

Current Grants

Note: Among Dowling College from 2002 to 2015, Rochester Institute of Technology from 2015 to 2019, and Ronin Institute for Independent Scholarship from 2018 to the present, have had 20 years of continuous external grant funding.

Subaward PI (October 2020 – June 2022), subaward to NIH 5P30GM133893 (Sean McSweeney, PI), “The Center for Biomolecular Structure at NSLS-II.” Total Subaward Amount 2020 – 2022: \$110,294.11. The goal of this sub-project is to transfer the High Data Rate Macromolecular Crystallography (HDRMX) project which runs a series of meetings on the subject to BNL, continuing an important part of the work under the Dectris grant, below.

PI/PD (October 2014 – September 2020) grant from DECTRIS of Baden-Dättwil, Switzerland for research on “Extensions and Improvements to Detector Data Formats.” Total Award Amount 2014 – 2020: \$150,000. The goal of this project was to create extensions and improvements to detector data formats with emphasis on interoperability of CBF and HDF5 via CBFlib, combining the crash recovery of CBF with the performance of HDF5, optimizing compression for high pixel-density MX data in EIGER support, and validation of Eiger HDF5 datasets.

Subaward PI and Co-Investigator (September 2017 – August 2019), subaward to 5R01GM117126 (Nicholas K. Sauter, PI), “DIALS: New Computational Methods to Enable Challenging Crystallographic Experiments.” Total Subaward Amount 2017 – 2019: \$91,000. Goals: For 2017-2018 subaward, instrument and test the best available version of Andrews-Bernstein Niggli-reduction-based NCDist in the context of cctbx and the nightly build system. For 2018-2019 subaward, improve the speed of Andrews-Bernstein Niggli-reduction-based NCDist by conversion to Delaunay reduction, forming “D7Dist” which involves only 7 boundary cases instead of 15, reducing the number of cases to be handled by a factor of $\frac{49}{225}$.

Co-PI (July 2015 – June 2017, September 2017 – August 2019) Consultant (August 2019 – August 2020) grants DUE-1503811 and DUE-1709170 from NSF for “Collaborative Research: Using protein function prediction to promote hypothesis-driven thinking in undergraduate biochemistry education”, with Paul Craig, PI, Jeffrey L. Mills, Co-PI, Suzanne O’Handley, Co-PI.

Total RIT Award Amount 2015 – 2020 \$208,374.

There are collaborative awards to

SUNY College at Oswego

(DUE-1709355, September 2017 – August 2020), Julia Koeppe, PI, \$26,948,

Ursinus College

(DUE-1709805, September 2017 – August 2020), Rebecca Roberts, PI, \$28,531,

(DUE-1503699, July 2015 – June 2017), Rebecca Roberts, PI, \$32,467,

Hope College

(DUE-1709278, September 2017 – August 2020), Michael Pikaart, PI, \$28,129,

(DUE-1503710, July 2015 – June 2017), Michael Pikaart, PI, \$21,227,

Purdue University

(DUE-1710051, September 2017 – August 2020), Trevor Anderson, PI, \$60,000,

(DUE-1503798, July 2015 – June 2017), Trevor Anderson, PI, \$23,974,

California Polytechnic State University Foundation

(DUE-1710538, September 2017 – August 2020), Anya Goodman, PI, Eric Jones, Co-PI, \$29,001,

(DUE-1503676, July 2015 – June 2017), Anya Goodman, PI, Ashley McDonald, Co-PI, \$36,294,

St Mary’s University San Antonio

(DUE-1709592, September 2017 – August 2020), Susan Colette Daubner, PI, \$29,985,

(DUE-1502720, July 2015 – June 2017), Susan Colette Daubner, PI, \$25,594,

Oral Roberts University

(DUE-1503734, July 2015 - June 2017), Robert Stewart, PI, \$23,783

Co-Investigator and sub-award PI (August 2018 – July 2020) subaward to 1R21GM129570 (Alexei Soares, PI) “Detecting Elusive Biologically Significant Structural Differences with Serial Crystallography.” Total Subaward Amount 2018 – 2020: \$110,880. The goals of this project were to produce a new parametrizable software framework combining the most sensitive and effective clustering techniques, firstly to detect structural differences among XFEL and synchrotron stills or synchrotron wedges and then to detect intensity similarities that will produce reasonably pure data to be merged and solved as single-species datasets or a single-state dataset. These will enable the recognition

of species in polymorphs, elucidation of state sequences, and recognition of differing ligands, as well as removal of datasets that might corrupt the single-species and single-state datasets. Our tools will leverage the investment in modern high-brilliance x-ray facilities (synchrotrons and XFELs) that can obtain data from proteins in different conformational and/or dynamic states. We will begin exploring potential strategies for optimal clustering using a two-stage approach that generates initial clusters using cell dimensions and then refines the clusters using intensities.

Scholarships and Fellowships

NSF Graduate Fellow, GSAS/New York University, 1966 – 67.

NSF Cooperative Graduate Fellow, GSAS/New York University, 1964 – 65, 1965 – 66.

New York State Regents Science Scholarship, WSC/NYU, 1961 – 64.

Honorary Societies

Phi Beta Kappa, Pi Mu Epsilon, Sigma Pi Sigma

Professional Societies

(1962 –) Mathematical Association of America (Life Member)

(1963 –) American Mathematical Society (Life Member)

(1974 –) American Crystallographic Association

(1978 –) Mathematical Association (UK) (Life Member)

(1983 –) Society for Industrial and Applied Mathematics

(1990 –) London Mathematical Society

(2019 –) International Society for Biocuration

Current Service Activities

Reviewer	(1975 –)	Math Reviews. 1 - 2 reviews per year
Chair Elect	(2020)	Best Practices Special Interest Group
Chair	(2021)	American Crystallographic Association
Member	(1999 –)	Committee for the Maintenance of the CIF Standard (COMCIFS)
		International Union of Crystallography (IUCr)
Member	(2017 –)	IUCr Committee on Data (IUCr CommDat)
		International Union of Crystallography (IUCr)
Member	(2012 –)	NeXus International Advisory Committee (NIAC)
Member	(August 2017 –)	Committee on Data (COMMDAT)
		International Union of Crystallography (IUCr)
Chair	(1998 –)	Image CIF (imgCIF/CBF) Dictionary Maintenance Group (IUCr)
Member	(2001 –)	Endowment Fund Committee and Cultural Enrichment Committee, Temple Beth El, Patchogue, NY

Earlier Grants while at Dowling College

At Dowling College from 2002 through 2015, brought in \$1,365,389 of continuous research funding, \$31,259 of workshop funding and helped bring in \$292,187 of scholarship funding.

PI/PD with P. Craig (Co-PI) (August 2006 – August 2015) on multiple awards on grant R15GM078077 from NIH/National Institute of General Medical Sciences. Total Award Amount 2006 – 2015: \$854,711.

“Algorithmic Assignment of Probable Function to Proteins of Previously Unknown Function”, 2011 – 2014 renewal, Grant 2R15GM078077-02 (MPI).

Supplements, 2011, Grant 3R15GM078077-02S1, 2013, Grant 3R15GM078077-02S2, Grant 3R15GM078077-02S3.

“SBEVSL – Structural Biology Extensible Visualization Scripting Language” 2006 – 2011, Grant 1R15GM078077-01.

Supplement for summer student research program, 2009, Grant 3R15GM078077-01S1.

PI/PD with R. Sweet (January 2006 – December 2008) “Workshop – imgCIF: The Management of Synchrotron Image Data, A Series of Three Workshops” project, supported by the Office of Science (BER), U.S. Department of Energy, Grant No. ER64212-1027708-0011962 (January 2006 – December 2008), the National Science Foundation, Grant No. DBI-0610407 (June 2006 – December 2007) and the National Institute of Research Resources, Grant No. 1R13RR023192-01A1 (June 2007 – May 2008). Award Amount: \$31,259.

PI/PD (September 2003 – August 2007) “ITR: Efficient Calculation of Molecular Surfaces”, research supported by National Science Foundation, Grant No. EF-0312612. Award Amount: \$147,414.

PI/PD (February 2002 – May 2007) “Accessible Retired Computers in Biology (ARCiB)” project, supported by the National Science Foundation, Grants No. DBI-0203064 and DBI-0315281. Award Amount: \$189,735.

PI/PD (August 2004 – July 2006) “New and Upgraded CIF Software”, research and software development supported by the International Union of Crystallography. Award Amount: \$30,593.

Co-PI with S. Monteferrante (PI) and F. Rispoli (Co-PI) (September 2004 – July 2008) “Computer Science & Mathematics Scholarship Program”, scholarship program supported by National Science Foundation, Grant DUE- 0422315. Award Amount: \$292,187.

PI/PD (August 2007 – October 2010) “New and Upgraded CIF Software”, research and software development supported by the International Union of Crystallography. Award Amount: \$41,409.

PI/PD (September 2003 – August 2011) “Local System Support for PDB Biological Unit Search and Display”, research supported by the Office of Science (BER), U.S. Department of Energy, Grant No. DE-FG02-03ER63601 with supplement in 2005 for “WPDB: Wide Protein Data Bank Format” and supplement in 2007 for “New Software Capabilities Relating to the Management of Image Data” and renewal in 2009. Total Award Amount: \$101,527 and custody of \$450,000 of government-owned computer equipment.

Teaching

At Rochester Institute of Technology, Rochester, NY

Fall 2018 – Spring 2021	SWEN 561/2	Serve as a customer for online software engineering project capstone course
Spring 2017	BIOL 670	Statistical Analysis for Bioinformatics (online course)
Spring 2017	BIOL 689.01	Rational Drug Design – Bioinformatics (special topics, online course)
Spring 2017	CHEM 789.03	Rational Drug Design – Cheminformatics (special topics, online course)
Fall 2016	BIOL 635	Bioinformatics Seminar (online course)
Spring 2016	BIOL 670	Statistical Analysis for Bioinformatics (online course)
Fall 2015	BIOL 635	Bioinformatics Seminar (online course)

At Dowling College, Oakdale, NY

Fall 2014	MTH 1002A	Fundamentals of Mathematics
	MTH 1007A	Operations Research (online course)
	MTH 4131A	Advanced Calculus
Spring 2014	CSC 1009	Introduction to Spreadsheets and Data Analysis
	CSC 2281	Network Flows and Queuing Theory
	MTH 1007A	Operations Research (online course)
Fall 2013	CSC 2025A	Data Structures (online course)
	CSC 2060N	Computer Organization (online course)
	MTH 1007A	Operations Research (online course)
	MTH 1014A	Pre-Calculus (online course)
Spring 2013	CSC 2281A	Network Design and Queuing Theory (online course)
	CSC 3072A	Database Systems (online course)
	CSC 3971N	Advanced Programming I (online course)
	CSC 3982N	Advanced Software Engineering II (online course)
	MTH 1014A	Pre-Calculus (online course)
Fall 2012	CSC 1009N	Introduction to Spreadsheets and Data Analysis (online course)
	CSC 2060N	Computer Organization (online course)
	CSC 3981N	Advanced Software Engineering I (online course)
	MTH 1002A	Fundamentals of Mathematics (online course)
Spring 2012	CSC 1023N	Introduction to Computer Science (online course)
	CSC 2281A	Network Design and Queuing Theory (online course)
	CSC 3080A	Operating Systems (online course)
	MTH 1007A	Operations Research (online course)
Fall 2011	CSC 1024N	Introduction to Programming
	CSC 3171A	Algorithms
	CSC 3971N	Advanced Programming
Spring 2011	CSC 1023N	Introduction to Computer Science
	CSC 2025A	Data Structures
	CSC 2281A	Network Design & Queuing Theory
Fall 2010	MTH 1002A	Fundamentals of Mathematics
	CSC 1023N	Introduction to Computer Science
	CSC 2060N	Computer Organization

January 2011, 2-week short course Programming for Structural Biology at Rochester Institute of Technology, Rochester, NY, <http://media.rit.edu/faculty/pac8612/1009-541/ProgrammingModule.html>

Spring 2010		(On sabbatical)
Fall 2009		(On sabbatical)
Spring 2009	MTH 1007A	Operations Research
	CSC 3149A	Compilers
	CSC 1009N	Introduction to Spreadsheets and Visual Basic
Fall 2008	NSM 6600	Technologies for Research and Instruction
	MTH 1002A	Fundamentals of Mathematics (2 sections)
Spring 2008	CSC 1009N	Introduction to Spreadsheets and Visual Basic
	CSC 3962N	Project-Oriented Computer Science
	CSC 4962N	Project-Oriented Computer Science Research
Fall 2007	NSM 6600	Technologies for Research and Instruction
	CSC 3961N	Project-Oriented Computer Science
	CSC 4961N	Project-Oriented Computer Science Research
Spring 2007	CSC 3171A	Algorithms
	CSC 3962N	Project-Oriented Computer Science
	CSC 4962N	Project-Oriented Computer Science Research
Fall 2006	NSM 6600	Technologies for Research and Instruction
	CSC 3961N	Project-Oriented Computer Science
	CSC 4961N	Project-Oriented Computer Science Research
Spring 2006	MTH 1002A	Fundamentals of Mathematics
	CSC 4181N	Project-Oriented Computer Science I
	CSC 4182N	Project-Oriented Computer Science II
Fall 2005	NSM 6600	Technologies for Research and Instruction
	CSC 4181N	Project-Oriented Computer Science I
	CSC 4182N	Project-Oriented Computer Science II
Spring 2005	CSC 3080	Operating Systems
	CSC 4175	Software Engineering
	CSC 4177	Senior Project
	MTH 1002	Fundamentals of Mathematics
Fall 2004	CSC 1012	Introduction to Computer Science
	NSM 6600	Technologies for Research and Instruction
	NSM 6602	Scientific Methods and Experimental Design
Spring 2004	CSC 1012	Introduction to Computer Science
	CSC 1071	Data Structures
Fall 2003	CSC 1012	Introduction to Computer Science
	CSC 1071	Data Structures
Spring 2003	CSC 080	Operating Systems
	MTH 002	Fundamentals of Mathematics
	MTH 014	Pre-Calculus
Fall 2002	CSC 181	Advanced Research Topics in Computer Science
	CSC 077	Intermediate Java Programming
	CSC 175	Software Engineering
	CSC 177	Senior Project
Spring 2002	CSC 080	Operating Systems
	CSC 182	Research Topics in Computer Science
	MTH 002	Fundamentals of Mathematics
Fall 01	CSC 012	Introduction to Computer Science

Also taught undergraduate computer science at St. Joseph's College and at Stony Brook, and graduate computer science at New York University.

Earlier Employment

Research Professor (April 2015 – August 2019) Consultant (August 2019 – March 2021), Rochester Institute of Technology, Rochester, NY 14623, working at Brookhaven National Laboratory, Upton, NY 11973

Research Professor (January 2015 – December 2015), Professor of Mathematics and Computer Science (January 2002 – January 2015) (title changed from Professor of Computer Science to Professor of Mathematics and Computer Science in 2011), Special Research Associate in Computer Science (October 2001 – January 2002), Dowling College, Oakdale, NY 11769 and Shirley, NY 11967.

Research Professor (September 2001 – December 2001), Computer Science Department, State University of New York at Stony Brook, Stony Brook, NY 11794.

Associate Professor (September 1999 – June 2000), Department of Mathematics and Computer Science, St. Joseph's College, 155 West Roe Boulevard, Patchogue, NY 11772-2603.

Senior Computer Analyst, (February 1994 – October 1997), Chemistry Department, (September 1993 – January 1994), Department of Applied Science, Research Collaborator (September 1983 – August 1993), Department of Applied Science and Chemistry Department, Brookhaven National Laboratory, Upton, L.I., New York 11973. Collaborated on data acquisition software for the Laser Electron Accelerator Facility (LEAF) in the Chemistry Department and on data management issues for new x-ray detectors of macromolecular crystallography at National Synchrotron Light Source-II. Provided consultation in matters related to computers and mathematics, laboratory automation, experiment design, networking, assisted in design of mass-spec system for radical-radical kinetics, FTIR, real-time reactor stack monitoring system, and airborne data acquisition system.

Senior Research Scientist (September 1983 – August 1991), Courant Institute of Mathematical Sciences, New York University, 251 Mercer Street, New York, New York 10012. Research activities included mapping of large flat texts to Hypermedia. Director of Administrative Computing (February 1989 – January 1990), New York University. Managed University Computer Center (with staff of 120) and provided advice to the University on matters concerning administrative computing. Administrator for Computing Projects and Technology Evaluation and Assessment (August 1985 – August 1989), Academic Computing Facility, CIMS/NYU. Assistant Director for Experimental Facilities (January 1984 – July 1985), Assistant Director for Systems Software Robotics Research Activity (September 1983 – June 1984), Computer Science Division, CIMS/NYU. Research in robotics, high speed parallel processing and numerical linear algebra. Administrative support for various computing projects at New York University, including representing NYU in consortia for supercomputing and data communications. Evaluate and assess computer related technology. Co-principal investigator (with J.T. Schwartz) and organizer of NSF funded Symposium on Factory Automation and Robotics, 9-11 September 1985, CIMS/NYU.

Adjunct Professor (September 1987 – August 1991), Adjunct Associate Professor (September 1982 – August 1987), Computer Science Department, Graduate School of Arts and Science, Courant Institute of Mathematical Sciences, New York University. Taught Data Communications, Network Design and Implementation, Biomedical Image Reconstruction, Laboratory Automation, and the Preparatory Accelerated Course on Data Structures and Assembly Language.

Trustee, Consortium for Scientific Computing (October 1984 – August 1991), a New Jersey not-for-profit corporation. Represented the interests of New York University.

Director, NYSErnet Inc. (New York State Education and Research Network), (January 1986 – November 1989), a New York not-for-profit corporation. Represented the interests of New York University in the establishment of a high speed data communications network for New York State. Member of the Executive Committee. Vice-Chairman (December 1987 – November 1989).

Visiting Member (February 1982 – August 1983), Courant Institute of Mathematical Sciences, New York University, 251 Mercer Street, New York, New York 10012. Research on high speed parallel computation, symbolic manipulation, robotics, and microcomputers.

Scientist (October 1978 – August 1983), Chemistry Department, Brookhaven National Laboratory, Upton, L.I., NY 11973. Associate Scientist (January 1974 – September 1978). Head, Chemistry Department Computing and Laboratory Automation Service Group. Chairman (January 1981 – January 1982), BNL Computer Users Organization. Provided laboratory automation and computation services for chemists. From 1975 to 1979 was scientific project officer on NIH-DOE IAG for support of various aspects of the NIH/EPA Chemical Information System, Operations Manager CIS (January 1978 – February 1979). Previously provided user support and software integration in CRYSTAL project.

Senior Computer Science Analyst (November 1971 – January 1974). Scientific Programmer Analyst II (October 1970 – November 1971). Applied Mathematics Department, Brookhaven National Laboratory. Major operating systems design, implementation and maintenance.

Associate Research Scientist (September 1968 – September 1970), AEC Computing and Applied Mathematics Center, Courant Institute of Mathematical Sciences, New York University, 251 Mercer Street. Symbolic manipulation, operating systems modification and maintenance, finite groups and near rings.

Adjunct Associate Professor of Mathematics (September 1968 – June 1969), New York University. Taught undergraduate course in computing for Washington Square College.

Assistant Research Scientist (February 1968 – August 1968), AEC Computing and Applied Mathematics Center, CIMS, New York University. Symbolic manipulation.

Lecturer (February 1968 – May 1968), part-time, Washington Square College of Arts and Science, Evening Division, New York University. Taught course in assembly language.

Operations Assistant (September 1967 – January 1968), part-time, AEC Computing and Applied Mathematics Center, CIMS, New York University. Symbolic Manipulation.

Earlier Service Activities

Consultant	(August 2011 – August 2017)	IUCr Diffraction Data Deposition Working Group (IUCr DDD WG) International Union of Crystallography (IUCr) Temple Beth El, Patchogue, NY
WebMaster	(2001 – 2015)	
Member	(February 2011 – October 2012)	Dowling College Middle States Self-Study Steering Committee
Member	(November 2010 – August 2012)	Dowling College Institutional Review Board
Coach	(September 2009)	Dowling College ACM Programming Contest team
Assistant Coach	(2008 – 2009)	Dowling College ACM Programming Contest team
Coach	(2003 – 2008)	Dowling College ACM Programming Contest team
Assistant Coach	(2002 – 2003)	Dowling College ACM Programming Contest team
Evaluator	(August 2010 – February 2011)	Dowling College School of Aviation Policy Project on Aviation Education Enhancement
Member	(Spring 2009)	Dowling College Faculty Personnel Committee
Member	(February 2009 – April 2010)	Dowling College NYSUT Negotiating Committee, Chair February 2010 – April 2010
Advisor	(September 2003 – May 2008)	Dowling College Computer Club
Chair	(September 2005 – January 2006)	Dowling College Human Subjects Committee
Webmaster	(May 2003 – May 2007)	Dowling College Chapter, NY State United Teachers web site (www.dcnysut.org)
Member	(1997 – 2001)	Macromolecular CIF (mmCIF) Dictionary Maintenance Group (IUCr)
Vice-Chairman, NYSERnet Inc.	(1987 – 1989)	NYSERnet Inc. (NY State Education and Research Network), New York, NY
Director, NYSERnet Inc.	(1986 – 1989)	NYSERnet Inc. (NY State Education and Research Network), New York, NY
Trustee	(1984 – 1991)	Consortium for Scientific Computing, Princeton, NJ

Publications

A. S. Soares, Y. Yamada, J. Jakoncic, S. McSweeney, R. M Sweet, J. Skinner, J. Foadi, M. R. Fuchs, D. K. Schneider, W. Shi, B. Andi, L. C. Andrews, H. J. Bernstein, 2022. "Serial crystallography with multi-stage merging of thousands

of images". *Acta Cryst*, F78:7 281 – 288. Preprint: H. J. Bernstein, L. C. Andrews, J. Foadi, M. R. Fuchs, J. Jakoncic, S. McSweeney, D. K. Schneider, W. Shi, J. Skinner, A. Soares, Y. Yamada, 2017. "Serial Crystallography with Multi-stage Merging of 1000s of Images". *bioRxiv*, p.141770.

<https://doi.org/10.1101/141770>

<https://doi.org/10.1107/S2053230X22006422>

E. O. Lazo, S. Antonelli, J. Aishima, H. J. Bernstein, D. Bhogadi, M. R. Fuchs, N. Guichard, S. McSweeney, S. Myers, K. Qian, D. Schneider, G. Shea-McCarthy, J. Skinner, R. Sweet, L. Yang and J. Jakoncic, 2021. "Robotic sample changers for macromolecular X-ray crystallography and biological small-angle X-ray scattering at the National Synchrotron Light Source II", *J. Synchrotron Rad.* 28 1649 – 1661

<https://doi.org/10.1107/S1600577521007578>

D. K. Schneider, W. Shi, B. Andi, J. Jakoncic, Y. Gao, D. K. Bhogadi, S. F. Myers, B. Martins, J. M. Skinner, J. Aishima, K. Qian, H. J. Bernstein, E. O. Lazo, T. Langdon, J. Lara, G. Shea-McCarthy, M. Idir, L. Huang, O. Chubar, R. M. Sweet, L. E. Berman, S. McSweeney and M. R. Fuchs, 2021. "FMX – the Frontier Microfocusing Macromolecular Crystallography Beamline at the National Synchrotron Light Source II", *J. Synchrotron Rad.* 28 650 – 665

<https://doi.org/10.1107/S1600577520016173>

T. Nguyen, K. L. Phan, D. E. Kreitler, L. C. Andrews, S. B. Gabelli, D. Kozakov, J. Jakoncic, R. M. Sweet, A. Soares, H. J. Bernstein, 2020. "A simple technique to classify diffraction data from dynamic proteins according to individual polymorphs". *bioRxiv*, p. 422680.

<https://doi.org/10.1101/2020.12.14.422680>, to appear in *Acta Cryst. D* in 2022

H. J. Bernstein, A. Förster, A. Bhowmick, A. S. Brewster, S. Brockhauser, L. Gelisio, D. R. Hall, F. Leonarski, V. Mariani, G. Santoni, C. Vonnrhein, G. Winter, 2020. "Gold Standard for Macromolecular Crystallography Diffraction Data", *IUCrJ* 7:5 784 – 792, <https://doi.org/10.1107/S2052252520008672>,

<https://doi.org/10.1107/S2052252520008672/ti5018sup1.pdf>,

<https://doi.org/10.1107/S2052252520008672/ti5018sup2.pdf>

H. J. Bernstein, L. C. Andrews, J. A. Diaz Jr., J. Jakoncic, T. Nguyen, N. K. Sauter, A. S. Soares, J. Y. Wei, M. R. Wlodek, and M. A. Xerri, 2020. "Best practices for high data-rate macromolecular crystallography (HDRMX)", *Structural Dynamics* 7:1 014302.

<https://aca.scitation.org/doi/10.1063/1.5128498>

L. C. Andrews, H. J. Bernstein, N. K. Sauter, 2020. "Converting three-space matrices to equivalent six-space matrices for Delone scalars in S_6 ", *Acta Cryst.* A76:1 79 – 83.

<https://doi.org/10.1107/S2053273319014542>

A. Ringer McDonald, H. J. Bernstein, S. C. Daubner, A. L. Goodman, S. M. Irby, J. R. Koeppe, J. L. Mills, S. F. O'Handley, M. Pikaart, R. Roberts, A. Sikora, P. A. Craig, 2019. "BASIL Biochemistry Curriculum,"

<https://basilbiochem.github.io/basil>

L.C. Andrews, H. J. Bernstein, N. K. Sauter, 2019. "A space for lattice representation and clustering", *Acta Cryst.* A75:3 593 – 599.

<https://doi.org/10.1107/S2053273319002729>

L.C. Andrews, H. J. Bernstein, N. K. Sauter, 2019. "Selling reduction versus Niggli reduction for crystallographic lattices", *Acta Cryst.* A75:1 115 – 120.

<https://doi.org/10.1107/S2053273318015413>

Y. Gao, W. Xu, W. Shi, A. Soares, J. Jakoncic, S. Myers, B. Martins, J. Skinner, Q. Liu, H. Bernstein, S. McSweeney, E. Nazaretskia, M. R. Fuchs, 2018. "High-speed raster-scanning synchrotron serial microcrystallography with a high-precision piezo-scanner", *J. Sync. Rad.* 25:5 1362 – 1370.

P. A. Craig, T. Anderson, H. J. Bernstein, C. Daubner, A. Goodman, S. M. Irby, J. Koeppe, J. L. Mills, M. Pikaart, A. R. McDonald, S. O'Handley, R. Roberts, R Stewart, 2018. "Using Protein Function Prediction to Promote Hypothesis-Driven Thinking in Undergraduate Biochemistry Education", *The Chemist* 91:1 1 – 8.

http://theaic.org/pub_thechemist_journals/Vol-91-No-1/Vol-91-No1-Article-1.html

H, J. Bernstein, B. Andi, K. Badalian, L. E. Berman, D. K. Bhogadi, S. Chodankar, J. DiFabio, M. R. Fuchs, J. Jakoncic, E. O. Lazo, S. McSweeney, L. Miller, S. Myers, D. K. Schneider, B. Seiva Martins, W. Shi, J. Skinner, H. Slepicka, A. S. Soares, V. Stojanoff, R. M. Sweet, R. Tappero, 2016. "Computing Infrastructure, Software Optimization, and Real Time Analysis for High Data-Rate MX", In *Scientific Data Summit (NYSDS) 2016*, New York pp. 1 – 4. IEEE.

- H. J. Bernstein, L. C. Andrews. 2016. "Accelerating k-nearest-neighbor searches", *J Appl. Cryst.* 49:5 1471 – 1477.
<https://doi.org/10.1107/S1600576716011353>
- L. C. Andrews, H. J. Bernstein, 2016. "*NearTree*, a data structure and a software toolkit for the nearest-neighbor problem", *J Appl. Cryst.* 49:3 756 – 761. <https://doi.org/10.1107/S1600576716004039> eCollection 2016 June 1. PubMed PMID: 27275134; PubMed Central PMCID: PMC4886977.
- H. J. Bernstein, J. C. Bollinger, I. D. Brown, S. Gražulis, J. R. Hester, B. McMahon, N. Spadaccini, J. D. Westbrook and S. P. Westrip, 2016. Specification of the Crystallographic Information File format, version 2.0. *J. Appl. Cryst.* 49:1 277 – 284.
<https://doi.org/10.1107/S1600576715021871>
- M. Osipovitch, M. Lambrecht, C. Baker, S. Madha, J. L. Mills, P. A. Craig, H. J. Bernstein, 2015. "Automated protein motif generation in the structure-based protein function prediction tool ProMOL", *J. Struct. Funct. Genomics* 16:3-4 101 – 111.
<https://doi.org/10.1007/s10969-015-9199-0> Epub 2015 November 16. PubMed PMID: 26573864; PubMed Central PMCID: PMC4684744
- C. C. Grills, J. A. Farrington, B. H. Layne, J. M. Preses, H. J. Bernstein, J. F. Wishart, 2015. "Development of nanosecond time-resolved infrared detection at the LEAF pulse radiolysis facility", *Rev. Sci. Instrum.* 86:4 044102.
<http://dx.doi.org/10.1063/1.4918728>
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- M. Rosa, P. A. Craig, H. J. Bernstein, 2009. "Lee-Richards Approximation by Intra-Residue Reentrant Surface Exclusion," talk (abstract 118), Rochester Institute of Technology 18th Annual Undergraduate Research Symposium, 7 August 2009, RIT, Rochester, NY.
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- H. J. Bernstein, 2008. "Designing Molecular Graphics Software for Teaching: Getting the Scripting Language Right," talk at 2008 MACTLAC Annual Meeting, Molecular Visualization: Do Our Students See What We See? October 17 – 18, 2008, University of Dubuque, Dubuque, IA.
- H. J. Bernstein, 2008. "Transition to object-oriented data representations: Interconversion between CIF and other formats," invited talk MS.96.3, XXI Congress of the International Union of Crystallography, 23 – 31 August 2008, Osaka, Japan, (see abstract in Acta Cryst. A64 (on-line supplement), page C160).
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- P. A. Craig, S. E. Mottarella, C. Wischmeyer, H. J. Bernstein, I. Awuah Asiamah, D. Boycheva, G. Darakev, N. Darakev, P. Gozo, J. Jemilawon, 2008. "Using RasMol, PyMol and Jmol with the Structural Biology Extensible Visualization Scripting Language (SBEVSL)," poster MP054 (abstract W0073), ACA 2008, American Crystallographic Association Meeting, 31 May – 5 June 2008, Knoxville, TN.
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H. J. Bernstein, 2001. "To Transpose or Not to Transpose; That is the Question – Performance Issues in the use of Java-based XML Software for Real-World Problems" presentation, Design and Analysis Research Seminar, Computer Science Department, SUNY at Stony Brook, 26 September 2001.

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