BIOGRAPHICAL SKETCH

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NAME: David S. Goodsell

eRA COMMONS USER NAME (credential, e.g., agency login): goodsell

POSITION TITLE: Professor of Computational Biology

EDUCATION/TRAINING *(Begin with baccalaureate or other initial professional education, such as nursing, include postdoctoral training and residency training if applicable. Add/delete rows as necessary.)*

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	Completion Date MM/YYYY	FIELD OF STUDY
University of California, Irvine	B.S.	1982	Chemistry
University of California, Irvine	B.S.	1982	Biology
University of California, Los Angeles	Ph.D.	1987	Biochemistry
The Scripps Research Institute	Postdoctoral	1987-1990	Advisor: A.J. Olson

A. Personal Statement

I currently hold a dual appointment as Professor of Computational Biology at the Scripps Research Institute and Research Professor at Rutgers University. I divide my time between research and science outreach. My research centers on methods for computational structural biology and their application to drug design, protein function prediction, and modeling of the molecular structure of entire cells. Current work includes development and applications of CellPACK, a new method for creating three-dimensional atomic models of large portions of cells, and continued development of AutoDock, a widely-used computational docking program used for drug design and virtual screening. I am applying these methods to the structural mechanisms of HIV-1 budding and maturation, and the structure and function of bacterial cells, with a strong focus on bacterial nucleoids. In my science outreach work, I have developed new visual methods for exploring molecular and cellular structure. This includes three decades of work on depiction of the cellular mesoscale, and development of non-photorealistic rendering methods for molecular and cellular subjects. Within the B-HIVE Center, I have produced a series of integrative visualizations of the viral lifecycle and during the pandemic focused on educational materials related to coronavirus biology and vaccines. I currently create outreach materials for the RCSB Protein Data Bank, including a popular monthly column that presents molecular structure and function for general audiences. I have written four general-interest books on molecular biology, cell biology and bionanotechnology, and have collaborated with science museums, filmmakers, educators and popular authors on the creation of educational and outreach materials.

Recent projects include a role as Principal Investigator on one NIH project, and Co-Investigator on two NIH projects:

R01-GM120604
Goodsell (PI)
09/15/16 - 07/31/26
NIH/NIGMS
Modeling and Interacting with the Visible Molecular Cell
Development and application of methods for the modeling of bacterial cells, with focus on challenging fibrous structures such as bacterial nucleoids.

R01-GM069832
Forli (PI), Role: Co-Investigator

01/01/04 - 07/31/26
NIH/NIGMS
AutoDock Suite: High Performance Software Environment for Drug Design
Continued development and maintenance of the AutoDock suite to expand its usefulness, its usability and its maintainability, within an evolvable software platform, for the broad diversity of its users.

U54-AI170855
Torbett (PD/PI), Role: Co-Investigator
06/22/22 - 03/31/27
NIH/NIGMS
Behavior of HIV in Viral Environments (B-HIVE)
Understanding of HIV-1 and HIV-1/cellular host factor macromolecular interactions within distinct cellular environments, which shape the HIVE replication cycle.

Citations:
1. Goodsell DS & Lasker K (2023) Integrative visualization of the molecular structure of a cellular microdomain. Protein Sci. 32, e4577. PMCID: PMC9926476.
2. Maritan M, Autin L, Karr J, Covert MW, Olson AJ & Goodsell DS (2022) Building structure models of a whole mycoplasma cell. J. Mol. Biol. 434, 167351. PMCID: PMC8752489.
3. Goodsell DS, Dutta S, Voigt M, Zardecki C & Burley, SK (2022) Molecular exploration of cancer biology and therapeutics at PDB-101. Oncogene 41, 4333-4335. PMCID: PMC9364277.
4. Goodsell DS, Autin L & Olson AJ. (2018) Lattice models of bacterial nucleoids. J. Phys. Chem. B 122, 5441-5447. PMCID: PMC5980677.

B. Positions, Scientific Appointments, and Honors

2020-present	Professor of Computational Biology, Department of Integrative Structural and Computational Biology, The Scripps Research Institute
2016-present	Research Professor, Center for Integrative Proteomics Research, Rutgers State University of New Jersey
2013-2019	Associate Professor of Molecular Biology, Department of Integrative Structural and Computational Biology, The Scripps Research Institute
2007-2012	Associate Professor of Molecular Biology, Department of Molecular Biology, The Scripps Research Institute
2001-2006	Associate Professor, Department of Molecular Biology, The Scripps Research Institute
1994-2001	Assistant Professor, Department of Molecular Biology, The Scripps Research Institute
1992-1994	Assistant Researcher, Molecular Biology Institute, University of California, Los Angeles
1987-1992	Research and Scientific Associate, Department of Molecular Biology, The Scripps Research Institute, La Jolla, CA. Postdoctoral Advisor: Arthur J. Olson.
1982-1987	Research and Teaching Assistant, Department of Chemistry and Biochemistry, University of California, Los Angeles. Graduate Advisor: Richard E. Dickerson.

C. Contributions to Science
1. I have a strong commitment to science outreach and have worked on several projects with this goal in mind. For several decades, I have created illustrations of molecules in cells, which have been presented to popular audiences in science museums, magazines, books, and presentations around the world. I also write a column at the RCSB Protein Data Bank, the "Molecule of the Month," that presents the structure and function of a different molecule each month. The goal of the column is to provide a gateway into the PDB archive for non-expert users.
a. Zardecki C, Dutta S, Goodsell DS, Lowe R, Voigt M & Burley SK (2022) PDB-101: Educational resources supporting molecular explorations through biology and medicine. Protein Sci. 31, 129-140. PMCID: PMC8740840.
b. Richardson JS, Richardson DC & Goodsell DS. (2021) Seeing the PDB. J. Biol. Chem. 296, 100742. PMCID: PMC8167287.
c. Goodsell DS, Voigt M, Zardecki C & Burley SK. (2020) Integrative illustration for coronavirus outreach. PLoS Biol. 18, e3000815. PMCID: PMC7433897.
d. Goodsell DS, Zardecki C, Berman HM & Burley SK. (2020) Insights from 20 years of the Molecule of the

Month. Biochem. Mol. Biol. Educ. 48, 350-355. PMCID: PMC7496199.

2. I have applied methods of computational chemistry to the study of HIV. In early work as part of a program project at TSRI, we developed methods for designing optimal inhibitors that evade drug resistance. Currently, as part of the HIVE Center, I am developing structural models of the HIV virion at multiple stages of the viral life cycle.

a. Goodsell DS, Jewett A, Olson AJ & Forli S. (2019) Integrative modeling of the HIV-1 ribonucleoprotein complex. PLoS Comput. Biol. 15: e1007150. PMCID: PMC6592547.
b. Craveur P, Gres AT, Kirby KA, Liu D, Hammond JA, Deng Y, Forli S, Goodsell DS, Williamson JR, Sarafianos SG & Olson AJ. (2019) Novel intersubunit interaction critical for HIV-1 core assembly defines a potentially targetable inhibitor binding pocket. Mbio 10, e02858-18. PMCID: PMC6414707.
c. Johnson GT, Goodsell DS, Autin L, Forli S, Sanner MF & Olson AJ. (2014) 3D molecular models of whole HIV-1 virions generated with cellPACK. Faraday Discuss. 169, 23-44. PMCID: PMC4569901.
d. Brik A, Alexandros J, Lin Y-C, Elder JH, Olson AJ, Wlodawer A, Goodsell DS & Wong, C-H. (2005) 1,2,3-Triazole as a peptide surrogate in the rapid synthesis of HIV protease inhibitors. ChemBioChem 6, 1167-1169.

3. We are developing methods to integrate experimental data from structural biology, microscopy, and proteomics to generate quantitative models of entire bacterial cells and eukaryotic organelles. The goal of this work is to create models that bridge cell biology and molecular biology, for hypothesis generation and simulation. This has included collaboration with computer scientists to address the challenges of visualization of these very complex models.

a. Goodsell DS (2022) Integrative illustration of a JCVI-syn3A minimal cell. J. Integr. Bioinform. 19, 20220013. PMCID: PMC9377704.
b. Gardner A, Autin L, Fuentes D, Maritan M, Barad BA, Medina M, Olson AJ, Grotjahn DA, Goodsell DS (2021) CellPAINT: turnkey illustration of molecular cell biology. Frontiers Bioinform. 1, 660936. PMCID: PMC8594902.
c. Jewett AI, Stelter D, Lambert J, Saladi SM, Roscioni OM, Ricci M, Autin L, Maritan M, Bashusqeh SM, Keyes T, Dame RT, Shea JE, Jensen GJ, Goodsell DS. (2021) Moltemplate: a tool for coarse-grained modeling of complex biological matter and soft condensed matter physics. J. Mol. Biol. 433, 166841. PMCID: PMC8119336.
d. Johnson GT, Autin L, Al-Alusi M, Goodsell DS, Sanner MF & Olson AJ. (2015) CellPACK: A virtual mesoscope to model and visualize structural systems biology. Nat. Methods 12, 85-91. PMCID: PMC4281296.

4. As part of postdoctoral work in 1990, I developed AutoDock, the first flexible ligand docking method, and subsequently have continued development and supported use of AutoDock by a large community of researchers, students, and educators. I have also developed methods for active site prediction, free energy estimation, and drug development. As a result of this work, AutoDock is currently the most widely cited free software for computational docking and virtual screening.

a. Holcomb M, Chang YT, Goodsell DS & Forli S (2023) Evaluation of AlphaFold2 structures as docking targets. Protein Sci. 32:e4530. PMCID: PMC9794023.
b. Goodsell DS, Sanner MF, Olson AJ & Forli S. (2021) The AutoDock suite at 30. Protein Sci. 30, 31-43. PMCID: PMC7737764.
c. Bianco G, Goodsell DS & Forli S (2020) Selective and effective: current progress in computational structure-based drug discovery of targeted covalent inhibitors. Trends Pharmacol. Sci. 41, 1038-1049. PMCID: PMC7669701.
d. Forli S, Huey R, Pique ME, Sanner MF, Goodsell DS & Olson AJ. (2016) Computational protein-ligand docking and virtual drug screening with the AutoDock suite. Nat. Protocols 11, 905-919. PMCID: PMC4868550.

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