

Publications (July 2021)

H index: 44; **i-10 index:** 87; **Citations:** 8872

A. Refereed Journal Papers

- (1) P. Koehl, H. Orland, and M. Delarue, “Parameterizing elastic network models to capture the dynamics of proteins”, *J. Chem. Phys.*, **43**, 1643 (2021).
- (2) P. Koehl, M. Delarue, and H. Orland, “Simultaneous identification of multiple binding sites in proteins: A statistical mechanics approach”, *J. Phys. Chem. B*, **125**, 5052 (2021).
- (3) P. Koehl and H. Orland, “Fast computation of exact solutions of generic and degenerate assignment problems”, *Phys. Rev. E*, **103**, 042101 (2021).
- (4) P. Koehl, M. Delarue, and H. Orland, “Physics approach to the variable-mass optimal-transport problem”, *Phys. Rev. E*, **103**, 012113 (2021).
- (5) P. Koehl, M. Delarue, and H. Orland, “Statistical physics approach to the optimal transport problem”, *Phys. Rev. Lett.*, **123**, 040603 (2019).
- (6) P. Koehl, M. Delarue, and H. Orland, “Optimal transport at finite temperature”, *Phys. Rev. E*, **100**, 013310 (2019).
- (7) P. Koehl and M. Delarue, “Coarse-grained dynamics of supramolecules: Conformational changes in outer shells of Dengue viruses”, *Prog. Biophys. Molec. Biol.*, **143**, 20 (2019).
- (8) J. Guan, F. Hsieh, and P. Koehl, “DCG++: A data-driven metric for geometric pattern recognition”, *PloS One*, **14**, e0217838 (2019).
- (9) F. Hsieh, O. Lee, C. Heitkamp, H. Heymann, S. E. Ebeler, R. B. Boulton, and P. Koehl, “Unraveling the regional specificities of Malbec wines from Mendoza, Argentina and from Northern California”, *Agronomy*, **9**, 234 (2019).
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- (12) S. Vaziri, P. Koehl, and S. Aviran, “Extracting information from RNA SHAPE data: Kalman filtering approach”, *PloS One*, **13**, e0207029 (2018).
- (13) P. Koehl, “Large eigenvalue problems in coarse-grained dynamic analyses of supra molecular systems”, *J. Chem. Theo. Comput.*, **14**, 3903-3919 (2018).
- (14) P. Koehl and M. Delarue, “Combined approaches from physics, statistics, and computer science for ab initio protein structure prediction: ex unitate vires (unity is strength)?”, *F1000 Research*, **7**, 1125 (2018).
- (15) T.E. Saunders, C.Y. He, P. Koehl, L.L.S. Ong, P.T.C. So, “Eleven quick tips for running an interdisciplinary short course for new graduate students”, *PLoS Comput. Biol.*, **14**, e1006039 (2018).

- (16) P. Koehl, “Minimum action principle and shape dynamics”, *J. R. Soc. Interface*, **14**, 20170031 (2017).
- (17) S. Nojoomi and P. Koehl, “A weighted string kernel for protein fold recognition”, *BMC Bioinformatics* **18**, 378 (2017).
- (18) J. Hass and P. Koehl, “Comparing shapes of genus-zero surfaces”, *J. Applied Comput. Topology*, **1**, 57 (2017).
- (19) M. Delarue, P. Koehl, H. Orland, “Ab initio sampling of transition paths by conditioned Langevin dynamics”, *J. Chem. Phys.*, **147**, 152703 (2017).
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B. Review articles and refereed papers in books

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