## **Supporting Information**

## Design, Synthesis and Biological Evaluation of Sugar-Derived Esters, $\alpha$ -Ketoesters and $\alpha$ -Ketoamides as Inhibitors for *Mycobacterium tuberculosis* Antigen 85C

Aditya K. Sanki, Julie Boucau, Francis E. Umesiri, Donald R. Ronning and

Steven J. Sucheck\*

The University of Toledo, Department of Chemistry, 2801 W. Bancroft Street, Toledo, OH, USA.

\**E-mail*: <u>Steve.Sucheck@UTNet.UToledo.Edu</u>

## **Supporting Information Contents**

Page S-1: Title of the paper, author's names, address, and table of contents Page S-2: Table of contents continued Page S-3: <sup>1</sup>H NMR of methyl 2,3-di-*O*-benzyl-5-*O*-trityl-β-D-arabinofuranoside (8) Page S-4: <sup>13</sup>C NMR of methyl 2,3-di-*O*-benzyl-5-*O*-trityl-β-D-arabinofuranoside (8) methyl Page S-5:  $^{1}H$ NMR of (5E)-2,3-di-O-benzyl-5,6-dideoxy-β-D-arabino-hept-5enofuranosiduronic acid methyl ester (10)  $^{13}C$ (5E)-2,3-di-O-benzyl-5,6-dideoxy-β-D-arabino-hept-5-Page S-6: NMR of methyl enofuranosiduronic acid methyl ester (10) Page S-7: <sup>1</sup>H NMR of methyl  $\beta$ -D-arabino-heptafuranosiduronic acid methyl ester (1) Page S-8: <sup>13</sup>C NMR of methyl  $\beta$ -D-arabino-heptafuranosiduronic acid methyl ester (1) Page S-9: <sup>1</sup>H NMR of methyl 2,3-di-*O*-benzyl-β-D-arabino-heptafuranosiduronic acid methyl ester (11) Page S-10: <sup>13</sup>C NMR of methyl 2,3-di-*O*-benzyl-β-D-arabino-heptafuranosiduronic acid methyl ester (11) Page S-11: <sup>1</sup>H NMR of methyl 2,3-di-*O*-benzyl-β-D-arabino-heptafuranosiduronic acid (12) Page S-12: <sup>13</sup>C NMR of methyl 2,3-di-*O*-benzyl-β-D-arabino-heptafuranosiduronic acid (12) Page S-13: <sup>1</sup>H NMR of methyl 2,3-di-*O*-benzyl-7-keto-β-D-arabino-nonafuranosiduronitrile (13) Page S-14: <sup>13</sup>C NMR of methyl 2,3-di-O-benzyl-7-keto-β-D-arabino-nonafuranosiduronitrile (13) Page S-15: <sup>31</sup>P NMR of methyl 2,3-di-*O*-benzyl-7-keto- $\beta$ -D-arabino-nonafuranosiduronitrile (13) Page S-16: <sup>1</sup>H NMR of methyl 2,3-di-O-benzyl-7-keto-β-D-arabino-octafuranosiduronic acid methyl ester (14) Page S-17: <sup>13</sup>C NMR of methyl 2,3-di-O-benzyl-7-keto-β-D-arabino-octafuranosiduronic acid methyl ester (14) Page S-18: <sup>1</sup>H NMR of methyl 7-keto-β-D-arabino-octafuranosiduronic acid methyl ester (2) Page S-19: <sup>13</sup>C NMR of methyl 7-keto-β-D-arabino-octafuranosiduronic acid methyl ester (2) Page S-20: <sup>1</sup>H NMR of methyl *N*-butyl-2,3-di-*O*-benzyl-7-keto-β-D-arabino-octafuranosiduronamide (15) Page S-21: <sup>13</sup>C NMR of methyl N-butyl-2,3-di-O-benzyl-7-keto-β-D-arabino-octafuranosiduronamide (15) Page S-22: <sup>1</sup>H NMR of methyl *N*-butyl-7-keto- $\beta$ -D-arabino-octafuranosiduronamide (3) Page S-23: <sup>13</sup>C NMR of methyl *N*-butyl-7-keto-β-D-arabino-octafuranosiduronamide (**3**) Page S-24: <sup>1</sup>H NMR of 6, 6'-di-*O*-tert-butyldiphenylsilyl- $\alpha$ -D-trehalose (18) Page S-25: <sup>13</sup>C NMR of 6, 6'-di-*O*-tert-butyldiphenylsilyl- $\alpha$ -D-trehalose (18) Page S-26: <sup>1</sup>H NMR of 2,2',3,3',4,4',6'-hepta-O-benzyl-6,6'-di-O-tert-butyldiphenylsilyl-α-Dtrehalose (20)

Page S-27: <sup>13</sup>C NMR of 2,2',3,3',4,4',6'-hepta-*O*-benzyl-6,6'-di-*O*-tert-butyldiphenylsilyl- $\alpha$ -D-trehalose (**20**)

Page S-28: <sup>1</sup>H NMR of 2,2',3,3',4,4'-hexa-O-benzyl-6,6'-di-O-tert-butyldiphenylsilyl- $\alpha$ -D-trehalose (**21**)

Page S-29: <sup>13</sup>C NMR of 2,2',3,3',4,4'-hexa-*O*-benzyl-6,6'-di-*O*-tert-butyldiphenylsilyl- $\alpha$ -D-trehalose (**21**)

Page S-30: <sup>1</sup>H NMR of bis(methyl- $\alpha$ -D-gluco-octopyranosyluronate) ether (4)

Page S-31: <sup>13</sup>C NMR of bis(methyl- $\alpha$ -D-*gluco*-octopyranosyluronate) ether (4)

Page S-32: <sup>1</sup>H NMR of bis(methyl-2,3,4-tri-*O*-benzyl- $\alpha$ -D-gluco-octopyranosyluronate) ether (24)

Page S-33: <sup>13</sup>C NMR of bis(methyl-2,3,4-tri-*O*-benzyl- $\alpha$ -D-*gluco*-octopyranosyluronate) ether (24)

Page S-34: <sup>1</sup>H NMR of bis(methyl-2,3,4-tri-*O*-benzyl- $\alpha$ -D-*gluco*-octopyranosyluronic acid) ether (25)

Page S-35: <sup>13</sup>C NMR of bis(methyl-2,3,4-tri-*O*-benzyl- $\alpha$ -D-*gluco*-octopyranosyluronic acid) ether (25)

Page S-36: <sup>1</sup>H NMR of bis(2,3,4-tri-*O*-benzyl-9-cyano-8-oxo-9-(triphenylphosphanylidene)- $\alpha$ -Dgluco-nonopyranosylurononitrile) ether (**26**)

Page S-37: <sup>13</sup>C NMR of bis(2,3,4-tri-*O*-benzyl-9-cyano-8-oxo-9-(triphenylphosphanylidene)- $\alpha$ -D-gluco-nonopyranosylurononitrile) ether (**26**)

Page S-38: <sup>31</sup>P NMR of bis(2,3,4-tri-*O*-benzyl-9-cyano-8-oxo-9-(triphenylphosphanylidene)- $\alpha$ -D-gluco-nonopyranosylurononitrile) ether (**26**)

Page S-39: <sup>1</sup>H NMR of bis(methyl-2,3,4-tri-*O*-benzyl-8-oxo- $\alpha$ -D-*gluco*-nonopyranosyluronate) ether (27)

Page S-40: <sup>13</sup>C NMR of bis(methyl-2,3,4-tri-*O*-benzyl-8-oxo- $\alpha$ -D-*gluco*-nonopyranosyluronate) ether (27)

Page S-41: <sup>1</sup>H NMR of  $bis(N-butyl-2,3,4-tri-O-benzyl-8-oxo-\alpha-D-gluco-nonapyranosyluronamide) ether (28)$ 

Page S-42:  ${}^{13}C$  NMR of bis(*N*-butyl-2,3,4-tri-*O*-benzyl-8-oxo- $\alpha$ -D-glucononapyranosyluronamide) ether (28)

Page S-43: <sup>1</sup>H NMR of trehalose-derived bicyclo-methyl ester (**29**)

Page S-44: <sup>13</sup>C NMR of trehalose-derived bicyclo-methyl ester (29)

Page S-45: <sup>1</sup>H NMR of trehalose-derived bicyclo-*N*-butylamide (**30**)

Page S-46: <sup>13</sup>C NMR of trehalose-derived bicyclo-*N*-butylamide (**30**)

<sup>1</sup>H NMR of methyl 2,3-di-*O*-benzyl-5-*O*-trityl-β-D-arabinofuranoside (8)



<sup>13</sup>C NMR of methyl 2,3-di-*O*-benzyl-5-*O*-trityl-β-D-arabinofuranoside (8)



<sup>1</sup>H NMR of methyl (5*E*)-2,3-di-*O*-benzyl-5,6-dideoxy-β-D-arabino-hept-5-enofuranosiduronic acid methyl ester (10)



<sup>13</sup>C NMR of methyl (5*E*)-2,3-di-*O*-benzyl-5,6-dideoxy-β-D-arabino-hept-5-enofuranosiduronic acid methyl ester (10)



<sup>1</sup>H NMR of methyl  $\beta$ -D-arabino-heptafuranosiduronic acid methyl ester (1)



<sup>13</sup>C NMR of methyl  $\beta$ -D-arabino-heptafuranosiduronic acid methyl ester (1)



<sup>1</sup>H NMR of methyl 2,3-di-*O*-benzyl-β-D-arabino-heptafuranosiduronic acid methyl ester (11)



<sup>13</sup>C NMR of methyl 2,3-di-*O*-benzyl-β-D-arabino-heptafuranosiduronic acid methyl ester (11)



<sup>1</sup>H NMR of methyl 2,3-di-*O*-benzyl-β-D-arabino-heptafuranosiduronic acid (12)



<sup>13</sup>C NMR of methyl 2,3-di-*O*-benzyl-β-D-arabino-heptafuranosiduronic acid (12)



<sup>1</sup>H NMR of methyl 2,3-di-*O*-benzyl-7-keto-β-D-arabino-nonafuranosiduronitrile (13)



<sup>13</sup>C NMR of methyl 2,3-di-*O*-benzyl-7-keto-β-D-arabino-nonafuranosiduronitrile (13)



<sup>31</sup>P NMR of methyl 2,3-di-*O*-benzyl-7-keto-β-D-arabino-nonafuranosiduronitrile (13)



<sup>1</sup>H NMR of methyl 2,3-di-*O*-benzyl-7-keto-β-D-arabino-octafuranosiduronic acid methyl ester (14)



<sup>13</sup>C NMR of methyl 2,3-di-*O*-benzyl-7-keto-β-D-arabino-octafuranosiduronic acid methyl ester (14)



<sup>1</sup>H NMR of methyl 7-keto-β-D-arabino-octafuranosiduronic acid methyl ester (2)



<sup>13</sup>C NMR of methyl 7-keto-β-D-arabino-octafuranosiduronic acid methyl ester (2)



<sup>1</sup>H NMR of methyl *N*-butyl-2,3-di-*O*-benzyl-7-keto-β-D-arabino-octafuranosiduronamide (15)



<sup>13</sup>C NMR of methyl *N*-butyl-2,3-di-*O*-benzyl-7-keto-β-D-arabino-octafuranosiduronamide (15)



<sup>1</sup>H NMR of methyl *N*-butyl-7-keto-β-D-arabino-octafuranosiduronamide (3)



<sup>13</sup>C NMR of methyl *N*-butyl-7-keto-β-D-arabino-octafuranosiduronamide (3)



<sup>1</sup>H NMR of 6, 6'-di-*O-tert*-butyldiphenylsilyl-α-D-trehalose (18)



<sup>13</sup>C NMR of 6, 6'-di-*O-tert*-butyldiphenylsilyl-α-D-trehalose (18)



<sup>1</sup>H NMR of 2,2',3,3',4,4',6'-Hepta-O-benzyl-6,6'-di-O-tert-butyldiphenylsilyl-α-D-trehalose (20)



<sup>13</sup>C NMR of 2,2',3,3',4,4',6'-hepta-*O*-benzyl-6,6'-di-*O*-tert-butyldiphenylsilyl-α-D-trehalose (20)



<sup>1</sup>H NMR of 2,2',3,3',4,4'-hexa-*O*-benzyl-6,6'-di-*O-tert*-butyldiphenylsilyl-α-D-trehalose (21)



<sup>13</sup>C NMR of 2,2',3,3',4,4'-hexa-*O*-benzyl-6,6'-di-*O-tert*-butyldiphenylsilyl-α-D-trehalose (21)



<sup>1</sup>H NMR of bis(methyl-α-D-*gluco*-octopyranosyluronate) ether (4)



<sup>13</sup>C NMR of bis(methyl-α-D-*gluco*-octopyranosyluronate) ether (4)



<sup>1</sup>H NMR of bis(methyl-2,3,4-tri-*O*-benzyl-α-D-*gluco*-octopyranosyluronate) ether (24)



<sup>13</sup>C NMR of bis(methyl-2,3,4-tri-*O*-benzyl-α-D-*gluco*-octopyranosyluronate) ether (24)



<sup>1</sup>H NMR of bis(methyl-2,3,4-tri-*O*-benzyl-α-D-*gluco*-octopyranosyluronic acid) ether (25)



<sup>13</sup>C NMR of bis(methyl-2,3,4-tri-*O*-benzyl-α-D-*gluco*-octopyranosyluronic acid) ether (25)



<sup>1</sup>H NMR of bis(2,3,4-tri-*O*-benzyl-9-cyano-8-oxo-9-(triphenylphosphanylidene)-α-D-*gluco*-nonopyranosylurononitrile) ether (26)



<sup>13</sup>C NMR of bis(2,3,4-tri-*O*-benzyl-9-cyano-8-oxo-9-(triphenylphosphanylidene)-α-D-*gluco*-nonopyranosylurononitrile) ether (26)



<sup>31</sup>P NMR of bis(2,3,4-tri-*O*-benzyl-9-cyano-8-oxo-9-(triphenylphosphanylidene)-α-D-*gluco*-nonopyranosylurononitrile) ether (26)



<sup>1</sup>H NMR of bis(methyl-2,3,4-tri-*O*-benzyl-8-oxo-α-D-*gluco*-nonopyranosyluronate) ether (27)



<sup>13</sup>C NMR of bis(methyl-2,3,4-tri-*O*-benzyl-8-oxo-α-D-*gluco*-nonopyranosyluronate) ether (27)



<sup>1</sup>H NMR of bis(*N*-butyl-2,3,4-tri-*O*-benzyl-8-oxo-α-D-*gluco*-nonapyranosyluronamide) ether (28)



<sup>13</sup>C NMR of bis(*N*-butyl-2,3,4-tri-*O*-benzyl-8-oxo-α-D-*gluco*-nonapyranosyluronamide) ether (28)



<sup>1</sup>H NMR of trehalose-derived bicyclo-methyl ester (29)



<sup>13</sup>C NMR of trehalose-derived bicyclo-methyl ester (29)



<sup>1</sup>H NMR of trehalose-derived bicyclo-*N*-butylamide (30)



<sup>13</sup>C NMR of trehalose-derived bicyclo-*N*-butylamide (30)

