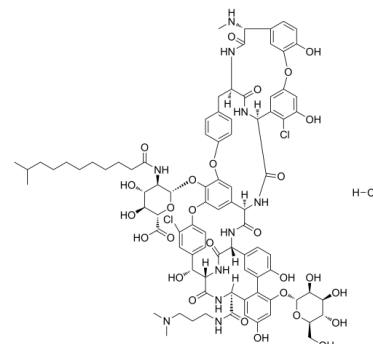


## Data Sheet

<b>Product Name:</b>	Dalbavancin (hydrochloride)
<b>Cat. No.:</b>	CS-3579
<b>CAS No.:</b>	2227366-51-8
<b>Molecular Formula:</b>	C <sub>88</sub> H <sub>101</sub> Cl <sub>3</sub> N <sub>10</sub> O <sub>28</sub>
<b>Molecular Weight:</b>	1853.15
<b>Target:</b>	Antibiotic; Bacterial
<b>Pathway:</b>	Anti-infection
<b>Solubility:</b>	DMSO : 250 mg/mL (134.91 mM; Need ultrasonic); H <sub>2</sub> O : 50 mg/mL (26.98 mM; Need ultrasonic)



### BIOLOGICAL ACTIVITY:

Dalbavancin hydrochloride (MDL-63397 hydrochloride) is a semisynthetic lipoglycopeptide antibiotic with potent bactericidal activity against **Gram-positive bacteria**. Dalbavancin hydrochloride inhibits **Staphylococcus aureus** and **Bacillus anthracis** with MIC<sub>90</sub>s of 0.06 µg/mL and 0.25 µg/mL, respectively<sup>[1][2]</sup>. **In Vitro:** Dalbavancin is a parenterally administered semisynthetic lipoglycopeptide developed to combat infections caused by resistant gram-positive pathogens. Dalbavancin exhibits potent in vitro bactericidal activity against gram-positive pathogens including *S. aureus* (MRSA), VISA, and non-VanA strains of VRE. Dalbavancin is developed for the treatment of complicated skin and skin structure infections (cSSSIs), predominantly those caused by MRSA and β-hemolytic streptococci, organisms against which it has shown greater potency than existing glycopeptide therapeutic agents<sup>[1][2]</sup>. **In Vivo:** Dalbavancin (15-240 mg/kg; intraperitoneal injection; every 36 h or 72 h; for 14 days; female BALB/c mice) treatment has a survival rate of 80% to 100% of mice with all dose regimens<sup>[1]</sup>.

### References:

- [1]. Heine HS, et al. Activity of dalbavancin against Bacillus anthracis in vitro and in a mouse inhalation anthrax model. *Antimicrob Agents Chemother.* 2010 Mar;54(3):991-6.
- [2]. Bennett JW, et al. Dalbavancin in the treatment of complicated skin and soft-tissue infections: a review. *Ther Clin Risk Manag.* 2008 Feb;4(1):31-40.

### CAIndexNames:

Ristomycin A aglycone, 5,31-dichloro-38-de(methoxycarbonyl)-7-demethyl-19-deoxy-56-O-[2-deoxy-2-[(10-methyl-1-oxoundecyl)amino]-β-D-glucopyranuronosyl]-38-[[[3-(dimethylamino)propyl]amino]carbonyl]-42-O-α-D-mannopyranosyl-N15-methyl- (hydrochloride)

### SMILES:

```
O[C@@H]([C@@H](O)[C@@H]1O)[C@H](O[C@@H]1CO)OC2=C(C3=CC([C@H](C4=O)([H])NC([C@@H](NC([C@H](NC5=O)([H])C6)=O)([H])C(C=C7OC(C=C8[C@H]5NC)=C(C=C8)O)=C(C(O)=C7)Cl)=O)([H])C9=CC%10=C(O[C@H](O[C@H](C(O)=O)[C@@H](O)[C@@H]11O)[C@@H]11NC(CCCCCCCC(C)C)=O)C(OC%12=CC=C6C=C%12)=C9)=O)=CC=C3O)C([C@@H](NC([C@H](N4)([H])[C@@H](C%13=CC=C(O%10)C)Cl)=C%13)O)=O)([H])C(NCCCN(C)C)=O)=CC(O)=C2.[H]Cl
```

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

Tel: 610-426-3128

Fax: 888-484-5008

E-mail: [sales@ChemScene.com](mailto:sales@ChemScene.com)

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA