

# Phytochemical Investigation and Biological Studies on Selected *Searsia* Species.

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## Moronic acid (1) and 21 $\beta$ -hydroxylolean-12-en-3-one (2)

**Table S1:** <sup>1</sup>H (400 MHz) and <sup>13</sup>C (100 MHz) NMR spectral data of C1 and C2 in CDCl<sub>3</sub>

No.	C1		C2	
	$\delta_H$ (mult, J)	$\delta_C$	$\delta_H$ (mult, J)	$\delta_C$
1	1.98 (m)	39.8		39.9
2	2.40 (m)	33.8	1.90 (m)	34.2
3		218.3	2.41 (m)	217.8
4		47.3		47.6
5	1.39(m)	55.3		55.3
6	1.38 (m)	19.6	1.33 (m)	19.6
7	2.49 (m)	33.9	1.51 (m)	33.8
8		40.6	2.37 (m)	41.3
9	1.39 (m)	50.5		50.6
10		36.8	1.34 (m)	37.1
11	1.33 (m)	21.4		20.1
12	1.28 (m)	26.0	1.46 (m)	122.4
13	2.27(m)	41.6	5.33 t, J = 7.08 Hz	143.6
14		42.6		41.7
15	1.27 (m)	29.3		29.7
16	1.48 (m)	33.7	1.27 (m)	29.6
17		47.9	1.36 (m)	36.7
18		136.6		46.8
19	5.19 (s)	132.4	0.78 (m)	45.8
20		32.1	1.19 (m)	36.7
21	2.22 (t)	33.4		78.9
22	2.19 (t)	33.3	3.22 dd, J = 11,2; 5.3 Hz)	45.2
23	1.05 (3H, s)	20.9	1.19 (m)	23.6
24	1.09 (3H, s)	26.8	0.96 3H, (s)	26.4
25	1.04 (3H, s)	15.8	0.86 (3H, s)	15.4
26	0.97 (3H, s)	16.7	0.79 (3H, s)	16.8
27	0.81 (3H, s)	14.8	0.84 (3H, s)	25.8
28		181.3	1.10 (3H, s)	27.8
29	0.99 (3H, s)	29.1	0.99 (3H, s)	28.0
30	1.02 (3H, s)	30.4	0.98 (3H, s)	15.3
C=O			0.79 (3H, s)	
CH <sub>3</sub>				

**Myricetin-3-*O*-β-galactopyranoside (3) and Rutin (4)**

**Table S2:** <sup>1</sup>H (400 MHz) and <sup>13</sup>C (100 MHz) NMR spectral data of **C3** and **C4** in CDOD<sub>3</sub>

<b>C3</b>			<b>C4</b>	
<b>No.</b>	<b>δ<sub>H</sub> (<i>mult</i>, <i>J</i>)</b>	<b>δ<sub>C</sub></b>	<b>δ<sub>H</sub> (<i>mult</i>, <i>J</i>)</b>	<b>δ<sub>C</sub></b>
<b>2</b>		157.2		157.1
<b>3</b>		134.5		134.3
<b>4</b>		177.9		178.0
<b>5</b>		161.6		161.5
<b>6</b>	6.2 ( <i>d</i> , <i>J</i> = 2.08 Hz)	98.4	6.23 ( <i>d</i> , <i>J</i> = 2.04 Hz)	98.6
<b>7</b>		164.6		164.6
<b>8</b>	6.39 ( <i>d</i> , <i>J</i> = 1.92 Hz)	93.2	6.42 ( <i>d</i> , <i>J</i> = 2.04 Hz)	93.5
<b>9</b>		156.9		158.0
<b>10</b>		105.7		104.2
<b>1`</b>		120.2		121.7
<b>2`</b>	7.38 <i>s</i> )	108.5	6.89 ( <i>d</i> , <i>J</i> = 8.5 Hz)	114.7
<b>3`</b>		144.9		144.3
<b>4`</b>		136.7		148.4
<b>5`</b>		144.9	7.69 ( <i>d</i> , <i>J</i> = 2.1 Hz)	116.3
<b>6`</b>	7.38 ( <i>s</i> )	108.5	7.65 ( <i>dd</i> , <i>J</i> = 8.4, 2.1 Hz)	122.2
<b>galactopyranoside</b>			<b>glucose</b>	
<b>1``</b>	5.21 ( <i>d</i> , <i>J</i> = 7.8 Hz)	104.1	5.09 ( <i>d</i> , <i>J</i> = 7.6 Hz)	103.6
<b>2``</b>	3.82	71.2	3.52	74.2
<b>3``</b>		73.2	3.44	76.7
<b>4``</b>	3.87 ( <i>d</i> , <i>J</i> = 3.36 Hz)	68.6	3.29	69.9
<b>5``</b>	3.49	75.8		75.7
<b>6``</b>		60.5		67.1
			<b>rhamnose</b>	
<b>1'''</b>			4.54 ( <i>d</i> , <i>J</i> = 1.2 Hz)	101.0
<b>2'''</b>				70.6
<b>3'''</b>			3.55 ( <i>d</i> , <i>J</i> = 2.3 Hz)	70.8
<b>4'''</b>			3.30	72.5
<b>5'''</b>			3.46 ( <i>d</i> , <i>J</i> = 2.4 Hz)	68.3
<b>6'''</b>			1.15 ( <i>d</i> , <i>J</i> = 6.2 Hz)	17.0

**Quercetin (5)**

**Table S3:**  $^1\text{H}$  (400 MHz) and  $^{13}\text{C}$  (100 MHz) NMR spectral data of compound **C5** in  $\text{CD}_3\text{OD}$

No.	$\delta_{\text{H}}$ ( <i>mult</i> , <i>J</i> )	$\delta_{\text{C}}$
<b>2</b>		147.4
<b>3</b>		135.8
<b>4</b>		175.9
<b>5</b>		161.1
<b>6</b>	6.08 ( <i>d</i> , <i>J</i> = 2.04 Hz)	97.8
<b>7</b>		164.2
<b>8</b>	6.29 ( <i>d</i> , <i>J</i> = 2.12 Hz)	92.9
<b>9</b>		156.8
<b>10</b>		103.1
<b>1'</b>		122.7
<b>2'</b>	7.63 ( <i>d</i> , <i>J</i> = 2.16 Hz)	114.8
<b>3'</b>		144.8
<b>4'</b>		146.6
<b>5'</b>	6.79 ( <i>d</i> , <i>J</i> = 8.48 Hz)	114.6
<b>6'</b>	7.54 ( <i>dd</i> , <i>J</i> = 2.16, 8.48 Hz)	120.2
<b>5-OH</b>	12.18, ( <i>brs</i> )	

**Apigenin (6)**

**Table S4:**  $^1\text{H}$  (400 MHz) and  $^{13}\text{C}$  (100 MHz) NMR spectral data of compound **C6** in DMSO

No.	$\delta_{\text{H}}$ ( <i>mult</i> , <i>J</i> )	$\delta_{\text{C}}$	$\delta_{\text{C}}$ (Lit. (Owen <i>et al.</i> , 2003))
<b>2</b>		162.0	165.30
<b>3</b>		104.5	103.78
<b>4</b>		183.4	183.07
<b>5</b>		165.9	166.46
<b>6</b>	6.1 ( <i>d</i> , <i>J</i> = 1.72 Hz)	99.8	99.71
<b>7</b>		155.2	159.6
<b>8</b>	6.2 ( <i>d</i> , <i>J</i> = 1.8 Hz)	94.4	93.99
<b>9</b>		154.5	157.33
<b>10</b>		109.5	103.6
<b>1'</b>		121.1	121.17
<b>2'</b>	7.6 ( <i>d</i> , <i>J</i> = 8.84 Hz)	129.1	128.48
<b>3'</b>	7.2 ( <i>d</i> , <i>J</i> = 8.60 Hz)	116.4	115.97
<b>4'</b>		161.7	162.9
<b>5'</b>	7.2 ( <i>d</i> , <i>J</i> = 8.60 Hz)	116.4	115.97
<b>6'</b>	7.6 ( <i>d</i> , <i>J</i> = 8.84 Hz)	129.1	128.48
<b>5-OH</b>	12.6 ( <i>s</i> )		

**Amentoflavone (7)**

**Table S5:** <sup>1</sup>H (400 MHz) and <sup>13</sup>C (100 MHz) NMR spectral data of compound **C7** in pyridine

Unit I			Unit II	
No.	$\delta_{\text{H}}$ ( <i>mult</i> , <i>J</i> )	$\delta_{\text{C}}$	$\delta_{\text{H}}$ ( <i>mult</i> , <i>J</i> )	$\delta_{\text{C}}$
<b>2</b>		166.1		162.7
<b>3</b>		102.4		102.4
<b>4</b>		183.2		183.5
<b>5</b>		163.02		162.7
<b>6</b>	6.65 ( <i>d</i> , <i>J</i> = 2.04 Hz)	100.3	6.89 ( <i>d</i> , <i>J</i> = 8.8 Hz)	99.8
<b>7</b>		165.6		165.4
<b>8</b>	6.54 ( <i>d</i> , <i>J</i> = 2.04 Hz)	94.6		103.9
<b>9</b>		155.7		154.5
<b>10</b>		109.4		109.4
<b>1'</b>		121.4		120.5
<b>2'</b>		129.1	7.88 ( <i>d</i> , <i>J</i> = 8.8 Hz)	129.1
<b>3'</b>	7.14 ( <i>d</i> , <i>J</i> = 8.8 Hz)	116.8	7.32 ( <i>d</i> , <i>J</i> = 8.56 Hz)	116.2
<b>4'</b>		161.2		159.1
<b>5'</b>		120.1	7.32 ( <i>d</i> , <i>J</i> = 8.65 Hz)	116.2
<b>6'</b>	7.65 ( <i>d</i> , <i>J</i> = 8.56 Hz)	132.4	7.88 ( <i>d</i> , <i>J</i> = 8.8 Hz)	129.1

**Quercetin-3-*O*- $\beta$ -glucoside (8)**

**Table S6:**  $^1\text{H}$  (400 MHz) and  $^{13}\text{C}$  (100 MHz) NMR spectral data of compound **C8** in  $\text{CD}_3\text{OD}$

No.	$\delta_{\text{H}}$ ( <i>mult</i> , <i>J</i> )	$\delta_{\text{C}}$	$\delta_{\text{C}}$ (Lit. (Zhang <i>et al.</i> , 2014))
<b>2</b>		157.05	156.79
<b>3</b>		134.36	133.99
<b>4</b>		178.14	177.97
<b>5</b>		161.61	161.71
<b>6</b>	6.23 ( <i>d</i> , <i>J</i> = 2.04 Hz)	98.53	99.16
<b>7</b>		164.74	164.66
<b>8</b>	6.42 ( <i>d</i> , <i>J</i> = 2.04 Hz)	93.34	93.98
<b>9</b>		157.40	156.79
<b>10</b>		104.22	104.39
<b>1'</b>		121.46	121.59
<b>2'</b>	7.86 ( <i>d</i> , <i>J</i> = 2.16 Hz)	116.39	115.67
<b>3'</b>		144.42	145.30
<b>4'</b>		148.56	148.95
<b>5'</b>	6.89 ( <i>d</i> , <i>J</i> = 8.52 Hz)	114.69	116.44
<b>6'</b>	7.62 ( <i>dd</i> , <i>J</i> = 2.16, 8.52 Hz)	121.53	122.46
<b>1''</b>	5.17 ( <i>d</i> , <i>J</i> = 7.76 Hz)	103.99	102.33
<b>2''</b>	3.58 ( <i>m</i> )	71.77	71.70
<b>3''</b>	3.84 ( <i>m</i> )	73.68	73.69
<b>4''</b>	3.87 ( <i>m</i> )	68.60	68.41
<b>5''</b>	3.49 ( <i>m</i> )	75.77	76.32
<b>6''</b>	3.65 ( <i>m</i> )	60.52	60.62

**$\alpha$  -Amyrin (9),  $\beta$ -Amyrin (10), and Lupeol (11)**

**Table S7:**  $^1\text{H}$  NMR (400 MHz) and  $^{13}\text{C}$  NMR (100 MHz) of compounds **C9**, **C10**, and **C11** in  $\text{CDCl}_3$

No.	C9		C10		C11	
	$\delta_{\text{H}}$ (mult, J)	$\delta_{\text{C}}$	$\delta_{\text{H}}$ (mult, J)	$\delta_{\text{C}}$	$\delta_{\text{H}}$ (mult, J)	$\delta_{\text{C}}$
1		38.8		38.7		38.6
2		28.7		27.2		27.5
3	3.22 (dd, J = 5.2, 10.8 Hz)	79.06	3.21 (dd, J = 4.8, 10.5 Hz)	79.03	3.17(d, J = 5.1 Hz)	79.0
4		38.7		38.5		39.8
5	0.76	55.3	0.72	55.3	0.69	55.1
6		18.4		18.6		19.0
7		32.2		32.4		34.3
8		40.7		39.8		41.7
9		47.7		47.6		50.7
10		36.6		36.9		37.2
11		23.3		23.6		21.2
12	5.13 (t, J = 3.6 Hz)	124.4	5.19 (t, J = 3.5 Hz)	121.7		25.3
13		139.6		145.2		38.6
14		42.1		41.7		42.8
15		27.2		26.2		27.2
16		26.6		26.1		35.9
17		33.7		32.6		43.0
18	1.31	59.1	1.54	47.8	2.39	48.3
19		39.6	1.92	47.3		47.7
20		39.6		31.0		150.9
21		31.2		34.7		30.1
22	1.85	41.5		37.1		40.8
23	0.83	28.1	0.77	28.0	0.80	28.7
24	0.76	15.6	0.90	15.5	0.77	15.7
25	0.73	15.6	0.73	15.4	0.84	16.2
26	0.83	16.9	0.93	16.1	1.04	16.1
27	1.01	23.2	1.19	25.9	0.96	14.5
28	0.94	28.1	1.07	28.4	0.80	18.1
29	0.79	17.9	0.87	33.8	4.69 (s)	109.3
					4.56 (s)	
30	0.86	19.4	0.80	23.7	1.70	19.8

## ANNEXURE ONE

### NMR SPECTRA OF COMPOUNDS ISOLATED FROM *RHUS LUCIDA*

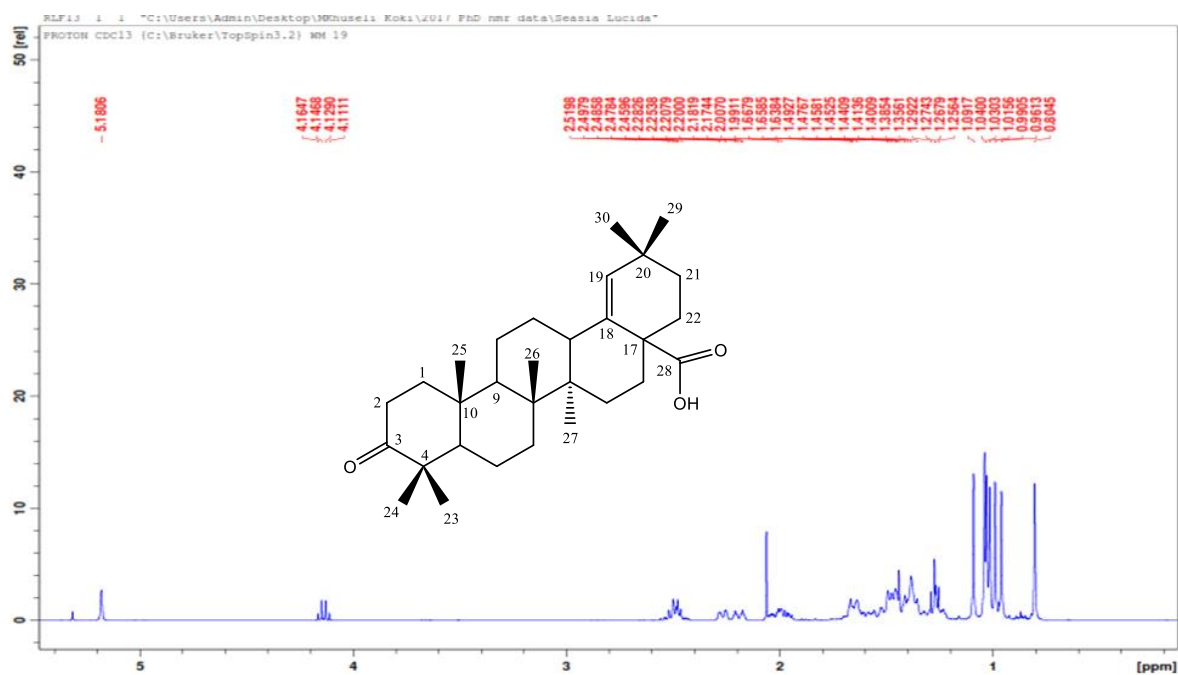


Figure S1: <sup>1</sup>H NMR moronic acid (C1) in CDCl<sub>3</sub>

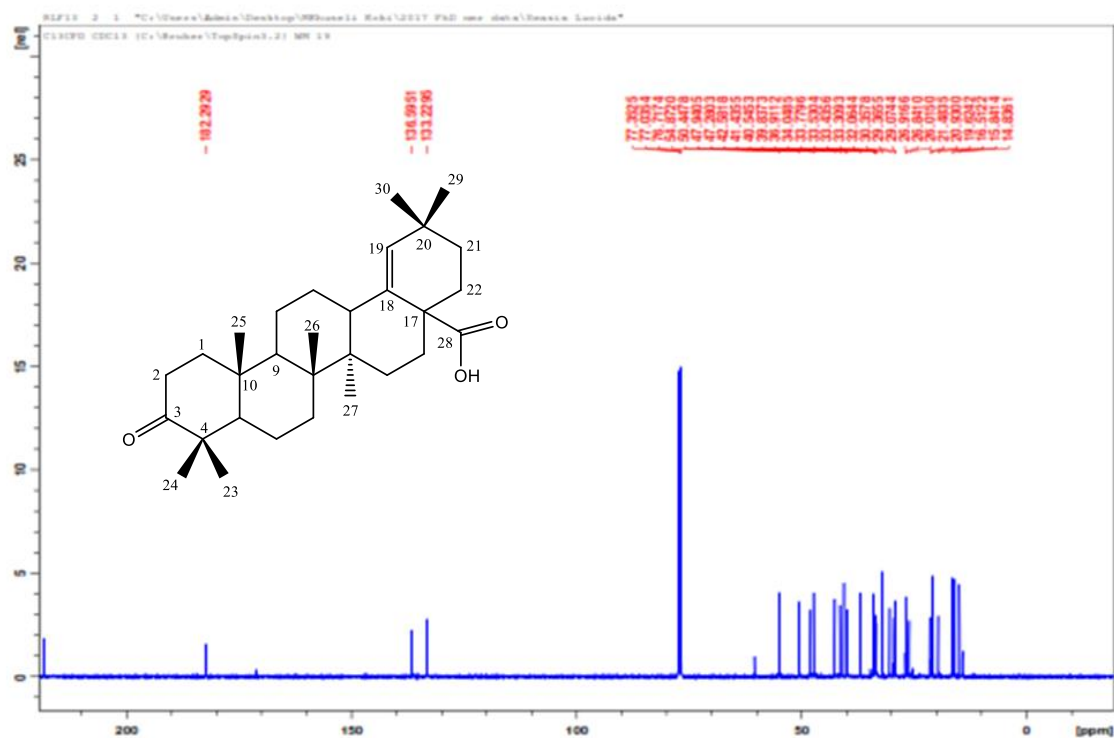


Figure S2: <sup>13</sup>C NMR of moronic acid (C1) in CDCl<sub>3</sub>



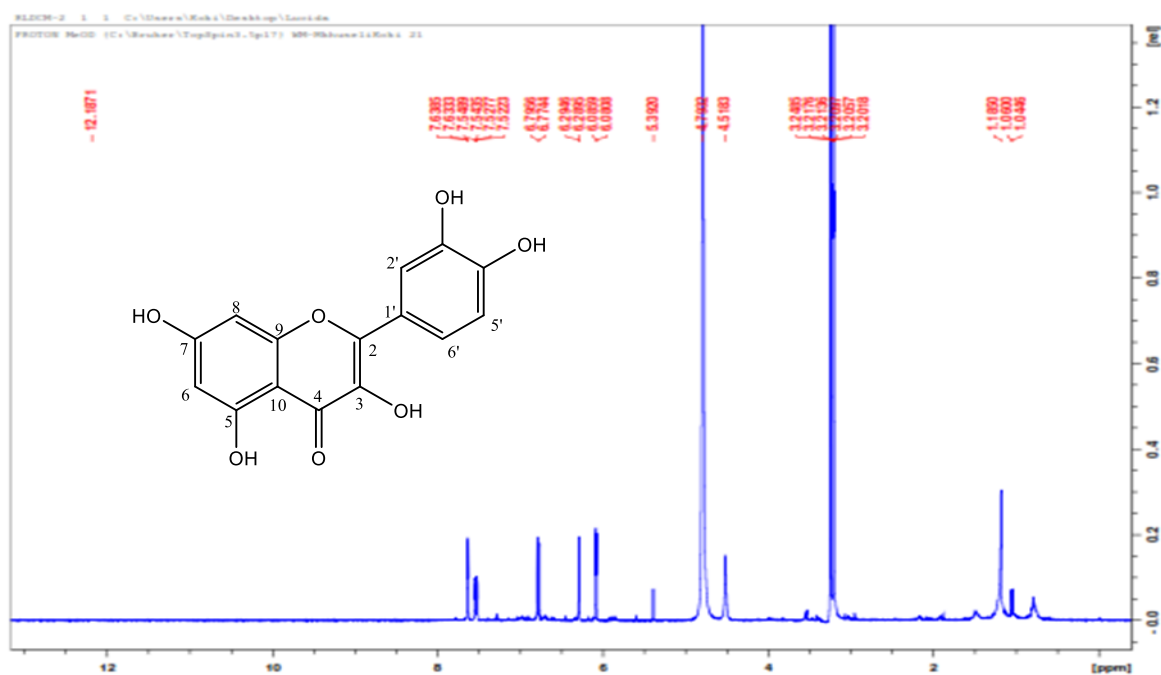


Figure S3:  $^1\text{H}$  NMR of quercetin (C5) in  $\text{CD}_3\text{OD}$

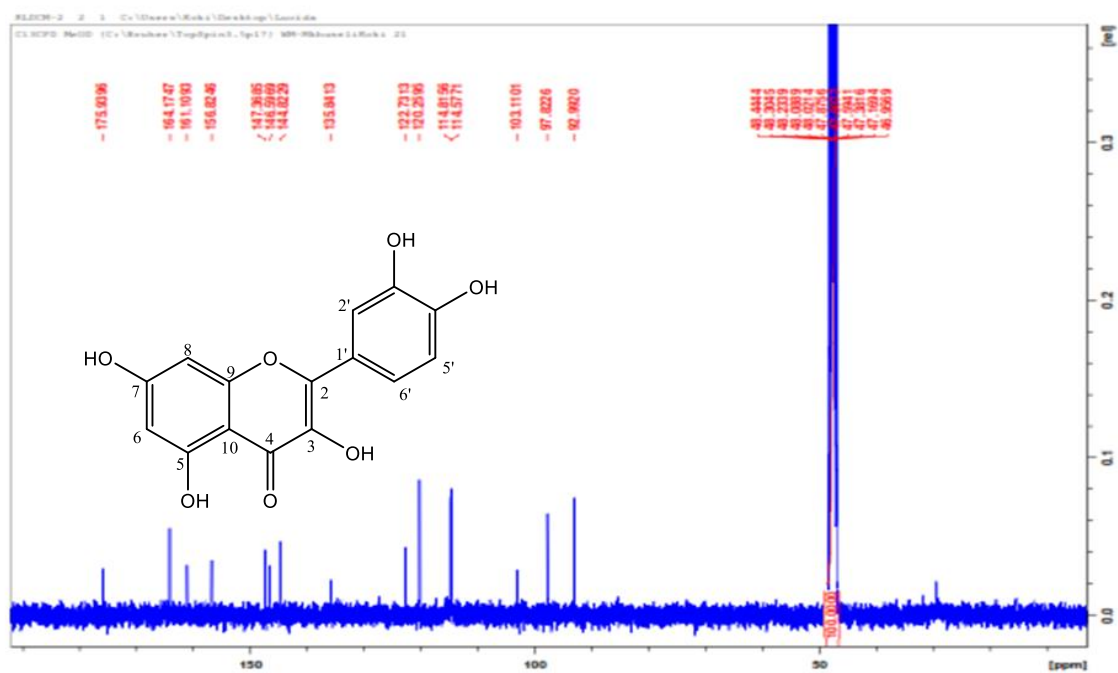


Figure S4:  $^{13}\text{C}$  NMR of quercetin C5 in  $\text{CD}_3\text{OD}$

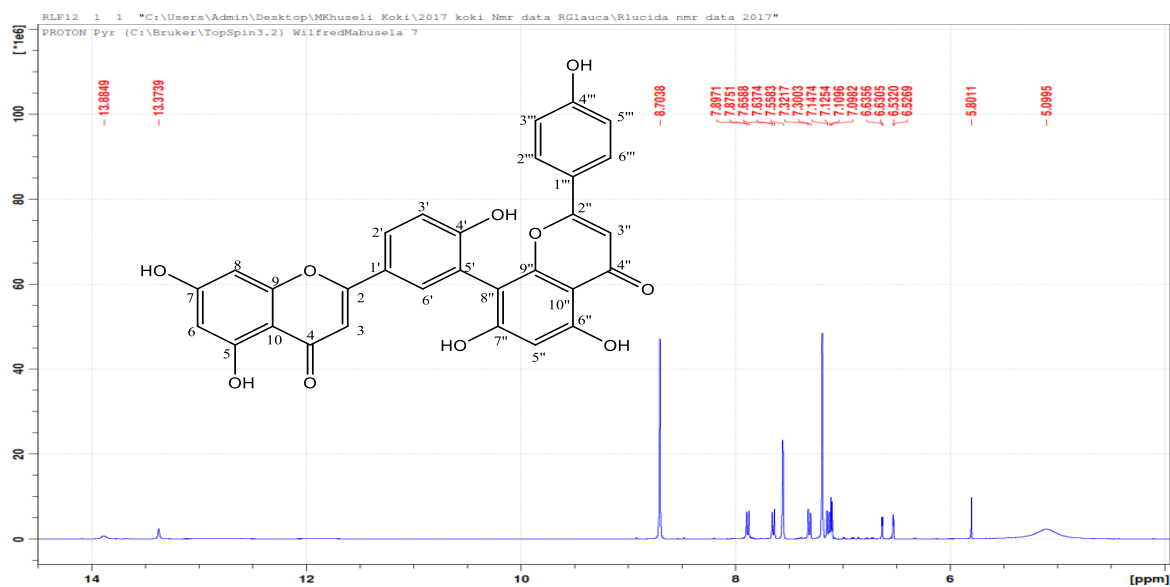


Figure S5:  $^1\text{H}$  NMR of amentoflavone (C7) in Pyridine- $\text{d}_5$

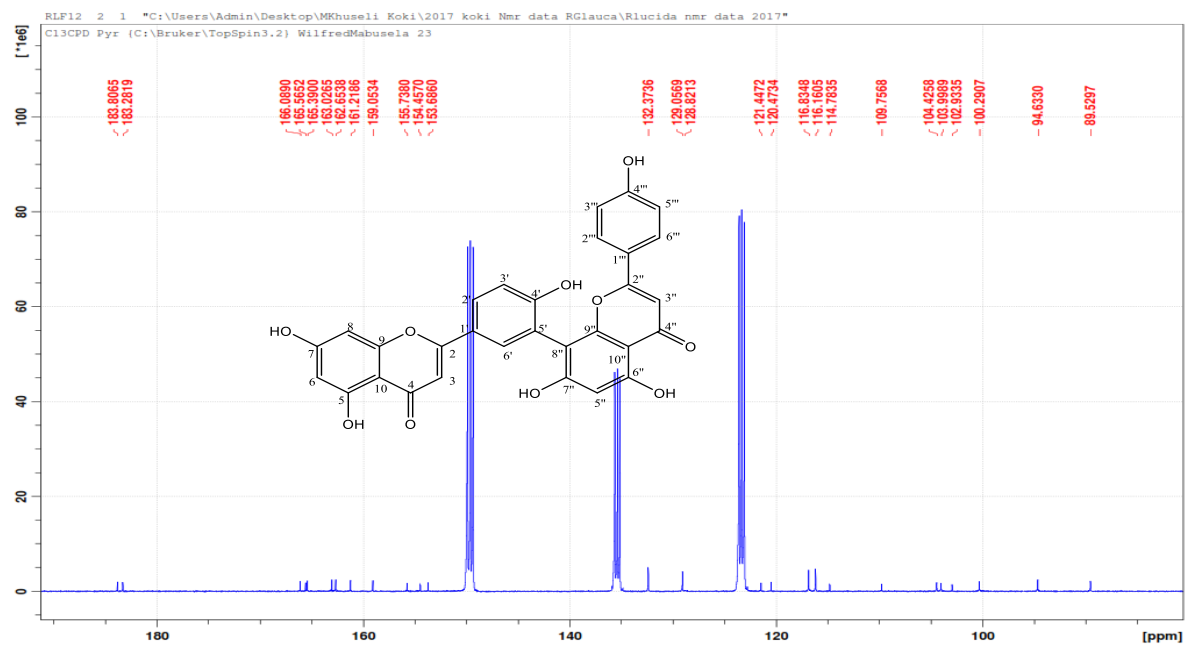


Figure S6:  $^{13}\text{C}$  NMR of amentoflavone (C7) in Pyridine- $\text{d}_5$

## ANNEXURE TWO

### NMR SPECTRA OF COMPOUNDS ISOLATED FROM *R. GLAUCA*

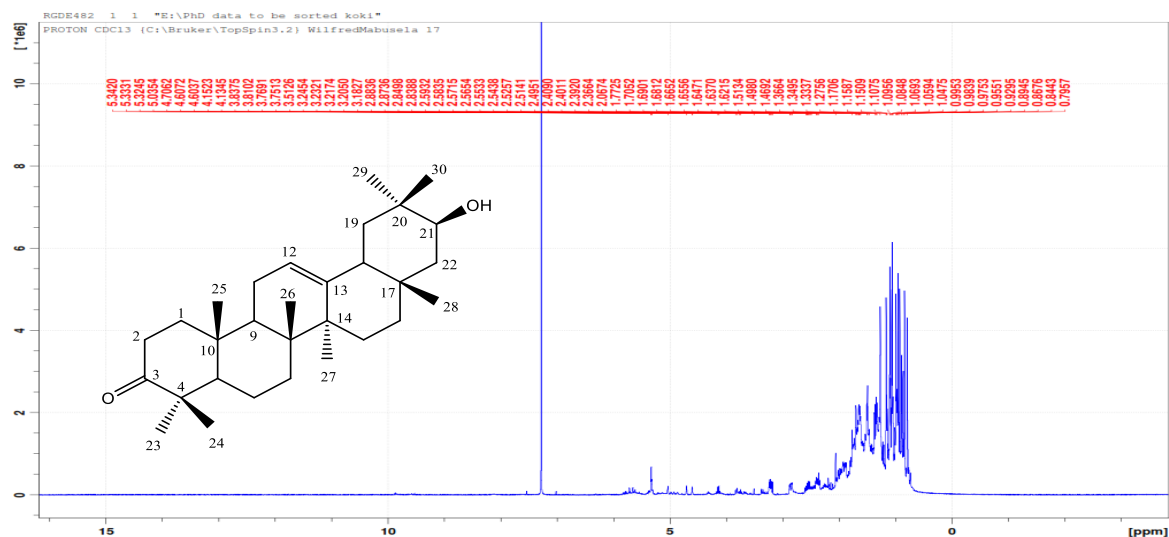


Figure S7:  $^1\text{H}$  NMR spectrum of 21- $\beta$ -hydroxylean-12-en-3-one (C2) in  $\text{CDCl}_3$

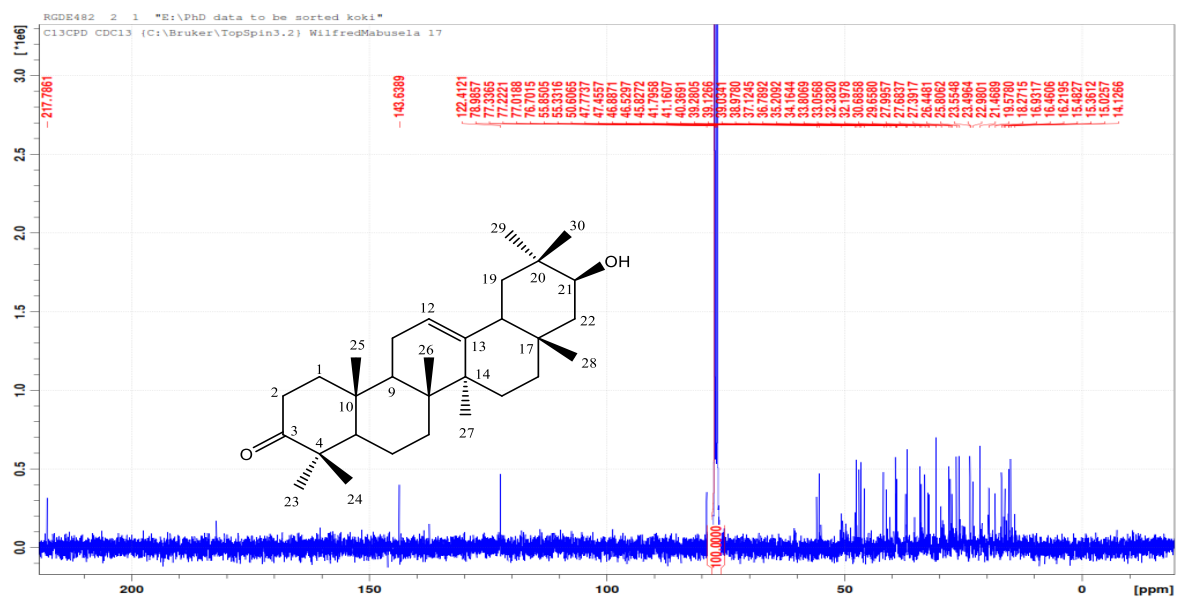


Figure S8:  $^{13}\text{C}$  NMR spectrum of 21- $\beta$ -hydroxylean-12-en-3-one (C2) in  $\text{CDCl}_3$

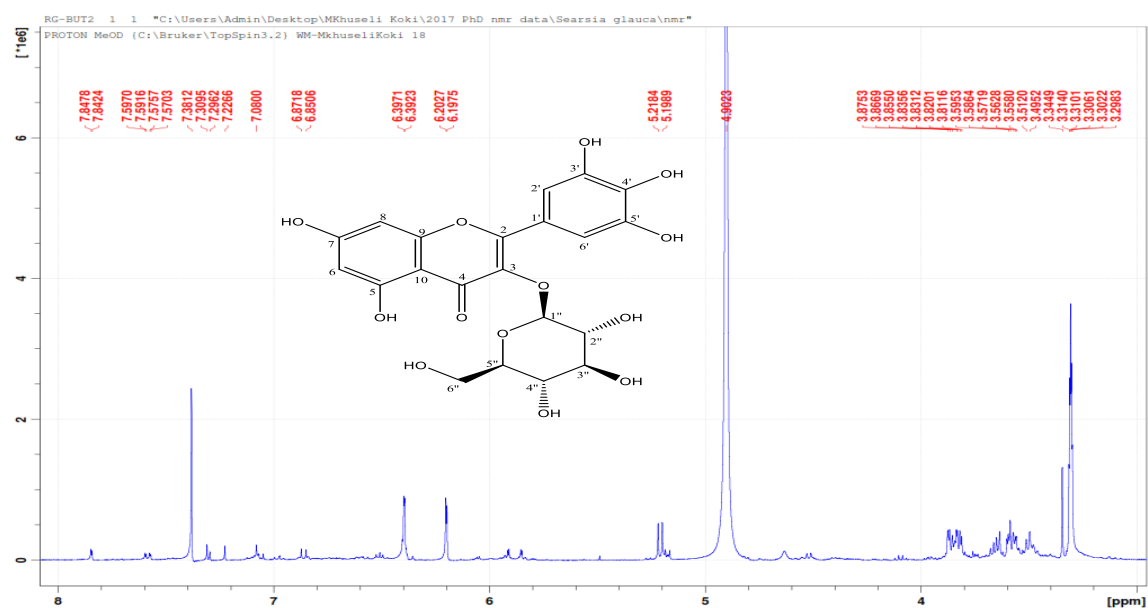


Figure S9:  $^1\text{H}$ -NMR of myricetin 3-O- $\beta$ -galactopyranoside (C3) in  $\text{CD}_3\text{OD}$

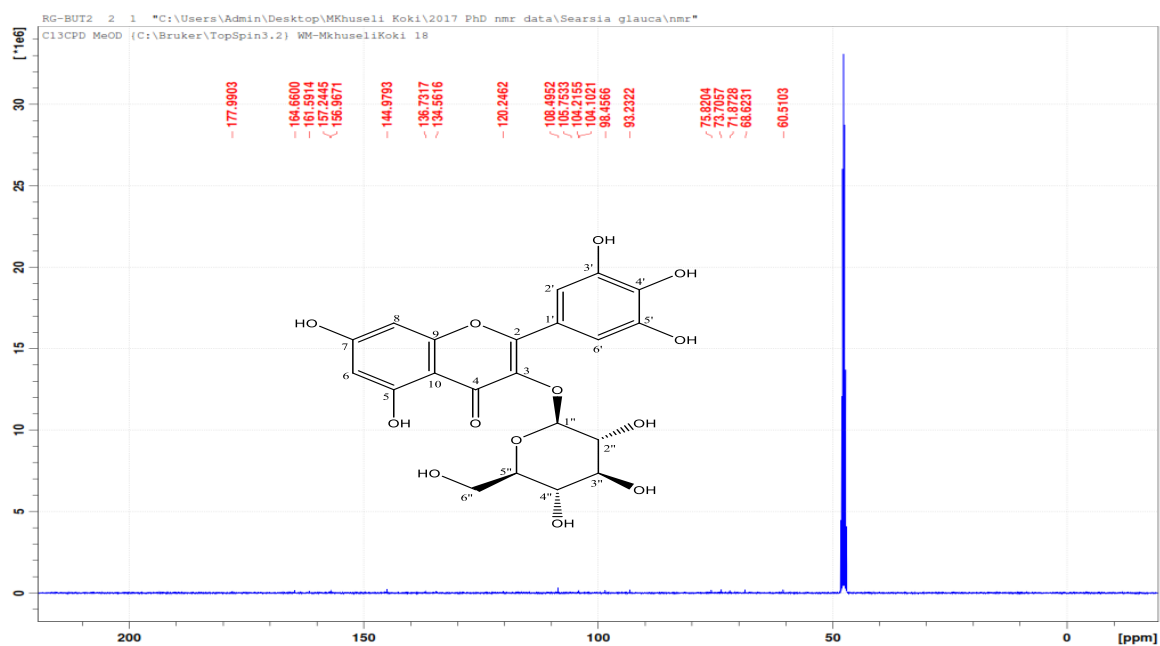


Figure S10:  $^{13}\text{C}$ -NMR of myricetin 3-O- $\beta$ -galactopyranoside (C3) in  $\text{CD}_3\text{OD}$

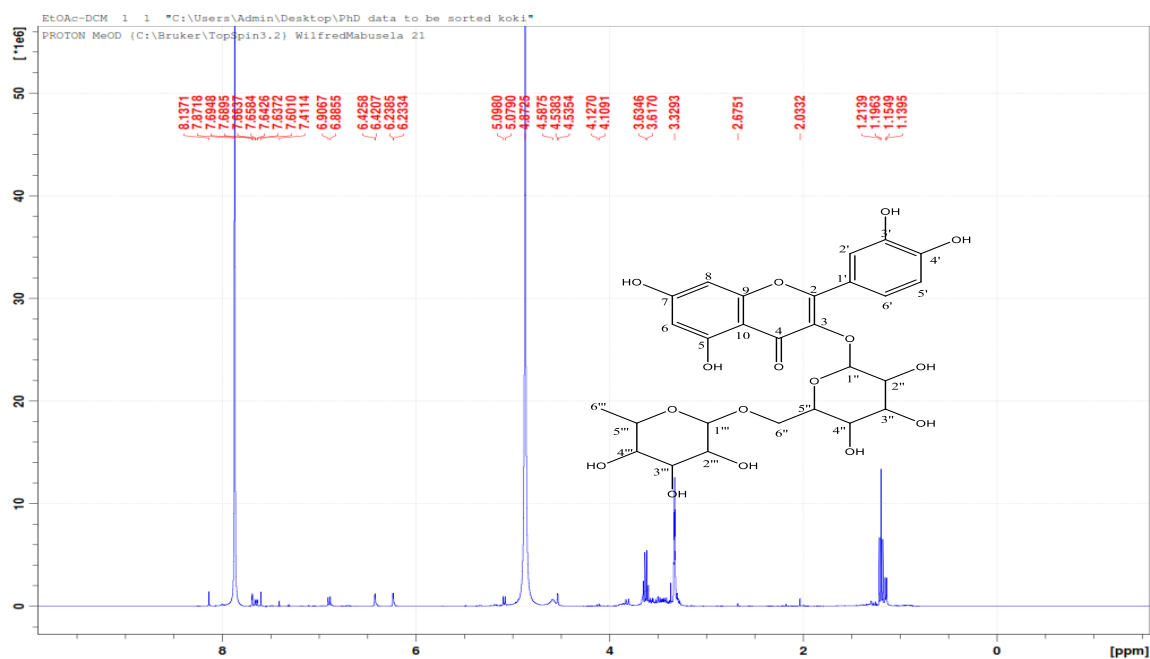


Figure S11:  $^1\text{H}$  NMR of Rutin (C4) in  $\text{CD}_3\text{OD}$

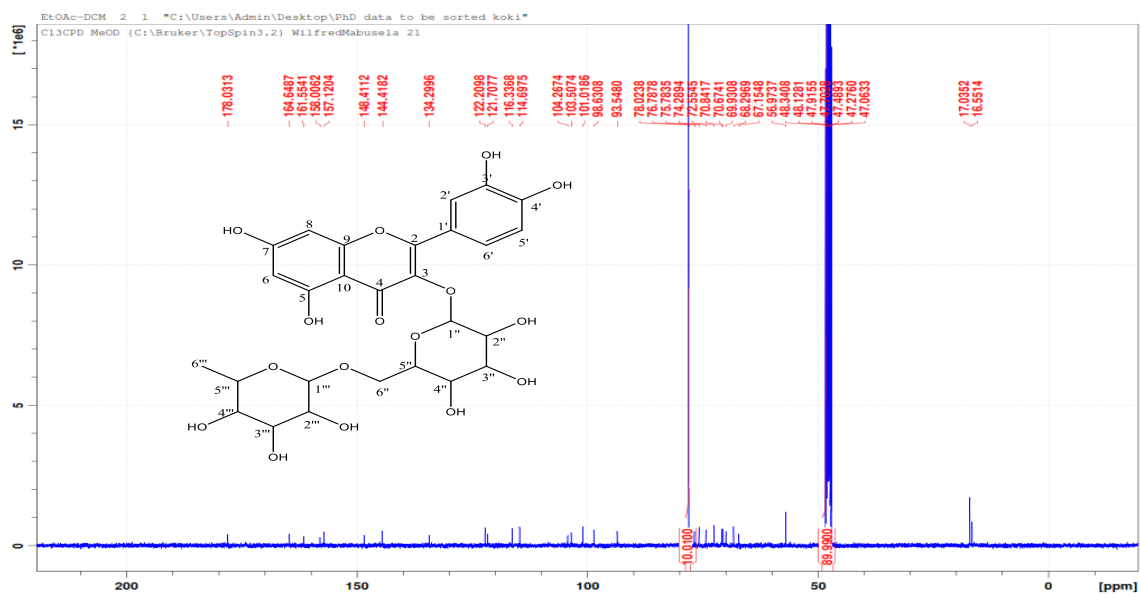


Figure S12:  $^{13}\text{C}$  NMR of Rutin (C4) in  $\text{CD}_3\text{OD}$

## ANNEXURE THREE

### NMR SPECTRA OF COMPOUNDS ISOLATED FROM *R. LAEVIGATA*

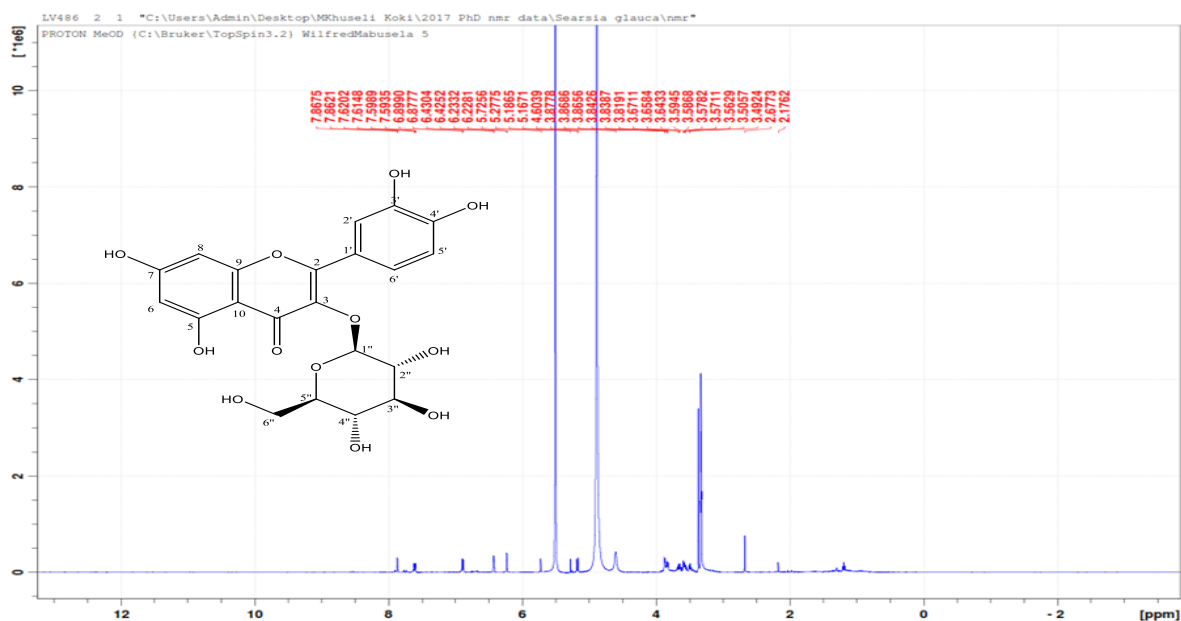


Figure S13:  $^1\text{H}$  NMR of Quercetin-3-O- $\beta$ -glucoside (C8) in  $\text{CD}_3\text{OD}$

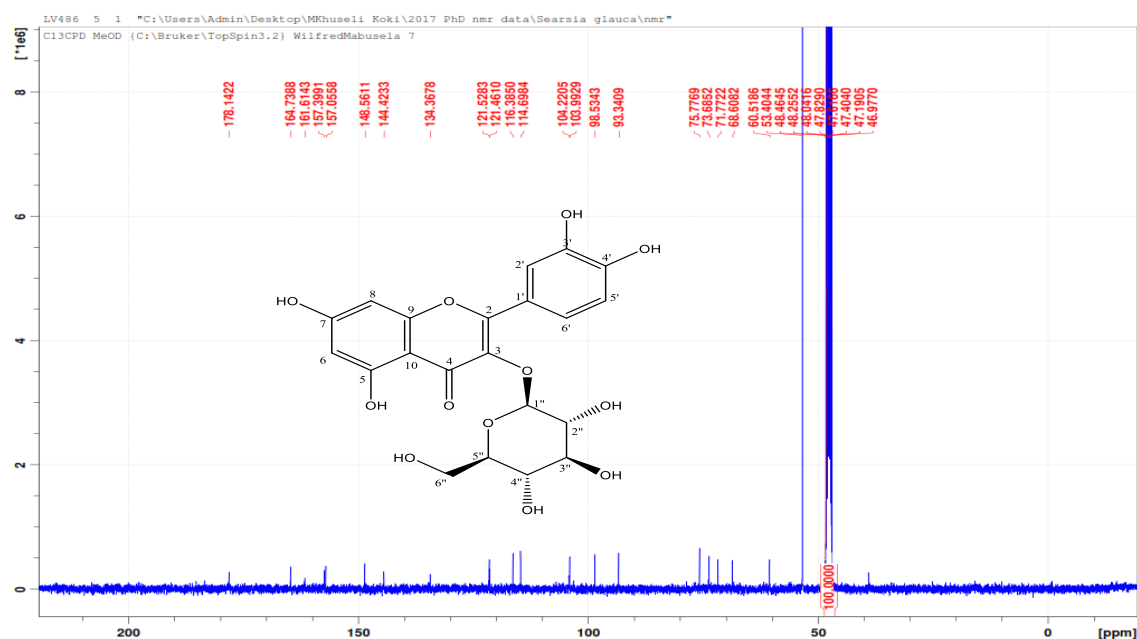


Figure S14:  $^{13}\text{C}$  NMR of Quercetin-3-O- $\beta$ -glucoside (C8) in  $\text{CD}_3\text{OD}$