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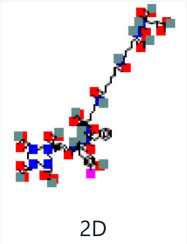
PubChem®

COMPOUND

Zadavotide guraxetan

Cite Download

PubChem CID	156596528
Structure	 2D
Molecular Formula	$C_{63}H_{92}IN_{11}O_{23}$
Synonyms	zadavotide guraxetan 45YI5BAE6Z RefChem:934478 PSMA inhibitor for imaging and therapy 2192281-54-0 View More...
Molecular Weight	1498.4 g/mol *Computed by PubChem 2.2 (PubChem release 2025.09.15)*
Dates	Create: 2021-09-16 Modify: 2026-08-08
Description	a DOTAGA-chelated urea-based PSMA inhibitor ▸ Medical Subject Headings (MeSH)

Patent Owner Exhibit 2141
IPR2025-01582

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2 Names and Identifiers
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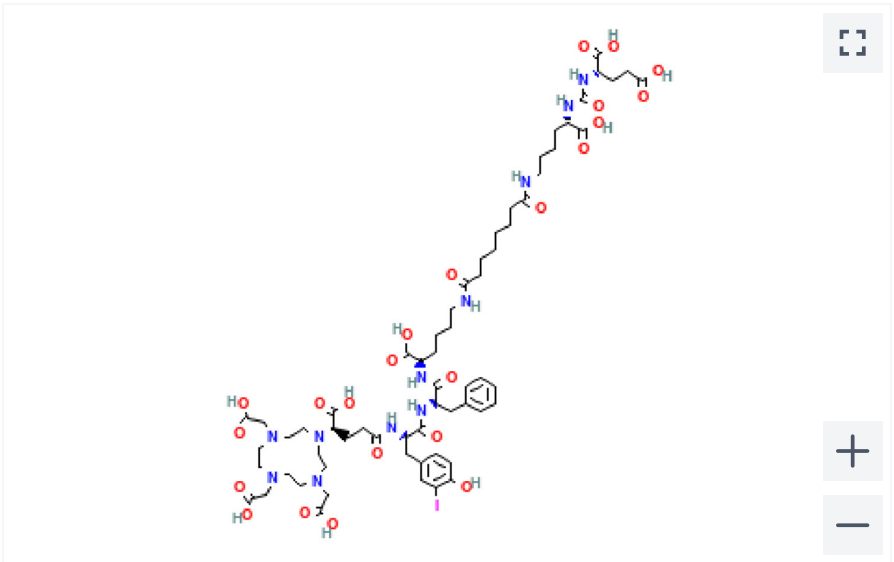
1 Structures

1.1 2D Structure

Chemical Structure Depiction



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1.2 3D Status

Conformer generation is disallowed since too many atoms, too flexible

PubChem

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

(2*S*)-2-[[(1*S*)-1-carboxy-5-[[8-[[(5*R*)-5-carboxy-5-[[(2*R*)-2-[[(2*R*)-2-[[(4*R*)-4-carboxy-4-[4,7,10-tris(carboxymethyl)-1,4,7,10-tetrazacyclododec-1-yl]butanoyl]amino]-3-(4-hydroxy-3-iodophenyl)propanoyl]amino]-3-phenylpropanoyl]amino]pentyl]amino]-8-oxooctanoyl]amino]pentyl]carbamoylamino]pentanedioic acid

Computed by Lexichem TK 2.9.3 (PubChem release 2025.09.15)

PubChem

2.1.2 InChI

InChI=1S/C63H92IN11O23/c64-42-34-41(18-21-49(42)76)36-46(67-52(79)22-20-48(62(96)97)75-32-30-73(38-55(84)85)28-26-72(37-54(82)83)27-29-74(31-33-75)39-56(86)87)57(88)69-47(35-40-12-4-3-5-13-40)58(89)68-43(59(90)91)14-8-10-24-65-50(77)16-6-1-2-7-17-51(78)66-25-11-9-15-44(60(92)93)70-63(98)71-45(61(94)95)19-23-53(80)81/h3-5,12-13,18,21,34,43-48,76H,1-2,6-11,14-17,19-20,22-33,35-39H2,(H,65,77)(H,66,78)(H,67,79)(H,68,89)(H,69,88)(H,80,81)(H,82,83)(H,84,85)(H,86,87)(H,90,91)(H,92,93)(H,94,95)(H,96,97)(H2,70,71,98)/t43-,44+,45+,46-,47-,48-/m1/s1

Computed by InChI 1.07.4 (PubChem release 2025.09.15)

PubChem

2.1.3 InChIKey

HPLNQICCRXHOIA-CIYKLJAQSA-N

Computed by InChI 1.07.4 (PubChem release 2025.09.15)

PubChem

2.1.4 SMILES

C1CN(CCN(CCN(CCN1CC(=O)O)CC(=O)O)[C@H](CCC(=O)N[C@H](CC2=CC(=C(C=C2)O)I)C(=O)N[C@H](CC3=CC=CC=C3)C(=O)N[C@H](CCCCNC(=O)CCCCCCC(=O)NCCCC[C@@H](C(=O)O)NC(=O)N[C@@H](CCC(=O)O)C(=O)O)C(=O)O)C(=O)O)CC(=O)O

Computed by OEChem 4.2.0 (PubChem release 2025.09.15)

PubChem

2.2 Molecular Formula

$C_{63}H_{92}IN_{11}O_{23}$

Computed by PubChem 2.2 (PubChem release 2025.09.15)

PubChem

2.3 Other Identifiers

2.3.1 CAS

2192281-54-0

FDA Global Substance Registration System (GSRS)

2.3.2 UNII

45YI5BAE6Z

FDA Global Substance Registration System (GSRS)

2.4 Synonyms

2.4.1 MeSH Entry Terms

PSMA I&T
PSMA inhibitor for imaging and therapy

Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

zadavotide guraxetan	SCHEMBL23862416
45YI5BAE6Z	EX-A5972A
RefChem:934478	EX-A7149
PSMA inhibitor for imaging and therapy	T207302
2192281-54-0	

PSMA I&T
2647371-60-4
PSMA-I&T
R-PSMA I&T
orb3027880

PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	1498.4 g/mol	Computed by PubChem 2.2 (PubChem release 2025.09.15)
XLogP3-AA	-7.7	Computed by XLogP3 3.0 (PubChem release 2025.09.15)
Hydrogen Bond Donor Count	16	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Hydrogen Bond Acceptor Count	27	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Rotatable Bond Count	45	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Exact Mass	1497.54123 Da	Computed by PubChem 2.2 (PubChem release 2025.09.15)
Monoisotopic Mass	1497.54123 Da	Computed by PubChem 2.2 (PubChem release 2025.09.15)
Topological Polar Surface Area	518 Å^2	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Heavy Atom Count	98	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	2590	Computed by Cactvs 3.4.8.24 (PubChem release 2025.09.15)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	6	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 2025.09.15)

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4 Related Records

4.1 Related Compounds with Annotation

Follow these links to do a live 2D search or do a live 3D search for this compound, sorted by annotation score. This section is deprecated (see the neighbor discontinuation help page for details), but these live search links provide equivalent functionality to the table that was previously shown here.

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4.2 Related Compounds

Same Connectivity Count	7
Same Parent, Connectivity Count	14
Same Parent, Exact Count	6
Mixtures, Components, and Neutralized Forms Count	5
Similar Compounds (2D)	View in PubChem Search
Similar Conformers (3D)	View in PubChem Search

PubChem

4.3 Substances

4.3.1 PubChem Reference Collection SID

516580386

PubChem

4.3.2 Related Substances

All Count	18
Same Count	10
Mixture Count	8

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4.3.3 Substances by Category

PubChem

5 Chemical Vendors

- PubChem

6 Drug and Medication Information

6.1 Clinical Trials

6.1.1 ClinicalTrials.gov

- ClinicalTrials.gov

6.1.2 EU Clinical Trials Register

- EU Clinical Trials Register

7 Patents

7.1 Depositor-Supplied Patent Identifiers

- PubChem

Link to all deposited patent identifiers

- PubChem

7.2 WIPO PATENTSCOPE

Patents are available for this chemical structure:

https://patentscope.wipo.int/search/en/result.jsf?inchikey=HPLNQICCRXHOIA-CIYKLJAQSA-N

- PATENTSCOPE (WIPO)

7.3 Chemical Co-Occurrences in Patents

PubChem

7.4 Chemical-Disease Co-Occurrences in Patents

PubChem

7.5 Chemical-Gene Co-Occurrences in Patents

PubChem

7.6 Chemical-Organism Co-Occurrences in Patents

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8 Classification

8.1 MeSH Tree

Medical Subject Headings (MeSH)

9 Information Sources

Filter by Source

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1. ## ClinicalTrials.gov

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https://clinicaltrials.gov/

2. ## EU Clinical Trials Register

https://www.clinicaltrialsregister.eu/

3. ## FDA Global Substance Registration System (GSRS)

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ZADAVOTIDE GURAXETAN

https://gsrs.ncats.nih.gov/ginas/app/beta/substances/45YI5BAE6Z

4. ## Medical Subject Headings (MeSH)

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PSMA I&T

https://id.nlm.nih.gov/mesh/M000750170.html

MeSH Tree

https://www.nlm.nih.gov/mesh/meshhome.html

5. PubChem

https://pubchem.ncbi.nlm.nih.gov

6. ## PATENTSCOPE (WIPO)

SID 484694869

https://pubchem.ncbi.nlm.nih.gov/substance/484694869