Supporting information for

A multi-disciplinary team-based classroom exercise for small molecule drug discovery

Charlotte A Dodson 1\*, Stephen E Flower 2\* & Mark Thomas 3

1 Department of Life Sciences, 2 Department of Chemistry, 3 Department for Health, University of Bath, Claverton Down, Bath BA2 7AY, UK

\* c.a.dodson@bath.ac.uk, s.e.flower@bath.ac.uk

**Virtual Drug Discovery Exercise Individual Report Mark Scheme**

**Written report marking scheme**

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| --- | --- | --- |
| **%** | **Achievement Descriptors and Attributes** | |
| *91-100* | **Exceptional**  Distinction | Exceptional report with all areas of the highest standard; excellent interpretation of data including critical comparison with other work and demonstrating conceptual understanding well beyond that expected at UG level. Complete and well laid out and explained synthesis with full justifications and understanding and high probability of real-world success. Rarely awarded and needs ***full and comprehensive*** justification. |
| *81-90* | **Outstanding**  Distinction | Exceptional report containing work of the highest standard; excellent interpretation of data including critical comparison with other work and demonstrating conceptual understanding beyond that expected at UG level. Needs ***full and comprehensive*** justification. |
| *76-80* | **Excellent**  Distinction | Very high quality report containing work of the highest standard; high level of conceptual understanding and critical appraisal clearly demonstrated; high level of originality demonstrated. |
| *70-75* | **Very Good**  Distinction | High quality report; clearly demonstrates good levels of conceptual understanding and reasoning; data critically and unambiguously discussed and placed within broader context; task area described with good breadth and depth. Detailed synthesis with high likelihood of real-world success. |
| *60-69* | **Distinction** | Very competent report with good quality explanation; demonstrates good levels of conceptual understanding and reasoning; critical discussion of data and task area included in some breadth and depth. Good synthesis although without being completely detailed, likelihood of real-world success not overly strong. |
| *58-59* | **Borderline** Distinction/Merit | Very close to Distinction standard but has not met all the requirements of the above. |
| *50-57* | **Merit** | Competent written report with reasonable quality of explanation of data, shows some evidence of conceptual understanding and reasoning, some critical discussion of data and their context, but this may lack breadth and depth. Synthesis not fully thought through – lacking detail and unlikely to be successful (incompatible reagents, incorrect reaction, shortcuts (v. expensive commercial material from unreliable supplier) etc.). |
| *48-49* | **Borderline** Merit / Pass | Very close to Merit standard but has not met all the requirements of the above. |
| *40-47* | **Pass** | Report of a passable standard, some understanding of the project area demonstrated, but clear deficiencies in the way that the data are communicated; deficiencies in explaining work which casts doubt on their understanding of the data. Synthesis shows lack of understanding or engagement with no chance of real-world success. Poor quality figures and schemes. |
| *0-39* | **FAIL:**  Not worthy  of credit. | Very little or no work reported; report demonstrates very little or no knowledge and understanding of the area; little attention to detail; little effort put into the report; work so poor as to make the report useless; overall, not worthy of a pass. Rarely awarded and needs ***full*** justification. |

**Written report marksheet**

* *Provide a mark* ***out of 100*** *for each of the following assessment criteria and justify your mark using the boxes provided.*
* *If an acceptable minimum of justification is not provided, the unit coordinator will contact you to request this.*

Student Name:

Assessor:

**Overall Mark** **%**

Abstract and Introduction (10%) /100

Include comments on the presence of an appropriate introduction pitched at the right level & a clear description of the experimental or computational methods and techniques.

Results and discussion (35%) /100

Include comments on the clarity and quality of the results, a critical discussion incorporating the chemistry, physical, structural and biochemical information, a discussion of the results within the context of previous work & the presence of justifiable conclusions.

Reaction (15%) /100

Include comments on the likely success of the route, quality of the reactions chosen and the student’s arguments for the synthetic route taken, the appropriateness of the reagents and price.

Assay methodology and data (15%) /100

Include comments on the assays selected, the extent to which they support a scientific question, and the breadth of data supporting the final compound

Layout (20%) /100

***Include co***m***ments on the quality of the figures and captions, number of typographical and grammatical errors.***

Citations (5%) / 100

Include comments on the quality of the referencing of all of the first three sections above.

**SIGNED………………………………………….. (ASSESSOR)**

**DATE……………………………………..**