

# PRODUCT INFORMATION



## Avoralstat

Item No. 35610

CAS Registry No.: 918407-35-9

Formal Name: 3-[2-[[[4-(aminoiminomethyl)phenyl]amino]carbonyl]-4-ethenyl-5-methoxyphenyl]-6-[[[(cyclopropylmethyl)amino]carbonyl]-2-pyridinecarboxylic acid

Synonym: BCX 4161

MF:  $C_{28}H_{27}N_5O_5$

FW: 513.6

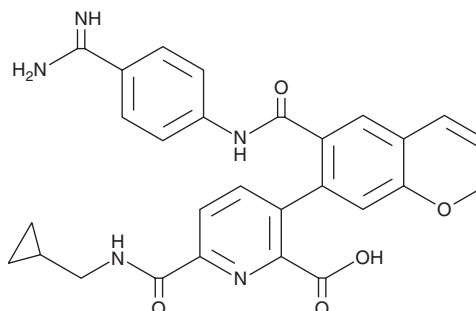
Purity:  $\geq 98\%$

UV/Vis.:  $\lambda_{max}$ : 218, 246, 286 nm

Supplied as: A solid

Storage:  $-20^\circ\text{C}$

Stability:  $\geq 4$  years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

## Laboratory Procedures

Avoralstat is supplied as a solid. A stock solution may be made by dissolving the avoralstat in the solvent of choice, which should be purged with an inert gas. Avoralstat is soluble in the organic solvent DMSO at a concentration of approximately 50 mg/ml.

## Description

Avoralstat is an inhibitor of kallikrein, a serine protease involved in the contact activation system.<sup>1</sup> It inhibits kallikrein activity in isolated human plasma ( $EC_{50}$ s = 1.14-11.1 nM). Avoralstat also inhibits transmembrane serine protease 2 (TMPRSS2;  $IC_{50}$  = 2.73 nM), a serine protease required for entry of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) into host cells.<sup>2,3</sup> It inhibits SARS-CoV-2 pseudovirus entry into Calu-3 2B4 cells ( $EC_{50}$  = 0.7  $\mu\text{M}$ ).<sup>2</sup> Avoralstat (30 mg/kg) reduces or prevents the accumulation of lung viral titers in mouse models of SARS-CoV-2 infection or prophylaxis, respectively, using Ad5-hACE2 mice that are sensitive to SARS-CoV-2 infection.

## References

1. Cornpropst, M., Collis, P., Collier, J., *et al.* Safety, pharmacokinetics, and pharmacodynamics of avoralstat, an oral plasma kallikrein inhibitor: Phase 1 study. *Allergy* **71**(12), 1676-1683 (2016).
2. Sun, Y.J., Velez, G., Parsons, D.E., *et al.* Structure-based phylogeny identifies avoralstat as a TMPRSS2 inhibitor that prevents SARS-CoV-2 infection in mice. *J. Clin. Invest.* **131**(10), e147973 (2021).
3. Hu, X., Shrimp, J.H., Guo, H., *et al.* Discovery of TMPRSS2 inhibitors from virtual screening as a potential treatment of COVID-19. *ACS Pharmacol. Transl. Sci.* **4**(3), 1124-1135 (2021).

### WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

### SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the [complete](#) Safety Data Sheet, which has been sent via email to your institution.

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