

Supplementary Material: Antiproliferative Activity of (-)-Rabdosiin Isolated from *Ocimum sanctum* L.

Alexandros Flegkas, Tanja Milosević Ifantis, Christina Barda, Pinelopi Samara, Ourania Tsitsilonis and Helen Skaltsa

Table 1. ¹H-NMR of 6 (CD₃OD, 400MHz).

δ (ppm)	n ^o H	J (Hz)	Interpretation
7.58	1	s	H-4
6.81	1	s	H-5
6.74	1	<i>d</i> (J = 2.0)	H-2''
6.68	1	<i>d</i> (J = 1.8)	H-2'''
6.67	1	<i>d</i> (J = 8.0)	H-5'''
6.66	1	<i>d</i> (J = 8.0)	H-5''
6.62	1	<i>d</i> (J = 8.2)	H-5'
6.58	1	<i>dd</i> (J = 8.0; 2.0)	H-6''
6.51	1	<i>dd</i> (J = 8.0; 2.0)	H-6'''
6.49	1	s	H-8
6.35	1	<i>dd</i> (J = 8.0; 2.0)	H-6'
6.32	1	<i>d</i> (J = 2.0)	H-2'
5.05	1	<i>dd</i> (J = 7.8; 4.4)	H-8'''
4.99	1	<i>dd</i> (J = 7.2; 5.2)	H-8''
4.44	1	brs	H-1
3.90	1	<i>d</i> (J = 2.0)	H-2
3.04	1	<i>dd</i> (J = 14.4; 4.2)	H-7'''a
2.98–2.88	2	<i>m</i>	H-7''a,b
2.93	1	<i>dd</i> (J = 14.0; 7.8)	H-7'''b

Table 2. ^{13}C -NMR of **6** (CD_3OD , 400MHz).

Position	δ (ppm)	Type of C
1	45.9	CH
2	48.1	CH
3	120.7	C
4	140.6	CH
5	116.8	CH
6	144.5	C
7	148.9	C
8	117.2	CH
9	131.0	C
10	124.2	C
1'	135.9	C
2'	115.2	CH
3'	144.1	C
4'	144.2	C
5'	115.8	CH
6'	119.6	CH
1''	128.9	C
2''	117.3	CH
3''	145.5	C
4''	144.4	C
5''	116.2	CH
6''	121.7	CH
7''	37.4	CH_2
8''	74.9	CH
9''	172.4	$\text{C}=\text{O}$
1'''	128.9	C
2'''	116.1	CH
3'''	145.5	C
4'''	144.4	C
5'''	116.7	CH
6'''	121.7	CH
7'''	37.4	CH_2
8'''	74.9	CH
9'''	173.3	$\text{C}=\text{O}$
2-COO	173.1	$\text{C}=\text{O}$
3-COO	167.8	$\text{C}=\text{O}$

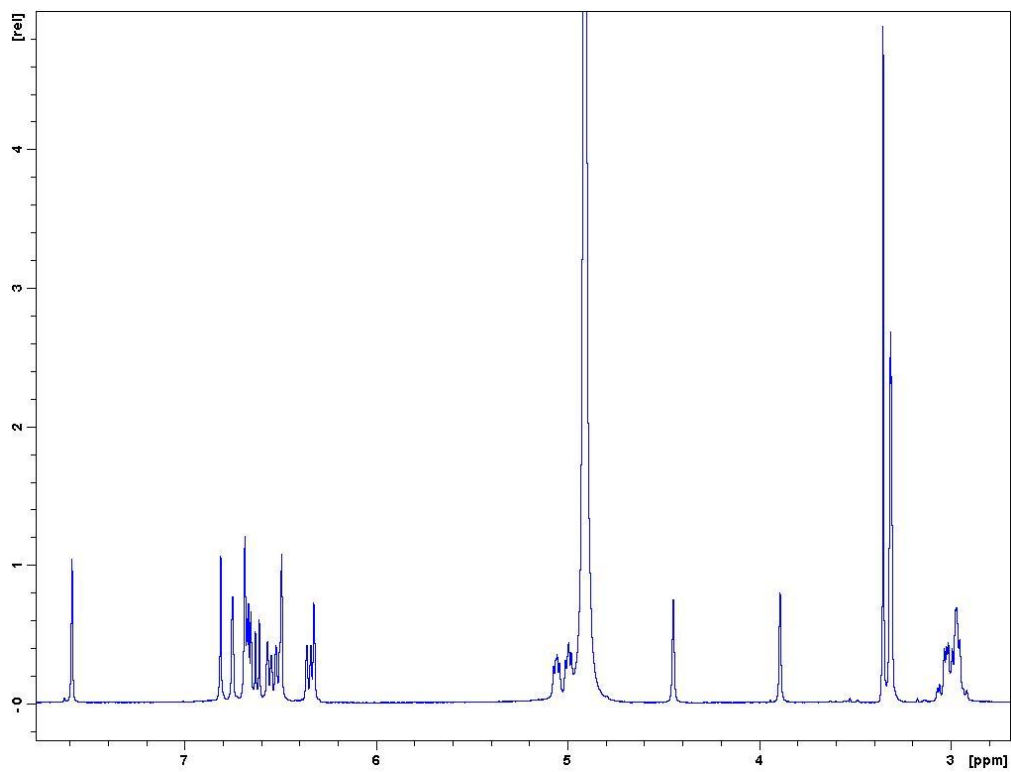


Figure 1. ¹H–NMR spectrum of **6** (CD₃OD, 400 Hz).

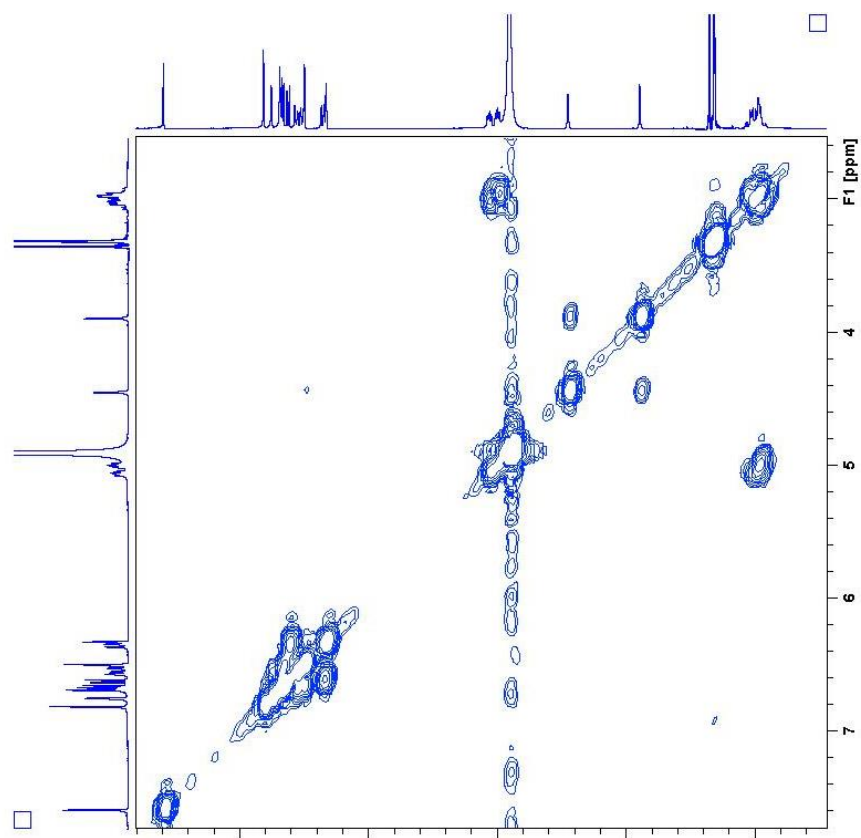


Figure 2. COSY spectrum of **6** (CD₃OD, 400 Hz).

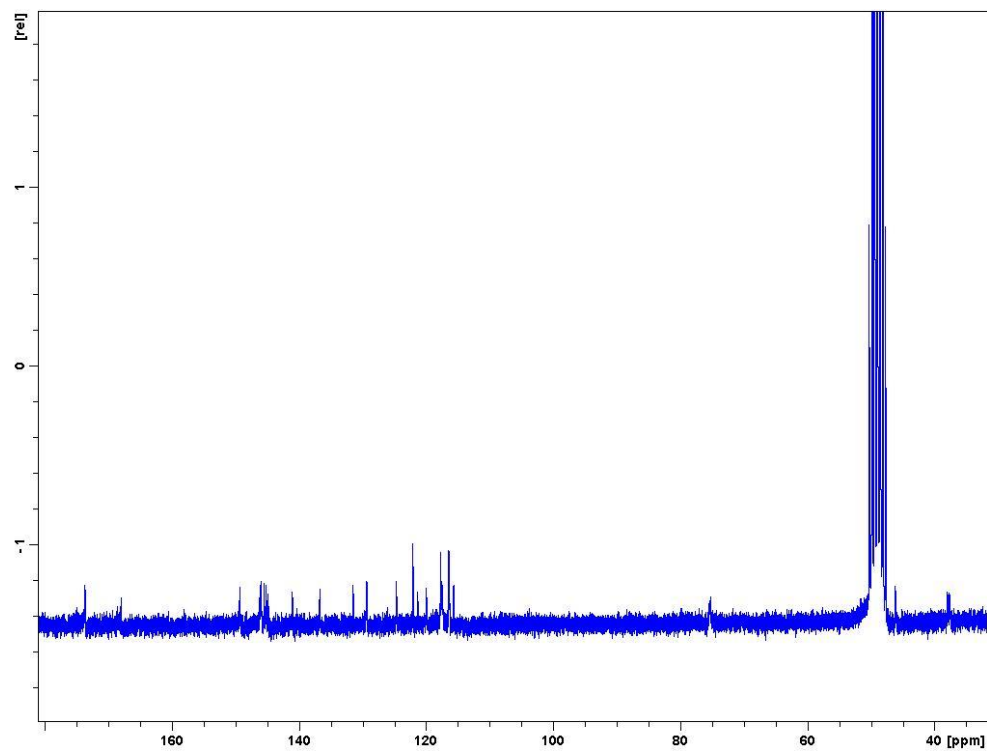


Figure S3. ¹³C NMR spectrum of 6 (CD₃OD, 400 Hz).

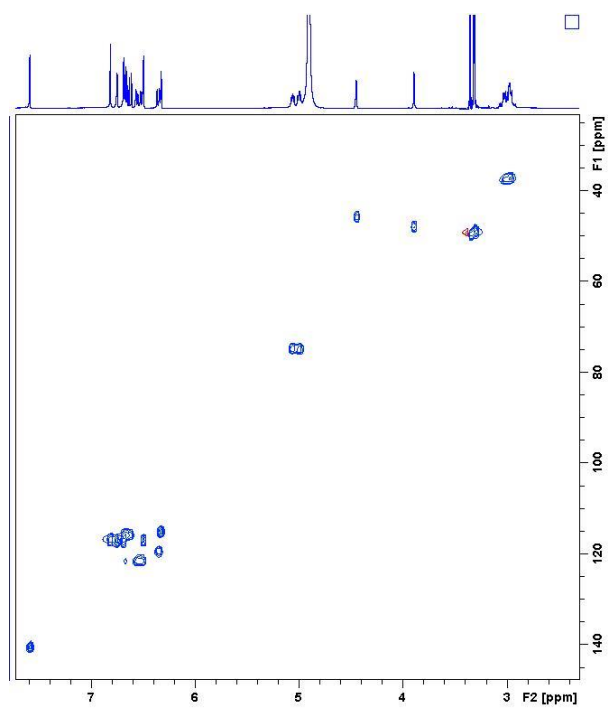


Figure 4. HSQC spectrum of 6 (CD₃OD, 400 Hz).

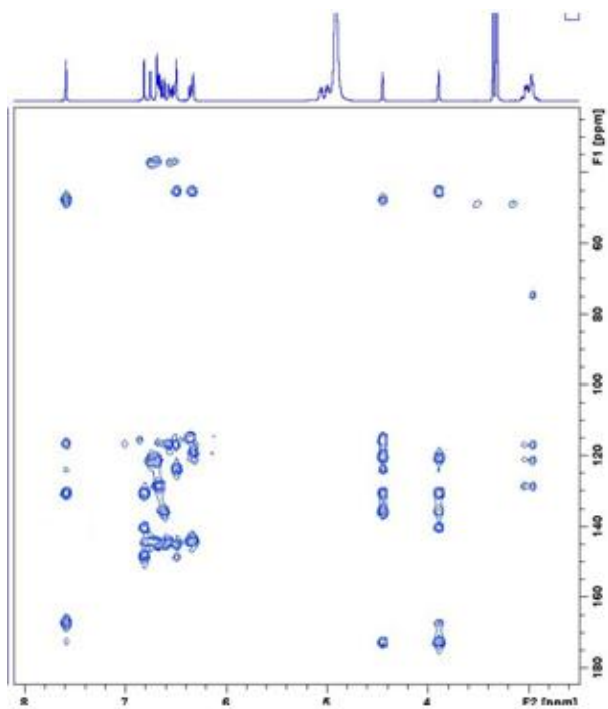


Figure 5. HMBC spectrum of 6 (CD₃OD, 400 Hz).

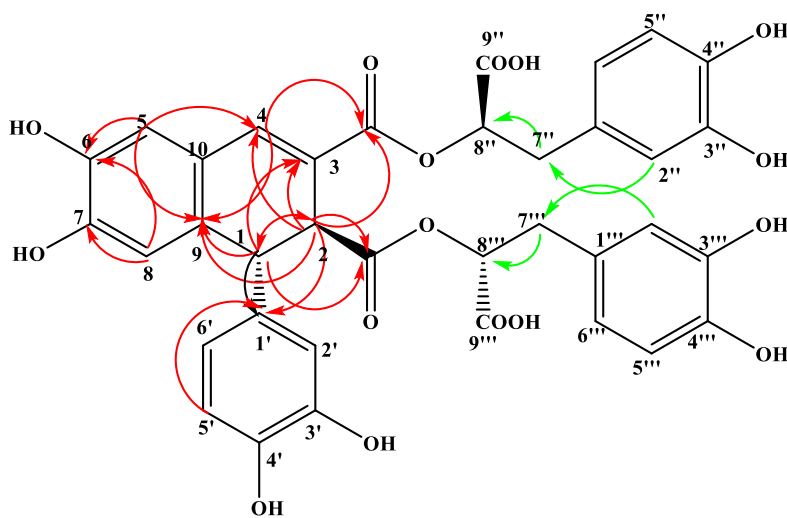


Figure 6. Most important HMBC signals of compound 6.