

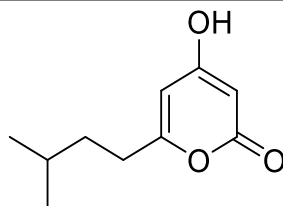
Supporting information

Secondary metabolites of actinomycetales as potent quorum sensing inhibitors targeting Gram-positive pathogens; *in vitro* and *in silico* study

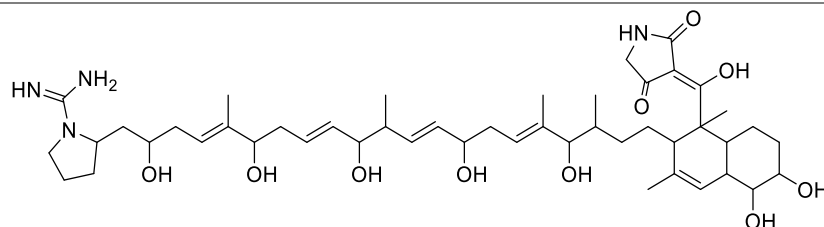
Said E. Desouky ^{1,2*}, Mohammed A Abu-Elghait ², Eman A. Fayed ³, Samy Selim ⁴, Basit Yousuf ¹, Yasuhiro Igarashi ⁵, Basel A. Abdel-Wahab ^{6,7}, Amnah Mohammed Alsuhaibani ⁸, Kenji Sonomoto ¹, Jiro Nakayama ¹

Table S1. Structures of the selected compounds.

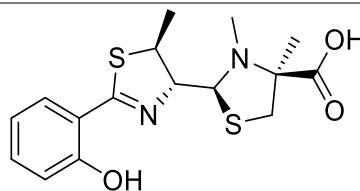
Fistupyrone



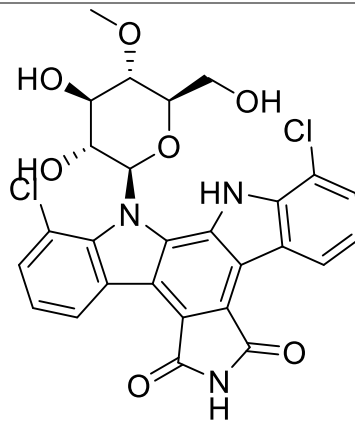
Lydicamycin



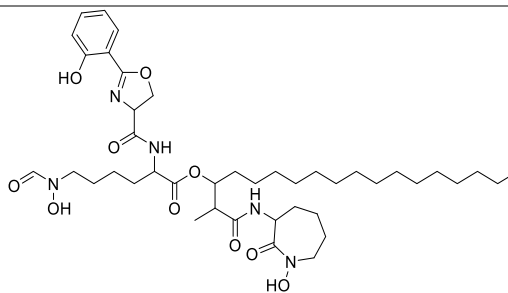
Watasemycin A



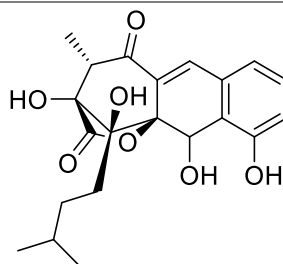
Rebeccamycin




Nocardimicin H



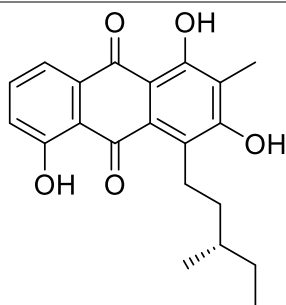
Rishirilide A



Lupinacidin C

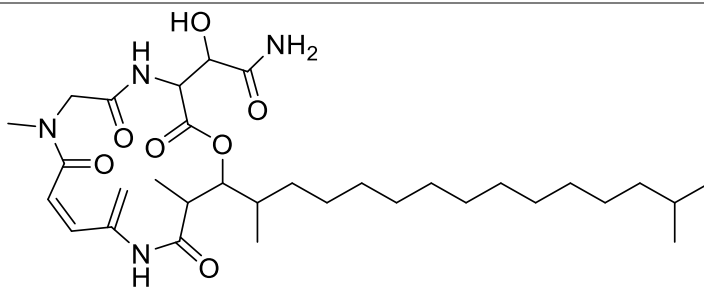


The chemical structure of Lupinacidin C is a dimeric naphthoquinone. It consists of two naphthoquinone units linked at their 2-positions. The left unit has a hydroxyl group at the 6-position. The right unit has hydroxyl groups at the 6 and 8 positions, a methyl group at the 7-position, and a 3-methylbutyl side chain at the 1-position. The 3-methylbutyl side chain is shown with a wedge bond to the chiral carbon, indicating its stereochemistry.

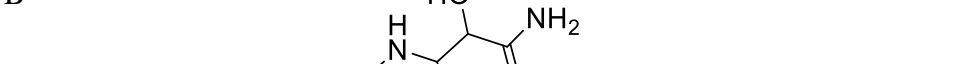
CC(C)CC[C@@H]1C=C2C(=C1)C(=O)C(=C2C3=CC=CC=C3C(=O)C4=CC=CC=C4O)O

Rakicidin A

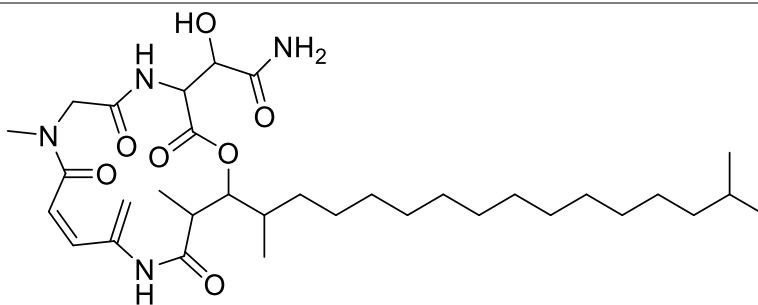
Chemical structure of Rakicidin A, a complex macrocyclic compound. The structure features a large 14-membered ring system containing multiple amide and ester linkages. A long, branched alkyl chain is attached to the ring, and a side chain with a hydroxyl group and an amide group is also present.



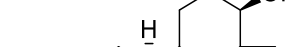
Rakicidin B



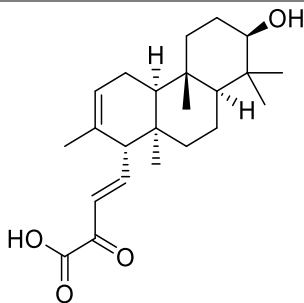
The chemical structure of Rakicidin B is a complex macrocyclic compound. It features a central 12-membered ring with a methyl group on one nitrogen atom. Attached to this ring are several side chains, including a long branched alkyl chain, a hydroxyl group, and an amide group. The structure is drawn in a skeletal format with explicit hydrogen atoms and lone pairs.




Phenalinolactone



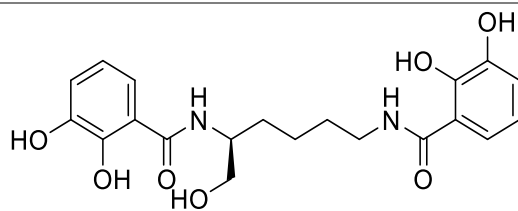
The chemical structure of Phenalinolactone is a complex polycyclic molecule. It features a phenanthrene-like core with a lactone ring fused to the C-10 and C-11 positions. The structure includes a methyl group at C-1, a hydroxyl group at C-13, and a carboxylic acid group at C-14. The stereochemistry is indicated by wedged and dashed bonds.



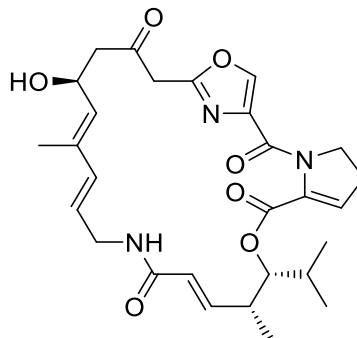
Myxochelinamide



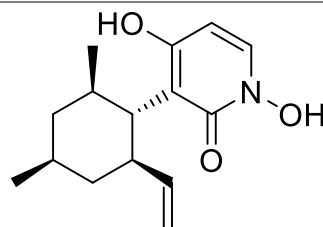
The chemical structure of Myxochelinamide is a symmetrical molecule. It features a central pentamethylene chain (-(CH₂)₅-) connecting two identical 2,4-dihydroxybenzoyl groups. Each benzoyl group is attached to the chain via an amide bond (-NH-CO-). The benzene rings are substituted with hydroxyl groups at the 2 and 4 positions. The stereochemistry at the chiral center of the amide linkage is indicated as (S) with a wedge bond to the hydrogen atom.

Oc1cc(O)cc(cc1C(=O)N[C@H](CCCCN[C@@H](C(=O)c2cc(O)cc(O)c2)C)C)C

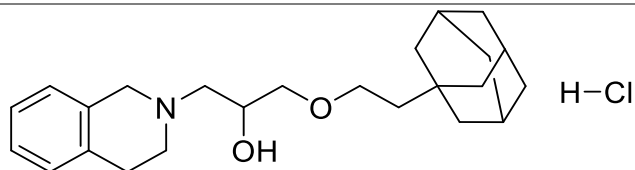
Pristinamycin IIA



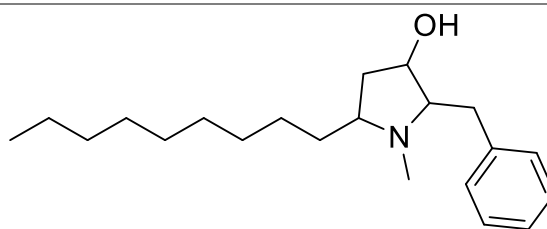
Pyridoxatin



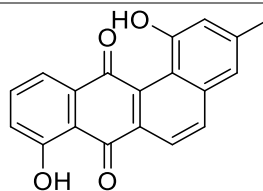
291-46



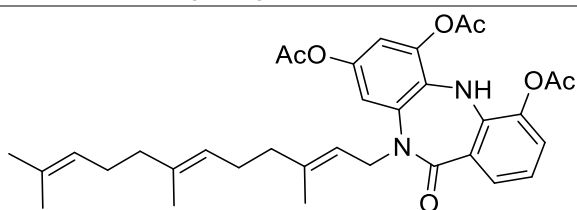
Preussin



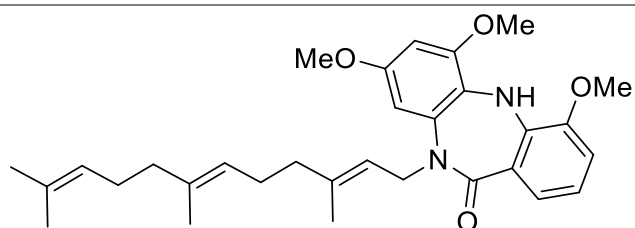
CHI15B
(Tetrangulol)



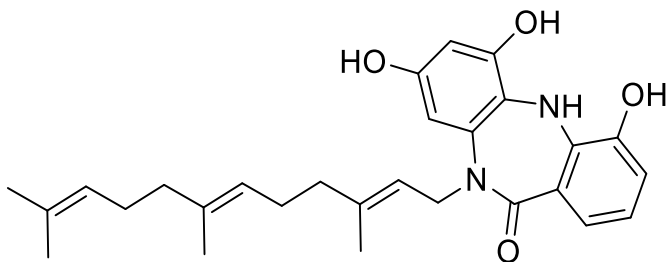
BU4664LAc



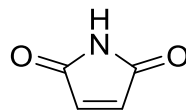
BU4664lMe



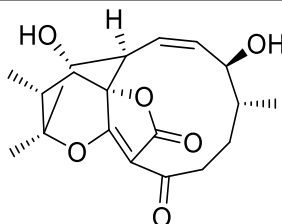
BU4664L



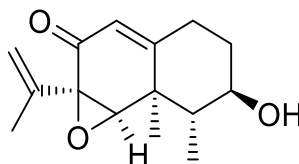
HF599 (maleimide)



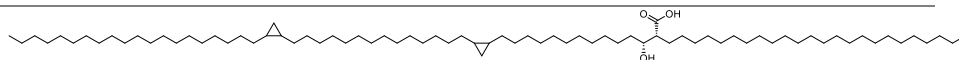
Abyssomicin I



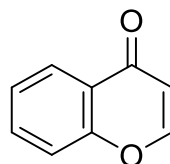
Sporogen AO-1



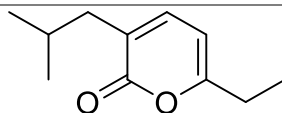
Mycolic acid



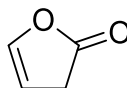
Chromone



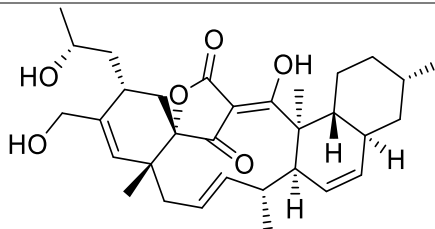
mucidone



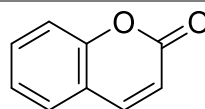
Furanone



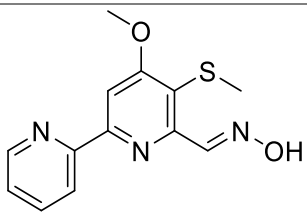
Maklamicin



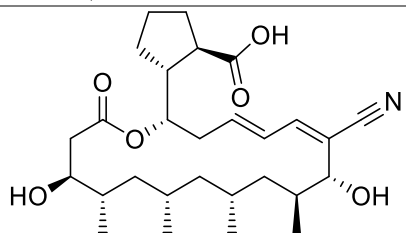
Coumarine



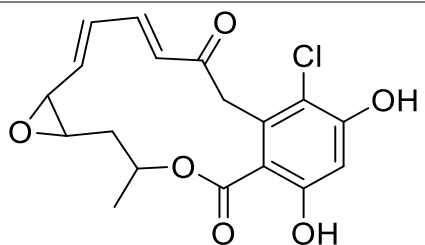
Collismycin



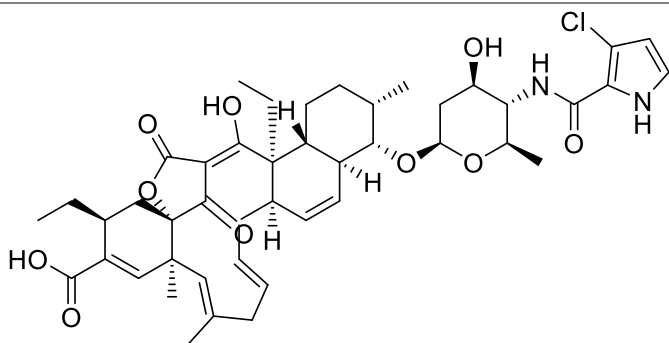
Borrelidin



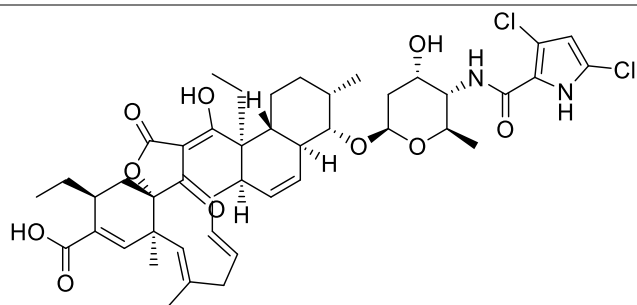
Radicicol



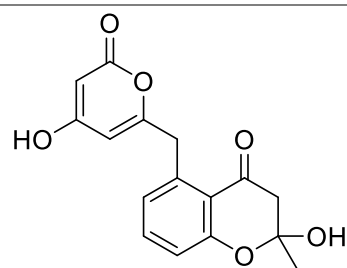
Decatromicin A



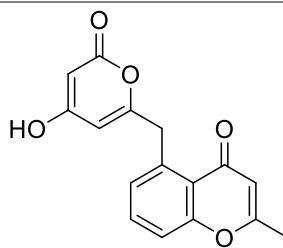
Decatromicin B



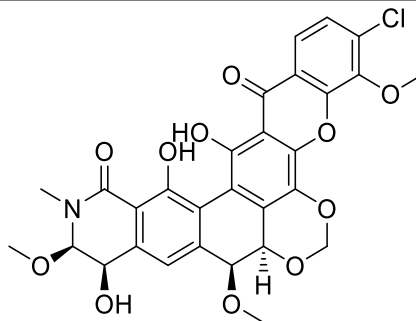
SEK34



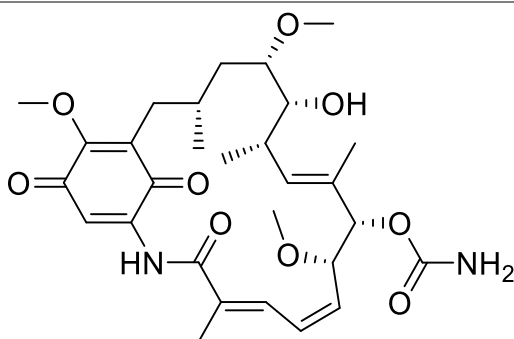
SEK34B



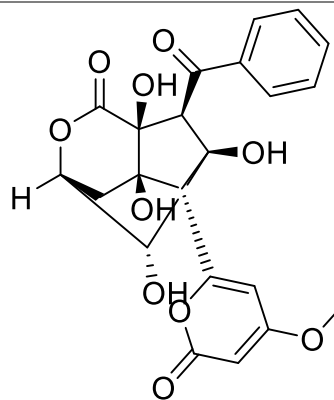
Lysolipin I



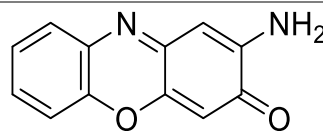
Geldanamycin



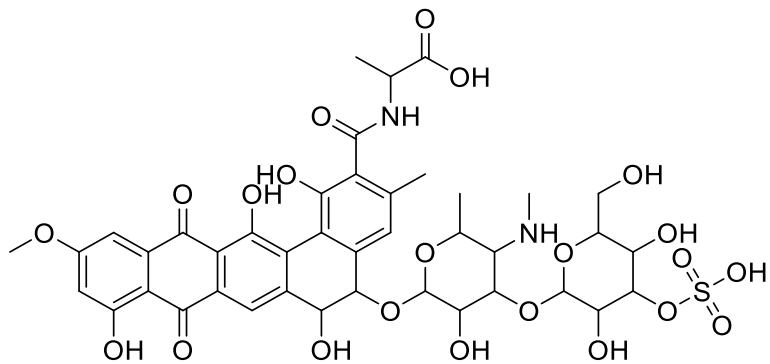
Enterocin



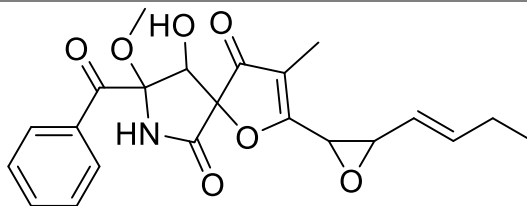
Questinomycin A



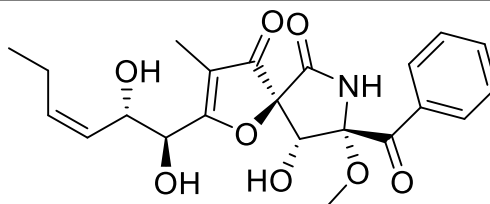
Pradimicin S



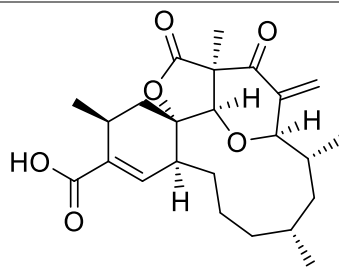
Synerazol



Pseurotin A



Okilactomycin



Leptomycin A

