^{11}	2.855	H8A	H11B^{10}	3.364
H8A	H11C^{10}	2.763	H8B	O2^{4}	3.129
H8B	C8^{11}	3.555	H8B	C10^{11}	3.523
H8B	H8A^{11}	2.864	H8B	H8B^{11}	3.416
H8B	H10A^{11}	2.821	H8B	H10B^{11}	3.391
H8B	H11B^{12}	3.476	H9	O3^{6}	3.395
H9	O4^{6}	2.903	H9	C6^{9}	3.510
H9	H4A^{6}	2.235	H9	H6A^{9}	2.976
H9	H6B^{9}	3.143	H9	H7^{6}	3.279
H9	H9^{6}	3.483	H10A	O1^{7}	3.522
H10A	O2^{7}	2.664	H10A	C1^{7}	3.393
H10A	C6^{11}	3.399	H10A	C8^{11}	3.389
H10A	H5B^{11}	3.032	H10A	H6B^{11}	2.608
H10A	H8A^{11}	3.117	H10A	H8B^{11}	2.821
H10B	C6^{11}	3.573	H10B	C8^{11}	3.533
H10B	C10^{12}	3.194	H10B	C11^{12}	3.093
H10B	H6B^{9}	3.387	H10B	H6B^{11}	2.624
H10B	H8A^{11}	2.855	H10B	H8B^{11}	3.391
H10B	H10B^{12}	2.472	H10B	H11B^{12}	2.753

H10B	H11C^{12}	2.936	H11A	O2^{13}	3.580
H11A	O3^{6}	3.003	H11A	C1^{13}	3.509
H11A	C4^{6}	3.197	H11A	H1^{6}	3.406

Table S13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H11A	H2[6]	3.236	H11A	H3C[13]	3.085
H11A	H4[6]	2.612	H11A	H5A[7]	3.521
H11B	O2[13]	2.904	H11B	C1[13]	3.379
H11B	H3A[12]	3.339	H11B	H3B[12]	3.219
H11B	H3C[13]	3.032	H11B	H6B[11]	3.115
H11B	H8A[9]	3.364	H11B	H8B[12]	3.476
H11B	H10B[12]	2.753	H11C	O2[13]	3.442
H11C	O3[6]	3.237	H11C	C6[9]	3.366
H11C	C7[9]	3.460	H11C	C8[9]	3.530
H11C	H4[6]	3.322	H11C	H6A[9]	3.397
H11C	H6B[9]	2.868	H11C	H7[9]	3.125
H11C	H7[6]	3.185	H11C	H8A[9]	2.763
H11C	H10B[12]	2.936			

Symmetry Operators:

(1) -X+1/2+1,Y+1/2-1,-Z+1/2
(2) -X+1/2+1,Y+1/2,-Z+1/2
(3) X,-Y,Z
(4) -X+1,Y,-Z+1/2
(5) X,-Y+1,Z
(6) -X+2,-Y+1,-Z+1
(7) X,-Y,Z+1
(8) -X+2,-Y,-Z+1
(9) X,Y+1,Z
(10) X,Y-1,Z
(11) -X+1,-Y,-Z+1
(12) -X+1,-Y+1,-Z+1
(13) X,-Y+1,Z+1

2. BMI1 promoter activity and cell viability of EtOAc layer.

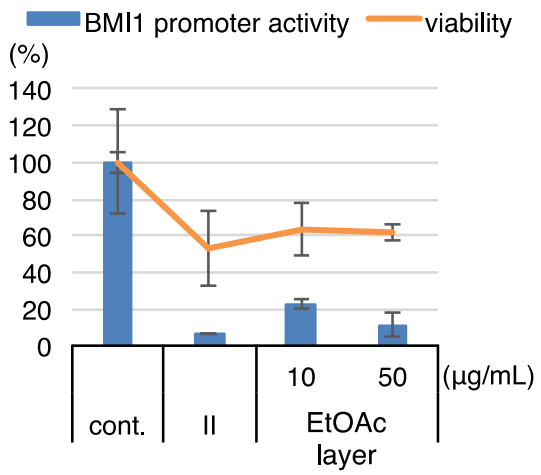

Fig. S1 BMI1 promoter activity and cell viability of EtOAc layer.

DMSO was used as a negative control (cont.) and 100 μM of *c*-Myc Inhibitor II 10074-G519 was used as a positive control (II). Data are presented as mean ± SD of n = 3 independent experiments.