

PROPERTIES AND REACTIONS IN REAXYFILESUB

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CAS

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American Chemical Society



Agenda

- REAXYSFILESUB/BIB Content and Coverage
- NEW! Properties and Reaction Data now available!
- Search Example: Ensifentrine
- Additional Resources

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- Additional Resources

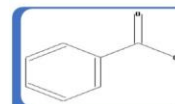
ReaxysFile Databases on CAS STNext

ReaxysFileBIB

- >57 million bibliographic records (2/2024)
- Patent and nonpatent literature records

ReaxysFileSUB

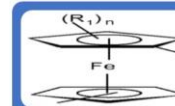
- >51 million chemical substances (2/2024)
 - Properties and reactions available
 - From 1771 to date
 - Both databases are updated twice weekly
- Same database architecture as REG-CAplus, DCR-DWPI - enabling a consistent workflow



Organic



Inorganic



Organometallic

ReaxysFileBIB – Chemistry Patent Coverage

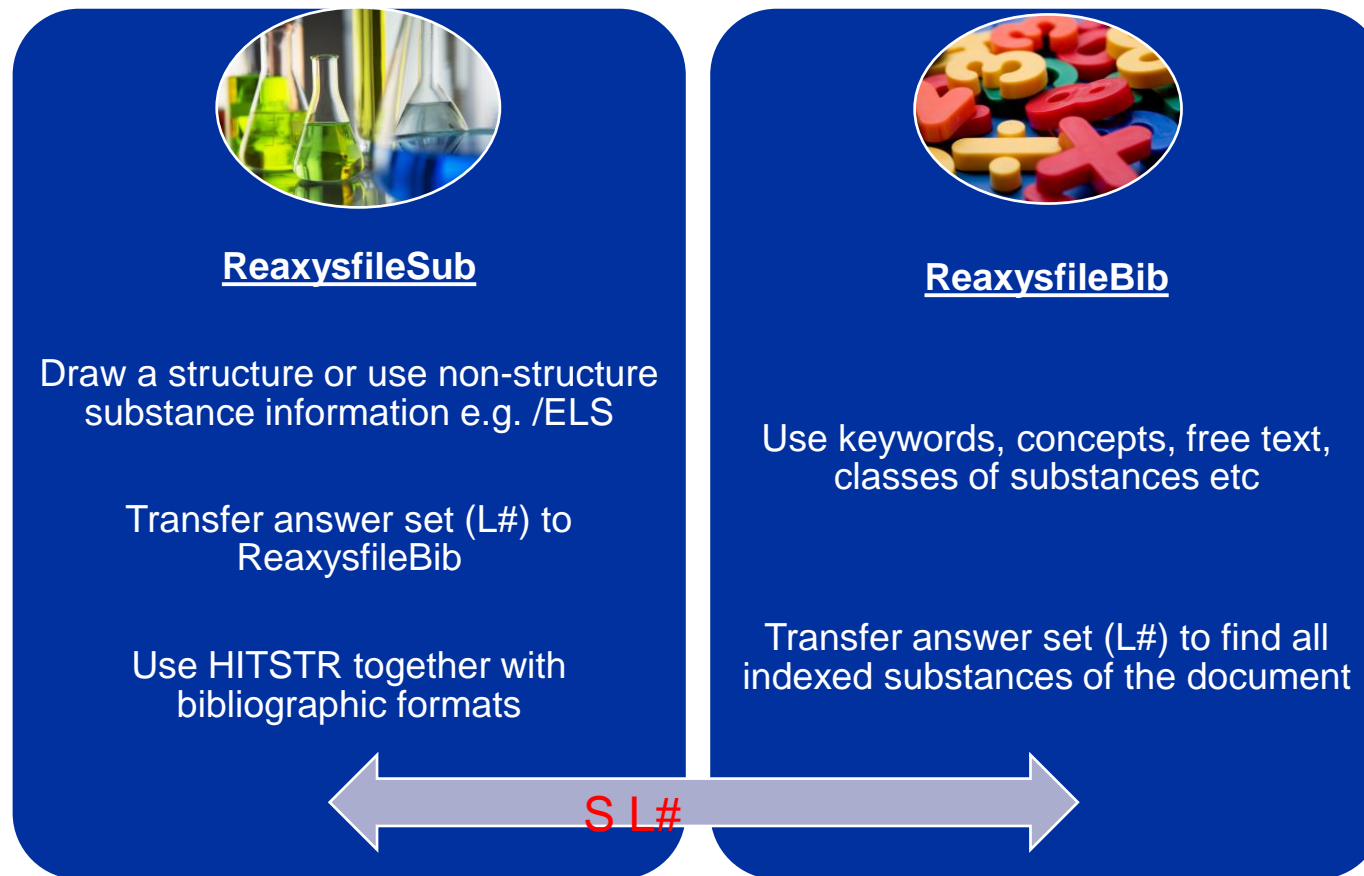
Patent coverage from 105 patent authorities (07/2023):

- 1803-present
- Significant increase of chemistry patent records to > 40 million over the last years
- Records available within 5 days after publication
- TI, AB available in English
- Substance indexing for priority patent authorities

In-depth patent information for:

- English language patents from US/EP/WO from 2001
- Asian patents of JP/KR from 2015 and CN/TW from 2016

Workflow crossfile searching



Please note: properties and reactions cannot be transferred

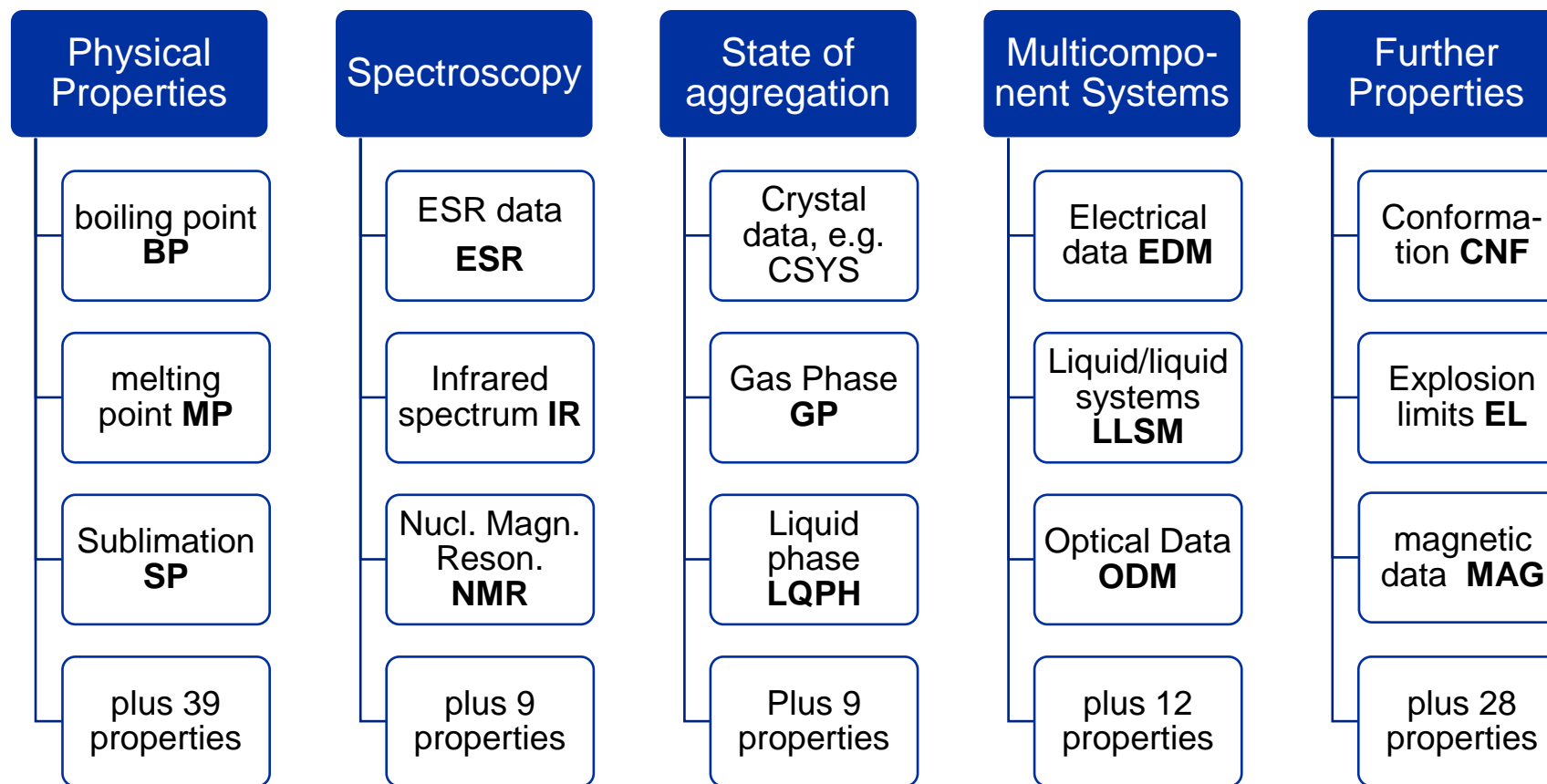
Agenda

- REAXYSFILESUB/BIB Content and Coverage
- **NEW! Properties and Reaction Data now available!**
- Search Example: Ensifentrine
- Additional Resources

NEW! Properties and Reaction Data Available!

- As of March 4, 2024, properties and reaction data have been added to REAXYSFILESUB
- Legacy REAXYSFILE has been disabled as of March 16, 2024

Property Sections cover 110 Properties



Consult => **HELP PROPERTIES**
=> **EXPAND A/FA.P**
To see available properties

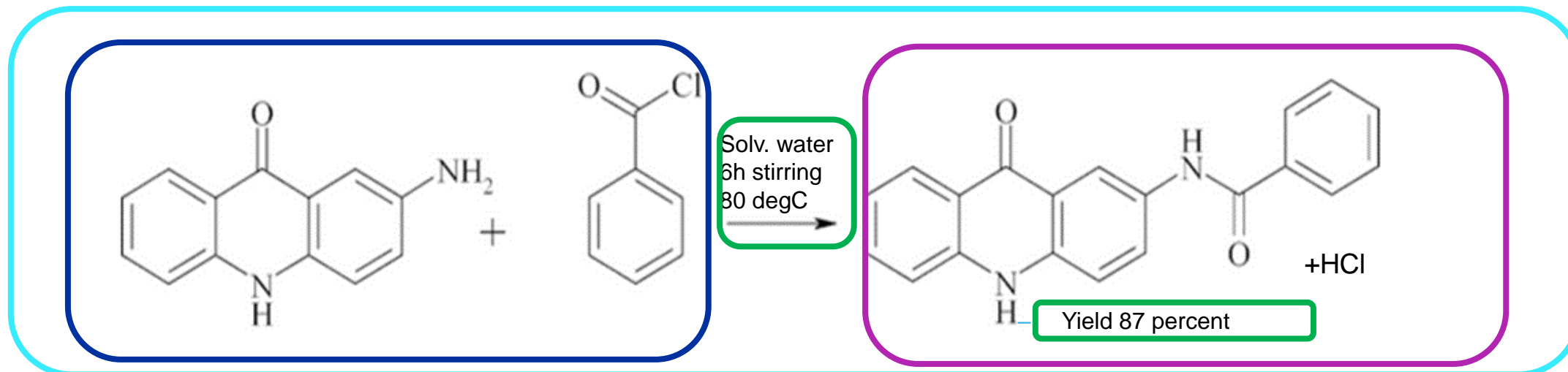
DISPLAY available properties by category

Kind of Property	Description	Example
PHYS	All physical properties	D PHYS
STATE	All state of aggregation properties	D STATE
FURTHER	All further properties	D FURTHER
MULTI	All multicomponent properties	D MULTI
SPEC	All spectroscopy properties	D SPEC

Search in Specialized Fields

– based on reaction scheme

Reaction Document RX.ID



Reactants
/RX.RAN

Reaction Details
/RX.Cl
/RX.CAAN
/RX.SOLAN
Yield, Time, ...*

Products
/RX.PAN

* not all reaction details are searchable

Reaction Data in ReaxysFileSub

- Reactions are available as part of a substance record
 - All reactions reported for a substance belong to one substance record
- Reactions are defined by reactants and products:
 - Reactant (.RCT) and Product (.PRO) name given
 - Reactant (.RAN) and Product (.PAN) accession numbers given

Reaction:

Reaction ID:	42969066
Reactant AN (.RAN):	27109425
Reactant (.RCT):	2-amino-4,5-bis[(2-methoxy)ethoxy]benzamide
Product AN (.PAN):	8798958
Product (.PRO):	erlotinib
Reference Count:	4

**Reaction
identification data**

Reaction data in ReaxysFileSub

- Reactions are available as part of a substance record
 - All reactions reported for a substance belong to one substance record
- Reactions are defined by reactants and products:
 - Reactant (.RCT) and Product (.PRO) name given
 - Reactant (.RAN) and Product (.PAN) accession numbers given
 - Reaction Details refer to the different reaction variations

Reaction:

Reaction Details:

```
Reaction RID: 42969066.1
Reaction Classification (.CL): Multi-step reaction
Reactant AN (.RCAN): 103233; 32472054; 4546405; 605268; 956581
Solvent AN (.SOLAN): 635639
Reagent: pyridine; C20H25IrN2O3; caesium
          carbonate; diethylamine;
          trichlorophosphate
Solvent: isopropyl alcohol
Reference(s): 73326449: Patent, CN 107337648 A
```

Reaction details

Reaction Data in ReaxysFileSub

Reaction data are clearly separated in two parts, reaction identification data and reaction details

Reaction:

Reaction ID:
Reactant AN (.RAN):
Reactant (.RCT):
Product AN (.PAN):
Product (.PRO):
Reference Count:

Reaction Details:

Reaction RID:
Reaction Classification (.CL):
Product AN (.PRAN)
Reactant AN (.RCAN):
Solvent AN (.SOLAN):



Catalyst AN (.CAAN): 8225498
Catalyst: bis(dibenzylideneacetone)-palladium(0)
Product: methyl 2-(4-(4-(4-...
Reagent: zinc(II) fluoride; tri-tert-butyl phosphine
Solvent: N,N-dimethyl-formamide
Temperature: 80 Cel
Time: 2 s
Yield: 62 percent
Yield Numerical: 62
Reference(s): 394900: Patent, US 20060063808 A1
...
Reaction RID: **23739860.2**
Reaction Classification (.CL): Preparation

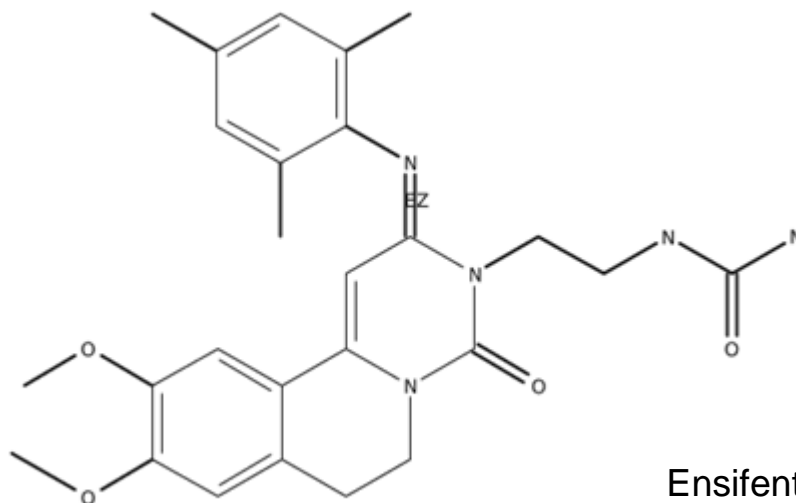
Agenda

- REAXYSFILESUB/BIB Content and Coverage
- NEW! Properties and Reaction Data now available!
- **Search Example: Ensifentrine**
- Additional Resources

Search Example: Ensifentrine

An investigational drug for the treatment of COPD

- What reaction details can be found?
- What spectroscopic and physicochemical data exist?



Search Example: Ensifentrine


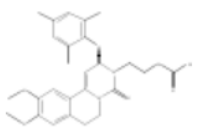
CAS STNext My Files Sarah Stokes

[Return to Session](#)

Structures (22)

Sort: Date Modified: Newest

Move to Folder

<input type="checkbox"/>  esifentrine <input type="text" value=""/>		<input type="button" value="Edit"/>	<input type="button" value="Upload"/> ...
7 Mar 2024 8:57 AM			

Structure files should be uploaded to an active, structure searchable database, like REAXYSFILESUB

Perform an EXACT structure search

L1 STRUCTURE UPLOADED

=> S L1 EXA FUL

FULL SEARCH INITIATED 11:17:52

FULL SCREEN SEARCH COMPLETED - 0 TO ITERATE

0.0% PROCESSED 50961552 ITERATIONS

SEARCH TIME: 00.00.06

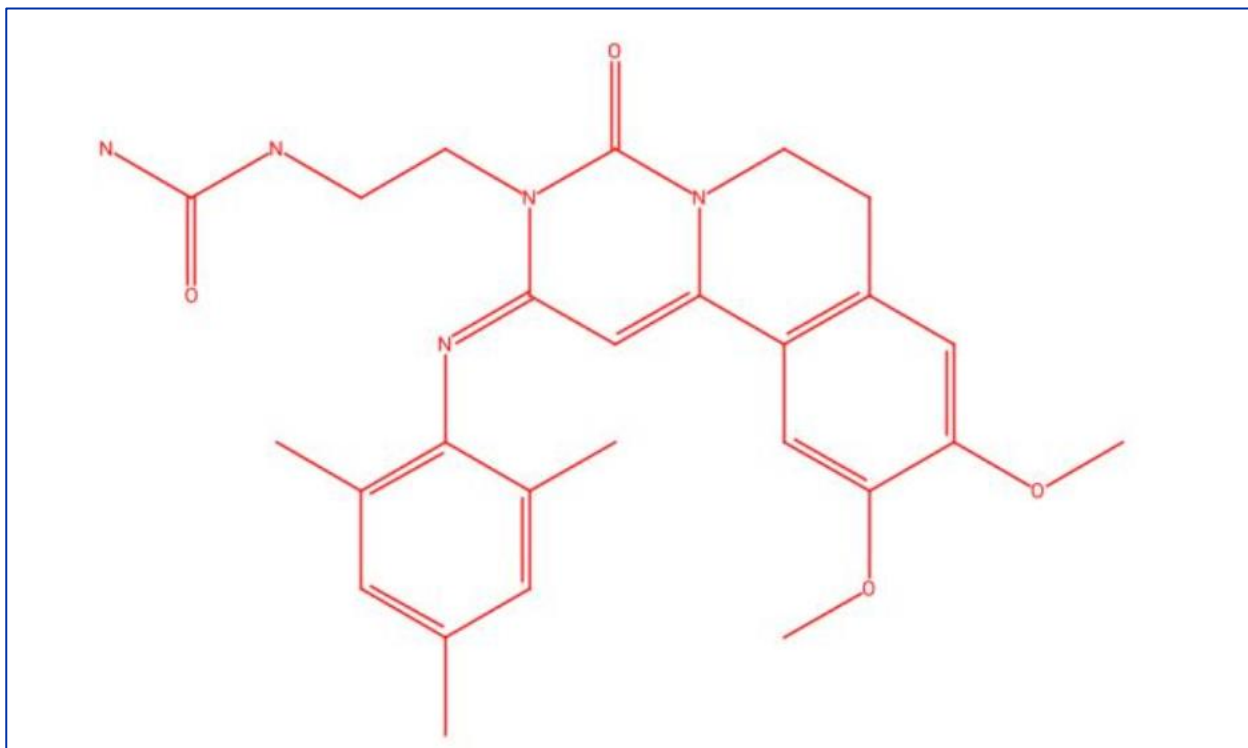
L2 5 SEA EXA FUL L1

=> D 1-5 ALL

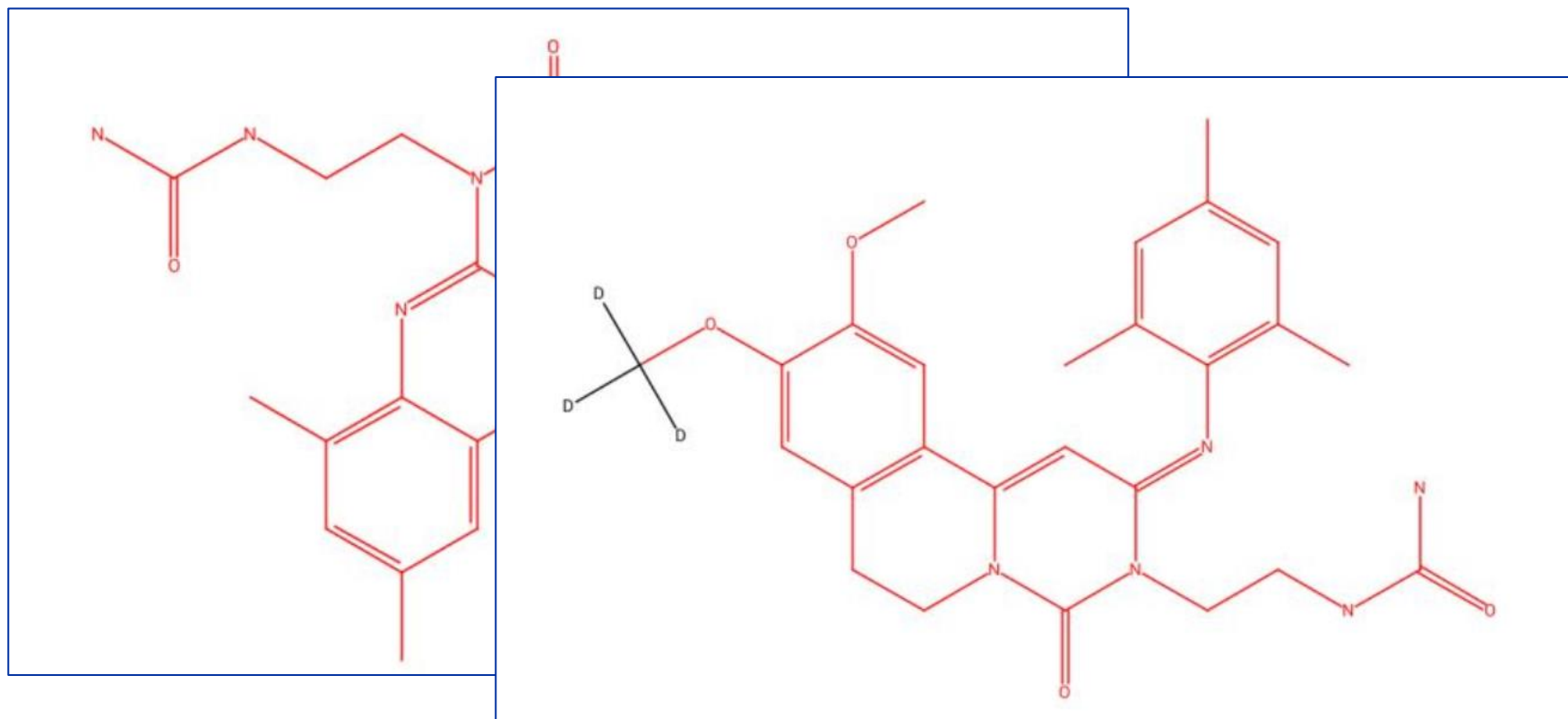
EXACT searching retrieves the
compound as drawn plus isomers
and radiolabeled forms

5 ANSWERS

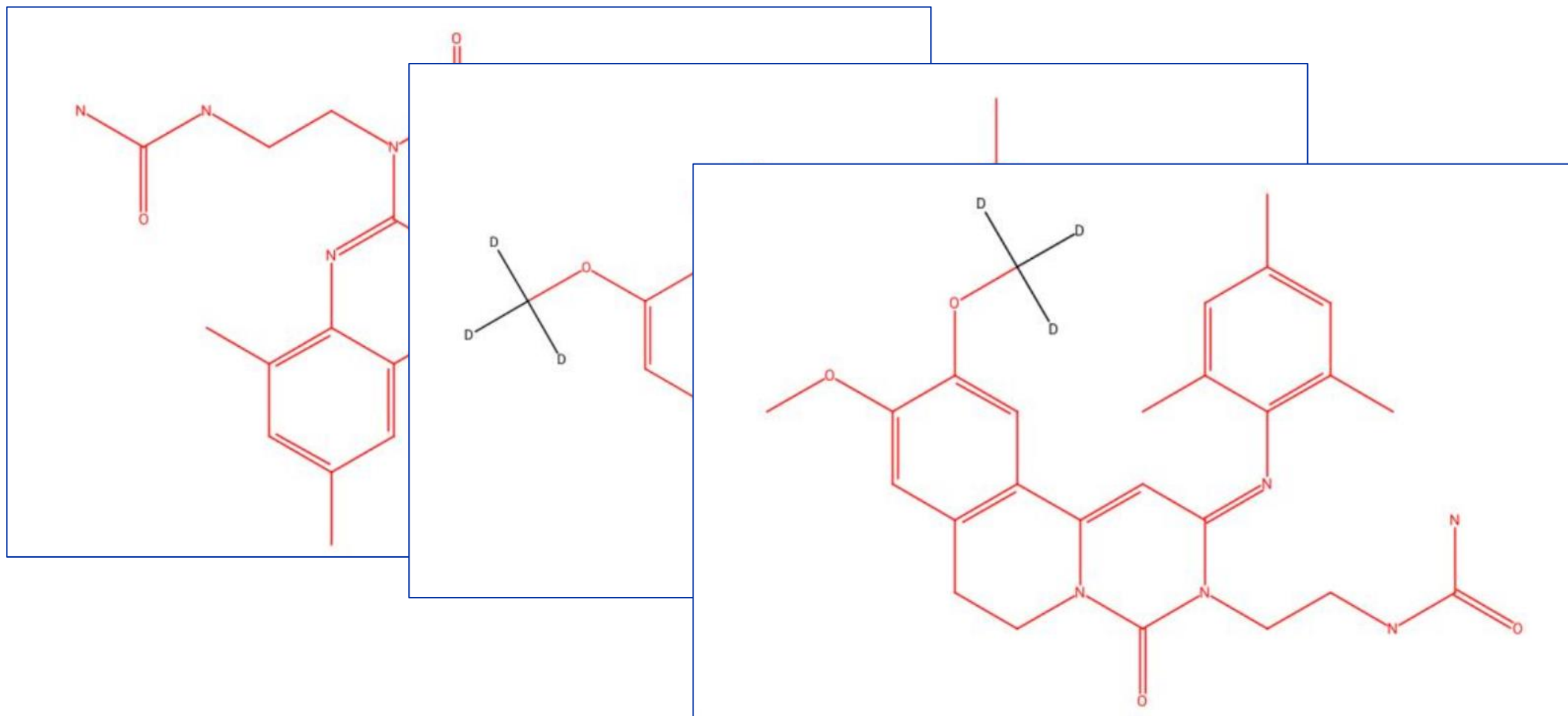
Ensifentrine and deuterated derivatives are retrieved



Ensifentrine and deuterated derivatives are retrieved



Ensifentrine and deuterated derivatives are retrieved



DISPLAY ALL provides substance data overview

```
L2      ANSWER 5 OF 5 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.  
AN      11001404  REAXYSFILESU  
CN      9,10-dimethoxy-2-(2,4,6-trimethylphenylimino)-3-(N-carbamoyl-2-  
        aminoethyl)-3,4,6,7-tetrahydro-2H-pyrimido[6,1-a]isoquinolin-4-one;  
        RPL554; N-{2-[(2E)-2-(mesitylimino)-9,10-dimethoxy-4-oxo-6,7-dihydro-2H-  
        pyrimido[6,1-a]-isoquinolin-3(4H)-yl]ethyl}urea  
MF      C26 H31 N5 O4  
CMF     C26 H31 N5 O4  
LSF     C26H31N5O4  
INCHI   CSOBIBXVIYAXFM-BYNJWEBRSA-N  
AINCHI  CSOBIBXVIYAXFM-DYLXTNJXDP  
MW      477.563  
MARKREF.CNT 0  
REC     298  
ED      Entered STN: 15 Jul 2020  
        Last updated on STN: 18 Mar 2024
```

Identification information, hit structure(s), and an overview of available property/reaction data

DISPLAY ALL provides substance data overview

L2 ANSWER 5 OF 5 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.

AN 11001404 REAXYSFILESU

CN 9,10-dimethoxy-2-(2,4,6-trimethylphenyliminoaminoethyl)-3,4,6,7-tetrahydro-2H-pyrimido[6,1-a]-isoquinolin-3(4H)-yl]ethyl

MF C26 H31 N5 O4

CMF C26 H31 N5 O4

LSF C26H31N5O4

INCHI CSOBIBXVIYAXFM-BYNJWEBRSA-N

AINCHI CSOBIBXVIYAXFM-DYLXTNJXDP

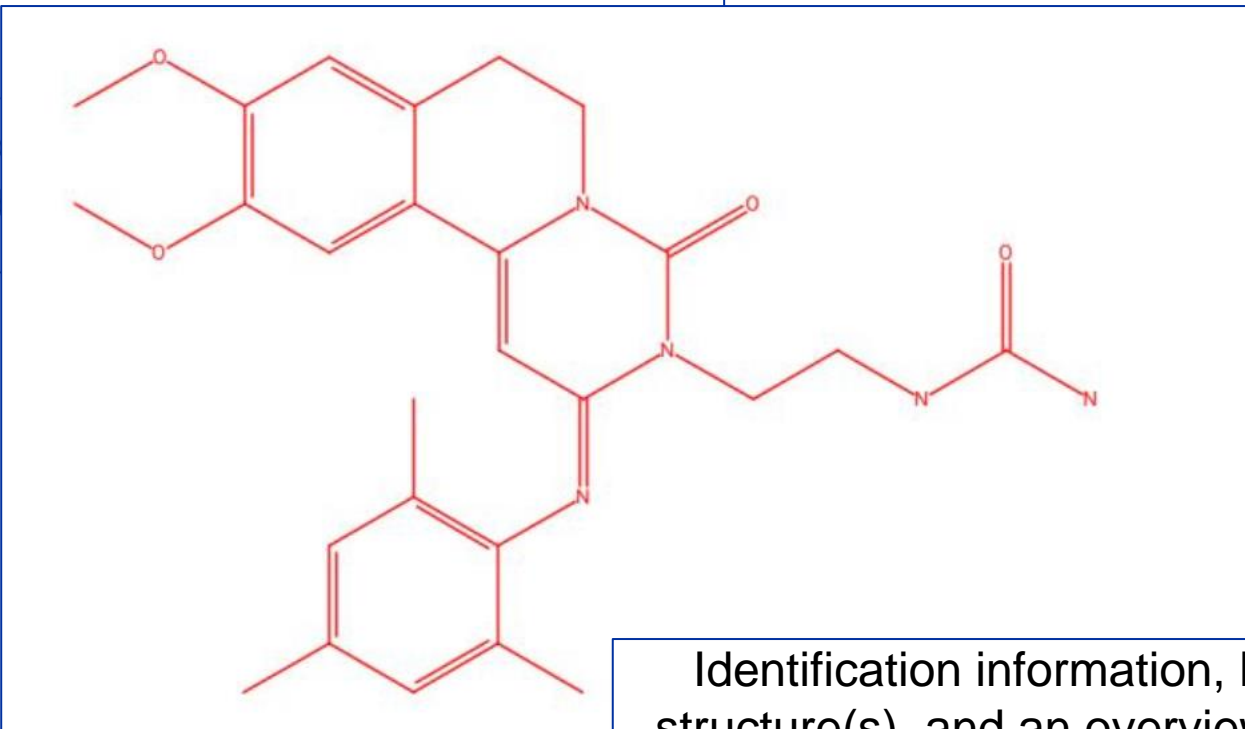
MW 477.563

MARKREF.CNT 0

REC 298

ED Entered STN: 15 Jul 2020

Last updated on STN: 18 Mar 2024



Identification information, hit structure(s), and an overview of available property/reaction data

DISPLAY ALL provides substance data overview

L2 ANSWER 5 OF 5 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.

AN 11001404 REAXYSFILESU

CN 9,10-dimethoxy-2-(2,4,6-trimethylphenyliminoaminoethyl)-3,4,6,7-tetrahydro-2H-pyrimido[6,1-a]-isoquinolin-3(4H)-yl]ethyl

MF C26 H31 N5 O4

CMF C26 H31 N5 O4

LSF C26H31N5O4

INCHI CSOBIBXVIYAXEM-BYNTWFBRSA-N

AINCHI CSOBIBXVIYAXEM-BYNTWFBRSA-N

MW 477.563

MARKREF.CNT 0

REC 298

ED Entered

Last up

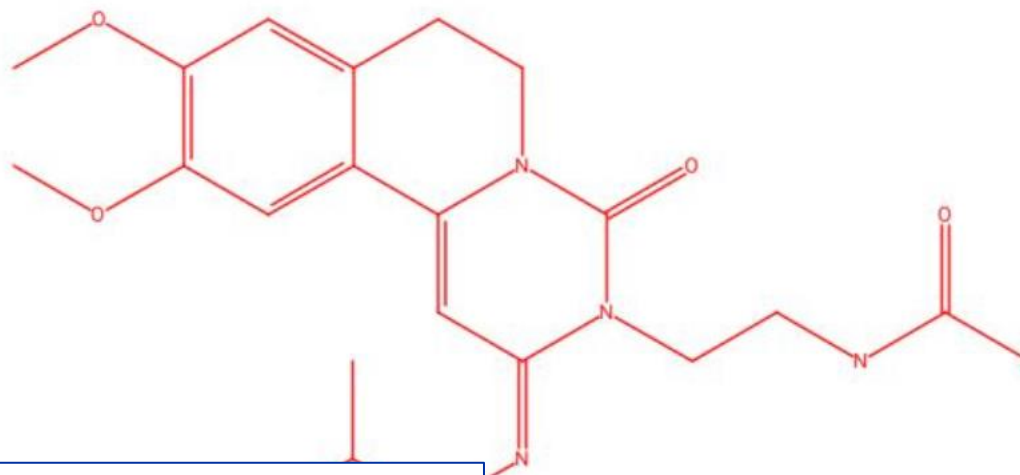
PROPERTIES

FINF02 Further Information (19) (FURTHER)

PSD Patent Specific Data (3) (FURTHER)

LB Substance Label (5) (FURTHER)

FA.RX RX.ID; RX.PAN; RX.RAN (4)



Identification information, hit structure(s), and an overview of available property/reaction data

Search for spectroscopic and melting point data

```
=> S L2 AND (MS OR NMR OR MP)/FA.P
```

```
12345919 MS/FA.P
```

```
14987160 NMR/FA.P
```

```
7704601 MP/FA.P
```

```
L3          3 L2 AND (MS OR NMR OR MP)/FA.P
```

```
=> D 1-3
```

Searching for property data types in /FA.P retrieves only results for which this data is available.

Property data is displayed in Table format

Mass Spectrometry (1)		
Keyword (.KW)	Location (.LO)	Ref(s) (REF)
liquid chromatograph y mass spectrometry (LCMS); electrospray ionisation (ESI); s pectrum	Page/Page column 32	1
1. AN 126517252: Patent, WO 2023109802 A1		

Property values, their location in the document, and related reference data are included.

Property data is displayed in Table format

```
Mass Spectrometry (1)
Keyword          | Location          | Ref(s)
(.KW)
=====
liquid          |                   |
y mass         |                   |
(LCMS)
ionis          |                   |
pectru        |                   |
1. AN 1       |                   |
```

```
NMR spectroscopy (1)
Keyword          | Nucleus          | Solvent          | Location          | Ref(s)
(.KW)            | (.NUC)           | (.SOL)           | (.LO)            | (REF)
=====+=====+=====+=====+=====
Chemical shifts | 1H               | CD3OD            | Paragraph 32     | 1
1. AN 126517252: Patent, WO 2023109802 A1
```

Property values, their location in the document, and related reference data are included.

Property data is displayed in Table format

```
Mass Spectrometry (1)
Keyword          | Location          | Ref(s)
(.KW)
=====
liquid
y mass
(LCMS)
ionis
pectru
1. AN 1

NMR spectroscopy (1)
Keyword          | Nucleus          | Solvent          | Location          | Ref(s)
(.KW)
=====
Melting Point (3)
Value           | Location          | Ref(s)
(MP)            | (.LO)            | (REF)
(Cel)           |                  |
=====+=====+=====
1. AN 1         | 246.1            | Page/Page column 36 | 1
1. AN          | 246.1            | Page/Page column 36 | 1
1. AN          | 246.1            | Page/Page column 36 | 1

1. AN 20082178: Patent, WO 2012020016 A1
```

Property values, their location in the document, and related reference data are included.

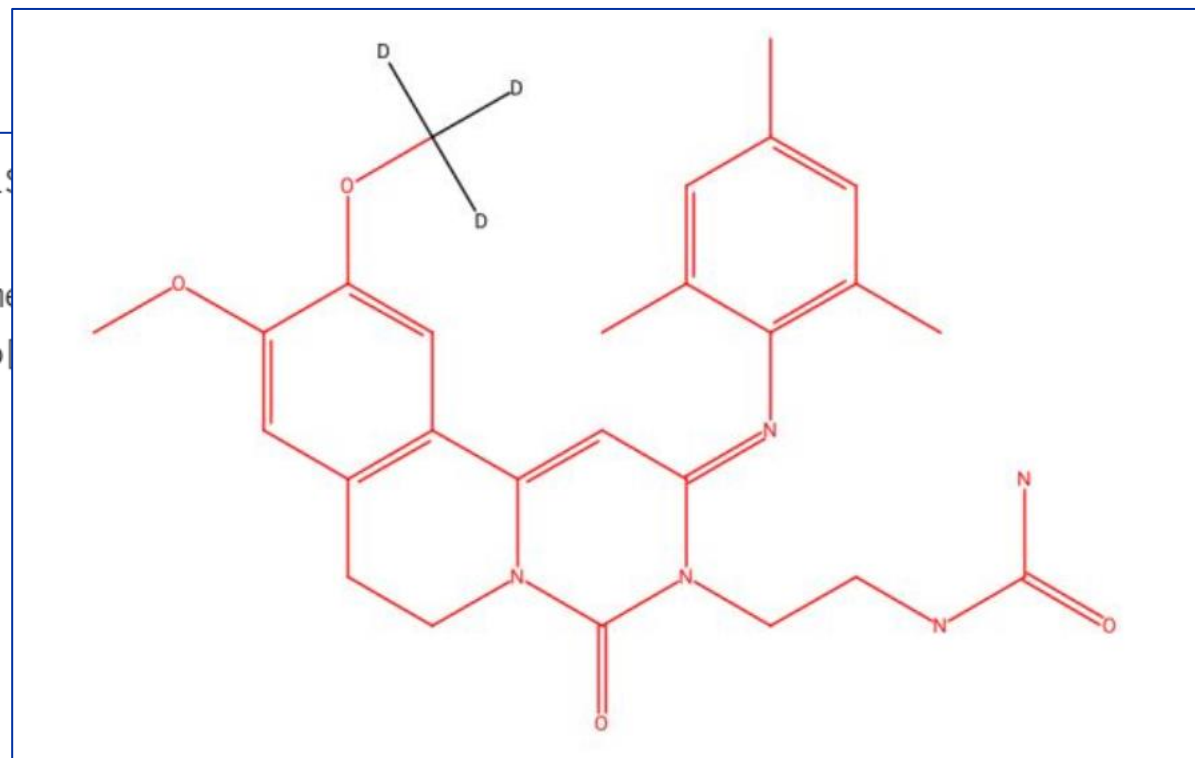
DISPLAY – QRD

L3 ANSWER 1 OF 3 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.
AN 55024098 REAXYSFILESU
CN (E)-1-(2-(2-(2,4,6-trimethylphenylimino)-9-methoxy-10-(methoxy-
d(sub)3(/sub))-4-oxo-6,7-dihydro-2H-pyrimido[6,1-a]isoquinolin-3(4H)-
yl)ethyl)urea
MF C26 H31 N5 O4
CMF C26 H31 N5 O4
LSF C26H28(2)H3N5O4
INCHI CSOBIBXVIYAXFM-QFJNNGLOSA-N
MW 480.539
MARKREF.CNT 2
REC 2
ED Entered STN: 17 Jul 2023
Last updated on STN: 19 Jan 2024

Query Related Display includes identification information, hit structure(s) and data requested in the search query

DISPLAY – QRD

L3 ANSWER 1 OF 3 REAXYSFILESU COPYRIGHT 2024 ELS
AN 55024098 REAXYSFILESU
CN (E)-1-(2-(2-(2,4,6-trimethylphenylimino)-9-methyl-
d(sub)3(/sub))-4-oxo-6,7-dihydro-2H-pyrimido[4,5-b]pyridin-
yl)ethyl)urea
MF C26 H31 N5 O4
CMF C26 H31 N5 O4
LSF C26H28(2)H3N5O4
INCHI CSOBIBXVIYAXFM-QFJNNGLOSA-N
MW 480.539
MARKREF.CNT 2
REC 2
ED Entered STN: 17 Jul 2023
Last updated on STN: 19 Jan 2024



Query Related Display includes identification information, hit structure(s) and data requested in the search query

DISPLAY – QRD

L3 ANSWER 1 OF 3 REAXYSFILESU COPYRIGHT 2024 ELS

AN 55024

CN (E)-1

d(sub

yl)et

MF C26 H

CMF C26 H

LSF C26H2

INCHI CSOBI

MW 480.5

MARKREF.CNT

REC 2

ED Enter

Last

Mass Spectrometry (1)

Keyword (.KW)	Location (.LO)	Ref(s) (REF)
---------------	----------------	--------------

liquid chromatograph	Page/Page column 32	1
y mass spectrometry		
(LCMS); electrospray		
ionisation (ESI); s		
pectrum		

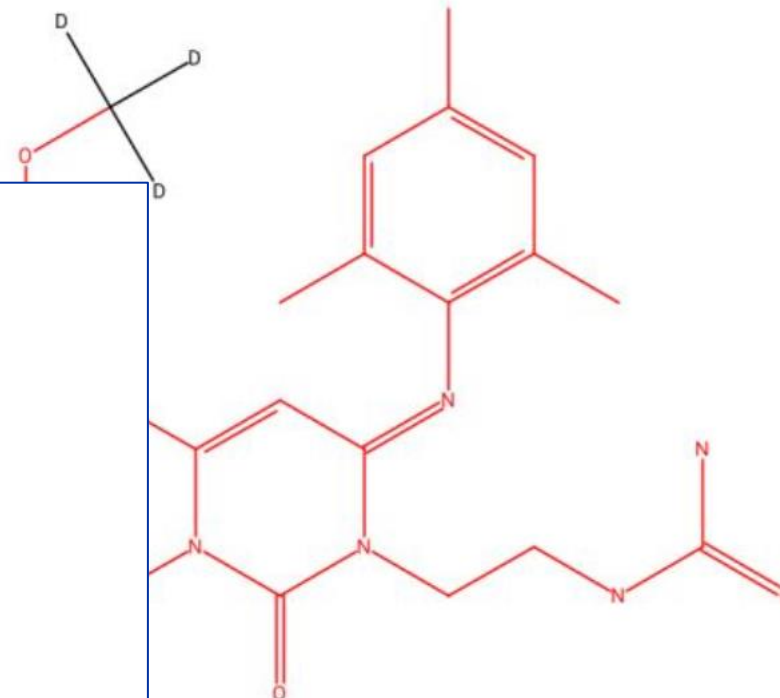
1. AN 126517252: Patent, WO 2023109802 A1

NMR spectroscopy (1)

Keyword (.KW)	Nucleus (.NUC)	Solvent (.SOL)	Location (.LO)	Ref(s) (REF)
---------------	----------------	----------------	----------------	--------------

Chemical shifts	1H	CD30D	Paragraph 32	1
-----------------	----	-------	--------------	---

1. AN 126517252: Patent, WO 2023109802 A1



Query Related Display includes identification information, hit structure(s) and data requested in the search query

Searchable Keywords within Property Data

```
=> S L2 AND ((ELECTROSPRAY? (3A) ION?) OR ESI)/KW
```

```
6273680 ELECTROSPRAY?/KW
```

```
6879671 ION?/KW
```

```
245207 ELECTROSPRAY? (3A) ION?
```

```
6273721 ESI/KW
```

```
L5          5 L2 AND ((ELECTROSPRAY? (3A) ION?) OR ESI)/KW
```

Searching in the /KW field retrieves records with specific terms listed as part of the property data table

Searchable Keywords within Property Data

=> S L2 AND			
	Keyword (.KW)	Location (.LO)	Ref(s) (REF)
6273	=====+=====+=====		
6879	liquid chromatograph	Page/Page column 32	1
245	y mass spectrometry		
6273	(LCMS); electrospray		
L5	ionisation (ESI); s		
	pectrum		
1. AN 126517252: Patent, WO 2023109802 A1			

Searching in the /KW field retrieves records with specific terms listed as part of the property data table

Search for Preparation Reactions

```
=> S L2 AND PREPARATION/RX.CL
```

```
23834706 PREPARATION/RX.CL
```

```
L4 3 L2 AND PREPARATION/RX.CL
```

Searching in /RX.CL retrieves only records where “preparation” is noted as the type of reaction.

Reaction search results

=> D 1-3

L4 ANSWER 1 OF 3 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.
AN 55024098 REAXYSFILESU
CN (E)-1-(2-(2-(2,4,6-trimethylphenylimino)-9-methoxy-10-(methoxy-
d(sub)3(/sub))-4-oxo-6,7-dihydro-2H-pyrimido[6,1-a]isoquinolin-3(4H)-
yl)ethyl)urea
MF C26 H31 N5 O4
CMF C26 H31 N5 O4
LSF C26H28(2)H3N5O4
INCHI CSOBIBXVIYAXFM-QFJNNGLOSA-N
MW 480.539
MARKREF.CNT 2
REC 2
ED Entered STN: 17 Jul 2023
Last updated on STN: 19 Jan 2024

Reaction search results

=> D 1-3

Reaction:

L4	Reaction ID:	64347951
AN	Reactant AN (.RAN):	1098379; 55475895
CN	Reactant (.RCT):	potassium cyanate; C25H27(2)H3N4O3
	Product AN (.PAN):	55024098
MF	Product (.PRO):	(E)-1-(2-(2-(2,4,6-trimethylphenylimino)-
CMF		9-methoxy
LSF		o-6,7-dihydro-2H-pyrimido[6,1-a]isoquinol
INCHI		in-3(4H)-yl)ethyl)urea
MW	Reference Count:	1

Reaction Identification information

REC 2

ED Entered STN: 17 Jul 2023

Last updated on STN: 19 Jan 2024

Reaction search results

=> D 1-3

Reaction:

Reaction Details:

L4
AN
CN

MF

CMF

LSF

INCHI

MW

MARKR

REC 2

ED Entere

Last u

Reaction RID: 64347951.1

Reaction Classification (.CL): **Preparation**

Product AN (.PRAN) 55024098

Reactant AN (.RCAN): 1098214

Solvent AN (.SOLAN): 3587155

Product: (E)-1-(2-(2-(2,4,6-trimethylphenylimino)-9-methoxy-10-(methoxy-d₃)-4-oxo-6,7-dihydro-2H-pyrimido[6,1-a]isoquinolin-3(4H)-yl)ethyl)urea

Reagent: hydrogenchloride

Solvent: water

Temperature: 80 Cel

Yield: 41 percent

Reference(s): 126517252: Patent, WO 2023109802 A1

Reaction Details

A key intermediate is found:

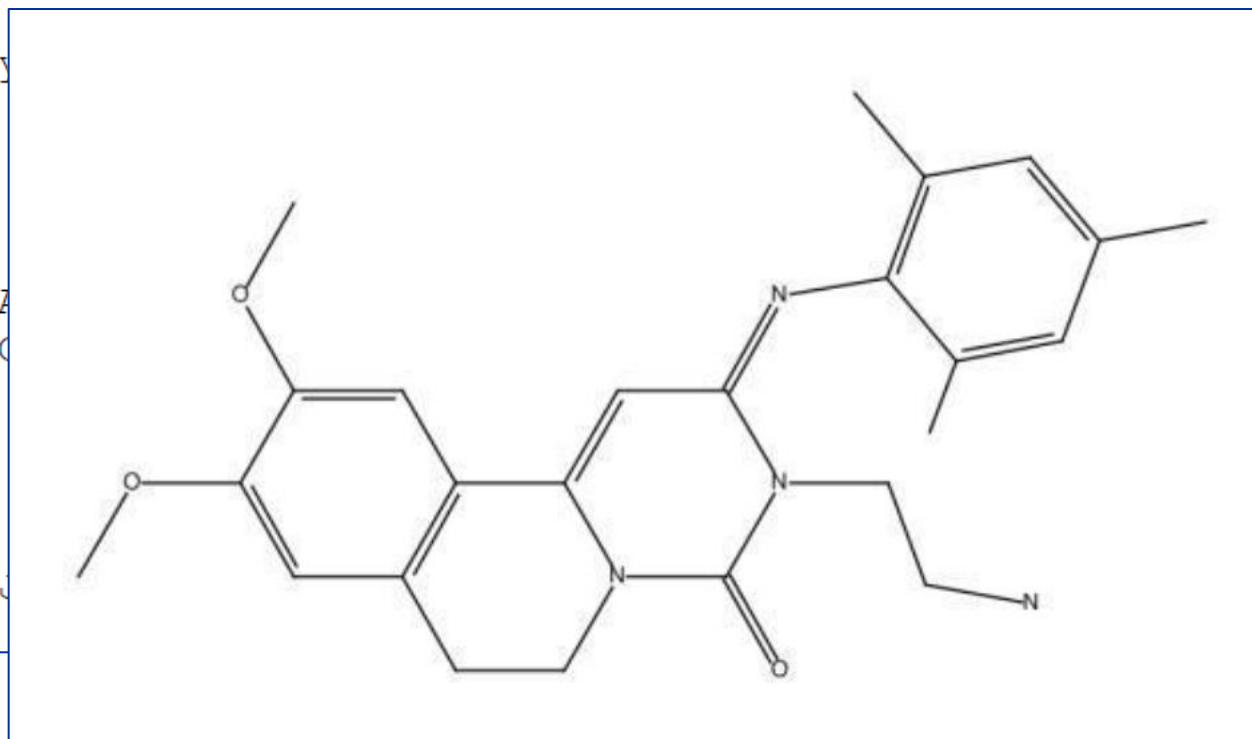
In addition to products and reactants, information about reagents, intermediates, etc., provides insight into reaction steps and conditions

```
L5      ANSWER 1 OF 1 REAXYSFILESU COPYRIGHT 2024 E
AN      14114306  REAXYSFILESU
CN
9,10-Dimethoxy-2-(2.4.6-trimethylphenylimino)-3-(2-aminoethyl)-3,4,6,7-tetrahydro-2H-py
rimido[6,1-a]isoquinolin-4-one
MF      C25 H30 N4 O3
CMF     C25 H30 N4 O3
LSF     C25H30N4O3
INCHI   XROHSSVKNYGALG-VYIQYICTSA-N
AINCHI  XROHSSVKNYGALG-VYIQYICTBO
MW      434.538
MARKREF.CNT 0
REC     1
ED      Entered STN: 14 Jul 2020
        Last updated on STN: 19 Jan 2024
```

A key intermediate is found:

In addition to products and reactants, information about reagents, intermediates, etc., provides insight into reaction steps and conditions

```
L5      ANSWER 1 OF 1 REAXYSFILESU COPYRIGHT 2024 E
AN      14114306  REAXYSFILESU
CN
9,10-Dimethoxy-2-(2,4,6-trimethyl
rimido[6,1-a]isoquinolin-4-one
MF      C25 H30 N4 O3
CMF     C25 H30 N4 O3
LSF     C25H30N4O3
INCHI   XROHSSVKNYGALG-VYIQYICTSA
AINCHI  XROHSSVKNYGALG-VYIQYICTBO
MW      434.538
MARKREF.CNT 0
REC     1
ED      Entered STN: 14 Jul 2020
        Last updated on STN: 19
```



2H-py

Search Reaction Data in Specialized Fields

Search Field Code	Long Name	How to Use
RX.ID	Reaction document	RX.ID/FA.RX
PAN	Product Accession Number	/RX.PAN
RAN	Reactant Accession Number	/RX.RAN
CL	Classification	/RX.CL
AAN	All Accession Numbers in reaction document	/RX.AAN
PRO, RCT	Chemical names or molecular formulas of products, reactants	Please use EXPAND!

Search for a substance in any reaction role

=> S 55024098/RX.AAN

L8 11 55024098/RX.AAN

Search for a substance in any reaction role

Reaction:

=>

L8

Reaction ID:	64348098
Reactant AN (.RAN):	55475905
Reactant (.RCT):	C20H20N2O5
Product AN (.PAN):	55024098
Product (.PRO):	(E)-1-(2-(2-(2,4,6-trimethylphenylimino)-9-methoxy-10-(methoxy-d ₃)-4-oxo-6,7-dihydro-2H-pyrimido[6,1-a]isoquinolin-3(4H)-yl)ethyl)urea
Reference Count:	1

Search for a substance in any reaction role

Reaction Details:

Reaction RID: 64348098.1
Reaction Classification (.CL): Multi-step reaction
Reactant AN (.RCAN): 1098214; 21730164; 3587189; 4267587;
4933273; 8127930; 956581
Solvent AN (.SOLAN): 1718733; 1731042; 3587155; 506104;
605365; 635639; 741880
Reagent: hydrogenchloride; Pd/C; hydrogen;
potassium carbonate; hydrazine hydrate;
sodium iodide; trichlorophosphate
Solvent: ethanol; chloroform; water; ethyl
acetate; N,N-dimethyl-formamide;
isopropyl alcohol; butanone
Reference(s): 126517252: Patent, WO 2023109802 A1

Search for products and reactants

```
=> s 56302858/RX.PAN (P) 14639110/RX.RAN
```

```
3 56302858/RX.PAN
```

```
3 14639110/RX.RAN
```

```
L9 3 56302858/RX.PAN (P) 14639110/RX.RAN
```

Search for products and reactants

```
L9      ANSWER 1 OF 3 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.  
AN      56302858  REAXYSFILESU  
CN      9,10-dimethoxy-2-(2,4,6-trimethylphenylimino)-3-(N-carbamoyl-2-  
        aminoethyl)-3,4,6,7-tetrahydro-2H-pyrimido(6,1-a)isoquinolin-4-one  
        ethane-1,2-disulfonate; ensifentrine ethane-1,2-disulfonate  
MF      C2 H6 O6 S2 . C26 H31 N5 O4  
CMF     C2 H6 O6 S2; C26 H31 N5 O4  
LSF     C26H31N5O4*C2H6O6S2  
INCHI   RDGBJTZHWWAGFL-UHFFFAOYSA-N  
MW      667.761  
MARKREF.CNT 0  
REC     1  
ED      Entered STN: 4 Nov 2023  
        Last updated on STN: 19 Jan 2024
```

Search for products and reactants

L9	AN	Reaction ID:	65005997
AN	56	Reactant AN (.RAN):	14639110 ; 1781377
CN	9	Reactant (.RCT):	9,10-dimethoxy-2-(2,4,6-trimethylphenylimino)-3-(N-carbamoyl-2-aminoethyl)-3,4,6,7-tetrahydro-2H-pyrimido[6,1-a]isoquinolin-4-one;
MF	C2		ethane-1,2-disulphonic acid
CMF	C2	Product AN (.PAN):	56302858
LSF	C2	Product (.PRO):	9,10-dimethoxy-2-(2,4,6-trimethylphenylimino)-3-(N-carbamoyl-2-aminoethyl)-3,4,6,7-tetrahydro-2H-pyrimido(6,1-a)isoquinolin-4-one
INCHI	RD		ethane-1,2-disulfonate
MW	66	Reference Count:	1
MARKREF.	C		
REC	1		
ED	EM		
La			

Closed Substructure search yields an additional unique structure hit

```
=> S L1 CSS FULL
```

```
FULL SEARCH INITIATED 08:45:34
```

```
FULL SCREEN SEARCH COMPLETED - 0 TO ITERATE
```

```
0.0% PROCESSED 50961552 ITERATIONS
```

```
6 ANSWERS
```

```
SEARCH TIME: 00.00.05
```

```
L6 6 SEA CSS FUL L1
```

```
=> S L6 NOT L2
```

```
L7 1 L6 NOT L2
```

Closed Substructure search yields an additional unique structure hit

=> S L1 CSS FULL

FULL SEARCH INITIATED 08:45:34

FULL SCREEN SEARCH COMPLETED - 0 TO ITERATE

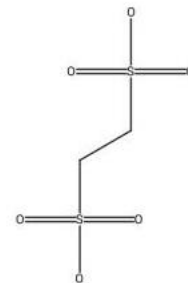
0.0% PROCESSED 50961552 ITERATIONS

SEARCH TIME: 00.00.05

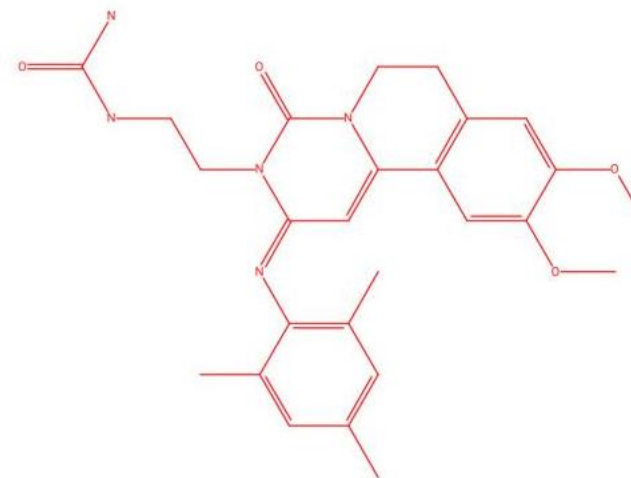
L6 6 SEA CSS FUL L1

=> S L6 NOT L2

L7 1 L6 NOT L2



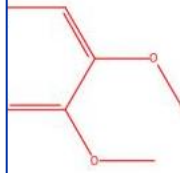
Expanding the search scope retrieves a disulfonate salt of ensifentrine.



Closed Substructure search yields an additional unique structure hit

	L7	ANSWER 1 OF 1 REAXYSFILESU COPYRIGHT 2024 ELSEVIER INC. on STN.
=> S L1	AN	56302858 REAXYSFILESU
FULL SEARCH	CN	9,10-dimethoxy-2-(2,4,6-trimethylphenylimino)-3-(N-carbamoyl-2-aminoethyl)-3,4,6,7-tetrahydro-2H-pyrimido(6,1-a)isoquinolin-4-one ethane-1,2-disulfonate; ensifentrine ethane-1,2-disulfonate
FULL SEARCH	MF	C2 H6 O6 S2 . C26 H31 N5 O4
0.0% FOUND	CMF	C2 H6 O6 S2; C26 H31 N5 O4
SEARCH	LSF	C26H31N5O4*C2H6O6S2
L6	INCHI	RDGBJTZHWWAGFL-UHFFFAOYSA-N
	MW	667.761
=> S L6	MARKREF.CNT	0
	REC	1
L7	ED	Entered STN: 4 Nov 2023
		Last updated on STN: 19 Jan 2024

Search scope retrieves a hit of ensifentrine.



FULL SSS search yields more substituted compounds

=> S L1 SSS FULL

FULL SEARCH INITIATED 08:45:59

FULL SCREEN SEARCH COMPLETED - 0 TO ITERATE

0.0% PROCESSED 50961552 ITERATIONS

37 ANSWERS

SEARCH TIME: 00.00.05

L8 37 SEA SSS FUL L1

=> S L8 NOT L6

L9 31 L8 NOT L6

Extending the scope to a full substructure search moves the search into the extended chemical space around the original compound of interest. SSS allows for substitution at any open site. 31 additional substances are retrieved.

FULL SSS search yields more substituted compounds

=> S L1 SSS FULL

FULL SEARCH INITIATED 08:45:59

FULL SCREEN SEARCH COMPLETED - 0 TO ITERATE

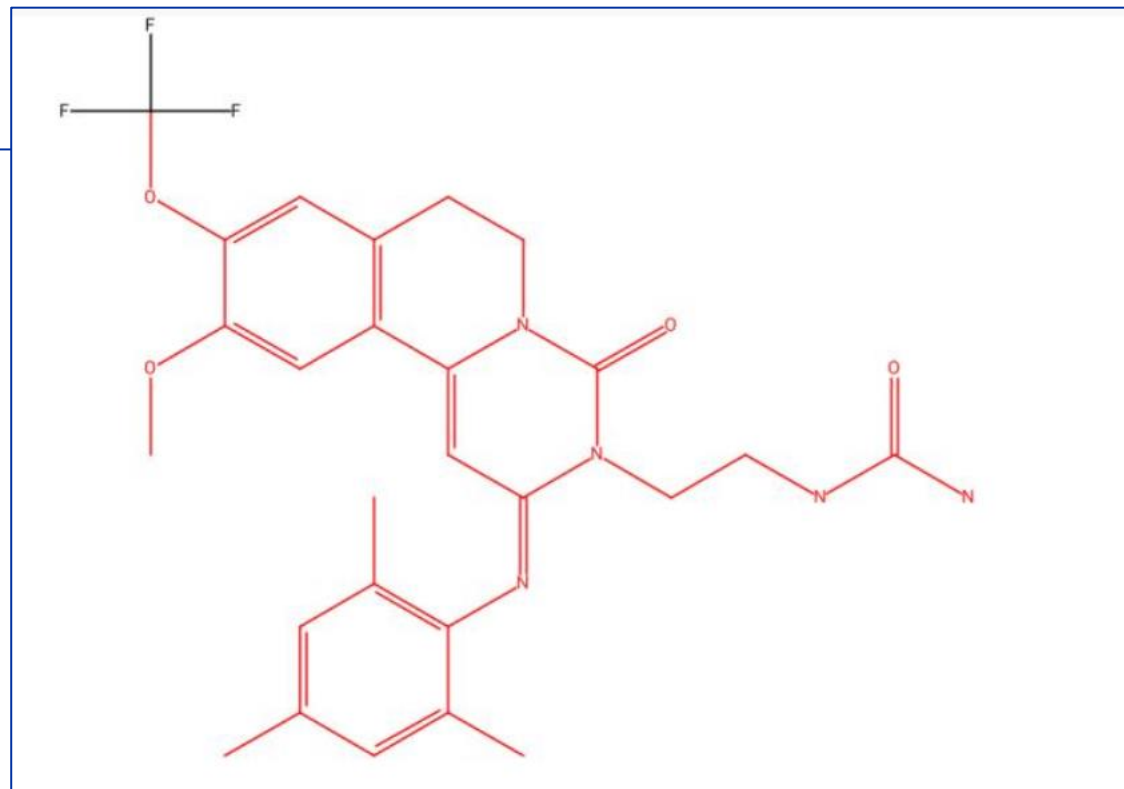
0.0% PROCESSED 50961552 ITERATIONS

SEARCH TIME: 00.00.05

L8 37 SEA SSS FUL L1

=> S L8 NOT L6

L9 31 L8 NOT L6



chemical space around the original compound of interest. SSS allows for substitution at any open site. 31 additional substances are retrieved.

FULL SSS search yields more substituted compounds

=> S L1 SSS FULL

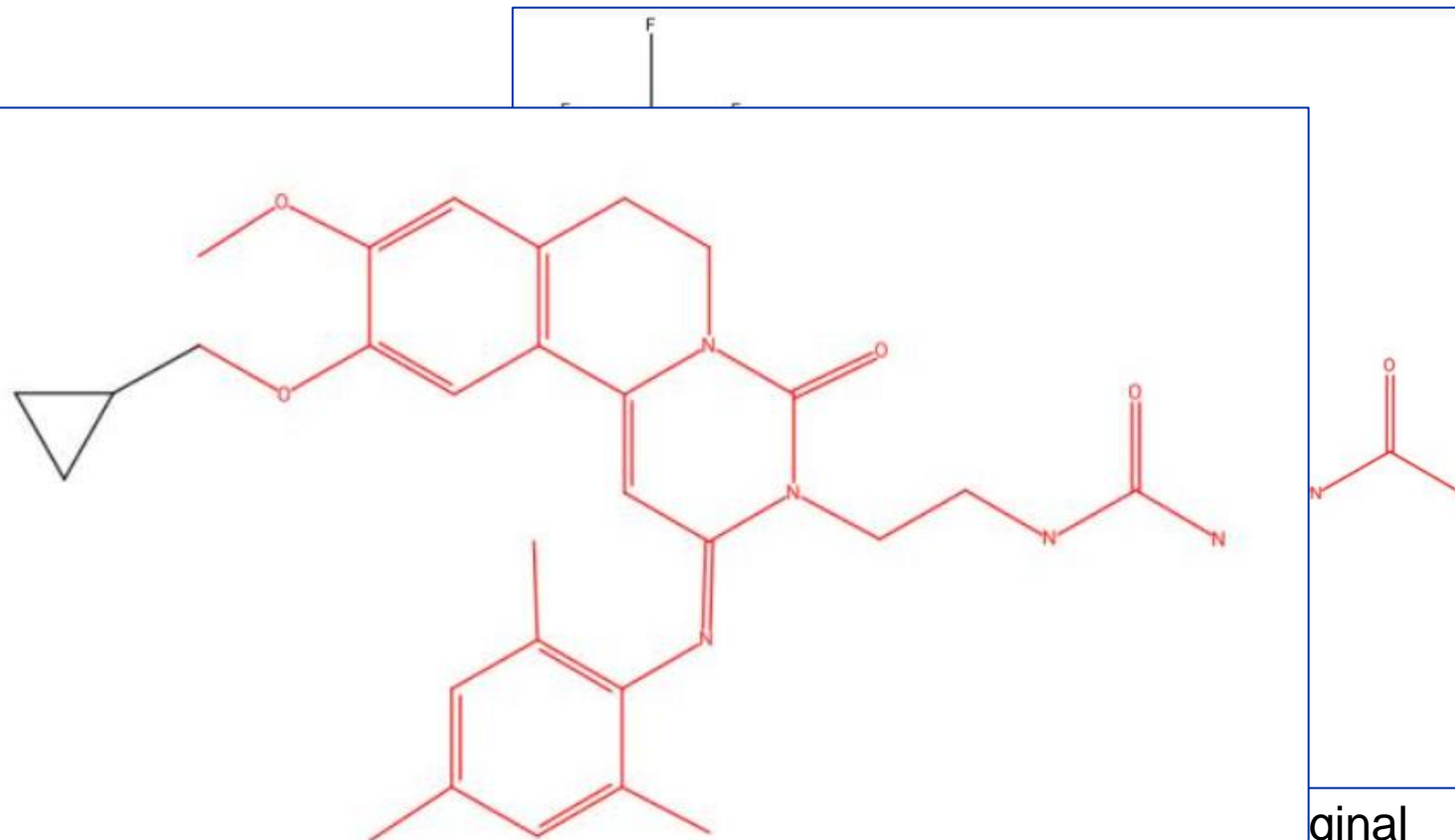
FULL SEARCH INITIATED 08:45
FULL SCREEN SEARCH COMPLETED

0.0% PROCESSED 50961552
SEARCH TIME: 00.00.05

L8 37 SEA SSS FULL

=> S L8 NOT L6

L9 31 L8 NOT L6



original
vs for

substitution at any open site. 31 additional
substances are retrieved.

FULL SSS search yields more substituted compounds

=> S L1 SSS FULL

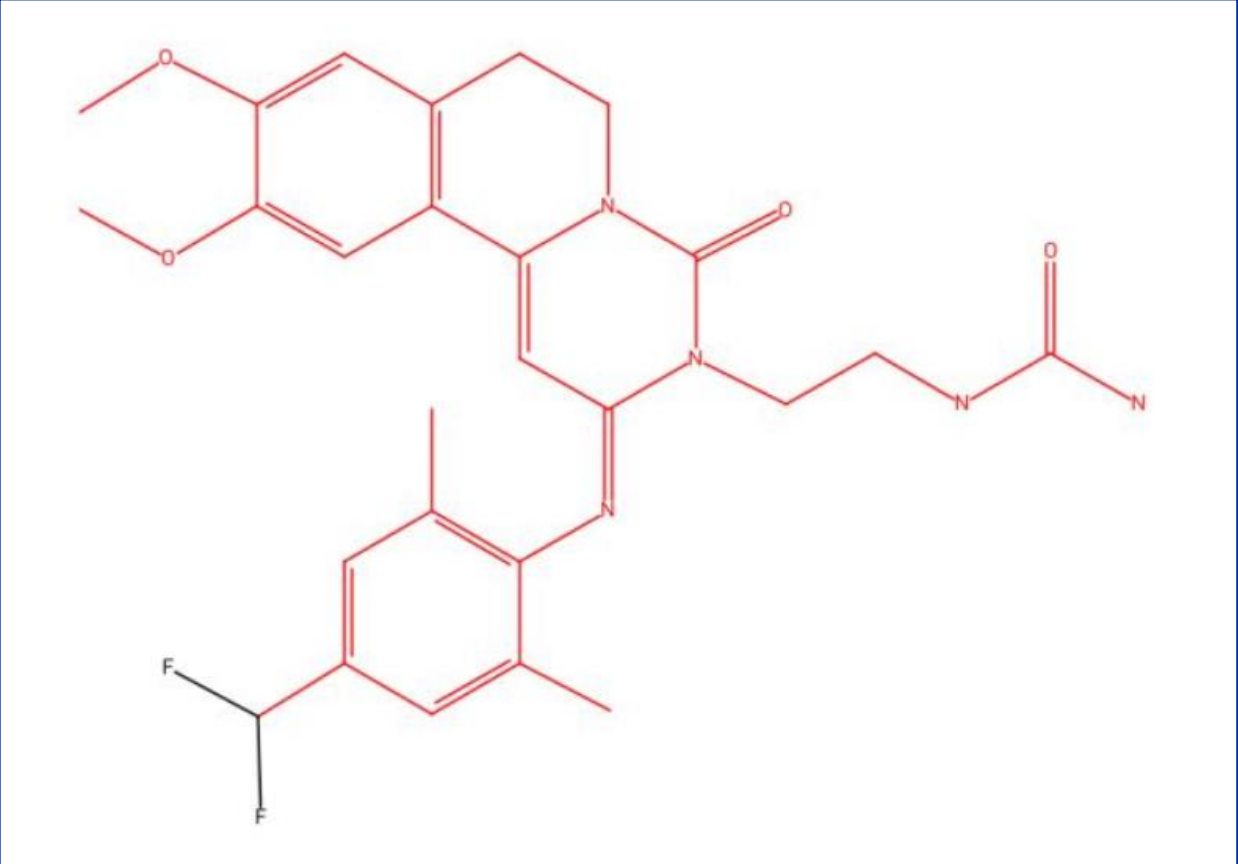
FULL SEARCH
FULL SCREEN

0.0% P
SEARCH T

L8

=> S L8 I

L9



original
vs for
ution at any open site. 31 additional
substances are retrieved.

Crossover to REAXYSFILEBIB

=> S L2 AND PATENT/DT

313 L2

41856739 PATENT/DT

L11 303 L2 AND PATENT/DT

=> S L2

L12 313 L2

=> S L12 NOT L11

L13 10 L12 NOT L11

Cross-file searching in REAXYSFILEBIB retrieves over 300 patent and nonpatent literature results

Patent Results

L11 ANSWER 1 OF 303 REAXYSFILEBI COPYRIGHT 2024 ELSEVIER INC. on STN.
AN 132357580 REAXYSFILEBI [Full-text](#)
TI SALT OF A PYRIMIDO[6,1-A]ISOQUINOLIN-4-ONE COMPOUND
IN SPARGO, PETER LIONEL; FRENCH, EDWARD JAMES; NORTHEN, JULIAN SCOTT;
MYKYTIUK, JOHN
PA VERONA PHARMA PLC

PI	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	---	-----	-----	-----
	AU 2016217674	A1	20170810		
	AU 2016217674	B2	20200430		
	AU 2020205281	A1	20200806		
	AU 2020205281	B2	20210715		
	CA 2974605	A1	20160818		
	CA 2974605 *	C	20240213	CA 2016-2974605	20160210

Patent Results

L11 ANSWER 1 OF 303 REAXYSFILEBI COPYRIGHT 2024 ELSEVIER INC. on STN.

AN	NZ 733926	A	20231027
TI	US 10463665	B2	20191105
IN	US 11491155	B2	20221108
	US 20180021337	A1	20180125
PA	US 20200016158	A1	20200116
	WO 2016128742	A1	20160818
PI	ZA201705112		20220525

* = indexed patent

DT **Patent**

LA English

SL English

ED Entered STN: 9 Mar 2024

Last updated on STN: 18 Mar 2024

Nonpatent Literature Results

L13 ANSWER 1 OF 10 REAXYSFILEBI COPYRIGHT 2024 ELSEVIER INC. on STN.
AN 131148564 REAXYSFILEBI [Full-text](#)
TI Beyond the heart - Exploring the therapeutic potential of PDE3
inhibitors
AU Trawally, Muhammed
SO Journal of Research in Pharmacy (2023), Volume 27, Number 6, pp.
2218-2241
ISSN: 2630-6344
DOI: <https://doi.org/10.29228/jrp.512>
Published by: Marmara University, Turkiye
DT Journal
LA English
SL English
ED Entered STN: 8 Jan 2024
Last updated on STN: 18 Mar 2024

Nonpatent Literature Results

L13 ANSWER 2 OF 10 REAXYSFILEBI COPYRIGHT 2024 ELSEVIER INC. on STN.
AN 128491880 REAXYSFILEBI [Full-text](#)
TI Ensifentrine as a Novel, Inhaled Treatment for Patients with COPD
AU Donohue, James F.; Rheault, Tara; Macdonald-Berko, Margot; Bengtsson, Thomas; Rickard, Kathleen
SO International Journal of COPD (2023), Volume 18, pp. 1611-1622
ISSN: 1178-2005
DOI: <https://doi.org/10.2147/COPD.S413436>
Published by: Dove Medical Press Ltd, New Zealand
DT Journal; General Review
LA English
SL English
ED Entered STN: 14 Oct 2023
Last updated on STN: 18 Mar 2024

Nonpatent Literature Results

L13 ANSWER 3 OF 10 REAXYSFILEBI COPYRIGHT 2024 ELSEVIER INC. on STN.
L13 AN 127290791 REAXYSFILEBI [Full-text](#)
AN TI Discovery of 2-(Methylcarbonylamino) thiazole as PDE4 inhibitors via
TI virtual screening and biological evaluation
AU AU Ma, Rui; Song, Na; Wang, Lveli; Gu, Xi; Xiong, Feng; Zhang, Shuqun;
Zhang, Jie; Yang, Weimin; Zuo, Zhili
SO SO Journal of Molecular Graphics and Modelling (2023), Volume 124, 108567
CODEN: JMGMFI ISSN: 1093-3263
DOI: <https://doi.org/10.1016/j.jmgm.2023.108567>
Published by: Elsevier Inc., United States
DT DT Journal
LA LA English
SL SL English
ED ED Entered STN: 20 Aug 2023
ED Last updated on STN: 18 Mar 2024
Last updated on STN: 18 Mar 2024

Summary

- REAXYFILESub contains more than 51 million records and covers all types of organic and inorganic substances, including alloys, coordination compounds, minerals, mixtures, polymers, and salts
- Substance properties and reaction data are now included in REAXYFILESUB's biweekly updates
- Simplified property and reaction searching and displays allow for efficient and thorough retrieval
- Legacy Database REAXYFILE has been discontinued – REAXYFILESUB and REAXYFILEBIB combine for a comprehensive replacement

Additional Resources and Materials

- User Guide:
<https://www.cas.org/sites/default/files/documents/CAS-STNext-ReaxysfileSUB-User%20Guide%20Properties-Reactions-2024-1.pdf>
- Database Summary Sheet: [REAXYSFILESU.pdf](#)
- Recorded training sessions: <https://www.stn-international.com/en/training-center>

For more information...

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