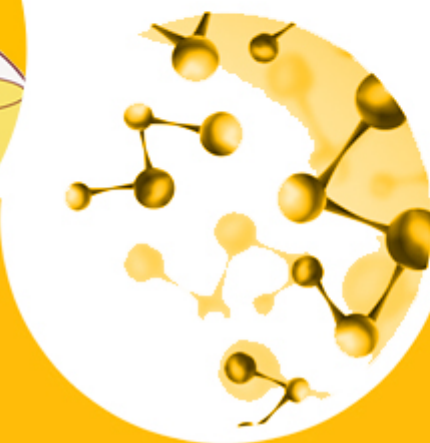




ChemRobotics

March 5, 2024

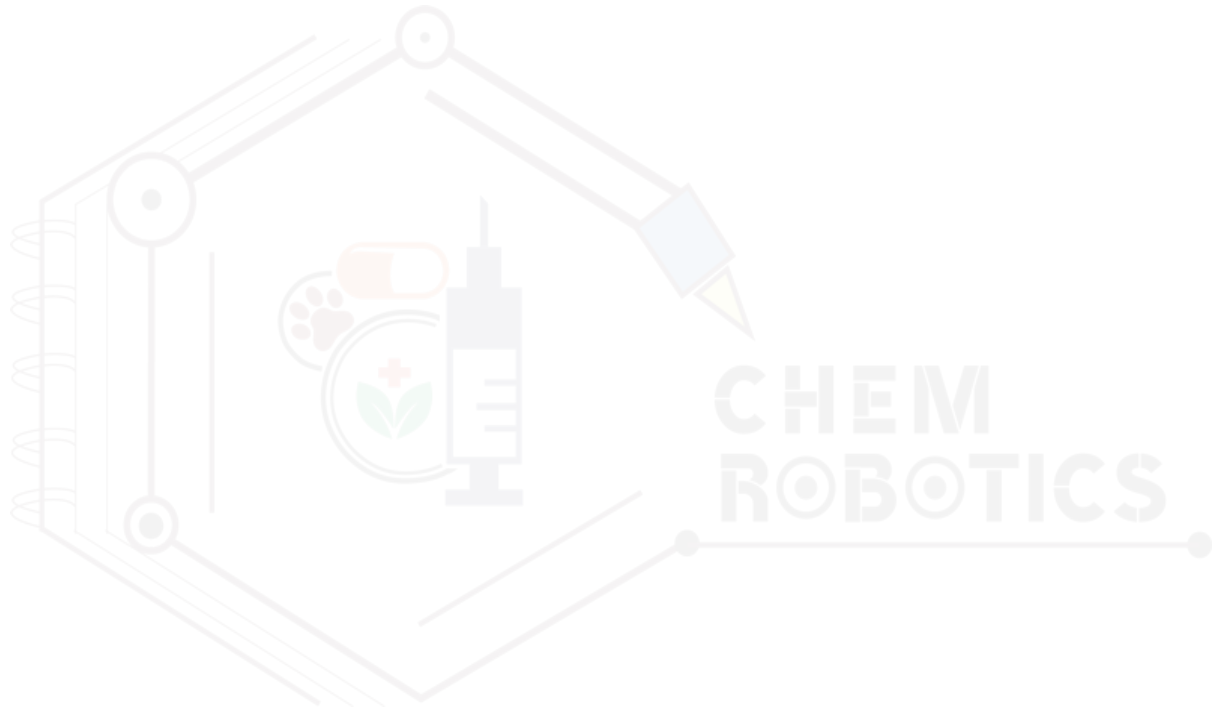
Agropat Product Landscape: TRIFLOXYSTROBIN



CHEM ROBOTICS

AGROPAT

PRODUCT LANDSCAPE



Content

• PRODUCT HIGHLIGHT
• DATA AVAILABILTY
• DESCRIPTION
• PRODUCT IDENTIFICATION
• PHYSICOCHEMICAL (COMPUTED PROPERTIES)
• PHYSICOCHEMICAL(EXPERIMENTAL PROPERTIES)
• KEYWORDS
• INVENT INFO
• JARVIS PATENT LANDSCAPE
• BIOLOGY
• APPROVAL STATUS
• COUNTRY WISE REGULATORY INFORMATION
• MAXIMUM RESIDUE LIMIT (MRL)
• INDIAN PESTICIDE DATABASE (IPD)
• AI PROCESS
• IMPURITIES
• CHEMICAL VENDORS
• FORMULATIONS / PREPARATIONS
• ANALYTICAL DATA
• MAMMALIAN TOXICOLOGY
• MAMMALIAN - HUMAN TOX
• SUPPLEMENTARY PROTECTION CERTIFICATE (SPC)
• DATA PROTECTION (Solo Product)
• KEY STARTING MATERIAL (KSM)
• ENVIRONMENTAL FATE
• METABOLITES
• GHS PICTOGRAM
• SALES DATA (Sales / Year (\$m.))
• SUPPLIER (S)
• PRICING
• PRODUCT TECHNOLOGIES
• LITERATURE REFERENCE
• GLOBAL SCIENTIFIC DOCUMENT ARCHIVAL (GSDA): REGULATORY & IP DOCUMENT ARCHIVAL

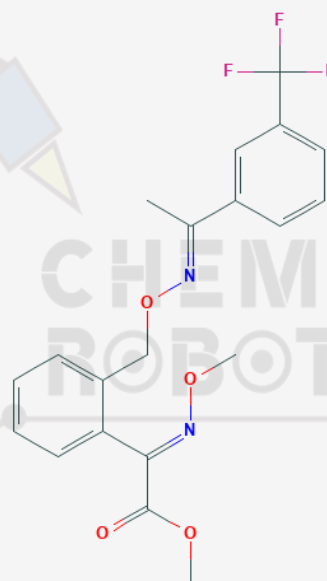
PRODUCT HIGHLIGHT

TRIFLOXYSTROBIN

INOVATORS LOGO



CHEMICAL STRUCTURE



NAME OF GENERIC CHEMISTRY

Strobilurin Fungicides

YEAR OF DISCOVERY

1990

LAUNCHING YEAR

2000

GB RN

504

LAUNCHING STATUS

LAUNCHED

INDICATION

FUNGICIDE

PRODUCT TYPE

AGROCHEMICAL

INNOVATOR(S)

IMPERIAL CHEMICAL

IUPAC

methyl (2E)-2-methoxyimino-2-[2-
 [[(E)-1-[3-(trifluoromethyl)phenyl]ethylideneamino]oxymethyl]phenyl]acetate

CAS RN

141517-21-7

CHEMICAL CLASSFungicides (Methoxyiminoacetate
Strobilurin Fungicides) [1]**RESISTANCE ACTION
COMMITTEE (RAC)**

MoA Code: C
 MoA: Respiration
 Target Code: C3
 Target Site: complex III: cytochrome
 bc1 (ubiquinol oxidase) at Qo site
 (cyt b gene)
 Group Name: QoI-fungicides
 (Quinone outside Inhibitors)
 Ref: FRAC Code List ©2020

PUBCHEM CID

11664966

SALES / YEAR (\$m.)

810

KEY MANUFACTURER / BRAND

Bayer (Flint, Stratego)

Application Rate (Rate g/ha)

Foliar, 62.5-187.5

APPLICATION TIMING

Foliar

**GENERIC CONSTRAINING DATE
(GCD)**

2011-08-16

**YEAR WISE OFF PATENT
MOLECULE**

2011

**GENERIC / PROPRIETARY /
DEVELOPING CANDIDATE /
WITHDRAWN**

GENERIC

MECHANISM OF ACTION (MOA)

Mitochondrial electron transport inhibition (MET III) by inhibition of ubiquinol oxidase at the Qo (quinone outside) binding site on cytochrome bc1 (complex III).

MAIN CROPS

Soybean
 Cereals
 F&V
 Maize
 Peanut
 Rice
 Turf
 Ornamentals

MAIN PESTS

Asian Rust
 Brown spot / Septoria leaf blight

Aerial Blight
 Leaf blight
 Powdery mildew
 Brown rust
 Septoria leaf spot
 Net blotch
 Leaf blotch
 Powdery mildew
 A wide range of diseases

COMBINING PARTNER / MIXTURE

EVERGOL Xtend (+ penflufen) (Bayer CropScience), Fox (+ prothioconazole) (Bayer CropScience), Nativo (+ tebuconazole) (Bayer CropScience), Prosper EverGol (+ metalaxyl+ penflufen+ clothianidin) (Bayer CropScience), Sphere (+ cyproconazole) (Bayer CropScience), Stratego (+ propiconazole) (Bayer CropScience)

Absolute (+ tebuconazole) (Bayer CropScience), Adament (+ tebuconazole) (Bayer CropScience), Agora (+ cyproconazole) (Bayer CropScience), Altus (+ triadimefon) (Bayer CropScience), Broadform (+ fluopyram) (Bayer CropScience), Consist Full (+ tebuconazole) (Bayer CropScience), Coronet (+ tebuconazole) (Bayer CropScience), Cripton (+ prothioconazole) (Bayer CropScience), Cripton Pro (+ bixafen + prothioconazole) (Bayer CropScience), Delaro (+ prothioconazole) (Bayer CropScience), Escolta (+ cyproconazole) (Bayer CropScience), Exteris Stressgard (+ fluopyram) (Bayer CropScience), Flint Max (+ tebuconazole) (Bayer CropScience), Flint Plus (+ captan) (Bayer CropScience), Flint Star (+ pyrimethanil) (Bayer CropScience), Fox Xpro (+ bixafen + prothioconazole) (Bayer CropScience), Interface Stressgard (+ iprodione) (Bayer CropScience), Jaunt (+ fluoxastrobin+ prothioconazole) (Bayer CropScience), Luna Sensation (+ fluopyram) (Bayer CropScience), Madison (+ prothioconazole) (Bayer CropScience), Mobius (+ prothioconazole) (Bayer CropScience), Mystic (+ pyrimethanil) (Bayer CropScience), Rombus (+ propiconazole) (Bayer CropScience), Sfera (+ cyproconazole) (Bayer CropScience), Stratego YLD (+ prothioconazole) (Bayer CropScience), Tartan Stressgard (+ triadimefon) (Bayer CropScience), Trigo (+ triadimefon) (Bayer CropScience), Trilex AL (+ metalaxyl) (Bayer CropScience), Trilex Optimum (+ metalaxyl+ captan) (Bayer CropScience), Trilex Star (+ thiophanate-methyl+ metalaxyl+ captan) (Bayer CropScience), Zephyr (+ prothioconazole) (Bayer CropScience), Éclair (+ cymoxanil) (Bayer CropScience)

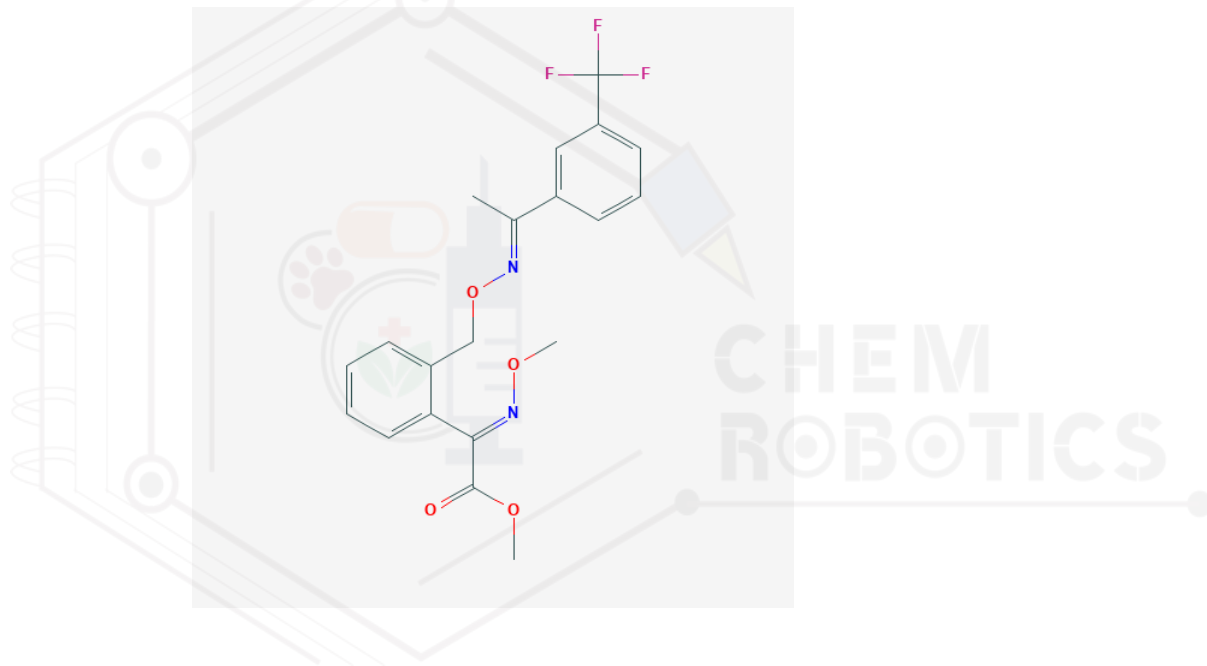
FORMULATION GLOBALLY

Flint (Bayer CropScience)

Further products, not always verified by the company. (Names that are a composite of company name and common name, and those used only in home and garden outlets, are not listed. Suffixes are omitted if they do not signify a difference in the a.i. components) Compass (Bayer CropScience), Consist (Bayer CropScience), Gate (Dofal), Gem (Bayer CropScience), Rapidox (Agri Sciences), Sphere Max (Bayer CropScience), Swift (Bayer CropScience), Tega (Bayer CropScience), Trilex (Bayer CropScience), Twist (Bayer CropScience), Zato (Bayer CropScience)

Active Ingredient	TRIFLOXYSTROBIN
Product Type	AGROCHEMICAL
CAS No.	141517-21-7
IUPAC	methyl (2E)-2-methoxyimino-2-[2-[[[(E)-1-[3-(trifluoromethyl)phenyl]ethylideneamino]oxymethyl]phenyl]acetate
Trade Names / Proprietary Name	Trifloxystrobin: 1. Flint (Bayer CropScience) 2. GEM (Bayer CropScience) 3. Gem RC (Bayer CropScience) 4. Gem 500 SC (Bayer CropScience) 5. Trifloxystrobin Technical (Bayer CropScience) 6. Stratego 7. Compass

CHEMICAL STRUCTURE



PRODUCT DESCRIPTION

Trifloxystrobin: It is the methyl ester of (2E)-(methoxyimino)[2-(((E)-{1-[3-(trifluoromethyl)phenyl]ethylidene}amino)oxy)methyl]phenyl]acetic acid. A foliar applied fungicide for cereals which is particularly active against Ascomycetes, Deuteromycetes and Oomycetes. It has a role as a mitochondrial cytochrome-bc1 complex inhibitor and an antifungal agrochemical. It is an oxime O-ether, an organofluorine compound, a methyl ester and a methoxyiminoacetate strobilurin antifungal agent. Trifloxystrobin is a systemic broad-spectrum foliar strobilurin fungicides that enters the aquatic environment during agricultural application.

PRODUCT IDENTIFICATION

CHEMICAL CLASS

Fungicides (Methoxyiminoacetate Strobilurin Fungicides) [1]

RESISTANCE ACTION COMMITTEE (RAC)

MoA Code: C

MoA: Respiration

Target Code: C3

Target Site: complex III: cytochrome bc1 (ubiquinol oxidase) at Qo site (cyt b gene)

Group Name: QoI-fungicides (Quinone outside Inhibitors)

Ref: FRAC Code List ©2020

MECHANISM OF ACTION (MOA)

Mitochondrial electron transport inhibition (MET III) by inhibition of ubiquinol oxidase at the Qo (quinone outside) binding site on cytochrome bc1 (complex III).

USE

Trifloxystrobin works by interfering with respiration in plant pathogenic fungi. The site of action of Strobilurin compounds is located in the mitochondrial respiration pathway as a result of this mode of action, Trifloxystrobin is a potent inhibitor of fungal spore germination and mycelial growth. Trifloxystrobin is a broad-spectrum foliar fungicide that has high levels of activity against many fungal pathogens within the ascomycete, deuteromycete, basidiomycete, and oomycete classes. Trifloxystrobin controls of Ascomycetes, Deuteromycetes, Basidiomycetes and Oomycetes in cereals, soybeans, maize, rice, cotton, peanuts, sugar beets, sunflowers, pome fruit, stone fruit, tropical fruit, bananas, grapes, soft fruit, ornamentals, turf and many vegetables, at 50–550 g/ha.

PRODUCT CLASSIFICATION

PESTICIDE

SYNONYMS / COMMON NAME

1. Trifloxystrobin
2. 141517-21-7
3. CHEBI: 81833
4. CGA 279202
5. methyl (2E)-2-methoxyimino-2-[2-[[[(E)-1-[3-(trifluoromethyl)phenyl]ethylideneamino]oxymethyl]phenyl]acetate
6. SCHEMBL19148
7. SCHEMBL9880011
8. CHEMBL1897483
9. AKOS030621531

10. NCGC00163847-01
11. NCGC00163847-02
12. NCGC00163847-03
13. SC-44613
14. Trifloxystrobin 10 microg/mL in Cyclohexane
15. C18562
16. A807769
17. Trifloxystrobin, PESTANAL(R), analytical standard
18. J-007507
19. (2E)-2-methoxyimino-2-[2-[[[(E)-1-[3-(trifluoromethyl)phenyl]ethylideneamino]oxymethyl]phenyl]acetic acid methyl ester
20. alpha-[[Z]-Methoxyimino]-2-[[[(1Z)-1-[3-(trifluoromethyl)phenyl]ethylidene]amino]oxy]methyl]benzeneacetic acid methyl ester
21. methyl (2E)-(methoxyimino)2-[[[(1E)-1-[3-(trifluoromethyl)phenyl]ethylidene]amino]oxy]methyl]phenyl]acetate
22. methyl (2E)-(methoxyimino)[2-[[[(E)-{1-[3-(trifluoromethyl)phenyl]ethylidene]amino]oxy]methyl]phenyl]acetate
23. methyl (2E)-2-methoxyimino-2-[2-[[[(E)-1-[3-(trifluoromethyl)phenyl]ethylideneamino]oxymethyl]phenyl]ethanoate
24. methyl (alphaE)-alpha-(methoxyimino)-2-[[[(1E)-1-[3-(trifluoromethyl)phenyl]ethylidene]amino]oxy]methyl]benzeneacetate
25. methyl (E)-methoxyimino-[(E)-alpha-[1-(alpha,alpha,alpha-trifluoro-m-tolyl)ethylideneamino]oxy]-o-tolyl]acetate
26. Methyl methoxyimino(alpha-(1-(alpha,alpha,alpha-trifluoro-3-tolyl)ethylideneamino)oxy)-2-tolyl]acetate

PubChem Substance and Compound databases - NCBI (U.S. National Library of Medicine) <https://pubchem.ncbi.nlm.nih.gov/>

PRODUCT TYPE

AGROCHEMICAL

TRADE NAMES / PROPRIETARY NAME

Trifloxystrobin:

1. Flint (Bayer CropScience)
2. GEM (Bayer CropScience)
3. Gem RC (Bayer CropScience)
4. Gem 500 SC (Bayer CropScience)
5. Trifloxystrobin Technical (Bayer CropScience)
6. Stratego
7. Compass

RELEATED COMPOUNDS (AI'S)

Methoxyiminoacetate Strobilurin Fungicides:

kresoxim-methyl
trifloxystrobin

CAS NAME

methyl (aE)-a-(methoxyimino)-2-[[[(1E)-1-[3-(trifluoromethyl)phenyl]ethylidene]amino]oxy]methyl]benzeneacetate

IUPAC

methyl (2E)-2-methoxyimino-2-[2-[[[(E)-1-[3-(trifluoromethyl)phenyl]ethylideneamino]oxymethyl]phenyl]acetate

GENERIC CONSTRAINING DATE :

2011-08-16

US EPA CHEMICAL CODE :

129112

PESTICIDE TYPE :

SYSTEMIC

SUBSTANCE ORIGIN :

Synthetic

YEAR OF DISCOVERY :

1990

REGISTERED PRODUCTS IN INDIA 9(4) :

LAUNCHED

INCHI :

InChI=1S/C20H19F3N2O4/c1-13(14-8-6-9-16(11-14)20(21,22)23)24-29-12-15-7-4-5-10-17(15)18(25-28-3)19(26)27-2/h4-11H,12H2,1-3H3/b24-13+,25-18+

INCHI KEY :

ONCZDRURRATYFI-TVJDWZFNSA-N

CANONICAL SMILES :CC(=NOCC1=CC=CC=C1C(=NOC)C(=O)OC)C2=CC(=CC=C2)C(F)(F)F**LAUNCH YEAR :**

2000

SMILES CODE :C/C(=N\OCC1=CC=CC=C1/C(=N\OC)/C(=O)OC)/C2=CC(=CC=C2)C(F)(F)F**MOLECULAR FORMULA :**

C20H19F3N2O4

EC. NO. :

604-237-6

PUBCHEM CID

11664966

INVENT INFO

COMPOUND PATENT / 1ST DISCLOSURE:

Patent Information:

COMPOUND PATENT

1. Patent Number: US5238956A

Assignee: Imperial Chemical Industries Ltd

Publication Date: 1993-08-24

Est. Exp.: 2011-08-16

Application Date: 1991-08-16

Equivalents: EP0472300A2; EP0472300A3; US5238956A; US5346902A

Indian Equivalents: Not Found

Title: Fungicidal aromatic dioxime

By: John M. Clough, Christopher R. A. Godfrey, Paul J. de Fraine

Abstract: Fungicidal compounds of the formula (I) and stereoisomers thereof, wherein Y is a specified small group or single atom and R1 and R2 are selected from a wide range of specified substituents.1. US 6326399 (BASF A.-G., Germany).

PROCESS PATENT

2. Patent Number: CN1560027A

Assignee: Tongji University

Publication Date: 2005-01-05

Est. Exp.: 2024-03-05

Application Date: 2004-03-05

Family: CN100357263C; CN1560027A

Indian Equivalents: Not Found

Title: Preparation process of oxime strain ester

Author: Zhuliang Zhu; Ronghua Zhang; Lili Yuan

Abstract: The invention discloses a trifloxystrobin preparing method, including the steps as follows: (a) using ortho-methyl hypnone as raw material and using potassium permanganate to oxidize so as to obtain 2-(2'-methyl-phenyl)-2-carbonyl acetic acid; (b) making the product in step (a) react with methanol to obtain 2-(2'-methyl-phenyl)-2-carbonyl methyl acetate; (c) bromizing the product in step (b) to obtain 2-(2'-bromomethyl-phenyl)-2-carbonyl methyl acetate; (d) making the product in step (c) react with methoxy amine to obtain (E)-2-(2'-bromomethyl-phenyl)-2-carbonyl methyl acetate-O-methyl ketone oxime; (e) making the product in step (d) react with meta-trifluoromethyl hypnone oxime to obtain the product trifloxystrobin. It reduces the discharge of large amount of waste water in course of oxidization reaction, avoids esterification by adopting methyl- chloroformate, most operating conditions are moderate.

COMBINATION PATENT

3. Patent Number: WO2002021918A1

Assignee: Syngenta Participations Ag

Publication Date: 2002-03-21

Est. Exp.: 2021-09-10

Application Date: 2001-09-10

Family: AR030637A1; AT266316T; AU1222702A; AU2002212227B2; BR0113815A; CA2421226A1; CN1455641A; CR6915A; DE60103292T2; ECSP034508A; EP1317178A1; EP1317178B1; ES2217194T3; GT200100182A; HU0301024A2; HU0301024A3; JP2004518623A; KR20030029977A; MXPA03002117A; PL360142A1; RU2270564C2; TWI220381B; WO0221918A1; ZA200301569B; US2003189958A1; IN348/CHENP/2003

Indian Equivalents: IN348/CHENP/2003 (Abandoned)

Title: Fungicidal compositions

Author: Cosima Nuninger; Martin Zeller

Abstract: It has now been found that the use of: A) a N-sulfonyl-valine-amide of formula (I) wherein R1 is hydrogen, C1-4alkyl, C3-6cycloalkyl or halophenyl, and R2 is C1-4alkyl; in association with B) either compounds of formulae II to XII is particularly effective in combating or preventing fungal diseases of crop plants. These combinations exhibit synergistic fungicidal activity. Prominent examples for the compounds of formulae II to XII are: acibenzolar-S-methyl, azoxystrobin, chlorothalonil, cymoxanil, dimethomorph, fluazinam, fludioxonil, imazalil, S-imazalil, mancozeb, metalaxyl, metalaxyl-M,

picoxystrobin, pyraclostrobin (BAS 500F) and trifloxystrobin.

COMBINATION PATENT

4. Patent Number: WO2003015515A1

Assignee: Bayer Cropscience Ag, Erdelen-Lubos, Angelika

Publication Date: 2003-02-27

Est. Exp.: 2022-08-05

Application Date: 2002-08-05

Family: AR041780A1; AR087990A2; AU2002333323B2; BR0211973A; BR0211973B1; CA2457570A1; CA2457570C; DE10140108A1; EG23362A; EP1423003A1; EP1423003B1; EP2301348A1; EP2316268A1; HU0401319A2; HU0401319A3; HU2304777B1; HU230849B1; HU230850B1; JP2004538325A; JP2010195815A; JP4810061B2; KR100944729B1; KR20040021687A; MX280562B; MXPA04001321A; PL209244B1; PL368404A1; US2005009703A1; US2012136032A1; US2012142528A1; US2013303527A1; US2014323525A1; US8101772B2; US8461349B2; US9326514B2; WO03015515A1; ZA200401182B

Indian Equivalents: Not Found

Title: Fungicidal active substance combinations containing trifloxystrobin

Author: Ulrike Wachendorff-Neumann; Astrid Mauler-Machnik; Hirohisa Ohtake; Christoph Erdelen

Abstract: The invention relates to novel active substance combinations comprised of a known oxime ether derivative (trifloxystrobin) and of known insecticidal active substances selected from the group consisting of imidacloprid, thiacloprid, acetamiprid, nitenpyram, thiamethoxam, clothiamidin and of dinotefuran, which are extremely well-suited for controlling phytopathogenic fungi and insects.

COMBINATION PATENT

5. Patent Number: WO2003073852A2

Assignee: Basf Aktiengesellschaft

Publication Date: 2003-09-12

Est. Exp.: 2023-02-26

Application Date: 2003-02-26

Family: AR038706A1; AT326844T; AT397860T; AU2003210354A1; AU2003210354B2; AU2003210354B9; AU2008229851A1; AU2008229851B2; AU2008229854A1; AU2008229854B2; BR0307729A; BR0307729B1; CA2477000A1; CA2477000C; CA2743460A1; CA2743460C; CA2812887A1; CA2812887C; CA2858118A1; CA2858118C; CL2010000658A1; CN1328956C; CN1638637A; CO5611068A2; DK1482798T3; DK1642499T3; EA011235B1; EA013641B1; EA014804B1; EA017870B1; EA200401133A1; EA200701899A1; EA200701900A1; EA201001208A1; EP1482798A2; EP1482798B1; EP1642499A2; EP1642499A3; EP1642499B1; EP1929868A2; EP1929868A3; EP1929868B1; ES2264768T3; ES2304657T3; ES2623443T3; IL163309A; JP2005526735A; JP4477358B2; KR100951210B1; KR20040096635A; MXPA04007477A; NZ534781A; NZ555498A; NZ567833A; PL210584B1; PL213742B1; PL219127B1; PL219750B1; PL372340A1; PL394171A1; PL398430A1; PL404554A1; PT1482798E; PT1642499E; SI1482798T1; SI1642499T1; UA78550C2; US10645930B2; US2005101639A1; US2015313226A1; US2015313227A1; US2016143282A2; WO03073852A2; WO03073852A3; ZA200407893B; IN2160/CHENP/2004

Indian Equivalents: IN222655B (IN2160/CHENP/2004)

Title: Fungicidal mixtures based on prothioconazole and a strobilurin derivative

Author: Eberhard Ammermann; Reinhard Stierl; Gisela Lorenz; Siegfried Strathmann; Klaus Schelberger; V. James Spadafora; Thomas Christen

Abstract: Disclosed is a fungicidal mixture containing (1) 2-[2-(1-chlorocyclopropyl)-3-(2-chlorophenyl)-2-hydroxypropyl]-2,4-dihydro-[1,2,4]-triazole-3-thion of formula (I) or the salts or adducts thereof, and at least one additional fungicidal compound or the salts or adducts thereof, selected among (2) trifloxystrobin of formula (II), (3) picoxystrobin of formula (III), (4) pyraclostrobin of formula (IV), (5) dimoxystrobin of formula (V), and (6) a strobilurin derivative of formula (VI), in a synergistically active quantity.

COMBINATION PATENT

6. Patent Number: WO2004000021A1

Assignee: Bayer Cropscience Ag

Publication Date: 2003-12-31

Est. Exp.: 2023-06-12

Application Date: 2003-06-12

Family: AR039701A1; AU2003237930A1; BR0312103A; CA2490303A1; DE10228102A1; EP1519651A1; GT200300123A; JP2005530831A; PL374390A1; RU2005101615A; RU2331192C2; TW200406153A; TWI274549B; US2006004070A1; WO2004000021A1; ZA200410269B; NZ537357A

Indian Equivalents: Not Found

Title: Fungicidal active substance combinations

Author: Ulrike Wachendorff-Neumann; Astrid Mauler-Machnik; Manfred Jautelat

Abstract: The invention relates to the novel active substance combination on the basis of 2-(alpha (((alpha-methyl-3-trifluoromethylbenzyl)imino)oxy)-o-tolyl) glyoxylic acid methylester-O-methyloxim of formula (I) (trifloxystrobin) and the active substance of formula (II) (prothioconazole) mentioned in the description which has excellent fungicidal properties.

Non-Pat. Reference:

Polymorphic study on trifloxystrobin

1. Role of solvent properties and composition on the solid-liquid equilibrium of trifloxystrobin and thermodynamic analysis

By: Qu, Haibin; Zhao, Yanxiao; Du, Shichao; Li, Peiyi; Wu, Songgu

This paper is to critically analyze the effects of solvent properties and compn. on the soly. of trifloxystrobin. The soly. of trifloxystrobin in eight mono-solvents and two binary solvents was detd. at temps. ranging from 283.15 K to 318.15 K. Among the selected mono-solvents, the soly. of trifloxystrobin in alcs. was greater than that in alkanes and obeyed the following order: n-propanol > ethanol > methanol > 2-propanol > n-butanol > n-hexane > n-heptane > n-octane. For the binary solvents, as the mole fraction of good solvent (methanol/ethanol) increased, the soly. of trifloxystrobin increased monotonically at the set temps. In addn., the obtained soly. data was correlated with the Apelblat, NRTL, Wilson and Apelblat Jouyban Acree model, and these models were in good agreement with the exptl. values. The NRTL model given the results of entropy, enthalpy and Gibbs free energy, which indicated that the dissoln. was spontaneous, endothermic and entropically driven. The powder X-ray diffraction patterns proved that there was no polymorphic transformation during the soly. measurement.

Source: Journal of Molecular Liquids. Volume 294, 111566 pp. Journal; Online Computer File, 2019

CODEN: JMLIDT

ISSN: 0167-7322

DOI: 10.1016/j.molliq.2019.111566

Company/Organization: State Key Laboratory of Chemical Engineering, School of Chemical Engineering and Technology, Tianjin University

Tianjin, Peop. Rep. China 300072

INNOVATOR (S) :

IMPERIAL CHEMICAL

HISTORY / DEVELOPMENT / LICENCING / COMMERCIALISATION :

Trifloxystrobin : Reported by P. Margot et al. (Proc. Br. Crop prot conf. Pests dis., 1998, 2, 375). Introduced by novartis crop protection ag (became syngenta ag) in Switzerland, South Africa and USA in 1999. All rights sold to Bayer AG in 2000.

Patents EP 00460575; there are also a series of production process, formulation, mixture, and application method patents.

Manufacturers Bayer CropScience.

Background

Novartis developed trifloxystrobin and first introduced the product in 2000, mainly under the brand names Flint and Twist. The product was subsequently acquired by Bayer on the formation of Syngenta. The key crop use was initially targeted at cereals, where the product benefited from its broad spectrum of control, although soybeans, maize, rice and fruit & vegetable use is now more significant. As with many other strobilurins, the main country is now Brazil, primarily for use on soybeans, whilst US maize is the next most significant market. Nativo (trifloxystrobin / tebuconazole) has been launched in a number of crop and country markets, with recent introductions including use on sugarcane in Brazil, representing Bayer's entry into the sugarcane fungicide sector.

In 2014 Bayer invested €100 million in an expansion of the production capabilities at its site in Muttenz, Switzerland, which is primarily used to produce the Nativo (trifloxystrobin / tebuconazole) range. In recent years trifloxystrobin has been incorporated in a number of mixture products with Bayer's SDHI fungicides fluopyram and penflufen, which has expanded usage into a number of niche crop sectors such as nuts, vegetables, fruit and other field crops.

2018 - In Chile, the Bayer introduced the fungicide Cripton Xpro (bixafen, prothioconazole and trifloxystrobin) for the control of various diseases on rapeseed and wheat.

2018 - The foliar Bayer fungicide product Luna Sensation (fluopyram and trifloxystrobin) was launched in Canada for the control of various diseases including Sclerotinia rot, powdery mildew, and Monilinia on stone fruit, root vegetables, cucurbits, leafy green vegetables, leafy petiole vegetables, brassicas and hops.

During 2019, the company launched its dry rice seed treatment fungicide Routine Start (trifloxystrobin / isotianil) in China, and Cripton Xpro (bixafen / prothioconazole / trifloxystrobin) in Chile for use on wheat and barley, while also registering its fungicide Delaro (prothioconazole / trifloxystrobin) in Canada for use on cereals.

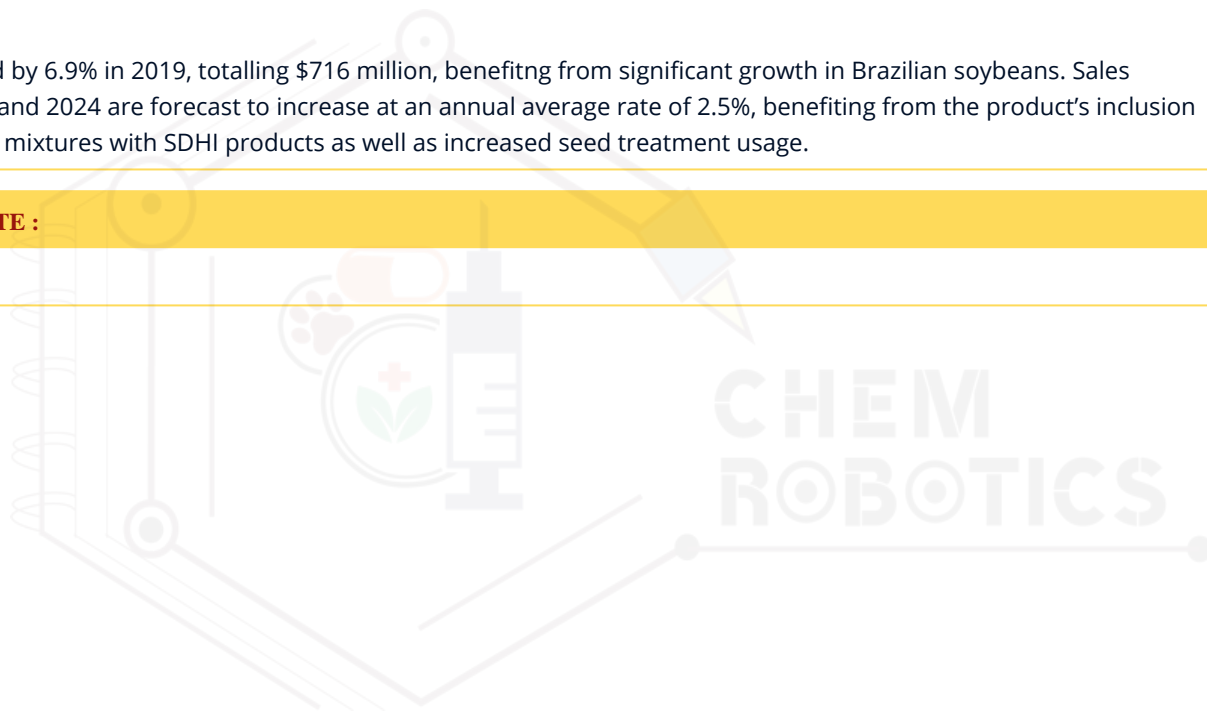
In 2020, Bayer gained approval in the US for Delaro Complete (fluopyram / trifloxystrobin / prothioconazole), representing the company's first fungicide in the US to possess three modes of action.

Sales

Sales increased by 6.9% in 2019, totalling \$716 million, benefiting from significant growth in Brazilian soybeans. Sales between 2019 and 2024 are forecast to increase at an annual average rate of 2.5%, benefiting from the product's inclusion in a number of mixtures with SDHI products as well as increased seed treatment usage.

PRIORITY DATE :

22.08.1990



PHYSICOCHEMICAL(COMPUTED PROPERTIES)

SUMMARY PHYSI CHEM (COMPUTED) :

Molecular Weight: 408.4
 XLogP3-AA: 4.9
 Hydrogen Bond Donor Count: 0
 Hydrogen Bond Acceptor Count: 9
 Rotatable Bond Count: 8
 Exact Mass: 408.12969158
 Monoisotopic Mass: 408.12969158
 Topological Polar Surface Area: 69.5 Å²
 Heavy Atom Count: 29
 Formal Charge: 0
 Complexity: 607
 Isotope Atom Count: 0
 Defined Atom Stereocenter Count: 0
 Undefined Atom Stereocenter Count: 0
 Defined Bond Stereocenter Count: 2
 Undefined Bond Stereocenter Count: 0
 Covalently-Bonded Unit Count: 1
 Compound Is Canonicalized: Yes

MOLECULAR WEIGHT

408.377 g/mol

HYDROGEN BOND DONOR COUNT

0

HYDROGEN BOND ACCEPTOR COUNT

9

ROTATABLE BOND COUNT

8

COMPLEXITY

607

TOPOLOGICAL POLAR SURFACE AREA

69.5 Å²

MONOISOTOPIC MASS

408.13 g/mol

EXACT MASS

408.13 g/mol

LOGP (COMPUTED)

4.9

COMPOUND IS CANONICALIZED

True

FORMAL CHARGE

0

HEAVY ATOM COUNT

29

DEFINED ATOM STEREOCENTER COUNT

0

UNDEFINED ATOM STEREOCENTER COUNT

0

DEFINED BOND STEREOCENTER COUNT

2

**UNDEFINED BOND
STEREOCENTER COUNT**

0

ISOTOPE ATOM COUNT

0

**COVALENTLY-BONDED UNIT
COUNT**

1

PHYSICOCHEMICAL(EXPERIMENTAL PROPERTIES)**SUMMARY PHYSICOCHEMICAL PROPERTIES (EXPERIMENTAL) :**

Physical Description:

Color: White powder

Odor: Odorless

MELTING POINT (°C): 72.9 deg C

BOILING POINT (°C): Approximately 312 deg C

DEGRADATION POINT (°C): 285

FLASHPOINT (°C): >70.00 deg C (>158.00 deg F)

AQUEOUS SOLUBILITY (mg/l): 0.61

SOLUBILITY IN METHANOL (mg/l): 76000

SOLUBILITY IN ACETONE (mg/l): 500000

SOLUBILITY IN ETHYL ACETATE (mg/l): 500000

DENSITY (g/ml): 1.36 g/mL at 21 deg C

BULK DENSITY (g/ml) / SPECIFIC GRAVITY: 1.36

VAPOR PRESSURE: 2.55X10-8 mm Hg at 25 deg C

LOGP (OCTANOL-WATER): log Kow = 4.5 at 25 deg C

Stability: : Stable under recommended storage conditions.

pH: 7.7 at 25 deg C

DISSOCIATION CONSTANTS (pKa): Trifloxystrobin does not show any dissociation in the pH ranges 2 to 12.

HENRYS LAW CONSTANT AT 25(C) (Pam3 mol-1): 2.30 X 10-03

GUS LEACHING POTENTIAL INDEX: -0.30

SCI-GROW GROUNDWATER INDEX (µg /l) for a 1Kg/ha or 1l/ha APPLICATION RATE: 1.43 X 10-05

MAXIMUM UV-VIS ABSORPTION l/mol/cm: 250.7nm = 17500, no absorption between 340-750nm

SURFACE TENSION (mN/m): 65.3

Ref: PubChem Substance and Compound databases - NCBI (U.S. National Library of Medicine) <https://pubchem.ncbi.nlm.nih.gov/>

Composition: Tech. is 97.5%.

Molecular Weight: : 408.4

Molecular formula: : C20H19F3N2O4

Physical form: Odourless, white powder.

M.p. (°C) : °C72.9

B.p. : c. 312 °C/760 mmHg with decomp. >285 °C

V.p. (mPa) : 0.0034 (25 °C)

log Kow: 4.5

Henry (Pa m3 mol-1, calc.) : (mg/l)0.0023

S.g./Bulk density (20-25 °C) : 1.36

Water solubility (mg/l, 20-25 °C) : 0.61

Organic solubility: (g/l, 20-25 °C)Organic solubility: in g/l given for each solvent at 20-25 °C.Soluble in acetone (>500), dichloromethane (>500), ethyl acetate (>500), n-hexane (11), methanol (76), n-octanol (18), toluene (500)

Stability: Hydrolysis stable (pH 5), DT50 39-40 d (pH 7), 1.2-2.3 d (pH 9) (25 °C). Aqueous photolysis DT50 2.6 d (pH 5), 5.8-9.5

d (pH 7).

Ref: Pesticide Manual 2020

ISOMERISM :

Geometric isomers

POLYMORPHISM :

POLYMORPHISM CHAPTER OF TRIFLOXYSTROBIN

IUPAC Name: methyl (2E)-2-methoxyimino-2-[2-[[[E]-1-[3-(trifluoromethyl)phenyl]ethylideneamino]oxymethyl]phenyl]acetate

CAS Number: 141517-21-7

Polymorph Summary:

The crystal structure of the title compound [(E,E)-a-(Methoxyimino)-2-[[{1-[3-(trifluoromethyl)phenyl]ethylidene}amino]oxymethyl]benzeneacetic acid], C₁₉H₁₇F₃N₂O₄, a metabolite of the fungicide trifloxystrobin (TFS), contains one molecule in the asymmetric unit. The CF₃ group is disordered over two positions. The important characteristics of the molecule are the two C=N bonds in an E,E configuration, one in the -methoxy system and the other in the oxymethyl side chain between the two aromatic rings.

Patents References:

Non-Patent Literature:

1. Trifloxystrobin - a new strobilurin fungicide with an outstanding biological activity

By: Ziegler, H.; Benet-Buchholz, J.; Etzel, W.; Gayer, H.

Abstract: A review. Structure and physico-chem. properties of trifloxystrobin are presented. Crystallog. studies depicts the binding of trifloxystrobin with cytochrome bc₁. NMR, UV/VIS, IR, and EI-MS spectroscopic data, and its crystal structure are described.

SOURCE: Pflanzenschutz-Nachrichten Bayer (English Edition). Volume56, Issue2, Pages213-230, Journal; General Review, 2003

ISSN: 0170-0405

COMPANY/ORGANIZATION: R&D Chemical Synthesis, Pentapharm Ltd. Basel, Switz. CH-4002

PUBLISHER: Bayer CropScience AG

2. (E,E)-[2-(Methoxyimino)-2-[[{1-[3-(trifluoromethyl)phenyl]ethylidene}amino]oxymethyl]benzeneacetic acid

By: Banerjee, Kaushik; Ligon, Axel Patrick; Schuermann, Markus; Preut, Hans; Spittler, Michael

Abstract: Crystals of the title compd., a metabolite of the fungicide trifloxystrobin (TFS), are monoclinic, space group P2₁/c, with a 13.6953(14), b 9.0282(15), c 16.302(2) Å, β 106.983(7)°; Z = 4, dc = 1.359; R = 0.036, Rw(F₂) = 0.094 for 3500 reflections. The CF₃ group is disordered over two positions. The important characteristics of the mol. are the two C=N bonds in an E,E configuration, one in the -methoxy system and the other in the oxymethyl side chain between the two arom. rings. The mols. are linked via an O-H...N H bond and an infinite spiral is formed along the b-axis direction.

SOURCE: Acta Crystallographica, Section E: Structure Reports Online. Volume61, Issue6, Pages o1528-o1529, Journal; Online Computer File, 2005

ISSN: 1600-5368

DOI: 10.1107/S1600536805012900

Company/Organization: Institut fuer Umweltforschung. Universitaet Dortmund, Dortmund, Germany 44221

PUBLISHER: International Union of Crystallography

AQUEOUS SOLUBILITY (mg/l) :

In water 610 µg/l (25 °C)

SOLUBILITY IN METHANOL (mg/l) :

methanol 76(all in g/l, 25 °C).

SOLUBILITY IN ACETONE (mg/l) :

> 500(all in g/l, 25 °C).

SOLUBILITY IN ETHYL ACETATE (mg/l) :

> 500(all in g/l, 25 °C).

STABILITY :

Hydrolysis OT50 27.1 h (pH 9), 11.4 w (pH 7); stable at pH 5 (all 20 °C). Aqueous photolysis OT50 1.7 d (pH 7, 25 °C), 1.1 d (pH 5, 25 °C)

POTENTIAL FOR PARTICLE BOUND TRANSPORT INDEX :

2011

KEYWORDS

1. Trifloxystrobin
2. 141517-21-7
3. CHEBI: 81833
4. CGA 279202
5. methyl (2E)-2-methoxyimino-2-[2-[[[E]-1-[3-(trifluoromethyl)phenyl]ethylideneamino]oxymethyl]phenyl]acetate
6. SCHEMBL19148
7. SCHEMBL9880011
8. CHEMBL1897483
9. AKOS030621531
10. NCGC00163847-01
11. NCGC00163847-02
12. NCGC00163847-03
13. SC-44613
14. Trifloxystrobin 10 microg/mL in Cyclohexane
15. C18562
16. A807769
17. Trifloxystrobin, PESTANAL(R), analytical standard
18. J-007507
19. (2E)-2-methoxyimino-2-[2-[[[E]-1-[3-(trifluoromethyl)phenyl]ethylideneamino]oxymethyl]phenyl]acetic acid methyl ester
20. alpha-[(Z)-Methoxyimino]-2-[[[[[1Z]-1-[3-(trifluoromethyl)phenyl]ethylidene]amino]oxy]methyl]benzeneacetic acid methyl ester
21. methyl (2E)-(methoxyimino)(2-[[[E]-1-[3-(trifluoromethyl)phenyl]ethylidene]amino]oxy)methyl]phenyl]acetate
22. methyl (2E)-(methoxyimino)[2-[[[E]-1-[3-(trifluoromethyl)phenyl]ethylidene]amino]oxy]methyl]phenyl]acetate
23. methyl (2E)-2-methoxyimino-2-[2-[[[E]-1-[3-(trifluoromethyl)phenyl]ethylideneamino]oxymethyl]phenyl]ethanoate
24. methyl (alphaE)-alpha-(methoxyimino)-2-[[[[[1E]-1-[3-(trifluoromethyl)phenyl]ethylidene]amino]oxy]methyl]benzeneacetate
25. methyl (E)-methoxyimino-[(E)-alpha-[1-(alpha,alpha,alpha-trifluoro-m-tolyl)ethylideneamino]oxy]-o-tolyl]acetate
26. Methyl methoxyimino(alpha-(1-(alpha,alpha,alpha-trifluoro-3-tolyl)ethylideneamino)oxy)-2-tolyl]acetate

PubChem Substance and Compound databases - NCBI (U.S. National Library of Medicine) <https://pubchem.ncbi.nlm.nih.gov/>

JARVIS PATENT LANDSCAPE

SUMMARY OF JARVIS PATENT LANDSCAPE

Patents:

1. WO2017085747 (GSP Crop Science Pvt. Ltd., India); Est. Exp.: 19 Nov, 2035; Equivalents: IN3957/MUM/2015; Process Claim
2. WO2013144924 (Rallis India Ltd); Equivalent: IN942/MUM/2012; Process Claim
1. CN105294490 (Jiangsu Changqing Agrochemical); Equivalent: No; Est. Exp.: 10 Sept, 2035, Granted)
2. CN103787916 (Jingbo Agrochemicals Technology); Equivalent: No; Est. Exp.: 15 Jan, 2034, Granted)
3. CN103524378, CN103524379 (Jiangsu Sevencontinent Green Chemical); Equivalent: No; Est. Exp.: 23 Oct., 2033, Granted)
4. CN102952036 (Dalian Joinking Biochem Technology); Equivalent: No; Est. Exp.: LAPSED - 3 Dec, 2014)
5. CN102659623 (Nantong Weilike Chemical); Equivalent: No; Est. Exp.: LAPSED - 6 Jan, 2016)
6. CN101941921 (Yueyang Dipu Chemical Technology); Equivalent: No; Est. Exp.: LAPSED - 3 Sept, 2014)
7. CN1793115 (Shanghai Tongna Environmental Protection Technology); Equivalent: No; Est. Exp.: LAPSED - 2 Feb, 2011)
8. CN1560027, CN1560028 (Tongji University); Equivalent: No; Est. Exp.: LAPSED - 11 May, 2011).

Non-Patents:

1. Synthesis process of trifloxystrobin. By Chen, Wei et al. From Huaxue Yanjiu, 25(1), 16-19; 2014.
2. Synthesis of trifloxystrobin. By Chai, Bing et al. From Nongyao, 52(4), 258-259, 262; 2013.
3. Synthesis of trifloxystrobin. By Lu, Cuijun et al. From Nongyao, 50(3), 187-191, 212; 2011.
4. Synthesis of (E)-N-(methoxyimino)-2-[[[(E)-[1-[3-(trifluoromethyl)phenyl]ethylidene]amino]oxy]methyl]benzeneacetic acid methyl ester (trifloxystrobin). By Zhang, Ronghua et al. From Nongyao, 46(1), 29-30, 35; 2007.
5. Studies on synthesis of trifloxystrobin as a new class of fluoro-fungicides. By Li, Yan et al. From Huazhong Shifan Daxue Xuebao Ziranxueban, 39(1), 54-56, 63; 2005.
6. Synthesis of 8-substituted 5H,9H-6-oxa-7-aza-benzocyclononene-10,11-dione-11-O-methyloximes, a new [1,2]-oxazonine ring system. By Pascual, Alfons et al. From Tetrahedron Letters, 41(9), 1381-1384; 2000.

DATA PROTECTION (Solo Product)

SUMMARY

Trifloxystrobin:

Annex I Inclusion Date: 01/10/2003

Data Protection Expiry Date: 30/09/2013

BIOLOGY

INDICATION :

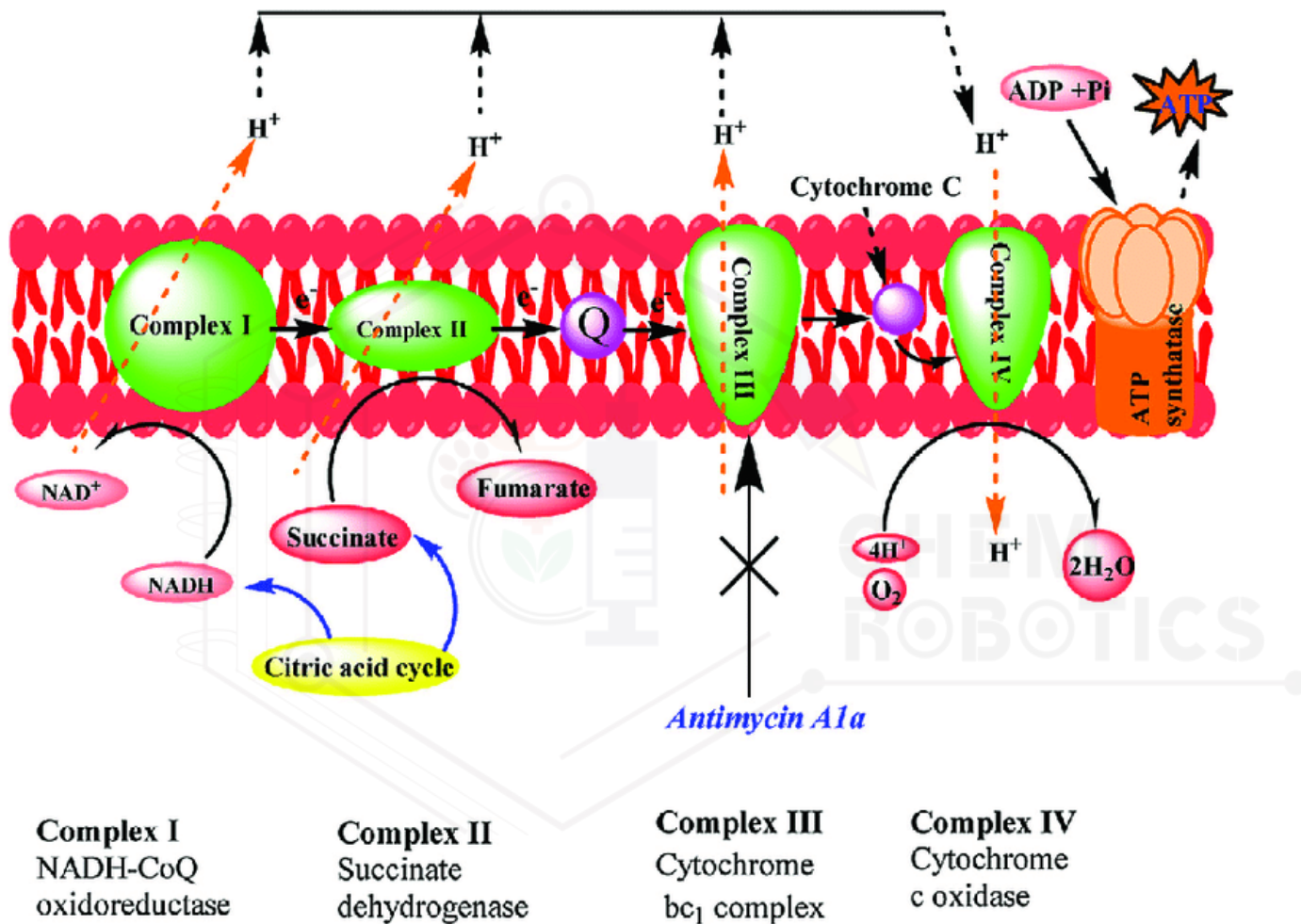
FUNGICIDE

USE :

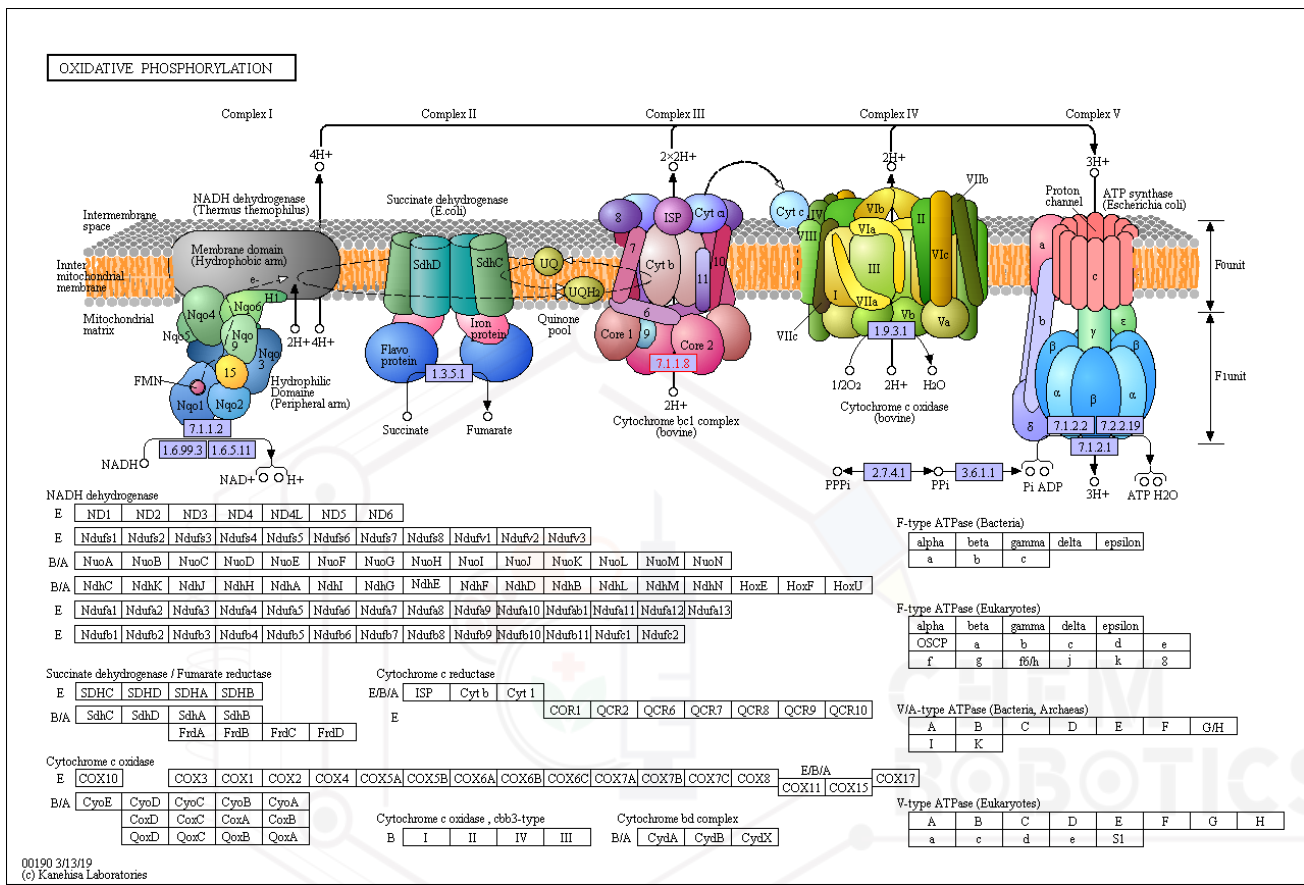
Trifloxystrobin works by interfering with respiration in plant pathogenic fungi. The site of action of Strobilurin compounds is located in the mitochondrial respiration pathway as a result of this mode of action, Trifloxystrobin is a potent inhibitor of fungal spore germination and mycelial growth. Trifloxystrobin is a broad-spectrum foliar fungicide that has high levels of activity against many fungal pathogens within the ascomycete, deuteromycete, basidiomycete, and oomycete classes. Trifloxystrobin controls of Ascomycetes, Deuteromycetes, Basidiomycetes and Oomycetes in cereals, soybeans, maize, rice, cotton, peanuts, sugar beets, sunflowers, pome fruit, stone fruit, tropical fruit, bananas, grapes, soft fruit, ornamentals, turf and many vegetables, at 50–550 g/ha.

MECHANISM OF ACTION (MOA) :

Mitochondrial electron transport inhibition (MET III) by inhibition of ubiquinol oxidase at the Q_o (quinone outside) binding site on cytochrome bc₁ (complex III).



KEGG PATHWAY :



PEST / PATHOGEN / SPECTRUM :

Trifloxystrobin Is A Broad-Spectrum Foliar Fungicide That Has High Levels Of Activity Against Many Fungal Pathogens Within The Ascomycete, Deuteromycete, Basidiomycete, And Oomycete Classes. Pests Controlled By This Active Ingredient Include Grape And Cucurbit Powdery Mildew, Apple Scab And Powdery Mildew, Peanut Leafspot, And Brown Patch Of Turfgrasses.

MAIN PESTS :

- Asian Rust
- Brown spot / Septoria leaf blight
- Aerial Blight
- Leaf blight
- Powdery mildew
- Brown rust
- Septoria leaf spot
- Net blotch
- Leaf blotch
- Powdery mildew
- A wide range of diseases

MAIN CROPS :

- Soybean
- Cereals
- F&V
- Maize
- Peanut

Rice
Turf
Ornamentals

CROP :

Soybean,Cereals,F&V,Maize,Peanut,Rice,Turf,Ornamentals, Almond, Apple, Banana, Barley, Calamint, Citrus, Cucurbit, Grapefruit, Hop, Mango, Melon, Nectarine, Nut, Oat, Ornamental, Peach, Peanut, Pear, Pecan, Pistachio, Potato, Rice, Rye Sugar Beet, Tea, Turf, Vine, Wheat

APPLICATION (APPLICATION TIMING) :

Foliar

COUNTRY WISE REGULATORY INFORMATION**COUNTRY WISE REGULATORY INFORMATION :**

Introduction & key dates: 1999, South Africa and USA UK/Greece

EU PESTICIDES DATA :

Substance: trifloxystrobin
Status: Date of Approval: 01/08/2018 Expiration of Approval: 31/07/2033
ADI: 0.1 mg/kg bw/day
ARfD: 0.5 mg/kg bw/day
AOEL: 0.06 mg/kg bw/day

USDA PESTICIDE DATA PROGRAM :

Appleauce: EPA tolerance level: 0.5 [ppm]
Apple: EPA tolerance level: 0.5 [ppm]
Cranberries Frozen: EPA tolerance level: 1.5 [ppm]
Cranberries: EPA tolerance level: 1.5 [ppm]
Cherries: EPA tolerance level: 2 [ppm]
Cucumbers: EPA tolerance level: 0.50 [ppm]
Cherries Frozen: EPA tolerance level: 2 [ppm]
Eggs: EPA tolerance level: 0.04 [ppm]
Green Beans: EPA tolerance level: NT [ppm]
Grapefruit: EPA tolerance level: 0.6 [ppm]
Grapes: EPA tolerance level: 2.0 [ppm]
Lettuce: EPA tolerance level: 30 [ppm]
Milk: EPA tolerance level: 0.02 [ppm]
Oranges: EPA tolerance level: 0.6 [ppm]
Olives Canned: EPA tolerance level: NT [ppm]
Pears: EPA tolerance level: 0.5 [ppm]
Potatoes: EPA tolerance level: 0.04 [ppm]
Spinach: EPA tolerance level: 30 [ppm]
Strawberries: EPA tolerance level: 1.5 [ppm]
Sweet Potatoes: EPA tolerance level: 0.04 [ppm]
Tomatoes Canned: EPA tolerance level: 0.5 [ppm]
Tomatoes: EPA tolerance level: 0.5 [ppm]

RESISTANCE ACTION COMMITTEE (RAC) / CLASSES**RESISTANCE ACTION COMMITTEE (RAC) :**

MoA Code: C
MoA: Respiration
Target Code: C3
Target Site: complex III: cytochrome bc1 (ubiquinol oxidase) at Qo site (cyt b gene)
Group Name: QoI-fungicides (Quinone outside Inhibitors)

Ref: FRAC Code List ©2020

COMBINATION

COMBINING PARTNER / MIXTURE :

EVERGOL Xtend (+ penflufen) (Bayer CropScience), Fox (+ prothioconazole) (Bayer CropScience), Nativo (+ tebuconazole) (Bayer CropScience), Prosper EverGol (+ metalaxyl+ penflufen+ clothianidin) (Bayer CropScience), Sphere (+ cyproconazole) (Bayer CropScience), Stratego (+ propiconazole) (Bayer CropScience)

Absolute (+ tebuconazole) (Bayer CropScience), Adament (+ tebuconazole) (Bayer CropScience), Agora (+ cyproconazole) (Bayer CropScience), Altus (+ triadimefon) (Bayer CropScience), Broadform (+ fluopyram) (Bayer CropScience), Consist Full (+ tebuconazole) (Bayer CropScience), Coronet (+ tebuconazole) (Bayer CropScience), Cripton (+ prothioconazole) (Bayer CropScience), Cripton Pro (+ bixafen + prothioconazole) (Bayer CropScience), Delaro (+ prothioconazole) (Bayer CropScience), Escolta (+ cyproconazole) (Bayer CropScience), Exteris Stressgard (+ fluopyram) (Bayer CropScience), Flint Max (+ tebuconazole) (Bayer CropScience), Flint Plus (+ captan) (Bayer CropScience), Flint Star (+ pyrimethanil) (Bayer CropScience), Fox Xpro (+ bixafen + prothioconazole) (Bayer CropScience), Interface Stressgard (+ iprodione) (Bayer CropScience), Jaunt (+ fluoxastrobin+ prothioconazole) (Bayer CropScience), Luna Sensation (+ fluopyram) (Bayer CropScience), Madison (+ prothioconazole) (Bayer CropScience), Mobius (+ prothioconazole) (Bayer CropScience), Mystic (+ pyrimethanil) (Bayer CropScience), Rombus (+ propiconazole) (Bayer CropScience), Sfera (+ cyproconazole) (Bayer CropScience), Stratego YLD (+ prothioconazole) (Bayer CropScience), Tartan Stressgard (+ triadimefon) (Bayer CropScience), Trigo (+ triadimefon) (Bayer CropScience), Trilex AL (+ metalaxyl) (Bayer CropScience), Trilex Optimum (+ metalaxyl+ captan) (Bayer CropScience), Trilex Star (+ thiophanate-methyl+ metalaxyl+ captan) (Bayer CropScience), Zephyr (+ prothioconazole) (Bayer CropScience), Éclair (+ cymoxanil) (Bayer CropScience)

AI PROCESS

(AI-DIUI)

TECHNICAL PURITY (AS PER EP REVIEW REPORT)

975 g/kg

Ref: EU - Pesticides database

IMPURITIES

IMPURITIES

AE 1344136 (max. 4 g/kg).

Ref: EU - Pesticides database

FORMULATION TYPES

SUMMARY FORMULATION TYPES

Flint (Bayer CropScience)

Further products, not always verified by the company. (Names that are a composite of company name and common name,

and those used only in home and garden outlets, are not listed. Suffixes are omitted if they do not signify a difference in the a.i. components Compass (Bayer CropScience), Consist (Bayer CropScience), Gate (Dolal), Gem (Bayer CropScience), Rapidox (Agri Sciences), Sphere Max (Bayer CropScience), Swift (Bayer CropScience), Tega (Bayer CropScience), Trilex (Bayer CropScience), Twist (Bayer CropScience), Zato (Bayer CropScience)

FORMULATION GLOBALLY

Trifloxystrobin: EC, SC, WG, FS

FORMULATIONS / PREPARATIONS

MANUFACTURERS

Bayer (Flint, Stratego), Manufacturers (Approved Importer for India): : \$\$

1. M/s Bayer CropScience AG at Muttenz, Switzerland, Through Supplier- Same .(By- M/s Bayer CropScience Pvt. Ltd., Mumbai, 96% w/w min. in 388th RC)
2. CAC Nantong,
3. Iprochem,
4. Sunjoy

Ref: :

1. SOURCE OF IMPORT AND LIST OF INDIGENOUS MANUFACTURERS OF INSECTICIDES: As on 29.02.2020 By Central Insecticide Board and Registration Committee (CIBRC), India

KEY MANUFACTURER / BRAND

Bayer (Flint, Stratego)

ANALYTICAL DATA

ANALYTICAL DATA

Residues Analysis: Residues and metabolites by gc/NPD (Resid. Anal. Methods); see also Pestic. Anal.Man., 2, 180.555

In Soil: In soil by hplc/uv (Environ. Chem. Methods). Methods for the determination of residues are also available from Bayer CropScience.

TOXICITY(EPA CLASS) :

Toxicity class: WHO (a.i.) III (company classification).

TOXICOLOGICAL & ENVIRONMENTAL REVIEWS :

Tox & Environment Reviews Summary of Trifloxystrobin:

Toxicological & environmental reviews JMPR Mtg. (2004), (2012), (2015), (2017); JMPR Evaln. I (2004), (2012), (2015), (2017); JMPR Evaln. II (2004); EU Rev. Rep. SANCO/4339/2000 (2003); EFSA Jou. 2017, 15(10), 4989; EPA Fact Sheet, Sep. 1999.

EU status (1107/2009): Approved

Legislation (EU) 2018/1060, (EU) 540/2011

EPA registration status Registered - Registration Under Review

Toxicity class: U

MAMMALIAN TOXICOLOGY

MAMMALIAN - NON-HUMAN ANIMALS TOX :

Ecotoxicology Summary of Trifloxystrobin :

Birds: Acute oral LD50 for bobwhite quail > 2000, mallard ducks >2250 mg/kg. Dietary LC50 for bobwhite quail and mallard ducks >5050 ppm.

Fish: LC50 (96 h) for rainbow trout 0.015, bluegill sunfish 0.054 mg/l.

Daphnia: LC50 (48 h) 0.016 mg/l.

Algae: EbC50 for *Scenedesmus subspicatus* 0.0053 mg/l.

Other aquatic spp.: Toxic to aquatic organisms in laboratory tests. but rapid dissipation in biotic environments. Low risk to aquatic ecosystems has been demonstrated in outdoor mesocosm tests.

Honey Bees: LD50 (oral and contact) >200 µg/bee.

Worms: LC50 (14 d) >1000 mg/kg soil.

Other beneficial spp.: Twist formulation caused 100% mortality to *Orius insidiosus* nymphs and *Aphidius colemani* adults at 250 g a.i./ha. However, field tests indicate low risk in normal use to a wide range of beneficial arthropods, including predatory mites, ground- and foliage-dwelling predators and parasitic wasps.

Ref: The Pesticide Manual (17th Edition)

ORAL :

GENERIC

CHRONIC :

MITOCHONDRIAL ELECTRON TRANSPORT INHIBITION (MET III) BY INHIBITION OF UBIQUINOL OXIDASE AT THE QO (QUINONE OUTSIDE) BINDING SITE ON CYTOCHROME BC1 (COMPLEX III).

MAMMALIAN - HUMAN TOX

SUMMARY OF MAMMALIAN - HUMAN TOX

Mammalian Tox Summary of Trifloxystrobin:

Oral: Acute oral LD50 for rats >5000 mg/kg.

Skin and eye: Acute percutaneous LD50 for rats > 2000 mg/kg. Classified as non-irritating to skin and eyes (rabbits). May cause sensitisation by skin contact.

Inhalation: LC50 for rats >4650 mg/m³.

NOEL: NOAEL (2 y) for rats 9.8 mg/kg b.w. daily (value used by EU); (2 generation for rats) 3.8 mg/kg b.w. daily (used by US, JMPR/WHO).

ADI/RfD: (JMPR) 0.04 mg/kg b.w. [2004]; (EC) 0.1 mg/kg b.w. (2003); (EPA), ARfD 2.5, cRfD 0.038 mg/kg b.w. [2003].

Other: Non-mutagenic, non-teratogenic, non-carcinogenic; no adverse effects on reproduction.

Toxicity class: WHO (a.i.) III (company classification).

EC classification: R43, N; R50, R53.

Ref. The Pesticide Manual (17th Edition)

ADI - ACCEPTABLE DAILY INTAKE (mg/kg BW PER DAY) :

ADI: 0.1 mg/kg bw/day

ARFD - ACUTE REFERENCE DOSE (mg/kg BW PER DAY) :

ARfD: 0.5 mg/kg bw/day

AOEL - ACCEPTABLE OPERATOR EXPOSURE LEVEL - SYSTEMIC (mg/kg BW PER DAY) :

AOEL : 0.06 mg/kg bw/day

ENVIRONMENTAL FATE

SUMMARY OF ENVIRONMENTAL FATE

Efate Summary of Trifloxystrobin :

Animals: Rapidly absorbed (60% in 48 h) and rapidly and extensively excreted (up to 96% in 48 h) in urine and faeces. Extensively and rapidly metabolised, by O-demethylation, oxidation and conjugation, and quickly and completely eliminated from the body.

Plants: Metabolic profile is similar for a range of crops. Based on wheat, apple, cucumber and sugar beet metabolism data, trifloxystrobin is considered as the residue of concern for food and feed commodities of plant origin.

Soil/Environment: Dissipates rapidly from soil and surface water. Soil DT50 4.2- 9.5 d. Koc 1642-3745. No leaching potential.

In water: DT50 0.3- 1 d, OT90 4-8 d.

Ref: The Pesticide Manual (17th Edition)

DISSIPATION STUDIES

APPLICATION RATE (Rate g/ha)

Foliar, 62.5-187.5

GHS PICTOGRAM

GHS PICTOGRAM

trifloxystrobin(ISO); methyl (E)-methoxyimino-{(E)- α -[1-(α,α,α -trifluoro-m-tolyl)ethylideneaminoxy]-o-tolyl}acetate

Substance identity

EC / List no.: 604-237-6

CAS no.: 141517-21-7

Mol. formula:

[

...

]

Hazard classification & labelling



Warning! According to the **harmonised classification and labelling** (CLP00) approved by the European Union, this substance is very toxic to aquatic life, is very toxic to aquatic life with long lasting effects and may cause an allergic skin reaction.

Properties of concern

Ss Skin sensitising

The InfoCard summarises the non-confidential data on substances as held in the databases of the European Chemicals Agency (ECHA), including data provided by third parties. The InfoCard is automatically generated. Information requirements under different legislative frameworks may therefore not be up-to-date or complete. Substance manufacturers and importers are responsible for consulting official publications. This InfoCard is covered by the ECHA Legal Disclaimer.



about INFOCARD - Last updated: 03/07/2019

SALES DATA (Sales / Year (\$m.))

SUMMARY SALES DATA (Sales / Year (\$m.))

810

SALES DATA

2017 Global Value (\$ m): 640.81

2017 Calculated Globally (based on formulated product) active price (\$/kg): 108.97

2017 Global Volume (x1000 kg): 5880.38

PRODUCT TECHNOLOGIES

KEY TECHNOLOGIES

Friedel Crafts Reaction
 Halogen exchange
 carbonylation
 esterification
 Methylation with dimethyl-sulphate
 Etherification
 Oxime formation

SAFETY DATA

FIRE FIGHTING MEASURES

Fire Fighting Measures

Fire fighting measures list suitable extinguishing techniques, equipment; chemical hazards from fire.
 Suitable extinguishing media: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.
 Sigma-Aldrich; Safety Data Sheet for Trifloxystrobin. Product Number: 46447, Version 5.2 (Revision Date 05/17/2016).
 Available from, as of December 20, 2016: <http://www.sigmaaldrich.com/safety-center.html>
 Advice for firefighters: Wear self-contained breathing apparatus for firefighting if necessary.
 Sigma-Aldrich; Safety Data Sheet for Trifloxystrobin. Product Number: 46447, Version 5.2 (Revision Date 05/17/2016).
 Available from, as of December 20, 2016: <http://www.sigmaaldrich.com/safety-center.html>
 PubChem Substance and Compound databases - NCBI (U.S. National Library of Medicine) <https://pubchem.ncbi.nlm.nih.gov/>

ACCIDENTAL RELEASE MEASURES

Accidental Release Measures

Accidental release measures lists emergency procedures; protective equipment; proper methods of containment and cleanup.

Cleanup Methods

Procedures for cleanup

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Avoid breathing dust. Environmental precautions: Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided. Methods and materials for containment and cleaning up: Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.
 Sigma-Aldrich; Safety Data Sheet for Trifloxystrobin. Product Number: 46447, Version 5.2 (Revision Date 05/17/2016).
 Available from, as of December 20, 2016: <http://www.sigmaaldrich.com/safety-center.html>

If the container is leaking or material spilled for any reason or cause, carefully sweep material into a pile. ... Do not walk through spilled material. ... In spill or leak incidents, keep unauthorized people away.

Bayer CropScience LP; Product Label for Trifloxystrobin Technical. Accepted by US EPA November 2016. Available from, as of December 21, 2016: <https://www.epa.gov/>

Disposal Methods

Disposal Methods for this chemical

SRP: Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the materials impact on air quality; potential migration in air, soil or water; effects on animal, aquatic and plant life; and conformance with environmental and public health regulations. If it is possible or reasonable use an alternative chemical product with less inherent propensity for occupational harm/injury/toxicity or environmental contamination.

Product: Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material; Contaminated packaging: Dispose of as unused product.

Sigma-Aldrich; Safety Data Sheet for Trifloxystrobin. Product Number: 46447, Version 5.2 (Revision Date 05/17/2016).
 Available from, as of December 20, 2016: <http://www.sigmaaldrich.com/safety-center.html>

Wastes resulting from the use of this product may be disposed of on site or at an approved facility.

Bayer CropScience LP; Product Label for Trifloxystrobin Technical. Accepted by US EPA November 2016. Available from, as of December 21, 2016: <https://www.epa.gov/>

Other Preventative Measures

Other information for Preventative Measures

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Avoid breathing dust. Environmental precautions: Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

Sigma-Aldrich; Safety Data Sheet for Trifloxystrobin. Product Number: 46447, Version 5.2 (Revision Date 05/17/2016).
 Available from, as of December 20, 2016: <http://www.sigmaaldrich.com/safety-center.html>

Precautions for safe handling: Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed.

Sigma-Aldrich; Safety Data Sheet for Trifloxystrobin. Product Number: 46447, Version 5.2 (Revision Date 05/17/2016).
 Available from, as of December 20, 2016: <http://www.sigmaaldrich.com/safety-center.html>

Appropriate engineering controls: Handle in accordance with good industrial hygiene and safety practice. Wash hands

before breaks and at the end of workday.

Sigma-Aldrich; Safety Data Sheet for Trifloxystrobin. Product Number: 46447, Version 5.2 (Revision Date 05/17/2016).

Available from, as of December 20, 2016: <http://www.sigmaaldrich.com/safety-center.html>

Gloves must be inspected prior to use. Use proper glove removal technique (without touching gloves outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Sigma-Aldrich; Safety Data Sheet for Trifloxystrobin. Product Number: 46447, Version 5.2 (Revision Date 05/17/2016).

Available from, as of December 20, 2016: <http://www.sigmaaldrich.com/safety-center.html>

SRP: Local exhaust ventilation should be applied wherever there is an incidence of point source emissions or dispersion of regulated contaminants in the work area. Ventilation control of the contaminant as close to its point of generation is both the most economical and safest method to minimize personnel exposure to airborne contaminants. Ensure that the local ventilation moves the contaminant away from the worker.

SRP: The scientific literature for the use of contact lenses by industrial workers is inconsistent. The benefits or detrimental effects of wearing contact lenses depend not only upon the substance, but also on factors including the form of the substance, characteristics and duration of the exposure, the uses of other eye protection equipment, and the hygiene of the lenses. However, there may be individual substances whose irritating or corrosive properties are such that the wearing of contact lenses would be harmful to the eye. In those specific cases, contact lenses should not be worn. In any event, the usual eye protection equipment should be worn even when contact lenses are in place.

PubChem Substance and Compound databases - NCBI (U.S. National Library of Medicine) <https://pubchem.ncbi.nlm.nih.gov/>

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

HANDLING AND STORAGE

Handling and Storage

Handling and storage lists precautions for safe handling and storage, including incompatibilities.

Storage Conditions

Information for Storage Conditions

Keep container tightly closed in a dry and well-ventilated place.

Sigma-Aldrich; Safety Data Sheet for Trifloxystrobin. Product Number: 46447, Version 5.2 (Revision Date 05/17/2016).

Available from, as of December 20, 2016: <http://www.sigmaaldrich.com/safety-center.html>

Store in a cool, dry place and in such a manner as to prevent cross contamination with other pesticides, fertilizers, food, and feed. Store in original container and out of the reach of children, preferably in a locked storage area.

Bayer CropScience LP; Product Label for Trifloxystrobin Technical. Accepted by US EPA November 2016. Available from, as of December 21, 2016: <https://www.epa.gov/>

Store in a well-ventilated, secure area out of reach of children and domestic animals. Do not eat, drink, smoke, or apply cosmetics; wash thoroughly after handling.

Crop Protection Handbook Volume 100, Meister Media Worldwide, Willoughby, OH 2014, p. 593

PubChem Substance and Compound databases - NCBI (U.S. National Library of Medicine) <https://pubchem.ncbi.nlm.nih.gov/>

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

EXPOSURE CONTROL AND PERSONAL PROTECTION

Exposure Control and Personal Protection

Exposure controls and personal protection list OSHAs Permissible Exposure Limits (PELs); Threshold Limit Values (TLVs); appropriate engineering controls; personal protective equipment (PPE) and more.

Allowable Tolerances

Allowable Tolerances

Tolerances are established for residues of trifloxystrobin, including its metabolites and degradates, in or on the commodities in the table below. Compliance with the tolerance levels specified below is to be determined by measuring only the sum of trifloxystrobin, benzeneacetic acid, (E,E)-a-(methoxyimino)-2-[[[1-[3-(trifluoromethyl) phenyl]ethylidene] amino]oxy]methyl]-, methyl ester, and the free form of its acid metabolite CGA-321113, (E,E)-methoxyimino-[2-[1-(3-trifluoromethyl-phenyl)-ethylideneamino]oxy]methyl]-phenyl]acetic acid, calculated as the stoichiometric equivalent of trifloxystrobin, in or on the commodity.

Commodity

Parts per million

Alfalfa, forage 0.01
Alfalfa, hay 0.01
Almond, hulls 9.0
Apple, wet pomace 5.0
Artichoke, globe 1.0
Asparagus 0.07
Banana (There are no USA registrations as of September 27, 1999 for use on banana.) 0.10
Barley, grain 0.05
Barley, hay 0.3
Barley, straw 5.0
Beet, sugar, dried pulp 0.4
Beet, sugar, molasses 0.2
Beet, sugar, roots 0.1
Beet, sugar, tops 4.0
Berry, low growing subgroup 13-07G 1.5
Brassica, head and stem, subgroup 5A 2.0
Brassica, leafy greens, subgroup 5B 30
Canistel 0.7
Cattle, fat 0.1
Cattle, meat 0.1
Cattle, meat byproducts 0.1
Citrus, dried pulp 1.0
Citrus, oil 38
Coffee, green bean (There are no USA registrations as of January 18, 2012 for use on coffee, green bean.) 0.02
Corn, field, forage 8.0
Corn, field, grain 0.05
Corn, field, stover 7
Corn, field, refined oil 0.1
Corn, pop, grain 0.05
Corn, pop, stover 7
Corn, sweet, cannery waste 0.6
Corn, sweet, forage 7.0
Corn, sweet, kernel plus cob with husks removed 0.04
Corn, sweet, stover 4.0
Cotton, gin byproducts 3.0
Cottonseed subgroup 20C 0.50
Dill, seed 30
Egg 0.04
Fruit, citrus, group 10 0.6
Fruit, pome 0.5
Fruit, small vine climbing, except fuzzy kiwifruit, subgroup 13-07F 2.0
Fruit, stone, group 12 2
Goat, fat 0.1
Goat, meat 0.1
Goat, meat byproducts 0.1
Grain, aspirated fractions 5.0
Grape, raisin 5.0
Grass, forage 12
Grass, hay 17
Herbs, subgroup 19A 200
Hog, fat 0.05
Hog, meat 0.05
Hog, meat byproducts 0.05
Hop, dried cones 11.0
Horse, fat 0.1

Horse, meat 0.1
Horse, meat byproducts 0.1
Leaf petioles subgroup 4B 9.0
Leafy greens, subgroup 4A 30
Mango 0.7
Milk 0.02
Nut, tree, group 14 0.04
Oat, forage 0.3
Oat, grain 0.05
Oat, hay 0.3
Oat, straw 5.0
Papaya 0.7
Pea, dry, seed 0.06
Pea, field, hay 15
Pea, field, vines 4
Peanut, hay 4.0
Peanut 0.05
Pistachio 0.04
Poultry, fat 0.04
Poultry, meat 0.04
Poultry, meat byproducts 0.04
Radish, tops 10
Rice, grain 3.5
Rice, hulls 8
Sapodilla 0.7
Sapote, black 0.7
Sapote, mamey 0.7
Sheep, fat 0.1
Sheep, meat 0.1
Sheep, meat byproducts 0.1
Soybean, forage 10.0
Soybean, hay 25.0
Soybean, seed 0.08
Star apple 0.7
Vegetable, cucurbit, group 9 0.50
Vegetable, fruiting 0.5
Vegetable, root, except sugar beet, subgroup 1B 0.1
Vegetable, tuberous and corm, subgroup 1C 0.04
Wheat, bran 0.15
Wheat, forage 0.3
Wheat, grain 0.05
Wheat, hay 0.2
Wheat, straw 5.0

40 CFR 180.555(a) (USEPA); U.S. National Archives and Records Administrations Electronic Code of Federal Regulations. Available from, as of December 6, 2016: <http://www.ecfr.gov>

Protective Equipment and Clothing

Protective Equipment and Clothing

Eye/face protection: Face shield and safety glasses. Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Sigma-Aldrich; Safety Data Sheet for Trifloxystrobin. Product Number: 46447, Version 5.2 (Revision Date 05/17/2016).

Available from, as of December 20, 2016: <http://www.sigmaaldrich.com/safety-center.html>

Skin protection: Handle with gloves.

Sigma-Aldrich; Safety Data Sheet for Trifloxystrobin. Product Number: 46447, Version 5.2 (Revision Date 05/17/2016).

Available from, as of December 20, 2016: <http://www.sigmaaldrich.com/safety-center.html>

Body Protection: Complete suit protecting against chemicals. The type of protective equipment must be selected according

to the concentration and amount of the dangerous substance at the specific workplace.

Sigma-Aldrich; Safety Data Sheet for Trifloxystrobin. Product Number: 46447, Version 5.2 (Revision Date 05/17/2016).

Available from, as of December 20, 2016: <http://www.sigmaaldrich.com/safety-center.html>

Respiratory protection: For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Sigma-Aldrich; Safety Data Sheet for Trifloxystrobin. Product Number: 46447, Version 5.2 (Revision Date 05/17/2016).

Available from, as of December 20, 2016: <http://www.sigmaaldrich.com/safety-center.html>

Protective clothing: Long-sleeved shirt and long pants. Shoes plus socks. Waterproof gloves.

Crop Protection Handbook Volume 100, Meister Media Worldwide, Willoughby, OH 2014, p. 593

EC CLASSIFICATION

EC classification: R43, N; R50, R53.

LITERATURE REFERENCE

INFORMATION SOURCE (S)

[1] Alan wood (<http://www.alanwood.net/pesticides/>)

[2] Pesticide Manual <http://tsime.uz.ac.zw/claroline/backends/download.php?url=L1BNMTYtc3VwcGxlbWVudGFyeS1CQ1BDLnBkZg%3D%3D&cidReq=MCP508>

[3] HRAC / FRAC / IRAC (<https://www.hracglobal.com/> / <https://www.frac.info/> / <https://www.irc-online.org>)

[4] United States Environmental Protection Agency (US EPA) <https://www.epa.gov/>

[5] CIBRC (GOVERNMENT OF INDIA MINISTRY OF AGRICULTURE & FARMERS WELFARE) <http://ppqs.gov.in/divisions/cibrc/news-update>

[6] PubChem Substance and Compound databases - NCBI (U.S. National Library of Medicine) <https://pubchem.ncbi.nlm.nih.gov/>

[7] UNITED STATES PATENT AND TRADEMARK OFFICE (uspto) <https://www.uspto.gov/>

[8] J-PlatPat : Japan platform for patent information <https://www.j-platpat.inpit.go.jp/>

[9] inPASS (Indian Patent Advanced Search System): Indian platform for patent information <https://ipindiaservices.gov.in/PublicSearch/>

[10] Pesticide Properties Data Base (PPDB) <https://sitem.herts.ac.uk/aeru/ppdb/en/atoz.htm>

[11] European chemical agency (ECHA) <https://echa.europa.eu/>

[12] Espacenet : European Patent Office platform for patent information https://worldwide.espacenet.com/?locale=en_EP

[13] Toxnet Toxicology data network <https://toxnet.nlm.nih.gov/cgi-bin/sis/search2/r?dbs+hsdb:@term+@rn+@rel+93-71-0>

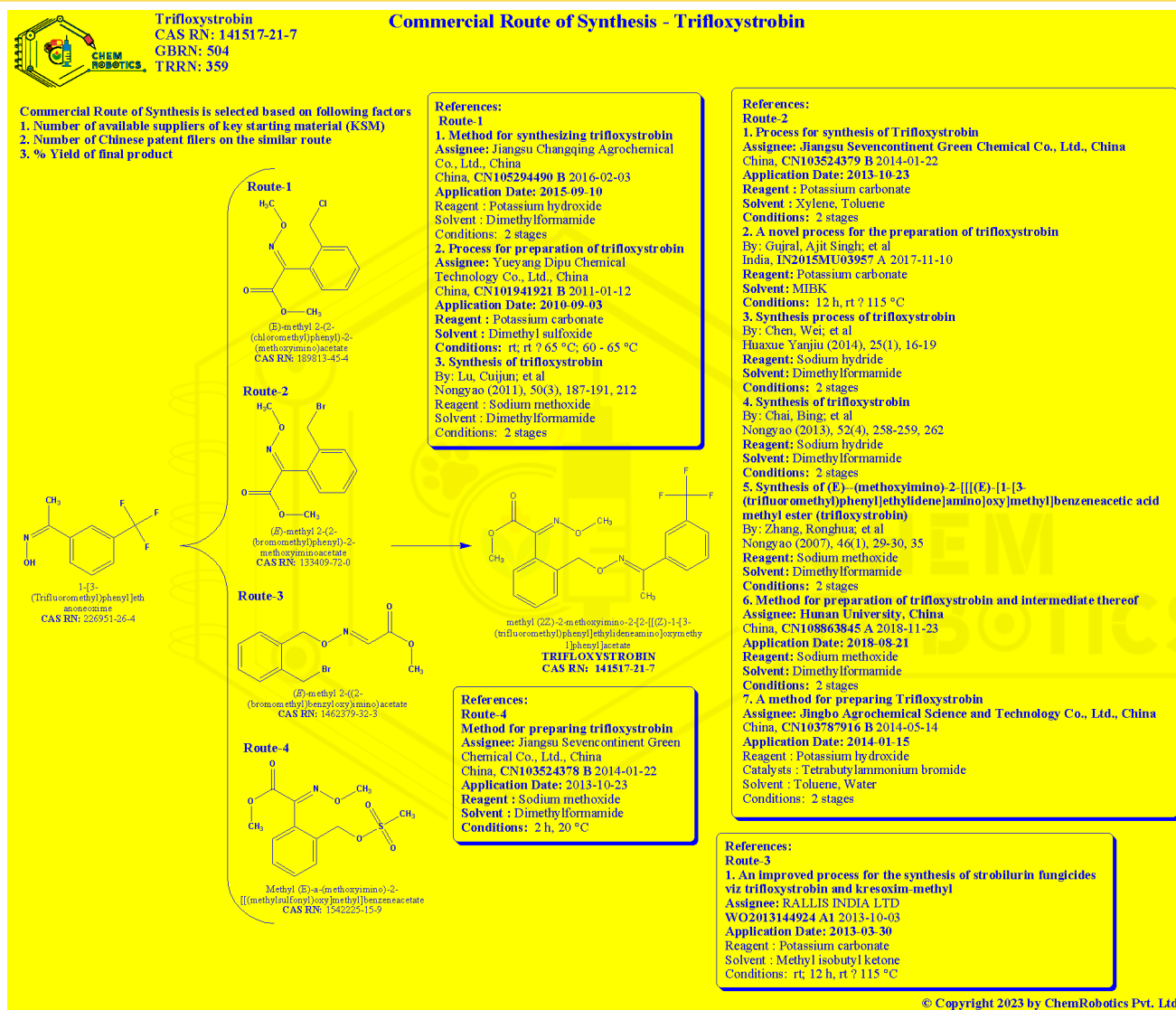
GLOBAL SCIENTIFIC DOCUMENT ARCHIVAL (GSDA): REGULATORY & IP DOCUMENT ARCHIVAL

REGULATORY & IP DOCUMENT ARCHIVE

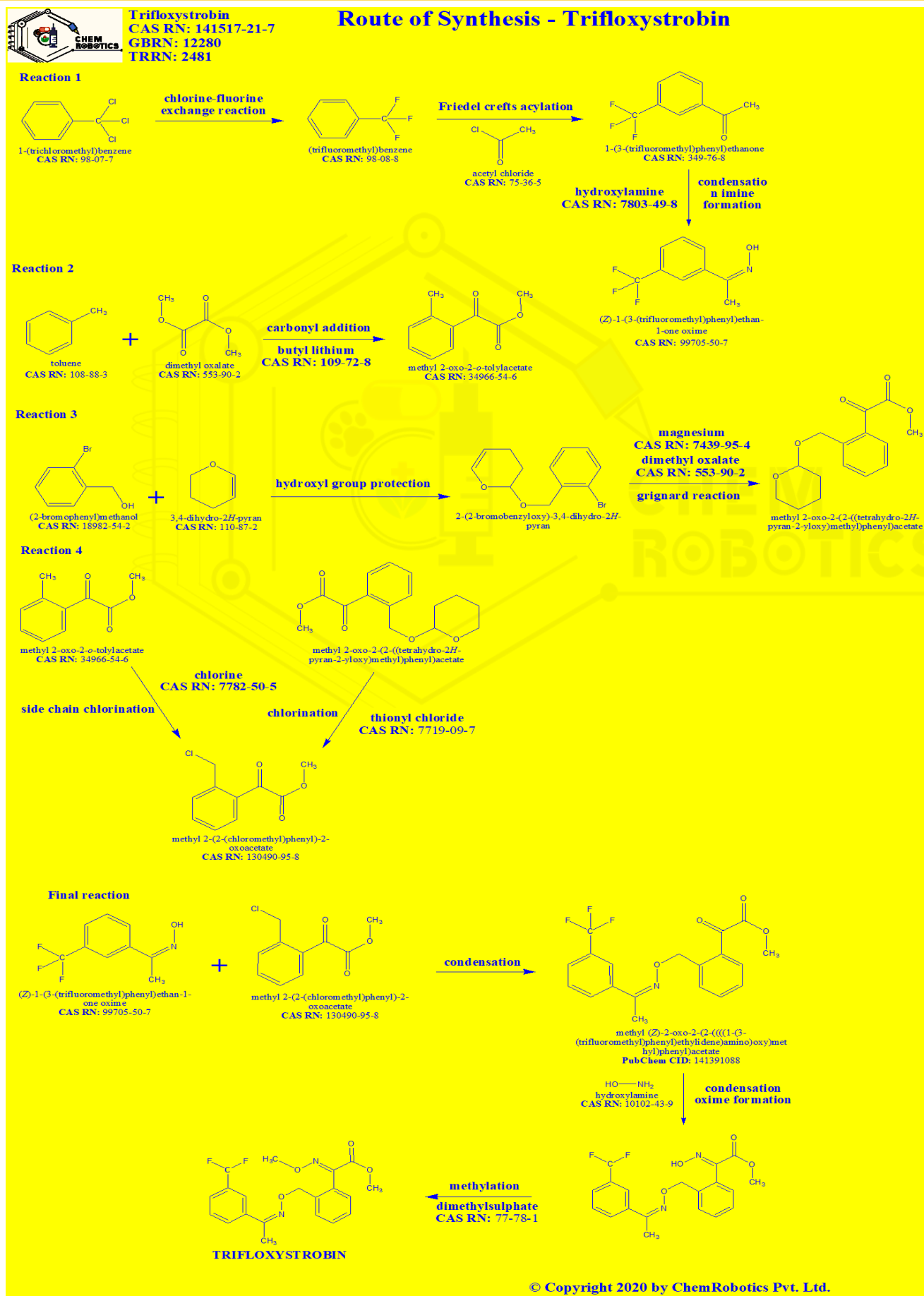
<https://patentscope.wipo.int/search/en/result.jsf?inchikey=ONCZDRURRATYFI-TVJDWZFNNSA-N>

ROUTE OF SYNTHESIS

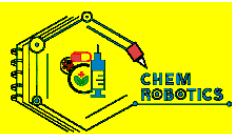
ROS - 1



ROS - 2



ROS - 3

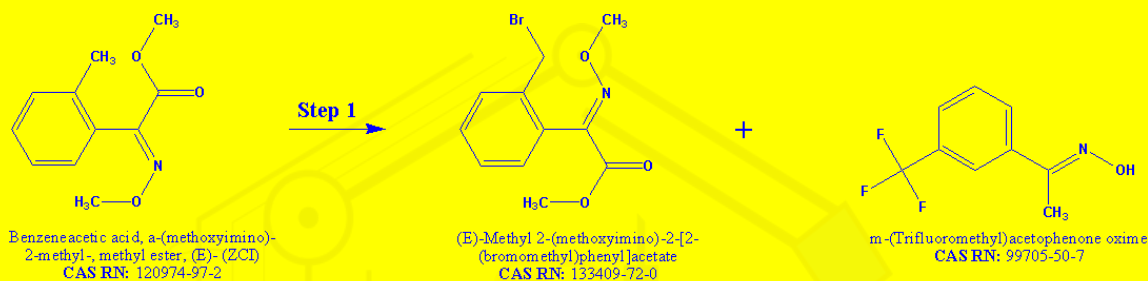


Trifloxystrobin
CAS RN: 141517-21-7
GBRN: 504
TRRN: 16144

Commercial Route of Synthesis - Trifloxystrobin

Commercial Route of Synthesis is selected based on following factors

1. Number of available suppliers of key starting material (KSM)
2. Number of Chinese patent filers on the similar route
3. % Yield of final product



Reference(s):

1.Method for preparation of trifloxystrobin and intermediate thereof

By: Hu, Aixi; et al China, CN108863845A 2018-11-23

Assignee:Hunan University, China

Reaction Summary:

1.1 Reagents: 1,3-Dibromo-5,5-dimethylhydantoin

Catalysts: Azobisisobutyronitrile

Solvents: 1,2-Dichloroethane ; 5 h, 80 °C

2.1 Reagents: Sodium methoxide

Solvents: Dimethylformamide ; 15 min, rt; rt 5 °C

2.2 5 h, rt

2.Process for preparation of trifloxystrobin

By: Zhang, Ronghua; et al China, CN1793115A 2006-06-28

Assignee:Shanghai Tongna Environment Protection Technology Co., Ltd., China

Reaction Summary:

1.1 Reagents: Benzoyl peroxide , N-Bromosuccinimide

Solvents: Carbon tetrachloride

2.1 Reagents: Sodium methoxide

Solvents: Tetrahydrofuran ; rt; 1 h, heated

2.2 Solvents: Dimethylformamide ; heated

3.Process for preparation of trifloxystrobin

By: Ni, Yuebiao; et al China, CN101941921A 2011-01-12

Assignee:Yueyang Dipu Chemical Technology Co., Ltd., China

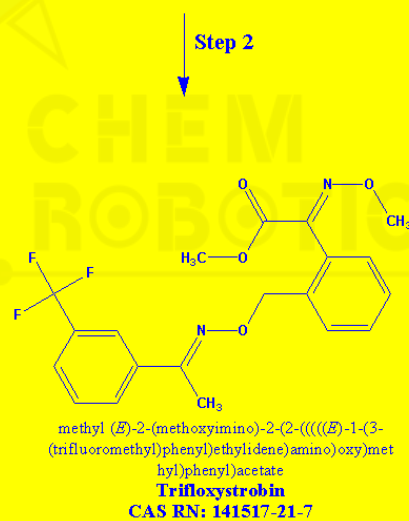
Reaction Summary:

1.1 Reagents: Chlorine

Solvents: 1,2-Dichloroethane ; rt 65 °C; 60 - 65 °C

2.1 Reagents: Potassium carbonate

Solvents: Dimethyl sulfoxide ; rt; rt 65 °C; 60 - 65 °C



© Copyright 2023 by ChemRobotics Pvt. Ltd.

ROS - 4



TRIFLOXYSTROBIN
CAS RN: 141517-21-7
GBRN : 12280

Commercial Route of Synthesis - TRIFLOXYSTROBIN

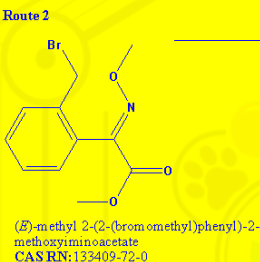
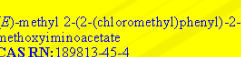
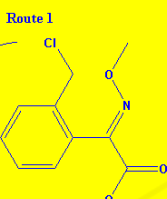
Commercial Route of Synthesis is selected based on following factors

- Number of available suppliers of key starting material (KSM)
- Number of Chinese patent filers on the similar route
- % Yield of final product

BLOCK 1



BLOCK 2



Route 1

Reference(s):

1. Method for synthesizing trifloxystrobin

By: Lv, Liangzhong, et al, China, CN105294490A 2016-02-03

Assignee: Jiangsu Changqing Agrochemical Co., Ltd., China

Reaction Summary:

Yield: 91%

1.1 Reagents: Potassium hydroxide
Solvents: Dimethylformamide , rt, 10 min, cooled
1.2 5 h, rt

2. Process for preparation of trifloxystrobin

By: Ni, Yuebiao, et al, China, CN101941921A 2011-01-12

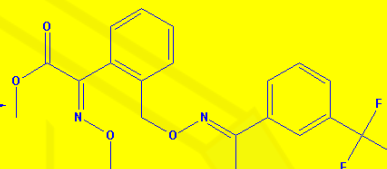
Assignee: Yueyang Dipu Chemical Technology Co., Ltd., China

Reaction Summary:

Yield: 74%

1.1 Reagents: Potassium carbonate
Solvents: Dimethylformamide , 65-80, 50-65, 80

2.1 Reagents: Potassium carbonate
Solvents: Toluene , 50, 80



Route 2

Reference(s):

1. Process for synthesis of Trifloxystrobin

By: He, Yongli, et al, China, CN103524379A 2014-01-22

Assignee: Jiangsu Sevencontinent Green Chemical Co., Ltd., China

Reaction Summary:

Yield: 90%

1.1 Reagents: Potassium carbonate
Solvents: Xylene , rt, reflux, 4 h, reflux
1.2 Solvents: Toluene , 0.5 h, rt, 3 h, 30 °C

2. A novel process for the preparation of trifloxystrobin

By: Gujral, Ajit Singh, et al, India, IN2015MU03957A 2017-11-10

Assignee: GSP Crop Science Pvt. Ltd., India

Reaction Summary:

Yield: 85%

1.1 Reagents: Potassium carbonate
Solvents: Methyl isobutyl ketone , 12 h, rt 115 °C

3. A novel process for the preparation of trifloxystrobin

By: Gujral, Ajit Singh, et al, World Intellectual Property Organization, WO201708574A2 2017-05-26

Assignee: GSP Crop Science Pvt. Ltd., India

Reaction Summary:

Yield: 85%

1.1 Reagents: Potassium carbonate
Solvents: Methyl isobutyl ketone , 12 h, rt, 115 °C

Route 3

Reference(s):

Method for preparing trifloxystrobin

By: He, Yongli, et al, China, CN103524378A 2014-01-22

Assignee: Jiangsu Sevencontinent Green Chemical Co., Ltd., China

Reaction Summary:

Yield: 85%

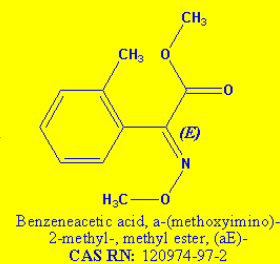
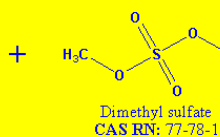
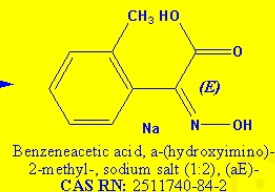
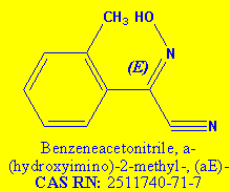
1.1 Reagents: Sodium methoxide
Solvents: Dimethylformamide , 2 h, 20 °C

© Copyright 2021 by ChemRobotics Pvt. Ltd.

ROS - 5



Trifloxystrobin
 CAS RN: 141517-21-7
 GBRN: 504;12280
 TRRN: 23465

Chinese Patent Route - Trifloxystrobin**References:****1. Synthesis method of intermediate for preparing trifloxystrobin**

By: Cai, Fanping; et al

China, CN111807990 A 2020-10-23

Assignee: Fuxin Fulongbao Pharmaceutical Technology Co., Ltd., China

Reaction Summary:

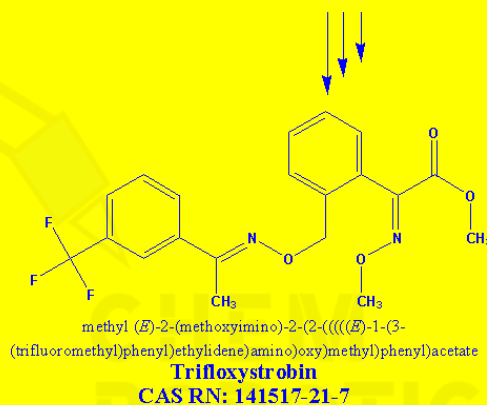
1.1 Reagents: Sodium hydroxide

Solvents: Methanol, Water; rt to reflux; 6 h, reflux to 106 °C; 106 °C to 0 °C

2.1 Solvents: Dimethylformamide; 45 min, -10 °C; 2 h, -10 °C; -10 °C to 0 °C; 2 h, 0 °C

2.2 Reagents: Hydrochloric acid

Solvents: Water; pH 7



© Copyright 2023 by ChemRobotics Pvt. Ltd.

ROS - 6



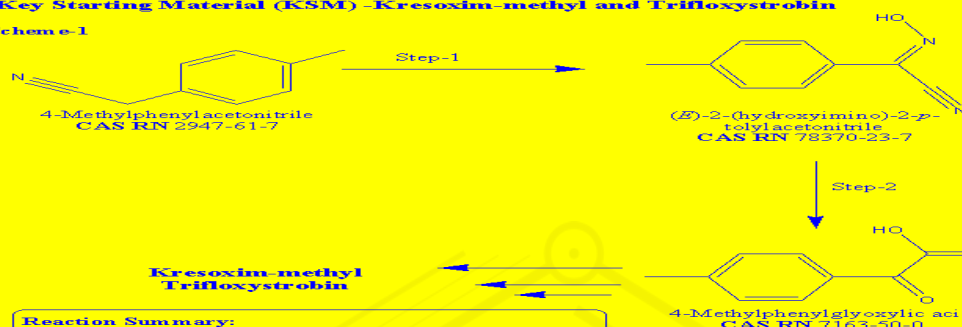
Kresoxim-methyl and Trifloxystrobin

CAS RN: 143390-89-0; 141517-21-7

GBRN: 503,504

Key Starting Material (KSM) -Kresoxim-methyl and Trifloxystrobin

Scheme-1



Reaction Summary:

1.1 Reagents: Sodium methoxide
Solvents: Methanol; rt, 0.5 h, rt; rt to 40 °C
1.2 Reagents: tert-Butyl nitrite; 1 h, 40 °C; 3 h, 40 °C
1.3 Reagents: Hydrochloric acid
Solvents: Water; pH 7, 40 °C
2.1 Catalysts: Sulfuric acid
Solvents: Water; 1 h, 100 °C; 5 h, 100 °C to 120 °C

Scheme-2



Reaction Summary:

1.1 Catalysts: Sulfuric acid
Solvents: Water; 1 h, 100 °C; 7 h, 100 °C
Yield: 96%

Scheme-3



Reaction Summary:

1.1 Catalysts: Sulfuric acid
Solvents: Water; 1 h, 100 °C; 6 h, 100 °C
Yield: 95%

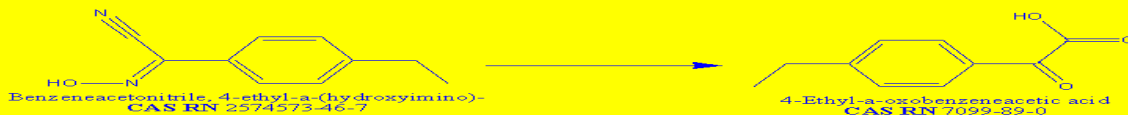
Scheme-4



Reaction Summary:

1.1 Catalysts: Sulfuric acid
Solvents: Water; 1 h, 100 °C; 6 h, 100 °C
Yield: 93%

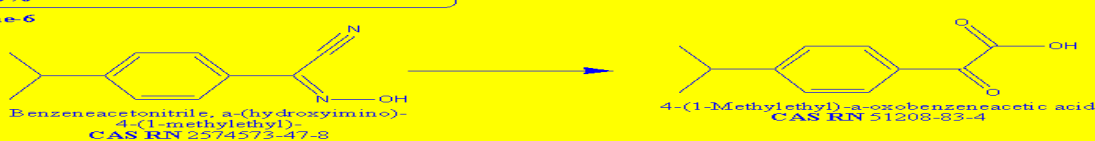
Scheme-5



Reaction Summary:

1.1 Catalysts: Sulfuric acid
Solvents: Water; 1 h, 100 °C; 5 h, 100 °C to 120 °C
Yield: 90%

Scheme-6



Reaction Summary:

1.1 Catalysts: Sulfuric acid
Solvents: Water; 1 h, 100 °C; 5 h, 100 °C to 120 °C
Yield: 83%

Scheme-7



Reaction Summary:

1.1 Catalysts: Sulfuric acid
Solvents: Water; 1 h, 100 °C; 5 h, 100 °C to 120 °C
Yield: 80%

References:

1. Green preparation of acetophenone acid and its application as chemical synthesis intermediate
By: Zhang, Hong, et al
China, CN112142587 A 2020-12-29
Assignee: Changsha Jiaqiao Biotechnology Co., Ltd., China

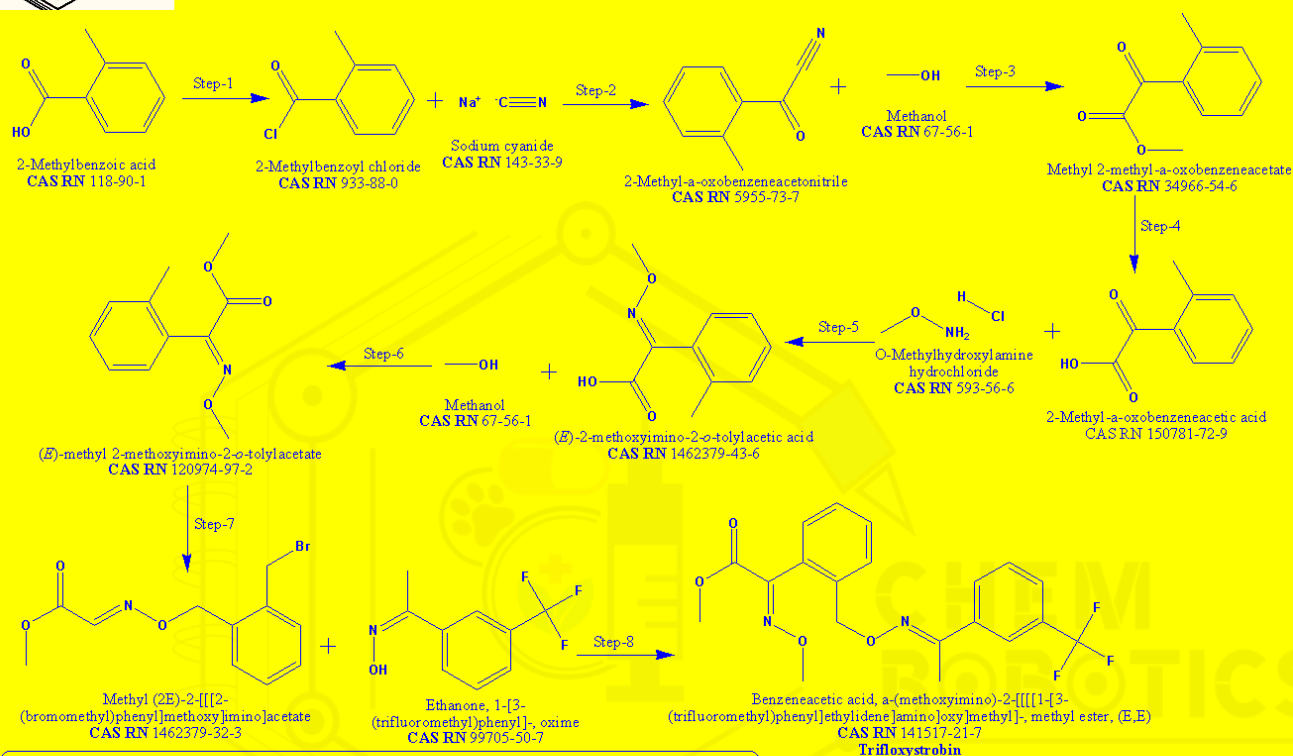
© Copyright 2021 by ChemRobotics Pvt. Ltd.

ROS - 7



Trifloxystrobin
CAS RN: 141517-21-7
GBRN: 504;12280

Route of Synthesis - Trifloxystrobin



References:

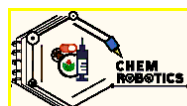
1. An improved process for the synthesis of strobilurin fungicides viz trifloxystrobin and kresoxim-methyl
By: Kamaraj, Pasumpon, et al
World Intellectual Property Organization, WO2013144924 A1 2013-10-03
Assignee: Rallis India Ltd., India

Reaction Summary:

1.1 Reagents: Thionyl chloride
Catalysts: Dimethylformamide
Solvents: Xylene, rt, 1 h, 50 °C
2.1 Catalysts: Tetrabutylammonium bromide
Solvents: Xylene, Water, < 20 °C, 2 h, rt
3.1 Reagents: Hydrochloric acid; 1 h, -5 - 0 °C
3.2 Reagents: Hydrochloric acid
Solvents: Methanol; 6 h, -5 - 0 °C, 15 - 20 °C, 20 °C to 45 °C
3.3 Reagents: Sulfuric acid
Solvents: Water; 3 h, 40 - 45 °C
3.4 Solvents: Methanol; 5 h, 60 - 65 °C, 65 °C to 40 °C
3.5 Solvents: Water; 10 min, 40 °C
4.1 Reagents: Methyl 2-methylbenzoate, Sodium hydroxide
Catalysts: Tetrabutylammonium bromide
Solvents: Water; 2 h, 45 °C
5.1 Solvents: Water; 1 h, rt
5.2 Solvents: Dichloromethane; 2 h, rt
5.3 Reagents: Hydrochloric acid
Solvents: Water; 10 min, rt
6.1 Reagents: Thionyl chloride, (aZ)-a-(Methoxyimino)-2-methylbenzeneacetic acid
Catalysts: Dimethylformamide; rt, 8 h, 40 - 45 °C
6.2 Solvents: Methanol; 1 h, 60 - 65 °C
7.1 Reagents: N-Bromosuccinimide
Catalysts: Azobisisobutyronitrile
Solvents: Acetonitrile; 6 h, rt to 60 °C
8.1 Reagents: Potassium carbonate
Solvents: Methyl isobutyl ketone; 12 h, rt to 115 °C

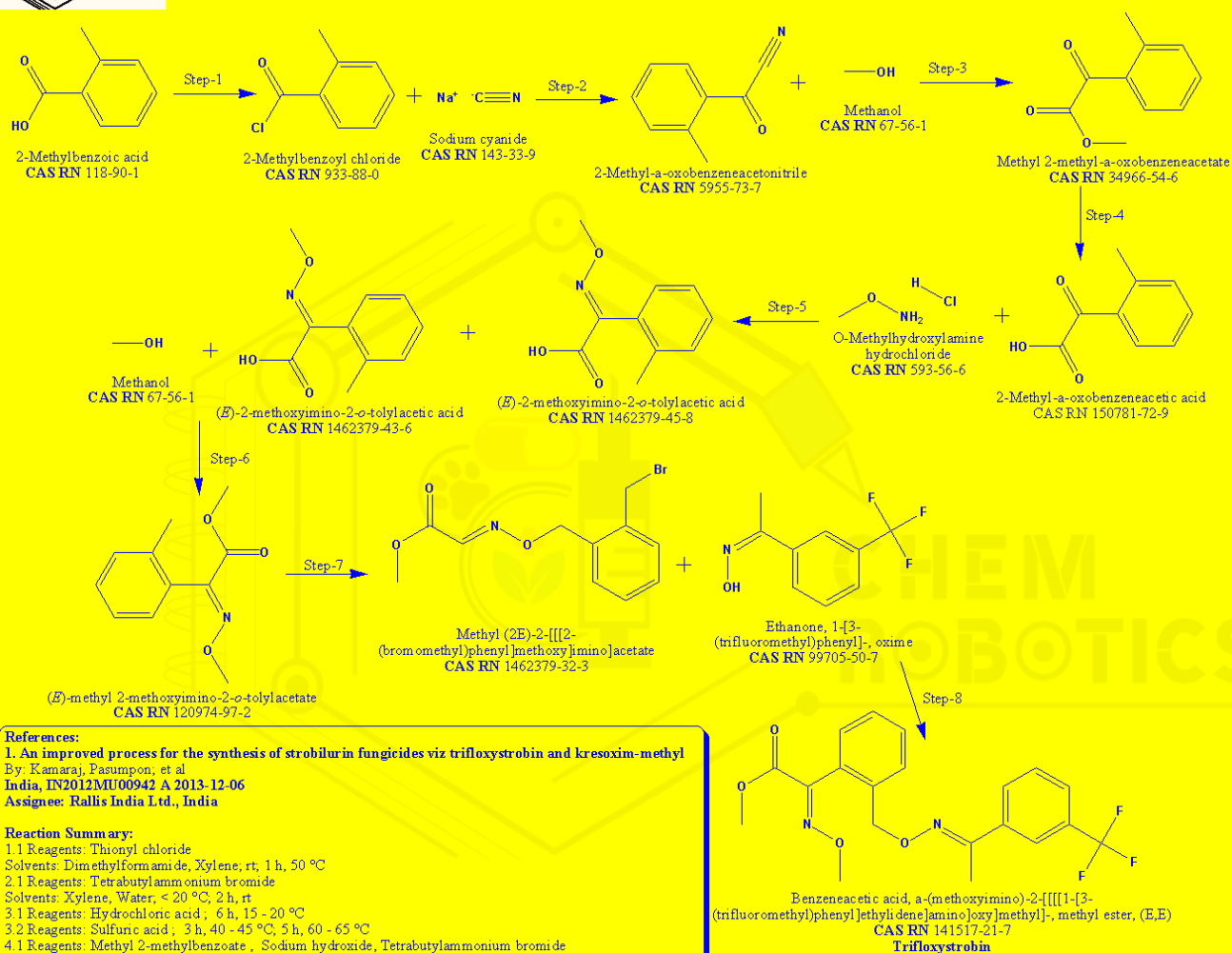
© Copyright 2022 by ChemRobotics Pvt. Ltd

ROS - 8



Trifloxystrobin
CAS RN: 141517-21-7
GBRN: 504;12280

Route of Synthesis - Trifloxystrobin



References:

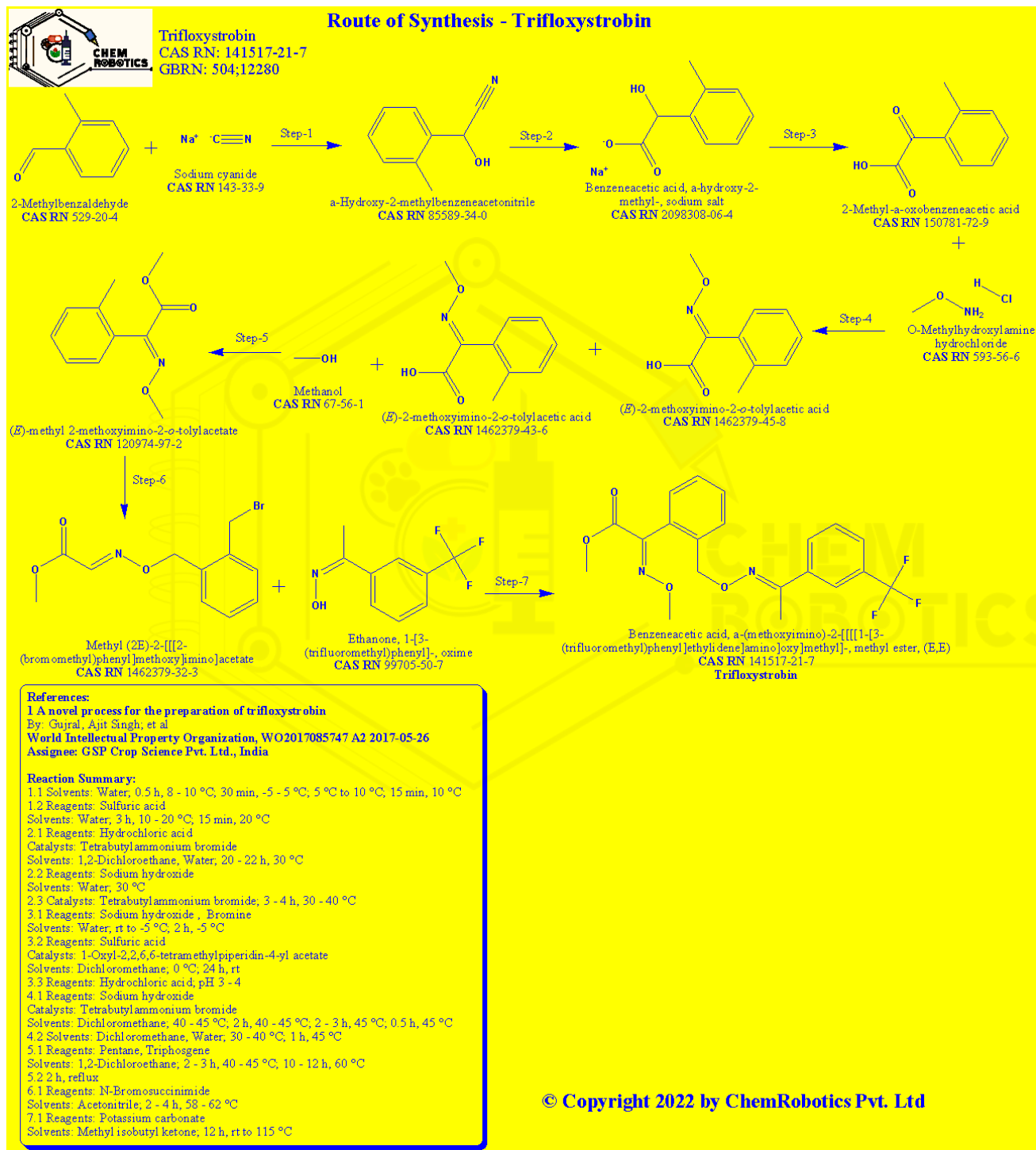
1. An improved process for the synthesis of strobilurin fungicides viz trifloxystrobin and kresoxim-methyl
By: Kamaraj, Pasumpon, et al
India, IN2012MU00942 A 2013-12-06
Assignee: Ralis India Ltd., India

Reaction Summary:

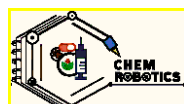
1.1 Reagents: Thionyl chloride
Solvents: Dimethylformamide, Xylene, rt, 1 h, 50 °C
2.1 Reagents: Tetrabutylammonium bromide
Solvents: Xylene, Water, < 20 °C, 2 h, rt
3.1 Reagents: Hydrochloric acid; 6 h, 15 - 20 °C
3.2 Reagents: Sulfuric acid; 3 h, 40 - 45 °C, 5 h, 60 - 65 °C
4.1 Reagents: Methyl 2-methylbenzoate, Sodium hydride, Tetrabutylammonium bromide
Solvents: Water, 2 h, 45 °C
5.1 Solvents: Water, 1 h, rt
5.2 Solvents: Dichloroethane; 2 h, rt
5.3 Reagents: Hydrochloric acid
Solvents: Water, 10 min, rt
6.1 Reagents: Thionyl chloride
Solvents: Dimethylformamide, rt, 8 h, 40 - 45 °C
6.2 1 h, 60 - 65 °C
7.1 Reagents: N-Bromosuccinimide
Catalysts: Azobisisobutyronitrile
Solvents: Acetonitrile, 6 h, rt to 60 °C
8.1 Reagents: Potassium carbonate
Solvents: Methyl isobutyl ketone, rt, 12 h, rt to 115 °C

© Copyright 2022 by ChemRobotics Pvt. Ltd

ROS - 9

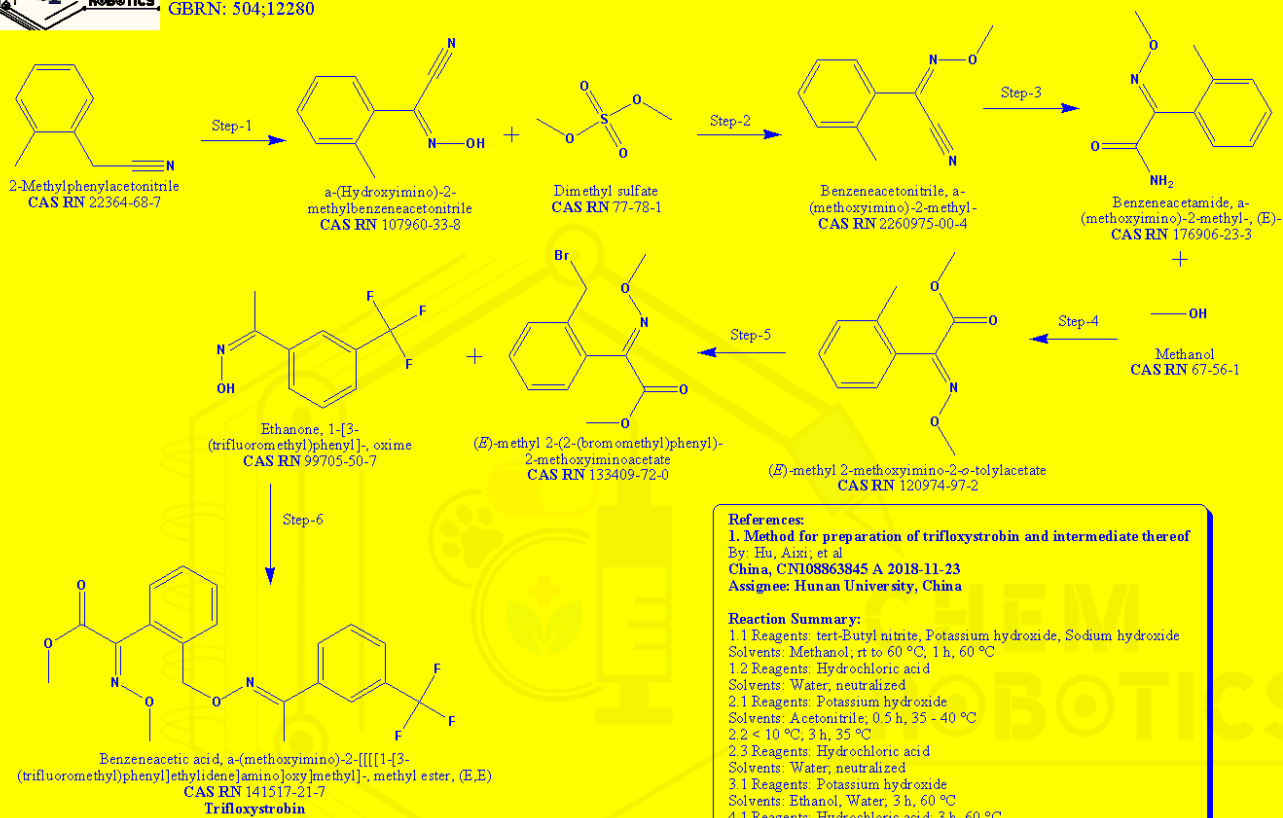


ROS - 10



Trifloxystrobin
CAS RN: 141517-21-7
GBRN: 504;12280

Route of Synthesis - Trifloxystrobin



© Copyright 2022 by ChemRobotics Pvt. Ltd

References:

1. Method for preparation of trifloxystrobin and intermediate thereof
By: Hu, Aisi; et al
China, CN108863845 A 2018-11-23
Assignee: Hunan University, China

Reaction Summary:

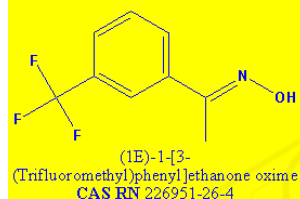
1.1 Reagents: tert-Butyl nitrite, Potassium hydroxide, Sodium hydroxide
Solvents: Methanol; rt to 60 °C, 1 h, 60 °C
1.2 Reagents: Hydrochloric acid
Solvents: Water, neutralized
2.1 Reagents: Potassium hydroxide
Solvents: Acetonitrile; 0.5 h, 35 - 40 °C
2.2 < 10 °C; 3 h, 35 °C
2.3 Reagents: Hydrochloric acid
Solvents: Water, neutralized
3.1 Reagents: Potassium hydroxide
Solvents: Ethanol, Water; 3 h, 60 °C
4.1 Reagents: Hydrochloric acid; 3 h, 60 °C
5.1 Reagents: 1,3-Dibromo-5,5-dimethylhydantoin
Catalysts: Azobisisobutyronitrile
Solvents: 1,2-Dichloroethane; 5 h, 80 °C
6.1 Reagents: Sodium methoxide
Solvents: Dimethylformamide; 15 min, rt, rt to 5 °C
6.2 5 h, rt

ROS - 11

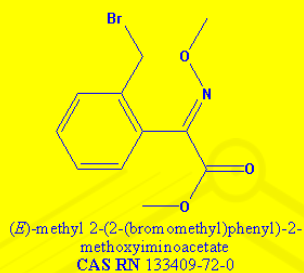


Trifloxystrobin
CAS RN: 141517-21-7
GBRN: 504;12280

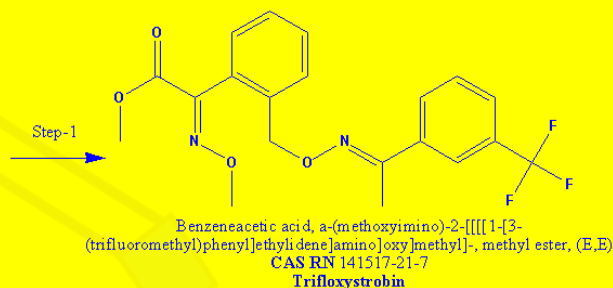
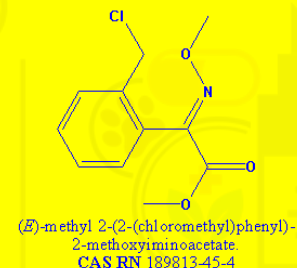
Route of Synthesis - Trifloxystrobin



Route-1



Route-2



References(Route-1):

1. Preparation of trifloxystrobin by microchannel reactor

By: Wang, Zhongyang, et al
China, CN113336668 A 2021-09-03

Assignee: Jingbo Agrochemicals Technology Co., Ltd., China

Reaction Summary:

1.1 Solvents: Dimethylformamide, rt

1.2 Reagents: Sodium methoxide

Solvents: Dimethylformamide, rt

Yield: 95%

2. Green preparation of trifloxystrobin

By: Xu, Hui, et al
China, CN112538029 A 2021-03-23

Assignee: Limin Chemical Co., Ltd., China

Reaction Summary:

1.1 Reagents: 1,8-Diazabicyclo[5.4.0]undec-7-ene

Solvents: Dimethylformamide, 10 min, < 5 °C; 2 h, 15 °C; 15 °C to rt

1.2 Reagents: Water, rt

Yield: 93%

3. Process for synthesis of Trifloxystrobin

By: He, Yongli, et al
China, CN103524379 A 2014-01-22

Assignee: Jiangsu Sevencontinent Green Chemical Co., Ltd., China

Reaction Summary:

1.1 Reagents: Potassium carbonate

Solvents: Xylene, rt to reflux; 4 h, reflux

1.2 Solvents: Toluene, 0.5 h, rt; 3 h, 30 °C

Yield: 90%

References(Route-2):

1. Preparation of trifloxystrobin by microchannel reactor

By: Wang, Zhongyang, et al
China, CN113336668 A 2021-09-03

Assignee: Jingbo Agrochemicals Technology Co., Ltd., China

Reaction Summary:

1.1 Solvents: Dimethylacetamide, rt

1.2 Reagents: Sodium methoxide

Solvents: Acetonitrile, rt

Yield: 95%

2. Method for synthesizing trifloxystrobin

By: Lv, Liangzhong, et al
China, CN105294490 A 2016-02-03

Assignee: Jiangsu Changqing Agrochemical Co., Ltd., China

Reaction Summary:

1.1 Reagents: Potassium hydroxide

Solvents: Dimethylformamide, rt, 10 min, cooled

1.2 5 h, rt

Yield: 91%

3. Process for preparation of trifloxystrobin

By: Ni, Yuebiao, et al
China, CN101941921 A 2011-01-12

Assignee: Yueyang Dipu Chemical Technology Co., Ltd., China

Reaction Summary:

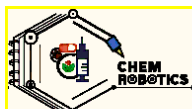
1.1 Reagents: Potassium carbonate

Solvents: Dimethyl sulfoxide, rt, rt to 65 °C; 60 - 65 °C

Yield: 74%

© Copyright 2022 by ChemRobotics Pvt. Ltd

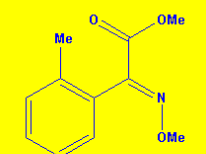
ROS - 12



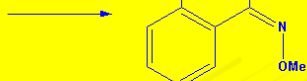
Trifloxystrobin
CAS RN: 141517-21-7
GBRN: 504

Chinese Patent Route

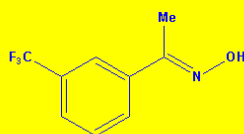
Patent Disclosure About Prior Arts-1 (PDPA-1)
 Route: 1



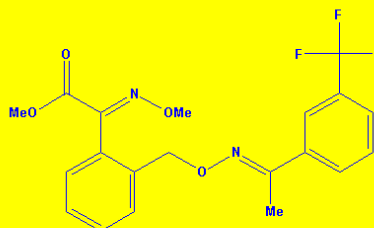
(*E*)-methyl 2-methoxyimino-2-*o*-tolylacetate
 PubChem CID: 14329206
 (I)



(II)



(*E*)-1-(3-(trifluoromethyl)phenyl)ethan-1-one oxime
 CAS RN: 99705-50-7
 (III)



methyl (*E*)-2-(methoxyimino)-2-(((((*E*)-1-(3-(trifluoromethyl)phenyl)ethylidene)amino)oxy)methyl)phenyl)acetate
TRIFLOXYSTROBIN
 CAS RN: 141517-21-7

References:

CN111807990A - Intermediate for preparing trifloxystrobin and synthetic method thereof

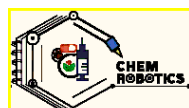
Assignee: Fuxin Fulongbao Pharmaceutical Technology Co Ltd

Application filed : 2020-07-24

Patent Disclosure About Prior Arts-1 (PDPA-1)

© Copyright 2022 by ChemRobotics Pvt. Ltd.

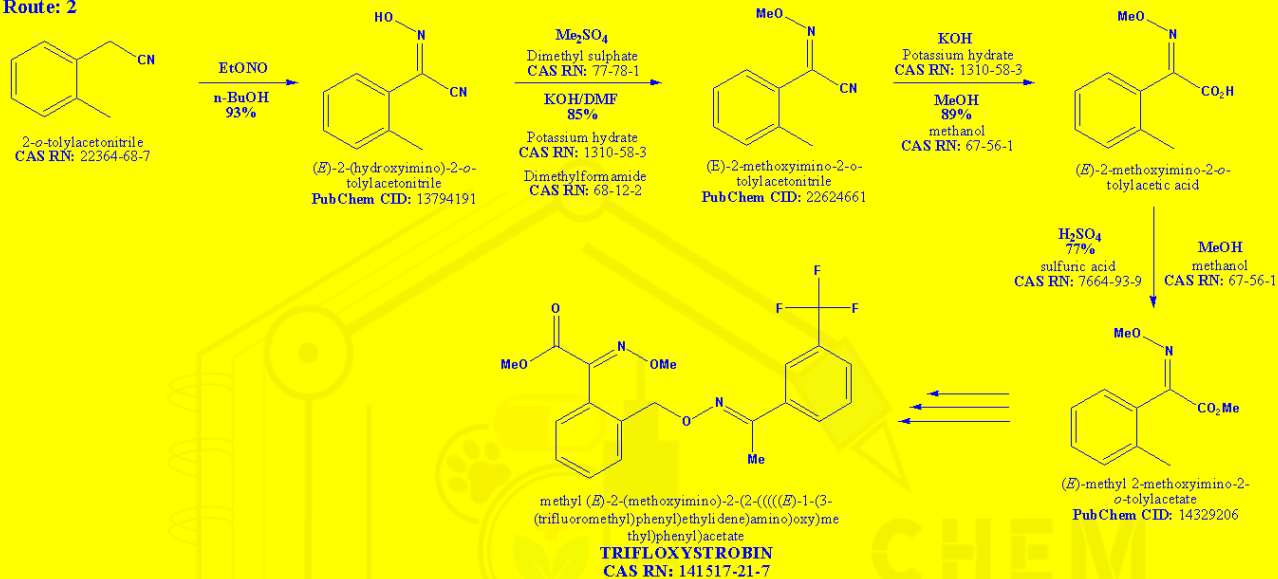
ROS - 13



Trifloxystrobine
CAS RN: 141517-21-7
GBRN: 504

Chinese Patent Route

Patent Disclosure About Prior Arts-2 (PDPA-2)
Route: 2



References:

CN111807990A - Intermediate for preparing trifloxystrobin and synthetic method thereof

Assignee: Fuxin Fulongbao Pharmaceutical Technology Co Ltd

Application filed : 2020-07-24

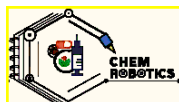
Patent Disclosure About Prior Arts-2 (PDPA-2)

Reaction Summary:

Li Renhong [Master Thesis of Hebei University of Science and Technology, 2015] reported a process for the preparation of trifloxystrobin intermediate I with readily available raw materials. They used *o*-tolyl acetonitrile as raw material, and obtained the trifloxystrobin intermediate I through a six-step reaction of oximation, acidification, etherification, hydrolysis, acidification and esterification. Although the raw material *o*-toluene acetonitrile is easy to obtain, the preparation route is long, and the equipment and labor required for production are large; and it is assumed that the reactions of each step are carried out quantitatively, and 1 molar equivalent is prepared from 1 molar equivalent of *o*-tolyl acetonitrile. Trifloxystrobin intermediate I at least needs more than 6 equivalents of sodium hydroxide or potassium hydroxide strong base, and the neutralization of the resulting salt intermediate needs to consume at least an equivalent of acid, which not only leads to the preparation of the trifloxystrobin intermediate by this process. Body I produces a large amount of three wastes, and the consumption of raw materials is large and the production cost is high. Further, even if the crude trifloxystrobin intermediate I prepared by this technique has undergone two-step purification operations of vacuum distillation and petroleum ether recrystallization to obtain the required (*E*)-2-(methoxyimino)-*o*-methyl. The purity of methyl phenylacetate is also only 93.77%. When the intermediate of this content is used for the preparation of trifloxystrobin, in order to obtain the trifloxystrobin product that meets the purity of market demand, the crude trifloxystrobin obtained also needs to be further re-used. Crystallization and other purification operations are carried out for purification, which leads to an important factor that the yield of trifloxystrobin is not high in the final preparation. The yields of each step were 93%, 85%, 89%, and 77%, respectively.

© Copyright 2022 by ChemRobotics Pvt. Ltd.

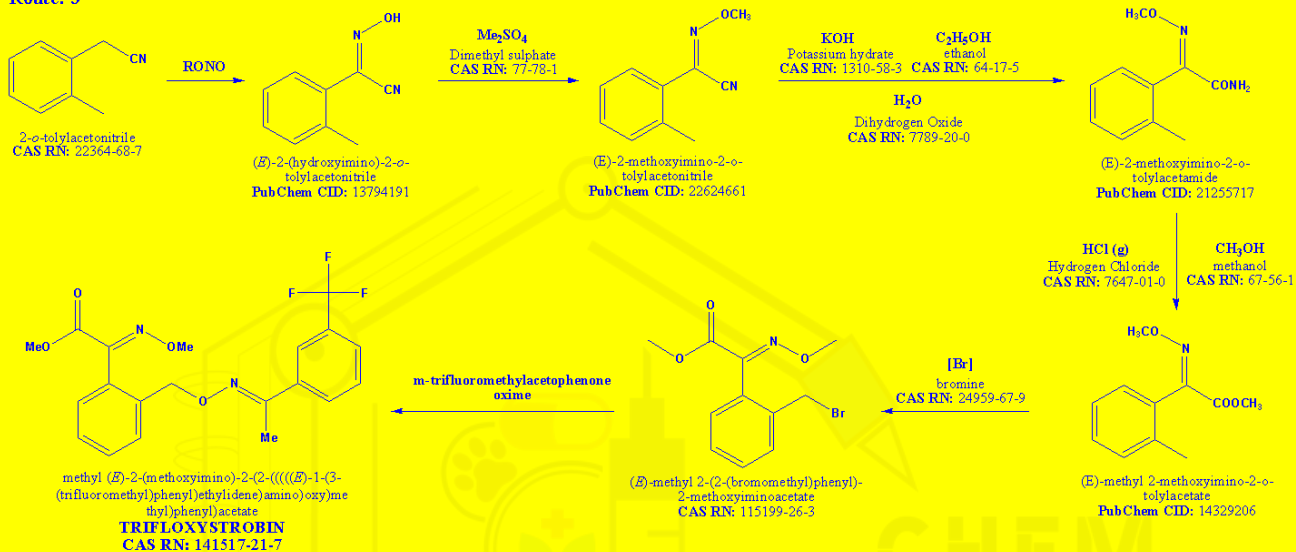
ROS - 14



Trifloxystrobin
CAS RN: 141517-21-7
GBRN: 504

Chinese Patent Route

Patent Disclosure About Prior Arts-3 (PDPA-3)
Route: 3



References:

CN111807990 A - Intermediate for preparing trifloxystrobin and synthetic method thereof

Assignee: Fuxin Fulongbao Pharmaceutical Technology Co Ltd

Application filed : 2020-07-24

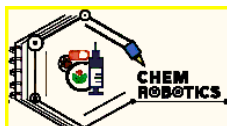
Patent Disclosure About Prior Arts-3 (PDPA-3)

Reaction Summary:

CN108863845 A discloses the following reaction process, which requires four steps, and the total yield of Example 4 is 75%; this patent divides the methyl esterification into two steps, and there is a process of repeatedly adjusting the base and then adjusting the acid, and the four steps consume a total of 5.4 equivalents of alkali, and 4.4 equivalents of acid, the amount of three wastes is large; each step requires an organic solvent to extract the product from the reaction system, and the cost is high.

© Copyright 2022 by ChemRobotics Pvt. Ltd.

ROS - 15

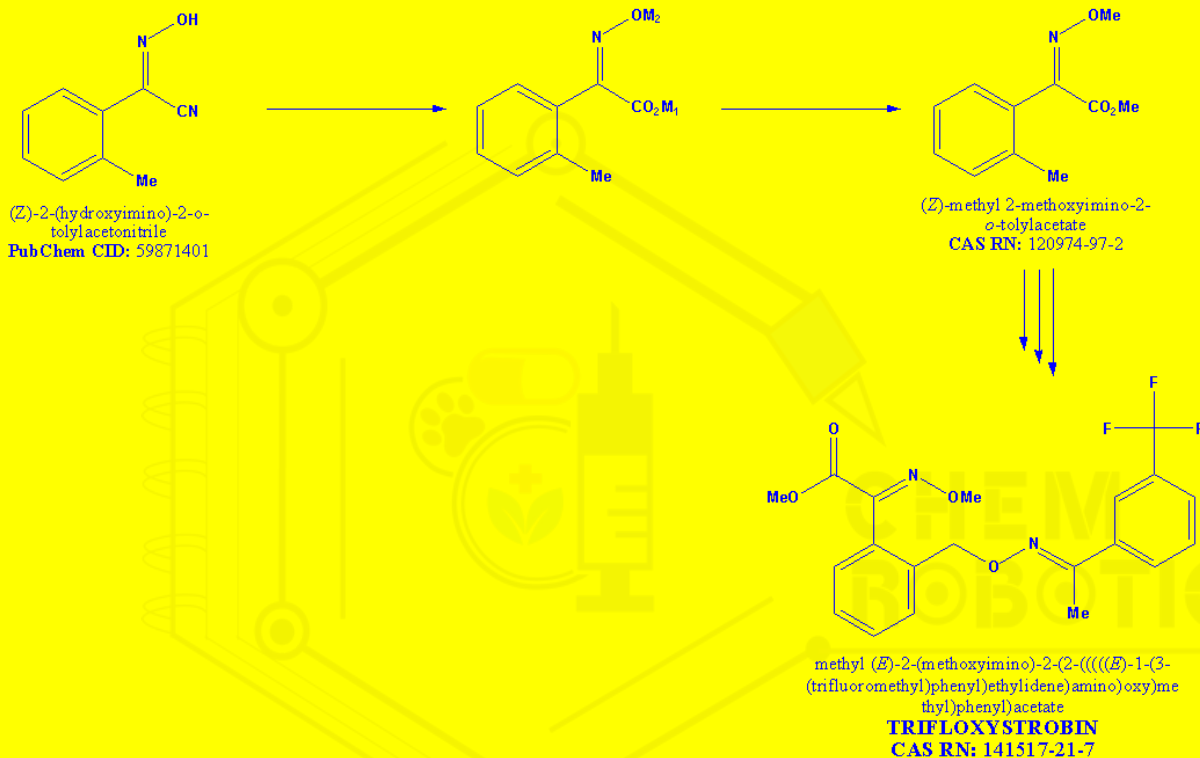


Trifloxystrobin

CAS RN: 141517-21-7
GBRN: 504

Chinese Patent Route

Accordingly to present Invention - 4 (API-4)
Route: 4



References:

CN111807990 A - Intermediate for preparing trifloxystrobin and synthetic method thereof

Assignee: Fuxin Fulongbao Pharmaceutical Technology Co Ltd

Application filed : 2020-07-24

Accordingly to present Invention - 4 (API-4)

Reaction Summary:

The invention relates to an intermediate for preparing trifloxystrobin and a synthesis method of the intermediate, wherein the synthesis method comprises the steps: by taking 2-oxime-o-methyl phenylacetonitrile as a raw material, heating and hydrolyzing in an alkaline aqueous solution to obtain 2-oxime-o-methyl phenylacetic acid or mono-sodium salt/mono-potassium salt or disodium salt/di-potassium salt of 2-oxime-o-methyl phenylacetic acid; and under an alkaline condition, carrying out a reaction with a methylation reagent to obtain (E)-2-(methoxyimino)-methyl o-methyl phenyl acetate. The method has the characteristics of easily available raw materials, single trans-configuration of the product, and simple operation, and is suitable for industrial production.

© Copyright 2022 by ChemRobotics Pvt. Ltd.

ROS - 16

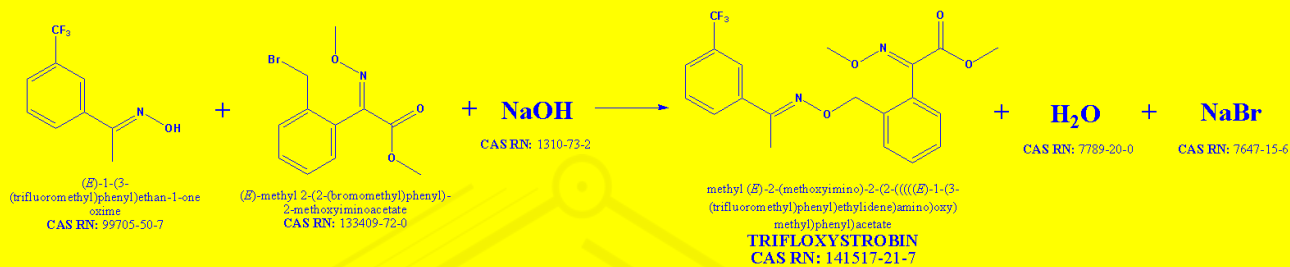


Trifloxystrobin
CAS RN: 141517-21-7
GBRN:504;12280

Chinese Patent Route

Kresoxim-Methyl
CAS RN: 143390-89-0
GBRN:503

Patent Disclosure About Prior Arts-1 (PDPA-1) Route 1



References:

CN113527137A - Preparation method of characteristic impurities of trifloxystrobin

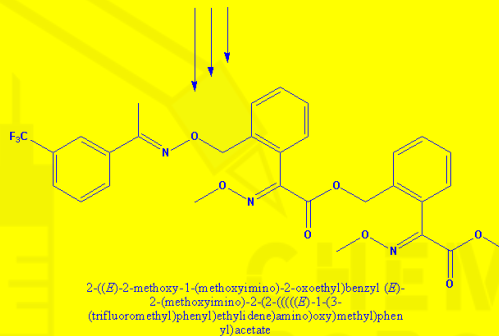
Assignee: Changsha Jiaqiao Biotechnology Co Ltd

Application filed by: 2020-04-13

Patent Disclosure About Prior Arts-1 (PDPA-1)

Reaction Summary:

The process for the preparation of Trifloxystrobin comprising, the reaction is condensed under the action of a base, because the base and (E)-2-(2-bromomethyl)phenyl)-2-methoxyiminoacetic acid methyl ester are all excessive in this reaction, and in an alkaline environment, trifloxystrobin will inevitably undergo saponification to form the intermediate salt (2E)-2-methoxyimino-2-[2-[[1-[3-(trifluoromethyl)phenyl] ethylene amino] oxymethyl] phenyl] sodium acetate, that is, sodium oxime. In the subsequent esterification reaction, sodium oxime reacts with methyl (E)-2-(2-bromomethyl)phenyl)-2-methoxyiminoacetate (bromooxime ether) to generate oxime. Characteristic impurities of pyraclostrobin (E)-2-((E)-2-methoxy-1-(methoxyimino)-2-ethoxy)phenyl-2-(methoxyimino)-2-(2-(((E)-1-(3-(trifluoromethyl)phenyl) ethyleneamino) methoxy) phenyl) methyl acetate, the structure of this characteristic impurity is as follows:



Trifloxystrobin Impurity

© Copyright 2022 by ChemRobotics Pvt. Ltd.

ROS - 17

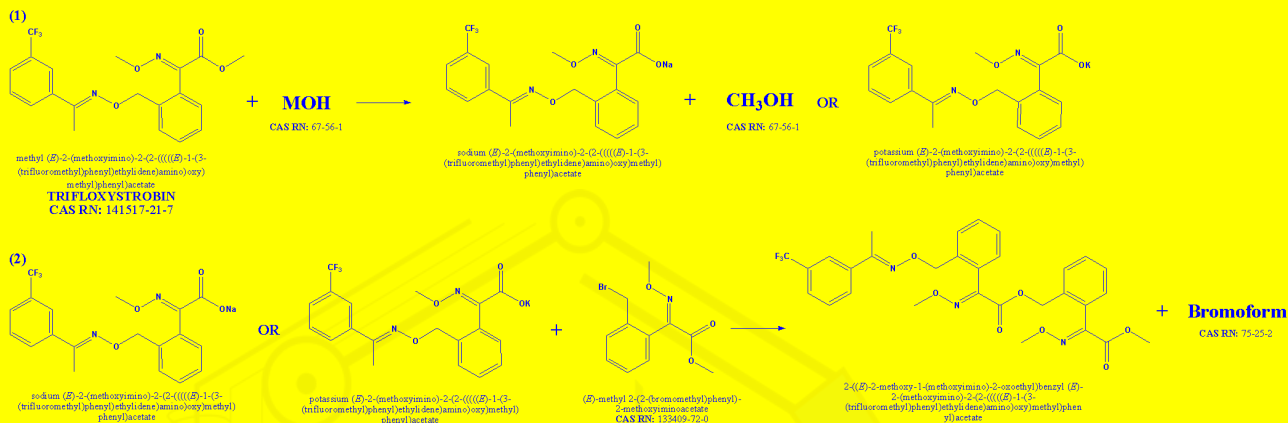


Trifloxystrobin
CAS RN: 141517-21-7
GBRN:504;12280

Chinese Patent Route

Kresoxim-Methyl
CAS RN: 143390-89-0
GBRN:503

Accordingly to present Invention - 1 (API-1)
Route 2



References:

CN113527137A - Preparation method of characteristic impurities of trifloxystrobin

Assignee: Changsha Jiaqiao Biotechnology Co Ltd

Application filed by: 2020-04-13

Accordingly to present Invention - 1 (API-1)

Reaction Summary:

The invention provides a preparation method of trifloxystrobin characteristic impurities, which comprises the following steps: (1) carrying out saponification reaction on trifloxystrobin and alkali to obtain trifloxystrobin salt, and (2) carrying out condensation reaction on the trifloxystrobin salt and bromo-oxime ether, and carrying out post-treatment on a generated crude product to obtain the trifloxystrobin characteristic impurity. According to the preparation method, the trifloxystrobin characteristic impurities are rapidly synthesized through saponification and condensation, the process steps are simple, the reaction conditions are mild, operation is easy, the raw material conversion rate is high, and no side reaction occurs; wherein the purity of the final product obtained through post-treatment is greater than 98.5%, and the yield can reach 87% or above. The trifloxystrobin characteristic impurity obtained by the preparation method provided by the invention has the characteristics of high purity and high yield, and can be used as a reference substance. The technology is beneficial to development of a trifloxystrobin analysis method and more beneficial to quality control of trifloxystrobin, and a new idea is provided for product quality control.

© Copyright 2022 by ChemRobotics Pvt. Ltd.

ROS - 18



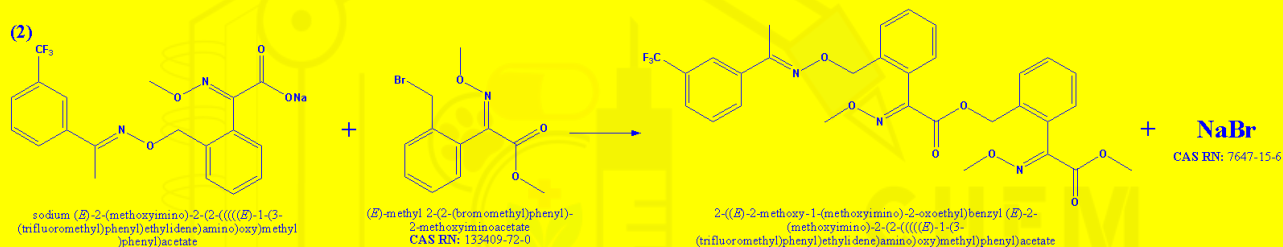
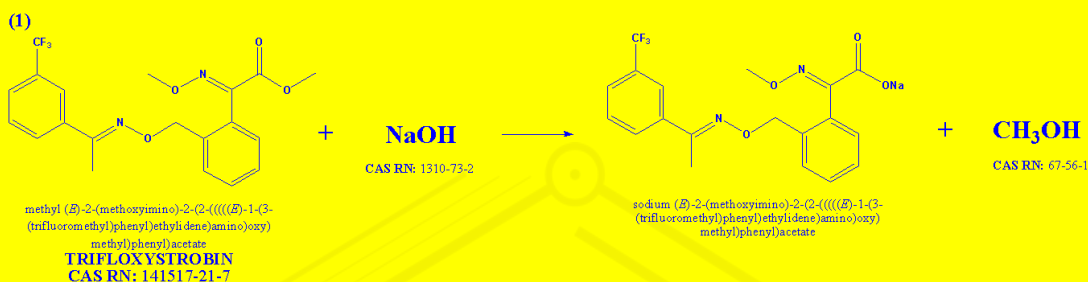
Trifloxystrobin
CAS RN: 141517-21-7
GBRN:504;12280

Chinese Patent Route

Kresoxim-Methyl
CAS RN: 143390-89-0
GBRN:503

Accordingly to present invention - 2 (API-2)

Example 1



Trifloxystrobin Impurity

References:

CN113527137A - Preparation method of characteristic impurities of trifloxystrobin

Assignee: Changsha Jiaqiao Biotechnology Co Ltd

Application filed by: 2020-04-13

Accordingly to present invention - 2 (API-2)

Reaction Summary:

The invention provides a preparation method of trifloxystrobin characteristic impurities, which comprises the following steps: (1) carrying out saponification reaction on trifloxystrobin and alkali to obtain trifloxystrobin salt; and (2) carrying out condensation reaction on the trifloxystrobin salt and bromo-oxime ether, and carrying out post-treatment on a generated crude product to obtain the trifloxystrobin characteristic impurity. According to the preparation method, the trifloxystrobin characteristic impurities are rapidly synthesized through saponification and condensation, the process steps are simple, the reaction conditions are mild, operation is easy, the raw material conversion rate is high, and no side reaction occurs; wherein the purity of the final product obtained through post-treatment is greater than 98.5%, and the yield can reach 87% or above. The trifloxystrobin characteristic impurity obtained by the preparation method provided by the invention has the characteristics of high purity and high yield, and can be used as a reference substance. The technology is beneficial to development of a trifloxystrobin analysis method and more beneficial to quality control of trifloxystrobin, and a new idea is provided for product quality control.

© Copyright 2022 by ChemRobotics Pvt. Ltd.

ROS - 19

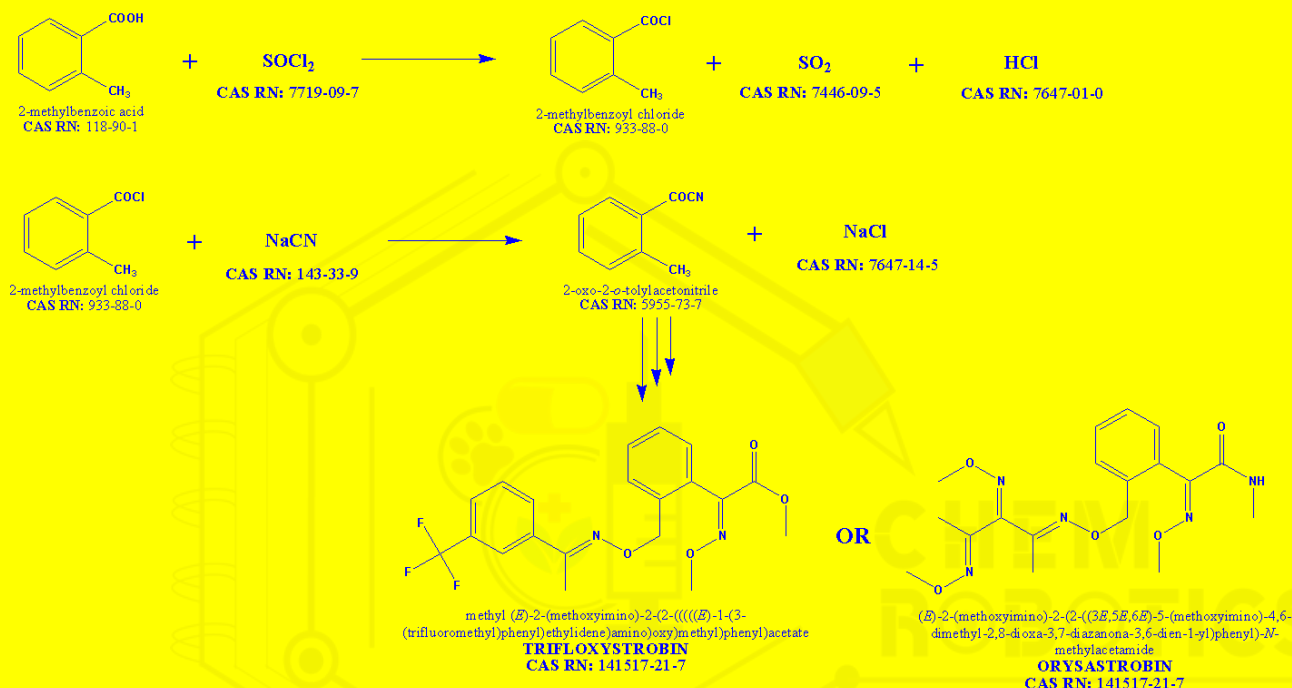


TRIFLOXYSTROBIN
CAS RN: 141517-21-7
GB RN: 504;12280

ORYSASTROBIN
CAS RN: 141517-21-7
GB RN: 423

Chinese Patent Route

Accordingly to present invention - 1 (API-1)
Route 1



References:

CN113666841A - Preparation method of o-methyl benzoyl nitrile

Assignee: Fushun Shunnum Chemical Co Ltd

Application filed: 2021-09-23

Accordingly to present invention - 1 (API-1)

Reaction Summary:

The invention discloses a preparation method of o-methyl benzoyl nitrile, the preparation method comprising the following steps: dissolving o-toluic acid in a toluene solvent, dropwise adding thionyl chloride for reaction, and removing a small amount of unreacted thionyl chloride at low temperature after the reaction is finished to obtain a solvent-containing intermediate o-methylbenzoyl chloride solution; then directly adding a catalyst, solid sodium cyanide and a reaction aid, continuing a second-step reaction, after the reaction is finished, adding a saturated sodium chloride solution into a reaction solution, pulping and splitting phases, and washing an organic phase once by using the saturated sodium chloride solution; and carrying out reduced pressure distillation on the organic phase to recover the solvent, and carrying out vacuum rectification to obtain the o-methylbenzoyl nitrile product with the purity of more than 99.0%.

According to the method, the o-methylbenzoyl nitrile is synthesized by taking o-toluic acid as an initial raw material through a one-pot method, the method is simple and feasible, a safe and environment-friendly treatment process is provided for waste gas and a byproduct sodium chloride salt generated in the reaction process, and the whole technological process is green and environment-friendly and is suitable for large-scale industrial enlarged production. a safe and environment-friendly treatment process is provided for waste gas and a byproduct sodium chloride salt generated in the reaction process, and the whole technological process is green and environment-friendly and is suitable for large-scale industrial enlarged production. a safe and environment-friendly treatment process is provided for waste gas and a byproduct sodium chloride salt generated in the reaction process, and the whole technological process is green and environment-friendly and is suitable for large-scale industrial enlarged production.

© Copyright 2022 by ChemRobotics Pvt. Ltd.

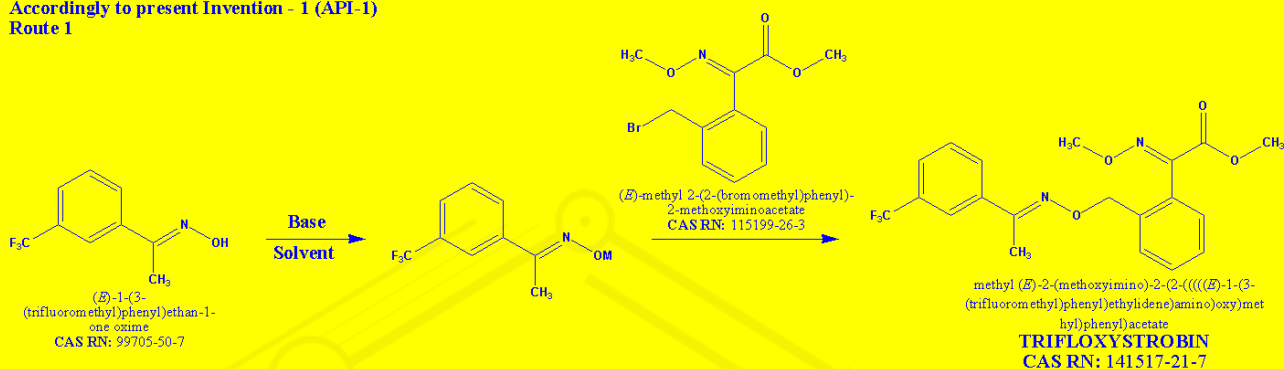
ROS - 20



Trifloxystrobin
CAS RN: 141517-21-7
GBRN: 504

Chinese Patent Route

Accordingly to present invention - 1 (API-1)
Route 1



References:

CN113683527A - Preparation method of trifloxystrobin

Assignee: Jiangsu Qizhou Green Technology Research Institute Co Ltd

Application filed: 2021-10-26

Family Equivalents: CN113683527A; CN113683527B

Accordingly to present invention - 1 (API-1)

Summary:

The invention provides a preparation method of trifloxystrobin. The preparation method comprises the following steps: (1) subjecting a raw material A to reacting with alkali at a first temperature; and (2) subjecting a substance obtained by the reaction in the step (1) to reacting with a raw material B at a second temperature to generate trifloxystrobin, wherein the first temperature is higher than the second temperature, the raw material A is *m*-trifluoromethylbenzene acetophenone oxime, and the raw material B is *(E)*-2-(2-(bromomethyl)phenyl)-2-methoxyiminoethyl acetate. According to the invention, the raw material A firstly reacts with a strong base to generate an intermediate, and then the intermediate reacts with the raw material B to generate the trifloxystrobin, so the decomposition of the raw material B and the trifloxystrobin is avoided, and the yield of the trifloxystrobin is improved; besides, water generated in a reaction system is removed, and then the raw material B is added for a reaction, so hydrolysis of the trifloxystrobin is avoided, and the yield of the trifloxystrobin is further improved; and the method is simple in process, a solvent is easy to recover, the preparation process is green and environment-friendly, and the method is suitable for industrial production. and the method is suitable for industrial production.

© Copyright 2022 by ChemRobotics Pvt. Ltd.

ROS - 21

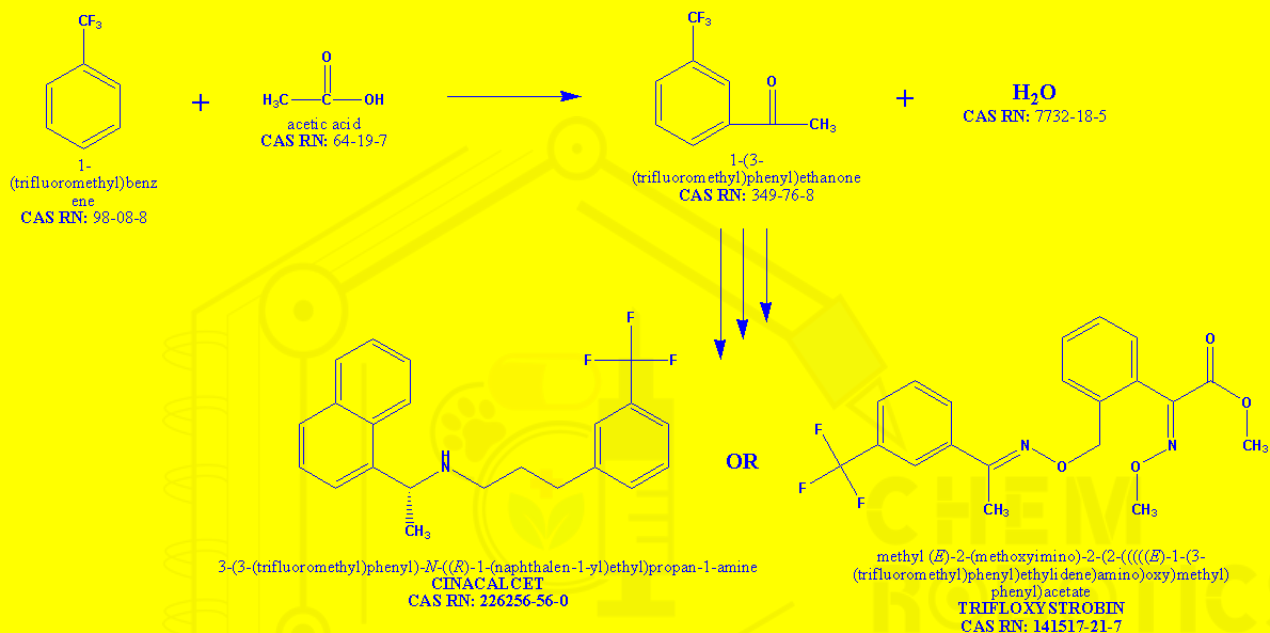


Cinacalcet
CAS RN: 226256-56-0
GBRN: 10342

Chinese Patent Route

Trifloxystrobin
CAS RN: 141517-21-7
GBRN: 504; 12280

Accordingly to present Invention - 1 (API-1)
Route 1



References:

CN113956143A - Preparation method of m-trifluoromethyl acetophenone

Assignee : Shandong Huayang Technology Co Ltd

Application filed :2021-11-15

Accordingly to present Invention - 1 (API-1)

Summary:

The invention discloses a preparation method of m-trifluoromethyl acetophenone, and relates to the technical field of chemical synthesis. According to the method, trifluoromethyl benzene and acetic acid are used as raw materials and subjected to a condensation reaction in a solvent under the action of a catalyst, the solvent is removed through distillation to obtain the m-trifluoromethyl acetophenone, the content of m-trifluoromethyl acetophenone is larger than or equal to 99.0%, and the total yield is larger than or equal to 95.0% in terms of trifluoromethyl benzene; and the method provided by the invention has the advantages of simple process flow, safety and convenience in operation, high product quality and yield of m-trifluoromethyl acetophenone, low consumption, low production cost and less amount of three wastes, relieves environmental protection pressure, meets the requirement of clean production, and is beneficial to large-scale industrial production.

© Copyright 2022 by ChemRobotics Pvt. Ltd.

ROS - 22



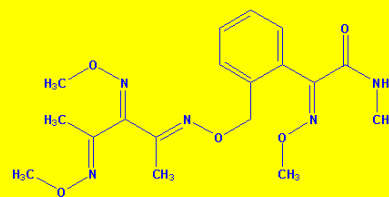
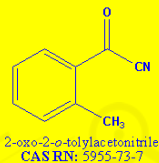
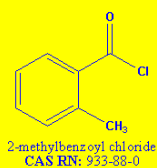
Orysastrubin
CAS RN: 248593-16-0
GBRN: 423

Mesotrione
CAS RN: 104206-82-8
GBRN: 410

Trifloxystrobin
CAS RN: 141517-21-7
GBRN: 504;12280

Chinese Patent Route

Accordingly to present Invention - 1 (API-1)
Route 1



(E)-2-(methoxyimino)-2-(2-(((3E,5E,6E)-5-(methoxyimino)-4,6-dimethyl-2,8-dioxa-3,7-diazanona-3,6-dien-1-yl)phenyl)-N-methylacetamide

Orysastrubin
CAS RN: 248593-16-0

OR

References:

CN114380713A - Synthesis method of o-methyl benzoyl cyanide

Assignee: Liaoning Zhonghui Biotechnology Co Ltd

Application filed: 2021-09-29

Accordingly to present Invention - 1 (API-1)

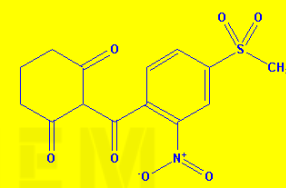
Summary:

The invention discloses a method for synthesizing o-toluy cyanide. The method uses o-toluy chloride as a raw material, potassium ferricyanide as a cyanating reagent, and is catalyzed by a copper catalyst in the presence or absence of solvent. In the preparation of o-toluy cyanide. The synthesis method avoids the use of highly toxic sodium cyanide, cuprous cyanide, etc., is green and safe, has cheap and easily available raw materials, mild reaction conditions, and has high industrial production value.



methyl (E)-2-(methoxyimino)-2-(2-(((E)-1-(3-(trifluoromethyl)phenyl)ethylidene)amino)oxy)methyl)phenyl)acetate
Trifloxystrobin
CAS RN: 141517-21-7

OR



2-(4-(methylsulfonyl)-2-nitrobenzoyl)cyclohexane-1,3-dione
Mesotrione
CAS RN: 104206-82-8

© Copyright 2023 by ChemRobotics Pvt. Ltd.

ROS - 23



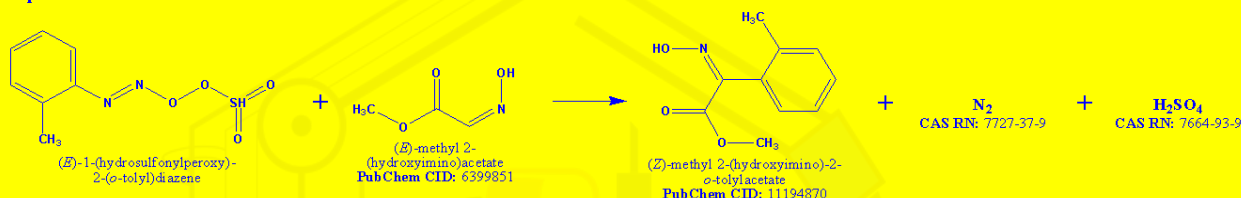
Trifloxystrobin
CAS RN: 141517-21-7
GBRN: 504;12280
TRRN: 75222

Indian Environment Clearance Disclosed Routes - Trifloxystrobin

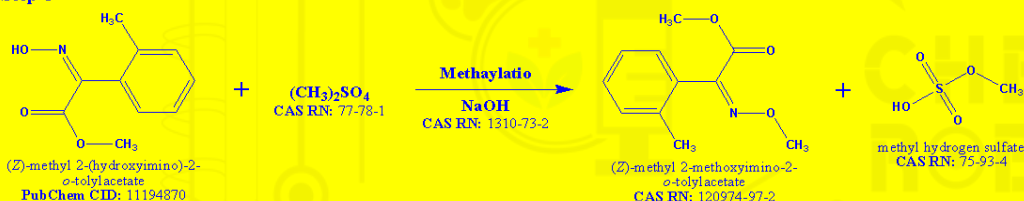
Step 1



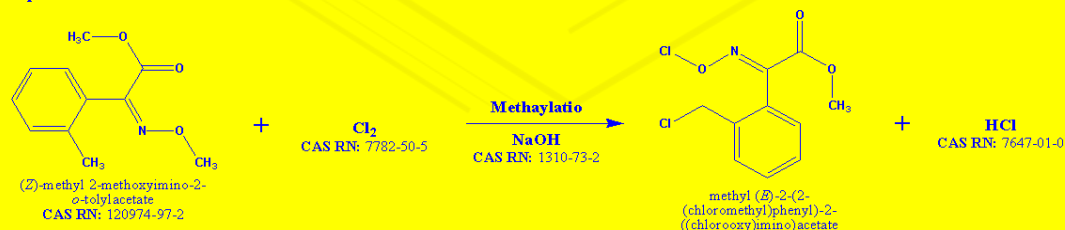
Step 2



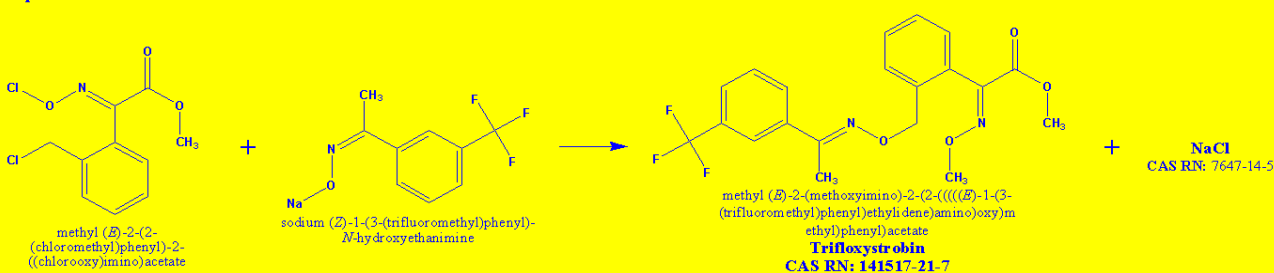
Step 3



Step 4



Step 4



References:

1. Environment Clearance Report, Ministry of Environment, Forest and Climate Change Government of India, Accessed on Aug 25, 2023.

Reaction Summary:

Trifloxystrobin

Manufacturing Process :-

Step 1 :- 2-Methyl Aniline is reacted with Sodium Nitrite and Hydrochloric acid to give 2-Methyl benzene Diazonium salt by diazotization.

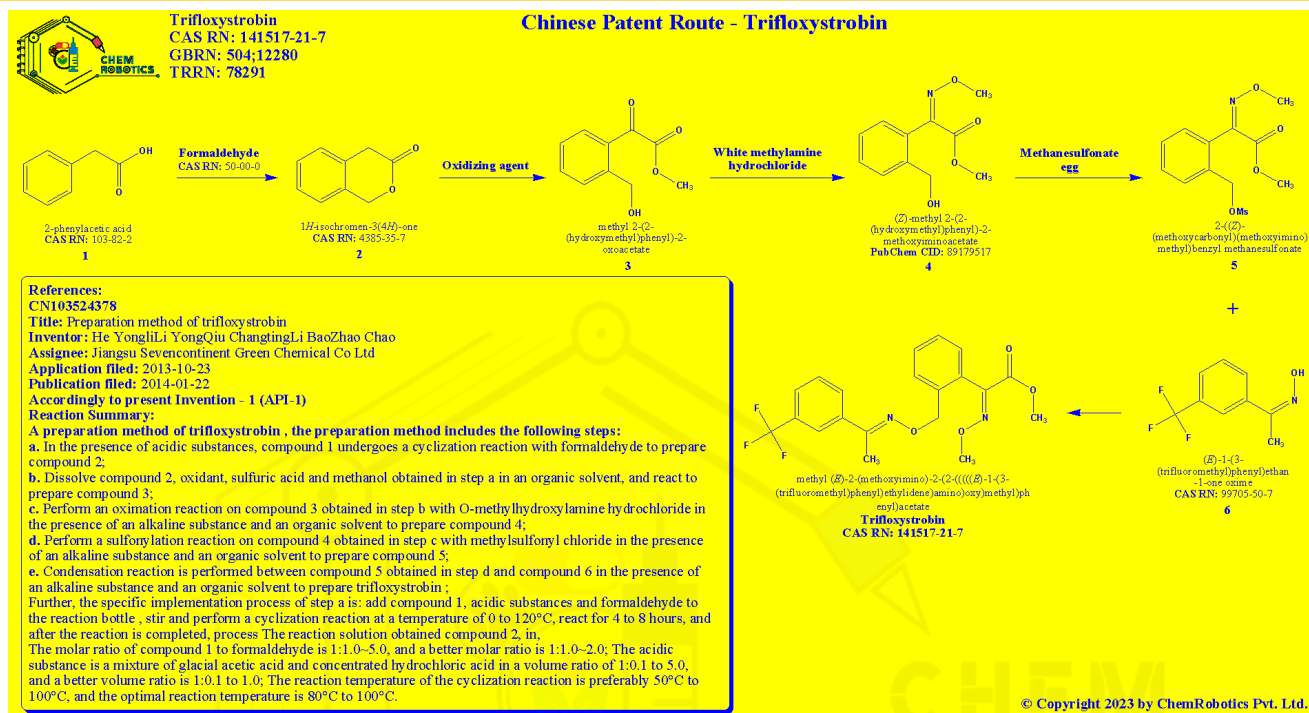
Step 2 :- 2-Methyl Benzene Diazonium salt further reacted with Glyoxylic Acid methyl ester Oxime to give 2-Methyl phenyl glyoxalin acid methyl ester Oxime.

Step 3 :- 2-Methyl Phenyl Glyoxylic Acid methyl ester Oxime reacted with Dimethyl sulfate in presence of Sodium Hydroxide to give 2-Methyl Phenyl Glyoxylate-o-methyl Oxime.

Step 4 :- 2-Methyl Phenyl Glyoxylate-o-methyl Oxime further on chlorination with chlorine gas in presence of Solvent - EDC gives 2-Methyl phenyl Glyoxylate-o-methyl Oxime.

Step 5 :- 2-Methyl Phenyl Glyoxylate-o-methyl Oxime reacted with Sodium [-1- [3- (Trifluoromethyl) Phenyl] Ethylene] Amine] Oxidamide in presence of Solvent - DMF to give final product Trifloxystrobin.

ROS - 24

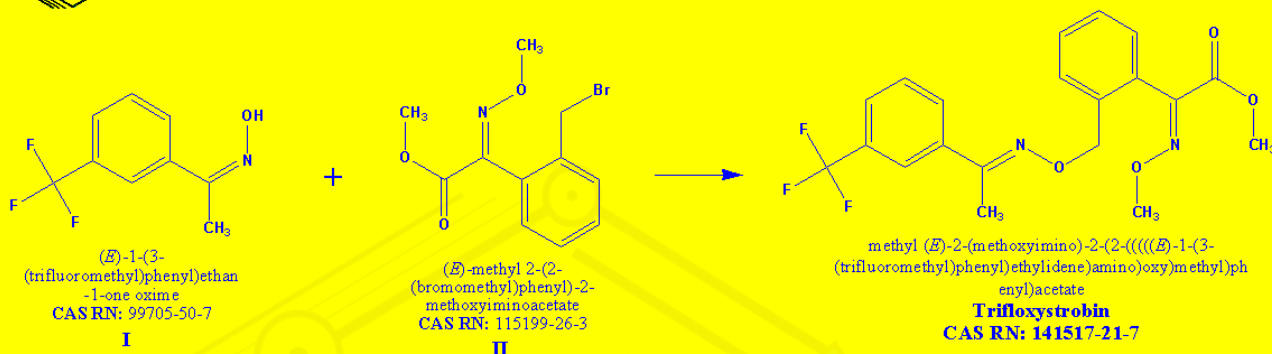


ROS - 25



Trifloxystrobin
 CAS RN: 141517-21-7
 GBRN: 504;12280
 TRRN: 78292

Chinese Patent Route - Trifloxystrobin



References:

CN103524379

Title: Synthesis method of trifloxystrobin

Inventor: He YongliDing FeiJu XiaodongCai Junyi

Assignee: Jiangsu Sevencontinent Green Chemical Co Ltd

Application filed: 2013-10-23

Publication filed: 2014-01-22

Accordingly to present Invention - 1 (API-1)

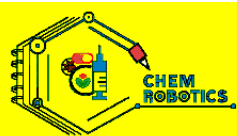
Reaction Summary:

A synthetic method of trifloxystrobin, the synthetic method includes the following steps:

a. To the nitrogen-substituted reaction bottle equipped with a stirrer, thermometer, water separator and condenser, add compound (I), alkaline substances and organic solvents and stir, and heat to reflux to separate water. The reflux separates. The water time is 5 to 6 hours. After the water separation is completed, the temperature is cooled to room temperature, and then the toluene solution of compound (II) is added dropwise to the above reaction solution. After the dropwise addition is completed, it is kept at room temperature for 2 to 4 hours, wherein, The molar ratio of the compound (I) to the alkaline substance is 1:1.0-3.0, the molar ratio of the compound (I) to the compound (II) is 1:0.9-2.0, and the toluene solution of the compound (II) The mass concentration is 30% to 70%;

© Copyright 2023 by ChemRobotics Pvt. Ltd.

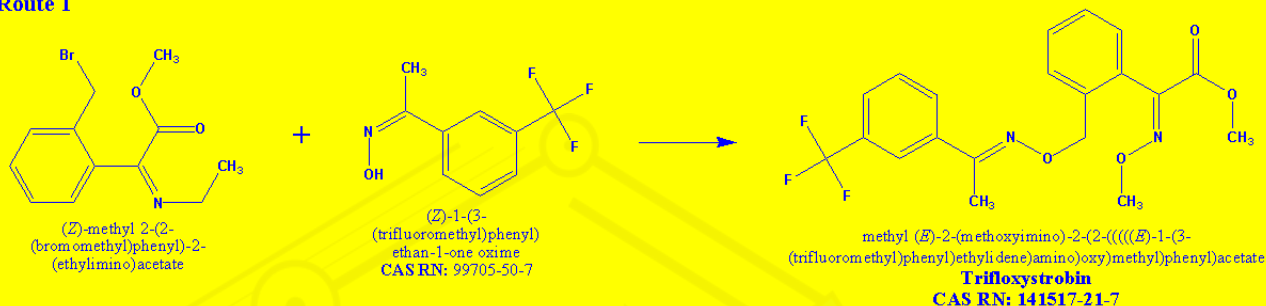
ROS - 26



Trifloxystrobin
CAS RN: 141517-21-7
GBRN: 504
TRRN: 78294

Chinese Patent Route - Trifloxystrobin

Accordingly to present Invention - 1 (API-1)
Route 1



References:

CN103787916A

Title: Preparation method of trifloxystrobin

Inventor: Wang Jiangang Wei Nengchun Wang Peng Wang Zongyuan Jinglin Cao Tongbo Liu Jiancheng Li Yonghong

Assignee: Jingbo Agrochemicals Technology Co Ltd

Application filed: 2014-01-15

Publication filed: 2014-05-14

Accordingly to present Invention - 1 (API-1)

Reaction Summary:

The invention provides a method for preparing trifloxystrobin, using m-trifluoromethylacetophenone oxime and (E)-2-(2'-bromomethylphenyl)-2-carboxylacetic acid methyl ester-O-Methyl ketoxime is used as the raw material. The raw material is added to a heterogeneous system composed of inorganic alkali solution and organic solvent, and then a catalyst is added to perform the etherification reaction. After the reaction is completed, the separated organic phase is directly subjected to liquid separation operation, and the pressure is reduced. Recrystallize, filter, and dry to obtain a white or off-white solid, which is trifloxystrobin. Compared with the existing technology, the present invention has the advantages of simple and easy operation, high yield and high purity. The use and recovery of solvents greatly reduce the generation of waste water, reduce environmental pollution, reduce production costs, and are suitable for industrialization. Production. The m-trifluoromethylacetophenone oxime and (E)-2-(2'-bromomethylphenyl)-2-carboxylacetic acid methyl ester-O-methyl ketone oxime of the present invention are best because they are difficult to preserve. It is currently used and prepared according to the reference "Research on the Synthesis Process of the Fungicides Trifloxystrobin and Pyraclostrobin" (Xu Pingping, Yang Guangfu, Master's Thesis of Central China Normal University, 2012).

© Copyright 2023 by ChemRobotics Pvt. Ltd.

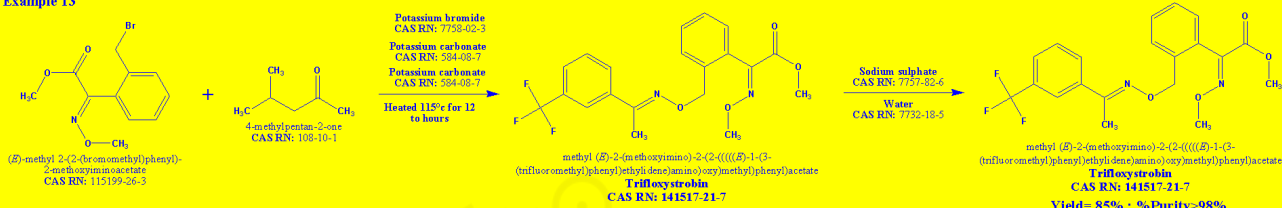
ROS - 27



Trifloxystrobin
CAS RN: 141517-21-7
GBRN: 504
TRRN: 78327

Patented Route - Trifloxystrobin

Accordingly to present invention - 1 (API-1)
Example 13



References:

WO2017085747A2

Title: A novel process for the preparation of trifloxystrobin

Inventor: Ajit Singh Gujral, Kenal V. Shah, Bhavesh V. Shah, Subhash KADAM, Nilesh N. JANIR, Ravindra Y SHINDE

Assignee: Gsp Crop Science Pvt. Ltd.

Application filed: 2016-11-18

Publication filed: 2017-05-26

Family Equivalents: CN108368033; CN108368033; WO2017085747; WO2017085747; WO2017085747

Accordingly to present invention - 1 (API-1)

Reaction Summary:

Example 13: Preparation of Trifloxystrobin

(2-Bromomethyl-phenyl)-methoxyimino 1-(3-(Trifluoromethyl-phenyl)-Methoxyimino-2-[1-(3-trifluoromethyl-phenyl)-acetic acid methyl ester]-ethanone oxime ethylideneaminooxymethyl]-phenyl)-acetic acid methyl ester

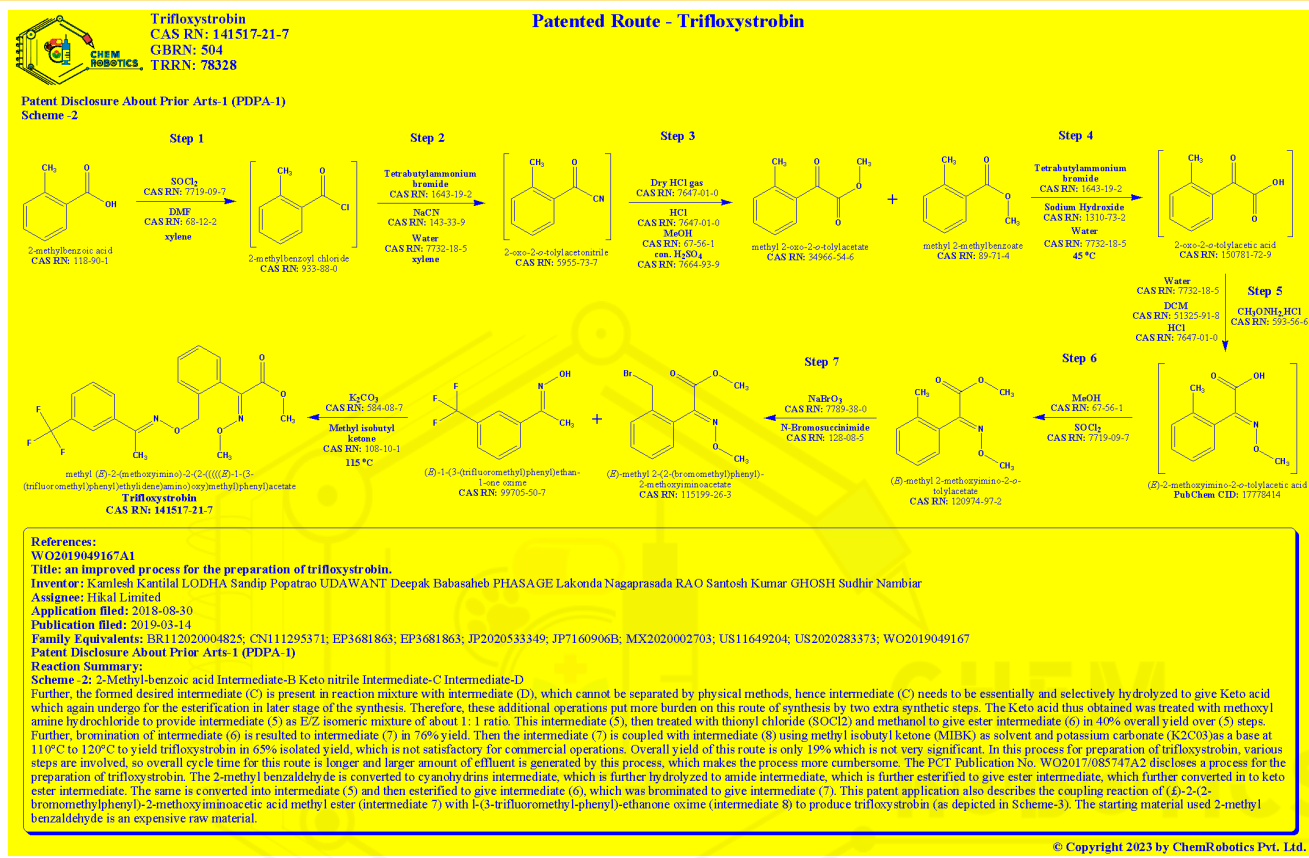
Formula (X) Formula (XI) (E-isomer)

Formula (I)

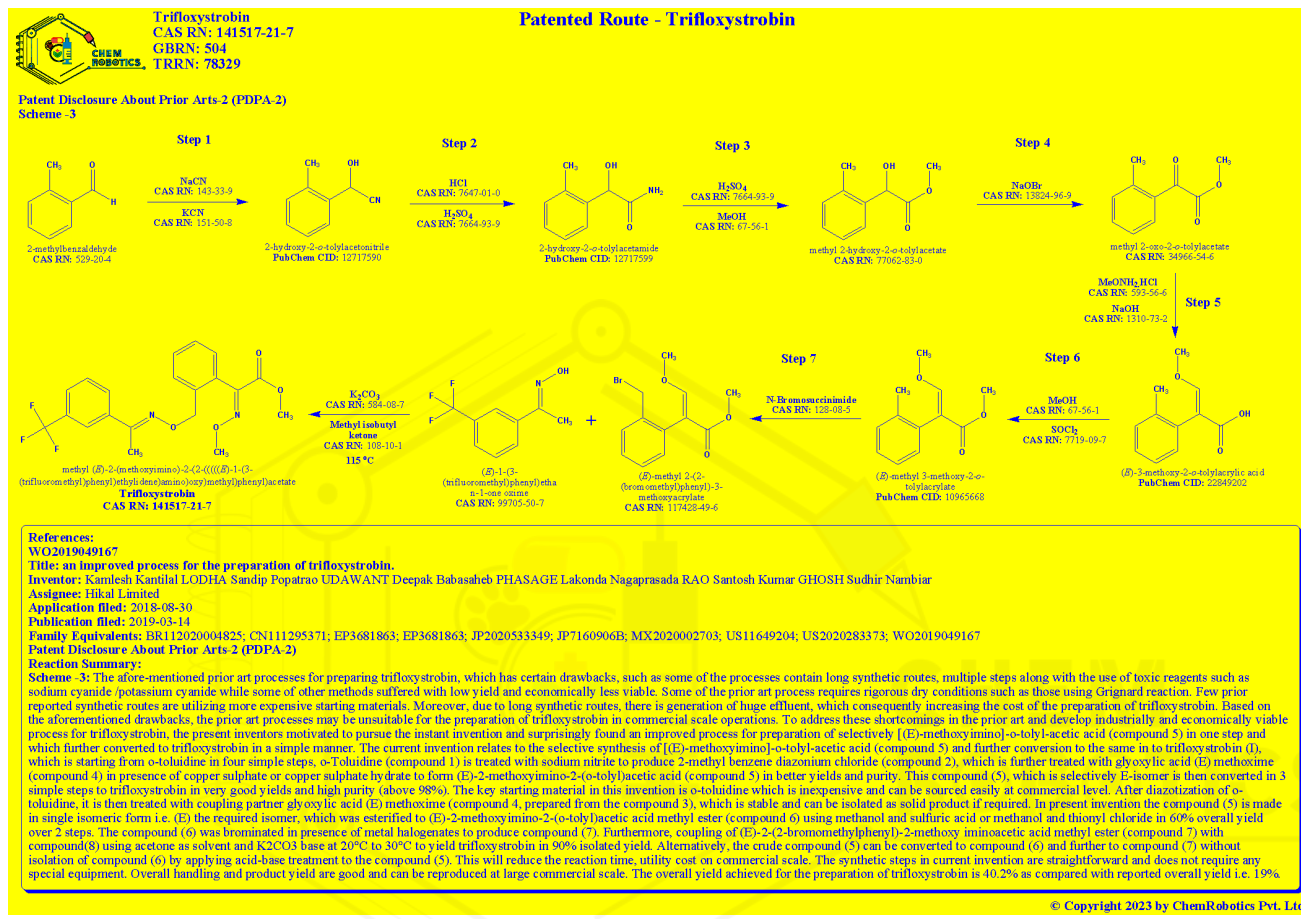
(2-bromomethyl-phenyl)-methoxyiminoacetic acid methyl ester (315 gm, 1.10 mole) was dissolved in 1500 ml methyl isobutyl ketone. To this solution was added Intermediate-II (203.16 gm, 1.0 mole) at room temperature followed by potassium carbonate (145 gm, 1.05 mole). The reaction mixture was heated to 115°C for 12 hours. After completion of reaction mixture was cooled to room temperature and filtered to remove potassium bromide by-product and excess potassium carbonate. The solid obtained after filtration was washed with methyl isobutyl ketone and recycled in next batch for the preparation of Trifloxystrobin. The filtrate was washed with water and dried over anhydrous sodium sulphate and concentrated under vacuum to obtain crude product. The crude product was recrystallized in methanol to give off white colored product of Trifloxystrobin = 348 gm. % Yield = 85%; % Purity > 98%

© Copyright 2023 by ChemRobotics Pvt. Ltd.

ROS - 28



ROS - 29



ROS - 30

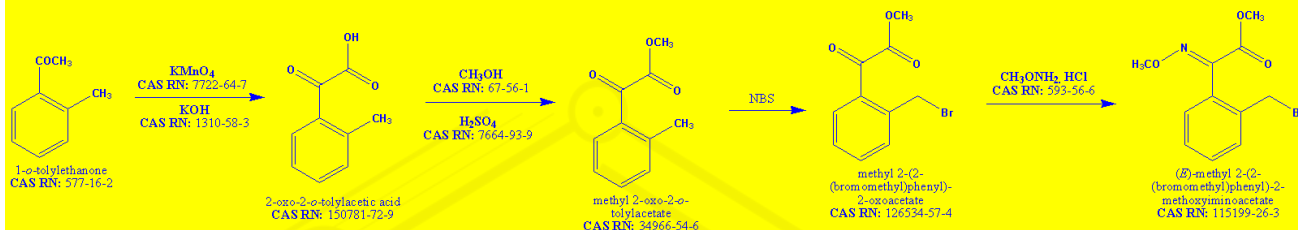


Trifloxystrobin
CAS RN: 141517-21-7
GBRN: 504
TRRN:

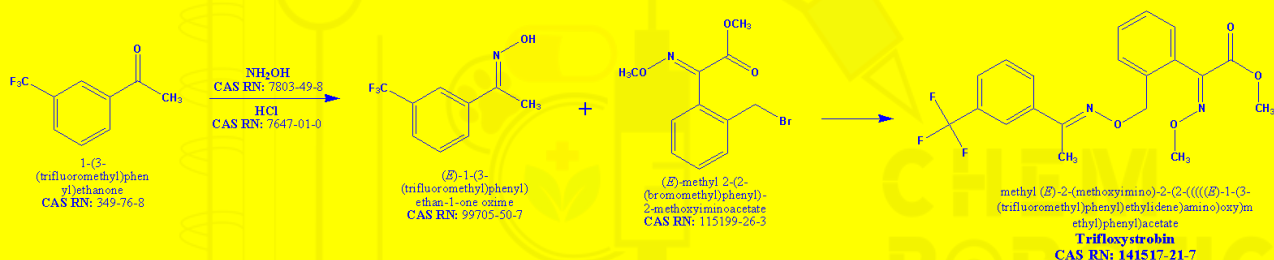
Chinese Patent Route - Trifloxystrobin

Patent Disclosure About Prior Arts-1 (PDPA-1) Route 1

Preparation of Intermediate: (E)-methyl 2-(2-(bromomethyl)phenyl)-2-methoxyiminoacetate; CAS RN: 115199-26-3



Preparation of Final: Trifloxystrobin; CAS RN: 141517-21-7



References:

CN101941921

Title: Method for preparing trifloxystrobin

Inventor: Ni Yuebiao, Sun JuhuiXu Jumping

Assignee: YUEYANG DIPU CHEMICAL TECHNOLOGY Co Ltd

Application filed: YUEYANG DIPU CHEMICAL TECHNOLOGY Co Ltd

Publication filed: 2011-01-12

Patent Disclosure About Prior Arts-1 (PDPA-1)

Reaction Summary:

- Documents J.Chem.Soc.1962:5298; Tetrahedron Lett., 1980, 21:4997; J.Org. Chem, 1981, 46(1); U.S. Patent US5194662 and others reported the preparation method of the fungicide trifloxystrobin, but the reported processes are all condensation processes in the last step, and there is no report on the preparation of its intermediates.
- Chinese invention patents CN200410016751.9 and CN200410016751.9 report using o-methylacetophenone as raw material, oxidation with potassium permanganate, esterification with methanol, bromination with NBS, and then oximation with methoxyamine hydrochloride. Finally, it is condensed with m-trifluoromethylacetophenone oxime to obtain trifloxystrobin. This process has the following problems during industrialization: (1) Potassium permanganate is highly oxidizing and can easily oxidize the carbonyl group, causing the carbon-carbon bond to break and obtain o-toluic acid as a by-product. Moreover, the methyl group on the benzene ring is also easy to oxidize to carboxyl group. The process parameters of this reaction can be controlled under laboratory small-scale conditions, but it is extremely difficult to control during industrialization, resulting in a low yield; (2) Use N-bromosuccinimide (NBS) Although bromination is relatively mild, the price of NBS is high, resulting in high product raw material costs; (3) When m-trifluoromethylacetophenone is oxidized, hydroxylamine hydrochloride is used as the oximation reagent, which seriously corrodes the equipment, and generally requires titanium equipment, resulting in high investment equipment costs.
- Chinese invention patent CN200510110511. The former is to first brominate the intermediate 2-(2'-methylphenyl)-2-carbonyl acetate methyl ester and then perform an oximation reaction with methoxyamine hydrochloride, while the latter is to first brominate 2-(2'-Methyl(methylphenyl)-2-carbonyl acetate is first subjected to oximation reaction with methoxyamine hydrochloride and then to bromination reaction.

© Copyright 2024 by ChemRobotics Pvt. Ltd.

ROS - 31



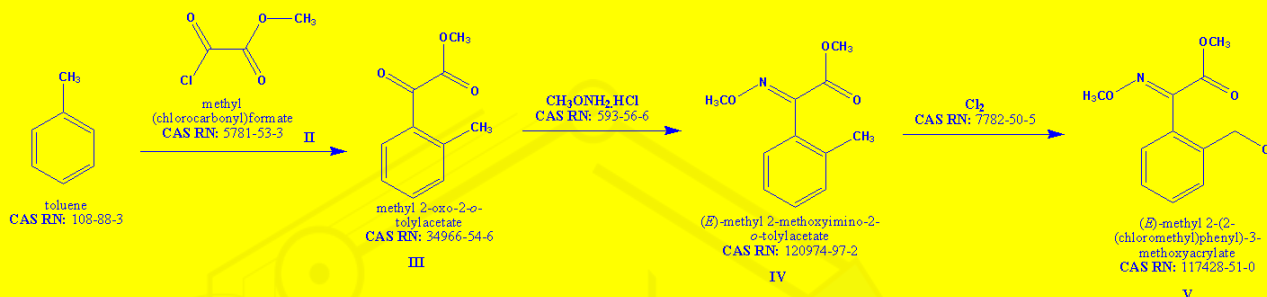
Trifloxystrobin
CAS RN: 141517-21-7
GBRN: 504
TRRN:

Chinese Patent Route - Trifloxystrobin

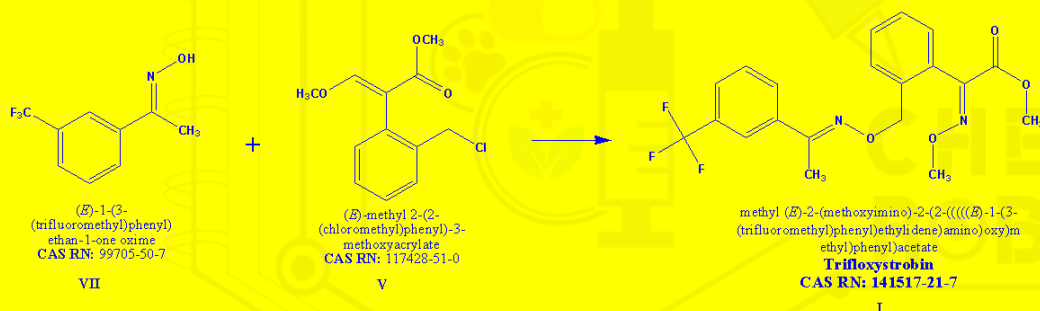
Accordingly to present invention - 1 (API-1)

Route 2

Preparation of Intermediate: (E)-methyl 2-(2-(chloromethyl)phenyl)-3-methoxyacrylate, CAS RN: 117428-51-0



Preparation of Final: Trifloxystrobin; CAS RN: 141517-21-7



References:

CN101941921

Title: Method for preparing trifloxystrobin

Inventor: Ni Yuebiao, Sun Juhui, Xu Junping

Assignee: YUEYANG DIPU CHEMICAL TECHNOLOGY Co Ltd

Application filed: YUEYANG DIPU CHEMICAL TECHNOLOGY Co Ltd

Publication filed: 2011-01-12

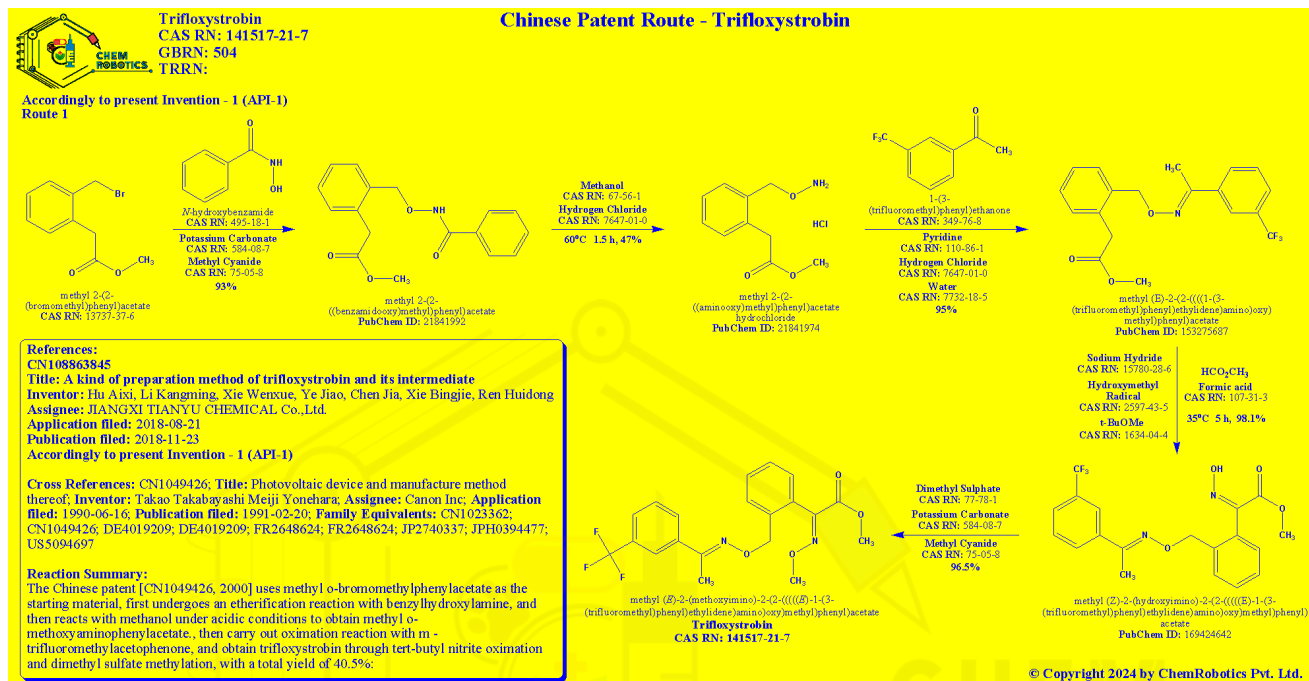
Accordingly to present invention - 1 (API-1)

Reaction Summary:

The invention discloses a method for preparing (E,E)-2-[1'-(3'-trifluoromethyl phenyl)-ethyl-imine-oxyl-tolyl]-2-carbonyl methyl acetate-O-ketoxime, following steps of: performing acylation reaction on toluene and methyl oxalyl chloride in the presence of anhydrous aluminum chloride to prepare 2-(2'-methyl phenyl)-2-carbonyl methyl acetate; reacting the 2-(2'-methyl phenyl)-2-carbonyl methyl acetate with methoxy amine hydrochloride to prepare (E)-2-(2'-methyl phenyl)-2-carbonyl methyl acetate-O-methyl ketoxime; and finally performing condensation reaction on the (E)-2-(2'-methyl phenyl)-2-carbonyl methyl acetate-O-methyl ketoxime and m-trifluoromethyl phenyl ethyl ketoxime under the action of alkaline substance to prepare the trifloxystrobin. The method has the advantages of a few reaction steps, simple synthesis process, readily available raw materials, mild reaction conditions, great industrial value and great social and economic benefit.

© Copyright 2024 by ChemRobotics Pvt. Ltd.

ROS - 32



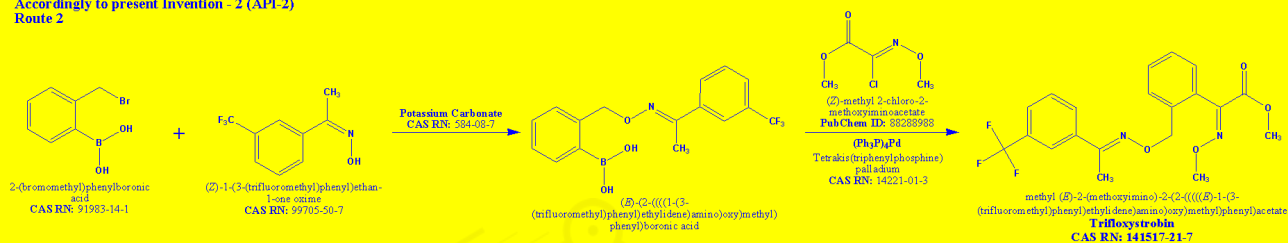
ROS - 33



Trifloxystrobin
CAS RN: 141517-21-7
GBRN: 504
TRRN:

Chinese Patent Route - Trifloxystrobin

Accordingly to present Invention - 2 (API-2)
Route 2



References:

CN108863845

Title: A kind of preparation method of trifloxystrobin and its intermediate

Inventor: Hu Aixi, Li Kangming, Xie Wensue, Ye Jiao, Chen Jia, Xie Bingjie, Ren Huidong

Assignee: JIANGXI TIANYU CHEMICAL Co.,Ltd.

Application filed: 2018-08-21

Publication filed: 2018-11-23

Accordingly to present Invention - 2 (API-2)

Cross References: WO9520569; Title: Process for the preparation of arylacetic ester derivatives via palladium-catalyzed cross coupling reaction; Inventor: Hugo ZieglerDenis NeffWolfgang Stutz; Assignee: Ciba-Geigy Ag; Application filed: 1995-01-16; Publication filed: 1995-08-03; Family Equivalents: ATE178047; AU1534495; BG100769; BR9506648; CA2181586; CN1139919; CZ220296; DE69508560; DK0741693; EP0741693; EP962953; HUT75179; JPH09508373; MXPA96003015; NO963126; PL315668; SK98296; US5726343; WO9520569; ZA95624

Reaction Summary:

The world patent [WO9520569, 1995] studied trifloxystrobin. First, o-bromomethylphenylboronic acid and m-trifluoromethylacetophenone oxime were etherified, and then reacted with 2-chloromethane under the catalysis of palladium. -The condensation reaction of methyl 2-methoxyiminoacetate produces trifloxystrobin.

This synthesis route is short, but the raw material o-bromomethylbenzeneboronic acid is expensive; the synthesis conditions of 2-chloro-2-methoxyimino methyl acetate are too harsh and there is isomerization, resulting in a low yield.

© Copyright 2024 by ChemRobotics Pvt. Ltd.

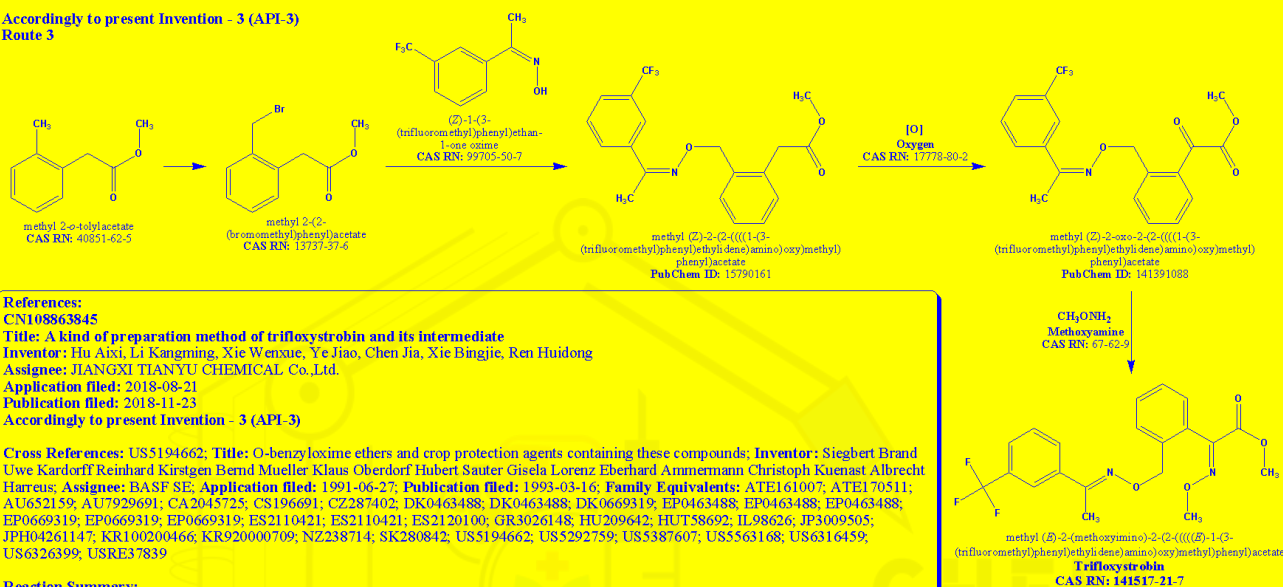
ROS - 34



Trifloxystrobin
CAS RN: 141517-21-7
GBRN: 504
TRRN:

Chinese Patent Route - Trifloxystrobin

Accordingly to present invention - 3 (API-3)
Route 3



References:

CN108863845

Title: A kind of preparation method of trifloxystrobin and its intermediate

Inventor: Hu Aixi, Li Kangming, Xie Wenxue, Ye Jiao, Chen Jia, Xie Bingjie, Ren Huidong

Assignee: JIANGXI TIANYU CHEMICAL Co., Ltd.

Application filed: 2018-08-21

Publication filed: 2018-11-23

Accordingly to present invention - 3 (API-3)

Cross References: US5194662; Title: O-benzyl oxime ethers and crop protection agents containing these compounds; Inventor: Siegbert Brand Uwe Kardorf Reinhard Kirstgen Bernd Mueller Klaus Oberdorf Hubert Sauter Gisela Lorenz Eberhard Ammermann Christoph Kuenast Albrecht Harreus; Assignee: BASF SE; Application filed: 1991-06-27; Publication filed: 1993-03-16; Family Equivalents: ATE161007; ATE170511; AU652159; AU7929691; CA2045725; CS196691; CZ287402; DK0463488; DK0463488; DK0669319; EP0463488; EP0463488; EP0669319; EP0669319; EP0669319; ES2110421; ES2110421; ES2120100; GR3026148; HU209642; HUT58692; IL98626; JP3009505; JPH04261147; KR100200466; KR920000709; NZ238714; SK280842; US5194662; US5292759; US5387607; US5563168; US6316459; US6326399; USRE37839

Reaction Summary:

The U.S. patent [US5194662, 1993] uses methyl o-toluene acetate as the initial raw material and obtains methyl o-bromomethyl phenylacetate after bromination reaction, and then condenses it with m-trifluoromethylacetophenone oxime, and then undergoes bromination reaction. Oxidation and oximation reactions yield trifloxystrobin:

The third step of the oxidation reaction in this route is difficult.

© Copyright 2024 by ChemRobotics Pvt. Ltd.

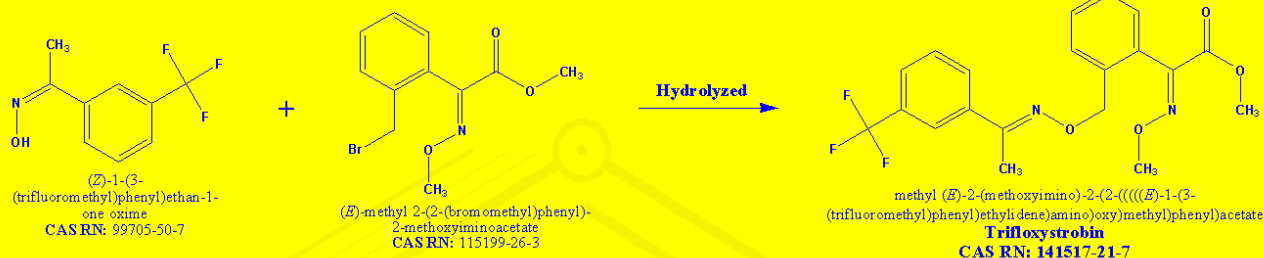
ROS - 35



Trifloxystrobin
CAS RN: 141517-21-7
GBRN: 504
TRRN:

Chinese Patent Route - Trifloxystrobin

Patent Disclosure About Prior Arts-1 (PDPA-1) Route 1



References:

CN115490612

Title: Synthesis method of trifloxystrobin

Inventor: Fan Li, Pantian, Xuefang, Xu Huishi, Wei, Li Linhu, Jia Chengguo

Assignee: Hebei Veyong Bio Chemical Co Ltd

Application filed: 2022-10-24

Publication filed: 2022-12-20

Patent Disclosure About Prior Arts-1 (PDPA-1)

Reaction Summary:

The synthesis of trifloxystrobin uses (E)-2-(2'-bromomethylphenyl)-2-carboxylacetate methyl ester-O-methylketoxime and m-trifluoromethylacetophenone oxime as raw materials, in the presence of alkaline substances and organic solvents, the above raw materials undergo a condensation reaction to obtain trifloxystrobin. However, the solvents used in these synthesis methods inevitably contain trace amounts of moisture, and a small amount of water is also generated during the reaction. This moisture is very easy for the generated trifloxystrobin to be hydrolyzed into the corresponding acid under alkaline conditions, resulting in low yield and low purity of trifloxystrobin.

© Copyright 2024 by ChemRobotics Pvt. Ltd.

ROS - 36

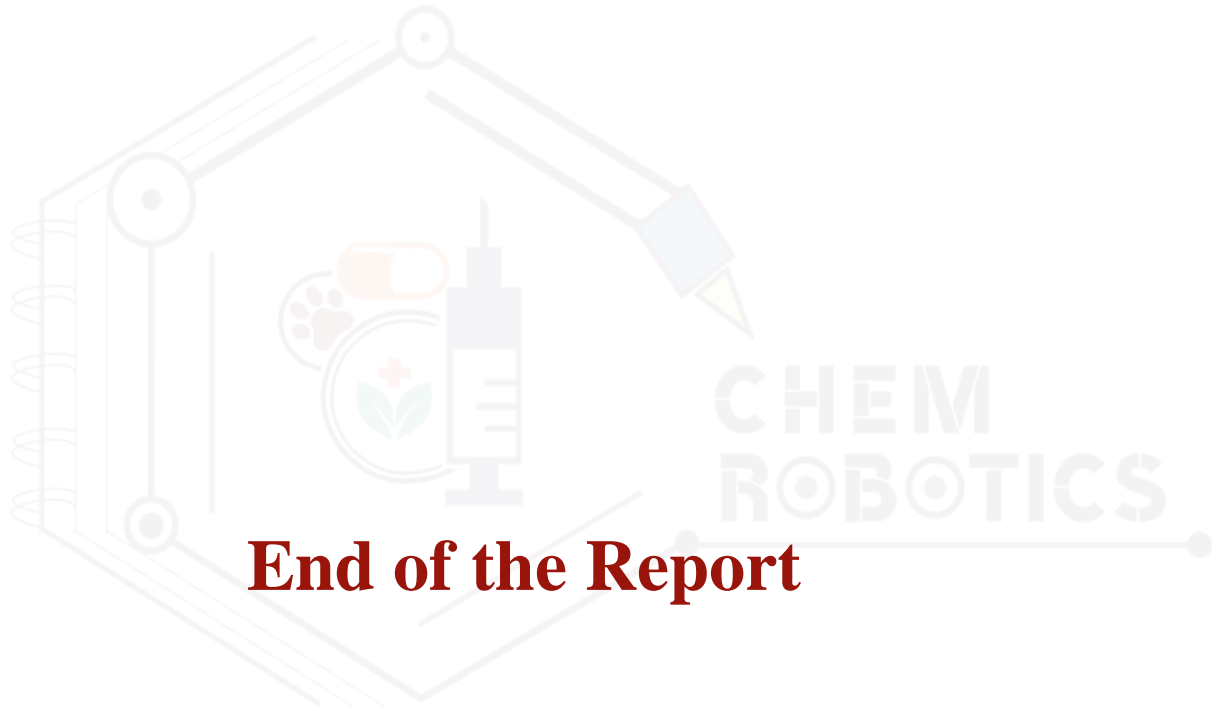
Chinese Patent Route-

Accordingly to present Invention-1 (API-1)
Embodiment 1

References:
CN1110677
Title: Synthetic technology of phenylacetic acid
Inventor: Pan Zelin, Zhao Ping
Application filed: 1994-12-15
Publication filed: 1995-10-25
Accordingly to present Invention-1 (API-1) Embodiment 1:
Reaction Summary:
Embodiment 1:
(1) cinnamic preparation: a cover water distilling apparatus is installed, add the deposed polystyrene 100g that pulverizes, control liquid temperature is more than 340 °, collect the overhead product more than 340 °, this overhead product is vinylbenzene, but color is dark, impurity is also more, leave standstill 3h after the virioli oil that can add 5% volume mixes, with the removal of impurity, then with saturated aqueous common salt and clear water respectively give a baby a bath on the third day after its birth time, behind the anhydrous sodium sulfate drying, add stopper, BP145-146 ° overhead product is collected in air distillation, gets vinylbenzene 89g, yield 89%, n 251.5436.
(2) preparation of phenylacetamide: in a reaction vessel, add vinylbenzene 21.7g, sulphur 37.5g, ammoniacal liquor 50ml, ethanol 30ml, under agitation, temperature of reaction is controlled at 93-95 °, reacts 3-4 hour.Reduce to room temperature then, change distillation into, steam liquid, stop heating, be cooled to room temperature, use 500ml water hot extraction 3 times, leave standstill adulerent plate crystal 26.7g after the solution decoloring after the extraction, yield is 94%, M.P.157-158 °, and B.P.280-290 ° (decomposition), C 8H 9NO(calculated value: C:71.11, H:6.67, N:10.37, O:11.85, measured value: C:71.18, H:6.59, N:10.29, O:11.95), IRv C=01680CM -1, v NH23350CM -1, 3180CM -1, v C6H51580CM -1
(3) preparation of tolylic acid: the phenylacetamide 100g with above-mentioned preparation, add water 150ml, hydrochloric acid 80ml, reflux 2h, being chilled to has precipitation to separate out after room temperature leaves standstill.After the filtration, get the glossiness crystallization 84g of white plates, yield 84%, M.P.76.5 °, B.P.265 ° (decomposition), IR v with 1: 2 aqueous ethanolic solution recrystallization C=01710CM -1, v OH3190CM -1, v C6H51586CM -1, C 8H 8O 2(calculated value: C:71.11, H:6.67, N:10.37, O:11.85, measured value: C:71.18, H:6.59, N:10.29, O:11.95).

ATORVASTATIN CALCIUM CAS RN: 134823-03-8 GBRN: 16263	FOSAMPRENAVIR CAS RN: 226700-81-8 GBRN: 17541	TRIFLOXYSTROBIN CAS RN: 141517-21-7 GBRN: 12280,504
ATROPINE SULFATE CAS RN: 55-48-1 GBRN: 18584	METHYLPHENIDATE HYDROCHLORIDE CAS RN: 298-59-9 GBRN: 18569	
AMRINONE CAS RN: 75898-90-7 GBRN: 10748	OSPEMIFENE CAS RN: 128607-22-7 GBRN: 10186	
BENALAXYL CAS RN: 71626-11-4 GBRN: 817	PHENINDIONE CAS RN: 83-12-5 GBRN: 17579	
CARBOPLATIN CAS RN: 41575-94-4 GBRN: 10667	PHENTHOATE CAS RN: 2597-03-7 GBRN: 185	
CYCLOBENZAPRINE HYDROCHLORIDE CAS RN: 6202-23-9 GBRN: 18419	PHENOBARBITAL CAS RN: 50-06-6 GBRN: 17708	
DEPTROPINE CAS RN: 604-51-3 GBRN: 16446	PRETOMANID CAS RN: 1187235-37-6 GBRN: 10025	
DEXMETHYLPHENIDATE CAS RN: 40431-64-9 GBRN: 18701	ROFECOXIB CAS RN: 162011-90-7 GBRN: 17164	
DIFETHALONE CAS RN: 104653-34-1 GBRN: 921	SULBENICILLIN CAS RN: 41744-40-5 GBRN: 17197	

© Copyright 2024 by ChemRobotics Pvt. Ltd.





Registered Office ChemRobotics Pvt. Ltd.

**House No. 9, Ward No. 23, Jawahar Ganj, District
Gwalior, Madhya Pradesh, 475110**

ChemRobotics Database: <http://chemrobotics.com>

ChemRobotics Times (News): <http://chemrobotics.in>

Support Email: support@chemrobotics.com

Sales Email: sales@chemrobotics.com

Promotion Email: promotion@chemrobotics.com

Cell: 91- 6266117944 / +91- 9407360810

What's App: +91- 9407360810

AGROPAT

PRODUCT LANDSCAPE

chemrobotics (C) 2020 | All Rights Reserved