



Hinweise zur

Literaturrecherche

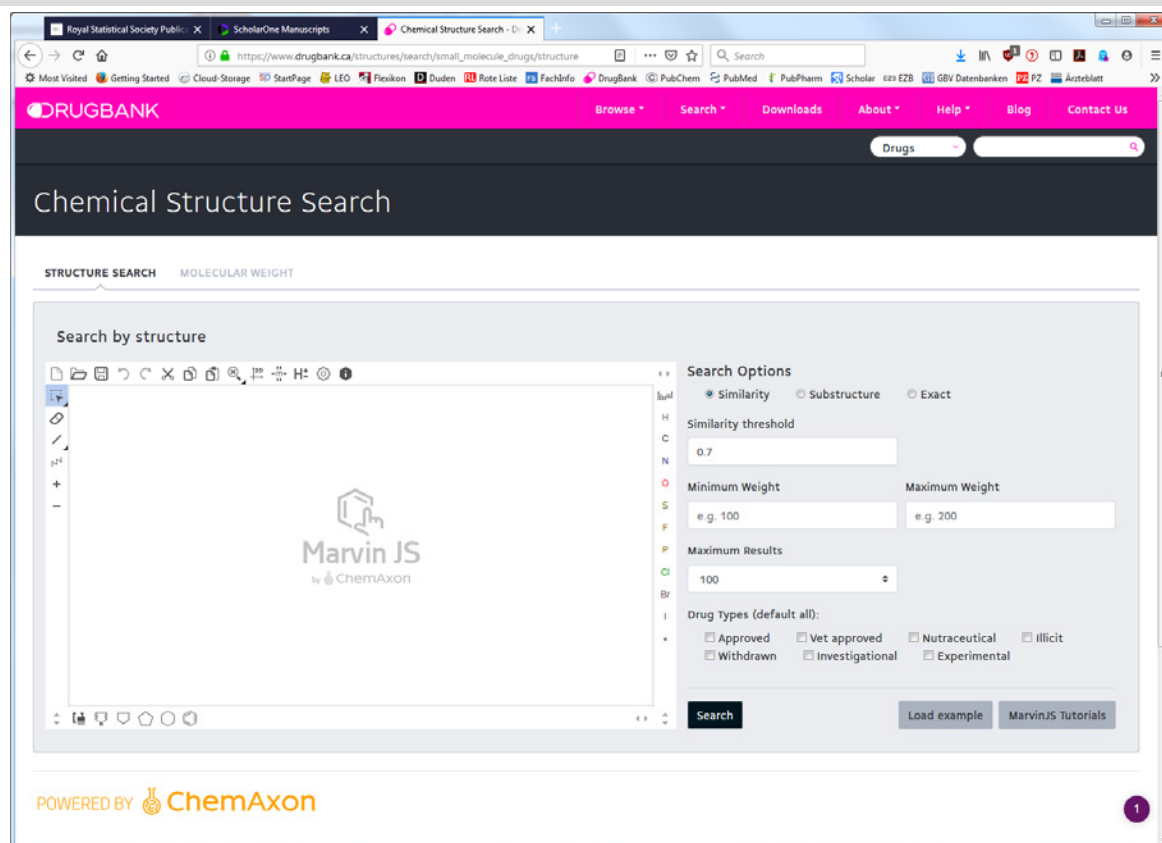
Knut Baumann

Aufgabe

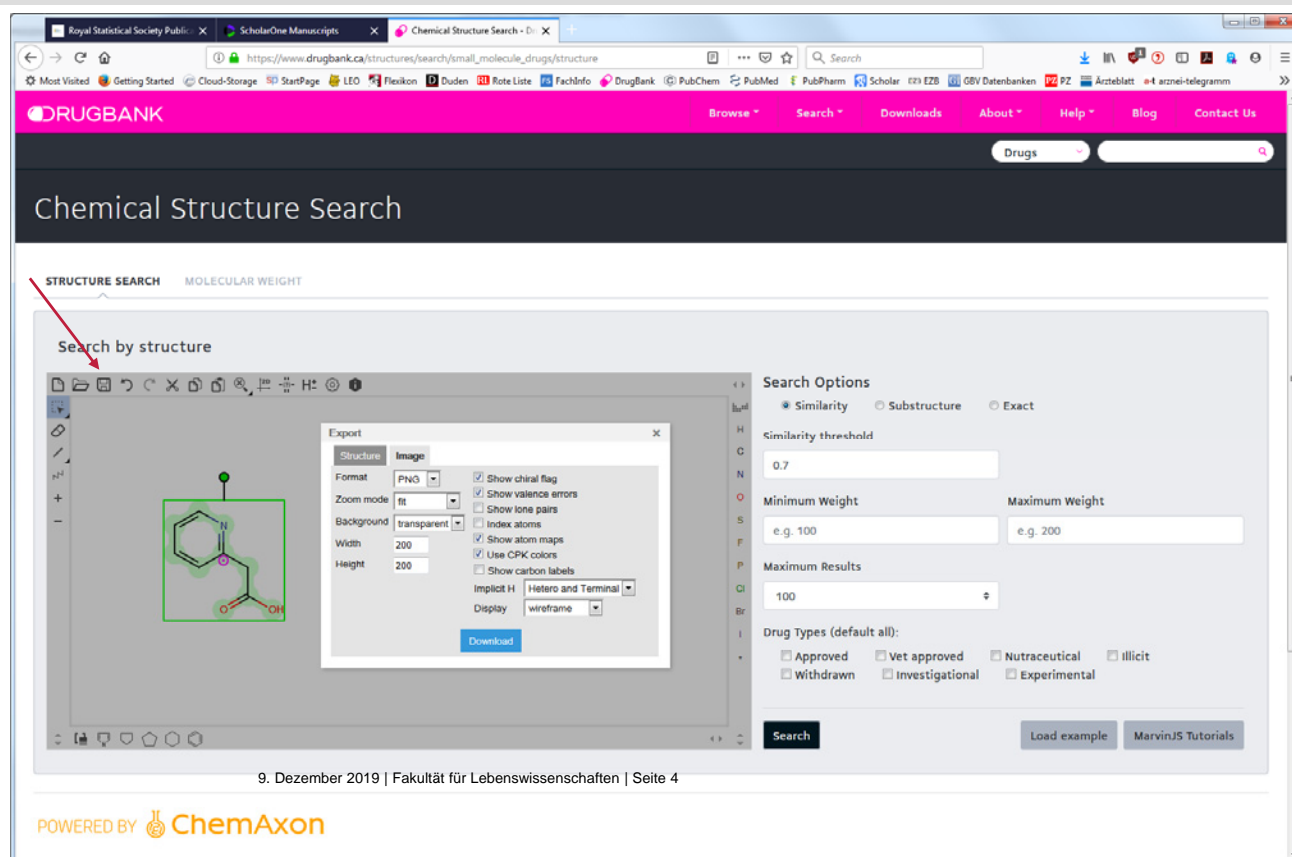
- 1) Erstellen einer Monographie, die in Inhalt und Struktur aktuellen Arzneibuchmonographien gleicht.
- 2) Erstellen eines Kommentars, der in Inhalt und Struktur einem aktuellen Arzneibuchkommentar gleicht.
- 3) Die Strukturformeln sollen selbst gezeichnet werden (Minimum: untersuchter Arzneistoff und Verunreinigungen; d.h. Ausnahme: ggf. komplexe Synthesen).
- 4) Es ist alle verwendete Literatur anzugeben. Die Literatur ist abweichend von der AB-Monographie im Monographietext als Literaturverweis anzugeben. Das Literaturverzeichnis muss die verwendeten Quellen in einheitlichem Stil zitieren.

Drugbank Struktureditor

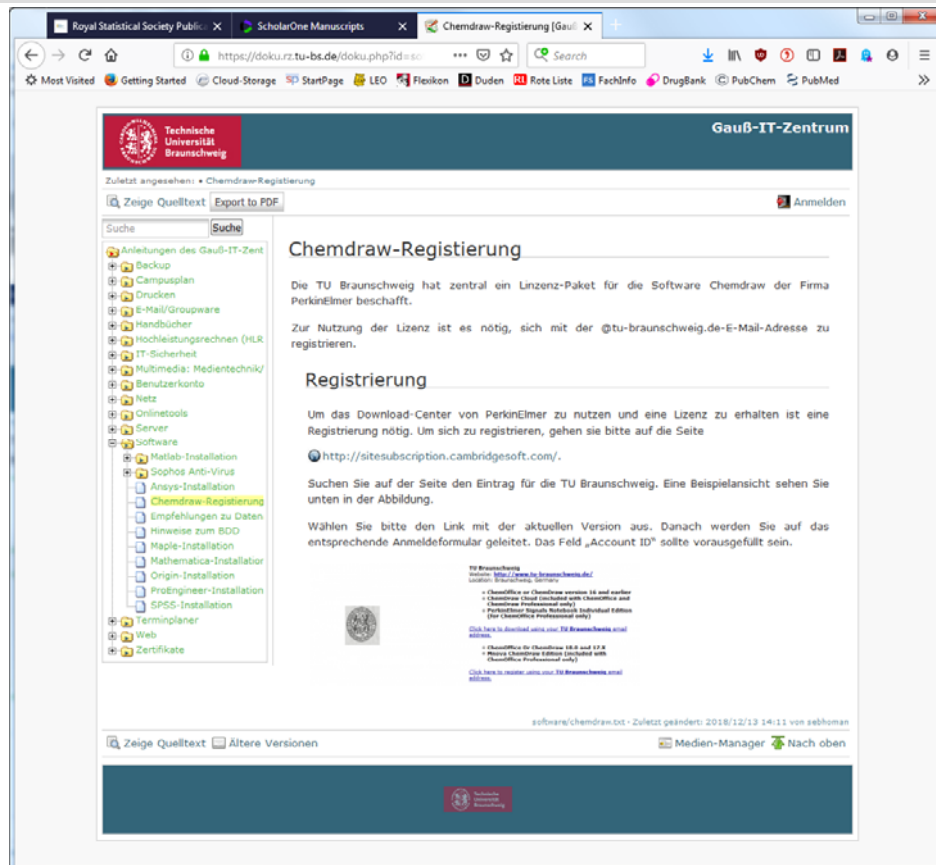
https://www.drugbank.ca/structures/search/small_molecule_drugs/structure



Drugbank Struktureditor – Speichern->Image



<https://doku.rz.tu-bs.de/...>
[...doku.php?id=software:chemdraw](https://doku.rz.tu-bs.de/doku.php?id=software:chemdraw)



Zitierstil I

Artikel (mit Titel)

1.) Buchwald, P.; Bodor, N. Computer-Aided Drug Design: The Role of Quantitative StructureProperty, Structure-Activity and Structure-Metabolism Relationships (QSPR, QSAR, QSMR). *Drugs Fut.* **2002**, 27, 577-588.

Format: Nachname, 1. Buchstabe Vorname. (alle Autoren nennen, Autoren durch „;“ getrennt) Titel des Artikels. Zeitschrift abgekürzt (kursiv) Jahr (fett), Jahrgang (kursiv), Seiten von-bis.

Zu den Artikeln ist wenn vorhanden ein **DOI** (Digital Object Identifier anzugeben) oder ein Link in PubMed (jeder Artikel in PubMed hat eine **PMID**)

Zitierstil II

Bücher

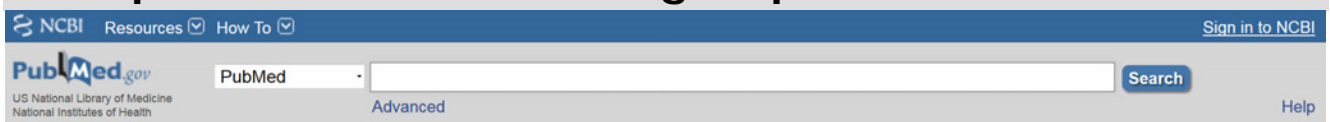
2.) Böhm, H.-J.; Klebe, G.; Kubinyi, H. *Wirkstoffdesign*, Spektrum Akademischer Verlag: Heidelberg, 1996.

Format: Nachname, 1. Buchstabe Vorname. (alle Autoren nennen, Autoren durch „;“ getrennt) Titel des Buchs (kursiv), Name des Verlags: Verlagsort, Erscheinungsjahr.

Wenn möglich mit **DOI** o.a. **permanenter Link**



<http://www.ncbi.nlm.nih.gov/pubmed/25440595>



Abstract ▾

Curr Vasc Pharmacol. 2015;13(5):566-77.

Platelet Inhibition Agents: Current and Future P2Y12 Receptor Antagonists.

Tang J, Li MP, Zhou HH, Chen XP¹.

Author information

Abstract

Percutaneous coronary intervention is widely used to reduce the risk of death or cardiovascular events in patients with acute coronary syndromes. Dual antiplatelet treatment with aspirin and clopidogrel has become routine practice to prevent thrombotic events after coronary surgery. Despite advances of significant reduction of thrombotic complications in this adjunctive therapy, major adverse cardiovascular events still occur, suggesting the need for development of novel antiplatelet agents that act as superior alternatives to current standard regimen. Recently developed antiplatelet agents (prasugrel, ticagrelor, cangrelor and elinogrel) efficiently antagonize P2Y12 receptor, a key platelet activating signaling pathway, and thereby inhibit aggregation induced by mediators such as ADP, collagen, thrombin and TXA2. We provide an evidence-based review on the pharmacological and clinical performance of clopidogrel and novel antiplatelet agents that antagonize P2Y12 receptors.

PMID: 25440595 [PubMed - indexed for MEDLINE]

Publication Types, MeSH Terms, Substances

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- Review** Novel platelet ADP P2Y12 inhibitors in the treatment of cardiovascular disease [Cardiovasc Ther. 2012]
- Third generation P2Y12 antagonists inhibit platelet aggregation [Thromb Haemost. 2014]
- Review** Clinical effects and outcomes with new P2Y12 [Fundam Clin Pharmacol. 2012]
- Review** A critical appraisal of the functional evolution of P2Y12 [Curr Pharm Des. 2012]
- Review** [Recent advances on the studies of the platelet's inhibition] [Recenti Prog Med. 2011]

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Current Vascular Pharmacology

ISSN (Print): 1570-1611

ISSN (Online): 1875-6212

Epub Full Text Article

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Price: \$95

Zeitschrift über EZB

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Platelet Inhibition Agents: Current and Future P2Y12 Receptor Antagonists

Author(s): Jie Tang, Mu-Peng Li, Hong-Hao Zhou and Xiao-Ping Chen

Abstract:

Percutaneous coronary intervention is widely used to reduce the risk of death or cardiovascular events in patients with acute coronary syndromes. Dual antiplatelet treatment and clopidogrel has become routine practice to prevent thrombotic events after coronary surgery. Despite advances of significant reduction of thrombotic complications in therapy, major adverse cardiovascular events still occur, suggesting the need for development of novel antiplatelet agents that act as superior alternatives to current strategies. Recently developed antiplatelet agents (prasugrel, ticagrelor, cangrelor and elinogrel) efficiently antagonize P2Y12 receptor, a key platelet activating signaling pathway, and aggregation induced by mediators such as ADP, collagen, thrombin and TXA2. We provide an evidence-based review on the pharmacological and clinical performance of novel antiplatelet agents that antagonize P2Y12 receptors.

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Thromb Haemost. 2013 Jan;109(1):93-101. doi: 10.1160/TH12-06-0377. Epub 2012 Nov 29.

Impact of clopidogrel and potent P2Y 12 -inhibitors on mortality and stroke in patients with acute coronary syndrome or undergoing percutaneous coronary intervention: a systematic review and meta-analysis.

Aradi D¹, Komócsi A, Vorobcsuk A, Serebruany VL.

Author information

Abstract

Administration of a P2Y 12 -receptor antagonist in addition to aspirin is mandatory in patients with acute coronary syndromes (ACS) or undergoing percutaneous coronary intervention (PCI) to reduce the occurrence of thrombotic events; however, their impact on mortality and stroke is unclear. We aimed to evaluate the influence of moderate (clopidogrel) or potent (prasugrel/ticagrelor) P2Y 12 -receptor inhibition on major cardiovascular outcomes among patients with ACS or undergoing PCI. Systematic literature search was performed to find randomised, controlled clinical trials comparing the clinical impact of clopidogrel with placebo or prasugrel/ticagrelor versus clopidogrel. Outcome measures included cardiovascular death, myocardial infarction (MI), total stroke and intracranial haemorrhage (ICH). Random-effects model with Mantel-Haenszel weighting was used to pool outcomes into a meta-analysis. Four studies comparing clopidogrel with placebo and five trials comparing clopidogrel with new P2Y 12 -receptor inhibitors were identified including a total of 107,473 patients. Compared to placebo, clopidogrel reduced the risk of cardiovascular death (odds

Full text links



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Related citations in PubMed

Relationship between post-tr [J Thromb Haemost. 2012]
Ticagrelor versus prasugrel in acute cc [J Am Coll Cardiol. 2012]
Discharge aspirin dose and clinical c [J Am Coll Cardiol. 2014]
Review Switching antiplatelet

<http://th.schattauer.de/en/contents/archive/issue/1623/manuscript/19048.html>

The screenshot shows the website of the journal 'Thrombosis and Haemostasis'. The header includes the journal title and a navigation bar with links: HOME, CONTENTS, SEARCH, SUBSCRIPTION, AUTHORS, ADVERTISING, ABOUT, and LOGIN. The 'CONTENTS' sidebar lists options like Current Issue, Ahead of Print, Archive, Search, Sponsored Content, Copyright permissions, Register for eTOC, and RSS. The main content area displays the article title, a thumbnail of the journal cover, and a table with metadata: Journal: Thrombosis and Haemostasis, ISSN: 0340-6245, DOI: <http://dx.doi.org/10.1160/TH12-06-0377>, Issue: 2013; 109/4 (Jan) pp. 1-173, and Pages: 93-101. Below this is a 'CONTACT PERSON' section for Dr. Elinor Switzer, Managing Editor, with contact details and a 'send an Email' button. The article abstract is also visible, starting with 'Administration of a P2Y 12 -receptor antagonist in addition to aspirin is mandatory in patients with acute coronary syndromes (ACS) or undergoing percutaneous coronary intervention (PCI) to reduce the occurrence of thrombotic events; however, their impact on mortality and stroke is unclear. We aimed to evaluate the influence of moderate (clopidogrel) or potent (prasugrel/ticagrelor) P2Y 12 -receptor inhibition on major cardiovascular outcomes among patients with ACS or undergoing PCI. Systematic literature search was performed to find randomised, controlled clinical trials comparing the clinical impact of clopidogrel with placebo or prasugrel/ticagrelor versus clopidogrel. Outcome measures included cardiovascular death, myocardial infarction (MI), total stroke and intracranial haemorrhage (ICH). Random effects model with Mantel-Haenszel weighting was used to pool outcomes from...

Zitierstil III

Online Ressourcen

Kurze Beschreibung und http-Adresse

4.) Prasugrel; <http://www.drugbank.ca/drugs/DB06209>; letzter Zugriff am 17.06.2016.

Keine Links in Datenbanken, die ein Login erfordern (SciFinder, Scopus etc.)

Allgemeine Recherche

Informationsquellen

- **Wissenschaftliche Literatur** \equiv „Die Literatur“
- Internetdatenbanken
- Arzneimittel-Hersteller (via DocCheck)
- Berufsverbände (Nds. Apothekerkammer, ABDA, ...)
- Behörden (BfArM, RKI, PEI, ...)
- Nachrichten (Internet)

Primärliteratur

Originalpublikationen, Basis des wissenschaftlichen Wissens

- Details
- Stark fokussiert
- Qualität: „Peer-Review-System“
- Beschaffung z.T. schwierig und teuer (PubMed und Google Scholar zeigen frei verfügbare Quellen)
- Nicht nur auf Zusammenfassung verlassen
 - ⇒ Hochaktuell, detailliert
 - ⇒ Kontrovers diskutierte Themen sind verstreut

Wichtige Journale

- Journal of Analytical Chemistry
- Journal of Chromatography A/B
- Journal of Pharmaceutical and Biomedical Analysis
- Analytical and Bioanalytical Chemistry
- Chromatographia
- Electrophoresis
- Analytica Chimica Acta
- Pharmaeuropa
- Journal of Medicinal Chemistry
- Bioorganic & Medicinal Chemistry
- ...u.v.m

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<http://rzblx1.uni-regensburg.de/ezeit/search.phtml?bibid=TUBS&colors=7&lang=de>



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Geben Sie bitte im folgenden Formular verschiedene Kriterien zu Ihrer gesuchten Zeitschrift ein. Informationen über verschiedene Suchmöglichkeiten finden Sie in der [Hilfe zur EZB](#). Hinweis: Sie können hier nicht nach Zeitschriftenartikeln suchen.

Erweiterte Suche nach Zeitschriften

Suchkriterien

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ISSN	<input type="text"/>	und	<input type="text"/>
Verlag	<input type="text"/>		
Treffer pro Seite:	<input type="text" value="50"/>		

Fachgebiete einschränken

Auswahl an Fachgebieten:

Allgemeine Sprach- und Literaturwissenschaft
Allgemeines, Fachübergreifendes
Anglistik, Amerikanistik
Archäologie
Architektur, Bauingenieur- und Vermessungswesen

Die Volltexte der Zeitschriften sind

- ☒ ☐ ☐ frei zugänglich
- ☒ ☐ ☐ für die TU Braunschweig campusweit freigeschaltet
- ☐ ☐ ☐ nur bei einem Teil der erschienenen Jahrgänge für die TU Braunschweig campusweit freigeschaltet
- ☒ ☐ ☐ nicht zugänglich (in vielen Fällen werden Abstracts angeboten)

[Nutzungsbedingungen](#)

<http://rzblx1.uni-regensburg.de/ezeit/search.phtml?bibid=TUBS&colors=7&lang=de>

Sekundärliteratur

- I. Indexierungs- und „Abstract“-Dienste
 - II. Themenbezogene Bewertungen und Übersichtsarbeiten („Reviews“)
 - Datenbanken
 - PubMed, SciFinder (\$), Scopus (\$), ...
 - Spezielle Zeitschriften
 - Pharmacon, Pharmazie in unser Zeit, ...
 - Drugs of the Future, ...
- ⇒ Vorauswahl, Wertung, weniger aktuell

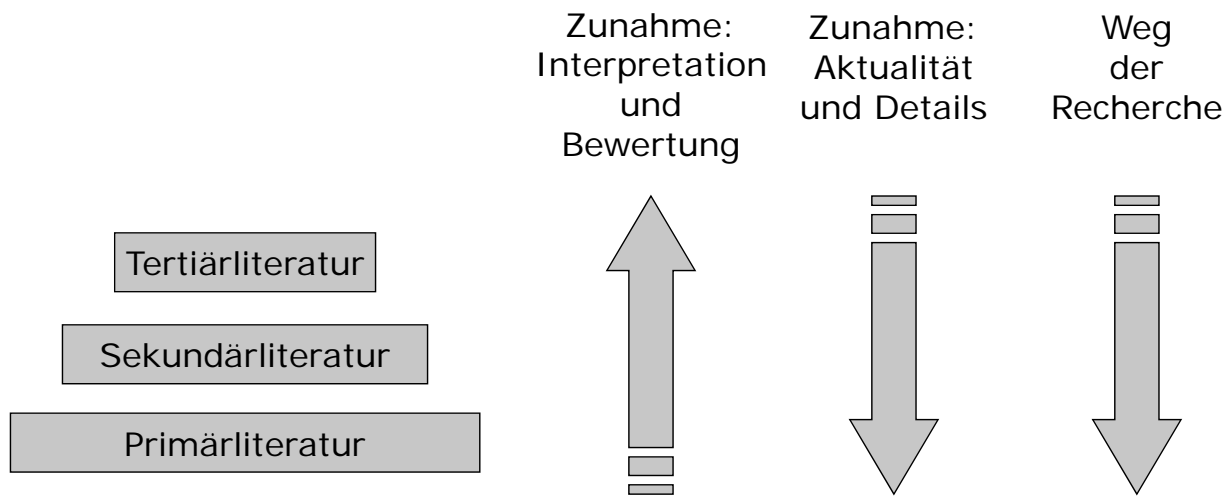
Tertiärliteratur

„Das“ etablierte Wissen in konzentrierter, strukturierter Form

- Nachschlagewerke
 - Hunnius, Pschyrembel, Hagers Handbuch, ...
 - Rote Liste, Fachinformation, ...
- Lehrbücher
 - Roth Eger Troschütz, Steinhilber et al., Mutschler, Gilman & Goodman, ...

⇒ Nachteil: zeitliche Verzögerung (5 – 10 Jahre)

Weg der Literaturrecherche



Datenbankrecherche I (PubMed o.ä.)

- Datenbankfelder: TI, AU, JN, MH, ...
- Schlagwort Vokabular: kontrolliert (MeSH) vs. unkontrolliert
 - Kontrolliertes Vokabular berücksichtigt:
Schreibweise, Wortendungen, Abkürzungen,
Synonyma
- Logische Operatoren (AND, OR, NOT, ggf. NEAR)
- Prioritäten „()“
(Ibuprofen OR Paracetamol) AND Kopfschmerzen
Ibuprofen OR (Paracetamol AND Kopfschmerzen)

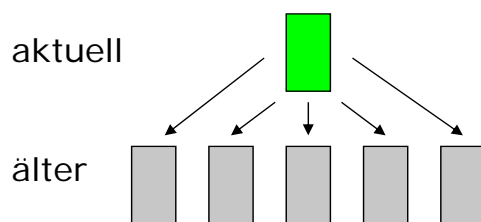
Datenbankrecherche II

- Phrasen: „Morbus Crohn“
- Eingrenzungen („Limits“) meist unter „Advanced Search“
- Expandieren von Suchen
 - Kontrolliertes Vokabular: eine Ebene höher
 - Platzhalter („*“, „?“): optimi*, optimi?ed
 - Achtung: Viele Arzneistoffe enden im Englischen auf „e“, z.B. „morphine“, „methylphenidate“, ...

Unterschiedliche Suchrichtung

„Rückwärtssuche“

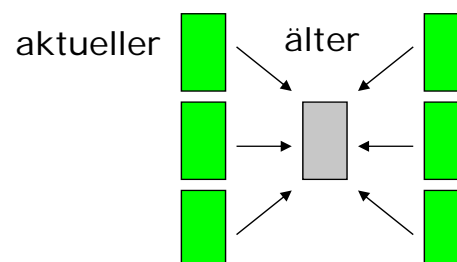
(Zitate in Aufsatz)



Grün zitiert Grau

„Vorwärtssuche“

(Scopus, Science Citation Index)



Grau wird von Grün zitiert

Bewerten speziell wissenschaftlicher Web-Sites

- Auffinden von „Web-Sites“
 - Suchmaschinen
- Bewerten einer Web-Site: Im Internet kann jeder alles schreiben! Bewertung ist somit zwingend nötig!
 - Wer bietet die Information an?
 - Wer ist für den Inhalt verantwortlich?
 - Wer finanziert das Angebot?
 - Letztes Update?
 - Inhaltliche Prüfung der Information?

Recherche zur Arzneibuchmonographie I

Unterpunkte des Kommentars

Allgemeine Hinweise

- Andere Arzneibücher (→ BP, USP, JAP, ...)
- Ähnliche Substanzen (z.B. Lehrbücher der Pharmakologie)
- CAS-Nr. (→ SciFinder)
- Darstellung (→ SciFinder: Kategorie „Preparation“, Drugs of the Future)
- Stereochemie (→ bestimmen)
- Stabilität/Lagerung (→ SciFinder: Suchbegriff „Degradation“)
- Synonyme (→ Pharmazeutische Stoffliste, PubChem)

Recherche zur Arzneibuchmonographie II

Eigenschaften

- Aussehen
- pK_a -Wert (→ SciFinder [berechnet])
- UV, IR, $^1\text{H-NMR}$, $^{13}\text{C-NMR}$, MS (→ SciFinder; Patente)
- Löslichkeit (→ SciFinder [berechnet])

Prüfung auf Identität

- Smt, IR, UV (s. Spektren)
- Farbreaktionen (→ Roth, Eger, Troschütz)
- DC (→ Apothekengerechte Prüfvorschriften, DAC, Monographien ähnl. Substanzen)

Recherche zur Arzneibuchmonographie III

Prüfung auf Reinheit

- Optische Drehung; nachrangig: Aussehen der Lösung, pH-Wert, ...
- Verwandte Substanzen
 - Auswahl verwandter Substanzen: Synthesezwischenprodukte, Abbauprodukte
 - Suche: → SciFinder Kategorie: „Analytical Study“ hier HPLC Methoden suchen für Ausgangssubstanz und ggf. für verwandte Substanzen
- Schwermetalle (allg.; speziell wenn Metall-Katalysatoren)
- Trocknungsverlust (nachrangig)

Recherche zur Arzneibuchmonographie IV

Gehaltsbestimmung

- Auf Basis von pK_a , UV-Spektrum, HPLC-Methode

Pharmakologische Eigenschaften

- Pharmakodynamik
 - Pharmakokinetik
 - Indikation
 - Dosierung
 - Intoxikation
 - Unerwünschte Wirkungen
 - Kontraindikation
 - ...
- Lehrbücher der Pharmakologie
 - Fachinformation
 - Rote Liste

Arzneibuchmonographie

Gegeben: Indikation

Gesucht: Arzneibuchmonographie plus Kommentar zu einem Arzneistoff mit der gegebenen Indikation

Nebenbedingungen:

- Der Arzneistoff darf noch nicht in Ph. Eur., USP, BP, JP, etc. monographiert sein (vgl. PM P820 (1)-(5)) für USP)

Taktisches:

- Der Arzneistoff sollte nicht zu jung sein!

Überblick verschaffen

- Pharmazeutische Zeitung ⇒ Arzneistoffe (alphabet., Jg.)
- DrugBank
- Google Scholar
- Schlüsselworte: HPLC, „stability indicating“, forced geradation“
- PubChem
- Wikipedia



<http://www.pharmazeutische-zeitung.de/index.php?id=46915&clid=29641>

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Start → Service → Arzneistoffe → Wirkstoff → Prasugrel|Efient™|79|2009

NEUE ARZNEISTOFFE

79 Thrombozytenaggregationshemmer

Prasugrel, Efient™ (Lilly Deutschland GmbH)

Mit Prasugrel kam im April 2009 ein weiterer Thrombozytenaggregationshemmer auf den Markt. Wie Clopidogrel ist der neue Arzneistoff zugelassen in Kombination mit Acetylsalicylsäure (ASS) zur Vorbeugung atherothrombotischer Ereignisse bei Erwachsenen mit einem akuten Koronarsyndrom, die sich einer perkutanen Koronarintervention unterziehen.

Die empfohlene Anfangsdosis beträgt 60 mg Prasugrel (Aufsättigungsdosis). Anschließend wird eine Erhaltungsdosis von einmal täglich 10 mg fortgesetzt. Die Filmtabletten können unabhängig von den Mahlzeiten eingenommen werden. Allerdings wird bei der Aufsättigungsdosis der schnellste Wirkeintritt erzielt, wenn die Filmtabletten nüchtern genommen werden. Empfohlen wird eine Behandlungsdauer von einem Jahr. Patienten, die Prasugrel einnehmen, müssen zudem täglich 75 bis 325 mg ASS einnehmen.

Prasugrel ist wie Clopidogrel ein Prodrug. Nach peroraler Applikation ist die Ausgangssubstanz im Plasma nicht nachweisbar. Sie wird schnell im Darm zu einem Thienolacton hydrolysiert

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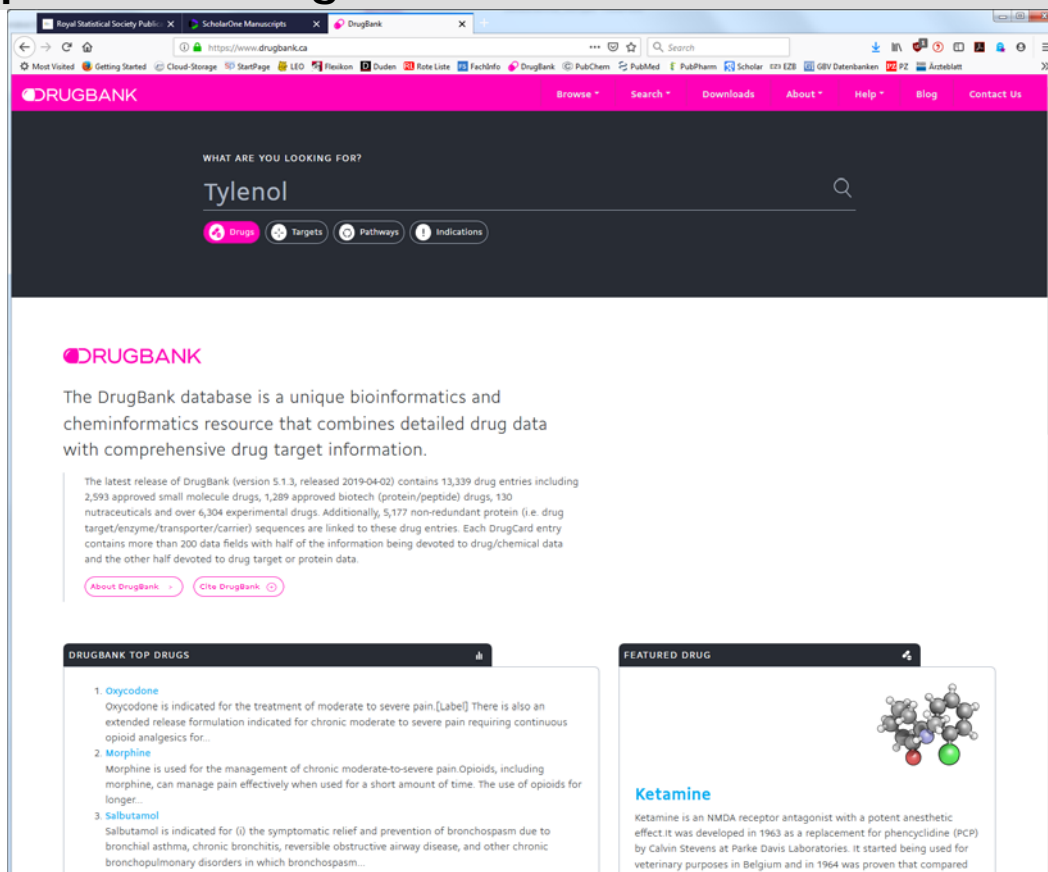
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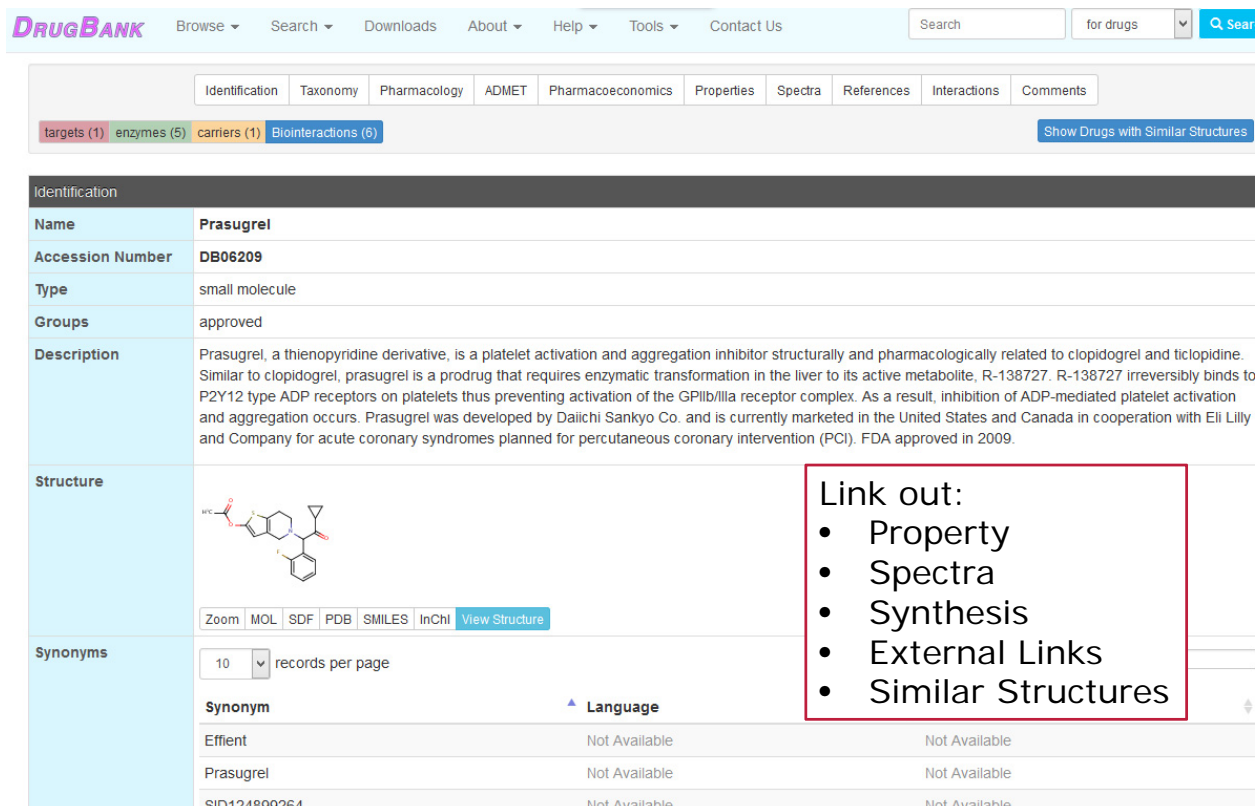
→ BfArM-Generikalist:
Schwierige Situation für Apotheker
Die Verwirrung ist groß:
Nachdem das...

<http://www.drugbank.ca/>



The screenshot shows the DrugBank homepage. At the top, there's a navigation bar with links like 'Browse', 'Search', 'Downloads', 'About', 'Help', 'Blog', and 'Contact Us'. Below this is a search bar with the text 'WHAT ARE YOU LOOKING FOR?' and a search icon. The main content area features a large heading 'Tylenol' and a description of the DrugBank database. It states that the database is a unique bioinformatics and cheminformatics resource that combines detailed drug data with comprehensive drug target information. A paragraph below this mentions the latest release of DrugBank (version 5.1.3, released 2019-04-02) contains 13,339 drug entries including 2,593 approved small molecule drugs, 1,289 approved biotech (protein/peptide) drugs, 130 nutraceuticals and over 6,304 experimental drugs. Additionally, 5,177 non-redundant protein (i.e. drug target/enzyme/transporter/carrier) sequences are linked to these drug entries. Each DrugCard entry contains more than 200 data fields with half of the information being devoted to drug/chemical data and the other half devoted to drug target or protein data. Below this, there are two sections: 'DRUGBANK TOP DRUGS' and 'FEATURED DRUG'. The 'TOP DRUGS' section lists three drugs: Oxycodone, Morphine, and Salbutamol. The 'FEATURED DRUG' section features Ketamine, which is described as an NMDA receptor antagonist with a potent anesthetic effect. It was developed in 1963 as a replacement for phencyclidine (PCP) by Calvin Stevens at Parke Davis Laboratories. It started being used for veterinary purposes in Belgium and in 1964 was proven that compared.

<http://www.drugbank.ca/drugs/DB06209>



The screenshot shows the DrugBank drug page for Prasugrel (DB06209). The page has a navigation bar with links like 'Browse', 'Search', 'Downloads', 'About', 'Help', 'Tools', and 'Contact Us'. Below this is a search bar with the text 'Search' and a search icon. The main content area features a large heading 'Prasugrel' and a description of the drug. It states that Prasugrel is a thienopyridine derivative, is a platelet activation and aggregation inhibitor structurally and pharmacologically related to clopidogrel and ticlopidine. Similar to clopidogrel, prasugrel is a prodrug that requires enzymatic transformation in the liver to its active metabolite, R-138727. R-138727 irreversibly binds to P2Y12 type ADP receptors on platelets thus preventing activation of the GPIIb/IIIa receptor complex. As a result, inhibition of ADP-mediated platelet activation and aggregation occurs. Prasugrel was developed by Daiichi Sankyo Co. and is currently marketed in the United States and Canada in cooperation with Eli Lilly and Company for acute coronary syndromes planned for percutaneous coronary intervention (PCI). FDA approved in 2009. Below this, there is a section for 'Structure' which shows the chemical structure of Prasugrel. To the right of the structure, there is a box with the text 'Link out:' and a list of links: 'Property', 'Spectra', 'Synthesis', 'External Links', and 'Similar Structures'. Below the structure, there is a section for 'Synonyms' which shows a table of synonyms and their corresponding language.

Synonym	Language
Effient	Not Available
Prasugrel	Not Available
SID124899264	Not Available

https://pubchem.ncbi.nlm.nih.gov/

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BioAssay Compound Substance

Go Advanced Search

Try the new PubChem Search

A revamped PubChem Compound Summary page is now released. [Read more...](#)

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BioActivity DataDicer
Structure Search
3D Conformer Tools
Structure Clustering
Classification
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https://www.ncbi.nlm.nih.gov/pccompound?term=%22prasugrel%22

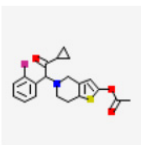
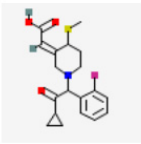
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1.  [Prasugrel; 150322-43-3; Efient ...](#)
MW: 373.441103 g/mol MF: C₂₀H₂₀FN₃S
IUPAC name: [5-[2-cyclopropyl-1-(2-fluorophenyl)-2-oxoethyl]-6,7-dihydro...
CID: 6918456
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component](#)
[Compounds](#) [PubMed \(MeSH Keyword\)](#) [Tested in 40 BioAssays](#)
2.  [Prasugrel hydrochloride; 389574-19-0; Prasugren hydrochloride ...](#)
MW: 409.902043 g/mol MF: C₂₀H₂₁ClFNO₃S
IUPAC name: [5-[2-cyclopropyl-1-(2-fluorophenyl)-2-oxoethyl]-6,7-dihydro...
CID: 10158453
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component](#)
[Compounds](#) [PubMed \(MeSH Keyword\)](#) [Active in 2 of 94 BioAssays](#)
3.  [Prasugrel Metabolite M5; SureCN5752091; R-106583 \(Prasugrel Metabolite\) ...](#)
MW: 363.446283 g/mol MF: C₁₉H₂₂FN₃O₃S
IUPAC name: (2Z)-2-[1-[2-cyclopropyl-1-(2-fluorophenyl)-2-oxoethyl]-4-me...
CID: 69553995
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#)

Actions on your results

-  **BioActivity Analysis**
Analyze the BioActivities of the compounds
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Cluster structures based on structural similarity
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Chemical Properties

Rule of 5 (6)

BioActivity Experiments

BioAssays, Active (1)
BioAssays, Tested (2)

BioMedical Annotation

Pharmacological Actions (3)
☒ Purinergic P2Y Receptor

Freiname	Prasugrel
Andere Namen	<ul style="list-style-type: none"> • IUPAC: (RS)-[5-[2-(Cyclopropyl-1-(2-fluorophenyl)-2-oxoethyl)-6,7-dihydro-4H- thieno[3,2-c]pyridin-2-yl]acetat
Summenformel	$C_{20}H_{20}FNO_3S$
CAS-Nummer	<ul style="list-style-type: none"> • 150322-43-3 (Prasugrel) • 389574-19-0 (Prasugrel Hydrochlorid)

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
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




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



















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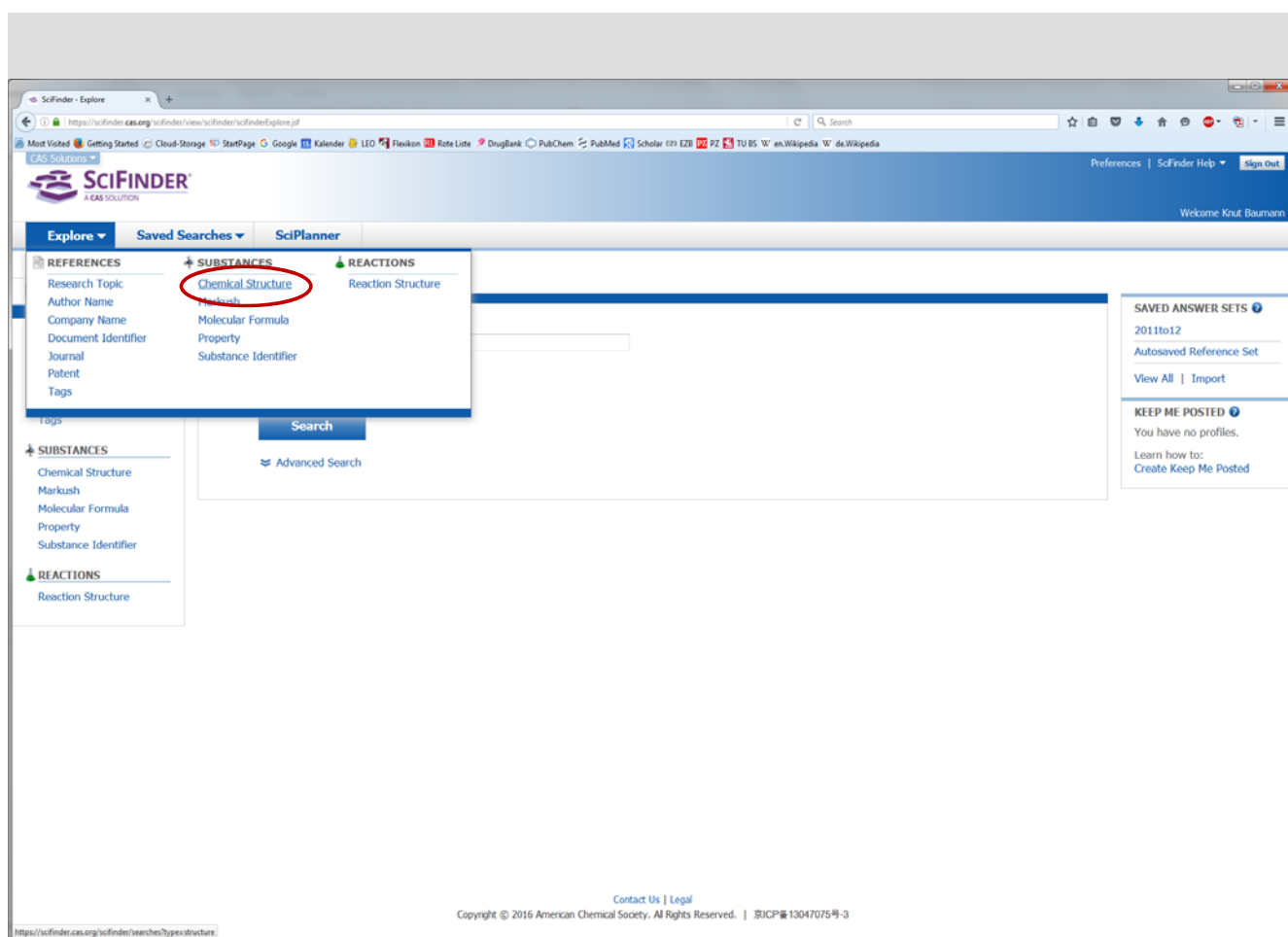
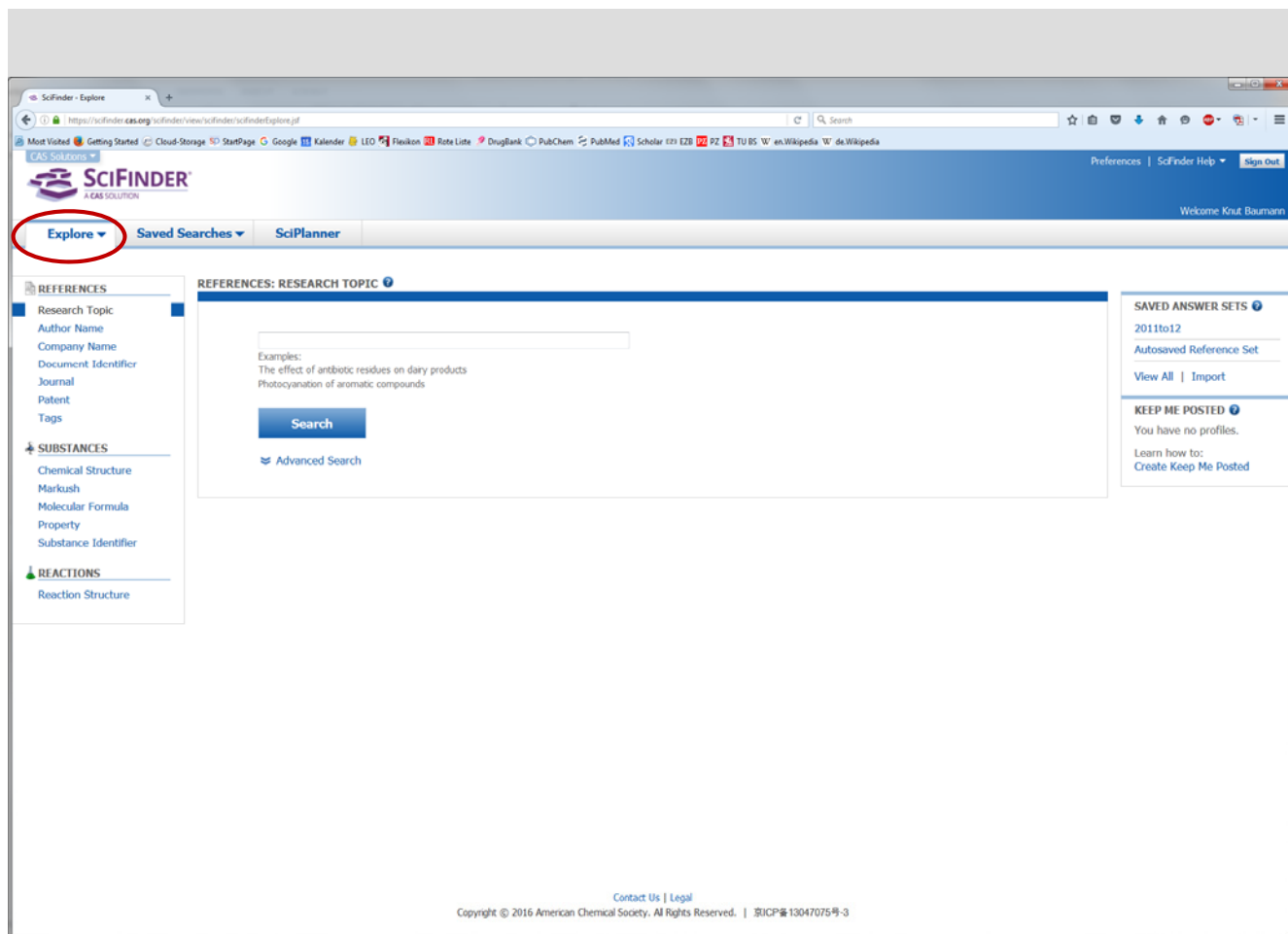
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logD 2.72 pH 9 Temp: 25 °C (2)

logP 2.718±0.904 Temp: 25 °C (2)

Mass Intrinsic Solubility Sparingly Soluble (6.3E-3 g/L) Temp: 25 °C (2)

Mass Solubility Slightly Soluble (2.1 g/L) pH 1 Temp: 25 °C (2)

Mass Solubility Sparingly Soluble (0.27 g/L) pH 2 Temp: 25 °C (2)

Mass Solubility Sparingly Soluble (0.034 g/L) pH 3 Temp: 25 °C (2)

Mass Solubility Sparingly Soluble (9.0E-3 g/L) pH 4 Temp: 25 °C (2)

Mass Solubility Sparingly Soluble (6.3E-3 g/L) pH 5 Temp: 25 °C (2)

Mass Solubility Sparingly Soluble (6.3E-3 g/L) pH 6 Temp: 25 °C (2)

Mass Solubility Sparingly Soluble (6.3E-3 g/L) pH 7 Temp: 25 °C (2)

Mass Solubility Sparingly Soluble (6.3E-3 g/L) pH 8 Temp: 25 °C (2)

Mass Solubility Sparingly Soluble (6.3E-3 g/L) pH 9 Temp: 25 °C (2)

Mass Solubility Sparingly Soluble (6.3E-3 g/L) pH 10 Temp: 25 °C (2)

Mass Solubility Sparingly Soluble (6.3E-3 g/L) Unbuffered Water pH 7.02 Temp: 25 °C (2)

Molar Intrinsic Solubility Sparingly Soluble (1.7E-5 mol/L) Temp: 25 °C (2)

Molar Solubility Sparingly Soluble (5.5E-3 mol/L) pH 1 Temp: 25 °C (2)

Molar Solubility Sparingly Soluble (7.3E-4 mol/L) pH 2 Temp: 25 °C (2)

Molar Solubility Sparingly Soluble (9.0E-5 mol/L) pH 3 Temp: 25 °C (2)

Molar Solubility Sparingly Soluble (2.4E-5 mol/L) pH 4 Temp: 25 °C (2)

Molar Solubility Sparingly Soluble (1.7E-5 mol/L) pH 5 Temp: 25 °C (2)

Molar Solubility Sparingly Soluble (1.7E-5 mol/L) pH 6 Temp: 25 °C (2)

Molar Solubility Sparingly Soluble (1.7E-5 mol/L) pH 7 Temp: 25 °C (2)

Molar Solubility Sparingly Soluble (1.7E-5 mol/L) pH 8 Temp: 25 °C (2)

Molar Solubility Sparingly Soluble (1.7E-5 mol/L) pH 9 Temp: 25 °C (2)

Molar Solubility Sparingly Soluble (1.7E-5 mol/L) pH 10 Temp: 25 °C (2)

Molar Solubility Sparingly Soluble (1.7E-5 mol/L) Unbuffered Water pH 7.02 Temp: 25 °C (2)

Molecular Weight 373.44 (2)

pKa 3.65±0.20 Most Basic Temp: 25 °C (2)

Vapor Pressure 7.01E-10 Torr Temp: 25 °C (2)

Notes

(2) Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2016 ACD/Labs)

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PREDICTED PROPERTIES

Biological Chemical Density Lipinski Structure Related Thermal

Lipinski Properties

Property	Value	Condition	Note
Freely Rotatable Bonds	6		(2)
H Acceptors	4		(2)
H Donors	0		(2)
H Donor/Acceptor Sum	4		(2)
logP	2.718±0.904	Temp: 25 °C	(2)
Molecular Weight	373.44		(2)

Notes

(2) Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2016 ACD/Labs)

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Occurrence		✓		
Preparation	✓	✓	✓	
Process	✓	✓		
Properties	✓	✓	✓	
Prophetic in Patents	✓			
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REFERENCES

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1. Analysis of prasugrel active metabolite R-138727 in human plasma: a sensitive, highly selective and fast LC-MS/MS method

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By Kakarla, Srekanth; Datta, Peda Varma; Kodali, Geetha; Senu, Ganapathy

From Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2016), 1020, 103-110. | Language: English, Database: CAPLUS

A cost effective, sensitive, simple, and rapid high-performance liq. chromatog.-tandem mass spectrometry method was developed and validated for the quantification of the prasugrel metabolite in human plasma. Following solid phase extrn., the analyte (prasugrel active metabolite; R-138727) and internal std. (emtricitabine) were sepd. using a mobile phase in an isocratic elution mode on a reverse phase C₁₈ column and were analyzed by an LC-MS/MS in the multiple reaction monitoring mode using the resp. [M + H]⁺ ions, m/z 498.3-206.0 for R-138727 and m/z 248.2-130.1 for the internal std. The assa...

2. Rapid Screening for Exposure to "Non-Target" Pharmaceuticals from Wastewater Effluents by Combining HRMS-Based Suspect Screening and Exposure Modeling

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By Singer, Heinz P.; Wossner, Annika E.; McArdell, Christa S.; Fenner, Kathrin

From Environmental Science & Technology (2016), Ahead of Print. | Language: English, Database: CAPLUS

Active pharmaceutical ingredients (APIs) have raised considerable concern over the past decade due to their widespread detection in water resources and their potential to affect ecosystem health. This triggered many attempts to prioritize the large no. of known APIs to target monitoring efforts and testing of fate and effects. However, so far, a comprehensive approach to screen for their presence in surface waters has been missing. We explore a combination of an automated suspect screening approach based on liq. chromatog. coupled to high-resoln. mass spectrometry and a model-based priori...

3. Chiral stationary phases and their relationship with enantiomer structures in enantioseparation research of analytical laboratory

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By He, Zhi-Jian; Song, Hong; Zhang, Yi-wen; Wang, Dao-cai; Yao, Shun

From Journal of the Mexican Chemical Society (2015), 59(1), 43-49. | Language: English, Database: CAPLUS

Chiral stationary phases (CSPs) and mol. structure of enantiomers are two independent but related aspects in enantiosepn., which are discussed on the basis of the exptl. data from the previous study. Two enantiosepn. expts. are performed to illustrate the relationship between enantiomer structures and chiral stationary phases, one is the resoln. of mandelic acid derivs. and the other is about prasugrel. Thermodyn. mechanism and theor. study with computational chem. method is helpful to understand the interactions of enantiomer and CSPs.

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Aim of the present work is to develop a rapid, simple, precise, accurate and reproducible reverse phase high performance liq. chromatog. method for simultaneous detn. of Aspirin and Prasugrel in tablet dosage form. The estn. was carried out on a HIBAR (Lichrospher C-18) column with the dimensions of 250mm × 4.6mm, 5µm. Combination of Acetonitrile and 0.5% Potassium dihydrogen phosphate buffer (adjusted to pH-3 using orthophosphoric acid) in the ratio of 60:40 was used as mobile phase. The flow rate is set at 1.0ml/min and eluents were monitored at 220 nm. Both drugs were properly resolved ...

7. Analysis of prasugrel by chromatography - review
 Quick View Other Sources
 By Housheh, Samer; Treffi, Saleh; Haroun, Mohammad; Chehna, M. Fawaz
 From International Journal of Pharmaceutical Sciences Review and Research (2014), 28(2), 180-186, 7 pp.. | Language: English, Database: CAPLUS
 A review. Prasugrel, being a potent platelet aggregation inhibitor, is used widely around the world to reduce cardiovascular risks in patients with stroke, myocardial infarction, and atherosclerosis. The aim of this review firstly to focus on a comprehensive update of chromatog. detn. of Prasugrel and its metabolites in human plasma, and in pharmaceutical preps. It has been described using TLC, HPLC/MS, RP-HPLC, and UV methods. Secondly to localize the chromatog. conditions for sepn. and quantification. This review provides detailed information on sepn. conditions for Prasugrel alone, wi...

8. Development and validation of stability indicating reverse-phase HPLC method for the determination of prasugrel hydrochloride and its related substances
 Quick View Other Sources
 By Reddy, K. Chandra Sekhar; Kothapalli, S. R. Pavani Kumar; Vundavilli, Jagadeesh Kumar; Sreenivas, N.; Sharma, Hemant Kumar; Mukkanti, K.
 From International Journal of Pharmaceutical Sciences and Research (2014), 5(3), 919-927, 9. | Language: English, Database: CAPLUS
 A gradient reverse-phase high performance liq. chromatog. (RP-HPLC) method has been developed and validated for the detn. of Prasugrel hydrochloride and its related substances. The well chromatog. sepn. of prasugrel from its seven related substances and degradn. products was achieved on Sunfire C18, 5µm (250mm × 4.6mm) column temp. maintained at 45°C with a mobile phase A: 0.1% vol./vol. orthophosphoric acid in water and mobile phase B: 0.1% vol./vol. orthophosphoric acid in acetonitrile. The flow rate was 1.0mL/min, and the detection wavelength was 220nm. The developed method was validated ...

9. Development and validation of a reverse-phase liquid chromatographic method for related substances of Prasugrel for 5 and 10 mg tablets
 Quick View Other Sources
 By Naresh Chandra Reddy, M.; Chandra Sekhar, K. B.; Kavitha, A.; Sasikiran Goud, E.
 From International Journal of Pharmacy and Pharmaceutical Sciences (2014), 6(1), 90-94, 5 pp.. | Language: English, Database: CAPLUS
 Objective: The main objective of current study was to develop and validate RP-HPLC, simple, precise, accurate and specific chromatog. method for the detn. of related substances of Prasugrel in pharmaceutical formulations. Methods: A high performance liq. chromatograph instrument and inert sustain C18, 75 × 4.6 mm, 3 µm were used for detn. of Prasugrel and its related substances. Buffer was prepd. by using 1.36 g of potassium phosphate monobasic in 1000 mL of water, adjust the pH of this soln. to 3.30 with dil. orthophosphoric acid soln. and mix well. Filter through 0.45 µm nylon filter and ...

10. Simultaneous determination of Prasugrel and Aspirin by second order and ratio first order derivative ultraviolet spectrophotometry
 Quick View Other Sources
 By Alvi, Shahabuddin N.; Patel, Mohul N.; Kathirya, Prakash B.; Patel, Bhavna A.; Parmar, Shraddha J.
 From Journal of Spectroscopy (New York, NY, United States) (2013), 705363/1-705363/8, 8 pp.. | Language: English, Database: CAPLUS
 Two simple, accurate, and precise UV deriv. spectrophotometric methods for the simultaneous detn. of Prasugrel and Aspirin in synthetic mixt. form were developed. The 1st method involves measurement of 2nd order deriv. spectra of Prasugrel and Aspirin. The zero crossing wavelengths 267.62 nm and 252.40 nm were selected for estn. of Prasugrel and Aspirin, resp. In the 2nd method, the 1st order derivs. of ratio spectra were calcd. and used for the detn. of Prasugrel and Aspirin by measuring the peak intensity at 268 nm and 290 nm, resp. The methods were validated as per the ICH guideline Q2 ...

11. Comparison of different sorbent materials for solid-phase extraction of selected drugs in human urine analyzed by UHPLC-UV
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 By Magiera, Sylwia; Hejnalak, Judyta; Baranowski, Jacek
 From Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2014), 958, 22-28. | Language: English, Database: CAPLUS

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A simple, rapid, cost-effective, sensitive, precise, and specific reversed phase high performance liq. chromatog. method was developed and validated for the detn. of prasugrel and aspirin in bulk and tablet dosage form. It was found that the excipient in the tablet dosage form does not interfere in the quantification of active drug by proposed method. The HPLC sepn. was carried out by reverse phase chromatog. on phenomenex C8 column(250 × 4.6 mm, 5 µ) with a mobile phase composed methanol: water 80:20 vol./vol. in isocratic mode of sepn. at flow rate 1mL/min. The detection was monitored at ...

16. Development and validation of RP-HPLC method for the estimation of Prasugrel in bulk as well in pharmaceutical dosages form
 Quick View Other Sources
 By Ashutosh Kumar, S.; Sridhargiri Rao, J. V. L. N.; Jharasi Reddy, K.; Jaya Pradipati, S. S.; Prasad, L. S. R. K. V.
 From International Research Journal of Pharmacy (2013), 4(3), 254-260. | Language: English, Database: CAPLUS
 This study was designed to develop and validate a simple, sensitive, precise, and specific reverse phase high-performance liq. chromatog. (HPLC) method for the detn. of Prasugrel in bulk and its tablet dosage forms. The HPLC sepn. was carried out by reverse phase chromatog. on XTerra column C18 (4.6 × 150 mm, 5 µm) with a mobile phase composed Potassium Dihydrogen phosphate and the pH was adjusted to 3.0 by Orthophosphoric Acid & Acetonitrile in the ratio of 40:60 vol./vol. in isocratic mode at a flow rate of 1.0 mL/min. The run time was maintained 5min. The detection was monitored at 210 n...

17. Identification, synthesis and characterization of related substances of Prasugrel
 Quick View Other Sources
 By Samprathi, A.; Reddy, V. Prabhakar; Govindhan, G.; Nagaraju, G.; Reddy, P. Pratap
 From Journal of Pharmaceutical Research and Opinion (2012), 2(9), 102-106. | Language: English, Database: CAPLUS
 During the process development of Prasugrel, six related substances (impurities) ranging from 0.05 to 0.15 % were detected by a gradient high performance liq. chromatog. (HPLC) method. Liq. chromatog.-mass spectrometry (LC-MS) was performed to identify the mol. mass of these impurities. A detailed study was undertaken to characterize all the impurities. These impurities were synthesized and co-injected with sample contg. the impurities and found the retention time match of the spiked impurities. Based on the spectral data (IR, NMR and MS), these impurities were characterized as 5-[2-cyclop...

18. Development and validation of analytical method for estimation of prasugrel Hydrochloride in bulk and in pharmaceutical formulations
 Quick View Other Sources
 By Modi, Viralkumar J.; Pingale, Prashant L.
 From International Journal of Pharma and Bio Sciences (2012), 3(4), 292-298. | Language: English, Database: CAPLUS
 A new, simple, specific, accurate, precise and rapid reverse phase high performance liq. chromatog. method was developed and validated for the detn. of prasugrel Hydrochloride in pure and tablet dosage forms. The HPLC sepn. was carried out by reverse phase chromatog. on Kromasil C18 (100 × 4.6 mm; 5µm) with a mobile phase consist of methanol buffer (600 mg potassium dihydrogen phosphate in 500 mL water, pH-2.1 adjusted with ortho phosphoric acid) in the ratio of 70:30 vol./vol. delivered in isocratic mode at a flow rate of 0.8 mL/min. The prasugrel Hydrochloride was quantified at 220 nm. Th...

19. RP-HPLC method for simultaneous estimation of Aspirin and Prasugrel in binary combination
 Quick View Other Sources
 By Jain, Deepak Kumar; Jain, Nilesh; Verma, Jitendra
 From International Journal of Pharmaceutical Sciences and Drug Research (2012), 4(3), 218-221. | Language: English, Database: CAPLUS
 A simple, reliable, rapid, precise, sensitive, and validated RP-HPLC method was developed to det. aspirin and prasugrel in synthetic mixt. form. Chromatog. sepn. achieved isocratically on Luna C₁₈ column (5µm, 150mm × 4.60mm) and acetonitrile:0.05M ammonium acetate buffer (pH 4.5) in the ratio of 75:25 (vol./vol.) as the mobile phase at a flow rate of 0.6 mL/min. Detection was carried out at 245 nm. Parameters such as linearity, precision, accuracy, recovery, specificity and ruggedness are studied as reported in the ICH guidelines. The retention times for Aspirin and Prasugrel was found T...

20. Development and validation of RP-HPLC method for prasugrel
 Quick View Other Sources
 By Parmar, S. J.; Patel, B. A.; Jain, A. P.
 From Journal of Chemical and Pharmaceutical Research (2012), 4(7), 3373-3376. | Language: English, Database: CAPLUS
 A reverse-phase liq. chromatog. (RP-LC) method was developed for the assay of prasugrel in bulk. The Chromatog. was performed on Kromasil C18 column. The eluted

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16. Development and validation of RP-HPLC method for the estimation of Prasugrel in bulk as well in pharmaceutical dosages form

By: Ashutosh Kumar, S.; Seshagiri Rao, J. V. L. N.; Jhansi Rani, K.; Jaya Madhuri, S. S. S.; Prasad, T. S. R. K. V.

This study was designed to develop and validate a simple, sensitive, precise, and specific reverse phase high-performance liq. chromatog. (HPLC) method for the detn. of Prasugrel in bulk and its tablet dosage forms. The HPLC sepn. was carried out by reverse phase chromatog. on XTerra column C18 (4.6 × 150 mm, 5 μm) with a mobile phase composed Potassium Dihydrogen phosphate and the pH was adjusted to 3.0 by Orthophosphoric Acid & Acetonitrile in the ratio of 40:60 vol./vol. in isocratic mode at a flow rate of 1.0 mL/min. The run time was maintained 5min. The detection was monitored at 210 nm. The Accuracy was calcd. and the % Recovery was found 99.0%-101.8% and reproducibility was found to be satisfactory. The calibration curve for prasugrel was linear from 20 to 60 μg/mL. The inter-day and intra-day precision was found to be within limits. The proposed method has adequate sensitivity, reproducibility, and specificity for the detn. of prasugrel in bulk and its tablet dosage forms. The limit of detection and limit of quantification for prasugrel were found to be 0.07 μg/mL and 0.2 μg/mL resp. The present work was undertaken with the aim to develop and validate a rapid and consistent RP-HPLC in which the peaks will be appear with a short period of time as per ICH guideline. The proposed method is simple, fast, accurate, and precise for the quantification of prasugrel in the dosage form, bulk drugs as well as for routine anal. in quality control.

Indexing

Pharmaceutical Analysis (Section64-3)

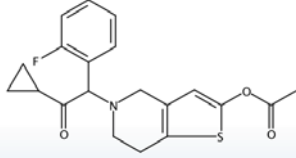
Concepts

Reversed-phase HPLC

development and validation of RP-HPLC method for detn. of prasugrel in bulk and pharmaceutical dosage form

Substances

150322-43-3 Prasugrel



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This study was designed to develop and validate a simple, sensitive, precise, and specific reverse phase high-performance liquid chromatographic (HPLC) method for the determination of Prasugrel in bulk and its tablet dosage forms. The HPLC separation was carried out by reverse phase chromatography on XTerra column C18 (4.6 x 150mm, 5 µm) with a mobile phase composed Potassium Dihydrogen phosphate and the pH has been adjusted to 3.0 by Orthophosphoric Acid & Acetonitrile in the ratio of 40:60 v/v in isocratic mode at a flow rate of 1.0 ml/min. The run time has been maintained 5mins. The detection was monitored at 210 nm. The Accuracy was calculated and the % Recovery was found 99.0%-101.8% and reproducibility was found to be satisfactory. The calibration curve for Prasugrel was linear from 20 to 600 µg/ml. The inter-day and intra-day precision was found to be within limits. The proposed method has adequate sensitivity, reproducibility, and specificity for the determination of Prasugrel in bulk and its tablet dosage forms. The limit of detection and limit of quantification for Prasugrel were found to be 0.07 µg/ml and 0.2 µg/ml respectively. The present work was undertaken with the aim to develop and validate a rapid and consistent RP-HPLC in which the peaks will be appear with a short period of time as per ICH guideline. The proposed



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22. Comparative Study of Forced Degradation Behavior of Prasugrel by UPLC and HPLC and the Development of Validated Stability Indicating Assay Method

By: Sahu, Kapendra; Karthikeyan, C.; Moorthy, N. S. Hari Narayana; Trivedi, Piyush

A novel stability-indicating ultra-performance liq. chromatog. (UPLC) assay method was developed and validated for prasugrel and its degradn. products. The UPLC sepn. was performed on Acquity UPLC BEH C₁₈ column (1.7 µm, 2.1 mm × 150 mm) using isocratic mode (acetonitrile:water, 80:20 vol./vol.) at flow rate of 0.1 mL/min and the high performance liq. chromatog. (HPLC) sepn. was achieved on Phenomenex C8 column using isocratic mode (acetonitrile:10 mM ammonium acetate, 85:15 vol./vol.) at flow rate of 0.9 mL/min. Prasugrel was found to degrade significantly in hydrolytic (acid, alkali, and neutral), and oxidative stress conditions and was stable in thermal and photolytic stress conditions. The RSD (%) values calcd. for the AUC of UPLC and HPLC are 0.0039 and 0.0015, resp. The UPLC and HPLC linearity of the proposed method were investigated in the range of 10-60 µg/mL. The r² value of UPLC and HPLC were found to be 0.9980 and 0.9983, resp. Method detection limit (MDL) and method quantification limit (MQL) were found to be 0.20 µg/mL and 1.00 µg/mL for UPLC and 0.50 µg/mL and 1.80 µg/mL for HPLC, resp. The RSD (%) values for intra-day and inter-day precision were <1.0%, confirming that the method is sufficiently precise. The validation studies were carried out fulfilling ICH requirements.

Indexing

Pharmaceutical Analysis (Section64-3)

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Reversed-phase HPLC

RP-UPLC; stability indicating behavior detn. of prasugrel by UPLC and HPLC

Decomposition Decomposition kinetics
Ultra-performance liquid chromatography

stability indicating behavior detn. of prasugrel by UPLC and HPLC

Substances

150322-43-3 Prasugrel

The chemical structure of Prasugrel is shown as a 2D skeletal formula. It features a central piperidine ring substituted with a cyclopropylmethyl group, a 2-fluorophenyl group, and a 2-(acetoxymethyl)-5-thienyl group.

stability indicating behavior detn. of prasugrel by UPLC and HPLC

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Journal of Liquid Chromatography & Related Technologies
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COMPARATIVE STUDY OF FORCED DEGRADATION BEHAVIOR OF PRASUGREL BY UPLC AND HPLC AND THE DEVELOPMENT OF VALIDATED STABILITY INDICATING ASSAY METHOD

DOI: 10.1080/10826076.2011.582209

Kapendra Sahu^a, C. Karthikeyan^a, N. S. Hari Narayana Moorthy^a & Piyush Trivedi^{a*}

pages 1870-1884

Publishing models and article dates explained

Published online: 12 Oct 2011

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Abstract

A novel stability-indicating ultra-performance liquid chromatographic (UPLC) assay method was developed and validated for prasugrel and its degradation products. The UPLC separation was performed on Acquity® UPLC BEH C18 column (1.7 µm, 2.1 mm x 150 mm) using isocratic mode (acetonitrile/water, 80:20 v/v) at flow rate of

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DOI: 10.1080/10826076.2011.582209

Kapendra Sahu^a, C. Karthikeyan^a, N. S. Hari Narayana Moorthy^a & Piyush Trivedi^{a*}

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1. Process for the preparation of prasugrel intermediate

Quick View | PATENTPAK

By Gao, Heyong; Chen, Lin; Zhong, Qichang
From Faming Zhuanli Shengqing (2016), CN 105272993 A 20160127. | Language: Chinese, Database: CAPLUS

The invention relates to process for the prepn. of prasugrel intermediate 5-[2-cyclopropyl-1-(2-fluorophenyl)-2-oxoethyl]-5,6,7,7a-tetrahydrothieno[3,2-c]pyridin-2(4H)-one (I). For example, compd. I was prepd. by amination reaction of 2-fluorobenzyl bromide with 2-(2-aminoethyl)thiophene to afford N-[(2-fluorophenyl)methyl]-2-thiopheneethanamine, which underwent cyclocondensation reaction with paraformaldehyde, followed by bromination, reaction with magnesium to form Grignard reagent and addn. reaction with cyclopropylcarbonitrile and oxidn. to afford compd. I. Prasugrel was prepd. by acylat...

2. Synthesis and structure characterization of prasugrel

Quick View | Other Sources

By Wu, Shimei; Cui, Bocheng; Zhong, Shi; Li, Yiyang
From Guangdong Huagong (2015), 42(8), 108-110. | Language: Chinese, Database: CAPLUS

Through the stepwise synthesis method, tested by sepn. and purifn. of HPLC-MS and pertinent matter, the writer of the paper finds out the structure characterization of NMR. The key exptl. data goes as follows: Chromatog. column is C18(Eclipse XDB-C18 4.6*150, 5 μ), column temp. is normal temp., moving phase is acetonitrile-water(vol. ratio: 70:30), velocity of flow is 1.0m L·min⁻¹, the inspection wavelength is 254 nm, and the sample vol. is 5 μL. The final results reveals that the purity quotient of the target is 98.9% after purifn., and by anal. of HNMR, CNMR, C13DEPT90, C13PEPT135, COSY, H...

3. Preparation of prasugrel

Quick View | PATENTPAK

By Sampath, Aalia; Metil, Dattatray Shanrao; Reddy, Jinna Rajender
From Indian Pat. Appl. (2015), IN 2013CH03945 A 20150807. | Language: English, Database: CAPLUS

The application relates to process for the prepn. of prasugrel (I) and its pharmaceutically acceptable salts. Compd. I was prepd. by alkylation of 5,6,7,7a-tetrahydrothieno[3,2-c]pyridin-2(4H)-one with 2-bromo-1-cyclopropyl-2-(2-fluorophenyl)ethanone followed by acetylation.

4. One-pot process for preparing prasugrel

Quick View | PATENTPAK

By Bai, Wenqin; Song, Zhengming; Zhao, Guilang
From Faming Zhuanli Shengqing (2015), CN 104725396 A 20150624. | Language: Chinese, Database: CAPLUS

The invention is related to one-pot process for prepg. prasugrel. The title process comprises the steps of: conducting a reaction on 5,6,7,7a-tetrahydrothieno[3,2-c]pyridin-2(4H)-one with 2-bromo-1-cyclopropyl-2-(2-fluorophenyl)ethanone followed by acetylation.

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1. Preparation of prasugrel

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By Sampath, Aalia; Metil, Dattatray Shamrao; Reddy, Jinna Rajender

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2. Process for the preparation of prasugrel and pharmaceutically acceptable salts thereof

Quick View PATENTPAK

By Patkar, Laxmikant Narhari; Mondkar, Harish Kashinath; Deshpande, Manoj Madhukarrao; Vengurlekar, Rupesh Sudhir

From Indian Pat. Appl. (2015), IN 2013MU00805 A 20150130. | Language: English, Database: CAPLUS

The invention relates to a process for the prepn. of prasugrel (I) and its pharmaceutically acceptable salts. The process for prepn. I comprising purifn. of the starting material 2-fluorobenzyl alc., 2-fluorotoluene or 2-fluorobenzyl cyanide and obtaining them substantially free from impurities is claimed. Compd. I was prepd. by bromination of 2-fluorobenzyl alc., followed by cyanation; the resulting 2-fluorobenzyl cyanide underwent purifn., followed by hydrolysis and alkylation with Et cyclopropylcarboxylate to give cyclopropyl 2-fluorobenzyl ketone, which underwent halogenation to give 2-f...

3. Improved process for the preparation of prasugrel and intermediate thereof

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By Nyulasi, Balint; Kovacs, Edina; Szabo, Eva; Pakaine Varga, Gabriella; Porcs-Maklay, Marta; Volk, Balazs; Lukacs, Gyula; Varady, Karolyne; Ruzsics, Gyorgy

From Pct Int. Appl. (2014), WO 2014114964 A2 20140731. | Language: English, Database: CAPLUS

The invention relates to an industrial scale process for the prepn. of 1-cyclopropyl-2-(2-fluorophenyl)-ethanone (I) and the use of this compd. for the prepn. of prasugrel (II). This process comprises reacting 2-fluorobenzyl chloride with magnesium followed by adding cyclopropane-carboxylic acid-dimethyl amide to thus formed the Grignard reactant (whereby the reaction is carried out in a mixt. of toluene and THF, in which mixt. the amt. of THF is 3-20 vol. %, or in methyl-tetrahydrofuran as solvent) to provide I. II was prepd. by halogenation, preferably bromination or chlorination of I foll...

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1. Comparison of different sorbent materials for solid-phase extraction of selected drugs in human urine analyzed by UHPLC-UV

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By Magiera, Sylwia; Hejnalik, Judyta; Baranowski, Jacek

From Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2014), 958, 22-28. | Language: English, Database: CAPLUS

A procedure based on solid-phase extrn. (SPE) followed by ultra-high-performance liq. chromatog. (UHPLC) with UV detection has been developed for the anal. of multiple drugs in human urine. The compds. evaluated were aliskiren, prasugrel, rivaroxaban, prednisolone, propranolol, ketoprofen, nifedipine, naproxen, terbinafine, ibuprofen, diclofenac, sildenafil and acenocoumarol. Seventeen different solid phase extrn. (SPE) cartridges were tested to evaluate their applicability for the isolation of drugs from human urine. Comparison were recovery of different drugs and reproducibility. The sampl...

2. Identification and synthesis of impurities formed during prasugrel hydrochloride preparation

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By Sastry, T. Umasankara; Rao, K. Nageswara; Reddy, T. Appi; Gandhi, P.

From Asian Journal of Chemistry (2013), 25(14), 7783-7789. | Language: English, Database: CAPLUS

Synthesis and characterization of impurities formed during prepn. of prasugrel hydrochloride(I-HCl) are described. Prasugrel hydrochloride is an important platelet inhibitor used for the redn. of thrombotic cardiovascular events.

3. An improvement to the preparation of prasugrel hydrochloride

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By Ou, Wenhua; Yi, Welyin; Liu, Feng; Pan, Xianhua; Peng, Xijiang

From Journal of Chemical Research (2013), 37(6), 369-371. | Language: English, Database: CAPLUS

An efficient synthesis of prasugrel, a thienopyridine ADP-receptor antagonists, is described. A thienopyridine intermediate was prepd. by N-protection, boric acid substitution and N-substitution. After acid hydrolysis of the Me ether and subsequent acetylation, prasugrel was obtained with a total yield of 50% after seven linear steps from 4,5,6,7-tetrahydrothieno [3,2-c]pyridine and 2-bromo-1-cyclopropyl-2-(2-fluorophenyl)ethan-1-one as raw materials.

4. Identification, synthesis and characterization of related substances of Prasugrel

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By Sampath, A.; Reddy, V. Prabhakar; Goverdhan, G.; Nagaraju, G.; Reddy, P. Pratap

From Journal of Pharmaceutical Research and Opinion (2012), 2(9), 102-106. | Language: English, Database: CAPLUS

During the process development of Prasugrel, six related substances (impurities) ranging from 0.05 to 0.15 % were detected by a gradient high performance liq. chromatog. (HPLC) method. Liq. chromatog.-mass spectrometry (LC-MS) was performed to identify the mol. mass of these impurities. A detailed study was undertaken to characterize all the impurities. These impurities were synthesized and identified with appropriate reagents and found that the synthetic routes of the impurities...

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Review

Synthetic approaches to the 2009 new drugs

Kevin K.-C. Liu^{a,†}, Subas M. Sakya^{b,†}, Christopher J. O'Donnell^{b,†}, Andrew C. Flick^{b,§}, Jin Li^{c,§}

^a Pfizer Inc., La Jolla, CA 92037, USA
^b Pfizer Inc., Groton, CT 06340, USA
^c Shenogen Pharma Group, Beijing, China

Received 12 November 2010; revised 15 December 2010; Accepted 16 December 2010. Available online 24 December 2010.

Abstract
New drugs are introduced to the market every year and each individual drug represents a privileged structure for its biological target. These new chemical entities (NCEs) provide insights into molecular recognition and also serve as leads for designing future new drugs. This review covers the syntheses of 21 NCEs marketed in 2009.

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Synthesis of pralatrexate (XVI).

18. Prasugrel (Effient®)

Prasugrel is a platelet inhibitor developed by Daiichi Sankyo Co. and is marketed in the United States in cooperation with Eli Lilly and Company for acute coronary syndromes planned for percutaneous coronary intervention (PCI).⁷² Prasugrel was approved for use in Europe in February 2009, and is currently available in the UK. In the U.S. prasugrel is also approved for the reduction of thrombotic cardiovascular events, including stent thrombosis, in patients with acute coronary syndrome who are to be managed with PCI. Prasugrel is a member of the thienopyridine class of ADP receptor inhibitors, and irreversibly binds to P2Y₁₂ receptors. The synthesis of prasugrel begins with the preparation of the α-ketocyclopropane **102** which is prepared as summarized in Scheme 17.⁷³ Conversion of 1-(bromomethyl)-2-fluorobenzene (**99**) to the corresponding Grignard reagent through reaction with magnesium followed by condensation with nitrile **100** resulted in ketone **101** in 72% yield. Chlorination of ketone **101** with CuCl₂ resulted in the key prasugrel coupling component **102** in 92% yield. The piperidine coupling partner was prepared by treating thiolactone **103** with TBDMSCl and triethylamine to give thiophene **104** in 91% yield. Treatment of piperidine **104** with α-chloroketone **102** resulted in enol silane **105** in 65% yield. Reaction of silylenol ether **105** with acetic anhydride in the presence of triethylamine and catalytic DMAP resulted in the preparation of prasugrel (**XVII**) in 60% yield.

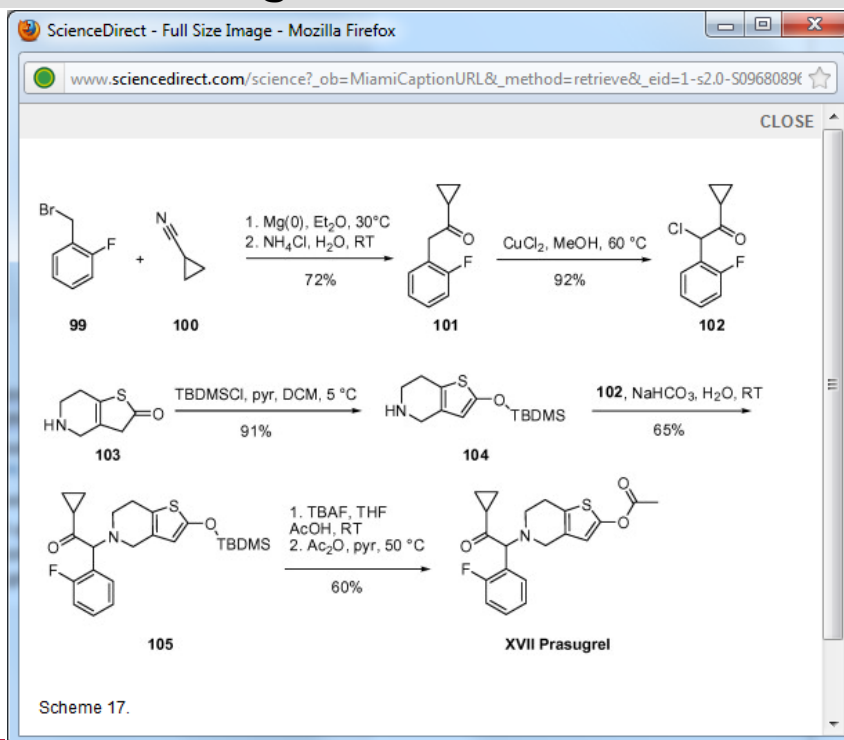
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Scheme 17.
Synthesis of prasugrel (XVII).

19. Saxagliptin (Onglyza®)

Saxagliptin, previously identified as BMS-477118, is an oral hypoglycemic of the dipeptidyl peptidase-4 (DPP-4) inhibitor class developed by Bristol-Myers Squibb for the treatment of type 2 diabetes.⁷⁴ DPP-IV is the primary enzyme responsible for degradation of incretins, such as glucagon-like peptide-1 (GLP-1), which is a hormone responsible for the glucose-dependent stimulation of insulin in humans.⁷⁵ Inhibitors of DPP-IV serve as effective glucose regulators by increasing the endogenous concentration of GLP-1. The initial discovery route to saxagliptin was a 15-step, convergent synthesis focused on the production and use of compounds **109** and **113** (Scheme 18a and Scheme 18b).^{(a), 76 and 77} While the strategy of early drug delivery involved rapid synthesis to support preclinical activities and Phase I clinical trials, as saxagliptin entered Phase II, a greater emphasis was placed on defining and demonstrating a commercially viable synthetic process. Scheme 18a describes a more expedient route to the preparation of adamantylamino acid

Synthese von Prasugrel



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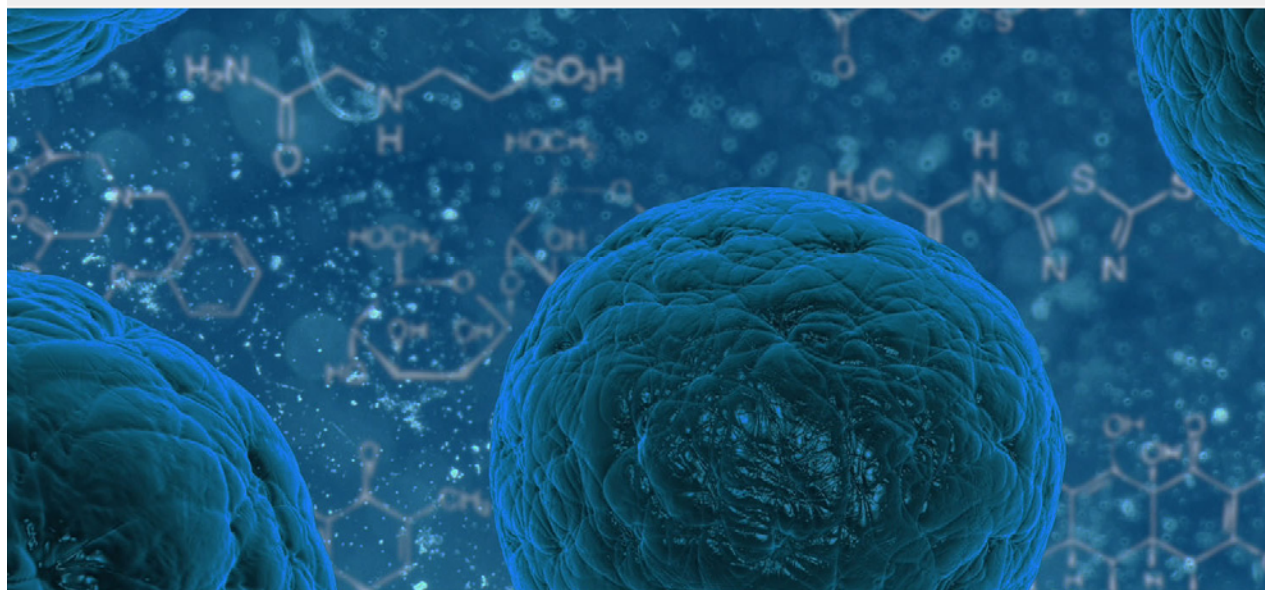
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The disposition of prasugrel, a novel thienopyridine, in humans.

Farid NA, Smith RL, Gillespie TA, Rash TJ, Blair PE, Kurihara A, Goldberg MJ.
Lilly Research Laboratories, Eli Lilly and Company, Lilly Corporate Center, Indianapolis, IN 46285, USA. nafarid@lilly.com

Abstract

Prasugrel, a prodrug, is a novel and potent inhibitor of platelet aggregation in vivo. The metabolism of prasugrel and the elimination and pharmacokinetics of its active metabolite, 2-[1-[2-cyclopropyl-1-(2-fluorophenyl)-2-oxoethyl]-4-mercapto-3-piperidinylidene]acetic acid (R-138727), three inactive metabolites, and radioactivity were determined in five healthy male subjects after a single 15-mg (100 microCi) p.o. dose of [(14)C]prasugrel. Prasugrel was rapidly absorbed, and maximum plasma concentrations of radioactivity and R-138727 were achieved in 30 min, indicating rapid formation of R-138727. Prasugrel was extensively metabolized in humans, first by hydrolysis to a thiolactone, followed by ring opening to form R-138727, which was further metabolized by S-methylation and conjugation with cysteine. Total radioactivity was higher in plasma than in blood, suggesting limited penetration of prasugrel metabolites into red blood cells. Approximately 70% of the dose was excreted in the urine and 25% in the feces.

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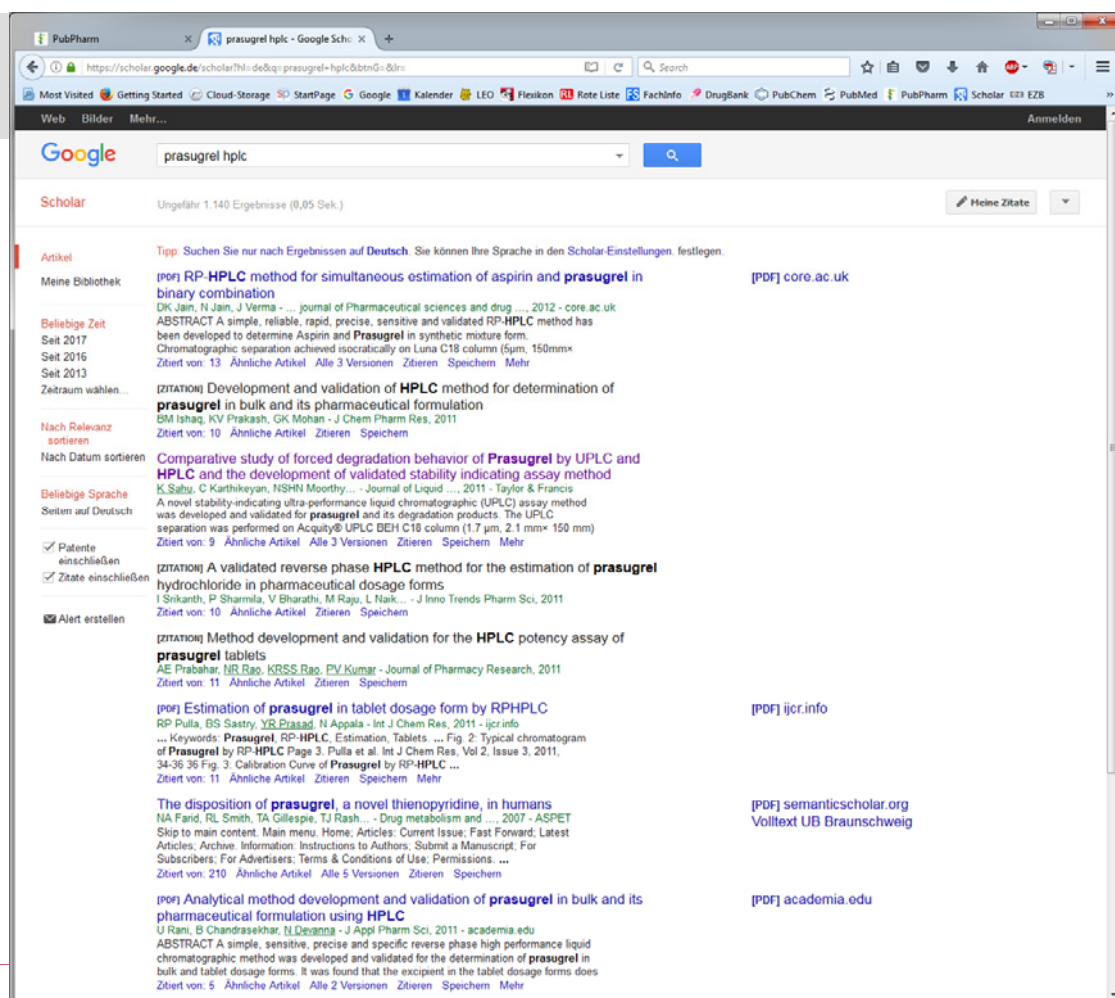
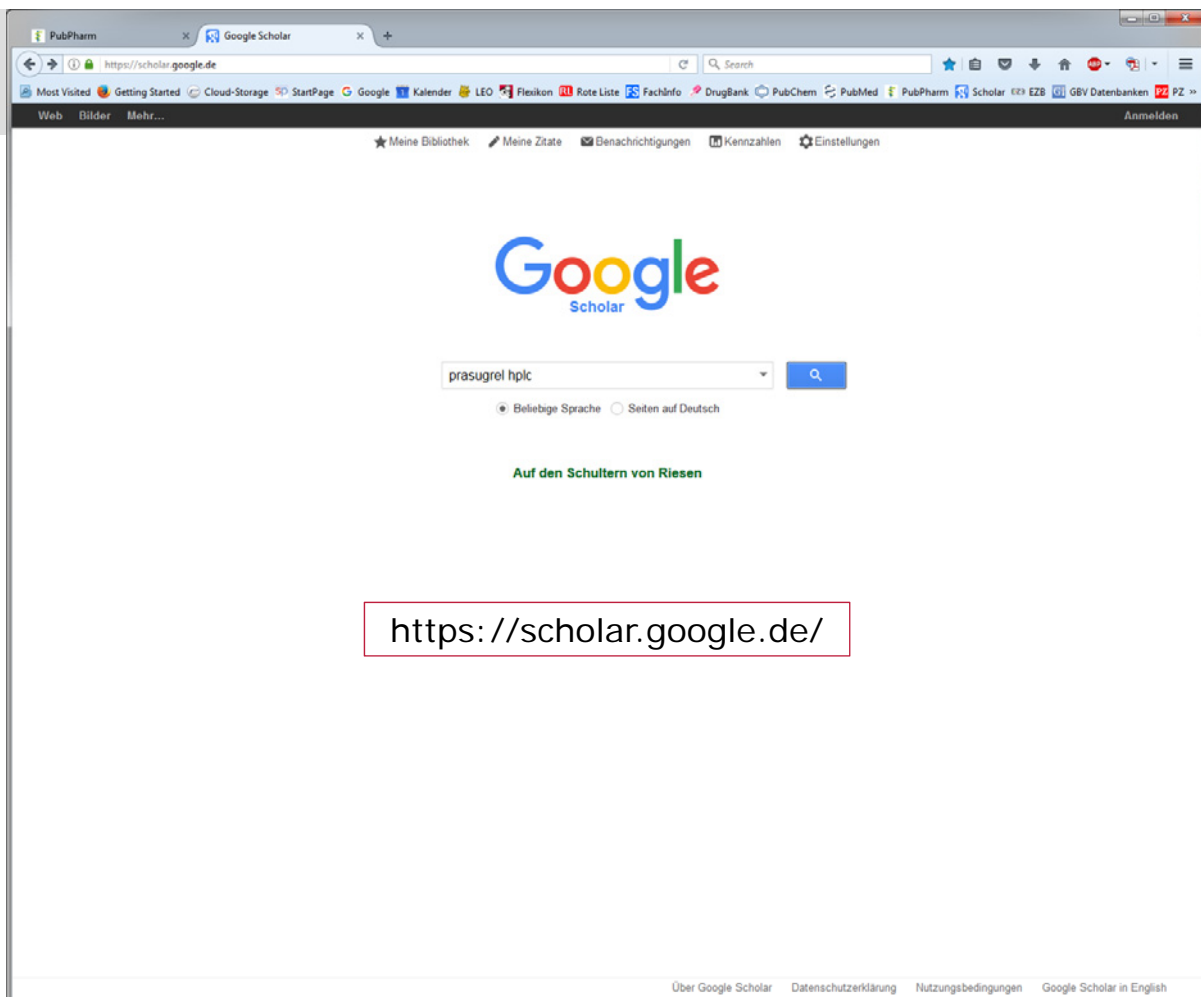
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Willkommen auf der neuen Webseite der ROTE LISTE® Online der Rote Liste® Service GmbH.

Wir haben die Seite aufgrund Ihrer Rückmeldungen in Umfragen, Telefonaten und Mails überarbeitet.

Unser Ziel ist es, Ihnen die Informationen übersichtlicher, freundlicher und zeitgemäßer darzustellen.

Ihre Recherchemöglichkeit

Die Suche ermöglicht Ihnen das Auffinden von Arzneimitteln/Medizinprodukten anhand von

- Name des Präparates
- Name des Pharmaunternehmens
- Name eines Wirkstoffes/Stoffes in Medizinprodukten
- Name einer Hauptgruppe
- Name einer Signatur

NEU

Die ROTE LISTE®
Medikamente App für iOS und
Android.

Zur App

DocCheck



DocCheck

Username

Password

- Passwort vergessen?
- Passwort beantragen

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http://www.fachinfo.de/


ROTE
LISTE

Fachinfo - Service®

Fachinformationsverzeichnis Deutschland

Suchbegriff eingeben ...

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Über den Fachinfo-Service®

ROTE LISTE® Online

Patienteninfo-Service®

Suche

Suche

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Unser Ziel ist es, Ihnen die Informationen übersichtlicher, freundlicher und zeitgemäßer darzustellen.

Ihre Recherchemöglichkeit

Die Suche ermöglicht Ihnen – wie bisher auch – das Auffinden von Fachinformationen anhand von

- Name der Fachinformation
- Name des Pharmaunternehmens

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Veranstaltungen

Fortbildungsveranstaltungen
der AkdÄ zu aktuellen Themen

► Mehr Informationen

Unerwünschte
Arzneimittelwirkung
melden

► Zum Meldebogen



Nutzenbewertung § 35a SGB V

► Mehr Informationen

Aktionsplan
Arzneimitteltherapiesicherheit
Initiative des BMG zur
Verbesserung der Arzneimittel-
therapiesicherheit in
Deutschland



AKTIONEN AN ZUM VERBESSERN NUTZ FÜR



100 Jahre Arzneimittelbewertung

Die AkdÄ 1911-2011: Im Einsatz für eine rationale
Arzneimitteltherapie.

Mehr erfahren

Aktuelle Meldungen

12.12.2014

Drug Safety Mail 2014-38

Rote-Hand-Brief zu Arzneimitteln, die Valproat und -verwandte Substanzen
enthalten: Risiko für Anomalien des Neugeborenen. Volltext

12.12.2014

Drug Safety Mail 2014-37

Aus der UAW-Datenbank: Cyanid-Intoxikation nach oraler Amygdalin-

Neue Arzneimittel

Ausgabe vom 25.11.2014:

Xarelto® (Rivaroxaban) ▼,
neu zugelassene Indikation

► Übersicht

Leitfaden

Orale Antikoagulation bei nicht
valvulärem Vorhofflimmern: