



# A Drug Optimization Pipeline that Spans Binary to Biology

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**6:00-7:15 pm**

**Main Theater, Building 4000**

***Free and open to the public***

**Abstract:** The blood-brain-barrier (BBB) is a special structure in the body that helps to protect the brain from unwanted toxins and germs. Unfortunately, this barrier can also make it extremely difficult for therapeutics to reach their intended target within brain. This requires the modification of the therapeutic drugs to allow them to cross the BBB and enter the brain where they can reach their target and be effective. Testing which chemical modifications act to improve accessibility of therapeutics to the brain can be a long and expensive process. At LLNL, we are using a drug optimization pipeline that combines several experimental techniques with computational methods, making use of some of the fastest supercomputers in the world. This allows us to speed up the process of optimizing therapeutics to cross the BBB.



Tim Carpenter received his combined Undergraduate/Masters degree in Biochemistry (MBiochem) from the University of Oxford in 2005, and his PhD in Biochemistry from the University of Oxford in 2008. Dr. Carpenter was a postdoctoral researcher at LLNL from 2009-2012. In 2012, he was converted to a Staff Scientist, and in 2017 was appointed Deputy Group Leader in the Biochemical and Biophysical Systems group within the Physical and Life Sciences Directorate at LLNL. He is interested in the modeling and

biomolecular simulation of cellular membranes and membrane proteins. Additionally, he has been working on small molecule permeability studies, to investigate the energetic barriers associated with crossing a lipid bilayer, with a view to developing screening methods to accurately predict blood-brain barrier permeability in drug design.