2-Hydroxy-5-(3,5,7-trihydroxy-4-oxo-4H-chromen-2-yl)phenyl (E)-3-(4-hydroxy-3-methoxyphenyl)acrylate: synthesis, in silico analysis and in vitro pharmacological evaluation

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Table of contents

S1-S2 ¹H- and ¹³C-NMR Quercetin.
S3-S4 ¹H- and ¹³C-NMR Ferulic acid.
S5-S8 ¹H- and ¹³C-NMR Compound 1.
S9-S10 HSQC Compound 1.
S11-S12 HMBC Compound 1.
S13 Table S1. K_Ca1.1 channel-compounds interaction network.
$^1$H-NMR (600 MHz, DMSO-$_d_6$) $\delta$: 12.48 (s, 1H, OH in 5), 10.76 (br s, 1H, OH in 3), 9.57 (br s, 1H, OH in 7), 9.33 (br s, 2H, OH in 3' and 4'), 7.67 (d, $J = 2.1$ Hz, 1H, H in 2'), 7.53 (dd, $J = 8.5$ Hz, 2.1 Hz, H in 6'), 6.88 (d, $J = 8.5$ Hz, 1H, H in 5'), 6.40 (d, $J = 2.0$ Hz, 1H, H in 8), 6.18 (d, $J = 1.8$ Hz, 1H, H in 6).
$^{13}$C-NMR (151 MHz, DMSO-$d_6$) $\delta$: 173.3 (C=O), 164.3 (C in 7), 161.2 (C in 5), 156.6 (C in 8a), 148.2 (C in 4'), 147.3 (C in 2), 145.5 (C in 3'), 136.2 (C in 3), 122.4 (C in 1'), 120.4 (C in 6'), 116.1 (C in 5'), 115.5 (C in 2'), 103.5 (C in 4a), 98.65 (C in 6), 93.8 (C in 8).
$^1$H-NMR (600 MHz, DMSO-$d_6$) $\delta$: 12.10 (br s, 1H, COOH), 9.52 (br s, 1H, OH in 4'), 7.48 (d, $J = 15.9$ Hz, 1H, -CH=CH-Ar), 7.27 (d, $J = 1.8$ Hz, 1H, H in 2'), 7.07 (dd, $J = 8.2$ Hz, 1.8 Hz, H in 6'), 6.78 (d, $J = 8.1$ Hz, 1H, H in 5'), 6.36 (d, $J = 15.9$ Hz, 1H, CO-CH=CH-Ar), 3.81 (s, 3H, OCH$_3$).
$^{13}$C-NMR (151 MHz, DMSO-$d_6$) $\delta$: 168.5 (C=O), 149.5 (C in 4'), 148.4 (C in 3'), 145.0 (-CH=CH-Ar), 126.2 (C in 1'), 123.3 (C in 6'), 116.1 (CO-CH=CH-Ar), 116.0 (C in 5'), 111.6 (C in 2'), 56.1 (OCH$_3$).
**Table S1.** $K_{Ca}1.1$ channel-compounds 1 and 2 interaction network. The *consensus* binding residues are marked in bold.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Hydrophobic Interaction</th>
<th>Hydrogen bond</th>
<th>Π-Stacking</th>
<th>Π- Cationic</th>
<th>ΔG (Kcal/mol)</th>
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