

Publications

A. Refereed Journal Papers

- (1) M. Carlsen, **P. Koehl**, and P. Røgen. “On the importance of the distance measures used to train and test knowledge-based potentials for proteins”, *PLoS One*, (2014: in press).
- (2) J. Li and **P. Koehl**, “3D representations of amino acids – applications to protein sequence comparison and classification”, *Comp. Struct. Biotech. J.*, (2014: in press).
- (3) C.-P. Chen, H. Fushing, R. Atwill, and **P. Koehl**, “biDCG: A new method for discovering global features of DNA microarray data via an iterative re-clustering procedure”, *PLoS One*, **9**, e102445 (2014).
- (4) H. Fushing, C. Chen, S.H. Liu, and **P. Koehl**, “Bootstrapping on undirected binary networks via statistical mechanics”, *J. Stat. Phys.* **156**, 853–862 (2014).
- (5) P. Francis-Lyon and **P. Koehl**, “Protein side-chain modeling with a protein dependent optimized rotamer library”, *Proteins: Struct. Func. Bioinfo.* **82**, 2000–2017 (2014).
- (6) **P. Koehl**, “Mathematics’s role in the grand challenge of deciphering the molecular basis of life”, *Frontiers in Biomolecular Sciences*, **1**, 00002 (2014).
- (7) V. Weinreb, L. Li, S.N. Chandrasekaran, **P. Koehl**, M. Delarue, and C.W. Carter Jr., “Enhanced amino acid selection in fully evolved tryptophanyl-tRNA synthetase, relative to ts urzyme, requires, domain motion sensed by the D1 switch, a remote dynamic packing motif”, *J. Biol. Chem.*, **289**, 4367-4376 (2014).
- (8) F. Xei, D. Tong, W. Lifeng, H. Dayong, C.H. Steven, **P. Koehl**, and L. Lu, “Identifying essential pairwise interactions in elastic network model using the alpha shape theory”, *J. Comp. Chem.*, **35**, 1111-1121 (2014).
- (9) **P. Koehl** and J. Hass, “Automatic alignment of genus-zero surfaces”, *IEEE Transactions on Pattern Analysis and Machine Intelligence*, **36**, 466-478 (2014).
- (10) **P. Koehl**, F. Poitevin, H. Orland, and M. Delarue, “Modified Poisson Boltzmann equations for characterizing biomolecular solvation”, *J. Theo. Comp. Chem.*, **13**, 1440001 (2014).
- (11) J. Li, P. Mach, and **P. Koehl**, “Measuring the shapes of macromolecules and why it matters”, *Comp. Struct. Biotech. J.*, **8**, e201309001 (2013).
- (12) A. Tsui, D. Fenton, P. Vuong, J. Hass, **P. Koehl**, N. Amenta, D. Coeurjolly, C. DeCarli, and O.T. Carmichael, “Globally optimal cortical surface matching with exact landmark correspondence”, in “Proc. Information Processing in Medical Imaging, IPMI 2013”, 487-498 (2013).
- (13) H. Fushing, H. Wang, K. VanderWaal, B. McCowan, and **P. Koehl**, “Multi-scale clustering by building a robust and self correcting ultrametric topology on data points”, *PLoS One*, **8**, e56259 (2013).
- (14) **P. Koehl** and P. Røgen. “Extracting knowledge from protein structure geometry”, *Proteins: Struct. Func. Bioinfo.*, **81**, 841-851 (2013).

- (15) P. Mach and **P. Koehl**, “Capturing protein sequence-structure specificity using computational sequence design”, *Proteins: Structure, Function, and Bioinformatics*, **81**, 1556-1570 (2013).
- (16) L. Sauguet, F. Poitevin, S. Murail, G. Moraga, C. van Renterghem, A.W. Thompson, **P. Koehl**, P.-J. Corringer, M. Baaden, and M. Delarue, “Structural basis for ion permeation mechanism in pentameric ligand-gated ion channels”, *EMBO J.*, **32**, 728-741 (2013).
- (17) M. R. Smaoui, F. Poitevin, M. Delarue, **P. Koehl**, H. Orland, and J. Waldispühl, “Computational assembly of polymorphic amyloid fibrils reveals stable aggregates”, *Biophys. J.*, **104**, 683-693 (2013).
- (18) B. Kabasakal and D.D. Gae and J. Li and J.C. Lagarias and **P. Koehl** and A.J. Fisher, “His74 conservation in the bilin reductase PcyA family reflects an important role in protein-substrate structure and dynamics”, *Biochim. Biophys. Acta*, **537**, 233-242 (2013).
- (19) **P. Koehl**, “Fast Recursive Computation of 3D Geometric Moments from Surface Meshes”, *IEEE Transactions on Pattern Analysis and Machine Intelligence*, **34**, 2158-2163 (2012).
- (20) P. Mach and **P. Koehl**. “An analytical method for computing atomic contact areas in biomolecules”, *J. Comp. Chem.*, **34**, 105-120 (2012).
- (21) S. Gu, **P. Koehl**, J. Hass, and N. Amenta. “Surface-histogram: A new shape descriptor for protein-protein docking”. *Proteins: Struct. Func. Bioinfo.*, **80**, 221-238 (2012).
- (22) E. DiLuccio and **P. Koehl**. “The H-factor as a novel quality metric for homology modeling”, *J. of Clin. Bioinfo.*, **2**, 18-26 (2012).
- (23) E. Kang and **P. Koehl**. “Identifying alpha-helices in proteins using the contact map and morphological operations”, *Journal of Korean Institute of Next Generation Computing (in Korean)*, **8**, 75-86 (2012).
- (24) **P. Koehl**, H. Orland, and M. Delarue. “Adapting Poisson-Boltzmann to the self-consistent mean field theory: Application to protein side-chain modeling”, *J. Chem. Phys.*, **135**, 055104 (2011).
- (25) P. Mach and **P. Koehl**. “Geometric measures of large biomolecules: Surface, volume, and pockets”, *J. Comp. Chem.*, **32**, 3023-3038 (2011).
- (26) C. Hu, **P. Koehl** and N. Max. “PackHelix: A tool for helix-sheet packing during protein structure prediction”, *Proteins: Struct. Func. Bioinfo*, **78**, 2828-2843 (2011).
- (27) L. Miao, H. Qin, **P. Koehl**, and J. Song. “Selective and specific ion binding on proteins at physiologically-relevant concentrations”. *FEBS letters* , **585**, 3126-3132 (2011).
- (28) F. Poitevin,, H. Orland, S. Doniach, **P. Koehl** and M. Delarue. “AquaSAXS: A web server for computation and fitting of SAXS profiles with a non-uniform hydration layer”. *Nucl. Acids. Res.* **39**, W184-W189 (2011).
- (29) X. Shi and **P. Koehl**. “Adaptive skin meshes coarsening for biomolecular simulation”, *Computer Aided Geometric Design*, **28**, 307-320 (2011).
- (30) E. DiLuccio and **P. Koehl**. “A quality metric for homology modeling: the H-factor.” *BMC Bioinformatics*: **12**, 48 (2011).

- (31) X. Shi and **P. Koehl**. “Geometry and topology for modeling biomolecular surfaces”. *Far East J. Applied Math.*, **50**, 1-34 (2011).
- (32) P. Francis-Lyon, S. Gu, J. Hass, N. Amenta and **P. Koehl**, “Sampling the conformation of protein surface residues for flexible protein docking”, *BMC Bioinformatics*, **11**, 575 (2010).
- (33) **P. Koehl** and M. Delarue. “AQUASOL: an efficient solver for the dipolar Poisson-Boltzmann-Langevin equation”, *J. Chem. Phys.*, **132**, 064101 (2010).
- (34) C. Hu and **P. Koehl**. “Helix-sheet packing in proteins”. *Proteins: Structure, Function and Bioinformatics*, **78**, 1736-1747 (2010).
- (35) **P. Koehl**, H. Orland and M. Delarue. “Computing ion solvation free energies using the Dipolar Poisson Model”. *J. Phys. Chem. B*, **113**, 5694-5697 (2009).
- (36) **P. Koehl**, H. Orland and M. Delarue. “Beyond Poisson-Boltzmann: Modeling biomolecule-water and water-water interactions”. *Phys. Rev. Lett.* **102**, 087801 (2009).
- (37) X. Shi and **P. Koehl**. “Adaptive surface meshes coarsening with guaranteed quality and topology”. In “Proceedings of the 2009 Computer Graphics International Conference”, editor S. Spence, pp 53-61 (2009).
- (38) P. Laowanapiban, M. Kapustina, C. Vornrhein, M. Delarue, **P. Koehl**, and C.W. Carter Jr. “Independent saturation of three TrpRS subsites generates a partially assembled state similar to those observed in molecular simulations.” *Proc. Natl. Acad. Sci. (USA)*, **106**, 1790-1795 (2009).
- (39) A. Azuara, H. Orland, M. Bon, **P. Koehl** and M. Delarue. “Incorporating dipolar solvents with variable density in Poisson-Boltzmann electrostatics”. *Biophys. J.*, **95**, 5587-5605 (2008).
- (40) Q. Le, G. Pollastri and **P. Koehl**. “Structural alphabets for protein structure classification: a comparison study”. *J. Mol. Biol.*, **387**, 431-450 (2008).
- (41) X. Shi and **P. Koehl**. “The geometry behind numerical solvers of the Poisson-Boltzmann equation”. *Commun. Comput. Phys.*, **3**, 1032-1050 (2008).
- (42) S. Gu, O. Poch, B. Hamann and **P. Koehl**. “A geometric representation of protein sequences”. *IEEE International Conference on Biology and Medicine, 2007*. BIBM, 135-142 (2007).
- (43) F. Chalmel, T. Leveillard, C. Jaillard, A. Lardenois, N. Berdugo, E. Morel, **P. Koehl**, G. Lambrou, A. Holmgren, J.A. Sahel and O. Poch. “Rod-derived cone viability factor-2 is a novel bifunctional thioredoxin like protein with therapeutic potential. *BMC Molecular Biology*, **8**, 74-85 (2007).
- (44) J. Franklin, **P. Koehl**, S. Doniach and M. Delarue. “MinActionPath: maximum likelihood trajectory for large-scale structural transitions in a coarse grained locally harmonic energy landscape”. *Nucleic Acids Res.* **35**, W477-W482 (2007).
- (45) L. McHale, X. Tan, **P. Koehl** and R. Michelmore. “Plant NBS-LRR proteins: adaptable guards.” *Genome Biology*. (published online April 26, 2006).

- (46) A. Zomorodian, L. Guibas and **P. Koehl**. “Geometric filtering of pairwise atomic interactions applied to the design of efficient statistical potentials. *Comput. Aided. Graph. Des.* **23**: 531-544 (2006).
- (47) E. Lindahl, C. Azuara, **P. Koehl** and M. Delarue. NORMAnDRef: Visualization, Deformation, and Refinement of Macromolecular Structures based on all-atom Normal Mode Analysis. *Nucleic. Acids. Res.* **34**: W52-W56 (2006).
- (48) C. Azuara, E. Lindahl, **P. Koehl**, H. Orland and M. Delarue. PDB_Hydro: Incorporating dipolar solvents with variable density in the Poisson-Boltzmann treatment of macromolecule electrostatics. *Nucleic Acids. Res.* **34**: W38-W42 (2006).
- (49) J.D. Thompson, **P. Koehl**, R. Ripp and O. Poch. “BAliBASE 3.0: Latest developments of the multiple sequence alignment benchmark”, *Proteins: Struct. Func Genet.*, **61**, 127-136 (2005).
- (50) J.D. Thompson, S.R. Holbrook, K. Katoh, **P. Koehl**, D. Moras, E. Westhof and O. Poch. “MAO: a multiple alignment ontology for nucleic acid and protein sequences”, *Nucleic Acids. Res.*, **33**, 4164-4171 (2005).
- (51) H. Edelsbrunner and **P. Koehl**. “The geometry of biomolecular solvation”. *Combinatorial and Computational Geometry*, (editors: *J.E. Goodman, J. Pach and E. Welz*) . MSRI Publications **52**, 243-275(2005).
- (52) **P. Koehl**. “Relaxed specificity in aromatic prenyltransferases.” *Nature Chem. Biol.*, **1**, 71-72 (2005).
- (53) R. Kolodny, L. Guibas, M. Levitt and **P. Koehl**. “Inverse kinematics in biology: the protein loop closure problem.” *Int. J. Robot. Res.* **24**:151-163 (2005).
- (54) R. Kolodny, **P. Koehl**, and M. Levitt. “Comprehensive Evaluation of Protein Structure Alignment Methods: Scoring by Geometric Measures.” *J. Mol. Biol.* , **346**: 1173-1188 (2005).
- (55) C. Birck, L. Damian, C. Marty-Detraves, A. Lougarre, C. Schulze Briese, **P. Koehl**, D. Fournier, L. Paquereau and J.P. Samama. “A new lectin family with structure similarity to actinoporins revealed by the crystal structure of *Xerocomus chrysenteron* Lectin XCL” *J. Mol. Biol.* . **344**, 1409-1420 (2004).
- (56) 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).
- (57) 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).
- (58) H. Edelsbrunner and **P. Koehl**. “The weighted volume derivative of a space filling diagram”, *Proc. Natl. Acad. Sci. (USA)*, **100**, 2203-2208 (2003).
- (59) **P. Koehl** and M. Levitt. “Sequence variations within protein families are linearly related to structural variations.”, *J. Mol. Biol.*, **323**, 551-562 (2002).
- (60) 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).

- (61) **P. Koehl** and M. Levitt. "Protein topology and Stability define the space of allowed sequences", *Proc. Natl. Acad. Sci. USA*, **99**, 1280-1285 (2002).
- (62) 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).
- (63) **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).
- (64) 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).
- (65) 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).
- (66) 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).
- (67) S.E. Brenner, **P. Koehl** and M. Levitt, "The Astral compendium for protein structure and sequence analysis", *Nucleic Acids Res.*, **28**, 254-256 (2000).
- (68) **P. Koehl** and M. Levitt, "De novo protein design. I. In search of stability and specificity", *J. Mol. Biol.*, **293**, 1161-1181 (1999).
- (69) **P. Koehl** and M. Levitt, "De novo protein design. II. Plasticity of protein sequence", *J. Mol. Biol.*, **293**, 1183-1193 (1999).
- (70) **P. Koehl** and M. Levitt, "Structure-based conformational preferences of amino acids", *Proc. Nat. Acad. Sci. USA*, **96**, 12524-12529 (1999).
- (71) 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).
- (72) 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).
- (73) **P. Koehl** and M. Delarue, "Building protein lattice models using self consistent mean field theory", *J. Chem. Phys.*, **108**, 9540-9549 (1998).
- (74) 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).
- (75) **P. Koehl**, C. Ling and J.F. Lefèvre, "Automatic phase correction of NMR spectra: statistics and limits", *J. Chim. Phys.*, **92**, 1929-1938 (1995).
- (76) 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).

- (77) **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).
- (78) 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).
- (79) **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).
- (80) **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).
- (81) **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).
- (82) **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).
- (83) G. Mohn, **P. Koehl**, H. Budzikiewicz and J.F. Lefèvre “Solution structure of pyoverdinin GM-II”, *Biochemistry*, **33**, 2843-2851 (1994).
- (84) 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).
- (85) 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).
- (86) B. Kieffer, **P. Koehl** and J.F. Lefèvre, “Modeling the dynamic of an antigenic peptide using NMR data”, *Biochimie*, **74**, 815-824 (1992).
- (87) **P. Koehl**, B. Kieffer and J.F. Lefèvre, “Computer-assisted assignment of biological macromolecule NMR spectra”, *J. Chim. Phys.*, **89**, 135-146 (1992).
- (88) **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).
- (89) **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).
- (90) **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).
- (91) **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).

- (92) 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).
- (93) **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).
- (94) 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

- (95) D.R. Weiss and **P. Koehl**, "Morphing methods to visualize coarse-grained protein dynamics", in *Methods in Molecular Biology : Protein Dynamics*, **1084**, 271-282 (2014).
- (96) **P. Koehl**, "Protein Structure Prediction", in *Biomedical applications of Biophysics*, Handbook of Modern Biophysics,, **3**, 1-34 (2010).
- (97) **P. Koehl**, "Molecular Force Fields", in *Protein Engineering and Design*, S. Park and J.R. Cochran editors, CRC Press, 255-277 (2009).
- (98) **P. Koehl**, H. Orland and M. Delarue. "Solvation of Ion Pairs: The Poisson-Langevin Model". *Proceedings of the International Conference on Applied Physics and Mathematics*, 917-923 (2009).
- (99) V. Natarajan, **P. Koehl**, Y. Wang and B. Hamann. "Visual analysis of biomolecular surfaces", in: Linsen, L., Hagen, H. and Hamann, B., eds., *Visualization in Medicine and Life Sciences*, Springer-Verlag, Heidelberg, Germany, pp. 237-255 (2008).
- (100) **P. Koehl**. "Protein Structure Classification". *Reviews Comput. Chem.*, **22**, 1-56 (2006).
- (101) **P. Koehl**. Electrostatics calculations: latest methodological advances. *Curr. Opin. Struct. Biol.*, **16**, 142-151 (2006).
- (102) 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).
- (103) **P. Koehl** "Recent progress in computational protein design", (editors M. Gromiha and S. Selvaraj) Research Signpost, Trivendrum, India , 307-324 (2002).
- (104) **P. Koehl** and Michael Levitt, "De novo protein design", (editors O. Jardetzky and M.D. Finucane), NATO ASI series, **315**, 57-75 (2001).
- (105) **P. Koehl** "Protein Structure Similarities", *Curr. Opin. Struct. Biol.* **11**, 348-353 (2001).
- (106) **P. Koehl** "Linear prediction spectral analysis of NMR data", *Progress in NMR spectroscopy.* **34**, 257-299 (1999).
- (107) **P. Koehl** and M. Levitt. "A brighter future for protein structure prediction". *Nature Struct. Biol.* **6**, 108-111 (1999).

- (108) **P. Koehl** and M. Levitt. “Theory and simulation: Can theory challenge experiment?”, *Curr. Opin. Struct. Biol.* **9**, 155-156 (1999).
- (109) **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).
- (110) 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).
- (111) **P. Koehl** and M. Delarue, “Mean field minimization methods for biological macromolecules”, *Curr. Opin. Struct. Biol.* **2**, 222-226 (1996).
- (112) **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).
- (113) **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).
- (114) **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).
- (115) **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).
- (116) 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).