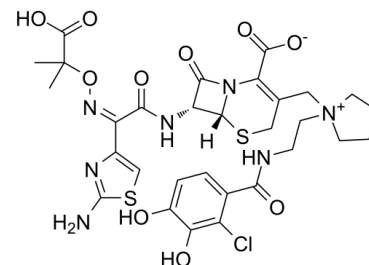


## Data Sheet

<b>Product Name:</b>	Cefiderocol
<b>Cat. No.:</b>	CS-0016784
<b>CAS No.:</b>	1225208-94-5
<b>Molecular Formula:</b>	C <sub>30</sub> H <sub>34</sub> ClN <sub>7</sub> O <sub>10</sub> S <sub>2</sub>
<b>Molecular Weight:</b>	752.21
<b>Target:</b>	Antibiotic; Bacterial
<b>Pathway:</b>	Anti-infection
<b>Solubility:</b>	Ethanol : < 1 mg/mL (ultrasonic;warming;heat to 60°C) (insoluble); DMSO : ≥ 125 mg/mL (166.18 mM); H <sub>2</sub> O : 1.06 mg/mL (1.41 mM; Need ultrasonic)



### BIOLOGICAL ACTIVITY:

Cefiderocol (S-649266) is a siderophore cephalosporin which has a potent activity against a broad range of aerobic Gram-negative bacterial species with MIC<sub>50</sub>s of 2 µg/mL or less. IC<sub>50</sub> & Target: MIC<sub>50</sub>: <2 µg/mL (Gram-negative bacteria)<sup>[1]</sup> **In Vitro:** Cefiderocol (S-649266), a novel parenteral siderophore cephalosporin conjugated with a catechol moiety, has a characteristic antibacterial spectrum with a potent activity against a broad range of aerobic Gram-negative bacterial species, including carbapenem-resistant strains of Enterobacteriaceae and nonfermenting bacteria such as *Pseudomonas aeruginosa* and *Acinetobacter baumannii*. Cefiderocol has affinity mainly for PBP3 of Enterobacteriaceae and nonfermenting bacteria similar to that of GR20263. A deficiency of the iron transporter PiuA in *P. aeruginosa* or both CirA and Fiu in *Escherichia coli* can cause 16-fold increases in cefiderocol MICs, suggesting that these iron transporters contribute to the permeation of cefiderocol across the outer membrane. The deficiency of OmpK35/36 in *Klebsiella pneumoniae* and the overproduction of efflux pump MexA-MexB-OprM in *P. aeruginosa* show no significant impact on the activity of cefiderocol<sup>[1]</sup>.

### PROTOCOL (Extracted from published papers and Only for reference)

**Cell Assay:** <sup>[1]</sup>For the determination of cefiderocol MIC, iron-depleted cation-adjusted Mueller-Hinton broth (ID-CAMHB) is prepared, except for the cases that are required to determine MICs under specific conditions. The quality control MIC ranges of **cefiderocol are 0.06 to 0.5 µg/mL for both E. coli ATCC 25922 and P. aeruginosa ATCC 27853**. For anaerobic bacteria, brucella agar supplemented with hemin, vitamin K1, and laked sheep blood is used<sup>[1]</sup>.

### References:

[1]. Ito A, et al. In Vitro Antibacterial Properties of Cefiderocol, a Novel Siderophore Cephalosporin, against Gram-Negative Bacteria. *Antimicrob Agents Chemother.* 2017 Dec 21;62(1).

### CAIndexNames:

Pyrrolidinium, 1-[[[(6R,7R)-7-[[[(2Z)-2-(2-amino-4-thiazolyl)-2-[(1-carboxy-1-methylethoxy)imino]acetyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]-1-[2-[(2-chloro-3,4-dihydroxybenzoyl)amino]ethyl]-], inner salt

### SMILES:

O=C(C(N12)=C(C[N+](C1)C(C2)C(C3)C(C4)=C(C5)C(O)=C4Cl)=O)CCCC3)CS[C@]2([H])[C@H](NC1(C5=CSC(N)=N5)=NOC(C)(C(O)=O)C)=O)C1=O][O-]

**Caution: Product has not been fully validated for medical applications. For research use only.**

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