

CURRICULUM VITAE

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TITLES AND DEGREES

- 2004** Associate Professor, Department of Computer Science, University of California, Davis
- 1995** Habilitation à diriger les recherches, Université Louis Pasteur, Strasbourg.
- 1989** PhD in Biophysics (Molecular Biology and NMR spectroscopy), Louis Pasteur University, Strasbourg.
- 1984** Diplôme d'ingénieur de l'Ecole Centrale des Arts et Manufactures de Paris. (Equivalent to M.S. in Engineering); Major: Bioengineering.

AWARDS AND FELLOWSHIPS

- 1997-1998** International Union against Cancer (UICC) long term fellowship for support of a sabbatical in Prof. Michael Levitt's laboratory in Stanford, California.
- 1997** Bronze Medal from the Centre National de la Recherche Scientifique, France (Young Investigator Award).
- 1991** Human Frontiers Science Program Organization (HSFPO) fellowship for support of a collaboration with Prof. Nobuhiro Go, University of Kyoto, Japan.
- 1990** International Union Against Cancer (UICC) fellowship for support of a collaboration with Prof. Jardetzky, Stanford University, California.
- 1986-1989** CNRS Doctoral Fellowship (France); PhD thesis supervised by Prof. J.F. Lefevre.
- 1984-1985** French Government, Ministry of Foreign Affairs Pre-doctoral fellowship.

EMPLOYMENT AND RESEARCH EXPERIENCE

- Since 2004** Associate Professor, Department of Computer Science and Genome Center, University of California, Davis.
Research project: "Computational Structural Biology"
- 2001-2004** Senior Research Associate in the Department of Structural Biology, Stanford University.
Research project: "A new computational method for protein design".

- 1998-2001** Senior Visiting Research Associate in the Department of Structural Biology, Stanford University.
Research project: “A new computational method for protein design”.
- 1997-1998** Visiting scholar in the department of Structural Biology, Stanford University
Research project: “A structure-dependent substitution matrix for the protein threading problem”.
- Since 1989** Tenured CNRS Staff Scientist Grade 1 in the Nuclear Magnetic Resonance Laboratory of the Molecular and Cellular Biology Institute, Strasbourg; on leave of absence
Research project: “Development of a strategy for structure determination by NMR, and development of theoretical models for protein folding and inverse folding problems”.
- Summer 1991** Visiting Scientist at the Molecular Modeling Laboratory of the University of Kyoto, Japan
Research project: “Normal mode analysis of nuclear magnetic resonance data on proteins”.
- Summer 1990** Visiting Scientist at the Stanford Magnetic Resonance Laboratory of the University of Stanford, California.
Research project: “Development of FILMAN, a new program for refining protein structures from Nuclear Magnetic Resonance data”.
- 1986-1989** Doctoral Research at the University Louis Pasteur of Strasbourg in the Molecular and Structural Carcinogenesis and Mutagenesis Group directed by Dr. R.P.P Fuchs. Supervisor: Prof. Jean-Francois Lefevre; Defense: April 11, 1989
Research project: “Molecular and structural studies of a hot-spot for acetylaminofluorene mutagenesis and a strategy for structure determination by NMR”.
- 1984-1986** Staff Scientist at the Lawrence Berkeley Laboratory, Berkeley, California, in the Biophysics Laboratory directed by Dr. A. Chatterjee.
Research project: “Interaction of ionizing heavy charged particles with dilute DNA solutions”.

TEACHING EXPERIENCE

- 1994-1997** Lecturer, “The Fourier transform and its applications”, Université Louis Pasteur, Strasbourg, Physics department, graduate level.
- 1992-1997** Lecturer, “Distance Geometry and protein structure”, Université Louis Pasteur, Strasbourg, Biophysics department, graduate level.
- 1988-1994** Lecturer, “Introduction to computer programming for biologists”, Ecole Supérieure de Biotechnologie de Strasbourg, undergraduate level.
- 1989-1991** Lecturer, “Calculus”, Ecole Supérieure de Biotechnologie de Strasbourg, undergraduate level.
- 1989** Lecturer, “Probability and statistics”, Université Louis Pasteur, Strasbourg, Biology Department, undergraduate level.

REVIEWING AND EDITING

Reviewer: Nature, Journal of Molecular Biology, Journal of Computational Biology, Journal of Magnetic Resonance, Journal of Biological NMR, Journal de Chimie Physique, Nucleic Acids Research, Proteins: Struct. Func. Genet., Protein Science, Proc. Natl. Acad. Sci. (USA).

Editor: Co-editor of section “Theory and Simulation” in Current Opinion in Structural Biology.

INTERESTS

Traveling, reading, writing, hiking, running, swimming, coaching soccer.

PUBLICATIONS

A. Refereed Journal Papers

- (1) R. Bryant, H. Edelsbrunner, P. Koehl and M. Levitt. "The weighted area derivative of a space filling diagram", *Discrete Comput. Geom.* **32**, 293-308 (2004).
- (2) J.M. Chandonia, N.S. Walker, L.L. Conte, P. Koehl, M. Levitt and S.E. Brenner. "Astral compendium enhancements", *Nucleic Acids Res.*, **32**, D189-D192 (2004).
- (3) H. Edelsbrunner and P. Koehl. "The weighted volume derivative of a space filling diagram", *Proc. Natl. Acad. Sci. (USA)*, **100**, 2203-2208 (2003).
- (4) P. Koehl and M. Levitt. "Sequence variations within protein families are linearly related to structural variations.", *J. Mol. Biol.*, **323**, 551-562 (2002).
- (5) R. Kolodny, P. Koehl, L. Guibas and M. Levitt. "Small libraries of protein fragments model native protein structures accurately", *J. Mol. Biol.*, **323**, 297-307 (2002).
- (6) P. Koehl and M. Levitt. "Protein topology and Stability define the space of allowed sequences", *Proc. Natl. Acad. Sci. USA*, **99**, 1280-1285 (2002).
- (7) J.M. Chandonia, N.S. Walker, L.L. Conte, P. Koehl, M. Levitt and S.E. Brenner. "Astral compendium enhancements", *Nucleic Acids Res.*, **30**, 260-263 (2002).
- (8) P. Koehl and M. Levitt. "Improved recognition of native-like protein structures using a family of designed sequences", *Proc. Nat. Acad. Sci. USA*, **99**, 691-696 (2002).
- (9) J.E. Wedeking, C.B. Trame, M. Dorywalska, P. Koehl, T.M. Raschke, M. McKee, D. FitzGerald, R.J. Collier and D.B. McKay, "Refined crystallographic structure of *Pseudomonas aeruginosa* exotoxin A and its implications for the molecular mechanism of toxicity" *J. Mol. Biol.* **314**, 823-837 (2001)
- (10) P. Rabier, B. Kieffer, P. Koehl and JF Lefevre. "Fast measurements of heteronuclear relaxation: frequency domain analysis of NMR accordion spectroscopy", *Mag Res Chem* **39**, 447-456 (2001)
- (11) R. Samudrala, E.S. Huang, P. Koehl and M. Levitt. "Constructing side-chains on near native main chains for ab initio protein structure prediction", *Prot. Eng.*, **13**, 453-457 (2000).
- (12) S.E. Brenner, P. Koehl and M. Levitt, "The Astral compendium for protein structure and sequence analysis", *Nucleic Acids Res.*, **28**, 254-256 (2000).
- (13) P. Koehl and M. Levitt, "De novo protein design. I. In search of stability and specificity", *J. Mol. Biol.*, **293**, 1161-1181 (1999)
- (14) P. Koehl and M. Levitt, "De novo protein design. II. Plasticity of protein sequence", *J. Mol. Biol.*, **293**, 1183-1193 (1999)
- (15) P. Koehl and M. Levitt, "Structure-based conformational preferences of amino acids", *Proc. Nat. Acad. Sci. USA*, **96**, 12524-12529 (1999).
- (16) E.S. Huang, P. Koehl, M. Levitt, R.V. Pappu and J.W. Ponder, "Accuracy of side-chain prediction upon near-native protein backbones generated by ab-initio folding methods", *Proteins: Struct. Funct. Genet.*, **33**, 204-217 (1998).

- (17) E. Furuichi and P. Koehl, "Influence of protein structure database on the predictive power of statistical pair potentials", *Proteins: Struct. Funct. Genet.*, **31**, 139-149 (1998).
- (18) P. Koehl and M. Delarue, "Building protein lattice models using self consistent mean field theory", *J. Chem. Phys.*, **108**, 9540-9549 (1998).
- (19) S. Sunada, N. Go and P. Koehl, "Calculation of NMR order parameters in proteins by normal mode analysis", *J. Chem. Phys.*, **104**, 4768-4775 (1996).
- (20) P. Koehl, C. Ling and J.F. Lefèvre, "Automatic phase correction of NMR spectra: statistics and limits", *J. Chim. Phys.*, **92**, 1929-1938 (1995).
- (21) M. Delarue and P. Koehl, "Atomic environment energies in proteins defined from statistics of accessible and contact surface areas", *J. Mol. Biol.*, **249**, 675-690 (1995).
- (22) P. Koehl and M. Delarue, "A self consistent mean field approach to simultaneous gap closure and side-chain positioning in homology modeling", *Nature Struct. Biol.*, **2**, 163-170 (1995).
- (23) G. Mer, C. Kellenberger, P. Koehl, R. Stote, O. Sorokine, A. Van Dorsselaer, B. Luu, H. Hietter and J.F. Lefèvre, "Disulphide bridge pairing and solution structure by 1H NMR of PMPD2, a 35 residue peptide isolated from *Locusta migratoria*", *Biochemistry*, **33**, 15397-15409 (1994).
- (24) P. Koehl and M. Delarue "Polar and non-polar atomic environments in the protein core: implications for folding and binding" *Protein: Struct. Funct. Genet.*, **20**, 264-278 (1994).
- (25) P. Koehl, C. Ling and J.F. Lefèvre, "Oversampling improves linear prediction quantification of magnetic resonance spectral parameters", *J. Chim. Phys.* **91**, 595-606 (1994).
- (26) P. Koehl and M. Delarue, "Application of a self-consistent mean field theory to predict protein side-chains conformation and estimate their conformational entropy", *J. Mol. Biol.*, **239**, 249-275 (1994).
- (27) P. Koehl, C. Ling and J.F. Lefèvre, "Linear prediction quantification of magnetic resonance spectral parameters: statistics and limits", *J. Magn. Reson.*, **A109**, 32-40 (1994).
- (28) G. Mohn, P. Koehl, H. Budzikiewicz and J.F. Lefèvre "Solution structure of pyoverdine GM-II", *Biochemistry*, **33**, 2843-2851 (1994).
- (29) B. Bersch, P. Koehl, Y. Nakatani, G. Ourisson, and A. Milon "1H nuclear magnetic resonance determination of the membrane-bound conformation of Senktide, a highly selective neurokinin B agonist" *J. Biol. NMR*, **3**, 443-461 (1993).
- (30) B. Kieffer, P. Koehl, S. Plaue and J.F. Lefèvre, "Structural and dynamic studies of two antigenic loops from Haemagglutinin: a relaxation matrix approach", *J. Biol. NMR*, **3**, 91-112 (1993).
- (31) B. Kieffer, P. Koehl and J.F. Lefèvre, "Modeling the dynamic of an antigenic peptide using NMR data", *Biochimie*, **74**, 815-824 (1992).
- (32) P. Koehl, B. Kieffer and J.F. Lefèvre, "Computer-assisted assignment of biological macromolecule NMR spectra", *J. Chim. Phys.*, **89**, 135-146 (1992).

- (33) P. Koehl, J.F. Lefèvre and O. Jardetzky, "Computing the geometry of a molecule in dihedral angle space using NMR-derived constraints: a new algorithm based on optimal filtering", *J. Mol. Biol.*, **223**, 299-315 (1992).
- (34) P. Koehl and J.F. Lefèvre, "The relaxation matrix reconstructed from an incomplete set of 2D-NOE data: Statistics and Limits", *Bull. Magn. Reson.*, **12**, 1/2, 23-29 (1990).
- (35) P. Koehl and J.F. Lefèvre, "The reconstruction of the relaxation matrix from an incomplete set of nuclear Overhauser effects", *J. Magn. Reson.*, **87**, 565-583 (1990).
- (36) P. Koehl, P. Valladier, J.F. Lefèvre and R.P.P. Fuchs, "Strong structural effect of the position of a single acetylaminofluorene adduct within a mutation hot spot", *Nucleic Acids Res.*, **17**, 9531-9541 (1989).
- (37) D. Burnouf, P. Koehl and R.P.P. Fuchs, "Single adduct mutagenesis : Strong effect of the position of a single acetylaminofluorene adduct within a mutation hot spot", *Proc. Nat. Acad. Sci. USA*, **86**, 4147-4151 (1989).
- (38) P. Koehl, D. Burnouf and R.P.P. Fuchs, "Construction of plasmids containing a unique acetylaminofluorene adduct located within a mutation hot spot: A new probe for frameshift mutagenesis", *J. Mol. Biol.*, **207**, 355-364 (1989).
- (39) A. Chatterjee, P. Koehl and J.L. Magee, "Theoretical consideration of the chemical pathways for radiation-induced strand breaks", *Adv. Space Res.*, **6**, 97-105 (1986).

B. Review articles and refereed papers in books

- (40) P. Agarwal, L.J. Guibas, H. Edelsbrunner, J. Erickson, M. Isard, S. Har-Peled, J. Hershberger, C. Jensen, L. Kavraki, P. Koehl, M. Lin, D. Manocha, D. Metaxas, B. Mirtich, D. Mount, S. Muthukrishnan, D. Pai, E. Sacks, J. Snoeyink, S. Suri, O. Wolfson, "Algorithmic Issues in Modeling Motion", *ACM Computing Surveys*, **34**, 550-572 (2002)
- (41) P. Koehl "Recent progress in computational protein design", (editors M. Gromiha and S. Selvaraj) Research Signpost, Trivendrum, India , 307-324 (2002)
- (42) P. Koehl and Michael Levitt, "De novo protein design", (editors O. Jardetzky and M.D. Finucane), NATO ASI series, **315**, 57-75 (2001).
- (43) P. Koehl "Protein Structure Similarities", *Curr. Opin. Struct. Biol.* **11**, 348-353 (2001)
- (44) P. Koehl "Linear prediction spectral analysis of NMR data", *Progress in NMR spectroscopy*. **34**, 257-299 (1999)
- (45) P. Koehl and M. Levitt. "A brighter future for protein structure prediction". *Nature Struct. Biol.* **6**, 108-111 (1999).
- (46) P. Koehl and M. Levitt. "Theory and simulation: Can theory challenge experiment?", *Curr. Opin. Struct. Biol.* **9**, 155-156 (1999)
- (47) P. Koehl and M. Delarue, "The native sequence determines sidechain packing in a protein, but does optimal sidechain packing determine the native sequence?", in "Proceedings of the Pacific Symposium on Biocomputing, 1997" 198-209 (eds. R.B. Altman, A.K. Dunker, L. Hunter and T. Klein), World Scientific, Singapore (1997).

- (48) M. Delarue and P. Koehl, "The inverse protein folding problem: self consistent mean field optimization of a structure specific mutation matrix", in "Proceedings of the Pacific Symposium on Biocomputing, 1997" 109-121 (eds. R.B. Altman, A.K. Dunker, L. Hunter and T. Klein), World Scientific, Singapore (1997).
- (49) P. Koehl and M. Delarue, "Mean field minimization methods for biological macromolecules", *Curr. Opin. Struct. Biol.* **2**, 222-226 (1996).
- (50) P. Koehl and J.F. Lefèvre, "Relaxation Matrix Refinement: Nucleic Acids", in "Encyclopedia of Nuclear Magnetic Resonance" (eds D.M. Grant and R.K. Harris), John Wiley, Chichester, England (1995).
- (51) P. Koehl and M. Delarue, "Modeling side-chain conformation in proteins: a self consistent mean field approach" in "Protein Engineering and Complementary Technologies" (eds M. Geisow and R. Epton), Mayflower Worldwide Ltd., Birmingham, England, 31-34 (1995).
- (52) P. Koehl, D. Burnouf and R.P.P. Fuchs, "Mutagenesis induced by a single acetylaminofluorene adduct within the NarI site is position dependent", in "Nitroarenes: Occurrence, Metabolism and Biological Impact", (eds P.C. Howard, S.S. Hecht and F.A. Beland), Plenum Press, New York, 105-112 (1991).
- (53) P. Koehl, B. Kieffer and J.F. Lefèvre, "The dynamics of oligonucleotides and peptides determined by proton NMR", in "Protein Structure and Engineering", (editor O. Jardetzky), NATO ASI series, **183**, 139-154 (1990).
- (54) D. Burnouf, P. Koehl and R.P.P. Fuchs, "Position of a single acetylaminofluorene adduct within a mutational hot spot is critical for the related mutagenic event", in "Antimutagenesis and Anticarcinogenesis Mechanisms II", (eds Y. Kuroda, D.M. Shankel and M.D. Waters) Plenum Press, New York, 277-288 (1990).