List of publications 2009-2017

Total citations: 31,613.

Over 110 publications in total, 3 above 5000, 4 above 1,000 citations, 25 above 100.

H-index 45, m-index 2.4, i10-index 72, more than 100 invited talks.

Citation data from Google scholar, public profile: https://goo.gl/zKzue2

Original articles last 8 years (chronological order)

1. Bjelkmar, P., Niemelä, P., Vattulainen, I., and **Lindahl, E.** (2009) Conformational changes and slow dynamics through microsecond polarized atomistic molecular simulation of an integral Kv1.2 ion channel, PLoS Comp. Biol. 5, e1000289. Number of citations: 102
2. Ollila, S., Risselada, HJ., Louhivuori, M., **Lindahl, E**., Vattulainen, I., and Marrink, SJ. (2009) 3D pressure fields in lipid membranes and membrane-protein complexes, Phys. Rev. Lett 102, 78101-4.
   Number of citations: 144
3. Johansson, A., and **Lindahl, E.** (2009) The role of lipid composition for insertion and stabilization ofamino acids in membranes, J. Chem. Phys. 130, 185101- 185108.
   Number of citations: 55
4. Johansson, A., and **Lindahl, E.** (2009) Protein contents in biological membranes can explain abnormal solvation of charged and polar residues, Proc. Natl. Acad. Sci., 106, 15684-89.
   Number of citations: 54
5. [1]Bjelkmar, P., Larsson, P. Cuendet, M. Hess, B., and **Lindahl, E.** (2010) Implementation of the CHARMM force field in GROMACS: Analysis of protein stability effects from correction maps, virtual interaction sites, and water models, J. Chem. Theor. Comput. 6, 459-466.
   Number of citations: 291
6. Niemelä, P. Miettinen, M., Monticelli, L., Hammeren, H., Bjelkmar, P., Murtola, T., **Lindahl, E.**, and Vattulainen, I. (2010) Membrane Proteins Diffuse as Dynamic Complexes with Lipids, J. Am. Chem. Soc. 132, 7574-75.
   Number of citations: 99
7. Bertaccini, EJ., Trudell, JR., and **Lindahl, E.** (2010) Normal mode gating motions of a ligand-gated ion channel persist in a fully hydrated lipid bilayer model, ACS Chem. Neurosci. 1, 552-558.
   Number of citations: 4

[1] Essential Science Indicators: Highly cited paper

8. Kasson, P., **Lindahl, E.**, and Pande, V. (2010) Atomic-resolution simulations predict a transition state for vesicle fusion defined by contact of a few lipid tails, PLoS Comp. Biol. 6, e1000829.
   Number of citations: 61
9. Larsson, P., and **Lindahl, E.** (2010) A high-performance parallel-generalized born implementation enabled by tabulated interaction rescaling, J. Comp. Chem. 31, 2593-2600.
   Number of citations: 17
10. Bertaccini, EJ., Wallner, B., Murail, S. Trudell, JR., and **Lindahl, E.** (2010) Modeling anesthetic binding sites within the glycine alpha one receptor based on prokaryotic ion channel templates: The problem with TM4, J. Chem. Inf. Model. 50, 2248-55.
    Number of citations: 20
11. Hennerdal, A., Falk, J., **Lindahl, E.**, and Elofsson, A. (2010) Internal duplications in alpha-helical membrane protein topologies, Prot. Sci. 19, 2305-18.
    Number of citations: 9
12. Ray, A., **Lindahl, E.**, and Wallner, B. (2010) Model quality assessment for membrane proteins, Bioinf. 26, 3067-74.
    Number of citations: 44
13. Kasson, P., **Lindahl, E.**, and Pande, V. (2011) Water ordering at membrane interfaces controls fusion dynamics. J. Am. Chem. Soc. 133, 3812-3815.
    Number of citations: 24
14. Schwaiger, S., Bjelkmar, P., Hess, B., and **Lindahl, E.** (2011) 3(10)-helix conformation facilitates the transition of a voltage sensor S4 segment toward the down state., Biophys. J. 100, 1446-54.
    Number of citations: 31
15. Murail, S., Wallner, B. Trudell, JR, Bertaccini, E., and **Lindahl E.** (2011) Microsecond simulations indicate that ethanol binds between subunits and could stabilize an open-state model of a glycine receptor, Biophys. J. 100, 1642-50.
    Number of citations: 60
16. Howard, RJ., Murail, S., Ondricek, KE., Corringer, PJ., **Lindahl, E.**, Trudell, JR., and Harris, RA. (2011) Structural basis for alcohol modulation of a pentameric ligand-gated ion channel, Proc. Natl. Acad. Sci. USA 108, 12149-12154.
    Number of citations: 75
17. Pronk, S., Larsson, P., Pouya, I., Bowman, G., Haque, I., Beauchamp, K., Hess, B., Pande, VS., Kasson, P., and **Lindahl, E.** (2011) Copernicus: A new paradigm for parallel adaptive molecular dynamics, Proc. ACM/IEEE High Performance Computing. Number of citations: 41

18. [2]Contreras, F., Ernst, A., Haberkant, P., Björkholm, P., **Lindahl, E.**, Gönen, B., Brodde, A., Tischer, C., Elofsson, A., von Heijne, G., Thiele, C., Pepperkok, R., Wieland, F., and Brügger, B. (2012) Molecular recognition of a single sphingolipid species by a protein's transmembrane domain, Nature 481, 525-529.
    Number of citations: 160

19. Henrion, U., Renhorn, J., Börjesson, SI., Nelson, EM., Schwaiger, CS., Bjelkmar, P., Wallner, B., **Lindahl, E.**, and Elinder, F (2012) Tracking a complete voltage-sensor cycle with metal-ion bridges, Proc. Natl. Acad. Sci. U S A 109, 8552-8557. Number of citations: 80

20. Ray, A., **Lindahl, E.**, and Wallner, B. (2012) Improved model quality assessment using ProQ2, BMC Bioinf. 13, 224-34. Number of citations: 73

21. Wacker, SJ., Jurkowski, W., Simmons, KJ., Fishwick, CW., Johnson, AP., Madge, D., **Lindahl, E.**, Rolland, JF., and de Groot, BL. (2012) Identification of selective inhibitors of the potassium channel Kv1.1-1.2((3)) by high-throughput virtual screening and automated patch clamp, Chem. Med. Chem. 7, 1775-1783.
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22. Murail, S., Howard, RJ., Brömstrup, T., Bertaccini, EJ., Harris, RA., Trudell, JR., and **Lindahl, E.** (2012) Molecular mechanism for the dual alcohol modulation of cys-loop receptors, PLoS Comput. Biol 8, e1002710.
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23. Schwaiger, CS., Börjesson, SI., Hess., B., Wallner, B., Elinder, F., and **Lindahl, E.** (2012) The free energy barrier for arginine gating charge translation is altered by mutations in the voltage sensor domain, PLoS One 7, e45880.
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24. Vargas, E., Yarov-Yarovoy, V., Khalili-Aragi, F., Catterall, WA., Klein, ML., Tarek, M., **Lindahl, E.**, Schulten, K., Perozo, E., Bezanilla, F., and Roux, B. (2012) Extremely long molecular dynamics simulations of K+ channel strengthen the consensus view of voltage gating, J. Gen. Physiol. 140, 587-594.
    Number of citations: 89

25. Schwaiger, CS., Liin, SI., Elinder, F., and **Lindahl, E.** (2013) The conserved phenylalanine in the K+ channel voltage sensor domain creates a barrier with unidirectional effects, Biophys J. 104, 75-84.
    Number of citations: 10

26. [3]Pronk, S., Pall, S., Schulz, R., Larsson, P., Bjelkmar, P., Apostolov, R., Shirts, MR., Smith, JC, Kasson, P, van der Spoel, D., Hess, B., and **Lindahl, E.** (2013) GROMACS 4.5: A high-throughput and highly parallel open source molecular simulation toolkit, Bioinformatics 29, 845-854.
    Number of citations: 2,293

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[2] Essential Science Indicators: Highly cited paper

[3] ESI: Top paper. Sweden's most cited paper in Web of Science 2014, 23rd higest in the world.

27. Paulsen, PA., Jurkowski, W., Apostolov, R., **Lindahl, E.**, Nissen, P., and Poulsen, H. (2012) The C-terminal cavity of the Na,K-ATPase analyzed by docking and electrophysiology, Mol. Membr. Biol. 30, 195-205.
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28. Kasson, P., Hess, B., and **Lindahl, E.** (2013) Probing microscopic material properties inside simulated membranes through spatially resolved three-dimensional local pressure fields and surface tensions, Chem. Phys. Lipids 169, 106-112.
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29. Wennberg, C., Murtola, T., Hess, B., and **Lindahl, E.** (2013) Lennard-Jones lattice summation in bilayer simulations has critical effects on surface tension and lipid properties, J. Chem. Theory Comput. 9, 3527-37.
    Number of citations: 24

30. Brömstrup, T., Howard, RJ., Trudell, JR., Harris, RA, and **Lindahl, E.** (2013) Inhibition versus potentiation of ligand-gated ion channels can be altered by a single mutation that moves ligands between intra- and intersubunit sites, Structure 21, 1307-16.
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31. Yoluk, Ö, Brömstrup, T., Bertaccini, EJ., Trudell, JR., and **Lindahl, E.** (2013) Stabilization effects on an open state of the GluCl ligand-gated ion channel in presence and absence of ivermectin, Biophys. J. 105, 640-47.
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32. Murugan, NA., Apostolov, R., Rinkevicius, Z., Kongsted, J., **Lindahl, E**., and Ågren, H. (2013) Association dynamics and linear and nonlinear optical properties of an N-acetylaladanamide probe in a POPC membrane, J. Am. Chem. Soc. 135, 13590-13597.
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33. Nyblom, M., Poulsen, H., Gourdon, P., Reinhard, L., Andersson, M., **Lindahl, E.**, Fedosova, N., and Nissen, P. (2013) Crystal structure of Na+,K+-ATPase in the NA+-bound state, Science 342, 123-127.
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34. Bertaccini, EJ., Yoluk, Ö., **Lindahl, E.**, and Trudell, JR. (2013) Assessment of Homology Templates and the Anesthetic Binding Sites within the GABA Receptor, Anesthesiology 119, 1087-1095.
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35. Heusser, SA., Howard, RJ., Borghese, CM., Cullins, MA., Broemstrup, T., Lee, U.S., **Lindahl, E.**, Carlsson, J., and Harris, RA. (2013) Functional validation of virtual screening for novel agents with general anesthetic action at ligand-gated ion channels, Mol. Pharmacol. 84, 670-678.
    Number of citations: 7

36. Åström, JA., Carter, A., Hetherington, J., Ioakimidis K., **Lindahl, E.**, Mozdzynski, G., Nash, RW., Schlatter, P., Signell, A., and Westerholm, J. (2013) Preparing scientific application software for exascale computing. Lect. Notes. Comp. Sci. 7782, 27-42. Number of citations: 1

37. Santacruz-Perez, C., Pegos, VR., Honorato, RV., Verli, H., **Lindahl, E.**, Barbosa, JA., and Balan, A. (2013) A specific interdomain interaction preserves the structural and binding properties of the ModA protein from the phytopathogen Xanthomonas citri domain interaction and transport in ModA, Arch. Biochem. Biophys. 539, 20-30. Number of citations: 1

38. Pronk, S., **Lindahl, E.**, and Kasson, P. (2014) Dynamic heterogeneity controls diffusion and viscosity near interfaces, Nature Comm. 5, 3034. Number of citations: 16

39. Lundborg, M., Apostolov, R., Spångberg, D., Gärdenäs, A., van der Spoel, D., and **Lindahl, E.** (2014) An efficient and extensible format, library and API for binary trajectory data from molecular simulations, J. Comp. Chem. 35, 260-269. Number of citations: 3

40. Olsen, R., Li, G., Wallner, M., Trudell, J., Bertaccini, E., **Lindahl, E.**, Miller, K., Alkana, R., and Davies, D. (2014), Structural models of ligand-gated ion channels: Sites of action for anesthetics and ethanol, Alcohol. Clin. Exp. Res. 38, 595-603. Number of citations: 31

41. Pall. S., Abraham, MJ., Kutzner, C., Hess, B., and **Lindahl, E.** (2014) Tackling exascale software challenges in molecular dynamics simulations with GROMACS, Lect. Notes Comp. Sci. 8759, 3-27. Number of citations: 59

42. Lundborg, M, and **Lindahl, E.** (2014), Automatic GROMACS topology generation and comparisons of force fields for solvation free energy calculations, J. Phys. Chem. B 119, 810-23. Number of citations: 4

43. **Lindahl, E.** (2015) Molecular dynamics simulations, Methods. Mol. Biol. 1215, 3-26. Number of citations: 9

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45. Pronk, S., Pouya, I., Lundborg, M., Rotskoff, G., Wesén, B., Kasson, P., and **Lindahl, E.** (2015) Molecular simulation workflows as parallel algorithms: The execution engine of Copernicus, a distributed high-performance computing platform, J. Chem. Theory Comput 11, 2600-08. Number of citations: 15

46. Yoluk, Ö., **Lindahl, E.**, and Andersson, M. (2015) Conformational gating dynamics in the GluCl anion-selective chloride channel, ACS Chem. Neurosci. 6, 1459-67. Number of citations: 3

47. Kimanius, D., Petters, I., Schluckebier, G., **Lindahl, E.**, and Andersson, M. (2015) SAXS-guided metadynamics, J. Chem. Theory Comput 11, 3491-98.
Number of citations: 3

48. [4]Abraham, MJ., Murtola, T., Schulz, R., Pall, S., Smith, JC., Hess, B., and **Lindahl, E.** (2015) GROMACS: High performance molecular simulations through multi-level parallelism from laptops to supercomputers, SoftwareX 1, 19-25.*
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49. Wennberg, CL., Murtola, T., Pall, S., Abraham, MJ., Hess, B., and **Lindahl, E.** (2015) Direct-space corrections enable fast and accurate Lorentz-Berthelot combination rule Lennard-Jones lattice summation, J. Chem. Theory Comput. 11, 5737-5746.
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50. Conti, L, Renhorn J., Gabrielsson A., Turesson F., Liin SI., **Lindahl, E.**, Elinder, F. (2016) Reciprocal voltage sensor-to-pore coupling leads to potassium channel C-type inactivation, Sci. Rep. 6, 27562
Number of citations: 1

51. Yazdi, S., Stein, M., Elinder, F., Andersson, M., and **Lindahl, E.** (2016) The molecular basis of polyunsaturated fatty acid interactions with the Shaker voltage-gated potassium channel. PLoS Comp. Biol. 12, e1004704.
Number of citations: 9

52. Heusser, SA., Yoluk, Ö., Klement, G., Riederer, EA., **Lindahl, E.**, and Howard RJ. (2016) Functional characterization of neurotransmitter activation and modulation in a nematode model ligand-gated ion channel. J. Neurochem. 138, 243-253.
Number of citations: 0

53. Orellana, L., Yoluk, Ö., Carrillo, O., Orozco, M., and **Lindahl, E.** (2016). Prediction and validation of protein intermediate states from structurally rich ensembles and coarse-grained simulations. Nature comm. 7, 12575.
Number of citations: 1

54. Öjemalm, K., Higuchi, T., Lara, P., **Lindahl, E.**, Suga, H., von Heijne, G. (2016) Energetics of side-chain snorkeling in transmembrane helices probed by nonproteinogenic amino acids. Proc. Natl. Acad. Sci. U S A 113, 10559-564.
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55. Nys, M., Wijckmans, E., Farinha, A., Yoluk, Ö., Andersson, M., Brams, M., Spurny, R., Peigneur, S., Tytgat, J., **Lindahl, E.**, Ulens, C. (2016). Allosteric binding site in a cys-loop receptor ligand-binding domain unveiled in the crystal structure of ELIC in complex with chlorpromazine. Proc. Natl. Acad. Sci. U S A 113, E6696-E6703.
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56. Kimanius, D., Forsberg, BO., Scheres, SHW., **Lindahl, E.** (2016) Accelerated cryo-EM structure determination with parallelisation using GPUs in RELION-2. eLife 5, e18722.
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[4] Most downloaded paper from SoftwareX

57. Grønberg, C., Sitsel, O., **Lindahl, E.**, Gourdon, P., Andersson, M. (2016) Membrane anchoring and ion-entry dynamics in P-type ATPase copper transport. Biophys J. 111, 2417-29
    Number of citations: 0
58. Pouya, I., Pronk, S., Lundborg, M., and **Lindahl, E.** (2017) Copernicus, a hybrid dataflow and peer-to-peer scientific computing platform for efficient large-scale ensemble sampling. Future Gen. Comp. Sys. 71, 18-31
    Number of citations: 0
59. Fourati, Z., Howard RJ., Heusser, SA., Sauguet, L., Hu, H., Ruza, RR., **Lindahl, E.**, Delarue, M. Structural basis for bimodal allosteric modulation by general anesthetics in a pentameric ligand-gated ion channel. Revision submitted.
60. Forsberg B., Aibara, S., Kimanius, D., Paul B., **Lindahl, E.**, Amunts, A. Cryo-EM structure determination of the chlororibosome to 3.2Å within 24 hours. In press, IUCrJ
61. Ottosson NE., Ejneby MS., Wu X., Yazdi S., Kondradsson P., **Lindahl, E.**, Elinder, F. Mapping a new binding site for small-molecule compounds and potential drugs targeting voltage-gated ion channels. Submitted.
62. Wennberg C., Narangifard A., Lundborg M., Norlén L., **Lindahl E**. Structural transitions in ceramide cubic phases during formation of the human skin barrier. Submitted.
63. Liin S., Gabrielsson A., Elinder F., **Lindahl E.** The Molecular Mechanism of the Dual Spider Toxin Effect on Voltage-gated Ion Channels. Submitted.

Review articles

1. Larsson, P., Hess, B., and **Lindahl, E.** (2011), Algorithm improvements for molecular dynamics simulations, Comp. Molec. Sci 1, 93-108.
   Number of citations: 22
2. **Lindahl, E.** (2012) Unraveling the strokes of ion channel molecular machines in computers, Proc. Natl. Acad. Sci. U S A 195 (52), 21186-21187.
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The five most highly cited publications regardless of publication year

1. [5]Hess, B., Kutzner, C., van der Spoel, D., and **Lindahl, E.** (2008) GROMACS 4: algorithms for highly efficient, load-balanced, and scalable molecular simulation. J.

[5] Essential Science Indicators: Highly cited paper & Research Front

Chem. Theory. Comput. 4, 435-447.
Number of citations: 8,126

2. **Lindahl, E.**, Hess, B., and van der Spoel, D. (2001) GROMACS 3.0: A package for molecular simulation and trajectory analysis. J. Mol. Mod. 7, 306-317.
Number of citations: 5,589

3. van der Spoel, D., **Lindahl, E**., Hess, B., Groenhof, G, Mark, AE., and Berendsen HJC. (2005) GROMACS: fast, flexible, and free. J. Comp. Chem. 26, 1701-1718.
Number of citations: 6,376

4. [6]Pronk, S., Pall, S., Schulz, R., Larsson, P., Bjelkmar, P., Apostolov, R., Shirts, MR., Smith, JC, Kasson, P, van der Spoel, D., Hess, B., and **Lindahl, E.** (2013) GROMACS 4.5: A high-throughput and highly parallel open source molecular simulation toolkit, Bioinformatics 29, 845-854.
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5. **Lindahl, E.**, and Edholm, O. (2000) Mesoscopic undulations and thickness fluctuations in lipid bilayers from molecular dynamics simulations. Biophys. J. 79, 426-433. Number of citations: 523

Books

1. Apol, E., Apostolov, R., Berendsen, HJC., van Buuren, A., Bjelkmar, P., van Drunen, R., Feenstra, A., Fritsch, S., Groenhof, G., Junghans, C., Hub, J., Kasson, P., Kutzner, C., Lambeth, B., Larsson, P., Lemkul, JA., Marklund, E., Meulenhoff, P., Murtola, T., Pall, S., Pronk, S., Schulz, R., Shirts, M., Sibjerts, A., Tieleman, P., Wennberg, C., Wolf, M., Abraham, M., Hess, B., van der Spoel, D., and **Lindahl, E.** (2008) GROMACS User Manual, Stockholm University, Sweden.
Number of citations: 827.

[6] ESI: Top paper. Sweden's most cited paper in Web of Science during 2014, 23rd higest in the world.