

CAS SciFinder®

CHEMSCAPE ANALYSIS

化学情報協会 情報事業部
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Chemscape Analysis とは

構造の類似性と物質関連特許の件数で 3D マップを作成する機能

The image shows the Chemscape Analysis interface. On the left, a window titled "物質の構造検索結果" (Search Results for Substance Structure) displays four chemical structures with their respective CAS numbers and associated data (References, Reactions, Suppliers). A blue arrow points from this window to the main "Chemscape Analysis" window. The main window features a 3D bar chart where the height of each bar represents the number of patents related to a specific chemical structure. A detailed information panel on the right shows the structure of 8-Hydroxypyrene-1,3,6-Trisulfonic acid, including its molecular formula (C₁₈H₁₀O₁₀S₃), SMILES string, and synonyms.

物質構造と関連特許を紐づけることで物質関連の特許解析や物質の用途探索に利用できる

Chemscape Analysis 作成の流れ (1/2)

① Substances (物質検索) を選択

The image illustrates the first step of the Chemscape Analysis workflow. On the left, a navigation menu shows "Substances" selected. Below it, a search bar is labeled "Search by Substance Name, Functional Group," and there are options for "Molecular Formula" and "Add Advanced Search Field". In the center, the "CAS Draw" window is open, showing a chemical structure of a complex molecule. A blue arrow points from the search bar to the "CAS Draw" window, and another blue arrow points from the "CAS Draw" window to the "Draw" button in the search bar. A blue box with the text "② 構造を作図して検索を実行" (2. Draw the structure and execute the search) is overlaid on the "CAS Draw" window. The molecular formula C₂₄H₂₉NO₃ (379.50) is displayed at the bottom of the window.

Chemscape Analysis 作成の流れ (2/2)

③ 目的に応じて Structure Match を選択*

④ Create Chemscape Analysis をクリック (上限 1,000 件)

Substances search for drawn structure

References - Reactions - Suppliers -

Structure Match

- As Drawn (396)
- Substructure (992)
- Similarity (417K)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful new tool. Learn more about Chemscape.

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Search Within Results

Reaction Role

Reference Role

Life Science Data

Commercial Availability

Number of Components

992 Results

Sort: Relevance - View: Partial -

1 120014-06-4

C24H29NO3
Donepezil

5,330 References 464 Reactions 87 Suppliers

2 142057-80-5

C24H29NO3
(-)-Donepezil

31 References 13 Reactions 33 Suppliers

3 142698-19-9

C24H29NO3
(+)-Donepezil

29 References 11 Reactions 33 Suppliers

4 286389-25-1

C24H29NO3
1H-Inden-1-one, 2,3-dihydro-5-methoxy-6-(methoxy-¹¹C)-2-[[1-(phenylmethyl)-4-pip...

5 References 1 Reaction 1 Supplier

5 1228545-52-5

C24H29DNO3
2,3-Dihydro-5,6-dimethoxy-2-[[1-(phenylmethyl)-4-piperidinyl)methyl]-1H-inden-1-...

4 References 4 Reactions 0 Suppliers

6 1215071-00-3

C24H29D7NO3
2,3-Dihydro-5,6-dimethoxy-2-[[1-(phenyl-2,3,4,5,6-d₅-methyl-d₂)-4-piperidinyl]me...

3 References 0 Reactions 10 Suppliers

*Structure Match の詳細は CAS SciFinder 構造作図ガイド p.8-9 参照

https://seminar.jaici.or.jp/doc/sf_str.pdf

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【参考】 Chemscape Analysis での便利な絞り込み

解析上限 (1,000 件) を超える場合には適宜回答を絞り込む

Reference Availability フィルター

- 関連文献を持つ文献に限定する

^ Reference Availability

Available (956)

Not Available (604)

物質の関連特許に対する解析機能であるため、Available がおすすめ

Number of Components フィルター

- 物質の成分数で限定する

^ Number of Components

1 (865)

2 (517)

3 (148)

4 (11)

5 or more (3)

作図した構造に対する類似度でマッピングするため、1 がおすすめ

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【参考】 Chemscape Analysis での便利な並び順

Substances search for drawn structure

References Reactions Suppliers

Structure Match

As Drawn (43)

Substructure (2,870)

Similarity (3,790)

Analyze Structure Precision

Chemscape Analysis

Visually explore structure similarity with a powerful tool.

Learn more about Chem

Create Chemscape Analysis

Filter Behavior

Filter by Exclude

Filtering: Number of Components: 1 X

1,812 Results

Sort: Number of References: Descending View: Partial

Number of References: Descending では関連文献の多い物質を優先して解析できる

Chemscape Analysis の対象は最初の 1,000 件の回答であるため、Sort で解析対象を変更できる

227 References 31 Reactions 10 Suppliers 129 References 5 Reactions 13 Suppliers 115 References 214 Reactions 2 Suppliers

Chemscape Analysis の見方 (1/2)

Structural Similarity

Less Similar

デフォルトは構造の類似度による色分け (類似度が高いものほど赤く表示される)

検索した構造質問式

カラムの高さは関連特許の数

物質情報はマップ上で確認できる (p.9)

特許に索引が無い物質は表示されない

Donepezil 120014-06-4

Patent Count 1,733

Molecular Formula

Synonyms 1-Benzyl-4-[(5,6-dimethoxy-1-oxoindan-2-

Chemscape Analysis の見方 (2/2)

The screenshot displays the Chemscape Analysis interface. On the left, a 3D bar chart shows the relative heights of various substances. A red box highlights a specific substance, Donepezil, with its CAS Registry Number 120014-06-4. A blue arrow points from this box to the detailed view on the right. The detailed view includes the chemical structure of Donepezil, its molecular formula $C_{24}H_{29}NO_3$, and its SMILES string: O=C1C2=CC(OC)=C(OC)C=C2CC1CC3CCN(CC=C4CC4)CC3. Below the structure, there are sections for 'References' and '関連特許の一覧' (List of Related Patents).

Chemscape Analysis の機能

Chemscape Analysis の機能はコントロールパネルで操作する

The screenshot shows the Chemscape Analysis interface with a focus on the Control Panel. On the left, a vertical list of buttons includes 'My Chemscape (p.11)', 'Substance (p.12-14)', 'Add Structure (p.15)', and 'Search (p.16-17)'. A blue box labeled 'コントロールパネル' (Control Panel) points to this list. The main area displays the 'Structural Similarity' tool, which features a color gradient bar from yellow (Less Similar) to red (More Similar). Below the bar, a slider is set to 33% similarity, with a range from 0% to 100%. The background shows a 3D bar chart of substances.

My Chemscape

保存したマップを呼び出す機能



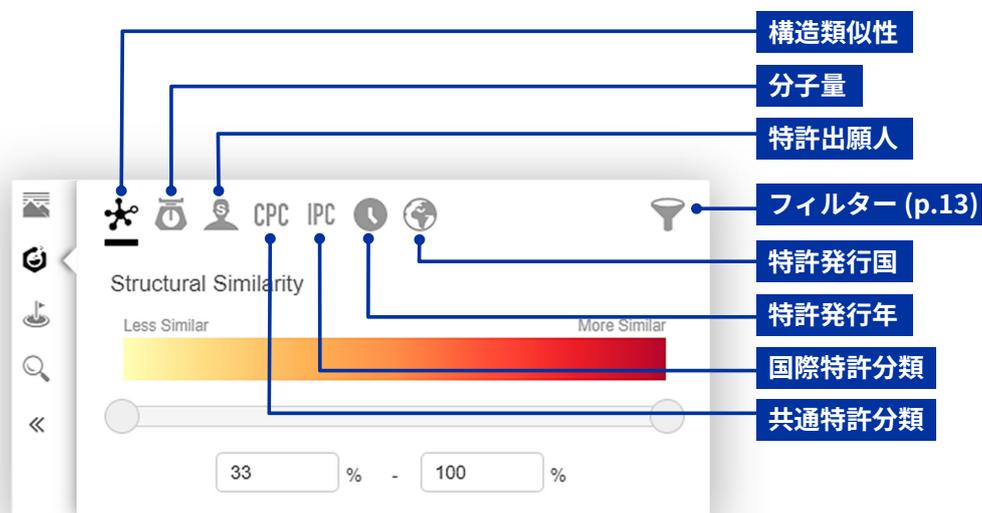
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Substance (1/3)

様々な解析項目でマップを解析できるSubstanceの解析項目

Substanceの解析項目



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Substance (2/3)

Substance のフィルター機能

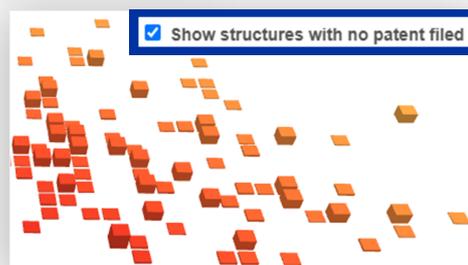
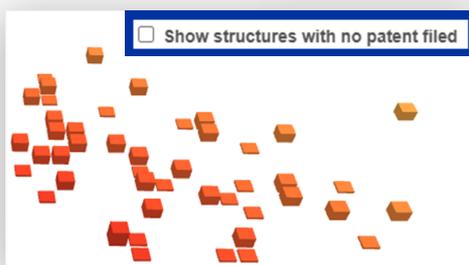
関連特許の数で表示するカラムを限定

Filter by patent count

1 - 1733 patents

Show structures with no patent filed

マップ上に関連特許を持たない物質を表示



Substance (3/3)

特許出願人での解析例

グループごとに色分けできる

Current Assignee

- エーザイ (EISAI CO., LTD.) 32
- スウェンライフサイエンス (SUVEN LIFE SCIENCES LIMITED) 31
- アウスベックス (AUSPEX PHARMACEUTICALS, INC.) 6
- Group 4 (Empty) 4

構造類似性のマッピングに対して特許出願人の特許分布を視覚化

2-Fluoro-2,3-Dihydro-2-[1-(Phenyl...]
290309-08-9

Patent Count: 3

Molecular Formula: C₂₈H₃₆FNO₃

SMILES: O=C1C2=CC(OCCC)=C(OCCC)C=C2CC1(F)CC3C CN(CC=4C=CC=CC4)CC3

Synonyms

■ エーザイ	82
■ スウェンライフサイエンス	1
■ アウスベックス	266

Add Structure

マップ上に指定した化学物質のフラグを追加する機能

追加されたフラグ

Donepezil

Donepezil
120014-06-4

フラグを付与したい物質を名称、CAS登録番号、構造から検索する

Search (1/2)

関連特許の全文情報または構造情報でマップを検索する機能

検索項目

- 全文
- 標題
- 抄録
- 詳細な説明
- クレーム
- 標題/抄録/クレーム
- 法的状況
- 特許発行日
- 特許出願人

Patent Structure 構造からの検索

All dementia

Title

Abstract

Description

Claims

Tit./Abs./Cla.

Simple legal status None

Pub. Date 年/月/日 年/月/日

Current Assignee

Search

Reset

物質と関連特許を紐づけたキーワード検索により類似構造を含めた用途探索に活用できる

Search (2/2)

検索を実行すると物質とヒットした関連特許の数が一覧で表示される

Results (291) Patents

Compound Name	Patent Count
Donepezil 120014-06-4	895
(-)-Donepezil 142057-80-5	7
(+)-Donepezil 142698-19-9	6
2-[[1-(3-Fluorophenyl)methyl]-4-piperidinyl]methyl]-2-oxoindan-5-yl]methyl]piperidine 120014-13-3	6
2,3-Dihydro-5,6-dimethoxy-2-[[1-(3-nitrophenyl)methyl]-4-piperidinyl]methyl]-2-oxoindan-5-yl]methyl]piperidine 120014-11-1	6
2,3-Dihydro-6-methoxy-5-(1-methylethoxy)-2-[[1-(phenylmethyl)-4-piperidinyl]methyl]-2-oxoindan-5-yl]methyl]piperidine 120014-15-5	5
5,6-Diethoxy-2,3-dihydro-2-[[1-(phenylmethyl)-4-piperidinyl]methyl]-2-oxoindan-5-yl]methyl]piperidine 120014-09-7	5
2,3-Dihydro-5,6-dimethoxy-2-[[1-oxido-1-(phenylmethyl)-4-piperidinyl]methyl]-2-oxoindan-5-yl]methyl]piperidine 120013-84-5	3

Donepezil
120014-06-4

Add mark

Patent Count
895

関連特許へのリンク

Molecular Formula
C₂₄H₂₉NO₃

SMILES
O=C1C2=CC(OC)=C(OC)C=C2CC1CC3CCN(CC=4C=CC(4)CC3

Synonyms
1-Benzyl-4-[[5,6-dimethoxy-1-oxoindan-2-yl]methyl]piperidine
2-[[1-Benzyl(piperidin-4-yl)methyl]-5,6-dimethoxy-2,3-

ヒットした物質はカラムが青くハイライトされる

Select Structure

選択した物質の表示と新たなマップの作成ができる

Select Structure からドラッグでマップを選択する

354 Selected Clear

New Chemscape 新たなマップを作成する

View Structures 選択した物質を表示する

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