

Multiscale modeling of Complex Bio Systems

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Research Projects

**Chemical and
biological warfare
agents**

***Biofuels* – Deconstruction of nature's
structural material**

***BioSecurity* - Antibiotic Resistance**

**Immune Escape in HIV/AIDS
& Vaccine design**

**Mechanistic modeling of
cell signaling molecules
and events**

Direct Relevance to LANL Missions

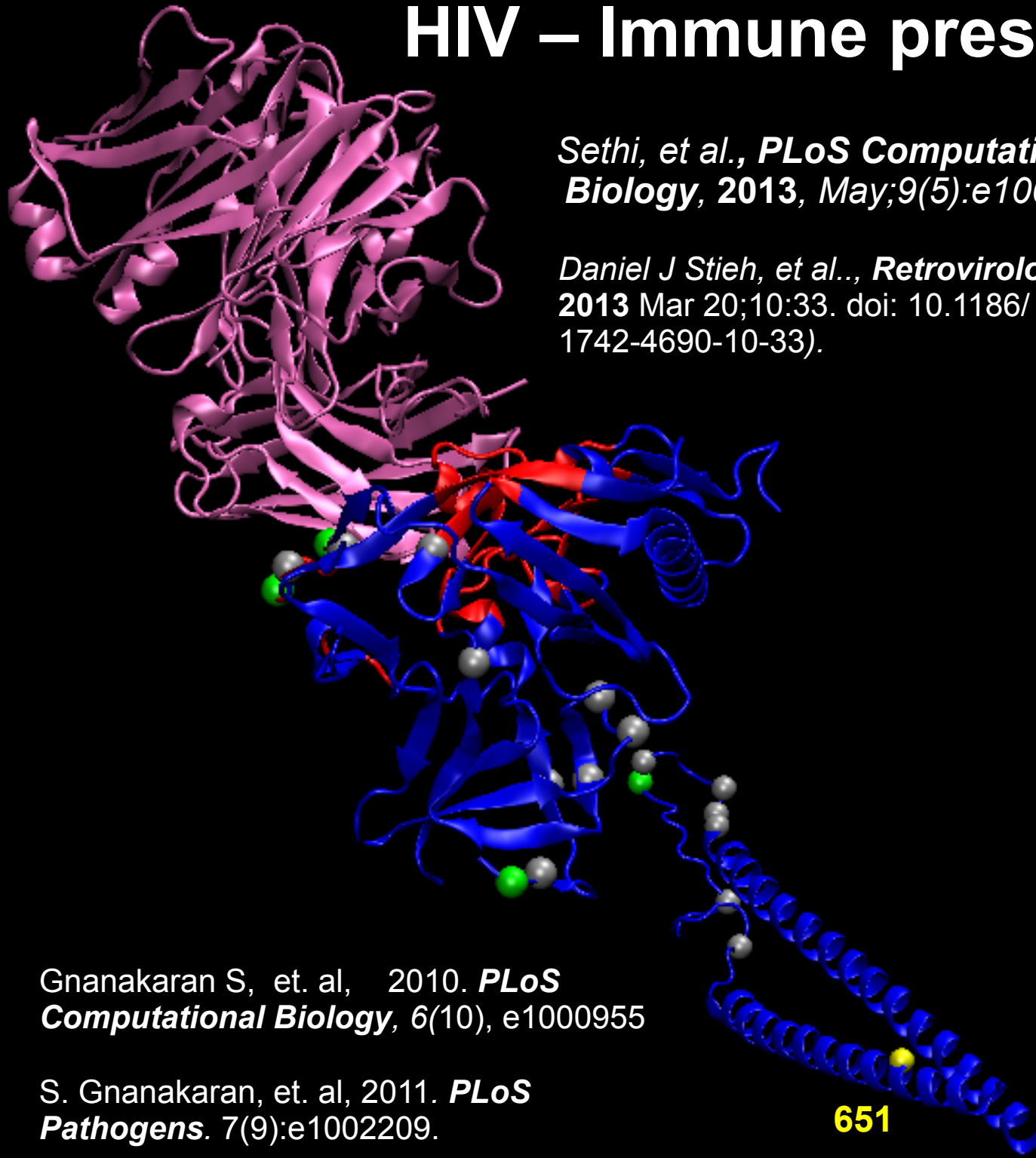
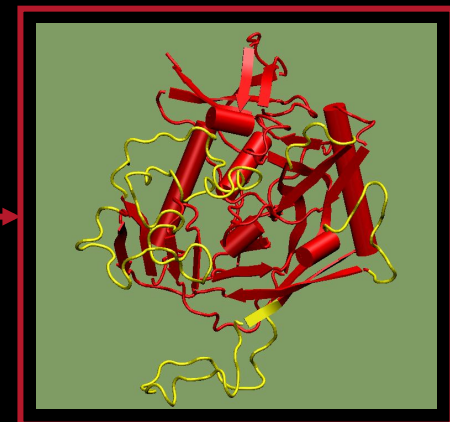
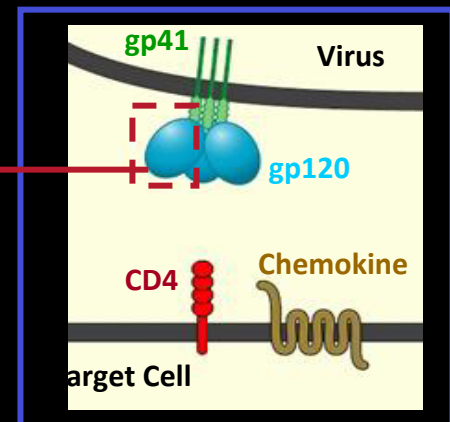
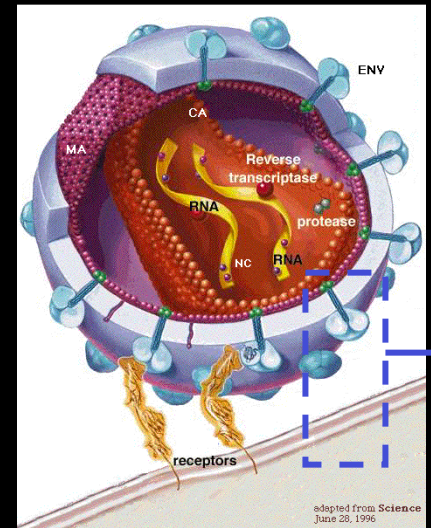
Basic

Applied

HIV – Immune pressure escape

Sethi, et al., *PLoS Computational Biology*, 2013, May;9(5):e1003046.

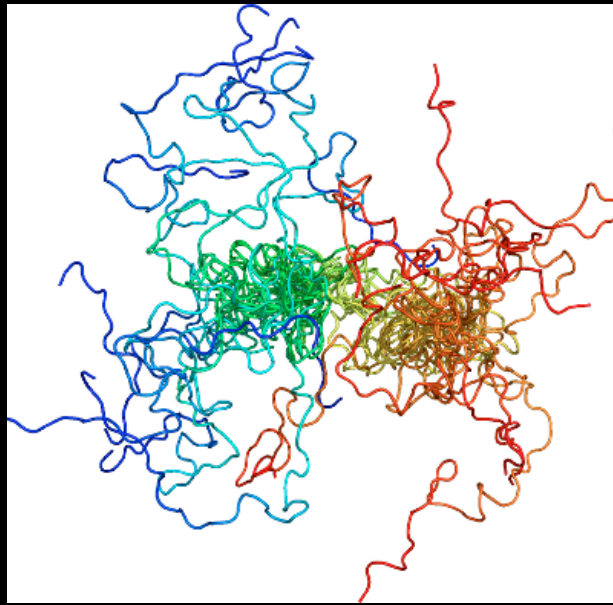
Daniel J Stieh, et al., *Retrovirology*. 2013 Mar 20;10:33. doi: 10.1186/1742-4690-10-33).



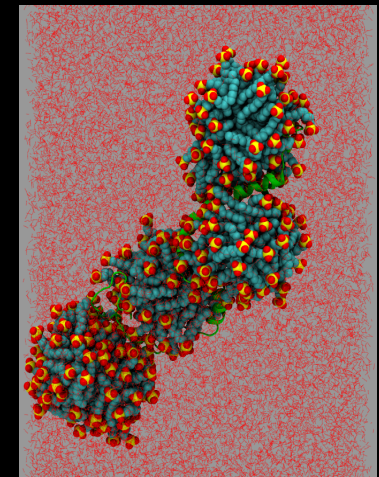
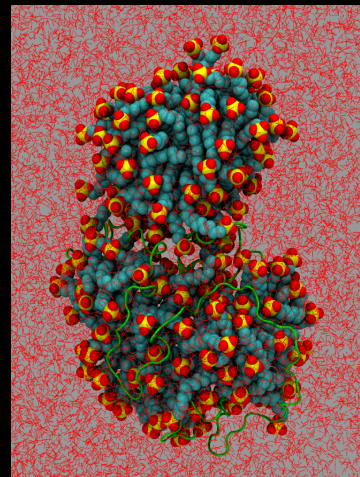
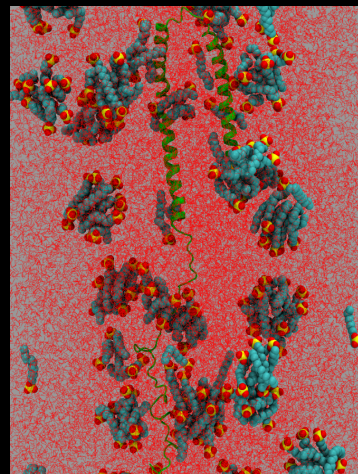
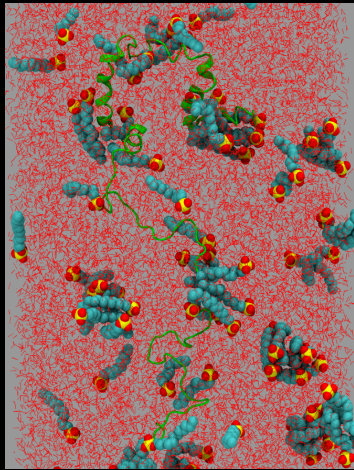
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S. Gnanakaran, et. al, 2011. *PLoS Pathogens*. 7(9):e1002209.

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Intrinsically disordered proteins



A Sethi, J Tian, D Vu, and S Gnanakaran, **Biophys J**, 2012 ; 103:748-57.

Tian J, Sethi A, Anunciado D, Vu DM, Gnanakaran S. J **Phys Chem B**. 2012. 116:4417-24

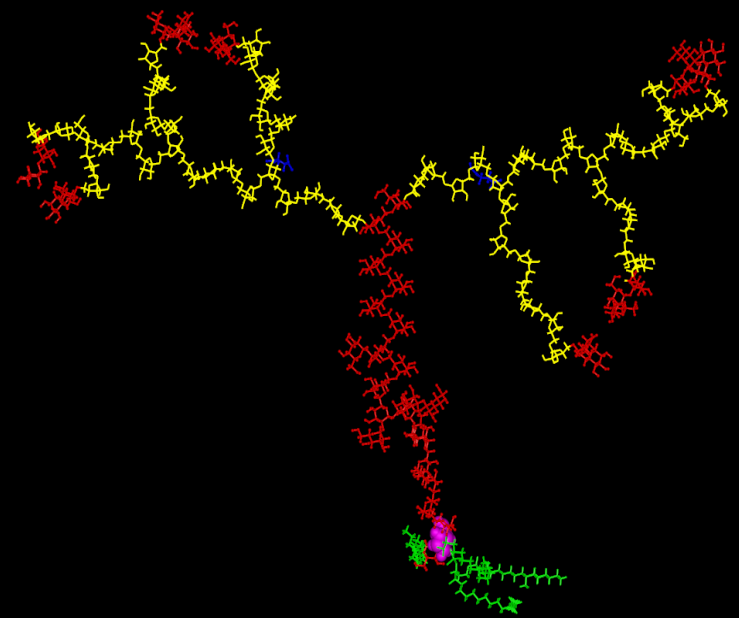
A. Sethi, D. Anunciado, J. Tian, D M Vu, and S Gnanakaran, **Chem. Phys.**, in Press (2013).

Host- Pathogen Interactions

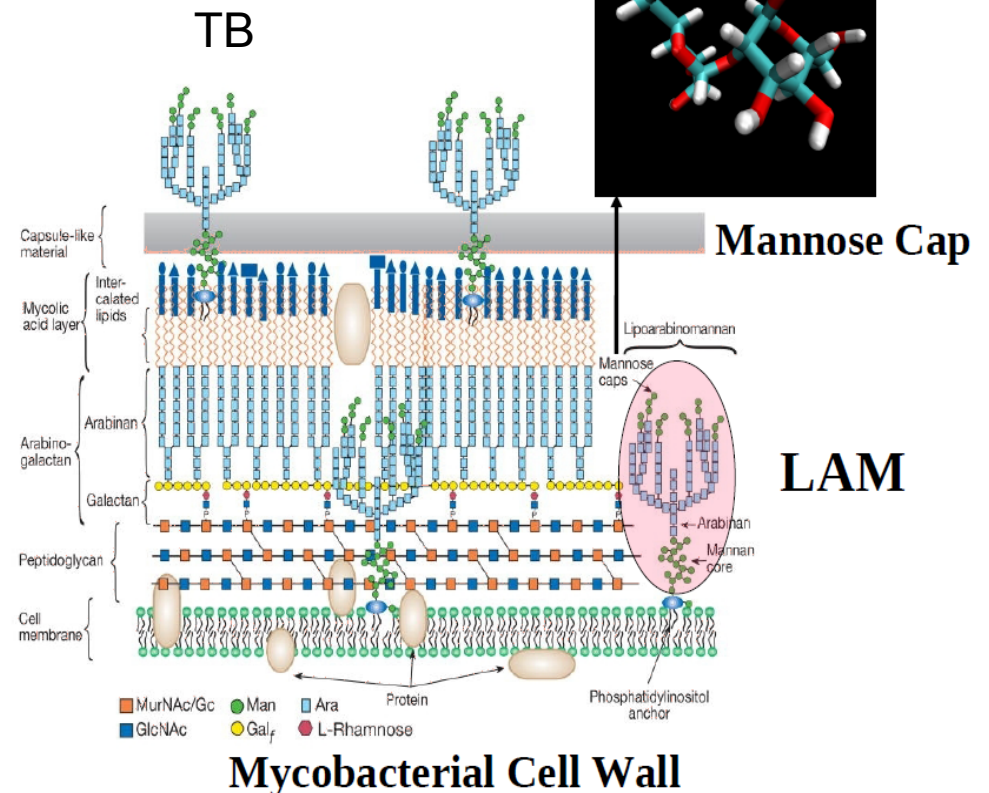
R. Parthasarathi, et al.,
J. Phys. Chem A. 2011. 115,
 12826-40.

Mukundan H, et al., *Tuberculosis.*
 (Jan 2012) ;92(1):38-47

Jianhui Tian, et al.
Biophys. J., 104, 622-632
 (Feb. 5, 2013).



Pathogen:



Increasing Spatial & Temporal Scales



PNAS, 2013, 110: 10922-7

J. Biol. Chem. 2013 (in press)

Biotechnol. Biofuels. 2012,5:55

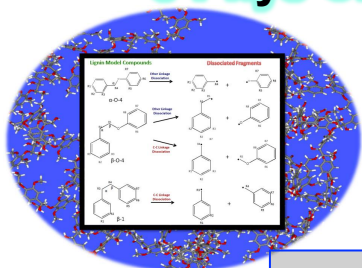
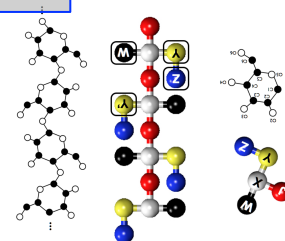
Optimal Cellulase Cocktails for Efficient Degradation of Cellulose

Biophys. J. 2009, 96:3032

Plasticity of Hydrogen Bond Network in Cellulose

J Phys Chem B. 2012 116:8031

Bulk Properties of Cellulose



Transformation of Cellulose I to III

J. Am. Chem. Soc. 2011 133, 11163

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Amorphous Cellulose

J. Am. Chem. Soc. 2009 131: 14786

Pyrolysis & Catalysis Lignin Models

J. Phys. Chem. Letters. 2011,2:2660

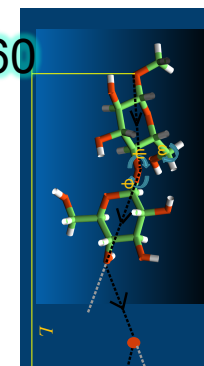
J Org Chem. 2010 75:6549

Stacking & Hydrogen Bonding in Cellulose

J. Phys. Chem. A. 2011 115: 14191

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Acta Crystal. D. 2010. 66:1184



Quantum Mechanical

Classical MD Simulations

Coarse-grained Simulations

Stat. Mech. Models

Rule-based Models

Multi-resolution Theoretical Approaches

Leaders – Biosimulations Track

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Week 1

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Week 2

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