

Antioxidants

Supporting Information

Peroxygenase-Catalyzed Selective Synthesis of Calcitriol Starting from Alfacalcidol

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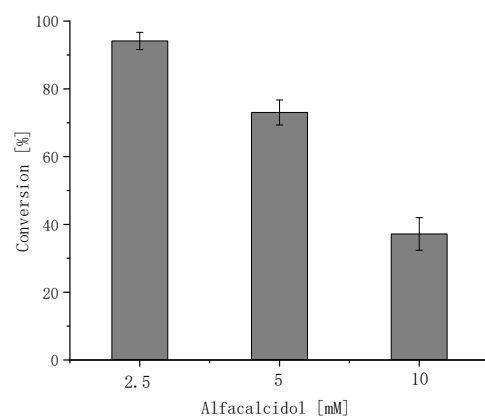


Figure S1. *Aae*UPO (Pada-I)-catalyzed oxyfunctionalization of alfacalcidol to calcitriol (path I) at various substrate loadings. Conditions: [*Aae*UPO] = 2.5 μ M, [substrate] = 2.5-10 mM, NaPi buffer (50 mM, pH 6), 40% (v/v) acetone, [H_2O_2] = 1.5 mM h^{-1} , 8 h, 25 $^\circ\text{C}$, 1 mL.

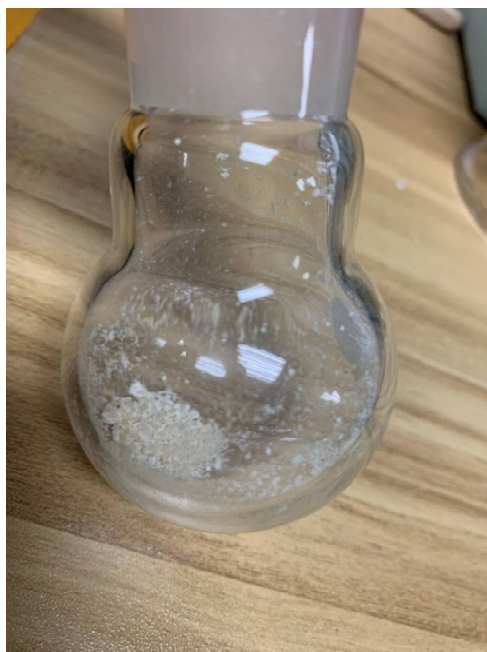


Figure S2. Image of the isolated product calcitriol (150 mg) obtained from a semi-preparative scale synthesis.

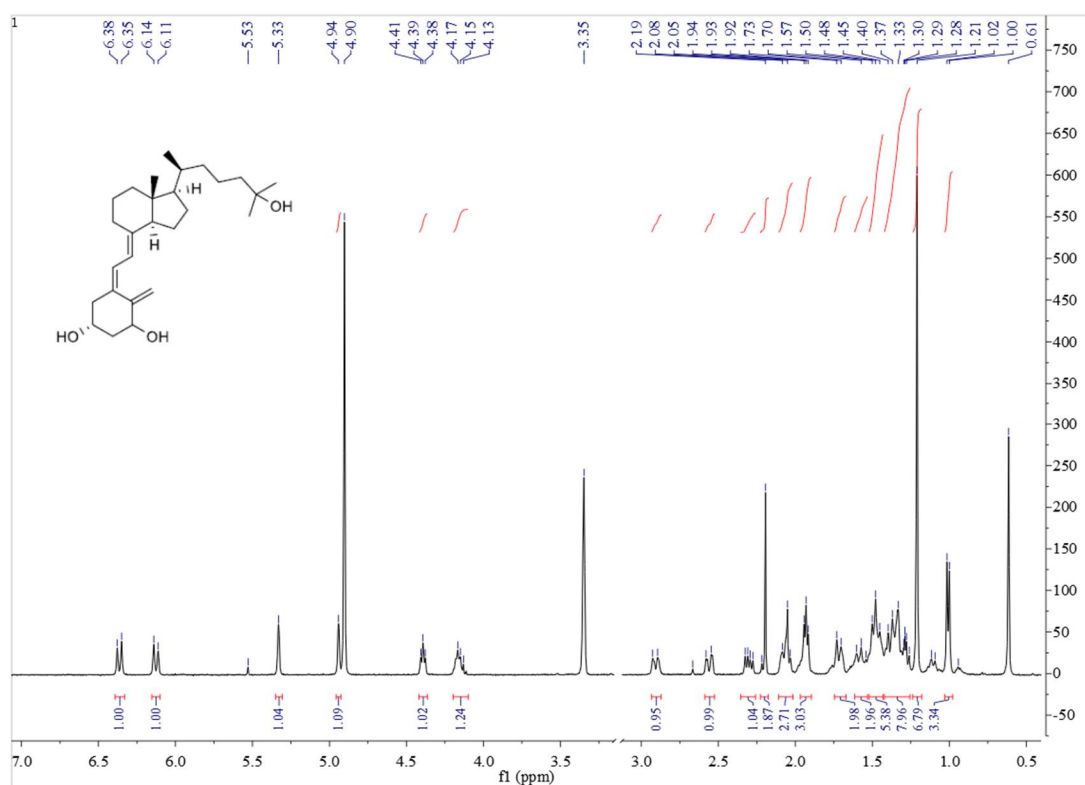


Figure S3. ¹H NMR of the isolated product calcitriol in CD₃OD: (400 MHz, δ, ppm: 6.36-6.39 (d, 1H), 6.00-6.03 (d, 1H), 5.32 (s, 1H), 5.00 (s, 1H), 4.41- 4.44 (m, 1H), 4.22- 4.24 (m, 1H), 1.00-1.60 (m, 28H), 0.90- 0.95 (m, 3H), 0.75- 0.92 (m, 4H), 0.54 (s, 3H)).

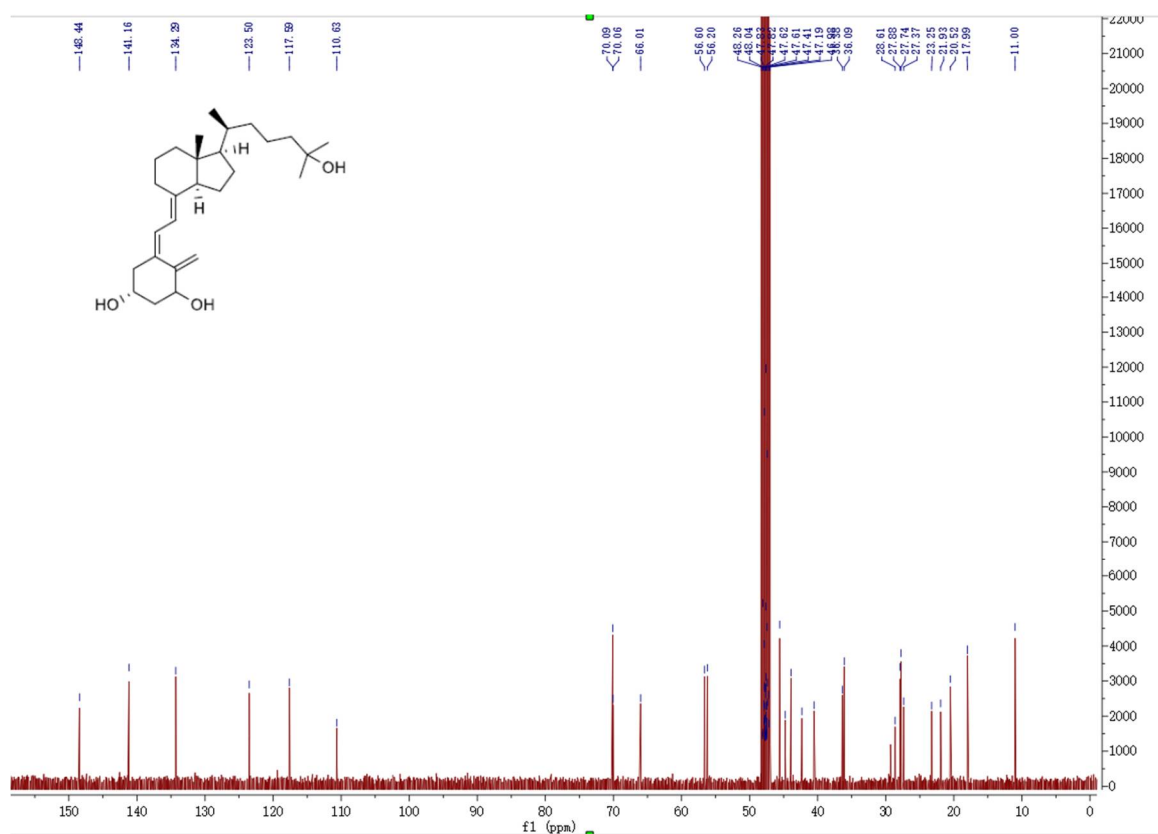


Figure S4. ¹³C NMR of the isolated product calcitriol in CD₃OD: (400 MHz, δ, ppm: 148.44, 141.16, 134.29, 123.50, 117.59, 110.63, 70.09, 70.06, 66.01, 56.60, 56.20, 45.59, 44.76, 43.91, 42.32, 40.54, 36.38, 36.09, 28.61, 27.88, 27.74, 27.37, 23.25, 21.93, 20.52, 17.99, 11.00).