

Complete list of publications

Complete list of publications (Marc Delarue, March 2021)

With Peer Reviews: 120

2021

Madru C., Tekpinar A., Rosario S., Brûlé S., Czernecki D., Sauguet L. & Delarue M.

Fast and efficient purification of SARS-CoV-2 RNA dependent RNA polymerase complex expressed in *Escherichia coli*.

PLoS One, accepted.

D. Czernecki, P. Legrand, M. Tekpinar, S. Rosario, P.A. Kaminski and M. Delarue

No A in DNA: how cyanophage S-2L extends the Watson-Crick base-pairing scheme in its DNA.

Nature Commun, accepted.

Koehl P, **Delarue M**, Orland H.

Statistical Physics solution of the unbalanced Optimal transport problem.

Phys Rev E. 2021 103:012113.

2020

Hu H, Howard RJ, Bastolla U, Lindahl E, and Delarue M.

Structural basis for allosteric transitions of a multidomain pentameric ligand-gated ion channel.

Direct submission.

Proc Natl Acad Sci USA. 2020 117 (24) 13437-13446; doi: 10.1073/pnas.1922701117.

Madru C, Henneke G, Raia P, Hugonneau-Beaufet I, Pehau-Arnaudet G, England P, Lindahl E, Delarue M, Carroni M, Sauguet L.

Structural basis for the increased processivity of D-family DNA Polymerases in complex with PCNA.

Nature Commun. 2020 11:1591. doi: 10.1038/s41467-020-15392-9.

Fourati Z, Sauguet L and Delarue M.

Structural evidence for mono- and di-carboxylates binding at pharmacologically relevant extracellular sites of a pentameric ligand gated ion channel.

Acta Cryst D 2020 76:668-675. doi: 10.1107/S205979832000772X.

Samson C, Legrand P, Tekpinar M, Rozenski J, Abramov M, Holliger P, Pinheiro VB, Herdewijn P, Delarue M.

Structural Studies of HNA Substrate Specificity in Mutants of an Archaeal DNA Polymerase Obtained by Directed Evolution.

Biomolecules. 2020 Dec 8;10(12):1647. doi: 10.3390/biom10121647.

2019

Koehl P, **Delarue M**, Orland H.

Statistical Physics Approach to the Optimal Transport Problem.

Phys Rev Lett. 2019 Jul 26;123(4):040603.

Koehl P, **Delarue M**, Orland H.

Optimal transport at finite temperature.

Phys Rev E. 2019 Jul;100(1-1):013310.

Loc'h J, Gerodimos CA, Rosario S, Tekpinar M, Lieber MR, Delarue M.

Structural evidence for an in trans base selection mechanism involving Loop1 in polymerase μ at an NHEJ double-strand break junction.

J Biol Chem. 2019 Jul 5;294(27):10579-10595.

Randrianjatovo-Gbalou I, Delarue M.

Rapid enzymatic synthesis of long RNA polymers: A simple protocol to generate RNA libraries with random sequences.

Methods. 2019 May 15;161:83-90.

Raia P, Carroni M, Henry E, Pehau-Arnaudet G, Brûlé S, Béguin P, Henneke G, Lindahl E, Delarue M, Sauguet L.

Structure of the DP1-DP2 PolD complex bound with DNA and its implications for the evolutionary history of DNA and RNA polymerases.

PLoS Biol. 2019 Jan 18;17(1):e3000122.

Raia P, Delarue M, Sauguet L.

An updated structural classification of replicative DNA polymerases.

Biochem Soc Trans. 2019 Feb 28;47(1):239-249. Review.

2018

Koehl P, Orland H, Delarue M.

Numerical Encodings of Amino Acids in Multivariate Gaussian Modeling of Protein Multiple Sequence Alignments.

Molecules. 2018 Dec 28;24(1).

Hu H, Ataka K, Menny A, Fourati Z, Sauguet L, Corringer PJ, Koehl P, Heberle J, Delarue M.

Electrostatics, proton sensor, and networks governing the gating transition in GLIC, a proton-gated pentameric ion channel.

Proc Natl Acad Sci U S A. 2018 Dec 26;115(52):E12172-E12181. Direct submission.

Koehl P. and Delarue M.

Coarse-grained dynamics of supramolecules: Conformational changes in Dengue viral capsids.

Progress in Biophysics and Molecular Biology 2018 143:20-37.

Delarue M. and Koehl P. Combined approaches from physics, statistics and computer science for ab-initio protein structure prediction: ex unitate vires.

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Randrianjatovo-Gbalou I, Rosario S, Sismeiro O, Varet H, Legendre R, Coppée JY, Huteau V, Pochet S, Delarue M.

Enzymatic synthesis of random sequences of RNA and RNA analogues by DNA polymerase theta mutants for the generation of aptamer libraries.

Nucleic Acids Res. 2018 Jul 6;46(12):6271-6284.

Fourati Z, Howard RJ, Heusser SA, Hu H, Ruza RR, Sauguet L, Lindahl E, Delarue M.

Structural Basis for a Bimodal Allosteric Mechanism of General Anesthetic Modulation in Pentameric Ligand-Gated Ion Channels.

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Terminal deoxynucleotidyltransferase: the story of an untemplated DNA polymerase capable of DNA bridging and templated synthesis across strands.

Curr Opin Struct Biol. 2018 Apr 12;53:22-31. Review.

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Nemecz Á, Hu H, Fourati Z, Van Renterghem C, **Delarue M**, Corringer PJ.

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Delarue M, Koehl P, Orland H.

Ab initio sampling of transition paths by conditioned Langevin dynamics.

J. Chem. Phys. 2017 Oct 21;147(15):152703. doi: 10.1063/1.4985651.

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Proc Natl Acad Sci U S A. 2017 May 23;114(21):E4158-E4167. doi: 10.1073/pnas.1617567114.

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Identification of a pre-active conformation of a pentameric channel receptor.

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Genuine open form of the pentameric ligand-gated ion channel GLIC

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Acta Cryst. D, 2015 Mar 1, 71(Pt 3):454-60. doi:10.1107/S1399004714026698.

Allosteric and hyperekplexic mutant phenotypes investigated on an alpha-glycine receptor transmembrane structure.

Gustavo Moraga-Cid*, Ludovic Sauguet*, Christèle Huon*, Laurie Malherbe, Christine Girard Blanc, Stéphane Petres, Samuel Murail, Antoine Taly, Marc Baaden, Marc Delarue, Pierre-Jean Corringer

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Enhanced amino acid selection in fully evolved tryptophanyl-tRNA synthetase, relative to its urzyme, requires domain motion sensed by the D1 switch, a remote dynamic packing motif.

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