



# ADVANCED SEARCHING CHEMICAL STRUCTURES IN PATENTS

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IP SOLUTIONS

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# WHAT IS A PATENT?

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- A patent is an agreement between inventors and the government in which the inventor is given an exclusive, monopoly right to make use of and exploit their inventions for a limited period of time. The patent owner has the legal authority to exclude others from making, using, or selling the claimed invention in that country without their consent, for a fixed period of time.
  - This authority does not extend to any other country. A patent needs to be obtained in each country where protection is sought.
- In exchange for the privilege of monopoly, the owner of the invention agrees to disclose the complete details of the invention.

## WHAT IS A PATENT? (contd.)

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- When an inventor seeks patent protection, she must submit an application to the patent office of the country in question. The application must show the details of the invention that can be understood by anyone who is skilled in that particular technology. It must be written in order to allow the invention to be duplicated.

# A PATENT IS BOTH A LEGAL DOCUMENT AND A SCIENTIFIC PAPER.

- It gives technical details describing the invention, including drawings, diagrams or chemical formulas, and is enforceable in court.



US006087380A

**United States Patent** [19] [11] **Patent Number:** 6,087,380  
Huel et al. [45] **Date of Patent:** \*Jul. 11, 2000

[54] DIS [30] **EXAMPLE 1**  
HET  
ANI  
PHA  
[75] Inven 3-Methyl-2-[2-(4-amidinophenyl)ethyl]-imidazo[4,5-b]-  
pyridine-6-carboxylic acid -N-phenyl-N-(2-  
ethoxycarbonyl)ethyl)-amide  
a) Methyl 6-methylamino-5-nitro-nicotinate  
[73] Assi 1.6 g (7.4 mMol) of methyl 6-chloro-5-nitro-nicotinate  
(see Bernie et al. in J. Chem. Soc. 1951, 2590) were stirred  
[\*] Noti in 20 ml of 40% aqueous methylamine solution at room  
temperature for 30 minutes. The reaction mixture was then  
diluted with ice water, the yellow precipitate formed was  
[21] App filtered off and dried. Yield: 1.2 g (80% of theory),  $R_f$  value:  
[22] Filed 0.66 (silica gel; ethyl acetate/ethanol/glacial acetic acid=  
90:5:5)  
[60] Provi b) Methyl 5-amino-6-methylamino-nicotinate  
[30] To a solution of 3.1 g (15 mMol) of methyl  
Nov. 24, 19 6-methylamino-5-nitro-nicotinate in 100 ml of ethanol/  
Feb. 18, 19 dichloromethane (3:1) was added 1 g of palladium on  
[51] Int. charcoal (10%) and the resulting suspension was hydroge-  
[52] U.S. nated at room temperature under 5 bar of hydrogen pressure  
[58] Filed for 1.5 hours. The catalyst was then filtered off and the  
solvent was distilled off in vacuo. The crude oily product  
[56] obtained was further reacted directly. Yield: 2.4 g (92% of  
theory),  $R_f$  value: 0.44 (silica gel; ethyl acetate/ethanol/  
4,675,4 ammonia=90:10:1)  
5,416,0 c) Methyl 5-[2-(4-cyanophenyl)ethylcarbonylamino]-6-  
methylamino-nicotinate  
A solution of 2.6 g (15 mMol) of 3-(4-cyanophenyl)  
propionic acid in 25 ml of absolute tetrahydrofuran was  
mixed with 2.4 g (15 mMol) of N,N'-carbonyldiimidazole

# THREE CATEGORIES OF INFORMATION IN A PATENT

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- **MONOPOLY RIGHTS** the legal limits which define how close another invention may come to the patented one before the inventor's rights are infringed.
- **TECHNICAL INFORMATION** this may include the nature of a manufacturing process, the composition of a new drug, the design of new pieces of machinery, etc. Such information helps to stimulate further progress on new ideas. At the same time, its availability avoids wasting time and money repeating already patented work. The monopoly right is given only in return for the disclosure of the invention in sufficient detail to enable someone "skilled in the art" (i.e. experienced in that particular craft or manufacture) to carry out the invention himself.
- **TECHNOLOGICAL INTELLIGENCE** much can be learned about industrial organizations from a study of their patents.

# WHY SEARCH PATENTS

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- In order to be patentable in the US, an invention has to be NEW, USEFUL and UNOBVIOUS. Therefore, the patent literature is full of useful ideas, but not necessarily theoretical ones
- Patent information is current, because (in most of the world) disclosure before patent application renders the invention unpatentable.
- Studies have shown that 70-90% of the information in patents is never published anywhere else.
- The technical content of a patent is often available in your local language, because protection in your country must be obtained in your country's patent office.

# PATENT FAMILIES

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- As stated earlier a patent only confers protection in one particular territory
  - So you have to file for a patent in each country you wish to seek patent protection
- This collection of patents for the same invention is called a patent family
- The markush structures stored in our database relate to a specific patent family (the individual patents can be seen in the XML datafeed of the DWPI record
  - So you can see where in the world the invention has patent protection



## Benefits of DWPI abstracts

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- Patents are legal documents which tend to be drafted by patent attorneys or patent agents
  - They are written in such a way as to maximise legal protection and to disguise the invention as much as possible using legal “jargon”
- The DWPI abstract is a concise summary of the invention written in plain English so that it should be easily understandable by a scientist familiar with the technology area

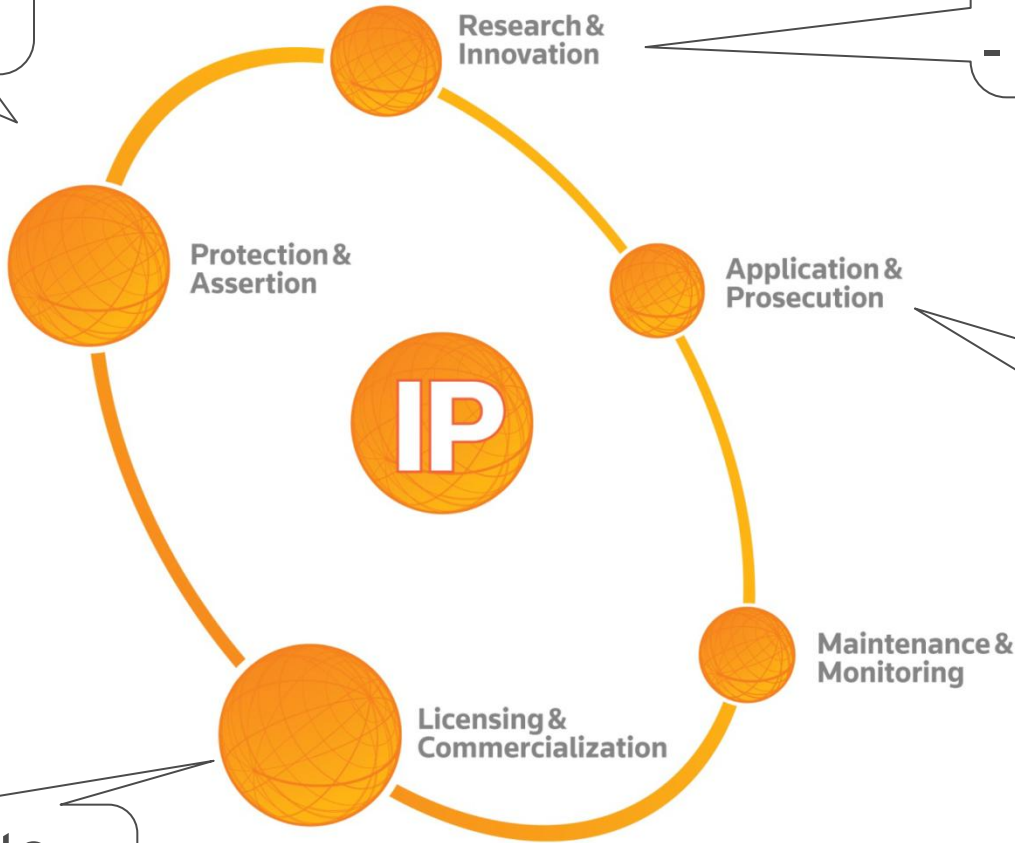


# SEARCHING THE IP LIFECYCLE

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- Validity
- Alerts

- State of the Art
- Alerts



- Patentability
- Validity

- Freedom to operate

# TYPES OF PATENT SEARCHES

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Research  
&  
Innovation

Application &  
Prosecution

Monitoring &  
Maintenance

Licensing &  
Commercialization

Protection &  
Assertion

- State-of-the-art research
- Collection searches with categorization
- Competitive and technical landscaping
- Alerts
- FTO

- Patentability / Novelty searching
- Accelerated Examination

- Legal status searches
- Patent family searches
- Patent watches

- Validity
- Assignee searching to identify target licensees

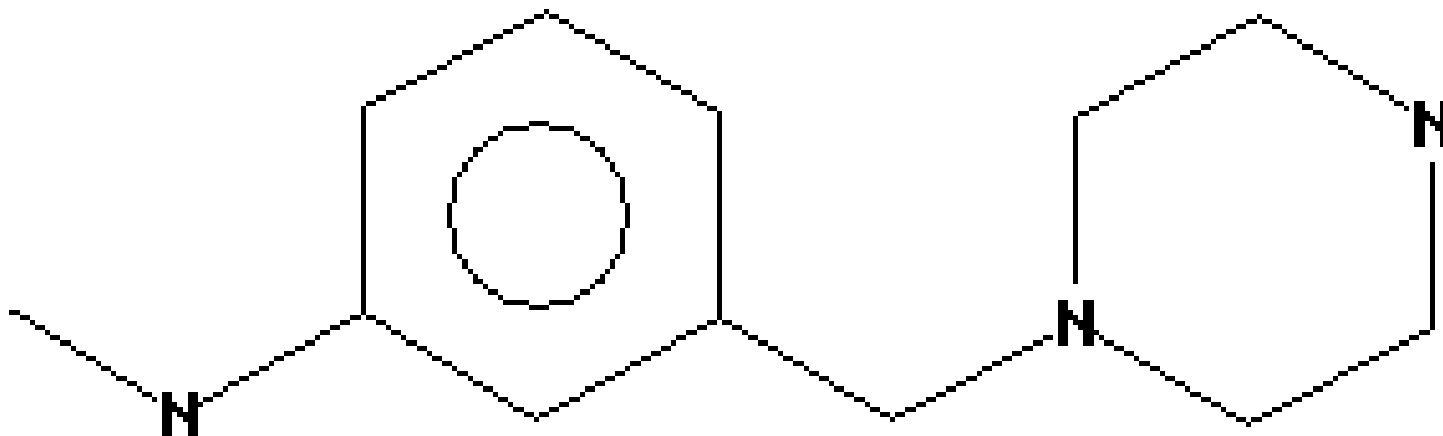
- FTO
- Validity/opposition research
- Claim strength analysis
- Patent watches



# CASE STUDY; A TYPICAL PATENT SEARCH

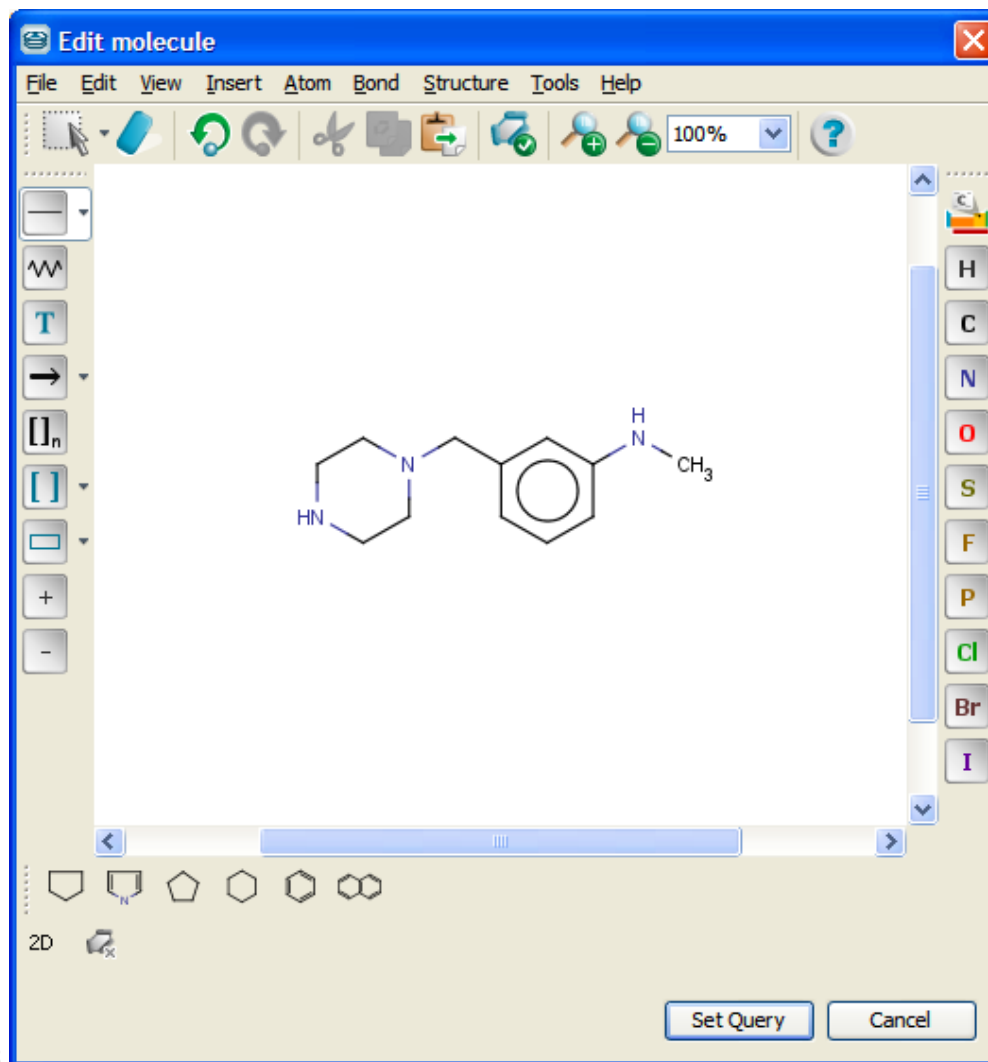
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- Have compounds containing structure I (below) been disclosed before?
  - If so, have they been disclosed for the treatment of diabetes? Schizophrenia?



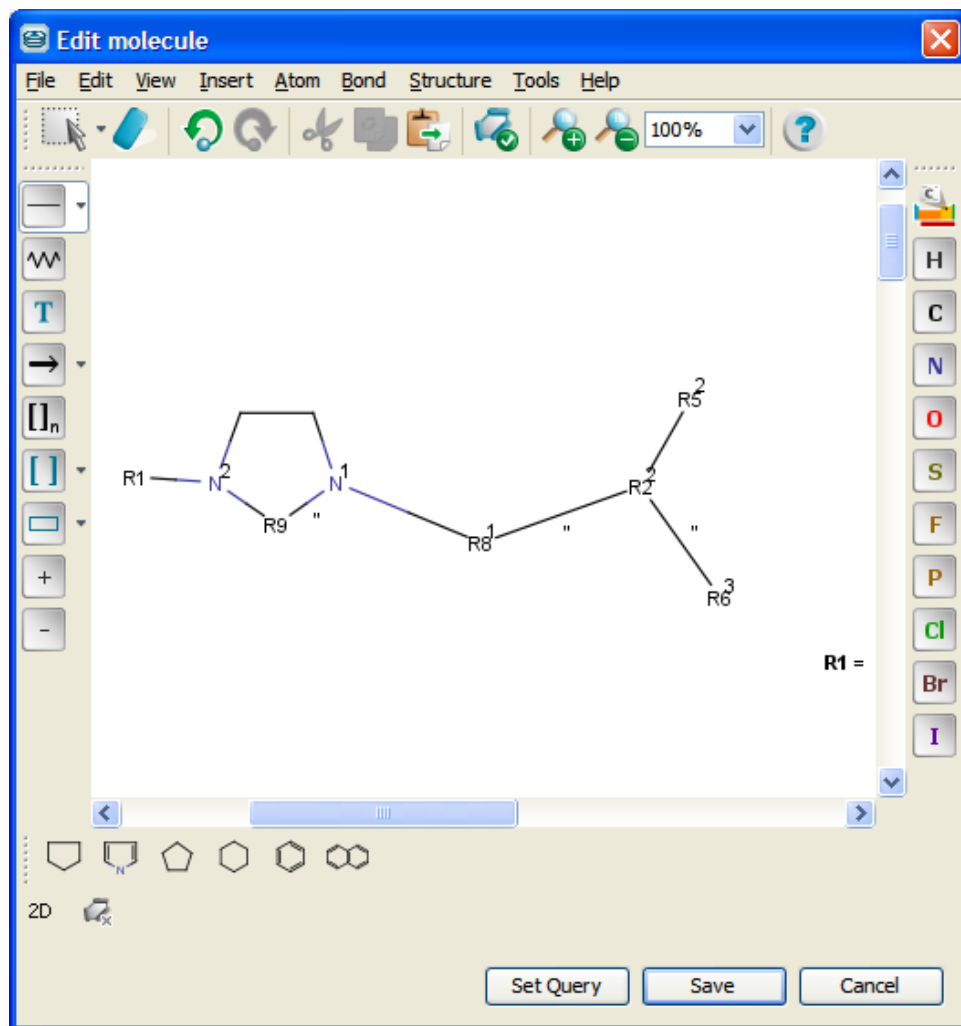
I

# WE SET UP THE QUERY ...





# ... OR, IN MORE DETAIL ...

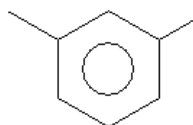


Which matches our query when

R1 = H

R9 = C-C

R8 = CHK (alkyl)

R2 = 

R5 = H

R6 = NR7R10

R7 = H

R10 = H

# ... AND WHICH COMES FROM THIS PATENT

Instant JChem 5.3.8

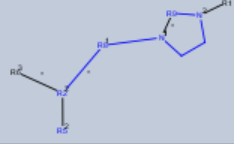
File Edit View Search Data Lists Tools Window Help

Welcome x Grid view for vmns x Form view for Inventions x Grid view for Inventions x

Design Query Browse Entity: Inventions

ID: 185

vmns

Markush structure	compound number
	0331-69601

Title: New substituted arylamine compounds are 5-hydroxytryptamine receptor modulators

Description: Substituted arylamine compounds of formula (I) and their salts and/or esters are new. A1 = a lower alkyl group; R1 = H or optionally substituted alkyl or aryl; R2 = H, halo, NO2, CN, lower alkoxy, carboxylate salt acid or its alkyl ester, a sulfone, haloalkyl or haloalkoxy, acetaldehyde, carboxamide, carbonyl, alkoxyaminocarbonyl or substituted arylalkylamino; either R3, R4 = H, optionally substituted alkyl, aryl, alkylaryl, heteroaryl or alkylheteroaryl; or R3+R4 = optionally substituted aryl, alkylaryl, heteroaryl or alkylheteroaryl group; B1 = lower alkyl (when present); X, Y1 = C or N; and n = 0-4.

Assignees: BECKER O, CHERUKU S R, DHANOA D S, EPIX DELAWARE INC, FICHMAN M, LOBERA M, MARANTZ Y

Novelty: Substituted arylamine compounds and their salts and/or esters are new.

Patents: WO2006081332-A1 \*, US20060205737-A1, NO200704324-A, AU2006209216-A1, EP1856075-A1, IN200703725-P4, KR2007097590-A, JP2008528517-W, CN101203500-A

Use: (I) are useful to treat 5-hydroxytryptamine related conditions, obesity related conditions (particularly cardiovascular disease, digestive disease, respiratory disease, cancer and type II diabetes) and schizophrenia (claimed). (I) are useful in the treatment, modulation and/or prevention of physiological or pathological conditions.

Activity: Anorectic; Cardiovascular; Respiratory-Gen.; Cytostatic; Neuroleptic; CNS-Gen.; Antidepressant; Anticonvulsant; Hypnotic; Antimigraine; Eating-Disorders-Gen.; Antiparkinsonian; Antidiarrheal; Gastrointestinal-Gen.; Anticancer

Mechanism Of Action: ...

Inventions: 70 out of 300 rows. vmns: 1 out of 579 rows.

## SOME FOLLOW UP POSSIBILITIES

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- If this were a Patentability search, the attorney will either decide not to file (because the compound we looked for was already claimed) or look for new patentable matter (synthesis, new uses, ...)
- If this were a Validity, the attorney might ask whether the patent was applied for before or after the invention date, or your filing date. You might have to license this patent.
- If this were a Freedom to Operate, the attorney would ask the legal status of this patent.



# SUMMARY

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- In this presentation we have looked at
  - What a patent is
  - What is meant by the term patent family
  - Why a DWPI abstract can help you understand the invention disclosed in the patent
  - How to search for a structure in the Markush database
  - How Instant JChem can help you better understand why you get this hit and what other structures are covered by the claim

# QUESTIONS?

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# THANK YOU

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