Electronic Supplementary Material (ESI) for Chemical Communications.

Supramolecular Scaffolds on Glass Slides as Sugar Based Rewritable Sensor for Bacteria

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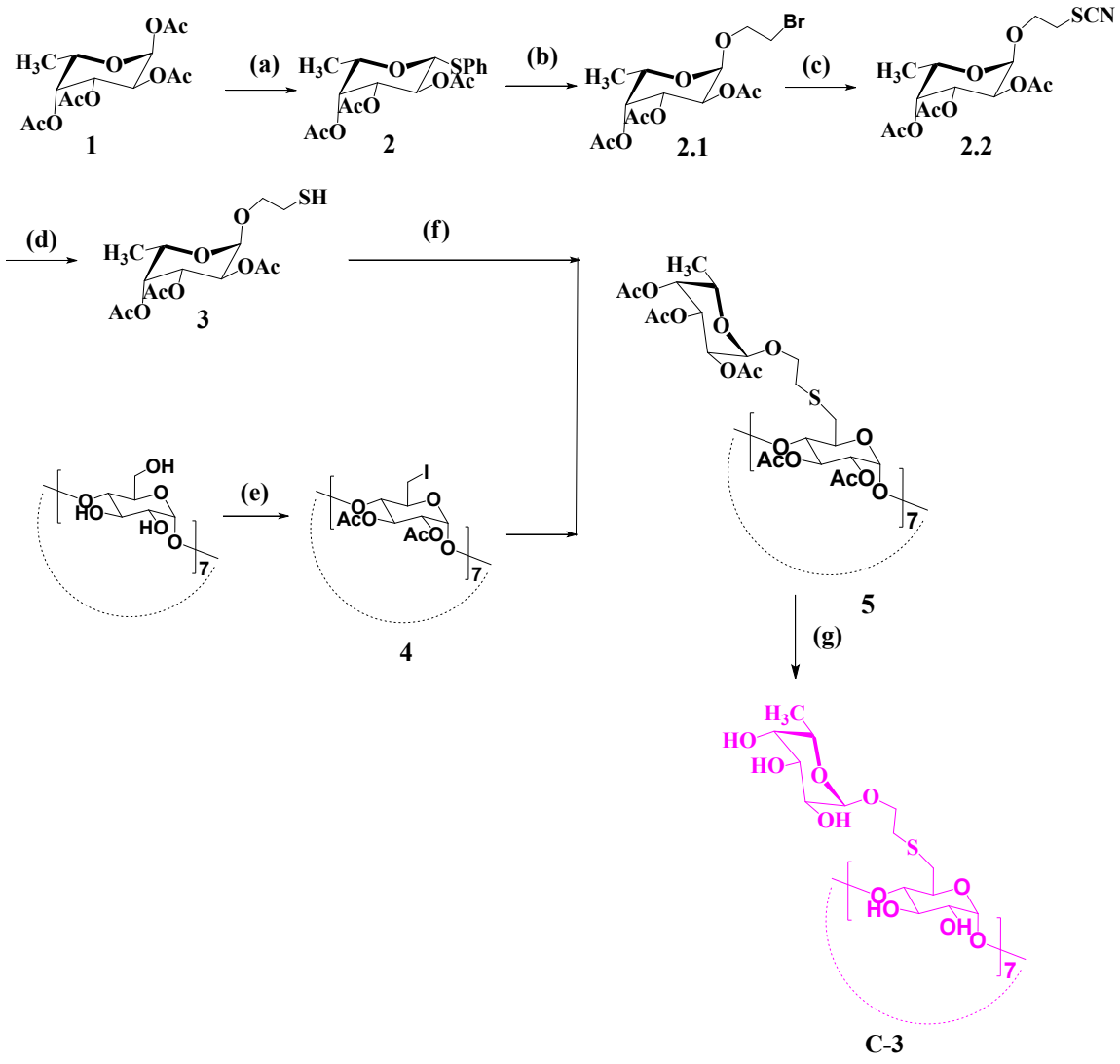
1. General Information

All chemicals were reagent grade and used as supplied except where noted. Analytical thin layer chromatography (TLC) was performed on Merck silica gel 60 F254 plates (0.25 mm). Compounds were visualized by UV irradiation or dipping the plate in CAM solution followed by heating. Column chromatography was carried out using force flow of the indicated solvent on Fluka Kieselgel 60 (230–400 mesh). ^{1}H and ^{13}C NMR spectra were recorded on Jeol 400 MHz using residual solvents signals as an internal reference ($CDCl_3$ δH, 7.26 ppm, δc 77.3 ppm and CD_3OH δH 3.31 ppm, δc 49.0 ppm). The chemical shifts (δ) are reported in *ppm* and

coupling constants (*J*) in Hz. XPS experiments were performed on a VG Micro Tech ESCA 3000 instrument at a pressure of < $1x10^{-9}$ Torr. The overall resolution was limited to the bandwidth of X - ray source (~ 1 eV). The spectra were recorded with monochromatic Al Kα radiation at pass energy of 50 eV and an electron take off angle of 60º. Bacterial images were collected from Zeiss optical microscope at 63X resolution and exciting DAPI, FITC and rhodamine by specific lazars.

1. **Synthesis of L-fucose β-CD (C-3).**



Scheme S1: Synthesis of comp **C-3**: (a) Thiophenol/$BF_3.Et_2O$, DCM, 0°C To RT, 12 h, 91% ; (b) NIS/TfOH/bromoethanol, DCM:ACN (2:1), -78°C to -50°C, 2hr, 38%; (c) KSCN/DMF, 80°C, 12hr, 95%; (d) Zn/AcOH, 80 °C, 4hr, 76%; (e) I_2, PhP_3, DMF, 80°C 16 hr; Ac_2O/Py, 12 hr, 72% (2 step); (f) **6**, Cs_2CO_3, DMF, RT, 72 hr, 57%; (f) NaOMe, MeOH, 2 hr, 51% .

Comp **2** was prepared by using procedure reported in literature.

Synthesis of Thiophenol-sugar derivatives (2).

Peracetylated L-fucose **1** (0.6 g, 1.80 mmol) thiophenol (0.2 mL, 0.98 mmol) were dissolved in DCM (10 mL) and maintained 0°C. To the reaction mixture $BF_3.Et_2O$ (0.5mL, 4.14 mmol) was slowly added for half hour and stirred overnight at RT. Completion of reaction was monitored by TLC. After completion, the reaction mixture was diluted with 20 mL DCM and washed with $NaHCO_3$ (2 X 20 mL) and brine (2 X 20 mL). Organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to give crude product, which was further purified on silica gel column chromatography using EtOAc/Pet-ether (1: 1) to get pure thiophenol sugar derivatives (Yield =0.41 g, 91%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53-7.50 (m, 2H), 7.35-7.30 (m, 3H), 5.30-5.26 (m, 1H), 5.21 (d, *J* = 8.0 Hz, 1H), 5.06 (dd, *J* = 3.66, 10.0 Hz, 1H), 4.72 (d, *J* = 10.7 Hz, 1H), 3.85 (q, *J* = 3.66, 8.0 Hz, 1H), 2.15 (s, 3H) 2.09 (s, 3H), 1.98 (s, 3H), 1.25 (d, *J* = 6.41 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ. 170.71, 170.24, 169.60, 132.98, 132.38, 128.95, 128.02, 86.55, 73.23, 72.50, 70.39, 67.42, 20.95, 20.75, 16.56. HRMS m/z calc'd for $C_{18}H_{22}O_7SNa$: 405.0984; found: 405.0979.

Synthesis of Bromoethanol-sugar derivatives (2.1)

L-fucose donor **2** (0.4 g, 1.04mmol) and bromoethanol (0.37 mL, 5.23mmol) were dissolved in 2:1 DCM:ACN mixture (10 mL). Then maintain -78 °C for 20 minutes, followed by NIS (0.58 g, 2.61mmol) and TfOH (0.13 mL, 1.04 mmol) were added at -78 °C. The reaction mixture was allowed to stir at -50 °C for 2 h. Completion of reaction was monitored by TLC. After completion, the reaction mixture was neutralized with triethyl amine, and then added DCM (50mL) to the reaction mixture, give washing two times with sodium thiosulphate $Na_2S_2O_3.5H_2O$ (10 mL) and two times with water (10 mL). Organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to give crude product, which was further purified on silica gel column chromatography using EtOAc/Pet-ether (70 : 30) to get pure bromoethanol sugar derivatives. ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.26-5.19 (m, 2H), 5.09 (dd, *J* =3.6, 10.1 Hz, 1H) 5.02 (d, *J* = 3.6 Hz, 1H), 4.07-4.02 (m, 1H), 3.83-3.76 (m, 2H), 3.46 (t, *J* = 11.2 Hz, 2H), 2.18 (s, 3H), 2.08 (s, 3H) 1.99 (s, 3H), 1.24 (d, *J* = 6.41 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ. 170.76, 170.33, 169.75, 96.40, 70.24, 70.21, 69.64, 68.38, 63.63, 62.5, 30.16, 29.76, 20.99, 20.72. HRMS m/z calc'd for $C_{14}H_{21}O_8BrNa$: 419.0317; found: 419.0317.

Synthesis of thiocyanate substituted sugar (2.2).

Per-acetylated bromoethanol-sugar derivative (0.2 g, 0.50 mmol) was dissolved in DMF (10 mL). Then potassium thiocyanate (0.19 g, 2.02 mmol) was added and stirred at 80 °C for 12 hr. The reaction mixture was diluted with 100 ml ethyl acetate and washed several times with water. The organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to give crude product, which was further purified by flash column using petroleum ether: ethylacetate (75 : 25) (Yield = 0.20 g, 95%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.26-5.14 (m, 2H), 5.11 (dd, *J* =3.6, 10.1 Hz, 1H) 4.98 (d, *J* = 3.6 Hz, 1H), 4.05-3.95 (m, 1H), 3.83-3.76 (m, 2H), 3.23-3.05 (m, 2H), 2.18 (s, 3H), 2.08 (s, 3H) 1.99 (s, 3H), 1.24 (d, *J* = 6.41 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ. 170.67, 170.22, 169.66, 111.82, 97.4, 71.17, 70.12, 69.84, 68.61, 63.02, 33.79, 29.73, 20.90, 20.73, 20.67, 16.06. HRMS m/z calc'd for $C_{15}H_{21}NO_8SNa$: 398.0885; found: 398.0883.

Synthesis of thio substituted sugar (3).

Peracetylated thiocynate-sugar derivative (0.23 g, 0.61 mmol) was dissolved in glacial acetic acid (30 mL). Then Zn dust (0.16 g, 2.45mmol) was added and refluxed at 80 °C for 4 h. The compound was filtered to remove zinc dust. The organic layer was quenched with water (50 mL). Then product was extracted with EtOAc (3 X 50 mL) and dried over anhydrous Na_2SO_4. Organic layer was concentrated under reduced pressure to give product, which was further used for next reaction without purification (Yield = 0.28 g, 76%). ^{1}H NMR (400 MHz, $CDCl_3$): δ δ 5.29-5.17 (m, 2H), 5.13 (dd, *J* = 3.66, 10.1 Hz, 1H), 5.01 (d, *J* = 3.6 Hz, 1H), 4.14-4.03 (m, 1H), 3.87-3.80 (m, 1H), 3.69-3.57 (m, 1H), 2.82-2.66 (m, 2H), 2.21 (s, 3H), 2.11 (s, 3H) 2.02 (s, 3H), 1.29 (d, *J* = 6.41 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ. 170.73, 170.15, 169.62, 98.08, 71.24, 70.28, 69.12, 68.86, 63.6, 29.67, 24.35, 20.63, 16.09. HRMS m/z calc'd for $C_{14}H_{22}O_8SNa$: 373.0933; found: 373.0932.

Synthesis of sugar substituted β-cyclodextrin (5).

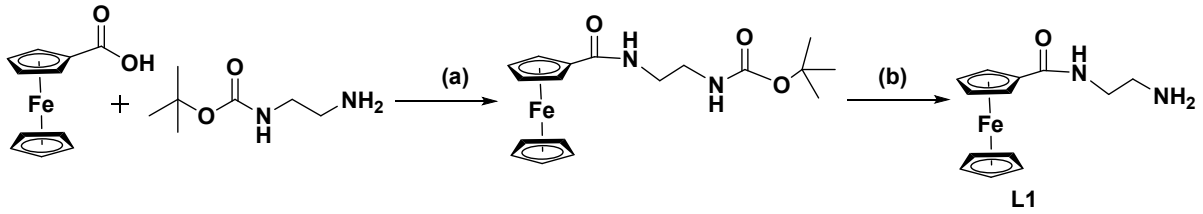
The per-acetylated thio-sugar (0.18 g, 0.52 mmol) in DMF (10 mL) was added to per-acetylated 6'-Iodo- β-cyclodextrin **4** (0.1 g, 0.04 mmol) and Cs_2CO_3 (0.168 g, 0.52 mmol) and stirred at room temperature for 72 h. The reaction mixture was diluted with 100 ml ethyl acetate and washed several times with water. The organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to give crude product, which was further purified by flash column using DCM:MeOH (5-7%) (Yield = 0.27 g, 57%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.23 (d, *J* = 3.21 Hz, 7H), 5.15-4.89 (m, 34H), 4.80-4.75 (m, 7H), 4.14-4.09 (m, 7H), 4.07-4.01 (m, 7H), 3.87-3.82 (m, 14H), 3.66-3.62 (m, 7H) 3.16-2.92 (m, 14H),2.87-

2.75 (m, 14), 2.17 (s, 18H), 2.09-2.03 (m, 66H), 1.96 (m, 21H), 1.21 (d, J = 6.41 Hz, 21H); ^{13}C NMR (100 MHz, $CDCl_3$): δ. 170.73, 170.15, 169.55, 101.08, 71.24, 70.28, 69.12, 68.86, 33.81, 31.90, 29.66, 22.67, 20.95, 20.79, 20.71, 20.63, 16.09. HRMS m/z calc'd for $C_{168}H_{238}O_{98}S_7Na$: 4070.1583; found: $[M+Na/2]^+$.2036.4113.

Deacetylation of Per-glycosylated β-cyclodextrin derivatives (C-3).

The sugar-substituted *β*-cyclodextrin (0.05 g, 0.01 mmol) was dissolved in methanol (10 mL). Then sodium methoxide (9 mg, 0.24 mmol) was added and stirred for 2 h at RT. The mixture was neutralized with amberlite–IR120H$^+$ resin, filtered and concentrated *in vacuo* to afford the final compound (**C-3**) (Yield = 51 mg, 51%). ^{1}H NMR (400 MHz, CD_3OD): δ 5.12-5.09 (m, 7H), 4.37 (d, J = 3.6 Hz, 7H),4.15-3.97 (m, 10H), 3.96-3.85 (m, 18H), 3.79-3.72(m, 17H), 3.64-3.61 (m, 17H), 3.55-3.51 (m, 7H), 3.49-3.46 (m, 7H), 3.27-3.25 (m, 7H) 3.02-2.89 (m, 21H),1.25 (bs, 21H); ^{13}C NMR (100 MHz, CD_3OD): δ. 120.87, 72.98, 72.96,72.95, 72.04, 71.98, 71.28, 70.90, 70.47, 68.97, 68.90, 68.79, 32.12, 32.07 15.70. HRMS m/z calc'd for $C_{24}H_{46}O_6$ Na: 2599.7987; found: 2599.81.

3. Synthesis of Ferrocene derivatives



Scheme S2: Synthesis of comp **L-1**: (a) EDC/HOBt/DIPEA, DMF, RT, 12 hr, 92%; (b) 40% TFA/DCM, 2hr, 83%.

Synthesis of ferrocene derivative (1).

Ferrocene carboxylic acid (0.5 g, 2.17 mmol) and mono-boc ethylene diamine (0.34 g, 2.17mmol) was dissolved in dry DMF (10 mL). Then HOBt (0.35 g, 2.60 mmol) and EDC (0.45 g, 2.60mmol) were added. The reaction mixture was stirred at RT for 12 hr. After completion, the reaction mixture was diluted with 50 ml water and extracted with ethyl acetate (3× 50mL). The organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to give crude product, which was further purified by flash column using petroleum ether: ethylacetate (Yield = 0.87 g 92%), . ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.81 (bs, 1H), 5.13 (s, 1H), 4.72 (bs,2H), 4.35(bs, 2H), 4.20 (s, 5H), 3.47 (q, J = 8.0 Hz, 2H),

3.36 (q, J = 8.0 Hz, 2H), 1.46 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ. 171.77, 79.99, 70.66, 69.89, 68.29, 41.32, 40.57, 28.50. HRMS m/z calc'd for $C_{18}H_{24}FeN_2O_3$: 373.1215; found: 373.1220.

Synthesis of L-1.

To ferrocene derivative 6 added 40% TFA in DCM was added, which was stirred for 2 hr. Then TFA was evaporated under reduced pressure which was further purified by column using DCM: Methanol (Yield = 0.87 g, 83%).

^{1}H NMR (400 MHz, CD_3OD): δ 4.85 (bs, 2H), 4.46 (bs, 2H), 4.24 (s, 5H), 3.63 (t, J = 12.0 Hz, 2H), 3.16 (t, J = 12.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ. 137.38, 123.70, 123.03, 49.56, 36.39, 32.01, 19.27, 13.29. HRMS m/z calc'd for $C_{13}H_{16}ON_2Fe$: 273.0690; found: 273.0691.

4. Surface Functionalization:

Immobilization of ferrocene derivatives : (Approx. 1x1 cm) glass were washed with piranha solution (Caution : Piranha solution reacts violently so use carefully) and immediately dipped in a solution of (3-glycidyloxypropyl) trimethoxysilane (GOPTMS) (0.5 M) in 2 ml toluene. The substrates were heated at 85 °C for 52 hrs in a pressure tube. Samples were then rinsed with toluene to remove excess of GOPTMS. Next, GOPTMS coated glass slides were dipped in a solution of **L-1** (0.02 M) in ethanol for 24 h and rinsed with ethanol to remove excess of ferrocene linker and to neutralize epoxide group.

Immobilization of cyclodextrin derivatives*:* Freshly prepared ferrocene glass substrate (modified with **L-1**) was washed twice with ethanol and immersed in solution of either **C-1** or **C-2 or C-3** (10 μM solution in deionized water) for 30 mins. The samples were rinsed with water, dried under a stream of nitrogen and used bacterial assay.

5. Time-of-Flight Secondary Ion Mass Spectrometer (SIMS-TOF) Characterization.

Time-of-Flight Secondary Ion Mass Spectroscopy (ToF SIMS) is a surface sensitive Spectroscopy that uses a pulsed Primary Ion beam to induce the desorption and ionization of atomic and molecular species from a solid sample surface. Approximate (20mmx20mmx20mm) silica wafer was coated with **L-1** followed by and the elementary composition was characterized by TOF-SIMs.

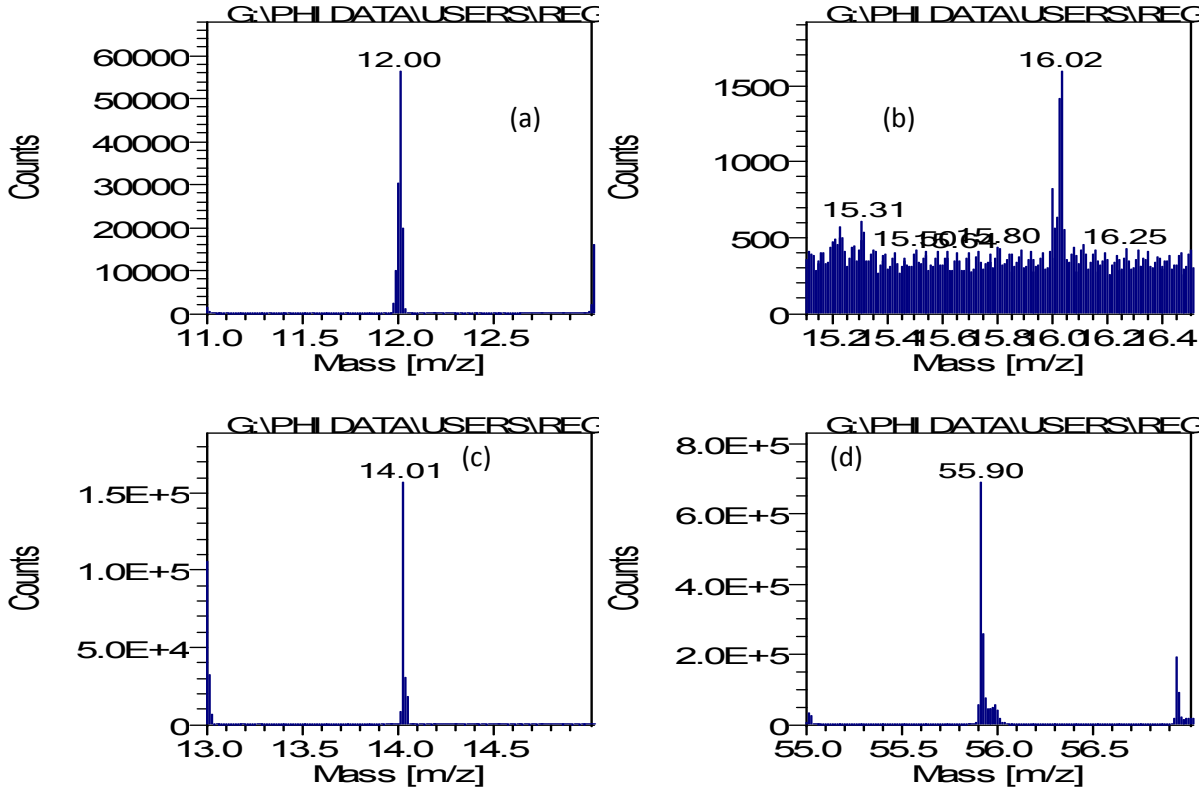


Figure S1. TOF-SIMS mass spectra of individual elements on L-1 coated surface: (a) carbon, (b) oxygen (c) nitrogen, (d) iron.

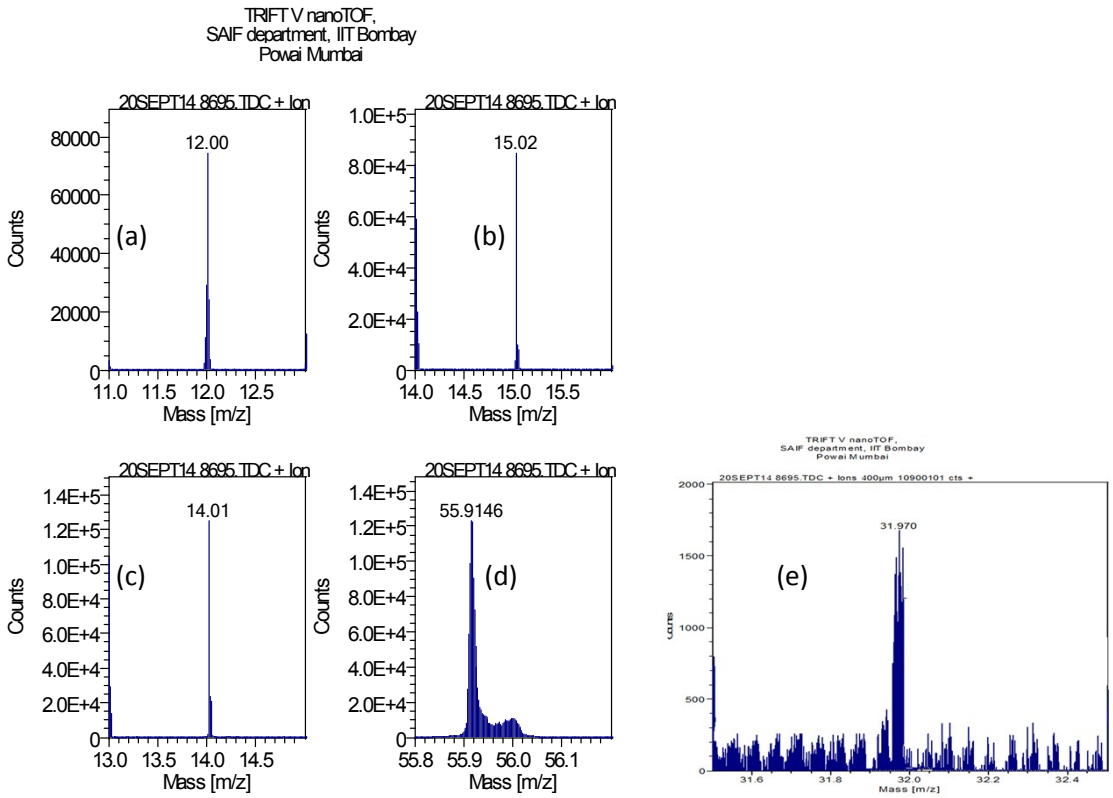


Figure S2. TOF-SIMS mass spectra of individual elements on L-1/C-3 coated surface: (a) carbon, (b) oxygen (c) nitrogen, (d) iron, (e) sulphur.

6. XPS Analysis

XPS is very important tool to analyse the chemical composition of molecules on surfaces. We used this method to confirm the conjugation of **L-1** and **C-2** on glass slides. Carbon 1s spectrum for **L-1** is deconvulated at 284.6 (C-C, C-H), 286.7(C-O), 287.5 (C-N) and 288.7eV(C=O) respectively. High resolution XPS spectrum of **L-1** revealed Fe $2p_{3/2}$ and $2p_{1/2}$ at 711.7 and 725.6 eV respectively, whereas nitrogen 1s spectrum was centered at 400.3 eV. This clearly indicates the presence of **L-1** linker on glass slides. Similarly, high resolution XPS of **C-2/L-1** confirm presence of sulphur 2P at 163.5 ev.

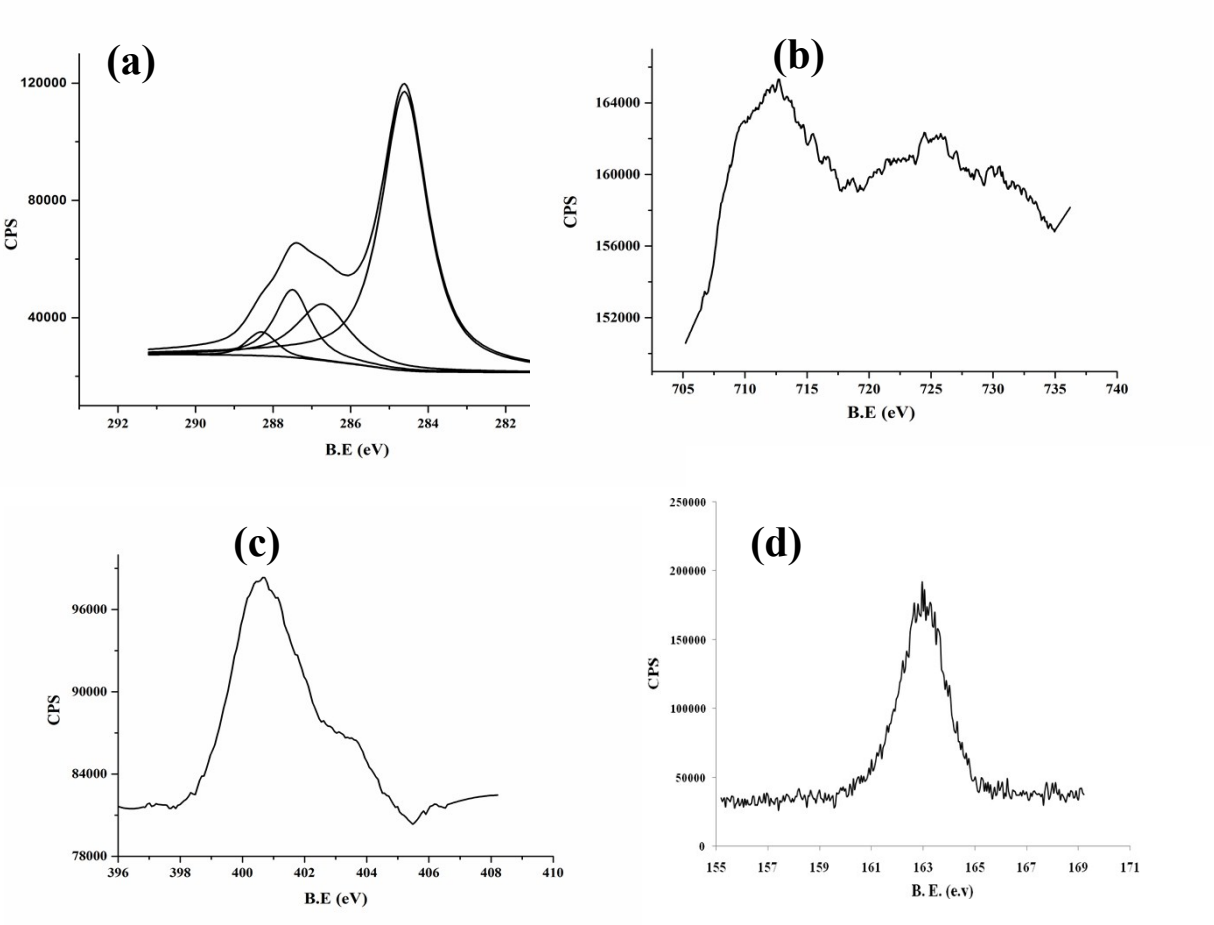


Fig. S3. XPS spectra of (a) C 1S ; (b) Fe 2P ; (c) N 1S of **L-1** coated glass slide and (D) S 2P of **C-2/L-1** glass slide.

7. Bacterial Strains growth. The mutants *E.coli ORN178 and ORN208* were provided by Prof. Orndorff (College of Veterinary Medicine, Raleigh, NC United States) and *P. aeruginosa* was obtained from NCL bacterial bank. The bacterial cultures were grown overnight at 37°C until they reached an approximate OD_{600} of 1.0.

Bacterial detection.

2 ml aliquot of bacteria of approximate OD_{600} of 1.0 was centrifuge to obtain a bacterial pellet. The resulting pellet was washed twice with PBS buffer and resuspended in 2 ml PBS and adjust the concentration to 10^8. Different sugar coated glass slides were dipped in this solution for 30 mins and the glass slides was rinsed with PBS, followed by distilled water to remove non-specific bindings. These slides were mounted on fluorescent microscopic slides to image the bacteria.

8. Concentration dependent studies. The concentration of the bacteria was calculated by using growth promotion curve. 2 ml solutions of different dilution of bacteria were prepared and sugar coated glass slides (**C-2/L-1** with *E. coli* ORN 178 and **C-3/L-1** with *P.aeruginosa*) were immersed for 30 mins. Slides were washed with distilled water and images were collected. Quantification of bacteria was done by measuring relative fluorescence unit.

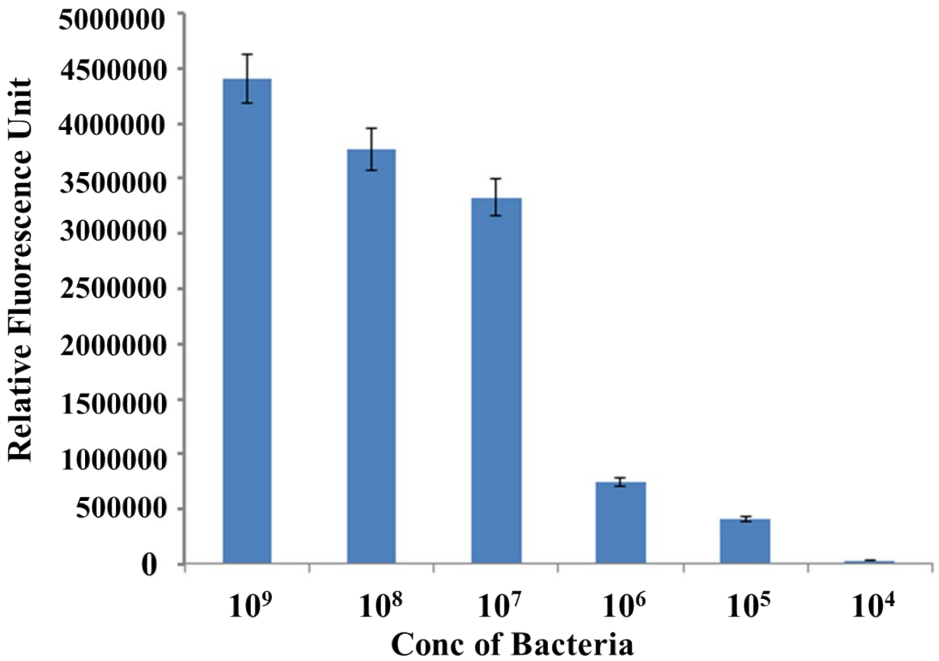


Fig. S4. Quantitative analysis of bacterial adhesion on **C-2/L-1** surface (200 X 200 μm) n =5.

9. Rewriting the sugar substrate for continuous bacterial sensor. A stock solution of 0.1 mM of adamantyl carboxylic acid in ethanol water was prepared. The glass substrate having bacteria and host-guest complex was immersed in above solution for 5 mins. The sample was then rinsed with PBS, deionized water and then dried under a stream of N_2. This substrate was once again incubated in a solution of **C-2** or **C-3** (10 μM) for 30 min, to obtain the regenerated substrate used for bacterial sensing.

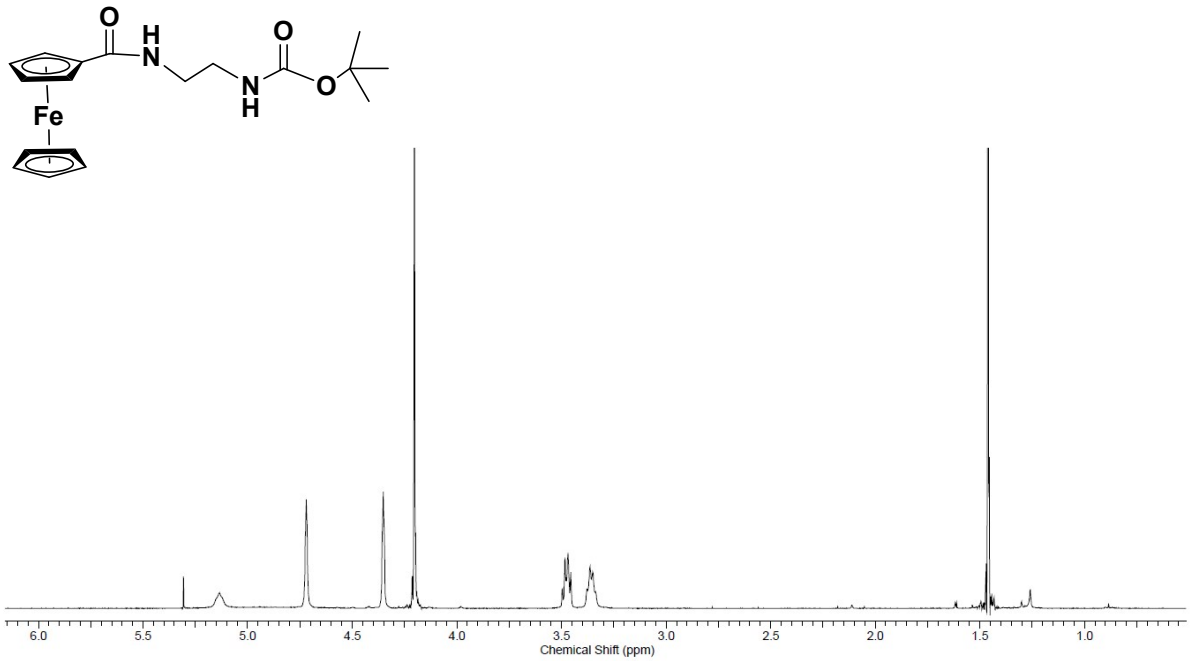
10. Estimation of the concentration of sugar on glass slides ;

The concentration of mannose sugar on glass slide was determined by the phenol-sulfuric acid method. A sugar functionalized-glass slides was dipped in 0.5 ml of adamantane carboxylic acid (0.1 M) containing solution, 100 μL of above solution, concentrated sulfuric acid (750 μL, 100%) and aqueous phenol solution (5% w/v, 100 μL) were added to the test tube and heated to 80°C. After 5 min, the plate was cooled to room temperature and the absorbance coefficient at 490 nm was measured. An adamantane carboxylic acid solution and sulfuric acid were used as a control. The mannose concentration was estimated by comparing the absorption of the sample with a standard curve. The number of sugar molecules per 1 X 1 cm plate was 0.56 ± 0.12 μM (n = 5). Same procedure was repeated during generation – degeneration processes to estimate the sugar concentration (Table S1).

Cycle (μM)	1st cycle	2nd cycle	3rd cycle	4th cycle	5th cycle
C-2	0.52 ± 0.04	0.45 ± 0.07	0.49 ± 0.06	0.51 ± 0.07	0.49 ± 0.08

Table S1. Concentration of mannose after each generation-degeneration process (value represents average of three parallel experiments).

10. NMR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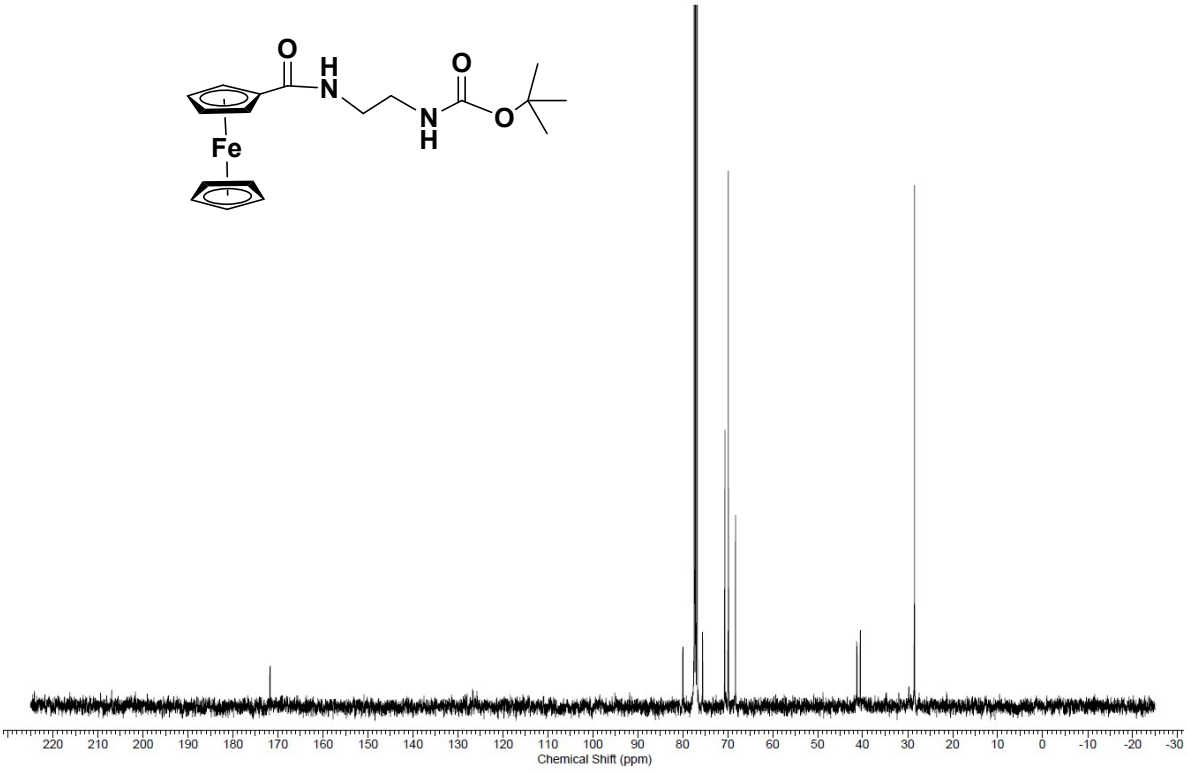
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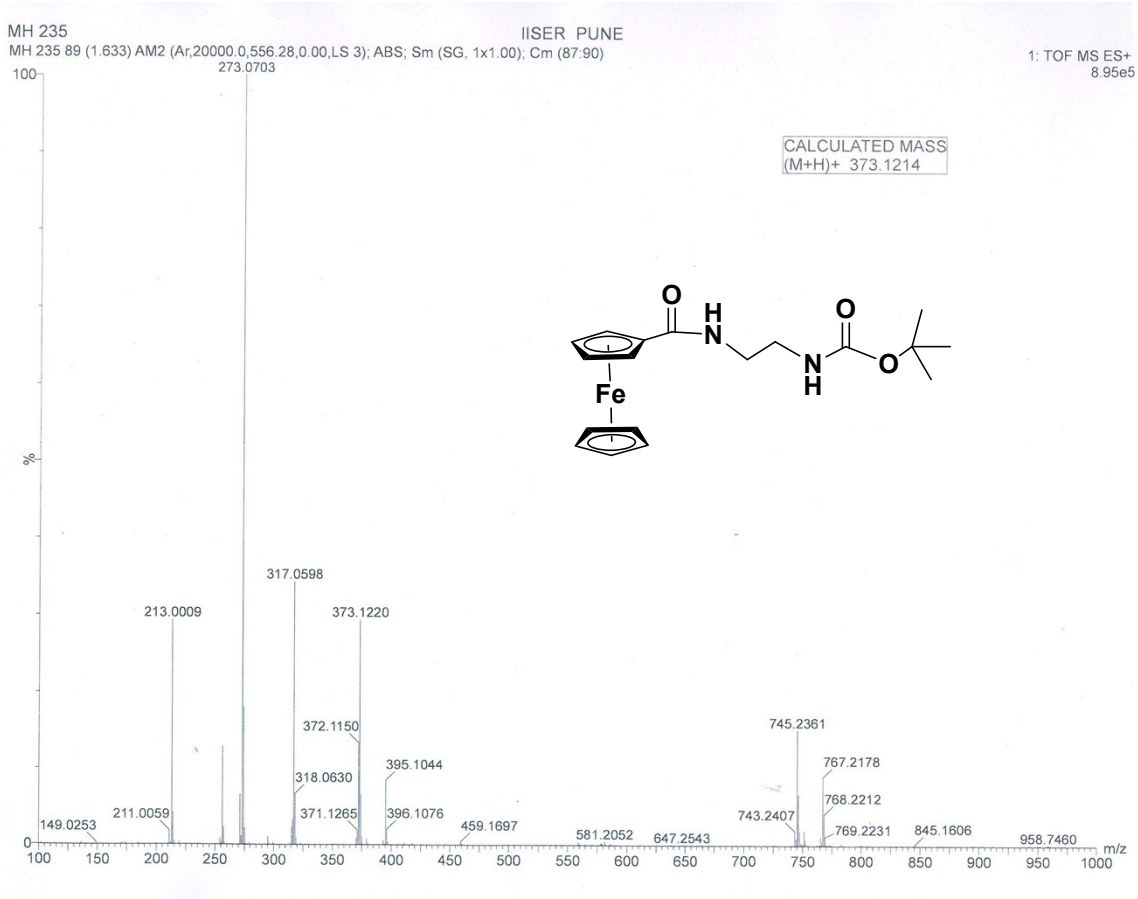
MH 235
IISER PUNE
MH 235 89 (1.633) AM2 (Ar,20000.0,556.28,0.00,LS 3); ABS; Sm (SG, 1x1.00); Cm (87:90)
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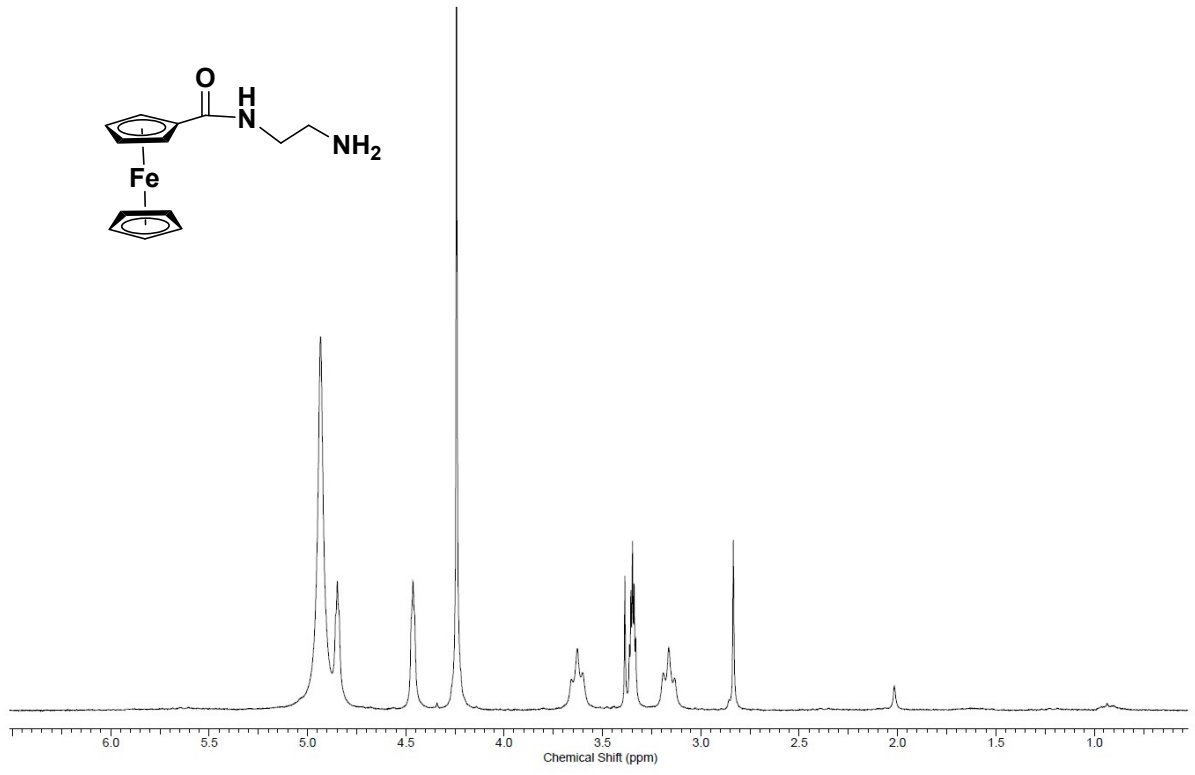
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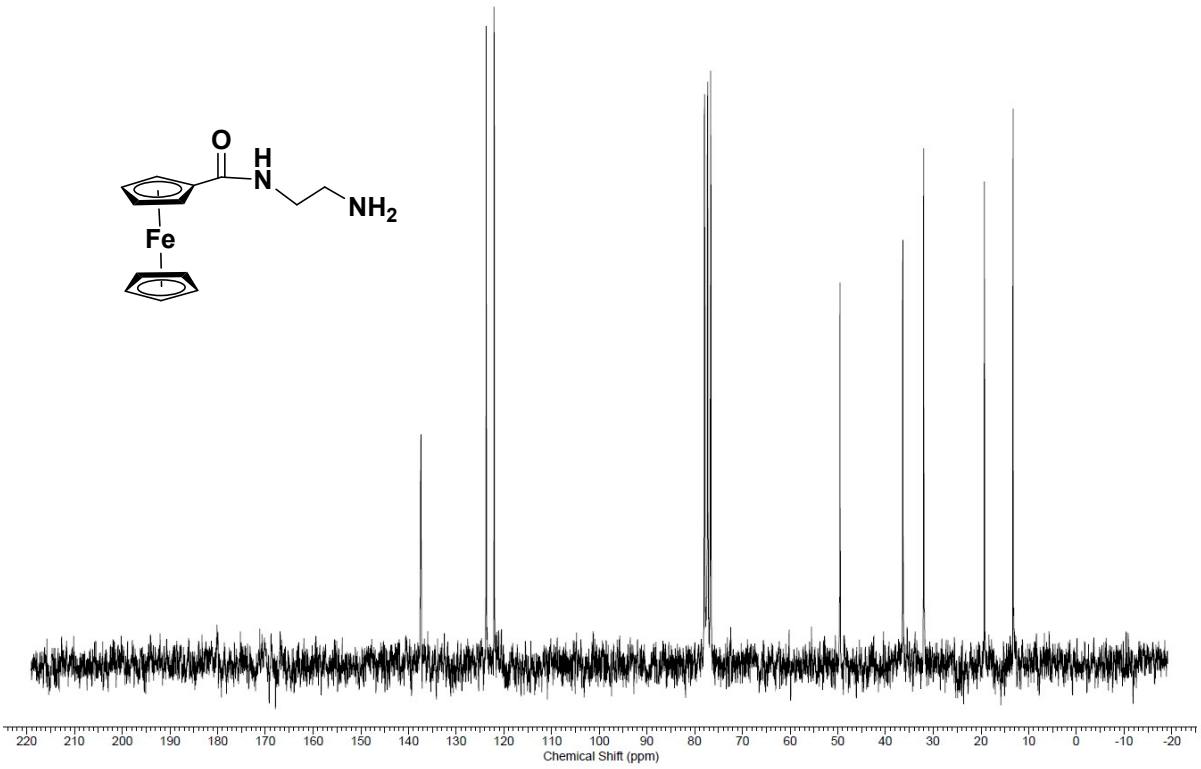
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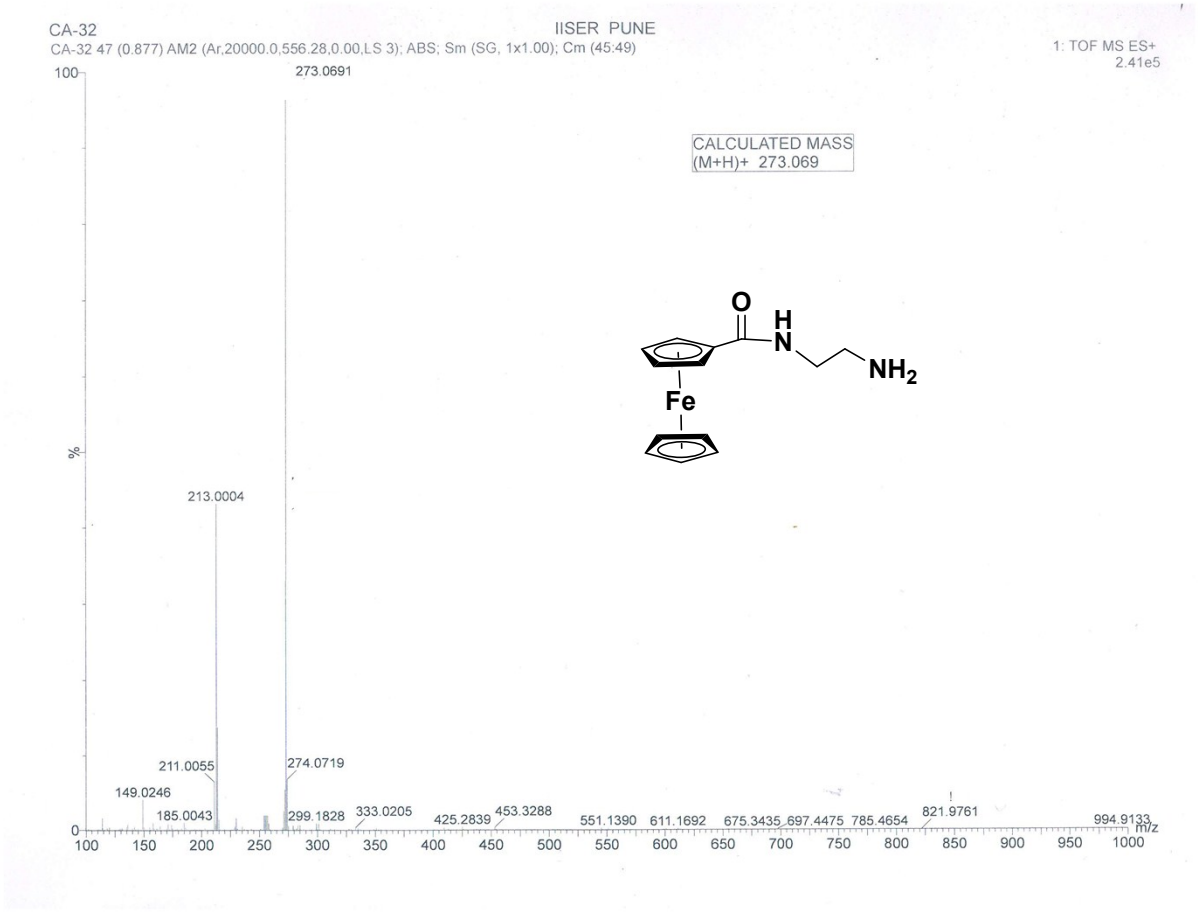
Chemical Shift (ppm)


CA-32
IISER PUNE
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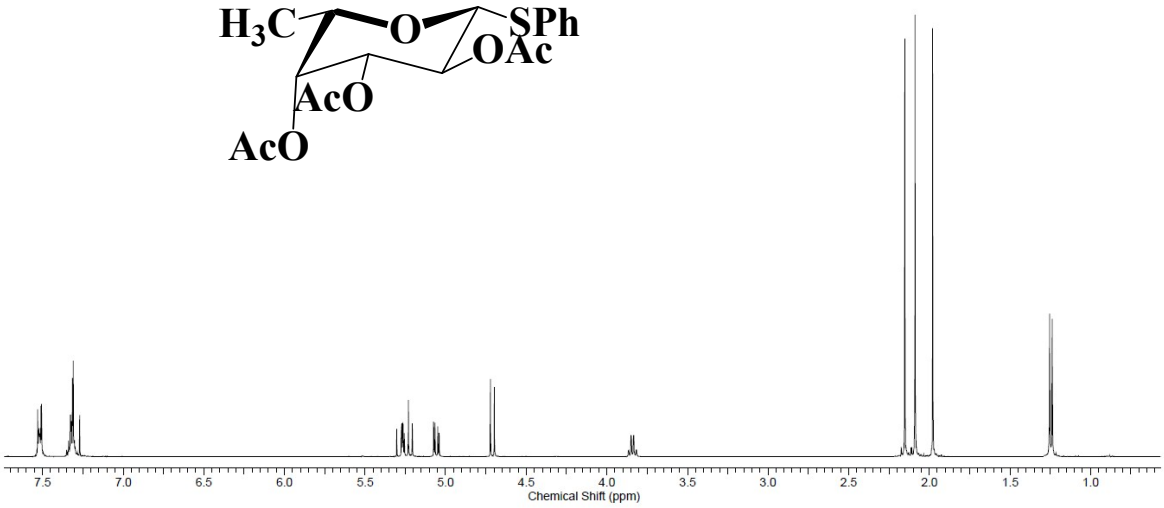
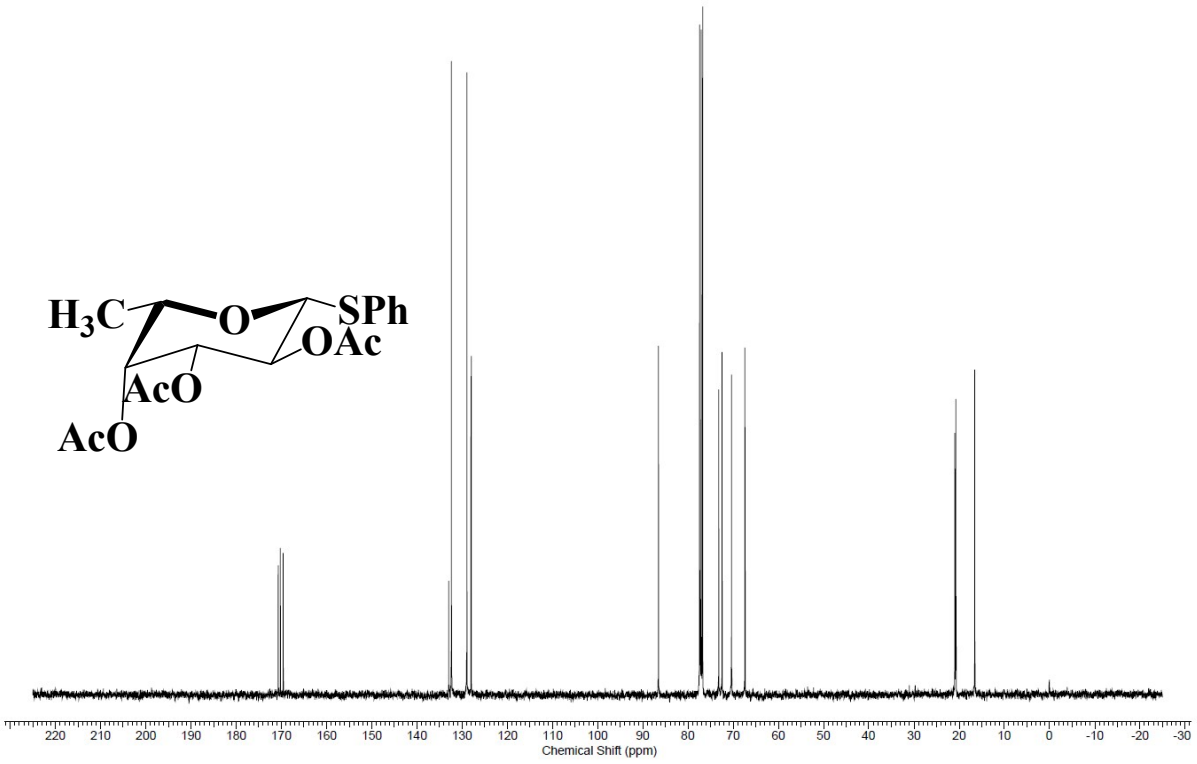
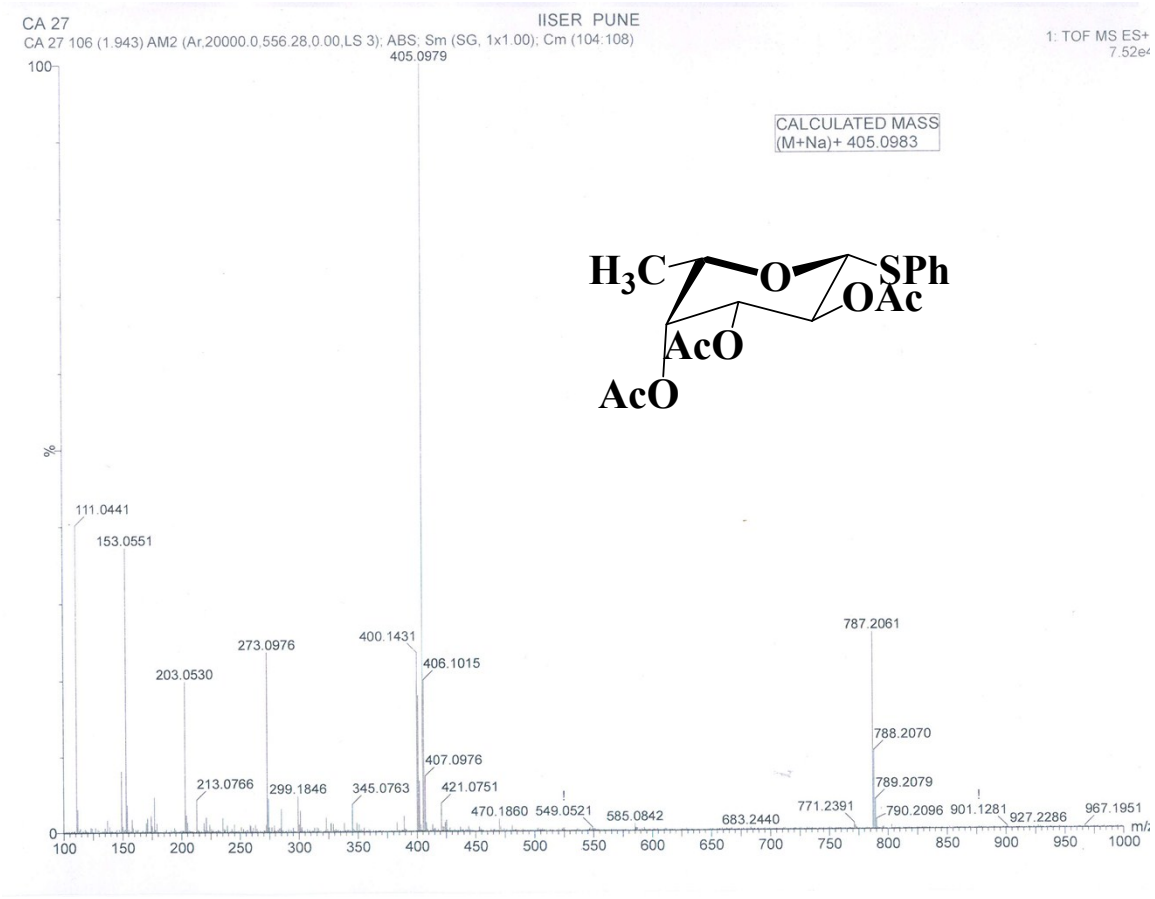
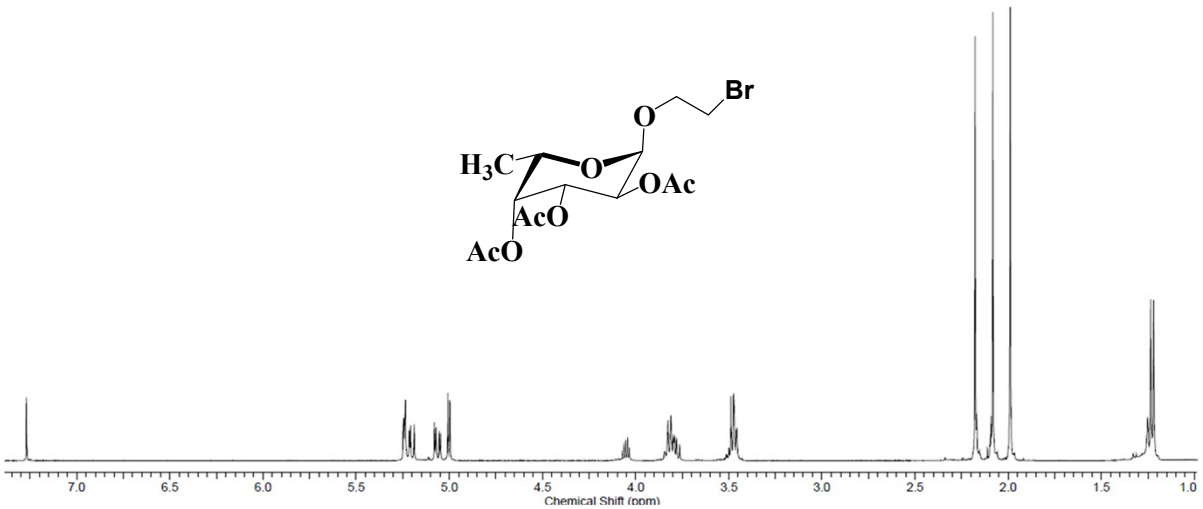
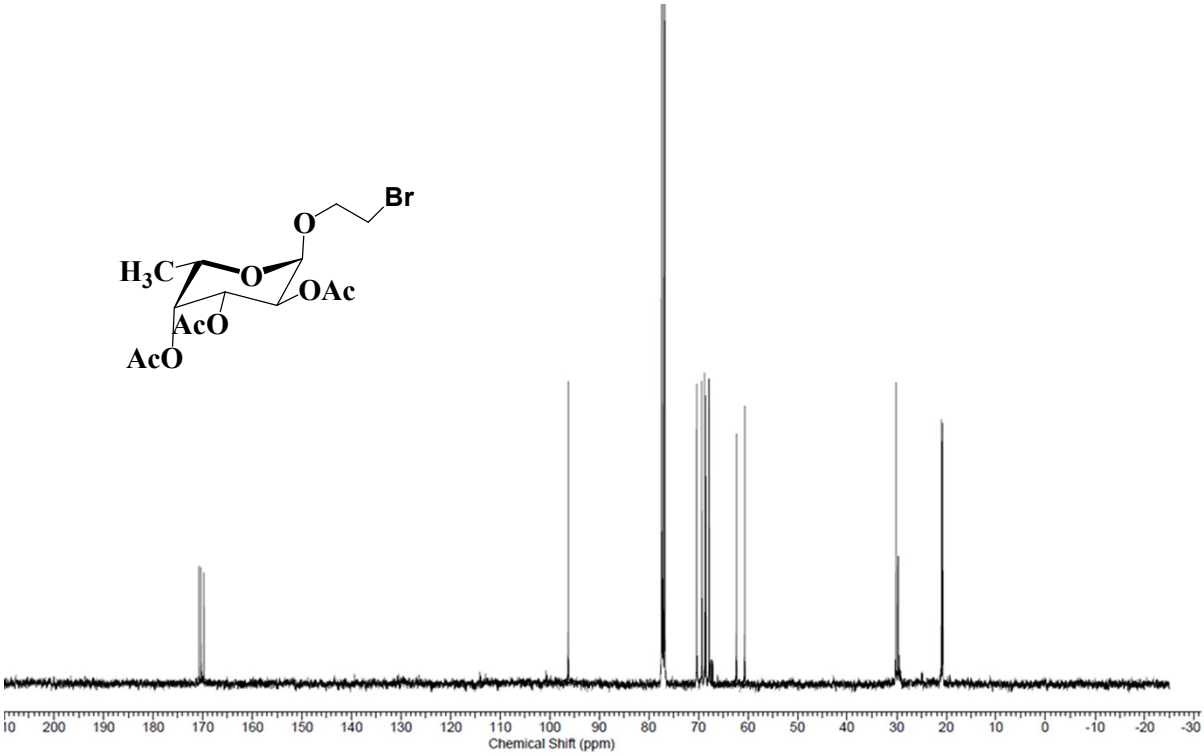
%
0
273.0691
CALCULATED MASS
(M+H)+ 273.069
O
H
N
NH2
Fe
213.0004
211.0055
274.0719
149.0246
185.0043
299.1828
333.0205
425.2839
453.3288
551.1390
611.1692
675.3435
697.4475
785.4654
821.9761
994.9133
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
m/z

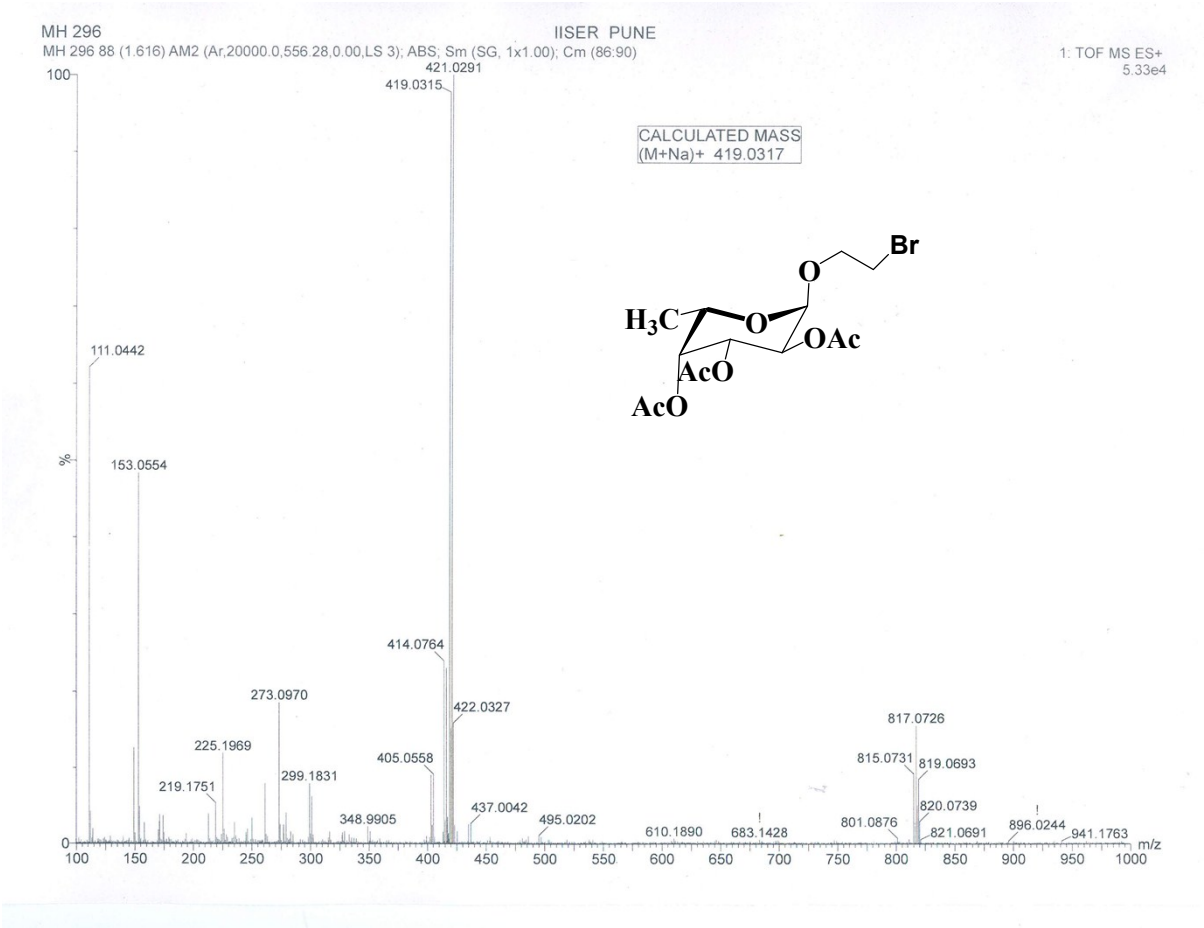

H3C
O
SPh
OAc
AcO
AcO
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
Chemical Shift (ppm)

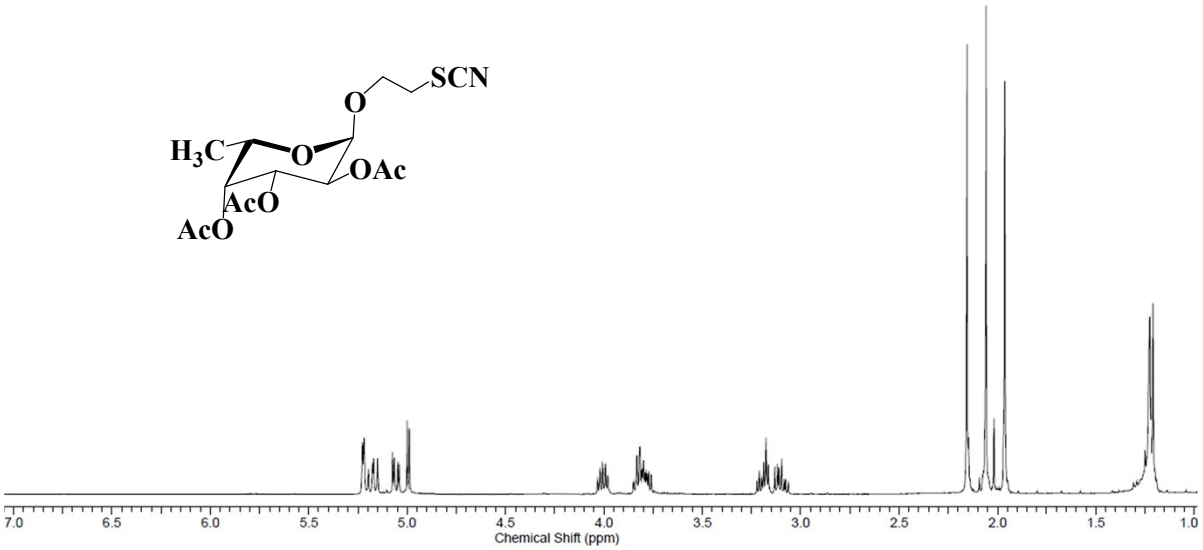

H3C
O
SPh
OAc
AcO
AcO
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
Chemical Shift (ppm)

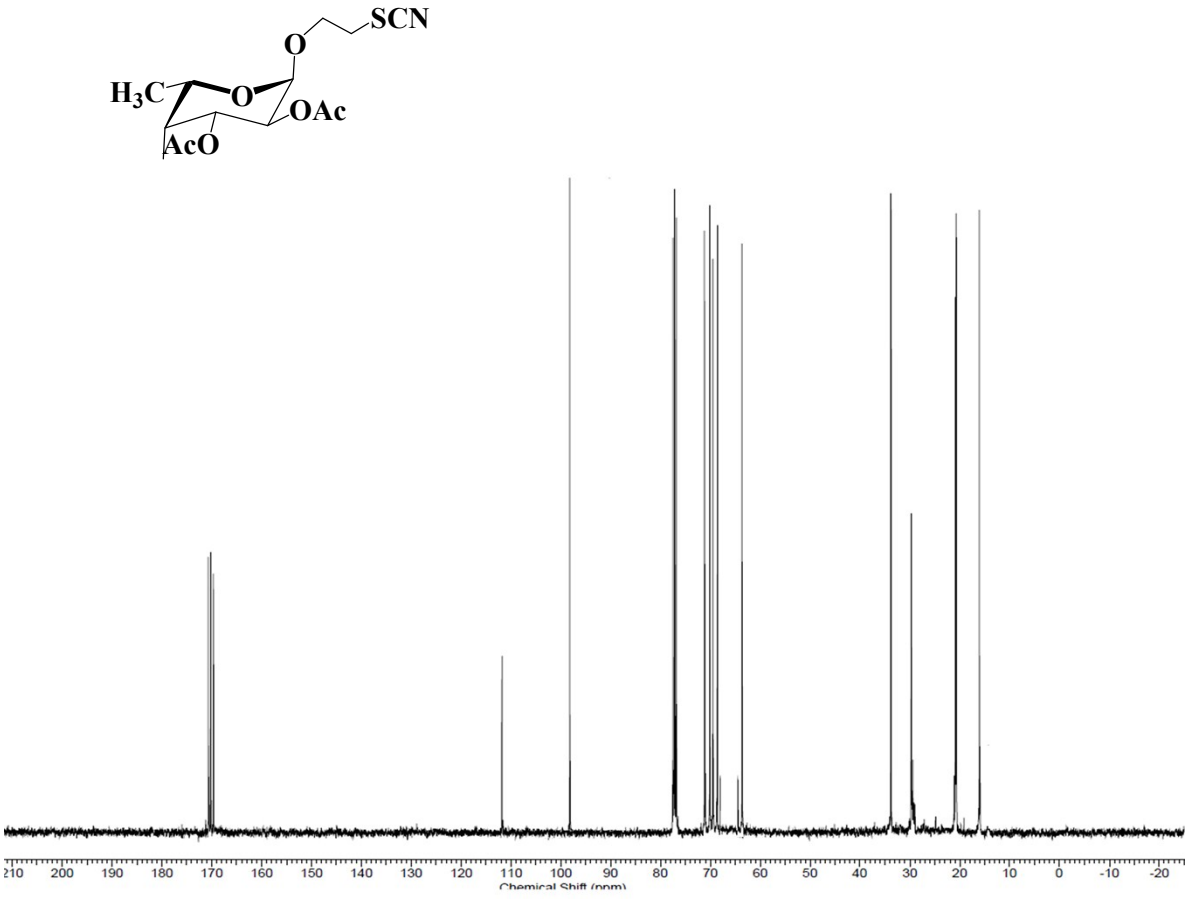

CA 27
IISER PUNE
CA 27 106 (1.943) AM2 (Ar,20000.0,556.28,0.00,LS 3); ABS; Sm (SG, 1x1.00); Cm (104:108)
1: TOF MS ES+
405.0979
CALCULATED MASS
(M+Na)+ 405.0983
H3C
O
SPh
OAc
AcO
AcO
%
111.0441
153.0551
203.0530
273.0976
400.1431
406.1015
787.2061
788.2070
407.0976
789.2079
213.0766
299.1846
345.0763
421.0751
470.1860
549.0521
585.0842
683.2440
771.2391
790.2096
901.1281
927.2286
967.1951
m/z

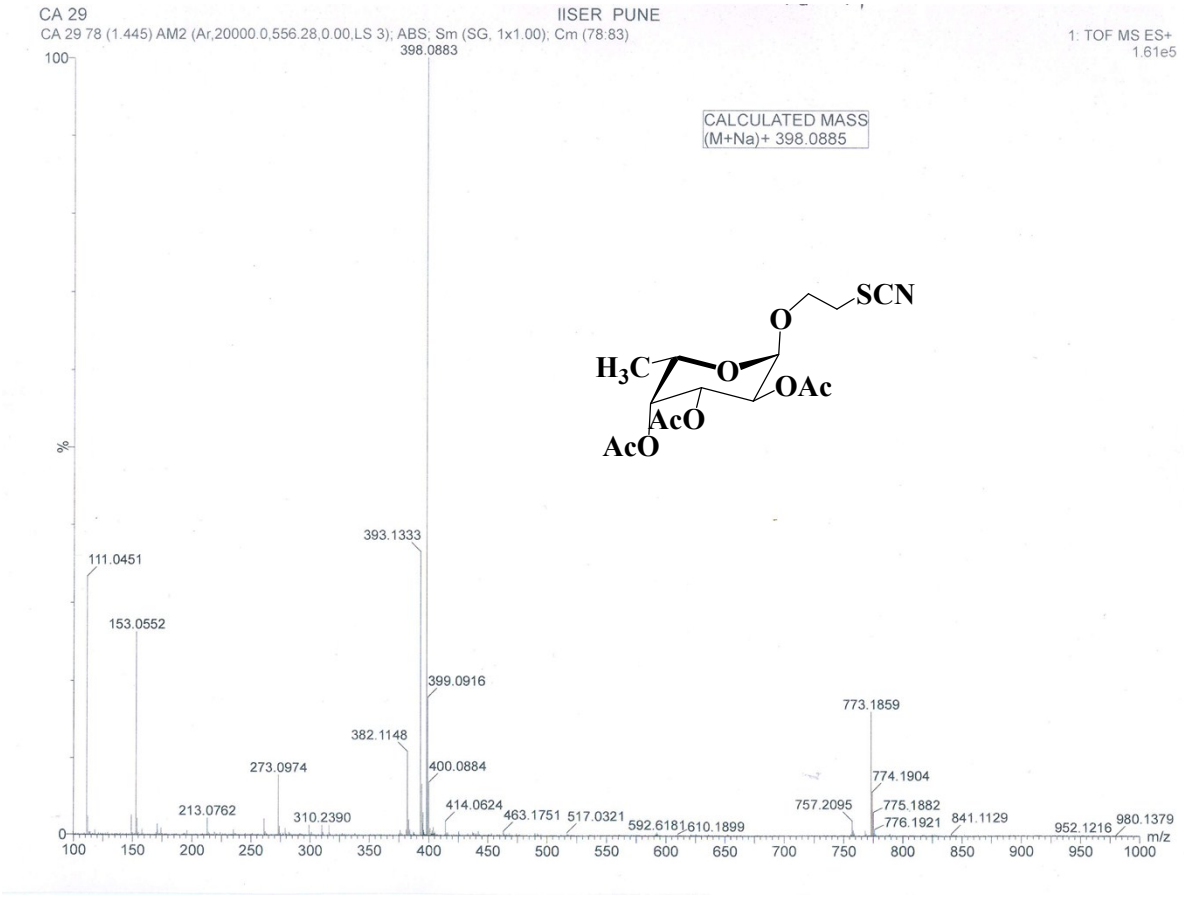

Br
O
H3C
O
OAc
AcO
AcO
Chemical Shift (ppm)

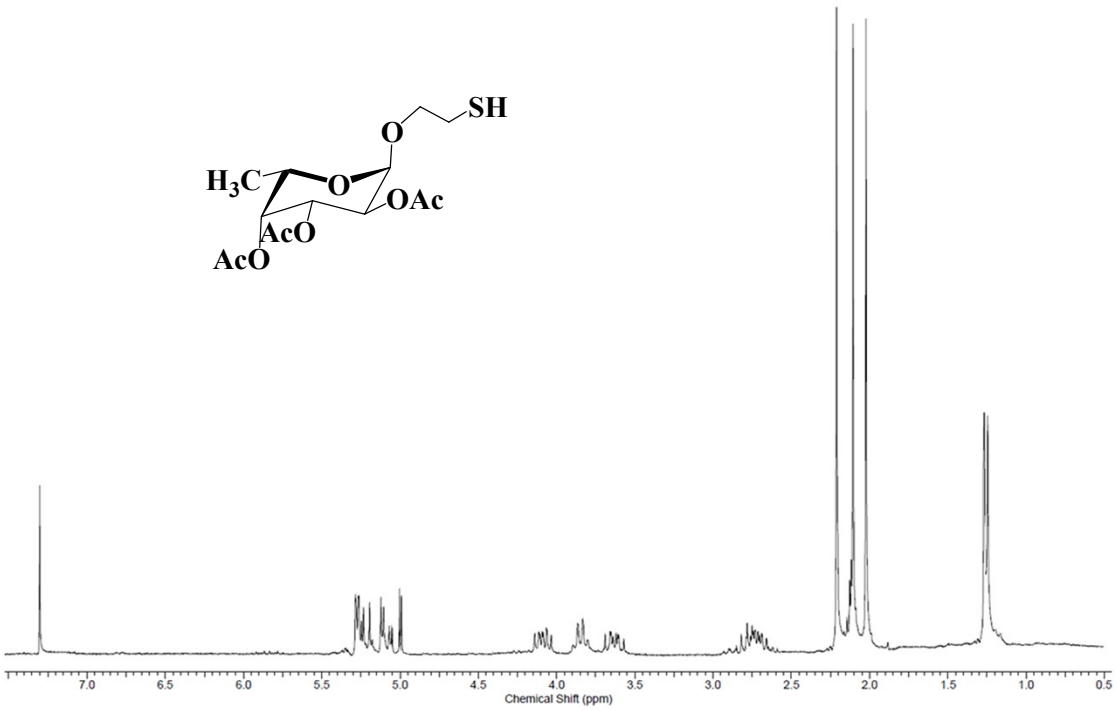

Br
O
H3C
O
OAc
AcO
AcO
Chemical Shift (ppm)

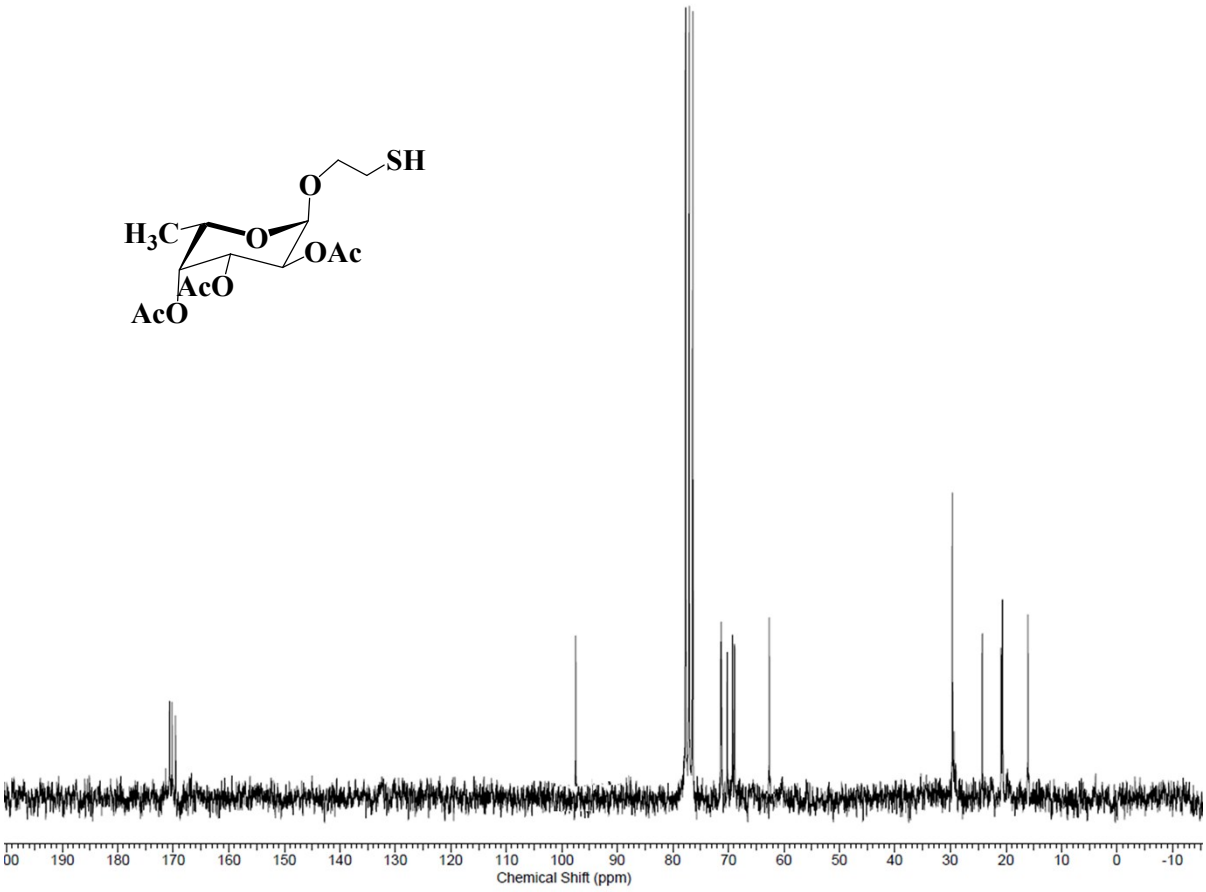

MH 296
IISER PUNE
MH 296 88 (1.616) AM2 (Ar,20000.0,556.28,0.00,LS 3); ABS; Sm (SG, 1x1.00); Cm (86:90)
1: TOF MS ES+
5.33e4
CALCULATED MASS
(M+Na)+ 419.0317
421.0291
419.0315
111.0442
153.0554
414.0764
273.0970
422.0327
225.1969
405.0558
299.1831
219.1751
437.0042
348.9905
495.0202
610.1890
683.1428
817.0726
815.0731
819.0693
820.0739
801.0876
821.0691
896.0244
941.1763
m/z
%

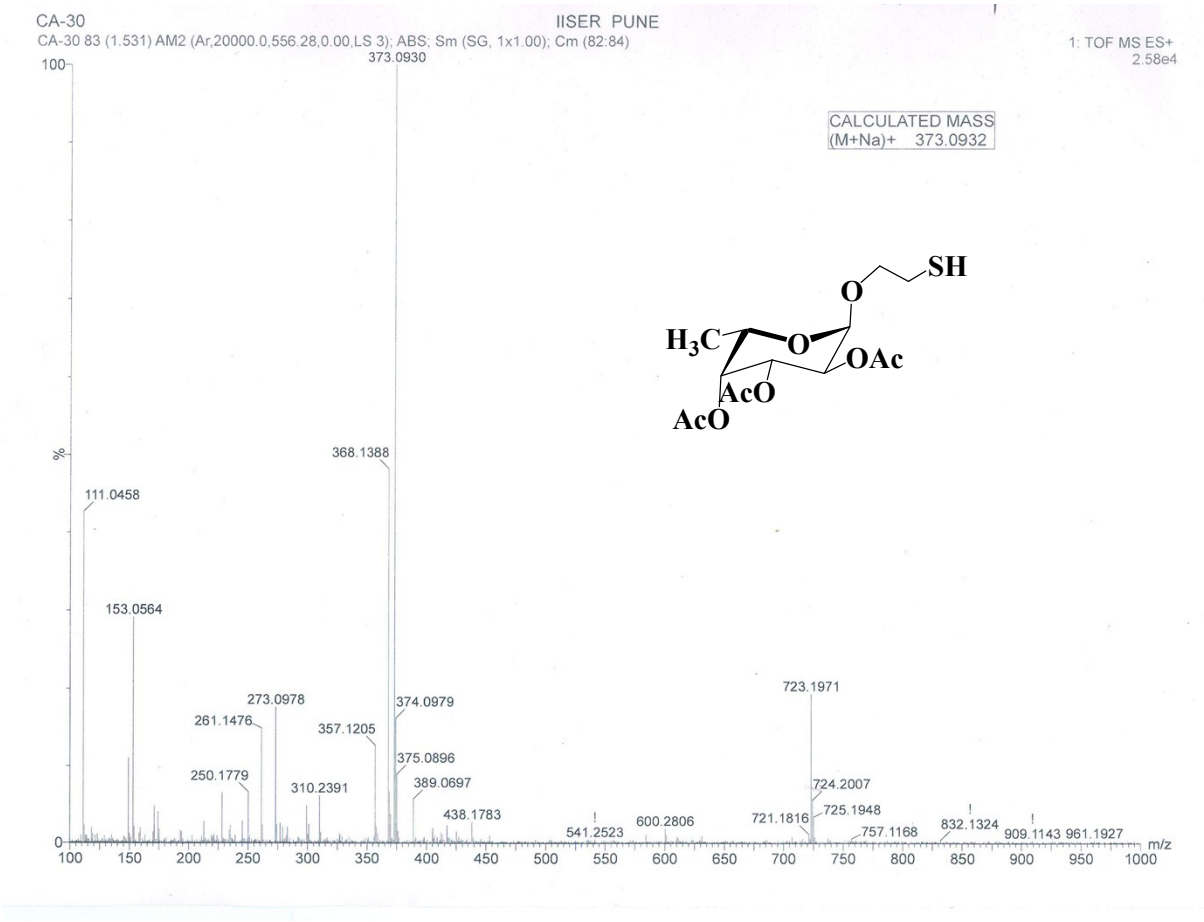

SCN
O
H3C
O
OAc
AcO
AcO
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
Chemical Shift (ppm)

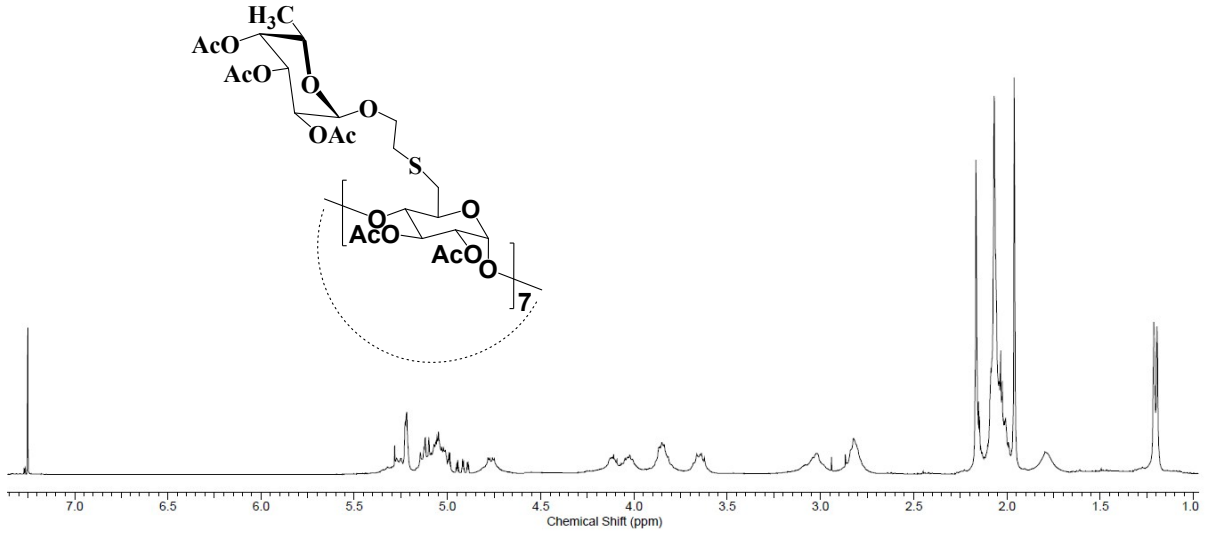

SCN
O
H3C
O
OAc
AcO
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20

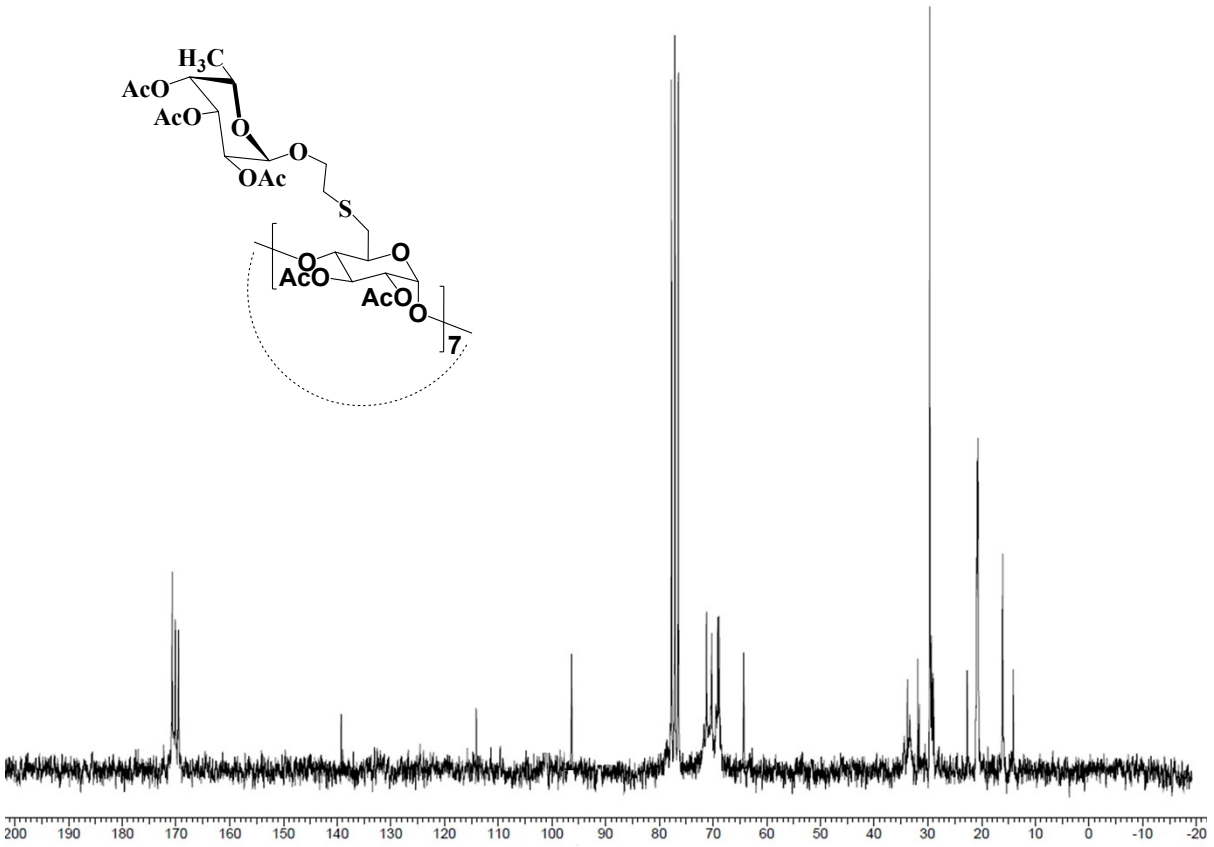

CA 29
IISER PUNE
CA 29 78 (1.445) AM2 (Ar,20000.0,556.28,0.00,LS 3); ABS; Sm (SG, 1x1.00); Cm (78:83)
1: TOF MS ES+
1.61e5
CALCULATED MASS
(M+Na)+ 398.0885
SCN
O
H3C
O
OAc
AcO
AcO
%
100
0
398.0883
393.1333
111.0451
153.0552
399.0916
773.1859
382.1148
400.0884
774.1904
273.0974
213.0762
310.2390
414.0624
463.1751
517.0321
592.6181
610.1899
757.2095
775.1882
776.1921
841.1129
952.1216
980.1379
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
m/z

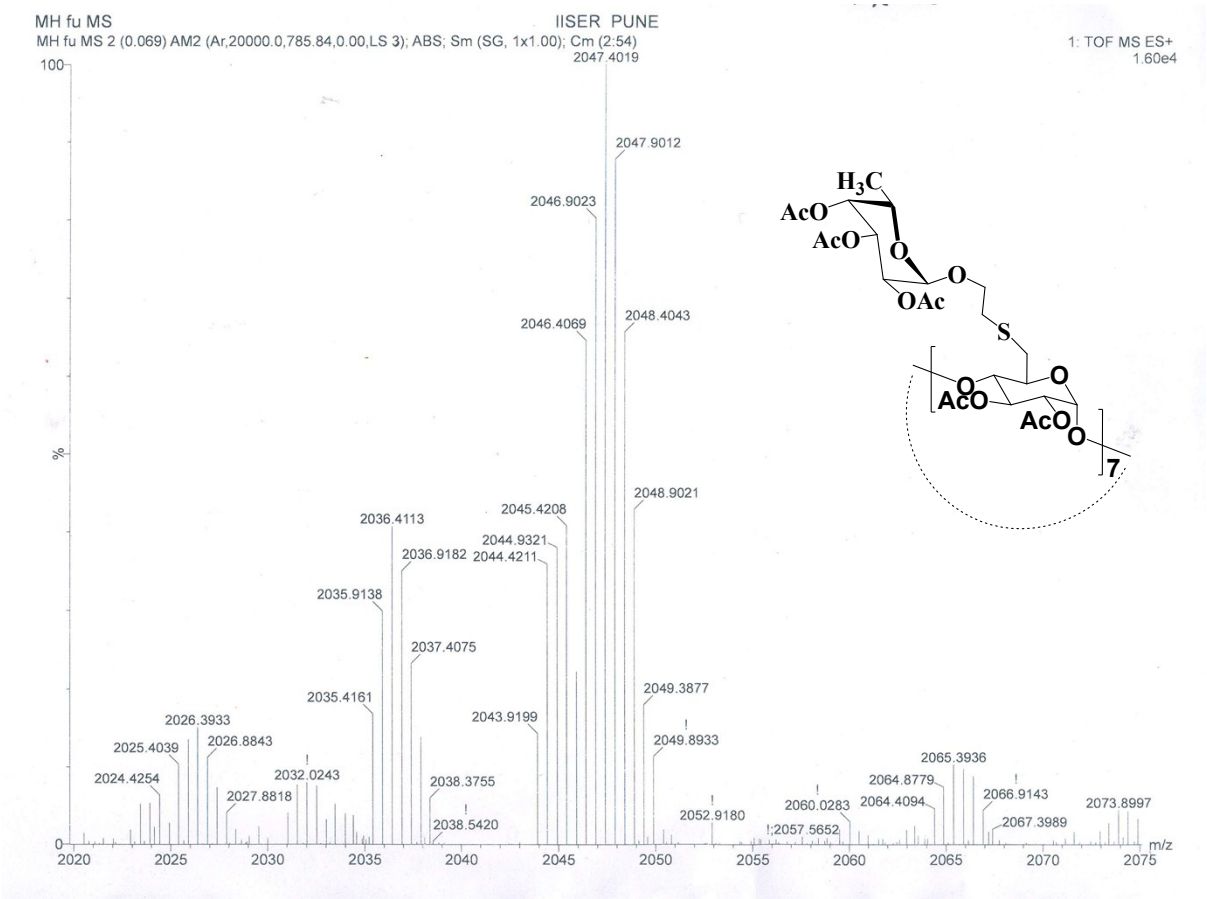

SH
O
H3C
O
OAc
AcO
AcO
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
Chemical Shift (ppm)

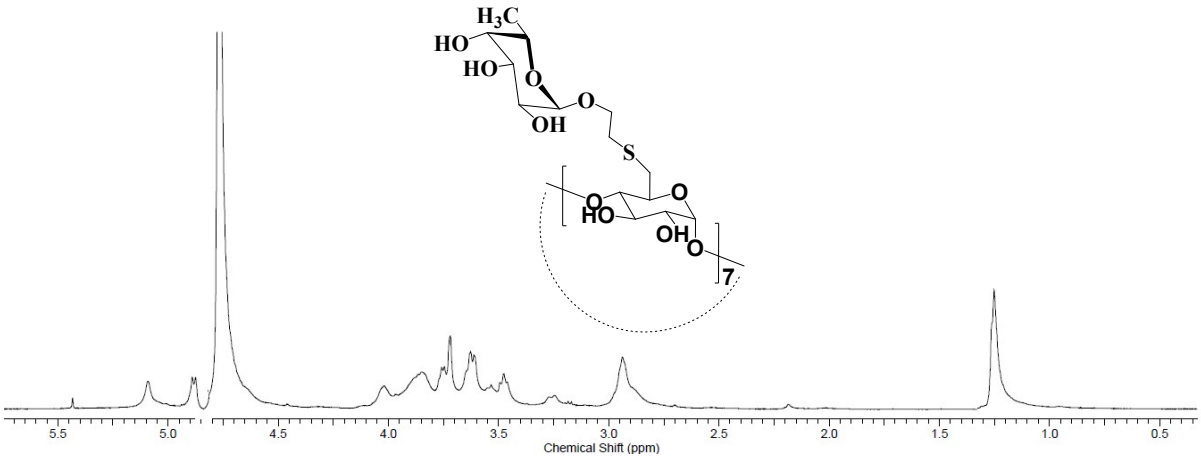

SH
O
H3C
O
OAc
AcO
AcO
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
Chemical Shift (ppm)

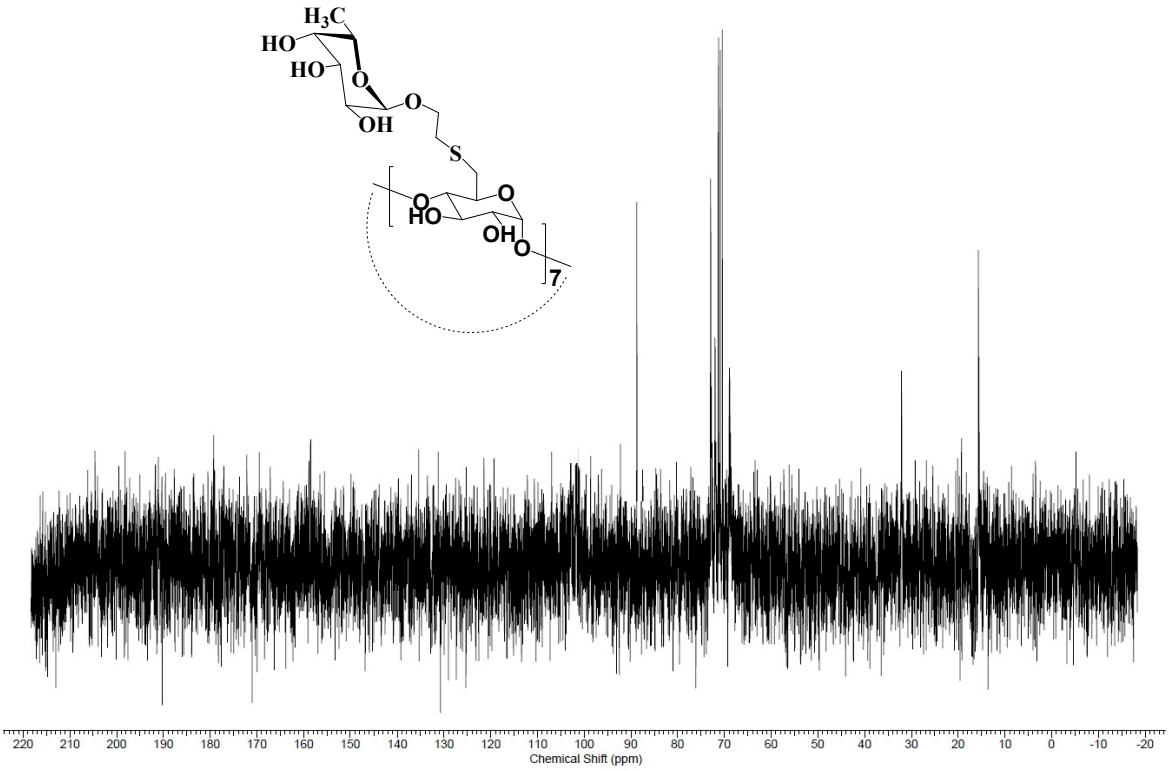

CA-30
IISER PUNE
CA-30 83 (1.531) AM2 (Ar,20000.0,556.28,0.00,LS 3); ABS; Sm (SG, 1x1.00); Cm (82:84)
1: TOF MS ES+
2.58e4
CALCULATED MASS
(M+Na)+ 373.0932
SH
O
H3C
O
OAc
AcO
AcO
373.0930
368.1388
111.0458
153.0564
273.0978
261.1476
357.1205
374.0979
375.0896
250.1779
310.2391
389.0697
438.1783
723.1971
724.2007
725.1948
721.1816
757.1168
832.1324
909.1143
961.1927
541.2523
600.2806
%
m/z

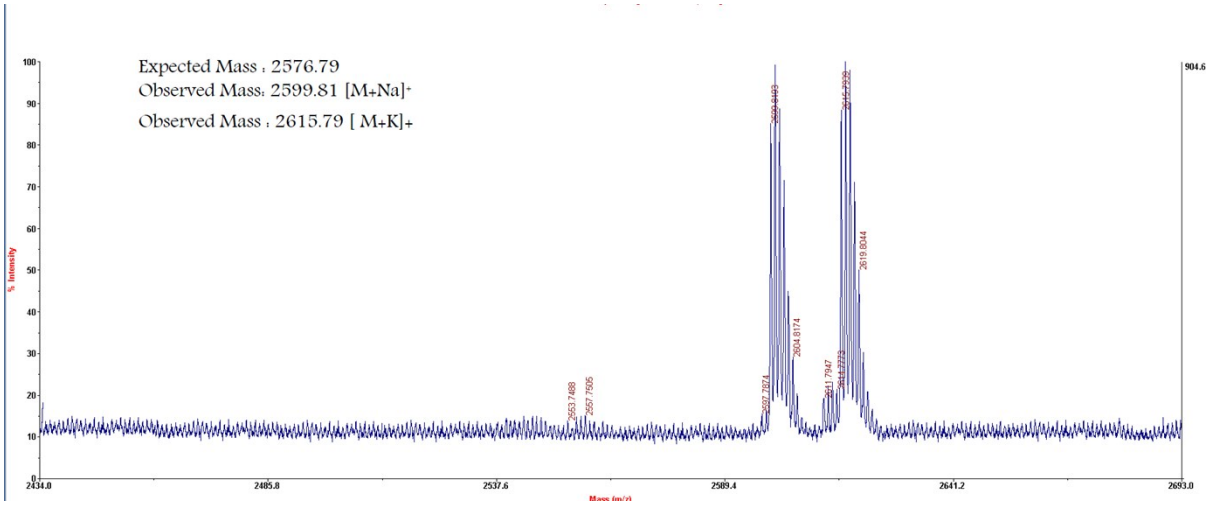

H3C
AcO
AcO
O
O
OAc
S
O
O
AcO
AcO
O
7
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
Chemical Shift (ppm)


H3C
AcO
AcO
O
O
OAc
S
O
O
AcO
AcO
O
7
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20


MH fu MS
IISER PUNE
MH fu MS 2 (0.069) AM2 (Ar,20000.0,785.84,0.00,LS 3); ABS; Sm (SG, 1x1.00); Cm (2:54)
1: TOF MS ES+
1.60e4
100
%
0
2047.4019
2047.9012
2046.9023
2048.4043
2046.4069
2048.9021
2045.4208
2036.4113
2044.9321
2036.9182
2044.4211
2035.9138
2037.4075
2049.3877
2035.4161
2043.9199
2049.8933
2026.3933
2025.4039
2026.8843
2024.4254
2032.0243
2027.8818
2038.3755
2038.5420
2052.9180
2060.0283
2057.5652
2065.3936
2064.8779
2064.4094
2066.9143
2067.3989
2073.8997
2020
2025
2030
2035
2040
2045
2050
2055
2060
2065
2070
2075
m/z
H3C
AcO
AcO
O
O
OAc
S
O
O
AcO
AcO
O
7


H3C
HO
HO
O
O
OH
S
O
HO
OH
O
7
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
Chemical Shift (ppm)


H3C
HO
HO
O
O
OH
S
O
HO
OH
O
7
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
Chemical Shift (ppm)


Expected Mass : 2576.79
Observed Mass: 2599.81 [M+Na]+
Observed Mass : 2615.79 [M+K]+
% Intensity
100
90
80
70
60
50
40
30
20
10
0
2434.0
2485.8
2537.6
2589.4
2641.2
2693.0
904.6
2653.7488
2557.7505
2597.7824
2599.8493
2604.8174
2611.7947
2615.7232
2619.6044