Charles Tapley Hoyt, Ph.D.

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Fields of Work

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

Employment

- 2023- **Research Fellow**, *Northeastern University*, Boston, MA, USA (remote).
- 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

- 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. The following are noted:

- † signifies first or co-first authorship
- ‡ signifies last or senior authorship
- 1. †Improving reproducibility and reusability in the Journal of Cheminformatics. *J Cheminform*, 2023. doi:10.1186/s13321-023-00730-y
- 2. Democratizing knowledge representation with BioCypher. *Nature Biotechnology*, 2023. doi:10.1038/s41587-023-01848-y
- 3. †Prediction and curation of missing biomedical identifier mappings with Biomappings. *Bioinformatics*, 2023. doi:10.1093/bioinformatics/btad130
- 4. (preprint) Experimental design for causal query estimation in partially observed biomolecular networks. arXiv, 2022. arxiv:2210.13423
- 5. †Unifying the identification of biomedical entities with the Bioregistry. Scientific Data, 2022. doi:10.1038/s41597-022-01807-3
- 6. A Simple Standard for Ontological Mappings 2022: Updates of data model and outlook. OM 2022
- 7. A review of biomedical datasets relating to drug discovery: a knowledge graph perspective. *Brief Bioinform*, 2022. doi:10.1093/bib/bbac404
- 8. ChemicalX: A Deep Learning Library for Drug Pair Scoring. KDD, 2022. doi:10.1145/3534678.3539023
- 9. Integrating multi-omics data reveals function and therapeutic potential of deubiquitinating enzymes. *eLife*, 2022. doi:10.7554/elife.72879
- 10. Understanding the Performance of Knowledge Graph Embeddings in Drug Discovery. *Artificial Intelligence in the Life Sciences*, 2022. doi:10.1016/j.ailsci.2022.100036
- 11. A Simple Standard for Sharing Ontological Mappings (SSSOM). Database, 2022. doi:10.1093/database/baac035
- 12. Gilda: biomedical entity text normalization with machine-learned disambiguation as a service. Bioinformatics Advances, 2022. doi:10.1093/bioadv/vbac034
- 13. ProtSTonKGs: A Sophisticated Transformer Trained on Protein Sequences, Text, and Knowledge Graphs. SWAT4HCLS 2022. ceur-ws:3127:13
- 14. (preprint) Mondo: Unifying diseases for the world, by the world. medRxiv, 2022. doi:10.1101/2022.04.13.22273750
- 15. **Do-calculus** enables estimation of causal effects in partially observed biomolecular pathways. *Bioinformatics*, 2022. doi:10.1093/bioinformatics/btac251
- 16. (preprint) †A Unified Framework for Rank-based Evaluation Metrics for Link Prediction in Knowledge Graphs. arXiv, 2022. arxiv:2203.07544
- 17. PyBioPAX: biological pathway exchange in Python. JOSS, 2022. doi:10.21105/joss.04136
- 18. (preprint) An Open Challenge for Inductive Link Prediction on Knowledge Graphs. arXiv, 2022. arxiv:2203.01520
- 19. STonKGs: A Sophisticated Transformer Trained on Biomedical Text and Knowledge Graphs. *Bioinformatics*, 2022. doi:10.1093/bioinformatics/btac001
- 20. Ontology Development Kit: a toolkit for building, maintaining and standardizing biomedical ontologies. *Database*, 2022. doi:10.1093/database/baac087
- 21. 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
- 22. The role of metadata in reproducible computational research. Patterns, 2021. doi:10.1016/j.patter.2021.100322
- 23. ‡CLEP: a hybrid data- and knowledge-driven framework for generating patient representations. *Bioinformatics*, 2021. doi:10.1093/bioinformatics/btab340

- 24. 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
- 25. †PyKEEN 1.0: A Python Library for Training and Evaluating Knowledge Graph Embeddings. *JMLR*, 2021. arxiv:2007.14175
- 26. Leveraging Structured Biological Knowledge for Counterfactual Inference: A Case Study of Viral Pathogenesis. *IEEE TBDATA*, 2021. doi:10.1109/tbdata.2021.3050680
- 27. (preprint) †Extension of Roles in the ChEBI Ontology. ChemRxiv, 2020. doi:10.26434/chemrxiv.12591221
- 28. The Minimum Information about a Molecular Interaction Causal Statement (MI2CAST). *Bioinformatics*, 2020. doi:10.1093/bioinformatics/btaa622
- 29. **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
- 30. **PS4DR:** a multimodal workflow for identification and prioritization of drugs based on pathway signatures. *BMC Bioinf.*, 2020. doi:10.1186/s12859-020-03568-5
- 31. 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
- 32. 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
- 33. The Impact of Pathway Database Choice on Statistical Enrichment Analysis and Predictive Modeling. *Frontiers in Genetics*, 2019. doi:10.3389/fgene.2019.01203
- 34. Quantifying mechanisms in neurodegenerative diseases (NDDs) using candidate mechanism perturbation amplitude (CMPA) algorithm. *BMC Bioinf.*, 2019. doi:10.1186/s12859-019-3101-1
- 35. The KEEN Universe. ISWC 2019. doi:10.1007/978-3-030-30796-71
- 36. Predicting Missing Links Using PyKEEN. ISWC 2019. ceur-ws:2456:64
- 37. RatVec: A General Approach for Low-dimensional Distributed Vector Representations via Domainspecific Rational Kernels. LWDA 2019
- 38. BioKEEN: a library for learning and evaluating biological knowledge graph embeddings. *Bioinformatics*, 2019. doi:10.1093/bioinformatics/btz117
- 39. PathMe: merging and exploring mechanistic pathway knowledge. *BMC Bioinf.*, 2019. doi:10.1186/s12859-019-2863-9
- 40. (preprint) †Integration of Structured Biological Data Sources using Biological Expression Language. bioRxiv, 2019. doi:10.1101/631812 biorxiv:631812
- 41. ComPath: an ecosystem for exploring, analyzing, and curating mappings across pathway databases. *NPJ Syst Biol Appl.*, 2019. doi:10.1038/s41540-018-0078-8
- 42. †Re-curation and rational enrichment of knowledge graphs in Biological Expression Language. *Database*, 2019. doi:10.1093/database/baz068
- 43. Challenges of Integrative Disease Modeling in Alzheimer's Disease. Frontiers in molecular biosciences, 2019. doi:10.3389/fmolb.2019.00158
- 44. †BEL Commons: an environment for exploration and analysis of networks encoded in Biological Expression Language. *Database*, 2018. doi:10.1093/database/bay126
- 45. **BEL2ABM:** agent-based simulation of static models in Biological Expression Language. *Bioinformatics*, 2018. doi:10.1093/bioinformatics/bty107
- 46. †PyBEL: a Computational Framework for Biological Expression Language. Bioinformatics, 2018. doi:10.1093/bioinformatics/btx66
- 47. †A systematic approach for identifying shared mechanisms in epilepsy and its comorbidities. *Database*, 2018. doi:10.1093/database/bay050
- 48. A Case Study on the Parametric Occurrence of Multiple Steady States. ISSAC 2017. doi:10.1145/3087604.3087622
- 49. 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.

Invited Presentations (Selected)

- 1. Axiomatizing Chemical Roles. Ontologies4Chem Workshop 2022 (September 7, 2022)
- 2. Knowledge Graph Embedding with PyKEEN in 2022. Knowledge Graph Conference (KGC 2022) (May 5, 2022)
- 3. The Biopragmatics Stack: Biomedical and Chemical Semantics for Humans. Machine-Actionable Data Interoperability for Chemical Sciences (MADICES) (February 8, 2022)
- 4. Current Issues in Theory, Reproducibility, and Utility of Graph Machine Learning in the Life Sciences. Graph Machine Learning in Industry (September 23, 2021)
- 5. Perspectives on Knowledge Graph Embedding Models in/out of Biomedicine. AstraZeneca (April 6, 2021)
- 6. Introduction to the Biological Expression Language and the Rational Enrichment Workflow. *CoronaWhy* (May 6, 2020)
- 7. **Applications of Knowledge Graphs in Drug Discovery**. *Computational Drug Discovery Group, University of Leiden* (November 5, 2019)
- 8. Generation and Application of Biomedical Knowledge Graphs. Harvard Medical School (July 19, 2019)

Talks and Posters (Selected)

- 1. Promoting the longevity of curated scientific resources through open code, open data, and public infrastructure. *Biocuration 2023* (April 26, 2023)
- 2. Using dashboards to monitor ontology standardisation and community activity. *Ontology Summit 2023* (February 15, 2023)
- 3. Introduction to WPCI 2022. 2022 Workshop on Prefixes, CURIEs, and IRIs (December 5, 2022)
- 4. The Bioregistry, CURIEs, and OBO Community Health. International Conference on Biomedical Ontology (ICBO) (September 26, 2022)
- 5. A Unified Framework for Rank-based Evaluation Metrics for Link Prediction in Knowledge Graphs. *Graph Learning Benchmarks (GLB 2022)* (April 26, 2022)
- 6. Introduction to WPCI 2021. 2021 Workshop on Prefixes, CURIEs, and IRIs (October 29, 2021)
- 7. **Biomappings: Community Curation of Mappings between Biomedical Entities**. 4th Session of the International Society of Biocuration 2021 Virtual Conference (October 5, 2021; poster)
- 8. **The Bioregistry: A Metaregistry for Biomedical Entities**. 12th International Conference on Biomedical Ontologies (September 17, 2021)
- 9. **Future Directions for WikiPathway Meta-curation**. *WikiPathways Developers Conference Call* (January 6, 2021)
- 10. The Biological Expression Language and PyBEL in 2020. COVID-19 Disease Map Community Meeting (July 10, 2020)
- 11. Maintenance and Enrichment of Disease Maps in Biological Expression Language. 4th Disease Maps Community Meeting (October 4, 2019; poster)
- 12. Identifying Drug Repositioning Candidates using Representation Learning on Heterogeneous Networks. *The Eighth Joint Sheffield Conference on Chemoinformatics* (June 19, 2019; poster)
- 13. The PyBEL Ecosystem in 2018. OpenBEL Community Meeting (May 14, 2018)
- 14. From Knowledge Assembly to Hypothesis Generation. Bio-IT World (April 22, 2018)
- 15. Knowledge Assembly in Systems and Networks Biology. Bio-IT World (April 23, 2018; poster)
- 16. **The Human Brain Pharmacome: An Overview**. *3rd European Conference on Translational Bioinformatics* (April 17, 2018; poster)
- 17. Gene Set Analysis using Phenotypic Screening Data. Research, Innovation and Scholarship Expo 2015 (April

Research Software (Selected)

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 A compiler for the Biological Expression Language (BEL)	O pybel/pybel
2.	Bio2BEL	O bio2bel/bio2bel
	A framework for reproducible data integration in BEL and knowledge graph construction	
3.	BEL Commons 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	O pykeen/pykeen
5.	SeMRA Automated assembly and inference of semantic mappings	• biopragmatics/semra
6.	Bioontologies Access and processing of ontologies on top of ROBOT and OBO Graphs	O biopragmatics/bioontologies
7.	PyOBO Harmonization of biological ontologies and controlled vocabularies	O pyobo/pyobo
8.	curies Idiomatic conversion between URIs and compact URIs (CURIEs)	O cthoyt/curies
9.	GuiltyTargets Target prioritization framework using gene expression and network representation	O guiltytargets/guiltytargets n learning
10.	RatVec Sequence-based representation learning	O ratvec/ratvec
11.	PS4DR Drug repositioning based on bioactivity pattern matching and GWAS	O ps4dr/ps4dr
12.	SeffNet Drug repositioning framework based on network representation learning	• seffnet/seffnet
13.	CLEP Patient stratification framework based on network representation learning	• hybrid-kg/clep
14.	BEL2SCM Generation of structural causal models (SCMs) from BEL	• bel2scm/bel2scm
15.	y0 Causal Inference Engine Representation and manipulating probabilistic expressions	O y0-causal-inference/y0
16.	STonKGs Multimodal Transformers for biomedical text and Knowledge Graph data	O stonkgs/stonkgs
17.	ChemicalX A deep learning library for drug-drug interaction, polypharmacy side effect, and s	• AstraZeneca/chemicalx synergy prediction
18.	PathMe Web application for exploration of pathway databases	• PathwayMerger/PathMe
19.	INDRA Automated knowledge assembly and modeling in biomedicine	$oldsymbol{\Omega}$ sorgerlab/indra
20.	INDRA CoGEx	• bgyori/indra_cogex

A 10^8 relation-scale knowledge graph extending on causal knowledge from INDRA 21. **MIRA** ndralab/mira Machine-assisted scientific modeling using meta-model templates and domain knowledge graphs 22. Gilda ndralab/gilda Biomedical named entity recognition and grounding using machine-learned disambiguation Databases (Selected) O bioregistry/bioregistry.io 1. Bioregistry An integrative meta-registry of biological databases, ontologies, and nomenclatures 2. Biomappings O biopragmatics/biomappings, https://biopragmatics.github.io/biomappings Predicted and curated mappings between named biological entities 3. Biolookup O biopragmatics/biolookup, http://biolookup.io Comprehensive database of identifiers, names, synonyms, cross-references, properties, and relations for biomedical entities O biopragmatics/bioversions 4. Bioversions Automated tracking of the current version for each biological database? 5. OBO Database Ingest O biopragmatics/obo-db-ingest Conversion of biomedical databases into ontologies

6. Chemical Roles Graph

Connecting roles in the ChEBI ontology to their targets

7. CONSO
Ontology of phenomena related to neurodegeneration

Ontology of phenomena related to neurodegeneration

CONIB

Curated knowledge graphs describing neurodegeneration in BEL

9. ComPath

O ComPath/ComPath, https://compath.scai.fraunhofer.de/

A data integration pipeline, manually curated dataset of mappings between pathway databases, and web application for integrative analysis of pathways

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

Funding

1. 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.

2. MIRA: Modeling with an Intelligent Reasoning Assistant

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

PI: Benjamin M. Gyori Role: Participant

3. Young Faculty Award / DARPA Director's Fellowship Award

• chemical-roles/chemical-roles

O pharmacome/conso

O pharmacome/conib

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

PI: Benjamin M. Gyori Role: Participant

4. (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

5. (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.

6. (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.

Community

Professional Affiliations

- International Society of Biocuration (2021 -)
- o CoronaWhy (2020 2021)
- OpenBEL Consortium (2017 -)
- Erasmus Student Network Bonn (2016 -)
- 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
- 2. Reproducibility Editor, Journal of Cheminformatics (pending)

Conference Organizing Committees

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

Teaching

Courses Taught

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)

Northeastern University

- 1. Drug Discovery and Development (Lecture; Teaching Assistant; Summer II 2015)
- 2. Organic Chemistry II for Majors (Lecture; Teaching Assistant; Spring 2015)
- 3. Organic Chemistry I for Majors (Lecture; Teaching Assistant; Fall 2014)
- 4. Organic Chemistry II for Majors (Lecture; Teaching Assistant; Spring 2014)
- 5. Organic Chemistry I for Majors (Lecture; Teaching Assistant; Fall 2013)

Supervision

CoronaWhy

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

Fraunhofer

- Lauren Nicole DeLong
 Student Research Assistant (September December 2019)
- Vinay Bharadhwaj D Student Research Assistant (July December 2019)
- Yojana Gadiya D 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)
- 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)
- Lingling Xu Master's Student (March December 2019)
- o Özlem Muslu 📵 Master's Student (May December 2018)