

SureChem

Patent chemistry when
and how **you** need it



Brought to you by the industry's most
advanced chemistry mining pipeline

SOFTWARE THAT UNDERSTANDS SCIENCE

We are an innovative technology company developing software and apps that change the way science is done.

[OUR STORY >](#)

Plasma Ball by Joetk75, under a CC-BY-2.0 license

SOFTWARE FOR SCIENCE

Browse our range of innovative products

Browse



Integrate your laboratory safety and regulatory compliance



Organise and discover the research relevant to you



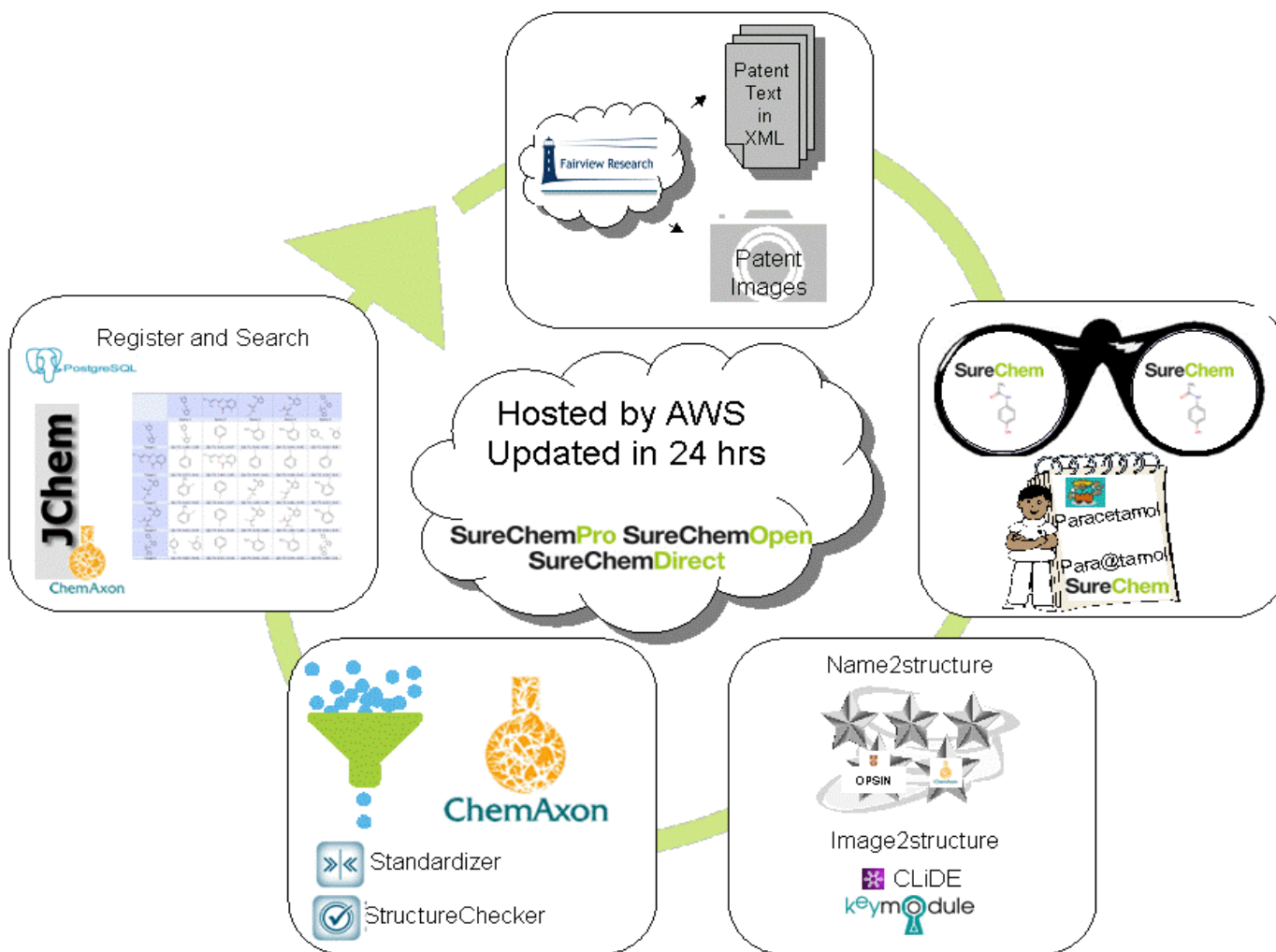
Publish all of your data in a citable, searchable and sharable manner



Dr. Eli Lewis explains how he has benefitted from using LabGuru at Ben-Gurion University

[LabGuru in practice](#)

SureChem Chemistry Mining Workflow



SureChem Data Collection

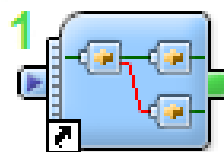
Database of automatically mined structures
from text and images

- ✧ 20M annotated **US, EP, WO** full text records and Japan patent abstracts
- ✧ **12M** unique chemical structures
- ✧ MEDLINE – 19M abstracts (coming Q4)

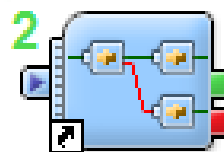
- ✧ Structures from **text** are available 24 hours from publication
- ✧ Structures from **images** are available 2 to 3 days from publication

SureChemDirect

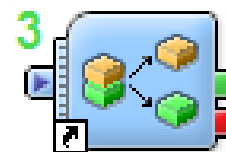
- API or Data Feed access to chemistry and full text
- Integrate with internal databases & workflows
- Off-the-shelf deployment including Pipeline Pilot support



SureChem
Query from
Text



SureChem
Query from
Molecule



SureChem
Matrix Query
from Text

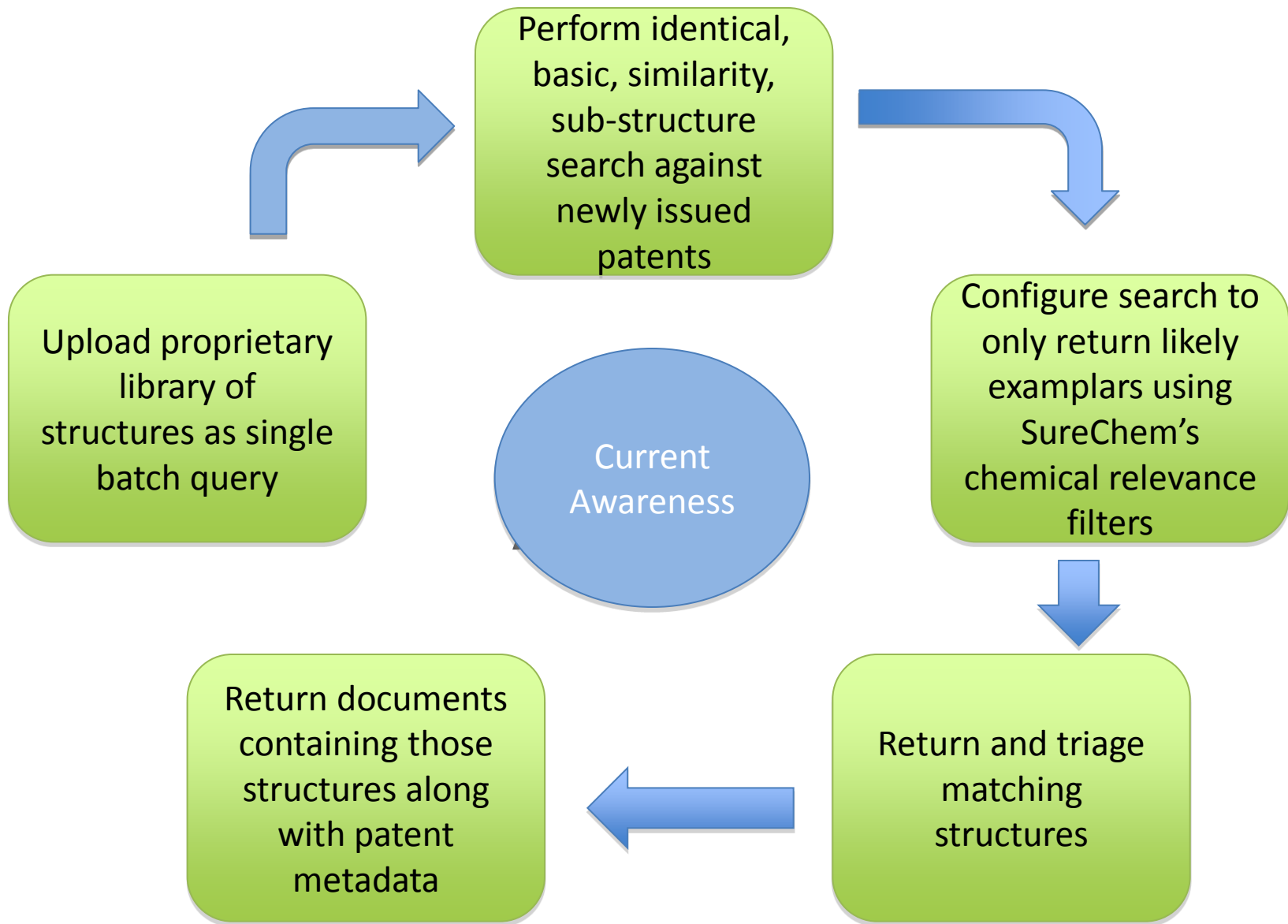
Innovative workflows:

Drug Discovery Fragment substitution

Can I perform bioisosteric replacement to improve binding and maintain freedom to operate?

1. Gather likely bioactive structures (similarity or substructure search) in combination with patent bibliographic/full text search.
2. Identify a substructure (fragment) candidate for bioisosteric replacement
3. Crop lead structure removing bioisosteric fragment
4. Perform a sub-structure search and look for hits that match compounds in your set of bioactive molecules
5. Identify matched molecular pairs of bioisosteric functional groups that maintain or improve bioactivity and are free of claims.
6. Export collected data and distribute to medicinal chemists

Batch Searching



Alerts and workflow integration

Set up daily, weekly, monthly structure and text alerts

Export structures, patent IDs and metadata to workflow tools and databases (Sharepoint, SpotFire, Seurat etc)

Distribute results to project scientists.
View structures in context using SureChemOpen/Pro

To a solution of 4-[3-(morpholin-4-ylcarbonyl)-5,6-dioxidothiopheno[4,3-c]pyrazol-4-(1H)-yl]phenyl]methanol (300 mg, 0.68 mmol, 1 eq.) in DCM (15 mL) is added triethylamine (190.28 μL, 1.37 mmol; 2 eq.) and methanesulfonyl chloride (105.67 μL, 1.37 mmol; 2 eq.) at 0°C under nitrogen. The reaction mixture is stirred at rt for 1 h. The reaction is stopped by addition of water and the product is extracted with DCM. The organic layers are dried over MgSO₄ and the solvents evaporated to afford 400 mg (quant) of the title compound as a beige oil. It is used in the next steps without further purification. MS (ESI⁺); 518.0.

Intermediate W.2: 3-[3-(Morpholin-4-ylcarbonyl)-5,5-dioxidothiopheno[4,3-c]pyrazol-4-(1H)-yl]benzyl methanesulfonate

Following the protocol outlined in procedure W (New: mesylate formation), 3-[3-(morpholin-4-ylcarbonyl)-5,5-dioxidothiopheno[4,3-c]pyrazol-4-(1H)-yl]benzyl methanesulfonate is obtained from 4-[3-(morpholin-4-ylcarbonyl)-5,6-dioxidothiopheno[4,3-c]pyrazol-4-(1H)-yl]phenyl]methanol to afford 1.85 g (quant) of the title compound. HPLC (max plot) 62.6%; Rt 3.69 min. HPLC (max plot) 29.4%; Rt 3.66 min. MS (ESI⁺); 517.9.

Compound **Chemical information**

Intermediate X.3: 1-Amino-3-[3-(morpholin-4-ylcarbonyl)-1,2,4-dithiazol-5-yl]pyrazole-5,5-dioxide (hydrochloride)

Structures generated for this name:

Procedure Y

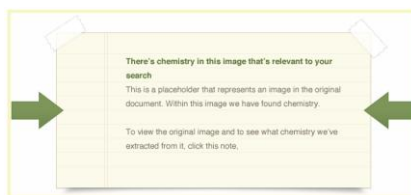
Intermediate Y.3

To ie E-butyl (1 in 1,4-dioxane under vacuum 3H), 3.02-4.89

Compound **Chemical information**

Obtained from

Name: 1-[4-(hydroxymethyl)phenyl]-3-[(morpholin-4-yl)carbonyl]-1H-4H-pyrazole-5,5-dione
 Name: 1-[4-(hydroxymethyl)phenyl]-3-[(morpholin-4-yl)carbonyl]-1H-4H-pyrazole-5,5-dione



STRUCTURE(S) EXTRACTED FROM THIS IMAGE

Chemical name:
1-methyl-3-[2-morpholin-4-ylcarbonyl-6-oxo-1H-5H-
[5H]-1,2-bisothienyl-3-yl]pyrazole-5,5-dione

SMILES:
CNC1C=C2C=CN(C)CC(=O)C1=C3C(=O)C=C1N=C3C(=O)C2=O

PubID:
ICM=18C19R1BACD0511-19-15-1018-1018-222-3-
151105221-2019-151101(1)-181162120-4-625-7-6-2562-
3-8-1-7-192-110

PubID:
DOI=10.26434/chemrxiv-2019-04

Mol Weight:
376.38993408201

In ChEMBL:
0

Chemical name:
1-methyl-3-[2-morpholin-4-ylcarbonyl-1H-4H-5H-1,2-
bisothienyl-3-yl]pyrazole-5,5-dione

SMILES:
CNC1C=C2C=CN(C)C=C3C(=O)C=C(C)C=C3C(=O)C2=O

PubID:
ICM=18C20G1ND04588-2224-18-12-29-13-11-2488-18-
15-2027-2819-4-6-4-1313211(1)R16323-2014-18-6-5-3-3-
18-1-8-10-19-2

PubID:
DOI=10.26434/chemrxiv-2019-04

Mol Weight:
422.444663515623

In ChEMBL:
0

Chemical name:
1-(2-methoxypropyl)-3-[2-morpholin-4-ylcarbonyl-1H-4H-
5H]-1,2-bisothienyl-3-yl]pyrazole-5,5-dione

SMILES:
COCOC1N(C)C=CN(C)C(=O)C1=C3C(=O)C=C1N=C3C(=O)C2=O

PubID:
ICM=18C19R1BACD0511-28-10-47-22-18-14-2-3-6-
16140524-2019-151101202(1)R163231-19-17-10-9-
21-2-3-8-1-7-192-110

PubID:
DOI=10.26434/chemrxiv-2019-04

Mol Weight:
414.444663515623

In ChEMBL:
0

SureChem Products

SureChemOpen

- ✦ **Free resource** for researchers to search, view and navigate through the relevant chemistry in the full text of patent documents
- ✦ Enables linking to public and proprietary content

SureChemPro

Coming in Q4:

- ✦ Professional search needs
- ✦ Structure and patent metadata export, alerts, patent family search, chemical relevance filters...

Enter your SureQuery™

SEARCH FOR KEYWORDS

PI3K inhibitors

BIBLIOGRAPHIC FIELDS

Assignees/Applicants merck serono

IPC Class C07D

PATENT AUTHORITIES

All chemically annotated authorities (7)

US Applications

US Granted

EP Applications

EP Granted

WO

JP

All authorities (Inc. DocDB) (1)

PUBLICATION DATE

[2002101] TO [2012925]

Our Chemistry Annotation Coverage **NEW!**

Chemistry annotations for US, EP, WO full text and all abstracts are now available as follows:

Structures from text annotations: from Jan 1, 1976 to date

Structures from image annotations: from Jan 1, 2012 to date

SELECT STRUCTURE SEARCH

Substructure

Duplicate

Exact

Similarity

SEARCH FOR STRUCTURE IN DOC SECTIONS

All

Title

Abstract

Claims

Description

Structure searches in document sections are coming soon

SureChemOpen Search Results

Your current query

Showing 1-32 of 595 total structure results

Structure search type: Substructure

Query: (c1cc(C2=CC=CC=C2)N(C2)C3=CC=CC=C3) OR desc: (PI3K inhibitors) AND (merck serono) AND s: (WO) AND (specify US OR EP OR WO OR JP) AND (patents (2002101 TO 2012925))

View results as: Matrix Table

Structure 1: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 2: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 3: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 4: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 5: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 6: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 7: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 8: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 9: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 10: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 11: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 12: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 13: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 14: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 15: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 16: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 17: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 18: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 19: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 20: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 21: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 22: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 23: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 24: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 25: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 26: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 27: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 28: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 29: Cc1ccc2c(c1)nc3c2c(=O)nc3

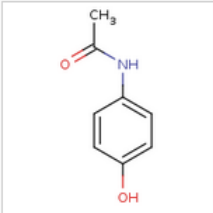
Structure 30: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 31: Cc1ccc2c(c1)nc3c2c(=O)nc3

Structure 32: Cc1ccc2c(c1)nc3c2c(=O)nc3

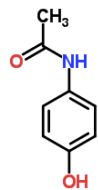
SureChem Partnering

Showing 1-32 of 65,982 total structure results View results as: [Matrix](#) | [Table](#)

Check	Structure image	Chemical information	Mol weight	External resources
<input type="checkbox"/>		Name: N-(4-hydroxyphenyl)acetamide SMILES: <chem>CC(=O)NC1=CC=C(O)C=C1</chem> InChi Key: RZVAJINKPMORJF-UHFFFAOYSA-N Inchi: InChI=1S/C8H9NO2/c1-6(10)9-7-2-4-8(11)5-3-7/h2-5,11H,1H3,(H,9,10)	151.162	54 168



[About](#) [More Searches](#) [Web APIs](#) [Help](#)



paracetamol
ChemSpider ID: 1906
Molecular Formula: C₈H₉NO₂
Average mass: 151.162598 Da
Monoisotopic mass: 151.063324 Da
Systematic name: N-(4-Hydroxyphenyl)acetamide
SMILES and InChIs
Cite this record

Names and Identifiers

Names and Synonyms [Database ID\(s\)](#)

Validated by Experts, Validated by Users, Non-Validated, Removed by Users, Red

- 103-90-2 [RN]
- 203-157-5 [EINECS]
- 4-(Acetylamino)phenol
- 4-13-00-01091 (Beilstein Handbook Reference) [Beilstein]
- 4-Acetaminophenol
- 4'-Hydroxyacetanilide
- 4-Hydroxyanilid kyseliny octove [Czech]
- Acetamide, N-(4-hydroxyphenyl)-
- Acetamide, N-(p-hydroxyphenyl)-
- Acetaminophen [Wiki] [USP] [JP15]
- More...

RSCPublishing

RSC | ChemSpider | Feedback | Login | Register

Advanced Search

Home > Search results >

Search results
You searched for: Keywords: csid:1906

Modify Search | Search History

All (168) | Journal Articles (168) | Book Chapters (0) | Non-RSC Articles (0)

Sort By: [Relevance] | Results Per Page: [25]

Page 1 of 7

Select All | Download Citation: [BibTex] | Go | Check Access | Expand All

- Direct analysis of dried blood spots utilizing desorption electrospray ionization (DESI) mass spectrometry
Justin M. Wiseman, Christopher A. Evans, Chester L. Bowen and Joseph H. Kennedy
Analyst, 2010, 135, 720-725
DOI: 10.1039/B922329K, Paper
From themed issue: Ambient mass spectrometry [Expand](#) [PDF](#) [Rich HTML](#)
- The biological potential of flavones
Alok Kumar Verma and Ran Prasad
Nat. Prod. Rep., 2010, 27, 1571-1593
DOI: 10.1039/C004698C, Review Article [Expand](#) [PDF](#) [Rich HTML](#)
- Polymorphic control by heterogeneous nucleation - A new method for selecting crystalline substrates
Keith Chadwick, Alan Myerson and Bernhard Trout
CrystEngComm, 2011, 13, 6625-6627
DOI: 10.1039/C1CE05871A, Communication [Expand](#) [PDF](#) [Rich HTML](#)
- Bacteria-based AND logic gate: a decision-making and self-powered biosensor
Zhonglan Li, Miran A. Rosenbaum, Arvind Venkataraman, Tsz Kin Tam, Evgeny Katz and Largus T. Angenent
Chem. Commun., 2011, 47, 3060-3062
DOI: 10.1039/C0CC05037G, Communication [Expand](#) [PDF](#) [Rich HTML](#)

Filters Applied
Content Type: all

Author
Craig E. Banks (5)
Alistair R. Lemmie (4)
Colin R. Pulham (4)
Iain D. H. Oswald (4)
John E. Warren (4)
More

Date Range
6 months-1 year (15)
1-2 years (74)
2-5 years (79)

Journal
Analyst (41)
Anal. Methods (18)
CrystEngComm (18)
Chem. Commun. (14)
Phys. Chem. Chem... (11)

SureChem – What's next?

- ✦ Complete backfile processing of structures from images
- ✦ Implement **chemical relevance filters** to improve chemistry relevance (SCD, SCPro)
 - Frequency counts of chemicals within patent corpus
 - Advanced chemical structure filters
 - Structure location and source
 - Identification of likely exemplar and medchem relevant compounds
- **SureChem** to deposit all structures into

**Please contact us to discuss
your requirements or set up a
free SureChemDirect
evaluation**

**www.surechem.com
<http://blog.surechem.com/>**

Elisabeth Piveteau
e.piveteau@digital-science.com
07801 133 928

SureChem