

Your SciFinderⁿ team

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Formulations in SciFinderⁿ and Formulus

hbz Online Meeting, July 1st 2020

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What are Formulations?

- Mixture of single components for a specific purpose
- Contains active ingredients and excipients (inactive ingredients)



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Who needs Formulations at Universities?

- Important research field in medicinal and pharmaceutical chemistry
- Publications with and without the collaboration of commercial companies
- Students working as Formulators after graduation

Method for preparing at least partially dried granules

By: Krumme, Markus; De Waard, Hans; Elbaz, Frantz; Kleinebudde, Peter; Moll, Klaus-Peter; Schmidt, Adrian
World Intellectual Property Organization, WO2019043615 A1 2019-03-07 | Language: English, Database: CPlus



In a method for preparing at least partially dried granules (56) an API (12), a base powder (14) and a granulation liquid (15) are fed to a granulator (16). The API (12), the base powder (14) and the granulation liquid (15) are mixed within the granulator (16) to produce an API/base powder/granulation liquid mixture. The API/base powder/granulation liquid mixture within the granulator (16) is heated to a heating temperature (TH) that exceeds an evaporation temperature (TE) of the granulation liquid (15) contained in the API/base powder/granulation liquid mixture. The API/base powder/granulation liquid mixture is discharged from the granulator (16) to produce the partially dried granules (56).

Universität Düsseldorf
& Novartis

Treatment for migraine with leucine and and/or acetylleucine

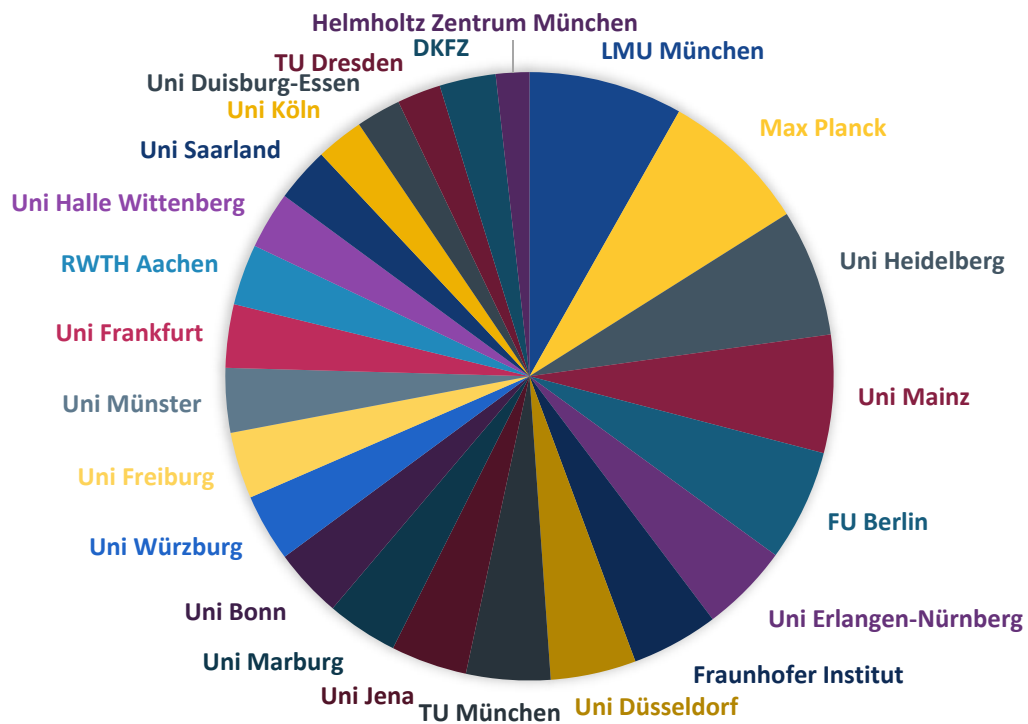
By: Strupp, Michael; Factor, Mallory
World Intellectual Property Organization, WO2018229738 A1 2018-12-20 | Language: English, Database: CPlus

A first aspect of the invention relates to leucine, acetylleucine, or a pharmaceutically acceptable salt thereof, for use in treating or preventing a migraine, or one or more symptoms associated therewith. A second aspect of the invention relates to a method of treating or preventing a migraine, or one or more symptoms associated therewith, in a subject, said method comprising administering to the subject a therapeutically or prophylactically effective amount of leucine, acetyl-leucine, or a pharmaceutically acceptable salt thereof.

LMU München
& Intrabio



Working with Formulations at Universities and in Gov. Research



Where are Formulations needed in industry?

- R&D
- Researcher who want to bring products to market
- Commonly discussed with this terminology in
 - Pharmaceutical industry
 - Agrochemistry
 - Cosmetic industry
- Also applicable for
 - Food, Paints, Adhesives, Cleaning Agents, ...

How can you search for formulations

- SciFinderⁿ
 - Text search for relevant terms
 - Combined text / substance search with active ingredient
 - **Inactive ingredients will most often NOT be indexed**

- Formulus
 - Specialized database and search tool for formulations
 - Active and inactive ingredients are searchable
 - Additional sources included (Drug Product inserts)
 - Refinement by purpose, physical form, a.o.

Available with
SciFinderⁿ access

Subscription to
Formulus needed

Formulations in SciFinderⁿ

The screenshot shows the SciFinderⁿ search interface. At the top, the SciFinderⁿ logo is on the left, followed by a search bar containing the text "Clofazimine and Clarithromycin and Rifabutin". To the right of the search bar are buttons for "References", "Draw", and a search icon. Below the search bar, the text "References (339)" is displayed. On the left side, there is a filter menu titled "CAS Solutions" with two options: "Formulus (90)" and "MethodsNow: Analysis (2)". A red line connects the "Formulus (90)" option to a central text box that reads "Limit to publications that contain indexed Formulations and refine by the formulation purpose". Below this menu is a yellow callout box with the text "Visible only with the respective subscription". On the right side, there is another filter menu titled "Formulation Purpose" with five options: "Antibacterial agents (22)", "Drugs (12)", "Antimicrobial agents (11)", "Anti-inflammatory agents (6)", and "Anti-infective agents (5)". A red line connects the top of this menu to the same central text box. Below this menu is a "View All" link and a yellow callout box with the text "Available with SciFinderⁿ access".

Formulations in SciFinderⁿ

Concepts

Antibiotics	Interleu
	Role: Bio
Cell cycle	
Colon carcinoma	Interleu
	Role: Bio
Combination chemotherapy	Interleu
	Role: Bio
Drug interactions, synergistic	Lung car
Drug screening	Lung ner
Homo sapiens	Mamma
Human	Matrix m
Immune checkpoint inhibitors	Metasta:
Immunomodulators	

Some formulation purposes coincident with a concept

Only active ingredients indexed as substances

Substances (16)

Sort: Relevance View: Partial

References Reactions Suppliers

1 23214-92-8 Absolute stereochemistry shown C ₂₇ H ₂₉ NO ₁₁ Doxorubicin 103K References 1,195 Reactions 56 Suppliers	2 59-05-2 Absolute stereochemistry shown C ₂₀ H ₂₂ N ₆ O ₅ Methotrexate 73K References 306 Reactions 110 Suppliers	3 50-07-7 Absolute stereochemistry shown C ₁₅ H ₁₈ N ₄ O ₅ Mitomycin C 25K References 187 Reactions 94 Suppliers
4 81103-11-9 	5 65271-80-9 	6 72559-06-9

Formulations in SciFinderⁿ

- ▼ Concepts
- ▼ Substances
- ▼ Formulations

Additional section
in Reference details

Information on
Formulations in SciFinderⁿ
available with standard
access

Partial information
available in SciFinderⁿ

Pharmaceutical Composition: Antibiotics

[View Formulus[®] Detail](#)

External link to Formulus –
Subscription needed

Location: Example Table 5

Purpose: Antibiotics

Target: cancer

Component	Function	Amount Reported
▲ Group: Erythromycin, 6-O-methyl-, mixt. with (9S,12E,14S,15R,16S,17R,18R,19R,20S,21S,22E,24Z)-16-(acetyloxy)-6,18,20-trihydroxy-14-methoxy-7,9,15,17,19,21,25-heptamethyl-1'-(2-methylpropyl)spiro[9,4-(epoxypentadeca[1,11,13]trienimino)-2H-furo[2',3':7,8]naphth[1,2-d]imidazole-2,4'-piperidine]-5,10,26(3H,9H)-trione and N,5-bis(4-chlorophenyl)-3,5-dihydro-3-[(1-methylethyl)imino]-2-phenazinamine	active agent, antibiotic	26.27 mg
Clarithromycin	active agent	10.00 mg/capsule
Rifabutin	active agent	45.00 mg/capsule
Clofazimine	active agent	10.00 mg/capsule
Polyethylene glycol	dispersing agent	50.00 mg/capsule
● Additional Components Reported in Full Text		
Ora Plus	vehicle	2.4 mL

Formulations in Formulus

Additional modul
Subscription needed to have access



Formulations ▾

+Clofazimine +Clarithromycin +Rifabutin



Searching directly in the formulations leads to more precise results

Filter by

- Industry
- Purpose
- Physical Form
- Information Included
- Document Type
- Organization
- Publication Year

No Min to No Max Apply

Purpose

- | | | |
|---|--|--|
| <input type="checkbox"/> Antibacterial agents (21) | <input type="checkbox"/> Otic solutions (3) | <input type="checkbox"/> Cardiovascular agents (1) |
| <input type="checkbox"/> Pharmaceutical formulations (21) | <input type="checkbox"/> Anesthetics (2) | <input type="checkbox"/> Dietary supplement formulations (1) |
| <input type="checkbox"/> Antimicrobial agents (15) | <input type="checkbox"/> Antidiabetic agents (2) | <input type="checkbox"/> Fungicides (1) |
| <input type="checkbox"/> Antiviral agents (14) | <input type="checkbox"/> Dermatological agents (2) | <input type="checkbox"/> Parasiticides (1) |
| <input type="checkbox"/> Anti-inflammatory agents (13) | <input type="checkbox"/> Drug delivery systems (2) | |
| <input type="checkbox"/> Antitumor agents (9) | <input type="checkbox"/> Imi | |
| <input type="checkbox"/> Anti-infective agents (8) | <input type="checkbox"/> Ne | |
| <input type="checkbox"/> Autoimmune disease medications (5) | <input type="checkbox"/> Wc | |
| <input type="checkbox"/> Antibiotics (4) | <input type="checkbox"/> An | |

Physical Form

- | | | |
|---|---|---|
| <input type="checkbox"/> Tablets (17) | <input type="checkbox"/> Candy (2) | <input type="checkbox"/> Inhalation drug delivery systems (1) |
| <input type="checkbox"/> Capsules (14) | <input type="checkbox"/> Elixirs (2) | <input type="checkbox"/> Lacquers (1) |
| <input type="checkbox"/> Solids (11) | <input type="checkbox"/> Grains (particles) (2) | <input type="checkbox"/> Liposomes (1) |
| <input type="checkbox"/> Suspensions (10) | <input type="checkbox"/> Particles (2) | <input type="checkbox"/> Medical plasters (1) |
| <input type="checkbox"/> Liquids (7) | <input type="checkbox"/> Pharmaceutical emulsions (2) | <input type="checkbox"/> Microemulsions (1) |
| <input type="checkbox"/> Powders (7) | <input type="checkbox"/> Pharmaceutical syrups (2) | <input type="checkbox"/> Nanoemulsions (1) |
| <input type="checkbox"/> Pharmaceutical ointments (6) | <input type="checkbox"/> Bandages (1) | <input type="checkbox"/> Oil-in-water emulsions (1) |
| <input type="checkbox"/> Sprays (6) | <input type="checkbox"/> Beads (1) | |

Specific refinement options



Formulations in Formulus

🧪 Formulation Detail

Formulation Ingredients

[Expand All Groups](#) | C

Component	Function	Amount Reported	Optionality
▲ Group: Erythromycin, 6-O-methyl-, mixt. with (9S,12E,14S,15R,16S,17R,18R,19R,20S,21S,22E,24Z)-16-(acetyloxy)-6,18,20-trihydroxy-14-methoxy-7,9,15,17,19,21,25-heptamethyl-1'-(2-methylpropyl)spiro[9,4-(epoxypentadeca[1,11,13]trienimino)-2H-furo[2',3':7,8]naphth[1,2-d]imidazole-2,4'-piperidine]-5,10,26(3H,9H)-trione and N,5-bis(4-chlorophenyl)-3,5-dihydro-3-[(1-methylethyl)imino]-2-phenazinamine	active agent, antibiotic	26.27 mg	Mandatory
Clarithromycin	active agent	10.00 mg/capsule	Mandatory
Rifabutin	active agent	45.00 mg/capsule	Mandatory
Clofazimine	active agent	10.00 mg/capsule	Mandatory
Polyethylene glycol	dispersing agent	50.00 mg/capsule	Mandatory
Polyoxyethylene sorbitan monooleate	wetting agent	6.66 mg/capsule	Mandatory
Cellulose	diluent	28.00 mg/capsule	Mandatory
Magnesium stearate	lubricant	4.68 mg/capsule	Mandatory
Sodium dodecyl sulfate	wetting agent	10.00 mg/capsule	Mandatory
Cellulose	diluent	60.42 mg/capsule	Mandatory
hard gelatin capsule	active agent	1 unit	Mandatory
Ora Plus	vehicle	2.4 mL	Mandatory

Pharmaceutical Composition: Antibiotics

Location: Example Table 5

Purpose: Antibiotics

Target: Neoplasm

Patent

Combination therapies for treating cancer

Assignee : RedHill Biopharma Ltd.
US20170095460
Language: English

[View Reference Detail](#)

[Patent PDF](#)

Formulations in Formulus

Formulation Detail

^ Process

dissolving 26.27 mg dry matter (corresponding to 8.64 mg API) in 2.4 milliliter Ora-plus and stirred (vortexed) at room temperature for 5 minutes followed by sonification until a homogenous suspension was achieved. the dosing solution was stored at ambient temperature, protected from light and used within the same dosing day (vortexed again before second application).

^ Effective Dose

Descriptor	Solvent	Details
rate of administration of RhB-104	-	36 mg/kg/day

Experimental Activity

Descriptor	Notes	Details
overall survival rate	overall survival rate of 3 pancreatic cancer mice treated with RhB-104 was evaluated. the results were expressed in the percentage of survived mice.	100 %

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Thank you for your kind attention- additional resources/support

- Videos:
 - [SciFinder-n short trainings \(Ø 10-15 Minutes recorded\)](#)
 - <https://www.cas.org/hbz/schulungseite>
 - [SciFinder-n extended trainings \(Ø 30 Minutes recoded- life sessions with Q and A\)](#)
 - <https://www.cas.org/about/events/scifinder-webinars>
- PDF material:
 - [SciFinder-n quick reference card](#)
 - <https://www.cas.org/sites/default/files/documents/SciFinder-n-ReferenceCard-HBZ.pdf>
 - [Differences SF Web and SciFinder-n incl. examples for all science areas](#)
 - <https://www.cas.org/sites/default/files/documents/HBZ-online-meeting0320final-rev.pdf>
 - [SciFinder-n tutorial in German \(big thank you! to the team at Univ Jena!\)](#)
 - <https://pinguin.biologie.uni-jena.de/pub3/1SciFinder-n/SciFinderNAnleitung.pdf>

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for your team, your co-scientists, your students, all of your BS or MS class