Electronic Supplementary Information for:

Phage-displayed Macrocyclic Glycopeptide Libraries

Simon Ng, Ratmir Derda*

Alberta Glycomics Centre and Department of Chemistry, University of Alberta, Edmonton, AB T6G 2G2, Canada

*Corresponding author: ratmir@ualberta.ca

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Abbreviations

AOB	Aminooxy-biotin
BIA	Biotin-PEG_2-iodoacetamide
DCA	1,3-Dichloroacetone
DCO	Dichloro-oxime derivatives
DMF	Dimethyl formamide
eq.	Equivalent
ESI	Electrospray ionization
h	Hour
HRMS	High-resolution mass spectrometry
min	Minute
MS	Mass spectroscopy
RT	Room temperature
TCEP	Tris(2-carboxyethyl)phosphine
Tris	Tris(hydroxymethyl)aminomethane
UPLC	Ultra-performance liquid chromatography
WT	Wild-type

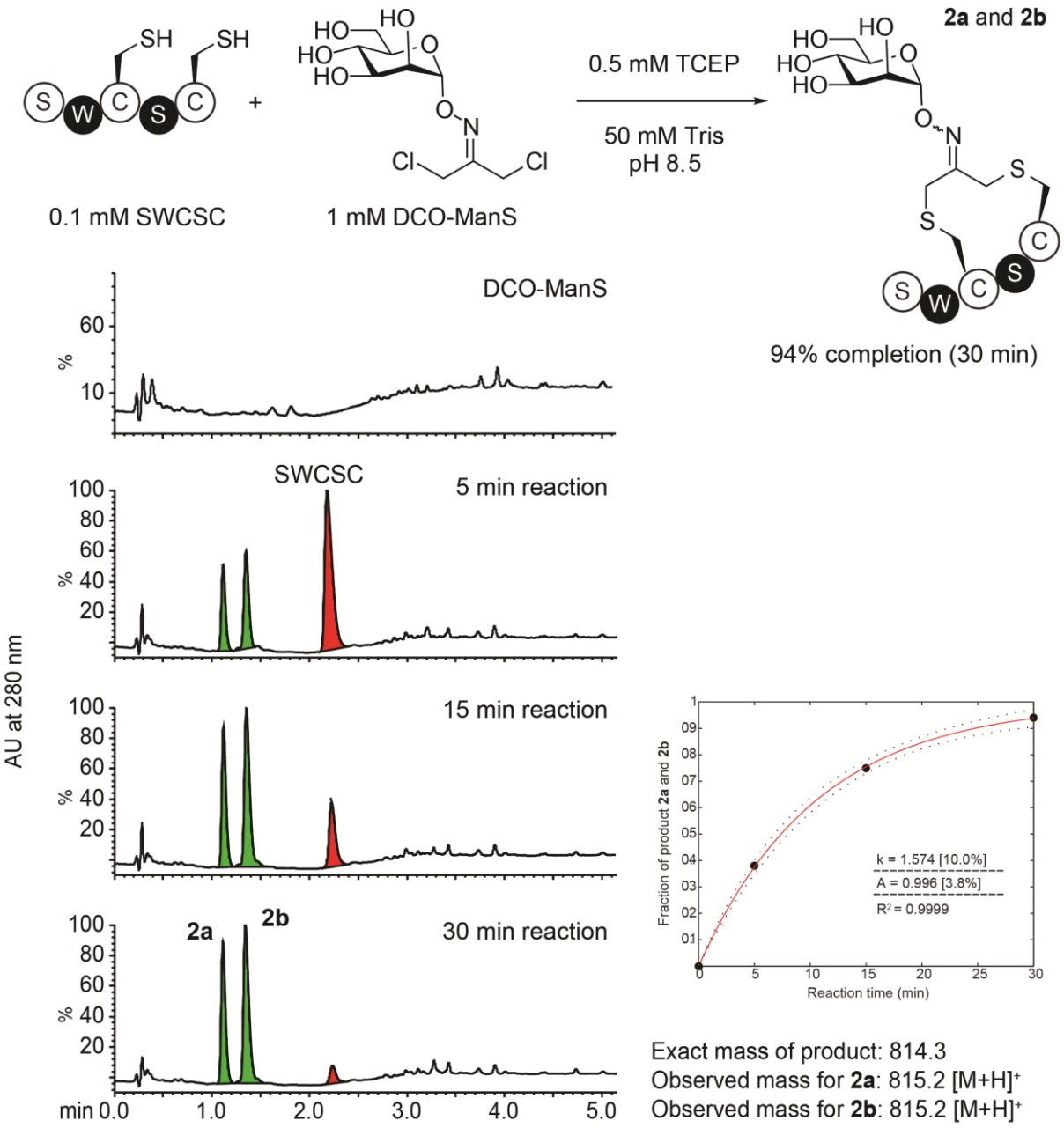


Figure S1. Reaction of SWCSC with DCO-ManS.

The reaction proceeded to near completion (94%) in 30 min as monitored by UPLC-MS. UV absorbance was detected at 280 nm. Red and green peaks represent SWCSC and the macrocyclic product (**2a** and **2b**) respectively. **2a** and **2b** are the oxime E/Z isomers and have the same m/z. The reaction was performed under pseudo-first-order condition. Fitting of the kinetic curve to the equation $A_t = 1 - e^{-k*[DCO\text{-}ManS]*t}$ yielded second-order rate constant k = 1.6 M^{-1} s^{-1}, where A_t is the fraction of the product at time t and [DCO-ManS] is 0.001 M.

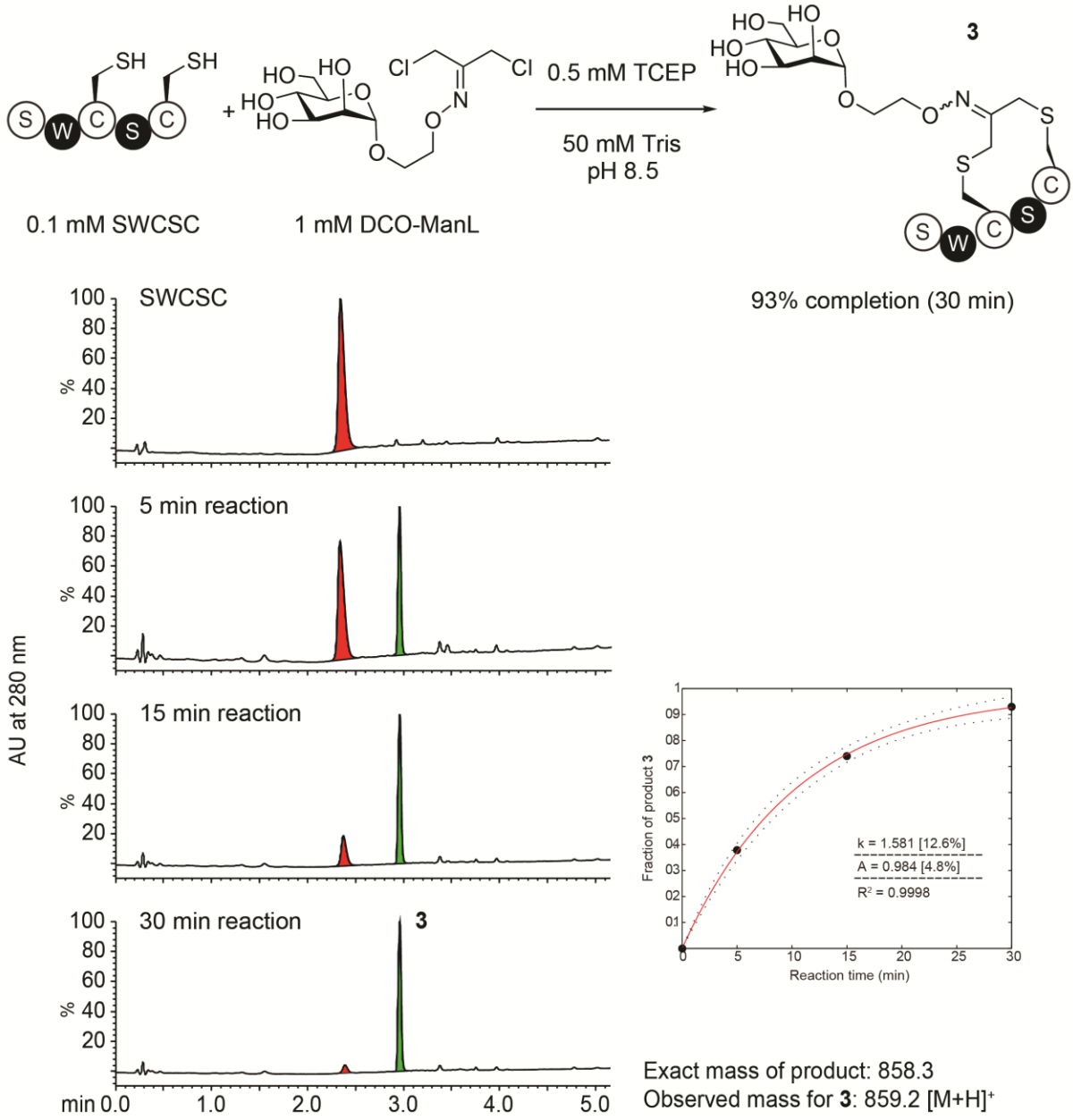


Figure S2. Reaction of SWCSC with DCO-ManL.

The reaction proceeded to near completion (93%) in 30 min as monitored by UPLC-MS. UV absorbance was detected at 280 nm. Red and green peaks represent SWCSC and the macrocyclic product (**3**) respectively. The product **3** is a mixture of E/Z isomers of oxime, but it appeared as a single peak on UPLC traces because they are inseparable. The reaction was performed under pseudo-first-order condition. Fitting of the kinetic curve to the equation $A_t = 1 - e^{-k*[DCO\text{-}ManL]*t}$ yielded second-order rate constant k = 1.6 M^{-1} s^{-1}, where A_t is the fraction of the product at time t and [DCO-ManL] is 0.001 M.

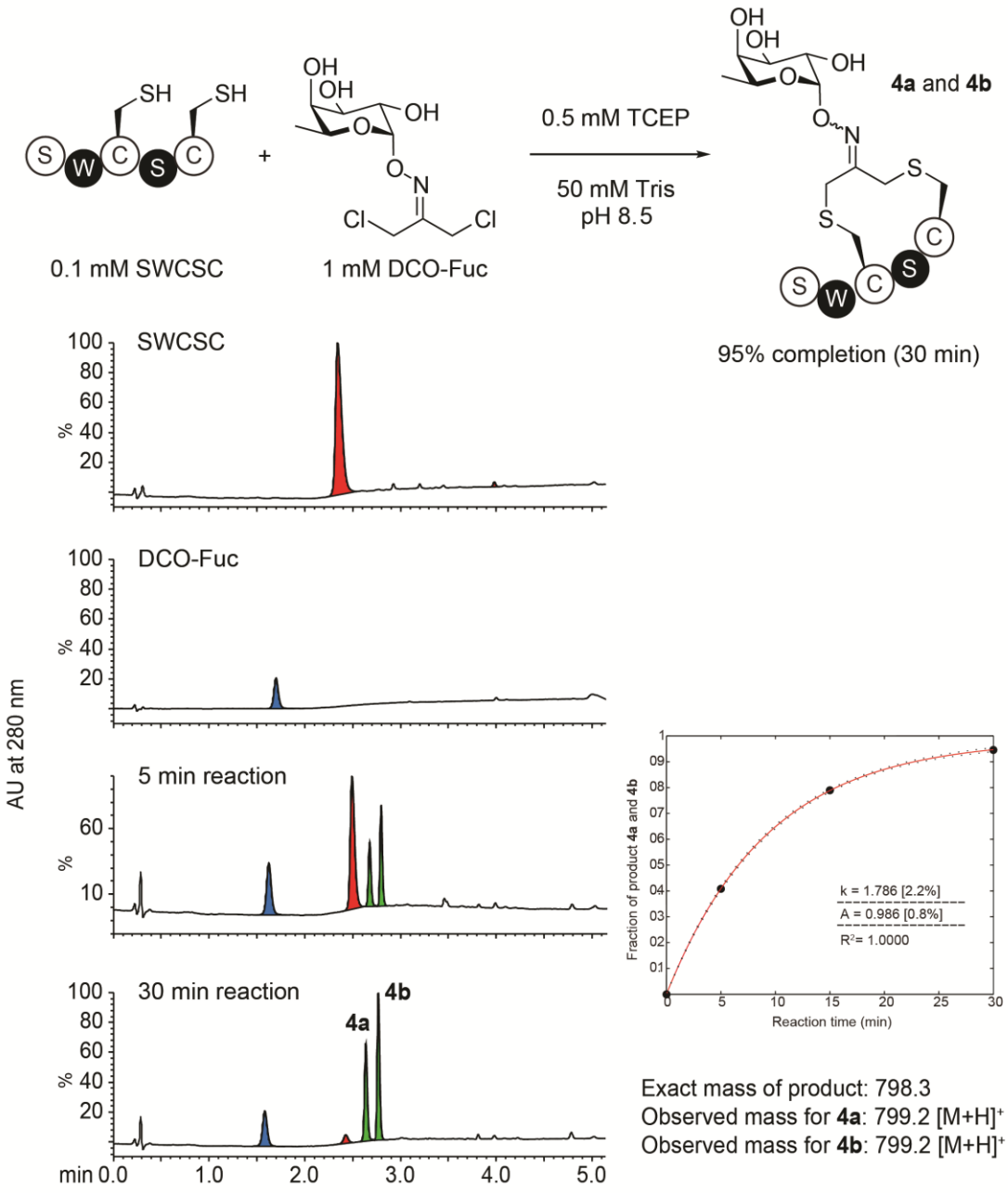


Figure S3. Reaction of SWCSC with DCO-Fuc.

The reaction proceeded to near completion (95%) in 30 min as monitored by UPLC-MS. UV absorbance was detected at 280 nm. Red and green peaks represent SWCSC and the macrocyclic product (**4a** and **4b**) respectively. **4a** and **4b** are the oxime E/Z isomers and have the same m/z. Blue peak was observed in the solution of DCO-Fuc but could not be identified unambiguously by MS, most likely due to poor ionization in electrospray. The reaction was performed under pseudo-first-order condition. Fitting of the kinetic curve to the equation $A_t = 1 - e^{-k*[DCO\text{-}Fuc]*t}$ yielded second-order rate constant k = 1.8 M^{-1} s^{-1}, where A_t is the fraction of the product at time t and [DCO-Fuc] is 0.001 M.

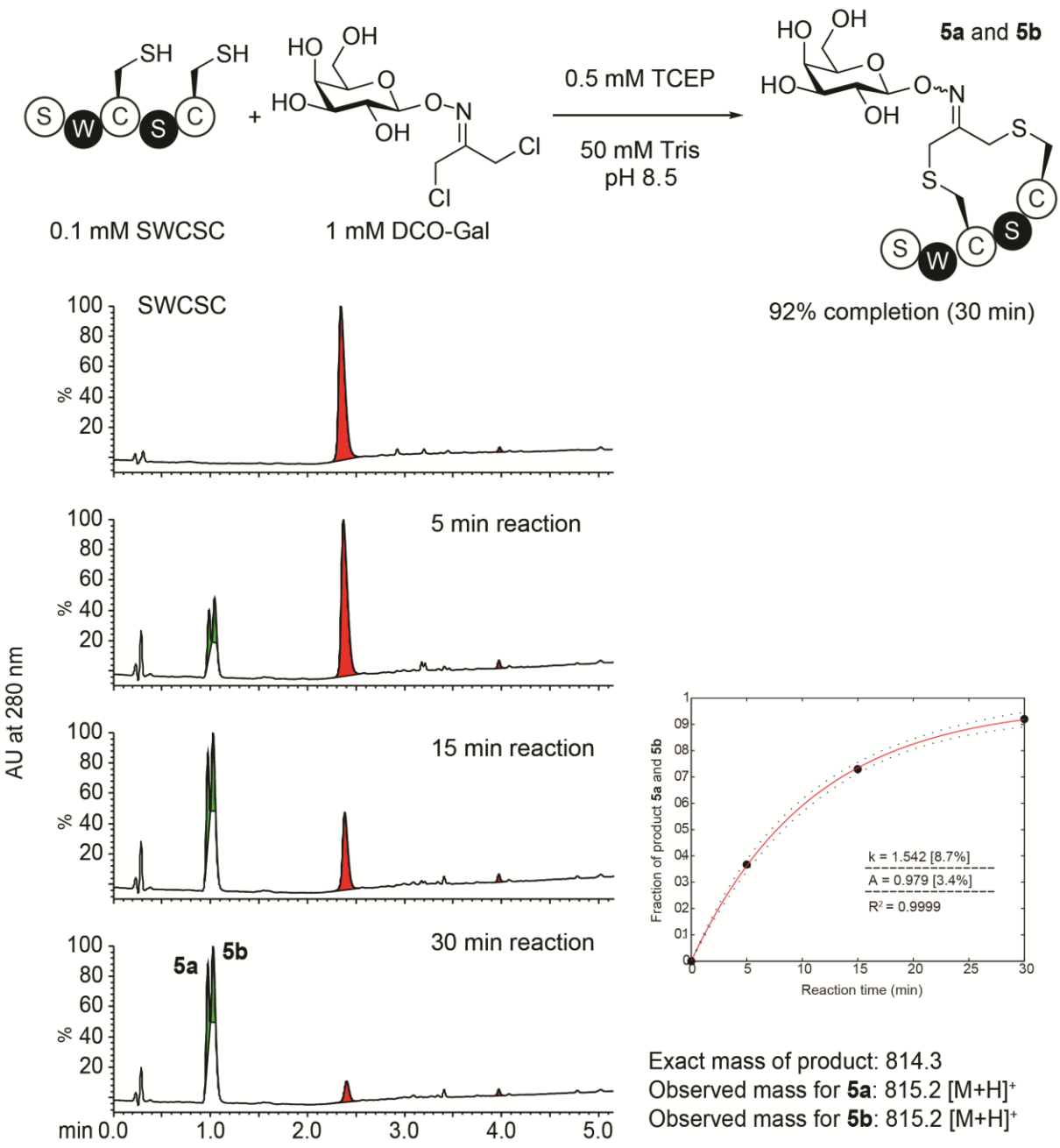


Figure S4. Reaction of SWCSC with DCO-Gal.

The reaction proceeded to near completion (92%) in 30 min as monitored by UPLC-MS. UV absorbance was detected at 280 nm. Red and green peaks represent SWCSC and the macrocyclic product (**5a** and **5b**) respectively. **5a** and **5b** are the oxime E/Z isomers and have the same m/z. The reaction was performed under pseudo-first-order condition. Fitting of the kinetic curve to the equation $A_t = 1 - e^{-k*[DCO\text{-}Gal]*t}$ yielded second-order rate constant k = 1.5 M^{-1} s^{-1}, where A_t is the fraction of the product at time t and [DCO-Gal] is 0.001 M.

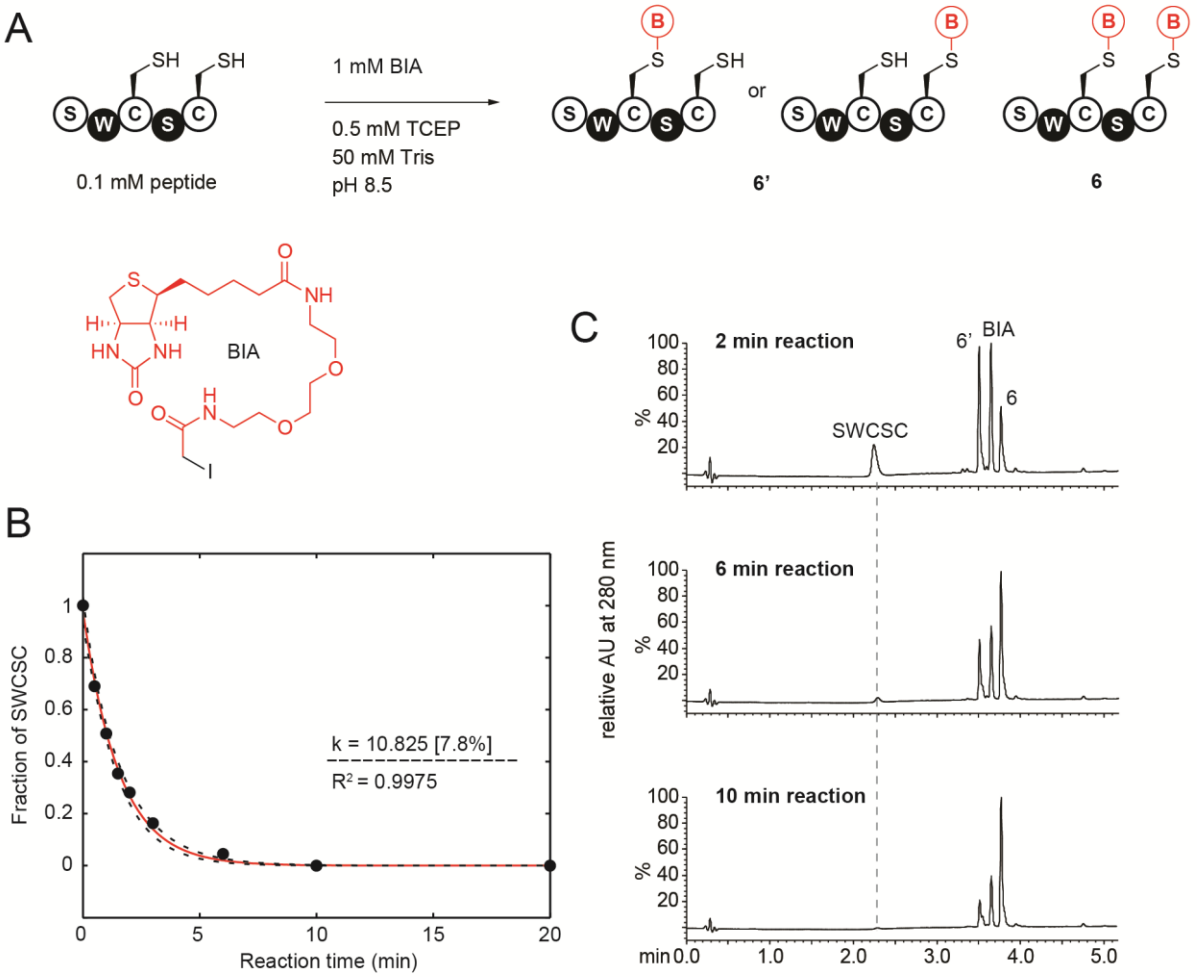


Figure S5. Kinetic profile of reaction between SWCSC and BIA.
(A) The reaction of SWCSC (0.1 mM) with 10 eq. of BIA (1 mM) proceeded to near completion in 10 min as monitor by UPLC-MS. (B) Fitting of the kinetic curve describing the disappearance of the thiol to the equation $R_t = e^{-k*[BIA]*t}$ yielded second-order rate constant k = 10.8 M^{-1} s^{-1}, where R_t is the fraction of the reactant (here peptide) remaining at time t and [BIA] is 0.001 M. (C) UPLC traces of the reaction mixture at selected time point.

Materials and general information

Tris buffer was prepared as a solution of 50 mM Tris at pH of 8.5. All solutions used for phage work were sterilized by filter sterilization (0.22 μm). The peptide (SWCSC) was synthesized on solid support according to standard protocol.[1] Aminooxy-biotin (AOB, #10009350) was purchased from Cayman Chemical. 1,3-Dichloroacetone (DCA, #168548) was purchased from Sigma-Aldrich. Biotin-PEG_2-iodoacetamide (BIA, #21334) was purchased from Thermo Fisher Scientific. Product purification was accomplished with automated chromatography machine (CombiFlash® Rf, Teledyne Isco, Inc.). ^{1}H and ^{13}C NMR spectra were acquired on Agilent/Varian VNMRS 500 MHz spectrometers. Chemical shifts (δ) are reported in ppm and coupling constants (*J*) are given in Hz. The following abbreviations classify the multiplet peaks in the ^{1}H NMR: s = singlet, d = doublet, m = multiplet or unresolved. HRMS (ESI) spectra were recorded on Agilent 6220 oaTOF mass spectrometer using either positive or negative ionization mode. Characterization of reaction crude was performed with UPLC-MS using a C18 column (Phenomenex Kinetex 1.7 μm EVO C18, 2.1×50 mm) running with a gradient of water/acetonitrile with 0.1% formic acid from 98/2 at 0 min to 40/60 at 5 min under a flow rate of 0.5 mL/min. The phage libraries ($SXCX_3C$ and $SXCX_4C$) were prepared according to literature protocol[2] using synthetic DNA oligos purchased from TriNucleotide Technologies.

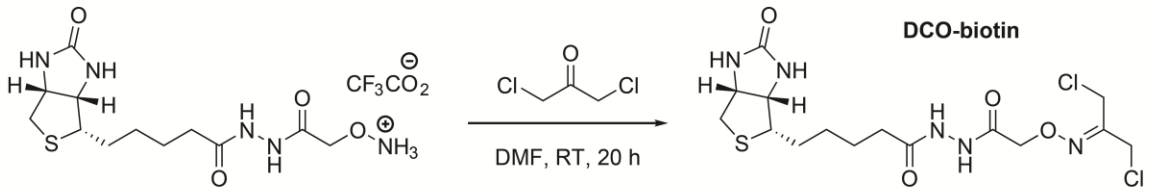
5’-CCCGGGTACCTTTCTATTCTCACTCT-TCT-X-TGT-XXX-TGT-GGTGGAGGT-TCGGCCGGGCGC-3’

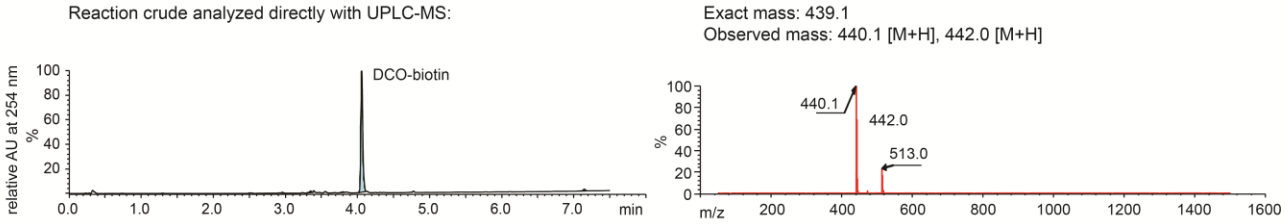
5’-CCCGGGTACCTTTCTATTCTCACTCT-TCT-X-TGT-XXXX-TGT-GGTGGAGGT-TCGGCCGGGCGC-3’

The X designates an equimolar mixture of 19 unique trinucleotide codons for all amino acids but cysteine. The synthetic oligonucleotide has been extended to form a dsDNA, and then cloned into M13KE vector using KpnI/EagI restriction enzyme cloning analogous to that described in our previous report.[2] The theoretical diversity of the $SXCX_3C$ library is 19^4=130,321 members and that of $SXCX_4C$ library is 19^5=2,476,099 members. During library production steps, we obtained transformation efficiencies of 1–2 million PFU, sufficient to cover the diversity of these libraries. Characterization of these libraries by deep sequencing and selection are beyond the scope of this report and will be described in our forthcoming publication.

Synthesis of dichloro-oxime-biotin (DCO-biotin)

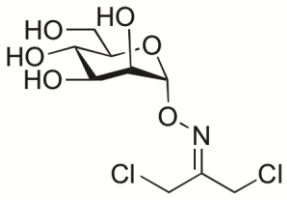
Slight excess of aminooxy-biotin (5 mg, 11 μmol, 1.1 eq.) was added to 1,3-dichloroacetone (1.3 mg, 10 μmol, 1 eq.) dissolved in DMF (100 μL). The reaction proceeded to completion within 20 h at RT. The reaction mixture was characterized by UPLC-MS (see below). The concentration of DCO-biotin produced *in situ* here was 100 mM. This solution (100× concentrated stock) was used directly for the modification of peptide or phage libraries without further purification—typically by adding 1 μL of DCO-biotin (100 mM) into 99 μL of reaction mixture containing peptide or phage.





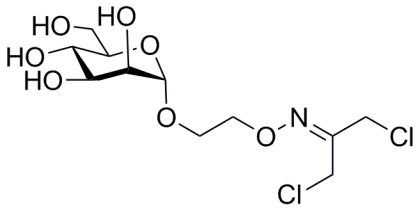
Synthesis of dichloro-oxime-carbohydrate derivatives (DCO-ManS/ManL/Fuc/Gal)

The synthesis of carbohydrate-hydroxylamine derivatives such as ManL-ONH_2 has been reported previously.[3] ManS-ONH_2, Fuc-ONH_2 and Gal-ONH_2 were synthesized using methods adapted from our previous publication.[3] To make a DCO-carbohydrate derivative, the carbohydrate-hydroxylamine derivative (40 μmol, 2 eq.) was added to 1,3-dichloroacetone (20 μmol, 1 eq.) dissolved in MeOH (0.5 mL). After 24 h reaction at RT, the solvent was evaporated. The residue was purified with silica-gel chromatography using a gradient of 0 to 10% MeOH in CH_2Cl_2 to afford the title compound as white solid in 60–90% yield.

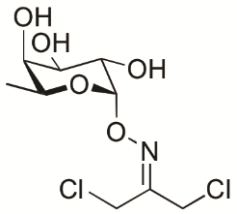


DCO-ManS: ^{1}H NMR (500 MHz, D_2O) δ = 5.49 (d, *J* = 1.5 Hz, 1 H), 4.52 (d, *J* = 12.5 Hz, 1 H), 4.42 – 4.35 (m, 3 H), 4.14 (dd, *J* = 1.5, 3.5 Hz, 1 H), 3.87 – 3.81 (m, 2 H), 3.78 – 3.73 (m, 2 H),

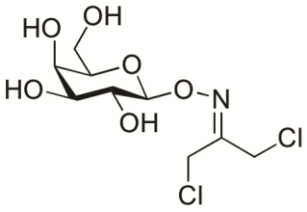
3.67 – 3.63 (m, 1H); ^{13}C NMR (125 MHz, D_2O) δ = 157.3, 102.9, 74.7, 71.6, 69.5, 67.3, 61.5, 42.7, 34.5; HRMS (ESI) calcd. for $C_9H_{15}Cl_2NO_6Na$ $[M+Na]^+$ *m/*z = 326.0169, found 326.0162.



DCO-ManL: ^{1}H NMR (500 MHz, D_2O) δ = 4.88 (d, *J* = 1.5 Hz, 1 H), 4.42 (s, 2 H), 4.38 – 4.35 (m, 4 H), 4.01 – 3.97 (m, 1 H), 3.95 – 3.94 (m, 1 H), 3.85 (dd, *J* = 2.0, 12.0 Hz, 1 H), 3.80 – 3.78 (m, 2 H), 3.75 (dd, *J* = 5.5, 12.0 Hz, 1 H), 3.68 – 3.61 (m, 2 H); ^{13}C NMR (125 MHz, D_2O) δ = 154.7, 100.9, 74.3, 73.7, 71.5, 70.9, 67.6, 66.8, 61.8, 42.9, 34.4; HRMS (ESI) calcd. for $C_{11}H_{19}Cl_2NO_7Na$ $[M+Na]^+$ *m/*z = 370.0431, found 370.0423.



DCO-Fuc: ^{1}H NMR (500 MHz, D_2O) δ = 5.53 (apparent s, 1 H), 4.59 (d, *J* = 12.5 Hz, 1 H), 4.44 – 4.35 (m, 3 H), 4.13 – 4.09 (m, 1 H), 3.96 (s, 2 H), 3.85 (s, 1 H), 1.19 (d, *J* = 6.5 Hz, 3 H); ^{13}C NMR (125 MHz, D_2O) δ = 157.4, 102.1, 72.7, 70.5, 68.8, 68.3, 42.7, 34.6, 16.2; HRMS (ESI) calcd. for $C_9H_{15}Cl_2NO_5Na$ $[M+Na]^+$ *m/*z = 310.0219, found 310.0217.



DCO-Gal: ^{1}H NMR (500 MHz, D_2O) δ = 5.03 (d, *J* = 8.0 Hz, 1 H), 4.51 (s, 2 H), 4.41 (s, 2 H), 3.97 (d, *J* = 2.5 Hz, 1 H), 3.80 – 3.74 (m, 5 H); ^{13}C NMR (125 MHz, D_2O) δ = 157.5, 105.2, 76.7, 73.6, 69.9, 69.4, 61.8, 42.4, 34.7; HRMS (ESI) calcd. for $C_9H_{15}Cl_2NO_6Na$ $[M+Na]^+$ *m/*z = 326.0169, found 326.0163.

Reaction of SWCSC with DCO derivatives

DCO derivatives (1 μL, 100 mM in water or in DMF for DCO-biotin, 10 eq.) were added to a solution of SWCSC peptide (99 μL, 0.1 mM, 1 eq.) in Tris buffer (pH 8.5) containing 0.5 mM TCEP. The reactions were incubated at RT. At each time interval, an aliquot of the mixtures (30 μL) was quenched by mixing with acetic acid (1 μL). The quenched mixtures were then analyzed by UPLC-MS to characterize the progress of the reaction. See Figure 2C and Figure S1–S4 for the spectra. All reactions were performed under pseudo-first-order condition. Fitting of the kinetic curve to the equation $A_t = 1 - e^{-k*[DCO]*t}$ yielded second-order rate constant k, where A_t is the fraction of the product at time t and [DCO] is 0.001 M. MATLAB script used to fit the kinetic curve is outlined below. It is also available as kineticFIT.m and DCO-biotin_kinetic.xls as part of the electronic supplementary information.

START OF SCRIPT

```
clear all
close all

%%%%%%%%%%%% define the data for fitting here %%%%%%%%%%%%%%%%%%%%%%%%%%%%

[Data,B,C]=xlsread('DCO-biotin_kinetic.xls');

x = Data(:,1);
y = Data(:,2);

conc = 0.001;  %concentration of the excess DCO (Molar)
sec = 60;      %60 second min-1

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

A0 = 0;
A  = 1;
k  = 0.001;

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%    End of Data section   %%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%%%%% define the fit options %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

s = fitoptions('Method','NonlinearLeastSquares',...
               'Lower',[0,  0 ],...
               'Upper',[1000,  1000],...
               'Startpoint',[A k ],...
               'TolFun', 1e-10 );
```

```
%%%%% define the fit equation (pseudo-first-order kinetics)%%%%%%%%%%%%%%%%%

ft = fittype( 'A*(1-exp(-k*x))','options',s );

[c2,gof2,output] = fit(x,y,ft);

%%%%% find the 95% confidence bounds and confidence interval  %%%%%%%%%%%%

CON = confint(c2);
x2=0:0.1:max(x);
p22 = predint(c2,x2,0.95,'functional','on');

%%%%% c2.k is the pseudo-first-order rate constant (min-1) %%%%%%%%%%%%%%%
%This step converts c2.k (min-1) into second-order rate constant (M-1 s-1)

fitk = c2.k / (conc*sec);

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%     End of Fit section    %%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%%%%% plot the raw data as black circle %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

plot(x,y,'o',...
         'MarkerEdgeColor','k',...
         'MarkerFaceColor','k',...
         'MarkerSize',7);

hold on;

%%%%% plot the fit data as black lines and 95% confidence bounds as dash %%

plot( c2,'r');
plot(x2,p22,'k:');
legend off;

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%  define the axis, re-scale them, label them  %%%%%%%%%%%%%

xmax = max(x)*1.3;
ymax = max(max(p22))*1.05;
ymin = min(min(p22));

%  display the results of the fit on the plot

STD(1) = 100*abs(CON(1,1) - CON(2,1))/2 / c2.A;
STD(2) = 100*abs(CON(1,2) - CON(2,2))/2 / c2.k;

TL{1} = [' k = ' num2str(fitk,'%0.3f') ...
         ' [' num2str(STD(2),'%0.1f')  '%]'];

TL{2} ='----------------';
TL{3} = [' A = ' num2str(c2.A,'%0.3f') ...
```

```
          ' [' num2str(STD(1),'%0.1f')  '%]'];

TL{4} ='----------------';
TL{5} = [' R^2= ' num2str(gof2.rsquare,'%0.4f') ];

text(0.4*xmax,0.3*(ymax-ymin)+ymin, char(TL));

hold off;
```

END OF SCRIPT

Kinetic studies of modification of phage with DCO-biotin

A mixture of phage libraries and WT phage ($SXCX_3C$/$SXCX_4C$/WT in 1:1:2 ratio) in Tris buffer (pH 8.5) was prepared to yield a final titer of 2×10^9 pfu mL^{-1}. To the mixture of phage (99 μL), TCEP (1 μL, 50 mM in water) was added, followed by DCO-biotin (1 μL, 100 mM in DMF). The reaction mixture was incubated at RT. At each time interval, the reaction was quenched by diluting 10^5 times an aliquot of the phage solution (10 μL). The efficiency of the modification was quantified by biotin-capture assay as described previously.[2, 3] The studies—modification and quantification—were repeated three times on separate days to validate the reproducibility of the experiments. The reactions were performed under pseudo-first-order condition. Fitting of the kinetic curve to the equation $A_t = 1 - e^{-k*[DCO\text{-}biotin]*t}$ yielded second-order rate constant k, where A_t is the fraction of the captured phage at time t and [DCO-biotin] is 0.001 M.

Pulse-chase reaction of SWCSC with DCO-ManL and BIA

DCO-ManL (1 μL, 100 mM in water, 10 eq.) was added to a solution of SWCSC peptide (99 μL, 0.1 mM, 1 eq.) in Tris buffer (pH 8.5) containing 0.5 mM TCEP. The reaction was incubated at RT. After pulsing for 5 or 60 min, BIA (1 μL, 100 mM in DMF, 10 eq.) was added immediately to the reaction mixture. After incubating at RT for 30 min, an aliquot of the mixture (30 μL) was quenched by mixing well with acetic acid (1 μL). The quenched mixtures were then analyzed by UPLC-MS to characterize the progress of the reactions. See Figure 4B for the spectra

Modification of phage libraries with DCO-carbohydrate derivatives

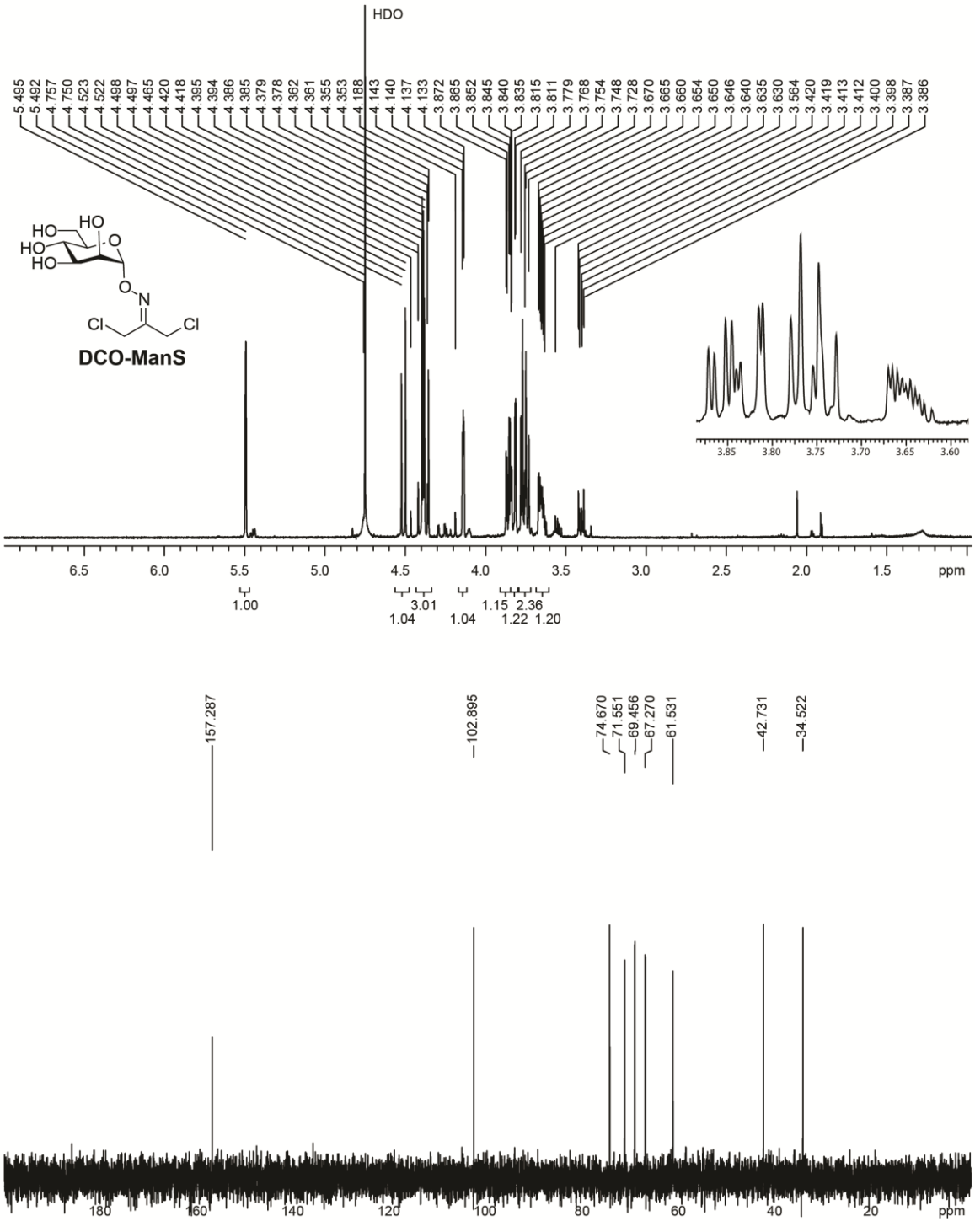
A mixture of phage libraries and WT phage ($SXCX_3C$/$SXCX_4C$/WT in 1:1:2 ratio) in Tris buffer (pH 8.5) was prepared to yield a final titer of 2×10^{11} pfu mL^{-1}. To the mixture of phage (99 μL), TCEP (1 μL, 50 mM solution in water) was added, followed by DCO-carbohydrate derivatives (1 μL, 100 mM in water). The reaction mixture was incubated at RT for 3 h and then an aliquot

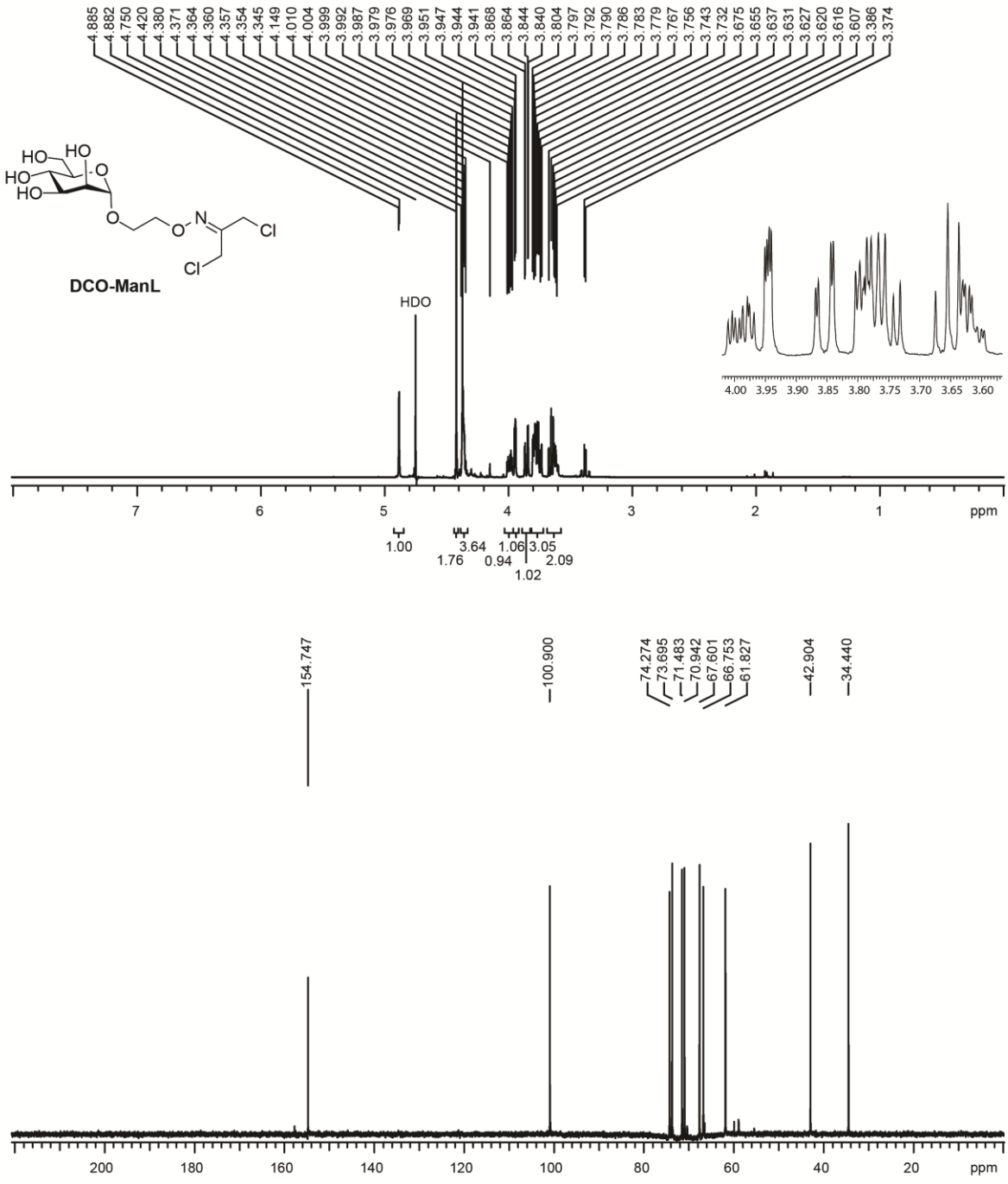
of the mixture (1 μL) was diluted immediately by 100-fold with Tris buffer containing 0.5 mM TCEP. To the diluted phage solution (100 μL), biotin−PEG_2−iodoacetamide (BIA, 1 μL, 100 mM in DMF) was added. The reaction mixture was incubated at RT for another 30 min and then quenched by diluting 10^5 times. The efficiency of the modification was quantified by biotin-capture assay as described previously.[2, 3]

Modification of phage libraries with DCA followed by AOB

A mixture of phage libraries and WT phage ($SXCX_3C$/$SXCX_4C$/WT in 1:1:2 ratio) in Tris buffer (pH 8.5) was prepared to yield a final titer of 2×10^{10} pfu mL^{-1}. To the mixture of phage (99 μL), TCEP (1 μL, 50 mM in water) was added, followed by 1,3-dichloroacetone (DCA, 1 μL, 100 mM in DMF). The reaction mixture was incubated at RT for 3 h, after which an aliquot of the DCA-labelled phage solution (6 μL) was mixed with aminooxy-biotin (AOB, 6 μL of 2 mM solution in 200 mM anilinium acetate, pH 4.7). The reaction mixture was incubated at RT for 17 h, and then quenched by diluting 10^5 times. The efficiency of the modification was quantified by biotin-capture assay as described previously.[2, 3]

NMR spectra of dichloro-oxime-carbohydrate derivatives

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4.364
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4.010
4.004
3.999
3.992
3.987
3.979
3.976
3.969
3.951
3.947
3.944
3.941
3.868
3.864
3.844
3.840
3.804
3.797
3.792
3.790
3.786
3.783
3.779
3.767
3.756
3.743
3.732
3.675
3.655
3.637
3.631
3.627
3.620
3.616
3.607
3.386
3.374
HO
HO
HO
HO
O
O
N
Cl
Cl
DCO-ManL
HDO
4.00 3.95 3.90 3.85 3.80 3.75 3.70 3.65 3.60
7
6
5
4
3
2
1
ppm
1.00
1.76
3.64
0.94
1.06
1.02
3.05
2.09
154.747
100.900
74.274
73.695
71.483
70.942
67.601
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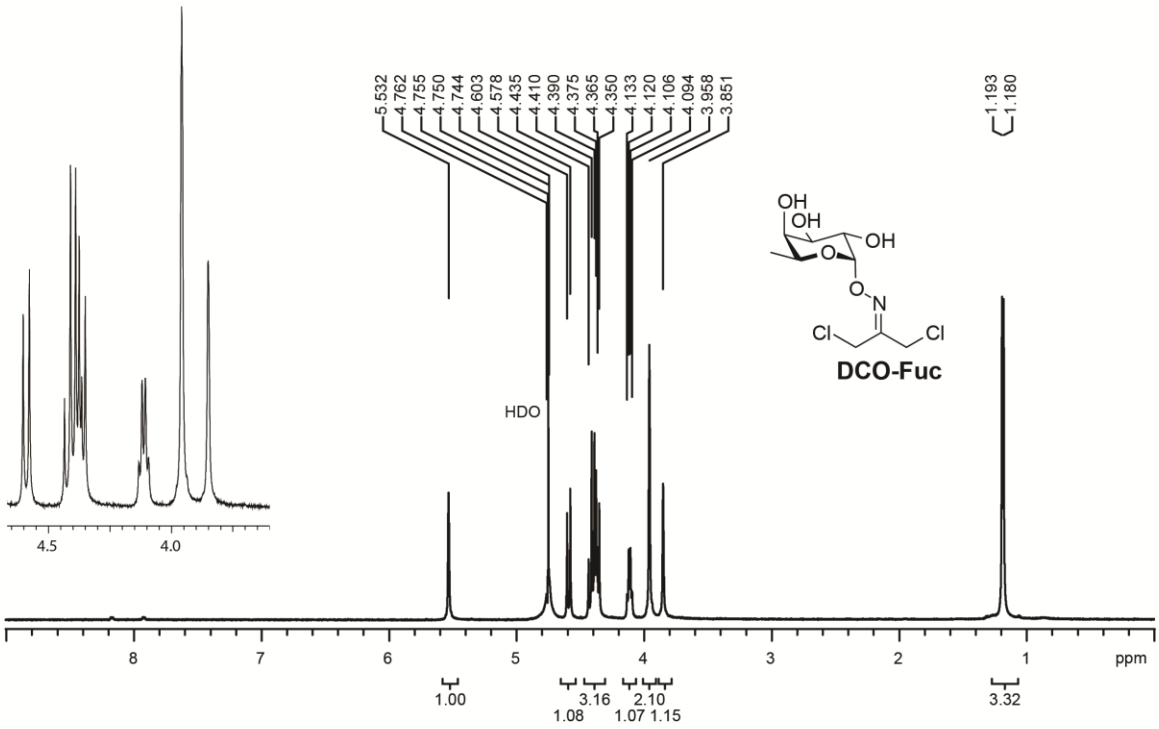
ppm


5.532
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4.755
4.750
4.744
4.603
4.578
4.435
4.410
4.390
4.375
4.365
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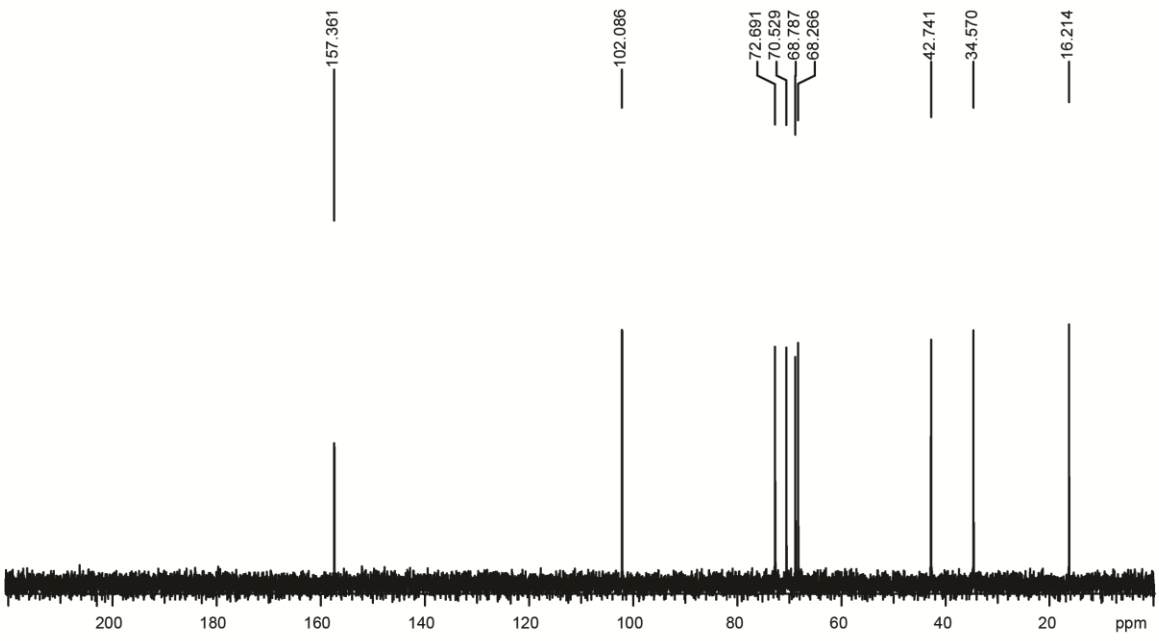
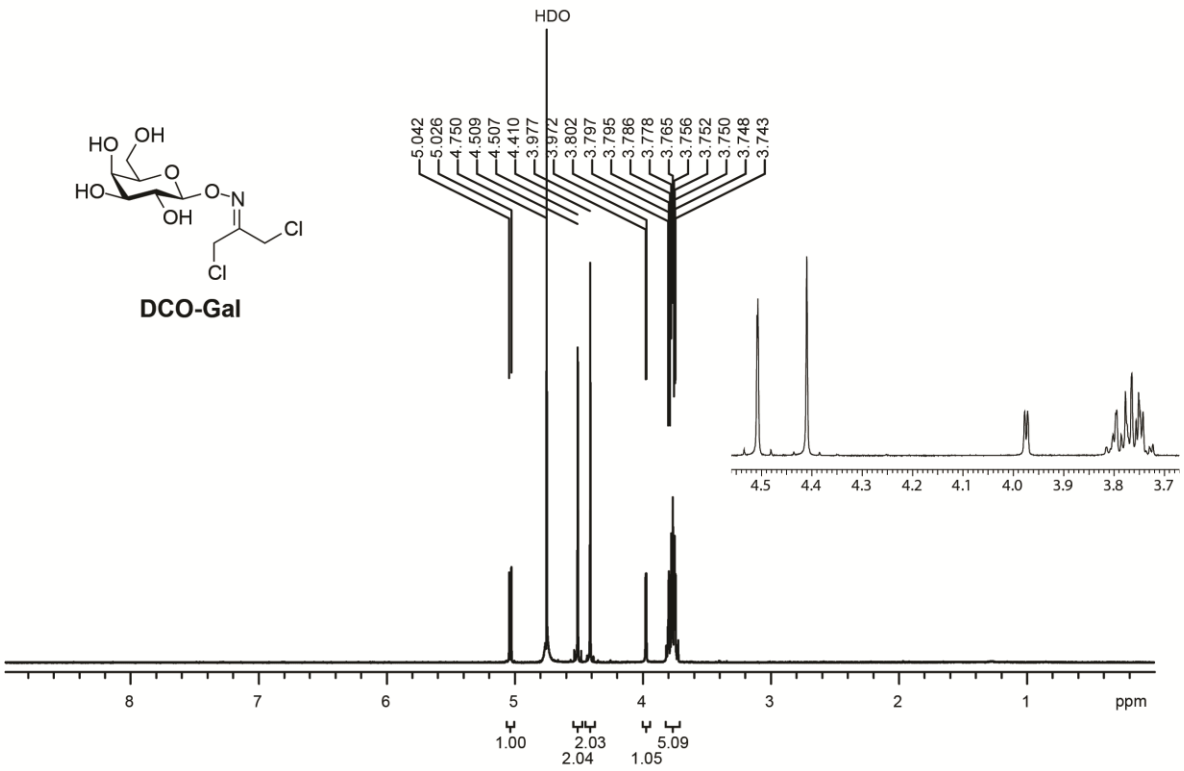
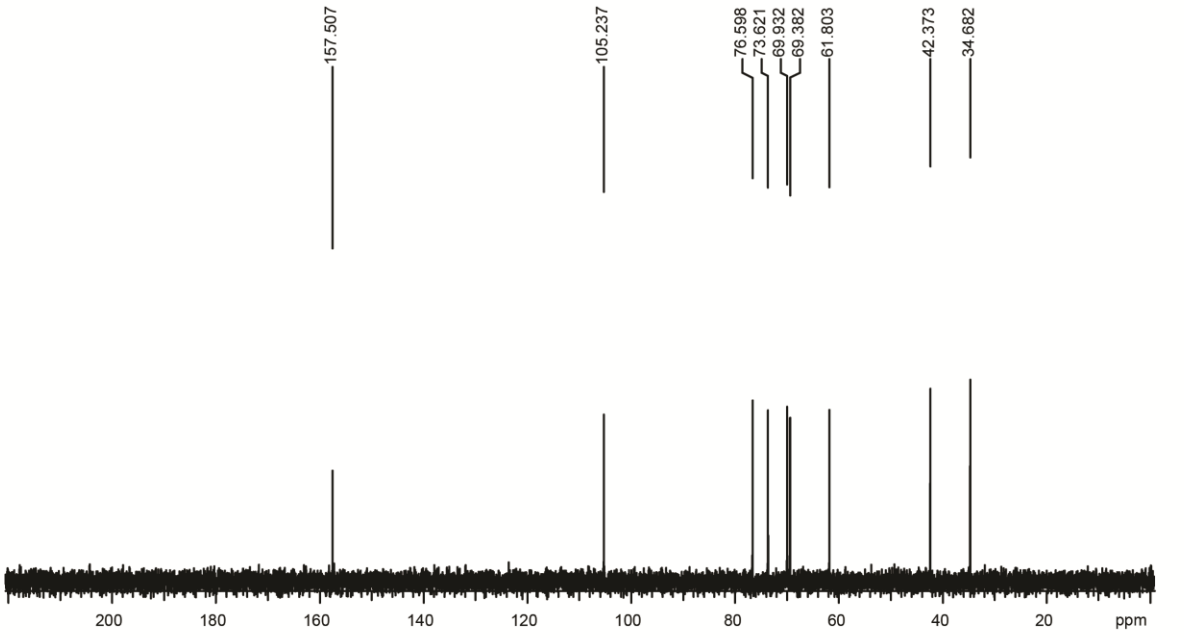
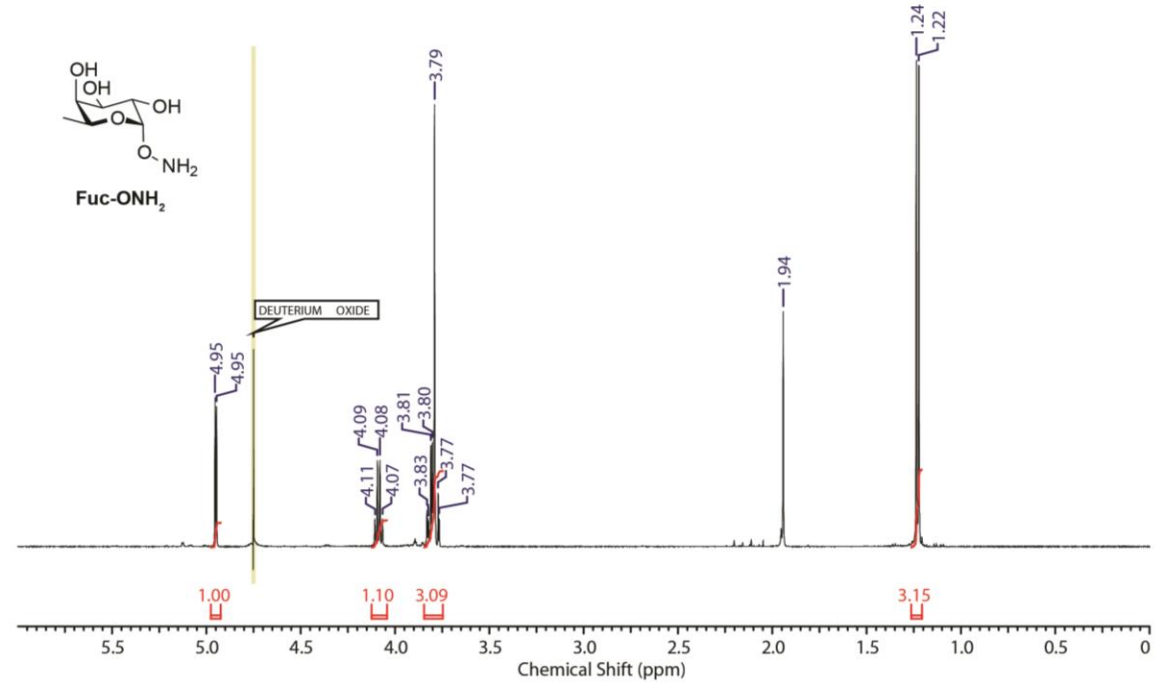
4.133
4.120
4.106
4.094
3.958
3.851
1.193
1.180
HDO
OH
OH
OH
O
O
N
Cl
Cl
DCO-Fuc
4.5
4.0
8
7
6
5
4
3
2
1
ppm
1.00
3.16
1.08
2.10
1.07
1.15
3.32

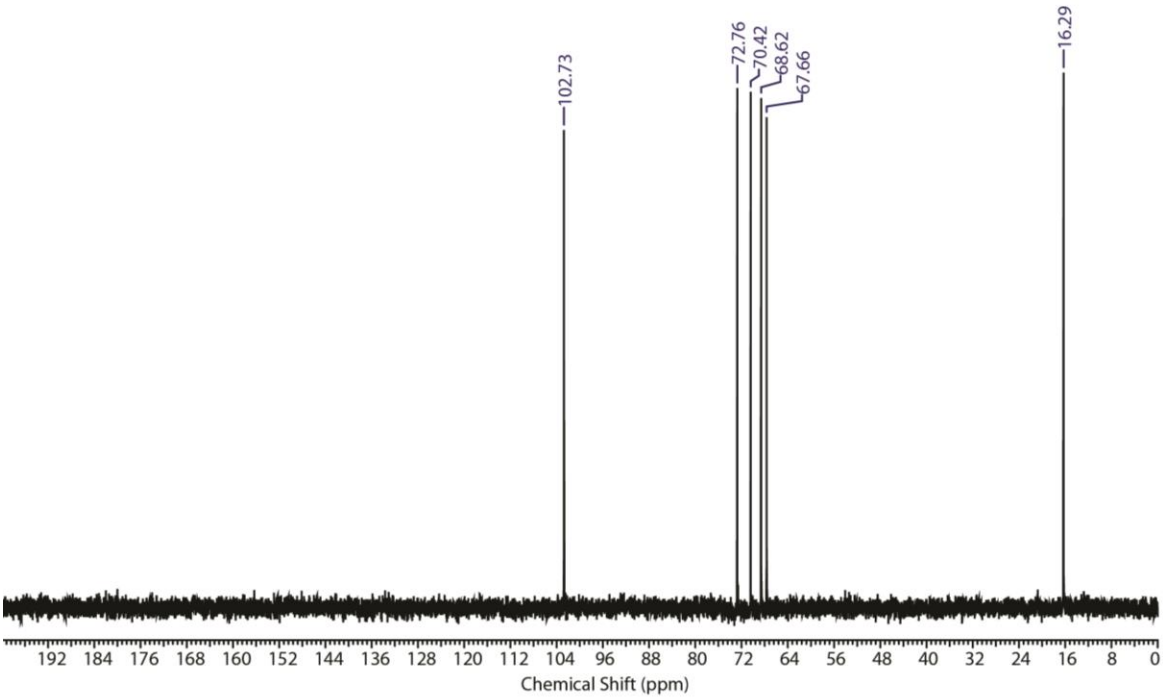

157.361
102.086
72.691
70.529
68.787
68.266
42.741
34.570
16.214
200
180
160
140
120
100
80
60
40
20
ppm

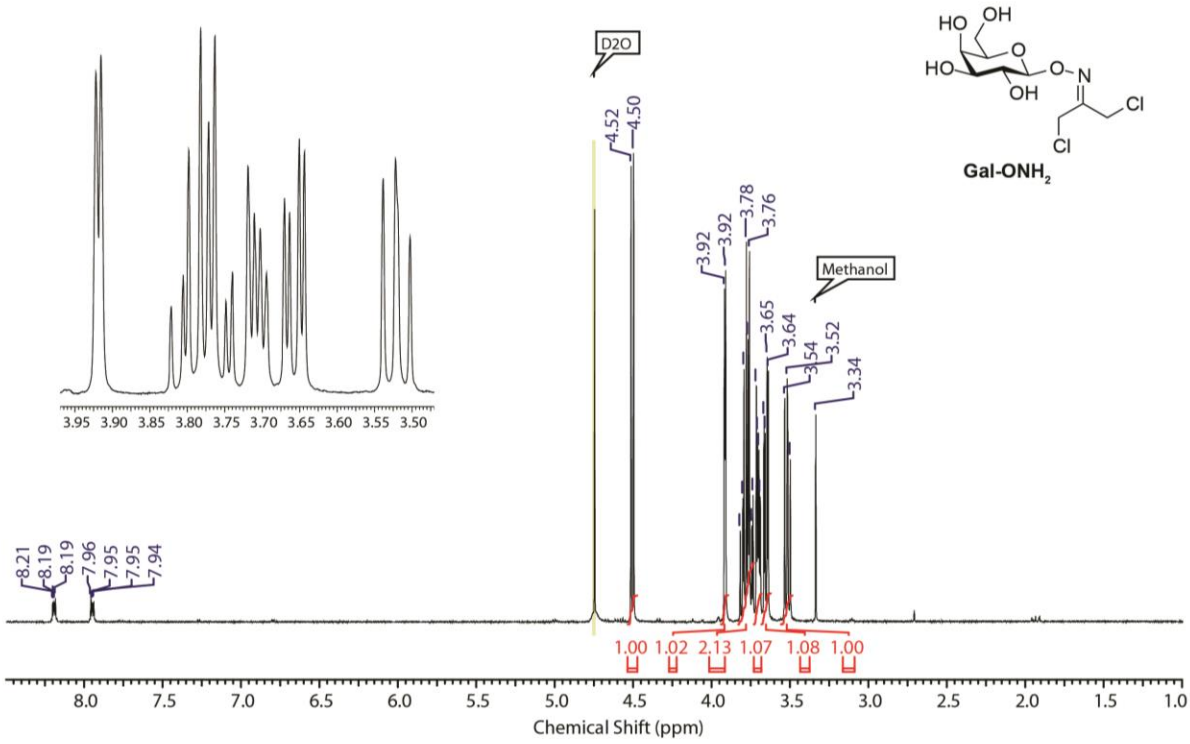

HDO
5.042
5.026
4.750
4.509
4.507
4.410
3.977
3.972
3.802
3.797
3.795
3.786
3.778
3.765
3.756
3.752
3.750
3.748
3.743
HO
OH
O
HO
O
N
OH
Cl
Cl
DCO-Gal
8
7
6
5
4
3
2
1
ppm
1.00
2.03
2.04
1.05
5.09

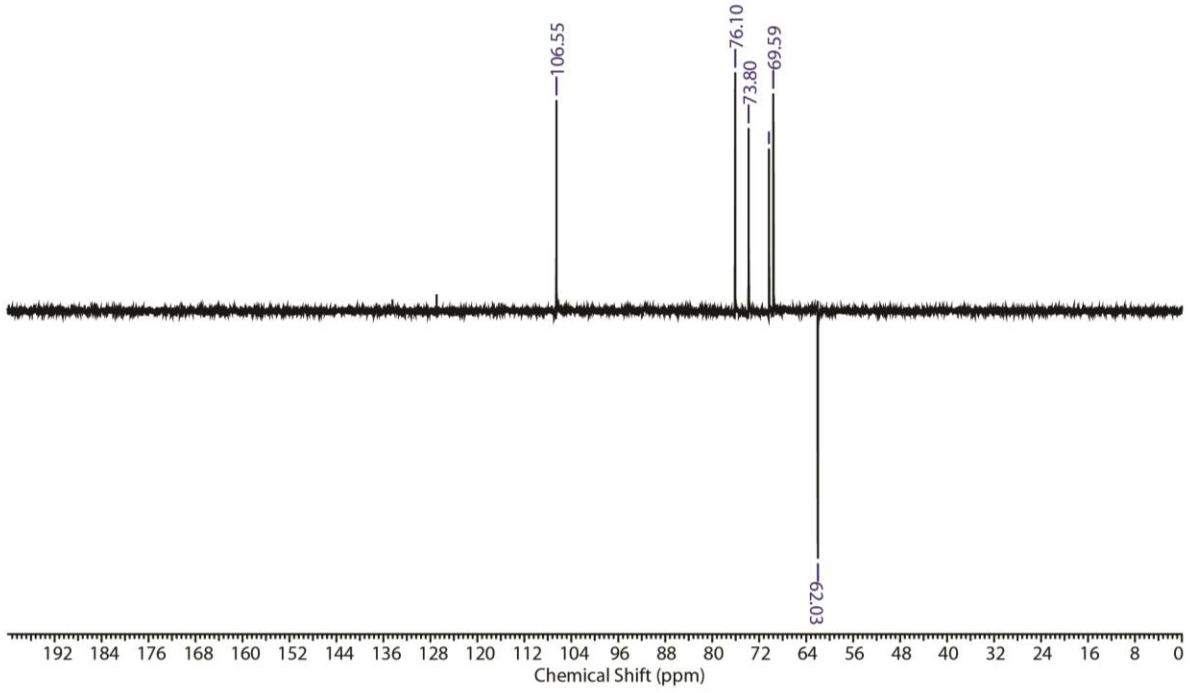

157.507
105.237
76.598
73.621
69.932
69.382
61.803
42.373
34.682
200
180
160
140
120
100
80
60
40
20
ppm

NMR spectra of carbohydrate-hydroxylamine derivatives






D2O
Methanol
Gal-ONH2
HO
OH
O
HO
OH
O
N
Cl
Cl
4.52
4.50
3.92
3.92
3.78
3.76
3.65
3.64
3.54
3.52
3.34
8.21
8.19
8.19
7.96
7.95
7.95
7.94
1.00 1.02 2.13 1.07 1.08 1.00
Chemical Shift (ppm)


106.55
76.10
73.80
69.59
62.03
Chemical Shift (ppm)

Supporting information references

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2. S. Ng, K. Tjhung, B. Paschal, C. Noren and R. Derda, in *Peptide Libraries*, ed. R. Derda, Springer New York, 2015, vol. 1248, ch. 11, pp. 155-172.
3. S. Ng, M. R. Jafari, W. L. Matochko and R. Derda, *ACS Chem. Biol.*, 2012, **7**, 1482–1487.