

## Supplementary material

# Inositol Derivatives and Phenolic Compounds from the Roots of *Taraxacum coreanum*

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**Table S1.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopic data for compound **3**

Carbon No	<b>3</b>	
	$^1\text{H}$	$^{13}\text{C}$
1, 4	5.08 (2H, dt, $J = 7.5, 2.0$ Hz)	74.2
2, 5	3.88 (2H, dd, $J = 7.0, 3.0$ Hz)	71.1
3, 6	4.03 (2H, d, $J = 2.0$ Hz)	69.9
1', 1''	-	125.7
2', 6', 2'', 6''	7.14 (4H, d, $J = 8.5$ Hz)	130.1
3', 5', 3'', 5''	6.74 (4H, d, $J = 8.5$ Hz)	114.8
4', 4''	-	156.1
7', 7''	3.65 (4H, s)	39.5
8', 8''	-	172.5

**Table S2.** <sup>1</sup>H spectroscopic data for compounds **4-6**

Carbon No	<b>4</b>	<b>5</b>	<b>6</b>
1	4.82 (1H, dd, <i>J</i> = 10.5, 3.5 Hz)	4.04 (1H, t, <i>J</i> = 3.5 Hz)	5.28 (1H, t, <i>J</i> = 3.5 Hz)
2	3.83 (1H, t, <i>J</i> = 9.5 Hz)	5.13 (1H, dd, <i>J</i> = 10.5, 3.0)	5.15 (1H, dd, <i>J</i> = 10.5, 3.0 Hz)
3	3.57 (1H, t, <i>J</i> = 9.5 Hz)	5.33 (1H, t, <i>J</i> = 9.5 Hz)	5.25 (1H, t, <i>J</i> = 10.0 Hz)
4	3.92 (1H, dd, <i>J</i> = 10.0, 3.5 Hz)	3.76 (1H, t, <i>J</i> = 9.5 Hz)	3.80 (1H, t, <i>J</i> = 10.0 Hz)
5	5.15 (1H, t, <i>J</i> = 4.0 Hz)	3.81 (1H, dd, <i>J</i> = 10.0, 3.0 Hz)	3.62 (1H, dd, <i>J</i> = 10.0, 3.0 Hz)
6	3.99 (1H, t, <i>J</i> = 4.0 Hz)	3.94 (1H, t, <i>J</i> = 3.5 Hz)	3.84 (1H, t, <i>J</i> = 3.5 Hz)
2', 6'	7.12 (2H, d, <i>J</i> = 8.5 Hz)	7.04 (2H, d, <i>J</i> = 8.5 Hz)	6.85 (2H, d, <i>J</i> = 8.0 Hz)
2'', 6''	7.14 (2H, d, <i>J</i> = 8.5 Hz)	7.07 (2H, d, <i>J</i> = 8.5 Hz)	7.10 (2H, d, <i>J</i> = 8.5 Hz),
2''', 6'''	-	-	7.14 (2H, d, <i>J</i> = 8.5 Hz)
3', 5'	6.75 (2H, d, <i>J</i> = 9.0 Hz)	6.73 (4H, d, <i>J</i> = 8.5 Hz)	6.69 (2H, d, <i>J</i> = 8.5 Hz)
3'', 5''	6.73 (2H, d, <i>J</i> = 8.5 Hz)	-	6.75 (2H, d, <i>J</i> = 8.0 Hz)
3''', 5'''	-	-	6.77 (2H, d, <i>J</i> = 8.5 Hz)
7'	3.65 (2H, m)	3.37 (4H, s)	3.50 (1H, s), 3.48 (1H, s)
7''	3.61 (2H, m),	-	3.44 (2H, d, <i>J</i> = 2.5 Hz)
7'''	-	-	2.86-2.96 (2H, m)

Recorded at 500MHz in CD<sub>3</sub>OD.

**Table S3.** <sup>1</sup>H spectroscopic data for compounds 7-12

Carbon No	7 <sup>a</sup>	8 <sup>b</sup>	9 <sup>a</sup>	10 <sup>a</sup>	11 <sup>b</sup>	12 <sup>b</sup>
1	-	-	-	-	-	-
2	7.79 (1H, d, <i>J</i> = 8.0 Hz)	7.44 (1H, m)	7.25 (1H, s)	7.43 (1H, m)	6.96 (1H, d, <i>J</i> = 8.5 Hz)	7.09 (1H, d, <i>J</i> = 8.5 Hz)
3	6.93 (1H, d, <i>J</i> = 8.4 Hz)	-	-	-	6.84 (1H, d, <i>J</i> = 8.5 Hz)	6.74 (1H, d, <i>J</i> = 8.5 Hz)
4	-	-	-	-	-	-
5	6.93 (1H, d, <i>J</i> = 8.4 Hz)	6.95 (1H, d, <i>J</i> = 8.5 Hz)	-	6.81 (1H, d, <i>J</i> = 8.8 Hz)	6.84 (1H, d, <i>J</i> = 8.5 Hz)	6.74 (1H, d, <i>J</i> = 8.5 Hz)
6	7.79 (1H, d, <i>J</i> = 8.0 Hz)	7.44 (1H, m)	7.25 (1H, s)	7.43 (1H, m)	6.96 (1H, d, <i>J</i> = 8.5 Hz)	7.09 (1H, d, <i>J</i> = 8.5 Hz)
7	9.78 (1H, s)	9.75 (1H, s)	9.76 (1H, s)	-	3.49 (2H, s)	3.54 (2H, s)
8					-	-
-OCH <sub>3</sub>		3.94 (3H, s)	3.94 (6H, s)	3.84 (3H, s)	3.74 (3H, s)	3.68 (3H, s)

<sup>a</sup> Recorded at 400MHz in CD<sub>3</sub>OD, <sup>b</sup> Recorded at 500MHz in CD<sub>3</sub>OD.

**Table S4.** <sup>1</sup>H spectroscopic data for compounds **13-15**

Carbon No	<b>13<sup>a</sup></b>	<b>14<sup>a</sup></b>	<b>15<sup>b</sup></b>
1	-	-	-
2	7.57 (1H, d, <i>J</i> = 2.0 Hz)	7.05 (1H, d, <i>J</i> = 2.0 Hz)	6.79 (1H, d, <i>J</i> = 2.0 Hz)
3	-	-	-
4	-	-	-
5	6.89 (1H, d, <i>J</i> = 8.4 Hz)	6.79 (1H, d, <i>J</i> = 8.0 Hz)	6.71 (1H, d, <i>J</i> = 8.0 Hz)
6	7.60 (1H, d, <i>J</i> = 8.4, 2.0 Hz)	6.96 (1H, dd, <i>J</i> = 8.0, 2.0 Hz)	6.64 (1H, dd, <i>J</i> = 8.0, 2.0 Hz)
7	-	7.56 (1H, d, <i>J</i> = 16.0 Hz)	2.61 (2H, t, <i>J</i> = 7.5 Hz)
8	3.18 (2H, t, <i>J</i> = 6.4 Hz)	6.28 (1H, d, <i>J</i> = 16.0 Hz)	1.82 (2H, m)
9	3.96 (2H, t, <i>J</i> = 6.4 Hz)	-	3.57 (2H, t, <i>J</i> = 6.5 Hz)
-OCH <sub>3</sub>	3.93 (3H, s)	3.77 (3H, s)	3.80 (3H, s)

<sup>a</sup> Recorded at 400MHz in CD<sub>3</sub>OD, <sup>b</sup> Recorded at 500MHz in CD<sub>3</sub>OD.

**Table S5.** <sup>1</sup>H spectroscopic data for compounds **17** and **18**

Carbon No	<b>17</b>	<b>18</b>
3	6.21 (1H, d, <i>J</i> = 9.6 Hz)	6.22 (1H, d, <i>J</i> = 9.2 Hz)
4	7.87 (1H, d, <i>J</i> = 9.6 Hz)	7.85 (1H, d, <i>J</i> = 9.2 Hz)
5	7.42 (1H, s)	7.37 (1H, s)
8	6.74 (1H, s)	6.72 (1H, s)
2'	4.78 (1H, t, <i>J</i> = 8.4 Hz)	
3'	3.27 (2H, m)	3.83 (1H, q, <i>J</i> = 6.8 Hz)
4'		3.12 (1H, dd, <i>J</i> = 16.8, 5.2 Hz)
		2.81 (1H, dd, <i>J</i> = 16.8, 6.8 Hz)
5'	1.31 (3H, s)	1.38 (3H, s)
6'	1.25 (3H, s)	1.34 (3H, s)

Recorded at 400MHz in CD<sub>3</sub>OD.

**Table S6.** <sup>1</sup>H spectroscopic data for compounds **19** and **20**

Carbon No	<b>19</b>	<b>20</b>
3	6.30 (1H, d, <i>J</i> = 10.0 Hz)	6.30 (1H, d, <i>J</i> = 10.0 Hz)
4	8.44 (1H, d, <i>J</i> = 9.6 Hz)	8.24 (1H, d, <i>J</i> = 10.0 Hz)
8	7.21 (1H, s)	
2'	7.80 (1H, d, <i>J</i> = 2.4 Hz)	7.84 (1H, d, <i>J</i> = 2.4 Hz)
3'	7.24 (1H, d, <i>J</i> = 2.4 Hz)	7.23 (1H, d, <i>J</i> = 2.4 Hz)
1''	4.81 (1H, dd, <i>J</i> = 10.0, 2.4 Hz)	4.58 (1H, dd, <i>J</i> = 10.4, 2.8 Hz)
	4.41 (1H, q, <i>J</i> = 9.6 Hz)	4.30 (1H, q, <i>J</i> = 10.4, 8.0 Hz)
2''	3.84 (1H, dd, <i>J</i> = 8.8, 2.8 Hz)	3.85 (1H, dd, <i>J</i> = 8.0, 2.8 Hz)
4''	1.31 (3H, s)	1.28 (3H, s)
5''	1.26 (3H, s)	1.24 (3H, s)
-OCH <sub>3</sub>		4.22 (3H, s)

Recorded at 400MHz in CD<sub>3</sub>OD.

**Table S7.** <sup>1</sup>H spectroscopic data for compounds **21 - 23**

Carbon No	<b>21</b>	Carbon No	<b>22</b>	<b>23</b>
2, 6	6.74 (2H, s)	2, 2'	6.68 (2H, s)	6.97 (2H, d, <i>J</i> = 1.6 Hz)
7	4.79 (1H, d, <i>J</i> = 4.0 Hz)	5, 5'	-	6.79 (2H, d, <i>J</i> = 8.0 Hz)
8	3.15 (1H, m)	6, 6'	6.68 (2H, s)	6.84 (2H, dd, <i>J</i> = 8.4, 1.6 Hz)
9	3.93 (2H, dd, <i>J</i> = 9.2, 3.2 Hz)	7, 7'	4.74 (2H, d, <i>J</i> = 4.4 Hz)	4.73 (2H, d, <i>J</i> = 4.4 Hz)
2', 6'	6.68 (2H, s)	8, 8'	3.17 (1H, m)	3.17 (1H, m)
7'	4.74 (1H, d, <i>J</i> = 4.4 Hz)	9, 9'	3.90 (2H, m)	3.86 (2H, m), 4.25 (2H, m)
8'	3.15 (1H, m)		4.29 (2H, m)	
9'	4.30 (2H, m)	3,3'-OCH <sub>3</sub>	3.87 (6H, s)	3.88 (6H, s)
1''	4.80 (1H, s)	5,5'-OCH <sub>3</sub>	3.87 (6H, s)	-
2''	3.50 (1H, m)			
3''	3.42 (1H, d, <i>J</i> = 2.8 Hz)			
4''	3.44 (1H, d, <i>J</i> = 2.8 Hz)			
5''	3.22 (1H, m)			
6''	3.80 (1H, dd, <i>J</i> = 12.0, 2.4 Hz)			
	3.68 (1H, dd, <i>J</i> = 12.0, 5.2 Hz)			
3,5-OCH <sub>3</sub>	3.88 (6H, s)			
3',5'-OCH <sub>3</sub>	3.86 (6H, s)			

Recorded at 400MHz in CD<sub>3</sub>OD.

**Table S8.** Antioxidant activity of compounds **1-23**.

Compounds	IC <sub>50</sub> (μM)	Compounds	IC <sub>50</sub> (μM)
<b>1</b>	>100	<b>13</b>	>100
<b>2</b>	>100	<b>14</b>	34.6
<b>3</b>	>100	<b>15</b>	>100
<b>4</b>	>100	<b>16</b>	>100
<b>5</b>	>100	<b>17</b>	>100
<b>6</b>	>100	<b>18</b>	>100
<b>7</b>	>100	<b>19</b>	>100
<b>8</b>	>100	<b>20</b>	>100
<b>9</b>	>100	<b>21</b>	81.6
<b>10</b>	30.4	<b>22</b>	75.4
<b>11</b>	>100	<b>23</b>	89.2
<b>12</b>	>100	quercetin <sup>a</sup>	19.8

<sup>a</sup>Quercetin was used as the positive control.