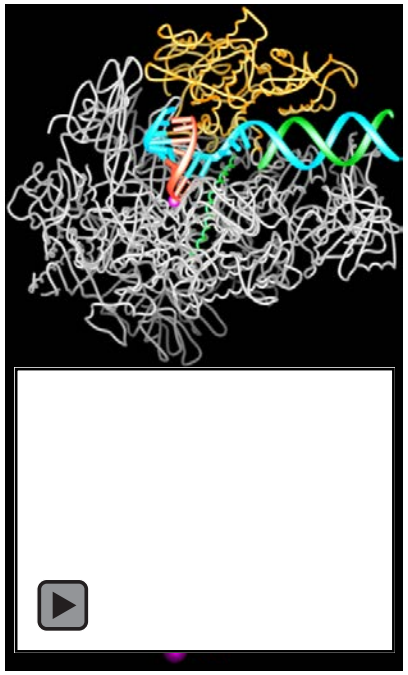
NIH, DOE, & WELLCOME TRUST DRIVE THE HUMAN GENOME PROJECT

Impact of Synchrotron Structural Biology; Enabling Nobel Prize-Winning Research

Membrane Channels

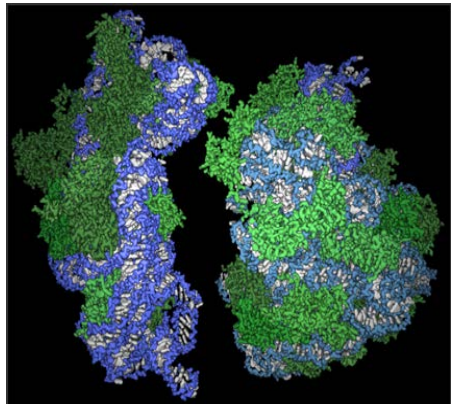
Roderick MacKinnon and Peter Agre – 2003 – K+ channel (KcsA)

Polymerases



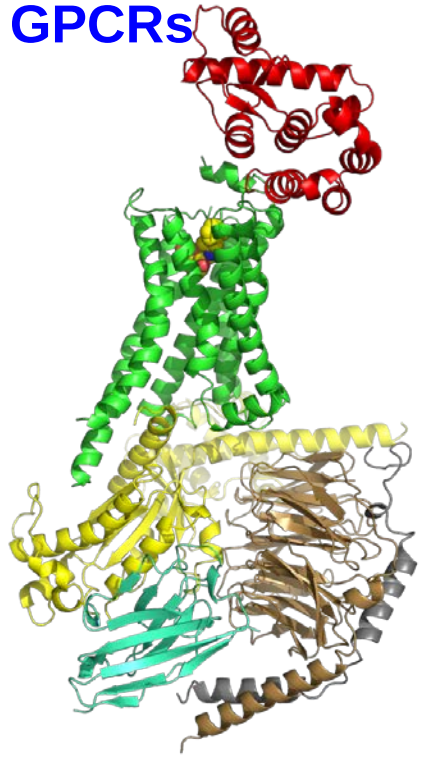
Roger Kornberg – 2006 - RNA Polymerase II

Ribosome



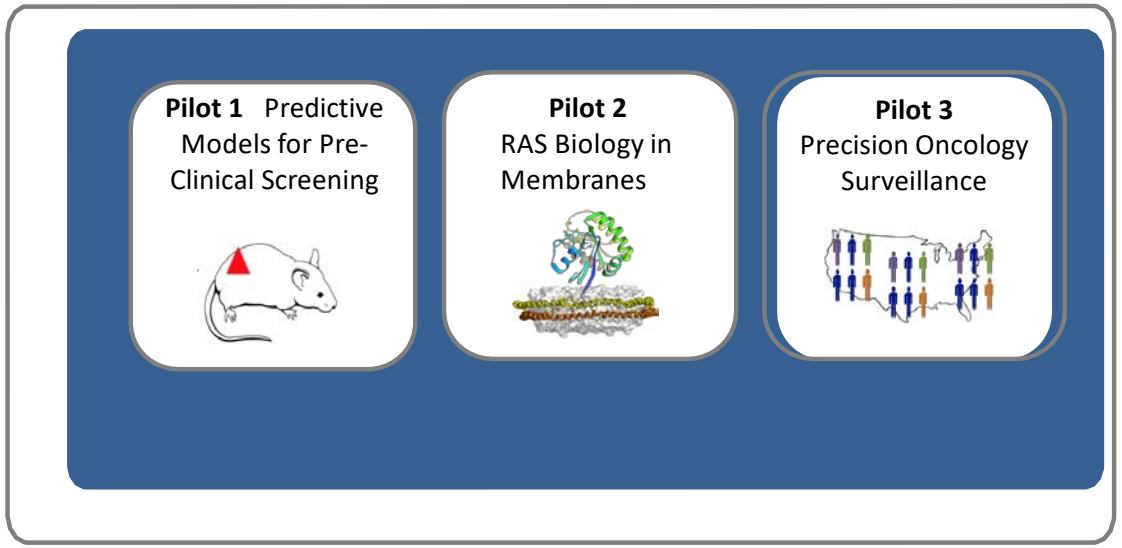
Venki Ramakrishnan, Thomas Steitz and Ada Yonath – 2009 - Ribosome

GPCRs



Brian Kobilka and Robert Lefkowitz – 2012 – β_2AR- beta adrenergic receptor

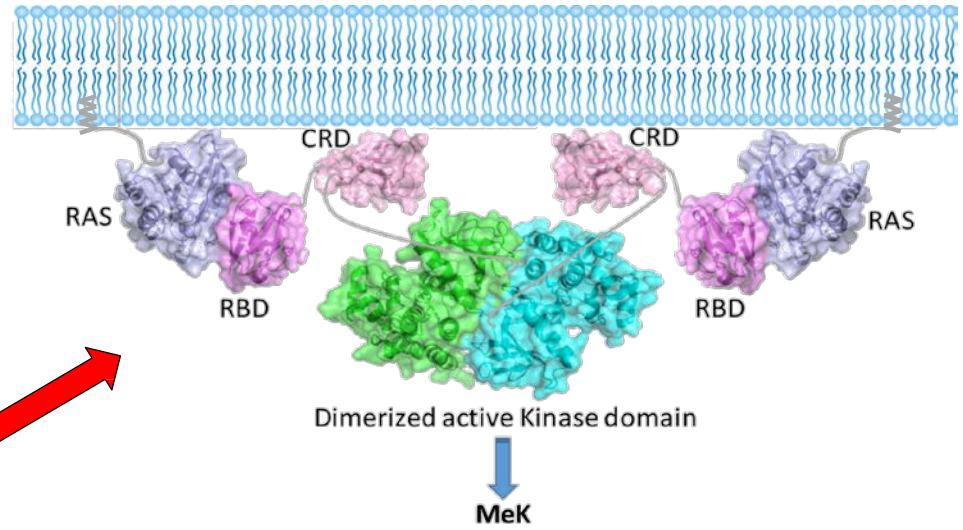
Joint Design of Advanced Computing Solutions for Cancer (DoE + NCI)



PILOT 2: SIMULATING THE BEHAVIOR OF RAS PROTEINS AT THE CELL MEMBRANE

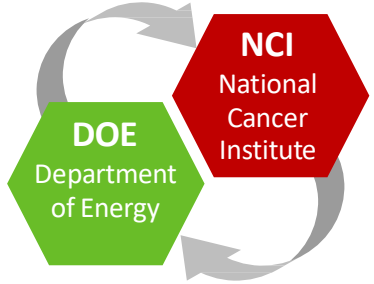
A problem of length and time scale:

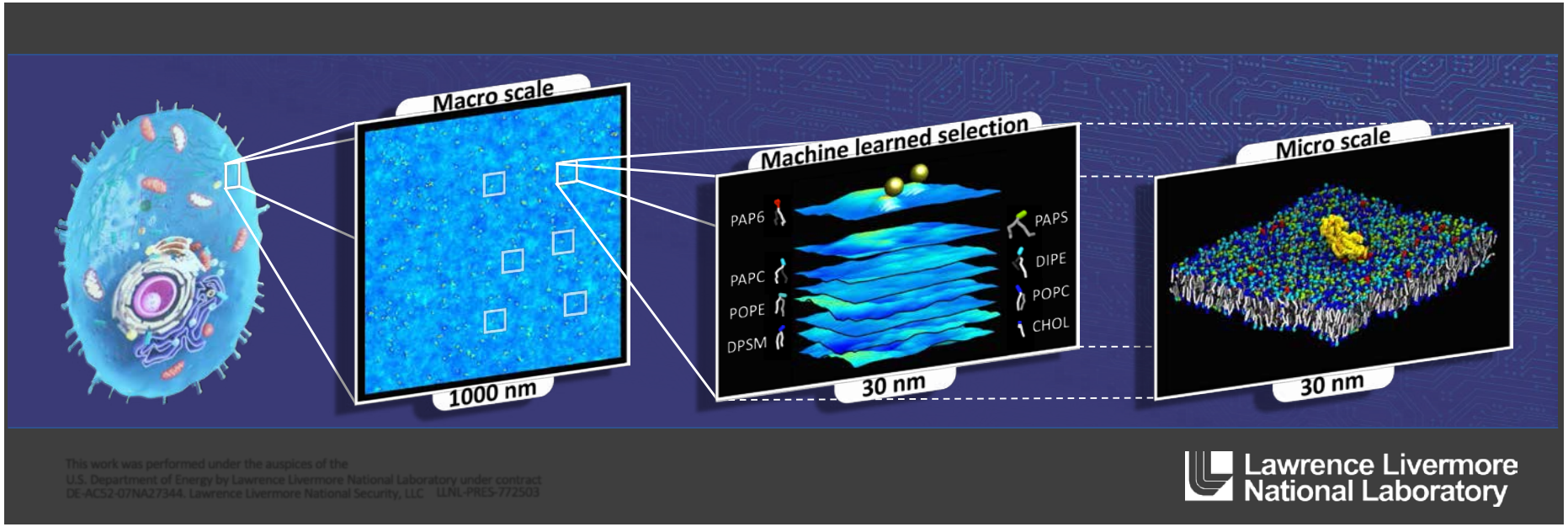
Membrane evolves on milli-second time frame across micro-meters



…while protein interactions occur in micro-seconds across nano-meters

Machine Learning Directed Multiscale Simulations To Explore RAS Biology





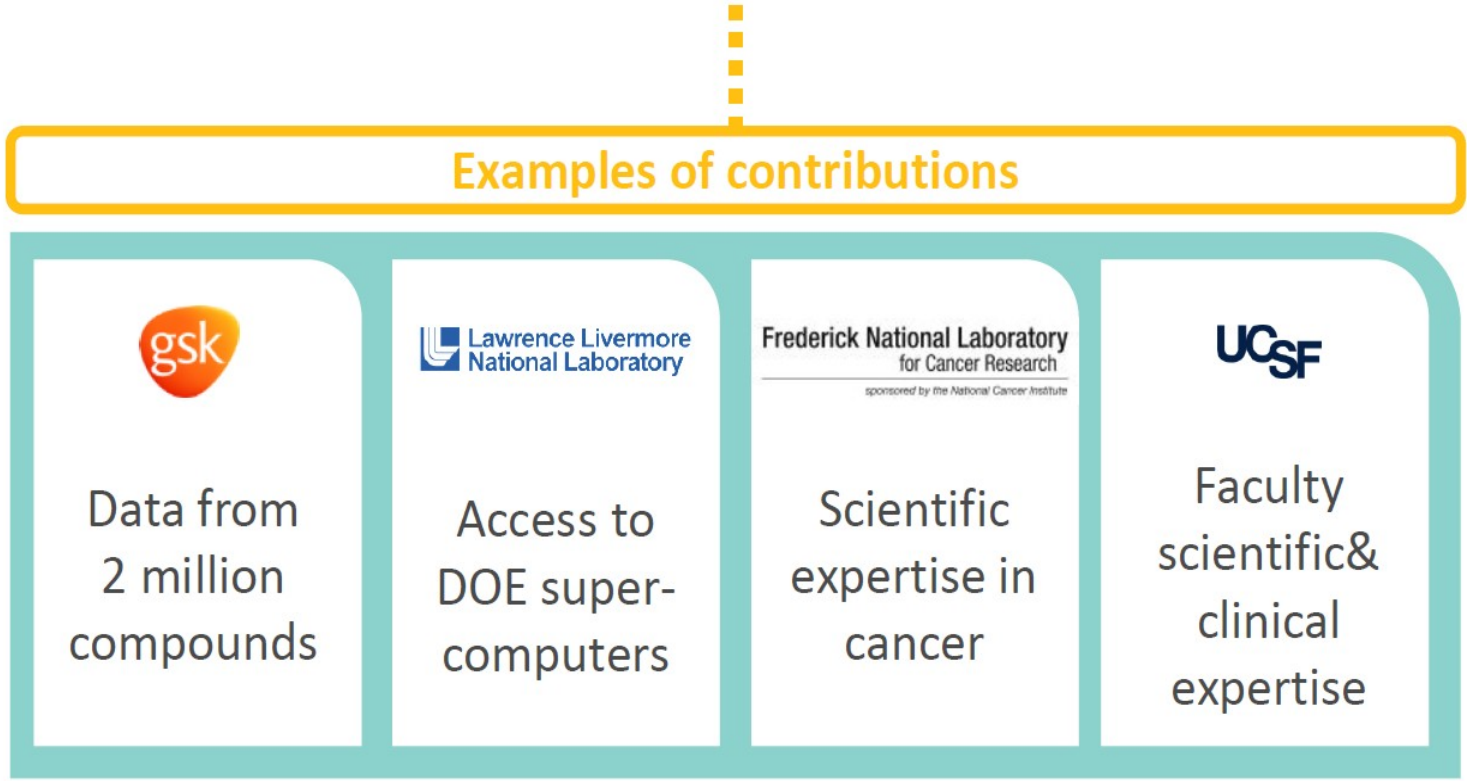
Senior Program Leaders Retreat
National Cancer Institute
January 21, 2020

JDACS4C- Pilot 2 Consortium

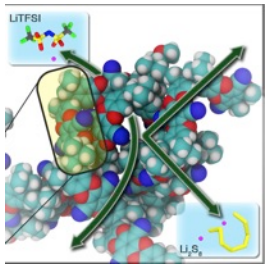
ATOM: Accelerating Therapeutics for Opportunities in Medicine

Highlights:

- Strong public-private partnership
- Builds on both NCI and DOE strengths



Diverse High Impact Science by Users and Staff…



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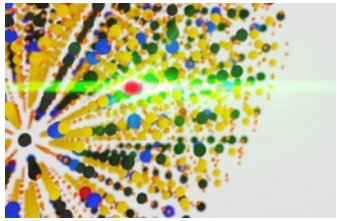
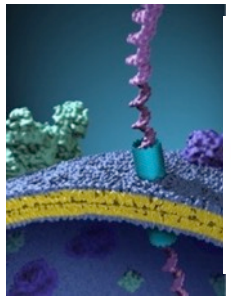
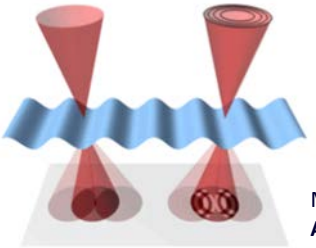


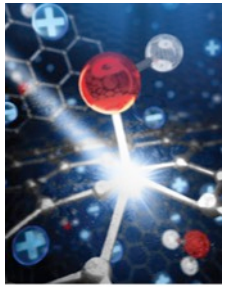
D. J. Gargas, et al. **Nature Nano.** (2014)



J. Geng *et al.,* **Nature** (2014)



C. Ophus, et al**. Nat Commun**. 2016



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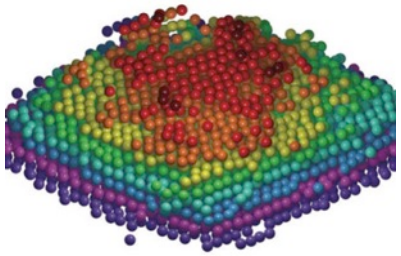

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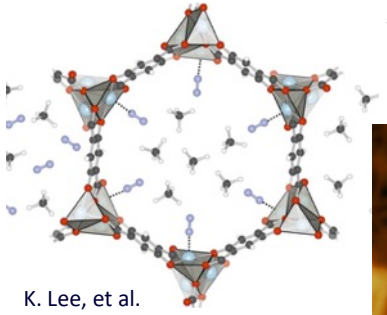
A. Llordés, et al. **Nature** (2013)



K. Lee, et al.
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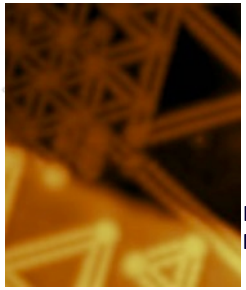

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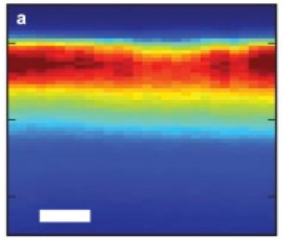

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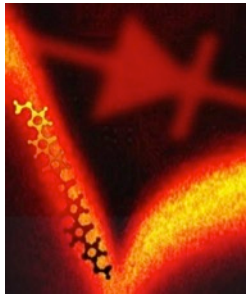

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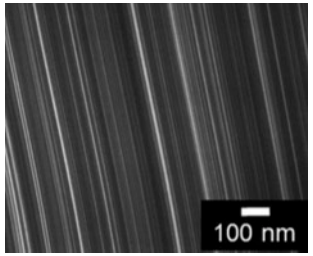

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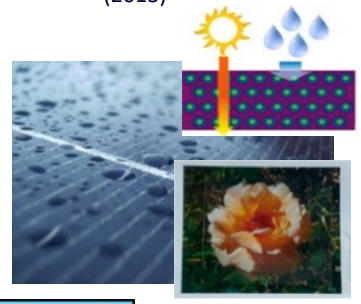

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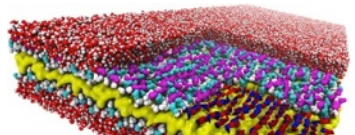

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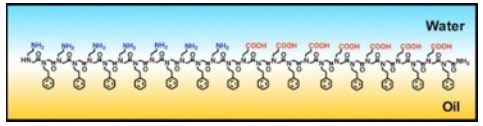

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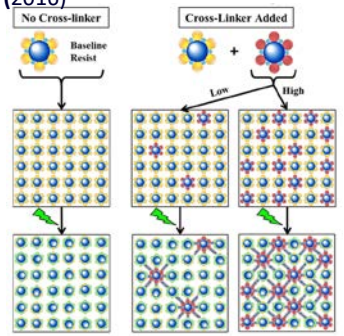

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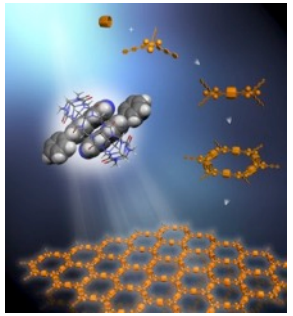

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…at LBL Molecular Foundry