## **Supplementary Information**

for

## Synthesis of selective inhibitors against V. *cholerae* sialidase and human cytosolic sialidase NEU2

Zahra Khedri,<sup>‡</sup><sup>a</sup> Yanhong Li,<sup>‡</sup><sup>a</sup> Hongzhi Cao,<sup>a,b</sup> Jingyao Qu,<sup>a</sup> Hai Yu,<sup>a</sup> Musleh M. Muthana,<sup>a</sup> Xi Chen<sup>\*a</sup>

<sup>a</sup> Department of Chemistry, University of California, One Shields Avenue, Davis, California 95616, USA. E-mail: chen@chem.ucdavis.edu; Fax: +1 530-752-8995; Tel: +1 530-754-6037
<sup>b</sup> Current address: National Glycoengineering Research Center, Shandong University, Jinan, Shandong 250012, China

<sup>‡</sup>These authors contributed equally.

\*Correspondence: Xi Chen, Ph. D.; Fax: 01-530-752-8995; Tel: 01-530-754-6037; E-mail: chen@chem.ucdavis.edu

Figure	<b>S1.</b>	Overlays	of	Neu5Ac2en	(1)	and	Neu5Ac9N <sub>3</sub> 2en	(3),	Neu5Gc9N <sub>3</sub> 2en	(4),	or
Neu5Ac	$N_39N$	[ <sub>3</sub> 2en ( <b>5</b> ) in	the	crystal structu	res o	of hum	an NEU2 and V. a	choler	ae sialidase		S2

<sup>1</sup> H NMR and <sup>13</sup> C NMR spectra of Neu5Ac9N <sub>3</sub> 2en <b>3</b>	S3–S4
<sup>1</sup> H NMR and <sup>13</sup> C NMR spectra of Neu5Gc9N <sub>3</sub> 2en <b>4</b>	S5–S6
<sup>1</sup> H NMR and <sup>13</sup> C NMR spectra of Neu5AcN <sub>3</sub> 9N <sub>3</sub> 2en <b>5</b>	S7–S8
<sup>1</sup> H NMR and <sup>13</sup> C NMR spectra of Neu5Ac9OMe2en 6	S9–S10
<sup>1</sup> H NMR and <sup>13</sup> C NMR spectra of Neu5Ac9NPro2en 7	S11–S12

Figure S1. Overlays of Neu5Ac2en (1) (C atoms: cyan) and Neu5Ac9N<sub>3</sub>2en (3), Neu5Gc9N<sub>3</sub>2en (4), or Neu5AcN<sub>3</sub>9N<sub>3</sub>2en (5) (Compounds 3–5, C atoms: green) in the crystal structures of human NEU2 (A) and *V. cholerae* sialidase (B). The surfaces of proteins are colored according to the electrostatic potential. Positive potentials are shown in blue, negative potentials are in red, and neutral potentials are in white.



<sup>1</sup>H NMR spectrum of Neu5Ac9N<sub>3</sub>2en (**3**)



<sup>13</sup>C NMR spectrum of Neu5Ac9N<sub>3</sub>2en (**3**)



<sup>1</sup>H NMR spectrum of Neu5Gc9N<sub>3</sub>2en (4)



<sup>13</sup>C NMR spectrum of Neu5Gc9N<sub>3</sub>2en (4)



<sup>1</sup>H NMR spectrum of Neu5AcN<sub>3</sub>9N<sub>3</sub>2en (5)



<sup>13</sup>C NMR spectrum of Neu5AcN<sub>3</sub>9N<sub>3</sub>2en (5)







<sup>13</sup>C NMR spectrum of Neu5Ac9OMe2en (6)







<sup>13</sup>C NMR spectrum of Neu5Ac9NPro2en (7)

