

## ORIGINAL RESEARCH ARTICLE

# Comparative evaluation of the therapeutic effects of *Schisandra chinensis* and *Schisandra sphenanthera* on vascular cognitive impairment and their drug-like compounds

## Supplementary File

**Table S1. Identified and characterized 71 compounds from *Schisandra chinensis* using ultraperformance liquid chromatography-quadrupole time-of-flight mass spectrometry**

Number	Retention time (min)	Name	Molecular formula	Measured molecular mass number (Da)	Adduct	Mass error (ppm)
1	2.20	4'-Demethylepipodophyllotoxin	C <sub>21</sub> H <sub>20</sub> O <sub>8</sub>	801.2352	2M+H	-4.69
2	2.94	Schisandroside B	C <sub>29</sub> H <sub>40</sub> O <sub>12</sub>	603.2399	M+Na	-2.27
3	3.42	Angeloylgomisin P	C <sub>28</sub> H <sub>34</sub> O <sub>9</sub>	515.2278	M+H	0.53
4	3.45	(-)-Tigloyl-deangeloyl-gomisin F	C <sub>28</sub> H <sub>34</sub> O <sub>9</sub>	515.2278	M+H	0.53
5	3.47	Gomisin F	C <sub>28</sub> H <sub>34</sub> O <sub>9</sub>	515.2278	M+H	0.53
6	3.50	Tigloylgomisin P	C <sub>28</sub> H <sub>34</sub> O <sub>9</sub>	515.2278	M+H	0.53
7	3.54	3,7-Dihydroxy-1,2,13, 14-tetramethoxydibenzocyclooctadiene 12-O-β-D-glucopyranoside	C <sub>24</sub> H <sub>30</sub> O <sub>9</sub>	463.1965	M+H	0.42
8	3.59	isoschisandrins	C <sub>32</sub> H <sub>40</sub> O <sub>8</sub>	591.2367	M+K	2.27
9	3.75	8,8'-Dihydroxypinoresinol	C <sub>20</sub> H <sub>22</sub> O <sub>8</sub>	391.1384	M+H	-0.77
10	3.89	Schindilactone A	C <sub>29</sub> H <sub>34</sub> O <sub>9</sub>	549.2099	M+Na	0.76
11	3.92	Schindilactone B	C <sub>29</sub> H <sub>34</sub> O <sub>9</sub>	549.2099	M+Na	0.76
12	3.96	Schintrilactone A	C <sub>29</sub> H <sub>36</sub> O <sub>9</sub>	529.2429	M+H	-0.63
13	3.98	Schintrilactone B	C <sub>29</sub> H <sub>36</sub> O <sub>9</sub>	529.2429	M+H	-0.63
14	4.00	D-Pantethine	C <sub>22</sub> H <sub>42</sub> N <sub>4</sub> O <sub>8</sub> S <sub>2</sub>	1131.48	2M+Na	2.42
15	4.18	Schindilactone D	C <sub>29</sub> H <sub>34</sub> O <sub>10</sub>	543.2224	M+H	-0.15
16	4.25	Gomisin S	C <sub>23</sub> H <sub>30</sub> O <sub>7</sub>	441.1886	M+Na	0.47
17	4.30	Schinlignins A	C <sub>23</sub> H <sub>30</sub> O <sub>7</sub>	441.1886	M+Na	0.47
18	4.40	Gomisin H	C <sub>23</sub> H <sub>30</sub> O <sub>7</sub>	441.1886	M+Na	0.47
19	4.60	Angeloyl-(+)-gomisin K3	C <sub>28</sub> H <sub>36</sub> O <sub>7</sub>	502.2822	M+NH <sub>4</sub>	1.04
20	4.61	Gomisin R	C <sub>22</sub> H <sub>24</sub> O <sub>7</sub>	401.1604	M+H	2.30
21	4.64	Schindilactone F	C <sub>29</sub> H <sub>36</sub> O <sub>10</sub>	545.2382	M+H	0.06
22	4.67	Schindilactone G	C <sub>29</sub> H <sub>36</sub> O <sub>10</sub>	545.2382	M+H	0.06
23	4.68	Schindilactone H	C <sub>29</sub> H <sub>36</sub> O <sub>10</sub>	545.2382	M+H	0.06
24	4.89	Schinlignins B	C <sub>21</sub> H <sub>26</sub> O <sub>6</sub>	375.1806	M+H	0.92
25	4.97	Schisanlactone C	C <sub>30</sub> H <sub>40</sub> O <sub>5</sub>	481.2950	M+H	0.34
26	4.99	Gomisin O	C <sub>23</sub> H <sub>28</sub> O <sub>7</sub>	439.1733	M+Na	1.30
27	5.00	Epigomisin O	C <sub>23</sub> H <sub>28</sub> O <sub>7</sub>	439.1733	M+Na	1.30
28	5.03	Gomisin A	C <sub>23</sub> H <sub>28</sub> O <sub>7</sub>	439.1733	M+Na	1.30
29	5.05	Schisandrins*	C <sub>24</sub> H <sub>32</sub> O <sub>7</sub>	455.2058	M+Na	4.14
30	5.09	Schineolignins B	C <sub>22</sub> H <sub>30</sub> O <sub>5</sub>	766.4533	2M+NH <sub>4</sub>	1.14

(Cont'd...)

Table S1. (Continued)

Number	Retention time (min)	Name	Molecular formula	Measured molecular mass number (Da)	Adduct	Mass error (ppm)
31	5.12	Schisanlactone J	C <sub>30</sub> H <sub>38</sub> O <sub>5</sub>	501.2589	M+Na	-4.79
32	5.15	schisanchinlactone C	C <sub>30</sub> H <sub>38</sub> O <sub>5</sub>	501.2589	M+Na	-4.79
33	5.24	Gomisin D*	C <sub>28</sub> H <sub>34</sub> O <sub>10</sub>	531.2251	M+H	4.99
34	5.34	Schindilactone E	C <sub>29</sub> H <sub>34</sub> O <sub>11</sub>	1155.3785	2M+K	-4.38
35	5.39	Pluviatolide	C <sub>20</sub> H <sub>20</sub> O <sub>6</sub>	357.1344	M+H	3.31
36	5.50	Gomisin J*	C <sub>22</sub> H <sub>28</sub> O <sub>6</sub>	406.2216	M+NH <sub>4</sub>	-2.00
37	5.60	Schisandrol B*	C <sub>23</sub> H <sub>28</sub> O <sub>7</sub>	439.1715	M+Na	-2.28
38	5.76	Nicotinoylgomisin Q	C <sub>30</sub> H <sub>34</sub> O <sub>9</sub>	539.2250	M+H	-4.77
39	5.79	8-Hydroxypinoresinol	C <sub>20</sub> H <sub>22</sub> O <sub>7</sub>	375.1455	M+H	4.59
40	5.91	Angeloylisogomisin O	C <sub>20</sub> H <sub>22</sub> O <sub>5</sub>	365.1370	M+Na	3.06
41	6.05	Wuweizidilactone H	C <sub>28</sub> H <sub>36</sub> O <sub>10</sub>	555.2199	M+Na	-0.82
42	6.08	Mesodihydroguaiaretci acid	C <sub>20</sub> H <sub>26</sub> O <sub>4</sub>	331.1914	M+H	3.07
43	6.10	Schineolignins A	C <sub>20</sub> H <sub>26</sub> O <sub>4</sub>	331.1914	M+H	3.07
44	6.13	Pregomisin	C <sub>22</sub> H <sub>30</sub> O <sub>6</sub>	391.2123	M+H	2.10
45	6.34	Schinchinenin F	C <sub>32</sub> H <sub>42</sub> O <sub>8</sub>	577.2775	M+Na	0.65
46	6.35	Schineolignins C	C <sub>21</sub> H <sub>28</sub> O <sub>5</sub>	361.2016	M+H	1.78
47	6.48	Schisanchinins C	C <sub>24</sub> H <sub>30</sub> O <sub>7</sub>	453.1897	M+Na	3.00
48	6.51	Benzoylgomisin H	C <sub>30</sub> H <sub>34</sub> O <sub>8</sub>	545.2153	M+Na	1.45
49	6.77	Schisanhenol B	C <sub>22</sub> H <sub>26</sub> O <sub>6</sub>	387.1809	M+H	1.75
50	6.88	Wuweizisu C	C <sub>22</sub> H <sub>24</sub> O <sub>7</sub>	418.1858	2M+NH <sub>4</sub>	-0.46
51	7.03	Gomisin N	C <sub>23</sub> H <sub>28</sub> O <sub>6</sub>	423.1784	M+Na	1.38
52	7.26	Gomisin K2	C <sub>23</sub> H <sub>30</sub> O <sub>6</sub>	425.1936	M+Na	0.42
53	7.29	Schisanchinins D	C <sub>23</sub> H <sub>30</sub> O <sub>6</sub>	425.1936	M+Na	0.42
54	7.35	Schisanhenol	C <sub>23</sub> H <sub>30</sub> O <sub>6</sub>	425.1936	M+Na	0.42
55	7.40	Schisantherin A	C <sub>30</sub> H <sub>32</sub> O <sub>9</sub>	559.1936	M+Na	-1.03
56	7.53	Schisantherin B*	C <sub>28</sub> H <sub>34</sub> O <sub>9</sub>	537.2097	M+Na	0.29
57	7.54	Schisantherin C	C <sub>28</sub> H <sub>34</sub> O <sub>9</sub>	1046.4744	2M+NH <sub>4</sub>	0.51
58	7.58	Desoxypodophyllotoxin	C <sub>22</sub> H <sub>22</sub> O <sub>7</sub>	399.1451	M+H	3.22
59	8.05	(-)-Gomisin L2	C <sub>22</sub> H <sub>26</sub> O <sub>5</sub>	371.1860	M+H	1.98
60	8.39	(R-biar)-12-angeloyloxy-6, 7, 8, 9-tetrahydro-1, 2, 3, 13, 14-pentamethoxy-7, 8-dimethyl-7-dibenzo[a, c] cyclooctenol	C <sub>28</sub> H <sub>36</sub> O <sub>8</sub>	523.2302	M+Na	-0.14
61	8.43	Angeloylgomisin H	C <sub>28</sub> H <sub>36</sub> O <sub>8</sub>	523.2302	M+Na	-0.14
62	8.51	19(R)-hydroxylwuwei-zidilactone H	C <sub>28</sub> H <sub>36</sub> O <sub>11</sub>	1097.4727	2M+H	-3.08
63	8.59	Isoschisandrins	C <sub>24</sub> H <sub>32</sub> O <sub>7</sub>	455.2041	M+Na	0.18
64	10.02	Schisandrins A*	C <sub>24</sub> H <sub>32</sub> O <sub>6</sub>	439.2097	M+Na	1.37
65	10.79	Schinchinenin D	C <sub>30</sub> H <sub>38</sub> O <sub>7</sub>	528.2960	M+NH <sub>4</sub>	0.91
66	11.52	Schinchinenin E	C <sub>30</sub> H <sub>40</sub> O <sub>7</sub>	530.3119	M+NH <sub>4</sub>	1.35
67	11.74	Schisandrins B*	C <sub>23</sub> H <sub>28</sub> O <sub>6</sub>	401.1970	M+H	1.69
68	11.76	Angeloylgomisin O	C <sub>28</sub> H <sub>34</sub> O <sub>8</sub>	521.2152	M+Na	1.28
69	11.82	Matairesinol	C <sub>20</sub> H <sub>22</sub> O <sub>6</sub>	359.1499	M+H	2.78
70	12.87	Schisandrins C*	C <sub>22</sub> H <sub>24</sub> O <sub>6</sub>	407.1467	M+Na	1.52
71	13.19	Benzoylgomisin O	C <sub>30</sub> H <sub>32</sub> O <sub>8</sub>	543.1987	M+Na	-0.38

Note: The compounds marked with an asterisk (\*) were identified as reference standards.

Table S2. Identified and characterized 63 compounds from *Schisandra sphenanthera* using ultraperformance liquid chromatography-quadrupole time-of-flight mass spectrometry

Number	Retention time (min)	Name	Molecular formula	Measured molecular mass number (Da)	Adduct	Mass error (ppm)
1	0.91	Glutamyltyrosine	C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>6</sub>	349.0796	M+K	-0.06
2	1.14	Epsilon-viniferin	C <sub>28</sub> H <sub>22</sub> O <sub>6</sub>	493.1065	M+K	3.74
3	1.25	Cis-resveratrol	C <sub>14</sub> H <sub>12</sub> O <sub>3</sub>	479.1484	2M+Na	4.24
4	1.30	3,4,5-Trihydroxystilbene	C <sub>14</sub> H <sub>12</sub> O <sub>3</sub>	479.1484	2M+Na	4.24
5	1.38	Anabasamine	C <sub>16</sub> H <sub>19</sub> N <sub>3</sub>	276.1461	M+Na	-4.01
6	1.44	Sinapic acid	C <sub>11</sub> H <sub>12</sub> O <sub>5</sub>	242.1018	M+NH <sub>4</sub>	-2.44
7	1.48	2',4,4'-Trihydroxychalcone	C <sub>15</sub> H <sub>12</sub> O <sub>4</sub>	513.1560	2M+H	3.19
8	1.74	Trans-piceid	C <sub>20</sub> H <sub>22</sub> O <sub>8</sub>	391.1380	M+H	-1.92
9	2.15	Gardnutine	C <sub>20</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>	361.1321	M+K	2.45
10	2.28	Rinderine	C <sub>15</sub> H <sub>25</sub> NO <sub>5</sub>	317.2070	M+NH <sub>4</sub>	-0.32
11	2.32	Palmatine	C <sub>21</sub> H <sub>22</sub> NO <sub>4</sub> <sup>+</sup>	743.2697	2M+K	-4.57
12	2.39	Matairesinol	C <sub>20</sub> H <sub>22</sub> O <sub>6</sub>	359.1487	M+H	-0.60
13	2.56	Trans-pterostilbene	C <sub>16</sub> H <sub>16</sub> O <sub>3</sub>	257.1173	M+H	0.24
14	2.58	N-fructosyl isoleucine	C <sub>12</sub> H <sub>23</sub> NO <sub>7</sub>	587.3004	2M+H	-3.03
15	2.89	Osthole	C <sub>15</sub> H <sub>16</sub> O <sub>3</sub>	245.1172	M+H	-0.24
16	2.93	E-resveratrol trimethyl ether	C <sub>17</sub> H <sub>18</sub> O <sub>3</sub>	309.0889	M+K	0.55
17	3.00	Koumine	C <sub>20</sub> H <sub>22</sub> N <sub>2</sub> O	345.1359	M+K	-1.57
18	3.83	Gelsemine	C <sub>20</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>	323.1751	M+H	-1.00
19	3.87	Vincanidine	C <sub>19</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub>	617.3129	2M+H	1.04
20	4.09	Homatropine	C <sub>16</sub> H <sub>21</sub> NO <sub>3</sub>	314.1159	M+K	2.35
21	4.20	3',4'-Dimethoxybenzoic-3-oxobutylester	C <sub>22</sub> H <sub>26</sub> O <sub>7</sub>	403.1761	M+H	2.49
22	4.50	Atropine	C <sub>17</sub> H <sub>23</sub> NO <sub>3</sub>	328.1319	M+K	3.27
23	4.55	Hyoscyamine	C <sub>17</sub> H <sub>23</sub> NO <sub>3</sub>	328.1319	M+K	3.27
24	4.65	Laudanosine	C <sub>21</sub> H <sub>27</sub> NO <sub>4</sub>	753.3517	2M+K	0.69
25	4.78	Methylgomisin O	C <sub>22</sub> H <sub>28</sub> O <sub>7</sub>	427.1724	M+Na	-0.78
26	4.79	Atractylenolide III	C <sub>15</sub> H <sub>20</sub> O <sub>3</sub>	271.1302	M+Na	-1.06
27	4.80	Schisandrone	C <sub>21</sub> H <sub>24</sub> O <sub>5</sub>	357.1712	M+H	4.28
28	4.85	L-oxonoreleagnine	C <sub>11</sub> H <sub>10</sub> N <sub>2</sub> O	373.1655	2M+H	-1.11
29	4.86	Epigomisin O	C <sub>23</sub> H <sub>28</sub> O <sub>7</sub>	417.1916	M+H	2.00
30	5.04	Cyclo-prolylglycine	C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>	177.0635	M+Na	0.10
31	5.05	Sempervirine	C <sub>19</sub> H <sub>16</sub> N <sub>2</sub>	562.2981	2M+NH <sub>4</sub>	2.93
32	5.06	Schisandrin *	C <sub>24</sub> H <sub>32</sub> O <sub>7</sub>	455.2050	M+Na	2.68
33	5.42	Indole-3-acetyl-L-valine	C <sub>15</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	587.2248	2M+K	-3.40
34	5.50	Gomisin J *	C <sub>22</sub> H <sub>28</sub> O <sub>6</sub>	411.1787	M+Na	2.42
35	5.94	Feruloyl lysine	C <sub>16</sub> H <sub>22</sub> N <sub>2</sub> O <sub>5</sub>	323.1588	M+H	-4.04
36	6.01	Gomisin M2	C <sub>22</sub> H <sub>26</sub> O <sub>6</sub>	387.1812	M+H	2.68
37	6.02	Meso-dihydroguaiaretic acid	C <sub>20</sub> H <sub>26</sub> O <sub>4</sub>	353.1713	M+Na	-3.25
38	6.13	Pregomisin	C <sub>22</sub> H <sub>30</sub> O <sub>6</sub>	391.2129	M+H	3.60
39	6.23	Schisphenlignan F	C <sub>22</sub> H <sub>30</sub> O <sub>6</sub>	391.2129	M+H	3.60
40	6.43	Hirsutine	C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>3</sub>	759.4071	2M+Na	-2.83

(Cont'd...)

Table S2. (Continued)

Number	Retention time (min)	Name	Molecular formula	Measured molecular mass number (Da)	Adduct	Mass error (ppm)
41	6.47	Ganschisandrin	C <sub>22</sub> H <sub>28</sub> O <sub>5</sub>	395.1839	M+Na	2.78
42	6.52	Harmalol	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O	401.1962	2M+H	-2.61
43	6.71	Rubrisadrin A	C <sub>44</sub> H <sub>56</sub> O <sub>12</sub>	799.3695	M+Na	3.95
44	6.75	p-Coumaraldehyde	C <sub>9</sub> H <sub>8</sub> O <sub>2</sub>	297.1108	2M+H	-4.63
45	6.79	Trans-cinnamic acid	C <sub>9</sub> H <sub>8</sub> O <sub>2</sub>	297.1108	2M+H	-4.63
46	6.83	Methylgomisin R	C <sub>23</sub> H <sub>26</sub> O <sub>7</sub>	437.1582	M+Na	2.65
47	6.87	Isofraxidin	C <sub>11</sub> H <sub>10</sub> O <sub>5</sub>	240.0877	M+NH <sub>4</sub>	4.91
48	6.93	Methyl cinnamate	C <sub>10</sub> H <sub>10</sub> O <sub>2</sub>	325.1447	2M+H	4.05
49	7.30	Schisphenlignan E	C <sub>22</sub> H <sub>26</sub> O <sub>8</sub>	837.3295	2M+H	-4.01
50	7.52	Harmol	C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O	397.1670	2M+H	2.88
51	7.53	(+)-Talaumidin	C <sub>20</sub> H <sub>22</sub> O <sub>5</sub>	343.1545	M+H	1.49
52	7.57	8-Methanesulfinyloctanenitrile	C <sub>9</sub> H <sub>17</sub> NOS	397.1950	2M+Na	-1.07
53	8.02	(-)-Machilusin	C <sub>21</sub> H <sub>24</sub> O <sub>5</sub>	379.1528	M+Na	3.28
54	8.03	Schiglaucin B	C <sub>22</sub> H <sub>26</sub> O <sub>5</sub>	371.1865	M+H	3.11
55	8.05	(-)-Epiaristoligone	C <sub>22</sub> H <sub>26</sub> O <sub>5</sub>	371.1865	M+H	3.11
56	8.08	(+)-1-Hydroxy pinoresinol	C <sub>22</sub> H <sub>26</sub> O <sub>6</sub>	387.1808	M+H	1.60
57	8.32	Chalcone	C <sub>15</sub> H <sub>12</sub> O	417.1842	2M+H	-1.59
58	8.49	Dihydroresveratrol	C <sub>14</sub> H <sub>14</sub> O <sub>3</sub>	483.1794	2M+Na	3.38
59	8.52	Lanceol	C <sub>15</sub> H <sub>24</sub> O	221.1909	M+H	4.19
60	9.27	Anwulignan*	C <sub>20</sub> H <sub>24</sub> O <sub>4</sub>	329.1735	M+H	-3.64
61	9.39	Coniferyl aldehyde	C <sub>10</sub> H <sub>10</sub> O <sub>3</sub>	357.1349	2M+H	4.46
62	9.44	Schisphenthin A	C <sub>30</sub> H <sub>46</sub> O <sub>5</sub>	509.3241	M+Na	0.78
63	9.99	Schisandrin A*	C <sub>24</sub> H <sub>32</sub> O <sub>6</sub>	855.4293	2M+Na	3.08

Note: The compounds marked with an asterisk (\*) were identified as reference standards.