Bioactivity-guided isolation of anticancer compounds from *Euphorbia lathyris*

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Supplementary information

Table S1. ^{13}C NMR spectroscopic data for compounds 1-6 in $CDCl_3$, compound 7 in DMSO (100 MHz)

No.	1	2	3	4	5	6	7
1	47.9	47.9	174.3	48.6	48.6	47.8	
2	37.7	37.8	34.1	37.7	37.9	37.6	161.3
3	79.6	80.7	24.9	81.9	80.9	79.3	112.0
4	52.9	49.9	27.2	52.3	52.2	52.9	144.9
5	64.2	65.2	27.2	65.5	66.5	64.5	112.8
6	142.0	58.9	29.1	144.4	144.6	142.1	143.3
7	78.6	33.6	29.3	34.9	34.9	78.9	150.9
8	28.7	20.1	29.7	21.0	21.7	28.7	103.1
9	31.6	34.8	130.0	35.4	35.4	31.4	149.0
10	24.7	25.6	129.7	25.4	25.3	24.7	111.2
11	27.8	29.1	31.9	28.5	28.6	27.7	

12	142.7	143.7	29.5	146.7	146.5	142.2	
13	135.5	136.0	29.1	134.2	134.2	135.8	
14	197.6	196.9	29.3	196.5	196.7	197.6	
15	92.0	91.8	29.1	92.5	92.5	91.9	
16	14.2	13.6	29.7	14.2	14.2	14.1	
17	119.8	55.5	22.7	115.5	115.4	119.4	
18	28.8	28.9	14.1	29.0	29.0	28.9	
19	16.7	16.8		16.9	16.8	16.6	
20	12.7	12.4		12.5	12.5	12.8	

Table S2. ^{1}H NMR data for compounds 1-6 in $CDCl_3$, compound 7 in DMSO (400 MHz)

position	1	2	3	4	5	6	7
1	3.5,dd	3.3,dd	4.2,dd	3.6,dd	3.6 ,dd	3.4,dd	
1’	1.8,dd	1.4,dd	4.2,dd	1.7,dd	1.7,dd	1.8,dd	
2	2.4,m	2.1,m	2.4,t	2.4.m	2.4,m	2,4,m	
3	5.8,t	5.5,t		5.9,t	5.9,t	5.8,t	6.1,d
4	3.0.dd	1.9,m		2.9,dd	2.9,dd	2.9.dd	7.8,d
5	6.4,d	6.3,d		6.2,d	6.,d	6.4,d	7.0,s
7	5.6,dd	1.0,t		2.2,dd	2.2,dd	5.6,dd	
7’		2.1.m		2.1,brdd	2.0,brdd		
8	2.4,m	2.2,m		2.0,dddd	2.0,dddd	2.4,m	6.8,s
8’	2,2,brdd	1.8,m		1.7,m	1.7,m	2.2,m	

9	1.4,dddd	1.1,m	5.3,dt	1.2,dddd	1.2,dddd	1.3,ddd	
11	1.5,dd	1.5,dd	2.0,m	1.4,dd	1.4,dd	1.6,dd	
12	6.6,dq	6.6,dd		6.6,dq	6.6,dq	6.5,dq	
16	1.0,d	0.7.d		0.9,d	1.0,d	1.0,d	
17	5.56,brs	2.5,d		5.0,d	5.0,d	5.5,s	
17’	5.3,brs	2.3,dd		4.8,brs	4.8,brs	5.3,s	
18	1.2,s	1.2,s	0.9,t	1.2,s	1.2,s	1.2,s	
19	1.3,s	1.3,s		1.2,s	1.2,s	1.3,s	
20	1.8,d	1.9,s			1.7,s	1.8,d	1.8,d

Table S3. Crystal data and structure refinement for compound 2

Compound	2
Empirical formula	$C_{32}H_{40}O_8$
Formula weight	552.64
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system，space group	Orthorhombic, $P2_12_12$
Unit cell dimensions	a = 8.2474(16)Å, α= 90.00
	b = 12.543(3)Å, β= 90.00
	c = 29.019(6)Å, γ= 90.00
Volume	3001.9(10) A^3
Z,Calculated density	4, 1.223 Mg/m^3
Absorption coefficient	0.064 mm^{-1}
F(000)	1184
Crystal size	0.25 × 0.20 × 0.15 mm
Theta range for data collection	3.04 to 25.50 deg.

Limiting indices	-8 ≦ h ≦ 9, -15 ≦ k ≦15, -34 ≦ l ≦ 35
Reflections collected / unique	24238 / 5565 [R(int) = 0.1286]
Completeness to theta = 25.50	99.7 %
Absorption correction	0.087 mm^{-1}
Max. and min. transmission	0.9871 and 0.9786
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5565/0/361
Goodness-of-fit on F^2	1.019
Final R indices [I>2sigma(I)]	R1 = 0.0668, ωR2 = 0.1111
R indices (all data)	R1 = 0.1205, ωR2 = 0.1260
Absolute structure parameter	-0.9(13)
Largest diff. peak and hole	0.149 and -0.169 e.$Å^{-3}$

Table S4. Selected Bond Lengths (Å) for compound 2

Bond	Dist.	Bond	Dist.	Bond	Dist.
O(1)-C(3)	1.458(4)	C(2)-C(16)	1.512(5)	C(11)-C(12)	1.451(5)
O(1)-C(21)	1.343(4)	C(2)-C(3)	1.528(4)	C(15)-C(1)	1.540(5)
O(2)-C(21)	1.195(4)	C(3)-C(4)	1.522(4)	C(9)-C(10)	1.500(4)
O(3)-C(5)	1.468(3)	C(4)-C(5)	1.531(4)	C(9)-C(11)	1.536(5)
O(3)-C(29)	1.359(4)	C(4)-C(15)	1.583(4)	C(11)-C(12)	1.451(5)
O(4)-C(29)	1.190(4)	C(5)-C(6)	1.520(5)	C(15)-C(1)	1.540(5)
O(5)-C(6)	1.455(4)	C(6)-C(17)	1.475(5)	C(2)-H(2A)	0.9800
O(5)-C(17)	1.443(4)	C(9)-C(8)	1.523(4)	C(3)-H(3A)	0.9800
O(6)-C(14)	1.217(4)	C(9)-C(10)	1.500(4)	C(5)-H(5A)	0.9800
O(7)-C(15)	1.450(4)	C(9)-C(11)	1.536(5)	C(9)-H(9A)	0.9800
O(7)-C(31)	1.353(4)	C(11)-C(12)	1.451(5)	C(11)-H(11A)	0.9800
O(8)-C(31)	1.199(4)	C(15)-C(1)	1.540(5)		

Table S5. Selected Bond Angles (°) for compound 2

Angle	(°)	Angle	(°)
C(21)-O(1)-C(3)	117.0(2)	C(5)–C(6)–C(7)	114.8(3)
C(29)-O(3)-C(5)	117.0(3)	C(8)–C(7)–C(6)	115.7(3)
C(17)-O(5)-C(6)	61.20(19)	C(9)–C(8)–C(7)	115.2(3)
C(31)-O(7)-C(15)	115.5(3)	C(8)–C(9)–C(10)	123.7(3)
C(2)–C(1)–C(15)	107.5(2)	C(8)–C(9)–C(11)	123.6(3)
C(3)–C(2)–C(16)	116.6(3)	C(10)–C(9)–C(11)	60.3(2)
C(3)–C(2)–C(1)	102.3(3)	C(19)–C(10)–C(9)	121.4(3)
C(16)–C(2)–C(1)	114.4(3)	C(19)–C(10)–C(11)	119.0(3)
O(1)–C(3)–C(2)	108.6(3)	C(9)–C(10)–C(11)	61.0(2)
O(1)–C(3)–C(4)	108.1(2)	C(19)–C(10)–C(18)	114.3(3)
C(2)–C(3)–C(4)	103.0(3)	C(9)–C(10)–C(18)	115.8(3)
C(3)–C(4)–C(5)	116.6(2)	C(11)–C(10)–C(18)	115.2(3)
C(3)–C(4)–C(15)	104.1(3)	C(12)–C(11)–C(10)	123.5(3)
C(5)–C(4)–C(15)	116.6(2)	C(12)–C(11)–C(9)	118.8(3)
O(3)–C(5)–C(6)	104.5(2)	C(10)–C(11)–C(9)	58.7(2)
O(3)–C(5)–C(4)	107.9(2)	C(12)–C(13)–C(14)	123.5(3)
C(6)–C(5)–C(4)	116.7(3)	C(12)–C(13)–C(20)	122.5(3)
O(5)–C(6)–C(17)	59.0(2)	C(14)–C(13)–C(20)	113.3(3)
O(5)–C(6)–C(5)	113.4(3)	O(6)–C(14)–C(13)	120.4(4)
C(17)–C(6)–C(5)	124.1(3)	O(6)–C(14)–C(15)	115.2(3)
O(5)–C(6)–C(7)	113.1(3)	C(13)–C(14)–C(15)	123.9(3)
C(17)–C(6)–C(7)	118.2(3)	C(1)–C(15)–C(4)	103.9(2)

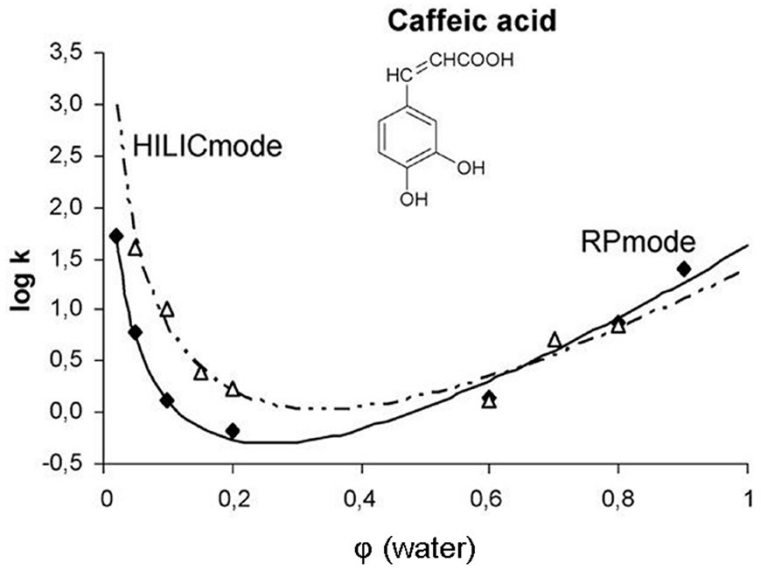

Figure S1. U-shape plots of the retention factors of caffeic acids, k, versus the volume fraction of water, φ (water).