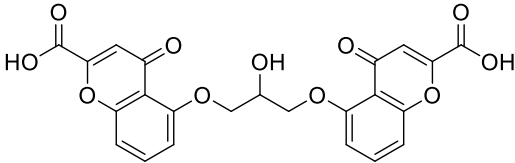
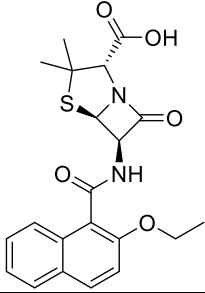
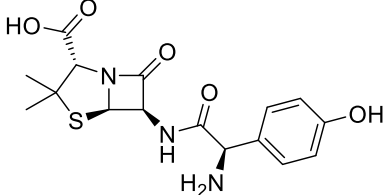
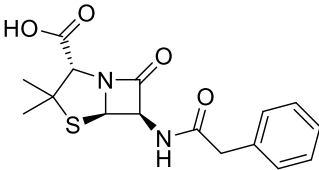
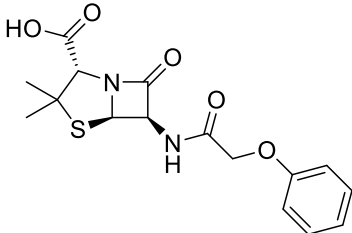


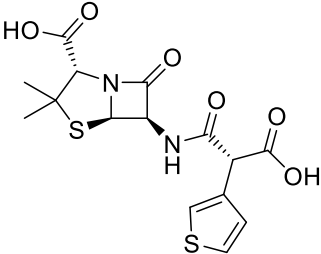
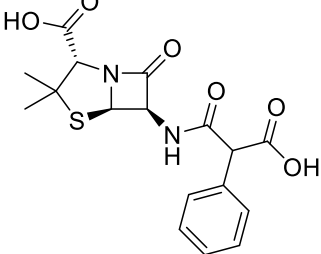
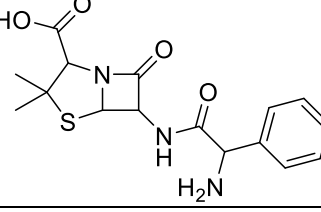
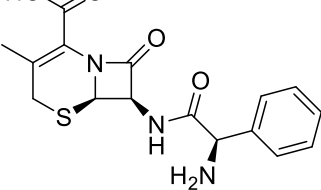
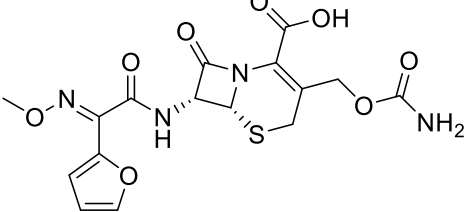
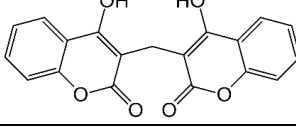
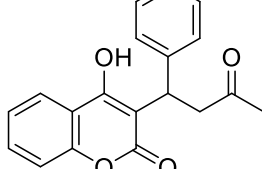
Supplementary Material

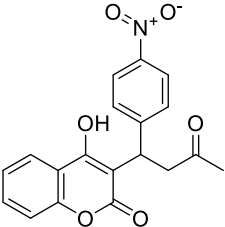
Scaffold Hopping of α -Rubromycin Enables Direct Access to the FDA-approved Cromoglicic acid as a SARS-CoV-2 M^{Pro} Inhibitor

Hani A. Alhadrami, Ahmed M. Sayed, Heba Alkhatabi, Nabil A. Alhakamy and Mostafa E. Rateb

Table S1. Results of ScafA similarity search in the FDA-approved drugs

Compound	Similarity Score	Structure	Class
Cromoglicic acid	0.84		Mast Cell stabilizer*
Nafcillin	0.3		β -Lactam antibiotic**
Amoxicillin	0.15		β -Lactam antibiotic**
Benzylpenicillin	0.11		β -Lactam antibiotic**
Phenoxymethylpenicillin	0.11		β -Lactam antibiotic**

Ticarcillin	0.11		β -Lactam antibiotic**
Carbenicillin	0.11		β -Lactam antibiotic**
Ampicillin	0.11		β -Lactam antibiotic**
Cefalexin	0.11		β -Lactam antibiotic**
Cefuroxime	0.11		β -Lactam antibiotic**
Dicoumarol	0.1		Anticoagulant [#]
Warfarin	0.1		Anticoagulant [#]

Acenocoumarol	0.1		Anticoagulant [#]
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*This is the most similar hit. In addition, it showed very low toxicity in vitro

** Frequent uncontrolled use of antibiotics can lead to the emergence of bacterial resistance [1].

[#]Anticoagulants are dangerous drugs with low therapeutic window [2].

References

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2. DUFF, I. F., & SHULL, W. H. (1949). Fatal Hemorrhage in Dicumarol® Poisoning. *Journal of the American Medical Association*, 139(12), 762-766.