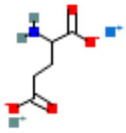
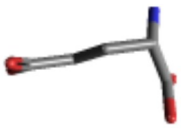
COMPOUND SUMMARY

Monosodium DL-glutamate

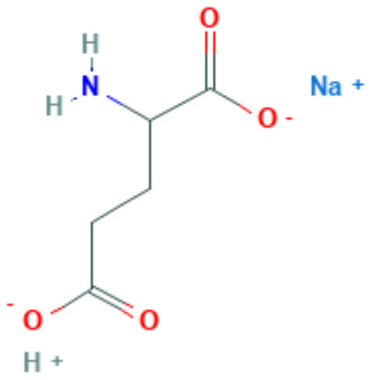
PubChem CID	21954795
Structure	 2D  3D
Molecular Formula	$C_5H_8NNaO_4$
Synonyms	Monosodium DL-glutamate LX3YQ006AP Glutamic acid, monosodium salt, DL- 32221-81-1 SCHEMBL1518007
Molecular Weight	169.11 g/mol *Computed by PubChem 2.1 (PubChem release 2021.05.07)*
Parent Compound	 CID 611 (DL-Glutamic acid)
Component Compounds	 CID 611 (DL-Glutamic acid) CID 5360545 (Sodium) CID 783 (Hydrogen)
Dates	Create: 2007-12-05 Modify: 2023-12-30

1 Structures

1.1 2D Structure

Structure Search | Get Image | Download Coordinates

Chemical Structure Depiction



PubChem

1.2 3D Conformer

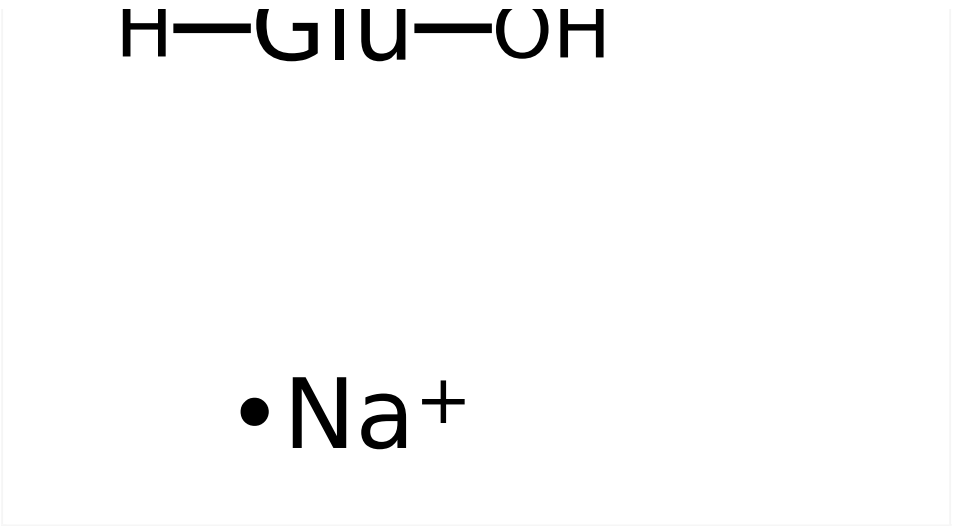
3D Conformer of Parent

UPDATING...

PubChem

2 Biologic Description

SVG Image



IUPAC Condensed	H-DL-Glu-OH.Na+
Sequence	E
IUPAC	DL-glutamic acid sodium salt

PubChem

3 Names and Identifiers

3.1 Computed Descriptors

3.1.1 IUPAC Name

sodium;2-aminopentanedioate;hydron

Computed by LexiChem 2.6.6 (PubChem release 2019.06.18)

PubChem

3.1.2 InChI

InChI=1S/C5H9NO4.Na/c6-3(5(9)10)1-2-4(7)8;/h3H,1-2,6H2,(H,7,8)(H,9,10);/q;+1/p-1

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

PubChem

3.1.3 InChIKey

LPUQAYUQRXPFSQ-UHFFFAOYSA-M

Computed by InChI 1.0.5 (PubChem release 2019.06.18)

PubChem

3.1.4 Canonical SMILES

[H+].C(CC(=O)[O-])C(C(=O)[O-])N.[Na+]

Computed by OEChem 2.1.5 (PubChem release 2019.06.18)

- PubChem

3.2 Molecular Formula

$C_5H_8NNaO_4$

Computed by PubChem 2.1 (PubChem release 2019.06.18)

- PubChem

3.3 Other Identifiers

3.3.1 CAS

32221-81-1

- European Chemicals Agency (ECHA); FDA Global Substance Registration System (GSRS)

3.3.2 European Community (EC) Number

608-719-7

- European Chemicals Agency (ECHA)

3.3.3 UNII

LX3YQ006AP

- FDA Global Substance Registration System (GSRS)

3.3.4 RXCUI

2049260

- NLM RxNorm Terminology

3.4 Synonyms

3.4.1 Depositor-Supplied Synonyms

Monosodium DL-glutamate
LX3YQ006AP
Glutamic acid, monosodium salt, DL-
32221-81-1
SCHEMBL1518007

▸ PubChem

4 Chemical and Physical Properties

4.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	169.11 g/mol	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Hydrogen Bond Donor Count	2	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Hydrogen Bond Acceptor Count	5	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Rotatable Bond Count	2	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Exact Mass	169.03510202 g/mol	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Monoisotopic Mass	169.03510202 g/mol	Computed by PubChem 2.1 (PubChem release 2021.05.07)
Topological Polar Surface Area	106Å^2	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Heavy Atom Count	11	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	134	Computed by Cactvs 3.4.6.11 (PubChem release 2019.06.18)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem