

SUPPLEMENT

References:

National Center for Biotechnology Information. The PubChem Project. Available from: <https://pubchem.ncbi.nlm.nih.gov/> (accessed 24.03.23) [Reference 181]

Kim S, Chen J, Cheng T, et al. PubChem 2023 update. *Nucleic Acids Res.* 2023;51(D1):D1373–D1380. [doi:10.1093/nar/gkac956](https://doi.org/10.1093/nar/gkac956) [Reference 182]

S-1. Cefiderocol

Chemical name: Cefiderocol

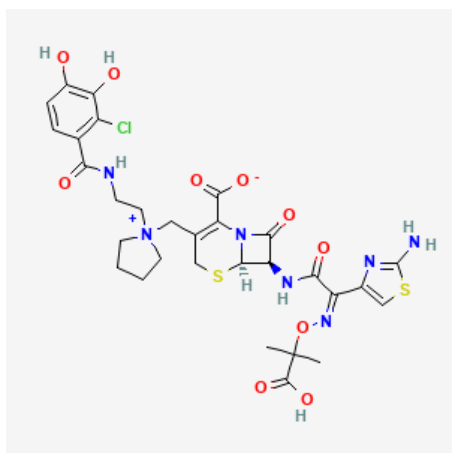
Pubchem CID: 77843966

Molecular formula: C₃₀H₃₄ClN₇O₁₀S₂

Molecular Weight: 752.2 g/mol

IUPAC Name: (6R,7R)-7-[[[(2Z)-2-(2-amino-1,3-thiazol-4-yl)-2-(2-carboxypropan-2-yl)oxyimino]acetyl]amino]-3-[[[1-[2-[(2-chloro-3,4-dihydroxybenzoyl)amino]ethyl]pyrrolidin-1-ium-1-yl]methyl]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylate

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/77843966> (accessed 24.03.23)

###

S-2. Imipenem-Cilastatin-Relebactam

Imipenem

Chemical name: Imipenem

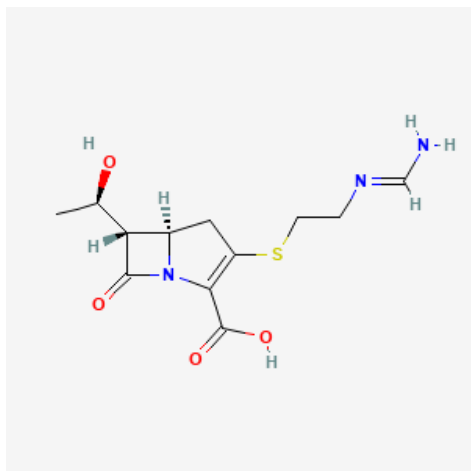
Pubchem CID: 104838

Molecular formula: C₁₂H₁₇N₃O₄S

Molecular Weight: 299.35g/mol

IUPAC Name: (5R,6S)-3-[2-(aminomethylideneamino)ethylsulfanyl]-6-[(1R)-1-hydroxyethyl]-7-oxo-1-azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/104838> (accessed 24.03.23)

Cilastatin

Chemical name: Cilastatin

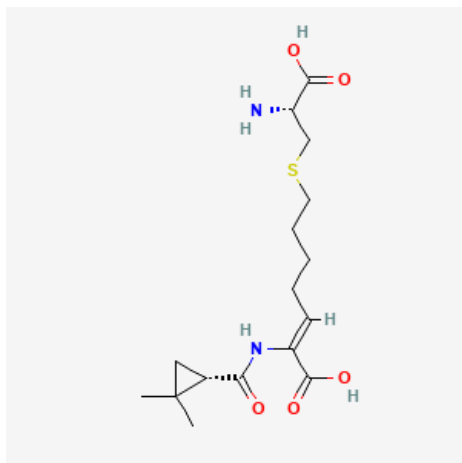
Pubchem CID: 6435415

Molecular formula: C₁₆H₂₆N₂O₅S

Molecular Weight: 358.5g/mol

IUPAC Name: (Z)-7-[(2R)-2-amino-2-carboxyethyl]sulfanyl-2-[[[(1S)-2,2-dimethylcyclopropanecarbonyl]amino]hept-2-enoic acid

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/6435415> (accessed 24.03.23)

Relebactam

Chemical name: Relebactam

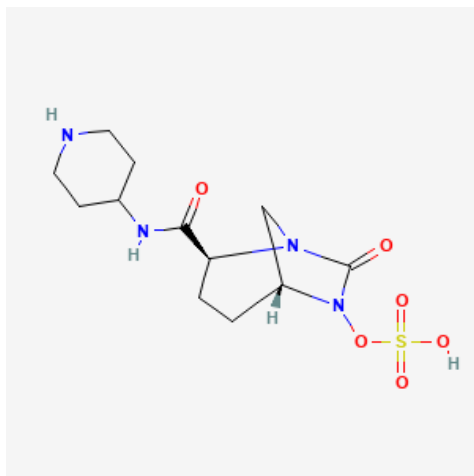
Pubchem CID: 44129647

Molecular formula: C₁₂H₂₀N₄O₆S

Molecular Weight: 348.38g/mol

IUPAC Name: [(2S,5R)-7-oxo-2-(piperidin-4-ylcarbamoyl)-1,6-diazabicyclo[3.2.1]octan-6-yl] hydrogen sulfate

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/44129647> (accessed 24.03.23)

###

S-3. Meropenem - Vaborbactam

Meropenem

Chemical name: Meropenem

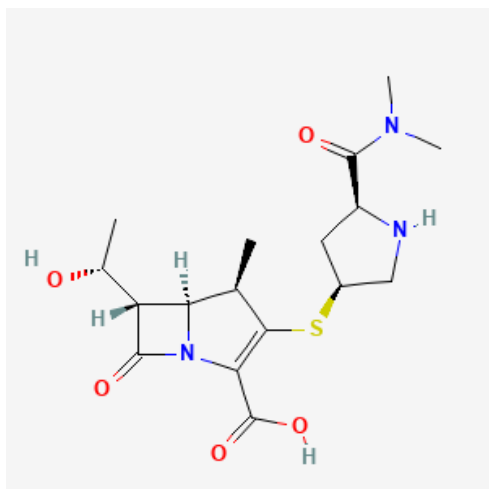
Pubchem CID: 441130

Molecular formula: C₁₇H₂₅N₃O₅S

Molecular Weight: 383.5g/mol

IUPAC Name: (4R,5S,6S)-3-[(3S,5S)-5-(dimethylcarbamoyl)pyrrolidin-3-yl]sulfanyl-6-[(1R)-1-hydroxyethyl]-4-methyl-7-oxo-1-azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/441130> (accessed 24.03.23)

Vaborbactam

Chemical name: Vaborbactam

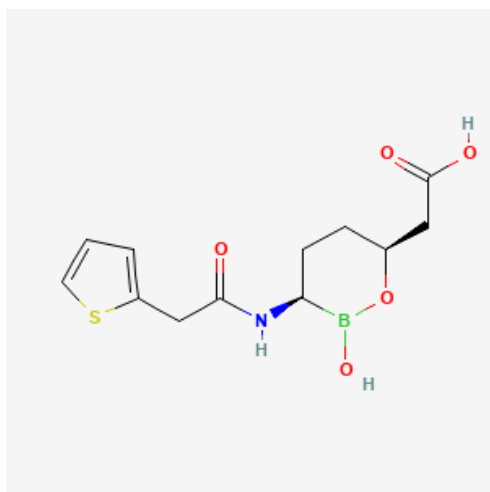
Pubchem CID: 56649692

Molecular formula: C₁₂H₁₆BNO₅S

Molecular Weight: 297.14g/mol

IUPAC Name: 2-[(3R,6S)-2-hydroxy-3-[(2-thiophen-2-ylacetyl)amino]oxaborinan-6-yl]acetic acid

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/56649692> (accessed 24.03.23)

###

S-4. Eravacycline

Chemical name: Eravacycline

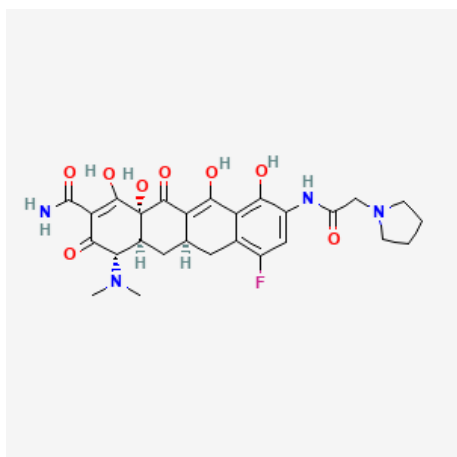
Pubchem CID: 54726192

Molecular formula: C₂₇H₃₁FN₄O₈

Molecular Weight: 558.6g/mol

IUPAC Name: (4S,4aS,5aR,12aR)-4-(dimethylamino)-7-fluoro-1,10,11,12a-tetrahydroxy-3,12-dioxo-9-[(2-pyrrolidin-1-ylacetyl)amino]-4a,5,5a,6-tetrahydro-4H-tetracene-2-carboxamide

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/56951485> (accessed 24.03.23)

###

S-5. Omadacycline

Chemical name: Omadacycline

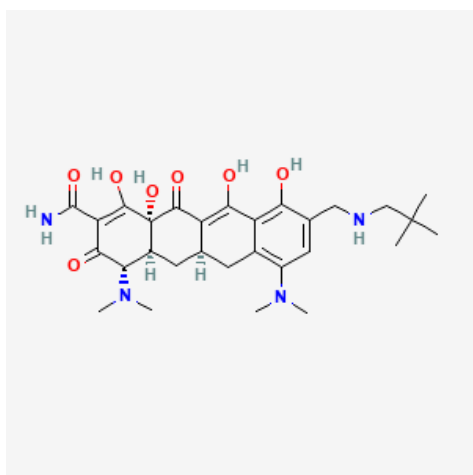
Pubchem CID: 54697325

Molecular formula: C₂₉H₄₀N₄O₇

Molecular Weight: 556.6g/mol

IUPAC Name: (4S,4aS,5aR,12aR)-4,7-bis(dimethylamino)-9-[(2,2-dimethylpropylamino)methyl]-1,10,11,12a-tetrahydroxy-3,12-dioxo-4a,5,5a,6-tetrahydro-4H-tetracene-2-carboxamide

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/54697325> (accessed 24.03.23)

###

S-6. Plazomicin

Chemical name: Plazomicin

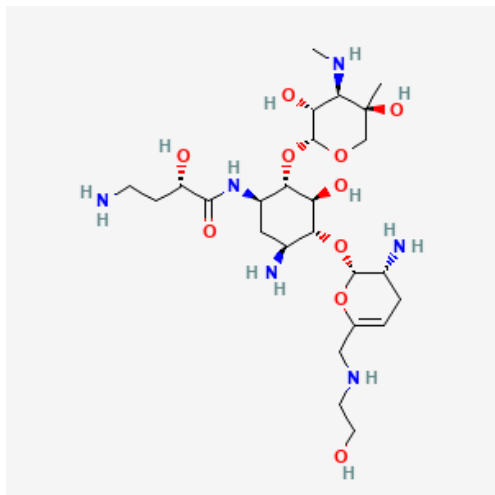
Pubchem CID: 42613186

Molecular formula: C₂₅H₄₈N₆O₁₀

Molecular Weight: 592.7g/mol

IUPAC Name: (2S)-4-amino-N-[(1R,2S,3S,4R,5S)-5-amino-4-[[[(2S,3R)-3-amino-6-[(2-hydroxyethylamino)methyl]-3,4-dihydro-2H-pyran-2-yl]oxy]-2-[(2R,3R,4R,5R)-3,5-dihydroxy-5-methyl-4-(methylamino)oxan-2-yl]oxy-3-hydroxycyclohexyl]-2-hydroxybutanamide

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/42613186> (accessed 24.03.23)

###

S-7. Aztreonam - Avibactam

Aztreonam

Chemical name: aztreonam

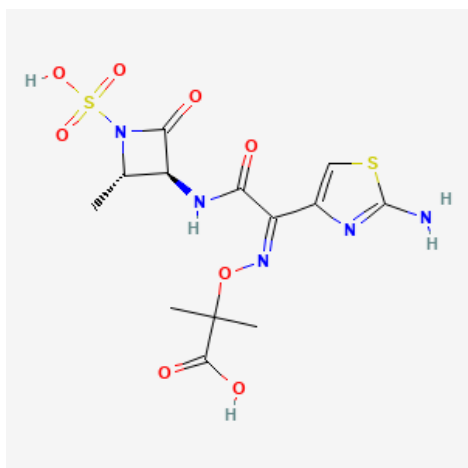
PubChem CID: 5742832

Molecular Formula: C₁₃H₁₇N₅O₈S₂

Molecular Weight: 435.4g/mol

IUPAC Name: 2-[(Z)-[1-(2-amino-1,3-thiazol-4-yl)-2-[[[(2S,3S)-2-methyl-4-oxo-1-sulfoazetidin-3-yl]amino]-2-oxoethylidene]amino]oxy-2-methylpropanoic acid

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/5742832> (accessed 24.03.23)

Avibactam

Chemical name: avibactam

PubChem CID: 9835049

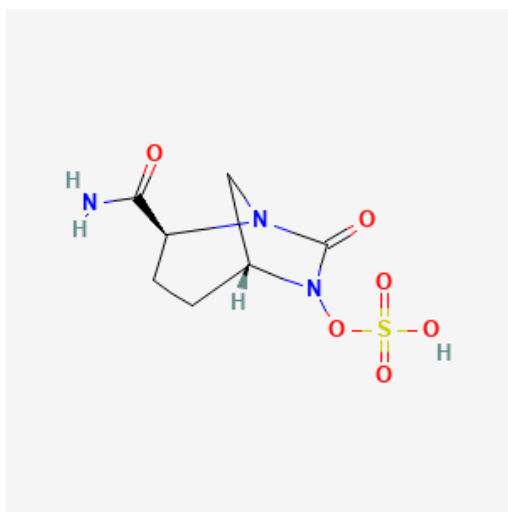
Molecular Formula: C₇H₁₁N₃O₆S

Molecular Weight: 265.25g/mol

IUPAC Name: [(2S,5R)-2-carbamoyl-7-oxo-1,6-diazabicyclo[3.2.1]octan-6-yl]

hydrogen sulfate

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/9835049> (accessed 24.03.23)

###

S-8. Cefepime - Enmetazobactam

S-9. Cefepime - Zidebactam

S.10. Cefepime - Taniborbactam

Cefepime

Chemical name: cefepime

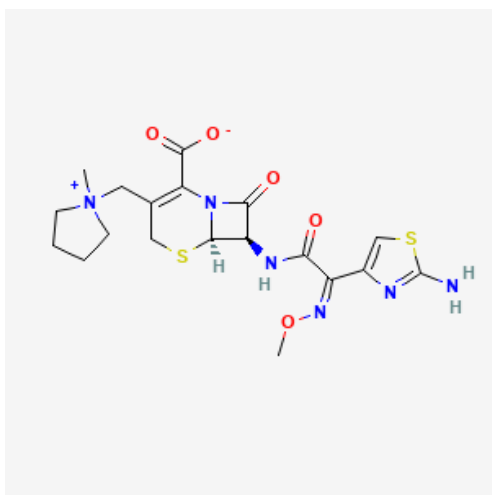
PubChem CID: 5479537

Molecular Formula: C₁₉H₂₄N₆O₅S₂

Molecular Weight: 480.6g/mol

IUPAC Name: (6R,7R)-7-[[[(2Z)-2-(2-amino-1,3-thiazol-4-yl)-2-methoxyiminoacetyl]amino]-3-[(1-methylpyrrolidin-1-ium-1-yl)methyl]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylate

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/5479537> (accessed 24.03.23)

Enmetazobactam

Chemical name: enmetazobactam

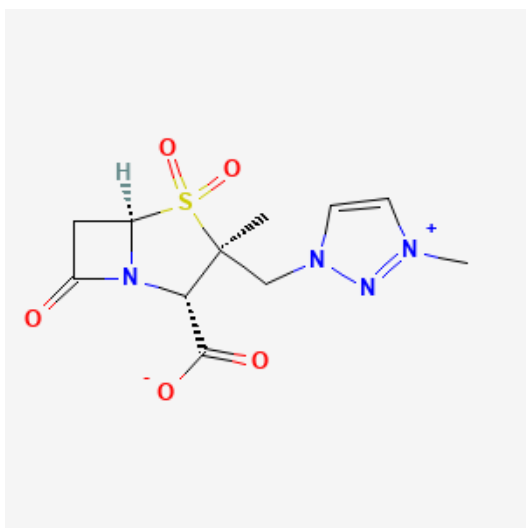
PubChem CID: 23653540

Molecular Formula: C₁₁H₁₄N₄O₅S

Molecular Weight: 314.32g/mol

IUPAC Name: (2S,3S,5R)-3-methyl-3-[(3-methyltriazol-3-ium-1-yl)methyl]-4,4,7-trioxo-4λ⁶-thia-1-azabicyclo[3.2.0]heptane-2-carboxylate

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/23653540> (accessed 24.03.23)

Zidebactam

Chemical name: zidebactam

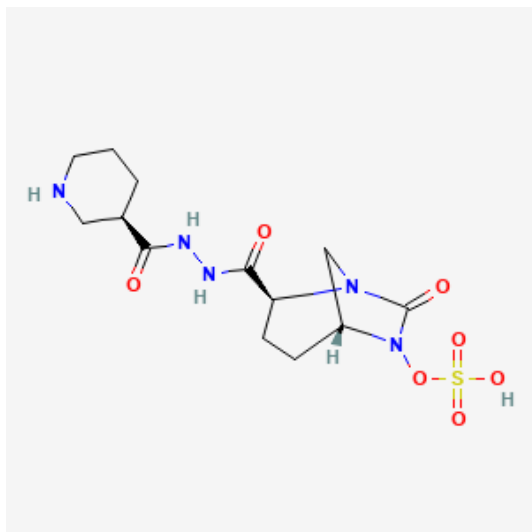
PubChem CID: 77846445

Molecular Formula: C₁₃H₂₁N₅O₇S

Molecular Weight: 391.4g/mol

IUPAC Name: [(2S,5R)-7-oxo-2-[[[(3R)-piperidine-3-carbonyl]amino]carbamoyl]-1,6-diazabicyclo[3.2.1]octan-6-yl] hydrogen sulfate

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/77846445> (accessed 24.03.23)

Taniborbactam

Chemical name: taniborbactam

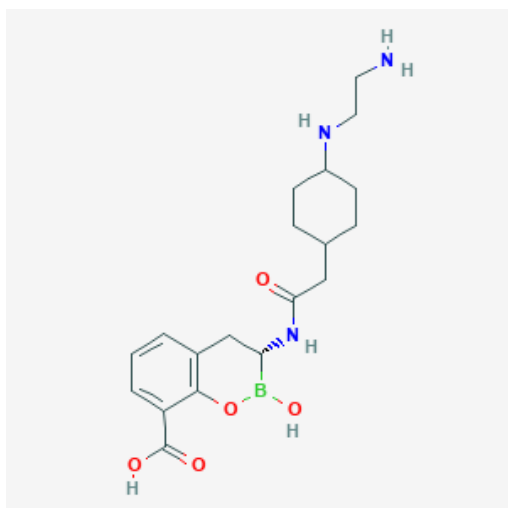
PubChem CID: 76902493

Molecular Formula: C₁₉H₂₈BN₃O₅

Molecular Weight: 389.3g/mol

IUPAC Name: (3R)-3-[[2-[4-(2-aminoethylamino)cyclohexyl]acetyl]amino]-2-hydroxy-3,4-dihydro-1,2-benzoxaborinine-8-carboxylic acid

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/76902493> (accessed 24.03.23)

###

S-11. Sulbactam - Durlobactam

Sulbactam

Chemical name: sulbactam

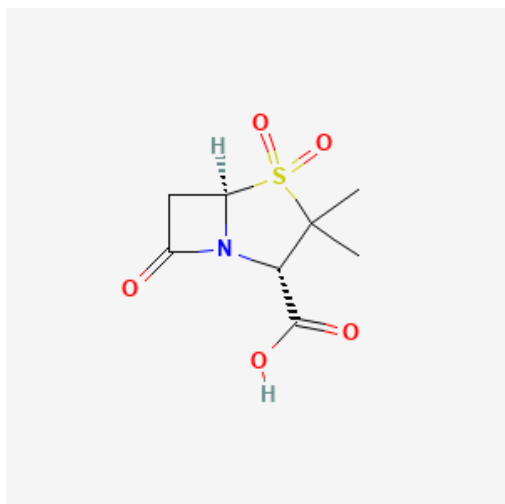
PubChem CID: 130313

Molecular Formula: C₈H₁₁NO₅S

Molecular Weight: 233.24g/mol

IUPAC Name: (2S,5R)-3,3-dimethyl-4,4,7-trioxo-4lambda6-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/130313> (accessed 24.03.23)

Durlobactam

Chemical name: durlobactam

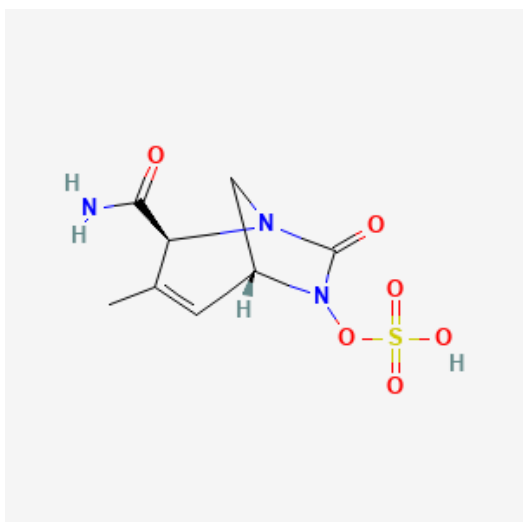
PubChem CID: 89851852

Molecular Formula: C₈H₁₁N₃O₆S

Molecular Weight: 277.26g/mol

IUPAC Name: [(2S,5R)-2-carbamoyl-3-methyl-7-oxo-1,6-diazabicyclo[3.2.1]oct-3-en-6-yl] hydrogen sulfate

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/89851852> (accessed 24.03.23)

###

S-12. Sulopenem

Chemical name: sulopenem

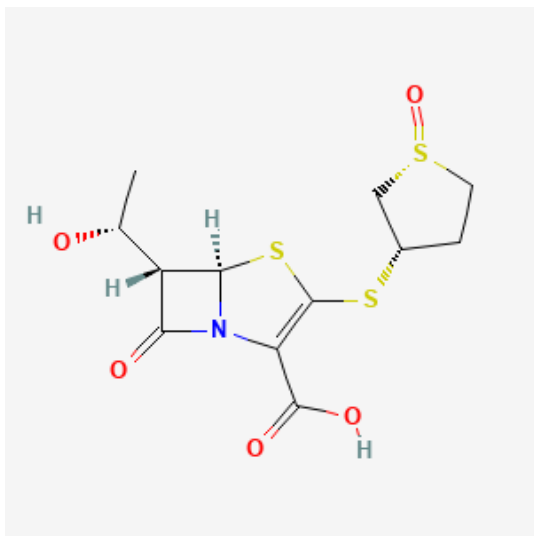
PubChem CID: 9950244

Molecular Formula: C₁₂H₁₅NO₅S₃

Molecular Weight: 349.5g/mol

IUPAC Name: (5R,6S)-6-[(1R)-1-hydroxyethyl]-7-oxo-3-[(1R,3S)-1-oxothiolan-3-yl]sulfanyl-4-thia-1-azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/9950244> (accessed 24.03.23)

###

S-13. Tebipenem

Chemical name: tebipenem

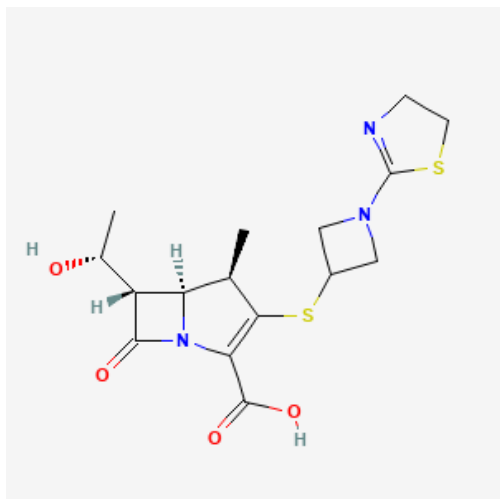
PubChem CID: 9800194

Molecular Formula: C₁₆H₂₁N₃O₄S₂

Molecular Weight: 383.5g/mol

IUPAC Name: (4R,5S,6S)-3-[1-(4,5-dihydro-1,3-thiazol-2-yl)azetidin-3-yl]sulfanyl-6-[(1R)-1-hydroxyethyl]-4-methyl-7-oxo-1-azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/9800194> (accessed 24.03.23)

###

S-14. Benapenem

Chemical name: benapenem

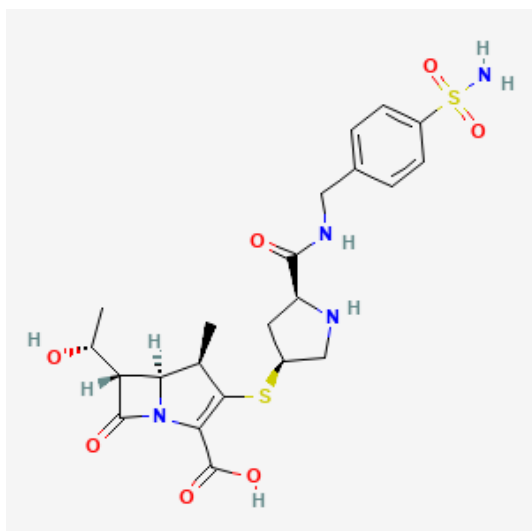
PubChem CID: 58326208

Molecular Formula: C₂₂H₂₈N₄O₇S₂

Molecular Weight: 524.6g/mol

IUPAC Name: (4R,5S,6S)-6-[(1R)-1-hydroxyethyl]-4-methyl-7-oxo-3-[(3S,5S)-5-[(4-sulfamoylphenyl)methylcarbamoyl]pyrrolidin-3-yl]sulfanyl-1-azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid

2D structure:



<https://pubchem.ncbi.nlm.nih.gov/compound/58326208> (accessed 24.03.23)