Novel Triterpenoids from the Aerial Roots of *Ficus microcarpa*

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^{13}C NMR spectrum of compound 1 (CDCl_3 , 100MHz)

IR spectrum of compound 1

MS spectrum of compound 1

HMQC spectrum of compound 1 (CDCl₃, 400MHz)

HMBC spectrum of compound 1 (CDCl₃, 400MHz)

COSY spectrum of compound 1 (CDCl₃, 400MHz)

NOESY spectrum of compound 1 (CDCl₃, 400MHz)

^1H spectrum of compound **2** (CDCl_3 , 400MHz)

^{13}C spectrum of compound 2 (CDCl_3 , 100MHz)

IR spectrum of compound 2

S12

MS spectrum of compound 2

S13

HMQC spectrum of compound 2 (CDCl₃, 400MHz)

HMBC spectrum of compound 2 (CDCl₃, 400MHz)

COSY spectrum of compound 2 (CDCl₃, 400MHz)

NOESY spectrum of compound 2 (CDCl₃, 400MHz)

Table 1. Crystal data and structure refinement for IC7921.

Identification code	ic7921
Diffractometer used	Nonius KappaCCD
Empirical formula	C ₃₀ H ₅₀ O ₂
Formula weight	442.70
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 ₁
Unit cell dimensions	a = 12.662(3) Å alpha = 90° b = 6.8170(14) Å beta = 94.87(3)° c = 15.405(3) Å gamma = 90°
Volume, Z	1324.9(5) Å ³ , 2
Density (calculated)	1.110 Mg/m ³
Absorption coefficient	0.067 mm ⁻¹
F(000)	492
Crystal size	0.35 x 0.20 x 0.20 mm
θ range for data collection	2.17 to 27.49°
Limiting indices	-16 ≤ h ≤ 16, -8 ≤ k ≤ 8, -19 ≤ l ≤ 19
Reflections collected	24606
Independent reflections	5869 (R _{int} = 0.0501)
Absorption correction	Multiscan(Sortav)
Max. and min. transmission	0.985 and 0.820
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5595 / 1 / 290
Goodness-of-fit on F ²	1.123
Final R indices [I > 2σ(I)]	R1 = 0.0523, wR2 = 0.1493
R indices (all data)	R1 = 0.0726, wR2 = 0.1664
Absolute structure parameter	-3(2)
Extinction coefficient	0.098(12)
Largest diff. peak and hole	0.228 and -0.197 eÅ ⁻³

Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 7921. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	9310(2)	10551(3)	1304(1)	90(1)
O(2)	9085(1)	8507(3)	8305(1)	77(1)
C(1)	9318(1)	7493(4)	5909(1)	57(1)
C(2)	9524(2)	7302(4)	6896(1)	65(1)
C(3)	8849(2)	8675(4)	7377(1)	55(1)
C(4)	7658(1)	8457(3)	7134(1)	51(1)
C(5)	7485(1)	8582(3)	6120(1)	45(1)
C(6)	6321(2)	8547(5)	5762(1)	71(1)
C(7)	6198(2)	9326(5)	4826(1)	71(1)
C(8)	6833(1)	8140(3)	4194(1)	47(1)
C(9)	7995(1)	7898(2)	4616(1)	37(1)
C(10)	8144(1)	7181(2)	5582(1)	41(1)
C(11)	8677(2)	6800(3)	3998(1)	51(1)
C(12)	8646(1)	7714(3)	3093(1)	49(1)
C(13)	7515(1)	7951(3)	2680(1)	45(1)
C(14)	6869(2)	9249(3)	3288(1)	52(1)
C(15)	5738(2)	9601(6)	2841(2)	94(1)
C(16)	5722(2)	10405(7)	1908(2)	106(1)
C(17)	6298(2)	8985(6)	1338(2)	88(1)
C(18)	7445(2)	8800(3)	1758(1)	53(1)
C(19)	8103(2)	7870(4)	1055(1)	60(1)
C(20)	9179(2)	8860(4)	1063(1)	62(1)
C(21)	7458(2)	8564(6)	187(1)	90(1)
C(22)	6532(2)	9787(7)	447(2)	104(1)
C(23)	7102(2)	10193(5)	7532(2)	90(1)
C(24)	7247(2)	6580(5)	7531(2)	76(1)
C(25)	7898(2)	4980(3)	5679(1)	68(1)
C(26)	6282(2)	6143(5)	4052(2)	79(1)
C(27)	7395(2)	11285(3)	3414(2)	72(1)
C(28)	5703(2)	7025(8)	1220(2)	125(2)
C(29)	10087(2)	7807(6)	714(2)	103(1)
C(30)	8208(2)	5624(4)	1094(2)	81(1)

Table 3. Bond lengths [Å] and angles [°] for 7921.

O(1)-C(20)	1.218(3)	O(2)-C(3)	1.440(2)
C(1)-C(2)	1.526(3)	C(1)-C(10)	1.543(2)
C(2)-C(3)	1.505(3)	C(3)-C(4)	1.530(2)
C(4)-C(24)	1.529(4)	C(4)-C(23)	1.531(3)
C(4)-C(5)	1.561(2)	C(5)-C(6)	1.529(2)
C(5)-C(10)	1.554(2)	C(6)-C(7)	1.531(3)
C(7)-C(8)	1.543(3)	C(8)-C(26)	1.537(3)
C(8)-C(9)	1.566(2)	C(8)-C(14)	1.592(3)
C(9)-C(11)	1.533(2)	C(9)-C(10)	1.562(2)
C(10)-C(25)	1.543(3)	C(11)-C(12)	1.524(3)
C(12)-C(13)	1.526(2)	C(13)-C(18)	1.529(3)
C(13)-C(14)	1.568(2)	C(14)-C(15)	1.553(3)
C(14)-C(27)	1.545(3)	C(15)-C(16)	1.537(4)
C(16)-C(17)	1.533(4)	C(17)-C(22)	1.529(4)
C(17)-C(18)	1.545(3)	C(17)-C(28)	1.537(6)
C(18)-C(19)	1.556(3)	C(19)-C(20)	1.519(3)
C(19)-C(30)	1.538(4)	C(19)-C(21)	1.579(3)
C(20)-C(29)	1.494(4)	C(21)-C(22)	1.519(5)
C(2)-C(1)-C(10)	113.1(2)	C(3)-C(2)-C(1)	112.5(2)
O(2)-C(3)-C(2)	111.1(2)	O(2)-C(3)-C(4)	110.7(2)
C(2)-C(3)-C(4)	114.1(2)	C(24)-C(4)-C(3)	110.2(2)
C(24)-C(4)-C(23)	107.6(2)	C(3)-C(4)-C(23)	107.7(2)
C(24)-C(4)-C(5)	115.0(2)	C(3)-C(4)-C(5)	106.96(14)
C(23)-C(4)-C(5)	109.2(2)	C(6)-C(5)-C(10)	110.1(2)
C(6)-C(5)-C(4)	114.15(14)	C(10)-C(5)-C(4)	117.68(14)
C(7)-C(6)-C(5)	110.6(2)	C(6)-C(7)-C(8)	113.3(2)
C(26)-C(8)-C(7)	107.4(2)	C(26)-C(8)-C(9)	111.4(2)
C(7)-C(8)-C(9)	108.39(14)	C(26)-C(8)-C(14)	109.9(2)
C(7)-C(8)-C(14)	111.1(2)	C(9)-C(8)-C(14)	108.56(13)
C(11)-C(9)-C(10)	114.19(13)	C(11)-C(9)-C(8)	110.67(13)
C(10)-C(9)-C(8)	117.47(13)	C(25)-C(10)-C(1)	107.4(2)
C(25)-C(10)-C(5)	115.1(2)	C(1)-C(10)-C(5)	106.68(14)
C(25)-C(10)-C(9)	112.8(2)	C(1)-C(10)-C(9)	107.68(13)
C(5)-C(10)-C(9)	106.82(13)	C(12)-C(11)-C(9)	113.3(2)
C(13)-C(12)-C(11)	112.0(2)	C(12)-C(13)-C(18)	113.9(2)
C(12)-C(13)-C(14)	109.27(13)	C(18)-C(13)-C(14)	110.4(2)
C(15)-C(14)-C(27)	106.7(2)	C(15)-C(14)-C(13)	109.3(2)
C(27)-C(14)-C(13)	109.9(2)	C(15)-C(14)-C(8)	111.6(2)
C(27)-C(14)-C(8)	111.1(2)	C(13)-C(14)-C(8)	108.1(2)
C(16)-C(15)-C(14)	114.1(2)	C(17)-C(16)-C(15)	110.0(3)
C(16)-C(17)-C(22)	115.2(3)	C(16)-C(17)-C(18)	106.7(2)
C(22)-C(17)-C(18)	99.1(2)	C(16)-C(17)-C(28)	111.4(3)
C(22)-C(17)-C(28)	109.6(3)	C(18)-C(17)-C(28)	114.4(3)
C(13)-C(18)-C(17)	113.5(2)	C(13)-C(18)-C(19)	120.0(2)
C(17)-C(18)-C(19)	106.3(2)	C(20)-C(19)-C(30)	111.6(2)
C(20)-C(19)-C(18)	110.3(2)	C(30)-C(19)-C(18)	115.4(2)
C(20)-C(19)-C(21)	105.8(2)	C(30)-C(19)-C(21)	111.6(2)
C(18)-C(19)-C(21)	101.4(2)	O(1)-C(20)-C(29)	118.4(3)
O(1)-C(20)-C(19)	121.4(2)	C(29)-C(20)-C(19)	120.1(3)
C(22)-C(21)-C(19)	107.2(2)	C(21)-C(22)-C(17)	104.6(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 7921.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^*b^*U_{12}]$$

	U11	U22	U33	U23	U13	U12
O(1)	98(1)	101(2)	73(1)	-16(1)	18(1)	-29(1)
O(2)	73(1)	111(1)	45(1)	-13(1)	-5(1)	17(1)
C(1)	39(1)	87(2)	46(1)	0(1)	4(1)	11(1)
C(2)	45(1)	98(2)	49(1)	-1(1)	0(1)	16(1)
C(3)	53(1)	68(1)	45(1)	-3(1)	0(1)	-2(1)
C(4)	44(1)	67(1)	44(1)	-6(1)	7(1)	5(1)
C(5)	36(1)	55(1)	44(1)	-4(1)	8(1)	5(1)
C(6)	39(1)	129(2)	46(1)	-9(1)	12(1)	14(1)
C(7)	42(1)	123(2)	48(1)	-7(1)	5(1)	32(1)
C(8)	32(1)	66(1)	44(1)	-7(1)	4(1)	2(1)
C(9)	32(1)	37(1)	44(1)	-2(1)	6(1)	2(1)
C(10)	38(1)	42(1)	44(1)	0(1)	8(1)	2(1)
C(11)	48(1)	61(1)	46(1)	2(1)	7(1)	19(1)
C(12)	42(1)	63(1)	42(1)	-3(1)	9(1)	10(1)
C(13)	43(1)	51(1)	42(1)	-6(1)	3(1)	2(1)
C(14)	43(1)	68(1)	44(1)	-5(1)	2(1)	18(1)
C(15)	59(1)	165(3)	55(1)	-1(2)	-3(1)	50(2)
C(16)	78(2)	180(4)	58(1)	4(2)	-7(1)	64(2)
C(17)	63(1)	149(3)	49(1)	-8(2)	-9(1)	24(2)
C(18)	53(1)	66(1)	39(1)	-5(1)	-1(1)	6(1)
C(19)	68(1)	74(1)	40(1)	-12(1)	2(1)	3(1)
C(20)	70(1)	82(2)	36(1)	4(1)	6(1)	-3(1)
C(21)	91(2)	136(3)	40(1)	-8(2)	-7(1)	-1(2)
C(22)	97(2)	163(3)	48(1)	7(2)	-15(1)	32(2)
C(23)	99(2)	119(2)	52(1)	-19(1)	4(1)	45(2)
C(24)	73(1)	106(2)	52(1)	5(1)	15(1)	-25(1)
C(25)	107(2)	45(1)	54(1)	1(1)	10(1)	-6(1)
C(26)	71(1)	104(2)	61(1)	-10(1)	6(1)	-45(1)
C(27)	111(2)	49(1)	56(1)	-2(1)	9(1)	24(1)
C(28)	66(2)	214(5)	93(2)	-45(3)	-8(1)	-31(2)
C(29)	93(2)	115(3)	107(2)	28(2)	47(2)	11(2)
C(30)	96(2)	76(2)	72(2)	-31(1)	26(1)	-10(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 7921.

	x	y	z	U(eq)
H(2A)	9550(1)	7681(3)	8409(1)	115
H(1A)	9748(1)	6537(4)	5633(1)	69
H(1B)	9538(1)	8787(4)	5735(1)	69
H(2B)	9382(2)	5963(4)	7065(1)	77
H(2C)	10265(2)	7574(4)	7063(1)	77
H(3A)	9041(2)	10010(4)	7216(1)	66
H(5A)	7731(1)	9898(3)	5980(1)	54
H(6A)	6054(2)	7215(5)	5774(1)	85
H(6B)	5907(2)	9349(5)	6128(1)	85
H(7A)	6431(2)	10681(5)	4826(1)	85
H(7B)	5454(2)	9298(5)	4617(1)	85
H(9A)	8282(1)	9234(2)	4635(1)	45
H(11A)	9405(2)	6777(3)	4251(1)	62
H(11B)	8433(2)	5453(3)	3943(1)	62
H(12A)	8987(1)	8989(3)	3135(1)	58
H(12B)	9042(1)	6892(3)	2722(1)	58
H(13A)	7188(1)	6647(3)	2647(1)	54
H(15A)	5351(2)	8372(6)	2828(2)	112
H(15B)	5370(2)	10519(6)	3191(2)	112
H(16A)	4994(2)	10570(7)	1667(2)	127
H(16B)	6066(2)	11677(7)	1915(2)	127
H(18A)	7704(2)	10150(3)	1827(1)	64
H(21A)	7906(2)	9341(6)	-160(1)	108
H(21B)	7201(2)	7438(6)	-153(1)	108
H(22A)	5922(2)	9637(7)	28(2)	124
H(22B)	6722(2)	11165(7)	487(2)	124
H(23A)	7345(2)	11396(5)	7294(2)	135
H(23B)	7263(2)	10193(5)	8153(2)	135
H(23C)	6350(2)	10077(5)	7400(2)	135
H(24A)	6500(2)	6459(5)	7374(2)	114
H(24B)	7374(2)	6636(5)	8154(2)	114
H(24C)	7608(2)	5468(5)	7315(2)	114
H(25A)	7171(2)	4737(3)	5480(1)	103
H(25B)	8020(2)	4608(3)	6280(1)	103
H(25C)	8351(2)	4225(3)	5337(1)	103
H(26A)	6660(2)	5368(5)	3660(2)	118
H(26B)	5567(2)	6341(5)	3806(2)	118
H(26C)	6275(2)	5474(5)	4599(2)	118
H(27A)	8098(2)	11134(3)	3690(2)	108
H(27B)	6984(2)	12084(3)	3773(2)	108
H(27C)	7428(2)	11903(3)	2857(2)	108
H(28A)	6082(2)	6167(8)	862(2)	187
H(28B)	5005(2)	7256(8)	945(2)	187
H(28C)	5650(2)	6428(8)	1779(2)	187
H(29A)	10703(2)	8632(6)	765(2)	154
H(29B)	9910(2)	7488(6)	112(2)	154
H(29C)	10230(2)	6622(6)	1040(2)	154
H(30A)	7516(2)	5045(4)	1089(2)	121
H(30B)	8624(2)	5254(4)	1618(2)	121
H(30C)	8549(2)	5170(4)	598(2)	121

^1H spectrum of compound **3** (CDCl_3 , 400MHz)

^{13}C spectrum of compound 3 (CDCl_3 , 400MHz)

IR spectrum of compound 3

S25

MS spectrum of compound 3

HMQC spectrum of compound 3 (CDCl_3 , 400MHz)

HMBC spectrum of compound 3 (CDCl₃, 400MHz)

COSY spectrum of compound **3** (CDCl₃, 400MHz)

NOESY spectrum of compound 3 (CDCl₃, 400MHz)