

# Database Developments

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*A Division of the American Chemical Society*

**Institute Ruđer Bošković**

**Paul Peters, 22 March 2000**

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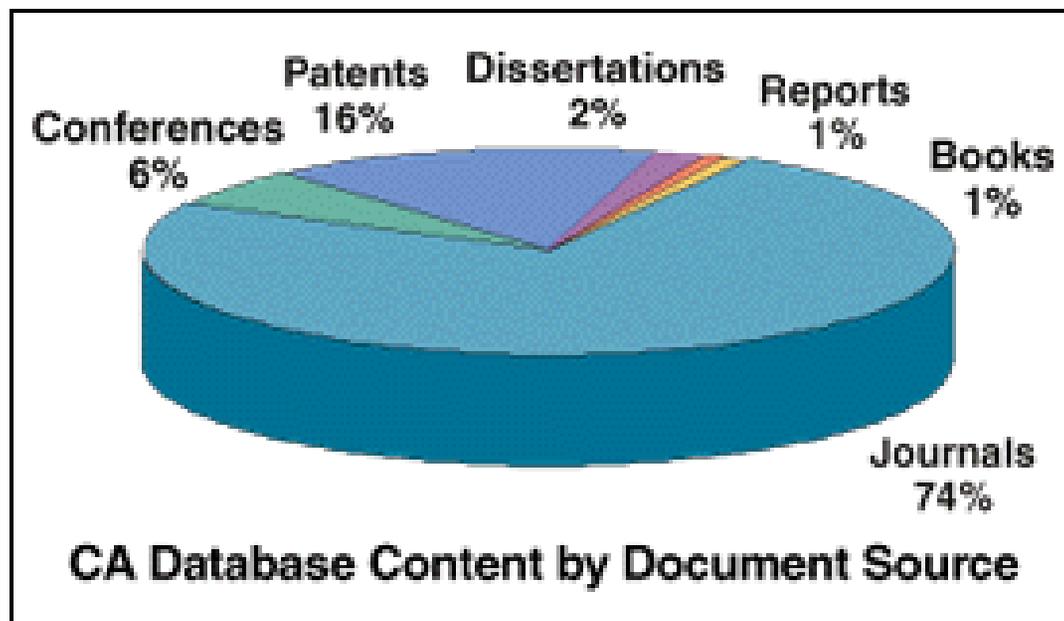
# ***CAS Scientists: Creating the CAS Databases for Scientists***



# CAplus: Comprehensive Abstracts in Science

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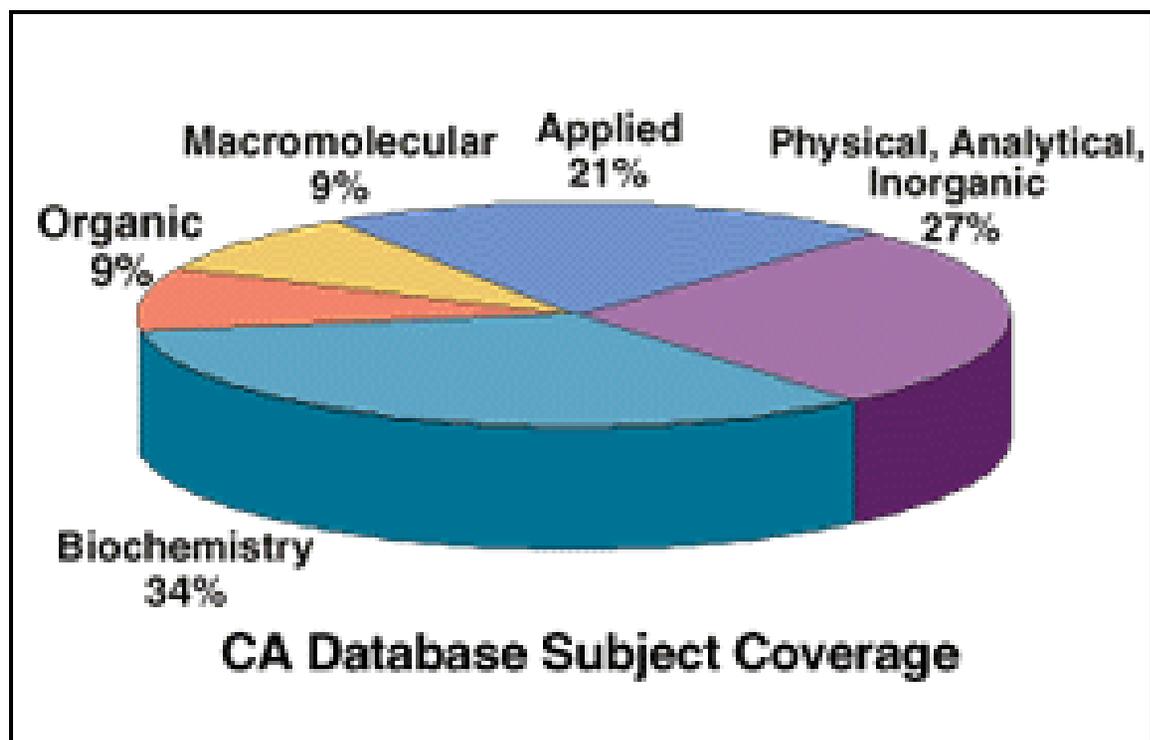
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# CAplus: Comprehensive Abstracts in Science

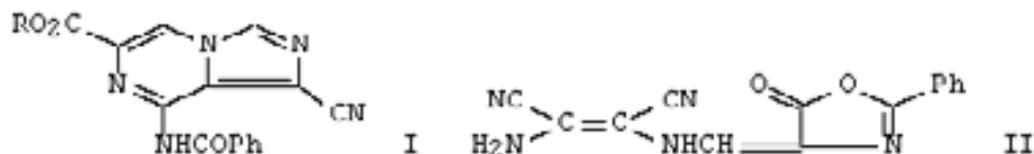
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- Large variety of subjects
- Chemistry related sciences



# CAplus: Sample Record

AN 1999:788576 CAPLUS [Full-text](#)  
DN 132:166211  
TI Use of diaminomaleonitrile in the synthesis of imidazo[1,5-a]pyrazines  
AU Trcek, Tomaz; Vercek, Bojan  
CS Fak. Kem. Kem. Tehnol., Univ. Ljubljana, Ljubljana, 1000, Slovenia  
SO Zb. Ref. Posvetovanja Slov. Kem. Dnevi (1999), 284-287. Editor(s):  
Glavic, Peter; Brodnjak-Voncina, Darinka. Publisher: Fakulteta za Kemijo  
in Kemijsko Tehnologijo Univerze v Mariboru, Maribor, Slovenia.  
CODEN: GOKMAE  
DT Conference  
LA Slovenian  
CC 20-17 (Heterocyclic Compounds (More Than One Hetero Atom))  
GI



AB Two new methods for the synthesis of imidazo[1,5-a]pyrazines (I; R = Et, Pr, Me<sub>2</sub>CH, Me<sub>2</sub>CHCH<sub>2</sub>, pentyl) are described. Both methods have the same starting material (II) but different sequences of opening of the oxazoline ring and formation of the imidazole ring.

# CAplus: Sample Record

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ST maleonitrile amino oxooxazolinylidenemethylamino conversion  
imidazopyrazine; imidazopyrazinecarboxylate benzamidocyano prepn

IT [122-51-0](#), Triethyl orthoformate CAS Registry  
number and Role  
RL: RCT (Reactant)  
(in imidazo[1,5-a]pyrazine deriv. prepn.)

IT [258338-24-8P](#) [258338-25-9P](#) [258338-26-0P](#) [258338-27-1P](#) [258338-28-2P](#)  
[258338-34-0P](#) [258338-35-1P](#) [258338-36-2P](#) [258338-37-3P](#) [258338-38-4P](#)  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and cyclization reaction with tri-Et orthoformate)

IT [258338-23-7P](#) [258338-29-3P](#) [258338-30-6P](#) [258338-31-7P](#) [258338-32-8P](#)  
[258338-33-9P](#)  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

IT [258338-22-6](#)  
RL: RCT (Reactant)  
(reaction with alcs. and with tri-Et orthoformate)



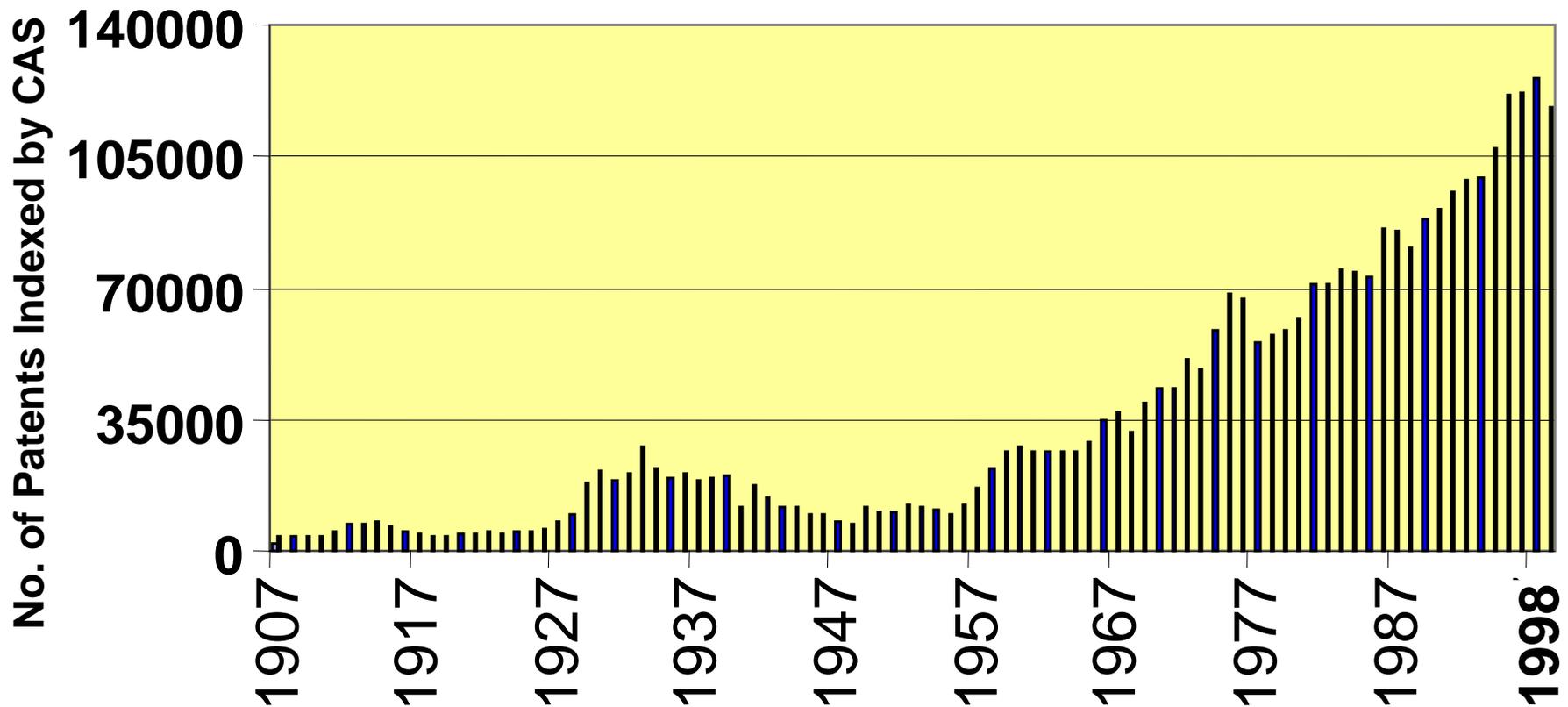
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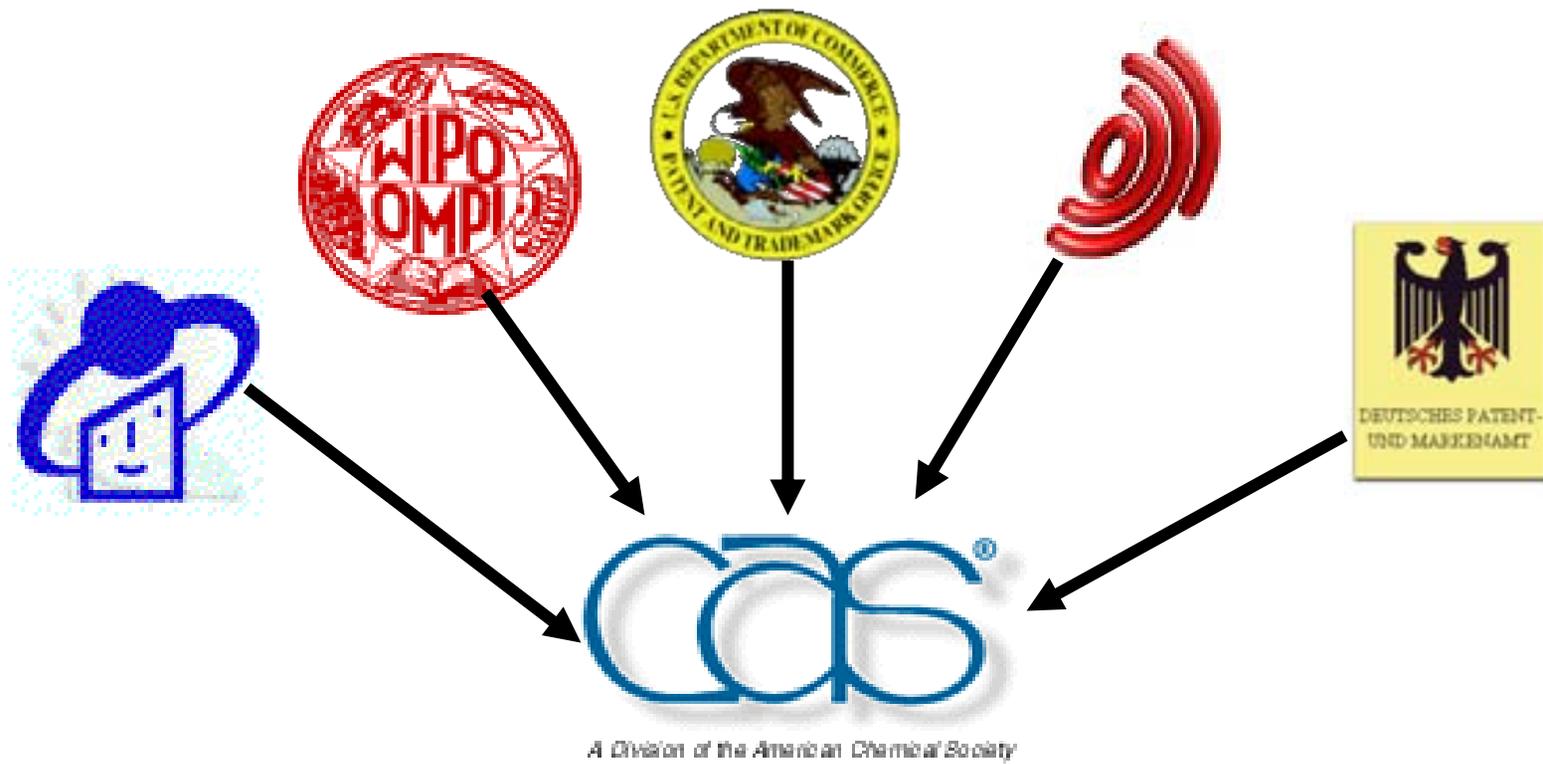


# Growth of Chemical Patents 1907-1999



# CAS works with patent offices to expedite addition of patent information into CAplus

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**Patent records are in CAplus database**

**2 days after issue**



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The following data was captured Mar 20th, 2000:

Patent Agency (ISO Code)	Fully indexed patent documents in CAplus are complete through issuing date:	CAplus is indexing patent information through:
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## Patent Coverage in Chemical Abstracts

### Summary

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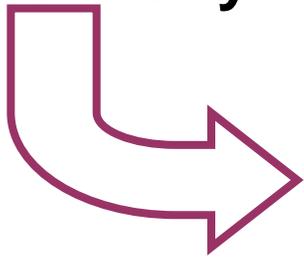
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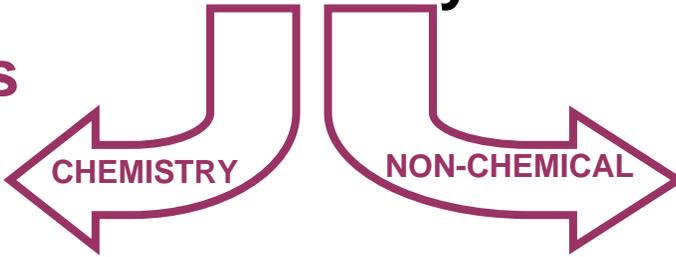
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# Links to Full-Text of Patents

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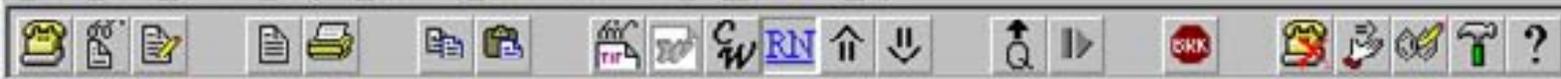
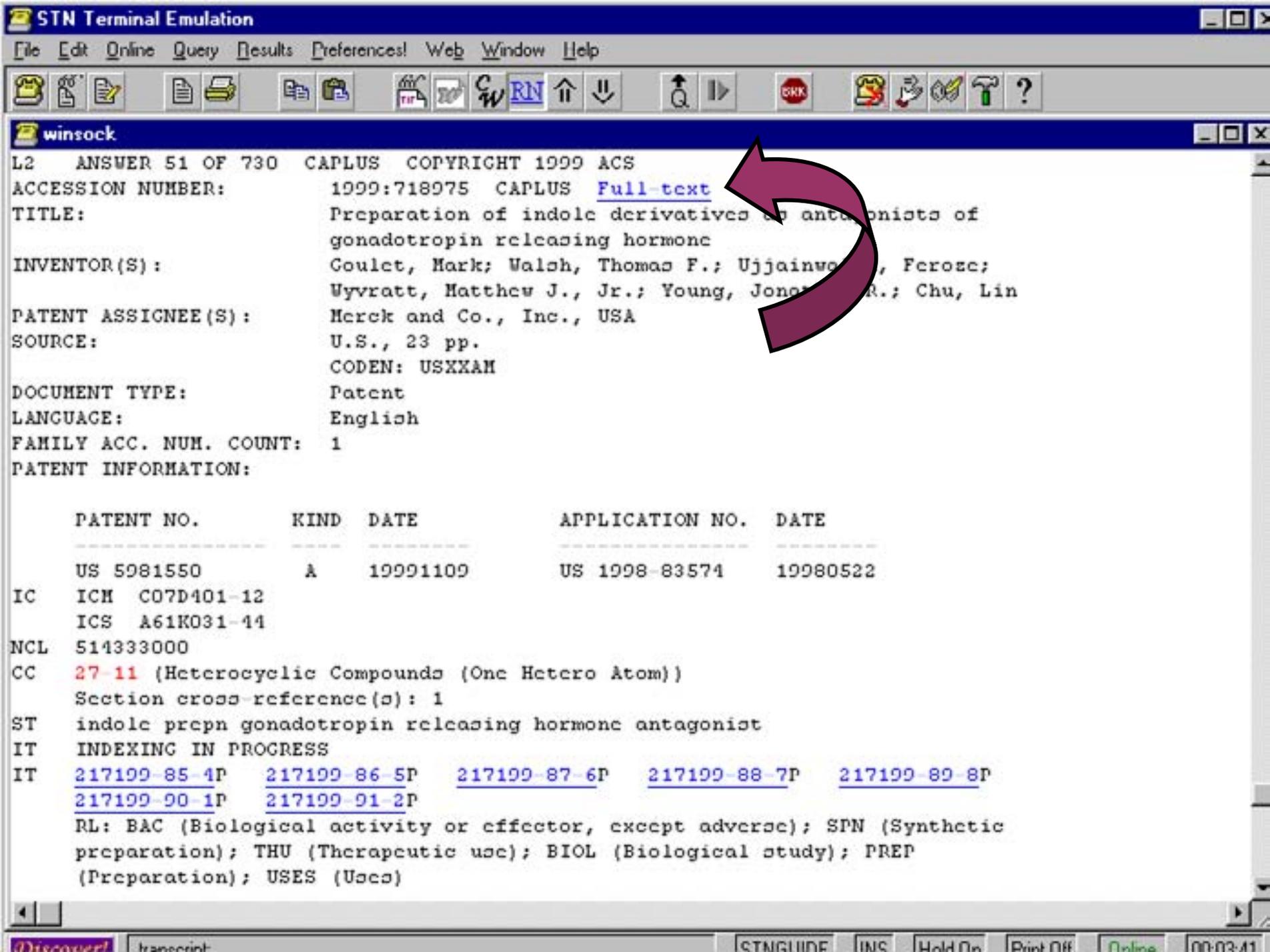
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- USPTO - from 1975 (partial 1972-1974)
- EPO

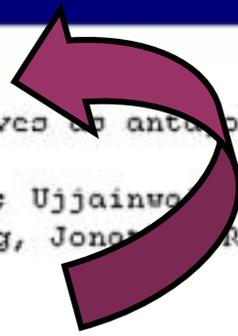
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L2 ANSWER 51 OF 730 CAPLUS COPYRIGHT 1999 ACS  
ACCESSION NUMBER: 1999:718975 CAPLUS [Full-text](#)  
TITLE: Preparation of indole derivatives as antagonists of  
gonadotropin releasing hormone  
INVENTOR(S): Coulet, Mark; Walsh, Thomas F.; Ujjainwal, Feroze;  
Wyvratt, Matthew J., Jr.; Young, Jonathan R.; Chu, Lin  
PATENT ASSIGNEE(S): Merck and Co., Inc., USA  
SOURCE: U.S., 23 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:



PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5981550	A	19991109	US 1998-83574	19980522

IC ICM C07D401-12  
ICS A61K031-44  
NCL 514333000  
CC 27-11 (Heterocyclic Compounds (One Hetero Atom))  
Section cross-reference(s): 1  
ST indole prepn gonadotropin releasing hormone antagonist  
IT INDEXING IN PROGRESS  
IT [217199-85-4P](#) [217199-86-5P](#) [217199-87-6P](#) [217199-88-7P](#) [217199-89-8P](#)  
[217199-90-1P](#) [217199-91-2P](#)  
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)



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**"Preparation of indole derivatives as antagonists of gonadotropin releasing hormone",**  
Patent Number: **US5981550**

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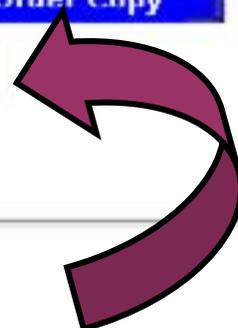
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United States Patent  
Goulet, et al.

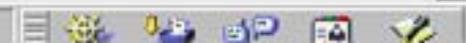
5,981,550  
November 9, 1999



### Antagonists of gonadotropin releasing hormone

#### Abstract

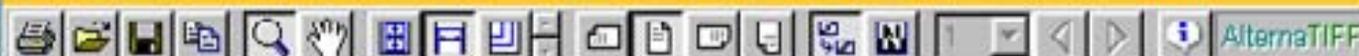
There are disclosed compounds of formula (I) ##STR.1## and pharmaceutically acceptable salts thereof which are useful as antagonists of GnRH and as such may be useful for the treatment of a variety of sex-hormone related and other conditions in both men and women.





Patent Number: 05981550

Section: Front Page 1 of 23 pages

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US0005981550A

**United States Patent** [19]

Goulet et al.

[11] Patent Number: **5,981,550**[45] Date of Patent: **Nov. 9, 1999**[34] ANTAGONISTS OF GONADOTROPIN  
RELEASING HORMONE[75] Inventors: **Mark Goulet**, Westfield; **Thomas F. Walsh**, Waching; **Feroze Ujjainwalla**, Edison; **Matthew J. Wyratt, Jr.**, Mountainside; **Jonathan R. Young**, Dayton; **Lin Chu**, Scotch Plains, all of N.J.[73] Assignee: **Merck & Co., Inc.**, Rahway, N.J.[21] Appl. No.: **09/083,574**[22] Filed: **May 22, 1998****Related U.S. Application Data**

[60] Provisional application No. 60/086,630, Jan. 5, 1997, and provisional application No. 60/048,742, Jan. 5, 1997.

[51] Int. Cl.<sup>5</sup> **C07D 401/12; A61K 31/44**[52] U.S. Cl. **514/333; 514/339; 514/361; 514/370; 514/365; 514/383; 514/372; 546/277.4; 546/256; 546/270.4; 546/270.7; 548/131; 548/128; 548/214; 548/184; 548/251**[58] Field of Search **546/277.4, 256; 546/270.4, 270.7; 548/131, 128, 214, 184, 251; 514/339, 333, 361, 370, 365, 383, 372**[56] **References Cited**

U.S. PATENT DOCUMENTS

4,544,063 10/1985 Manning et al. 314/378

0 219 292 A2 4/1987 European Pat. OE .  
 0 679 642 A1 11/1995 European Pat. OE .  
 2181559 12/1973 France .  
 WO90/05721 5/1990 WIPO .  
 WO95/70900 11/1995 WIPO .  
 WO97/21703 6/1997 WIPO .  
 WO97/21707 6/1997 WIPO .

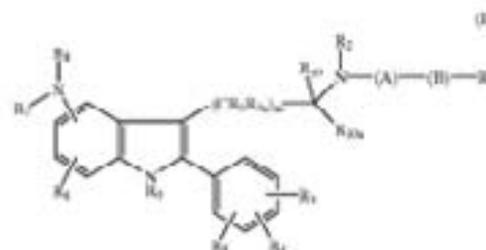
**OTHER PUBLICATIONS**

CA 124-233030, Bru-Magniere et al., 1996.  
 J. Med. Chem., vol. 32, pp. 2036-2038 (1989), by Clark, et al.

*Primary Examiner*—Jane Fan  
*Attorney, Agent, or Firm*—Elliott Kosen; Mark R. Daniel

[57] **ABSTRACT**

There are disclosed compounds of formula (I)



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Go to Page:

 Go


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# New to CAS Databases in 2000

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Citations  
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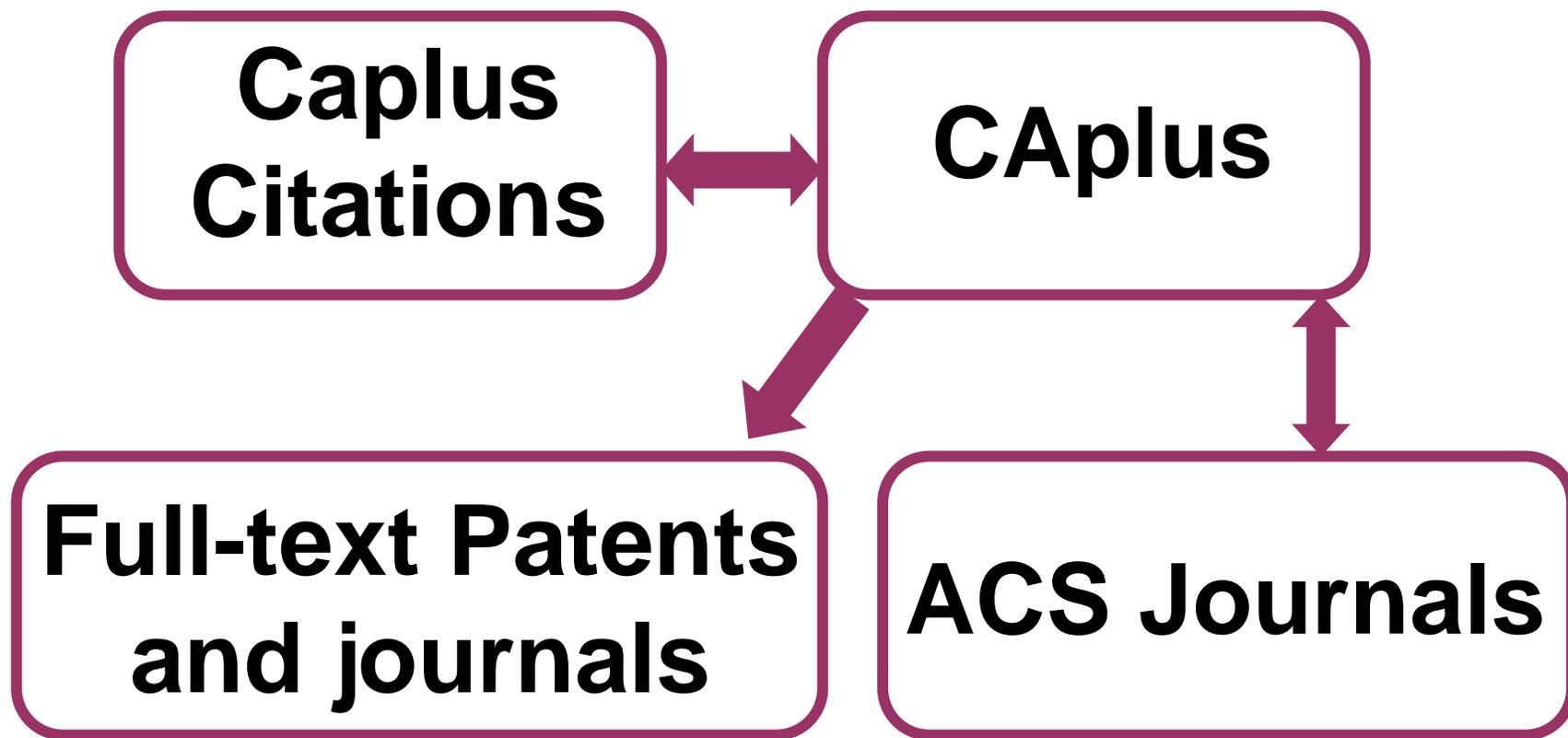
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# CAplus Citation -> Caplus Record

AN 1999:607401 CAPLUS  
TI Radical chain reactions of .alpha.-azido-.beta.-keto esters with tributyltin hydride. A novel entry to amides and lactams through regiospecific nitrogen insertion  
AU Benati, Luisa; Nanni, Daniele; Sangiorgi, Corrado; Spagnolo, Piero  
CS Dipartimento di Chimica Organica A. Mangini, Universita di Bologna, Bologna, I-40136, Italy  
SO J. Org. Chem. (1999), 64(21), 7836-7841

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RE.CNT 41

RE

- (1) Abramovitch, R; The Chemistry of The Azido Group 1971
- (2) Antkowiak, R; Bull Acad Polon Sci, Ser Sci Chim 1975, V23, P723
- (3) Antkowiak, R; 1976
- (4) Benati, L; J Chem Soc, Perkin Trans 1 1997, P457
- (5) Benati, L; J Org Chem 1998, V63, P4679
- (6) Benati, L; J Org Chem 1999, V64, P5132
- (7) Benati, L; Tetrahedron Lett 1978, P815

o o o



# CAplus Record -> Full-text

AN 1999:379050 CAPLUS [Full-text](#) ←

DN 131:144332

TI Reactions of Benzocyclic .beta.-Keto Esters with Sulfonyl Azides. 2. Further Insight into the Influence of Azide Structure and Solvent on the Reaction Course

AU Benati, Luisa; Nanni, Daniele; Spagnolo, Piero

CS Dipartimento di Chimica Organica A. Mangini, Universita di Bologna, Bologna, I-40136, Italy

SO J. Org. Chem. (1999), 64(14), 5132-5138  
CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

OS [CASREACT 131:144332](#)

AB The reactions of 2-ethoxycarbonyl-1-benzosuberone with 4-methoxybenzenesulfonyl, 2,4,6-triisopropylbenzenesulfonyl, methanesulfonyl, and trifluoromethanesulfonyl azide, in the presence of triethylamine, have been investigated in N,N-dimethylformamide, acetonitrile, or THF with the intent of clarifying the influence of both the azide electrophile and solvent on the reaction course. The present findings, in addn. to those previously obtained with tosyl and

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*J. Org. Chem.*, **64** (14), 5132 -5138, 1999. 10.1021/jo9901541 S0022-3263(99)00154-1

Web Release Date: June 17, 1999

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## Reactions of Benzocyclic $\beta$ -Keto Esters with Sulfonyl Azides. 2.<sup>1</sup> Further Insight into the Influence of Azide Structure and Solvent on the Reaction Course

Luisa Benati,<sup>\*</sup> Daniele Nanni, and Piero Spagnolo

*Dipartimento di Chimica Organica "A. Mangini", Università di Bologna, Viale Risorgimento 4, I-40136 Bologna, Italy*

*Received January 27, 1999*

### Abstract:

The reactions of 2-ethoxycarbonyl-1-benzosuberone with 4-methoxybenzenesulfonyl, 2,4,6-triisopropylbenzenesulfonyl, methanesulfonyl, and trifluoromethanesulfonyl azide, in the presence of triethylamine, have been investigated in *N,N*-dimethylformamide, acetonitrile, or tetrahydrofuran with the intent of clarifying the influence of both the azide electrophile and solvent on the reaction course. The present findings, in addition to those previously obtained with tosyl and 4-nitrobenzenesulfonyl azide, indicate that both the electronic features of the sulfonyl azide and the solvent polarity greatly affect

# Full-text Citation -> CAplus

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\* In papers with more than one author, the asterisk indicates the name of the author to whom inquiries about the paper should be addressed.

1. Part 1: Benati, L.; Calestani, G.; Nanni, D.; Spagnolo, P. *J. Org. Chem.* **1998**, *63*, 4679. [\[Full text - ACS\]](#)[\[CAS\]](#)
2. Doyle, M. P.; McKervey, M. A.; Ye, T. *Modern Catalytic Methods for Organic Synthesis with Diazo Compounds*, Wiley-Interscience: New York, 1998, Chapter 1. Ye, T.; McKervey, M. A. *Chem. Rev.* **1994**, *94*, 1091. Regitz, M.; Maas, G. *Diazo Compounds: Properties and Synthesis*, Academic Press: New York, 1986, Chapter 13.
3. Lombardo, L.; Mander, L. N. *Synthesis* **1980**, 368. [\[CAS\]](#) Coates, R. M.; Kang, H.-Y. *J. Org. Chem.* **1987**, *52*, 2065. [\[CAS\]](#) Uyehara, T.; Takehara, N.; Ueno, M.; Sato, T. *Bull. Chem. Soc. Jpn.* **1995**, *68*, 2687. [\[CAS\]](#) 
4. Evans, D. A.; Britton, T. C.; Ellman, J. A.; Dorow, R. L. *J. Am. Chem. Soc.* **1990**, *112*, 4011. [\[CAS\]](#)
5. Cavender, C. J.; Shiner, V. J., Jr. *J. Org. Chem.* **1972**, *37*, 3567. [\[CAS\]](#)
6. Zaloom, J.; Roberts, D. C. *J. Org. Chem.* **1981**, *46*, 5173. [\[CAS\]](#)



# Patent Citation Searching

AN 1999:460467 CAPLUS Full-text  
DN 131:88355  
TI Grafted poly(ethylene oxide) compositions  
IN Wang, James H.; Soerens, Dave A.; Schertz, David M.  
PA Kimberly-Clark Worldwide, Inc., USA

o o o

FAN.CNT 1

	<u>PATENT NO.</u>	<u>KIND DATEAPPLICATION NO.</u>	<u>DATE</u>
PI	WO 9933921 A1	19990708 WO 1998-US27703	19981229

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,  
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CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRAI US 1997-1831 19971231

AB The title poly(ethylene oxide) compns. Have polydispersity index less than

o o o

RE.CNT 5

- (1) Bayer Ag; EP 515949 A 1992
- (2) Chu Nan, S; US 3963805 A 1976
- (3) Michael, S; US 5700872 A 1997
- (4) Nippon Catalytic Chem Ind; EP 639592 A 1995
- (5) Vasta, J; US 5008322 A 1991



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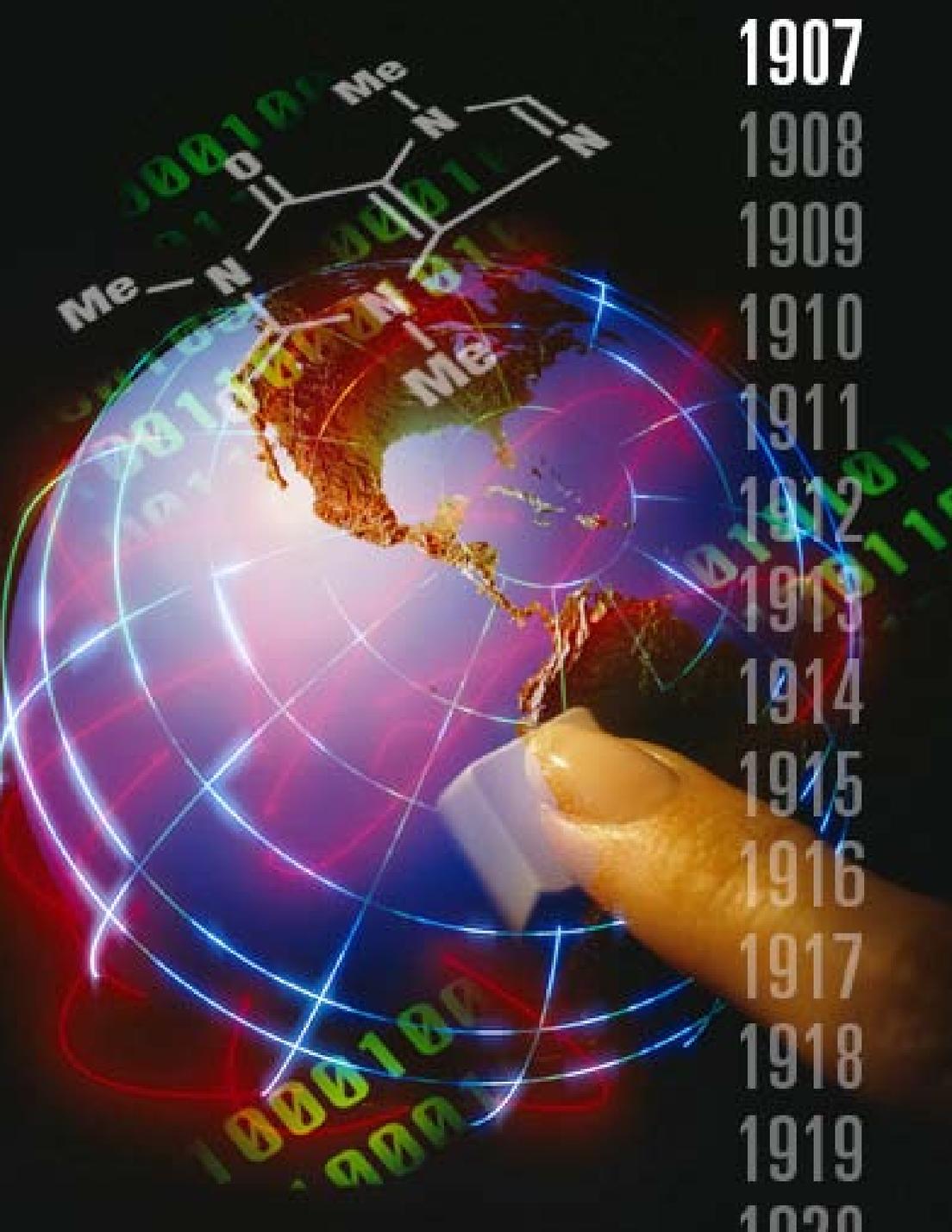
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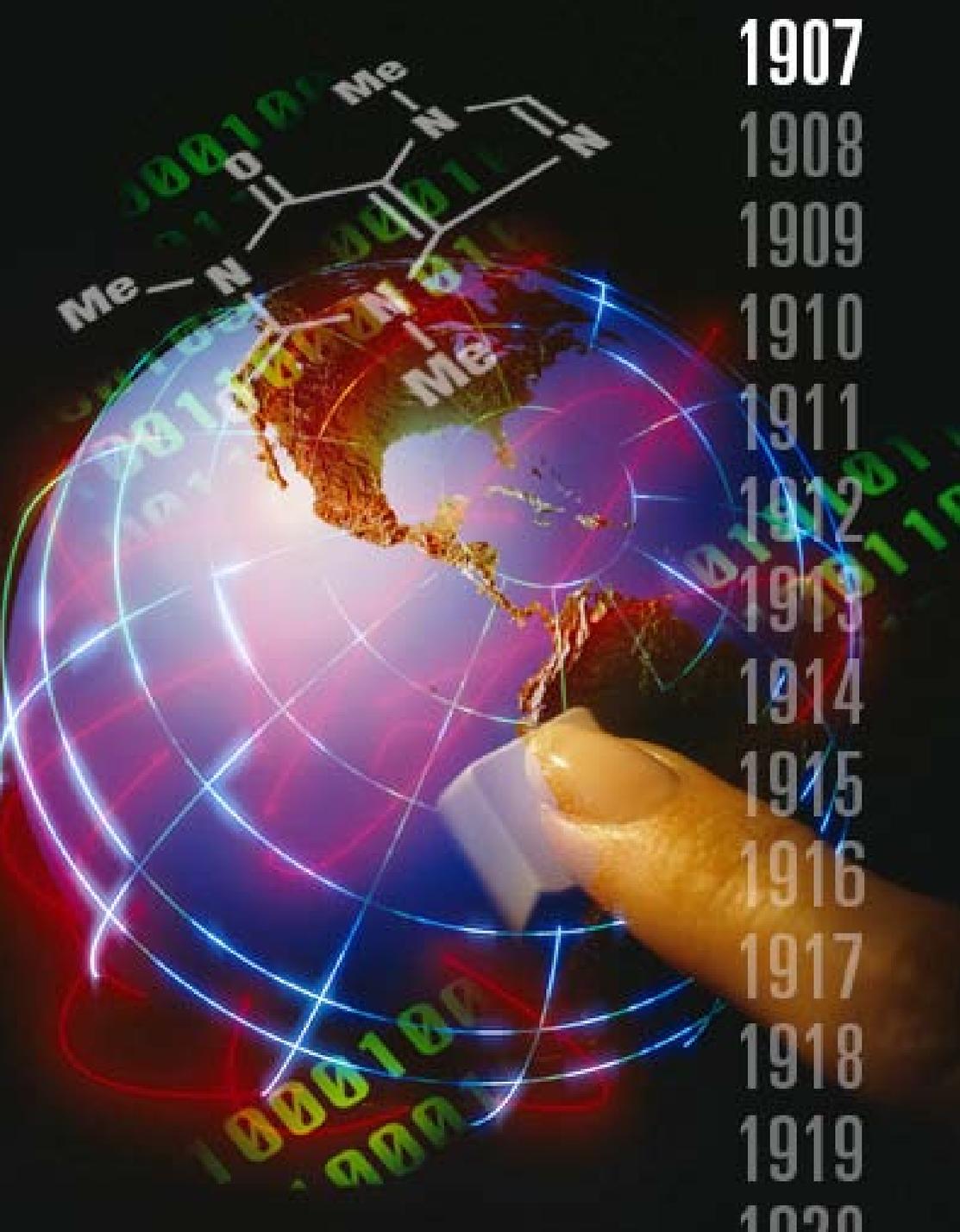
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DT  Patent
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7912

Vol. 63, 1965

ble that 2 OH groups be in these activating agents are not ads. The activating compd. stoichiometric proportion of the acid. The soln. so obtained of an aliphatic amine, such as acetic acid and 10 g. pyrogallol in 10 ml. aq. MeNH<sub>2</sub> (25-30% a

This soln. has a resistivity of 33, 4979 $\Omega$ . J. B. Doe

pure nickel strike. John A. U.S. 3,186,925 (Cl. 204-160; 3 pp. A pure Ni layer

the conventional dual layer Ni plating process. This results in

forming of Cr plated parts. free of all codeposited sub-

employed while the part to be plated. Bipolar effects, inorg.

and brighteners, believed to be causes causing poor adhesion,

the Ni layer. Watts-type Ni plating Ni layer. However, other

activating NiSO<sub>4</sub>, or contg. Ni-purifying methods such as

iodic dummying can be em-

4,7-Phenanthroline-5,6-dione. PLIVA Tvrnica Farmaceutskih i Kemijskih Proizvoda. Fr. 1,382,542 (Cl. C 07d), Dec. 18, 1964; Czech. Appl. April 9, 1963; 5 pp. The title compd. (I) is prepd. by electrolytic oxidn. of 6-methoxy-4,7-phenanthroline (II). The best results are obtained with a Pb electrode in an H<sub>2</sub>SO<sub>4</sub> medium at ambient temp. Thus, 10 wt. % II was introduced into the anode compartment of an electrolytic bath divided by a porous ceramic wall into anode and cathode compartments provided with Pb electrodes. The electrolytic oxidn. was begun at ambient temp. with mixing of the anodic electrolytic during application of d.c. of low c.d. The current was applied longer than the calcd. time. The anodic electrolyte was then neutralized with a Na<sub>2</sub>CO<sub>3</sub> soln. and filtered. The crude product was recrystd. from MeOH and dried at about 110° *in vacuo* to const. wt. I was obtained in good yield, m.p. 293-5°.

R. T. Stewart

Manufacture of lithium. Metallgesellschaft A.-G. (by Erich Thieler). Ger. 1,194,588 (Cl. C 22d), June 10, 1965, Appl. March 6, 1964; 2 pp. Li is made by fusion electrolysis of molten LiCl-contg. salt mixts. Gaseous Cl formed in the electrolysis is reacted in the electrolysis cell with O-contg. Li salts, preferably Li<sub>2</sub>CO<sub>3</sub>, and the salt mixt. is replenished with the formed LiCl. Preferably, Li<sub>2</sub>CO<sub>3</sub> is reacted with Cl in the anode compartment, LiCl forming on the surface of the melt.

Friedrich Epstein

# CAS Database Developments

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- CAplus
  - Patents
  - Citations
- CAOLD
- **Registry File**



# Registry contains >23 million substances of all types

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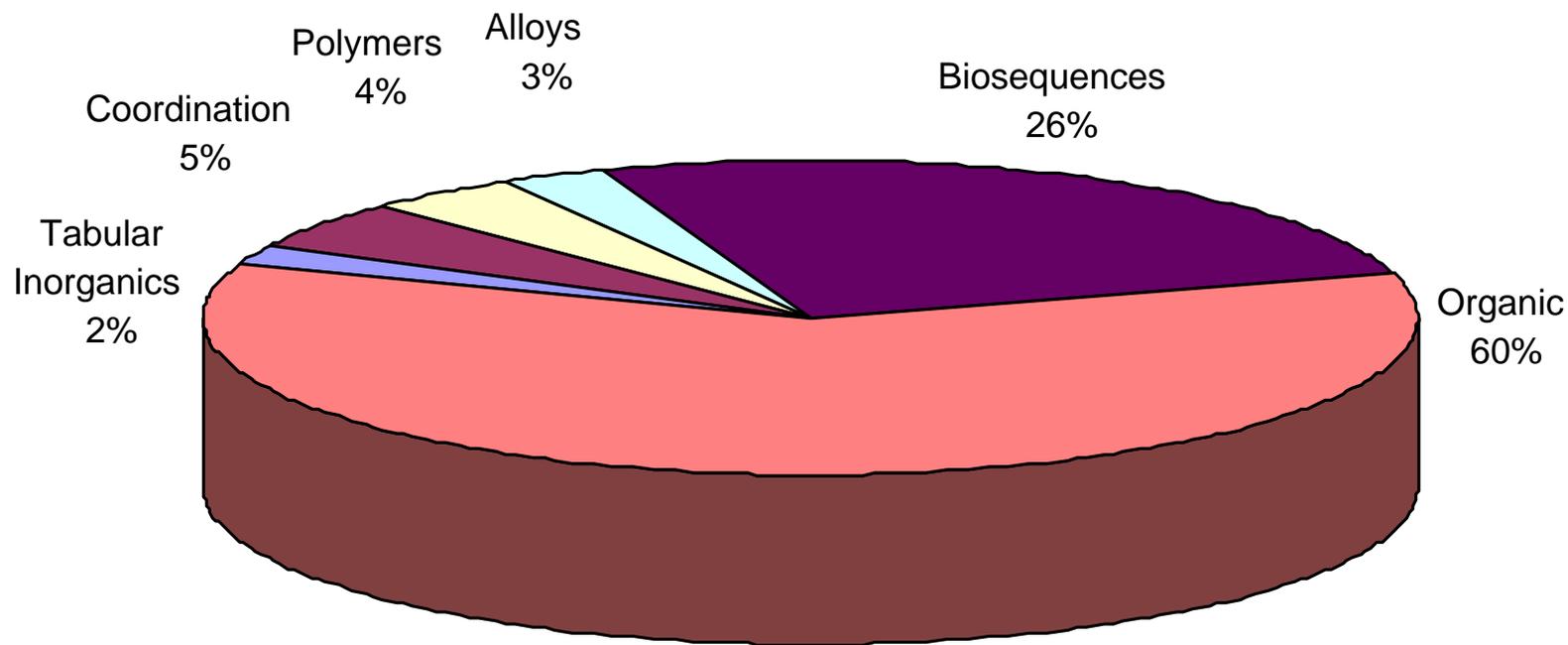
## The Latest CAS Registry Number® and Substance Count

Date	Sun Mar 19 08:36:09 EST 2000
Count	16,643,365 organic and inorganic substances
	6,547,778 sequences
Total	23,191,143 chemical substance registrations
CAS RN	259274-28-7 is the most recent CAS Registry Number



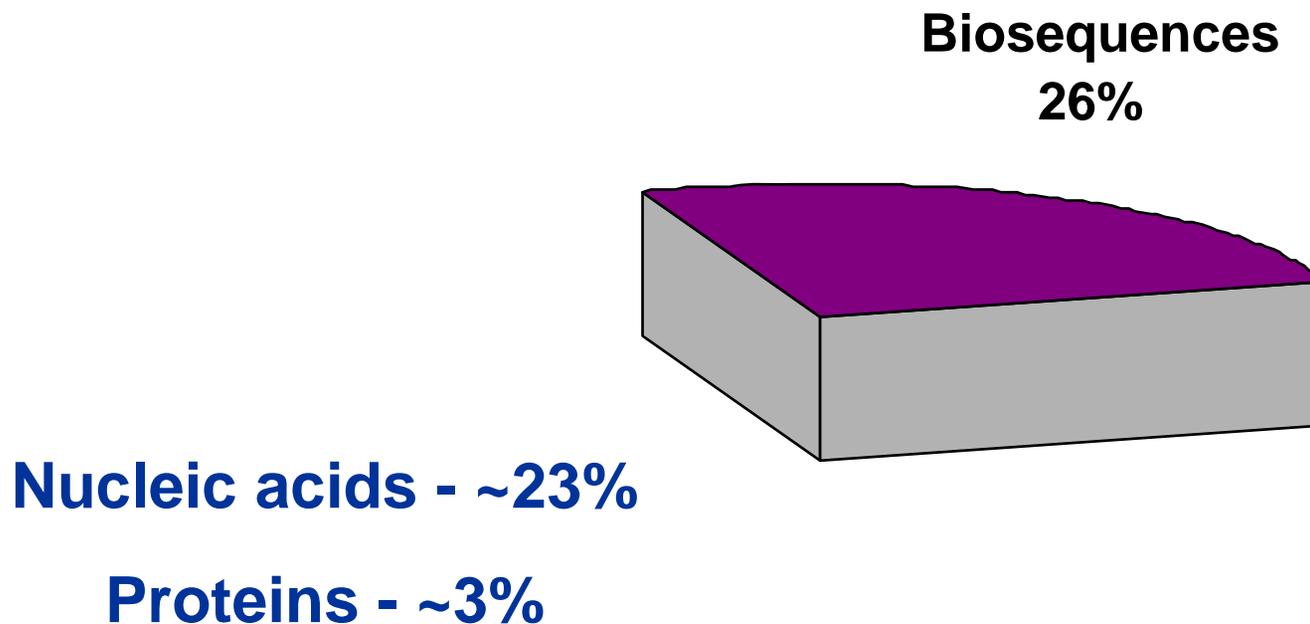
# Registry contains >23 million substances of all types

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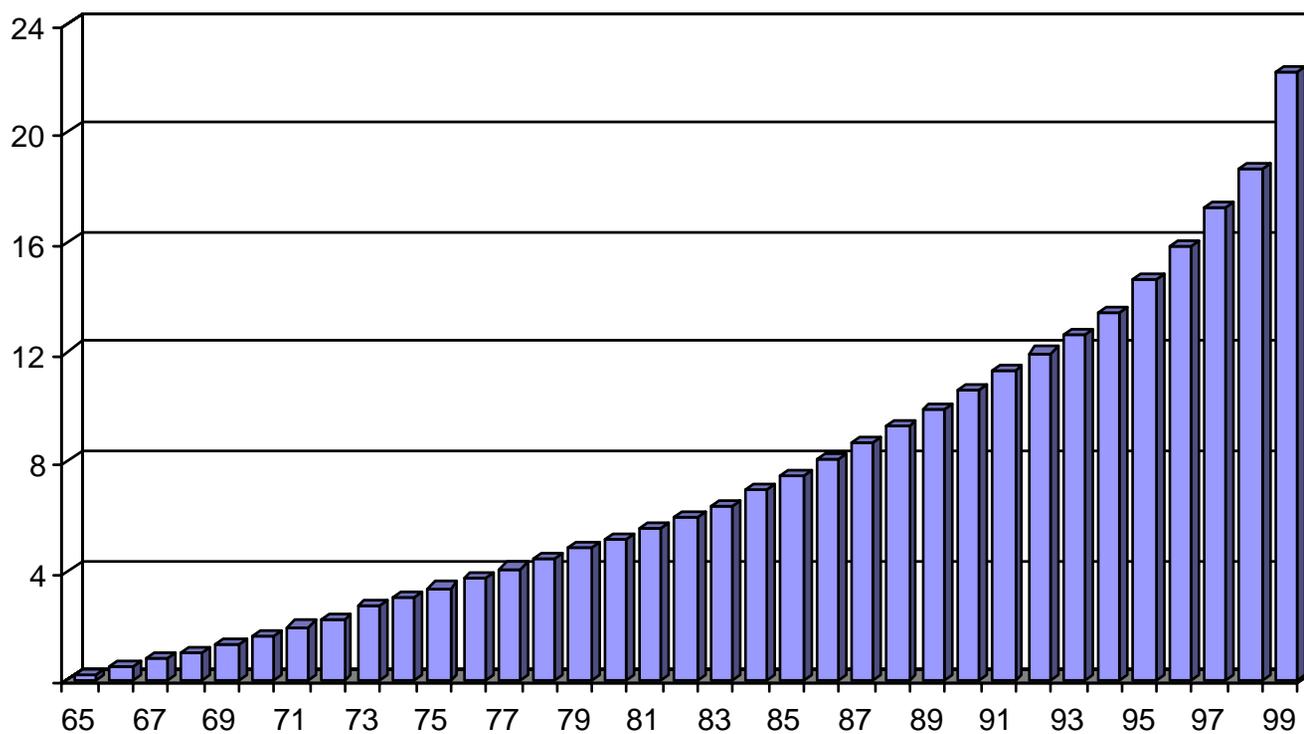
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# Every working day, we add nearly 11,000 substance registrations

---

Number of Substances in the Registry Database  
1965-1999



# Sequence Enhancements

---

- All sequences in patents are now assigned RN's (as of Oct 1999)
- The CN field now includes
  - the patent number
  - the location of the sequence in the patent

RN 97263-66-6 REGISTRY

CN Aequorin (Aequorea victoria precursor protein moiety reduced) (9CI)  
(CA INDEX NAME)

OTHER NAMES:

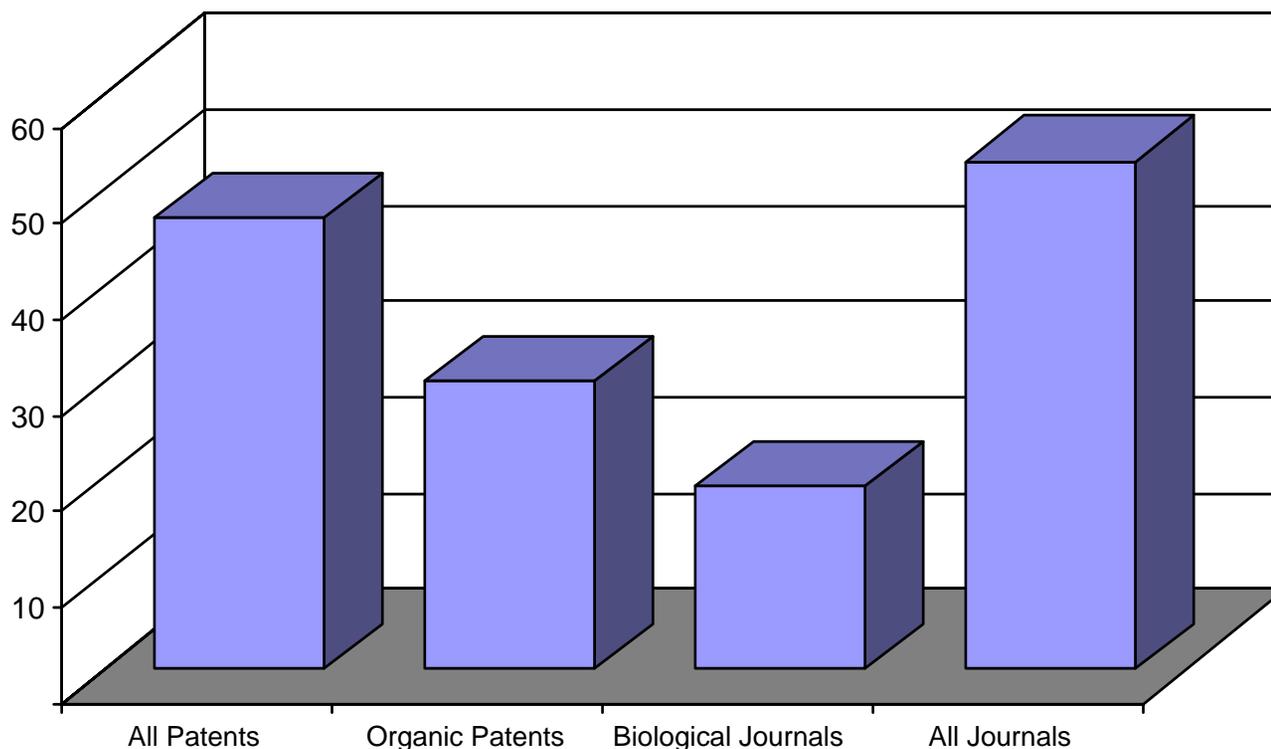
CN PN: WO9949019 SEQID: 5 unclaimed protein



# Organic Patents are a Significant Source of New Substance Registrations from the Literature

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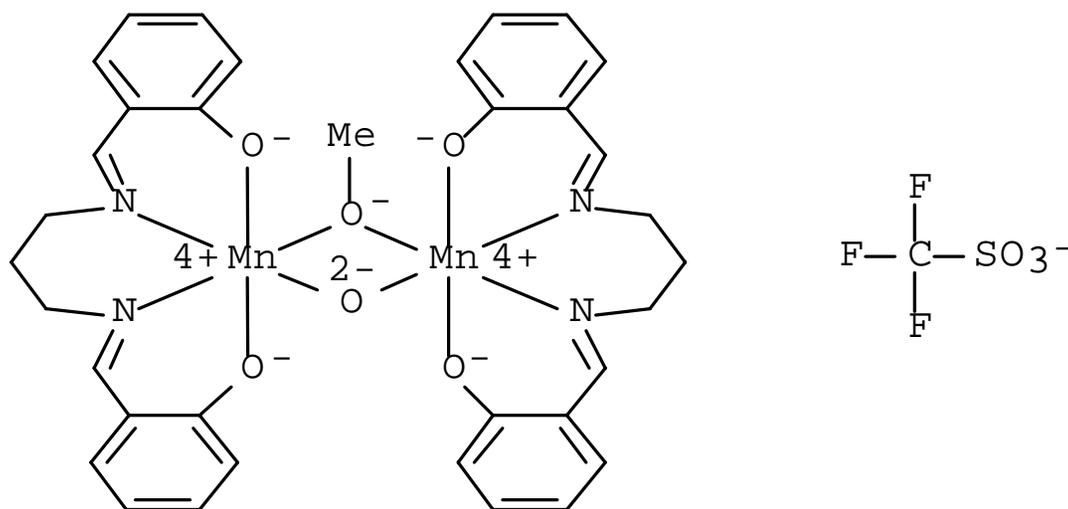
Percent of New Substance Registrations  
from 1998 Literature



# 22,000,000<sup>th</sup> Registry Record Assigned November 18, 1999

---

RN 247577-81-7



Manganese(1+), .mu.-methoxy-.mu.-oxobis[[2,2'-[1,3-propanediylbis[(nitrilo-  
.kappa.N)methylidyne]]bis[phenolato-.kappa.O]](2-)]di-, stereoisomer, salt  
with trifluoromethanesulfonic acid (1:1)

# 23,000,000<sup>th</sup> Registry Record Assigned March 2nd, 2000

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RN 257260-79-0

```
1 ggtaccatat ttgggtaaac actcttttgg tataatttat gtttttagtcc
51 aatgtcttgg gatgaaaatg acaggtgggc cacttatgat ctccagagaa
101 attcagggca atttgggtgtg ggagtaggca tggtagagga gagcagcatc
151 taagaagtcc ccagcagagg ctctcagctt gtcttgaggc atctggggcgg
201 agggctatga tactggcccc atcctgcaga aggtggcaga tattggcagc
251 tggcaccagt gcggttccat tgtgatcatc atttctcgaa cgtcagactg
301 ttgaagggtc ccccaacaga ctttctgtgc aactttctgt cttcacaaa
351 ttcagtcac agtaaggaag tgaattaat ttcagaggtg tagggagggc
401 ttaagggagt gtggtaaaat tagaggtgt tcagaaacag aaatctgacc
451 gcttggggcc accttgcagg gagagtttt ttgatgatcc ctcacttggt
501 tctttgcatg ttggcttagc ttggcgggct cccaactggt gactgggttag
551 tgatgaggct gtgtgcttct gagctgggca tccgaaggca tccttgggga
601 agctgagggc acgaggaggg gctgccagac tccgggagct gctgcctggc
651 tgggattc
```

Nucleotide found in patent US6022741, "DNA regulating expression of class II transactivator (CIITA) gene, chimeric genes containing CIITA regulatory element, and cells containing the chimeric genes", assigned to the University of North Carolina at Chapel Hill, granted on Feb. 8th, 2000



# Research in Croatia

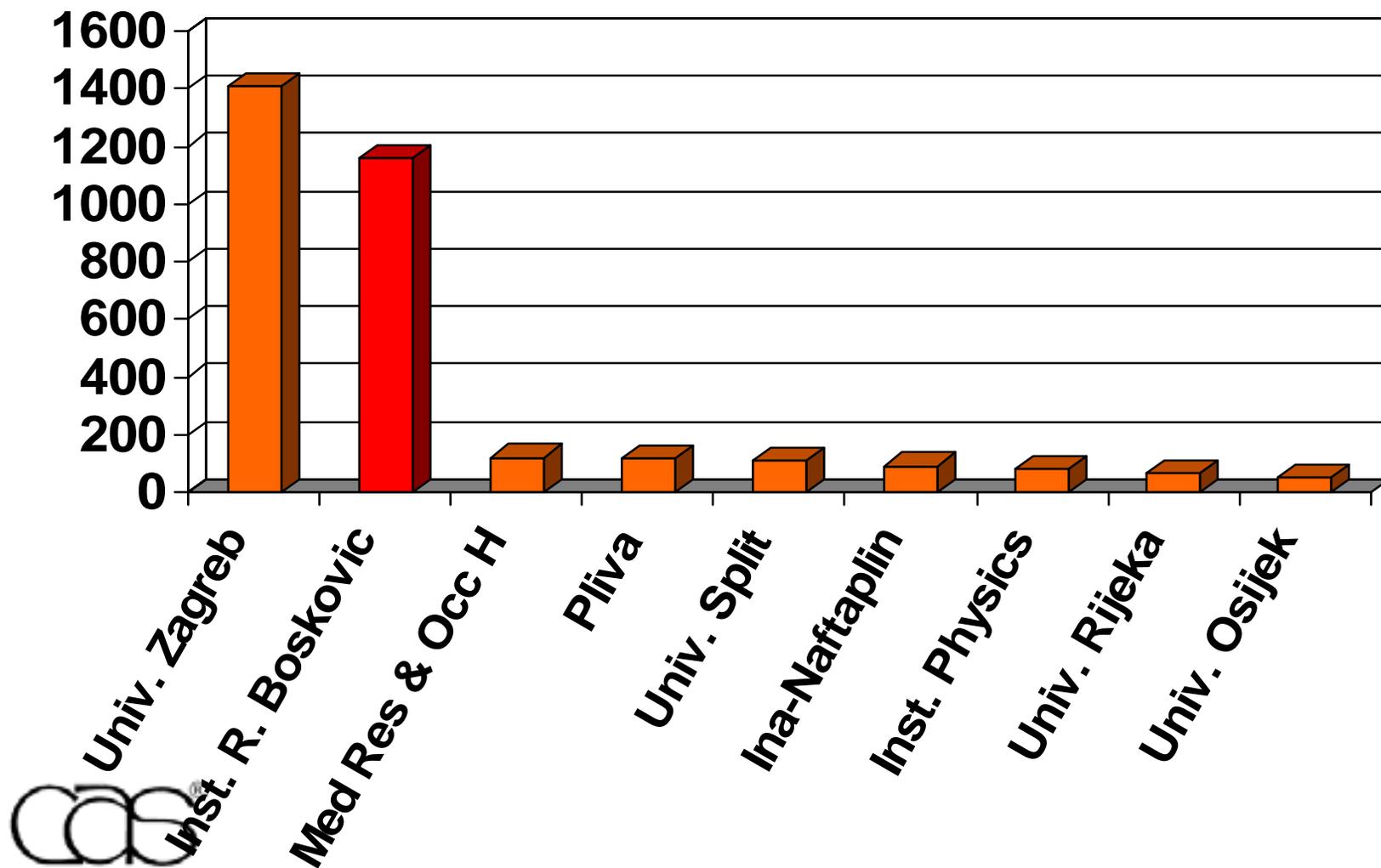
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- **Publications by Croatian organisations in CAplus (1995-)**
- **Publications by departments at Inst. Ruđer Bošković**
- **Publications by selected authors at Dept of Marine Research**

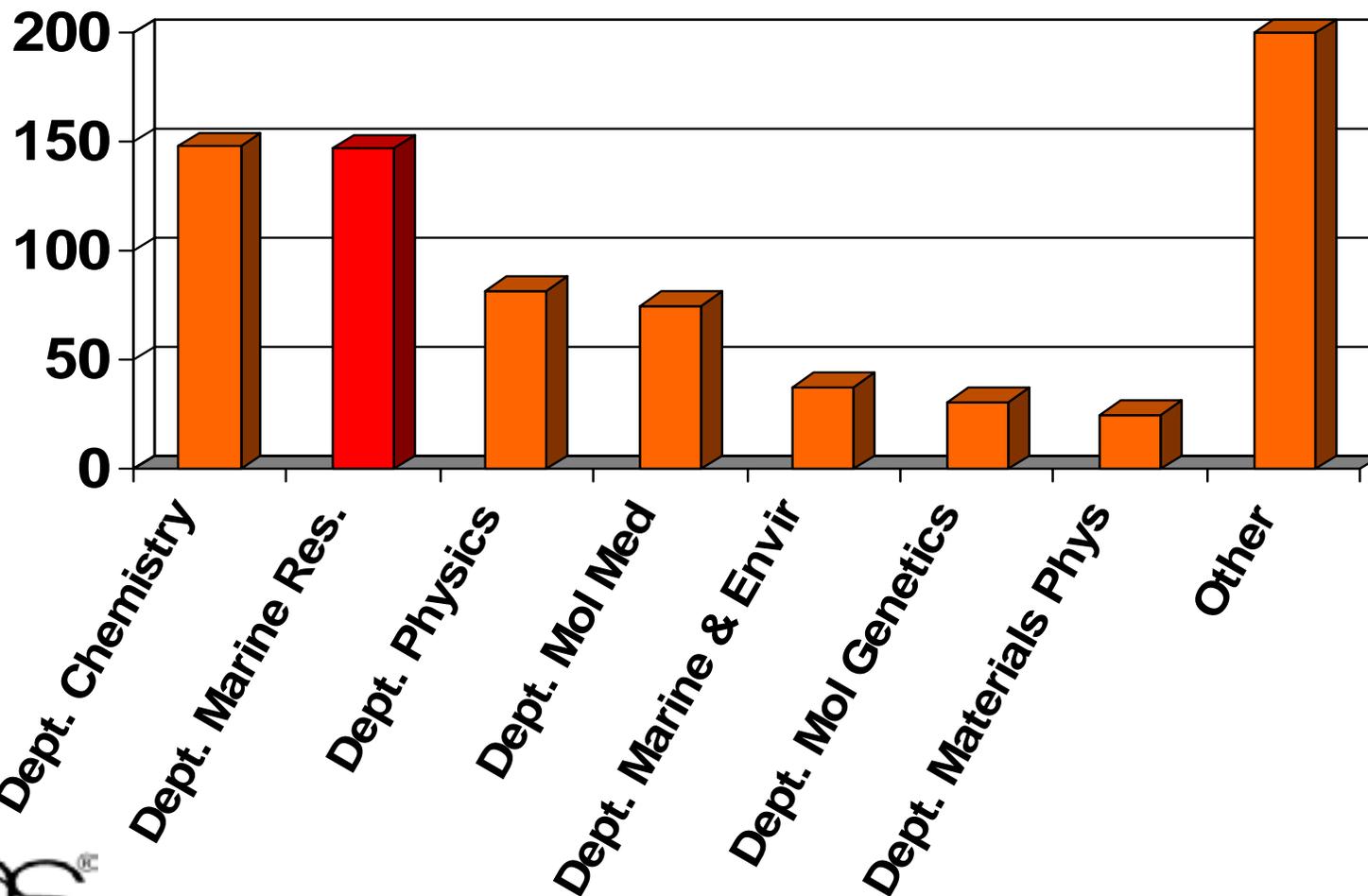
# Research in Croatia (1995-)

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# Research at Institute Ruđer Bošković (1995-)

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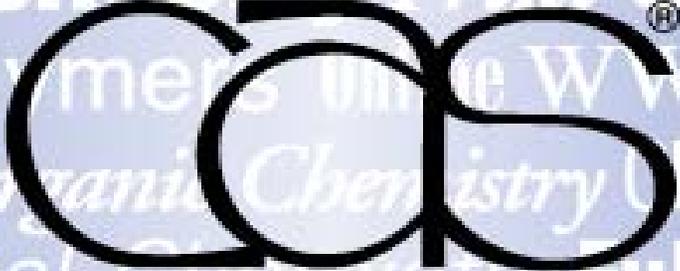
# Authors in Dept. of Marine Res, Institute Ruđer Bošković

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Author	CAplus	Biosis	SciSearch	Aquasci
	1967-	1969-	1974-	1978-
LOVRIC, M.	106	12	101	3
COSOVIC, B.	91	42	74	27
KOMORSKY-LOVIC	67	8	55	0
BRANICA, M.	225	64	140	155
RASPOR, B.	41	21	29	21
PRAVDIC, V.	59	15	46	21
AHEL, M.	48	37	39	19

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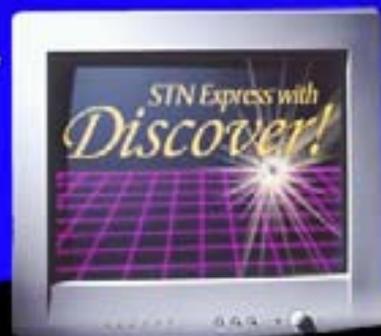
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  - 4 collectives on CD 1982-1996
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# Easy Access to Substance Information with Hyperlinked CAS RN's

```
SUPPL. TERM:      manjiejing emulsion miticide anticocccoideal agent
INDEX TERM:       Tea products
                  (chaku: prodn. of manjiejing emulsion for getting rid of
                  mite and coccoidea)
INDEX TERM:       Acaricides
                  Coccidiostats
                  Detergents
                  Diesel fuel
                  (prodn. of manjiejing emulsion for getting rid of mite
                  and coccoidea)
INDEX TERM:       Alums
                  Resin
                  ROLE: AGR (Agricultural use); BIOL (Biological study); USES
                  (Uses)
                  (prodn. of manjiejing emulsion for getting rid of mite
                  and coccoidea)
INDEX TERM:       532-32-1, Sodium benzoate 1310-73-2, Sodium hydroxide,
                  biological studies 7704-34-9, Sulfur, biological studies
                  ROLE: Get additional data from STN use); BIOL (Biological study); USES
                  (Uses)
                  (prodn. of manjiejing emulsion for getting rid of mite
                  and coccoidea)
INDEX TERM:       67-64-1, Acetone, uses
                  ROLE: NUU (Nonbiological use, unclassified); USES (Uses)
                  (prodn. of manjiejing emulsion for getting rid of mite
```



# Quickly Find Additional Patent Information

ACCESSION NUMBER: 1999:226159 CAPLUS [Full-text](#)  
DOCUMENT NUMBER: 130:219478  
TITLE: Production of manjiejing emulsion for getting rid of mite and coccoidea  
INVENTOR(S): Jiang, Tuling  
PATENT ASSIGNEE(S): Peop. Rep. China  
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 5 pp.  
CODEN: CNXKEV  
DOCUMENT TYPE: Patent  
LANGUAGE: Chinese  
INT. PATENT CLASSIF.:  
MAIN: A01N065-00  
CLASSIFICATION: S-4 (Agrochemical Bioregulators)  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE
CN 1123603	A	19960605

You have selected PN CN 1123603

Get Legal Status  
Get English Language Equivalents  
Get Extended Patent Family Information

## ABSTRACT:

The title manjiejing emulsion is composed of pine gum powder 15-23.5, withered tea 7-15, sulfur and diesel oil 2-3, NaOH 4-4.5, Na benzoate and alum 0.4-0.5, acetone and detergent 0.8-1.1%. The emulsion is prepd. by heating water and diesel oil in iron barrel at 55.degree., adding sulfur powder, alum, NaOH, pine gum powder, and **filtered** withered tea (chaku) ext., stirring at 100.degree. for 10 min, and keeping for 20-40 min, adding Na benzoate, acetone



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<input type="checkbox"/> <a href="#">Chemistry &amp; Chemicals</a>	<input checked="" type="checkbox"/> <a href="#">Patents</a>	<input checked="" type="checkbox"/> <a href="#">CAplus (Patents focus)</a>
<input checked="" type="checkbox"/> <a href="#">Intellectual Property (Patents)</a> ▶▶▶	<input type="checkbox"/> <a href="#">Patents, Citations</a>	<input checked="" type="checkbox"/> <a href="#">CAOLD (Patents focus)</a>
<input type="checkbox"/> <a href="#">Agriculture &amp; Food</a>	<input type="checkbox"/> <a href="#">Patents, Fulltext</a>	<input checked="" type="checkbox"/> <a href="#">DPCI database</a>
<input type="checkbox"/> <a href="#">Business</a>	<input type="checkbox"/> <a href="#">Patents, International</a>	<input checked="" type="checkbox"/> <a href="#">EUROPATFULL database</a>
<input type="checkbox"/> <a href="#">Energy &amp; Environment</a>	<input type="checkbox"/> <a href="#">Patents, National</a>	<input checked="" type="checkbox"/> <a href="#">IFIPAT database</a>
<input type="checkbox"/> <a href="#">General</a>		<input checked="" type="checkbox"/> <a href="#">INPADOC database</a>
<input type="checkbox"/> <a href="#">Health &amp; Medicine</a>		<input checked="" type="checkbox"/> <a href="#">JAPIO database</a>
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<input type="checkbox"/> <a href="#">Regulatory</a>		<input checked="" type="checkbox"/> <a href="#">UISPATFULL database</a>
<input type="checkbox"/> <a href="#">Technology &amp; Engineering</a>		<input checked="" type="checkbox"/> <a href="#">WPINDEX database</a>
		<input type="checkbox"/> Make these selections my default.

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# Bringing CAS database to the end-user's desktop

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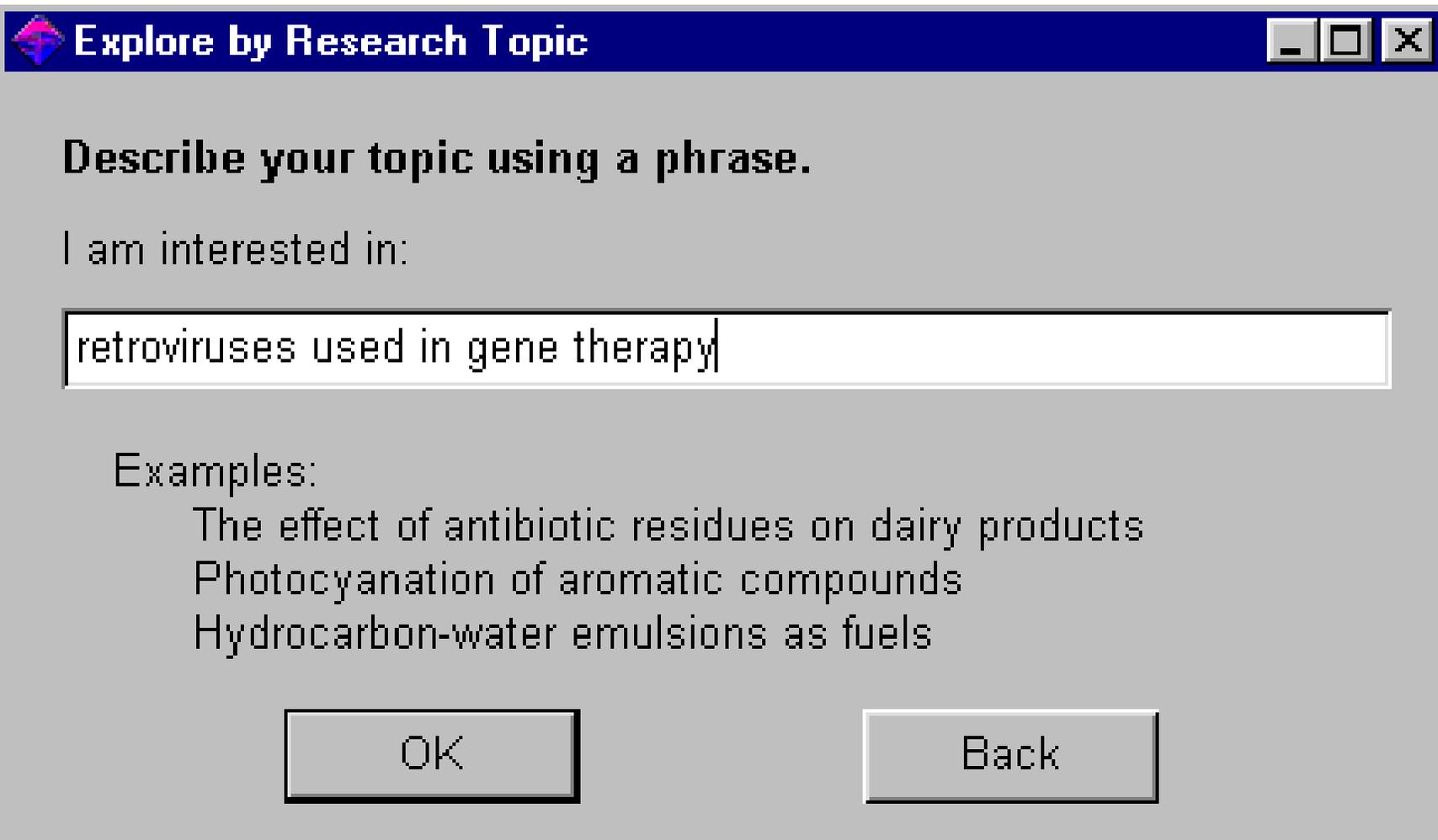
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# Explore by Research Topic



**Explore by Research Topic** [-] [ ] [X]

**Describe your topic using a phrase.**

I am interested in:

Examples:

- The effect of antibiotic residues on dairy products
- Photocyanation of aromatic compounds
- Hydrocarbon-water emulsions as fuels

CCB

# Explore by Research Topic

The image shows a web browser interface with two main panels. The left panel displays a list of search results, and the right panel shows the detailed view of a selected reference.

**Left Panel (Search Results):**

- Lebouloch, Philippe; Westerman, Karen. **Novel h** WO 9958701 A1 19991118 AN 1999:736961
- Matsukura, Norio; Hoshino, Arichika; Igarashi, Tak Osamu; Akiyama, Katsuhiko; Goto, Takashi; Taku **suicide gene therapy of gastric cancer induce** (1999), 90(9), 1039-1049. CODEN: JICREP ISS
- Schlom, Jeffrey; Hodge, James W. **The diversity** Immunol Rev. (1999), 170 73-84. CODEN: IMRI
- Kuriyama, S.; Mitoro, A.; Yamazaki, M.; Tsujinori Fukui, H. **Comparison of gene therapy with th** **cytosine deaminase gene for the treatment of** 1033-1041. CODEN: SJGRA4 ISSN:0036-5521.
- Tang, Zhanyun; Sun, Wenchang; Chen, Shishu. **HSV-TK gene.** Zhonghua Zhongliu Zazhi (1999) CAPLUS
- Amara, Jane F.; Courage, Nancy L.; Gilman, Mich **chimeric human protein.** Hum. Gene Ther. (1 1999:728826 CAPLUS
- Sacco, MG; Benedetti, S.; Calo, E; Mira, Caniatti, Vezzoni, P. **Retrovirus-mediated IL-4 gene the** **mice.** Gene Ther (1999), 6(11), 1893-1897. C
- Yu, H.; Eton, D.; Wang, Y.; Kumar, SR; Tang, L.; **vitro gene transfer into vascular tissues using** Ther. (1999), 6(11), 1876-1883. CODEN: GETH
- Uto, Hirofumi; Ido, Akio; Hori, Takeshi; Hirono, Shi **Hepatoma Specific Gene Therapy through Rel** **Carrying the Ecotropic Receptor Gene.** Biocl BBRC99 ISSN:0006-291X. AN 1999:720681 C
- Rigden, Justin E.; Ely, Julie A.; Macpherson, Jane **ribozyme gene therapy for the inhibition of HI** (1999) 255-270. CODEN: BRWAY AN 1999:7

**Right Panel (Detail of Reference 34):**

**Bibliographic Information**

**Cloning, sequence, expression and therapeutic use of human DNA topoisomerase I  $\alpha$**  Wei, Ying-fei; Adams, Mark D.; Fleischmann, Robert D. (Human Genome Sciences, Inc., USA). U.S. (1999), 27 pp. CODEN: USXXAM US: 5968803 A 19991019 Patent written in English. Application: US 98-33153 19980302. CAN 131 297112 AN 1999:670091 CAPLUS

**Patent Family Information**

**Abstract**

Disclosed is a human is a DNA topoisomerase I  $\alpha$  (hTopI- $\alpha$ ) polypeptide and DNA (RNA) encoding such hTopI- $\alpha$  polypeptide. Also provided is a procedure for producing such polypeptide by recombinant techniques and antibodies and antagonists against such polypeptide. Also provided are methods of using the antibodies and antagonist inhibitors to inhibit the action of hTopI- $\alpha$  for therapeutic purposes such as an antitumor agent, to detect an autoimmune disease, or retroviral infections and to treat adenocarcinoma of the colon. Diagnostic methods for detecting mutations in the coding sequence and alterations in the concn. of the polypeptides in a sample derived from a host are also disclosed.

**Patent Classifications**

**Main IPC:** C12N009-90. **U.S.:** 435233000. **Secondary IPC:** C07K014-435.

**Indexing** - Section 7-5 (Enzymes)  
Section cross-reference(s): 1, 3, 13, 63

Primers (nucleic acid)  
Role: BIU (Biological use, unclassified); PRP (Properties); BIOL (Biological study); USES (Uses)  
(DNA: cloning, sequence, expression and therapeutic use of human DNA topoisomerase I  $\alpha$ )

Antitumor agents  
Diagnostic agents  
Drug screening  
Drugs  
Gene expression  
Gene therapy  
Lung  
Molecular cloning  
Ovary

# Explore by Structure

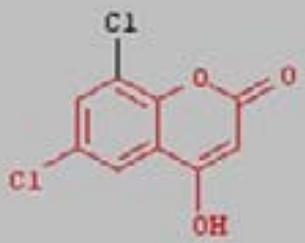
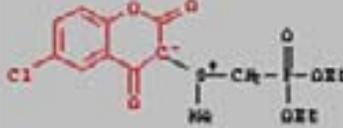
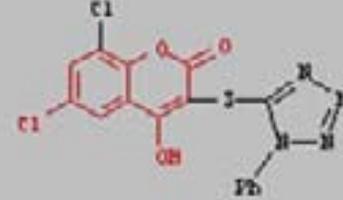
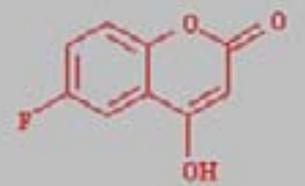
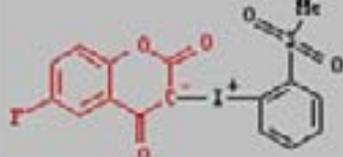
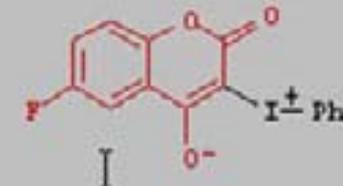
The image shows a screenshot of a chemical software interface. The main window displays a chemical structure of a benzofuran derivative with a substituent 'A' on the benzene ring and a hydroxyl group (-OH) on the furan ring. A dialog box titled "Get Substances" is open in the foreground, asking the user to specify the search criteria. The dialog box contains the following text and options:

Get substances where this structure is:

- an exact match or a related structure
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Buttons for "OK" and "Cancel" are visible at the bottom of the dialog box. The main window has a menu bar (File, Edit, View, Tools, Template, Help) and a toolbar with various drawing tools. A status bar at the bottom left shows "Formula not available".

# Explore by Structure

<input type="checkbox"/>  36051-82-8  ~4 References REGISTRY	<input type="checkbox"/>  188474-04-6  ~2 References REGISTRY	<input type="checkbox"/>  88331-43-5  ~1 Reference REGISTRY
<input type="checkbox"/>  1994-13-4  ~6 References REGISTRY	<input type="checkbox"/>  142911-25-9  ~1 Reference REGISTRY	<input type="checkbox"/>  188474-67-1  ~2 References REGISTRY

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# Analysis Tools - Gain Unique Insights

36051-80

**Analyze**

Use Analyze to view a subset of your answers.

Analyze by one of these methods:

- Real-atom attachments
- Variable group (A, Q, X, and M) composition
- R-group composition
- Precision

Analyze only selected substances

Analyze all substances

OK Cancel

~4 Refe  
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1994-13

~6 References  
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~1 Reference  
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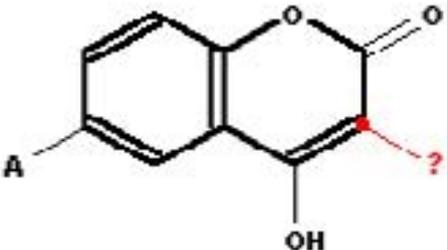
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# Analysis Tools - Gain Unique Insights

**View Real-atom Attachments**

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Select any real atom in your structure to view the atom's attachments.



Atom attachments:

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<input type="checkbox"/>	C	640
<input type="checkbox"/>	N	120
<input checked="" type="checkbox"/>	O	24
<input checked="" type="checkbox"/>	I	15
<input checked="" type="checkbox"/>	S	10
<input type="checkbox"/>	Br	4
<input type="checkbox"/>	Cl	2
<input type="checkbox"/>	A - Any (not H)	815
<input type="checkbox"/>	Q - Any (not C, H)	1/5
<input type="checkbox"/>	...	...

? = O, I, S

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# Reference Information

SciFinder Scholar

File Edit View Task Tools Help

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Tao, Zhi-Fu; Fujiwara, Tsuyoshi; Saito, Isao; Sugiyama, Hiro. **Duocarmycin A and Pyrrole-Imidazole Hairpin Polyamides.** CAN 131:73584; AN 1999:294284 CAPLUS

Tao, Zhi-Fu; Fujiwara, Tsuyoshi; Saito, Isao; Sugiyama, Hiro. **Duocarmycin A and pyrrole/imidazole diamide.** Ange 131:1795; AN 1999:192822 CAPLUS

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Herman, David M.; Turner, James M.; Baird, Eldon E.; Dervan Chem. Soc. (1999), 121(6), 1121-1129. CODEN: JACSAT

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Dervan, Peter B. **Preparation of DNA-binding pyrrole an** 9849142 A1 981105 CAN 129:343723; AN 1998:721676

Hashimoto, Shigeki; Yamamoto, Kazuo; Yamada, Takao; Nal **and effective DNA cleavage by their vanadyl complex** 129:136473; AN 1998:361758 CAPLUS

König, Burkhard; Rodel, Martin. **Synthesis of DNA-binding** (1998), (5), 605-606. CODEN: CHCOFS ISSN:1359-7345

Brown, George Robert; Newcombe, Nicholas John; Stokes, **pyrimidinylpiperidinylcarbonylpiperazines and related** PXXXX2 WO 9806705 A1 980219 CAN 128:192661; AN

Cozzi, Paolo; Beria, Italo; Biasoli, Giovanni; Caldarelli, Manr **derivatives as antitumor and antiviral agents.** PCT Int. 1999:107045 CAPLUS

Refine References

References 1-12 of 67

**Detail of Reference 1**

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**Rational Design of Sequence-Specific DNA Alkylating Agents Based on Duocarmycin A and Pyrrole-Imidazole Hairpin Polyamides.** Tao, Zhi-Fu; Fujiwara, Tsuyoshi; Saito, Isao; Sugiyama, Hiroshi. Division of Biofunctional Molecules Institute of Biomaterials and Bioengineering, Tokyo Medical and Dental University, Tokyo, Japan. J. Am. Chem. Soc. (1999), 121(21), 4961-4967. CODEN: JACSAT ISSN: 0002-7863. Journal written in English. CAN 131:73584 AN 1999:294284 CAPLUS

**Abstract**

Synthesis of novel conjugates between segment A of Duocarmycin A (Du) and N-methylimidazole (Im)-N-methylpyrrole (Py) hairpin polyamides and their DNA alkylation are described. The conjugates PyPyPpyImPyPyDu and ImPyPpyImPyPyDu were designed to alkylate the target sequences (AT)G(AT)2N(AVG) and (AT)G(AT)CN(AVG), resp., according to Dervan's ring-pairing rule. High-resoln. denaturing gel electrophoresis indicated that PyPyPpyImPyPyDu exclusively alkylated the A of the 5'-TGTAAAA-3' within a approx 400 bp DNA fragment. Similarly, alkylation by ImPyPpyImPyPyDu occurred exclusively at the G of the 5'-AGTCAGA-3' sequence with efficiency at nanomolar concn. To better understand the structure of the alkylated DNA by these conjugates, the alkylation of non-self-complementary duplex decanucleotides, ODN1 and ODN2, was investigated. HPLC and ESMS analyses of the reaction of these ODNs with PyPyPpyImPyPyDu and ImPyPpyImPyPyDu demonstrated that both conjugates efficiently and selectively alkylate N3 of the purine bases of their target sequences.

**Indexing** -- Section 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1, 26

DNA  
Role: BPR (Biological process); BIOL (Biological study); PROC (Process)  
(DNA alkylating agents; design of sequence-specific DNA alkylating agents based on duocarmycin A and pyrrole-imidazole hairpin polyamides)

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