

EMCR Symposium at Westmead Abstract Submission Form

Abstract details:

Presentation title: Making Molecules That Matter: Open Source Drug Discovery In Undergraduate Laboratories

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Presenting author career stage (PhD student; early career, 0–10 years post-PhD; mid-career, 10–15 years post-PhD: early career

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Abstract:

The Breaking Good Project (www.breakinggoodproject.com) has been working with high school and undergraduate students from around the world, involving them in crowdsourced citizen science projects where they make molecules that matter. In this presentation, I will share the latest achievements of undergraduate students from The University of Sydney and their contributions to the Open Source Mycetoma project.

Mycetoma was first recognised by the World Health Organisation as a neglected tropical disease in 2016. It is endemic to tropical and subtropical areas though the true burden of the condition is unknown. Currently, actinomycetoma (bacterial infection) can be effectively treated with a course of antibiotics at a 90% curative rate. Eumycetoma (fungal infection) treatment options, on the other hand are less effective with curative rates between 25-35%. Open Source Mycetoma (https://github.com/OpenSourceMycetoma) is an open source drug discovery collaboration searching for a viable treatment for eumycetoma.

In 2021, first year students at The University of Sydney focused on the synthesis of compounds in the 2-aminothiazole family (series 2), a hit identified from screening of the statis box against *Madurella mycetomatis*. Working as open scientists, the students synthesised and characterised 11 novel compounds. In all bar one instance, final products were obtained in >99% purity (HPLC) and in moderate yields without the need from further purification. Furthermore, biological evaluation of the compounds against *Madurella mycetomatis* provided evidence of a key structural elements required for potent activity.

- 1. World Health Organization. Neglected tropical diseases. http://www.who.int/neglected_diseases/diseases/en/ (accessed 29/04/2021)
- 2. W. W. J. van de Sande, *et al.* (2014). *PLOS Negl Trop Dis.* 7: e2550. DOI: 10.1371/journal.pntd.0002667