Fig. S1. Iron coordination for vibriobactin and enterobactin.

Fig. S2. The predicted iron coordination of ferric-vulnibactin.



Fig. S1. Iron coordination for vibriobactin and enterobactin. A. The common viewpoint for chemical coordination of iron and vibriobactin. B. Our result demonstrated that one nitrogen atom BN3' from the second oxazoline ring instead of oxygen coordinated with iron. C. The chemical coordination of enterobactin and ferric atom. Six oxygen atoms of the catecholate are chemically coordinated with the iron.

Figure S2



Fig. S2. The predicted iron coordination of ferric-vulnibactin. Left represents the chemical structure of vulnibactin, and the right shows that vulnibactin has to use two different nitrogen atoms from the oxazoline ring to coordinate with the ferric atom, because it lacks two of the hydroxyl groups compared with vibriobactin.