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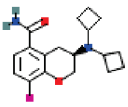
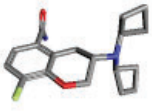
COMPOUND SUMMARY

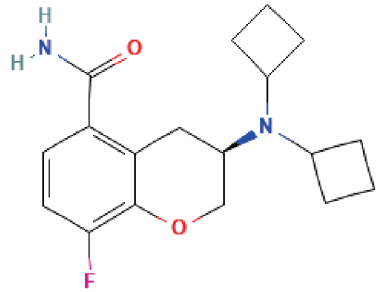
Robalzotan

PubChem CID	3055171
Structure	 2D  3D Find Similar Structures
Molecular Formula	$C_{18}H_{23}FN_2O_2$
Synonyms	Robalzotan 169758-66-1 UNII-I18M56OGME NAD-299 NAD 299 More...
Molecular Weight	318.4
Dates	Modify 2021-10-02 Create 2005-08-09

1 Structures

1.1 2D Structure

Chemical Structure Depiction



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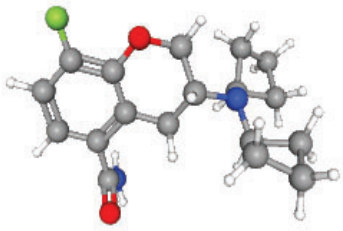
1.2 3D Conformer

Interactive Chemical Structure Model

- (•) Ball and Stick
- ( ) Sticks
- ( ) Wire-Frame
- ( ) Space-Filling
- [x] Show Hydrogens
- [ ] Animate



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2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

(3*R*)-3-[di(cyclobutyl)amino]-8-fluoro-3,4-dihydro-2*H*-chromene-5-carboxamide

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

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2.1.2 InChI

InChI=1S/C18H23FN2O2/c19-16-8-7-14(18(20)22)15-9-13(10-23-17(15)16)21(11-3-1-4-11)12-5-2-6-12/h7-8,11-13H,1-6,9-10H2,(H2,20,22)/t13-/m1/s1

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

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2.1.3 InChI Key

MQTUXRKNJYPMCG-CYBMUJFWSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

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2.1.4 Canonical SMILES

C1CC(C1)N(C2CCC2)C3CC4=C(C=CC(=C4OC3)F)C(=O)N

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

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2.1.5 Isomeric SMILES

C1CC(C1)N([C@@H]2CC3=C(C=CC(=C3OC2)F)C(=O)N)C4CCC4

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

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2.2 Molecular Formula

C18H23FN2O2

Computed by PubChem 2.1 (PubChem release 2021.05.07)

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2.3 Other Identifiers

2.3.1 CAS

169758-66-1

CAS Common Chemistry; ChemIDplus; DrugBank; EPA DSSTox

2.3.2 UNII

I18M56OGME

FDA/SPL Indexing Data

2.3.3 DSSTox Substance ID

DTXSID30168743

EPA DSSTox

2.3.4 Wikipedia

Robalzotan

Wikipedia

2.4 Synonyms

2.4.1 MeSH Entry Terms

3-N,N-dicyclobutylamino-8-fluoro-3,4-dihydro-2H-1-benzopyran-5-carboxamide hydrogen tartrate monohydrate
NAD 299
NAD-299
robalzotan

Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

Robalzotan	SCHEMBL115079
169758-66-1	NAD299
UNII-I18M56OGME	CHEMBL1628569
NAD-299	DTXSID30168743
NAD 299	ZINC3811952
I18M56OGME	DB06538
AZD-7371	VC30713
(R)-3-(Dicyclobutylamino)-8-fluoro-5-chromancarboxamide	NCGC00370859-01
(3R)-3-[di(cyclobutyl)amino]-8-fluoro-3,4-dihydro-2H-chromene-5-carboxamide	3-N,N-dicyclobutylamino-8-fluoro-3,4-dihydro-2H-1-benzopyran-5-carboxamide hydrogen
(R)-3-(Dicyclobutylamino)-8-fluorochroman-5-carboxamide	A13092
Robalzotan [INN:BAN]	Q7340703
GTPL72	(R)-3-(Dicyclobutylamino)-8-fluoro-5-chromancarboxamide.

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3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	318.4	Computed by PubChem 2.1 (PubChem release 2021.05.07)
XLogP3-AA	2.8	Computed by XLogP3 3.0 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	1	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Hydrogen Bond Acceptor Count	4	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Rotatable Bond Count	4	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Exact Mass	318.17435614	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	318.17435614	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	55.6 Å^2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Heavy Atom Count	23	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	438	Computed by Cactvs 3.4.8.18 (PubChem release 2021.05.07)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	1	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.05.07)

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