






# 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: 3.95/4.0 (Summa Cum Laude)  
Research Advisor: Prof. Dr. Michael P. Pollastri

## Awards

- 2023 **Nominated, 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. (preprint) **Democratising Knowledge Representation with BioCypher.** *arXiv*, 2022. doi:10.48550/arxiv.2212.13543
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
14. **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
20. **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](https://arxiv.org/abs/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:10.1007/978-3-030-30796-7\_1
35. **Predicting Missing Links Using PyKEEN.** *ISWC 2019*. ceur-ws:2456:64
36. **RatVec: A General Approach for Low-dimensional Distributed Vector Representations via Domain-specific 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](https://doi.org/10.1101/631812)
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. **Using dashboards to monitor ontology standardisation and community activity.** *Ontology Summit 2023* (February 15, 2023)
2. **Introduction to WPCI 2022.** *2022 Workshop on Prefixes, CURIEs, and IRIs* (December 5, 2022)
3. **The Bioregistry, CURIEs, and OBO Community Health.** *International Conference on Biomedical Ontology (ICBO)* (September 26, 2022)
4. **Axiomatizing Chemical Roles.** *Ontologies4Chem Workshop 2022* (September 7, 2022)
5. **Knowledge Graph Embedding with PyKEEN in 2022.** *Knowledge Graph Conference (KGC 2022)* (May 5, 2022)
6. **The Biopragnatics Stack: Biomedical and Chemical Semantics for Humans.** *Machine-Actionable Data Interoperability for Chemical Sciences (MADICES)* (February 8, 2022)
7. **Introduction to WPCI 2021.** *2021 Workshop on Prefixes, CURIEs, and IRIs* (October 29, 2021)
8. **Current Issues in Theory, Reproducibility, and Utility of Graph Machine Learning in the Life Sciences.** *Graph Machine Learning in Industry* (September 23, 2021)
9. **Perspectives on Knowledge Graph Embedding Models in/out of Biomedicine.** *AstraZeneca* (April 6, 2021)
10. **Future Directions for WikiPathway Meta-curation.** *WikiPathways Developers Conference Call* (January 6, 2021)
11. **The Biological Expression Language and PyBEL in 2020.** *COVID-19 Disease Map Community Meeting* (July 10, 2020)
12. **Introduction to the Biological Expression Language and the Rational Enrichment Workflow.** *CoronaWhy* (May 6, 2020)
13. **Applications of Knowledge Graphs in Drug Discovery.** *Computational Drug Discovery Group, University of Leiden* (November 5, 2019)
14. **Generation and Application of Biomedical Knowledge Graphs.** *Harvard Medical School* (July 19, 2019)
15. **The PyBEL Ecosystem in 2018.** *OpenBEL Community Meeting* (May 14, 2018)










## 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. **A Unified Framework for Rank-based Evaluation Metrics for Link Prediction in Knowledge Graphs.** *Graph Learning Benchmarks (GLB 2022)* (April 26, 2022)
3. **Biomappings: Community Curation of Mappings between Biomedical Entities.** *4th Session of the International Society of Biocuration 2021 Virtual Conference* (October 5, 2021; poster)
4. **The Bioregistry: A Metaregistry for Biomedical Entities.** *12th International Conference on Biomedical Ontologies* (September 17, 2021)
5. **Maintenance and Enrichment of Disease Maps in Biological Expression Language.** *4th Disease Maps Community Meeting* (October 4, 2019; poster)
6. **Identifying Drug Repositioning Candidates using Representation Learning on Heterogeneous Networks.** *The Eighth Joint Sheffield Conference on Chemoinformatics* (June 19, 2019; poster)
7. **From Knowledge Assembly to Hypothesis Generation.** *Bio-IT World* (April 22, 2018)
8. **Knowledge Assembly in Systems and Networks Biology.** *Bio-IT World* (April 23, 2018; poster)
9. **The Human Brain Pharmacome: An Overview.** *3rd European Conference on Translational Bioinformatics* (April 17, 2018; poster)
10. **Gene Set Analysis using Phenotypic Screening Data.** *Research, Innovation and Scholarship Expo 2015* (April 9, 2015; poster)

## Research Software

1. **PyBEL**  [pybel/pybel](#)  
A compiler for the Biological Expression Language (BEL)
2. **Bio2BEL**  [bio2bel/bio2bel](#)  
A framework for reproducible data integration in BEL and knowledge graph construction
3. **BEL Commons**  [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**  [biopragnatics/semra](#)  
Automated assembly and inference of semantic mappings
6. **Bioontologies**  [biopragnatics/bioontologies](#)  
Access and processing of ontologies on top of ROBOT and OBO Graphs
7. **PyOBO**  [pyobo/pyobo](#)  
Harmonization of biological ontologies and controlled vocabularies
8. **curies**  [cthoit/curies](#)  
Idiomatic conversion between URIs and compact URIs (CURIEs)
9. **GuiltyTargets**  [guiltytargets/guiltytargets](#)  
Target prioritization framework using gene expression and network representation learning
10. **RatVec**  [ratvec/ratvec](#)  
Sequence-based representation learning
11. **PS4DR**  [ps4dr/ps4dr](#)  
Drug repositioning based on bioactivity pattern matching and GWAS
12. **SeffNet**  [seffnet/seffnet](#)  
Drug repositioning framework based on network representation learning
13. **CLEP**  [hybrid-kg/clep](#)  
Patient stratification framework based on network representation learning
14. **BEL2SCM**  [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**  [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
18. **PathMe**  [PathwayMerger/PathMe](#)  
Web application for exploration of pathway databases
19. **INDRA**  [sorgerlab/indra](#)  
Automated knowledge assembly and modeling in biomedicine
20. **INDRA CoGEx**  [bgyori/indra\\_cogex](#)  
A  $10^8$  relation-scale knowledge graph extending on causal knowledge from INDRA
21. **MIRA**  [indralab/mira](#)  
Machine-assisted scientific modeling using meta-model templates and domain knowledge graphs
22. **Gilda**  [indralab/gilda](#)  
Biomedical named entity recognition and grounding using machine-learned disambiguation

## Databases

1. **Bioregistry**  bioregistry/bioregistry , <https://bioregistry.io>  
An integrative meta-registry of biological databases, ontologies, and nomenclatures
2. **Biomappings**  biopragnatics/biomappings , <https://biopragnatics.github.io/biomappings>  
Predicted and curated mappings between named biological entities
3. **Biolookup**  biopragnatics/biolookup , <http://biolookup.io>  
Comprehensive database of identifiers, names, synonyms, cross-references, properties, and relations for biomedical entities
4. **Bioversions**  biopragnatics/bioversions  
Automated tracking of the current version for each biological database?
5. **OBO Database Ingest**  biopragnatics/obo-db-ingest  
Conversion of biomedical databases into ontologies
6. **Chemical Roles Graph**  chemical-roles/chemical-roles  
Connecting roles in the ChEBI ontology to their targets
7. **CONSO**  pharmacome/conso  
Ontology of phenomena related to neurodegeneration
8. **CONIB**  pharmacome/conib  
Curated knowledge graphs describing neurodegeneration in BEL
9. **ComPath**  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

EHDA2, BFO, GO, ECO, OMO, FYPO, COB, RO, HSAPDV, MMUSDV, MP, AGRO, CIDO, EUPATH, HANCES-TRO, OBA, PDUMDV, GEO, HTN, TTO, MOD, CL, CDAO, AISM, HAO, ONS, PCL, SWO, TO, TAXRANK, WBBT, WBL, OLATDV, PECO, UPHENO, XCO, IAO, PO, OGMS, OHD, OBI, MIAPA, MONDO, LPAO, 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  
Role: Key Person. Co-wrote proposal with PNNL collaborators. Responsible for design and implementation of research plan.
2. **MIRA: Modeling with an Intelligent Reasoning Assistant**  
DARPA ASKE Program, (HR00112220036), \$2.1M, 2022-2026 (42 months)  
Role: Participant
3. **Young Faculty Award / DARPA Director's Fellowship Award**  
DARPA, (W911NF2010255), \$750K, 2020-2023 (36 months)  
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)  
Role: Participant
5. (past) **Interdisciplinary Research Award**  
Fraunhofer Center for Machine Learning, \$40K 2019 (3 months)  
Role: Key person. Co-wrote proposal. Responsible for design and implementation of research plan.
6. (past) **PYBEL2NDEX**  
University of California, San Diego, \$28K 2018 (6 months)

Role: Key person. Wrote proposal. Responsible for design and implementation of research plan.

## Community

### Professional Affiliations

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

#### Northeastern University

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

## 5. Organic Chemistry I for Majors (Lecture; Fall 2013)

### Supervision





#### CoronaWhy

- Aman Choudhri  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)
- Rana Aldisi  Student Research Assistant (July 2018 - March 2019)
- Lingling Xu  Student Research Assistant (July 2018 - March 2019)
- Kristian Kolpeja  Student Research Assistant (July - November 2018)
- Esther Wollert  Student Research Assistant (July 2018 - August 2019)
- 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)
- Özlem Muslu  Master's Student (May - December 2018)