THE UNIVERSITY of EDINBURGH
School of Biological Sciences

MSc Research or Work Based Project/Dissertation Feedback

Exam number:	B134006
MSc Programme:	Drug Discovery and Translational Biology
Project Title:	Performance Improvements on LIDAEUS through Comparison with AutoDock Vina in Virtual Screening Evaluation

Feedback – Marker 1

This is a very good report which describes a significant amount of work and analysis. It is well structured but in places is overly long (the introduction could perhaps have had some summary figures to pull it together). There is a clear understanding of the methodology and the field as a whole. The results are well presented with detailed figures throughout. The discussion could have benefited from some suggestions for future prospects and comparison with similar studies. The conclusion is a little basic.

Feedback – Marker 2

The abstract and introduction are nicely written and reasonably well referenced and provides a good background to the project. The descriptions of the two virtual screening programs are clear and concise. The preamble does however become more of a broad review of ligand docking in general. More relevant is the discussion on Enrichment Factors and on the evaluation of how well a screening program performs; this is well described. The methods section is well organised and describes a significant number of small programs developed in the course of the project. The program to implement an entropy factor to account for water displacement is impressive even though subsequent evaluation suggested this approach does not improve docking scores. Figures 8 and 9 provide an excellent objective and quantitative evaluation of the docking results of the two programs. The discovery that far better docking scores can be achieved by implementation of different weighting schemes is a really impressive result In summary this is a very well written if somewhat wordy account of the merits of Lidaeus and contains a very substantial amount of original work. The results are clearly and objectively presented and evaluated. The dissertation shows a a very good understanding of the field and presents the development some very original and general methods for evaluating docking and virtual screening programs