Assessment of your knowledge

(a) Answer the following questions to assess your command on terminology, facts, concepts, and theories learned in this chapter:

1. What is the difference between hypothesis led and high throughput materials discovery?
2. What experimental circumstances are best suited to high throughput screening approaches?
3. What are the key requirements of a supporting substrate and its coating for high throughput materials discovery platforms?
4. Which material properties need to be considered when developing a new biomaterial?
5. What key consideration must be made when developing a library of materials where a single property is intended to be varied systematically?
6. What is synergy in a materials discovery context and why is it important to consider?
7. How many experiments would be necessary if assessing five different experimental parameters using a Design of Experiments approach?
8. What makes a biological assay compatible with a high throughput screening experiment?
9. What are the four main steps in generating a QSPR model?
10. What are the most important factors that determine the robustness and predictivity of QSPR models?
11. Why is feature selection so important in QSPR models?
12. How are QSPR models assessed for their ability to predict new data?
13. What determines how reliably strong QSPR models can predict the properties of very large libraries of virtual materials?
14. What are the disadvantages of using experimentally determined descriptors, such as ToF-SIMS ion peaks, as descriptors in QSPR models?
15. Why are evolutionary methods needed in biomaterials discovery?
16. What is the difference between a black box and a white box model?
17. Give an example of a black box model and a white box model.
18. What are the three main model components of a white box model?
19. What are the advantages of white box modeling for biomaterials discovery?
20. Which checks are typically done to check the model implementation before starting to simulate "what if" scenarios?

(b) Answer the following questions to assess your ability to apply the concepts and theories learned in this chapter in real life, clinical, and scientific situations:

1. What are the biggest obstacles to the rationale design of biomaterials?
2. Describe the different approaches to developing a materials library and their advantages and disadvantages for biomaterials discovery.
3. Why is it possible to reduce the number of experiments required by applying a Design of Experiments approach?
4. Think about a system with four experimental parameters, which combinations of experimental conditions should be selected in order to create a balanced design for a Design of Experiments approach using a partial factorial design with $P = 1$?
5. Using Fig. 9.10, describe what different biological assays might be used at different stages of a materials discovery project.
6. Why are computational methods useful in biomaterials discovery?
7. Describe why machine learning models are more efficient than hard coded rules-based models.
8. Considering a library of materials, for example, a collection of 100 different polyacrylates that each had different chemical pendant groups, design an experiment to apply evolutionary methods to biomaterials discovery.
9. Give two examples of white box models and their findings in the field of biomaterials discovery.
10. If given unlimited resources, describe what the ultimate biomaterials discovery project would look like.