**Introduction:**

Thank you for choosing to continue the application process at Accendero Software, Inc. The task below is both open ended and relatively straight forward. It is designed to evaluate your abilities on three axes:

1.) Tool-based strategies for interacting with complex pharmaceutical compounds and your personal knowledge of the current pharmaceutical informatic ecosystem.

2.) Communication of complex scientific code to collaborators or other engineering team members.

3.) Ability to work on open ended scientific tasks and return with actionable data and information.

Please note that we are not providing you with a novel pharmaceutical compound or construction during this practical. A google search of the canonical smile provided below will likely provide you most of the information you would need. Because of that, please realize we are not evaluating the *results*, but rather, the code and methodology that you generate to provide the results.

**Task:**

Using commonly available open-source methodologies and packages, characterize the following pharmaceutical compound:

CC1=C(C=C(C=C1)NC(=O)C2=CC=C(C=C2)CN3CCN(CC3)C)NC4=NC=CC(=N4)C5=CN=CC=C5

Please note that we understand that the instruction here is somewhat open-ended. Potential pharmaceutical characterizations could (but are not required to) include:

* Pharmacophore Identification
* PK/PD
* Predicted Stability
* Predicted Functional Targets

**Requirements:**

1.) Upload your code to git or a similar online VCS solution and add [ahoneycutt@accendero.com,](mailto:ahoneycutt@accendero.com) [ashiromani@accendero.com](mailto:ashiromani@accendero.com), [arastogi@accendero.com](mailto:arastogi@accendero.com), and [lbbateman@accendero.com](mailto:lbbateman@accendero.com) as reviewers and/or contributors so your code can be evaluated.

You should utilize at least one of Python or R.

2.) ***COMMENT YOUR CODE.*** If we do not know what it is doing, we cannot evaluate what you are attempting to accomplish.

3.) Provide a readme.md for running your code locally, as well as a list of all pertinent requirements for running any packages or tools that you use to characterize the molecule.

Code being difficult to run does not necessarily disqualify your submission, but it will be evaluated beneath those that provide clear instructions sufficient for an engineer to run your submission locally.

**Pluses:**

1.) Demonstrable knowledge of unit or integration test cases present in your code.

2.) Complex mathematical or biostatistics calculations outside of those run specifically by included packages.

3.) Utilization of **both** Python and R.

**Submitting Your Work and Final Steps:**

Please note that this is a limited task, it is not meant to be an exhaustive study of a compound. Submissions should demonstrate reasonable knowledge of packages, project initialization, and basic characterization techniques. It is not expected to be of publishable quality. This is about showing the team here your knowledge and ability, not crossing off an enormous imaginary checklist.

After you have completed your work, please e-mail [mbarber@accendero.com](mailto:mbarber@accendero.com) so that the review process can begin. We would like to have all submissions no later than October 17th, 2022 so that finalists can be contacted by October 19th. 2022.

We will select 2-3 finalists for final interviews the week of October 17th and October 24th and expect to make an offer no later than October 28th. In the case your submission is not selected to move to the final round, you will be contacted the week of final interviews with an evaluation and a note explaining the choice to not move forward with your application.

Please contact [mbarber@accendero.com](mailto:mbarber@accendero.com) with any questions.