Molecular Simulation Assignment Marksheet Y…

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|  | 1g | 1a | 2i | 2ii | 3 | u |  |
| **1 Title/Abstract** |  |  |  |  |  |  |  |
| Title: concise and informative |  |  |  |  |  |  | Not so |
| Abstract: concise and self-contained |  |  |  |  |  |  | Not so, too long or inadequate |
| Clear summary of results |  |  |  |  |  |  | Missing or poor summary of results |
| **2 Introduction** |  |  |  |  |  |  |  |
| Background context explained |  |  |  |  |  |  | Missing background context |
| Appropriate references |  |  |  |  |  |  | Lack of references |
| Purpose and aims set out and explained |  |  |  |  |  |  | Missing clear aims and purpose |
| Includes an outline of the investigation |  |  |  |  |  |  | Aims not clearly given or explained |
| **3 Theory** |  |  |  |  |  |  | Not given, ends abruptly |
| Detailed explanation of the relevant theory |  |  |  |  |  |  | Insufficient explanation of the theory |
| Key equations given and explained |  |  |  |  |  |  | Missing key equations |
| Application of the model justified |  |  |  |  |  |  | No justification given for the model |
| **4. Method** |  |  |  |  |  |  |  |
| Detailed method and program for block averaging |  |  |  |  |  |  | Missing details/program for block avgs |
| Detailed method and program for fluctuation calculations |  |  |  |  |  |  | Missing or inadequate method for fluctuation calculations |
| Detailed account and justification of simulation parameters used sufficient to repeat the work |  |  |  |  |  |  | Missing / poorly explained simulation and parameter details |
| **5 Results and discussion** |  |  |  |  |  |  |  |
| Complete set of results |  |  |  |  |  |  | Missing, incorrect or incomplete results |
| Well-presented figures with labels and captions |  |  |  |  |  |  | Poor figures, missing units, captions |
| Good level of text linking figures and tables |  |  |  |  |  |  | Overly brief description of results |
| Critical analysis and discussion of results |  |  |  |  |  |  | Missing or poor discussion of results |
| **6 Conclusions** |  |  |  |  |  |  |  |
| Clear summary of results |  |  |  |  |  |  | Missing summary of results |
| Conclusions drawn and justified |  |  |  |  |  |  | Unsubstantiated/ invalid conclusions |
| Critical analysis of results and comparison with published results |  |  |  |  |  |  | Results not put into context |
| Clear assessment of suitability of method and further work |  |  |  |  |  |  | No discussion of parameters and no suggestions for further work |
| **7 Overall Factors** |  |  |  |  |  |  |  |
| Outstanding presentation |  |  |  |  |  |  | Presentation disorganised, scruffy |
| Well-structured report |  |  |  |  |  |  | Missing or inappropriate structure |
| Excellent standard of scientific investigation |  |  |  |  |  |  | Unsatisfactory or flawed investigation |
| Fluent accurate writing style |  |  |  |  |  |  | Poor style, errors in grammar/spelling |
| Good original references in APS format |  |  |  |  |  |  | Missing/poor unformatted references |
| **8 Code** |  |  |  |  |  |  |  |
| Clear and easy to follow coding style |  |  |  |  |  |  | Missing code or poor coding style |
| Excellent code comments and documentation |  |  |  |  |  |  | Missing code comments and documentation |

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| *General comments on the project report justifying the overall mark* |

**Report Mark %**