ISMS-PL01 **Robot Scientists: Automating Drug Design** Ross D. KING University of Manchester

A Robot Scientist is a physically implemented robotic system that applies techniques from artificial intelligence to execute cycles of automated scientific experimentation. A Robot Scientist can automatically execute cycles of: hypothesis formation, selection of efficient experiments to discriminate between hypotheses, execution of experiments using laboratory automation equipment, and analysis of results. The motivation for developing Robot Scientists is to better understand science, and to make scientific research more efficient. The Robot Scientist 'Adam' was the first machine to autonomously discover novel scientific knowledge. Our new Robot Scientist, 'Eve', is designed to automate and integrate drug screening, hit conformation, and QSAR development. Its combination of novel automation with synthetic biology assays enables faster and cheaper drug design. Eve's focus was originally on neglected tropical diseases, and Eve has discovered hits and leads against targets in multiple parasites. We are now adapting Eve to work with and learn about human cancer cell lines. There is currently a 'replication crisis' in biology, and many scientific results have been shown to difficult to replicate. We argue that the formalisation of protocols, combined with the automation of experiments, is the best way to replicate results.