Charles Tapley Hoyt

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Fields of Work

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

Spoken Languages

English, German

Education

- 2018-19 **Doctor Of Philosophy**, University of Bonn, Germany.
- 2015-17 Master Of Science, University of Bonn, Germany.
- 2011-15 Bachelor Of Science, Northeastern University, United States of America.
- 2007-11 High School Diploma, North Haven High School, United States of America.

Work

- 2021- Research Fellow, Harvard Medical School, Bonn, Germany.
- 2020 Computational Biologist, Enveda Biosciences, Bonn, Germany.
- 2018-19 Lecturer, University of Bonn, Bonn, Germany.
- 2016-19 **Research Fellow**, Fraunhofer Institute for Algorithms and Scientific Computing, Sankt Augustin, Germany.
 - 2014 Intern, Novartis, Cambridge, United States of America.
- 2013-14 Intern, Pfizer, Cambridge, United States of America.
 - 2013 Intern, GlaxoSmithKline, Waltham, United States of America.
- 2012-15 **Teaching Assistant**, Northeastern University, Boston, United States of America.

Research Output

Software

SSSOM-py, Python package.

https://github.com/mapping-commons/sssom-py/, https://mapping-commons.github.io/sssom-py/

PyBEL, Python library for Biological Expression Language.

https://github.com/pybel/pybel, https://pybel.github.io

Integrated Network and Dynamical Reasoning Assembler, *Text mining and systems biology modeling software*.

https://github.com/sorgerlab/indra, https://www.indra.bio/

PyKEEN, Learning, evaluation and applications of knowledge graph embeddings...

https://github.com/pykeen/pykeen, https://pykeen.github.io

Articles 2022

1. Unifying the Identification of Biomedical Entities with the Bioregistry

bioRxiv, 2022

doi:10.1101/2022.07.08.499378 biorxiv:2022.07.08.499378

2. Ontology Development Kit: a toolkit for building, maintaining, and standardising biomedical ontologies

arXiv, 2022

arxiv:2207.02056

3. Integrating multi-omics data reveals function and therapeutic potential of deubiquitinating enzymes

eLife, 2022

doi:10.7554/elife.72879

4. Understanding the performance of knowledge graph embeddings in drug discovery

Artificial Intelligence in the Life Sciences, 2022

doi:10.1016/j.ailsci.2022.100036

5. A Simple Standard for Sharing Ontological Mappings (SSSOM)

Database, 2022

doi:10.1093/database/baac035

6. ProtSTonKGs: A Sophisticated Transformer Trained on Protein Sequences, Text, and Knowledge Graphs

SWAT4HCLS 2022

ceur-ws:3127:13

7. **Do-calculus enables estimation of causal effects in partially observed biomolecular pathways** *Bioinformatics*, 2022

doi:10.1093/bioinformatics/btac251

8. A Unified Framework for Rank-based Evaluation Metrics for Link Prediction in Knowledge Graphs

arXiv, 2022

arxiv:2203.07544

9. PyBioPAX: biological pathway exchange in Python

JOSS, 2022

doi:10.21105/joss.04136

10. An Open Challenge for Inductive Link Prediction on Knowledge Graphs

arXiv, 2022

arxiv:2203.01520

11. ChemicalX: A Deep Learning Library for Drug Pair Scoring

arXiv, 2022

arxiv:2202.05240

12. STonKGs: A Sophisticated Transformer Trained on Biomedical Text and Knowledge Graphs Bioinformatics, 2022

PMID:34986221 PMC8896635 doi:10.1093/bioinformatics/btac001

Articles 2021

13. Bringing Light Into the Dark: A Large-scale Evaluation of Knowledge Graph Embedding Models Under a Unified Framework

TPAMI, 2021

 $\mathsf{doi:} 10.1109/\mathsf{tpami.} 2021.3124805$

14. Gilda: biomedical entity text normalization with machine-learned disambiguation as a service bioRxiv, 2021

doi:10.1101/2021.09.10.459803 biorxiv:2021.09.10.459803

15. The role of metadata in reproducible computational research

Patterns, 2021

PMID:34553169 PMC8441584 doi:10.1016/j.patter.2021.100322

16. Wavelet-Packet Powered Deepfake Image Detection

arXiv, 2021

arxiv:2106.09369

17. A Review of Biomedical Datasets Relating to Drug Discovery: A Knowledge Graph Perspective arXiv, 2021

arxiv:2102.10062

18. A Systems Biology Approach for Hypothesizing the Effect of Genetic Variants on Neuroimaging Features in Alzheimer's Disease

JAD, 2021

PMID:33554913 PMC8075382 doi:10.3233/jad-201397

19. PyKEEN 1.0: A Python Library for Training and Evaluating Knowledge Graph Embeddings *JMLR*, 2021

arxiv:2007.14175

20. Leveraging Structured Biological Knowledge for Counterfactual Inference: A Case Study of Viral Pathogenesis

IEEE TBDATA, 2021

doi:10.1109/tbdata.2021.3050680

Articles 2020

21. CLEP: A Hybrid Data- and Knowledge- Driven Framework for Generating Patient Representations

bioRxiv, 2020

doi:10.1101/2020.08.20.259226 biorxiv:2020.08.20.259226

22. Extension of Roles in the ChEBI Ontology

ChemRxiv, 2020

doi:10.26434/chemrxiv.12591221

23. The Minimum Information about a Molecular Interaction Causal Statement (MI2CAST)

Bioinformatics, 2020

PMID:32637990 doi:10.1093/bioinformatics/btaa622

24. GuiltyTargets: Prioritization of Novel Therapeutic Targets with Deep Network Representation Learning

IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2020

PMID:32750869 doi:10.1109/tcbb.2020.3003830

25. PS4DR: a multimodal workflow for identification and prioritization of drugs based on pathway signatures

BMC Bioinf., 2020

PMID:32503412 PMC7275349 doi:10.1186/s12859-020-03568-5

26. A Computational Approach for Mapping Heme Biology in the Context of Hemolytic Disorders Frontiers in Bioengineering and Biotechnology, 2020

Articles 2019

27. The Impact of Pathway Database Choice on Statistical Enrichment Analysis and Predictive Modeling

Frontiers in Genetics, 2019

PMID:31824580 PMC6883970 doi:10.3389/fgene.2019.01203

28. Quantifying mechanisms in neurodegenerative diseases (NDDs) using candidate mechanism perturbation amplitude (CMPA) algorithm

BMC Bioinf., 2019

PMID:31604427 PMC6788110 doi:10.1186/s12859-019-3101-1

29. The KEEN Universe

ISWC 2019

 $\mathsf{doi:} 10.1007/978\text{--}3\text{--}030\text{--}30796\text{--}7_1$

30. Predicting Missing Links Using PyKEEN

ISWC 2019

ceur-ws:2456:64

31. RatVec: A General Approach for Low-dimensional Distributed Vector Representations via Domain-specific Rational Kernels

LWDA 2019

32. BioKEEN: a library for learning and evaluating biological knowledge graph embeddings *Bioinformatics*, 2019

PMID:30768158 doi:10.1093/bioinformatics/btz117

33. PathMe: merging and exploring mechanistic pathway knowledge

BMC Bioinf., 2019

PMID:31092193 PMC6521546 doi:10.1186/s12859-019-2863-9

34. Integration of Structured Biological Data Sources using Biological Expression Language bioRxiv, 2019

doi:10.1101/631812 biorxiv:631812

35. ComPath: an ecosystem for exploring, analyzing, and curating mappings across pathway databases

NPJ Syst Biol Appl., 2019

PMID:30564458 PMC6292919 doi:10.1038/s41540-018-0078-8

36. Re-curation and rational enrichment of knowledge graphs in Biological Expression Language *Database*, 2019

PMID:31225582 PMC6587072 doi:10.1093/database/baz068

37. Challenges of Integrative Disease Modeling in Alzheimer's Disease

Frontiers in molecular biosciences, 2019

PMID:31993440 PMC6971060 doi:10.3389/fmolb.2019.00158

Articles 2018

38. BEL Commons: an environment for exploration and analysis of networks encoded in Biological Expression Language

Database, 2018

PMID:30576488 PMC6301338 doi:10.1093/database/bay126

39. BEL2ABM: agent-based simulation of static models in Biological Expression Language

Bioinformatics, 2018

PMID:29949955 PMC6022644 doi:10.1093/bioinformatics/bty107

40. PyBEL: a Computational Framework for Biological Expression Language

Bioinformatics, 2018

PMID:29048466 PMC5860616 doi:10.1093/bioinformatics/btx660

41. A systematic approach for identifying shared mechanisms in epilepsy and its comorbidities

Database, 2018

PMID:29873705 PMC6007221 doi:10.1093/database/bay050

Articles 2017

42. A Case Study on the Parametric Occurrence of Multiple Steady States

ISSAC 2017

doi:10.1145/3087604.3087622

Articles 2014

43. 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

PMID:25127163 PMC4155488 doi:10.1016/j.bmcl.2014.07.063

Reviews

Note that this section is automatically generated from Wikidata and is not necessarily complete.

1. The LOTUS initiative for open knowledge management in natural products research *eLife*, 2022

PMID:35616633 doi:10.7554/elife.70780

2. New reasons for biologists to write with a formal language

Database, 2022

doi:10.1093/database/baac039

3. PecanPy: a fast, efficient and parallelized Python implementation of node2vec

Bioinformatics, 2021

PMID:33760066 doi:10.1093/bioinformatics/btab202

Acknowledgements

Note that this section is automatically generated from Wikidata and is not necessarily complete.

1. Automated assembly of molecular mechanisms at scale from text mining and curated databases bioRxiv, 2022

doi:10.1101/2022.08.30.505688 biorxiv:2022.08.30.505688

2. PecanPy: a fast, efficient and parallelized Python implementation of node2vec

Bioinformatics, 2021

PMID:33760066 doi:10.1093/bioinformatics/btab202

3. The status of causality in biological databases: data resources and data retrieval possibilities to support logical modeling

Briefings in Bioinformatics, 2020

PMID:33378765 doi:10.1093/bib/bbaa390

4. Multimodal Mechanistic Signatures for Neurodegenerative Diseases (NeuroMMSig): a web server for mechanism enrichment

Bioinformatics, 2017

PMID:28651363 doi:10.1093/bioinformatics/btx399

Mentees

- 1. Aman Choudhri 10 0000-0003-4963-6651
 - O Student Research Assistant (June October 2020)
- 2. Lauren Nicole DeLong 0 0000-0001-6618-3370
 - O Student Research Assistant (September December 2019)
- 3. Vinay Bharadhwaj 0 0000-0002-9901-9494
 - O Student Research Assistant (July December 2019)
- 4. Mauricio Pio de Lacerda © 0000-0002-1770-3007
 - O Master's Student (March December 2019)
- 5. Yojana Gadiya 10 0000-0002-7683-0452
 - O Student Research Assistant (April May 2019)
- 6. Trusha Adeshara @ 0000-0002-8929-4724
 - O Student Research Assistant (April May 2019)
- 7. Rana Aldisi 0 0000-0002-3034-9970
 - O Master's Student (March December 2019)
 - O Student Research Assistant (July 2018 March 2019)
- 8. Lingling Xu 0 0000-0002-0303-8616
 - O Master's Student (March December 2019)
 - O Student Research Assistant (July 2018 March 2019)
- 9. Özlem Muslu 10 0000-0003-0408-6190
 - O Master's Student (May December 2018)
- 10. Kristian Kolpeja @ 0000-0001-9661-5277
 - O Student Research Assistant (July November 2018)
- 11. Esther Wollert © 0000-0002-7128-929X
 - O Student Research Assistant (July 2018 August 2019)
- 12. Sandra Spalek @ 0000-0002-6117-4413
 - O Student Research Assistant (July 2018 August 2019)
- 13. Keerthika Lohanadan
 - O Student Research Assistant (July September 2018)
- 14. Colin Birkenbihl (1) 0000-0002-7212-7700
 - O Student Research Assistant (July October 2017)
- 15. Aram Grigoryan
 - O Student Research Assistant (July December 2017)

Courses

- Mechanism Enrichment Using Neurommsig (Practical; Winter 2020-2021)
 University of Bonn
- 2. Mechanism Enrichment Using Neurommsig (Practical; Winter 2019-2020)

University of Bonn

3. Mathematics Meets Life Sciences (Lecture; Winter 2019-2020)

University of Bonn

4. Enzyme Technology Internship (Practical; Summer 2019)

University of Bonn

5. Life Sciences Knowledge Discovery (Lecture; Summer 2019)

University of Bonn

6. Knowledge Assembly, Data Integration, and Modeling in Systems and Networks Biology (Seminar; Winter 2018-2019)

University of Bonn

7. Biological Databases (Lecture; Winter 2018-2019)

University of Bonn

8. Life Sciences Knowledge Discovery (Lecture; Summer 2018)

University of Bonn

9. Biological Databases (Lecture; Winter 2017-2018)

University of Bonn

10. Life Sciences Knowledge Discovery (Lecture; Summer 2017)

University of Bonn

11. Biomedical Database Lab (Practical; Winter 2016-2017)

University of Bonn

12. Drug Discovery and Development (Lecture; Summer II 2015)

Northeastern University

13. Organic Chemistry II for Majors (Lecture; Spring 2015)

Northeastern University

14. Organic Chemistry I for Majors (Lecture; Fall 2014)

Northeastern University

15. Organic Chemistry II for Majors (Lecture; Spring 2014)

Northeastern University

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

Northeastern University