COSC 2P03 Advanced Data Structures: Assignment 3

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1 DrugBank and Drug Design

In this assignment, we continue to play with the DrugBank data using heap. You are expected to finish the following tasks.

2 Your Tasks (Total: 8 marks)

You should define classes named `Drug` and `DrugHeap` with the following requirements (feel free to define extra variables, classes, and methods if needed). Please note that, `DrugHeap` is actually a class for min-heap.

1. Define the class `Drug` with data attributes `drugBankID`, (this is used as key), `genericName`, `SMILES`, `url`, `drugGroups`, and `score`. This class has at least one method, named `displayDrug` to print out the information on the screen. You may reuse your code for this class from Assignment 2. **(0.5 mark)**

2. Define a method named `readData` under the `DrugHeap` class to load all the provided information from the given text file to an array variable (named `data` which is an attribute of the class). Note that, you should not use the Brock basic IO package anymore, otherwise, 0.5 mark will be deducted. **(0.5 mark)**

3. Define a method named `trickleDown (int i)` under the `DrugHeap` class to trickle down the `i`-th node in the heap to restore heap-order, where `i` is the index of an object in the array. **(1 mark)**

4. Define a method named `buildHeap` under the `DrugHeap` class to convert the array `data` into a heap. **(1 mark)**

5. Define a method named `removeMin` under the `DrugHeap` class to remove the Drug object with the minimal key. **(1 mark)**

6. Define a recursive method named `inOrderTraverse` under the `DrugHeap` class to perform inorder traversal over the nodes in the heap. In this method, you should write your results into a text file named `dockedApprovedInOrder.tab` where each row contains the information of a drug with same format as the given text file. **(1 mark)**

7. Define a method named `heapSort` under the `DrugHeap` class to sort the Drug objects in array `data`. Note that, you should not save the result in array `data`. Instead, you should save the result in a text file named `dockedApprovedSorted.tab` which has the same format as the given text file. **(2 mark)**

8. In the **main** function, instance (named `dh`) of the `DrugHeap` should be created. The following methods of this instance should be called sequentially:

   (a) `dh.buildHeap()`
   (b) `dh.inOrderTraverse()`
   (c) `db.heapSort()`

   , **(0.5 mark)**

9. Your code should be well commented. **(0.5 mark)**

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3   Submission

- Your source code.

- A PDF printout of your source code.

- Output text files `dockedApprovedInOrder.tab` (from Task 6) and `dockedApprovedSorted.tab` (from Task 7).

- Compress the above files in a zipped folder named `COSC2P03_A3_Firstname_Lastname_StudentNumber.zip` and submit it through Brightspace before indicated due time.

- If any of the above require files are not submitted, 0 mark will be given to the whole assignment.

- Late submissions will not be accepted.

4   Academic Integrity

This assignment should be tackled individually. Outsourcing or teamwork is not allowed. Violation of this requirements will be seriously processed in accordance with university policies.