

Supporting information:

## From COX-2 inhibitor nimesulide to potent anti-cancer agent: synthesis, *in vitro* and *in vivo*, and pharmacokinetic evaluation

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### HPLC analysis of the purity of the compounds

For the HPLC analysis, a 1.00 mg/mL stock solution of each standard was prepared in either methanol or acetonitrile. The Beckman HPLC system consists of two LC-20AD pumps, a DGU-20A<sub>3</sub> degasser, a SIL-20AC autosampler, and a CBM-20A module (Shimadzu, Tokyo, Japan). The chromatographic separation was performed on a Luna C18 column (2.0 mm × 150 mm, 5 μm) with a guard column (2 mm × 40 mm, 5 μm) from Phenomenex (Torrance, CA, USA) at room temperature with a flow rate of 0.2 mL/min. Two mobile phases with 10mM ammonium acetate (10% water, 90% methanol; 20% water, 80% acetonitrile) were employed to run 15 min. An injection volume of 5-15μL was used. The UV detector was set up at 290 and 256nm.

H <sub>2</sub> O/CH <sub>3</sub> OH (10%/90%)			H <sub>2</sub> O/CH <sub>3</sub> CN (20%/80%)	
Compd	Retention time (R <sub>t</sub> ) in minutes	Purity	Retention time (R <sub>t</sub> ) in minutes	Purity
<b>1</b>	3.3	95.1%	4.0	94.1%
<b>2</b>	3.3	95.3%	4.1	92.0%
<b>3</b>	3.7	95.4%	4.7	92.8%
<b>4</b>	4.8	96.5%	6.6	96.9%
<b>5</b>	3.9	97.6%	5.4	92.7%
<b>6</b>	4.3	95.3%	6.3	97.8%
<b>7</b>	3.0	96.0%	3.6	82.1%
<b>8</b>	3.0	97.7%	3.7	96.4%

<b>9</b>	3.9	100.0%	5.3	100.0%
<b>10</b>	3.1	99.7%	3.7	97.9%
<b>11</b>	3.0	99.5%	3.7	98.4%
<b>12</b>	2.9	100.0%	3.2	96.7%
<b>14</b>	3.5	99.1%	5.0	99.3%
<b>15</b>	3.7	100.0%	5.2	99.5%
<b>16</b>	3.0	99.6%	3.5	99.2%
<b>17</b>	2.8	100.0%	3.2	99.4%
<b>18</b>	3.2	99.6%	3.9	98.5%
<b>19</b>	3.3	100.0%	4.6	99.3%
<b>20</b>	3.2	99.2%	4.0	99.0%
<b>21</b>	3.5	99.9%	4.7	99.8%
<b>22</b>	3.4	98.1%	4.4	100.0%
<b>23</b>	3.4	99.4%	4.3	98.4%
<b>24</b>	3.2	99.2%	3.8	98.7%
<b>25</b>	3.4	95.4%	4.8	95.2%
<b>26</b>	5.0	99.8%	7.6	99.7%
<b>27</b>	3.9	99.9%	5.4	98.3%
<b>28</b>	3.8	98.2%	5.0	99.1%
<b>29</b>	4.0	99.7%	5.6	98.9%
<b>30</b>	3.5	99.6%	4.6	99.7%
<b>31</b>	3.3	93.7%	4.2	94.5%
<b>32</b>	3.5	99.2%	4.5	99.8%
<b>33</b>	3.8	97.9%	5.3	97.9%
<b>34</b>	3.7	99.5%	5.2	98.6%
<b>35</b>	3.8	99.2%	5.4	99.5%
<b>36</b>	3.4	98.8%	4.5	98.0%
<b>37</b>	2.9	99.9%	3.4	99.3%
<b>38</b>	3.1	99.7%	3.8	99.1%

**39**      2.8                              99.5%    3.2                              97.9%

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\*Compound 13 was not subjected to HPLC analysis due to its poor solubility.

## Growth inhibitory effect of CSUOH0901 on 60 human tumor cell lines

This screening service was provided by the Developmental Therapeutics Program at National Cancer Institute. A sulforhodamine B (SRB) protein assay was used to estimate cell viability or growth.

