



Reaxysの概要と特徴

*The Shortest Path from Chemistry
Question to Insight Reaxys*

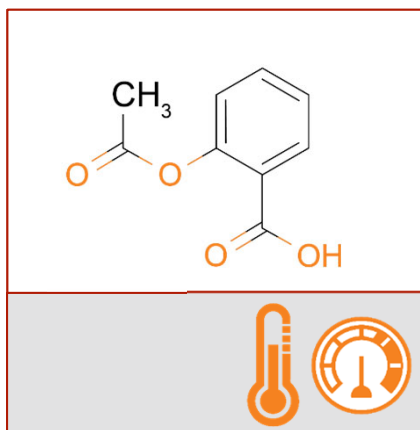
2021年7月7日
エルゼビア・ジャパン
磯辺 隆



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- 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ス
デ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検索機能を搭載



3,368万以上の化合物と
その物性（物性値、ス
ペクトル、生物活性
データなど）5億5千万
件を収録

収録データ



5,454万件以上の反応情
報（反応条件、溶媒、
触媒、収率など）を収
録

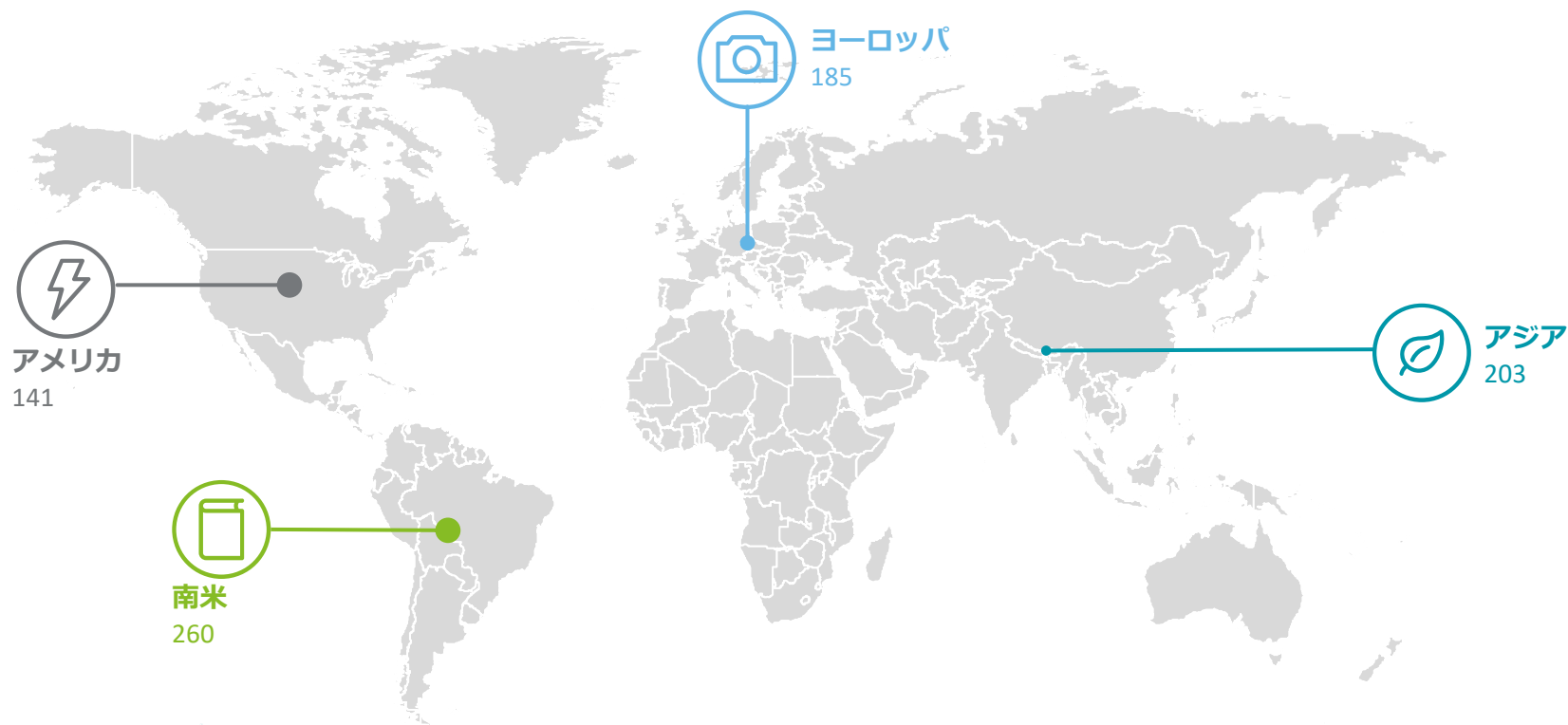


6,153万件以上のライフサイエ
ンス、マテリアル、エンジニ
アリング、薬理学、環境科学
などに関連する文献を15,000
誌のジャーナルや特許から収
録

情報源

導入実績

789の大学・公的機関に導入されています。
(2019年1月現在、企業を除く)



The Times Higher Education 上位50校のうち42校がReaxysを導入しています。

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16,000誌を追加
- ✓ 化合物に関わる必須の特許情報
- ✓ **5億5千万件以上の実測物性値・同定情報**
- ✓ 約5,601万の反応情報（すべて異なる反応）
- ✓ 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
- ✓ PubChemやeMoleculesに収録されている化合物データも同時検索可能
- ✓ Gmelin Handbook, Belistein Handbookを収載

2021年7月現在のコンテンツ

- 収録反応数： 約5,601万
- 収録化合物： 約3,440万
- **実測物性値： 5億5千万件以上**

収録対象の大幅な拡大

ライフサイエンス、エンジニアリング、薬理学、環境科学などの多岐にわたる分野の書籍、学会抄録などを含む約16,000誌の定期刊行物における構造情報や化学関連情報



- 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**

(例) 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。化合物名や構造のみが文献・特許中に記載されているような場合は収録対象外

<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

Reaxys®

The screenshot displays the Reaxys interface. At the top, a chemical reaction is shown: (R)-phenyl-pyridin-2-yl-acetic acid methyl ester reacts with sodium hydroxide in water to form 3(5)-aminopyrazole. Below the reaction, the experimental conditions are listed: Stage #1: (R)-phenyl-pyridin-2-yl-acetic acid methyl ester, palladium/activated carbon in methanol; water at 45 - 50°C; Stage #2: With sodium hydroxide in water. The compound details for 3(5)-aminopyrazole are shown on the right, including its molecular formula (C₆H₆N₂), molecular weight (83.0928), and CAS number (605752). The physical data section is expanded, showing the melting point (36°C) and references (Ege; Arnold - [Angewandte Chemie, 1974, vol. 86, p. 237] and BASF - CH599162, 1974, DE2400415 [Chem.Abstr., vol. 83, # 179101]).

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. At the top, a reaction is shown with the ID 28096702. Below the reaction, there are icons for search, filters, and a shopping cart. A red box highlights the left sidebar area, which contains a list of reaction IDs (e.g., 28096702, 28500901) and a 'Find Similar' button. On the right, a 'Sort search results' dropdown menu is open, showing various sorting criteria. The 'Reaxys Ranking' option is selected and highlighted with a red box. Other options include 'No of References', 'Reactant Availability', 'Product Availability', 'MW of product', 'Yield', and 'Publication Year'.

Reaction ID: 28096702

1

Reaction ID: 28500901

2

4 Conditions Find Similar

Sort search results

- ✓ Reaxys Ranking
- No of References
- Reactant Availability
- Product Availability
- MW of product
- Yield
- Publication Year

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⇒容易に比較

原著にあたる前に、検索結果の画面上で基本情報が得られる

反応の実験項・実施例をワンクリックで表示⇒複数の実施例の比較も容易

Chemical reaction scheme showing the synthesis of a benzimidazole derivative.

Reaxys Ranking 

Hide All Details  Find Similar Reactions 

Yield	Conditions	Reference
3.5%	With $C_{68}H_{72}N_4O_{10}Ti_2$; 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-cholestone-3 β -tert-butylidiphenylsilyloxy 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, 3x5 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.		

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

1

The screenshot displays the Reaxys Query Builder interface. At the top, the 'Query builder' tab is selected and highlighted with a red box (1). Below it, the 'Search in:' section shows 'Substances' selected with a red box (2). The 'Structure' icon is also highlighted with a red box (2). The search term 'natura' is entered in the search bar, highlighted with a red box (3). The chemical structure of a natural product derivative is shown in the main area, highlighted with a red box (4). The 'Isolation from Natural Product' filter is selected in the right sidebar, highlighted with a red box (3). The 'Find any' checkbox is checked in the bottom left, highlighted with a red box (4). The 'Synthesis plan' tab is highlighted with a yellow circle (5).

Reaxys[®] Quick search Query builder^{New} Results Synthesis plan⁵ 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
Q natura

Structure

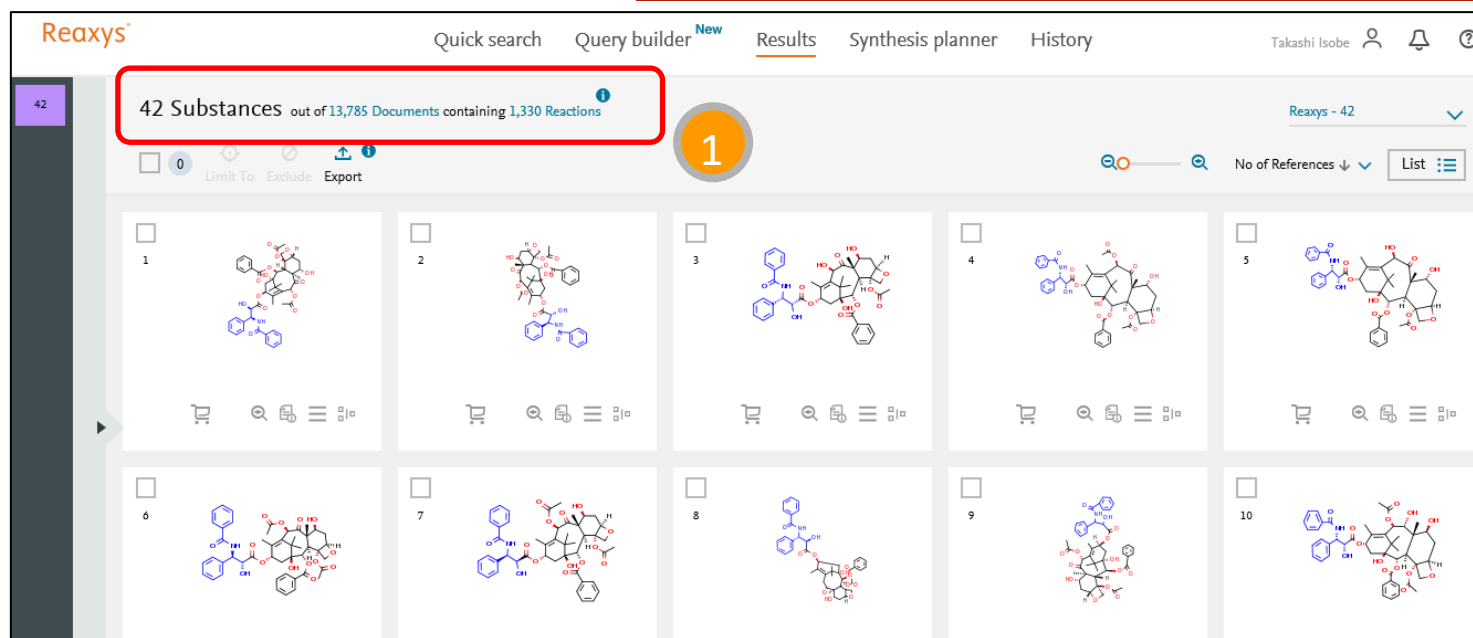
On all atoms

AND Isolation from Natura... Find any Show fields (Isolation from Natural Product)

Isolation from Natural Product

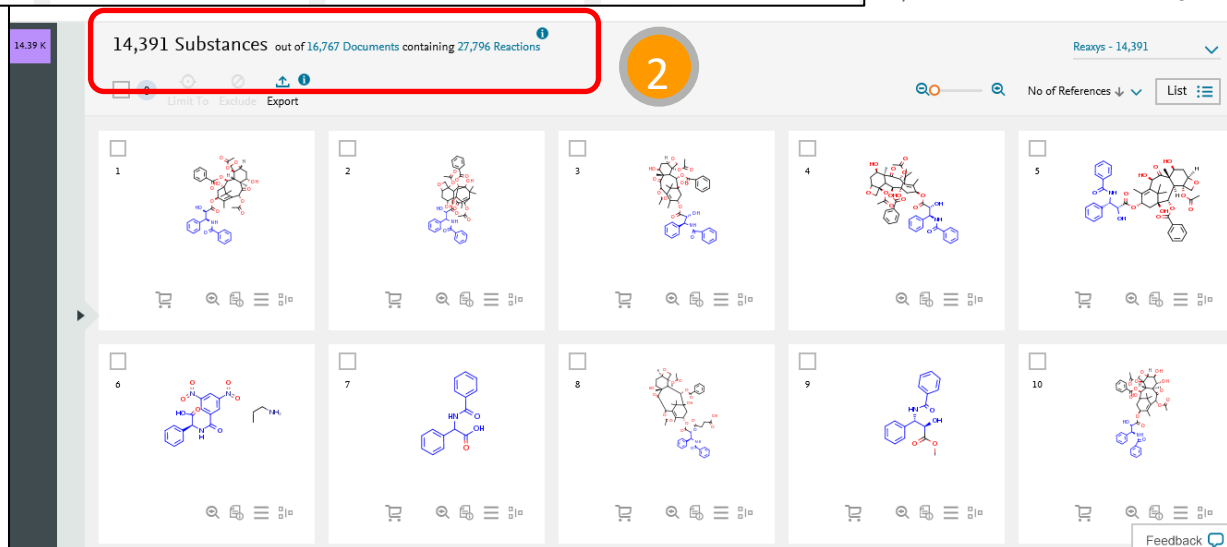
天然物に限定した化合物・反応あるいは文献・特許検索を行うことができます。

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



1 天然物に限定した化合物検索結果

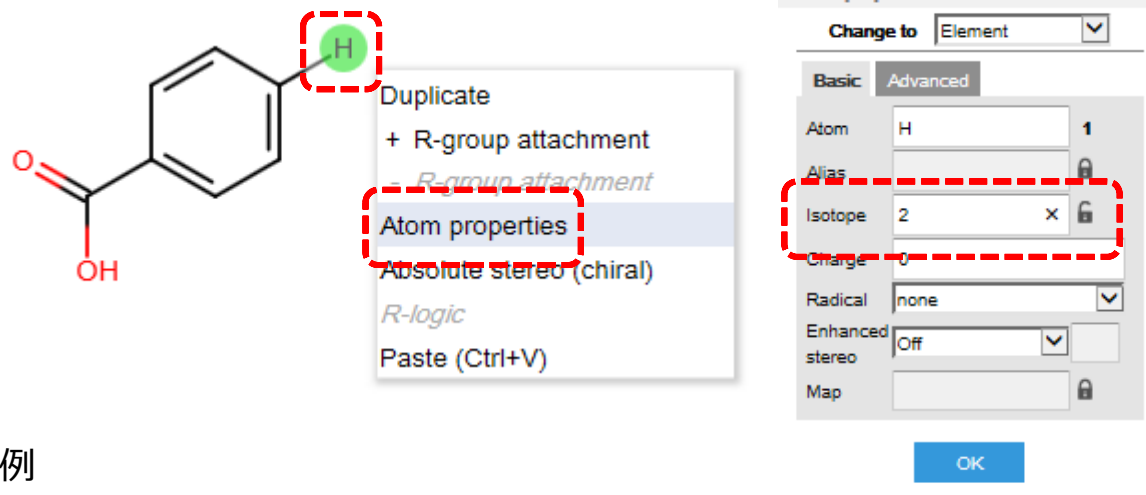
2 限定しない場合の化合物検索結果



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。



■ 検索結果例

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 > Cited 3 times > 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 > Cited 32 times > 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 -

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。

The screenshot displays the Reaxys search results interface. On the left, the 'Filters and Analysis' panel is visible, featuring a red box around the 'Exclude >' button. Below this, a list of reagents/catalysts is shown with checkboxes and counts:

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

The main panel shows '4,638 Reactions out of 4,766 Documents containing 4,571 Substances'. Below this, a toolbar includes 'Limit To', 'Exclude', 'Export', and 'Syn-Plan' buttons. A specific reaction is highlighted with 'Reaction ID: 28332007'. The reaction scheme shows a phenylboron trifluoride complex reacting with a potassium cation to form biphenyl. At the bottom, there are tabs for 'Yield' and 'Conditions', and a 'Find Similar' button.

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	Crystal Phase
Boiling Point	Crystal System
Sublimation	Decomposition
Refractive Index	Triple Point
Density	Transition Point(s) of Crystalline Modification(s)
Conformation	Crystal System
Interatomic Distances and Angles	Space Group
Electrical Moment	Density of the Crystal
Electrical Polarizability	Liquid Phase
Molecular Deformation	Transition Point(s) of Liquid Modification(s)
Energy Barriers	Critical Temperature
Dissociation Energy	Critical Pressure
Ionization Potential	Critical Density
Electron Binding	Critical Volume
Crystal Property Description	Vapour Pressure

5.5億件以上の実測物性値・スペクトル情報

複数条件を満たす化合物・反応の検索：
部分構造、融点100℃以上、屈折率1以上の化合物

The screenshot shows the Reaxys search interface. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. The search bar is set to 'Reactions' > 'Substances' > 'Documents'. The search criteria are defined in the 'Query builder' section:

- Structure:** A chemical structure of benzoic acid is shown in a red box.
- Melting Point:** Set to 'Find any' with a condition of '≥ 100'.
- Refractive Index:** Set to 'Find any' with a condition of '≥ 1'.

The right sidebar shows a list of search fields and forms, including 'Basic Indexes', 'Identification', 'Physical Properties', 'Spectra', 'Pharmacological Data', 'Ecotoxicology', 'Other', 'Reactions', and 'Bibliography'.

The screenshot shows the search results page for '100 Substances' out of 108,823 documents containing 109,044 reactions. The results are displayed in a table with columns for 'Substance', 'Hit Data', and 'Physical Data'. The first two results are highlighted:

- benzoic acid** (C₆H₅CO₂H): 122.123, 636131, 65-85-0. Hit Data - 110. Physical Data - 2,978.
- salicylic acid** (C₆H₄(OH)CO₂H): 138.123, 774890, 69-72-7. Hit Data - 46. Identification.

The 'Hit Data' section for the first result is highlighted in a red box, showing 'Melting Point - 100 hits out of 103' and 'Refractive Index - 10 hits out of 10'.

Hit Data - 110

Melting Point - 100 hits out of 103

Melting Point, °C	Solvent (Melting Point)	Location	Reference
124 - 126		supporting information	Maitly, 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	Maitly, 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

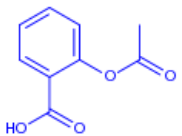
Refractive Index - 10 hits out of 10

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	Wolffmann; Skatetzki; Schaaf - [Die Pharmazie, 1974, vol. 29, # 10-11, p. 708 - 711] Full Text Details Abstract

ヒットした物性値

5.5億件以上の実測物性値・スペクトル情報

1



aspirin

C₆H₄OOCCH₃COOH 180.16 779271 50-78-2

Identification

Physical Data - 563

Spectra - 189

Bioactivity - 4,158

Other Data - 3,799

Preparations - 96 >

Reactions - 1,191 >

Documents - 17,793 >

aspirin

Identification

Physical Data - 563

Spectra - 189

NMR Spectroscopy - 53

情報の掲載箇所（ページ数やSI等）

核種

測定溶媒

Description (NMR Spectroscopy)	Nucleus (NMR Spectroscopy)	Coupling Nuclei	Solvents (NMR Spectroscopy)	Temperature (NMR Spectroscopy), °C	Frequency (NMR Spectroscopy), MHz	Location	Reference
Chemical shifts, Spectrum	1H		dimethylsulfoxide-d ₆			supporting information	Banti, Christina N.; Papatriantafyllopoulou, Constantina; Tasiopoulos, Anastasios J.; Hadjikakou, Sotiris K. - [European Journal of Medicinal Chemistry, 2018, vol. 143, p. 1687 - 1701] Full Text > Cited 4 times > Details > Abstract >
Chemical shifts	1H		dimethylsulfoxide-d ₆ , water-d ₂	25		supporting information	Biancalana, Lorenzo; Batchelor, Lucinda K.; Funaioli, Tiziana; Zacchini, Stefano; Bortoluzzi, Marco; Pampaloni, Guido; Dyson, Paul J.; Marchetti, Fabio - [Inorganic Chemistry, 2018, vol. 57, # 11, p. 6669 - 6685] Full Text > Cited 6 times > Details > Abstract >

15

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. The main search area is titled 'Search in:' with buttons for 'Reactions', 'Substances', and 'Documents'. Below this, there are icons for 'Import', 'Save', 'Reset form', and 'Delete all'. The central panel shows a search criteria table for 'NMR Spectroscopy' (highlighted with a red box). The table has columns for 'Find any', 'Hide fields', and a list of search criteria. The criteria include 'Description (NMR Spectroscopy)', 'Nucleus (NMR Spectroscopy)', 'Coupling Nuclei', 'Solvents (NMR Spectroscopy)', 'Temperature (NMR Spectroscopy), °C', 'Frequency (NMR Spectroscopy), MHz', and 'Original Text (NMR Spectroscopy)'. To the right, a sidebar titled 'Find search fields and forms' shows a list of search fields: 'Basic Indexes', 'Identification', 'Physical Properties', 'Spectra' (highlighted with a red box), 'NMR Spectroscopy', 'IR Spectroscopy', 'Mass Spectrometry', and 'UV/VIS Spectroscopy'. The bottom of the interface features a 'Create Structure / Reaction Drawing' button.

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)

スペクトル情報の迅速な入手: Luminescence, Fluorescence, Phosphorescenceいずれかを持つレコードの検索(1/2)

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 TI, AB & KW

Structure

As drawn

AND Luminescence Spectroscopy Find any Show fields (Description)

AND Fluorescence Spectroscopy Find any Show fields (Description...Temperature, °C)

AND Phosphorescence Spect... Find any Show fields (Description...Temperature, °C)

ドラッグ&ドロップによるグループ化

Group 1 Ungroup

AND Luminescence Spectroscopy Find any Show fields (Description)

AND Fluorescence Spectroscopy Find any Show fields (Description...Temperature, °C)

AND Phosphorescence Spect... Find any Show fields (Description...Temperature, °C)

OR

OR

Find search fields and forms

Fields Forms History

Topics and Keywords

Identification

Physical Properties

Spectra

NMR Spectroscopy

IR Spectroscopy

Mass Spectrometry

UV/VIS Spectroscopy

Raman Spectroscopy

ESR Spectroscopy

NQR Spectroscopy

Rotational Spectroscopy

Luminescence Spectroscopy

Fluorescence Spectroscopy

Phosphorescence Spectroscopy

ダブルクリック

スペクトル情報の迅速な入手: Luminescence, Fluorescence, Phosphorescenceいずれかを持つレコードの検索(2/2)

スペクトルの絞り込みを行わない場合

812 Substances out of 17,022 Documents containing 6,208 Reactions

59 Substances out of 16,635 Documents containing 5,994 Reactions

anthracene
C6H4C6H4CHCH 178.233 1905429 120-12-7

Hit Data - 434
Identification

Physical Data - 3,077
Spectra - 883

Bioactivity - 1,149
Other Data - 2,227

Preparations - 1,036
Reactions - 5,933
Documents - 16,372

Hit Data - 434

- ✓ Luminescence Spectroscopy - 143 hits out of 143
- ✓ Fluorescence Spectroscopy - 273 hits out of 273
- ✓ Phosphorescence Spectroscopy - 18 hits out of 18

Description (Phosphorescence Spectroscopy)	Solvent (Phosphorescence Spectroscopy)	Temperature (Phosphorescence Spectroscopy), °C	Comment (Phosphorescence Spectroscopy)	Reference
Triplet state quenching				Adam, Waldemar; Schneider, Katrin; Stapper, Marion; Steenken, Steen [Journal of the American Chemical Society, 1997, vol. 119, # 14, p. 3280 - 3287] Full Text Cited 23 times Details Abstract Flors, Cristina; Ogilby, Peter R.; Luis, Javier G.; Grillo, Teresa A.; Izquierdo, Laura R.; Gentili, Pier-Luigi; Bussotti, Laura; Nonell, Santi

Reaxys

Quick search Query builder Results Synthesis planner History

Search in: Reactions Substances Documents

Structure Molecular Formula CAS RN TL AB & KW

Structure

As drawn

AND Group 1 Ungroup

- Luminescence Spectroscopy Find any Show fields (Description)
- Fluorescence Spectroscopy Find any Show fields (Description...Temperature, °C)
- Phosphorescence Spectroscopy Find any Show fields (Description...Temperature, °C)

Find search fields and forms

Fields Forms History

Physical Properties

Spectra

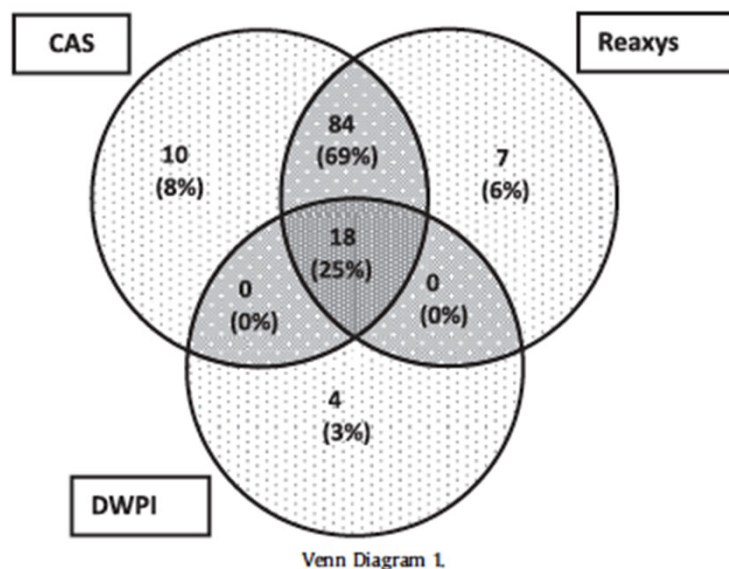
- NMR Spectroscopy
- IR Spectroscopy
- Mass Spectrometry
- UV/VIS Spectroscopy
- Raman Spectroscopy
- ESR Spectroscopy
- NQR Spectroscopy
- Rotational Spectroscopy
- Luminescence Spectroscopy
- Fluorescence Spectroscopy
- Phosphorescence Spectroscopy
- Other Spectroscopic Methods

Pharmacological Data

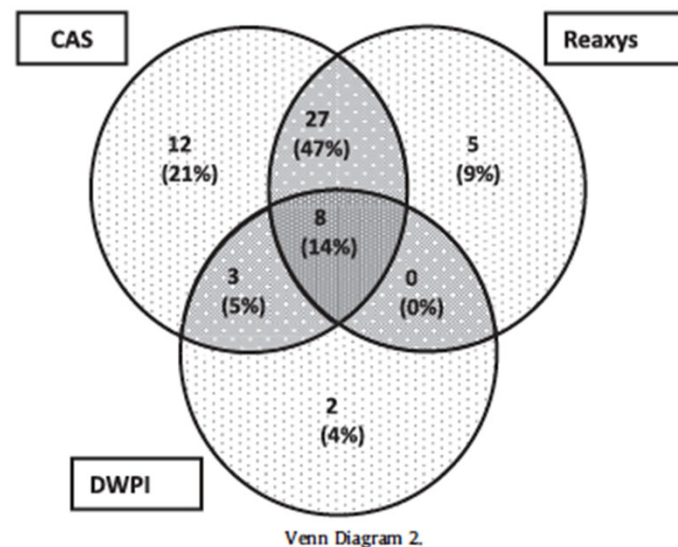
Feedback

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)



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



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。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。