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October 25th – 28th, 2016

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Discipline areas – 61%
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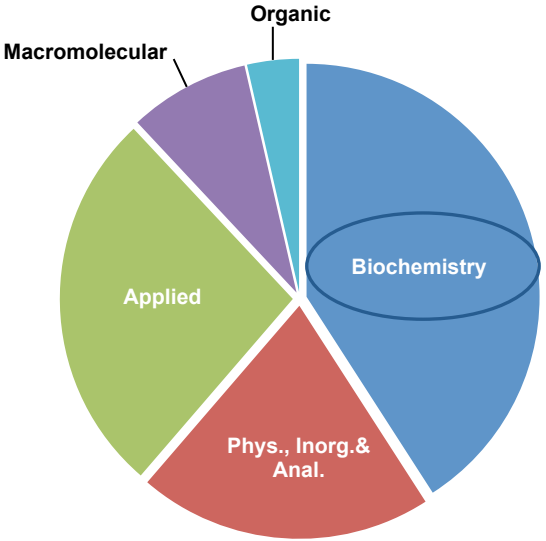
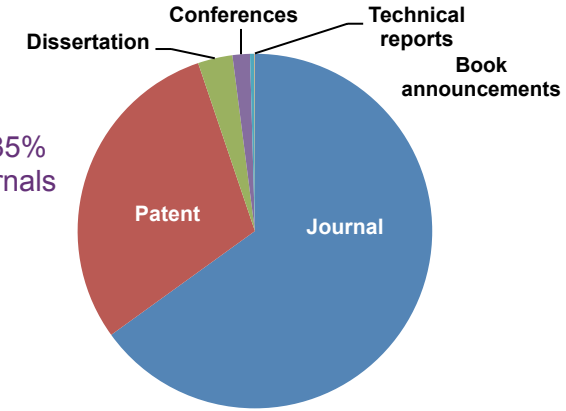
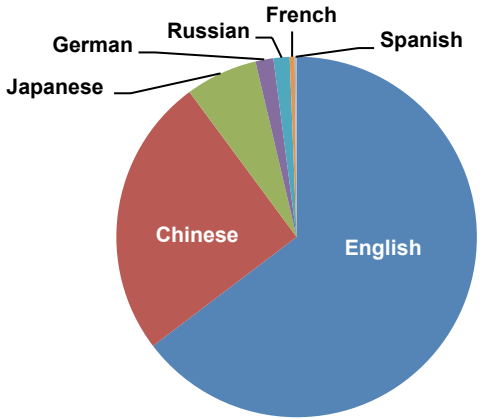


Disclosure types – 35%
not published in journals





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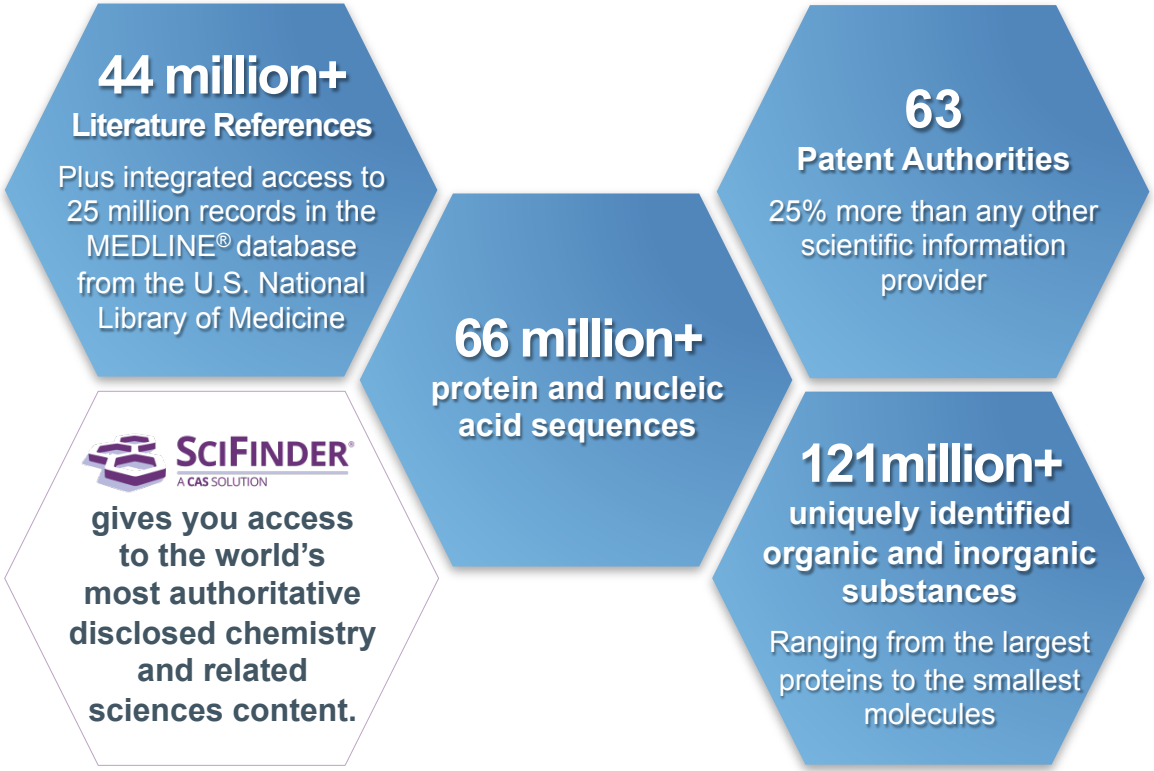

Data as of March 2016

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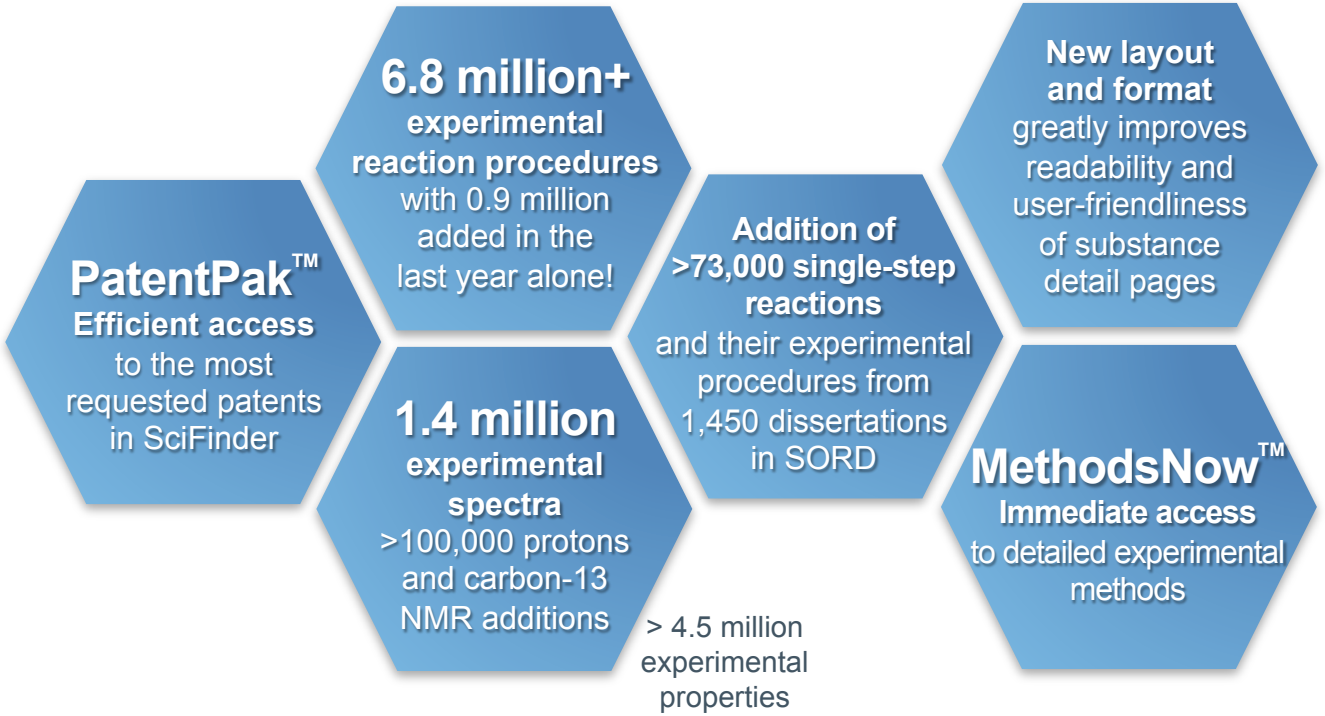

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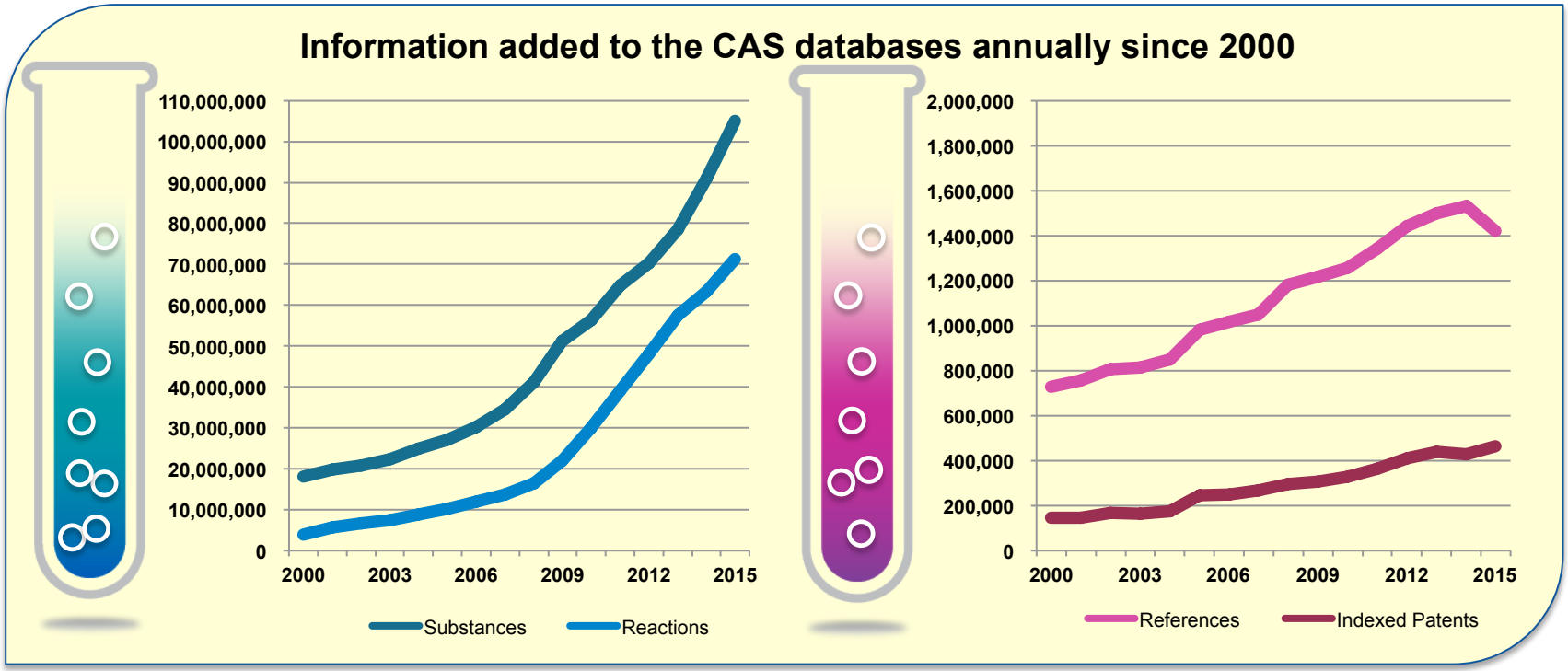

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48. CAS Registry Number 50-23-7

~55,285 ~205

$C_{21}H_{30}O_5$

Pregn-4-ene-3,20-dione, 11,17,21-trihydroxy-, (11β)-

Molecular Weight
362.46

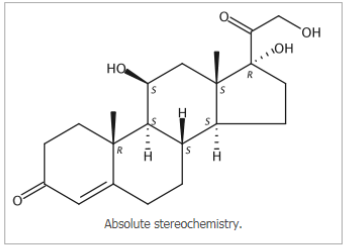
pKa (Predicted)
Value: 12.47±0.70 | Condition: Most Acidic Temp: 25 °C

Melting Point (Experimental)
Value: 217-220 °C (decomp)

Boiling Point (Predicted)
Value: 566.4±50.0 °C | Condition: Press: 760 Torr

Density (Experimental)
Value: 1.4 g/cm3

Other Names
Cortisol (8CI)
11β,17,21-Trihydroxypregn-4-ene-3,20-dione
11β,17,21-Trihydroxyprogesterone
11β,17α,21-Trihydroxypregn-4-ene-3,20-dione
11β-Hydroxycortisone
View more...



Absolute stereochemistry.

Indexing in other search tools can be
- unpredictable
- less-detailed
- non-existent

BIOACTIVITY INDICATORS

Indicators	References
Anti-infective agents (all) > > > Antibacterial agents	220
Anti-infective agents (all) > > Antibiotics	338
Anti-infective agents (all) > > Antimicrobial agents	122
Anti-infective agents (all) > > > Antiviral agents	179
Anti-infective agents (all) > > Fungicides	226
Anti-inflammatory agents (all) > Antiarthritics	64
Anti-inflammatory agents (all) > Anti-inflammatory agents	871
Anti-inflammatory agents (all) > Antirheumatic agents	98
Anti-inflammatory agents (all) > Nonsteroidal anti-inflammatory drugs	265
Antitumor agents (all) > Antiangiogenic agents	60
Antitumor agents (all) > Antitumor agents	404
Dermatological agents (all) > Dermatological agents	73
Immune agents (pharmaceutical) > Allergy inhibitors	83
Immune agents (pharmaceutical) > > Immunomodulators	117
Immune agents (pharmaceutical) > > Immunosuppressants	213
Natural products, pharmaceutical	89
Nervous system agents (all) > > > Analgesics	216
Nervous system agents (all) > > Anesthetics	209
Receptor antagonists (all) > > Antihistamines	124
Respiratory system agents (all) > Antiasthmatics	104
Wound healing promoters	55

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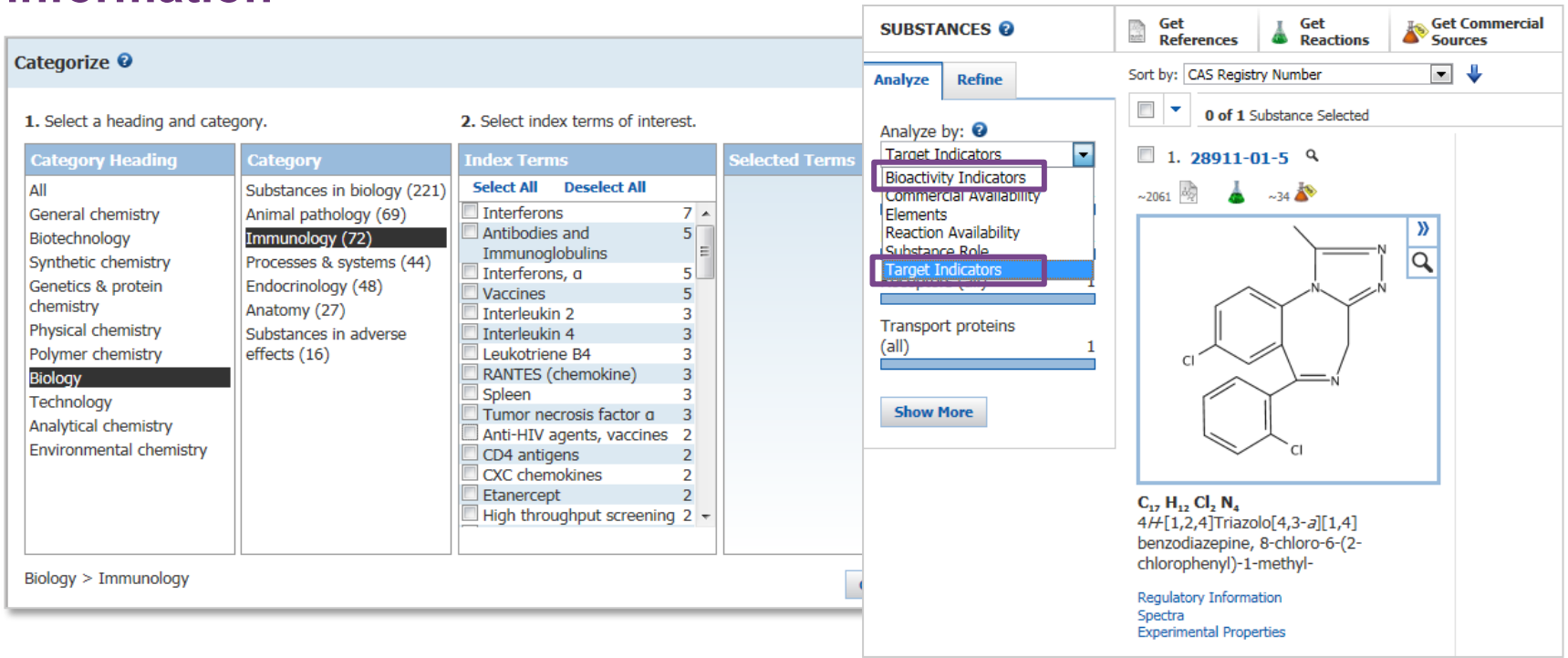

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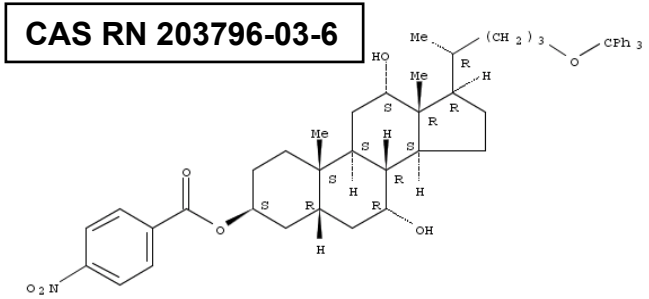
CAS scientists find the chemistry, and save you time!

Compound 34: Diisopropyl azodicarboxylate (DIAD) (1.20 mL, 6.08 mmol) was added to triphenylphosphine (1.60 g, 6.08 mmol) in THF (100 mL) at 0 °C. and was stirred for half an hour during which time the yellow solution became a paste. Compound 14 (2.58 g, 4.06 mmol) and p-nitrobenzoic acid (0.81 g, 4.87 mmol) were dissolved in THF (50 mL) and added to the paste. The resulted mixture was stirred at ambient temperature overnight. Water (100 mL) was added and the mixture was made slightly basic by adding $NaHCO_3$ solution followed by extraction with EtOAc (3x50 mL). The combined extracts were washed with brine once and dried over anhydrous Na_2SO_4. The desired product (2.72 g, 85% yield) was obtained as white powder after SiO_2 chromatography (Et_2O/hexanes 1:2). m.p. 207-209 °C.; IR (KBr) 3434, 3056, 2940, 2868, 1722, 1608, 1529,1489, 1448, 1345 cm^{-1} ; ^1H NMR ($CDCl_3$, 300 MHz) δ 8.30-8.26 (m, 2 H), 8.21-8.16 (m, 2 H), 7.46-7.42 (m, 6 H), 7.31-7.18 (m, 9 H)5.33 (bs, 1 H), 4.02 (bs, 1 H), 3.90 (bs, 1 H), 3.09-2.97 (m, 2 H), 2.68 (td, J=14.95, 2.56 Hz, 1 H), 2.29-2.19 (m, 1 H), 2.07-1.06 (series of multiplets, 24 H), 1.01 (s, 3 H), 0.98 (d, J=6.6 Hz, 3 H), 0.70 (s, 3 H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 164.21, 150.56, 144.70, 136.79, 130.77, 64.22, 47.79, 46.79, 42.1 28.74, 27.71, 26.85, 26.3 (thioglycerol+Na^+ matrix

CAS RN 203796-03-6



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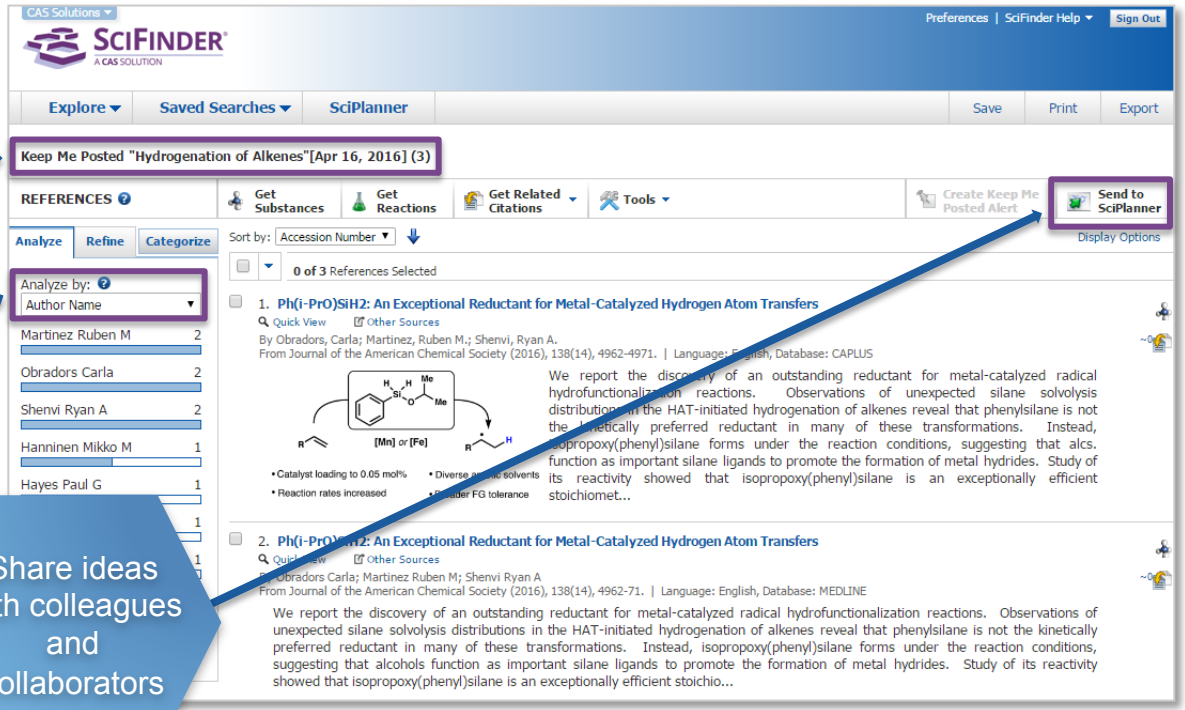

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Unlike its competitors, CAS covers patents in many languages, with enhanced translations

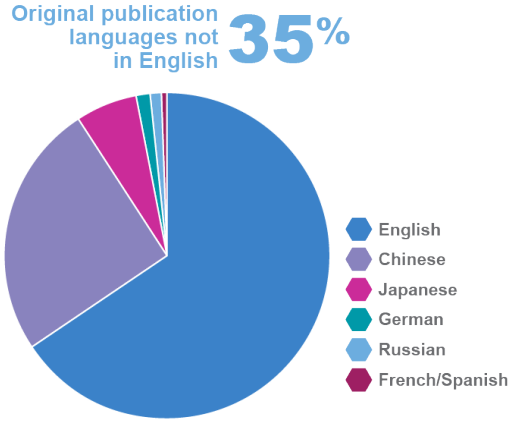
9. **Process for the preparation of favipiravir**

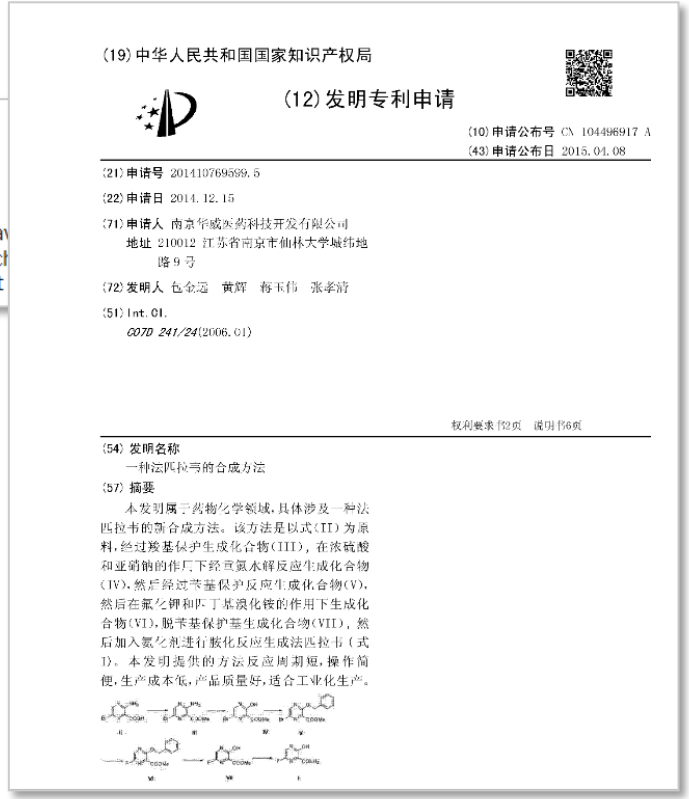
Quick View PATENTPAK

Patent No.	Kind	Language
CN 104496917	A	Chinese

By Bao, Jinyuan; H…qing
From Faming Zhua… A 20150408. | Language: Chinese, Database: CAPLUS

The inventio… prepn. of favipiravir. For example, favipirav… bromopyrazine-2-carboxylic acid to afford Me 3-amino-6-bromopyrazine-2-carboxylate, which… and fluorination to afford Me 3-(benzyloxy)-6-fluoropyrazine-2-carboxylate, which underwent …





(19)中华人民共和国国家知识产权局

(12)发明专利申请

(10)申请公布号 CN 104496917 A
(43)申请公布日 2015.04.08

(21)申请号 201410769599.5

(22)申请日 2014.12.15

(71)申请人 南京华威医药科技开发有限公司
地址 210012 江苏省南京市仙林大学城纬地路9号

(72)发明人 包金远 黄辉 梅玉伟 张孝清

(51)Int.Cl.
C07D 241/24(2006.01)

权利要求书2页 说明书6页

(54)发明名称
一种法匹拉韦的合成方法

(57)摘要
本发明属于药物化学领域，具体涉及一种法匹拉韦的新合成方法。该方法是以式(II)为原料，经过羧基保护生成化合物(III)，在浓硫酸和亚硝酸钠的作用下经亚氨水解反应生成化合物(IV)，然后经过苄基保护反应生成化合物(V)，然后在氟化钾和四丁基溴化铵的作用下生成化合物(VI)，脱苄基保护基生成化合物(VII)，然后加入氨气进行胺化反应生成法匹拉韦(式I)。本发明提供的方法反应周期短，操作简便，生产成本低，产品质量好，适合工业化生产。

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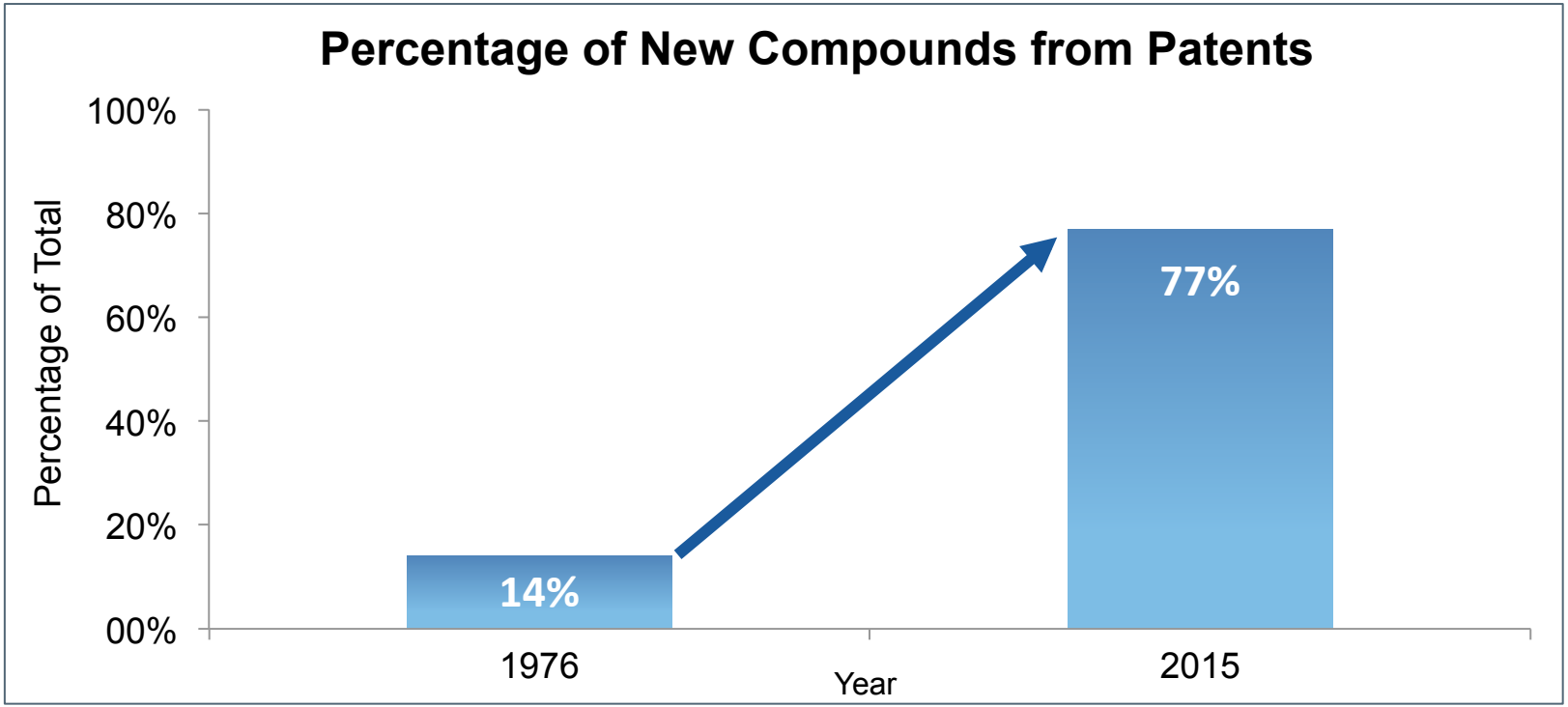
Increasingly, new compounds in the literature are first disclosed in patents



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SciFinder PatentPak – Patent Family information

57. **Fluorine-containing substituted 5-[2-(pyrid-3-yl)-ethyl]-2,3,4-tetrahydro-1H-pyrido[4,3-b]indoles and hydrochlorides and hydrobromides thereof as agents for reducing uncontrolled protein aggregation in the nervous system, pharmacological agent based thereon and method for preparation and using thereof**

Quick View PATENTPAK

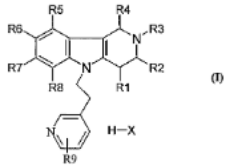
By **Bachurin, S. O.**; Ustyugov, A. A.; Ninkina, N. N.; Sokolov, V. B.; Aksinenko, A. Yu
From Russ. (2013), RU 2490268 C2 20130820. | Language: Russian, Database: CAP

Present invention refers to org. chem., namely to new fluorine-contg. (C1-C_6H_4) alkyl; R^2, R^3, R^4, R^5 = H, F, Cl, Br, (C1-C6) alkyl, (C1-C6) al method of decreasing uncontrolled protein aggregation in the nervou patient.

61. **Fluorine-containing substituted 5-[2-(pyrid-3-yl)-ethyl]-2,3,4-tetra uncontrolled protein aggregation in the nervous system, pharmacologic**

Quick View PATENTPAK

By **Bachurin, Sergey Olegovich**; Ustugov, Aleksey Anatolyevich; Ninkina, Natalya N Aleksey Viktorovich
From PCT Int. Appl. (2013), WO 2013070117 A2 20130516. | Language: Russian, Da



(I)

The invention provides the alkynyl, C_1-C_6 alkoxy, etc.; R^9 = F, 2F, CHF_2, $CClF_2$, reducing uncontrolled pro same relate to the field of

Patent Information

Patent No.		Kind	Language	Date
WO 2013070117	PATENTPAK	A2		May 16, 2013
WO 2013070117	PATENTPAK	A3	Russian	Jul 18, 2013
RU 2490268	PATENTPAK	C2	Russian	Aug 20, 2013
AU 2012336451		A1		Jul 3, 2014
EP 2781518	PATENTPAK	A2	English	Sep 24, 2014
CN 104105698	PATENTPAK	A	Chinese	Oct 15, 2014
JP 2014533266	PATENTPAK	T	Japanese	Dec 11, 2014
US 20150038526	PATENTPAK	A1	English	Feb 5, 2015

Priority Application

RU 2011-145513	A		Nov 10, 2011
WO 2012-RU894	W		Nov 1, 2012

62. **Agent for neutralizing toxic effect of tumor necrosis factor on the basis of tetrahydro-pyrido(4,3-b)indole derivatives and method for the treatment of autoimmune diseases**

Quick View PATENTPAK

By Alesenko, A. V.; **Bachurin, S. O.**; Grigor'ev, V. V.; Gur'yanova, S. V.; Guss, F. V.; Lukina, G. V.; Lyangus, A. P.; Nasonov, E. L.; Sigidin, Ya. A.
From Russ. (2013), RU 2477131 C1 20130310. | Language: Russian, Database: CAPLUS

Agent for neutralizing toxic effect of tumor necrosis factor on the basis of tetrahydro-pyrido(4,3-b)indole derivs. and method for the treatment of autoimmune diseases are disclosed. The invention relates to pharmacol. and involves agents for neutralizing toxic action of tumor necrosis factor on the basis of tetrahydro-pyrido(4,3-b)indole derivs. of

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US 2008-61046712	P	Apr 21, 2008
WO 2009-US41276	W	Apr 21, 2009
JP 2011-505263	A3	Apr 21, 2009

CAPLUS

LANGUAGE
English

Indexing

Pharmacology (Section1-12)

Section cross-reference(s): 8, 9, 34, 63

Concepts

Transcription factors

Antennapedia, of Drosophila, conjugates with polydentate ligands; selective high-affinity polydentate ligands of target mols. and methods of making such and uses for diagnosis and therapeutics in relation to delivery of effectors

Biological study, unclassified; Diagnostic use; Pharmacological activity; Therapeutic use; Biological study; Uses

Viral transcription factor Tat

HIV, protein transduction domain, conjugates; selective high-affinity polydentate ligands of target mols. and methods of making such and uses for diagnosis and therapeutics in relation to delivery of effectors

Biological study, unclassified; Diagnostic use; Pharmacological activity; Therapeutic use; Biological study; Uses

Histocompatibility antigen HLA-D

HLA-DR, target mols.; selective high-affinity polydentate ligands of target mols. and methods of making such and uses for diagnosis and therapeutics in relation to delivery of effectors

Adverse effect, including toxicity; Biological study, unclassified; Diagnostic use; Biological

Substances

170908-81-3 — Page 104 in PatentPak

DOTA-NHS-ester; selective high-affinity polydentate ligands of target mols. and methods of making such and uses for diagnosis and therapeutics in relation to delivery of effectors

Reactant; Reactant or reagent

83-44-3 Deoxycholic acid — Page 84 in PatentPak
495-69-2 Hippuric acid — Page 123 in PatentPak
744-59-2 Hippuryl-L-phenylalanine — Page 123 in PatentPak
15307-86-5 2-[(2,6-Dichlorophenyl)amino]benzeneacetic acid
21811-74-5 — Page 123 in PatentPak
26129-32-8 — Page 123 in PatentPak
40843-25-2 2-[4-(2,4-Dichlorophenoxy)phenoxy]propanoic acid
54857-86-2 5-(Tetradecyloxy)-2-furoic acid
58594-74-4
63058-21-9 — Page 84 in PatentPak
69335-91-7 — Page 123 in PatentPak
69806-34-4 — Page 123 in PatentPak
74051-80-2 Sethoxydim
76578-12-6
89131-11-3 — Page 84 in PatentPak
94588-27-9 — Page 123 in PatentPak

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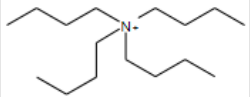
Key Substances in Patent

CAS RN 1643-19-2



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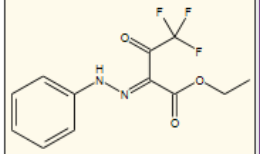
Analyst Markup Locations (1)

page 9

CAS RN 1494-98-0



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Analyst Markup Locations (2)

page 10

page 15

см$^{-1}$: 3150, 1625 (NH), 1680 (C=O), 1620, 1540, 1510 (C=N, C=C), 1250-1100 (C-F). Спектр ЯМР ^{1}H ($CDCl_3$, δ, м.д., J/Гц): 1.42 т (3H, OCH_2Me, $^3J_{H,H}$ 7.1), 4.41 к (2H, OCH_2CH_3, $^3J_{H,H}$ 7.1), 7.24-7.26 и 7.43-7.46 оба м (5H, C_6H_5), 13.49 уш.с (1H, NH). Найдено, %: C 50.01, H 3.87, F 19.88, N 9.80. $C_{12}H_{11}F_3N_2O_3$. Вычислено, %: C 50.01, H 3.85, F 19.77, N 9.72.

Пример 2. Этиловый эфир 2-[(4-метилфенил)гидразоно]-3-оксо-4,4,4-трифторбутановой кислоты (2). (Соединение формулы I, где R^1=CF_3, R^2=Et, R_3=4-Me). Получают аналогично примеру 1 из 1.07 г п-толуидина (10 ммоль) и 1.84 г (10 ммоль) этилового эфира 3-оксо-4,4,4-трифторбутановой кислоты. Выход 2.45 г (81%), желтый порошок, т.пл. 75-76°C. ИК спектр (DRA), ν, см$^{-1}$: 3100, 1590 (NH), 1690 (C=O), 1630, 1520, 1500 (C=N, C=C), 1200-1080 (C-F). Спектр ЯМР ^{1}H (ДМСО-d_6, δ, м.д., J/Гц): 1.28 т (3H, OCH_2Me, $^3J_{H,H}$ 7.1), 2.28 с (3H, Me), 4.30 к (2H, OCH_2CH_3, $^3J_{H,H}$ 7.1), 7.18-7.36 м (4H, C_6H_4), 11.65 уш.с (1H, NH). Найдено, %: C 51.89, H 4.59, F 18.58, N 9.15. $C_{13}H_{13}F_3N_2O_3$. Вычислено, %: C 51.66, H 4.34, F 18.86, N 9.27.

Пример 3. Этиловый эфир 2-(4-метоксифенил)гидразоно-3-оксо-4,4,4-трифторбутановой кислоты (3). (Соединение формулы I, где R^1=CF_3, R^2=Et, R_3=4-OMe). Получают аналогично примеру 1 из 1.23 г (10 ммоль) п-анизидина и 1.84 г (10 ммоль) этилового эфира 3-оксо-4,4,4-трифторбутановой кислоты. Выход 2.70 г (85%), желтые кристаллы, т.пл. 130-131°C. ИК спектр (DRA), ν, см$^{-1}$: 3090 ($NH^{вал}$), 1690 (C=O), 1640,

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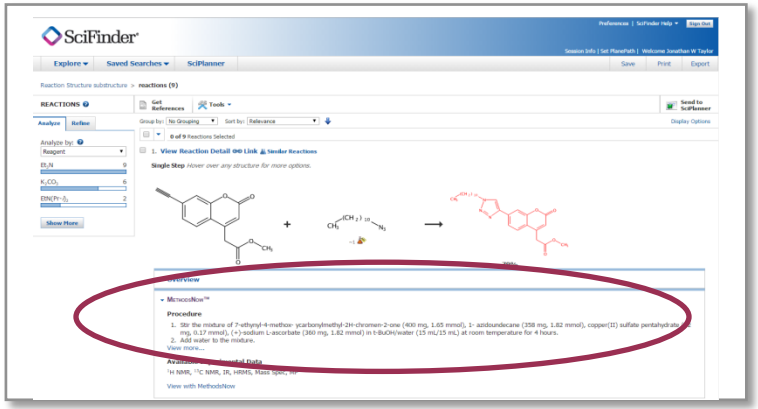

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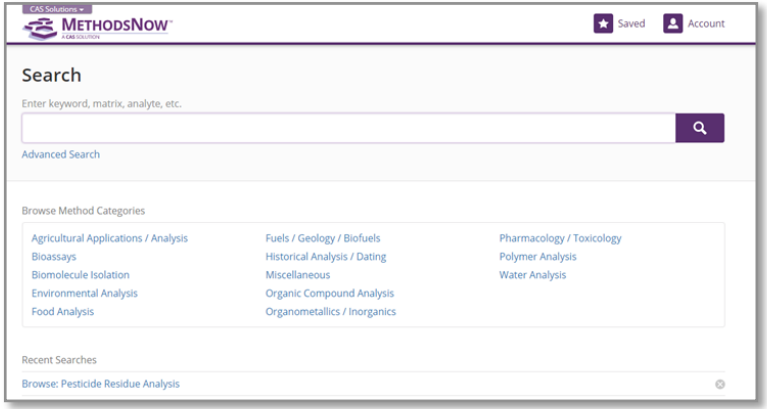

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Focus	Small molecule-centric
Example journal titles	Food Chemistry, Journal of Chromatography A and B, Journal of Agricultural and Food Chemistry, Talanta, Analytica Chimica Acta
Language	English only

SciFinder® A CAS SOLUTION

MethodsNow – Analysis: Main Categories

Method categories	Primary content in these categories
active-pharmaceutical-ingredient	Pharmacology, toxicology, SAR, analysis of drugs
bioassay	Pharmacology, toxicology, biochemical methods
biomolecule-isolation-assay	Biochemical methods, mammalian hormones
bioorganism-isolation-assay	Biochemical genetics
element-detection	Inorganic analytical chemistry
environmental-analysis	Essential oils/cosmetics
food-analysis	Additives, food processing, contaminants, GMO
forensic-analysis	Toxicology
natural-product-isolation-analysis	Analysis of drugs
organic-compound-analysis	Organic analytical chem.
pesticide-residue-analysis	Food, feed, toxicology, agrochemical bioregulators
trace-element-analysis	Inorganic analytical chemistry, benzene
water-wastewater-sludge-analysis	Chemical water analysis (i.e. contaminants in water)

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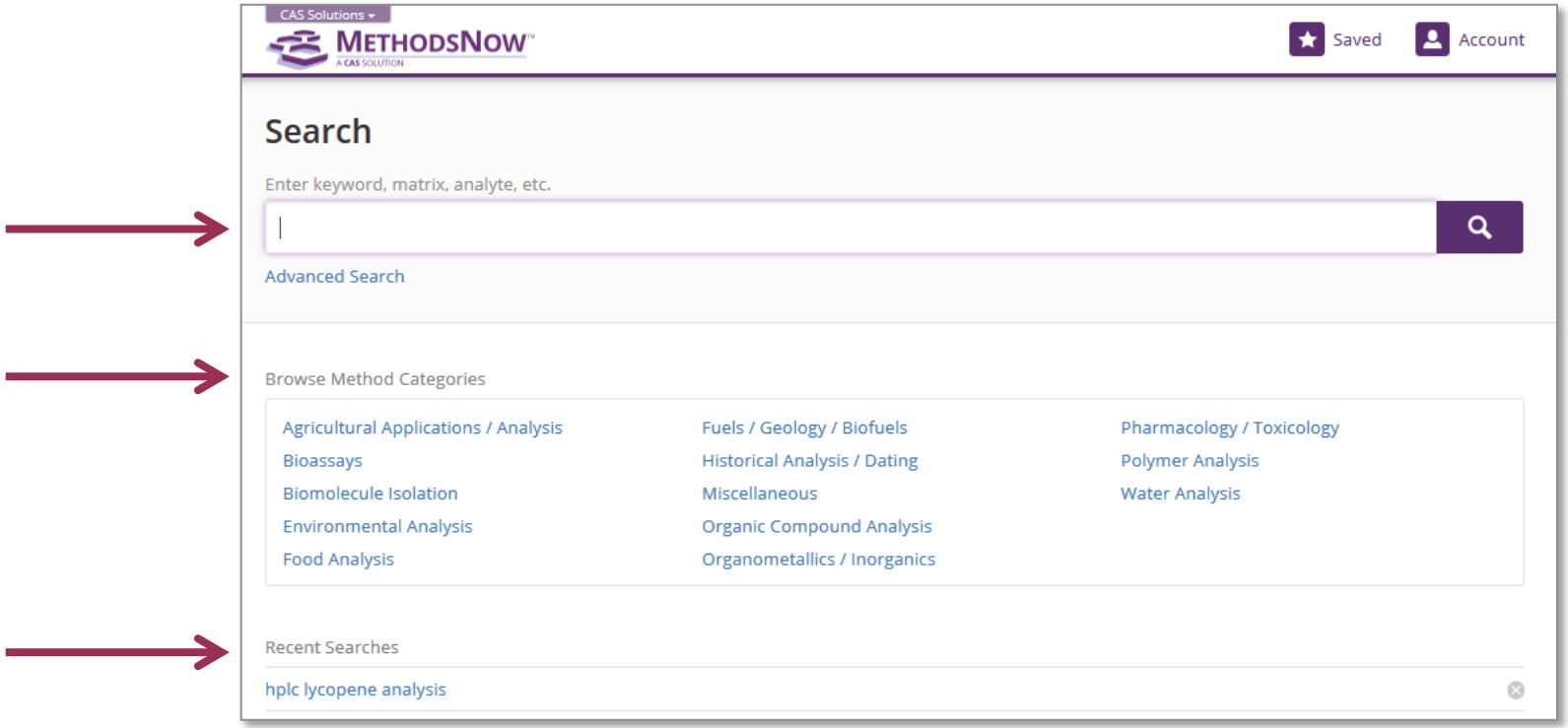
MethodsNow – Analytical Scientist Interface



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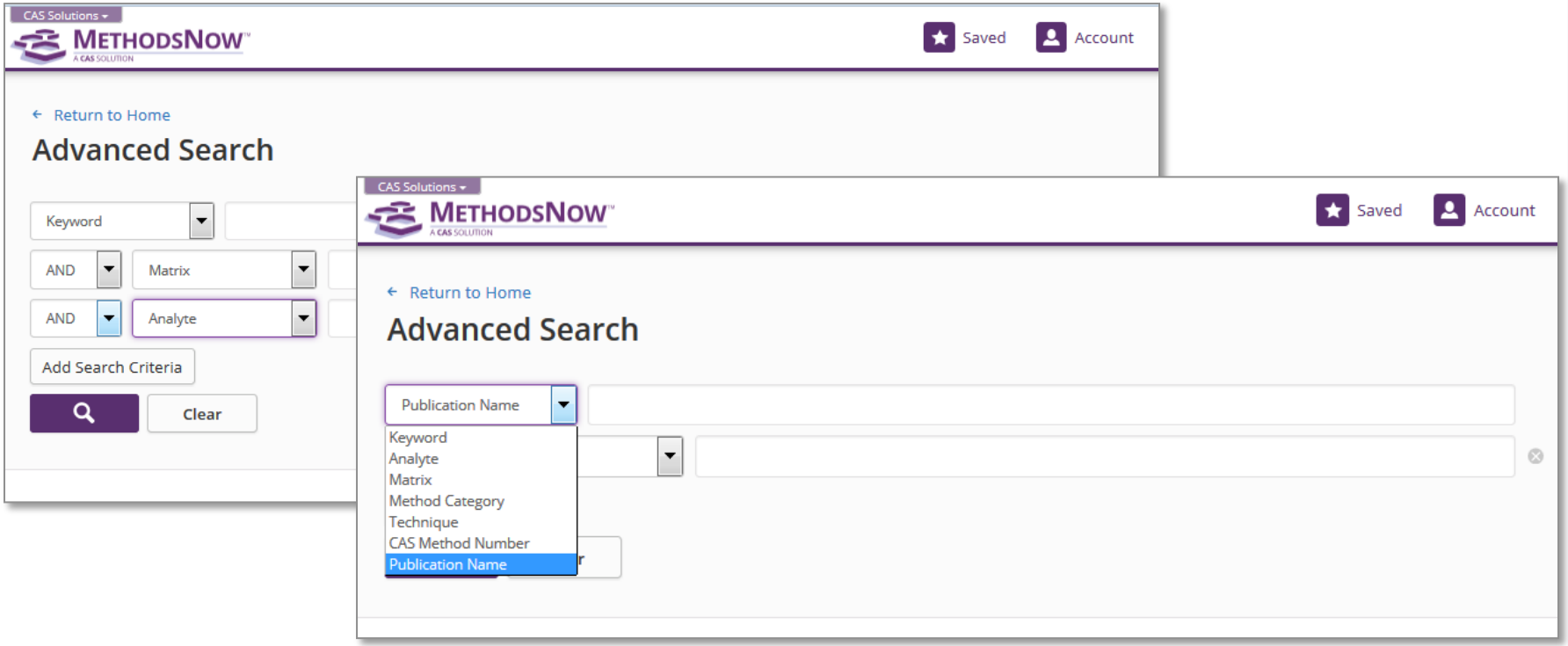
Specify one or many advanced search fields



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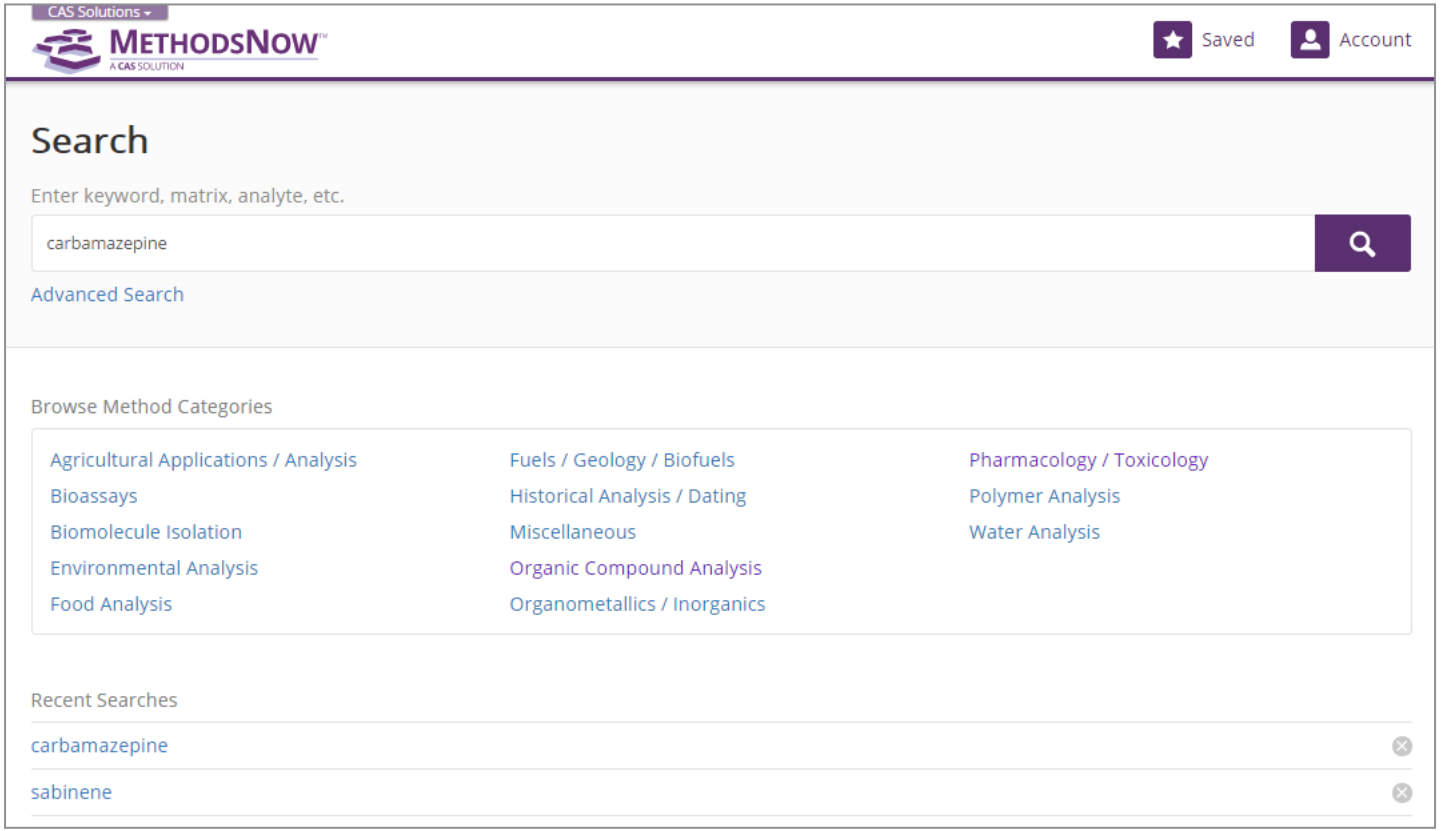

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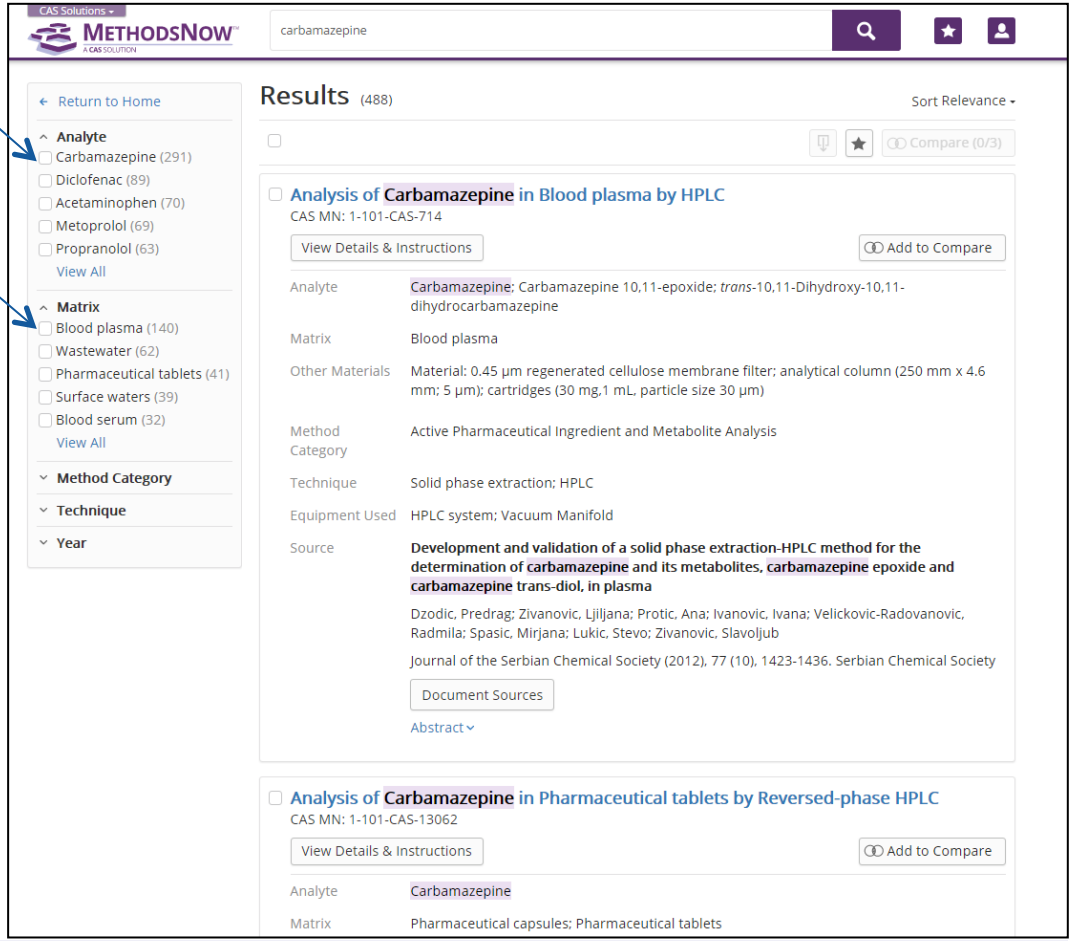

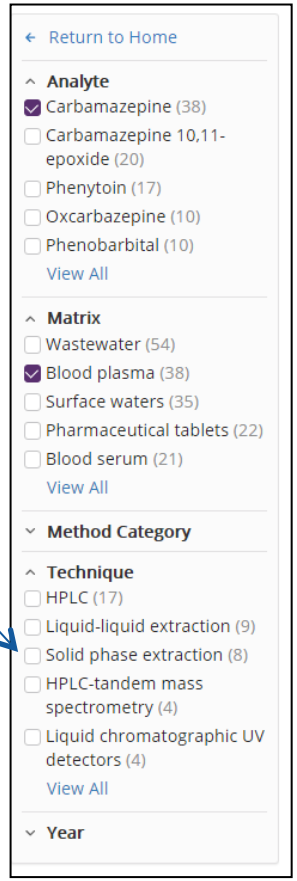

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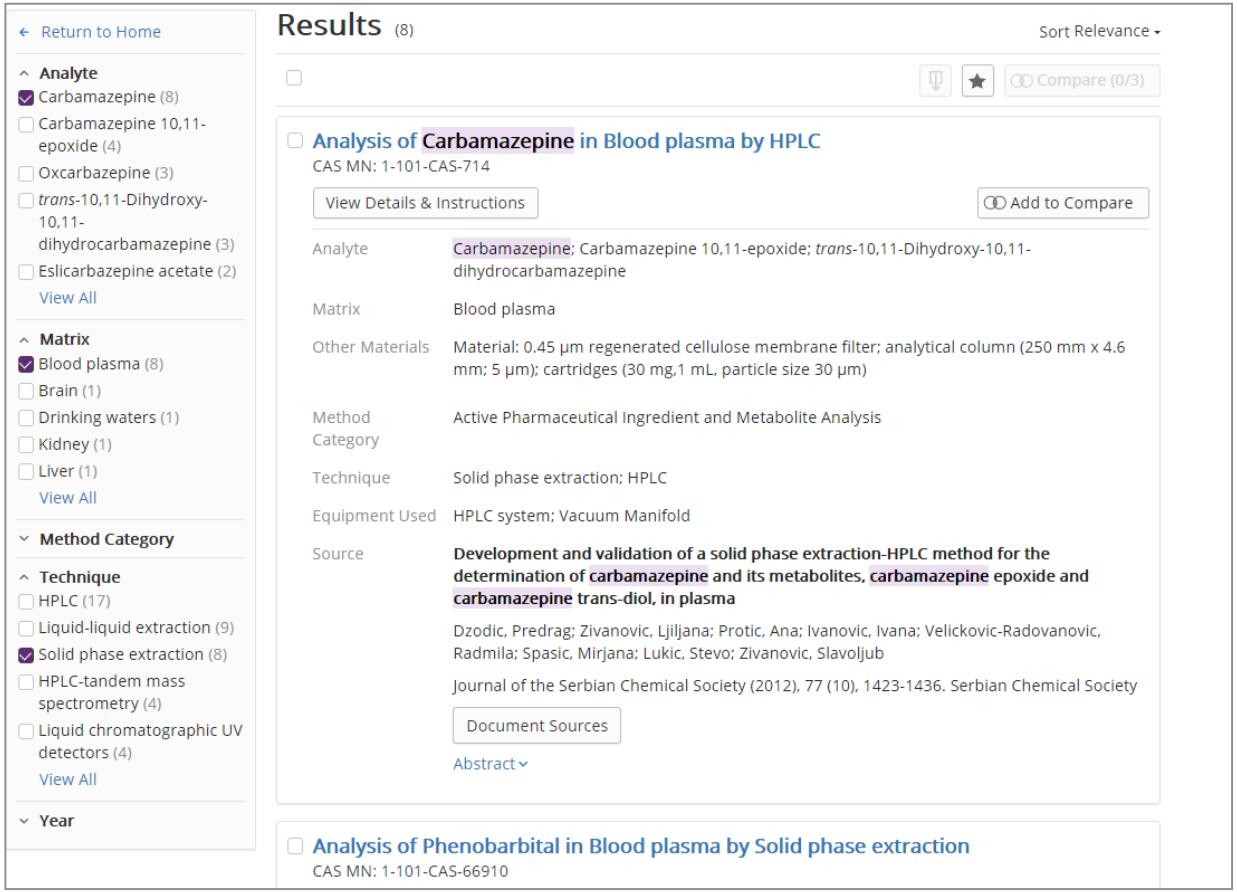
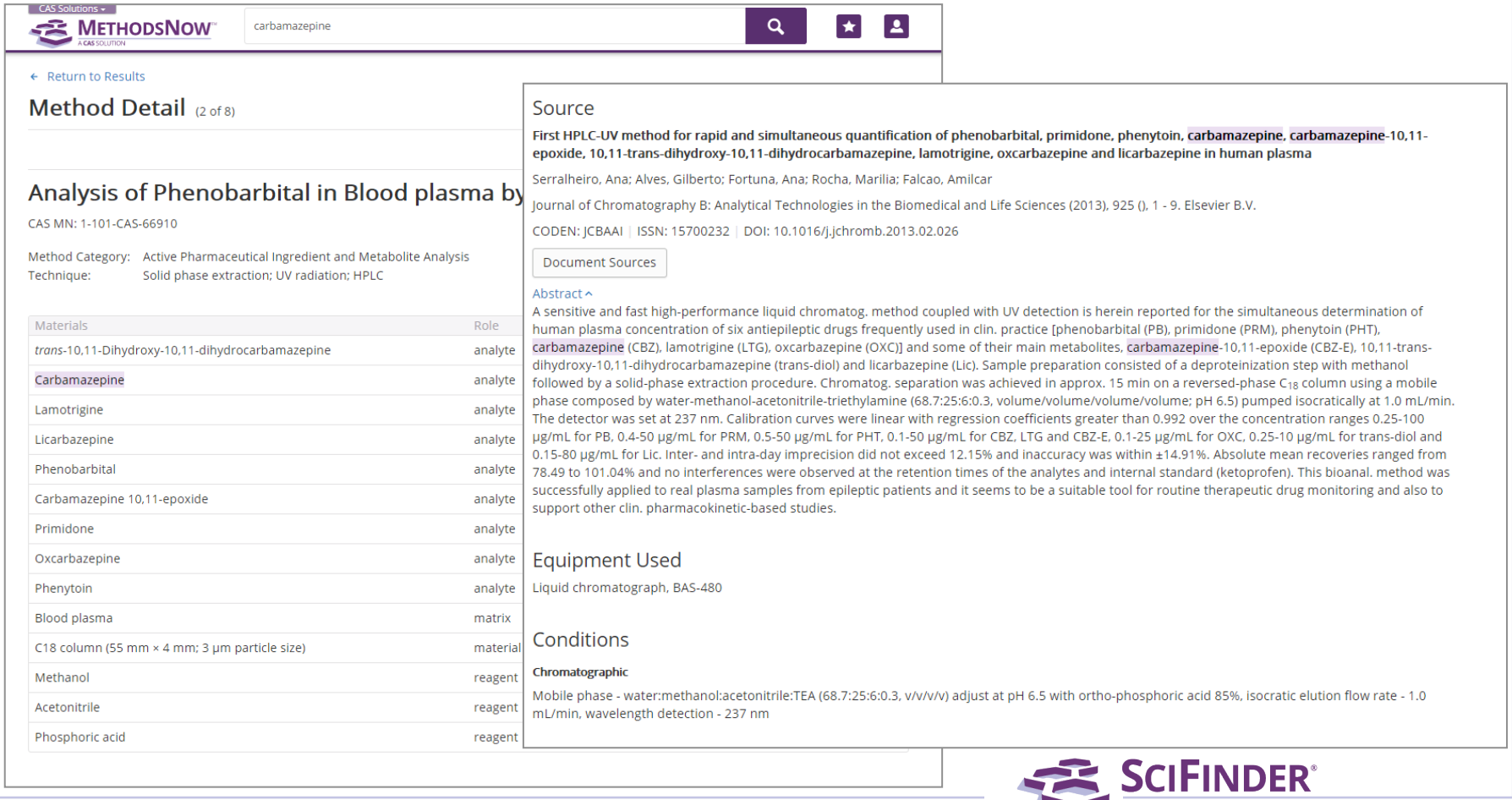

Return to Home
Analyte
Carbamazepine (8)
Carbamazepine 10,11-epoxide (4)
Oxcarbazepine (3)
trans-10,11-Dihydroxy-10,11-dihydrocarbamazepine (3)
Eslicarbazepine acetate (2)
View All
Matrix
Blood plasma (8)
Brain (1)
Drinking waters (1)
Kidney (1)
Liver (1)
View All
Method Category
Technique
HPLC (17)
Liquid-liquid extraction (9)
Solid phase extraction (8)
HPLC-tandem mass spectrometry (4)
Liquid chromatographic UV detectors (4)
View All
Year
Results (8)
Sort Relevance
Compare (0/3)
Analysis of Carbamazepine in Blood plasma by HPLC
CAS MN: 1-101-CAS-714
View Details & Instructions
Add to Compare
Analyte
Carbamazepine; Carbamazepine 10,11-epoxide; trans-10,11-Dihydroxy-10,11-dihydrocarbamazepine
Matrix
Blood plasma
Other Materials
Material: 0.45 µm regenerated cellulose membrane filter; analytical column (250 mm x 4.6 mm; 5 µm); cartridges (30 mg,1 mL, particle size 30 µm)
Method Category
Active Pharmaceutical Ingredient and Metabolite Analysis
Technique
Solid phase extraction; HPLC
Equipment Used
HPLC system; Vacuum Manifold
Source
Development and validation of a solid phase extraction-HPLC method for the determination of carbamazepine and its metabolites, carbamazepine epoxide and carbamazepine trans-diol, in plasma
Dzodic, Predrag; Zivanovic, Ljiljana; Protic, Ana; Ivanovic, Ivana; Velickovic-Radovanovic, Radmila; Spasic, Mirjana; Lukic, Stevo; Zivanovic, Slavoljub
Journal of the Serbian Chemical Society (2012), 77 (10), 1423-1436. Serbian Chemical Society
Document Sources
Abstract
Analysis of Phenobarbital in Blood plasma by Solid phase extraction
CAS MN: 1-101-CAS-66910



SCIFINDER® A CAS SOLUTION

Instructions

Preparation of standard solution

1. Prepare stock solutions of Phenobarbital (PB 20 mg/mL), Primidone (PRM 10 mg/mL), Phenytoin (PHT 10 mg/mL), Carbamazepine (CBZ 10 mg/mL), Lamotrigine (LTG 10 mg/mL), Oxcarbazepine (OXC 5 mg/mL), Carbamazepine-10,11-epoxide (CBZ-E 10 mg/mL), *trans*-diol (10 mg/mL), Licarbazepine 20 mg/mL) and IS (1 mg/mL) individually by dissolving appropriate amounts of each compound in methanol.
2. Dilute these solutions adequately with methanol to obtain the corresponding working solutions.
3. Mix stock and working solutions of drugs and metabolites properly to afford six combined spiking solutions with final concentrations of 6.25, 12.5, 5(250, 100 and 2500 µg/mL for PB; 10, 20, 50, 125, 500 and 1250 µg/mL for PRM; 12.5, 25, 50, 125, 500 and 1250 µg/mL for PHT; 2.5, 5, 12.5, 50, 250 an 1250 µg/mL for CBZ, LTG and CBZ-E; 2.5, 5, 12.5, 25, 125 and 625 µg/mL for OXC; 6.25, 12.5, 25, 50, 100 and 250 µg/mL for trans-diol and 3.75, 7.5, 2(100, 500 and 2000 µg/mL for Lic.

Solid phase extraction

1. Add an aliquot of human plasma (500 µL) of 20 µL of the IS working solution and mix with 1 mL of methanol in order to precipitate plasma proteins.
2. After centrifuging at 13,400 rpm for 10 min, evaporate the resulting supernatant under a gentle nitrogen stream at 80 °C for 10 min.
3. Dilute the residual volume of supernatant with 1.5 mL of water and vortex-mix for 30 s.
4. Subject the pre-treated sample to a solid-phase extraction (SPE) on the Oasis® HLB (30 mg, 1 mL) cartridge (Waters, Milford, MA, USA), which is previously conditioned with 1 mL of methanol, 1 mL of acetonitrile and 1 mL of water-acetonitrile (95:5, v/v).
5. Submit the loaded cartridge subsequently to -60 kPa and wash four times with 1 mL of water.
6. After drying the sorbent under airflow for 5 min, elute the analytes with 1 mL of ethyl acetate using gentle vacuum.
7. Evaporate the eluate to dryness at 45 °C under a gentle stream of nitrogen gas and reconstitute with 500 µL of mobile phase by vortexing and ultrasonication.
8. Inject 20 µL of the final mixture into the chromatographic system.

Method or Procedure

1. Perform the chromatographic analysis on a BAS-480 liquid chromatograph equipped with a PM-80 pump, a Rheodyne manual injector with a 20 µL loop, a BAS UV-116 UV-vis detector, a BAS DA-5 chromatography control and a data system interface (Bioanalytical Systems, West Lafayette, IN, USA)
2. Achieve the data acquisition by means of BAS Chromgraph Control and Chromgraph Report software version 2.30.
3. Perform the chromatographic analysis of all the six drugs, metabolites and IS at room temperature.
4. Carry out the separation on reversed-phase LiChroCART® Purospher Star® C18 column (55 mm × 4 mm; 3 µm particle size) purchased from Merck KGaA (Darmstadt, Germany).
5. Apply an isocratic elution at a flow rate of 1.0 mL/min with a mobile phase compose of water-methanol-acetonitrile-TEA (68.7:25:6:0.3, v/v/v/v) and adjust at pH 6.5 with ortho-phosphoric acid 85%.
6. Set the wavelength detection at 237 nm.

Validation

Linearity Range	0.40 - 50 µg/mL, Primidone
	0.10 - 50 µg/mL, Lamotrigine
	0.25 - 10 µg/mL, 10,11-*trans*-Dihydroxy-10,11-dihydrocarbamazepine
	0.25 - 100 µg/mL, Phenobarbital
	0.15 - 80 µg/mL, Licarbazepine
	0.10 - 50 µg/mL, Carbamazepine-10,11-epoxide
Limit of Quantitation	0.40 µg/mL, Primidone
	0.10 µg/mL, Lamotrigine
	0.25 µg/mL, 10,11-*trans*-Dihydroxy-10,11-dihydrocarbamazepine
	0.25 µg/mL, Phenobarbital
	0.15 µg/mL, Licarbazepine
	0.10 µg/mL, Carbamazepine-10,11-epoxide
	0.10 µg/mL, Oxcarbazepine
	0.50 µg/mL, Phenytoin
	0.10 µg/mL, Carbamazepine
Recovery	92.24 ± 3.99%, 80.17 ± 2.84%, 94.47 ± 2.80% spiked in 1.2 µg/mL, 25 µg/mL, 45 µg/mL respectively, Primidone
	84.87 ± 5.89%, 84.16 ± 3.20%, 85.96 ± 2.41% spiked in 0.3 µg/mL, 25 µg/mL, 45 µg/mL respectively, Lamotrigine
	83.57 ± 3.94%, 83.13 ± 2.57%, 88.68 ± 2.48% spiked in 0.75 µg/mL, 5 µg/mL, 9 µg/mL respectively, 10,11-*trans*-Dihydroxy-10,11-dihydrocarbamazepine
	89.77 ± 4.77%, 81.35 ± 2.60%, 83.80 ± 2.60% spiked in 0.75 µg/mL, 50 µg/mL, 90 µg/mL respectively, Phenobarbital
	101.04 ± 3.83%, 87.45 ± 3.05%, 91.42 ± 2.67% spiked in 0.45 µg/mL, 40 µg/mL, 72 µg/mL respectively, Licarbazepine
	89.43 ± 6.02%, 85.27 ± 3.05%, 90.46 ± 2.67% spiked in 0.3 µg/mL, 25 µg/mL, 45 µg/mL respectively, Carbamazepine-10,11-epoxide
	82.88 ± 1.95%, 86.96 ± 2.98%, 89.01 ± 2.47% spiked in 0.3 µg/mL, 12.5 µg/mL, 22.5 µg/mL respectively, Oxcarbazepine
	84.19 ± 7.42%, 82.81 ± 3.63%, 78.49 ± 2.60% spiked in 1.5 µg/mL, 25 µg/mL, 45 µg/mL respectively, Phenytoin
	88.89 ± 9.37%, 88.46 ± 3.35%, 86.37 ± 2.57% spiked in 0.3 µg/mL, 25 µg/mL, 45 µg/mL respectively, Carbamazepine
Accuracy	7.38% (%bias, Inter-day); 1.94% (%bias, Intra-day), Primidone
	5.78% (%bias, Inter-day); 16.43% (%bias, Intra-day), Lamotrigine
	5.46% (%bias, Inter-day); 6.09% (%bias, Intra-day), 10,11-*trans*-Dihydroxy-10,11-dihydrocarbamazepine
	-1.58% (%bias, Inter-day); -13.93% (%bias, Intra-day), Phenobarbital
	-5.28% (%bias, Inter-day); 5.47% (%bias, Intra-day), Licarbazepine
	9.24% (%bias, Inter-day); 10.87% (%bias, Intra-day), Carbamazepine-10,11-epoxide
	6.26% (%bias, Inter-day); 0.43% (%bias, Intra-day), Oxcarbazepine
	1.22% (%bias, Inter-day); -0.17% (%bias, Intra-day), Phenytoin
	10.88% (%bias, Inter-day); 14.74% (%bias, Intra-day), Carbamazepine
Precision	13.48% (%CV, Inter-day); 3.31% (%CV, Intra-day), Primidone
	14.95% (%CV, Inter-day); 14.29% (%CV, Intra-day), Lamotrigine
	9.6% (%CV, Inter-day); 2.42% (%CV, Intra-day), 10,11-*trans*-Dihydroxy-10,11-dihydrocarbamazepine
	18.27% (%CV, Inter-day); 8.09% (%CV, Intra-day), Phenobarbital
	17.93% (%CV, Inter-day); 7.62% (%CV, Intra-day), Licarbazepine
	10.22% (%CV, Inter-day); 10.41% (%CV, Intra-day), Carbamazepine-10,11-epoxide
	12.4% (%CV, Inter-day); 7.04% (%CV, Intra-day), Oxcarbazepine
	12.05% (%CV, Inter-day); 4.66% (%CV, Intra-day), Phenytoin
	12.31% (%CV, Inter-day); 14.85% (%CV, Intra-day), Carbamazepine

Analysis of Phenobarbital in Blood plasma by Solid phase extraction

CAS MN: 1-101-CAS-66910

View Details & Instructions | Remove from Compare

Analyte	*trans*-10,11-Dihydroxy-10,11-dihydrocarbamazepine; Carbamazepine; Lamotrigine; Licarbazepine; Phenobarbital; Carbamazepine 10,11-epoxide; Primidone; Oxcarbazepine; Phenytoin
Matrix	Blood plasma
Other Materials	Reagent: Methanol; Acetonitrile; Phosphoric acid Material: C18 column (55 mm × 4 mm; 3 µm particle size)
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis
Technique	Solid phase extraction; UV radiation; HPLC
Equipment Used	Liquid chromatograph
Source	**First HPLC-UV method for rapid and simultaneous quantification of phenobarbital, primidone, phenytoin, carbamazepine, carbamazepine-10,11-epoxide, 10,11-trans-dihydroxy-10,11-dihydrocarbamazepine, lamotrigine, oxcarbazepine and licarbazepine in human plasma** Serralheiro, Ana; Alves, Gilberto; Fortuna, Ana; Rocha, Marilia; Falcao, Amilcar Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences (2013), 925 (), 1-9. Elsevier B.V. Document Sources Abstract

Analysis of Carbamazepine in Blood plasma by Solid phase extraction

CAS MN: 1-101-CAS-133183

View Details & Instructions | Remove from Compare

Analyte	Carbamazepine
Matrix	Drinking waters; Urine; Blood plasma

chromatographic analysis

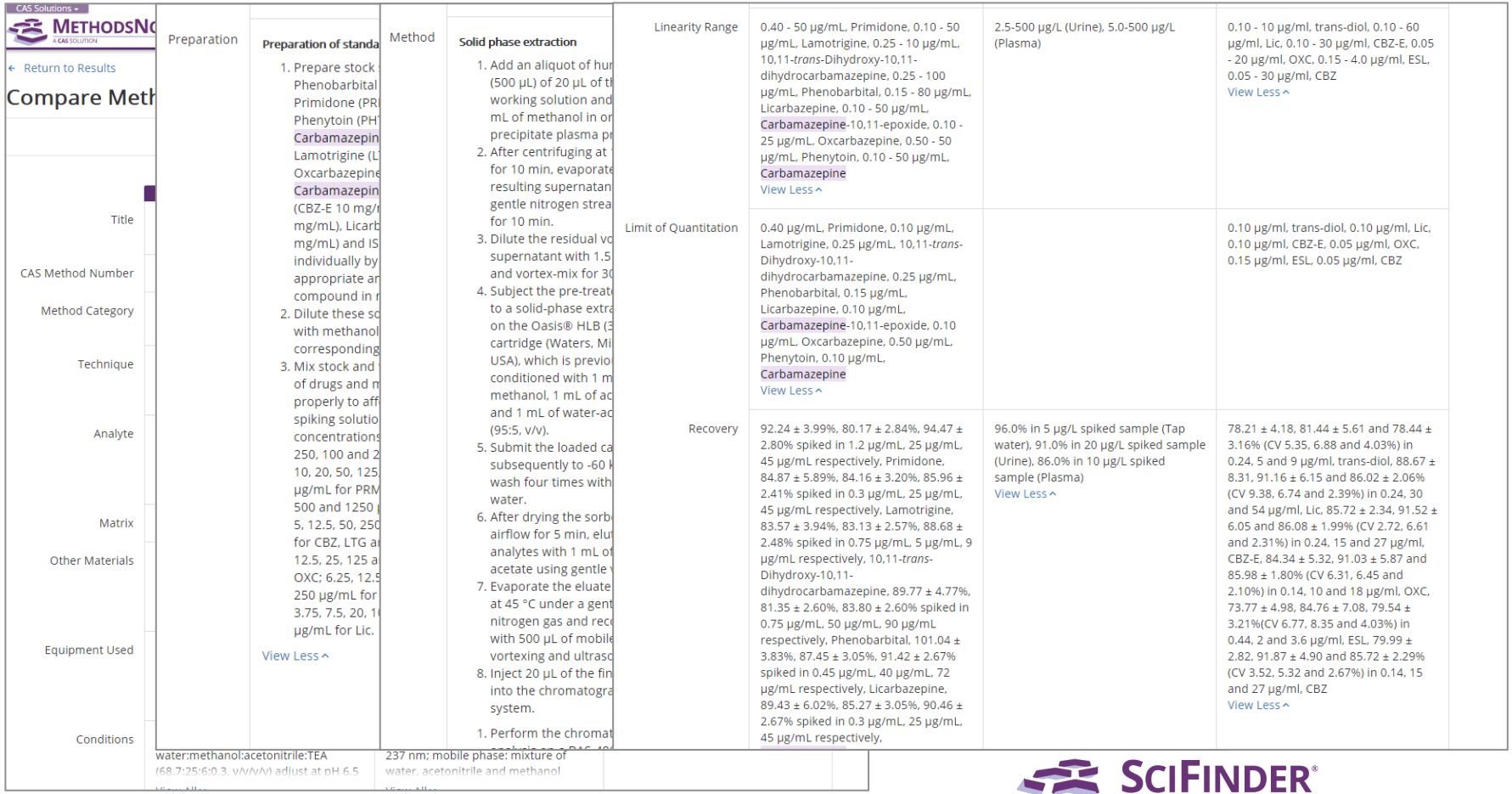
Source	**Solid-phase extraction combined with dispersive liquid-liquid microextraction as an efficient and simple method for the determination of carbamazepine in biological samples** Rezaee, Mohammad; Mashayekhi, Hossein Ali Analytical Methods (2012), 4 (9), 2887-2892. Royal Society of Chemistry Document Sources Abstract

Analysis of Carbamazepine in Blood plasma by Reversed-phase HPLC

CAS MN: 1-101-CAS-60070

View Details & Instructions | Remove from Compare

Analyte	Licarbazepine; Oxcarbazepine; Eslicarbazepine acetate; *trans*-10,11-Dihydroxy-10,11-dihydrocarbamazepine; Carbamazepine 10,11-epoxide; Carbamazepine
Matrix	Blood plasma
Other Materials	Material: Oasis® HLB (30 mg, 1 ml) cartridges; LiChroCART® Purospher® Star (C_{18}, 3 µm, 55 mm x 4 mm)
Method Category	Active Pharmaceutical Ingredient and Metabolite Analysis
Technique	Solid phase extraction; Reversed-phase HPLC
Equipment Used	liquid chromatograph
Source	**Development and validation of an HPLC-UV method for the simultaneous quantification of carbamazepine, oxcarbazepine, eslicarbazepine acetate and their main metabolites in human plasma** Fortuna, Ana; Sousa, Joana; Alves, Gilberto; Falcao, Amilcar; Soares-da-Silva, Patricio Analytical and Bioanalytical Chemistry (2010), 397 (4), 1605-1615. Springer Document Sources Abstract


CAS Solutions
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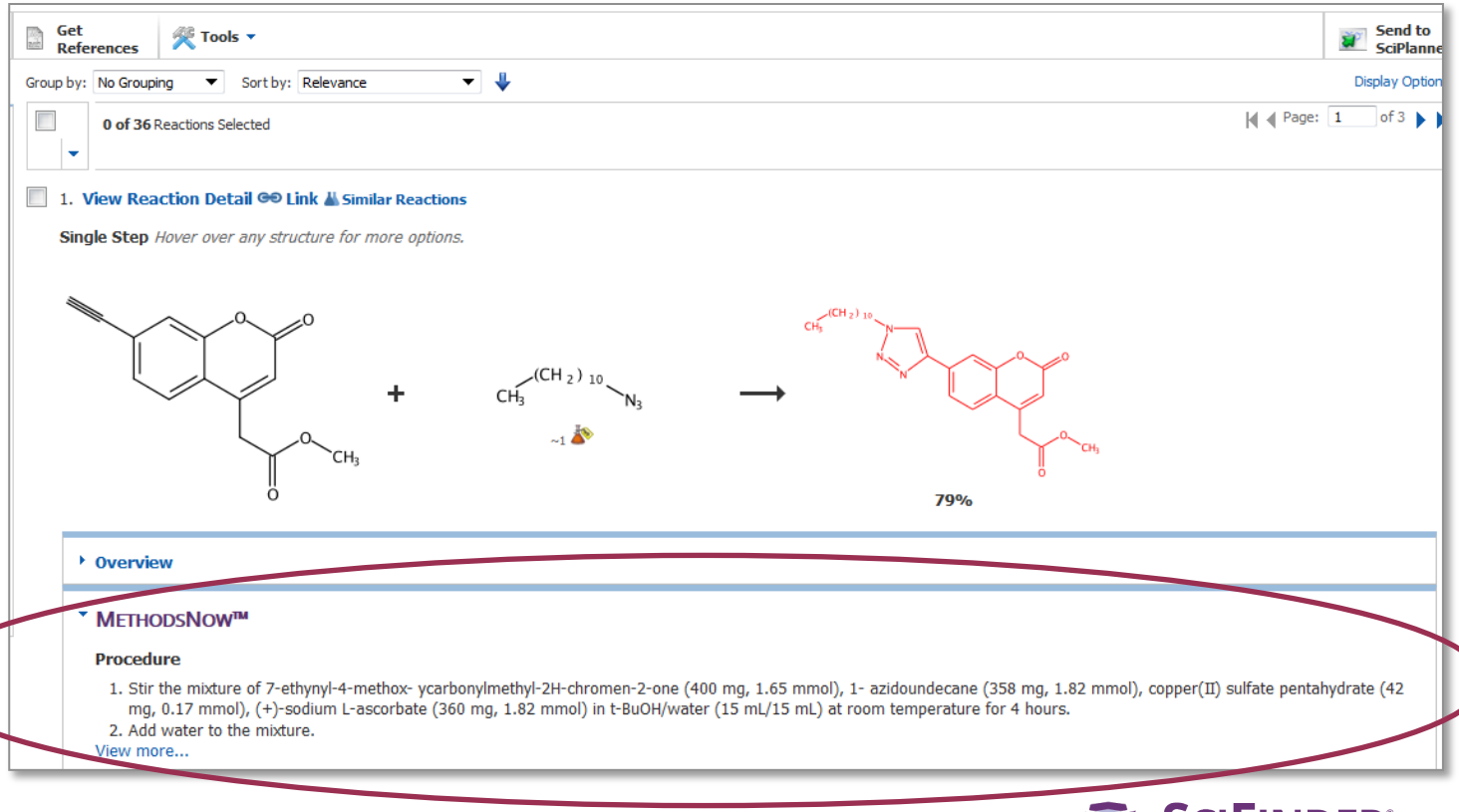
Return to Results
Compare Meth
Title
CAS Method Number
Method Category
Technique
Analyte
Matrix
Other Materials
Equipment Used
Conditions
Preparation
Preparation of standa
1. Prepare stock
Phenobarbital
Primidone (PR
Phenytoin (PH
Carbamazepin
Lamotrigine (L
Oxcarbazepine
Carbamazepin
(CBZ-E 10 mg/
mg/mL), Licarb
mg/mL) and IS
individually by
appropriate ar
compound in
2. Dilute these sc
with methanol
corresponding
3. Mix stock and
of drugs and m
properly to aff
spiking solutio
concentrations
250, 100 and 2
10, 20, 50, 125,
µg/mL for PRM
500 and 1250
5, 12.5, 50, 250
for CBZ, LTG a
12.5, 25, 125 a
OXC; 6.25, 12.5
250 µg/mL for
3.75, 7.5, 20, 1
µg/mL for Lic.
View Less
Method
Solid phase extraction
1. Add an aliquot of hur
(500 µL) of 20 µL of t
working solution and
mL of methanol in or
precipitate plasma pr
2. After centrifuging at
for 10 min, evaporate
resulting supernatan
gentle nitrogen strea
for 10 min.
3. Dilute the residual vo
supernatant with 1.5
and vortex-mix for 30
4. Subject the pre-treat
to a solid-phase extra
on the Oasis® HLB (3
cartridge (Waters, Mi
USA), which is previo
conditioned with 1 m
methanol, 1 mL of ac
and 1 mL of water-ac
(95:5, v/v).
5. Submit the loaded ca
subsequently to -60 k
wash four times with
water.
6. After drying the sorb
airflow for 5 min, elu
analytes with 1 mL of
acetate using gentle
7. Evaporate the eluate
at 45 °C under a gent
nitrogen gas and rec
with 500 µL of mobile
vortexing and ultrasc
8. Inject 20 µL of the fin
into the chromatogra
system.
1. Perform the chromat
Linearity Range
0.40 - 50 µg/mL, Primidone, 0.10 - 50 µg/mL, Lamotrigine, 0.25 - 10 µg/mL, 10,11-trans-Dihydroxy-10,11-dihydrocarbamazepine, 0.25 - 100 µg/mL, Phenobarbital, 0.15 - 80 µg/mL, Licarbazepine, 0.10 - 50 µg/mL, Carbamazepine-10,11-epoxide, 0.10 - 25 µg/mL, Oxcarbazepine, 0.50 - 50 µg/mL, Phenytoin, 0.10 - 50 µg/mL, Carbamazepine
View Less
2.5-500 µg/L (Urine), 5.0-500 µg/L (Plasma)
0.10 - 10 µg/ml, trans-diol, 0.10 - 60 µg/ml, Lic, 0.10 - 30 µg/ml, CBZ-E, 0.05 - 20 µg/ml, OXC, 0.15 - 4.0 µg/ml, ESL, 0.05 - 30 µg/ml, CBZ
View Less
Limit of Quantitation
0.40 µg/mL, Primidone, 0.10 µg/mL, Lamotrigine, 0.25 µg/mL, 10,11-trans-Dihydroxy-10,11-dihydrocarbamazepine, 0.25 µg/mL, Phenobarbital, 0.15 µg/mL, Licarbazepine, 0.10 µg/mL, Carbamazepine-10,11-epoxide, 0.10 µg/mL, Oxcarbazepine, 0.50 µg/mL, Phenytoin, 0.10 µg/mL, Carbamazepine
View Less
0.10 µg/ml, trans-diol, 0.10 µg/ml, Lic, 0.10 µg/ml, CBZ-E, 0.05 µg/ml, OXC, 0.15 µg/ml, ESL, 0.05 µg/ml, CBZ
Recovery
92.24 ± 3.99%, 80.17 ± 2.84%, 94.47 ± 2.80% spiked in 1.2 µg/mL, 25 µg/mL, 45 µg/mL respectively, Primidone, 84.87 ± 5.89%, 84.16 ± 3.20%, 85.96 ± 2.41% spiked in 0.3 µg/mL, 25 µg/mL, 45 µg/mL respectively, Lamotrigine, 83.57 ± 3.94%, 83.13 ± 2.57%, 88.68 ± 2.48% spiked in 0.75 µg/mL, 5 µg/mL, 9 µg/mL respectively, 10,11-trans-Dihydroxy-10,11-dihydrocarbamazepine, 89.77 ± 4.77%, 81.35 ± 2.60%, 83.80 ± 2.60% spiked in 0.75 µg/mL, 50 µg/mL, 90 µg/mL respectively, Phenobarbital, 101.04 ± 3.83%, 87.45 ± 3.05%, 91.42 ± 2.67% spiked in 0.45 µg/mL, 40 µg/mL, 72 µg/mL respectively, Licarbazepine, 89.43 ± 6.02%, 85.27 ± 3.05%, 90.46 ± 2.67% spiked in 0.3 µg/mL, 25 µg/mL, 45 µg/mL respectively,
96.0% in 5 µg/L spiked sample (Tap water), 91.0% in 20 µg/L spiked sample (Urine), 86.0% in 10 µg/L spiked sample (Plasma)
View Less
78.21 ± 4.18, 81.44 ± 5.61 and 78.44 ± 3.16% (CV 5.35, 6.88 and 4.03%) in 0.24, 5 and 9 µg/ml, trans-diol, 88.67 ± 8.31, 91.16 ± 6.15 and 86.02 ± 2.06% (CV 9.38, 6.74 and 2.39%) in 0.24, 30 and 54 µg/ml, Lic, 85.72 ± 2.34, 91.52 ± 6.05 and 86.08 ± 1.99% (CV 2.72, 6.61 and 2.31%) in 0.24, 15 and 27 µg/ml, CBZ-E, 84.34 ± 5.32, 91.03 ± 5.87 and 85.98 ± 1.80% (CV 6.31, 6.45 and 2.10%) in 0.14, 10 and 18 µg/ml, OXC, 73.77 ± 4.98, 84.76 ± 7.08, 79.54 ± 3.21%(CV 6.77, 8.35 and 4.03%) in 0.44, 2 and 3.6 µg/ml, ESL, 79.99 ± 2.82, 91.87 ± 4.90 and 85.72 ± 2.29% (CV 3.52, 5.32 and 2.67%) in 0.14, 15 and 27 µg/ml, CBZ
View Less
water:methanol:acetonitrile:TEA (68.7:25:6:0.3, v/v/v/v) adjust at pH 6.5
237 nm; mobile phase: mixture of water, acetonitrile and methanol

MethodsNow synthetic chemistry content sources

Content from years	2000 - present
Number of protocols	2.1 million; 3 million later this year
Content Coverage	Small molecule synthesis
Source Focus	180+ journals titles including new coverage from Wiley, RSC and Elsevier in addition to ACS, Springer, Taylor&Francis, WO patents (2010-present)
Example journal titles	Organic Letters, Catalysis Letters, Journal of Coordination Chemistry, Journal of Medicinal Chemistry, Journal of the American Chemical Society, Angewandte Chemie, Tetrahedron, Chemical Science
Language	English only

MethodsNow – Synthetic Chemist Interface



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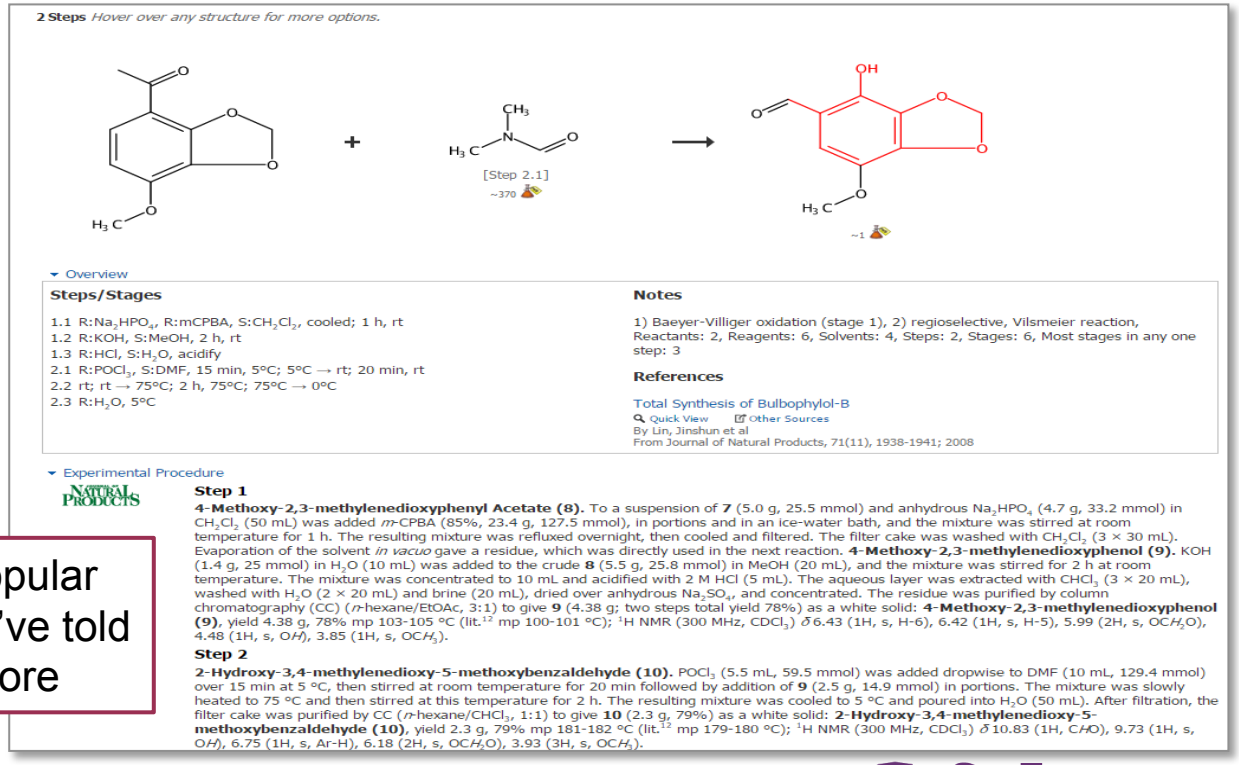

2 Steps *Hover over any structure for more options.*

[Step 2.1]
~370

~1

Overview

Steps/Stages

1.1 R:Na_2HPO_4, R:mCPBA, S:CH_2Cl_2, cooled; 1 h, rt
1.2 R:KOH, S:MeOH, 2 h, rt
1.3 R:HCl, S:H_2O, acidify
2.1 R:$POCl_3$, S:DMF, 15 min, 5°C; 5°C → rt; 20 min, rt
2.2 rt; rt → 75°C; 2 h, 75°C; 75°C → 0°C
2.3 R:H_2O, 5°C

Notes

1) Baeyer-Villiger oxidation (stage 1), 2) regioselective, Vilsmeier reaction, Reactants: 2, Reagents: 6, Solvents: 4, Steps: 2, Stages: 6, Most stages in any one step: 3

References

Total Synthesis of Bulbophylol-B
Quick View Other Sources
By Lin, Jinshun et al
From Journal of Natural Products, 71(11), 1938-1941; 2008

Experimental Procedure

JOURNAL OF NATURAL PRODUCTS

Step 1

4-Methoxy-2,3-methylenedioxyphenyl Acetate (8). To a suspension of **7** (5.0 g, 25.5 mmol) and anhydrous Na_2HPO_4 (4.7 g, 33.2 mmol) in CH_2Cl_2 (50 mL) was added *m*-CPBA (85%, 23.4 g, 127.5 mmol), in portions and in an ice-water bath, and the mixture was stirred at room temperature for 1 h. The resulting mixture was refluxed overnight, then cooled and filtered. The filter cake was washed with CH_2Cl_2 (3 × 30 mL). Evaporation of the solvent *in vacuo* gave a residue, which was directly used in the next reaction. **4-Methoxy-2,3-methylenedioxyphenol (9).** KOH (1.4 g, 25 mmol) in H_2O (10 mL) was added to the crude **8** (5.5 g, 25.8 mmol) in MeOH (20 mL), and the mixture was stirred for 2 h at room temperature. The mixture was concentrated to 10 mL and acidified with 2 M HCl (5 mL). The aqueous layer was extracted with $CHCl_3$ (3 × 20 mL), washed with H_2O (2 × 20 mL) and brine (20 mL), dried over anhydrous Na_2SO_4, and concentrated. The residue was purified by column chromatography (CC) (*n*-hexane/EtOAc, 3:1) to give **9** (4.38 g; two steps total yield 78%) as a white solid: **4-Methoxy-2,3-methylenedioxyphenol (9)**, yield 4.38 g, 78% mp 103-105 °C (lit.[12] mp 100-101 °C); ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.43 (1H, s, H-6), 6.42 (1H, s, H-5), 5.99 (2H, s, OCH_2O), 4.48 (1H, s, O*H*), 3.85 (1H, s, OCH_3).

Step 2

2-Hydroxy-3,4-methylenedioxy-5-methoxybenzaldehyde (10). $POCl_3$ (5.5 mL, 59.5 mmol) was added dropwise to DMF (10 mL, 129.4 mmol) over 15 min at 5 °C, then stirred at room temperature for 20 min followed by addition of **9** (2.5 g, 14.9 mmol) in portions. The mixture was slowly heated to 75 °C and then stirred at this temperature for 2 h. The resulting mixture was cooled to 5 °C and poured into H_2O (50 mL). After filtration, the filter cake was purified by CC (*n*-hexane/$CHCl_3$, 1:1) to give **10** (2.3 g, 79%) as a white solid: **2-Hydroxy-3,4-methylenedioxy-5-methoxybenzaldehyde (10)**, yield 2.3 g, 79% mp 181-182 °C (lit.[12] mp 179-180 °C); ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.83 (1H, C*H*O), 9.73 (1H, s, O*H*), 6.75 (1H, s, Ar-H), 6.18 (2H, s, OCH_2O), 3.93 (3H, s, OCH_3).

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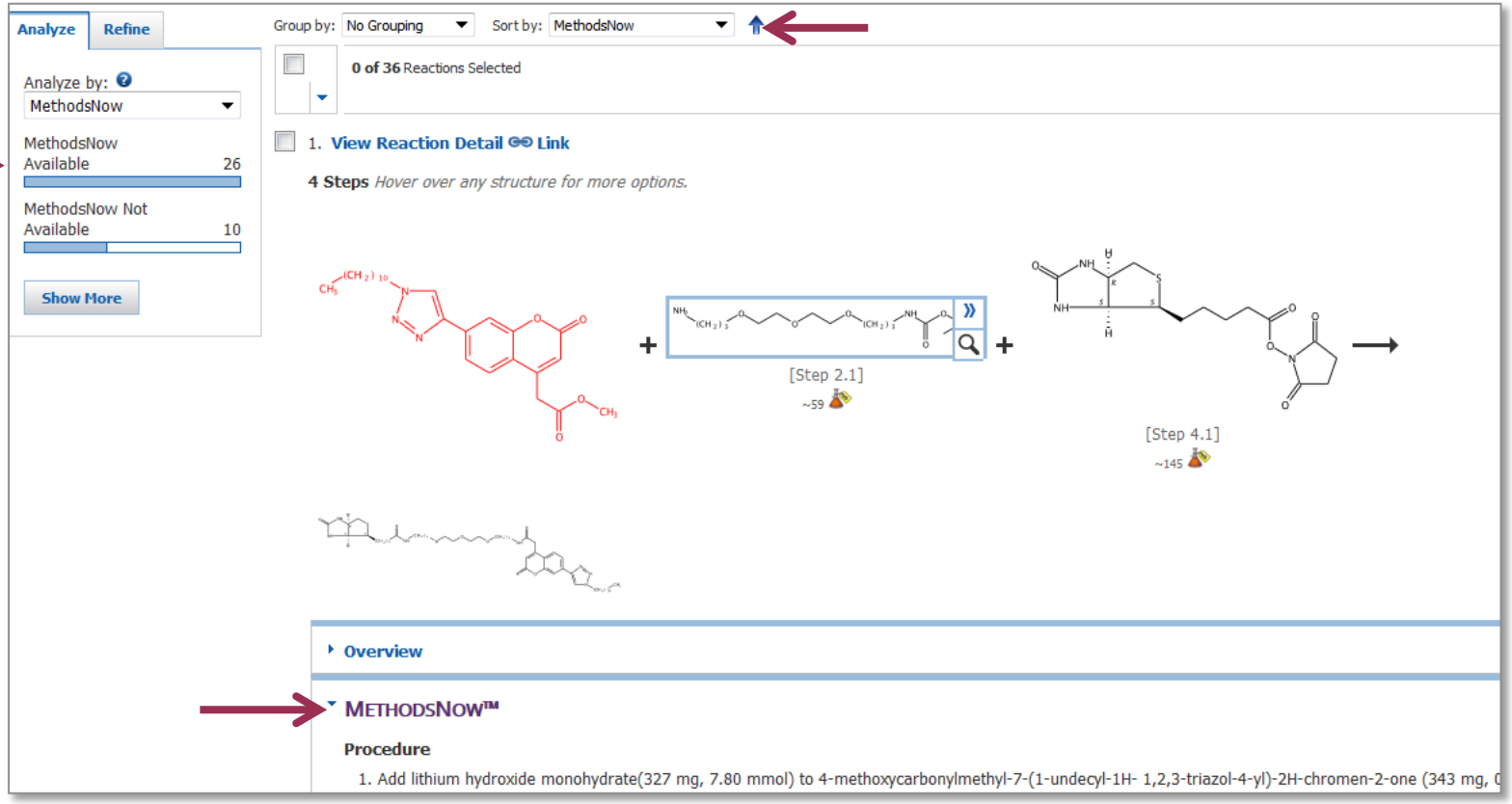
Analyze
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[Step 2.1]
~59
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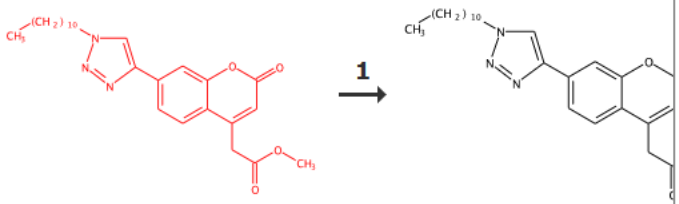
~145
Overview
METHODSNOW™
Procedure
1. Add lithium hydroxide monohydrate(327 mg, 7.80 mmol) to 4-methoxycarbonylmethyl-7-(1-undecyl-1H- 1,2,3-triazol-4-yl)-2H-chromen-2-one (343 mg,

MethodsNow

7-Triazolylcoumarin-based fluorescent tag system for stepwise, comparative assessment of small molecule microarrays

By Jeon, Moon-Kook; Kang, Myoung-Ku; Park, Koon Ha
From Tetrahedron, 68(30), 6038-6053; 2012
Published by Elsevier Ltd.

Reaction Steps 1 2 3 4



Products	2*H*-1-Benzopyran-4-acetic acid, 2-oxo-7-(1-undecyl-1*H*-1,2,3-tria 1384966-77-1
Reactants	2*H*-1-Benzopyran-4-acetic acid, 2-oxo-7-(1-undecyl-1*H*-1,2,3-tria 1384966-75-9
Reagents	Hydrochloric acid, CAS RN: 7647-01-0 Lithium hydroxide, CAS RN: 1310-65-2
Solvents	Water, CAS RN: 7732-18-5 Tetrahydrofuran, CAS RN: 109-99-9

MethodsNow

Procedure	1. Add lithium hydroxide monohydrate(327 mg, 7.80 mmol) to 4-methoxycarbonylmethyl-7-(1-undecyl-1H- 1,2,3-triazol-4-yl)-2H-chromen-2-one (343 mg, 0.780 mmol) in THF/water(25 mL/25 mL) at room temperature. 2. Stir the reaction mixture for 3 hours at room temperature. 3. Adjust pH 3-4 to the reaction mixture by adding 1 N hydrochloric acid. 4. Partition the reaction mixture between ethyl acetate and water. 5. Extract the aqueous layer with ethyl acetate. 6. Dry the combined organic layer over magnesium sulfate.
Scale	milligram
^{1}H NMR	^{1}H NMR (300 MHz, acetone- d_6): δ = 7.83 (s, 1H), 8.58 (s, 1H), 7.92 (d, *J* = 8.1 Hz, 1H), 7.84 (d, *J* = 8.1 Hz, 1H), 6.47 (s, 1H), 4.50 (t, *J* = 7.2 Hz, 2H), 3.99 (s, 2H), 2.00 (quintet, *J* = 7.2 Hz, 2H), 1.32-1.43 (m, 4H), 1.22-1.32 (m, 12H), 0.87 ppm (t, *J* = 6.8 Hz, 3H).
^{13}C NMR	^{13}C NMR (125 MHz, DMF-d_7, 60 °C): δ = 161.0, 155.1, 154.2, 146.5, 136.0, 127.2, 123.7, 122.1, 120.4, 115.3, 113.5, 51.1, 32.8, 29.9, 27.3, 23.5, 18.7, 14.7 ppm (decarboxylation occurred to give the corresponding 4-methyl derivative).
IR	IR (ATR, neat): ν = 3423, 2922, 2851, 1702 (2C=O, overlapped), 1619, 1561, 1375, 1154, 936, 852, 809 cm^{-1}.
HRMS	HRMS (EI): m/z calculated for $C_{24}H_{31}N_3O_4$: 425.2315 [M$^+$]; found: 425.2315.
Mass Spec	MS (ESI): m/z: 426 [M+H$^+$].
MP	235.5±0.8 °C.
CAS Method Number	3-352-CAS-78415

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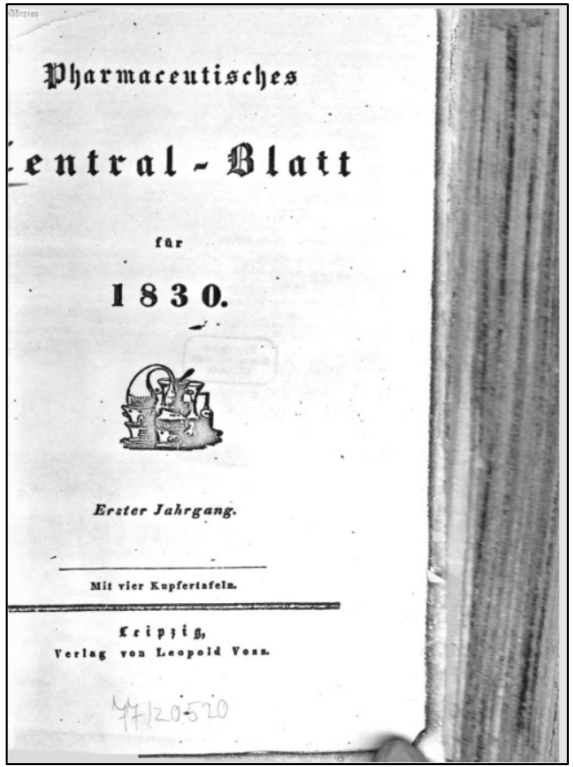
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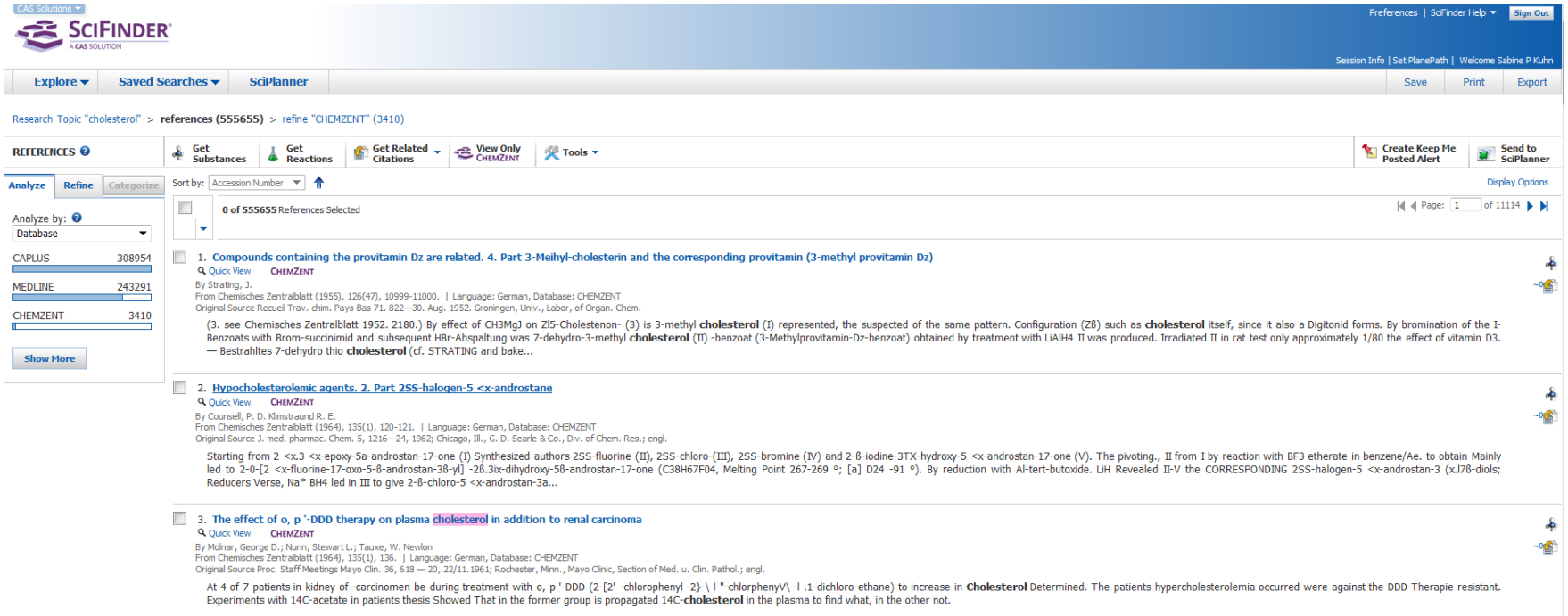

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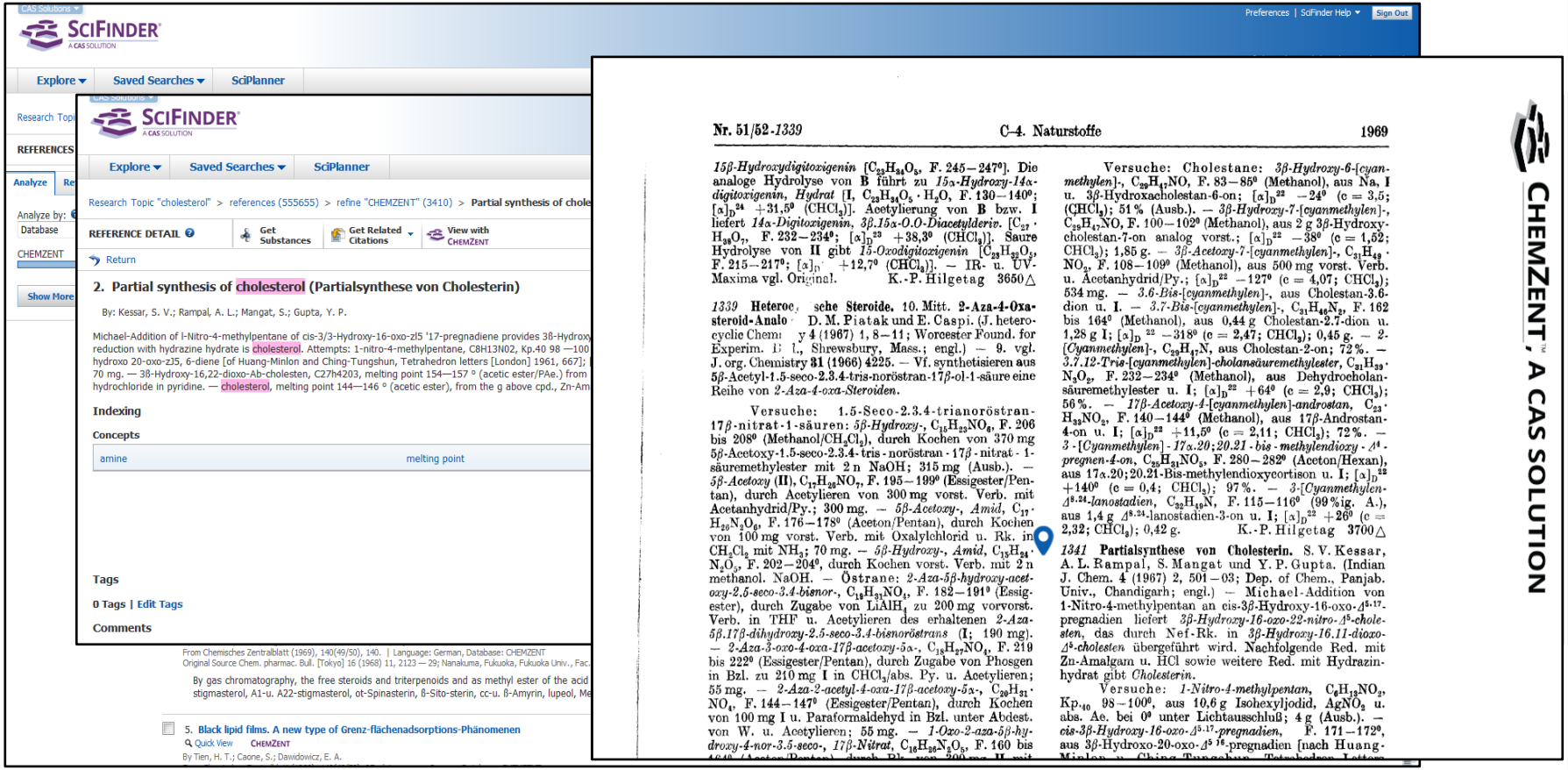

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