

Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

A cationic cysteine-hydrazide as an enrichment tool for the mass spectrometric characterization of bacterial free oligosaccharides

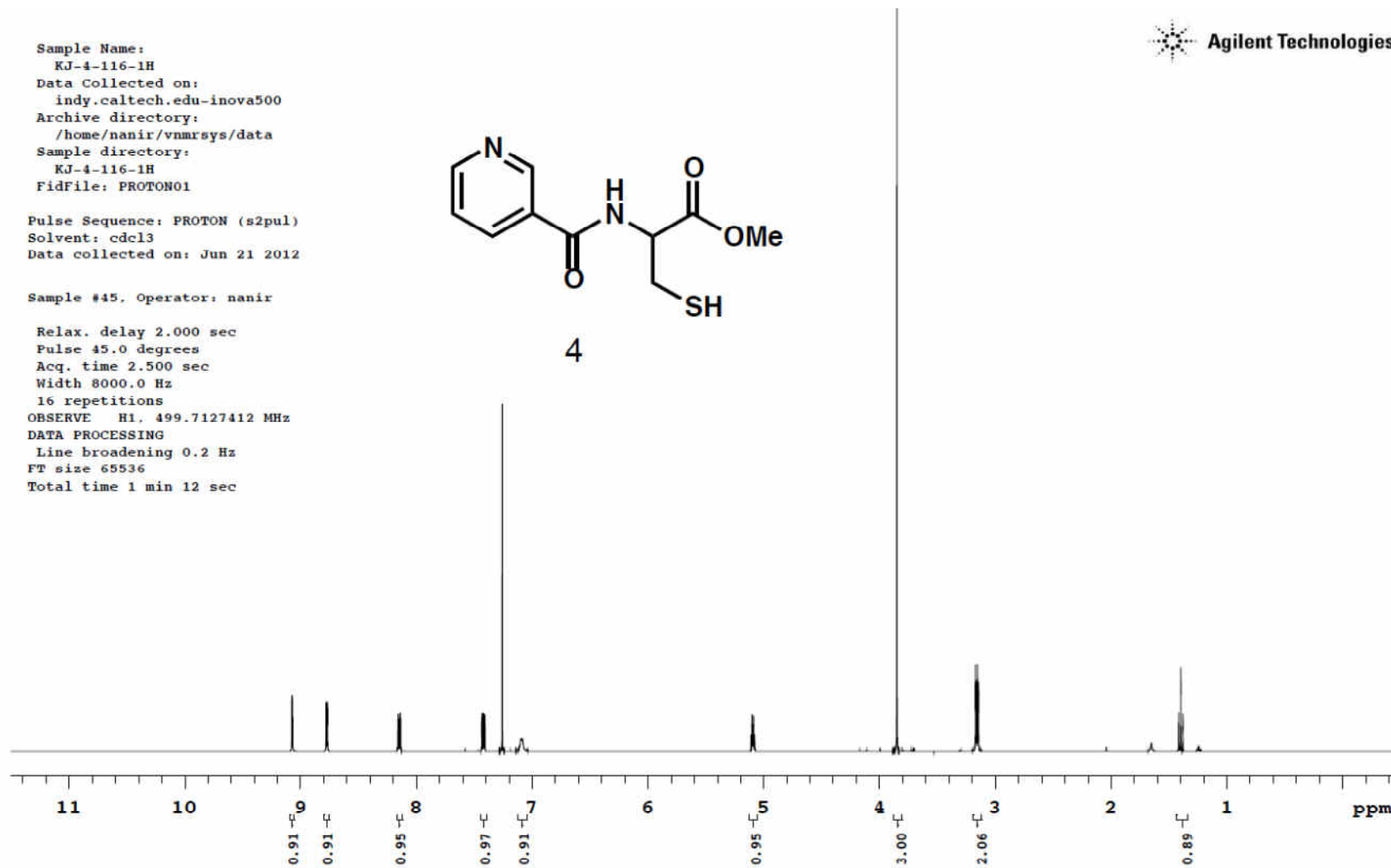
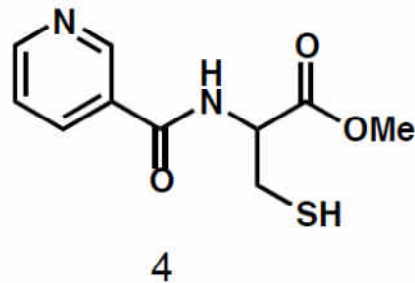
Kyoung-Soon Jang, Roger R. Nani, Anastasia Kalli, Sergiy Levin, Axel Müller, Sonja Hess, Sarah E. Reisman, William M. Clemons, Jr.

Sample Name:
 KJ-4-116-1H
 Data Collected on:
 indy.caltech.edu-inova500
 Archive directory:
 /home/nanir/vnmrsys/data
 Sample directory:
 KJ-4-116-1H
 FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Jun 21 2012

Sample #45, Operator: nanir

Relax. delay 2.000 sec
 Pulse 45.0 degrees
 Acq. time 2.500 sec
 Width 8000.0 Hz
 16 repetitions
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 DATA PROCESSING
 Line broadening 0.2 Hz
 FT size 65536
 Total time 1 min 12 sec



Plotname: --Not assigned--

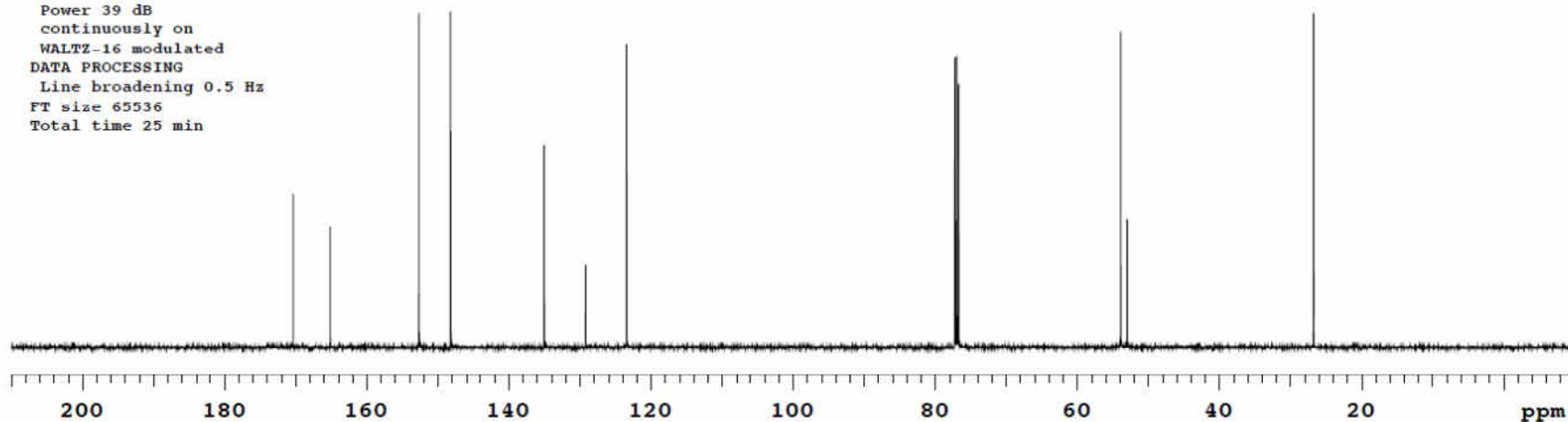
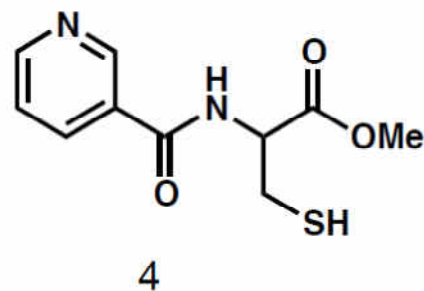
Fig. S1 NMR spectra of cysteine methyl ester nicotinamide

Sample Name:
 KJ-4-116-13C
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 indy.caltech.edu-inova500
 Archive directory:
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 Sample directory:
 KJ-4-116-13C
 FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
 Solvent: cdcl3
 Data collected on: Jun 21 2012

Sample #45, Operator: nanir

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.000 sec
 Width 31446.5 Hz
 512 repetitions
 OBSERVE C13, 125.6528748 MHz
 DECOUPLE H1, 499.7152303 MHz
 Power 39 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 65536
 Total time 25 min



Plotname: --Not assigned--

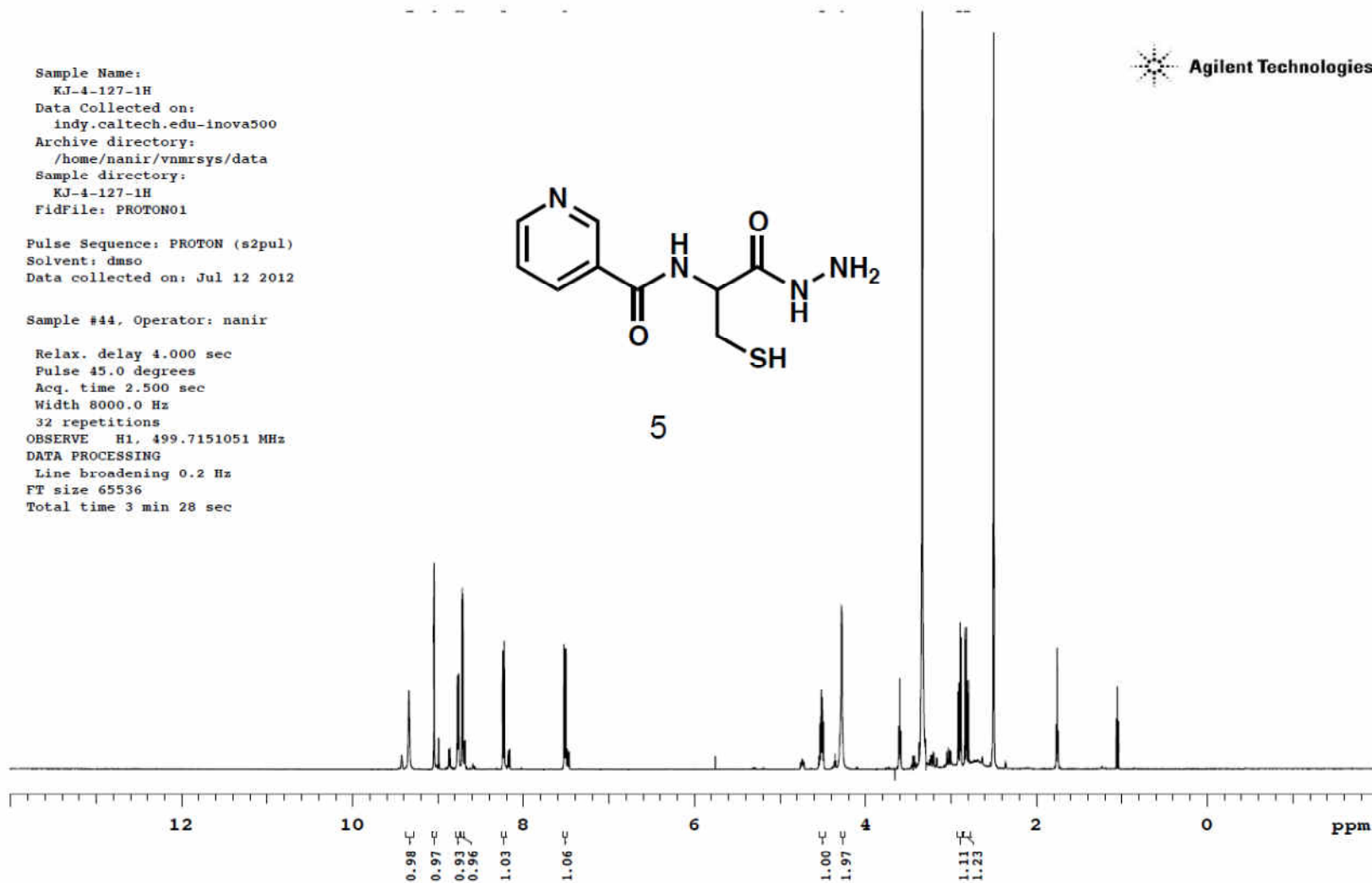
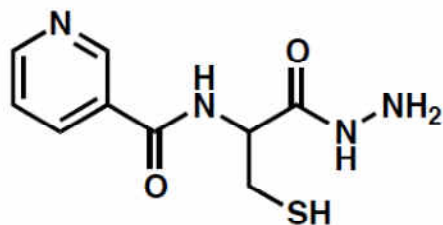
Fig. S1 (continued) NMR spectra of cysteine methyl ester nicotinamide

Sample Name:
KJ-4-127-1H
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/nanir/vnmrsys/data
Sample directory:
KJ-4-127-1H
FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)
Solvent: dms0
Data collected on: Jul 12 2012

Sample #44, Operator: nanir

Relax. delay 4.000 sec
Pulse 45.0 degrees
Acq. time 2.500 sec
Width 8000.0 Hz
32 repetitions
OBSERVE H1, 499.7151051 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 3 min 28 sec



Plotname: --Not assigned--

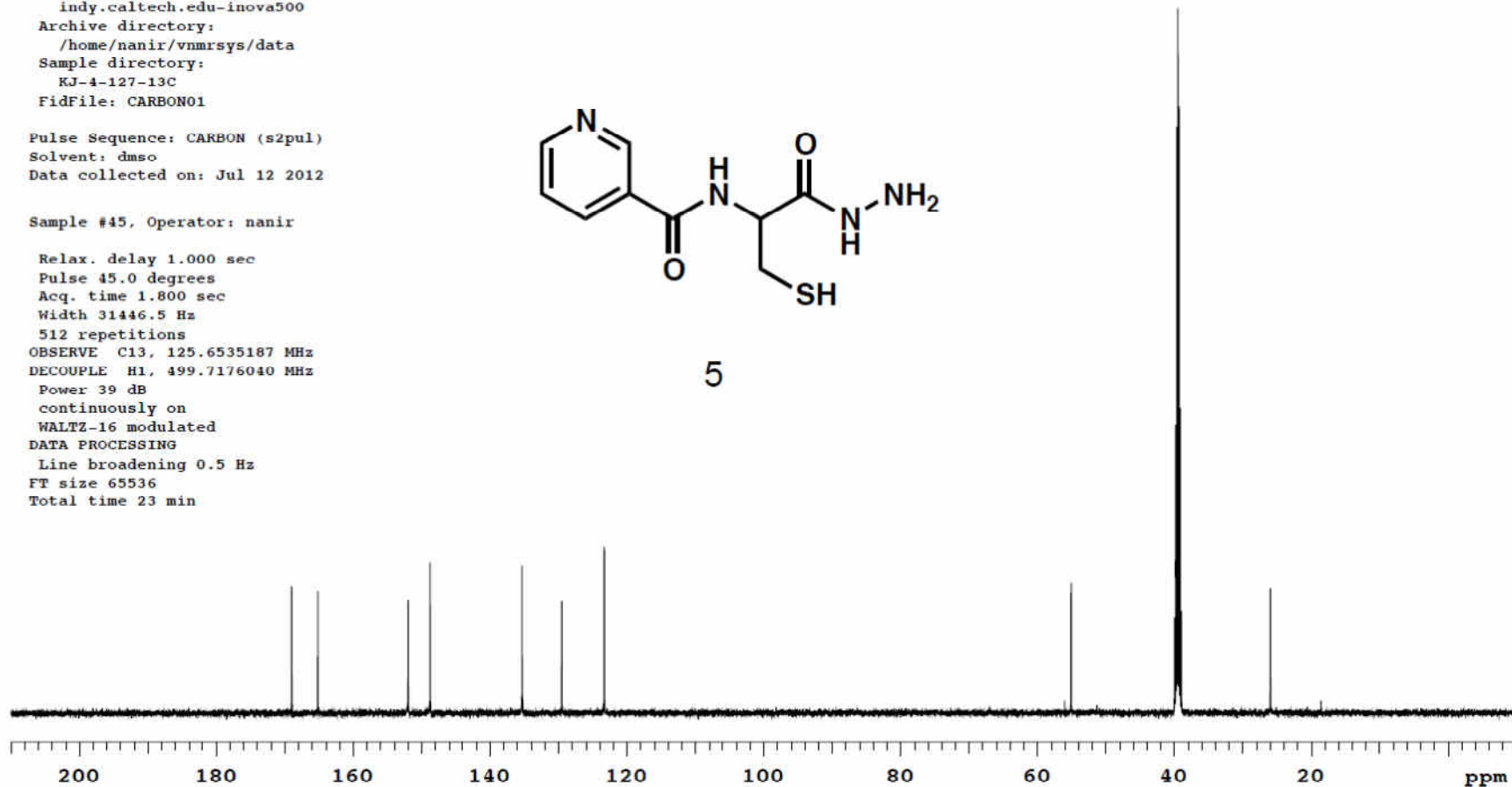
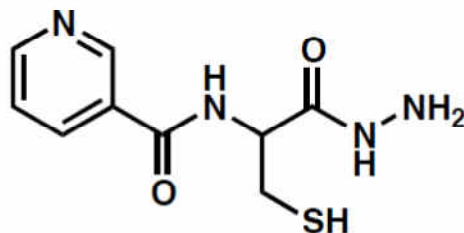
Fig. S2 NMR spectra of cysteine hydrazone nicotinamide

Sample Name:
 KJ-4-127-13C
 Data Collected on:
 indy.caltech.edu-inova500
 Archive directory:
 /home/nanir/vnmrsys/data
 Sample directory:
 KJ-4-127-13C
 FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
 Solvent: dmsd
 Data collected on: Jul 12 2012

Sample #45, Operator: nanir

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.800 sec
 Width 31446.5 Hz
 512 repetitions
 OBSERVE C13, 125.6535187 MHz
 DECOUPLE H1, 499.7176040 MHz
 Power 39 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 65536
 Total time 23 min



Plotname: --Not assigned--

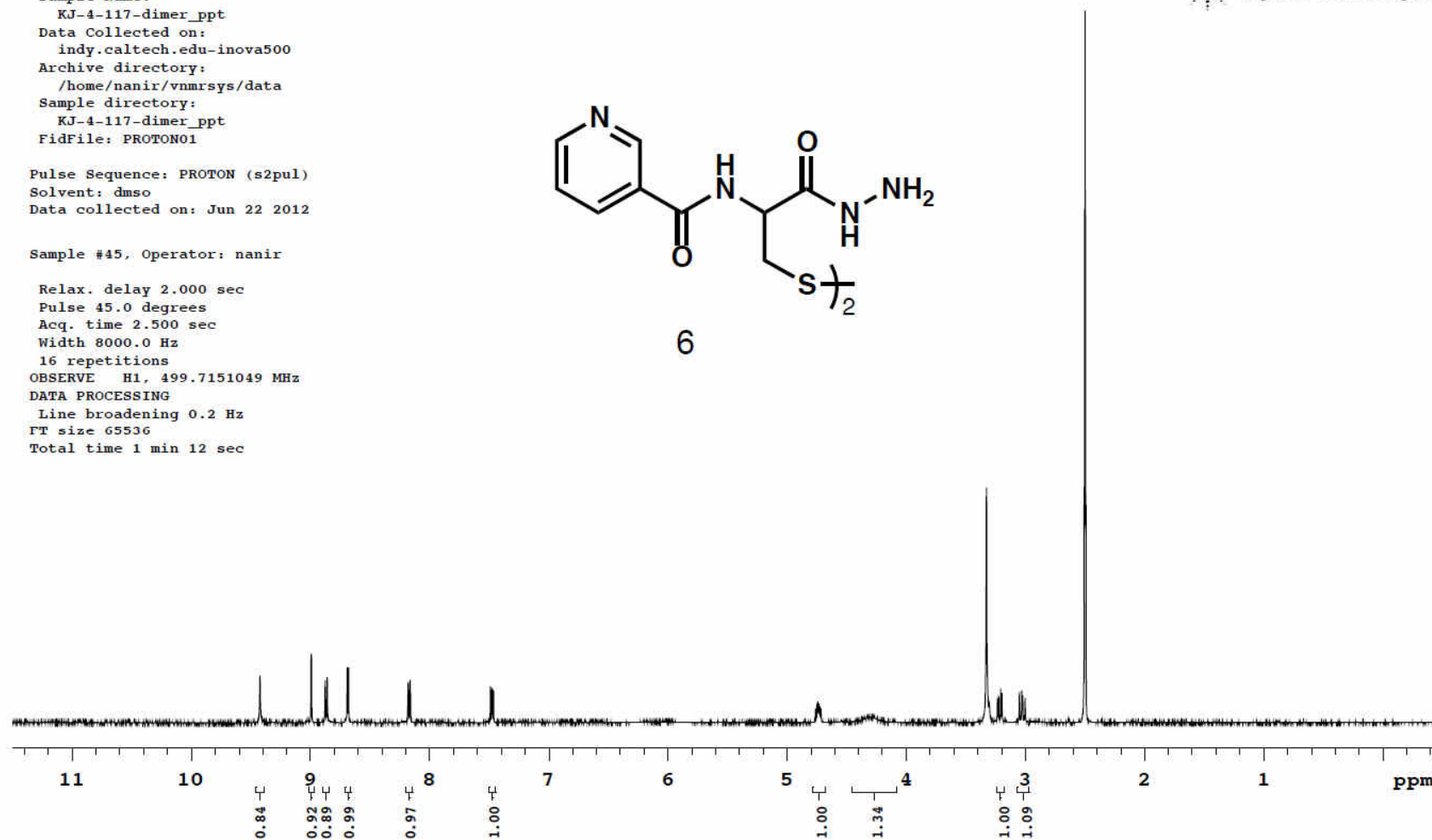
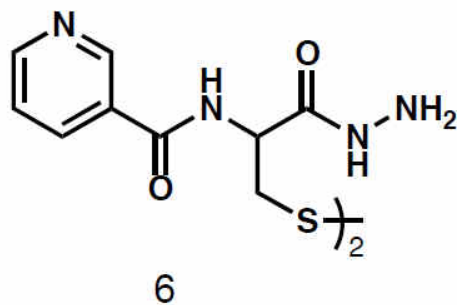
Fig. S2 (continued) NMR spectra of cysteine hydrazone nicotinamide

Sample Name:
 KJ-4-117-dimer_ppt
 Data Collected on:
 indy.caltech.edu-inova500
 Archive directory:
 /home/nanir/vnmrsys/data
 Sample directory:
 KJ-4-117-dimer_ppt
 FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)
 Solvent: dms0
 Data collected on: Jun 22 2012

Sample #45, Operator: nanir

Relax. delay 2.000 sec
 Pulse 45.0 degrees
 Acq. time 2.500 sec
 Width 8000.0 Hz
 16 repetitions
 OBSERVE H1, 499.7151049 MHz
 DATA PROCESSING
 Line broadening 0.2 Hz
 FT size 65536
 Total time 1 min 12 sec



Plotname: --Not assigned--

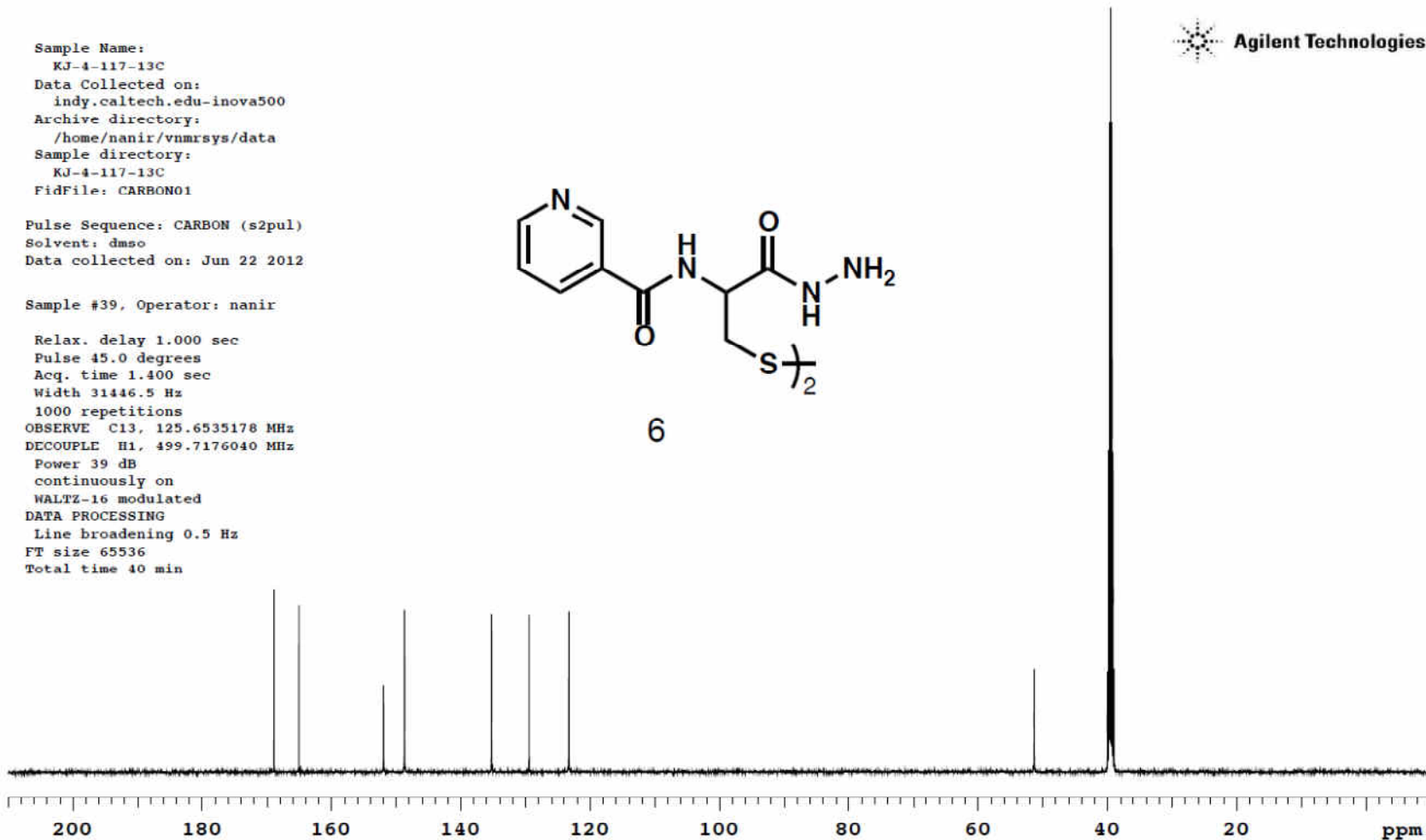
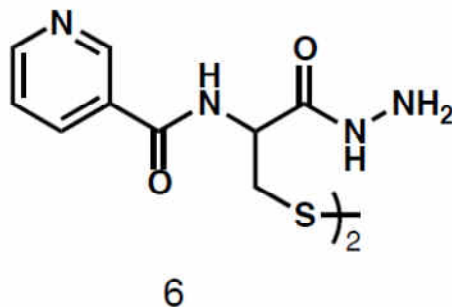
Fig. S3 NMR spectra of cystine dihydrazide nicotinamide

Sample Name:
KJ-4-117-13C
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/nanir/vnmrsys/data
Sample directory:
KJ-4-117-13C
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
Solvent: dms0
Data collected on: Jun 22 2012

Sample #39, Operator: nanir

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.400 sec
Width 31446.5 Hz
1000 repetitions
OBSERVE C13, 125.6535178 MHz
DECOUPLE H1, 499.7176040 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 40 min



Plotname: --Not assigned--

Fig. S3 (continued) NMR spectra of cystine dihydrazide nicotinamide

a (CID)

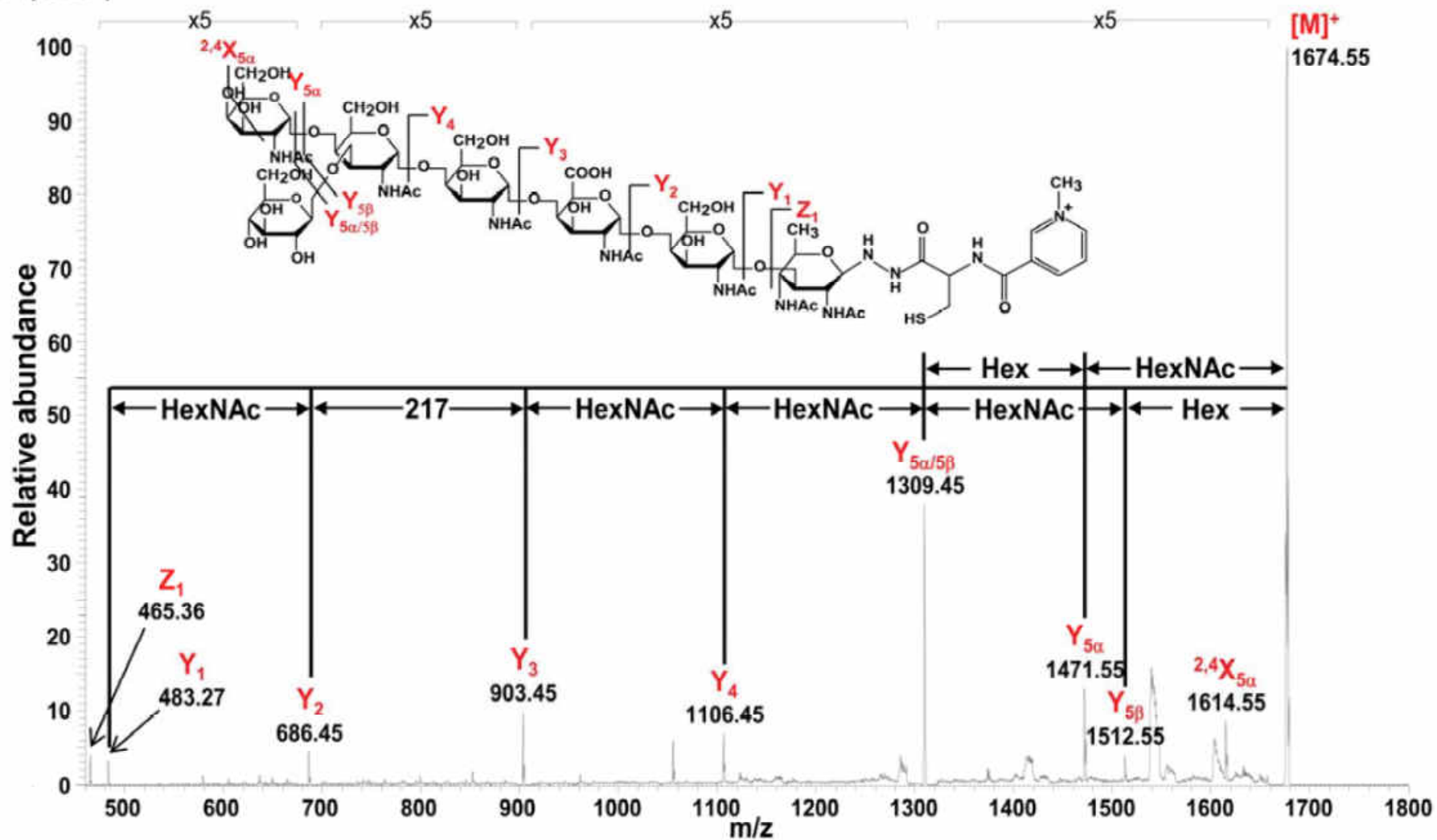


Fig. S4 Selected tandem MS spectra of the fOS_{CC}. (a) CID (30-ms with 15% collision energy)

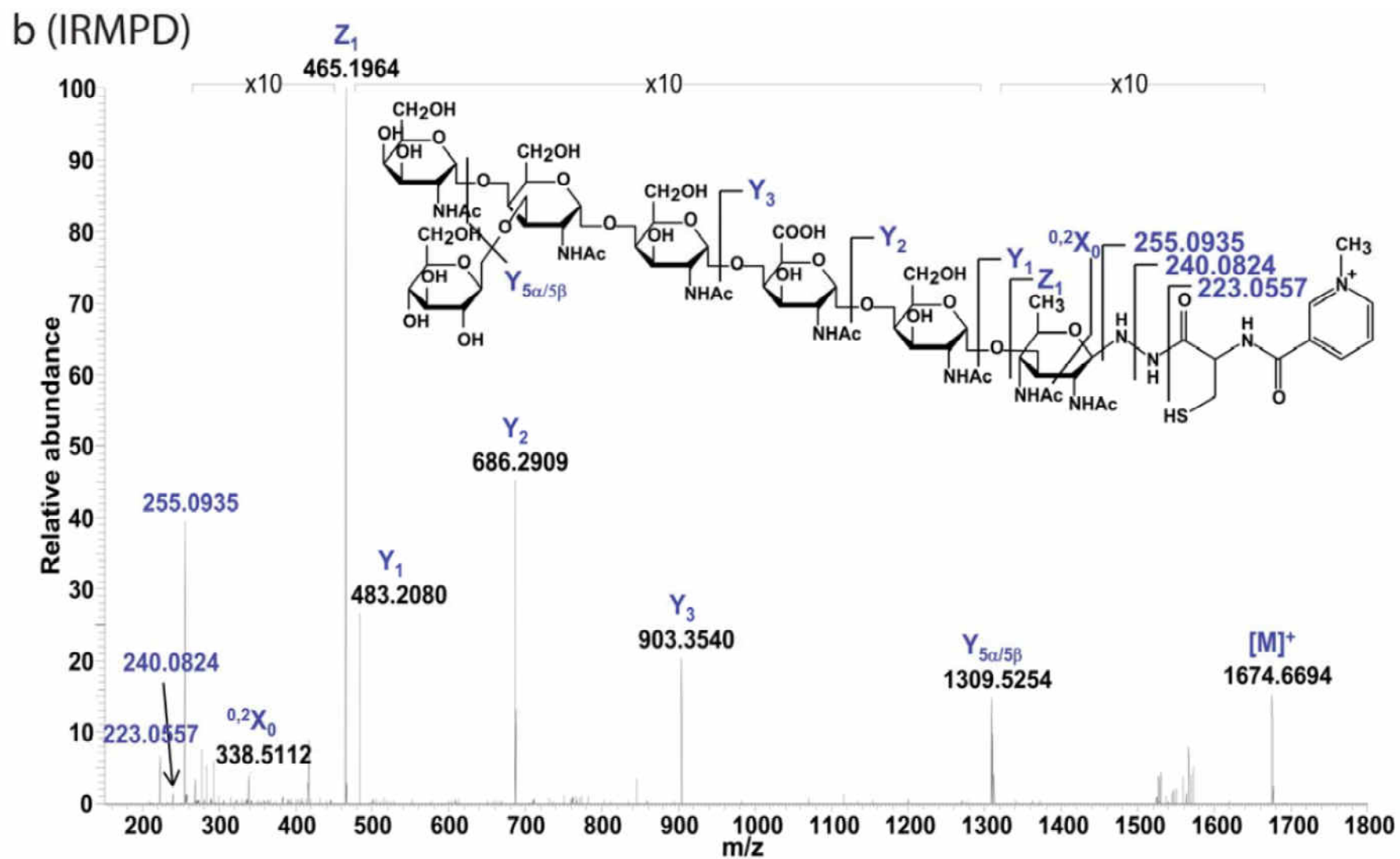
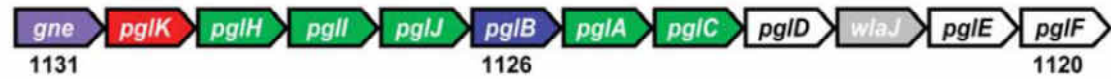


Fig. S4 (continued) Selected tandem MS spectra of the fOS_{Cc} . (b) IRMPD (50-ms with 10-W laser power) MS/MS spectra

C. jejuni NCTC11168



C. concisus RM5485



Fig. S5 Selected bacterial protein N-glycosylation (*pgl*) gene clusters. Blue, oligosaccharyltransferase gene (*pglB*); red, flippase gene (*pglK*); green, glycosyltransferase (GT) gene; purple, UDP-sugar epimerase gene (*gne* or *galE*); white, sugar biosynthesis gene. GT-25, group 25 family glycosyltransferase; UDP-DH, UDP-sugar dehydrogenase.