

SciFinder®
インターネットセミナー

SciFinder 生物活性情報の 調べ方

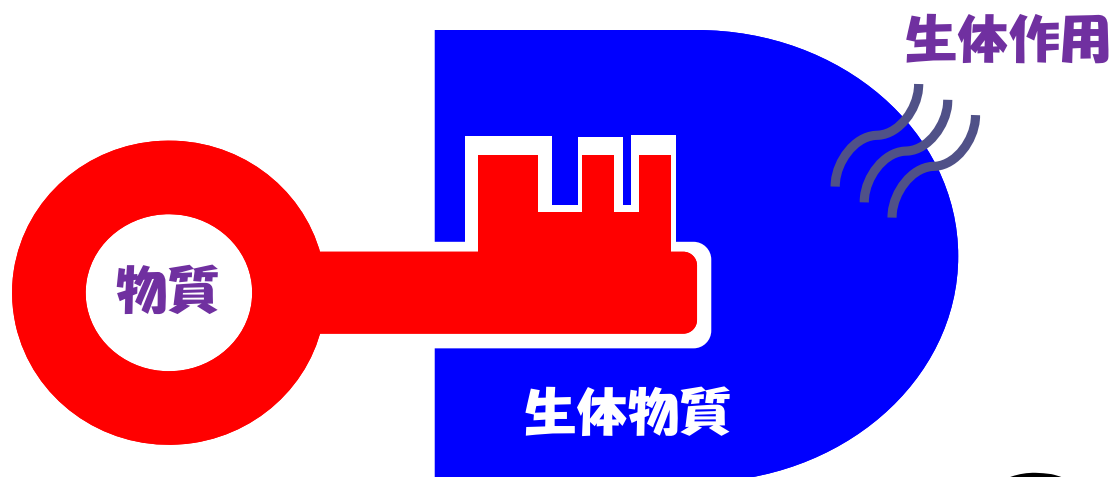
JAICI
化学情報協会



本日の流れ

1. 物質の生物活性情報
2. Bioactivity Indicators と Target Indicators
3. テータの作成方法
4. 検索例

1. 物質の生物活性情報



・ドッキングプログラム
・スクリーニング



医薬品候補物質



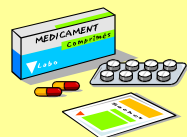
3

この物質には？



どんな効用があるだろう？

抗がん剤??



睡眠薬？

糖尿病治療薬？

作用する対象はなんだろう？

Bioactivity Indicators



注目する物質の生物活性

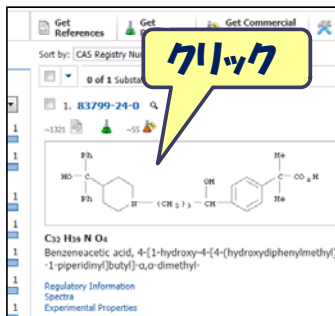
Target Indicators



注目する物質が作用する
受容体・酵素など

4

2. Bioactivity Indicators & Target Indicators



Deleted CAS Registry Numbers: 76815-58-2, 159389-12-5

Fexofenadine (アレグラ)

Source of Registration: CA

~1,321 References
~55 Commercial Sources

Document Types: Conference, Dissertation, Journal, Patent, Report

CAS Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Analytical Study	✓	✓		
Biological Study	✓	✓	✓	✓
Prophetic in Patents	✓		✓	
Reaction Uses			✓	

Bioactivity Indicators

Indicator	References
Anti-inflammatory agents (all) > Anti-inflammatory agents	63
Immune agents (pharmaceutical) > Allergy inhibitors	120
Receptor antagonists (all) >> Antihistamines	276
Receptor antagonists (all) >> H1-antihistamines	173
Respiratory system agents (all) > Decongestants	59

Target Indicators

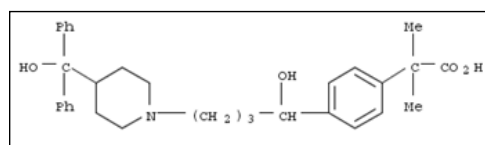
Indicator	References
Cytokines (all) >> Tumor necrosis factor α	12
Cytokines (all) >> Tumor necrosis factor α	12
Enzymes (all) >>>> ATP-binding cassette transporters	15
Enzymes (all) >>>>> 3',5'-Cyclic AMP phosphodiesterase	14
Enzymes (all) >>> Cyclooxygenase 2	22
Enzymes (all) >>>> Cyclooxygenase 2	22
Enzymes (all) >>> Hydroxymethylglutaryl-CoA	11
(all) >>>>> Multidrug resistance-related proteins	12
Enzymes (all) >>>>> P-glycoproteins	80

最初は折いたたまっています

文献数

文献数でみると

Bioactivity Indicators	
Antihistamines	276
H1-antihistamines	173
Allergy inhibitors	120
Anti-inflammatory agents	63
Decongestants	59



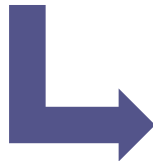
鼻炎薬



Target Indicators	
P-glycoproteins	80
Histamine H1 receptors	50
Voltage-gated potassium channels, Kv11	30
Organic anion transporters	27
Cyclooxygenase 2	22
Cytochrome P450 CYP3A4	20

3. データの作成方法

論文・特許etc



索引作成



46. Anti-inflammatory activity of H1-receptor antagonists: review of recent experimental research

By: Gelfand, Erwin W.; Appajoyula, Sireesh; Meeves, Suzanne

A review. Objective: To compare the anti-inflammatory effects of fexofenadine with other H₁-receptor antagonists in vitro. Data sources: Published literature. Study selection: Recent exptl. studies on anti-inflammatory effects of H₁-receptor antagonists. Databases searched: Medline, Medscape. Period covered: 1990-2003. Search terms: second-, third-generation antihistamines; sedating, nonsedating antihistamines; in vitro ant inflammatory activity; cetirizine; ebastine; loratadine; fexofenadine; desloratadine. Results: Second- and third-generation H₁-receptor antagonists may demonstrate significant in vitro anti-inflammatory activity at concns. considered to be clin. relevant. In some instances, higher (supraclin.) concns. are required to achieve comparable effects. Conclusions: Exptl. research suggests that second- and third-generation H₁-receptor antagonists may achieve anti-inflammatory effects in a clin. context. Further studies are required to support this conclusion.

Indexing

Pharmac

キーワード索引

物質索引

Concepts

Antihistamines

H1; second- and third-generation H1-receptor antagonists may demonstrate significant anti-inflammatory activity in human cell lines at concns. considered to be clin. relevant but in some instances required higher concn.

Allergy inhibitors Anti-inflammatory agents
Drug targets Human

second- and third-generation H1-receptor antagonists may demonstrate significant anti-inflammatory activity in human cell lines at concns. considered to be clin. relevant but in some instances required higher concn.

Histamine H1 receptors

second- and third-generation H1-receptor antagonists may demonstrate significant anti-inflammatory activity in human cell lines at concns. considered to be clin. relevant but in some instances required higher concn.

Biological study, unclassified; Biological study

Substances

83799-24-0 Fexofenadine

third-generation H1-receptor antagonist fexofenadine may demonstrate significant anti-inflammatory activity in human cell lines at concns. considered to be clin. relevant but in some instances required higher concn.

Adverse effect, including toxicity; Pharmacological activity; Therapeutic use; Biological study; Uses

キーワード、CAS 番号は厳密に統制

キーワード索引

Concepts

Antihistamines

H1; second- and third-generation H1-receptor antagonists may demonstrate significant anti-inflammatory activity in human cell lines at concns. considered to be clin. relevant but in some instances required higher concn.

Allergy inhibitors Anti-inflammatory agents
Drug targets Human

second- and third-generation H1-receptor antagonists may demonstrate significant anti-inflammatory activity in human cell lines at concns. considered to be clin. relevant but in some instances required higher concn.

Histamine H1 receptors

second- and third-generation H1-receptor antagonists may demonstrate significant anti-inflammatory activity in human cell lines at concns. considered to be clin. relevant but in some instances required higher concn.

Biological study, unclassified; Biological study

物質索引

Substances

83799-24-0 Fexofenadine

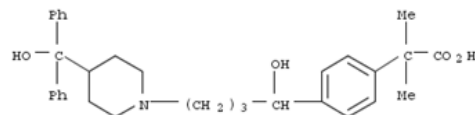
third-generation H1-receptor antagonist fexofenadine may demonstrate significant anti-inflammatory activity in human cell lines at concns. considered to be clin. relevant but in some instances required higher concn.

Adverse effect, including toxicity; Pharmacological activity; Therapeutic use; Biological study; Uses

薬効・生物学的研究

Bioactivity Indicators

Target Indicators



Bioactivity Indicators

生物活性を表すキーワード (約 260 種)

注目する物質がどのような生物活性をもつか

例:

抗がん剤
血管収縮剤 など



Target Indicators

受容体や酵素を表すキーワード (約 5,800 種)

注目する物質がどのような受容体や酵素に作用するか

例:

α -アミラーゼ
前立腺特異抗原 など

注)

いずれも将来的に
増えます

9

ご注意

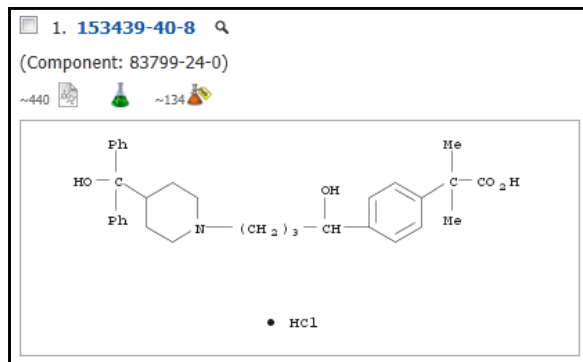
1. 過去に文献がなければ情報なし
2. 同一文献中のキーワードと直接関連性のない物質が結び付けられることがある

※同一文献中に該当キーワードと物質があることは間違いはない

<p>Histamine H1 receptors</p> <p>H1-antagonist olopatadine significantly reduced serum substance P, while other H1-antagonists cetiridine and fexofenadine increased serum substance P and epinastine had no effect on serum substance P in peripheral blood of AD patient</p> <p>Biological study, unclassified; Biological study</p>	<p>83881-51-0 Cetirizine 🔍 ①</p> <p>H1-antagonist cetirizine increased serum substance P that was unrelated to deterioration of atopic dermatitis but rather associated with clinical improvement in atopic dermatitis patient</p> <p>Pharmacological activity; Therapeutic use; Biological study; Uses</p>
<p>Interleukin 2 receptors</p> <p>blood severity markers including soluble forms of interleukin-2 were reduced in atopic dermatitis patient treated with cetirizine</p> <p>Biological study, unclassified; Biological study</p>	<p>9001-60-9 Lactate dehydrogenase 🔍 ②</p> <p>blood severity marker lactate dehydrogenase were reduced in atopic dermatitis patient treated with cetirizine</p> <p>Biological study, unclassified; Biological study</p>

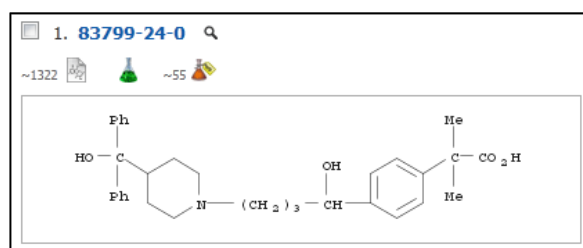
10

一般的なご注意



Allegra(アレグラ)
(Fexofenadine hydrochloride)

⇒ **文献数 440**



Fexofenadine

⇒ **文献数 1322**

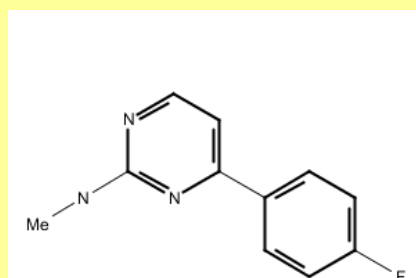
物質名称検索だけでは情報を取り逃がすことがあります

11

4. 検索例

(例) 下記骨格をもつ物質についての生物活性情報を調査する。

1. 部分構造検索を行う。
2. 得られた物質の Bioactivity Indicator および Target Indicator を確認する。
3. 解析機能を用いて、この骨格をもつ物質群の情報を確認する。
4. 構造検索した物質のうち、抗ガン作用をもつものだけに絞りさらに情報を追跡する。



※ 環の縮合は禁止

まとめ

Bioactivity Indicators

Target Indicators



**注目する物質の生物活性に関する情報を
把握できます！
化学構造と薬効・作用する対象の相関関係を
大局的に把握するのに役立ちます**