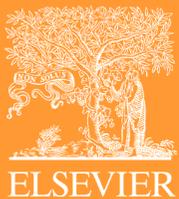




# MDL Patent Chemistry Database

A new end-user database  
for more effective synthesis planning  
and better bioactivity profiling

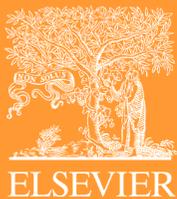
Presented by: Eva Seip  
Title: Senior Product Manager  
Date: 1-November-2004



# Agenda

- What is the MDL Patent Chemistry Database?
- Why do users want this database ?
- What will Patent Chemistry Database deliver ?
  - Unique content & competitive advantages
- How does this database complement other DiscoveryGate sources ?
  - MDL Databases
  - Derwent Databases
- Technical Information
- Competitive Advantage Summary
- Value Analysis for ROI Calculation



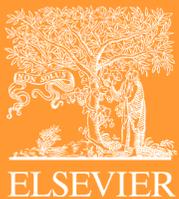


# MDL® Patent Chemistry Database

## What is it?

- A new structure-searchable CrossFire database
  - mainly for end-users, but with interesting features for information professionals also
  - indexing chemical reactions, substances and substance related information from Chemistry and LifeScience patents (World, U.S. and European) since 1976
  - addressing the following business critical issues:
    - **More effective synthesis planning**
    - **Better bioactivity profiling**
    - **Easy patent relevance check**
- **Integrated with other data sources on DiscoveryGate**

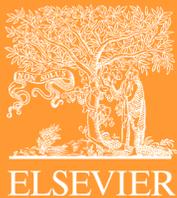




# Agenda

- What is MDL Patent Chemistry Database?
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- What will Patent Chemistry Database deliver ?
  - Unique content & competitive advantages
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  - MDL Databases
  - Derwent Databases
- Technical Information
- Competitive Advantage Summary
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# Patent Chemistry Database - More Effective Synthesis Planning

## Customers request: Make reactions from patents accessible

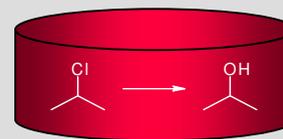
- Many novel reactions published *only* in patents
- Search State-of-the-Art
- Review similar reactions in other MDL databases (via InfoChem ClassCodes)
- Better synthesis planning

## MDL's answer:

### 1.5 Million Reactions (1976 onwards)

- Complete Reaction Descriptions
- Structure searchable Reactions incl. Reagents & Solvents
- InfoChem ClassCodes
- Markush Reaction Display (Dec 2003-)

DG today: 140,000 reactions from patents

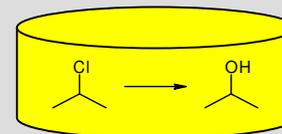


Synthetic Methodology  
Databases

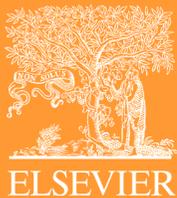


Primary Literature

Major Reference  
Works



Patent Chemistry  
Database

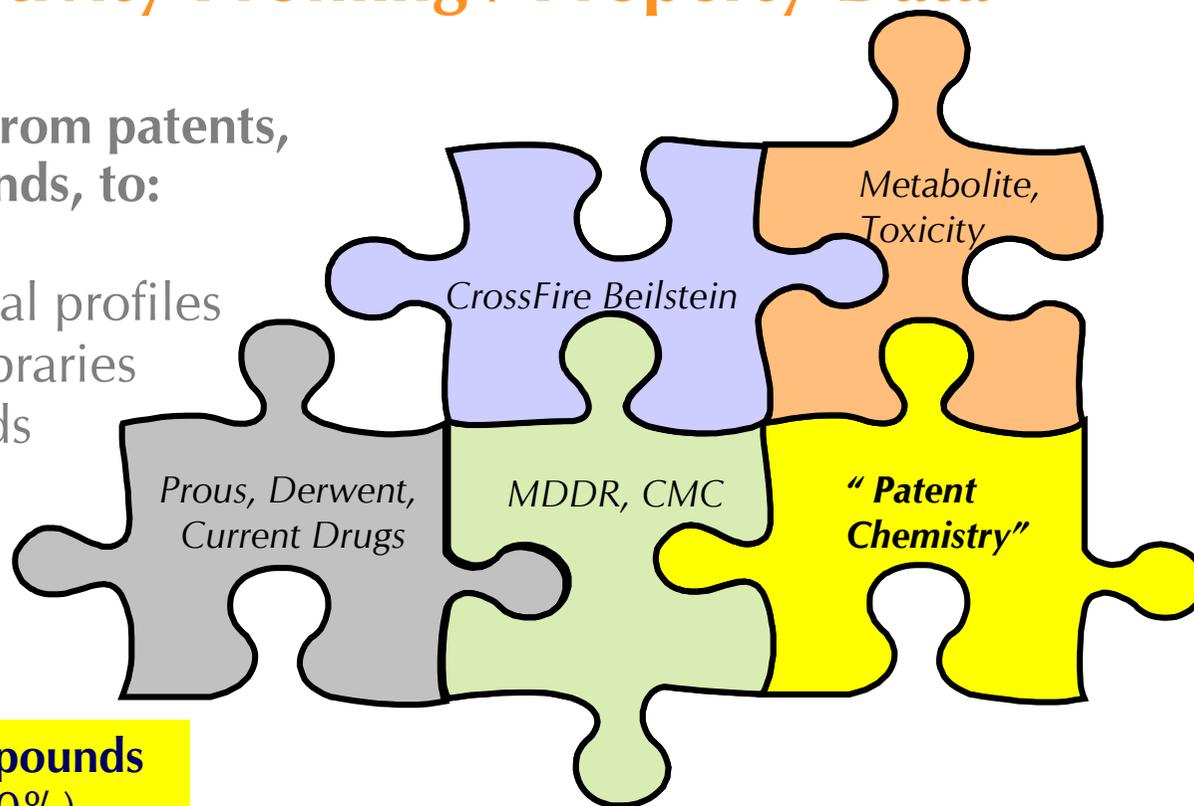


# Patent Chemistry Database - Better Bioactivity Profiling / Property Data

## Customers request:

Include structures and data from patents,  
including prophetic compounds, to:

- Search State-of-the-Art
- Develop pharmacological profiles
- Design combinatorial libraries
- Select and optimize leads
- Competitor Watch
- Industry trends

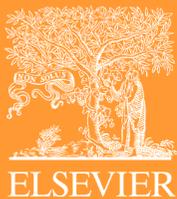


**DiscoveryGate**

## MDL's answer: 1.6 million compounds

- Prophetic Compounds (> 20%)
- Claims text
- Markush Structure Display\*
- Property data
  - Spectral & Physical Data (logP)
  - Formulation\*, Application\*
  - Bioactivity\* (EC/IC50)

\* Patents published Dec 2003 onwards



# MDL Patent Chemistry Database

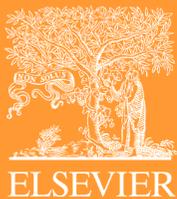
MDL Patent Chemistry Database is the first database for end-users to index

- not only reactions and compounds with data,
- but also prophetic compounds and analogous reactions from 28 years of Patent Chemistry
- the complete experimental text (example section) for reactions from patents
- the claims text with display of main Markush\* structures for easy relevance check
- measured numerical bioactivity\* data from patents

\*From December 2003 onwards



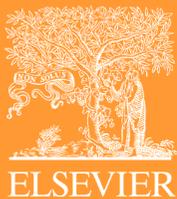
Reactions, Substances and related Data and more ...



## Agenda

- What is MDL Patent Chemistry Database?
- Why do users want this database ?
- What will Patent Chemistry Database deliver ?
  - Unique content & competitive advantages
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  - MDL Databases
  - Derwent Databases
- Technical Information
- Competitive Advantage Summary
- Value Analysis for ROI Calculation





# Content and Coverage

- **Covered International Patent Classes [IPC]**

**C07**      Organic Chemistry\*

**A61K**      Drugs [Medicinal, Dental, Cosmetic Preparations]

**A01N**      Biocides [Agrochemicals, Disinfectants, etc.]

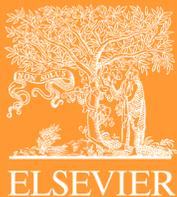
**C09B**      Dyes [can be pharmacological active]

\* Polymers indexed from 2004 onwards, when mentioned in these 4 IPC's (e. g. formulations)

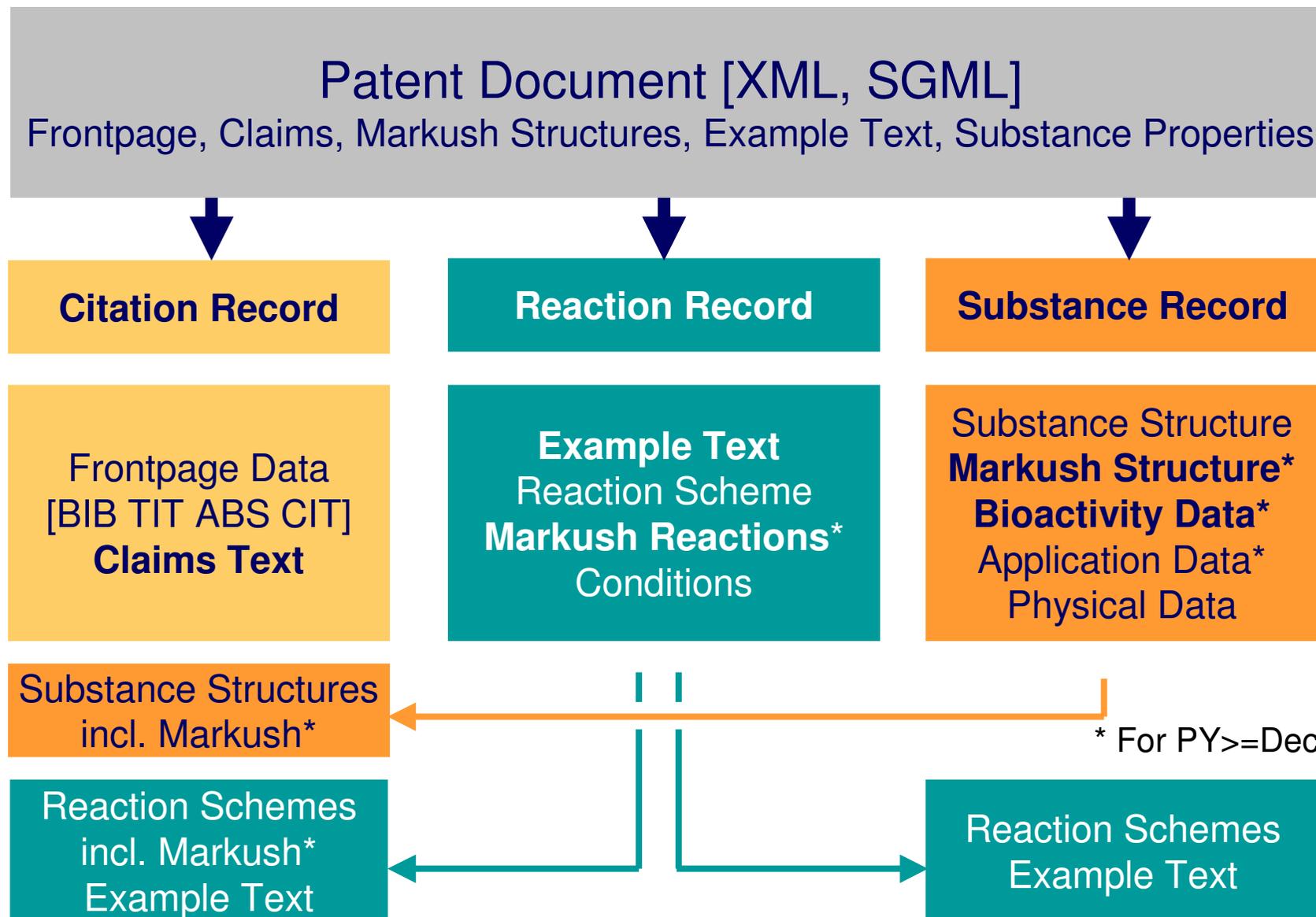
- **Covered Patent Agencies**

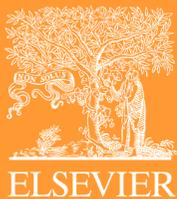
- World (WO), United States (US), European (EP) patents from Publication Year 1976 onwards
- Japanese and German patents in discussion
- Further patent countries according to customer needs





# Database Design – Three “Contexts”





# Competitive Advantages - Citations

## Database Content:

At release: approx. 340,000 Patent Citations

Anticipated Growth: 35,000 Patents / Year

## Your Benefits: Easy Relevance Check

Without time consuming access to original patent document

- **Full claims text** together with display of main Markush\* structures and main Markush\* Reactions
- **Expanded Markush\* Structure** with full substituent list
- **Referencing Compounds** - View compounds being a representative of a Markush\* structure in a patent

\* On release, available for patents published since December 2003





# Claim & Markush Structures to explore fast scope of patent

## Title / Abstract / Claims

Title 1-substituted 2,5-dithienyl pyrrole derivatives and film-forming materials

Abstract A 1-substituted 2,5-dithienylpyrrole derivative having the following formula (I), in which R is hydrogen, a substituted or non-substituted alkyl group, or a substituted or non-substituted aromatic group, Y is hydrogen or cyano group, it can be involved the case that one of Ys may be hydrogen and the other may be cyano group, and n is an integer of 1 to 3. The derivative is used for forming films.

## Claims

What is claimed is:

1. A 1-substituted 2,5-dithienylpyrrole derivative having the following formula (I).

[Figure]

in which R, is hydrogen, a substituted or non-substituted alkyl group, or a substituted or non-substituted aromatic group, Y is hydrogen or cyano group, provided that one of Ys may be hydrogen and the other may be cyano group, and n is an integer of 1 to 3.

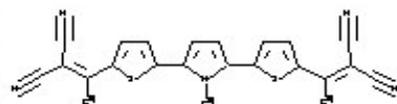
Claim Text

Language English  
Number of pages 8  
Manually excerpted yes

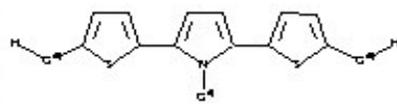
## Markush Structures

Markush PRN [19](#), [48](#), [49](#), [50](#)

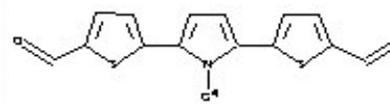
PRN=19



PRN=48



PRN=49



Markush  
Structure  
Display\*

\* On release, available for patents published Dec 2003 onwards

# Highlight: Expanded Markush Structure\*

**Substance Characterization**

Patent Compound Registry Number **305**

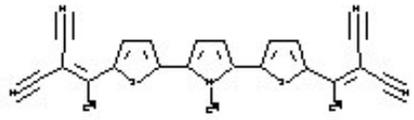
Substance Type **Markush**  
organic compound

Entry Date (YYYY/MM/DD) 2003/10/16

Update Date (YYYY/MM/DD) 2003/10/16

Referencing Compounds [click here](#)

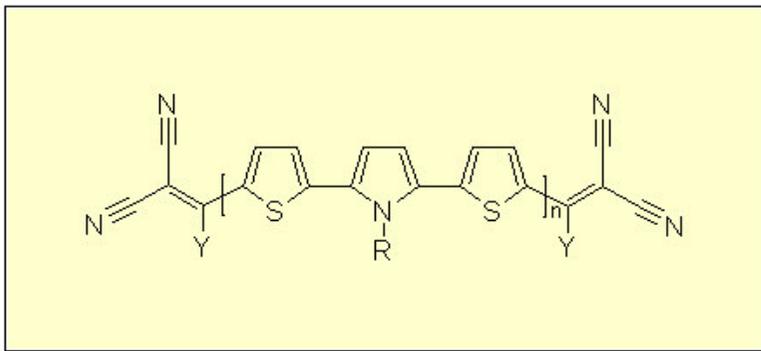
PRN=19



Compressed MARKUSH: Click to expand details

Markush Viewer

To Report Print Help OK



Label	Value	Size	Attributes	Substitution	Frequency
Y	H				
	CN				
R	H				
	alkyl	1-30C	os		
	aromatic group		os		
	formyl				
	acyl				
n	alkoxycarbonyl				
	alkenyl				
	1-3				

**Generic Symbols as written in Full-text**

# Defined Substances related to Markush\* - Easy relevance check

## Substance Characterization

Patent Compound Registry Number **305**

Substance Type **Markush**

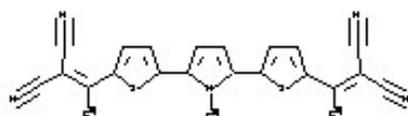
organic compound

Entry Date (YYYY/MM/DD) 2003/10/16

Update Date (YYYY/MM/DD) 2003/10/16

Referencing Compounds **[click here](#)**

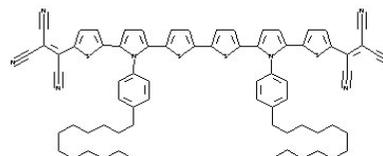
PRN=19



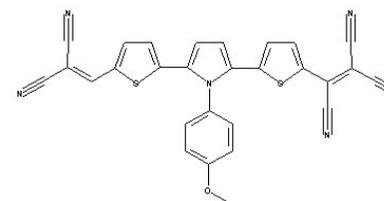
Compressed MARKUSH: Click to expand details

## Representatives of the given Markush Structure:

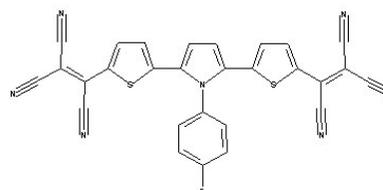
Hit 1 PRN=9 C<sub>70</sub>H<sub>70</sub>Ne<sub>8</sub>S<sub>4</sub>



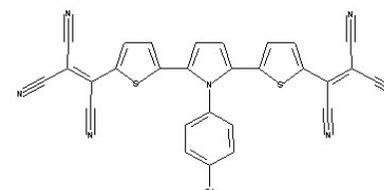
Hit 2 PRN=11 C<sub>28</sub>H<sub>14</sub>Ne<sub>6</sub>O<sub>8</sub>S<sub>2</sub>

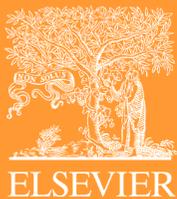


Hit 3 PRN=13 C<sub>28</sub>H<sub>10</sub>FN<sub>7</sub>S<sub>2</sub>



Hit 4 PRN=14 C<sub>28</sub>H<sub>10</sub>ClN<sub>7</sub>S<sub>2</sub>





## Competitive Advantages - Reactions

Approx. 1.5 M reactions (structure-searchable; 1976 onwards)

Strong growth anticipated: ~ 500,000 reactions/year

### Your Benefit: More Effective Synthesis Planning

- **Complete Reaction Descriptions**

Immediately reproduce chemistry without the need to order the patent document

- **InfoChem ClassCodes**

- Similar reactions get same class code (15-digit number)
- All MDL reaction db's are classified with ClassCodes
- Find Similar Reactions in same/other MDL database
- Grouping of similar reactions

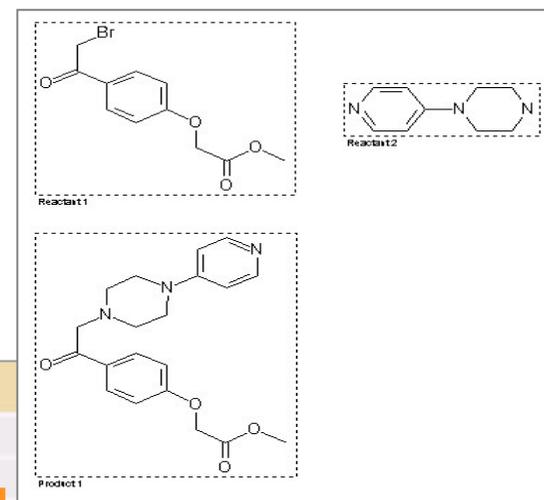
- **Markush Reaction Display\***

Explore the scope of patent coverage and reaction scope

\* On release, available for patents published since December 2003 —



# Experimental Text



## Reaction Details

Reaction Classification

Preparation

Example Text

EXAMPLE 1

methyl 4-[2-[4-(4-pyridyl)piperazin-1-yl]acetyl]phenoxyacetate

A solution of methyl 4-bromoacetylphenoxyacetate (4.3 g) in acetonitrile (50 ml) was added dropwise over 40 minutes to a stirred solution of 1-(4-pyridyl)piperazine (4.9 g) in acetonitrile (100 ml).

Stirring was continued for a further 1.5 hours, then the solution was filtered and the filtrate evaporated in vacuo.

The solid residue was triturated with water (50 ml), then dried and suspended in methylene chloride (50 ml).

The suspension was then filtered and the filtrate concentrated to a small volume.

Purification by flash chromatography on neutral alumina eluting first with dichloromethane, then 0.

5percent w/v methanol/dichloromethane and finally 1 percent w/v methanol/dichloromethane gave the title

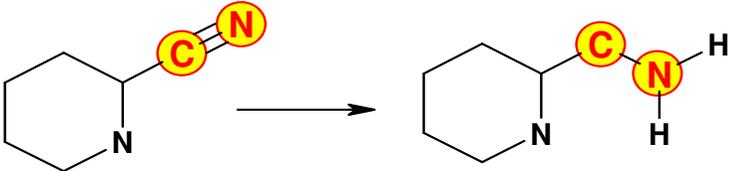
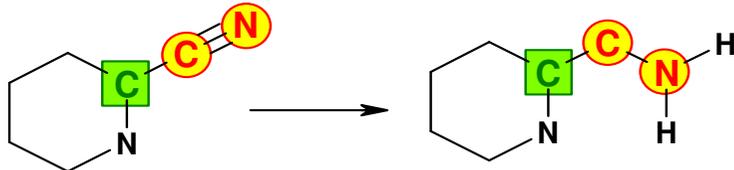
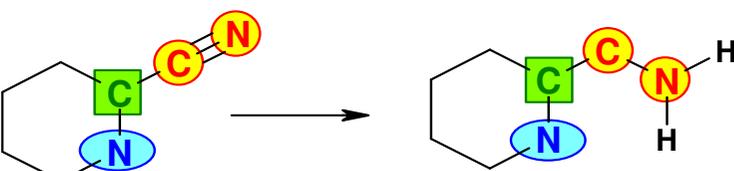
compound, 1.93 g, as a solid: m.p. 150.deg.-152.deg. C.; NMR(d6DMSO)  $\delta$  8.14(2H,d), 7.98(2H,d), 7.03(2H,d), 6.78(2H,d), 4.90(2H,s), 3.83(2H,s), 3.72(3H,s), 3.34(4H,br), 2.65(4H,br); m/e 370 (M+H)+; calculated for C<sub>20</sub>H<sub>23</sub>N<sub>3</sub>O<sub>4</sub>: C, 65.0; H, 6.3; N, 11.4. found: C, 65.2; H, 6.4; N, 11.3percent.

## Easy relevance check

- Example Number
- Example Title
- Example Text
- Spectral Data (Product)

# InfoChem Reaction Classification

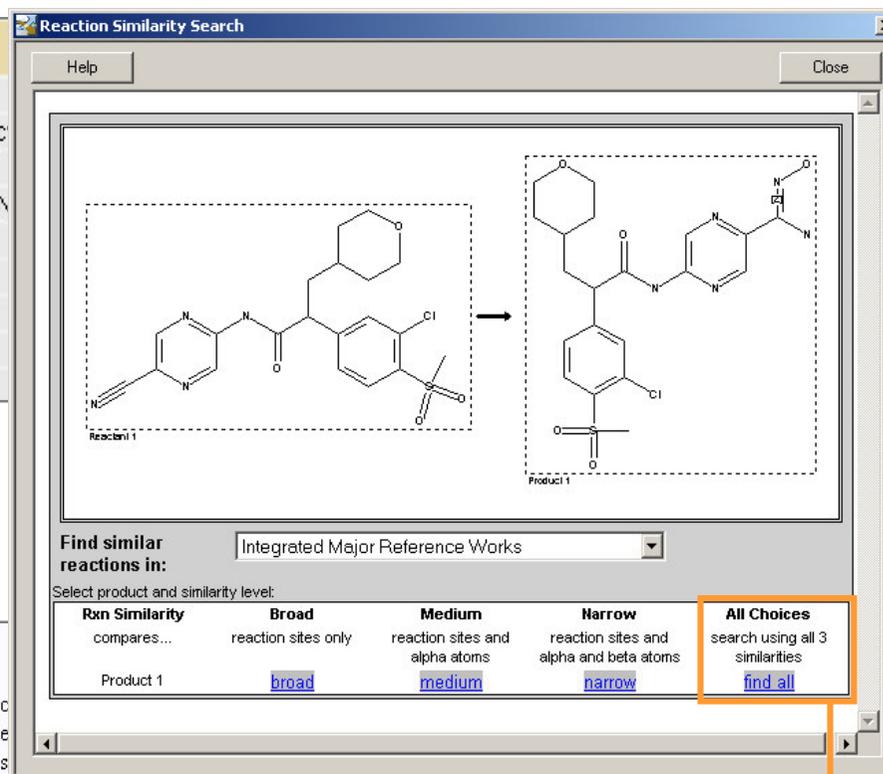
All MDL reaction databases are indexed with InfoChem ClassCodes  
 Similar Reactions have same ClassCode in different databases.

	<p><b>Reaction Similarity: <u>Broad</u> ClassCode</b>          Only reaction centers are compared</p>
	<p><b>Reaction Similarity: <u>Medium</u> ClassCode</b>          Reaction centers and alpha atoms and bonds are compared</p>
	<p><b>Reaction Similarity: <u>Narrow</u> ClassCode</b>          Reaction centers and alpha + beta atoms and bonds are compared</p>

# Find Similar Reactions in same/other db's

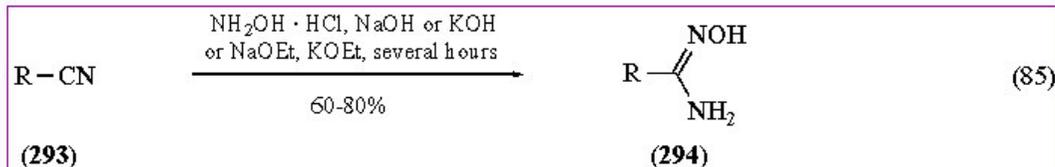
## Reaction Identification

Reaction RN	<b>4966189</b>
Reactant PRN	<b>3259400</b> 2-(3-Chloro-4-methanesulfonylphenyl)-N-(5-(tetrahydro-pyran-4-yl)-propionamide
Product PRN	<b>3412781</b> 2-(3-chloro-4-methanesulfonylphenyl)-N-[5-(N-pyrazin-2-yl)-3-(tetrahydropyran-4-yl)propionamide
Reaction Specification	full reaction
Entry Date (YYYY/MM/DD)	2004/03/28
Update Date (YYYY/MM/DD)	2004/03/28
Find Similar Reactions	<a href="#">click here</a>



### 5.21.2.4.1 From nitriles

Nitriles (**293**) are the most frequently employed starting materials for this class of compounds. They are typically prepared from hydrochloride with sodium carbonate, sodium or potassium hydroxide, or sodium ethoxide and sodium cyanide to give (**294**) (Equation (85)) [8]. To avoid the separation of the product from starting materials, anhydrous methanol or ethanol is used [130]. The highest yields are obtained when 15% excess of hydroxylamine in butanol is used and the mixture is left for 48 h at 60 °C. The product separates as a practically pure crystalline material [189]. Diamidoximes (**297**) can, in principle, be prepared according to the same method from dinitriles, such as cyanogen (**295**) with hydroxylamine or alternatively, from its addition compounds with aniline, for example, diphenyloxamidine (**296**), which is treated with hydroxylamine hydrochloride (Scheme 34) [16] [17][26]. The best yields and the purest products are obtained if gaseous cyanogen is led directly in an aqueous hydroxylamine solution at 0 °C [62CVR155]. Polyoxymidic amides [172] and polymers containing the oxymidic amide function have been prepared from polyacrylonitrile of low molecular weight with a slight excess of hydroxylamine [158] [164].



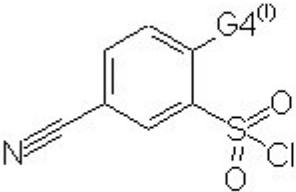
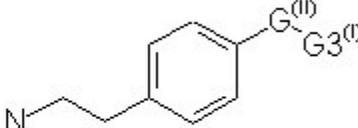
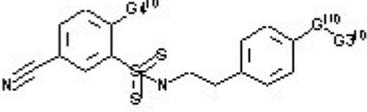
# Markush Reaction Display

Reaction Identification	
Reaction RN	<b>16</b>
Reactant PRN	<b>286</b>
	<b>367</b>
Product PRN	<b>285</b>
Reaction Specification	Markush Reaction
Entry Date (YYYY/MM/DD)	2003/10/16
Update Date (YYYY/MM/DD)	2003/10/16
Find Similar Reactions	not available

Hitset Family Go [ ] [ ] [ ]

## Markush Reaction Display\*

[\* available for patents published Dec 2003 onwards]

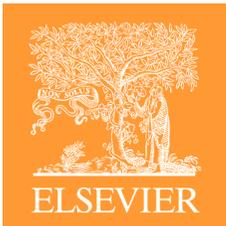
<p>PRN=286</p>  <p>Compressed MARKUSH: Right-click to expand details</p>	<p>PRN=367</p>  <p>Compressed MARKUSH: Right-click to expand details</p>	<p>PRN=285</p>  <p>Compressed MARKUSH: Right-click to expand details</p>
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Reaction Details	
Topic of Interest	Preparation
Example Name	Scheme B
Location in Patent	Page 7
Product PRN	<b>285</b>
Stage Number	1
Reactant PRN	<b>286</b>
	<b>367</b>

[ ] [ ] [ ]

## Location in Patent\* "Page Number"

Ref. 1	Frontpage/Claim: <b>13</b> , Fulltext: <a href="#">LitLink</a> ; Patent, Publ.: EP1174421 A1 (2002/01/23), Appl.: EP00911405.9 (20000328)
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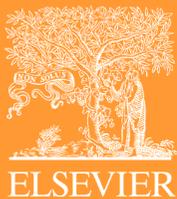
## Competitive Advantages - Compounds

- **1.6 million compounds with data since 1976**
- **Strong growth anticipated: ~ 800,000 Compounds/Year**

### **Your Benefit: Compounds rarely covered elsewhere**

- **800,000 Prophetic Compounds since 1976**
  - could be made analogously to given methods
  - have a structure, but no data associated
  - normally only accessible via Markush Structure Search





# Competitive Advantages - Substances

## Prophetic Compounds

### Synthesis of methyl-(S)-2-(2-naphthalenesulfonylamino)-3-(4-hydroxyphenyl)propionate

[0029] Methyltyrosinate(1g, 4.32mmol) was suspended in 5ml of methylene chloride, pyridine(1.4ml, 17.28mmol) was added thereto, and the reaction mixture was allowed to stand until the mixture became thoroughly transparent. After the reaction solution became transparent, trimethylsilylchloride(1.1ml, 8.64mmol) was slowly added thereto at room temperature. After 1 hour, 2-naphthalenesulfonylchloride(1.08g, 4.75mmol) was added and the resulting mixture was stirred for 24 hours. To this mixture was added 3N HCl solution, which was then stirred for about 2 hours. The organic layer was separated, the aqueous layer was extracted with methylene chloride, and the organic layers were combined. The combined organic layer was dried over Na<sub>2</sub>SO<sub>4</sub> and the organic solvent was removed by distillation under reduced pressure. The resulting residue was recrystallized from toluene to give 1.29g(Yield 79%) of the title compound as a white solid.

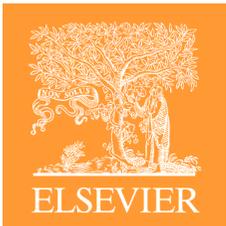
### Compounds with data (e.g. yield, spectra)

<sup>1</sup>H NMR(CDCl<sub>3</sub>, 300MHz) δ 8.33(s, 1H), 7.91(m, 3H), 7.68(m, 3H), 6.90(d, J=8.4Hz, 2H), 6.62(d, J=8.4Hz, 2H), 5.18(d, J=9.1Hz, 1H), 4.92(br.s, 1H), 4.21(dt, J=15, 6.0Hz, 1H), 3.37(s, 3H), 3.00(dd, J=13.5, 5.7Hz, 1H), 2.93(dd, J=14.3, 6.5Hz, 1H).

The following compounds could be prepared according to the similar procedure as Preparation 2 above

Methyl-(S)-2-(*p*-toluenesulfonylamino)-3-(4-hydroxyphenyl)propionate.  
Methyl-(S)-2-(benzenesulfonylamino)-3-(4-hydroxyphenyl)propionate.  
Methyl-(S)-2-(benzothiazole-2-sulfonylamino)-3-(4-hydroxyphenyl)propionate,

**Prophetic  
Compounds**



# Competitive Advantages - Compounds

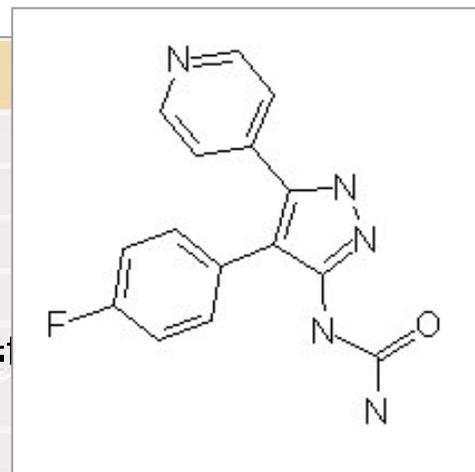
## Your Benefit: Better Bioactivity Profiling

- **Measured numerical bioactivity data (e.g. IC50, EC50)**
- **Toxicology & metabolism data, application & formulation**
- Data export to **structure-activity-relationship table (SAR)**
- Many **Predefined Export Formats**
- Definition of own export formats and user-views possible
- **Substance profiles:** A substance record accumulates data from different patents



# Numerical Bioactivity Data\*

Bioactivity Data 1 of 2	
Effect	inhibition of human P38 kinase alpha
Class of Effect	Pharmacology
Type	IC50
Value of Type (mole conc.-unit)	1.98 µmol/l
Species (Scientific Name)	PHAS-I (phosphorylated heat and acid stable protein kinase inducible)
Named Method	In Vitro Assay: PHAS-I
Method Details	96 well plates; biotinylated PHAS-I was used as substrate (c=1.5 µM); activated human p38 kinase alpha (c=0.3 µM); gamma 32P-ATP (activity 1.2 µCi per 50 µl); title comp. prediluted in DMSO (1percent final conc.); incubation either for 1 hour or overnight at 30 degC; capture of biotinylated PHAS-I with 32P incorporated using high capacity streptavidin coated filter place; scintillation detection.
Location in Patent	Table 1
Ref. 1	Frontpage/Claim: <a href="#">192</a> , Fulltext: <a href="#">LilLink</a> ; G.D. Searle and Company; Publ.: US6335336 B1 (2002/01/01), Appl.: US09561423 (2000/04/28)

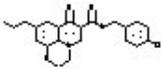
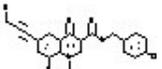
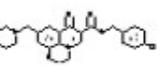


**Location in Patent\***  
**“Page Number”**

\* On release, available for patents published Dec 2003 onwards

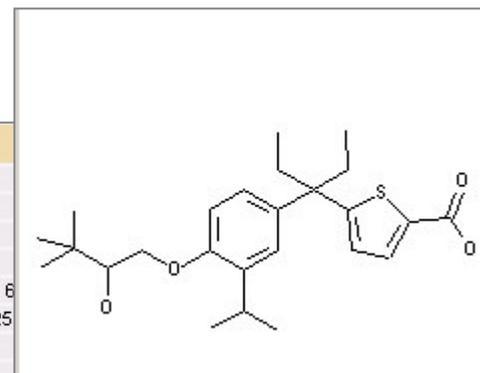


# Export to Structure-Activity-Relationship Table

Structure	Compound RegNo	Molecular Formula	Class of Effect	Effect	Type	Value (µMol/l)	Species (Scientific Name)	Location in Patent	Citation
	<a href="#">179361</a>	C22H21ClN2O3	Pharmacology	antiviral	IC50	1.8	HCMV polymerase	Page column 7-8	<a href="#">253; Patent; Pharmacia and Upjohn Company; Publ.: US6340680; B1; (2002/01/22), Appl.: US2000-672472; (2000/09/28)</a>
	<a href="#">179360</a>	C22H21ClN2O4	Pharmacology	antiviral	IC50	0.31	HCMV polymerase	Page column 7-8	<a href="#">253; Patent; Pharmacia and Upjohn Company; Publ.: US6340680; B1; (2002/01/22), Appl.: US2000-672472; (2000/09/28)</a>
	<a href="#">179359</a>	C22H17ClN2O4	Pharmacology	antiviral	IC50	1.2	HCMV polymerase	Page column 7-8	<a href="#">253; Patent; Pharmacia and Upjohn Company; Publ.: US6340680; B1; (2002/01/22), Appl.: US2000-672472; (2000/09/28)</a>
	<a href="#">179351</a>	C24H24ClN3O4	Pharmacology	antiviral	IC50	0.48	HCMV polymerase	Page column 7-8	<a href="#">253; Patent; Pharmacia and Upjohn Company; Publ.: US6340680; B1; (2002/01/22), Appl.: US2000-672472; (2000/09/28)</a>

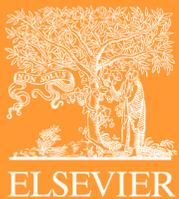
Predefined Export Forms

# Substance Profile



NMR	
Nucleus	1H
Signals given	yes
Solvent PRN	<a href="#">502</a> chloroform-d1
Location in Patent	Page 231; 236
Original String	H-NMR (ppm, [CDC13]): 7.69 (1H, d, 4.0 Hz), 7.06 (1H, s), 6.99 (1H, d, 6 Hz), 4.08 (1H, d, 8.0 Hz), 3.84 (1H, t, 8.0 Hz), 3.73 (1H, d, 8.0 Hz), 3.25 (1H, t, 8.0 Hz), 1.02 (9H, s), 0.72 (6H, t, 7.0 Hz).
Ref. 1	Frontpage/Claim: <a href="#">240650</a> , Fulltext: <a href="#">LitLink</a> ; Patent; ELI LILLY AND COMPANY; Publ.: WO2003/101978 A1 (2003/12/11), Appl.: WO2003-US14539 (2003/05/22)
Bioactivity Data 1 of 2	
Class of Effect	Pharmacology
Effect	osteocalcin activation
Type	EC50
Value of Type (mole conc.-unit)	0.07535 $\mu$ mol
Cell Line / Test System	osteoblast-like cell line RG-15 (ROS 17/2.8)
Method Name	OCN (osteocalcin) Promoter Assay
Method Details	rat osteoblast-like cell line; cell were trypsinized (0.25percent trypsin) and plated into white opaque 96-well plates; after 24 h cells treated with title comp., after 48 h treatment cells were lysed and assayed for luciferase activity using Luciferase Reporter Gene Assay kit
Location in Patent	Page 353-364; 368-376
Ref. 1	Frontpage/Claim: <a href="#">240650</a> , Fulltext: <a href="#">LitLink</a> ; Patent; ELI LILLY AND COMPANY; Publ.: WO2003/101978 A1 (2003/12/11), Appl.: WO2003-US14539 (2003/05/22)
Application Data	
Area of Use	Pharmaceuticals
Use	Drug acting on osteoporosis useful for treating or preventing disease states responsive to Vitamin D receptor ligands; displays the desirable cell differentiation and antiproliferative effects of Vitamin D receptor ligand with reduced calcium mobilization (calcemic) effects
Preferred Administration Form	Emulsion, Ointment, Tablet, Capsule, Pill, Powder, Lozenge, Syrup, Aerosol
Preferred Route of Application	oral
Preferred Dosage (nonnumeric)	0.0001 - 50 mg/(kg*d)
Formulation Given	yes

A substance record accumulates data from different patents



## Agenda

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# Synergies with other Databases

## - Reactions

Reaction related data	Discovery Knowledge Databases			Other vendors	
	Patent Chemistry Database		Other	Integrity (Prous)	SciFinder (CAS)
Patent Coverage					
Patent Reactions	> 1,5 Mio structure-searchable reactions from ~ 340.000 patents since 1976		JSM: ~ 9,000 SPORE: ~ 1,000	Synthesis of > 5,000 selected drugs	Unknown number taken from ~ 70,000 patents since 1982
Markush Reactions	Display [Published Dec 2003- ]		No	No	No
Experimental Section	Yes		No	Yes	No
Claims Text	Yes		No	No	No

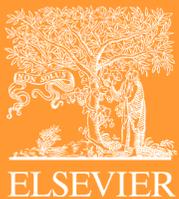


# Synergies with other Databases

## - Compounds

Compound related Data	Discovery Knowledge Databases			Other vendors
	"Patent Chemistry Database"	Derwent WPI / DCR in CompoundIndex	MDDR	
Patent Coverage				SciFinder (CAS)
Patent compounds	> 1,5 M from Org.Chem. Patents since 1976	> 507,000 selected targets since 1999	> 150,000 bioactive compounds	Unknown Number (Millions) from all areas of chemistry since 1957
Prophetic Compounds	> 800.000	No	No	No?
Markush structures	Display [Published Dec 2003- ]	No (in MMS)	No	No (in MARPAT)
Compound Properties	Measured numerical Bioactivity Data (EC50, LD50 etc) Application, formulation, spectral & physical data [Published Dec 2003- ]	High Value Thesaurus for bioactivity and diseases	High value thesaurus for therapeutic groups and diseases, drug Profiles	Controlled vocabulary for compound properties, calculated and measured physical data, no numerical bioactivity data

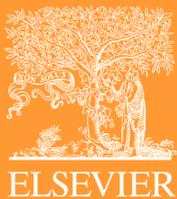
Status: June 2004



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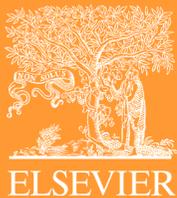


## Technical Details

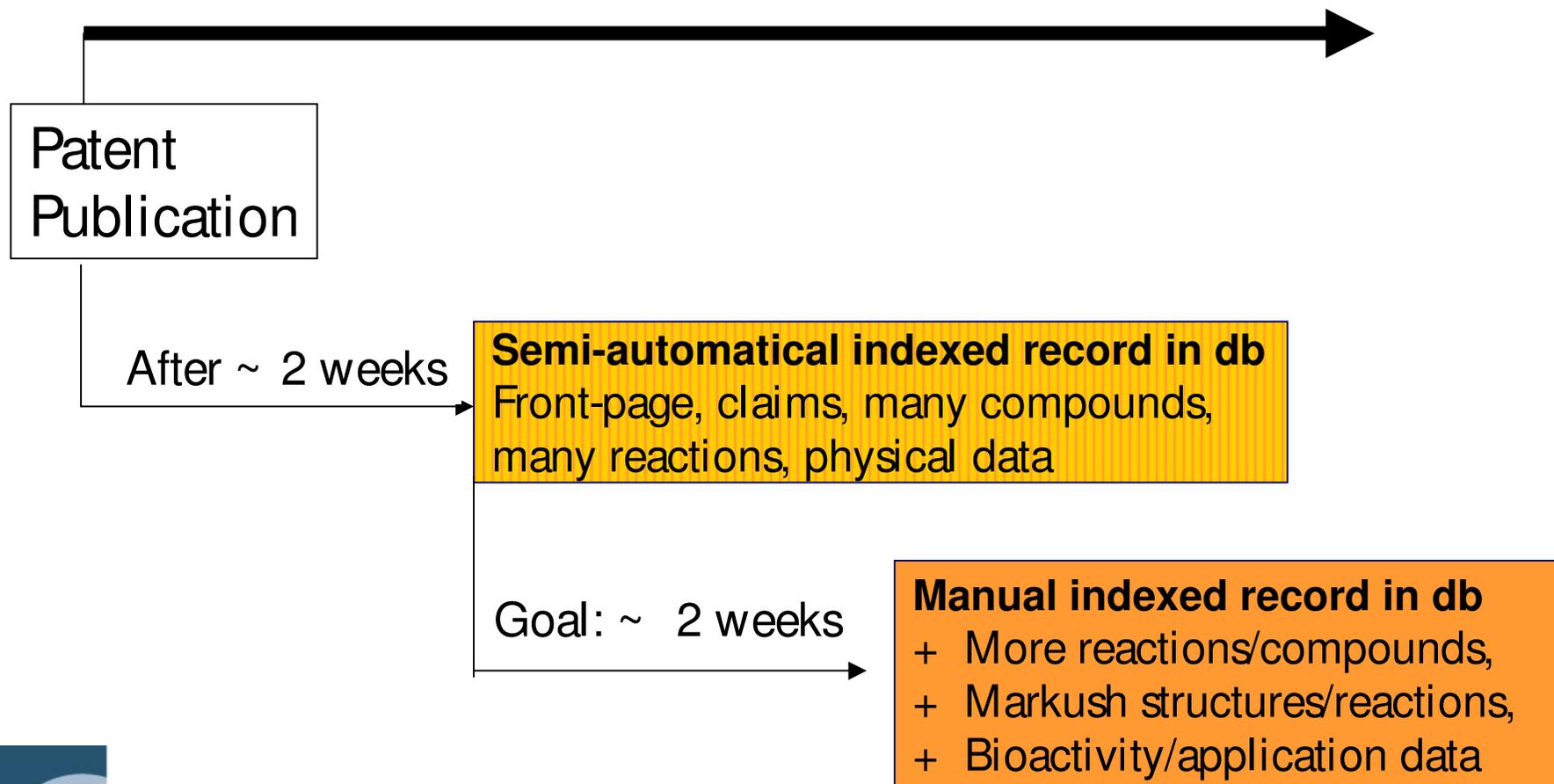
- **Database for use with**
  - CrossFire Direct
  - in-house CrossFire Server [delivery via tape, FTP]
  - DiscoveryGate
    - Database Browser
    - CompoundIndex (May 2005)
- **Size and Anticipated Yearly Growth**

1.5 Million reactions	+ 500,000 reactions/year
1.6 Million substances	+ 800,000 substances/year
340,000 citations	+ 35,000 citations/year
- **Updates / Timeliness**
  - Bi-weekly updates on CrossFire Direct and DatabaseBrowser
  - **Semi-automatically indexed patents already 2 weeks after publication** incl. front-page, claims, many reactions, compounds and physical data
  - Fully indexed record a few weeks later incl. Markush structures/ reactions and bioactivity data





## Update Process – Final Database\*



\* In the first year after release some manual indexed records may be delayed as final productivity has not been reached yet.



# Added Value Content by time

**Patent  
Publication  
Year**

**1976** (semi-automatically indexed)

**Dec 2003** (manually indexed)

**Citations**

Bibliographic Data, IPC, Title, Abstract

**Claim Text**

**Markush Structure Display**

**Markush Reaction Display**

**Reactions\***

Reaction Scheme (structure searchable),

**Example Text, InfoChem Class Codes**

**Markush Reaction Display**

**Substances\***

Spectral Data (Signals) & Phys. Data

**Prophetic Compounds**

**Markush Structure Display**

**Application & Formulation**

**Bioactivity Data (e.g. IC50)**

**Metabolism, Toxicity (LD50)**

\* Publication < Dec 2003 : Selected reactions (which have data) & selected substances **including prophetic compounds**

\* Publication > = Dec 2003: All compounds/reactions with data; **selected prophetic compounds & analogous reactions**



# Alert Service – to stay up-to-date

MDL CrossFire Commander

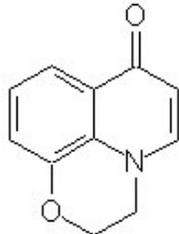
Query Results Reports Alerts AutoNom

Query History | Open Query | Save Query | Print Query | Clear Query | Select Database | Draw Structure | Modify Alert | **Create Alert** | Start Search

Alert Profile: Morpholino (Alert hitsets see "Results")

Query Search Context: Substances

impl. free sites



Query Options:

Free sites on all atoms	Allow: mixtures
Stereo: off	Allow: related Markush
	Allow: salts
	Allow: additional rings
	Allow: isotopes
	Allow: charges
	Allow: radicals

Text Search

**and** Text Search: antivir\* or biocid\* Automatic truncation right

Alert  
Conditions

Database: Patents Frequency: After each update

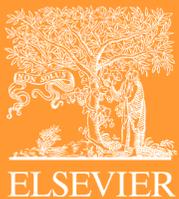
First run [date]: 2004-Feb-20 Last run: Hits [last run]: Show

Send results to: e.seip@mdl.com

Send a copy to: J.Tannemann@mdl.com

Comment: Morpholino Structures with antiviral activity Save Profile

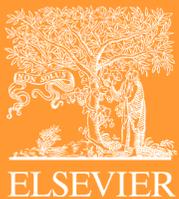




## CrossFire Commander 7.0 SP1

For CrossFire users of MDL Patent Chemistry Database is recommended:  
**CrossFire Commander 7.0 SP1** (= “patent-enabled” Commander 7)

Commander 7.0 <b>SP1</b>	<b><u>Recommended</u></b> for MDL Patent Chemistry Database = Standard-version Commander 7 <b>plus</b> add. patent-specific files (help files, predefined export formats, predefined user views, predefined search forms (PDS= former EDS))
Commander <b>7.0</b>	<b><u>Usable, but not recommended</u></b> for MDL Patent Chemistry DB Additional features compared to Commander 6: Markush display, grouping sorting, Find Similar Reactions, handling of long texts, MDL Standard Look&Feel similar to DG
Commander <b>6</b>	<b><u>Not usable</u></b> for MDL Patent Chemistry Database as the following features are missing: Markush Display, Grouping/Sorting, Find Similar Reactions, Handling of long texts (claims)



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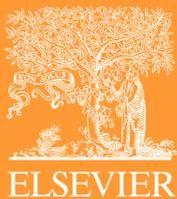
# Competitive Advantages - Summary

Aspect	Advantage
Reactions	<b>More Effective Synthesis Planning</b> <ul style="list-style-type: none"><li>1.5 Million Structure-Searchable Reactions</li><li>Strong growth anticipated: + 500,000 reactions/year</li><li>Complete Experimental Section</li><li>InfoChem ClassCodes [Find/ Group Similar Reactions]</li><li>Markush Reaction Display*</li><li>Location in Patent*</li></ul> <p>* For patents published Dec 2003 onwards</p>
Substances	<b>Better Bioactivity Profiling</b> <ul style="list-style-type: none"><li>1.6 Million Structure-Searchable Substances</li><li>Strong growth anticipated: + 800,000/Year</li><li>800,000 Prophetic Compounds</li><li>Numerical Bioactivity Data [Structure-Activity-Relationship-Table]*</li><li>Substance Profiles: Properties &amp; reactions accumulated in one record</li><li>Related Markush Structure*</li><li>Compound Identifier in Patent* &amp; Location in Patent*</li></ul>
Citations	<b>Easy Relevance Check</b> <ul style="list-style-type: none"><li>Full Claims Text – searchable together with structures/reactions</li><li>Markush Structure/ Reaction Display* [Expanded Form: Substituent List]</li><li>Defined Substances related to a Markush structure* [“Representatives”]</li></ul>



## Competitive Advantages - Summary

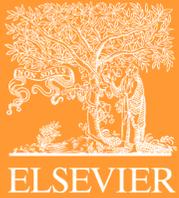
Aspect	Advantage
<b>Timeliness</b>	<ul style="list-style-type: none"><li>▪ Bi-weekly Update</li><li>▪ Semi-automatically indexed patents already 2 weeks after publication incl. front-page, claims, many compounds, many reactions and physical data</li><li>▪ Fully indexed record a few weeks later incl. Markush structures, Markush reactions and bioactivity/application data</li><li>▪ Alert Service [Export/Import Alert Profiles]</li></ul>
<b>User-Interface</b>	<b>Better Integration</b> <ul style="list-style-type: none"><li>▪ Integration into DiscoveryGate</li><li>▪ MDL Standard Look &amp; Feel</li><li>▪ Find Similar Reactions in all MDL databases [InfoChem Class Codes]</li><li>▪ Grouping &amp; Sorting</li><li>▪ Query &amp; Hitset History</li><li>▪ Easy to Use: Find Field Name; Predefined Search Forms</li><li>▪ Expert Search Mode: Command Language [STN Field Names]</li><li>▪ Predefined Export/Report Formats [List and Table Views]</li></ul>
<b>Costs</b>	Fixed User Fee [All-You-Can-Eat] <ul style="list-style-type: none"><li>▪ Subscription; Alert included in Fixed Fee</li></ul>



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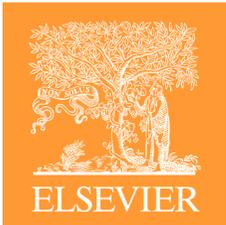


# Value Analysis for ROI calculation

## Large cost savings

- **Easy relevance check**
  - Full-text access is seldom needed as claim text, experimental section, numerical data are given and compounds are correlated to their properties.
  - Relevance check of 1 patent (~ 15 min): 40 \$  
20 scientists/5 patents/week: 160,000 \$ savings/year
- **Cost-free Alert Service**
  - Alert is included in fixed fee.
  - No additional payments for documents/search time.
  - 50 Alerts at an official host cost a company about 100,000\$/year
- **Fixed User Fee [“All-you-can-eat”]  
No Task Pricing**
  - Costs independent of search time and number of searches / documents





**Many Thanks for Your Interest!**

**Any Questions?**

