

FARMASÖTİK KİMYA UYGULAMA IV DERSİ



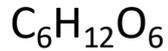
**Kemoenformatik, Literatür Tarama
ve Reaxys Veri Tabanının Kullanımı**

Kemoenformatik

- Bilişim teknolojilerinin kullanılması yoluyla kimyasal bilginin kayıt altına alınması ve işlenmesi ile ilgili disipline verilen addır.
- İlaç keşfinde kullanım alanlarından bazıları aşağıdaki gibi özetlenebilir.
 - 1B, 2B veya 3B moleküler yapıların kayıt altına alınması,
 - kimyasal veritabanlarının oluşturulması,
 - ilgili yapıların kimyasal veritabanlarından taranması,
 - Kimyasal yapının biyolojik etkisinin veya fizikokimyasal özellik üzerine etkisinin tahminine yönelik hesaplamalar
 - (İnhibitör/Aktivatör konsantrasyonların tahmini, ADME-T özelliklerinin tahmini),
 - kimyasal uzayın haritalanması

Kimyasal Gösterim/Boyut Kavramı

0 D

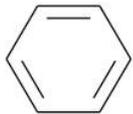


1 D

SMILES (Canonical / Isomeric)

smi dosya formatı

InChI (Value / Key)



Benzene



c1ccccc1

SMILES

```
Benzen
12 12 0 1 0          999 V2000
-0.0167  1.3781  0.0096 C  0 00 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 0.0021 -0.0041  0.0020 C  0 00 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 1.1709  2.0855  0.0021 C  0 00 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 1.2084 -0.6789 -0.0132 C  0 00 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 2.3960  0.0285 -0.0212 C  0 00 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 2.3773  1.4107 -0.0131 C  0 00 0 0 0 0 0 0 0 0 0 0 0 0 0 0
-0.9592  1.9054  0.0170 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
-0.9258 -0.5567  0.0083 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 1.1563  3.1654  0.0077 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 1.2231 -1.7588 -0.0184 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 3.3385 -0.4987 -0.0324 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 3.3051  1.9634 -0.0197 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 1  2  02  0  1  0  0
 1  3  01  0  1  0  0
 1  7  1  0  0  0  0
 2  4  01  0  1  0  0
 2  8  1  0  0  0  0
 3  6  02  0  1  0  0
 3  9  1  0  0  0  0
 4  5  02  0  1  0  0
 4 10  1  0  0  0  0
 5  6  01  0  1  0  0
 5 11  1  0  0  0  0
 6 12  1  0  0  0  0
M  END
$$$$
```

2 D

mol dosya formatı

sdf dosya formatı

2,5 D

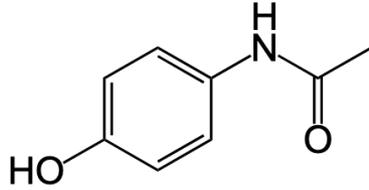
Konfigürasyon özelliklerinin kayıt altına alınması

3 D

Konformasyon özelliklerinin kayıt altına alınması

Literatür Tarama Çalışması İş Akışı

1. İlaç molekülünün verilmesi (Kimyasal formülü ve Adı)



Örnek: Parasetamol

2. Kimyasal formül ve ilaç adından yola çıkılarak ana ilaç hedefi ve farmakolojik özellikleri ile ilgili literatür tarama çalışmasının yapılması



3. İlaç molekülünün ana hedefi ile olan moleküler etkileşimlerinin PDB verileri kullanılarak incelenmesi

4. Tüm bulguların kısa bir sunum haline getirilmesi ve sunulması

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Başlıca ařağıdaki amaçlar için kullanılabilir:

- ✓ **Kimyasal Reaksiyonlar ve Yöntemler:** Kimyasal reaksiyonları, reaksiyon koşullarını, kullanılan reaktifleri ve bunların verimleri
- ✓ **Moleküler Yapı ve Fizikokimyasal Özellikler:** Kimyasal bileşiklerin yapıları, moleküler özellikleri, fiziksel özellikler ve spektral veriler (NMR, IR, MS vb.)
- ✓ **Biyolojik Aktivite Bulguları:** Veri tabanında yer alan bileşiklere ait biyolojik bulgular
- ✓ **Benzerlik Taraması:** Yapısal benzerlik analizleri yapılarak kimyasal yapılar arasında ilişkiler kurulabilir
- ✓ **Patent ve Literatür Tarama:** Bilimsel literatüre erişim sağlanarak, arařtırmacıların daha önce yapılmıř çalıřmaları ve patentli buluşlar incelenebilmektedir.



Bilgi, geleceğimizi aydınlatan ışıktır...

Anahtar Kelime Ara

Katalog Tarama Tüm Kaynaklarda Arama

Elsevier ClinicalKey Veri Tabanı İçerik Erişimi

Elsevier ClinicalKey veri tabanı ile "Gray's Anatomy", "Netter", "Sobotta" serileri gibi dünyaca ünlü kitapların da bulunduğu 900'den fazla kitaba, kullanıcı sınırlı olmadan ve her zaman yenilenmiş / son edisyonlarına erişiminiz bulunmaktadır.

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Bilgiyi

Hızlı Bağlantılar

- Elektronik Kaynakların Kullanım Kuralları
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- Veri Tabanları
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- Referans Yöneticileri
- Atrf Veri Tabanları
- H-İndeks Nedir? Atrf İndekslerde Nasıl Sorgulanır?
- EKUAL Veri Tabanlarında Tarama
- Deneme Veri Tabanları
- Kareller
- Kütüphanelerarası İşbirliği
- Diğer E-Kaynaklar
- Kütüphaneler ve Bilgi Merkezleri
- Ulusal Toplu Katalog (TO-KAT)
- Ulusal Tez Merkezi

Duyurular

- 07.03.2023 Complete Anatomy Veri Tabanı Deneme Erişimine Açıldı
- 07.03.2023 Oxford Academic Journals Online Eğitimi
- 06.03.2023 Osmosis Veri Tabanı Deneme Erişimine Açıldı
- 28.02.2023 Uptodate ve Clinical Key Online Eğitimleri
- 27.02.2023 Oxford Oku-Yayınla Anlaşması
- 27.02.2023 Proquest Online Eğitimleri
- 22.02.2023 Web of Science Araştırmacı Profilleri ve Araştırmacı Kayıt Düzeltme Kılavuzları

@gazikutuphane adlı kullanıcının Tweetleri

Takip et



Gazi Kütüphane @gazikutuphane · 8s
Değerli Tıp Kullanıcısı,

Osmosis Veri Tabanı deneme erişimine açıldı.

Detay bilgi; lib.gazi.edu.tr/view/announcem...

İyi Çalışmalar...

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@MBahcelioglu

OSMOSIS



Tümü ▶

ProQuest Digital Dissertations	
Proquest Public Available Content Database (Proquest Açık Erişim Veri Tabanı)	
Reaxys	
Regional Business News (EBSCO)	
Royal Society of Chemistry (RSC) 2022 yılında aboneliğine son verilmiştir. Sürekli erişime açık olan dergiler ve yıl bilgileri için tıklayınız .	
Royal Society of Chemistry (RSC) E-Books 2013	
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Search substances, reactions, documents and bioactivity data

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RELX Group™

Feedback

Verilen ilaç moleküllerinin formülü reaxys veri tabanında çizilir.
Bu aşamada ekran görüntüsü alınarak laboratuvar raporuna eklenmelidir.

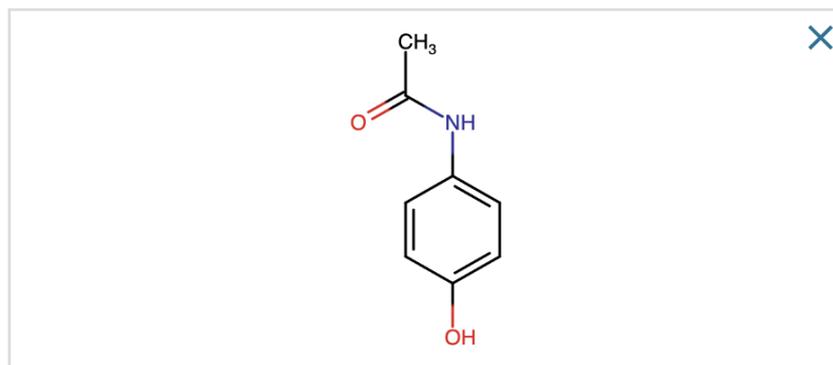
The screenshot displays the Reaxys software interface. At the top left is the Reaxys logo. The navigation bar includes 'Quick search', 'Query builder', 'Results', and 'Retrosynthesis'. On the right, there are 'Register' and 'Sign in' buttons. Below the navigation bar, the 'Structure editor selected:' section shows 'MarvinJS' as the active editor. A search bar labeled 'Insert structure from name' is present. The main workspace contains a chemical structure of N-(4-hydroxyphenyl)acetamide, represented as a benzene ring with a hydroxyl group (-OH) at the para position and an acetamido group (-NHCOCH₃) at the other para position. To the right of the workspace is a search options panel titled 'Search this structure as:'. It includes radio buttons for 'As drawn' (selected), 'As substructure', and 'Similar'. Below these are several checked checkboxes: 'Tautomers', 'Stereo', 'Additional ring closures', 'Salts', 'Mixtures', 'Isotopes', 'Charges', and 'Radicals'. A '+ More Options' link is at the bottom of this panel. At the bottom of the workspace, there are 'Clear' and 'Cancel' buttons, and a 'Transfer to query >' button which is highlighted with a red box and a red arrow pointing to it.

Search Reaxys

Substance Properties, e.g. ferroelectric materials

Find >

AND



As drawn 

ilaç molekülüne ait bilgile substances sekmesinde görülebilmektedir.

	3	Substances	Structure :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	242	Targets	Structure :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	46,318	Documents	Structure :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	3,398	Substances	Structure :  average similarity Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	295	Reactions	Reaction Query :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	1	Commercial Substances	Structure :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	2,150	Commercial Substances	Structure :  average similarity Edit in Query Builder  Create Alert 	Preview Results 	View Results 

4-acetaminophenol
HO₆H₄NHCOCH₃ 151.165 2208089 103-90-2

Identification Bioactivity (All) Spectra - 538
Druglikeness Physical Data - 1.032 Other Data - 1.819

Preparations - 242 >
Reactions - 4.076 >
Targets - 242 >
Documents - 46.318 >

4-acetaminophenol

Identification

Chemical Names: 4-acetaminophenol • N-acetyl-para-aminophenol • Acetaminophen • paracetamol • p-hydroxyacetanilide • APAP • N-(4-hydroxyphenyl)acetamide

+ Show all chemical names

Reaxys ID: 2208089

CAS Registry Number(s): 103-90-2

Molecular Formula: C₈H₉NO₂

Molecular Weight: 151.165

InChIKey: RZVAJINJKPMORJF-UHFFFAOYSA-N

Substance type: isocyclic

Linear Structure Formula: HO₆H₄NHCOCH₃

No of references: 46346

Bu bölümde bileşiğe ait biyoaktivite bulguları, ilaç olabilirlik özellikleri, fiziksel data, IR, NMR spekturumu gibi bir çok bilgiye ulaşılabilir

Rapora yazılması gerekenler:

Kimyasal adı (Chemical Name): 4-asetaminofenol (4-acetaminophenol)

Kapalı formül (Molecular Formula): C₈H₉NO₂

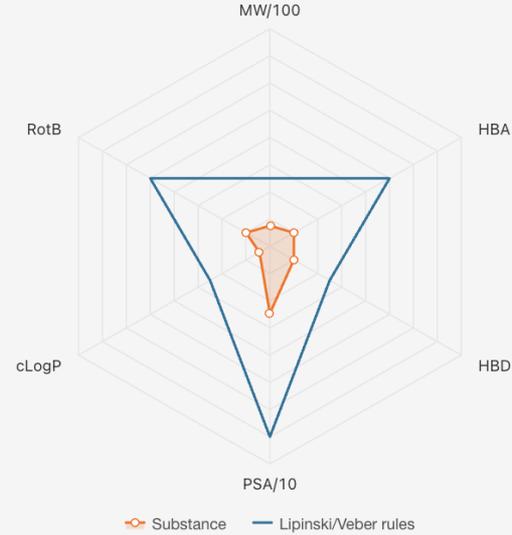
Druglikeness

Lipinski rules component

Molecular Weight	151.165
cLogP	0.87
HBA	2
HBD	2
Matching Lipinski Rules	4

Weber rules component

Polar Surface Area (PSA)	49.33
Rotatable Bond (RotB)	2
Matching Weber Rules	2



Rapora yazılması gerekenler:

İlaç olabilirlik Özellikleri;

Molekül ağırlığı:

LogP:

HBA (Hidrojen bağ akseptörü) sayısı:

HBD (Hidrojen bağ donörü) sayısı:

Polar yüzey alanı (Polar surface area (PSA)):

Döner Bağ (Rotatable Bond) sayısı:

Molekülünüzün Lipinski ve Weber kurallarına uyup uymadığını Matching Lipinski Rules ve Weber rules sayılarına bakarak belirtiniz!

^ Bioactivity (All)

^ In vitro: Efficacy - 2302

Quantitative Results

Show/Hide columns v

pX	Parameter	Value (qual)	Value (quant)	Unit	Effect	Reference
10.6	concentration (parameter) (Plasma interleukin-4)	=	4.2	pg/mL	antiinflammatory agent	Sparkenbaugh, Erica M.; Saini, Yogesh; Greenwood, Krista K.; LaPres, John J.; Luyendyk, James P.; Copple, Bryan L.; Maddox, Jane F.; Ganey, Patricia E.; Roth, Robert A. Journal of Pharmacology and Experimental Therapeutics, 2011, vol. 338, # 2, p. 492 - 502 Full Text Cited 38 times Details Abstract
10.5	concentration (parameter) (Plasma)	=	4.4	pg/mL	antiinflammatory agent	Sparkenbaugh, Erica M.; Saini, Yogesh; Greenwood, Krista K.; LaPres, John J.; Luyendyk, James P.; Copple, Bryan L.; Maddox, Jane F.; Ganey, Patricia E.; Roth, Robert A. Journal of Pharmacology and Experimental Therapeutics, 2011, vol. 338, # 2, p. 492 - 502 Full Text Cited 38 times Details Abstract
10.5	concentration (parameter) (Plasma interleukin-4)	=	4.5	pg/mL	antiinflammatory agent	Sparkenbaugh, Erica M.; Saini, Yogesh; Greenwood, Krista K.; LaPres, John J.; Luyendyk, James P.; Copple, Bryan L.; Maddox, Jane F.; Ganey, Patricia E.; Roth, Robert A. Journal of Pharmacology and Experimental Therapeutics, 2011, vol. 338, # 2, p. 492 - 502 Full Text Cited 38 times Details Abstract
10.4	concentration (parameter) (Plasma)	=	6.5	pg/mL	antiinflammatory agent	Sparkenbaugh, Erica M.; Saini, Yogesh; Greenwood, Krista K.; LaPres, John J.; Luyendyk, James P.; Copple, Bryan L.; Maddox, Jane F.; Ganey, Patricia E.; Roth, Robert A. Journal of Pharmacology and Experimental Therapeutics, 2011, vol. 338, # 2, p. 492 - 502 Full Text Cited 38 times Details Abstract

Show Less ^

+ Show next 100

Bu bölümde bileşiğe ait *in vitro* ve *in vitro* etkinlik çalışmaları, toksisite, ADME çalışmaları gibi birçok biyoaktivite datası incelenebilir.

Rapora yazılması gerekenler:

In vitro efficacy (*in vitro* efikasite) bölümünde yer alan Etki (Effect) kolonunda yazan bilgiler derlenecektir.

Örnek: Parasetamolün antiinflamatuvar etkisi incelenmiştir.

4-acetaminophenol
CC(=O)Nc1ccc(O)cc1 151.165 2208089 103-90-2

Identification Bioactivity (All) Spectra - 538
 Druglikeness Physical Data - 1.032 Other Data - 1.819

Preparations - 242 >
 Reactions - 4.076 >
 Targets - 242 >
 Documents - 46.318 >

Preparations sekmesine tıklanarak ilaç molekülünün nasıl sentezlendiği ile ilgili verilere ulaşılabacaktır.

1

CC(=O)c1ccc(O)cc1 $\xrightarrow{\text{H}_2\text{N-OH}}$ CC(=O)Nc1ccc(O)cc1

113 129

21 Conditions Find Similar Reaction ID: 3799095

Conditions	Yield	Reference
With hydroxylamine hydrochloride in acetanitrile at 110°C; for 1h; Solvent; Time; chemoselective reaction;	100%	Rancan, Elio; Aricò, Fabio; Quartarone, Giuseppe; Ronchin, Lucio; Tundo, Pietro; Vavasori, Andrea Catalysis Communications , 2014, vol. 54, p. 11 - 16 Full Text Cited 21 times Details Abstract
With hydroxylamine hydrochloride ; tetrachlorosilane at 160°C; for 0.0583333h; microwave irradiation;	92%	Srinivas; Mahender; Das, Biswanath Chemistry Letters , 2003, vol. 32, # 8, p. 738 - 739 Full Text Cited 14 times Details Abstract
With mesitylenesulfonylhydroxylamine in acetanitrile at 20°C; for 6h; Experimental Procedure	92%	Chandra, Dinesh; Verma, Saumya; Pandey, Chandra Bhan; Yadav, Ajay K.; Kumar, Puneet; Tiwari, Bhagendra; Jai, Jawahar L. Tetrahedron Letters , 2020, vol. 61, # 18, art. no. 151822 Full Text Cited 13 times Details Abstract

Rapora yazılması gerekenler:
Çıkan sentez yöntemlerinden birinin ekran görüntüsü alınacaktır.

1



113



129



21 Conditions ^ Find Similar > Reaction ID: 3799095

Conditions	Yield	Reference
With hydroxylamine hydrochloride In acetonitrile at 110°C; for 1h; Solvent; Time; chemoselective reaction;	100%	Rancan, Elia; Aricò, Fabio; Quartarone, Giuseppe; Ronchin, Lucio; Tundo, Pietro; Vavasori, Andrea Catalysis Communications , 2014, vol. 54, p. 11 - 16 Full Text ↗ Cited 21 times ↗ Details > Abstract >
With hydroxylamine hydrochloride ; tetrachlorosilane at 160°C; for 0.0583333h; microwave irradiation;	92%	Srinivas; Mahender; Das, Biswanath Chemistry Letters , 2003, vol. 32, # 8, p. 738 - 739 Full Text ↗ Cited 14 times ↗ Details > Abstract >
With mesitylenesulfonylhydroxylamine In acetonitrile at 20°C; for 6h; Experimental Procedure ^	92%	Chandra, Dinesh; Verma, Saumya; Pandey, Chandra Bhan; Yadav, Ajay K.; Kumar, Puneet; Tiwari, Bhoopendra; Jat, Jawahar L Tetrahedron Letters , 2020, vol. 61, # 18, art. no. 151822 Full Text ↗ Cited 13 times ↗ Details > Abstract >

General procedure for the preparation of amides from ketones

General procedure: To a round bottom flask, equipped with a magnetic stirring bar, was added ketone 1 (0.5 mmol, 1.0 equiv.) and acetonitrile (2 mL) at room temperature. To this stirred solution, freshly prepared O-(Mesitylsulfonyl)hydroxylamine 2 (2.0 equiv.) was added. The reaction mixture was stirred for the specified duration and temperature. The progress of the reaction was monitored by TLC. After completion, the reaction mixture was diluted with ethyl acetate (10 mL) and washed with a saturated aqueous NaHCO₃ solution (3 x 5 mL). The combined organic layer was washed with brine solution and dried over anhydrous Na₂SO₄. Solvent was removed under reduced pressure to get the crude product. The reaction that required elevated temperature was stirred first at room temperature for 2 hours after addition of MSH and then heated at 70 °C for the specified time.

Bu bölümde kullanılacak başlangıç maddesi (reaktan), rejan ve çözücünün hangi şartlarda (sıcaklık, basınç, süre) reaksiyonun gerçekleştirildiği literatürde belirtilen şekilde yer almaktadır.

ilaç molekülüne ait hedefler Targets (Hedefler) bölümünde incelenecektir.

	731	Substances	Structure :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	250	Targets	Structure :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	46,714	Documents	Structure :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	3,398	Substances	Structure :  average similarity; included: tautomers, only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	340	Reactions	Reaction Query :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	140	Commercial Substances	Structure :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	2,150	Commercial Substances	Structure :  average similarity; included: tautomers, only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals Edit in Query Builder  Create Alert 	Preview Results 	View Results 

İlaç molekülüne ait hedefler Targets (Hedefler) bölümünde incelenecektir.

Single protein
1 Cyclooxygenase (sheep, Wild)
Synonyms: cyclooxygenase
Mutant/chimera Details: Wild
[Show target details](#) ▾

Substances - 18 >
Documents - 1 >

Parasetamolün Cyclooxygenase hedefi için ilgili document sekmesine tıklayarak makale incelenebilir.

1 Documents with 18 Substances, 0 Reactions, 1 Targets

Sort by Rel

0 selected
Limit To Exclude Export

🔍 — 🔍

Bioactivity

1 Prostaglandin-H synthase inhibition by malonamides. Ring-opened analogues of phenylbutazone

Vennerstrom; Holmes Jr.

Journal of Medicinal Chemistry, 1987, vol. 30, # 2, pp. 185-190, 185a031

Index Terms ▾ Substances 18 ▾ Target ▾ Full Text ↗

Hit Substances 1 ▾



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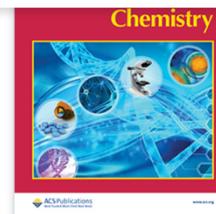
ARTICLE | February 1, 1987

Prostaglandin-H synthase inhibition by malonamides. Ring-opened analogs of phenylbutazone

Jonathan L. Vennerstrom, and Thomas J. Holmes Jr.

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Journal of Medicinal ChemistryCite this: *J. Med. Chem.* 1987, 30, 2, 434–437
<https://doi.org/10.1021/jm00385a031>

Published February 1, 1987 ▾

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Prostaglandin-H Synthase Inhibition by Malonamides. Ring-Opened Analogues of Phenylbutazone

Jonathan L. Vennerstrom and Thomas J. Holmes, Jr.*

 Department of Medicinal Chemistry, College of Pharmacy, University of Minnesota, Minneapolis, Minnesota 55455.
 Received January 14, 1986

Recent reports of serious concern regarding the safe clinical use of phenylbutazone and its hydroxylated metabolite (oxyphenbutazone) as antiinflammatory agents have prompted the further investigation of ring-opened (malonamide) derivatives as potentially preferable therapeutic derivatives. Earlier reports have claimed reduced toxicity among similar derivatives. These studies reveal the relative degree of prostaglandin-H (PGH) synthase inhibitory activity among a series of malonamide derivatives. Contrary to observations in the pyrazolidinedione series, incorporation of a nonpolar butyl side chain in these malonamides was not beneficial but, rather, detrimental to enzyme-inhibitory activity. Although none of the reported nonbutylated malonamides was as potent an inhibitor of this enzyme as phenylbutazone, they all showed some inhibitory activity. PGH synthase inhibitory activity was especially pronounced in the bis(*p*-hydroxy anilide) derivatives, even extending to succinamide and adipamide derivatives. Of some interest is the observation that all of these *p*-hydroxy anilide derivatives were more potent inhibitors of this enzyme than acetaminophen.

The history of phenylbutazone (1) as a nonsteroidal antiinflammatory (NSAI) agent began in 1949 when the drug (which had been originally used as a solubilizing agent for aminopyrine) was introduced for the treatment of rheumatoid arthritis, acute gout, and allied disorders.¹ Clinically, phenylbutazone is 6 times more potent than the salicylates, but 5 times less potent than indomethacin. Phenylbutazone is an effective NSAI agent, but serious toxicity (especially aplastic anemia and agranulocytosis) limits its use in long-term therapy.^{1,2}

A significant concern has been expressed about the toxicity of phenylbutazone (1) and oxyphenbutazone (2)

in a number of recent reports^{3,4} and letters to the editor.^{5–8} Phenylbutazone and oxyphenbutazone have, in fact, been removed from the market in Bahrain, Jordan, and Norway.⁸ Similar decisions are pending in Australia, the United States, and several other countries.^{5,8} Meanwhile, the product labeling of phenylbutazone and oxyphenbutazone in the United States is being revised to reflect concern about the serious toxicity mentioned above.⁴ A recent report in the *Drug and Therapeutics Bulletin*³ acknowledged that while some physicians consider phenylbutazone to have special value in acute gout and an-

- (1) Flower, R. J.; Moncada, S.; Vane, J. R. In *The Pharmacological Basis of Therapeutics*, 7th ed.; Gilman, A. G., Goodman, L. S., Rall, T. W., Murad, F., Eds.; Macmillan: New York, 1985; pp 674–715.
- (2) McEvoy, G. K.; McQuarrie, G. M. Eds. *Drug Information—85*; American Hospital Formulary Service, American Society of Hospital Pharmacists, Bethesda, MD, 1985.

- (3) *Drug Ther. Bull. (London)* 1984, 22, 5–6.
- (4) *FDA Drug Bull.* 1984, 14, 23–24.
- (5) Auerbach, E. *Med. J. Aust.* 1984, 141, 261–262.
- (6) Smith, G. I. *Med. J. Aust.* 1984, 141, 551–552.
- (7) Loshak, D. *Lancet* 1985, No. 8425, 410.
- (8) Herxheimer, A.; Collier, J.; Rawlins, M. D.; Schonhofer, P.; Medawar, C.; Melrose, C.; Bannenberg, W.; Beardshaw, V. *Lancet* 1985, No. 8428, 580.

Get References

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118 Documents with 10,050 Substances, 13,095 Reactions, 550 Targets Reaxys - 118

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1 Beyond the Rule of 5: Impact of PEGylation with Various Polymer Sizes on Pharmacokinetic Properties, Structure-Properties Relationships of mPEGylated Small Agonists of TGR5 Receptor
Hoguet, Vanessa; Lasalle, Manuel; Maingot, Mathieu; Dequirez, Geoffrey; Boulahjar, Rajaa; Leroux, Florence; Piveteau, Catherine; (...) Tailleux, Anne; Charton, Julie [Journal of Medicinal Chemistry, 2021, vol. 64, # 3, p. 1593 - 1610]
Abstract Index Terms Substances 44 Reactions 100 Targets Full Text ↗
Hit Substances 1

2 Antimalarial Benzimidazole Derivatives Incorporating Phenolic Mannich Base Side Chains Inhibit Microtubule and Hemozoin Formation: Structure-Activity Relationship and in Vivo Oral Efficacy Studies
Dziwornu, Godwin Akpeko; Coertzen, Dina; Leshabane, Meta; Korkor, Constance M.; Cloete, Cleavon K.; Njoroge, Mathew; Gibhard, Liesl; (...) Birkholtz, Lyn-Marie; Chibale, Kelly [Journal of Medicinal Chemistry, 2021, vol. 64, # 8, p. 5198 - 5215]
Abstract Index Terms Substances 112 Reactions 318 Full Text ↗
Hit Substances 1

3 Effects of Replacing Oxygenated Functionality with Fluorine on Lipophilicity
Glyn, Richard J.; Pattison, Graham [Journal of Medicinal Chemistry, 2021, vol. 64, # 14, p. 10246 - 10259]
Abstract Index Terms Substances 225 Full Text ↗
Hit Substances 1

Vanessa Hoguet : Yazar
Beyond the Rule..... : Yayın başlığı
Journal of Medicinal Chemistry : Dergi ismi
2021 : Basım yılı
64(3) : Dergi volümü (sayısı)
1593-1610 : Sayfa sayısı

İlaç molekülüne ait hedefler Makale, Patent gibi çalışmalar Document bölümünde de incelenebilir.

	731	Substances	Structure :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	250	Targets	Structure :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	46,714	Documents	Structure :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	3,398	Substances	Structure :  average similarity; included: tautomers, only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	340	Reactions	Reaction Query :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	140	Commercial Substances	Structure :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	2,150	Commercial Substances	Structure :  average similarity; included: tautomers, only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals Edit in Query Builder  Create Alert 	Preview Results 	View Results 

Dokümanlar yıl, doküman türü, makale adı gibi özelliklere göre filtrelenebilmektedir.

The image shows a screenshot of a chemical database search results page. A red box highlights the left sidebar, which contains a 'Filters' section with various filter options. The main content area displays search results for '16,318 Documents with 3 Substances, 4,076 Reactions, 242 Targets'. The results are sorted by relevance and include details such as document titles, authors, publication years, and patent information. The filters sidebar includes options for Publication Year, Document Type, Authors of Scientific Documents, Current Affiliation, Inventors of Patents, Current Patent Assignee, Patent Office, Journal Title, Substance Classes, Reaction Classes, Index Terms (List), and Index Terms (ReaxysTree). There is also a checkbox for 'Manually curated content only'.

Filters

- Limit to > Exclude >
- Publication Year
- Document Type
- Authors of Scientific Documents
- Current Affiliation
- Inventors of Patents
- Current Patent Assignee
- Patent Office
- Journal Title
- Substance Classes
- Reaction Classes
- Index Terms (List)
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16,318 Documents with 3 Substances, 4,076 Reactions, 242 Targets

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Sort by Relevance

Bioactivity Visualizatic

No title
Della,E.W.; Jefferies,P.R.
Australian Journal of Chemistry, 1961, vol. 14, p. 610 - 618
Index Terms Substances 33 Reactions 31 Full Text
Hit Substances 1

Cleansing articles for skin and/or hair which also deposit skin care actives
US6338855, 2002, B1
Current Patent Assignee: PROCTER GAMBLE
Office: US View full patent family
Abstract Index Terms Claims Bibliographic Info Substances 423 Full Text
Hit Substances 1

Heterocyclic compounds
Current Patent Assignee: ASTRAZENECA - EP355049, 1990, A3
Patent Family Members: GB8819660 D0; GB8914041 D0; DK405489 D0; NO893304 D0; GB8916722 D0; ...
Abstract Claims Bibliographic Info Substances 35 Reactions 19 Full Text
Hit Substances 1

New serotonin 5-HT1F agonists
Current Patent Assignee: ELI LILLY - EP835869, 1998, A2
Patent Family Members: EP835869 A2; CA2268164 A1; WO1998/15545 A1; AU4652697 A; EP835869 A3; ...
Abstract Claims Bibliographic Info Substances 506 Reactions 459 Targets Full Text
Hit Substances 1

Substituted pyridinyloxy(thio)phenyl -acetamides, -ureas and urea derivatives
Current Patent Assignee: DOW CHEMICAL - US3931201, 1976, A
Patent Family Members: DE2501648 A1; JP5501/1534 A; FR2258382 A1; BR7500308 A; US3931201 A; ...
Abstract Claims Bibliographic Info Substances 20 Reactions 4 Full Text
Hit Substances 1

4-Ethers of 3-amino-5-sulfamoylbenzoic acids
Current Patent Assignee: CIBA GEIGY - US3939267, 1976, A

46,318 Documents with 3 Substances, 4,076 Reactions, 242 Targets

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Limit to > exclude >

Publication Year	Count
<input checked="" type="checkbox"/> 2026	376
<input type="checkbox"/> 2025	2,967
<input type="checkbox"/> 2024	2,403
<input type="checkbox"/> 2023	3,312
<input type="checkbox"/> 2022	5,086
<input type="checkbox"/> 2021	5,028
<input type="checkbox"/> 2020	4,840

Document Type

Authors of Scientific Documents

Current Affiliation

Inventors of Patents

Current Patent Assignee

Patent Office

Journal Title

Substance Classes

Reaction Classes

Index Terms (List)

Index Terms (ReaxysTree)

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No title
Della, E.W.; Jefferies, P.R.
Australian Journal of Chemistry, 1961, vol. 14, p. 610 - 618
Index Terms Substances 33 Reactions 31 Full Text
Hit Substances 1

Cleansing articles for skin and/or hair which also deposit skin care actives
US6338855, 2002, B1
Current Patent Assignee: PROCTER GAMBLE
Office: US View full patent family
Abstract Index Terms Claims Bibliographic Info Substances 423 Full Text
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Heterocyclic compounds
3
Current Patent Assignee: ASTRAZENECA - EP355049, 1990, A3
Patent Family Members: GB8819660 D0; GB8914041 D0; DK405489 D0; NO893304 D0; GB8916722 D0; ...
Abstract Claims Bibliographic Info Substances 35 Reactions 19 Full Text
Hit Substances 1

New serotonin 5-HT1F agonists
4
Current Patent Assignee: ELI LILLY - EP835869, 1998, A2
Patent Family Members: EP835869 A2; CA2268164 A1; WO1998/15545 A1; AU4652697 A; EP835869 A3; ...
Abstract Claims Bibliographic Info Substances 506 Reactions 459 Targets Full Text
Hit Substances 1

Substituted pyridinyloxy(thio)phenyl -acetamides, -ureas and urea derivatives
5
Current Patent Assignee: DOW CHEMICAL - US3931201, 1976, A
Patent Family Members: DE2501648 A1; JP5501/1534 A; FR2258382 A1; BR7500308 A; US3931201 A; ...
Abstract Claims Bibliographic Info Substances 20 Reactions 4 Full Text
Hit Substances 1

4-Ethers of 3-amino-5-sulfamoylbenzoic acids
6
Current Patent Assignee: CIBA GEIGY - US3939267, 1976, A

Notlar Açıklamalar Adobe Acrobat

İngilizce (ABD) Erişilebilirlik: Önerilere göz atın

Quick search kısmına molekül formülüne ek olarak anahtar kelimeler yapılarak arama daraltılabilir.

Search for "analgesic" AND 

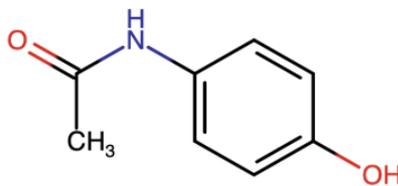
Search Reaxys

"analgesic"



Find >

AND



As drawn 

Hedef sayısı bu şekilde 9 adete kadar düştü!

	9	Targets	Structure :  as drawn Effect(s) : analgesic Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	1	Substances	Structure :  as drawn Effect(s) : analgesic Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	9,149	Documents	Structure :  as drawn Titles, Abstracts, Keywords : "analgesic" Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	1,420	Targets	Effect(s) : analgesic Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	43,027	Substances	Effect(s) : analgesic Edit in Query Builder  Create Alert 	Preview Results 	View Results 
	3	Substances	Structure :  as drawn Edit in Query Builder  Create Alert 	Preview Results 	View Results 

Artık anahtar kelimeyi içeren dokümanlar işaretli bir şekilde ekrana gelecektir.

The screenshot displays the Reaxys search results interface. At the top, the Reaxys logo is on the left, and navigation links for 'Quick search', 'Query builder', 'Results', and 'Retrosynthesis' are in the center. On the right, there are icons for refresh, help, and a 'Register' button. Below the navigation, a search bar shows '413,86 K' results. A 'Filters' sidebar on the left lists various criteria like 'Publication Year', 'Document Type', and 'Substance Classes'. The main content area shows a list of search results. The first result is 'Analgesic effect of non-narcotic herbal remedies' from *Herba Polonica*, 2023, with keywords 'analgesic' and 'herbal remedies' highlighted. The second result is 'ANALGESIC NON-NARCOTIC MEDICINE' from RU2008112511, 2009, A, with keywords 'analgesic' and 'non-narcotic' highlighted. The third result is 'Tracing analgesic constituents from crude and vinegar-processed resin of Boswellia carterii...' from *Biomedical Chromatography*, 2022, with keywords 'analgesic' and 'Boswellia carterii' highlighted. Each result includes an 'Abstract hit' snippet with the highlighted keywords.

Reaxys

Quick search Query builder Results Retrosynthesis

413,86 K

413,863 Documents with 1,617,253 Substances, 935,628 Reactions, 6,434 Targets

0 selected Limit To Exclude Export

Sort by Relevance Bioactivity Visual

Analgesic effect of non-narcotic herbal remedies
1
Gutowski, Mateusz; Aleksandrak, Justyna; Przerwa, Filip; Bieniewicz, Arkadiusz; Warkocz, Szymon; Byrski, Jakub; Kotrych, Katarzyna; Ziłek, Paweł; Uzar, Izabela
Herba Polonica, 2023, vol. 69, # 4, p. 33 - 44, [10.5604/01.3001.0054.1402](#)
Abstract Index Terms Substances 1 Full Text

Abstract hit:
{...effects and analgesic activity. The aim of this publication is to summarise the...}

Index Terms hit:
{...Reaxys Index Terms: analgic agent, anticoagulant agent...}

ANALGESIC NON-NARCOTIC MEDICINE
2
RU2008112511, 2009, A
Office: RU [View full patent family](#)
Abstract Bibliographic Info Full Text

Abstract hit:
{...1. The analgesic non-narcotic medicine, which contains active material - paracetamol and auxiliary...}

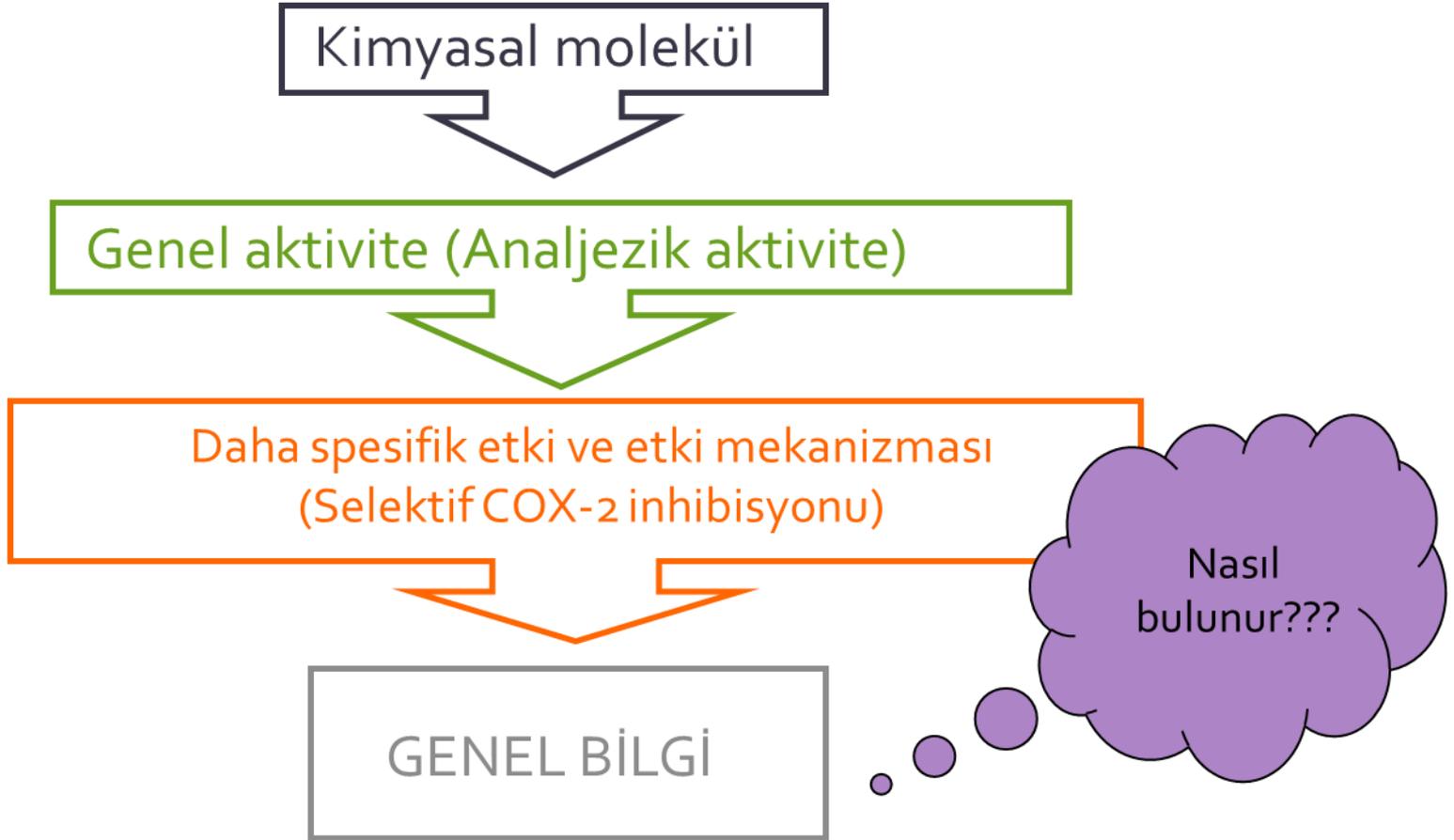
Tracing analgesic constituents from crude and vinegar-processed resin of Boswellia carterii by integrating ultra-performance liquid chromatography tandem mass spectrometry-based determination, analgesic evaluation in mice, and gray relationship analysis
3
Xie, Xiaoyang; Liu, Qing; Zhu, Fei; Zhang, Tingjun; Xu, Xiangwei; Tao, Yi
Biomedical Chromatography, 2022, vol. 36, # 9, art. no. e5430, [10.1002/bmc.5430](#)
Abstract Index Terms Substances 6 Full Text

Abstract hit:
{...The analgesic effect of the resin of Boswellia carterii (BC) is well...}

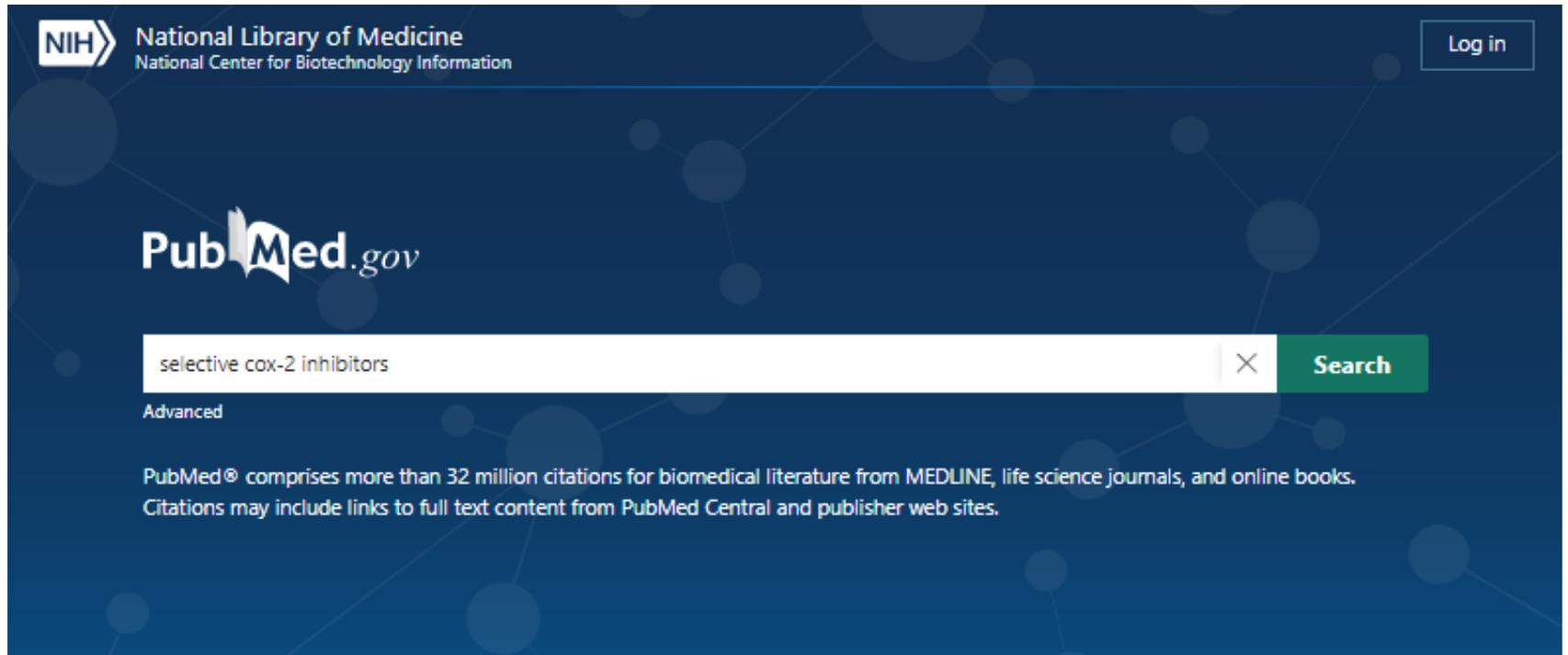
İstenirse Query Builder kısmından farklı filtreleme ve aramalar yapılabilir.

The screenshot displays the Reaxys Query Builder interface. At the top left, the Reaxys logo is visible. The navigation bar includes 'Quick search', 'Query builder' (highlighted with a red box), 'Results', 'Retrosynthesis', and 'History'. On the right side of the navigation bar, there are 'Register >' and 'Sign in' buttons. Below the navigation bar, the 'Search in:' section contains buttons for 'Reactions >', 'Targets >', 'Substances >', and 'Documents >' (highlighted with a red box). A toolbar below this section includes 'Import', 'Save', 'Reset form', and 'Delete all' buttons, along with icons for 'Current Patent Assignee', 'Structure', 'Molecular Formula', 'CAS RN', and 'TI, AB & KW'. The main search area features a dropdown menu for 'Authors/Inventors' and a search input field containing the text 'banglu, erden' (highlighted with a red box). To the right, a 'Search fields' sidebar is visible, listing various search criteria: 'MedChem', 'Other', 'Reactions', 'Bibliography' (highlighted with a red box), 'Document Type', 'Authors/Inventors' (highlighted with a red box), 'Current Patent Assignee', 'Original Patent Assignee', 'Journal Title', 'Publication Year', 'Common Patent Number', and 'Journal Publication Status'.

Genel biyolojik aktivite hakkında bilgi edinme



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The image shows a screenshot of the PubMed.gov website. The background is dark blue with a faint molecular structure pattern. At the top left, there is the NIH logo and the text "National Library of Medicine National Center for Biotechnology Information". At the top right, there is a "Log in" button. In the center, the "PubMed.gov" logo is displayed. Below the logo is a search bar containing the text "selective cox-2 inhibitors". To the right of the search bar is a green "Search" button. Below the search bar, the word "Advanced" is written. At the bottom, there is a paragraph of text: "PubMed® comprises more than 32 million citations for biomedical literature from MEDLINE, life science journals, and online books. Citations may include links to full text content from PubMed Central and publisher web sites."

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Log in

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selective cox-2 inhibitors

Search

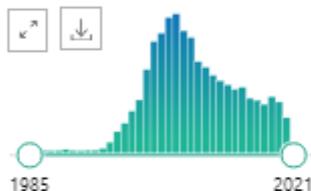
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- Associated data

ARTICLE TYPE

- Books and Documents
- Clinical Trial
- Meta-Analysis
- Randomized Controlled Trial
- Review
- Systematic Review

6,384 results

Selective COX-2 inhibitors as anticancer agents: a patent review (2014-2018).

1 Mahboubi Rabbani SMI, Zarghi A.

Cite Expert Opin Ther Pat. 2019 Jun;29(6):407-427. doi: 10.1080/13543776.2019.1623880. Epub 2019 May 27. PMID: 31132889 Review.

Share AREAS COVERED: It is well established that **COX-2** is overexpressed in many different cancers and treatment with **selective COX-2 inhibitors** could relieve their symptoms and limit their adverse sequences. EXPERT OPINION: The diversity of ...

Structural investigation on the selective COX-2 inhibitors mediated cardiotoxicity: A review.

2 Arora M, Choudhary S, Singh PK, Sapra B, Silakari O.

Cite Life Sci. 2020 Jun 15;251:117631. doi: 10.1016/j.lfs.2020.117631. Epub 2020 Apr 3. PMID: 32251635 Review.

Share This review discusses the key structural features of the **selective COX-2 inhibitors** and underlying mechanisms that are responsible for the cardiotoxicity. This report also unfolds different strategies that have been reported in the last 10 years to com ...

Update on COX-2 Selective Inhibitors: Chemical Classification, Side Effects and their Use in Cancers and Neuronal Diseases.

3 Rayar AM, Lagarde N, Ferroud C, Zagury JF, Montes M, Sylla-Iyarreta Veitia M.

Cite Curr Top Med Chem. 2017;17(26):2935-2956. doi: 10.2174/1568026617666170821124947. PMID: 28828990 Review.

Share Inflammation is a complex phenomenon necessary in human defense mechanisms but also involved in the development of some human diseases. The discovery of **cyclooxygenase-2 (COX- 2)** improved the pharmacology of nonsteroidal anti-inflammatory drugs (NSAID) ...

Selective COX-2 inhibitors are safe and effective.



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- Book chapters (6,631)

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Design, synthesis and biological assessment of new selective COX-2 inhibitors including methyl sulfonyl moiety
European Journal of Medicinal Chemistry, 9 October 2020, ...
Begüm Nurpelin Sağlık, Derya Osmaniye, ... Zafer Asım Kaplancıklı

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Symmetrical and un-symmetrical curcumin analogues as selective COX-1 and COX-2 inhibitor
European Journal of Pharmaceutical Sciences, 1 February 2021, ...
Monisha Mohan, Mulla Althaf Hussain, ... Roy Anindya

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1

of 143



1 Pyridazinones as selective cyclooxygenase-2 inhibitors

Li, CS; Brideau, C; (...); Prasit, P

Feb 24 2003 | [Bioorganic & Medicinal Chemistry Letters](#)

Pyridazinone was found to be an excellent core template for selective COX-2 inhibitors. Two potent, selective and orally active COX-2 inhibitors, which were highly efficacious in rat paw edema and rat paresis models, have been obtained. (C) 2003 Elsevier Science Ltd. All rights reserved.

[Full Text at Publisher](#) ***

61

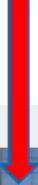
Citations

14

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[Mozilla Firefox Proxy Ayarları](#)

[Mac Bilgisayar Proxy Ayarları](#)

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Yeni sekme
Yeni pencere
Yeni gizli pencere
Geçmiş
İndirilenler
Yer İşaretleri
Yakınlaştır
Yazdır...
Bul...
Diğer araçlar
Düzenle Kes Kopyala Yapıştır
Ayarlar
Çıkış

AYARLAR SEÇENEĞİNE TIKLAYIN

Google'da Ara Kendimi Şanslı Hissediyorum

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Chrome Ayarlar

chrome://settings

Ayarlarda ara

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Belirli bir sayfayı veya sayfaları aç. Sayfaları ayarla

Görünüm

Tema al Varsayılan temaya sıfırla

Ana Sayfa düğmesini göster

Yer işaretleri çubuğunu her zaman göster

Ara

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Kişi 1 (şu andaki)

Misafir olarak göz atmayı etkinleştir

Herhangi birinin Chrome'a kişi eklemesine izin ver

Kişi ekle... Düzenle... Kaldır... Yer işaretlerini ve ayarları içe aktar...

Varsayılan tarayıcı

Varsayılan tarayıcı şu anda Google Chrome.

Gelişmiş ayarları göster...

**GELİŞMİŞ AYARLARI
GÖSTER SEÇENEĞİNE
TIKLAYIN**

3. Adım

Chrome Ayarlar

chrome://settings

Ayarlarda ara

Geçmiş

Uzantılar

Ayarlar

Hakkında

Ayarlar

Yazı tipi boyutu: Orta Yazı tiplerini özelleştir...

Sayfa yakınlaştırma: %100

Ağ

Google Chrome, ağa bağlanmak için bilgisayarınızın sistem proxy ayarlarını kullanır.

Proxy ayarlarını değiştir...

PROXY AYARLARINI DEĞİŞTİR SEÇENEĞİNE TIKLAYIN

Diller

Chrome uygulamasının dilleri işleme ve görüntüleme biçimini değiştir. [Daha fazla bilgi edinin](#)

Dil ve giriş ayarları...

Okuduğum dilde olmayan sayfaları çevirmeyi öner. Dilleri yönetin

İndirilenler

İndirme konumu: C:\Users\mustafa\Downloads Değiştir...

İndirmeden önce her dosyanın nereye kaydedileceğini sor

HTTPS/SSL

Sertifikaları yönet...

Google Cloud Print

Google Cloud Print içinde yazıcılar kurun ve yönetin. [Daha fazla bilgi edinin](#)

Yönet

A4 üzerinde yeni yazıcılar alıldığında bildirim göster

4. Adım



5. Adım

Yerel Ağ (LAN) Ayarları

Otomatik Yapılandırma

Otomatik yapılandırma, yaptığınız ayarları değiştirebilir. Bu ayarların kullanılması için otomatik yapılandırmayı devre dışı bırakın.

Ayarları otomatik olarak algıla

Otomatik yapılandırma komut dosyası kullan

Adres:

Ara sunucu

Yerel ağınız için bir proxy sunucu kullanın (Bu ayarlar çevirmeli bağlantılarda ve da VPN bağlantılarında geçerli olmaz).

Adres: B. Nok.: Gelişmiş

Yerel adresler için proxy sunucuya ara

KUTUCUĞU İŞARETLEYİN

YUKARIDAKİ İKİ KUTUCUĞU ŞEKİLDEKİ GİBİ DOLDURUN

6. Adım

Yerel Ağ (LAN) Ayarları



Otomatik Yapılandırma

Otomatik yapılandırma, yaptığınız ayarları değiştirebilir. Bu ayarların kullanılması için otomatik yapılandırmayı devre dışı bırakın.

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Yerel ağınız için bir proxy sunucu kullanın (Bu ayarlar çevirmeli bağlantılarda ya da VPN bağlantılarında geçerli olmaz).

Adres:

B. Nok.:

Yerel adresler için proxy sunucuyu atla

**TAMAM BUTONUNA
TIKLAYIN**

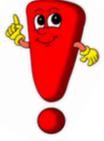


← → X Google üzerinde arayın veya bir URL yazın

Uygulamalar Click2Drug Determination and... https://akademikyo...

☆ 🗑️ 🌐 S

Gmail Görseller S



Kullanıcı adı: Öğrenci numarası
Şifre: Oluşturulan proxy şifresi

Oturum açın

http://proxy2.gazi.edu.tr:2001 proxy'si için kullanıcı adı ve şifre gerekiyor.
Bu siteme bağlantınız gizli değil

Kullanıcı adı:

Şifre:

Oturum açın İptal

Q Google'da arama yapın veya bir URL yazın

