Supporting Information

for

Triazole-linked transition state analogs as selective inhibitors against V. cholerae sialidase

Teri J. Slack,^{#a} Wanqing Li,^{#a} Dashuang Shi,^b John B. McArthur,^a Gengxiang Zhao,^b Yanhong Li,^aAn Xiao,^a Zahra Khedri,^a Hai Yu,^a Yang Liu,^{b,&} and Xi Chen^{a,*}

^aDepartment of Chemistry, University of California-Davis, One Shields Avenue, Davis, CA 95616, USA

^bCenter for Genetic Medicine Research, Children's National Medical Center, 111 Michigan Ave, NW, Washington DC 20012, USA

[#] These authors contributed equality to this work.

- [&] Current address: Division of Immunotherapy, Institute of Human Virology, University of Maryland, Baltimore, MD 21201, United States
- * Corresponding author. Tel: +1 530 754 6037; fax: +1 530 752 8995. *E-mail address:* <u>xiichen@ucdavis.edu</u> (X. Chen).

Table of Contents

Figure S1. Multiple sequence alignment (MSA) of sialidases tested in the current study......S2

Figure S1. Multiple sequence alignment (MSA) of sialidases tested in the current study. The MSA was generated using CLC Sequence Viewer 7.0 and constructed with an open gap cost of 5.0, gap extension cost of 1.0, and cheap end gap cost. The site of interest is marked with an asterisk "*" on the top.

| | | | | | | * | | |
|---------------|------------|------------|-------------------------|--------------|------------|-------------|------------|----------------|
| V cholerae | GSNWQTGSTL | PIPER | WKSSSI | LETLEPSEAD | MVELQNGD | - LLLTARLDE | NQIVNGVNYS | PROOFLSKDG 65 |
| CpNanH | GETWTMGNKV | PNS | | NTSENM | VIEL - DG | ALIMSTRYDY | S G | YRAAYISHDL 26 |
| SpNanA | GKTWHAGEAN | NDNRQVDGQK | HSSTM NN | KRAQNT - EST | VVQLNNG | DVKLEMR | GL TG | DLOVATSKDG 60 |
| SpNanB | GQTW | K | KSSASIPFEN | ATAEAQ | MVELRDG | VIRTEER | TT TG | KIAYMTSRDS 57 |
| SpNanC | GASW | K | VKVVPLP-SS | WSAEAQ | FVELSPG | MIQAYMR | TN NG | KIAYLTSKDA 53 |
| A ureafaciens | GNTWHKGANN | GDRMD | | ENK | TVELSDG | RVELNSR | DNANQG | YRKVAVSTDG 31 |
| BiNanH2 | GATWHAGTPN | GDHMD | | ENK | VVELSDG | RVMLNSR | SSDGNG | CRYNALSRDG 26 |
| hNEU2 | GRTWARGHEV | | · · · · · · · · · · · · | AQDTLECQ | VAEVETGEOR | VVTLNAR | SHL - RA | RVQAQSTND - 25 |
| Consensus | GATWHAG V | | | A E X Q | VVELSDG | VVLLNXR | SN NG | XRXVATSKDG |
| Conservation | | 000000000 | | | | | | |

¹H and ¹³C NMR spectra of (propargyl)-A (**3**)





¹H and ¹³C NMR spectra of (propargyl)-AdE (4)





¹H and ¹³C NMR spectra of E-(propargyl)-AKE (**5**)





¹H and ¹³C NMR spectra of (TriazoNeu5Ac2en)-A (6)













