



Reaxysの概要と特徴

*The Shortest Path from Chemistry
Question to Insight Reaxys*

2026年2月
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目次

1. Reaxysの特徴概要
2. コンテンツ概要
3. 効率的なデータ取得のためのインターフェース例
 - ✓ Reaxys Ranking
 - ✓ 同一反応に紐づく複数の実験条件を並べて表示
 - ✓ 天然物に限定した検索
 - ✓ 同位体や異性体を考慮した検索
 - ✓ 特定条件レコードの除外機能による検索結果refine
4. 5.5億件以上の実測物性値・スペクトル情報
5. 網羅性

1. Reaxysの特徴概要

- 反応、化合物データベース
- 化学関連論文や特許から反応、物性、スペクトルデータなどをサイエンティストが手順書に従って抽出
- コンテンツ：一定の網羅性を保ちつつ、ノイズを排除し、研究者にとって有用なデータを収録
- インターフェース：
 - 効率的かつノイズの少ない結果を得るための検索機能を搭載
 - 反応条件など、必要な情報へたどり着くまでのクリック数を最小限にする設計
 - ユーザーの視認性を意識した設計（反応条件を一画面に並べて表示、スペクトルデータは核種や測定溶媒を記載等）

反応：

同一ページ内に複数の条件を並べて表示

Yield	Conditions	Reference
93.5%	With $C_{64}H_{72}N_4O_{23}Ti_{12}$ dihydrogen peroxide In water; ethyl acetate at 0°C for 24h Reagent/catalyst Experimental part	Tsai, Evgenii P.; Brylakov, Konstantin P. - Catalysis Today, 2017, vol. 279 Full Text Show details
86%	With N-methyl-6-aza-5 β ,6 ϵ -epoxy-cholestone-3 β -tert-butylidiphenylsilyloxy tetrafluoroborate In dichloromethane at -70 - 20°C for 3h Inert atmosphere	Zhou, Guobin; Guan, Yueqing - Heterocyclic Communications, 2016, vol. 22, # 1, p. 17 - 19 Full Text Show details
	With tert-butylhydroperoxide In water; toluene at -20°C for 12h	RATIOPHARM GMBH - US2008/319195, 2008, A1 Location in patent: Page/Page column 5 Full Text Show details

スペクトル：

核種や溶媒等実験条件を掲載

Description	Nucleus	Solvents	Temperature	Frequency	Original file	Location	Reference
DEPT (Distortionless Enhancement by Polarization Transfer), Spectrum	^{13}C	chloroform-d1		100		supporting information	Barbosa, Sandro L.; Nelson, David Lee; Freitas, Mili dos Santos; Williams Torres Pao Klein, Daniel L.; Ciesinski, Giuliano C.; Caires, Franco J.; Wenta, Alex [Molecules, 2022, vol. 27, # 15, art.no. 4767] Full Text Cited 2 times Details About
Chemical shifts	1H	dimethylsulfoxide-d6				Paragraph 0074	Current Patent Assignee: ZHEJIANG UNIVERSITY C TECHNOLOGY - CN115433076, 2022, A Full Text Details Abstract
Chemical shifts	^{13}C	dimethylsulfoxide-d6				Paragraph 0074	Current Patent Assignee: ZHEJIANG UNIVERSITY C TECHNOLOGY - CN115433076, 2022, A Full Text Details Abstract

2. コンテンツ概要

- ✓ 収録ジャーナル： 合成化学関連450誌
 + 幅広い分野の約18,000誌
- ✓ 化合物に関わる必須の特許情報
- ✓ **5.5億件以上の実測物性値・スペクトル情報**
- ✓ 約7,200万の反応情報（すべて異なる反応式）
- ✓ 論文ガイドにとどまらず、原著参照する前に必要な反応条件や実測物性値を得られるファクトデータベース

2026年2月現在のコンテンツ

- 収録反応数： 約7,200万
- 収録化合物： 約3億5,300万
- 収録文献・特許： 約1億2,000万件
- 実測物性値： 5.5億件以上

Physical Data - 565

Melting Point - 63

Melting Point, °C	Solvent (Melting Point)	Location	Reference
141			Lun, Hullin; Ouyang, Jing; Ya Full Text Full Text Cited 39 times Darwish, Shaza; Zeglinski, Jac Growth and Design, 2018, vol Full Text Full Text Details Details
130.5			Dichi, Emma; Sghaier, Mehre Full Text Full Text Cited 1 times
133 - 134			Sarief, Abdulla; Haque, SK Ma 1104 - 1109 Full Text Full Text Details Details
150	ethanol		Singh, Navneet; Garg, Geetika Full Text Full Text Details Details

1

Conditions [Find Similar](#) Reaction ID: 22871426 [Full Text](#)

Conditions	Yield	Reference
With sodium hydrogencarbonate In water; isopropyl alcohol at 20°C; for 3h; Experimental Procedure Experimental Procedure	88%	Biancalana, Lorenzo; Pampaloni, Guido; Zacchini, Stefano; Marchetti, Fabio [Journal of Organometallic Chemistry, 2018, vol. 869, p. 201 - 211] Full Text Full Text Cited 1 times Full Text Details Details Abstract Abstract
Na[aspCO₂]₂. The preparation of the title compound was adapted from the literature [1]. In a 10 mL round-bottom flask, a H₂O:iPrOH 85:15 v/v solution (1.0 mL) was added dropwise, with stirring, to a mixture of aspCO₂H (542 mg, 3.00 mmol) and NaHCO₃ (271 mg, 3.23 mmol). The bubbling suspension was stirred at room temperature for 3 hours in an open system. The resulting colorless solution (pH ≈ 7-8) was diluted with iPrOH (8 mL), stirred for further 30' then filtered over celite. The filtrate solution was concentrated under vacuum (V ≈ 1-2 mL, opalescent mixture) then settled aside at -20 °C overnight. The colorless crystals (Na[aspCO₂]₂·2H₂O [1]) were collected by filtration, washed with iPrOH (2 mL, -20 °C), Et₂O then dried under vacuum (50 °C over P₂O₅). Loss of crystallinity of the material was observed during these operations, possibly associated to the removal of water of crystallization [1]. The resulting colorless solid was stored under dry N₂ in sealed glass vials. Yield: 534 mg, 88 percent. All attempts to obtain Na[aspCO₂] by different procedures led to partial or complete deacetylation of the starting material [2].		
With sodium hydride In N,N-dimethyl-formamide for 0.5h;		Laboratori Alchemica S.r.l.; Nicox SA US6369260, 2002, B1 Location In patent: Example 13 Full Text Full Text Details Details Abstract Abstract

- サイエンティストが人手で実用的な価値を持つ実験データを抽出
- 一定の網羅性を担保しつつ、ノイズを低減させ、研究者によって有用と思われるデータを収録**
- 2段階の収録方法**

(1)機械による化合物情報収録

機械学習により、網羅性を担保しつつノイズを低減させる手法を継続改良
化合物に紐づくデータがなくても収録

(2)手作業による化合物情報収録

化合物は、物性、スペクトルあるいは反応情報といった化合物に紐づくデータが記載されている場合に収録する。

<反応情報>

- 反応式、収率、反応条件、実施例

<化合物情報>

- 物性値
 - ✓ 融点、沸点、溶解度、分配係数
- 400種類以上
- スペクトルデータ
 - ✓ NMR、UVスペクトル、マスマスペクトル

*** 約500項目、5億5000万件以上のデータ**

- 市販情報

The screenshot displays the Reaxys interface. On the left, a chemical reaction scheme shows the conversion of (R)-phenyl-pyridin-2-yl-acetic acid methyl ester to a cyclic product. Below the reaction, the 'Conditions' section lists two stages: Stage #1 involves (R)-phenyl-pyridin-2-yl-acetic acid methyl ester with perchloric acid in methanol/water at 45-50°C, and Stage #2 involves sodium hydroxide in water. On the right, the compound '3(5)-aminopyrazole' is detailed. It includes its molecular formula (C₄H₄N₃), CAS number (83-0928), and EINECS number (605752). The 'Identification' section lists 'Physical Data - 8' and 'Spectra - 5'. The 'Physical Data - 8' section is expanded, showing 'Melting Point - 2' with a table of values and references.

Melting Point, °C	Reference
36	Ege; Arnold - [Angewandte Chemie, 1974, vol. 86, p. 237] Full Text Details
	BASF - CH599162, 1974, DE2400415 [Chem.Abstr., vol. 83, # 179101] Full Text Details
36 - 38	Dorn et al. - [Angewandte Chemie, 1964, vol. 76, p. 920]

3. 効率的なデータ取得のためのインターフェース例：Reaxys Ranking

収率、副生成物の有無、実験条件の情報量等のパラメータから、有用と思われるレコード順に表示されます。

The screenshot displays the Reaxys web interface. On the left, a red box highlights the reaction details for Reaction ID: 28096702, which includes a chemical reaction scheme and a 'Conditions' tab. On the right, a sorting menu titled 'Sort search results' is open, with a red box highlighting the 'Reaxys Ranking' option, which is selected with a checkmark. Other sorting options listed include 'No of References', 'Reactant Availability', 'Product Availability', 'MW of product', 'Yield', and 'Publication Year'. The interface also shows a 'Find Similar' button and a 'Reaction ID: 28500901' entry at the bottom.

3. 効率的なデータ取得のためのインターフェース例： 同一反応に紐づく複数の実験条件を並べて表示

年代順ではなく、ユーザーが必要とする順に検索結果を表示することで迅速に必要なデータにアクセス。収率、副生成物の有無、反応条件における情報量等で重み付け

条件違いの同一反応を並べて表示⇒
条件毎に異なるページにするとページ間の行き来が発生するため、それを避けたUI設計

Reaxys Ranking 

Hide All Details  Find Similar Reactions 

Yield	Conditions	Reference
3.5%	With $C_{48}H_{72}N_4O_{10}Ti_2$; dihydrogen peroxide In water; ethyl acetate at 0°C for 24h Reagent/catalyst Experimental part	Talsi, Evgenii P.; Bryliakov, Konstantin P. - Catalysis Today, 2017, vol. 279 Full Text  Show details 
Experimental Procedure 		
86%	With N-methyl-6-aza-5 β ,6 β -epoxy-cholestane-3 β -tert-butyl(diphenylsilyloxy tetrafluoroborate In dichloromethane at -70 - 20°C for 3h Inert atmosphere Experimental part	Zhou, Guobin; Guan, Yueqing - Heterocyclic Communications, 2016, vol. 22, # 1, p. 17 - 19 Full Text  Show details 
	With tert-butylhydroperoxide In water; toluene at -20°C for 12h	RATIOPHARM GMBH - US2008/319195, 2008, A1 Location in patent: Page/Page column 5 Full Text  Show details 
Experimental Procedure 		
Experimental Procedure Titanium tetraisopropoxide (4.5 mg, 0.016 mmol) was added to a solution of (S,S)-1,2-bis-(2-bromophenyl)ethane-1,2-diol (12 mg, 0.032 mmol) in toluene (2 ml) at 25° C. The solution was stirred for 10 minutes, water (5.7 mg, 0.32 mmol) was added, and the solution was stirred for another 10 minutes. 5-methoxy-2-[[[4-methoxy-3,5-dimethyl-2-pyridinyl]-methyl]thio]-1H-benzimidazole (105 mg, 0.32 mmol) was then added to the solution, and the temperature was adjusted to -20° C. Thereafter, t-butyl hydroperoxide (70percent, 96 μl, 0.064 mmol) was slowly added. After 12 hours at -20° C., the solution was extracted three times with aqueous ammonium hydroxide (12.5percent NH3, 3x.5 ml). Thereafter, the methyl isobutyl ketone (5 ml) was added to the combined aqueous extracts. After this, the pH of the aqueous phase was adjusted using acetic acid, the aqueous phase was separated and extracted with an additional amount of methyl isobutyl ketone (5 ml). The organic solution was cooled to -10° C. over night, and the neutral form of R-omeprazole was precipitated as a solid to obtain the title compound. The enantiomeric excess of R-omeprazole was 93percent.		

3. 効率的なデータ取得のためのインターフェース例： 天然物に限定した検索

The screenshot displays the Reaxys search interface with several numbered annotations (1-5) and red boxes highlighting key features:

- 1**: Points to the **Query builder** tab in the top navigation bar.
- 2**: Points to the **Structure** tab in the search criteria panel.
- 3**: Points to the **Search fields** input box containing the text **natural**.
- 4**: Points to the **Find any** checkbox in the search criteria panel.
- 5**: Points to the **Substances >** tab in the search criteria panel.

The main search area shows a chemical structure of a benzamide derivative. The search criteria panel on the right includes the filter **Isolated from Natural Source**. The bottom of the interface shows a search bar with the text **Isolated from Natural L...** and a **Show fields** dropdown menu.

天然物に限定した化合物・反応あるいは文献・特許検索を行うことができます。

3. 効率的なデータ取得のためのインターフェース例： 天然物に限定した検索

Reaxys® Quick search Query builder ^{New} Results Synthesis planner History Takashi Isobe

42 Substances out of 13,785 Documents containing 1,330 Reactions

1

Limit To Exclude Export

Reaxys - 42

No of References ↓ List

1 2 3 4 5 6 7 8 9 10

1 天然物に限定した化合物検索結果

2 限定しない場合の化合物検索結果

Reaxys® Quick search Query builder ^{New} Results Synthesis planner History Takashi Isobe

14,391 Substances out of 16,767 Documents containing 27,796 Reactions

2

Limit To Exclude Export

Reaxys - 14,391

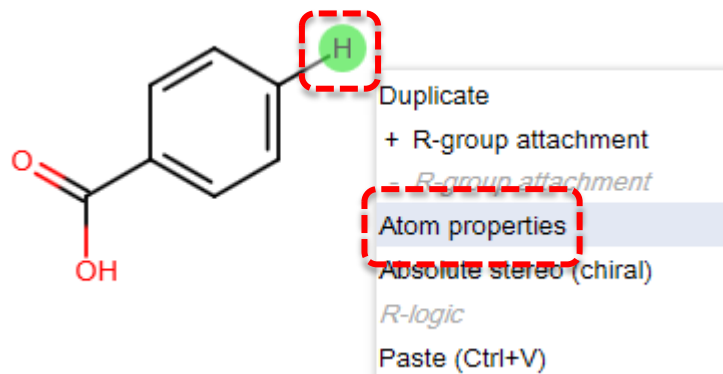
No of References ↓ List

1 2 3 4 5 6 7 8 9 10

3. 効率的なデータ取得のためのインターフェース例： 同位体や電荷を考慮した検索

■ 検索例：アレーンの重水素化反応

立体異性体、電荷、原子価、ラジカル、同位体等、様々な観点から化合物や反応の検索を行うことができます。



Atom properties

Change to: Element

Basic | Advanced

Atom: H 1

Alias: [locked]

Isotope: 2 [x] [locked] (highlighted with a red dashed box)

Charge: 0

Radical: none [v]

Enhanced stereo: Off [v]

Map: [locked]

OK

直接Dとタイプしても可

Reaction ID: 9743270

2

3 Conditions Find Similar >

Yield	Conditions	References
94%	With deuterated hypophosphorous acid; palladium 10 on activated carbon; sodium carbonate In water-d2 at 50°C; for 1.5h; regioselective reaction;	Oba, Makoto - Journal of Labelled Compounds and Radiopharmaceuticals, 2015, vol. 58, # 5, p. 215 - 219 Full Text [v] Cited 3 times [v] Details > Abstract >
79%	With hydrogen; water-d2; triethylamine; palladium on activated charcoal In methanol at 20°C; for 24h;	Sajiki, Hironao; Kurita, Takanori; Esaki, Hiroyoshi; Aoki, Fumiyo; Maegawa, Tomohiro; Hirota, Kosaku - Organic Letters, 2004, vol. 6, # 20, p. 3521 - 3523 Full Text [v] Cited 32 times [v] Details > Abstract >
79%	With 10 Pd/C; hydrogen; water-d2; triethylamine In methanol at 20°C; for 24h; chemoselective reaction;	Kurita, Takanori; Aoki, Fumiyo; Mizumoto, Takuto; Maejima, Toshihide; Esaki, Hiroyoshi; Maegawa, Tomohiro; Monguchi, Yasunari; Sajiki, Hironao -

3. 特定条件レコードの除外機能による検索結果refine

必要なレコードに絞り込むだけでなく、不要なレコードのみ除外する機能を実装しています。

Filters and Analysis

Limit to > **Exclude >**

By Structure ▼

Yield ▼

Reagent/Catalyst 1 ^

☒ palladium diacetate	391
☐ tetrakis(triphenylphosphine) palladium ⁽⁰⁾	270
☐ potassium carbonate	198
☐ triphenylphosphine	187
☐ palladium dichloride	167

4,638 Reactions out of 4,766 Documents containing 4,571 Substances

☐ 0 selected Limit To Exclude Export Syn-Plan

☐ Reaction ID: 28332007 +□□

1 🔍 📄 ☰ 🔍 📄 ☰

Fc1ccccc1.[K+].c1ccccc1>>c1ccccc1-c2ccccc2

+□□ +□□

5 Conditions ^ Find Similar >

Yield Conditions

4. 5.5億件以上の実測物性値・スペクトル情報

収録物性値抜粋

Melting Point

Boiling Point

Sublimation

Refractive Index

Density

Conformation

Interatomic Distances and Angles

Electrical Moment

Electrical Polarizability

Molecular Deformation

Energy Barriers

Dissociation Energy

Ionization Potential

Electron Binding

Crystal Property Description

Crystal Phase

Crystal System

Decomposition

Triple Point

Transition Point(s) of Crystalline
Modification(s)

Crystal System

Space Group

Density of the Crystal

Liquid Phase

Transition Point(s) of Liquid
Modification(s)

Critical Temperature

Critical Pressure

Critical Density

Critical Volume

Vapour Pressure

4. 5.5億件以上の実測物性値・スペクトル情報

Reaxys® Quick search Query builder Results Synthesis planner History Takashi Isobe

Search in: Reactions Substances Documents

Import Save Reset form Delete all

Structure Molecular Formula CAS RN Doc. Index

Find search fields and forms

Fields Forms History

Reaxys

Basic Indexes

Identification

Physical Properties

Spectra

Pharmacological Data

Ecotoxicology

Other

Reactions

Bibliography

PubChem

eMolecules

LabNetwork

Structure

On all atoms

Melting Point

Find any Hide fields

>= 100

is Solvent (Melting Point)

Refractive Index

Find any Hide fields

>= 1

= Wavelength (Refractive Index), nm

= Temperature (Refractive Index), °C

100 Substances out of 108,823 Documents containing 109,044 Reactions

Limit To Exclude Export

benzoic acid
(C₆H₅CO₂H) 122.123 636131 65-85-0

Hit Data - 110

Identification

Physical Data - 2,978

Hit Data - 110

Melting Point - 100 hits out of 103

Refractive Index - 10 hits out of 10

salicylic acid
(C₆H₄(OH)(CO₂H)) 138.123 774890 69-72-7

Hit Data - 46

Identification

Hit Data - 110

Melting Point - 100 hits out of 103

Melting Point, °C	Solvent (Melting Point)	Location	Reference
124 - 126		supporting information	Maly, Asim; Hyun, Sung-Min; Wortman, Alan K.; Powers, David C. - [Angewandte Chemie - International Edition, 2018, vol. 57, # 24, p. 7205 - 7209, Angew. Chem., 2018, vol. 130, p. 7323 - 7327,5] Full Text Details Abstract
126 - 129		supporting information	Maly, Asim; Hyun, Sung-Min; Wortman, Alan K.; Powers, David C. - [Angewandte Chemie - International Edition, 2018, vol. 57, # 24, p. 7205 - 7209, Angew. Chem., 2018, vol. 130, p. 7323 - 7327,5] Full Text Details Abstract

Hit Data - 110

Melting Point - 100 hits out of 103

Refractive Index - 10 hits out of 10

Refractive Index	Wavelength (Refractive Index), nm	Temperature (Refractive Index), °C	Reference
1.539	589	15	Dutshak; Panchenko - [J. Gen. Chem. USSR (Engl. Transl.), 1977, vol. 47, p. 1771, Zhurnal Obshchei Khimii, 1977, vol. 47, p. 1936] Full Text Details
1.54	589	20	Wollmann; Skaletzki; Schaaf - [Die Pharmazie, 1974, vol. 29, # 10-11, p. 708 - 711] Full Text Details Abstract

4. 5.5億件以上の実測物性値・スペクトル情報

1

CC(=O)Oc1ccccc1C(=O)O

aspirin

C6H4OOCCH3COOH 180.16 779271 50-78-2

Identification

Bioactivity - 4,158

Physical Data - 563

Other Data - 3,799

Spectra - 189

Preparations - 96 >

Reactions - 1,191 >

Documents - 17,793 >

aspirin

Identification

Physical Data - 563

Spectra - 189

情報の掲載箇所（ページ数やSI等）

核種

測定溶媒

NMR Spectroscopy - 53									
Description (NMR Spectroscopy)	Nucleus (NMR Spectroscopy)	Chemical Shift (ppm)	Solvents (NMR Spectroscopy)	Temperature (NMR Spectroscopy), °C	Frequency (NMR Spectroscopy), MHz	Original Text (NMR Spectroscopy)	Location	Content (NMR Spectroscopy)	Reference
DEPT (Distortionless Enhancement by Polarisation Transfer), Spectrum	¹³ C		chloroform-d1		100		supporting information		Full Text Cited 2 times Details Abstract Barbosa, Sandro L.; Nelson, David Lee; Freitas, Mil dos Santos, Wallans Torres Pio; Klein, Stanley I.; Clososki, Giuliano C.; Caires, Franco J.; Wentz, Alex [Molecules, 2022, vol. 27, # 15, art. no. 4767] Full Text Cited 2 times Details Abstract
Chemical shifts	¹ H		dimethylsulfoxide-d6				Paragraph 0074		Current Patent Assignee: ZHEJIANG UNIVERSITY C TECHNOLOGY - CN115433076, 2022, A Full Text Details Abstract
Chemical shifts	¹³ C		dimethylsulfoxide-d6				Paragraph 0074		Current Patent Assignee: ZHEJIANG UNIVERSITY C TECHNOLOGY - CN115433076, 2022, A Full Text Details Abstract

4. 5.5億件以上の実測物性値・スペクトル情報

核種等スペクトルデータを指定した検索インターフェース

The screenshot displays the Reaxys Query builder interface. The top navigation bar includes 'Quick search', 'Query builder' (highlighted with a red box), 'Results', 'Synthesis planner', and 'History'. The user 'Takashi Isobe' is logged in. Below the navigation bar, there are tabs for 'Reactions', 'Substances', and 'Documents'. A search bar is present with the text 'Search in:'. Below the search bar, there are icons for 'Import', 'Save', 'Reset form', and 'Delete all'. The main area is divided into two sections. The left section, titled 'NMR Spectroscopy', contains a table of search criteria. The right section, titled 'Find search fields and forms', contains a list of search fields. The 'Spectra' section in the right sidebar is highlighted with a red box, showing 'NMR Spectroscopy', 'IR Spectroscopy', 'Mass Spectrometry', and 'UV/VIS Spectroscopy'. The 'NMR Spectroscopy' section in the main area is also highlighted with a red box, showing a table of search criteria.

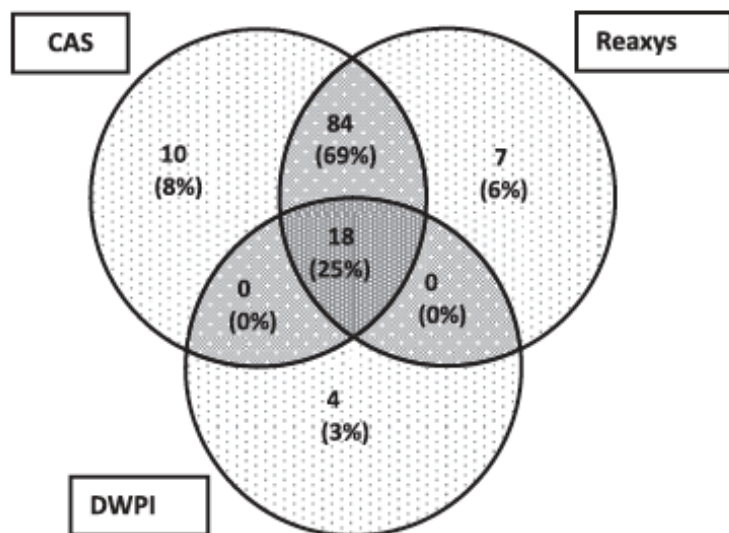
Find any	Hide fields
is	Description (NMR Spectroscopy)
is	Nucleus (NMR Spectroscopy)
is	Coupling Nuclei
is	Solvents (NMR Spectroscopy)
=	Temperature (NMR Spectroscopy), °C
=	Frequency (NMR Spectroscopy), MHz
is	Original Text (NMR Spectroscopy)

AND Structure

Create Structure / Reaction Drawing

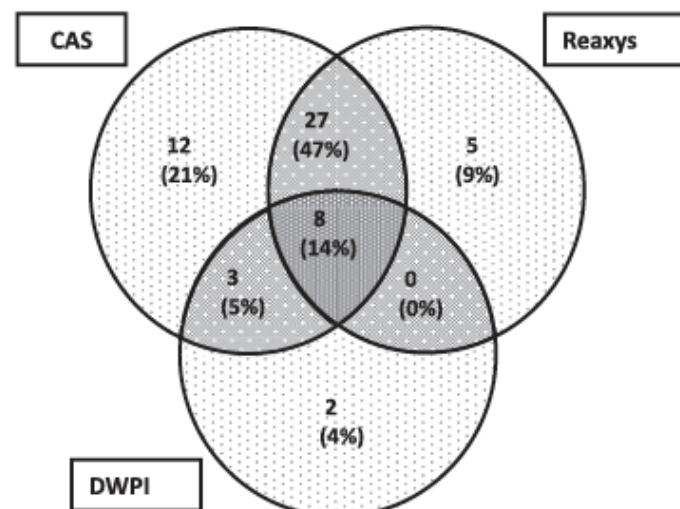
5. 網羅性：データベース間収録コンテンツの差異

4. Case study- WO2010026122 (Novartis – Heterocyclic PIM-Kinase Inhibitors)



Venn Diagram 1.

5. Case study – WO20100106249 (Servier Laboratoires - Benzothiadiazepine Derivatives Used as AMPA and NMDA Receptor Modulators)



Venn Diagram 2.

Mark Ede, John Endacott, Mark Harper, David Rees

Indexing chemical structures: Exemplified compound indexing in patents by the vendors Thomson Reuters, Chemical Abstracts and Elsevier – A comparative study by the Patent Documentation Group (PDG)

World Patent Information, Volume 44, 2016, 48–52

<https://doi.org/10.1016/j.wpi.2015.12.003>

ある2つの特許に含まれる化合物がReaxys、CAS、DWPIで網羅されているかどうかを調査し、ベン図に示したものの。それぞれユニークな化合物収録があり、網羅的に検索する場合は、これらすべてを検索することが理想的。