SUPPORTING INFORMATION

Newly synthesized curcumin derivatives: crosstalk between chemico-physical properties and biological activity.

Erika Ferrari,[1] Francesca Pignedoli,[1] Carol Imbriano,[2] Gaetano Marverti,[3] Valentina Basile,[2] Ettore Venturi,[1] Monica Saladini[1*]

[1]*Department of Chemistry, University of Modena and Reggio Emilia, Via Campi 183, 41125 Modena (Italy).*
[2]*Department of Biology, University of Modena and Reggio Emilia, Via Campi 213/D, 41125 Modena (Italy).*
[3]*Department of Biomedical Science, University of Modena and Reggio Emilia, Via Campi 287, 41125 Modena (Italy).*

* corresponding author: Prof. Monica Saladini, e-mail: monica.saladini@unimore.it; Tel. +39 059 2055040; fax: +39 059373543.

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Table S1- Elemental analysis details for the compounds **3-10**
(3) calculated (experimental) for $C_{25}H_{26}O_4$: C 76.90 (75.75); H 6.71 (6.67).
(4) calculated (experimental) for $C_{27}H_{30}O_8$: C 67.21 (65.83); H 6.27 (6.89).
(**5**) calculated (experimental) for $C_{27}H_{30}O_6$: C 71.98 (71.70); H 6.71 (7.24).
(**6**) calculated (experimental) for $C_{31}H_{34}O_{10}$: C 65.71 (65.10), H 6.05 (5.33).
(**7**) calculated (experimental) for $C_{21}H_{18}O_4$: C 75.43 (75.27); H 5.43 (5.61).
(**8**) calculated (experimental) for $C_{23}H_{22}O_8$:C 64.78 (63.86); H, 5.20 (5.47).
(**9**) calculated (experimental) for $C_{23}H_{22}O_6$: C 70.04 (69.89), H 5.62 (5.86).
(**10**) calculated (experimental) for $C_{27}H_{26}O_{10}$: C 63.53 (62.94), H 5.13 (5.48).

Table S2. Crystal data and structure refinement for **5**.

Identification Code	**5**
Empirical formula	$C_{27}H_{30}O_6$
Formula weight	450.51
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic P-1
Unit Cell dimensions	a = 10.3080(10) Å α = 63.957(4) deg.
	b = 10.9062(9) Å β= 82.789(3) deg.
	c = 12.1041(9) Å γ = 86.318(3) deg.
Volume	1212.86(18) $Å^3$
Z, Calculated density	2, 1.234 g/Cm^3
Absorption Coefficient	0.086 mm^{-1}
F(000)	480
Crystal size	0.3 × 0.2 × 0.3 mm
Theta range for data Collection	3.77 to 19.19 deg.
Limiting indices	-9<=h<=9, -9<=k<=10, -11<=l<=10
Reflections Collected / unique	5076 / 1946 [R(int) = 0.0449]
Completeness to θ = 19.19	96.6 %
Absorption Correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1946 / 0 / 389
Goodness-of-fit on F^2	0.800
Final R indices [I>2σ (I)]	R_1 = 0.0399, wR_2 = 0.0943
R indices (all data)	R_1 = 0.0761, wR_2 = 0.1167
Extinction Coefficient	0.0000(12)
Largest diff. peak and hole	0.106 and -0.103 $e.Å^{-3}$

Table S3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **5**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	3318(3)	5811(4)	10001(3)	93(1)
O(2)	2421(3)	5867(3)	8218(3)	87(1)
O(3)	6291(3)	8673(3)	5576(3)	94(1)
O(4)	6881(3)	8046(3)	7475(2)	64(1)
O(5)	66(3)	6431(3)	2683(3)	92(1)
O(6)	7816(3)	9812(4)	11432(3)	110(1)
C(1)	3944(4)	7487(4)	8003(4)	57(1)
C(2)	3144(4)	6915(5)	7504(4)	62(1)
C(3)	3058(4)	7417(5)	6188(5)	65(1)
C(4)	2311(4)	6873(5)	5718(4)	65(1)
C(5)	2176(4)	7299(4)	4406(4)	60(1)
C(6)	1228(4)	6710(5)	4088(5)	64(1)
C(7)	1053(5)	7079(5)	2873(5)	67(1)
C(8)	1831(5)	8050(6)	1939(5)	76(1)
C(9)	2784(5)	8634(5)	2252(5)	90(2)
C(10)	2979(5)	8263(5)	3462(5)	77(1)
C(11)	-128(6)	6750(7)	1441(6)	105(2)
C(12)	4715(4)	8774(5)	7159(4)	61(1)
C(13)	6038(4)	8499(4)	6624(5)	60(1)
C(14)	8221(4)	7594(5)	7219(4)	66(1)
C(15)	8166(6)	6408(6)	6914(6)	96(2)
C(16)	8971(5)	8785(6)	6197(5)	99(2)
C(17)	8753(5)	7153(7)	8439(5)	99(2)
C(18)	4017(4)	6867(5)	9284(5)	67(1)
C(19)	4848(4)	7333(5)	9918(5)	66(1)
C(20)	4943(4)	6695(5)	11109(5)	76(1)
C(21)	5729(4)	7077(6)	11834(5)	71(1)
C(22)	5745(5)	6242(6)	13087(6)	93(2)
C(23)	6454(7)	6606(8)	13788(5)	106(2)
C(24)	7152(6)	7781(8)	13272(6)	92(2)
C(25)	7148(5)	8612(6)	12037(6)	77(1)
C(26)	6439(5)	8267(6)	11325(5)	78(1)
C(27)	8656(6)	10171(7)	12097(6)	114(2)

Table S4. Bond lengths [Å] and angles [deg] for **5**.

O(1)-C(18)	1.293(4)	C(6)-C(7)	1.377(6)
O(2)-C(2)	1.299(4)	C(7)-C(8)	1.369(6)
O(3)-C(13)	1.194(4)	C(8)-C(9)	1.378(6)
O(4)-C(13)	1.335(5)	C(9)-C(10)	1.375(6)
O(4)-C(14)	1.478(5)	C(12)-C(13)	1.506(6)
O(5)-C(7)	1.371(5)	C(14)-C(15)	1.500(7)
O(5)-C(11)	1.424(6)	C(14)-C(17)	1.503(6)
O(6)-C(25)	1.368(5)	C(14)-C(16)	1.514(6)
O(6)-C(27)	1.430(6)	C(18)-C(19)	1.464(6)
C(1)-C(2)	1.398(5)	C(19)-C(20)	1.311(5)
C(1)-C(18)	1.403(5)	C(20)-C(21)	1.464(6)
C(1)-C(12)	1.525(5)	C(21)-C(26)	1.381(6)
C(2)-C(3)	1.452(6)	C(21)-C(22)	1.386(6)
C(3)-C(4)	1.318(5)	C(22)-C(23)	1.379(7)
C(4)-C(5)	1.468(6)	C(23)-C(24)	1.361(7)
C(5)-C(6)	1.381(5)	C(24)-C(25)	1.366(6)
C(5)-C(10)	1.385(6)	C(25)-C(26)	1.376(6)

C(13)-O(4)-C(14)	121.9(3)	O(3)-C(13)-C(12)	124.0(4)
C(7)-O(5)-C(11)	118.0(4)	O(4)-C(13)-C(12)	110.9(4)
C(25)-O(6)-C(27)	118.5(5)	O(4)-C(14)-C(15)	109.9(3)
C(2)-C(1)-C(18)	119.2(4)	O(4)-C(14)-C(17)	101.9(4)
C(2)-C(1)-C(12)	120.0(4)	C(15)-C(14)-C(17)	110.7(5)
C(18)-C(1)-C(12)	120.8(4)	O(4)-C(14)-C(16)	109.5(4)
O(2)-C(2)-C(1)	120.8(4)	C(15)-C(14)-C(16)	112.5(4)
O(2)-C(2)-C(3)	115.4(4)	C(17)-C(14)-C(16)	111.8(4)
C(1)-C(2)-C(3)	123.8(4)	O(1)-C(18)-C(1)	120.5(4)
C(4)-C(3)-C(2)	123.8(4)	O(1)-C(18)-C(19)	114.8(5)
C(3)-C(4)-C(5)	127.5(4)	C(1)-C(18)-C(19)	124.7(5)
C(6)-C(5)-C(10)	118.1(4)	C(20)-C(19)-C(18)	123.3(5)
C(6)-C(5)-C(4)	119.4(4)	C(19)-C(20)-C(21)	127.8(5)
C(10)-C(5)-C(4)	122.5(4)	C(26)-C(21)-C(22)	117.9(5)
C (7)-C(6)-C(5)	121.8(4)	C(26)-C(21)-C(20)	122.5(5)
C(8)-C(7)-O(5)	123.9(5)	C(22)-C(21)-C(20)	119.6(5)
C(8)-C(7)-C(6)	120.1(4)	C(23)-C(22)-C(21)	120.2(5)
O(5)-C(7)-C(6)	116.0(5)	C(24)-C(23)-C(22)	121.1(5)
C(7)-C(8)-C(9)	118.3(5)	C(23)-C(24)-C(25)	119.3(5)
C(10)-C(9)-C(8)	122.2(5)	C(24)-C(25)-O(6)	123.8(6)
C(9)-C(10)-C(5)	119.5(4)	C(24)-C(25)-C(26)	120.3(5)
C(13)-C(12)-C(1)	113.8(4)	O(6)-C(25)-C(26)	115.9(5)
O(3)-C(13)-O(4)	125.1(4)	C(21)-C(26)-C(25)	121.2(5)

Table S5. Anisotropic displacement parameters ($Å^2$ x 10^3) for **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(1)	110(2)	111(3)	58(2)	-30(2)	-4(2)	-51(2)
O(2)	93(2)	96(2)	70(2)	-31(2)	-1(2)	-46(2)
O(3)	92(2)	142(3)	49(2)	-44(2)	-9(2)	17(2)
O(4)	53(2)	85(2)	48(2)	-24(2)	-7(2)	-8(2)
O(5)	90(2)	118(3)	84(3)	-54(2)	-24(2)	-16(2)
O(6)	120(3)	117(3)	100(3)	-46(2)	-25(2)	-35(2)
C(1)	55(3)	66(3)	50(3)	-25(3)	-6(2)	-6(2)
C(2)	55(3)	72(3)	61(4)	-31(3)	-4(3)	-12(3)
C(3)	64(3)	68(3)	62(4)	-27(3)	-2(2)	-15(2)
C(4)	65(3)	72(3)	64(4)	-34(3)	-13(3)	-12(2)
C(5)	56(3)	62(3)	69(4)	-34(3)	-10(3)	-1(2)
C(6)	65(3)	70(3)	59(4)	-28(3)	-7(2)	-12(2)
C(7)	66(3)	70(3)	72(4)	-37(3)	-10(3)	0(3)
C(8)	81(3)	88(4)	66(4)	-37(4)	-20(3)	7(3)
C(9)	105(5)	96(4)	60(5)	-26(3)	5(3)	-28(3)
C(10)	76(3)	78(4)	82(4)	-37(3)	-10(3)	-18(3)
C(11)	111(5)	133(5)	96(5)	-65(4)	-38(4)	-5(4)
C(12)	60(3)	68(3)	63(3)	-33(3)	-8(2)	-13(3)
C(13)	55(3)	63(3)	57(3)	-22(3)	-3(3)	-10(2)
C(14)	54(3)	74(3)	60(3)	-21(3)	-5(2)	-7(3)
C(15)	93(4)	89(5)	101(4)	-38(4)	-7(3)	6(3)
C(16)	62(3)	101(5)	106(4)	-26(4)	22(3)	-24(4)
C(17)	70(3)	129(6)	92(5)	-37(4)	-25(3)	-9(4)
C(18)	59(3)	76(4)	68(4)	-34(3)	7(3)	-15(3)
C(19)	68(3)	79(3)	58(4)	-36(3)	-2(3)	-20(2)
C(20)	83(3)	85(4)	59(4)	-30(3)	-4(3)	-16(3)
C(21)	80(3)	81(4)	54(4)	-30(3)	-6(3)	-3(3)
C(22)	109(4)	94(4)	70(4)	-29(4)	-11(3)	-15(3)
C(23)	137(5)	115(6)	61(4)	-30(4)	-31(4)	-4(4)
C(24)	100(4)	115(5)	80(5)	-57(4)	-29(3)	11(4)
C(25)	81(3)	95(4)	65(4)	-42(4)	-15(3)	-1(3)
C(26)	84(3)	90(4)	58(3)	-28(3)	-11(3)	-12(3)
C(27)	97(4)	149(6)	136(6)	-91(5)	-46(4)	-3(4)

Table S6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for **5**.

	x	y	z	U(eq)
H(1)	2810(40)	5650(40)	9380(50)	110
H(2)	3570(30)	8100(30)	5690(30)	42
H(3)	1770(30)	6050(30)	6260(30)	51
H(4)	730(30)	6090(30)	4680(30)	57
H(5)	1730(30)	8350(40)	1100(30)	66
H(6)	3360(40)	9230(40)	1650(40)	89
H(7)	3690(30)	8660(40)	3710(30)	76
H(8)	-790(50)	6290(50)	1460(50)	115
H(9)	680(40)	6580(50)	1000(40)	111
H(10)	-300(40)	7740(50)	970(40)	114
H(11)	4210(40)	9410(40)	6430(40)	94
H(12)	4880(30)	9260(30)	7610(30)	61
H(13)	7560(40)	5780(50)	7530(40)	113
H(14)	7710(40)	6670(50)	6160(40)	113
H(15)	8980(50)	6000(50)	6850(40)	115
H(16)	8920(40)	9500(40)	6460(40)	93
H(17)	8480(40)	9020(50)	5340(50)	132
H(18)	9800(50)	8550(50)	6130(50)	128
H(19)	8730(40)	7880(50)	8690(40)	99
H(20)	8270(40)	6490(50)	9080(40)	113
H(21)	9620(50)	6920(50)	8440(40)	120
H(22)	5330(30)	8140(40)	9420(40)	81
H(23)	4430(40)	5720(50)	11510(40)	122
H(24)	5140(40)	5440(40)	13390(30)	80
H(25)	6460(50)	6010(50)	14580(50)	116
H(26)	7660(40)	8040(40)	13750(40)	100
H(27)	6530(40)	8890(40)	10440(40)	95
H(28)	8100(50)	10210(50)	12880(50)	135
H(29)	9380(60)	9520(60)	12390(60)	172
H(30)	9090(60)	11030(60)	11320(60)	177