

Total citations: 61,146. Citation data from Google scholar, public profile: <https://goo.gl/zKzue2>
~130 peer-reviewed publications in total. 2 >10,000 citations, 4 >5000, 6 >1,000, 40 above 100.
H-index 59, M-index 2.5 (H/years-since-first-paper), i10-index 115, more than 100 invited talks.

Selected recent publications of relevance for the proposal

1. Lycksell M, Rovšnik U, Bergh C, Johansen NT, Martel A, Porcar L, Arleth L, Howard RJ, **Lindahl E** (2021). Probing solution structure of the pentameric ligand-gated ion channel GLIC by small-angle neutron scattering. <https://doi.org/10.1101/2021.04.10.439285>
The first successful application of small-angle neutron scattering to probe solution-phase structure of small conformational changes in ligand-gated ion channels, which we propose to apply to DeCLIC.
2. Sridhar A, Lummis SCR, Pasini D, Mehregan A, Brams M, Kambara K, Bertrand D, **Lindahl E**, Howard RJ, Ulens C (2021). A cationic lipid site at the outward transmembrane face of a pentameric ligand-gated ion channel. <https://doi.org/10.1101/2021.03.24.436810>
Identification of a new binding site where cationic lipids modulate gating of the ELIC channel through headgroup cation-π interactions from simulations and electrophysiology validation.
3. Bergh C, Heusser SA, Howard RJ, **Lindahl E** (2021) Markov State Models of Proton- and Gate-Dependent Activation in a Pentameric Ligand-Gated Ion Channel.
<https://doi.org/10.1101/2021.03.12.435097>
Markov state models of GLIC gating, quantification of the small fraction of open channels, open/activated states as secondary local free energy minima, and electrophysiology to show how the MSM-predicted gain-of-function I233T does indeed open the channel.
4. Kim JJ, Gharpure A, Teng J, Zhuang Y, Howard RJ, Zhu S, Noviello CM, Walsh Jr RM, **Lindahl E**, Hibbs RE. (2020). Shared structural mechanisms of general anesthetics and benzodiazepines. *Nature* 585, 303-308 <https://www.nature.com/articles/s41586-020-2654-5>
Cryo-EM structures and simulations explaining the shared molecular mechanism of anesthetics and benzodiazepines (valium) on a human heteropentameric receptor, and how the flumazenil antagonist has allosteric modulation effects on the subunits.
5. Rovsnik U, Zhuang Y, Forsberg BO, Carroni M, Yvonne'sdotter L, Howard RJ, **Lindahl E**. Dynamic closed states of a ligand-gated ion channel captured by cryo-EM and simulations. Revision submitted to Life Sci. Alliance, <https://doi.org/10.1101/2021.01.04.425171>
Structure of the GLIC channel at resting and activating conditions, providing the highest-resolution closed state to date and illustrating how the closed state appears to be an ensemble of flexible states.
6. Forsberg B, Aibara S, Howard RJ, Mortezaei N, **Lindahl E**. (2020) Arrangement and symmetry of the fungal E3BP-containing core of the Pyruvate Dehydrogenase Complex. *Nature Commun.* 11, 4667 <https://www.nature.com/articles/s41467-020-18401-z>
First application of new classification methods that better capture small populations of states (here used to solve the PDC complex core), which we are proposing to apply to ligand-gated ion channels.
7. Hu H, Howard RJ, Bastille U, **Lindahl E**, Delarue M. (2020). Structural basis for allosteric transitions of a multidomain pentameric ligand-gated ion channel. *Proc. Natl. Acad. Sci. U S A.* 117(24), 13437-46 <https://www.pnas.org/content/117/24/13437>
First report of structure and functional characterization of the new DeCLIC channel.
8. Gharpure A, Teng J, Zhuang Y, Noviello CM, Walsh RM, Cabuco R, Howard RJ, Zaveri NT, **Lindahl E**, Hibbs RE. (2019). Agonist Selectivity and Ion Permeation in the a3b4 Ganglionic Nicotinic Receptor. *Neuron* 104 (3), 501-11 <https://doi.org/10.1016/j.neuron.2019.07.030>
Structures showing specific agonist displacement of nicotine in a heteropentameric acetylcholine receptor combined with simulations illustrating stabilization, closure of the binding site, and lipid stabilization of the intracellular domain.
9. Fourati, Z., Howard RJ., Heusser, SA., Sauguet, L., Hu, H., Ruza, RR., **Lindahl, E.**, Delarue, M. (2018) Structural basis for bimodal allosteric modulation by general anesthetics in a pentameric ligand-gated ion channel. *Cell reports* 23, 993
<https://doi.org/10.1016/j.celrep.2018.03.108>
First evidence for close-state conformational selection due to pore binding, and identification of two potentiating sites inter- and intrasubunit that create bimodal allosteric modulation.
10. ¹Heusser SA, Lycksell, M, Wang X, McComas S, Howard RJ, **Lindahl E**. (2018) Allosteric potentiation of a ligand-gated ion channel is mediated by access to a deep membrane-facing cavity. *Proc. Natl. Acad. Sci. U S A.* 115, 10672-677 <https://doi.org/10.1073/pnas.1809650115>
Observation of the persistent potentiation of LGICs from a TMD mutation that alters access to membrane-facing binding site, which helped reconcile lipid- and LGIC-mediated models of anesthesia.

¹ Faculty of 1000 research highlight

Original peer-reviewed articles 2013-2021 (reverse chronological order)

1. Bergh C, Heusser SA, Howard RJ, **Lindahl E** (2021) *Markov State Models of Proton- and Gate-Dependent Activation in a Pentameric Ligand-Gated Ion Channel*. To appear in eLife, available on BioRxiv. <https://doi.org/10.1101/2021.03.12.435097>
2. Lycksell M, Rovšnik U, Bergh C, Johansen NT, Martel A, Porcar L, Arleth L, Howard RJ, **Lindahl E** (2021). *Probing solution structure of the pentameric ligand-gated ion channel GLIC by small-angle neutron scattering*. Proc. Natl. Acad. Sci. USA 118 (37), e2108006118
3. Gossen J, et al. (2021). *A blueprint for high affinity SARS-CoV-2 Mpro inhibitors from activity-based compound library screening guided by analysis of protein dynamics*. ACS Pharmacol. Transl. Sci. 4 (3), 1079-95
4. Sridhar A, Lummis SCR, Pasini D, Mehregan A, Brams M, Kambara K, Bertrand D, **Lindahl E**, Howard RJ, Ulens C (2021). *A cationic lipid site at the outward transmembrane face of a pentameric ligand-gated ion channel*. J. Biol. Chem. 297 (2), 100899.
5. Rovsnik U, Zhuang Y, Forsberg BO, Carroni M, Yvonneesdotter L, Howard RJ, **Lindahl E**. *Dynamic closed states of a ligand-gated ion channel captured by cryo-EM and simulations*. Life Sci. Alliance, 4(8), e202101011
6. Masrati G, Mondal R, Rimon A, Kessel A, Padan E, **Lindahl E**, Ben-Tal N (2021). *An angular motion of a conserved four-helix bundle facilitates alternating access transport in the TtNapA and EcNhaA transporters*. Proc. Natl. Acad. Sci. USA 117, 31850.
7. Van Sorge NM, Bonsor DA, Deng L, **Lindahl E**, Schmitt V, Lyndin M, Schmidt A, Nilsson OR, Brizuela J, Boero E, Sundberg EJ, van Strijp JAG, Doran KS, Singer BB, Lindahl G, McCarthy AJ (2021). *Bacterial protein domains with a novel Ig-like fold bind human CEACAM receptors*. EMBO J 40, e106103.
8. Páll S, Zhmurov A, Bauer P, Abraham M, Lundborg M, Gray A, Hess B, **Lindahl E** (2020) *Heterogeneous Parallelisation and Acceleration of Molecular Dynamics Simulations in GROMACS*. J Chem. Phys. 153(13), 134110.
9. Narangifard A, Wennberg C, den Hollander L, Wai I, Lundborg M, Masich S, **Lindahl E**, Daneholt B, Norlén L. (2020). *Molecular reorganization during formation of the human skin barrier studied in situ*. J. Invest. Dermat. doi:10.1016/j.jid.2020.07.040
10. Forsberg B, Aibara S, Howard RJ, Mortezaei N, **Lindahl E**. (2020) *Arrangement and symmetry of the fungal E3BP-containing core of the Pyruvate Dehydrogenase Complex*. Nature Commun. 11, 4667.
11. Kim JJ, Gharpure A, Teng J, Zhuang Y, Howard RJ, Zhu S, Noviello CM, Walsh Jr RM, **Lindahl E**, Hibbs RE. (2020). *Shared structural mechanisms of general anesthetics and benzodiazepines*. Nature 585, 303-308
12. Madru C, Henneke G, Raia P, Hugonneau-Beaufet I, Pehau-Arnaudet G, England P, **Lindahl E**, Delarue M, Carroni M, Sauguet L. (2020). *Structural basis for the increased processivity of D-family DNA polymerases in complex with PCNA*. Nature Comm. 11 (1), 1-12
13. Hu H, Howard RJ, Bastille U, **Lindahl E**, Delarue M. (2020). *Structural basis for allosteric transitions of a multidomain pentameric ligand-gated ion channel*. Proc. Natl. Acad. Sci. U S A. 117(24), 13437-46
14. De la Rosa-Trevin JM, Viga H, Otón J, **Lindahl E**. (2020). *Development of basic building blocks for cryo-EM: the encore and Elvis software libraries*. Acta Cryst D. 76 (4), 350-6
15. Grottessi A, Besker N, Emerson A, Manelfi C, Beccari AR, Frigerio D, **Lindahl E**, Cerchia C, Talarico C. (2020). *Computational Studies of SARS-CoV-2 3CLpro: Insights from MD Simulations*. Int. J. Mol. Sci. 21(15), 5346.
16. Gharpure A, Teng J, Zhuang Y, Noviello CM, Walsh RM, Cabuco R, Howard RJ, Zaveri NT, **Lindahl E**, Hibbs RE. (2019). *Agonist Selectivity and Ion Permeation in the a3b4 Ganglionic Nicotinic Receptor*. Neuron 104 (3), 501-11
17. Abraham, MJ, Apostolov R, Barnoud J, Bauer P, Blau C, Bonvin A, Chavent, Matthieu, Chodera J, Čondić-Jurkić C, Delemotte L, Grubmüller H, Howard RJ, Jordan EJ, **Lindahl E**, Ollila O, Salent J, Smith D, Stansfeld P, Tiemann J, Trellet M, Woods, C, Zhmurov A. (2019). *Sharing Data From Molecular Simulations*. J. Chem. Inf. Model. 59(10), 4093-99
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25. Gómez-Blanco, J., de la Rosa-Trevín J.M., Marabini, R., Del Cano, L., Jiménez, A., Martínez, M., Melero, R., Majtner, T., Maluenda, D., Mota, J. Rancel, Y., Ramírez-Aportela, E. Vilas, J.L., Carroni, M., Fleischmann, S., **Lindahl, E.**, Ashton, A.W., Basham, M., Clare, D.K., Savage, K., Siebert, C.A., Sharov, G.G., Sorzano, C.O.S., Conesa, P., Carazo, J.M. (2018) *Using Scipion for Stream Image Processing at Cryo-EM Facilities* *J. Struct. Biol.* 204(3), 457-463
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35. Fourati, Z., Howard RJ., Heusser, SA., Sauguet, L., Hu, H., Ruza, RR., **Lindahl, E.**, Delarue, M. (2018) *Structural basis for bimodal allosteric modulation by general anesthetics in a pentameric ligand-gated ion channel*. *Cell reports* 23, 993
36. Wennberg C., Narangifard A., Lundborg M., Norlén L., **Lindahl E**. (2018) *Structural transitions in ceramide cubic phases during formation of the human skin barrier*. *Biophys J* 114, 1116
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39. 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
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41. ³Kimanius, 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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51. Yoluk, Ö., **Lindahl, E.**, and Andersson, M. (2015) *Conformational gating dynamics in the GluCl anion-selective chloride channel*, ACS Chem. Neurosci. 6, 1459-67.
52. 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.
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55. 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.
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57. 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.
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³ Faculty of 1000 research highlight⁴ Most downloaded paper ever from SoftwareX

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62. Heusser, SA., Howard, RJ., Borghese, CM., Collins, 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.
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71. ⁵Pronk, 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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Review articles

73. Larsson P, Pouya I, and **Lindahl E.** (2014) *From side chains rattling on picoseconds to ensemble simulations of protein folding*, Israel J. Chem. DOI: 10.1002/ijch.201400020.

Books

74. **Lindahl E.**, editor-in-chief, with The PRACE Scientific Steering Committee (2018). *The Scientific Case for Computing in Europe*. Insight Publishers, Bristol, UK. ISBN 9789082169492.

⁵ ESI: Top paper. Sweden's most cited paper in Web of Science 2014, 23rd highest in the world.