

Complete Assignments of Flavonol Derivatives

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Abstract

Even though over 4,000 flavonoids have been known, novel flavonoids are discovered still. Their identification can be performed based on instrumental analysis. A comparison of NMR data may help us decide the novelty. One of the most abundant flavonoid classes is flavonols which are 2-(3-hydroxyphenyl)-4H-chromen-4-one. Their common substitution patterns are 5 and 7 positions. 7-mono-substitutions are not observed frequently. In addition, 6-monosubstitutions are rare. The natural sources producing flavonols are plants. However, the discovery of methyltransferases to metabolite flavonols from microorganisms can produce novel methylated flavonols. One of the methods to identify the substrates by the enzymes is HPLC. Because it requires authentic samples to compare, HPLC cannot be the best method. NMR experimental results can be alternative method. We tried to report complete assignments of ^1H and ^{13}C NMR data of 6 or 7 mono-substituted flavonols. Here we report four hydroxylated flavonol derivatives and four methylated flavonol derivatives with 6 or 7 substitution.

Reference

1. Harborne JB. (1994) *The Flavonoids: Advances in Research*. Chapman & Hall, London.