

CURRICULUM VITAE

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TITLES AND DEGREES

- 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 under the supervision of Prof. J.F. Lefevre.
1984-1985 French Government, Ministry of Foreign Affairs Pre-doctoral fellowship.

EMPLOYMENT AND RESEARCH EXPERIENCE

- Since 2001** Senior Research Associate in the Department of Structural Biology, Stanford University.
Research project: "A new computational method for protein design".
- Since 1998** 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
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.
Research project: Supervisor: Prof. Jean-Francois Lefevre; Defense: April 11, 1989
 “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: Journal of Molecular Biology, Journal of Computational Biology, Journal of Magnetic Resonance, Journal of Biological NMR, Journal de Chimie Physique, Nucleic Acids Research.

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) P. Koehl and M. Levitt. "Sequence variations within protein families are linearly related to structural variations.", *J. Mol. Biol.*, **323**, 551-562 (2002).
- (2) 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).
- (3) P. Koehl and M. Levitt. "Protein topology and Stability define the space of allowed sequences", *Proc. Natl. Acad. Sci. USA*, **99**, 1280-1285 (2002).
- (4) 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).
- (5) 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).
- (6) 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)
- (7) 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)
- (8) 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).
- (9) S.E. Brenner, P. Koehl and M. Levitt, "The Astral compendium for protein structure and sequence analysis", *Nucleic Acids Res.*, **28**, 254-256 (2000).
- (10) P. Koehl and M. Levitt, "De novo protein design. I. In search of stability and specificity", *J. Mol. Biol.*, **293**, 1161-1181 (1999)
- (11) P. Koehl and M. Levitt, "De novo protein design. II. Plasticity of protein sequence", *J. Mol. Biol.*, **293**, 1183-1193 (1999)
- (12) P. Koehl and M. Levitt, "Structure-based conformational preferences of amino acids", *Proc. Nat. Acad. Sci. USA*, **96**, 12524-12529 (1999).
- (13) 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).
- (14) 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).
- (15) P. Koehl and M. Delarue, "Building protein lattice models using self consistent mean field theory", *J. Chem. Phys.*, **108**, 9540-9549 (1998).

- (16) 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).
- (17) P. Koehl, C. Ling and J.F. Lefèvre, "Automatic phase correction of NMR spectra: statistics and limits", *J. Chim. Phys.*, **92**, 1929-1938 (1995).
- (18) 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).
- (19) 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).
- (20) 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).
- (21) 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).
- (22) 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).
- (23) 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).
- (24) 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).
- (25) G. Mohn, P. Koehl, H. Budzikiewicz and J.F. Lefèvre "Solution structure of pyoverdinin GM-II", *Biochemistry*, **33**, 2843-2851 (1994).
- (26) 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).
- (27) 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).
- (28) B. Kieffer, P. Koehl and J.F. Lefèvre, "Modeling the dynamic of an antigenic peptide using NMR data", *Biochimie*, **74**, 815-824 (1992).
- (29) P. Koehl, B. Kieffer and J.F. Lefèvre, "Computer-assisted assignment of biological macromolecule NMR spectra", *J. Chim. Phys.*, **89**, 135-146 (1992).
- (30) 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).
- (31) 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).
- (32) 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).

- (33) 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).
- (34) 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).
- (35) 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).
- (36) 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

- (37) P. Koehl "Recent progress in computational protein design", (editors M. Gromiha and S. Selvaraj) Research Signpost, Trivendrum, India , 307-324 (2002)
- (38) P. Koehl and Michael Levitt, “De novo protein design”, (editors O. Jardetzky and M.D. Finucane), NATO ASI series, **315**, 57-75 (2001).
- (39) P. Koehl "Protein Structure Similarities", *Curr. Opin. Struct. Biol.* **11**, 348-353 (2001)
- (40) P. Koehl “Linear prediction spectral analysis of NMR data”, *Progress in NMR spectroscopy.* **34**, 257-299 (1999)
- (41) P. Koehl and M. Levitt. "A brighter future for protein structure prediction". *Nature Struct. Biol.* **6**, 108-111 (1999).
- (42) P. Koehl and M. Levitt. "Theory and simulation: Can theory challenge experiment?", *Curr. Opin. Struct. Biol.* **9**, 155-156 (1999)
- (43) 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).
- (44) 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).
- (45) P. Koehl and M. Delarue, “Mean field minimization methods for biological macromolecules”, *Curr. Opin. Struct. Biol.* **2**, 222-226 (1996).
- (46) 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).

- (47) 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).
- (48) 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).
- (49) 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).
- (50) 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).