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Total conversion of lupeol by iodobenzene diacetate catalyzed by a Mn-porphyrin in green conditions

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Natural Products and their structurally modified counterparts are a prolific source for the development of potential drugs, representing 28% of the first in class drugs approved by de FDA between 1999 and 2013[1]. Lupeol is a pentacyclic triterpene found in plants and, like several of its derivatives, exhibits cytotoxic, antiviral, and antifungal activity[2]. Hence, modifying the structure of lupeol is of interest for new drug discovery. In this work, the use of the meso-tetrakis(4-carbomethoxyphenyl)porphyrinatemanganese(III), [Mn(T4CMPP)Cl], as a biomimetic catalyst, and iodobenzene diacetate ($PhI(OAc)_2$) as an oxidizing agent for the structural modification of lupeol was investigated. The reactions were performed in 10 mL glass vials using a 1:33 molar ratio of [Mn(T4CMPP)Cl]:lupeol, and 2 mL of ethyl acetate as a green solvent under magnetic stirring for 24 hours at 50 °C. Different equivalents of [Mn(T4CMPP)Cl]:iodobenzene diacetate were used: 1:100, 1:200, 1:300 and 1:400 (TCM-100, TCM-200, TCM-300, and TCM-400, respectively). GC-MS analysis indicates partial lupeol conversion for the reaction TCM-100, and full conversion for the reactions TCM-200, TCM-300, and TCM-400. Furthermore, by comparing chromatograms, the signals obtained indicate that at least four products were obtained for each condition, in which TCM-200, TCM-300, and TCM-400 lead to the same products, whereas TCM-100 lead to formation of different products. Two products, previously reported in literature[3], were successfully identified by ^1H and ^{13}C NMR for the TCM-100 reaction as shown in Figure 1, and further purification steps have been performed for the identification of all products obtained in all four tested conditions. UV-Vis analysis showed partial destruction of the catalyst for the TCM-100 reaction and full destruction of the porphyrin for the TCM-200, TCM-300 and TCM-400 reactions. In conclusion, the use of porphyrins as biomimetic catalysts for the structural modification of lupeol can be a promising strategy for the discovery of new potential bioactive substances.

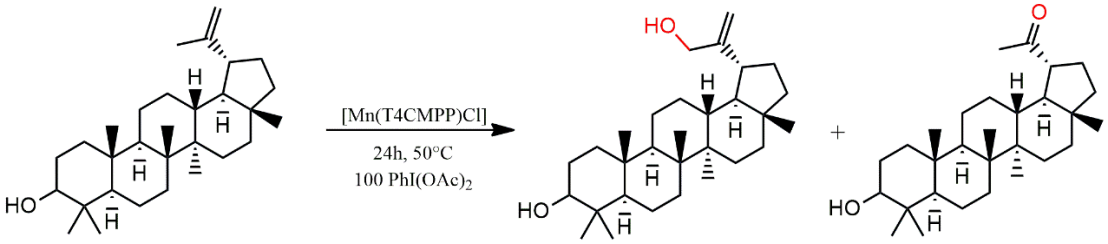

Figure 1- Reaction scheme using 100 equivalents of $PhI(OAc)_2$, with lupeol modifications highlighted in red.

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