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http://en.wikipedia.org/wiki/Philip_Bourne *Last Update February 11, 2013*

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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

- **2012- Associate Vice Chancellor for Innovation and Industrial Alliances** University of California, San Diego.
- **2001- Professor Skaggs School of Pharmacy & Pharmaceutical Sciences** University of California, San Diego.
- **2001-2004 Director** Integrated Biosciences Program, San Diego Supercomputer Center, San Diego.
- **2000-2004 Adjunct Professor** The Keck Graduate Institute, Claremont.
- **1997- 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, University of California, San Diego.
- **1998- Associate Director** Protein Data Bank, University of California, San Diego
- **1996-2000 Adjunct Associate Professor** Dept. of Pharmacology, University of California, San Diego.
- **1995-1998 Senior Staff Scientist** San Diego Supercomputer Center, San Diego.
- **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.

TEACHING EXPERIENCE (General Areas)

1974- Biochemistry; structural biology; physical and inorganic chemistry; bioinformatics, 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.

COMMERCIAL EXPERIENCE (Major)

- **2007 Co-Founder** SciVee Inc. San Diego.
- **2004 Co-Founder** FilmFrontiers Inc. UK.
- **2001 Co-Founder** Protein Vision Inc. San Diego.
- **1991 Founder** ViSoft Inc., New York NY.

PROFESSIONAL ACTIVITIES (Major)

- **2011 - Advisory Board**, Receptos Pharmaceuticals Inc.
- **2010 - Advisory Board**, National Library of Medicine, PubMed Central.
- **2010 - Advisory Board**, Microsoft External Research.
- **2010- Editor**, Journal of Biomedical Semantics.
- **2009 - Advisory Board**, Interpro.
- **2006-2010 Advisory Board**, Crossref.
- **2006-2010 Advisory Board**, EcoCyc.
- **2005-2010 Advisory Board**, PharmGKB.
- **2004- 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- 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** – Herbert Irving Comprehensive Cancer Center, Columbia University.
- **1999-2002 Representative** to the American Association for the Advancement of Science on behalf of the American Crystallography Association.

- **1997-1999 Chairman** - American Crystallography Association Computing and Data Committee.
- **1997-1999 Chairman** - American Crystallography Association Computing and Data Committee.
- **1997-2000 Editor** - Web Alert, Current Opinions in Structural Biology.
- **1996- Member** - Review Panel - NSF Database Activities Program.
- **1996-1999 Chairman** - International Union of Crystallography Computing Commission.
- **1991-2005 Member** - Macromolecular CIF Working Group - International 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.

UNIVERSITY COMMITTEES – NOTEWORTHY

- **2009-2011 Co-Chair** UCSD University Industry Relations Task Force.
- **2009- Chair** UCSD Library Committee.
- **2007- Member** UCSD Senate Representative.
- **2003- Chair** Second Year Bioinformatics Program Qualifying Exam Committee.
- **2001- Member** Pharmacy School Planning Committee.
- **2000-2008 Member** MD/PhD Admissions Committee.
- **2000- Member** Bioinformatics Graduate Student Program Steering Committee.
- **2000- Member** Ad hoc Promotions Committee, San Diego Supercomputer Center

AWARDS

- **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, Flinders University of South Australia.
- **2002** Convergence Award from Sun Microsystems Inc.
- **2002** Elected Fellow of the American Medical Informatics Association
- **2001** Second 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.

MEMBERSHIP OF SOCIETIES (Not necessarily current)

- American Association for the Advancement of Science.
- American Medical Informatics Association.
- IEEE.
- International Society for Computational Biology.
- American Chemical Society.

- American Crystallography Association.
- Biophysical Society.
- Protein Society.

CURRENT GRANTS

- PDB Management of the Research Collaboratory for Structural Bioinformatics (PI of subcontract) 3/1/09 – 2/28/14 Total subcontract \$9.5M. Non-competitive 5-year renewal in preparation.
- Conceptualization and Analysis of a 3D Virtual Cell (PI) NSF Awarded 08/01/12 - 07/31/13. \$675,000.
- Changing Scholarly Communication (PI) Alfred P. Sloan Foundation Awarded 04/01/12 - 03/31/13. \$250,000.
- Collaborative Research: Discovery Informatics: Accelerating Science by Coupling Human and Machine Intelligence (Hirsh PI; Bourne Co-PI) NSF Pending.
- A Structural View of Biology: Interdisciplinary Theme-Based Short Courses (PI York; Bourne Co-PI) NIH Pending.
- A Structural Systems Biology Approach to Analyzing Functional Sequence Variants (PI Xie; Bourne Co-PI) NIH Pending
- High-throughput, High resolution Pathogen-Host Protein-Protein Interactions (PI Xie; Co-PIs Brinkman and Bourne) NIH Pending.

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(thiosemicarbazonato)]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 Acetylcholinesterases, 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, I.N. 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. D.S. Greer, J.D. Westbrook and P.E. Bourne 2002 An Ontology Driven Architecture for Derived Representations of Macromolecular Structure *Bioinformatics* 18:1280-1281.
69. P. Craig, P. Yang and P.E. 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. Watenpugh, 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. Adress, 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.
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PUBLICATIONS – Books

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PUBLICATIONS – Reports

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INVITED LECTURES (Since 2004)

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 Principle 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](#)]
- Its 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 Carabean*, 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](#)]