

## Project proposal

<i>Project title</i>	A twenty first century approach to detecting doping in sport: maximising computational predictions for novel drugs	
<i>First Supervisor</i>	Dr <input type="text" value=""/>	<input type="text" value="Jean-Christophe Nebel"/>
<i>Second Supervisor</i>	<input type="text" value="Prof. Declan Naughton"/>	
<i>School</i>	<input type="text" value="Computing and Information Systems"/>	
<i>Other member of supervisory team (no more than three KU supervisors in total)</i>	<input type="text" value="Prof. Andrea Petroczi"/>	
<i>Specific requirements beyond 2:1 degree</i>	<input type="text" value=""/>	

### Project summary (max 4,000 characters)

MSc by Research

Anabolic androgenic steroids (AAS) are prohibited by sport governing bodies and governments signatories to the WADA Anti-Doping Code. Not only does their usage flout sports ethics and gives unfair advantage during competition, but they are harmful to athletes' health. Although top level athletes are subject to in and out of competition testing regimens, these tests are usually unable to detect drugs which are unknown to the relevant authorities, resulting in a controller-type game with cheaters usually a step ahead. Thus new approaches are required to predict new drug appearances to inform testing. The main aim of this bioinformatics project is to design a machine learning based software which would predict the composition of future illegal 'designer' performance-enhancing drugs. This will be achieved by, first, predicting the structures of potentially new AAS. A set of drug candidates will be generated by combining analysis of the existing drug network and the automatic evolution of new compounds using a genetic algorithm. Secondly, the potency of those putative drugs will be estimated by calculating their affinity with human androgen receptor using molecular mechanics.