

## Fighting malaria with the help of personal computing power

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UCD researchers, Dr Anthony Chubb and PhD student Kevin O'Brien, working with Conway Fellow, Professor Denis Shields in the Complex Adaptive Systems Laboratory (CASL) are harnessing the donated computational power of personal computers to find new targets for antimalarial drugs.

Most computers only use a fraction of their available CPU power for dayto-day computation. The UCD team have built a BOINC server that distributes jobs to donated 'client' computers, which then carry out the work in the background.

Malaria kills a child every 45 seconds. The parasite responsible, Plasmodium falciparum, continues to evolve resistance to available medication. New replacement drugs that target new proteins in the parasite are urgently needed.

Large pharmaceutical organisations such as GSK and Novartis have already tested millions of compounds and found nearly 19,000 hits that show promising activity against <u>Plasmodium falciparum</u>. However, they do not know which <u>target protein(s)</u> is actually being affected by these compounds.

If the target protein for each of these hits is identified, the process of drug discovery and development would be significantly enhanced. The FightMalaria@Home project is aimed at finding these new targets by distributed computation or crowd-sourcing.



Dr Anthony Chubb says, "We plan to dock each of the 19,000 hits into structures of each of the 5,363 proteins in the <u>malaria parasite</u>. The <u>computational power</u> needed is enormous.

By connecting thousands of computers, we can harness the equivalent <u>power</u> of large supercomputers to help us with our research.

We have over 2000 computers from 63 countries around the world signed on already. This is allowing us to do about 300,000 docking calculations per day, but need to get to closer to 1 million per day."

The UCD team are appealing to people all over Ireland to donate computing time by logging onto <u>www.fight-malaria.org</u> and following the simple setup instructions. On this website, you can also monitor the leader board, top teams and project statistics.

Malaria infects 216 million people and kills 650,000 each year, mostly African children under 5 years old [WHO].

Provided by University College Dublin

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