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| **Date** | **Task** | **Remark** |
| June 8th | Installed Schrodinger on Windows machine. Just invoke the license.  Waiting for the new licencese file fie for Schrdoinger. Will get it running today  30 mis to 1 hrs job.  -----------------------------------------------  The rest time will be also used to modelling the Sirt3/AADPr product complex with an open loop conformation in Prime. This task includes side chain prediction, model refinement using Prime and model validation. The protocol employed by Ping would be followed for consistency purpose. | In the interest of saving time we are using the windows machine as the license server until the problem with slave003 is resolved.  Will discuss in detail with you later the advantage of having the Windows machine as the server and using the gpu node as the client machines in a separate email communication after the paper work gets completed. |
| 9th -10th June | Modelling the Sirt3/AADPr product complex with an open loop conformation in Prime. This task includes side chain prediction, model refinement using Prime and model validation. The protocol employed by Ping would be followed for consistency purpose. |  |
| June 11th  **(WEEKEND)** | Setting up an MD simulation for the modelled system.  I have accommodated this task into a single day schedule (really tight assuming that I will have no issues during structure preparation).Since, I will have prior experience in creating parameters for AADPr, I think it should be easy to replicate here too, because the AADPR is the same. | This includes parametrizing non-standard residues and obtaining QM partial charges followed by minimization and equilibration. |
| June 12th **(WEEKEND)** | Analyzing if the system has equilibrated and then launch the production simulation for the sirt3/AADPr production complex with open loop conformation. | This will be done over the weekend to effectively utilize the weekends for the run time. |
| June 13-16th | Compute MM-PBSA and MM/GBSA binding energies for Sirt3/OAADPr/ deace-peptide complex of the complex with an open loop conformation.  ------------------------------------------------  Compiling a report of the MD work, in particular updating the MM/PBSA table, generating MD based B fac plots, and generating time vs energy plots as done for other Sirt3/INT/NAM complexes contained in the manuscript | A detailed list of miscellaneous task is listed at the end of the document |
| June 17th | Completion of other works related to manuscript draft will be undertaken. It includes writing up the method section ( It has not been touched upon till date)   1. Adding references for the supplementary method section. 2. Any other pending work related to manuscript like image editing, formatting reference style etc if any 3. Creating ligand interaction plots | A detailed list of miscellaneous task is listed at the end of the document |
| June 21 and 22nd | Reserve day, to complete any task if behind schedule. | Some of the miscellaneous tasks will be undertaken when the MD simulation is running. |

**Miscellaneous task list**

The following are the tasks for the paper.

Fig ------Simulated B factor values for Sirt3/OAADPRr complexes modeled based on native closed conformation (4BVH) and an open loop conformation as see in apo enzyme (3GLS).

Per-residue RMSD values for the cofactor binding loop region calculated with respect to

MD averaged structure of Sirt3/OADPr complex modeled based on an open and closed loop conformation.

Fig Ligand interaction diagrams for the product interacting with open and closed loop conformation and for Sirt3/INT/NAM complex

Table …..MM/GBSA and MM/PBSA conformational energies and binding affinity calculation based on the new simulation results

Time series plot of MM/GBSA and MM/PBSA energies for Sirt3/OAADPr with open and closed loop conformation.

Creating probability density distribution plots based on the energies of each frame in the MD simulation.

SI Fig ------: Plot showing crystallographic B-factor values of the Cα atoms belonging to the co-factor binding loop region of Sirt2 in different states.

Method for Ligand/NAM placement needs to be worked out for the supplementary section

MD simulation method in particular treatment of non-standard residues has to worked out

Working with Alok and Guan in editing the graphic image files.