

Structure-function relationships, 3D printing and public engagement: developing teaching exercises to integrate core principles and communication skills with a modern technological approach



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Background context

- The UG Pharmacology curriculum at the University of Aberdeen was aligned with the British Pharmacological Society (BPS) core curriculum
- This identified some areas for development:
 - Public engagement
 - Science communication
 - Drug design
 - Structure-activity relationships
 - Big data engagement

- In response to this, an Honours year practical project was designed to deliver these key topics in an integrated manner

Aim

- To create an exercise which integrates less identified strands of pharmacology within the curriculum in Aberdeen
- To emphasise the links between structure and function

The 3D project

- Groups of 3 students research a known drug target
- With a chosen target, groups must research the 3D molecular structure and produce models for 3D printing
- Individuals examine different drugs that influence the chosen target and prepare those files for printing
- Groups design a “new synthetic” for potential development and define the molecular structure and how it relates to the PK and PD of the drugs

Assessment 1:

Lay person justification of target choice:

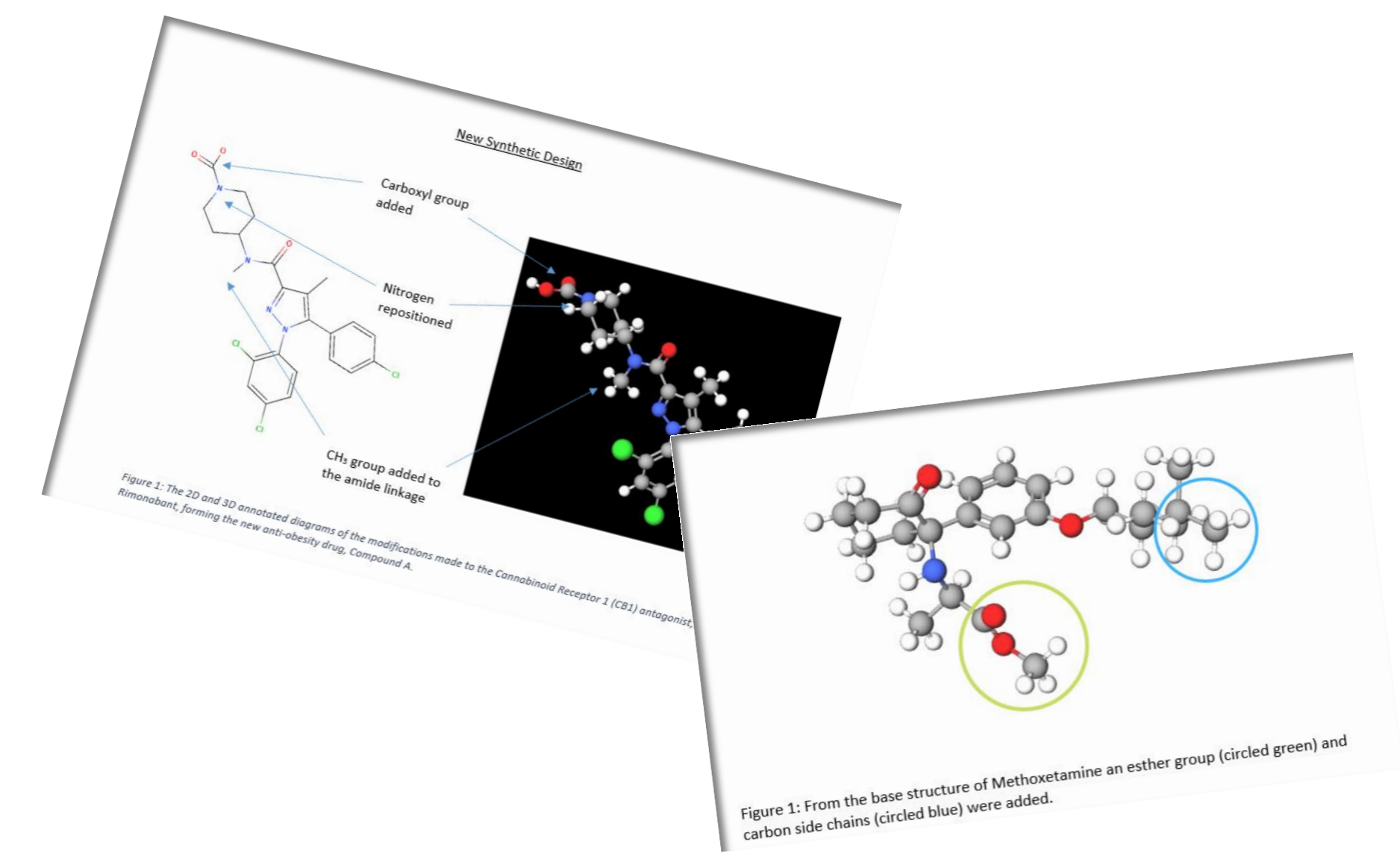
- Individual explanation of target
- Examples of drugs that interact
- Effects of interaction
- Pitched to public audience
- Public information – freedom of design
- Submitted examples:



Assessment 3:

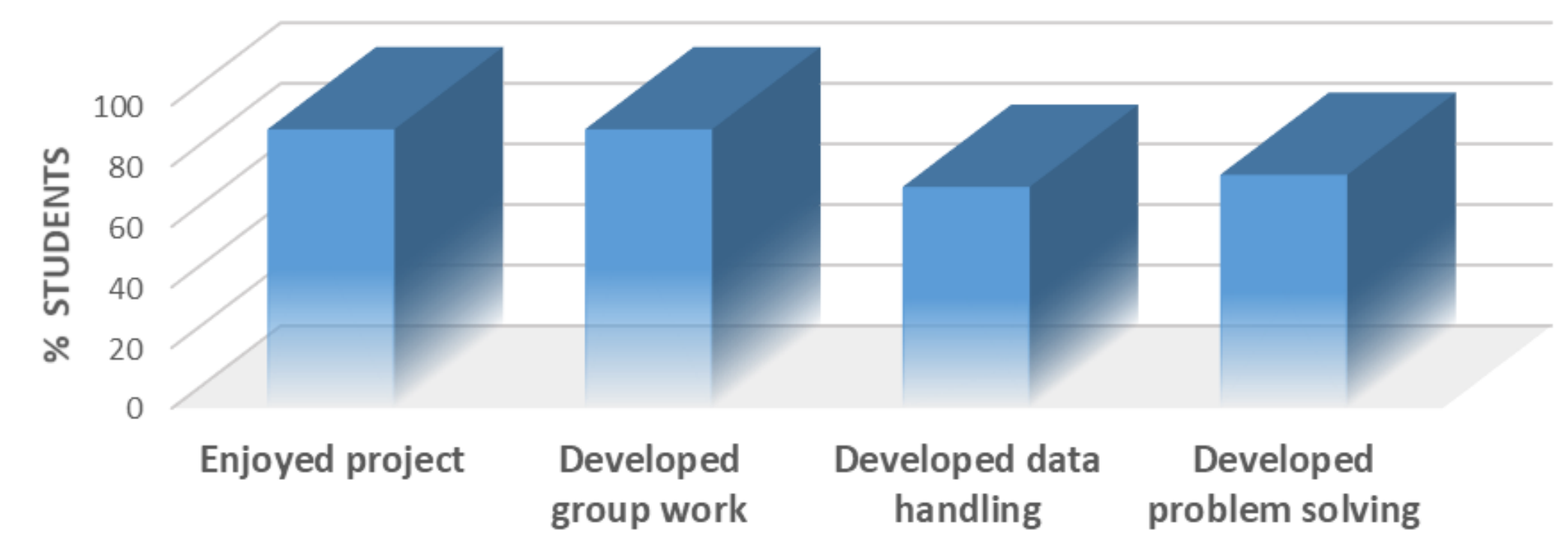
Design of new synthetic drug for target:

- Group design
- Use of 3D molecular software
- Design to be annotated to indicate new structural moieties
- 300 word narrative explaining the new PK and PD profile
- Example new synthetics:

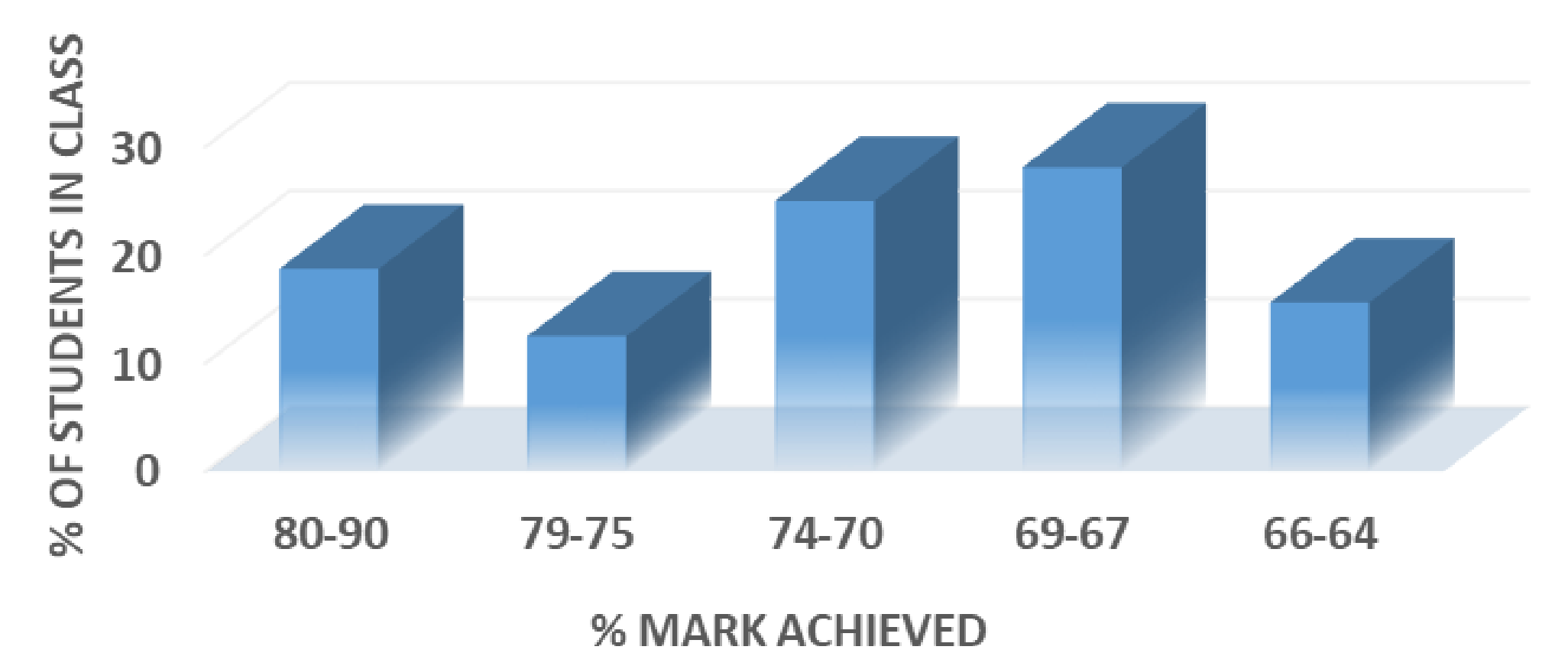


Evaluation

% OF CLASS RATING 4 OR 5



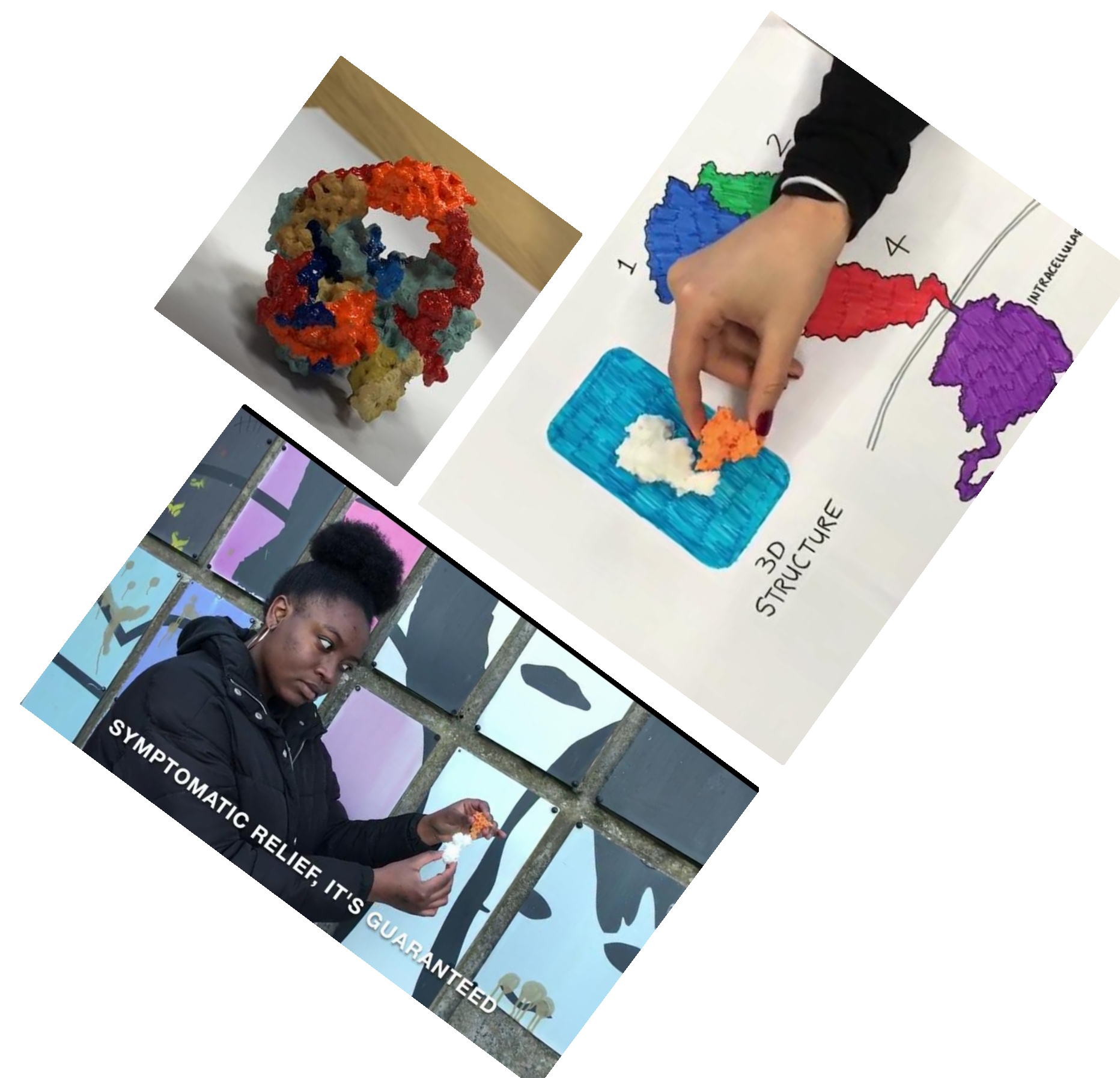
GRADE DISTRIBUTION



Assessment 2:

Lay person public information video:

- Group video
- Use of 3D models
- Pitched to public audience
- 4 min maximum
- Staff and peer marked
- Video screenshots:



- “enjoyed combination of group and individual exercises, and the variety of assessments”
- “fun and informative”
- “made me think about how to approach explaining complex concepts to the public”
- “unique and enjoyable experience”
- “good experience of 3D molecular interactions and drug design”

Outcomes

- Structure-function relationship emphasis
- Visual, tangible and interactive approach
- Focus on public engagement and produces materials for outreach
- Applicable to all areas of medical science

UNIVERSITY OF ABERDEEN
PA4302
Molecular Toxicology
Practical 3D Modelling and Drug Design Project
Dr S Tucker