

## Anti-glycating and anti-oxidant compounds from traditionally used anti-diabetic plant *Geigeria alata* (DC) Oliv. & Hiern.

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### Abstract

A new sesquiterpene lactone geigerianoloide (**1**) and four known flavonoids axillarin (**2**), quercetin (**3**), 3-methoxy-5,7,3',4'-tetrahydroxy-flavone (**4**) and hispidulin (**5**) were isolated from *Geigeria alata* (DC) Oliv. & Hiern. (Asteraceae). Structures were deduced using <sup>1</sup>H- and <sup>13</sup>C- NMR spectroscopy, mass spectrometry, while the structure of compound **1** was also deduced using X-ray crystallography technique.

*Geigeria alata* is traditionally used for diabetes, therefore compounds were tested for anti-glycation activity, in which compounds **2** and **3** showed potent activities (IC<sub>50</sub> values of 246.97±0.83 and 262.37±0.22 μM, respectively) compared to IC<sub>50</sub> value 294.50±1.5 μM of rutin. Moreover, compound **4** exhibited a comparable activity to rutin (IC<sub>50</sub> = 293.28±1.34 μM). Compound **5** showed a weak activity.

Compounds **2**, **3** and **4** exhibited potent DPPH radical scavenging activity (IC<sub>50</sub> = 0.1±0.00, 0.13±0.00 and 0.15±0.01 μM, respectively). Compounds **2**, **3** and **4** demonstrated significant superoxide anion scavenging activity with IC<sub>50</sub> values of 0.14±0.001, 0.17±0.00 and 0.11±0.006 μM, respectively.

**Keywords:** *Geigeria alata* (DC) Oliv. & Hiern.; Geigerianoloide; Antioxidant; Anti-glycation, axillarin.

## Supplementary Material

List of supporting information:

Table S1.  $^1\text{H}$ , and  $^{13}\text{C}$ -NMR chemical shift data of compound **1**.

Figure S2. IR Spectrum of compound **1**.

Figure S3. UV Spectrum of compound **1**.

Figure S4. EI MS Spectrum of compound **1**.

Figure S5.  $^1\text{H}$  NMR Spectrum of compound **1**.

Figure S6.  $^{13}\text{C}$  NMR Spectrum of compound **1**.

Figure S7. Key COSY and HMBC correlations in compound **1**.

Figure S8. HR-MS spectrum of compound **1**.

**Table S1.**  $^1\text{H}$  and  $^{13}\text{C}$ -NMR chemical shift data of compound **1** recorded in  $\text{CDCl}_3$  at 300, and 125MHz, respectively.

C.No.	$\delta_c$	$\delta_H$ (J, Hz)
1	50.0	2.30 m
2	42.1	2.04 dd (18.5, 1.5), 2.61 dd (18.5, 6.5)
3	207.8	-
4	137.6	-
5	170.1	-
6	31.2	2.22 t (12.0), 3.02 dd (12.0, 4.5)
7	43.0	2.30 m
8	80.8	4.40 m
9	37.0	1.87 m, 1.94 m
10	39.7	1.24 m
11	40.8	2.38 m
12	178.0	-
13	22.8	1.12 d (6.5)
14	14.4	1.32 d (7.0)
15	7.8	1.67 s

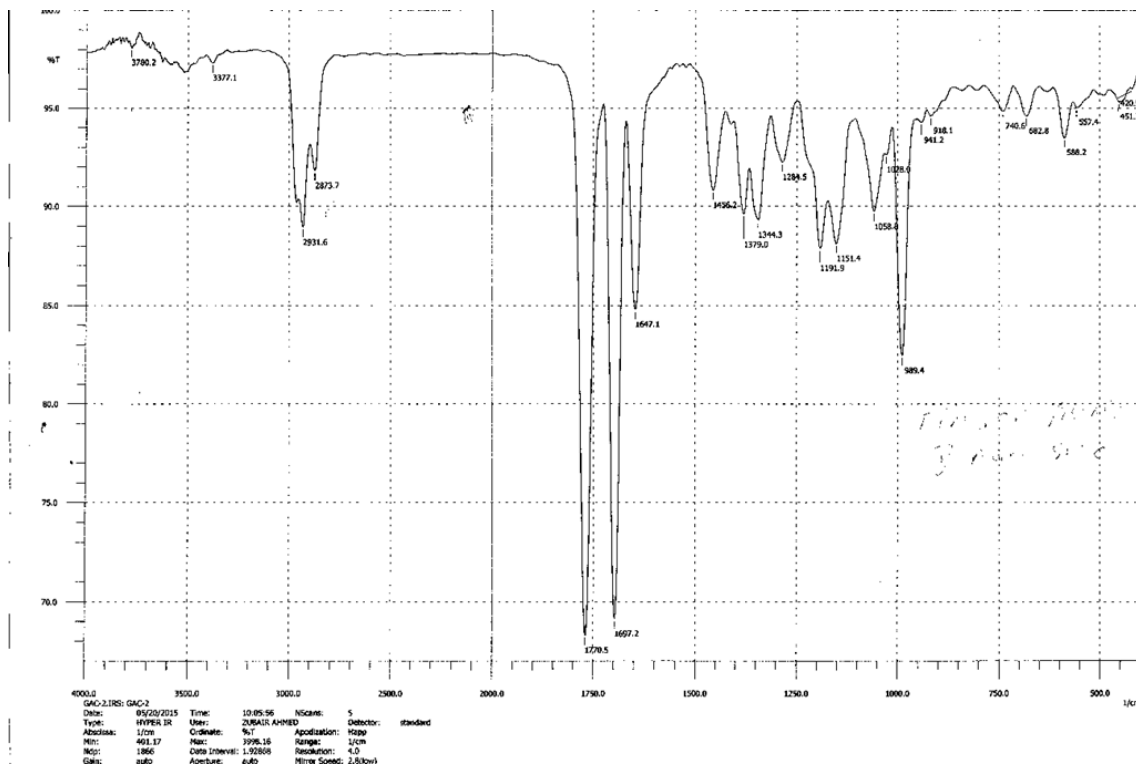


Figure S2. IR Spectrum of compound 1.

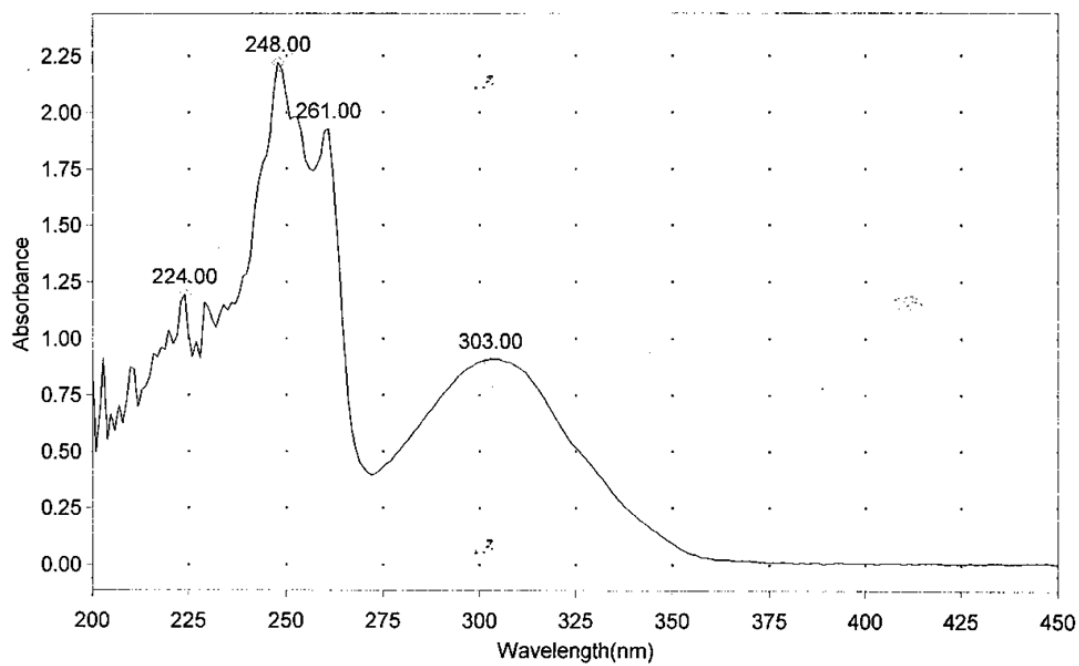


Figure S3. UV Spectrum of compound 1.

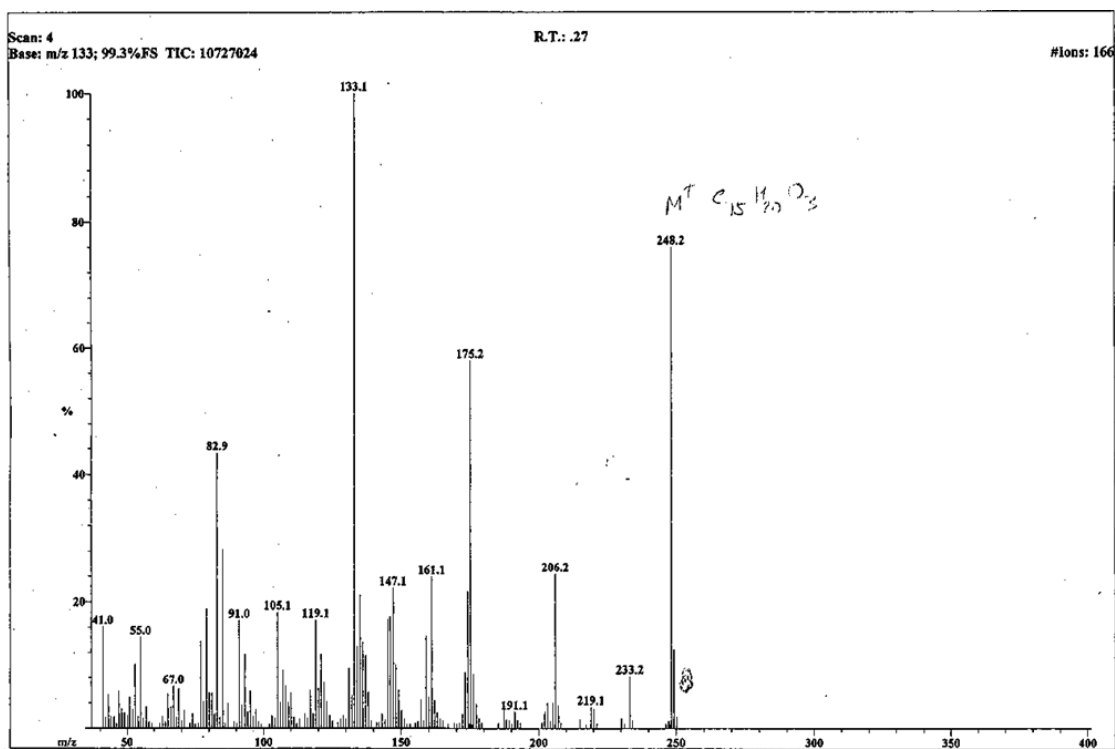


Figure S4. EI-MS Spectrum of compound 1.

ELTAYEB / DR. IQBAL / GAC2  
1H

AVANCE AV - III  
300 MHz, LAB # 116

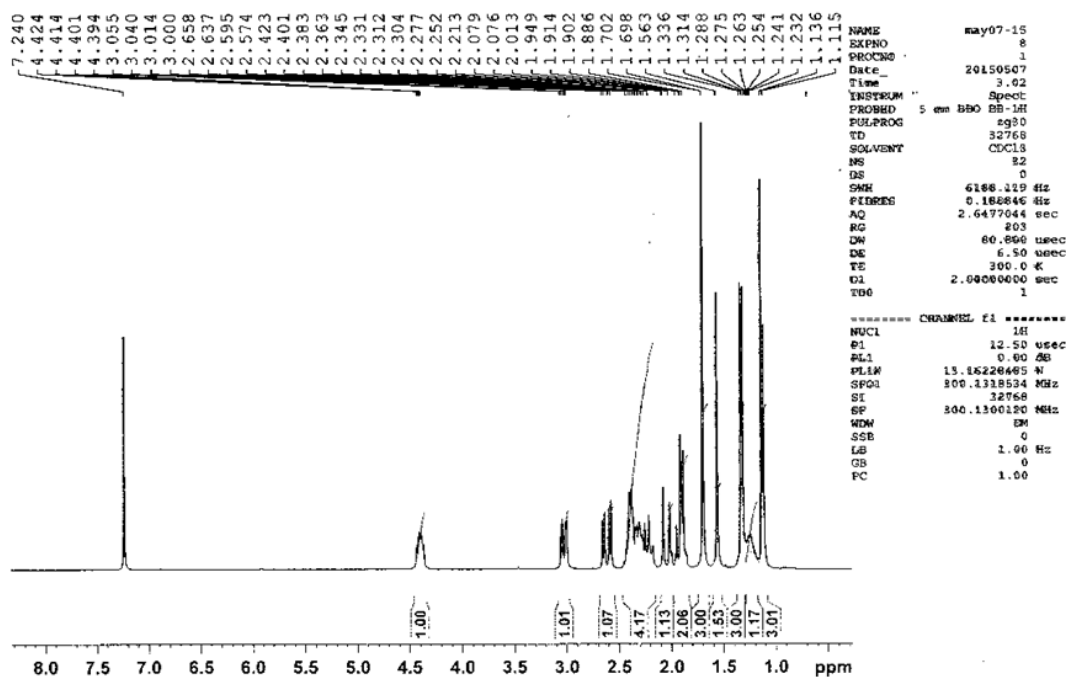


Figure S5. <sup>1</sup>H-NMR spectrum of compound 1.

ELTAYEB/DR. IQBAL/GAC-2/CDCL3  
ICCBS/U.O.K

AVANCE AV-500  
LAB NO:118

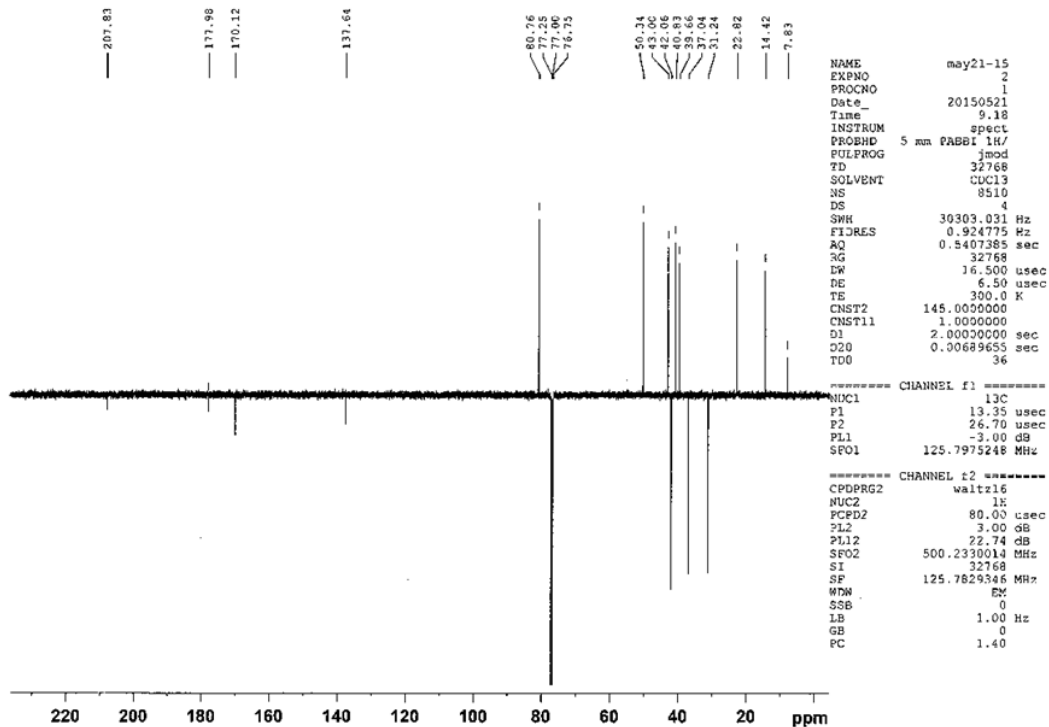


Figure S6.  $^{13}\text{C}$ -NMR spectrum of compound 1.

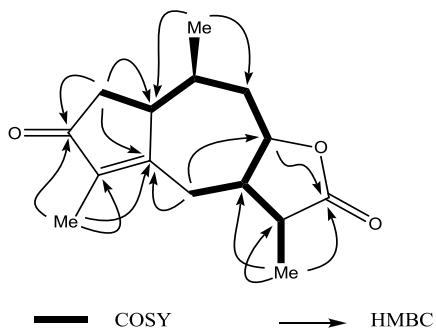


Figure S7. Key COSY and HMBC correlations in compound 1.

File : C:\Xcalibur\data\gac-2-150515-c2.RAW  
 Full ms [ 39.500 - 700.500 ] - Range: 69.000 - 700.500  
 Scan No. 1 of 1

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
69.0333	4.6	69.0340	-11.3	-0.8	2.5	C <sub>4</sub> H <sub>5</sub> O <sub>1</sub>
69.0702	2.5	69.0704	-3.2	-0.2	1.5	C <sub>5</sub> H <sub>9</sub>
71.0356	1.1					
76.9848	15.1					
77.9859	4.1					
79.9907	3.6	79.9898	11.2	0.9	5.0	C <sub>4</sub> O <sub>2</sub>
82.8622	2.0					
84.8533	1.2					
90.9688	17.6					
91.9794	3.2					
92.9195	5.9					
94.9964	1.4	94.9980	-17.9	-1.7	0.5	C <sub>1</sub> H <sub>3</sub> O <sub>5</sub>
95.0324	2.7					
103.0646	2.4					
104.0743	1.3					
105.0821	14.4					
106.0872	2.1					
107.0593	1.4					
107.0963	4.5					
108.0664	3.0					
108.1014	1.5					
109.0717	1.6					
110.0771	2.1					
115.0563	3.3	115.0548	13.5	1.6	6.5	C <sub>9</sub> H <sub>12</sub> O <sub>2</sub>
116.0630	1.2	116.0626	3.7	0.4	6.0	C <sub>9</sub> H <sub>8</sub>
117.0715	4.3	117.0704	9.0	1.1	5.5	C <sub>9</sub> H <sub>9</sub>
118.0780	1.4	118.0783	-1.8	-0.2	5.0	C <sub>9</sub> H <sub>10</sub>
119.0870	9.0	119.0861	8.0	1.0	4.5	C <sub>9</sub> H <sub>11</sub>
120.0940	2.9	120.0939	0.5	0.1	4.0	C <sub>9</sub> H <sub>12</sub>
121.0650	3.3	121.0653	-2.6	-0.3	4.5	C <sub>9</sub> H <sub>9</sub> O <sub>1</sub>
121.1015	2.0	121.1017	-2.0	-0.2	3.5	C <sub>9</sub> H <sub>13</sub>
122.0741	2.3	122.0732	7.7	0.9	4.0	C <sub>9</sub> H <sub>10</sub> O <sub>1</sub>
123.0815	1.4	123.0810	4.1	0.5	3.5	C <sub>9</sub> H <sub>11</sub> O <sub>1</sub>
128.0639	1.5	128.0626	9.9	1.3	7.0	C <sub>10</sub> H <sub>8</sub>
129.0709	2.0	129.0704	4.0	0.5	6.5	C <sub>10</sub> H <sub>9</sub>
131.0863	6.1	131.0861	1.9	0.2	5.5	C <sub>10</sub> H <sub>11</sub>
132.0928	2.4	132.0939	-8.5	-1.1	5.0	C <sub>10</sub> H <sub>12</sub>
133.0665	31.2	133.0653	8.9	1.2	5.5	C <sub>9</sub> H <sub>9</sub> O <sub>1</sub>
133.1027	4.8	133.1017	7.6	1.0	4.5	C <sub>10</sub> H <sub>13</sub>
134.0705	3.8	134.0732	-19.5	-2.6	5.0	C <sub>9</sub> H <sub>10</sub> O <sub>1</sub>
134.1097	1.3	134.1096	0.8	0.1	4.0	C <sub>10</sub> H <sub>14</sub>
135.0802	7.3	135.0810	-6.1	-0.8	4.5	C <sub>9</sub> H <sub>11</sub> O <sub>1</sub>
136.0884	4.8	136.0888	-2.8	-0.4	4.0	C <sub>9</sub> H <sub>12</sub> O <sub>1</sub>
137.0968	5.1	137.0966	0.8	0.1	3.5	C <sub>9</sub> H <sub>13</sub> O <sub>1</sub>
138.1028	1.8	138.1045	-11.9	-1.6	3.0	C <sub>9</sub> H <sub>14</sub> O <sub>1</sub>
143.0852	1.2	143.0861	-6.5	-0.9	6.5	C <sub>11</sub> H <sub>11</sub>
145.0633	5.4	145.0653	-14.3	-2.1	6.5	C <sub>10</sub> H <sub>9</sub> O <sub>1</sub>
145.1005	2.7	145.1017	-8.7	-1.3	5.5	C <sub>11</sub> H <sub>13</sub>
146.0723	1.2	146.0732	-5.9	-0.9	6.0	C <sub>10</sub> H <sub>10</sub> O <sub>1</sub>
146.1100	5.6	146.1096	3.3	0.5	5.0	C <sub>11</sub> H <sub>14</sub>
147.0801	4.3	147.0810	-6.0	-0.9	5.5	C <sub>10</sub> H <sub>11</sub> O <sub>1</sub>
147.1170	6.5	147.1174	-2.6	-0.4	4.5	C <sub>11</sub> H <sub>15</sub>
148.0884	2.7	148.0888	-2.9	-0.4	5.0	C <sub>10</sub> H <sub>12</sub> O <sub>1</sub>
148.1222	1.1					
149.0958	1.4	149.0966	-5.6	-0.8	4.5	C <sub>10</sub> H <sub>13</sub> O <sub>1</sub>
157.1016	1.7	157.1017	-1.0	-0.2	6.5	C <sub>12</sub> H <sub>13</sub>
159.0816	3.6	159.0810	3.8	0.6	6.5	C <sub>11</sub> H <sub>11</sub> O <sub>1</sub>
159.1187	1.4	159.1174	8.1	1.3	5.5	C <sub>12</sub> H <sub>15</sub>
160.0864	1.8	160.0888	-15.2	-2.4	6.0	C <sub>11</sub> H <sub>12</sub> O <sub>1</sub>
161.0963	6.4	161.0966	-2.1	-0.3	5.5	C <sub>11</sub> H <sub>13</sub> O <sub>1</sub>
162.1028	1.3	162.1045	-10.6	-1.7	5.0	C <sub>11</sub> H <sub>14</sub> O <sub>1</sub>
173.0968	2.3	173.0966	0.8	0.1	6.5	C <sub>12</sub> H <sub>13</sub> O <sub>1</sub>
174.1053	4.4	174.1045	4.5	0.8	6.0	C <sub>12</sub> H <sub>14</sub> O <sub>1</sub>
175.1124	12.2	175.1123	0.9	0.2	5.5	C <sub>12</sub> H <sub>15</sub> O <sub>1</sub>
176.1174	2.1	176.1201	-15.4	-2.7	5.0	C <sub>12</sub> H <sub>16</sub> O <sub>1</sub>
203.1429	1.0	203.1436	-3.2	-0.7	5.5	C <sub>14</sub> H <sub>19</sub> O <sub>1</sub>
206.0949	5.2	206.0943	2.8	0.6	6.0	C <sub>12</sub> H <sub>14</sub> O <sub>3</sub>

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
233.1175	1.5	233.1178	-1.0	-0.2	6.5	C <sub>14</sub> H <sub>17</sub> O <sub>3</sub>
248.1409	13.4	248.1412	-1.2	-0.3	6.0	C <sub>15</sub> H <sub>20</sub> O <sub>3</sub>
249.1456	2.5	249.1491	-13.7	-3.4	5.5	C <sub>15</sub> H <sub>21</sub> O <sub>3</sub>

Figure S8. HR- MS spectrum of compound 1.