

Discovery Studio Client

File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help

Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores **Small Molecules** X-ray My Tools

Tools Files # bisdimethoxy

Index	Name	Visible	Tagged	Visibility Locked	StdInChI	StdInChIKey	AuxInfo	Formula	Mw	SMILES	CSID	Clean Energy
1	Molecule	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	InChI=1S/C...	PREBVFJCNPEK...	1/0/N:9,13...	C19H16O4	308.328	O=C(C=C...	4,474,770	9.83512

Molecule: 22 columns (9 columns hidden) - no current row

Jobs

localhost:9943 20.1.0.19295

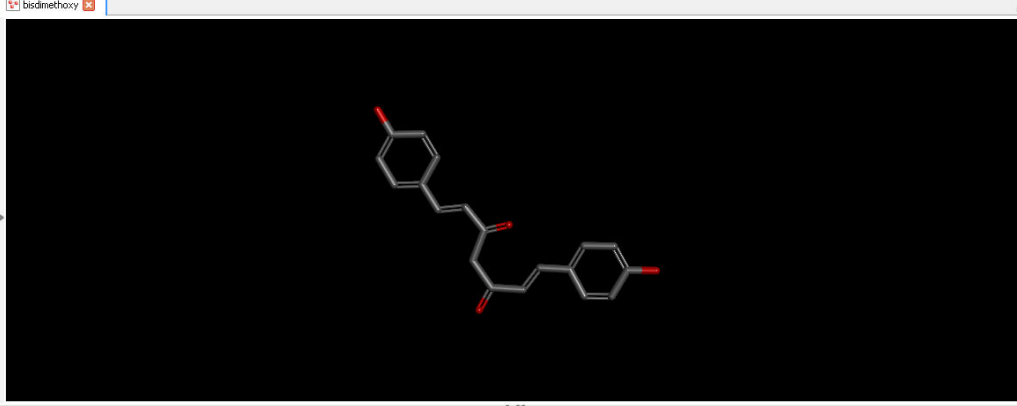
3:35 PM 6/25/2020

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Molecule / Atom / Bond

Jobs

Use the Select tool to select one or more objects. Click to select an object, drag to select multiple objects.

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Search product features

Tools Files

Sketch Molecules
Build Fragment
Prepare or Filter Ligands
Search Small Molecule Conform...
Minimize Ligands
Align Small Molecules
Calculate Molecular Properties
ADMET
ADMET Descriptors...
Toxicity Prediction...
Property Calculation
Basic Arithmetic...
Calculate RMSD...
Calculate Molecular Properties...
Calculate Ligand Efficiency...
Analysis
Correlation and Statistics...
Calculate ROC Curve...
For further analysis, you can Calculate Principal Components or run Filter By Property on the data.
Create QSAR Model
Study SAR
Design and Analyze Libraries
Select Subset Libraries
Molecule Browser

ADMET Descriptors

Parameter Name	Parameter Value
Input Ligands	bidimethoxyVisible
ADMET Descriptors	Aqueous Solubility,Blood Brain Barrier Penetratio...

Show Parameter Help

Run Options Cancel Help

Index	Name	Visible	Tagged	Visibility Locked	StdInChi	StdInChiKey	AuxInfo	Formula	Mw	SMILES	CSD	Clean Energy
1	Molecule	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	InChi=15/C...	PREBVFJICNPEK...	1/0/N-9,13...	C19H16O4	308.328	O=C(C=C...	4,474,770	9.83512

Molecule \ Atom \ Bond

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ADMET Descriptors

Do you want to display the ADMET plot?

Yes No More

Do not show this message again.

Index	Name	Visible	Tagged	Visibility Locked	StdInChi	StdInChiKey	AuxInfo	Formula	Mw	SMILES	CSD	Clean Energy	ADMET_Solubility	ADM
1	Molecule	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	InChi=15/C...	PREBVFJICNPEK...	1/0/N-9,13...	C19H16O4	308.328	O=C(C=C...	4,474,770	9.83512	-3.396	3

Molecule \ Atom \ Bond

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Search product features

Tools Files

Sketch Molecules Build Fragment Prepare or Filter Ligands Search Small Molecule Conform... Minimize Ligands Align Small Molecules Calculate Molecular Properties

ADMET

ADMET Descriptors... Toxicity Prediction...

Property Calculation

Basic Arithmetic... Calculate RMSD... Calculate Molecular Properties... Calculate Ligand Efficiency...

Analysis

Correlation and Statistics... Calculate ROC Curve... For further analysis, you can Calculate Principal Components or run Filter By Property on the data. Create QSAR Model Study SAR

Design and Analyze Libraries Select Subset Libraries Molecule Browser

Jobs

Chemical structure of bisdimethoxy

ADMET_AlogP98 vs ADMET_PSA_2D scatter plot

Legend	Color
ADMET_AlogP98	Blue
Absorption-95	Red
Absorption-99	Green
B88-95	Magenta
B88-99	Cyan

Index	Name	Visible	Tagged	Visibility Locked	StdInChI	StdInChIKey
1	Molecule	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	InChI=1S/C...	PREBVFJICNPE

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ADMET

ADMET Descriptors... Toxicity Prediction...

Property Calculation

Basic Arithmetic... Calculate RMSD... Calculate Molecular Properties... Calculate Ligand Efficiency...

Analysis

Correlation and Statistics... Calculate ROC Curve... For further analysis, you can Calculate Principal Components or run Filter By Property on the data. Create QSAR Model Study SAR

Design and Analyze Libraries Select Subset Libraries Molecule Browser

Jobs

Chemical structure of bisdimethoxy

Chemical structure of bisdimethoxy (1)

Chemical structure of bisdimethoxy

Toxicity Prediction (Extendable)

Information User: R130255

Molecule

C11H16O2
Molecular Weight: 308.3274
MolWt: 3.027
Protonable Bonds: 6
Acceptable: 4
Donors: 2

Model Prediction
Prediction: Non-Mutagen
Report Score: 1.0
Manhattan Distance: 10.1
Manhattan Distance (over): 0.282
Prediction: Studies the Report score to assess the whether predicted data best matching the test set and use the current job.
Decision Score: The standard Laplacian-modified Decision score.

Model Applicability
Default: Features are fingerprint features in the query molecule, but not found or appearing too infrequently in the training set.
1. All properties and QSP components are within expected ranges.

Structural Similar Compounds (TOPKAT_Ames_Mutagenicity)

Name	488-317	488-317	488-312
Structure			
Actual Property	Non-Mutagen	Non-Mutagen	Non-Mutagen
Expected Property	Non-Mutagen	Non-Mutagen	Non-Mutagen
Distance	0.442	0.442	0.442
Reference	Parsons et al. 1985, Chem (1985) 48, 315-330	12 Environmental Protection Agency at 100-70000-200-000000	Parsons et al. 1985, Chem (1985) 48, 315-330

Information User: R130255

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