Supporting Information

***Rec. Nat. Prod.* X:X (2021) XX-XX**

Jatroidaine A, A New Tetranortirucallane Type Triterpene from *Jatropha multifida*

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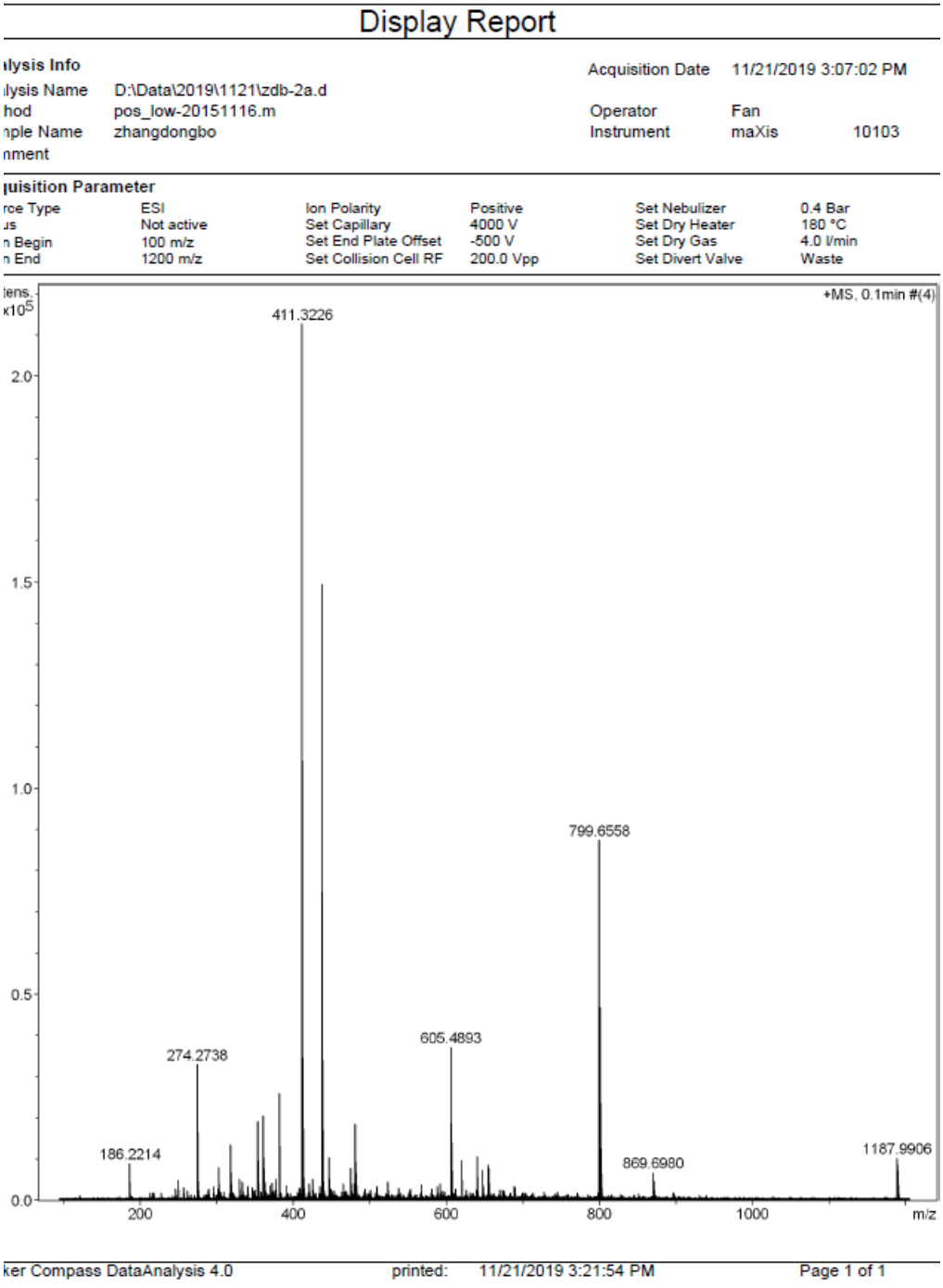

Figure S1: HR-ESI-MS spectrum of **1**

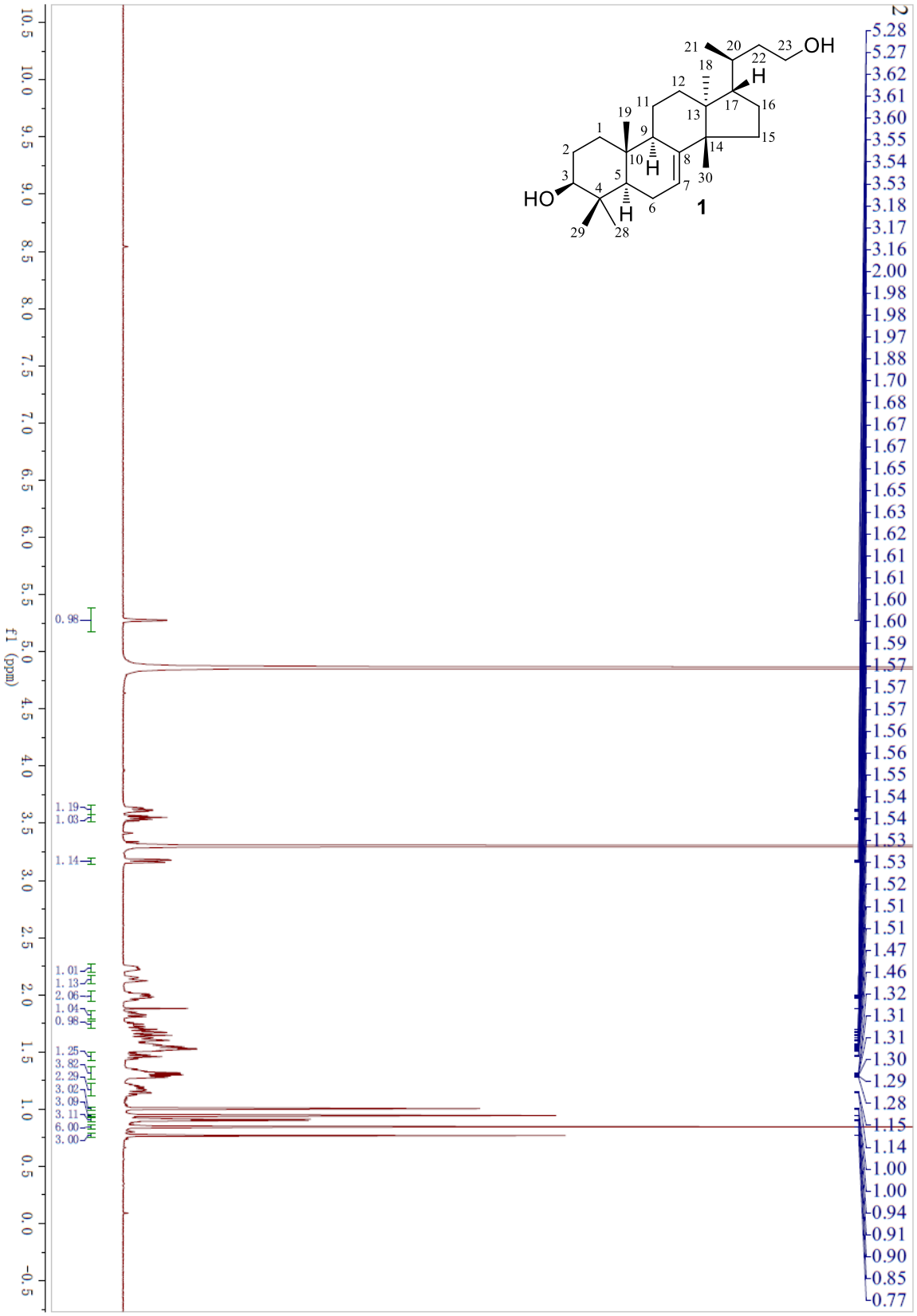

Figure S2: ^{1}H NMR (600 MHz, CD_3OD) spectrum of **1**

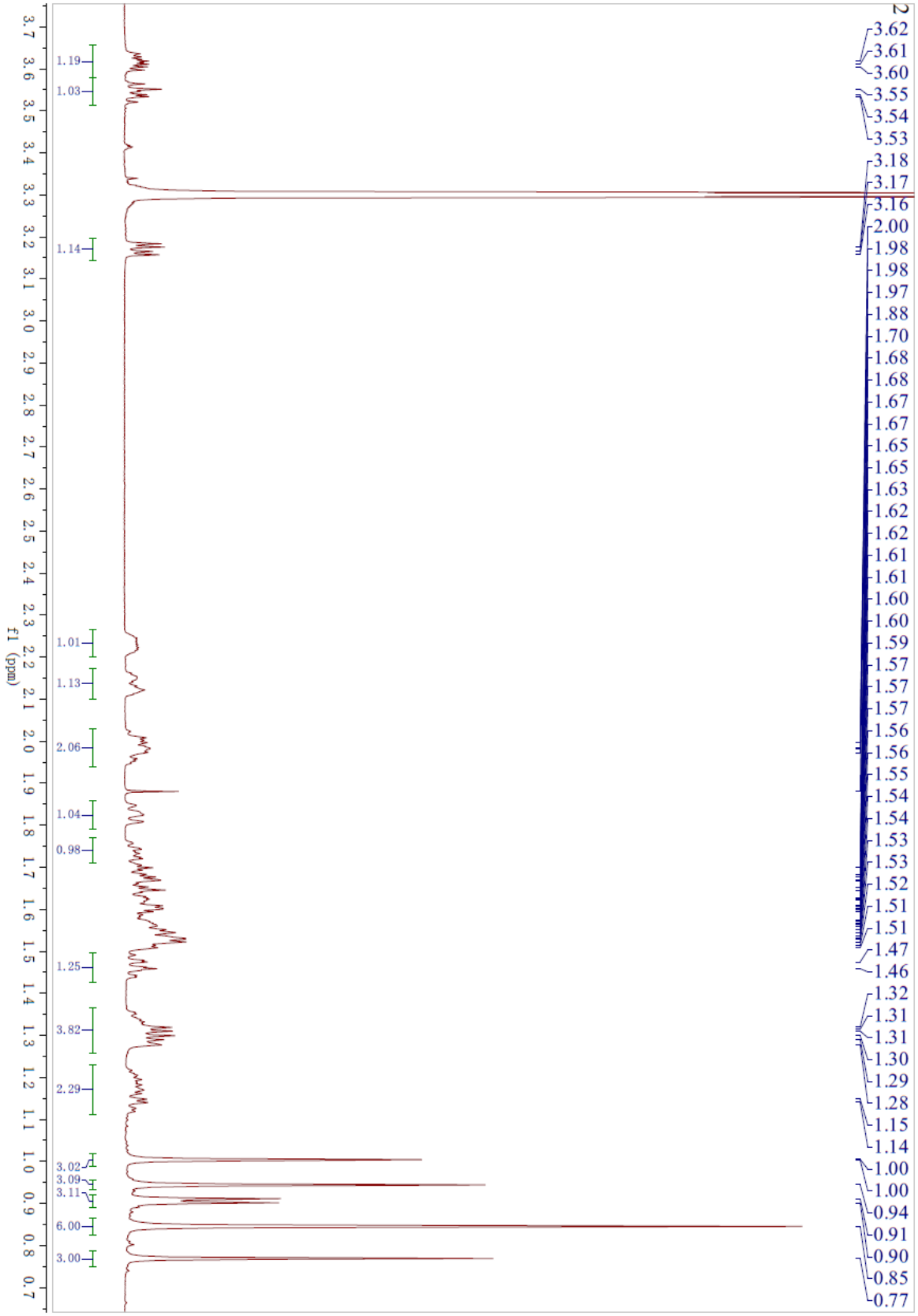

Figure S3: ^{1}H NMR (600 MHz, CD_3OD) spectrum of **1** (from δ_H 0.7 ppm to δ_H 3.7 ppm)

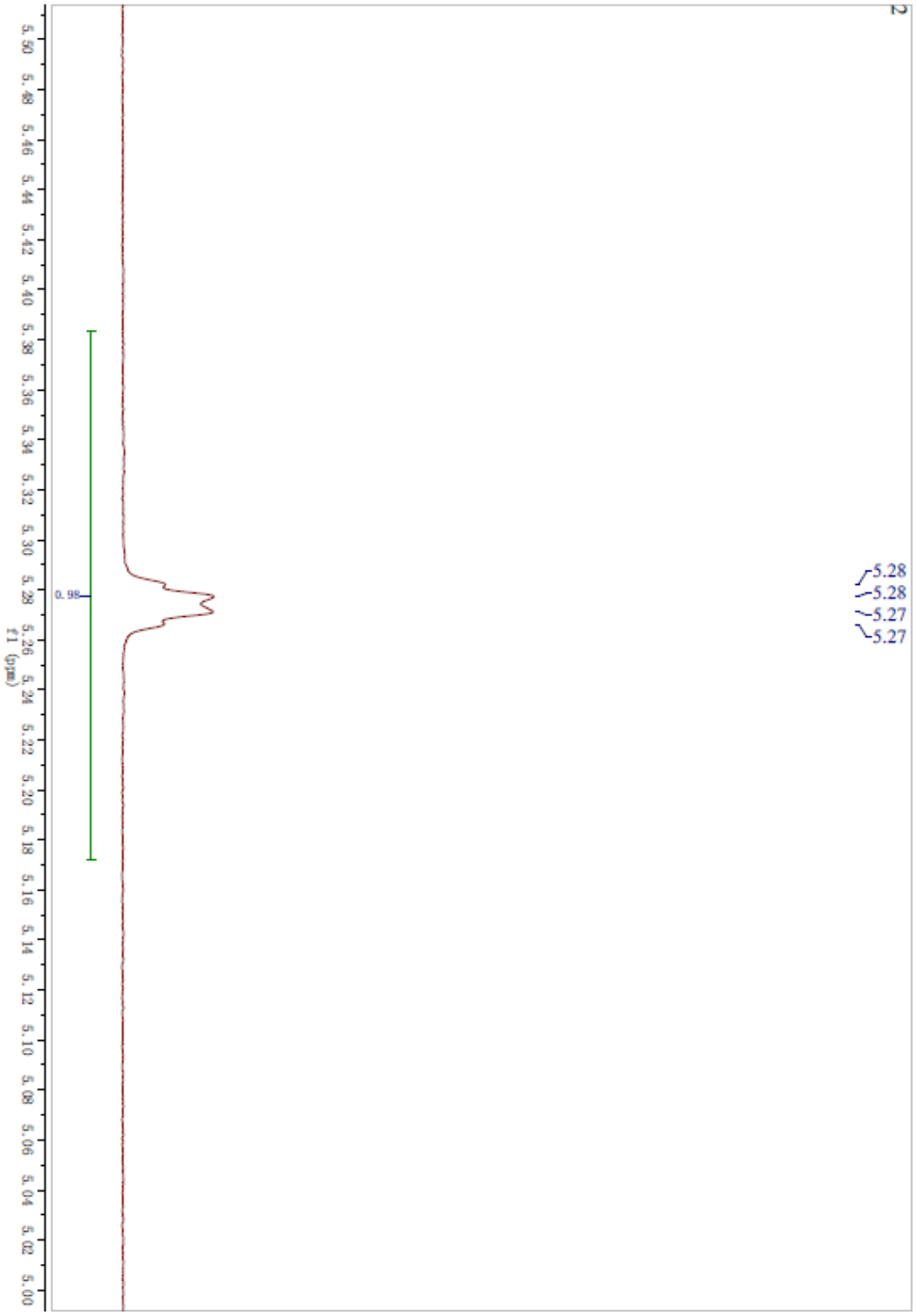

Figure S4: ^{1}H NMR (600 MHz, CD_3OD) spectrum of **1** (from δ_H 5.0 ppm to δ_H 5.5 ppm)

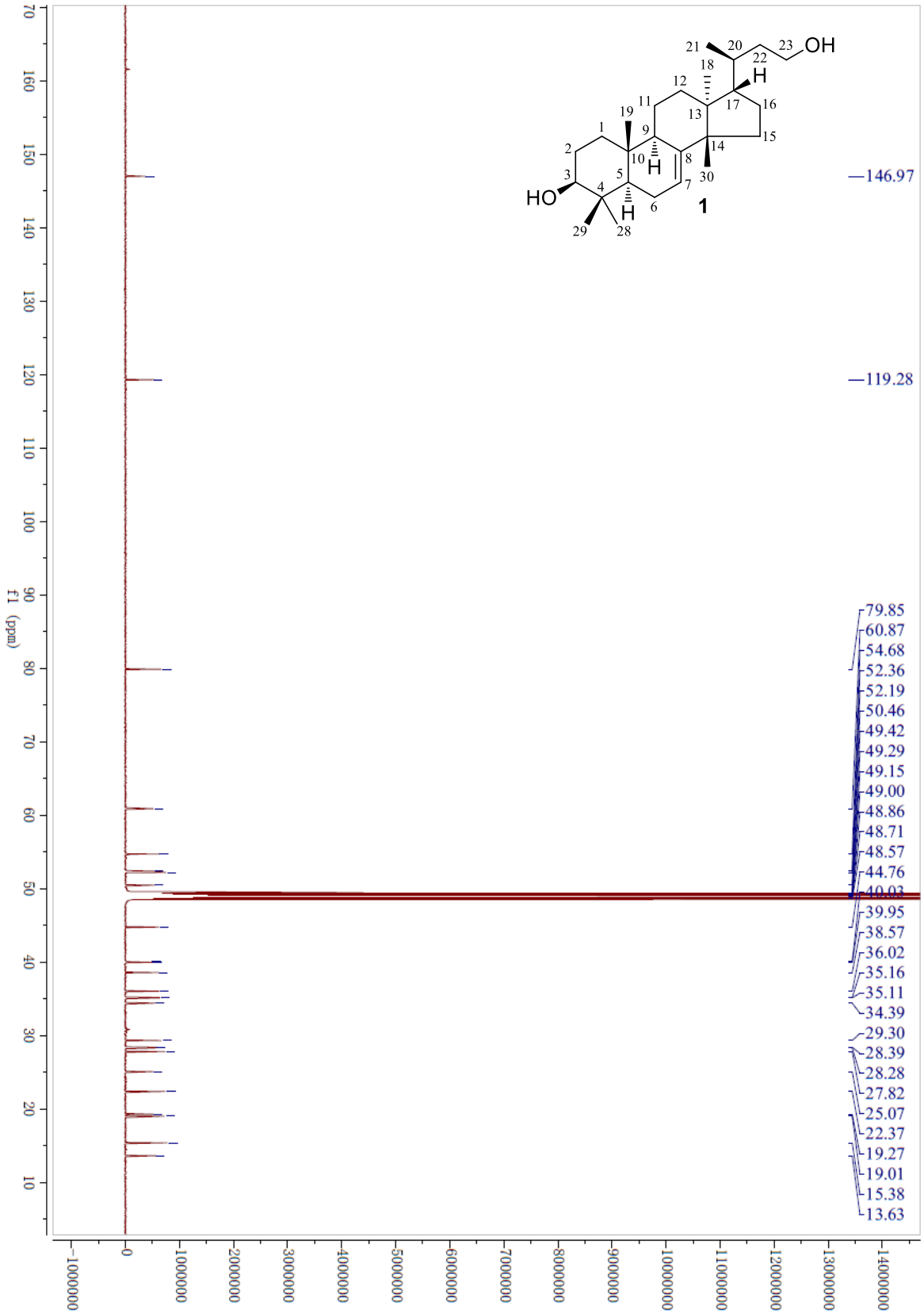

Figure S5: ^{13}C NMR (150 MHz, CD_3OD) spectrum of **1**

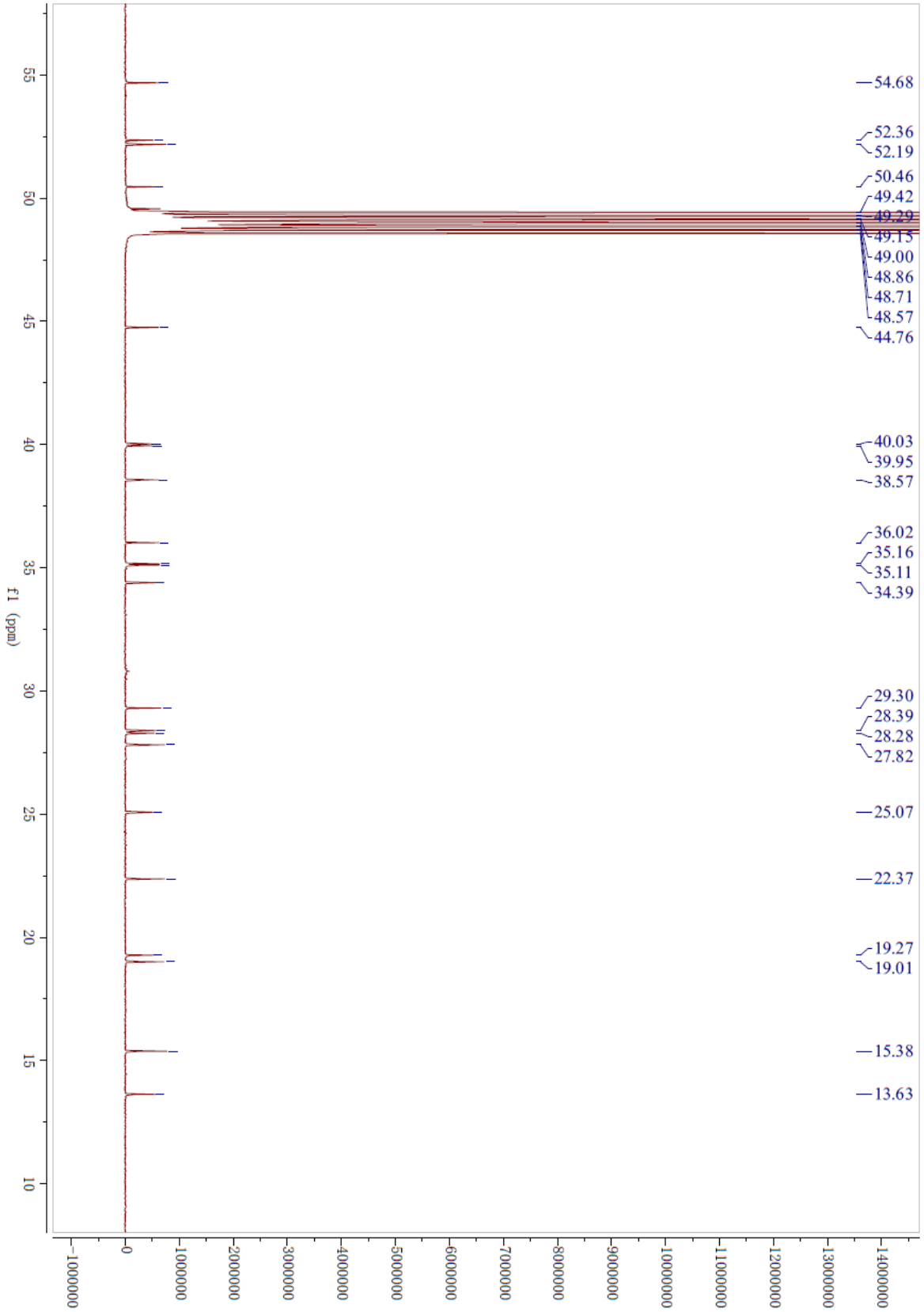

Figure S6: ^{13}C NMR (150 MHz, CD_3OD) spectrum of **1** (from δ_C 10 ppm to δ_C 55 ppm)

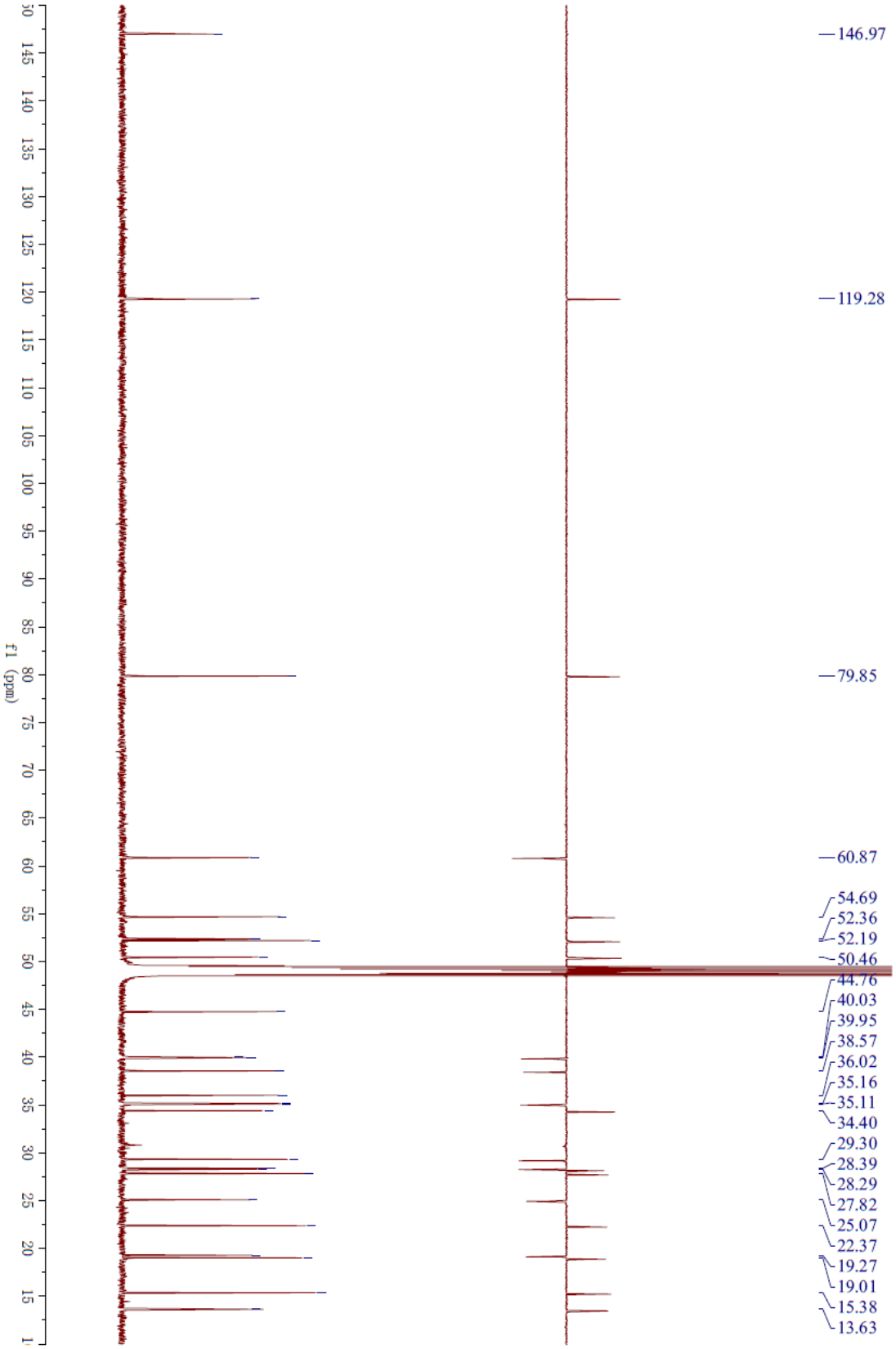

Figure S7: DEPT135 (150 MHz, CD_3OD) spectrum of **1**

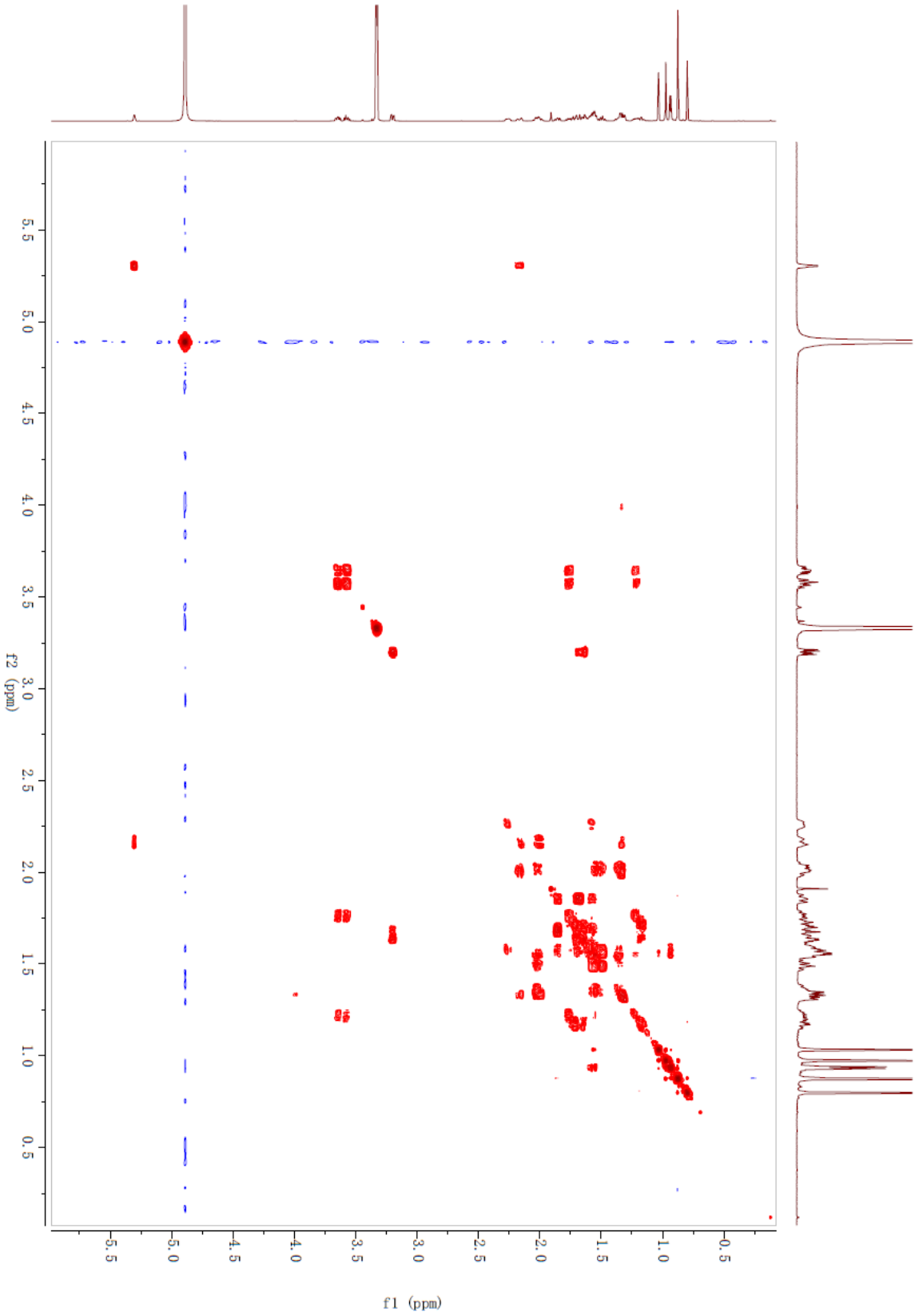

Figure S8: ^{1}H-^{1}H COSY (CD_3OD) spectrum of **1**

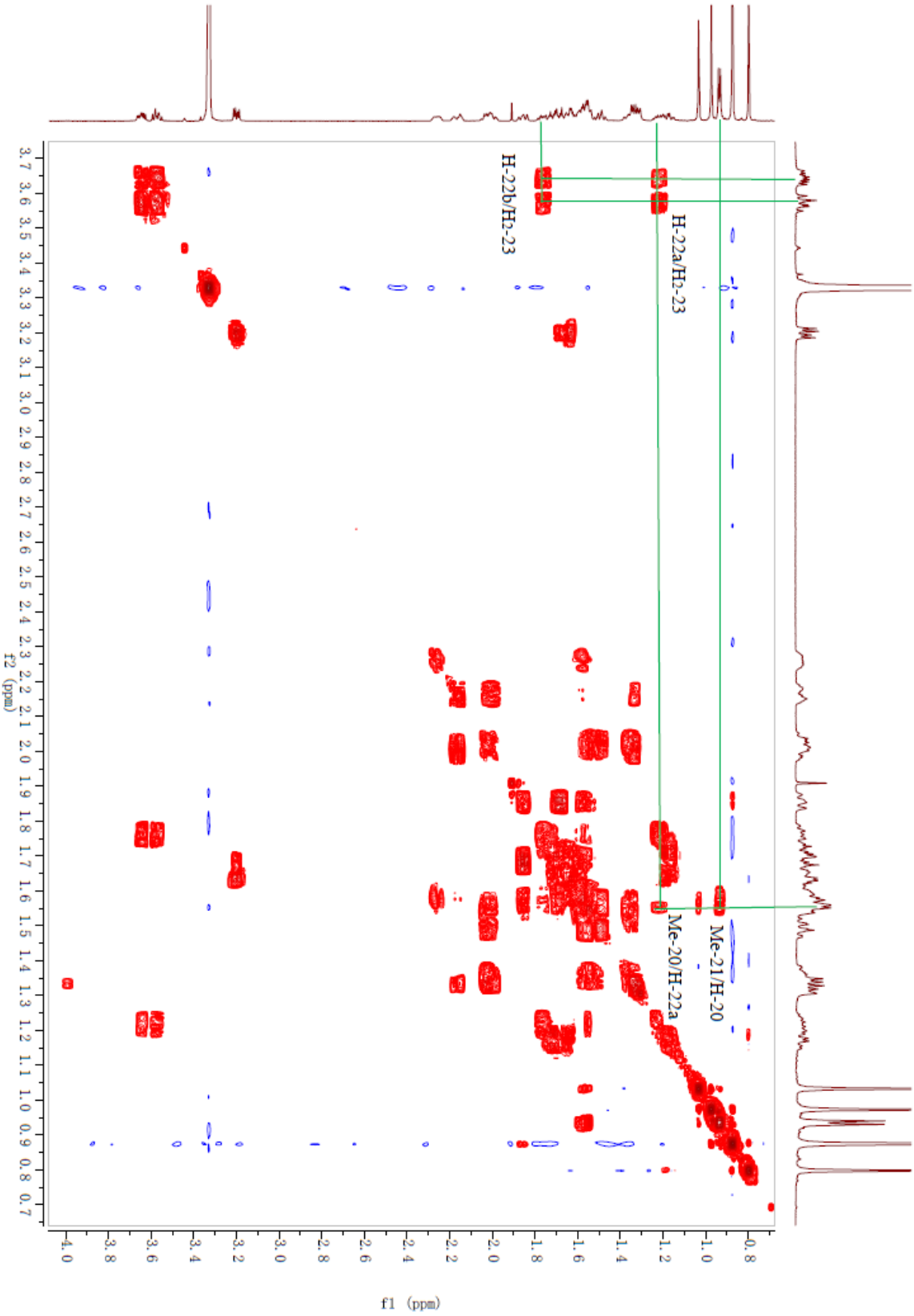

Figure S9: The enhanced ^{1}H-^{1}H COSY (CD_3OD) spectrum of **1**

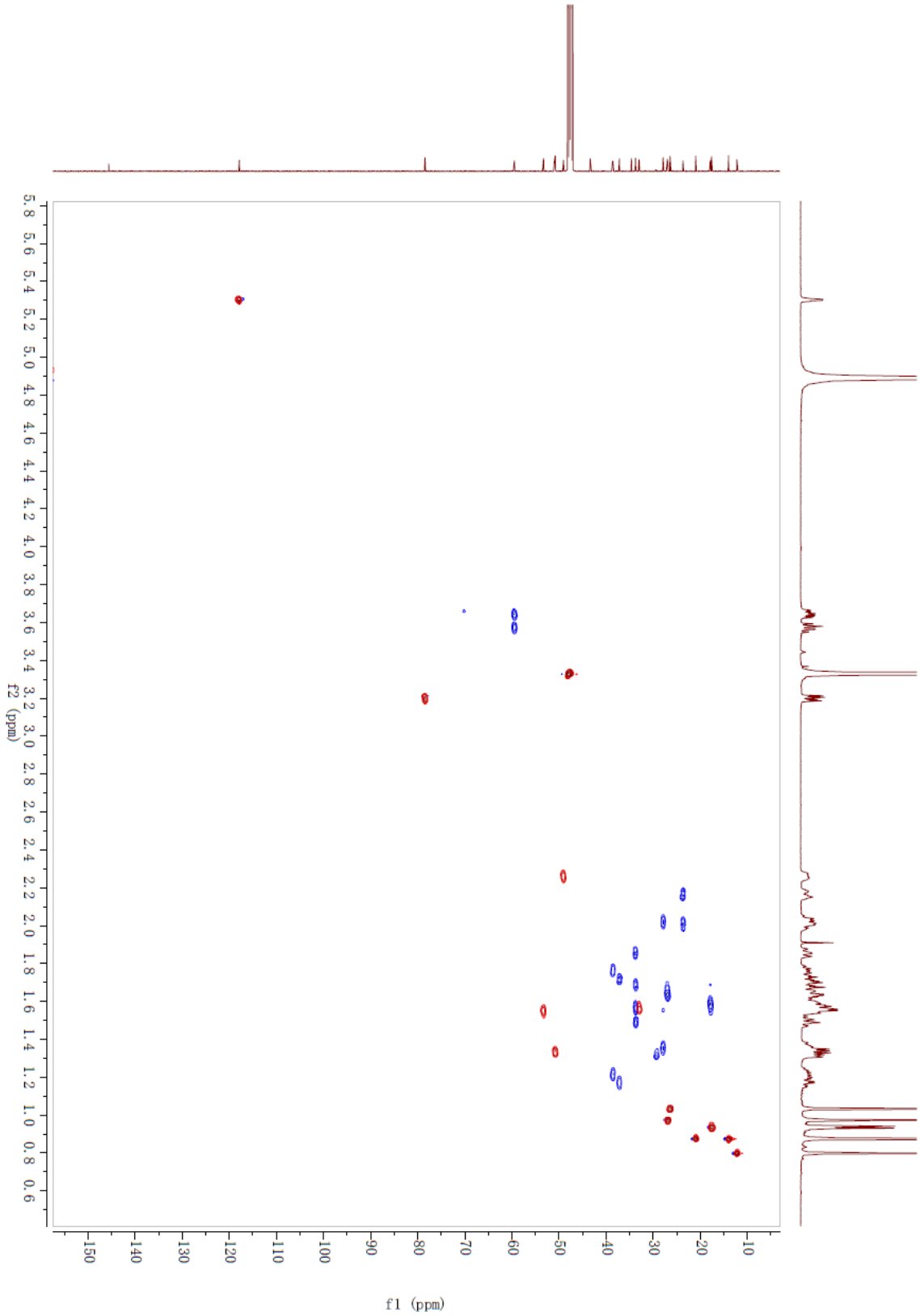

Figure S10: HSQC (CD_3OD) spectrum of **1**

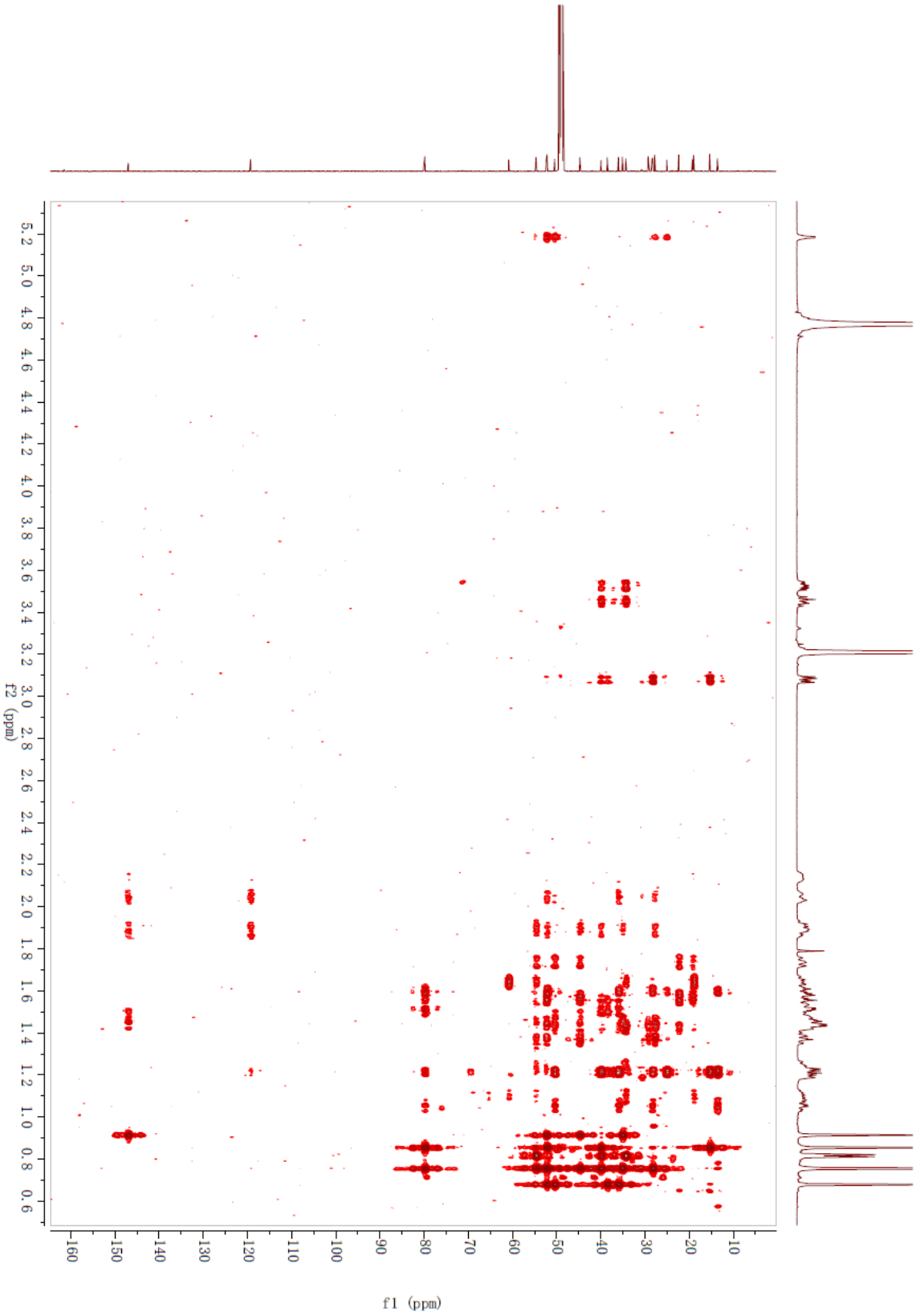

Figure S11: HMBC (CD_3OD) spectrum of **1**

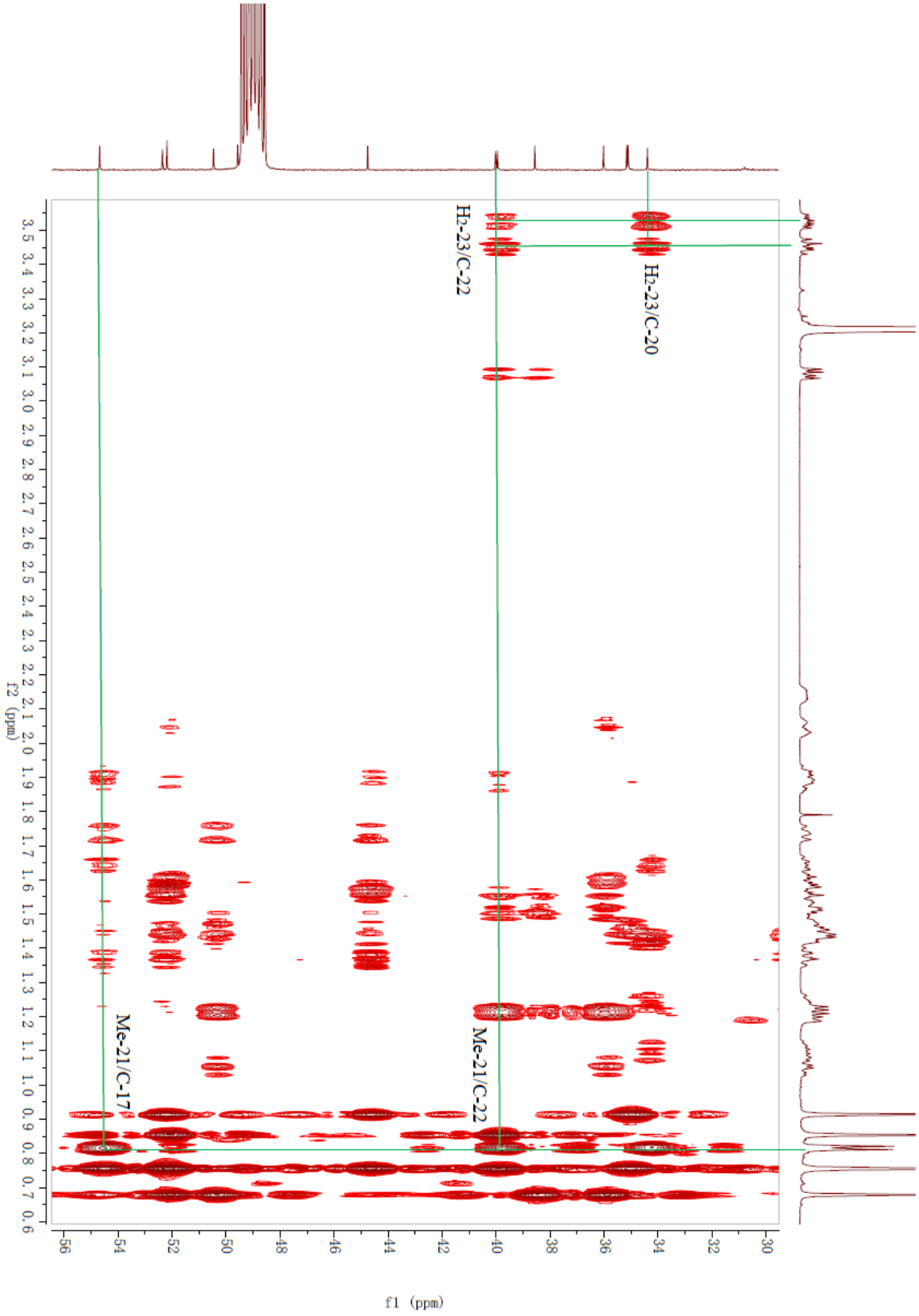

Figure S12: The enhanced HMBC (CD_3OD) spectrum of **1**

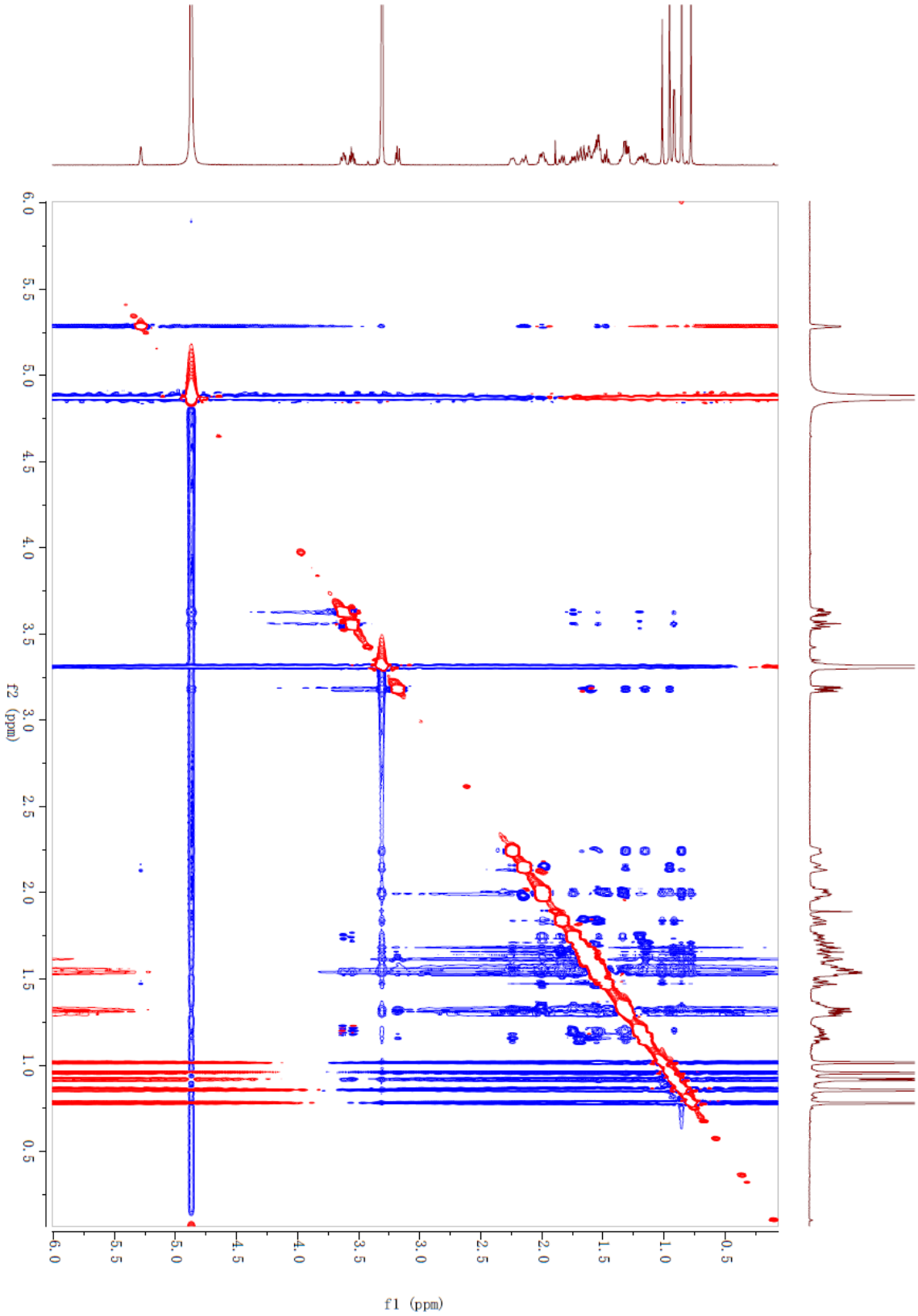

Figure S13: NOESY (CD_3OD) spectrum of **1**

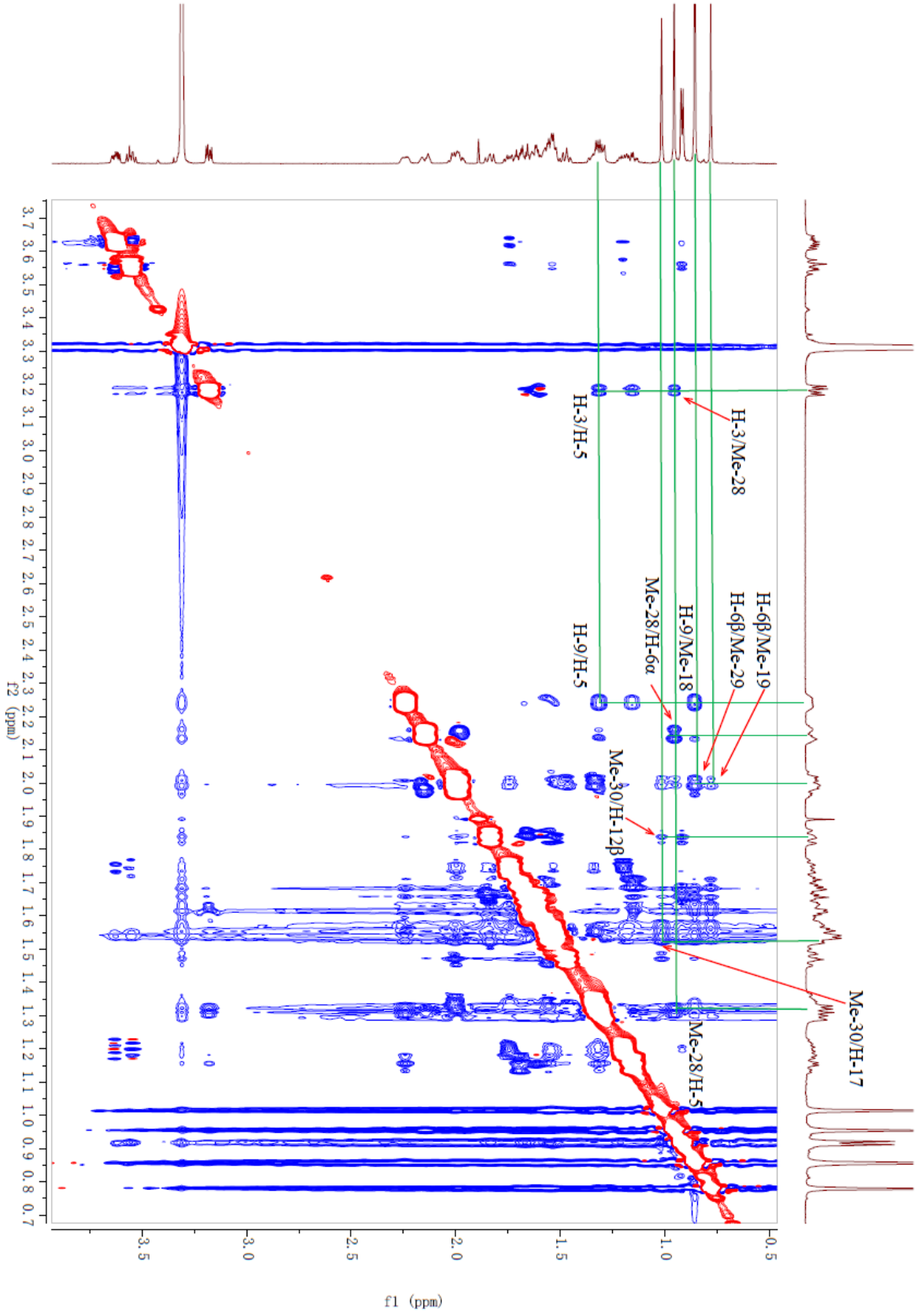

Figure S14: The enhanced NOESY (CD_3OD) spectrum of **1**

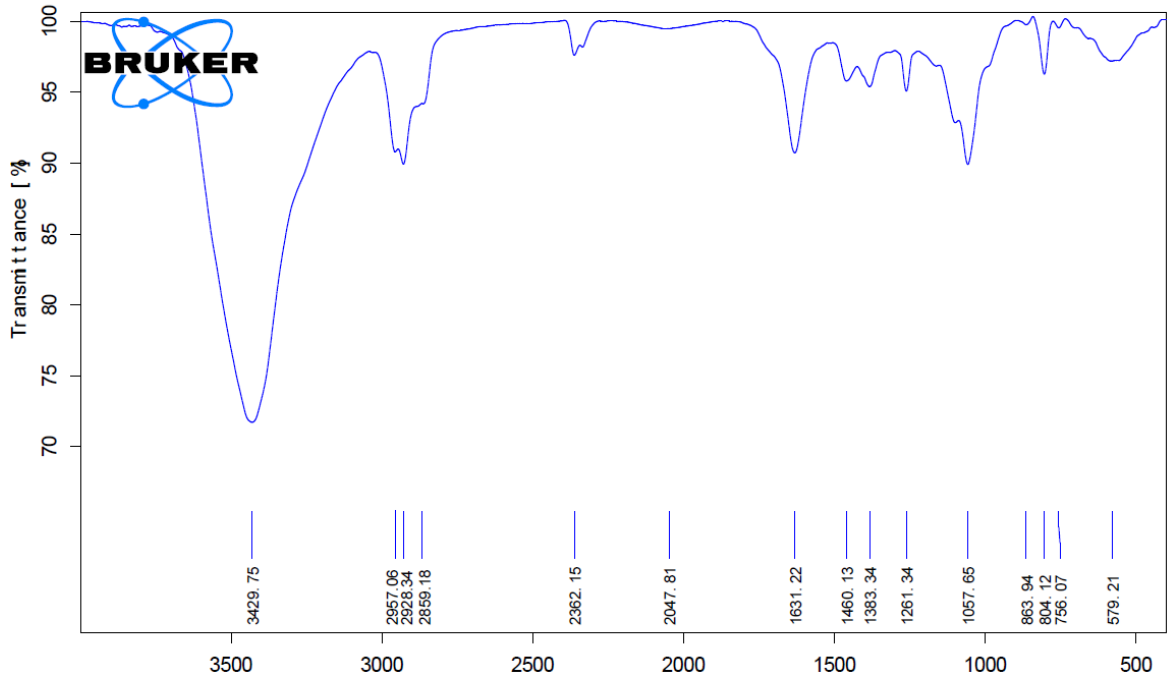

Figure S15: IR spectrum of **1**

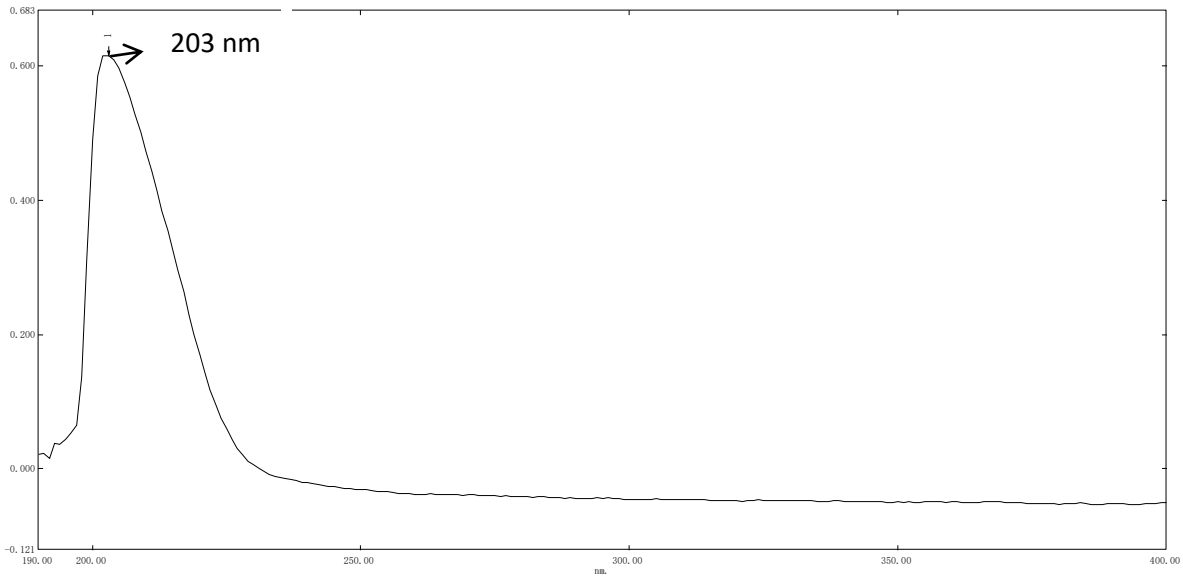

Figure S16: UV spectrum of **1**

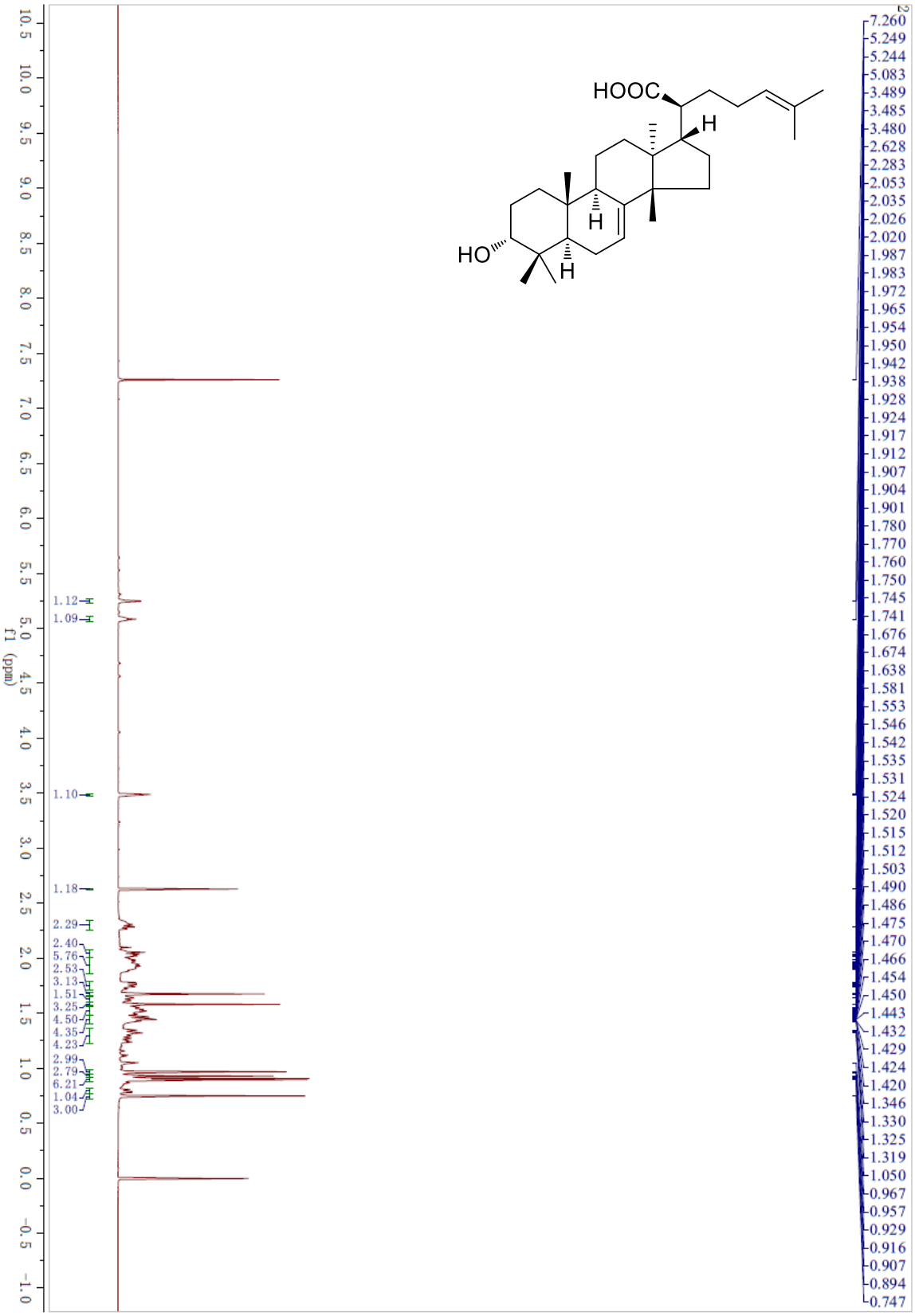

Figure S17: ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **2**

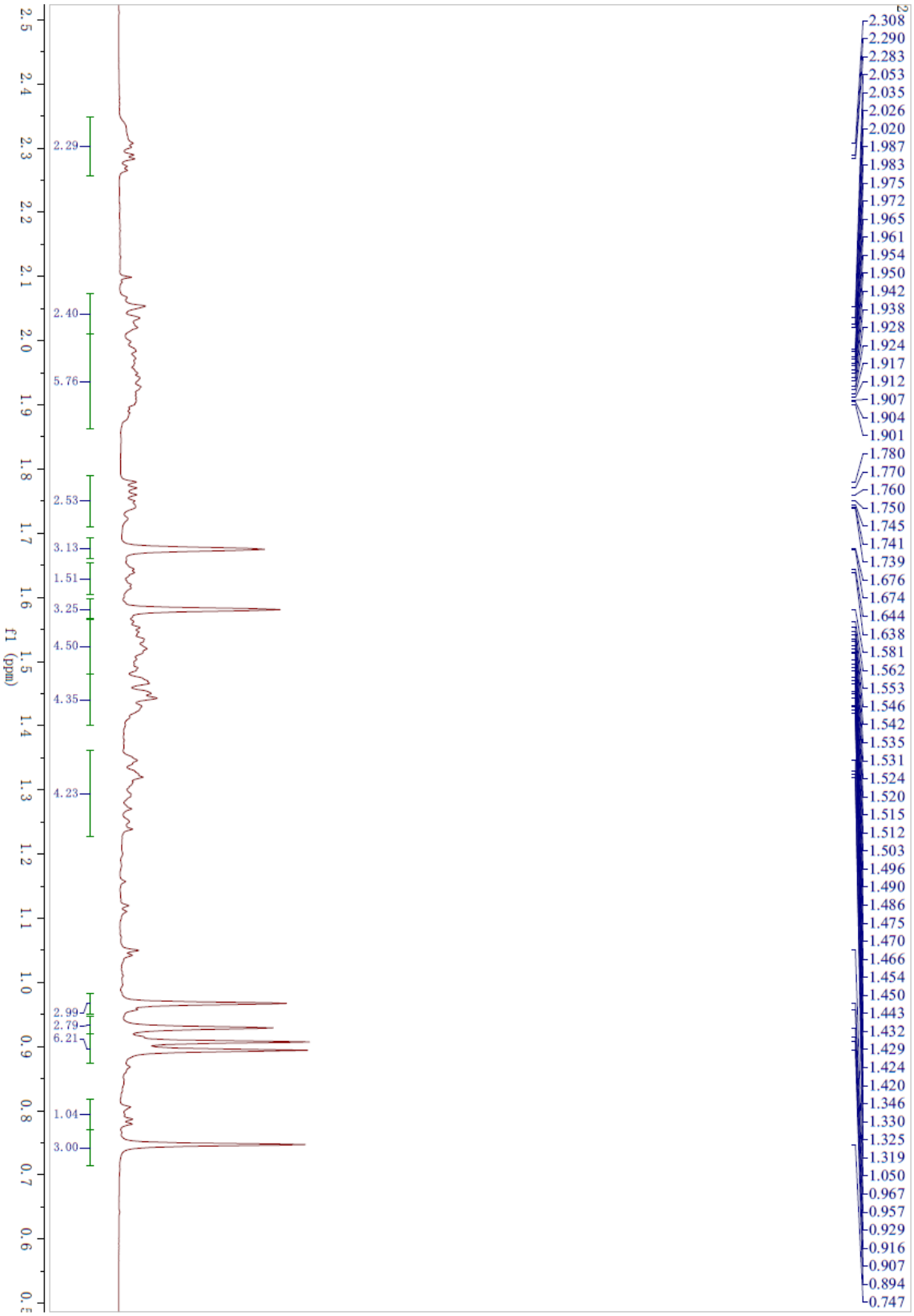

Figure S18: ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **2** (from δ_H 0.5 ppm to δ_H 2.5 ppm)

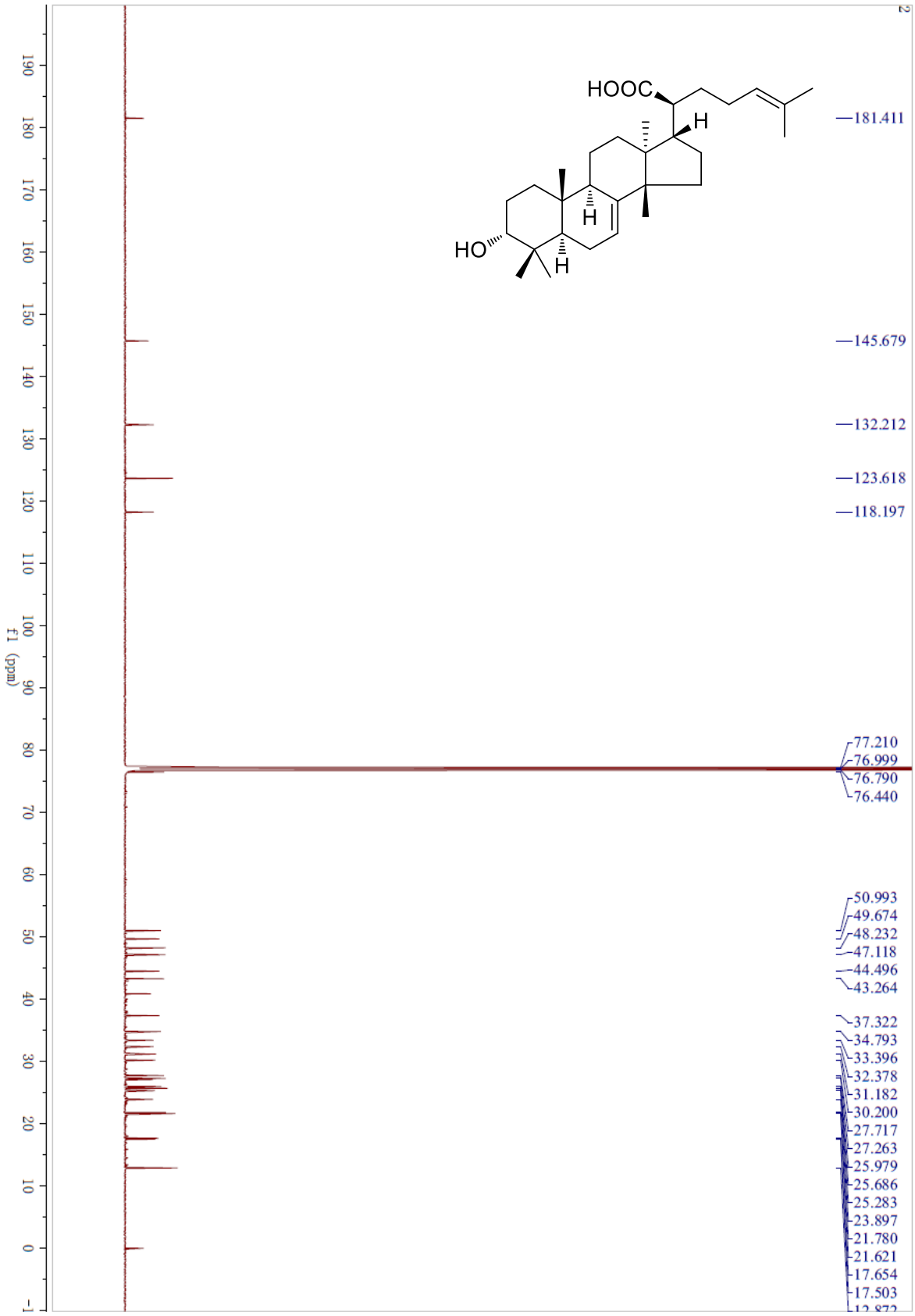

Figure S19: ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **2**

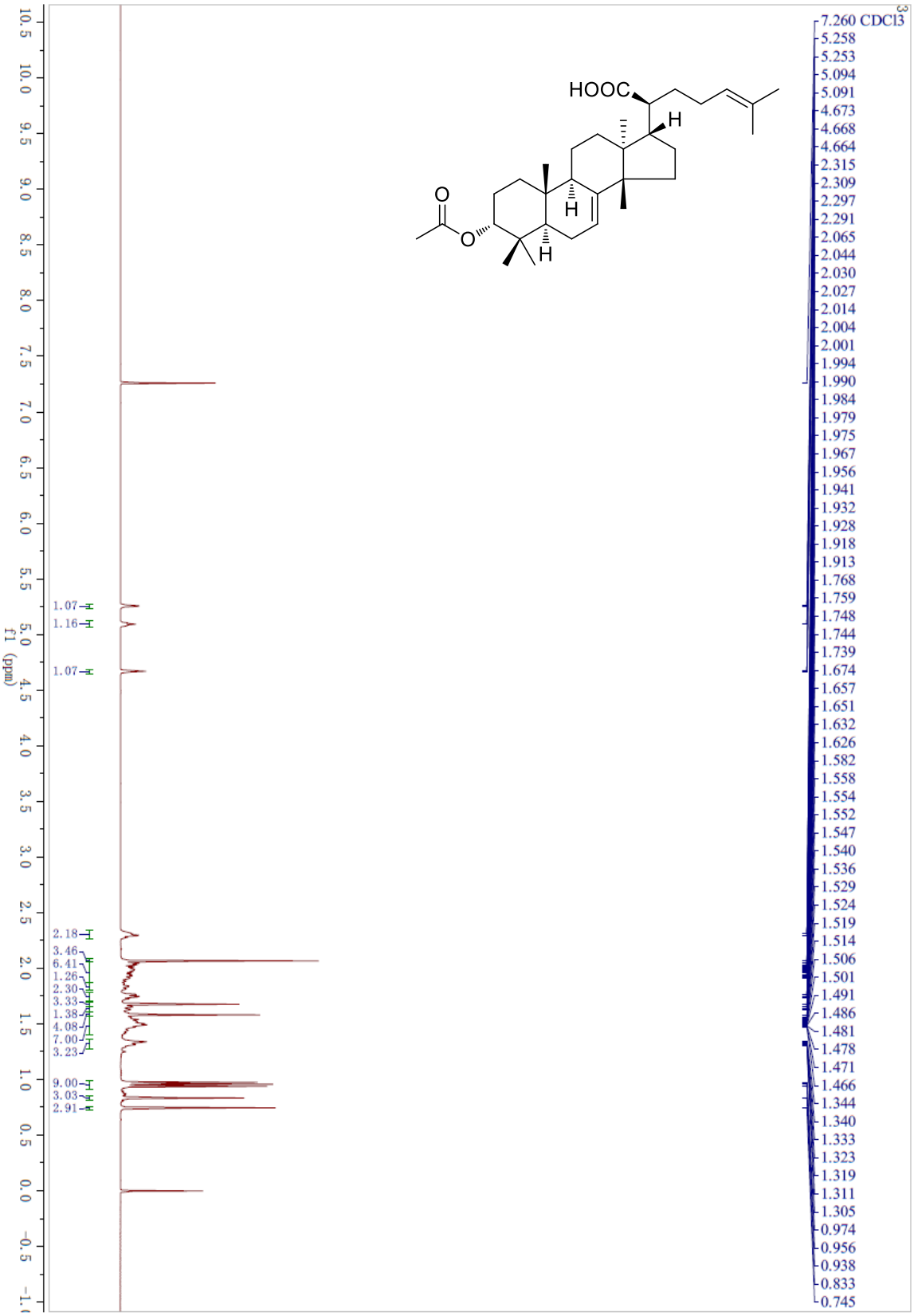

Figure S20: ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3**

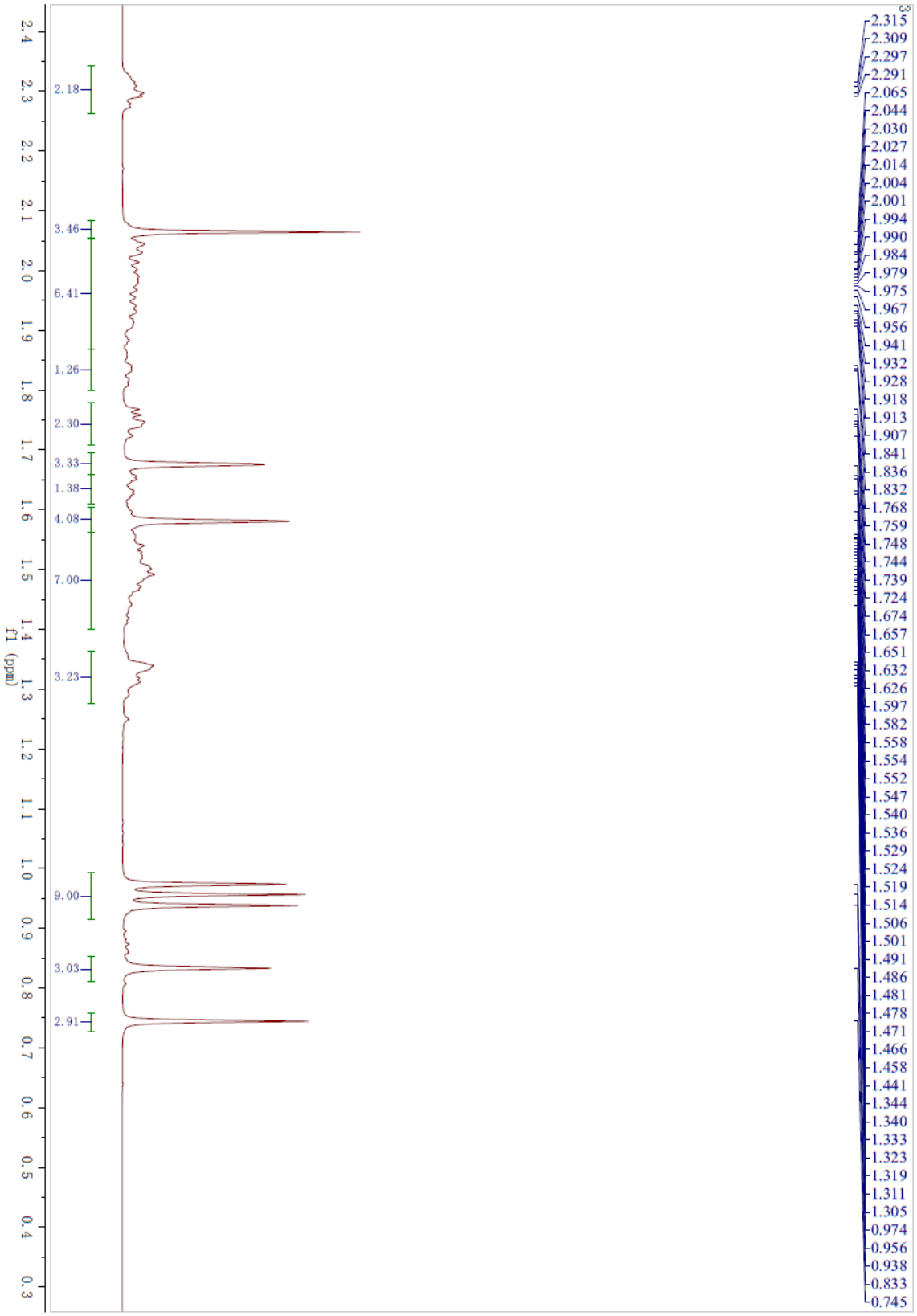

Figure S21: ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3** (from δ_H 0.3 ppm to δ_H 2.4 ppm)

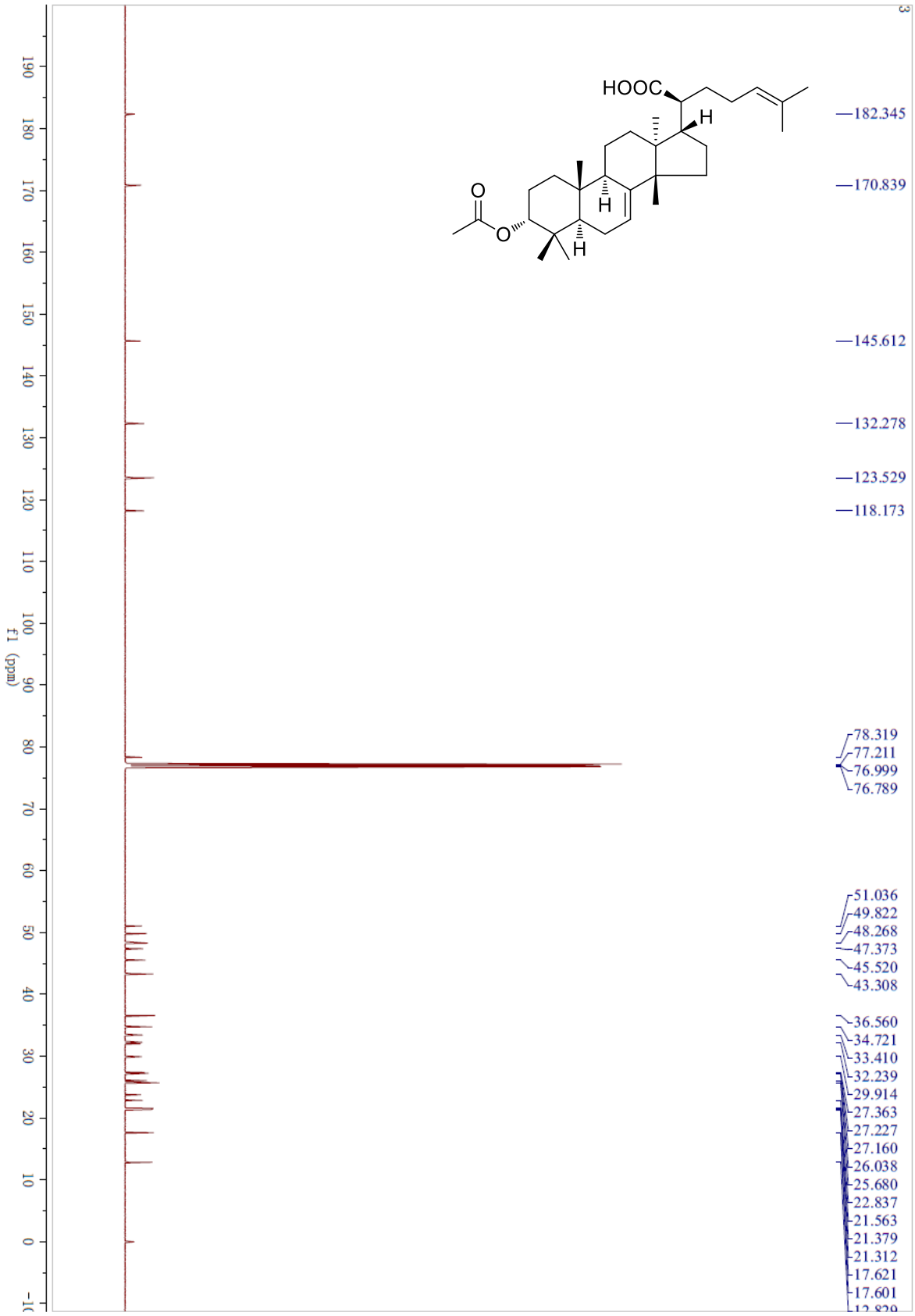

Figure S22: ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of **3**

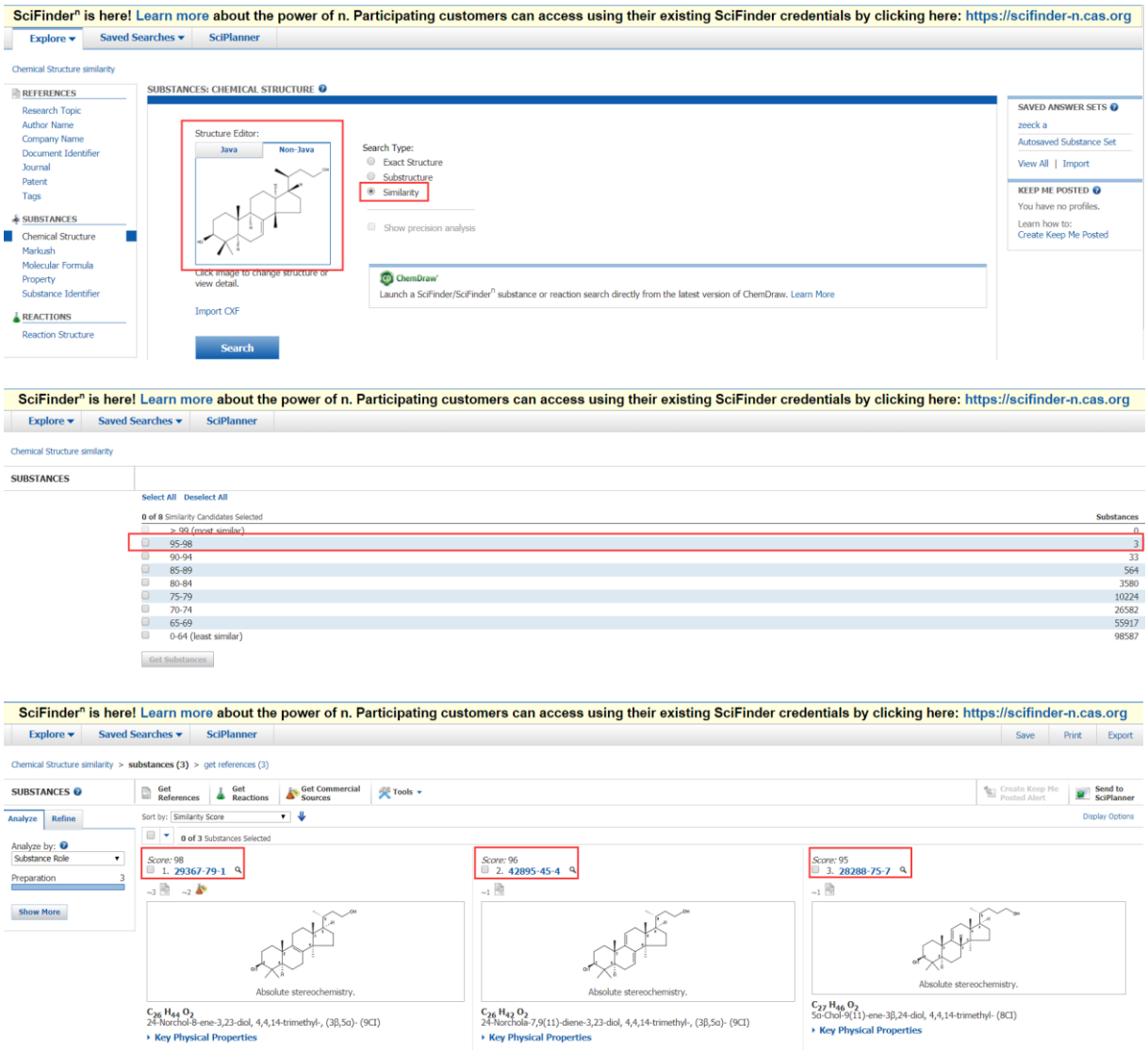

Figure S23: The Scifinder similarity report for new compound **1**

Table S1. The ^{13}C NMR data for **1** and 24,25-epoxy-3β,23-dihydroxy-7-tirucallene.

No.	**1**[a]	24,25-epoxy-3β,23-dihydroxy-7-tirucallene[b]
1a	38.6 (t)	37.2 (t)
1b	—	—
2	28.4 (t)	27.2 (t)
3	79.9 (d)	79.2 (d)
4	40.0 (s)	39.0 (s)
5	52.2 (d)	50.7 (d)
6*β*	25.1 (t)	23.9 (t)
6*α*	—	—
7	119.3 (d)	118.1 (d)
8	147.0 (s)	145.6 (s)
9	50.5 (d)	49.0 (d)
10	36.0 (s)	35.0 (s)
11	19.3 (t)	18.1 (t)
12*β*	35.2 (t)	33.8 (t)
12*α*	—	—
13	44.8 (s)	43.6 (s)
14	52.4 (s)	51.2 (s)
15a	35.1 (t)	34.0 (t)
15b	—	—
16a	29.3 (t)	28.7 (t)
16b	—	—
17	54.7 (d)	53.3 (d)
18	22.4 (q)	21.7 (q)
19	13.6 (q)	13.1 (q)
20	34.4 (d)	33.6 (d)
21	19.0 (q)	19.9 (q)
22a	39.9 (t)	40.8 (t)
22b	—	—
23a	60.9 (t)	69.3 (d)
23b	—	—
24	—	68.5 (d)
25	—	60.3 (s)
26	—	24.87 (q)
27	—	19.8 (q)
28	28.3 (q)	27.6 (q)
29	15.4 (q)	14.7 (q)
30	27.8 (q)	27.2 (q)

[a] Recorded at 150 MHz in CD_3OD. [b] Recorded at 100 MHz in $CDCl_3$.

Table S2. X-ray data of new compound **1**.

Identification code	s
Empirical formula	$C_{26}H_{44}O_2$
Formula weight	388.61
Temperature/K	162.0
Crystal system	triclinic
Space group	P1
a/Å	10.9288(3)
b/Å	11.7408(4)
c/Å	15.7438(5)
α/°	84.345(2)
β/°	69.749(2)
γ/°	66.639(2)
Volume/Å^3	1738.14(10)
Z	3
ρ_{calc}g/cm^3	1.114
μ/mm^{-1}	0.513
F(000)	648.0
Crystal size/mm^3	0.5 × 0.4 × 0.3
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	5.99 to 136.916
Index ranges	$-11 \leq h \leq 13$, $-14 \leq k \leq 14$, $-18 \leq l \leq 18$
Reflections collected	46387
Independent reflections	12355 [R_{int} = 0.0777, R_{sigma} = 0.0634]
Data/restraints/parameters	12355/3/781
Goodness-of-fit on F^2	1.059
Final R indexes [I>=2σ (I)]	R_1 = 0.0562, wR_2 = 0.1499
Final R indexes [all data]	R_1 = 0.0737, wR_2 = 0.1658
Largest diff. peak/hole / e Å^{-3}	0.70/-0.25
Flack parameter	0.03(14)

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

Atom	*x*	*y*	*z*	U(eq)
O1	10195(3)	4668(3)	-187(2)	55.6(8)
O2	3587(4)	825(3)	376(2)	56.8(8)
O3	2013(4)	5871(3)	9261(2)	60.3(8)
O4	1145(4)	2109(3)	9875(2)	57.3(8)
O5	4873(4)	8283(3)	9630(2)	58.9(8)
C1	2392(4)	2678(3)	4512(3)	40.8(8)
C2	5219(4)	5462(3)	5477(3)	41.4(9)
C3	6351(4)	4205(3)	5062(3)	40.5(8)
C4	6309(4)	5049(3)	3526(3)	40.5(8)
C5	5830(4)	6390(3)	3872(3)	43.3(9)
C6	2791(4)	2371(3)	2623(3)	40.9(8)
C7	7207(4)	4131(3)	4071(3)	42.1(9)
O6	12865(6)	7131(4)	164(3)	90.1(13)
C8	10131(4)	8417(4)	4570(3)	44.5(9)
C9	2315(4)	3656(3)	3988(3)	43.5(9)
C10	7838(4)	8574(3)	5874(3)	41.9(9)
C11	7225(4)	8959(4)	6898(3)	45.7(9)
C12	2496(5)	503(3)	5714(3)	45.2(9)
C13	7131(5)	9534(4)	5280(3)	49.3(10)
C14	4974(5)	5610(4)	6501(3)	44.0(9)
C15	2619(5)	3611(4)	2987(3)	45.7(9)
C16	10152(5)	7533(4)	6088(3)	51.0(10)
C17	1185(5)	4003(4)	6030(3)	50.1(10)
C18	1486(4)	1854(3)	6045(3)	42.5(9)
C19	6628(4)	3230(4)	5580(3)	43.7(9)
C20	9444(4)	8118(3)	5534(3)	44.2(9)
C21	7884(4)	7785(4)	7398(3)	45.8(9)
C22	3216(5)	2288(4)	1571(3)	45.3(9)

C23	2757(4)	1414(3)	4105(3)	41.0(8)
C24	63(5)	2152(4)	5917(3)	46.3(9)
C25	5607(5)	9357(4)	7233(3)	50.6(10)
C26	3650(5)	6795(4)	6902(3)	48.8(10)
C27	3653(5)	1254(4)	3083(3)	44.7(9)
C28	3357(5)	343(4)	4689(3)	46.4(9)
C29	3217(5)	1033(4)	1329(3)	47.8(10)
C30	9370(4)	8308(4)	3935(3)	46.8(9)
C31	5001(5)	4768(4)	3634(3)	47.2(9)
C32	3036(5)	6877(4)	7928(3)	51.5(10)
C33	1294(5)	1639(4)	9031(3)	51.3(10)
C34	4664(4)	4467(3)	6961(3)	41.1(8)
C35	5918(5)	3250(4)	6572(3)	46.0(9)
C36	159(5)	1798(4)	7817(3)	49.6(10)
C37	7776(5)	2889(4)	3539(3)	48.7(10)
C38	5056(5)	4439(5)	8516(3)	57.2(11)
C39	1186(5)	2224(4)	7046(3)	45.4(9)
C40	7978(5)	4675(4)	833(3)	48.6(10)
C41	7206(5)	7819(4)	8443(3)	51.2(10)
C42	5594(5)	8236(4)	8676(3)	50.7(10)
C43	4048(5)	4519(4)	8012(3)	46.6(9)
C44	7827(5)	9263(4)	4243(3)	50.7(10)
C45	5485(5)	6545(4)	4904(3)	50.0(10)
C46	9027(5)	5289(4)	605(3)	49.4(10)
C47	10081(5)	9750(4)	4618(3)	52.5(10)
C48	3791(5)	34(4)	2697(3)	49.0(10)
C49	2185(5)	2758(4)	5507(3)	44.7(9)
C50	3654(5)	2457(4)	5595(3)	51.0(10)
C51	3592(5)	3422(4)	8309(3)	54.0(11)
C52	6779(5)	5130(4)	1741(3)	47.7(9)
C53	7336(4)	4680(4)	2543(3)	43.6(9)

C54	2075(5)	3344(4)	1286(3)	52.3(10)
C55	4226(5)	-60(4)	1666(3)	52.6(10)
C56	11671(5)	7584(4)	4079(3)	53.8(11)
C57	9506(5)	7348(4)	7070(3)	54.9(11)
C58	2711(5)	5738(4)	8305(3)	49.8(10)
C59	9386(5)	6998(4)	3945(4)	59.5(12)
C60	5125(5)	1229(4)	2952(3)	51.2(10)
C61	8030(5)	3236(4)	2543(3)	47.8(9)
C62	8521(5)	4394(4)	4006(3)	50.7(10)
C63	4945(5)	9429(4)	8256(3)	55.4(11)
C64	-23(5)	2263(4)	8760(3)	51.6(10)
C65	690(5)	3659(4)	7032(3)	52.0(11)
C66	6282(5)	5682(4)	6615(3)	50.2(10)
C67	7509(6)	8636(5)	8975(4)	66.5(13)
C68	4631(5)	2386(5)	1024(4)	57.7(11)
C69	10364(5)	8489(5)	2998(3)	57.2(11)
C70	7597(5)	10043(4)	7049(3)	54.5(11)
C71	11871(5)	7746(5)	3069(4)	58.8(12)
C72	586(6)	379(5)	7803(3)	58.2(11)
C73	5985(5)	6537(4)	1765(3)	55.4(11)
C74	10267(6)	8206(6)	2097(4)	73.0(15)
C75	7759(6)	6489(5)	8764(4)	69.0(14)
C76	8763(6)	8703(7)	2071(4)	80.7(17)
C77	11183(8)	8791(8)	1312(5)	92(2)
C78	11601(8)	8331(7)	367(5)	93(2)

Table S2-2. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for new compound **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}
O1	47.7(18)	50.6(17)	55.4(19)	-0.3(14)	-9.9(14)	-11.8(14)
O2	64(2)	51.1(17)	51.7(18)	-0.8(13)	-24.1(15)	-13.8(15)
O3	63(2)	61(2)	51.0(18)	-1.2(15)	-9.9(15)	-25.4(17)
O4	63(2)	50.8(17)	56.9(19)	0.1(14)	-26.8(16)	-14.1(16)
O5	63(2)	54.7(18)	50.3(18)	1.3(14)	-14.8(15)	-17.2(16)
C1	38(2)	28.7(18)	57(2)	3.0(16)	-22.0(18)	-8.9(15)
C2	41(2)	32.4(19)	50(2)	4.1(16)	-16.8(18)	-12.0(16)
C3	40(2)	33.8(18)	49(2)	3.0(15)	-19.0(17)	-12.7(16)
C4	43(2)	31.9(19)	47(2)	5.5(15)	-16.0(17)	-14.4(16)
C5	41(2)	28.7(18)	55(2)	5.5(16)	-14.8(18)	-9.7(15)
C6	39(2)	35.6(19)	47(2)	0.4(15)	-16.5(17)	-10.9(16)
C7	41(2)	33.3(19)	52(2)	6.3(16)	-18.6(18)	-13.2(16)
O6	119(4)	85(3)	73(3)	-3(2)	-32(3)	-46(3)
C8	36(2)	35.7(19)	57(2)	2.5(16)	-17.5(18)	-7.3(16)
C9	43(2)	30.1(18)	58(2)	-0.4(16)	-20.9(19)	-10.1(16)
C10	36(2)	31.9(18)	57(2)	4.8(16)	-18.6(18)	-10.3(15)
C11	39(2)	35(2)	60(3)	5.9(17)	-20.7(19)	-8.6(16)
C12	52(2)	31.7(19)	54(2)	5.2(16)	-26(2)	-11.5(17)
C13	42(2)	43(2)	57(3)	7.3(18)	-20(2)	-9.2(18)
C14	47(2)	33.8(19)	53(2)	6.4(16)	-20.1(19)	-15.9(17)
C15	52(2)	31.9(19)	54(2)	4.3(16)	-25(2)	-11.0(17)
C16	36(2)	44(2)	67(3)	1.5(19)	-21(2)	-6.0(17)
C17	57(3)	36(2)	57(3)	-0.1(18)	-25(2)	-11.9(18)
C18	42(2)	35(2)	50(2)	1.8(16)	-20.9(18)	-9.3(17)
C19	40(2)	31.7(18)	57(2)	1.9(16)	-18.4(18)	-10.1(16)
C20	39(2)	31.6(19)	62(3)	1.5(17)	-21.0(19)	-10.4(16)
C21	41(2)	31.5(18)	61(3)	0.8(17)	-22.0(19)	-5.8(16)
C22	46(2)	34.6(19)	55(2)	0.1(16)	-21.0(19)	-12.2(17)

C23	42(2)	32.0(18)	49(2)	0.6(15)	-18.5(17)	-11.1(16)
C24	44(2)	42(2)	55(2)	2.0(17)	-22.0(19)	-14.0(18)
C25	40(2)	45(2)	57(3)	3.0(18)	-16.9(19)	-6.6(18)
C26	48(2)	35(2)	56(3)	1.9(17)	-15.7(19)	-10.6(18)
C27	46(2)	33.1(19)	54(2)	3.3(16)	-22.8(19)	-9.6(17)
C28	50(2)	33.3(19)	53(2)	0.1(16)	-21.9(19)	-9.2(17)
C29	50(2)	45(2)	46(2)	-2.5(17)	-16.5(19)	-14.5(19)
C30	39(2)	40(2)	56(2)	-3.9(17)	-16.6(18)	-9.3(17)
C31	43(2)	45(2)	55(2)	7.3(17)	-20.1(19)	-16.4(18)
C32	51(2)	40(2)	59(3)	-0.2(18)	-17(2)	-12.7(18)
C33	52(3)	45(2)	54(3)	0.9(18)	-24(2)	-10.7(19)
C34	39(2)	36.2(19)	47(2)	3.0(15)	-14.4(17)	-13.6(16)
C35	45(2)	33.6(19)	56(3)	5.1(16)	-19.9(19)	-10.0(17)
C36	44(2)	51(2)	49(2)	0.9(18)	-18.8(19)	-11.2(19)
C37	44(2)	35(2)	58(3)	3.8(17)	-17.6(19)	-6.7(17)
C38	55(3)	60(3)	57(3)	4(2)	-24(2)	-19(2)
C39	43(2)	40(2)	53(2)	2.8(17)	-22.3(19)	-10.9(17)
C40	49(2)	41(2)	51(2)	5.7(17)	-16.6(19)	-14.1(18)
C41	48(2)	42(2)	59(3)	2.0(18)	-24(2)	-8.2(19)
C42	51(2)	49(2)	52(2)	1.7(18)	-18(2)	-17.8(19)
C43	46(2)	39(2)	54(2)	4.8(17)	-18.7(19)	-14.4(18)
C44	39(2)	48(2)	62(3)	8.0(19)	-21(2)	-11.1(18)
C45	59(3)	33(2)	55(3)	6.0(17)	-18(2)	-17.2(19)
C46	48(2)	42(2)	49(2)	2.8(17)	-11.9(19)	-11.4(18)
C47	52(3)	43(2)	61(3)	0.1(18)	-12(2)	-21.7(19)
C48	56(3)	34(2)	52(2)	0.8(17)	-21(2)	-9.8(18)
C49	48(2)	33.6(19)	55(2)	3.8(16)	-24.9(19)	-11.9(17)
C50	51(3)	47(2)	64(3)	6.6(19)	-29(2)	-21(2)
C51	58(3)	47(2)	55(3)	7.3(19)	-16(2)	-22(2)
C52	46(2)	43(2)	55(2)	7.7(18)	-19.5(19)	-16.3(18)
C53	41(2)	42(2)	49(2)	5.9(16)	-16.5(18)	-16.1(17)

C54	58(3)	43(2)	55(3)	3.1(18)	-27(2)	-13(2)
C55	57(3)	38(2)	56(3)	-1.4(18)	-22(2)	-9.5(19)
C56	38(2)	47(2)	73(3)	-8(2)	-20(2)	-10.0(19)
C57	47(2)	48(2)	66(3)	5(2)	-29(2)	-7.3(19)
C58	47(2)	45(2)	52(2)	2.2(18)	-15.4(19)	-12.7(19)
C59	56(3)	45(2)	84(4)	-5(2)	-33(3)	-16(2)
C60	41(2)	53(2)	57(3)	5.2(19)	-21(2)	-13.3(19)
C61	46(2)	39(2)	50(2)	-2.3(17)	-13.2(19)	-9.0(17)
C62	44(2)	52(2)	61(3)	9.7(19)	-23(2)	-19.9(19)
C63	41(2)	51(3)	60(3)	4(2)	-16(2)	-4.7(19)
C64	48(2)	47(2)	52(3)	-0.3(18)	-17(2)	-10.7(19)
C65	61(3)	40(2)	54(3)	-5.1(18)	-24(2)	-13(2)
C66	54(3)	49(2)	56(3)	2.5(18)	-24(2)	-24(2)
C67	64(3)	74(3)	67(3)	-5(3)	-28(3)	-26(3)
C68	55(3)	56(3)	58(3)	6(2)	-16(2)	-21(2)
C69	47(3)	56(3)	59(3)	-7(2)	-17(2)	-9(2)
C70	61(3)	37(2)	66(3)	1.9(19)	-23(2)	-18(2)
C71	40(2)	57(3)	70(3)	-13(2)	-15(2)	-8(2)
C72	68(3)	57(3)	59(3)	3(2)	-22(2)	-34(2)
C73	45(2)	50(2)	54(3)	5.5(19)	-15(2)	-3.3(19)
C74	51(3)	86(4)	65(3)	-16(3)	-20(2)	-4(3)
C75	71(3)	58(3)	60(3)	12(2)	-24(3)	-7(3)
C76	57(3)	109(5)	63(3)	-2(3)	-24(3)	-15(3)
C77	75(4)	111(5)	73(4)	3(4)	-18(3)	-24(4)
C78	90(5)	89(5)	87(5)	9(4)	-29(4)	-22(4)

Table S2-3. Bond Lengths for new compound **1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C46	1.434(5)	C18	C49	1.564(6)
O2	C29	1.431(5)	C19	C35	1.481(6)
O3	C58	1.423(5)	C21	C41	1.550(6)
O4	C33	1.421(5)	C21	C57	1.539(6)
O5	C42	1.429(6)	C22	C29	1.558(6)
C1	C9	1.337(6)	C22	C54	1.531(6)
C1	C23	1.522(5)	C22	C68	1.532(7)
C1	C49	1.510(6)	C23	C27	1.551(6)
C2	C3	1.522(5)	C23	C28	1.546(6)
C2	C14	1.556(6)	C25	C63	1.516(7)
C2	C45	1.549(6)	C26	C32	1.515(6)
C3	C7	1.507(6)	C27	C48	1.543(6)
C3	C19	1.334(6)	C27	C60	1.538(6)
C4	C5	1.539(5)	C29	C55	1.515(6)
C4	C7	1.557(5)	C30	C44	1.543(6)
C4	C31	1.541(6)	C30	C59	1.530(6)
C4	C53	1.545(6)	C30	C69	1.554(7)
C5	C45	1.547(6)	C32	C58	1.530(6)
C6	C15	1.535(5)	C33	C64	1.522(6)
C6	C22	1.558(6)	C34	C35	1.528(6)
C6	C27	1.561(5)	C34	C43	1.553(6)
C7	C37	1.541(6)	C36	C39	1.538(7)
C7	C62	1.553(6)	C36	C64	1.552(6)
O6	C78	1.495(9)	C36	C72	1.542(6)
C8	C20	1.518(6)	C37	C61	1.537(6)
C8	C30	1.546(6)	C38	C43	1.536(7)
C8	C47	1.552(6)	C39	C65	1.552(6)
C8	C56	1.526(6)	C40	C46	1.511(6)

C9	C15	1.496(6)	C40	C52	1.531(6)
C10	C11	1.552(6)	C41	C42	1.543(7)
C10	C13	1.531(6)	C41	C67	1.527(7)
C10	C20	1.521(6)	C41	C75	1.539(7)
C11	C21	1.559(5)	C42	C63	1.502(6)
C11	C25	1.540(6)	C43	C51	1.535(6)
C11	C70	1.544(6)	C43	C58	1.550(6)
C12	C18	1.543(5)	C48	C55	1.527(6)
C12	C28	1.547(6)	C49	C50	1.555(6)
C13	C44	1.548(7)	C52	C53	1.545(6)
C14	C26	1.540(6)	C52	C73	1.528(6)
C14	C34	1.563(5)	C53	C61	1.559(6)
C14	C66	1.536(6)	C56	C71	1.532(8)
C16	C20	1.327(6)	C69	C71	1.567(7)
C16	C57	1.496(7)	C69	C74	1.535(7)
C17	C49	1.535(6)	C74	C76	1.525(8)
C17	C65	1.549(7)	C74	C77	1.589(10)
C18	C24	1.534(6)	C77	C78	1.486(10)
C18	C39	1.563(6)			

Table S2-4. Bond Angles for new compound **1**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C9	C1	C23	120.2(4)	C48	C27	C23	108.9(3)
C9	C1	C49	122.4(3)	C60	C27	C6	112.5(4)
C49	C1	C23	117.3(3)	C60	C27	C23	110.2(4)
C3	C2	C14	112.1(3)	C60	C27	C48	110.3(4)
C3	C2	C45	111.8(3)	C23	C28	C12	115.6(3)
C45	C2	C14	114.3(3)	O2	C29	C22	113.0(3)
C7	C3	C2	117.7(3)	O2	C29	C55	108.0(3)
C19	C3	C2	120.5(4)	C55	C29	C22	111.6(4)
C19	C3	C7	121.6(4)	C8	C30	C69	101.2(4)
C5	C4	C7	109.5(3)	C44	C30	C8	110.0(3)
C5	C4	C31	109.5(3)	C44	C30	C69	116.7(4)
C5	C4	C53	117.4(3)	C59	C30	C8	110.2(4)
C31	C4	C7	110.2(3)	C59	C30	C44	109.5(4)
C31	C4	C53	108.4(3)	C59	C30	C69	108.9(4)
C53	C4	C7	101.4(3)	C26	C32	C58	112.0(4)
C4	C5	C45	114.7(3)	O4	C33	C64	113.3(4)
C15	C6	C22	113.3(3)	C35	C34	C14	111.3(3)
C15	C6	C27	111.0(3)	C35	C34	C43	112.8(3)
C22	C6	C27	117.7(3)	C43	C34	C14	117.4(3)
C3	C7	C4	111.4(3)	C19	C35	C34	113.9(3)
C3	C7	C37	117.7(3)	C39	C36	C64	111.7(4)
C3	C7	C62	107.1(3)	C39	C36	C72	113.3(4)
C37	C7	C4	101.9(3)	C72	C36	C64	109.7(4)
C37	C7	C62	106.4(3)	C61	C37	C7	104.8(3)
C62	C7	C4	112.4(3)	C36	C39	C18	118.8(4)
C20	C8	C30	111.4(3)	C36	C39	C65	112.7(4)
C20	C8	C47	106.5(3)	C65	C39	C18	102.6(3)
C20	C8	C56	117.5(3)	C46	C40	C52	114.2(4)

C30	C8	C47	112.1(3)	C42	C41	C21	108.0(3)
C56	C8	C30	102.7(3)	C67	C41	C21	115.7(4)
C56	C8	C47	106.8(4)	C67	C41	C42	110.0(4)
C1	C9	C15	124.8(4)	C67	C41	C75	107.3(4)
C13	C10	C11	114.8(3)	C75	C41	C21	108.4(4)
C20	C10	C11	110.6(3)	C75	C41	C42	107.1(4)
C20	C10	C13	114.0(4)	O5	C42	C41	112.2(4)
C10	C11	C21	106.7(3)	O5	C42	C63	111.7(4)
C25	C11	C10	109.4(3)	C63	C42	C41	113.1(4)
C25	C11	C21	109.2(3)	C38	C43	C34	116.2(4)
C25	C11	C70	109.9(4)	C38	C43	C58	110.1(4)
C70	C11	C10	109.7(4)	C51	C43	C34	108.6(3)
C70	C11	C21	111.8(4)	C51	C43	C38	106.4(4)
C18	C12	C28	114.2(3)	C51	C43	C58	108.2(4)
C10	C13	C44	116.5(4)	C58	C43	C34	107.1(3)
C2	C14	C34	106.4(3)	C30	C44	C13	114.6(4)
C26	C14	C2	108.6(3)	C5	C45	C2	115.8(3)
C26	C14	C34	108.3(3)	O1	C46	C40	108.9(4)
C66	C14	C2	109.8(4)	C55	C48	C27	114.9(4)
C66	C14	C26	111.0(4)	C1	C49	C17	117.7(3)
C66	C14	C34	112.5(3)	C1	C49	C18	110.6(3)
C9	C15	C6	113.3(3)	C1	C49	C50	107.8(4)
C20	C16	C57	125.6(4)	C17	C49	C18	102.1(3)
C49	C17	C65	104.7(3)	C17	C49	C50	106.4(3)
C12	C18	C39	116.7(3)	C50	C49	C18	112.0(3)
C12	C18	C49	109.3(3)	C40	C52	C53	111.0(4)
C24	C18	C12	110.2(3)	C73	C52	C40	110.5(3)
C24	C18	C39	108.2(3)	C73	C52	C53	113.5(4)
C24	C18	C49	110.5(3)	C4	C53	C52	119.9(3)
C39	C18	C49	101.5(3)	C4	C53	C61	103.2(3)
C3	C19	C35	125.1(4)	C52	C53	C61	112.2(3)

C8	C20	C10	116.4(3)	C29	C55	C48	110.7(4)
C16	C20	C8	124.1(4)	C8	C56	C71	105.0(4)
C16	C20	C10	119.5(4)	C16	C57	C21	114.1(4)
C41	C21	C11	117.4(3)	O3	C58	C32	111.7(4)
C57	C21	C11	110.7(4)	O3	C58	C43	112.5(4)
C57	C21	C41	113.4(4)	C32	C58	C43	111.8(4)
C29	C22	C6	106.4(3)	C37	C61	C53	106.9(3)
C54	C22	C6	108.7(3)	C42	C63	C25	112.5(4)
C54	C22	C29	108.2(4)	C33	C64	C36	113.5(4)
C54	C22	C68	106.7(4)	C17	C65	C39	107.6(3)
C68	C22	C6	116.4(4)	C30	C69	C71	102.6(4)
C68	C22	C29	110.3(4)	C74	C69	C30	122.8(5)
C1	C23	C27	112.5(3)	C74	C69	C71	112.4(4)
C1	C23	C28	112.0(3)	C56	C71	C69	106.9(4)
C28	C23	C27	114.9(3)	C69	C74	C77	108.0(5)
C63	C25	C11	113.6(4)	C76	C74	C69	114.1(4)
C32	C26	C14	114.6(4)	C76	C74	C77	109.1(5)
C23	C27	C6	105.9(3)	C78	C77	C74	117.5(7)
C48	C27	C6	108.9(3)	C77	C78	O6	110.5(6)

Table S2-5. Torsion Angles for new compound **1**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O2	C29	C55	C48	-173.9(4)	C26	C32	C58	C43	58.3(5)
O4	C33	C64	C36	177.2(4)	C27	C6	C15	C9	-40.9(5)
O5	C42	C63	C25	-174.7(4)	C27	C6	C22	C29	53.0(5)
C1	C9	C15	C6	9.8(6)	C27	C6	C22	C54	169.3(4)
C1	C23	C27	C6	-55.0(4)	C27	C6	C22	C68	-70.3(5)
C1	C23	C27	C48	-172.0(3)	C27	C23	C28	C12	178.6(3)
C1	C23	C27	C60	66.9(4)	C27	C48	C55	C29	-55.5(5)
C1	C23	C28	C12	48.7(5)	C28	C12	C18	C24	86.3(4)
C2	C3	C7	C4	-33.3(5)	C28	C12	C18	C39	-149.7(4)
C2	C3	C7	C37	-150.3(4)	C28	C12	C18	C49	-35.3(5)
C2	C3	C7	C62	90.0(4)	C28	C23	C27	C6	175.4(3)
C2	C3	C19	C35	-0.7(6)	C28	C23	C27	C48	58.4(4)
C2	C14	C26	C32	163.6(4)	C28	C23	C27	C60	-62.8(4)
C2	C14	C34	C35	61.4(4)	C30	C8	C20	C10	-38.2(5)
C2	C14	C34	C43	-166.5(3)	C30	C8	C20	C16	144.2(4)
C3	C2	C14	C26	-170.2(3)	C30	C8	C56	C71	35.0(4)
C3	C2	C14	C34	-53.7(4)	C30	C69	C71	C56	-18.8(5)
C3	C2	C14	C66	68.3(4)	C30	C69	C74	C76	45.4(8)
C3	C2	C45	C5	47.3(5)	C30	C69	C74	C77	167.0(5)
C3	C7	C37	C61	157.3(4)	C31	C4	C5	C45	85.5(4)
C3	C19	C35	C34	7.9(6)	C31	C4	C7	C3	-58.3(4)
C4	C5	C45	C2	-18.0(5)	C31	C4	C7	C37	68.0(4)
C4	C7	C37	C61	35.3(4)	C31	C4	C7	C62	-178.5(4)
C4	C53	C61	C37	-18.4(4)	C31	C4	C53	C52	49.4(5)
C5	C4	C7	C3	62.3(4)	C31	C4	C53	C61	-76.3(4)
C5	C4	C7	C37	-171.4(3)	C34	C14	C26	C32	48.4(5)
C5	C4	C7	C62	-57.9(4)	C34	C43	C58	O3	177.7(3)
C5	C4	C53	C52	-75.3(5)	C34	C43	C58	C32	-55.5(5)

C5	C4	C53	C61	159.0(4)	C35	C34	C43	C38	61.7(5)
C6	C22	C29	O2	179.8(3)	C35	C34	C43	C51	-58.1(5)
C6	C22	C29	C55	-58.2(4)	C35	C34	C43	C58	-174.8(4)
C6	C27	C48	C55	46.6(5)	C36	C39	C65	C17	-147.5(4)
C7	C3	C19	C35	174.7(4)	C38	C43	C58	O3	-55.1(5)
C7	C4	C5	C45	-35.5(5)	C38	C43	C58	C32	71.6(5)
C7	C4	C53	C52	165.5(3)	C39	C18	C49	C1	-172.4(3)
C7	C4	C53	C61	39.8(4)	C39	C18	C49	C17	-46.3(4)
C7	C37	C61	C53	-10.6(5)	C39	C18	C49	C50	67.2(4)
C8	C30	C44	C13	-33.4(5)	C39	C36	C64	C33	-69.4(5)
C8	C30	C69	C71	39.7(4)	C40	C52	C53	C4	179.1(3)
C8	C30	C69	C74	167.2(4)	C40	C52	C53	C61	-59.6(5)
C8	C56	C71	C69	-9.9(5)	C41	C21	C57	C16	-169.1(4)
C9	C1	C23	C27	26.6(5)	C41	C42	C63	C25	57.6(5)
C9	C1	C23	C28	157.7(4)	C43	C34	C35	C19	-173.5(3)
C9	C1	C49	C17	30.7(6)	C44	C30	C69	C71	159.1(4)
C9	C1	C49	C18	147.5(4)	C44	C30	C69	C74	-73.4(6)
C9	C1	C49	C50	-89.6(5)	C45	C2	C3	C7	-20.4(5)
C10	C11	C21	C41	-166.6(3)	C45	C2	C3	C19	155.2(4)
C10	C11	C21	C57	61.0(4)	C45	C2	C14	C26	61.2(5)
C10	C11	C25	C63	165.0(4)	C45	C2	C14	C34	177.6(3)
C10	C13	C44	C30	-18.5(6)	C45	C2	C14	C66	-60.3(4)
C11	C10	C13	C44	172.7(4)	C46	C40	C52	C53	-70.2(5)
C11	C10	C20	C8	-145.2(3)	C46	C40	C52	C73	56.6(5)
C11	C10	C20	C16	32.6(5)	C47	C8	C20	C10	84.3(4)
C11	C21	C41	C42	50.4(5)	C47	C8	C20	C16	-93.4(5)
C11	C21	C41	C67	-73.4(5)	C47	C8	C30	C44	-56.5(5)
C11	C21	C41	C75	166.1(4)	C47	C8	C30	C59	-177.3(4)
C11	C21	C57	C16	-34.8(5)	C47	C8	C30	C69	67.5(4)
C11	C25	C63	C42	-55.1(5)	C47	C8	C56	C71	-83.1(4)
C12	C18	C39	C36	-76.7(5)	C49	C1	C9	C15	175.1(4)

C12	C18	C39	C65	158.2(4)	C49	C1	C23	C27	-151.0(3)
C12	C18	C49	C1	63.6(4)	C49	C1	C23	C28	-19.9(5)
C12	C18	C49	C17	-170.2(3)	C49	C17	C65	C39	-10.1(5)
C12	C18	C49	C50	-56.7(4)	C49	C18	C39	C36	164.5(4)
C13	C10	C11	C21	170.0(3)	C49	C18	C39	C65	39.4(4)
C13	C10	C11	C25	52.0(5)	C51	C43	C58	O3	60.8(5)
C13	C10	C11	C70	-68.6(4)	C51	C43	C58	C32	-172.5(4)
C13	C10	C20	C8	-14.2(5)	C52	C40	C46	O1	171.9(4)
C13	C10	C20	C16	163.6(4)	C52	C53	C61	C37	-148.9(4)
C14	C2	C3	C7	-150.3(3)	C53	C4	C5	C45	-150.3(4)
C14	C2	C3	C19	25.3(5)	C53	C4	C7	C3	-173.0(3)
C14	C2	C45	C5	176.2(4)	C53	C4	C7	C37	-46.7(4)
C14	C26	C32	C58	-54.9(5)	C53	C4	C7	C62	66.8(4)
C14	C34	C35	C19	-39.1(5)	C54	C22	C29	O2	63.1(5)
C14	C34	C43	C38	-69.7(5)	C54	C22	C29	C55	-174.9(4)
C14	C34	C43	C51	170.5(4)	C56	C8	C20	C10	-156.2(4)
C14	C34	C43	C58	53.8(5)	C56	C8	C20	C16	26.1(6)
C15	C6	C22	C29	-175.3(3)	C56	C8	C30	C44	-170.7(4)
C15	C6	C22	C54	-59.0(5)	C56	C8	C30	C59	68.5(4)
C15	C6	C22	C68	61.4(5)	C56	C8	C30	C69	-46.7(4)
C15	C6	C27	C23	62.9(4)	C57	C16	C20	C8	172.7(4)
C15	C6	C27	C48	179.8(4)	C57	C16	C20	C10	-4.9(7)
C15	C6	C27	C60	-57.6(5)	C57	C21	C41	C42	-178.5(4)
C18	C12	C28	C23	-19.5(5)	C57	C21	C41	C67	57.7(5)
C18	C39	C65	C17	-18.5(4)	C57	C21	C41	C75	-62.8(5)
C19	C3	C7	C4	151.2(4)	C59	C30	C44	C13	87.8(5)
C19	C3	C7	C37	34.1(6)	C59	C30	C69	C71	-76.3(4)
C19	C3	C7	C62	-85.5(5)	C59	C30	C69	C74	51.2(6)
C20	C8	C30	C44	62.7(4)	C60	C27	C48	C55	-77.3(5)
C20	C8	C30	C59	-58.1(5)	C62	C7	C37	C61	-82.7(4)
C20	C8	C30	C69	-173.3(3)	C64	C36	C39	C18	-179.3(3)

C20	C8	C56	C71	157.6(4)	C64	C36	C39	C65	-59.3(5)
C20	C10	C11	C21	-59.3(4)	C65	C17	C49	C1	156.0(4)
C20	C10	C11	C25	-177.4(3)	C65	C17	C49	C18	34.7(4)
C20	C10	C11	C70	62.0(4)	C65	C17	C49	C50	-82.9(4)
C20	C10	C13	C44	43.7(5)	C66	C14	C26	C32	-75.6(5)
C20	C16	C57	C21	6.1(7)	C66	C14	C34	C35	-58.9(5)
C21	C11	C25	C63	48.5(5)	C66	C14	C34	C43	73.2(5)
C21	C41	C42	O5	179.3(3)	C67	C41	C42	O5	-53.5(5)
C21	C41	C42	C63	-53.2(5)	C67	C41	C42	C63	73.9(5)
C22	C6	C15	C9	-175.8(3)	C68	C22	C29	O2	-53.1(5)
C22	C6	C27	C23	-164.4(3)	C68	C22	C29	C55	68.9(5)
C22	C6	C27	C48	-47.4(5)	C69	C30	C44	C13	-147.9(4)
C22	C6	C27	C60	75.2(5)	C69	C74	C77	C78	162.2(6)
C22	C29	C55	C48	61.3(5)	C70	C11	C21	C41	73.4(5)
C23	C1	C9	C15	-2.4(6)	C70	C11	C21	C57	-58.9(5)
C23	C1	C49	C17	-151.7(4)	C70	C11	C25	C63	-74.5(5)
C23	C1	C49	C18	-34.9(5)	C71	C69	C74	C76	168.6(5)
C23	C1	C49	C50	88.0(4)	C71	C69	C74	C77	-69.9(6)
C23	C27	C48	C55	161.6(4)	C72	C36	C39	C18	56.2(5)
C24	C18	C39	C36	48.2(5)	C72	C36	C39	C65	176.3(4)
C24	C18	C39	C65	-76.9(4)	C72	C36	C64	C33	57.1(5)
C24	C18	C49	C1	-57.8(4)	C73	C52	C53	C4	53.9(5)
C24	C18	C49	C17	68.3(4)	C73	C52	C53	C61	175.3(4)
C24	C18	C49	C50	-178.2(4)	C74	C69	C71	C56	-152.7(5)
C25	C11	C21	C41	-48.4(5)	C74	C77	C78	O6	-80.9(8)
C25	C11	C21	C57	179.2(4)	C75	C41	C42	O5	62.8(5)
C26	C14	C34	C35	178.0(4)	C75	C41	C42	C63	-169.8(4)
C26	C14	C34	C43	-49.9(5)	C76	C74	C77	C78	-73.1(8)
C26	C32	C58	O3	-174.5(4)					

Table S2-6. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for new compound **1**.

Atom	*x*	*y*	*z*	U(eq)
H1	10748.88	5042.38	-344.46	83
H2A	2872.19	1207.73	219.95	85
H3	2468.18	6078.88	9507.13	90
H4	959.92	2874.73	9849.19	86
H5	4586.12	9006.82	9843.79	88
H2	4315.3	5474.27	5445.79	50
H5A	4978.03	6918.52	3717.45	52
H5B	6585.4	6696.79	3548.37	52
H6	1813.92	2375.84	2853.16	49
H6A	13571.17	7255.21	162.36	135
H9	2047.67	4435.61	4272.78	52
H10	7628.09	7831.51	5829.43	50
H12A	1933.37	-19	5852.15	54
H12B	3162.69	193.67	6057.15	54
H13A	7108.79	10347.56	5419.17	59
H13B	6137.8	9614.05	5455.36	59
H15A	3497.54	3757.87	2675.86	55
H15B	1837.53	4290.04	2839.25	55
H16	11156.17	7202.6	5839.31	61
H17A	369.25	4415.69	5814.16	60
H17B	1688.37	4565.33	5957.55	60
H19	7334.92	2462.28	5289.95	52
H21	7710.79	7114.88	7173.12	55
H23	1834.11	1399.1	4136.04	49
H24A	202.62	2130.17	5268.4	69
H24B	-599.97	2981.51	6184.34	69
H24C	-322.62	1535.84	6215.81	69
H25A	5179.64	10180.97	6999.25	61

H25B	5378.52	8758.32	6978.99	61
H26A	3894.92	7525.74	6696.67	59
H26B	2913.06	6837.86	6656.52	59
H28A	4331.03	249.51	4612.01	56
H28B	3421.55	-436.49	4452.15	56
H29	2240.77	1049.37	1633.36	57
H31A	4438.34	4824.94	4278.47	71
H31B	5308.32	3928.22	3385.6	71
H31C	4425.92	5371.44	3307.9	71
H32A	2154.89	7632.08	8124.75	62
H32B	3716.48	6953.18	8178.49	62
H33A	1514.49	735.87	9067.11	62
H33B	2102.39	1755.06	8553.95	62
H34	3899.87	4449.45	6757.96	49
H35A	6619.88	3099.68	6876.65	55
H35B	5583.54	2561.11	6711.31	55
H36	-787.2	2183.18	7735.57	59
H37A	8669.49	2307.3	3623.77	58
H37B	7076.55	2496.88	3740.15	58
H38A	5936.84	3707.25	8284.49	86
H38B	4608	4369.56	9165.8	86
H38C	5266.36	5188.41	8420.33	86
H39	2113.96	1889.71	7152.01	54
H40A	8491.65	3767.11	844.99	58
H40B	7560.92	4824.68	345.8	58
H42	5454.41	7580.77	8405.21	61
H44A	7254.46	8955.66	4030.77	61
H44B	7801.26	10051.79	3945.88	61
H45A	4633.99	7316.41	5133.64	60
H45B	6279.78	6654.58	5001.84	60
H46A	8565.74	6176.27	491.86	59

H46B	9367.89	5239.51	1119.62	59
H47A	9097.56	10348.02	4782.63	79
H47B	10634.98	9939.52	4025.52	79
H47C	10479.92	9802.99	5075.23	79
H48A	4498.29	-669.39	2890.65	59
H48B	2871.46	-54.41	2964.88	59
H50A	4268.44	1590.24	5397.16	76
H50B	3535.13	2587.97	6229.05	76
H50C	4083.96	3004.71	5215.67	76
H51A	2997.97	3398.05	7971.65	81
H51B	3052.9	3522.53	8959.68	81
H51C	4432.22	2645.44	8186.17	81
H52	6092.88	4744.28	1784.04	57
H53	8095.65	4993.65	2459.73	52
H54A	1148.95	3309.48	1614.83	79
H54B	2283.02	3254.07	632.52	79
H54C	2064.56	4143.07	1426.29	79
H55A	5197.78	-79.37	1389.2	63
H55B	4228.21	-842.53	1480.65	63
H56A	11854.25	6706.84	4233.06	65
H56B	12319.51	7844.27	4245.56	65
H57A	9761.3	7803.6	7433.41	66
H57B	9918.04	6454.14	7184.29	66
H58	2034.2	5686.37	8030.35	60
H59A	9000.73	6785.82	4571.47	89
H59B	10360.21	6402.62	3669.69	89
H59C	8805.87	6966.59	3598.85	89
H60A	5587.79	563.96	3300.31	77
H60B	5025.8	2028.67	3164.52	77
H60C	5700.21	1079.04	2308.07	77
H61A	7594.31	2856.6	2259.05	57

H61B	9056.75	2935.59	2200.01	57
H62A	8210.33	5215.25	4285.99	76
H62B	9095.37	4372.31	3367.41	76
H62C	9086.92	3760.01	4322.61	76
H63A	5059.86	10106.41	8507.84	66
H63B	3918.72	9635.46	8420.4	66
H64A	-271.45	3170.72	8754.69	62
H64B	-820.32	2110.73	9222.39	62
H65A	-353.19	4056.77	7299.26	62
H65B	1109.02	3949.77	7388.43	62
H66A	7110.59	4921.08	6353.49	75
H66B	6124.59	5769.92	7261.59	75
H66C	6445.77	6400.1	6304.54	75
H67A	7104.73	9504.2	8820.98	100
H67B	8533.94	8370.45	8819.7	100
H67C	7081.8	8559.06	9625.96	100
H68A	4640.48	3153.49	1210.74	87
H68B	4751.55	2397.01	376.87	87
H68C	5405.41	1670.86	1133.16	87
H69	10222.27	9384.85	2994.57	69
H70A	8571.09	9717.92	7053.23	82
H70B	6947.5	10480.06	7631.47	82
H70C	7509.45	10621	6559.46	82
H71A	12310.76	6925.67	2743.67	71
H71B	12490.14	8208.13	2798.89	71
H72A	497.02	113.63	7263.53	87
H72B	-36.05	155.94	8347.77	87
H72C	1568.67	-34.27	7787.35	87
H73A	6564.46	6950.83	1842.03	83
H73B	5089.22	6786.1	2272.21	83
H73C	5793.78	6775.78	1195.18	83

H74	10690.4	7284.35	1983.22	88
H75A	7226.36	6469.54	9406.04	104
H75B	8764.79	6221.4	8682.13	104
H75C	7636.88	5928.03	8407.15	104
H76A	8210.14	8303.01	2527.91	121
H76B	8788.78	8522.95	1468.93	121
H76C	8322.72	9602.99	2199.81	121
H77A	10642.38	9700.15	1345.7	110
H77B	12056.79	8650.5	1438.77	110
H78A	11824.22	8955.62	-60.23	112
H78B	10803.62	8209.02	282.7	112