

# Erich Hellemann, Ph.D.

Email: ehellemann@gmail.com  
LinkedIn: Erich Hellemann  
Google Scholar: Erich Hellemann

## EDUCATION

### University of Pittsburgh

PA, USA

Ph.D. in Molecular Biophysics and Structural Biology

2017–2022

Advisor: Jacob D. Durrant, Ph.D.

- Developed a tool that uses weighted ensemble path sampling to sample protein pocket conformations in an efficient way
- Used molecular dynamics of proteins in their *apo* and *holo* states to elucidate allosteric communications within proteins for the understanding of different types of behaviors

### Carnegie Mellon University

PA, USA

M. S. in Chemistry

2014–2016

Advisor: Roberto R. Gil, Ph.D.

- Developed methodologies for the use of anisotropic NMR parameters in structural elucidation of small molecules

### Universidad Nacional Autónoma de México

Mexico City, México

B. S. in Chemistry

2006–2011

Advisor: Raúl G. Enríquez Habib, Ph.D.

- Thesis: “The use of NMR to study the structure of small organic molecules: isotropic exchange, keto/enol equilibrium of β-dicarbonyl systems”

## EXPERIENCE

### BIOVIA, Dassault Systems

Remote, USA

BIOVIA Customer Success Engineering Specialist

Jan 2023 - Present

- Resolved customer issues promptly, ensuring minimal downtime and a positive customer experience
- Gathered customer feedback and communicated insights to the product team for continuous improvement of the product offering
- Managed escalated customer issues, ensuring swift resolution and maintaining positive relationships
- Performed state of the art computational tools to deliver results for a Contract Research project

### New Mexico State University

NM, USA

Director of the analytical core facility at the Chemistry and Biochemistry Department

Aug 2022–Dec 2022

- Maintaining instrumentation
- Help researchers with their research projects
- Research in the binding mode of the drug Napabucasin to a zinc finger protein
- Mentoring of graduate and undergraduate students

### University of Pittsburgh

PA, USA

Research Assistant

2018–Present

- Development of a computational tool to sample protein conformational space using path sampling techniques for their use in computer-aided drug design
- Use of molecular dynamics to elucidate the effects of mutations or small molecule binding in biologically relevant proteins
- Mentoring of undergraduate students

<b>University of Pittsburgh</b>	PA, USA
Teaching Assistant	Spring 2020
– Course –Biochemistry Laboratory (Biosc 1830)	
<b>University of Pittsburgh</b>	PA, USA
Research Technician in Prof. Andrew P. Hinck laboratory	2016–2017
– Recombinant protein expression and purification	
– Structural studies of TGF- $\beta$ receptors using NMR	
– NMR fragment-based screening of recombinant proteins	
<b>Carnegie Mellon University</b>	PA, USA
Research Assistant	2014 –2016
– Use of anisotropic NMR parameters to determine relative configuration of small molecules	
– Development of methodologies for the use of anisotropic NMR parameters in structural elucidation of small molecules	
<b>Universidad Nacional Autónoma de México</b>	Mexico City, México
Research Assistant	2009 –2011
– NMR studies of natural products	
– Extraction, purification, modification and characterization of natural products	

## PUBLICATIONS

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1. **E. Hellemann**, J.D. Durrant, "Worth the Weight: Sub-Pocket EXplorer (SubPEx), a Weighted Ensemble Method to Enhance Binding-Pocket Conformational Sampling", *J Chem Theory Comput*, 2023, 19, 17, 5677–5689
2. **E. Hellemann**, A. Nallathambi, J.D. Durrant, "Allosteric inhibition of TEM-1  $\beta$ -lactamase: microsecond molecular dynamics simulations provide mechanistic insights", *Protein Sci*, 2023, 32(4), e4622
3. **E. Hellemann\***, J. L. Walker\*, M. A. Lesko\*, D. G. Chandrashekharappa, M. C. Schmidt, A. F. O'Donnell, J. D. Durrant, "Novel mutation in hexokinase 2 confers resistance to 2-deoxyglucose by altering protein dynamics", *PLoS Comput Biol*, 2022, 18(3):e1009929. \*equal contribution
4. S. Ottlie<sup>1</sup>, M.R. Luth<sup>1</sup>, **E. Hellemann**<sup>2</sup>, G.M. Goldgof<sup>2</sup>, *et al.*, "Adaptive laboratory evolution in *S. cerevisiae* highlights role of transcription factors in fungal xenobiotic resistance", *Commun. Biol.*, 2022, 5, 128. <sup>1,2</sup>equal contribution
5. Y. Kochnev, **E. Hellemann**, K.C. Cassidy, J. D. Durrant, "Webina: An Open-Source Library and Web App that Runs AutoDock Vina Entirely in the Web Browser", *Bioinformatics*, 2020, 36(16), 4513–4515
6. **E. Hellemann**, R.R. Gil, "New Stretching Method for Aligning Gels: Its Application to the Measurement Residual Chemical Shift Anisotropies (RCSAs) without the Need for Isotropic Shift Correction", *Chem-Eur J*, 2018, 24(15), 3689–3693
7. F. Hallwass, R.R. Teles, **E. Hellemann**, C. Griesinger, R.R. Gil, A. Navarro-Vázquez, A., "Measurement of residual chemical shift anisotropies in compressed polymethylmethacrylate gels. Automatic compensation of gel isotropic shift contribution", *Magn Reson Chem*, 2018, 56, 321–328
8. W. Waratchareeyakul, **E. Hellemann**, R.R. Gil, K. Chantrapromma, M.K. Langat, Moses, D.A. Mulholland, "Application of Residual Dipolar Couplings and Selective Quantitative NOE to Establish the Structures of Tetranortriterpenoids from *Xylocarpus rumphii*", *J Nat Prod*, 2017, 80(2), 391–402
9. M.E. García, S.R. Woodruff, **E. Hellemann**, N.V. Tsarevsky, R.R. Gil, "Di(ethylene glycol) methyl ether methacrylate (DEGMEMA)-derived gels align small organic molecules in methanol", *Magn Reson Chem*, 2017, 55(3), 206–209

10. L. Castañar, M.E. García, **E. Hellemann**, P. Nolis, R.R. Gil, T. Parella, "One-Shot Determination of Residual Dipolar Couplings: Application to the Structural Discrimination of Small Molecules Containing Multiple Stereocenters", *J Org Chem*, 2016, 81(22), 11126-11131
11. **E. Hellemann**, R.R. Teles, F. Hallwass, W. Barros, A. Navarro-Vázquez, Armando, R.R. Gil, "Mechanical Behavior of Polymer Gels for RDCs and RCSAs Collection: NMR Imaging Study of Buckling Phenomena", *Chem-Eur J*, 2016, 22(46), 16632-16635
12. J.C. Worch, **E. Hellemann**, G. Pros, C. Gayathri, T. Pintauer, R.R. Gil, K.J.T. Noonan, "Stability and Reactivity of 1,3-Benzothiaphosphole: Metalation and Diels-Alder Chemistry", *Organometallics*, 2015, 34(22), 5366-5373

## GRANTS AND INVITED TALKS

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1. Invited speaker at the MBSB Symposium 2021, with the talk: Sub-Pocket Explorer: a Weighted ensemble algorithm to sample protein pocket conformations, Online meeting, May 14 2021
2. Invited speaker at the Just Another (Chemistry) Webinar Series (JAWSChem), with the talk: Sub-Pocket Explorer: Leveraging weighted ensemble simulations to enhance the conformational search of binding-pocket conformations, January 19, 2021
3. XSEDE Startup Allocation, "Sub-Pocket EXplorer (SubPEx): a Weighted ensemble algorithm to sample protein conformations", Jacob D. Durrant (PI), **Erich Hellemann (Co-PI)**, 50,000.0 SUs, 2020

## POSTER PRESENTATIONS

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1. **E. Hellemann**, J.D. Durrant, "Sub-Pocket EXplorer(SubPEx): Leveraging weighted ensemble simulations to enhance the conformational search of binding-pocket conformations", *ACS Spring 2022 National Meeting*, San Diego, USA, 2022
2. **E. Hellemann**, J. L. Walker, M. A. Lesko1, D. G. Chandrashekappa, M. C. Schmidt, A. F. O'Donnell1, J. D. Durrant, "Novel mutation in hexokinase 2 confers resistance to 2-deoxyglucose by altering protein dynamics", *LatinXChem Chemistry Twitter Conference*, Online meeting, 2021
3. **E. Hellemann**, J.D. Durrant, "Sub-Pocket EXplorer(SubPEx): Leveraging weighted ensemble simulations to enhance the conformational search of binding-pocket conformations", *LatinXChem Chemistry Twitter Conference*, Online meeting, 2020
4. **E. Hellemann**, J.D. Durrant, "Sub-Pocket EXplorer(SubPEx): Leveraging weighted ensemble simulations to enhance the conformational search of binding-pocket conformations", *ACS Spring 2020 National Meeting*, Online meeting, 2020
5. **E. Hellemann**, R. Telles, F. Hallwass, A. Navarro-Vázquez, R.R. Gil, "RCSAs: Compressed versus stretched gels. Automatic correction of the isotropic component", *57<sup>th</sup> Experimental Nuclear Magnetic Resonance Conference*, Pittsburgh, PA, USA, 2016
6. L.F. Gil-Silva, R. Santamaría-Fernández, **E. Hellemann**, R.R. Teles, F. Hallwass, W. Barros Jr., A. Navarro-Vázquez, R.R. Gil, "Collection of NMR Scalar and Residual Dipolar Couplings Using a Single Experiment, and Imaging Study of the Aligning Gels", *57<sup>th</sup> Experimental Nuclear Magnetic Resonance Conference*, Pittsburgh, PA, USA, 2016
7. **E. Hellemann**, W. Waratchareeyakul, D.A. Mulholland, R.R. Gil, "Unambiguous Determination of Protolimonoids Side Chain Configuration Assisted by Residual Dipolar Couplings and Quantitative NOE", *Small Molecules Are Still Hot*, Baveno, Italy, 2015
8. **E. Hellemann**, R.R. Teles, F. Hallwass, W. Barros Jr., A. Navarro-Vázquez, R.R. Gil, "NMR imaging studies explain the presence of isotropic solvent at full degree of compression of PMMA gels", *Small Molecules Are Still Hot*, Baveno, Italy, 2015

9. L. Ezra, W. Waratchareeyakul, K. Chantrapromma, S. Chantrapromma, M.K. Langat, S.L. Schwikkard, **E. Hellemann**, R.R. Gil Dulcie A. Mulholland, “Chemical Constituents from *Xylocarpus rumphii* (Meliaceae)”, *International Congress and Annual Meeting of the Society for Medicinal Plant and Natural Product Research*, Budapest, Hungary, 2015
10. M.E. García, S.R. Woodruff, **E. Hellemann**, N.V. Tsarevsky, R.R. Gil, “Di(ethylene glycol) methyl ether methacrylate (DEGMA) gels align small organic molecules in methanol”, *Small Molecules Are Still Hot*, Atlanta, GA, USA, 2014
11. **E. Hellemann**, M.E. García, C. Gayathri, R.R. Gil, “Pure Shift F1 Proton-Coupled J-Scaled BIRD HSQC to Measure RDCs with Higher Accuracy and Sensitivity: Features and Limitations”, *Small Molecules Are Still Hot*, Atlanta, GA, USA, 2014
12. **E. Hellemann**, R. Gaviño, R.G. Enríquez-Habib, “NMR spectroscopy in the study of natural product curcumin”, *Small Molecules Are Still Hot*, Providence, RI, USA, 2012

## SKILLS

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- **Programming:** Python, Bash, Pipeline Pilot
- **Applications:** Discovery Studio, Generative Therapeutics Design, Schrödinger (Maestro, Glide), Autodock Vina, NAMD, Amber, I-TASSER, Topspin, MNova, MSpin, Gaussian09
- **Tools/Techs:** LaTeX, Git
- **Instrumentation:** Nuclear Magnetic Resonance (NMR), CD spectroscopy, Infrared spectroscopy (IR), Gas Chromatography (GS), High-Performance Liquid Chromatography (HPLC), UV-Vis, PCR, Transmission electron microscopy (TEM)
- **Languages:** Spanish (Native), English(bilingual), German (Conversational)

## AWARDS AND LEADERSHIP

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- Travel scholarship to attend Small Molecules Are Still Hot (SMASH) meeting in Atlanta, US, 2014
- Travel scholarship to attend SMASH meeting in Providence, US, 2012
- CONACyT scholarship to work as research assistant, 2009-2011
- Cofounder of the student fraction of the Mexican Chemical Society at the Faculty of Chemistry UNAM, with the secretary position, 2011