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Bio-Guided of Active New Alkaloids from Alstonia Brassi Toxicity Antitumour Activity in Silico and Molecular Modeling

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Abstract : Alstonia, which are tropical plants with a wide geographical distribution, have been divided into different sections by different authors based on previous studies of several species within the genus. Monachino divides Alstonia into 5 sections, while Pichon divides it into 3 sections. Several plants belonging to this genus, such as Alstonia brassii, have been used in traditional folk medicine to treat ailments such as fever, malaria and dysentery]. Previous studies focusing on the chemical composition of these plants have successfully identified indol alkaloids with cytotoxic, anti-diabetic and anti-inflammatory properties. The newly discovered monomers are structurally similar to the backbones of picralin, affinisin and macrolin. On the other hand, all recently isolated dimeric compounds have a macrolin moiety. In this study, a computational analysis was performed on a series of novel molecules, including both monomeric and dimeric compounds with different structural frameworks. This investigation represents the first computational study of these molecules using an in silico approach incorporating 2D-QSAR data. The analysis involved various computational techniques, including 2D-QSAR modelling, molecular docking studies and subsequent validation by molecular dynamics simulation and assessment of ADMET properties. The chemical composition was identified by 1D and 2D NMR. Eight new alkaloids were isolated, 5 monomers and 3 dimers. In this section, we focus on the biological activity of 4 new alkaloids belonging to two different skeletons, the affinisine skeleton.

Keywords : affinisine, talcarpine, macroline, cytotoxicity, alkaloids
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