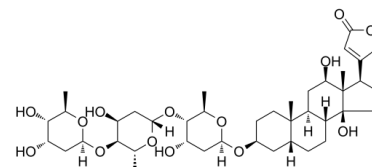


## Data Sheet

Product Name:	Digoxin
Cat. No.:	CS-4571
CAS No.:	20830-75-5
Molecular Formula:	C <sub>41</sub> H <sub>64</sub> O <sub>14</sub>
Molecular Weight:	780.94
Target:	Na <sup>+</sup> /K <sup>+</sup> ATPase
Pathway:	Membrane Transporter/Ion Channel
Solubility:	DMSO : ≥ 28 mg/mL (35.85 mM)



### BIOLOGICAL ACTIVITY:

Digoxin is a cardiac glycoside that blocks the **sodium-potassium ATPase**, as a potent inhibitor of chikungunya virus (CHIKV) infection. IC<sub>50</sub> & Target: Na<sup>+</sup>/K<sup>+</sup> ATPase<sup>[1]</sup> **In Vitro:** Digoxin, a sodium-potassium ATPase inhibitor, has a negative Z score of -26.67, suggesting a function for the sodium-potassium ATPase in CHIKV infection. Relative to DMSO-treated cells, treatment of U-2 OS cells with Digoxin results in a dose-dependent decrease in CHIKV infection with a half-maximal effective concentration (EC<sub>50</sub>) of 48.8 nM. Digoxin treatment similarly decreases CHIKV infection of primary human synovial fibroblasts (HSFs) and Vero African green monkey kidney cells with EC<sub>50</sub>s of 43.9 nM and 67.3 nM, respectively. Digoxin treatment significantly diminishes CHIKV infection in these cell types, with EC<sub>50</sub>s of 16.2 μM in ST2 cells and 23.2 μM in C2C12 cells, values 330 and 475 times the EC<sub>50</sub> of Digoxin in U-2 OS cells. Cell viability is only modestly impaired at 24 h posttreatment with 1 μM Digoxin, a dose 20 times the Digoxin EC<sub>50</sub> for CHIKV antiviral activity in these cells<sup>[1]</sup>.

### PROTOCOL (Extracted from published papers and Only for reference)

**Cell Assay:** Digoxin is dissolved in DMSO and then diluted with appropriate media<sup>[1]</sup>. U-2 OS cells seeded in 60-mm-diameter dishes are incubated with DMSO, 10 μM STS as an inducer of apoptosis, or increasing concentrations of Digoxin at 37°C for 6 h. Cells are washed with fluorescence-activated cell sorter (FACS) buffer (PBS with 2% FBS) and stained with PI. Cell staining is quantified using a BD LSRII flow cytometer and FlowJo software. Alternatively, U-2 OS cells seeded in 96-well plates are incubated with DMSO, STS, or increasing concentrations of Digoxin at 37°C for 6 or 24 h. PrestoBlue reagent is added to supernatants of compound-treated cells, and cells are incubated at 37°C for 30 min. Fluorescence as a surrogate for cell viability is quantified using a Synergy H1 plate reader<sup>[1]</sup>.

### References:

[1]. Ashbrook AW, et al. Antagonism of the Sodium-Potassium ATPase Impairs Chikungunya Virus Infection. MBio. 2016 May 24;7(3). pii: e00693-16.

### CAIndexNames:

Card-20(22)-enolide, 3-[(O-2,6-dideoxy-β-D-ribo-hexopyranosyl-(1→4)-O-2,6-dideoxy-β-D-ribo-hexopyranosyl-(1→4)-2,6-dideoxy-β-D-ribo-hexopyranosyl)oxy]-12,14-dihydroxy-, (3β,5β,12β)-

### SMILES:

O[C@]1([C@@]2(CC[C@@]1([H])[C@@]2(CC[C@H](O[C@@](O[C@H](C)[C@H]3O[C@@](O[C@H](C)[C@H]4O[C@@](O[C@H](C)[C@H]5O)([H])C[C@@H]5O)([H])C[C@@H]4O)([H])C[C@@H]3O)C1)C)([H])[C@]2([H])C[C@H]6O)(CC[C@H]7C(CO8)=CC8=O)[C@]67C

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

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