

Supporting Information

Rec. Nat. Prod. 10:1 (2016) 83-92

Isolation, Identification and Cytotoxic Activity of Triterpenes and Flavonoids from Green Walnut (*Juglans regia* L.) Pericarps

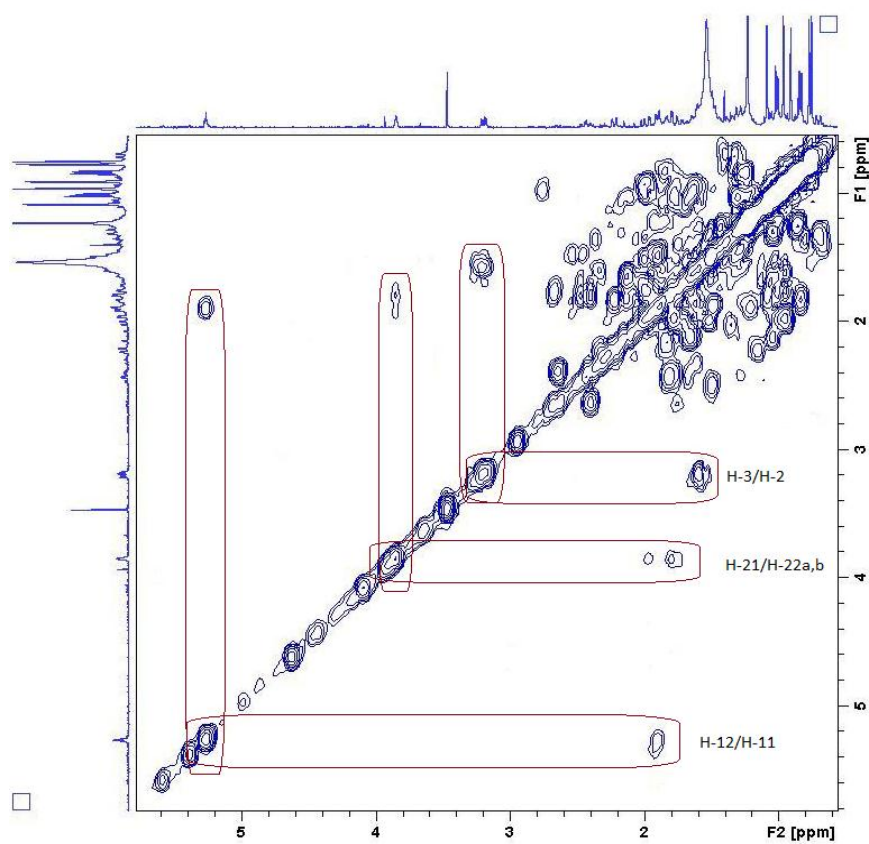
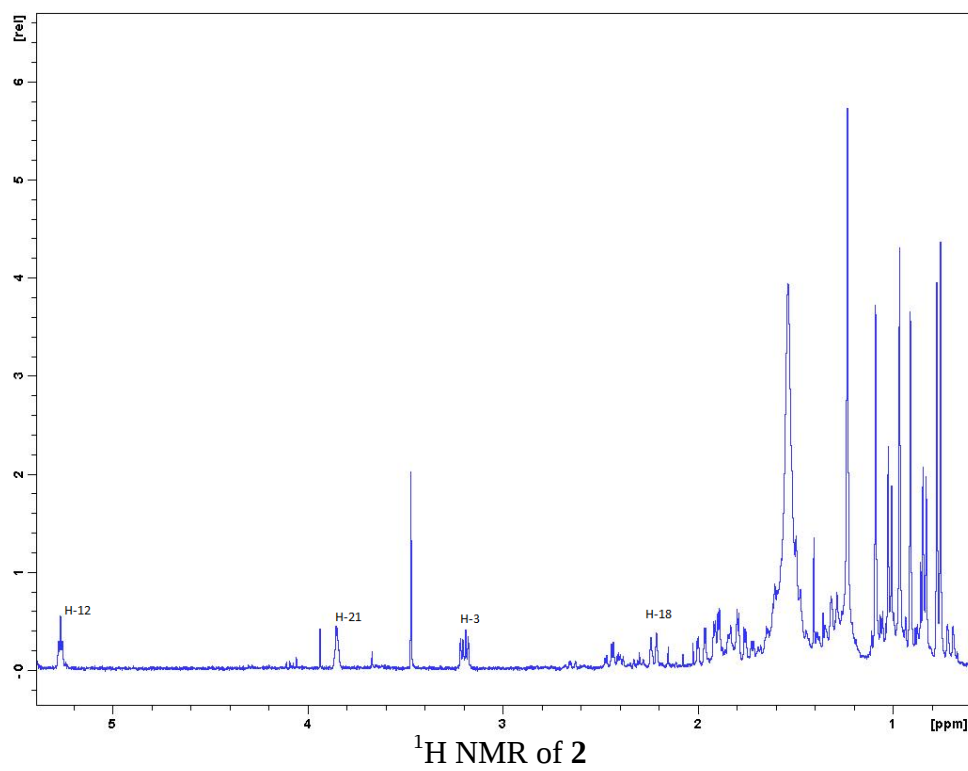
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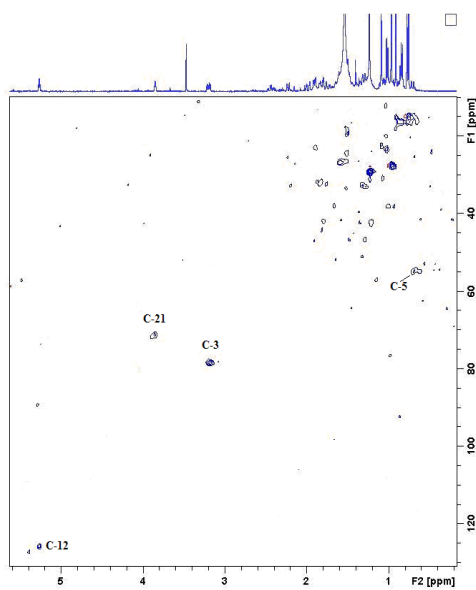
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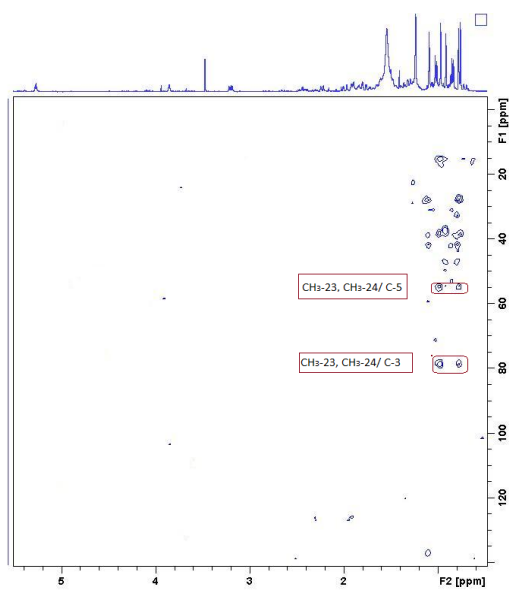
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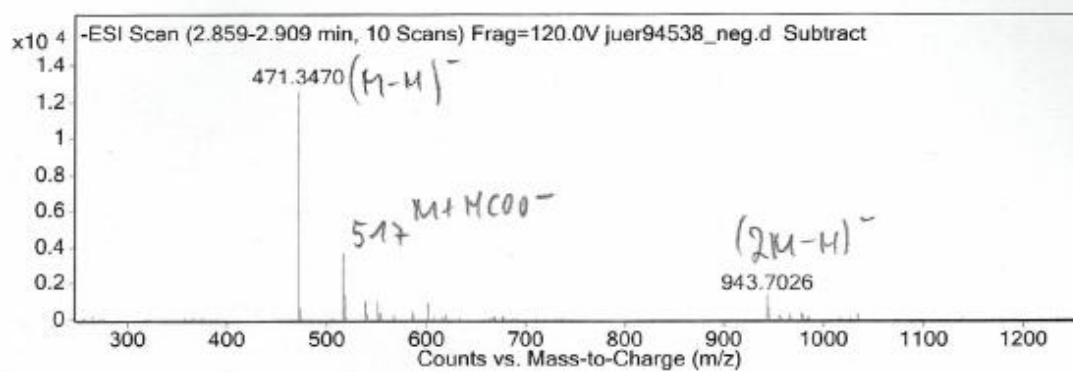
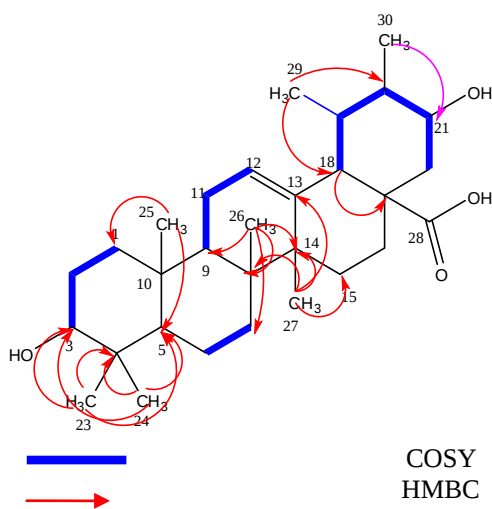




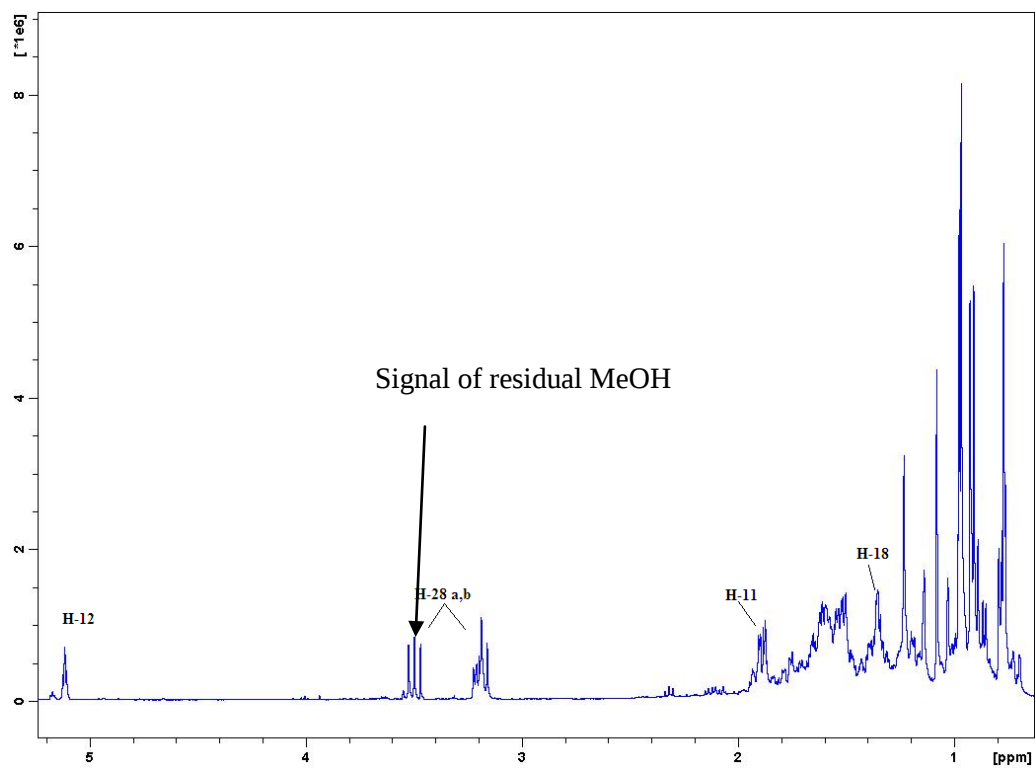
HSQC of 2



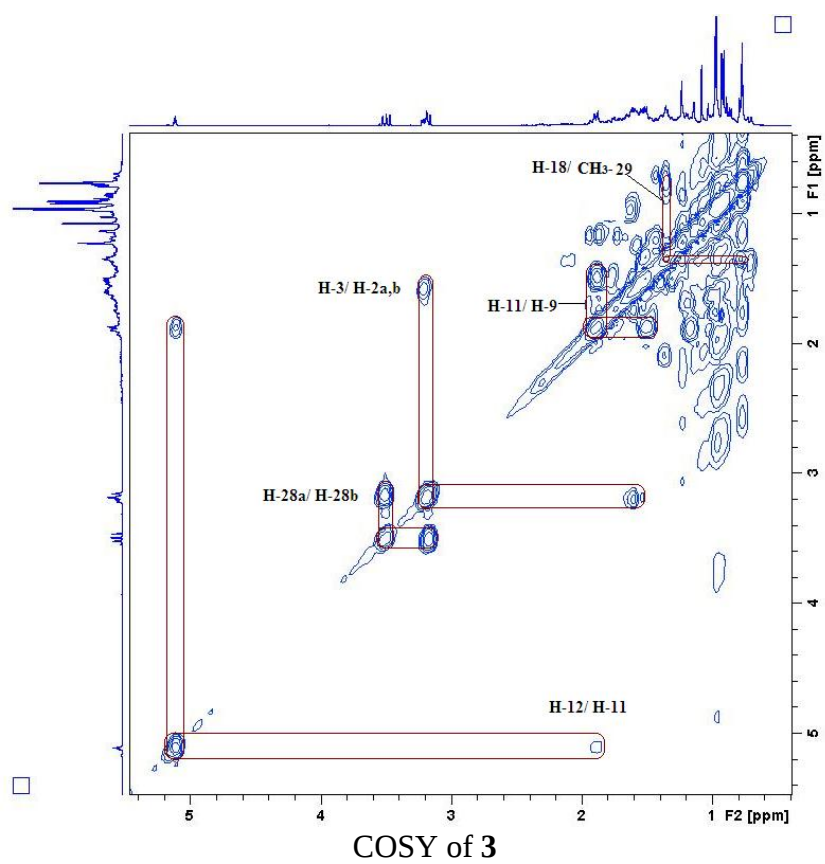
HMBC of 2

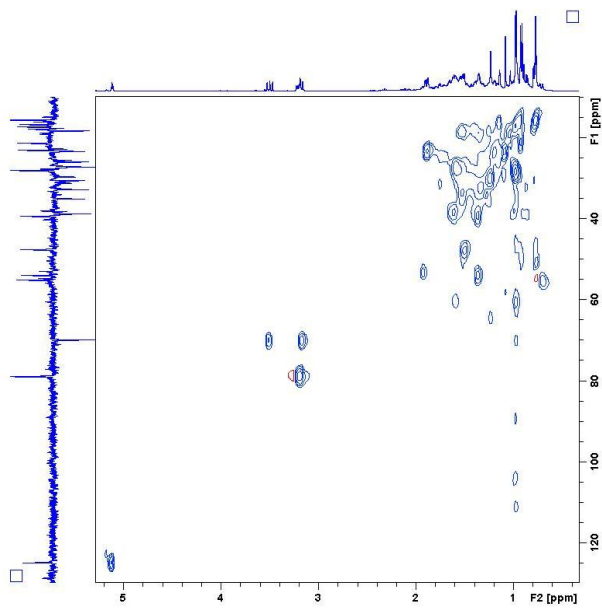


ESI MS of 2

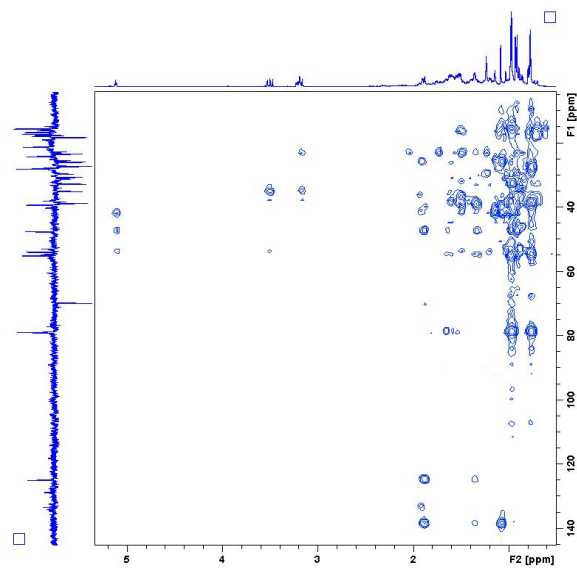


^1H NMR of 3

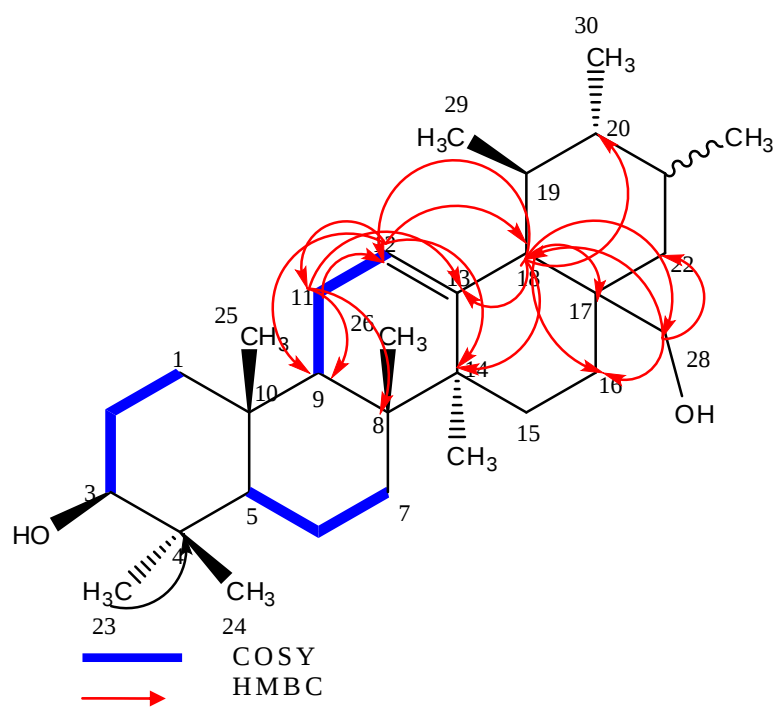


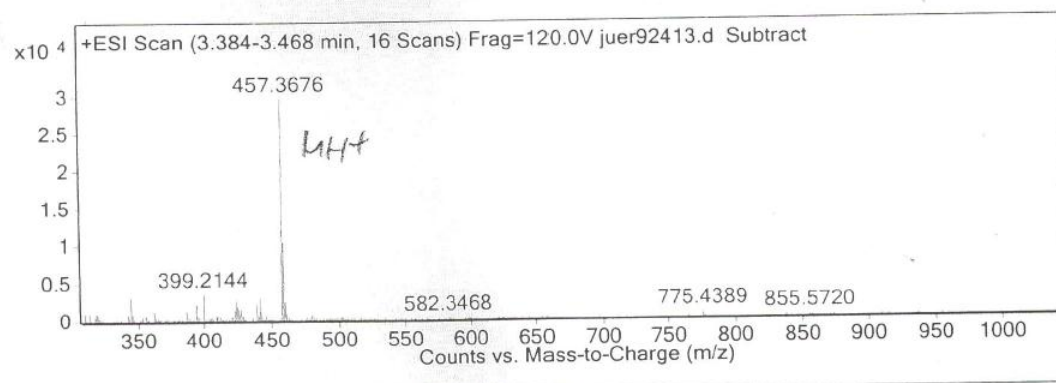
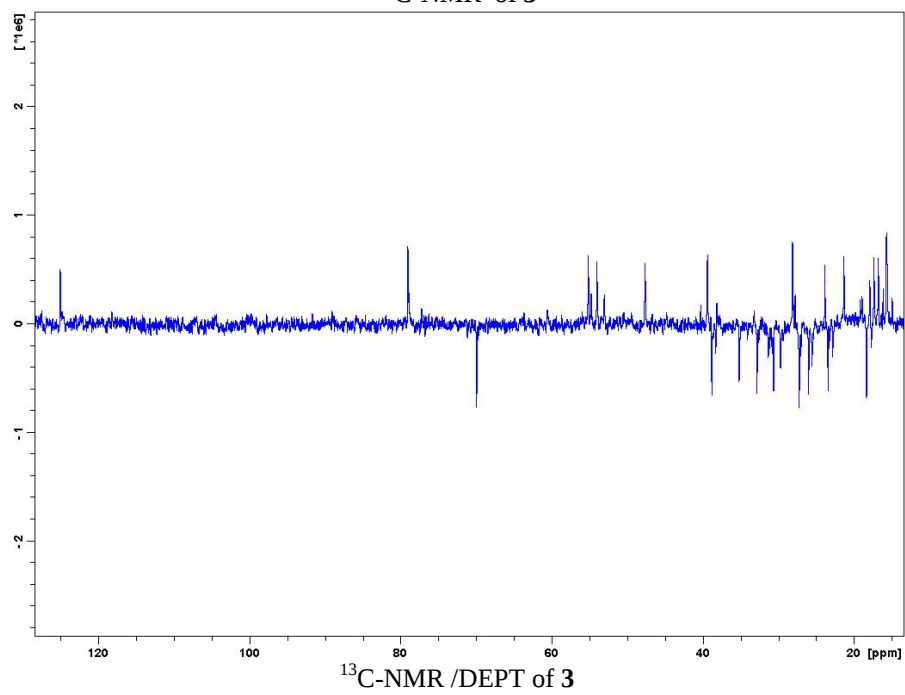
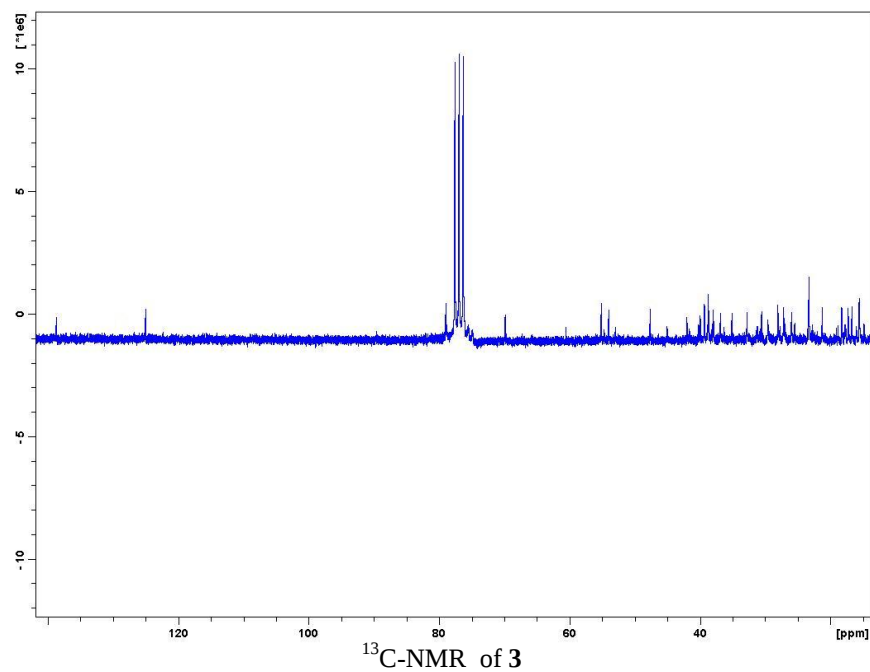


HSQC of **3**



HMBC of **3**



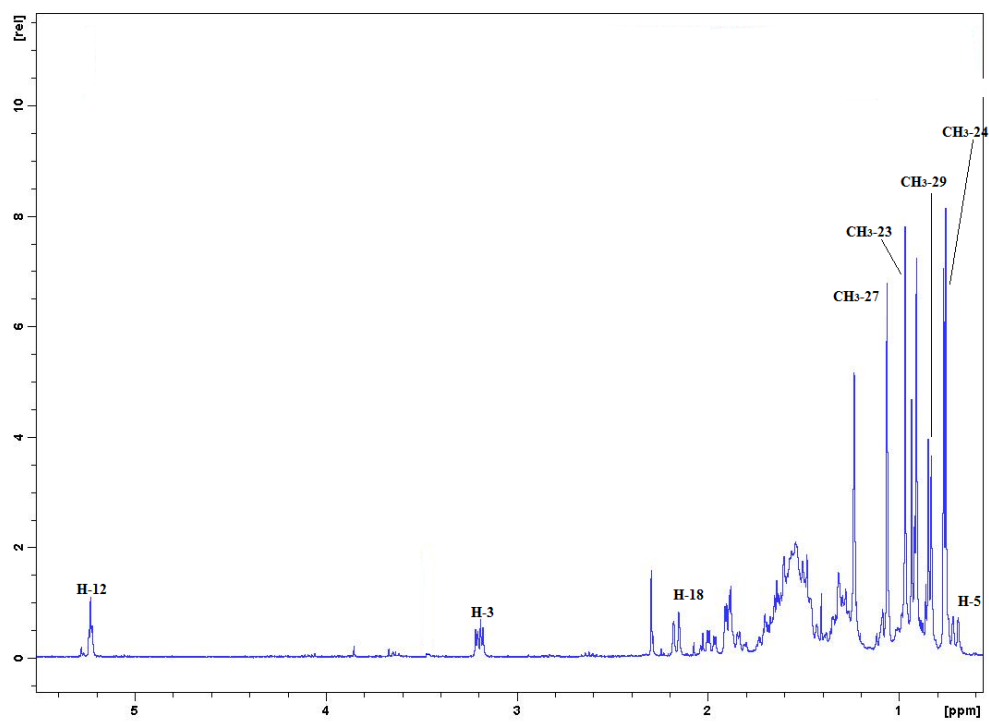
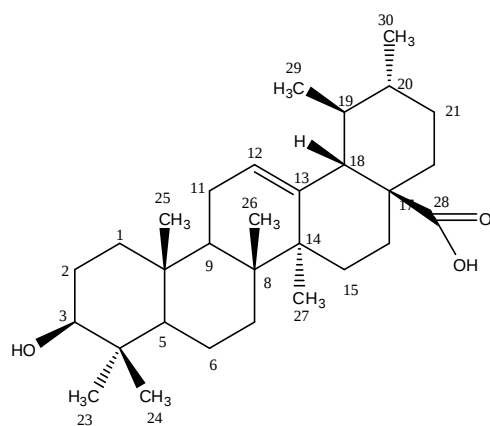


ESI MS of **3**

Table 3: ^1H - and ^{13}C -NMR spectroscopic data of compounds **1** (ursolic acid) in CDCl_3 .

Position	δ_{C}	δ_{H}	J (Hz)
1a	38.9	1.31	m
1b		1.00	m
2	27.2	1.63- 1.54	m
3	78.8	3.19	dd (J =4.5, 10.0)
4		-	-
5	55.1	0.69	dd
6a, b	18.1	1.39-1.32	m
7a,b	33.1	1.46-1.33	m
8	39.5	-	-
9	47.5	1.48	m
10	38.2	-	-
11a,b	23.0	1.89	dd (J= 3.5, 9.0)
12	125.4	5.23	t (J= 3.5)
13	137.8	-	-
14	41.9	-	-
15	27.6	*	
16a	23.7	2.01-1.08	dd (J= 4.3, 12.9)
16b		2.02	brd (J= 4.3)
17	47.5	-	-
18	52.5	2.16	d (J= 10.7)
19	38.8	1.30	m
20	39.2		
21a	32.8	1.45	m
21b		1.34	m
22	36.5	1.70	m
23	28.1	0.96	s
24	15.3	0.74	s
25	15.4	0.90	s
26	16.8	0.76	s
27	23.5	1.05	s
28	180.4	-	-
29	16.8	0.83	d (J= 6.4)
30	21.3	0.91	d (J= 6.4)

* Overlapped signal

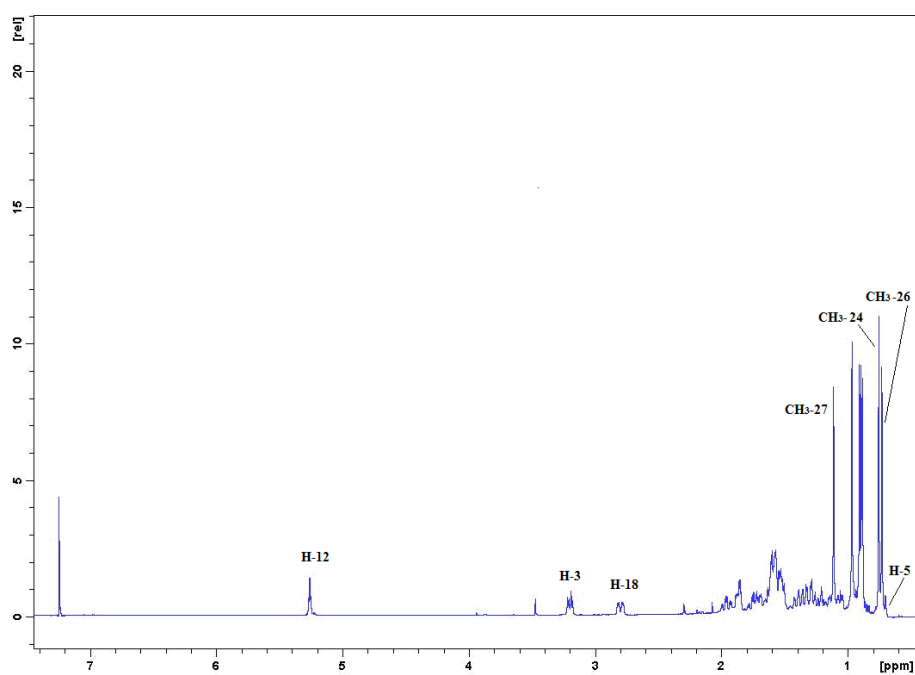
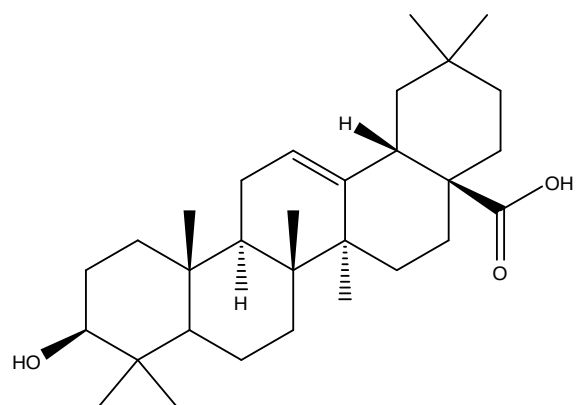


^1H NMR of 1

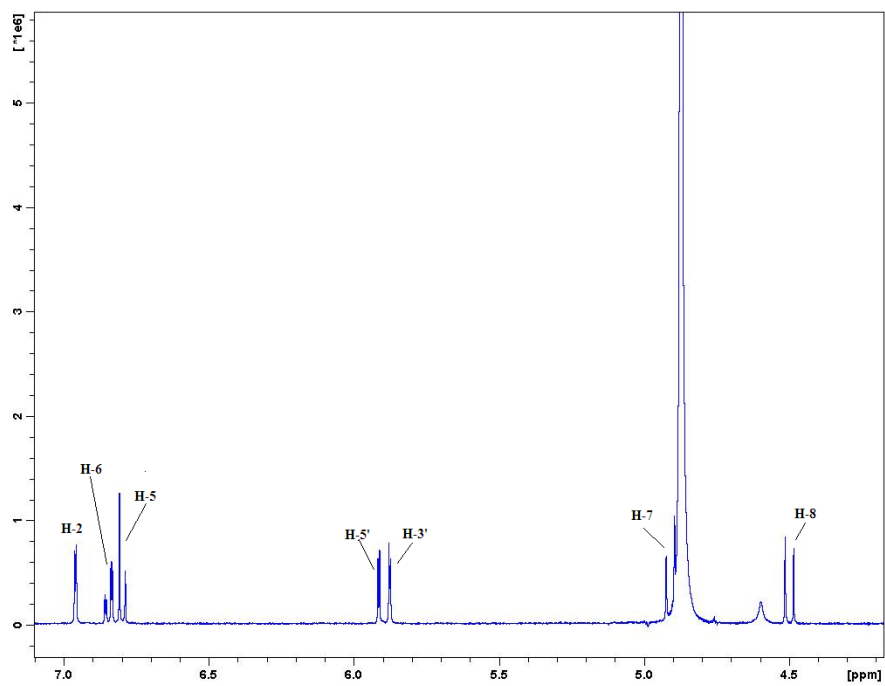
Table 4: ^1H - and ^{13}C -NMR spectroscopic data of compounds **4** (oleanolic acid) in CDCl_3 .

Position	δ_{C}	δ_{H}	J (Hz)
1	38.4	1.55-1.63	m
2a		1.58	m
2b	27.1	*	
3	78.5	3.21	dd (J= 10.2, 4.8)
4	38.3	-	-
5	55.3	0.70	brs
6a		1.52	m
6b	18.8	1.37	m
7a		1.18	m
7b	32.6	1.44	m
8	39.3	-	-
9	47.7	1.54	m
10	36.8	-	-
11	23.1	1.85	m
12	122.7	5.25	t (J=3.5)
13	143.6	-	-
14	41.3	-	-
15	28	1.56	m
16a		1.90	*
16b	22.3	1.82	*
17	45.8	-	-
18	40.6	2.79	dd (J=4.3, 13.7)
19a		1.60	
19b	46.4	1.15	m
20	30.6	-	-
21	33.8	1.65-1.48	m
22a		1.73	m
22b	32.5	1.29	m
23	27.8	0.96	s
24	15.6	0.75	s
25	15.3	0.89	s
26	17.1	0.72	s
27	25.8	1.11	s
28	183.4	-	-
29	32.9	0.88	s
30	23.9	0.90	s

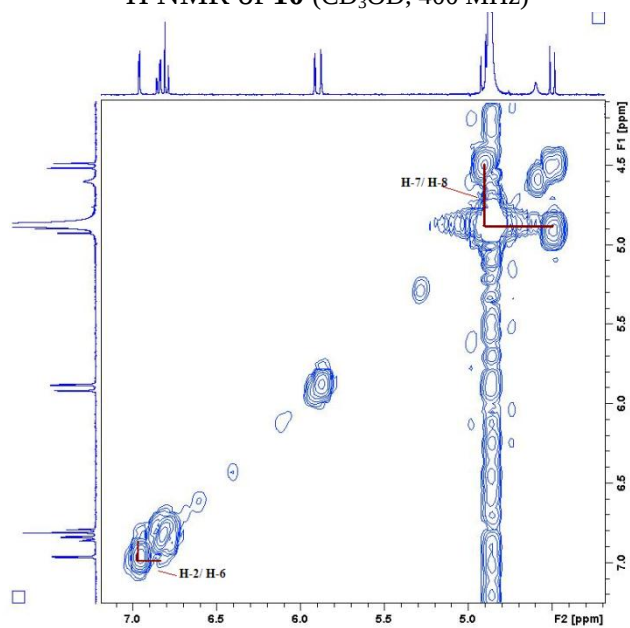
* Overlapped signal



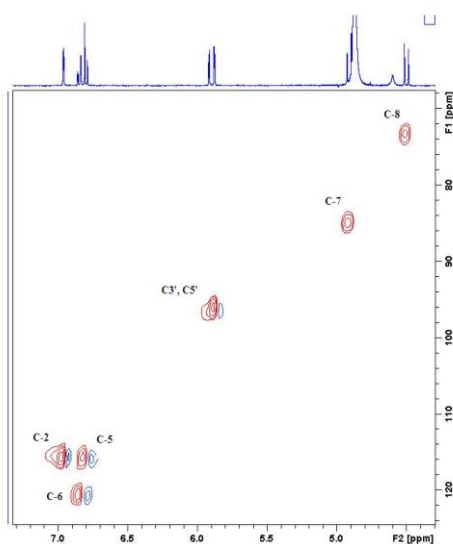
^1H NMR of 4



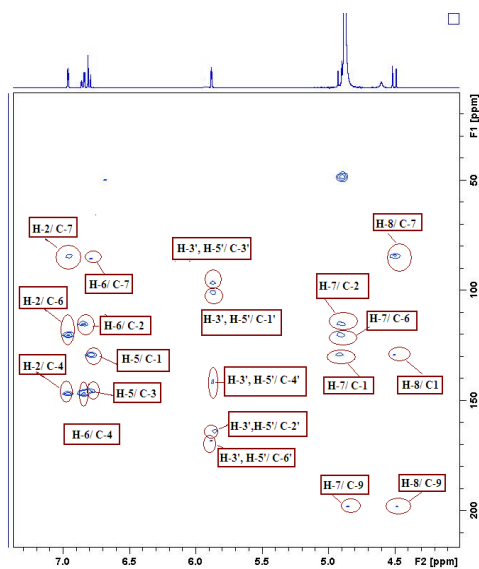
^1H NMR of **10** (CD_3OD , 400 MHz)



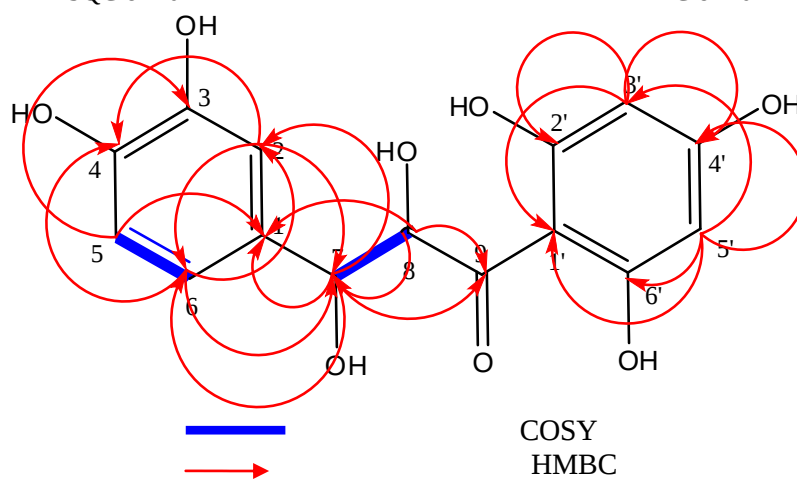
COSY of **10**



HSQC of 10



HMBC of 10



Structures of isolated compounds	
Ursolic acid (1)	3β, 21α-dihydroxy-urs-12-en-28-oic acid (2)
28-hydroxymethylene-21-methyl-urs-12-ene (3)	oleanolic acid (4)
apigenin (5)	5,6,4'-trihydroxy-7,3'-dimethoxy-flavone (6)
cirsilioneol (7)	sudachitin (8)
apigenin 7-O-β-D-glucuronide (9),	cilicione-b (10)