

# The Use of Computational Methods for Investigating Potential Off- target Bindings and Their Implications in the Treatment of Spinal Muscular Atrophy

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Xiaolong Qiu

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University of California, San Diego., U.S.A.

Monash University, Caulfield Campus., Australia



# Project Goal

To identify potential off-target bindings and their implications in the treatment of spinal muscular atrophy through computational methods

To investigate these off-targets and their intrinsic ligands through their ligand chemistry and binding activities

# Progress to Date

- Chose sequences selected by PSI-BLAST for further analysis based on their e-values
- Ran selected sequences in SMAP successfully, and compared these sequences with 3BL7\_A, 3BL9\_A, and 3BLA\_A, which are PDB IDs for DcpS
- Ranked the results generated by SMAP according to the p-value and raw score of each pair-wise comparison



# Tentative Plans

- Continue reading literature regarding off-target bindings
- Keep reading research papers about SMAP
- Further analyze the preliminary off-targets list by checking if there are any biological significance present in the selected pair-wise comparisons
- Discuss my project and problems that I might encounter with my UCSD mentors



Sydney Opera House, Sydney, New South Wales



Shrine of Remembrance, Melbourne, Victoria



Albert Park, Melbourne, Victoria



The Esplanade, Cairns, Queensland



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