

Philip E. Bourne, Ph.D., FACMI

Stephenson Founding Dean, School of Data Science
Professor of Data Science
Professor of Biomedical Engineering
The University of Virginia
Cell: 858 354 8301; peb6a@virginia.edu

http://en.wikipedia.org/wiki/Philip_Bourne
Google Scholar: <https://scholar.google.com/citations?hl=en&user=Y9q2zZAAAAAJ>
<https://engineering.virginia.edu/faculty/philip-e-bourne>
<https://datascience.virginia.edu/people/phil-bourne>

Last Update: May 2024
Citations: 87,731; h-index 84; [i10-index](#) 236 (source Google Scholar)
In the top ten most cited scholars in the history of The University of Virginia

EDUCATION

- **1976-1980 Ph.D. Major - Chemistry** X-ray structure analysis of anti-cancer drugs, nucleic acid-metal complexes and caged hydrocarbons. Software development for small molecule crystallography. The Flinders University, South Australia.
- **1975 B.Sc.(Hon.) Major - Chemistry** X-ray structure analysis of drugs in the treatment of diabetes mellitus. The Flinders University, South Australia.
- **1971-1974 B.Sc. Major - Chemistry** The Flinders University, South Australia.

ACADEMIC EXPERIENCE

- **2019- Founding Dean**, School of Data Science, University of Virginia.
- **2019- Professor of Data Science**, University of Virginia.
- **2017- Stephenson Professor of Data Science**, University of Virginia.
- **2017-2019 Director Data Science Institute**, University of Virginia.
- **2017- Professor of Biomedical Engineering**, University of Virginia.
- **2014- 2017 Associate Director for Data Science**, National Institutes of Health.
- **2014- 2017 Senior Investigator**, National Center for Biotechnology Information.
- **2012- 2014 Associate Vice Chancellor for Innovation and Industrial Alliances**, UCSD.
- **2001-2014 Professor**, Skaggs School of Pharmacy & Pharmaceutical Sciences, UCSD.
- **2001-2004 Director**, Integrated Biosciences Program, San Diego Supercomputer Center.
- **2000-2004 Adjunct Professor**, The Keck Graduate Institute, Claremont.
- **1997-2014 Adjunct Professor**, The Sanford Burnham Medical Research Institute, San Diego.
- **1998-2001 Senior Principal Scientist**, San Diego Supercomputer Center, San Diego.
- **2000 Professor in Residence**, Dept. of Pharmacology, UCSD.
- **1998-2014 Associate Director**, RCSB Protein Data Bank, UCSD.
- **1996-2000 Adjunct Associate Professor**, Dept. of Pharmacology, UCSD.
- **1995-1998 Senior Staff Scientist**, San Diego Supercomputer Center.

- **1994-1995 Senior Research Scientist**, Dept. of Biochemistry & Molecular Biophysics, Columbia University, New York.
- **1987-1995 Senior Associate**, Howard Hughes Medical Institute, Columbia University, New York.
- **1987-1994 Research Scientist**, Dept. of Biochemistry & Molecular Biophysics, Columbia University, New York.
- **1985-1986 Director**, Basic Science Information Systems, Health Sciences Administration, Columbia Presbyterian Medical Center, New York.
- **1984-1986 Director**, Health Sciences Computer Facility, Columbia University, New York.
- **1982-1986 Director**, Cancer Center Computing Facility, Dept. of Biochemistry & Molecular Biophysics, Columbia University, New York.
- **1981-1982 Senior Research Associate**, Dept. of Biochemistry & Molecular Biophysics, Columbia University, New York.
- **1981 Visiting Scientist**, Dept. of Chemistry, Adelaide University, South Australia.
- **1979-1981 Postdoctoral Fellow**, Dept. of Biochemistry, Sheffield University, U.K.

AWARDS - NOTABLE

- **2022** Special [Honoree Issue of Biomolecules](#) ISSN 2218-273X
- **2018** Elected Fellow Am. Inst. for Biomedical and Medical Engineering.
- **2017** Special Director's Recognition Award for Data Science, NHGRI, NIH.
- **2017** FedHealthIT100 Awardee.
- **2011** Elected Fellow International Society for Computational Biology.
- **2010** Elected Fellow American Association for the Advancement of Science.
- **2010** Jim Gray eScience Award.
- **2009** Benjamin Franklin Award.
- **2005** Editors Choice Award, Science Magazine.
- **2004** Convocation Medal, The Flinders University of South Australia.
- **2002** Convergence Award from Sun Microsystems Inc.
- **2002** Elected Fellow of the American Medical Informatics Association.
- **2001** 2nd most cited paper in biology for 2000 according to Science Watch®.
- **1997** UCSD Connect Award for New Inventions.
- **1996** UCSD Connect Award for New Inventions.
- **1982** National Institutes of Health, Senior Research Scientist.
- **1981** ARGC Visiting Fellowship, Australia.
- **1979** Science Research Council, Post-doctoral Research Fellowship, UK.
- **1974** Commonwealth Postgraduate Research Award, Australia.

COMMERCIAL EXPERIENCE (Major)

- **2022** **Co-Founder** Dark Matter LLC
- **2007** **Co-Founder** SciVee Inc., San Diego.
- **2004** **Co-Founder** Film Frontiers Inc., UK.
- **2001** **Co-Founder** Protein Vision Inc., San Diego.
- **1991** **Founder** ViSoft Inc., New York NY.

PATENTS

- Multimedia user interfaces for documents and associated digital videos, 2008 [WO2008134658A](#)
- Methods for the determination of protein three-dimensional structure employing

PROFESSIONAL ACTIVITIES (Major)

- 2023- **Advisory Board** Metaphysic.
- 2023- **External Advisory Board** USC Viterbi.
- 2022- **Scientific Advisory Board** La Jolla Labs.
- 2022- **Board Member**, eLwazi ODSP (Africa).
- 2022- **Board Member**, Jefferson Science Associates LLC.
- 2021- **Board Member**, Nat. Advisory Environmental Health Sciences Council.
- 2021- **Editorial Board**, Biomolecules.
- 2021- **Scientific Advisory Board**, Global Biodata Coalition.
- 2021- **Advisory Board**, University of Arizona NSF ER2.
- 2021- **Advisory Board**, The Academic Data Science Alliance.
- 2021- **Advisory Board**, Online Ethics Center for Engineering and Science.
- 2019-2024 **Board of Science Councilors**, The Jackson Laboratory.
- 2019 -2023 **Advisory Board**, Data Science Institute, Maastricht University.
- 2019 - **Co-chair Scientific Advisory Board**, ELIXIR.
- 2019-2020 **Scientific Advisory Board**, uBiome.
- 2019-2020 **Advisory Board**, School of Pharm. Sci. & Tech., Tianjin University
- 2019 - **Advisory Board**, Harvard Review of Data Science.
- 2018- **Editor**, Data Science, Methods, Infrastructure and Applications.
- 2018-2021 **Board of Directors**, ASAPbio.
- 2018-2019 **Scientific Advisory Committee**, Oak Ridge National Laboratory.
- 2018-2021 **Committee Member**, Open Research Fund, Wellcome Trust.
- 2016-2020 **Faculty**, F1000.
- 2014- **Editor**, Database.
- 2013-2014 **President**, FORCE11.
- 2011-2014 **Scientific Advisory Board**, Receptos Pharmaceuticals Inc.
- 2010-2015 **Advisory Board**, National Library of Medicine, PubMed Central.
- 2010-2014 **Advisory Board**, Microsoft External Research.
- 2010- 2014 **Editorial Board**, Journal of Biomedical Semantics.
- 2009-2014 **Advisory Board**, Interpro.
- 2006-2010 **Advisory Board**, Crossref.
- 2006-2010 **Advisory Board**, EcoCyc.
- 2005-2010 **Advisory Board**, PharmGKB.
- 2004-2011 **Founding Editor in Chief**, PLOS Computational Biology.
- 2004-2008 **Editor**, IEEE Trends in Computational Biology and Bioinformatics.
- 2003-2007 **Editor**, Proteins: Structure, Function and Bioinformatics.
- 2003-2005 **Associate Editor**, Bioinformatics.
- 2003-2008 **Consulting Editor**, BioSilico.
- 2002-2014 **Advisory Board**, NCCR Resource RVBI at UCSF.
- 2002-2003 **President** International Society for Computational Biology.
- 2001- **Advisory Board**, Biopolymers.
- 2000-2003 **Editor**, Bioinformatics.
- 2000 **Consultant**, Structural GenomiX Inc. San Diego CA.
- 2000-2001 **Secretary**, International Society for Computational Biology.
- 1999-2005 **Advisory Board**, Irving Comprehensive Cancer Center, Columbia Uni.
- 1999-2002 **Representative to the AAAS**, American Crystallography Assoc.
- 1997-1999 **Chairman**, Am. Crystallography Assoc. Comp. and Data Committee.
- 1997-1999 **Chairman**, Am. Crystallography Assoc. Computing and Data Committee.
- 1997-2000 **Editor**, Web Alert, Current Opinions in Structural Biology.
- 1996-2005 **Member**, Review Panel - NSF Database Activities Program.

- **1996-1999 Chairman** – Int. Union of Crystallography Computing Commission.
- **1991-2005 Member** - mmCIF Working Group – Int. Union of Crystallography.
- **1994 Consultant** - Smith Kline Beecham Pharmaceuticals.
- **1991-1993 Consultant** - Ontario Hydro, Canada.
- **1990 Consultant** - European Database Bridge Project, Belgium.
- **1988-1997 Editor** - *Digital Age Magazine* (formally *The DEC Professional*).
- **1979-1981 Member** - Collaborative Computational Project for Protein Crystallography, Science Research Council, UK.

PRIOR UNIVERSITY COMMITTEES – NOTEWORTHY

- **2023 Chair** UVA Biocomplexity Institute 5 year review.
- **2022 Chair** UVA Search Committee AVP Research Computing.
- **2021 UVA Representative** to the NASEM Committee on Open Knowledge.
- **2021 Member** UVA Interdisciplinary Research Building Committee.
- **2021 Member** UVA Dean of Engineering Search Committee.
- **2019 Member** UVA Strategic Planning Committee.
- **2019 Member** UVA Provost Search Committee.
- **2018 Chair** UVA Committee on Data Science Credentials.
- **2017 Chair** UVA Cluster hire in Biomedical Data Science.
- **2009-2011 Co-Chair** UCSD University Industry Relations Task Force.
- **2009-2012 Chair** UCSD Library Committee.
- **2007- 2010 Member** UCSD Senate Representative.
- **2003-2010 Chair** Second Year Bioinformatics Program Qualifying Exam Committee.
- **2001-2005 Member** Pharmacy School Planning Committee.
- **2000-2008 Member** MD/PhD Admissions Committee.
- **2000-2014 Member** Bioinformatics Graduate Student Program Steering Committee.
- **2000-2010 Member** Ad hoc Promotions Committee, San Diego Supercomputer Center.

MEMBERSHIP OF SOCIETIES (Not necessarily current)

- American Institute for Biomedical and Medical Engineering (AIMBE).
- American Association for the Advancement of Science (AAAS).
- American Medical Informatics Association (AMIA).
- Institute of Electrical and Electronics Engineers (IEEE).
- International Society for Computational Biology (ISCB).
- American Chemical Society (ACS).
- American Crystallography Association (ACA).
- Biophysical Society.
- Protein Society.

GRANTS ~\$50M in prior grants; average ~\$2M per year

- *2018 – Research supported by the Stephenson and Quantitative Foundation Endowments to the Founding Dean of the School of Data Science, University of Virginia.*
- *2014 – 2017 Research funded by the NIH Intramural Program while the Associate Director for Data Science (ADDS).*
- NSF 0829586 (Co-PI) PDB Management by the Research Collaboratory for Structural Bioinformatics 2009-13 \$32,076,399.
- NSF 1216893 Conceptualization and Analysis of a 3D Virtual Cell 2012-3 \$625,830
- Sloan Foundation (PI) Beyond the PDF Workshop 2012 \$214,720.

- [5R01GM078596-04](#) (PI) NIH-NIGMS Protein Functional Site Characterization and Analysis (PI) 2007-2011 \$548,820.
- NSF 0732706 (PI) SGER: ScTube.tv: Video Delivery of Papers Published in PLOS 2009-10 \$177,620.
- [1R41 RR025720](#) (PI) NIH-NCRR SciVee Pubcasts – New Modes of Scientific Dissemination (PI) 2009 \$141,026.
- NSF 0737714 (PI) Cyberbridge 2007-10 \$1,195,636
- [5P01 GM063208](#) (PI) NIH-NIGMS Tools and Data Resources in Support of Structural Genomics (PI) 2002-2009 \$5,000,000
- NSF 0620405 (PI) ISMB 2006 Conference Support for Students and Young Investigators 2006 \$40,000.
- NSF 0544575 (PI) BioLit: Open Source Tools for Integrating Biological Literature and Databases 2006-2008 \$953,466.
- NSF 0505980 (PI) ISMB 2005 Conference Support for Students and Young Investigators 2006 \$30,000.
- NSF 0440678 (PI) ISMB 2005 Conference Support for Students and Young Investigators 2006 \$55,200.
- NSF 0331648 (Co-PI) ITR Collaborative Research Building the Tree of Life 2003-6 \$5,122,999.
- NSF 0111710 (PI) A Public Database Linking Protein Sequence and Structure Mutation Data 2005-7 \$542,739.
- NSF 0111709 (PI) Voltage-gated Ion Channel Protein Resource Database 2001-3 \$240,000
- NSF 0078296 (Co-PI) Computational Quantum Mechanical Biological Framework in Conjunction with the Protein Data Bank 2000-3 \$549,283.
- NSF 0078296 (PI) A Public Database Resource for Apoptosis Research and Education 2000-3 \$518,821.
- NSF 0078274 (PI) A Public Protein Mutation Database 2000-3 \$460,718.
- NSF 9808706 (Co-PI) Database of Classified Proteins based Upon a Composite Property Description 1998-2001 \$450,000.
- NIH 5P41RR008605-08 Molecular Interactive Collaborative Environment (MICE) (PI) 1997-2000 \$450,149.
- NSF 9529557 International Summer School on Macromolecular Crystallographic Computing (PI) 1995 \$5,000.
- NSF 9507625 (PI) Continued Development of a Software Framework to Maintain and Query Features of Biological Macromolecules 1995-6 \$141,007.
- NSF 9630339 (PI) A Portable Client-Server Data Management System for the Comparative Analysis of Proteins 1996-9 \$424,355.
- NSF 9310154 (PI) CIFters: Object Oriented Tools for Manipulating Crystallographic Information Files 1993-6 \$391,935.
- NSF 9116798 (PI) An Object-oriented Toolbox for Use with the Protein Data Bank (PDB) 1992-5 \$1,251,150.

TEACHING EXPERIENCE

General Areas

1974- Biochemistry; biophysics; structural biology; physical and inorganic chemistry; bioinformatics, medical informatics, computational biology, pharmaceutical sciences, scholarly communication, professional development, operating system design; network design; high-level languages; expert systems; database design; object-oriented programming; real-time graphics; scientific programming; hardware architectures; system management; network management; data science; science ethics and policy; health systems science; data science.

Example Courses

- BME 8315 – Systems Bioengineering and Multi-scale Models (2019-2020 UVA)
- BIMS 7100 – Research Ethics (UVA 2020-2021)
- DS 6002 – Ethics of Big Data (UVA 2018)
- Pharm 201 – Biological Data and Analysis (UCSD 2004-2014)
- SSPPS 205 – Pharmacy Informatics (UCSD 2008-2014)

PUBLICATIONS – Peer Reviewed Research Articles

1. G.A.Clegg, R.F.D.Stansfield, P.E.Bourne & P.M.Harrison, *Biochemical Society Transactions* (1980) 8(5), 654-655. The Structure and Heavy Metal Ion Binding Sites of Horse Spleen Apoferritin.
2. G.A.Clegg, R.F.D.Stansfield, P.E.Bourne & P.M.Harrison, *Nature* (1980) 288, 298-300. Helix Packing and Subunit Conformation in Horse Spleen Apoferritin.
3. J.R.Helliwell, A.Achari, A.C.Bloomer, P.E.Bourne, P.Carr, G.A.Clegg, R.Cooper et al., *Acta Cryst.* (1981) A37Sup., C311. Protein Crystal Oscillation Film Data Processing: A Comparative Study.
4. D.Akrigg, T.N.Bhat, P.E.Bourne, J.Campbell, M.Elder, P.R.Evans, J.R. Helliwell et al., *Acta Cryst.* (1981) A37Sup., C8. The Collaborative Computational Project for Protein Crystallography.
5. P.E.Bourne, G.A.Clegg, P.M.Harrison, J.M.A.Smith & R.F.D.Stansfield, *Acta Cryst.* (1981) A37Sup., C26. Inter-Subunit Interactions and Metal Binding Sites in Horse Spleen Apoferritin.
6. P.E.Bourne, G.A.Clegg, P.M.Harrison, J.M.A.Smith & R.F.D.Stansfield, *Acta Cryst.* (1981) A37Sup., C14. X-ray Crystallographic Analysis of Horse Spleen Apoferritin.
7. P.E.Bourne & M.R.Taylor, *Acta Cryst.* (1982) B36, 2143-2145. The Structure of Aqua[3-ethoxy-2-oxobutylaldehyde bis(thiosemicarbazone)]zinc(II).
8. P.E.Bourne & M.R.Taylor, *Acta Cryst.* (1983) C39, 430-432. Dicytosinium Tetrachlorozincate.
9. P.E.Bourne & M.R.Taylor, *Acta Cryst.* (1983) C39, 266-268. 3-Thioxo-2-pyridinecarboxylic Acid C₆H₅NO₂S. Redetermination of the Structure.
10. P.E.Bourne, S.Ginell, B.W.Low & L.Lessinger, *Acta Cryst.* (1984) A40 Sup, C83. Caracurine-II Dimethochloride Octahydrate, A Potent Neuromuscular Blocking Agent.
11. P.E.Bourne, S.Ginell, B.W.Low & L.Lessinger, *J. Cryst. & Spec. Res.* (1985) 15, 453-471. The Structure of a Potent Neuromuscular Blocking Agent: Caracurine-II Dimethochloride Octahydrate.
12. P.E.Bourne, A.Sato, P.W.R.Corfield, L.S.Rosen, S.Birken & B.W.Low, *Eur. J. Biochem.* (1985) 153, 521-527. Erabutoxin b: Initial Protein Refinement and Sequence Analysis at 0.140-nm Resolution.
13. P.E.Bourne & N.Desai, *Comp. Methods & Programs in Biomed.* (1987) 24, 27-38. PRONUC: A Software Package for the Analysis of Protein and Nucleic Acid Sequences.
14. P.E.Bourne, *Acta Cryst. Supp.* (1987) A43, C292. Desktop Crystallography - The Next Generation of Computers.
15. P.E.Bourne & W.A.Hendrickson, *Comput. Biol. Med.* (1988) 18, 341-349. Selecting a Processor for Computations in Molecular Biophysics.
16. P.E.Bourne & W.A.Hendrickson, *Comput. Biol. Med.* (1990) 20(4), 219-230. A CPU Benchmark for Protein Crystallographic Refinement.
17. P.E.Bourne, P.L.Marquess, & W.A.Hendrickson, *Acta Cryst. Supp.* (1991) A46, C34-C3. The Crystallographic Workbench.
18. W.Chang, I.N.Shindyalov, C.Pu, & P.E.Bourne, *CABIOS*(1994) 10(6), 575-586. Design and Application of PDBlib, a C++ Macromolecular Class Library.
19. P.Zhang, E.A.Schon, S.G.Fischer, E. Cayanis, J. Weiss, S. Kistler & P.E.Bourne, *CABIOS* (1994) 10(3), 309-317. An Algorithm Based on Graph Theory for the Assembly

- of Contigs in the Physical Mapping of DNA.
20. W.Chang, I.N.Shindyalov, C.Pu, & P.E.Bourne, *Proceedings of the Second International Conference on Intelligent Systems in Molecular Biology* (1994) 70-77. Design and Application of a C++ Macromolecular Class Library.
 21. I.N.Shindyalov, W.Chang, C. Pu, & P.E.Bourne *Protein Engineering* (1994) 7(11), 1311-1322. MMQL An Object Oriented Macromolecular Query Language: Prototype Data Model and Implementation.
 22. I.N.Shindyalov, J.Cooper, W.Chang & P.E.Bourne *Proceedings of the 28th Annual Hawaii International Conference on System Sciences* (1995), 207-217 IEEE Computer Society Press. Design and Use of a Software Framework to Obtain Information Derived from Macromolecular Structure Data.
 23. I.N.Shindyalov & P.E.Bourne *J. App. Cryst.* (1995), 28(6) 847-852. WPDB – PC windows-based Interrogation of Macromolecular Structure.
 24. J.Biggs, C.Pu, A Groeniger & P.E.Bourne *J. App. Cryst.* (1996), 29(4) 484-490. PDBtool: An Interactive Browser and Geometry Checker for Protein Structures
 25. P.E.Bourne & I.N. Shindyalov *Acta Cryst. Sup.* (1996), C78 C-78. A Local Macromolecular Structure Database for Crystallography Laboratories.
 26. Ponomarenko, I.N.Shindyalov & P.E.Bourne *Proceedings of the International Summer School on Crystallographic Computing* (1996) P.E.Bourne & K.Watenpaugh, (Eds.), Fast Substructure Searching Using the Conformational Likeness Method.
 27. P.E.Bourne, H.M.Berman, B. McMahon, K. Watenpaugh, J. Westbrook & P.M.D. Fitzgerald. *Methods in Enzymology.* (1997) 277, 571-590. The Macromolecular CIF Dictionary (mmCIF).
 28. P.E. Bourne, I.N. Shindyalov, J. Moreland G. Johnson, M. Gribskov *FASEB J.* (1997) 11(9) 1564. New Developments in Internet Technology Important to Biochemistry and Molecular Biology.
 29. I.N.Shindyalov and P.E. Bourne *CABIOS* (1997) 13, 487-496. Protein Data Representation and Query Using Optimized Data Decomposition.
 30. J. Biggs, C. Pu, and P.E. Bourne *Fifth International Conference on Intelligent Systems for Molecular Biology* Ed. T. Gaasterland et al. 1997, 52-55. AAAI Press. Code Generation Through Annotation of Macromolecular
 31. C. Smith, M. Gribskov, I.N. Shindyalov, S.S Taylor, L. Ten Eyck, S. Veretnik, P.E.Bourne *TIBS* 1997 22(11) 444-446. The Protein Kinase Resource (PKR).
 32. I.N. Shindyalov and P.E. Bourne *Protein Engineering* 1998, 11(9) 739-747. Protein Structure Alignment by Incremental Combinatorial Extension of the Optimum Path.
 33. P.E.Bourne and I.N. Shindyalov 1998 *Proceedings of ACHE-98*. Ed. D.P. Doctor, D.M. Quinn, R.L. Rotundo, and P. Taylor. A Database of Pairwise Aligned 3-D Structures for the Aceylcholinesterases, Lipases and Other Homologous Proteins p 455-460. Plenum Press NY.
 34. H. Weissig, I.N. Shindyalov, and P.E. Bourne *Acta Cryst* 1998 D54 1085-1094. Macromolecular Structure Databases: Past Progress and Future Challenges.
 35. P.E. Bourne, M. Gribskov, G. Johnson, J. Moreland, and H. Weissig *Pacific Symposium on Biocomputing* 1998 Ed. R Altman, K. Dunker, L.Hunter, and T. Klein pp.118-129. A Prototype Molecular Interactive Collaborative Environment (MICE).
 36. W. Chang and P.E. Bourne *J. App. Cryst.* 1998 31, 505 - 509. CIF Applications: A New Approach for Representing and Manipulating STAR Files.
 37. H.J. Bernstein, F.C. Bernstein, and P.E. Bourne *J. App. Cryst.* 1998, 31, 282 - 295. CIF Applications. pdb2cif: Translating PDB Entries into mmCIF Format.
 38. M.P. Ponomarenko, I.N. Shindyalov, P.E. Bourne, and N.A. Kolchanov LIKENESS: a real-time system for searching and aligning protein spatial structures. *Biofizika*. 1999. V. 44. N. 5. pp. 821-831 (Russ).
 39. P.E.Bourne *Bioinformatics* 15(9) 715-716. Editorial

40. J.G. Tate, J. Moreland and P.E. Bourne *J. App. Cryst.* 32, 1026-1027. MSG (Molecular Scene Generator): A Web-based Application for the Visualization of Macromolecular Structures.
41. G. Quinn, A. Taylor, H-P Wang and P.E. Bourne 1999 *TIBS* 24 321-324. Development of Internet-based Multimedia Applications.
42. H. Weissig, and P.E. Bourne 1999 *Bioinformatics* 15(10) 807-831. An Analysis of the Protein Data Bank in Search of Temporal and Global Trends.
43. G. Quinn, H-P. Wang, D. Martinez, P.E. Bourne 1999 *Pacific Symposium on Biocomputing* Developing Protein Documentaries and other Multimedia Presentations for Molecular Biology. Ed. R Altman, K. Dunker, L. Hunter, T. Klein, and K. Lauderdale pp. 380-391.
44. H.M. Berman, J. Westbrook, Z. Feng, G. Gilliland, T.N. Bhat, H. Weissig, I.N. Shindyalov, and P.E. Bourne 2000 *Nucleic Acid Research* 28(1), 235-242. The Protein Data Bank.
45. I. Tsigelny, I. N. Shindyalov, P. E. Bourne, T. Südhof and P. Taylor *Protein Science* 2000 9(1) 180-185 Common EF-hand Motifs in Cholinesterases and Neuroligins Suggest a Role for CA²⁺ Binding in Cell Surface Associations.
46. J.D. Westbrook and P.E. Bourne *Bioinformatics* 2000 16(2) 159-168. STAR/mmCIF: An Ontology for Macromolecular Structure and Beyond.
47. P.E. Bourne and Michael Gribskov 2000 *Bioinformatics* Editorial 16 749. ISMB2000: Bioinformatics Enters a New Millennium.
48. H.M. Berman, T.N. Bhat, P.E. Bourne, G. Gilliland, H. Weissig, and J. Westbrook 2000 *Nature Structure Biology*, 7sup. 957-959. The Protein Data Bank and the Challenge of Structural Genomics.
49. P.E. Bourne 2000 *Trends in Biotechnology* 2000 18(6), 228-230. Bioinformatics Meets Data Mining, Time to Dance? A Report of the Data Mining Conference held at the EBI from Nov. 10-12, 1999.
50. I.N. Shindyalov and P.E. Bourne 2000 *Proteins: Structure, Function and Genetics* 38(3), 247-260. An Alternative View of Protein Fold Space.
51. B.V.B Reddy, W. Li, I.N. Shindyalov, and P.E. Bourne 2001 *Proteins: Structure, Function and Genetics* 42(2) 148-163. Conserved key amino acid positions (CKAAPs) derived from the analysis of common substructures in proteins.
52. W.W. Li, B.V.B. Reddy, I.N. Shindyalov and P.E. Bourne 2001 *Nucleic Acids Research*, 29(1) 329-331. CKAAPs DB: A Conserved Key Amino Acid Position Database.
53. I.N. Shindyalov and P.E. Bourne 2001 *Nucleic Acids Research*, 29(1) 228-229. A Database and Tools for 3-D Protein Structure Comparison and Alignment Using the Combinatorial Extension (CE) algorithm.
54. H.M. Berman, T.N. Bhat, P.E. Bourne, G. Gilliland, H. Weissig, and J. Westbrook 2001 *Nucleic Acids Research*, 29(1) 214-218, The PDB Uniformity Project.
55. C. Guda, E.D. Scheeff, P.E. Bourne and I.N. Shindyalov 2001 *Pacific Symposium on Biocomputing* 6: 275-286. A New Algorithm for Alignment of Multiple Protein Structures Using Monte Carlo Optimization.
56. J.G. Tate, J. Moreland, and P.E. Bourne 2001 *J. Mol. Graphics* 19 280-287. Design and Implementation of a Collaborative Molecular Graphics Environment.
57. H.M. Berman, J. Westbrook, Z. Feng, G. Gilliland, T.N. Bhat, H. Weissig, I.N. Shindyalov, and P.E. Bourne 2001 *International Tables Chapter 24 Crystallographic Databases* 675-681. The Protein Data Bank.

58. I.N.Shindyalov and P.E.Bourne 2001 The 2001 International Conference on Mathematics and Engineering Techniques in Medicine and Biological Sciences (METMBS'2001). Protein Sequence-Structure Space and Data Redundancy in The Protein Data Bank 139-145.
59. A. Kuller, W. Fleri, W.F. Bluhm, J.L. Smith, J. Westbrook and P.E.Bourne 2001. Announcement of the BioSync Web Site. *Nature Structure Biology* 8(8) 663.
60. H.M. Berman, T. Battistuz, T.N.Bhat, W.F. Bluhm, P.E. Bourne, K. Burkhardt, Z. Feng, G.L. Gilliland, L. Iype, S. Jain, P. Fagan, J. Marvin, V. Ravichandran, B. Schneider, N. Thanki, D. Padilla, H. Weissig, J.D. Westbrook, C. Zardecki 2002 The Protein Data Bank *Acta Cryst.* D58, 899-907.
61. A. Kuller, W. Fleri, W.F. Bluhm, J.L. Smith, J. Westbrook and P.E.Bourne 2001. BioSync: A Biologist's Guide to Synchrotron Resources *TIBS* 27(4):213-215
62. H.M. Berman, D. Goodsell and P.E. Bourne 2002 Proteins Structures: From Famine to Feast *American Scientist* 90: 350-359.
63. J. Westbrook, Z.Feng, S. Jain, T.N.Bhat, N. Thanki, V.Ravichandran, G.L.Gilliland, W.Bluhm, H. Weissig, D.S.Greer, P.E.Bourne, and H.M.Berman 2002 The Protein Data Bank: Unifying the Archive. *Nucleic Acids Research*, 30:245-248.
64. W. Li, BVB Reddy, J. Tate, IN Shindyalov and P.E.Bourne 2002 CKAAPs DB: A Conserved Key Amino Acid Positions Database. *Nucleic Acids Research* 30: 409-411.
65. BVB Reddy, W. Li, and P.E.Bourne 2002 Conserved Key Amino Acid Positions Used to Morph Protein Folds. *Biopolymers* 64(3):139-145.
66. H.Weissig and P.E. Bourne 2002 Protein Structure Resources *Acta Cryst.* D 58(6) 908-915.
67. P.E. Bourne 2002 Science's Policy on Data Deposition. *Science* 296, 1609.
68. DS. Greer, JD. Westbrook and PE. Bourne 2002 An Ontology Driven Architecture for Derived Representations of Macromolecular Structure *Bioinformatics* 18:1280-1281.
69. P Craig, P Yang and PE Bourne 2002 BioEditor A Tool for Structure Annotation *FASEB J* 16 (5): A741-A742.
70. J.V. Ponaramenko, I.N. Shindyalov and P.E. Bourne 2002 Building an Automated Classification of DNA-binding Protein Domains *Bioinformatics* 18:S192-201.
71. P.E.Bourne 2003 Free access to publicly funded databases is vital *Nature* 421, 786.
72. P. Yang, P.A. Craig, D. Goodsell and P.E. Bourne 2002 BioEditor - Simplifying Macromolecular Structure Annotation *Bioinformatics*. 19(7) 897-898.
73. K.S. Doctor, J. Reed, A. Godzik and P.E. Bourne 2002 The Apoptosis Database *Cell Death and Differentiation* 10(6), 621-633.
74. P.E. Bourne 2003 The Status of Structural Genomics *Targets* 2(5) 1181-1182 (Editorial).
75. W.G Krebs and P.E. Bourne 2003 Statistical and Visual Morph Movie Analysis of Crystallographic Mutant Selection Bias in Protein Mutation Resource Data. *Proceedings of the 2003 IEEE Computer Society Bioinformatics Conference Proceedings* 180-189.
76. P.M.D. Fitzgerald, J. Westbrook, P.E. Bourne, B. McMahon, K.D. Watenpaugh, and H.M. Berman 2003 The Macromolecular Crystallographic Information File (mmCIF) *The International Tables for X-ray Crystallography* Volume G.
77. W.W. Li, G.B. Quinn, N. N. Alexandrov, P.E. Bourne and I.N. Shindyalov 2003 Proteins of *Arabidopsis thaliana* (PAT) database: A resource for comparative proteomics *Genome Biology* 4(8), R51.

78. Y. Jia, G.T. Dewey, I.N. Shindyalov and P.E. Bourne 2004 A New Scoring Function and Associated Statistical Significance for Structure Alignment by CE. *J. Comp. Biol.* 11(5) 787-799.
79. W.G Krebs and P.E. Bourne 2004 Statistical and Visual Morph Movie Analysis of Crystallographic Mutant Selection Bias in Protein Mutation Resource Data. *J. Bioinformatics and Computational Biology*, 2(1) 61-75.
80. C. Guda, S. Lu, E.D. Scheeff, P.E. Bourne and I.N. Shindyalov 2004 CE-MC: A multiple protein structure alignment server. *Nucleic Acids Research*, 32 W100-W103.
81. S. Verentik, P.E. Bourne, N.N. Alexandrov, I.N. Shindyalov 2004. Towards consistent assignment of structural domains in proteins. *Journal of Molecular Biology*, 339(3), 647-678.
82. D. Pekurovsky, I.N. Shindyalov, P.E. Bourne 2004 High Throughput Biological Data Processing on Massively Parallel Computers. A Case Study of Pairwise Structure Comparison and Alignment Using the Combinatorial Extension (CE) Algorithm. *Bioinformatics*, 20(12) 1940-1947.
83. P.E. Bourne, J. Westbrook and H.M. Berman 2004. The Protein Data Bank and Lessons Learned in Data Management. *Briefings in Bioinformatics*. 5(1), 23-30.
84. W.G. Krebs and P.E. Bourne 2004 Statistically Rigorous Automated Protein Annotation *Bioinformatics* 10(7) 1066-1073.
85. H.M. Berman, P.E. Bourne and J. Westbrook 2004 The Protein Data Bank: A Case Study in the Management of Community Data. *Current Proteomics* 1, 49-57.
86. P.E. Bourne, K.J. Address, W.F. Bluhm, L. Chen, N. Deshpande, Z. Feng³, R. Kramer Green, J. C. Merino-Ott, W. Townsend-Merino, H. Weissig, J. Westbrook, H. M. Berman 2004. The Distribution and Query Systems of the RCSB Protein Data Bank *Nucleic Acids Research*, 32, D223-225.
87. P.E. Bourne, C.K.J. Allerston, W. Krebs, W. Li, I.N Shindyalov, A. Godzik, I. Friedberg, T. Liu, D. Wild, S. Hwang, Z. Ghahramani L. Chen, and J. Westbrook 2004. The Status of Structural Genomics through the analysis of current targets and structures. 2004 *Pacific Symposium on Biocomputing* 404-416.
88. B. Peters, J. Sidney, P.E. Bourne, H-H Bui, S. Buus, G. Doh, W. Fleri, M. Kronenberg, R. Kubo, O. Lund, D. Nemazee, J.V. Ponomarenko, M. Sathiamurthy, S. Schoenberger, S. Stewart, P. Surko, S. Way, S. Wilson, A. Sette 2005 The Immune Epitope Database and Analysis Resource: From Vision to Blueprint. *PLoS Biology*, 3(3) e91.
89. Shahab, A., Chuon, D., Suzumura, T., Li, W. W., Byrnes, R. W., Tanaka, K., Ang, L., Matsuoka, S., Bourne, P. E., Miller, M. A. & Arzberger, P. W. 2005. Grid Portal Interface for Interactive Use and Monitoring of High-Throughput Proteome Annotation. *Lecture Notes In Computer Science*, 3370:53-67.
90. Birnbaum, A., Hayes, J., Li, W. W., Miller, M. A., Arzberger, P.W., Bourne, P. E. & Casanova, H. 2005. Grid Workflow Software for High-Throughput Proteome Annotation Pipeline. *Lecture Notes In Computer Science*, 3370: 68-61.
91. J.L. Moreland, A.Gramada, O.V. Buzko and P.E. Bourne 2005 The Molecular Biology Toolkit (mbt): A Modular Platform for Developing Molecular Visualization Applications. *BMC Bioinformatics*, 6:21.
92. J.V. Ponomarenko, P.E. Bourne and I.N. Shindyalov 2005 Assigning New GO Annotations to Protein Data Bank Sequences by Structural Homology *Proteins: Structure, Function and Bioinformatics* 58: 855-865.
93. S. Yang, R.F. Doolittle and P.E. Bourne 2005 Phylogeny Determined through Protein Domain Content *Proc. Nat. Acad. Sci. (USA)* 102(2): 373-378.
94. N. Deshpande, K.J. Address, W.F. Bluhm, J.C. Merino-Ott, W. Townsend-Merino, Q. Zhang, C. Knezevich, L. Chen, Z. Feng, R. Kramer Green, J.L. Flippen-Anderson, J. Westbrook, H.M. Berman and P.E. Bourne 2005 The RCSB Protein Data Bank: A

- Redesigned Query System and Relational Database Based on the mmCIF Schema *Nucleic Acids Research*. 33: D233-D237.
95. PC Babbitt, PE Bourne, SD Mooney 2005 Introduction to informatics approaches in structural genomics: modeling and representation of function from macromolecular structure. *Pacific Symposium on Biocomputing* 319-321.
 96. B. Peters, J. Sidney, P.E. Bourne, H-H Bui, S. Buus, G. Doh, W. Fleri, M. Kronenberg, R. Kubo, O. Lund, D. Nemazee, J.V. Ponomarenko, M. Sathiamurthy, S. Schoenberger, S. Stewart, P. Surko, S. Way, S. Wilson, A. Sette 2005 The Design and Implementation of the Immune Epitope Data Base and Analysis Resource *Immunogenetics*. 57(5): 326-36.
 97. P.E. Bourne, S.E. Brenner, M.B. Eisen (2005) PLoS Computational Biology: A New Community Journal. *PLoS Comp Biol* 1(1): e4
 98. L. Xie and P.E. Bourne 2005 Functional Coverage of the Human Genome by Existing Structures, Structural Genomics Targets and Homology Models. *PLoS Comp Biol* 1(3) e31
 99. M. Sathiamurthy, B. Peters, H. Bui, J. Sidney, J.Mokili, S.S. Wilson, W. Fleri, D.L. McGuinness, P.E. Bourne and A. Sette 2005 An Ontology for Immune Epitopes: Application to the Design of a Broad Scope Database of Immune Reactivities *Immunome Research* 1:2
 100. P.E. Bourne 2005 In the Future will a Biological Database Really be Different from a Biological Journal? *PLoS Comp. Biol.* 1(3) e34
 101. P.E. Bourne 2005 Ten Simple Rules for Getting Published *PLoS Comp. Biol.* 1(5) e57.
 102. E. Scheeff and P.E. Bourne 2005 Structural Evolution of the Protein Kinase-Like Superfamily *PLoS Comp. Biol.* 1(5): e49.
 103. A. Kouranov, L. Xie, J. de la Cruz, L. Chen, J. Westbrook, P.E. Bourne and H.M. Berman 2006 The RCSB PDB Information Portal for Structural Genomics *Nucleic Acids Research*, 34 D302-5.
 104. E.D Scheeff and P.E. Bourne 2006 Application of Protein Structure Alignments to Iterated Hidden Markov Model Protocols for Structure Prediction. *BMC Bioinformatics*, 7:410.
 105. P.E.Bourne and L.M.Chalupa 2006 Ten Simple Rules for Getting a Grant *PLoS Comp. Biol.*, (Editorial) 2(2) e12.
 106. H.M. Berman, S.K. Burley, W. Chiu, A. Sali, A. Adzhubei, P.E. Bourne, S.H. Bryant, R.L. Dunbrack, Jr., K. Fidelis, J. Frank, A. Godzik, K. Henrick, A. Joachimiak, B. Heymann, D. Jones, J.L. Markley, John Moul, G.T. Montelione, C. Orengo, M.G. Rossmann, B. Rost,²¹ H. Saibil, T. Schwede, D.M. Standley, J.D. Westbrook 2006 Archiving Structural Models of Biological Macromolecules. *Structure*, 14:1211-1217.
 107. P.E.Bourne 2006 One Year of PLoS Computational Biology *PLoS Comp. Biol.*, (Editorial) 2(8):e111.
 108. R. Vita, K. Vaughan, L. Zarebski, N. Salimi, W. Fleri, H. Grey, M. Sathiamurthy, J. Mokili, H-H. Bui, P.E Bourne, J. Ponomarenko, R. DE Castro Jr, R.K Chan, J. Sidney, S.S Wilson, S. Stewart, S. Way, B. Peters and A. Sette 2006 Curation of Complex, Content-dependant Immunological Data *BMC Bioinformatics*, 7(1), 341.
 109. J-L Chung, W. Wang and P.E. Bourne 2006 Exploiting Sequence and Structure Homology to Identify Protein-Protein Binding Sites *Proteins: Structure, Function and Bioinformatics* 62(3) 630-640.
 110. P.E. Bourne and S. Brunak 2006 ISMB 2006 (Editorial) *Bioinformatics* 22(14):e1-2.
 111. J. Gu, M. Gribskov and P.E. Bourne 2006 Wiggle – Predicting Functionally Flexible Regions from Primary Sequence *PLoS Comp. Biol.*, 2(7) e90.

112. P.E.Bourne and A. Korngreen 2006 Ten Simple Rules for Reviewers. *PLoS Comp. Biol.*, (Editorial), 2(9) e110.
113. A. Gramada and P.E. Bourne 2006 Multipolar Representation of Protein Structure *BMC Bioinformatics*, 7:242.
114. T. Holland, S. Veretnik, I.N. Shindyalov, P.E. Bourne 2006 A Benchmark for Domain Assignment from Protein 3-dimensional Structure and it's Applications *J. Mol. Biol.*, 361(3), 562-590.
115. P.E.Bourne and J. McEntyre 2006 Biocurators: Contributors to the World of Science *PLoS Comp. Biol.*, (Editorial) 2(10) e142.
116. P Guda, P.E. Bourne and C. Guda 2006 Conserved Motifs in Voltage-sensing and Pore-forming Modules of Voltage-gated Ion Channel Proteins *Biochem. Biophys. Res. Com.* 352(2) 292-8.
117. P.E. Bourne and I. Friedberg 2006 Ten Simple Rules for Getting a Post Doc. *PLoS Comp. Biol.*, 2(11) e121
118. C.L. Dupont, S. Yang, B. Palenik and P.E. Bourne 2006 Putative Imprints in Modern Proteomes of Ancient Shifts in Trace Metal Geochemistry *Proc Nat Acad Sci (USA)*, 103(47) 17822-17827.
119. P.E.Bourne and J. McEntyre 2006 Biocurators: Contributors to the World of Science *PLoS Comp. Biol.*, (Editorial) 2(10) e142
120. E.D Scheeff and P.E. Bourne 2006 Application of Protein Structure Alignments to Iterated Hidden Markov Model Protocols for Structure Prediction. *BMC Bioinformatics*, 7:410
121. H.M. Berman, S.K. Burley, W. Chiu, A. Sali, A. Adzhubei, P.E. Bourne, S.H. Bryant, R.L. Dunbrack, Jr., K. Fidelis, J. Frank, A. Godzik, K. Henrick, A. Joachimiak, B. Heymann, D. Jones, J.L. Markley, John Moul, G.T. Montelione, C. Orengo, M.G. Rossmann, B. Rost, H. Saibil, T. Schwede, D.M. Standley, J.D. Westbrook 2006 Archiving Structural Models of Biological Macromolecules. *Structure*, 14:1211-1217.
122. P.E.Bourne and A. Korngreen 2006 Ten Simple Rules for Reviewers. *PLoS Comp. Biol.*, 2(9) e110
123. P.E.Bourne 2006 One Year of PLoS Computational Biology *PLoS Comp. Biol.*, 2(8):e111.
124. J. Gu and P.E. Bourne 2007 Ten Simple Rules for Graduate Students. *PLoS Comp. Biol.* 3(11) e229.
125. L. Xie, J. Wang and P.E. Bourne 2007 In Silico Elucidation of the Molecular Mechanism Defining the Adverse Effect of Selective Estrogen Receptor Modulators. *PLoS Comp. Biol.*, 3(11) e217.
126. T.C. Erren, P. Cullen, M. Erren and P.E. Bourne 2007 Ten Simple Rules for Doing Your Best Research, According to Hamming *PLoS Comp. Biol.*, 3(10): e21.
127. P.E. Bourne and S.E. Brenner 2007 Developing Computational Biology *PLoS Comp. Biol* 3(9):e157]
128. J. Ponomarenko and P.E. Bourne 2007 Antibody-Protein Interactions: Benchmark Datasets and Prediction Tools Evaluation *BMC Structural Biology* 7(1):64.
129. J-L Chung, J. Beaver, E.D. Scheeff and P.E. Bourne 2007 Con-Struct Map: a Comparative Contact Map Analysis Tool *Bioinformatics* 23:2491-2492.
130. J.L. Fink and P.E. Bourne 2007 Reinventing Scholarly Communication for the Electronic Age. *CT Watch*, 3(3) 26-31.

131. H.M. Berman, K. Hendrick, H. Nakamura, J. Markley, P.E. Bourne, J. Westbrook (2007) Realism about PDB *Nature Biotechnology*, 25(8) 845-6.
132. L. Hunter, R.B. Altman and P.E. Bourne 2007 The International Society for Computational Biology 10th Anniversary *PLoS Comp. Biol.* 3(6) e135.
133. J-L Chung, W Wang and P.E. Bourne 2007 High-throughput identification of Interacting Protein-Protein Binding Sites. *BMC Bioinformatics*, 8(1): 223.
134. L. Xie and P.E. Bourne 2007 A Robust and Efficient Algorithm for the Shape Description of Protein Structures and Its Application in Predicting Ligand Binding Sites *BMC Bioinformatics*, 8(Suppl 4):S9.
135. P.E. Bourne 2007 Ten Simple Rules for Making Good Oral Presentations, *PLoS Comp. Biol.*, 3(4)e77.
136. J.E Beaver, P.E Bourne and J.V Ponomarenko 2007 EpitopeViewer: a Java Application for the Visualization and Analysis of Immune Epitopes in the IEDB database. *Immunome Research*, 3(1):3.
137. Q. Vicens and P.E. Bourne 2007 Ten Simple Rules for Collaboration *PLoS Comp. Biol.*, 3(3) e44.
138. J. Gu and P.E. Bourne 2007 Allosteric Fluctuation Transitions as Applied to Cyclin Dependent Kinase 2 *BMC Bioinformatics* 8(1):45.
139. P.E. Bourne and J.L. Fink 2008 I am Not a Scientist I am a Number *PLoS Comp. Biol.* 4(12):e1000247.
140. J.V. Ponomarenko, H-H. Bui, W. Li, N. Fusseder, P.E. Bourne, A. Sette and B. Peters 2008 ElliPro: A New Structure-based Tool for the Prediction of Antibody Epitopes, *BMC Bioinformatics* 9:514.
141. A. Gramada and P.E. Bourne 2008 Resolving a Distribution of Charge into Intrinsic Multipole Moments: A Rankwise Distributed Multipole Analysis. *Physical Review E*, 78, 066601.
142. P.D. Karp, G. Sherlock, J.A. Gerlt, I. Sim, I. Paulsen, P.C. Babbitt, K. Laderoute, L. Hunter, P. Sternberg, J. Wooley, P.E. Bourne 2008 Changes to NIH Grant System May Backfire *Science* 322(5905) 1187-1188.
143. M. Corpas, N. Gehlenborg, S. Chandra Janga and P. E. Bourne 2008 Ten Simple Rules for Organizing a Scientific Meeting *PLoS Comp. Biol.* 4(5) e1000024.
144. S. Veretnik, J.L. Fink, and P.E. Bourne 2008 Computational Biology Resources Lack Persistence and Usability. *PLoS Comp. Biol.* . 4(7): e1000136.
145. P.E. Bourne and L.M. Chalupa 2008 A New Approach to Scientific Dissemination *Materials Today* 11(6) 48.
146. R. Bauer, P.E. Bourne, A. Formella, C. Fr  mmel, G. Cornelius G. Christoph, G. Andrean, A. Aysam, A. Hoppe, E-W Knapp, T. Paschel, B. Wittig, V. Ziegler, R. Preissner 2008 Superimpose: A 3D structural superposition server *NAR* 36(S2) W47-54.
147. J.L. Fink, S. Kushch, P. Williams & P.E. Bourne 2008 BioLit: Integrating Biological Literature with Databases *Nucleic Acids Research* 36(S2) W385-389.
148. Q. Zhang, P. Wang, Y. Kim, P. Haste-Andersen, J. Beaver, P.E. Bourne, H-H. Bui, S. Buus, S. Frankild, J. Greenbaum, O. Lund, C. Lundegaard, M. Nielsen, J. Ponomarenko, A. Sette, Z. Zhu, B. Peters 2008 Immune Epitope Database Analysis Resource (IEDB-AR) *Nucleic Acids Research*. 36(S2) W513-W518.
149. P.E. Bourne, J.L. Fink, M. Gerstein 2008 Open Access: Taking Full Advantage of the Content *PLoS Comp. Biol.* 4(3) e1000037.
150. L. Xie and P.E. Bourne 2008 Detecting Evolutionary Linkages Across Fold and Functional Space with Sequence Order Independent Profile-profile Alignments. *Proc. Nat. Acad. Sci. (USA)*, 105(14) 5441-5446.
151. R. Valas and P.E. Bourne 2008 Rethinking Proteasome Evolution: Two Novel

- Bacterial Proteasomes. *J. Mol. Evol.* 66(5) 494-504
152. K. Briedis, A. Starr and P.E. Bourne 2008 Analysis of the Human Kinome Using Methods Including Fold Recognition Reveals Two Novel Kinases *PLoS ONE*, 3(2): e1597.
153. J.G. Caporaso, N. Deshpande, J.L. Fink, P.E. Bourne, K.B. Cohen and L. Hunter 2008 Intrinsic Evaluation of Text Mining Systems May Not Predict Performance on Realistic Tasks. *Pacific Symposium on Biocomputing*, 640-651.
154. S. Gunther, M. Kuhn, M. Dunkel, M. Campillos, C. Senger, E. Petsalaki, J. Ahmed, E. Garcia Urdiales, A. Gewiss, L. Juhl Jensen, R. Schneider, R. Skoblo, R.B. Russell, P.E. Bourne, P. Bork and R. Preissner 2007 SuperTarget and Matador: Resources for exploring drug-target relationships *Nucleic Acids Research*, 36:D919-922.
155. Q. Vicens and P.E. Bourne 2009 Ten Simple Rules for Combining Teaching and Research *PLoS Comp. Biol.* 5(4): e1000358.
156. S.L. Kinnings, N. Liu, N. Buchmeier, P.J. Tonge L. Xie and P.E. Bourne 2009 Drug Discovery Using Chemical Systems Biology: Repositioning the Safe Medicine Comtan to Treat Multi-drug and Extensively Drug resistant Tuberculosis. *PLoS Comp. Biol.* 5(7) e1000423.
157. L. Xie, L. Xie and P.E. Bourne 2009 A Unified Statistical Model to Support Local Sequence Order Independent Similarity Searching for Ligand-binding Sites and Its Application in Genome-based Drug Discovery 2009 *Bioinformatics* 25(12) 305-312.
158. S. Yang and P.E. Bourne 2009 The Evolutionary History of Protein Domains Viewed by Species Phylogeny, *PLoS ONE*, 4(12): e8378.
159. L. Xie, J. Li, L. Xie, and P.E. Bourne 2009 Drug Discovery Using Chemical Systems Biology: Identification of the Protein-Ligand Binding Network To Explain the Side Effects of CETP Inhibitors, *PLoS Comp. Biol.* 5(5).
160. S. Veretnik, C. Wills, P. Youkharibache, R. Valas & P.E. Bourne 2009 Sm/Lsm genes provide a glimpse into the early evolution of the spliceosome, *PLoS Comp. Biol.* 5(3) e10000315.
161. E. Browne, R. Dickin, P.E. Bourne 2009 A Review of 2008 for PLoS Computational Biology *PLoS Comp. Biol.* 5(1) e100027.
162. A. Bateman & P.E. Bourne 2009 Ten Simple Rules for Chairing a Scientific Session *PLoS Comp. Biol.* 5(9):e1000517.
163. R.E. Valas & P.E. Bourne 2009 Structural Analysis of Polarizing Indels: An Emerging Consensus on the Root of the Tree of Life. *Biology Direct*. 4(1) 30.
164. R.E. Valas, S. Yang and P.E. Bourne 2009 Nothing in Protein Structure Classification Makes Sense Except in the Light of Evolution *Current Opinions in Structural Biology* 19:1-6.
165. R.S. Datta, M.W. Lux and P.E. Bourne. 2010 PLoS Computational Biology Postcards from PSB 2010 *PLoS Comp. Biol.* 6(4) e1000746.
166. H. Zhang, P. Wang, N. Papangelopoulos, Y. Xu, A. Sette, P.E. Bourne, O. Lund, J. Ponomarenko, M. Nielsen and B. Peters 2010 Limitations of ab initio Predictions of Peptide Binding to MHC class II Molecules *PLoS ONE* 5(2): e9272.
167. A. Prlic, M.A. Martinez, B.T. Yukich, D. Dimitropoulos, B. Beran, P.W. Rose, P.E. Bourne, J.L. Fink 2010 Integration of Open Access Literature into the RCSB Protein Data Bank Using BioLit. *BMC Bioinformatics* 11:220.
168. J.L. Fink, P. Fericola, R. Chandran, S. Parastatidis, A. Wade, O. Naim, G.B. Quinn & P.E. Bourne 2010 Word Add-in for Ontology Recognition: Semantic Enrichment of Scientific Literature. *BMC Bioinformatics* 11:103.
169. P.E. Bourne, B. Beran, C. Bi, W. Bluhm, R. Dunbrack, A. Prlic, G. Quinn, P. Rose, R. Shah, W. Tao, B. Weitzner, Ben Yukich 2010 Will Widgets and Semantic Tagging Change Computational Biology? *PLoS Comp. Biol.* 6(2) e1000673.
170. R. Dickin, C. Marden, C. Nancarrow & P.E. Bourne 2010 A Review of 2009 for PLoS Computational Biology *PLoS Comp. Biol.* 6(2) e1000687.

171. J.D. Durant, R.E. Amaro, L. Xie, M.D. Urbaniak, M.A.J. Ferguson, A. Haapalainen, Z-J. Chen, A.M. Di Guilmi, F. Wunder, A. Tersteegen. P.E. Bourne & J.A. McCammon 2010 A Multidimensional Strategy to Detect Secondary Pharmacological Targets in the Absence of Global Structure and Sequence Homology *PLoS Comp Biol.* 6(1): e1000648.
172. P.E. Bourne 2010 What Do I Want from the Publisher of the Future? *PLoS Comp Biol* 6(5): e1000787.
173. K. Alden, S. Veretnik, P.E. Bourne 2010 dConsensus: a tool for displaying domain assignments by multiple structure-based algorithms and for construction of a consensus assignment. *BMC Bioinformatics*, 11:310
174. P.E. Bourne, K. Briedis, C. Dupont, R. Valas, S. Yang 2008 Evolution of Molecular Repertoires: Genome Evolution in Evolutionary Genomics and Systems Biology G. Caetano-Anolles (Ed.) Wiley-Blackwell Inc. p153-164.
175. R.S. Datta, M.W. Lux and P.E. Bourne. 2010 PLoS Computational Biology Postcards from PSB 2010 *PLoS Comp. Biol.* 6(4) e1000746.
176. H. Zhang, P. Wang, N. Papangelopoulos, Y. Xu, A. Sette, P.E. Bourne, O. Lund, J. Ponomarenko, M. Nielsen and B. Peters 2010 Limitations of ab initio Predictions of Peptide Binding to MHC class II Molecules *PLoS ONE* 5(2): e9272.
177. A. Prlic, M.A. Martinez, B.T. Yukich, D. Dimitropoulos, B. Beran, P.W. Rose, P.E. Bourne, J.L. Fink 2010 Integration of Open Access Literature into the RCSB Protein Data Bank Using BioLit. *BMC Bioinformatics* 11:220.
178. J.L. Fink, P. Fericola, R. Chandran, S. Parastatidis, A. Wade, O. Naim, G.B. Quinn & P.E. Bourne 2010 Word Add-in for Ontology Recognition: Semantic Enrichment of Scientific Literature. *BMC Bioinformatics* 11:103.
179. P.E. Bourne, B. Beran, C. Bi, W. Bluhm, R. Dunbrack, A. Prlic, G. Quinn, P. Rose, R. Shah, W. Tao, B. Weitzner, Ben Yukich 2010 Will Widgets and Semantic Tagging Change Computational Biology? *PLoS Comp. Biol.* 6(2) e1000673.
180. R. Dickin, C. Marden, C. Nancarrow & P.E. Bourne 2010 A Review of 2009 for PLoS Computational Biology *PLoS Comp. Biol.* 6(2) e1000687.
181. J.D. Durant, R.E. Amaro, L. Xie, M.D. Urbaniak, M.A.J. Ferguson, A. Haapalainen, Z-J. Chen, A.M. Di Guilmi, F. Wunder, A. Tersteegen. P.E. Bourne & J.A. McCammon 2010 A Multidimensional Strategy to Detect Secondary Pharmacological Targets in the Absence of Global Structure and Sequence Homology *PLoS Comp Biol.* 6(1): e1000648.
182. C. L. Dupont, A Butcher, R. Valas, P.E. Bourne, and G. Caetano-Anolles 2010 The Impact of Trace Metal Chemistry on the Evolution of Life *PNAS*, doi: 10.1073/pnas.0912491107.
183. P.E. Bourne 2010 What Do I Want from the Publisher of the Future? *PLoS Comp Biol* 6(5): e1000787.
184. J. Ren, L. Xie, W. Li & P.E. Bourne 2010 SMAP-WS: A Parallel Web Service for Structural Proteomic-wide Ligand-Binding Site Comparison. *NAR*, doi: 10.1093/nar/gkq400.
185. G.B Quinn, G. Berger and P.E. Bourne 2010 Data Encapsulation and Mobile Access to the Protein Data Bank *m-Science Sensing, Computing and Dissemination* Eds E Canessa and M Zennaro, ICTP, Italy ISBN 92-95003-43-8, p189-203.
186. A. Prlic, S. Bliven, P.W. Rose, W.F. Bluhm, C. Bizon, A. Godzik, P.E. Bourne 2010 Precalculated Protein Structure Alignments at the RCSB PDB website. *Bioinformatics* 10.1093/bioinformatics/btq572.
187. R.E. Valas & P.E. Bourne 2010 Save the Tree of Life or Get Lost in the Woods *Biology Direct*, 5:44.
188. K. Alden, S. Veretnik, P.E. Bourne 2010 dConsensus: a tool for displaying domain assignments by multiple structure-based algorithms and for construction of a consensus assignment. *BMC Bioinformatics*, 11:310

189. S.L. , L. Xie, K.H.Fung, R.M. Jackson, L. Xie and P.E. Bourne 2010 The *Mycobacterium tuberculosis* Drugome and its Pharmaceutical Implications. *PLoS Comp. Biol.* 6(11): e1000976.
190. R.L Chang, L. Xie, L. Xie, P.E. Bourne B.O. Palsson 2010 Drug Off-Target Effects Predicted Using Structural Analysis in the Context of a Metabolic Network Model. *Plos Comp. Biol.* 6(9): e1000938
191. P.E. Bourne, K. Briedis, C. Dupont, R. Valas, S. Yang 2010 Genome Evolution Studied through Protein Structure in Evolutionary Genomics and Systems Biology G. Caetano-Anolles (Ed.) Wiley-Blackwell Inc. p153-164.
192. P.E.Bourne 2011 Digital research/analog publishing - one scientist's view *Serials* 24(2) 119-122.
193. F. Lewitter and P.E. Bourne 2011 Teaching Bioinformatics at the Secondary School Level *PLoS Comp Biol* 7(10): e1002242.
194. P.E. Bourne and V. Barbour 2011 Ten Simple Rules for Building and Maintaining a Scientific Reputation *PLoS Comp Biol* 7(6) e1002108.
195. J. Wang, P.E. Bourne, N. Bandeira 2011 Peptide Identification by Database Search of Mixture Tandem Mass Spectra *Mol. Cell Proteomics* 10(12):M111.010017.
196. J. von Eichborn, P.E. Bourne and R. Preissner 2011 Cobweb: A Java Applet for Network Exploration and Visualization *Bioinformatics* 7(12):1725-6.
197. P.W. Rose, W.F. Bluhm, B. Beran, C. Bi, D. Dimitropoulos, D.S. Goodsell, A. Prlic, G.B. Quinn, B. Yukich, H.M. Berman & P.E. Bourne 2011, The RCSB Protein Data Bank: Site Functionality and Bioinformatics Use Cases. *National Cancer Institute, Nature Pathways Interaction Database* doi:10.1038/pid.2011.1.
198. L. Xie, L. Xie and P.E.Bourne 2011 Structure-based Systems Biology for Analyzing Off-target Binding. *Curr. Opinions. in Struct. Biol.* 21:1-11.
199. W.F. Bluhm, B. Beran, C. Bi, D. Dimitropoulos, A. Prlic, G. Quinn, P.W. Rose, C. Shah, B. Yukich, H.M. Berman, P.E. Bourne 2011 Quality Assurance for the Query and Distribution Systems of the RCSB Protein Data Bank, *Database* doi: 10.1093/database/bar003.
200. P.E. Bourne, B. Beran, C. Bi, W.F. Bluhm, D. Dimitropoulos, Z. Feng, D.S. Goodsell, A. Prlic, G. Quinn, P.W. Rose, J. Westbrook, B. Yukich, J. Young, C. Zardecki, and H.M.Berman, 2011 The Evolution of the RCSB Protein Data Bank Website. *WIRE Computational Molecular Science*, DOI: 10.1002/wcms.57.
201. R.E. Valas and P.E. Bourne 2011 The Origin of the Derived Superkingdom: How a Gram-positive Bacterium Crossed the Desert to Become an Archaeon, *Biology Direct* 6:16.
202. G.M. Kuo, J.D. Ma, K.C. Lee and P.E. Bourne 2011 Telemedicine, Genomics and Personalized Medicine: Synergies and Challenges *Current Pharmacogenomics and Personalized Medicine* 9(1), 6-13.
203. S.L. Kinnings, N. Liu, P.J. Tonge, R.M. Jackson, L. Xie and P.E.Bourne 2011 A Machine Learning Based Method to Improve Docking Scoring Functions and its Application to Drug Repurposing *J. Chem. Info. Model.* 51(2), 408-419.
204. L. Xie, T. Evangelidis, L. Xie and P.E. Bourne 2011 Drug Discovery Using Chemical Systems Biology: Weak inhibition of multiple kinases may contribute to the anti-cancer effect of Nelfinavir *PLoS Comp. Biol.* 7(4) e1002037 [Science 2011 332(6030) 648-649].
205. A. Gramada and P.E. Bourne 2011 Coarse-graining the Electrostatic Potential via Distributed Multipole Expansions. *Comp. Phys. Communications*, 182, 1455-1462.
206. G.M. Kuo, J.D. Ma, K.C.Lee, J.R. Halpert, P.E. Bourne, T.G. Ganiats and P.W. Taylor, 2011 Institutional Profile: University of California San Diego Pharmacogenomics Education Program (PharmGenEd): Bridging the Gap Between Science and Practice. *Pharmacogenomics* 12(2), 149-153.

207. R. Dicken, C. Marden, A.M. Collins, R. Nussinov and P.E. Bourne 2011 A Review of 2010 for PLoS Computational Biology, *PLoS Comp. Biol.*, 7(1) e1002003.
208. P.E. Bourne 2011 Ten Simple Rules for Getting Ahead as a Computational Biologist in Academia. *PLoS Comp. Biol.* 7(1) e1002001.
209. J. von Eichborn, M.S. Murgueitio, M. Dunkel, S. Koerner, P.E. Bourne and R. Preissner 2011 PROMISCUOUS: A Database for Network-based Drug Repositioning, *NAR* 39 D1060-6.
210. P.W. Rose, B. Beran, C. Bi, W.F. Bluhm, D. Dimitropoulos, D.S. Goodsell, A. Prlic, M. Quesada, G. Quinn, J.D. Westbrook, J. Young, B. Yukich, C. Zardecki, H.M. Berman, P.E. Bourne 2011 The RCSB Protein Data Bank: Redesigned Website and Web Services *NAR* 39 D392-401.
211. J. Ponomarenko, N. Papangelopoulos, D.M Zajonc, B. Peters, A. Sette, P.E. Bourne 2011 IEDB-3D: Structural Data within the Immune Epitope Database *NAR* 39, D1164-70.
212. N. Rifai, J. Sack, M.A. Keller, A. Acharya, P.E. Bourne, M. Rossner, and S. Wills 2012 Communication of Scientific Information: is it Time to Reassess? *Clinical Chemistry*, 59:4.
213. M. Jolly, A.C. Fletcher & P.E. Bourne 2012 Ten Simple Rules to Protect Your Intellectual Property. *PLoS Comp. Biol.* 8(11): e1002766.
214. P.W. Rose, C. Bi, W.F. Bluhm, D. Dimitropoulos, D.S. Goodsell, A. Prlic, M. Quesada, G.B. Quinn, A. Ramos, J.D. Westbrook, J. Young, C. Zardecki, H.M. Berman & P.E. Bourne 2012 An Update on the RCSB Protein Data Bank. *NAR* 41(D1):D475-D482.
215. P.E. Bourne 2012 Seven Years; Its Time for a Change. *PLoS Comp. Biol.* 8(10): e1002728.
216. A.C. Fletcher & P.E. Bourne 2012 Ten Simple Rules to Commercialize Scientific Research *PLoS Comp. Biol.* 8(9): e1002712.
217. A. Prlic, A. Yates, S.E. Bliven, P.W. Rose, J. Jacobsen, P.V. Troshin, M. Chapman, J. Gao, C.H. Koh, S. Foisy, R. Holland, G. Rimsa, M.L. Heuer, H. Brandstatter, Muller, P.E. Bourne & S. Willis 2012 BioJava: An Open-source Framework for Bioinformatics in 2012, *Bioinformatics*. 10.1093/bioinformatics/bts494.
218. P.E. Bourne 2012 The Reaming of Life: Based on the 2010 Jim Gray eScience Award Lecture. *Concurrency and Computation: Practice and Experience*, 25(4), 445-453.
219. Y. Kim, J. Ponomarenko, Z. Zhu, D. Tamang, P. Wang, J. Greenbaum, A. Sette, O. Lund, P.E. Bourne, M. Nielsen, & B. Peters 2012 Immune Epitope Database Analysis Resource *NAR* 40(W1): W525-530.
220. S.J. Wodak, D. Mietchen, A.M. Collings, R.B. Russell & P.E. Bourne 2012 PLoS Computational Biology Meets Wikipedia *PLoS Comp. Biol.* 8(3): e1002446.
221. P.E. Bourne 2012 The RCSB Protein Data Bank: An Interview with Phil. Bourne, Associate Director RCSB Protein Data Bank. Interviewed by Wendy Warr *J. Comput. Aided Mol. Des.* 26:165-167.
222. M.J. Costello, W.K. Michener, M. Gahegan, Z-Q. Zhang, P.E. Bourne & V. Chavan 2012 Quality Assurance and Intellectual Property Rights in Advancing Biodiversity Data Publication *Global Biodiversity Information Facility* Pp. 33, ISBN: 87-92020-49-6.
223. A.C. Fletcher & P.E. Bourne 2012 Ten Simple Rules for Starting a Company *PLoS Comp Biol.* 8(3): e1002439.
224. R. Dicken, C.J. Hall, L.K. Taylor, A.M. Collins, R. Nussinov & P.E. Bourne 2012 A Review of 2011 for PLoS Computational Biology *PLoS Comp Biol.* 8(1): e10022387.
225. B.K. Rana, P.E. Bourne and P. Insel 2012 Receptor Databases and Computational Websites for Ligand Binding. *Receptor Binding Techniques, Methods in Molecular Biology* A.P. Davenport (Ed.). Springer. 897:1-13.
226. S.J. Ho Sui, R. Lo, A.R. Fernandes, M.DG.Caulfield, J.A Lerman, L. Xie, P.E. Bourne, D.L.Baillie and F.S.L.Brinkman 2012 Raloxifene Attenuates *Pseudomonas*

- aeruginosa* Pyocyanin Production and Virulence. *Int. J. of Antimicrobial Agents* (40)3: 246-251.
227. L. Xie, L. Xie, S.L. Kinnings and P.E. Bourne 2012 Novel Computational Approaches to Polypharmacology as a Means to Define Responses to Individual Drugs, *Annual Review of Pharmacology and Toxicology* 52: 361-379.
228. N. Hecker, J. Ahmed, J. von Eichborn, M. Dunkel, K. Macha, A. Eckert, M.K. Gilson, P.E. Bourne, and R. Preissner 2012 SuperTarget goes quantitative: update on drug-target interactions *Nucleic Acids Res.* 40 (D1) D1113-D1117.
229. T. Alexandrov & P.E. Bourne 2013 Learning How to Run a Lab: Interviews with principle Investigators, *PLOS Comp. Biol.*, 9(11): e1003349.
230. R. Chang, P.E. Bourne & B.O. Palsson 2013 Antibacterial Mechanisms Identified through Structural Systems Pharmacology *BMC Systems Biology*, 7:102.
231. H. Masum, A. Rao, B.M. Good, M.H. Todd, A.M. Edwards, L. Chan, B.A. Bunin, A.I. Su, Z. Thomas, P.E. Bourne 2013 Ten Simple Rules for Cultivating Open Science and Collaborative R&D *PLOS Comp. Biol.* 9(9) e1003244.
232. F(.
233. M.J. Costello, W.K. Michener, M. Gahegan, Z-Q. Zhang, & P.E. Bourne 2013 Biodiversity Data Should be Published, Cited and Peer Reviewed *Trends in Ecology and Evolution*, <http://dx.doi.org/10.1016/j.tree.2013.05.002>.
234. L. Xie, T. Ali, R. Valencia, B.L. Ferreira, V. Xue, M. Tanweer, D. Zhou, G.G. Hahhah, P.E. Bourne & L. Xie 2013 Multiscale Modeling of the Causal Functional Roles of nsSNPs in a Genome-wide Association Study: Application to Hypoxia *BMC Genomics* 14(Suppl 3):S9 doi:10.1186/1471-2164-14-S3-S9.
235. D. Garijo, S. Kinnings, L. Xie, L. Xie, P.E. Bourne & Y. Gil 2013 Quantifying Reproducibility in Computational Biology: The Case of the Tuberculosis Drugome, *PLOS ONE*,8(11): e80278.
236. P.E. Bourne 2013 Lets Make Those Book Chapters Open Too! *PLOS Comp. Biol.* 9(2) e1002941.
237. C. Ng, Y. Zhang, P.E. Bourne & L. Xie 2014 Anti-infectious Drug Repurposing Using an Integrated Chemical Genomics and Structural Systems Biology Approach, *Pacific Symposium on Biocomputing*, 19:136-47.
238. J. Wang, V.G. Anania, J. Knott, J. Rush, J.R Lill, P.E. Bourne & N. Bandeira 2014 A Turn-key Approach for Large-scale Identification of Complex Post-translational Modifications, *J. Proteomics Research* 13 (3): 1190-1199.
239. P.E. Bourne 2014 What Big Data Means to Me *J. Am. Med. Inform. Assoc.* 21:194.
240. J. Wang, V.G. Anania, J. Knott, J. Rush, J.R Lill, P.E. Bourne & N. Bandeira 2014 Combinatorial Approach for Large-scale Identification of Linked Peptides from MS/MS Spectra, *Mol. Cell. Proteomics* 13(4):1128-36.
241. L. Xie, X. Ge, H. Tan, L. Xie Y. Zhang, T. Hart, X. Yang & P.E. Bourne 2014 Towards Structural Systems Pharmacology to Study Complex Diseases and Personalized Medicine *PLOS Comp. Biol.*, 10(5): e1003554.
242. P.E. Bourne 2014 Ten Simple Rules for Approaching a Job Interview, *PLOS Comp. Biol.*, 10(6): e1003660.
243. D. Myers-Turnbull, S.E. Bliven, P.W. Rose, Z.K. Azizd, P. Youkharibache, P.E. Bourne & Andreas Prlic, 2014 Systematic Detection of Internal Symmetry in Proteins using CE-Symm, *J. Mol. Biol.*, <http://dx.doi.org/10.1016/j.jmb.2014.03.010>.
244. J. Wang, P.E. Bourne & N. Bandeira 2014 MixGF: Spectral Probabilities for Mixture Spectra from More Than One Peptide *Mol. Cell Proteomics*, 10.1074/mcp.O113.037218
245. N.P. Rougier M. Droettboom & P.E. Bourne 2014 Ten Simple Rules for Better Figures, *PLOS Comp. Biol.* 10(9): e1003833.

246. G.B. Quinn, C. Bi, C.H. Christie, K. Pang, A. Prlić, T. Nakane, C. Zardecki, M. Voigt, P.E. Bourne, & P.W. Rose 2014 RCSB PDB *Mobile*: iOS and Android mobile apps to provide data access and visualization to the RCSB Protein Data Bank, *Bioinformatics*, 10.1093/bioinformatics/btu596.
247. S. Bliven, P.E. Bourne & A. Prilic 2014 Detection of Circular Permutations within Protein Structures using CE-CP *Bioinformatics*, 10.1093/bioinformatics/btu823.
248. H. Dashnow, A. Lonsdale & P.E. Bourne 2014 Ten Simple Rules for Writing a PLOS Ten Simple Rules Article, *PLOS Comp Biol*, 10(10): e1003858.
249. I. Samish, P.E. Bourne & R. Najmanovich 2014 Achievements and Challenges in Structural Bioinformatics and Computational Biophysics, *Bioinformatics*, 10.1093/bioinformatics/btu769.
250. P.W. Rose, A. Prlić, C. Bi, W.F. Bluhm, C.H. Christie, S. Dutta, R. Kramer Green, D.S. Goodsell, J.D. Westbrook, J. Woo, J. Young, C. Zardecki, H.M. Berman, P.E. Bourne, S.K. Burley 2015 The RCSB Protein Data Bank: Views of Structural Biology for Basic and Applied Research and Education *NAR*, 43 (D1): D345-D356.
251. P. Prins, J. de Light, A. Tarasov, E. Cuppen & P.E. Bourne 2015 Towards Effective Software Solutions for Big Biology, *Nature Biotechnology*, 33(7) 686-7.
252. T.C. Erren, T.E. Slanger, J.V. Groß, P.E. Bourne, & P. Cullen, 2015 Ten Simple Rules for Lifelong Learning According to Hamming, *PLOS Comp Biol*, 11(2) e1004020.
253. P.E. Bourne 2015 DOIs for DICOM raw images – Enabling Science Reproducibility, *Radiology*, 275(1) 3-4.
254. P.E. Bourne 2015 Confronting the Challenges of Big Data in Public Health *PLOS Comp Biol*, 11(2): e1004073.
255. P.E. Bourne, S.E. Brenner & M.B. Eisen, 2015 Ten Years of PLoS‡ Computational Biology: A Decade of Appreciation and Innovation. 10.1371/journal.pcbi.1004317.
256. F.D. Berman & P.E. Bourne 2015 Lets Get Gender Diversity in Science a Priority Right from the Start, *PLOS Biology*, 13(7): e1002206.
257. P.E. Bourne, J.R. Lorsch & E.D. Green 2015 Perspective: Sustaining the Big-Data Ecosystem, *Nature* 527 S16-S17.
258. L. Xie & P.E. Bourne 2015 Opinion: Developing Multi-target Therapeutics to Fine-tune the Evolutionary Dynamics of the Cancer Ecosystem *Frontiers in Pharmacology*, doi: 10.3389/fphar.2015.00209.
259. L.L. Tsai, L. Xie, K. Dore, L. Xie, G. Martinez-Ariza, C. Hulme, R. Malinow, P.E. Bourne, A.C. Newton 2015 Zeta Inhibitory Peptide Disrupts Electrostatic Interactions That Maintain Atypical Protein Kinase C in Its Active Conformation on the Scaffold p62, *JBC*, 10.1074/jbc.M115.676221.
260. P.E. Bourne, V. Bonazzi, M. Dunn, E.D. Green, M. Guyer, G. Komatsoulis, J. Larkin. B. Russell 2015 The Big Data to Knowledge Initiative *JAMIA* 22(6) 1114 10.1093/jamia/ocv136.
261. Z. Zhao, C. Martin, R. Fan, P.E. Bourne & L. Xie, 2016 Drug Repurposing to Target Ebola Virus Replication and Virulence Using Structural Systems Pharmacology, *BMC Bioinformatics*, 17:90 DOI: 10.1186/s12859-016-0941-9.
262. C. Krishna, Li Xie, C. DerMarderosian & P.E. Bourne 2016 Combating Chagas Disease Through Inhibition of Tiam1, a Rho GTPase Guanine Nucleotide Exchange Factor, *bioRxiv*, doi: <http://dx.doi.org/10.1101/040121>.
263. E. Brunk, N. Mih, J. Monk, Z. Zhang, E.J. O'Brien, S.E. Bliven, K. Chen, R.L. Chang, P.E. Bourne, & B.O. Palsson 2016 Systems Biology of the Structural Proteome, *BMC Systems Biology*, 10:26. DOI: 10.1186/s12918-016-0271-6.
264. M.D. Wilkinson, M. Dumontier, I.J. Aalbersberg, G. Appleton, M. Axton, A. Baak, N. Blomberg, J-W. Boiten, L. Bonino da Silva Santos, P.E. Bourne, J. Bouwman, A.J. Brookes, T. Clark, M. Crosas, I. Dillo, O. Dumon, S. Edmunds, C. Evelo, R. Finkers, A. Gonzalez-Beltran, A.J.G. Gray, P. Groth, C. Goble, J.S. Grethe, J. Heringa, P.A.C. 't

- Hoehn, R. Hooft, T. Kuhn, R. Kok, J. Kok, S.J. Lusher, M.E. Martone, A. Mons, A.L. Packer, B. Persson, P. Rocca-Serra, M. Roos, R. Schaik, S-A. Sansone, E. Schultes, T. Sengstag, T. Slater, G. Strawn, M.A. Swertz, M. Thompson, J. van der Lei, E. van Mulligen, J. Velterop, A. Waagmeester, P. Wittenburg, K. Wolstencroft, J. Zhao, and B. Mons, 2016, The FAIR Guiding Principles for Scientific Data Management and Stewardship, *Scientific Data* 3,160018, doi:10.1038/sdata.2016.18.
265. Z. Zhao, L. Xie, L. Xie, P.E. Bourne 2016 Characterizing Kinase-ligand Interactions Across the Human Structural Kinome Using a Functional Site Interaction Fingerprint Approach, *J. Med. Chem.* 59(9) 4326-4341.
266. J.M. Berg, N. Bhalla, P.E. Bourne, M. Chalfie, D.G. Drubin, J.S. Fraser, C.W. Greider, M. Hendricks, C. Jones, R. Kiley, S. King, M.W. Kirschner, H.M. Krumholz, R. Lehmann, M. Leptin, B. Pulverer, B. Rosenzweig, J.E. Spiro, M. Stebbins, C. Strasser, S. Swaminathan, P. Turner, R.D. Vale, K. VijayRaghavan, C. Wolberger 2016 Preprints for the Life Sciences, *Science*, 352(6288) 899-901.
267. E. McKiernan, P.E. Bourne, C. Titus Brown, S. Buck, A. Kendall, J. Lin, D. McDougall, B.A. Nosek, K. Ram, C.K. Soderberg, J. Spies, K. Thaney, A. Updegrave, K.H. Woo, & T. Yarkoni 2016 How Open Science Helps Researchers Succeed, *eLife*, 10.7554/eLife.16800.
268. H.K. Krumholz, P.E. Bourne, K.B. DeSalvo, R.E. Kuntz, H.L. Paz, S.F. Terry, J. Waldstreicher 2016 *Data Acquisition, Curation and Use for a Continuously Learning Health Care System*, Perspectives, National Academy of Medicine, <https://nam.edu/data-acquisition-curation-and-use-for-a-continuously-learning-health-system-a-vital-direction-for-health-and-health-care/>.
269. Y. Zhang, L. Xie, L. Xie & P.E. Bourne 2016 The *Plasmodium falciparum* Drugome and its Polypharmacological Implications *BioRxiv*, doi: <http://dx.doi.org/10.1101/042481>.
270. L. Xie, E.J. Draizen & P.E. Bourne 2017 Harnessing Big Data for Systems Pharmacology, *Annual Review of Pharmacology and Toxicology*, 57: 245-262 doi: 10.1146/annurev-pharmtox-010716-104659. Preprint at: <http://biorxiv.org/content/early/2016/09/23/077115>
271. J. Gao, A. Prlic, C. Bi, W.F. Bluhm, D. Dimitropoulos, D. Xu, P.E. Bourne & P.W. Rose 2017 Biojava-ModFinder: Identification of Protein Modifications in 3D Structures from the Protein Data Bank, *Bioinformatics*, doi: 10.1093/bioinformatics/btx101.
272. X. Zhang, E.J. Pérez-Stable, P.E. Bourne, E. Peprah, K. Duru, N. Breen, D. Berrigan, F. Wood, J.S. Jackson, D.W. Wong, J. Denny 2017 Big Data Science: Opportunities and Challenges to Address Minority Health and Health Disparities in the 21st Century, *Ethnicity and Disease*, 27(2):95-106; doi:10.18865/ed.27.2.95.
273. Z. Zhao, L. Xie & P.E. Bourne 2017 Insights into the Binding Mode of MEK Type-III inhibitors. A Step Towards Discovering and Designing Allosteric Kinase Inhibitors Across the Human Kinome, *PLOS ONE* 12(6): e0179936 <http://biorxiv.org/content/early/2016/09/22/076711>
274. P.E. Bourne, J.K. Polka, R. Kiley, R.D. Vale 2017 Ten Simple to Consider Regarding Preprint Submission. *PLOS Comp. Biol.* 13(5):e1005473. doi: 10.1371/journal.pcbi.1005473. Peerj Preprints <https://peerj.com/preprints/2669.pdf>
275. P.E. Bourne 2017 Ten Simple Rules in Considering a Career in Academia Versus Government *PLOS Comp. Biol.* 13(10): e1005729. <https://doi.org/10.1371/journal.pcbi.1005729>
276. V.R. Bonazzi, P.E. Bourne 2017 Should Biomedical Research be Like Airbnb? *PLOS Biology*. <http://dx.doi.org/10.1371/journal.pbio.2001818>.
277. Z. Zhao, L. Xie, Q. Liu, & P.E. Bourne 2017 Which Cysteines Can Covalently Interact with Irreversible Inhibitors Across the Human Kinome? *J. Med. Chem.* doi: 10.1021/acs.jmedchem.6b01815.

278. P.E. Bourne 2017 Life is 3-dimensional and it begins with Molecules *PLOS Biology* 15(3): e2002041. doi:10.1371/journal.pbio.2002041.
279. E. Kittrie, A.A. Atienza, D. Mietchen, R. Kiley, D. Carr, A. MacFarlane, V. Pai, J. Couch, J. Bajkowski, J.F. Bonner & P.E. Bourne 2017 Developing International Open Science Collaborations – Funder Reflections on the Open Science Prize. *PLOS Biology*, 15(8): e2002617. <https://doi.org/10.1371/journal.pbio.2002617>.
280. M.C. Dunn & P.E. Bourne 2017 Building the Biomedical Data Science Workforce. *PLOS Biology*, 15(7): e2003082 <https://doi.org/10.1371/journal.pbio.2003082>.
281. Z. Zhao & P.E. Bourne 2018 Progress with Covalent Small-molecule Kinase Inhibitors. *Drug Discovery Today*, 23(3) 727-735 <https://doi.org/10.1016/j.drudis.2018.01.035>.
282. V. Navale & P.E. Bourne 2018 Cloud Computing Applications for Biomedical Science: A Perspective *PLOS Comp. Biol.*, 14(6): e1006144. <https://doi.org/10.1371/journal.pcbi.1006144>
283. P. Youkharibache, S. Veretnik, Q. Li, K.A. Stanek, C. Mura & P.E. Bourne 2018 The Small β -barrel Domain: A Survey-based Structural Analysis. *Structure*, in press. <https://doi.org/10.1016/j.str.2018.09.012>
284. P.E. Bourne 2018 Ten Simple Rules When Considering Retirement, *PLOS Comp. Biol.*, 14(10): e1006411 <https://doi.org/10.1371/journal.pcbi.1006411>.
285. C. Mura, E.J Draizen & P.E. Bourne 2018 Structural Biology Meets Data Science: Does Anything Change? *Curr. Op. in Struct. Biol.*, 52: 95-102 <https://doi.org/10.1016/j.sbi.2018.09.003>.
286. P.E. Bourne, F. Lewitter, S. Markel & J.A Papin 2018 One Thousand Simple Rules. *PLOS Comp. Biol.* 14(12): e1006670. <https://doi.org/10.1371/journal.pcbi.1006670>.
287. C. Dreisbach, T.A. Koleck, P.E. Bourne & S. Bakken 2019 Natural Language Processing of Symptoms Documented in Free-text Narratives of Electronic Health Records: A Systematic Review, *JAMIA*, 26(4), 364-379 <https://doi.org/10.1093/jamia/ocy173>
288. F. Lewitter, P.E. Bourne & T.K. Attwood 2019 Ten Simple Rules for Avoiding and Resolving Conflicts with Your Colleagues *PLOS Comp Biol.*, 15(1): e1006708 <https://doi.org/10.1371/journal.pcbi.1006708>
289. S.E. Bliven, A. Lafita, P.W. Rose, G. Capitani, A. Prlic & P.E. Bourne 2019 Analyzing the Symmetrical Arrangement of Structural Repeats in Proteins with CE-Symm *PLOS Comp Biol.* <https://doi.org/10.1371/journal.pcbi.1006842>
290. T.A. Koleck, C. Dreisbach, P.E. Bourne & S. Bakken 2019 A systematic review of natural language processing and text mining of symptoms from electronic patient-authored text data. *Int. J. of Medical Informatics* 125:37-46. <https://doi.org/10.1016/j.ijmedinf.2019.02.008>
291. S. Mullane, Ruoyan Chen, Sri V. Vemulapalli, E.J. Draizen, C. Mura & P.E. Bourne 2019 Machine Learning for Classification of Protein Helix Capping Motifs <https://arxiv.org/abs/1905.00455>.
292. C. Mura, S. Veretnik & P.E. Bourne 2019 The Urfold: Structural Similarity Just Above the Superfold Level? *Protein Science*, 28(12) 2119-2126. doi: 10.1002/pro.3742.
293. N. Breen, D. Berrigan, J.S. Jackson, D.W.S. Wong, F. Wood, J.C. Denny, X. Zhang, & P.E. Bourne 2019 Translational Health Disparities in a Data Rich World. *Health Equity* 3(1), 588-600. <https://doi.org/10.1089/hecq.2019.0042>.
294. P.E. Bourne 2019 Ten Simple Rules to Aid in Achieving a Vision *PLOS Comp Biol.*, 15(10): e1007395. <https://doi.org/10.1371/journal.pcbi.1007395>.
295. Z. Zhao & P.E. Bourne 2020 Revealing Acquired Resistance Mechanisms of Kinase-targeted Drugs Using an On-the-Fly Function-Site Interaction Fingerprint Approach, *J. Chem. Theory & Computation*, 12;16(5):3152-3161. doi: 10.1021/acs.jctc.9b01134

296. G.A. Komatsoulis, N. Weber, D. Tenenbaum & P.E. Bourne 2019 The Commons Credit Model: A New Funding Approach with Potential to Improve Computational Biomedicine. *PLOS Biology*, submitted.
297. A.C. Fletcher, G.A. Wagner & P.E. Bourne 2020 Ten Simple Rules for More Objective Decision Making, *PLOS Comp. Biol.* 16(4):e1007706 <https://doi.org/10.1371/journal.pcbi.1007706>.
298. M. Jaiswal, S. Saleem, Y. Kweon, E.J. Draizen, S. Veretnik, C. Mura, P. E. Bourne 2020 Deep Learning of Protein Structural Classes: Any Evidence for an Urfold? <https://arxiv.org/abs/2005.08443>
299. Hoe-Han Goh & P.E. Bourne 2020 Ten Simple Rules for Researchers While in Isolation from a Pandemic. *PLOS Comp Biol.* 16(6): e1007946. <https://doi.org/10.1371/journal.pcbi.1007946>.
300. C. Mura, M. Chalupa, A.M. Newbury, J. Chalupa & P.E. Bourne 2020 Ten Simple Rules for Starting Research in Your Late Teens. *PLOS Comp. Biol.* 16(11): e1008403. <https://doi.org/10.1371/journal.pcbi.1008403>.
301. Z. Zhao & P.E. Bourne 2020 Structural insights into the binding modes of viral RNA-dependent RNA polymerases using a function-site interaction fingerprint method for RNA virus drug discovery. *J. Proteome Res.* 19(11) 4698-4705 <https://pubs.acs.org/doi/10.1021/acs.jproteome.0c00623>.
302. Hoe-Han Goh & P.E. Bourne 2020 Ten Simple Rules for Writing Scientific Op-Ed Articles. *PLOS Comp. Biol.* 16(9): e1008187. <https://doi.org/10.1371/journal.pcbi.1008187>
303. R. Abel, M.P. Ramos, Q. Chen, H.P. Sánchez, F. Coluzzi, M. Rocco, P. Marchetti, C. Mura, M. Simmaco, P.E. Bourne, R. Preissner and P. Banerjee 2020 Computational prediction of potential inhibitors of the main protease of SARS-CoV-2. *Frontiers in Chemistry.* 8:590263. <https://www.frontiersin.org/articles/10.3389/fchem.2020.590263/full>
304. U. Seeland, F. Coluzzi, M. Simmaco, C. Mura, P.E. Bourne, R. Preissner, S. Preissner 2020 Evidence for treatment with estradiol for women with SARS-CoV-2 infection. *BMC Medicine* 18, 369 <https://doi.org/10.1186/s12916-020-01851-z>
305. M. Parker, A. Burgess & P.E. Bourne 2021 Ten Simple Rules for Starting (and Maintaining) a Data Science Initiative. *PLOS Comp. Biol.* 17(2): e1008628. <https://doi.org/10.1371/journal.pcbi.1008628>.
306. P.E. Bourne 2021 Is Bioinformatics Dead? *PLOS Biology*, 19(3): e3001165. <https://doi.org/10.1371/journal.pbio.3001165>.
307. A.N. Donlan, T.E. Sutherland, C. Marie, S. Preissner, B.T. Bradley, R.M. Carpenter, J.M. Sturek, J.Z. Ma, G.B. Moreau, J.R. Donowitz, G.A. Buck, M. Serrano⁹, S.L. Burgess, M.M. Abhyankar, C. Mura, P.E. Bourne, R. Preissner, M.K. Young, G.R. Lyons, J.J. Loomba, S.J. Ratcliffe, M.D. Poulter, A.J. Mathers, A. Day, B.J. Mann, J.E. Allen, W.A. Petri, Jr 2021 IL-13 is a Driver of COVID-19 Severity 2021 *JCI Insight* 6(15):e150107. <https://doi.org/10.1172/jci.insight.150107>.
308. R.S. Valdez, D. Detmer, P.E. Bourne, K. Kim, R. Austin, A. McCollister, C.C. Rogers & K.C. Walters-Wicks 2021 Informatics-enabled Citizen Science to Advance Health Equity. *JAMIA*, [10.1093/jamia/ocab088](https://doi.org/10.1093/jamia/ocab088).
309. C. Mura, S. Preissner, S. Nahles, M. Heiland, P.E. Bourne, R. Preissner 2021 Real-world Evidence for Improved Outcomes with Histamine Antagonists and Aspirin in 22,560 COVID-19 Patients. *Signal Transduction & Targeted Therapy*, 6:267 <https://doi.org/10.1038/s41392-021-00689-y>.
310. C. Mura, S. Preissner, R. Preissner, P.E. Bourne 2021 A birds-eye (re)view of acid suppression drugs, COVID-19, and the highly variable literature. *Frontiers in Pharmacology*, 12, 2012-. <https://doi.org/10.3389/fphar.2021.700703>.
311. B-O Gohlke, F. Zincke, A. Eckert, D. Kobelt, S. Preissner, J. Liebeskind, N. Gunkel, J. Lewis, S. Preissner, B. Kortium, W. Walther, C. Mura, P.E. Bourne, U. Stein &

- R. Preissner 2022 Real-world Evidence for Preventive Effects of Statins on Cancer Incidence: A transatlantic Analysis, *Clinical and Translational Medicine*. 12(2):e726 doi: 10.1002/ctm2.726. <https://www.medrxiv.org/content/10.1101/2021.07.20.21260891v1>
312. K. Gallo, A. Goede, C. Mura, R. Abel. B. Moahamed. S. Preissner. S. Nahles, M. Heiland, P.E. Bourne, R. Preissner, M. Mallach, 2022 A Comparative Analysis of COVID-19 Vaccines Based on over 580,000 Cases from the Vaccination Adverse Event Reporting System. *Vaccines* 2022, 10, 408. <https://doi.org/10.3390/vaccines10030408>.
313. M. Hertel, M. Heiland, S. Nahles, M. von Laffert, C. Mura, P.E. Bourne, R. Preissner, S. Preissner 2022 Real-world Evidence for Over One-million COVID-19 Vaccinations is Consistent with Reactivation of the Varicella-zoster Virus. *JEADV*, 36(8) 1342-1348 <https://doi.org/10.1111/jdv.18184>.
314. C. Bautista, N. Alfuraiji, A. Drangowska-Way, K. Gangwani, A. de Flamingh & P.E. Bourne 2022 Ten Simple Rules for Improving Communication Among Scientists, *PLOS Comp. Biol.* 18(6) e1010130.
315. C. Borgman & P.E. Bourne 2022 Why It Takes a Village to Manage and Share Data. *Harvard Data Science Review*, 4(3). <https://doi.org/10.1162/99608f92.42eec111>
316. M. Bawn, D. Dent & P.E. Bourne 2022 Ten Simple Rules for using Entrepreneurship Skills to Improve Research Careers and Culture, *PLOS Comp. Biol.* 18(4) e1009946..
317. B.A. Corliss, T.R. Brown, T. Zhang, K.A. Janes, H. Shakeri & P.E. Bourne 2022 The Most Difference in Means: A statistic for Null and Near-Zero Results *Science*, submitted <https://arxiv.org/abs/2201.01239>.
318. N.C. Sheffield, P.E. Bourne, T. Burden, T. Clark, R.L. Grossman, O. Spjuth & A.D. Yates 2022 From Biomedical Cloud Platforms to Microservices: Next Steps in FAIR data and analysis, *Sci Data* 9, 553 <https://doi.org/10.1038/s41597-022-01619-5>
319. P.E. Bourne, V. Bonazzi, A. Brand, B. Carrol, I. Foster, R.V. Guha, R. Hanisch, S.A. Keller, M.L. Kennedy, C. Kirkpatrick, B. Mons, S.M. Nusser, M. Stebbins, G. Strawn, & A. Szalay 2022 A Call to Funders and Policy Makers – Establish an Open Research Commons. *Science*, 377(6603), 256-258. <https://www.science.org/doi/10.1126/science.abo5947>.
320. P.E. Bourne 2022 Ten Simple Rules for Good Leadership. *PLOS Comp. Biol.* 18(6), e1010133.
321. Z. Zhao & P.E. Bourne 2022 Harnessing Systematic Protein-ligand Interaction Fingerprints for Personalized Drug Discovery. *Drug Discovery Today*, 27(10) 103319 <https://doi.org/10.1016/j.drudis.2022.07.004>.
322. E.J. Draizen, S. Veretnik, C. Mura & P.E. Bourne 2022 Deep Generative Models of Protein Structure Uncover Distant Relationships Across a Continuous Fold Space. *Nature Commun.* Submitted. <https://www.biorxiv.org/content/10.1101/2022.07.29.501943v1>
323. D. Chicco & P.E. Bourne 2022 Ten Simple Rules for Organizing a Special Session at a Scientific Conference. *PLOS Comp. Biol.*, 18(8): e1010395. <https://doi.org/10.1371/journal.pcbi.1010395>
324. Z. Zhao & P.E. Bourne 2022 Systematic exploration of privileged warheads for covalent kinase drug discovery. *Pharmaceuticals* 15(11) 1322. <https://doi.org/10.3390/ph15111322>.
325. P.E. Bourne, E.J. Draizen & C. Mura 2022 The Curse of the Ribbon. *PLOS Biol.* 20(12): e3001901. <https://doi.org/10.1371/journal.pbio.3001901>.
326. E.J. Draizen, C. Mura, P.E. Bourne 2022 Explainable Deep Generative Models, Ancestral Fragments and Murky Fragments of the Protein Structure Universe NeurIPS 2022 Accepted. <https://www.biorxiv.org/content/10.1101/2022.11.16.516787v1>
327. T. Cai, L. Xie, S. Zhang, M. Chen, D. He, A. Badkul, Y. Liu, H. K. Namballa, M. Dorogan, W. W. Harding, C. Mura, P. E. Bourne, & L. Xie 2023 End-to-end sequence-structure-function meta-learning predicts genome-wide chemical-protein interactions for

- dark proteins *PLOS Comp. Biol.* 19(1): e1010851.
<https://doi.org/10.1371/journal.pcbi.1010851>
328. C. Mura, E. Darizen, S. Veretnik & P.E. Bourne 2023 Deep Generative Models of Protein Structure: A Method to Uncover Distant Relationships Across a Continuous Fold Space 2023 <https://www.researchsquare.com/article/rs-2834307/v1>.
329. Z. Zhao, N. Bohidar & P.E. Bourne 2023 Analysis of KRAS-ligand Interaction Modes and Flexibilities Reveals the Binding Characteristics *J. Chem. Info. Mode.* 63,4, 1362-1370. <https://doi.org/10.1021/acs.jcim.3c00097>
330. Z. Zhao and P.E. Bourne 2023 Advances in Reversible Covalent Kinase Inhibitors *Medical Research Reviews*, Submitted. <https://arxiv.org/pdf/2106.11698.pdf>
331. C. Mura & P.E. Bourne 2023 Ten Simple Rules for Serving as an Editor *PLOS Comp. Biol.* 19(3): e1010911 <https://doi.org/10.1371/journal.pcbi.1010911>.
332. A. Weisenberger, C. Keppel, T. Atanasijevic, S. Wang, G. Zubal, J. Buchsbaum, Martin Brechbiel [Emeritus], Jacek Capala, Freddy Escorcia, Ceferino Obecamea, A. Boehnlein, G. Heyes, P.E. Bourne, S. Cherry, E. Colby, G. El Fakhri, J. Gillo, R. Gropler, P. Gueye, G. Tourassi, S. Peggs, & C. Woody 2023 The United States Department of Energy and National Institutes of Health Collaboration: Medical Care Advances via Discovery in Physical Sciences *Medical Physics*, 50(3) e53-e61 <https://aapm.onlinelibrary.wiley.com/doi/10.1002/mp.16252>.
333. E.J. Draizen, J. Readey, C. Mura & P.E. Bourne 2024 Prop3D: A flexible, Python-based platform for machine learning with protein structural properties and biophysical data *BMC Bioinformatics* 25, 11 <https://doi.org/10.1186/s12859-023-05586-5>
334. Z. Zhao & P.E. Bourne 2023 Rigid Scaffolds are Promising for Designing Macrocyclic Kinase Inhibitors *ACS Pharmacol. Transl. Sci.* 6,8, 1182-1191 <https://pubs.acs.org/doi/10.1021/acsptsci.3c00078>
335. B.A. Corliss, Y. Wang, H. Shakeri & P.E. Bourne 2023 Contra-Analysis: Prioritizing Meaningful Size Effect in Scientific Research. Submitted <https://arxiv.org/abs/2210.04867>.
336. L. Felipe Murillo, C. Wylie, P.E. Bourne 2023 Critical Data Ethics Pedagogies: Three (non-rival) Approaches *Big Data & Society* 10(2), <https://doi.org/10.1177/20539517231203666>.
337. Z. Zhao & P.E. Bourne 2023 How Ligands Interact with the Kinase Hinge. *ACS Med. Chem. Letters* <https://pubs.acs.org/doi/epdf/10.1021/acsmchemlett.3c00212>.
338. E.C. McKiernan, L. Barba, P.E. Bourne, C. Carter, Z. Chandler⁵, S. Choudhury, S. Jacobs, D. Katz, S. Lieggi, B. Plale, G. Tananbaum 2023 Policy Recommendations to Ensure that Research Software is Accessible and Reusable *PLoS Biol* 21(7): e3002204. <https://doi.org/10.1371/journal.pbio.3002204>.
339. C-T. Berezin, L.U. Aguilera, S. Billerbeck, P.E. Bourne, D. Densmore, P. Freemont, T. Gorochocki, S.I. Hernandez, N.J. Hillson, C.R. King, M. Köpke, S. Ma, K. Miller¹, T. Seok Moon, J. Moore, B. Munsky¹, C.J. Myers, D.A. Nicholas, S. Peccoud, W. Zhou, & J. Peccoud 2023 Ten Simple Rules for Managing Laboratory Information *PLoS Comput Biol* 19(12): e1011652. <https://doi.org/10.1371/journal.pcbi.1011652>.
340. H. Masum & P.E. Bourne 2023 Ten Simple Rules for Humane Data Science *PLOS Comput Biol* 19(12): e1011698. <https://doi.org/10.1371/journal.pcbi.1011698>.
341. B.A. Corliss, Y. Wang, F.P. Driscoll, H. Shakeri & P.E. Bourne 2024 MAD-FC: A Fold Change Visualization with Readiness, Proportionality and Symmetry *PLOS ONE*, accepted. <https://arxiv.org/abs/2303.10829>.
342. Z. Zhao & P.E. Bourne 2024 Exploring Extended Warheads of Reversible and Irreversible Cysteine-Targeted Covalent Kinase Inhibitors *J. Med. Chem.* Submitted. <https://chemrxiv.org/engage/chemrxiv/article-details/6622898a418a5379b0325b80>.
343. T.R. Johnson & P.E. Bourne 2024 The Biological Data Sustainability Paradox. *Science*, under consideration <https://arxiv.org/abs/2311.05668>.

PUBLICATIONS – Book Chapters

1. P.E.Bourne, P.M.Harrison, W.G.Lewis, D.W.Rice, J.M.A.Smith & R.F.D.Stansfield, *The Biochemistry and Physiology of Iron* (1982) P.Saltman & J.Hegenauer (Eds.), Elsevier, North Holland, 345-351. The Structure and Function of Ferritin: Past Progress and Future Promise.
2. P.E.Bourne, P.M.Harrison, D.W.Rice, J.M.A.Smith & R.F.D.Stansfield, *The Biochemistry and Physiology of Iron* (1982) P.Saltman & J.Hegenauer (Eds.), Elsevier, North Holland, 427-429. The Apoferritin Shell and its Assembly: Some 3-Dimensional Views.
3. P.E.Bourne, *Crystallographic Computing IV* (1988) N.W. Isaacs and M.R. Taylor (Eds.), Oxford University Press, 426-439. Networking for Crystallographers.
4. P.E.Bourne, *Crystallographic Computing VI* (1993) H.D.Flack, L.Parkanyi and K.Simon (Eds.), Oxford University Press, 266-280. Advances in Computing for Macromolecular Crystallography.
5. P.E.Bourne, *Crystallographic Computing VI* (1993), H.D.Flack, L.Parkanyi and K.Simon (Eds.), Oxford University Press. 199-211. User Interface Management Systems for Crystallography.
6. M. Gribskov, P.E. Bourne, C.M Smith PKR - The Protein Kinase Resource *Genetics Databases* Ed. Martin J. Bishop Hardcourt Press pp 241-246.
7. P.E. Bourne 2000 *Encyclopedia of Life Sciences* Macmillian Reference Ltd. Primary Protein and Nucleic Acid Three-dimensional Databases.
8. I.N. Shindyalov and P.E. Bourne 2002 New Insights into Protein Fold Space and Sequence-Structure Relationships. *Structure Prediction: Bioinformtic Approach*, Chapter 17, pp 417-428, Ed. I. Tsigelny. Int'l University Line, La Jolla, CA.
9. C. Guda, E.D. Scheeff, P.E. Bourne, and I.N. Shindyalov 2002, Comparative Analysis of Protein Structure: New Concepts and Approaches for Multiple Structure Alignment. *Structure Prediction: Bioinformtic Approach*. Chapter 19, pp 449-459. Ed. I. Tsigelny, Int'l University Line, La Jolla, CA.
10. E.D. Scheeff, P.E. Bourne, and I.N. Shindyalov 2002 Comparative Analysis of Protein Structure: Automated vs. Manual Alignment of the Protein Kinase Family. *Protein Structure Prediction: Bioinformtic Approach*, Chapter 20, pp 463-475. Ed. I. Tsigelny, Int'l University Line, La Jolla, CA.
11. I.N. Shindyalov and P.E. Bourne 2002 Structure Structure Comparison and Alignment *Structural Bioinformatics* Chapter 16 Ed. H. Weissig and P.E. Bourne Wiley and Associates, NY.
12. H. Wessig and P.E. Bourne 2002 Other Structure Based Databases *Structural Bioinformatics* Chapter 11 Ed. H. Weissig and P.E. Bourne Wiley and Associates, NY.
13. B.V.B Reddy and P.E. Bourne 2002 A User's Perspective on the Structure Classification of Proteins (SCOP) *Structural Bioinformatics* Chapter 12 Ed. H. Weissig and P.E. Bourne Wiley and Associates, NY.
14. H.M. Berman, P.E. Bourne, J.D. Westbrook and C. Zardecki 2003 The Protein Data Bank pp 389-406 from *Structure* (ed.) Chasman Marcel Decker Inc. NY.
15. K. Baldridge and P.E. Bourne 2003 The New Biology and the Grid. Chapter 40 pp 907-922 from *Grid Computing - Making the Global Infrastructure a Reality* (eds) F.Berman, G. Fox and T.Hey Wiley, New York.
16. P.M.D Fitzgerald, J. Westbrook, P.E. Bourne, B. McMahon, K. Watenpaugh, H.M. Berman 2001 *The International Tables for X-ray Crystallography*, In Press, The Macromolecular Crystallographic Information File.

17. P.E.Bourne 2004. Protein Resources in *Encyclopedia of Biological Chemistry*, Eds W.J. Lennarz & M.D. Lane, Elsevier, Oxford, Vol. 3 pp 478-483.
18. Li, W. W., Byrnes, R. W., Hayes, J., Birnbaum, A., Reyes, V. M., Shahab, A., Mosley, C., Pekurovsky, D., Quinn, G. B., Shindyalov, I. N., Casanova, H., Ang, L., Berman, F., Arzberger, P. W., Miller, M. A. & Bourne, P. E. 2004. The Encyclopedia of Life Project: Grid Software and Deployment. *New Generation Computing*, 22: 127-136.
19. Q. Zhang, S. Veretnik and P.E.Bourne 2005 Structural Bioinformatics in Bioinformatics Technologies, pp. 15-40, Ed. Y-P.P. Chen, Springer-Verlag, Berlin.
20. P.M.D. Fitzgerald, J. Westbrook, P.E. Bourne, B. McMahon, K.D. Watenpugh, and H.M. Berman 2006 The Macromolecular Crystallographic Information File (mmCIF) *The International Tables for X-ray Crystallography* Volume G. Chapter 4.5 295-443.
21. A.Sette, H.H.Bui, J.Sidney, P.E.Bourne, S. Buus, W. Fleri, R.Kubo, O.Lund, D.Nemazee, J.V.Ponomarenko, M.Sathiamurthy, S. Stewart, S.Way, S.S.Wilson and B. Peters 2006 The Immune Epitope Database and Analysis Resource Pattern Recognition in Bioinformatics, Springer, Jagath C. Rajapakse, Limsoon Wong, Raj Acharya (Eds)
22. P.E. Bourne and A. Godzik 2007 Structural Genomics in Bioinformatics “From Genomes to Therapies” T. Lengauer (Ed.) Wiley-VCH. p419-438.
23. J.L. Fink, H. Weissig and P.E. Bourne 2009 Other Structure Based Databases in Structural Bioinformatics 2nd Edition J. Gu and P.E. Bourne (Eds.) John Wiley and Sons NJ 321-338.
24. M.A. Marti-Renom, E. Capriotti, I.N. Shindyalov and P.E. Bourne 2009 Structure Comparison and Alignment in Structural Bioinformatics 2nd Edition J. Gu and P.E. Bourne (Eds.) John Wiley and Sons NJ 397-417.
25. S. Yang, R. Valas and P.E. Bourne 2009 Evolution Studies Through Protein Structure in Structural Bioinformatics 2nd Edition J. Gu and P.E. Bourne (Eds.) John Wiley and Sons NJ 559-571.
26. J. Gu and P.E. Bourne 2009 CASP and Other Community-wide Assessments to Advance the Field of Structure Prediction in Structural Bioinformatics 2nd Edition J. Gu and P.E. Bourne (Eds.) John Wiley and Sons NJ 665-678.
27. H. Asher & P.E. Bourne 2009 Drivers of Change - Emergent Information and Biotechnologies in Pharmacy Informatics P.H. Anderson, S.M. McGuinness & P.E. Bourne (Eds.) Taylor & Francis Chapter 2, pp 7-19.
28. P.E. Bourne 2009 Computer and Informatics Basics in Pharmacy Informatics P.H. Anderson, S.M. McGuinness & P.E. Bourne (Eds.) Taylor & Francis, Chapter 3, pp23-35.
29. P.E. Bourne & S.M. McGuinness 2009 Controlled Vocabularies in Pharmacy Informatics P.H. Anderson, S.M. McGuinness & P.E. Bourne (Eds.) Taylor & Francis, Chapter 4, pp37-52.
30. P.E. Bourne 2009 Pharmaceutical Sciences in a Virtual World in Pharmacy Informatics P.H. Anderson, S.M. McGuinness & P.E. Bourne (Eds.) Taylor & Francis Chapter 17, pp251-259.
31. P.O. Anderson, S.M. McGuinness & P.E. Bourne 2009 What is Pharmacy Informatics in Pharmacy Informatics P.H. Anderson, S.M. McGuinness & P.E. Bourne (Eds.) Taylor & Francis, Chapter 1, pp3-5.
32. L. Xie, S.L. Kinnings, L. Xie and P.E. Bourne 2012 Predicting the Polypharmacology of Drugs: Identifying New Uses Through Cheminformatics, Structural Informatics and Molecular Modeling-based Approaches in *Drug Repurposing* M. Barrett and D. Frail (Eds.) Chap. 7, 163-194, Wiley and Sons.
33. L.R. Hardy and P.E. Bourne 2017 Data Science: Transformation of Research and Scholarship in *Big Data-Enabled Nursing* ed. C.W. Delaney, C.A. Weaver, J.L. Warren,

- T.R. Clancy & R.L. Simpson. Chap. 10. In: Delaney C, Weaver C, Warren J, Clancy T, Simpson R (editors), pp 183-196. Springer.
34. M. Grabowski, I.G. Shabalin, P. Porebski, M.J. Domagalski, H. Zheng, D. Cooper, B.S. Venkataramany, P.E. Bourne, & W. Minor 2018 Data Sharing in Structural Biology: Advances and Challenges, In *Data Sharing*, Ed. Y.I. Daradkeh et al., Nova Science Publishers Inc. ISBN 978-1-53614-677-6.
35. Z. Zhao & P.E. Bourne 2020 Overview of Current Type I/II Kinase Inhibitors *Next Generation Kinase Inhibitors: Moving Beyond the ATP Binding/Catalytic Sites* P. Shapiro (Ed.), pp13-28. ISBN 978-3-030-48283-1
<https://link.springer.com/book/10.1007%2F978-3-030-48283-1>
36. Z. Zhao & P.E. Bourne 2021 Using the Structural Kinome to Systematize Kinase Drug Discovery ISBN 978-1-83880-907-2 <https://www.intechopen.com/online-first/78606>.
37. R. Alvarado & P.E. Bourne 2022 AI in the Broader Context of Data Science IEEE, accepted.
38. N.H. Krishna, N.G. Kotla, P.E. Bourne & S.R. Bonam 2022 Successful Funding of Proposals in Pharmaceutical Sciences, under review.

PUBLICATIONS – Books

39. P.E. Bourne, *UNIX for VMS Users* 1990 Digital Press, Maynard, MA. ISBN 1-55558-034-DP.
40. P.E. Bourne *A Cookbook for Serving the Internet - UNIX Version* 1997 Prentice Hall Englewood Cliffs NJ ISBN 0-13-519992-1.
41. R. Holstein, J. McMullen, and P.E. Bourne *Unix for OpenVMS Users* (2nd Edition) 1998 Digital Press MA ISBN: 1555581552.
42. D. Hart and P.E. Bourne *A Cookbook for Serving the Internet - Mac Version* 1998 Prentice Hall NJ, ISBN: 0135200164.
43. P.E. Bourne, R. Holstein, J. McMullen *Unix for OpenVMS Users* 2003 (3rd Edition) HP Technologies ISBN: 1-55558-276-1.
44. P.E. Bourne and H. Weissig *Structural Bioinformatics* 2003 John Wiley and Sons ISBN: 0-471-20200-2.
45. J. Gu and P.E. Bourne *Structural Bioinformatics* (2nd Edition) 2009 John Wiley and Sons ISBN: 978-0-470-18105-8.
46. P.A. Anderson, S.M. McGuinness and P.E. Bourne *Pharmacy Informatics* 2010 Taylor & Francis 978-1-42007175-7.
47. P.E. Bourne *Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins* 2020 A.D Baxevanis & B.F.F Oullette (eds.) Forward John Wiley & Sons (in press).
48. C. Mura and L. Xie *Biomolecular Data Science – in Honor of Philip E. Bourne* 2023 Biomolecules <https://doi.org/10.3390/books978-3-0365-8610-6>.
49. P.E. Bourne *Celebrating the Life of an Average Scientist* 2021 MIT Press in preparation.

PUBLICATIONS – Reports

50. C. Pu, K.P. Sheka, J. Ong, L. Chang, A. Chang, E. Alessio, I.N. Shindyalov, W. Chang, & P.E. Bourne, *Technical Report CUCS-048-92*, Department of Computer Science, Columbia University (1992). PDBtool: A Prototype Object Oriented Toolkit for Protein Structure Verification.
51. P.E. Bourne (Ed.) *Proceedings of The Macromolecular CIFtools Workshop*, Tarrytown NY, (1993).

52. J. Stewart & P.E. Bourne *Proceedings of the International Summer School on Crystallographic Computing* (1996) P.E. Bourne & K. Watenpaugh, (Eds.), International Union of Crystallography Computing Schools.
53. P.E. Bourne, C. Smith, I.N. Shindyalov, and H. Weissig *ACA Transactions* 1997 Invited. What Does Database Federation Mean to Crystallography?
54. D.S. Greer, J. Westbrook, P.E. Bourne 2001 Proceedings NETTAB - Network Tools and Applications in Biology CORBA and XML: Towards a Bioinformatics Integrated Network Environment. An Ontology Driven Architecture for Macromolecular Structure.
55. P.E. Bourne, T.W. Clark, R. Dale, A. de Waard, I. Herman, E.H. Hovy and D. Shotton (eds.), on behalf of the Force11 community 2011. Improving the Future of Research Communication and e-Scholarship. *Dagstuhl Perspectives Workshop 11331*. 10.4230/DagMan.1.1.41.
56. J.J Holt & P.E. Bourne 2019 New Masters or Doctoral Data Science and Analytics Programs II AmstatNews <http://magazine.amstat.org/blog/2019/01/02/new-masters-or-doctoral-data-science-and-analytics-programs-ii/>
57. P.E. Bourne 2019 A School of Data Science at UVA – The Right Place at the Right Time *Cavalier Daily* <http://www.cavalierdaily.com/article/2019/01/bourne-a-school-of-data-science-at-u-va-the-right-place-at-the-right-time>
58. P.E. Bourne 2019 Launching a New School: Five Things We Have Learned *Times Higher Education* <https://www.timeshighereducation.com/blog/launching-a-new-school-five-things-weve-learned>

SELECTED INVITED LECTURES (Since 2004)

This is a partial list emphasizing uniqueness and assumed impact. Many presentations are available at <http://www.slideshare.net/pebourne>.

2021

- Data to Advance Sustainability *NASEM Workshop, Virtual, September 9, 2021*. [PPT]
- SWOT Analysis – What Does it Tell Us about Federally Supported Data Repositories? *NITRD Big Data Interagency Working Group: Pioneering the Future of Federally Supported Data Repositories, Virtual, 13 Jan, 2021*. [PPT]

2020

- The Analytics & Data Science Landscape *Analytics in Modern Taxation Meeting, Virtual, 16, November, 2020*. [PPT]
- The Most Important Ten Simple Rules, *ECML PKDD Conference, Virtual, 14 Sept., 2020*. [PPT]
- Biomedical Data Sciences – New Name with New Opportunities for Change? 4th *IIC/Open Health Systems Colloquium, New Delhi, February 7, 2020*. [PPT]

2019

- What Does Responsible Data Science Mean? *Data Science for the Public Good Symposium, Arlington VA, Aug 9, 2019*. [PPT]
- Its Just Not FAIR. *ISMB BD2K Special Session, Basil, July 23, 2019*. [PPT]
- What is it Going to Cost and What is in it for Me? *Forecasting Costs and Preserving, Archiving & Promoting Access to Biomedical Data, National Academy of Sciences, Washington DC, 22 July, 2019*. [PPT]

2018

- Structural Systems Pharmacology (with Zheng Zhao and Cam Mura). *Department meeting, University of Virginia, December 10, 2018*. [PPT]
- Implications of the Fourth Paradigm *American Society of Human Genetics, San Diego, Oct 16, 2018*. [PPT]
- Data Science Meets Structural Biology, *Lunch & Learn, University of Virginia, Aug 31, 2018*. [PPT]

- Veteran Suicide: Exemplifying the DSI Mission, *Data Science Meeting, Uni. of Manchester, May 22, 2018*. [[PPT](#)]
- Implications of Big Data & Data Science on Publishing, *American Association of Publishers Meeting Feb 8, 2018 Washington DC* [[PPT](#)]

2017

- Biomedical Engineering in a Changing Scholarly Landscape, *50th Anniversary of the UVA Biomedical Engineering Department November 2, 2017* [[PPT](#)]
- A Perspective on Preprints *ASAPbio Meeting, Washington DC July 19, 2017* [[PPT](#)]
- Reproducibility: A Funder and Data Science Perspective *NetSci Pre Workshop June 19, 20-17* [[PPT](#)]
- Will Biomedical Research Fundamentally Change in the Era of Big Data *University of N. Carolina, Chapel Hill, June 7, 2017* [[PPT](#)]

2016

- Making Biomedical Research More Like Airbnb, *International Data Week, Denver, Sept. 14, 2016* [[PPT](#)]
- Systems Biology and Pharmacology from a Structural Perspective, *University of Virginia, August 30, 2016* [[PPT](#)]
- From Where Have We Come & Where Are We Going? *FORCE16 Portland Oregon, April 20, 2016*. [[PPT](#)]
- The Levinthal Lecture – There is no Intelligent Life Down Here, *Open Eye, Santa Fe, March 8, 2016*. [[PPT](#)].
- A SWOT Analysis of Data Science @ NIH *Pacific Symposium on Biocomputing, Hawaii, January 7, 2016* [[PPT](#)].

2015

- BD2K Update, *Advisory Committee to the NIH Director, NIH, December 11, 2015* [[PPT](#)].
- The Commons: Leveraging the Power of the Cloud for Big Data *US GAO December 10, 2015* [[PPT](#)].
- Big Data an NIH Perspective *Johns Hopkins University, October 16, 2015* [[video](#)].
- Big Data in Biomedicine Where are We Headed *University of Georgia, October 12, 2015* [[PPT](#)].
- A Few Thoughts on Open Science Relevant to PCORI, *Washington DC October 8, 2015* [[PPT](#)].
- Ten Simple Rules for Changing How Scholars Communicate *National Information Standards Organization Virtual Seminar September 23, 2015* [[PPT](#)].
- Sharing, reproducibility, Replication – AN NIH View. *American Chemical Society, Denver March 24, 2015* [[PPT](#)].
- Biomedicine – From Stethoscope to Computer *Emerging Researchers National Conference in STEN, Washington DC February 20, 2015* [[PPT](#)].
- Training Quantitative Scientists for Biomedical Science Through the BD2K Initiative *AAAS Washington DC, February 16, 2015* [[PPT](#)].
- The NIH as a Digital Enterprise: Implications for PAG, *Plant and Animal Genomics Meeting, San Diego January 11, 2015* [[PPT](#)].

2014

- Societal Aspects of Big Data: Some general Statements *Big Data in Biomedicine Barcelona November 11, 2014* [[PPT](#)]
- The Future of Open Science *Keynote at the NIAID Festival on Open Science, NIH, April 8, 2014*.
- Some Early Thoughts *BISTI Group NIH, April 1, 2014*.
- Biomedical Research as Part of the Digital Enterprise *ABRF Keynote Address, Albuquerque MN, Mar 25, 2014*.
- Next Generation Data and Opportunities for Clinical Pharmacologists *ASCP Annual*

Meeting, Atlanta GA, Mar 19, 2014.

- Where is Open Going? *SPARC Annual Meeting Keynote Address, Kansas City MI, Mar 1, 2014.*
- Bioinformatics in the Era of Open Science and Big Data *Keynote Swiss Institute of Bioinformatics, Biel, Switzerland, Jan 28, 2014.*
- A Vision for Biomedical Research *Pacific Symposium on Biocomputing, Hawaii, January 4, 2014.*

2013

- I Cannot Reproduce Work from My Own Laboratory, *Data Literature Integration Workshop, EBI, UK December 11, 2013* [[PPT](#)].
- A Recipe for Sustainable Software *Keynote WSSSPE, Denver, November 17, 2013* [[PPT](#)].
- Is a Biological Database Really Different from a Biological Journal? *IDASH virtual seminar October 18, 2013* [[PPT](#)] [[video](#)].
- From B Student to Associate Vice Chancellor and Professor *ACS Student Group, UC San Diego October 16, 2013* [[PPT](#)].
- UCSD Progress in Innovation *CONNECT Commercialization Council San Diego, October 3, 2013* [[PPT](#)].
- The Era of Open *Keynote WikiSymm Conference, Hong Kong, August 7, 2013* [[PPT](#)].
- Drug Repurposing Against Infectious Diseases By Integrating Chemical Genomics and Structural Systems Biology, *ISMB, Berlin July 21, 2013* [[PPT](#)].
- A Few Overarching Thoughts on Digital Publishing and How You Can Participate, *ISMB, Berlin July 21, 2013* [[PPT](#)].
- The 3D Virtual Cell Project *NSF Washington DC, June 28, 2013* [[PPT](#)].
- Thoughts from the Biomedical Sciences *Second Open Economics Workshop, Boston, March 11, 2013* [[PPT](#)].
- Best Practices for Data: A Biologists View *Research Data Alliance, Keynote Gothenburg, Sweden, March 20, 2013* [[PPT](#)].

2012

- Towards Systems Pharmacology *BIOTEC Forum, Dresden, Germany, December 5, 2012* [[PPT](#)].
- Open Access Panel Discussion *Universities Allied for Essential Medicines Conference, UC Irvine, November 3, 2012.*
- Open Data - Where Do We Stand from A Researcher's Perspective? *Kansas State University, Manhattan, Kansas, October 23, 2012* [[PPT](#)].
- Towards Accelerating Innovation at UCSD (with Sandra Brown) *CONNECT Advisory Board Meeting, San Diego, September 26, 2012* [[PPT](#)].
- Near Term Scientific Impact of the Data Web Forum *National Academy of Sciences, Washington DC, August 29, 2012.* [[PPT](#);[MP3](#)].
- Hiring and Supervising *ISMB Workshop - From Postdoc to Principal Investigator 2012 Long Beach CA, July 17, 2012* [[PPT](#)].
- Open Participatory Science *Transforming Opportunities in Scholarly Discourse, Birmingham UK July 6, 2012* [[PPT](#)].
- Using Bioinformatics and Systems Biology to Enable Early Stage Drug Discovery *CIBCB, San Diego, May 10, 2012.*

- Bioinformatics in the Bourne Lab *BILD94 Undergraduate Lecture, UCSD, May 3, 2012.*
- Communicating Systems Biology - Why and How We Should Do Better in a Digital World *ICBP Workshop, Houston, April 27, 2012* [[PPT](#)].
- The Story of Meridith Sage *Bionetworks Congress San Francisco, April 20, 2012* [[Video](#)].
- What Happens When We Take a Drug? *VANBUG, Vancouver, April 12, 2012.* [[Powerpoint](#)].
- A Career in Computational Biology *Kearny High School March 5, 2012.*
- Computational Approaches in Network Pharmacology *Tri-Con San Francisco Feb. 22, 2012* [[Powerpoint](#)].
- One Scientist's Wish List for Scientific Publishers. *Conference of American Chemical Society Editors, La Jolla Jan. 6, 2012* [[Powerpoint](#)].

2011

- Open Data Driven Scholarly Communication in 2020 *7th International Data Curation Conference, Bristol, UK, Dec 7, 2011* [[Powerpoint](#)].
- It's Not Just About Papers Anymore *Elsevier Labs on Line Webinar November 14, 2011* [[Powerpoint](#)].
- Searching Deeply for Data, Results and Tools. What is Stopping Us? *Berlin 9 Washington DC November 9, 2011* [[Powerpoint](#)].
- SciVee & BioLIT Demo *2011 eScience Workshop Transforming Scholarly Communication Harvard University, Oct. 24, 2011* [[Video](#)]
- What Will Be The Impact of Future Changes in Digital Scholarship on Marine Biodiversity? *Marine Biodiversity Conference, Aberdeen Sept 30, 2011* [[Powerpoint](#)].
- Using Open Access Content *New Trends for Scientific Dissemination Trieste Italy Sept 26, 2011* [[Powerpoint](#)].
- PLoS Why it is a Model to be Emulated *New Trends for Scientific Dissemination Trieste Italy Sept 26, 2011* [[Powerpoint](#)].
- Ten Simple Rules for Open Access Publishers *Open Access Scholarly Publishers Association Tallinn, Estonia Sept 21* [[Powerpoint](#)].
- Making Beyond the PDF Current Practice *Dagstuhl Workshop, Germany, 16 Aug 2011* [[Powerpoint](#)].
- Collaboration, *PopTech Washington DC, August 5, 2011.*
- The Path to Open Science with Illustrations from Computational Biology *Microsoft Research Faculty Summit, Cartagena, Columbia, May 18, 2011* [[Powerpoint](#)] [[Video](#)].
- Bioinformatics Meets Systems Biology for Early Stage Drug Discovery *NBIC The Netherlands, April 22, 2011* [[Powerpoint](#)].
- What Open Access Potentially Means to a Scientist *National Bioinformatics Center Workshop, The Netherlands, April 21, 2011* [[Powerpoint](#)].
- CV Talk *NBIC Regional Student Group, The Netherlands, April 20, 2011* [[Powerpoint](#)].
- Digital Research Analog Publishing - One Scientist's View *UKSG, Harrogate Yorkshire, April 4, 2011* [[Powerpoint](#)].
- A Few RDAP Thoughts Based on Experience with the RCSB Protein Data Bank *Research Data Access and Preservation (RDAP) Summit 2011, Denver March 31, 2011* [[Powerpoint](#)].
- Mining Databases for Understanding Target Recognition *Workshop in Allosteric and Orthosteric Ligands in Drug Action UCSD Mar 12, 2011* [[Powerpoint](#)].

- The Changing Face of Scholarly Communication and the Opportunities it Affords the Bioinformatics/Systems Biology Student *UCSD Student Expo* Feb 28, 2011 [[Powerpoint](#)].
- Computational Biology Feb. 7, 2011, *Chattanooga Research Institute*, Chattanooga [[Powerpoint](#)].
- What Do I want from a Publisher of the Future? Jan 20, 2011, *Elsevier VPs Meeting* [[Powerpoint](#)].
- High Throughput Computational Strategies for Proteomics Jan 13, 2011, *PepTalk*, San Diego [[Powerpoint](#)].
- Hybrid Journals: Two Domain Scientist / Faculty Member Perspectives *American Library Association*, Jan 8, 2011, San Diego [[Powerpoint](#)].

2010

- Polypharmacology Studied Using Structural Bioinformatics and Systems Biology December 8, 2010 *University College London* UK [[Powerpoint](#)].
- Addressing the Discontinuity between Doing Research and Disseminating Research *STM Innovations Seminar* December 3, 2010 London, UK [[Powerpoint](#)].
- Polypharmacology - The Good News and Bad News of Possible Cancer Therapy *UCSD Cancer Center* November 23, 2010 [[Powerpoint](#)].
- Professional Development Workshop - Collaboration *University of the Central Caribbean*, Puerto Rico November 19, 2010 [[Powerpoint](#)].
- The Reaming of Life *Jim Gray Award Lecture* Microsoft eResearch Summit Berkeley CA Oct 12, 2010 [[Video](#)] [[Powerpoint](#)] [[Blog post](#)].
- The Future of Data Sharing Platforms in Academic Medicine *Physician Scientist Career Development Meeting* New York Nov 4, 2010 [[Powerpoint](#)].
- Writing a Good Paper *ISMB* July 13, 2010 Boston [[Powerpoint](#)].
- What I want from a Publisher of the Future *STM Meeting Keynote* April 28, 2010 Boston. [[Powerpoint](#)].
- A Career of Computers in Biology *Chula Vista High School*, March 15, 2010. A Nifty One-Fifty Presentation as Part of the San Diego Science Festival [[Powerpoint](#)].
- Who Owns the Data? *Center for Ethics Seminar Series*, Ruben H. Fleet Science Center, March 3, 2010. [[Powerpoint](#)] [[Video](#)].
- Telling Research Stories through SciVee *AAAS Annual Meeting*, San Diego, February 21, 2010 [[Powerpoint](#)].
- New Targets for Old Drugs: Ideas from In silico Analysis, *WPS-AMEFAR Meeting*, San Diego, February 10, 2010 [[Powerpoint](#)].
- Experiences with Rich Media in the Dissemination and Comprehension of Science (Dumbing Down or Opening New Horizons?) *ICSTI Winter Meeting* Paris, February 8, 2010 [[Powerpoint](#)].

2009

- Polypharmacology: Drug Discovery in the Era of Genomics and Proteomics *Rocky 09 Keynote*, Snowmass Colorado, December 10, 2009 [[Powerpoint](#)].
- The Evolution of Protein Structure and Function as Studied through Structural Bioinformatics *BHT Keynote* Hamilton Ontario November 6, 2009 [[Powerpoint](#)].
- Using Protein Structure to Study Network Pharmacology *HWI Buffalo*, November 5, 2009 [[Powerpoint](#)].
- The Changing Landscape of Scholarly Communication as it Relates to the Biosciences *Keck Symposium Keynote*, Houston October 29, 2009 [[Powerpoint](#)].
- PLoS, Semantic Enrichment Tools, Database and Literature Integration *Trieste* October 2009 [[Powerpoint](#)].

- Some Thoughts on Open Science Ben Franklin Award Lecture *BioIT World* Boston April 2009 [[Powerpoint](#)].
- Changes in Scholarly Communication and the Potential Impact on Biocuration *3rd International Biocurators Conference* Berlin April 2009 [[Powerpoint](#)].
- Nothing in Biology {Including Drug Discovery} Makes Sense Except in the Light of Evolution *Purdue & UI* April 2009 [[Powerpoint](#)].
- I am Not a Scientist I am a Number *Allen Press*, National Press Club Washington DC April 2009 [[Powerpoint](#)] [[Meeting Details](#)].
- Finding Ligand Binding Sites on a Protein-wide scale and its implications *HUPO San Diego* February 2009 [[Powerpoint](#)].
- Open Science: One Persons View and What we are Doing About It Keynote Lecture *PSB* January 2009 Hawaii [[Powerpoint](#)].

2008

- Machine Learning in the New World of Scholarly Communication Keynote Lecture The Seventh International Conference on Machine Learning and Applications *La Jolla* December 2008 [[Powerpoint](#)].
- Open Access Day Webcast from *UCSD* October, 2008 [[Powerpoint](#)] [[Video](#)].
- BioPathways Keynote *Toronto ISMB* July 2008 [[Powerpoint](#)].
- 3Dsig Keynote *Toronto ISMB* July 2008 [[Powerpoint](#)].
- Bioontologies Keynote *Toronto ISMB* July 2008 [[Powerpoint](#)].
- Automated Functional Prediction *Toronto ISMB* July 2008 [[Powerpoint](#)].
- Professional Development Tutorial *Toronto ISMB* July 2008 [[Powerpoint](#)].

- 2004-2007

- Evolutionary Insights from Protein Structure *Dalhousie University* December 2007 [[Powerpoint](#)].
- Thinking Outside the Box: Applications Including Finding Off-targets for Major Pharmaceuticals *Winter School in Mathematical and Computational Biology Plenary Lecture* Brisbane Australia June 2007 [[Powerpoint](#)].
- Thoughts on the Future of Scientific Dissemination *eResearch Australasia* Keynote Lecture Brisbane Australia June 2007 [[HTML](#)].
- The RCSB Protein Data Bank: Teaching an Old Dog New Tricks *Swiss-Prot 20th Anniversary* Fortaleza, Brazil, July-Aug, 2006. [[Powerpoint](#)].
- Machine Learning as Applied to Structural Bioinformatics: Results and Challenges *DIMACS Workshop on Machine Learning Techniques in Bioinformatics* July 2006 [[Powerpoint](#)].
- The Future of Structure Genomics *Pacific Symposium on Biocomputing*, Jan. 8, 2004 [[Powerpoint](#)].
- Keynote: The Future of Bioinformatics *The 2nd Asia-Pacific Bioinformatics Conference* (APBC'04), Jan. 19, 2004 [[Powerpoint](#)].
- The Future of Bioinformatics *World University Network Broadcast* Feb. 25, 2004 [[Powerpoint](#)].
- The Future of Bioinformatics *Michael Conrad Memorial Lecture* Wayne State University April 13, 2004 [[Powerpoint](#)] [[Video](#)].
- Biological Databases *ISMB 2004 Introductory Session*, Glasgow August 4, 2004 [[Powerpoint](#)].
- A Royal Wedding - The Marriage between PLoS and the International Society for Computational Biology *Emerging Trends Seminar*, Allen Press Washington DC April 13, 2005 [[Powerpoint](#)].

- How to Write a Scientific Paper *ISMB 2005* On Behalf of the Student Council, Detroit, June 28, 2005 [[Powerpoint](#)].