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| **Date** | **Task** | **Remark** |
| June 20th | Setting up and calculating MM/GBSA scores from the **1ns** trajectory   1. **Sirt3/INT/NAM - 4FVT rec/loop** 2. **Sirt3/INT/NAM - 4FVT recp/4BVG loop** 3. **Sirt3/2’-OAADPr- 4BVH rec/ loop** 4. **Sirt3/2’-OAADPr- 4BVH recp/3GLS loop** 5. **Sirt3/2’-OAADPr/Ac-cs2 deac-4FVT rec/loop** 6. **Sirt3/2’-OAADPr/ Ac-cs2 deac -4FVT rec/4BVG loop** | **STATUS:**  **Trajectories are available for systems**  **A to E**, but for **system F only modelling has been complete.**  **NB: MM/GBSA and MM/PBSA scores for**  **systems A-E will be complete by the end of the day** (both 1ns and Equilibration) |
| June 21st | Setting up Equilibration and 1ns MD simulation for **system F**  Sirt3/AADPr/2’-OAADPr/ Ac-cs2 deac -4FVT rec/4BVG loop  Computing MM/GBSA values from the equilibration and 1 ns simulation trajectory in the evening | Send out a complete 1ns and equilibration data results to Dr.Raj to decide which systems to be subjected for an 12 ns simulation |
| June 22nd | Launching a 12 ns MD simulation of the systems decided by Dr.Raj ( **30 mins work, just need to extend the simulation setup**)  The rest of the day will be used for carrying out the Miscellaneous task listed at the end | 12 ns MD simulation will be running in the background |
| June 23rd | Miscellaneous task items 1,2  ( needs to write a Perl script ) | A 12 ns MD simulation will be running in the background |
| June 24-26 th | Miscellaneous task items  3,8 and 10  Mostly methodology write-up work | MD simulation will be running |
| June 25th  **(WEEKEND)** | Compute MM-PBSA and MM/GBSA binding energies from the 12ns MD trajectories on the system that will be decided | MD simulations will be completed on Friday (24th June). |
| June 27th | Miscellaneous task items  4 -9 |  |
| June 28th | Miscellaneous task items  4-9  Continued .. |  |
| June 29-30 th | Work on side chain validation data  Presenting the data  Miscellaneous task 12 |  |

**The following are the tasks for the paper based on the priority and the time of availability of the data.**

1. Creating probability density distribution plots based on the energies of each frame in the MD simulation. (Perl script needs to be written). Sirt3/INT/NAM complex data available. Sirt3/AADPr product complex data will be computed upon completion of the MD simulation.
2. Ligand interaction diagrams for Sirt3/INT/NAM complex (data available) the other system (Sirt3/AADPr closed and open product complex data not available).
3. Incorporating the references for the computational section and a draft of the methodology has to be written (Will be adapted from the previous PLOS one paper).
4. Fig ------Simulated B factor values for Sirt3/OADPr product complex modeled based on native and closed conformation (4BVH). Note Sirt3/INT/NAM Bfac data already completed.
5. Fig ------ Per-residue RMSD values for the cofactor binding loop region calculated with respect to MD averaged structure of Sirt3/OADPr complex based on open/closed loop conformation. Note Sirt3/INT/NAM rmsd plot already completed.
6. Revise the Table …..MM/GBSA and MM/PBSA conformational energies and binding affinity calculation based on the new simulation results (Sirt3/OADPr closed loop). Also revise the earlier MM/GBSA and MM/PBSA table prepared for Sirt3/INT/NAM as suggested by Dr.Raj because NAM data shows insufficient sampling leading to convergence issue.
7. Time series plot of MM/GBSA and MM/PBSA energies for Sirt3/OAADPr closed/open loop conformation. Also revise the old plot (Sirt3/INT/NAM) with 2 or 3 traces as suggested by Dr.Raj (I guess we can show only 2 traces and not 3 traces).
8. Receptor with INT
9. Receptor with NAM
10. NOT SURE if INT/NAM with receptor can be calculated anyways will give it a try).
11. Also consider showing a plot form t=0
12. Method for Ligand/NAM placement needs to identified and written for the completeness of supplementary section
13. Identify B factors for any Sir2 simulations available from PL’s data if any to make the plot analogous to that for SIRT3.
14. MD simulation method protocol and particular treatment of non-standard residues has to be written. ( This will be linked to the MD methodology section)
15. Starting structures for simulations (for SI)
16. Identifying all data on side chain validation carried out by Ping and present the data in a format so as to distinguish sampling/energy errors.