

Stability and Photoisomerization of Stilbenes Isolated From the Bark of Norway Spruce Roots

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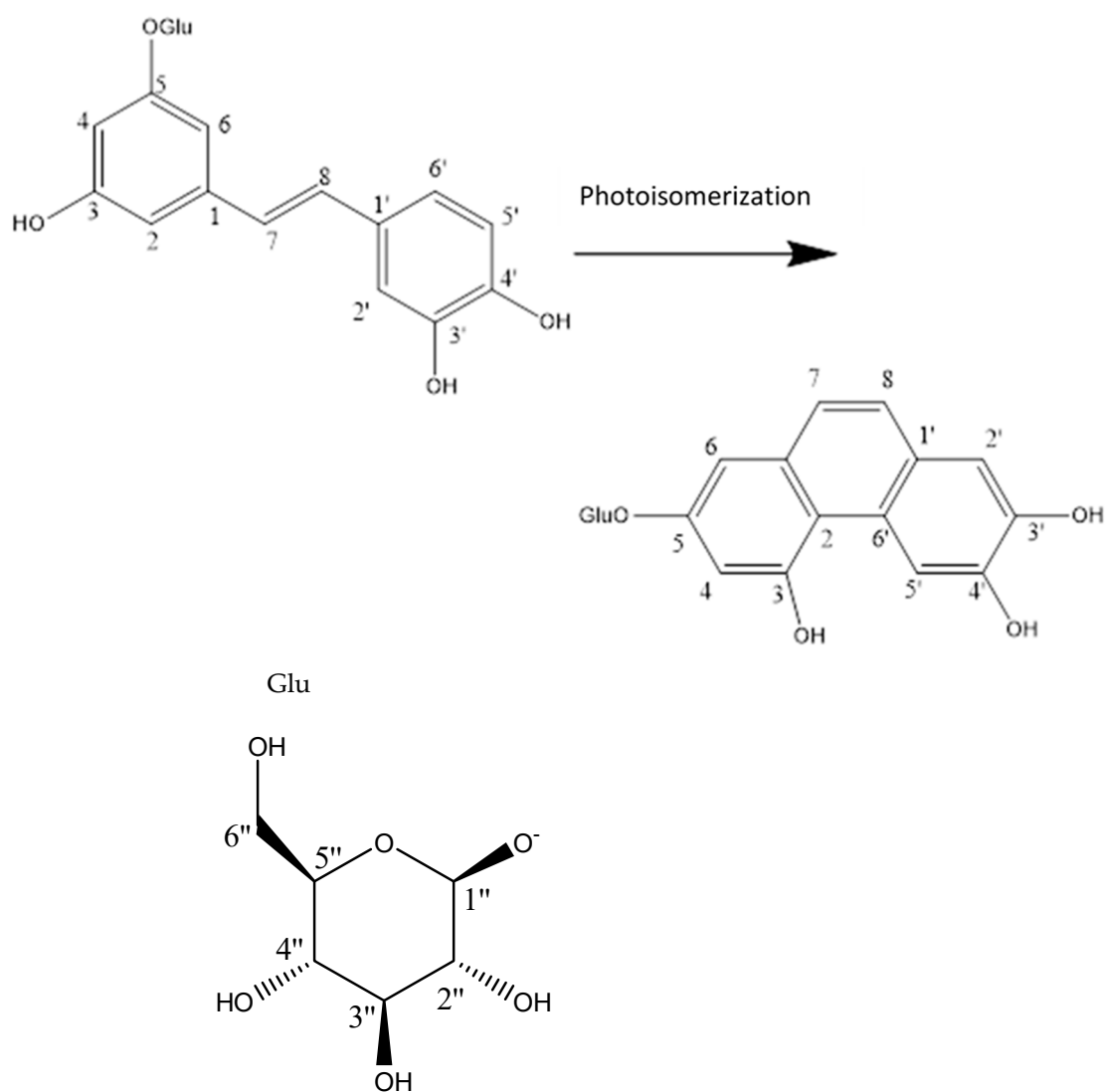


Figure S1. F3.2 fraction: The phenanthrene structure formed in the photoisomerization of *trans* – isorhapotin.

The NMR analyses were performed by Bruker Avance III 500 MHz and Varian Mercury 300 MHz spectrometers. The ¹H and ¹³C spectra were recorded in CD₃OD (300

MHz, 500MHz). ¹H and ¹³C chemical shifts were referenced to solvent signals of CD₃OD, δ (¹H) = 3.31 ppm and δ (¹³C) = 49.86 ppm.

F1.2 ¹H-NMR (300 MHz, CD₃OD): 9.01 (H-5', 1H, s), 7.44 (H-8, 1H, d, J= 9Hz), 7.32 (H-7, 1H, d, J= 9Hz), 7.13 (H-2', 1H, s), 6.97 (H-6, 1H, d, J= 2.5 Hz), 6.84 (H-4, 1H, d, J=2.5 Hz), 5.26 (1 H, d, J=7.8 Hz); ¹³C -NMR (500 MHz, CD₃OD) 136.40 (C-1), 128.53 (C-2), 156.04 (C-3), 103.45 (C-4), 158.19 (C-5), 107.31 (C-6), 125.12 (C-7), 128.36 (C-8), 126.06 (C-1'), 116.06 (C-2'), 146.40 (C-3'), 145.62 (C-4'), 113.04 (C-5'), 114.33 (C-6'), 102.72 (C-1''), 75.01 (C-2''), 78.45 (C-3''), 78.72 (C-4''), 71.38 (C-5''), 62.60 (C-6'').

F1.3 ¹H-NMR (300 MHz, CD₃OD): 6.75 (H-2', 1H,d, J= 1.8Hz), 6.66 (H-5', 1H, d, J=8.2 Hz), 6.61 (H-6', 1H, dd, J=8.2, 1.8 Hz), 6.55 (H-2, 1H, br s), 6.44 (H-7, 1H, d, J= 12.4 Hz), 6.39 (H-6, 1H, br s), 6.73 (H-4, 1H, t, J=2.1 Hz), 6.33 (H-8, 1H, d, 12.4 Hz), 4.67 (H-1'', 1H, d, J= 7.7 Hz); ¹³C -NMR (500 MHz, CD₃OD) 141.80 (C-1), 110.04 (C-2), 160.93 (C-3), 104.96 (C-4), 160.93 (C-5), 112.22 (C-6), 131.42 (C-7), 129.97 (C-8), 132.46 (C-1'), 117.04 (C-2'), 146.72 (C-3'), 147.69 (C-4'), 117.84 (C-5'), 123.06 (C-6'), 103.34 (C-1''), 75.70 (C-2''), 78.57 (C-3''), 71.83 (C-4''), 78.79 (C-5''), 62.99 (C-6'').

F.3.2 ¹H-NMR (500 MHz, CD₃OD): 9.17 (H-5', 1H, s), 7.57 (H-8, 1H, d, J= 8.5 Hz), 7.44 (H-7, 1H, d= 8.5 Hz), 7.28 (H-2', 1H, s), 7.04 (H-4, 1H, d, J= 2.25 Hz), 6.85 (H-6, 1H, d= 2.25 Hz), 5.04 (H-1'', 1H, d, J= 7.5Hz), 3.99 (OCH₃, 3H, s); ¹³C -NMR (500 MHz, CD₃OD) 137.11 (C-1), 128.02 (C-2), 157.48 (C-3), 104.70 (C-4), 159.13 (C-5), 106.95 (C-6), 126.46 (C-7), 128.97 (C-8), 129.23 (C-1'), 115.01 (C-2'), 148.92 (C-3'), 147.78 (C-4'), 117.27 (C-5'), 110.10 (C-6'), 103.23 (C-1''), 75.86 (C-2''), 79.00 (C-3''), 79.13 (C-4''), 72.36 (C-5''), 63.51 (C-6''), 56.99 (OCH₃).

F3.4 ¹H-NMR (500 MHz, CD₃OD): 6.85 (H-2', d, J=2.0Hz), 6.72 (H-6', dd, J= 8.0, 1.5 Hz), 6.68 (H-5', d, J=8.0Hz), 6.53 (H-4, br, s), 6.48 (H-8, d, J= 12.3 Hz), 6.42 (H-6, br, s), 6.41 (H-2, br, s), 6.39 (H-7, d, J= 12.3 Hz), 4.71 (H-1'', d, J=7.0 Hz), 3.78 & 3.70 (H-6'', dd, J=12.3, 2.25), 3.63 (OCH₃, 3H, s) 3.46 (H-4'', m) 3.41-3.37 (H-2'', overlap), 3.35 (H-5'', overlap), 3.25 (H-3'', m); ¹³C-NMR (500 MHz, CD₃OD) 142.03 (C-1), 104.79 (C-2), 160.25 (C-3), 110.15 (C-4), 161.08 (C-5), 111.94 (C-6), 129.98 (C-7), 131.09 (C-8), 132.37 (C-1'), 114.26 (C-2'), 149.27 (C-3'), 147.90 (C-4'), 116.83 (C-5'), 124.50 (C-6'), 103.28 (C-1''), 75.66 (C-2''), 78.71 (C-3''), 78.78 (C-4''), 71.93 (C-5''), 63.10 (C-6''), 61.34 (OCH₃, 3H, s).

F3.5 ¹H-NMR (500 MHz, CD₃OD): 7.45 (H-6', 2H, d, J= 8.5Hz), 7.45 (H-8, 2H, d, J= 8.8 Hz), 7.26 (H-7, 1H, d, J=8.8. Hz), 7.13 (H-5', 1H, d, J=8.5 Hz), 6.86 (H-4, 1H, d, J= 2.4 Hz), 6.83 (H-6, 1H, d, J=2.4 Hz), 5.22 (H-1'', 1H, J=7.5Hz), 3.48 (OCH₃, 3H, s) ; ¹³C-NMR (500 MHz, CD₃OD) 138.67 (C-1), 113.90 (C-2), 157.66 (C-3), 103.70 (C-4), 159.02 (C-5), 106.64 (C-6), 124.61 (C-7), 129.51 (C-8), 130.0 (C-1'), 125.33 (C-2'), 151.23 (C-3'), 145.38 (C-4'), 117.59 (C-5'), 126.11 (C-6'), 102.39 (C-1''), 75.80 (C-2''), 79.10 (C-3''), 78.51 (C-4''), 72.16 (C-5''), 63.33 (C-6''), 61.34 (OCH₃, 3H, s).