

Supporting Information for

**Comparison of zwitterionic *N*-alkylaminomethanesulfonic acids to related compounds in the Good buffer series**

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Additional supporting information (in separate files): S2.CIF, S3.CIF

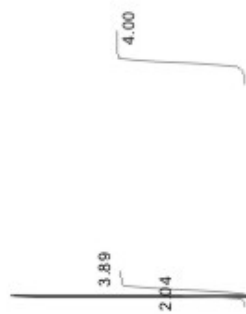
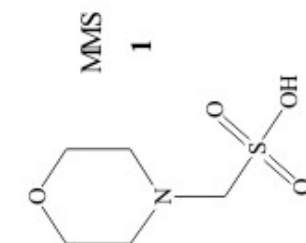
## Protocols and methods

Optical absorbance spectra of 0.2 M solutions were recorded from 700 to 200 nm using a Perkin Elmer Lambda 35 dual beam spectrophotometer. Elemental composition was determined by combustion analysis at Texas Tech University, Lubbock, TX, USA. Melting points were determined using a Stanford Research Systems MPA-100 Optimelt melting point apparatus and are uncorrected. Infrared absorption spectra were recorded as KBr pellets using a Nicolet Magna 560 FT-IR. X-ray crystallographic analysis of MMS 1 was obtained by Robert Long during an ACS/PRF workshop entitled “X-ray Crystallography for Organic Chemists” at UCSD in Aug 2004. X-ray crystallographic analysis of HEPMS 2 was conducted by Tatiana Timofeeva and associates of New Mexico Highlands University. Crystals for X-ray analysis were obtained by recrystallization from saturated methanol solutions of the products. NMR analyses were conducted on 250 and 500 MHz instruments at Texas Tech University and University of New Mexico.

**Growth Study protocol.** *Escherichia coli* strain HB101 was cultured overnight in LB media at 37 °C with shaking. Filter sterilized stock solutions were made for each buffer. Each stock solution was adjusted to pH 7.2 (the pH of LB media) prior to sterilizing. Sterile buffer was added to culture tubes containing fresh LB media to final concentrations of 10, 20 and 50 mM. Each tube was inoculated from the overnight culture and shaken at 37 °C for ~18 h. Culture growth was estimated by measuring the optical density at 600 nm.

TTU\_05042006\vrh050406.2.fid\processed\_fid  
MMS in D2O SW Prober\h050406.2  
May 4 2006  
USER:

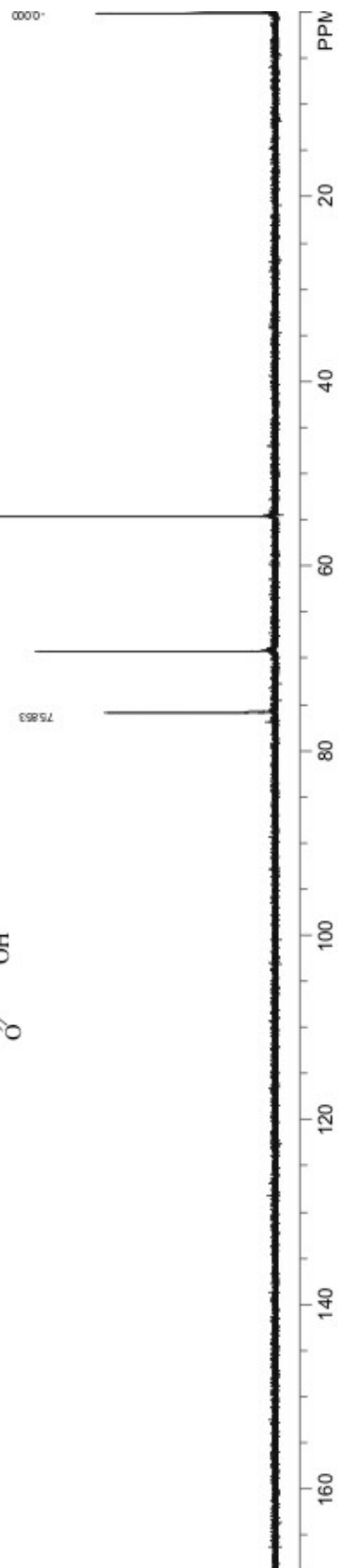
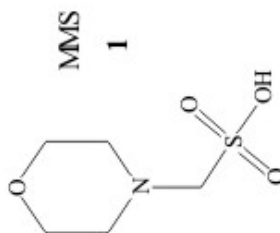
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F2 = 499.711945 MHz  
SW1 = 8000.00 Hz  
AT1 = 8.19 sec  
Hz per Pt 1stD = 0.12 Hz  
SW2 = 1.00 Hz  
Hz per Pt 2ndD = 1.00 Hz  
O1 = 2560.42 Hz  
O2 = -0.50 Hz  
LB1 = 0.00 Hz  
TP A = 26.69  
B = 10.40



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May 4 2006

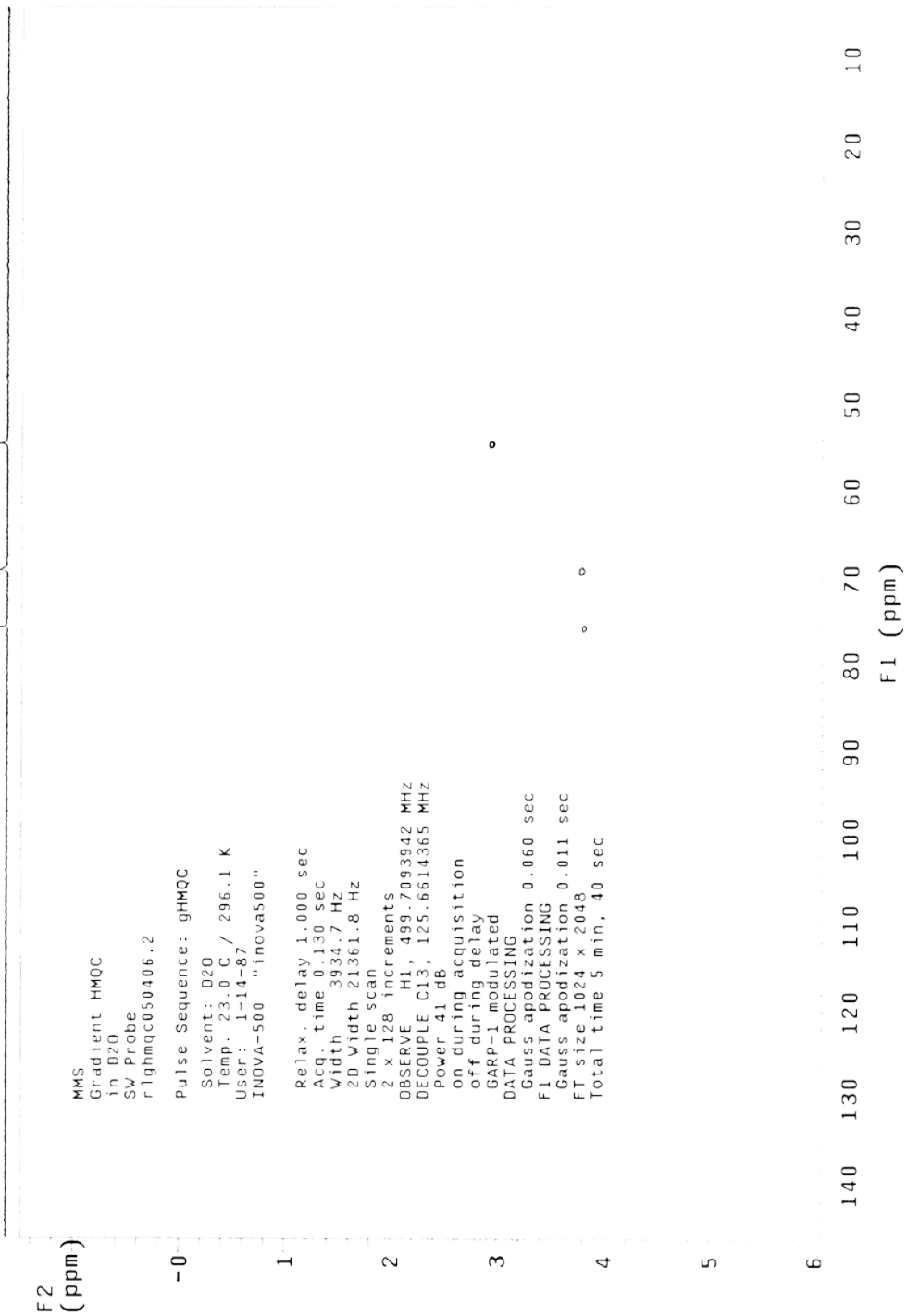
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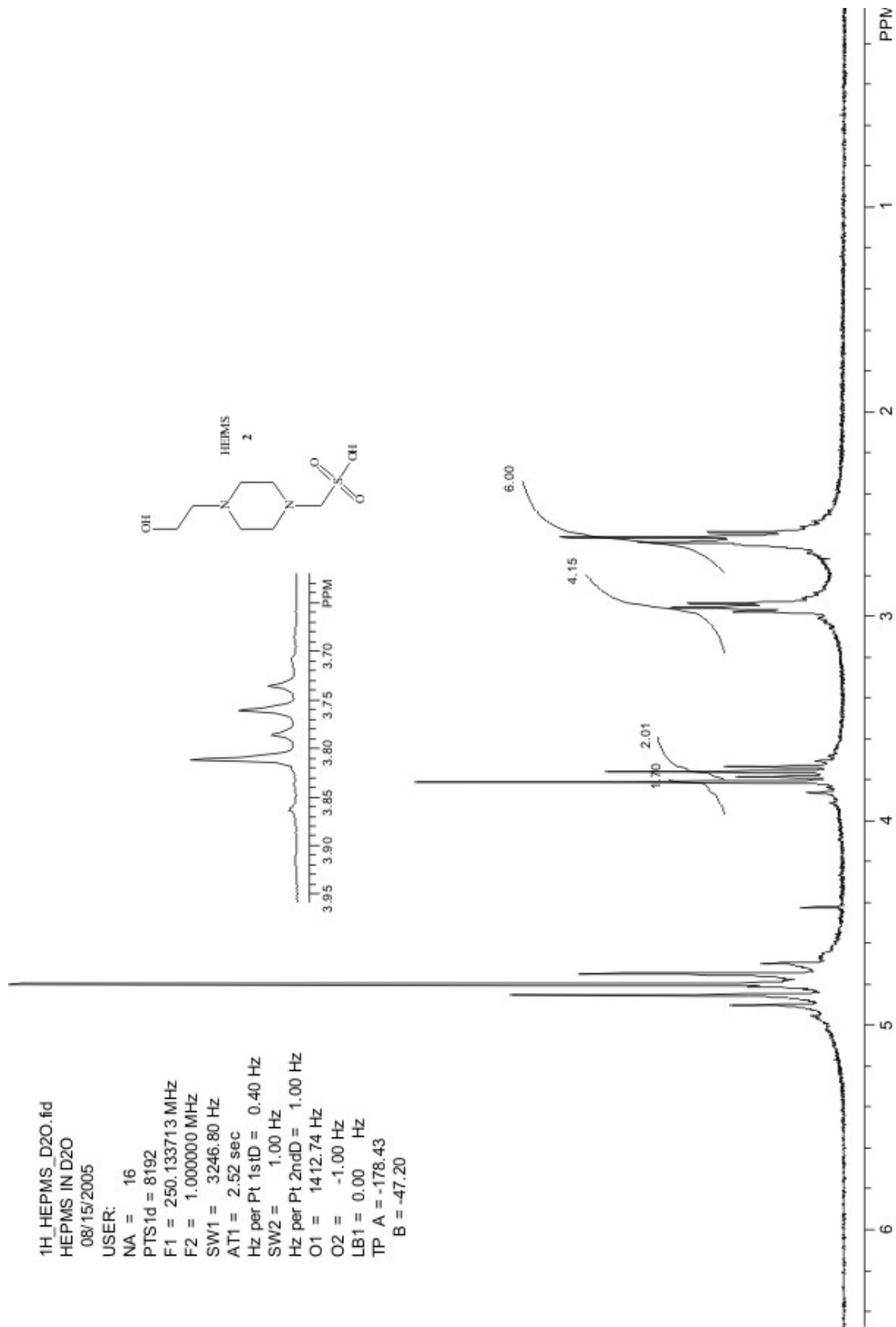
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SW1 = 32520.33 Hz  
AT1 = 2.02 sec  
Hz per Pt 1d = 0.50 Hz  
SW2 = 1.00 Hz  
Hz per Pt 2nd = 1.00 Hz  
O1 = 14164.01 Hz  
O2 = -0.50 Hz  
LB1 = 0.00 Hz  
TP A = -173.65  
B = 78.90



125 MHz  $^{13}\text{C}$  NMR of MMS 1 in  $\text{D}_2\text{O}$  with TSP reference

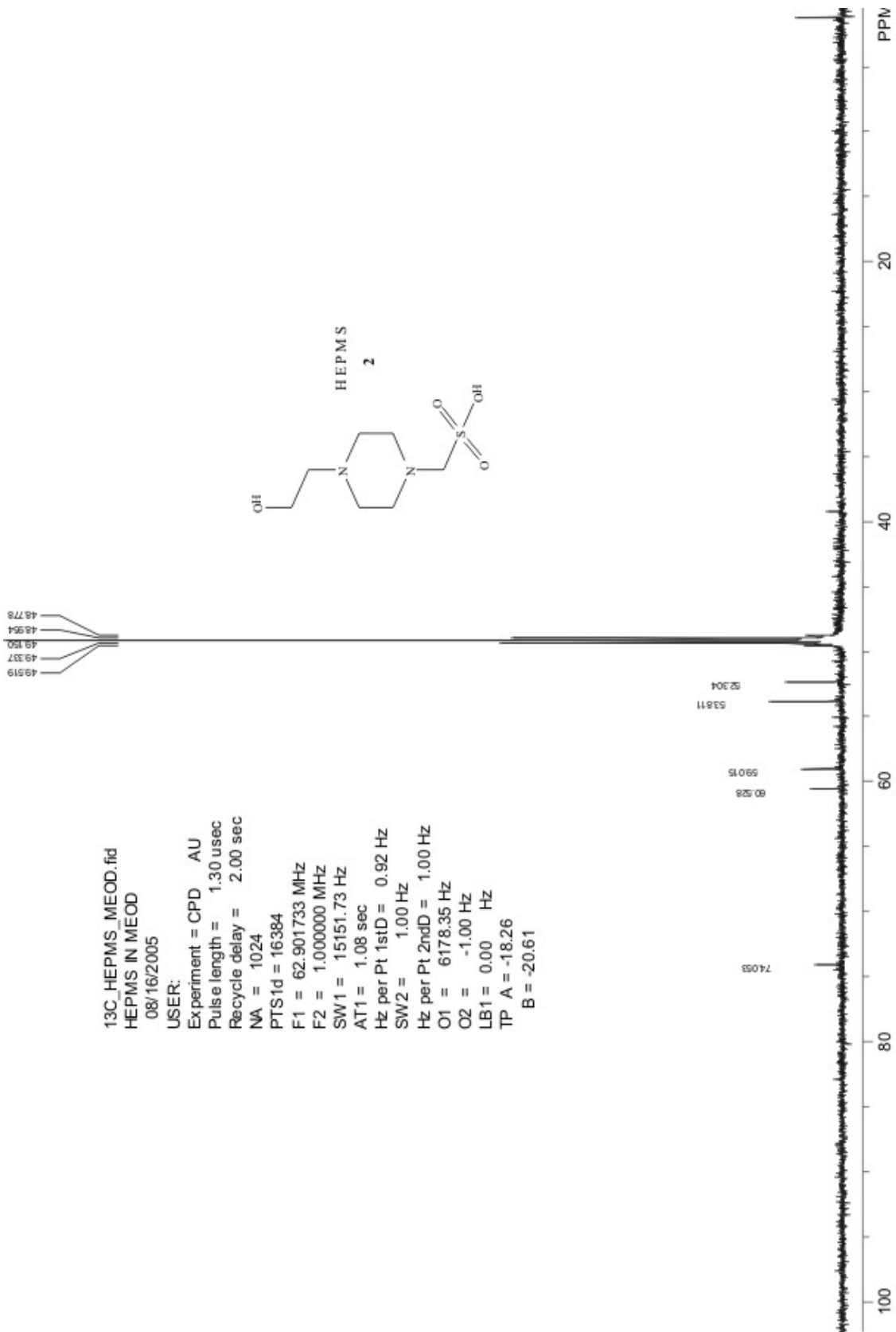
gHMQC of MMS 1 in D<sub>2</sub>O on 500 MHz NMR





250 MHz <sup>1</sup>H NMR of HEPMS 2 in D<sub>2</sub>O

63 MHz <sup>13</sup>C NMR of HEPMS 2 in MeOD

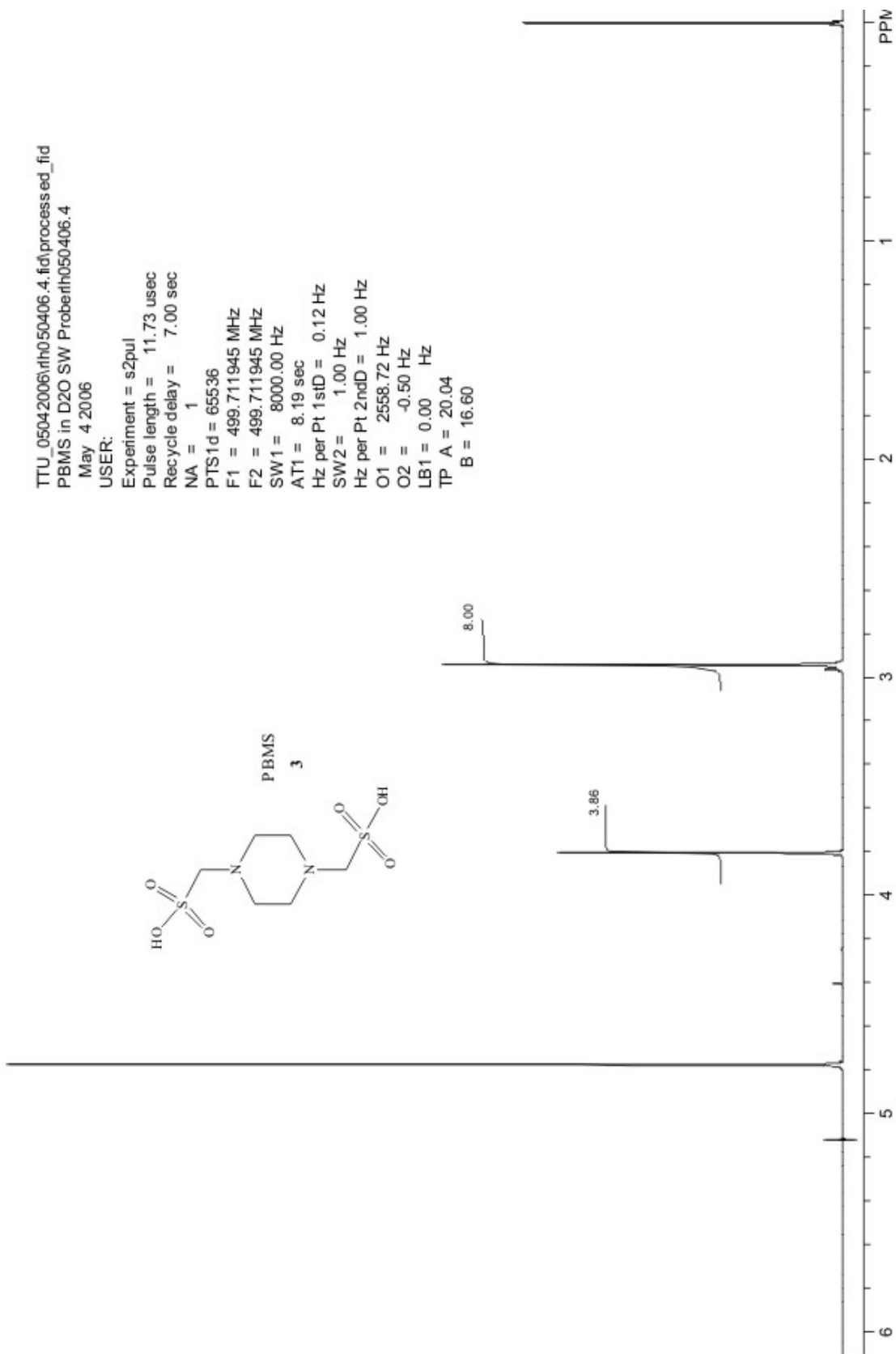
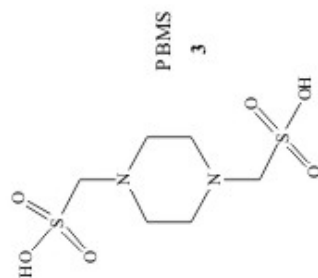




TTU\_05042006\rh050406.4.fid\processed\_fid  
PBMS in D2O SW Prober\rh050406.4  
May 4 2006

USER:

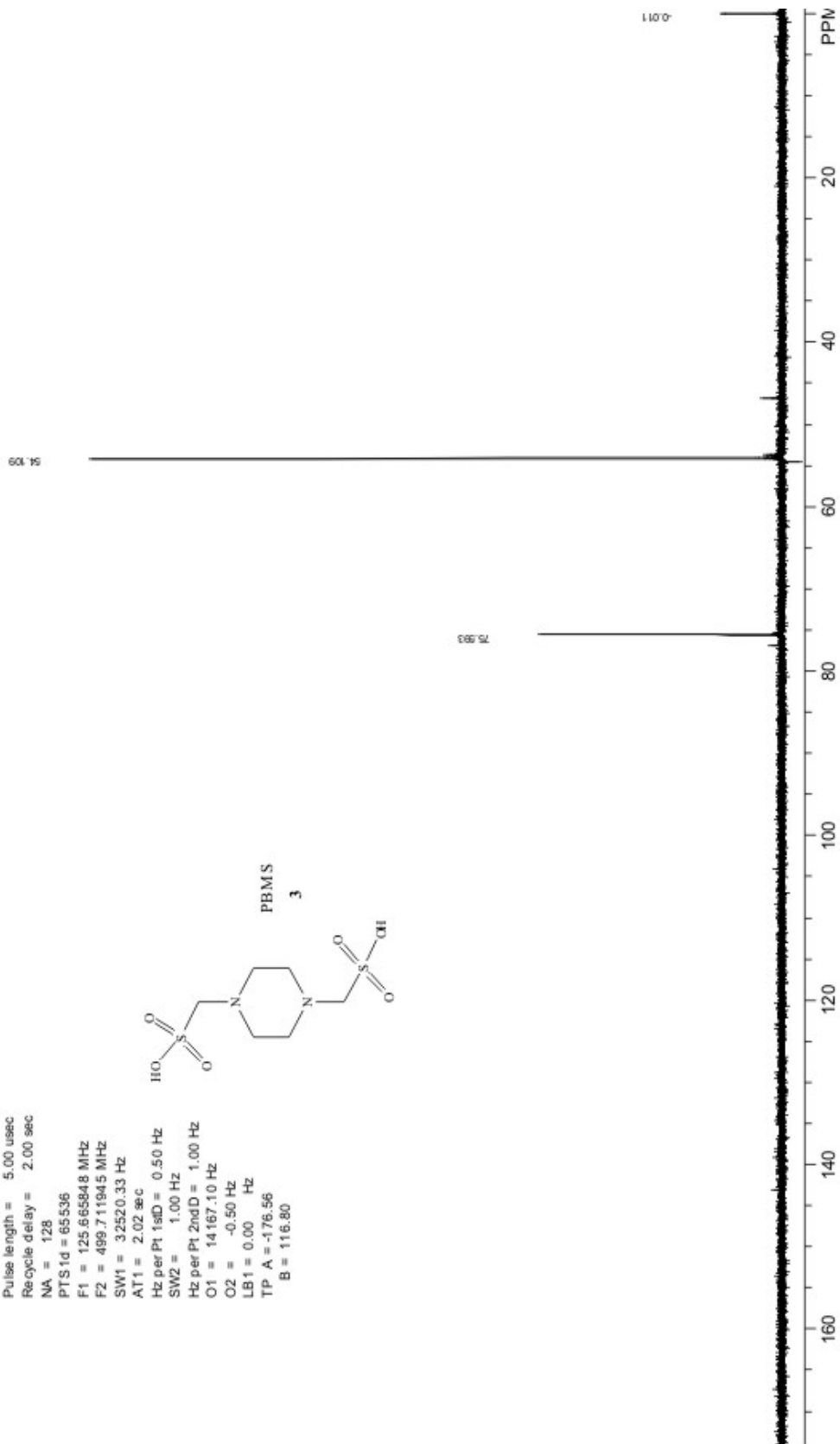
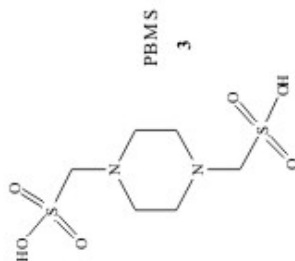
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F2 = 499.711945 MHz  
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SW2 = 1.00 Hz  
Hz per Pt 2ndD = 1.00 Hz  
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LB1 = 0.00 Hz  
TP A = 20.04  
B = 16.60



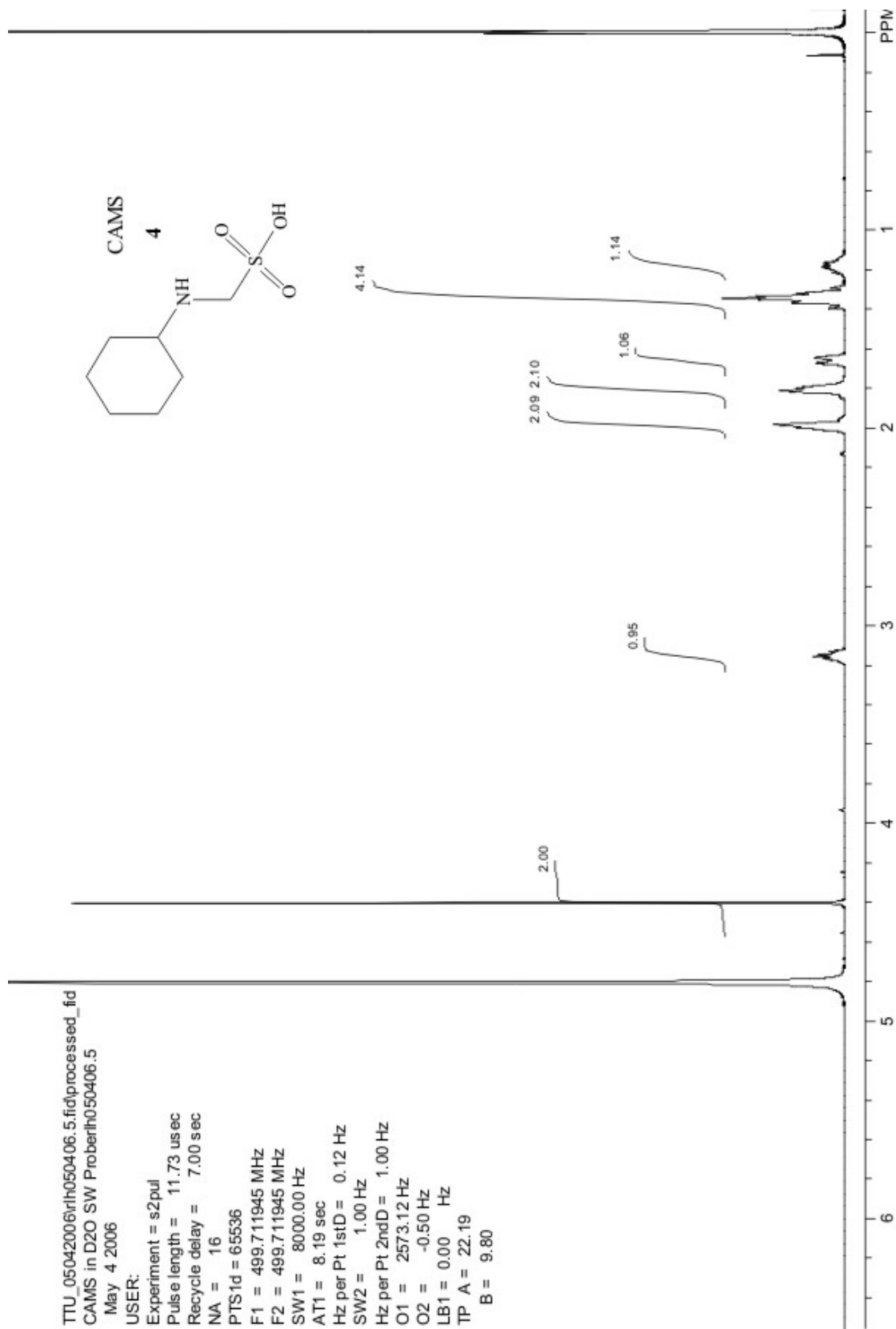
500 MHz  $^1\text{H}$  NMR of PBMS 3 in  $\text{D}_2\text{O}$  with TSP reference

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PBMS in D2O SW Probe\lc050406\_4  
May 4 2006  
USER:

Experiment = s2pul  
Pulse length = 5.00 usec  
Recycle delay = 2.00 sec  
NA = 128  
PTS1d = 65536  
F1 = 125.665848 MHz  
F2 = 499.711945 MHz  
SW1 = 32520.33 Hz  
AT1 = 2.02 sec  
Hz per Pt 1stD = 0.50 Hz  
SW2 = 1.00 Hz  
Hz per Pt 2ndD = 1.00 Hz  
O1 = 14167.10 Hz  
O2 = -0.50 Hz  
LB1 = 0.00 Hz  
TP A = -176.56  
B = 116.80



125 MHz  $^{13}\text{C}$  NMR of PBMS 3 in  $\text{D}_2\text{O}$  with TSP reference



500 MHz  $^1\text{H}$  NMR of CAMS 4 in  $\text{D}_2\text{O}$  with TSP reference

TTU\_05042006\rlc050406.5.fid\processed\_fid  
 CAMS in D2O SW Proberfc050406.5

May 4 2006

USER:

Experiment = s2pul

Pulse length = 5.00 usec

Recycle delay = 2.00 sec

NA = 256

PTS1d = 65536

F1 = 125.665848 MHz

F2 = 499.711945 MHz

SW1 = 32520.33 Hz

AT1 = 2.02 sec

Hz per Pt 1stID = 0.50 Hz

SW2 = 1.00 Hz

Hz per Pt 2ndID = 1.00 Hz

O1 = 14176.53 Hz

O2 = -0.50 Hz

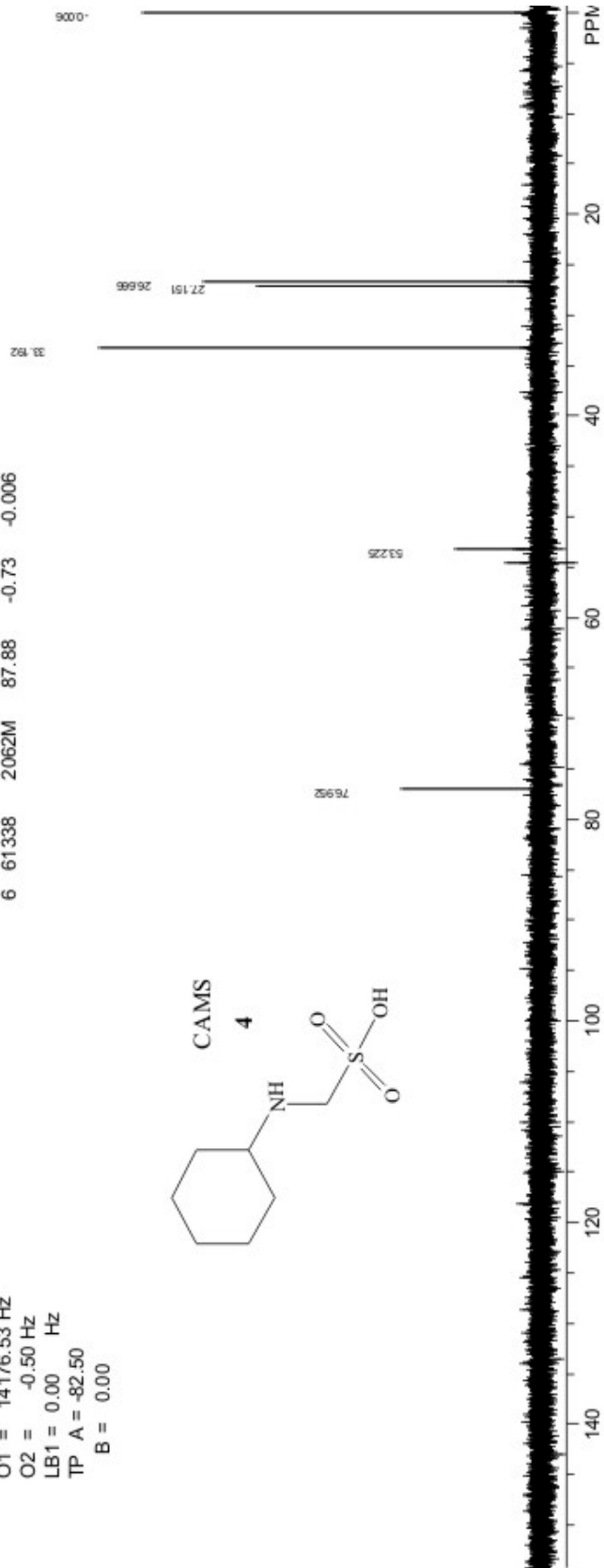
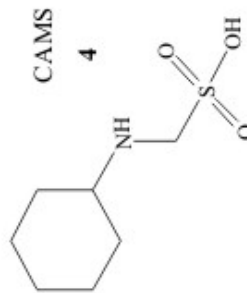
LB1 = 0.00 Hz

TP A = -82.50

B = 0.00

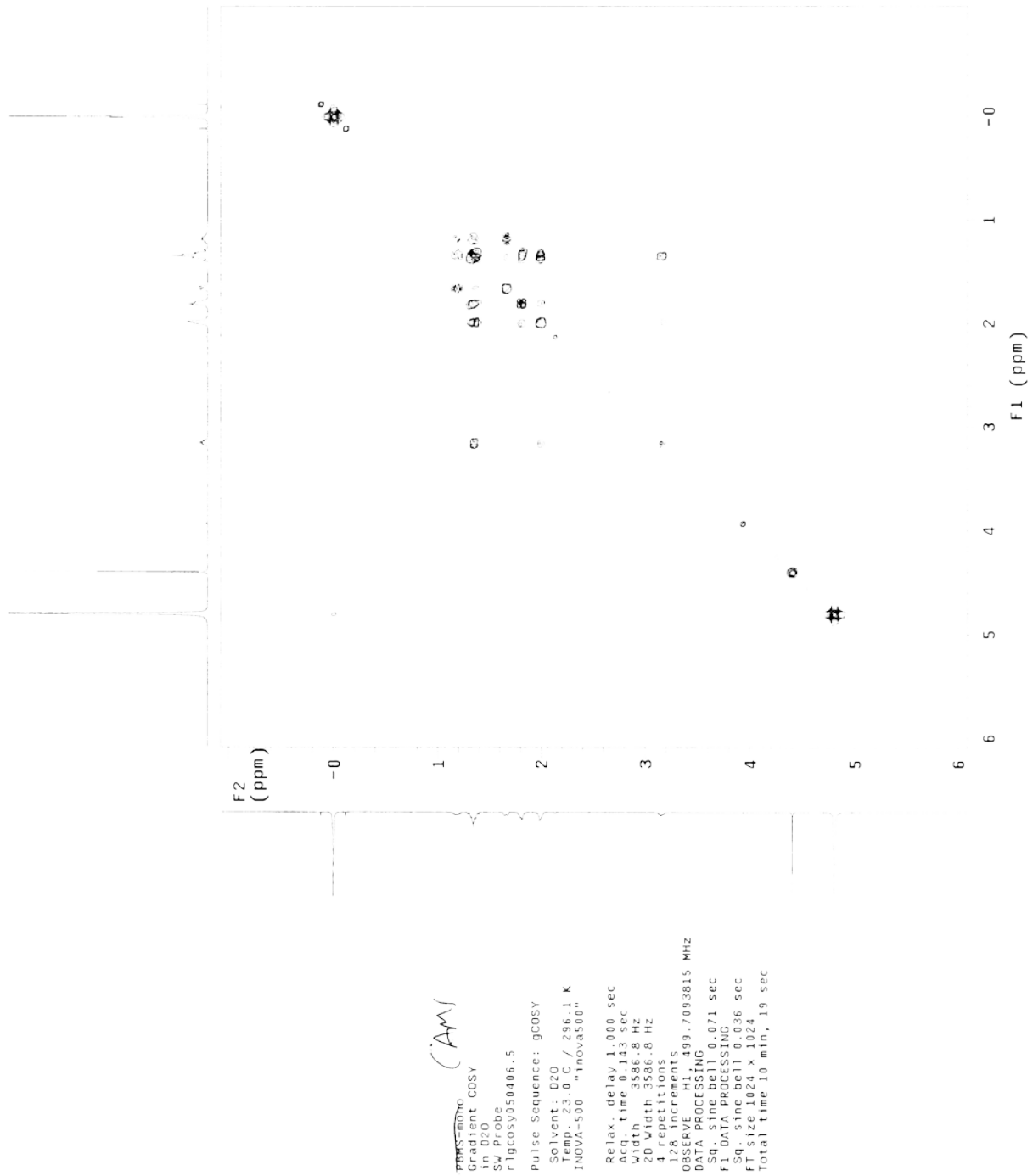
Interpolated Peak Listing

| PEAK | POINT | HEIGHT  | REL. HT | HT      | HZ     | PPM |
|------|-------|---------|---------|---------|--------|-----|
| 1    | 41849 | 777436K | 33.13   | 9670.18 | 76.952 |     |
| 2    | 47858 | 462563K | 19.71   | 6688.54 | 53.225 |     |
| 3    | 52931 | 2597M   | 110.67  | 4171.11 | 33.192 |     |
| 4    | 54461 | 1655M   | 70.52   | 3411.94 | 27.151 |     |
| 5    | 54584 | 1727M   | 73.60   | 3351.02 | 26.666 |     |
| 6    | 61338 | 2062M   | 87.88   | -0.73   | -0.006 |     |



125 MHz <sup>13</sup>C NMR of CAMS 4 in D<sub>2</sub>O with TSP reference

COSY of CAMS 4 in D<sub>2</sub>O on 500 MHz NMR



gHMQC of CAMS 4 in D<sub>2</sub>O on 500 MHz NMR

CAMS

~~PHAS-echo~~  
Gradient HMQC

in D<sub>2</sub>O

SW Probe

r1ghmqc050406.5

Pulse Sequence: gHMQC

Solvent: D<sub>2</sub>O

Temp: 23.0 C / 296.1 K

User: 1-14-87

INOVA-500 "inova500"

Relax. delay 1.000 sec

Acq time 0.129 sec

Width 3971.6 Hz

2D Width 21361.8 Hz

4 repetitions

2 x 128 increments

OBSERVE HI, 499.7093815 MHz

DECOUPLE C13, 125.6614365 MHz

Power 41 dB

on during acquisition

off during delay

GARP-1 modulated

DATA PROCESSING

Gauss apodization 0.060 sec

F1 DATA PROCESSING

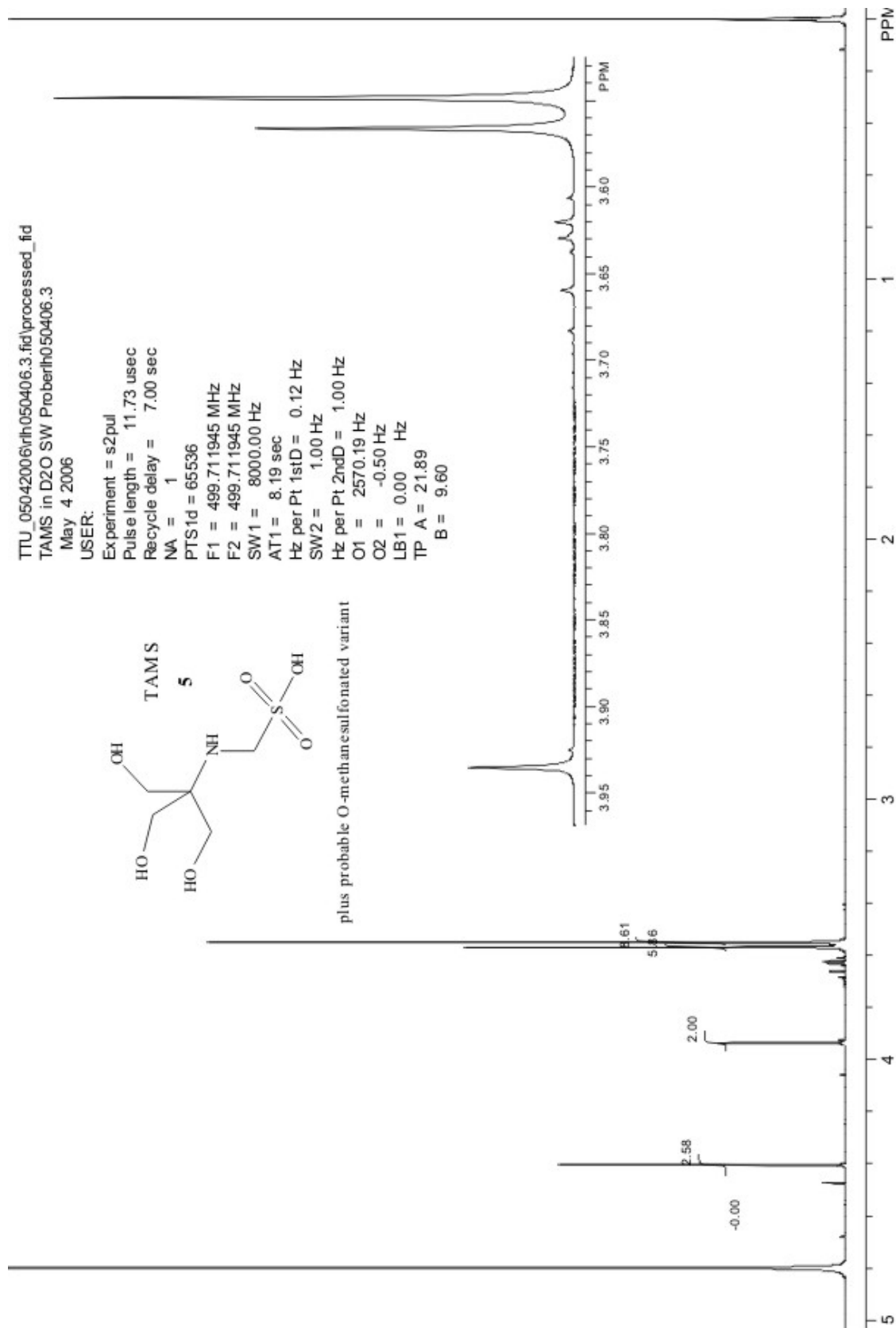
Gauss apodization 0.011 sec

FT size 1024 x 2048

Total time 20 min, 49 sec

F2 (ppm)  
1.0  
1.5  
2.0  
2.5  
3.0  
3.5  
4.0  
4.5  
5.0  
5.5  
6.0  
6.5

140 130 120 110 100 90 80 70 60 50 40 30 20 10  
F1 (ppm)



500 MHz <sup>1</sup>H NMR of TAMS 5 in D<sub>2</sub>O with TSP reference (with byproduct)



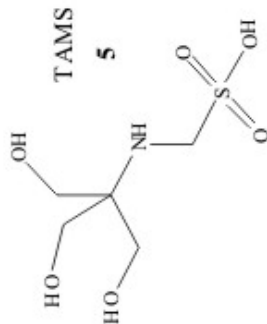
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TAMS in D2O SW Proberic050406.3  
May 4 2006

USER:

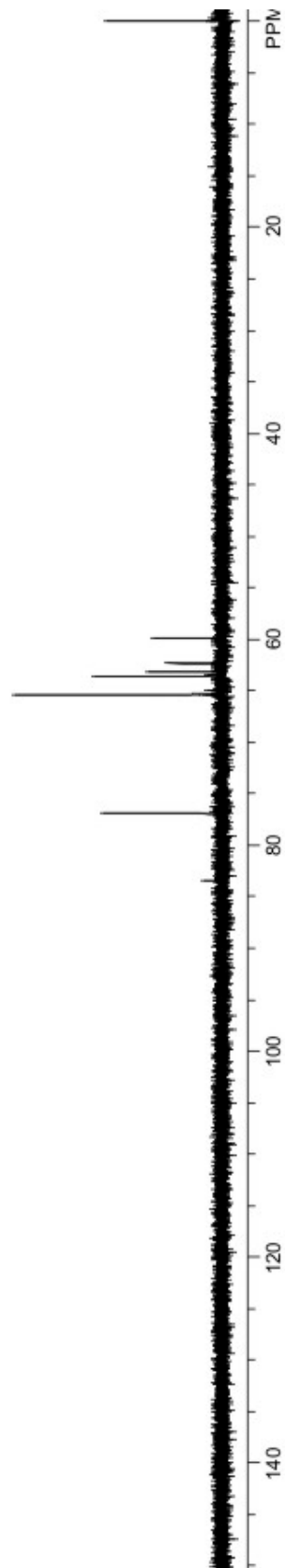
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Recycle delay = 2.00 sec  
NA = 128  
PTS1d = 65536  
F1 = 125.665848 MHz  
F2 = 499.711945 MHz  
SW1 = 32520.33 Hz  
AT1 = 2.02 sec  
Hz per Pt 1stID = 0.50 Hz  
O1 = 14175.04 Hz  
O2 = -0.50 Hz  
LB1 = 0.00 Hz  
TP A = -97.55  
B = -10.84

Interpolated Peak Listing

| PEAK | POINT | HEIGHT  | REL. HT | HT       | HZ     | PPM |
|------|-------|---------|---------|----------|--------|-----|
| 1    | 40201 | 134384K | 10.98   | 10486.75 | 83.449 |     |
| 2    | 41848 | 708486K | 57.87   | 9669.46  | 76.946 |     |
| 3    | 44773 | 123744K | 10.11   | 8217.97  | 65.395 |     |
| 4    | 44784 | 1139M   | 93.03   | 8212.14  | 65.349 |     |
| 5    | 45233 | 708190K | 57.84   | 7989.33  | 63.576 |     |
| 6    | 45325 | 420489K | 34.34   | 7944.13  | 63.216 |     |
| 7    | 45545 | 331581K | 27.08   | 7834.90  | 62.347 |     |
| 8    | 46156 | 443181K | 36.20   | 7531.66  | 59.934 |     |
| 9    | 61336 | 673989K | 55.05   | -1.27    | -0.010 |     |



plus probable O-methanesulfonated variant

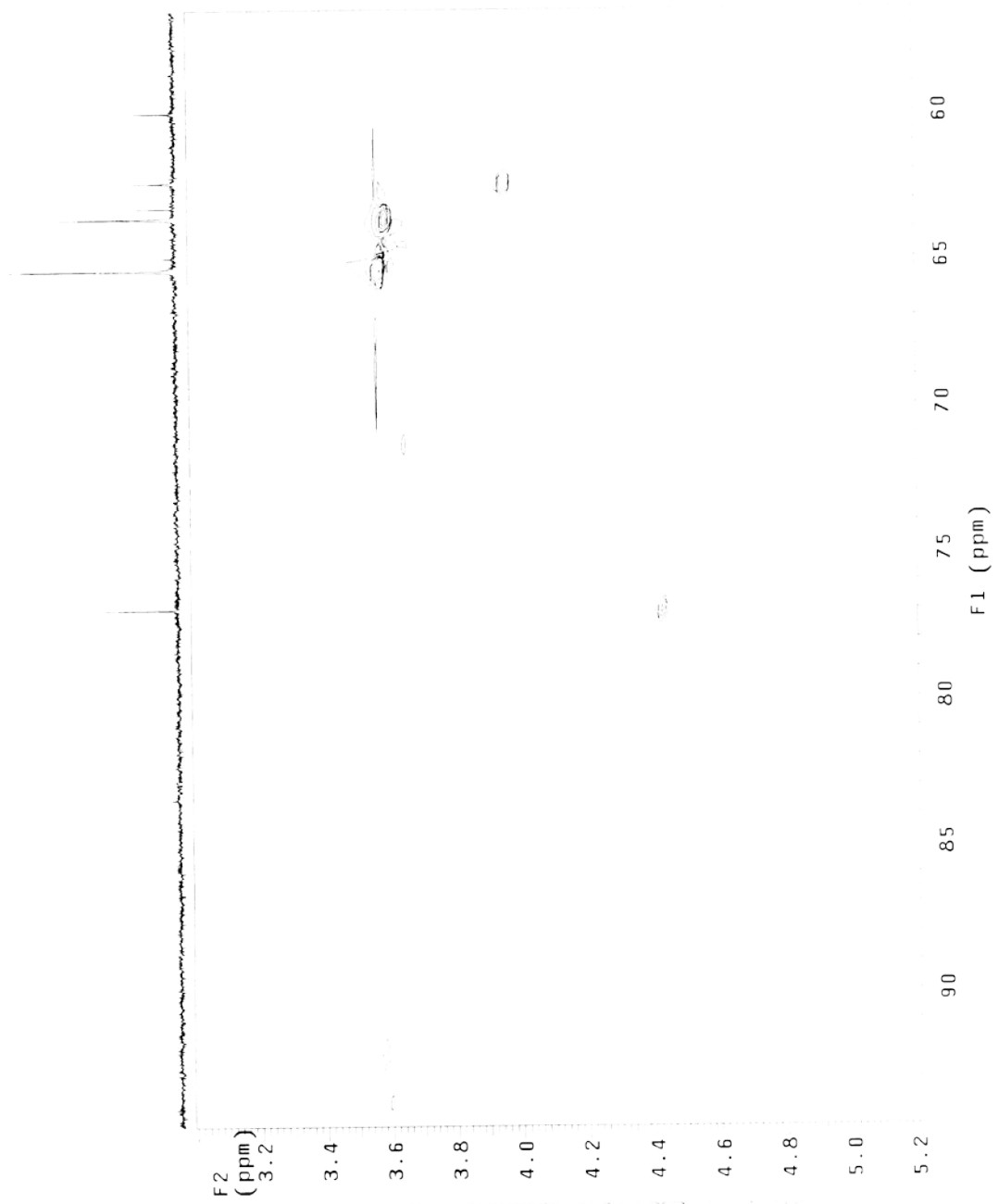


125 MHz <sup>13</sup>C NMR of TAMS 5 in D<sub>2</sub>O with TSP reference (with byproduct)

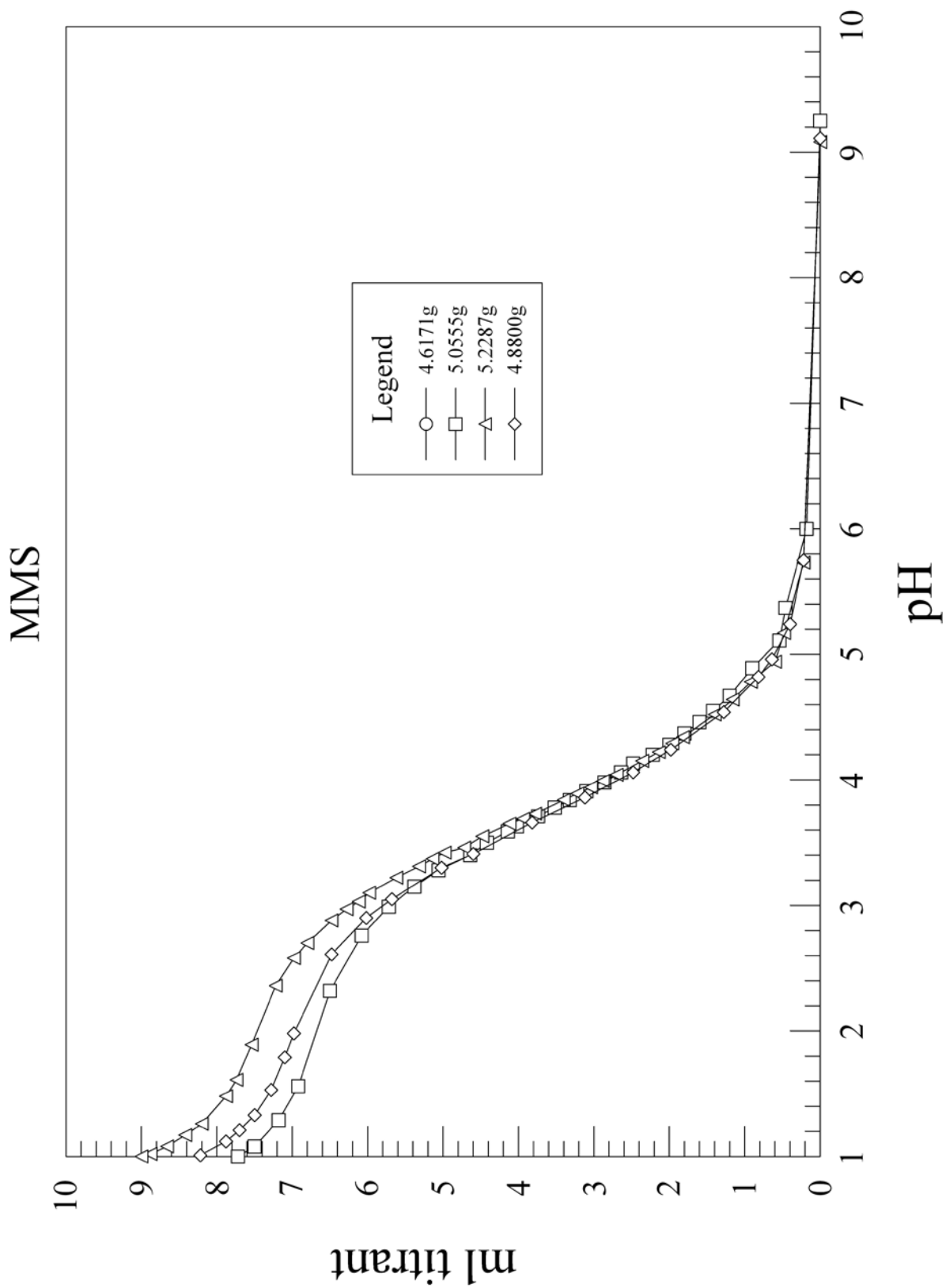


TAMS  
 Gradient HMQC  
 in D2O  
 SW Probe  
 r1ghmqc050405.3  
 Pulse Sequence: gHMQC

Solvent: D2O  
 Temp: 23.0 C / 296.1 K  
 User: 1-14-87  
 INOVA-500 "Inova500"  
 Relax. delay 1.000 sec  
 Acq. time 0.144 sec  
 Width 3565.1 Hz  
 2D Width 21361.8 Hz  
 4 repetitions  
 2 x 128 increments  
 OBSERVE H1, 499.7093844 MHz  
 DECOUPLE C13, 125.6614365 MHz  
 Power 41 dB  
 on during acquisition  
 off during delay  
 GARP-1 modulated  
 DATA PROCESSING  
 Gauss apodization 0.066 sec  
 F1 DATA PROCESSING  
 Gauss apodization 0.011 sec  
 FT size 1024 x 2048  
 Total time 21 min, 4 sec

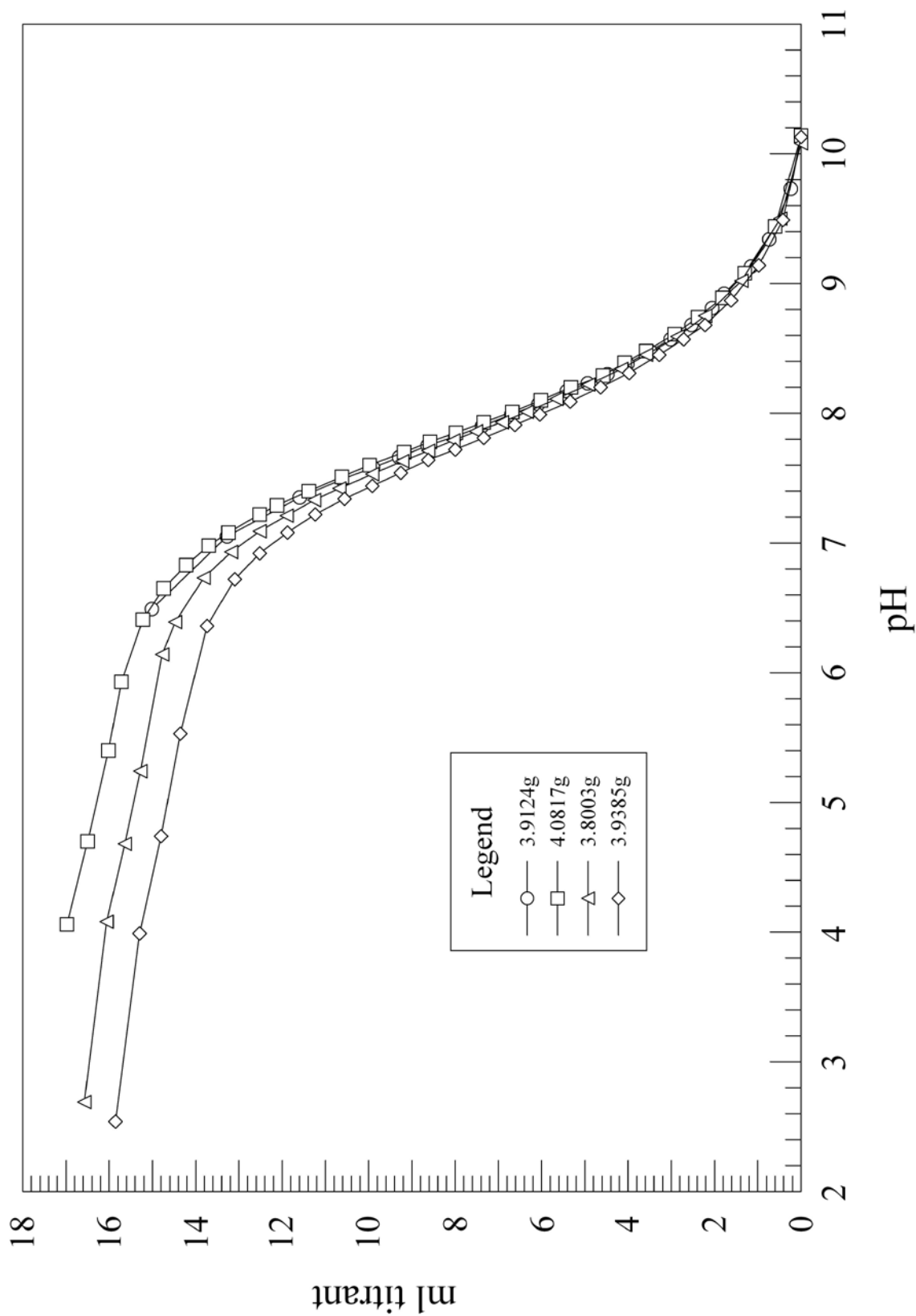


gHMQC of TAMS 5 sample in D<sub>2</sub>O (with byproduct)



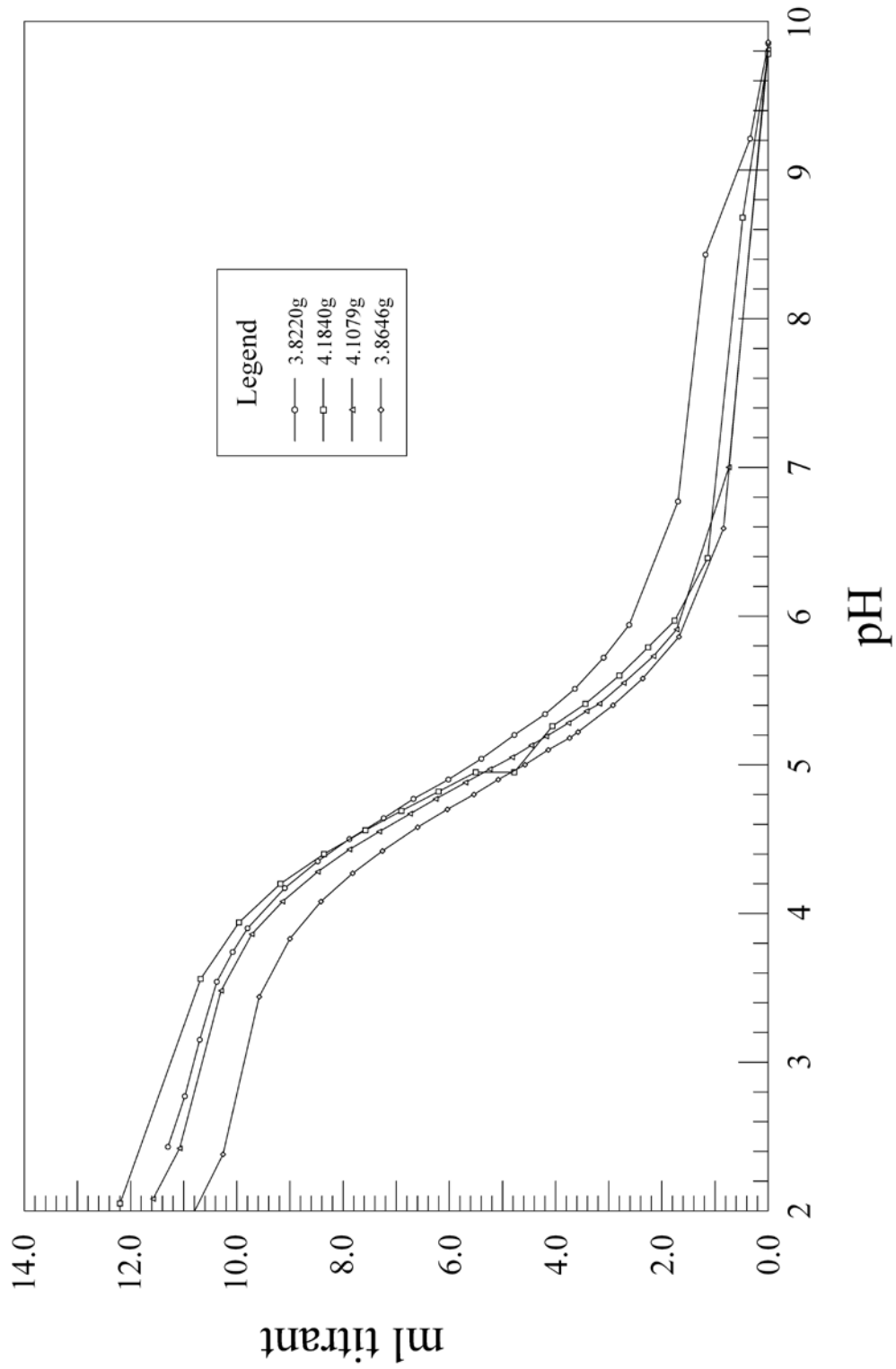
Titration curve of MMS 1 with 1M HCl

# HEPMS

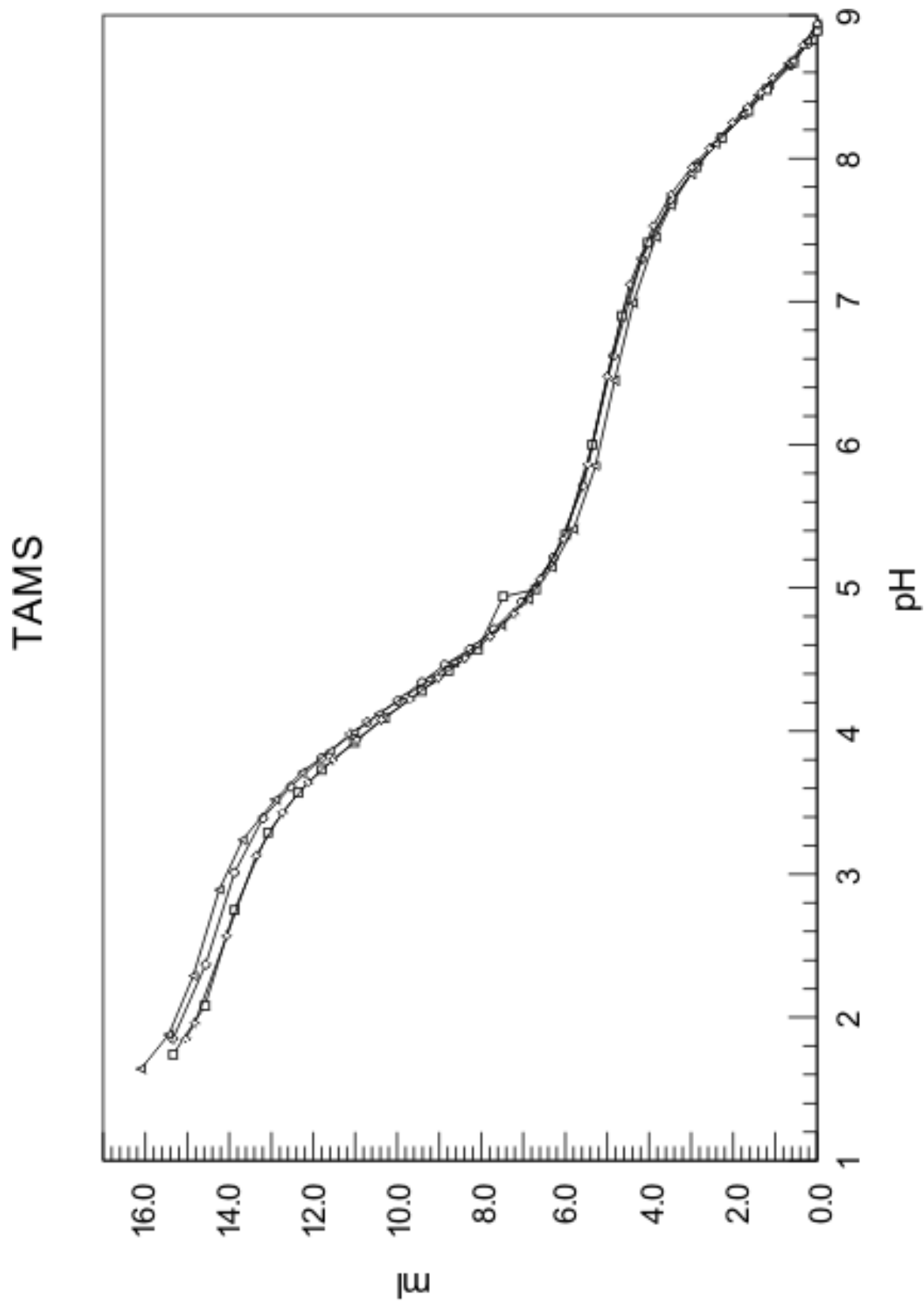


Titration curve of HEPMS 2 with 1M HCl

# PBMS



Titration curve of PBMS 3 with 1M HCl

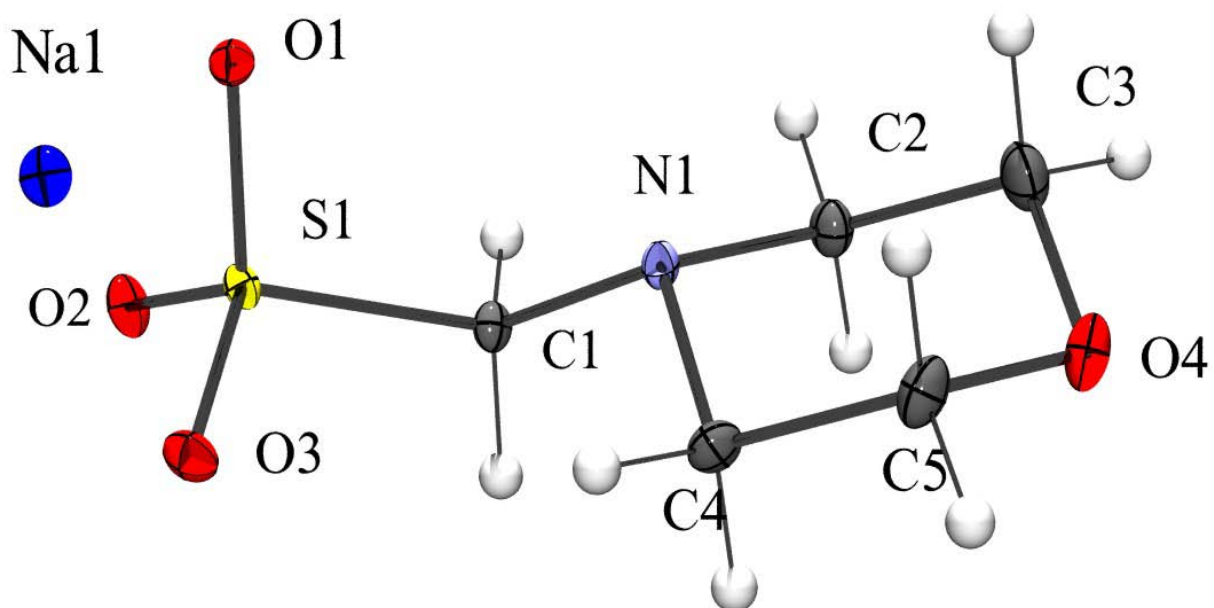


Titration curve of TAMS 5 (impure as synthesized) showing a probable  $pK_a$  of  $\approx 4.1$

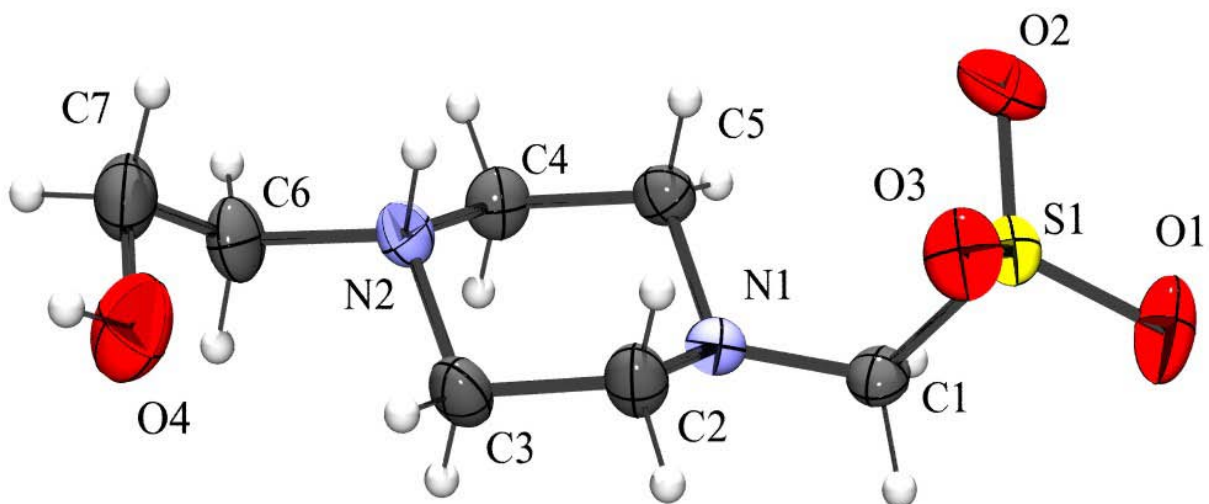
## Summary of Titration Data

|                 | Number of samples | Avg $pK_a$ | Std Error |
|-----------------|-------------------|------------|-----------|
| <b>MMS 1</b>    | 7                 | 3.87       | 0.076     |
| <b>HEPMS 2</b>  | 4                 | 7.88       | 0.069     |
| <b>PBMS 3</b>   | 4                 | 4.90       | 0.049     |
| <b>CAMS 4</b>   | 3                 | 6.92       | 0.56      |
| * <b>TAMS 5</b> | 6                 | 4.11       | 0.13      |

\*TAMS is contaminated with unreacted Tris (observable in titration curves at pH 7–10)



POV-Ray rendering of ORTEP3 figure for MMS 1 at 50% probability level



POV-Ray rendering of ORTEP3 figure for HEPMS 2 at 50% probability level