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Computational and Experimental Study of Neuroglobin and Mutants[1] LAUREN NELSON, Wake Forest University Department of Physics, SAMUEL CHO, Wake Forest University Departments of Physics and Computer Science, DANIEL KIM-SHAPRIO, Wake Forest University Department of Physics

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Neuroglobin (Ngb) is a hexacoordinated heme protein that is closely related to hemoglobin and myoglobin and normally found in the brain and nervous systems. It is involved in cellular oxygen homeostasis and reversibly binds to oxygen with a higher binding affinity than hemoglobin. To protect the brain tissue from hypoxic or ischemic conditions, Ngb increases oxygen availability. We have previously shown that a mutant form of Ngb reduces nitrite to nitric oxide 50x faster than myoglobin and 500x faster than hemoglobin. It also tightly binds to carbon monoxide (CO) with an association rate that is 500x faster than hemoglobin. To analyze the structure of neuroglobin and the characteristics causing these phenomena, we performed 3 sets of 1 microsecond molecular dynamic (MD) simulations of wild-type oxidized and reduced human Ngb and their C46A, C55A, H64L, and H64Q mutants. We also directly compare our MD simulations with time-resolved absorption spectroscopy. These studies will help identify treatments for diseases involving low nitric oxide availability and carbon monoxide poisoning.

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