ChemInform RX (CIRX) and Current Synthetic Methodology (CSM)
New Reaction Databases from Molecular Design Limited

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Introduction

Molecular Design Limited (MDL) introduced REACCS in the early '80s and soon after began producing reaction databases to meet the requirements of its new user community. The decision to develop particular databases was dictated by the availability of source material and by customer demand. The result? MDL now provides a collection of databases, each specializing in a particular area of synthetic methodology. The recent release of Comprehensive Heterocyclic Chemistry filled in the remaining gap in the collection and the set of available databases now thoroughly covers all areas of synthetic organic chemistry (~~see Figure 1~~).

With the help of the German research organization, Fachinformationszentrum Chemie GmbH (FIZ Chemie), MDL will continue to provide high-quality reaction information, but in a more consistent manner and consolidated form. MDL plans to update its existing pool of historical data with information from *ChemInform*, a high-quality compendium of reaction information published by FIZ Chemie. The two newest MDL reactions databases, ChemInform RX and Current Synthetic Methodology, will be available in the fall of 1992. This marketing bulletin contains historical data on FIZ Chemie and *ChemInform*, information on the ChemInform project, and a detailed discussion of the two new databases and their contents. Attached are 11 figures and a list of the journals abstracted for *ChemInform*.

The History of FIZ Chemie [1]

FIZ Chemie, founded in 1981, is a relatively young company, but it represents an important link between historical and current chemical services in Germany. Its roots go back to 1830, when the venerable abstracting journal *Chemisches Zentralblatt* was founded. This respected journal ceased publication in 1969, but German activities in the information field were maintained by the German Chemical Society through its division, Chemie-Information and -Dokumentation Berlin (CIDB). In cooperation with BAYER AG, the division published *Chemischer Informationsdienst*, a new abstracting journal that was renamed *ChemInform*. CIDB established close working links with Chemical Abstract Services (CAS) and Internationale Dokumentationsgesellschaft für Chemie (IDC).

FIZ Chemie was established as a non-profit organization in 1981 by the Federal German government, the Senate of Berlin, and several learned societies. As a direct successor to CIDB, its charter is to provide scientific and technical information services in chemistry and related fields to the German public and interested organizations. FIZ Chemie and its partners, Deutsches Kunstoffinstitut and Deutsche Gesellschaft für Chemisches Apparatewesen, Chemische Technik und Biotechnologie (DECHEMA), offer printed information services, magnetic tape services and software, specialized information, profile services, and customer searches for chemistry, chemical engineering, and chemical economics. In addition, the organization is a marketing representative for CAS ONLINE and CJACS, and offers training support and search help to online users.

Background on ChemInform

Twenty years after CIDB first published the journal, *ChemInform* remains one of the most important printed services produced by FIZ Chemie. The chemical community—particularly in German speaking countries—respects the quality and coverage of the weekly abstracting service, which reports recent publications in the fields of organic, organometallic, bio-organic, inorganic, and physical chemistry. FIZ Chemie, BAYER AG and the German Chemical Society publish the journal jointly, ensuring that it reflects high quality, current information; abstracts usually appear in *ChemInform* only three or four months after publication of the original article.

The selection process is rigorous. The FIZ Chemie editorial staff works with a scientific advisory board of university professors and research directors from industry to abstract information from approximately 250 journals (see Appendix). Under the supervision and guidance of the editorial board, a highly qualified team of industrial chemists from BAYER AG and professional documentation specialists at FIZ Chemie select about 20,000 abstracts, 11,000 of them with reaction equations, for inclusion in *ChemInform*. Although *ChemInform* covers the areas of physical-inorganic, inorganic, physical-organic, and organic chemistry, the journal emphasizes novel syntheses and preparative methods in organic, and to a lesser degree, inorganic chemistry. The main aspects covered are:

- New reactions and syntheses, including enzymatic or microbial processes
- Applications of known reactions in the synthesis of known compounds or classes of substances
- Improved synthetic methods and new reagents
- Syntheses of natural products of general importance
- Syntheses of novel organo-element compounds and new catalysts

ChemInform does not include syntheses of new compounds that are based upon trivial derivations similar, previously prepared compounds. In addition, the journal does not normally abstract data from conferences, proceedings, or patents.

Abstractors for *ChemInform* select individual reactions represented by up to three examples or reaction sequences leading to important compounds. In the latter, abstractors frequently summarize consecutive trivial steps within a sequence as one multistep reaction. The same procedure is used for "one-pot" reactions involving several steps. In choosing relevant examples for a given methodology, abstractors place the highest priority on good representation of substituent effects, and secondly consider examples resulting in different yields (high, medium, low) or providing for different product ratios. Abstractors also pay close attention to how different catalysts, reagents, or reaction conditions are applied within a given transformation. By including reaction sequences, scientists can look at individual reactions in their proper environment; multiple examples with different substituents give researchers a good feel for the scope and limitations of a given reaction. Both reaction sequences and multiple examples give scientists important information, which they can use to locate the most relevant analogy to a synthetic problem.

The journal places great importance on the distinctiveness, clarity, and compactness of graphic reaction schemes to allow users to grasp complicated schemes at a glance (~~see Figure 2~~). Despite its wealth of high-quality data, chemists use the journal as any other printed service: as an awareness tool and for browsing purposes. To make full use of the information and to provide for easy retrospective searches, FIZ Chemie and its partners initiated the ChemInform project in 1988.

The ChemInform Project [2-6]

Realizing the tremendous potential of the *ChemInform* reaction data as an unequaled source for a electronic database, the German Ministry for Research and Technology (BMFT) decided to fund the ambitious ChemInform project in 1988. The objective of the project, now close to completion, is to generate both a printed publication and an electronic version of *ChemInform* from a central database, requiring data entry only once (~~see Figure 3~~). Besides FIZ Chemie and BAYER AG, two other German partners, CHEMODATA GmbH and GTS-GRAL, are collaborating in the project. The project coordinator is Professor J. Gasteiger of the Technical University Munich. Although ChemInform RX will eventually contain all the information available in the hard copy, some of the data conversion, particularly for ee yields and product ratios, will not be completed for the first release. This converted data will be included in subsequent releases.

The production flow (~~see Figure 4~~) begins with journal registration, after which editors can select suitable publications and enter the appropriate bibliographical data. Abstractors then prepare the abstracts, assign classification codes, and create the graphic reaction scheme, while adhering to strict guidelines. Technicians then enter

the entire reaction scheme, including all information taken from the original publication, using an input program (CAESAR) developed by a team at BAYER AG.[7] This sophisticated software system based on DEC-Windows[8] processes the data, checks the input, generates connection tables and stores the data in SMD files. It even processes generic structures (e.g. R-groups as variable substructures defined elsewhere in the scheme), stereochemical information, and strings or abbreviations for groups. The generated information is stored in a "workfile" from which both the printed version and the database can be prepared. For the former, the layout module developed by GTS-GRAL reads the information and generates a graphic metafile. This metafile contains the complete reaction scheme, complete with chained multistep syntheses, eliminating all redundant information. These files are joined with textual bibliographical data in subsequent typesetting processes.

Further processing is required to use the original SMD files in the reaction database. A conversion program developed by CHEMODATA resolves the compact information (e.g. generic reactions and alternate reaction conditions) into single reactions, each including uniquely defined reaction partners and associated data (~~see Figure 5~~). Because the layout in the printed version differs markedly from that of individual reactions in the database, the program also generates new coordinates for all molecules. In addition, the data from the SMD files are enriched by computer-generated information, such as keywords for reactions and molecules, stereochemical descriptors, and reaction center perception. The enhanced data are stored in internal workfiles, which can be transformed by conversion routines into the file format of retrieval systems such as REACCS or ORAC. To complete the database generation process, the program assigns CAS registry numbers to molecules and generates data specific to the particular retrieval system involved. For example, the program automatically generates EXTREG, PATH and STEP data for REACCS overall reactions. Quality control checks are incorporated at all levels of data generation and processing to ensure accuracy.

The ChemInform RX database

Impressed by the high quality and the scientific contents of *ChemInform*, MDL acquired exclusive marketing rights for a reaction database produced from the central database, called ChemInform RX (CIRX). By adding CIRX to the current collection of proven MDL databases, MDL can begin to generate a higher degree of consistency in coverage, style, and scientific content for future databases and provide a unified source for smaller subsets. The first release of CIRX is scheduled for 1992 and will contain 60,000 reactions (excluding REACCS-specific overall reactions), as published in the 1991 hard copy issues of *ChemInform*. Subsequent releases early each year will offer the same number of reactions, representing electronically the reactions found in the previous year's hard copy version. With the exception of the abstract, individual reactions in the database will contain the same information available in the hard copy, including all bibliographic data.

To allow for global searching, MDL modeled the data structure of CIRX after other REACCS databases. In addition, CIRX contains several new data types to accommodate additional information from *ChemInform*. These data types include:

- Title and the language of the publication
- Where the research took place
- *ChemInform* classification index numbers (~~see Figure~~ 6)
- *ChemInform* abstract number and identification numbers

These additional data allow chemists to view individual reactions in the database in the context of the full abstract. For example, a broader perspective on the chemistry associated with a retrieved reaction can be obtained through the use of the title of the publication and the classification number. As with the title, the classification number indexes the main topics described in the abstracted paper. These numbers (SYSNO) are assigned to every abstract by the abstractors based on the classification index developed by FIZ Chemie[9]. Since all reactions from a given abstract have the same classification numbers, chemists can search for all of the reactions studied in the course of a certain project. For example, a chemist might search for information relating to a compound or reaction class (e.g. oxazole derivatives or microbiological synthesis) or to the role or occurrence of certain compounds (e.g. pheromones, flavor etc.).

All reactions from one abstract are also tied together by the abstract number (REFNO). This number in combination with the identification number (ID) allows researchers to correlate reactions within a synthetic sequence or from a set of generic reactions. Each reaction within a sequence points to the reactions immediately preceding (PRERXN) or succeeding (SUCCRXN) it. Reactions that describe identical methodology but differ in the substitution pattern of participating molecules (generic reactions) point to the first reaction of the set (BASERXN), providing easy access to information about how variations in the substrate structure influence the outcome of a reaction. The use of reaction IDs in the BASERXN, PRERXN and SUCCRXN data fields facilitates vertical or horizontal searching within a reaction scheme (~~see Figure 7~~). Naturally, these data are supplementary to standard REACCS information on reaction sequences EXTREG, PATH, and STEP.

Obviously, the annual addition of 60,000 reactions to CIRX will change the way researchers use databases and the information they contain. When chemists are limited to a relatively small set of selective, representative reactions, researchers attempt to find structurally relevant answers to their questions, turning to the primary literature for further details. Because CIRX contains many more examples for a given methodology, an increasingly varied amount of reaction condition data (reagents, catalysts, solvents, temperature etc.) becomes available. This opens the door to meaningful searching for these data (e.g. reduction with LAH in THF at -50° or the use of a specific reagent in a specified solvent) and greatly enhances the usefulness of any reaction retrieval system. These searches may be possible in principle with existing databases, but they very often lead to irrelevant hits because

the correlation of individual data does not exist in reactions with more than one operation (multistep or one-pot reactions). This situation has been remedied in CIRX by inserting an additional parent data type (STEPNO) into the affected data types within the CIRX hierarchy (~~see Figure 8~~). This important change in the data structure will not affect global searching in REACCS.

In other changes, MDL redefined REACTANT in CIRX to represent any molecule that contributes at least one carbon atom to the product(s). As previously, the CATALYST field contains information on both reagents and catalysts, in the chemical sense, but the addition of the CATALYST:CAT flag to the database allows chemists to search for chemically meaningful catalysts. In addition, CIRX contains a broader definition of the reagents stored under CATALYST, encompassing all molecules that contribute any noncarbon atom to the product(s). For example, H_2 (hydrogenations) and O_2 (oxygenations), are stored and can be searched for under CATALYST. Gases (e.g. N_2) that participate in a reaction but are inert are mentioned in RXNTEXT; the ATMOSPHERE field no longer exists in CIRX.

The Current Synthetic Methodology (CSM) database

This new database fulfills MDL customer requests for a smaller database highlighting new developments in synthetic organic chemistry in a timely fashion. CIRX will serve as the data source for such a database, CSM. The selection criteria applied to CSM, however, are closely related to those formerly established when MDL began selecting reactions for the Current Literature File, CHIRAS™, and METALYSIS™. These three databases will be replaced by CSM in 1992. CSM will build upon the tradition established by its predecessors by combining information from various areas of organic synthesis into a single source, which will give chemists a fast way to access primary literature selected from the frontiers of synthetic methodology.

Applying stringent selection criteria, abstractors will select about 8,000 reactions annually from the pool of 60,000 reactions in CIRX. These reactions will be released two times a year, approximately 4,000 at a time. Since CSM is a direct subset of CIRX, selected reactions and their data will be exact copies of the corresponding reactions in the larger database. The first release of CSM, planned for early fall of 1992, will contain reactions from issues 1-26 of *ChemInform*, 1992.

CSM will serve as a current awareness tool to alert chemists of emerging new synthetic methodologies. CSM will only include those reactions that describe novel methodology, regardless of yield. The database will also include reactions that employ new reagents or illustrate an important modification of known reagent (~~see Figure 9~~). Because of the increasingly complex nature of synthesized compounds, special emphasis will be placed on regio-, chemo- and stereo-selective reactions carried out on multifunctional molecules. Reactions NOT included in the database include:

- Modifications or improvements to existing techniques achieved by varying the reaction conditions (temperature, time, or solvent)
- Reactions that simply apply known methods to prepare new molecules
- Reactions that focus more on the product than on the methodology
- Reactions that describe mechanistic details or analytical results
- Steps that describe the preparation of reactive or unisolated intermediates. The reaction conditions leading to such intermediates may be included in a multistep reaction resulting in an isolable product if the reaction meets other selection criteria.

In general, abstractors will favor reactions that show the potential for general use. For example, they will not consider reactions that employ conditions specific to preparing one particular molecule, with the possible exception of the synthesis of a specific heterocyclic ring system. Similarly, new methodology developed and tailored to the completion of a key step in a multistep synthesis will only be included if the methodology has wider-reaching benefits in other syntheses, and in this case, only the key step will be selected. Exceptions to the single reaction rule might include examples from the area of protecting group chemistry and asymmetric synthesis. In these cases the full sequence will be registered with protection and deprotection (attachment and detachment) steps so that chemists can search for the unprotected functionality of the molecule.

Scope and limitations of a new methodology are very often documented in the literature by several examples. In most cases one example will be chosen to represent the method in CSM, but if functionality, substitution pattern, or other skeletal differences vary greatly and give different results, the database may include several examples to illustrate the broad applicability of the method (~~see Figure~~ 10). The same holds true if the use of different reagents leads to significantly different product distribution; in this case the different examples will be stored as VARIATIONS (~~see Figure 11~~).

References and Notes:

(1) Weiske, C. Fachinformationszentrum Chemie in Berlin. To be published.

(2) Parlow, A. ChemInform-Printed Issue and Database. In *Chemical Structures;* Warr, W.A., Ed.; Springer: Berlin, 1988; pp 409-411

(3) Blücher, I.; Christoph, B.; Ehrhardt.F.; Parlow, A. "Elektronisches Publizieren von Text und chemischen Strukturen am Beispiel des *ChemInform.*" In *Software-Entwicklung in der Chemie 2;* Gasteiger, J., Ed.; Springer: Berlin, 1988; pp 395-398.

(4) Gasteiger, J.; Weiske, C. "*ChemInform*-An Integrated Information System on Chemical Reactions." In *Proceedings of the 13th International Online Information Meeting; Learned Information;* Oxford, 1989; pp 147-154.

(5) Parlow, A.; Weiske, C.; Gasteiger, J. "*ChemInform*-An Integrated Information System on Chemical Reactions." *J.Chem.Inf.Comput.Sci.* 1990, 30, 400-402.

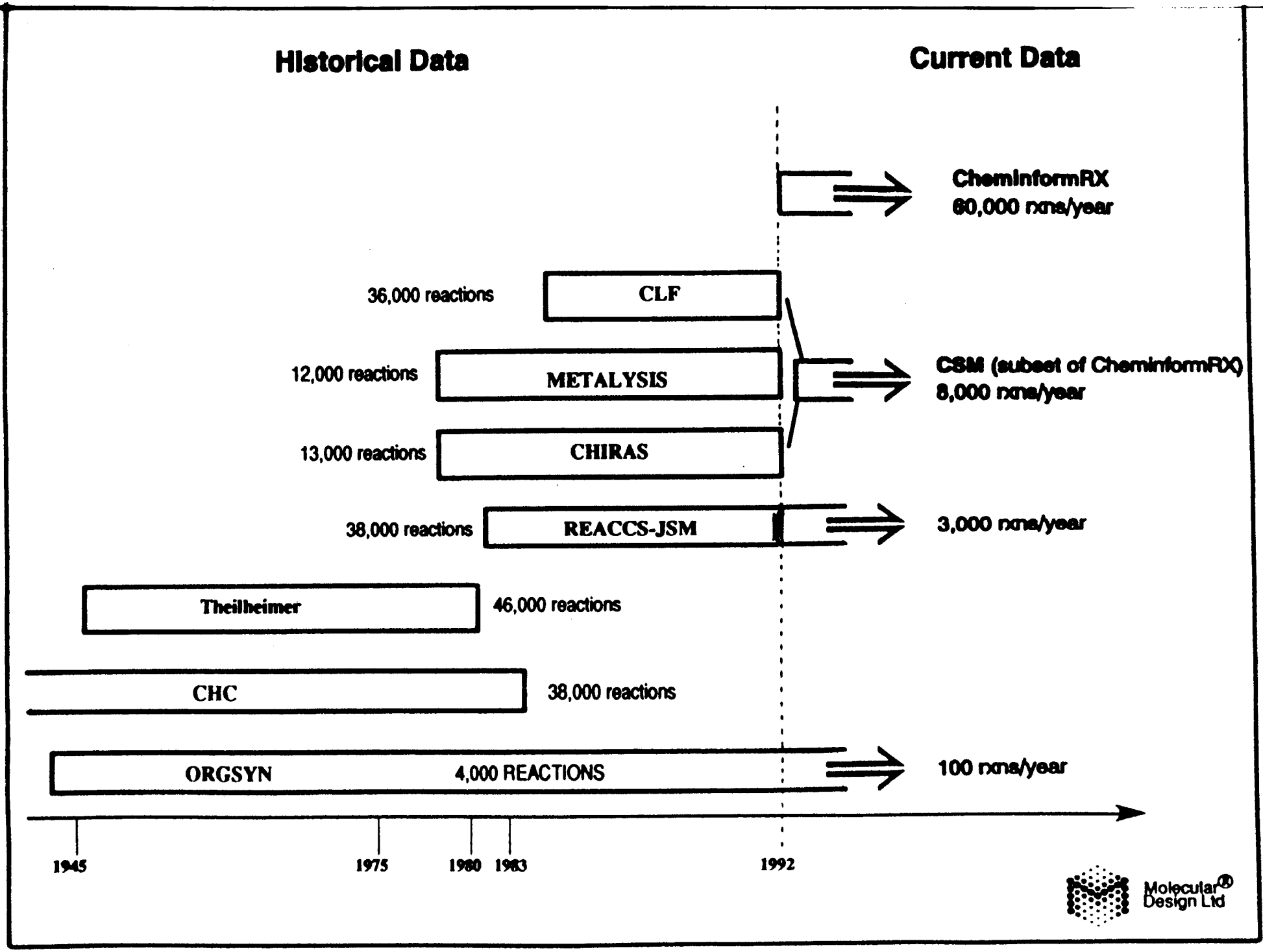
(6) Bohlen, J.; Parlow, A.; Weiske, C.; Gasteiger, J. "*ChemInform*-An Integrated Production Process for the Building of a Reaction Database and the Publishing of a Printed Abstracts Service." In *Software Development in Chemistry 5;* Gmehling, J., Ed.; Springer: Berlin, 1991; pp 37-43.

(7) Donner, W.T.; Hess-Pohl, N.; Roden, G.; Römelt, J.; Wagner, A.; Zirz, C. "CAESAR-Ein neuartiges System zur Computer Assistierten Eingabe und Speicherung Allgemeiner Reaktionen am Beispiel des *ChemInform.*" Mitteilungsblatt, Gesellschaft Deutscher Chemiker, Fachgruppe Chemie-Information-Computer (CIC) 1991, 18, 31-50.

(8) Barnard, J. "Draft Specification for Revised Version of the Standard Molecular Data (SMD) Format." *J.Chem.Inf.Comput.Sci.* 1990, 30, 81-96.

(9) Weiske, C. *Das Klassifikationssystem des* ChemInform, *DK-Mitteilungen 21;* DIN (Deutsches Institut für Normung): Berlin, 1977; pp 11-15.

(10) In this and the following examples, reactions selected for CSM from a ChemInform abstract are highlighted.


Historical Data
Current Data
ChemInformRX
60,000 rxns/year
36,000 reactions
CLF
12,000 reactions
METALYSIS
CSM (subset of ChemInformRX)
8,000 rxns/year
13,000 reactions
CHIRAS
38,000 reactions
REACCS-JSM
3,000 rxns/year
Theilheimer
46,000 reactions
CHC
38,000 reactions
ORGSYN
4,000 REACTIONS
100 rxns/year
1945
1975
1980
1983
1992
Molecular Design Ltd

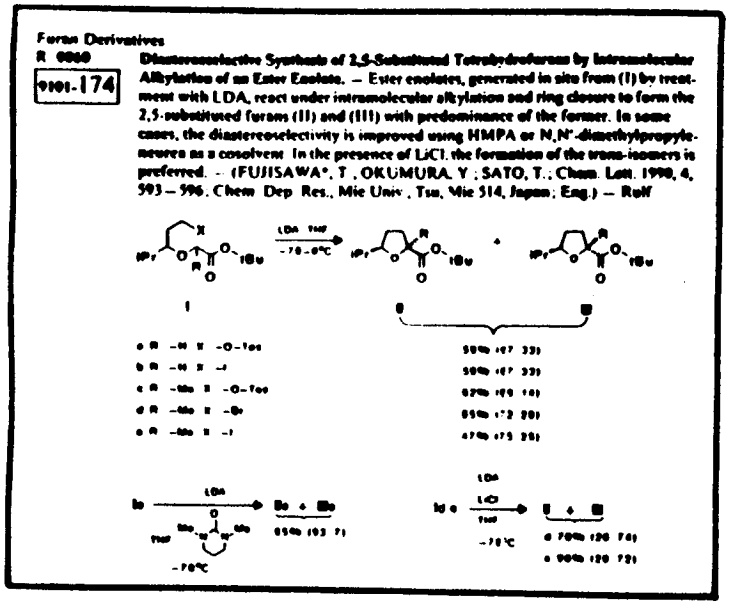
FIZ CHEMIE FIZ BERLIN

Molecular Design Ltd

Helping You Communicate Good Chemistry

ChemInform

REACCS / ORAC / ISIS



Furan Derivatives

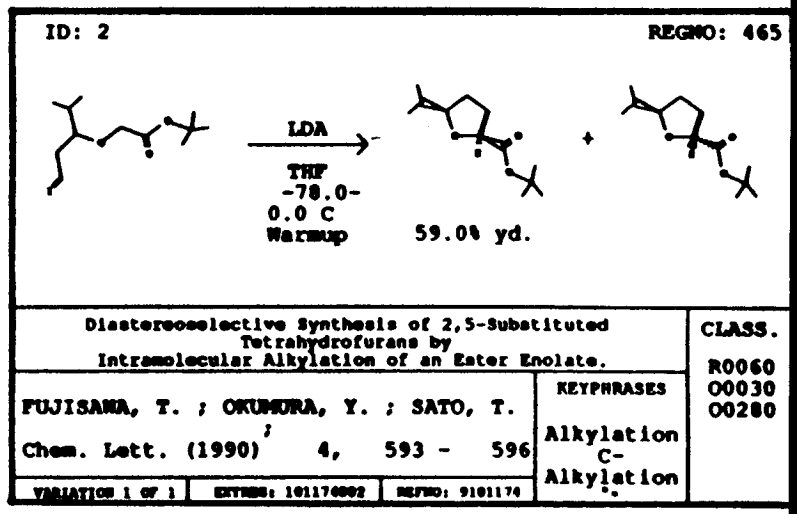
R 0060

9101-174

Diastereoselective Synthesis of 2,5-Substituted Tetrahydrofurans by Intramolecular Alkylation of an Ester Enolate. – Ester enolates, generated in situ from (I) by treatment with LDA, react under intramolecular alkylation and ring closure to form the 2,5-substituted furans (II) and (III) with predominance of the former. In some cases, the diastereoselectivity is improved using HMPA or N,N'-dimethylpropyleneurea as a cosolvent. In the presence of LiCl, the formation of the trans-isomers is preferred. – (FUJISAWA*, T.; OKUMURA, Y.; SATO, T.; Chem. Lett. 1990, 4, 593 – 596; Chem. Dep. Res., Mie Univ., Tsu, Mie 514, Japan; Eng.) – Ruff

ChemInform RX

CIRX



ID: 2 REGNO: 465

LDA

THF

-78.0-

0.0 C

Warmup

59.0% yd.

Diastereoselective Synthesis of 2,5-Substituted Tetrahydrofurans by Intramolecular Alkylation of an Ester Enolate.

CLASS. R0060 O0030 O0280

FUJISAWA, T. ; OKUMURA, Y. ; SATO, T.

Chem. Lett. (1990) 4, 593 - 596

KEYPHRASES: Alkylation C- Alkylation

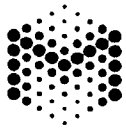
VARIATION 1 OF 1 | ENTRY#: 101174002 | REFNO: 9101174

Current Synthetic Methodology

CSM

What is ChemInform - Facts and Figures

- printed reaction information since 1970
- abstracted from approx. 250 primary journals
- industrial chemists at BAYER AG and documentation specialists at FIZ Chemie provide annually:
  - ≈ 19,000 abstracts
  - ≈ 11,000 abstracts with reaction equations
  - ≈ 70,000 reactions
  - ≈ 145,000 compounds
- professional editors oversee critical selection of data and ensure high-quality contents
- Advisory Board of university professors and research directors from industry provide guidance and supervision



ChemInform - Selection Criteria

Main areas covered:

- new reactions and syntheses, including enzymatic or microbial processes
- applications of known reactions to the synthesis of new compounds or classes of substances
- improved synthetic methods, new reagents
- syntheses of natural products of general importance
- syntheses of novel organo-element compounds, new catalyst, applications

Other topics covered in ChemInform, but not in CIRX:

- theoretical, physicochemical and analytical studies
- topics from interdisciplinary areas
- reviews

Topics not covered:

- polymers and polymerizations
- routine use of known reactions
- biochemical subjects not involving new preparative methods

Classification Code

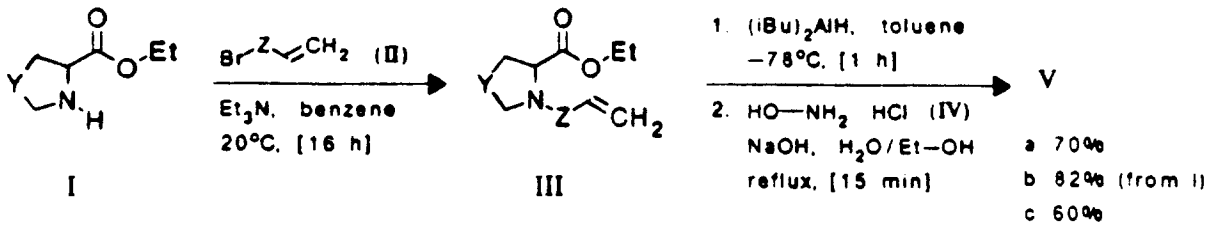
Isoxazole Derivatives

R 0240

9141-153

ChemInform Abstract

Cycloadditions. Part 46. Thermally-Induced Intramolecular Oxime Olefin Cycloadditions (IOOC) Leading to N-Bridgehead Systems. Stereochemistry and Molecular Mechanics Calculations. — The amino esters (I) are converted to the oximes (V) by successive coupling with the alkenyl bromides (II), DIBAL reduction, and condensation reaction with hydroxylamine hydrochloride (IV). Thermolysis of (V) in toluene forms diastereoselectively the cyclization products (VI) and/or (VII). Wittig olefination of the aldehydes (VIII), further deprotection, and reaction with ethyl bromoacetate (X) yields the esters (XI) which are converted to the oximes (XII) and then thermolyzed to give the fused ring systems (XIII). — (HASSNER*, A.; MAURYA, R.; PADWA, A.; BULLOCK, W. H.; J. Org. Chem. 56 (1991) 8, 2775—2781; Dep. Chem., Bar-Ilan Univ., Ramat-Gan 52100, Israel; Eng.) — Kaletta



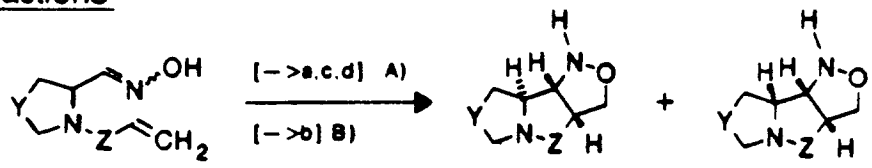
I III

a Y: $-CH_2-$
b Y: $-(CH_2)_2-$

a	Y, Z: $-CH_2-$	83%
b	Y: $-CH_2-$; Z: $-(CH_2)_2-$	–
c	Y: $-(CH_2)_2-$; Z: $-CH_2-$	73%
d	Y, Z: $-(CH_2)_2-$	–

Multiple Reaction

Generic Reactions

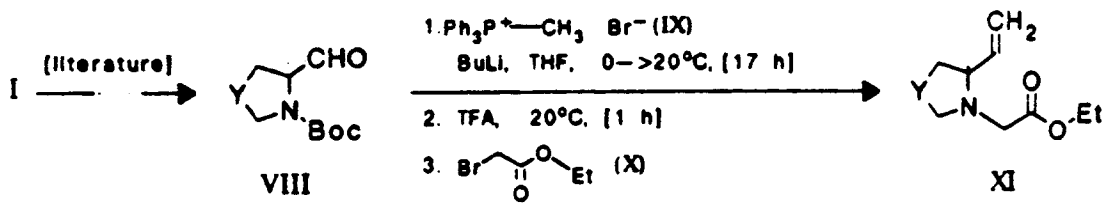


V VI VII

A): toluene, 180—185°C, [8—18 h]
B): toluene, 110°C, [24 h]

a 60% (100 : 0)
b 75% (75 : 25)
c 74% (0 : 100)
d 69% (0 : 100)

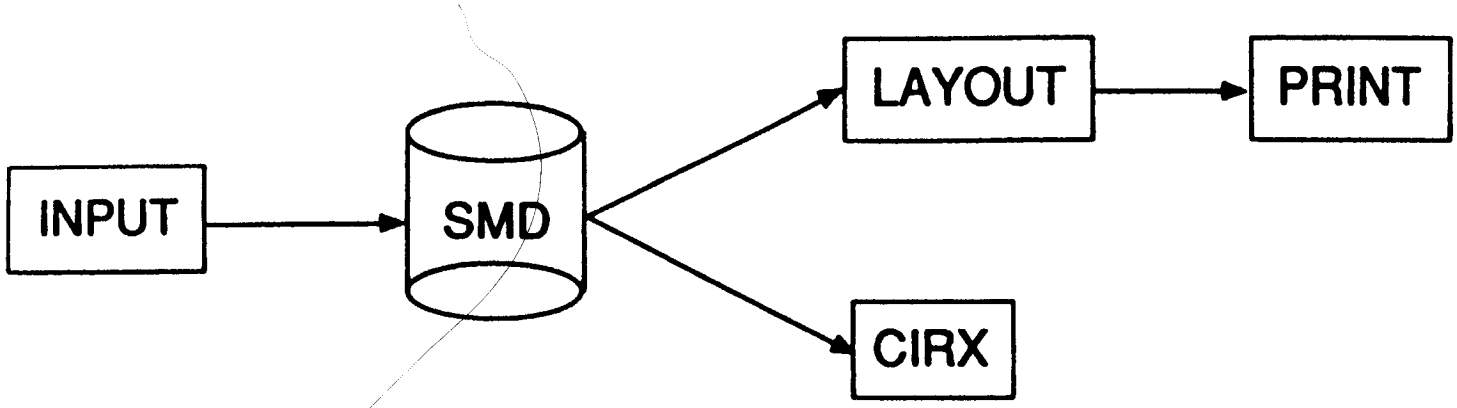
Alternative Conditions



VIII XI

a 29%
b 34%

ChemInform Project



Fachinformationszentrum Chemie GmbH, Berlin
BAYER AG, Leverkusen
CHEMODATA Computer-Chemie GmbH, Munich
GTS-GRAL GmbH, Darmstadt

Project Leader: Prof. J. Gasteiger, TU Munich
Funding: German Ministry for Research and Technology (BMFT)

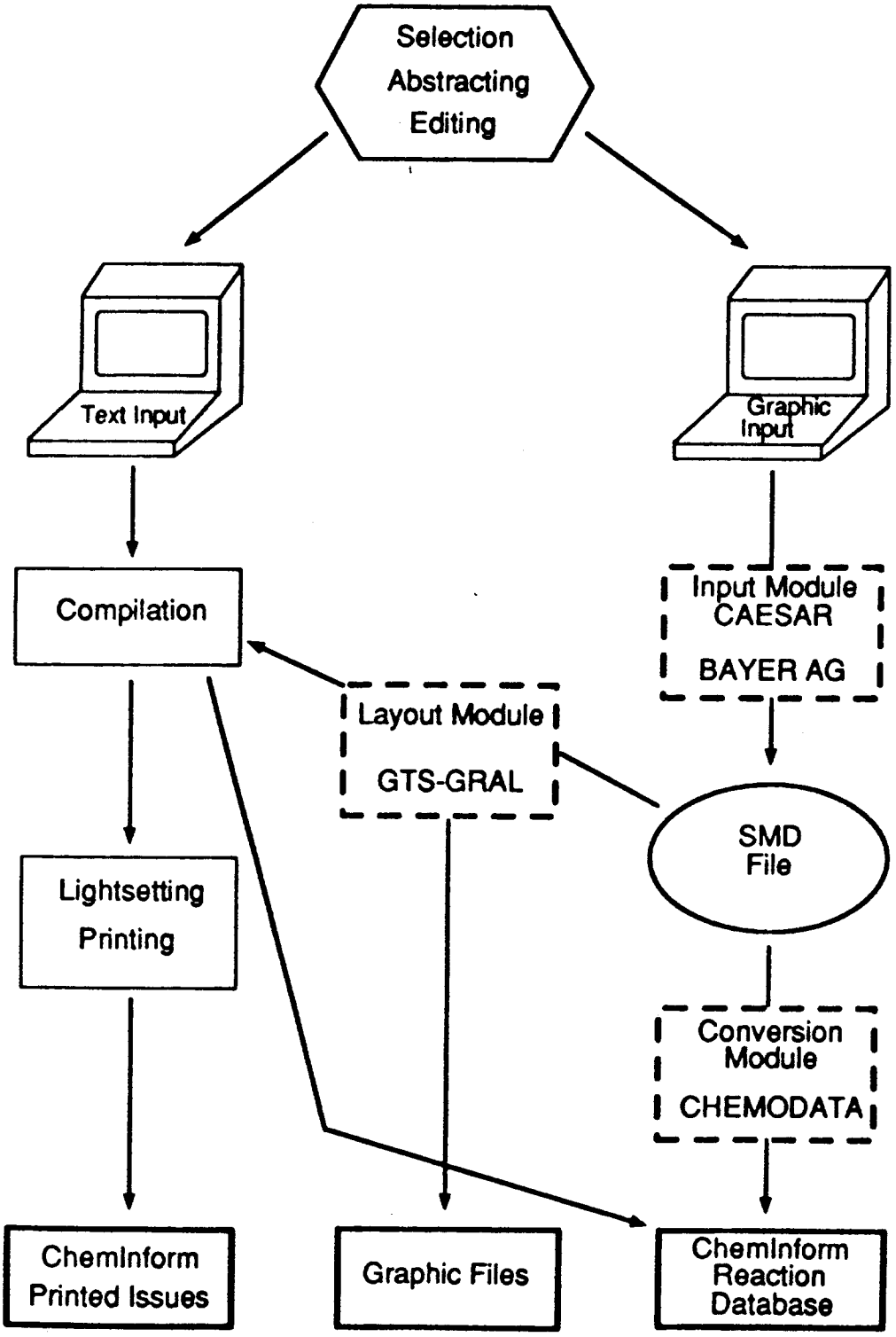
FIZ CHEMIE BERLIN

GTS-GRAL GmbH * Darmstadt

BAYER

CHEMODATA

ChemInform Project - Flowchart



Molecular Design Ltd®

Current Synthetic Methodology (CSM)

- A Subset of ChemInform RX

- Selection Criteria -

What is CSM?

The overall goal of CSM is to be a current awareness tool and to alert chemists of the emergence of new synthetic methodologies and important trends in organic, organoelement and low-molecular bioorganic chemistry. Annually, approximately 8,000 carefully selected reactions will be added to the database in two installments.

Selection Criteria:

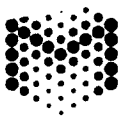
- Only reactions which describe new synthetic methodology, regardless of yield, are incorporated into the database. Strong consideration is given to the potential of a reaction for general use.

- Reactions involving the use of a new reagent or an important modification of a known one are included. The synthesis of the reagent will not be registered in the database.

- Reactions which focus more on products than on the methodology are not taken into account. Exceptions to this criterion might be found in heterocyclic chemistry in the synthesis of specific ring systems. Furthermore, because of the increasingly complex nature of compounds to be synthesized, special emphasis is placed on regio-, chemo-, and stereoselective reactions carried out on multifunctional molecules.

- In general, only single-step reactions will be selected. Exceptions might include examples from the area of protecting group chemistry and asymmetric synthesis where it might be necessary to register several steps of a sequence.

- Frequently, new methodology is developed and tailored to the completion of a keystep in the multistep synthesis of an organic compound. Should this particular reaction meet the criteria of general applicability then it will be selected.

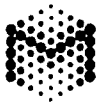


ChemInform RX 1991 - Literature References

- 60532 reactions/year abstracted from approximately 250 journals
- 9681 references - 6.25 reactions/reference

Number of references for 25 of the most cited journals:

J.Org.Chem	884	9.1%
Tetrahedron Lett.	830	8.6%
Tetrahedron	541	5.6%
J.Am.Chem.Soc.	437	4.5%
J.Chem.Soc.,Perkin I	390	4.0%
J.Heterocycl.Chem.	344	3.6%
Syn.Commun.	331	3.4%
J.Chem.Soc.,Chem.Commun.	298	3.1%
Synthesis	292	3.0%
J.Med.Chem.	255	2.6%
Zh.Org.Khim.	252	2.6%
Chem.Ber.	244	2.5%
Heterocycles	200	2.1%
Liebigs Ann.Chem.	193	2.0%
Bull.Chem.Soc.Jpn.	188	1.9%
Syn.Letters	163	1.7%
Chem.Pharm.Bull.	155	1.6%
J.Organomet.Chem.	150	1.5%
Angew.Chem	145	1.5%
Chem.Lett.	137	1.4%
Tetrahedron Asymmetry	119	1.2%
J.Indian Chem.Soc.	115	1.2%
Helv.Chim.Acta	101	1.0%
Can.J.Chem.	90	1.0%
Organometallics	89	0.9%
		71.6%



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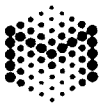
Current Synthetic Methodology 92/1 - Literature References

Number of reactions / citations and coverage (endpoint) for 20 of the most cited journals

Tetrahedron Lett.	491/255	15.3%	(91/44)
Tetrahedron	220/116	7.6%	(92/10)
J.Am.Chem.Soc.	240/90	7.5%	(92/5)
J. Org. Chem.	224/116	7.0%	(92/3)
Synthesis	220/54	6.9%	(91/12)
J.Chem.Soc., Perkin Trans I	208/92	6.5%	(92/5)
J.Chem.Soc., Chem.Commun.	151/89	4.7%	(92/3)
J. Heterocycl. Chem.	138/58	4.3%	(91/8)
Synlett	124/66	3.9%	(91/12)
Tetrahedron: Asymmetry	109/55	3.4%	(92/2)
Synth.Commun.	101/60	3.1%	(92/3)
Bull.Chem.Soc.Jpn.	76/37	2.4%	(92/2)
Phosphorus, Sulfur Silicon.....	62/28	1.9%	(92)
Chem.Lett.	59/36	1.8%	(91/8)
Angew.Chem.	56/24	1.8%	(92/3)
Zh.Org.Khim.	56/33	1.7%	(91/9)
Heterocycles	55/31	1.7%	(92/1)
Helv.Chim.Acta	54/22	1.7%	(92/2)
Chem.Ber.	51/23	1.6%	(92/3)
Liebigs Ann.Chem.	39/19	1.2%	(92/3)
		86.0%	

Additional journals: Acta.Chem.Scand.; Acta Crystallogr.,Sect.C:; Aust.J.Chem.; Bioorg.Med.Chem.Lett.; Bull.Korean Chem.Soc.; Bull.Soc.Chim.Belg.; C.R.Acad.Sci,Ser.II; Can.J.Chem.; Chem.Express; Chem.Ind.(London); Chem.Pharm.Bull.; Chem-Ztg.; Collect.Czech.Chem.Commun.; Eur.J.Med.Chem.; Farmaco, Ed.Sci.; Gazz.Chim.Ital.; Heteroat.Chem.; Indian J Chem, Sect.B; Inorg.Chem.; Izv.Akad.Nauk SSSR,Ser.Khim; J.Chem.Soc.,Perkin II; J Fluorine Chem.; J.Mat.Chem.; J.Organomet.Chem.; J.Prakt.Chem.; Khim.Geterotsikl.Soedin.; Khim-Farm.Zh.; Mendeleev Commun.; Monatsh.Chem.; New J.Chem.; Org.Prep.Proced.Int.; Organometallics; Recl.Trav.Chim.Pays-Bas; Sib.Khim.Zh.; Z.Anorg.Allg.Chem.; Z.Naturforsch., B:Chem.Sci.



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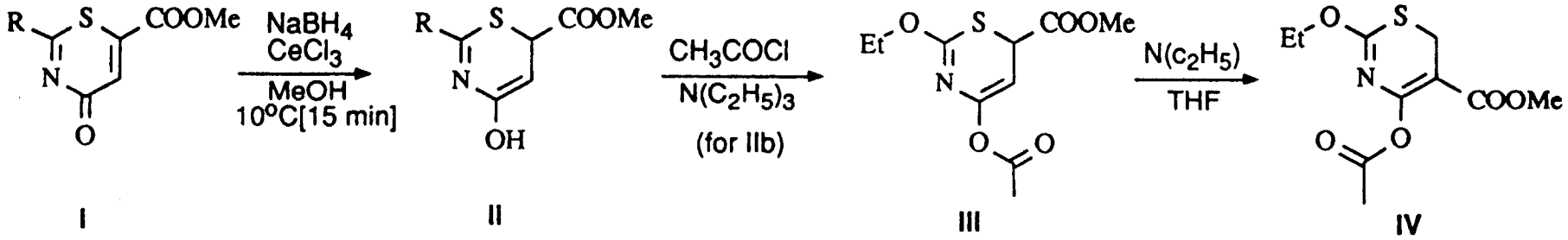
Reaction Correlation Within One Abstract

9137-188 ← Abstract Number [REFNO]



I

II

III

IV

a. R: -Ph
b. R: -OEt

a. 50% [1]
b. 57% [2]

78% [3]

87% [4]

	ID	BASERXN	PRERXN	SUCCRXN	PRIMARY
Ia → IIa	[1]	[1]	-	-	[Y]
Ib → IIb	[2]	[1]	-	[3]	-
IIb → III	[3]	-	[2]	[4]	[Y]
III → IV	[4]	-	[3]	-	[Y]

[n] = ID's of individual reactions

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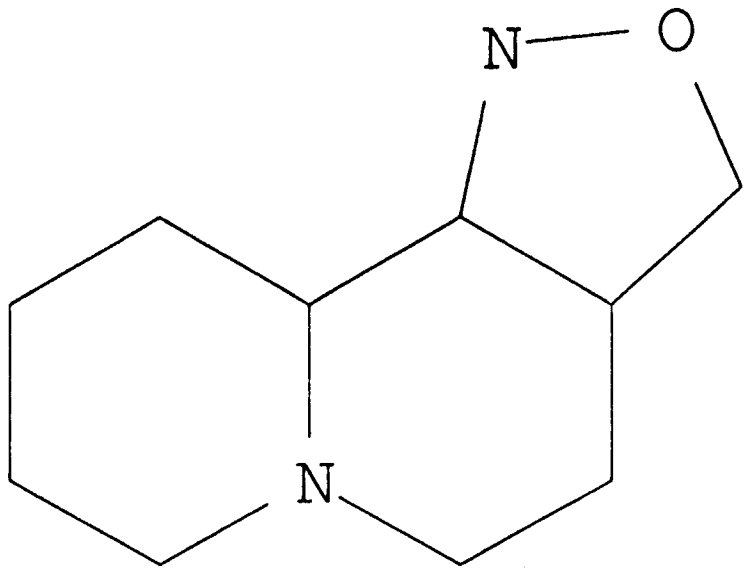
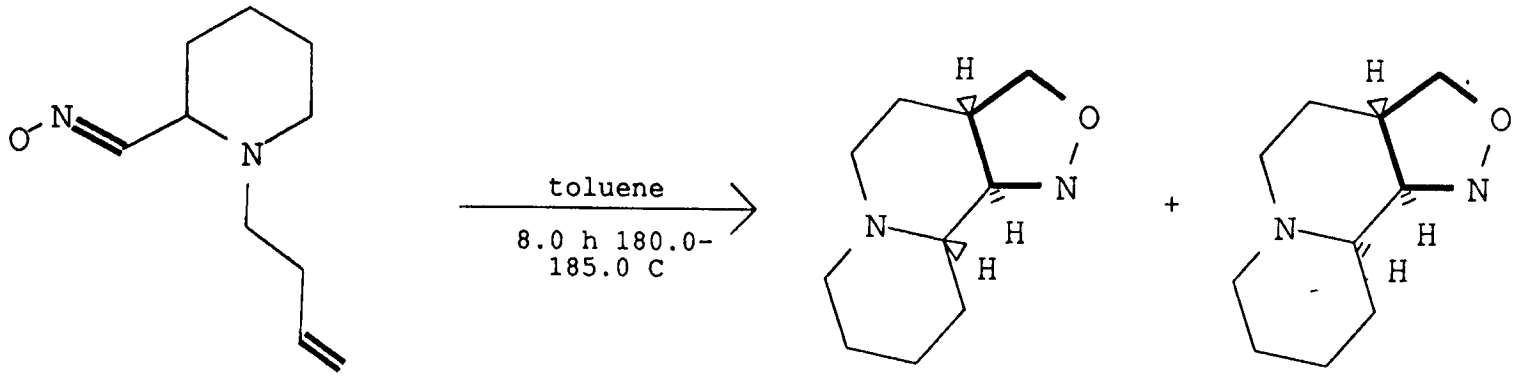


SSS AS PRODUCT NOT SSS AS REACTANT

MDL NO: RXCI91064425 RXN ID: 12 CIRX REGNO: 61196



BASERXN: 9

Cycloadditions. Part 46. Thermally-Induced Intramolecular Oxime Olefin Cycloadditions (IOOC) Leading to N-Bridgehead Systems. Stereochemistry and Molecular Mechanics Calculations.

EN

PR	SR
8	

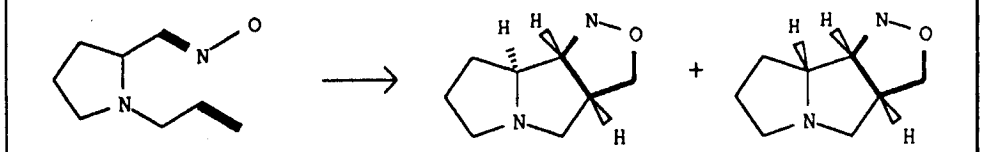
HASSNER, A. ; MAURYA, R. ; PADWA, A. ; BULLOCK, W. H. ;
J. Org. Chem. 56 (1991) 8, 2775 - 2781

CLASS

Dep. Chem., Bar-Ilan Univ., Ramat-Gan 52100, Israel

R0240
R0450

VARIATION 1 OF 1 | REFNO: 9141153 | EXTREG: 914115304 | PATH: A | 3 OF 3



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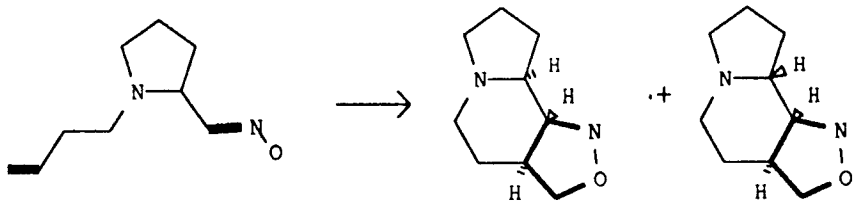

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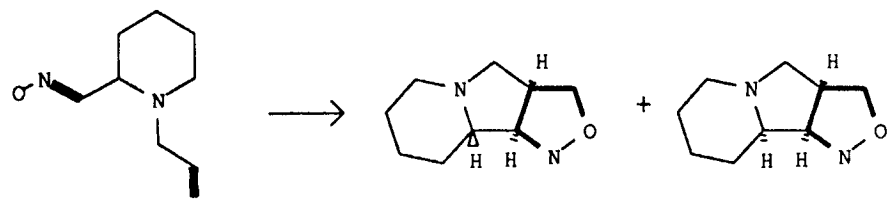

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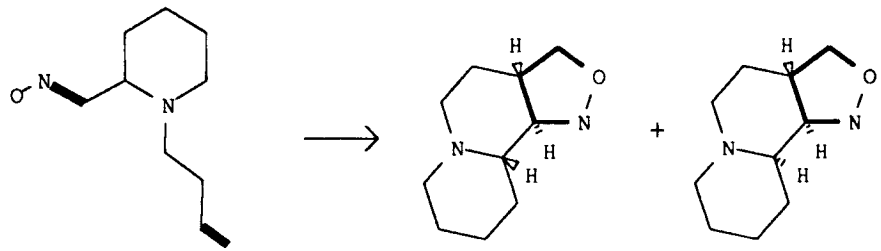

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