

Supporting Information

Antibacterial Balsacones J-M, Hydroxycinnamoylated

Dihydrochalcones from *Populus balsamifera* Buds

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Table of Content

Figure S-1. ^1H NMR spectrum (acetone- d_6 , 400 MHz) of (+)- 1	S3
Figure S-2. ^{13}C NMR spectrum (acetone- d_6 , 100 MHz) of (+)- 1	S4
Figure S-3. ^1H NMR spectrum (acetone- d_6 , 400 MHz) of (–)- 1	S5
Figure S-4. ^{13}C NMR spectrum (acetone- d_6 , 100 MHz) of (–)- 1	S6
Figure S-5. ^1H NMR spectrum (acetone- d_6 , 400 MHz) of (+)- 3	S7
Figure S-6. ^{13}C NMR spectrum (acetone- d_6 , 100 MHz) of (+)- 3	S8
Figure S-7. ^1H NMR spectrum (acetone- d_6 , 400 MHz) of (–)- 3	S9
Figure S-8. ^{13}C NMR spectrum (acetone- d_6 , 100 MHz) of (–)- 3	S10
Figure S-9. ^1H NMR spectrum (acetone- d_6 , 400 MHz) of (+)- 4	S11
Figure S-10. ^{13}C NMR spectrum (acetone- d_6 , 100 MHz) of (+)- 4	S12
Figure S-11. ^1H NMR spectrum (acetone- d_6 , 400 MHz) of (–)- 4	S13
Figure S-12. ^{13}C NMR spectrum (acetone- d_6 , 100 MHz) of (–)- 4	S14
Figure S-13. ^1H NMR spectrum (acetone- d_6 , 400 MHz) of (±)- 5	S15
Figure S-14. ^{13}C NMR spectrum (acetone- d_6 , 100 MHz) of (±)- 5	S16
X-ray crystallographic supplementary data of compound (–)- 1	S17
References	S20

Figure S-1. ^1H NMR spectrum (acetone- d_6 , 400 MHz) of (+)-**1**

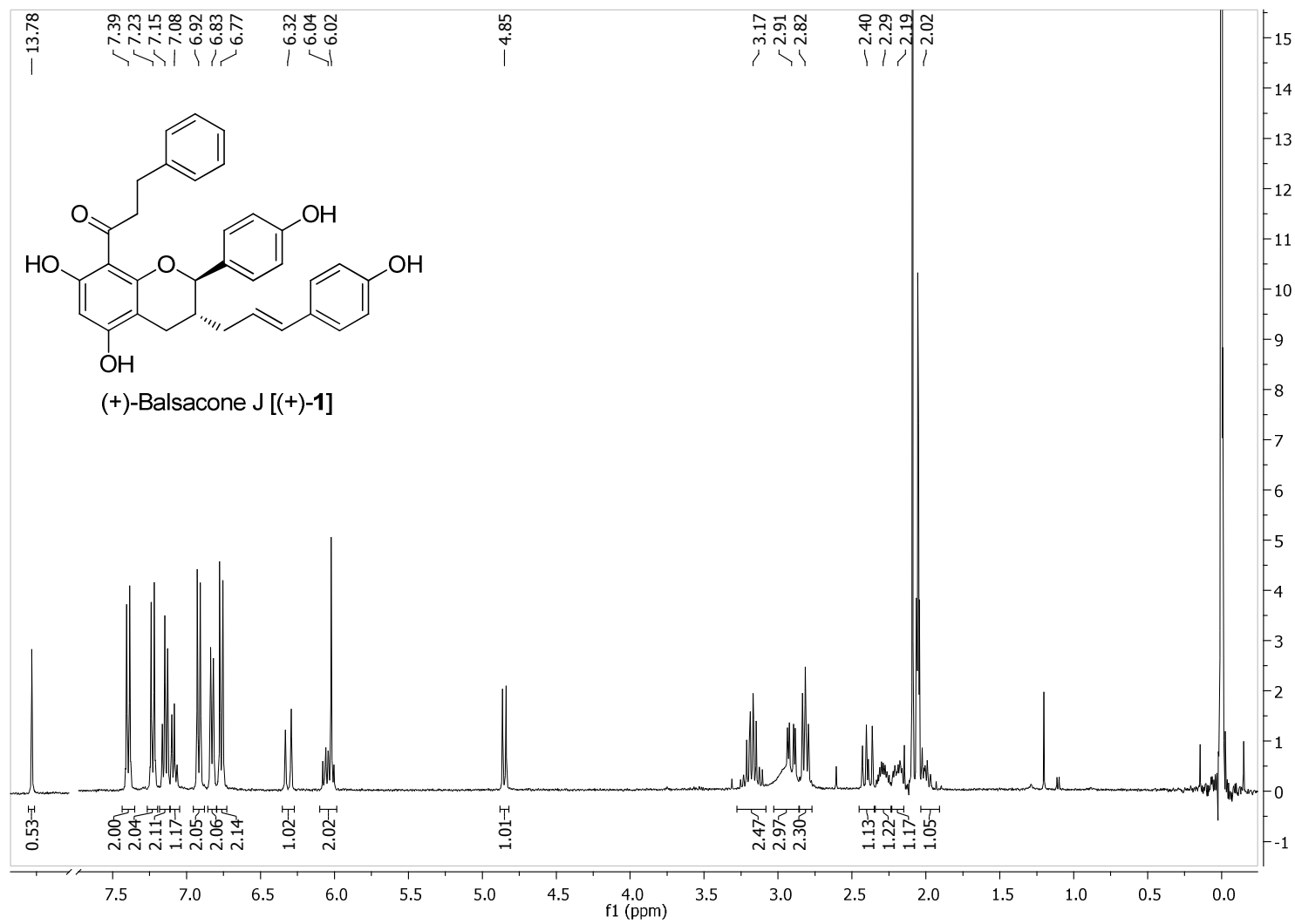


Figure S-2. ^{13}C NMR spectrum (acetone- d_6 , 100 MHz) of (+)-**1**

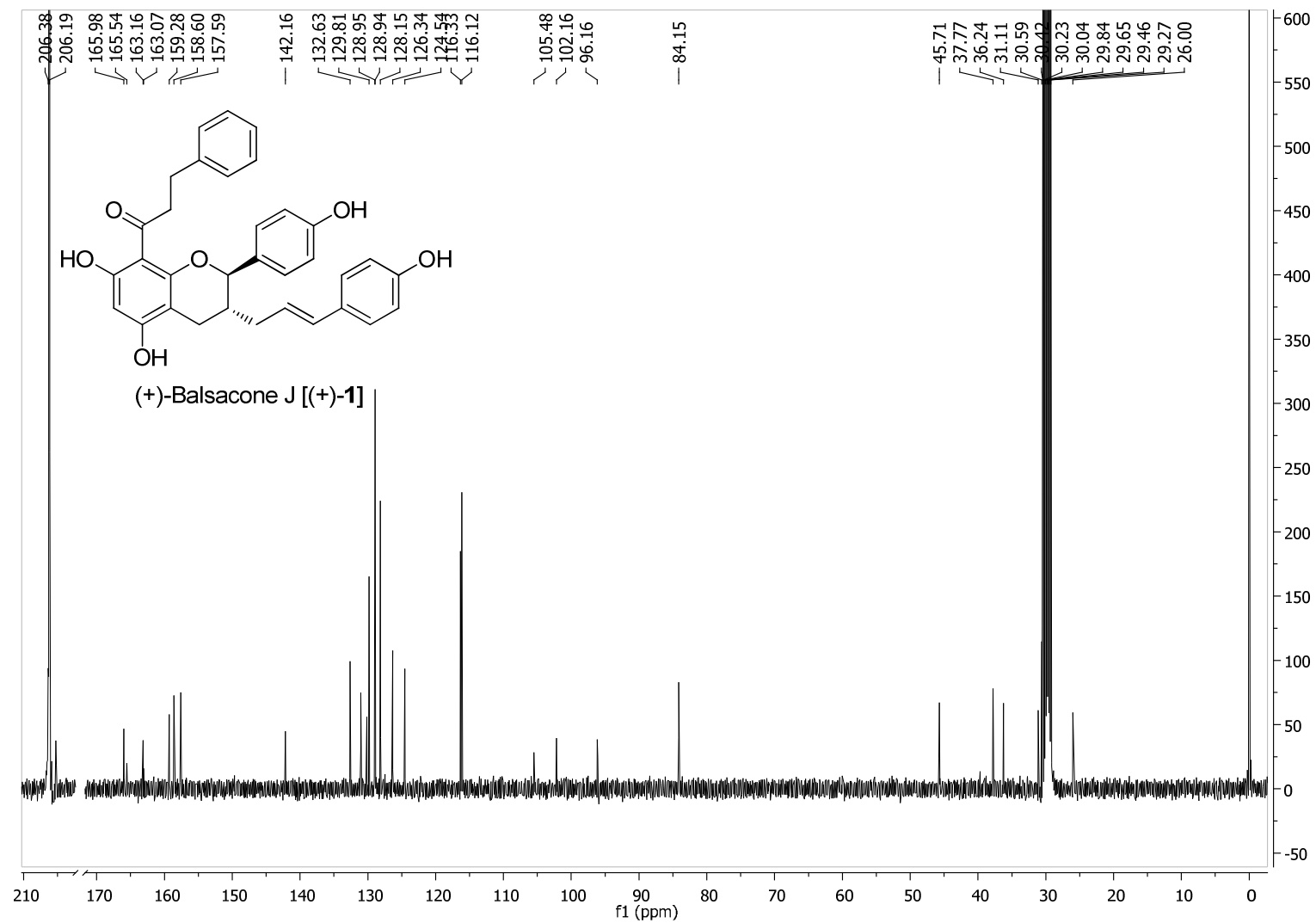


Figure S-3. ^1H NMR spectrum (acetone- d_6 , 400 MHz) of (-)-**1**

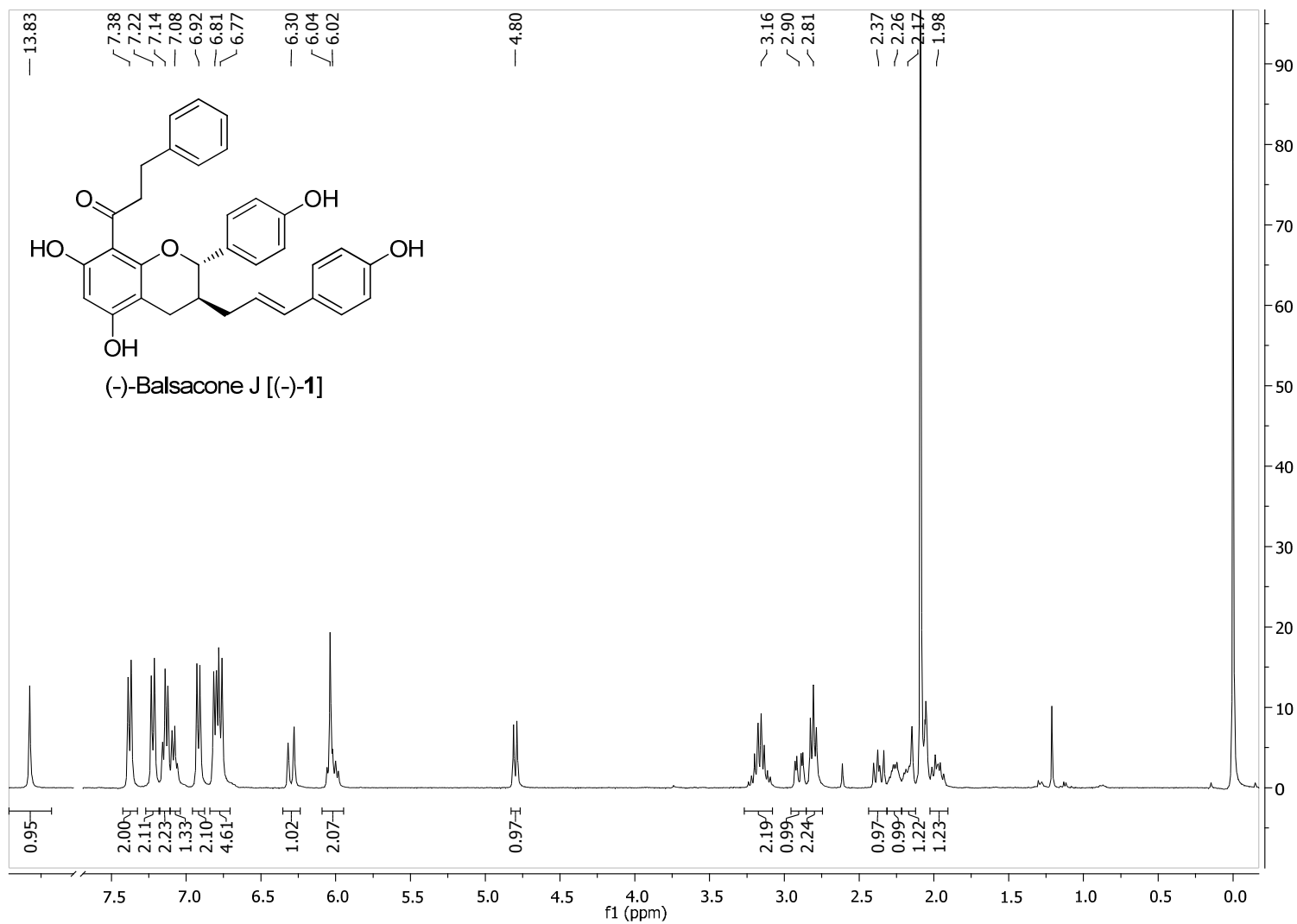


Figure S-4. ^{13}C NMR spectrum (acetone- d_6 , 100 MHz) of (-)-1

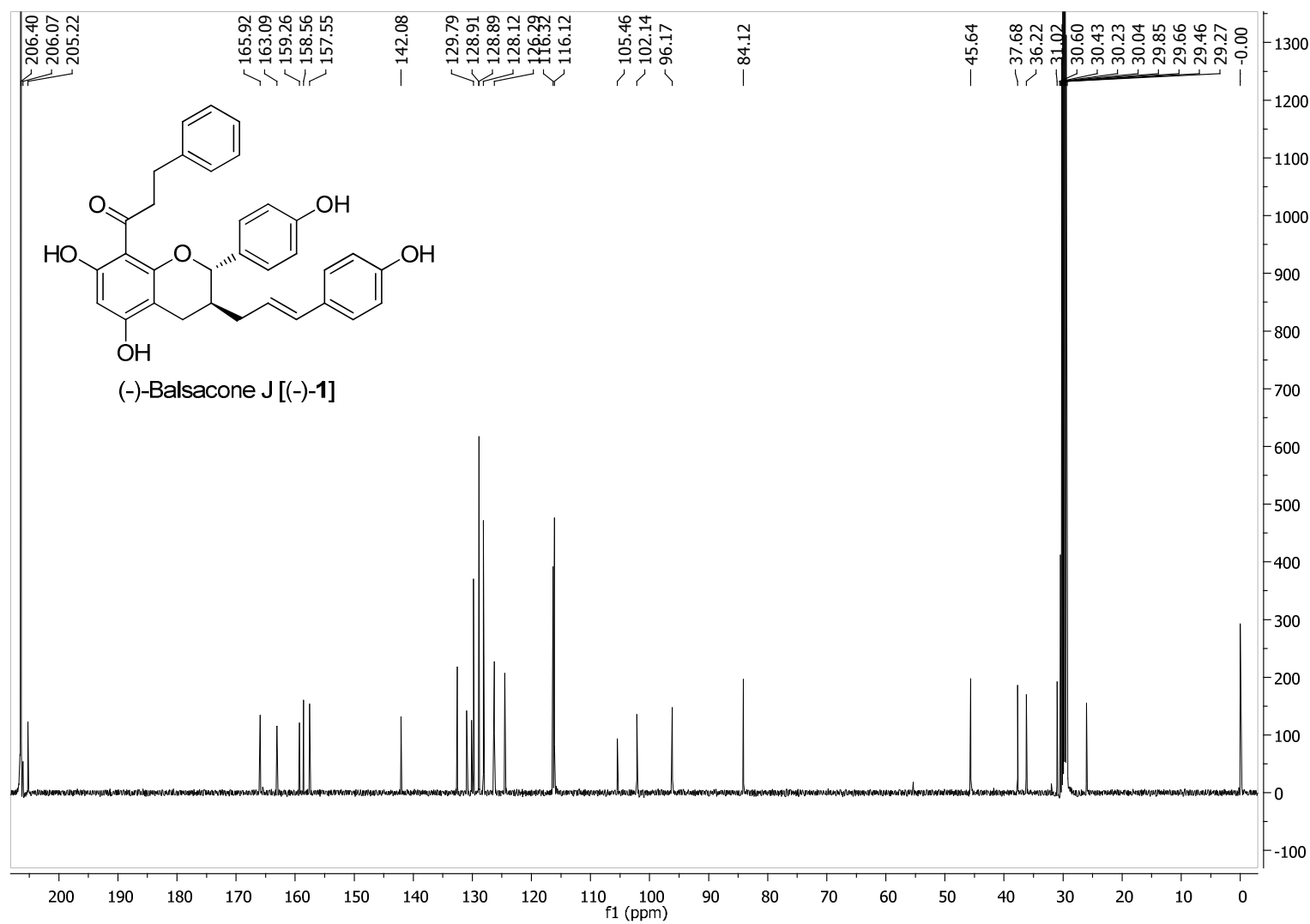


Figure S-5. ^1H NMR spectrum (acetone- d_6 , 400 MHz) of (+)-**3**

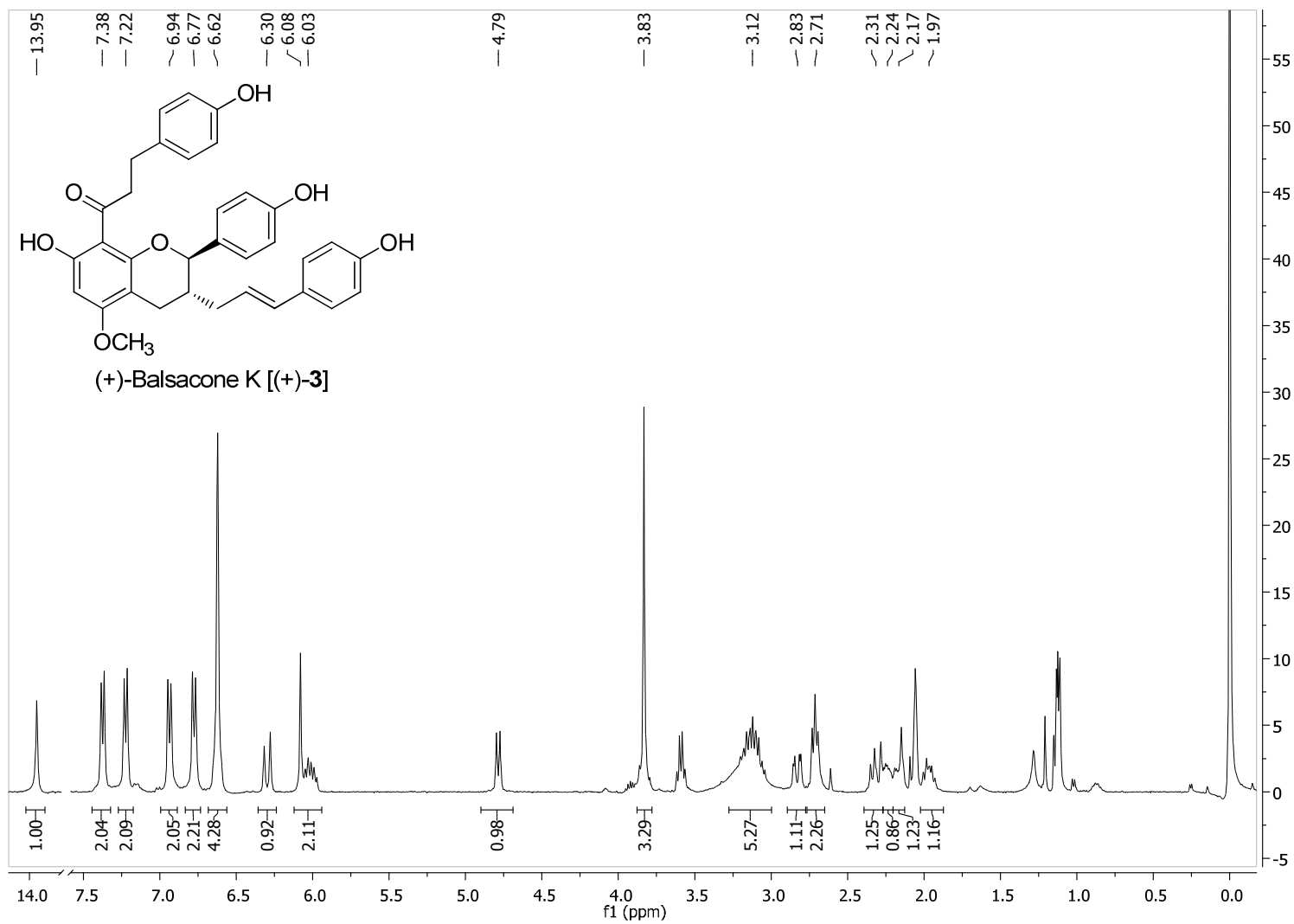


Figure S-6. ^{13}C NMR spectrum (acetone- d_6 , 100 MHz) of (+)-**3**

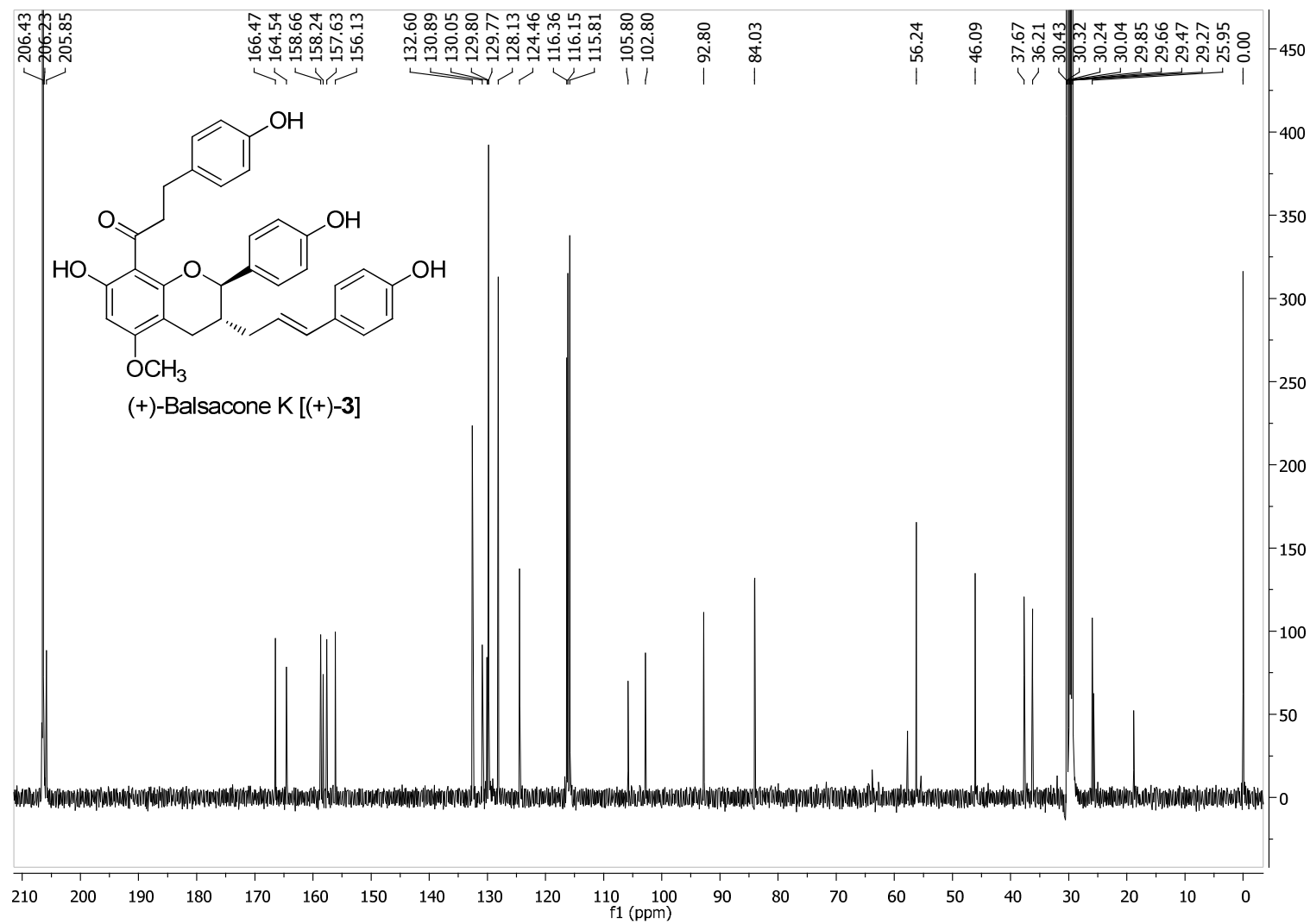


Figure S-7. ^1H NMR spectrum (acetone- d_6 , 400 MHz) of (-)-**3**

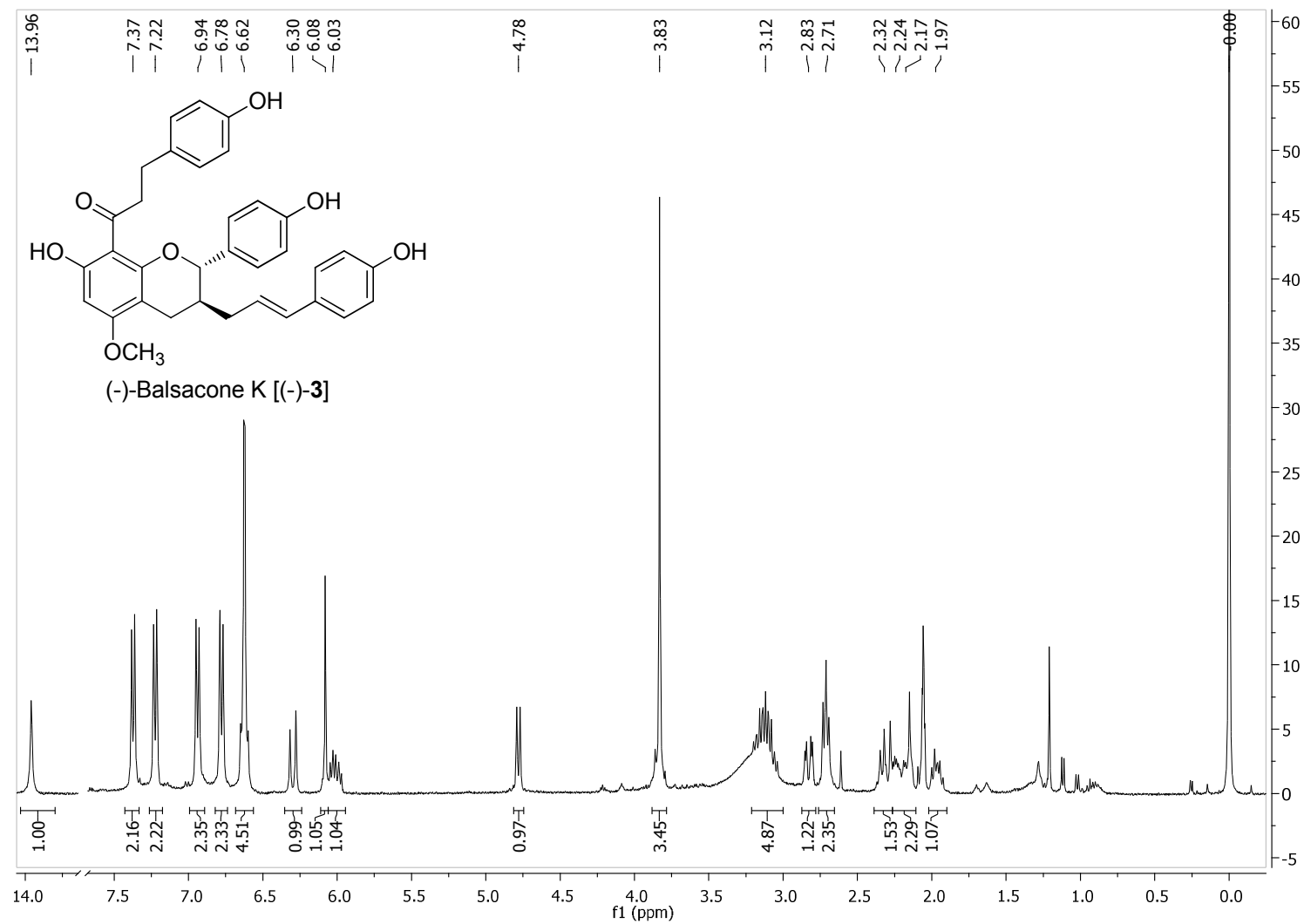


Figure S-8. ^{13}C NMR spectrum (acetone- d_6 , 100 MHz) of (-)-**3**

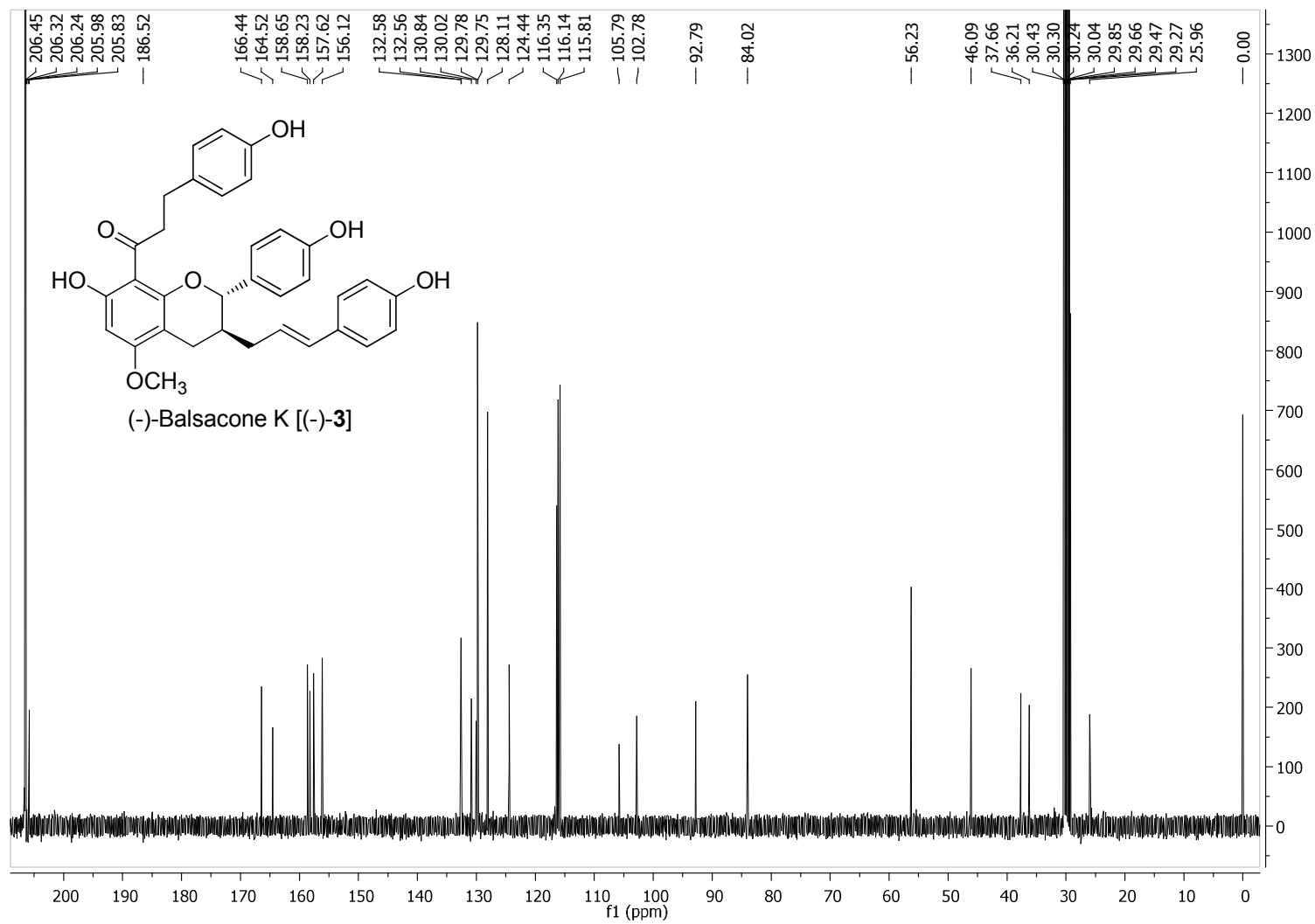


Figure S-9. ^1H NMR spectrum (acetone- d_6 , 400 MHz) of (+)-4

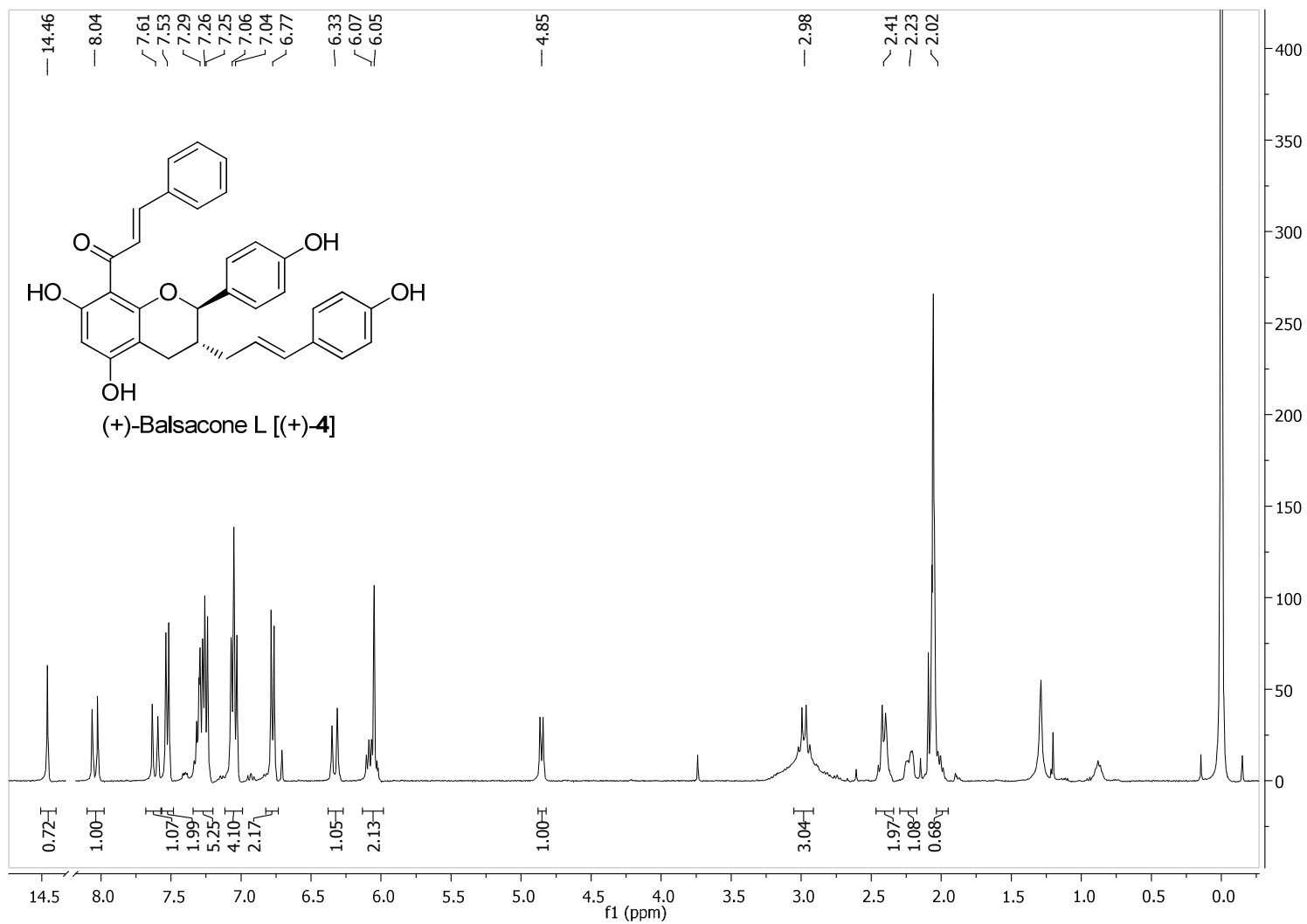


Figure S-10. ^{13}C NMR spectrum (acetone- d_6 , 100 MHz) of (+)-**4**

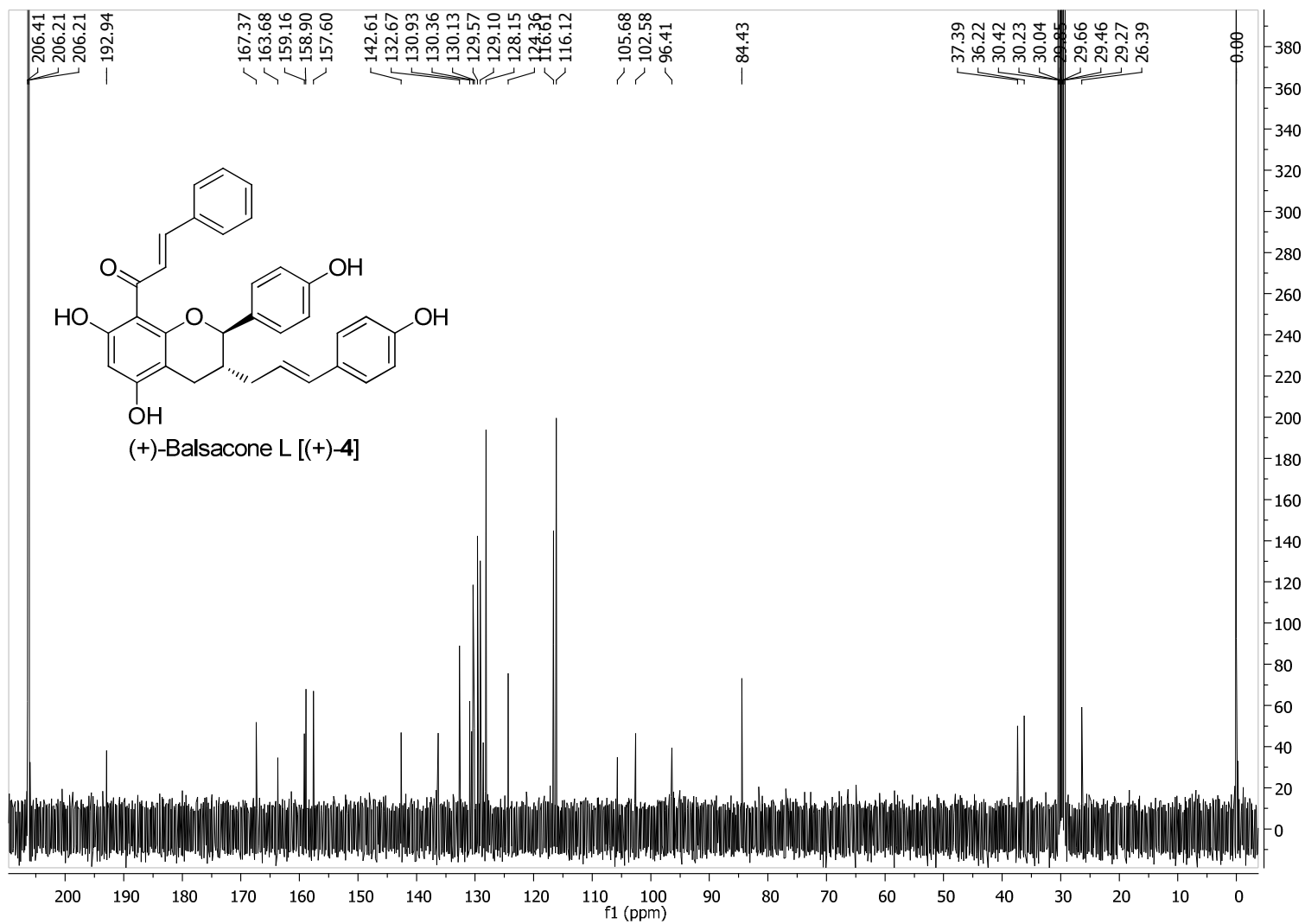


Figure S-11. ^1H NMR spectrum (acetone- d_6 , 400 MHz) of (-)-**4**

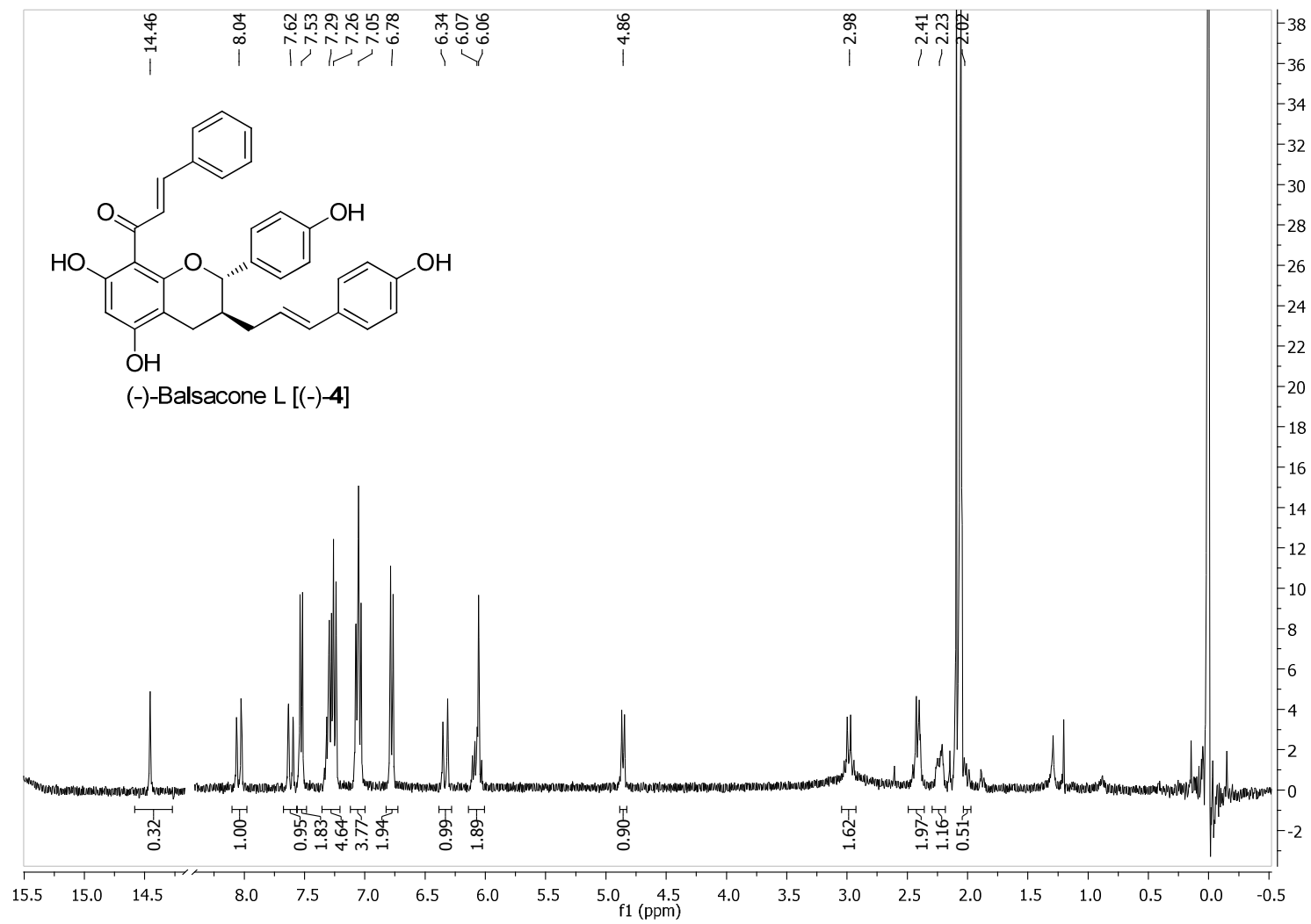


Figure S-12. ^{13}C NMR spectrum (acetone- d_6 , 100 MHz) of (-)-4

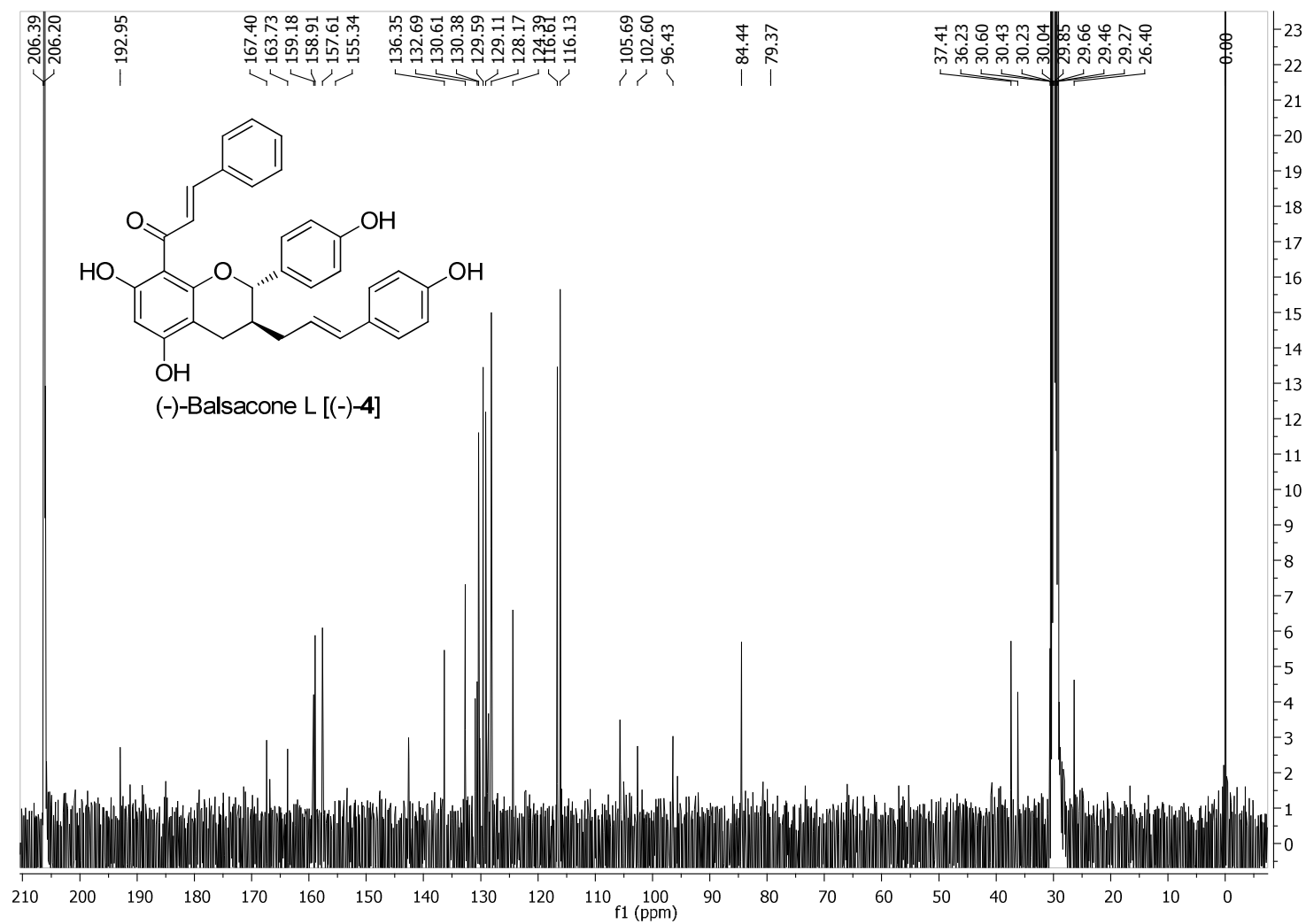


Figure S-13. ^1H NMR spectrum (acetone- d_6 , 400 MHz) of ($\pm$)-**5**

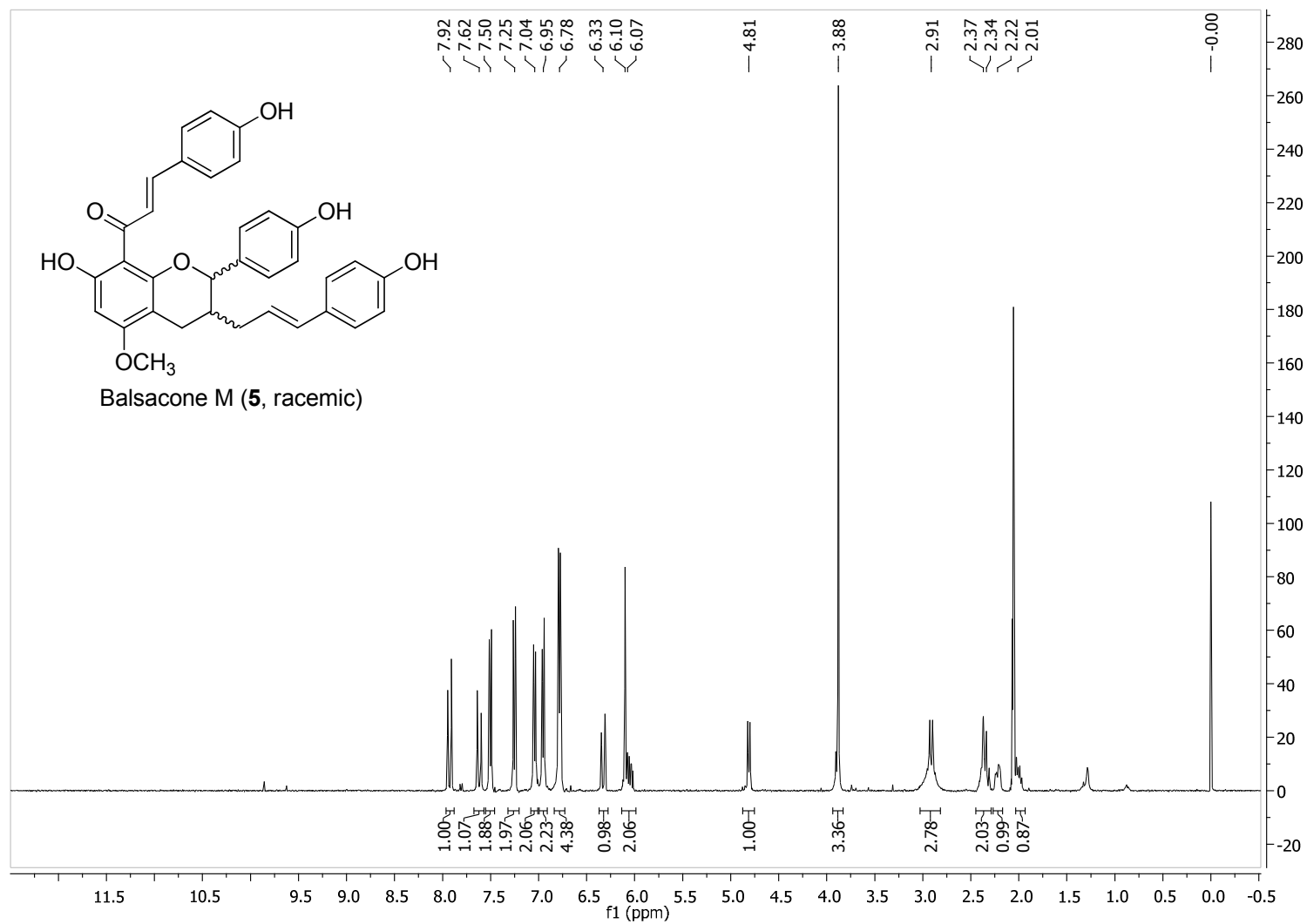
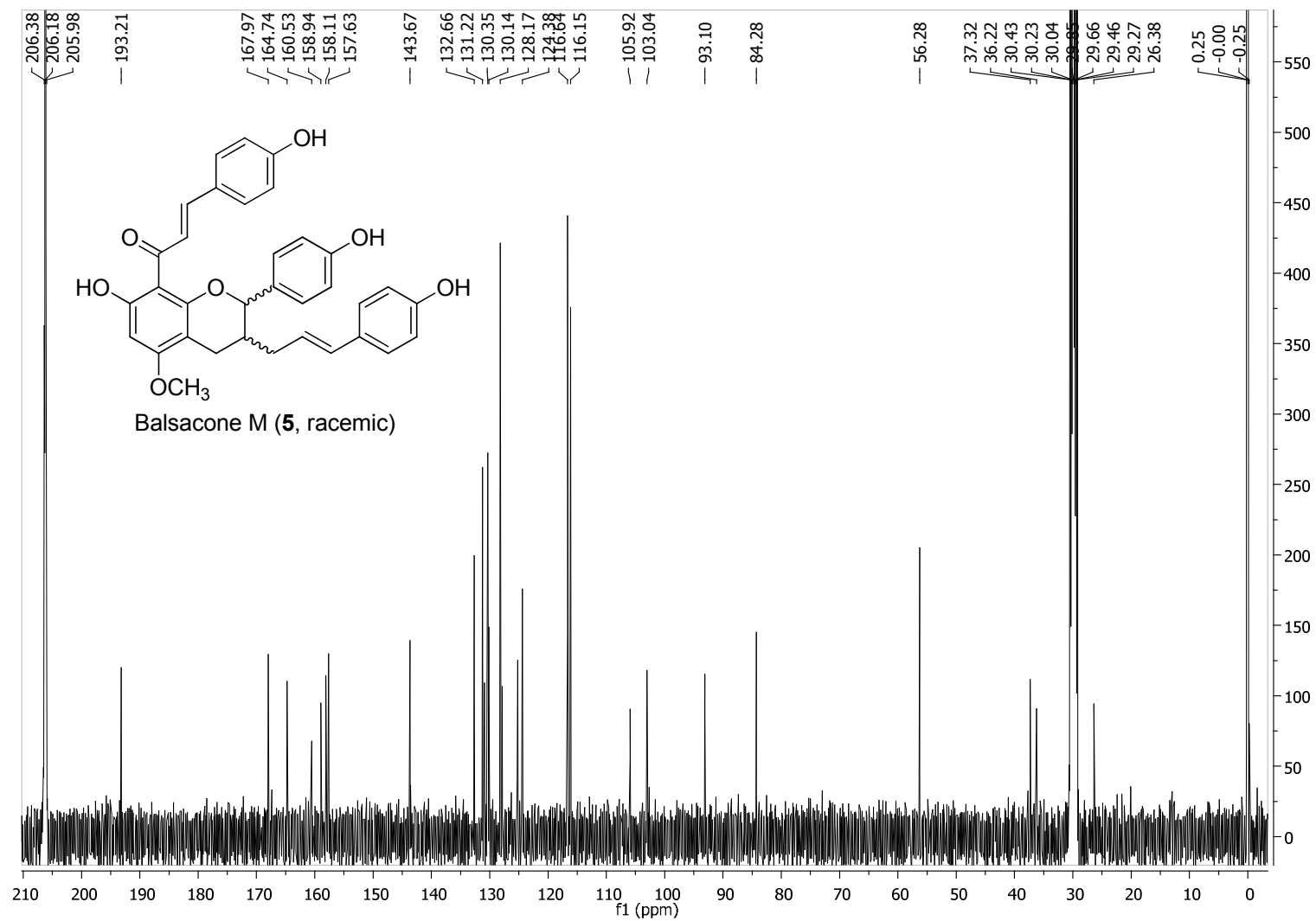


Figure S-14. ^{13}C NMR spectrum (acetone- d_6 , 100 MHz) of ($\pm$)-**5**



X-ray crystallographic supplementary data of compound (–)-1.

Chemical formula	C ₄₂ H ₅₄ O ₉
Formula weight	702.85
Crystal system	Monoclinic
Space group	C2
Unit cell dimensions	a = 32.5740(12) Å α = 90° b = 6.0055(2) Å β = 95.689(2)° c = 19.9952(7) Å γ = 90°
Z	4
Calculated density	1.199 g/cm ³
Radiation	Cu K α (λ = 1.54178 Å) at 100 K

Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for C42 H54 O9.

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	Occ.	x	y	z	U _{eq}
O(1)	1	1287(1)	1686(2)	1923(1)	37(1)
O(5)	1	1032(1)	-2212(3)	-127(1)	50(1)
O(7)	1	180(1)	-3507(3)	1625(1)	58(1)
O(11)	1	245(1)	-1031(3)	2608(1)	59(1)
O(23)	1	2320(1)	8645(2)	3657(1)	44(1)
O(4')	1	1704(1)	6558(3)	-3182(1)	47(1)
C(2)	1	1692(1)	2292(3)	1728(1)	33(1)
C(3)	1	1644(1)	3035(3)	994(1)	34(1)
C(4)	1	1502(1)	1010(3)	574(1)	39(1)
C(5)	1	923(1)	-1824(4)	500(1)	42(1)
C(6)	1	605(1)	-2962(4)	759(1)	48(1)
C(7)	1	497(1)	-2407(4)	1391(1)	47(1)
C(8)	1	709(1)	-708(4)	1786(1)	41(1)
C(9)	1	1055(1)	263(3)	1513(1)	36(1)
C(10)	1	1160(1)	-203(3)	874(1)	37(1)
C(11)	1	542(1)	-2(4)	2403(1)	45(1)
C(12)	1	700(1)	2010(4)	2791(1)	45(1)
C(13)	1	428(1)	2703(5)	3333(1)	55(1)
C(14)	1	588(1)	4612(5)	3769(1)	50(1)
C(15)	1	400(1)	5084(6)	4348(1)	69(1)
C(16)	1	531(1)	6840(6)	4757(1)	76(1)
C(17)	1	849(1)	8172(6)	4612(1)	66(1)
C(18)	1	1044(1)	7729(5)	4037(1)	57(1)

C(19)	1	913(1)	5968(5)	3629(1)	53(1)
C(20)	1	1862(1)	3975(3)	2239(1)	33(1)
C(21)	1	1668(1)	6005(3)	2309(1)	36(1)
C(22)	1	1822(1)	7547(3)	2786(1)	37(1)
C(23)	1	2178(1)	7054(3)	3203(1)	35(1)
C(24)	1	2372(1)	5023(3)	3146(1)	37(1)
C(25)	1	2214(1)	3504(3)	2664(1)	35(1)
C(1')	1	2013(1)	4753(3)	-1180(1)	35(1)
C(2')	1	2082(1)	3289(3)	-1698(1)	38(1)
C(3')	1	1974(1)	3847(3)	-2369(1)	39(1)
C(4')	1	1806(1)	5901(3)	-2528(1)	38(1)
C(5')	1	1738(1)	7401(3)	-2019(1)	43(1)
C(6')	1	1842(1)	6819(4)	-1357(1)	42(1)
C(7')	1	2113(1)	4032(3)	-476(1)	36(1)
C(8')	1	1964(1)	4914(3)	59(1)	36(1)
C(9')	1	2039(1)	4050(4)	764(1)	38(1)
O(30)	1	3156(1)	8444(3)	4110(1)	43(1)
C(30)	1	3274(1)	9341(4)	4780(1)	43(1)
C(31)	1	2999(1)	11280(5)	4868(1)	74(1)
C(32)	1	3248(1)	7580(5)	5303(1)	72(1)
O(40)	1	1317(1)	323(3)	6251(1)	50(1)
C(40)	1	990(1)	1073(4)	6627(1)	53(1)
C(41)	1	766(1)	2883(5)	6226(2)	75(1)
C(42)	1	717(1)	-825(5)	6779(2)	68(1)
O(50)	0.55	4496(3)	10107(17)	770(5)	83(4)
C(50)	0.55	4398(3)	7860(14)	849(5)	48(2)
C(51)	0.55	4764(2)	6577(12)	749(5)	98(2)
C(52)	0.55	4152(4)	7332(19)	1399(5)	134(4)
O(50')	0.45	4493(2)	10003(15)	800(6)	65(4)
C(50')	0.45	4364(4)	7940(20)	1045(6)	77(4)
C(51')	0.45	4697(3)	6287(15)	1169(5)	91(3)
C(52')	0.45	4187(4)	8600(30)	1681(5)	146(6)

Hydrogen coordinates (x 10⁴) and isotropic displacement parameters (Å² x 10³) for C42 H54 O9.

	Occ.	x	y	z	U _{eq}
H(5)	1	852	-3013	-339	75
H(7)	1	143	-3027	2009	87
H(23)	1	2572	8435	3772	66
H(4')	1	1769	5553	-3444	71

H(2)	1	1873	942	1768	40
H(3)	1	1421	4186	939	40
H(4A)	1	1404	1494	112	47
H(4B)	1	1737	-14	546	47
H(6)	1	463	-4113	506	58
H(12A)	1	719	3266	2475	54
H(12B)	1	981	1696	3004	54
H(13A)	1	153	3112	3112	65
H(13B)	1	391	1401	3624	65
H(15)	1	178	4180	4463	82
H(16)	1	396	7131	5148	92
H(17)	1	936	9381	4897	79
H(18)	1	1266	8637	3927	68
H(19)	1	1049	5676	3240	64
H(21)	1	1425	6347	2025	43
H(22)	1	1685	8929	2828	44
H(24)	1	2612	4668	3436	45
H(25)	1	2349	2116	2625	42
H(2')	1	2205	1883	-1591	45
H(3')	1	2017	2812	-2715	47
H(5')	1	1621	8820	-2128	51
H(6')	1	1796	7855	-1013	51
H(7')	1	2300	2827	-398	44
H(8')	1	1795	6200	-11	43
H(9'1)	1	2134	5283	1069	45
H(9'2)	1	2258	2905	787	45
H(30)	1	3319	7410	4031	64
H(30A)	1	3565	9883	4801	51
H(31A)	1	3045	12427	4535	111
H(31B)	1	3060	11893	5321	111
H(31C)	1	2710	10796	4806	111
H(32A)	1	2962	7069	5298	108
H(32B)	1	3339	8196	5747	108
H(32C)	1	3425	6323	5208	108
H(40)	1	1438	-762	6450	75
H(40A)	1	1115	1718	7061	64
H(41A)	1	962	4060	6134	113
H(41B)	1	551	3505	6481	113
H(41C)	1	640	2271	5800	113
H(42A)	1	599	-1501	6357	102
H(42B)	1	495	-276	7031	102
H(42C)	1	879	-1941	7047	102
H(50)	0.55	4661	10520	1096	124
H(50A)	0.55	4207	7524	438	57
H(51A)	0.55	4825	6719	280	147
H(51B)	0.55	4717	5007	851	147

H(51C)	0.55	4998	7139	1047	147
H(52A)	0.55	4335	6909	1797	201
H(52B)	0.55	3965	6093	1267	201
H(52C)	0.55	3990	8640	1503	201
H(50')	0.45	4699	10464	1047	97
H(50B)	0.45	4140	7306	722	92
H(51D)	0.45	4946	7024	1378	136
H(51E)	0.45	4755	5615	742	136
H(51F)	0.45	4611	5126	1471	136
H(52D)	0.45	4073	10104	1632	219
H(52E)	0.45	4405	8564	2056	219
H(52F)	0.45	3968	7552	1770	219

The structure was solved by direct methods SHELXS-97¹ and refined with full-matrix least-squares calculations on F² using SHELX-97¹.

References

1. Sheldrick, G. M., A short history of SHELX. *Acta Crystallographica Section A* **2008**, 64, (1), 112-122.