ONTOFORCE

CHEMISTRY USE CASE IN LIFE SCIENCES

Use Case

SEARCH FOR SIMILAR MOLECULE STARTING FROM « MY » COMPOUND :

CARMUSTINE

DISQOVER

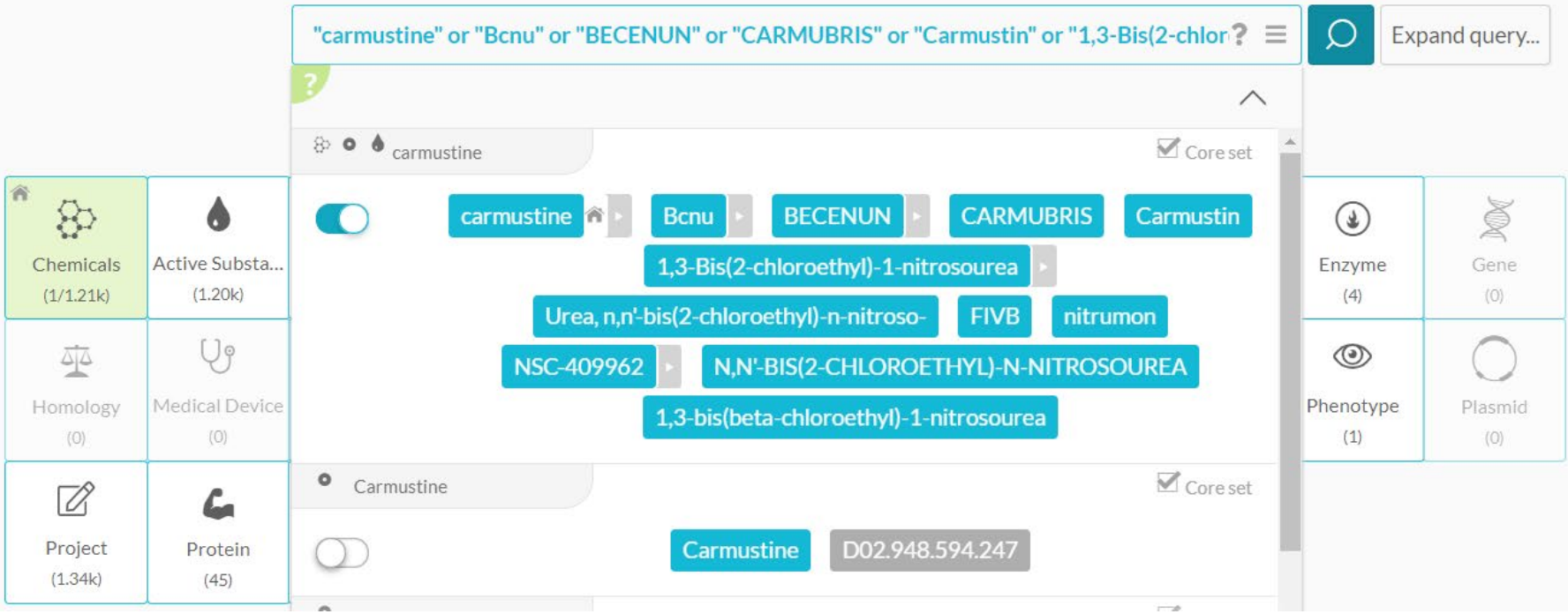
Text Search | Chemistry Search by Chemaxon

I am looking for...

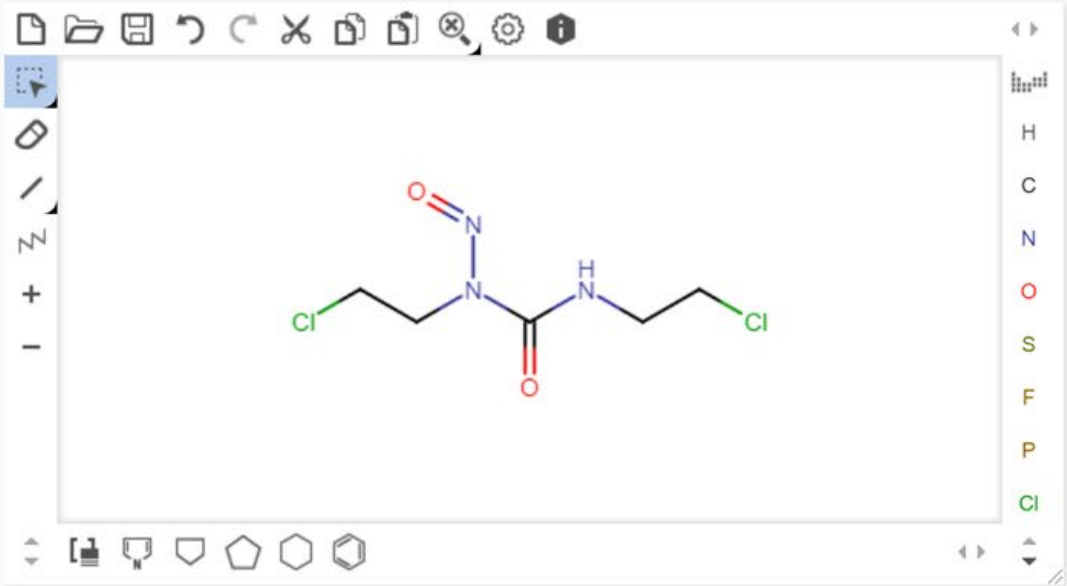
Chemicals (7.77M)	Active Substa... (16.1k)	Adverse Event (9.47M)	Antibody (1.76M)	Assay (15.3M)	Biospecimen (4.16k)	Cell line (332k)	Clinical study (552k)	Disease (287k)	Enzyme (8.05k)	Gene (21.9M)
Homology (44.2k)	Medical Device (2.50M)	Medicine (374k)	Model Organi... (42.7k)	Organism (1.84M)	Organization (10.6M)	Patent (364k)	Pathway (25.5k)	Person (27.4M)	Phenotype (10.5k)	Plasmid (29.6k)
Project (2.88M)	Protein (598k)	Publication (29.7M)	Transcript (1.44M)	Variant (13.9M)						

DISQOVER

Text Search | Chemistry Search by Chemaxon



Text Search | Chemistry Search by Chemaxon



Search Strategy:

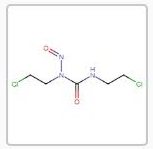
Similarity

Maximum number of results: 101

Similarity Threshold: 70%

Search

Chemicals (28)	Active Substa... (3)	Adverse Event (0)	Antibody (0)	Assay (0)	Biospecimen (0)	Cell line (0)	Clinical study (0)	Disease (0)	Enzyme (0)	Gene (0)
Homology (0)	Medical Device (0)	Medicine (0)	Model Organi... (0)	Organism (0)	Organization (0)	Patent (0)	Pathway (0)	Person (0)	Phenotype (0)	Plasmid (0)
Project (0)	Protein (0)	Publication (0)	Transcript (0)	Variant (0)						



Chemicals
28

Links
(26k)

Open in Visual Analytics

Data Sources (26)

In-House

27	Chemaxon

Public

28	Chemantics
27	ChEMBL
27	PubChem

1/5

Substance Type (4)

28	Original Material
27	Small_molecule
3	Organic
2	Synthetic organic

Group (4)

25	not annotated
3	Investigational
2	Approved
1	Experimental

Mechanism of Action

26	not annotated
2	INHIBITOR
2	DNA inhibitor

MeSH Classification

25	not annotated
3	Organic Chemicals
3	Nitroso Compoun...
3	Nitrosourea Co...
2	Lomustine
1	Carmustine

Bemis-Murcko Framework (6)

1	not annotated
15	c1ccccc1
8	C
2	C1CCCC1
1	C(c1ccccc1)c1ccccc1
1	C1CCCCCCCCCCC1

Reduced Molecular Framew... (5)

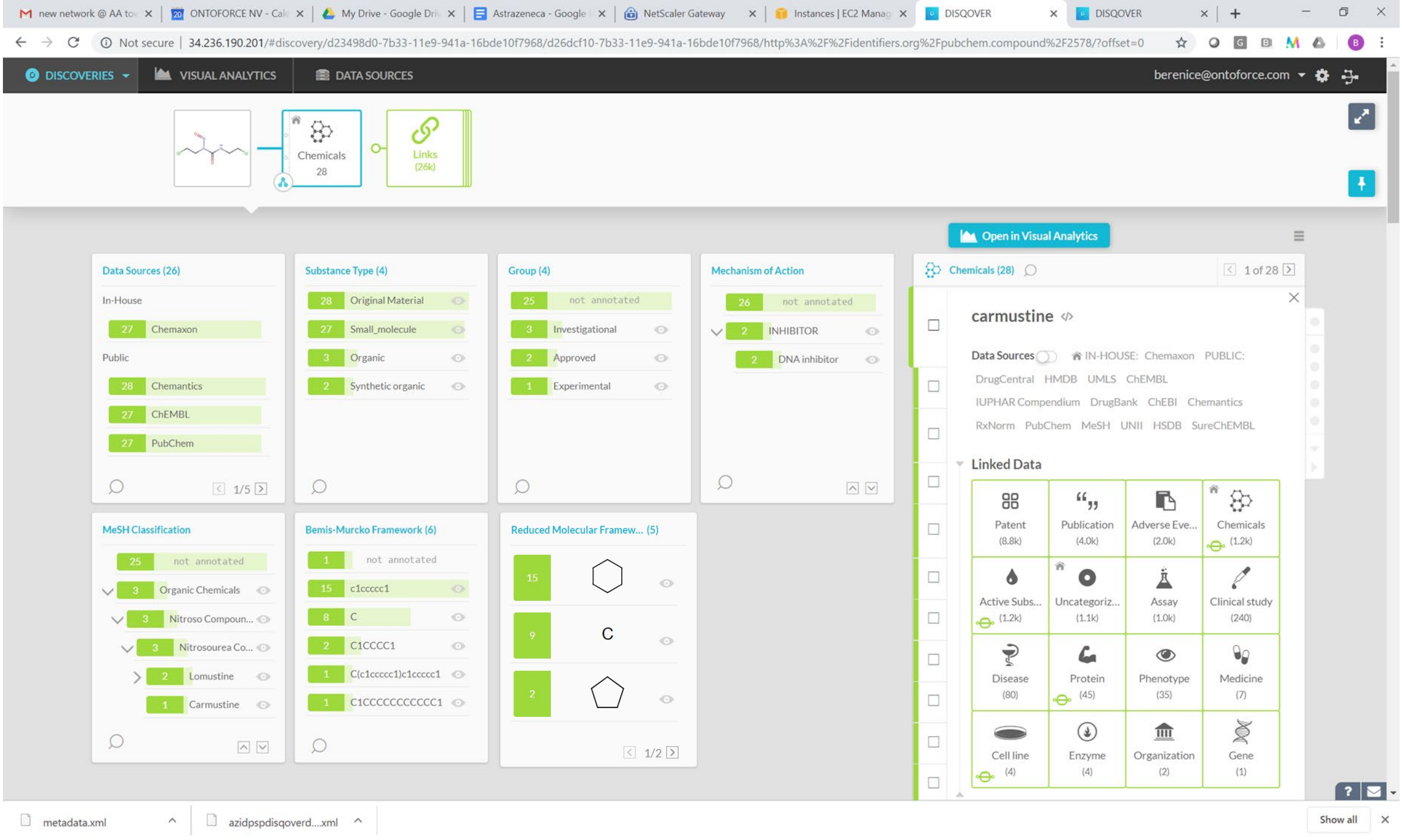
15	
9	C
2	

1/2

Chemicals (28)

1-20 of 28

carmustine **Molecular Formula** : C5H9Cl2N3O2 **Source** : DrugCentral ; HMDB ; UMLS ; ChEMBL ; IUPHAR Compendium ; DrugBank ; ChEBI ; Chemantics ; RxNorm ; PubChem ; MeSH ; UNII ; HSDB ; SureChEMBL ; Chemaxon	100.0% *similar*
Nitrosochloroethyldimethylurea **Source** : ChEMBL ; Chemantics ; PubChem ; Chemaxon	87.27% *similar*
Pentamustine **Molecular Formula** : C8H16ClN3O2 **Source** : ChEMBL ; Chemantics ; PubChem ; UNII ; SureChEMBL ; Chemaxon	82.53% *similar*
Springer12044259-77685716 **Source** : Chemantics	82.3% *similar*
Elmustine **Molecular Formula** : C5H10ClN3O3 **Source** : ChEMBL ; Chemantics ; PubChem ; UNII ; SureChEMBL ; MeSH ; Chemaxon	80.0% *similar*
13908-92-4 **Source** : ChEMBL ; Chemantics ; PubChem ; Chemaxon	79.38% *similar*
NSC 93184 **Source** : ChEMBL ; Chemantics ; PubChem ; Chemaxon	78.78% *similar*
1-(2-Chloroethyl)-1-nitrosourea **Source** : ChEMBL ; Chemantics ; PubChem ; Chemaxon	77.27% *similar*
1-(2-Chloroethyl)-3-cyclopentyl-1-nitrosourea **Source** : ChEMBL ; Chemantics ; PubChem ; Chemaxon	71.42% *similar*
BRN 2270948 **Source** : ChEMBL ; Chemantics ; PubChem ; Chemaxon	70.94% *similar*
1-(2-Chloroethyl)-3-cyclododecyl-1-nitrosourea	70.94%


DISCOVERIES
VISUAL ANALYTICS
DATA SOURCES
berenice@ontoforce.com
Chemicals
28
Links
(26k)
Open in Visual Analytics
Data Sources (26)
In-House
27 Chemaxon
Public
28 Chemantics
27 ChEMBL
27 PubChem
1/5
Substance Type (4)
28 Original Material
27 Small_molecule
3 Organic
2 Synthetic organic
Group (4)
25 not annotated
3 Investigational
2 Approved
1 Experimental
Mechanism of Action
26 not annotated
2 INHIBITOR
2 DNA inhibitor
Chemicals (28)
1 of 28
carmustine
Data Sources
IN-HOUSE: Chemaxon
PUBLIC:
DrugCentral HMDB UMLS ChEMBL
IUPHAR Compendium DrugBank ChEBI Chemantics
RxNorm PubChem MeSH UNII HSDB SureChEMBL
Linked Data
Patent (8.8k)
Publication (4.0k)
Adverse Eve... (2.0k)
Chemicals (1.2k)
Active Subs... (1.2k)
Uncategoriz... (1.1k)
Assay (1.0k)
Clinical study (240)
Disease (80)
Protein (45)
Phenotype (35)
Medicine (7)
Cell line (4)
Enzyme (4)
Organization (2)
Gene (1)
MeSH Classification
25 not annotated
3 Organic Chemicals
3 Nitroso Compoun...
3 Nitrosourea Co...
2 Lomustine
1 Carmustine
Bemis-Murcko Framework (6)
1 not annotated
15 c1ccccc1
8 C
2 C1CCCC1
1 C(c1ccccc1)c1ccccc1
1 C1CCCCCCCCCC1
Reduced Molecular Framew... (5)
15
9
C
2
1/2
metadata.xml
azidpspdisqoverd....xml
Show all

Structure	ClCCNC(=O)N(CCCl)N=O
Mol Weight	214.05
Formula	C5H9Cl2N3O2
InChi Key	InChIKey=DLGOEMSEDOSKAD-UHFFFAOYSA-N
Log P	1.02
Log D	1.02
TPSA	61.77
Atom Count	21
Heavy Atom Count	12
Ring Count	0
Rotatable Bonds	5
H Bond Acceptors	2
H Bond Donors	1
Lipinski rule of 5 (4 of 4)	true
Polarizibility	17
Bemis-Murcko Framework	C

Identification

Structure

Identification

Structure

Molecular Formula	C5H9Cl2N3O2

Scope Note

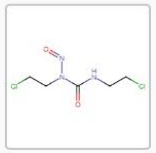
A cell-cycle phase nonspecific alkylating antineoplastic agent. It is used in the treatment of brain tumors and various other malignant neoplasms. (From Martindale, The Extra Pharmacopoeia, 30th ed, p462) This substance

Description

A member of the class of N-nitrosoureas that is 1,3-bis(2-chloroethyl)urea in which one of the nitrogens is substituted by a nitroso group.

A cell-cycle phase nonspecific alkylating antineoplastic agent. It is used in the treatment of brain tumors and various other malignant

Iupac Name	1,3-bis(2-chloroethyl)-3-nitrosourea
CAS Registry Number	154-93-8
InChIKey	DLGOEMSEDOSKAD-UHFFFAOYSA-N
INCHI	InChI=1S/C5H9Cl2N3O2/c6-1-3-8-5(11)10(9-12)4-2-7/h1-4H2,(H,8,11)
Smiles Representation	ClCCNC(=O)N(CCCl)N=O



Chemicals
28

Links
(26k)

Open in Visual Analytics

Data Sources (26)

In-House

- 27 Chemaxon

Public

- 28 Chemantics
- 27 ChEMBL
- 27 PubChem

1/5

Substance Type (4)

- 28 Original Material
- 27 Small_molecule
- 3 Organic
- 2 Synthetic organic

Group (4)

- 25 not annotated
- 3 Investigational
- 2 Approved
- 1 Experimental

Mechanism of Action

- 26 not annotated
- 2 INHIBITOR
  - 2 DNA inhibitor

MeSH Classification

- 25 not annotated
- 3 Organic Chemicals
  - 3 Nitroso Compoun...
    - 3 Nitrosourea Co...
      - 2 Lomustine
      - 1 Carmustine

Bemis-Murcko Framework (6)

- 1 not annotated
- 15 c1ccccc1
- 8 C
- 2 C1CCCC1
- 1 C(c1ccccc1)c1ccccc1
- 1 C1CCCCCCCCCCC1

Reduced Molecular Framew... (5)

- 15 
- 9 C
- 2 

1/2

Chemicals (28)

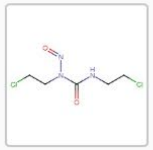
22 of 28

lomustine

Data Sources: IN-HOUSE: Chemaxon PUBLIC: ChEMBL HMDB UMLS DrugBank DrugCentral IUPHAR Compendium ChEBI RxNorm PubChem MeSH UNII HSDB SureChEMBL

Linked Data

Patent (7.5k)	Publication (1.9k)	Chemicals (1.1k)	Active Subs... (1.1k)
Uncategoriz... (955)	Adverse Eve... (904)	Assay (784)	Clinical study (121)
Disease (44)	Protein (37)	Phenotype (19)	Medicine (8)
Enzyme (4)			



Chemicals 28 | Iomustine | Clinical study 121 | Links (5.0k)

Open in Visual Analytics

Data Sources (9)

- 120 Countries
- 74 ClinicalTrials.gov
- 74 MeSH
- 69 WHO: International ...
- 56 ChEMBL
- 55 EudraCT

1/2

MeSH Condition Classificati...

- 48 not annotated
- 73 Neoplasms
  - 65 Neoplasms by His...
    - 54 Neoplasms, Ger...
    - 54 Neoplasms, Ner...
    - 51 Neoplasms, Gla...
    - 9 Lymphoma
    - 3 Leukemia
    - 3 Nevi and Melan...
    - 1 Neoplasms, Co...
    - 1 Neoplasms, Pla...
  - 34 Neoplasms by Site
  - 2 Neoplastic Proces...
- 30 Nervous System Dis...
- 10 Hemic and Lymphati...

Study Record Type (2)

- 74 Trial
- 47 Protocol

Condition (144)

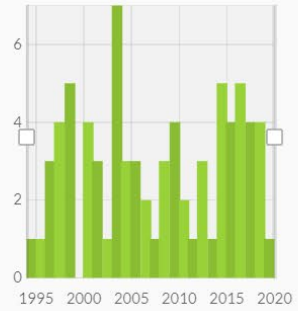
- 50 Glioblastoma
- 23 Medulloblastoma
- 21 Central Nervous Syst...
- 21 Nervous System Neo...
- 20 Glioma
- 16 Brain and Central Ne...

1/24

MeSH Intervention

- 48 not annotated
- 72 Organic Chemicals
- 49 Heterocyclic Compo...
- 20 Amino Acids, Peptid...
- 12 Polycyclic Compoun...
- 11 Carbohydrates

Start Year



From 1994 To 2019

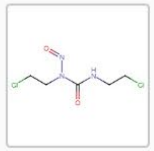
Study Phase (6)

- 61 Phase 2
- 48 Phase 3
- 9 Phase 1
- 6 Not Applicable
- 5 Phase 2/Phase 3
- 4 Phase 1/Phase 2

Clinical study (121)

1-20 of 121

- Radiation Therapy With or Without Chemotherapy in Treating Patients With Anaplastic Oligodendroglioma
  Source : ClinicalTrials.gov ; MeSH ; WHO: ICTRP ; Countries
- Chemotherapy Followed by Radiation Therapy in Treating Adults With Supratentorial Glioma
  Source : ClinicalTrials.gov ; MeSH ; WHO: ICTRP ; Countries
- Radiation Therapy With and Without Combination Chemotherapy in Patients With Resected Anaplastic Oligodendroglioma
  Source : ClinicalTrials.gov ; MeSH ; WHO: ICTRP ; Countries
- Radiation Therapy Plus Combination Chemotherapy in Treating Children With Medulloblastoma
  Source : ClinicalTrials.gov ; MeSH ; WHO: ICTRP ; Countries
- Combination Chemotherapy in Treating Children With Progressive Brain Tumors
  Source : ClinicalTrials.gov ; MeSH ; WHO: ICTRP ; Countries
- Combination Chemotherapy and Bone Marrow Transplantation or Peripheral Stem Cell Transplantation in Treating Patients With Oligodendroglioma
  Source : ClinicalTrials.gov ; MeSH ; WHO: ICTRP ; Countries
- Oral Combination Chemotherapy in Treating Elderly Patients With Intermediate or High-Grade Non-Hodgkin's Lymphomas
  Source : ClinicalTrials.gov ; MeSH ; WHO: ICTRP ; Countries
- Combination Chemotherapy in Treating Patients With AIDS-Related Hodgkin's Disease
  Source : ClinicalTrials.gov ; MeSH ; WHO: ICTRP ; Countries



Open in Visual Analytics

Data Sources (3)

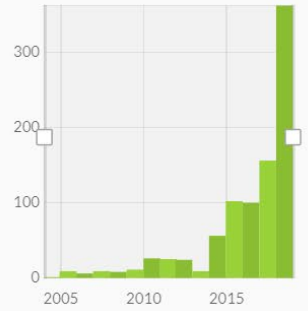
904	OpenFDA Drug Adve...
887	Countries
860	UMLS

Adverse Event (724)

106	Nausea
101	Fatigue
60	Death (finding)
52	Disease Progression
49	Decreased platelet c...
43	Vomiting

1/121

Creation Date



From 2004 To 2018

Drug Indication (262)

44	not annotated
325	Malignant neoplasm ...
234	Product used for unk...
114	Glioblastoma
114	Glioblastoma - categ...
49	Hodgkin^S Disease

1/44

Country

Category Of Reporter (5)

57	not annotated
353	Physician
302	Other Health Profess...
114	Consumer Or Non-H...
78	Pharmacist

Event Seriousness (5)

533	not annotated
200	Hospitalization
184	Death
20	Life-Threatening
12	Disabled

Adverse Event (904)

1-20 of 904

- FDA drug-event: DECADRON, CLOBAZAM, SENOKOT, AVASTIN, CHLOROPHYLL, ZOPICLONE, TYLENOL, ONDANSETRON, KEPPRA, LOMUSTINE [10005435]
  Source : OpenFDA Drug Adverse Events ; UMLS ; Countries
- FDA drug-event: ETOPOSIDE (ETOPOSIDE), AVASTIN, CALBOLCAL, FRISIUM (UNKNOWN), DECADRON/0016001, NYSTATIN, ASA (UNKNOWN), VITAMIN D/00107901/(UNKNOWN), FOSAMAX (UNKNOWN), KEPPRA, LOMUSTINE [10011278]
  Source : OpenFDA Drug Adverse Events ; UMLS ; Countries
- FDA drug-event: PAXIL (CANADA), FISH OIL, AVASTIN, LOMUSTINE., DEXAMETHASONE. [10020115]
  Source : OpenFDA Drug Adverse Events ; UMLS ; Countries
- FDA drug-event: RADIOTHERAPY, CYCLOPHOSPHAMIDE, CISPLATIN, CARBOPLATIN, LOMUSTINE [10033227]
  Source : UMLS ; OpenFDA Drug Adverse Events ; Countries
- FDA drug-event: CISPLATIN, CYCLOPHOSPHAMIDE, CARBOPLATIN, LOMUSTINE [10040701]
  Source : UMLS ; OpenFDA Drug Adverse Events ; Countries
- FDA drug-event: TEMOZOLOMIDE, VINBLASTINE, VINCRISTINE, CARBOPLATIN, LOMUSTINE [10097329]
  Source : OpenFDA Drug Adverse Events ; UMLS ; Countries
- FDA drug-event: TEMODAL, AVASTIN, STEMETIL, LOMUSTINE [10142567]
  Source : OpenFDA Drug Adverse Events ; UMLS ; Countries
- FDA drug-event: TEGRETOL, KEPPRA (LEVETIRACETAM), VOGALENE (METOPIMAZINE), INEXIUM (ESOMEPRAZOLE MAGNESIUM)

DASHBOARDS | DATA SOURCES

Search in dashboards

New search

Created today:

- > Chemical
- >...> Disease
- >...> Adverse Event
- > Chemical
- > Clinical Study
- > Chemical

> Chemical

Substance Type

4.99k	Small_molecule
3.07k	Original Material
205	Synthetic organic
186	Organic
126	Metabolite

Filter 21 values 1 / 5

Group

7.76M	< Missing >
5.02k	Experimental
3.79k	Investigational
3.70k	Approved
602	Labelled

Filter 9 values 1 / 2

MeSH Classification

4.82k	< Missing >
97	Organic Chemicals
74	Heterocyclic Compounds
27	Polycyclic Compounds
25	Amino Acids, Peptides, and Proteins

Filter

Chemical Properties

Mechanism of Action

4.99k	< Missing >
15	INHIBITOR
4	Cyclin-dependent kinase 2 inhibitor
3	Cyclin-dependent kinase 4 inhibitor
3	MAP kinase p38 alpha inhibitor
2	Cyclooxygenase inhibitor
1	11-beta-hydroxysteroid dehydrogenase...

Molecular Framework

1.95k	< Missi...	61	
460		60	
269		34	

Molecular Graph

1.95k	< Missing >	5	HBr	2	
22	Na^+	3	NH_3	2	Ca^{2+}
17	HCl	2		2	K^+
5	H_2O	2		2	

Search in 5.02k results

- (5Z)-3-benzyl-5-[(2-hydroxy-3-nitrophenyl)methylidene]-2-sulfanylidene-1,3-thiazolidin-4-one
- MLS000911622
- 2-OXO-3-PENTENOIC ACID
- 4-{5-[(Z)-(2,4-dioxo-1,3-thiazolidin-5-ylidene)methyl]furan-2-yl}benzenesulfonamide
- Biliverdin Ix Gamma Chromophore
- Ceftazidime Batsi
- STK004775
- AC1O07NV
- N,N-dimethyl-4-(4-phenyl-1H-pyrazol-3-yl)-1H-pyrrole-2-carboxamide
- D&C Red No. 28
- CHEMBL62836
- CHEMBL62492
- 2-benzenesulfonamido-5-methylbenzoic acid

Key Takeaways

- **Ability to have competitive and new insights in minutes.**
- Bridge between big data storage/data lake and analytic possibilities
- Helps you handle your growing data problems
- Make your data **actionable** by enabling: searching, data linking, harmonization and cataloguing