

Supporting Information for:

Porphyrin Architectures Tailored for Studies of Molecular Information Storage

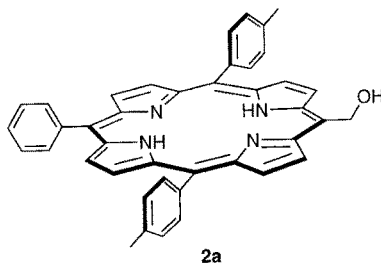
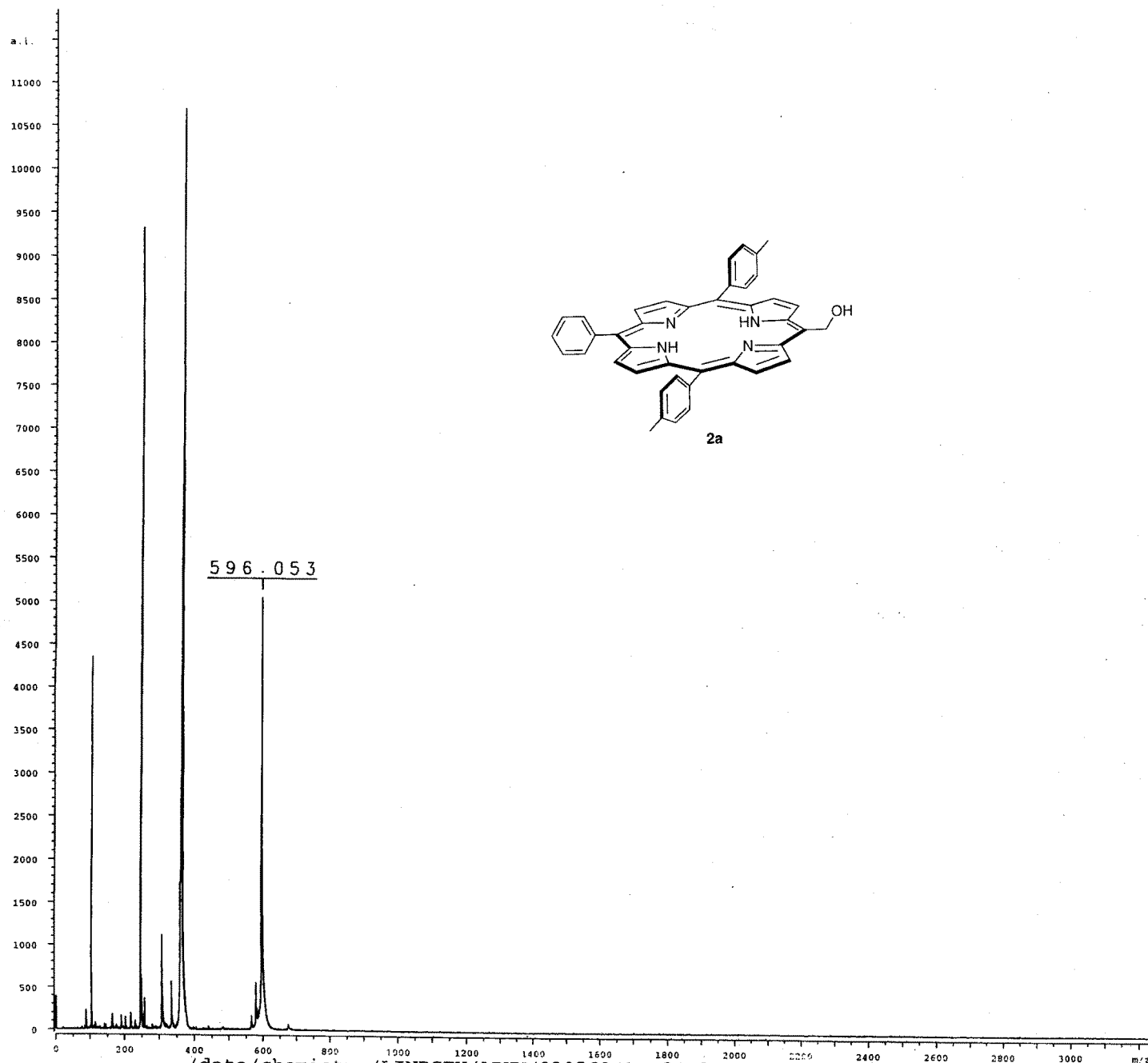
Carole M. Carcel, Joydev K. Laha, Robert S. Loewe, Patchanita Thamyongkit, Karl-Heinz Schweikart, Veena Misra, David F. Bocian, and Jonathan S. Lindsey

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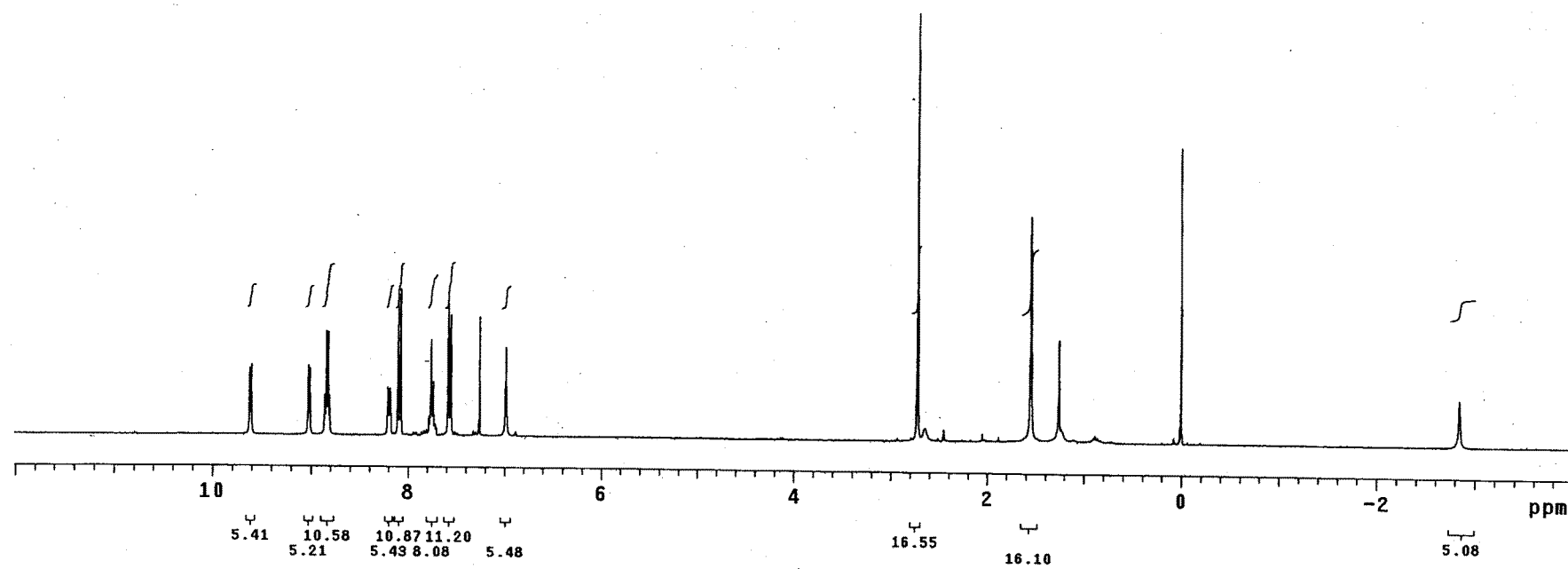
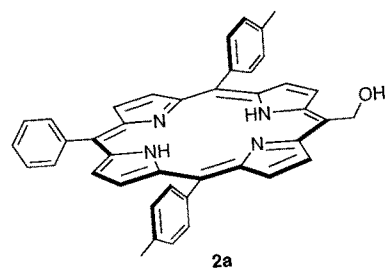
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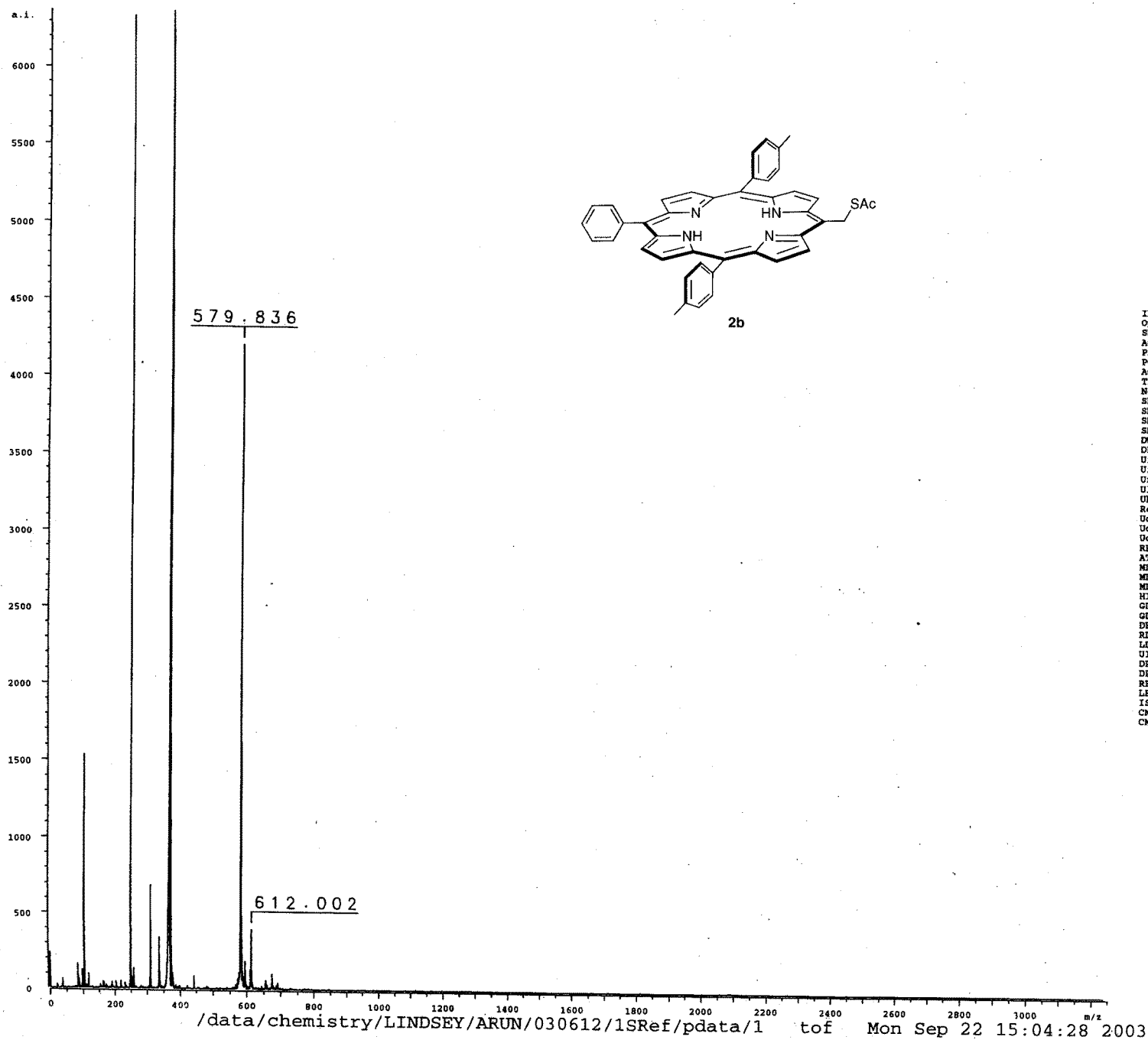
General. All ^1H NMR spectra (300 or 400 MHz) and ^{13}C NMR (75 MHz) were collected in CDCl_3 unless noted otherwise. Absorption and fluorescence spectra were collected in toluene at room temperature. Mass spectra of porphyrins were obtained via laser desorption mass spectrometry (LD-MS) without a matrix³² or by matrix-assisted laser desorption ionization mass spectrometry (MALDI-MS), and by high-resolution fast atom bombardment mass spectrometry (FAB-MS) using a matrix of nitrobenzyl alcohol and polyethylene glycol. Melting points are uncorrected. Kugelrohr distillation was performed by a standard-size Kugelrohr short path distillation apparatus. Silica gel (40 μm average particle size) was used for column chromatography. All GC chromatograms were collected using a phenyl methyl siloxane column (30.0 m x 32 μm x 0.5 μm), thermal programming (oven at 35 $^\circ\text{C}$ for 5 min; ramp to 325 $^\circ\text{C}$ at 10 $^\circ\text{C}/\text{min}$; oven at 325 $^\circ\text{C}$ for 5 min), and a flame ionization detector.²⁹ THF was freshly distilled from sodium as required. Toluene was distilled from CaH_2 . CHCl_3 was stabilized with 0.8% ethanol.



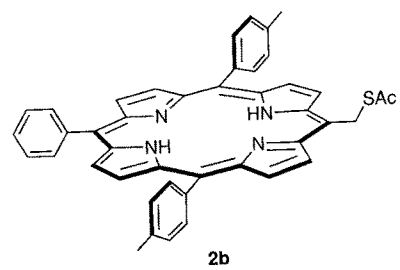
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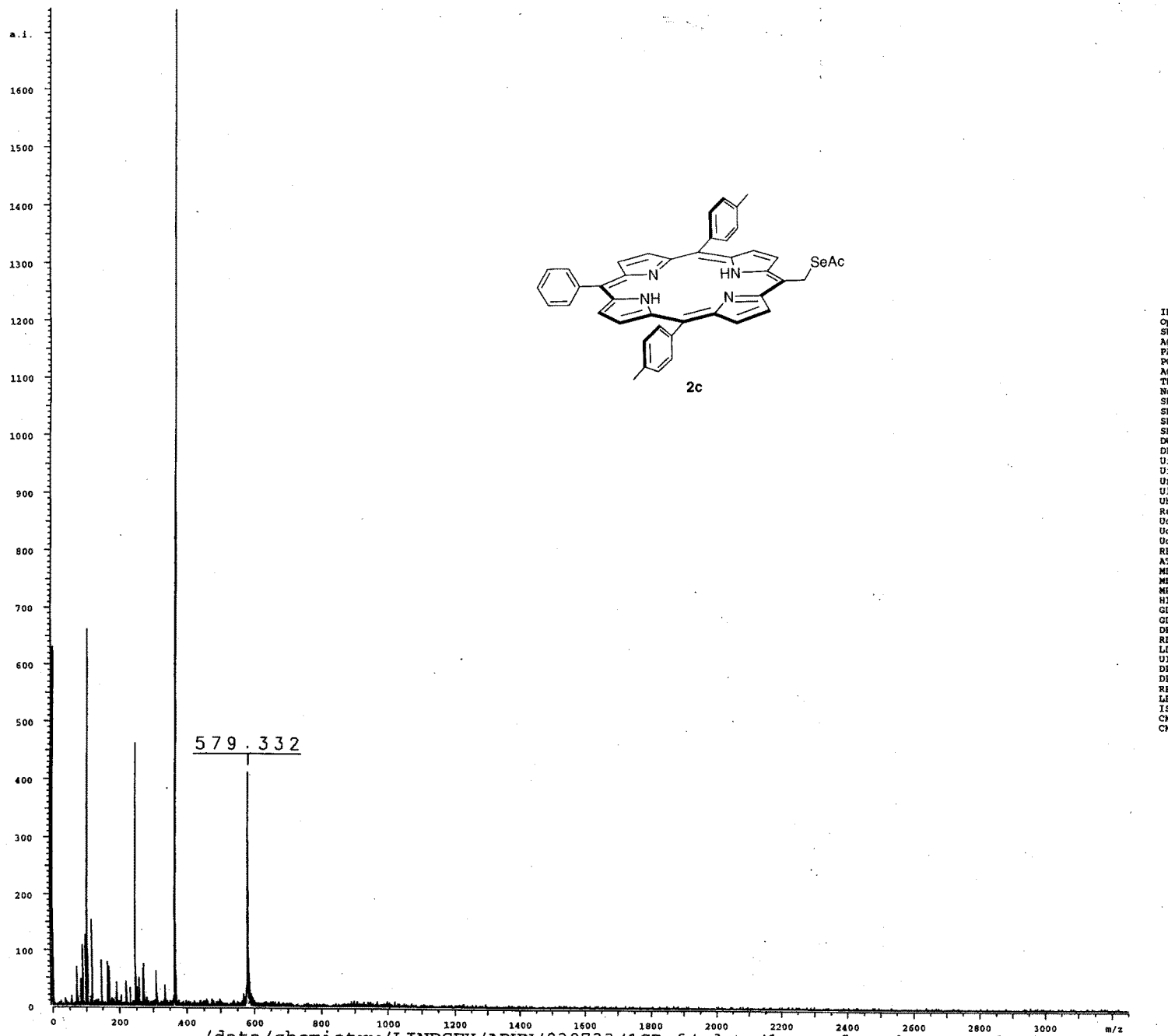
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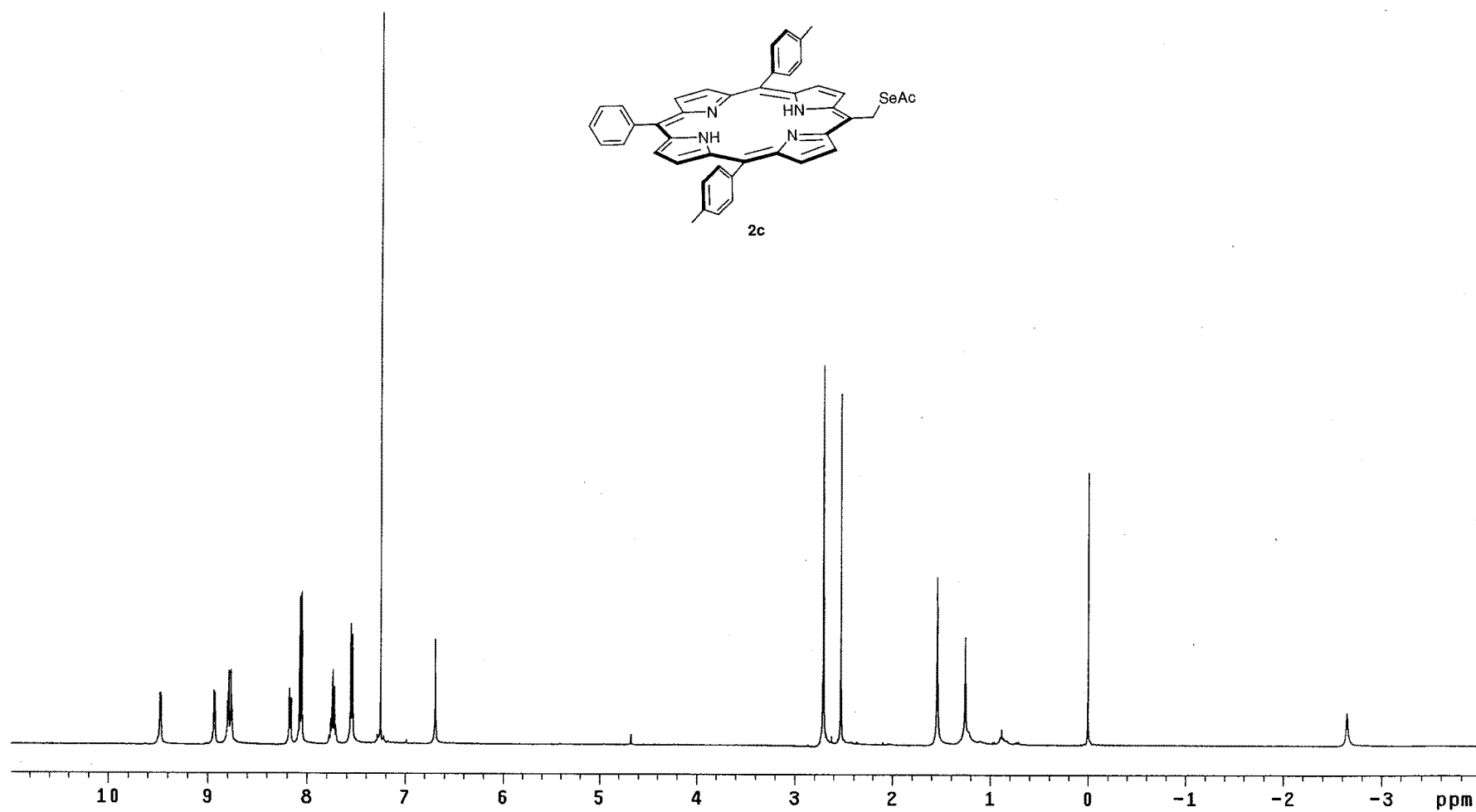
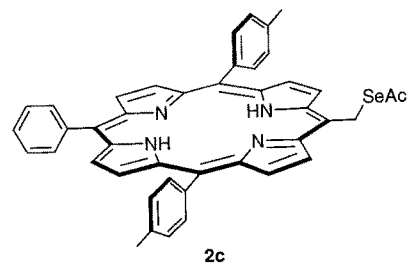


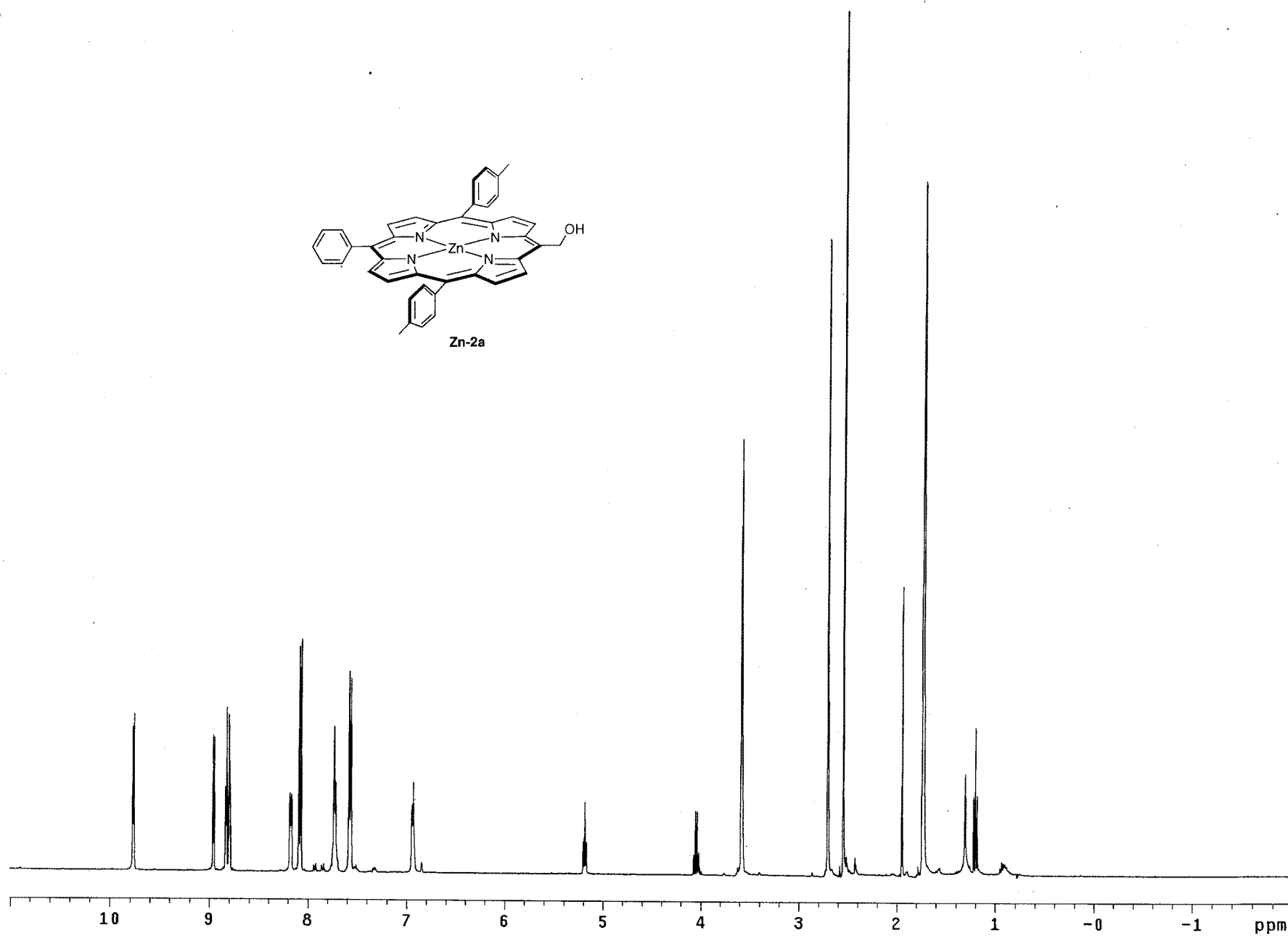
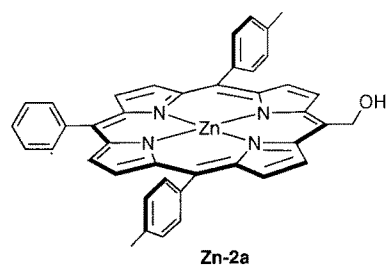
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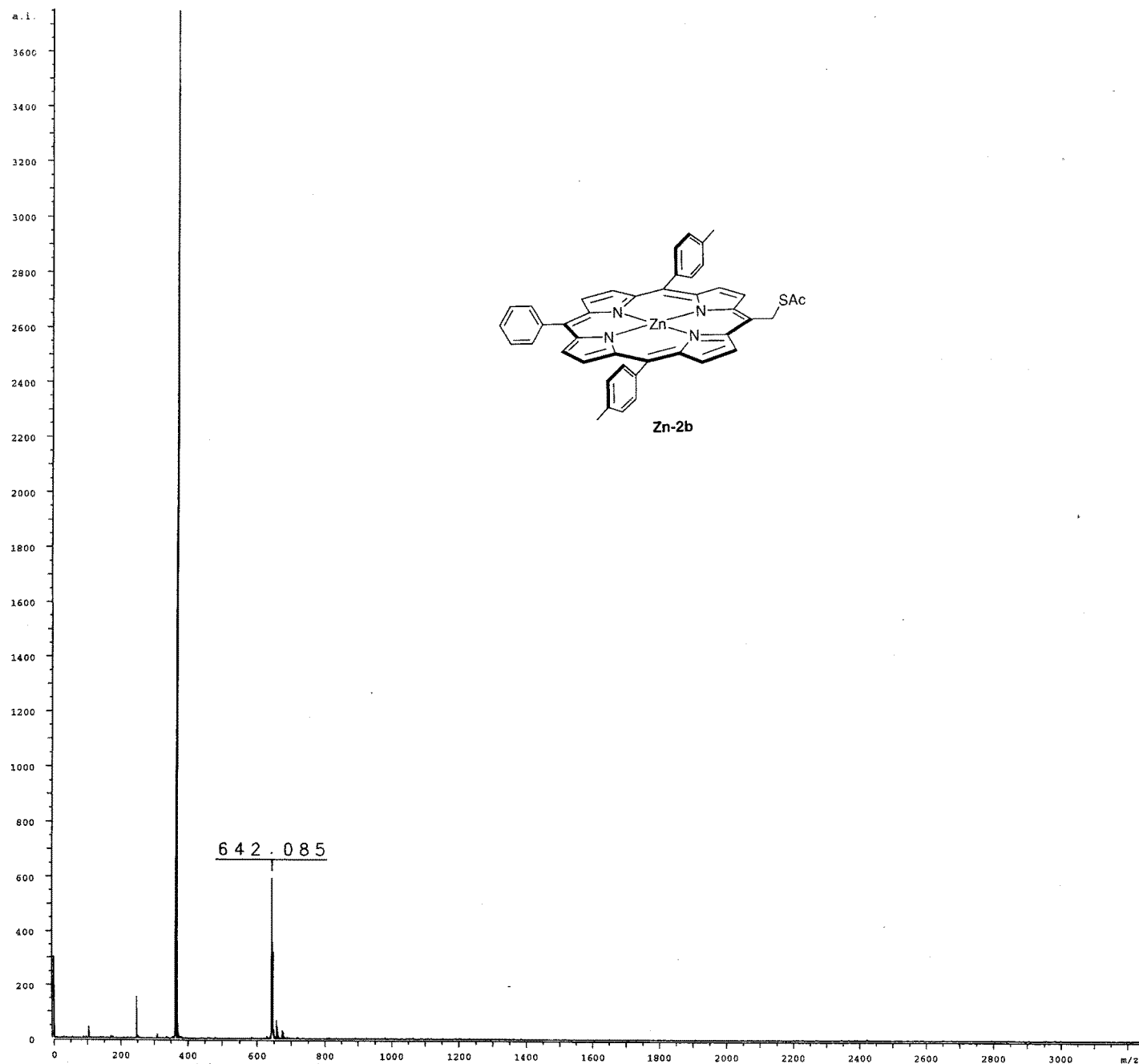
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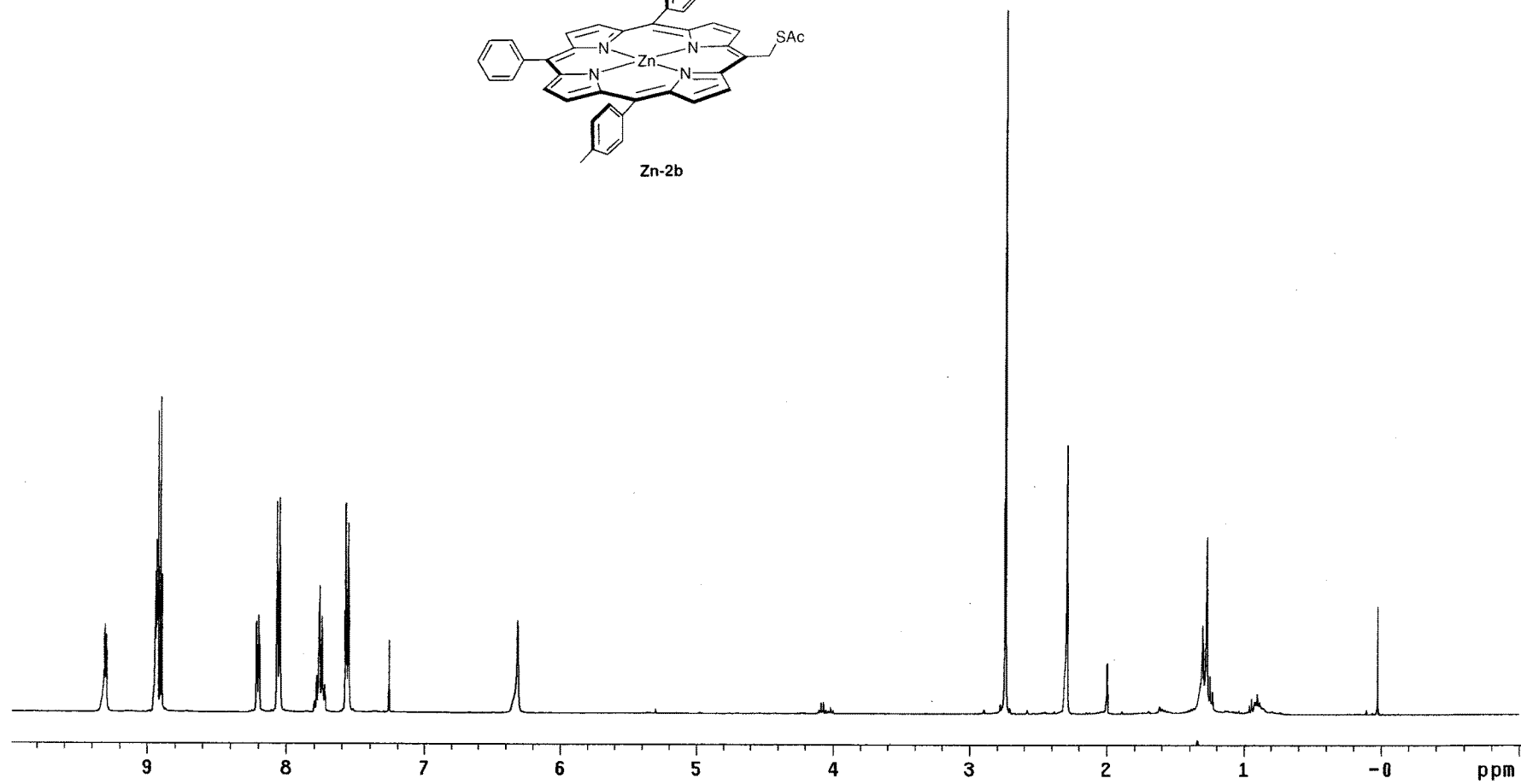
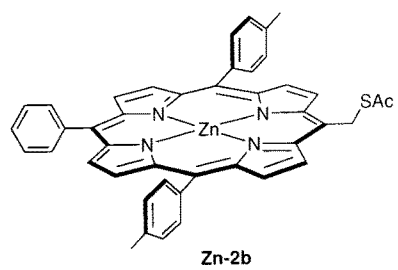


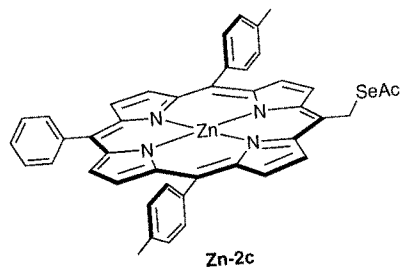
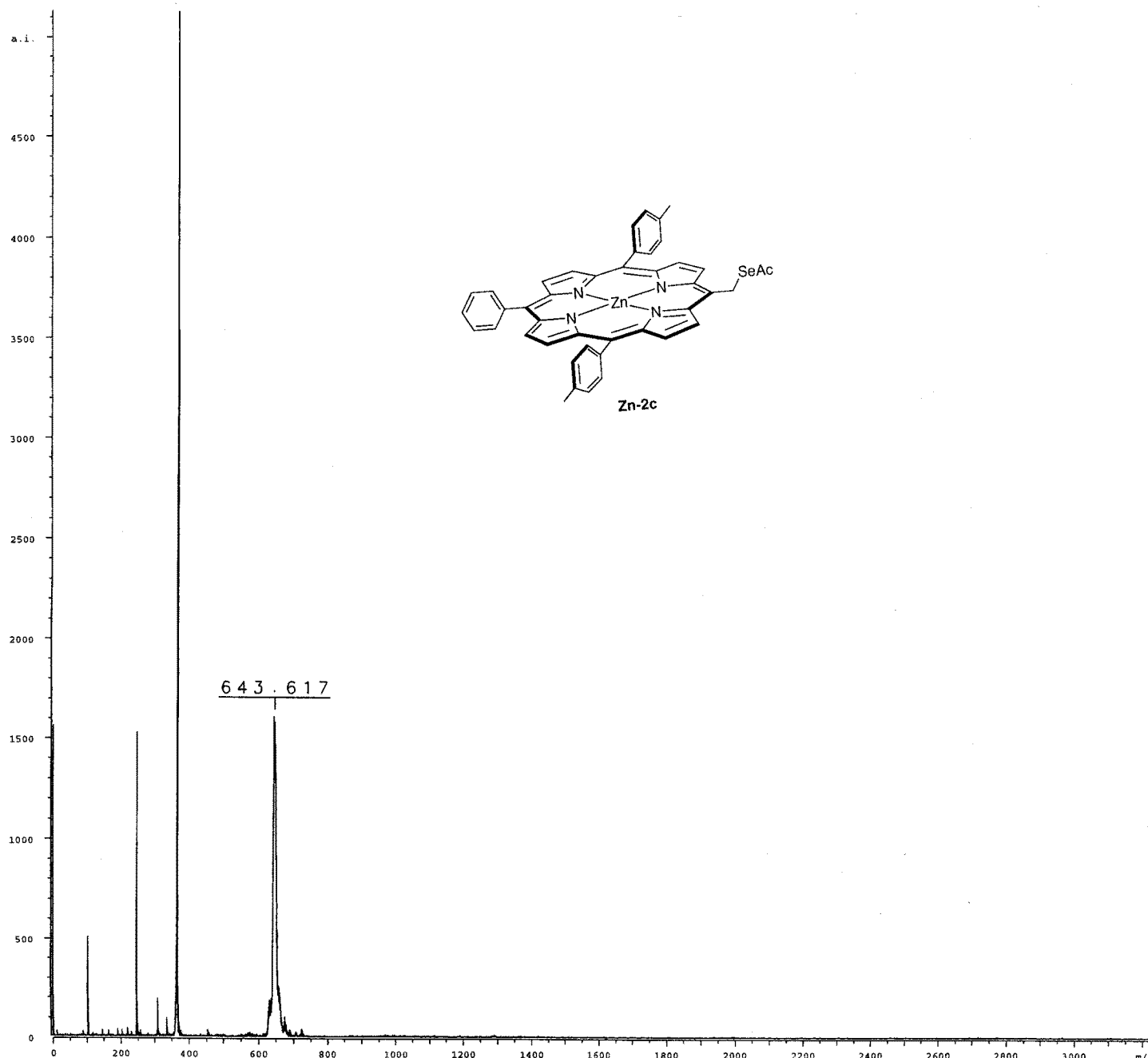
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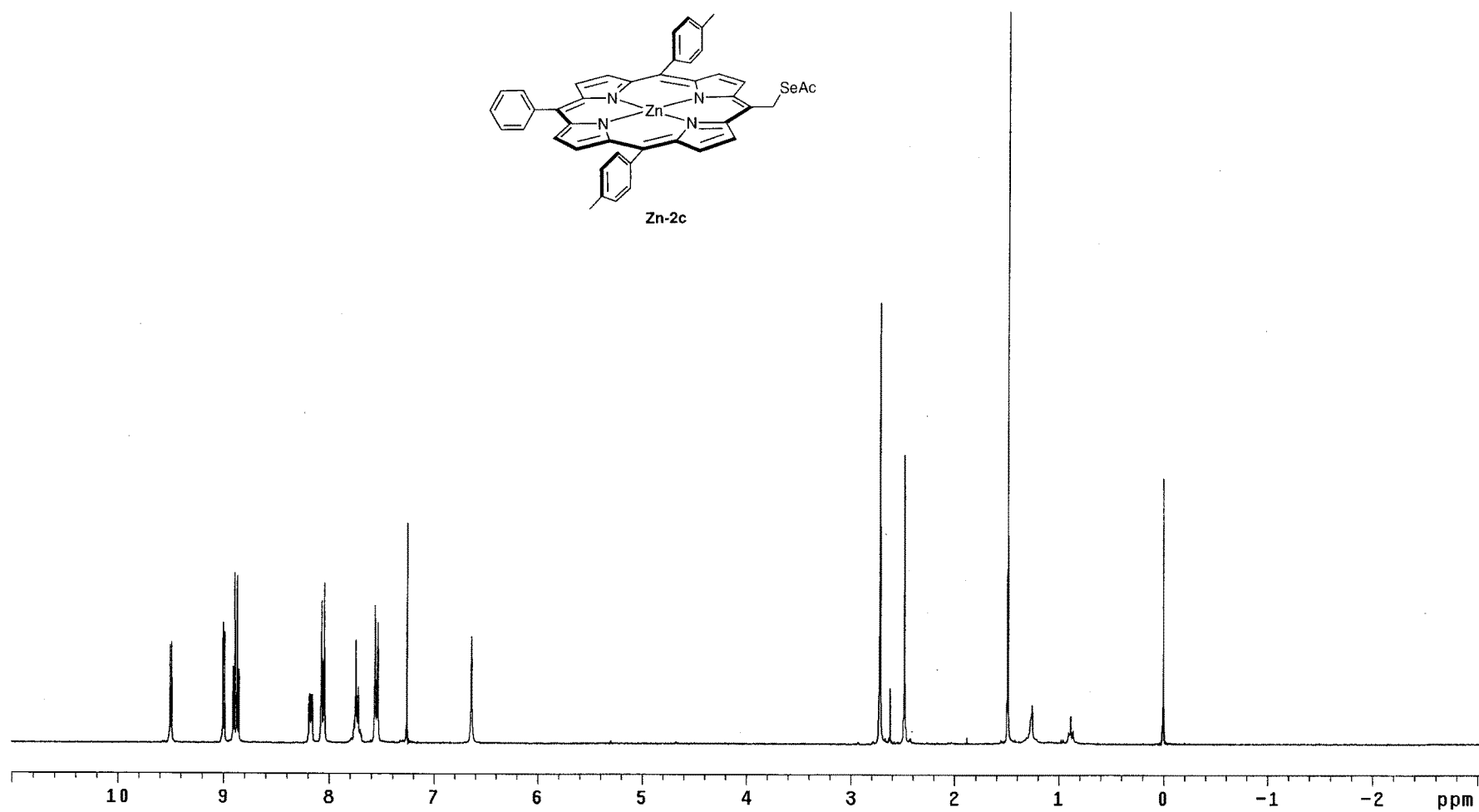
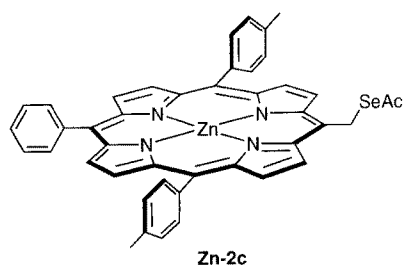


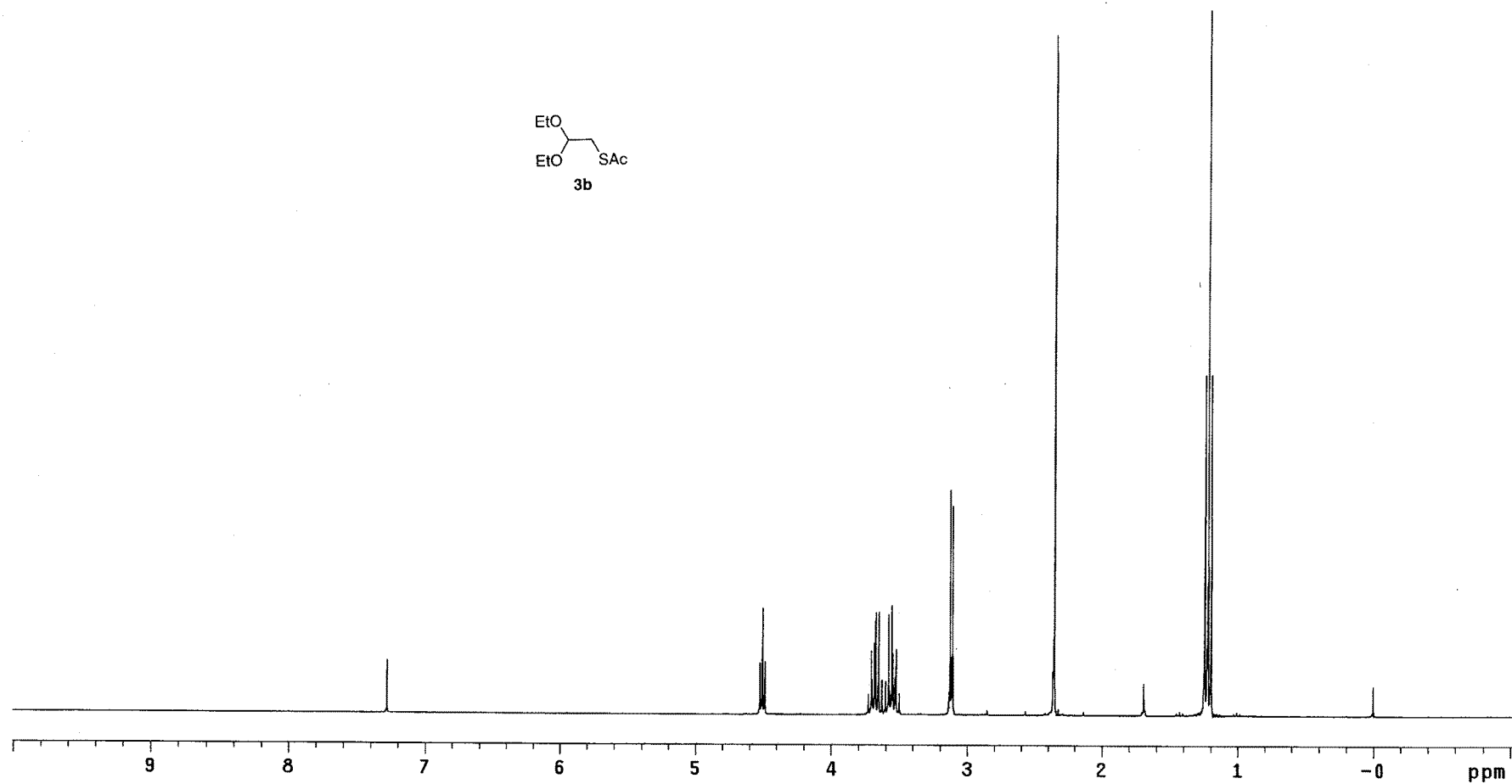
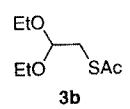


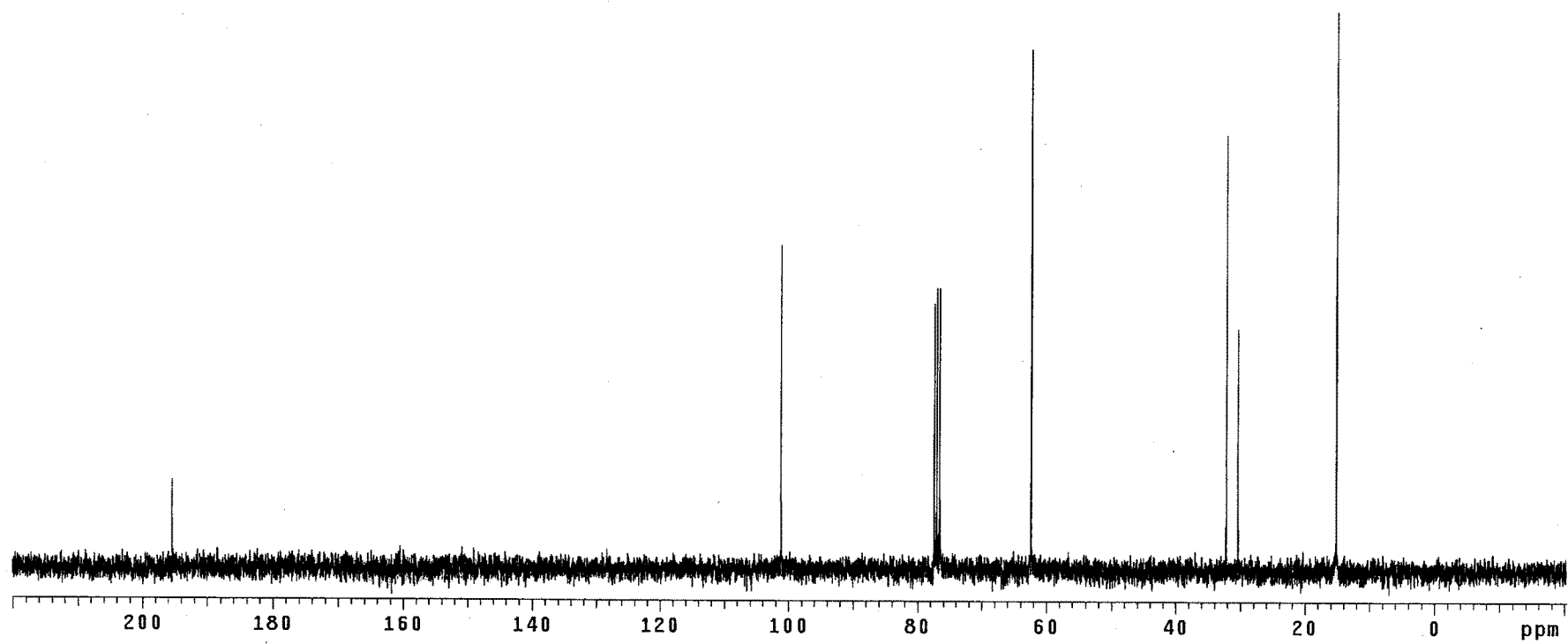
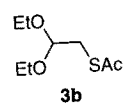
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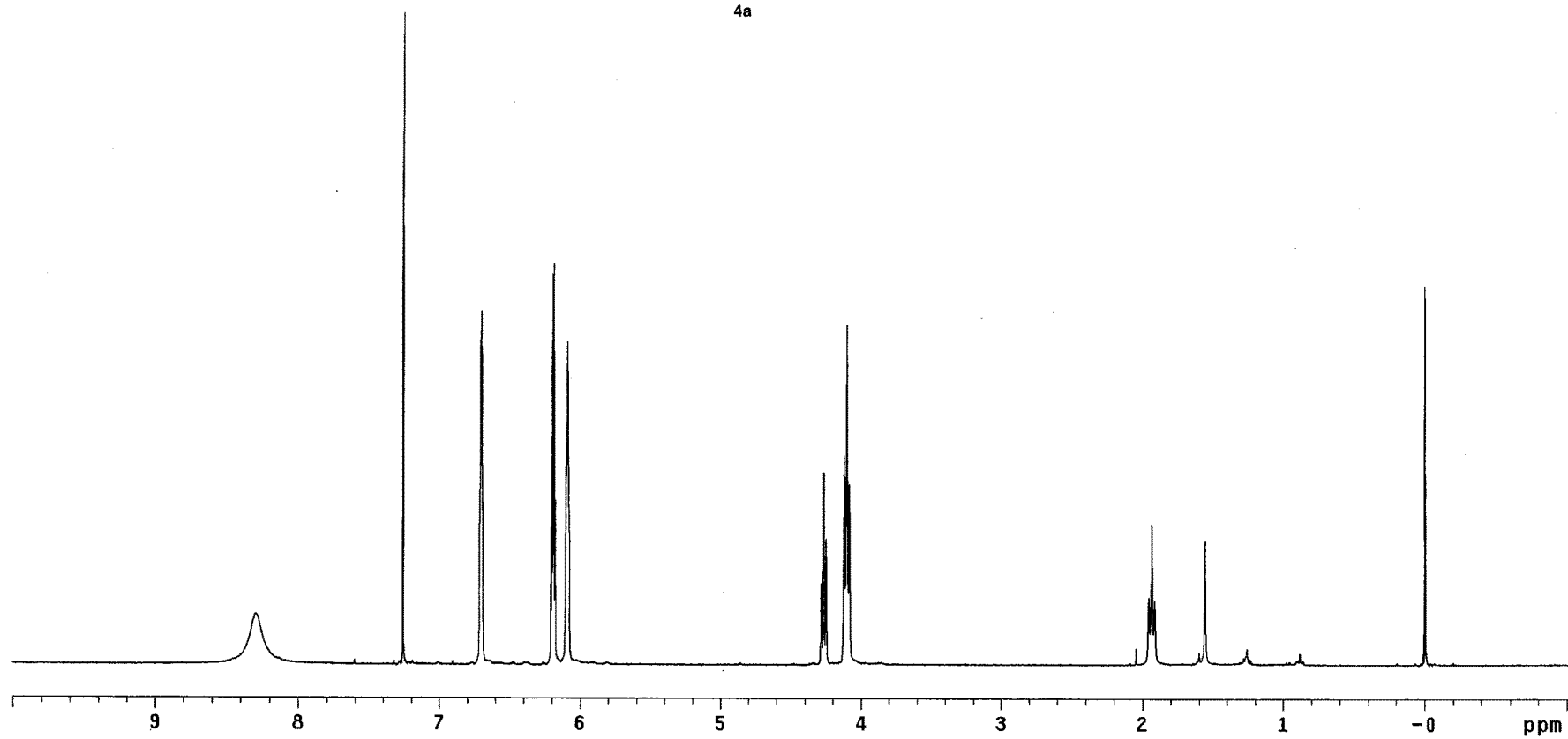
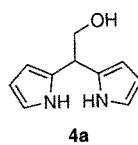
INSTRUM TOP
OpId N. Srinivasan
SMPNAM 030736
AQ_DATE Fri Oct 17 14:41:34 2003
PATH /data/chemistry/LINDSEY/ARUN
POLARI POS
AQOP_m Reflector
TD 40000
NoSHOTS 80
SHOWMUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 0 [ns]
Uis1 20.00 [kV]
Uis2 18.70 [kV]
Uref1 0.00 [kV]
Ulen5 7.50 [kV]
Uhinmass 10.00 [kV]
RefPull 0.00 [kV]
UdetL 1.50 [kV]
UdetR 0.00 [kV]
Udef1 2.00 [kV]
REPHZ 1.00 [Hz]
ATTEN 33.0
ML1 2067125.193
ML2 333.982
ML3 0.000
HITURBO no
GDEON yes
GDEDL short
DEFLON no
RLNSEND no
LLNSEND no
UISSEND no
DPCALL 510.84
DPMAS 700.00 [Da]
RENDVAL 0.33
LENDVAL 0.28
ISSENDV 0.91
CMT1 AcSe-zn-por
CMT2 matrix
  
```

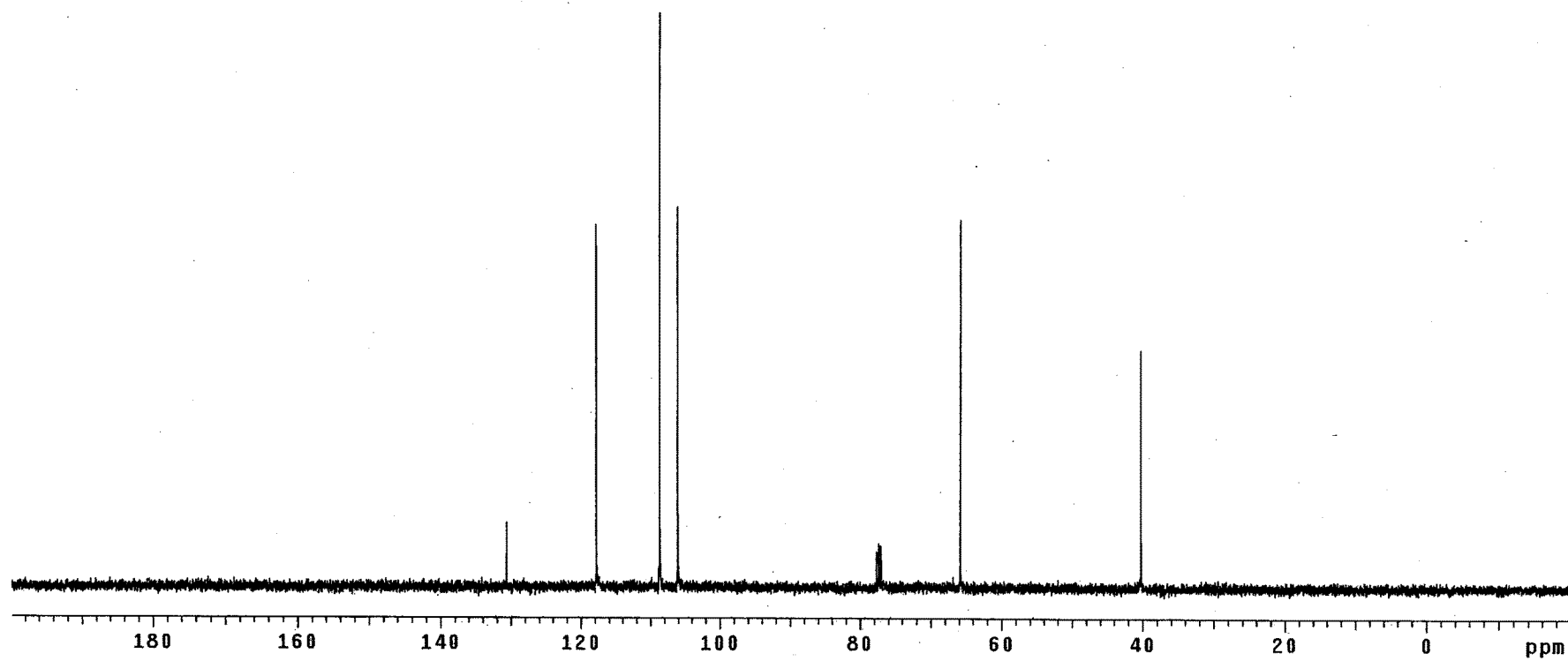
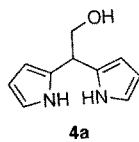
/data/chemistry/LINDSEY/ARUN/030736/1SRef/pdata/1 tof Fri Oct 17 14:41:59 2003

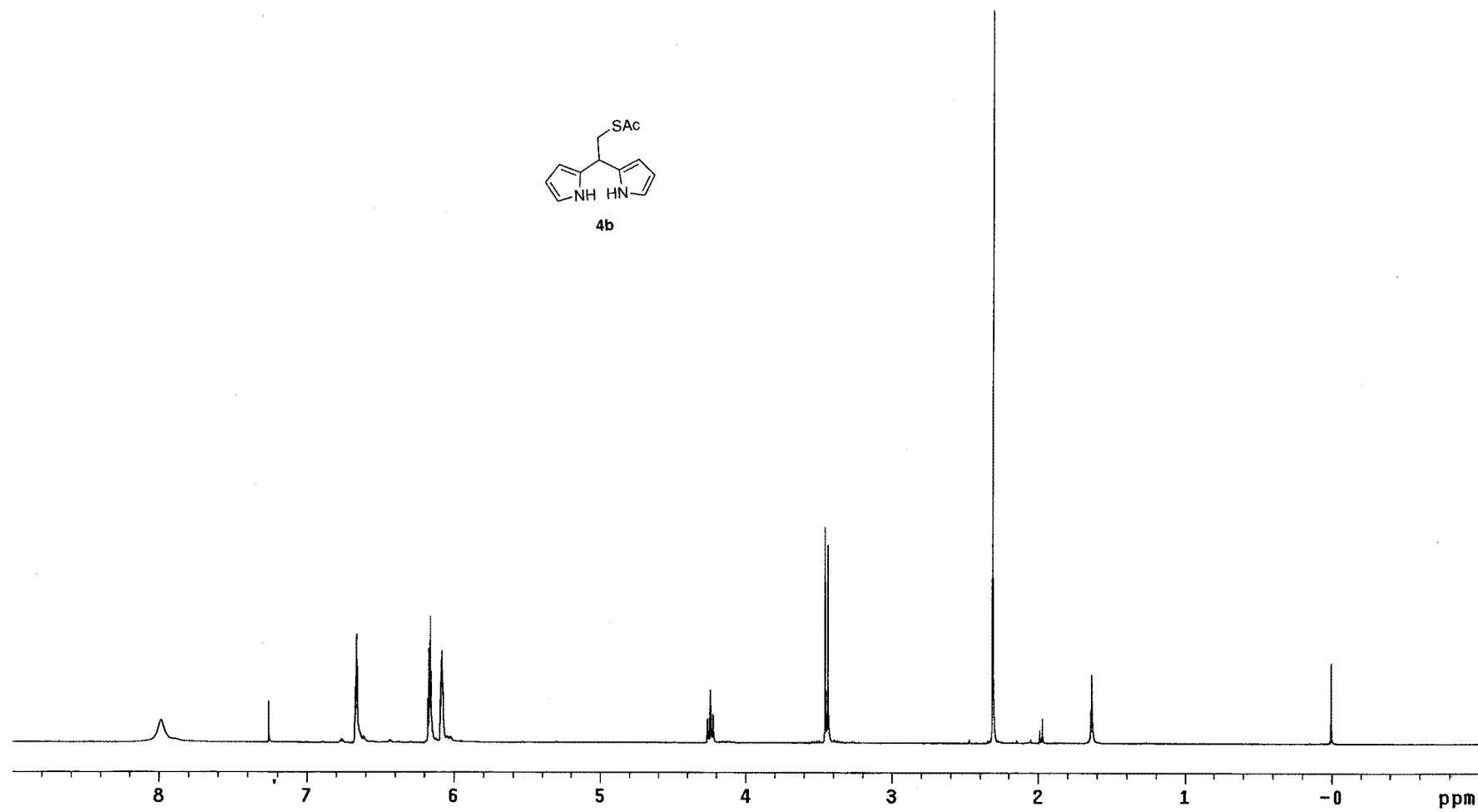
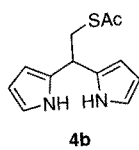


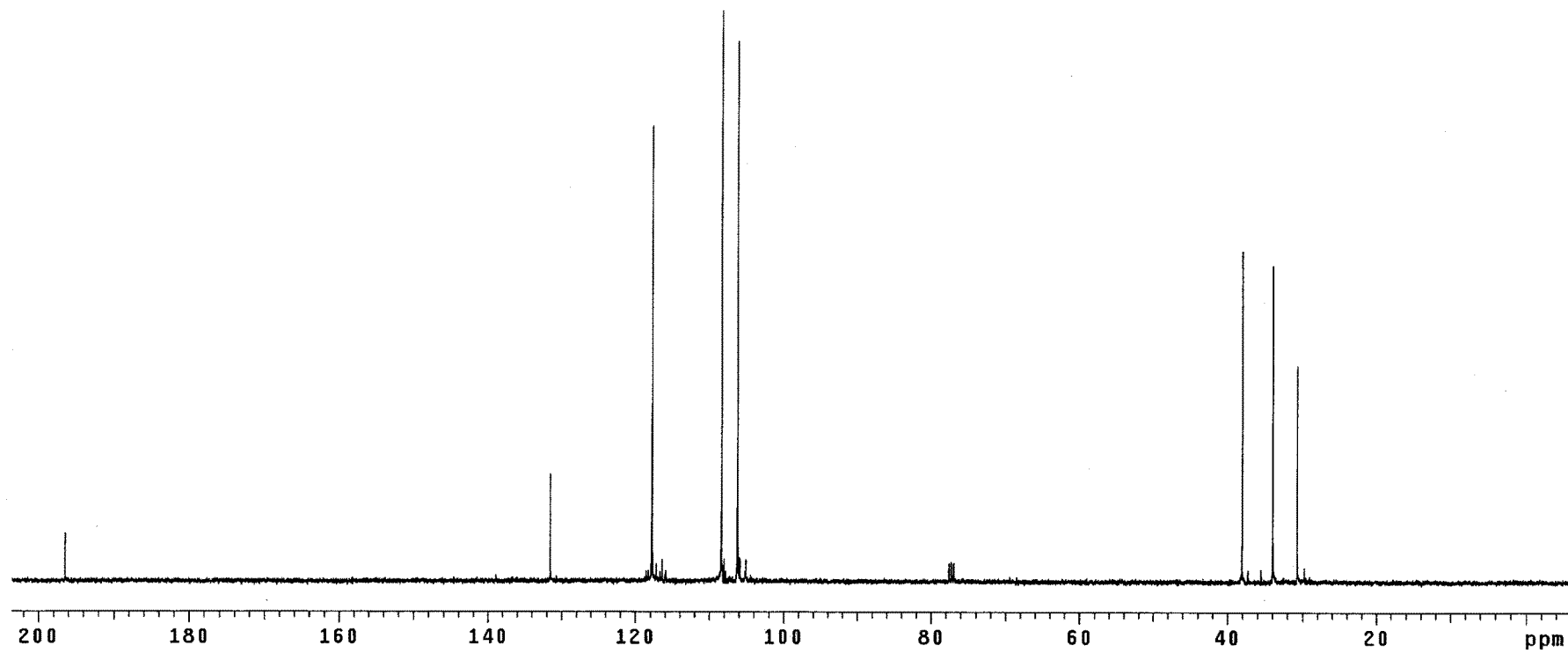
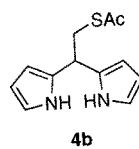


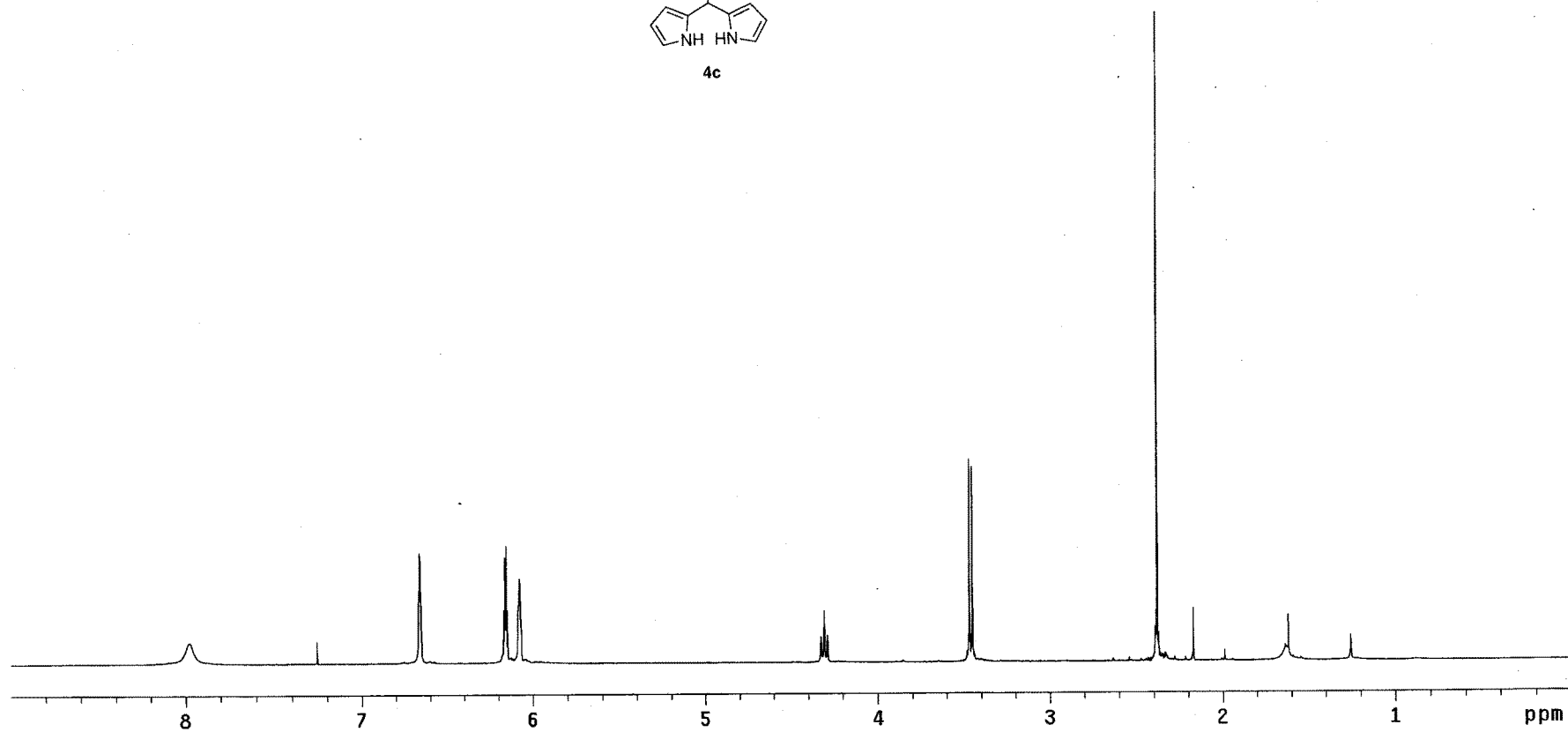


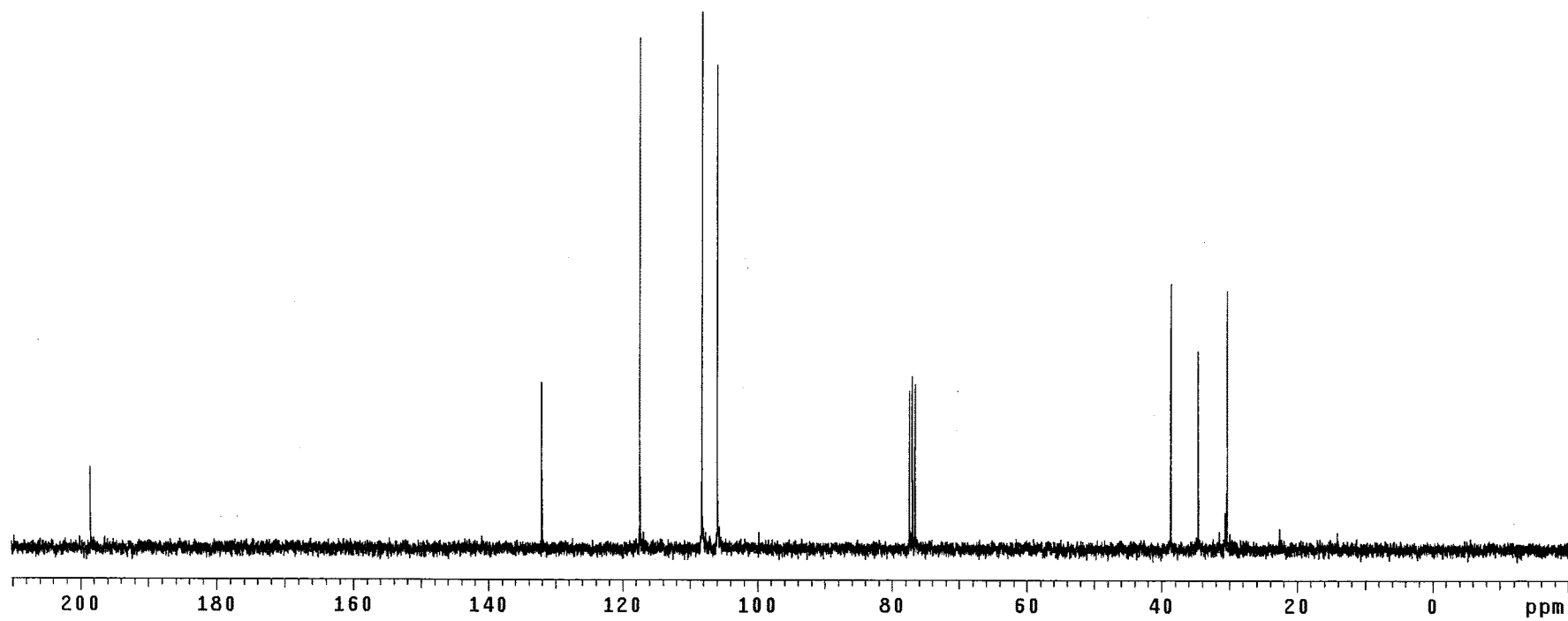


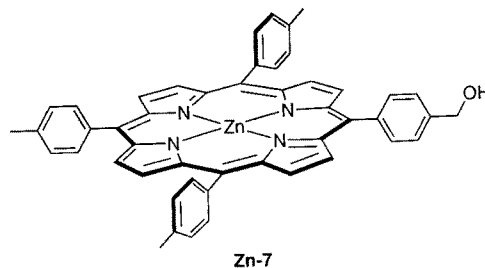
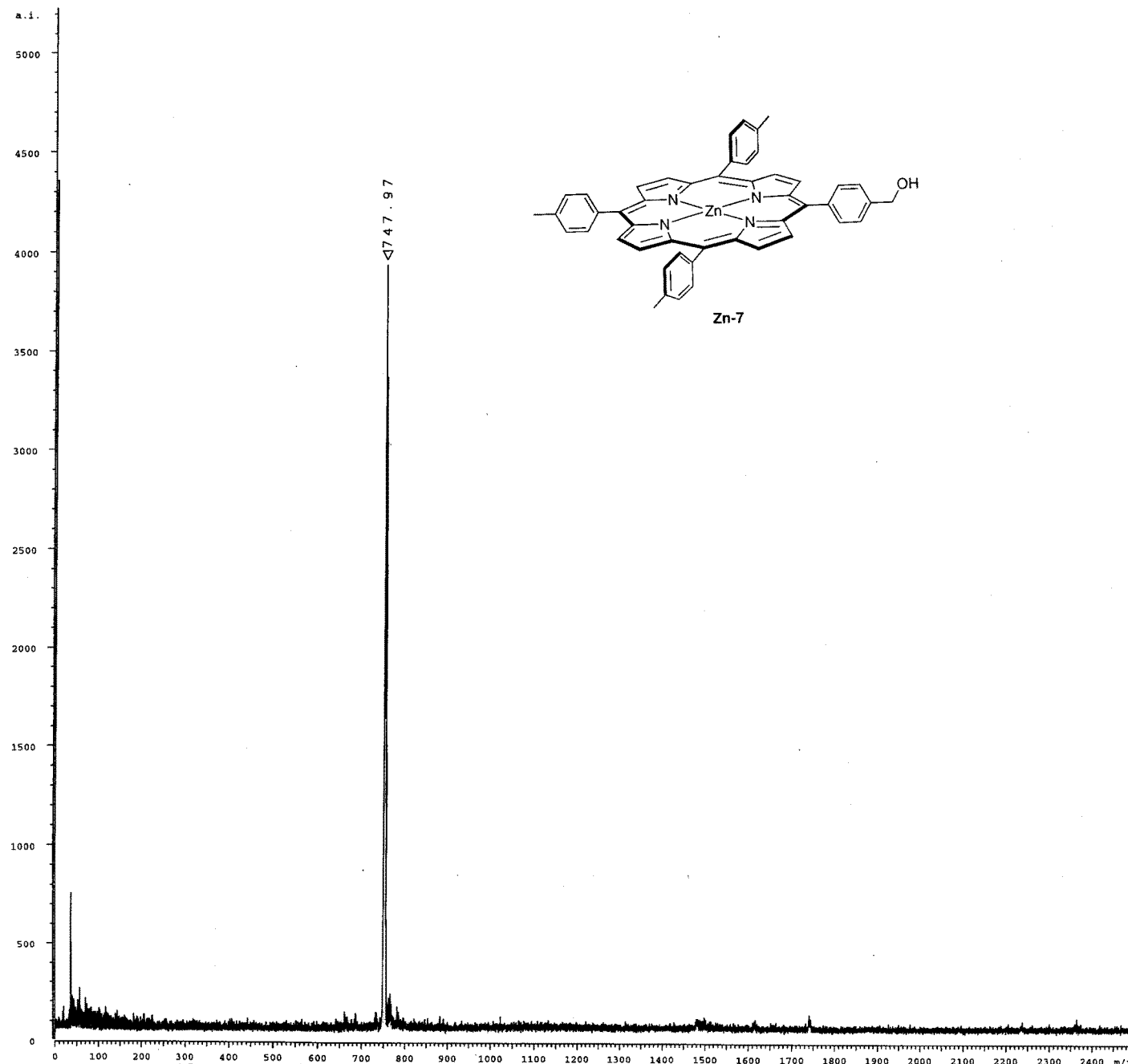








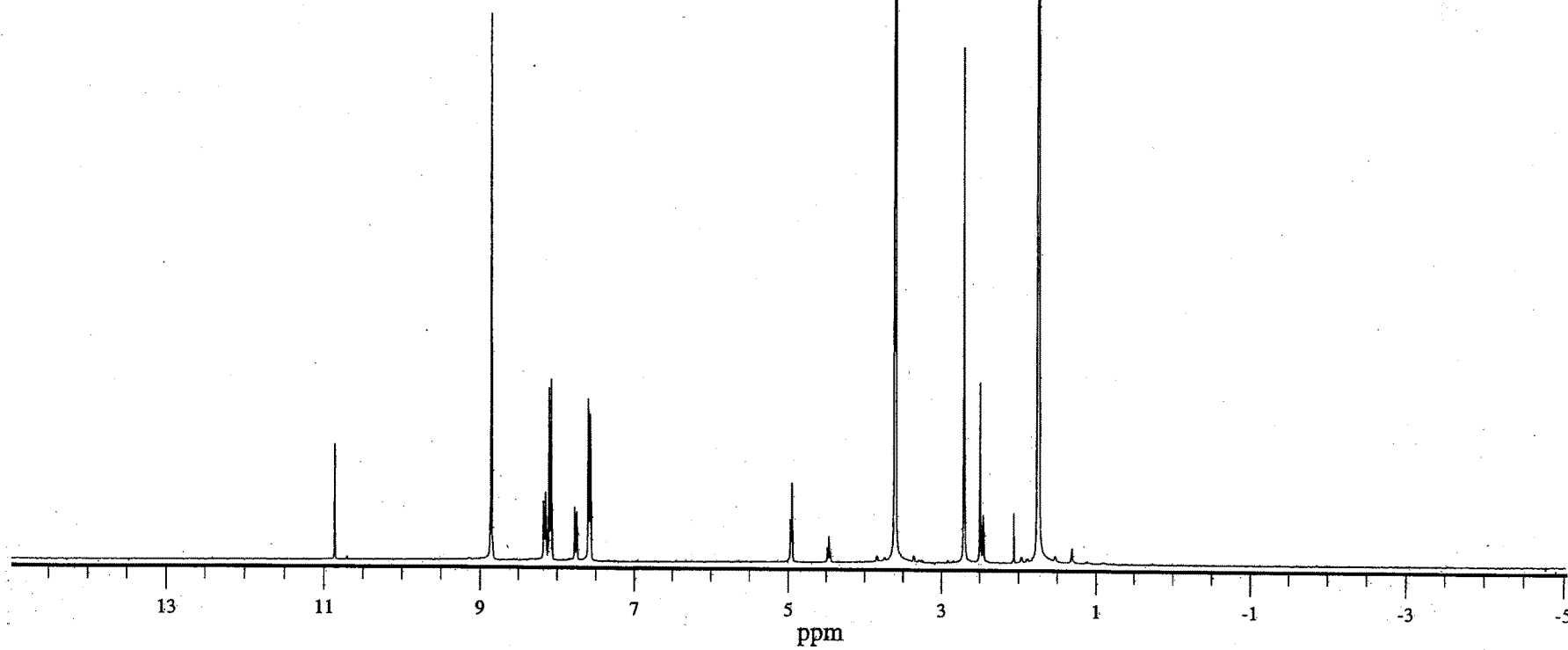
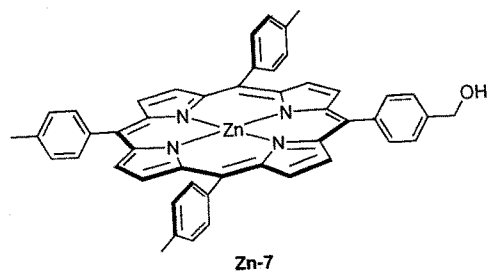


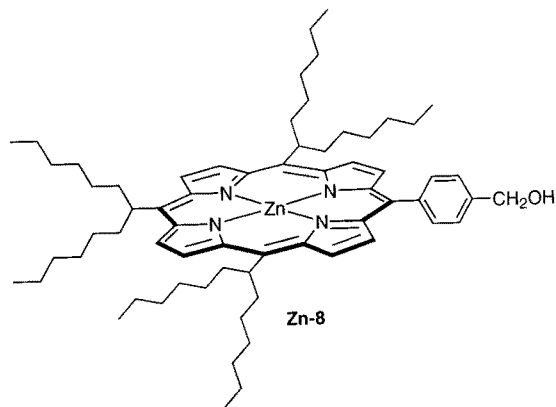


```

INSTRUM TOF
OpId Unknown
SMPNAM 148125
AQ_DATE Mon Mar 5 16:03:07 2001
PATH /data/chemistry/LINDSEY/SCHWEIKART
POLARI POS
AQCF_m Reflector
TD 35000
NoSHOTS 200
SMONUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 0 [ns]
Uis1 20.00 [kV]
Uis2 18.50 [kV]
Uref1 0.00 [kV]
Ulen 7.50 [kV]
Uhimass 10.00 [kV]
RefFull 0.00 [kV]
UdetL 1.55 [kV]
UdetR 0.00 [kV]
Udef1 2.00 [kV]
REPHZ 1.00 [Hz]
ATTEN 37.0
ML1 2077751.567
ML2 353.368
ML3 0.000
HITURBO no
GDEON yes
GDEOLY short
DEFLON no
RLNSND no
LLNSND no
UISZND no
DPCALL 510.84
DPMAS 200.00 [Da]
RENDVAL 0.33
LENDVAL 0.28
ISZENDV 0.91
CMT1 Synthesis 72: trisTol-OHPorZn pure
CMT2 attn = 37, 200 shots
  
```

/data/chemistry/LINDSEY/SCHWEIKART/148125/1SRef/pdata/1 tof Mon Mar 5 16:17:04 2001

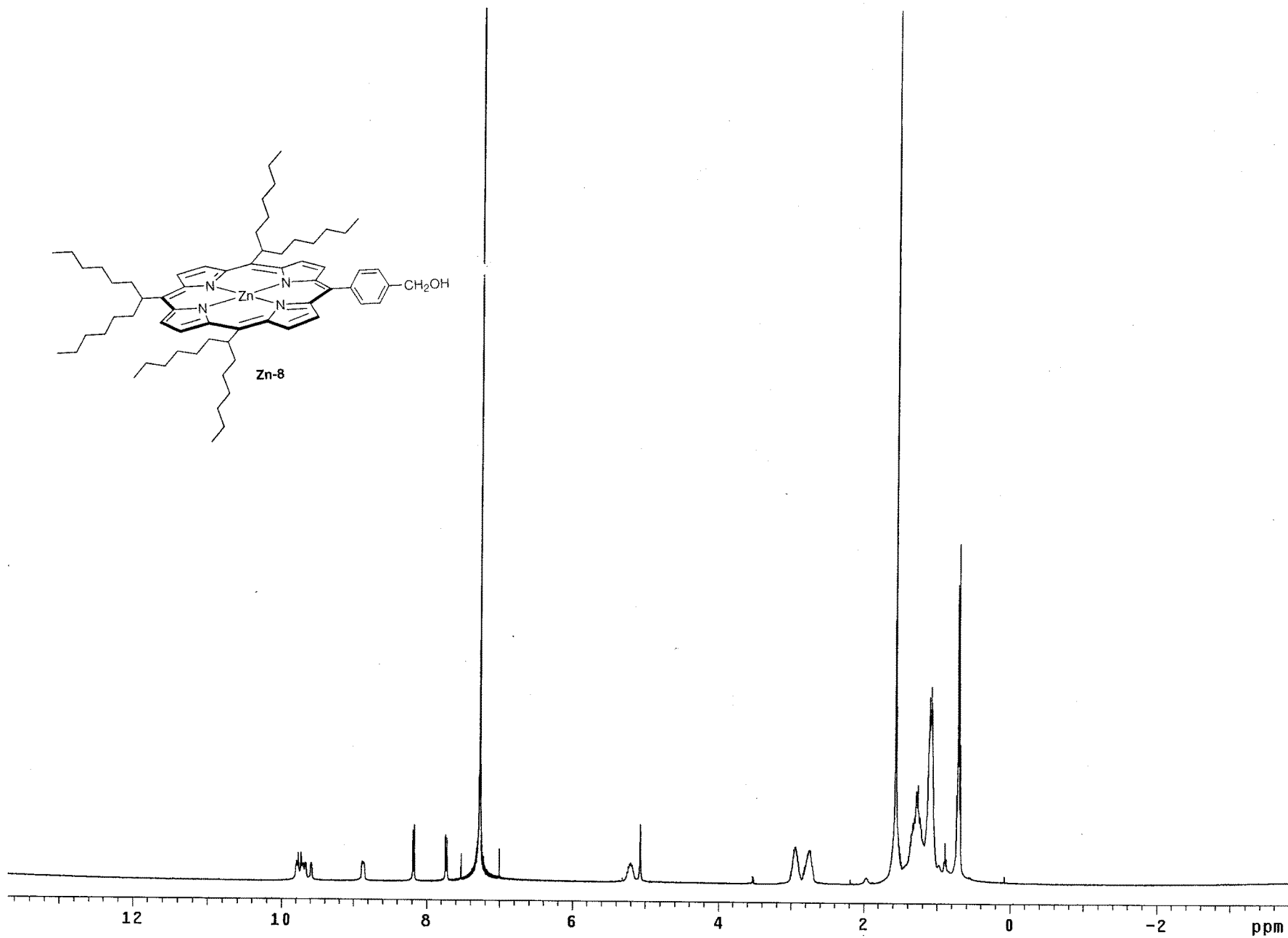


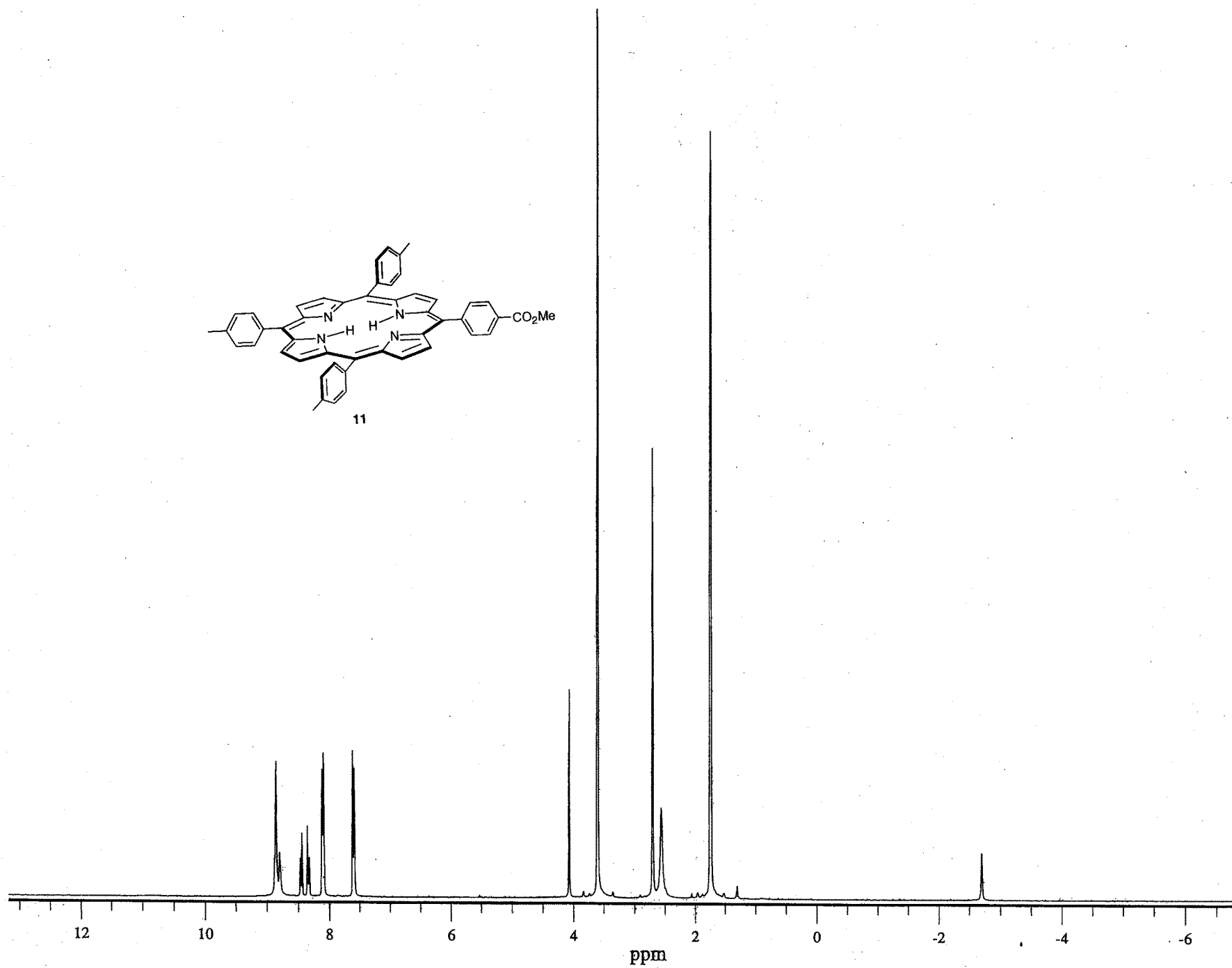


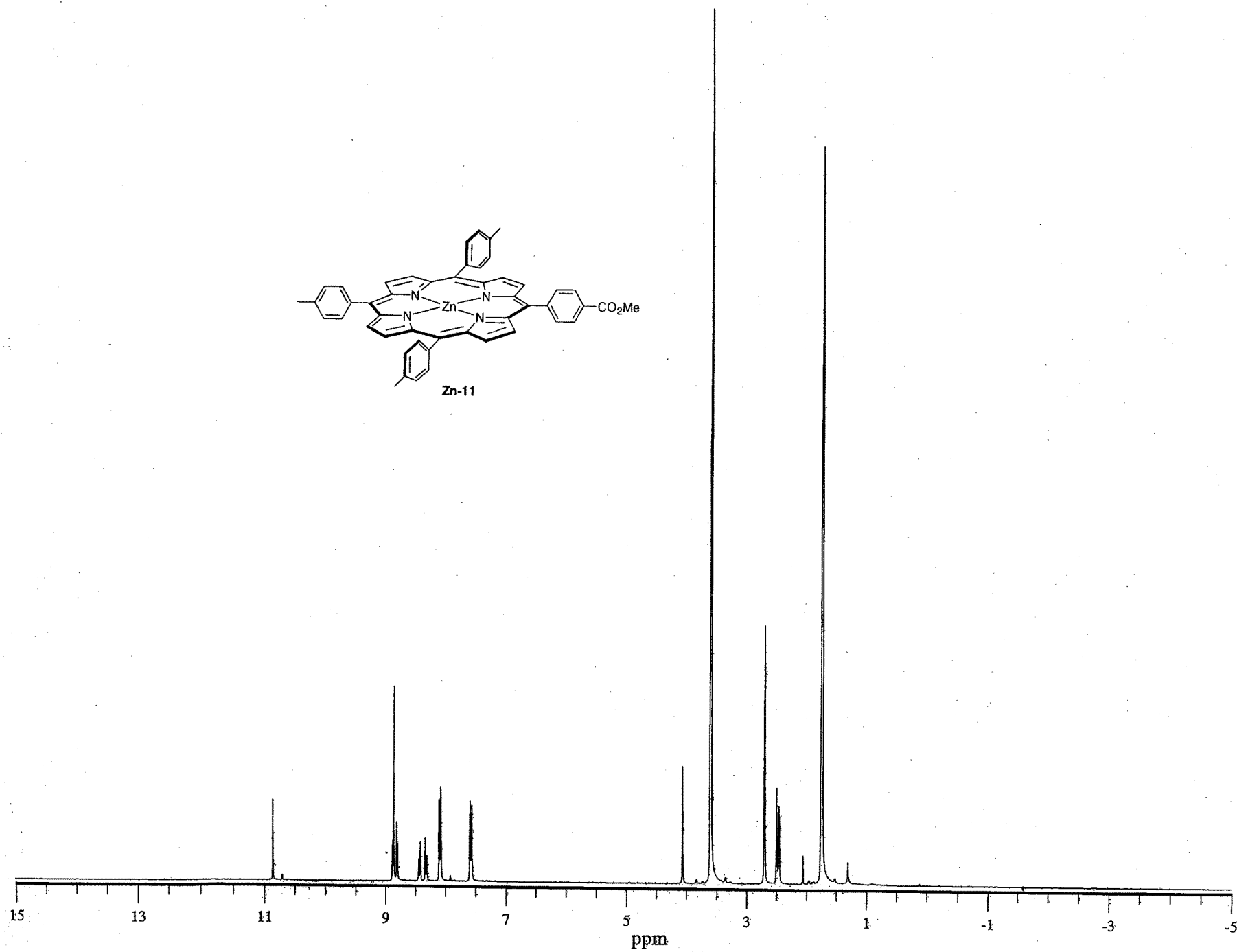
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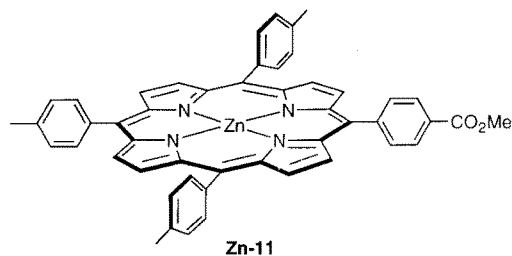
/data/chemistry/LINDSEY/SCHWEIKART/030302/1SRef/pdata/1  tof  Wed May 7 12:42:01 2003

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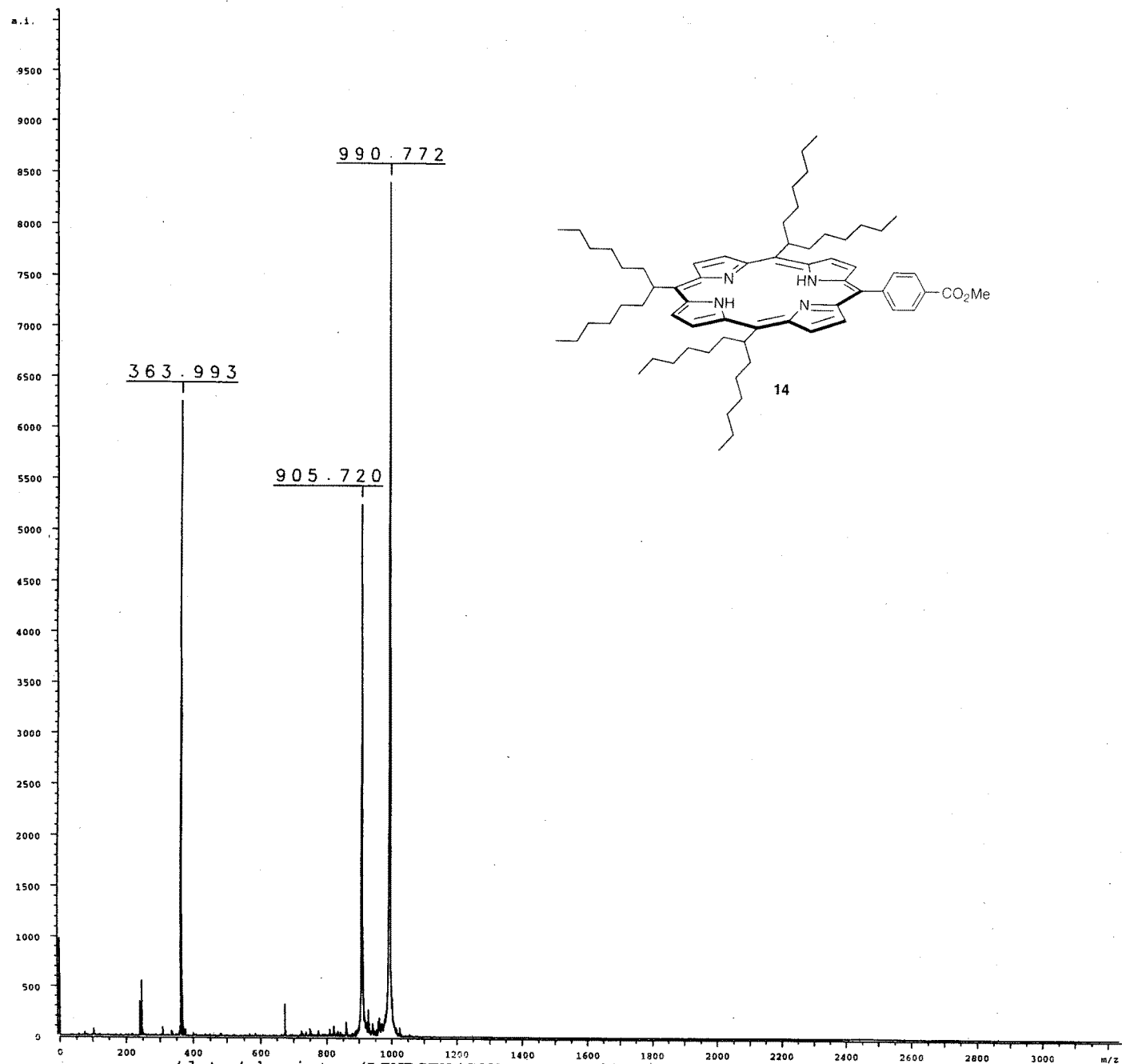




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200      300      400      500      600      700      800      900      1000      1100      1200      1300      1400      m/z
/data/chemistry/LINDSEY/SCHWEIKART/0148149/1SRef/pdata/1  tof  Mon Mar 12 14:26:19 2001

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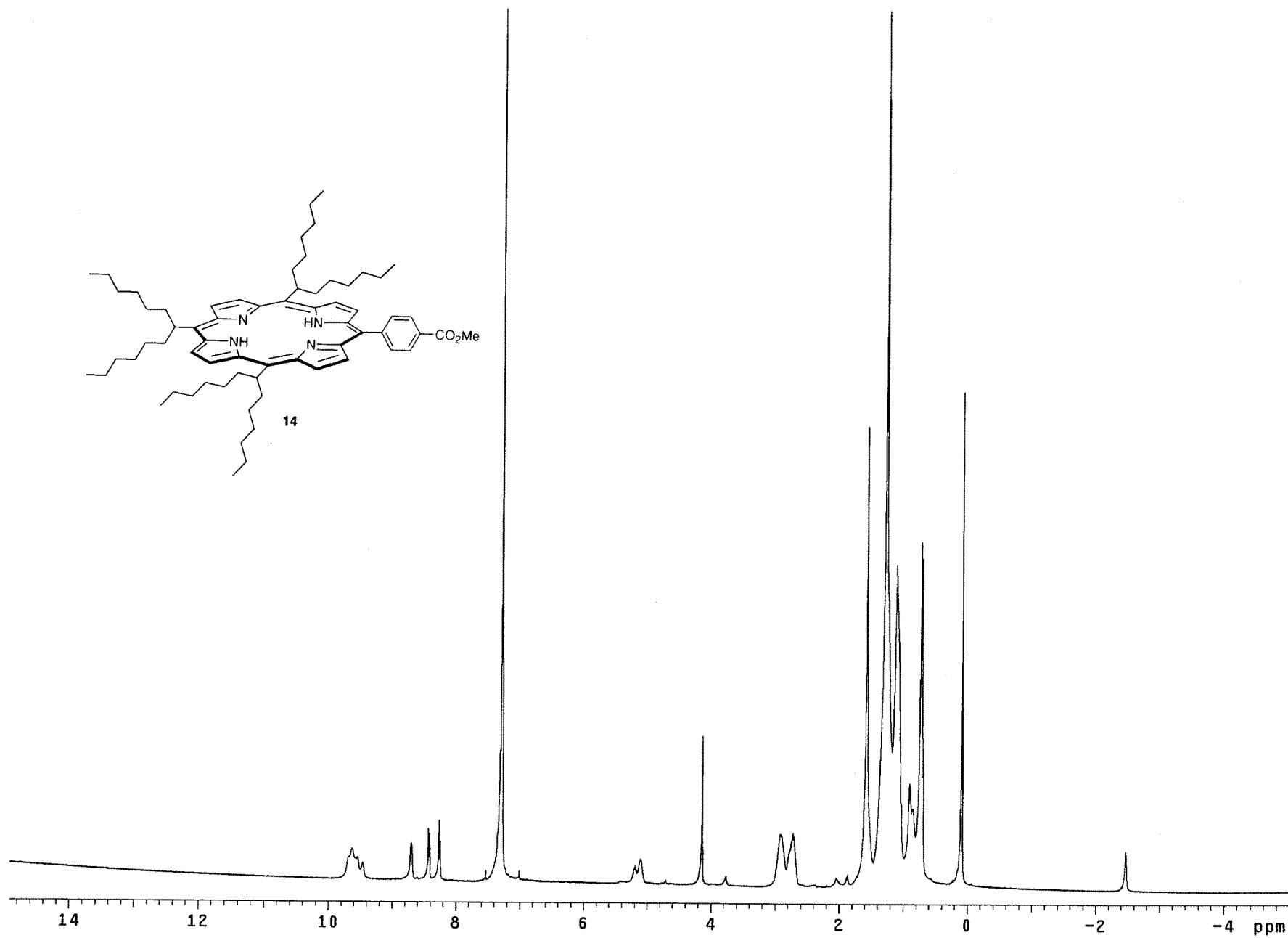
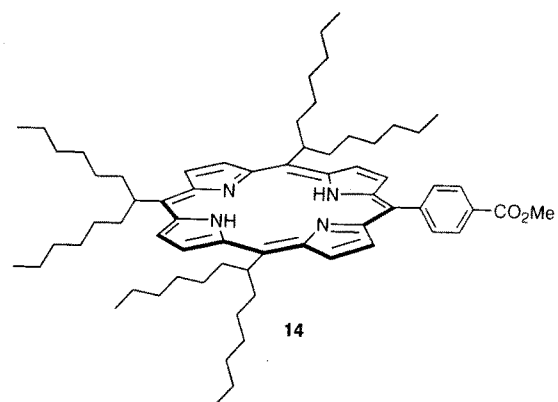


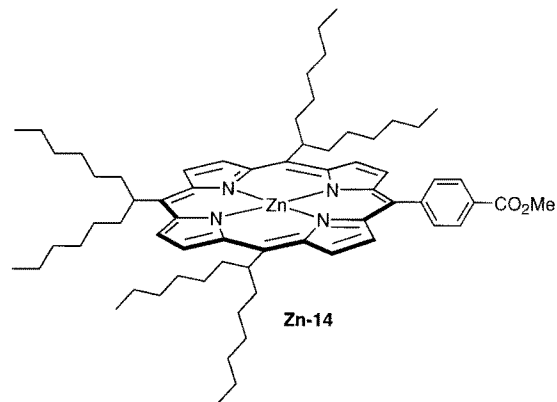
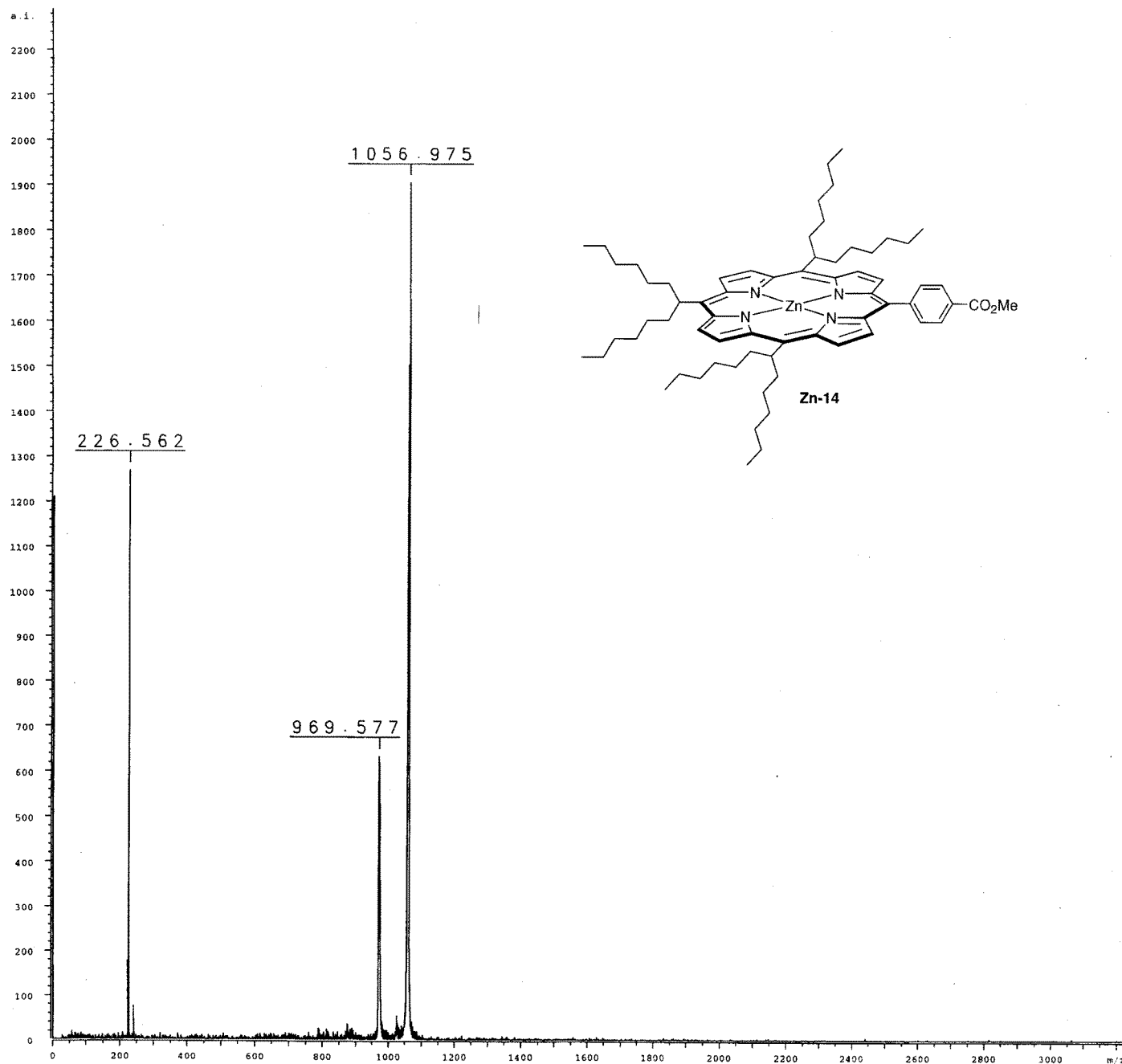
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INSTRUM TOP
OpId N. Srinivasan
SMPNAM 030303
AQ_DATE Wed May 7 12:29:33 2003
PATH /data/chemistry/LINDSEY/SCHWEIKART
POLARI POS
AQOP_m Reflector
TD 40000
NoSHOTS 80
SMCRUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
EW 1.00 [ns]
DELAY 0 [ns]
Uis1 20.00 [kV]
Uis2 18.70 [kV]
Uref1 0.00 [kV]
Uiams 7.50 [kV]
Ulimass 10.00 [kV]
RefFull 0.00 [kV]
UdetL 1.50 [kV]
UdetR 0.00 [kV]
Udefl 2.00 [kV]
REPH2 1.00 [Hz]
ATTEN 54.0
ML1 2067125.193
ML2 333.982
ML3 9.000
RITUREBO no
GDEON yes
GDEEDLY short
DEFLON no
RLNSRND no
LINSRND no
UIS2RND no
DPCAL1 510.84
DPMAS 700.00 [Da]
RENDVAL 0.33
LRENDVAL 0.28
IS2RNDV 0.91
CMT1 Fb1SWT-est (POPOP)
CMT2 MW=991.5206

```

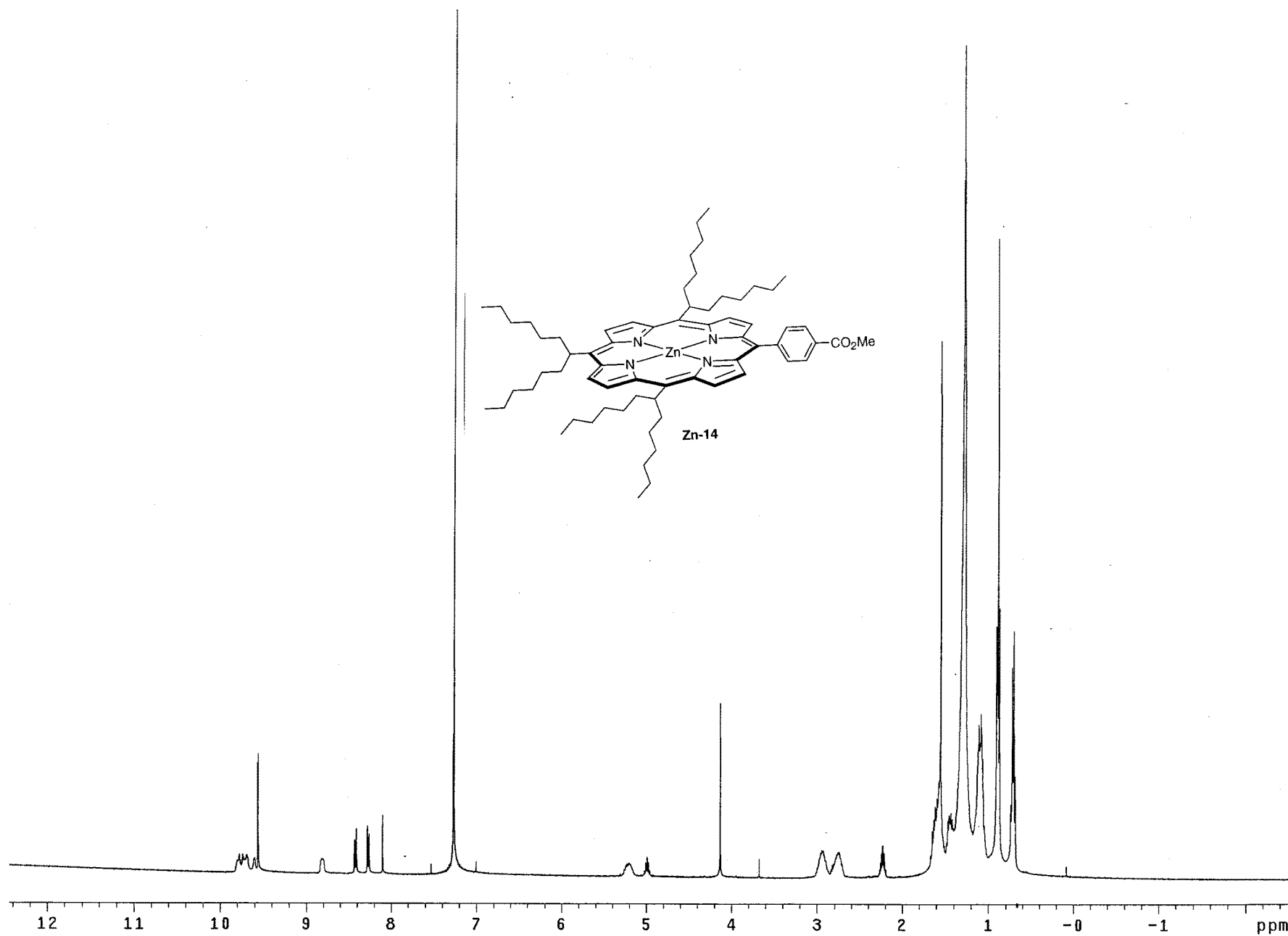
/data/chemistry/LINDSEY/SCHWEIKART/030303/1SRef/pdata/1 tof Wed May 7 12:41:37 2003

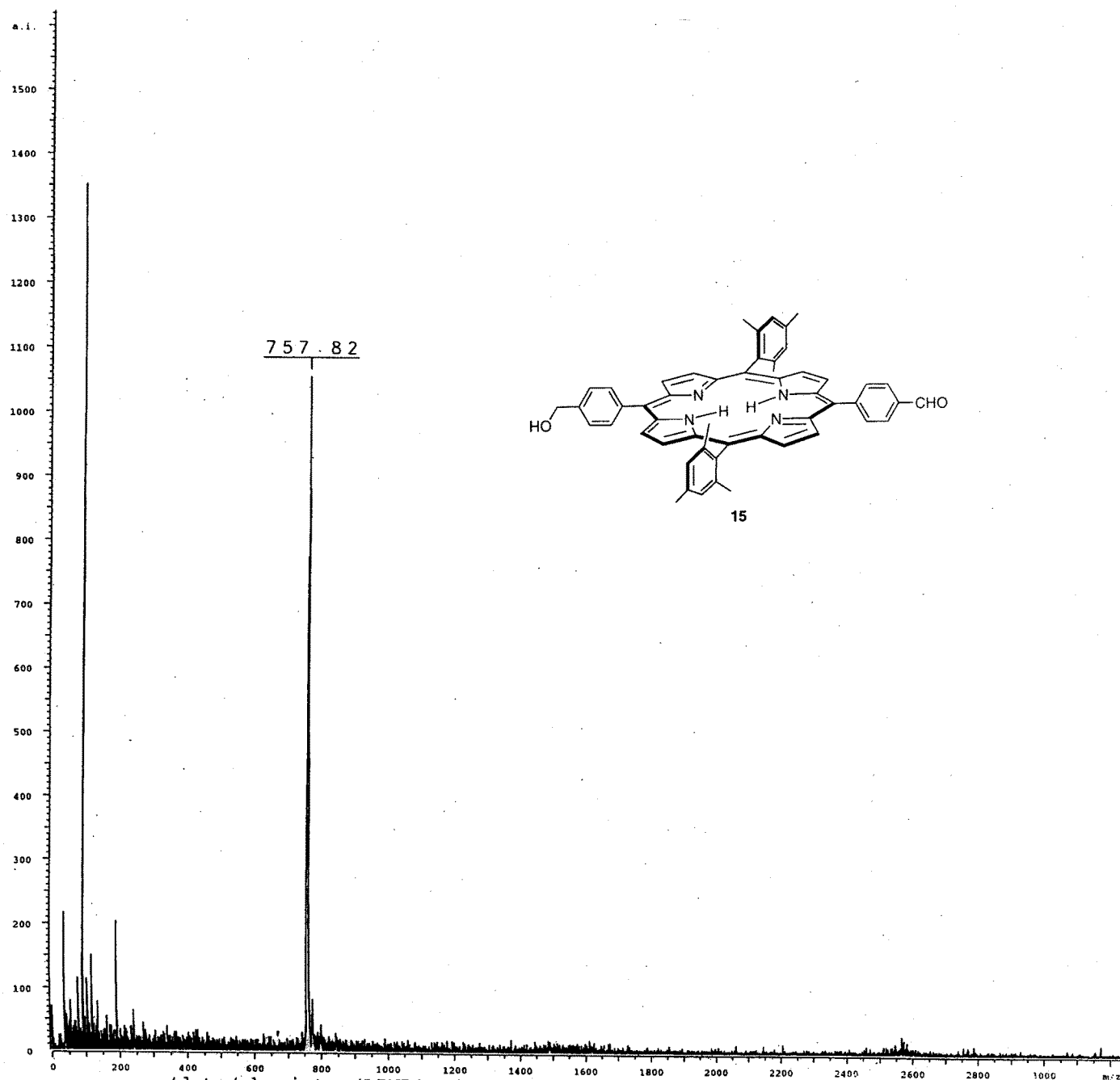




INSTRUM TOP
 OpId N. Srinivasan
 SMPNAM 030261
 AQ_DATE Tue Apr 15 14:20:59 2003
 PATH /data/chemistry/LINDSEY/SCHWEIKART
 POLARI POS
 AQOP_n Reflector
 TD 40000
 NoSHOTS 100
 SMOPT1 0
 SMOPT2 0
 SMOPT3 0
 DW 1.00 [ns]
 DELAY 0 [ns]
 Uis1 20.00 [kV]
 Uis2 18.70 [kV]
 Uref1 0.00 [kV]
 Uisens 7.50 [kV]
 Ulimass 10.00 [kV]
 RefPull 0.00 [kV]
 UdetL 1.50 [kV]
 UdetR 1.55 [kV]
 Udef1 2.00 [kV]
 REPfHZ 1.00 [Hz]
 APTEZ 38.9
 ML1 2064271.968
 ML2 342.177
 ML3 0.000
 HITVRBO no
 GDEON yes
 GDEELY short
 DEFLON no
 RINSRND no
 LINSRND no
 UIS2RND no
 DPCALL 510.84
 DPMASS 700.00 [Da]
 RENDVAL 0.13
 LENDVAL 0.28
 IS2RNDV 0.91
 CMT1 3SWTCOOMe (dithranol)
 CMT2 1054.8947

/data/chemistry/LINDSEY/SCHWEIKART/030261/1SRef/pdata/1 tof Tue Apr 15 14:21:26 2003



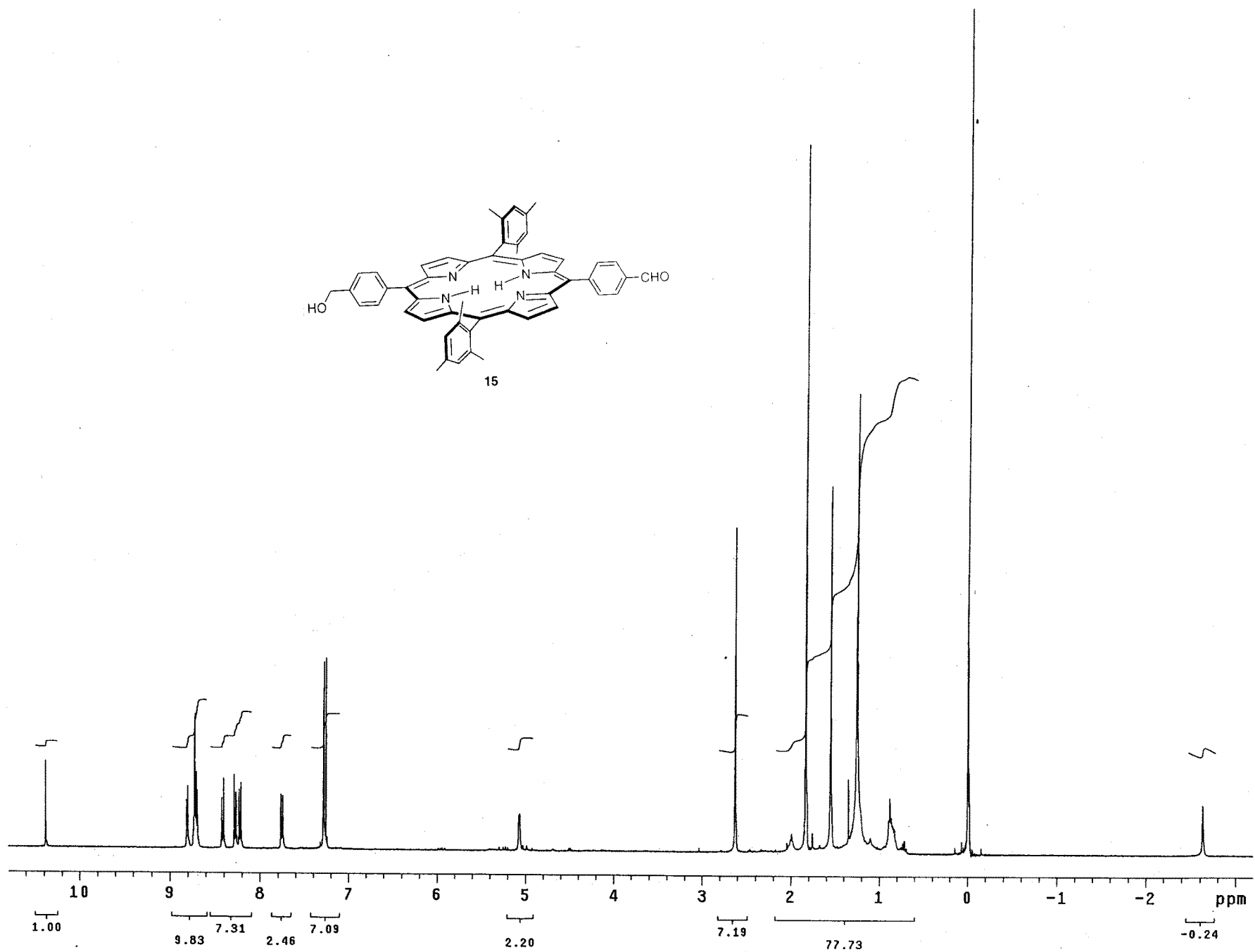
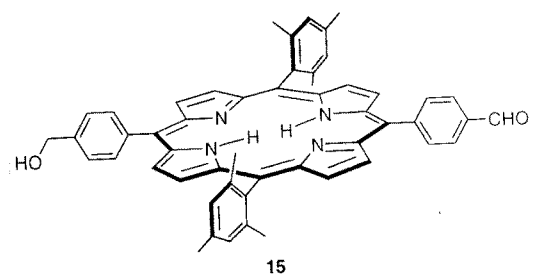


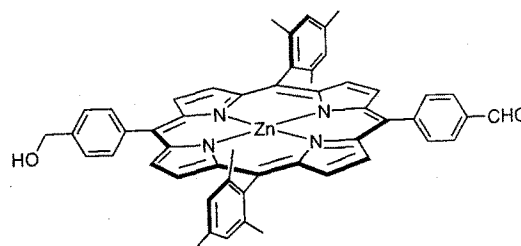
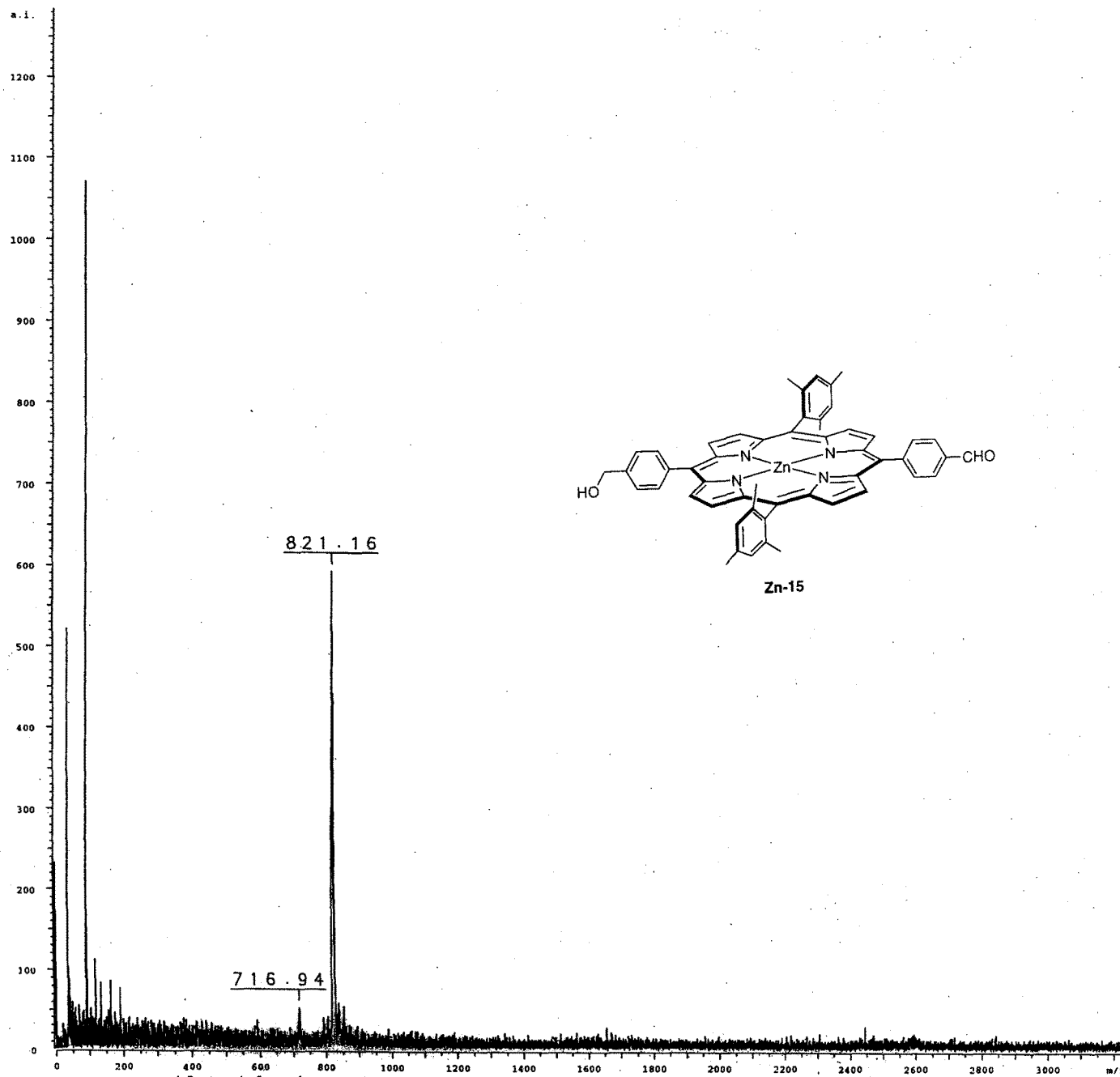
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INSTRUM TOP
OpId N. Srinivasan
SMPNAM 020462
AQ_DATE Mon Apr 22 10:06:23 2002
PATH /data/chemistry/LINDSEY/MALYNOVSKYY
POLARI POS
AQOP_m Reflector
TD 40000
NoSHOTS 9
SMONUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 0 [ns]
Uis1 20.00 [KV]
Uis2 18.70 [KV]
Uref1 0.00 [KV]
Ulen5 7.50 [KV]
Uhimass 10.00 [KV]
RefPull 0.00 [KV]
UdetL 1.50 [KV]
UdetR 0.00 [KV]
Udef1 2.00 [KV]
REPHZ 1.00 [Hz]
ATTEN 31.0
ML1 2067125.193
ML2 333.982
ML3 0.000
HITURBO no
GDEON yes
GDEDLY short
DEFLON no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 510.84
DPMAS5 700.00 [Da]
RBNDVAL 0.33
LBNDVAL 0.28
IS2BNDV 0.91
CNT1 target 8
CNT2 shots =9, attn = 31

```

/data/chemistry/LINDSEY/MALYNOVSKYY/020462/2SRef/pdata/1 tof Mon Apr 22 10:06:41 2002





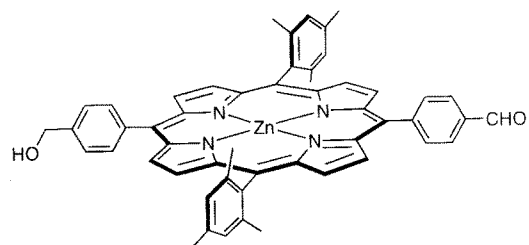
Zn-15

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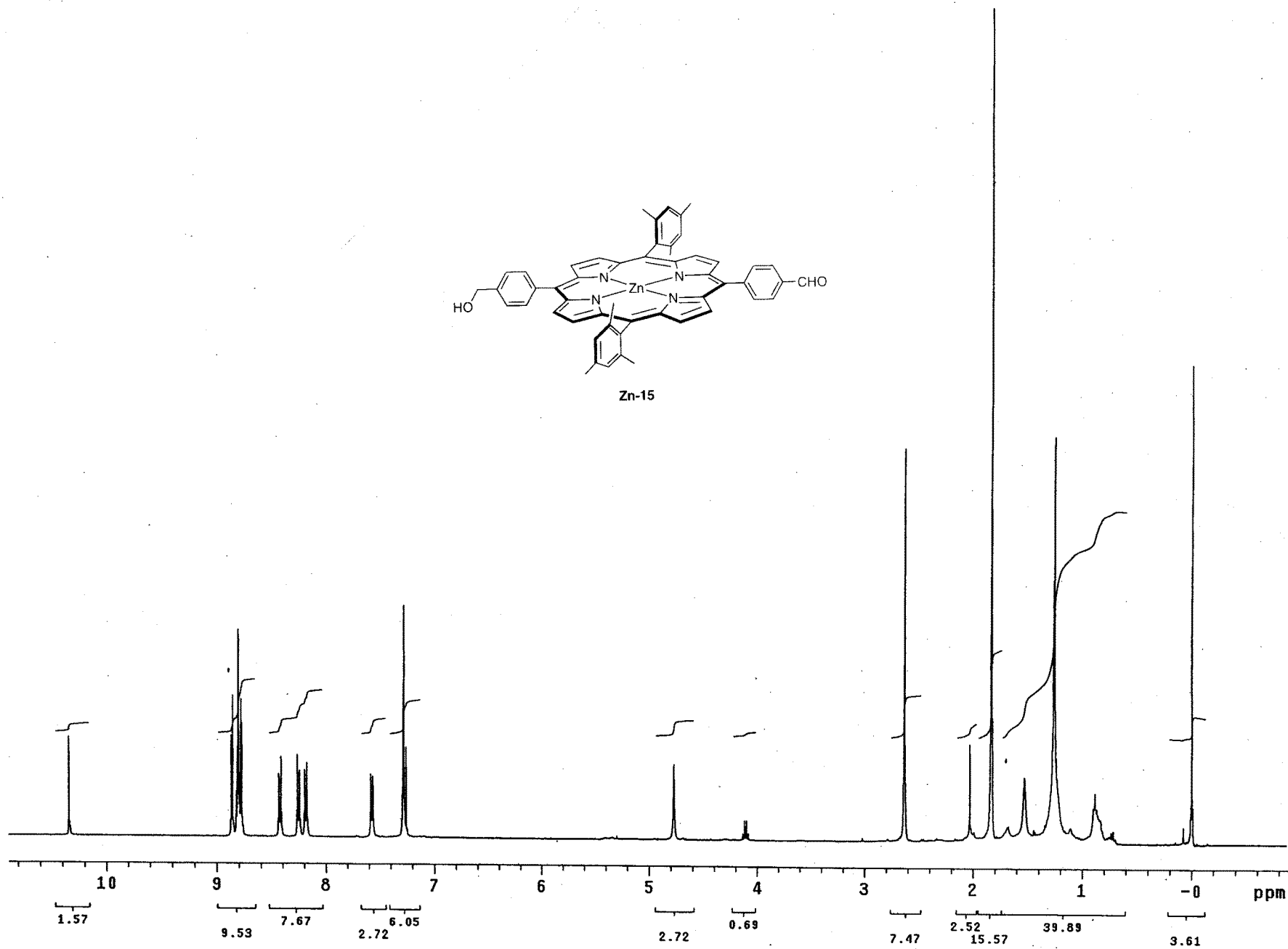
INSTRUM TOP
OpId N. Srinivasan
SMPNAM 020462
AQ_DATE Mon Apr 22 10:04:37 2002
PATH /data/chemistry/LINDSEY/MALYNOVSKYY
POLARI POS
AQOP_m Reflector
TD 40000
NoSHOTS 30
SMORUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 0 [ns]
Uis1 20.00 [KV]
Uis2 18.70 [KV]
Uref1 0.00 [KV]
Ulen5 7.50 [KV]
Uhimass 10.00 [KV]
RefPull 0.00 [KV]
UdetL 1.50 [KV]
UdetR 0.00 [KV]
Udefl 2.00 [KV]
REPHZ 1.00 [Hz]
ATTEN 31.0
ML1 2067125.193
ML2 333.982
ML3 0.000
HITURBO no
GDEON yes
GDEELY short
DEFLON no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 510.84
DPWASS 700.00 [Da]
RBNDVAL 0.33
LBNDVAL 0.28
IS2BNDV 0.91
CMT1 target 6
CMT2 shots =30, attn = 31

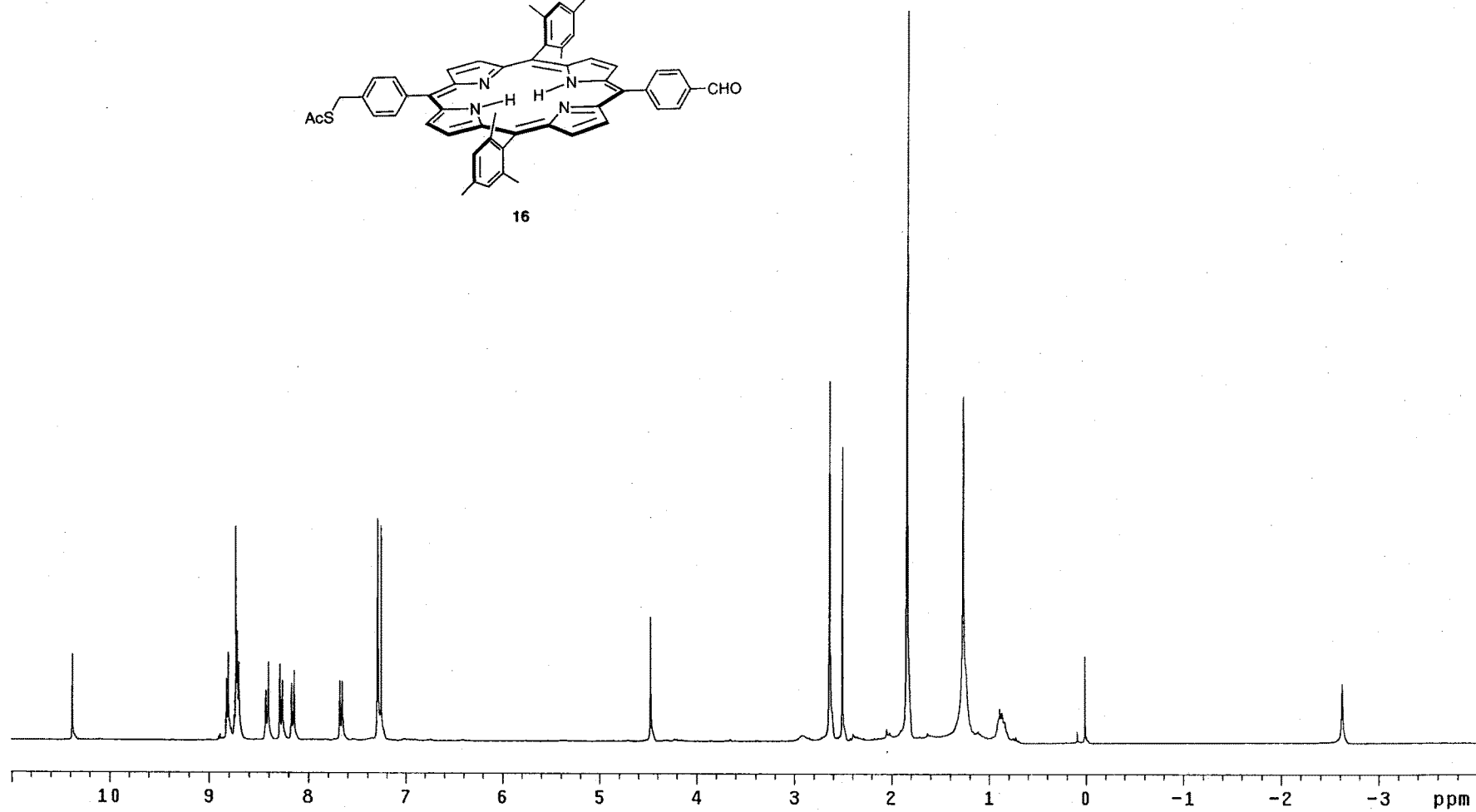
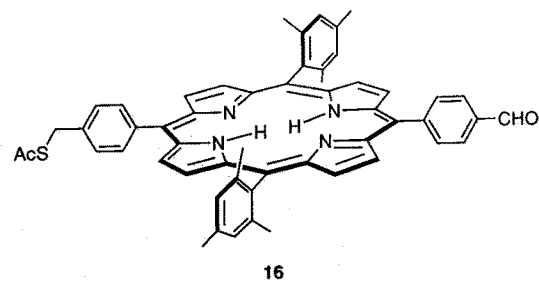
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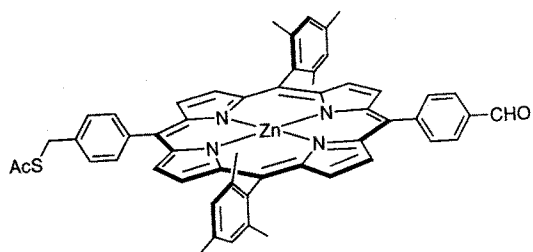
/data/chemistry/LINDSEY/MALYNOVSKYY/020462/1SRef/pdata/1 tof Mon Apr 22 10:05:05 2002



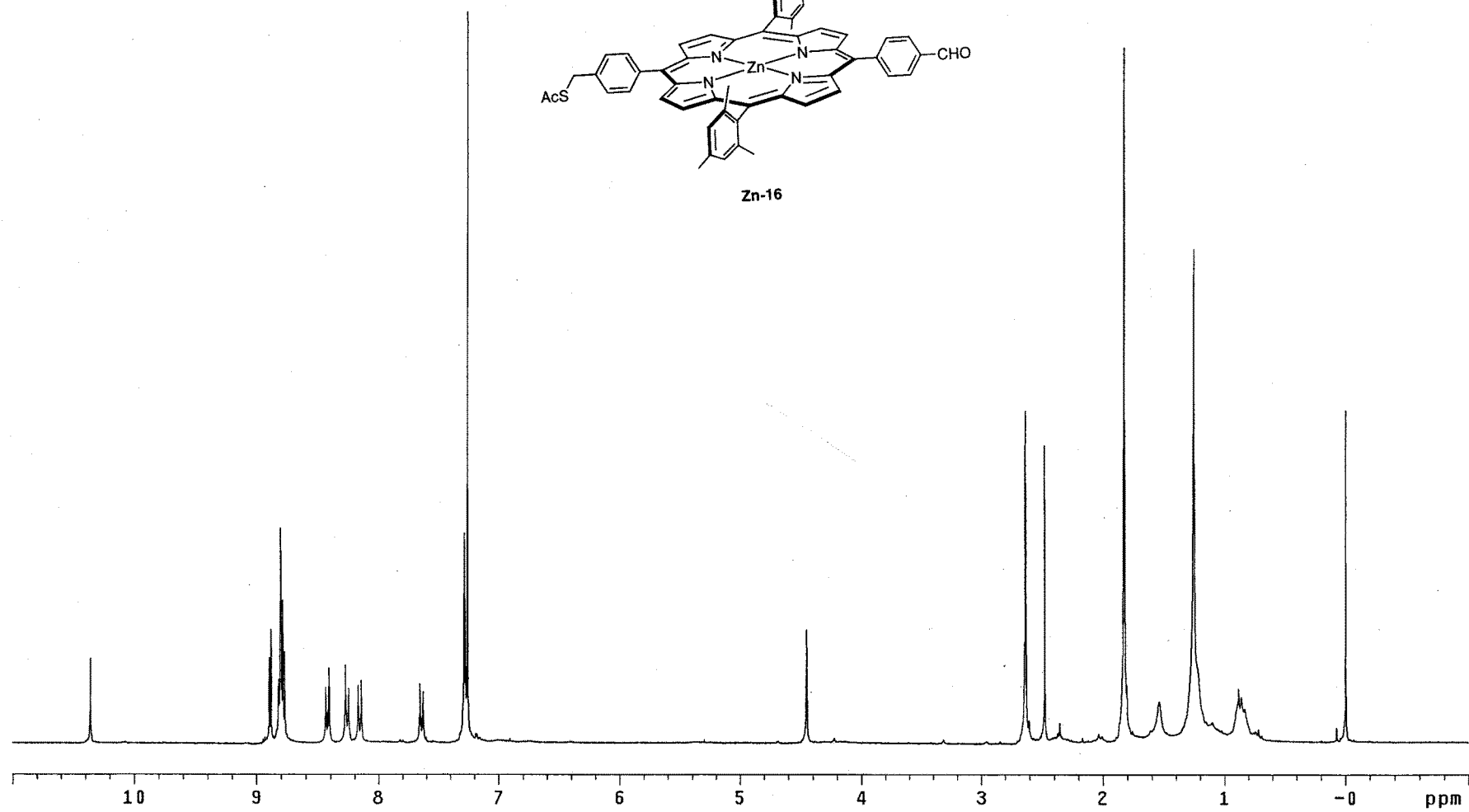
Zn-15

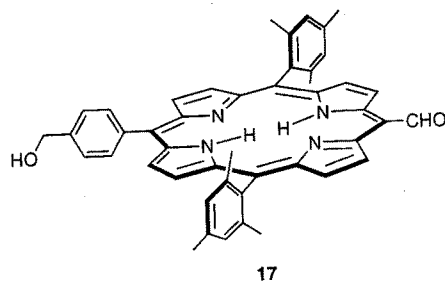
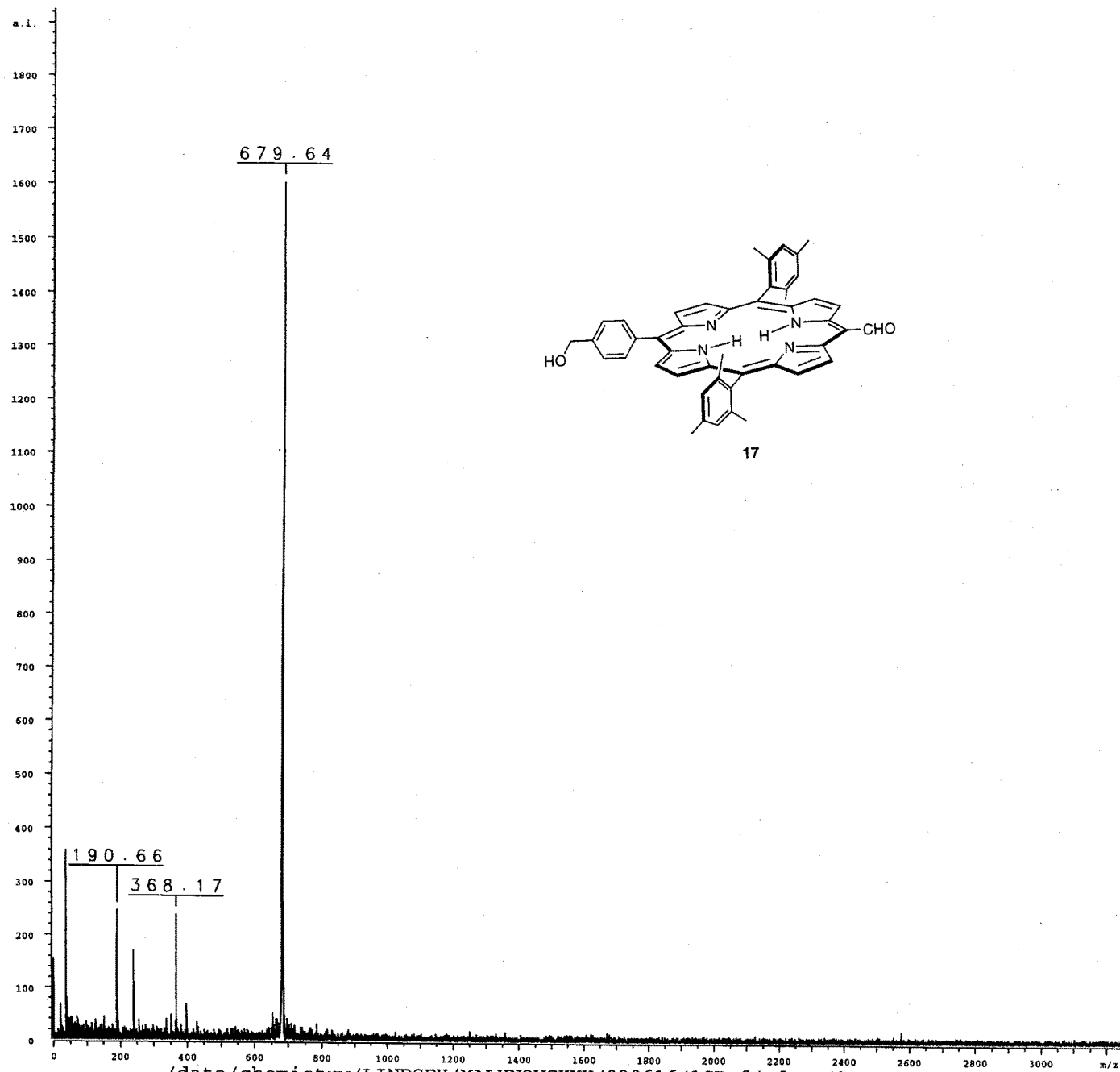






Zn-16



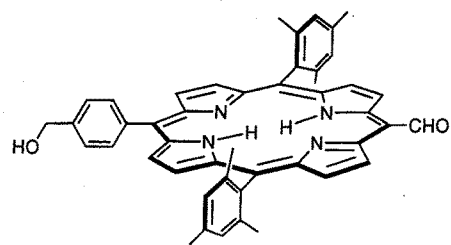


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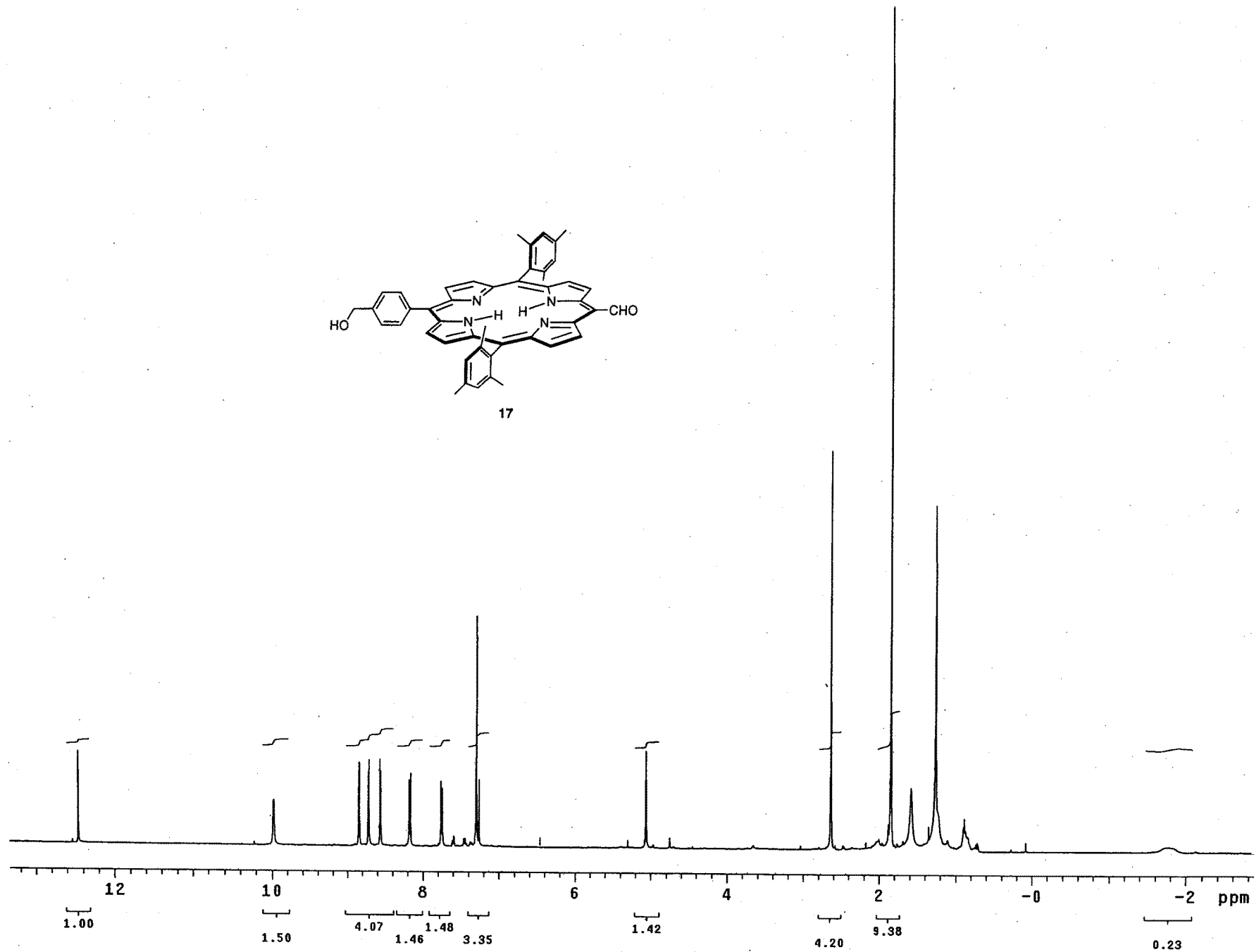
INSTRUM TOF
OpId N. Srinivasan
SMPNAM 020616
AQ_DATE Tue May 28 14:14:42 2002
PATH /data/chemistry/LINDSEY/MALYNOSKY
POLARI POS
AQOP_m Reflector
TD 40000
NoSHOTS 28
SMONUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 0 [ns]
Uls1 20.00 [kV]
Uls2 18.70 [kV]
Uref1 0.00 [kV]
Ulenz 7.50 [kV]
Uhimass 10.00 [kV]
RefPull 0.00 [kV]
UdetL 1.50 [kV]
UdetR 0.00 [kV]
Udef1 2.00 [kV]
REPHZ 1.00 [Hz]
ATTEN 33.0
ML1 2068825.350
ML2 331.982
ML3 0.000
HITURBO no
GDEON yes
ODEELY short
DEFLON no
RLSEND no
LLSEND no
UISEND no
DPCAL1 510.84
DPMAS 700.00 [Da]
RBNVAL 0.33
LBNVAL 0.28
IS2BNDV 0.91
CMT1 suruki coupling after column
CMT2 att 33 shot 28

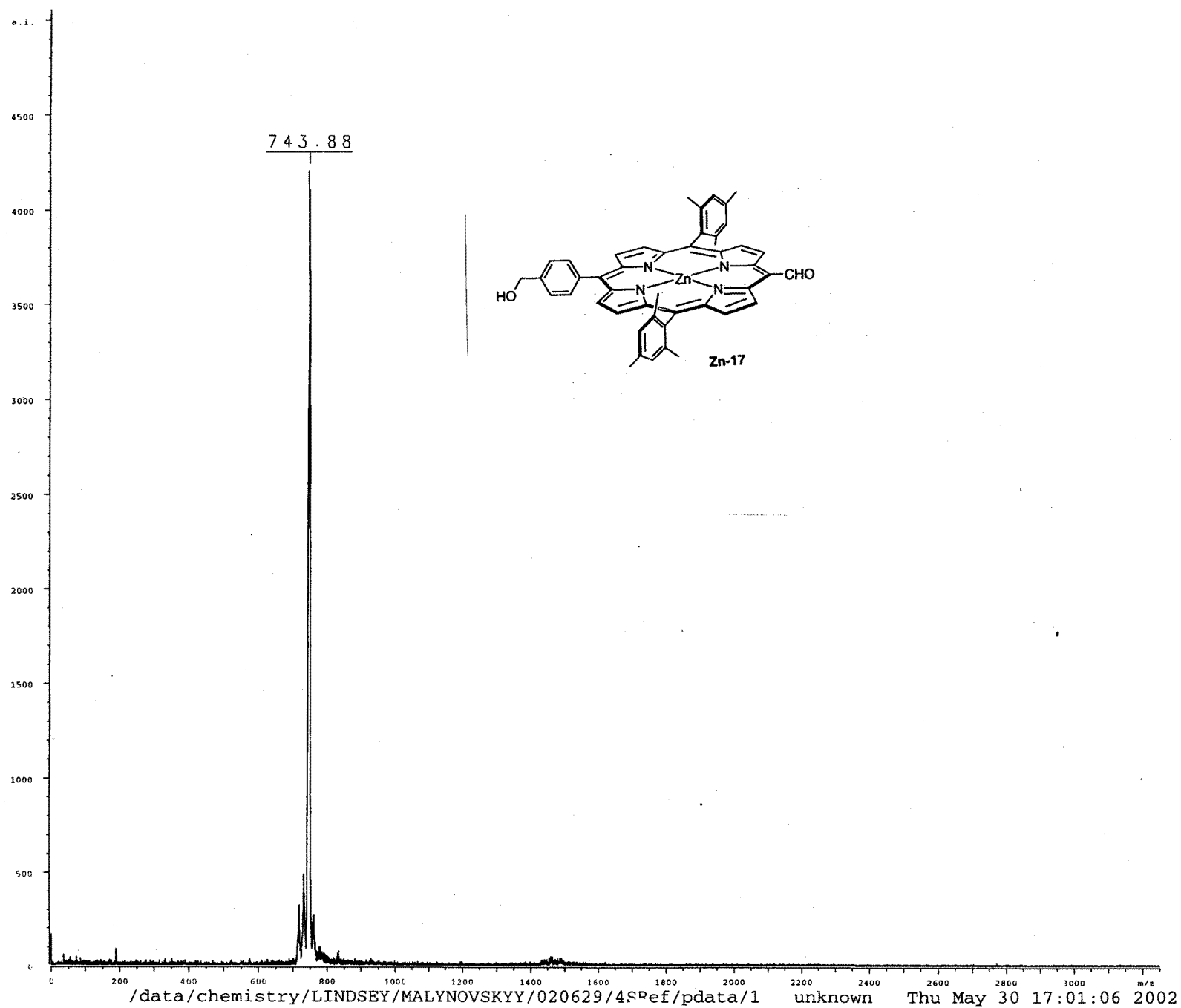
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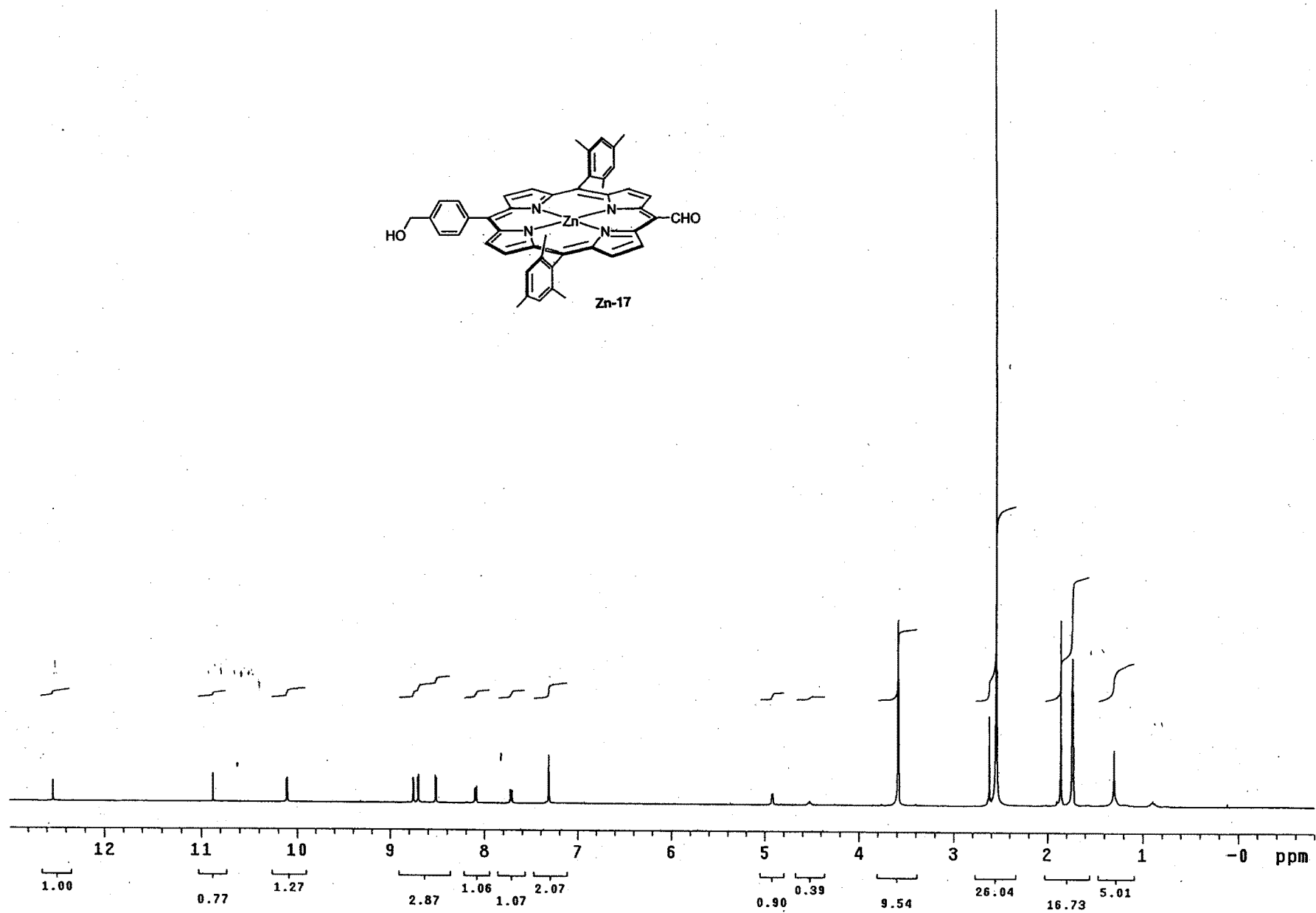
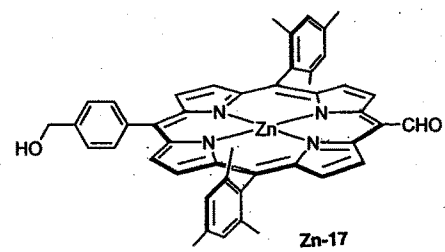
/data/chemistry/LINDSEY/MALYNOSKY/020616/1SRef/pdata/1 tof Tue May 28 14:15:28 2002

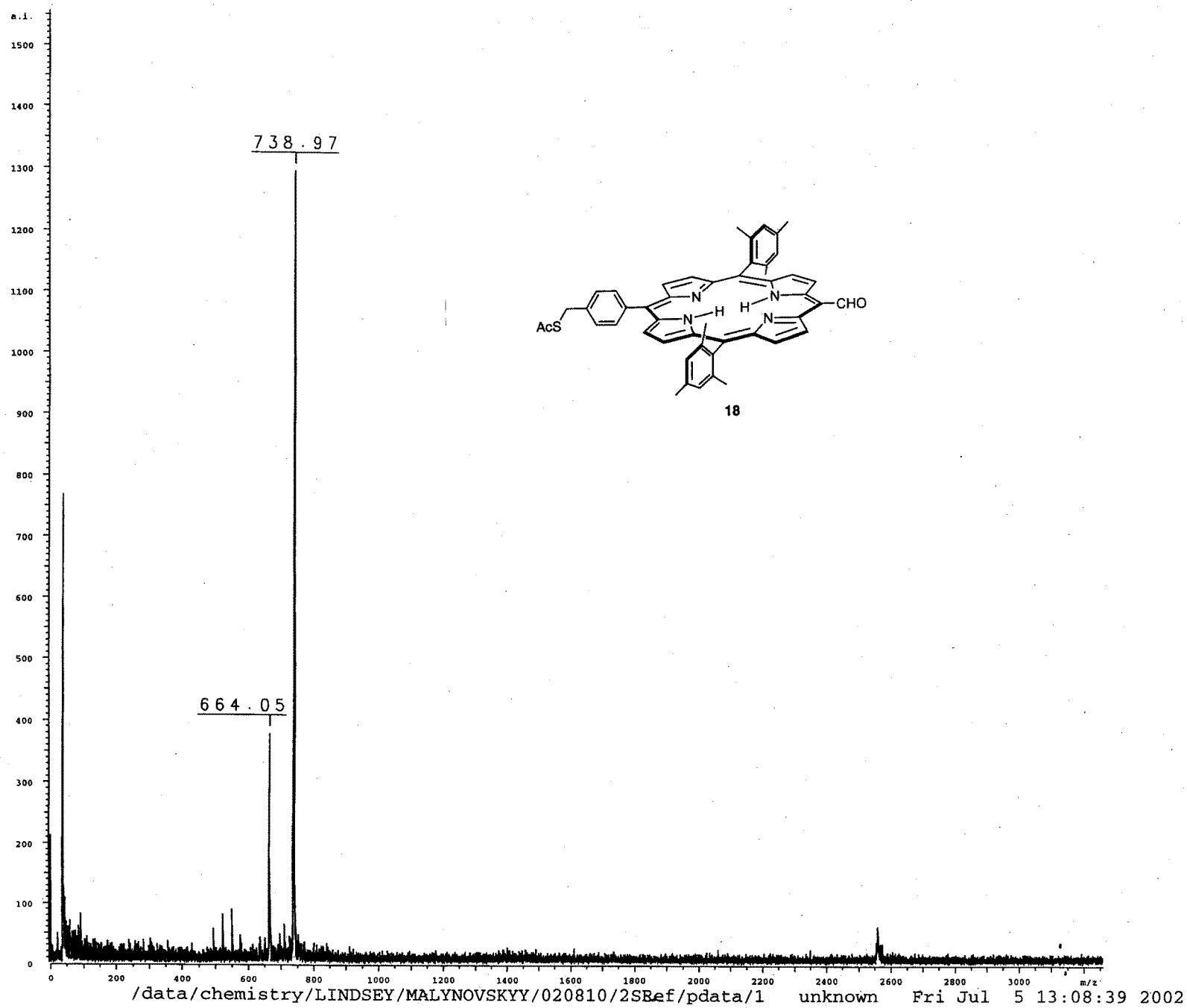


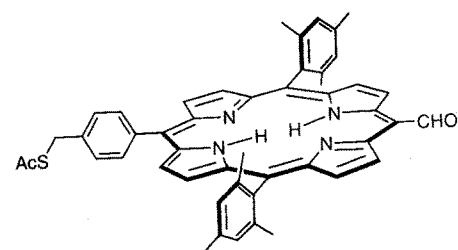
17



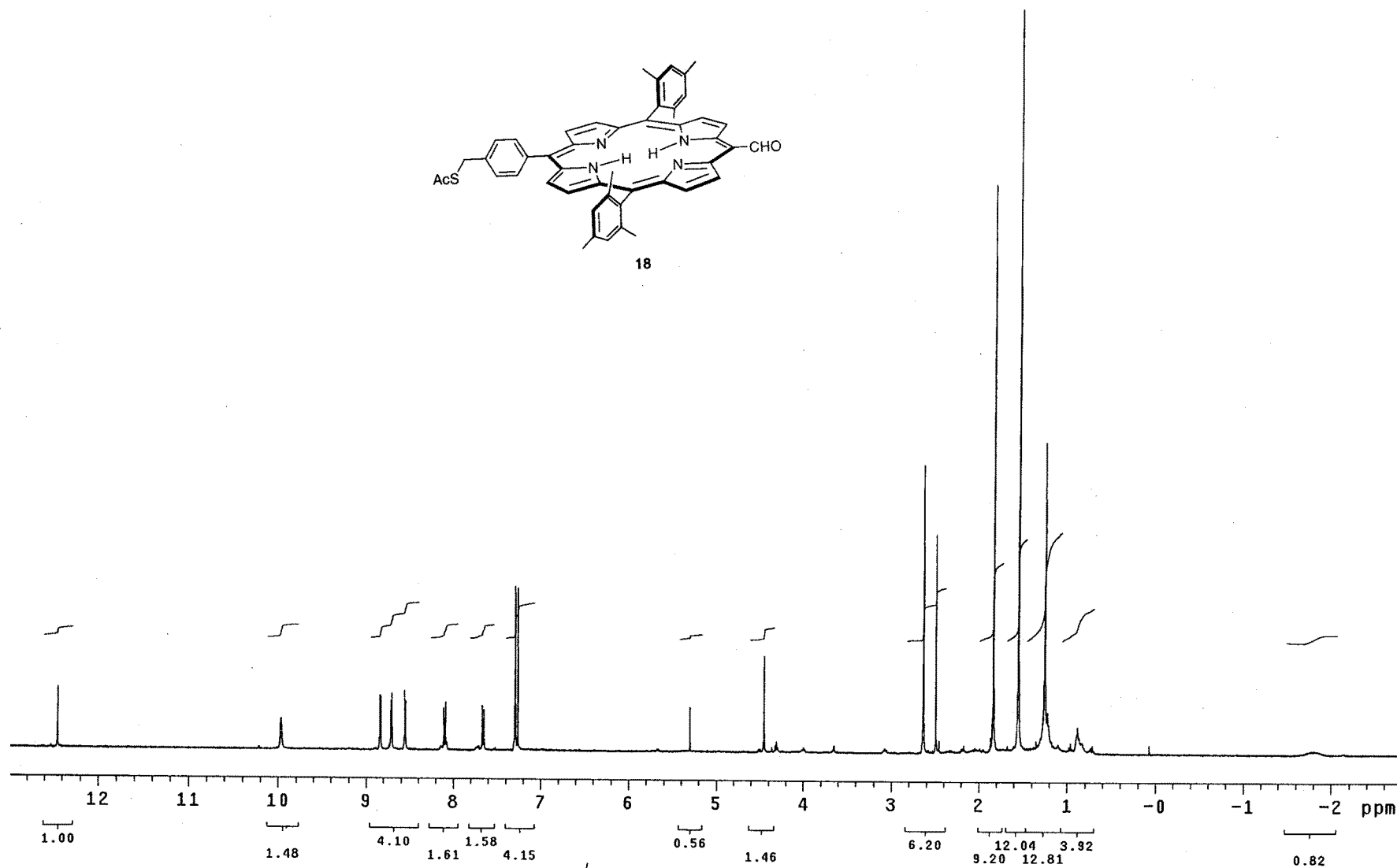


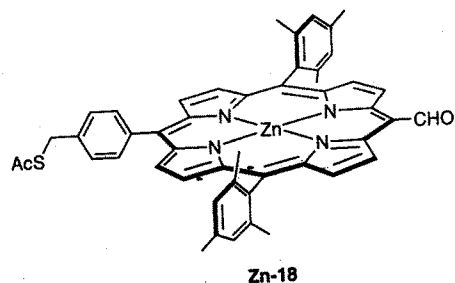
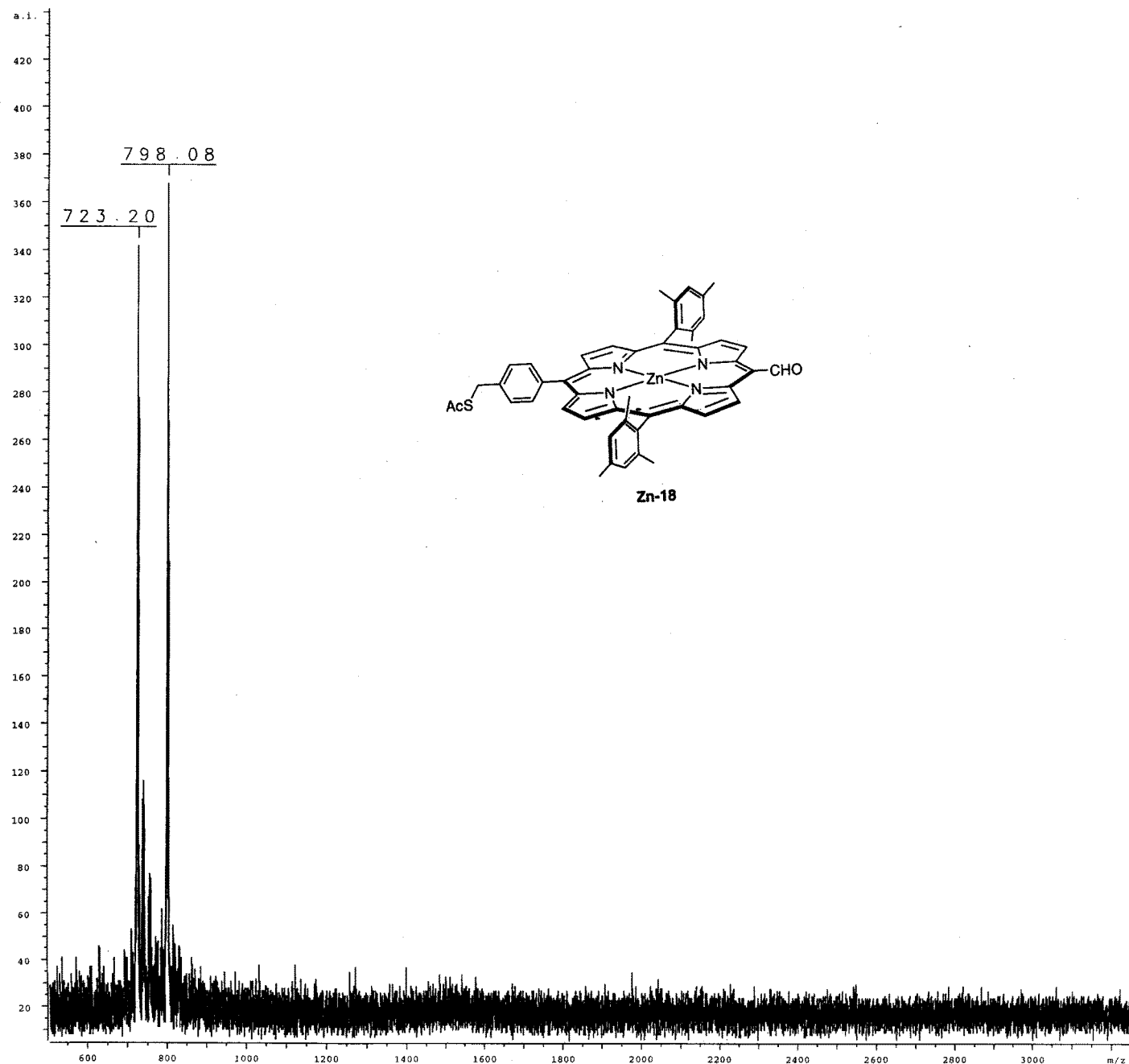






18



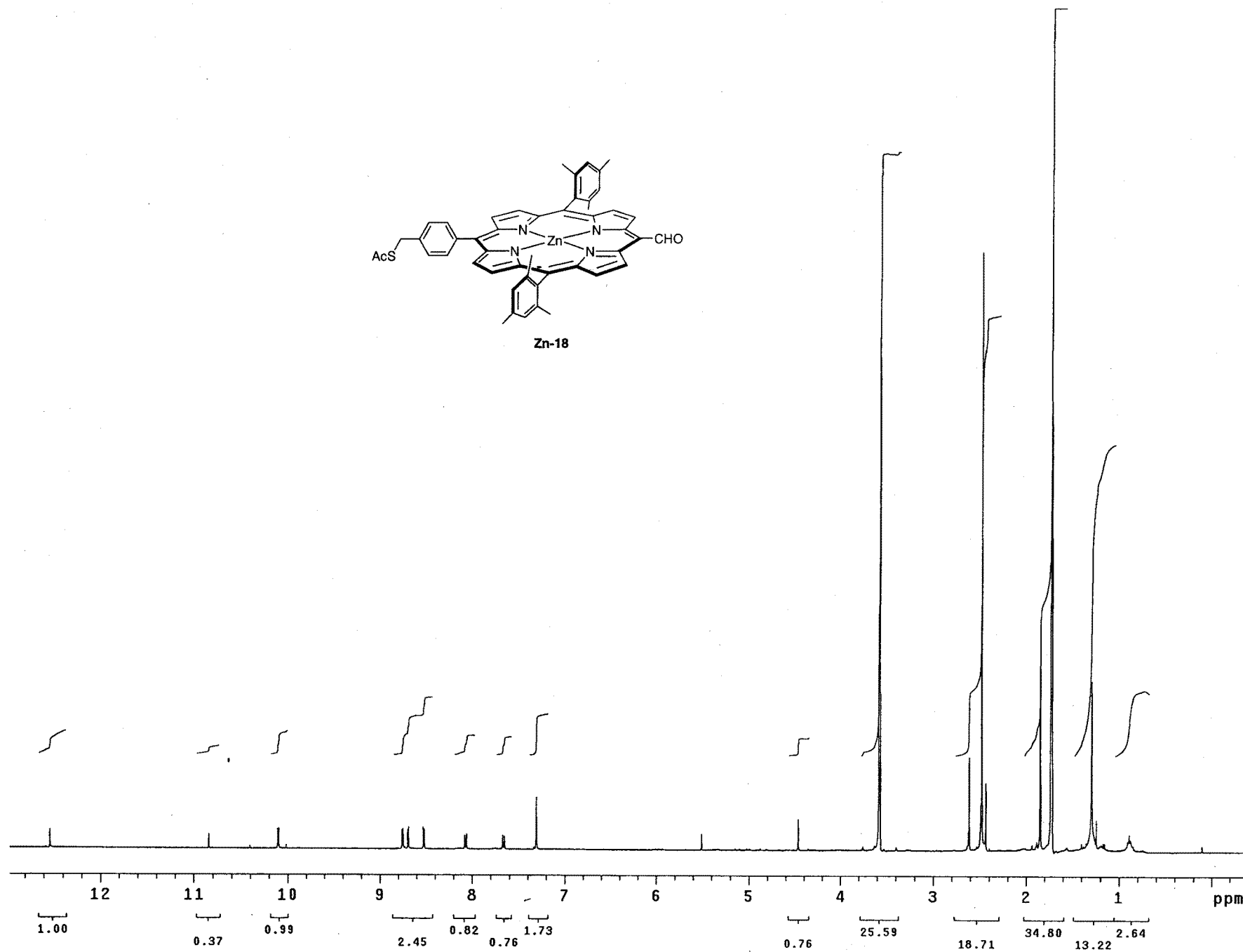
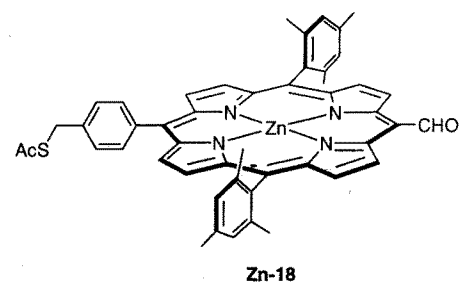


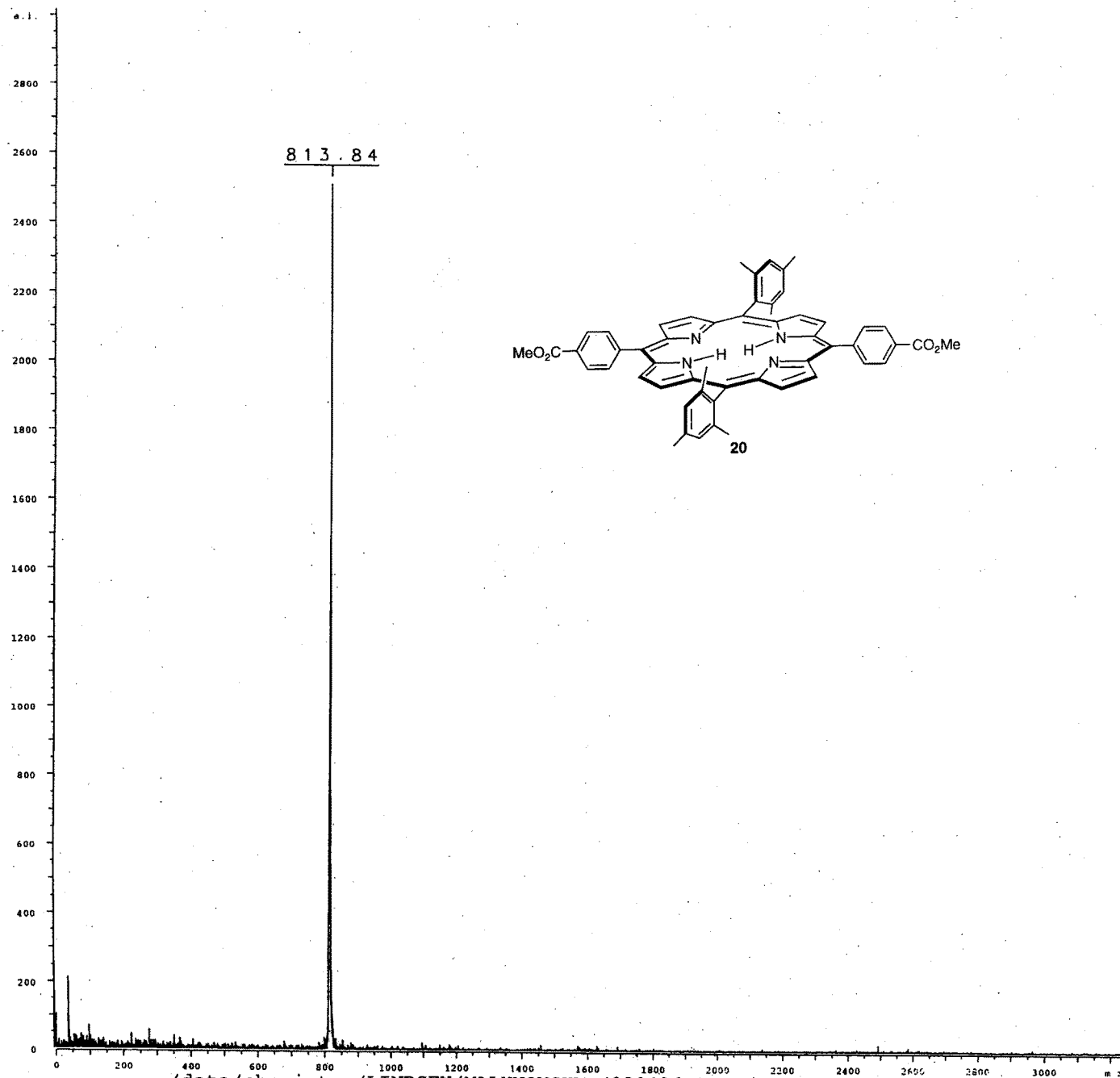
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INSTRUM TOP
Cpld N. Srinivasan
SMPNAM 020837
AQ_DATE Tue Jul 9 13:47:30 2002
PATH /data/chemistry/LINDSEY/MALYNOVSKYY
POLARI POS
AQOP_m Reflector
TD 40000
NoSHOTS 45
SMONUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 0 [ns]
Uls1 20.00 [kV]
Uls2 18.70 [kV]
Urefl 0.00 [kV]
Ulenz 7.50 [kV]
Uhlmass 10.00 [kV]
RefFull 0.00 [kV]
UdetL 1.50 [kV]
UdetR 0.00 [kV]
Udefl 2.00 [kV]
REPHZ 1.00 [Hz]
ATTEN 28.0
ML1 2067125.193
ML2 333.982
ML3 0.000
HITURBO no
GDEON yes
GDEOLY short
DEFLON no
RLNSND no
LLNSND no
UIS2ND no
DPCAL1 510.84
DPMAS 700.00 [Da]
RENDVAL 0.33
LENDVAL 0.28
IS2ENDV 0.91
CMT1 zn insertion
CMT2

```

/data/chemistry/LINDSEY/MALYNOVSKYY/020837/2CRef/pdata/1 tof Tue Jul 9 13:47:57 2002



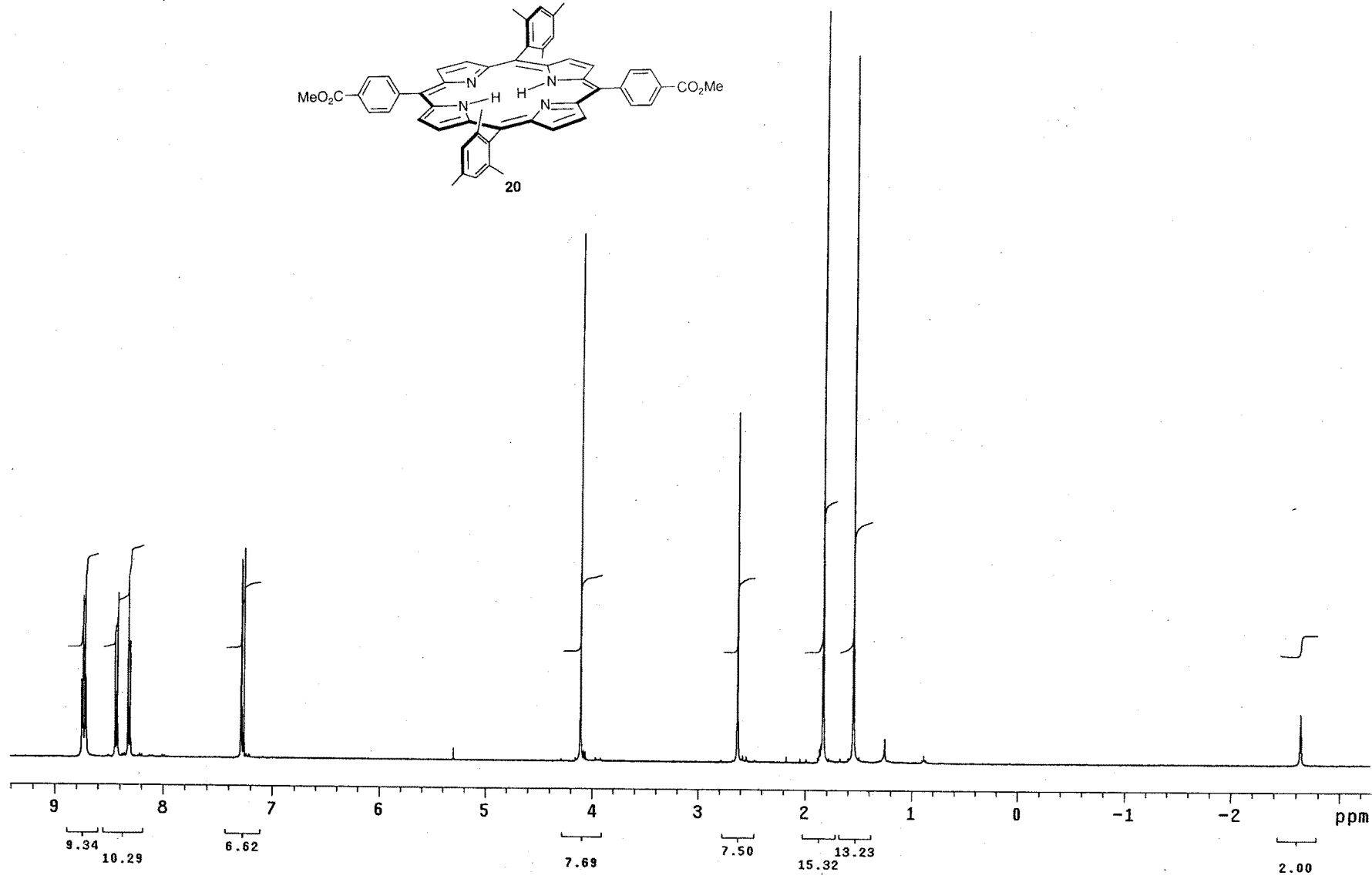
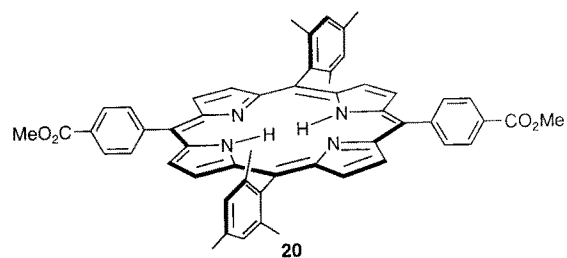


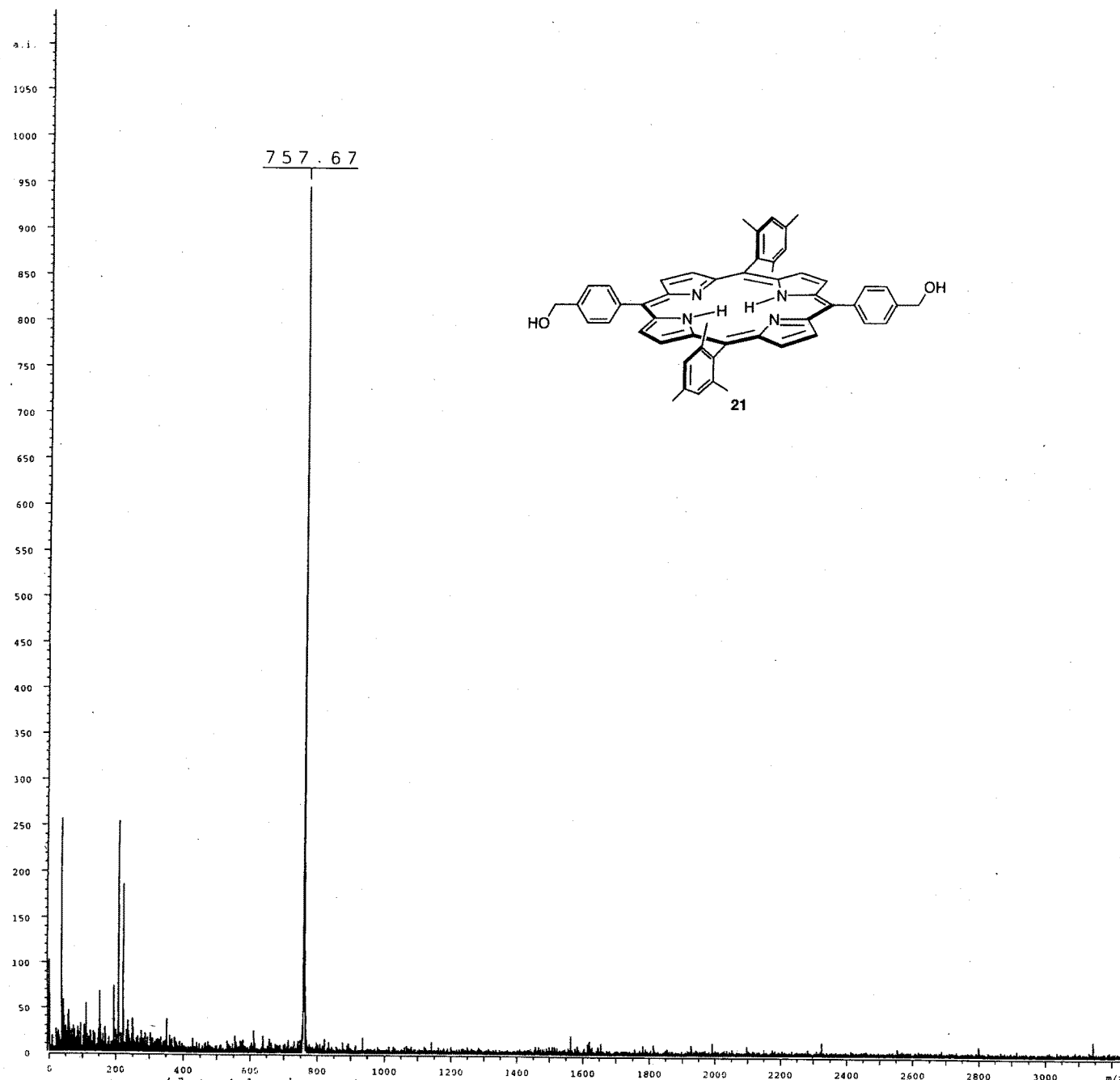
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INSTRUM TOP
OpId      N. Srinivasan
SMPNAM    020426
AQ_DATE   Thu Apr 11 16:24:04 2002
PATH      /data/chemistry/LINDSEY/MALYNOSKY
POLARI    FOS
AQOP_m    Reflector
TD        40000
NoSHOTS   16
SMONUM    0
SMOPTS1   0
SMOPTS2   0
SMOPTS3   0
DW         1.00 [ns]
DELAY     0 [ns]
U1a1      20.00 [kV]
U1a2      18.70 [kV]
Uref1     0.00 [kV]
U1a3      7.50 [kV]
U1a4      10.00 [kV]
RefPull   0.00 [kV]
UdetL     1.50 [kV]
UdetR     0.00 [kV]
Udef1     2.00 [kV]
REPHZ     1.00 [Hz]
ATTEN     31.0
ML1       2069529.231
ML2       333.982
ML3       0.000
HITURBO   no
GDEON     yes
CODELY    short
DEFLON    no
RLNSEND   no
LINSEND   no
UISZEND   no
OPCAL1    510.84
DPHASS    700.00 [Da]
RBNDVAL   0.33
LBNDVAL   0.28
ISZBNDV   0.91
CMT1      por diester dimesityl
CMT2      attn = 31, shot = 16

```

/data/chemistry/LINDSEY/MALYNOSKY/020426/'Sref/pdata/1 tof Thu Apr 11 16:24:25 2002



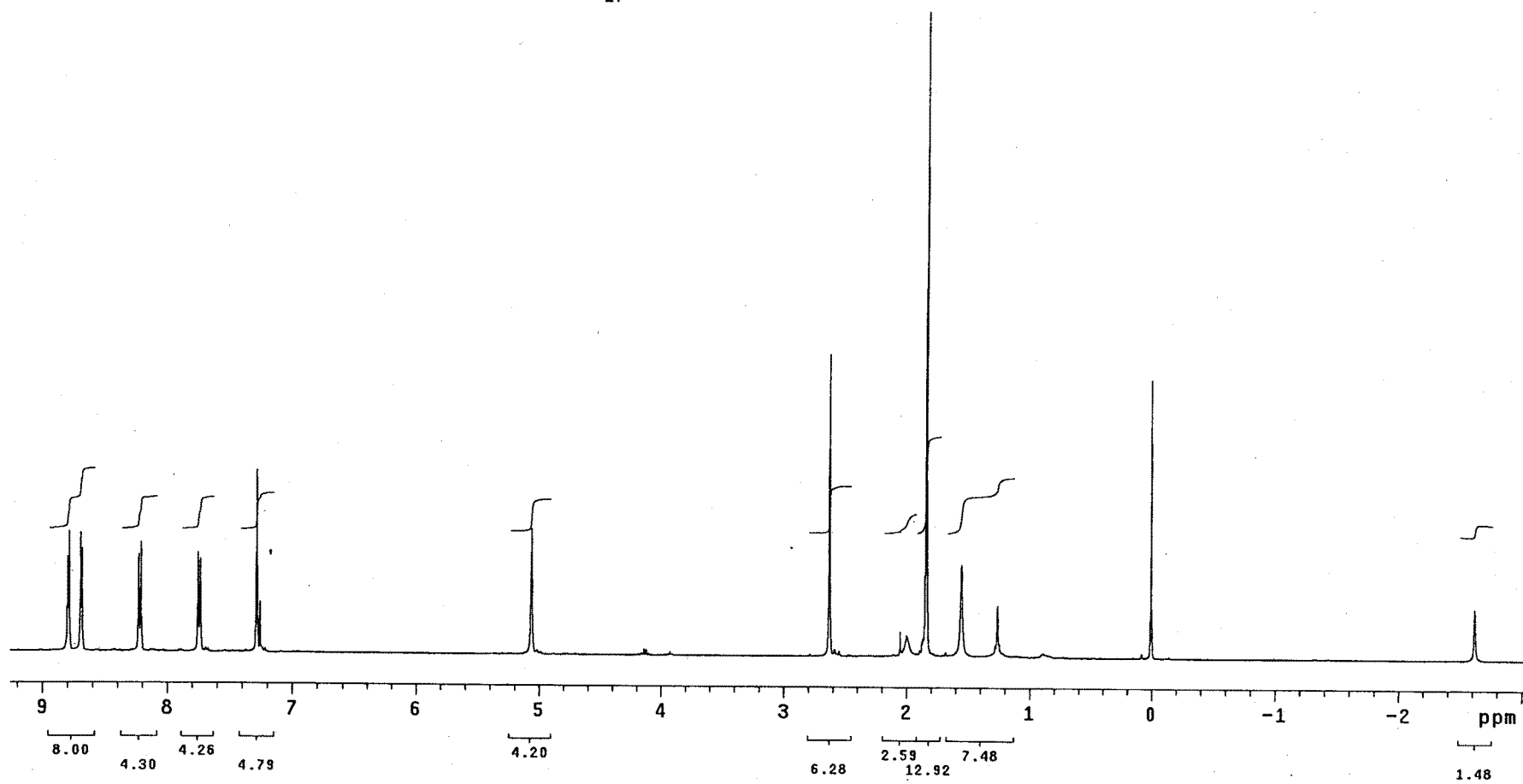
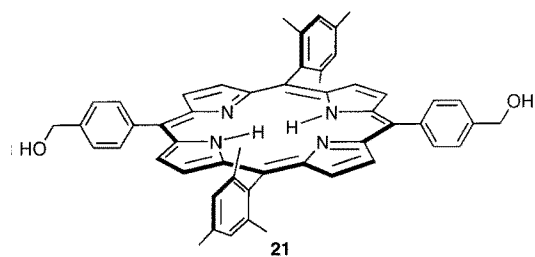


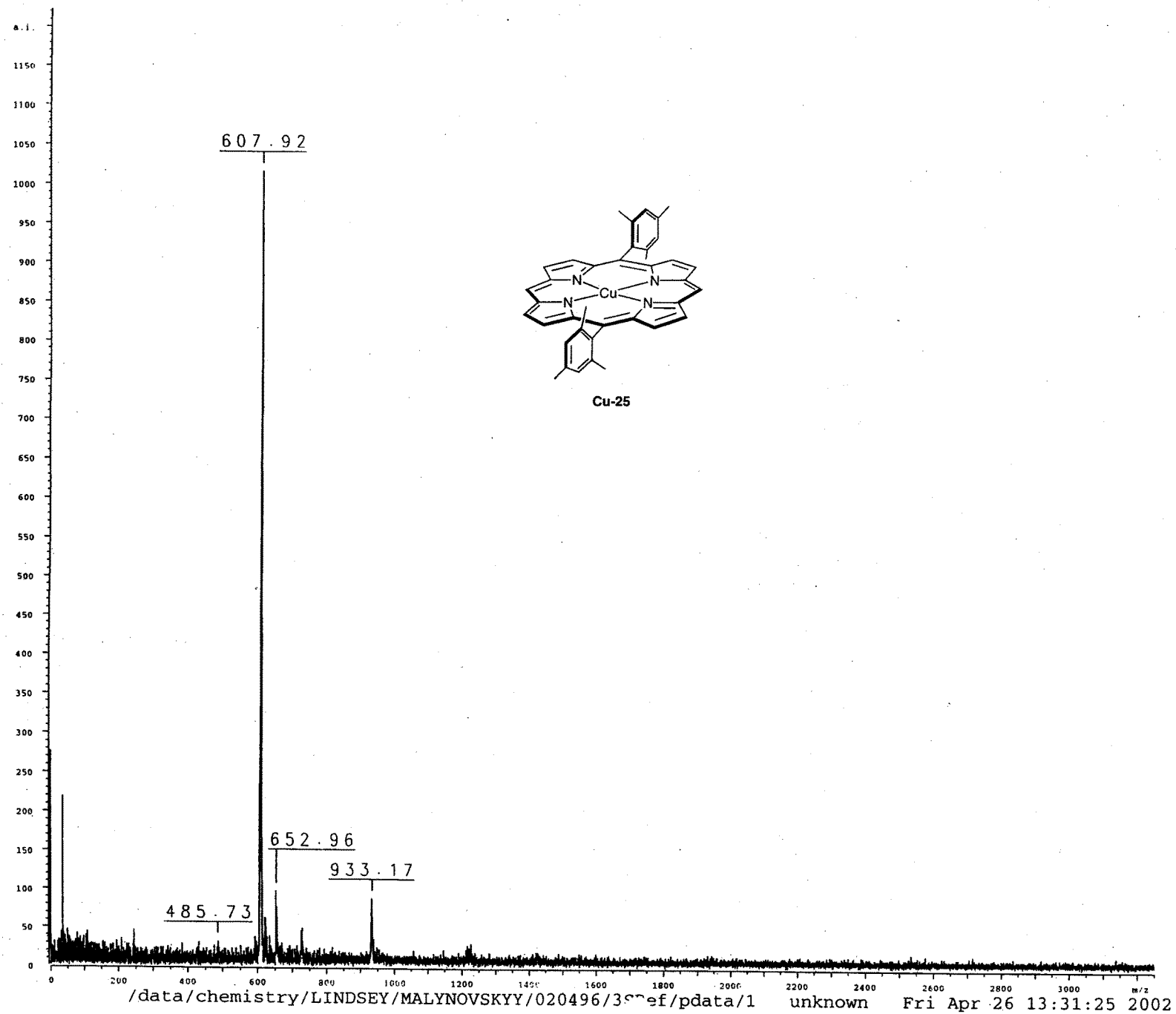
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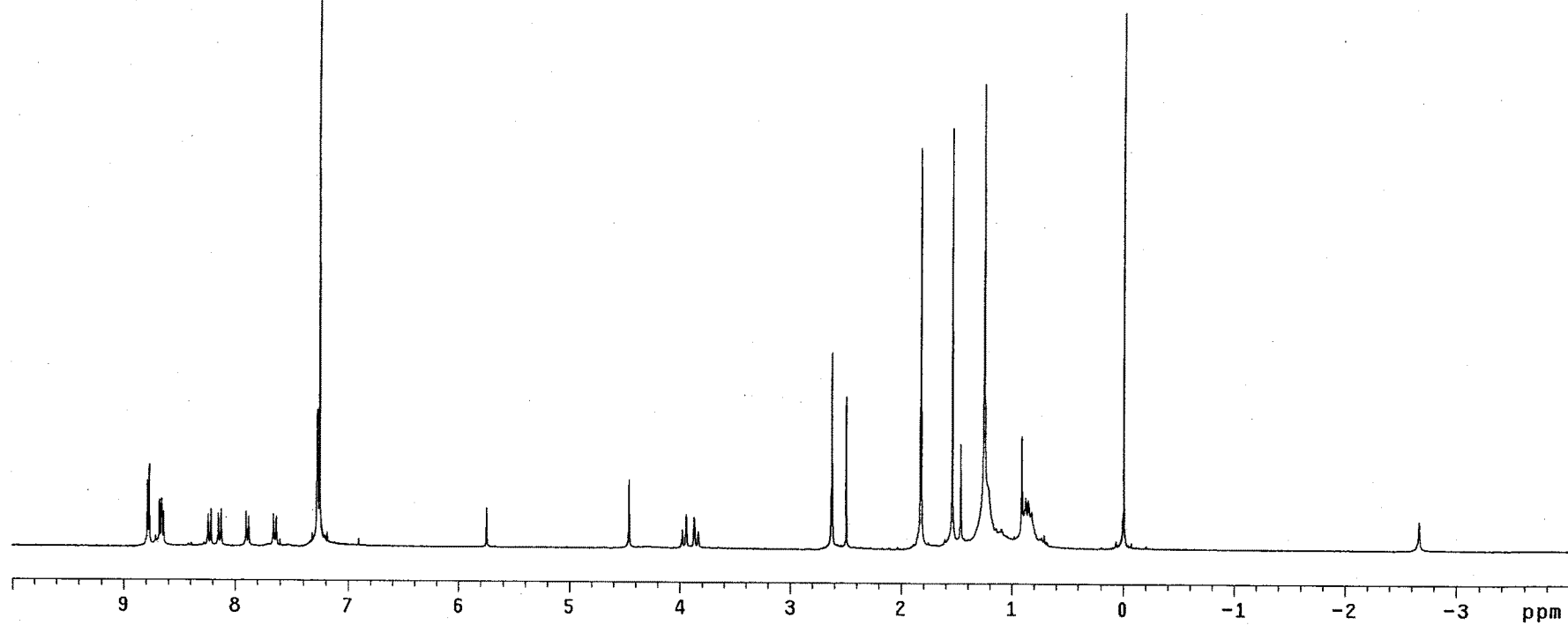
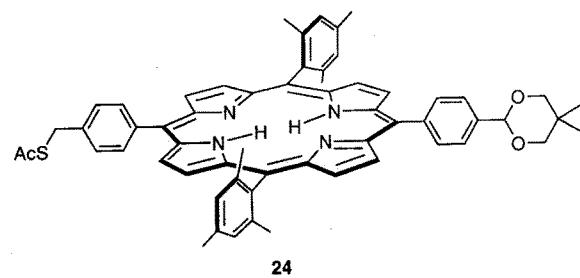
INSTRUM TOF
OpId N. Srinivasan
SMPNAM 020433
AQ_DATE Fri Apr 12 15:36:00 2002
PATH /data/chemistry/LINDSEY/MALYNOVSKYY
POLARI POS
AQOP_m Reflector
TD 40000
NoSHOTS 14
SNOUUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 0 [ns]
Uis1 20.00 [kV]
Uis2 18.70 [kV]
Uref1 0.00 [kV]
Uilens 7.50 [kV]
Uhimass 10.00 [kV]
RefFull1 0.00 [kV]
UdetL 1.50 [kV]
UdetR 0.00 [kV]
Udef1 2.00 [kV]
REPHZ 1.00 [Hz]
ATTEN 32.0
ML1 2069529.231
ML2 333.982
ML3 0.000
HITURBO no
GDEON yes
GDEDLY short
DEFLON no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 510.84
DPMAS 700.00 [Da]
RBNDVAL 0.33
LBNDVAL 0.28
IS2BNDV 0.91
CMT1 por diol dimesityl
CMT2 shots = 14, attn = 32

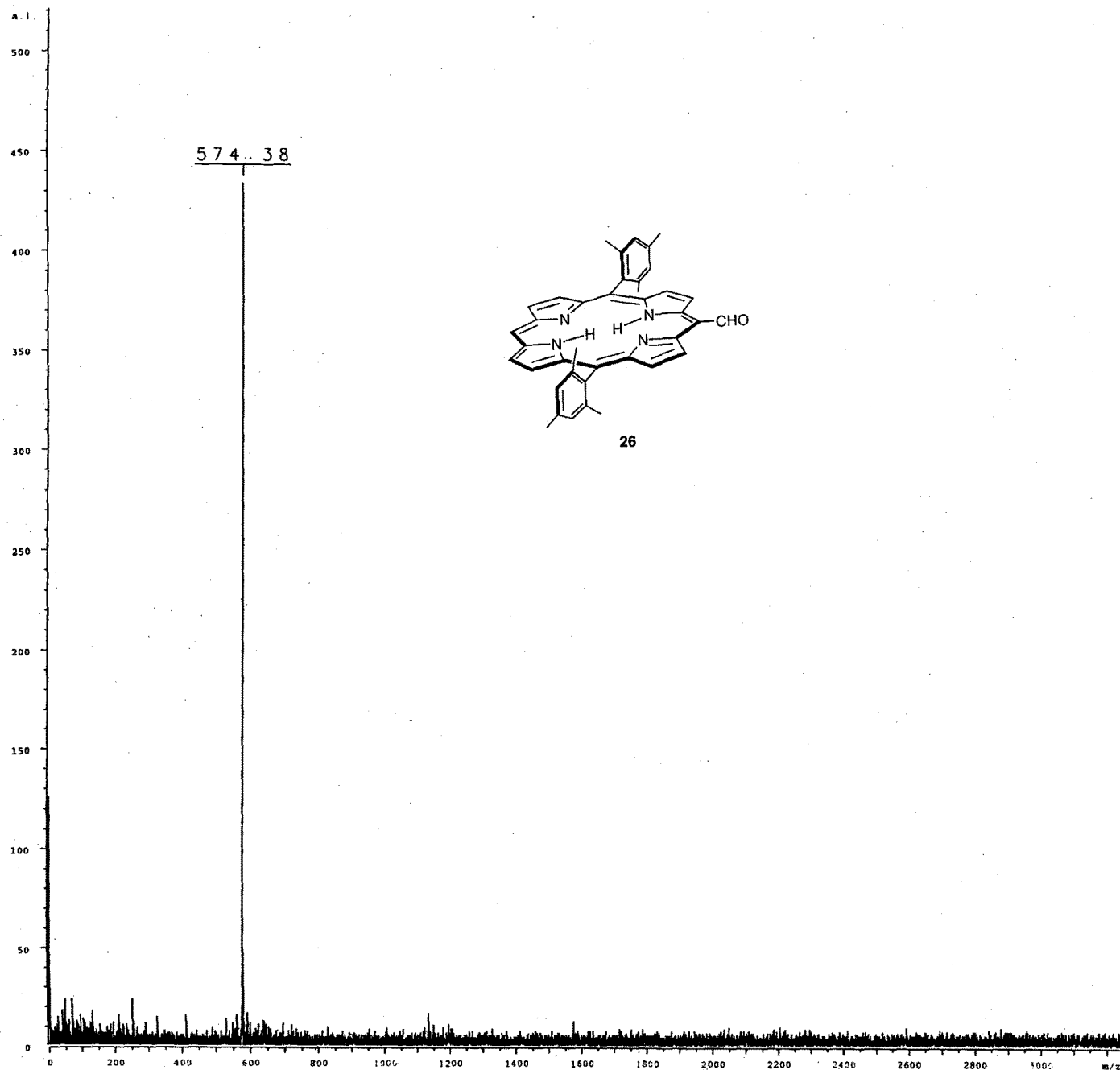
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/data/chemistry/LINDSEY/MALYNOVSKYY/020433/1SRef/pdata/1 tof Fri Apr 12 15:36:23 2002







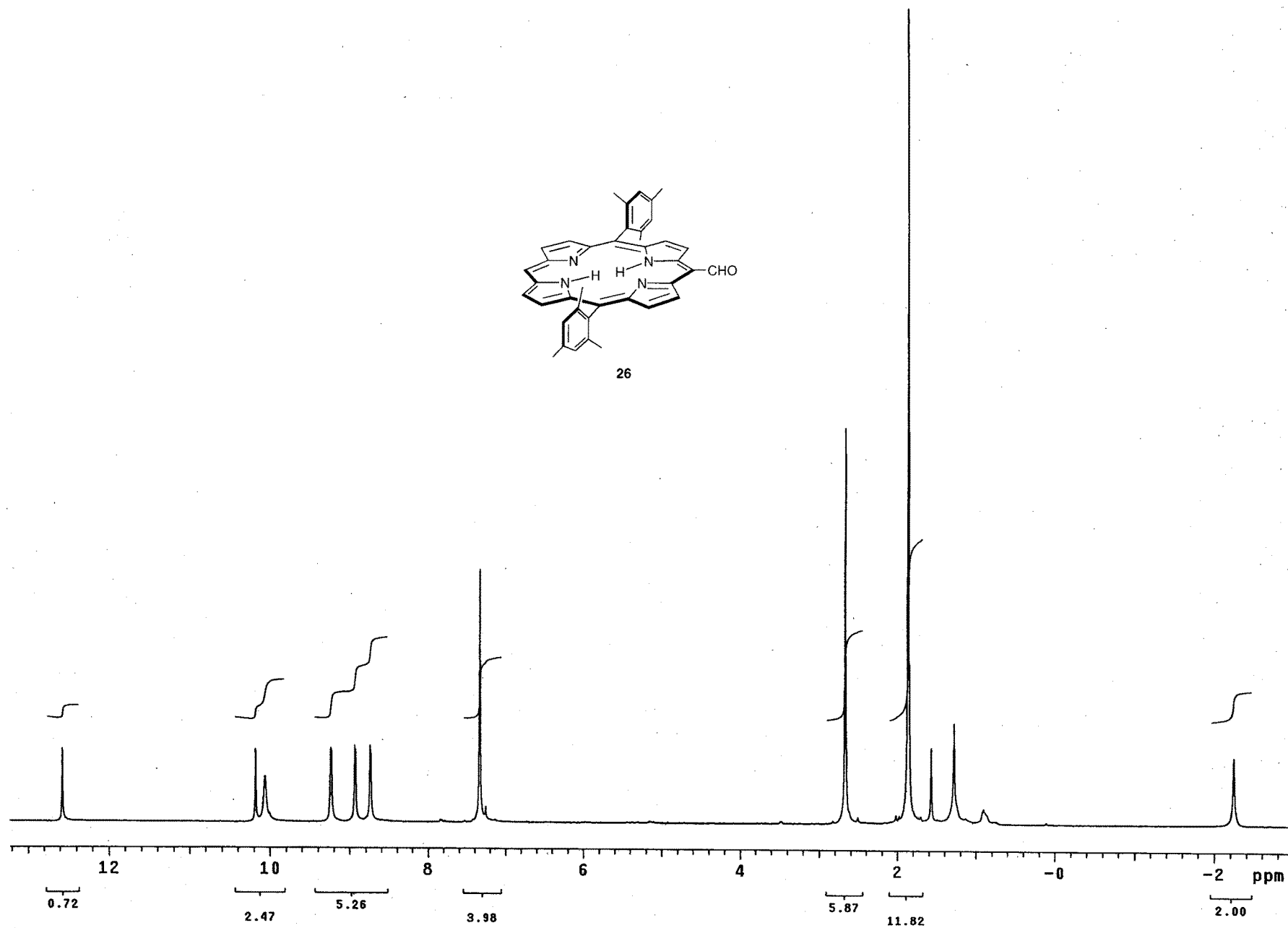
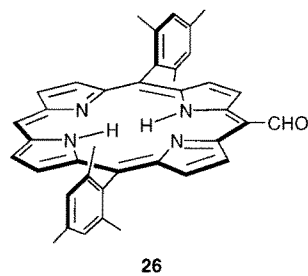


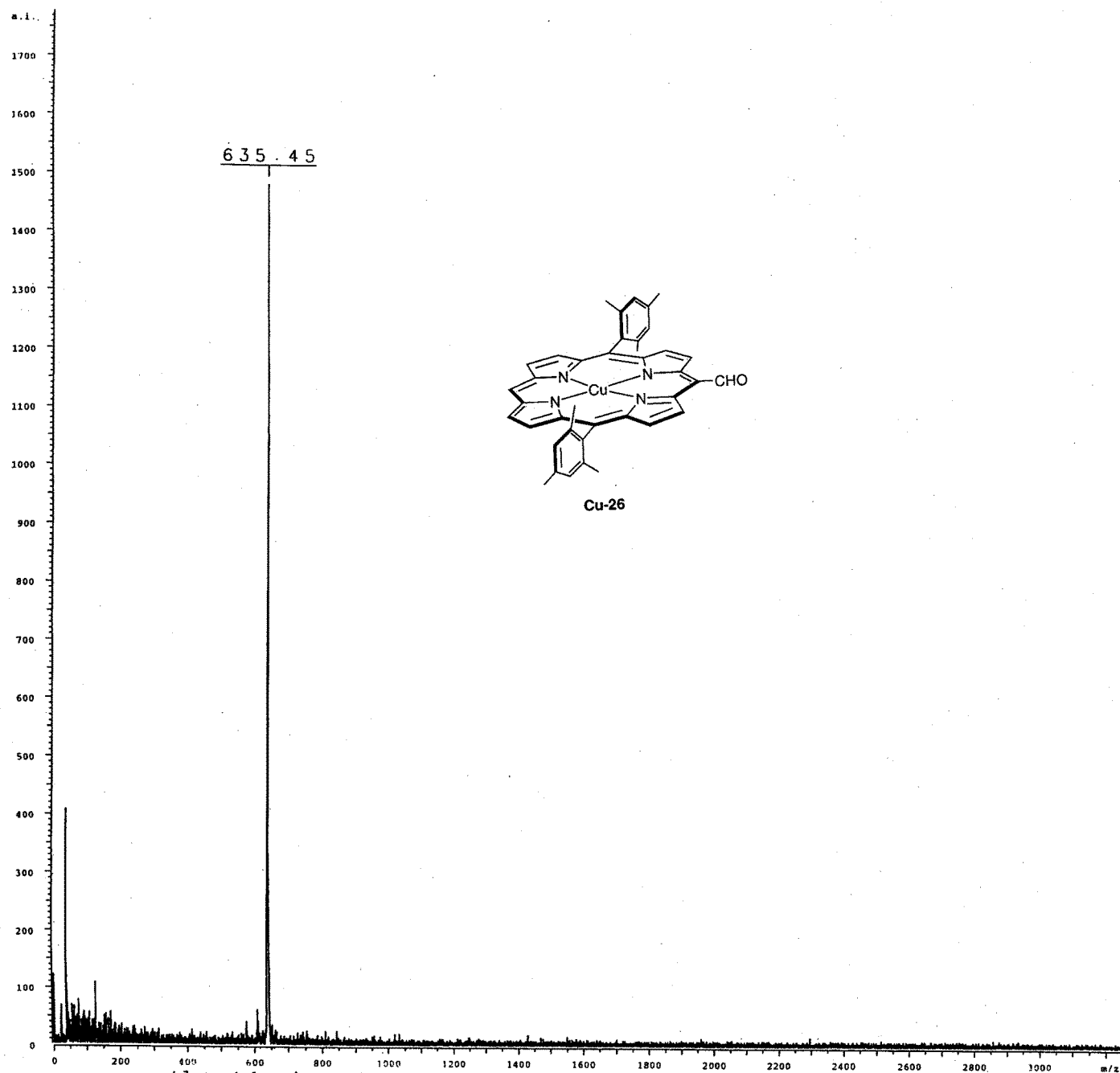
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INSTRUM TOP
OpId      N. Srinivasan
SMPNAM    020524
AQ_DATE   Fri May 3 15:18:45 2002
PATH      /data/chemistry/LINDSEY/MALYNOVSKYY
POLARI    POS
AQOP_m    Reflector
TD         40000
NoSHOTS   16
SNOPTM    0
SNOPTS1   0
SNOPTS2   0
SNOPTS3   0
DM         1.00 [ns]
DELAY     0 [ns]
Uis1      20.00 [kV]
Uis2      18.70 [kV]
Uref1     0.00 [kV]
Ulen5     7.50 [kV]
Uhlmas5   10.00 [kV]
RefFull   0.00 [kV]
UdetL     1.50 [kV]
UdetR     0.00 [kV]
Udef1     2.00 [kV]
REPHZ     1.00 [Hz]
ATTEN     32.0
ML1        2071938.026
ML2        333.982
ML3         0.000
HITURBO   no
GDECON    yes
GDEELY    short
DEFLON    no
RLASBND   no
LLASBND   no
UIS2BND   no
DPCAL1    510.84
DPMAS5    700.00 [Da]
RENDVAL   0.33
LENDVAL   0.28
IS2BNDV   0.91
CMT1      formulation after column
CMT2      shot., 16; att., 32

```

/data/chemistry/LINDSEY/MALYNOVSKYY/020524/^SRef/pdata/1 tof Fri May 3 15:19:17 2002



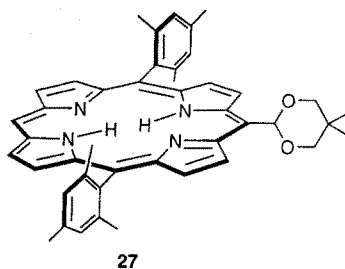
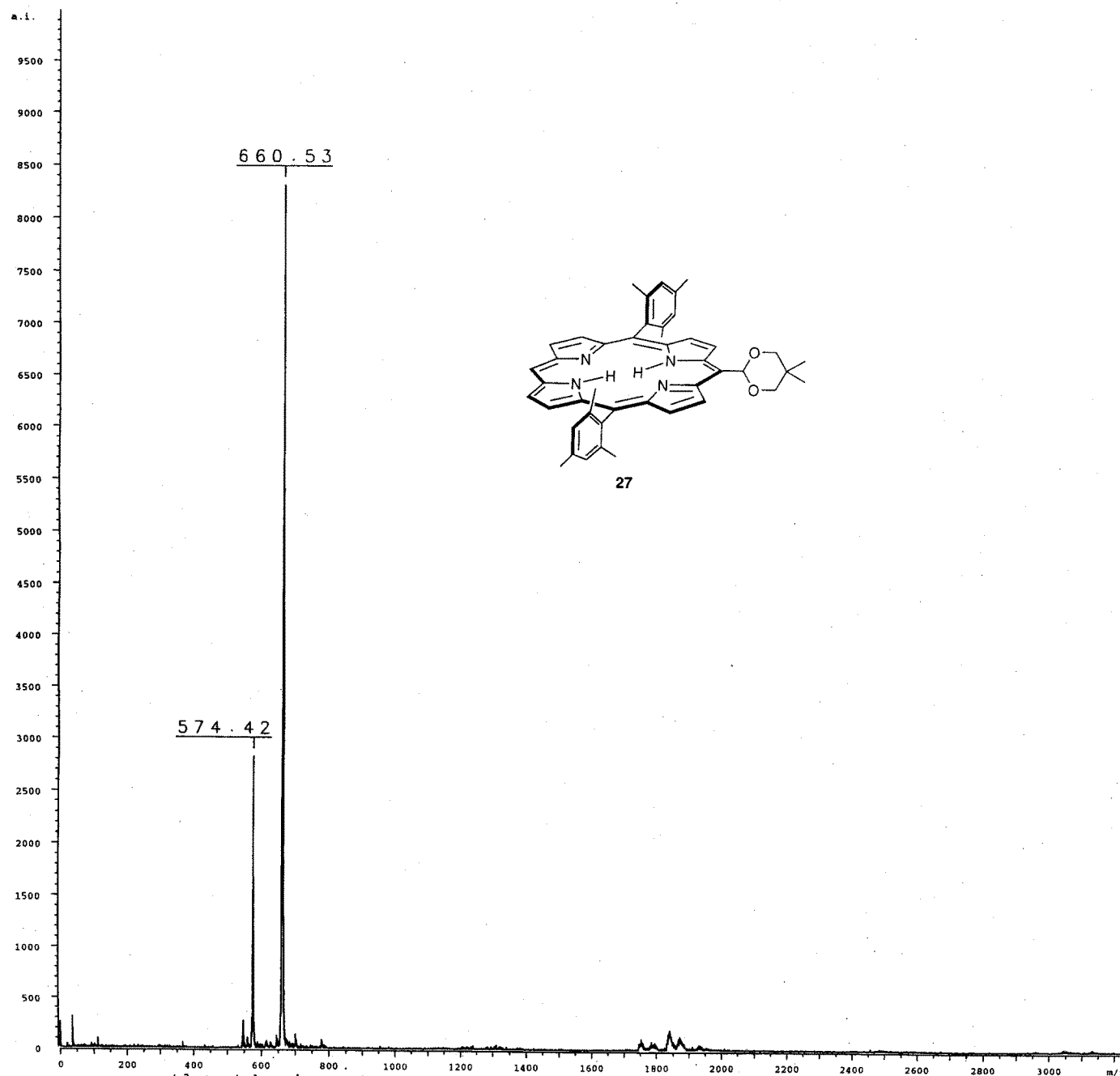


```

INSTRUM TOP
OpId N. Srinivasan
SMPNAM 020511
Acq_DATE Tue Apr 30 15:14:38 2002
PATH /data/chemistry/LINDSEY/MALYNOVSKYY
POLARI POS
AQOP_m Reflector
TO 40000
NoSHOTS 16
SNOPT1 0
SNOPT2 0
SNOPT3 0
DW 1.00 [ns]
DELAY 0 [ns]
Uis1 20.00 [kV]
Uis2 18.70 [kV]
Uref1 0.00 [kV]
Uisns 7.50 [kV]
Uisns 10.00 [kV]
RefFull 0.00 [kV]
UdetL 1.50 [kV]
UdetR 0.00 [kV]
Udef1 2.00 [kV]
REPHZ 1.00 [Hz]
ATTEN 31.0
ML1 2071938.026
ML2 333.982
ML3 0.000
HITURBO no
GDEON yes
GDEPLY short
DEFLON no
RLNSND no
LLNSND no
UIS2BND no
DPCAL1 510.84
DPMAS 700.00 [Da]
RENDVAL 0.33
LENDVAL 0.28
IS2ENDV 0.51
CMT1 formylation f7 to f14
CMT2 shot., 16; att., 31

```

/data/chemistry/LINDSEY/MALYNOVSKYY/020511/'SRef/pdata/1 tof Tue Apr 30 15:15:15 2002

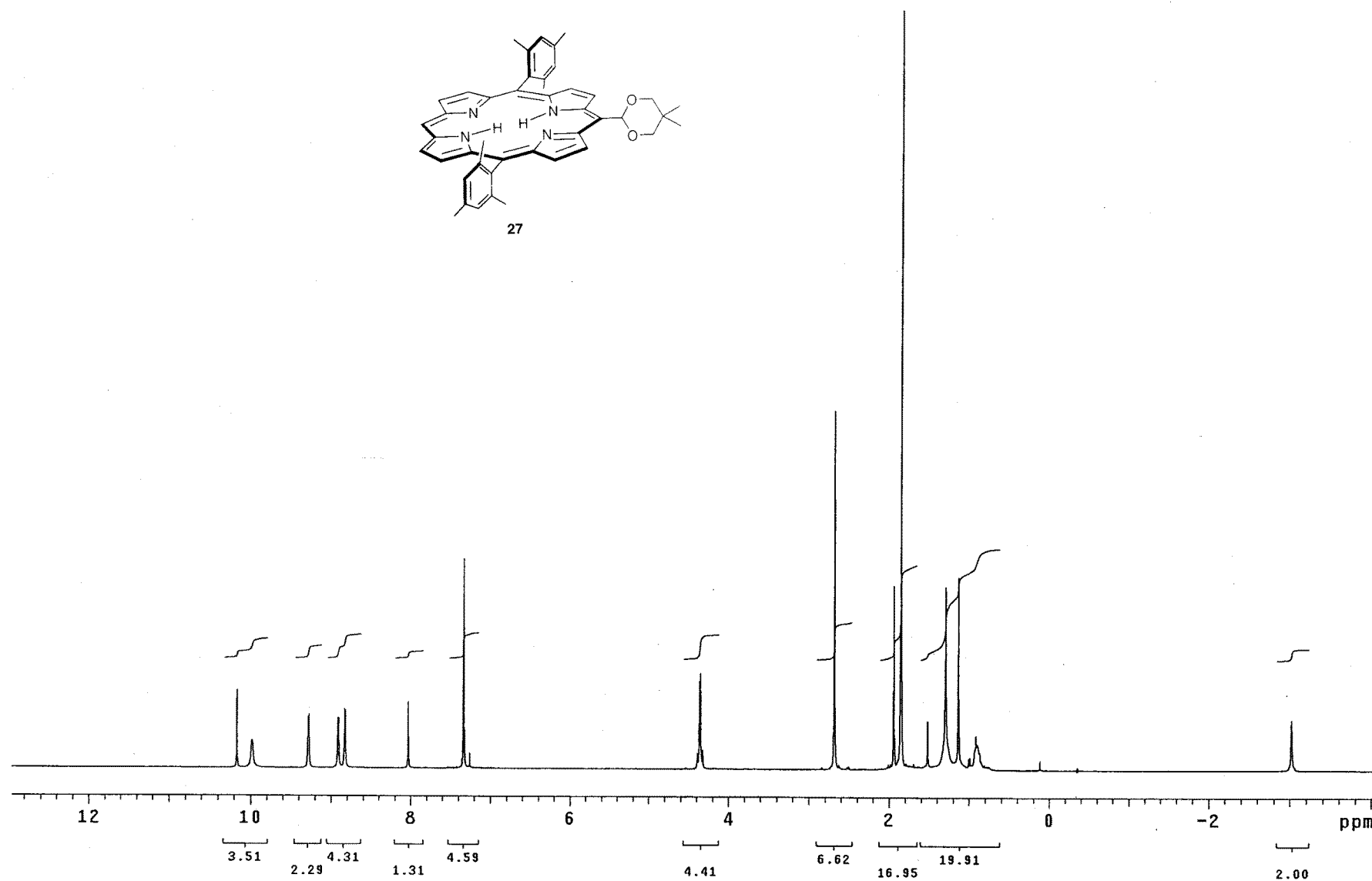
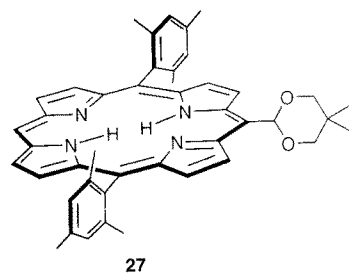


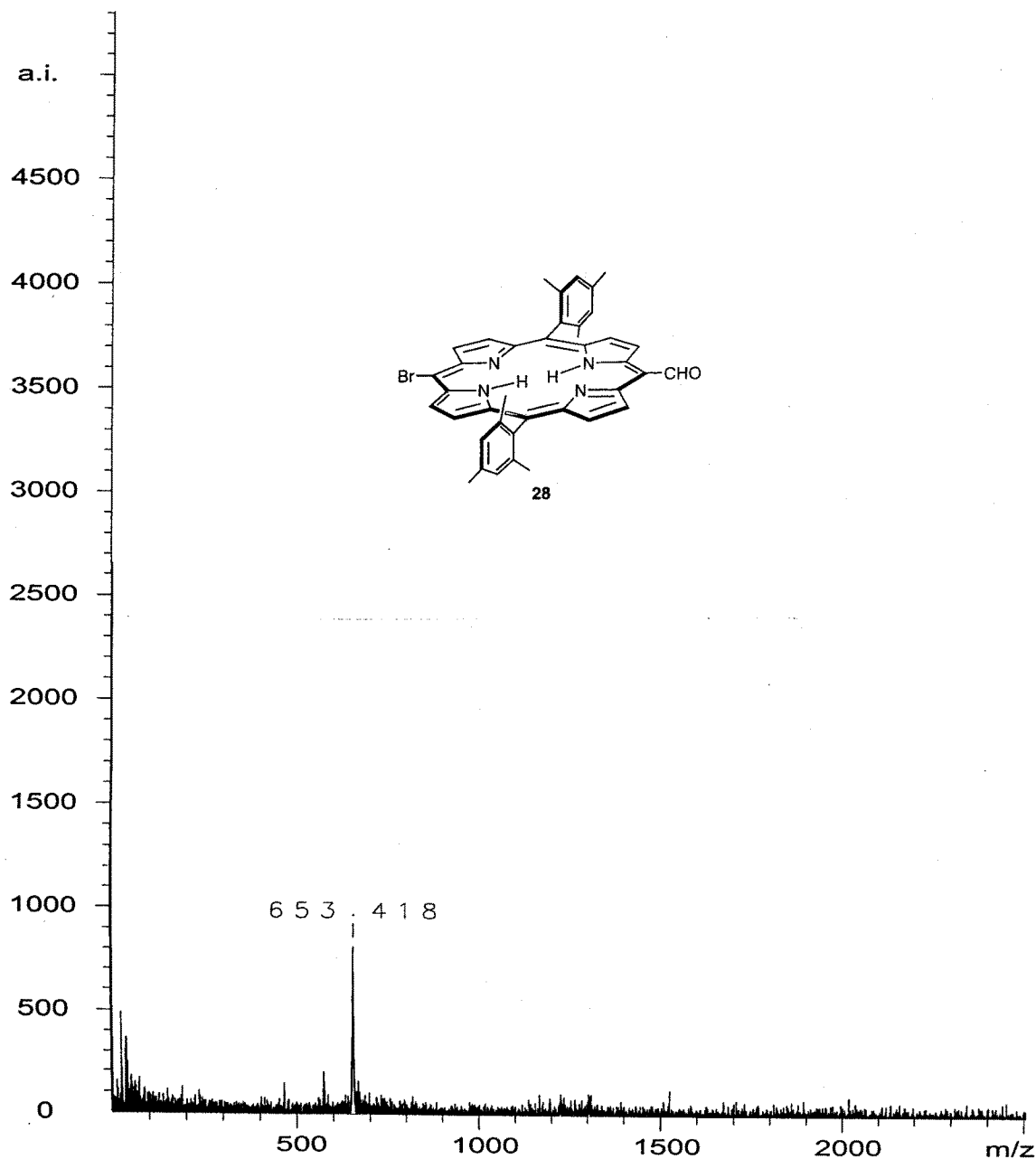
```

INSTRUM TOF
OpId N. Srinivasan
SMPNAM 020556
AQ DATE Tue May 14 13:24:17 2002
PATH /data/chemistry/LINDSEY/MALYNOVSKYY
POLARI POS
AQOP_m Reflector
TD 40000
NoSHOTS 49
SMONUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 0 [ns]
Uis1 20.00 [kV]
Uis2 18.70 [kV]
Uref1 0.00 [kV]
Ulen1 7.50 [kV]
Ulinmass 10.00 [kV]
RefFull 0.00 [kV]
UdetL 1.50 [kV]
UdetR 0.00 [kV]
Udef1 2.00 [kV]
REPHZ 1.00 [Hz]
ATTEN 31.0
ML1 2067125.193
ML2 333.982
ML3 0.000
HITURBO no
GDEON yes
GDEDLV short
DEFLON no
RLS2END no
LINS2END no
UIS2END no
DPCALL 510.84
DPHASS 700.00 [Da]
RENDVAL 0.33
LENDVAL 0.28
IS2ENDV 0.91
CMT1 after 2h30
CMT2

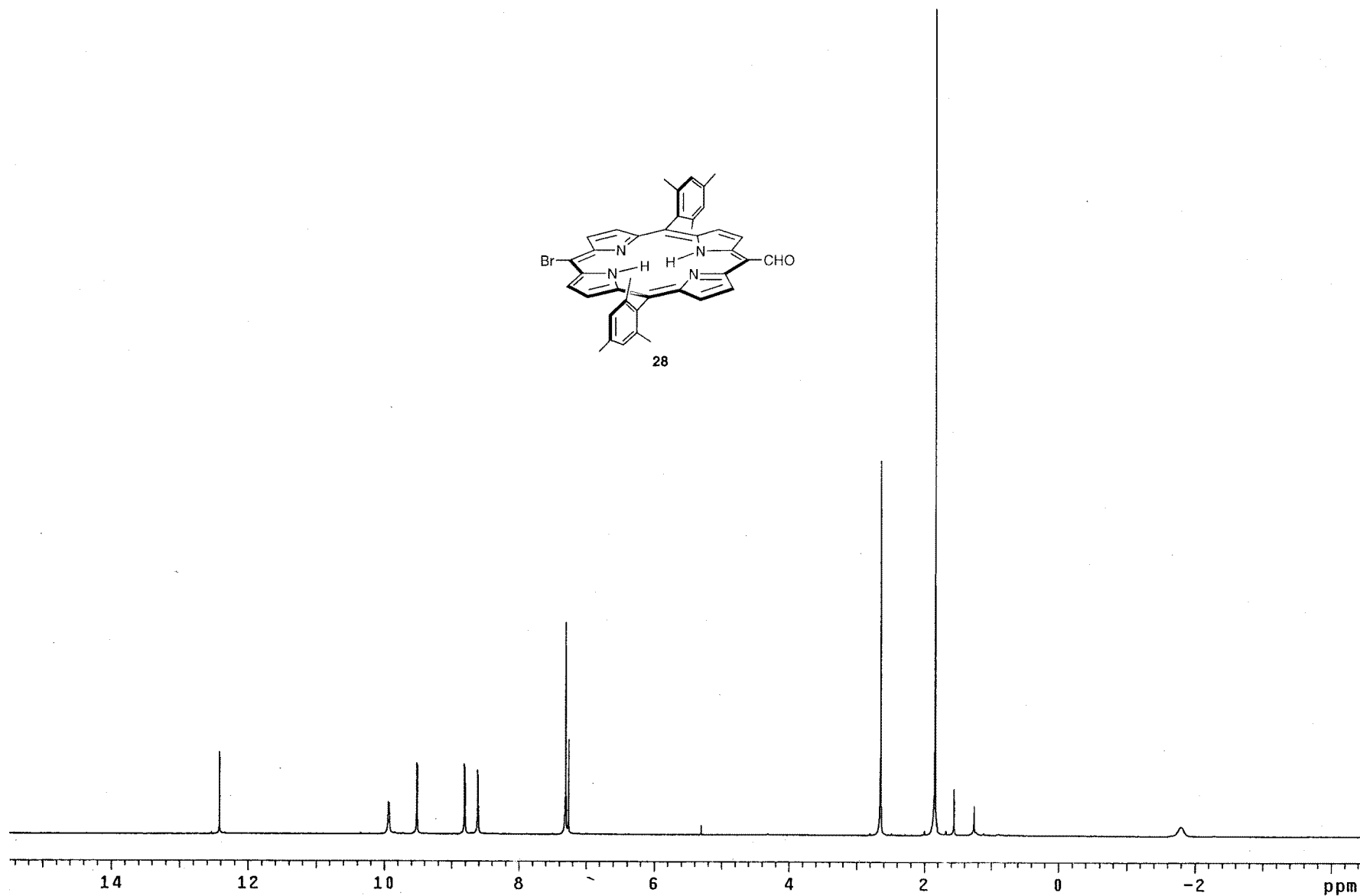
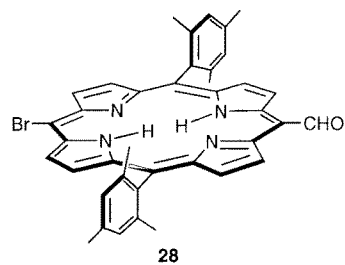
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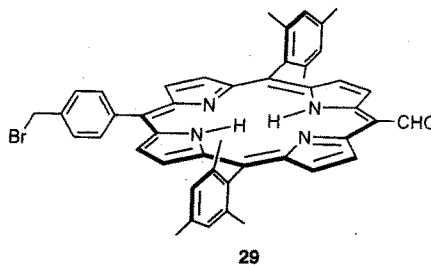
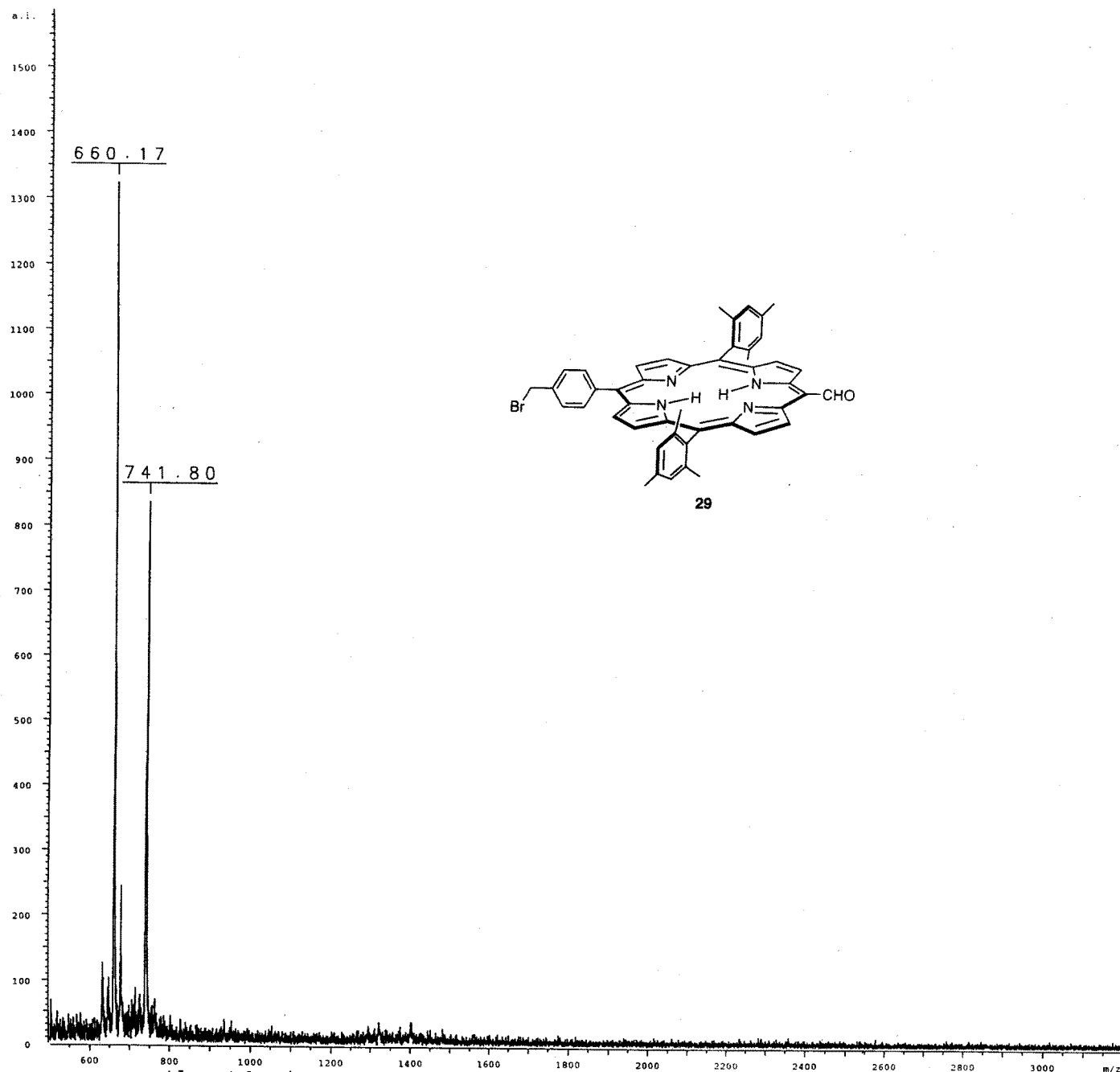
/data/chemistry/LINDSEY/MALYNOVSKYY/020556/2SRef/pdata/1 tof Tue May 14 13:24:37 2002





INSTRUM OMNIFLEX
 OpId tof
 SMPNAM CC-Br-CHO
 AQ_DATE 2004-01-16 09:04:32
 PATH D:\data\Chemistry\Lindsey\Patchanita
 POLARI POS
 AQOP_m Linear
 TD 78614
 NoSHOTS 60
 SMONUM 0
 SMOPTS1 0
 SMOPTS2 0
 SMOPTS3 0
 DW 1.00 [ns]
 DELAY 252 [ns]
 Uis1 19.00 [kV]
 Uis2 13.15 [kV]
 Urefl 20.00 [kV]
 Ulens 9.40 [kV]
 Uhimass 0.00 [kV]
 RefFull 0.00 [kV]
 UdetL 1.65 [kV]
 UdetR 1.70 [kV]
 Udefl 0.00 [kV]
 REPHZ 3.00 [Hz]
 ATTEN 41.0
 ML1 789620.245
 ML2 252.162
 ML3 0.000
 HITURBO no
 GDEON yes
 GDEDLY short
 DEFLON no
 RLNSBND no
 LLNSBND no
 UIS2BND no
 DPCAL1 0.38
 DPMASS 500.00 [Da]
 RBNDVAL 0.00
 LBNDVAL 0.00
 IS2BNDV 0.00
 CMT1 FLEXControl generated XMASS data
 CMT2 (c) 2000 Bruker Daltonics





```

INSTRUM TOP
OpId N. Srinivasan
SMPNAM 020777
AQ_DATE Mon Jul 1 13:06:20 2002
PATH /data/chemistry/LINDSEY/MALYNOVSKYY
POLARI POS
AQOP_m Reflector
TD 40000
NoSHOTS 25
SMONUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 0 [ns]
Uis1 20.00 [kV]
Uis2 18.70 [kV]
Uref1 0.00 [kV]
Ulen5 7.50 [kV]
Uhimass 10.00 [kV]
RefFull 0.00 [kV]
UdetL 1.50 [kV]
UdetR 0.00 [kV]
Udef1 2.00 [kV]
REPHZ 1.00 [Hz]
ATTEN 10.0
ML1 2067125.193
ML2 331.982
ML3 0.000
HITURBO no
GDEON yes
GDECLY short
DEFLON no
RLNSBND no
LLNSBND no
UIS2BND no
DPCALL 510.84
DPMASS 700.00 [Da]
RENOVAL 0.33
LBNDVAL 0.28
IS2BNDV 0.91
CMT1 pbr3 reaction
CMT2
  
```

/data/chemistry/LINDSEY/MALYNOVSKYY/020777/1stRef/pdata/1 tof Mon Jul 1 13:06:57 2002

