RESEARCH & PUBLICATIONS

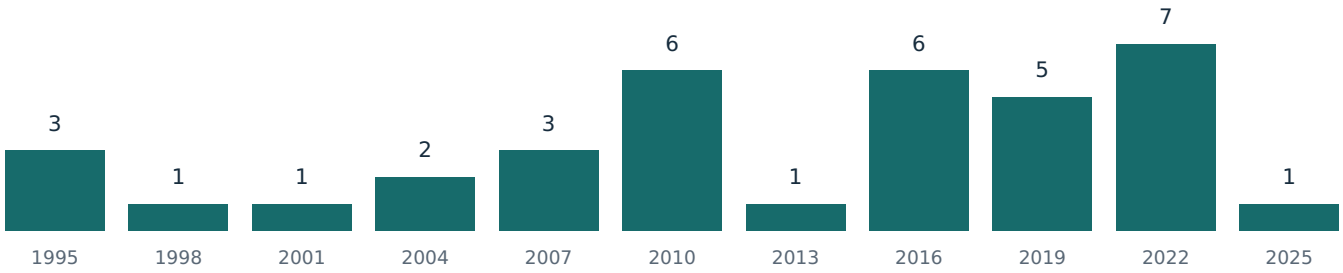
Ian J. Bruno

A publication record at a glance

36	24,565	17
ARTICLES	CITATIONS	h-INDEX

PUBLICATION ACTIVITY

Articles grouped into 3-year periods



MOST CITED IN THIS LIST

The Cambridge Structural Database. — 10,174
2016 Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials

Mercury CSD 2.0 – New Features for the Visualization and Investigation of Crystal Structures — 8,719
2008 Journal of Applied Crystallography

New Software for Searching the Cambridge Structural Database and Visualizing Crystal Structures — 3,141
2002 Acta Crystallographica Section B: Structural Science

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Ordered by publication year, newest first

2025

01 **FAIRSpec-Ready Spectroscopic Data Collections – Advice for Researchers, Authors, and Data Managers (IUPAC Technical Report)**
2 citations
Pure and Applied Chemistry · 97, 1479-1510
https://exaly.com/article/206123565

2024

02 **The Interoperability of Crystallographic Data and Databases**
9 citations
IUCrJ · 11, 9-15
https://exaly.com/article/174133578

03 **Chemistry Digital Standards: Tools for an Increasingly Digital Research Culture**
0 citations
Chemistry International · 46, 16-19
https://exaly.com/article/175742431

04 **Digital Standards: A Path to Sustainable and Interoperable Chemical Data Exchange**
1 citations
Chemistry International · 46, 43-47
https://exaly.com/article/187373612

2023

05 **Chemical Data Evaluation: General Considerations and Approaches for IUPAC Projects and the Chemistry Community (IUPAC Technical Report)**
5 citations
Pure and Applied Chemistry · 95, 1107-1120
https://exaly.com/article/167241349

2022

06 **IUPAC Specification for the FAIR Management of Spectroscopic Data in Chemistry (IUPAC FAIRSpec) – Guiding Principles**
17 citations
Pure and Applied Chemistry · 94, 623-636
https://exaly.com/article/145146807

07 **Mindestinformationsstandards in der Chemie: Ein Appell zum besseren Umgang mit Forschungsdaten**
2 citations
Angewandte Chemie · 134, e202203038
https://exaly.com/article/156471015

08 **Minimum Information Standards in Chemistry: A Call for Better Research Data Management Practices**
36 citations
Angewandte Chemie - International Edition · 61, e202203038
https://exaly.com/article/156487476

Ordered by publication year, newest first

2021

09 **FAIR Enough?**
Spectroscopy Europe
https://exaly.com/article/79659246
2 citations

10 **FAIR and Open Data in Science: The Opportunity for IUPAC**
Chemistry International · 43, 12-16
https://exaly.com/article/81581694
9 citations

2020

11 **The Impact of the Cambridge Structural Database and the Small Molecule Crystal Structures It Contains: A Bibliographic and Literature Study**
CrystEngComm · 22, 7233-7241
https://exaly.com/article/76906092
9 citations

12 **Growing the FAIR Community at the Intersection of the Geosciences and Pure and Applied Chemistry**
Data Intelligence · 2, 139-150
https://exaly.com/article/86272743
8 citations

2019

13 **“Particle Informatics”: Advancing Our Understanding of Particle Properties Through Digital Design**
Crystal Growth and Design · 19, 5258-5266
https://exaly.com/article/71913010
30 citations

2017

14 **The Next Dimension of Structural Science Communication: Simple 3D Printing Directly From a Crystal Structure**
CrystEngComm · 19, 690-698
https://exaly.com/article/66723944
21 citations

15 **From Experiments to Knowledge: Reproducibility, Validation and Reuse of Crystal Structure Data**
Chemistry International · 39, 41-42
https://exaly.com/article/67376744
1 citations

16 **Connecting Chemistry With Global Challenges Through Data Standards**
Chemistry International · 39, 5-8
https://exaly.com/article/68225260
6 citations

Ordered by publication year, newest first

2017 / continued

17 **Crystallography and Databases** — 52 citations
Data Science Journal
https://exaly.com/article/90235583

2016

18 **The Cambridge Structural Database.** — 10,174 citations
Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials · 72, 171-9
https://exaly.com/article/64148480

19 **Defining the Scholarly Commons - Reimagining Research Communication. Report of Force11 SCWG Workshop, Madrid, Spain, February 25-27, 2016** — 1 citations
Research Ideas and Outcomes · 2, e9340
https://exaly.com/article/89270101

2014

20 **A Crystallographic Perspective on Sharing Data and Knowledge** — 28 citations
Journal of Computer-Aided Molecular Design · 28, 1015-1022
https://exaly.com/article/59090083

2012

21 **Mining the Cambridge Structural Database for Bioisosteres** — 5 citations
Journal unavailable
https://exaly.com/article/53130935

22 **One in Half a Million: A Solid Form Informatics Study of a Pharmaceutical Crystal Structure** — 47 citations
CrystEngComm · 14, 2391-2403
https://exaly.com/article/54378988

2011

23 **New Software for Statistical Analysis of Cambridge Structural Database Data** — 193 citations
Journal of Applied Crystallography · 44, 882-886
https://exaly.com/article/51444563

24 **Deducing Chemical Structure From Crystallographically Determined Atomic Coordinates** — 24 citations
Acta Crystallographica Section B: Structural Science · 67, 333-349
https://exaly.com/article/51444993

Ordered by publication year, newest first

2010

25 **WebCSD: The Online Portal to the Cambridge Structural Database**
Journal of Applied Crystallography · 43, 362-366
https://exaly.com/article/48383972
135 citations

26 **Bond Lengths in Organic and Metal-Organic Compounds Revisited: X—H Bond Lengths From Neutron Diffraction Data**
Acta Crystallographica Section B: Structural Science · 66, 380-386
https://exaly.com/article/48384556
517 citations

2009

27 **Polymer-Rückgrat-Konformation – eine schwierige Aufgabe für Datenbank-Suchaktionen**
Angewandte Chemie · 121, 9774-9776
https://exaly.com/article/46096284
5 citations

28 **Polymer Backbone Conformation—A Challenging Task for Database Information Retrieval**
Angewandte Chemie - International Edition · 48, 9596-9598
https://exaly.com/article/46098402
7 citations

2008

29 **Mercury CSD 2.0 – New Features for the Visualization and Investigation of Crystal Structures**
Journal of Applied Crystallography · 41, 466-470
https://exaly.com/article/43359098
8,719 citations

2005

30 **Factors Affecting d-Block Metal–Ligand Bond Lengths: Toward an Automated Library of Molecular Geometry for Metal Complexes**
Journal of Chemical Information and Modeling · 45, 1727-48
https://exaly.com/article/39312514
34 citations

2004

31 **Retrieval of Crystallographically-Derived Molecular Geometry Information**
Journal of Chemical Information and Computer Sciences · 44, 2133-44
https://exaly.com/article/37336004
998 citations

Ordered by publication year, newest first

2002

32 **New Software for Searching the Cambridge Structural Database and Visualizing Crystal Structures**

3,141 citations

Acta Crystallographica Section B: Structural Science · 58, 389-397

https://exaly.com/article/34644176

1999

33 **The Development and Application of Knowledge-Based Approaches to Molecular Design**

0 citations

Journal unavailable

https://exaly.com/article/106522238

1997

34 **IsoStar: A Library of Information About Nonbonded Interactions**

311 citations

Journal of Computer-Aided Molecular Design · 11, 525-537

https://exaly.com/article/28608203

35 **Representation and Searching of Carbohydrate Structures Using Graph-Theoretic Techniques**

16 citations

Carbohydrate Research · 304, 61-67

https://exaly.com/article/28823348

1995

36 **Knowledge Acquisition From Crystallographic Databases**

0 citations

AIP Conference Proceedings · 330, 647-666

https://exaly.com/article/26129744

End of list · 36 articles. Citation counts use Exaly's peer-reviewed cohort.