

## Supplementary Materials

# Molecular Docking and Molecular Dynamics Studies Reveal the Anticancer Potential of Medicinal-Plant-Derived Lignans as MDM2-P53 Interaction Inhibitors

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**Table S1.** List of *Justica Procumbens* and *Ferula sinkiangensis* lignans

Compound Name	Mol. Wt.	Mol. Formula
Justicidin A	394	C <sub>22</sub> H <sub>18</sub> O <sub>7</sub>
6'-Hydroxy justicidin A	410	C <sub>22</sub> H <sub>18</sub> O <sub>8</sub>
Justicidin B	364	C <sub>21</sub> H <sub>16</sub> O <sub>6</sub>
6'-Hydroxy justicidin B	380	C <sub>21</sub> H <sub>16</sub> O <sub>7</sub>
Neojusticin B = Justicidin C	394	C <sub>22</sub> H <sub>18</sub> O <sub>7</sub>
Neojusticin A = Justicidin D	378	C <sub>21</sub> H <sub>14</sub> O <sub>7</sub>
6'-Hydroxy justicidin C	410	C <sub>22</sub> H <sub>18</sub> O <sub>8</sub>
Neojusticin C	380	C <sub>21</sub> H <sub>16</sub> O <sub>7</sub>
Justicidin E	348	C <sub>20</sub> H <sub>12</sub> O <sub>6</sub>
Phyllamyricin C	394	C <sub>22</sub> H <sub>18</sub> O <sub>7</sub>
Taiwanin C = Lignan J <sub>1</sub>	378	C <sub>21</sub> H <sub>14</sub> O <sub>7</sub>
Taiwanin E	364	C <sub>20</sub> H <sub>12</sub> O <sub>7</sub>
Taiwanin E methyl ether	378	C <sub>21</sub> H <sub>14</sub> O <sub>7</sub>
Chinensinaphthol	380	C <sub>21</sub> H <sub>16</sub> O <sub>7</sub>
Chinensinaphthol methyl ether	394	C <sub>22</sub> H <sub>18</sub> O <sub>7</sub>
4'-Demethylchinensinaphthol methyl ether	380	C <sub>21</sub> H <sub>16</sub> O <sub>7</sub>
Procumphthalide A	394	C <sub>22</sub> H <sub>18</sub> O <sub>7</sub>
Cilinaphthalide A	396	C <sub>22</sub> H <sub>20</sub> O <sub>7</sub>
Cilinaphthalide B	410	C <sub>23</sub> H <sub>22</sub> O <sub>7</sub>
Pronaphthalide A	396	C <sub>22</sub> H <sub>20</sub> O <sub>7</sub>
5'-Methoxy retrochinensin	394	C <sub>22</sub> H <sub>18</sub> O <sub>7</sub>
Diphyllin	380	C <sub>21</sub> H <sub>16</sub> O <sub>7</sub>
Isodiphyllin	380	C <sub>21</sub> H <sub>16</sub> O <sub>7</sub>
Tuberculatin (Diphyllin-1-O-β-D-apiofuranoside)	512	C <sub>26</sub> H <sub>24</sub> O <sub>11</sub>
Diphyllin apioside-5-acetate	554	C <sub>28</sub> H <sub>26</sub> O <sub>12</sub>
Justicidin A (Justicidin C 6'-O-glucopyranoside)	572	C <sub>28</sub> H <sub>28</sub> O <sub>13</sub>
Justicidin B (Justicidin A 6'-O- glucopyranoside)	572	C <sub>28</sub> H <sub>28</sub> O <sub>13</sub>
Justicidin C (Justicidin B 6'-O- glucopyranoside)	542	C <sub>27</sub> H <sub>26</sub> O <sub>12</sub>
Procumbenoside A (4-O-α-L-Arabinopyranosyl-(1'''→2'')- β-D-apiofuranosyldiphyllin	644	C <sub>31</sub> H <sub>32</sub> O <sub>15</sub>
Procumbenoside B = Procumphthalide B (4-O-β-D-Glucopyranosyl-(1'''→2'')-β-D-apiofuranosyldiphyllin)	674	C <sub>32</sub> H <sub>34</sub> O <sub>16</sub>
Procumbenoside C	526	C <sub>26</sub> H <sub>22</sub> O <sub>12</sub>
Procumbenoside D	542	C <sub>27</sub> H <sub>26</sub> O <sub>12</sub>

Procumbenoside H (4-O-β-D-Xylopyranosyl-(1''' → 5'')-β-D-apiofuranosyl diphyllin)	644	C <sub>31</sub> H <sub>32</sub> O <sub>15</sub>
Procumbenoside E (4-O-β-D-Bis-xylopyranosyl-(1''' → 5'', 1'''→2'')-β-D-apiofuranosyl diphyllin)	776	C <sub>36</sub> H <sub>40</sub> O <sub>19</sub>
Procumbenoside I	528	C <sub>26</sub> H <sub>24</sub> O <sub>12</sub>
Procumbenoside J	552	C <sub>29</sub> H <sub>28</sub> O <sub>11</sub>
Procumbenoside K	532	C <sub>26</sub> H <sub>28</sub> O <sub>12</sub>
Procumbenoside L	502	C <sub>25</sub> H <sub>26</sub> O <sub>11</sub>
Procumbenoside M	738	C <sub>37</sub> H <sub>38</sub> O <sub>16</sub>
Procumbenoside N (7-O-[β-D-Xylopyranosyl-(1'''→2'')-β-D-glucopyranosyl]-diphyllin)	674	C <sub>32</sub> H <sub>34</sub> O <sub>16</sub>
Procumbenoside O (7-O-[β-D-Glucopyranosyl-(1''''→5'')-β-D-xylopyranosyl-(1'''→2'')-β-D-apiofuranosyl]-diphyllin)	806	C <sub>37</sub> H <sub>42</sub> O <sub>20</sub>
Cleistanthin B	542	C <sub>27</sub> H <sub>26</sub> O <sub>12</sub>
Ciliatoside A (4-O-[α-L-Arabinopyranosyl-(1'''→2'')-β-D-xylopyranosyl-(1''''→5'')-β-D-apiofuranosyl]diphyllin)	776	C <sub>36</sub> H <sub>40</sub> O <sub>19</sub>
Ciliatoside B (4-O-[[β-D-Apiofuranosyl-(1''''→3'')-α-L-arabinopyranosyl-(1'''→2'')][β-D-xylopyranosyl-(1''''→5'')]-β-D-apiofuranosyl]diphyllin)	908	C <sub>41</sub> H <sub>48</sub> O <sub>23</sub>
Azizin (4-O-[β-D-Xylopyranosyl-(1'''→2'')-β-D-xylopyranosyl-(1''''→5'')-β-D-apiofuranosyl]diphyllin)	776	C <sub>36</sub> H <sub>40</sub> O <sub>19</sub>
Justatropmer A (4-O-β-D-Apiofuranosyl-6'-hydroxydiphyllin)	528	C <sub>26</sub> H <sub>24</sub> O <sub>12</sub>
Justatropmer B (4-O-β-D-apiofuranosyl-6'-hydroxydiphyllin)	528	C <sub>26</sub> H <sub>24</sub> O <sub>12</sub>
Justatropmer C (4-O-[β-D-Xylopyranosyl-(1→2)-β-D-apiofuranosyl]-6'-hydroxydiphyllin)	660	C <sub>31</sub> H <sub>32</sub> O <sub>16</sub>
Justatropmer D (4-O-[β-D-Xylopyranosyl-(1→2)-β-D-apiofuranosyl]-6'-hydroxydiphyllin)	660	C <sub>31</sub> H <sub>32</sub> O <sub>16</sub>
Justatropmer E (4-O-[Bis-β-D-xylopyranosyl-(1→2, 1→5)-β-D- apiofuranosyl]-6'-hydroxydiphyllin)	792	C <sub>36</sub> H <sub>40</sub> O <sub>20</sub>
Justatropmer F (4-O-[Bis-β-D-xylopyranosyl-(1→2, 1→5)-β-D- apiofuranosyl]-6'-hydroxydiphyllin)	792	C <sub>36</sub> H <sub>40</sub> O <sub>20</sub>
Justatropmer G (4-O-[[β-D-Apiofuranosyl-(1→3)-β-D-xylopyranosyl-(1→2)][β-D-xylopyranosyl-(1 → 5)]-β-D-apiofuranosyl]-6'-hydroxydiphyllin)	924	C <sub>41</sub> H <sub>48</sub> O <sub>24</sub>
Justatropmer H (4-O-[[β-D-Apiofuranosyl-(1→3)-β-D-xylopyranosyl-(1→2)][β-D-xylopyranosyl-(1 → 5)]-β-D-apiofuranosyl]-6'-hydroxydiphyllin)	924	C <sub>41</sub> H <sub>48</sub> O <sub>24</sub>
Justatropmer I (6'-O-β-D-Glucopyranosyldiphyllin)	558	C <sub>27</sub> H <sub>26</sub> O <sub>13</sub>
Justatropmer J (4-O-β-D-Glucopyranosyl-6'-hydroxyl-diphyllin)	558	C <sub>27</sub> H <sub>26</sub> O <sub>13</sub>
Justatropmer K (4-O-β-D-Glucopyranosyl-6'-hydroxyl-diphyllin)	558	C <sub>27</sub> H <sub>26</sub> O <sub>13</sub>

Justatropmer L (6'-O-[[β-D-6-O-Acetylglucopyranosyl]-justicidin B)	584	C <sub>29</sub> H <sub>28</sub> O <sub>13</sub>
Justatropmer M (6'-O-β-D-Glucopyranosyl-retro-justicidin A)	572	C <sub>28</sub> H <sub>28</sub> O <sub>13</sub>
Justin A	444	C <sub>24</sub> H <sub>28</sub> O <sub>8</sub>
Justin B	474	C <sub>25</sub> H <sub>30</sub> O <sub>9</sub>
Justin C	490	C <sub>26</sub> H <sub>34</sub> O <sub>9</sub>
(-)-Dihydroclusin	404	C <sub>22</sub> H <sub>28</sub> O <sub>7</sub>
(-)-Dihydroclusin diacetate	488	C <sub>26</sub> H <sub>32</sub> O <sub>9</sub>
Secoisolariciresinol	362	C <sub>20</sub> H <sub>26</sub> O <sub>6</sub>
Secoisolariciresinol dimethyl ether	390	C <sub>22</sub> H <sub>30</sub> O <sub>6</sub>
Secoisolariciresinol dimethyl ether monoacetate	432	C <sub>24</sub> H <sub>32</sub> O <sub>7</sub>
Secoisolariciresinol dimethyl ether diacetate	474	C <sub>26</sub> H <sub>34</sub> O <sub>8</sub>
5-Methoxy-4,4'-di-O-methylsecolariciresinol	420	C <sub>23</sub> H <sub>32</sub> O <sub>7</sub>
5-Methoxy-4,4'-di-O-methylsecolariciresinol monoacetate	462	C <sub>25</sub> H <sub>34</sub> O <sub>8</sub>
5-Methoxy-4,4'-di-O-methylsecolariciresinol diacetate	504	C <sub>27</sub> H <sub>36</sub> O <sub>9</sub>
2,3-Demethoxysecisolintetralin acetate	458	C <sub>25</sub> H <sub>30</sub> O <sub>8</sub>
Hemiariensin	400	C <sub>22</sub> H <sub>24</sub> O <sub>7</sub>
Ariensin	442	C <sub>24</sub> H <sub>26</sub> O <sub>8</sub>
Rostellulin A	472	C <sub>25</sub> H <sub>28</sub> O <sub>9</sub>
Hinokinin	354	C <sub>20</sub> H <sub>18</sub> O <sub>6</sub>
Procumbiene	368	C <sub>20</sub> H <sub>16</sub> O <sub>7</sub>
Juspurpudin	368	C <sub>20</sub> H <sub>16</sub> O <sub>7</sub>
Pinoresinol	372	C <sub>21</sub> H <sub>24</sub> O <sub>6</sub>
(-)-Syringaresinol	418	C <sub>22</sub> H <sub>26</sub> O <sub>8</sub>
Lariciresinol	360	C <sub>20</sub> H <sub>24</sub> O <sub>6</sub>
5'-Methoxy-4'-O-methylariciresinol	418	C <sub>23</sub> H <sub>30</sub> O <sub>7</sub>
(7'S,8'R)-5,3'-Dimethoxy-4,4',9'-trihydroxy-2-8',9-O-7'-neolignan	360	C <sub>20</sub> H <sub>24</sub> O <sub>6</sub>
Arctigenin	372	C <sub>21</sub> H <sub>24</sub> O <sub>6</sub>
Matairesinol	358	C <sub>20</sub> H <sub>22</sub> O <sub>6</sub>
Secoisolariciresinol	362	C <sub>20</sub> H <sub>26</sub> O <sub>6</sub>
(7,8-cis-8,8'-trans)-2-4-Dihydroxyl-3,5-dimethoxy-lariciresinol	360	C <sub>20</sub> H <sub>24</sub> O <sub>6</sub>
(+)-Ferulasinkin A (7R, 8R, 7'R, 8'R)	362	C <sub>19</sub> H <sub>22</sub> O <sub>7</sub>
(-)-Ferulasinkin A (7S, 8S, 7'S, 8'S)	362	C <sub>19</sub> H <sub>22</sub> O <sub>7</sub>
(+)-Ferulasinkin B (7S, 8S, 7'R, 8'R)	362	C <sub>19</sub> H <sub>22</sub> O <sub>7</sub>
(-)-Ferulasinkin B (7R, 8R, 7'S, 8'S)	362	C <sub>19</sub> H <sub>22</sub> O <sub>7</sub>
(+)-Ferulasinkin C (7S, 8S, 7'R, 8'S)	362	C <sub>19</sub> H <sub>22</sub> O <sub>7</sub>
(-)-Ferulasinkin C (7R, 8R, 7'S, 8'R)	362	C <sub>19</sub> H <sub>22</sub> O <sub>7</sub>

(+)-Ferulasinkin D (7R, 8S, 7'S, 8'S)	362	C <sub>19</sub> H <sub>22</sub> O <sub>7</sub>
(-)-Ferulasinkin D (7S, 8R, 7'R, 8'R)	362	C <sub>19</sub> H <sub>22</sub> O <sub>7</sub>
(+)-Sinkianlignan A (7''S, 8''R)	518	C <sub>30</sub> H <sub>30</sub> O <sub>8</sub>
(-)-Sinkianlignan A (7''R, 8''S)	518	C <sub>30</sub> H <sub>30</sub> O <sub>8</sub>
(+)-Sinkianlignan B (7S, 8S, 7''S, 8''R)	552	C <sub>30</sub> H <sub>32</sub> O <sub>10</sub>
(-)-Sinkianlignan B (7R, 8R, 7''R, 8''S)	552	C <sub>30</sub> H <sub>32</sub> O <sub>10</sub>
(+)-Sinkianlignan C (7R, 8R, 9S, 7''R)	524	C <sub>30</sub> H <sub>36</sub> O <sub>8</sub>
(-)-Sinkianlignan C (7S, 8S, 9R, 7''S)	524	C <sub>30</sub> H <sub>36</sub> O <sub>8</sub>
(+)-Sinkianlignan D (7S, 8R, 9''S)	430	C <sub>23</sub> H <sub>26</sub> O <sub>8</sub>
(-)-Sinkianlignan D (7R, 8S, 9''R)	430	C <sub>23</sub> H <sub>26</sub> O <sub>8</sub>
(+)-Sinkianlignan E (7S, 8S)	358	C <sub>21</sub> H <sub>26</sub> O <sub>5</sub>
(-)-Sinkianlignan E (7R, 8R)	358	C <sub>21</sub> H <sub>26</sub> O <sub>5</sub>
(+)-Sinkianlignan F (7R, 8S)	358	C <sub>21</sub> H <sub>26</sub> O <sub>5</sub>
(-)-Sinkianlignan F (7S, 8R)	358	C <sub>21</sub> H <sub>26</sub> O <sub>5</sub>
(+)-Sinkianlignan G (7R, 8S, 7'R, 8'S)	376	C <sub>20</sub> H <sub>24</sub> O <sub>7</sub>
(-)-Sinkianlignan G (7S, 8R, 7'S, 8'R)	376	C <sub>20</sub> H <sub>24</sub> O <sub>7</sub>
(+)-Sinkianlignan H (7S, 8R, 7'R, 8'S)	376	C <sub>20</sub> H <sub>24</sub> O <sub>7</sub>
(-)-Sinkianlignan H (7R, 8S, 7'S, 8'R)	376	C <sub>20</sub> H <sub>24</sub> O <sub>7</sub>
(+)-Sinkianlignan I (7R, 8R, 7'S, 8'S)	376	C <sub>20</sub> H <sub>24</sub> O <sub>7</sub>
(-)-Sinkianlignan I (7S, 8S, 7'R, 8'R)	376	C <sub>20</sub> H <sub>24</sub> O <sub>7</sub>
(+)-Sinkianlignan J (7R, 8R, 7'R, 8'R)	376	C <sub>20</sub> H <sub>24</sub> O <sub>7</sub>
(-)-Sinkianlignan J (7S, 8S, 7'S, 8'S)	376	C <sub>20</sub> H <sub>24</sub> O <sub>7</sub>
(+)-Sinkianlignan K (7R, 8S, 7'S, 8'R)	376	C <sub>20</sub> H <sub>24</sub> O <sub>7</sub>
(-)-Sinkianlignan K (7S, 8S, 7'R, 8'S)	376	C <sub>20</sub> H <sub>24</sub> O <sub>7</sub>
Neoarctin A	742	C <sub>42</sub> H <sub>46</sub> O <sub>12</sub>
Arctiin	534	C <sub>27</sub> H <sub>34</sub> O <sub>11</sub>