Fundamentals of Biochemistry 6th edition Heilman Solutions Manual

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Chapter 1: Bioinformatics Exercise 1.1

The Periodic Table of the Elements and Domains of Life

Exercise Objectives

- Retrieve specific chemical information using online periodic tables.
- Identify the elements essential to biology.
- Distinguish the three domains of life.

Difficulty

- 9 questions
- Computer-Related: Easy
- Subject-Related: Easy

Resources & Websites

- Figure 1.9, Chapter 1
- Ptable:
  - http://www.ptable.com
- Web Elements:
  - http://webelements.com
- Periodic Videos:
  - http://www.periodicvideos.com
- Google Scholar:
  - http://scholar.google.com
- Related Scientific Article:
  - http://onlinelibrary.wiley.com/doi/10.1111/1462-2920.12249/full

Exercise

The periodic table is perhaps the most recognizable of tables within the field of chemistry. Indeed, the organization of the elements and the related elemental properties provide the framework for the study of chemistry and the molecular underpinnings of biology. As an introductory exercise to the field of cheminformatics, online periodic tables will be reviewed and explored for elemental information relevant to biochemistry. The focus of this exercise is the dynamic periodic table provided at http://ptable.com, which uses a straightforward graphical interface that collates elemental information obtained from several online sources. For instance, Ptable.com includes embedded links to http://webelements.com and http://periodicvideos.com, which are popular online tools that provide additional information and videos, respectively. The questions below demonstrate the use of various online tools to explore some of the foundations of biochemistry: the elements required for biology and the three domains of life.

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Chapter 1: Bioinformatics Exercise 1.1

Instructions

1. Go to http://ptable.com.
2. Use the dynamic periodic table to navigate to specific elements.
3. Use the "Database" or first tab (upper left corner of the window) to select the type and source of information; the first tab should be labeled "Wikipedia" as the default).
4. Use the "Properties" tab to explore each element. To choose a property, select the desired radio button. In some cases, controls at the upper right provide more options.
5. Use the "Orbitals" tab to explore the oxidation states and electronic configuration of each element.
6. Use the "Compounds" tab to explore specific compounds containing the highlighted element.

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Chapter 1: Bioinformatics Exercise 1.1

Assessment Questions

1. Using the table and the Wikipedia database, which of the following elements is not listed as "other non-metals"?

    A. Carbon
    B. Phosphorous
    C. Selenium
    D. Boron

Answer: D
Feedback: Boron is categorized as a metalloid in this table.

2. Among the "other non-metals," which element is present in certain amino acids and is required in the elemental and mineral form by plants and animals?

    A. Phosphorus
    B. Selenium
    C. Nitrogen
    D. Boron

Answer: B
Feedback: According to the Wikipedia-based links, selenium is the only element on this list that is chemically incorporated into the structure of certain amino acids and is a nutrient in the mineral and elemental form.

3. Which of the following elements are not utilized in specific biological processes?

    I. Nickel
    II. Molybdenum
    III. Rhodium
    IV. Tungsten
    V. Chromium
    VI. Silicon
    VII. Scandium

    A. I–VII
    B. III and VII
    C. I, II, IV, V, and VI
    D. II, III, and VII

Answer: B

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Feedback: According to the WebElements-based links, all of the listed metals except rhodium and scandium have known roles in biology.

4. A sample of pure carbon would be in what state at 3823 K?

    A. gas
    B. liquid
    C. solid
    D. plasma

Answer: B
Feedback: When using the "state at…" tool on the Properties tab and the corresponding slider, a sample of pure carbon would be a liquid at 3823 K.

5. What are the most common oxidation states for iron and what are the corresponding electronic configurations?

    A. Oxidation states of +2 and +3, which are $[Ar]3d^6$ and $[Ar]3d^5$, respectively.
    B. Oxidation states of –2 and –3, which are $[Ar]3d^6$ and $[Ar]3d^5$, respectively.
    C. Oxidation states of +2 and +3, which are $[Ar]4s^23d^4$ and $[Ar]4s^23d^3$, respectively.
    D. Oxidation states of –2 and –3, which are $[Ar]4s^23d^4$ and $[Ar]4s^23d^3$, respectively.

Answer: A
Feedback: The oxidation states of "2,3" are listed below Fe in the table. Since these oxidation states represent the loss of electrons, the overall charge of the element is positive, or +2 and +3. Further, electrons are lost from the outermost orbital first, which for iron is the 4s orbital. Hence, the electronic configurations are $[Ar]3d^6$ and $[Ar]3d^5$.

6. According to the textbook, which of the following oxidation states of iron is also relevant in biological processes?

    A. Fe^{+1}
    B. Fe^{+4}
    C. Fe^{+5}
    D. Fe^{+6}

Answer: B
Feedback: Fe(IV) is used in many biological processes.

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7. Which of the following is the most abundant isotope of Mo?

    A. ^{100}Mo
    B. ^{92}Mo
    C. ^{95}Mo
    D. ^{98}Mo

Answer: D
Feedback: ^{98}Mo is the most abundant isotope of Mo.

8. As described in the abstract for the scientific article published by A. Pol *et al.* in *Environmental Microbiology* (http://onlinelibrary.wiley.com/doi/10.1111/1462-2920.12249/full), what type of element is incorporated into the structure of the protein known as methanol dehydrogenase?

    A. an actinide
    B. a lanthanide

Answer: B
Feedback: This article describes the incorporation of rare earth elements, such as cerium, in the protein; rare earth elements are lanthanides.

9. The microorganism described by A. Pol *et al.* in *Environmental Microbiology* (volume 16, pages 255–264; http://onlinelibrary.wiley.com/doi/10.1111/1462-2920.12249/full) is a member of which domain of life?

    A. Bacteria
    B. Archaea
    C. Eukarya

Answer: A
Feedback: This article describes *Methylacidiphilum fumariolicum* SolV as a bacterium.

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Organic Functional Groups and the Three-Dimensional Structure of Vitamin C

Exercise Objectives

- Visualize organic molecules using cheminformatics freeware.
- Identify organic functional groups.
- Review hybridization and its impact on three-dimensional structure.

Difficulty

- 10 questions
- Computer-Related: Moderate
- Subject-Related: Easy

Resources & Websites

- ChemAxon:
  - https://www.chemaxon.com
- Marvin from ChemAxon:
  - https://chemaxon.com/products/marvin
- Installation Instructions:
  - https://docs.chemaxon.com/display/docs/marvin_installation-and-upgrade.md

Exercise

In this exercise, vitamin C will be visualized and analyzed using Marvin, which is a free, open-source software developed by ChemAxon for chemical education and research. The aim of this exercise is to successfully download, install, and use the package of Marvin applications including MarvinSketch and MarvinView. In this exercise, the subject is Vitamin C, which is an organic molecule used as a cofactor for several cellular processes. Vitamin C is defined as a biological metabolite due its low molecular weight; in contrast, the major biomolecules (e.g., proteins, nucleic acids, carbohydrates, and lipids) have higher molecular weights and tend to associate with other biomolecules involved in cell structure and metabolism. Organic metabolites are often acquired through dietary intake (e.g., vitamins and essential nutrients) and are typically modified by biosynthetic pathways in the cell. To better understand the biochemistry of metabolites, such as vitamin C, researchers often study their molecular structures and three-dimensional properties using cheminformatics tools.

Instructions

The following instructions are for **MarvinSketch 20.3**.

Download MarvinSuite

1. Go to https://www.chemaxon.com/.

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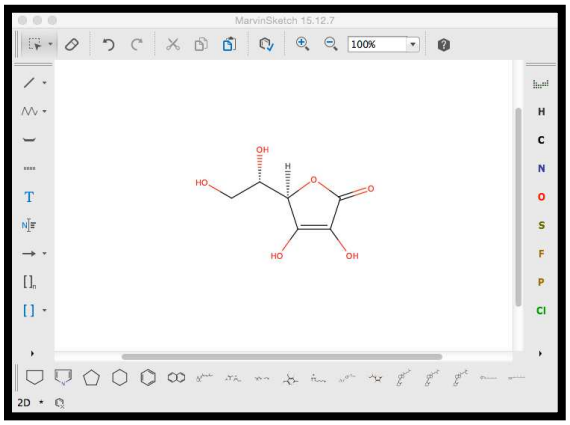
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2. Go to the "Profile" menu.
3. Create a free account using your campus email address (or any other email address).
4. Log into your new account on the home page.
5. Go to the "Downloads" area and then scroll down to Standalone Application called "Marvin."
6. Click on "Download."
7. The ensuing page will be titled "Download Marvin."
8. Click on the link that indicates the "DOWNLOAD LATEST…," which should provide the application for your OS system (*i.e.*, PC or Mac)
9. Follow all prompts to allow and install the download.
10. Alternatively, go to the Downloads folder and open the respective installation file (for example, ".exe" for PC, and ".dmg" for Mac).

Visualize the two-dimensional structure of vitamin C

1. Open MarvinSketch. A new work window appears automatically.
2. Go to the Insert menu and click on the Template submenu.
3. The Template Library Manager window will now open.
4. Scroll down to "Vitamins" in the left window of the Template Library Manager.
5. Click on "Vitamins."
6. Scroll down to "Vitamin C" in the right window of the Template Library Manager.
7. Click on "Vitamin C."
8. Click on "Close."
9. The structure of vitamin C is visible in the MarvinSketch work window, and the structure is linked to the movement of the mouse (**Figure 1**).
10. Click the mouse after centering the structure in the work window.
11. This series of actions adds the structure of vitamin C to the work window.
12. Now press "Esc" on the keyboard to resume all normal functions of the mouse.

Figure 1



13. If you wish to ***enlarge the structure***, click and drag the mouse across the molecule; this action should highlight all atoms of the molecule; if not, then

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perform the selection process again using a larger selection area. To enlarge the structure, drag one corner of the "selection box" until a suitable size is obtained. Press "Esc" to deselect the structure and to resume all normal functions of the mouse.

14. If you wish to ***move the structure***, repeat the selection process, click within the center of the "selection box" (a centering box should appear), and drag the structure to the desired location. Press "Esc" to deselect the structure and to resume all normal functions of the mouse.

Analyze vitamin C structure

1. This section must be completed with vitamin C added to the work window, as described above.
2. To obtain the official IUPAC name for vitamin C, go to the "Structure" menu and choose "Generate Name" and "Preferred IUPAC Name."
3. To obtain the molecular weight, go to the "Calculations" menu and choose "Elemental Analysis," which opens the Elemental Analysis Option window.
4. Make sure that the radio buttons for "Mass," "Exact Mass," and "Formula" are all checked.
5. Click "OK."
6. This series of actions opens an Elemental Analysis window.
7. Use the information in this window to answer the questions below.
8. To exit this function, click on "Cancel" in the Elemental Analysis Option window.

Visualize the three-dimensional structure of vitamin C

1. In MarvinSketch, save the vitamin C structure; use the file name "vitaminC.mrv" (file format = ChemAxon Marvin Documents / MRV).
2. Now, open MarvinView. A new work window will appear automatically.
3. Under the File menu in MarvinView, open the vitamin C structure (for example, the open the "vitaminC.mrv" file).
4. Once the file is open is MarvinView, go to the "View" menu and select "Open MarvinSpace."
5. These actions will open a new window, where the three-dimensional structure of vitamin C will be displayed.
6. To rotate the structure, click and drag the mouse as desired.
7. To show the hydrogen atoms, right click on the mouse, select "Draw Type," and choose "Hydrogens".
8. Use the rotation tool to answer the questions below.

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Chapter 1: Bioinformatics Exercise 1.2

Assessment Questions

1. What is the molecular weight of vitamin C to 5 significant figures?

    A. 176.124 g/mol
    B. 176.1 g/mol
    C. 176.12 g/mol
    D. 176.13 g/mol

Answer: C
Rationale: The molecular weight is 176.124 g/mol, which rounds to 176.12 for 5 significant figures.

2. Why do the mass and exact mass of vitamin C differ?

    A. The exact mass does not consider the mass of the electrons.
    B. The exact mass is obtained from theoretical calculations, while the mass is experimentally obtained using an analytical balance.
    C. The exact mass term includes contributions from the stable isotopes of all elements in the molecule, while the mass term considers only the most abundant isotope of each element.
    D. The mass term includes contributions from the stable isotopes of all elements in the molecule, while the exact mass term considers only the most abundant isotope of each element.

Answer: D
Rationale: The measured mass, or mass term, includes all contributions from the stable isotopes of carbon, hydrogen, and oxygen.

3. Which of the following functional groups is not present in vitamin C?

    A. tertiary alcohol
    B. secondary alcohol on an sp^3 hybridized carbon
    C. secondary alcohol on an sp^2 hybridized carbon
    D. primary alcohol

Answer: A
Rationale: Vitamin C has no tertiary alcohols.

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4. According to IUPAC rules, which of the following atoms is a chiral center (note, a furan is an aromatic 5 membered heterocycle)?

    A. Atom 1 of the dihydrofuran ring and carbon 1 of the dihydroxyethyl substituent
    B. Atom 1 of the dihydrofuran ring and carbon 5 of the dihydroxyethyl substituent
    C. Atom 5 of the dihydrofuran ring and carbon 2 of the dihydroxyethyl substituent
    D. Atom 5 of the dihydrofuran ring and carbon 1 of the dihydroxyethyl substituent

Answer: D
Rationale: According to the MarvinSketch tool, the full IUPAC name is (5*R*)-5-[(1*S*)-1,2-dihydroxyethyl]-3,4-dihydroxy-2,5-dihydrofuran-2-one, which indicates that (A) the root structure is furan, (B) atom 2 of the furan ring is the carbonyl carbon, (C) atom 5 of the furan ring is chiral, and (D) carbon 1 of the dihydroxyethyl substituent is chiral.

5. Which of the following functional groups most appropriately describes the type of acyl group in vitamin C?

    A. lactone
    B. lactam
    C. ester
    D. ether

Answer: A
Rationale: Vitamin C contains a cyclic ester, which is most appropriately referred to as a lactone.

6. Which of the following statements best describes the hybridization of vitamin C?

    A. Vitamin C has 3 sp^2 and 3 sp^3 hybridized carbons.
    B. Vitamin C has 3 sp^2 and 2 sp^3 hybridized carbons.
    C. Vitamin C has 2 sp^2 and 4 sp^3 hybridized carbons.
    D. Vitamin C has 2 sp^2 and 3 sp^3 hybridized carbons.

Answer: A
Rationale: Vitamin C contains 3 sp^2 and 3 sp^3 hybridized carbons.

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7. Which of the following statements best describes the modified furan ring of vitamin C?

    A. The chiral center and double bond are conjugated.
    B. The ether group and double bond are conjugated.
    C. The carbonyl group and double bond are conjugated.
    D. The carbonyl group and chiral center are conjugated.

Answer: C
Rationale: The carbonyl group and double bond of vitamin C are conjugated.

8. The modified furan ring in vitamin C is planar.

    A. True
    B. False

Answer: A
Rationale: As visualized in MarvinSpace, the dihydrofuranone of vitamin C is planar.

9. The three-dimensional character of vitamin C is mostly imparted by the _____.

    A. sp^2 hybridized carbons of the dihydrofuranone ring.
    B. chiral sp^3 hybridized carbons of vitamin C.
    C. carbonyl group of vitamin C.
    D. nonchiral sp^3 hybridized carbons of vitamin C.

Answer: B
Rationale: As visualized in MarvinSpace, the three-dimensional aspects of vitamin C are imparted by the chirality of the sp^3 carbons.

10. When an oxidant is present, vitamin C can be converted to a product described as (5*R*)-5-[(1*S*)-1,2-dihydroxyethyl]-3,4-dihydroxy-furan-2,3,4(5H)-trione, which retains the furan-based nomenclature of vitamin C and describes the hydrogen placement

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at atom 5 of the ring. Which of the following statements best describes this vitamin C derivative?

A. Vitamin C is reduced to yield a furan ring with 1 carbonyl group and no double bonds.
B. Vitamin C is oxidized to yield a furan ring with 3 carbonyl groups and no double bonds.
C. Vitamin C is reduced to yield a furan ring with 4 carbonyl groups and no double bonds.
D. Vitamin C is oxidized to yield a furan ring with 3 carbonyl groups and 1 double bond.

Answer: B
Rationale: Oxidation of the enediol component of vitamin C yields a furan ring containing a total of 3 carbonyl groups and no double bonds.

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