Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

A Series of Meroterpenoids with Rearranged Skeletons from an Endophytic Fungus *Penicillium* sp. GDGJ-285

Tu-Xiang Mo[a, #], Xi-Shan Huang[a, #], Wen-Xiu Zhang[a], Till F. Schäberle[b,c], Jiang-Ke Qin[a], De-Xiong Zhou[a], Xiao-Ya Qin[a], Zhao-Long Xu[a], Jun Li[a], and Rui-Yun Yang[a*]

[a]State Key Laboratory for Chemistry and Molecular Engineering of Medicinal Resources, College of Chemistry and Pharmaceutical Sciences, Guangxi Normal University, Guilin 541004, P. R. China

[b]Institute of Insect Biotechnology, Justus-Liebig-University Giessen, Giessen 35392, Germany

[c]Branch for Bioresources, Fraunhofer Institute for Molecular Biology and Applied Ecology, Giessen 35392, Germany

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Table S1. Crystal data and structure refinement for **1**.

Identification code	**1**
Empirical formula	$C_{25}H_{24}O_{10}$
Formula weight	484.44
Temperature/K	102.0(7)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	8.52210(10)
b/Å	12.37940(10)
c/Å	11.00760(10)
α/°	90
β/°	107.4100(10)
γ/°	90
Volume/Å^3	1108.08(2)
Z	2
ρ_{calc}g/cm^3	1.452
μ/mm^{-1}	0.957
F(000)	508.0
Crystal size/mm^3	? × ? × ?
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.418 to 149.028
Index ranges	$-10 \le h \le 8$, $-15 \le k \le 15$, $-13 \le l \le 13$
Reflections collected	10864
Independent reflections	4345 [R_{int} = 0.0235, R_{sigma} = 0.0229]
Data/restraints/parameters	4345/1/323

Goodness-of-fit on F^2	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0456, wR_2 = 0.1303
Final R indexes [all data]	R_1 = 0.0461, wR_2 = 0.1309
Largest diff. peak/hole / e $Å^{-3}$	0.50/-0.59
Flack parameter	0.13(5)

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **1**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O3	-1048(3)	5691(2)	5182(2)	23.4(5)
O5	727(3)	6090.4(19)	7023(2)	21.0(5)
O8	35(3)	5038(2)	9128(2)	24.6(5)
O4	181(3)	3736.2(19)	5082(2)	21.4(5)
O9	-378(3)	3420(2)	8196(2)	25.9(5)
O7	4899(3)	5914(2)	9096(2)	24.4(5)
O2	3456(3)	4960(2)	3115(2)	24.8(5)
O1	3912(3)	6430(2)	2130(2)	29.9(6)
O6	3523(3)	7231(2)	7884(3)	32.2(6)
C11	224(4)	5462(3)	5982(3)	18.9(6)
C1	3336(4)	6038(3)	2911(3)	22.6(7)
C00C	451(4)	4211(3)	8468(3)	20.3(6)
C10	1291(4)	4524(3)	5764(3)	17.4(6)
C22	4137(4)	4395(2)	7041(3)	18.7(6)
C3	2233(4)	6217(3)	4705(3)	20.2(6)
C17	3494(4)	4246(3)	9415(3)	19.5(6)
C12	1928(4)	5725(3)	8165(3)	18.7(6)
C23	2432(4)	4016(2)	7021(3)	16.3(6)
C2	2601(4)	6671(3)	3732(3)	22.7(7)
C15	3526(4)	6343(3)	8343(3)	22.7(7)
C16	2082(4)	4493(2)	8216(3)	17.1(6)
C8	4185(4)	4897(3)	5981(3)	20.3(6)
C6	2331(4)	4418(3)	3714(3)	21.3(7)

Atom	*x*	*y*	*z*	U(eq)
C14	1184(4)	5937(3)	9257(3)	23.3(7)
C5	610(4)	4481(3)	2737(3)	25.8(7)
C18	3351(4)	3621(3)	10354(3)	26.8(7)
C21	5527(4)	4232(3)	8236(3)	22.2(6)
C7	2964(4)	3270(3)	3885(3)	25.7(7)
C24	2352(4)	2771(3)	7035(3)	21.8(7)
C4	2487(4)	5019(3)	5004(3)	17.5(6)
C19	5095(4)	4736(3)	9366(3)	21.6(7)
C9	5717(4)	5317(3)	5753(4)	30.2(8)
C20	6493(4)	4680(3)	10600(3)	30.2(8)
C13	270(5)	6976(3)	9225(4)	31.8(8)
O0AA	3036(12)	8885(9)	6268(11)	171(4)

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **1**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O3	14.3(10)	32.4(12)	22.6(11)	4.3(10)	4.3(8)	3.0(9)
O5	22.0(11)	22.3(11)	18.4(10)	2.6(9)	5.3(8)	4.3(9)
O8	21.3(11)	30.7(12)	25.4(12)	0.5(10)	12.6(9)	2.7(10)
O4	18.9(11)	21.5(11)	22.4(11)	-1.8(9)	4.0(9)	-5.7(9)
O9	20.2(11)	33.8(13)	24.9(12)	2.0(10)	8.6(9)	-6.3(10)
O7	19.5(11)	24.7(12)	26.4(11)	-1.1(10)	2.7(9)	-4.9(9)
O2	26.6(12)	26.2(12)	26.3(12)	-0.3(10)	14.8(10)	-2.6(10)
O1	31.9(13)	36.5(13)	24.3(12)	2.7(10)	12.9(11)	-8.0(11)
O6	35.0(14)	20.8(12)	37.5(15)	0.9(11)	5.8(12)	-5.1(10)
C11	17.3(14)	23.5(15)	18.1(14)	-0.1(12)	8.6(12)	-2.0(12)
C1	23.4(15)	26.6(16)	19.0(14)	0.3(13)	7.9(12)	-3.5(13)
C00C	15.8(14)	27.2(16)	17.7(14)	2.9(12)	4.9(11)	2.4(13)
C10	13.8(13)	20.5(14)	17.3(14)	-0.6(11)	3.6(11)	-2.6(11)
C22	12.7(13)	20.6(15)	23.2(16)	-2.2(12)	6.0(12)	-0.4(11)
C3	18.1(14)	21.3(15)	21.7(15)	-1.9(12)	6.9(12)	-0.7(12)
C17	15.5(14)	24.7(15)	17.5(14)	0.8(12)	3.7(11)	1.5(12)
C12	19.5(14)	20.8(14)	15.8(13)	-0.1(11)	5.3(11)	2.0(12)
C23	14.9(13)	18.0(14)	17.7(15)	-0.4(11)	7.2(11)	0.5(11)
C2	23.6(15)	22.3(16)	23.4(16)	1.0(12)	9.0(13)	-1.0(12)
C15	23.5(16)	22.2(15)	22.6(15)	-5.1(13)	7.3(13)	-2.8(13)
C16	13.1(14)	20.7(14)	17.8(14)	1.0(11)	5.3(11)	0.3(11)
C8	12.6(13)	24.6(15)	24.1(15)	-1.2(12)	6.2(11)	-0.7(12)
C6	22.5(15)	24.2(16)	20.3(15)	-1.9(12)	11.1(12)	-4.3(13)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C14	24.5(16)	26.5(16)	20.1(15)	-1.4(13)	8.5(12)	2.4(13)
C5	25.5(16)	34.3(18)	18.5(14)	-3.5(13)	8.1(13)	-4.0(14)
C18	23.7(16)	34.0(19)	23.3(17)	2.6(14)	8.2(13)	0.4(14)
C21	12.6(13)	28.4(16)	24.5(16)	-0.3(14)	4.2(12)	-0.3(12)
C7	26.2(16)	24.4(17)	30.3(18)	-5.5(14)	14.2(14)	-4.1(13)
C24	22.9(16)	18.6(15)	24.7(16)	-1.5(12)	8.3(13)	-0.3(12)
C4	14.8(14)	21.2(14)	17.5(14)	-0.6(11)	6.6(11)	-1.0(12)
C19	16.6(14)	24.2(16)	22.5(15)	0.3(12)	3.7(12)	0.6(12)
C9	18.1(16)	40(2)	32.8(18)	7.8(16)	8.1(14)	-4.6(14)
C20	19.3(16)	44(2)	23.9(17)	0.7(15)	1.1(13)	-3.4(14)
C13	35.3(19)	34(2)	27.8(18)	-0.6(15)	11.6(15)	12.5(16)
O0AA	137(7)	161(8)	215(11)	13(8)	49(7)	8(6)

Table S4. Bond Lengths for **1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O3	C11	1.208(4)	C22	C21	1.498(4)
O5	C11	1.345(4)	C3	C2	1.328(5)
O5	C12	1.436(4)	C3	C4	1.521(4)
O8	C00C	1.363(4)	C17	C16	1.527(4)
O8	C14	1.460(4)	C17	C18	1.325(5)
O4	C10	1.409(4)	C17	C19	1.509(4)
O9	C00C	1.193(4)	C12	C15	1.522(4)
O7	C15	1.326(4)	C12	C16	1.531(4)
O7	C19	1.487(4)	C12	C14	1.541(4)
O2	C1	1.353(4)	C23	C16	1.550(4)
O2	C6	1.477(4)	C23	C24	1.542(4)
O1	C1	1.212(4)	C8	C4	1.530(4)
O6	C15	1.210(5)	C8	C9	1.494(4)
C11	C10	1.537(4)	C6	C5	1.539(5)
C1	C2	1.470(5)	C6	C7	1.512(5)
C00C	C16	1.536(4)	C6	C4	1.573(4)
C10	C23	1.566(4)	C14	C13	1.499(5)
C10	C4	1.618(4)	C21	C19	1.533(5)
C22	C23	1.521(4)	C19	C20	1.517(5)
C22	C8	1.333(5)			

Table S5. Bond Angles for **1**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C11	O5	C12	121.7(3)	C24	C23	C16	110.6(3)
C00C	O8	C14	110.5(2)	C3	C2	C1	121.1(3)
C15	O7	C19	122.9(3)	O7	C15	C12	117.8(3)
C1	O2	C6	119.7(3)	O6	C15	O7	121.1(3)
O3	C11	O5	118.2(3)	O6	C15	C12	120.9(3)
O3	C11	C10	120.4(3)	C00C	C16	C23	118.7(3)
O5	C11	C10	121.2(3)	C17	C16	C00C	108.7(2)
O2	C1	C2	116.7(3)	C17	C16	C12	105.5(3)
O1	C1	O2	119.1(3)	C17	C16	C23	110.8(2)
O1	C1	C2	124.1(3)	C12	C16	C00C	99.2(2)
O8	C00C	C16	108.6(3)	C12	C16	C23	112.6(2)
O9	C00C	O8	121.5(3)	C22	C8	C4	113.0(3)
O9	C00C	C16	129.9(3)	C22	C8	C9	124.5(3)
O4	C10	C11	105.8(2)	C9	C8	C4	122.6(3)
O4	C10	C23	109.4(2)	O2	C6	C5	105.9(3)
O4	C10	C4	114.4(2)	O2	C6	C7	103.1(3)
C11	C10	C23	113.9(3)	O2	C6	C4	107.3(2)
C11	C10	C4	106.8(2)	C5	C6	C4	114.4(3)
C23	C10	C4	106.8(2)	C7	C6	C5	111.4(3)
C8	C22	C23	114.3(3)	C7	C6	C4	113.7(3)
C8	C22	C21	127.5(3)	O8	C14	C12	102.4(2)
C21	C22	C23	118.2(3)	O8	C14	C13	108.8(3)
C2	C3	C4	122.3(3)	C13	C14	C12	117.4(3)
C18	C17	C16	123.9(3)	C22	C21	C19	109.8(3)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C18	C17	C19	123.9(3)	C3	C4	C10	114.2(3)
C19	C17	C16	112.1(3)	C3	C4	C8	106.9(3)
O5	C12	C15	109.3(3)	C3	C4	C6	107.3(2)
O5	C12	C16	112.1(3)	C8	C4	C10	102.1(2)
O5	C12	C14	106.1(2)	C8	C4	C6	113.2(3)
C15	C12	C16	115.6(3)	C6	C4	C10	113.0(2)
C15	C12	C14	112.1(3)	O7	C19	C17	110.6(3)
C16	C12	C14	101.0(3)	O7	C19	C21	106.1(3)
C22	C23	C10	103.0(2)	O7	C19	C20	103.6(3)
C22	C23	C16	107.2(2)	C17	C19	C21	107.7(3)
C22	C23	C24	110.7(3)	C17	C19	C20	115.2(3)
C16	C23	C10	111.7(2)	C20	C19	C21	113.1(3)
C24	C23	C10	113.1(3)				

Table S6. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **1**.

Atom	*x*	*y*	*z*	U(eq)
H4	442	3144	5414	32
H3	1804	6647	5222	24
H2	2391	7402	3567	27
H14	2049	5876	10074	28
H5A	100	5153	2837	39
H5B	-51	3892	2871	39
H5C	709	4439	1892	39
H21A	6517	4565	8146	27
H21B	5736	3466	8385	27

Atom	*x*	*y*	*z*	U(eq)
H7A	2972	2984	3077	39
H7B	2261	2836	4225	39
H7C	4060	3261	4462	39
H24A	1245	2547	6949	33
H24B	3073	2505	7824	33
H24C	2687	2487	6339	33
H9A	6565	5386	6551	45
H9B	5501	6010	5347	45
H9C	6069	4824	5214	45
H20A	7433	5055	10499	45
H20B	6776	3938	10810	45
H20C	6157	5010	11271	45
H13A	-622	7016	8449	48
H13B	1003	7573	9266	48
H13C	-156	7005	9939	48

Table S7. Crystal data and structure refinement for **2**.

Identification code	**2**
Empirical formula	$C_{24}H_{26}O_8$
Formula weight	442.45
Temperature/K	106.15
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	8.33180(10)
b/Å	14.6050(2)
c/Å	17.4015(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2117.52(5)
Z	4
ρ_{calc}g/cm^3	1.388
μ/mm^{-1}	0.870
F(000)	936.0
Crystal size/mm^3	0.22 × 0.2 × 0.18
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.904 to 148.828
Index ranges	$-9 \leq h \leq 9$, $-15 \leq k \leq 17$, $-21 \leq l \leq 21$
Reflections collected	10171
Independent reflections	4147 [R_{int} = 0.0305, R_{sigma} = 0.0346]

Data/restraints/parameters	4147/0/312
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	$R_1 = 0.0305$, $wR_2 = 0.0809$
Final R indexes [all data]	$R_1 = 0.0315$, $wR_2 = 0.0820$
Largest diff. peak/hole / e $Å^{-3}$	0.23/-0.17
Flack parameter	0.08(7)

Table S8. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **2**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	5133.9(19)	2874.9(10)	4308.6(8)	28.7(3)
O2	4817.6(18)	3817.8(9)	5279.1(8)	22.7(3)
O3	1097.4(16)	2976.7(9)	7052.7(8)	21.3(3)
O4	2286.1(16)	4355.4(9)	7350.2(7)	18.0(3)
O5	4022.3(19)	5932.2(10)	7894.4(9)	28.2(3)
O6	5173.0(17)	4973.4(9)	8698.7(8)	24.3(3)
O7	-32.9(16)	4295.0(9)	8682.6(8)	24.3(3)
C8	66(3)	5639.3(15)	7888.1(13)	28.4(5)
C1	4697(2)	2977.1(13)	4967.4(11)	22.1(4)
C2	4137(2)	2236.0(13)	5466.8(11)	22.3(4)
C3	3801(2)	2382.0(13)	6202.0(11)	20.1(4)
C4	3901(2)	3313.5(13)	6575.6(11)	18.3(4)
C5	3793(2)	4074.1(13)	5943.7(11)	19.8(4)
C6	2103(3)	4176.3(14)	5622.0(12)	23.0(4)
C7	4457(3)	5009.6(13)	6166.6(12)	23.7(4)
C0AA	5417(2)	3356.8(13)	7080.5(12)	20.8(4)
C9	7072(3)	3388.9(16)	6743.4(13)	28.3(5)
C10	5052(2)	3267.7(12)	7825.4(11)	19.6(4)
C11	3302(2)	3037.7(12)	7955.8(11)	17.9(4)
C12	3061(3)	2021.0(13)	8143.5(12)	23.0(4)
C13	2567(2)	3393.0(12)	7204.2(11)	18.0(4)
C14	2579(2)	3682.5(13)	8570.8(11)	18.2(4)
C15	2500(2)	4586.3(12)	8140.5(11)	17.1(4)

Atom	*x*	*y*	*z*	U(eq)
C16	3964(2)	5209.2(13)	8225.3(11)	20.2(4)
C17	819(2)	3514.6(13)	8765.3(11)	20.8(4)
O18	194.6(19)	2820.5(10)	8987.9(9)	29.1(3)
C19	982(2)	5056.4(13)	8448.0(11)	21.0(4)
C20	6102(2)	3398.0(15)	8513.4(12)	24.1(4)
C21	5298(3)	4066.8(14)	9082.0(11)	22.9(4)
C22	6368(3)	4245.4(16)	9770.5(13)	30.4(5)
C23	3626(2)	3731.1(13)	9276.4(11)	20.1(4)
C24	3172(3)	3470.1(14)	9972.1(12)	25.9(4)

Table S9. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **2**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	36.0(9)	30.6(7)	19.5(7)	-0.9(6)	4.4(6)	7.7(7)
O2	27.4(8)	21.7(7)	19.0(6)	-0.4(5)	4.8(6)	0.1(6)
O3	18.2(7)	26.3(7)	19.6(6)	-3.5(5)	-1.0(5)	-4.0(5)
O4	22.1(7)	15.7(6)	16.1(6)	-1.2(5)	-1.2(5)	2.0(5)
O5	35.2(8)	21.8(7)	27.7(7)	2.9(6)	-2.0(7)	-6.9(6)
O6	21.6(7)	23.8(7)	27.6(7)	-1.2(6)	-3.4(6)	-2.8(6)
O7	20.0(7)	23.9(7)	29.0(7)	0.7(6)	3.5(6)	1.6(6)
C8	30.0(12)	26.5(10)	28.7(10)	0.2(8)	-0.9(10)	9.2(9)
C1	22.5(9)	23.8(9)	20.1(9)	-1.6(7)	1.0(8)	5.8(8)
C2	24.9(10)	19.4(9)	22.6(9)	-2.4(7)	0.3(8)	3.3(8)
C3	18.7(9)	18.3(9)	23.2(9)	-1.0(7)	-0.6(8)	2.1(7)
C4	19.7(9)	17.2(8)	18.1(8)	-2.3(7)	-0.2(7)	0.9(7)
C5	22.2(10)	19.7(9)	17.6(8)	-1.4(7)	3.8(7)	0.8(7)
C6	26.8(10)	21.6(9)	20.5(9)	1.1(8)	-0.6(8)	1.6(8)
C7	28.8(10)	20.2(9)	22.3(9)	0.9(7)	2.3(8)	-3.4(8)
C0AA	21.0(10)	19.5(8)	22.0(9)	-2.5(7)	-0.5(8)	1.0(7)
C9	21.3(10)	36.8(11)	26.9(10)	-1.6(9)	-0.1(8)	1.9(9)
C10	18.8(9)	17.8(9)	22.2(9)	-0.9(7)	-0.4(8)	3.5(7)
C11	18.9(9)	17.6(8)	17.2(9)	-0.3(7)	0.3(7)	1.9(7)
C12	28.4(10)	18.1(9)	22.5(9)	1.5(7)	0.2(8)	2.0(8)
C13	17.8(9)	16.9(8)	19.2(9)	-1.2(7)	-0.6(7)	0.0(7)
C14	19.9(9)	17.5(8)	17.0(9)	-0.6(7)	-0.8(7)	0.2(7)
C15	18.2(9)	17.6(9)	15.6(8)	-1.5(7)	-0.7(7)	0.4(7)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C16	21.9(10)	20.4(9)	18.2(8)	-3.3(7)	1.6(7)	-1.9(7)
C17	22.3(10)	21.3(9)	18.7(9)	-0.4(7)	1.7(8)	1.1(7)
O18	29.4(8)	26.0(7)	31.9(8)	3.3(6)	7.8(7)	-5.6(6)
C19	22.1(9)	18.8(9)	22.0(9)	-0.9(7)	0.5(8)	0.5(7)
C20	18.7(10)	30.3(10)	23.3(9)	-1.8(8)	-1.7(8)	4.6(8)
C21	22.5(10)	25.1(9)	21.1(9)	0.0(8)	-3.7(8)	3.6(8)
C22	25.6(11)	40.1(12)	25.4(10)	-6.7(9)	-5.7(9)	4.2(9)
C23	22.4(10)	18.5(8)	19.4(9)	-1.8(7)	-0.9(8)	4.9(8)
C24	31.2(11)	24.1(10)	22.5(10)	0.7(8)	-1.4(9)	5.5(8)

Table S10. Bond Lengths for **2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.212(2)	C5	C7	1.524(3)
O2	C1	1.346(2)	C0AA	C9	1.499(3)
O2	C5	1.485(2)	C0AA	C10	1.338(3)
O3	C13	1.392(2)	C10	C11	1.514(3)
O4	C13	1.447(2)	C10	C20	1.495(3)
O4	C15	1.427(2)	C11	C12	1.533(3)
O5	C16	1.204(2)	C11	C13	1.535(3)
O6	C16	1.346(2)	C11	C14	1.547(2)
O6	C21	1.486(2)	C14	C15	1.519(2)
O7	C17	1.350(2)	C14	C17	1.524(3)
O7	C19	1.456(2)	C14	C23	1.508(3)
C8	C19	1.502(3)	C15	C16	1.529(3)
C1	C2	1.465(3)	C15	C19	1.535(3)
C2	C3	1.327(3)	C17	O18	1.204(2)
C3	C4	1.510(2)	C20	C21	1.543(3)
C4	C5	1.566(3)	C21	C22	1.516(3)
C4	C0AA	1.540(3)	C21	C23	1.515(3)
C4	C13	1.564(3)	C23	C24	1.324(3)
C5	C6	1.523(3)			

Table S11. Bond Angles for **2**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	O2	C5	120.06(15)	O3	C13	C11	111.39(15)
C15	O4	C13	112.25(13)	O4	C13	C4	108.04(14)
C16	O6	C21	123.69(15)	O4	C13	C11	104.07(14)
C17	O7	C19	111.66(15)	C11	C13	C4	106.71(15)
O1	C1	O2	118.11(18)	C15	C14	C11	101.82(14)
O1	C1	C2	124.47(19)	C15	C14	C17	101.98(15)
O2	C1	C2	117.31(17)	C17	C14	C11	115.47(16)
C3	C2	C1	121.36(18)	C23	C14	C11	111.51(15)
C2	C3	C4	123.26(17)	C23	C14	C15	112.67(16)
C3	C4	C5	109.49(15)	C23	C14	C17	112.52(16)
C3	C4	C0AA	109.12(15)	O4	C15	C14	105.96(14)
C3	C4	C13	109.21(15)	O4	C15	C16	109.46(15)
C0AA	C4	C5	114.73(16)	O4	C15	C19	109.81(15)
C0AA	C4	C13	100.43(14)	C14	C15	C16	115.78(16)
C13	C4	C5	113.46(15)	C14	C15	C19	104.63(15)
O2	C5	C4	109.59(14)	C16	C15	C19	110.94(14)
O2	C5	C6	105.66(15)	O5	C16	O6	119.12(18)
O2	C5	C7	102.44(15)	O5	C16	C15	120.55(18)
C6	C5	C4	112.37(16)	O6	C16	C15	120.26(16)
C6	C5	C7	109.96(16)	O7	C17	C14	110.26(16)
C7	C5	C4	115.88(16)	O18	C17	O7	121.19(18)
C9	C0AA	C4	122.18(17)	O18	C17	C14	128.52(18)
C10	C0AA	C4	111.25(18)	O7	C19	C8	108.63(16)
C10	C0AA	C9	126.23(19)	O7	C19	C15	103.57(14)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C0AA	C10	C11	112.69(17)	C8	C19	C15	116.48(17)
C0AA	C10	C20	129.12(18)	C10	C20	C21	109.89(16)
C20	C10	C11	118.14(16)	O6	C21	C20	107.84(16)
C10	C11	C12	111.88(15)	O6	C21	C22	104.03(16)
C10	C11	C13	100.46(15)	O6	C21	C23	108.93(15)
C10	C11	C14	110.10(15)	C22	C21	C20	111.10(17)
C12	C11	C13	117.18(16)	C23	C21	C20	109.72(17)
C12	C11	C14	113.03(16)	C23	C21	C22	114.84(17)
C13	C11	C14	103.20(14)	C14	C23	C21	111.42(16)
O3	C13	O4	108.38(15)	C24	C23	C14	124.4(2)
O3	C13	C4	117.40(15)	C24	C23	C21	124.05(19)

Table S12. Torsion Angles for **2**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C1	C2	C3	174.4(2)	C12	C11	C13	O3	36.7(2)
O2	C1	C2	C3	-1.7(3)	C12	C11	C13	O4	153.29(15)
O4	C15	C16	O5	59.0(2)	C12	C11	C13	C4	-92.60(19)
O4	C15	C16	O6	-123.93(18)	C12	C11	C14	C15	-162.82(16)
O4	C15	C19	O7	86.09(17)	C12	C11	C14	C17	-53.3(2)
O4	C15	C19	C8	-33.1(2)	C12	C11	C14	C23	76.8(2)
O6	C21	C23	C14	56.8(2)	C13	O4	C15	C14	-12.6(2)
O6	C21	C23	C24	-126.4(2)	C13	O4	C15	C16	112.92(16)
C1	O2	C5	C4	49.7(2)	C13	O4	C15	C19	-125.06(15)
C1	O2	C5	C6	-71.6(2)	C13	C4	C5	O2	-165.93(14)
C1	O2	C5	C7	173.23(16)	C13	C4	C5	C6	-48.8(2)
C1	C2	C3	C4	2.5(3)	C13	C4	C5	C7	78.8(2)
C2	C3	C4	C5	21.4(3)	C13	C4	C0AA	C9	-174.60(18)
C2	C3	C4	C0AA	-105.0(2)	C13	C4	C0AA	C10	11.7(2)
C2	C3	C4	C13	146.14(19)	C13	C11	C14	C15	-35.27(18)
C3	C4	C5	O2	-43.7(2)	C13	C11	C14	C17	74.27(19)
C3	C4	C5	C6	73.5(2)	C13	C11	C14	C23	-155.66(16)
C3	C4	C5	C7	-158.92(17)	C14	C11	C13	O3	-88.18(18)
C3	C4	C0AA	C9	70.7(2)	C14	C11	C13	O4	28.40(18)
C3	C4	C0AA	C10	-103.02(18)	C14	C11	C13	C4	142.51(15)
C3	C4	C13	O3	-36.4(2)	C14	C15	C16	O5	178.67(18)
C3	C4	C13	O4	-159.26(14)	C14	C15	C16	O6	-4.3(2)
C3	C4	C13	C11	89.35(17)	C14	C15	C19	O7	-27.24(18)
C4	C0AA	C10	C11	6.9(2)	C14	C15	C19	C8	-146.41(17)

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C4	C0AA	C10	C20	-170.57(18)	C15	O4	C13	O3	108.32(17)
C5	O2	C1	O1	157.25(18)	C15	O4	C13	C4	-123.50(16)
C5	O2	C1	C2	-26.4(2)	C15	O4	C13	C11	-10.3(2)
C5	C4	C0AA	C9	-52.6(2)	C15	C14	C17	O7	-16.4(2)
C5	C4	C0AA	C10	133.72(17)	C15	C14	C17	O18	166.0(2)
C5	C4	C13	O3	86.0(2)	C15	C14	C23	C21	-55.0(2)
C5	C4	C13	O4	-36.8(2)	C15	C14	C23	C24	128.2(2)
C5	C4	C13	C11	-148.22(15)	C16	O6	C21	C20	84.5(2)
C0AA	C4	C5	O2	79.41(19)	C16	O6	C21	C22	-157.41(17)
C0AA	C4	C5	C6	-163.44(16)	C16	O6	C21	C23	-34.5(2)
C0AA	C4	C5	C7	-35.8(2)	C16	C15	C19	O7	-152.78(15)
C0AA	C4	C13	O3	-151.06(16)	C16	C15	C19	C8	88.0(2)
C0AA	C4	C13	O4	86.10(16)	C17	O7	C19	C8	142.27(16)
C0AA	C4	C13	C11	-25.29(18)	C17	O7	C19	C15	17.8(2)
C0AA	C10	C11	C12	102.58(19)	C17	C14	C15	O4	-89.94(17)
C0AA	C10	C11	C13	-22.5(2)	C17	C14	C15	C16	148.53(16)
C0AA	C10	C11	C14	-130.85(17)	C17	C14	C15	C19	26.10(18)
C0AA	C10	C20	C21	127.4(2)	C17	C14	C23	C21	-169.66(16)
C9	C0AA	C10	C11	-166.55(19)	C17	C14	C23	C24	13.5(3)
C9	C0AA	C10	C20	16.0(3)	C19	O7	C17	C14	-1.0(2)
C10	C11	C13	O3	158.10(15)	C19	O7	C17	O18	176.86(18)
C10	C11	C13	O4	-85.33(16)	C19	C15	C16	O5	-62.3(2)
C10	C11	C13	C4	28.79(17)	C19	C15	C16	O6	114.73(18)
C10	C11	C14	C15	71.26(18)	C20	C10	C11	C12	-79.7(2)
C10	C11	C14	C17	-179.20(15)	C20	C10	C11	C13	155.25(17)

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C10	C11	C14	C23	-49.1(2)	C20	C10	C11	C14	46.9(2)
C10	C20	C21	O6	-64.1(2)	C20	C21	C23	C14	-61.1(2)
C10	C20	C21	C22	-177.49(17)	C20	C21	C23	C24	115.7(2)
C10	C20	C21	C23	54.4(2)	C21	O6	C16	O5	-174.43(17)
C11	C10	C20	C21	-49.9(2)	C21	O6	C16	C15	8.5(3)
C11	C14	C15	O4	29.63(19)	C22	C21	C23	C14	172.96(17)
C11	C14	C15	C16	-91.89(18)	C22	C21	C23	C24	-10.2(3)
C11	C14	C15	C19	145.67(15)	C23	C14	C15	O4	149.19(16)
C11	C14	C17	O7	-125.82(17)	C23	C14	C15	C16	27.7(2)
C11	C14	C17	O18	56.5(3)	C23	C14	C15	C19	-94.77(18)
C11	C14	C23	C21	58.8(2)	C23	C14	C17	O7	104.61(18)
C11	C14	C23	C24	-118.0(2)	C23	C14	C17	O18	-73.0(3)

Table S13. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **2**.

Atom	*x*	*y*	*z*	U(eq)
H3	988	2914	6587	32
H8A	614	6082	7765	43
H2	4013	1651	5264	27
H3A	3489	1886	6502	24
H6A	2119	4595	5197	34
H6B	1404	4407	6015	34
H6C	1721	3591	5451	34
H7A	5432	4932	6454	36
H7B	3684	5328	6476	36
H7C	4676	5358	5710	36
H9A	7313	2812	6506	43
H9B	7838	3509	7143	43
H9C	7125	3867	6365	43
H12A	3677	1655	7792	34
H12B	1945	1868	8096	34
H12C	3411	1903	8660	34
H19	1260	5424	8900	25
H20A	7134	3640	8355	29
H20B	6281	2813	8763	29
H22A	7357	4516	9601	46
H22B	6590	3678	10028	46
H22C	5835	4655	10118	46
H24A	2090(40)	3280(18)	10055(16)	37(7)

Atom	*x*	*y*	*z*	U(eq)
H24B	3820(30)	3500(17)	10406(15)	27(6)
H8B	-240(30)	5286(19)	7396(16)	35(7)
H8C	-940(30)	5868(18)	8145(16)	35(7)

Table S14. Crystal data and structure refinement for **3**.

Identification code	**3**
Empirical formula	$C_{25}H_{26}O_8$
Formula weight	454.48
Temperature/K	101.8(6)
Crystal system	monoclinic
Space group	C2
a/Å	20.3188(2)
b/Å	8.20450(10)
c/Å	13.22130(10)
α/°	90
β/°	91.3740(10)
γ/°	90
Volume/Å^3	2203.43(4)
Z	4
ρ_{calc}g/cm^3	1.3699
μ/mm^{-1}	0.853
F(000)	963.5
Crystal size/mm^3	0.22 × 0.2 × 0.18
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.7 to 148.32
Index ranges	-25 ≤ h ≤ 24, -9 ≤ k ≤ 9, -16 ≤ l ≤ 16
Reflections collected	11749
Independent reflections	3823 [R_{int} = 0.0298, R_{sigma} = 0.0290]

Data/restraints/parameters	3823/1/388
Goodness-of-fit on F^2	0.823
Final R indexes [I>=2σ (I)]	R_1 = 0.0295, wR_2 = 0.0880
Final R indexes [all data]	R_1 = 0.0299, wR_2 = 0.0886
Largest diff. peak/hole / e $Å^{-3}$	0.37/-0.17
Flack parameter	-0.08(8)

Table S15. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **3**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
O0aa	3216.6(5)	5068.1(12)	5796.9(7)	22.1(2)
O	2189.7(4)	5255.9(12)	7961.4(7)	20.9(2)
O2aa	1137.3(5)	4162.4(13)	6452.0(7)	24.8(2)
O3aa	1716.1(5)	3205.2(12)	5165.6(7)	24.8(2)
O4aa	1946.4(5)	2987.0(13)	9620.7(7)	26.2(2)
O5aa	5378.6(6)	6605(2)	8976.5(8)	44.3(4)
O6aa	4929.3(5)	5039.3(17)	7796.3(7)	31.8(3)
O1aa	2570.5(5)	7182.1(13)	6956.4(8)	25.3(2)
C1aa	1971.7(6)	2561.3(17)	8750.7(10)	21.0(3)

Atom	*x*	*y*	*z*	U(eq)
C2aa	3097.6(6)	4599.1(16)	6796.8(9)	19.1(3)
C3aa	1657.3(6)	3365.6(16)	6057.8(10)	19.7(3)
C4aa	2585.1(6)	5778.1(17)	7213.2(9)	20.1(3)
C5aa	3733.3(6)	4695.4(17)	7556.5(9)	21.1(3)
C6aa	4881.2(7)	6175(2)	8525.7(10)	31.9(4)
C7aa	3688.4(7)	6054.6(18)	8338.6(10)	23.5(3)
C8aa	1871.6(6)	3702.9(16)	7832.3(9)	19.5(3)
C	2110.5(7)	850.9(17)	8336.4(10)	22.0(3)
C0ba	3168.5(6)	2172.8(18)	7809.9(9)	20.8(3)
C1ba	3673.7(6)	3093.2(18)	8142.4(10)	21.7(3)
C2ba	2855.0(6)	2794.3(17)	6826.8(9)	18.9(3)
C1	1814.1(7)	-507.5(18)	8947.4(11)	26.6(3)
C4ba	2095.1(6)	2727.4(16)	6926.5(9)	19.0(3)
C5ba	1879.3(6)	1022.8(17)	7242.4(9)	20.2(3)
C6ba	4217.0(7)	6748(2)	8763.0(11)	28.7(3)
C7ba	1533.4(7)	-36.3(18)	6690.5(10)	24.6(3)
C8ba	2882.0(7)	701.4(18)	8306.8(10)	24.6(3)
C9ba	4403.4(6)	4948(2)	7004.6(10)	27.1(3)
C0ca	1138.7(6)	3987.2(18)	7551.2(10)	22.7(3)
C1ca	4457.3(8)	6518(2)	6386.4(12)	33.5(4)
C2ca	3064.0(7)	1760.5(19)	5923.8(10)	24.2(3)
C0aa	811.4(7)	5442(2)	8019.4(12)	30.1(3)
C9aa	4125.7(7)	2673(2)	9021.9(11)	27.0(3)
C2	4610.3(7)	3502(3)	6376.9(12)	34.5(4)

Table S16. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **3**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O0aa	25.7(4)	22.6(5)	17.9(4)	-0.9(4)	0.8(3)	2.2(4)
O	23.1(4)	17.8(5)	21.9(4)	-3.1(4)	3.5(3)	-3.5(4)
O2aa	21.2(4)	27.4(5)	25.8(5)	4.4(4)	-2.1(4)	-0.1(4)
O3aa	29.1(5)	24.5(5)	20.5(4)	-0.7(4)	-2.4(4)	0.8(4)
O4aa	33.0(5)	25.9(5)	19.9(4)	-3.6(4)	2.2(4)	-1.9(4)
O5aa	28.4(5)	77.7(10)	26.6(5)	-19.0(6)	-3.2(4)	2.1(6)
O6aa	19.8(4)	51.6(7)	23.9(5)	-2.9(4)	-1.7(4)	3.2(5)
O1aa	29.1(5)	19.7(5)	27.1(5)	0.3(4)	0.8(4)	1.0(4)
C1aa	20.1(6)	23.1(7)	19.8(6)	-3.7(5)	1.8(5)	-0.4(5)
C2aa	19.0(5)	21.0(6)	17.5(5)	0.1(5)	1.8(4)	0.3(5)
C3aa	20.9(6)	14.8(6)	23.2(6)	-2.3(4)	-1.5(5)	0.9(5)
C4aa	18.9(5)	21.9(7)	19.3(5)	-1.8(5)	-2.8(4)	-1.3(5)
C5aa	18.2(6)	27.7(7)	17.4(5)	-0.3(5)	-0.2(4)	1.2(5)
C6aa	25.4(7)	48.9(10)	21.2(6)	-12.4(6)	-2.1(5)	6.3(6)
C7aa	25.4(7)	25.2(7)	19.7(6)	-3.6(5)	-1.7(5)	2.9(5)
C8aa	20.1(6)	16.8(7)	21.6(6)	-1.4(5)	1.6(5)	-0.9(5)
C	27.0(6)	19.4(7)	19.5(6)	-0.2(5)	1.2(5)	1.9(5)
C0ba	20.2(6)	22.2(7)	20.1(6)	5.4(5)	1.1(4)	0.9(5)
C1ba	20.5(6)	25.7(7)	19.1(5)	3.4(5)	2.0(5)	1.2(5)
C2ba	19.3(6)	20.0(7)	17.6(5)	1.2(5)	0.7(4)	0.6(5)
C1	34.7(7)	21.1(7)	23.9(6)	-3.5(5)	1.4(5)	3.2(5)
C4ba	18.5(6)	19.2(6)	19.1(5)	0.9(5)	-1.2(4)	0.7(5)
C5ba	21.8(6)	19.3(7)	19.8(6)	2.0(5)	2.7(4)	0.2(5)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C6ba	30.4(7)	33.1(8)	22.3(6)	-8.9(6)	-3.4(5)	0.1(6)
C7ba	28.8(6)	22.0(7)	22.9(6)	-2.1(5)	0.4(5)	0.3(5)
C8ba	27.8(6)	21.8(7)	24.1(6)	2.8(5)	-0.9(5)	4.1(5)
C9ba	16.6(5)	44.5(9)	20.0(6)	-1.2(6)	-0.8(5)	2.0(6)
C0ca	19.9(6)	24.4(7)	24.0(6)	-0.5(5)	2.8(5)	-1.0(5)
C1ca	25.5(7)	48.9(10)	26.1(7)	-13.1(7)	-0.4(5)	8.7(7)
C2ca	25.0(6)	24.8(7)	23.1(6)	3.8(5)	3.1(5)	-3.3(6)
C0aa	25.9(7)	27.9(8)	36.6(7)	5.4(6)	4.1(6)	-2.3(6)
C9aa	25.4(6)	31.9(8)	23.3(6)	4.5(5)	-4.4(5)	3.4(6)
C2	24.4(7)	53.0(11)	26.5(7)	4.9(6)	4.8(6)	-2.1(7)

Table S17. Bond Lengths for **3**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O0aa	C2aa	1.4034(14)	C5aa	C9ba	1.5739(18)
O	C4aa	1.3585(16)	C6aa	C6ba	1.470(2)
O	C8aa	1.4370(16)	C7aa	C6ba	1.3280(19)
O2aa	C3aa	1.3571(17)	C8aa	C4ba	1.5189(17)
O2aa	C0ca	1.4604(15)	C8aa	C0ca	1.5440(17)
O3aa	C3aa	1.1958(16)	C	C1	1.510(2)
O4aa	C1aa	1.2044(16)	C	C5ba	1.5167(17)
O5aa	C6aa	1.2134(18)	C	C8ba	1.5739(18)
O6aa	C6aa	1.346(2)	C0ba	C1ba	1.3399(19)
O6aa	C9ba	1.4795(15)	C0ba	C2ba	1.5217(16)
O1aa	C4aa	1.2010(18)	C0ba	C8ba	1.499(2)
C1aa	C8aa	1.5431(18)	C1ba	C9aa	1.5044(16)
C1aa	C	1.5349(18)	C2ba	C4ba	1.5537(16)
C2aa	C4aa	1.5332(18)	C2ba	C2ca	1.5327(17)
C2aa	C5aa	1.6191(16)	C4ba	C5ba	1.5269(18)
C2aa	C2ba	1.5614(18)	C5ba	C7ba	1.3254(19)
C3aa	C4ba	1.5283(16)	C9ba	C1ca	1.531(2)
C5aa	C7aa	1.525(2)	C9ba	C2	1.513(2)
C5aa	C1ba	1.5321(19)	C0ca	C0aa	1.506(2)

Table S18. Bond Angles for **3**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C8aa	O	C4aa	117.73(10)	C5ba	C	C1	117.42(11)
C0ca	O2aa	C3aa	110.60(10)	C8ba	C	C1aa	105.76(10)
C9ba	O6aa	C6aa	118.58(12)	C8ba	C	C1	111.47(11)
C8aa	C1aa	O4aa	124.58(13)	C8ba	C	C5ba	105.63(11)
C	C1aa	O4aa	128.19(12)	C2ba	C0ba	C1ba	113.15(12)
C	C1aa	C8aa	107.22(10)	C8ba	C0ba	C1ba	127.78(12)
C4aa	C2aa	O0aa	107.41(10)	C8ba	C0ba	C2ba	119.03(11)
C5aa	C2aa	O0aa	114.71(10)	C0ba	C1ba	C5aa	112.76(11)
C5aa	C2aa	C4aa	106.56(10)	C9aa	C1ba	C5aa	122.22(12)
C2ba	C2aa	O0aa	110.22(10)	C9aa	C1ba	C0ba	124.98(13)
C2ba	C2aa	C4aa	111.82(10)	C0ba	C2ba	C2aa	102.33(10)
C2ba	C2aa	C5aa	106.15(10)	C4ba	C2ba	C2aa	110.53(10)
O3aa	C3aa	O2aa	121.93(11)	C4ba	C2ba	C0ba	108.19(10)
C4ba	C3aa	O2aa	108.72(11)	C2ca	C2ba	C2aa	114.29(11)
C4ba	C3aa	O3aa	129.31(13)	C2ca	C2ba	C0ba	111.20(11)
O1aa	C4aa	O	119.82(13)	C2ca	C2ba	C4ba	109.94(10)
C2aa	C4aa	O	118.76(11)	C8aa	C4ba	C3aa	103.44(10)
C2aa	C4aa	O1aa	121.06(12)	C2ba	C4ba	C3aa	119.07(11)
C7aa	C5aa	C2aa	113.36(11)	C2ba	C4ba	C8aa	111.39(10)
C1ba	C5aa	C2aa	101.55(10)	C5ba	C4ba	C3aa	110.71(10)
C1ba	C5aa	C7aa	106.13(10)	C5ba	C4ba	C8aa	100.01(10)
C9ba	C5aa	C2aa	113.89(10)	C5ba	C4ba	C2ba	110.37(10)
C9ba	C5aa	C7aa	106.54(11)	C4ba	C5ba	C	105.17(11)
C9ba	C5aa	C1ba	115.28(12)	C7ba	C5ba	C	127.74(13)

Atom Atom Atom	Angle/°	Atom Atom Atom	Angle/°
O6aa C6aa O5aa	118.65(16)	C7ba C5ba C4ba	127.00(12)
C6ba C6aa O5aa	124.05(16)	C7aa C6ba C6aa	120.67(15)
C6ba C6aa O6aa	117.20(12)	C0ba C8ba C	110.23(10)
C6ba C7aa C5aa	122.61(14)	C5aa C9ba O6aa	107.27(10)
C1aa C8aa O	113.22(10)	C1ca C9ba O6aa	105.97(12)
C4ba C8aa O	114.76(10)	C1ca C9ba C5aa	115.59(13)
C4ba C8aa C1aa	105.32(11)	C2 C9ba O6aa	102.85(11)
C0ca C8aa O	108.85(11)	C2 C9ba C5aa	113.95(13)
C0ca C8aa C1aa	112.91(11)	C2 C9ba C1ca	110.04(13)
C0ca C8aa C4ba	101.23(10)	C8aa C0ca O2aa	103.48(10)
C1 C C1aa	113.88(11)	C0aa C0ca O2aa	109.91(12)
C5ba C C1aa	101.53(10)	C0aa C0ca C8aa	116.97(11)

Table S19. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **3**.

Atom	*x*	*y*	*z*	U(eq)
H0aa	3124(10)	6034(7)	5723(4)	33.1(3)
H1a	1947(5)	-390(9)	9645.2(19)	39.8(4)
H1b	1342.8(7)	-457(9)	8887(8)	39.8(4)
H1c	1964(5)	-1538.8(19)	8698(6)	39.8(4)
H2a	4350(9)	3450(30)	5725(14)	25(4)
H7ba	1406(10)	200(30)	5978(15)	35(5)
H6ba	4193(9)	7540(30)	9277(15)	30(5)
H1ca	4243(11)	7420(30)	6681(17)	40(6)
H8ba	2997(8)	-360(30)	7930(13)	23(4)
H1cb	4888(12)	6790(30)	6341(16)	44(6)
H0ca	887(8)	2940(30)	7686(13)	23(4)
H2ca	2927(8)	2230(30)	5283(13)	23(4)
H2cb	3550(10)	1600(30)	5902(15)	37(5)
H9aa	4539(10)	2440(30)	8763(15)	31(5)
H0ab	1058(10)	6370(30)	7886(15)	34(5)
H2b	4582(10)	2580(30)	6767(18)	38(6)
H7aa	3245(9)	6340(20)	8610(14)	24(4)
H2c	5081(11)	3620(30)	6202(15)	39(5)
H9ab	4203(10)	3600(30)	9517(16)	37(5)
H8bb	3080(10)	510(30)	9020(16)	36(5)
H0ac	339(11)	5490(30)	7776(17)	44(6)
H9ac	3976(11)	1700(30)	9400(18)	46(6)
H0ad	840(11)	5380(30)	8764(17)	41(5)

Atom	*x*	*y*	*z*	U(eq)
H2cc	2855(11)	650(30)	6029(16)	36(5)
H1cc	4306(11)	6410(30)	5709(17)	37(5)
H7bb	1399(9)	-1130(30)	6984(13)	24(4)

Table S20 Crystal data and structure refinement for **4**

Identification code	**4**
Empirical formula	$C_{26}H_{34}O_8$
Formula weight	474.53
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	8.70681(4)
b/Å	12.24332(6)
c/Å	21.97785(9)
α/°	90

β/°	90
γ/°	90
Volume/Å^3	2342.844(18)
Z	4
ρ_{calc}g/cm^3	1.345
μ/mm^{-1}	0.818
F(000)	1016.0
Crystal size/mm^3	? × ? × ?
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.046 to 148.808
Index ranges	-10 ≤ h ≤ 10, -15 ≤ k ≤ 14, -27 ≤ l ≤ 27
Reflections collected	29855
Independent reflections	4734 [R_{int} = 0.0323, R_{sigma} = 0.0185]
Data/restraints/parameters	4734/0/325
Goodness-of-fit on F^2	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0294, wR_2 = 0.0772
Final R indexes [all data]	R_1 = 0.0297, wR_2 = 0.0775
Largest diff. peak/hole / e Å^{-3}	0.23/-0.19
Flack parameter	-0.05(4)

Table S21 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **4**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O4	2717.2(15)	8000.2(10)	6018.2(5)	22.4(3)
O2	5713.9(15)	3794.6(11)	5550.6(6)	25.3(3)
O6	-380.4(16)	9023.7(11)	6323.9(6)	27.6(3)
O5	4217.3(16)	8062.2(12)	7202.0(6)	31.1(3)
O3	832.2(16)	4057.5(11)	5617.4(7)	28.9(3)
O8	5483.5(16)	8859.5(12)	5878.6(7)	31.2(3)
O1	7859.9(15)	4496.9(13)	5194.7(7)	32.2(3)
O7	-1916.8(17)	7625.9(12)	6091.5(7)	34.1(3)
C009	6500(2)	4622.2(16)	5304.8(8)	24.6(4)
C00A	3386(2)	5193.9(14)	6403.2(8)	21.7(4)
C00B	2227(2)	5690.3(14)	6698.7(8)	21.6(4)
C00C	4267(2)	5810.4(15)	5406.2(8)	23.0(4)
C00D	-734(2)	7952.4(15)	6312.1(8)	24.8(4)
C00E	1659(2)	5030.2(15)	5469.1(8)	22.5(4)
C00F	742(2)	6089.1(14)	6403.7(8)	21.5(3)
C00G	4002(2)	3789.6(15)	5527.1(9)	23.1(4)
C00H	5700(2)	5658.4(16)	5212.8(8)	25.5(4)
C00I	313(2)	7333.3(15)	7313.6(8)	24.8(4)
C00J	1927(2)	8080.2(15)	6567.3(8)	21.7(4)
C00K	1906(2)	7118.9(16)	7558.6(8)	25.3(4)
C00L	2884(2)	7810.7(15)	7130.8(8)	23.7(4)

C00M	3322(2)	4932.7(14)	5715.7(8)	20.9(3)
C00N	2331(2)	5918.6(15)	7379.4(8)	25.1(4)
C00O	3628(2)	3484.4(16)	4870.9(9)	26.8(4)
C00P	834(2)	6041.3(14)	5705.6(8)	22.5(3)
C00Q	1089(2)	9195.9(15)	6634.5(9)	25.4(4)
C00R	4892(2)	4964.2(18)	6729.3(9)	30.0(4)
C00S	523(2)	7301.7(15)	6620.4(8)	22.6(4)
C00T	3592(2)	2856.8(16)	5953.6(10)	29.2(4)
C00U	1875(3)	10169.4(16)	6364.5(10)	30.3(4)
C00V	-629(2)	5400.4(16)	6629.5(9)	28.6(4)
C00W	2182(3)	7322.5(17)	8230.1(9)	32.1(4)
C00X	-954(3)	7562.0(18)	7619.1(10)	33.8(5)
C00Y	5875(3)	9835.0(19)	6185.5(11)	37.6(5)

Table S22 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **4**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O4	23.1(6)	23.9(6)	20.3(6)	-1.7(5)	2.5(5)	-2.4(5)
O2	20.0(6)	26.0(7)	30.0(6)	0.5(5)	0.2(5)	3.6(5)
O6	27.3(7)	22.5(6)	32.9(7)	-0.3(5)	-2.5(5)	5.4(5)
O5	29.3(7)	35.0(8)	29.1(7)	-1.4(6)	-3.9(6)	-4.3(6)
O3	21.8(6)	21.2(6)	43.8(8)	-3.4(5)	-2.8(6)	-2.2(5)
O8	26.6(7)	30.5(7)	36.5(7)	2.6(6)	-0.2(6)	1.0(6)
O1	20.1(7)	40.3(8)	36.3(7)	-4.7(6)	0.5(6)	1.1(6)

O7	25.0(7)	31.9(8)	45.3(8)	-4.5(6)	-5.5(6)	5.4(6)
C009	21.9(9)	29.8(10)	22.2(8)	-3.2(7)	-1.1(7)	-0.8(7)
C00A	22.1(8)	20.0(8)	23.1(8)	2.9(7)	-1.7(7)	0.5(7)
C00B	24.2(9)	18.0(8)	22.5(8)	1.4(6)	-0.6(7)	0.2(7)
C00C	25.4(9)	21.4(8)	22.0(8)	-0.1(6)	-1.0(7)	-0.1(7)
C00D	23.8(9)	24.0(9)	26.7(9)	-2.4(7)	1.9(7)	2.6(7)
C00E	21.3(9)	19.9(8)	26.4(8)	-0.7(7)	-2.7(7)	0.3(7)
C00F	20.1(8)	19.5(8)	24.9(8)	-0.2(7)	0.4(7)	0.8(7)
C00G	18.4(8)	22.1(9)	28.9(9)	0.1(7)	-0.1(7)	1.6(7)
C00H	26.4(9)	24.8(9)	25.5(9)	-0.2(7)	1.1(7)	-3.7(8)
C00I	29.3(10)	19.9(8)	25.2(9)	1.3(7)	4.1(7)	1.1(7)
C00J	24.2(9)	21.5(8)	19.5(8)	-0.9(6)	2.7(7)	-0.7(7)
C00K	28.8(10)	24.3(9)	22.6(9)	0.4(7)	2.2(7)	2.2(8)
C00L	27.1(9)	21.6(9)	22.3(8)	-2.8(6)	0.5(7)	0.1(7)
C00M	20.0(8)	20.2(8)	22.5(8)	0.1(7)	-0.3(7)	1.0(7)
C00N	28.7(9)	23.5(9)	23.0(9)	2.2(7)	1.1(7)	2.5(7)
C00O	25.3(9)	22.7(9)	32.4(10)	-6.0(8)	-0.3(8)	2.2(7)
C00P	21.4(8)	20.3(8)	25.7(8)	0.8(7)	-2.7(7)	1.8(7)
C00Q	29.1(10)	21.5(9)	25.7(9)	-1.8(7)	-0.6(7)	2.1(7)
C00R	26.5(10)	38.6(11)	25.0(8)	-2.1(8)	-3.9(8)	7.0(8)
C00S	23.2(9)	20.4(8)	24.1(8)	0.8(7)	1.1(7)	1.4(7)
C00T	28.7(10)	20.8(9)	38.2(11)	4.8(8)	3.0(8)	3.1(7)
C00U	35.9(11)	21.8(9)	33.4(10)	-0.4(7)	0.9(9)	1.2(8)
C00V	24.6(9)	26.6(9)	34.6(10)	1.0(8)	4.2(8)	-2.7(8)
C00W	41.8(11)	32.3(10)	22.3(9)	-0.8(8)	1.6(8)	6.1(9)
C00X	33.6(11)	34.8(11)	33.2(11)	1.7(9)	9.0(9)	4.2(9)

C00Y	32.1(11)	36.1(11)	44.6(11)	-3.7(9)	3.0(9)	-1.3(9)

Table S23 Bond Lengths for **4**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O4	C00J	1.392(2)	C00E	C00M	1.551(2)
O2	C009	1.337(2)	C00E	C00P	1.523(2)
O2	C00G	1.492(2)	C00F	C00P	1.538(2)
O6	C00D	1.348(2)	C00F	C00S	1.571(2)
O6	C00Q	1.465(2)	C00F	C00V	1.543(3)
O5	C00L	1.211(2)	C00G	C00M	1.575(2)
O3	C00E	1.429(2)	C00G	C00O	1.525(3)
O8	C00Y	1.413(3)	C00G	C00T	1.520(3)
O1	C009	1.218(2)	C00I	C00K	1.511(3)
O7	C00D	1.206(2)	C00I	C00S	1.535(2)
C009	C00H	1.461(3)	C00I	C00X	1.321(3)
C00A	C00B	1.345(3)	C00J	C00L	1.529(3)
C00A	C00M	1.546(2)	C00J	C00Q	1.556(2)
C00A	C00R	1.521(3)	C00J	C00S	1.555(3)
C00B	C00F	1.526(2)	C00K	C00L	1.525(3)
C00B	C00N	1.525(2)	C00K	C00N	1.566(3)
C00C	C00H	1.331(3)	C00K	C00W	1.516(3)
C00C	C00M	1.515(2)	C00Q	C00U	1.497(3)
C00D	C00S	1.513(3)			

Table S24 Bond Angles for **4**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C009	O2	C00G	120.06(14)	C00X	C00I	C00S	127.52(19)
C00D	O6	C00Q	110.39(14)	O4	C00J	C00L	114.68(15)
O2	C009	C00H	118.03(16)	O4	C00J	C00Q	112.08(15)
O1	C009	O2	118.85(18)	O4	C00J	C00S	114.24(14)
O1	C009	C00H	123.03(19)	C00L	C00J	C00Q	111.61(15)
C00B	C00A	C00M	122.59(16)	C00L	C00J	C00S	103.61(14)
C00B	C00A	C00R	120.19(16)	C00S	C00J	C00Q	99.34(14)
C00R	C00A	C00M	116.96(15)	C00I	C00K	C00L	101.32(15)
C00A	C00B	C00F	125.08(16)	C00I	C00K	C00N	106.88(16)
C00A	C00B	C00N	120.81(16)	C00I	C00K	C00W	117.66(16)
C00N	C00B	C00F	114.10(15)	C00L	C00K	C00N	103.54(14)
C00H	C00C	C00M	123.59(17)	C00W	C00K	C00L	114.86(17)
O6	C00D	C00S	109.79(16)	C00W	C00K	C00N	111.20(16)

O7	C00D	O6	121.68(18)	O5	C00L	C00J	124.90(17)
O7	C00D	C00S	128.51(18)	O5	C00L	C00K	126.62(17)
O3	C00E	C00M	109.06(14)	C00K	C00L	C00J	108.37(15)
O3	C00E	C00P	111.21(15)	C00A	C00M	C00E	111.06(14)
C00P	C00E	C00M	112.58(14)	C00A	C00M	C00G	115.32(14)
C00B	C00F	C00P	111.58(15)	C00C	C00M	C00A	105.82(14)
C00B	C00F	C00S	106.06(14)	C00C	C00M	C00E	107.19(14)
C00B	C00F	C00V	110.10(15)	C00C	C00M	C00G	107.95(14)
C00P	C00F	C00S	110.17(14)	C00E	C00M	C00G	109.11(14)
C00P	C00F	C00V	109.89(15)	C00B	C00N	C00K	113.88(15)
C00V	C00F	C00S	108.94(15)	C00E	C00P	C00F	113.33(14)
O2	C00G	C00M	111.27(14)	O6	C00Q	C00J	103.83(14)
O2	C00G	C00O	104.31(14)	O6	C00Q	C00U	109.21(15)
O2	C00G	C00T	102.50(15)	C00U	C00Q	C00J	116.55(16)
C00O	C00G	C00M	112.72(15)	C00D	C00S	C00F	116.73(15)
C00T	C00G	C00M	114.66(15)	C00D	C00S	C00I	110.20(15)
C00T	C00G	C00O	110.42(16)	C00D	C00S	C00J	102.25(14)
C00C	C00H	C009	121.59(18)	C00I	C00S	C00F	109.83(14)
C00K	C00I	C00S	103.91(15)	C00I	C00S	C00J	98.78(14)
C00X	C00I	C00K	128.45(18)	C00J	C00S	C00F	117.44(15)

Table S25 Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å2×103) for **4**

Atom	***x***	***y***	***z***	**U(eq)**

H4	3565	8284	6054	34
H3	-55	4111	5495	43
H8	6190	8420	5910	47
H00C	3822	6493	5348	28
H00E	1714	5084	5025	27
H00H	6204	6225	5014	31
H00A	3370	5768	7515	30
H00B	1649	5422	7592	30
H00D	3856	4091	4609	40
H00F	2557	3305	4839	40
H00G	4234	2865	4752	40
H00I	-199	6055	5541	27
H00J	1365	6686	5559	27
H00Q	894	9335	7067	31
H00K	5312	5636	6881	45
H00L	5605	4637	6450	45
H00M	4711	4474	7062	45
H00N	4098	2202	5821	44
H00O	2501	2746	5950	44
H00P	3918	3034	6359	44
H00R	2191	10004	5956	46
H00S	2759	10351	6605	46
H00T	1179	10777	6359	46
H00U	-467	4648	6524	43
H00V	-1556	5657	6441	43
H00W	-716	5468	7063	43

H00X	1872	8053	8331	48
H00Y	3254	7233	8319	48
H	1595	6811	8466	48
H00	5321	10435	6009	56
HA	6958	9963	6147	56
HB	5610	9769	6608	56
H00Z	-1910(30)	7680(20)	7403(12)	43(7)
HC	-900(30)	7630(20)	8060(13)	45(7)

Table S26 Crystal data and structure refinement for **5**

Identification code	**5**
Empirical formula	$C_{26}H_{30}O_8$
Formula weight	472.54
Temperature/K	296.15
Crystal system	triclinic
Space group	P1
a/Å	8.30120(10)
b/Å	8.44520(10)
c/Å	9.7416(2)
α/°	88.4430(10)
β/°	68.237(2)
γ/°	69.518(2)
Volume/Å^3	590.02(2)
Z	1

ρ_{calc}g/cm^3	1.3298
μ/mm^{-1}	0.812
F(000)	252.9
Crystal size/mm^3	0.22 × 0.2 × 0.18
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.84 to 148.28
Index ranges	-10 ≤ h ≤ 10, -10 ≤ k ≤ 10, -12 ≤ l ≤ 12
Reflections collected	11370
Independent reflections	4466 [R_{int} = 0.0150, R_{sigma} = 0.0142]
Data/restraints/parameters	4466/3/324
Goodness-of-fit on F^2	1.108
Final R indexes [I>=2σ (I)]	R_1 = 0.0303, wR_2 = 0.0812
Final R indexes [all data]	R_1 = 0.0303, wR_2 = 0.0813
Largest diff. peak/hole / e Å^{-3}	0.34/-0.35
Flack parameter	0.09(8)

Table S27 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **5**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O5	5608.3(12)	5734.5(11)	6592.9(10)	19.51(19)
O8	5960.7(13)	2636.3(11)	7558.1(10)	22.3(2)
O6	4066.4(13)	9452.3(12)	7962.4(10)	22.2(2)
O3	9443.3(13)	4598.9(12)	4086.8(11)	23.8(2)
O7	5029.9(13)	10677.0(11)	5923.8(10)	22.7(2)
O2	8781.5(13)	1887.3(11)	740.4(10)	20.39(19)
O1	9131.8(14)	-810.3(12)	902.5(11)	28.2(2)
O4	2058.3(14)	5188.8(12)	7486.2(12)	28.1(2)
C13	8127.3(17)	5158.0(16)	3716.2(13)	17.8(2)
C24	4411.0(17)	9628.4(16)	6515.8(14)	18.3(2)
C11	4992.2(17)	7657.2(15)	4186.0(13)	16.1(2)
C10	4329.9(17)	6245.9(15)	3948.6(13)	15.9(2)
C1	8926.3(17)	519.8(17)	1506.1(14)	21.1(3)
C20	1776.1(17)	9176.9(16)	6176.2(13)	17.1(2)
C15	2215.0(17)	6801.5(16)	4494.7(14)	18.4(2)
C8	4646.8(18)	3360.5(16)	3113.0(14)	18.9(2)
C25	3861.3(17)	8384.5(15)	5868.9(13)	15.7(2)
C2	8705.7(18)	774.5(16)	3055.5(15)	21.3(3)
C19	3856.8(17)	7031.1(16)	6965.5(13)	17.0(2)
C9	5440.8(16)	4634.0(15)	3376.5(13)	15.6(2)
C18	2303.4(17)	6437.7(16)	6965.9(14)	18.8(3)
C12	7118.9(17)	7024.9(16)	3793.5(14)	18.3(2)
C3	8020.4(17)	2320.2(16)	3778.1(13)	18.2(3)
C14	4536.0(19)	9053.1(16)	3187.6(14)	20.3(3)

C23	3226.7(18)	8156.9(17)	8432.9(14)	20.6(3)
C16	1219.5(17)	7658.9(16)	6146.8(14)	18.2(2)
C21	726.8(19)	10815.6(17)	6416.6(15)	22.2(3)
C4	7552.9(17)	3923.8(15)	3035.5(13)	16.2(2)
C17	-850.5(18)	7972.8(17)	6784.2(15)	23.7(3)
C26	5714(2)	2244.5(19)	9040.2(15)	24.9(3)
C6	10863.1(17)	3172.1(18)	943.7(15)	24.0(3)
C5	8808.2(18)	3476.6(16)	1318.1(14)	18.3(2)
C7	8056(2)	4772.0(17)	385.7(14)	23.5(3)
C22	3858(2)	7275(2)	9603.5(16)	30.4(3)

Table S28 Anisotropic Displacement Parameters (Å2×103) for **5**. The Anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+2hka*b*U12+…].

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{12}**	**U_{13}**	**U_{23}**
O5	15.3(4)	18.2(4)	23.9(5)	-4.5(4)	-8.1(4)	5.5(4)
O8	25.3(5)	19.3(4)	26.2(5)	-8.4(4)	-14.0(4)	3.4(4)
O6	23.5(5)	25.4(5)	19.9(4)	-9.9(4)	-9.7(4)	-0.6(4)
O3	16.1(4)	28.0(5)	27.6(5)	-5.9(4)	-10.5(4)	-1.6(4)
O7	25.2(5)	20.8(5)	24.6(4)	-11.4(4)	-9.4(4)	-1.0(4)
O2	21.1(5)	19.9(4)	18.8(4)	-7.2(4)	-6.3(4)	-1.1(3)
O1	26.3(5)	22.6(5)	28.5(5)	-10.3(4)	-0.9(4)	-6.3(4)
O4	24.6(5)	26.5(5)	36.3(5)	-13.1(4)	-12.1(4)	12.1(4)
C13	15.0(6)	22.3(6)	16.6(5)	-8.7(5)	-4.7(5)	0.7(5)
C24	14.6(6)	19.0(6)	19.2(6)	-3.2(5)	-6.7(5)	-2.7(5)
C11	17.6(6)	15.1(6)	17.1(5)	-7.4(5)	-7.0(5)	0.1(5)

C10	16.8(6)	16.7(6)	17.3(5)	-7.6(5)	-8.6(5)	3.1(5)
C1	14.6(6)	19.3(6)	23.3(6)	-5.0(5)	-1.5(5)	-1.0(5)
C20	16.1(6)	19.7(6)	16.4(5)	-6.0(5)	-7.6(5)	1.4(5)
C15	15.4(6)	18.4(6)	23.2(6)	-6.1(5)	-9.4(5)	-0.1(5)
C8	16.1(6)	16.3(6)	24.1(6)	-5.5(5)	-7.6(5)	-2.5(5)
C25	15.2(6)	13.9(6)	18.4(5)	-5.0(5)	-7.3(5)	1.1(5)
C2	18.6(6)	18.4(6)	24.5(6)	-4.4(5)	-8.1(5)	5.0(5)
C19	13.4(6)	18.4(6)	18.7(6)	-4.5(5)	-6.9(5)	2.6(5)
C9	15.2(6)	18.2(6)	15.1(5)	-7.5(5)	-6.4(5)	2.3(5)
C18	15.1(6)	19.6(6)	20.5(6)	-6.2(5)	-5.6(5)	1.8(5)
C12	16.4(6)	19.3(6)	20.8(5)	-9.4(5)	-6.0(5)	-0.6(5)
C3	14.8(6)	21.2(6)	17.7(6)	-5.4(5)	-6.4(5)	2.2(5)
C14	25.2(7)	17.6(6)	19.7(6)	-9.4(5)	-9.1(5)	3.3(5)
C23	20.2(6)	22.8(6)	19.1(6)	-7.7(5)	-8.0(5)	2.3(5)
C16	15.5(6)	17.6(6)	21.7(6)	-5.7(5)	-7.5(5)	0.1(5)
C21	20.8(7)	18.9(6)	25.1(6)	-4.4(6)	-9.5(5)	0.7(5)
C4	14.8(6)	16.1(6)	17.2(5)	-5.3(5)	-6.1(5)	1.3(4)
C17	14.7(6)	25.6(7)	29.0(6)	-5.6(5)	-7.8(5)	-1.3(5)
C26	23.3(7)	29.9(7)	22.7(6)	-9.6(6)	-9.9(5)	-1.2(5)
C6	16.5(7)	30.0(7)	22.7(6)	-9.6(6)	-3.2(5)	-1.4(6)
C5	18.6(6)	18.0(6)	17.9(5)	-7.5(5)	-5.6(5)	-0.6(5)
C7	26.5(7)	23.8(7)	18.9(6)	-9.3(6)	-7.3(5)	4.2(5)
C22	32.9(8)	38.1(8)	21.2(6)	-10.1(7)	-14.2(6)	5.1(6)

Table S29 Bond Lengths for **5**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O5	C19	1.4003(15)	C1	C2	1.4639(18)
O8	C26	1.4276(16)	C20	C25	1.5329(16)
O6	C24	1.3451(15)	C20	C16	1.5113(17)
O6	C23	1.4705(15)	C20	C21	1.3234(19)
O3	C13	1.2120(16)	C15	C16	1.5671(17)
O7	C24	1.2048(17)	C8	C9	1.5145(16)
O2	C1	1.3517(17)	C25	C19	1.5431(16)
O2	C5	1.4798(15)	C2	C3	1.3253(19)
O1	C1	1.2101(17)	C19	C18	1.5381(17)
O4	C18	1.2064(16)	C19	C23	1.5467(17)
C13	C12	1.4927(18)	C9	C4	1.5451(16)
C13	C4	1.5405(16)	C18	C16	1.5324(17)
C24	C25	1.5145(16)	C3	C4	1.5150(17)
C11	C10	1.5311(15)	C23	C22	1.5010(18)
C11	C25	1.5672(16)	C16	C17	1.5190(17)
C11	C12	1.5488(16)	C4	C5	1.5791(16)
C11	C14	1.5419(16)	C6	C5	1.5315(17)
C10	C15	1.5264(16)	C5	C7	1.5166(17)
C10	C9	1.3400(18)			

Table S30 Bond Angles for **5**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C23	O6	C24	110.64(9)	C18	C19	C25	103.87(9)
C5	O2	C1	121.31(10)	C23	C19	O5	113.03(10)
C12	C13	O3	121.97(11)	C23	C19	C25	100.24(9)
C4	C13	O3	119.59(12)	C23	C19	C18	110.72(10)
C4	C13	C12	118.29(10)	C8	C9	C10	120.84(11)
O7	C24	O6	121.26(11)	C4	C9	C10	123.25(10)
C25	C24	O6	109.55(10)	C4	C9	C8	115.81(10)
C25	C24	O7	129.18(12)	C19	C18	O4	124.59(11)
C25	C11	C10	105.28(9)	C16	C18	O4	127.38(12)
C12	C11	C10	113.27(10)	C16	C18	C19	107.98(10)
C12	C11	C25	111.29(9)	C11	C12	C13	117.51(10)
C14	C11	C10	109.45(10)	C4	C3	C2	122.68(11)
C14	C11	C25	110.31(10)	C19	C23	O6	103.76(9)
C14	C11	C12	107.25(10)	C22	C23	O6	108.62(11)
C15	C10	C11	113.90(10)	C22	C23	C19	115.94(11)
C9	C10	C11	125.20(11)	C15	C16	C20	106.24(10)
C9	C10	C15	120.85(10)	C18	C16	C20	101.80(10)

O1	C1	O2	118.47(12)	C18	C16	C15	104.05(10)
C2	C1	O2	117.45(11)	C17	C16	C20	117.34(11)
C2	C1	O1	123.96(12)	C17	C16	C15	112.41(10)
C16	C20	C25	103.93(10)	C17	C16	C18	113.64(11)
C21	C20	C25	127.34(11)	C9	C4	C13	111.75(10)
C21	C20	C16	128.73(12)	C3	C4	C13	105.20(10)
C16	C15	C10	111.76(9)	C3	C4	C9	109.02(10)
C11	C25	C24	118.11(10)	C5	C4	C13	108.77(10)
C20	C25	C24	109.15(10)	C5	C4	C9	113.52(9)
C20	C25	C11	109.79(9)	C5	C4	C3	108.18(10)
C19	C25	C24	102.91(10)	C4	C5	O2	110.07(9)
C19	C25	C11	114.96(10)	C6	C5	O2	105.93(10)
C19	C25	C20	100.30(9)	C6	C5	C4	113.96(10)
C3	C2	C1	121.45(12)	C7	C5	O2	102.99(10)
C25	C19	O5	112.71(10)	C7	C5	C4	112.93(10)
C18	C19	O5	114.95(10)	C7	C5	C6	110.16(11)

Table S31 Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å2×103) for **5**.

Atom	***x***	***y***	***z***	**U(eq)**
H5	5486(3)	4904(9)	7011(18)	29.3(3)
H8	5440(30)	3663(4)	7571(3)	33.4(3)
H15a	1773.3(17)	7599.6(16)	3861.8(14)	22.1(3)
H15b	1893.4(17)	5817.2(16)	4419.1(14)	22.1(3)

H8a	4283(15)	2820(11)	3996(4)	28.3(4)
H8b	3579(10)	3938(3)	2875(12)	28.3(4)
H8c	5575(5)	2516(8)	2301(8)	28.3(4)
H2	9054.2(18)	-169.2(16)	3543.5(15)	25.6(3)
H12a	7322.5(17)	7601.7(16)	4525.9(14)	22.0(3)
H12b	7689.3(17)	7382.7(16)	2837.3(14)	22.0(3)
H3	7818.2(17)	2424.7(16)	4782.0(13)	21.8(3)
H14a	5183(13)	8576(4)	2162.0(15)	30.4(4)
H14b	3218(3)	9501(10)	3425(9)	30.4(4)
H14c	4924(14)	9951(7)	3354(9)	30.4(4)
H23	1865.5(18)	8709.0(17)	8849.4(14)	24.7(3)
H17a	-1387(4)	8442(14)	7810(4)	35.5(4)
H17b	-1449(3)	8758(12)	6234(9)	35.5(4)
H17c	-1023.8(18)	6917(3)	6712(12)	35.5(4)
H26a	5509(18)	1190(8)	9169(4)	37.4(4)
H26b	6810(7)	2141(16)	9214(5)	37.4(4)
H26c	4658(11)	3139(8)	9734.9(15)	37.4(4)
H6a	11322(5)	2359(12)	1546(10)	36.1(4)
H6b	11573(3)	2742(15)	-89(4)	36.1(4)
H6c	10983(3)	4225(4)	1140(13)	36.1(4)
H7a	8810(10)	4392(8)	-650.1(15)	35.3(4)
H7b	6794(6)	4896(12)	579(10)	35.3(4)
H7c	8088(16)	5849(4)	638(10)	35.3(4)
H22a	5186(3)	6694(14)	9185(4)	45.7(5)
H22b	3523(16)	8100(3)	10417(7)	45.7(5)
H22c	3268(14)	6466(12)	9958(10)	45.7(5)

H21a	-640(30)	11260(20)	6598(19)	19(4)
H21b	1210(30)	11720(20)	6400(20)	27(4)

Figure S1. HRESIMS spectrum of **1**

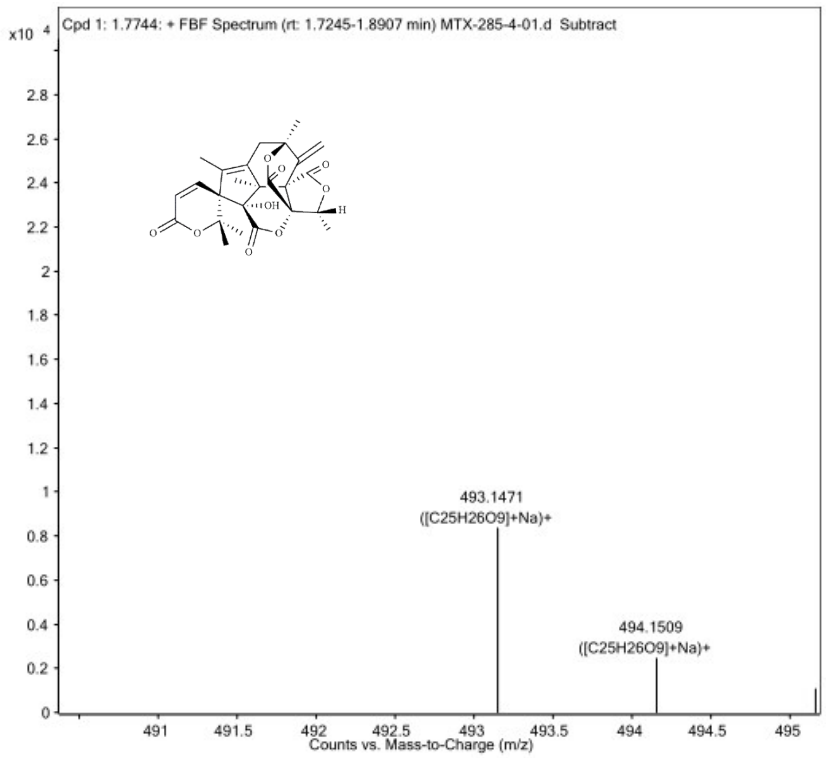


Figure S2. ^{1}H NMR spectrum of **1** in DMSO-d_6.

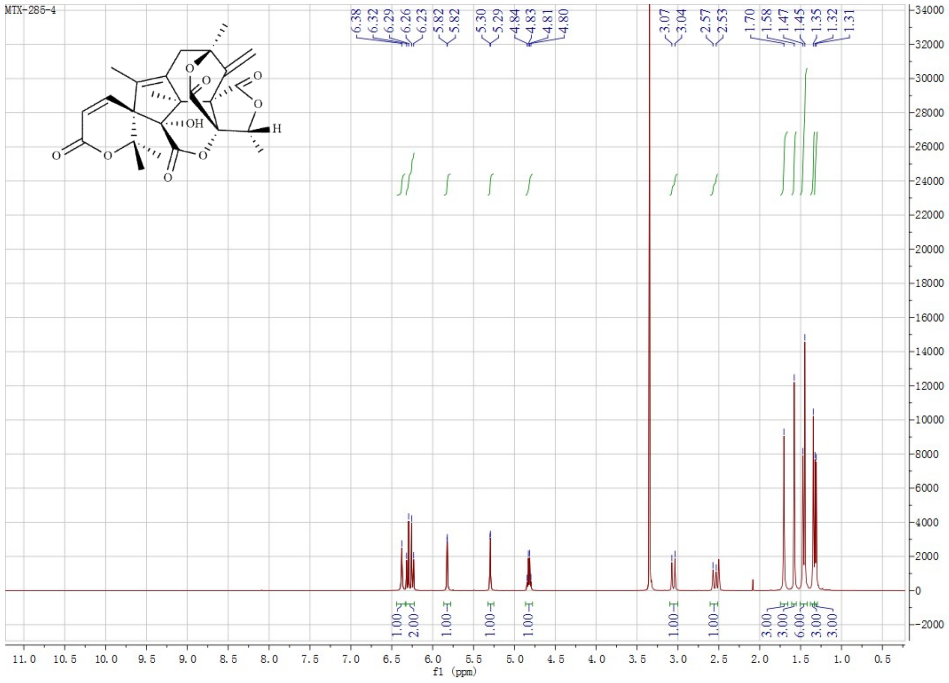


Figure S3. ^{13}C NMR spectrum of **1** in DMSO-d_6

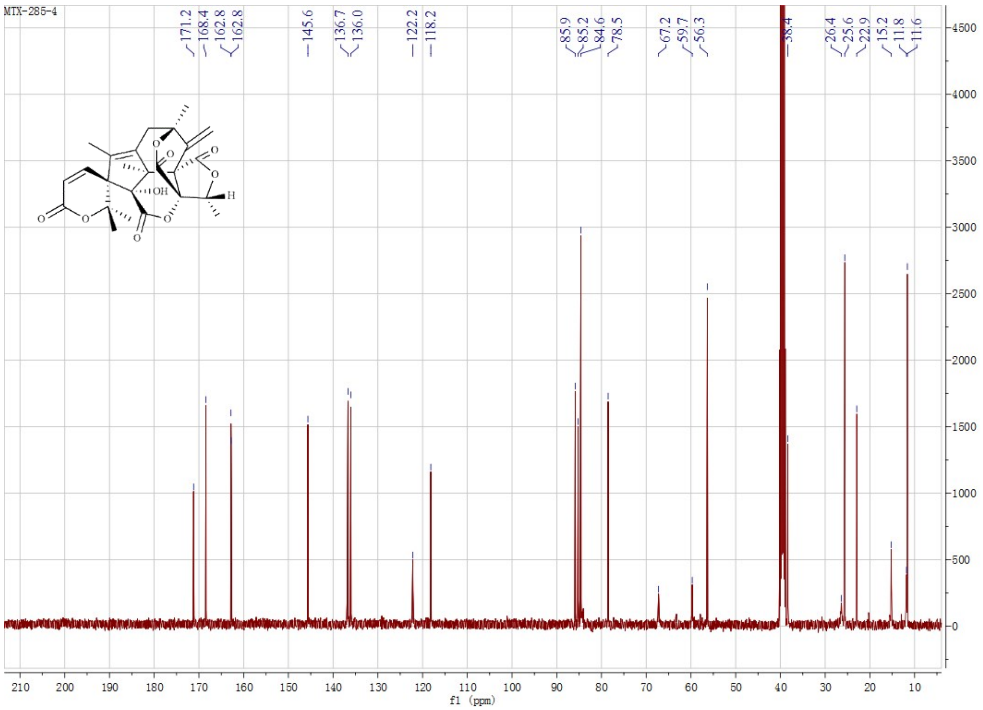


Figure S4. COSY spectrum of **1** in DMSO-d_6

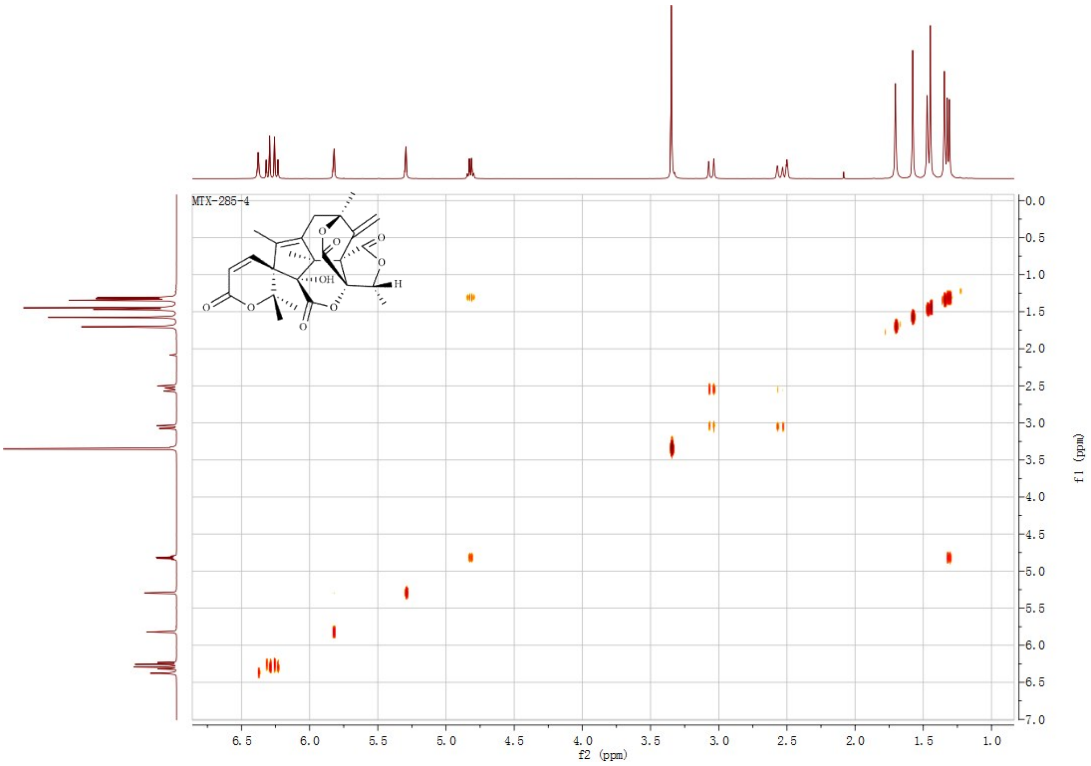


Figure S5. HSQC spectrum of **1** in DMSO-d_6.

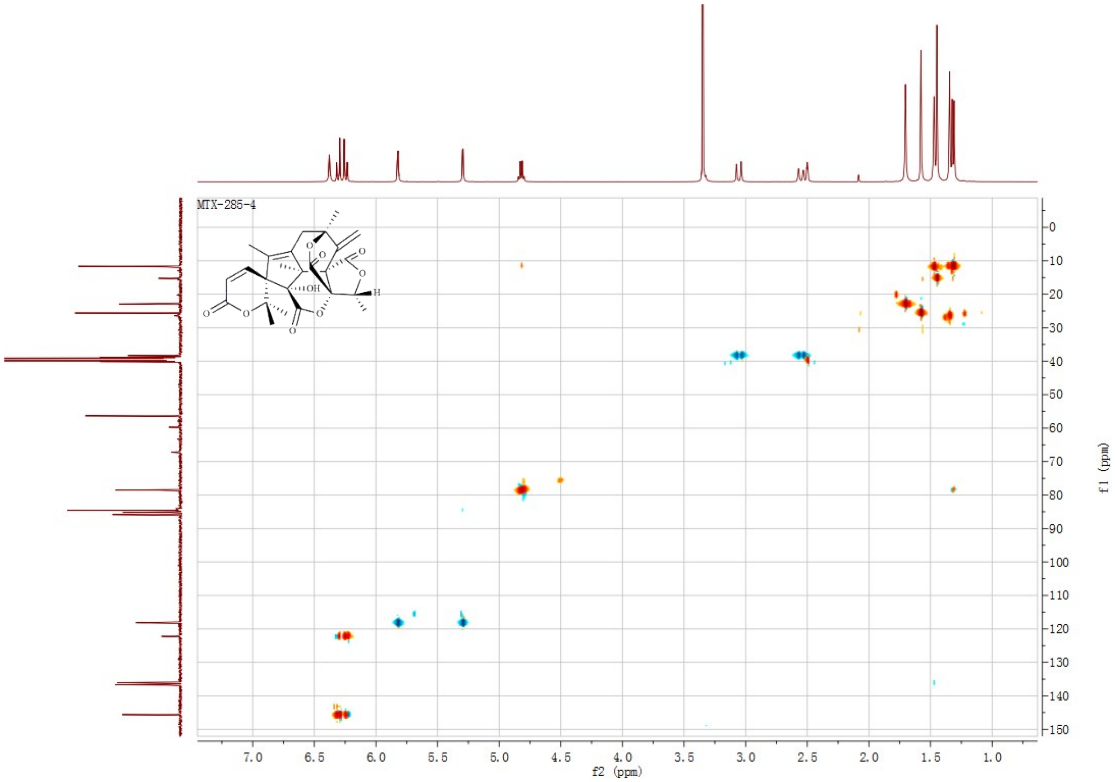


Figure S6. HMBC spectrum of **1** in DMSO-d_6.

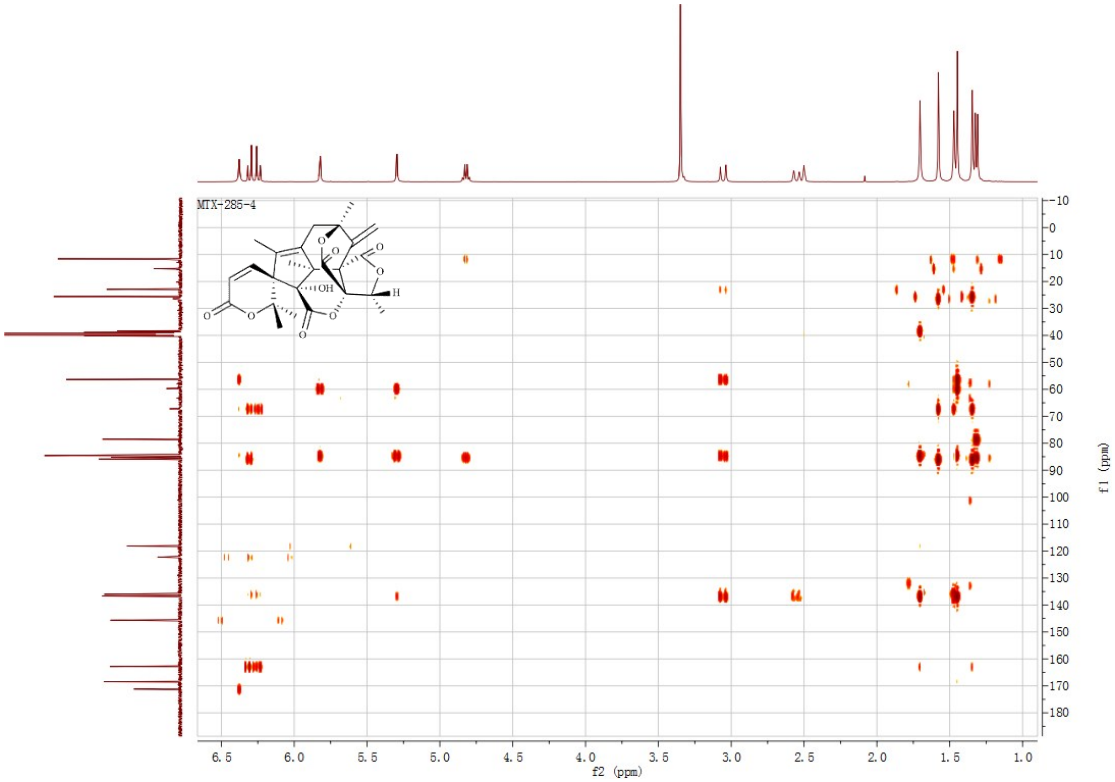


Figure S7. NOESY spectrum of **1** in DMSO-d_6.

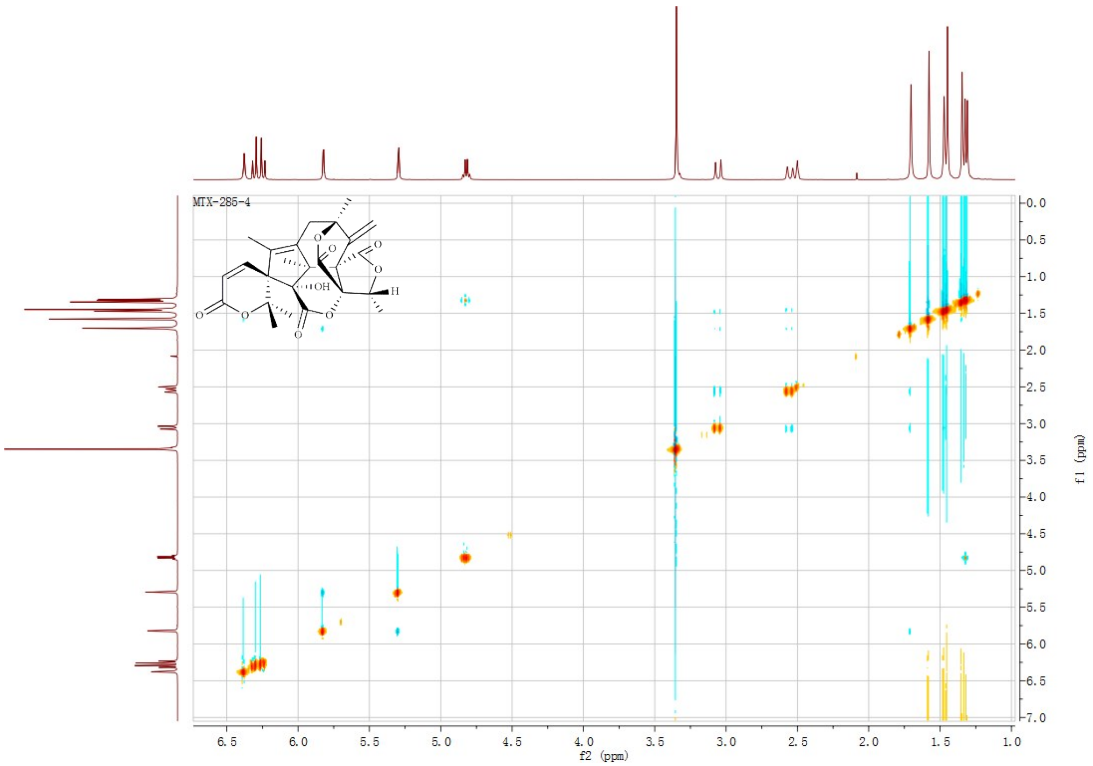


Figure S8. IR data of **1** in KBr

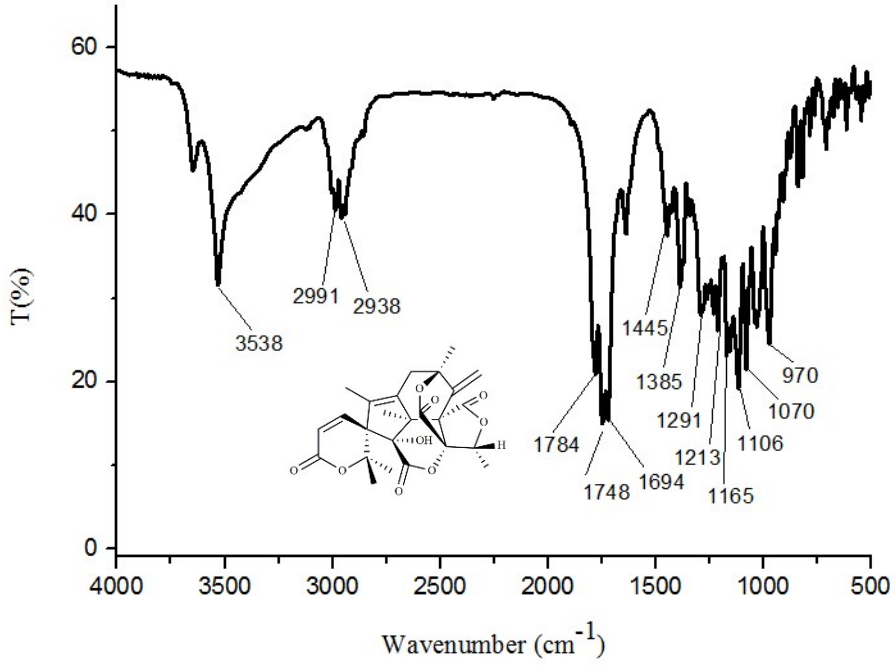


Figure S9. X-ray ORTEP drawing of **1**

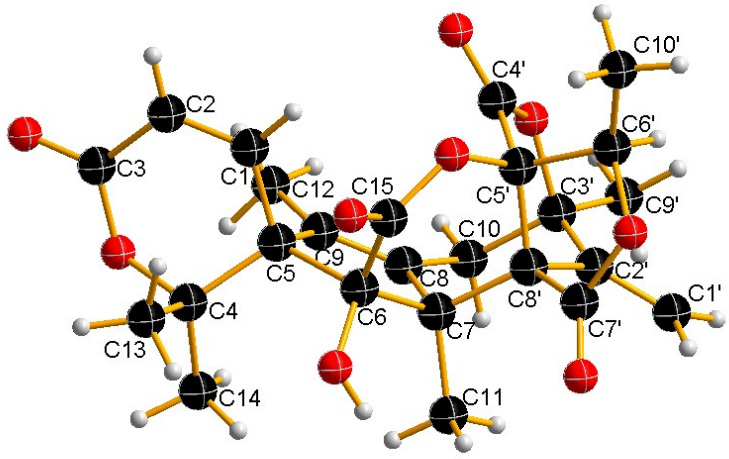


Figure S10. HRESIMS spectrum of **2**

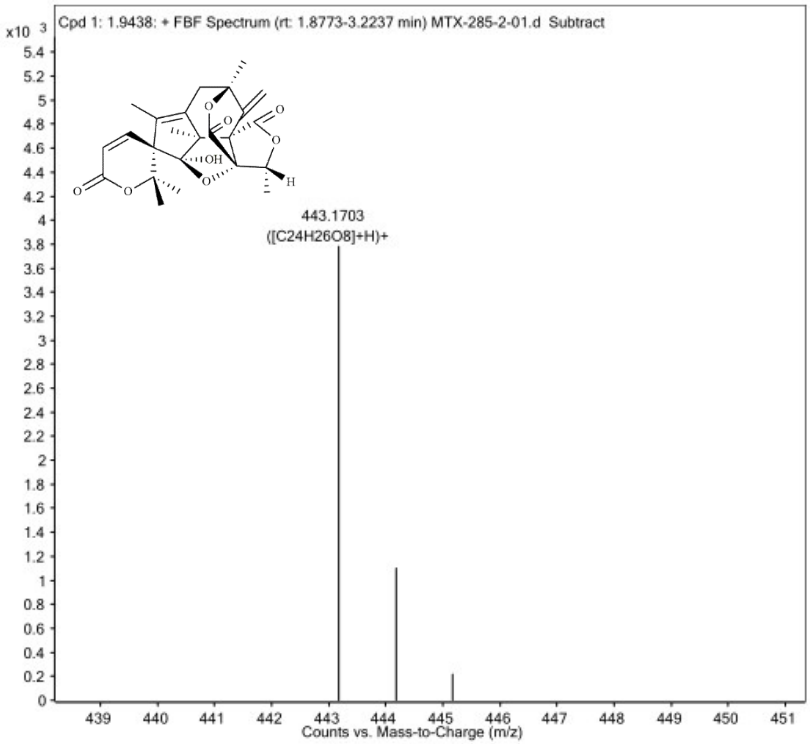


Figure S11. ^{1}H NMR spectrum of **2** in acetone-d_6.

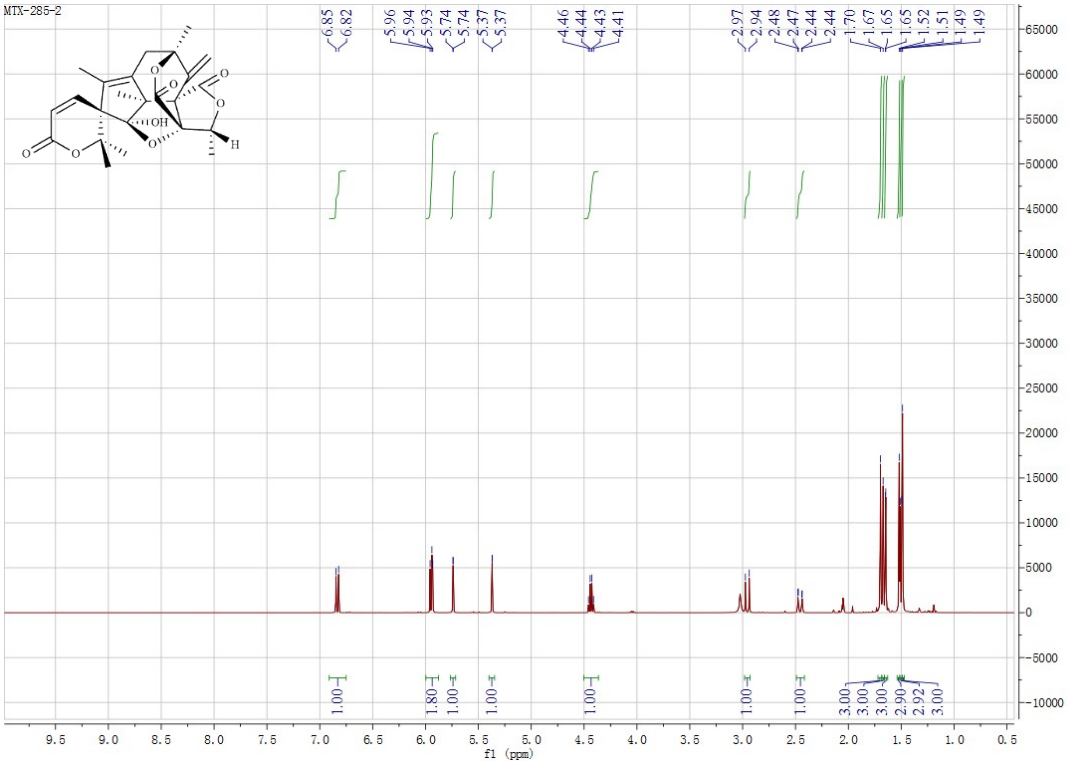


Figure S12. ^{13}C NMR spectrum of **2** in acetone-d_6.

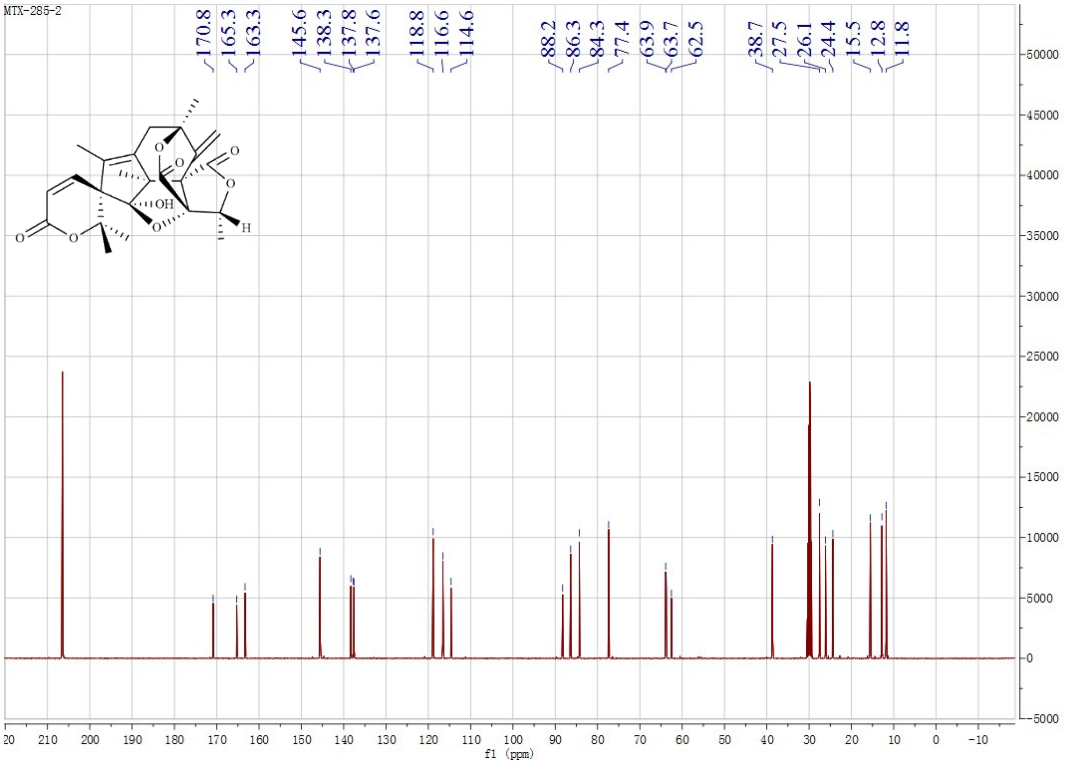


Figure S13. COSY spectrum of **2** in acetone-d_6

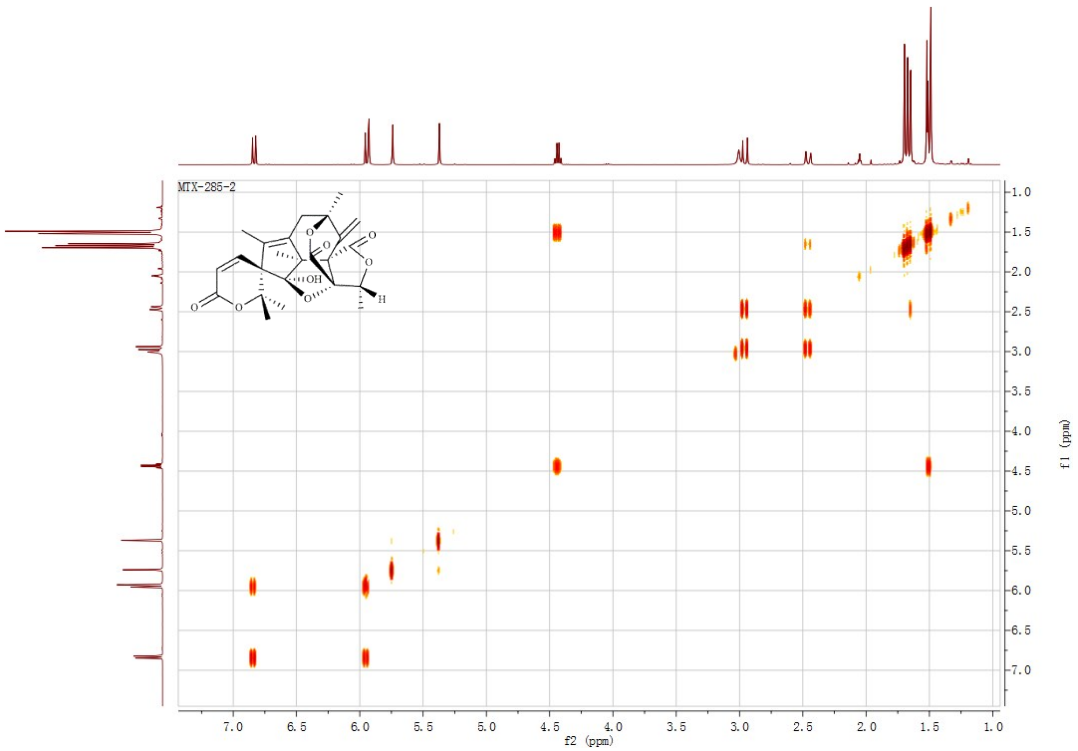


Figure S14. HSQC spectrum of **2** in acetone-d_6

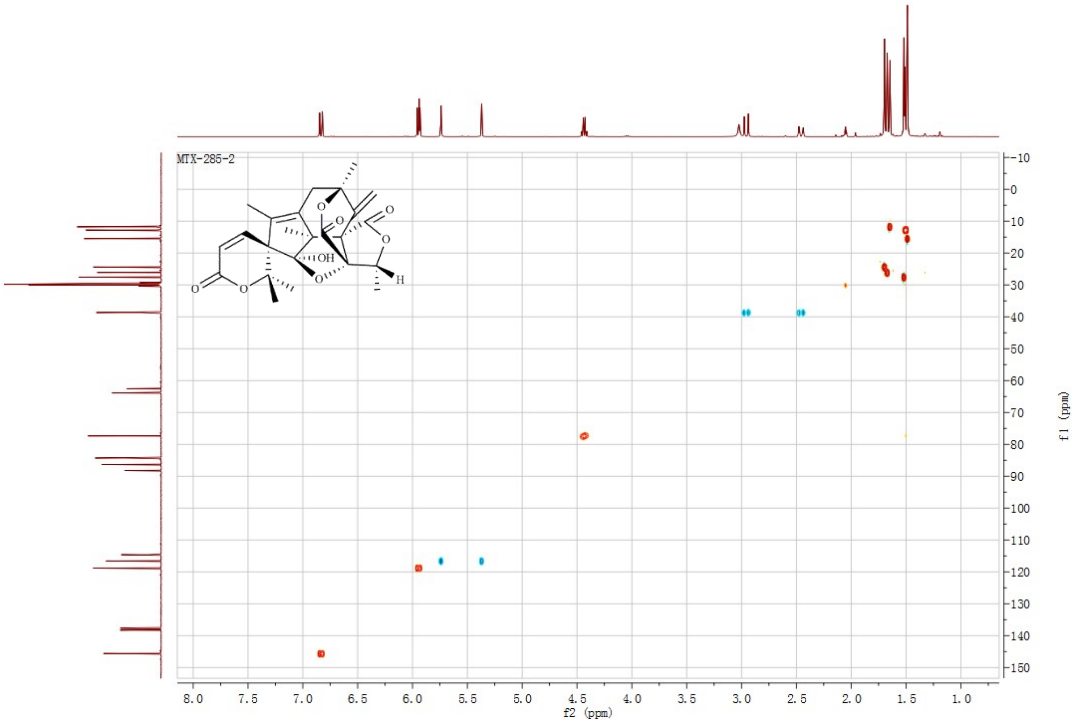


Figure S15. HMBC spectrum of **2** in acetone-d_6

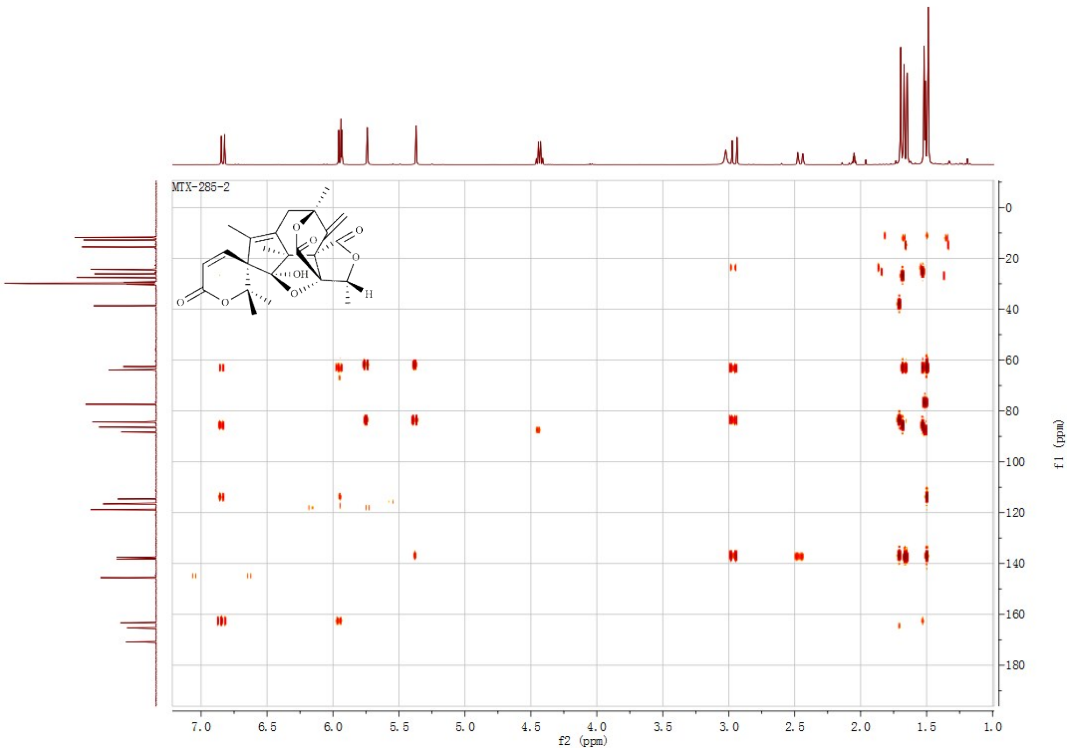


Figure S16. NOESY spectrum of **2** in acetone-d_6

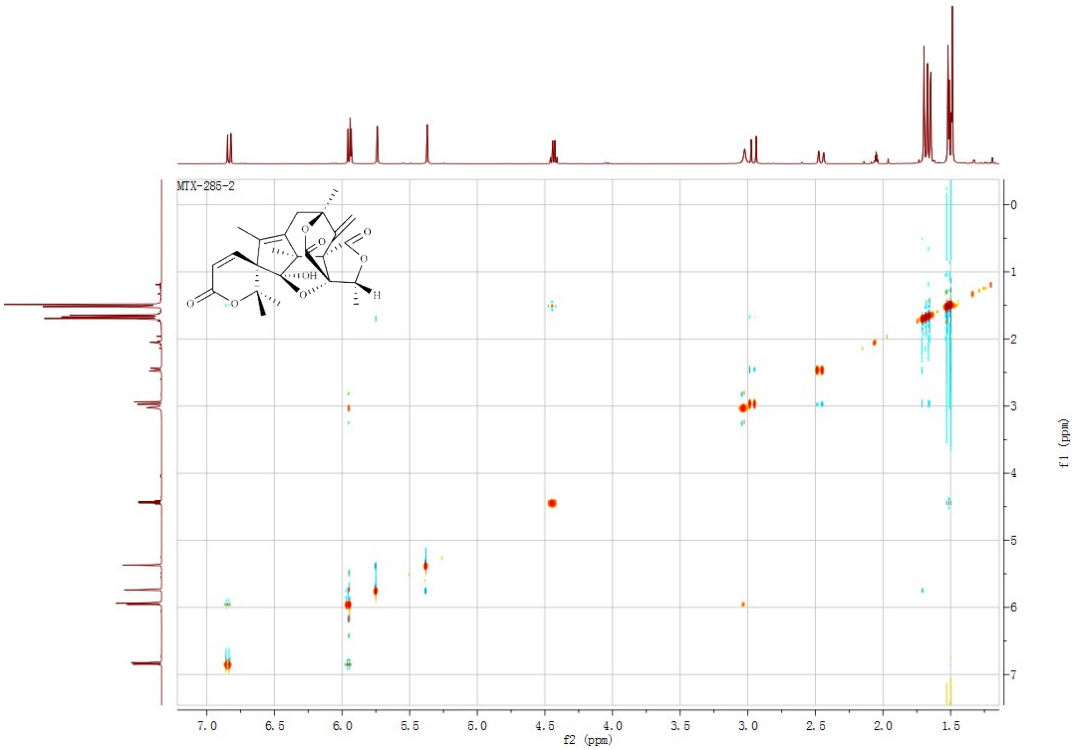


Figure S17. IR data of **2** in KBr

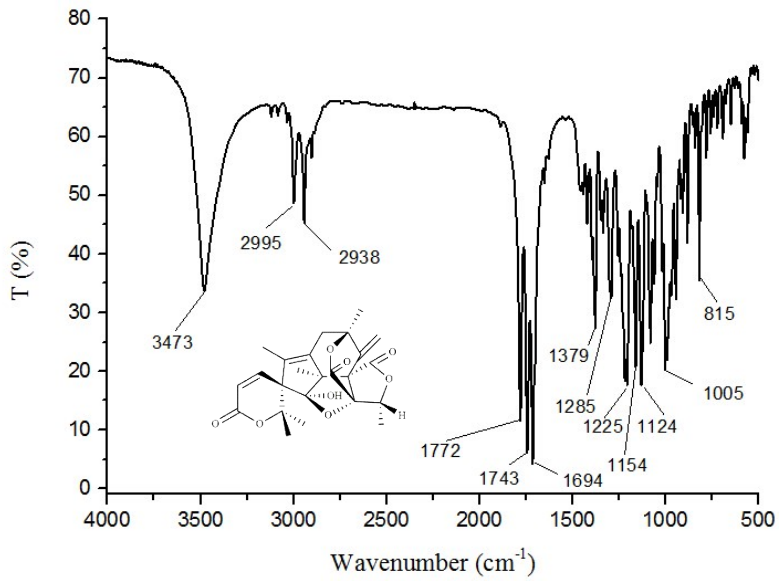


Figure S18. X-ray ORTEP drawing of **2**.

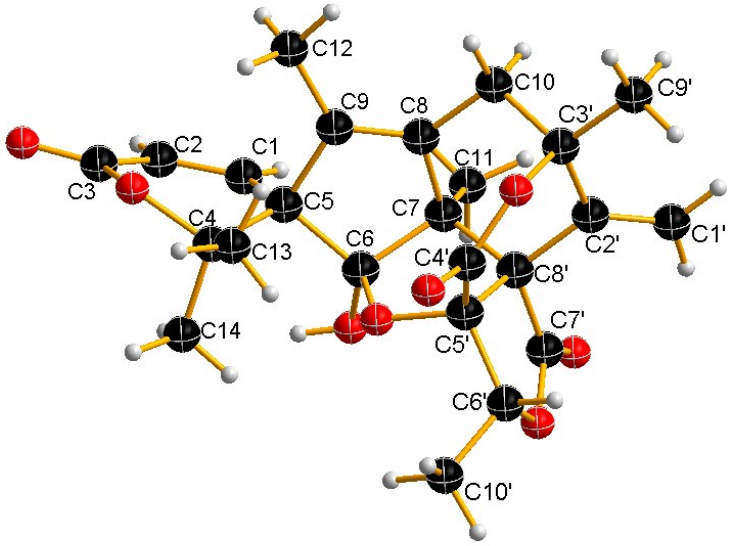


Figure S19. HRESIMS spectrum of **3**

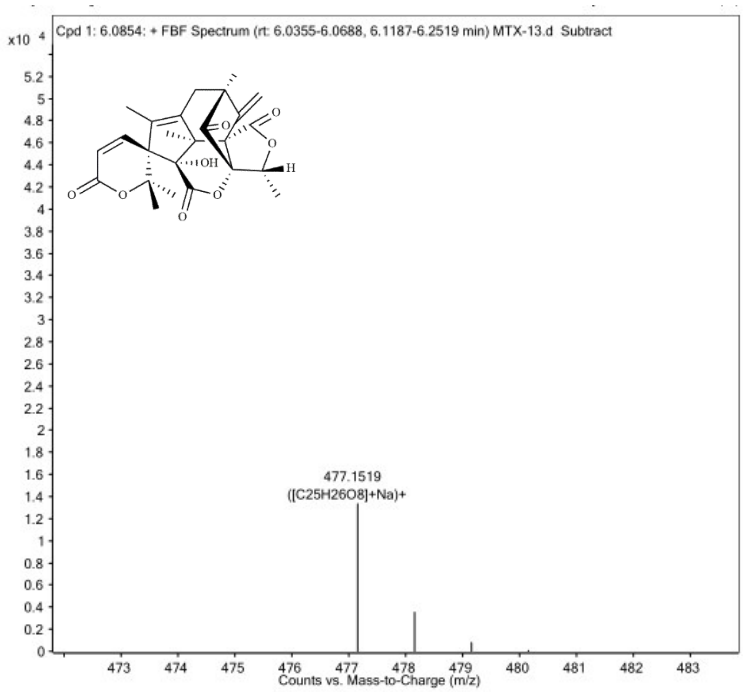


Figure S20. ^{1}H NMR spectrum of **3** in DMSO-d_6.

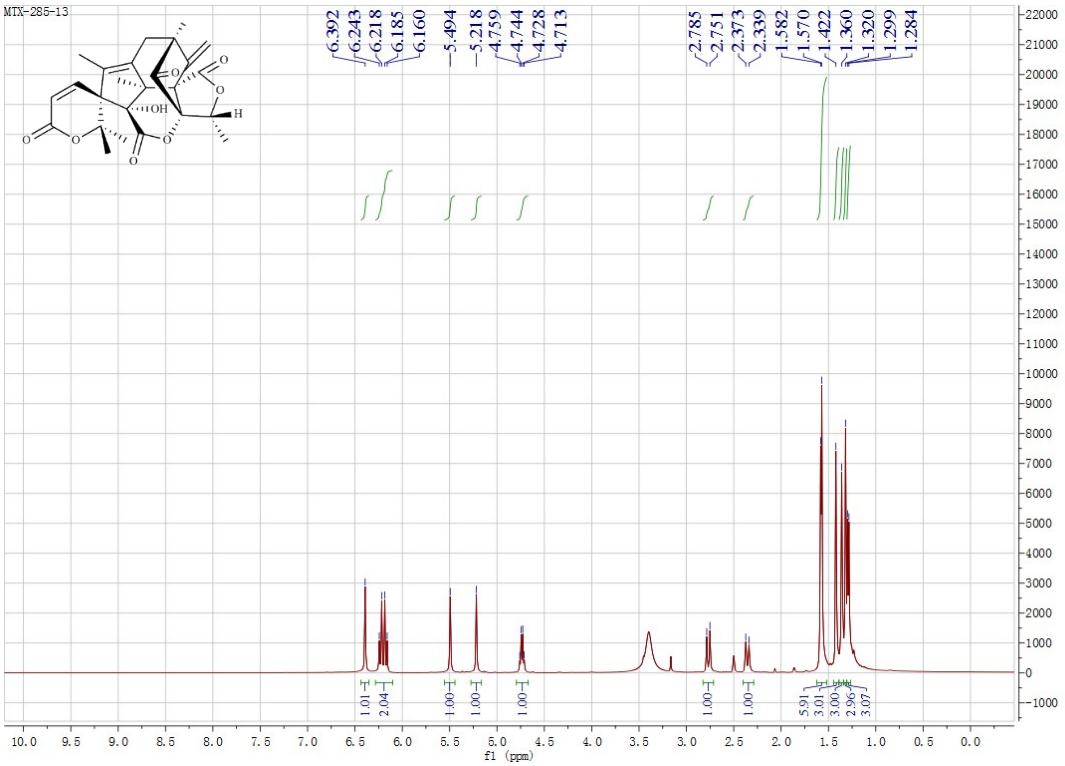


Figure S21. ^{13}C NMR spectrum of **3** in DMSO-d_6

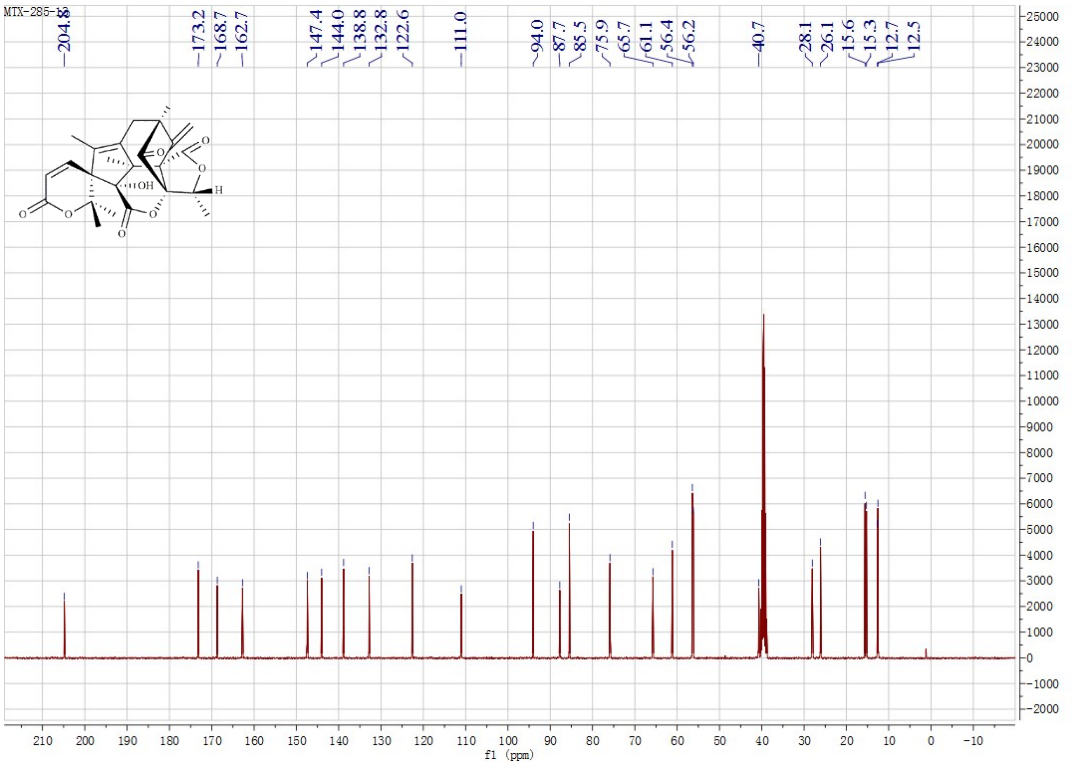


Figure S22. COSY spectrum of **3** in DMSO-d_6.

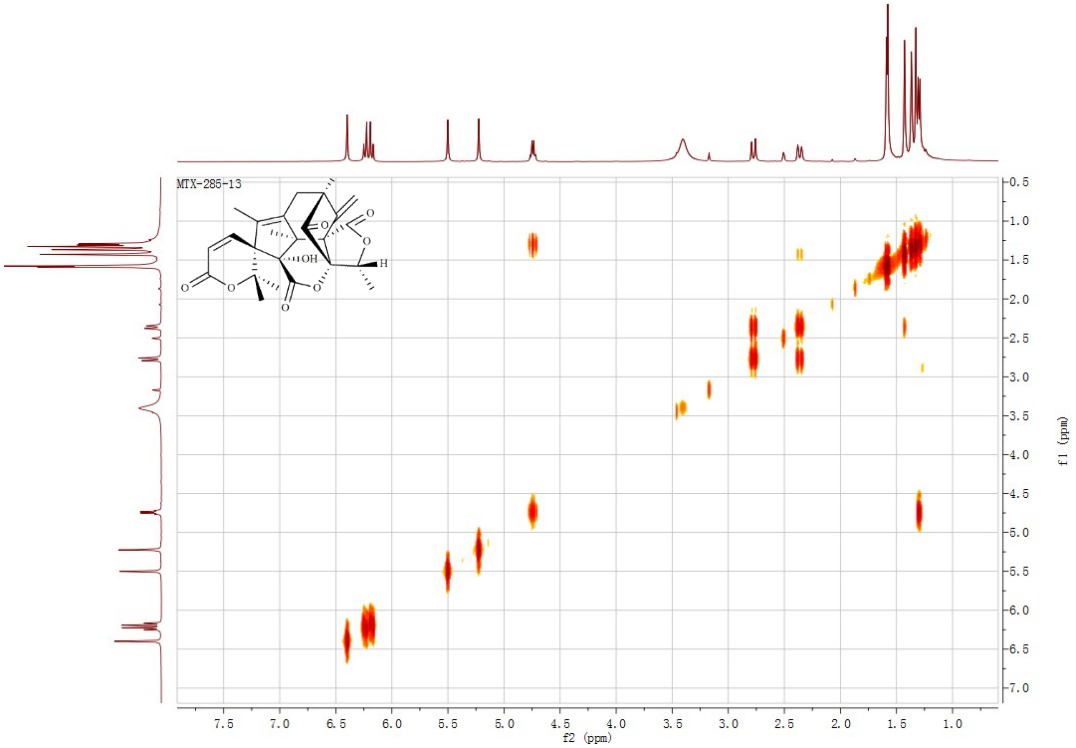


Figure S23. HSQC spectrum of **3** in DMSO-d_6.

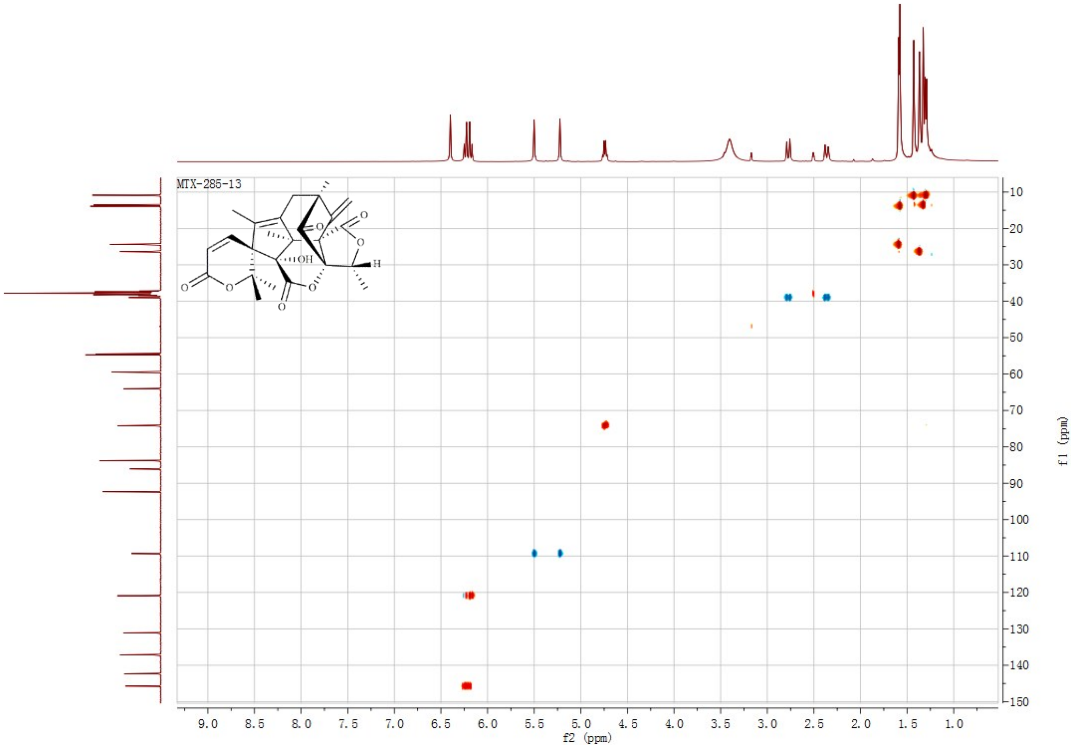


Figure S24. HMBC spectrum of **3** in DMSO-d_6

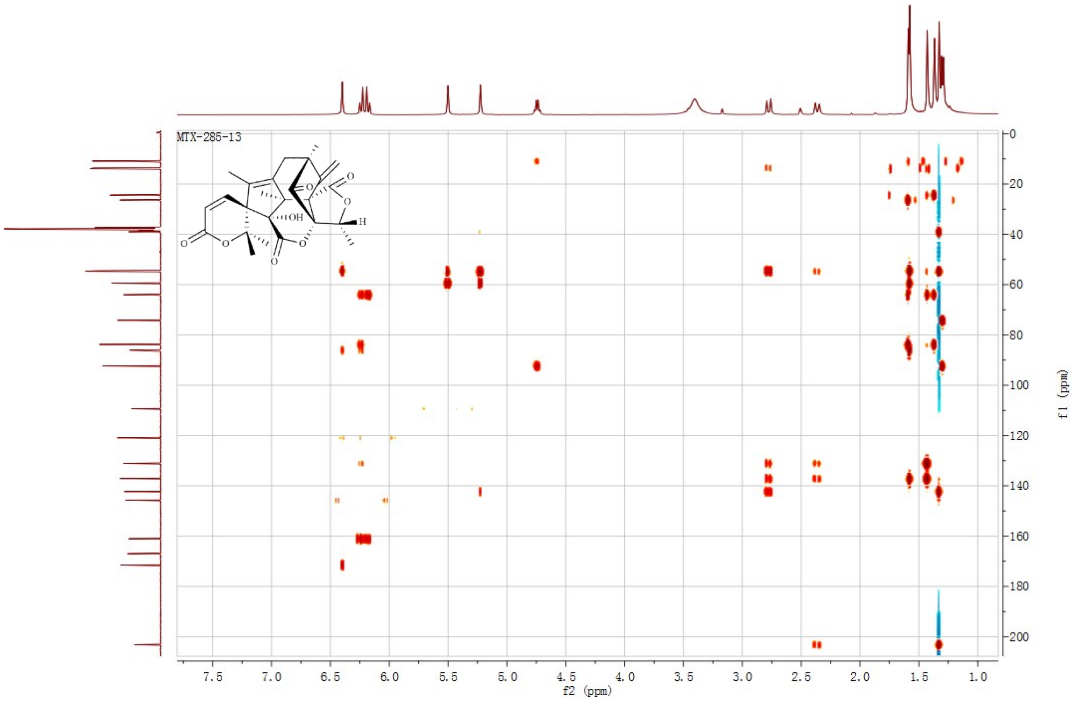


Figure S25. NOESY spectrum of **3** in DMSO-d_6

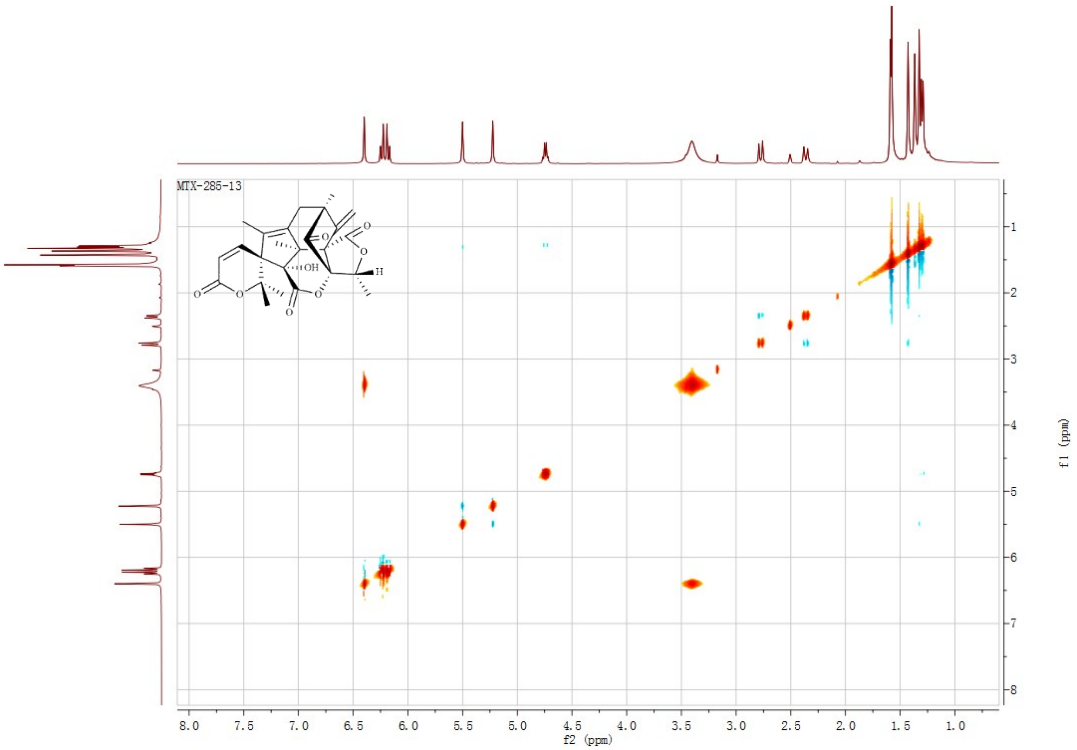


Figure S26. IR data of **3** in KBr

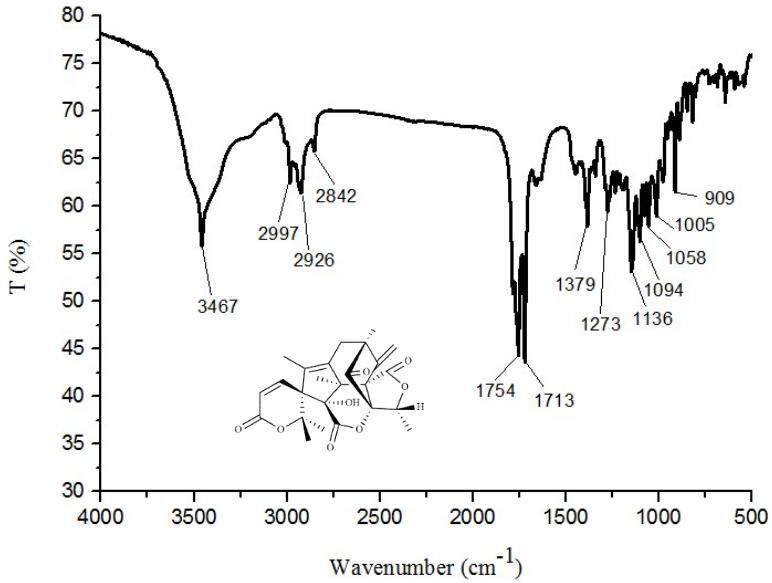


Figure S27. X-ray ORTEP drawing of **3**

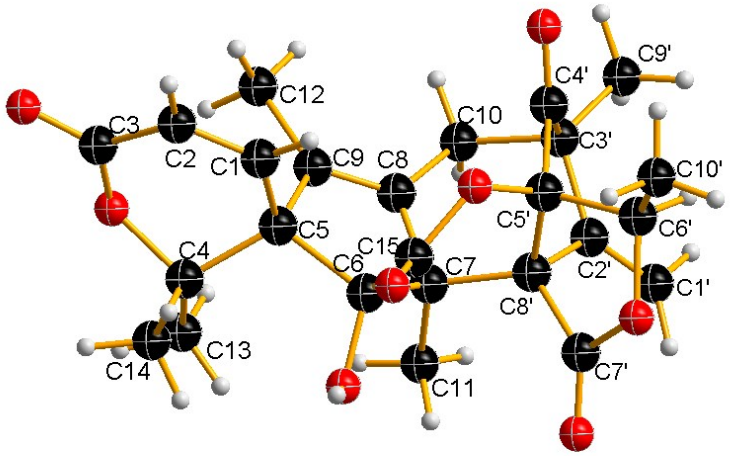


Figure S28. HRESIMS spectrum of **4**

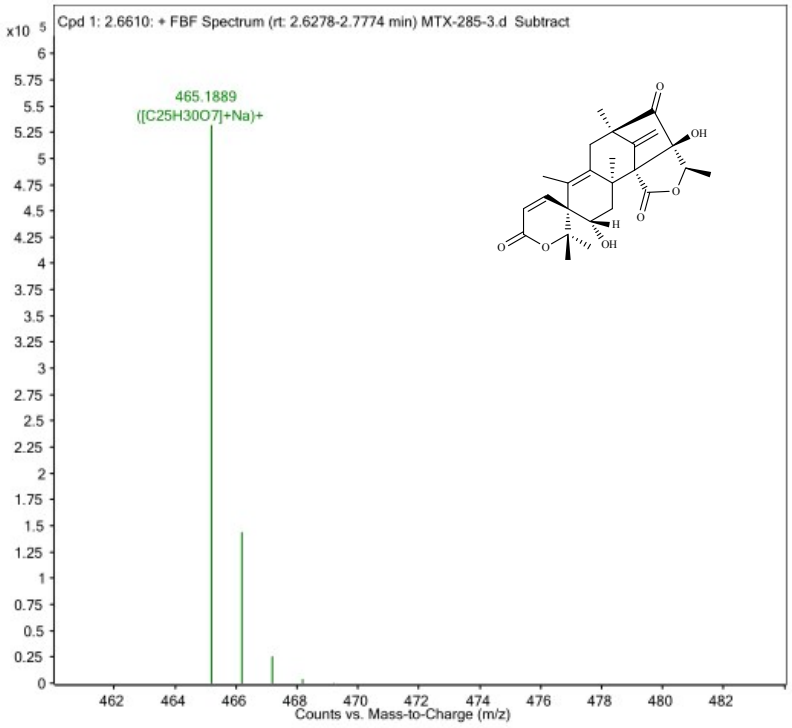


Figure S29. ^{1}H NMR spectrum of **4** in DMSO-d_6.

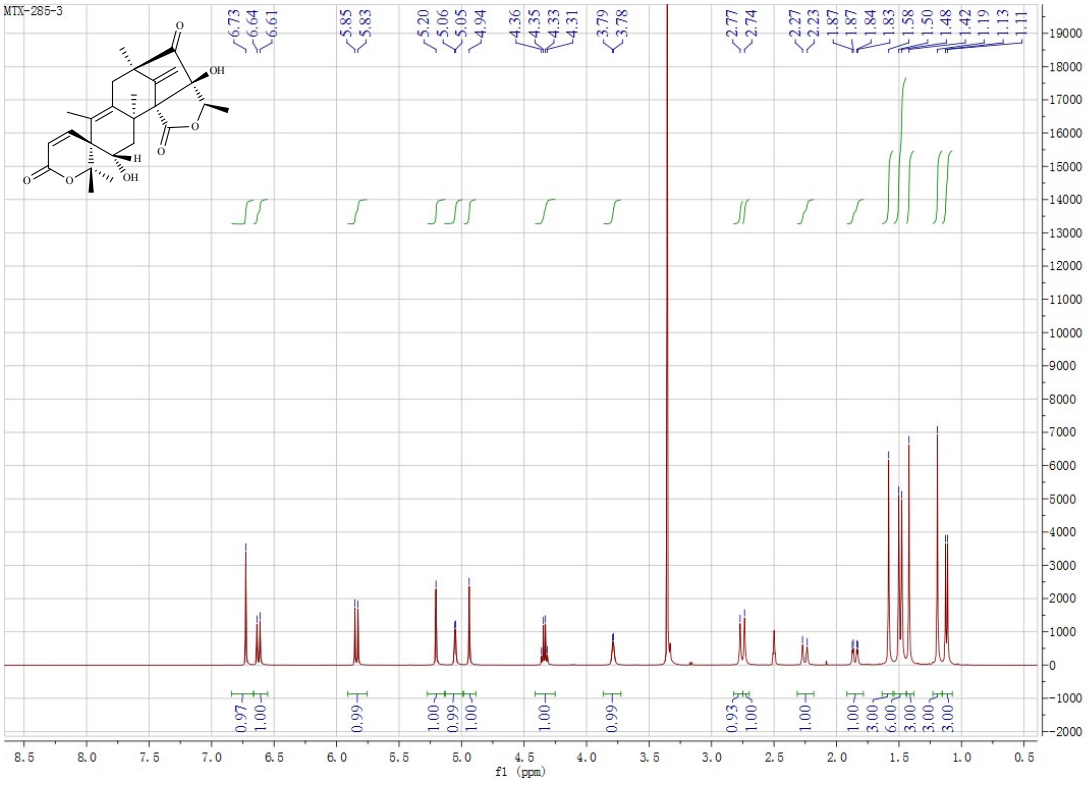


Figure S30. ^{13}C NMR spectrum of **4** in DMSO-d_6.

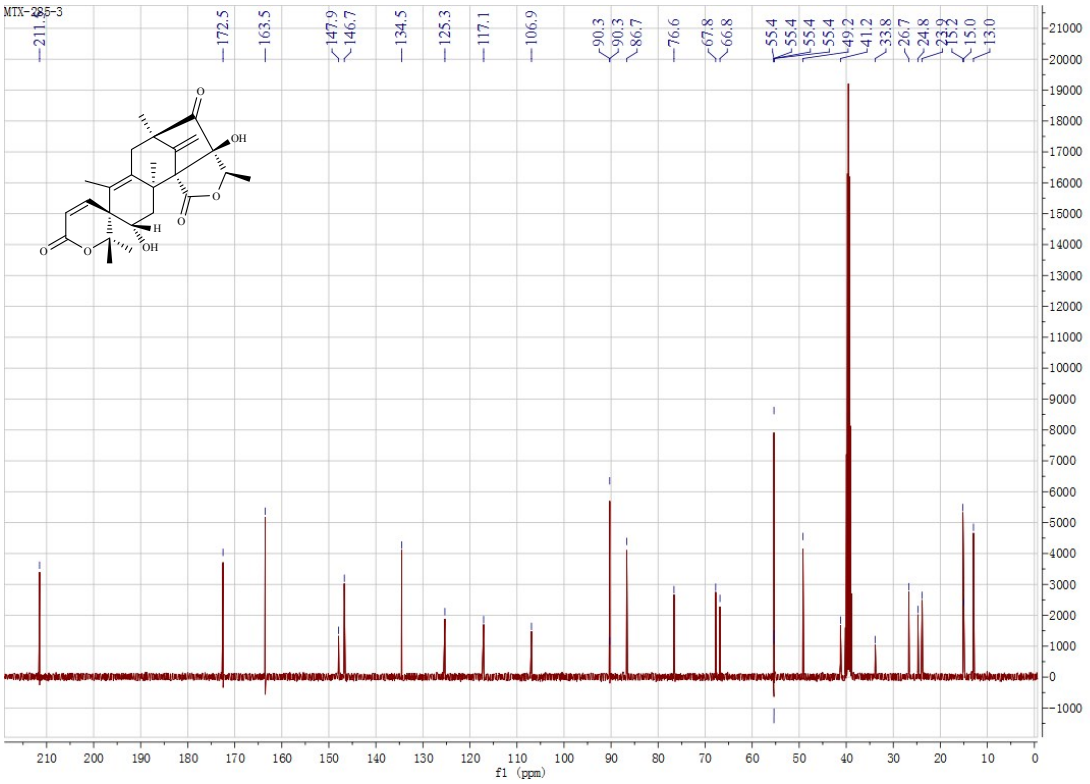


Figure S31. COSY spectrum of **4** in DMSO-d_6.

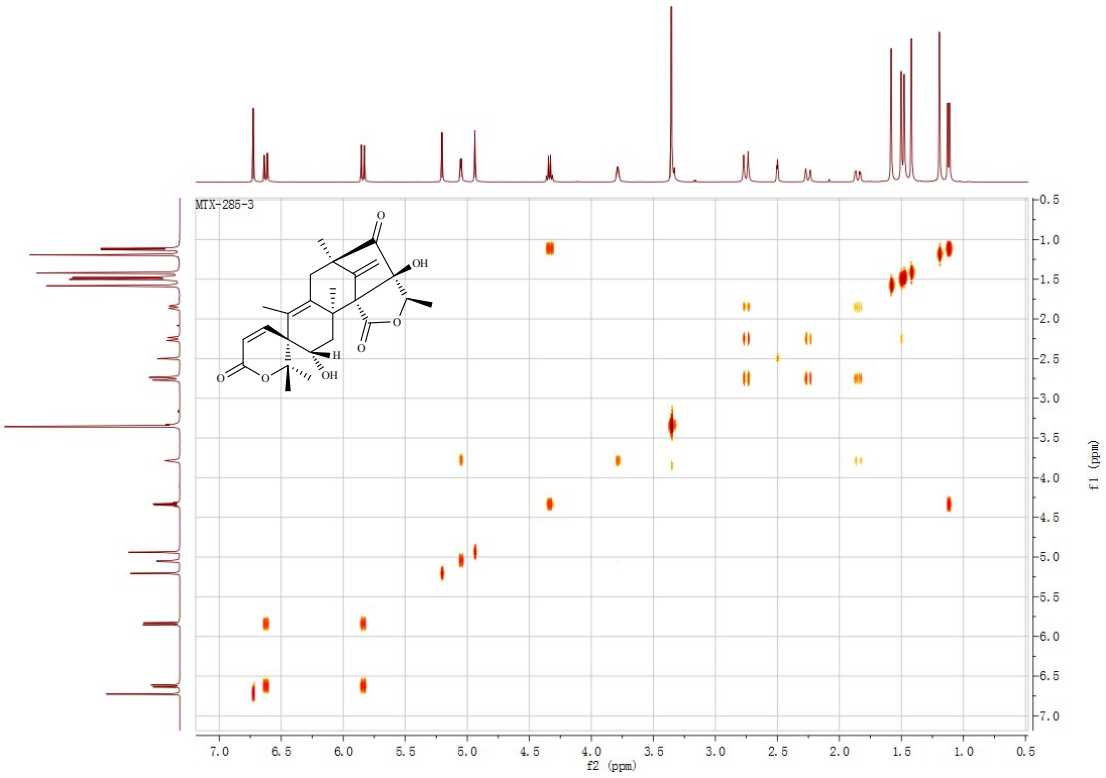


Figure S32. HSQC spectrum of **4** in DMSO-d_6.

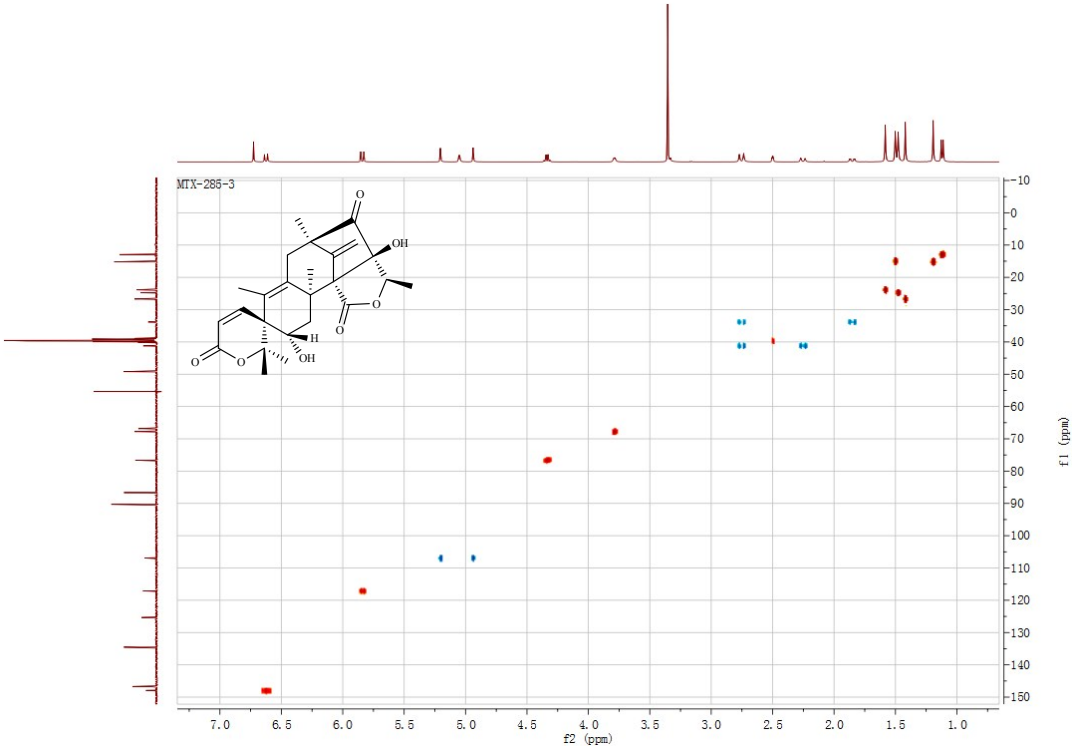


Figure S33. HMBC spectrum of **4** in DMSO-d_6.

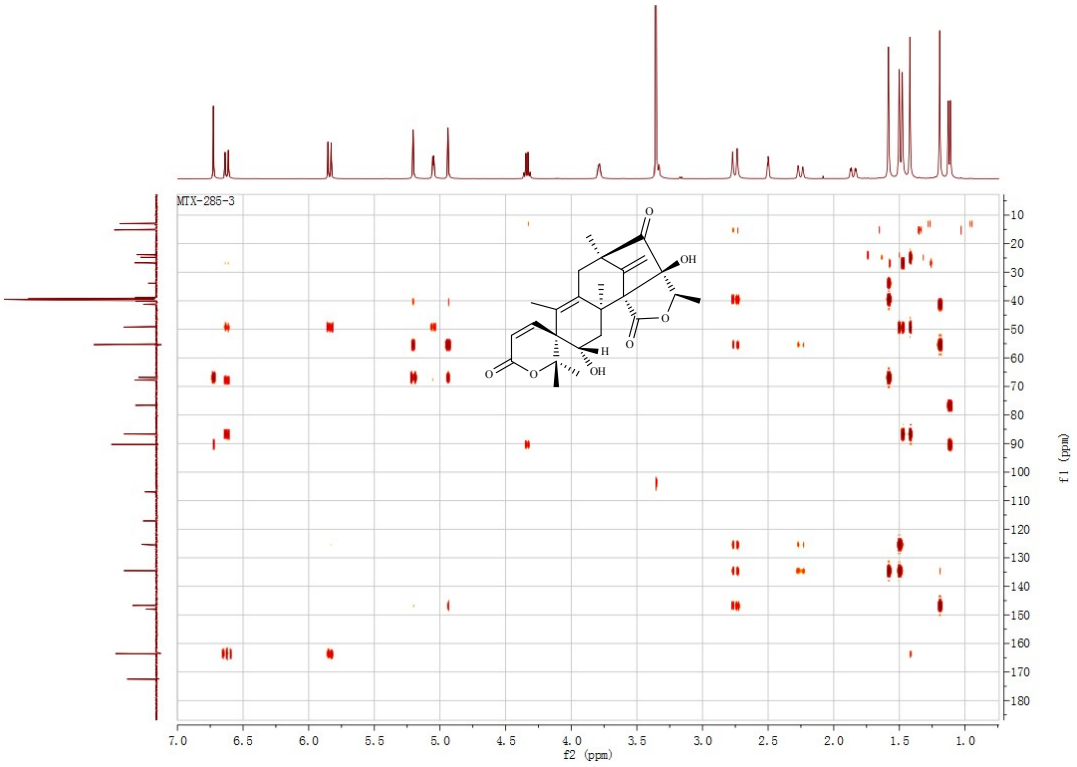


Figure S34. NOESY spectrum of **4** in DMSO-d_6

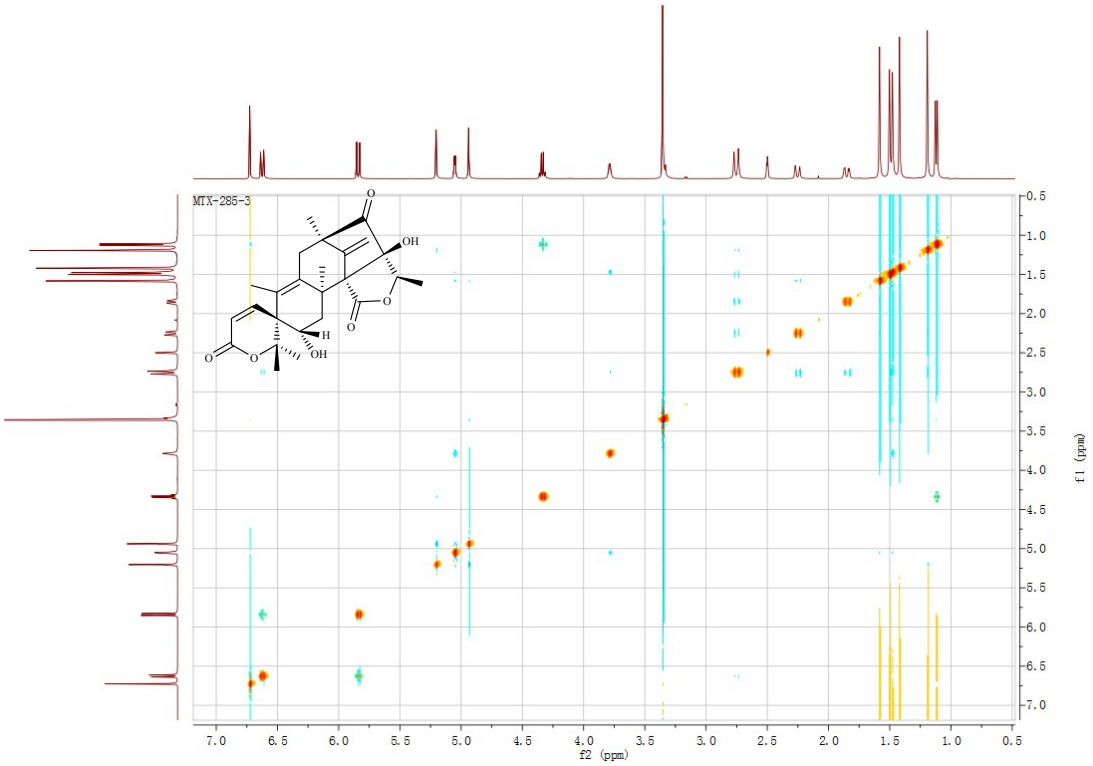


Figure S35.IR data of **4** in KBr

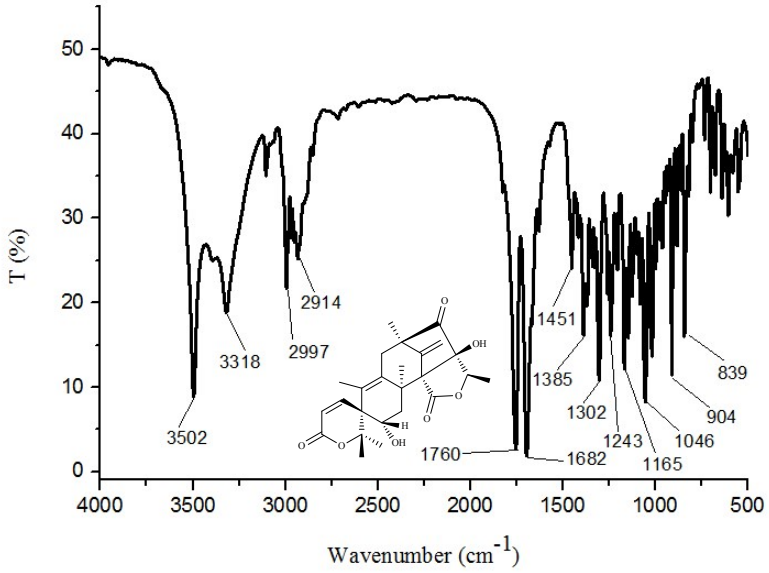


Figure S36. X-ray ORTEP drawing of **4**

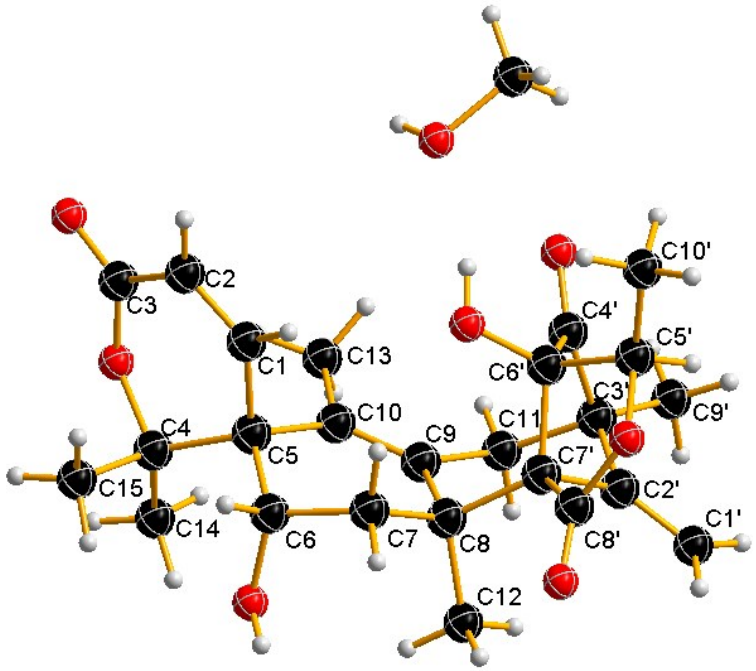


Figure S37. HRESIMS spectrum of **5**

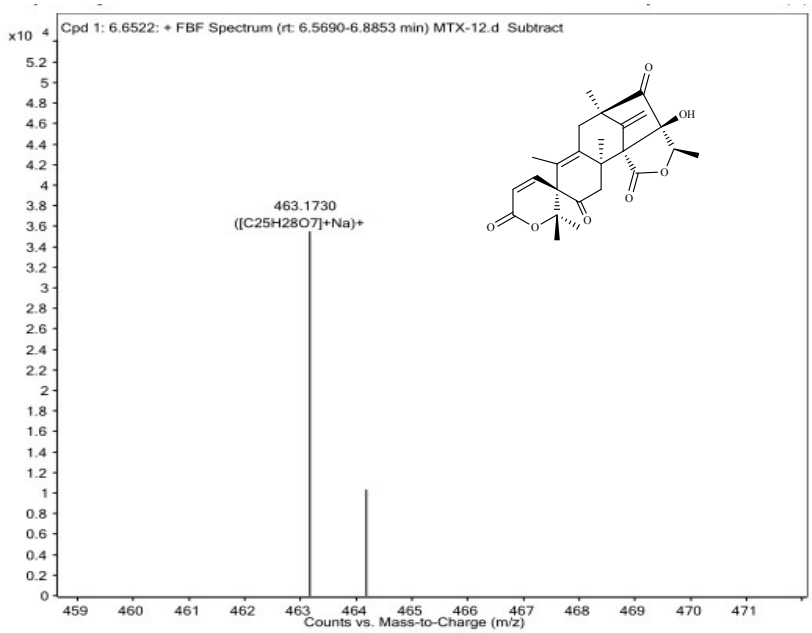


Figure S38. ^{1}H NMR spectrum of **5** in DMSO-d_6.

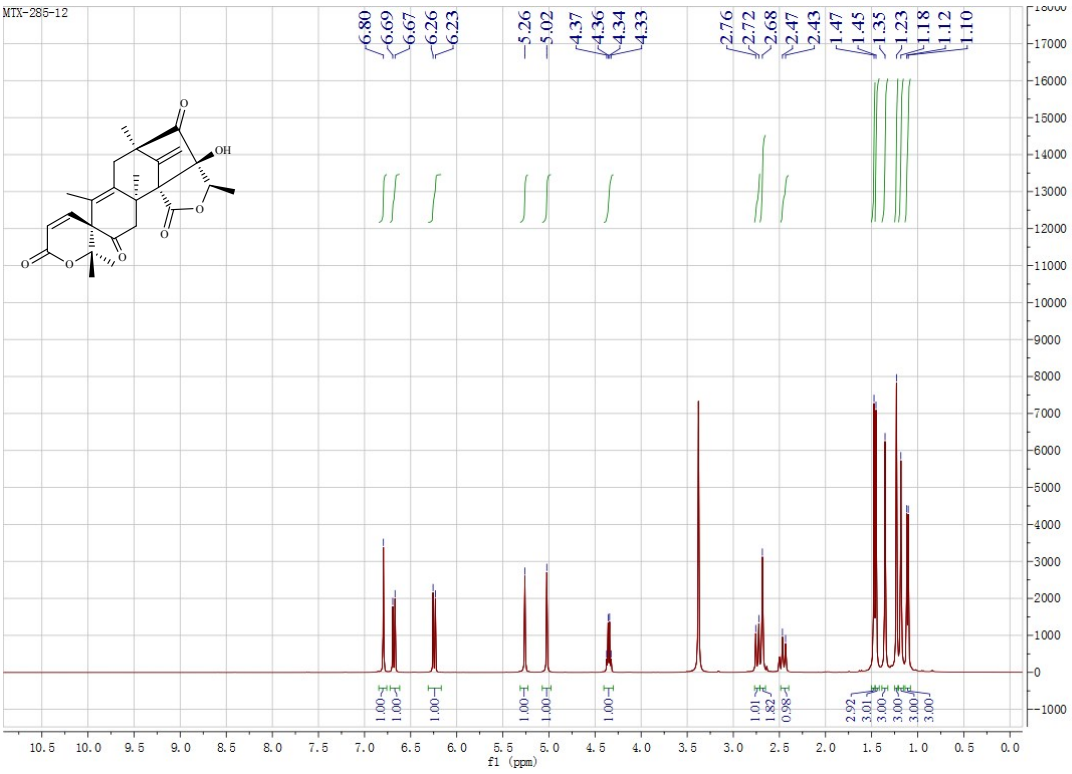


Figure S39. ^{13}C NMR spectrum of **5** in DMSO-d_6

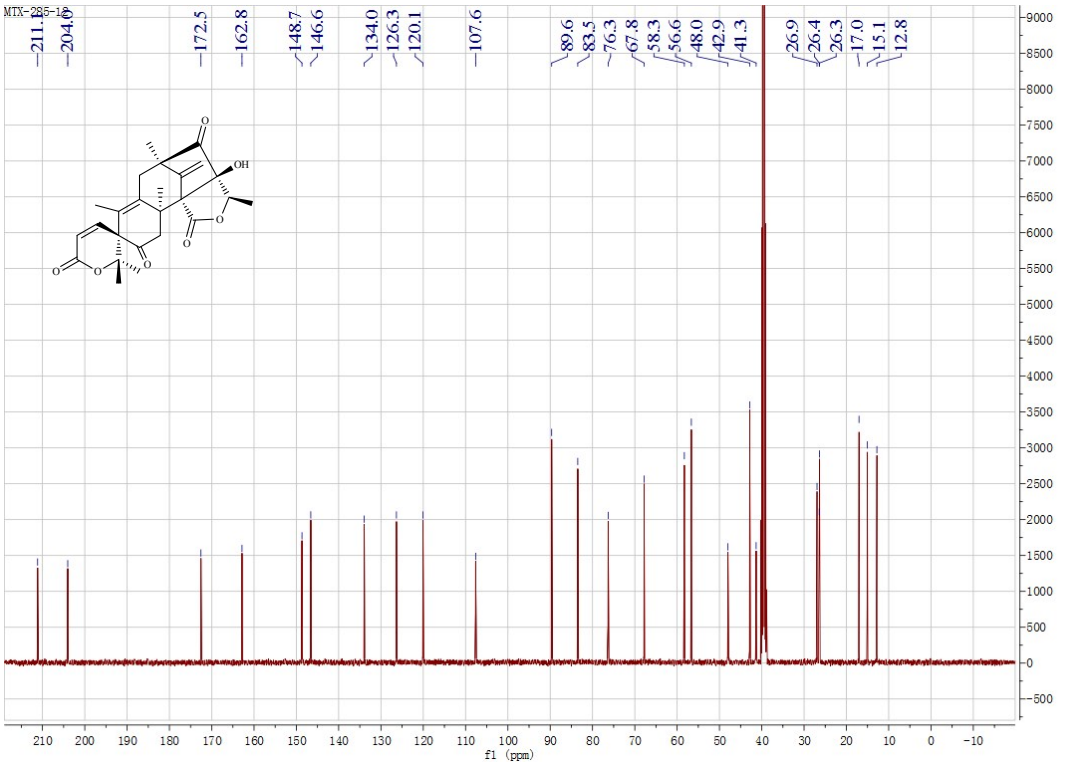


Figure S40. COSY spectrum of **5** in DMSO-d_6.

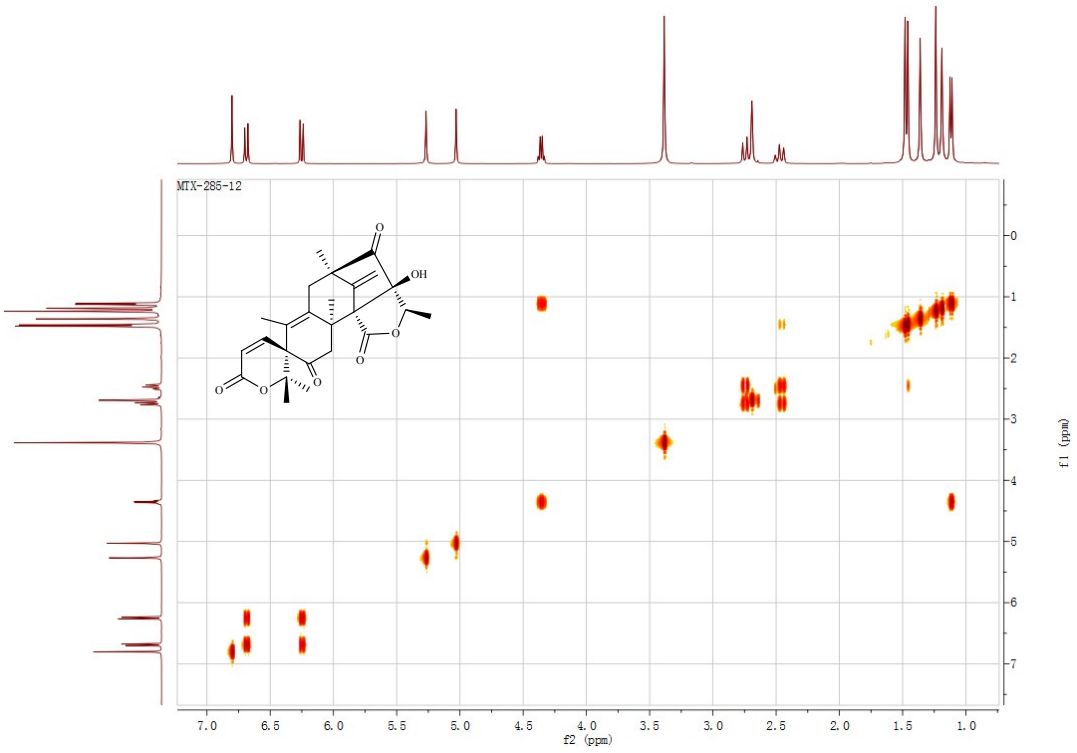


Figure S41. HSQC spectrum of **5** in DMSO-d_6.

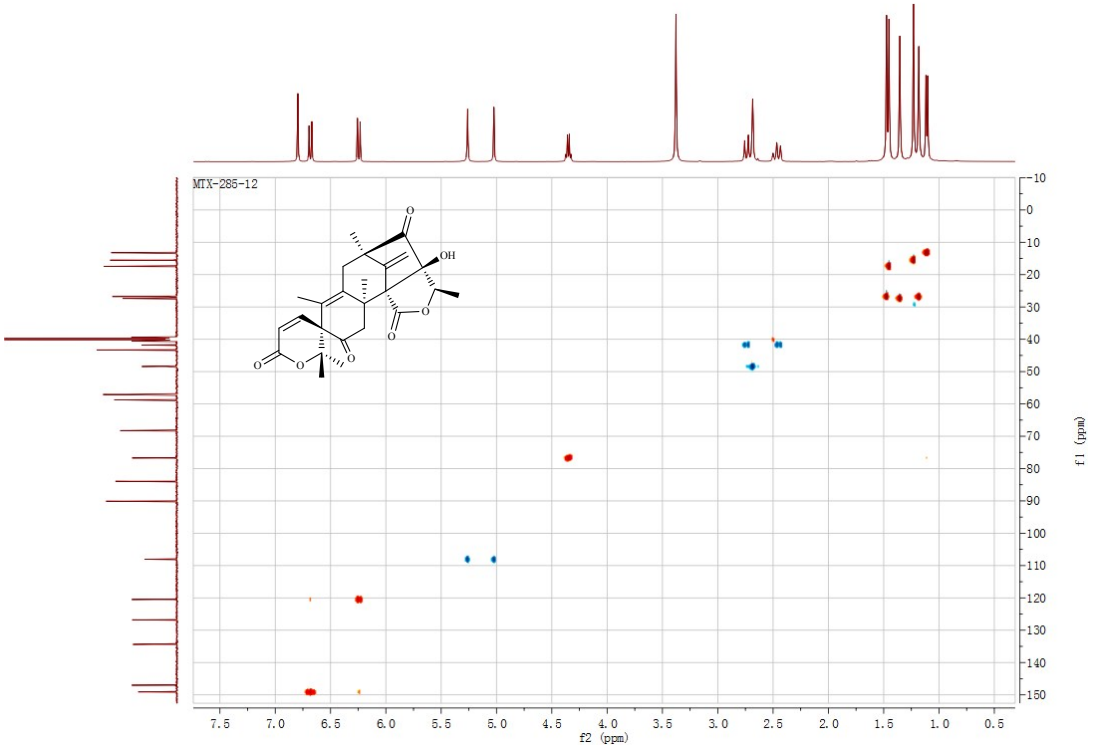


Figure S42. HMBC spectrum of **5** in DMSO-d_6.

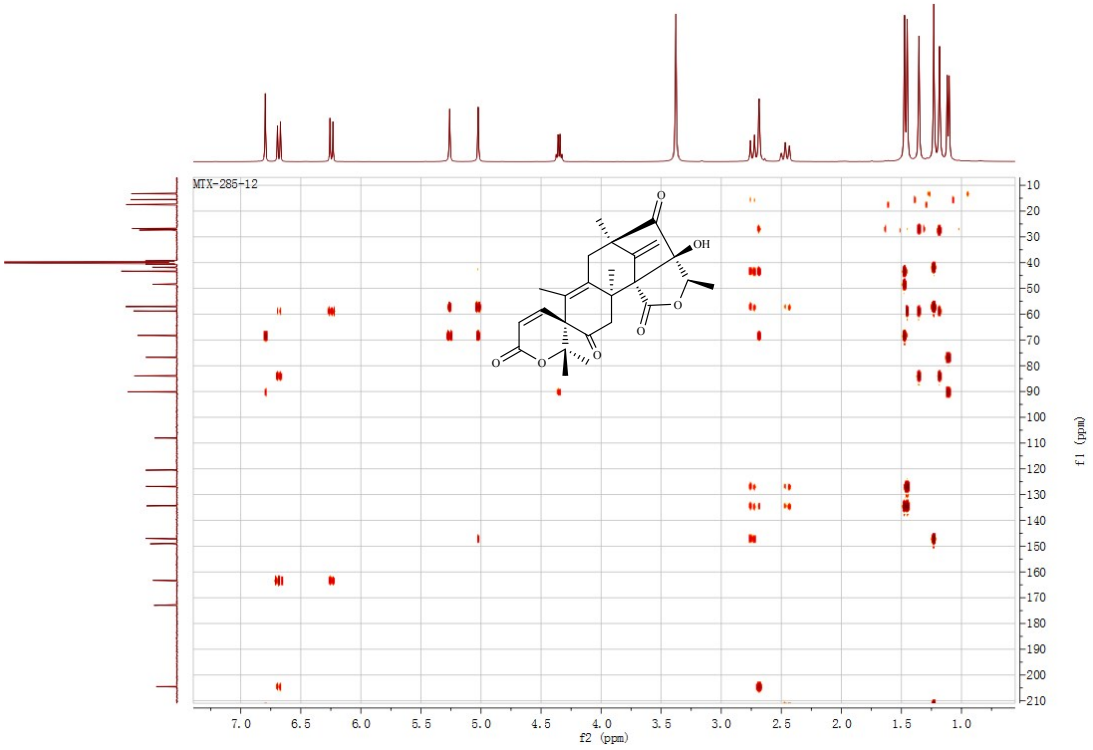


Figure S43. NOESY spectrum of **5** in DMSO-d_6

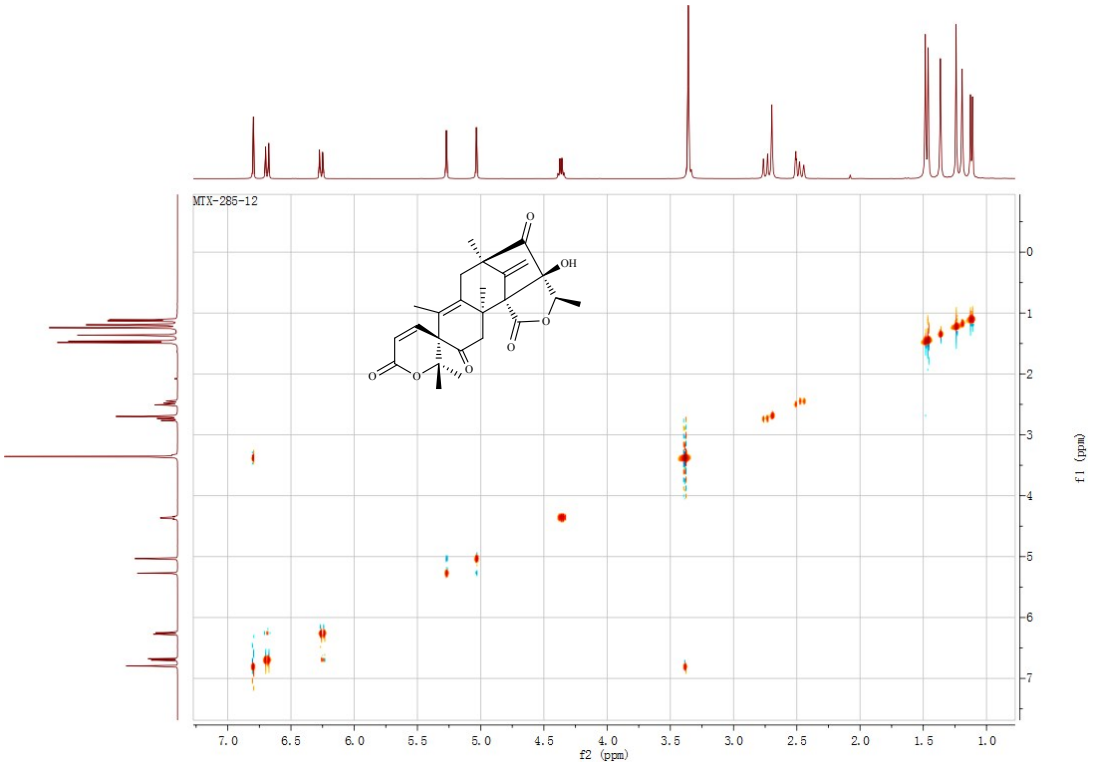


Figure S44.IR data of **5** in KBr

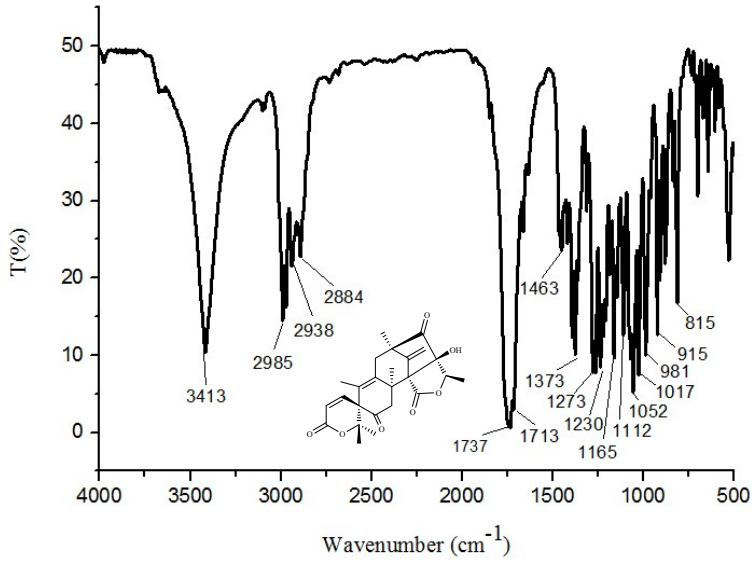


Figure S45. X-ray ORTEP drawing of **5**

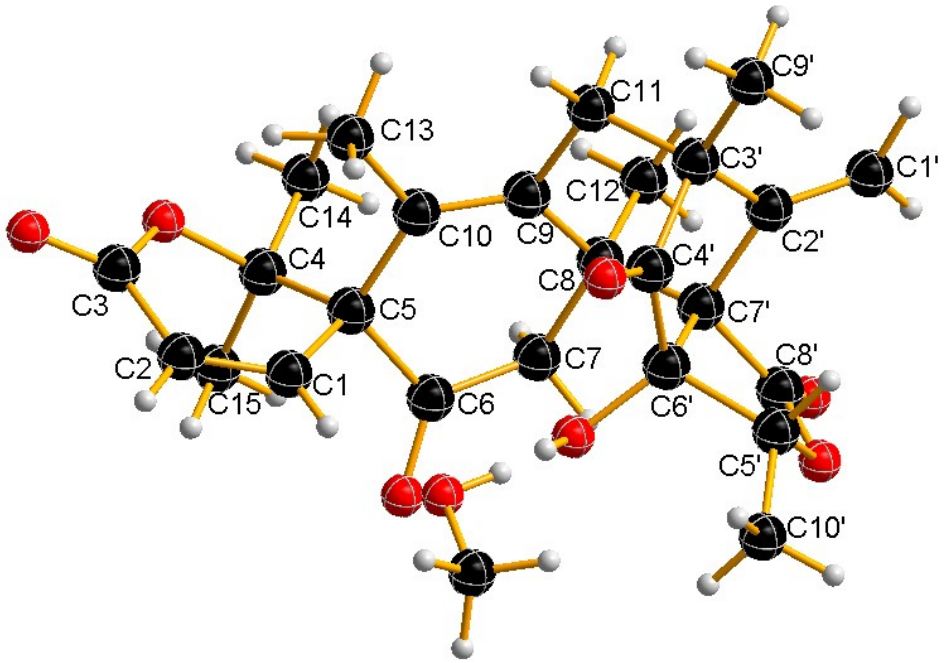
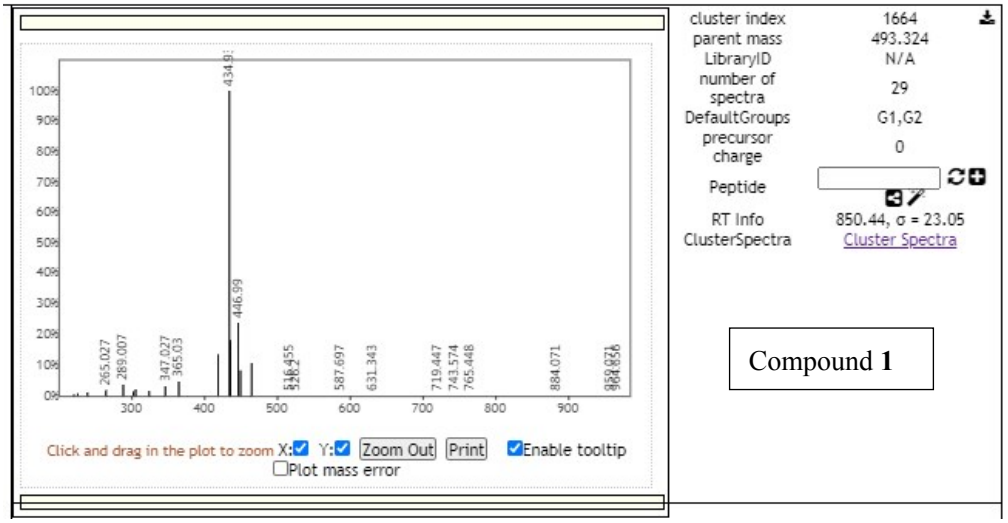
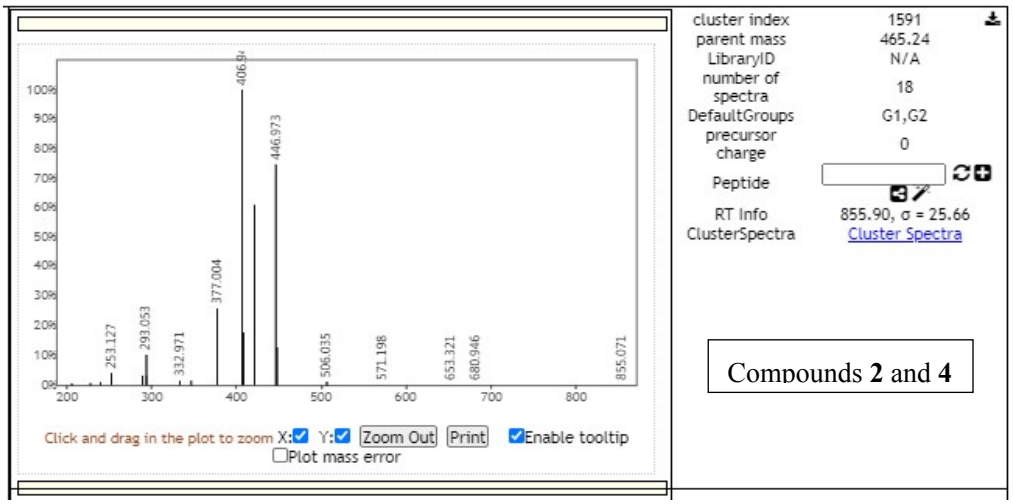
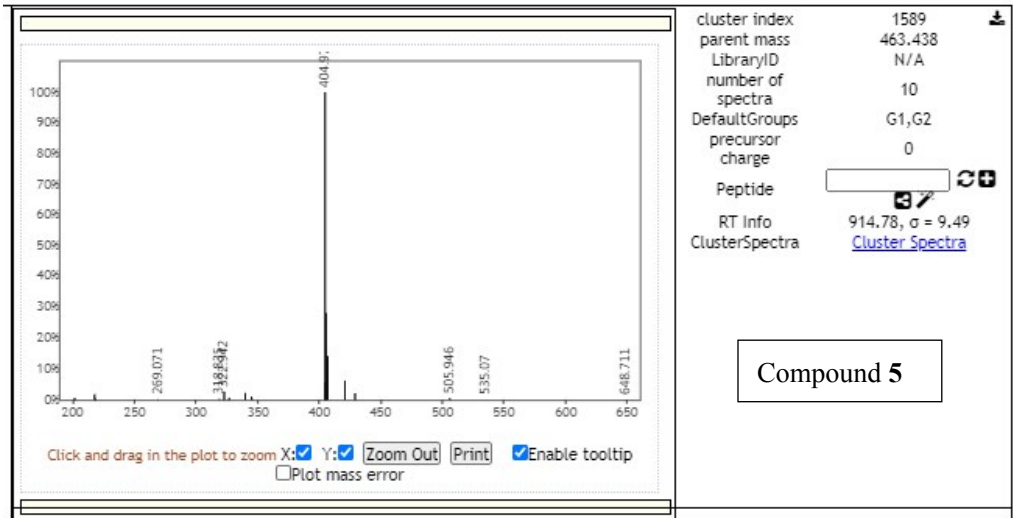
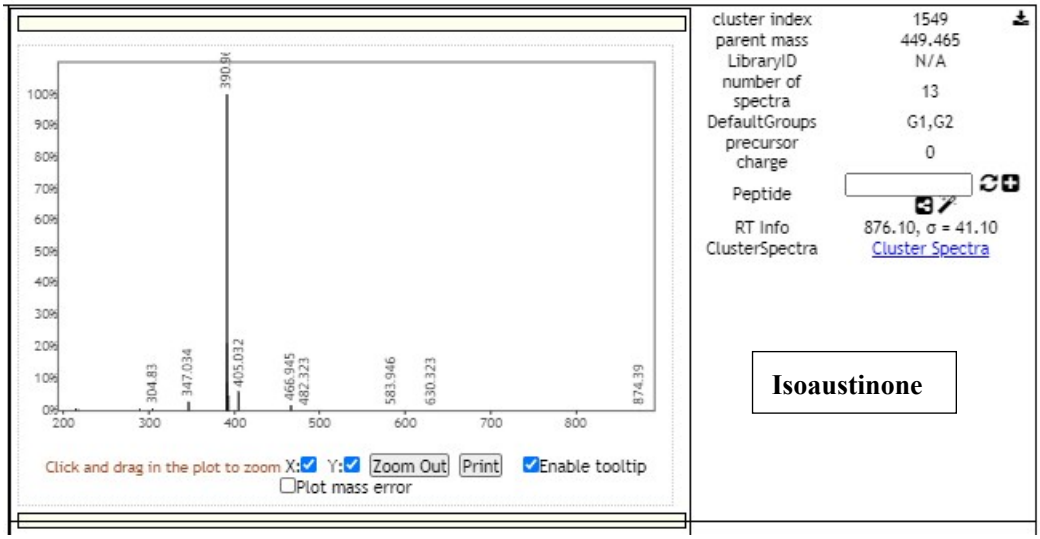


Figure S46. MS/MS spectrum of compounds 1, 2, 4, 5 and isoaustinone.





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405.032
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482.323
583.946
630.323
874.39
Click and drag in the plot to zoom X: Y: Zoom Out Print Enable tooltip
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Isoaustinone