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

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

- 24. †PyKEEN 1.0: A Python Library for Training and Evaluating Knowledge Graph Embeddings. *JMLR*, 2021. arxiv:2007.14175
- 25. Leveraging Structured Biological Knowledge for Counterfactual Inference: A Case Study of Viral Pathogenesis. *IEEE TBDATA*, 2021. doi:10.1109/tbdata.2021.3050680
- 26. (preprint) †Extension of Roles in the ChEBI Ontology. ChemRxiv, 2020. doi:10.26434/chemrxiv.12591221
- 27. The Minimum Information about a Molecular Interaction Causal Statement (MI2CAST). Bioinformatics, 2020. doi:10.1093/bioinformatics/btaa622
- 28. **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
- 29. **PS4DR:** a multimodal workflow for identification and prioritization of drugs based on pathway signatures. *BMC Bioinf.*, 2020. doi:10.1186/s12859-020-03568-5
- 30. 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
- 31. 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
- 32. The Impact of Pathway Database Choice on Statistical Enrichment Analysis and Predictive Modeling. *Frontiers in Genetics*, 2019. doi:10.3389/fgene.2019.01203
- 33. Quantifying mechanisms in neurodegenerative diseases (NDDs) using candidate mechanism perturbation amplitude (CMPA) algorithm. *BMC Bioinf.*, 2019. doi:10.1186/s12859-019-3101-1
- 34. The KEEN Universe. ISWC 2019. doi:10.1007/978-3-030-30796-71
- 35. Predicting Missing Links Using PyKEEN. ISWC 2019. ceur-ws:2456:64
- 36. RatVec: A General Approach for Low-dimensional Distributed Vector Representations via Domainspecific Rational Kernels. LWDA 2019
- 37. BioKEEN: a library for learning and evaluating biological knowledge graph embeddings. *Bioinformatics*, 2019. doi:10.1093/bioinformatics/btz117
- 38. PathMe: merging and exploring mechanistic pathway knowledge. *BMC Bioinf.*, 2019. doi:10.1186/s12859-019-2863-9
- 39. (preprint) †Integration of Structured Biological Data Sources using Biological Expression Language. *bioRxiv*, 2019. doi:10.1101/631812 biorxiv:631812
- 40. ComPath: an ecosystem for exploring, analyzing, and curating mappings across pathway databases. NPJ Syst Biol Appl., 2019. doi:10.1038/s41540-018-0078-8
- 41. †Re-curation and rational enrichment of knowledge graphs in Biological Expression Language. *Database*, 2019. doi:10.1093/database/baz068
- 42. Challenges of Integrative Disease Modeling in Alzheimer's Disease. Frontiers in molecular biosciences, 2019. doi:10.3389/fmolb.2019.00158
- 43. †BEL Commons: an environment for exploration and analysis of networks encoded in Biological Expression Language. *Database*, 2018. doi:10.1093/database/bay126
- 44. BEL2ABM: agent-based simulation of static models in Biological Expression Language. *Bioinformatics*, 2018. doi:10.1093/bioinformatics/bty107
- 45. †PyBEL: a Computational Framework for Biological Expression Language. Bioinformatics, 2018. doi:10.1093/bioinformatics/btx66
- 46. †A systematic approach for identifying shared mechanisms in epilepsy and its comorbidities. *Database*, 2018. doi:10.1093/database/bay050
- 47. A Case Study on the Parametric Occurrence of Multiple Steady States. ISSAC 2017. doi:10.1145/3087604.3087622
- 48. 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. 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 9, 2015; poster)

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.

pybel/pybel 1. PyBEL A compiler for the Biological Expression Language (BEL) O bio2bel/bio2bel A framework for reproducible data integration in BEL and knowledge graph construction 3. BEL Commons O bel-commons/bel-commons A web application for the interactive exploration of networks encoded in BEL 4. PyKEEN pykeen/pykeen The most expansive knowledge graph embedding framework to date 5. SeMRA O biopragmatics/semra Automated assembly and inference of semantic mappings 6. Bioontologies O biopragmatics/bioontologies Access and processing of ontologies on top of ROBOT and OBO Graphs pyobo/pyobo 7. **PyOBO** Harmonization of biological ontologies and controlled vocabularies C cthoyt/curies 8. curies Idiomatic conversion between URIs and compact URIs (CURIEs) **O** guiltytargets/guiltytargets 9. GuiltyTargets Target prioritization framework using gene expression and network representation learning 10. RatVec ? ratvec/ratvec Sequence-based representation learning ns4dr/ps4dr 11. **PS4DR** Drug repositioning based on bioactivity pattern matching and GWAS 12. SeffNet • seffnet/seffnet Drug repositioning framework based on network representation learning nybrid-kg/clep Patient stratification framework based on network representation learning 14. BEL2SCM O bel2scm/bel2scm Generation of structural causal models (SCMs) from BEL 15. y0 Causal Inference Engine • y0-causal-inference/y0 Representation and manipulating probabilistic expressions 16. STonKGs O stonkgs/stonkgs Multimodal Transformers for biomedical text and Knowledge Graph data 17. ChemicalX AstraZeneca/chemicalx A deep learning library for drug-drug interaction, polypharmacy side effect, and synergy prediction • PathwayMerger/PathMe 18. PathMe Web application for exploration of pathway databases 19. INDRA Sorgerlab/indra Automated knowledge assembly and modeling in biomedicine 20. INDRA CoGEx O bgyori/indra_cogex

A 10^8 relation-scale knowledge graph extending on causal knowledge from INDRA

21.	21. MIRA Machine assisted scientific modeling using meta model templates and domain	ndralab/mira
22.	Machine-assisted scientific modeling using meta-model templates and domain 22. Gilda Biomedical named entity recognition and grounding using machine-learned dis	ndralab/gilda 🕜
	Databases (Selected)	
1.	1. Bioregistry An integrative meta-registry of biological databases, ontologies, and nomencla	istry , https://bioregistry.ic
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.ic omprehensive database of identifiers, names, synonyms, cross-references, properties, and relations for biomedical ntities	
4.	4. Bioversions Automated tracking of the current version for each biological database?	O biopragmatics/bioversions
5.	 OBO Database Ingest Conversion of biomedical databases into ontologies 	O biopragmatics/obo-db-ingest
6.	 Chemical Roles Graph Connecting roles in the ChEBI ontology to their targets 	• chemical-roles/chemical-roles
7.	7. CONSO Ontology of phenomena related to neurodegeneration	• pharmacome/consc
8.	8. CONIB Curated knowledge graphs describing neurodegeneration in BEL	• pharmacome/conib
9.	9. ComPath A data integration pipeline, manually curated dataset of mappings between path 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

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, \$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, \$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
 - eLife
 - 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 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)