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Applications of GastroPlus® Software in Toxicokinetic Studies: A Case Study on Atractyloside

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Abstract

This study aims to predict the toxicokinetics of atractyloside, the principal toxic compound found in Atractylis gummifera, utilizing GastroPlus software. Key parameters such as maximum concentration (Cmax), half-life (t1/2), area under the curve (AUC), and bioavailability (F) were determined. These findings have significant implications for enhancing the management and treatment of Atractylis gummifera poisoning cases.

Keywords: GastroPlus, toxicokinetics, atractyloside, Atractylis gummifera.

Résumé

Cette étude vise à prédire la toxicocinétique de l'atractyloside, le principal composé toxique trouvé dans Atractylis gummifera, en utilisant le logiciel GastroPlus. Des paramètres clés comme la concentration maximale (Cmax), la demi-vie (t1/2), l'aire sous la courbe (AUC) et la biodisponibilité (F) ont été déterminés. Ces résultats ont des implications importantes pour améliorer la gestion et le traitement des cas d'intoxication par Atractylis gummifera.

Mots-clés : GastroPlus, toxicocinétique, atractyloside, Atractylis gummifera.

الملخص

تهدف هذه الدراسة إلى التنبؤ بالسميات الحيوية للأتركتيلوسيد، المركب السام الرئيسي الموجود في نبات الأتركتيلس غميفيرا، باستخدام برنامج GastroPlus.تم تحديد المعلمات الرئيسية مثل التركيز الأقصى (Cmax) ، ونصف العمر (t1/2) ، والمساحة تحت المنحنى(AUC) ، و التوافر البيولوجي (F) .تحمل هذه النتائج تبعات هامة لتعزيز إدارة وعلاج حالات التسمم بنبات الأتركتيلس غميفيرا.

الكلمات الدالة: GastroPlus، السميات الحيوية، الأتركتيلوسيد، الأتركتيلس غميفيرا.

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