

## 2015

Structural basis for a novel mechanism of DNA bridging and alignment in eukaryotic DSB DNA repair

Jérôme Gouge, Sandrine Rosario, Félix Romain, Frédéric Poitevin, Pierre Béguin and Marc Delarue\* (2015)

**EMBO J.**, 2015 Mar 11, pii: e201489643. [Epub ahead of print]

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

Fourati, Z., Sauguet, L. and Delarue, M. (2015).

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

Allosteric and hyperekplexic mutant phenotypes investigated on an  $\alpha_1$  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<sup>#</sup>, Pierre-Jean Corringer<sup>#</sup> (2015)

**Proc Natl Acad Sci U S A.** 2015, 112(9):2865-70. doi: 10.1073/pnas.1417864112.

## 2014

[Crystallographic studies of pharmacological sites in pentameric ligand-gated ion channels.](#)

Sauguet L, Shamsavar A, **Delarue M.**

**Biochim Biophys Acta.** 2015 Mar;1850(3):511-523. Epub 2014.

[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.](#)

Weinreb V, Li L, Chandrasekaran SN, Koehl P, Delarue M, Carter CW Jr.

**J Biol Chem.** 2014 Feb 14;289(7):4367-76.

[Crystal structures of a pentameric ligand-gated ion channel provide a mechanism for activation.](#)

Sauguet L, Shamsavar A, Poitevin F, Huon C, Menny A, Nemečz À, Haouz A, Changeux JP, Corringer PJ, **Delarue M.**

**Proc Natl Acad Sci U S A.** 2014 Jan 21;111(3):966-71. Direct Submission (Track 2), A. Karlin Editor.

## 2013

Costi R, Cuzzucoli Crucitti G, Pescatori L, Messori A, Scipione L, Tortorella S, Amoroso A, Crespan E, Campiglia P, Maresca B, Novellino, E, Gouge J, Delarue M, Maga G, di Santo R. (2013) [New nucleotide-](#)

[competitive non-nucleoside inhibitors of terminal deoxynucleotidyl transferase: discovery, characterization, and crystal structure in complex with the target.](#)

**J. Med. Chem.** 2013, 56(18):7431-41.

Gouge J, Rosario S, Romain F, Beguin P, Delarue M. (2013) Structures of Intermediates along the Catalytic Cycle of Terminal Deoxynucleotidyltransferase: Dynamical Aspects of the Two-Metal Ion Mechanism.

**J. Mol. Biol.**, 2013, 425(22):4334-52.

Sauguet L, Howard RJ, Malherbe L, Lee US, Corringer PJ, Harris RA, Delarue M. (2013)

Structural basis for potentiation by alcohols and anaesthetics in a ligand-gated ion channel.

**Nat Comm.** 2013, 4:1697.

Smaoui MR, Poitevin F, Delarue M., Koehl P, Orland H, Waldispühl J. (2013) Computational assembly of polymorphic amyloid fibrils reveals stable aggregates.

**Biophys J.** 2013, 104(3):683-93.

Sauguet L, Poitevin F, Murail S, Van Renterghem C, Moraga-Cid G, Malherbe L, Thompson AW, Koehl P, Corringer PJ, Baaden M, Delarue M. (2013) Structural basis for ion permeation mechanism in pentameric ligand-gated ion channels.

**EMBO J.** 2013, 32(5):728-41.

## 2012

Giraut A, Abu El-Asrar R, Marlière P, Delarue M., Herdewijn P. (2012) 2'-Deoxyribonucleoside phosphoramidate triphosphate analogues as alternative substrates for E. coli polymerase III.

**Chembiochem.** 13(16):2439-44. Epub 2012 Sep 28.

Gouge J, Ralec C, Henneke G, Delarue M. (2012) Molecular recognition of canonical and deaminated bases by P. abyssi family B DNA polymerase.

**J. Mol. Biol.** 2012, 423(3):315-36.

Prevost MS, Sauguet L, Nury H, Van Renterghem C, Huon C, Poitevin F, Baaden M, Delarue M, Corringer PJ. (2012) A locally closed conformation of a bacterial pentameric proton-gated ion channel.

**Nat Struct Mol Biol.** 2012, 19(6):642-9.

[Structure and pharmacology of pentameric receptor channels: from bacteria to brain.](#)

Corringer PJ, Poitevin F, Prevost MS, Sauguet L, Delarue M, Changeux JP. (2012)

**Structure**, 2012, 20(6):941-56. Review.

## 2011

Koehl P, Orland H, **Delarue M**. (2011) Adapting Poisson-Boltzmann to the self-consistent mean field theory: application to protein side-chain modeling.

**J. Chem. Phys.** 2011, 135(5):055104.

Poitevin F, Orland H, Doniach S, Koehl P, Delarue M. (2011) AquaSAXS: a web server for computation and fitting of SAXS profiles with non-uniformly hydrated atomic models.

**Nucleic Acids Res.** 2011, 39:W184-9.

Nury H, Van Renterghem C, Weng Y, Tran A, Baaden M, Dufresne V, Changeux JP, Sonner JM, Delarue M, Corringer PJ. (2011) X-ray structures of general anaesthetics bound to a pentameric ligand-gated ion channel.

**Nature**, 2011, 469(7330):428-31.

Nury H, Delarue M, Corringer PJ. (2011)

X-ray structures of general anesthetics bound to their molecular targets

**Med Sci (Paris)**, 2011, 27(12):1056-7. Review.

## 2010

### [Structural insights into the quinolone resistance mechanism of Mycobacterium tuberculosis DNA gyrase.](#)

Piton J, Petrella S, Delarue M, André-Leroux G, Jarlier V, Aubry A, Mayer C.

**PLoS One.** 2010 Aug 18;5(8):e12245.

### [One-microsecond molecular dynamics simulation of channel gating in a nicotinic receptor homologue.](#)

Nury H, Poitevin F, Van Renterghem C, Changeux JP, Corringer PJ, Delarue M, Baaden M.

**Proc Natl Acad Sci U S A.** 2010 Apr 6;107(14):6275-80. Epub 2010 Mar 22.

### [AQUASOL: An efficient solver for the dipolar Poisson-Boltzmann-Langevin equation.](#)

Koehl P, Delarue M.

**J. Chem. Phys.** 2010 Feb 14;132(6):064101.

### [Atomic structure and dynamics of pentameric ligand-gated ion channels: new insight from bacterial homologues.](#)

Corringer PJ, Baaden M, Bocquet N, Delarue M, Dufresne V, Nury H, Prevost M, Van Renterghem C.

**J Physiol.** 2010 Feb 15;588(Pt 4):565-72. Epub 2009 Dec 7. Review.

### [Crystal structure of the extracellular domain of a bacterial ligand-gated ion channel.](#)

Nury H, Bocquet N, Le Poupon C, Raynal B, Haouz A, Corringer PJ, Delarue M.

**J Mol Biol.** 2010 Feb 5;395(5):1114-27. Epub 2009 Nov 13.

## 2009

### [Computing ion solvation free energy using the Dipolar Poisson model.](#)

Koehl P, Orland, H and Delarue M.

**J. Phys. Chem. B** 2009 113(17):5694-7

### [Conferring a template-dependent polymerase activity to terminal deoxynucleotidyltransferase by mutations in the Loop1 region.](#)

Romain F, Barbosa I, Gouge J, Rougeon F, Delarue M.

**Nucleic Acids Res.** 2009 Aug;37(14):4642-56. Epub 2009 Jun 5.

### [Computing ion solvation free energies using the dipolar Poisson model.](#)

Koehl P, Orland H, Delarue M.

**J Phys Chem B.** 2009 Apr 30;113(17):5694-7.

### [Insights into the enzymatic mechanism of 6-phosphogluconolactonase from Trypanosoma brucei using structural data and molecular dynamics simulation.](#)

Duclert-Savatier N, Poggi L, Miclet E, Lopes P, Ouazzani J, Chevalier N, Nilges M, Delarue M, Stoven V.

**J Mol Biol.** 2009 May 22;388(5):1009-21. Epub 2009 Apr 1.

[Structure of the archaeal pab87 peptidase reveals a novel self-compartmentalizing protease family.](#)

Delfosse V, Girard E, Birck C, Delmarcelle M, Delarue M, Poch O, Schultz P, Mayer C.

**PLoS One.** 2009;4(3):e4712. Epub 2009 Mar 5.

[Beyond the Poisson-Boltzmann model: modeling biomolecule-water and water-water interactions.](#)

Koehl P, Orland H, Delarue M.

**Phys Rev Lett.** 2009 Feb 27;102(8):087801. Epub 2009 Feb 24.

[Independent saturation of three TrpRS subsites generates a partially assembled state similar to those observed in molecular simulations.](#)

Laowanapiban P, Kapustina M, Vonrhein C, Delarue M, Koehl P, Carter CW Jr.

**Proc Natl Acad Sci U S A.** 2009 Feb 10;106(6):1790-5. Epub 2009 Jan 27.

[X-ray structure of a pentameric ligand-gated ion channel in an apparently open conformation.](#)

Bocquet N, Nury H, Baaden M, Le Poupon C, Changeux JP, Delarue M\*, Corringer PJ\*.

**Nature.** 2009 Jan 1;457(7225):111-4. Epub 2008 Nov 5.

## 2008

[Incorporating dipolar solvents with variable density in Poisson-Boltzmann electrostatics.](#)

Azuara C, Orland H, Bon M, Koehl P, Delarue M.

**Biophys J.** 2008 Dec 15;95(12):5587-605. Epub 2008 Sep 26. Erratum in: *Biophys J.* 2009 Mar 4;96(5):2043.

[Dealing with structural variability in molecular replacement and crystallographic refinement through normal-mode analysis.](#)

Delarue M.

**Acta Crystallogr D Biol Crystallogr.** 2008 Jan;64(Pt 1):40-8. Epub 2007 Dec 5.

## 2007

[MinActionPath: maximum likelihood trajectory for large-scale structural transitions in a coarse-grained locally harmonic energy landscape.](#)

Franklin J, Koehl P, Doniach S, Delarue M.

**Nucleic Acids Res.** 2007 Jul;35(Web Server issue):W477-82. Epub 2007 Jun 1.

[Three dimensional structure and implications for the catalytic mechanism of 6-phosphogluconolactonase from Trypanosoma brucei.](#)

Delarue M, Duclert-Savatier N, Miclet E, Haouz A, Giganti D, Ouazzani J, Lopez P, Nilges M, Stoven V.

**J Mol Biol.** 2007 Feb 23;366(3):868-81. Epub 2006 Nov 22.

[An asymmetric underlying rule in the assignment of codons: possible clue to a quick early evolution of](#)

[the genetic code via successive binary choices.](#)

Delarue M.

**RNA**. 2007 Feb;13(2):161-9. Epub 2006 Dec 12.

## 2006

[NOMAD-Ref: visualization, deformation and refinement of macromolecular structures based on all-atom normal mode analysis.](#)

Lindahl E, Azuara C, Koehl P, Delarue M.

**Nucleic Acids Res.** 2006 Jul 1;34(Web Server issue):W52-6.

[PDB\\_Hydro: incorporating dipolar solvents with variable density in the Poisson-Boltzmann treatment of macromolecule electrostatics.](#)

Azuara C, Lindahl E, Koehl P, Orland H, Delarue M.

**Nucleic Acids Res.** 2006 Jul 1;34(Web Server issue):W38-42.

[Determination of dihedral Psi angles in large proteins by combining NH\(N\)/C\(alpha\)H\(alpha\) dipole/dipole cross-correlation and chemical shifts.](#)

Loth K, Abergel D, Pelupessy P, Delarue M, Lopes P, Ouazzani J, Duclert-Savatier N, Nilges M, Bodenhausen G, Stoven V.

**Proteins**. 2006 Sep 1;64(4):931-9.

## 2005

[Refinement of docked protein-ligand and protein-DNA structures using low frequency normal mode amplitude optimization.](#)

Lindahl E, Delarue M.

**Nucleic Acids Res.** 2005 Aug 8;33(14):4496-506.

[Normal mode analysis suggests a quaternary twist model for the nicotinic receptor gating mechanism.](#)

Taly A, Delarue M, Grutter T, Nilges M, Le Novère N, Corringer PJ, Changeux JP.

**Biophys J**. 2005 Jun;88(6):3954-65. Epub 2005 Apr 1.

## 2004

[On the use of low-frequency normal modes to enforce collective movements in refining macromolecular structural models.](#)

Delarue M\*, Dumas P.

**Proc Natl Acad Sci U S A**. 2004 May 4;101(18):6957-62. Direct submission, Michael Levitt Editor.