Faggruppe for Organisk Kjemi (FOK)

Selective Synthesis in Chemical Biology

21. Organisk kjemiske høstmøte (OKH21)

21st National Autumn Meeting in Organic Chemistry

20.th of October 2017

Christiania Qvartalet Møtesenter, Oslo

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09.00-09.25	**Registration**	
09.30-09.40	**Opening remarks**	Trond V. Hansen
09.40-10.40	**Professor Petri Pihko** University of Jyväskylä, Jyväskylä, Finland. *Can we design organocatalysts?*	Chair: Trond V. Hansen
10.40-11.40	**Professor Stuart Conway** University of Oxford, Oxford, UK *The Development of Potent CREBBP Bromodomain Ligands*	Chair: Bengt Erik Haug
11.40-12.00	**Coffee and refreshments**	
12.00-13.00	**Professor Mercedes Amat** University of Barcelona, Barcelona, Spain *Chiral Tricyclic Lactams as Multipurpose Scaffolds for the Efficient Synthesis of Decahydroquinoline alkaloids*	Chair: Anne Fiksdahl
13.00-13.45	**Lunch**	
13.45-14.45	**Professor Soai** *Tokyo University of Science, Tokyo, Japan* *Asymmetric Autocatalysis and the Origin of Homochirality*	Chair: Mohamed Amedjkouh
14.45-15.00	**Coffee and refreshments**	
15.00-16.00	**Professor Karl-Heinz Altmann** ETH Zürich, Zürich, Switzerland. *Total Synthesis and Functional Exploration of Bioactive Natural Macrocycles*	Chair: Annette Bayer
16.00-16.05	**Concluding remarks**	Trond V. Hansen

Organizing Committee

The Board of the Norwegian Chemical Society – Section for organic chemistry (NKS-FOK):

Trond Vidar Hansen

Inger Reidun Aukrust

Annette Bayer

Anne Fiksdahl

Bengt Erik Haug

Associate committee member for OKH21

Mohamed Amedjkouh

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2016 - OKH20 *New Trends, Topics and methods in organic chemistry,* Christiania Qvartale Møtesenter, Oslo.

Abstracts

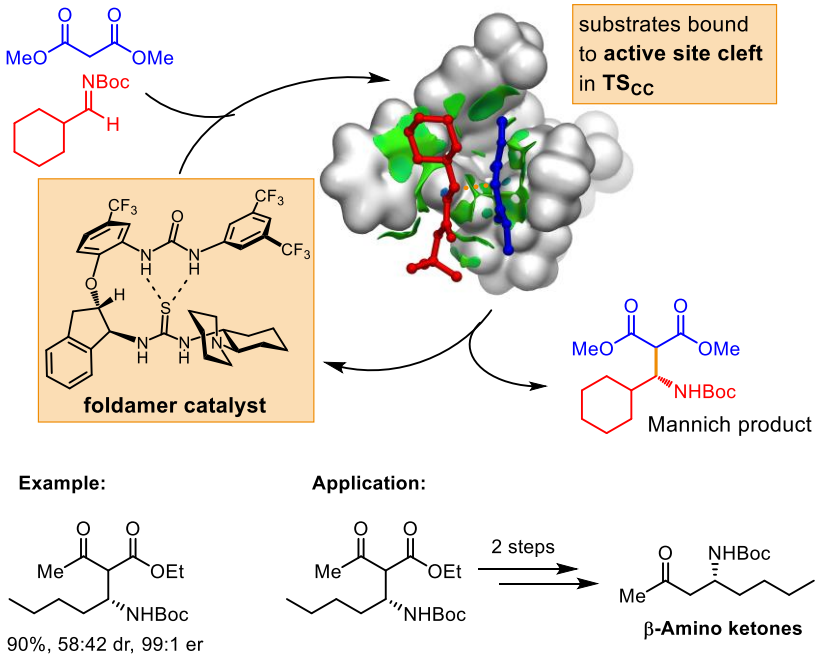
Can we design organocatalysts?

Petri M. Pihko

Department of Chemistry and NanoScience Center, University of Jyväskylä, Finland,
Petri.Pihko@jyu.fi

Keywords: organocatalysis, hydrogen bonding, noncovalent interactions, enantioselectivity, foldamers

Noncovalent interactions play very important roles in determining the enantioselectivities and rates of catalytic enantioselective reactions. In addition, the conformational preferences, or *folding* patterns in catalysts that can exist in different folds, may be important for selectivity and activity. In this talk, recent examples of enantioselective organocatalytic reaction and mechanistic insights into their design – or the prospects for their design – are discussed.[1,2]



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The Development of Potent CREBBP Bromodomain Ligands

Stuart J. Conway

Department of Chemistry, University of Oxford, Oxford, UK
stuart.conway@chem.ox.ac.uk

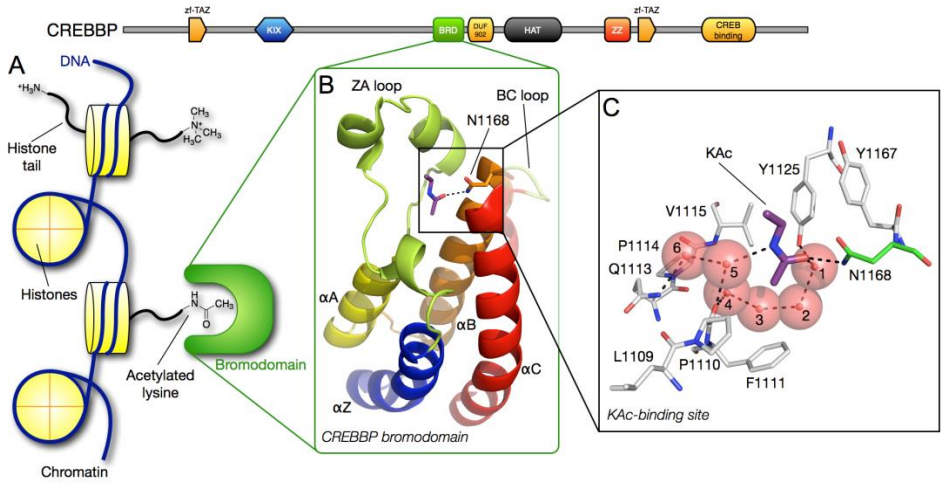

Figure 1. (A) Histone tails are subjected to multiple PTMs, including lysine acetylation. Lysine acetylation state is "read" by bromodomains, protein modules that exist as part of a more complex protein architecture. cAMP response element-binding protein- (CREB)-binding protein (CREBBP or CBP) is shown. (B) An X-ray crystal structure of the CREBBP bromodomain in complex with KAc (carbon = purple, PDB ID, 3P1C). (C) The KAc residue binds in a well-defined pocket and, in CREBBP, forms interactions with N1168 and Y1125.

Epigenetics, defined as "stably heritable phenotype resulting in changes in a chromosome without alterations in the DNA sequence", comprises regulatory mechanisms of chromatin state that control access to DNA, mediated by noncoding RNA, DNA methylation, nucleosome remodelling histone variants, and some histone post-translational modifications (PTMs). Histone PTMs are dynamic, with cellular machinery identified that can add these modifications and that can remove them. A third class of proteins, termed "readers", has been identified (Figure 1A), that binds to PTMs and thus stabilise large protein assemblies, which are often involved in transcriptional regulation. Bromodomains (Figure 2B), protein modules that act as readers of lysine acetylation state, have emerged as important therapeutic targets for a number indication, especially in oncology.[1,2] We have developed small molecule inhibitors of the bromodomain and extra terminal domain (BET) family of bromodomain-containing proteins,[3-5] and the CREB-binding protein (CREBBP) bromodomain.[6,7] Recent developments in the optimisation of these probes will be discussed, with a focus on the development of potent and selective CREBPP bromodomain ligands.

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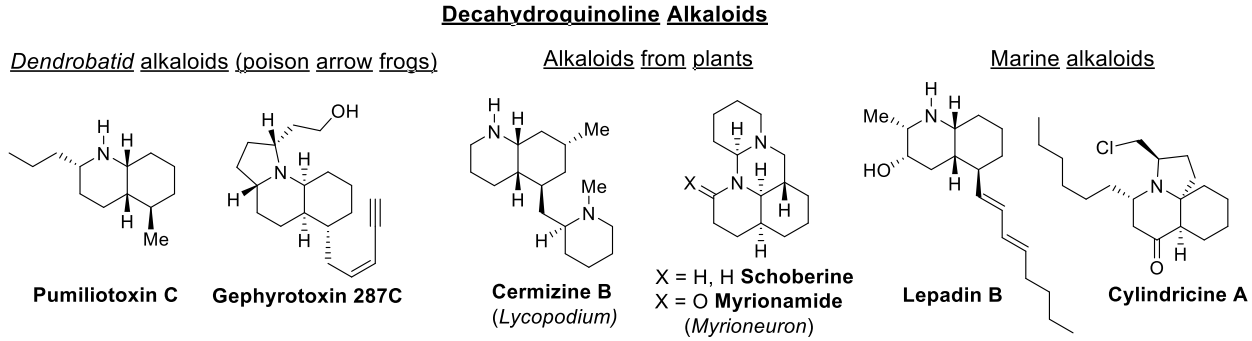
Chiral Tricyclic Lactams as Multipurpose Scaffolds for the Efficient Synthesis of Decahydroquinoline alkaloids

Mercedes Amat

Laboratory of Organic Chemistry, Faculty of Pharmacy and Institute of Biomedicine (IBUB), University of Barcelona, Av. Joan XXIII 27-31, 08028-Barcelona, Spain
amat@ub.edu

In the last years we have focused our attention on the development of new and efficient procedures for the enantioselective synthesis of nitrogen heterocycles with the final goal of applying them to the total synthesis of natural products and biologically active compounds. To this end, we originally explored a methodology based on the use of chiral, conformationally rigid and highly functionalized aminoalcohol-derived bicyclic lactams as enantiomeric scaffolds and carried out a systematic study on their scope and limitations for the enantioselective synthesis of nitrogen-derivatives.[1] As a result of this work, we have now in hand a flexible and versatile tool for the preparation of a broad range of chiral piperidines that allows the generation of new stereocenters with a high degree of stereoselectivity and a predictable absolute configuration. This methodology has enabled us to complete the enantioselective synthesis of a variety of piperidine-containing alkaloids, indole and oxindole alkaloids, and macrolactams.
As an extension of this work, more recently, we have also reported the stereoselective generation of aminoalcohol-derived tricyclic lactams as chiral scaffolds for the preparation of *cis*-decahydroquinolines (DHQs) and octahydroindoles. The application of this methodology to the enantioselective synthesis of structurally diverse DHQ alkaloids will be discussed.[2]



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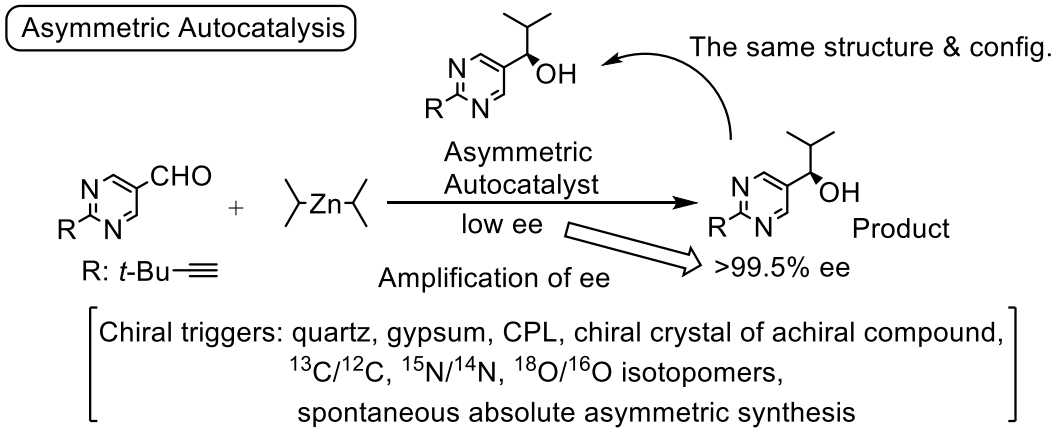
Asymmetric Autocatalysis and the Origin of Homochirality

Kenso Soai

Department of Applied Chemistry, Tokyo University of Science,
Kagurazaka, Shinjuku-ku, Tokyo, Japan
soai@rs.kagu.tus.ac.jp

Asymmetric autocatalysis is a reaction in which chiral product acts as a chiral catalyst for its own formation. The process is a catalytic self-replication of chiral molecule, and has advantages over usual asymmetric catalysis: (1) because the product becomes catalyst, the amount of catalyst increases and no decrease in the catalytic activity, (2) because the structure of the asymmetric autocatalyst and the product is the same, no need to separate the product from catalyst.

We found asymmetric autocatalysis of enantiomeric excess of pyrimidyl alkanol in the enantioselective addition of diisopropylzinc to pyrimidine-5-carbaldehyde.[1] Significant amplification of ee is observed in the asymmetric autocatalysis. Starting from pyrimidyl alkanol with only ca. 0.00005% ee as asymmetric autocatalyst, pyrimidyl alkanol with >99.5% ee was formed in consecutive asymmetric autocatalysis.[2]



We have been studying the origin of homochirality by using asymmetric autocatalysis. Chiral inorganic crystal, chiral isotopomers,[3] chiral crystals composed of achiral organic compounds, circularly polarized light (CPL), enantiotopic face of achiral mineral, i.e., gypsum,[4] act as chiral triggers in asymmetric autocatalysis. Pyrimidyl alkanol of the corresponding absolute configuration with those of chiral triggers was obtained.

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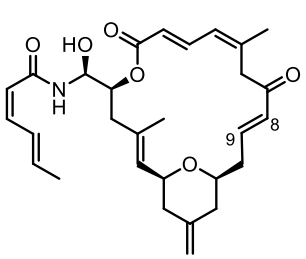
Total Synthesis and Functional Exploration of Bioactive Natural Macrocycles

Karl-Heinz Altmann

ETH Zürich,
Zürich, Switzerland
karl-heinz.altmann@pharma.ethz.ch

Macrocyclic secondary metabolites are a diverse group of bioactive natural products and many of these compounds have been, and continue to be important leads for drug discovery and development. This contribution will discuss selected aspects of the synthetic chemistry, medicinal chemistry and chemical biology of two macrocyclic natural products, the marine macrolide zampanolide (**1**) and the mycobacterial toxins mycolactones A/B (**2**). (-)-Zampanolide (**2**) is a microtubule-stabilizing agent (MSA) and it is a potent inhibitor of human cancer cell proliferation *in vitro*; mycolactones A/B (**2**) are produced by the human pathogen *M. ulcerans* and are the causative pathogenic agents for Buruli ulcer, but their molecular target(s) have not been elucidated.



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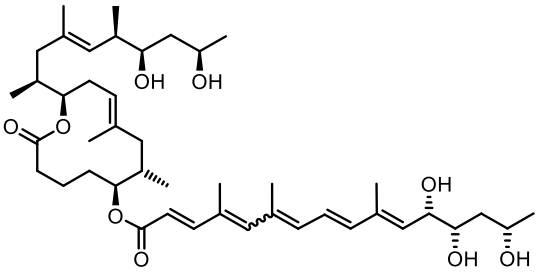

2

We have developed efficient modular total syntheses for both of the above natural products. For **1**, macrocyclic ring-closure was based on an intramolecular Horner-Wittig-Emmons reaction between C8 and C9, which proceeded in high yield and with excellent selectivity. The same overall approach was employed in the synthesis of analogs of **1** for SAR studies. A high resolution crystal structure of the complex of **1** with tubulin has provided fundamentally new insights into the molecular mechanism of MSA-induced tubulin assembly. **2** was prepared *via* ring-closing olefin metathesis (RCM) as one of the key steps, followed by elaboration of the upper and lower side chain, respectively. Conjugates of **2** have been prepared that have allowed the exploration of the mechanistic pathways responsible for mycolactone toxicity.

List of participants

Altmann, Karl-Heinz
ETH Zürich
karl-heinz.altmann@pharma.ethz.ch

Amat Tuson, Maria Mercedes
University of Barcelona
amat@ub.edu

Amedjkouh, Mohamed
Universitetet i Oslo
mamou@kjemi.uio.no

Antonsen, Simen
NMBU
simen.antonsen@nmbu.no

Aukrust, Inger Reidun
Synthetica AS
ira@synthetica.no

Austli, Guro Buaas
NTNU
guroba@stud.ntnu.no

Balcells, David
Universitetet i Oslo
david.balcells@kjemi.uio.no

Bayer, **Annette**
Universitetet i Tromsø – Norges Arktiske Universitet
annette.bayer@uit.no

Bero, Rawan
Universitetet i Oslo
rawanb@student.farmasi.uio.no

Bolsønes, Marianne
Forsvarets Forskningsinstitutt
marianne.bolsones@ffi.no

Boomgarden, Marc
Universitetet i Tromsø – Norges Arktiske Universitet
marc.boomgarden@uit.no

Brondz, Anton
Synthetica AS
ab@synthetica.no

Conway, Stuart
University of Oxford
stuart.conway@chem.ox.ac.uk

Due-Hansen, Maria-Elisabeth
Forsvarets Forskningsinstitutt
maria-elisabeth.due-hansen@ffi.no

Espeseth, Ørjan
Matriks
orjan.espeseth@matriks.no

Eilertsen, Ingar
Teknolab AS
ie@teknolab.no

Fiksdahl, Anne
NTNU
anne.fiksdahl@chem.ntnu.no

Gammelsæter Johnson, Lars Inge
Universitetet i Oslo
l.i.g.johnsen@farmasi.uio.no

Garnås, Fredrik
NMBU
Fredrik.garnås@nmbu.no

Gjessing, Gard
NMBU
gard.gjessing@nmbu.no

Glessi, Christiano
Universitetet i Oslo
cristiano.glessi@smn.uio.no

Grøssereid, Ingrid
NTNU
ingridgrossereid@gmail.com

Hansen, Trond Vidar
Universitetet i Oslo
t.v.hansen@farmasi.uio.no

Halvorsen, Harald
ThermoFisher Scientific
harald.halvorsen@thermofisher.com

Halsvik, Beate
Universitetet i Bergen
beate.halsvik@uib.no

Haug, Bent Erik
Universitetet i Bergen
bengt-erik.haug@farm.uib.no

Hoff, Bård Helge
NTNU
bard.helge.hoff@chem.ntnu.no

Holmsen, Marte Sofie
Universitetet i Oslo
m.s.holmsen@kjemi.uio.no

Hofsløkken, Rune
Nerliens Meszansky AS
rune.hofslokken@nmas.no

Hoster, Norman Emanuel
NTNU
Norman.Hoster@uni-duesseldorf.de

Hustad, Jan Arild
ChemSupport AS
jah@chemsupport.no

Ihle Aarhus, Thomas
NTNU
thomas.i.aarhus@ntnu.no

Jacobsen, Øyvind
Oslo Universitets Sykehus
oyvind.jacobsen@farmasi.uio.no

Johannessen, Tonje
NMBU
Tonje.johannessen@nmbu.no

Johansson, Silje
Universitetet i Oslo
silje.johansson@farmasi.uio.no

Johansson Solum, Eirik
Nord universitet
eirik.j.solum@nord.no

Jørgensen, Kåre
Universitetet i Stavanger
kare.b.jorgensen@uis.no

Kampesæther, Arne
Nerliens Meszansky AS
arne.kampesaeter@nmas.no

Kania, Jindrich
ThermoFisher Scientific
jindrich.kania@thermofisher.com

Kildahl-Andersen, Geir
Universitetet i Oslo
geir.kildahl-andersen@farmasi.uio.no

Kjus, Nini Unn Hofsløkken
ThermoFisher Scientific
nini.kjus@thermofisher.com

Kristensen, Tor Erik
Forsvarets forskningsinstitutt
tor-erik.kristensen@ffi.no

Kristianslund, Renate
Universitetet i Oslo
renate.kristianslund@farmasi.uio.no

Levchenko, Vladimir
Universitetet i Oslo
volodymyr.levchenko@smn.uio.no

Madland, Marte Størdal
Thermo Fisher Scientific
marte.stordal@thermofisher.com

Mortansson Jelstrup Nolsøe, Jens
NMBU
jens.mj.nolsoe@nmbu.no

Neerbye Berntsen, Linn
Universitetet i Oslo
l.n.berntsen@kjemi.uio.no

Nesman, Jannicke Irene
Universitetet i Oslo
j.i.nesman@farmasi.uio.no

Olavesen, Ida Karoline
NMBU
ida.karoline.olavesen@nmbu.no

Pavlovic, Bojana
Universitetet i Oslo
bojanapavlovic83@gmail.com

Peeters, Sara
Universitetet i Oslo
sara.peeters@kjemi.uio.no

Pihko, Petri
University of Jyväskylä
petri.pihko@jyu.fi

Primdahl, Karoline
Universitetet i Oslo
k.g.primdahl@farmasi.uio.no

Ringheim-Bakka, Thomas Aleksander
BIOZEP AS
ta.bakka@biozep.com

Rongved, Pål
Universitetet i Oslo
pal.rongved@farmasi.uio.no

Rotunno, Giuseppe
Universitetet i Oslo

Schnaars, Christian
Universitetet i Oslo
Christian.schnaars@farmasi.uio.no

Soai, Kenso
Tokyo University of Science
soai@rs.kagu.tus.ac.jp

Solbakken, Erlend
Universitetet i Oslo
erlensau@kjemi.uio.no

Solli, Anders
NMBU
anders.solli@nmbu.no

Skotte, Christian
Chemical Abstract Services - ACS
cskotte@acs-i.org

Stenstrøm, Yngve
NMBU
yngve.stenstrom@nmbu.no

Suarez, Lluis Artus
Universitetet i Oslo
l.a.suarez@kjemi.uio.no

Suissa, **Michal Rachel**
Høgskolen i Oslo og Akershus
rachel.suissa@hioa.no

Tannæs, Bjørg Siw Møller
Høgskolen i Oslo og Akershus
bjorgm.tannas@hioa.no

Thoresen, Erik Mydske
Universitetet i Oslo
e.m.thoresen@kjemi.uio.no

Tilset, Mats
Universitetet i Oslo
mats.tilset@kjemi.uio.no

Torp Lien, Vegard
Universitetet i Oslo
v.t.lien@farmasi.uio.no

Trones, Roger
Teknolab AS
rt@teknolab.no

Tungen, Jørn Eivind
Universitetet i Oslo
j.e.tungen@farmasi.uio.no

Vik, Anders
Universitetet i Oslo
anders.vik@farmasi.uio.no

Wåhlander, Jakob
Universitetet i Oslo
j.k.k.wahlander@kjemi.uio.no

Åstrand, Alexander
Universitetet i Oslo
o.a.astrand@farmasi.uio.no

Norsk Kjemisk Selskap - Faggruppe for Organisk Kjemi

Innkalling til generalforsamling 2017

Sted: Skeikampen Høifjellshotell **Tid: Lørdag 13. januar 2018**

Dagsorden:

1. Konstituering
2. Valg av møteleder og referent
3. Styrets årsberetning 2017
4. Regnskap 2017
5. Innkomne saker
6. Arrangør neste Organisk kjemisk vintermøte
7. Valg av styre, revisor og valgkomité

Saker som ønskes behandlet under punkt 5 må være styret i hende senest 2 uker før generalforsamlingen.

Oslo, 13.10.2017
Styret

Organisk kjemisk Vintermøte på Skeikampen Høifjellshotell

Faggruppen for organisk kjemi, Norsk Kjemisk Selskap, inviterer til det 33. Organisk kjemiske vintermøte - OKV 2018 - fra 11. til 14. januar 2018.

Inviterte foredragsholdere:

Professor Andreas Kirschning, Leibniz University of Hannover, Germany
Professor Valentine P. Ananikov, Zelinsky Institute of Organic Chemistry, Russia
Professor Harry Anderson, University of Oxford, UK
Professor Tanja Gaich, University Konstanz, Germany

Praktiske opplysninger:
Program, informasjon om priser, transport, reisestipend og påmelding samt innsending av sammendrag av foredrag og plakater **er tilgjengelig** på møtets hjemmesider, se http://www.kjemi.no/organisk/okv33/.
Påmeldingsfrist er 1. Desember 2017. Ytterligere informasjon kommer på email.

Arrangør: Professor Bård Helge Hoff, NTNU, bard.helge.hoff@chem.ntnu.no

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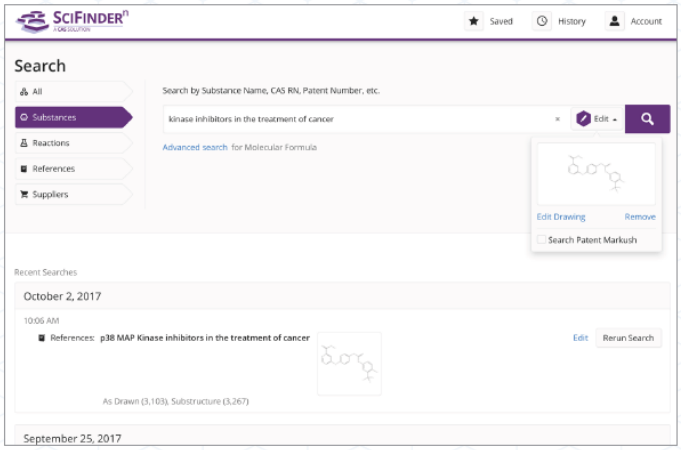

Get actionable results faster with a streamlined new interface

- Add important chemical context to your keyword search with chemical structures
- Search all reactions, substances and references at once
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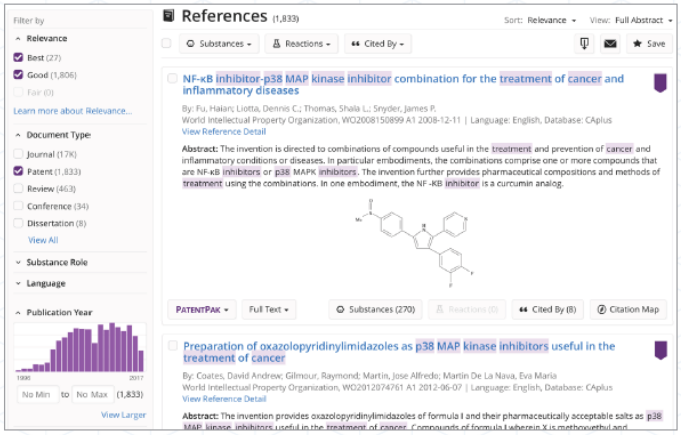

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- Powerful, comprehensive filters for rapid focus
- Results are displayed in a format designed for quick comprehension
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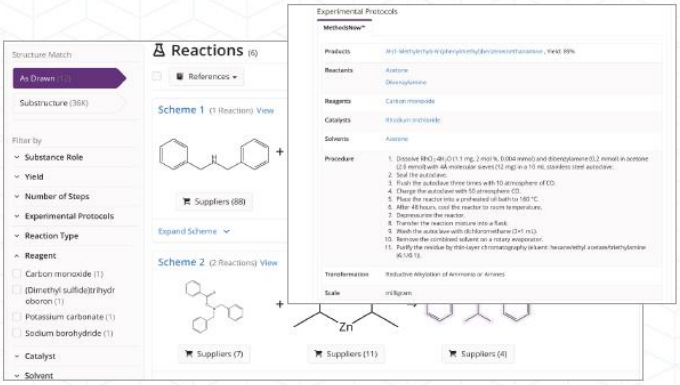
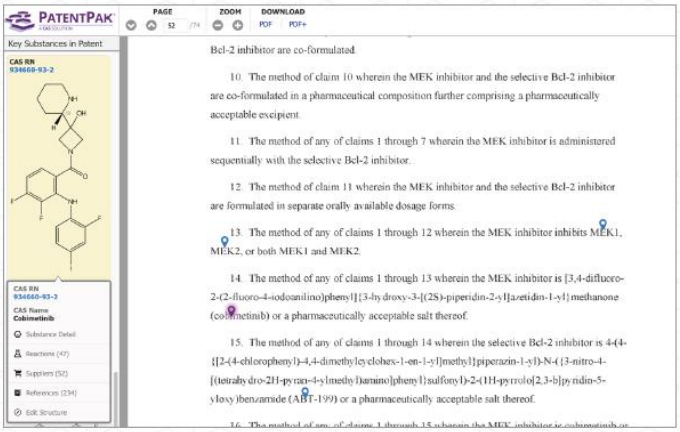


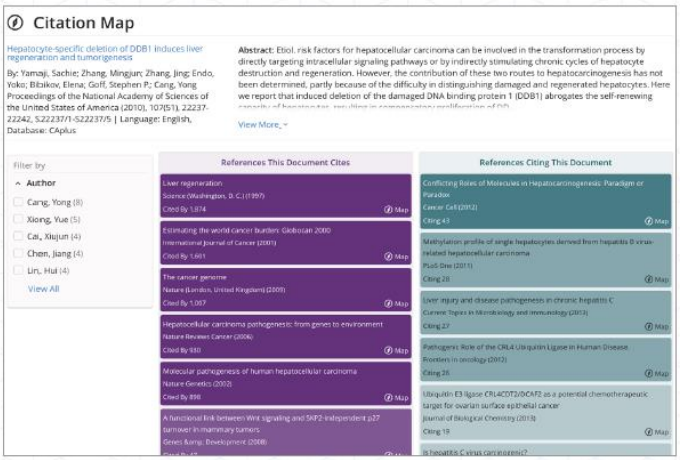
Step-by-step synthetic procedures, extracted and summarized

- Save time with procedures summarized by CAS scientists
- Take step-by-step instructions directly to the lab
- Key chemical components of reactions are identified and linked to additional information



Go straight to the chemistry in patents

- Patent chemistry is fully annotated with structures, nomenclature and more
- CAS expert scientists have identified chemistry locations, so SciFinder^n reveals what patents usually obscure



Citation Mapping shows you other important literature

- Interactive map quickly identifies important research
- Trace the "family tree" of important papers
- Locate potential collaborators, funding sources or competition
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