

## **Julien Roche, Ph.D.**

Roy J. Carver Department of Biochemistry, Biophysics and Molecular Biology  
Iowa State University  
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### **Academic position**

Associate Professor, Roy J. Carver Department of Biochemistry, Biophysics & Molecular Biology, Iowa State University (2022 - present)

Assistant Professor, Roy J. Carver Department of Biochemistry, Biophysics & Molecular Biology, Iowa State University (2016 - 2022)

### **Education**

University of Montpellier (France)	Biophysics	Ph.D. 2012
University of Montpellier (France)	Biophysics	M.S 2008
University of Montpellier (France)	Biology	B.S. 2006

### **Research Experience**

June 2016 - present

**Roy J. Carver Department of Biochemistry, Biophysics & Molecular Biology, ISU**

*Research focus: Structure, function and assembly of large scaffold proteins. Order/Disorder transitions.*

*Other affiliations: Bioinformatics & Computational Biology, Molecular, Cellular and Developmental Biology, Toxicology*

September 2012 – June 2016

**Postdoctoral Research Associate, The National Institutes of Health, Bethesda, MD**

*In the laboratory of Dr. Adriaan Bax*

September 2008 – June 2012

**Graduate Research Assistant, Centre de Biochimie Structurale, Montpellier, France**

*In the laboratory of Dr. Christian Roumestand and Dr. Catherine A. Royer*

January 2008 – June 2008

**Undergraduate Research Assistant, Rensselaer Polytechnic Institute, Troy, NY**

*In the laboratory of Dr. Angel E. Garcia*

### **Secured Funding**

National Institutes of Health, NIGMS R01 (1R01GM132561-01): \$1,624,518

*Structure and Function of DISC1 in the cAMP pathway*

9/1/2019-8/31/2024,

Role: Sole PI.

## Awards

- **LAS Award for Impact on Student Success (2023)**
- **LAS Award for Early Achievement in Research (2022)**
- Young researcher award from the French Biophysical Society (2014)
- Intramural AIDS Research Fellowship, NIH, renewal, one-year funding (2014)
- Intramural AIDS Research Fellowship, NIH, one-year funding (2014)
- Fellows Award for Research Excellence, NIH, travel grant (2013)
- Fulbright scholarship, 6 months stay in Prof. Angel E. Garcia's lab, RPI, NY (2011)
- Grant for Excellency, University of Montpellier, France (2007)

**Publications** (total: 41, first author: 16, corresponding author: 11, total number of citations: 1767)

### **1. Publications after joining ISU (17)**

Kramer D.A, Narvaez-Ortiz, H.Y, Patel U, Shi R, Shen K, Nolen B.J, **Roche J\***, Chen B\*. (2023) The intrinsically disordered cytoplasmic tail of a dendrite branching receptor uses two distinct mechanisms to regulate the actin cytoskeleton. **eLife** (In press) *\*corresponding author*

Siang S, Underbakke E, **Roche J\*** (2022) Intricate coupling between the transactivation and basic-leucine zipper domains governs phosphorylation of transcription factor ATF4 by casein kinase 2. **J. Biol. Chem** 298: 101633 *\*corresponding author*

Dershwitz P, Gu W, **Roche J**, Kang-Yun C.S, Semrau J.D, Bobik T.A, Fulton B, Zischka H, DiSpirito A.A (2022) MbnC is not required for the formation of the N-terminal oxazolone in the methanobactin from *Methylosinus trichosporium* OB3b. **Appl. Environ. Microbiol.** 88: e01841-21

Nguyen T. T, Siang S, **Roche J\*** (2021) High-pressure NMR experiments for detecting protein low-lying conformational states. **J. Vis. Exp** 172: doi: 10.3791/62701 *\*corresponding author*

Nguyen T. T, Ghirlando R, **Roche J\***, Venditti V.\* (2021) Structure elucidation of the elusive Enzyme I monomer reveals the molecular mechanisms linking oligomerization and enzymatic activity. **Proc. Natl. Acad. Sci. USA.** 118: e2100298118 *\*corresponding author*

Levengood J, Peterson J, Tolbert B, **Roche J.\*** (2021) Thermodynamic stability of hnRNP A1 low complexity domain revealed by high-pressure NMR. **Proteins** 89: 781-791 *\*corresponding author*

**Roche J**, Potoyan D.A. (2019) Disorder mediated oligomerization of DISC1 proteins revealed by coarse-grained molecular dynamics simulations. **J. Phys. Chem. B.** 45: 9567-9575

**Roche J.\*** (2019) High-pressure NMR of biological systems in solution. **eMagRes** 8: 121-126 *\*corresponding author*

**Roche J**, Royer C.A, Roumestand C. (2019) Exploring protein conformational landscapes using high-pressure NMR. **Methods in Enzymology** 614:293-320

Alderson R.T, **Roche J**, Gastall H.Y, Pristisanac I, Bax A, Benesch J.L.P, Baldwin A.J. (2019) Local unfolding of the HSP27 monomer regulates chaperone activity. **Nature Commun.** 10: 1068

Andrews R, **Roche J**, Moss W. (2018) ScanFold: an approach for genome-wide discovery of local RNA structural elements – applications to Zika virus and HIV. **PeerJ**. 6: e6136

**Roche J**, Royer C.A (2018) Lessons from Pressure Denaturation of Proteins. **J. R. Soc. Interface** 15: pii 20180244

Baweja L.K, **Roche J.\*** (2018) Pushing the limits of structure-based models: prediction of non-globular protein folding and fibrils formation with Go-model simulations. **J. Phys. Chem. B**. 122: 2525-2535 *\*corresponding author*

**Roche J**, Royer C.A, Roumestand C. (2017) Monitoring protein folding through high pressure NMR. **Prog. Nucl. Magn. Reson. Spectrosc.** 102-103: 15-31

Nguyen L.M, **Roche J.\*** (2017) High-pressure NMR techniques for the study of protein dynamics, folding and aggregation. **J. Magn. Reson.** 277: 179-185 *\*corresponding author*

Shen Y, **Roche J**, Grishaev A, Bax A. (2017) Prediction of nearest neighbor effects on backbone torsion angles and NMR scalar coupling constants in disordered proteins. **Protein Sci.** 27: 146-158

Agniswamy J, Louis J.M, **Roche J**, Harrison R.W, Weber I.T (2016) Structural studies of a rationally selected multi-drug resistant HIV-1 protease reveal synergistic effect of distal mutations on flap dynamics. **PLoS One**. 11: e0168616

## 2. Publications before joining ISU (24)

Louis J.M, Baber J.L, Ghirlando R, Aniana A, Bax A, **Roche J.\*** (2016) Insights into the conformation of the membrane proximal regions critical to the trimerization of the HIV-1 gp41 ectodomain bound to dodecyl phosphocholine micelles. **PLoS One**. 11: e0160597 *\*corresponding author*

Louis J.M, **Roche J.\*** (2016) Evolution under drug pressure remodels the folding free-energy landscape of mature HIV-1 protease. **J. Mol. Biol.** 428: 2780-2792 *\*corresponding author*

**Roche J**, Ying J, Shen Y, Torchia D.A, Bax A. (2016) ARTSY-J: convenient and precise measurement of  $^3J_{\text{HNH}\alpha}$  couplings in medium-size proteins from TROSY-HSQC spectra. **J. Magn. Reson.** 268: 73-81

**Roche J**, Shen Y, Jung Ho L, Jinfa Y, Bax A. (2016) Monomeric  $\text{A}\beta^{1-40}$  and  $\text{A}\beta^{1-42}$  peptides in solution adopt very similar ramachandran map distributions that closely resemble random coil. **Biochemistry** 55: 762-775 (cited > 100 times)

**Roche J**, Ying J, Bax A. (2015) Accurate measurement of  $^3J_{\text{HNH}\alpha}$  couplings in small or disordered proteins from WATERGATE-optimized TROSY spectra. **J. Biomol. NMR** 64: 1-7

**Roche J**, Louis J.M, Bax A, Best R. (2015) Pressure-induced structural transition of mature HIV-1 Protease from a combined NMR/MD simulation approach. **Proteins**. 83: 2117-2123

**Roche J**, Dellarole M, Royer C.A, Roumestand C. (2015) Exploring the protein folding pathway with high-pressure NMR: steady-state and kinetics studies. **High pressure Bioscience: basic concepts, applications and frontiers (Subcell Biochem.)** 72: 261-278

Tugarinov V, Libich D.A, Meyer V, **Roche J**, Clore G.M. (2015) The energetics of a three-state protein folding system probed by high-pressure relaxation NMR from 1 to 2500 bar. **Angew. Chem. Int. Ed.** 54: 11157-11161

Dellarole M, Caro J.A, **Roche J**, Fossat M, Barthe P, Garcia-Moreno B, Royer C.A, Roumestand C (2015) Evolutionary conserved pattern of interactions in a protein revealed by local thermal expansion properties. **J. Am. Chem. Soc.** 137: 9354-9362

**Roche J**, Louis J.M, Aniana A, Ghirlando R, Bax A. (2015) Complete dissociation of the HIV-1 gp41 ectodomain and membrane proximal regions upon phospholipid binding. **J. Biomol. NMR** 61: 235-248

**Roche J**, Louis J.M, Bax A. (2014) Conformation of inhibitor-free HIV-1 protease derived from NMR spectroscopy in a weakly oriented solution. **Chembiochem.** 16: 214-218

Louis J.M, Aniana A, Lohith K, Sayer J.M, **Roche J**, Bewley C.A, Clore G.M. (2014) Binding of HIV-1 gp41-directed neutralizing and non-neutralizing fragment antibody binding domain (Fab) and single chain variable fragment (ScFv) antibodies to the ectodomain of gp41 in the pre-hairpin and six-helix bundle conformations. **PLoS One.** 9: e104683

Maltsev A.S, Grishaev A, **Roche J**, Zasloff M, Bax A. (2014) Improved cross validation of a static ubiquitin structure derived from high precision residual dipolar couplings measured in a drug-based liquid crystalline phase. **J. Am. Chem. Soc.** 136: 3752-3755

**Roche J**, Louis J.M, Grishaev A, Ying J, Bax A. (2014) Dissociation of the trimeric gp41 ectodomain at the lipid-water interface suggests an active role in HIV-1 Env-mediated membrane fusion. **Proc. Natl. Acad. Sci. USA.** 111: 3425-3430

Ying J, **Roche J**, Bax A. (2013) Homonuclear decoupling for enhancing resolution and sensitivity in NOE and RDC measurements of peptides and proteins. **J. Magn. Reson.** 241: 97-102 (cited > 100 times)

Louis. J.M, Tozser J, **Roche J**, Matuz K, Aniana A, Sayer J.M. (2013) Enhanced stability of monomer fold correlates with extreme drug resistance of HIV-1 Protease. **Biochemistry** 52: 7678-7688

**Roche J**, Dellarole M, Caro J.A, Norberto D.E, Garcia A.E, Garcia-Moreno B, Roumestand C, Royer C.A. (2013) Effect of internal cavities on folding rates and routes revealed by real-time pressure-jump NMR spectroscopy. **J. Am. Chem. Soc.** 135: 14610-14618

**Roche J**, Ying J, Maltsev A.S, Bax A. (2013) Impact of hydrostatic pressure on an intrinsically disordered protein: a high-pressure NMR study of  $\alpha$ -synuclein. **Chembiochem.** 14: 1754-1761

Dellarole M, Kobayashi K, Rouget J-B, Caro J.A, **Roche J**, Islam M.M, Garcia-Moreno B, Kuroda Y, Royer C.A. (2013) Probing the physical determinants of thermal expansion of folded proteins. **J. Phys. Chem. B.** 117: 12742-12749

**Roche J**, Caro J.A, Dellarole M, Guca E, Royer C.A, Garcia-Moreno B, Garcia A.E, Roumestand C. (2013) Structural, energetic and dynamic responses of the native state ensemble of staphylococcal nuclease to cavity-creating mutations. **Proteins** 81: 1069-1080

**Roche J**, Dellarole M, Caro J.A, Guca E, Norberto D.E, Yang T, Garcia A.E, Roumestand C, Garcia-Moreno B, Royer C.A. (2012) Remodeling of the folding free-energy landscape of staphylococcal nuclease by cavity-creating mutations. **Biochemistry** 51: 9535-9546

**Roche J**, Caro J.A, Norberto D.E, Barthe P, Roumestand C, Schlessman J.L, Garcia A.E, Garcia-Moreno B, Royer C.A. (2012) Cavities determine the pressure unfolding of proteins. **Proc. Natl. Acad. Sci. USA.** 109: 6945-6950 (cited > 300 times)

Rouget J-B, Aksel T, **Roche J**, Saldana J.L, Garcia A.E, Barrick D, Royer C.A. (2011) Size and sequence and the volume change of protein folding. **J. Am. Chem. Soc.** 133: 6020-6027 (cited > 100 times)

Kitahara R, Hata K, Maeno A, Akasaka K, Chimenti M.S, Garcia-Moreno B, Schroer M.A, Jeworrek C, Tolan M, Winter R, **Roche J**, Roumestand C, Montet de Guillen K, Royer C.A. (2011) Structural plasticity of staphylococcal nuclease probed by perturbation with pressure and pH. **Proteins** 79: 1293-1305

### **Conferences & seminars** (33)

- Cornell University, Extreme Biology workshop at CHESS, 2022 (Ithaca, NY): **Invited talk**
- Extreme Biophysics RCN, 2022 (Santa Fe, NM): **Invited Talk**
- Cornell University, Biology under extreme conditions workshop at CHESS, 2021 (virtual): **Invited talk**
- University of California San Diego, Department of Chemistry seminar, 2021 (virtual): **Invited talk**
- University of Illinois at Chicago, Department of Chemistry seminar, 2021 (virtual): **Invited talk**
- CUNY Advanced Science Research Center, Biochemistry seminar, 2021 (virtual): **Invited talk**
- Rensselaer Polytechnic Institute, Department of Biological Sciences, seminar, 2021 (virtual): **Invited talk**
- University of Illinois at Urbana-Champaign, Department of Chemistry seminar, 2021 (virtual): **Invited talk**
- Mississippi State University, Chemistry Department seminar, 2021 (virtual): **Invited talk**
- Johns Hopkins University, Biophysics Department seminar, 2021 (virtual): **Invited talk**
- Brown University, MCB Department seminar, 2021 (virtual): **Invited talk**
- Extreme Biophysics RCN, 2020 (Virtual): **Talk**
- 34<sup>th</sup> Gibbs Conference on Biological Thermodynamics, 2020 (Virtual): **Poster**
- Extreme Biophysics RCN, 2019 (San Diego, CA, USA): **Talk**
- RESOLV, 2019 (Bochum, Germany): **Invited talk**
- GRASP NMR, 2018 (Lawrence, KS, USA): **Invited talk**
- 62<sup>nd</sup> Biophysical Society Meeting, 2018 (San Francisco, CA, USA): **Poster**
- 61<sup>st</sup> Biophysical Society Meeting, 2017 (New Orleans, LA, USA): **Talk**
- 252<sup>nd</sup> ACS National Meeting, 2016 (Philadelphia, PA, USA): **Invited Talk**
- 60<sup>th</sup> Biophysical Society Meeting, 2016 (Los Angeles, CA, USA): **Talk**
- DCO workshop on extreme biophysics, 2015 (Washington, DC, USA): **Invited talk**
- 56<sup>th</sup> ENC, 2015 (Pacific Grove, USA): **Poster**
- 59<sup>th</sup> Biophysical society meeting, 2015 (Baltimore, MD, USA): **Talk**
- 7<sup>th</sup> IMBP, 2014 (Montpellier, France): **Invited talk.**
- Biomolecular structure, dynamics and function: membrane proteins, 2014 (Nashville, TN, USA): **Talk**
- 58<sup>th</sup> Biophysical society meeting, 2014 (San Francisco, CA, USA): **Poster**
- 51<sup>st</sup> EHPRG, 2013 (London, UK): **Invited talk.**
- 56<sup>th</sup> Biophysical Society meeting, 2012 (San Diego, CA, USA): **Talk.**
- 6<sup>th</sup> IMBP, 2011 (Otsu, Japan): **Talk.**

- 49<sup>th</sup> EHPRG, 2011 (Budapest, Hungary): **Poster**
- 8<sup>th</sup> EBSA, 2011 (Budapest, Hungary): **Talk**.
- GERM conference, 2011 (Sitges, Spain): **Talk**.

## Advising Activities

### Research Advisor

#### Graduate Students

- Luan Nguyen (Fall 17 – Summer 19). Master Thesis: “*Conformational change upon phosphorylation at S713 site of Disrupted-in-schizophrenia-1 (DISC1) leads to a change in the oligomeric state*”.  
Graduated 07/10/19
- Tung Mei Khu (Summer 20 – Summer 22). Master Thesis: “*DISC1 as a sensor for oxidative stress*”.  
Graduated 08/16/22
- Steven Siang (Fall 17 – present) Received a **BBMB Research Excellence Award** (Spring 22)
- Urval Patel (Spring 22 – present)
- Manuela Chavez Mejia (Spring 23 – present)

#### Undergraduate Students

- Mai Huong (Fall 16)
- Sam Kuhn (Fall 16 – Spring 17)
- Bete Ranzi (Fall 16 – Spring 17)
- Steven Siang (Fall 16 - Spring 17)
- Isaac Stine (Fall 18)
- Richard Weerts (Spring 19)
- Henry Anderson (Fall 18 - Fall 19)
- Juyoung Shin (Winter 20 - Spring 21)
- Grant Warren (Winter 20 - Spring 23) Received a **Thilo Scholarship** (Summer 22)
- Austin Petfalsi (Spring 23 - present)

### Doctoral Committees

- Timothy Egner (Chemistry Dept. Pr. Venditti) “*Nuclear Magnetic Resonance Methodologies for the Study of Nanoparticle Surface Adsorbed Ligands*” Graduated 11/15/19
- Trang Nguyen (Chemistry Dept. Pr. Venditti) “*Allosteric regulation of bacterial Enzyme I: Toward the discovery of a new class of antimicrobial compounds*” Graduated 04/07/21
- Phan Phong Tuan (BBMB. Pr. Dipali) “*Defining the effects of mismatches on type I-E CRISPR immunity and phage escape*” Graduated 07/16/21
- Kristin Roach (BBMB, Pr. Peters) “*Investigations into the underlying mechanisms of Class II Diterpene Cyclases*” Graduated 04/15/22
- Ambuj Kumar (BBMB. Pr. Jernigan) “*New Computational Methods to Study the Relationship between Protein Structure and Function*” Graduated 06/03/22
- Suresh Shrivanti (BBMB. Pr. Dipali) “*Cas4 and host exonucleases such as DinG facilitate adaptation in type I-C CRISPR-Cas systems*” Graduated 06/24/22
- Philip Dershwitz (BBMB, Pr. Dispirito) “*Methanobactin Biosynthesis and Redox Activity*” Graduated 08/11/22
- Jake Peterson (BBMB, Pr. Moss)
- Christopher Gayvert (Chemistry Dept. Pr. Potoyan)
- Monica Hepker (Vet. Med. Pr. Kanthasamy)

- SeongSoo Lee (Chemistry Dept. Pr. Anderson)
- Dulitha Prasanna (Chemistry Dept. Pr. Potoyan)
- Dan Burn (Chemistry Dept. Pr. Potoyan & Pr. Venditti)
- Chuan Ping (Chemistry Dept. Pr. Potoyan)
- Rachel Murphy (Biochemistry Dept. Pr. Chen)
- Kyle Malcom (Chemistry Dept. Pr. Venditti)
- Yijun Liu (Biochemistry Dept. Pr. Chen)
- Rachel Murphy (Biochemistry Dept. Pr. Chen)
- William Brown (Chemistry Dept. Pr. Potoyan)
- Baboucarr Faal (Chemistry Dept. Pr. Venditti)
- Sayan Das (Chemistry Dept. Pr. Venditti)
- Dilini Dissanayake (Chemistry Dept. Pr. Venditti)

### **Teaching Activities**

- Instructor for BBMB 301 – Survey of Biochemistry (Fall 21, Spring 22, Summer 22, Fall 22, Spring 23, Summer 23, Fall 23)
- Instructor for BBMB 461/561 and 561L - Molecular Biophysics (Spring 20, Spring 21, Spring 22, Spring 23)
- Instructor for BBMB 549 – NMR spectroscopy (Spring 22, Spring 23)
- Instructor for BBMB 221 – Structure and Reactions in Biochemical Processes (Fall 17, Spring 19, Fall 19, Fall 20, Fall 21)
- Instructor for HON 322V – Biochemistry of Drug Addiction (Spring 19)

### **Other Teaching Activities**

Guest Lecturer for the Life Skills Curriculum. Iowa Correctional Institution for Women in Mitchellville, IA.  
Lecture on Biochemistry of Drug Addiction (Summer 19)

### **Institutional Service**

- BBMB Oral Research Proposition Exam (ORPE) Committee (2019 – present)
- BBMB Postdoctoral Committee (2019 – present)
- BBMB Graduate Affairs Committee (2018 – present)
- BBMB Seminar Committee (2016 – present)

### **Professional Service**

- **Ad hoc reviewer for the Biophysics of Neural Systems (BPNS) NIH study section (2021)**
- Reviewer for Scientific Rep., J. Phys. Chem., Biophys. J., BBA - Proteins and Proteomics, J. Mol. Biol., PloS One, J. Am. Chem. Soc., Nature Commun., J. Biomol.NMR, Proteins, Biochemistry, eLife