PhD placement/PIPS: Natural Products for Human Health

Placement supervisor:

Dr Melanie-Jayne Howes, m.howes@kew.org
Dr Adam Richard-Bollans, a.richard-bollans@kew.org

Placement overview and objective:

Project idea 1: 'Mining Medicinal Molecules'. This project involves developing an Artificial Intelligence (AI) method to predict plant species that contain bioactive molecules to facilitate drug discovery. Large and unique plant 'trait' datasets are needed for the AI model being developed. This placement will involve mining data from published literature (including data on bioactive plants and their chemical constituents for malaria), documenting and co-ordinating datasets. The outcome will be the acquisition and documentation of a range of plant 'trait' data for the AI model.

Project idea 2: 'Heterogeneity in Antiplasmodial Plant Assays': One of the big challenges of applying Artificial Intelligence (AI) techniques in plant and biological sciences is the current state of the data. A particular challenge is data heterogeneity, which we see in collected data on antiplasmodial activity of plants in Gentianales. There are many ways antiplasmodial tests on the same plant species may differ: using different plant parts, extraction methods, *in vitro/vivo* tests, living/dried material, plasmodium strains etc. This heterogeneity complicates the quantification of antiplasmodial activity in plants and poses challenges for the application of AI predictive approaches.

This placement will involve extending datasets on antiplasmodial activity held by Kew, analysing the variation found in test outcomes and identifying trends relating types of tests to antiplasmodial activity. The outcomes will be (1) insights into how different antiplasmodial test procedures influence test outcomes and (2) recommendations for antiplasmodial test procedures to maximise the likelihood of finding new antiplasmodial compounds in future bioassays.

Tasks to be undertake/Possible projects:

Project idea 1: 'Mining Medicinal Molecules'.

- Search available online databases to mine published 'trait' data on plants and their chemical constituents with antimalarial properties.
- Review and document the mined plant 'trait' data (including ethnobotanical and pharmacological data) on bioactive plants and their chemical constituents to generate and database plant 'trait' data.
- Co—ordinate project 'trait' data available for inclusion in an AI model.

Project idea 2: 'Heterogeneity in Antiplasmodial Plant Assays':

- Update existing collated data on antiplasmodial activity to include identified sources of heterogeneity e.g. plant parts
- Analyse within-species variation of test outcomes and evaluate consistency of results
- Provide recommendations for which test conditions are most likely to result in finding active species
- Present findings to working group and potentially wider seminars within Kew

Required skills and experience:

Project idea 1: 'Mining Medicinal Molecules'.

- Experience or understanding of pharmacology.
- Experience or understanding of chemistry.
- Experience of documenting and analysing data using software packages.

Project idea 2: 'Heterogeneity in Antiplasmodial Plant Assays':

- Experience or understanding of pharmacology.
- Experience of documenting and analysing data using software packages

Skills and areas of knowledge that can be developed:

Project idea 1: 'Mining Medicinal Molecules'.

- Develop skills in searching and reviewing published literature.
- Develop skills in co-ordinating large datasets and databasing.
- Develop knowledge of plant traits.
- Develop teamworking and communication skills by working with the multidisciplinary (chemistry, pharmacology, plant taxonomy, AI) project team.

Project 2: 'Heterogeneity in Antiplasmodial Plant Assays':

- Develop teamwork and communication skills by collaborating with an interdisciplinary team to compile new data
- Develop data analysis skills
- Develop skills in reviewing literature
- Develop knowledge of natural product drug discovery
- Develop reporting and presentation skills

Location of work:

Kew, Richmond, hybrid working possible

Length of placement:

3 months

Provisional start date:

Before August/September 2024