Competenze bibliografiche in Chimica

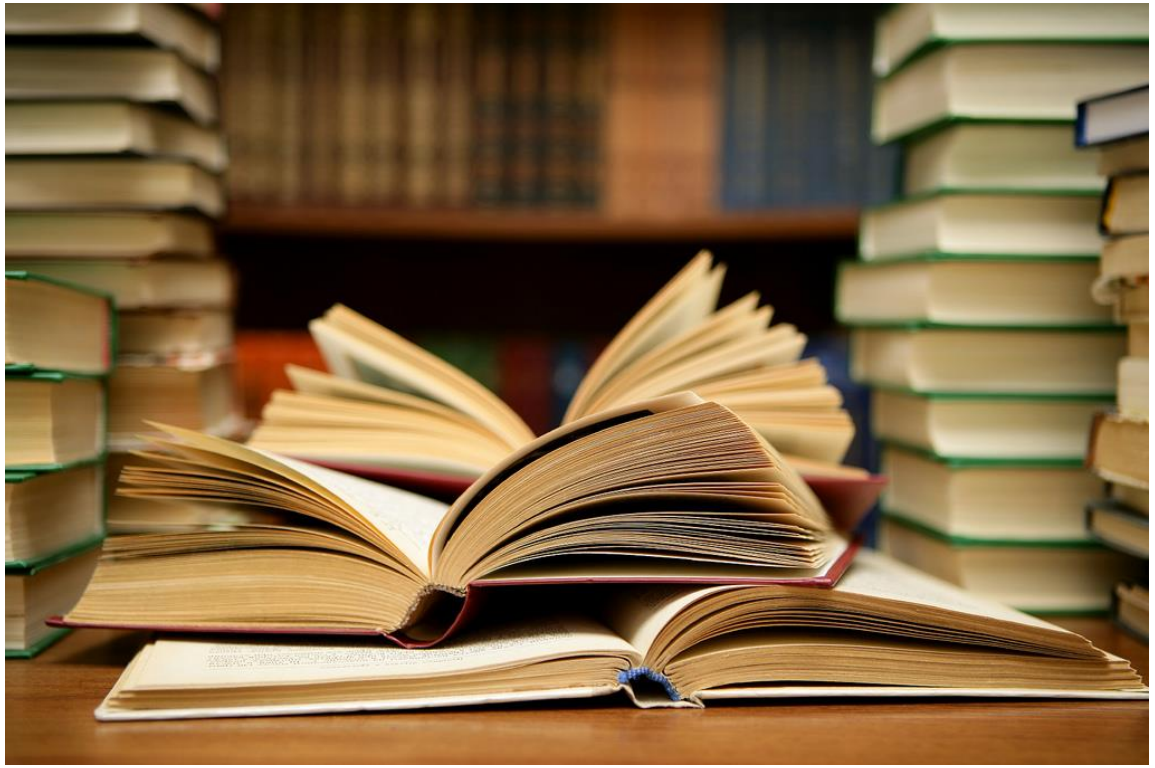
Debora Zanolla

PhD STUDENT (XXXI Ciclo)

debora.zanolla@gmail.com

Che cosa si può trovare in letteratura?

- Libri
- Articoli
- Comunicazioni
- Review
- Brevetti (Patent)



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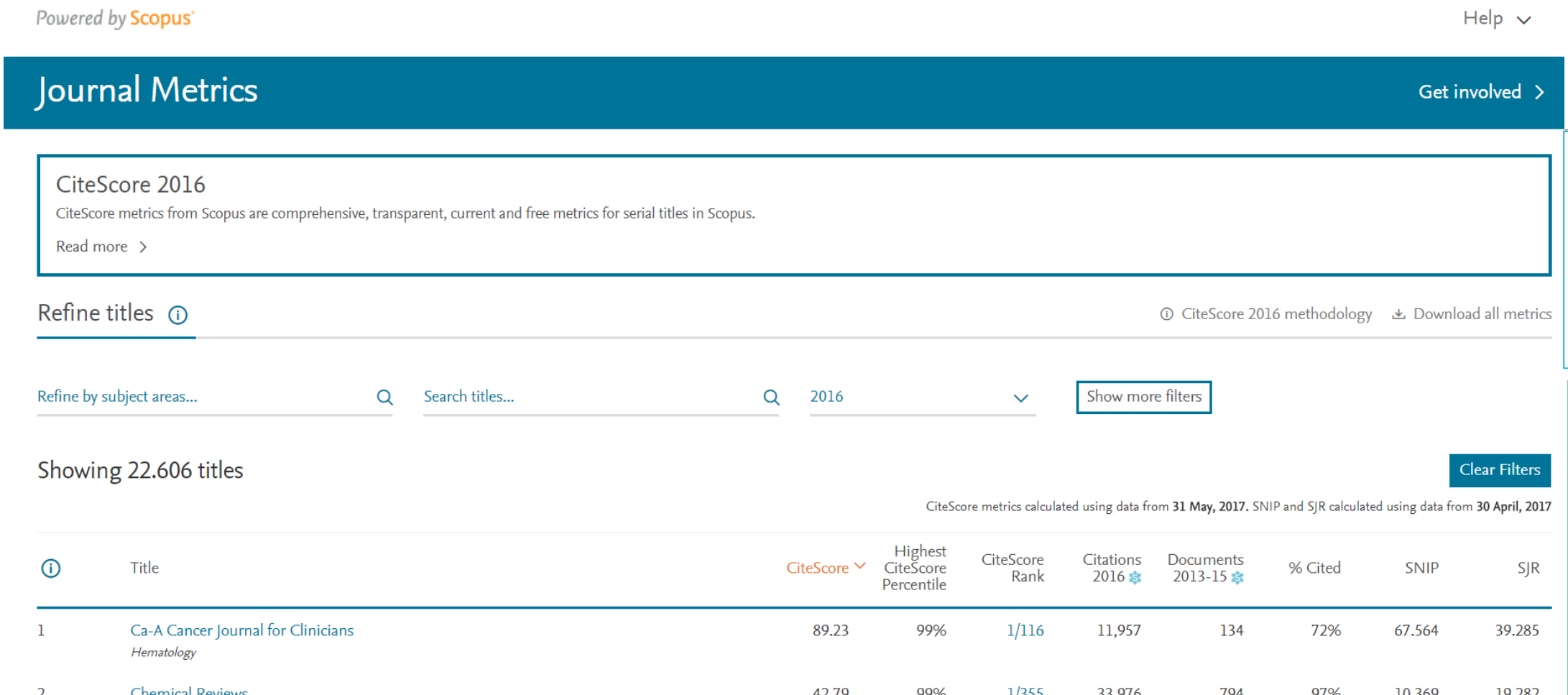

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Article

- Title
- Authors and affiliations
- Abstract - Keywords
- Introduction
- Materials & Methods
- Results
- Discussion
- Conclusions
- Acknoledgements
- References

European Journal of Pharmaceutics and Biopharmaceutics 127 (2018) 19–28

Contents lists available at ScienceDirect

European Journal of Pharmaceutics and Biopharmaceutics

journal homepage: www.elsevier.com/locate/ejpb

Rivista, fascicolo, pagine, anno…

Research paper

A new soluble and bioactive polymorph of praziquantel

Debora Zanolla[a], Beatrice Perissutti[a,*], Nadia Passerini[b], Michele R. Chierotti[c], Dritan Hasa[d], Dario Voinovich[a], Lara Gigli[e], Nicola Demitri[e], Silvano Geremia[a], Jennifer Keiser[f], Paolo Cerreia Vioglio[g], Beatrice Albertini[b]

[a] Department of Chemical and Pharmaceutical Sciences, University of Trieste, P.le Europa 1/via L. Giorgieri 1, 34127 Trieste, Italy
[b] Department of Pharmacy and BioTechnology, University of Bologna, Via S. Donato 19/2, 40127 Bologna, Italy
[c] Department of Chemistry and NIS Centre, University of Torino, V. Giuria 7, 10125 Torino, Italy
[d] Leicester School of Pharmacy, De Montfort University, The Gateway, LE1 9BH Leicester, United Kingdom
[e] Elettra – Sincrotrone Trieste, S.S. 14 Km 163.5 in Area Science Park, 34149 Basovizza, Trieste, Italy
[f] Helminth Drug Development Unit, Department of Medical Parasitology and Infection Biology, Swiss Tropical and Public Health Institute, Socinstr. 57, CH-4051 Basel, Switzerland
[g] Aix-Marseille Université, CNRS, ICR (UMR 7273), 13397 Marseille cedex 20, France

ARTICLE INFO

Keywords:
Praziquantel
Mechanochemistry
Solid-state reactions
Polymorphism
Solubility
Bioactivity
Crystal structure solution
DFT-D calculations
Neglected tropical diseases

ABSTRACT

Praziquantel is the only available drug to treat Schistosomiasis. However, its utilization is limited by many drawbacks, including the high therapeutic dose needed, resulting in large tablets and capsules difficult to be swallowed, especially from pediatric patients. In this study, an alternative option to overcome these disadvantages is proposed: to switch to a novel crystalline polymorph of racemic compound praziquantel. The preparation of the crystalline polymorph was realized via a neat grinding process in a vibrational mill. The new phase (Form B) was chemically identical to the starting material (as proved by HPLC, ^{1}H NMR, and polarimetry) but showed different physical properties (as evaluated by SEM, differential scanning calorimetry, thermogravimetry, ATR-FTIR spectroscopy, X-ray powder diffraction, and solid-state NMR). Furthermore, the crystal structure of the new phase was solved from the powder synchrotron X-ray diffraction pattern, resulting in monoclinic *C*2/*c* cell and validated by DFT-D calculation. Moreover the simulated solid-state NMR ^{13}C chemical shifts were in excellent agreement with the experimental data. The conversion of original praziquantel into Form B showed to affect positively the water solubility and the intrinsic dissolution rate of praziquantel. Both the in vitro and in vivo activity against *Schistosoma mansoni* were maintained. Our findings suggest that the new phase that proved to be physically stable for at least one year, is a promising product for designing a new praziquantel formulation.

1. Introduction

Praziquantel (PZQ) is an antihelmintic drug largely used for the treatment of Schistosomiasis. It is estimated that at least 230 million people worldwide are infected by the genus Schistosoma [1], mainly with *Schistosoma haematobium*, *S. japonicum* and *S. mansoni*. Praziquantel is included in the WHO Model List of Essential Drug for the schistosomiasis is 20 mg/kg three times a day which has to be repeated after 4 to –6 weeks. For at-risk populations a 40 mg/kg single dose is used as preventive chemotherapy. Since children are the main target of treatment, research is needed to enhance the solubility and the bioavailability of PZQ, in order to reduce the high therapeutic doses and therefore the dimension of tablets, which are difficult to swallow particularly for pediatric patients [5]. Several studies aimed to enhance

2. Materials and methods

2.1. Materials

Praziquantel (PZQ) Ph. Eur. grade ((11bRS)-2-(Cyclohexylcarbonyl)-1,2,3,6,7,11b-hexahydro-4-H-pyrazino[2,1-a]isoquinolin-4-one) was kindly donated by Fatro S.p.A. (Bologna, Italy). PZQ impurity A (2-Benzoyl-1,2,3,6,7,11b-hexahydro-4-H-pyrazino[2,1-a]isoquinolin-4-one) and impurity B (2-Cyclohexanecarbonyl-2,3,6,7-tetrahydro-pyrazino[2,1-a]isoquinolin-4-one) were Ph. Eur. grade and purchased from Endotherm Gmbh (Saarbruecken, Germany). HiPersolv Chromanorm Methanol (Ph. Eur. for HPLC Gradient Grade) and Ethanol (Ph. Eur.) were purchased from VWR Chemicals BHD PROLABO®.

2.1.1. Preparation of Form B

Praziquantel was milled on its own, by neat grinding, in a vibrational mill-Retsch MM400 (Retsch GmbH) which was equipped by 2 screw-type zirconium oxide jars, each with a capacity of 35 ml. A ceramic material like zirconium oxide was selected due to its high

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Article

- Title
- Authors and affiliations
- Abstract - Keywords
- Introduction
- Results and discussion
- Conclusion
- Experimental

Tetrahedron 74 (2018) 2143–2150

Contents lists available at ScienceDirect

Tetrahedron

journal homepage: www.elsevier.com/locate/tet

Syntheses of cyclopentyl nucleoside (−)-neplanocin A throu tetrazole-fragmentation from cyanophosphates

Hiroki Yoneyama, Kenji Uemura, Yoshihide Usami, Shinya Harusawa*

Osaka University of Pharmaceutical Sciences, 4-20-1 Nasahara, Osaka, 569-1094, Japan

ARTICLE INFO

Article history:
Received 20 February 2018
Received in revised form
7 March 2018
Accepted 9 March 2018
Available online 10 March 2018

Keywords:
Neplanocin A
Carbocyclic nucleoside
Cyanophosphate
Neutral condition
[1,5]-C–H insertion
Alkylidene carbene

ABSTRACT

We recently reported a novel synthetic method for five-membered ketones involving cyanophosphates (CPs) under neutral condit generated through tetrazole-fragmentation undergo [1,5]-C–H in pounds. The present paper describes the use of the tetrazole-fragm practical syntheses of (−)-neplanocin A and a protected tetrol, synthetic precursor of both (−)-neplanocin A and its analogues. F dihydropyran derivative was observed during the synthetic study

(−)-Neplanocin A (NPA: **1**) is a naturally occurring carbocyclic nucleoside that was first isolated from the culture filtrate of the soil fungus *Ampullariella regularis* in 1981.[1] NPA and other natural

Diels-Alder adducts,[12] intramo zirconocene-mediated ring cons Baylis-Hillman reaction.[15]

tetrol **2α**, formation of an unusual dihydropyran derivative **17** was newly observed.[23]

1. Synthesis of (−)-neplanocin A from CP 16

Ketone **3**, which was prepared via triphenylmethyl (Tr) ether **15**[25] from D-ribose in five steps (71% overall yield),[26] was subjected to the CP method, as illustrated in Scheme 3. Reaction of ketone **3** with diethyl phosphorocyanidate (DEPC, 3.0 equiv.)[21] in the presence of LiCN (3.0 equiv.) easily afforded CP **16** in 95% yield.[27] Reaction of CP **16** with $TMSN_3$ (3.0 equiv.) in the presence of Bu_2SnO (0.3 equiv.) in refluxing toluene for 24 h afforded an inseparable mixture of epimeric cyclopentenes **5αβ**,[22] which was the result of the C–H insertion reaction of alkylidene-carbene **4a**, along with unexpected compound **17**. The ratio of **5αβ** to **17** was 3:1

2. Synthesis of (−)-neplanocin A f

We next investigated the synth adenine-containing ketone **6**, propylidene-adenosine (**18**) using M Matsuda used the reductive tetrahyd reported by Maki.[30] Treatment of hydride (DIBAL) in THF afforded yield.[31] Meanwhile, we found that ether (CPME)-toluene (1:1, v/v) s cleavage reaction of **18** led to impro much easier extraction. After sele primary hydroxyl group of **19** with secondary alcohol **20** with *o*-iodoxy

3. Experimental

3.1. General information

All reactions were carried out under an inert argon atmosphere. Anhydrous solvents (THF, toluene, CH_2Cl_2, DMF, CPME and MeCN) were purchased from Wako Chemical Company. During organic workup, solvent extracts were dried over Na_2SO_4 and subsequently removed in a rotary evaporator under reduced pressure. Fuji Silysia FL-60D silica gel was used for flash column chromatography. **8α** and **8β** were chromatographed over spherical silica gel (Fuji Silysia PSQ 100 B silica gel). TLC was performed using precoated plates (Wako silica gel 70 F254). ^1H NMR spectra were recorded on a Varian Mercury-300 or an Agilent 400-MR-DD2 spectrometer in $CDCl_3$ spectrometer (Jeol Ltd., Tokyo, Japan) operating in positive-ion mode, with 3-nitrobenzyl alcohol (NBA)–NaCl or triethanolamine (TEOA)–NaCl as matrices.[33]

3.2. Synthesis of (−)-neplanocin A from CP16

3.2.1. (2S,3S)-[4-(tert-Butyldimethylsilyloxymethyl)-2,3-isopropylidenedioxy-1-cyanobutyl diethyl phosphate (16)

DEPC (831 mg, 5.1 mmol) and LiCN (168 mg, 5.1 mmol) were added to a solution of ketone **3** (944 mg, 1.7 mmol) in THF (20 mL) at rt. After it was stirred for 30 min, the reaction mixture was treated with water (60 mL), and then extracted with EtOAc-hexane (1:1, 100 mL). The organic layer was washed with brine, dried over Na_2SO_4, filtered, and concentrated. Purification via silica gel column

chromatography (EtOAc-hexane, 1:4) afforded CP **16** (1165 mg, 95%, oil).

^1H NMR (300 MHz, $CDCl_3$): δ 0.09 (s, 3H), 0.10 (s, 1.5H), 0.11 (s, 1.5H), 0.91 (s, 4.5H), 0.91 (s, 4.5H), 1.22–1.33 (m, 10.5H), 1.43 (s, 1.5H), 3.60 (d, 0.5H, J = 8.4 Hz), 3.61 (d, 0.5H, J = 10.2 Hz), 3.76 (d, 0.5H, J = 8.4 Hz), 3.89–4.27 (m, 6.5H), 4.40–4.48 (m, 1H), 4.59 (d, 0.5H, J = 6.3 Hz), 4.71 (dd, 0.5 Hz, J = 6.3, 4.5 Hz), 7.24–7.34 (m, 9H), 7.45–7.49 (m, 6H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ −5.2, −5.0, 15.9, 16.0, 18.4, 24.9, 25.1, 25.9, 26.4, 26.8, 61.4, 61.5, 63.1, 63.9, 64.4, 64.5, 64.6, 64.7, 64.8, 64.9, 75.5, 75.6, 75.9, 76.0, 79.1, 79.3, 87.5, 87.7, 109.2, 109.4, 115.7, 115.8, 116.0, 127.3, 127.8, 127.9, 128.7, 128.8, 142.8, 142.9; HRMS (FAB + NaCl): m/z $[M+Na]^+$ calcd for $C_{38}H_{52}NO_8PSiNa$: 732.3098; found: 732.3099.

3.2.2. (4R,5S)-4,5-O,O-Isopropylidene-3-(trityloxymethyl)-2-cyclopenten-1-ol (2αβ); (3aS,7aR)-2,2-dimethyl-7-(trityloxymethyl)-6-tert-butyldimethylsilyl-3a,7a-dihydro-4H-[1,3]dioxolo[4,5-c]pyran (17)

$TMSN_3$ (0.20 mL, 1.50 mmol) and Bu_2SnO (37 mg, 0.15 mmol) were added to a solution of CP **16** (355 mg, 0.50 mmol) in toluene. After it was refluxed for 24 h, the reaction mixture was concentrated to give a residue, which was purified using silica gel column chromatography to give an inseparable 3:1 mixture of **5αβ** (**5α**/**5β** = 1/3) and **17** (210 mg). To a solution of the mixture in THF (5 mL), 1 M solution of TBAF in THF (1.2 mL, 1.20 mmol) was added. After 1 h, saturated aqueous NH_4Cl was added to the reaction mixture to quench it. After the mixture was extracted with EtOAc (30 mL), the organic layer was washed with H_2O and then brine, dried over Na_2SO_4, filtrated, and concentrated to give a residue, which was purified using silica gel column chromatography (EtOAc–hexane, 1:4) to give **2αβ** (139 mg, 65%, yellow amorphous) and **17** (54 mg, 20%, oil). In addition, **2β** could be partially resolved by use of the above solvent system.

2β: ^1H NMR (300 MHz, $CDCl_3$): δ 1.30 (s, 3H), 1.33 (s, 3H), 2.06 (br, 1H), 3.70 (d, 1H, J = 15.0 Hz), 3.89 (d, 1H, J = 15.0 Hz), 4.51 (d, 1H, J = 5.7 Hz), 4.78 (br, 1H), 5.08 (d, 1H, J = 5.7 Hz), 6.00 (br, 1H), 7.20–7.32 (m, 9H), 7.45–7.48 (m, 6H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 26.1, 27.4, 61.3, 76.6, 79.9, 83.7, 86.4, 111.8, 127.0, 127.8, 128.5, 143.8, 147.4; HRMS (EI): m/z $[M^+]$ calcd for $C_{28}H_{28}O_4$: 428.1988; found: 428.1990.

17: ^1H NMR (400 MHz, $CDCl_3$): δ −0.44 (s, 3H), −0.16 (S, 3H), 0.67 (s, 9H), 1.48 (s, 3H), 1.55 (s, 3H), 3.20 (dd, 1H, J = 10.0, 10.0 Hz), 3.52 (dd, 1H, J = 5.7 Hz), 6.44–6.46 (m, 1H), 7.23–7.36 (m, 9H), 7.40–7.47 (m, 6H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 26.3, 27.5, 62.5, 77.7, 78.1, 87.4, 115.4, 127.4, 128.0, 128.2, 128.4, 143.3, 174.6, 201.9; HRMS (EI+): m/z $[M]^+$ calcd for $C_{28}H_{26}O_4$: 426.1831; found: 426.1828.

3.2.5. (1S,4R,5S)-4,5-O,O-Isopropylidene-3-(trityloxymethyl)-2-cyclopenten-1-ol (2α)

A solution of **22** (81 mg, 0.19 mmol) in THF (2 mL) was added dropwise to a suspension of LAH (36 mg, 0.96 mmol) in THF (2 mL) at 0 °C. After the reaction was stirred at rt for 2 h, H_2O (1 mL) was added to quench it. After the mixture was stirred at rt for 1 h, $MgSO_4$ was added, and the resulting mixture was filtered through Celite and concentrated to give a residue, which was purified using silica gel column chromatography (EtOAc–hexane 1:3) to give **2α** (79 mg, 98%, white solid).[16]

2α: ^1H NMR (300 MHz, $CDCl_3$): δ 1.36 (s, 3H), 1.37 (s, 3H), 2.74 (d, 1H, J = 10.2 Hz), 3.65 (dt, 1H, J = 14.4, 1.8 Hz), 3.88 (d, 1H, J = 14.4 Hz), 4.59 (br, 1H), 4.75 (t, 1H, J = 5.4 Hz), 4.88 (d, 1H, J = 5.4 Hz), 6.00 (br, 1H), 7.20–7.32 (m, 9H), 7.44–7.48 (m, 6H).

3.2.6. Reaction of ketone 3 with TMSC(Li)N_2

A 1.6 M solution of *n*-BuLi in hexane (1.1 mL, 1.71 mmol) was added dropwise to a solution of diisopropylamine (0.29 mL, 1.71 mmol) in THF (3 mL) at −78 °C. After the mixture was stirred at −78 °C for 10 min, 0.6 M solution of $TMSCHN_2$ in hexane (2.8 mL, 1.71 mmol) was added dropwise. After 30 min at −78 °C, a solution of ketone **3** (315 mg, 0.57 mmol) in THF (3 mL) was added dropwise at −78 °C. After the reaction mixture was stirred at 0 °C for 1 h, H_2O was added to quench it. The mixture was extracted twice with Et_2O (50 mL), and the combined organic layers were washed with H_2O and then brine, dried over Na_2SO_4, filtered, and concentrated to give a residue, which was purified by silica gel column chromatography (EtOAc–hexane 1:19) to give an inseparable mixture (188 mg, 61%) of **5αβ** (**5α**/**β** = 1/3) and **17**.

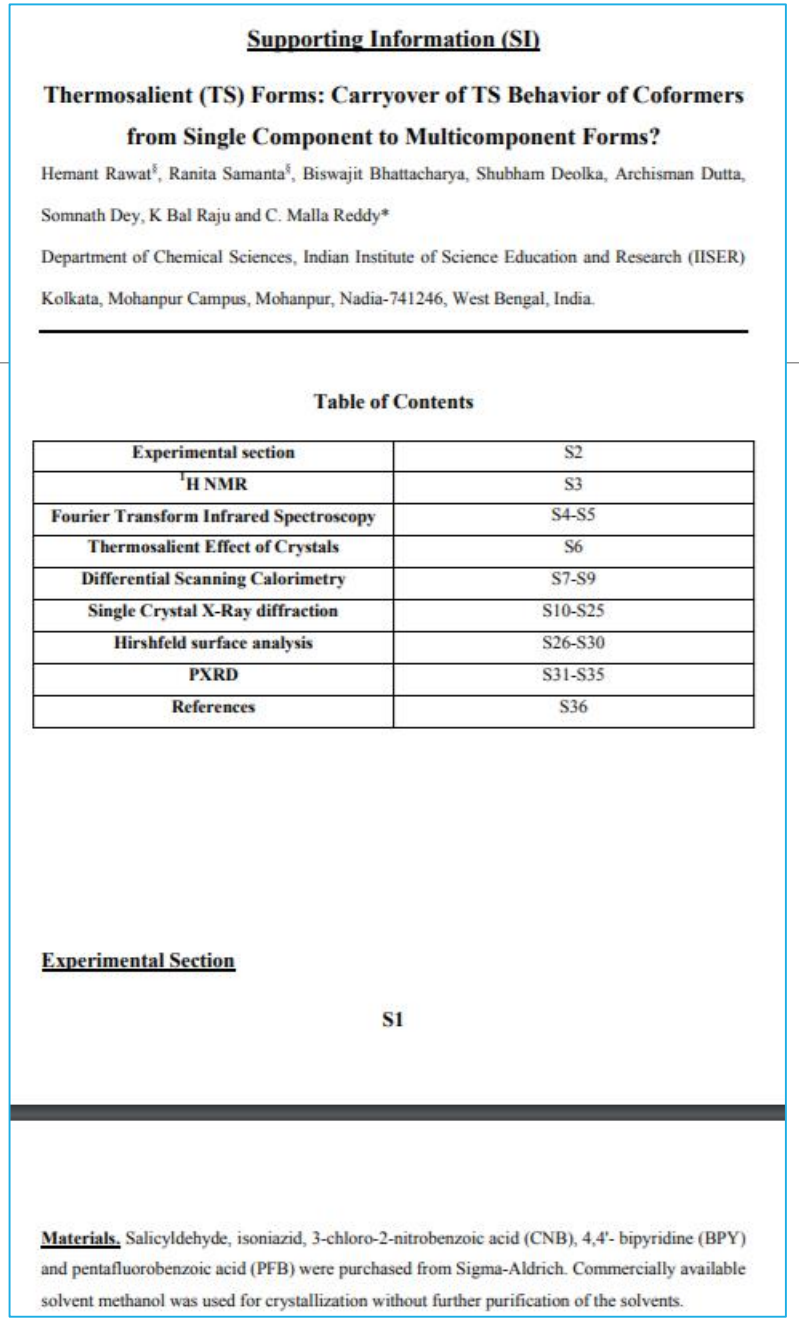
3.3. Synthesis of (−)-neplanocin A from CP 21

3.3.1. 9-[(2S,3R,4R)-(5,4-Dihydroxy-2,3-isopropylidenedioxy)pentyl]adenine (19)

A 1 M solution of DIBAL-H in toluene (82 mL, 81.5 mmol) was added dropwise to a solution of 2′,3′–*O*-isopropylideneadenosine **18** (5.0 g, 16.3 mmol) in CPME (80 mL) at 0 °C. After the reaction

Altre sezioni eventuali

- Supplementary information/supporting material: strutture chimiche, analisi ulteriori, metodi dettagliati
- Funding sources, conflict of interests…



Supporting Information (SI)

Thermosalient (TS) Forms: Carryover of TS Behavior of Coformers from Single Component to Multicomponent Forms?

Hemant Rawat[§], Ranita Samanta[§], Biswajit Bhattacharya, Shubham Deolka, Archisman Dutta, Somnath Dey, K Bal Raju and C. Malla Reddy*

Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur Campus, Mohanpur, Nadia-741246, West Bengal, India.

Table of Contents

Experimental Section

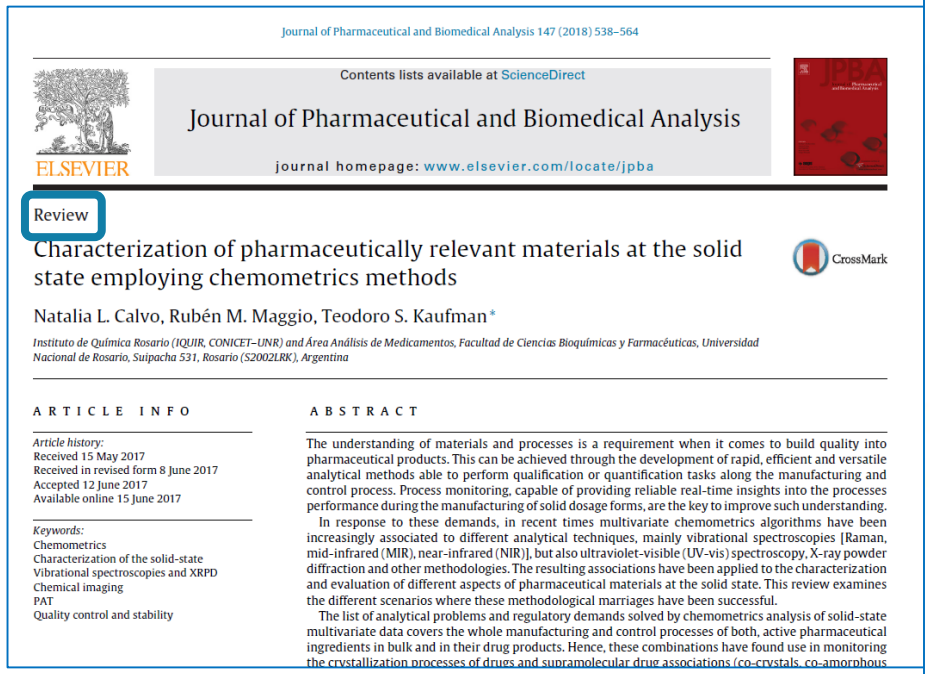
S1

Materials. Salicyldehyde, isoniazid, 3-chloro-2-nitrobenzoic acid (CNB), 4,4'- bipyridine (BPY) and pentafluorobenzoic acid (PFB) were purchased from Sigma-Aldrich. Commercially available solvent methanol was used for crystallization without further purification of the solvents.

Review

- Non solo in giornali specifici

- Abstract
- Contents
- “Main”
- References



Journal of Pharmaceutical and Biomedical Analysis 147 (2018) 538–564

Contents lists available at ScienceDirect

Journal of Pharmaceutical and Biomedical Analysis

journal homepage: www.elsevier.com/locate/jpba

Review

Characterization of pharmaceutically relevant materials at the solid state employing chemometrics methods

Natalia L. Calvo, Rubén M. Maggio, Teodoro S. Kaufman *

Instituto de Química Rosario (IQUIR, CONICET–UNR) and Área Análisis de Medicamentos, Facultad de Ciencias Bioquímicas y Farmacéuticas, Universidad Nacional de Rosario, Suipacha 531, Rosario (S2002LRK), Argentina

ARTICLE INFO

Article history:
Received 15 May 2017
Received in revised form 8 June 2017
Accepted 12 June 2017
Available online 15 June 2017

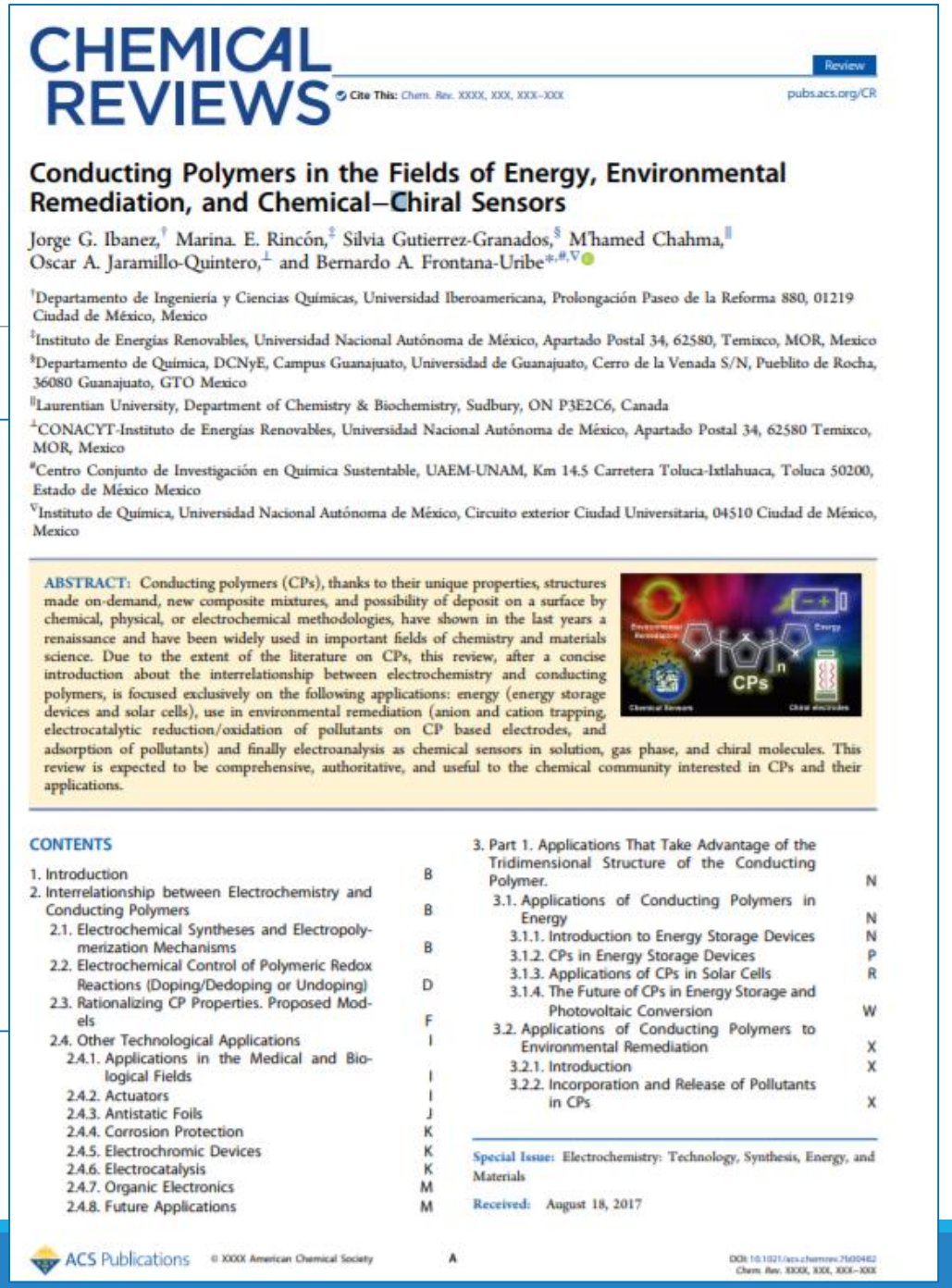
Keywords:
Chemometrics
Characterization of the solid-state
Vibrational spectroscopies and XRPD
Chemical imaging
PAT
Quality control and stability

ABSTRACT

The understanding of materials and processes is a requirement when it comes to build quality into pharmaceutical products. This can be achieved through the development of rapid, efficient and versatile analytical methods able to perform qualification or quantification tasks along the manufacturing and control process. Process monitoring, capable of providing reliable real-time insights into the processes performance during the manufacturing of solid dosage forms, are the key to improve such understanding.

In response to these demands, in recent times multivariate chemometrics algorithms have been increasingly associated to different analytical techniques, mainly vibrational spectroscopies [Raman, mid-infrared (MIR), near-infrared (NIR)], but also ultraviolet-visible (UV-vis) spectroscopy, X-ray powder diffraction and other methodologies. The resulting associations have been applied to the characterization and evaluation of different aspects of pharmaceutical materials at the solid state. This review examines the different scenarios where these methodological marriages have been successful.

The list of analytical problems and regulatory demands solved by chemometrics analysis of solid-state multivariate data covers the whole manufacturing and control processes of both, active pharmaceutical ingredients in bulk and in their drug products. Hence, these combinations have found use in monitoring the crystallization processes of drugs and supramolecular drug associations (co-crystals, co-amorphous



CHEMICAL REVIEWS

Review

Cite This: Chem. Rev. XXXX, XXX, XXX−XXX

pubs.acs.org/CR

Conducting Polymers in the Fields of Energy, Environmental Remediation, and Chemical–Chiral Sensors

Jorge G. Ibanez,[†] Marina. E. Rincón,[‡] Silvia Gutierrez-Granados,[§] M'hamed Chahma,[∥] Oscar A. Jaramillo-Quintero,[⊥] and Bernardo A. Frontana-Uribe*[,#,▽]

[†]Departamento de Ingeniería y Ciencias Químicas, Universidad Iberoamericana, Prolongación Paseo de la Reforma 880, 01219 Ciudad de México, Mexico

[‡]Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Apartado Postal 34, 62580, Temixco, MOR, Mexico

[§]Departamento de Química, DCNyE, Campus Guanajuato, Universidad de Guanajuato, Cerro de la Venada S/N, Pueblito de Rocha, 36080 Guanajuato, GTO Mexico

[∥]Laurentian University, Department of Chemistry & Biochemistry, Sudbury, ON P3E2C6, Canada

[⊥]CONACYT-Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Apartado Postal 34, 62580 Temixco, MOR, Mexico

[#]Centro Conjunto de Investigación en Química Sustentable, UAEM-UNAM, Km 14.5 Carretera Toluca-Ixtlahuaca, Toluca 50200, Estado de México Mexico

[▽]Instituto de Química, Universidad Nacional Autónoma de México, Circuito exterior Ciudad Universitaria, 04510 Ciudad de México, Mexico

ABSTRACT: Conducting polymers (CPs), thanks to their unique properties, structures made on-demand, new composite mixtures, and possibility of deposit on a surface by chemical, physical, or electrochemical methodologies, have shown in the last years a renaissance and have been widely used in important fields of chemistry and materials science. Due to the extent of the literature on CPs, this review, after a concise introduction about the interrelationship between electrochemistry and conducting polymers, is focused exclusively on the following applications: energy (energy storage devices and solar cells), use in environmental remediation (anion and cation trapping, electrocatalytic reduction/oxidation of pollutants on CP based electrodes, and adsorption of pollutants) and finally electroanalysis as chemical sensors in solution, gas phase, and chiral molecules. This review is expected to be comprehensive, authoritative, and useful to the chemical community interested in CPs and their applications.

CONTENTS

Special Issue: Electrochemistry: Technology, Synthesis, Energy, and Materials

Received: August 18, 2017

DOI: 10.1021/acs.chemrev.7b00482
Chem. Rev. XXXX, XXX, XXX−XXX

Communications

- Brevi
- Proteggere un risultato originale da eventuali altre pubblicazioni

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Cite this: DOI: 10.1039/c8cc01787e

Received 5th March 2018,
Accepted 25th March 2018

DOI: 10.1039/c8cc01787e

rsc.li/chemcomm

Manganese catalyzed reductive amination of aldehydes using hydrogen as a reductant†

Duo Wei, [a] Antoine Bruneau-Voisine, [ab] Dmitry A. Valyaev, [b] Noël Lugan [b] and Jean-Baptiste Sortais [*bc]

A one-pot two-step procedure was developed for the alkylation of amines *via* reductive amination of aldehydes using molecular dihydrogen as a reductant in the presence of a manganese pyridinyl-phosphine complex as a pre-catalyst. After the initial condensation step, the reduction of imines formed *in situ* is performed under mild conditions (50–100 °C) with 2 mol% of catalyst and 5 mol% of tBuOK under 50 bar of hydrogen. Excellent yields (>90%) were obtained for a large combination of aldehydes and amines (40 examples), including aliphatic aldehydes and amino-alcohols.

In the last two years, the use of manganese as a sustainable alternative to precious transition metals in hydrogenation and hydrogen borrowing reactions has achieved an impressive explosion.[1] Starting from the hydrogenation of aldehydes, ketones and nitriles,[2] the scope of reducible functional groups was rapidly expanded to esters,[2d,3] amides,[3c,4] and CO_2.[5] Soon after, hydrogen transfer reactions using isopropanol as a reductant[6] and asymmetric reduction[2d,7] have been disclosed. In the case of hydrogen borrowing reactions, the first manganese-catalyzed dehydrogenative coupling of alcohols and amines to form imines[8] was rapidly complemented by the synthesis of esters[9] from alcohols, and amides[10] from alcohols and amines. In the case of C–C bond forming reactions, α-alkylation of ketones with alcohols,[11] and olefination of nitriles[12] were also achieved. Interestingly, the upgrading of ethanol into butanol,[13] the dehydrogenation of methanol[14] to H_2 and CO_2, and the deoxygenation of alcohols[15] were also found to be catalyzed by manganese complexes. Finally, the access to various higher amine derivatives using alcohols

Reductive amination[22] is one of the chemical reactions in the chemist's tool-box for the preparation of amines.[23] It relies on the *in situ* condensation of a ketone or aldehyde with an amine to form the corresponding imine, which is subsequently reduced to the desired amine. When using molecular hydrogen as a reductant, it appears that the key step in the reaction sequence is the hydrogenation of the intermediate imine.

In line with our previous work on manganese catalyzed reactions[24] and catalytic amine synthesis using first-row transition metal complexes,[25] we report here the first alkylation of amines *via* reductive amination of aldehydes using molecular hydrogen as a reductant and well-defined manganese complexes as pre-catalysts.

We have selected complexes **1–4** as candidates for this study (Scheme 1) as we recently demonstrated that manganese(I) bromotricarbonyl complexes bearing bidentate pyridinyl–phosphine ligands were good catalysts for the hydrogenation of carbonyl derivatives, and especially complex **2** featuring a diphenyl-(2-aminopyridinyl)-phosphine ligand.[26]

We initially focused on the direct hydrogenation of *N*-benzylideneaniline **c1** as a model substrate, using catalyst **2** and a base, under 50 bar of H_2, based on previously optimized conditions for the hydrogenation of ketones. First, we found that alcohols, and notably ethanol, were suitable solvents for the hydrogenation step (see Table S1 in the ESI†) as a green solvent alternative to toluene. It then appeared that the nature of the base had little influence on the reaction, NaO*t*Bu, KO*t*Bu, KHMDS, or Cs_2CO_3, leading to satisfactory conversions (**2** (1 mol%), base (2 mol%), 100 °C, EtOH, 22 h, 41% to 64% yield, see Table S2 in

References

- L. Liu, X. Wang, Improved dissolution of oleanolic acid with ternary solid dispersion, AAPS PharmSciTech 8 (2007) 267-271

(1) (a) Trost, B. M. Angew. Chem., Int. Ed. Engl. **1995**, 34, 259−281. (b) Han, L.-B.; Tanaka, M. Chem. Commun. **1999**, 395−402. (c) Shimizu, Y.; Kanai, M. Tetrahedron Lett. **2014**, 55, 3727−3737. (d) Ansell, M. B.; Navarro, O.; Spencer, J. Coord. Chem. Rev. **2017**, 336, 54−77.

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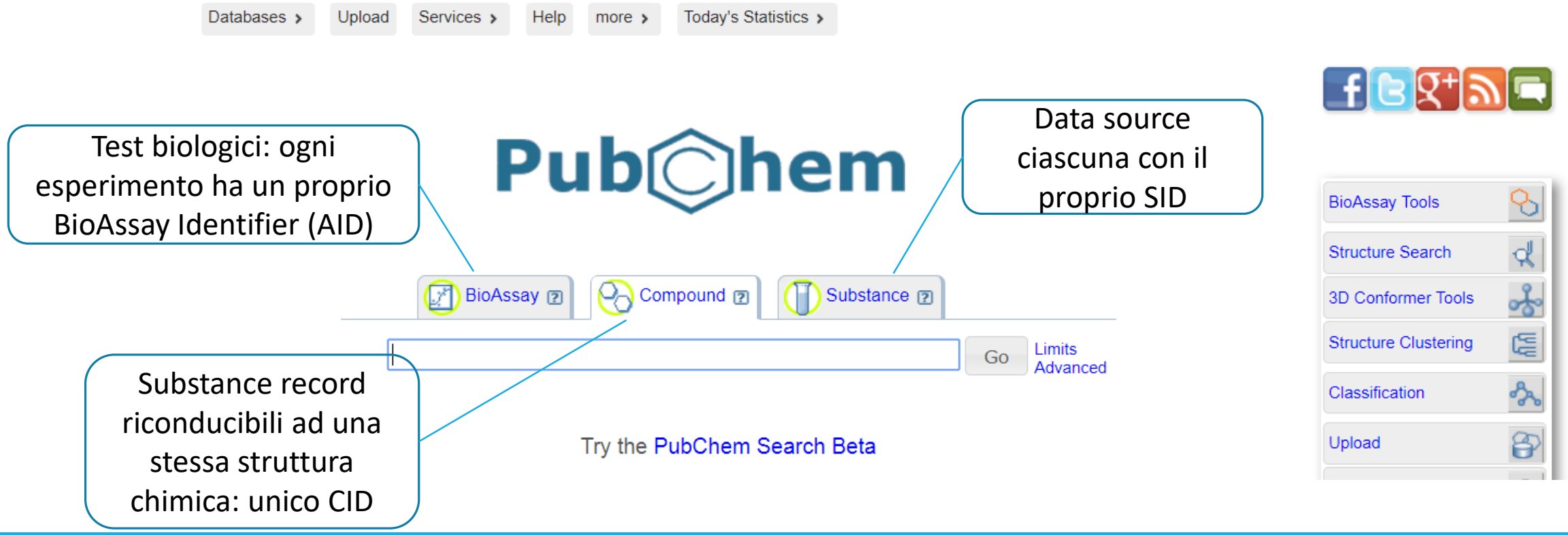

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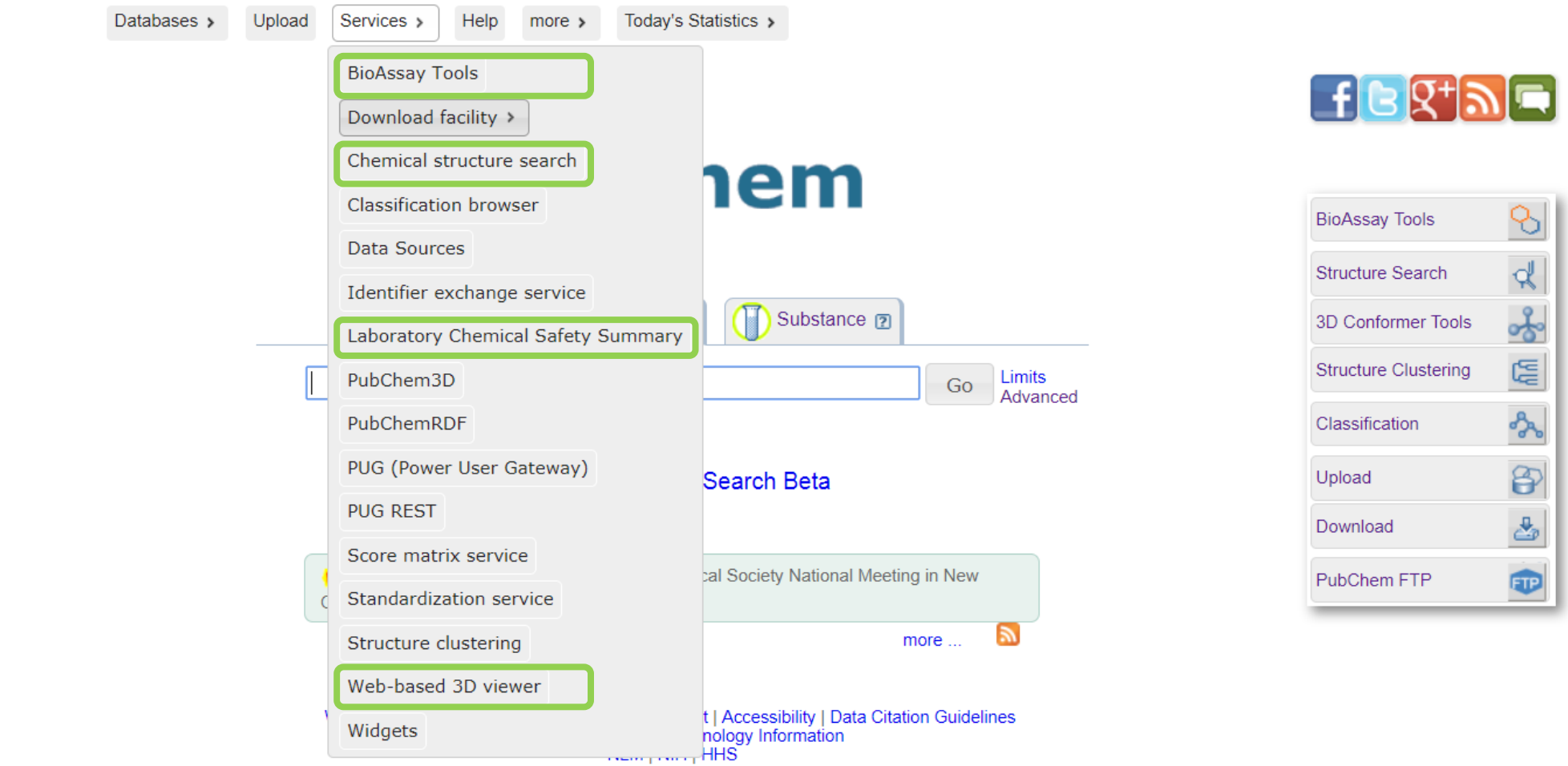

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Acetaminophen

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PubChem CID:	1983
Chemical Names:	Acetaminophen; 4-Acetamidophenol; Paracetamol; 103-90-2; APAP; N-(4-Hydroxyphenyl)acetamide More...
Molecular Formula:	$C_8H_9NO_2$ or $HOC_6H_4NHCOCH_3$
Molecular Weight:	151.165 g/mol
InChI Key:	RZVAJINKPMORJF-UHFFFAOYSA-N
Drug Information:	Drug Indication | Therapeutic Uses | Clinical Trials | FDA Orange Book | FDA UNII
Safety Summary:	Laboratory Chemical Safety Summary (LCSS)

Analgesic antipyretic derivative of acetanilide. Acetaminophen has weak anti-inflammatory properties and is used as a common analgesic, but may cause liver, blood cell, and kidney damage

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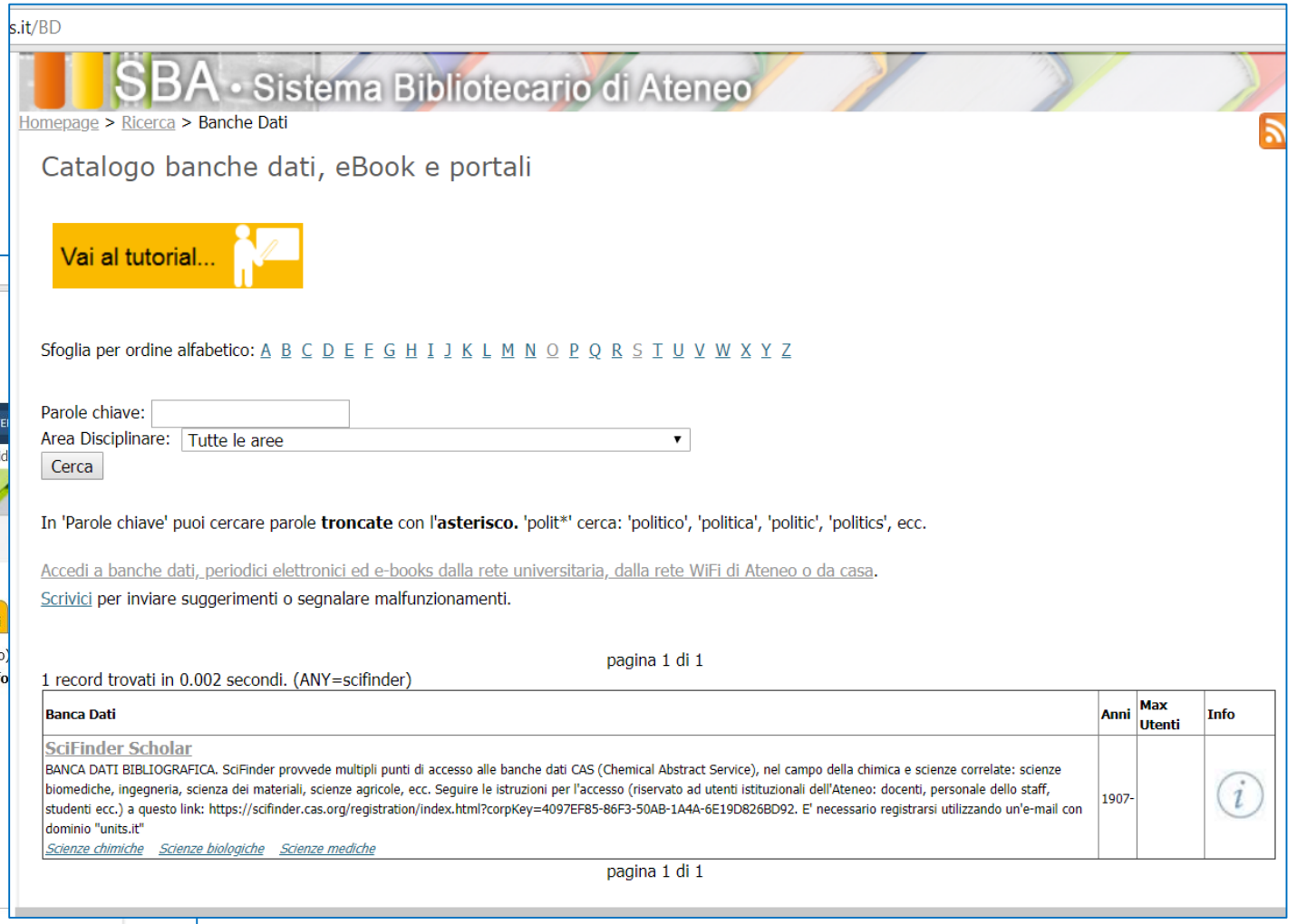

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1. **The effects of subcurative praziquantel treatment on life-history traits and trade-offs in drug-resistant Schistosoma mansoni**
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By Viana, Mafalda; Faust, Christina L.; Haydon, Daniel T.; Webster, Joanne P.; Lamberton, Poppy H. L.
From Evolutionary Applications (2018), 11(4), 488-500. | Language: English, Database: CAPLUS
Natural selection acts on all organisms, including parasites, to maximize reproductive fitness. Drug resistance traits are often assocd. with life-history costs in the absence of treatment. Schistosomiasis control programs rely on mass drug administration to reduce human morbidity and mortality. Although hotspots of reduced drug efficacy have been reported, resistance is not widespread. Using Bayesian state-space models (SSMs) fitted to data from an in vivo lab. system, we tested the hypothesis that the spread of resistant Schistosoma mansoni may be limited by life-history costs not presen...

2. **Insights into the mode of action of 1,2,6,7-tetraoxaspiro [7.11] nonadecane (N-89) against adult Schistosoma mansoni worms**
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By Blay, Emmanuel Awusah; Kumagai, Takashi; Yamabe, Masafumi; Hino, Akina; Shimogawara, Rieko; Kim, Hye-Sook; Sato, Akira; Ichimura, Koichiro; Ayi, Irene; Iwanaga, Shiroh; et al
From Parasitology International (2018), 67(4), 403-412. | Language: English, Database: CAPLUS
Control of morbidity assocd. with schistosomiasis via chemotherapy largely relies on the drug **praziquantel**. Repeated therapy with **praziquantel** has created concerns about the possible selection of resistant worms and necessitated the search for novel drugs to treat schistosomiasis. Here, a murine model was infected with Schistosoma mansoni and treated with oral 1,2,6,7-tetraoxaspiro [7.11] nonadecane (N-89), which caused a significant redn. in fecundity and egg burden and reduced morbidity when administered at 5-wk post-infection. The anal. showed that the mode of action occurred through the...

3. **Control of Hymenolepis nana infection as a measure to improve mouse colony welfare**
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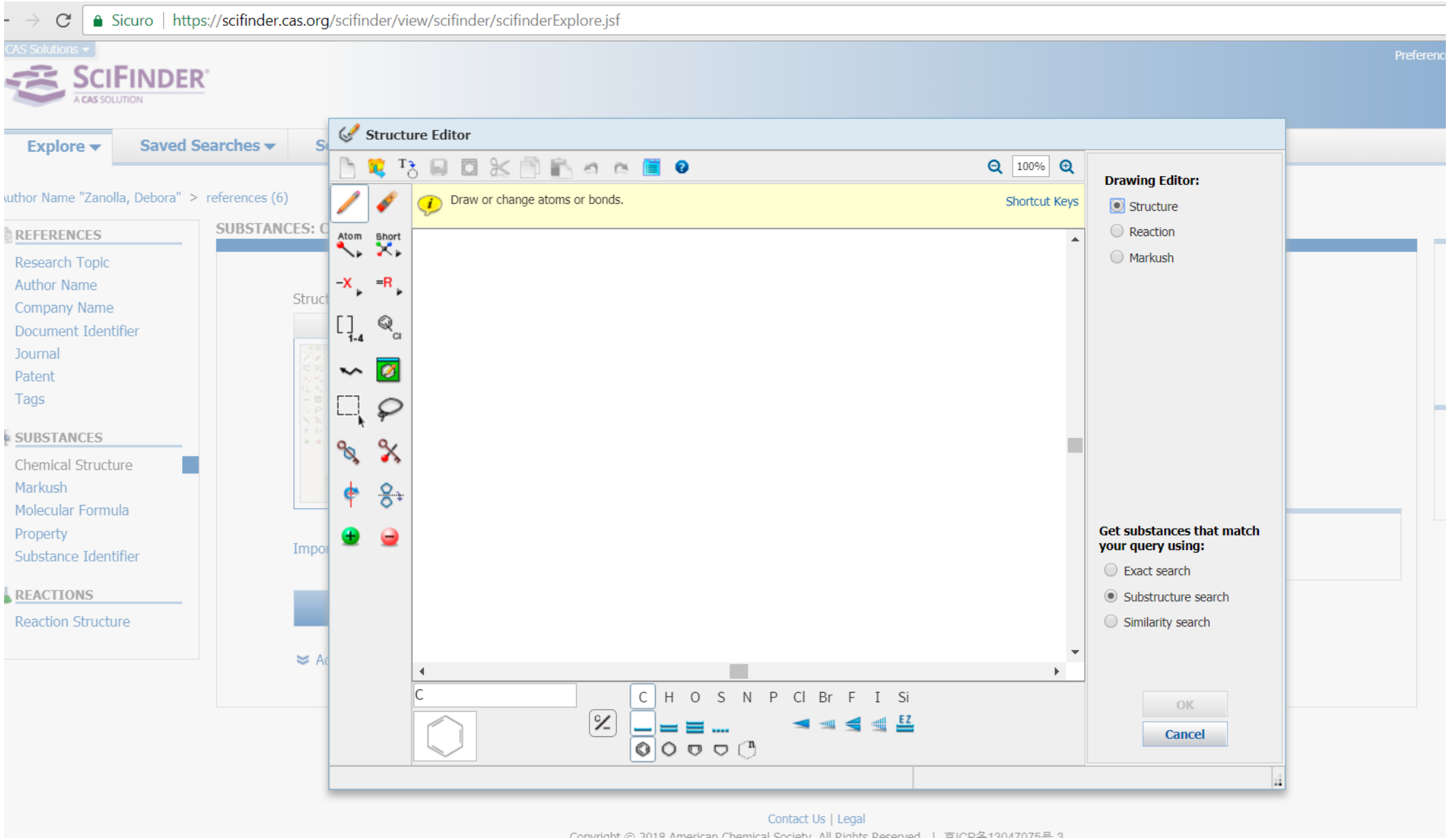
By Dovc, Alenka; Gracner, Gordana Greguric; Tomazic, Iztok; Vlahovic, Ksenija; Pavlak, Marina; Knific, Renata Lindtner; Kralj, Klemen; Stvarnik, Mateja; Rataj, Aleksandra Vergles
From Acta Veterinaria Hungarica (2017), 65(2), 208-220. | Language: English, Database: CAPLUS
After cannibalism had appeared in the reproductive units of a white mouse colony, treatment against confirmed Hymenolepis nana, a tapeworm with zoonotic potential, was performed on 67 mice in the reproductive and nursery units. Faecal droppings were evaluated by flotation and sedimentation methods. The sedimentation method revealed a higher no. of pos. results before, during and after the treatment, but the flotation method yielded some addnl. pos. cases. In the reproductive unit, H. nana eggs were confirmed in 50% of the tested mice by the flotation and in 70% by the sedimentation method. ...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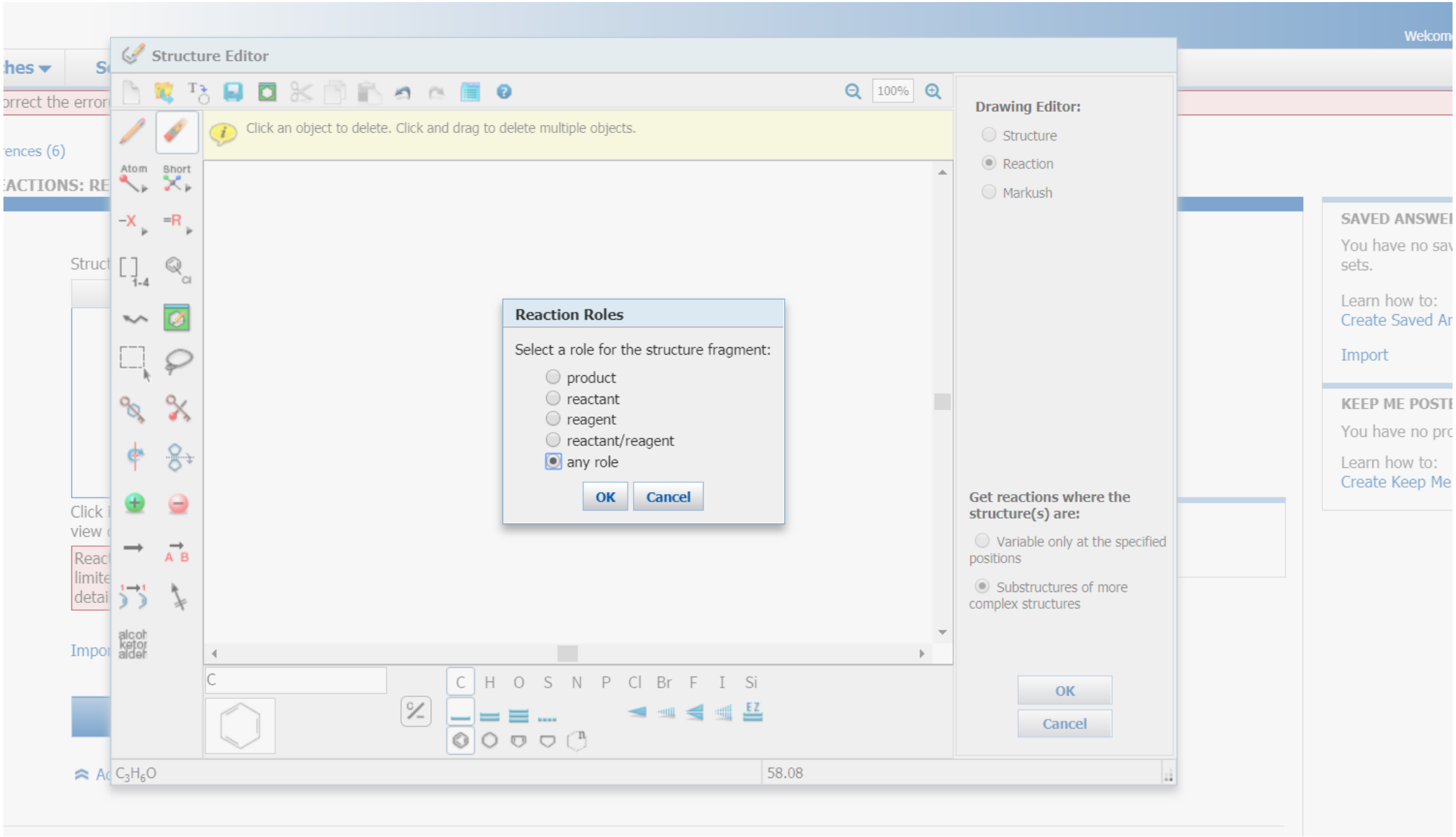
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Steps/Stages

1.1 R:H_2, C:1160618-74-5, S:THF, 1 h, rt, 20 bar

Notes

reaction in an autoclave, %ee = 99, high pressure, stereoselective, Reactants: 1, Reagents: 1, Catalysts: 1, S
1, Most stages in any one step: 1

References

Process for asymmetric hydrogenation of enol esters
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By Francio, Giancarlo et al
From Ger. Offen., 102013107421, 15 Jan 2015

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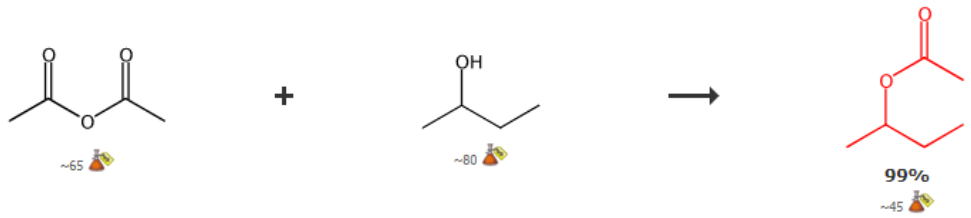

Overview

Steps/Stages

1.1 C:36968-17-9, 4 h, 90°C

Notes

catalyst prepared and used, Reactants: 2, Catalysts: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Catalyst and method for preparing acetate by acid anhydride method
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By Liu, Lianghui et al
From Faming Zhuanli Shenqing, 105363492, 02 Mar 2016

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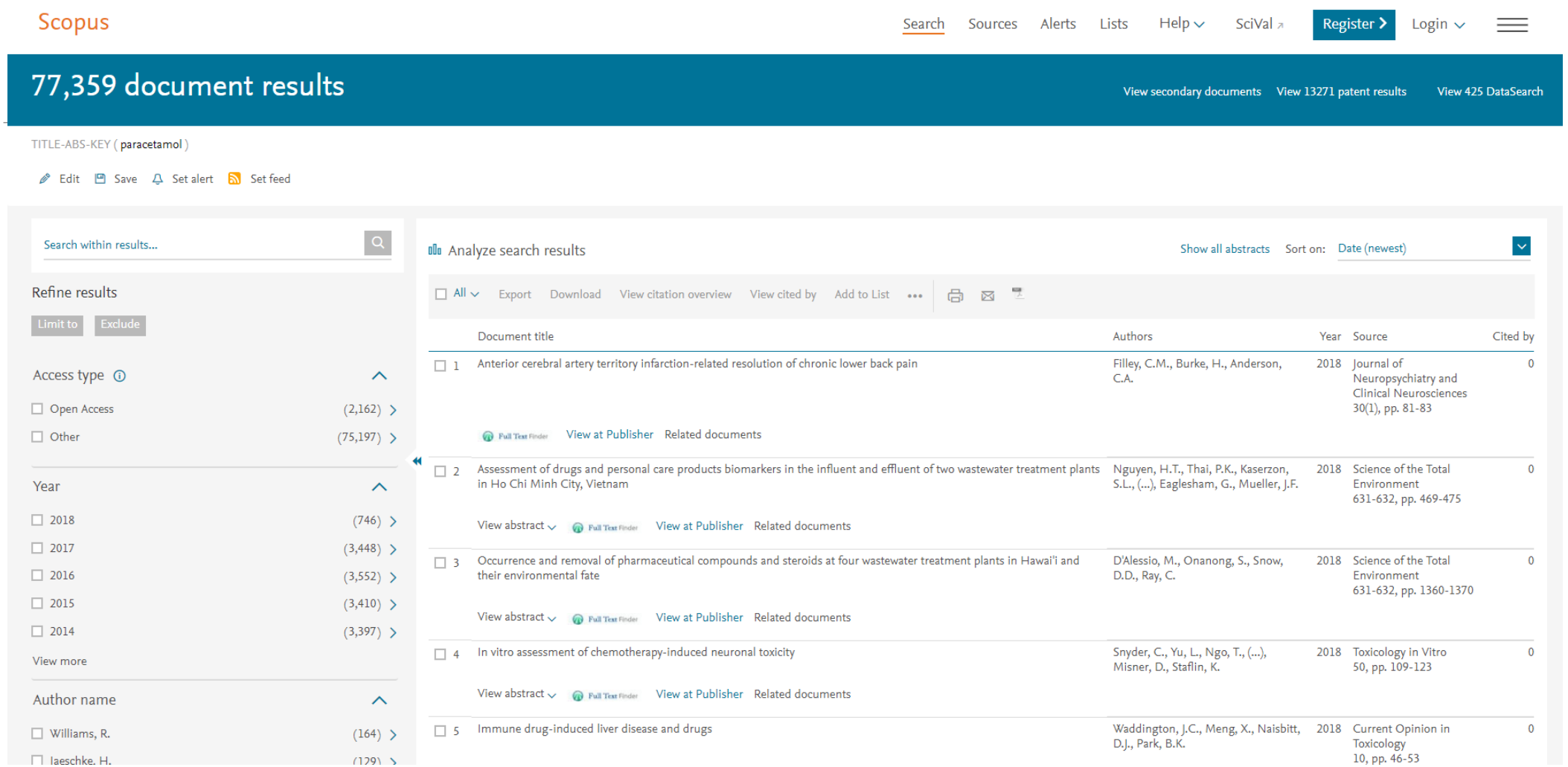
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Journal of Molecular Structure
Volume 1154, 15 February 2018, Pages 196-203

Structural study of salt forms of amides; paracetamol, benzamide and piperine (Article)

Kennedy, A.R.[a], King, N.L.C.[a], Oswald, I.D.H.[b], Rollo, D.G.[a], Spiteri, R.[a], Walls, A.[a]

[a]Westchem, Department of Pure & Applied Chemistry, University of Strathclyde, 295 Cathedral Street, Glasgow, Scotland, United Kingdom
[b]Strathclyde Institute of Pharmacy and Biomedical Sciences, University of Strathclyde, 161 Cathedral Street, Glasgow, Scotland, United Kingdom

Abstract

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Single crystal x-ray diffraction has been used to investigate the structures of six complexes containing O-atom protonated cations derived from the pharmaceutically relevant amides benzamide (BEN), paracetamol (PAR) and piperine (PIP). The structures of the salt forms [PAR(H)][$SO_3C_6H_4Cl$], [BEN(H)][$O_3SC_6H_4Cl$] and [BEN(H)][Br]·H_2O are reported along with those of the hemi-halide salt forms [PAR(H)][I_3]. PAR, [PIP(H)][I_3]·PIP and [PIP(H)][I_3]$_{0.5}$[I]$_{0.5}$·PIP. The structure of the cocrystal BEN. $HOOCCH_2Cl$ is also presented for comparison. The geometry of the amide group is found to systematically change upon protonation, with the C[dbnd]O distance increasing and the C[sbnd]N distance decreasing. The hemi-halide species all feature strongly hydrogen bonded amide(H)/amide pairs. The amide group C[dbnd]O and C[sbnd]N distances for both elements of each such pair are intermediate between those found for simple neutral amide and protonated amide forms. It was found that crystallising paracetamol from aqueous solutions containing Ba^{2+} ions gave orthorhombic paracetamol.

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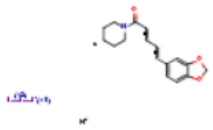

Reaxys RN	32039550
Chemical Name	
CAS Number	
Mol. Formula	$C_{34}H_{39}I_3N_2O_6$
Mol. Weight	952.407
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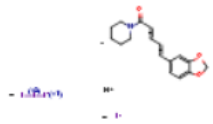

Reaxys RN	32039551
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Mol. Weight	825.502
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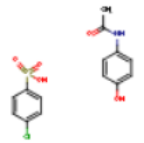

Reaxys RN	32039552
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CAS Number	
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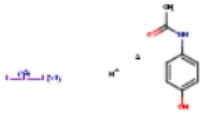

Reaxys RN	32039553
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Mol. Weight	684.051
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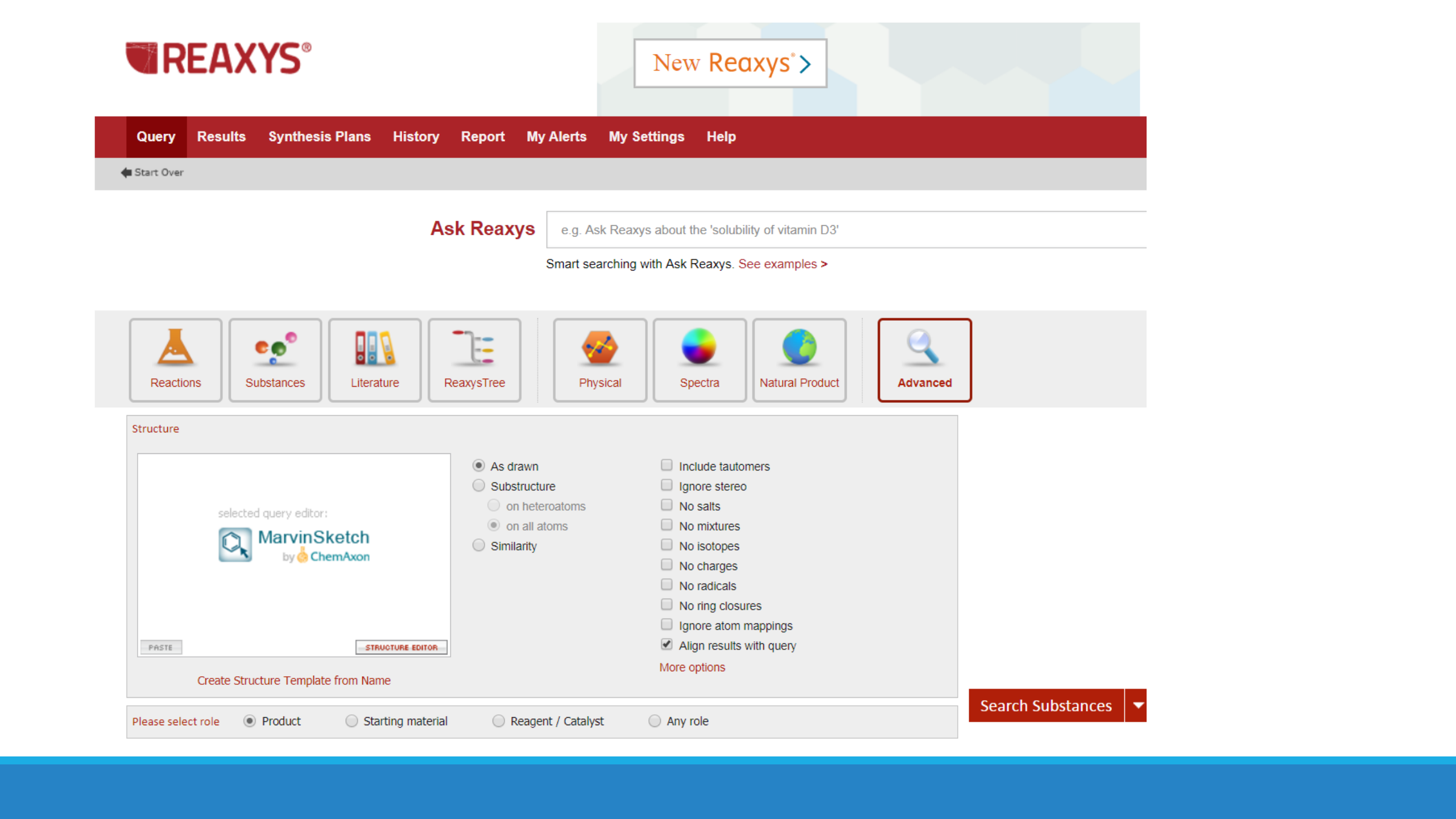
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Bands Spectrum	potassium bromide			**Dametto; Polese; Ribeiro; Chorilli; de Freitas, Osvaldo** Journal of Thermal Analysis and Calorimetry, **2017** , vol. 127, # 2 p. 1693 - 1706 Title/Abstract Full Text View citing articles Show Details
Spectrum	neat (no solvent, solid phase)			**Sánchez-Guadarrama, Obdulia; Mendoza-Navarro, Fabiola; Cedillo-Cruz, Alberto; Jung-Cook, Helgi; Arenas-García, Jenniffer I.; Delgado-Díaz, Alejandra; Herrera-Ruiz, Dea; Morales-Rojas, Hugo; Höpfl, Herbert** Crystal Growth and Design, **2016** , vol. 16, # 1 p. 307 - 314 Title/Abstract Full Text View citing articles Show Details
Bands Spectrum	potassium bromide	at 3460 cm^{-1}, 3277 cm^{-1}, 3065 cm^{-1}, 3048 cm^{-1}, 3021 cm^{-1}, 3003 cm^{-1}, 2932 cm^{-1}, 2853 cm^{-1}, 2660 cm^{-1}, 1651 cm^{-1}, 1645 cm^{-1}, 1622 cm^{-1}, 1576 cm^{-1}, 1570 cm^{-1}, 1558 cm^{-1}, 1541 cm^{-1}, 1533 cm^{-1}, 1522 cm^{-1}, 1506 cm^{-1}, 1497 cm^{-1}, 1489 cm^{-1}, 1472 cm^{-1}, 1456 cm^{-1}, 1437 cm^{-1}, 1418 cm^{-1}, 1387 cm^{-1}, 1364 cm^{-1}, 1339 cm^{-1}, 1323 cm^{-1}, 1296 cm^{-1}, 1285 cm^{-1}, 1263 cm^{-1}, 1254 cm^{-1}, 1242 cm^{-1}, 1217 cm^{-1}, 1190 c	Page/Page column 11	**TONGLI BIOMEDICAL CO., LTD; Qian, Mingxin; Ho, Rodney JY; Qiao, Chunsheng; Shi, Junwei** **Patent:** US2016/272636 A1, **2016** ; Title/Abstract Full Text Show Details
Bands				**Cedillo-Cruz, Alberto; Aguilar, Maria Isabel; Flores-Alamo, Marcos; Palomares-Alonso, Francisca; Jung-Cook, Helgi** Tetrahedron Asymmetry, **2014** , vol. 25, # 2 p. 133 - 140 Title/Abstract Full Text View citing articles Show Details
ATR (attenuated total reflectance) Bands				**Seki, Maki; Ogiku, Tsuyoshi** Tetrahedron, **2014** , vol. 70, # 25 p. 3864 - 3870 Title/Abstract Full Text View citing articles Show Details
Bands			supporting	**Tsang, Althea S.K.; Ingram, Katrin; Keiser**

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Compound name	sulfadiazine
DOI	A single publication DOI or CSD DOI
Authors	e.g. F.H.Allen
Journal	e.g. Journal of the American Chemical Society
Publication details	Year / Volume / Page

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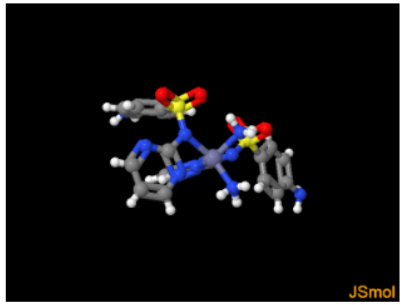
Results

Database Identifier	Deposition Number
CAXPUM	1121077

Download

CAXPUM : Diammine-bis(2-sulfanilamidopyrimidinato)-zinc(ii)
Space Group: P n 2_1 a (33), **Cell:** *a* 13.894(1)Å *b* 14.221(1)Å *c* 12.608(1)Å, *α* 90° *β* 90° *γ* 90°

3D viewer



H | Disorder | Menu | Open

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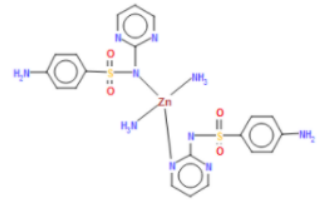
Ball and Stick	No Labels	None	None

Chemical diagram



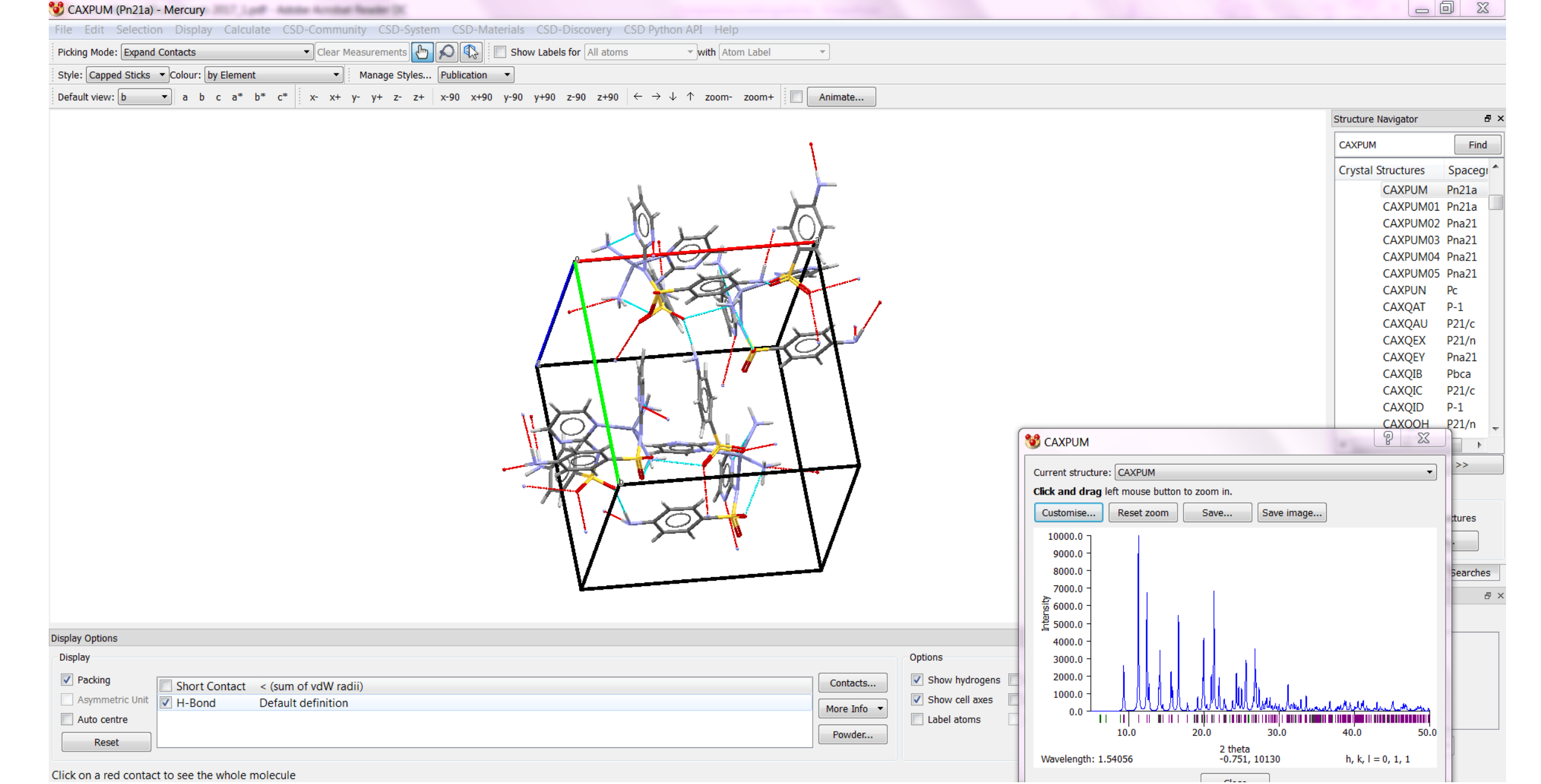
View group symbols key

Additional details

Deposition Number	1121077
Synonyms	Diammine-zinc sulfadiazine
Deposited on	23/08/1984

Associated publications

N.C.Baenziger, S.L.Modak, C.L.Fox Junior, *Acta Crystallographica,Section C: Crystal Structure Communications*, 1983, 39, 1620, DOI: 10.1107/S0108270183009506


CAXPUM (Pn21a) - Mercury
File Edit Selection Display Calculate CSD-Community CSD-System CSD-Materials CSD-Discovery CSD Python API Help
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x- x+ y- y+ z- z+ x-90 x+90 y-90 y+90 z-90 z+90
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CAXPUM04 Pna21
CAXPUM05 Pna21
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CAXQAT P-1
CAXQAU P21/c
CAXQEX P21/n
CAXQEY Pna21
CAXQIB Pbca
CAXQIC P21/c
CAXQID P-1
CAXQOH P21/n
CAXPUM
Current structure: CAXPUM
Click and drag left mouse button to zoom in.
Customise... Reset zoom Save... Save image...
Intensity
10000.0
9000.0
8000.0
7000.0
6000.0
5000.0
4000.0
3000.0
2000.0
1000.0
0.0
10.0 20.0 30.0 40.0 50.0
2 theta
Wavelength: 1.54056
-0.751, 10130
h, k, l = 0, 1, 1
Display Options
Display
Packing
Asymmetric Unit
Auto centre
Reset
Short Contact < (sum of vdW radii)
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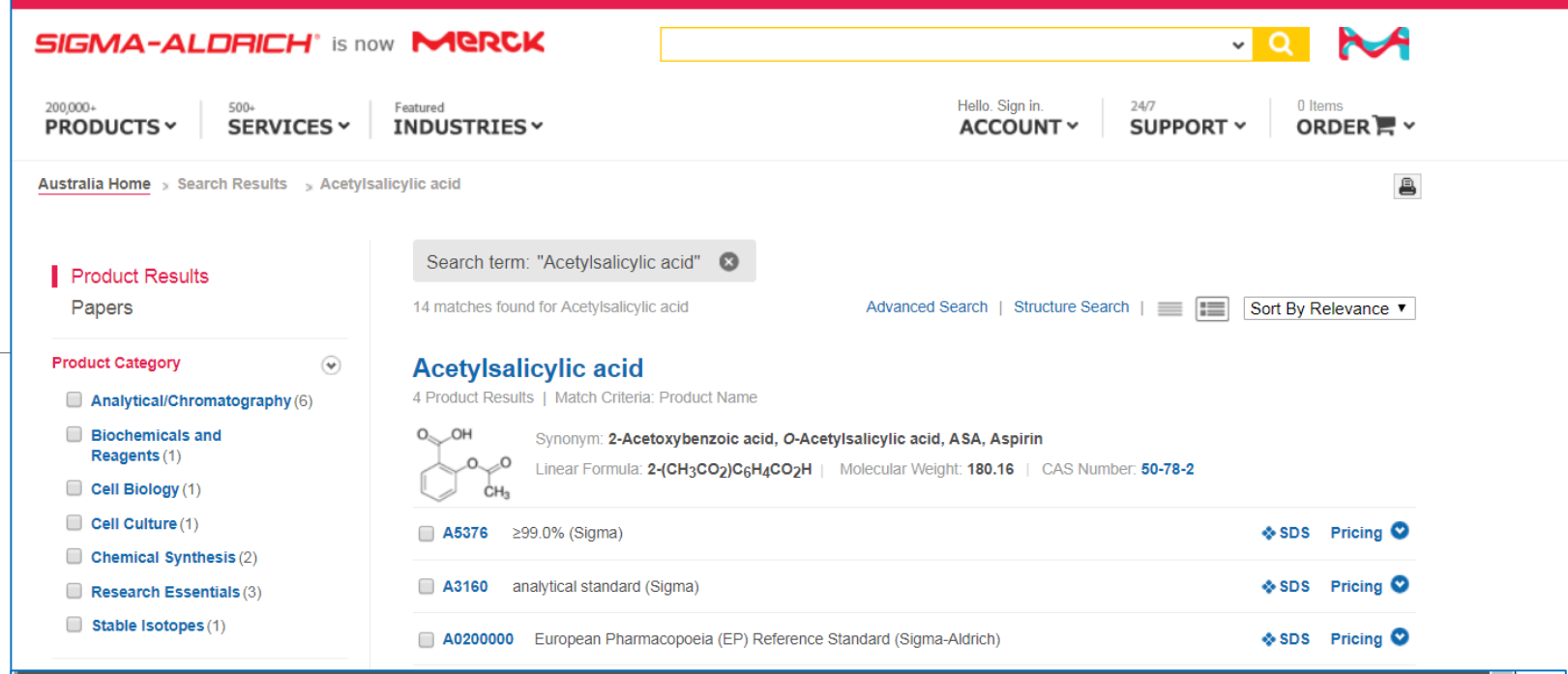
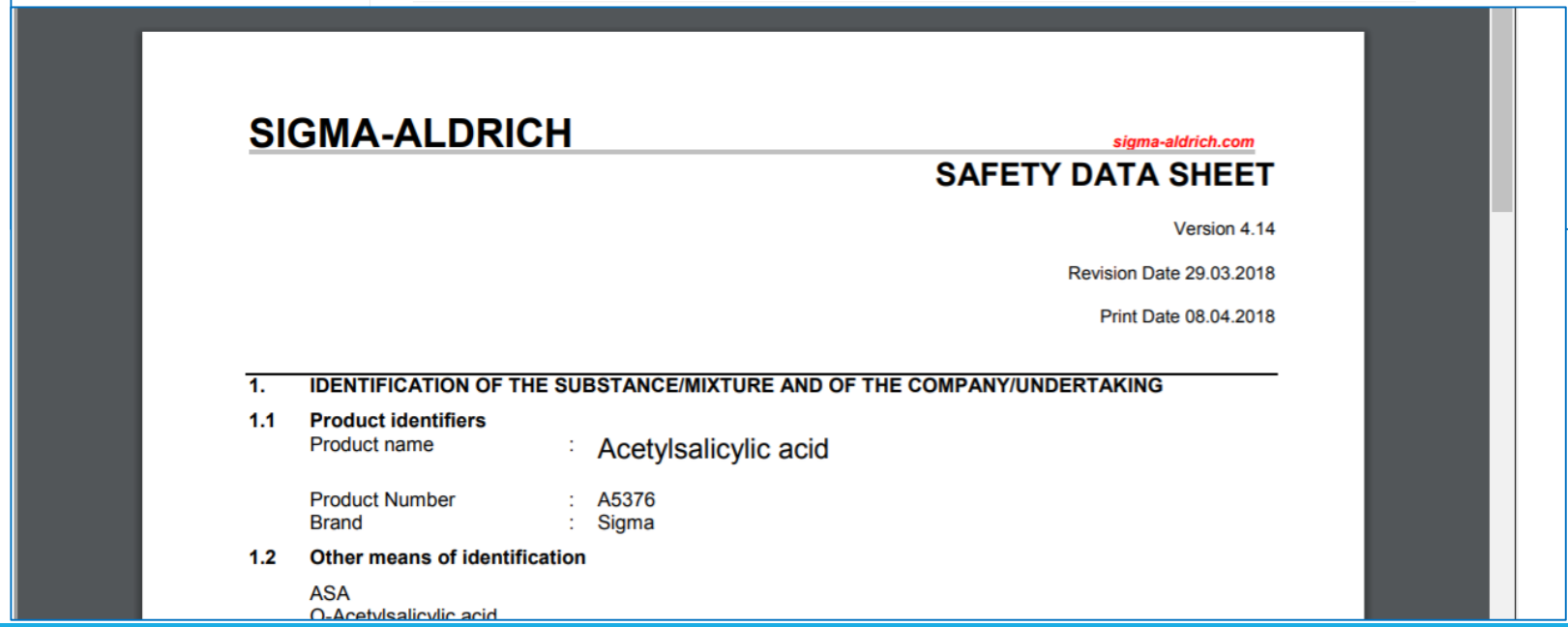
- Diversi gradi di purezza
- Schede di sicurezza!





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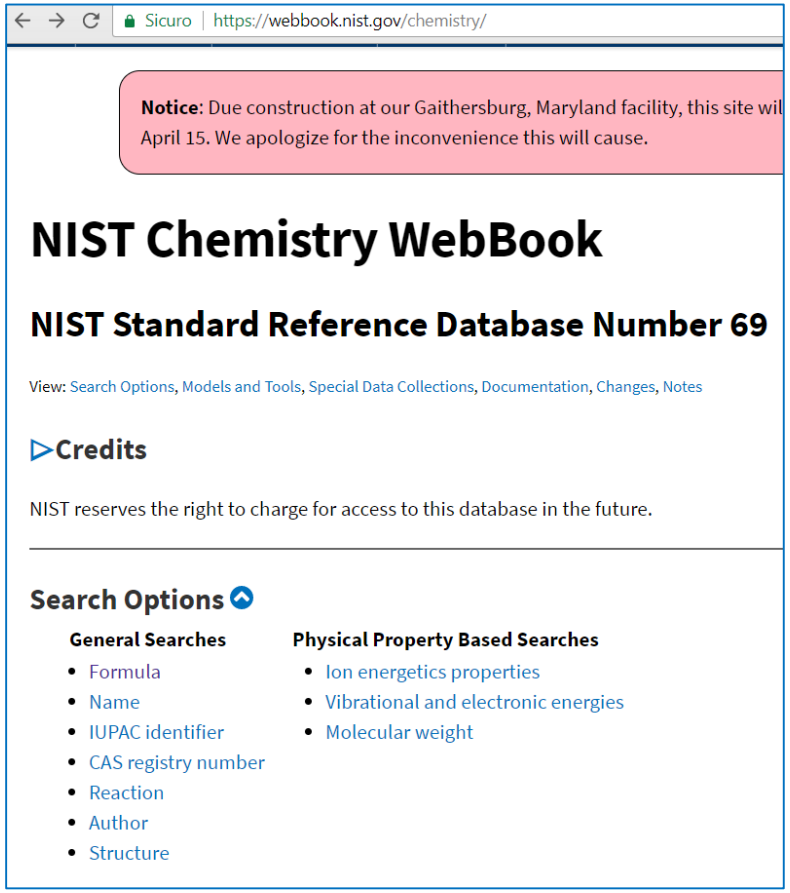
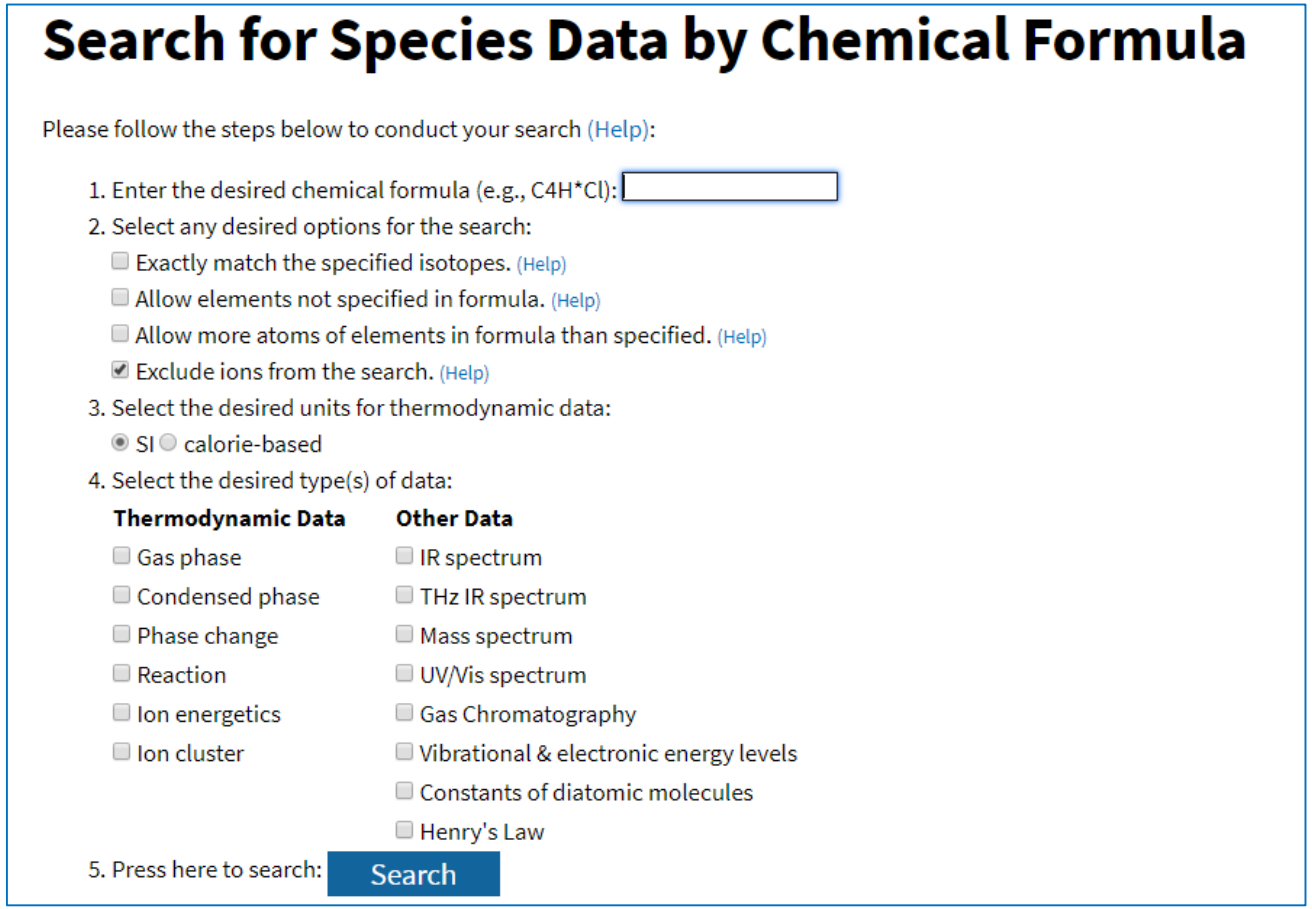
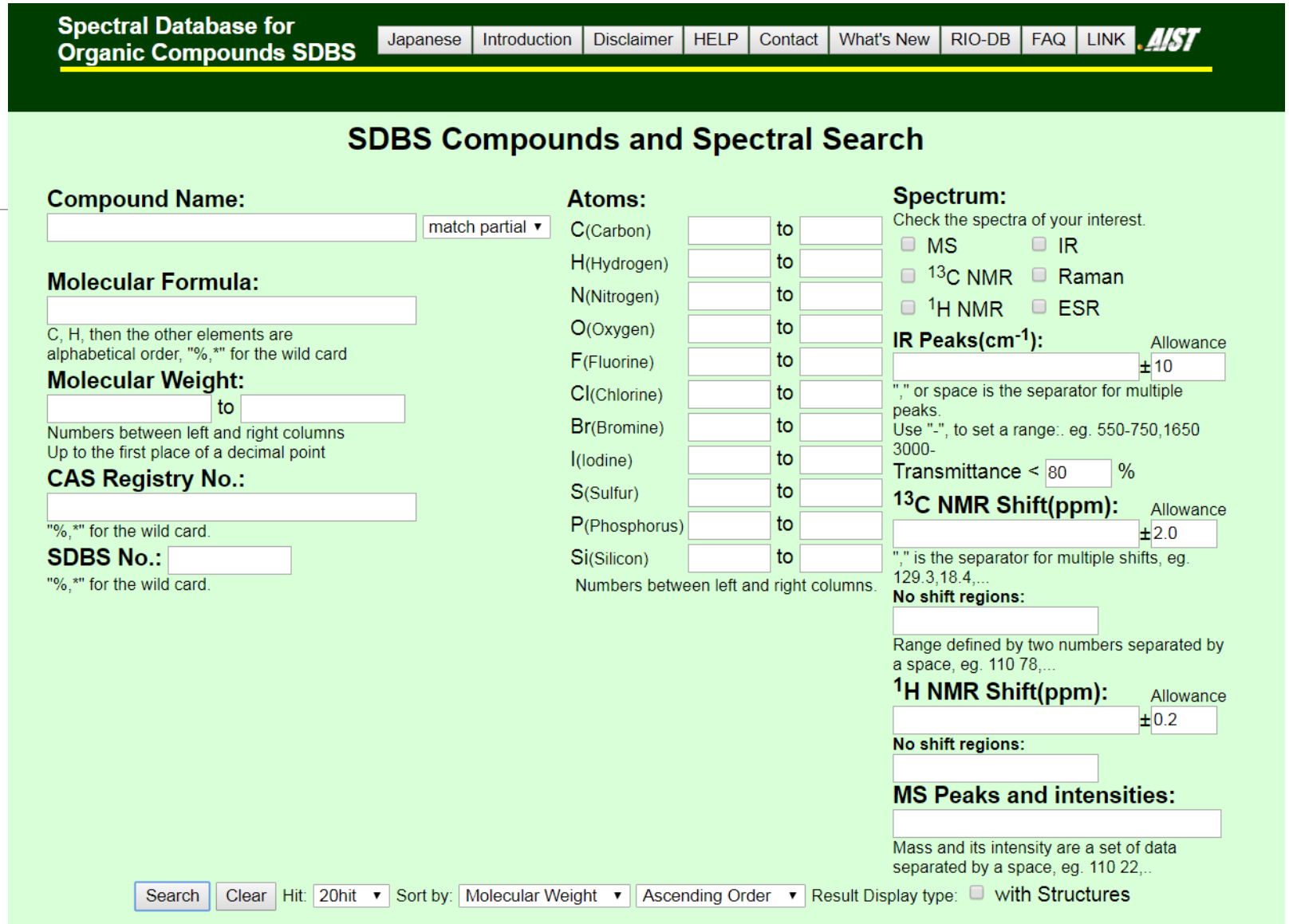




Spectral Database of Organic Compounds



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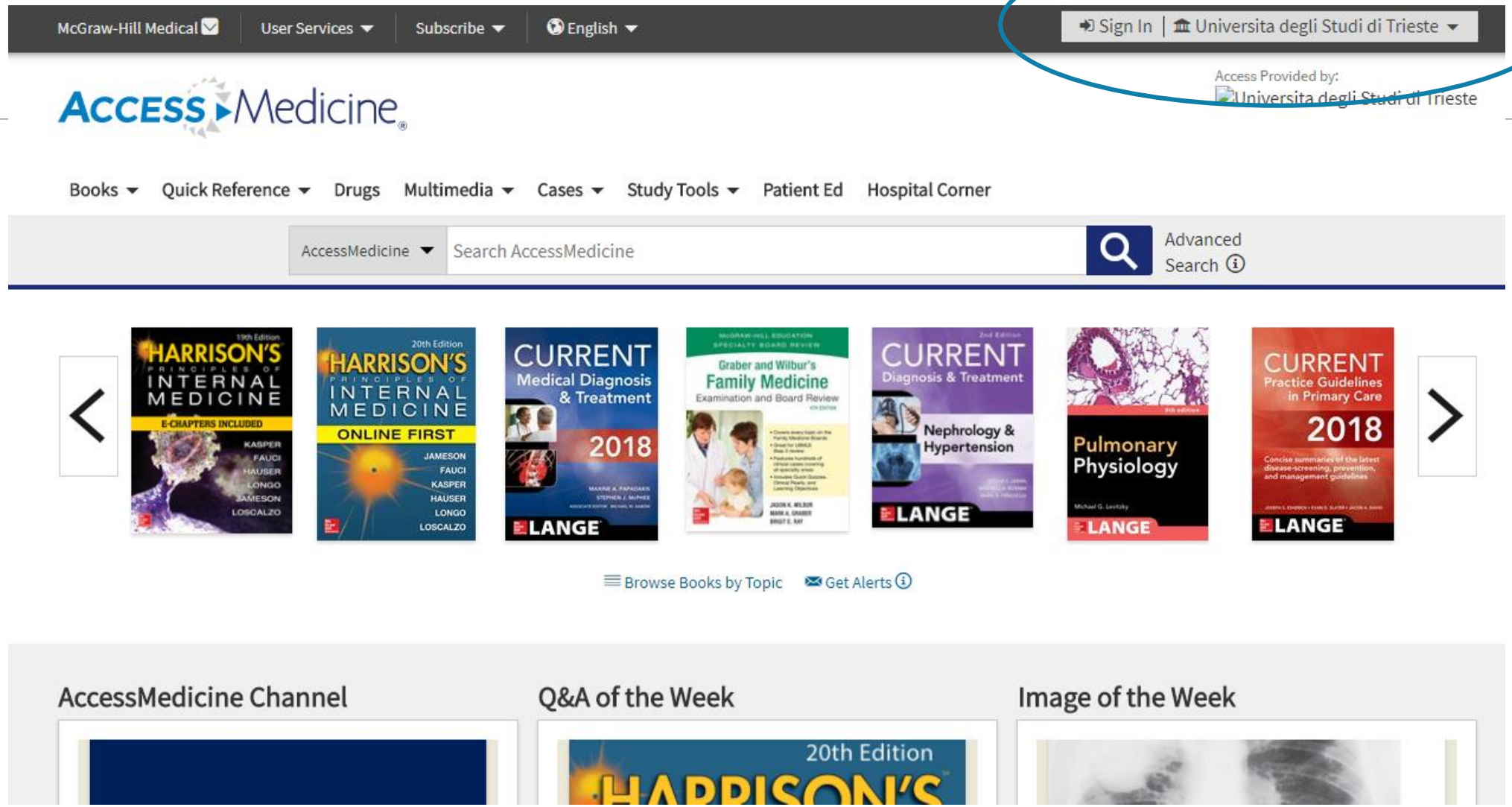

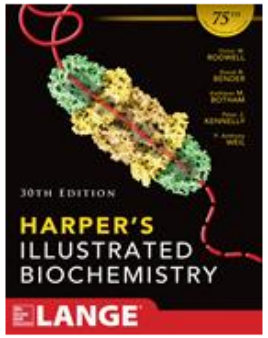

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CHAPTER 7

INTRODUCTION

BIOMEDICAL IMPORTANCE

ENZYMES ARE EFFECTIVE & HIGHLY SPECIFIC CATALYSTS

CHAPTER 7: Enzymes: Mechanism of Action

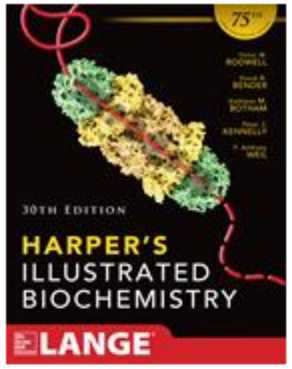
Peter J. Kennelly; Victor W. Rodwell

INTRODUCTION

OBJECTIVES

After studying this chapter, you should be able to:

- Appreciate and describe the structural relationships between specific B vitamins and certain coenzymes.
- Outline the four principal mechanisms by which enzymes achieve catalysis and how these mechanisms combine to facilitate catalysis.
- Describe the concept of an "induced fit" and how it facilitates catalysis.



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CHAPTER 7

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BIOMEDICAL IMPORTANCE

ENZYMES ARE EFFECTIVE & HIGHLY SPECIFIC CATALYSTS

ENZYMES ARE CLASSIFIED BY REACTION TYPE

PROSTHETIC GROUPS, COFACTORS, & COENZYMES PLAY IMPORTANT ROLES IN CATALYSIS

CATALYSIS OCCURS AT THE ACTIVE SITE

ENZYMES EMPLOY MULTIPLE MECHANISMS TO FACILITATE CATALYSIS

SUBSTRATES INDUCE CONFORMATIONAL CHANGES IN ENZYMES

HIV PROTEASE ILLUSTRATES ACID-BASE CATALYSIS

CHYMOTRYPSIN & FRUCTOSE-2, 6-BISPHOSPHATASE ILLUSTRATE COVALENT CATALYSIS