Erich Hellemann

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Education

University of Pittsburgh — PA, USA
PhD Candidate in the Molecular Biophysics and Structural Biology program — 2017–Present
Advisor: Jacob D. Durrant PhD

- Research interests focus on computer-aided drug discovery, virtual screening, molecular dynamics simulations, and weighted ensemble path sampling

Carnegie Mellon University — PA, USA
M. S. in Chemistry — 2014–2016
Advisor: Roberto R. Gil PhD

- 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

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

Relevant experience

University of Pittsburgh — PA, USA
Research Assistant — 2018–Present

- Development of a computational tool to sample protein conformational space using rare event 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 biological important proteins
- Mentoring of undergraduate students

University of Pittsburgh — PA, USA
Teaching Assistant — Spring 2020

- Course –Biochemistry Laboratory (Biosc 1830)

University of Pittsburgh — PA, USA
Research Technician in Prof. Andrew P. Hinck laboratory — 2016–2017

- Recombinant protein expression and purification
- Structural studies of TGF–β receptors using NMR
- NMR fragment–based screening of recombinant proteins

Carnegie Mellon University — 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

Universidad Nacional Autónoma de México — Mexico City, México
Research Assistant — 2009 –2011

- NMR studies of natural products
- Extraction, purification and characterization of natural products

Publications

1. S Ottilie, M.R. Luth, **E. Hellemann**, G.M. Goldgof, *et al.*, "Defining the Yeast Resistome through in vitro Evolution and Whole Genome Sequencing", *Under review*, 2021. Preprint in bioRxiv

2. 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

3. **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

4. 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

5. 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

6. 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

7. 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

8. **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

9. 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

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)**, *38,450.0 SUs*, 2020

Posters

1. **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

2. **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

3. **E. Hellemann**, R. Telles, F. Hallwass, A. Navarro-Vázquez, R.R. Gil, "RCSAs: Compressed versus stretched gels. Automatic correction of the isotropic component", *57th Experimental Nuclear Magnetic Resonance Conference*, Pittsburgh, PA, USA, 2016

4. 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", *57th Experimental Nuclear Magnetic Resonance Conference*, Pittsburgh, PA, USA, 2016

5. **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

6. **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

7. 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

8. 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

9. **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

10. **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

- **Programming:** Python, Bash, Golang
- **Applications:** Autodock Vina, NAMD, Amber, I-TASSER, Schrödinger (Maestro), Topspin, MNova, MSpin, Gaussian09
- **Tools/Techs:** LaTeX, Git
- **Instruments:** Nuclear Magnetic Resonance (NMR), 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

- 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