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Abstract

Modelling the Controlled Release of Toxins in a Rumen Environment †

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Abstract: *Pimelea* poisoning in grazing cattle, also known as St George or Marree Disease, has been a long-time pestilence for the pastoral industry throughout arid regions of inland Australia. The causative species *Pimelea* (Thymelaeaceae), native to Queensland, New South Wales and South Australia, have been confirmed, with the secondary metabolite simplexin, a daphnane orthoester, being extracted and identified as the principal toxin. Despite the lack of effective prevention or treatment for *Pimelea* poisoning, naïve calves have previously been demonstrated to develop detoxification capability following prolonged low-dose simplexin intake. A variety of composites are being fabricated by encapsulating *Pimelea* plant material or a crude extract in biodegradable and biocompatible polyesters, aiming to develop a sustained toxin release mechanism. Studies on screening potential rumen microflora able to decompose simplexin during rumen-fluid fermentation are being conducted simultaneously. In this project, a quantification method for simplexin within these biocomposites was developed and validated utilising solid-phase extraction combined with UHPLC-Q-Orbitrap MS/MS. Reliable simplexin measurement in matrices will allow investigations into the material composition, geometry and rumen microorganism's effects on the controlled release kinetics of simplexin *in vitro*. The degradation patterns of toxin delivery systems when exposed to simulated rumen environments will also be thoroughly assessed on both microscopic and chemical scales. Mathematical models of the underlying mass transport mechanisms will ultimately be established through approaches ranging from simple empirical correlations to stochastic simulations, which hold the potential to facilitate future design, optimisation, and prediction of other intra-ruminal devices based on biodegradable polymers.

Keywords: *Pimelea* poisoning; biodegradable biocomposite; slow release; modelling

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