



Towards the Next Level: Chemical Information @ Springer Nature

Steffen Pauly, J. Eiblmaier, [H. Kraut](#)

16 August 2017

SPRINGER NATURE

#springer175



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Springer – Driving academic publishing since 1842

Commemorating Julius Springer's passion for chess, the knight chess piece – Springer in German – was the natural choice for the company logo. Over the years, the logo changed with the company.

1881 1976 1995 2006

#springer 175

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About Springer Nature

- Formed in 2015 through the merger of Nature Publishing Group, Palgrave Macmillan, Macmillan Education and Springer Science+Business Media.
- The company numbers almost 13,000 staff in over 50 countries
- A leading global research, educational and professional publisher, home to an array of respected and trusted brands providing quality content through a range of innovative products and services
- The world's largest academic book publisher, publisher of the world's most influential journals and a pioneer in the field of open research



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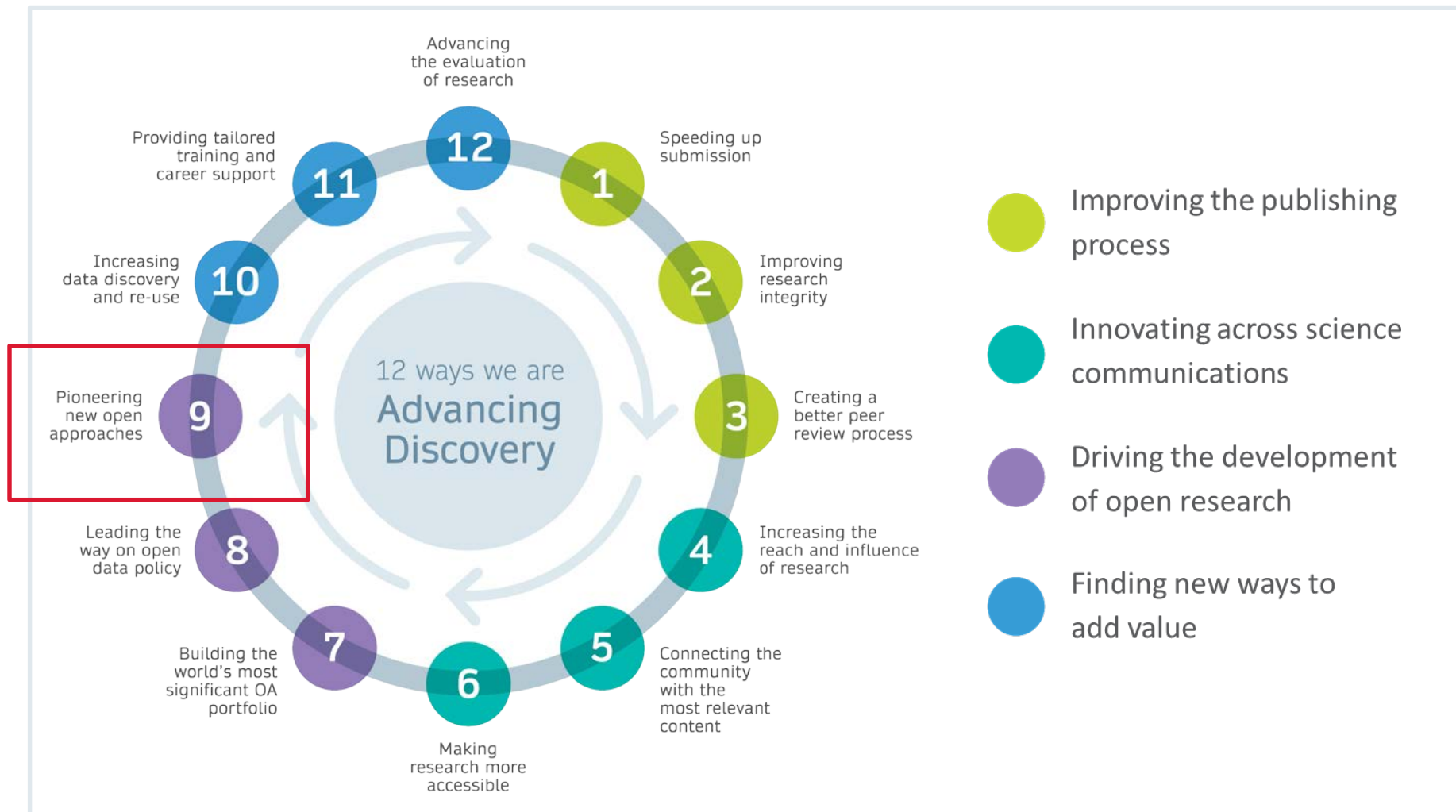
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Our simple ambition

To help researchers, students,
teachers and professionals to
learn, discover and achieve more

12 ways we are helping researchers to advance discovery



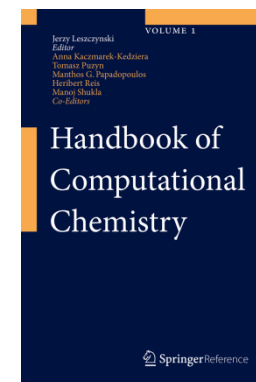
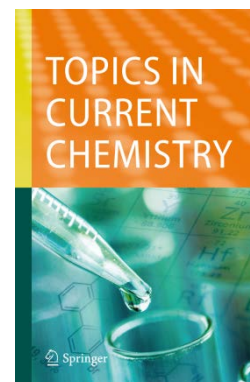
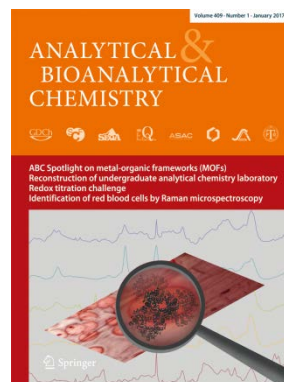
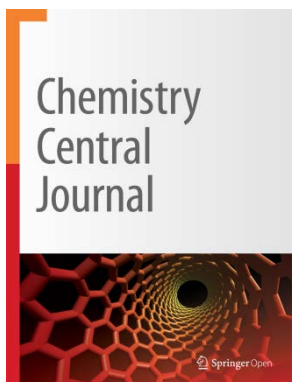
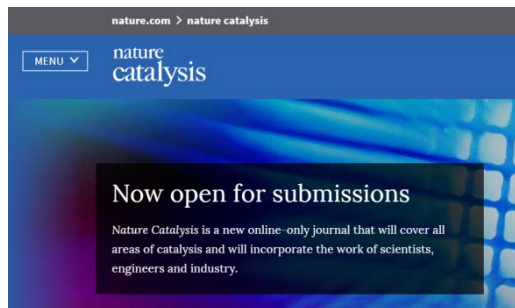
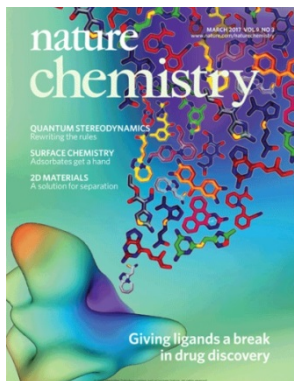
9 Pioneering new open approaches



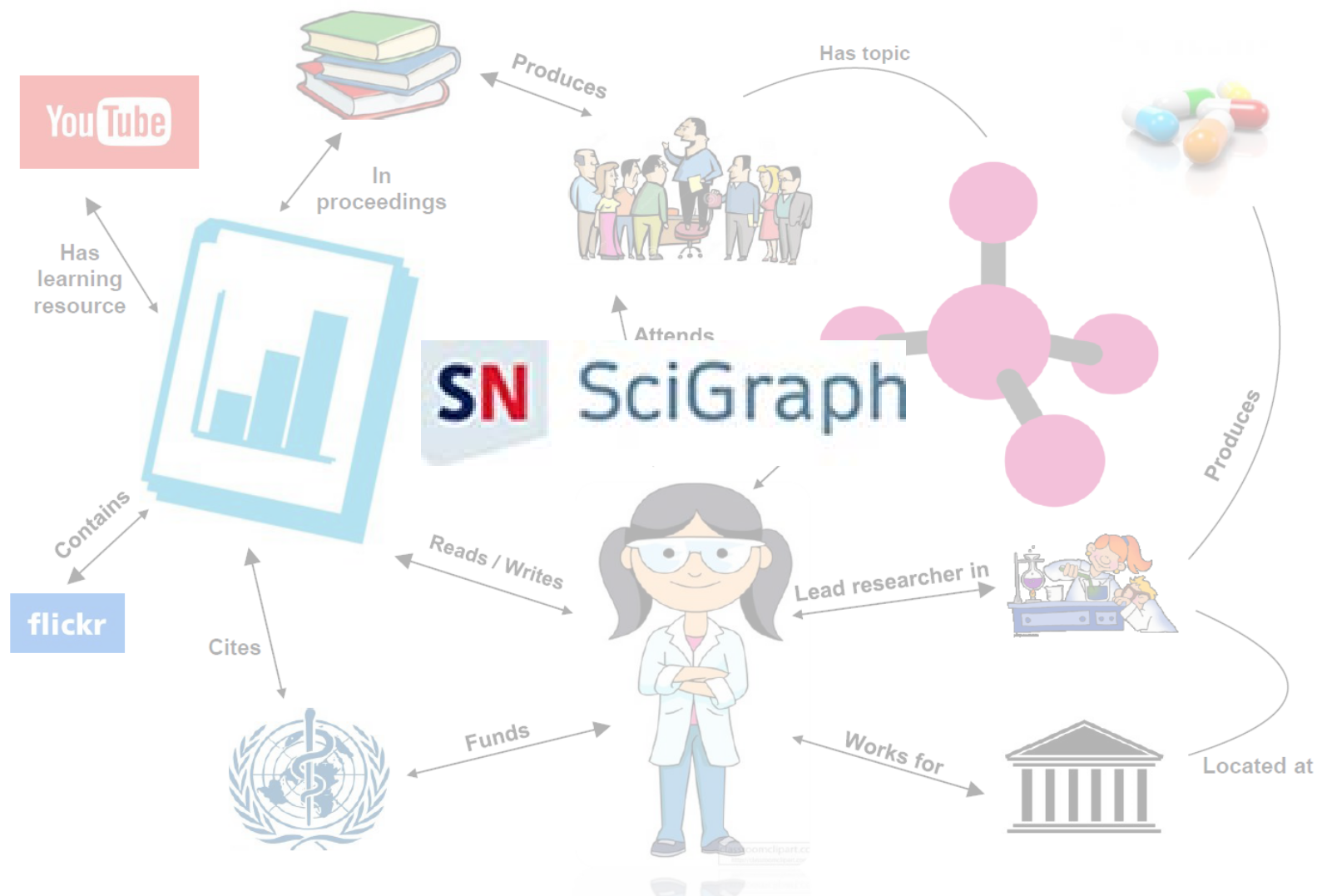
12 ways we are Advancing Discovery

- One pioneering new approach to open is Springer Nature **SciGraph** – a Linked Open Data (LOD) platform that aggregates data sources from Springer Nature and cooperating partners, making it easier to analyse information related to Springer Nature publications. SciGraph collates information from across the research landscape, such as funders, research projects and grants, conferences, affiliations, and publications. Currently the knowledge graph contains 155 million facts about objects of interest to the scholarly domain

Chemical Information @ Springer Nature so far (examples)



From Publishing Chemistry to Managing Knowledge



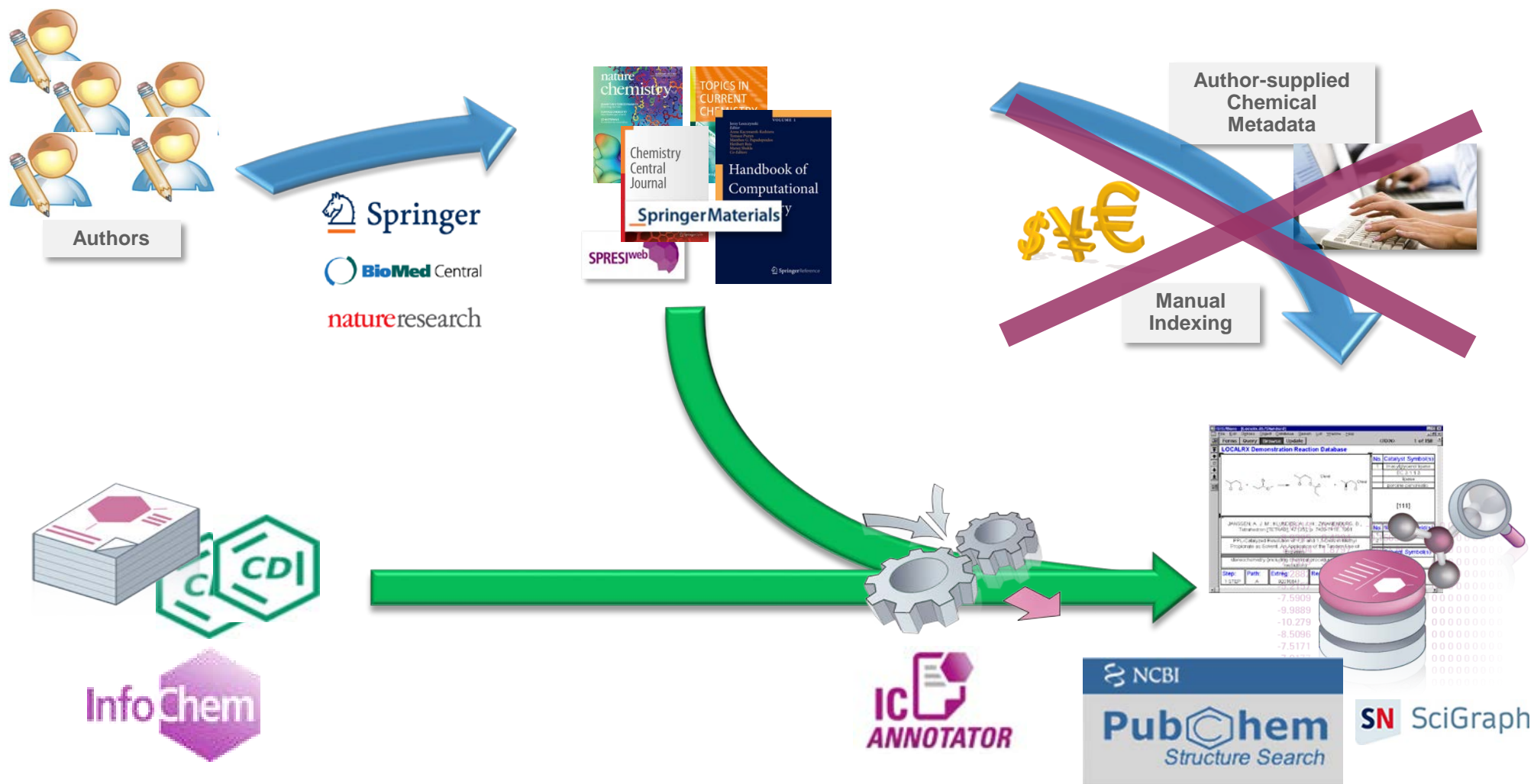
Examples of Data on SciGraph



InChI/InChIKey



Chemical Entity Recognition and Annotation



PubChem Compound

Summary 20 per page Sort by Default order

Send to: Filters: [Manage Filters](#)

Actions on your results

- BioActivity Analysis: Analyze the BioActivities of the compounds
- Structure Clustering: Cluster structures based on structural similarity
- Structure Download: Download the structures in various formats

Refine your results - What's this?

Chemical Properties: Rule of 5 (610)

BioActivity Experiments: BioAssays, Active (35); BioAssays, Tested (89)

BioMedical Annotation: Pharmacological Actions (2); Antineoplastic Agents (1); Antineoplastic Agents, Alkylating (1)

Depositor Category: Chemical Vendors (72); NIH Molecular Libraries (2)

Find related data: Database: Select; Find items

Recent activity: Turn Off Clear; PubMed: The Bibliographic Database - The NCBI Handbook; See more...

1. **temozolomide; 85622-93-1; Temodar ...**
 MW: 194.150840 g/mol MF: C₈H₈N₆O₂
 IUPAC name: 3-(2-chloroethyl)-4-oxoimidazo[5,1-d][1,2,3,5]tetrazine-8-carboxamide
 Create Date: 2005-03-26
 CID: 5394
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#) [PubMed \(MeSH Keyword\)](#) [Active in 29 of 831 BioAssays](#)

2. **Mitozolomide; Azolastone; Mitozolamide ...**
 MW: 242.622480 g/mol MF: C₇H₇ClN₆O₂
 IUPAC name: 3-(2-chloroethyl)-4-oxoimidazo[5,1-d][1,2,3,5]tetrazine-8-carboxamide
 Create Date: 2005-03-26
 CID: 71766
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [PubMed \(MeSH Keyword\)](#) [Active in 20 of 322 BioAssays](#)

3. **113942-32-8; 3-(2-Chloroethyl)-4-oxo-3H-imidazo(5,1-d)-1,2,3,5-tetrazine-8-carboxylic acid, imidazo[5,1-d]-1,2,3,5-tetrazine-8-carboxylic acid, 3-(2-chloroethyl)-3,4-dihydro-4-oxo- ...**
 MW: 243.607240 g/mol MF: C₇H₆ClN₆O₃
 IUPAC name: 3-(2-chloroethyl)-4-oxoimidazo[5,1-d][1,2,3,5]tetrazine-8-carboxylic acid
 Create Date: 2005-03-26
 CID: 124241
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [PubMed \(MeSH Keyword\)](#) [Active in 2 of 27 BioAssays](#)

4. **Ethazolastone; 3-ethyl-4-oxo-3,4-dihydroimidazo[5,1-d][1,2,3,5]tetrazine-8-carboxamide; 97716-74-0 ...**
 MW: 208.177420 g/mol MF: C₇H₈N₆O₂
 IUPAC name: 3-ethyl-4-oxoimidazo[5,1-d][1,2,3,5]tetrazine-8-carboxamide
 Create Date: 2005-03-26
 CID: 126798
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [PubMed \(MeSH Keyword\)](#) [Tested in 9 BioAssays](#)

5. **8-(N-Methyl)mitozolomide; 3-(2-chloroethyl)-n-methyl-4-oxo-3,4-dihydroimidazo[5,1-d][1,2,3,5]tetrazine-8-carboxamide; 85622-96-4 ...**
 MW: 256.649060 g/mol MF: C₈H₉ClN₆O₂
 IUPAC name: 3-(2-chloroethyl)-N-methyl-4-oxoimidazo[5,1-d][1,2,3,5]tetrazine-8-carboxamide
 Create Date: 2005-08-08
 CID: 128723
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#) [PubMed \(MeSH Keyword\)](#) [Tested in 32 BioAssays](#)

8-(N-Dimethyl)mitozolomide; 3-(2-Chloroethyl)-N,N-dimethyl-4-oxo-3,4-dihydroimidazo[5,1-d][1,2,3,5]tetrazine-8-carboxamide; 85622-97-5 ...

statistics Hervorheben Groß-/Kleinschreibung 1 von 1 Übereinstimmung

Compound Summary for CID 5394

1 2D Structure

2 3D Conformer

3 Names and Identifiers

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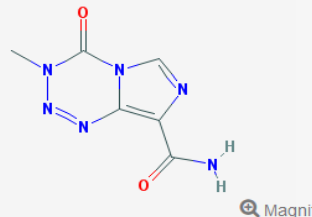
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14 Classification

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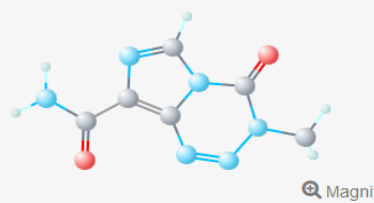


Magnify

from PubChem

2 3D Conformer

Search Download Get Image



Magnify

Show Hydrogens Show Atoms Animate

Compound Summary for CID 5394

Contents

- 2D Structure
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- Biomolecular Interactions and Pathways
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10.7 SpringerLink

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Title

Anaplastic ependymoma of the cerebrum of an adult

Targeting pattern recognition receptors in cancer immunotherapy

A Phase II trial of 17-allyl-17-demethoxygeldanamycin in metastatic breast cancer

Targeting the mTOR pathway in cancer

Pharmacologic inhibition of the cytotoxic activity of CD8+ T cells in cancer

Regulatory T Cells in Cancer

F10 gene hypomethylation is associated with poor prognosis in gastric cancer

Wechselwirkungen zwischen Kinetin und Kinetin-Phosphatase

A simultaneous analysis of the cytotoxic activity of CD8+ T cells and the expression of CD137 in cancer

The value of 18F-FDG PET/CT in the diagnosis of malignant melanoma

11 Patents

2066313 Canada

2476494 Canada

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2 months prior to consulting our hospital, she began to experience difficulty in understanding the names of objects as well as difficulty in finding adequate words while talking. Because these symptoms gradually progressed, she was admitted to our hospital. Mild right hemiparesis and aphasia of mixed type were noted on admission, and magnetic resonance (MR) imaging of the

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Review
Targeted Oncology
March 2012, Volume 7, Issue 1, pp 29-54
First online: 08 March 2012

Targeting pattern recognition receptors in cancer immunotherapy

Nadège Goutagny, Yann Estomes, Uzma Hasan, Serge Lebecque, Christophe Caux

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Abstract

Pattern recognition receptors (PRRs) are known for many years for their role in the recognition of microbial products and the subsequent activation of the immune system. The 2011 Nobel Prize for medicine indeed rewarded J. Hoffmann/B. Beutler and R. Steinman for their revolutionary findings concerning the activation of the immune system, thus stressing the significance of understanding the mechanisms of activation of the innate immunity. Such immunostimulatory activities are of major interest in the context of cancer to induce long-term antitumoral responses. Ligands for the toll-like receptors (TLRs), a well-known family of PRR, have been shown to have antitumoral activities in

from DrugBank

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A quick word about InfoChem

- **InfoChem** is a subsidiary of **Springer Nature** working in the field of ChemInformatics
- A leading force in retrieval and handling of chemical structures and reactions with more than 20 years of experience
- InfoChem contributes to the extension of InChI for chemical reactions
- Join the RInChI discussion on Thursday morning

My Question to the Audience:

Which use cases do you foresee for linking our (meta-)data to your data?



Thank you

Steffen Pauly

Editorial Director Chemistry

Springer

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