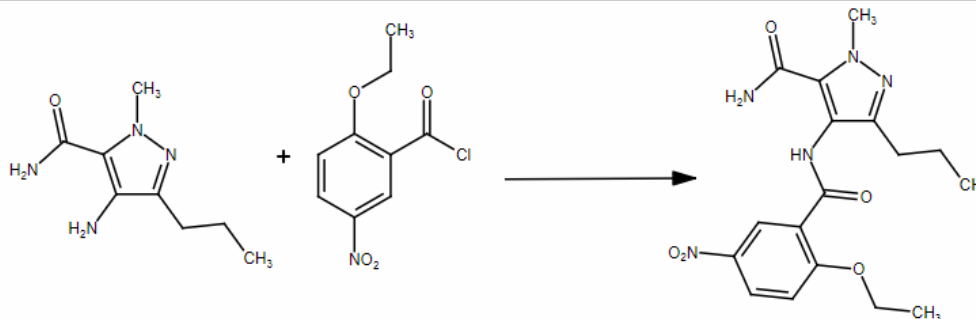


IDBS & ChemAxon: Our Strategic Partnership



Overview

Total reaction mass
46.398 g
Total reaction volume
141.354 mL



- Edit reaction
- Find component
- Print worksheet
- Clear reaction

Components Conditions Health & Safety Procedure Registration Analytical

Columns

Reactants	+ Add new	Limit	Equiv.	Mass	Volume	MW (g/mol)	Purity (%)	Quantifier	n	Supplier ID	Batch ID	CAS Number	Synonym
(R1) 4-amino-2-methyl-5-propylpyrazo...			1	10 g		182.227	100		54.877 mmol	Internal			
(R2) 2-ethoxy-5-nitrobenzoyl chloride			1.2	15.121 g	12.601 mL	229.62	100	1.2 g/mL	65.852 mmol				

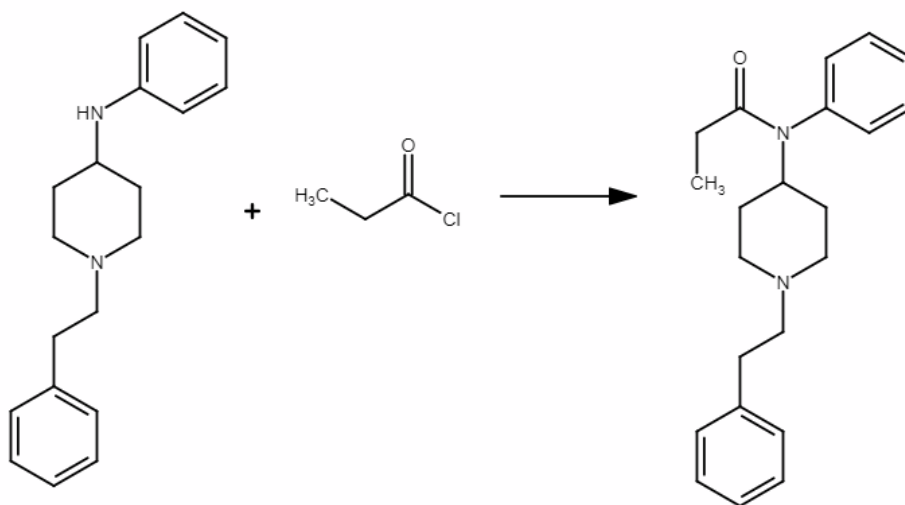
Agents	+ Add new	Limit	Equiv.	Mass	Volume	Purity (%)	Quantifier	n	MW (g/mol)	IUPAC name
(A1) DIPEA			3	21.277 g	28.753 mL	100	0.74 g/mL	164.63 mmol	129.243	N,N-diisopropylethylamine

Solvents	+ Add new	Volume	Molarity	Solvent Vols	Comment
(S1) DCE		100 mL	0.549 M	10	

Catalysts	+ Add new

Products	+ Add new	Formula	Mass [expected]	Mass [actual]	Purity (%)	n [expected]	n [actual]	Yield
(P1) 4-(2-ethoxy-5-nitrobenzamido)-2-...		C ₁₇ H ₂₁ N ₅ O ₅	20.6 g	19.8 g	97	54.877 mmol	51.163 mmol	

Stoichiometry with integrations to reagent sources, analytical services and registration



MarvinJS , with integration
to MarvinSketch,
ChemDraw & BioviaDraw

Integration to
Compliance
Checker for risk
analysis

Compliance checker



We have identified that some of the compounds have legal documents associated to them.

Last run on: 20 Mar 2019 11:05:34

Run compliance checker again

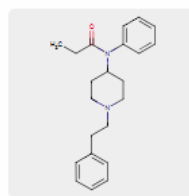
fentanyl :

- IT Decreto del Presidente della Repubblica del 9 ottobre 1990, n. 309 TABELLA II SEZIONE A
- FR Arrête du 22 fevrier 1990 fixant la listedes substances classees comme stupefiants ANNEXE I
- DE Gesetz über den Verkehr mit Betäubungsmitteln (Betäubungsmittelgesetz - BtMG) Anlage III
- AT Suchtgiftverordnung Anhang I
- US ARCOS NDC Dictionary File
- UK Misuse of Drugs Act Part I Class A Drugs
- IE MISUSE OF DRUGS REGULATIONS 1988 Schedule II
- US Controlled Substance Act Schedule II
- DK Bekendtgørelse om euforiserende stoffer Liste B
- ES LEY 17/1.967, DE 8 DE ABRIL LISTA I
- UK The Misuse of Drugs Regulations 2001



Tree Browser

- ▼ CXN319
 - ▼ CXN319A
 - CXN319-001
 - CXN319-002**

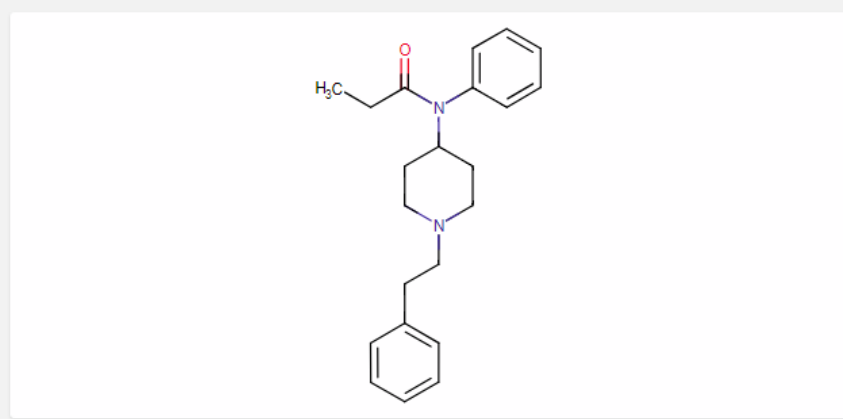


CXN319-002

Using source REGISTRAR • Created on 2019-03-20 11:14:00

[Edit](#) [More actions](#)

LnbRef CXN319-002	Created by Ian	Molecular Formula C22H28N2O	Mol Weight 336.479	Submitter Ian
----------------------	-------------------	--------------------------------	-----------------------	------------------



Additional Data

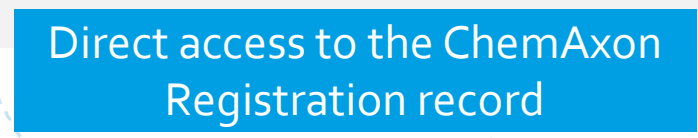
Project	Comment
	--

Characterization

NMR
structure consistent with spectrum

Uncategorized Data

% Yield 96.07	Experiment ID Ian-0069	Mass 6.41
Project ID aaa31f40350011e99fe40000a0e0159		



Search for Reactions Hide detail (3)

Options

Match ALL search terms

+ New...

Reaction chemistry
Structure
Defined
Substructure (Ignore stereo)

Experiment
Created by
is
Ian

Reaction chemistry
Yield of Product
greater than
70 %

Download ...

Reaction	Title	Created By	Created At	Product Yield
<input type="checkbox"/>	lan-0046	Ian	18 Jul 2018 14:59 19s	88.151% (P1)
	EXP-Ian1189	Ian	28 Mar 2018 11:17 8s	98.078% (P1)
	EXP-Ian1393	Ian	26 Feb 2018	88.800% (P1)

Search combining experimental and chemical information (JCHEM backend)

🔍 Search

Search Bioregistry for registered biomolecule

Search Bioregistry

📄 Upload

Upload a sequence file of one of the [following file formats](#)

Choose a file to upload

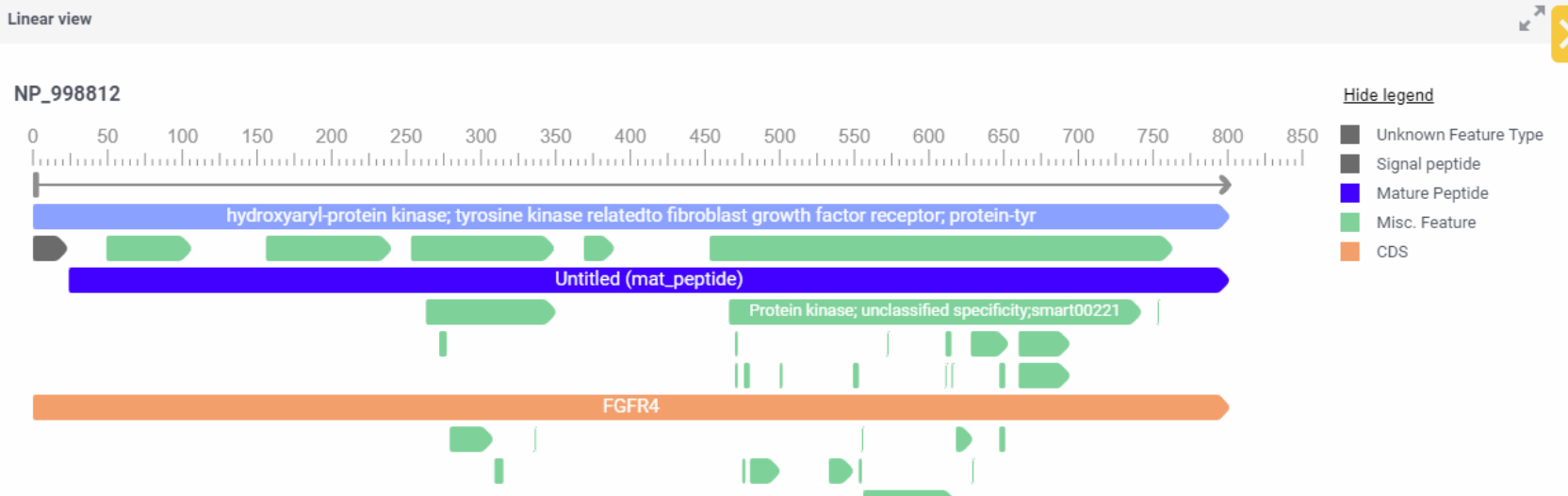
or drag a file to this page

➕ Create new

Create a new biomolecule using the BioEddie editor

Open BioEddie

Ability to load GenBank, GenPept, FASTA or HELM formats, draw HELM and query bio-registration



Sequence

```

1  MRLLALLGV  LLSVPGPPVL  SLEAEEVEL  EPCLAPSLQ  QEQLTVALG  QPVRLCCGRA
61  ERGGHWYKEG  SRLAPAGRVR  GWRGRLEIAS  FLPEDAGRYL  CLARGSMIVL  QNLTITGDS
121  LTSSNDDDEP  KSHRDPSNRH  SYPQQAPYWT  HPQRMEKKLH  AVPAGNTVKF  RCPAAGNPTP
181  TIRWLKDGQA  FHGENRIGGI  RLRHQHWSLV  MESVVPSDRG  TYTCLVENAV  GSIRYNYLLD
241  VLERSPHRPI  LQAGLPANTT  AVVGSDEVLL  CKVYSDAQPH  IQWLKHIVIN  GSFSGADGFP
301  YVQVLKTADI  NSSEVEVLYL  RNVAEDAGE  YTCLAGNSIG  LSYQSAWLTV  LPEEDPTWTA
361  AAPEARYTDI  ILYASGSLAL  AVLLLAGLY  RGQALHGRHP  RPPATVQKLS  RFPLARQFSL
421  ESGSSGKSSS  SLVRGVRLSS  SGPALLAGLV  SLDLPLDPLW  EFPRDRLVLG  KPLGEGCFGQ
481  VVRAEAFGMD  PARPDQASTV  AVKMLKDNAS  DKDLADLVSE  MEVMKLGIRH  KNIIINLLGVC
541  TQEGPLYVIV  ECAAKGNLRE  FLRARRPPGP  DLSPDGRSS  EGPLSFPVLV  SCAYQVARGM
601  QYLESRKCII  RDLAARNVLV  TEDNVMKIAD  FGLARGVHHI  DYYKKTNSGR  LPVKWMAPEA
661  LFDREVYTHQS  DVWSFGILLW  EIFTLGGSPY  PGIPVEELFS  LLREGHRMDR  PPHCPPPELYG
721  LMRECHHAAP  SQRPTFKQLV  EALDKVLLAV  SEEYDLRLT  FGPYSPSGGD  ASSTCSSSDS
781  VFSHDPLPLG  SSSFPFGSGV  QT
  
```

- Annotations
- Features
 - Homo sapiens (Source)
 - hydroxyaryl-protein kinase; tyrosine kinase related to fibroblast growth factor receptor; pr...
 - Untitled Feature (Signal peptide)
 - Untitled Feature (Mature Peptide)
 - Immunoglobulin domain; c11960 (Misc. Feature)
 - Immunoglobulin domain; c11960 (Misc. Feature)
 - Immunoglobulin V-set domain; pfam07686 (Misc. Feature)
 - Third immunoglobulin (Ig)-like domain of fibroblast growth factor receptor 2 (FGFR2); ad...

Tools

Download & upload ?

Use to edit the biomolecule in an external editor

Download Upload

Registration

Register the biosequence to the biology registration system

Register

Sequence renderer (linear/cyclic)

E-WorkBook Biomolecule Show title ?

+ ↶ ↷ ↗ 📁 💾 ⋮

1 I 2 C 3 E 4 C 5 R 6 E 7 A 8 M NH₂

Library ×

Search

Peptide	CHEM	Nucleic acid	BLOB
X	A	C	D
E	F	G	H
I	K	L	M
N	O	P	Q
R	S	T	V
W	Y	U	dA
dC	dD	dE	dF
dH	dI	dK	dL
dM	dN	dP	dQ
dR	dS	dT	dV
dW	dY	Aib	B-Aia

Tools

Registration

Register the biomolecule to the biology registration system

Register

HELM Details ×

BioEddie sequence editor
(BMT backend)

Search results

Search for a biomolecule | by properties

Refine results

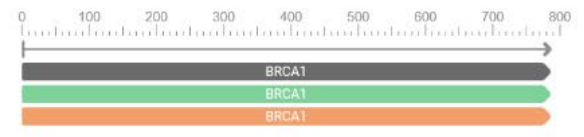
Clear all

Type

- Clear
- Protein
- Vector
- Antibody
- Enzyme

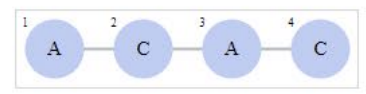
BA_Ab1

Sequence ID CXN32
Type Antibody
Species Arabidopsis thaliana
Accession Number BA123



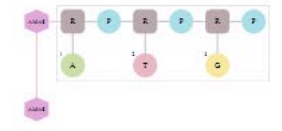
d

Sequence ID CXN24
Type Antibody
Species
Accession Number



Delic

Sequence ID CXN18
Type Enzyme
Species Escherichia coli
Accession Number BHB12



Drosophila melanogaster MIP31231 full insert cDNA

Sequence ID CXN15
Type Antibody
Species
Accession Number BT128753



Bio-Registration search
by sequence/type
(BMT backend)

Thank you!

