

## Supporting Information

### Semisynthetic blastidicin S ester derivatives show enhanced antibiotic activity

Cole Gannett,<sup>a,c</sup> Paige Banks,<sup>a</sup> Christina Chuong,<sup>b</sup> Emily Mevers,<sup>a,c,d</sup> James Weger-Lucarelli,<sup>b,c</sup>

Andrew N. Lowell<sup>a,c,d,\*</sup>

<sup>a</sup> Department of Chemistry, Virginia Polytechnic Institute and State University (Virginia Tech), Blacksburg, VA 24061, United States

<sup>b</sup> Department of Biomedical Sciences and Pathobiology, Virginia Tech, VA-MD Regional College of Veterinary Medicine, Blacksburg, VA 24061, USA

<sup>c</sup> Center for Emerging, Zoonotic, and Arthropod-borne Pathogens, Virginia Polytechnic Institute and State University (Virginia Tech), Blacksburg, VA 24061, United States

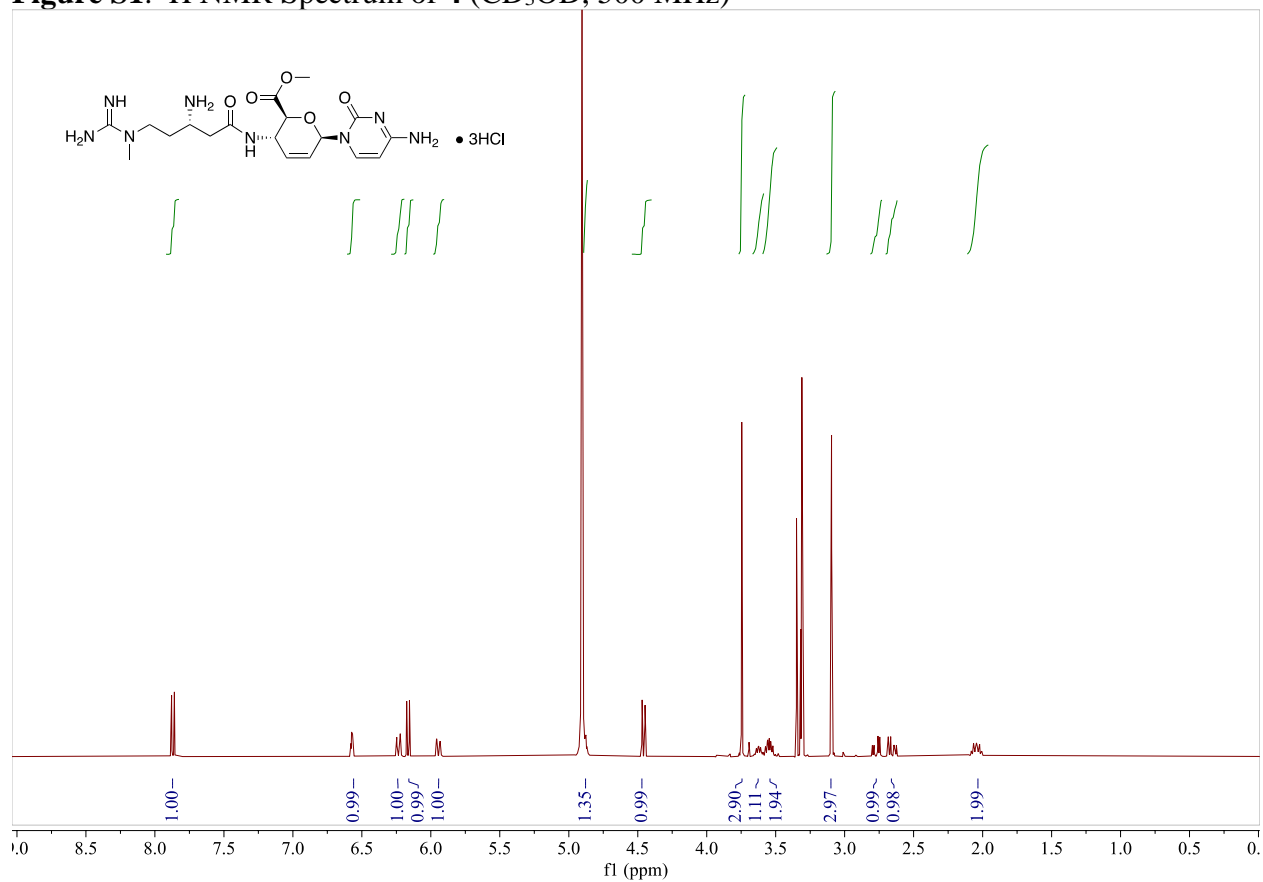
<sup>d</sup> Faculty of Health Sciences, Virginia Polytechnic Institute and State University (Virginia Tech), Blacksburg, VA 24061, United States

\*Corresponding author; email for A.N.L., [alowell@vt.edu](mailto:alowell@vt.edu)

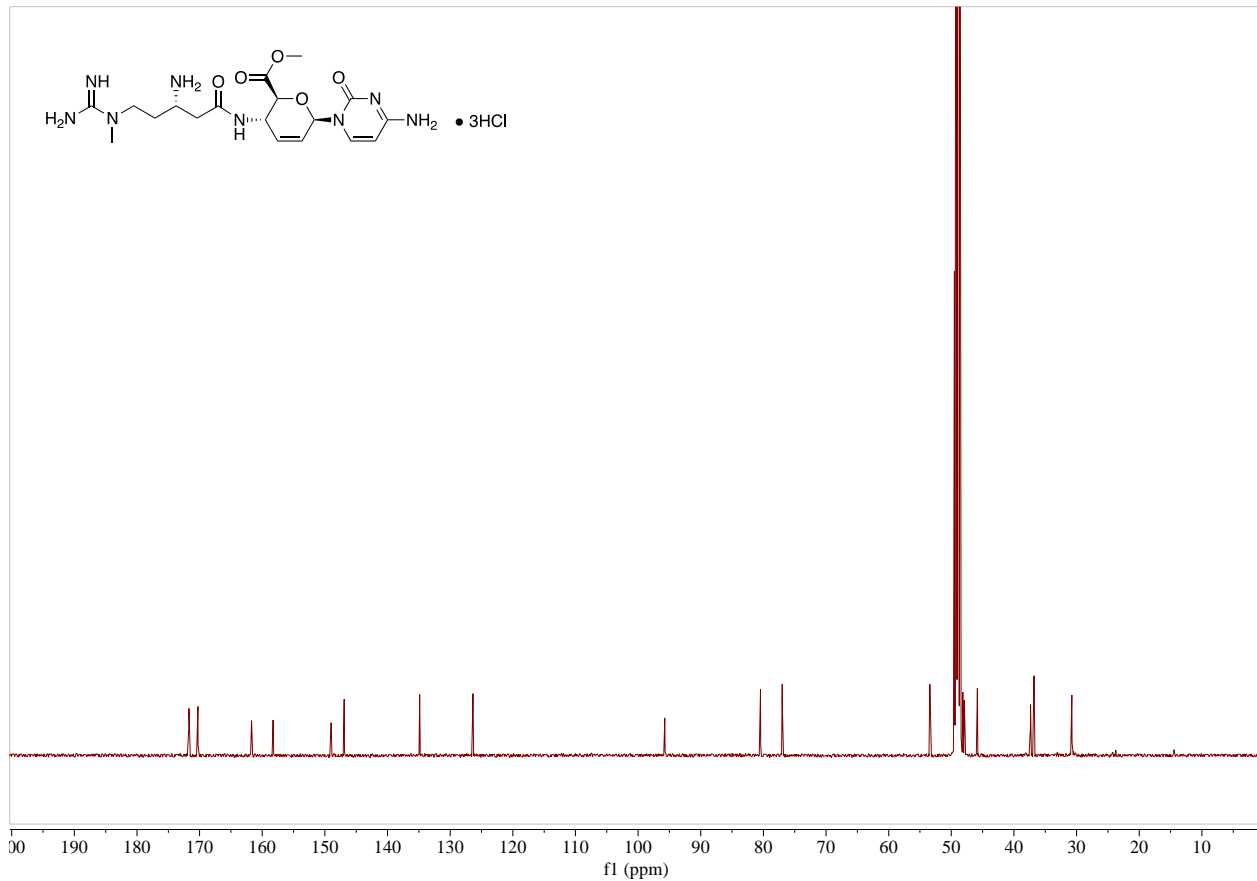
## Table of Contents

<sup>1</sup> H and <sup>13</sup> C NMR Spectra for Compounds <b>4-11</b> .....	S3
Media Recipes.....	S11
Bacterial Inhibition Curves Naming Key.....	S11
Bacterial Inhibition Curves.....	S12-S28

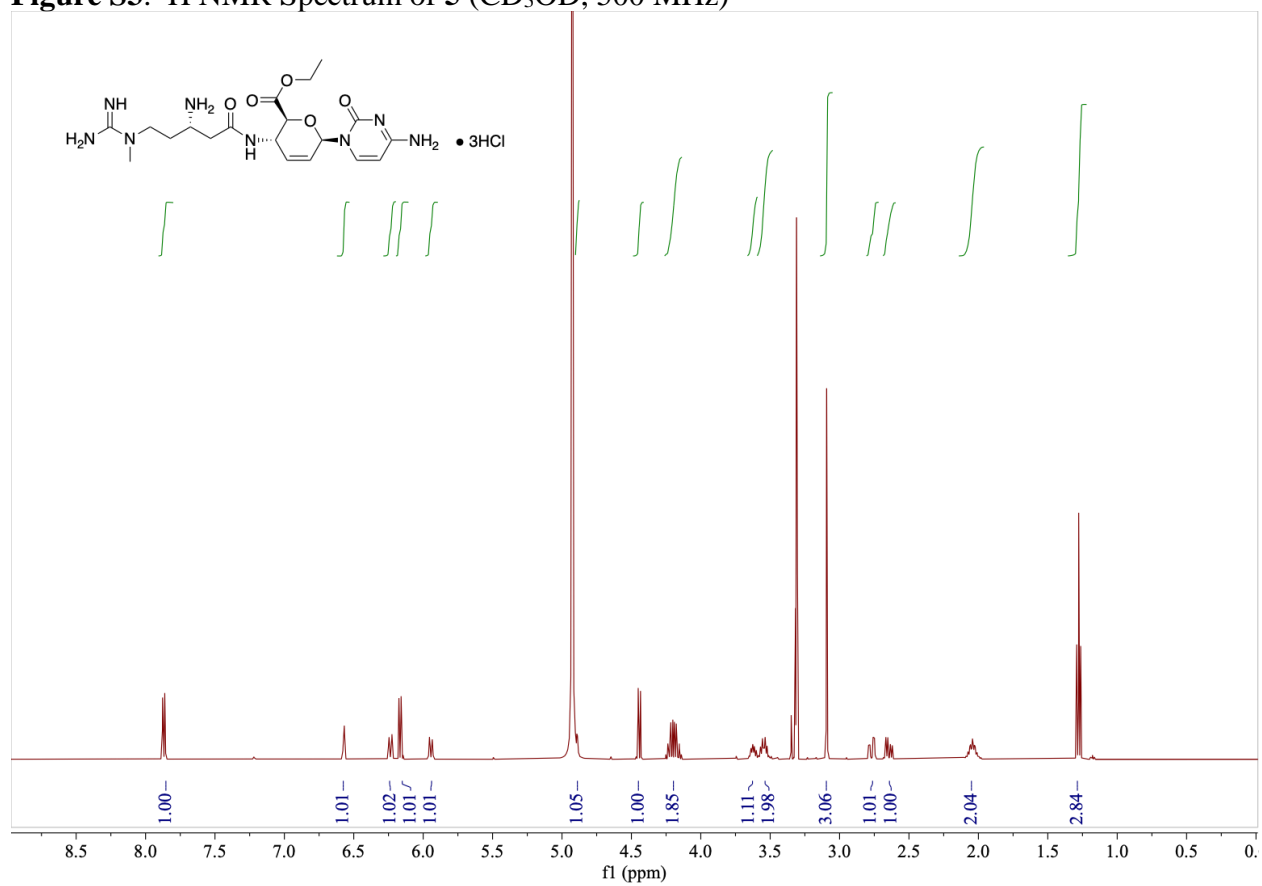
**Figure S1.**  $^1\text{H}$  NMR Spectrum of **4** ( $\text{CD}_3\text{OD}$ , 500 MHz)



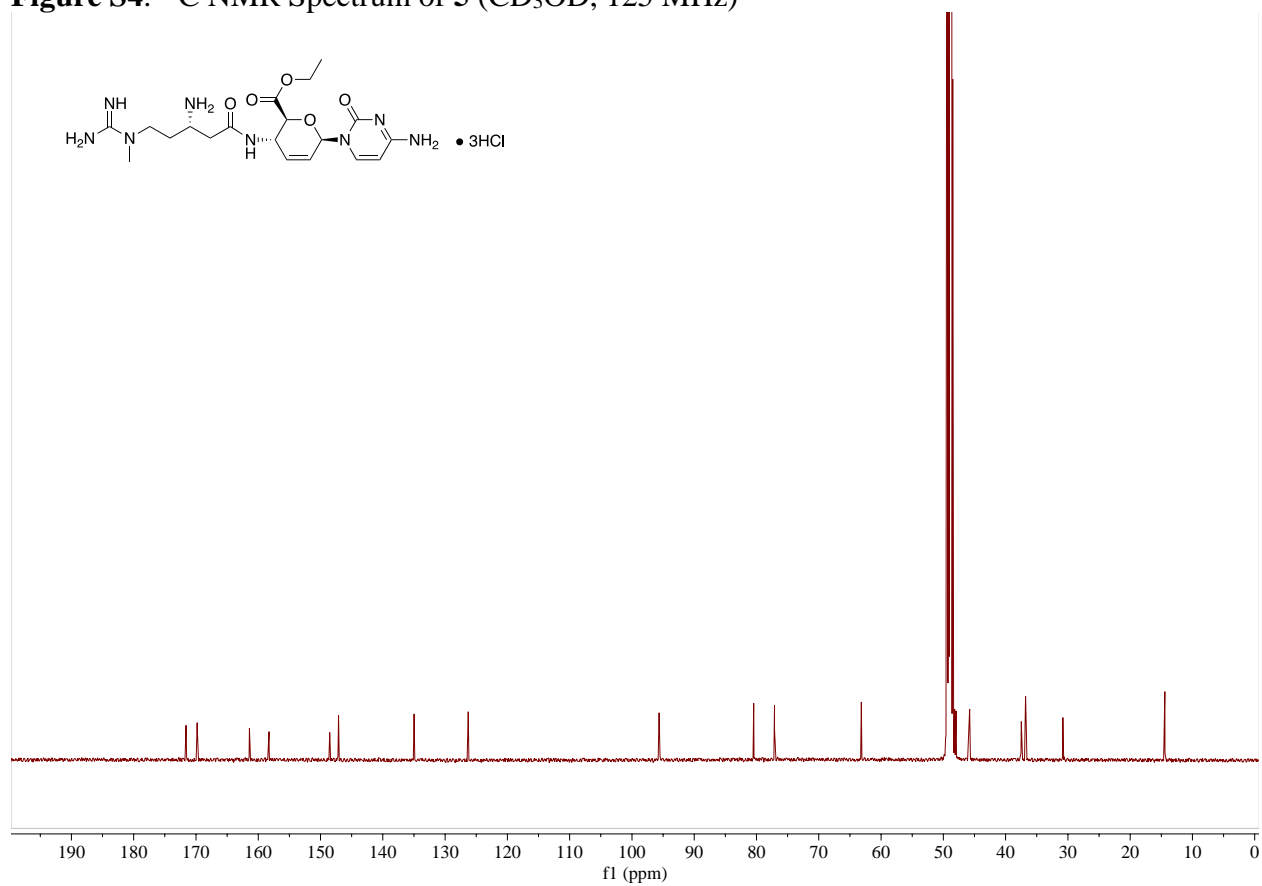
**Figure S2.**  $^{13}\text{C}$  NMR Spectrum of **4** ( $\text{CD}_3\text{OD}$ , 125 MHz)



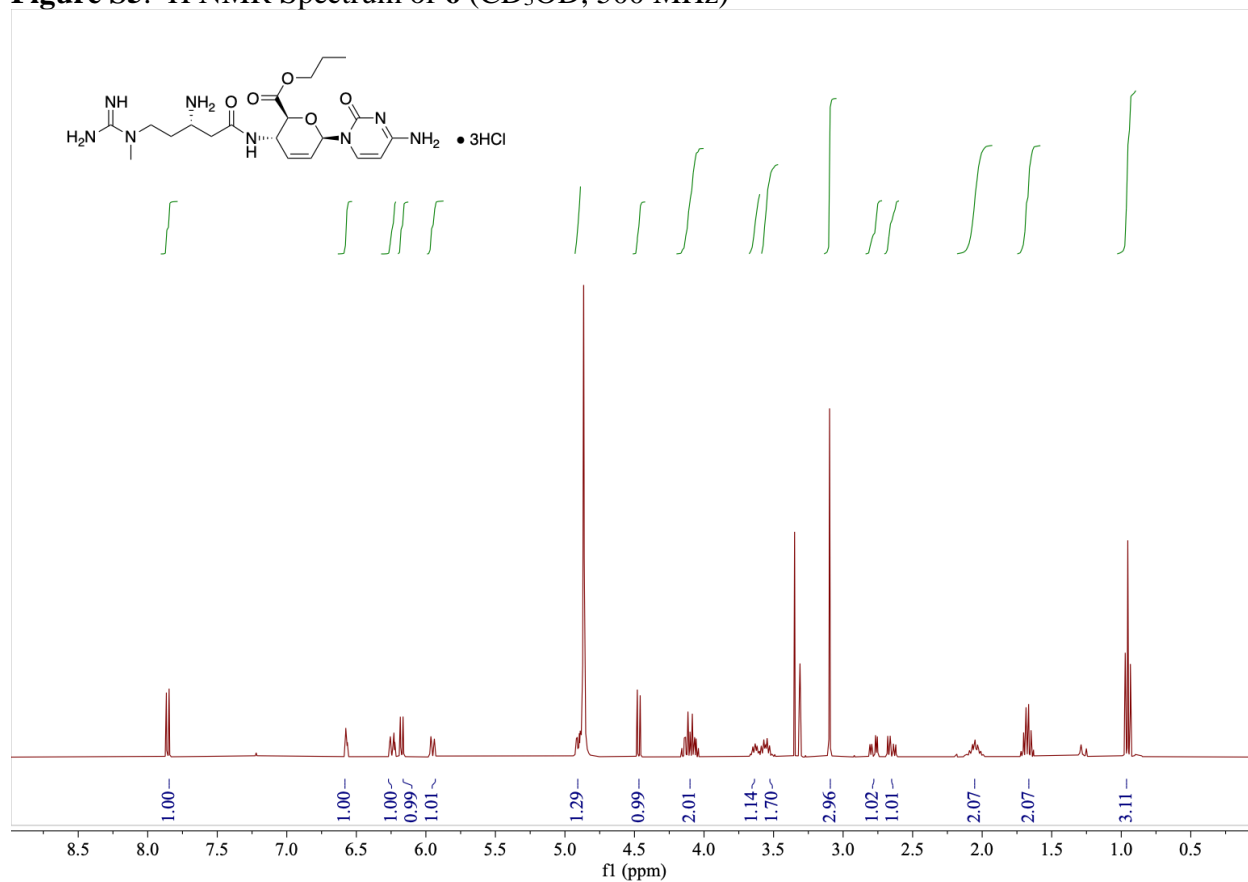
**Figure S3.**  $^1\text{H}$  NMR Spectrum of **5** ( $\text{CD}_3\text{OD}$ , 500 MHz)



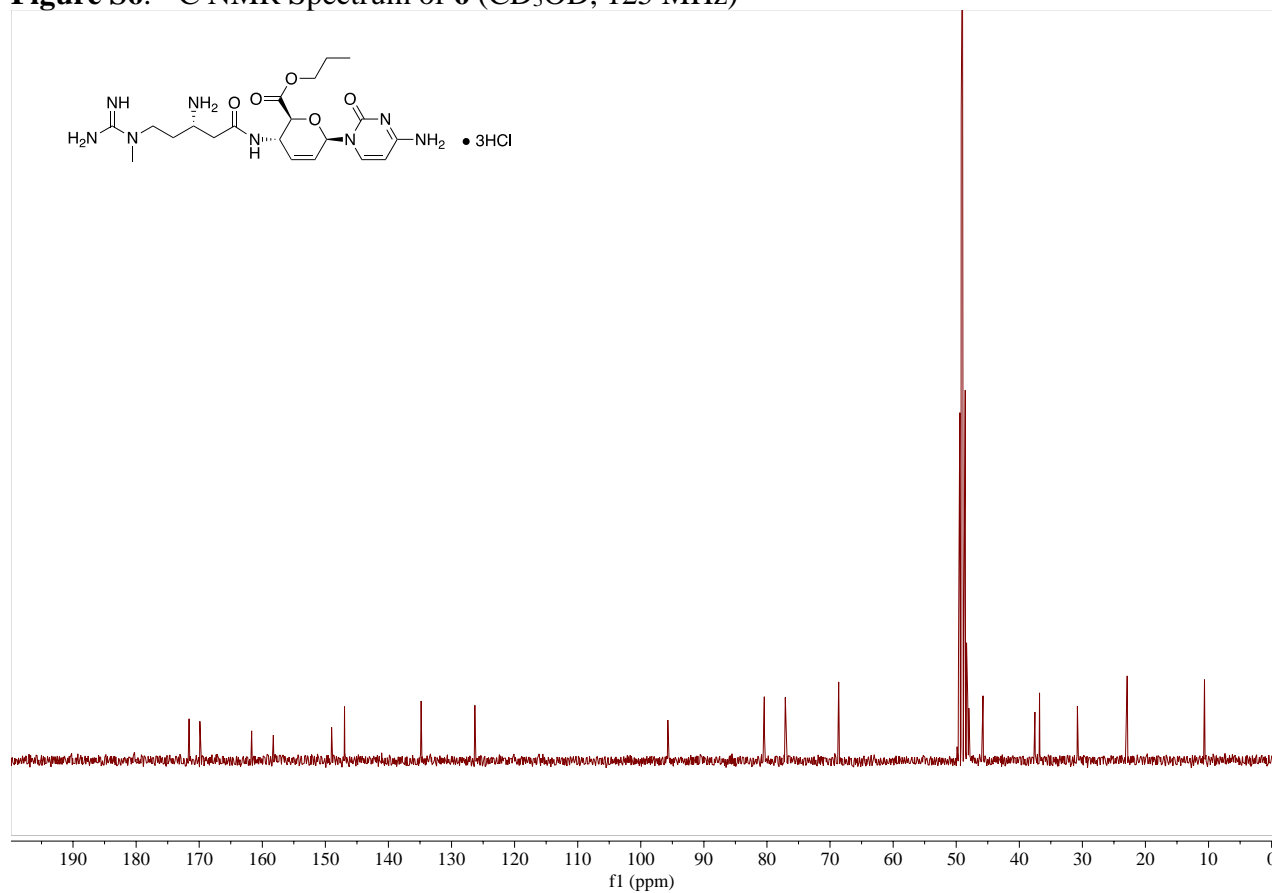
**Figure S4.**  $^{13}\text{C}$  NMR Spectrum of **5** ( $\text{CD}_3\text{OD}$ , 125 MHz)



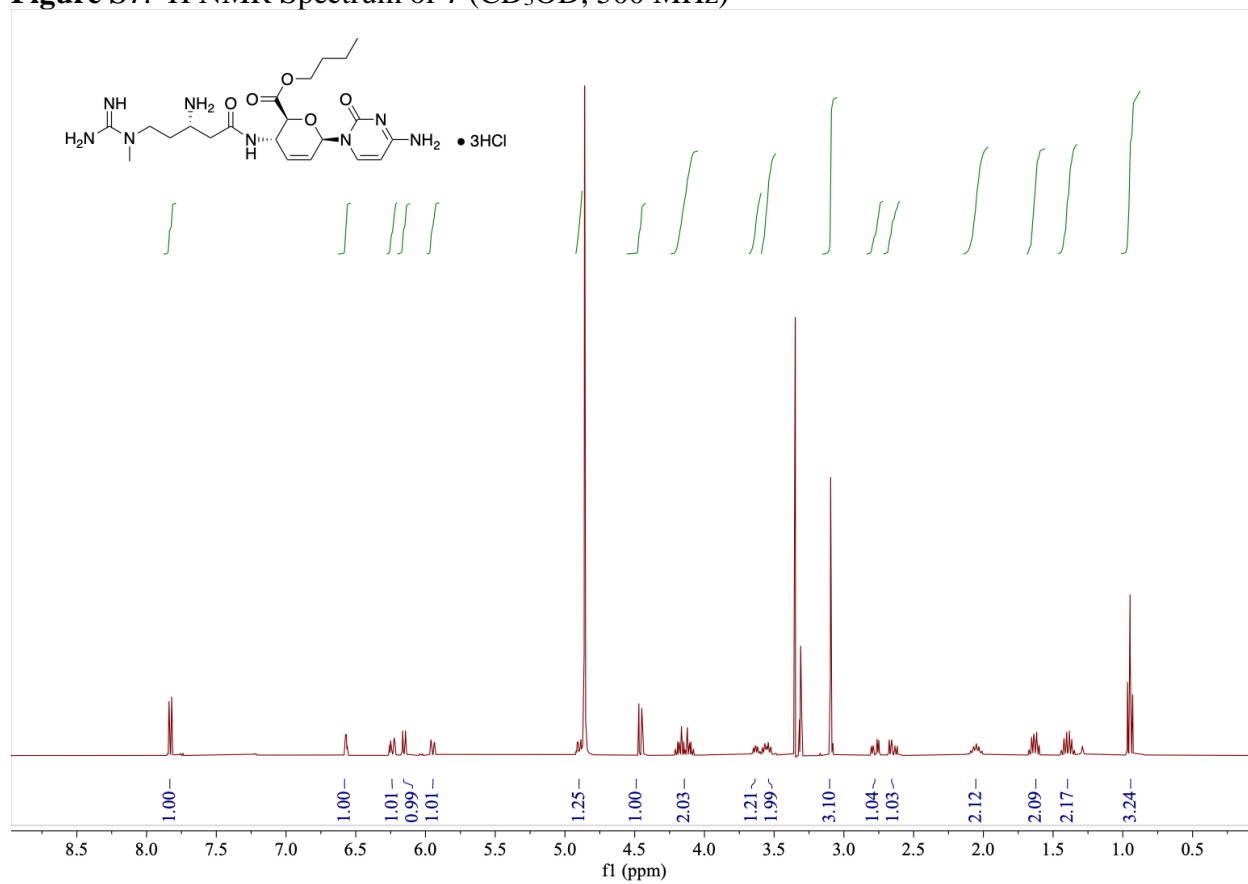
**Figure S5.**  $^1\text{H}$  NMR Spectrum of **6** ( $\text{CD}_3\text{OD}$ , 500 MHz)



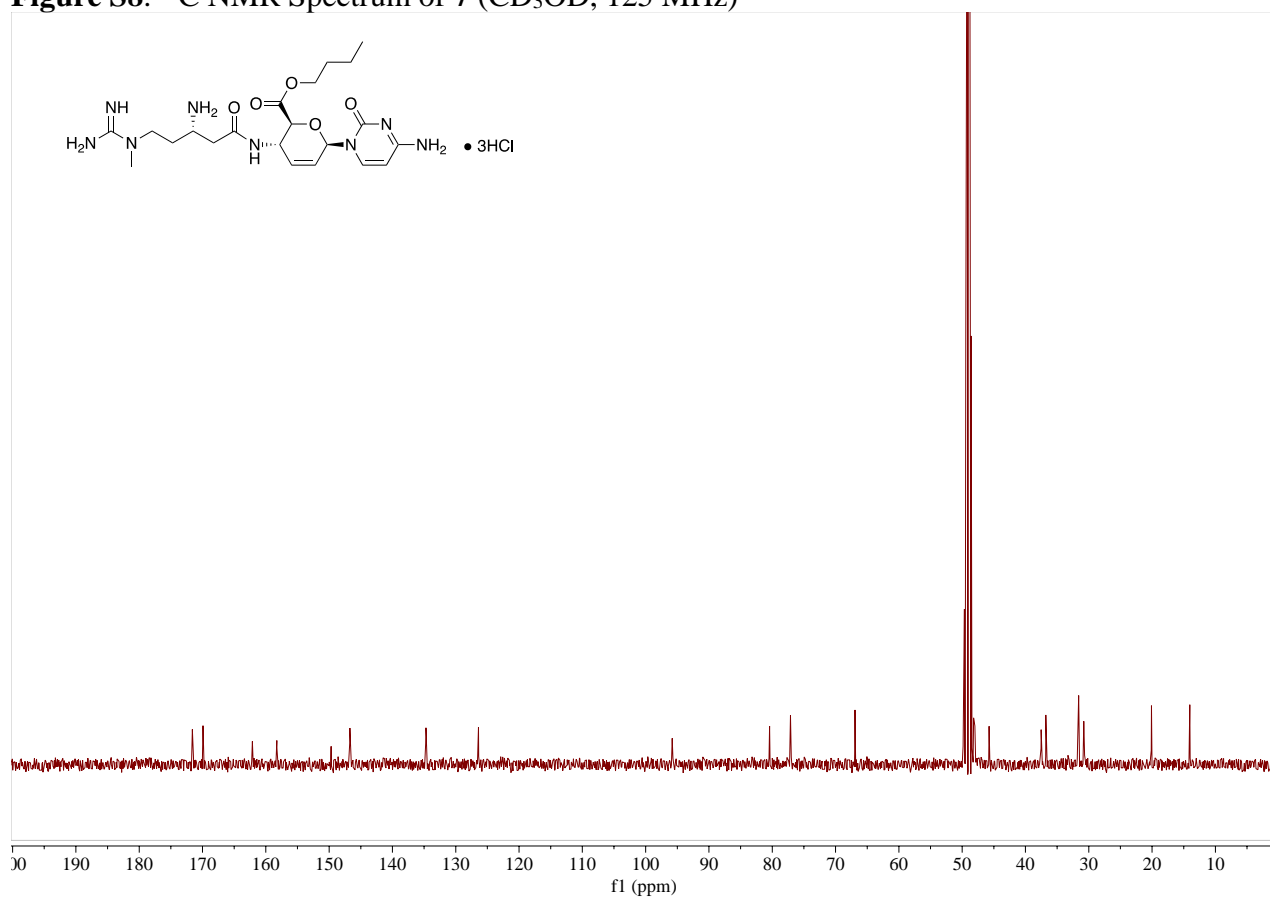
**Figure S6.**  $^{13}\text{C}$  NMR Spectrum of **6** ( $\text{CD}_3\text{OD}$ , 125 MHz)



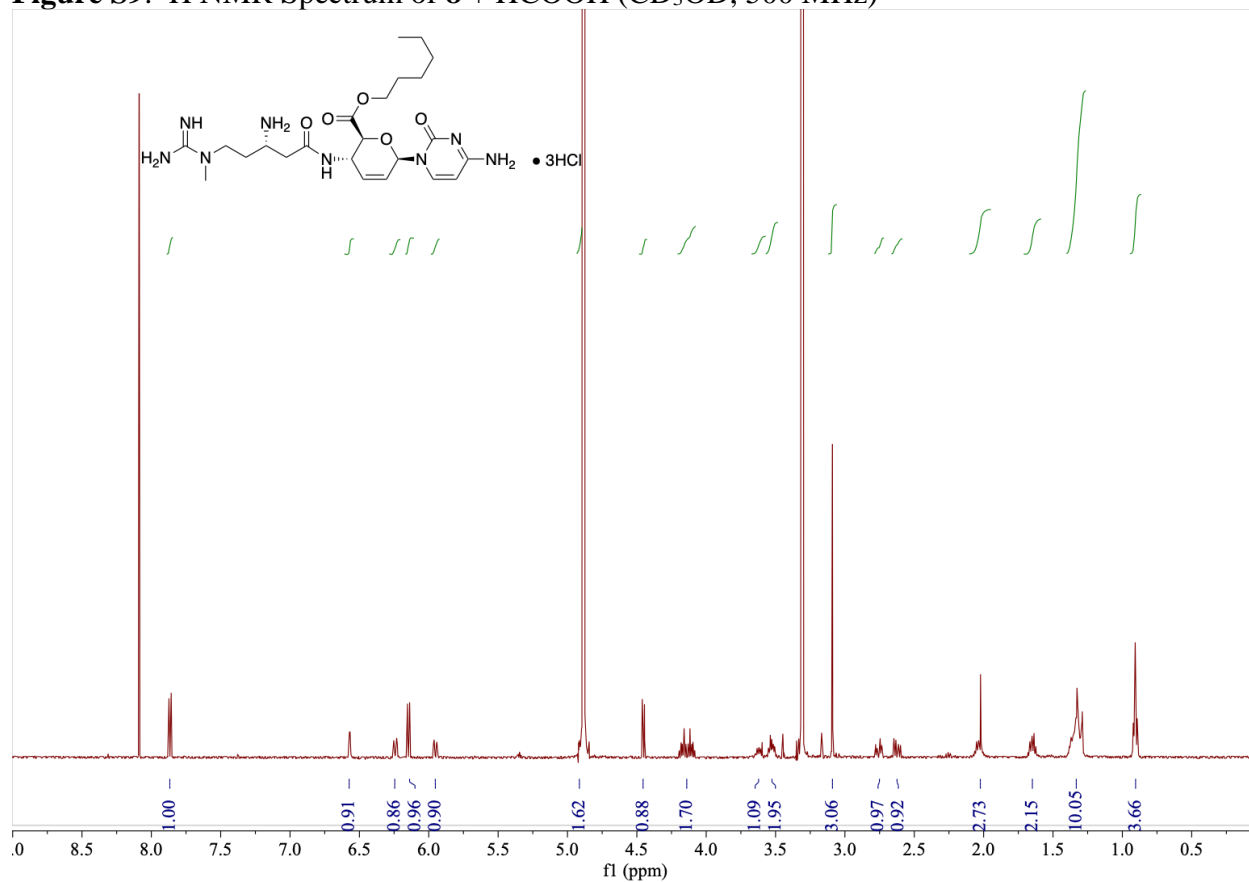
**Figure S7.**  $^1\text{H}$  NMR Spectrum of **7** ( $\text{CD}_3\text{OD}$ , 500 MHz)



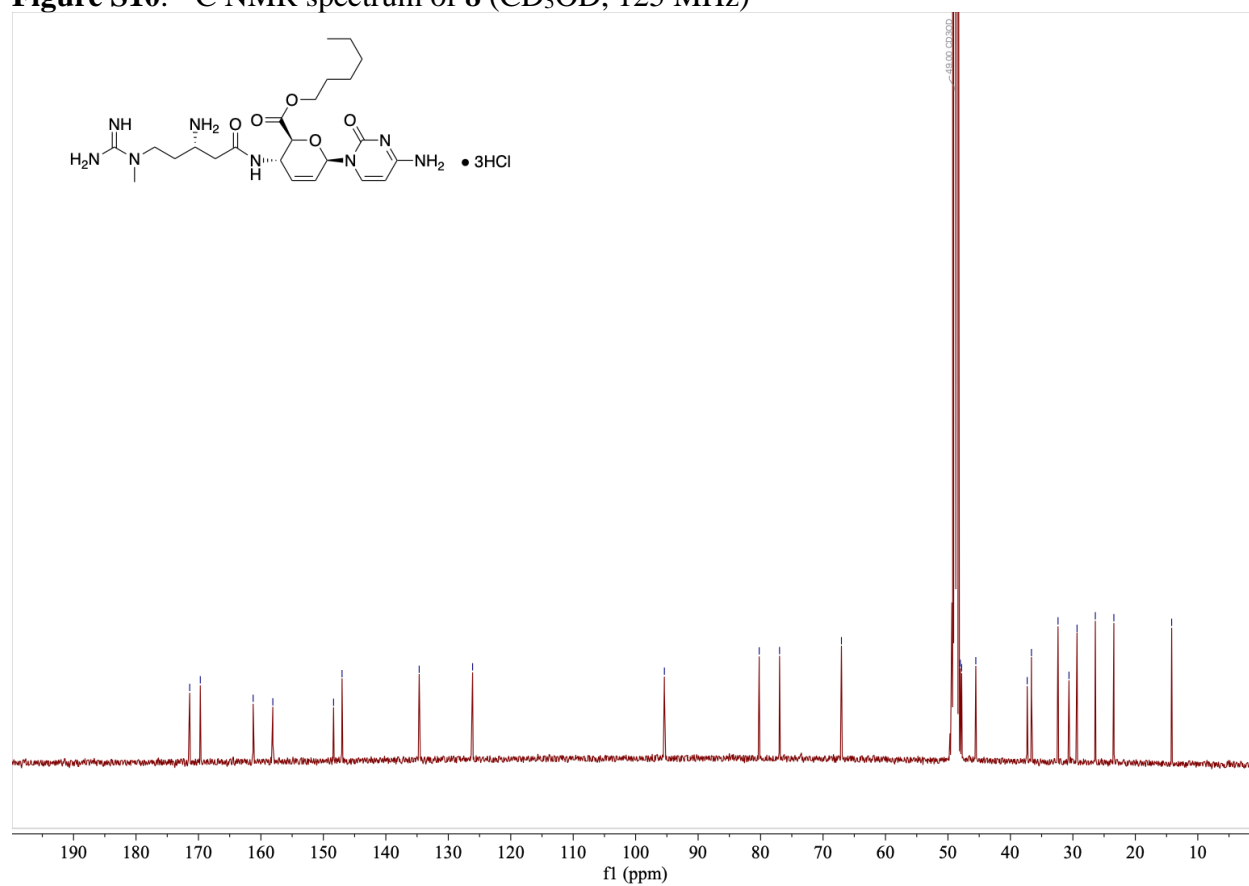
**Figure S8.**  $^{13}\text{C}$  NMR Spectrum of **7** ( $\text{CD}_3\text{OD}$ , 125 MHz)



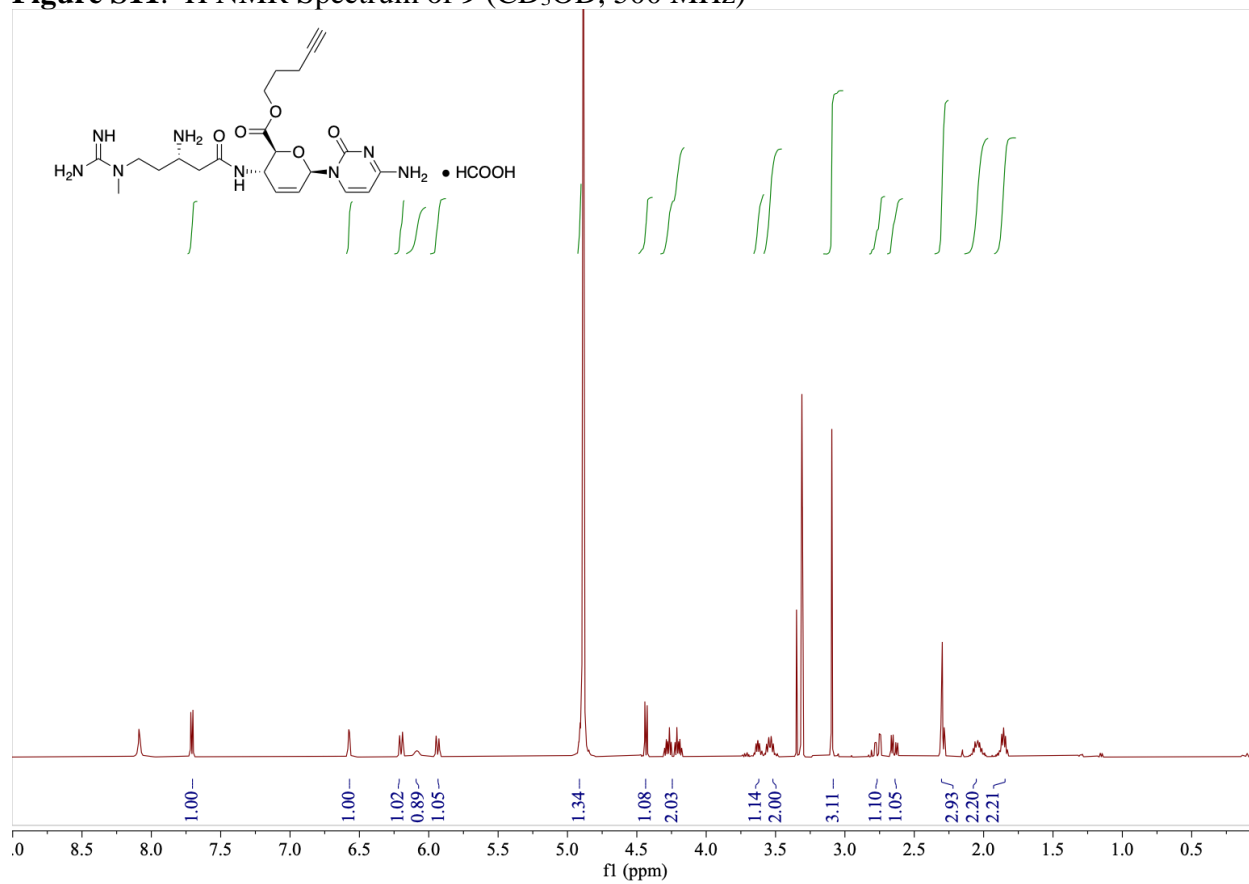
**Figure S9.**  $^1\text{H}$  NMR Spectrum of **8** +  $\text{HCOOH}$  ( $\text{CD}_3\text{OD}$ , 500 MHz)



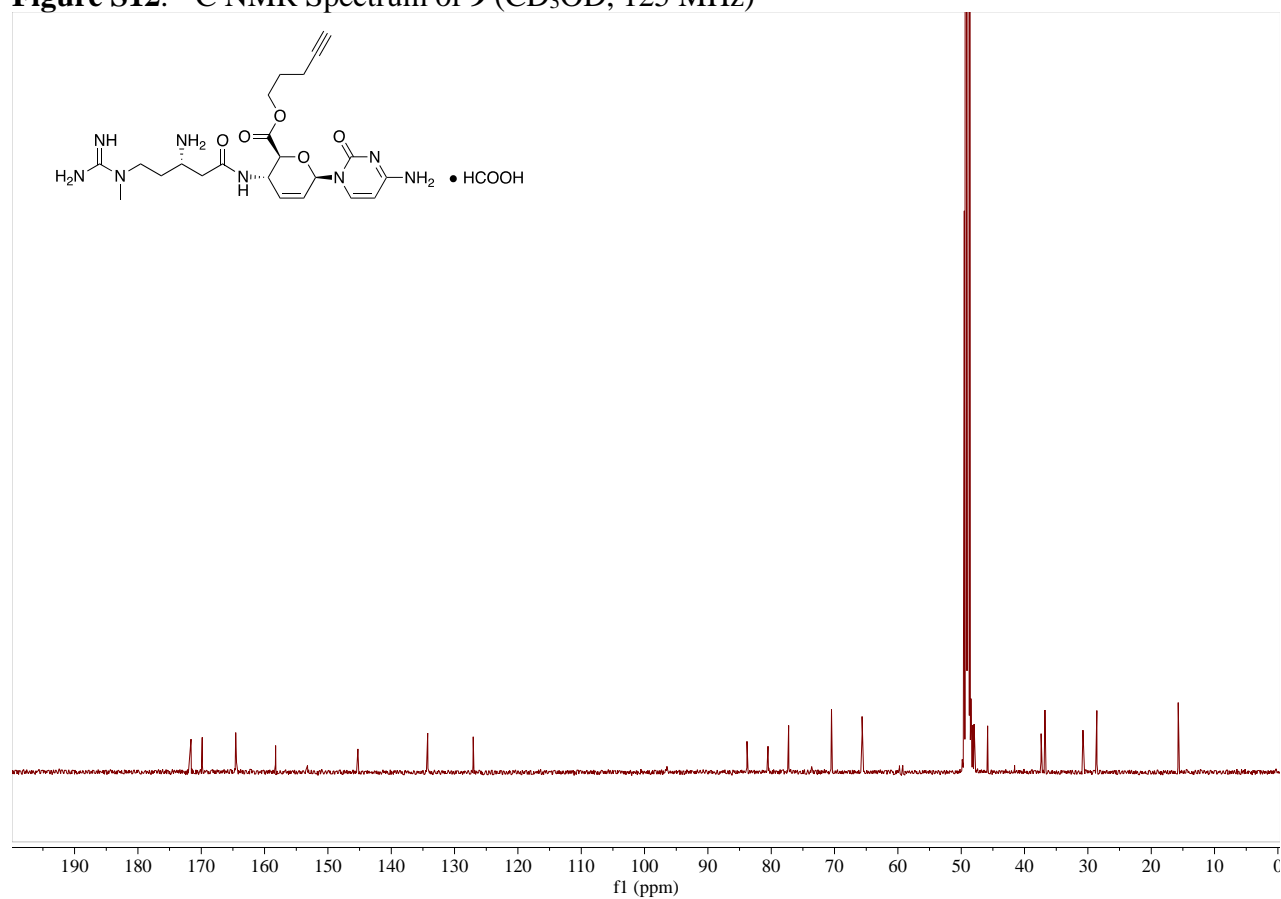
**Figure S10.**  $^{13}\text{C}$  NMR spectrum of **8** ( $\text{CD}_3\text{OD}$ , 125 MHz)



**Figure S11.**  $^1\text{H}$  NMR Spectrum of **9** ( $\text{CD}_3\text{OD}$ , 500 MHz)

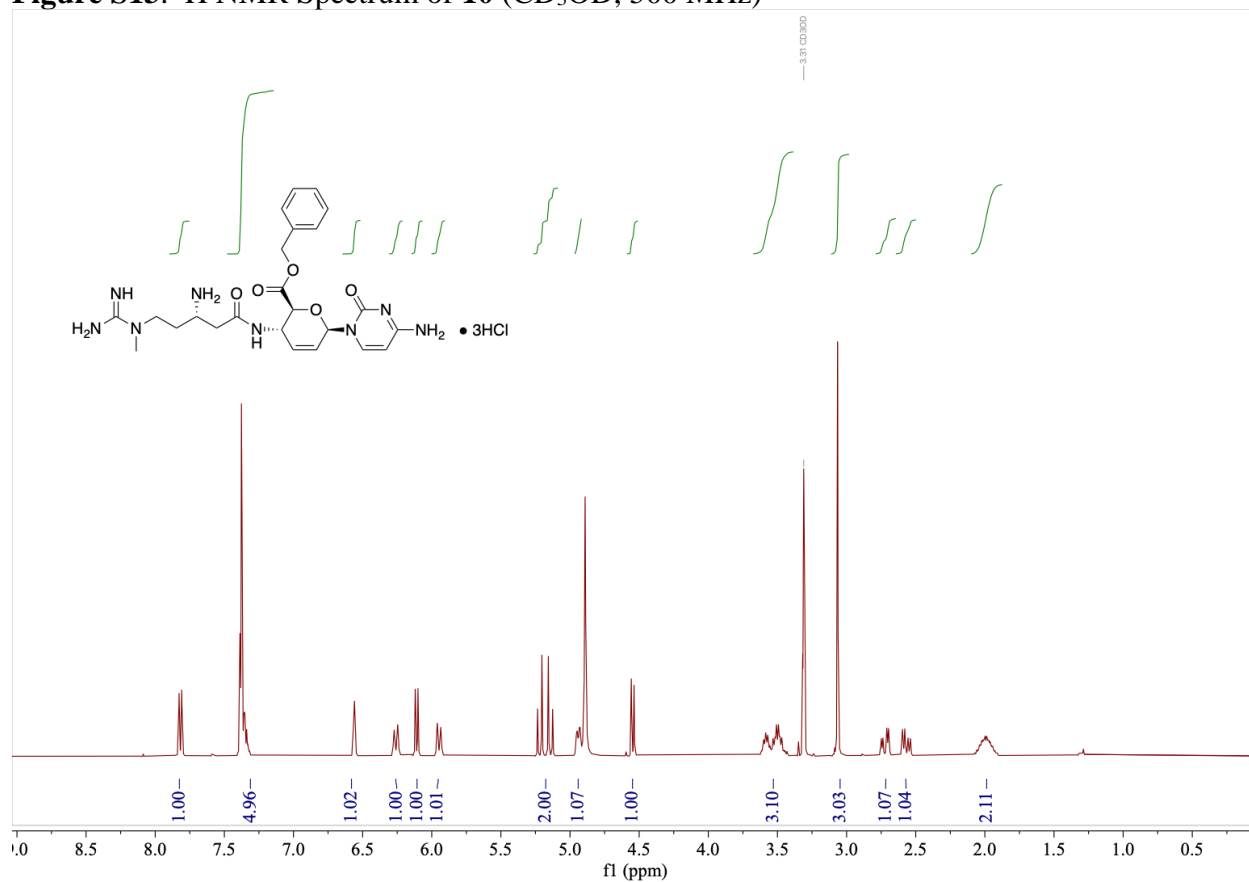


**Figure S12.**  $^{13}\text{C}$  NMR Spectrum of **9** ( $\text{CD}_3\text{OD}$ , 125 MHz)

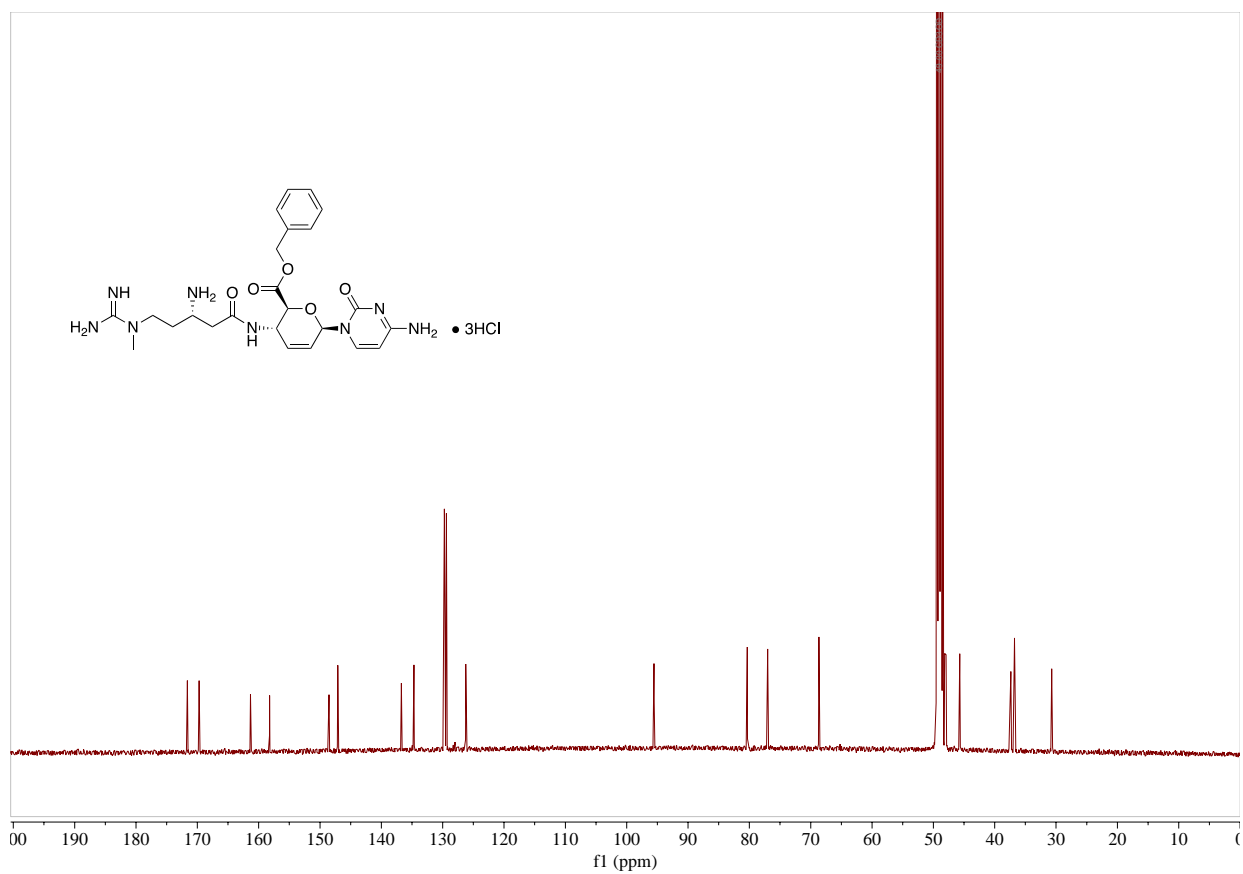




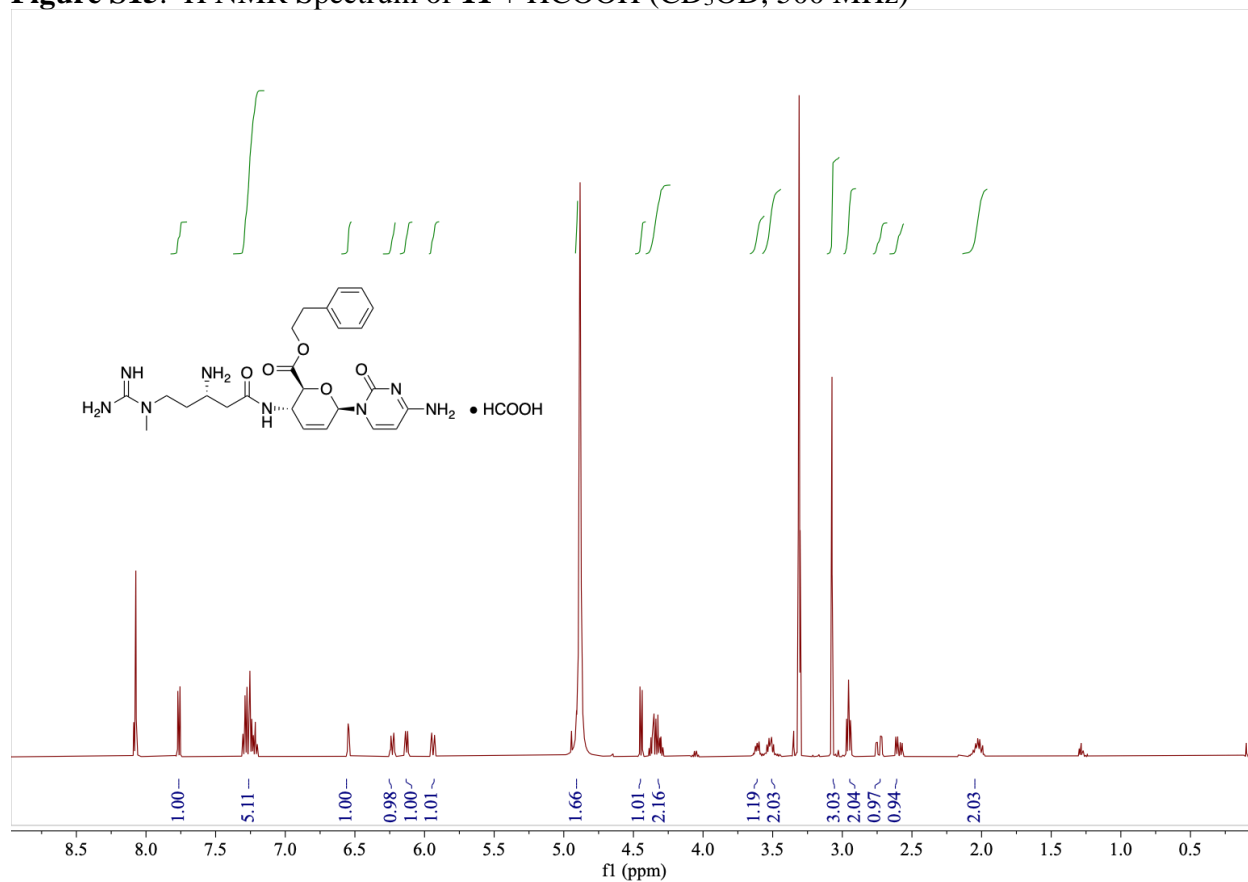
**Figure S13.**  $^1\text{H}$  NMR Spectrum of **10** ( $\text{CD}_3\text{OD}$ , 500 MHz)



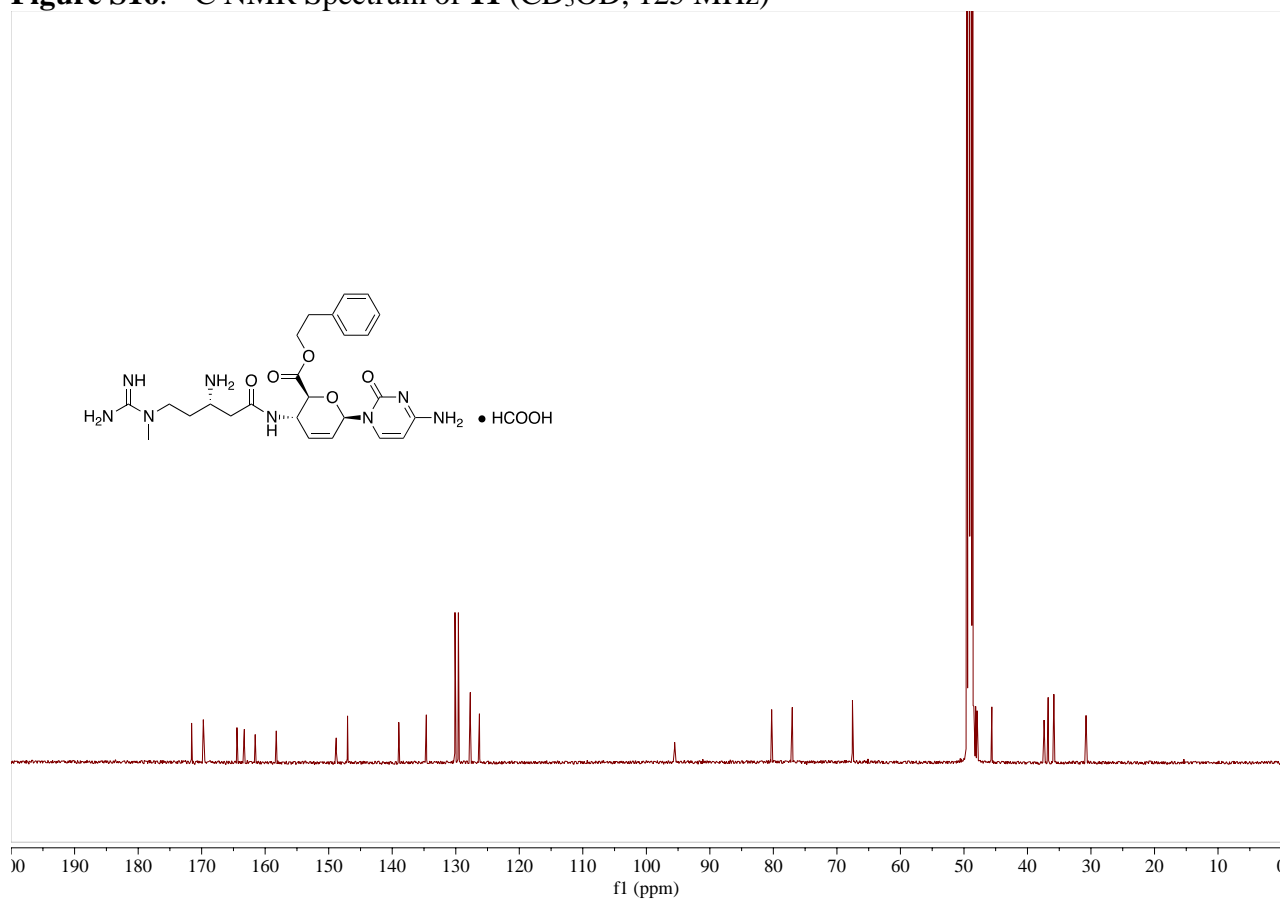
**Figure S14.**  $^{13}\text{C}$  NMR Spectrum of **10** ( $\text{CD}_3\text{OD}$ , 125 MHz)



**Figure S15.**  $^1\text{H}$  NMR Spectrum of **11** +  $\text{HCOOH}$  ( $\text{CD}_3\text{OD}$ , 500 MHz)



**Figure S16.**  $^{13}\text{C}$  NMR Spectrum of **11** ( $\text{CD}_3\text{OD}$ , 125 MHz)



## Media Recipes

ATCC 1245 YPD Medium:

Yeast Extract – 10.0g

Peptone – 20.0g

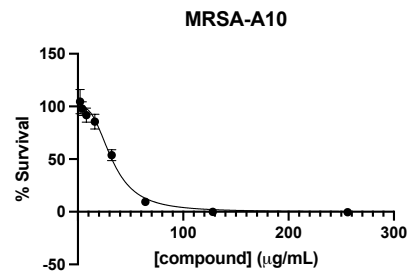
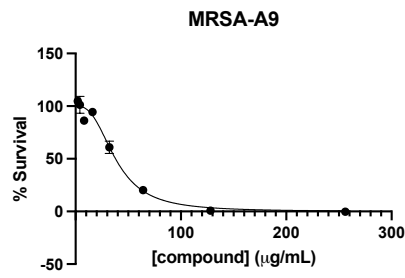
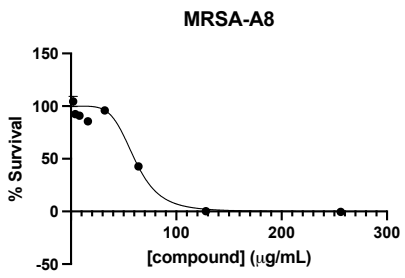
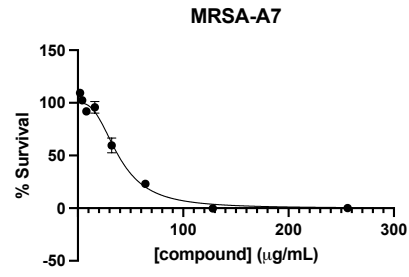
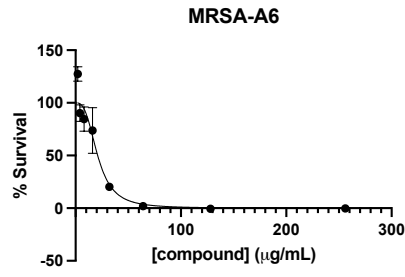
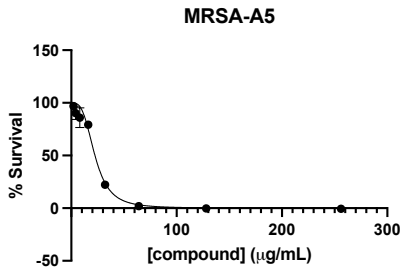
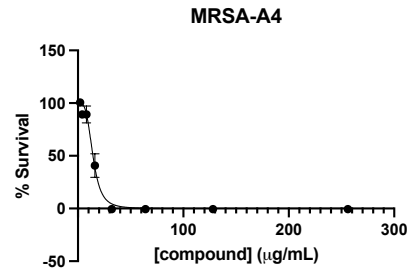
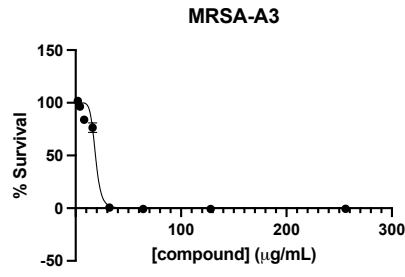
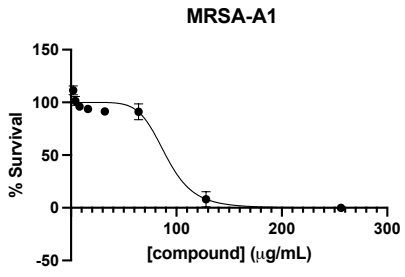
Dextrose – 20.0g

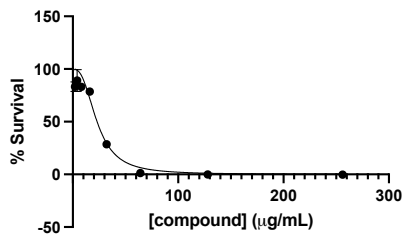
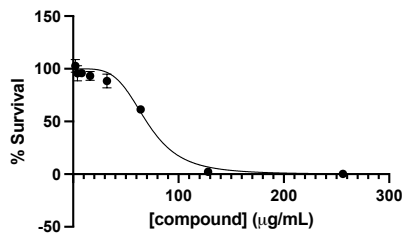
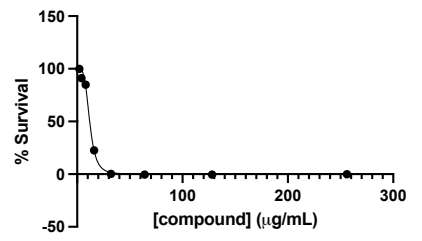
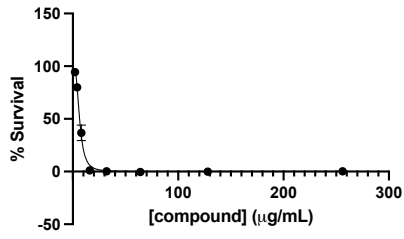
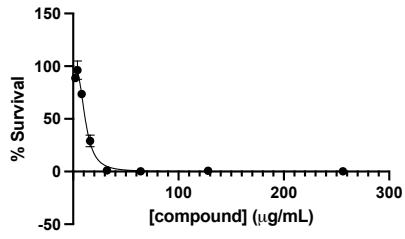
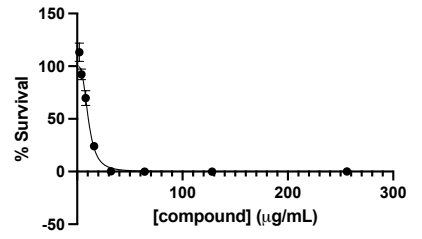
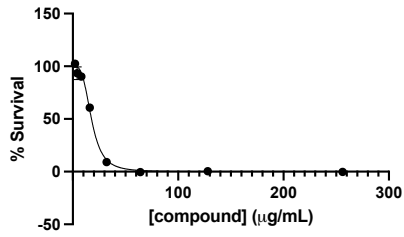
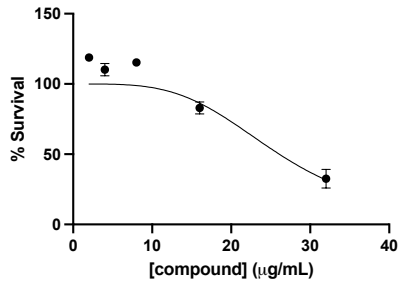
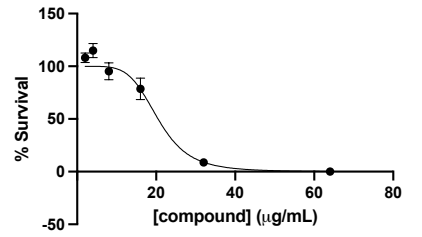
DI Water – 1000 mL

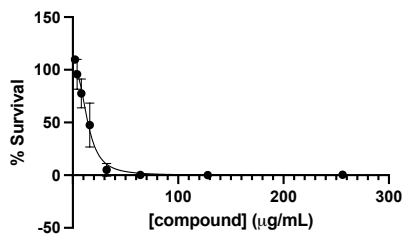
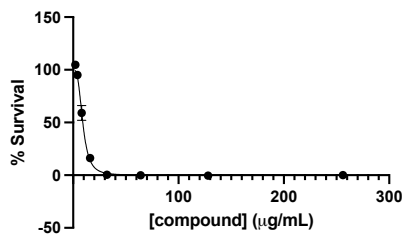
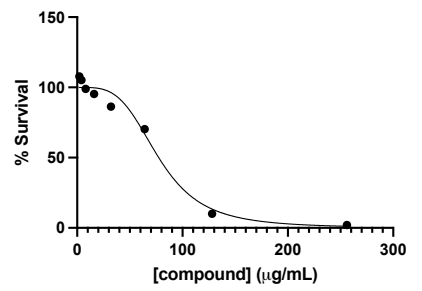
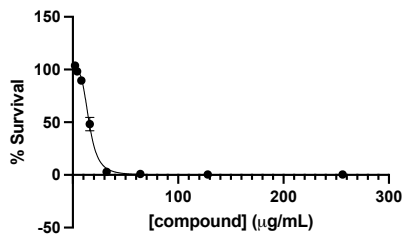
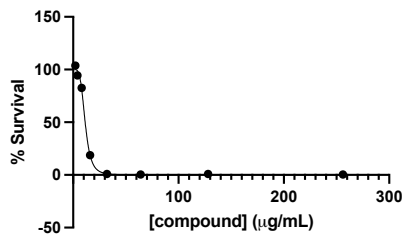
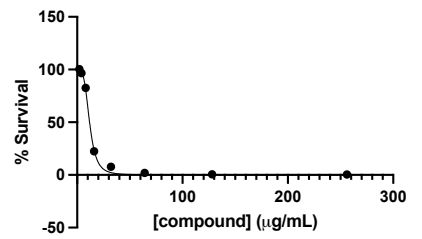
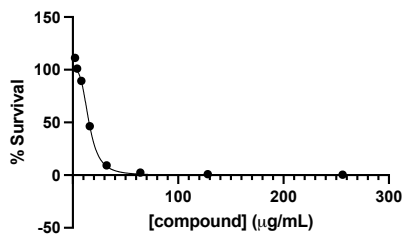
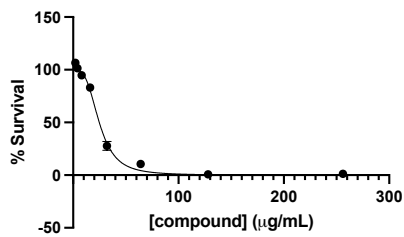
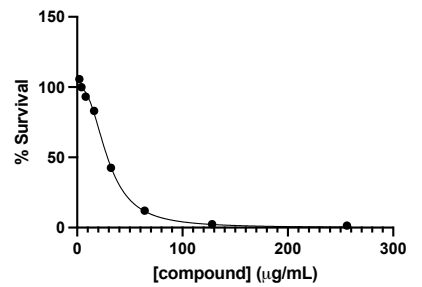
## Bacterial Inhibition Curves

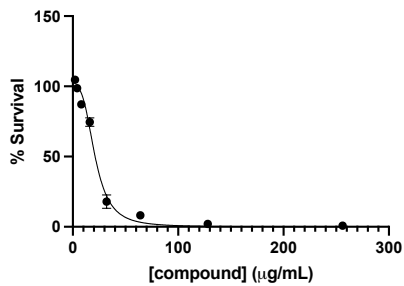
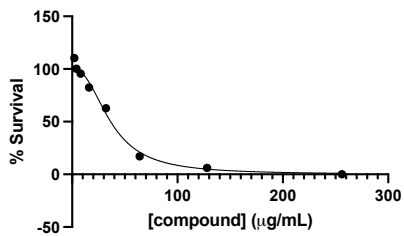
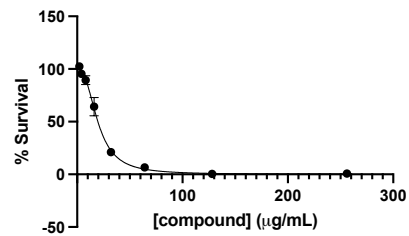
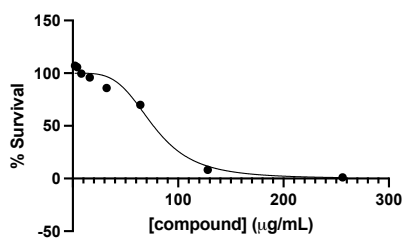
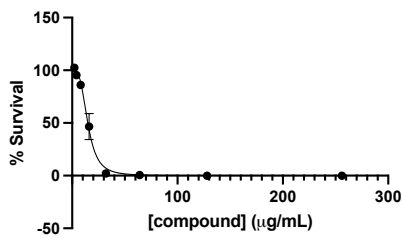
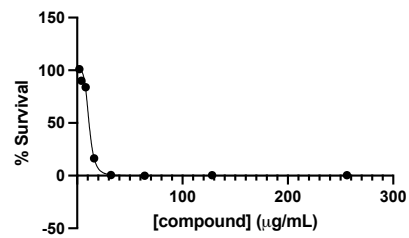
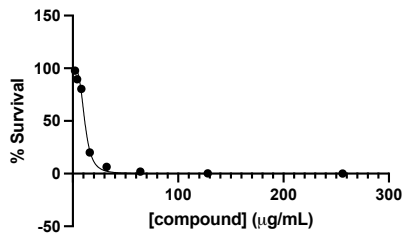
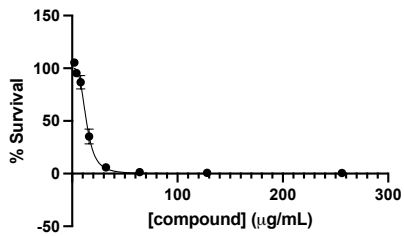
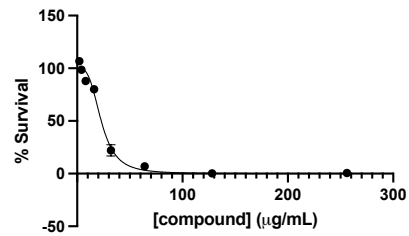
The curves for each biological replicate are shown below. The title of the graphs are [organism]-[biological replicate A or B][compound number]. The organisms are described using acronyms according to the table below.

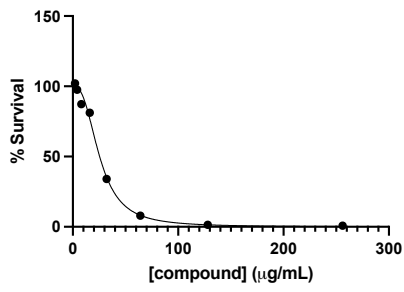
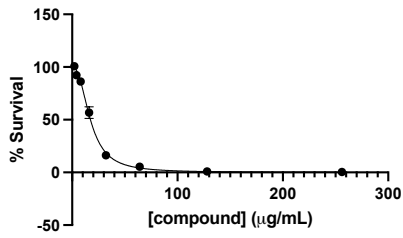
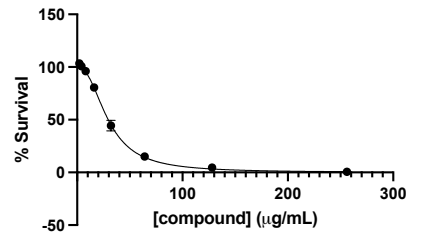
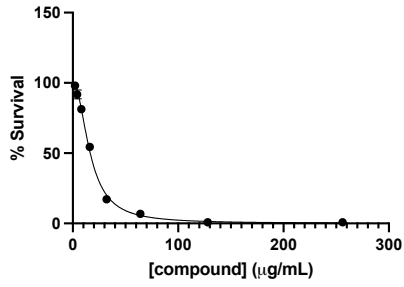
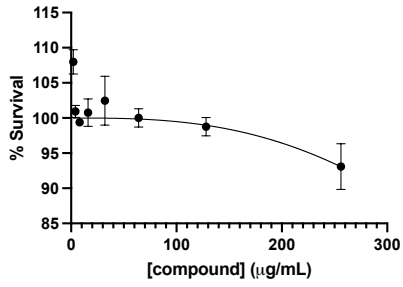
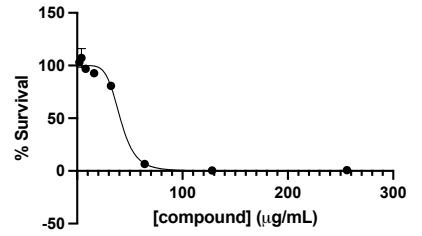
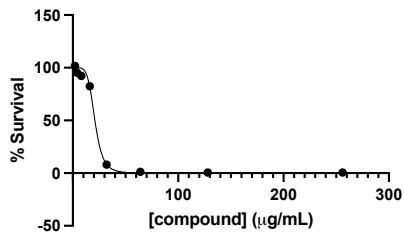
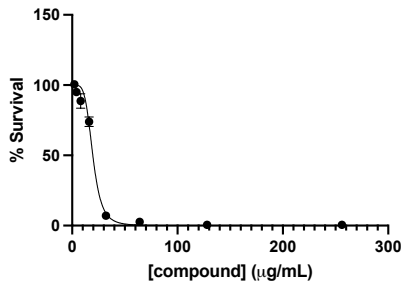
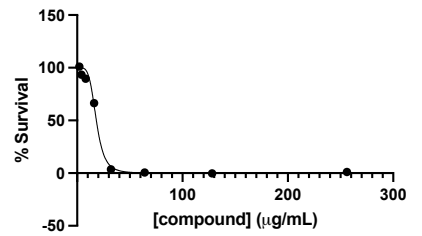
Organism	Acronym
<i>S. aureus</i> $\Delta$ NorA	NorA
<i>S. aureus</i> 8810	8810
<i>S. aureus</i> MRSA	MRSA
<i>E. faecalis</i>	EF
VRE	VRE
<i>K. pneumoniae</i>	KP
<i>P. aeruginosa</i> $\Delta$ MexAB-OprM	PA
<i>A. baumannii</i>	AB



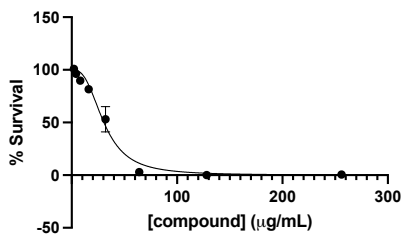
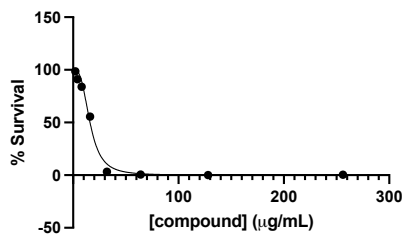
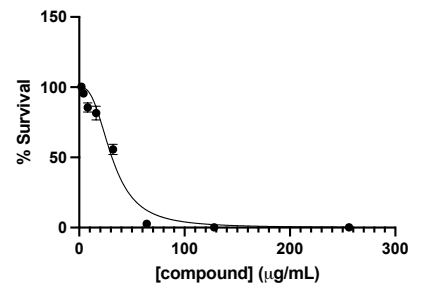
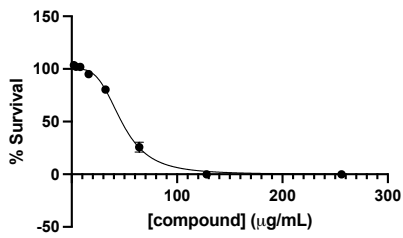
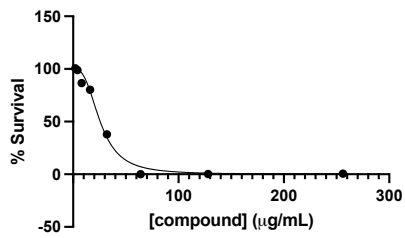
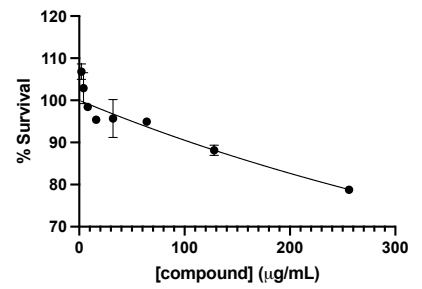
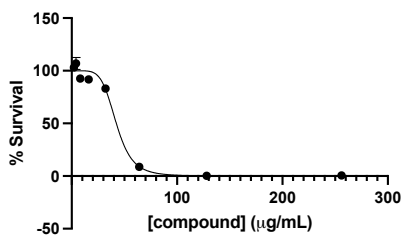
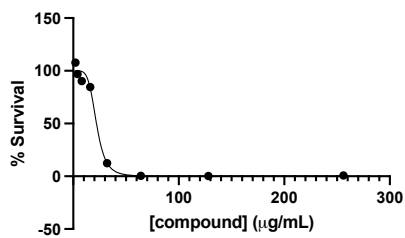
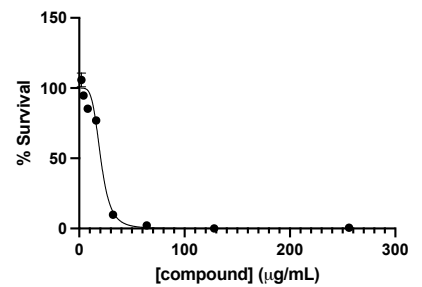
**MRSA-A11****MRSA-B1****MRSA-B3****MRSA-B4****MRSA-B5****MRSA-B6****MRSA-B7****MRSA-B8****MRSA-B9**

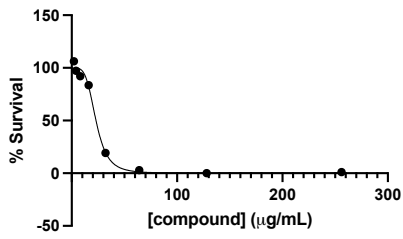
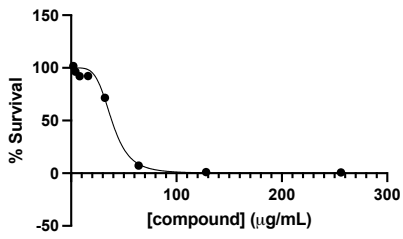
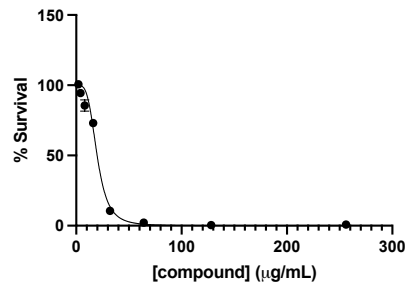
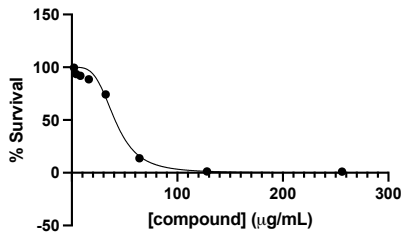
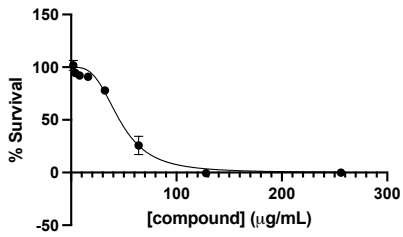
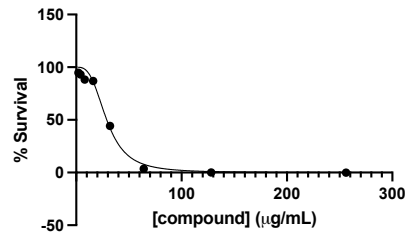
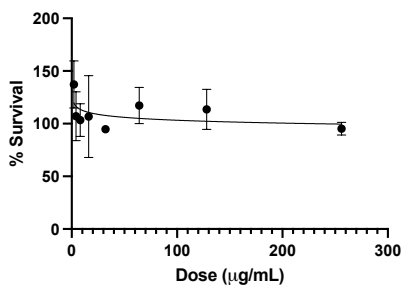
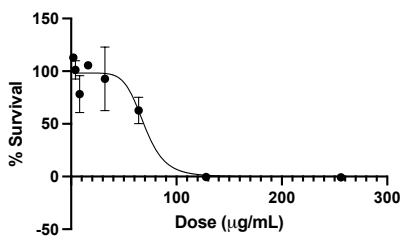
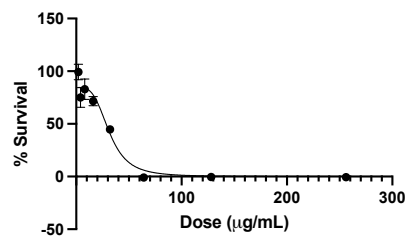
**MRSA-B10****MRSA-B11****8810-A1****8810-A3****8810-A4****8810-A5****8810-A6****8810-A7****8810-A8**

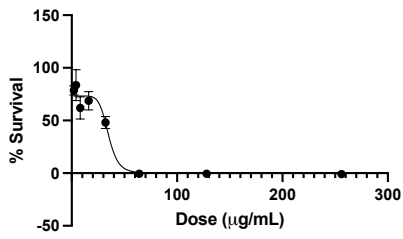
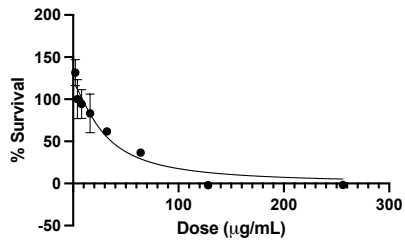
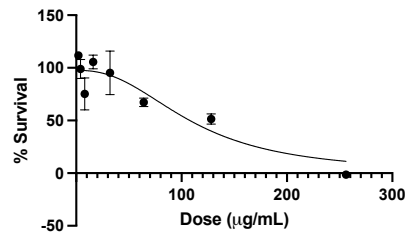
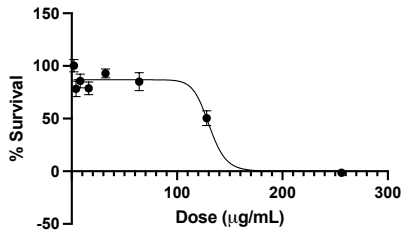
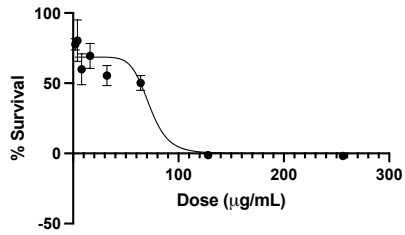
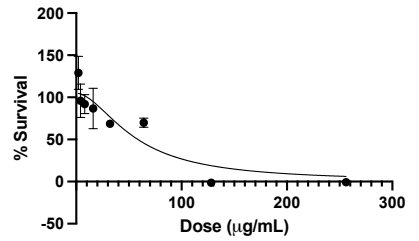
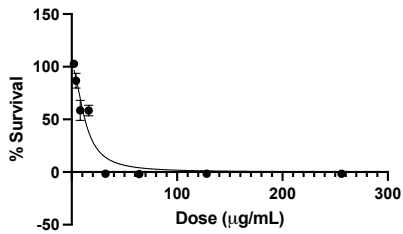
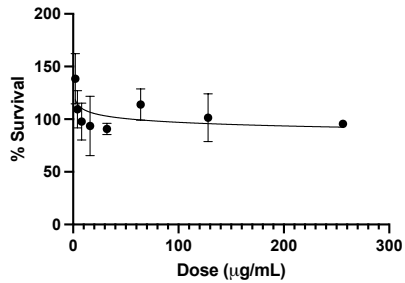
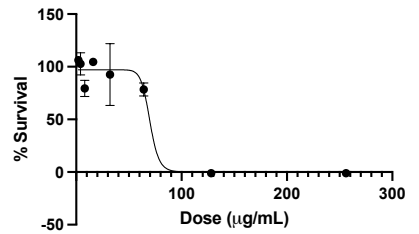
**8810-A9****8810-A10****8810-A11****8810-B1****8810-B3****8810-B4****8810-B5****8810-B6****8810-B7**

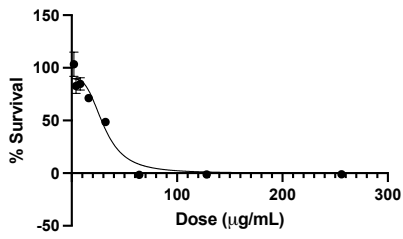
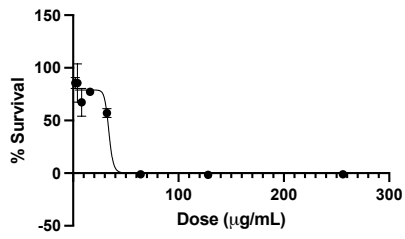
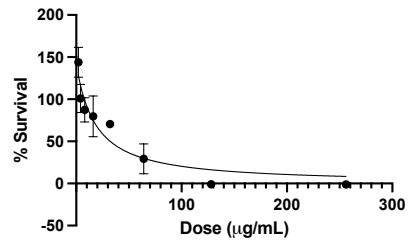
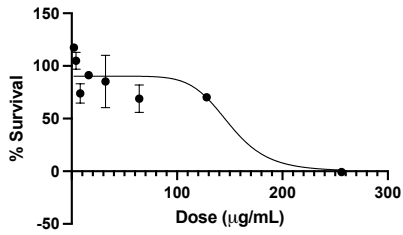
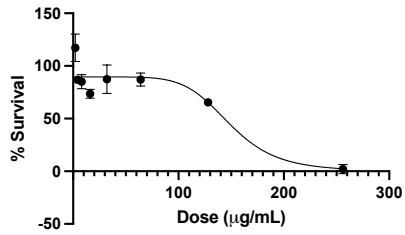
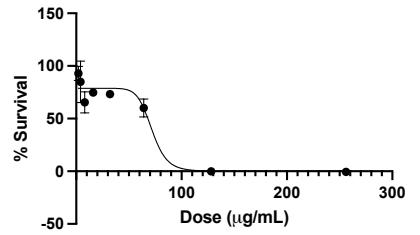
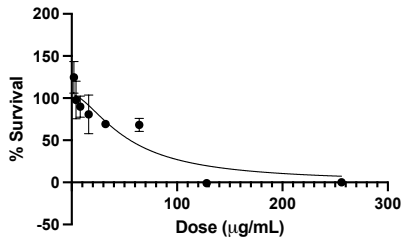
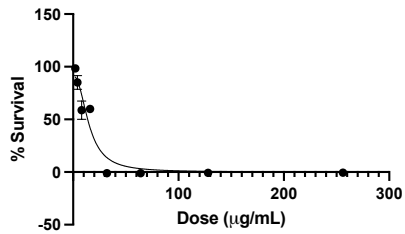
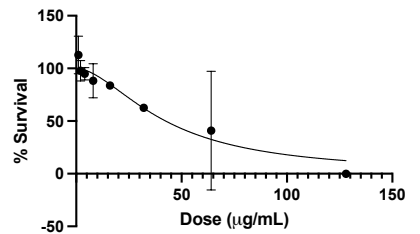
**8810-B8****8810-B9****8810-B10****8810-B11****NorA-A1****NorA-A3****NorA-A4****NorA-A5****NorA-A6**

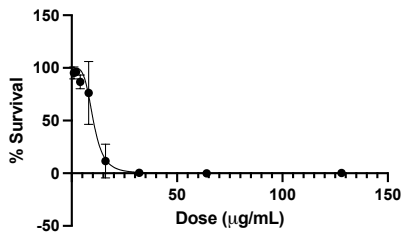
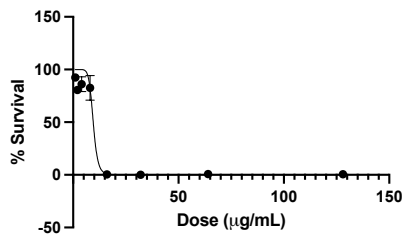
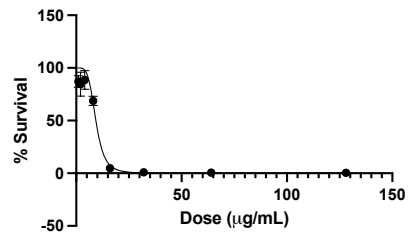
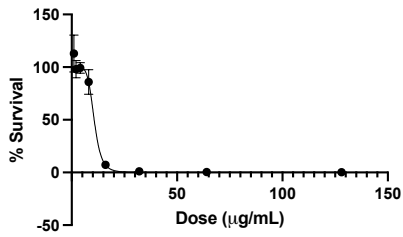
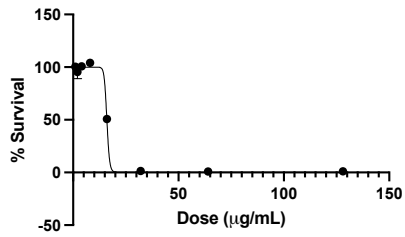
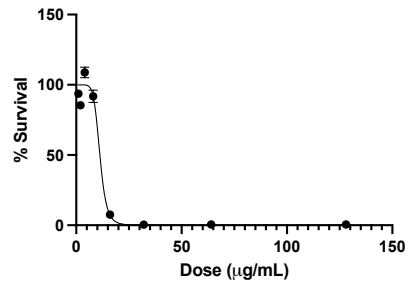
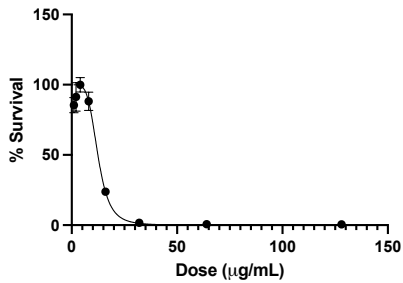
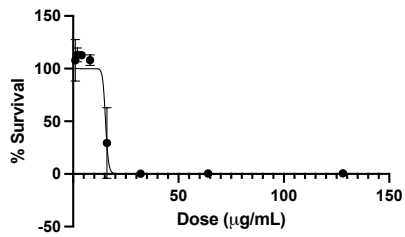
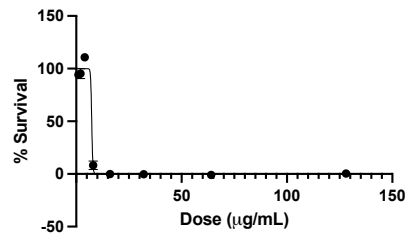


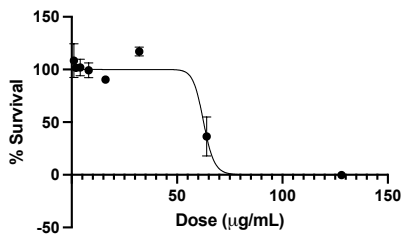
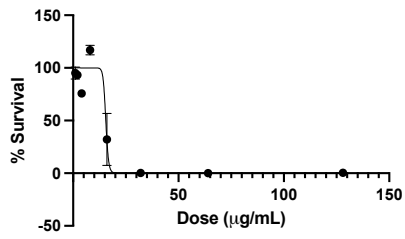
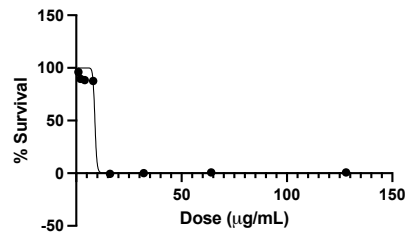
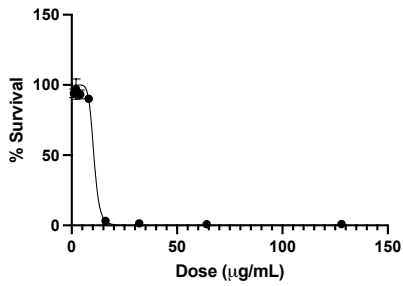
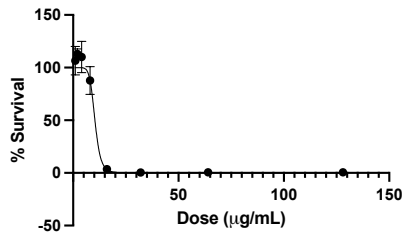
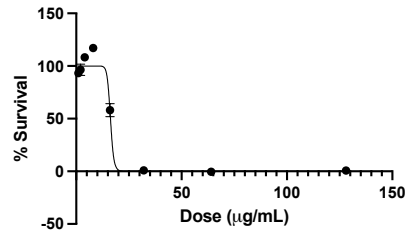
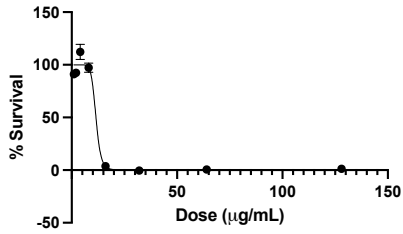
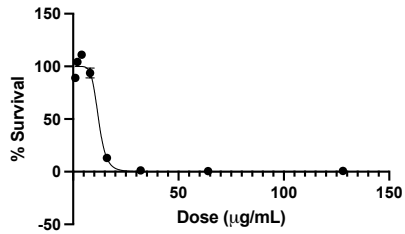
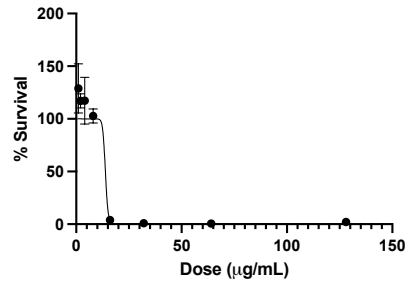
**NorA-A7****NorA-A8****NorA-A9****NorA-A10****NorA-A11****NorA-B1****NorA-B3****NorA-B4****NorA-B5**

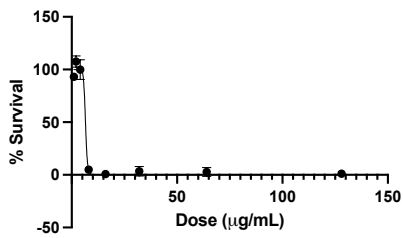
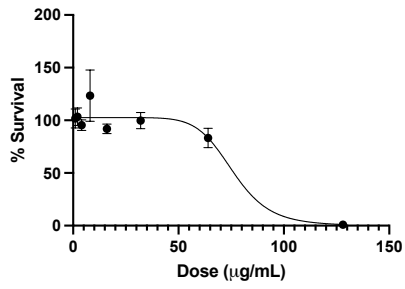
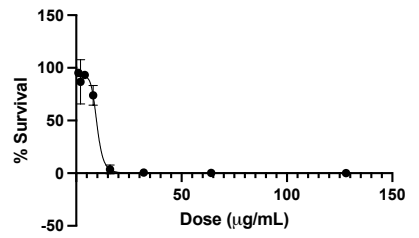
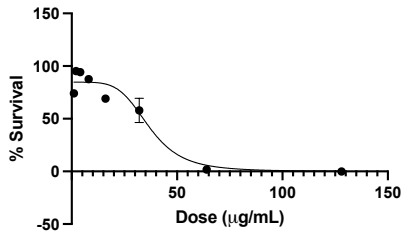
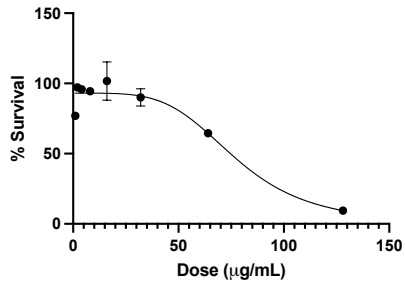
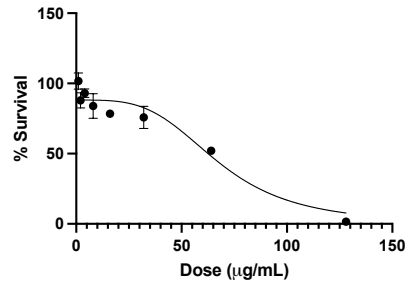
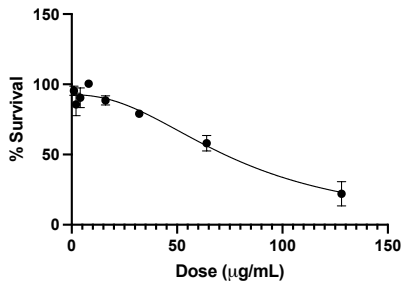
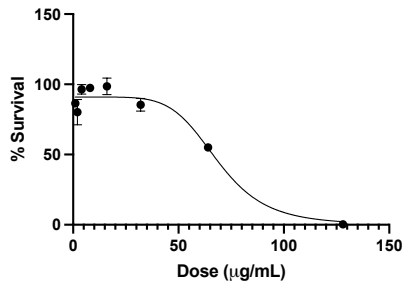
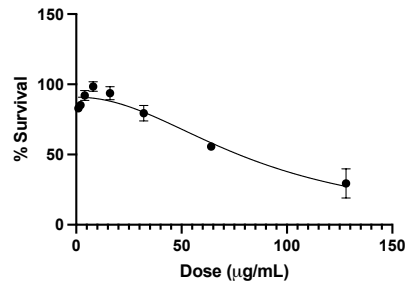
**NorA-B6****NorA-B7****NorA-B8****NorA-B9****NorA-B10****NorA-B11****VRE-A1****VRE-A3****VRE-A4**

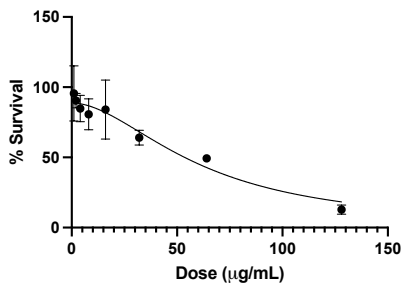
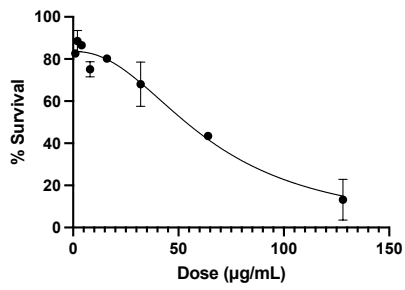
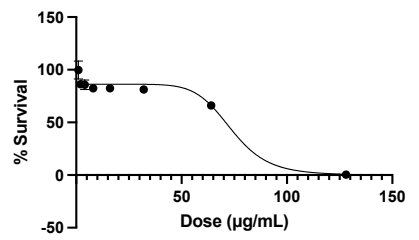
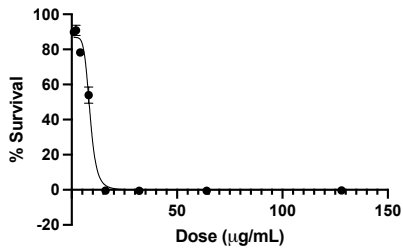
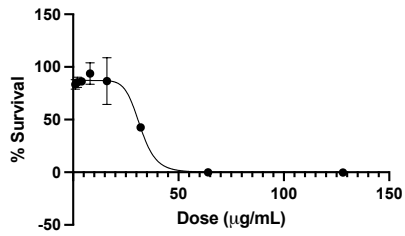
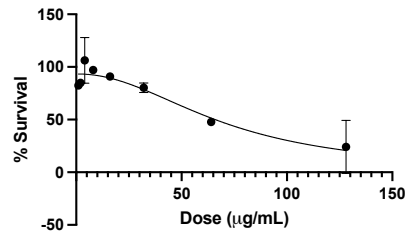
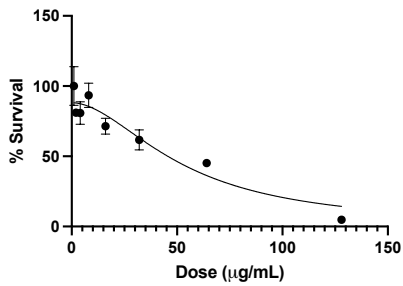
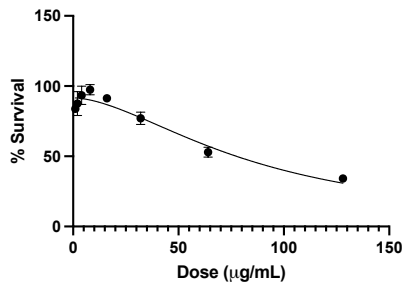
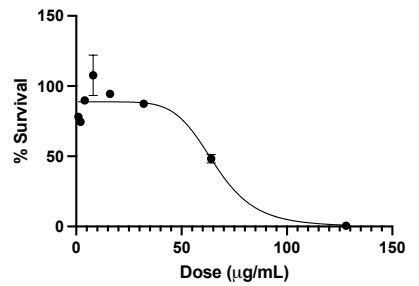
**VRE-A5****VRE-A6****VRE-A7****VRE-A8****VRE-A9****VRE-A10****VRE-A11****VRE-B1****VRE-B3**

**VRE-B4****VRE-B5****VRE-B6****VRE-B7****VRE-B8****VRE-B9****VRE-B10****VRE-B11****EF-A1**

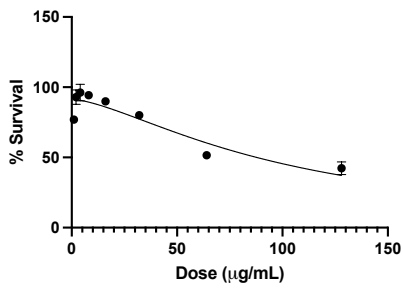
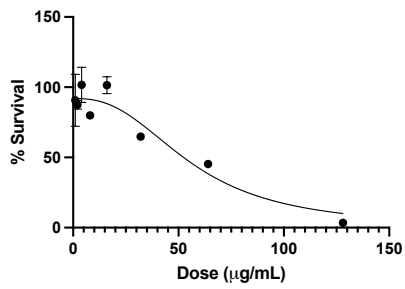
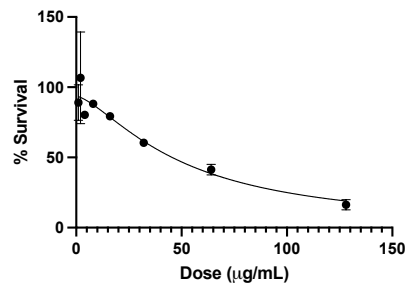
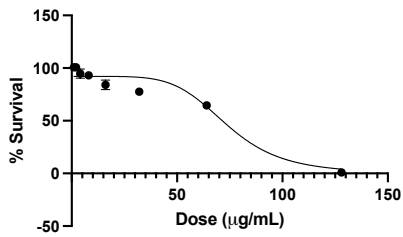
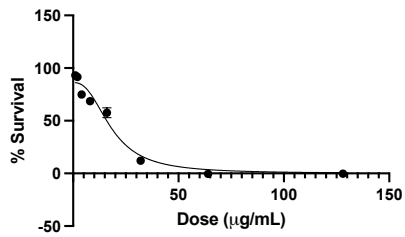
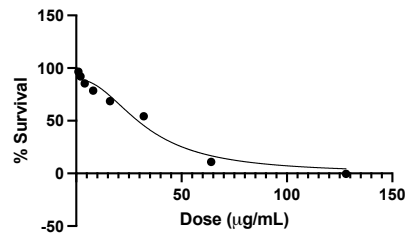
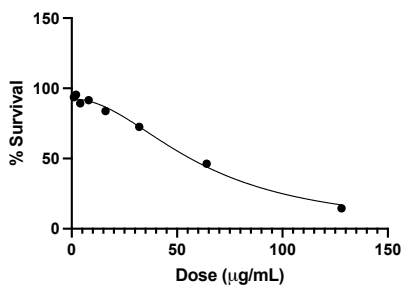
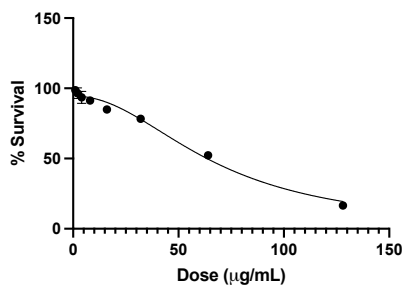
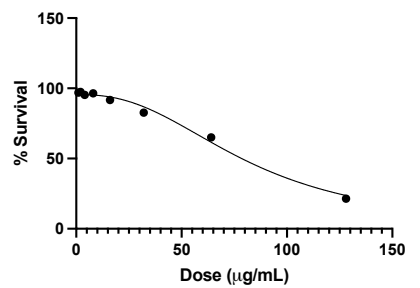
**EF-A3****EF-A4****EF-A5****EF-A6****EF-A7****EF-A8****EF-A9****EF-A10****EF-A11**

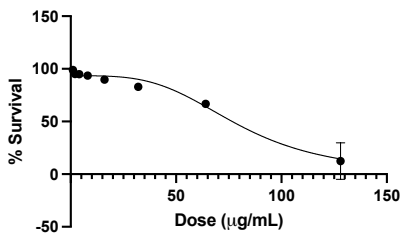
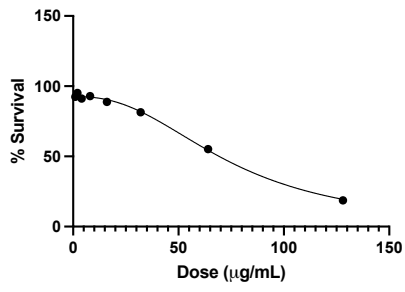
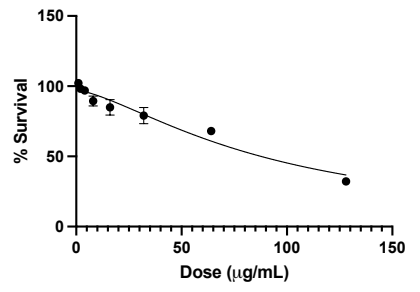
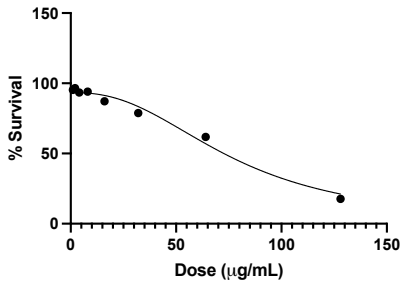
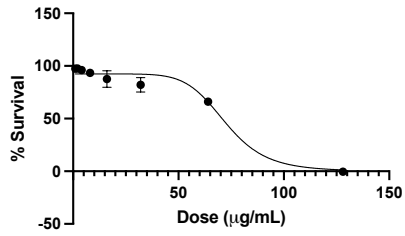
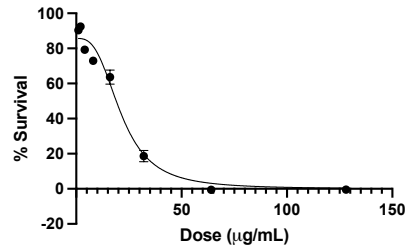
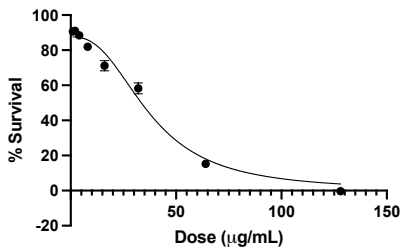
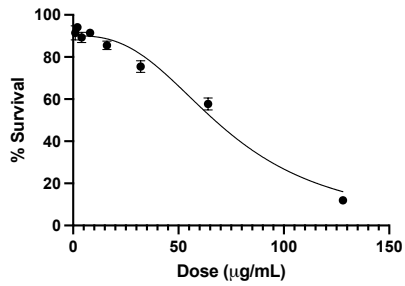
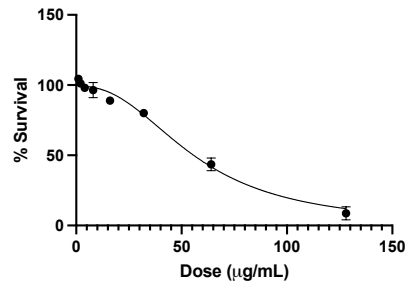
**EF-B1****EF-B3****EF-B4****EF-B5****EF-B6****EF-B7****EF-B8****EF-B9****EF-B10**

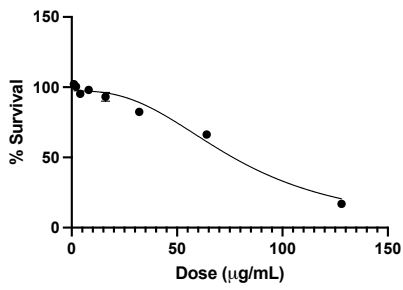
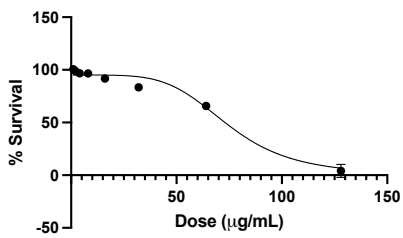
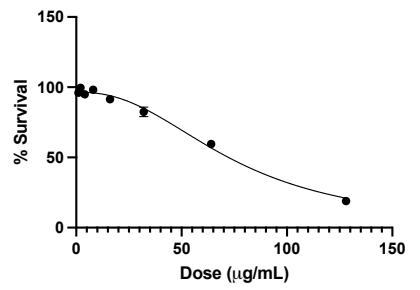
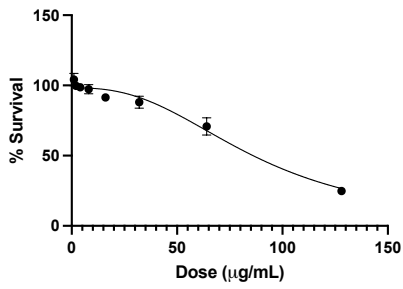
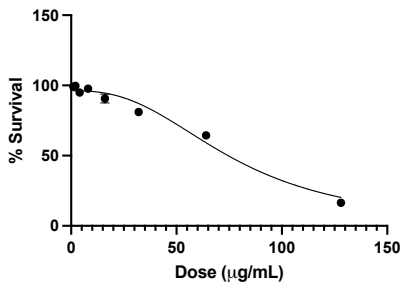
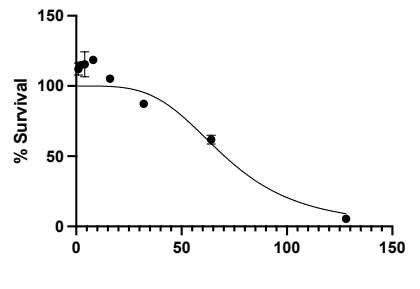
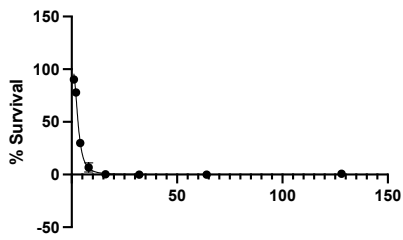
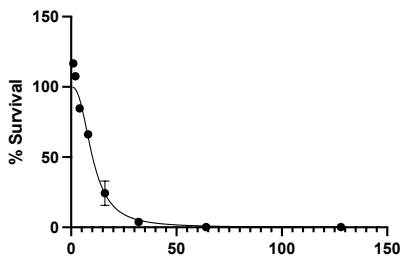
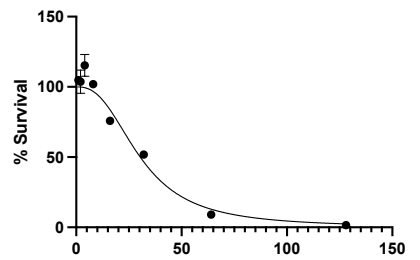
**EF-B11****KP-A1****KP-A3****KP-A4****KP-A5****KP-A6****KP-A7****KP-A8****KP-A9**

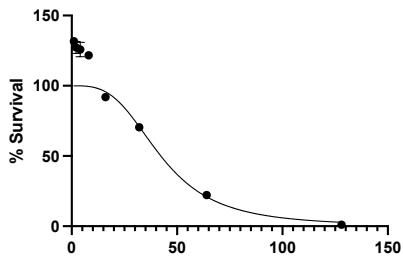
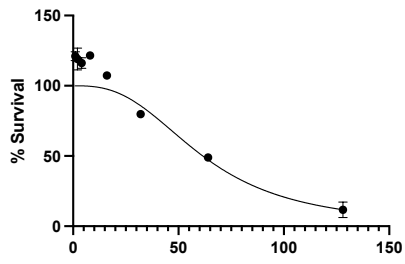
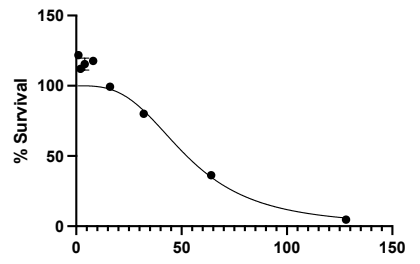
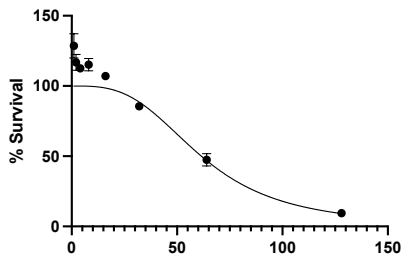
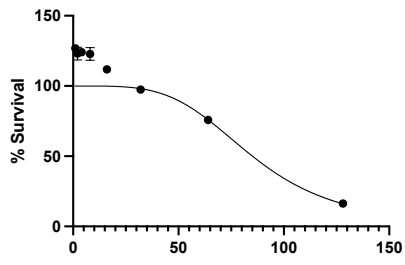
**KP-A10****KP-A11****KP-B1****KP-B3****KP-B4****KP-B5****KP-B6****KP-B7****KP-B8**



**KP-B9****KP-B10****KP-B11****PA-A1****PA-A3****AP-A4****PA-A5****PA-A6****PA-A7**

**PA-A8****PA-A9****PA-A10****PA-A11****PA-B1****PA-B3****PA-B4****PA-B5****PA-B6**

**PA-B7****PA-B8****PA-B9****PA-B10****PA-B11****AB1****AB3****AB4****AB5**

**AB6****AB7****AB8****AB9****AB10****AB11**