

# Chemistry and the Law

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# NEWSLETTER

## CHAIR'S MESSAGE

JEN BLOUNT



Welcome to the Chemistry and the Law (CHAL) Division of the ACS! It is my privilege and honor to serve as Chair of CHAL this year, and I am very much looking forward to attending the upcoming national meetings in San Francisco and Washington, D.C. I hope that you will join us for what promise to be dialogue, informative presentations, and ample opportunity for networking at two spectacular

venues. Also, I also encourage current and prospective members to attend our happy hour networking reception on Monday, April 3, from 6-8 pm, at Jillian's Restaurant.

CHAL is truly diverse, and I hope that this year will bring further growth and expansion to our division. The diversity of our members is reflected in the variety of our symposiums, with topics including deproliferation, tracking and proper destruction of chemical weapons, the changing scope of patentable subject matter around the world, legal considerations for collaborative research, strategic planning for small- to mid-size chemical and pharmaceutical companies, forensic science and the law, and legal updates regarding the generic drug and ANDA process.

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# COUNCILORS' REPORT

## CHAIR'S MESSAGE (CONT'D)

As a division of the ACS, we constantly strive to enrich the many facets of CHAL and to broaden our reach to our members. In that regard, we have started a new webinar series with division members at its target audience. Please consider attending any or all of the upcoming webinars (4/11 -Webinar #3: Collaborative Research Considerations; 5/9 - Webinar #4: Considerations for License Agreements; 6/13 - Webinar #5: Joint Inventorship of Patents). I want to particularly thank Krista Bianco for all her phenomenal work on launching this program.

In our constant effort to best serve our members, we value your feedback and input regarding CHAL's programming, and CHAL as a whole. If you have any questions or suggestions for our division, please do not hesitate to contact me or any member of the Executive Committee.

Last, but not least, I would like to thank every member of our Executive Committee, and all the past Chairs of the division, who have helped shape CHAL into what it is today: an actively growing division with passionate people and places to go!

I hope to see all of you in San Francisco.

*Jen Blount*

## COUNCILORS' REPORT

ALAN EHRLICH & JIM CARVER

### Upcoming Meeting, San Francisco, April 2-6, 2017.

The Council will listen to four nominees for President-Elect and choose two candidates for the Fall ballots. The nominees are: Bonnie Charpentier, Cytokinetics, Inc., South San Francisco, California; Mark Frishberg, Custom Organic Synthesis Consultant, Santa Rosa, California (retired from Eastman Chemical Company); Anne Gaffney, Idaho National Laboratory, Idaho Falls, Idaho; and Willie E. May, Emeritus Director, National Institute of Standards and Technology, Gaithersburg, Maryland. The 2 selected candidates will be on the ballot along with any petition candidates who file petitions by July 15. You can hear the 4 nominees at a Town Hall Meeting, Sunday, April 2, 2017, 4:30-5:30, Hilton San Francisco Union Square Hotel, Imperial Ballroom B, or review information on the candidates' webpages.

A Joint Board of Directors-Council Policy Committee Task Force on Governance Design was established at the previous Philadelphia Meeting and has been hard at work. They are sponsoring a Special Discussion Item at this Council Meeting, ACS Yesterday and Today: Paving the Way to Tomorrow.

A petition for Removal of Officers and Councilors [for neglect of duties, misconduct,

# COUNCILORS' REPORT

or conduct that reflects on the SOCIETY] will be up for action by the Council. If approved, the petition will become effective upon approval of a companion set of specific procedures that will be acted upon by the Council, and confirmation by the Board of Directors.

A second petition on International Chemical Sciences Chapters has been filed and is on the Agenda for consideration. The petition will be up for action at the Council Meeting in Washington in August. The petition will allow International Chemical Sciences Chapters to receive funds from the SOCIETY, which is not now permitted for these chapters.

The Council will also consider a proposal to raise dues for 2018 from 2017's \$166 to \$171. The proposal is derived from an inflation formula, but does not go into force until formal approval by the Council.

At least once every three years, at a spring national meeting, the Divisional Activities Committee must bring to Council a formula for allocating funds dedicated to divisions. The current formula places the funds in six categories. The Committee is proposing keeping the current formula.

Finally, a number of administrative issues are on the agenda that we don't normally report on because of time or space. One item of interest, however, is the Santa Clara Valley Section, one of the primary sources of support for creation of CHAL 30 years ago, is proposing a name change

to Silicon Valley Section. This more closely reflects the nature of the Section's current activities related to high technology subjects rather than their original concentration in agricultural chemistry and more accurately reflects the geography of the Section.

## Report from 252nd National Meeting, Philadelphia, August 2016.

We are proud to announce that Brian Meadows, CHAL's candidate, was named an ACS Fellow for 2016. CHAL has a good record in nominations for Fellows. Each year of the Fellows program, at least one CHAL member or someone with CHAL connections has been named a Fellow – for a total of 15 in the 8 years of the program.

The Council elected *Harmon B. Abrahamson, Lissa A. Dulany, Andrea B. Twiss-Brooks, and Sally B. Peters* for a 2017-2019 term, *Martin D. Rudd* for a 2017-2018 term, and *Karl S. Booksh and Ella L. Davis* for a one-year term, 2017, on the Council Policy Committee.

The Council elected *Lisa M. Balbes, Thomas H. Lane, Amber S. Hinkle, Alan M. Ehrlich, and Alan A. Hazari* for a 2017-2019 term and *Neil D. Jespersen* for a one-year term, 2017, on the Committee on Nominations and Elections.

The Council elected *Wayne E. Jones, Jr., D. Richard Cobb, Stephanie J. Watson, Dee Ann Casteel, and Emilio X. Esposito* for three year terms, 2017-2019, on the Committee on Committees.

# COUNCILORS' REPORT

The Council also approved a petition to amend the ACS Bylaws to extend the Unemployed Members' Dues Waiver, which will extend waivers for unemployed members' dues from the current two years to three years, subject to confirmation by the Board of Directors.

## Special Discussion

The Council conducted a special discussion to gather input on proposed recommendations from the ACS Presidential Task Force on the U.S. Employment of Chemists. The task force has been examining and considering all known influences that can impact employment in the chemical sciences. Councilors were invited to share their thoughts, comments, and suggestions on the proposed suggestions to date, in preparation for the report's expected release later this year.

As of Tuesday evening, August 23, the total meeting attendance, all categories together, was 12,800. The final number is 12,989.

On the recommendation of the Society Committee on Budget and Finance, the Board voted to approve the advance member registration fee of \$445 for national meetings held in 2017 and also authorized several program funding requests.

The Board is seeking ways to engage ACS stakeholders to identify opportunities and issues for governance improvement

that will enable ACS to advance its mission in a streamlined and simplified manner. As mentioned above, the Board and the Council Policy Committee have created a new task force that will look at the Society's future governance needs. Per the Board's discussion, the chair's report to Council provided additional details on a proposed Society-wide initiative to ensure an agile, efficient, and effective ACS. The task force is comprised of equal numbers of people nominated by the Chairman of the Board and by the Vice-Chair of CPC (at the time, Alan Ehrlich) in consultation with each other. Jim Carver, who is continuing for a third year as Chair of the Committee on Constitution and Bylaws, was named as one of the representatives to the Task Force.

The Board held a well-attended regular session which featured a discussion on ACS National Meetings of the Future. Board Chair Pat Confalone opened the discussion by stating ACS National Meetings are a key way that ACS fulfills its obligation to deliver scientific information. These National Meetings are successful, but we are always looking for ways to improve and to anticipate what members' future needs – as to these meetings and other subjects – will be. Almost two dozen audience members came forward to offer comments, observations, and suggestions, prompted by a list of questions designed to help focus the discussion.



# SCHEDULE OF EVENTS

Sunday  
April  
02

**1:00 PM- 2:30 PM**  
**Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions**

*Organizers and Presiding: X. Pillai and A. Berks*  
Stanford Conference Room, Park Central San Francisco Hotel

**5:00 PM- 7:00 PM**  
**CHAL Executive Committee Meeting,**  
Jillian's, 175 Fourth St., San Francisco

Monday  
April  
03

**9:00 AM-10:00 PM**  
**Non-Traditional Careers in Chemistry**  
*Organizer: K. Bianco*  
*Presiding: R. Franz*

Stanford Conference Room, Park Central San Francisco Hotel

**10:30 AM- 11:45 AM Patent Challenges & Chocolate: A Sweet & Sour Symposium**  
*Organizer and Presiding: J. Hasford*  
Stanford Conference Room, Park Central San Francisco Hotel

**12:00 PM - 1:30 PM CHAL Luncheon**  
Mourad, 140 New Montgomery St., San Francisco

**1:30 PM-4:30 PM The Use of Scientific Information in IP-Related Matters**  
*Organizer and Presiding: E. Cheeseman*  
Stanford Conference Room, Park Central San Francisco Hotel

**6:00 PM- 8:00 PM CHAL Reception**  
Jillian's, 175 Fourth St., San Francisco

**8:00 PM- 10:00 PM**  
**Sci-Mix - Hall D Moscone Center**

Tuesday  
April  
04

**9:00 AM- 11:00 AM**  
**An International Perspective: Patent Eligible Subject Matter & Opposition Procedures**  
*Organizers and Presiders: J. Gledhill and K. Bianco*

Stanford Conference Room, Park Central San Francisco Hotel

**11:00 AM-11:30 AM Resources and outreach available through Silicon Valley Regional Office of the U.S. Patent and Trademark Office,**  
*John Cabeca, Director,* Stanford Conference Room, Park Central San Francisco Hotel

**12:00 PM- 1:30 PM Protecting & Capitalizing on Your Intellectual Property**  
*Organizer and Presiding: J. Kennedy*  
Stanford Conference Room, Park Central San Francisco Hotel

**2:30 PM - 4:30 PM Recent Developments in TSCA Regulation: New Requirements for Chemicals in Commerce**  
*Organizer and Presiding: I. Hantman*  
Stanford Conference Room, Park Central San Francisco Hotel

Wednesday  
April  
05

**9:00 AM - 11:30 AM**  
**Cannabis Law: Navigating Complex Regulatory & Legal Issues in States with Legal Cannabis Programs**  
*Organizer and Presiding: J. Marcu*

Stanford Conference Room, Park Central San Francisco Hotel

**1:00 PM - 2:30 PM The Many Faces of CHAL: Where Chemistry Meets the Law**  
*Organizer and Presiding: K. Bianco*  
Stanford Conference Room, Park Central San Francisco Hotel

**2:45 PM - 3:45 PM A Decade of U.S. Supreme Court Patent Jurisprudence**  
*Organizer and Presiding: R. Bone*  
Stanford Conference Room, Park Central San Francisco Hotel

# CHAL AWARDS & CHAL FEATURED PUBLICATION

## The Howard and Sally Peters Award for Non-Traditional Careers in Chemistry

The Chemistry and the Law (CHAL) Division of ACS has established an award regarding nontraditional careers in chemistry in honor of chemists Howard and Sally Peters—long-term members of the Santa Clara Valley Local Section. The award was first presented

in 2012 to both Howard and Sally to recognize their significant lifetime contributions to non-traditional careers in chemistry.

Additional information about nominations for the Howard & Sally Peters Award can be found on the CHAL website (<http://www.chemistryandthelaw.org/category/announcements/>). The next deadline is May 31, 2017.

## CHAL Featured Publication



### America Invents Acts Primer

By Sarah Hasford (CHAL member since 2005)

Since its passage in 2011, the Leahy-Smith America Invents Act (“AIA”) has brought many significant changes to U.S. patent law. Accordingly, to assist readers in developing an in-depth understanding of these changes, the America Invents Act Primer provides discussions of each and every one of the AIA’s substantive

provisions. More specifically, and whenever possible, each discussion of the AIA’s provisions includes the following key features:

- An identification of the AIA section’s effective date, including the statutory basis for such dates;
- A direct comparison of relevant pre- and post-AIA statutes;
- An analysis of the similarities and differences between pre- and post-AIA statutes;
- A discussion of the legislative goals that were addressed by the AIA section; and
- An analysis of the practical implications of the changes made by the AIA section

The America Invents Act Primer additionally highlights a number of free resources that can be utilized by readers to attain a deeper understanding of the AIA, including resources that explain how the U.S. Patent and Trademark Office is applying the new law.

Overall, the America Invents Act Primer provides a unique and practical desk reference on the AIA that is sure to be useful for years to come.

# CHAL PROGRAMMING

The Division of Chemistry and the Law is currently accepting papers and symposia for the 253rd National Meeting of the American Chemical Society, to be held August 20-24, 2017 in Washington, DC.

CHAL welcomes submissions on all legal topics impacting the chemical sciences, including, but not limited to, intellectual property, patents, copyrights, trademarks, trade secrets, forensic chemistry, food and drug law, regulatory law, product liability, tort law, environmental law, employment agreements, professional ethics, expert witnesses, chemical consulting, chemical health and safety, chemical information, administrative law and rule making, biotechnology, pharmaceuticals,

licensing and technology transfers, and litigation.

Please submit abstracts for individual presentations or Sci-Mix posters on-line through MAPS at <https://acsmaps.abstractcentral.com/members/client/acs.jsp> under the session entitled "The Many Faces of CHAL: Where Chemistry Meets the Law." Abstracts must be submitted by April 10, 2017.

For submission of half-day or full-day symposia with multiple speakers, please contact Krista Bianco at [krista.bianco@finnegan.com](mailto:krista.bianco@finnegan.com) or Jonathan Kennedy at [jonathan.kennedy@ipmvs.com](mailto:jonathan.kennedy@ipmvs.com).

## This Newsletter is Published in the United States of America

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A primary version of this newsletter is published twice yearly as Adobe pdf prior to ACS national meetings. It is sent to CHAL members via e-mail. Copies as print-on-paper are for distribution at those meetings, and are for U.S. Postal Service mailing to CHAL members who so request. Opinions expressed are those of the authors and not necessarily of CHAL or ACS. While great effort is made for accuracy, factual errors are possible; CHAL and ACS bear no liability for such errors, and CHAL invites correction for future publication.

References, including internet sites, cited as bibliography or for general interest, are intended for readers' convenience only, and are not endorsed as to opinions or for detailed accuracy or timeliness, which are the responsibilities of the authors and publishers of those references. Internet site citations were thought to be timely within a few weeks before this newsletter would be fixed for publication; however, some may have become stale. Mention of publications, products, or services is intended for readers' convenience only and not as commercial endorsement. Discussion of legal issues is for information and educational purposes and is not legal advice; legal advice should be sought from licensed lawyers formally consulted for that purpose. Readers' comments are welcome and future articles from them are invited -- especially to broaden the range of topics and viewpoints -- address all inquiries to [chal@chemistryandthelaw.org](mailto:chal@chemistryandthelaw.org).

# CHAL NETWORKING & MEETING HIGHLIGHTS

Monday  
April  
03

## CHAL Drug & Power Luncheon

12:00-1:30 PM

Mourad, 140 New Montgomery St., San Francisco

### **Innovation Elevated: Taking Your Patents to the Next Level**

by Rod Wittenberg, Reed Tech®, a LexisNexis® Company

Sponsor: Reed Tech®

(Note: a ticket is required for this event)

Monday  
April  
03

## CHAL Reception

6:00-8:00 PM

Jillian's, 175 Fourth St., San Francisco

### **Premium Open Bar and Hors D'oeuvres**

Sponsors: CAS and Division of Chemical Health & Safety

All Attendees welcome -- No ticket required!

## Meeting Highlights

**Monday afternoon, April 3**

**What exactly are you looking for?**

**Searching for chemical information**

*Elaine N. Cheeseman, echeesema@cas.org.*

*Science IP, Chemical Abstracts Service*

As the official research service of CAS, a division of the American Chemical Society, Science IP® works closely with clients to understand their unique information needs. Searching is generally an iterative process – to maintain sufficient breath while generating a manageable number of retrieved results. For example, when a search request for a chemical structure is submitted, Science IP experts consult with the client to precisely determine what is needed. Should the search be broadened or narrowed? Should it include exemplified compounds plus Markush structures? Is the client

interested in a particular use for that compound or is a particular formulation needed? Frequently requested search types on small molecules will be illustrated with examples.

**Patent claims reciting scientific information: The now heightened definiteness requirement**

*Todd A. Ostomel, tostomel@gmail.com. Squire Patton Boggs*

The claims of an issued patent describe the metes-and-bounds of the invention being claimed. Quite often, scientific information is the basis for these claims. However, scientific information, in all its forms, does not always meet the definiteness requirement for obtaining a patent. In the US, the claims must be definitely described so the public knows what activities do or do not constitute patent infringement. In 2015, the Supreme Court and Federal Circuit bolstered the ability of patent challengers to invalidate issued US patents for



# CHAL MEETING HIGHLIGHTS

failure to meet the definiteness requirement for claim terms such as “molecular weight.” This talk will discuss the now heightened definiteness requirement, as a consequence of these cases, as it relates to claims reciting scientific information and the validity of the patents which include these claims.

## **Your next breakthrough starts here – CAS content and solutions foster discovery and innovation**

*Kurt Zielenbach, kzielenbach@cas.org. CAS*

Patent professionals and researchers around the world rely on CAS solutions to fuel discovery and protect intellectual property. Curated by expert analysts with years of experience and made available through market-leading, state of the art tools like STN and SciFinder, CAS delivers the world’s most comprehensive, timely and accurate collection of chemical information. Every day, scientists, technologists and business leaders at CAS build on more than 100 years of tradition that supports insight and discovery. Customers know and trust CAS solutions to make confident research and business decisions. This presentation will highlight the breadth and depth of CAS content as well as examine various new solutions designed to facilitate the world’s research to fuel tomorrow’s innovations.

## **Survey of biosequence in patent claims and the impact on biosequence search methods**

*Kenneth L. Hoppe, khoppe@cas.org. Science IP, CAS*

Business decisions are only as good as

the information upon which they are based, and information acquisition must be weighed against cost, time and complexity of a project. Nowhere is this more critical than in the pharmaceutical and biotechnology industries. For IP projects that require biological sequence data, multiple resources must be consulted to obtain the most comprehensive information possible. The wording of patent claims will impact: (1) whether the sequence gets into a database; (2) how the sequence is indexed; and (3) how a sequence search should be conducted. For a comprehensive biosequence patent search, technical knowledge of the science is needed, but also in-depth knowledge and experience of biosequence patent databases and searching are critical for a comprehensive search.

This presentation will discuss examples of sequences in patent claims, history of patent office rules for sequences in claims, and considerations for which search algorithms may need to be used to account for these issues.

## **Patents and basic scientific research: Discovery versus invention**

*Patricia Campbell, pcampbell@jonesday.com.  
Jones Day*

Scientific discovery plays an important role in innovation. Patents can incentivize in bringing innovations to market. In biotechnology, a surge in innovation, notably by start-ups, benefited greatly from patents, which attracted capital needed in this area. The dividing line between scientific discoveries and inventions can be difficult to determine. Further, not all inventions are patentable. For

# CHAL MEETING HIGHLIGHTS

an invention to be patentable, it must be: (1) patent eligible; (2) useful; (3) new; (4) non-obviousness; and (5) sufficiently described so that people of skill in the relevant field can understand what the invention is, and make it and use it without undue experimentation. This presentation will address the differences between discoveries and inventions, and the use of scientific information in patenting inventions. This presentation will also address recent developments in U.S. patent law in the area of patent subject matter eligibility.

## Importance of Markush searching for FTO purposes

*Peter F. Blasi, pblasi@cas.org. CAS*

When advising clients on freedom to operate, having confidence in your search results is imperative. For intellectual property related to chemical substances, it is important to consider not only patents claiming specific substances, but also those covering generic chemical structures. Markush structures allow inventors to claim multiple substances by using variables at specific positions in the chemical structure to represent multiple chemical moieties. By omitting Markush structures

from a substance search, you risk missing vital information. The MARPAT database is produced by CAS and contains more than 1.1 million searchable Markush structures from patents and patent applications from the early 1960s to the present. In this presentation we will discuss patent and claim coverage in MARPAT, the impact MARPAT and other Markush databases can have on patentability and validity/invalidity, and why MARPAT is key for confidently advising your clients on freedom to operate.

## Tuesday Morning, April 4 Silicon Valley Regional Office of the U.S. Patent and Trademark Office

*John Cabeca, john.cabeca@uspto.gov. U.S. Patent & Trademark Office*

In October 2014, the U.S. Patent and Trademark Office opened a regional office in Silicon Valley to serve inventors, entrepreneurs, startups, researchers, and others in California, Nevada, Oregon, Washington, Arizona, and Hawaii. In this presentation, the Director of the Silicon Valley Regional Office will discuss what resources and outreach services are available through that office.

## CHAL Spring Webinar Series

CHAL is pleased to offer a five-part webinar series focused on patent-related topics of interest to every chemist. Please mark your calendars for the following upcoming webinar dates at 2-3 pm EST:

**4/11 - Webinar #3: Collaborative Research Considerations**

**5/9 - Webinar #4: Considerations for License Agreements**

**6/13 - Webinar #5: Joint Inventorship of Patents**

If you missed the first or second webinar, the recordings are available at the links below:

"Patents 101: The Nuts and Bolts of Obtaining a Patent,"

<https://www.youtube.com/watch?v=XHP1d3DRRM0&feature=youtu.be>.

"Lifecycle Management and Research Opportunities for Patentable Inventions,"

[https://youtu.be/Xga\\_vubK7k8](https://youtu.be/Xga_vubK7k8)

# CHAL FEATURED ARTICLE

Elaine Cheeseman  
Science IP

## The Anatomy of CAS Value-Added Summaries: Intellectual Indexing Makes the Difference!

One of the greatest challenges faced by intellectual property professionals is the ability to balance the need for comprehensive search results with the need for speed and precision. Fortunately, curated content offers a solution. Searchers can leverage intellectual analysis and indexing of primary literature sources to increase the precision of search results while maximizing the comprehensiveness of the information that is retrieved.

enhanced titles and abstracts as well as intellectually assigned structure and concept indexing. A staff of more than 1,400 scientists indexes the world's literature according to CAS's indexing guidelines. The CAS content collection covers 63 patent authorities and thousands of journals.

This article illustrates portions of the value-added indexing for patent application WO2014177977. All of this information can be searched and displayed.

The CAS content collection contains

### Patent family members plus filing details

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2014177977	A1	20141106	WO 2014-IB60945	20140423
W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BN, BR, BW, BY, ...				
CA 2910759	A1	20141106	CA 2014-2910759	20140423
AU 2014261070	A1	20151029	AU 2014-261070	20140423
CN 105164134	A	20151216	CN 2014-80024798	20140423
IL 242165	A	20151231	IL 2014-242165	20140423
KR 2016003234	A	20160108	KR 2015-7034216	20140423
MD 20150103	A2	20160229	MD 2015-103	20140423 ...

### Enhanced titles and abstracts - The following abstract was enhanced by CAS scientists.

AB The invention is directed to a class of triazine derivs. of formula I and to the use of the compds. as PDE10 inhibitors. Compds. of formula I wherein ring A-X forms (un)substituted C6-10 aryl and (un)substituted 5- to 10-membered heteroaryl; X is N and C; R1 is (un)substituted C1-6 alkyl, (un)substituted C6-1- aryl, and (un)substituted 5- to 6-membered heterocyclyl; R2 and R3 are independently H, (un)substituted C1-6 alkyl and (un)substituted C1-6 alkoxy; R4 is 0 - 2 substituents and is independently F, OH, (un)substituted C1-6 alkyl and (un)substituted C1-6 alkoxy; and pharmaceutically acceptable salt thereof are claimed. Example compound II was prepared by a multistep procedure (procedure given). The invention compds. were evaluated for their PDE10 inhibitory activity. From the assay, it was determined that compound II exhibited IC50 values in the range of 4.23 nm to 5.93 nm.

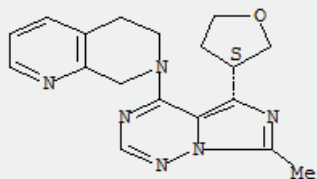
# CHAL FEATURED ARTICLE

## Chemical structure indexing

One of the substances shown below was retrieved in a substructure search and displayed in the HITSTR format. This patent application had 360 indexed substances.

RN 1636158-56-9 HCAPLUS  
CN 1,7-Naphthyridine, 5,6,7,8-tetrahydro-7-[7-methyl-5-[(3S)-tetrahydro-3-furanyl]imidazo[5,1-f][1,2,4]triazin-4-yl]- (CA INDEX NAME)

Absolute stereochemistry.



## Concept indexing

The following is an example of a portion of the detailed intellectual concept indexing which includes supplementary terms, indexing terms, and free text terms.

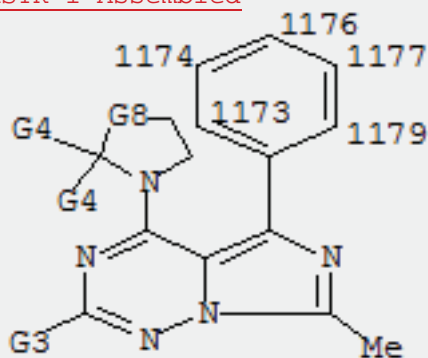
ST imidazotriazine prepn PDE10 inhibitor  
IT Homo sapiens  
Human  
Pharmaceutical excipients  
(preparation of imidazotriazine derivs. as PDE10 inhibitors)  
IT 1349749-10-5, PDE10  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(preparation of imidazotriazine derivs. as PDE10 inhibitors)  
IT 1636158-56-9P  
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of imidazotriazine derivs. as PDE10 inhibitors) ...

# CHAL FEATURED ARTICLE

## MARPAT®

MARPAT is a structure searchable database of Markush structures. The structure below was retrieved from a substructure search in MARPAT, and was displayed in the QHIT format.

### MSTR 1 Assembled



1173, 1174, 1176, 1177, 1179: opt. substd. by G15

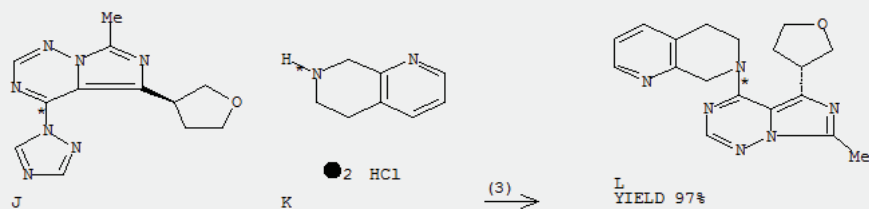
G8 = heteroarylene <containing up to 10 atoms,  
1 or more heteroatoms, 1 or more N, zero or more O,  
zero or more S (no other heteroatoms), 1 or more C,  
attached through 1 or more C> (opt. substd. by G27)

Patent location: claim 1  
Note: or pharmaceutically acceptable salts  
Note: additional derivatization also claimed

## CASREACT®

CASREACT is a reaction database which covers both single- and multi-step reactions, plus synthetic preparations. The following result from a reaction search was displayed in the FHIT format. 2503 reactions were indexed for this patent application.

RX(3) OF 2503 ...J + K ==> L



RX(3) RCT J 1636161-20-0, K 351038-62-5  
RGT H 121-44-8 Et3N  
PRO L 1636158-56-9  
SOL 75-09-2 CH2Cl2  
CON 3 days, room temperature

# CHAL FEATURED ARTICLE

## PatentPak™

A patent workflow solution that offers one-click access go to indexed substances in a patent. It is available in CAPlusSM/HCAplus on STN® and SciFinder®.

PATENTPAK  
A CAS SOLUTION

PAGE 53 / 165 ZOOM DOWNLOAD PDF

Key Substances in Patent

CAS RN 1636158-56-9

Analyst Markup Locations (2)  
page 53  
page 139

CAS RN 351038-62-5

• 2 HCl

Analyst Markup Locations (1)  
page 53

WO 2014/177977 PCT/IB2014/060945

-51-

Step 7. Synthesis of 7-{7-methyl-5-[(3S)-tetrahydrofuran-3-yl]imidazo[5,1-f][1,2,4]triazin-4-yl}-5,6,7,8-tetrahydro-1,7-naphthyridine (**3**).

A solution of **C17** (150 mg, 0.553 mmol), 5,6,7,8-tetrahydro-1,7-naphthyridine, dihydrochloride salt (126 mg, 0.608 mmol), and triethylamine (0.308 mL, 2.21 mmol) in dichloromethane (5 mL) was stirred at room temperature for 3 days. The reaction mixture was diluted with additional dichloromethane and washed sequentially with saturated aqueous sodium bicarbonate solution, water and saturated aqueous sodium chloride solution. The organic layer was dried over magnesium sulfate, filtered, and concentrated *in vacuo*. Silica gel chromatography (Gradient: 5% to 10% methanol in ethyl acetate) provided the product as a yellow solid. Yield: 181 mg, 0.538 mmol, 97%. LCMS *m/z* 337.3 [M+H]<sup>+</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 8.42-8.45 (m, 1H), 7.88 (s, 1H),

The CAS content collection provides access to chemically-related patent and non-patent literature which is enhanced with CAS value-added indexing. The scientists at CAS enhance document titles and abstracts as needed, add the structure and concept indexing according to the CAS indexing guidelines, and put this information in a searchable format for comprehensive search and display. The entire CAS content collection is available on STN.

For more information about STN (which provides access to the CAS databases as well as other scientific and technical databases) and Science IP® (the official research service of CAS), please visit the CAS website or contact the CAS Customer Center at 1-800-753-4227 (in North America).

# CHAL FEATURED ARTICLE

**Figure 1 (cont'd):** A CAPlus record with the three PatentPak options in the bibliography, HITPPAK, and HITSTR format

PI

PATENT NO. KIND DATE APPLICATION NO. DATE

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WO 2011123890 A1 20111013 WO 2011-AU392 20110406

...

CA 2795370 A1 20111013 CA 2011-2795370 20110406  
AU 2011238421 A1 20121025 AU 2011-238421 20110406  
IL 222176 A 20121129 IL 2011-222176 20110406  
CN 102933557 A 20130213 CN 2011-80027758 20110406  
EP 2556058 A1 20130213 EP 2011-764947 20110406

...

PPAK  
1339044-80-2P, Pg 206  
1339044-67-5P, Pg 44  
1339044-77-7P, Pg 206

IT

1339044-80-2P

The links in the PPAK field in the CAPlus record, as shown in Figure 1, takes you to the place in the Interactive PDF where the specific compound of interest was indexed by the CAS scientist, as shown in Figure 2.

**Figure 2:** The link to CAS RN 1339044-80-2 leads directly to the location in the Interactive PDF where this compound was indexed.

The screenshot displays the PatentPak interface. On the left, a sidebar titled 'Key Substances in Patent' lists three entries: CAS RN 1339047-52-7, CAS RN 1339044-80-2 (highlighted), and CAS RN 1339044-77-7. Each entry includes a chemical structure and a 'Patent Location' link. The main text area on the right shows patent claims, with claim 9 containing a chemical structure of a benzimidazole derivative. A red location marker is placed on the text '4-Methoxy-2-(5'-(4'''-methylpiperazin-1'''-yl)benzimidazol-2''-yl)pyridine' in claim 9, and a blue arrow points from the 'Highlighted Location Marker' label to this marker. A 'Marked Patent' label is also present on the right side of the interface.

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