







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

- 2023–24 **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 60 manuscripts (50 peer-reviewed, 7 pre-printed, and 3 in preparation). The following are noted:

- † signifies first or co-first authorship
- ‡ signifies last or senior authorship

1. (preprint) †**Computational Tools and Data Integration to Accelerate Vaccine Development: Challenges, Opportunities, and Future Directions.** *OSF Preprints*, 2024
2. **Eliater: A Python package for estimating outcomes of perturbations in biomolecular networks.** *Bioinformatics*, 2024. doi:10.1093/bioinformatics/btae527
3. †**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
4. **An open source knowledge graph ecosystem for the life sciences.** *Scientific Data*, 2024. doi:10.1038/s41597-024-03171-w
5. ‡**ptwt - The PyTorch Wavelet Toolbox.** *JMLR*, 2024
6. (in preparation) †**SeMRA: Assembly and Reasoning over Semantic Mappings at Scale for Biomedical Data Integration.** *in preparation*, 2024
7. (in preparation) †**Improving reproducibility of cheminformatics workflows with 'chembl-downloader'.** *in preparation for J. Chem. Inf*, 2024
8. (in preparation) †**Causal inference with Y_0 .** *in preparation for JOSS*, 2024
9. **A simple standard for ontological mappings 2023: updates on data model, collaborations and tooling.** *OM 2023*
10. **The Human Phenotype Ontology in 2024: phenotypes around the world.** *NAR*, 2023. doi:10.1093/nar/gkad1005
11. †**Improving reproducibility and reusability in the Journal of Cheminformatics.** *J Cheminform*, 2023. doi:10.1186/s13321-023-00730-y
12. **Democratizing knowledge representation with BioCypher.** *Nature Biotechnology*, 2023. doi:10.1038/s41587-023-01848-y
13. **Optimal adjustment sets for causal query estimation in partially observed biomolecular networks.** *Bioinformatics*, 2023. doi:10.1093/bioinformatics/btad270
14. †**Prediction and curation of missing biomedical identifier mappings with Biomappings.** *Bioinformatics*, 2023. doi:10.1093/bioinformatics/btad130
15. (preprint) **Experimental design for causal query estimation in partially observed biomolecular networks.** *arXiv*, 2022. arxiv:2210.13423
16. †**Unifying the identification of biomedical entities with the Bioregistry.** *Scientific Data*, 2022. doi:10.1038/s41597-022-01807-3
17. **A Simple Standard for Ontological Mappings 2022: Updates of data model and outlook.** *OM 2022*
18. **A review of biomedical datasets relating to drug discovery: a knowledge graph perspective.** *Brief Bioinform*, 2022. doi:10.1093/bib/bbac404
19. **ChemicalX: A Deep Learning Library for Drug Pair Scoring.** *KDD*, 2022. doi:10.1145/3534678.3539023
20. **Integrating multi-omics data reveals function and therapeutic potential of deubiquitinating enzymes.** *eLife*, 2022. doi:10.7554/elife.72879
21. **Understanding the Performance of Knowledge Graph Embeddings in Drug Discovery.** *Artificial Intelligence in the Life Sciences*, 2022. doi:10.1016/j.ailsci.2022.100036
22. **A Simple Standard for Sharing Ontological Mappings (SSSOM).** *Database*, 2022. doi:10.1093/database/baac035
23. **Gilda: biomedical entity text normalization with machine-learned disambiguation as a service.** *Bioinform-*

matics Advances, 2022. doi:10.1093/bioadv/vbac034

24. **ProtSTonKGs: A Sophisticated Transformer Trained on Protein Sequences, Text, and Knowledge Graphs.** *SWAT4HCLS* 2022. ceur-ws:3127:13
25. (preprint) **Mondo: Unifying diseases for the world, by the world.** *medRxiv*, 2022. doi:10.1101/2022.04.13.22273750
26. **Do-calculus enables estimation of causal effects in partially observed biomolecular pathways.** *Bioinformatics*, 2022. doi:10.1093/bioinformatics/btac251
27. (preprint) **†A Unified Framework for Rank-based Evaluation Metrics for Link Prediction in Knowledge Graphs.** *arXiv*, 2022. arxiv:2203.07544
28. **PyBioPAX: biological pathway exchange in Python.** *JOSS*, 2022. doi:10.21105/joss.04136
29. (preprint) **An Open Challenge for Inductive Link Prediction on Knowledge Graphs.** *arXiv*, 2022. arxiv:2203.01520
30. **STonKGs: A Sophisticated Transformer Trained on Biomedical Text and Knowledge Graphs.** *Bioinformatics*, 2022. doi:10.1093/bioinformatics/btac001
31. **Ontology Development Kit: a toolkit for building, maintaining, and standardising biomedical ontologies.** *Database*, 2022. doi:10.1093/database/baac087
32. **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
33. **The role of metadata in reproducible computational research.** *Patterns*, 2021. doi:10.1016/j.patter.2021.100322
34. **†CLEP: a hybrid data- and knowledge-driven framework for generating patient representations.** *Bioinformatics*, 2021. doi:10.1093/bioinformatics/btab340
35. **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
36. **†PyKEEN 1.0: A Python Library for Training and Evaluating Knowledge Graph Embeddings.** *JMLR*, 2021. arxiv:2007.14175
37. **Leveraging Structured Biological Knowledge for Counterfactual Inference: A Case Study of Viral Pathogenesis.** *IEEE TBDATA*, 2021. doi:10.1109/tbdata.2021.3050680
38. (preprint) **†Extension of Roles in the ChEBI Ontology.** *ChemRxiv*, 2020. doi:10.26434/chemrxiv.12591221
39. **The Minimum Information about a Molecular Interaction Causal Statement (MI2CAST).** *Bioinformatics*, 2020. doi:10.1093/bioinformatics/btaa622
40. **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
41. **PS4DR: a multimodal workflow for identification and prioritization of drugs based on pathway signatures.** *BMC Bioinf.*, 2020. doi:10.1186/s12859-020-03568-5
42. **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
43. **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
44. **The Impact of Pathway Database Choice on Statistical Enrichment Analysis and Predictive Modeling.** *Frontiers in Genetics*, 2019. doi:10.3389/fgene.2019.01203
45. **Quantifying mechanisms in neurodegenerative diseases (NDDs) using candidate mechanism perturbation amplitude (CMPA) algorithm.** *BMC Bioinf.*, 2019. doi:10.1186/s12859-019-3101-1
46. **The KEEN Universe.** *ISWC 2019*. doi:10.1007/978-3-030-30796-7_1
47. **Predicting Missing Links Using PyKEEN.** *ISWC 2019*. ceur-ws:2456:64
48. **RatVec: A General Approach for Low-dimensional Distributed Vector Representations via Domain-specific Rational Kernels.** *LWDA 2019*
49. **BioKEEN: a library for learning and evaluating biological knowledge graph embeddings.** *Bioinformatics*, 2019. doi:10.1093/bioinformatics/btz117

50. **PathMe: merging and exploring mechanistic pathway knowledge.** *BMC Bioinf.*, 2019. doi:10.1186/s12859-019-2863-9
51. (preprint) †**Integration of Structured Biological Data Sources using Biological Expression Language.** *bioRxiv*, 2019. doi:10.1101/631812 biorxiv:631812
52. **ComPath: an ecosystem for exploring, analyzing, and curating mappings across pathway databases.** *NPJ Syst Biol Appl.*, 2019. doi:10.1038/s41540-018-0078-8
53. †**Re-curation and rational enrichment of knowledge graphs in Biological Expression Language.** *Database*, 2019. doi:10.1093/database/baz068
54. **Challenges of Integrative Disease Modeling in Alzheimer's Disease.** *Frontiers in molecular biosciences*, 2019. doi:10.3389/fmolb.2019.00158
55. †**BEL Commons: an environment for exploration and analysis of networks encoded in Biological Expression Language.** *Database*, 2018. doi:10.1093/database/bay126
56. **BEL2ABM: agent-based simulation of static models in Biological Expression Language.** *Bioinformatics*, 2018. doi:10.1093/bioinformatics/bty107
57. †**PyBEL: a Computational Framework for Biological Expression Language.** *Bioinformatics*, 2018. doi:10.1093/bioinformatics/btx660
58. †**A systematic approach for identifying shared mechanisms in epilepsy and its comorbidities.** *Database*, 2018. doi:10.1093/database/bay050
59. **A Case Study on the Parametric Occurrence of Multiple Steady States.** *ISSAC 2017*. doi:10.1145/3087604.3087622
60. **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 Biopragnatics 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. **Assembly and Reasoning over Semantic Mappings at Scale.** *Biocuration 2024* (March 7, 2024)
2. **Introduction to WPCI 2023.** *Winter 2023 Workshop on Prefixes, CURIEs, and IRIs* (November 27, 2023)
3. **Standardization of chemical prefixes, CURIEs, URIs, and semantic mappings.** *Ontologies4Chem Workshop 2023* (October 12, 2023)
4. **Improving the reproducibility of cheminformatics workflows with chembl-downloader.** *RDKit User Group Meeting 2023* (September 21, 2023)
5. **Promoting the longevity of curated scientific resources through open code, open data, and public infrastructure.** *Biocuration 2023* (April 26, 2023)
6. **Using dashboards to monitor ontology standardisation and community activity.** *Ontology Summit 2023* (February 15, 2023)
7. **Introduction to WPCI 2022.** *2022 Workshop on Prefixes, CURIEs, and IRIs* (December 5, 2022)
8. **The Bioregistry, CURIEs, and OBO Community Health.** *International Conference on Biomedical Ontology (ICBO)* (September 26, 2022)
9. **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)
10. **A Unified Framework for Rank-based Evaluation Metrics for Link Prediction in Knowledge Graphs.** *Graph Learning Benchmarks (GLB 2022)* (April 26, 2022)
11. **Introduction to WPCI 2021.** *2021 Workshop on Prefixes, CURIEs, and IRIs* (October 29, 2021)
12. **Biomappings: Community Curation of Mappings between Biomedical Entities.** *4th Session of the International Society of Biocuration 2021 Virtual Conference* (October 5, 2021; poster)
13. **The Bioregistry: A Metaregistry for Biomedical Entities.** *12th International Conference on Biomedical Ontologies* (September 17, 2021)
14. **Future Directions for WikiPathway Meta-curation.** *WikiPathways Developers Conference Call* (January 6, 2021)
15. **The Biological Expression Language and PyBEL in 2020.** *COVID-19 Disease Map Community Meeting* (July 10, 2020)
16. **Maintenance and Enrichment of Disease Maps in Biological Expression Language.** *4th Disease Maps Community Meeting* (October 4, 2019; poster)
17. **Identifying Drug Repositioning Candidates using Representation Learning on Heterogeneous Networks.** *The Eighth Joint Sheffield Conference on Chemoinformatics* (June 19, 2019; poster)
18. **The PyBEL Ecosystem in 2018.** *OpenBEL Community Meeting* (May 14, 2018)
19. **From Knowledge Assembly to Hypothesis Generation.** *Bio-IT World* (April 22, 2018)
20. **Knowledge Assembly in Systems and Networks Biology.** *Bio-IT World* (April 23, 2018; poster)
21. **The Human Brain Pharmacome: An Overview.** *3rd European Conference on Translational Bioinformatics* (April 17, 2018; poster)
22. **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.

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**  [biopragnatics/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-kb/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 10⁸ 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 (Selected)

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

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, 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, LPAO, EXO, BSPO, DDPHENO, UBERON, FBBT, ENVO, SYMP, CHMO, OAE, 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), €17.8M 2014-2018 (4 years)
PI: Martin Hofmann-Apitius
Role: Participant. Note: Joined in 2016.

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 (*ad hoc*) in:
 - Bioinformatics
 - Database
 - BMC Bioinformatics
 - Journal of Cheminformatics
 - Journal of Biomedical Semantics
 - eLife
 - MATCH Communications in Mathematical and in Computer Chemistry
 - PeerJ
2. Guest Reproducibility Editor, Journal of Cheminformatics (2023-)
3. Grant reviewer for:
 - 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

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





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)

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- 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)