

OR-3**Structural Elucidation and Computational Study of Limonoids from *Chisocheton Erythrocarpus* (Meliaceae)**Chong Soon Lim^{1,*}, Khalit Mohamad² and Khalijah Awang¹

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Limonoid is a type of modified triterpenes that are abundant in the family Meliaceae. Their production is confined to several closely related families in the order Riales such as Rutaceae, Simaroubaceae, Cneoraceae, and Meliaceae. Among them, Meliaceae family produces the most variety of limonoid skeletons. Biosynthetically, limonoids are derived from triterpenes by having lost four carbon atoms in the final product. Hence they are formally known as tetranortriterpenoids. Structural elucidations were based on spectroscopic methods; NMR, UV, IR, and mass spectrometry. The absolute stereochemistry of some new and novel limonoids will be discussed. In order to determine the absolute configuration of limonoids, we employed the most widely used chiroptical technique; electronic circular dichroism (ECD). For optically active organic compound, it is an excellent tool for probing the chirality of chromophores through CD cotton effect, from which the determination of the absolute configuration can be achieved. Along with the experimental results, the simulation of CD curves using density functional theory (DFT) calculations was provided to compare and verify the assigned absolute configurations of new limonoids.

Keywords: Meliaceae, Limonoids, NMR, Circular Dichroism, Density Functional Theory.
