

# Multi-Scale GranSim - CBM

# **TECHNOLOGY NUMBER: 2021-039**



## **OVERVIEW**

GranSim Multiscale Models Available

- Original GranSim Models first released 2004, continually updated
- Substantial Publication History

## BACKGROUND

GranSim-CBM is a multi-scale model combining a constraint-based metabolic model of Mycobacterium tuberculosis with an agent-based model of bacterial growth and host immunity within TB granulomas. Multi-scale Gransim is a computational model that simulates the formation, function and treatment of tuberculosis (TB) granulomas in the lung that builds on GranSim which we published on previously and is listed under different Invention Report. It is a hybrid model: ordinary differential equations describe the kinetics of molecular interactions and action of antibiotics; partial differential equations describe diffusion of molecules within the lung; an agent-based model captures the actions of individual immune cells and bacteria in a stochastic framework. The model is multi-scale, including molecular and cellular events that produce emergent behavior at the tissue scale. The framework accommodates multiple antibiotics, includes accounting of their pharmacokinetics and pharmacodynamics, and thus can predict the impact of antibiotic treatment on TB granulomas. The model is calibrated and validated against multiple datasets from non-human primates and humans.

# **Technology ID**

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### Category

Software Software & Content

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