# Charles Tapley Hoyt, Ph.D.

cthoyt.com · in linkedin.com/in/cthoyt · • github.com/cthoyt · • @ @cthoyt@scholar.social · IIIII Q47475003 
bhttps://orcid.org/0000-0003-4423-4370 · IIII Q47475003

I'm working towards building a research group in the Institute of Inorganic Chemistry at RWTH Aachen University focused on software development, data standardization, FAIRification, integration, and applications of ML/AI in the chemical, biological, and health sciences. Therefore, I'm interested in **building academic collaborations** that can lead to grant opportunities and **securing project contracts** for unmet business needs addressed by my semantic technologies, capabilities, and experience.

#### Fields of Work

Bioinformatics, Pathway Analysis, Machine Learning, Natural Language Processing, Ontology, Knowledge Graph, Proteochemometrics, Drug Repositioning, Systems Biology, Cheminformatics

## Employment

- 2025- Wissenschaftlicher Mitarbeiter, RWTH Aachen University, Aachen, Germany.
- 2023–24 **Senior Scientist**, *Northeastern University*, Boston, MA, USA (remote). Moved with the Gyori Lab from Harvard Medical School
- 2021–23 **Research Fellow**, *Harvard Medical School, Laboratory of Systems Pharmacology*, Boston, MA, USA (remote).
  - Biocuration, data standardization, natural language processing, data integration, and automated assembly of knowledge and models (Gyori/INDRA Lab)
  - 2020 **Computational Biologist**, *Enveda Biosciences*, Boulder, CO, USA (remote). Biomedical data integration, knowledge graph construction, and analysis
- 2018–19 Lecturer, University of Bonn, Bonn, Germany.
- 2016–19 **Research Fellow**, Fraunhofer SCAI, Dept. of Bioinformatics, Sankt Augustin, Germany. Systems biology modeling and analysis with the Biological Expression Language
- 2012–15 **Teaching Assistant**, Northeastern University, Boston, MA, USA.
  - 2014 in Silico Lead Discovery Co-op, Novartis, Cambridge, MA, USA.
    Mechanism of action deconvolution in high-throughput black-box phenotypic screens
- 2013–14 **Molecular Informatics Internship**, *Pfizer*, Cambridge, MA, USA. Software development and database development for cancer genomics data
  - 2013 **Post-Selection Chemistry Co-op**, *GlaxoSmithKline*, Waltham, MA, USA. Lead optimization of antivirals identified by ultra-high-throughput screening
  - 2012 **Research Assistant**, *Pollastri Laboratory*, *Northeastern University*, Boston, MA, USA. Medicinal synthetic chemistry for repurposing PDE4 inhibitors against *T. Brucei*

#### Education

2018–19 **Doctor of Philosophy**, *Computational Life Sciences*, University of Bonn.

Thesis: Generation and Applications of Knowledge Graphs in Systems and Networks Biology

Research Advisor: Prof. Dr. Martin Hofmann-Apitius

GPA: 1,3 (Magna Cum Laude)

2015–17 Master of Science, Life Science Informatics, University of Bonn.

Thesis: PyBEL: a Computational Framework for Biological Expression Language

Research Advisor: Prof. Dr. Martin Hofmann-Apitius

GPA: 1,6

2011–15 Bachelor of Science, Chemistry, Northeastern University.

GPA: 3.93/4.0 (Summa Cum Laude)

Research Advisor: Prof. Dr. Michael P. Pollastri

#### Awards

- 2023 Excellence in Biocuration Early Career Award, International Society of Biocuration.
- 2015 Bernie Lemire Award, Department of Chemistry, Northeastern University.
- 2011 **Presidential Scholarship**, Northeastern University.

# Research

## Publications

Author lists have been omitted to reduce visual clutter. There are a total of 62 manuscripts (53 peer-reviewed, 8 pre-printed/submitted, and 1 in preparation). The following are noted:

- † signifies first or co-first authorship
- ‡ signifies last or senior authorship
- 1. †Assembly and reasoning over semantic mappings at scale for biomedical data integration. *Bioinformatics*, 2025. doi:10.1093/bioinformatics/btaf542
- 2. †Improving reproducibility of cheminformatics workflows with chembl-downloader. JOSS, 2025. doi:10.21105/joss.08844
- 3. (preprint) †Causal identification with Y0. arXiv, 2025. doi:10.48550/arxiv.2508.03167
- 4. (preprint) The Cell Ontology in the age of single-cell omics. arXiv, 2025. doi:10.48550/arxiv.2506.10037
- 5. †Computational tools and data integration to accelerate vaccine development: challenges, opportunities, and future directions. Front Immunol, 2025. doi:10.3389/fimmu.2025.1502484
- 6. (in preparation) †Assembly and application of coherent biomedical lexica. in preparation for Database, 2025
- 7. (submitted) **OmniPath: integrated knowledgebase for multi-omics analysis**. *submitted to Nucleic Acids Research*, 2025. biorxiv:2025.09.11.675512
- 8. (submitted) VO: The Vaccine Ontology. submitted to Scientific Data, 2025. biorxiv:2025.08.12.669998
- 9. (submitted) ‡More Rigorous Software Engineering Would Improve Reproducibility in Machine Learning Research. submitted to TMLR, 2025. arxiv:2502.00902
- 10. (in preparation) **Teaching RDM in a smart advanced inorganic lab course and its provision in the DALIA platform**. *in preparation for Nature Computational Science*, 2025
- 11. Eliater: A Python package for estimating outcomes of perturbations in biomolecular networks. *Bioinformatics*, 2024. doi:10.1093/bioinformatics/btae527
- 12. †The O3 guidelines: open data, open code, and open infrastructure for sustainable curated scientific resources. *Scientific Data*, 2024. doi:10.1038/s41597-024-03406-w
- 13. An open source knowledge graph ecosystem for the life sciences. *Scientific Data*, 2024. doi:10.1038/s41597-024-03171-w
- 14. ‡ptwt The PyTorch Wavelet Toolbox. JMLR, 2024
- 15. A simple standard for ontological mappings 2023: updates on data model, collaborations and tooling. *OM 2023*
- 16. The Human Phenotype Ontology in 2024: phenotypes around the world. NAR, 2023. doi:10.1093/nar/gkad1005
- 17. †Improving reproducibility and reusability in the Journal of Cheminformatics. *J Cheminform*, 2023. doi:10.1186/s13321-023-00730-y
- 18. Democratizing knowledge representation with BioCypher. *Nature Biotechnology*, 2023. doi:10.1038/s41587-023-01848-y
- 19. Optimal adjustment sets for causal query estimation in partially observed biomolecular networks. *Bioinformatics*, 2023. doi:10.1093/bioinformatics/btad270
- 20. †Prediction and curation of missing biomedical identifier mappings with Biomappings. *Bioinformatics*, 2023. doi:10.1093/bioinformatics/btad130
- 21. (preprint) Experimental design for causal query estimation in partially observed biomolecular networks.

- arXiv, 2022. arxiv:2210.13423
- 22. †Unifying the identification of biomedical entities with the Bioregistry. *Scientific Data*, 2022. doi:10.1038/s41597-022-01807-3
- 23. A Simple Standard for Ontological Mappings 2022: Updates of data model and outlook. OM 2022
- 24. A Review of Biomedical Datasets Relating to Drug Discovery: A Knowledge Graph Perspective. Brief Bioinform, 2022. doi:10.1093/bib/bbac404
- 25. ChemicalX: A Deep Learning Library for Drug Pair Scoring. KDD, 2022. doi:10.1145/3534678.3539023
- 26. Integrating multi-omics data reveals function and therapeutic potential of deubiquitinating enzymes. *eLife*, 2022. doi:10.7554/elife.72879
- 27. Understanding the Performance of Knowledge Graph Embeddings in Drug Discovery. Artificial Intelligence in the Life Sciences, 2022. doi:10.1016/j.ailsci.2022.100036
- 28. A Simple Standard for Sharing Ontological Mappings (SSSOM). Database, 2022. doi:10.1093/database/baac035
- 29. **Gilda:** biomedical entity text normalization with machine-learned disambiguation as a service. *Bioinformatics Advances*, 2022. doi:10.1093/bioadv/vbac034
- 30. ProtSTonKGs: A Sophisticated Transformer Trained on Protein Sequences, Text, and Knowledge Graphs. SWAT4HCLS 2022. ceur-ws:3127:13
- 31. (preprint) Mondo: Unifying diseases for the world, by the world. medRxiv, 2022. doi:10.1101/2022.04.13.22273750
- 32. **Do-calculus enables estimation of causal effects in partially observed biomolecular pathways**. *Bioinformatics*, 2022. doi:10.1093/bioinformatics/btac251
- 33. (preprint) †A Unified Framework for Rank-based Evaluation Metrics for Link Prediction in Knowledge Graphs. arXiv, 2022. arxiv:2203.07544
- 34. PyBioPAX: biological pathway exchange in Python. JOSS, 2022. doi:10.21105/joss.04136
- 35. (preprint) An Open Challenge for Inductive Link Prediction on Knowledge Graphs. arXiv, 2022. arxiv:2203.01520
- 36. STonKGs: A Sophisticated Transformer Trained on Biomedical Text and Knowledge Graphs. *Bioinformatics*, 2022. doi:10.1093/bioinformatics/btac001
- 37. Ontology Development Kit: a toolkit for building, maintaining, and standardising biomedical ontologies. *Database*, 2022. doi:10.1093/database/baac087
- 38. Bringing Light Into the Dark: A Large-scale Evaluation of Knowledge Graph Embedding Models Under a Unified Framework. TPAMI, 2021. doi:10.1109/tpami.2021.3124805
- 39. The role of metadata in reproducible computational research. Patterns, 2021. doi:10.1016/j.patter.2021.100322
- 40. ‡CLEP: a hybrid data- and knowledge-driven framework for generating patient representations. Bioinformatics, 2021. doi:10.1093/bioinformatics/btab340
- 41. A Systems Biology Approach for Hypothesizing the Effect of Genetic Variants on Neuroimaging Features in Alzheimer's Disease. *JAD*, 2021. doi:10.3233/jad-201397
- 42. †PyKEEN 1.0: A Python Library for Training and Evaluating Knowledge Graph Embeddings. *JMLR*, 2021. arxiv:2007.14175
- 43. Leveraging Structured Biological Knowledge for Counterfactual Inference: A Case Study of Viral Pathogenesis. *IEEE TBDATA*, 2021. doi:10.1109/tbdata.2021.3050680
- 44. (preprint) †Extension of Roles in the ChEBI Ontology. ChemRxiv, 2020. doi:10.26434/chemrxiv.12591221
- 45. The Minimum Information about a Molecular Interaction Causal Statement (MI2CAST). *Bioinformatics*, 2020. doi:10.1093/bioinformatics/btaa622
- 46. GuiltyTargets: Prioritization of Novel Therapeutic Targets with Deep Network Representation Learning. *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, 2020. doi:10.1109/tcbb.2020.3003830
- 47. **PS4DR:** a multimodal workflow for identification and prioritization of drugs based on pathway signatures. *BMC Bioinf.*, 2020. doi:10.1186/s12859-020-03568-5

- 48. Identifying the parametric occurrence of multiple steady states for some biological networks. *Journal of Symbolic Computation*, 2020. doi:10.1016/j.jsc.2019.07.008
- 49. A Computational Approach for Mapping Heme Biology in the Context of Hemolytic Disorders. Frontiers in Bioengineering and Biotechnology, 2020. doi:10.3389/fbioe.2020.00074
- 50. The Impact of Pathway Database Choice on Statistical Enrichment Analysis and Predictive Modeling. *Frontiers in Genetics*, 2019. doi:10.3389/fgene.2019.01203
- 51. Quantifying mechanisms in neurodegenerative diseases (NDDs) using candidate mechanism perturbation amplitude (CMPA) algorithm. *BMC Bioinf.*, 2019. doi:10.1186/s12859-019-3101-1
- 52. The KEEN Universe An Ecosystem for Knowledge Graph Embeddings with a Focus on Reproducibility and Transferability. *ISWC 2019*. doi:10.1007/978-3-030-30796-7<sub>1</sub>
- 53. Predicting Missing Links Using PyKEEN. ISWC 2019. ceur-ws:2456:64
- 54. RatVec: A General Approach for Low-dimensional Distributed Vector Representations via Domain-specific Rational Kernels. LWDA 2019
- 55. BioKEEN: a library for learning and evaluating biological knowledge graph embeddings. *Bioinformatics*, 2019. doi:10.1093/bioinformatics/btz117
- 56. PathMe: merging and exploring mechanistic pathway knowledge. *BMC Bioinf.*, 2019. doi:10.1186/s12859-019-2863-9
- 57. (preprint) †Integration of Structured Biological Data Sources using Biological Expression Language. *bioRxiv*, 2019. doi:10.1101/631812 biorxiv:631812
- 58. ComPath: an ecosystem for exploring, analyzing, and curating mappings across pathway databases. *NPJ Syst Biol Appl.*, 2019. doi:10.1038/s41540-018-0078-8
- 59. †Re-curation and rational enrichment of knowledge graphs in Biological Expression Language. *Database*, 2019. doi:10.1093/database/baz068
- 60. Challenges of Integrative Disease Modeling in Alzheimer's Disease. Frontiers in molecular biosciences, 2019. doi:10.3389/fmolb.2019.00158
- 61. †BEL Commons: an environment for exploration and analysis of networks encoded in Biological Expression Language. *Database*, 2018. doi:10.1093/database/bay126
- 62. BEL2ABM: agent-based simulation of static models in Biological Expression Language. *Bioinformatics*, 2018. doi:10.1093/bioinformatics/bty107
- 63. †PyBEL: a Computational Framework for Biological Expression Language. *Bioinformatics*, 2018. doi:10.1093/bioinformatics/btx660
- 64. †A systematic approach for identifying shared mechanisms in epilepsy and its comorbidities. *Database*, 2018. doi:10.1093/database/bay050
- 65. A Case Study on the Parametric Occurrence of Multiple Steady States. ISSAC 2017. doi:10.1145/3087604.3087622
- Repurposing human PDE4 inhibitors for neglected tropical diseases: design, synthesis and evaluation of cilomilast analogues as Trypanosoma brucei PDEB1 inhibitors. Bioorg Med Chem Lett, 2014. doi:10.1016/j.bmcl.2014.07.063

# Invited Presentations (Selected)

- 1. Modern software development practice with Python. May Institute (May 7, 2024)
- 2. Assembly and inference over semantic mappings to support the NFDI Terminology Service. *TS4NFDI Community Workshop* (April 9, 2024)
- 3. **Assembly of Domain Knowledge at Scale in Biomedicine and Beyond**. *Harvard Medical School Laboratory of Systems Pharmacology Meeting* (January 19, 2024)
- 4. Machine-assisted integration of data and knowledge at scale to support biomedical discovery. *NIH BISTI Seminar* (December 7, 2023)
- 5. **Democratizing Biocuration, or, How I Learned to Love the Drive-by Curation**. *International Society of Biocuration Annual General Meeting* (October 18, 2023)

- 6. **Improving ontology interoperability with Biomappings**. *OBO Academy Monarch Training Series* (September 19, 2023)
- 7. **Modern prefix management with the Bioregistry and 'curies'**. *OBO Academy Monarch Training Series* (September 5, 2023)
- 8. Axiomatizing Chemical Roles. Ontologies4Chem Workshop 2022 (September 7, 2022)
- 9. Modern Scientific Software Development Practice in Python. May Institute (May 20, 2022)
- 10. Knowledge Graph Embedding with PyKEEN in 2022. Knowledge Graph Conference (KGC 2022) (May 5, 2022)
- 11. The Biopragmatics Stack: Biomedical and Chemical Semantics for Humans. Machine-Actionable Data Interoperability for Chemical Sciences (MADICES) (February 8, 2022)
- 12. Reusable Science in Python. May Institute (July 28, 2021)
- 13. Current Issues in Theory, Reproducibility, and Utility of Graph Machine Learning in the Life Sciences. *Graph Machine Learning in Industry* (September 23, 2021)
- 14. Perspectives on Knowledge Graph Embedding Models in/out of Biomedicine. AstraZeneca (April 6, 2021)
- 15. Introduction to the Biological Expression Language and the Rational Enrichment Workflow. *CoronaWhy* (May 6, 2020)
- 16. **Applications of Knowledge Graphs in Drug Discovery**. *Computational Drug Discovery Group, University of Leiden* (November 5, 2019)
- 17. Generation and Application of Biomedical Knowledge Graphs. Harvard Medical School (July 19, 2019)

# Talks and Posters (Selected)

- 1. Bioregistry Workshop at Biocuration 2025. Bioregistry Workshop @ Biocuration 2025 (April 6, 2025)
- 2. Bioregistry and the NFDI in 2024. 3rd Ontologies4Chem Workshop (December 9, 2024)
- 3. Assembly and Reasoning over Semantic Mappings at Scale. Biocuration 2024 (March 7, 2024)
- 4. Introduction to WPCI 2023. Winter 2023 Workshop on Prefixes, CURIEs, and IRIs (November 27, 2023)
- 5. Standardization of chemical prefixes, CURIEs, URIs, and semantic mappings. *Ontologies4Chem Workshop* 2023 (October 12, 2023)
- 6. Improving the reproducibility of cheminformatics workflows with chembl-downloader. RDKit User Group Meeting 2023 (September 21, 2023)
- 7. Promoting the longevity of curated scientific resources through open code, open data, and public infrastructure. *Biocuration 2023* (April 26, 2023)
- 8. Using dashboards to monitor ontology standardisation and community activity. *Ontology Summit 2023* (February 15, 2023)
- 9. Introduction to WPCI 2022. 2022 Workshop on Prefixes, CURIEs, and IRIs (December 5, 2022)
- 10. The Bioregistry, CURIEs, and OBO Community Health. International Conference on Biomedical Ontology (ICBO) (September 26, 2022)
- 11. Closing the Semantic Gap: Identifying Missing Mappings and Merging Equivalent Concepts to Support Knowledge Graph Assembly. Harvard Medical School Sorger Lab Meeting (August 1, 2022)
- 12. A Unified Framework for Rank-based Evaluation Metrics for Link Prediction in Knowledge Graphs. *Graph Learning Benchmarks (GLB 2022)* (April 26, 2022)
- 13. Introduction to WPCI 2021. 2021 Workshop on Prefixes, CURIEs, and IRIs (October 29, 2021)
- 14. **Biomappings: Community Curation of Mappings between Biomedical Entities**. 4th Session of the International Society of Biocuration 2021 Virtual Conference (October 5, 2021; poster)
- 15. **The Bioregistry: A Metaregistry for Biomedical Entities**. *12th International Conference on Biomedical Ontologies* (September 17, 2021)

- 16. Future Directions for WikiPathway Meta-curation. WikiPathways Developers Conference Call (January 6, 2021)
- 17. **The Biological Expression Language and PyBEL in 2020**. *COVID-19 Disease Map Community Meeting* (July 10, 2020)
- 18. Maintenance and Enrichment of Disease Maps in Biological Expression Language. 4th Disease Maps Community Meeting (October 4, 2019; poster)
- 19. Identifying Drug Repositioning Candidates using Representation Learning on Heterogeneous Networks. *The Eighth Joint Sheffield Conference on Chemoinformatics* (June 19, 2019; poster)
- 20. The PyBEL Ecosystem in 2018. OpenBEL Community Meeting (May 14, 2018)
- 21. From Knowledge Assembly to Hypothesis Generation. Bio-IT World (April 22, 2018)
- 22. Knowledge Assembly in Systems and Networks Biology. Bio-IT World (April 23, 2018; poster)
- 23. **The Human Brain Pharmacome: An Overview**. *3rd European Conference on Translational Bioinformatics* (April 17, 2018; poster)
- 24. **Gene Set Analysis using Phenotypic Screening Data**. *Research, Innovation and Scholarship Expo 2015* (April 9, 2015; poster)

# Research Software (Selected)

12. **SeffNet** 

Achieving reproducibility and reusability in the computational sciences heavily depends on code that is developed, tested, documented, and distributed according to best software development practices. I aim to make as much of my research as possible available and reusable in the form of open source software. Accordingly, I have pushed tens of thousands of commits to GitHub across my own and external projects to which I have contributed. I have also written extensively on teaching best practices to scientists on my blog.

1.	PyBEL (DEL)	<b>O</b> pybel/pybel
2	A compiler for the Biological Expression Language (BEL)  Bio2BEL	hio2hal/hio2hal
۷.	A framework for reproducible data integration in BEL and knowledge graph cons	<b>♀</b> bio2bel/bio2bel truction
3.	<b>BEL Commons</b> A web application for the interactive exploration of networks encoded in BEL	• bel-commons/bel-commons
4.	PyKEEN The most expansive knowledge graph embedding framework to date	• pykeen/pykeen
5.	SeMRA Automated assembly and inference of semantic mappings	• biopragmatics/semra
6.	<b>Bioontologies</b> Access and processing of ontologies on top of ROBOT and OBO Graphs	• biopragmatics/bioontologies
7.	PyOBO Harmonization of biological ontologies and controlled vocabularies	<b>O</b> pyobo/pyobo
8.	curies Idiomatic conversion between URIs and compact URIs (CURIEs)	• biopragmatics/curies
9.	<b>GuiltyTargets</b> Target prioritization framework using gene expression and network representation	$\begin{tabular}{l} \Omega \ \mbox{guiltytargets/guiltytargets} \\ \mbox{learning} \end{tabular}$
10.	RatVec Sequence-based representation learning	• ratvec/ratvec
11.	<b>PS4DR</b> Drug repositioning based on bioactivity pattern matching and GWAS	<b>O</b> ps4dr/ps4dr

Seffnet/seffnet

	Drug repositioning framework based on network representation le	earning
13.	<ol> <li>CLEP         Patient stratification framework based on network representation     </li> </ol>	$\label{eq:clephase} \ensuremath{ f O} \mbox{ hybrid-kg/clep}$ learning
14.	14. <b>BEL2SCM</b> Generation of structural causal models (SCMs) from BEL	• bel2scm/bel2scm
15.	15. <b>y0 Causal Inference Engine</b> Representation and manipulating probabilistic expressions	• y0-causal-inference/y0
16.	16. <b>STonKGs</b> Multimodal Transformers for biomedical text and Knowledge Gra	• stonkgs/stonkgs
17.	17. <b>ChemicalX</b> A deep learning library for drug-drug interaction, polypharmacy s	• AstraZeneca/chemicalx side effect, and synergy prediction
18.	18. <b>PathMe</b> Web application for exploration of pathway databases	• PathwayMerger/PathMe
19.	19. <b>INDRA</b> Automated knowledge assembly and modeling in biomedicine	• sorgerlab/indra
20.	20. INDRA CoGEx A $10^8$ relation-scale knowledge graph extending on causal knowledge	• bgyori/indra_cogex edge from INDRA
21.	21. MIRA  Machine-assisted scientific modeling using meta-model templates	$oldsymbol{\Omega}$ indralab/miras and domain knowledge graphs
22.	22. <b>Gilda</b> Biomedical named entity recognition and grounding using machi	$oldsymbol{\Omega}$ indralab/gilda ne-learned disambiguation
	Databases (Selected)	
1.		egistry/bioregistry , https://bioregistry.io
2.	2. <b>Biomappings</b> • D biopragmatics/biomappings , https Predicted and curated mappings between named biological entiti	://biopragmatics.github.io/biomappings
3.	3. <b>Biolookup</b> Comprehensive database of identifiers, names, synonyms, cross-reentities	pragmatics/biolookup , http://biolookup.io ferences, properties, and relations for biomedical
4.	4. <b>Bioversions</b> Automated tracking of the current version for each biological date.	$oldsymbol{\Omega}$ biopragmatics/bioversions tabase?
5.	5. <b>OBO Database Ingest</b> Conversion of biomedical databases into ontologies	$oldsymbol{\Omega}$ biopragmatics/obo-db-ingest
6.	6. Chemical Roles Graph Connecting roles in the ChEBI ontology to their targets	$oldsymbol{\Omega}$ chemical-roles/chemical-roles
7.	7. <b>CONSO</b> Ontology of phenomena related to neurodegeneration	• pharmacome/conso
8.	8. <b>CONIB</b> Curated knowledge graphs describing neurodegeneration in BEL	• pharmacome/conib
9.	9. <b>ComPath</b> A data integration pipeline, manually curated dataset of mappings for integrative analysis of pathways	h , https://compath.scai.fraunhofer.de/ between pathway databases, and web application

## **External Contributions**

Manually and semi-automatically curated resources benefit greatly from open governance models that enable external contribution. Instead of creating siloed or single use improvements to resources I consume, I aim to make as many upstream contributions as possible. Accordingly, I have made hundreds of small contributions across 50+ ontologies in the OBO Foundry and other resources including:

EHDAA2, SSSOM, MIAPA, DDPHENO, BFO, ECO, OMO, GO, FYPO, OAE, HSAPDV, COB, RO, MMUSDV, MP, AGRO, CIDO, EUPATH, GEO, TTO, OGMS, BSPO, OLATDV, FBBT, PECO, XCO, UPHENO, CL, CDAO, AISM, HAO, HANCESTRO, ONS, PCL, SWO, OBA, PDUMDV, HTN, MOD, PO, OHD, OBI, LEPAO, EXO, MONDO, UBERON, ENVO, SYMP, IAO, CHMO, TO, TAXRANK, WBBT, WBLS, HP, MAXO, COLAO

## Funding

## 1. Advancing Data Integration and Discovery in Biomedicine with the Bioregistry

Chan Zuckerberg Initiative (CZI), (2023-329850), \$250K overall, 2023-2025 (24 months), Grant: 2023-329850 PI: Benjamin M. Gyori

Role: Key person. Co-wrote proposal, responsible for design and implementation of research plan.

#### 2. (past) Rapid Assessment of Platform Technologies to Expedite Response

Defense Threat Reduction Agency (DTRA), (FP00012844), \$623K (subcontract) / \$15M overall, 2022-2024 (18 months), Grant: HDTRA1242031

PI: Benjamin M. Gyori

Role: Participant. Co-wrote proposal with PNNL collaborators. Responsible for design and implementation of research plan. Lead developer of semantic and analytical technologies. Note: left position before project completion.

#### 3. (past) MIRA: Modeling with an Intelligent Reasoning Assistant

DARPA ASKEM Program, (HR00112220036), \$2.1M, 2022-2026 (42 months)

PI: Benjamin M. Gyori

Role: Participant. Note: left position before project completion.

#### 4. (past) Young Faculty Award / DARPA Director's Fellowship Award

DARPA, (W911NF2010255), \$750K, 2020-2023 (36 months)

PI: Benjamin M. Gyori Role: Participant

#### 5. (past) Ecosystem of Machine-maintained Models with Automated Assembly

DARPA Automating Scientific Knowledge Extraction (ASKE) / Artificial Intelligence Exploration (AIE) program, (HR00111990009), \$2M, 2018-2020 (18 months + extension)

PI: Benjamin M. Gyori

Role: Participant. Note: Joined in 2021

#### 6. (past) Interdisciplinary Research Award

Fraunhofer Center for Machine Learning, (Internal), \$40K 2019 (3 months)

PI: Martin Hofmann-Apitius

Role: Key person. Co-wrote proposal. Responsible for design and implementation of research plan including applications of PyKEEN in biomedicine.

## 7. (past) Fraunhofer Service Contract

Philip Morris International, (Contract), €80K 2019-2020 (4 months)

PI: Martin Hofmann-Apitius

Role: Key Person. Co-responsible for design and implementation of visual analytics software for the Biological Expression Language.

### 8. (past) Human Brain Pharmacome

Fraunhofer, under the MAVO Scheme, 2018-2021 (4 years)

PI: Martin Hofmann-Apitius

Role: Participant. Lead project on Fraunhofer SCAI team. Note: left position before project completion.

## 9. (past) PYBEL2NDEX

University of California, San Diego, (Contract), \$28K 2018 (6 months)

PI: Martin Hofmann-Apitius

Role: Key person. Wrote proposal. Responsible for design and implementation of research plan for implementing interoperability between PyBEL and NDEx.

#### 10. (past) AETIONOMY

European Union (EU), European Federation of Pharmaceutical Industries and Associations (EFPIA), and Innovative Health Initiative (IMI), (115568), equiv 17.8M 2014-2018 (4 years)

PI: Martin Hofmann-Apitius

Role: Participant. Note: Joined in 2016.

# Community

## Professional Affiliations

- International Society of Biocuration (2021 -)
- o CoronaWhy (2020 2021)
- o OpenBEL Consortium (2017 -)
- Erasmus Student Network Bonn (2016 -)
- o American Chemical Society (2011 2022)

# Service to the Community

## Scholarly Journals

- 1. Scientific article reviewer (ad hoc) in:
  - Bioinformatics
  - Database
  - BMC Bioinformatics
  - Journal of Cheminformatics
  - Journal of Biomedical Semantics
  - o el ife
  - MATCH Communications in Mathematical and in Computer Chemistry
  - Peer.J
- 2. Guest Reproducibility Editor, Journal of Cheminformatics (2023-)
- 3. Grant reviewer for:
  - o CZI Essential Open Source Software (EOSS) Cycle 6 (2023)

## Conference Organizing Committees

- 1. ICBO 2024 (Program Committee)
- 2. 2023 Workshop on Prefixes, CURIEs, and IRIs (Organizer)
- 3. Biocuration 2024 (Organizing Committee)
- 4. Biocuration 2023 (Co-chair)
- 5. 2022 Workshop on Prefixes, CURIEs, and IRIs (Organizer)
- 6. ICBO 2022 Workshop on Ontology Tools (Co-organizer)
- 7. ICBO 2022 (Program Committee)
- 8. ISMB 2022 (Bio-Ontologies/BOSC joint session) (Program Committee)
- 9. Biocuration 2022 (Organizing Committee)
- 10. 2021 Workshop on Prefixes, CURIEs, and IRIs (Organizer)

#### Other Service

1. International Society of Biocuration (Executive Committee)

# **Teaching**

## Courses Taught

I have given 11 lectures, 1 seminars, and 7 practicals / labs as either the primary or a guest instructor.

#### Northeastern University

- 1. Modern software development practice with Python (Practical; Instructor; Summer 2024)
- 2. Modern Scientific Software Development Practice in Python (Practical; Instructor; Summer 2022)
- 3. Reusable Science in Python (Practical; Instructor; Summer 2021)
- 4. Drug Discovery and Development (Lecture; Teaching Assistant; Summer II 2015)
- 5. Organic Chemistry II for Majors (Lecture; Teaching Assistant; Spring 2015)
- 6. Organic Chemistry I for Majors (Lecture; Teaching Assistant; Fall 2014)
- 7. Organic Chemistry II for Majors (Lecture; Teaching Assistant; Spring 2014)
- 8. Organic Chemistry I for Majors (Lecture; Teaching Assistant; Fall 2013)

### University of Bonn

- 1. Mechanism Enrichment Using NeuroMMSig (Practical; Guest Lecturer; Winter 2020-2021)
- 2. Mechanism Enrichment Using NeuroMMSig (Practical; Guest Lecturer; Winter 2019-2020)
- 3. Mathematics Meets Life Sciences (Lecture; Guest Lecturer; Winter 2019-2020)
- 4. Enzyme Technology Internship (Practical; Instructor; Summer 2019)
- 5. Life Sciences Knowledge Discovery (Lecture; Guest Lecturer; Summer 2019)
- 6. Knowledge Assembly, Data Integration, and Modeling in Systems and Networks Biology (Seminar; Instructor; Winter 2018-2019)
- 7. Biological Databases (Lecture; Guest Lecturer; Winter 2018-2019)
- 8. Life Sciences Knowledge Discovery (Lecture; Guest Lecturer; Summer 2018)
- 9. Biological Databases (Lecture; Guest Lecturer; Winter 2017-2018)
- 10. Life Sciences Knowledge Discovery (Lecture; Guest Lecturer; Summer 2017)
- 11. Biomedical Database Lab (Practical; Teaching Assistant; Winter 2016-2017)

## Supervision

## Northeastern University

- o Aria Agarwal D Undergraduate Research Assistant (January May 2024)
- Sara Taheri
   Doctoral Student (July 2023 April 2024)

## CoronaWhy

o Aman Choudhri D Student Research Assistant (June - October 2020)

#### Fraunhofer

- Lauren Nicole DeLong
   Student Research Assistant (September December 2019)
- Vinay Bharadhwaj
   Student Research Assistant (July December 2019)
- Yojana Gadiya
   Student Research Assistant (April May 2019)
- Trusha Adeshara
   Student Research Assistant (April May 2019)
- o Rana Aldisi D Student Research Assistant (July 2018 March 2019)
- Lingling Xu Student Research Assistant (July 2018 March 2019)
- o Kristian Kolpeja D Student Research Assistant (July November 2018)
- Sandra Spalek Student Research Assistant (July 2018 August 2019)
- Keerthika Lohanadan Student Research Assistant (July September 2018)
- Colin Birkenbihl Student Research Assistant (July October 2017)
- Aram Grigoryan Student Research Assistant (July December 2017)

#### University of Bonn

- Mauricio Pio de Lacerda
   Master's Student (March December 2019)
- Rana Aldisi Master's Student (March December 2019)
- o Lingling Xu Master's Student (March December 2019)
- o Özlem Muslu 📵 Master's Student (May December 2018)