Supporting Information for:

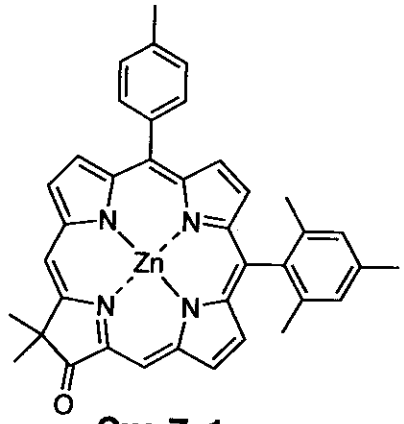
Synthesis and Electronic Properties of Regioisomerically Pure Oxochlorins

Masahiko Taniguchi, Han-Je Kim, Doyoung Ra,

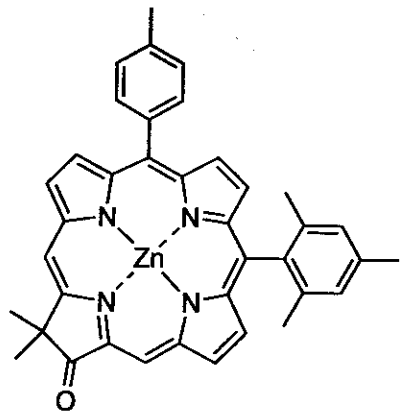
Jennifer K. Schwartz, Christine Kirmaier, Eve Hindin, James R. Diers,

Sreedharan Prathapan, David F. Bocian, Dewey Holten, and Jonathan S. Lindsey

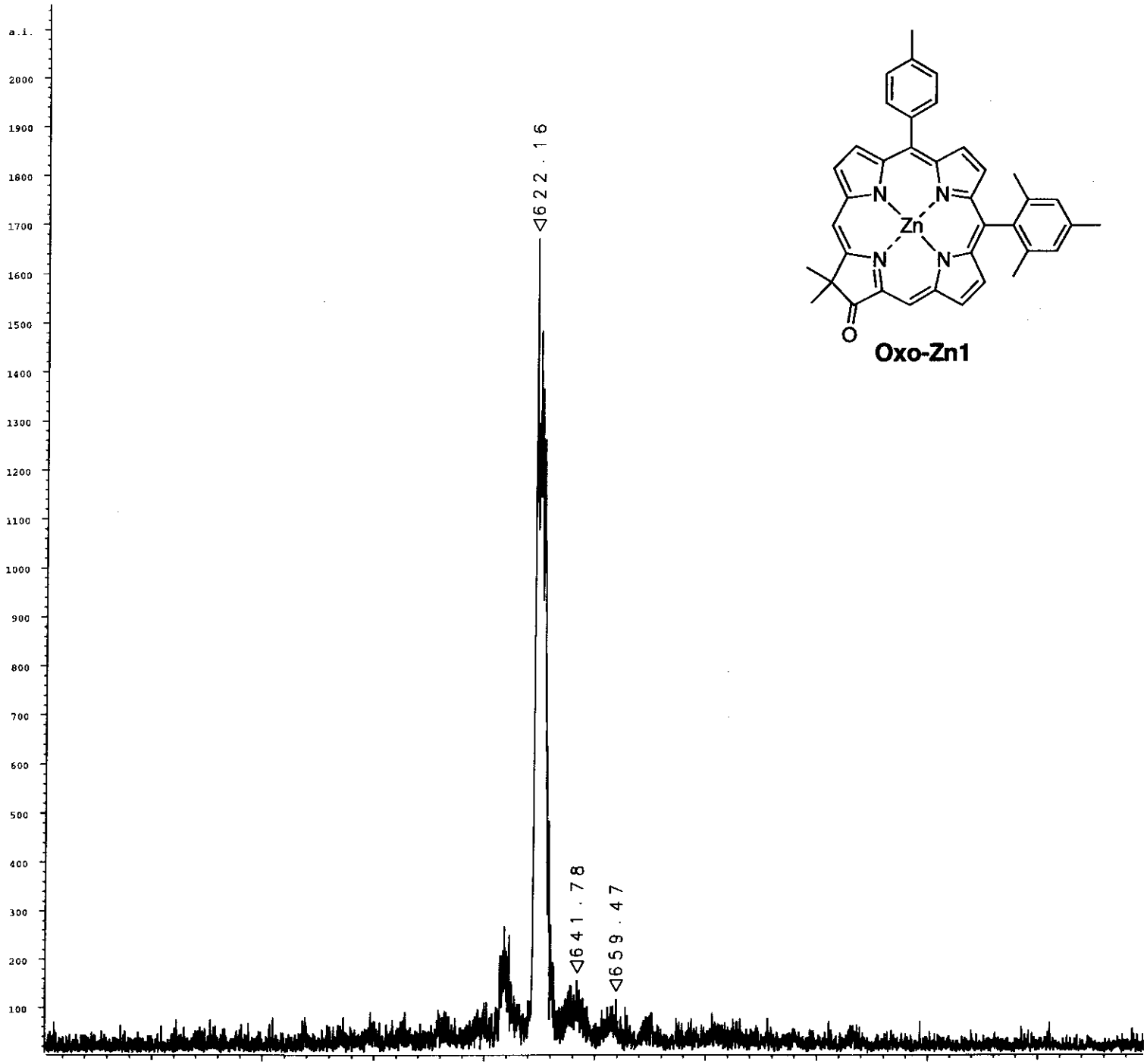
Table of contents:



Oxo-Zn1



Oxo-Zn1



Oxo-Zn1

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SMOPTS2             0
SMOPTS3             0
DW                  1.00  [ns]
DELAY               0 [ns]
Uis1               20.00  [kV]
Uis2               18.50  [kV]
Uref1               0.00  [kV]
Ulens               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              30.0
ML1           2067510.748
ML2               353.368
ML3                 0.000
HITURBO no
GDEON   yes
GDEDLY  short
DEFLON  no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1            510.84
DPMASS            200.00  [Da]
RBNDVAL             0.33
LBNDVAL             0.28
IS2BNDV             0.91
CMT1
CMT2
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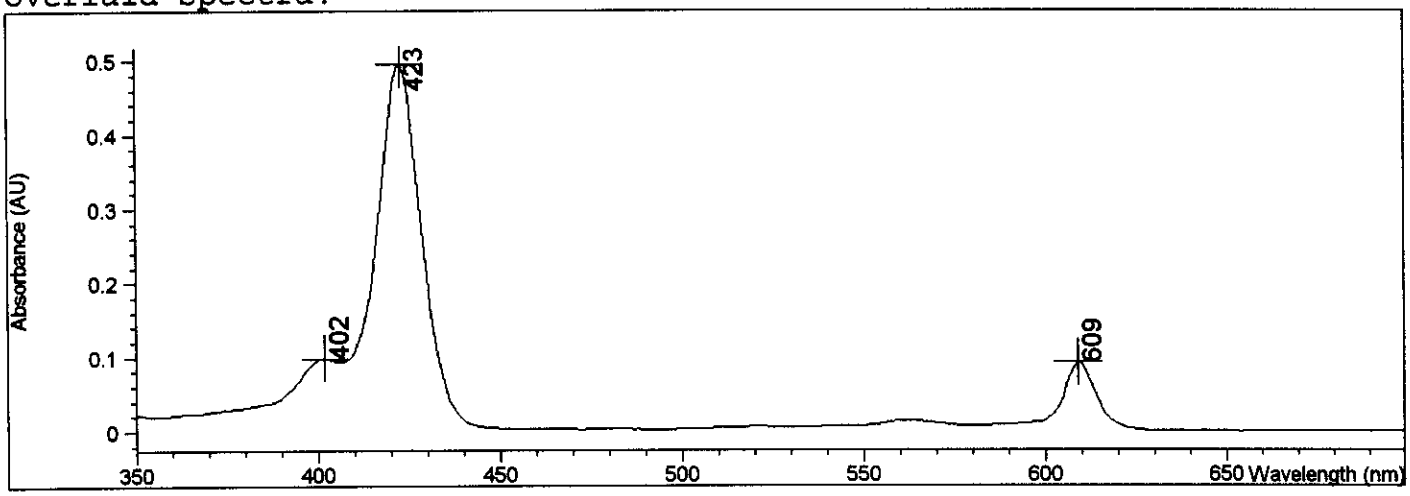

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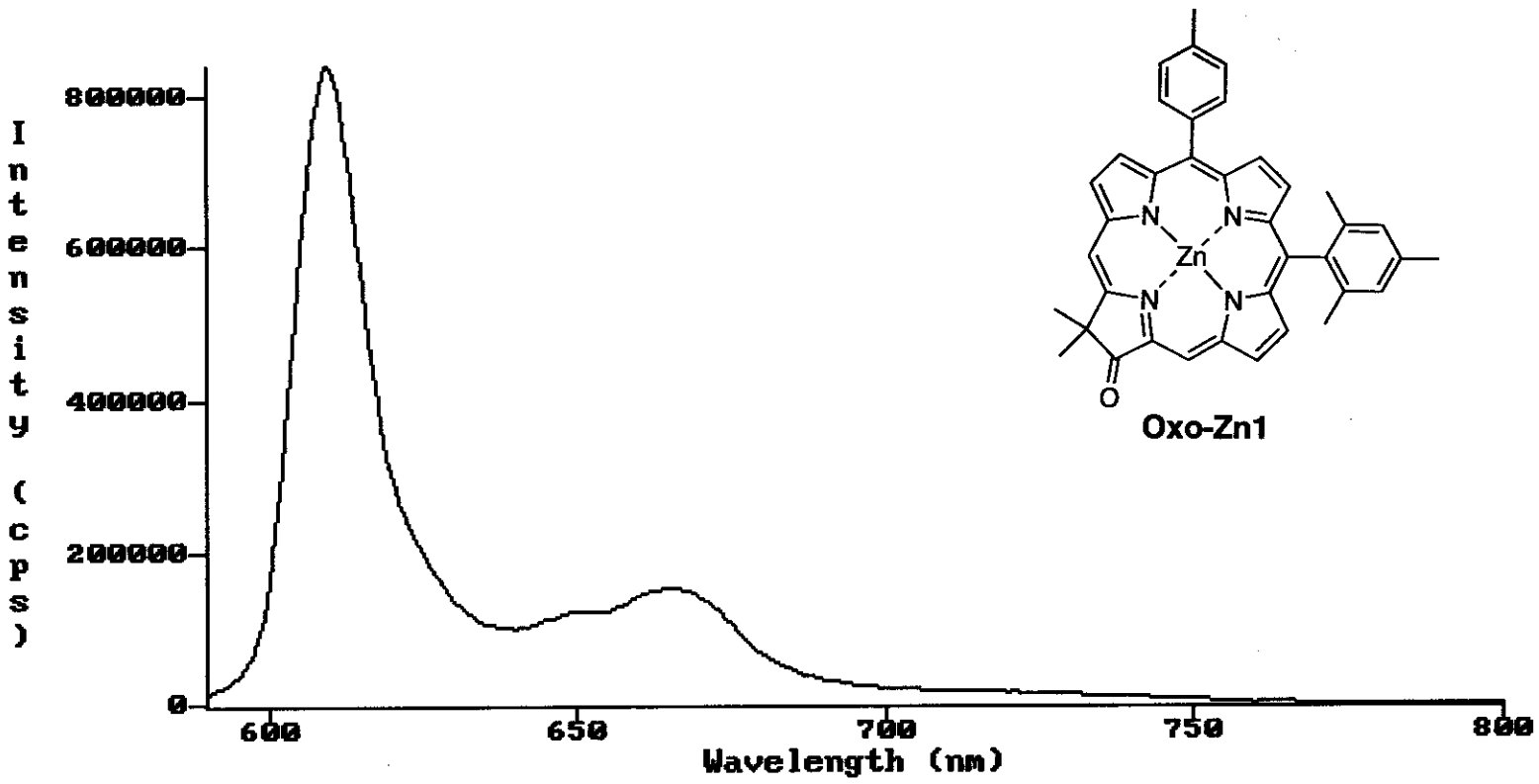
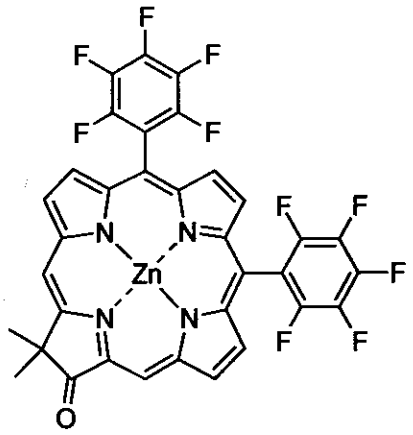
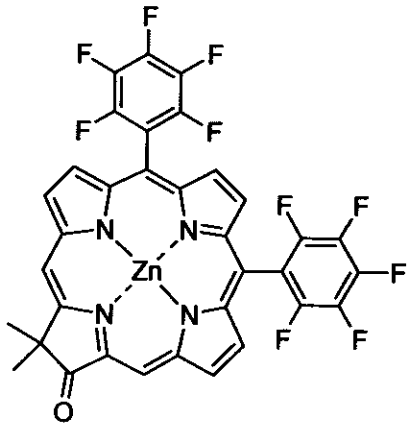


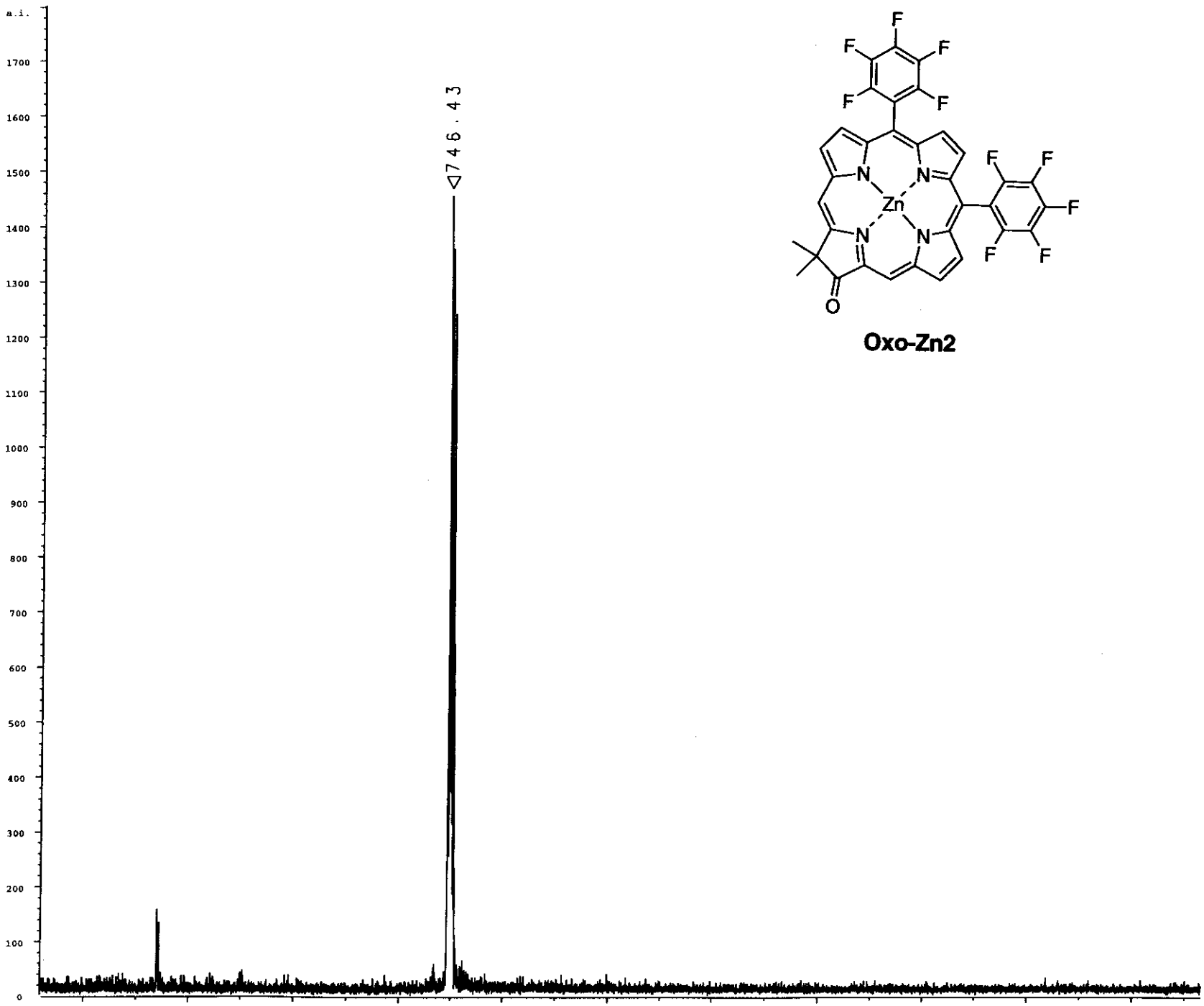
Oxo-Zn1



Oxo-Zn2



Oxo-Zn2


a.i.
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1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
746.43
500
700
900
1100
1300
m/z
/data/chemistry/LINDSEY/PRATHAPAN/015068/1SRef/pdata/1 unknown Tue Apr 10 12:12:43 2001

F
F
F
F
F
N
N
Zn
N
N
F
F
F
F
F
O

Oxo-Zn2

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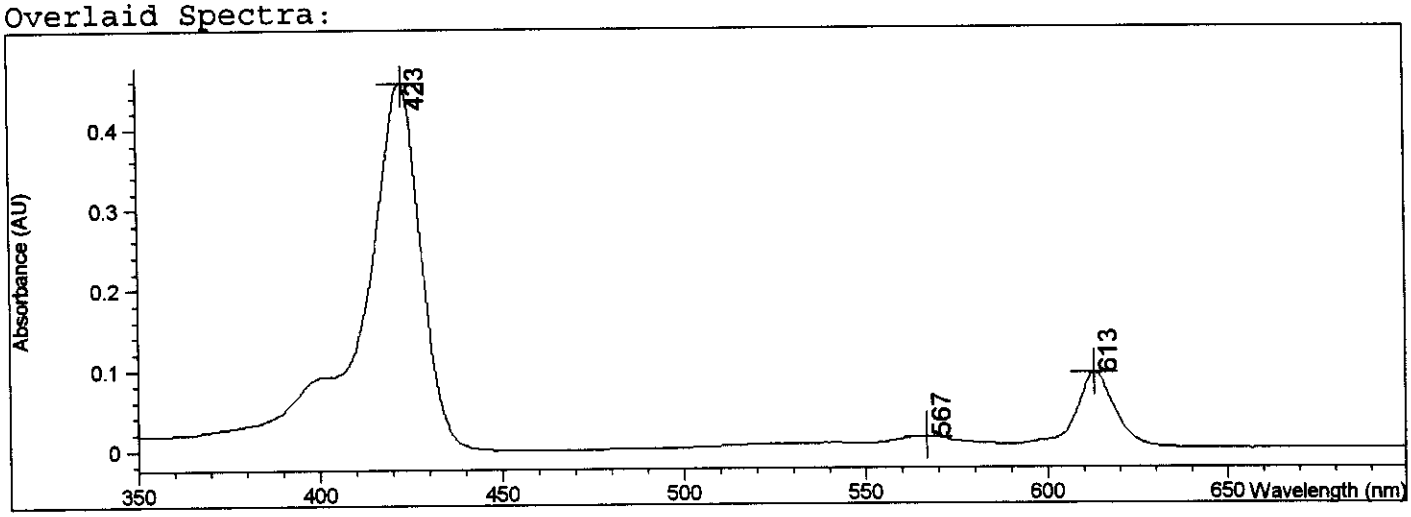

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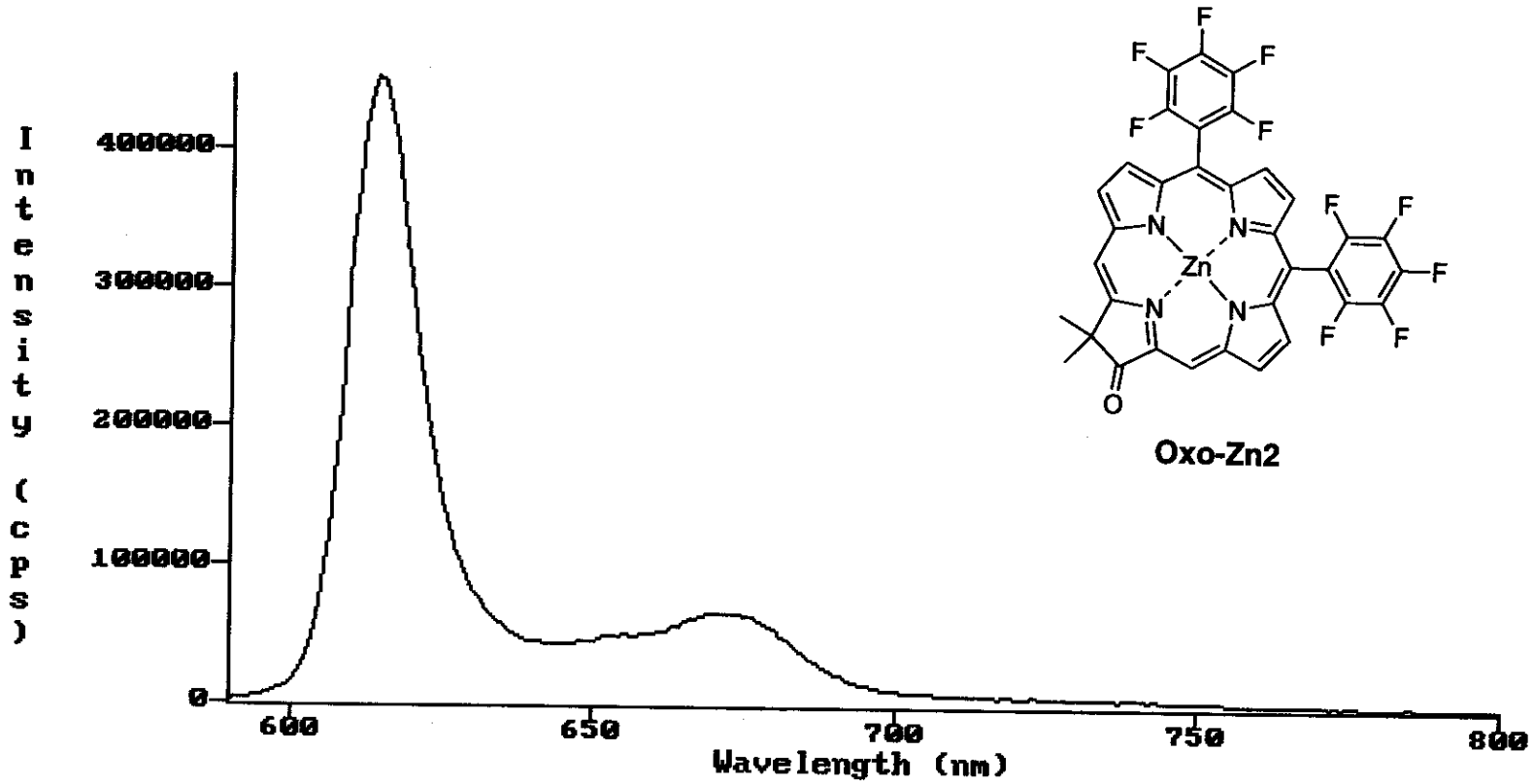
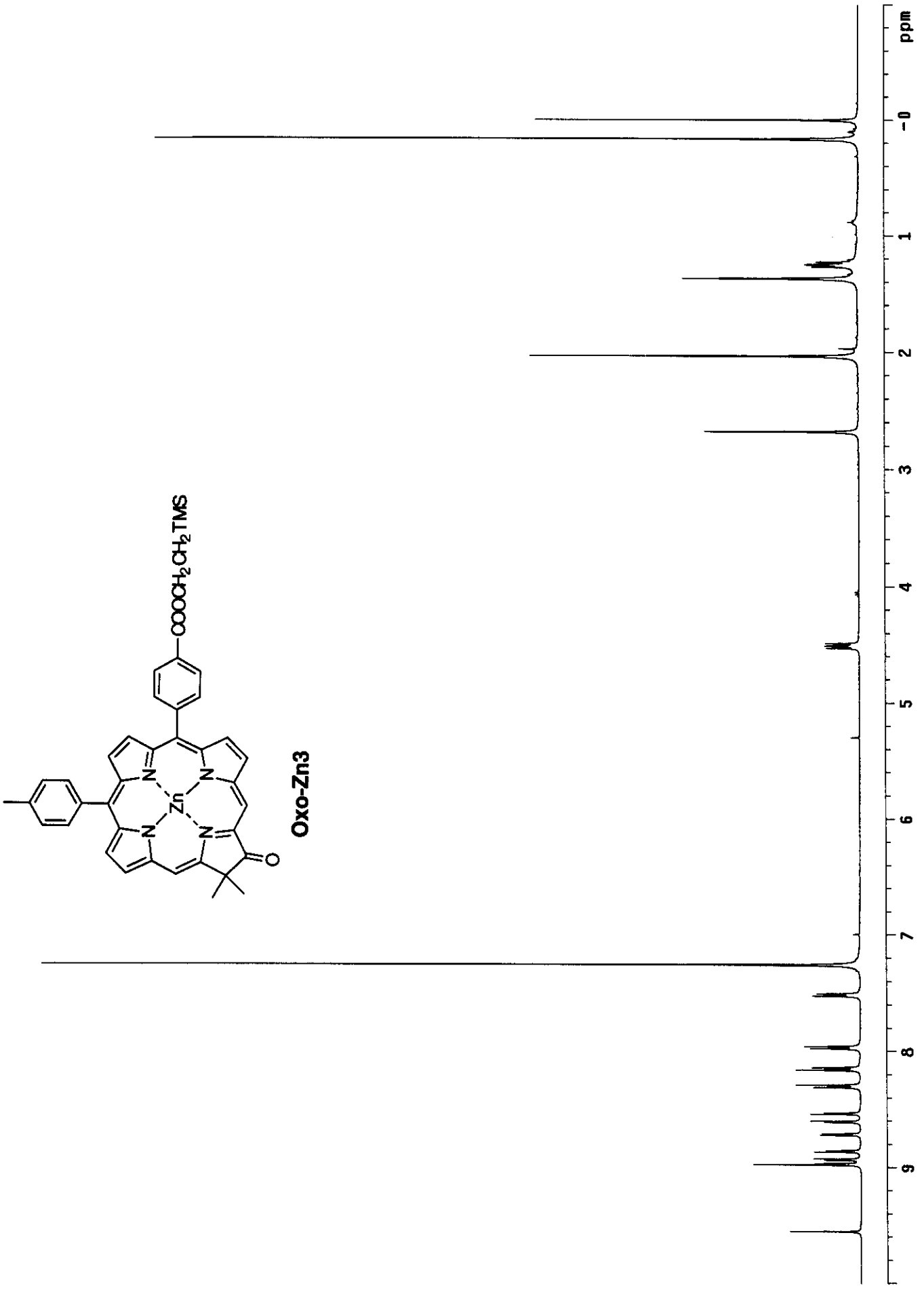
1		567.0	1.4304E-2



Oxo-Zn2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O
Oxo-Zn3
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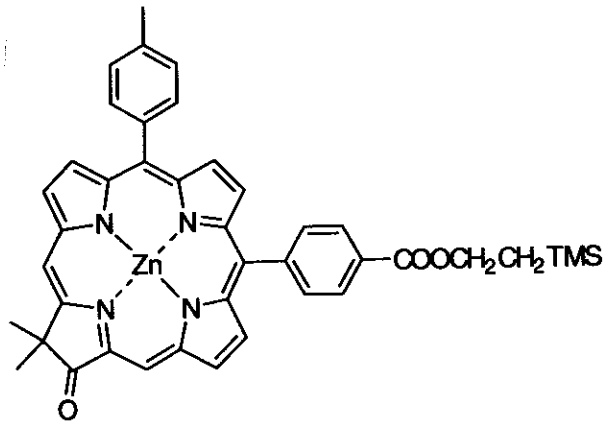
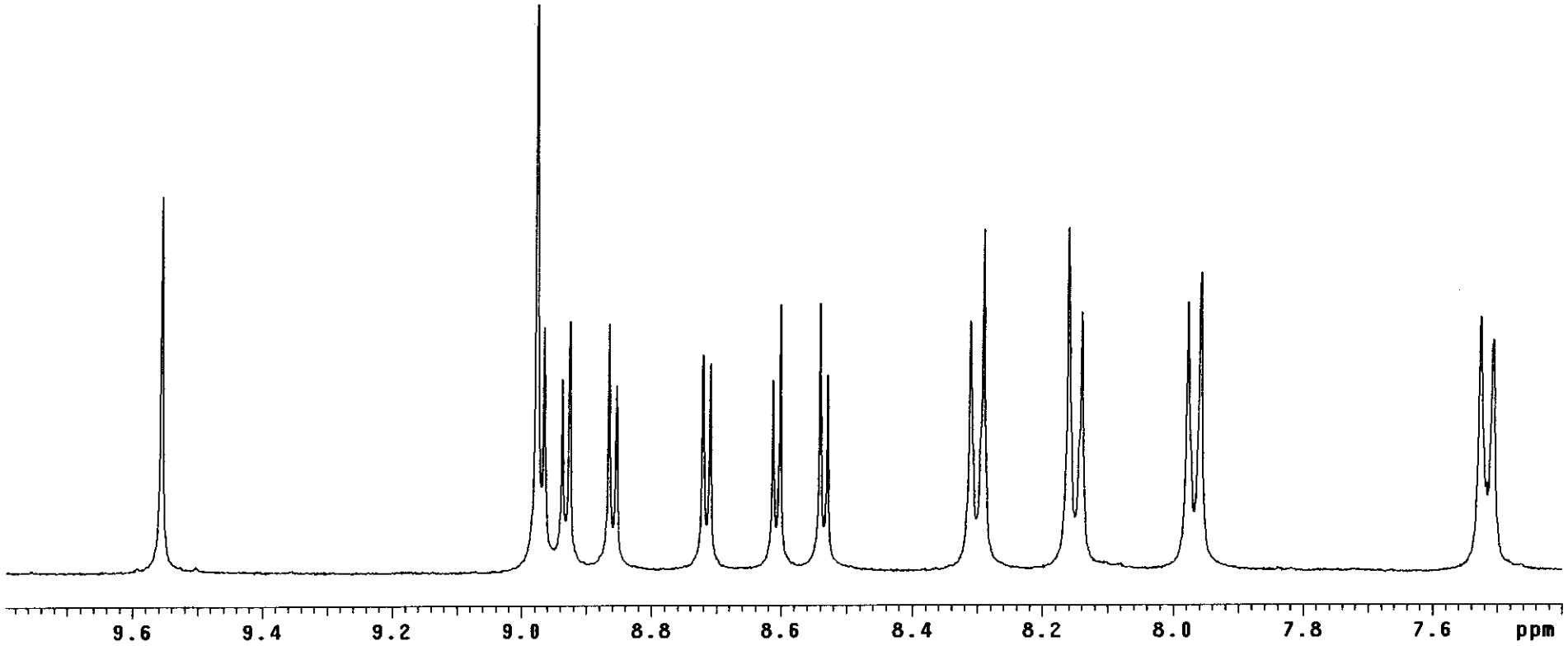
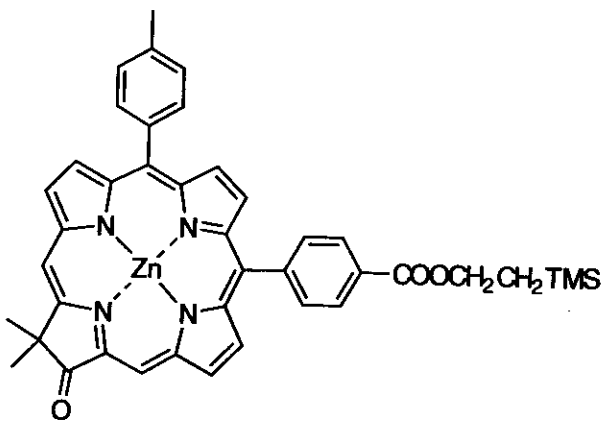
2
3
4
5
6
7
8
9



Oxo-Zn3





Oxo-Zn3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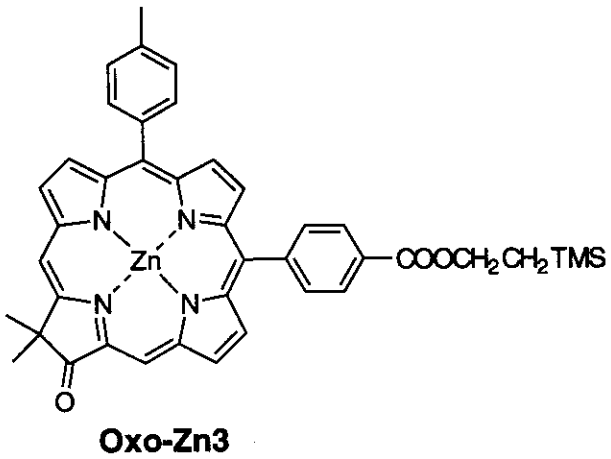
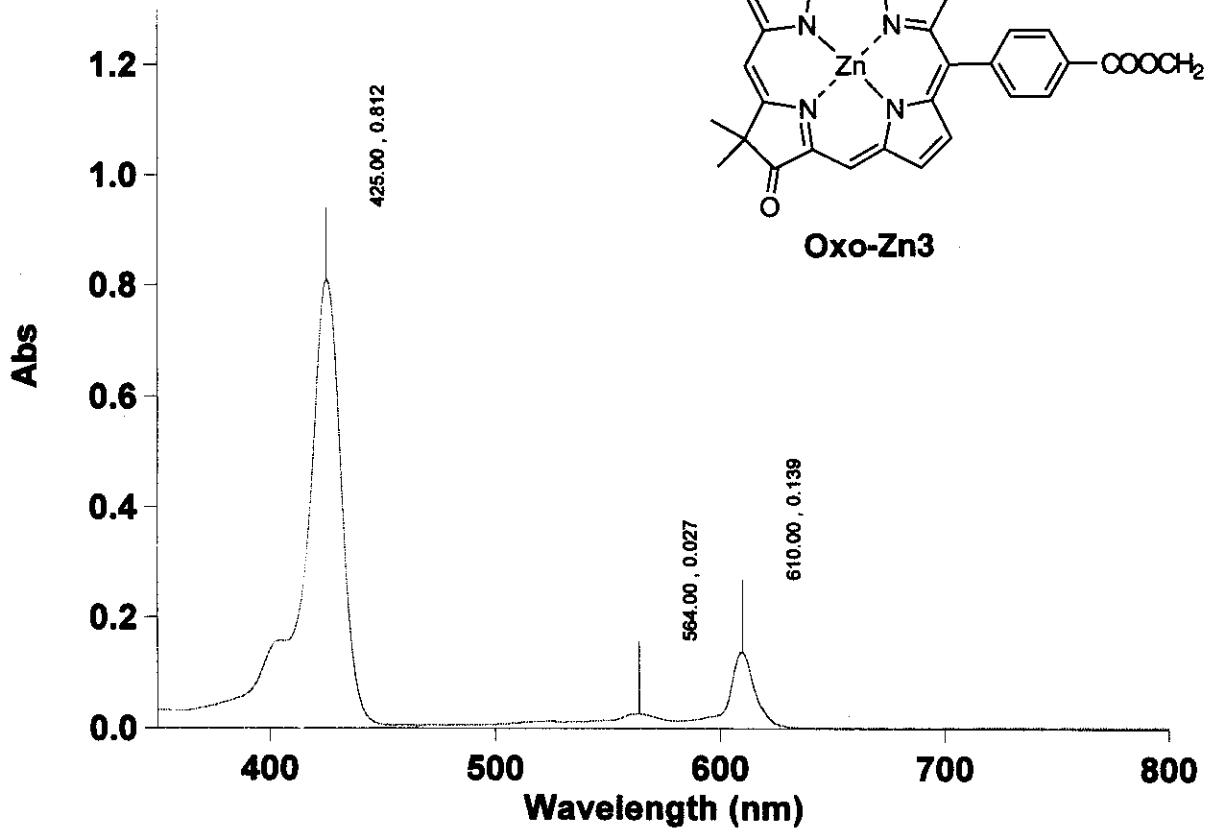
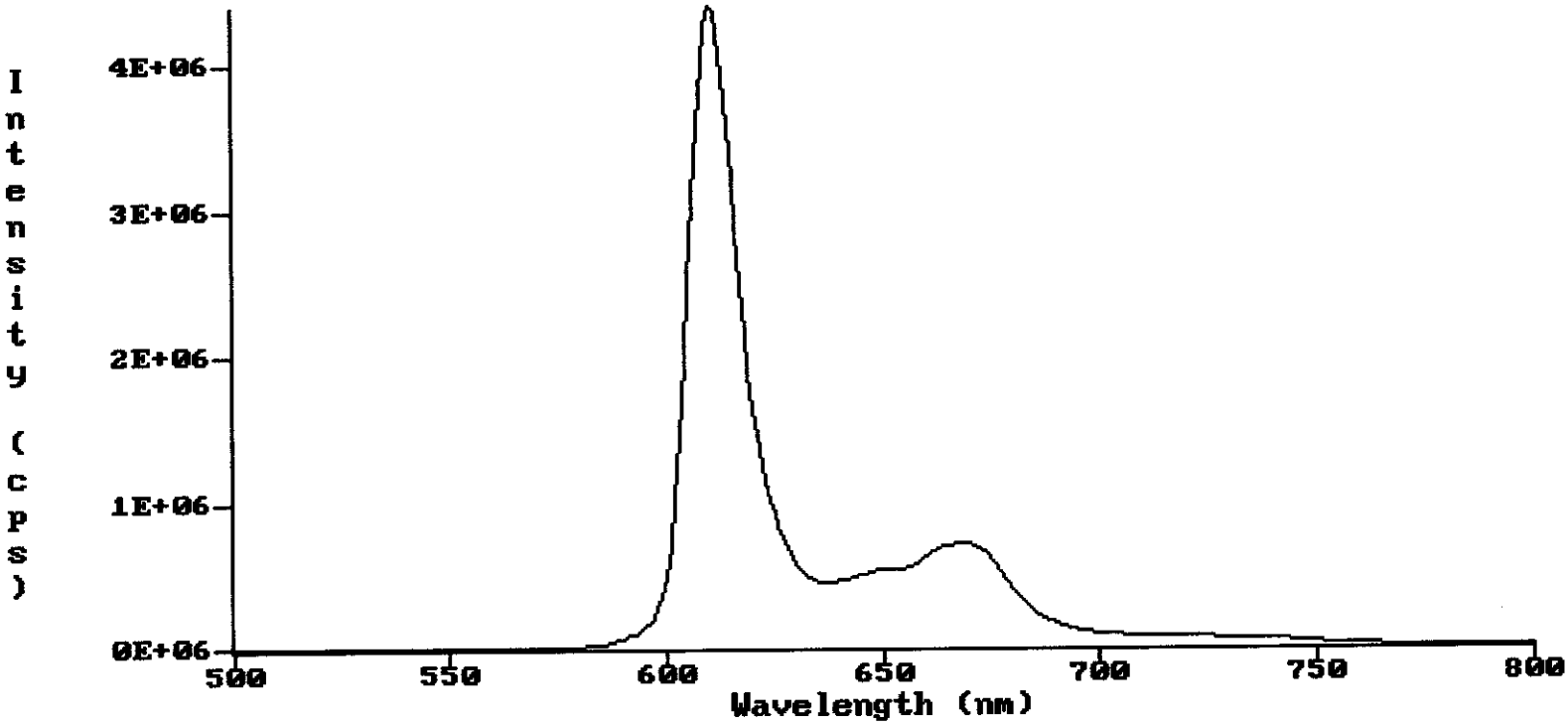
SMONUM          0
SMOPTS1         0
SMOPTS2         0
SMOPTS3         0
DW              1.00  [ns]
DELAY           0 [ns]
Uis1           20.00  [kV]
Uis2           18.70  [kV]
Urefl           0.00  [kV]
Ulens           7.50  [kV]
Uhimass        10.00  [kV]
RefFull         0.00  [kV]
UdetL           1.50  [kV]
UdetR           0.00  [kV]
Udefl           2.00  [kV]
REPHZ           1.00  [Hz]
ATTEN           39.0
ML1        2071110.891
ML2          323.058
ML3            0.000
HITURBO no
GDBON   yes
GDEDLY  short
DEFLON  no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1         510.84
DPMASS         700.00  [Da]
RBNDVAL          0.33
LBNDVAL          0.28
IS2BNDV          0.91
CMT1    Zn-Oxo-Chl-COOCCTMS
CMT2    Att=39, 35shots
```

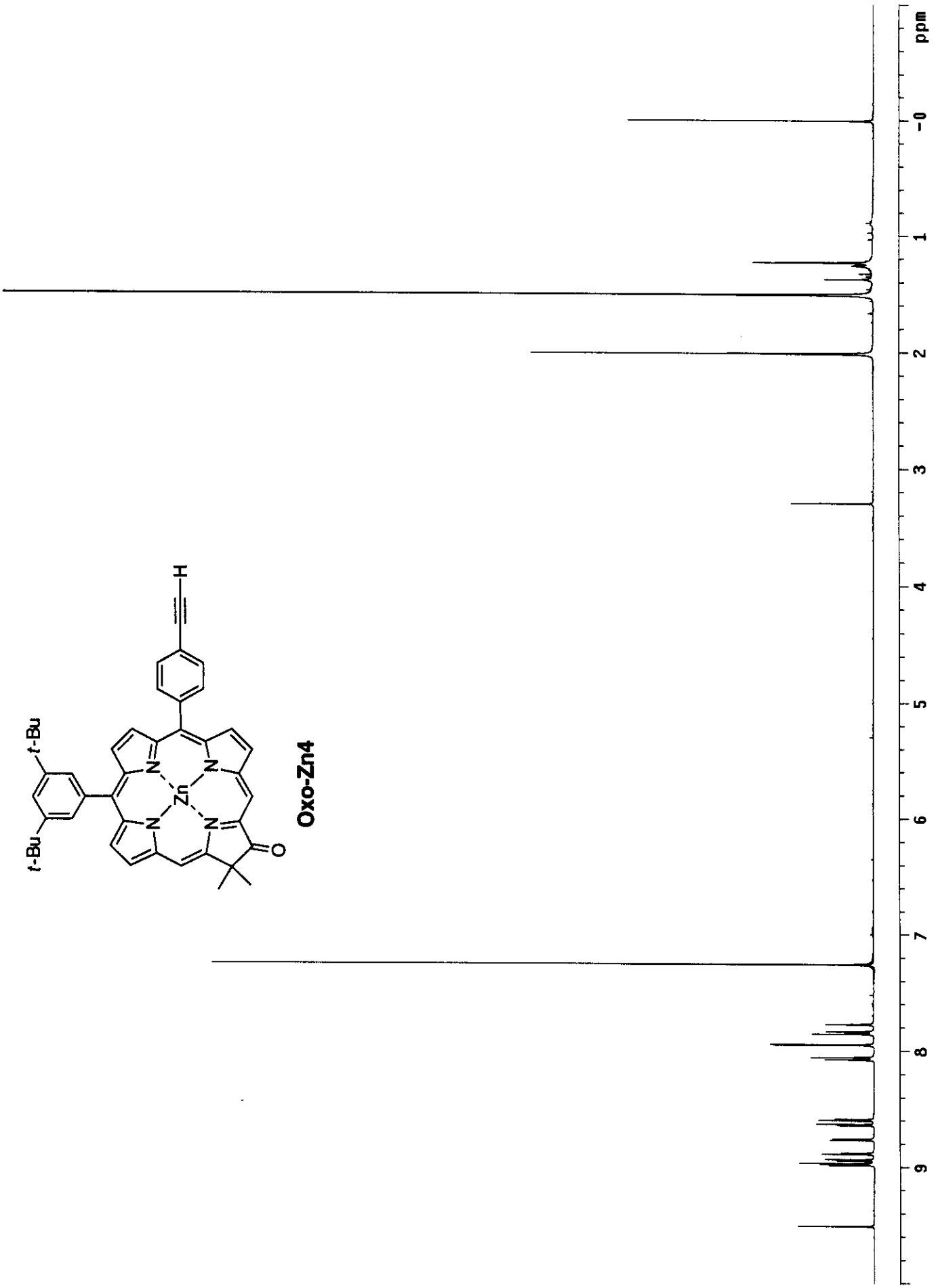
NCSU Chemistry
Instrument Serial Number 0051477



Oxo-Zn3






t-Bu
t-Bu
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N
Zn
N
N
O
H
Oxo-Zn4
ppm
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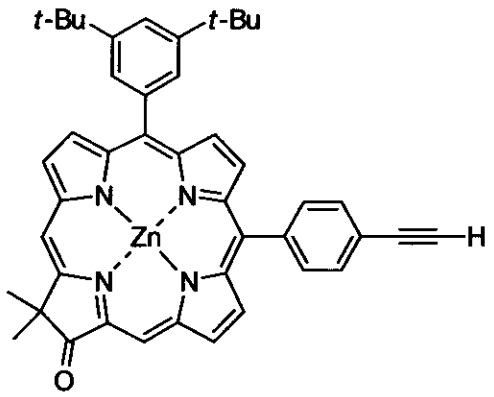
1
2
3
4
5
6
7
8
9



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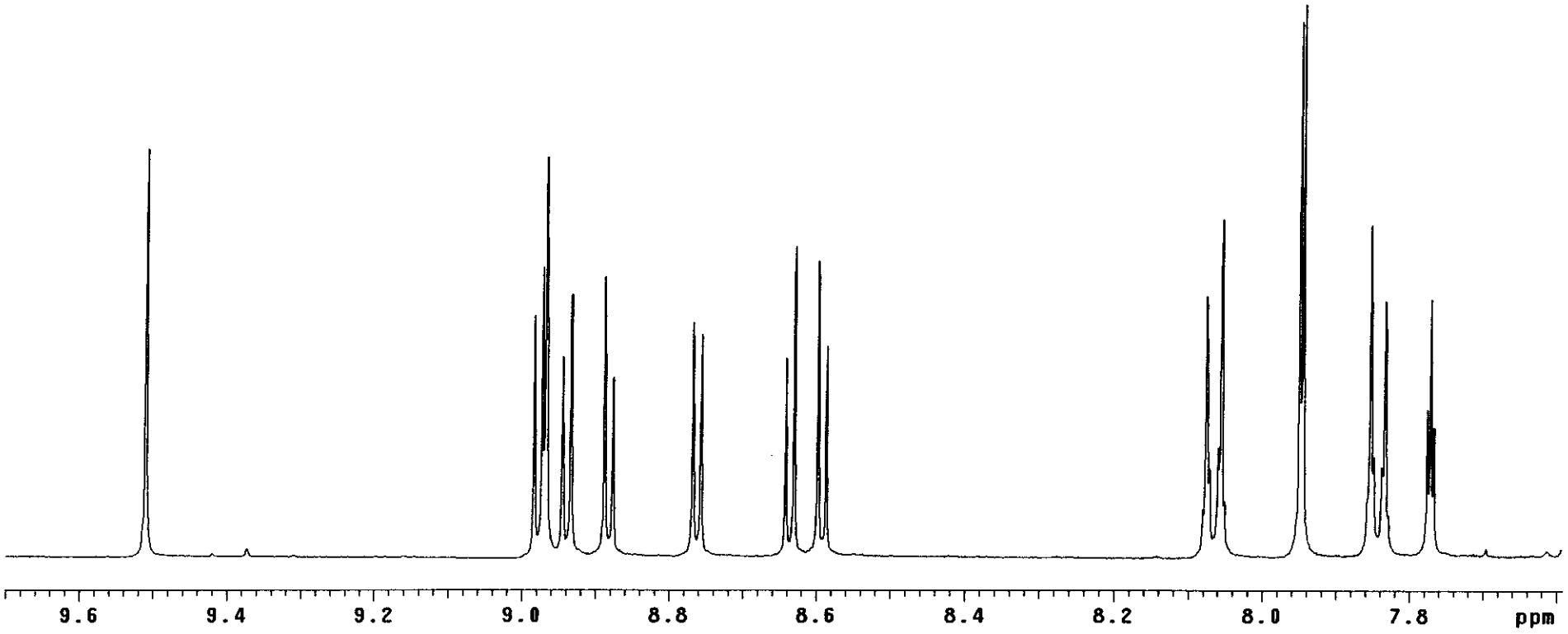

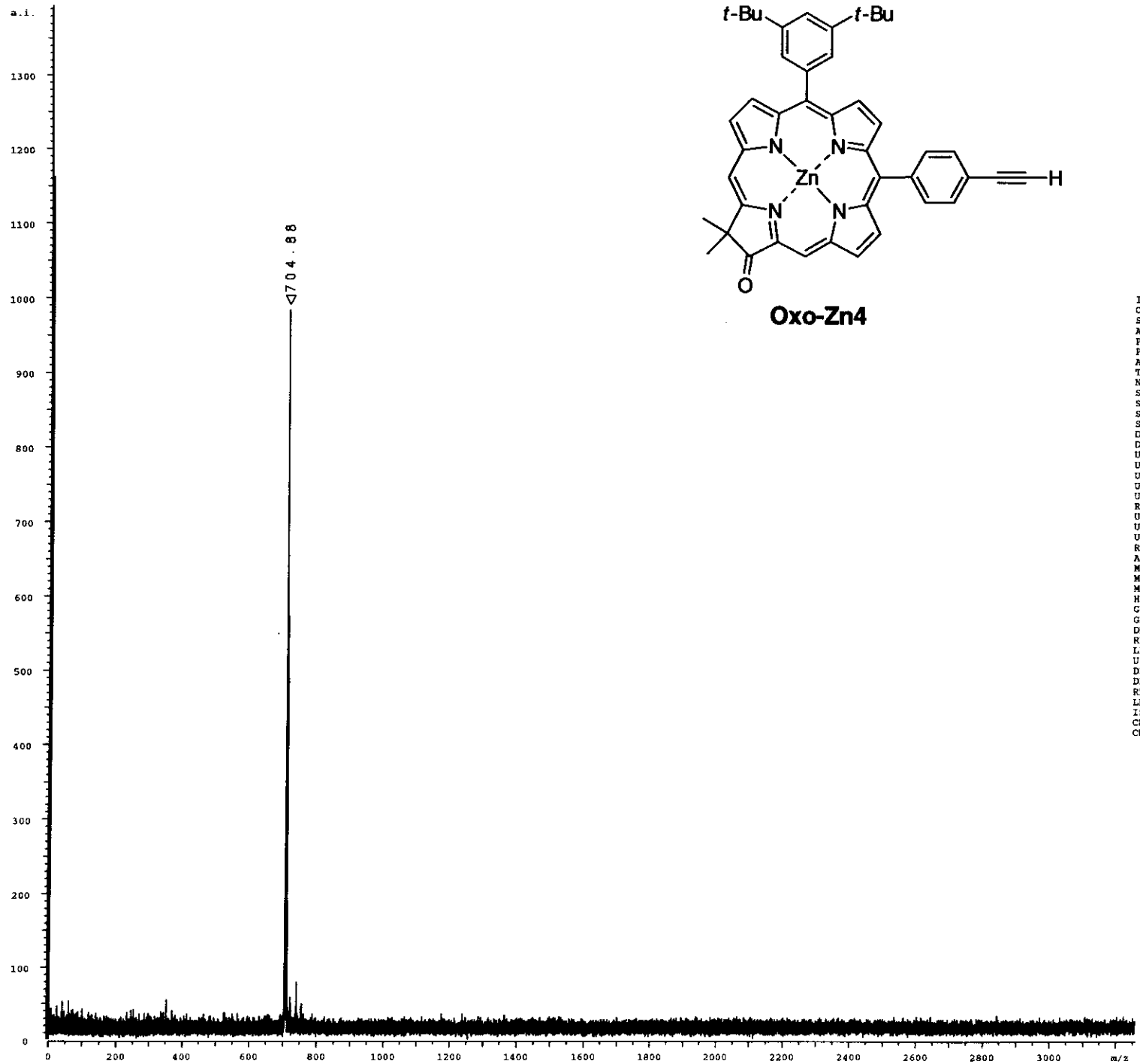

Oxo-Zn4

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AQOP_m  Reflector
TD              40000
NoSHOTS            51
SMONUM              0
SMOPTS1             0
SMOPTS2             0
SMOPTS3             0
DW                  1.00  [ns]
DELAY               0 [ns]
Uis1               20.00  [kV]
Uis2               18.70  [kV]
Urefl               0.00  [kV]
Ulens               7.50  [kV]
Uhimass            10.00  [kV]
RefFull             0.00  [kV]
UdetL               1.50  [kV]
UdetR               0.00  [kV]
Udefl               2.00  [kV]
REPHZ               1.00  [Hz]
ATTEN               35.0
ML1          2071110.891
ML2              323.058
ML3                0.000
HITURBO no
GDEON   yes
GDEDLY  short
DEFLON  no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1           510.84
DPMASS           700.00  [Da]
RSNDVAL            0.33
LSNDVAL            0.28
IS2SNDV            0.91
CMT1    Zn-Oxo-Chl-CCH
CMT2    Att=35, 100shots
```
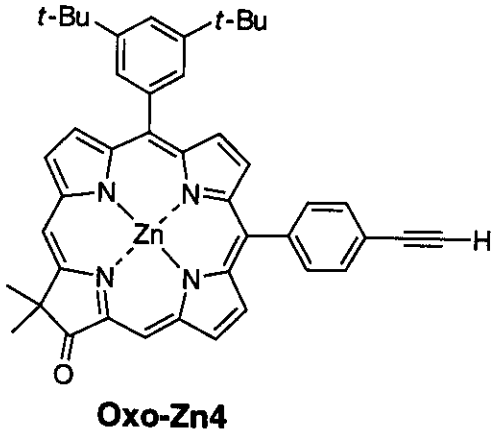
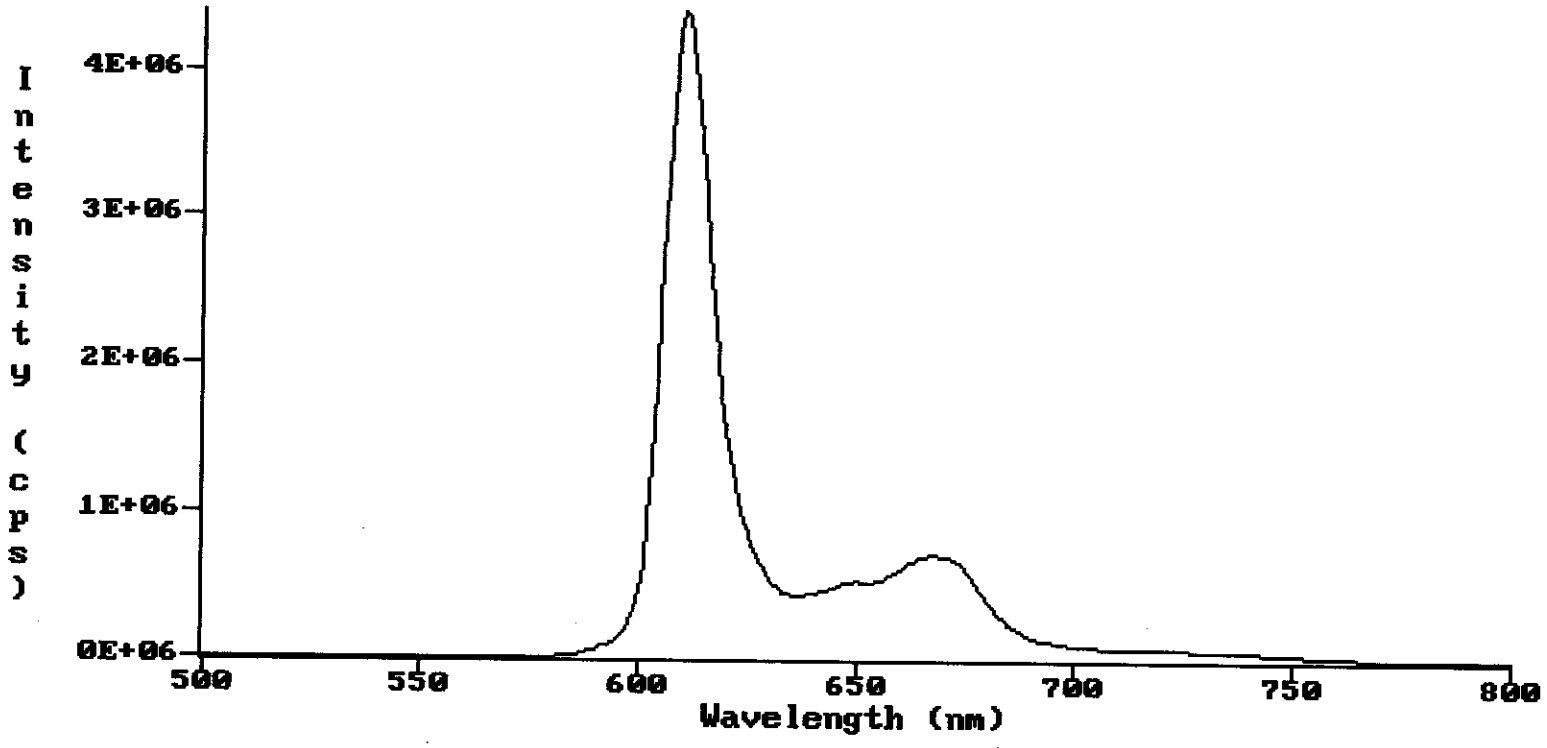
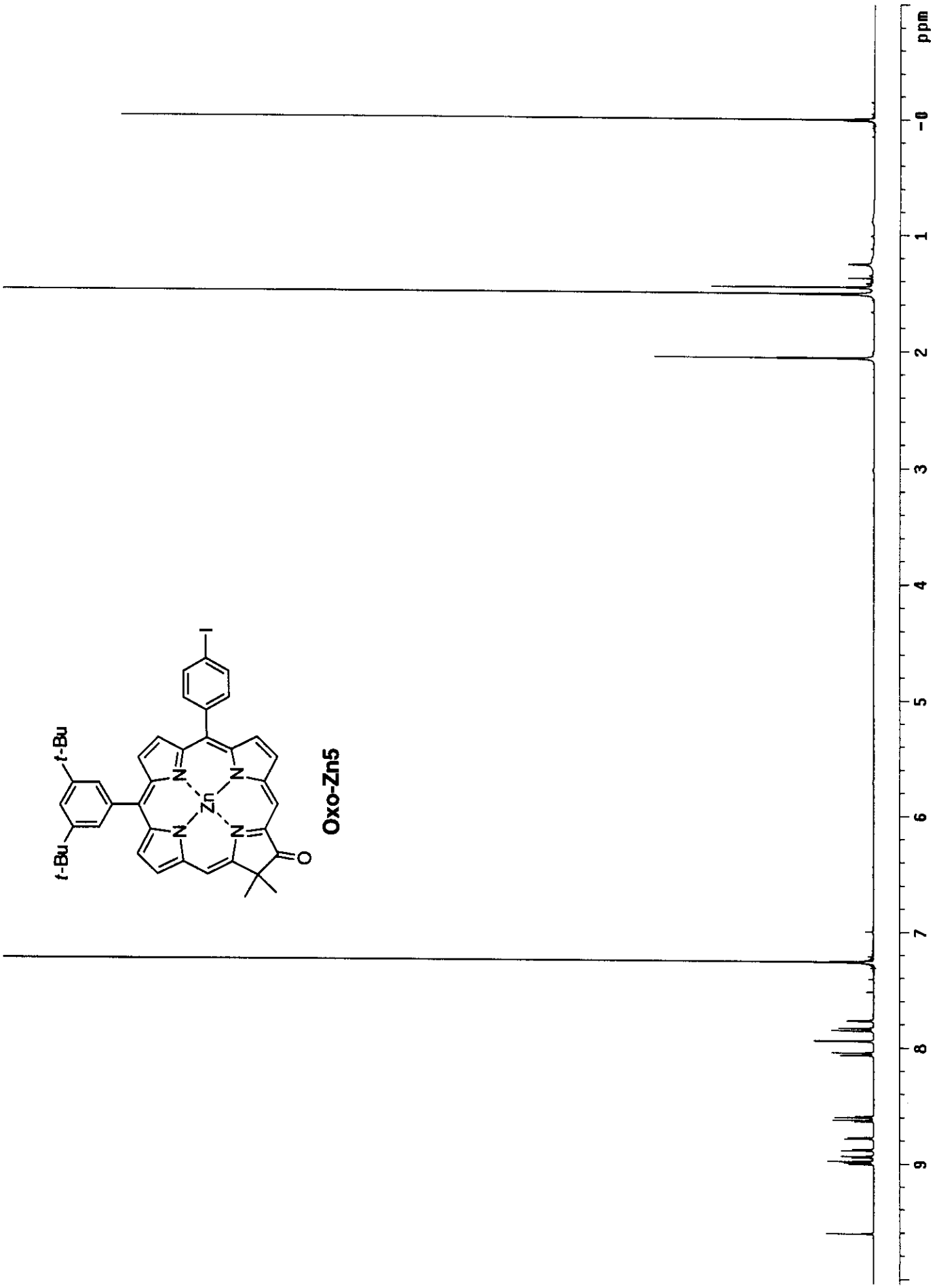

NCSU Chemistry
Instrument Serial Number 0051477



Oxo-Zn4




t-Bu
t-Bu
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N
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Zn
N
N
O
Oxo-Zn5
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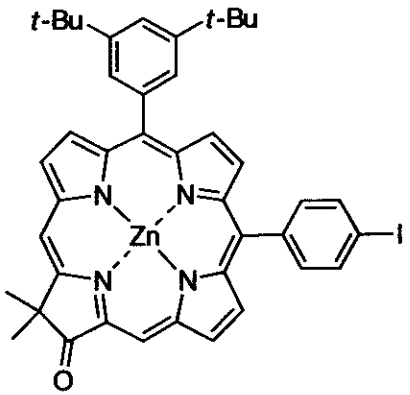
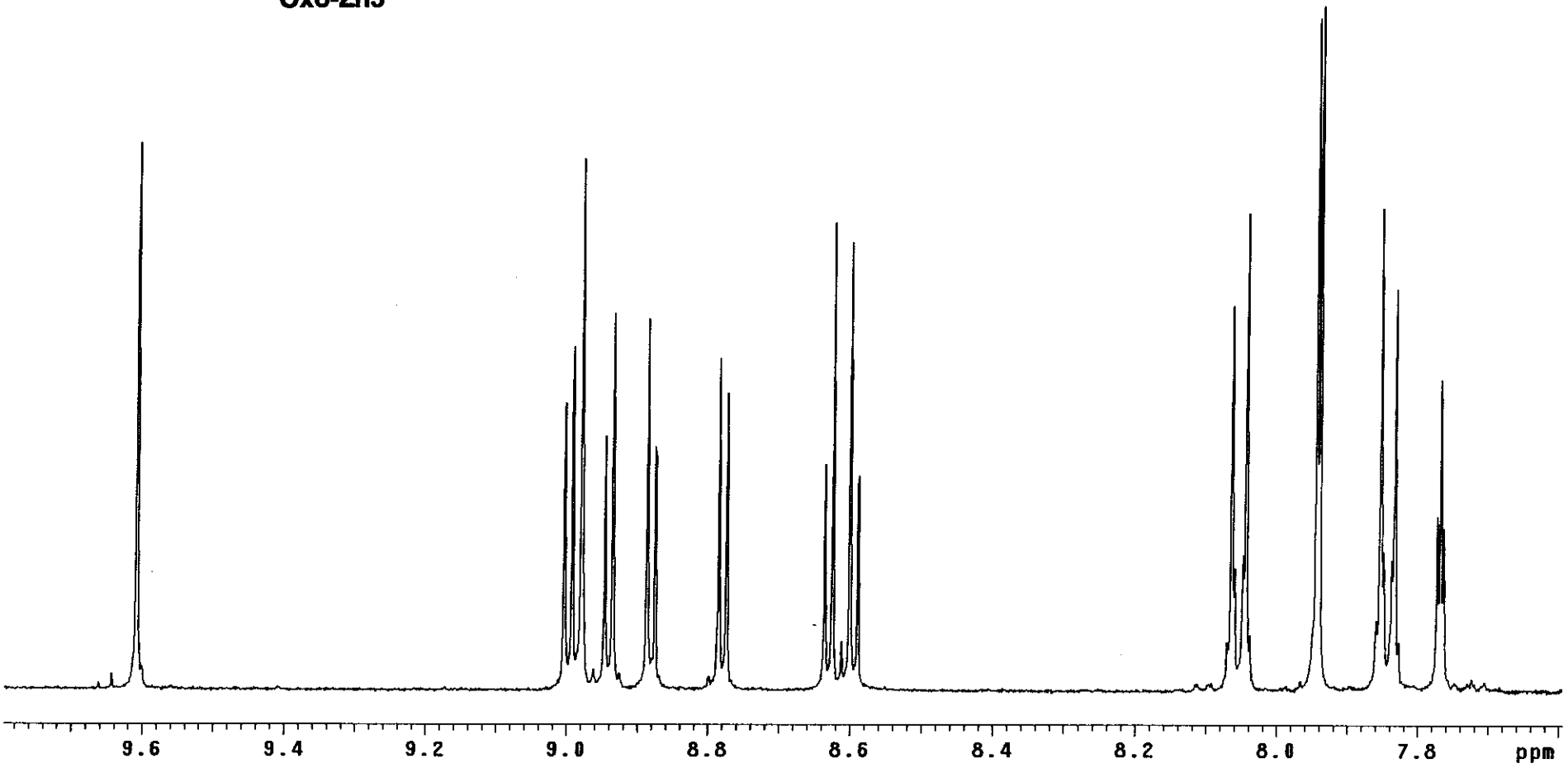
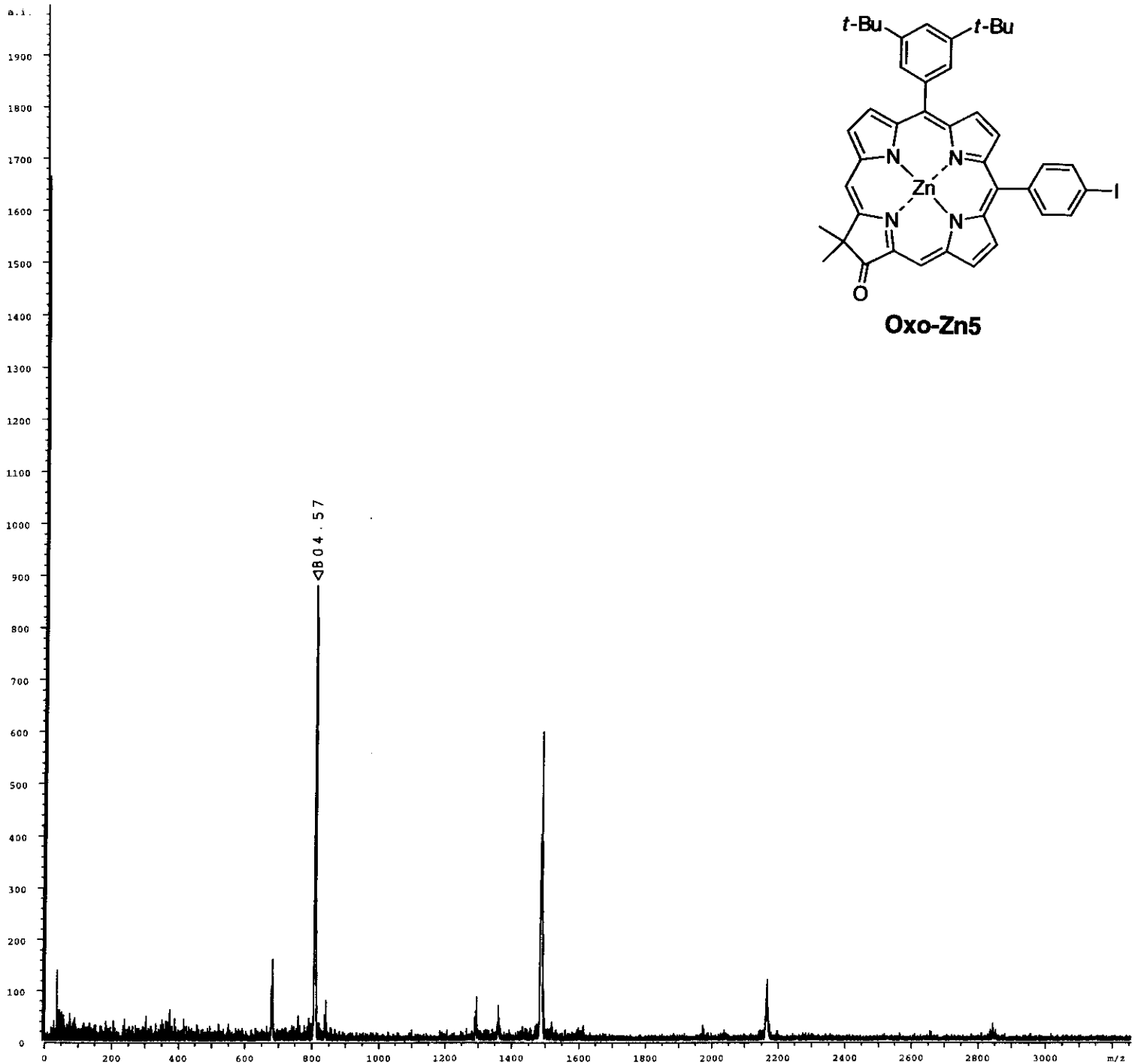
2
3
4
5
6
7
8
9



Oxo-Zn5





Oxo-Zn5

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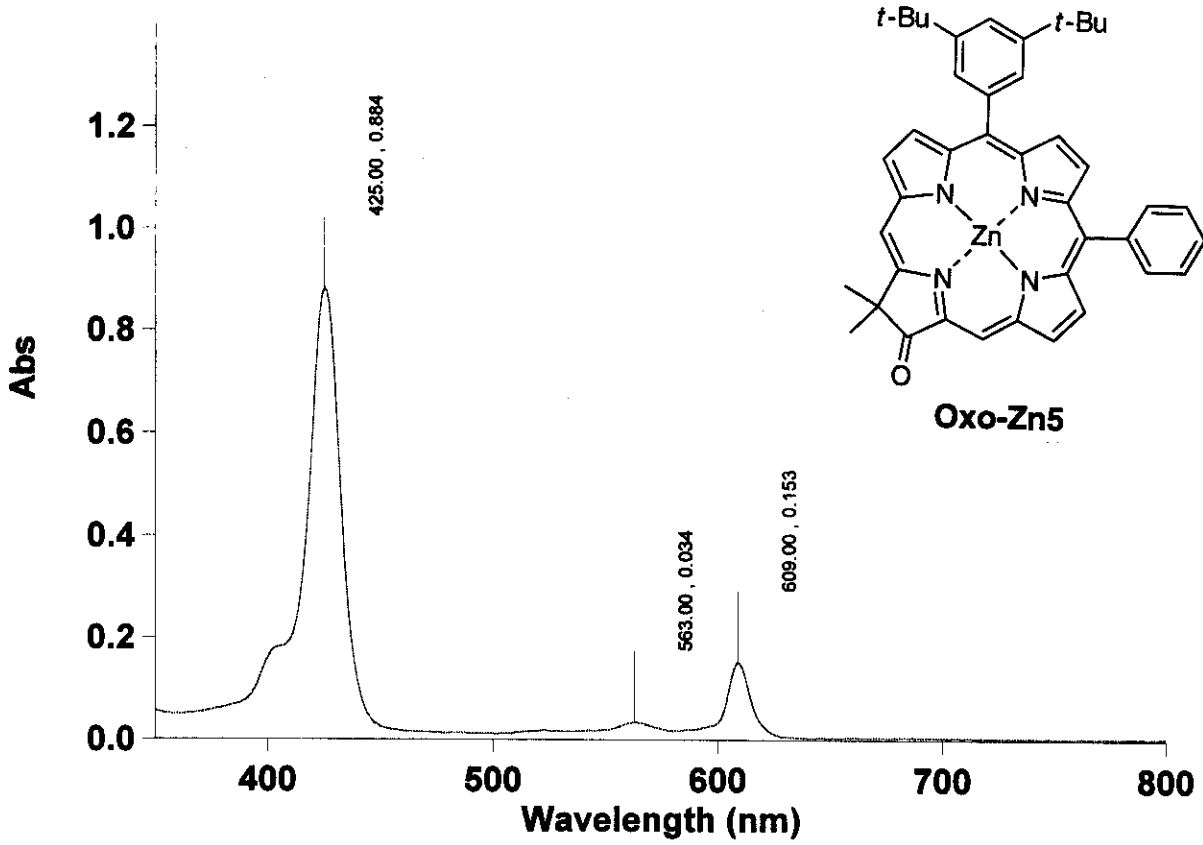
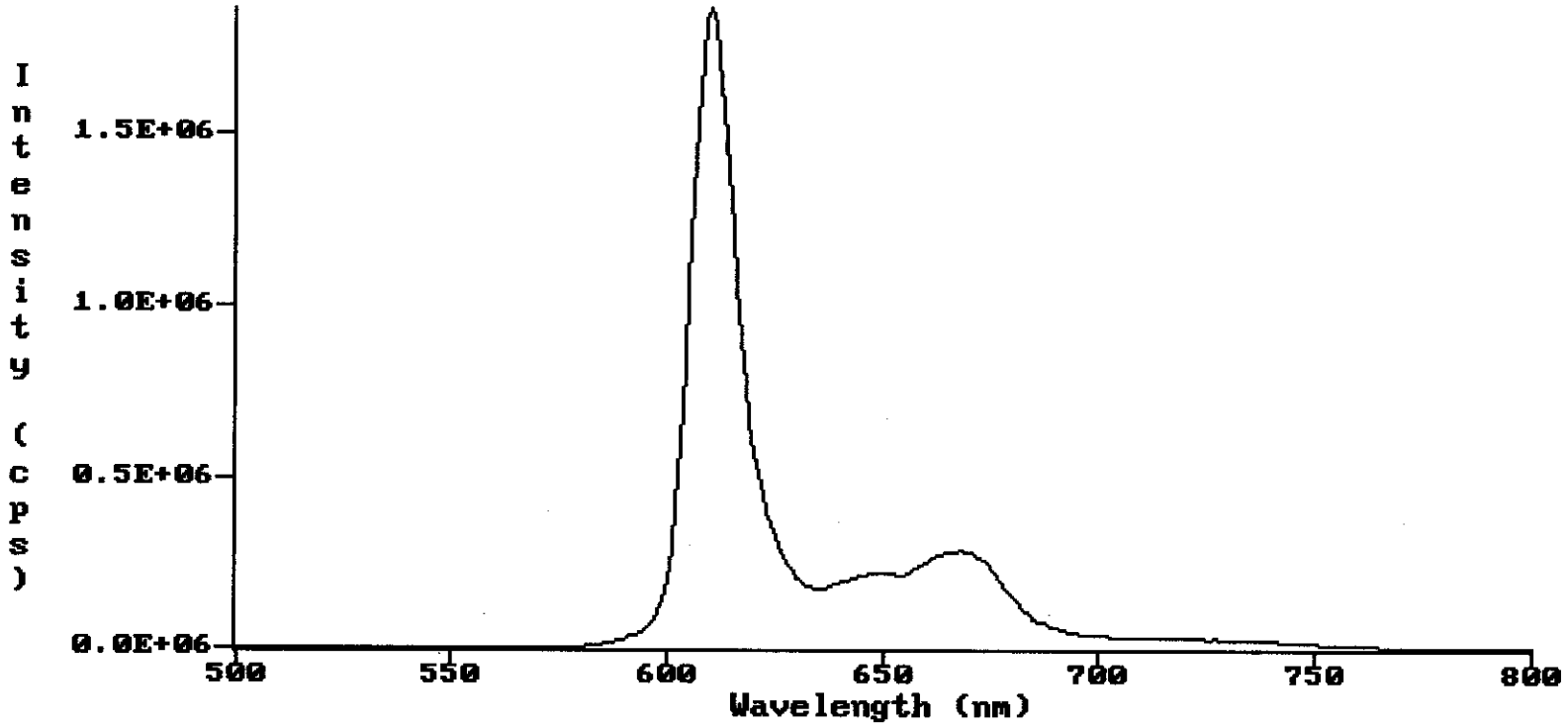
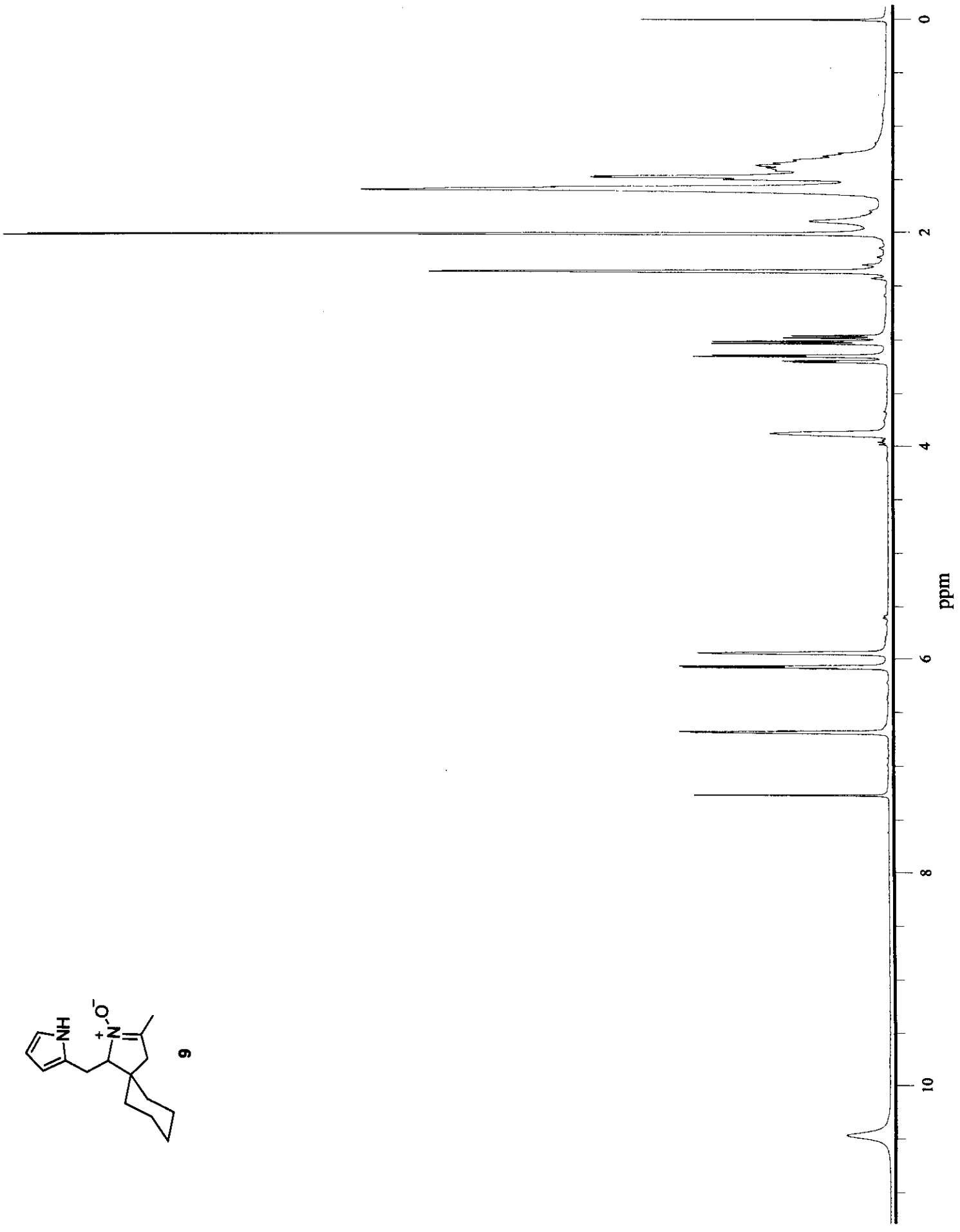
SMONUM          0
SMOPTS1         0
SMOPTS2         0
SMOPTS3         0
DW              1.00   [ns]
DELAY           0 [ns]
Uis1           20.00   [kV]
Uis2           18.50   [kV]
Urefl           0.00   [kV]
Ulens           7.50   [kV]
Uhimass        10.00   [kV]
RefFull         0.00   [kV]
UdetL           1.55   [kV]
UdetR           0.00   [kV]
Udefl           2.00   [kV]
REPHZ           1.00   [Hz]
ATTEN           35.0
ML1       2074469.941
ML2           355.586
ML3             0.000
HITURBO no
GDEON   yes
GDEDLY  short
DEFLON  no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1        510.84
DPMASS        200.00   [Da]
RBNDVAL         0.33
LBNDVAL         0.28
IS2BNDV         0.91
CMT1    Zn-OXO-PhI-tbu
CMT2    attn35 70 shots
```

NCSU Chemistry
Instrument Serial Number 0051477



Oxo-Zn5





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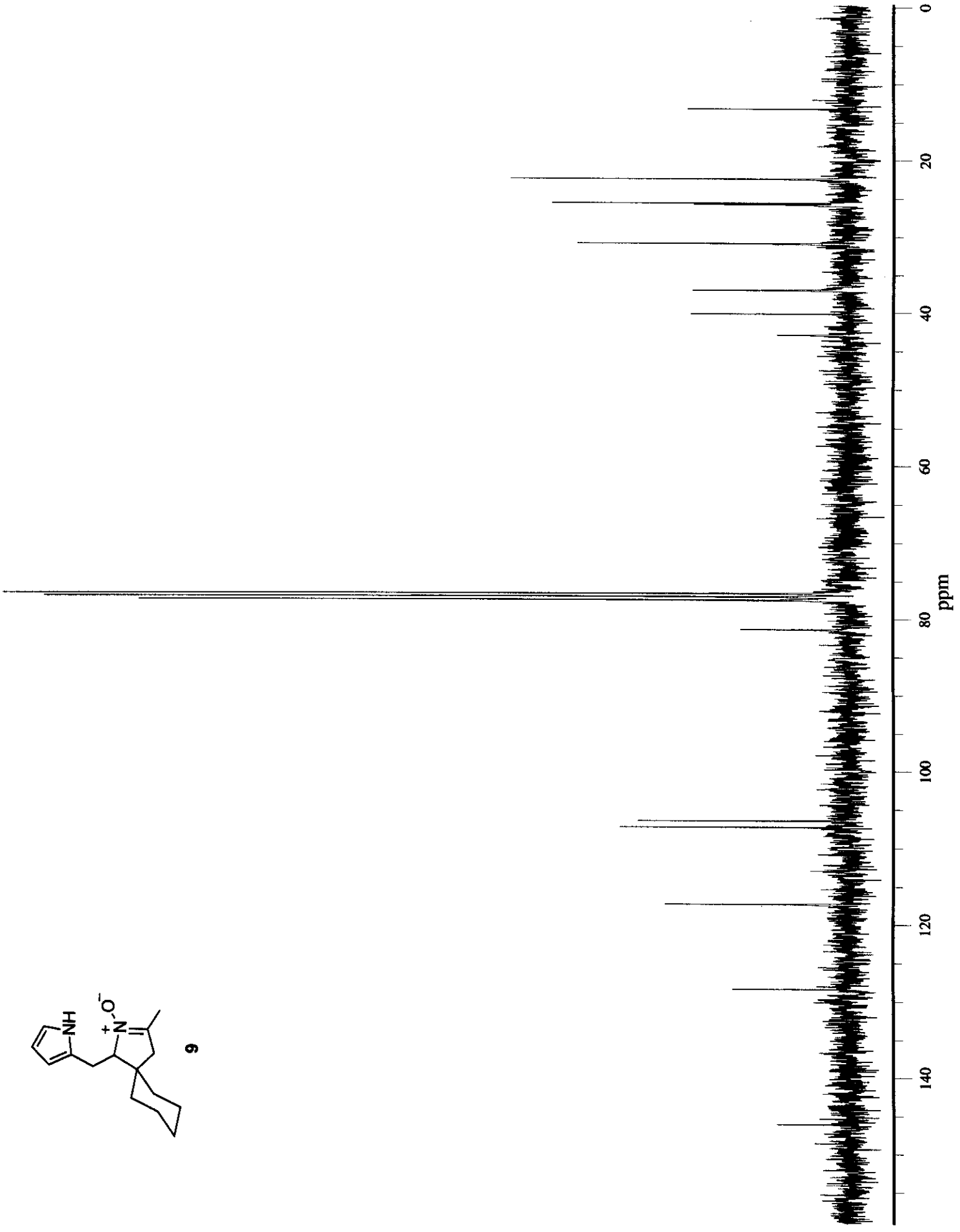

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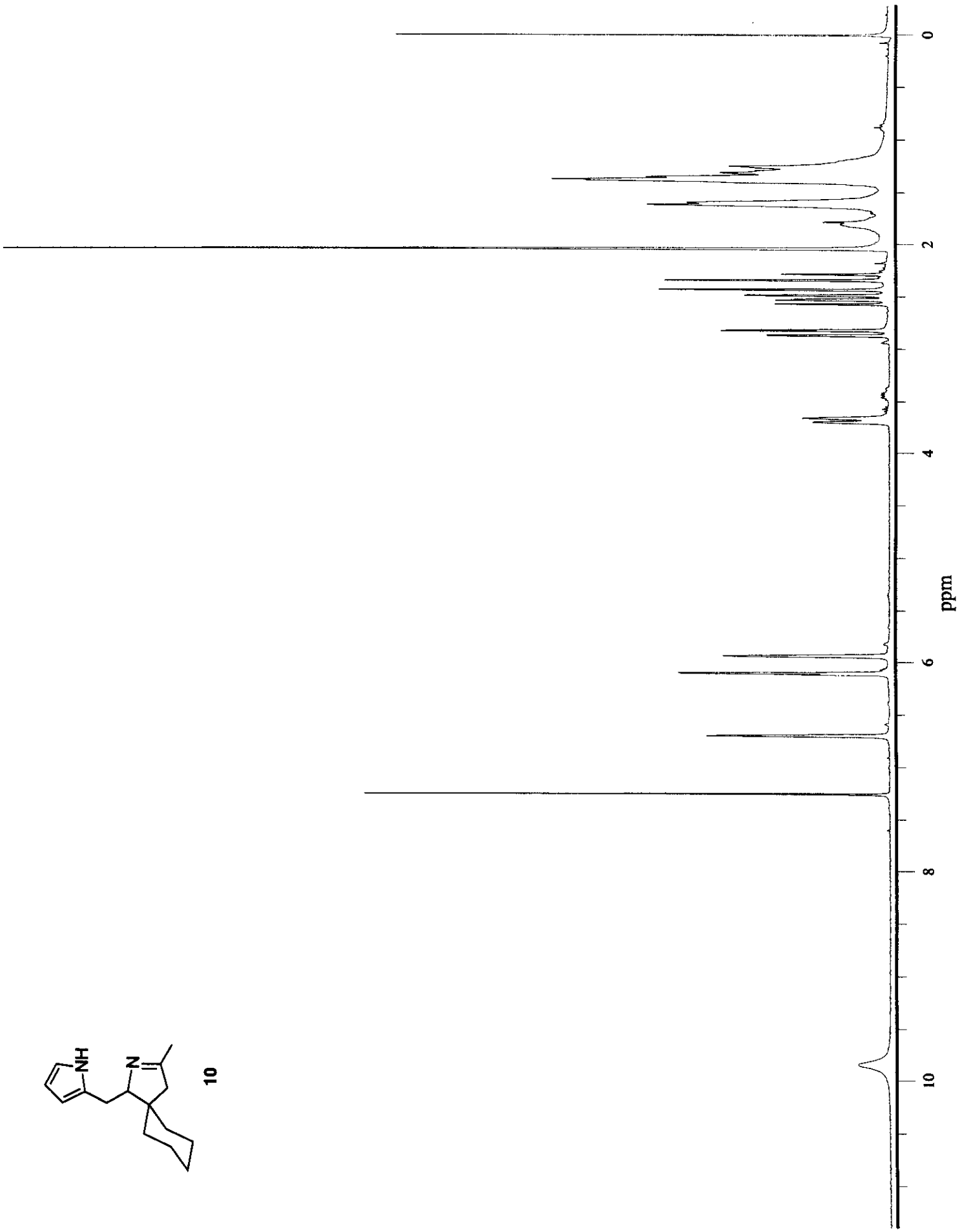

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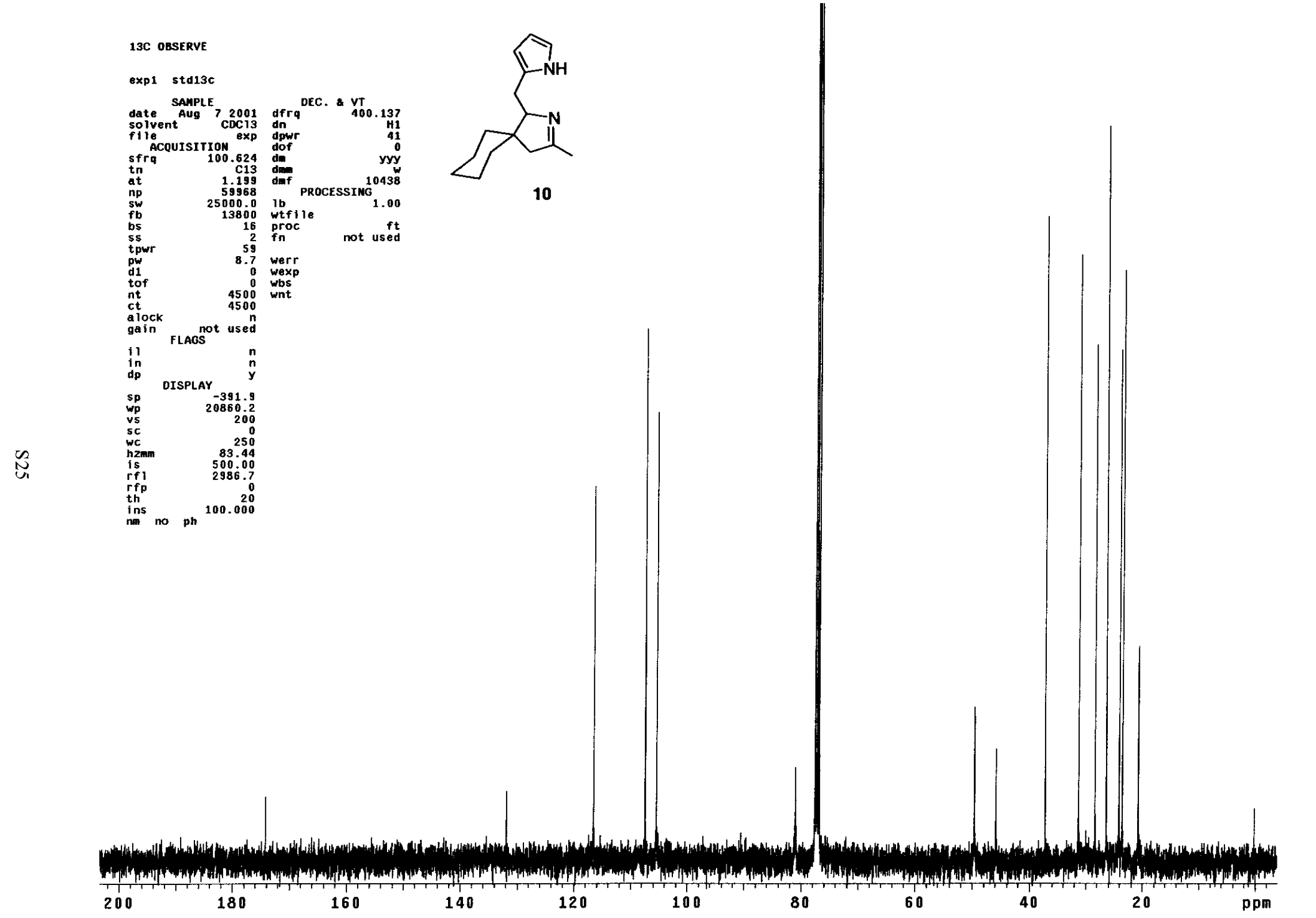
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SAMPLE
date Aug 7 2001
solvent CDCl3
file exp
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tn C13
at 1.199
np 59968
sw 25000.0
fb 13800
bs 16
ss 2
tpwr 59
pw 8.7
d1 0
tof 0
nt 4500
ct 4500
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -391.9
wp 20860.2
vs 200
sc 0
wc 250
hzmm 83.44
is 500.00
rfl 2986.7
rfp 0
th 20
ins 100.000
nm no ph
DEC. & VT
dfrq 400.137
dn H1
dpwr 41
dof 0
dm yyy
dmm w
dmf 10438
PROCESSING
lb 1.00
wtfile
proc ft
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wnt
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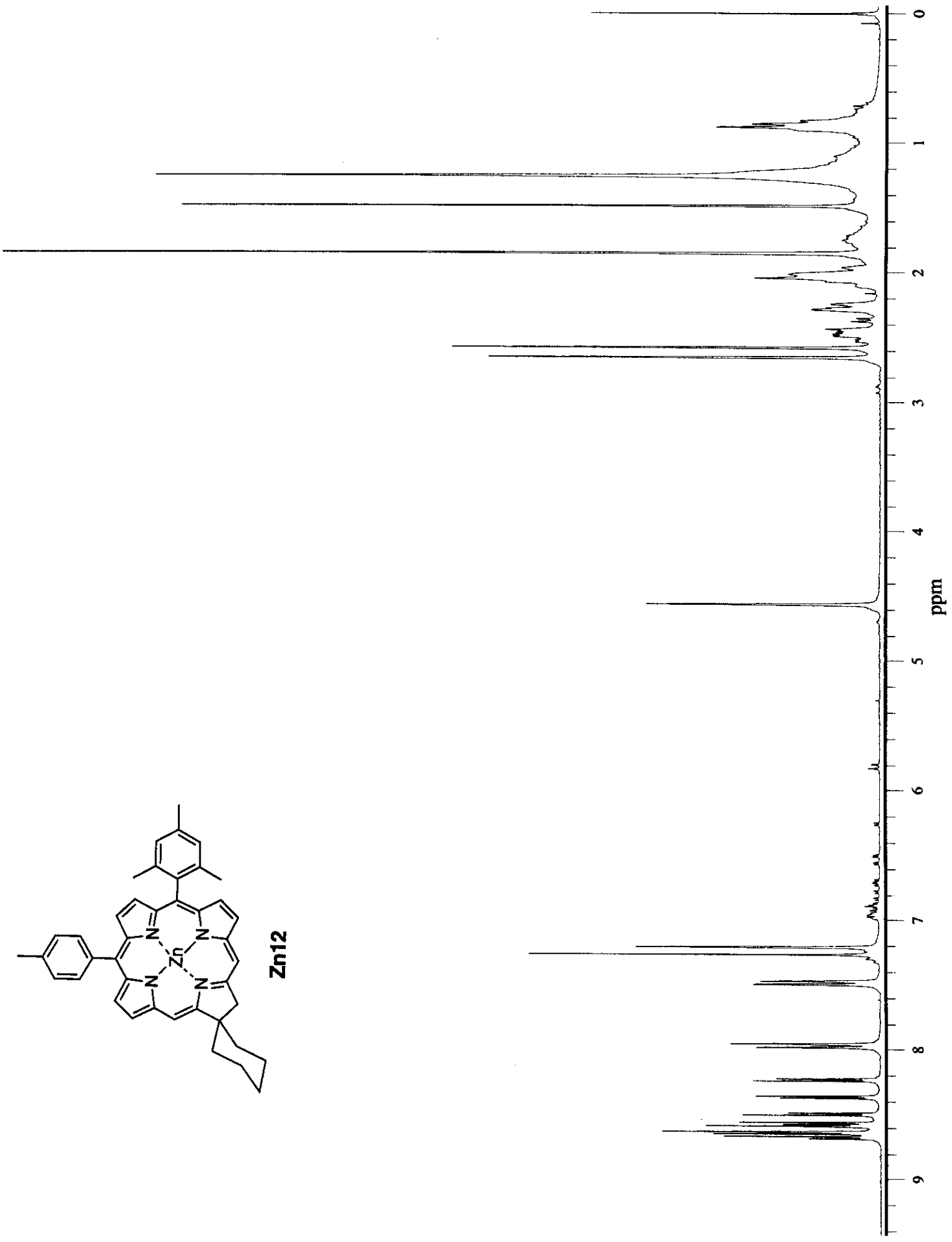
20
ppm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ppm

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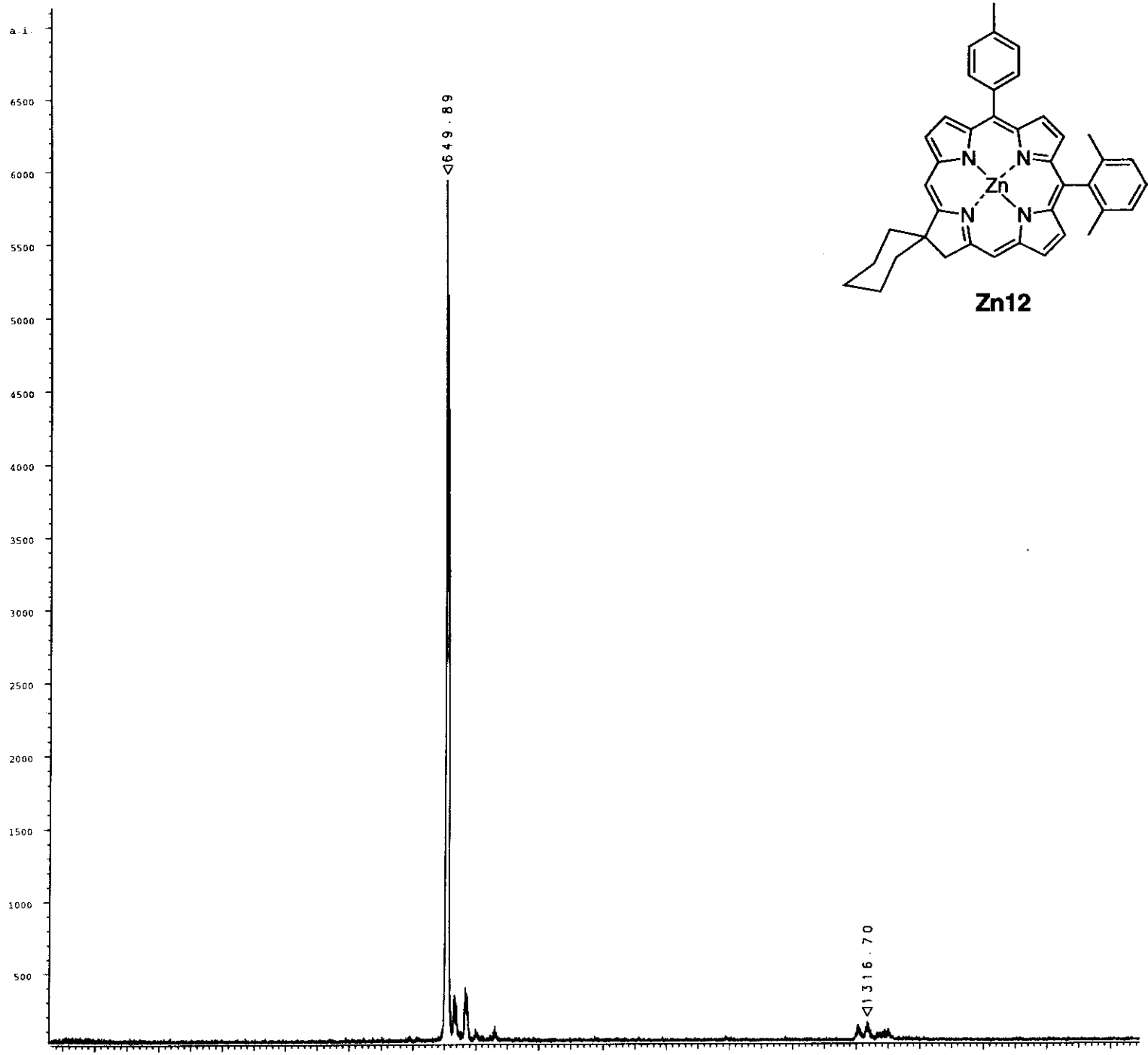

Zn12

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NoSHOTS           100
SMONUM              0
SMOPTS1             0
SMOPTS2             0
SMOPTS3             0
DW                1.00  [ns]
DELAY             0 [ns]
Uis1             20.00  [kV]
Uis2             18.70  [kV]
Urefl             0.00  [kV]
Ulens             7.50  [kV]
Uhimass          10.00  [kV]
RefFull           0.00  [kV]
UdetL             1.50  [kV]
UdetR             0.00  [kV]
Udefl             2.00  [kV]
REPHZ             1.00  [Hz]
ATTEN             35.0
ML1         2067125.193
ML2             333.982
ML3               0.000
HITURBO no
GDEON   yes
GDEDLY  short
DEFLON  no
RLNSEND no
LLNSEND no
UIS2END no
DPCAL1          510.84
DPMASS          700.00  [Da]
RENDVAL           0.33
LENDVAL           0.28
IS2ENDV           0.91
CMT1    Zn-spirochlorin
CMT2    attn =35, shot =100
```

/data/chemistry/LINDSEY/PRATHAPAN/015605/1SRef/pdata/1 tof Mon Aug 13 10:27:09 2001

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Information : Default Method
Data File : <untitled>

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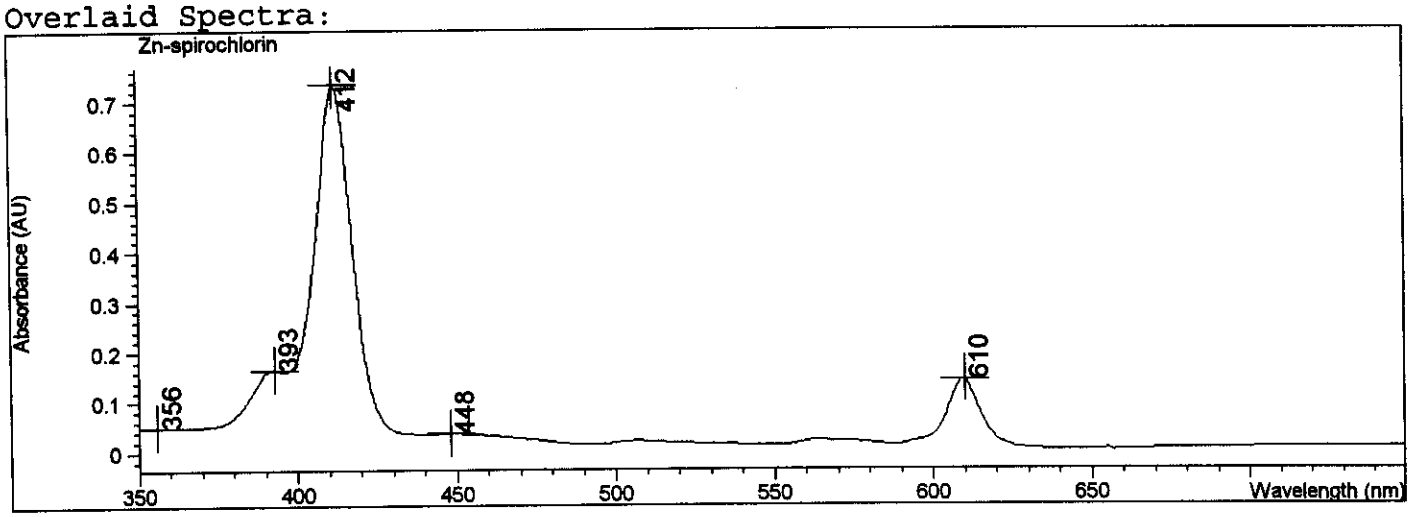
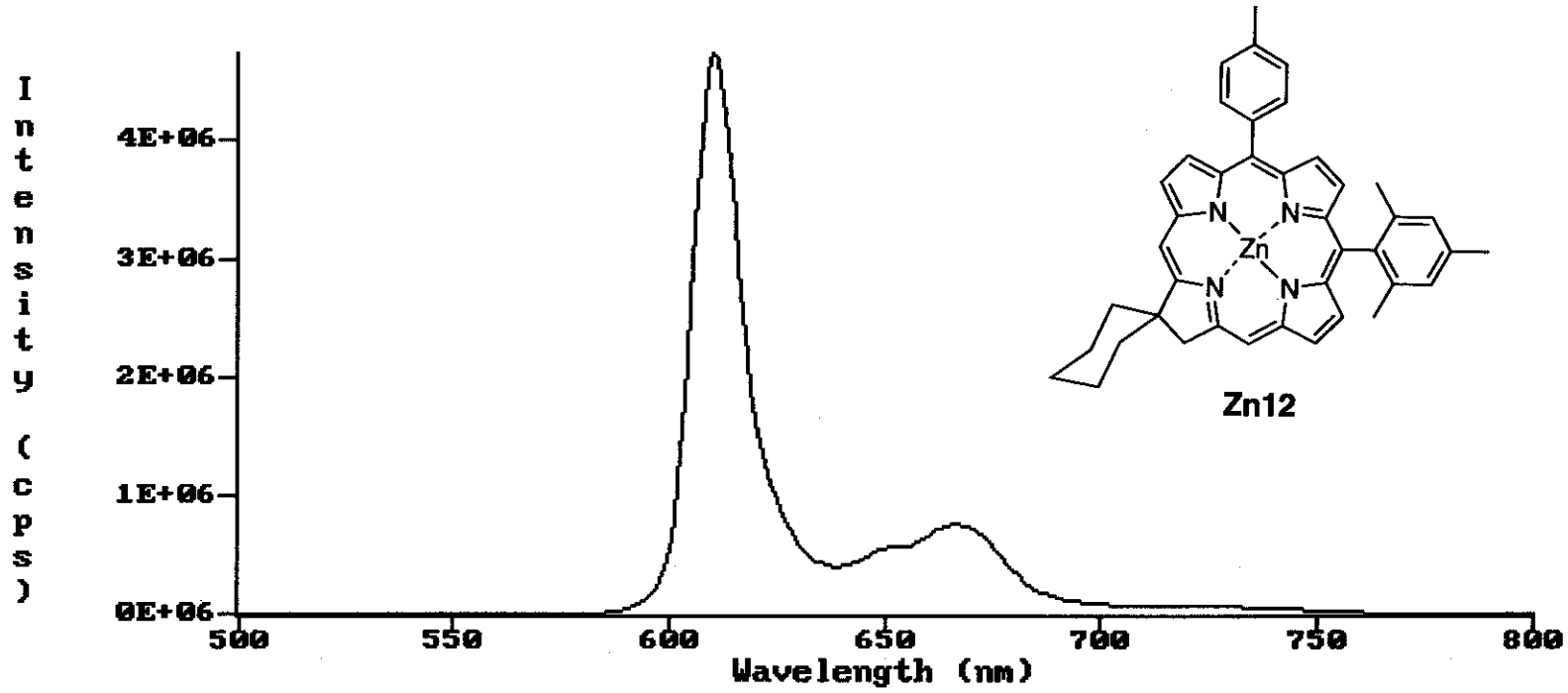
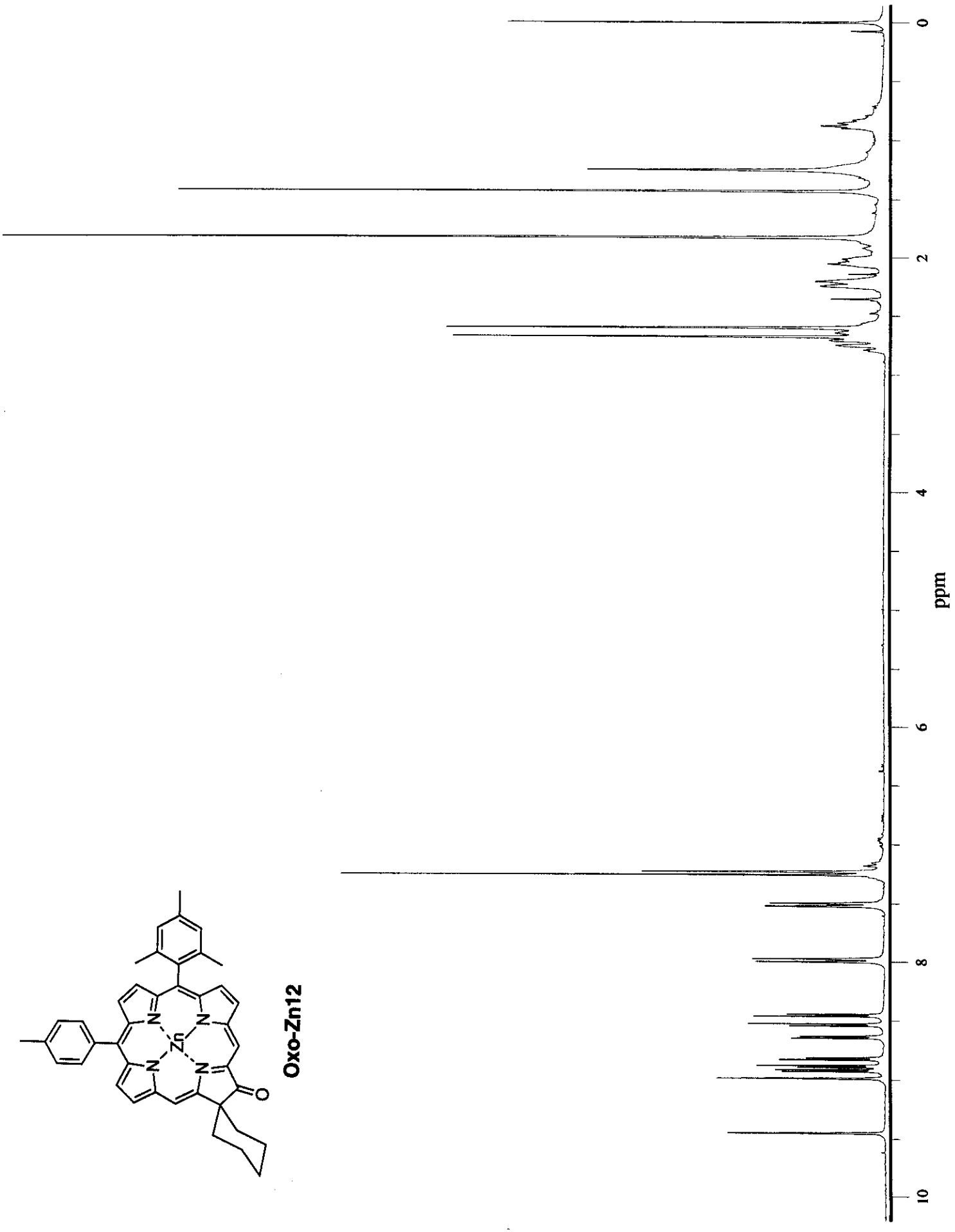
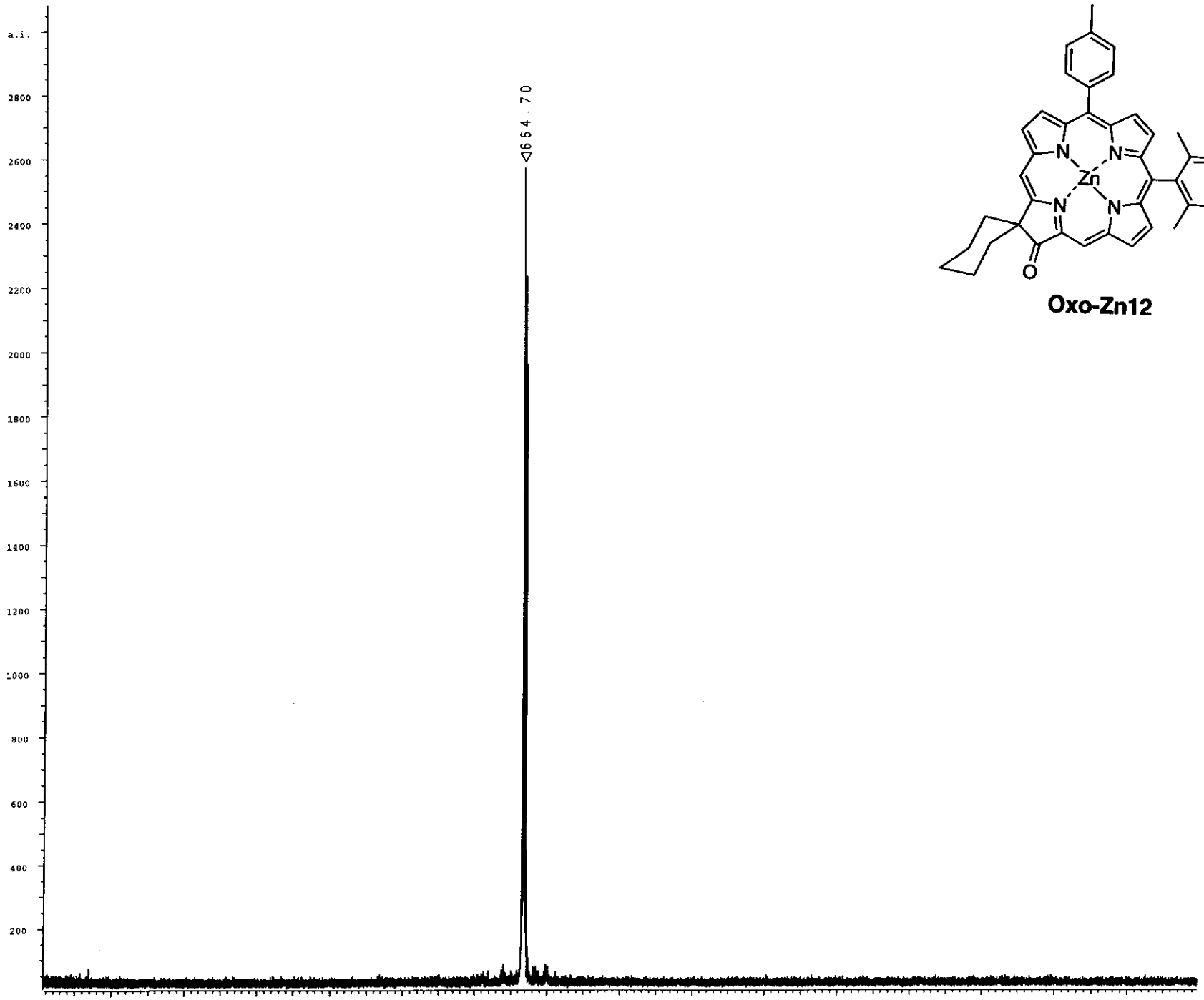


#	Name	Peaks (nm)	Abs (AU)
1	Zn-spirochlorin	412.0	0.73442
1		393.0	0.16490
1		610.0	0.14187
1		356.0	5.0785E-2
1		448.0	3.6520E-2





Oxo-Zn12

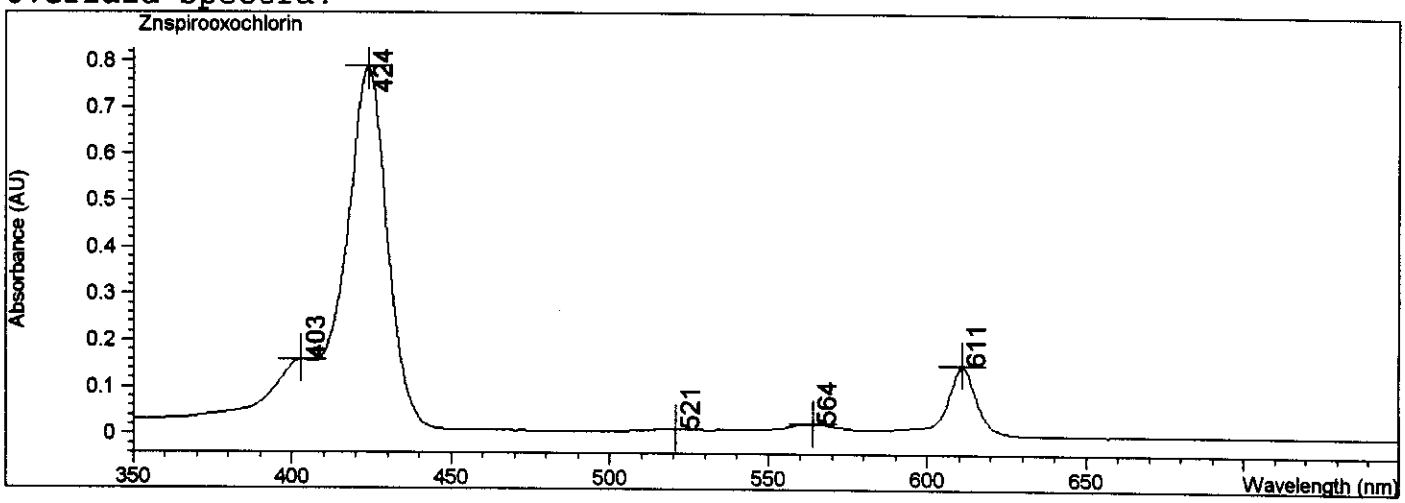

a.i.
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
664.70
100
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
1500
m/z
/data/chemistry/LINDSEY/PRATHAPAN/015606/1SRef/pdata/1 unknown Mon Aug 13 10:35:51 2001

N
N
Zn
N
N
O

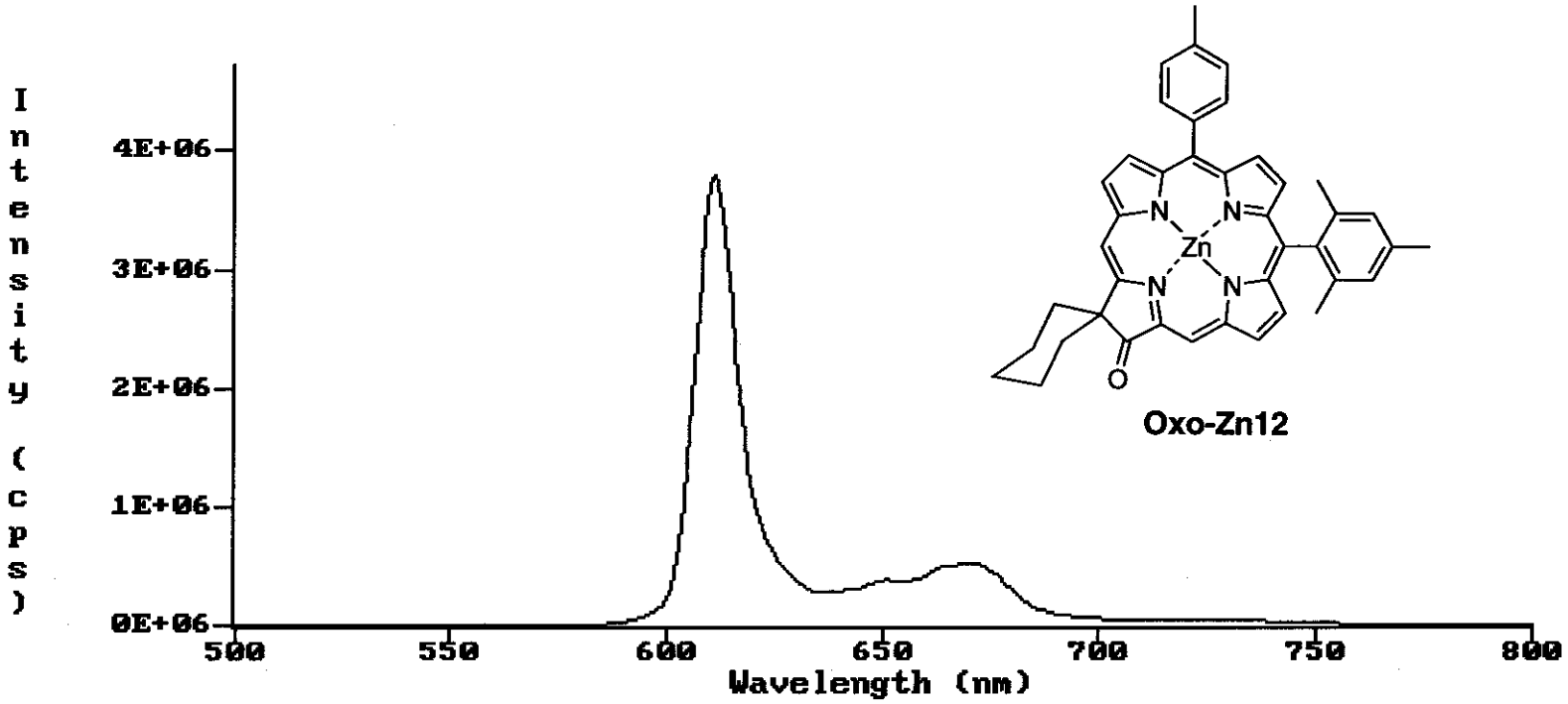
Oxo-Zn12

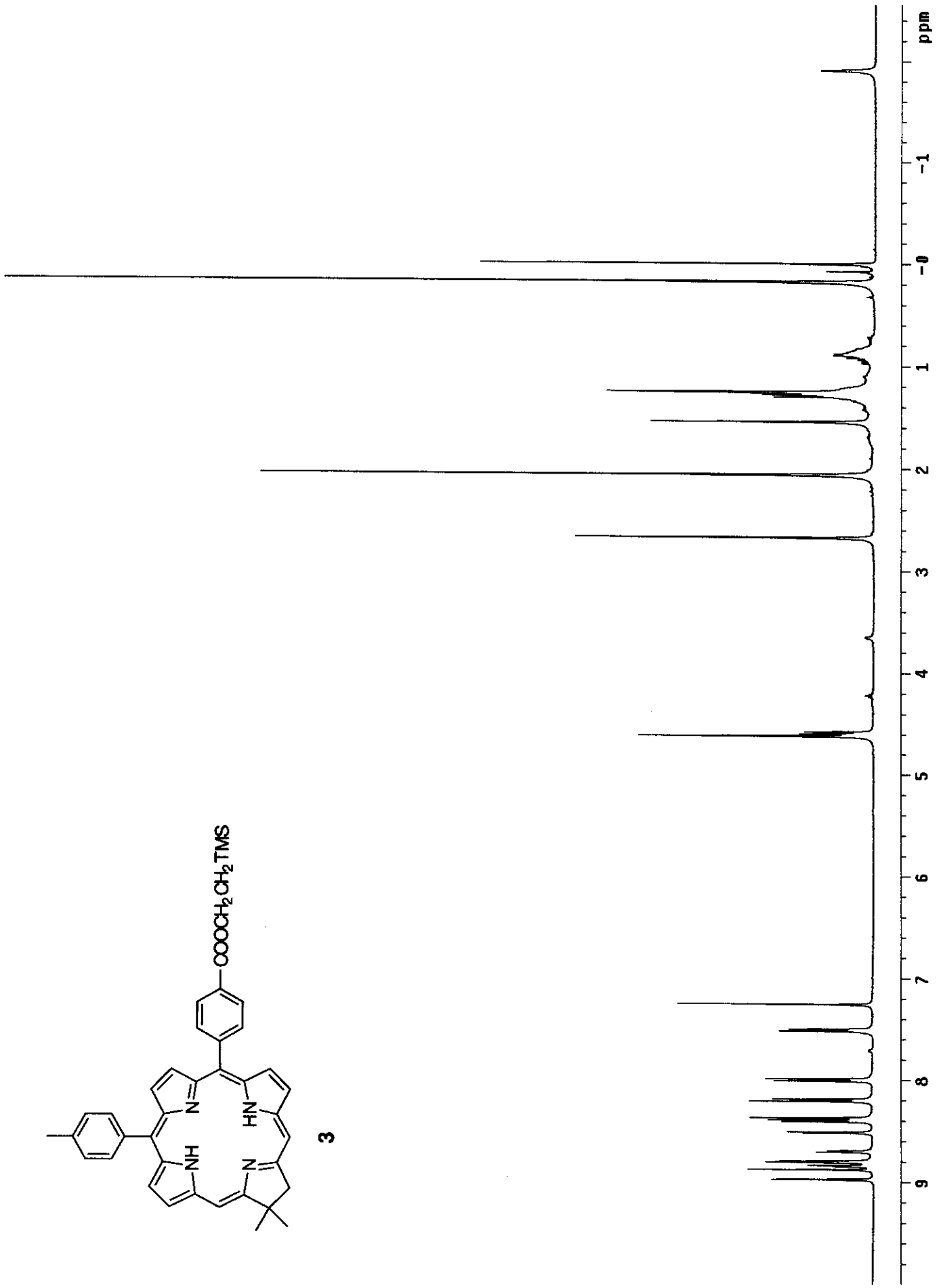
Method file : <untitled>
Information : Default Method
Data File : <untitled>

Overlaid Spectra:



#	Name	Peaks(nm)	Abs(AU)
1	Znspirooxochlori	424.0	0.78796
1		403.0	0.15892
1		611.0	0.15093
1		564.0	2.3799E-2
1		521.0	1.1910E-2




COOCH2CH2TMS
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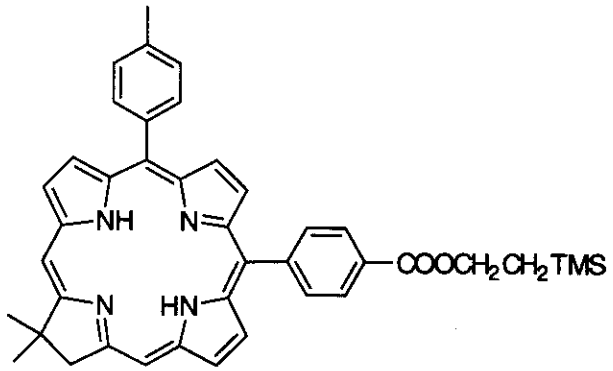
HN
NH
N
3
ppm
9
8
7
6
5
4
3
2
1
-0
-1



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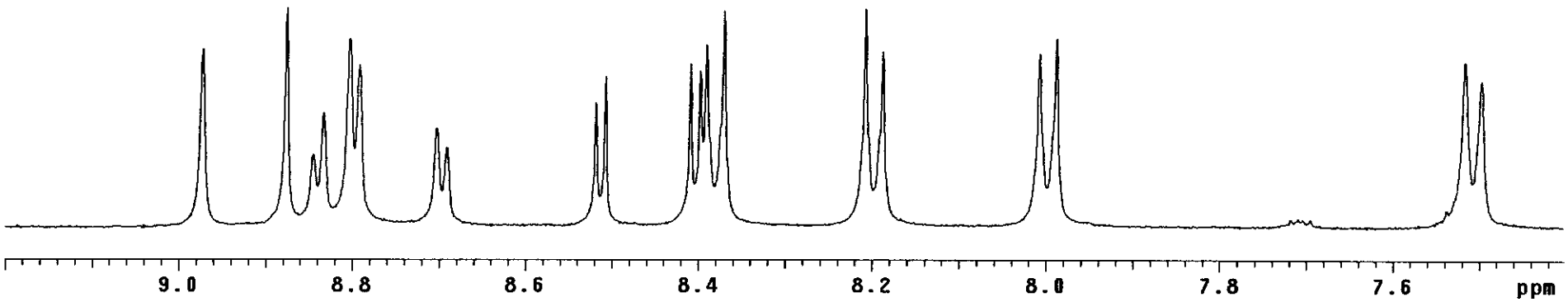

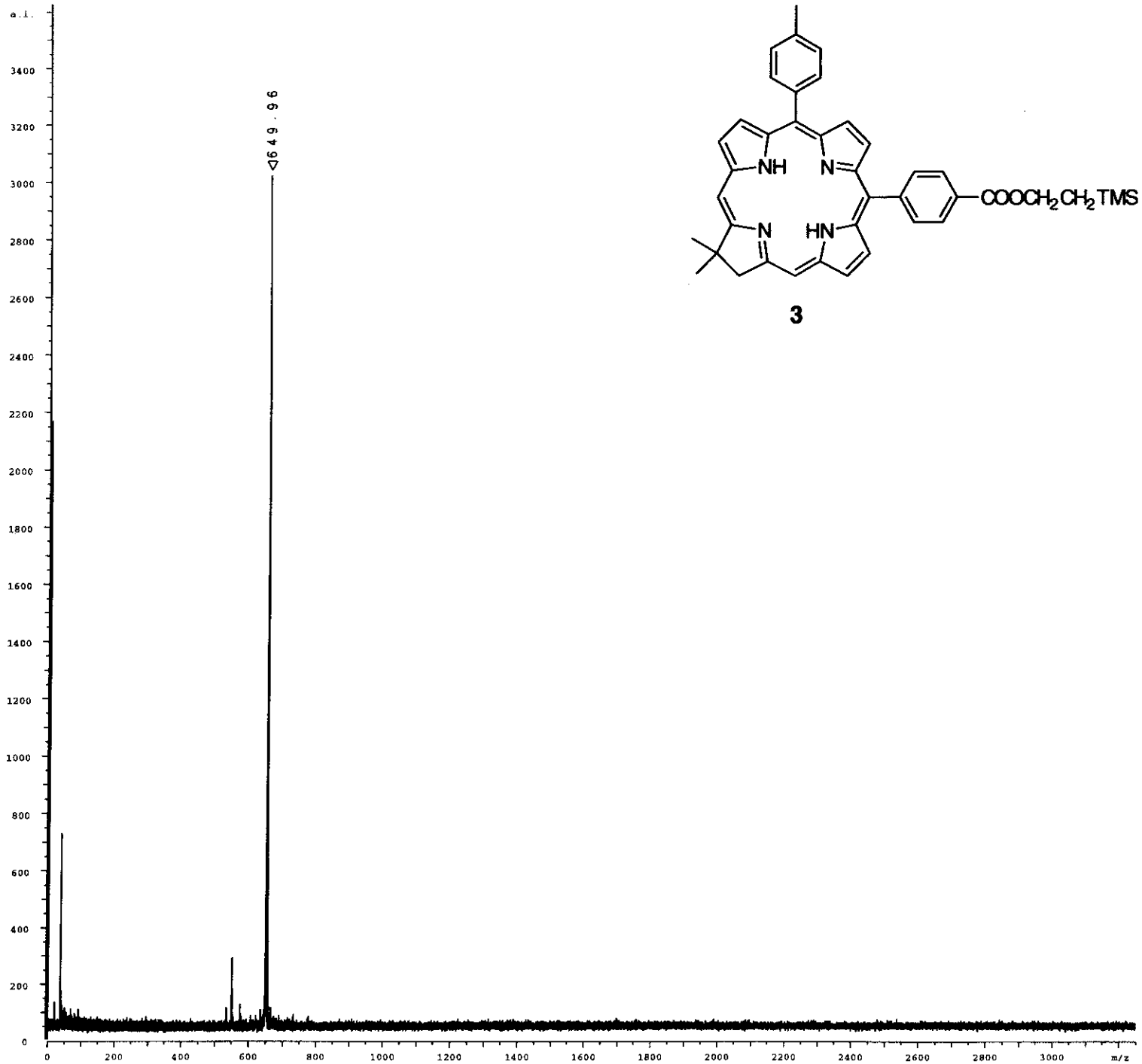

3

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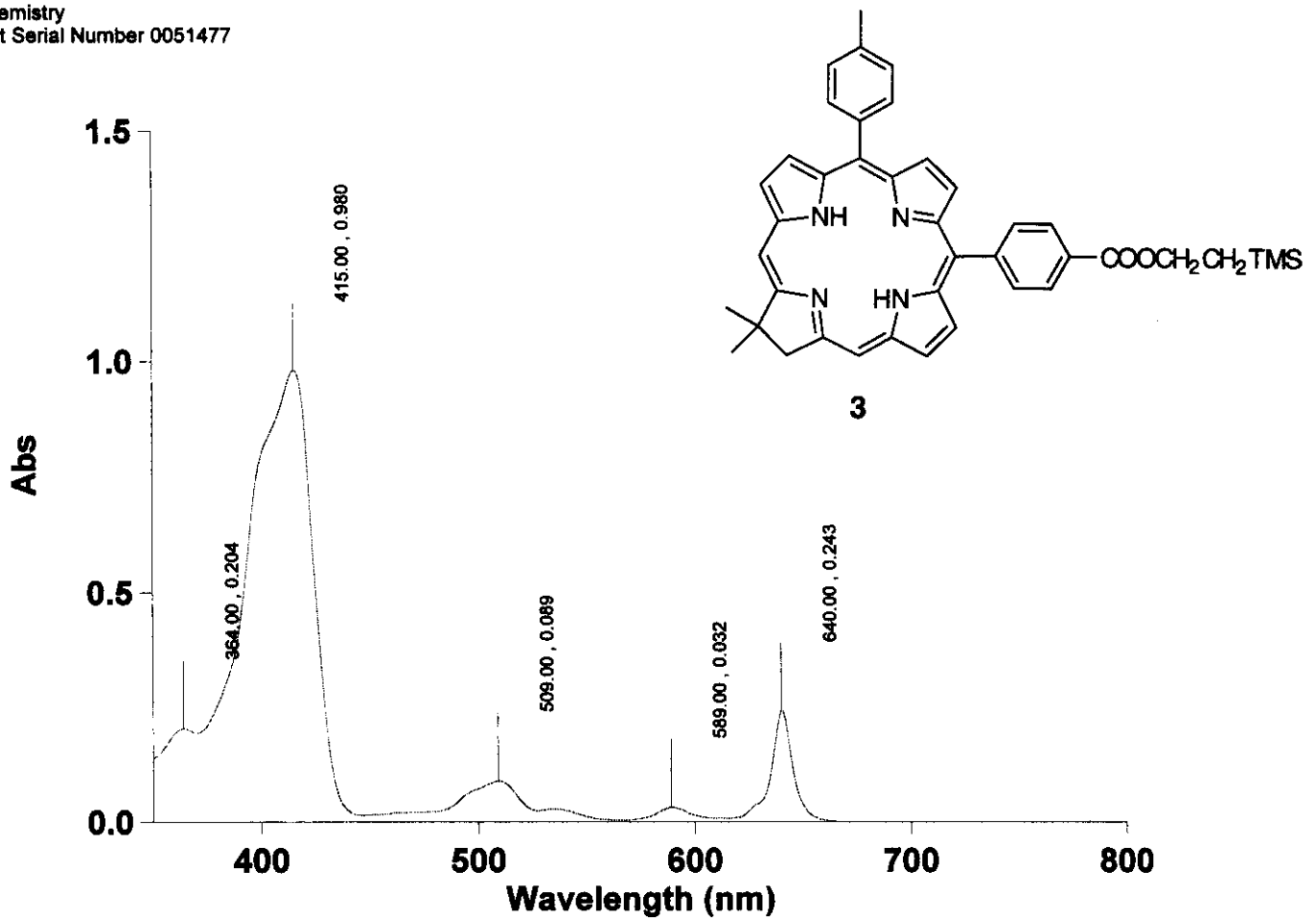
INSTRUM TOF
OpId    N. Srinivasan
SMPNAM  015499
AQ_DATE Wed Jul 18 16:25:41 2001
PATH    /data/chemistry/LINDSEY/TANIGUCHI
POLARI  POS
AQOP_m  Reflector
TD          40000
NoSHOTS       100
SMONUM          0
SMOPTS1         0
SMOPTS2         0
SMOPTS3         0
DW              1.00   [ns]
DELAY           0 [ns]
Uis1           20.00   [kV]
Uis2           18.70   [kV]
Urefl           0.00   [kV]
Ulens           7.50   [kV]
Uhimass        10.00   [kV]
RefFull         0.00   [kV]
UdetL           1.50   [kV]
UdetR           0.00   [kV]
Udefl           2.00   [kV]
REPHZ           1.00   [Hz]
ATTEN           40.0
ML1       2065947.190
ML2           327.134
ML3             0.000
HITURBO no
GDEON   yes
GDEDLY  short
DEFLON  no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1        510.84
DPMASS        700.00   [Da]
RBNDVAL         0.33
LBNDVAL         0.28
IS2BNDV         0.91
CMT1    Pb-Chl-COOCCTMS
CMT2    att 40,shots100
```

/data/chemistry/LINDSEY/TANIGUCHI/015499/1SRef/pdata/1 tof Wed Jul 18 16:27:06 2001

NCSU Chemistry
Instrument Serial Number 0051477



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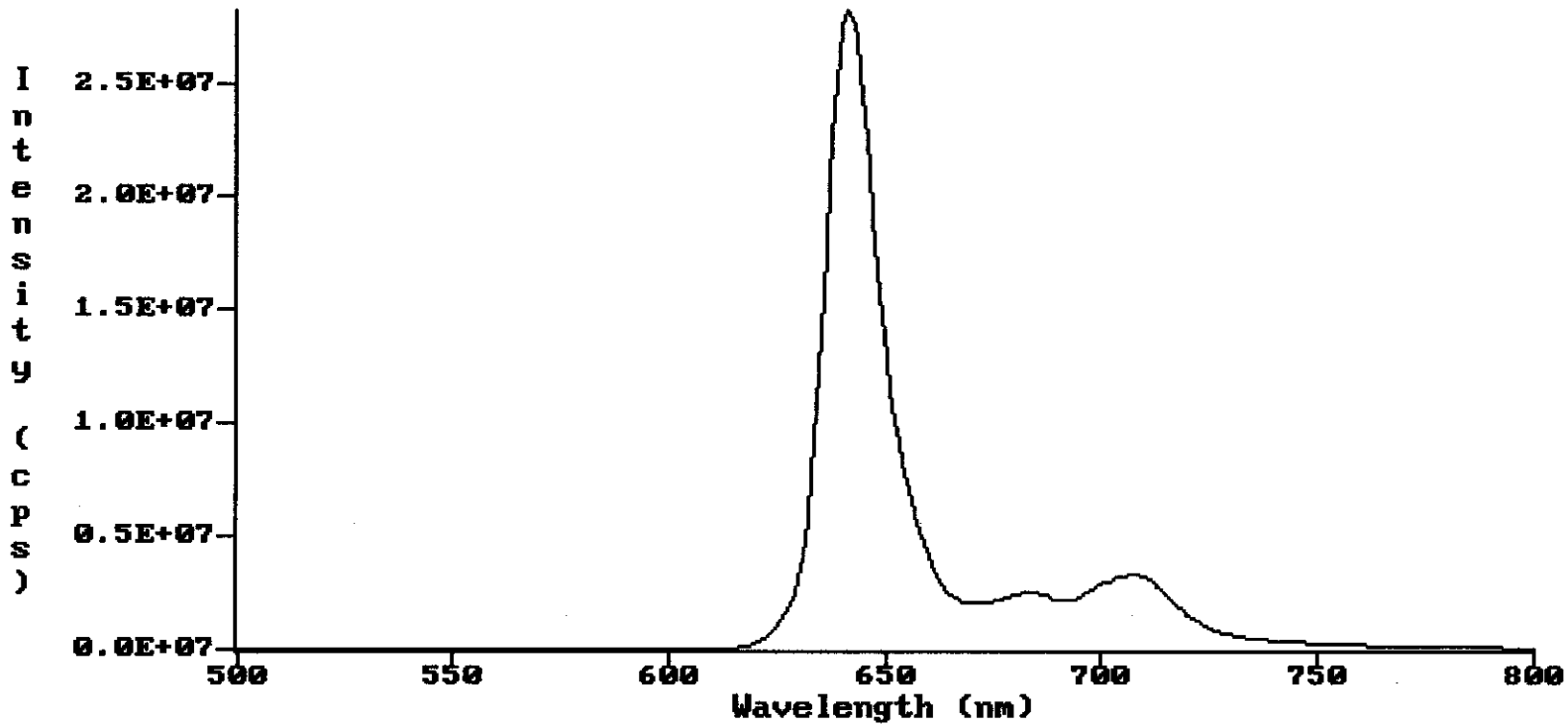

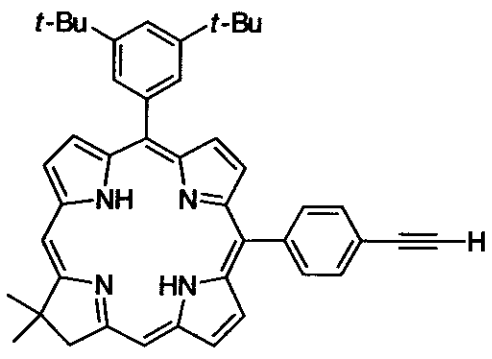

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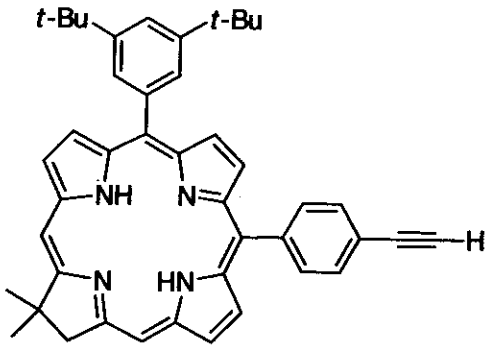

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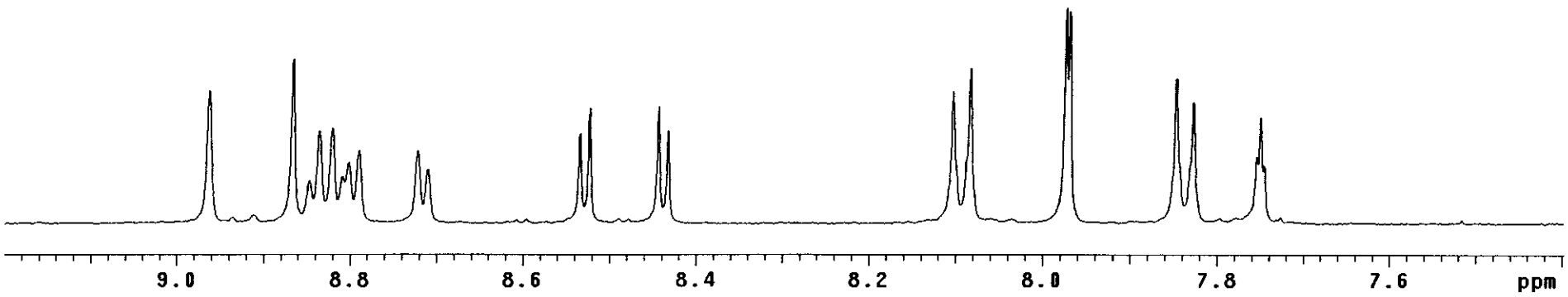

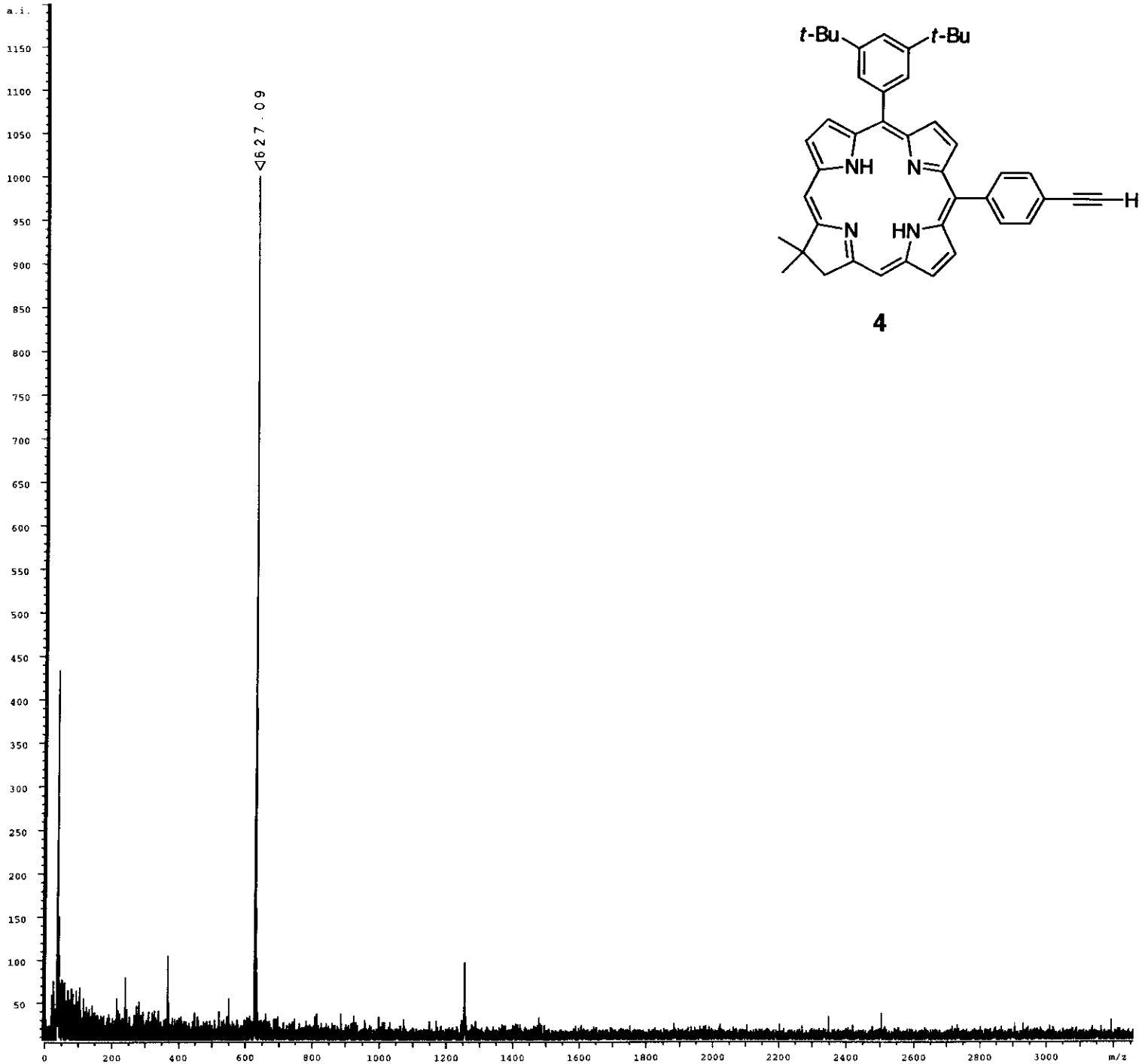

4

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INSTRUM TOF
OpId    N. Srinivasan
SMPNAM  015089
AQ_DATE Mon Apr 16 23:53:51 2001
PATH    /data/chemistry/LINDSEY/TANIGUCHI
POLARI  POS
AQOP_m  Reflector
TD          40000
NoSHOTS       100
SMONUM          0
SMOPTS1         0
SMOPTS2         0
SMOPTS3         0
DW              1.00  [ns]
DELAY           0 [ns]
Uis1           20.00  [kV]
Uis2           18.70  [kV]
Urefl           0.00  [kV]
Ulens           7.50  [kV]
Uhimass        10.00  [kV]
RefFull         0.00  [kV]
UdetL           1.50  [kV]
UdetR           0.00  [kV]
Udefl           2.00  [kV]
REPHZ           1.00  [Hz]
ATTEN           24.0
ML1       2074469.941
ML2           355.586
ML3             0.000
HITURBO no
GDEON   yes
GDEDLY  short
DEFLON  no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1        510.84
DPMASS        700.00  [Da]
RBNDVAL         0.33
LBNDVAL         0.28
IS2BNDV         0.91
CMT1    Pb Chl CCH
CMT2    atten 26, shots 100
```
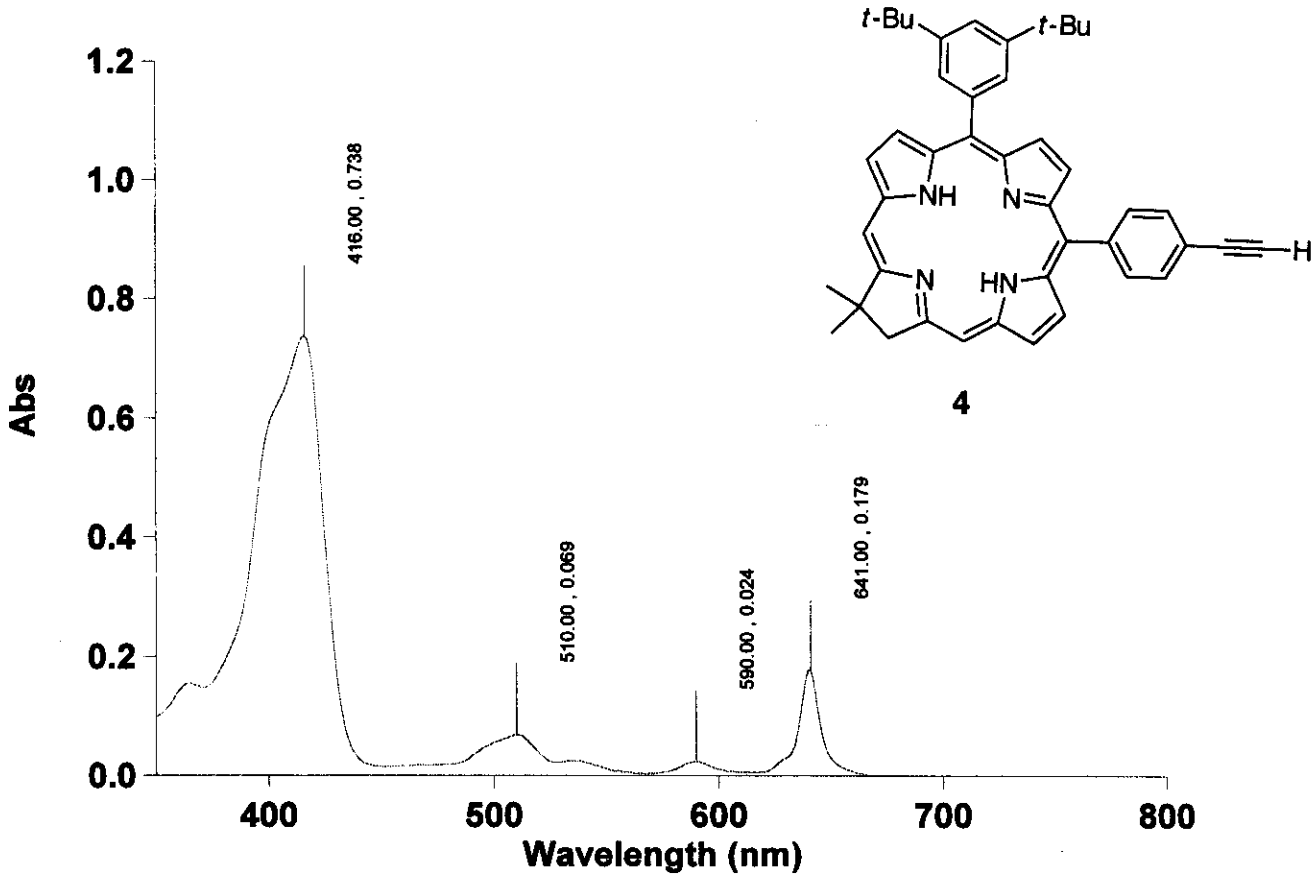
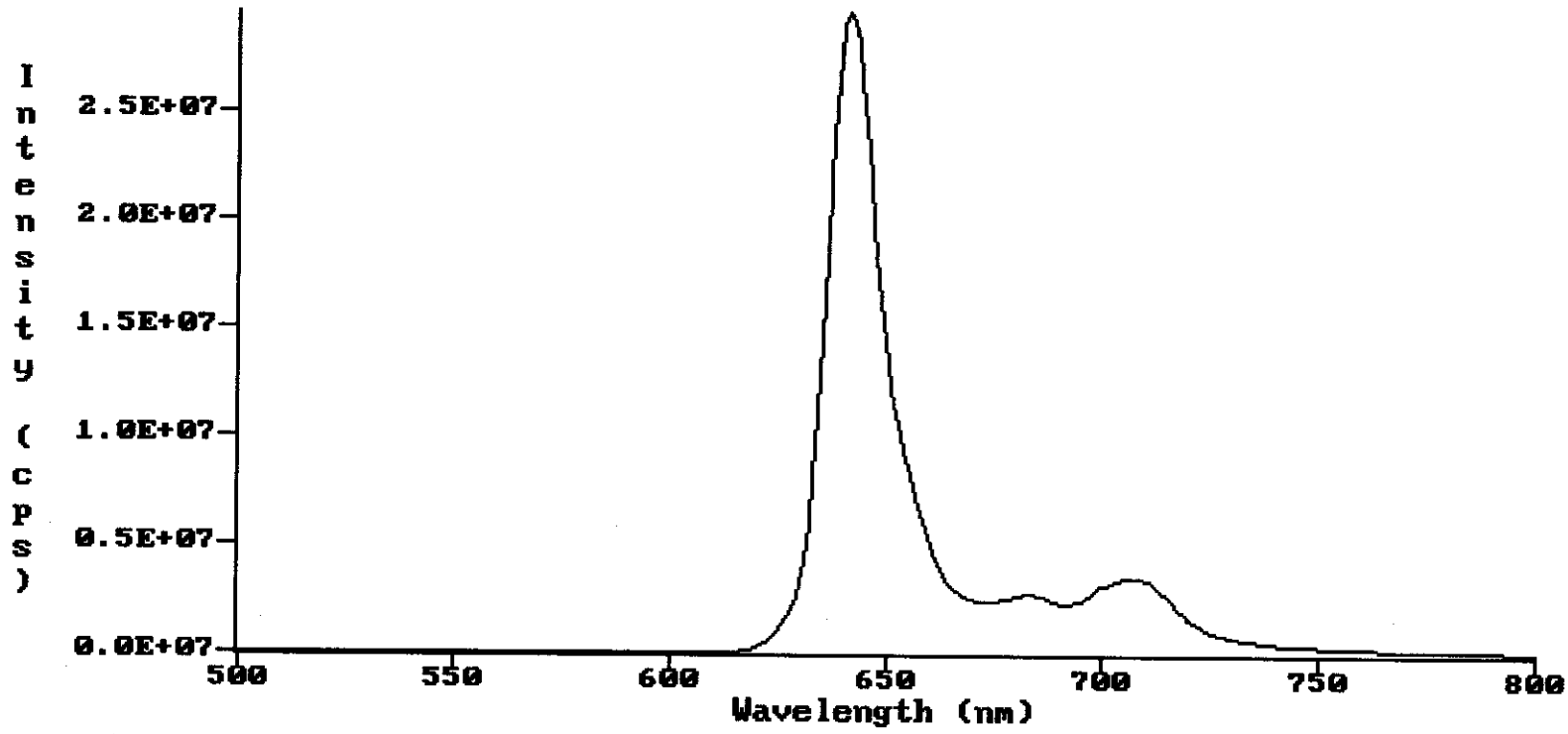
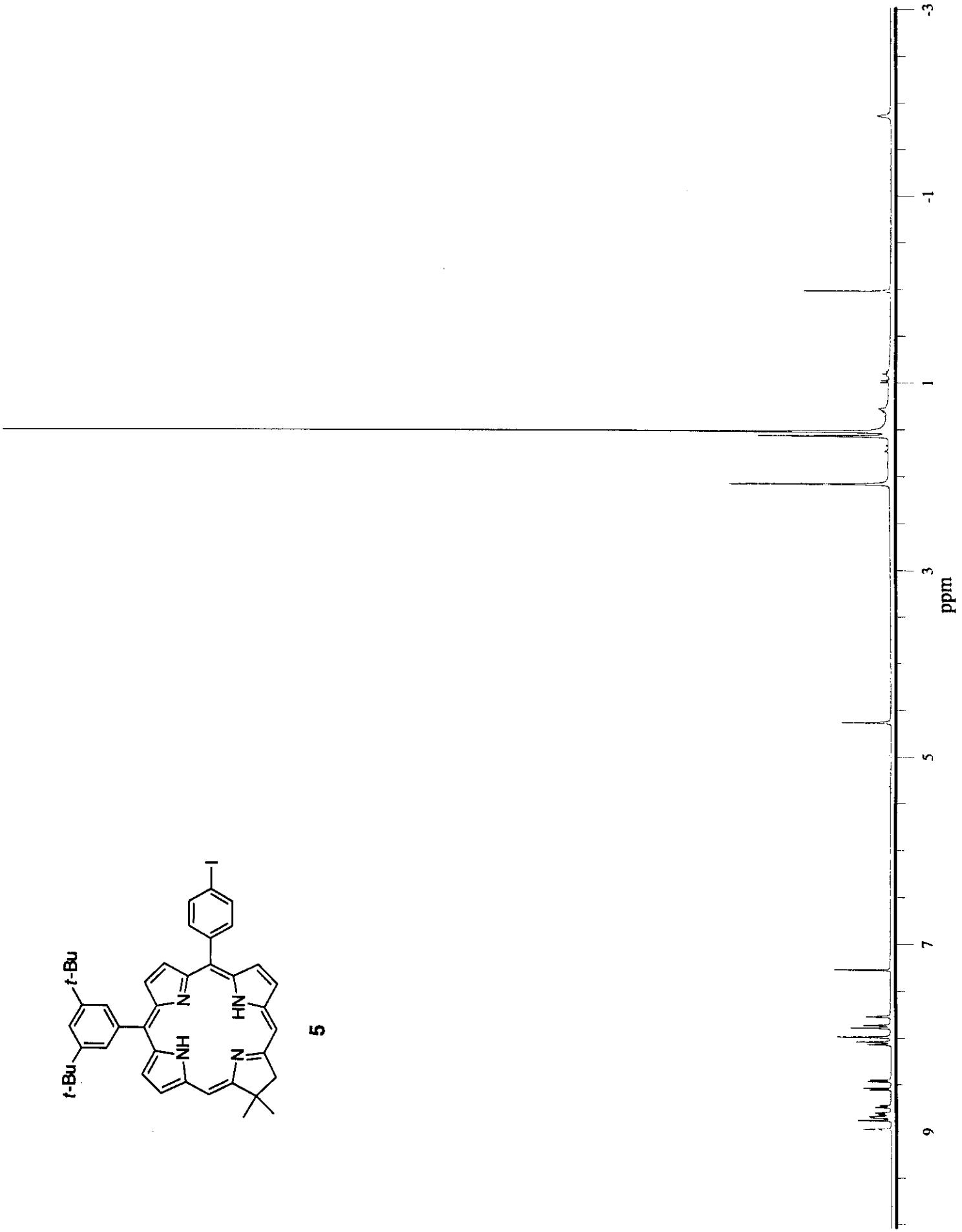

NCSU Chemistry
Instrument Serial Number 0051477







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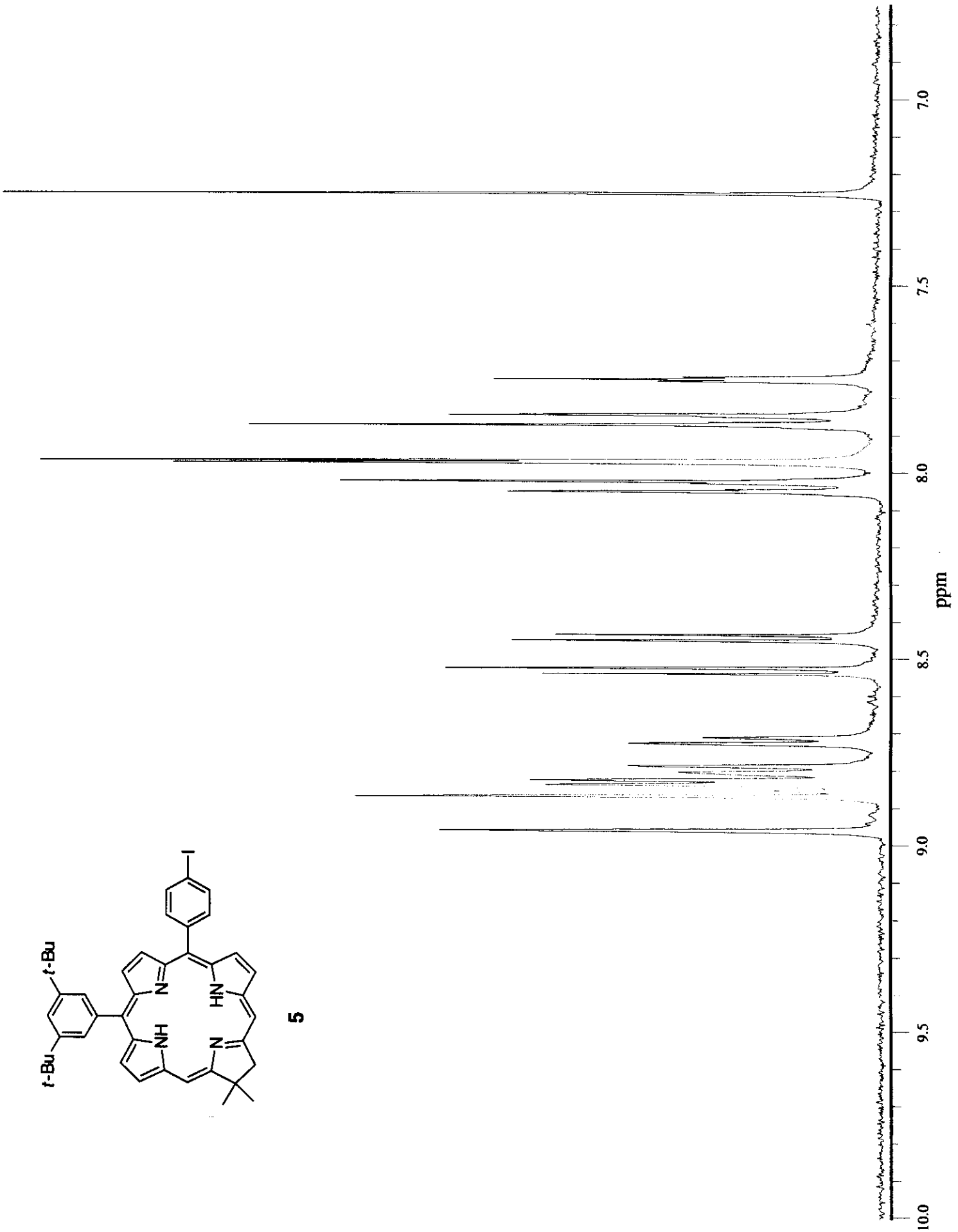

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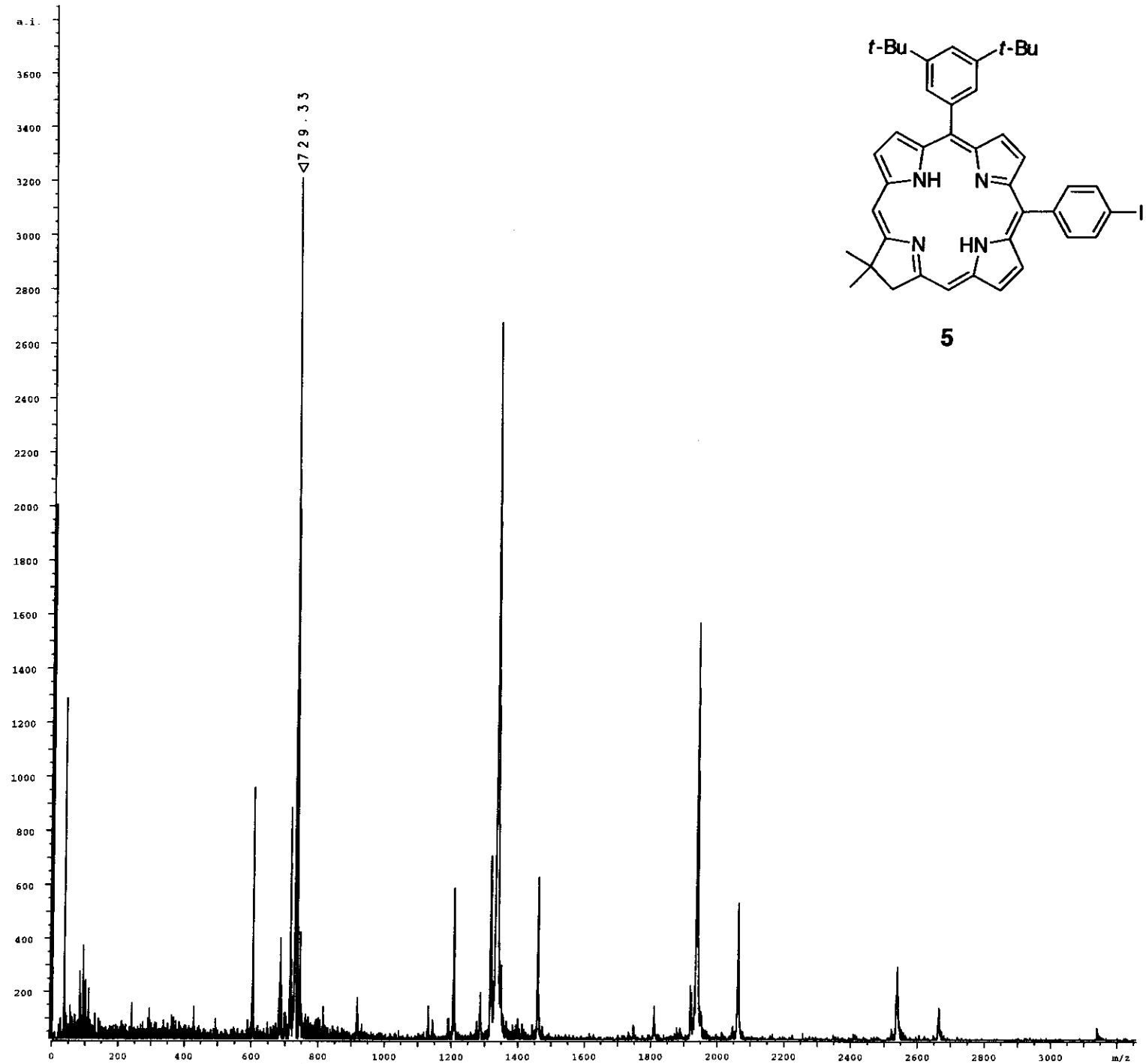

5

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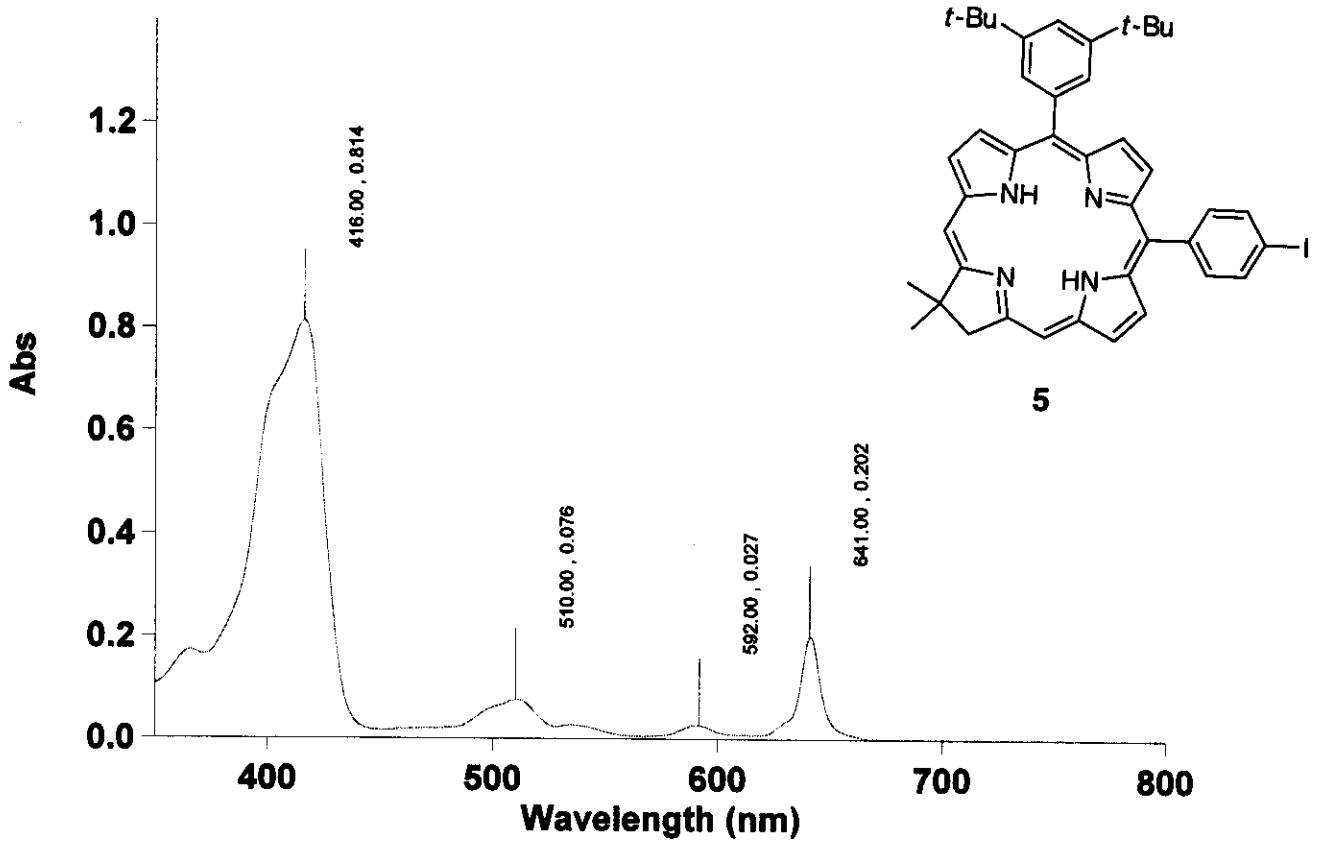
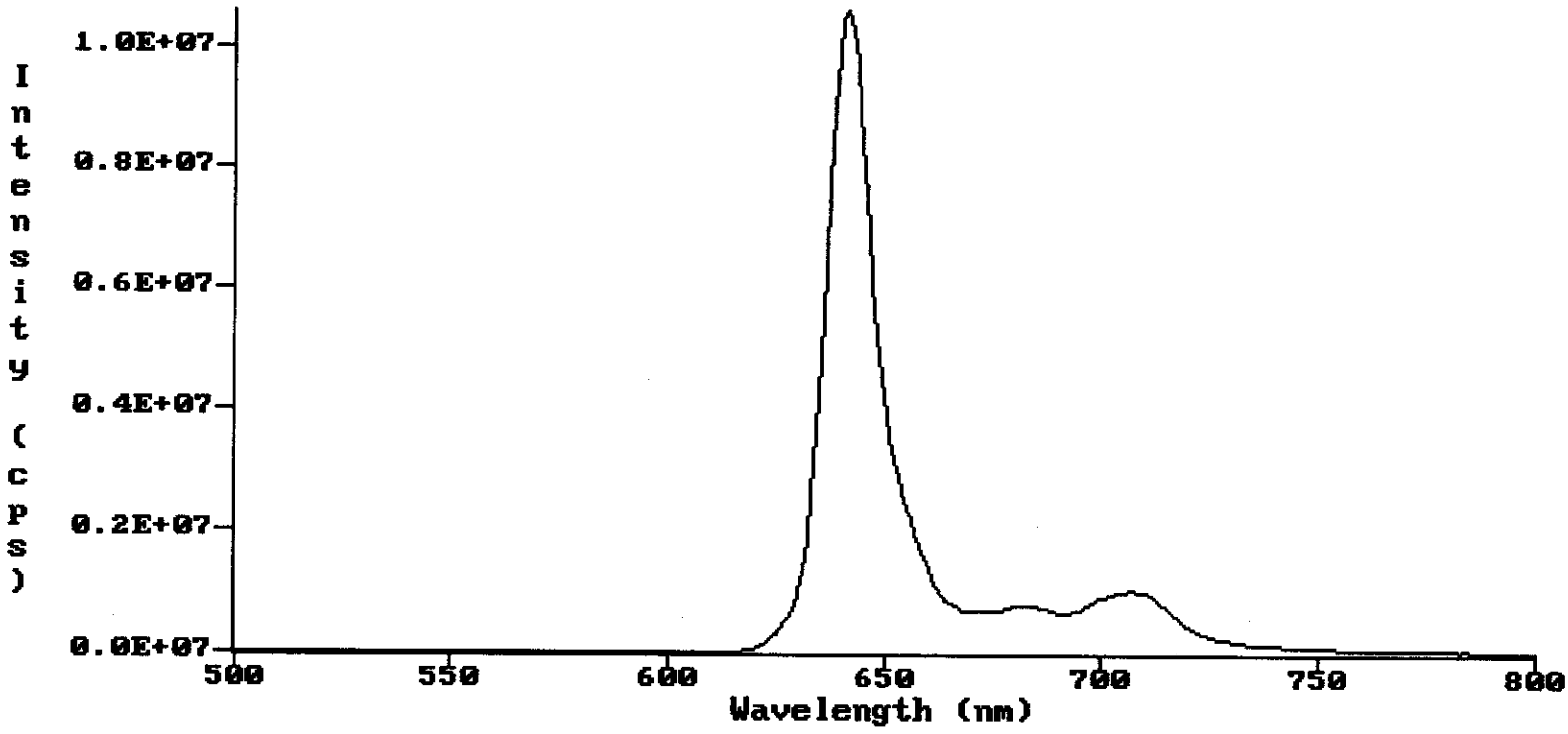
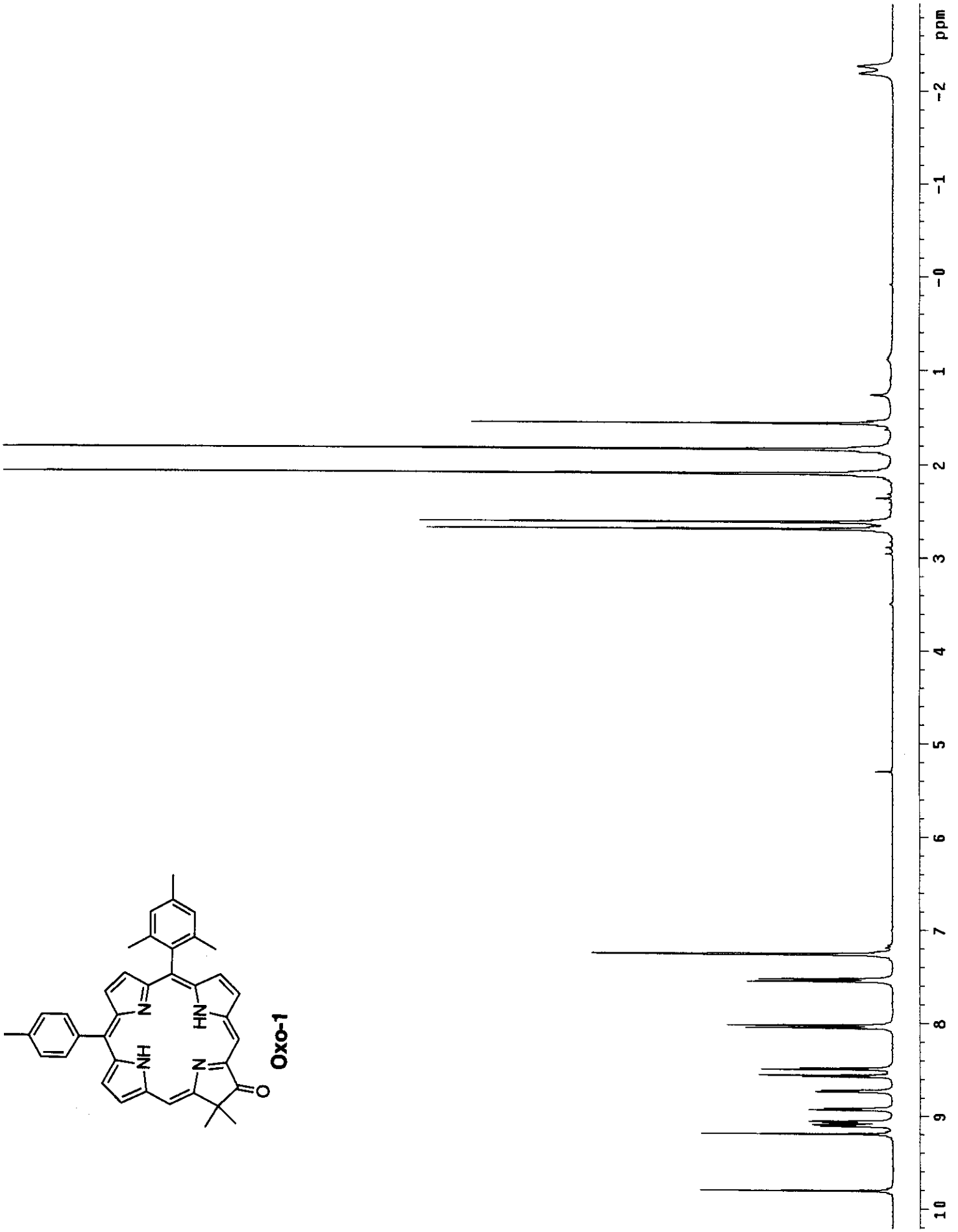
INSTRUM TOF
OpId    Unknown
SMPNAM  015099
AQ_DATE Sun Apr 22 17:44:45 2001
PATH    /data/chemistry/LINDSEY/TANIGUCHI
POLARI  POS
AQOP_m  Reflector
TD          40000
NoSHOTS        87
SMONUM          0
SMOPTS1         0
SMOPTS2         0
SMOPTS3         0
DW              1.00  [ns]
DELAY           0 [ns]
Uis1           20.00  [kV]
Uis2           18.50  [kV]
Urefl           0.00  [kV]
Ulens           7.50  [kV]
Uhimass        10.00  [kV]
RefFull         0.00  [kV]
UdetL           1.55  [kV]
UdetR           0.00  [kV]
Udefl           2.00  [kV]
REPHZ           1.00  [Hz]
ATTEN           34.0
ML1       2074469.941
ML2           355.586
ML3             0.000
HITURBO no
GDEON   yes
GDEDLY  short
DEFLON  no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1          510.84
DPMASS          200.00  [Da]
RBNDVAL           0.33
LBNDVAL           0.28
IS2BNDV           0.91
CMT1    fbchlphi
CMT2    attn34 80 shots
```

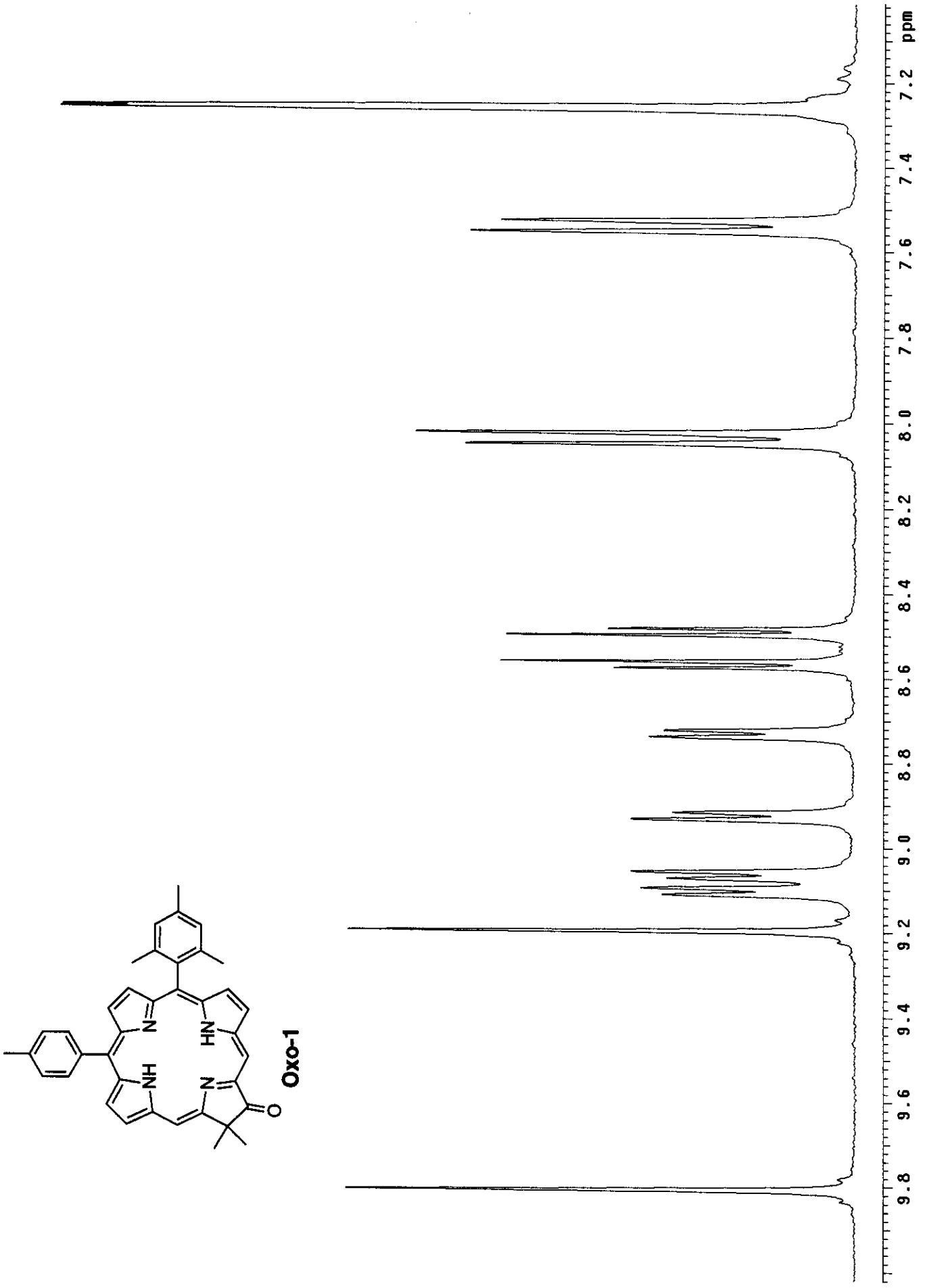
NCSU Chemistry
Instrument Serial Number 0051477

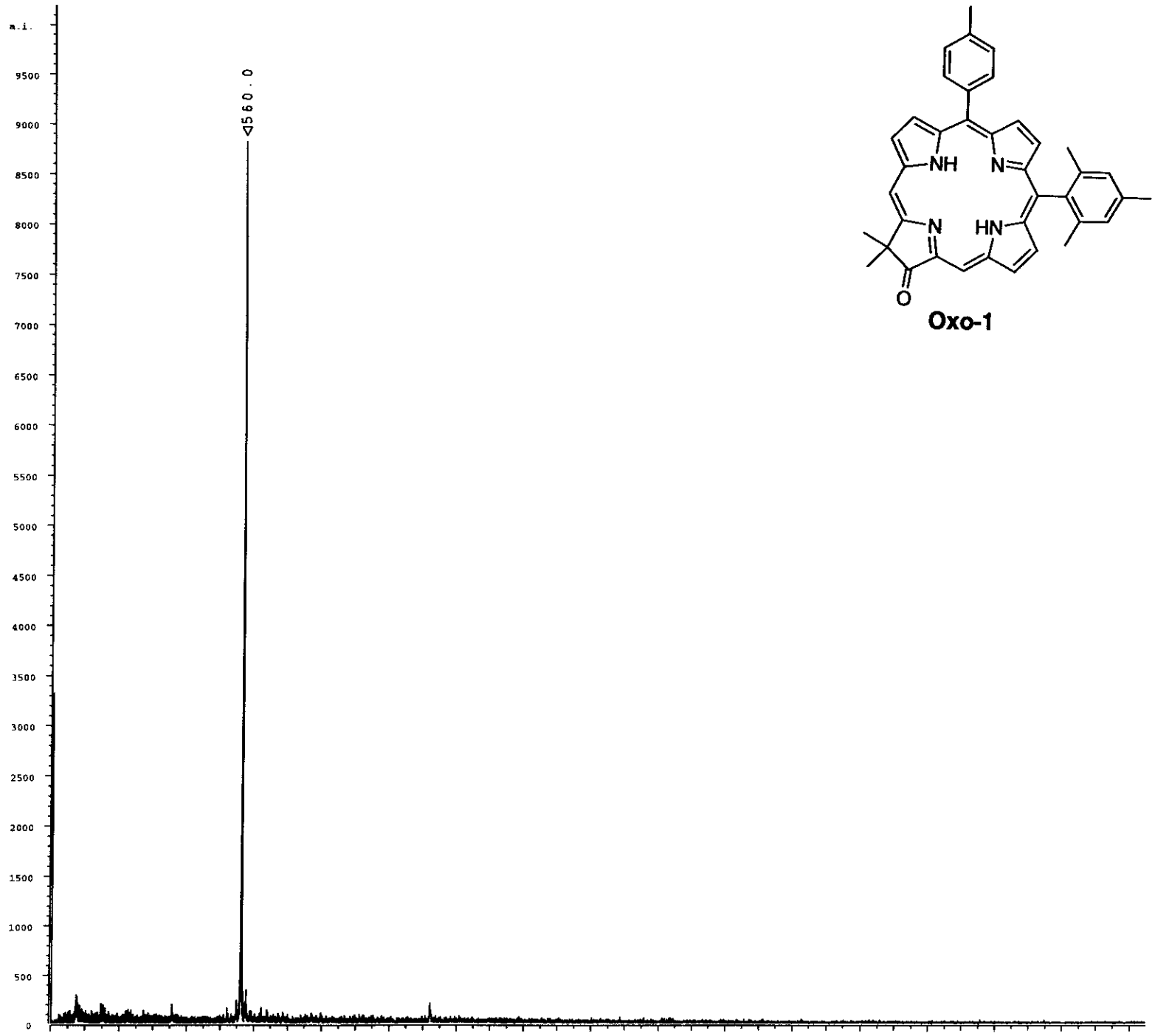






Oxo-1


Oxo-1
HN
NH
N
N
O
9.8
9.6
9.4
9.2
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
ppm

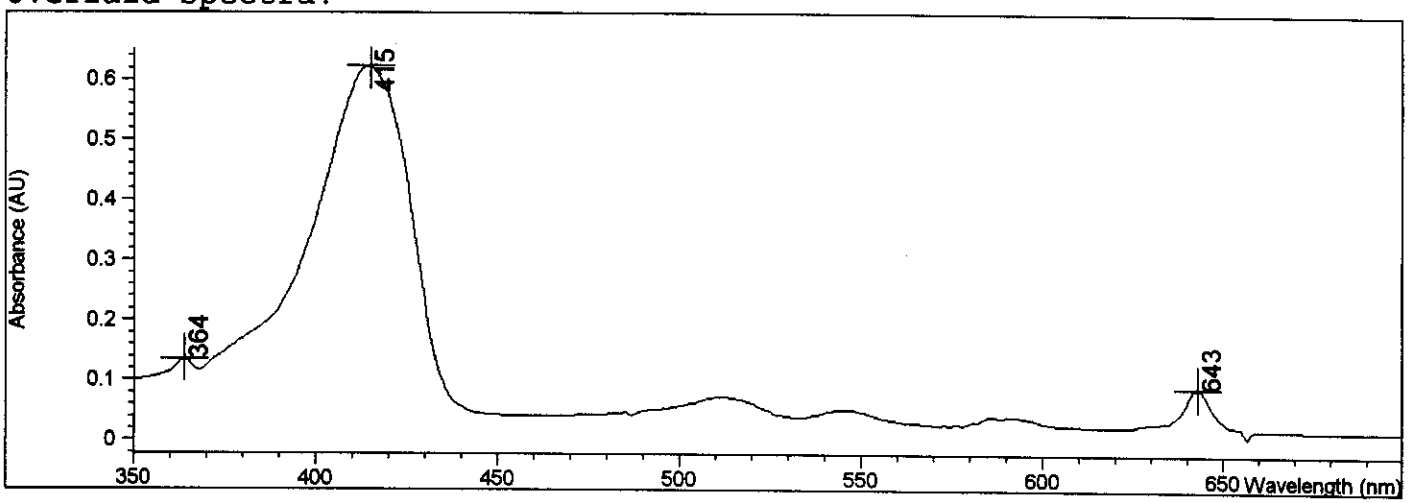

a.i.
9500
9000
8500
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
560.0
0
200
400
600
800
1000
1200
1400
1600
1800
2000
2200
2400
2600
2800
3000
m/z
/data/chemistry/LINDSEY/ARUN/014993/2SRef/pdata/1 unknown Thu Mar 29 14:23:38 2001

NH
N
N
HN
O

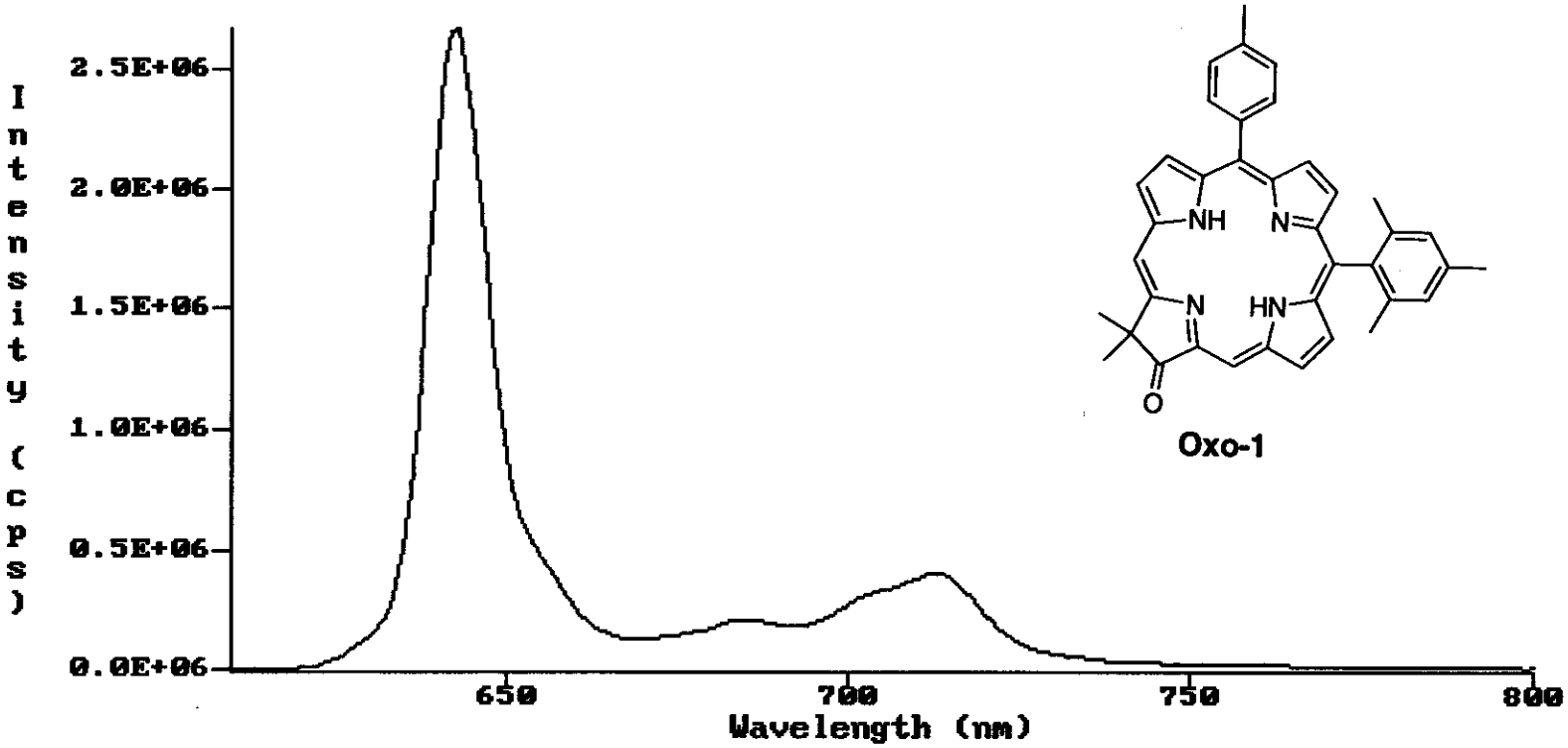
Oxo-1

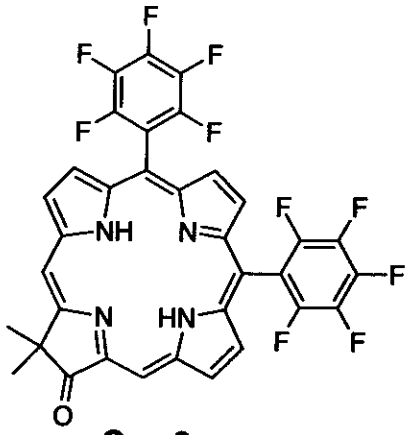
Method file : <untitled>
Information : Default Method
Data File : C:\RSLSPE~1\04230102.SD Created : 4/23/01 17:36:37

Overlaid Spectra:

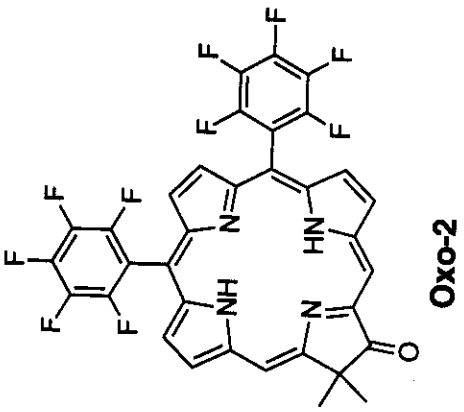


#	Name	Peaks (nm)	Abs (AU)
1	Mes-Fb-Oxo	415.0	0.62237
1		364.0	0.13570
1		643.0	8.9929E-2

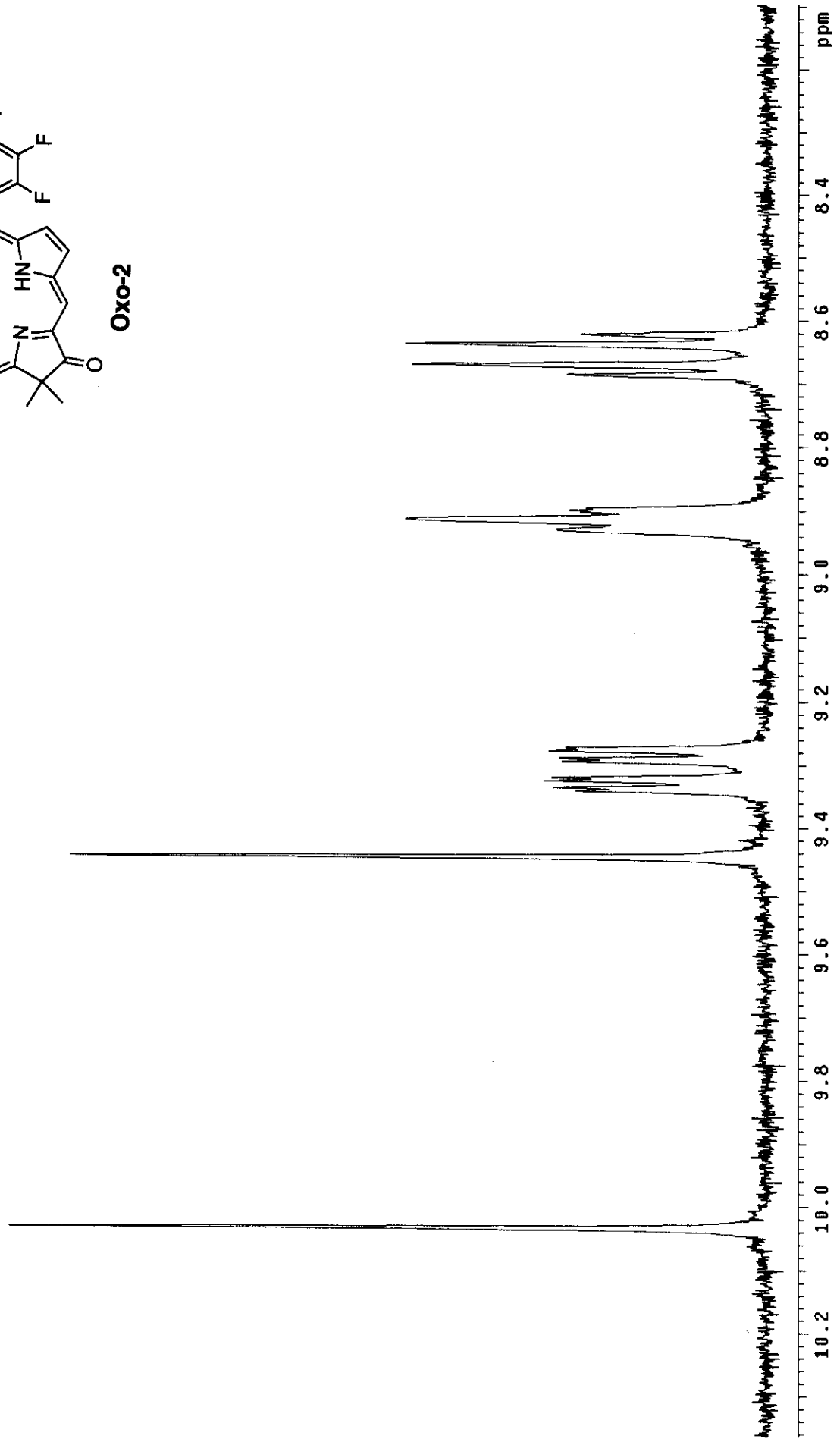


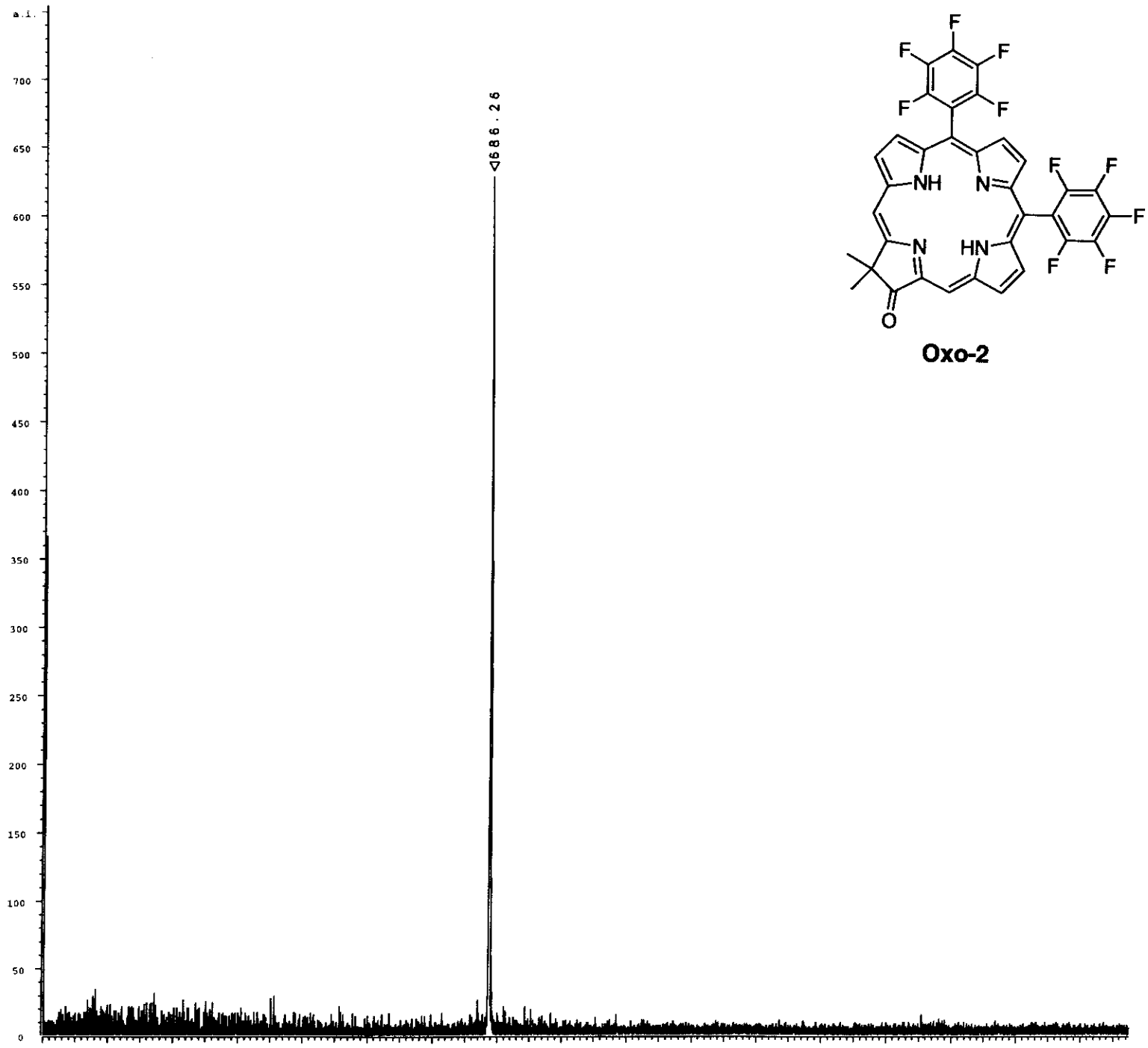


Oxo-2



Oxo-2





Oxo-2

```
INSTRUM TOF
OpId    N. Srinivasan
SMPNAM  015034
AQ_DATE Wed Apr  4 11:26:08 2001
PATH    /data/chemistry/LINDSEY/PRATHAPAN
POLARI  POS
AQOP_m  Reflector
TD          40000
NoSHOTS        20
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]
Ulens           7.50   [kV]
Uhimass        10.00   [kV]
RefFull         0.00   [kV]
UdetL           1.50   [kV]
UderR           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
GDEDLY  short
DEFLON  no
RLNSEND no
LLNSEND no
UIS2END no
DPCAL1         510.84
DPMASS         700.00   [Da]
RENDVAL          0.33
LENDVAL          0.28
IS2ENDV          0.91
CMT1    (PPP)2FBChlorin
CMT2    attn 33, shots 20
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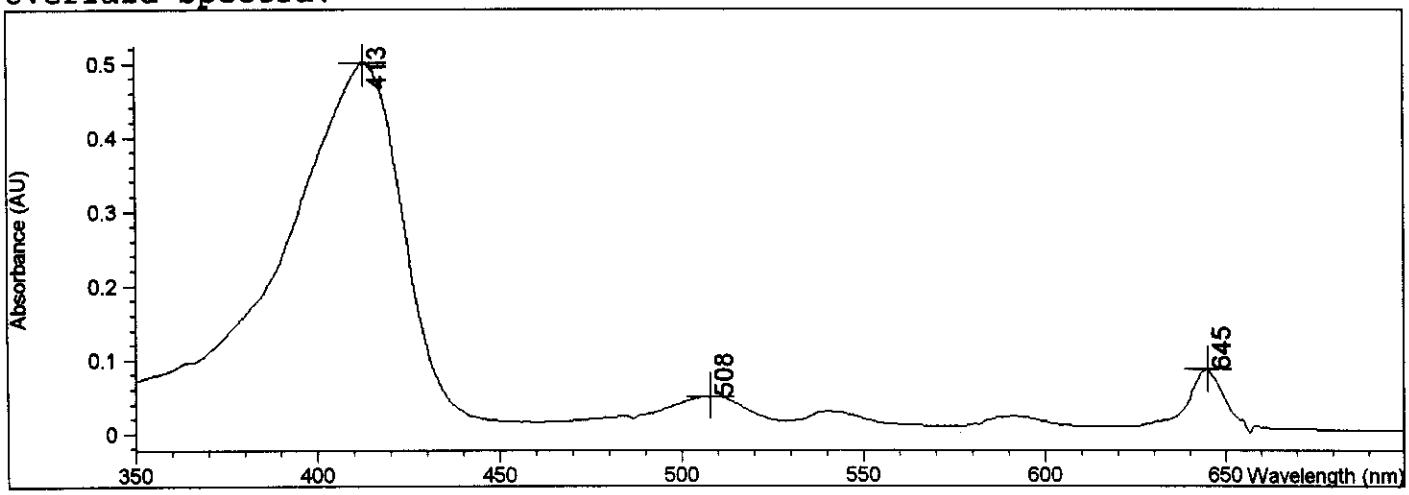
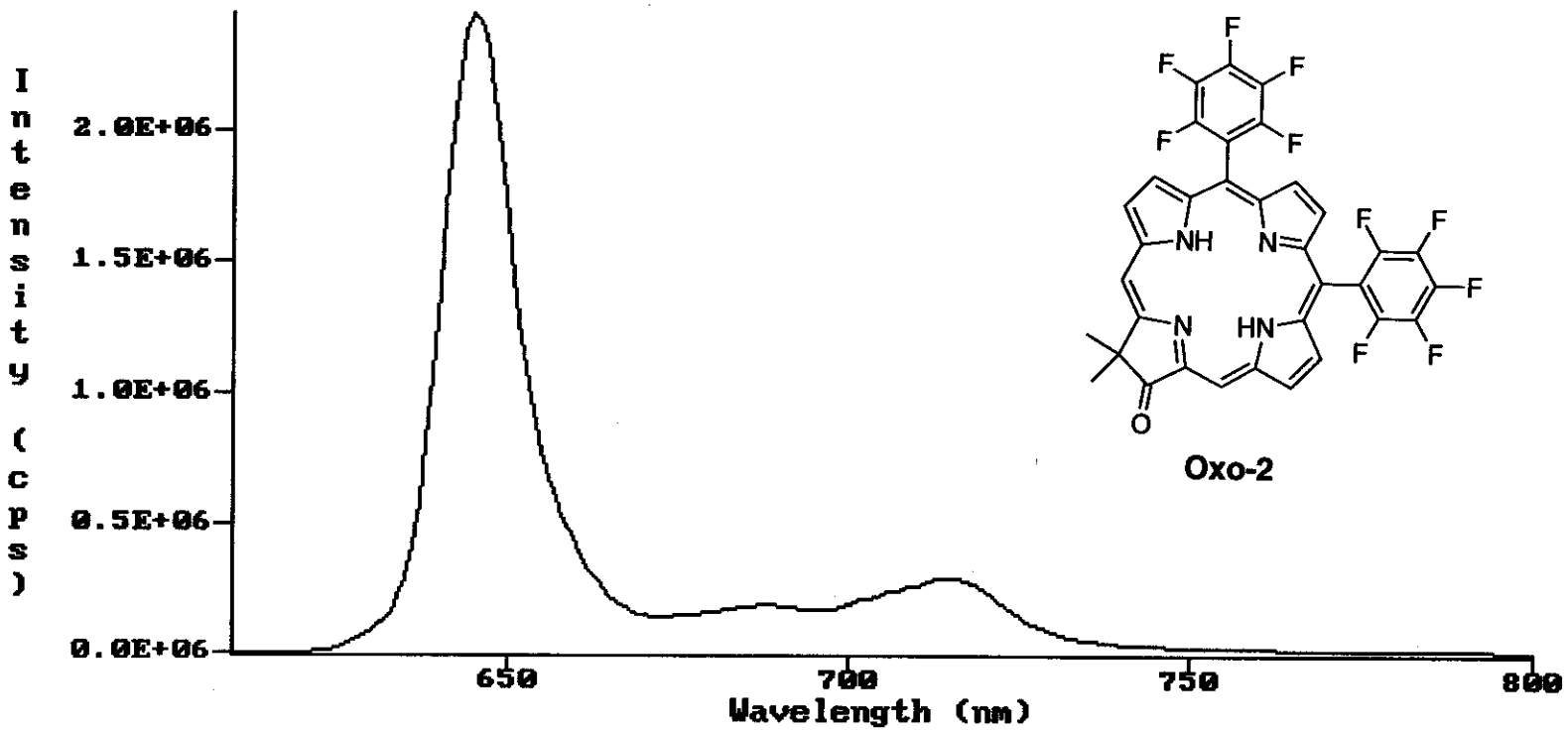
Method file : <untitled>
Information : Default Method
Data File : C:\RSLSPE~1\04230103.SD Created : 4/23/01 18:02:39

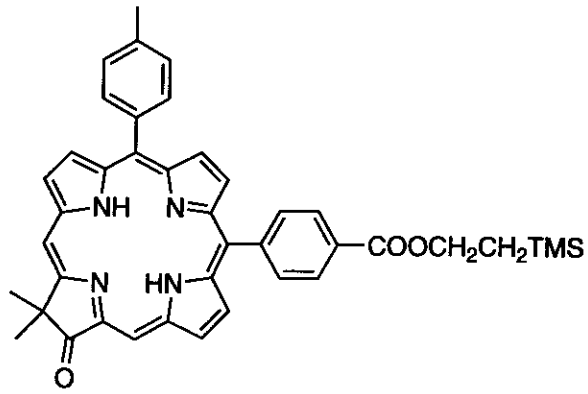
Overlaid Spectra:



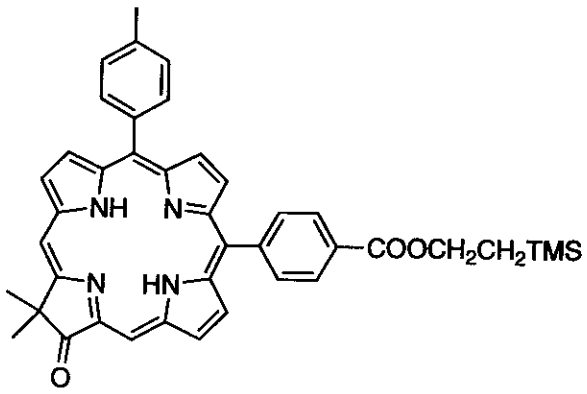
#	Name	Peaks(nm)	Abs(AU)
1	F5-Fb-Oxo	413.0	0.50016
1		645.0	8.6864E-2
1		508.0	5.0235E-2



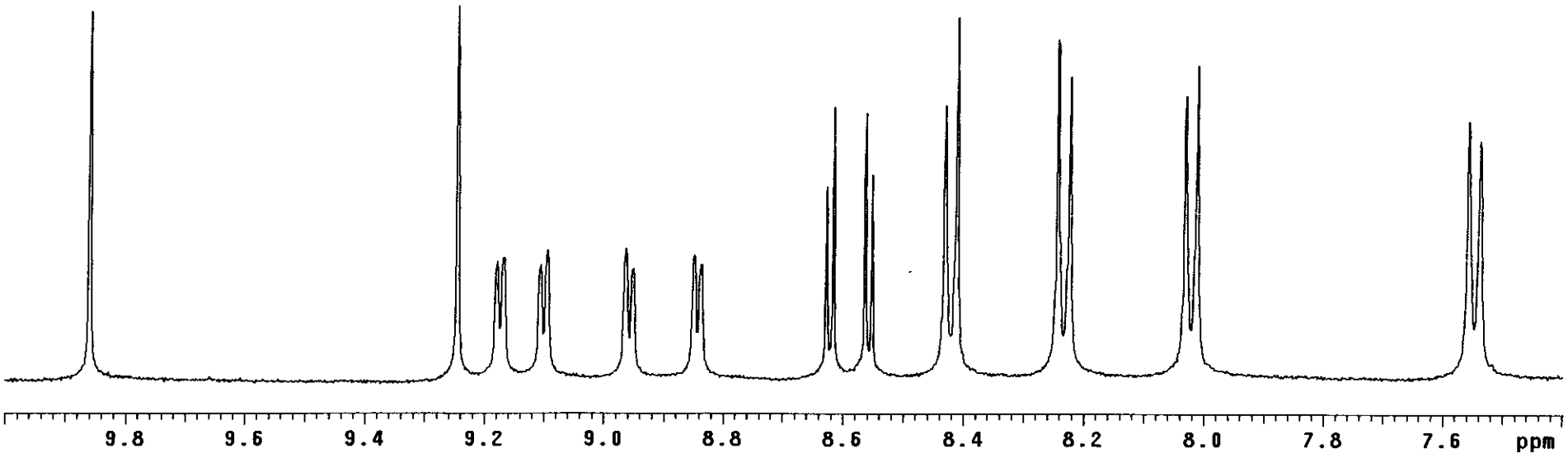
Oxo-2

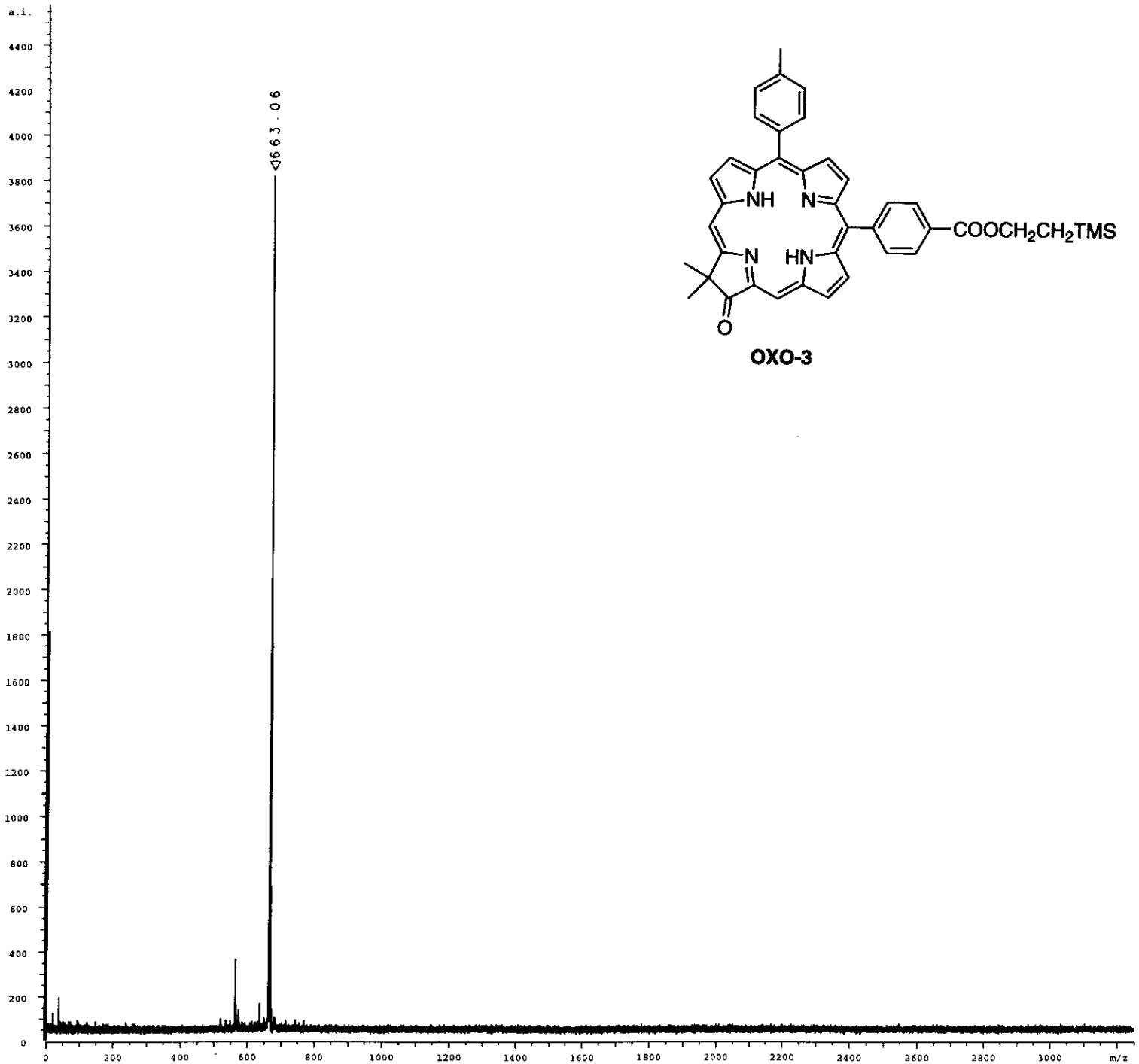


OXO-3



OXO-3



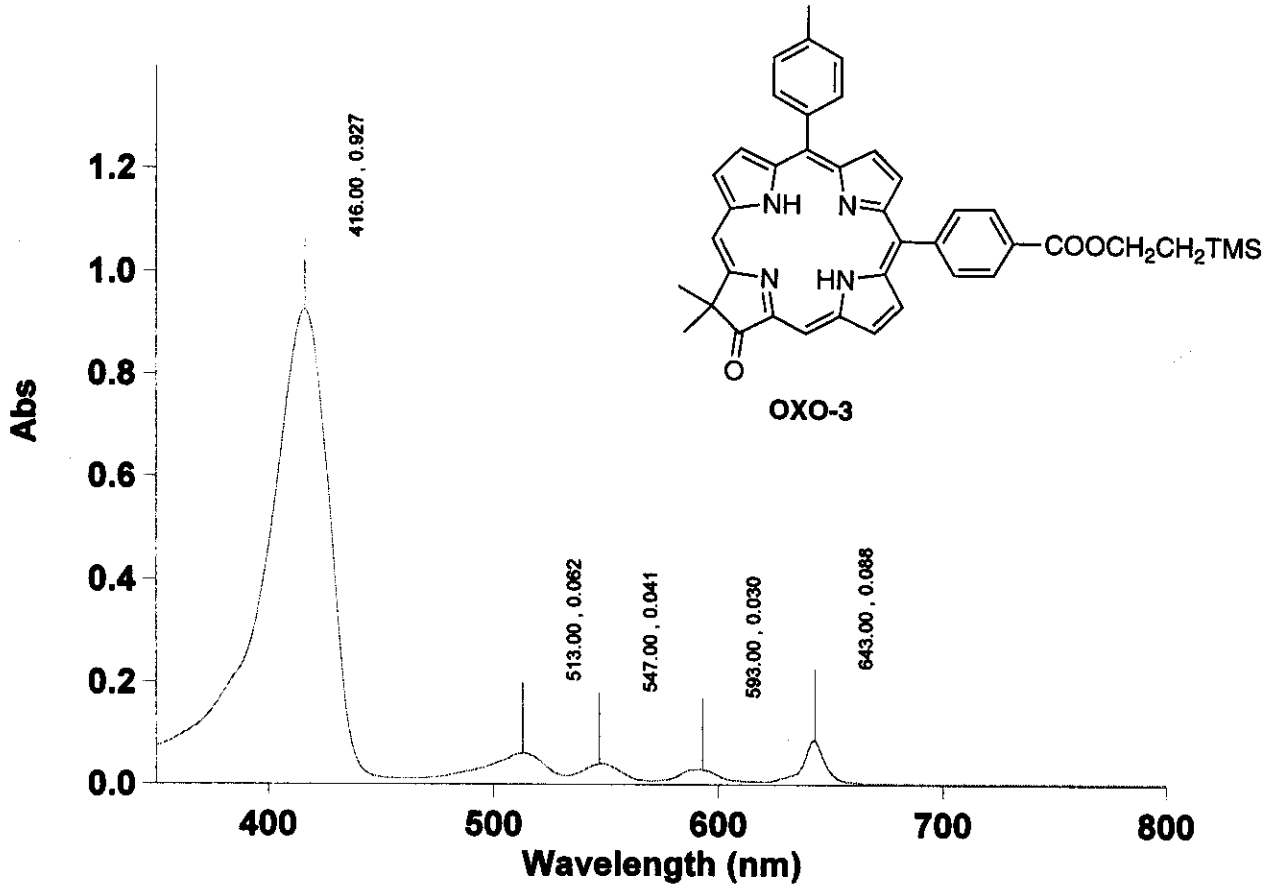


OXO-3

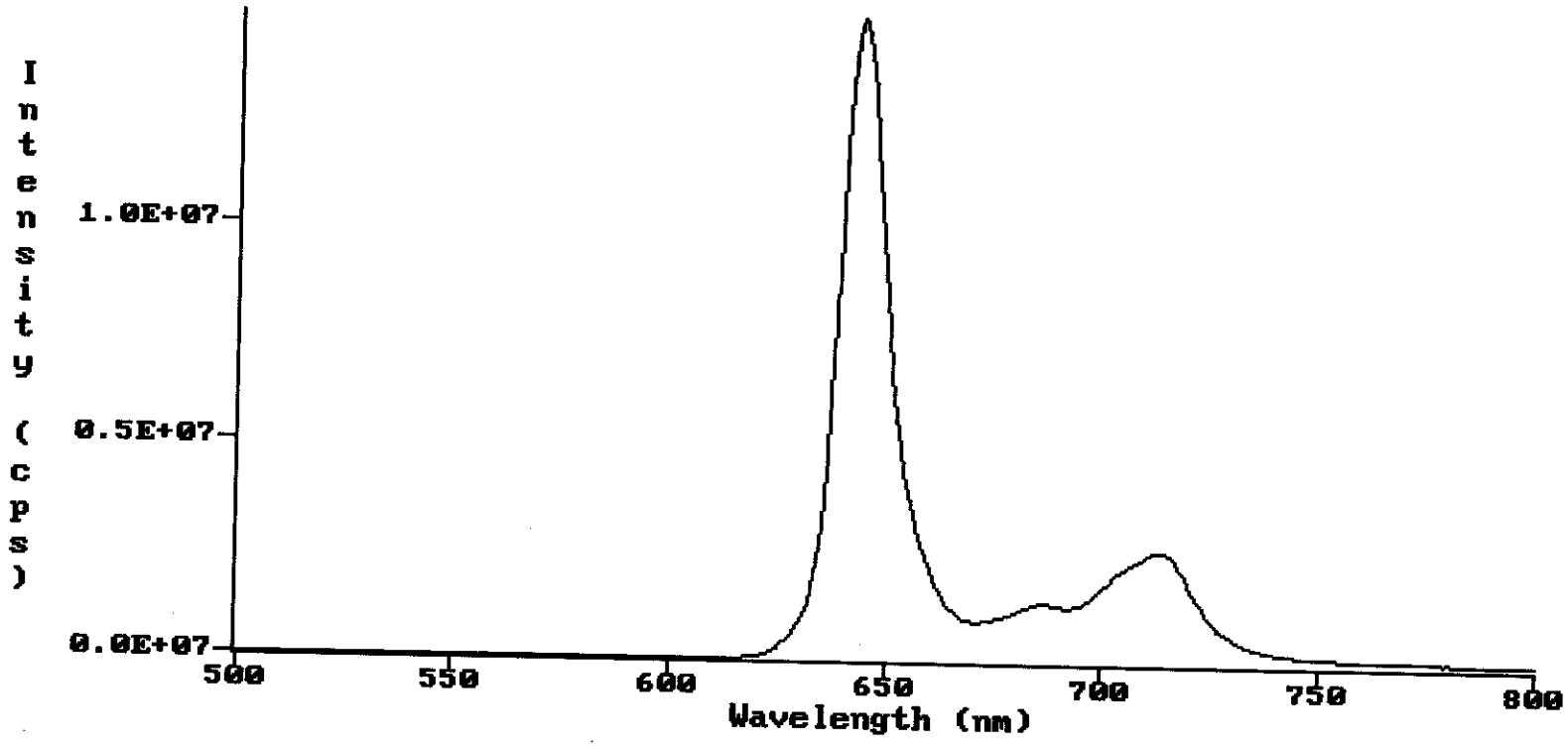
```
INSTRUM TOF
OpId    N. Srinivasan
SMPNAM  015498
AQ_DATE Wed Jul 18 16:14:40 2001
PATH    /data/chemistry/LINDSEY/TANIGUCHI
POLARI  POS
AQOP_m  Reflector
TD          40000
NoSHOTS       100
SMONUM          0
SMOPTS1         0
SMOPTS2         0
SMOPTS3         0
DW              1.00   [ns]
DELAY           0 [ns]
Uis1           20.00   [kV]
Uis2           18.70   [kV]
Urefl           0.00   [kV]
Ulens           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           44.0
ML1       2065947.190
ML2           327.134
ML3             0.000
HITURBO no
GDEON   yes
GDEDLY  short
DEFLON  no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1        510.84
DPMASS        700.00   [Da]
RENDVAL         0.33
LENDVAL         0.28
IS2BNDV         0.91
CMT1    Fb-OXO-COOCCTMS
CMT2    att 44,shots50
```

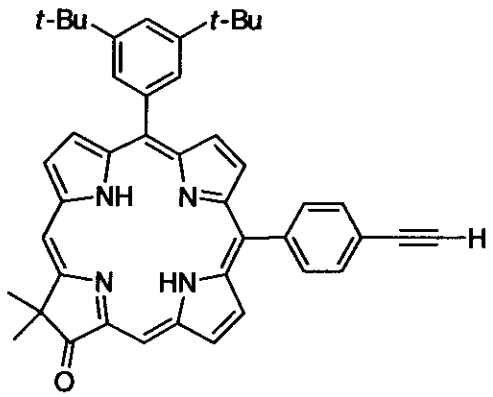
/data/chemistry/LINDSEY/TANIGUCHI/015498/1SRef/pdata/1 tof Wed Jul 18 16:17:31 2001

NCSU Chemistry
Instrument Serial Number 0051477

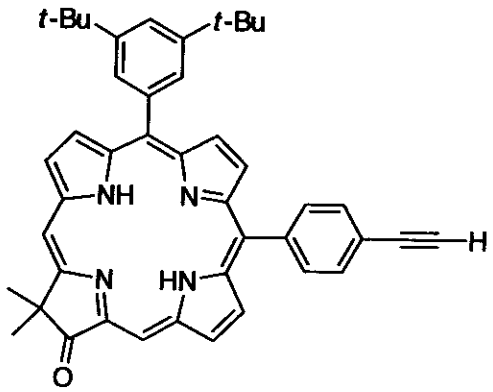


OXO-3

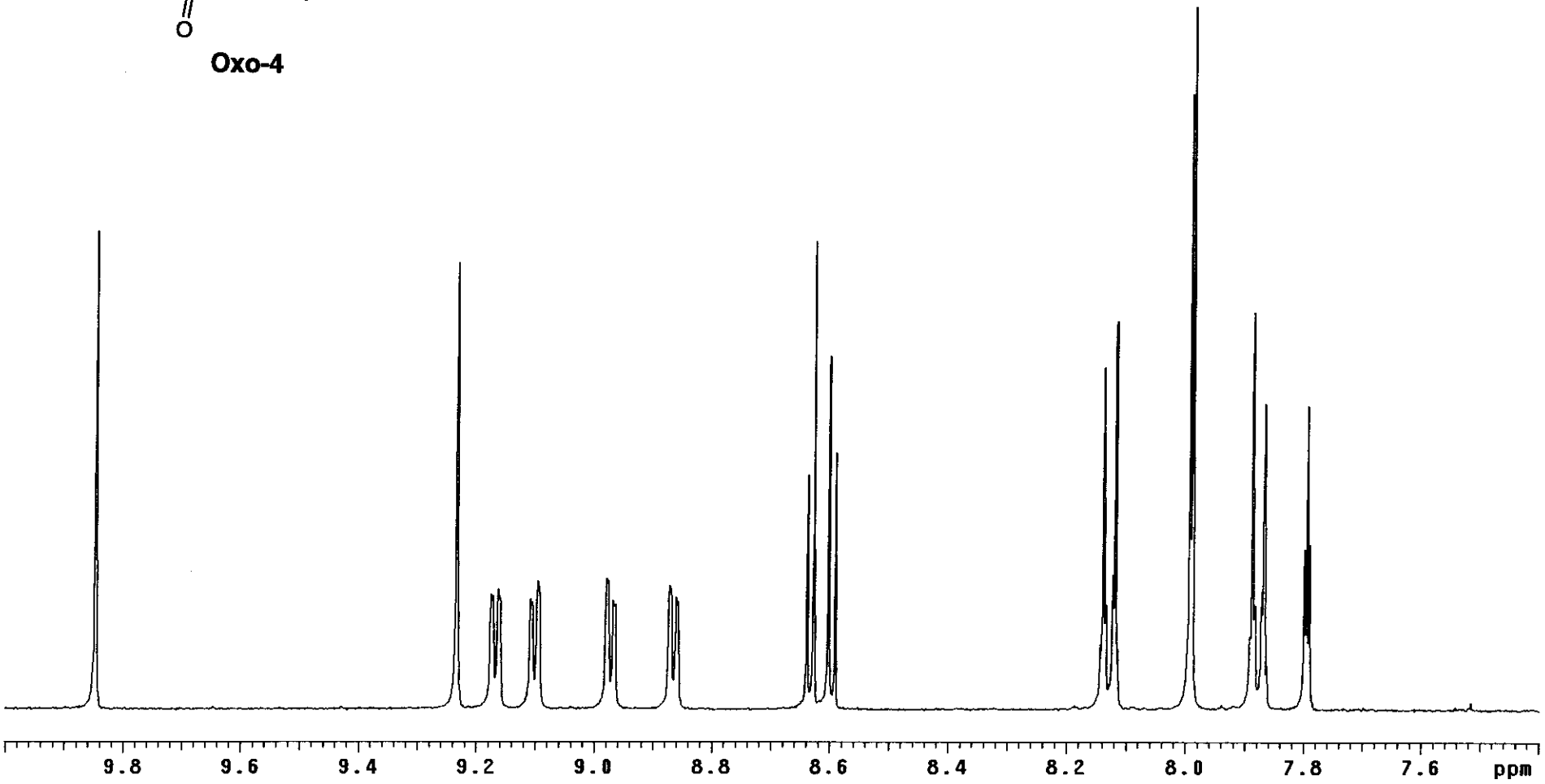


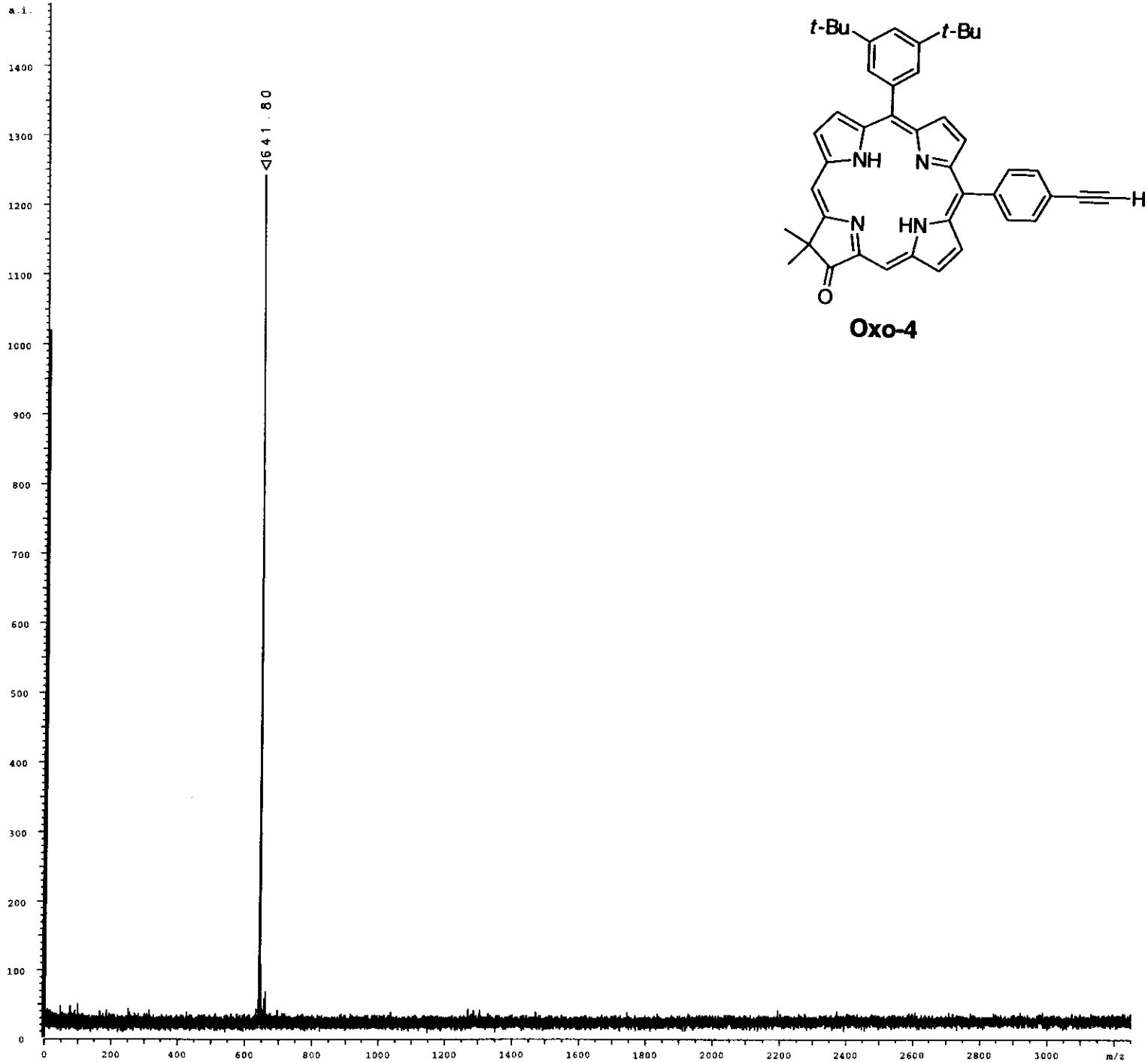


Oxo-4



Oxo-4

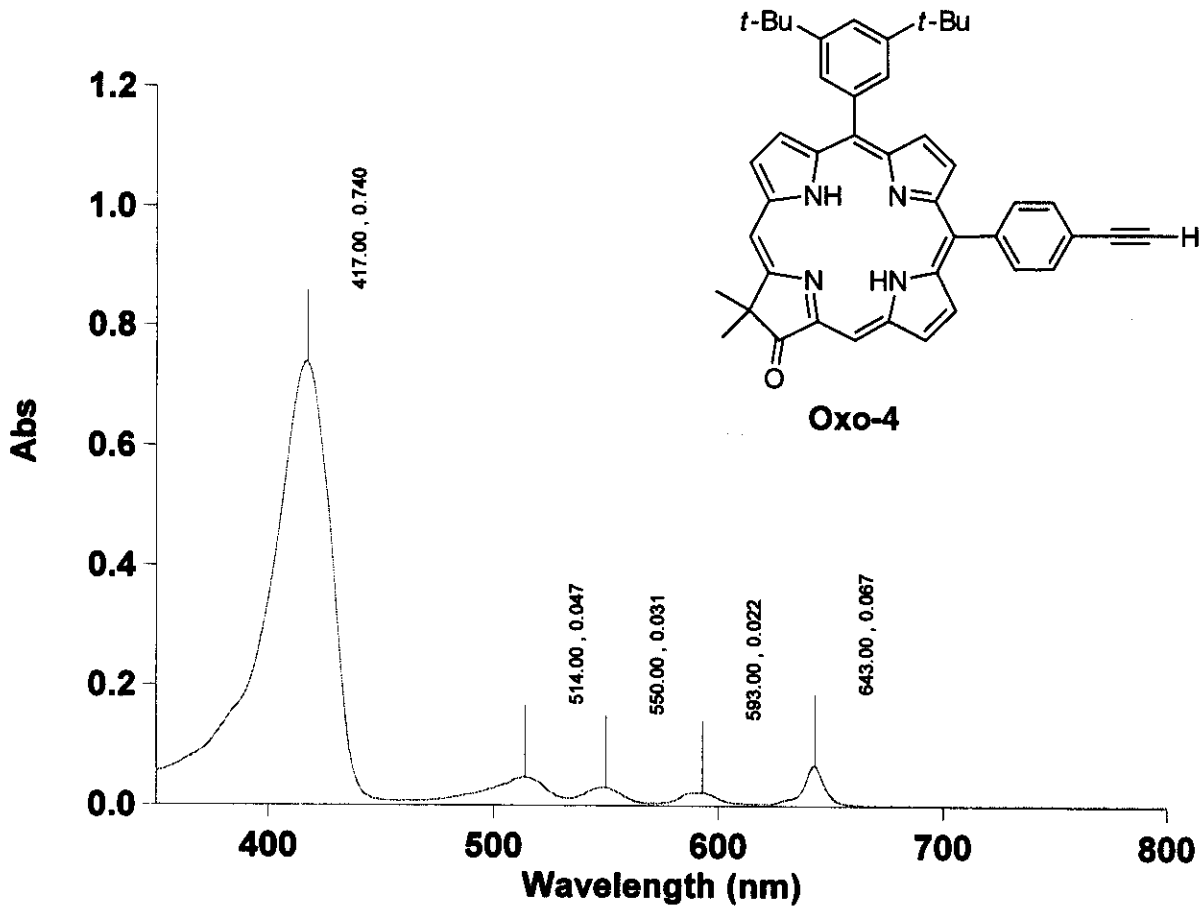


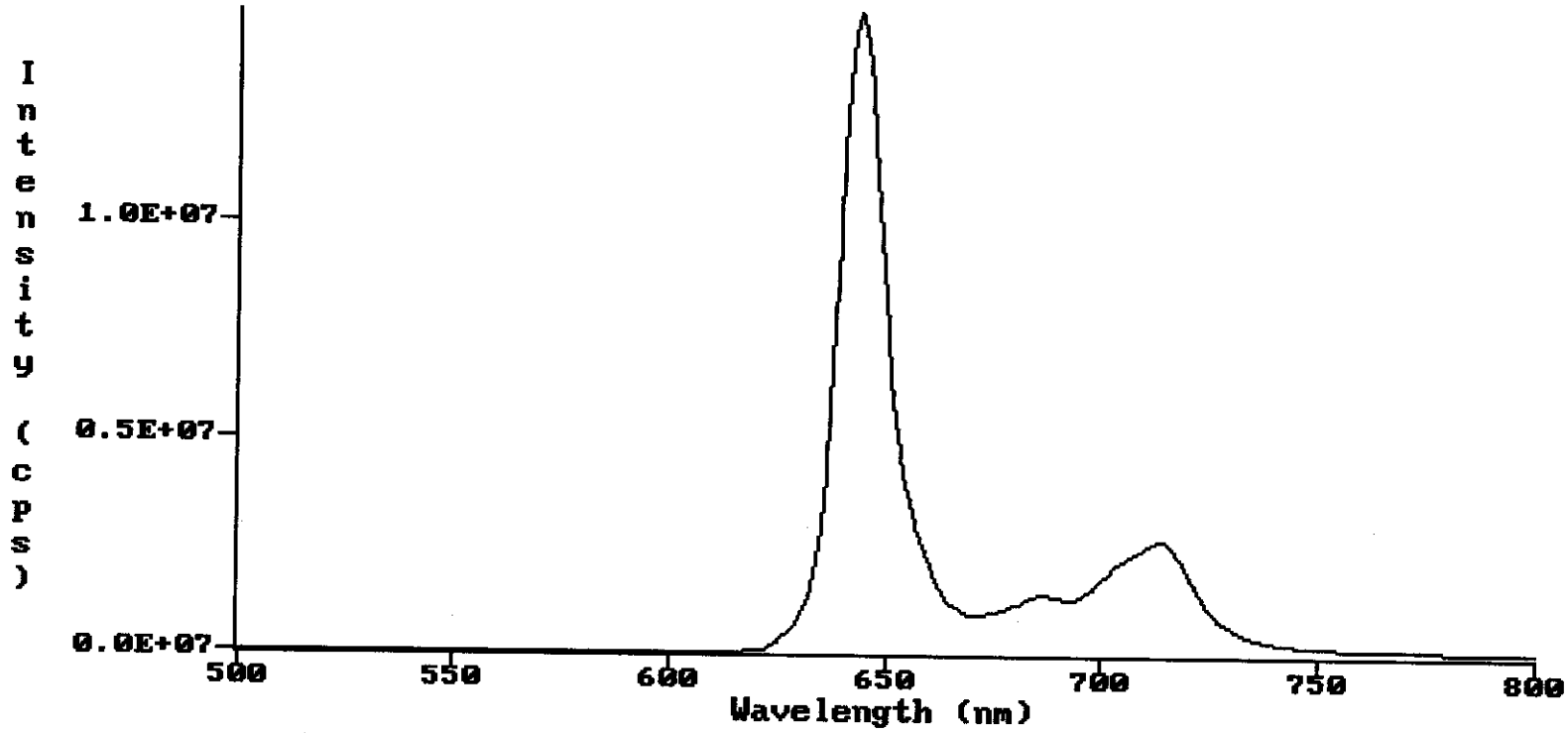


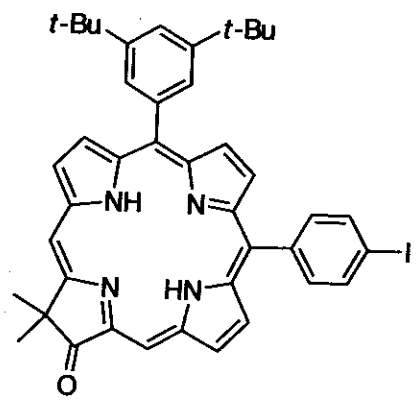
Oxo-4

```
INSTRUM TOF
OpId    N. Srinivasan
SMPNAM  015496
AQ_DATE Wed Jul 18 16:02:07 2001
PATH    /data/chemistry/LINDSEY/TANIGUCHI
POLARI  POS
AQOP_m  Reflector
TD              40000
NoSHOTS            50
SMONUM              0
SMOPTS1             0
SMOPTS2             0
SMOPTS3             0
DW                  1.00  [ns]
DELAY               0 [ns]
Uis1               20.00  [kV]
Uis2               18.70  [kV]
Urefl               0.00  [kV]
Ulens               7.50  [kV]
Uhimass            10.00  [kV]
RefFull             0.00  [kV]
UdetL               1.50  [kV]
UdetR               0.00  [kV]
Udefl               2.00  [kV]
REPHZ               1.00  [Hz]
ATTEN               42.0
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
DPMASS           700.00  [Da]
RBNDVAL            0.33
LBNDVAL            0.28
IS2BNDV            0.91
CMT1    Pb-OXO-CCH
CMT2    att 42,shots50
```

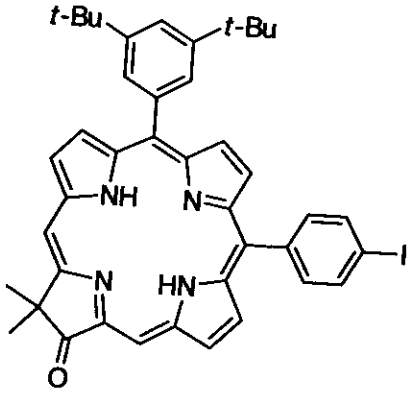
NCSU Chemistry
Instrument Serial Number 0051477



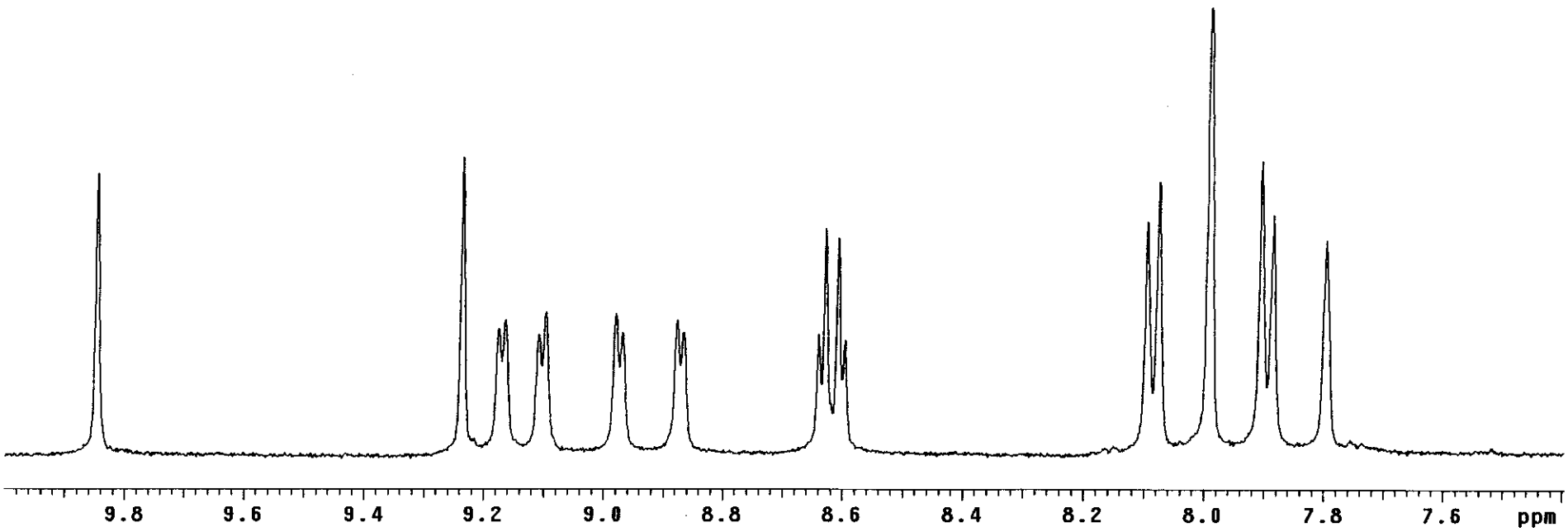


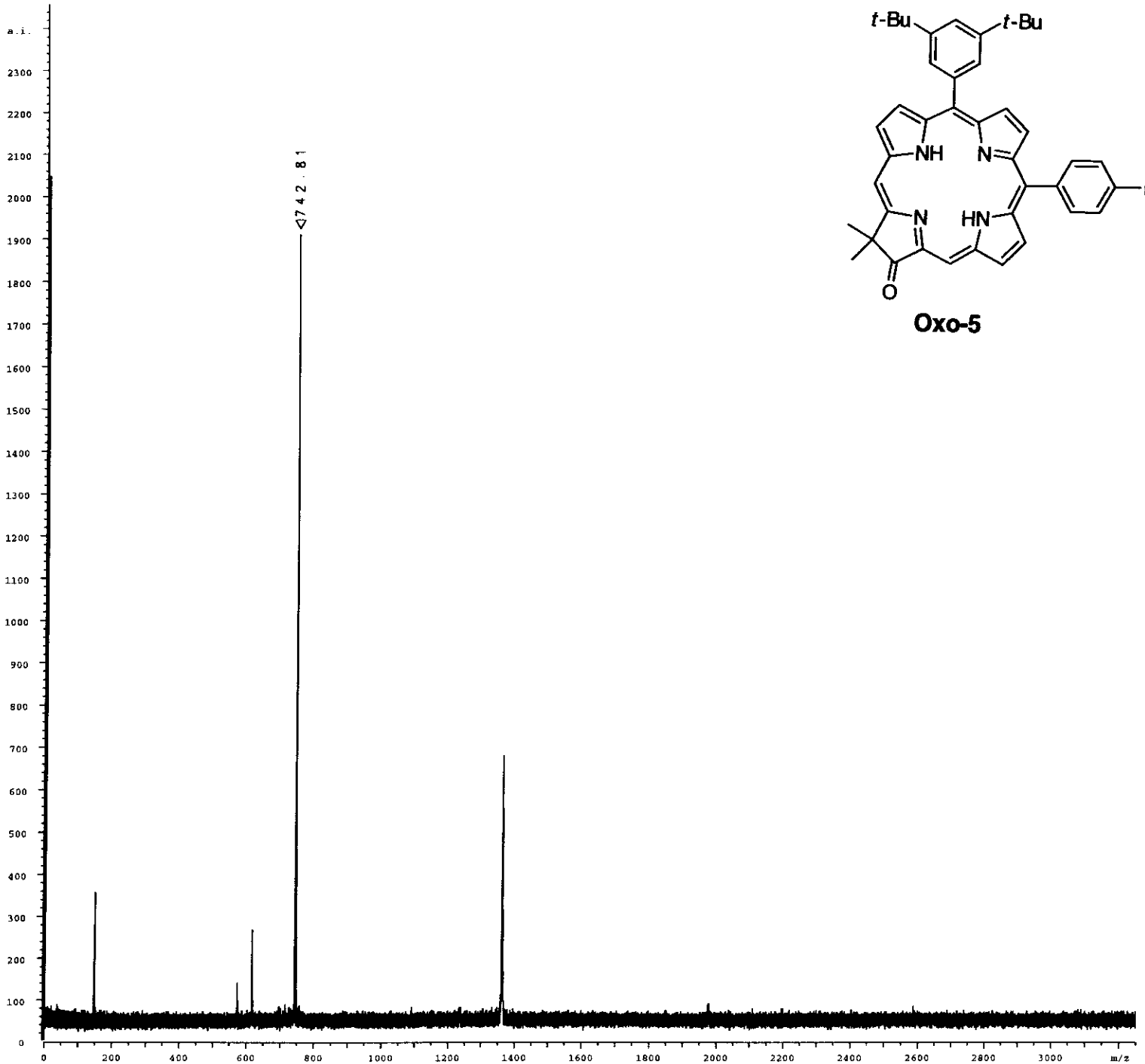


Oxo-5



Oxo-5



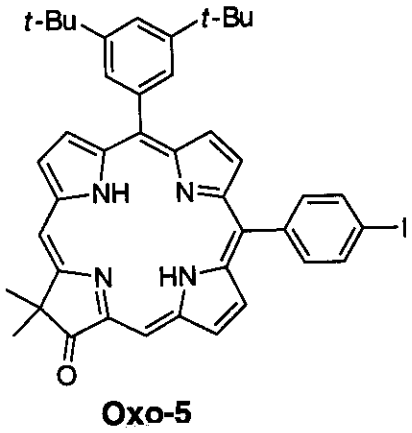


Oxo-5

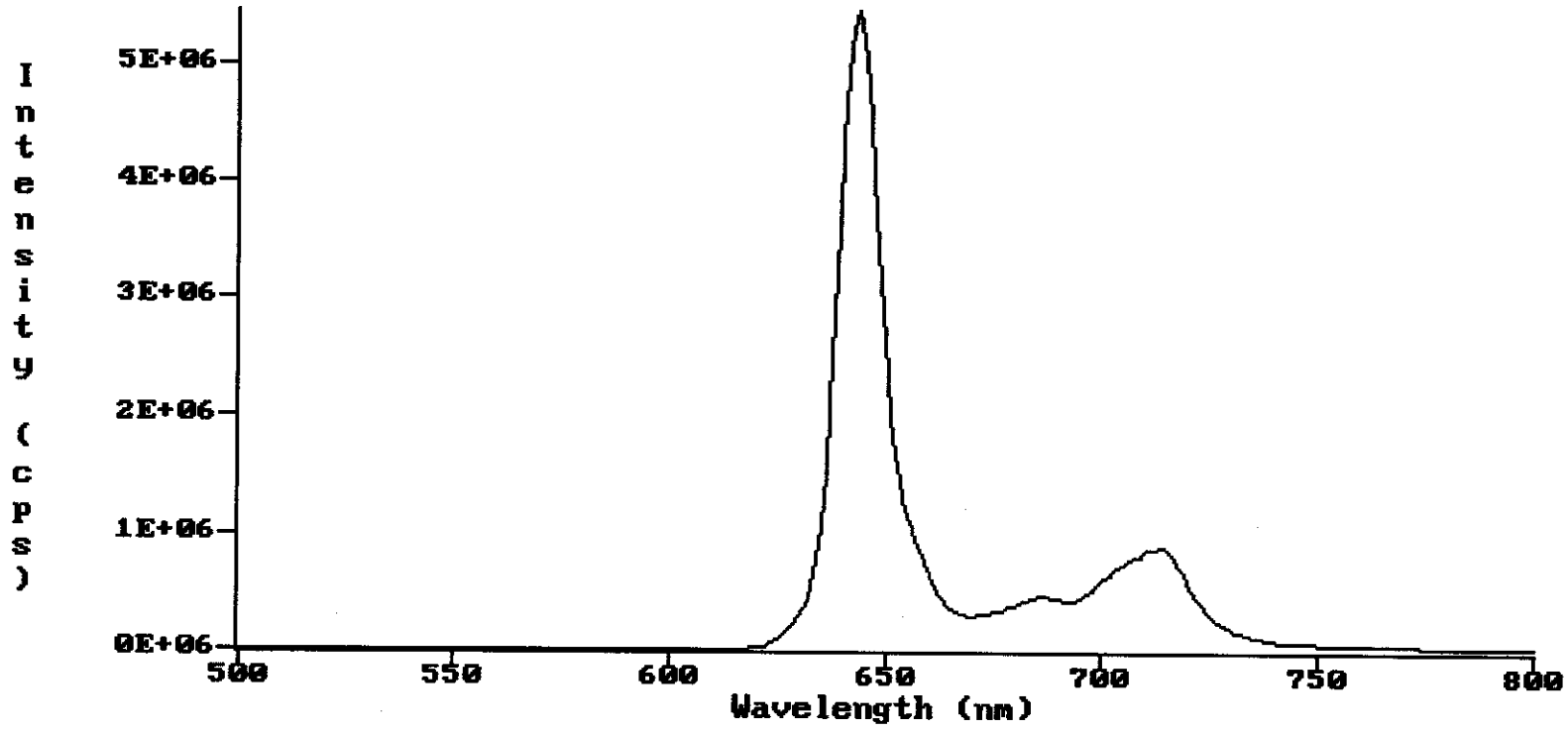
```
INSTRUM TOF
OpId    N. Srinivasan
SMPNAM  015497
AQ_DATE Wed Jul 18 16:08:40 2001
PATH    /data/chemistry/LINDSEY/TANIGUCHI
POLARI  POS
AQOP_m  Reflector
TD              40000
NoSHOTS           100
SMONUM              0
SMOPTS1             0
SMOPTS2             0
SMOPTS3             0
DW                1.00  [ns]
DELAY             0 [ns]
Uis1             20.00  [kV]
Uis2             18.70  [kV]
Urefl             0.00  [kV]
Ulens             7.50  [kV]
Uhimass          10.00  [kV]
RefFull           0.00  [kV]
UdetL             1.50  [kV]
UdetR             0.00  [kV]
Udefl             2.00  [kV]
REPRZ             1.00  [Hz]
ATTEN             43.0
ML1          2067125.193
ML2              333.982
ML3                0.000
HITURBO no
GDBON   yes
GDEDLY  short
DEFLON  no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1           510.84
DPMASS           700.00  [Da]
RBNDVAL            0.33
LBNDVAL            0.28
IS2BNDV            0.91
CMT1    Fb-OXO-PhI
CMT2    att 43,shots100
```

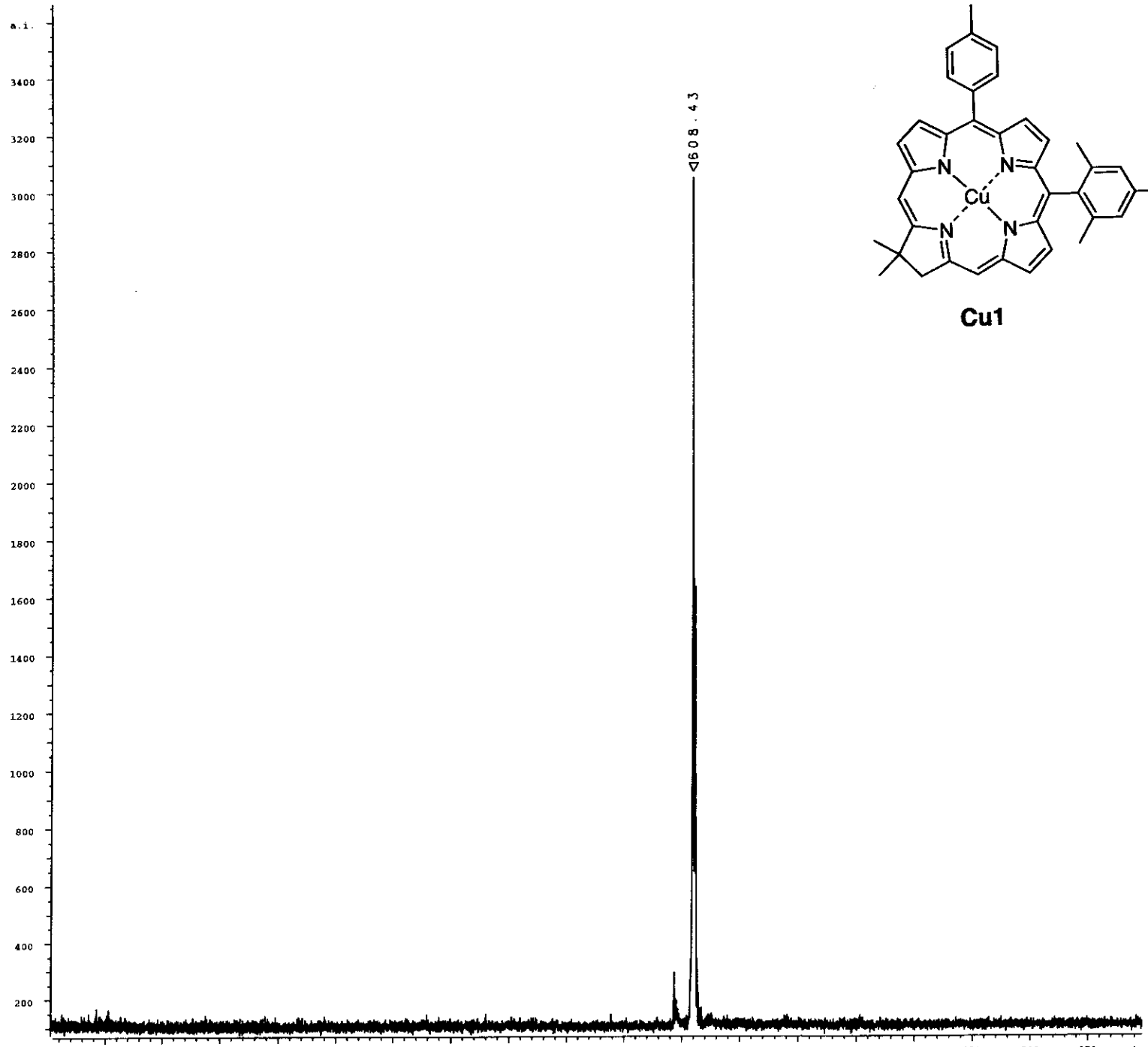
/data/chemistry/LINDSEY/TANIGUCHI/015497/1SRef/pdata/1 tof Wed Jul 18 16:09:31 2001

NCSU Chemistry
Instrument Serial Number 0051477



Oxo-5





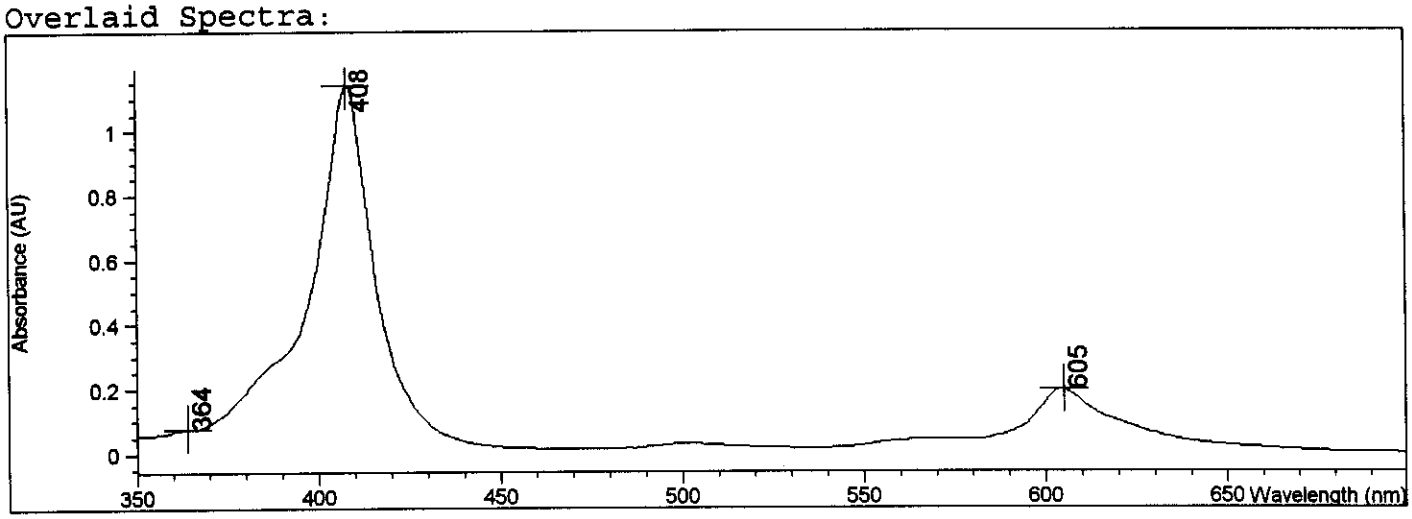
Cu1

```
INSTRUM TOP
OpId    N. Srinivasan
SMPNAM  015461
AQ_DATE Wed Jul 11 17:44:05 2001
PATH    /data/chemistry/LINDSEY/PRATHAPAN
POLARI  POS
AQQP_m  Reflector
TD              40000
NoSHOTS           250
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]
Ulens               7.50  [kV]
Uhimass            10.00  [kV]
RefFul1             0.00  [kV]
UdetL               1.50  [kV]
UdetR               0.00  [kV]
Udef1               2.00  [kV]
REPHZ               1.00  [Hz]
ATTEN               41.0
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
DPMASS            700.00  [Da]
RBNDVAL             0.33
LBNDVAL             0.28
IS2BNDV             0.91
CMT1    MsTolCuChlorin
CMT2    att 35, 150 shots
```

Spectrum/Peak Report Date 08/27/01 Time 18:55:42 Page 1 of 1

Method file : <untitled>
Information : Default Method
Data File : C:\HPCHEM\1\DATA\07120101.SD Created : 7/12/01 10:44:56

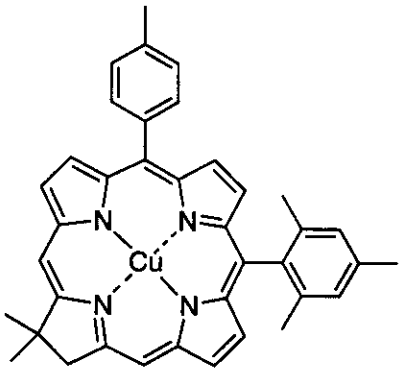
Overlaid Spectra:



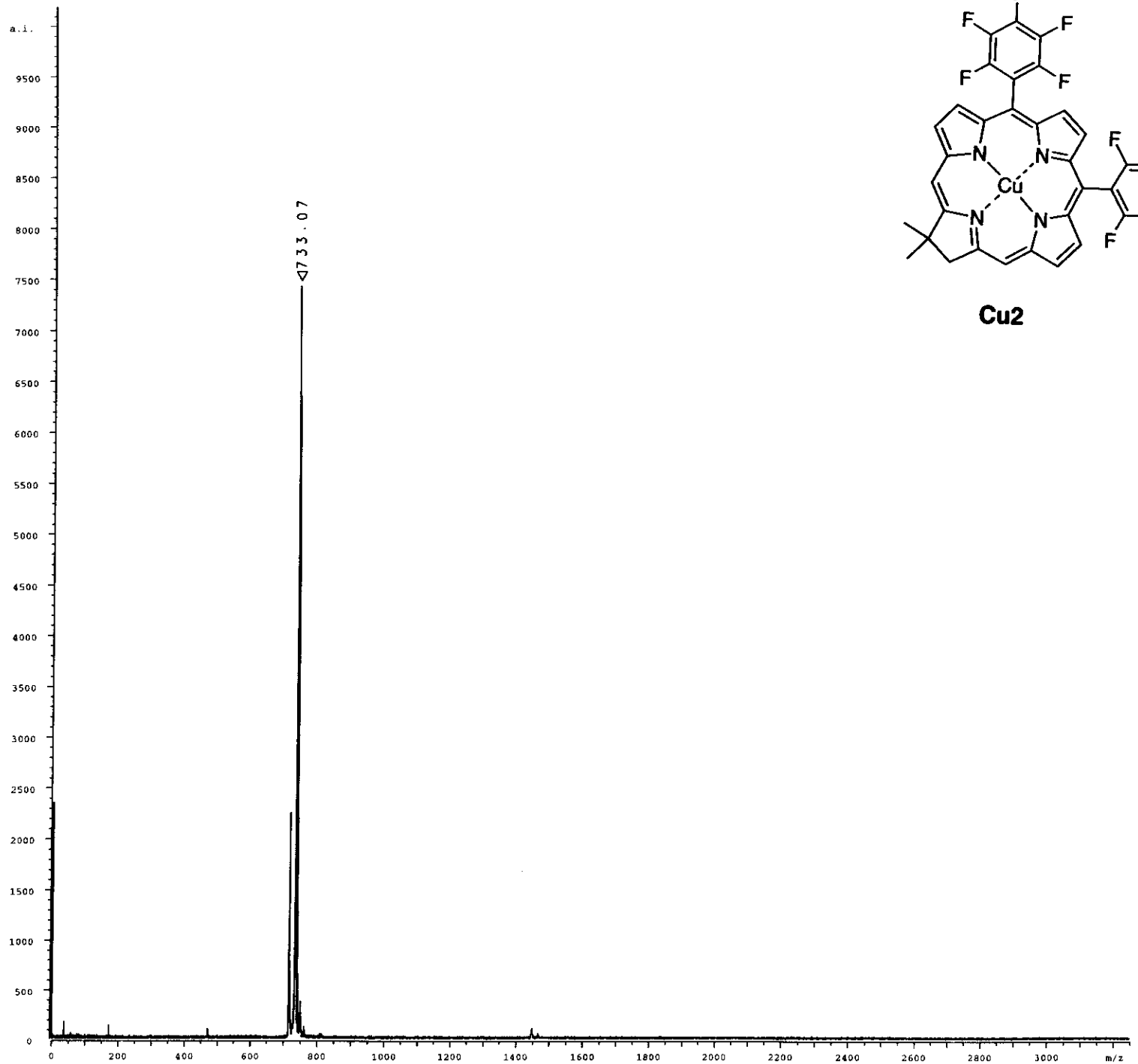
#	Name	Peaks (nm)	Abs (AU)
1	Mes-Cu-Chl	408.0	1.14090
1		605.0	0.19516
1		364.0	7.9418E-2

Report generated by : Signature: .....

*** End Spectrum/Peak Report ***



Cu1



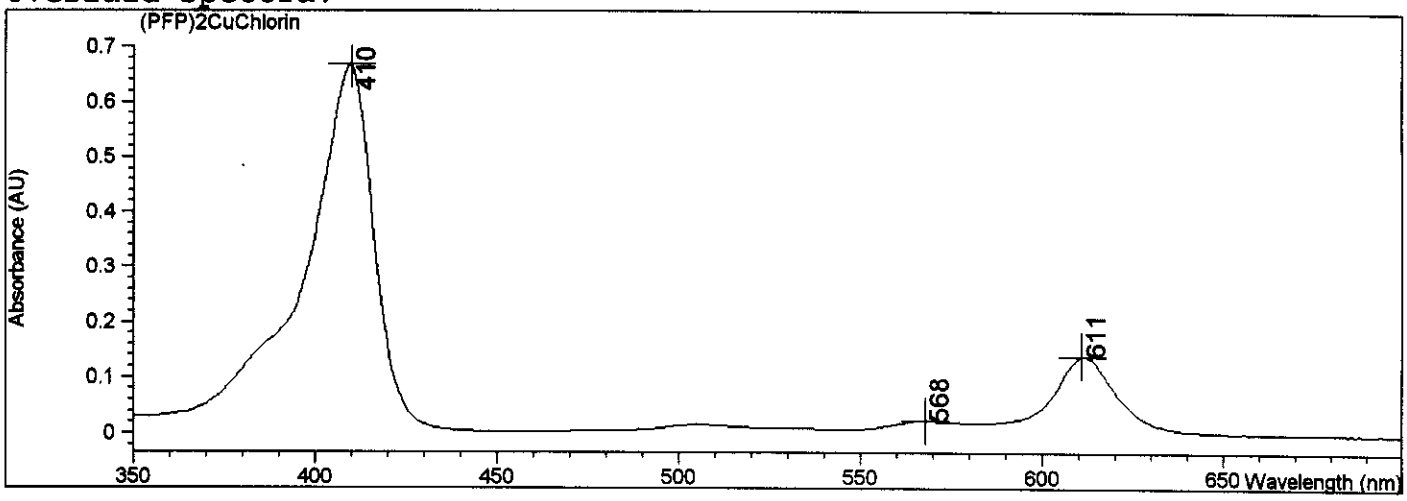
Cu2

```
INSTRUM TOF
OpId    N. Srinivasan
SMPNAM  015503
AQ_DATE Fri Jul 20 13:07:01 2001
PATH    /data/chemistry/LINDSEY/PRATHAPAN
POLARI  POS
AQOP_m  Reflector
TD          40000
NoSHOTS       100
SMONUM          0
SMOPTS1         0
SMOPTS2         0
SMOPTS3         0
DW              1.00  [ns]
DELAY           0 [ns]
Uis1           20.00  [kV]
Uis2           18.50  [kV]
Urefl           0.00  [kV]
Ulens           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           35.0
ML1       2065947.180
ML2           327.134
ML3             0.000
HITURBO no
GDEON   yes
GDEDLY  short
DEFLON  no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1        510.84
DPMASS        700.00  [Da]
RBNDVAL         0.33
LBNDVAL         0.28
IS2BNDV         0.91
CMT1    (PFP)2CuChlorin
CMT2    Attn35. shots100
```

Spectrum/Peak Report Date 08/27/01 Time 18:47:10 Page 1 of 1

Method file : <untitled>
Information : Default Method
Data File : C:\HPCHEM\1\DATA\MASA\07270101.SD Created : 7/27/01 10:17:39

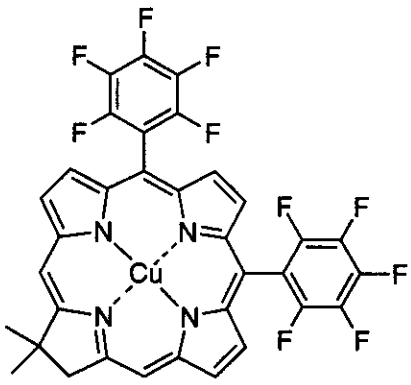
Overlaid Spectra:



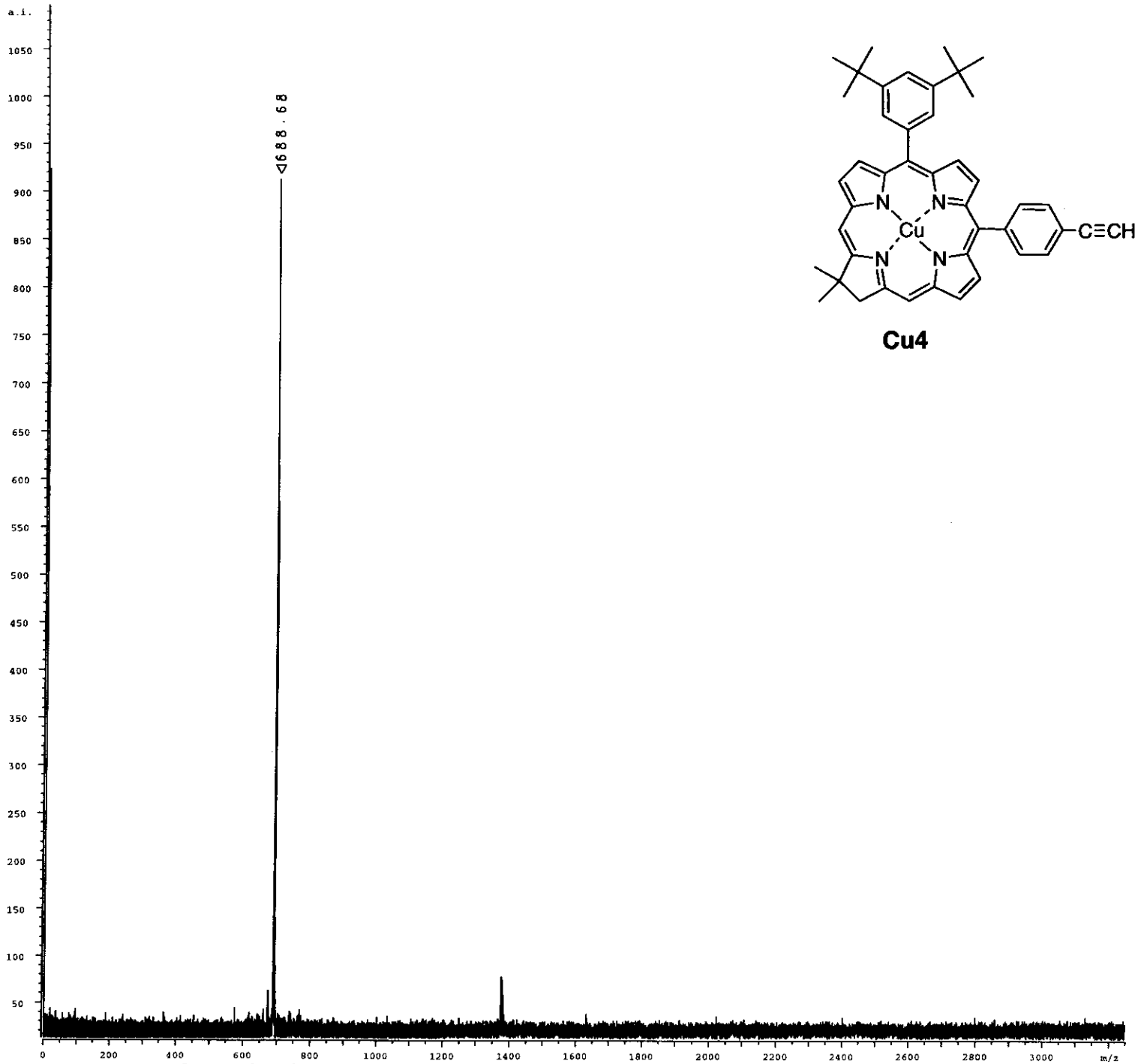
#	Name	Peaks(nm)	Abs(AU)
1	(PFP)2CuChlorin	410.0	0.66764
1		611.0	0.13924
1		568.0	2.2439E-2

Report generated by : Signature: .....

*** End Spectrum/Peak Report ***



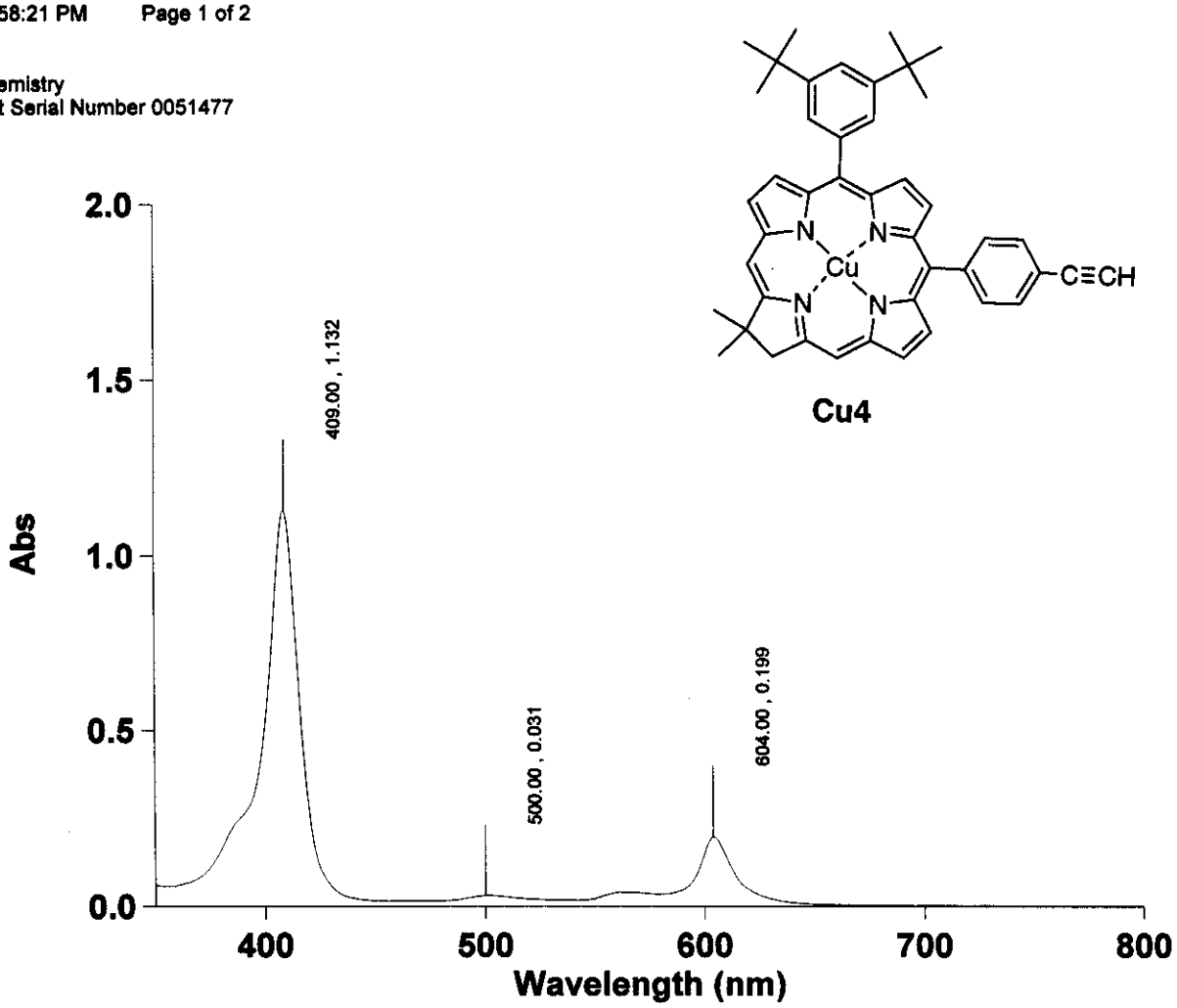
Cu2



Cu4

```
INSTRUM TOF
OpId    N. Srinivasan
SMPNAM  015491
AQ_DATE Wed Jul 18 12:28:16 2001
PATH    /data/chemistry/LINDSEY/TANIGUCHI
POLARI  POS
AQOP_m  Reflector
TD              40000
NoSHOTS            50
SMONUM              0
SMOPTS1             0
SMOPTS2             0
SMOPTS3             0
DW                  1.00  [ns]
DELAY               0 [ns]
Uis1               20.00  [kV]
Uis2               18.70  [kV]
Urefl               0.00  [kV]
Ulens               7.50  [kV]
Uhimass            10.00  [kV]
RefFull             0.00  [kV]
UdetL               1.50  [kV]
UdetR               0.00  [kV]
Udefl               2.00  [kV]
REPHZ               1.00  [Hz]
ATTEN              42.0
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
DPMASS            700.00  [Da]
RBNDVAL             0.33
LBNDVAL             0.28
IS2BNDV             0.91
CMT1    Cu-Chl-CCH
CMT2    att 42,shots50
```

NCSU Chemistry
Instrument Serial Number 0051477



Cu4

Scan Analysis Report

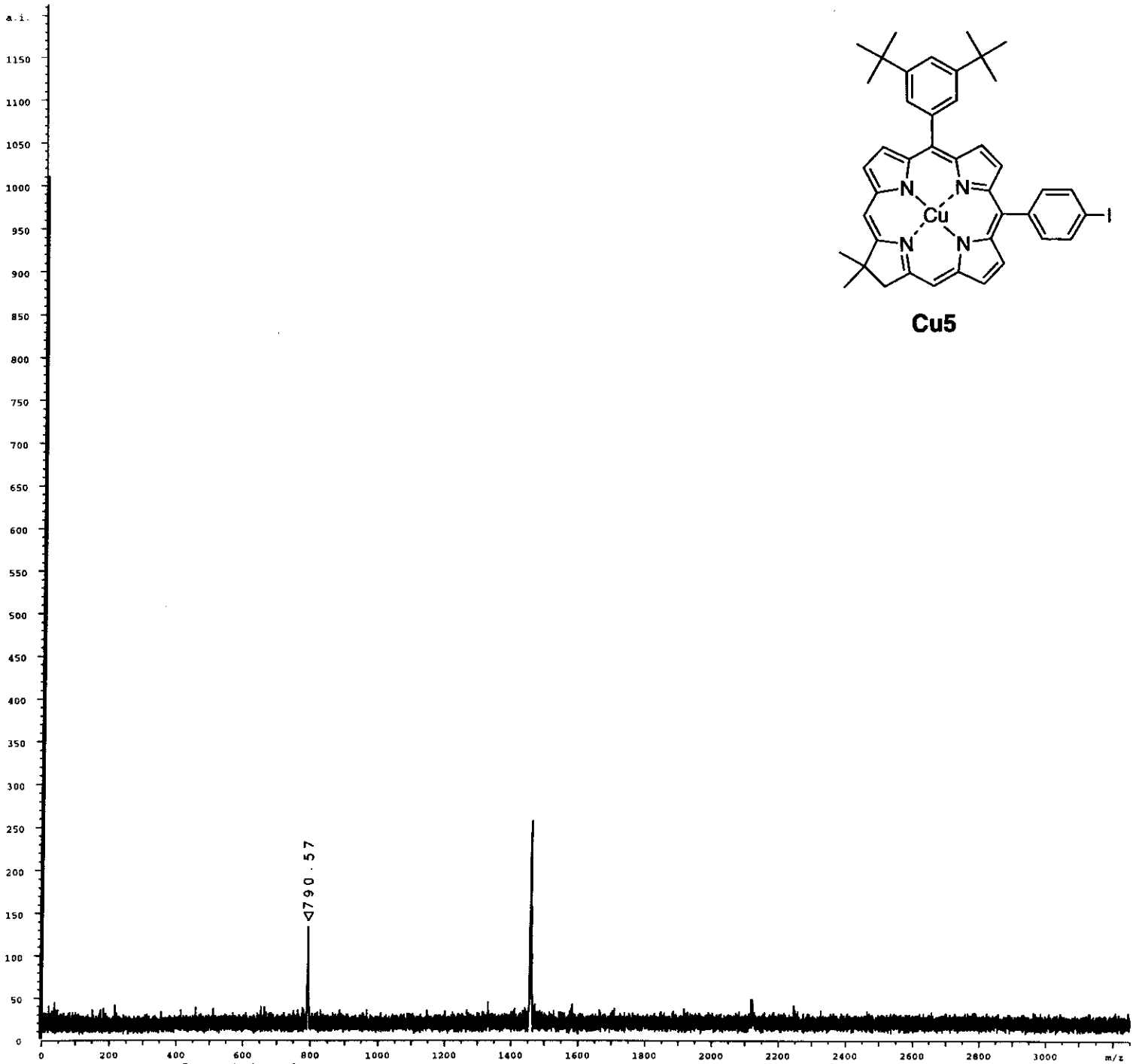
Report Time : Mon 16 Jul 01:39:56 PM 2001
Batch:
Software version: 02.00(25)
Operator:

Sample Name: sample1
Collection Time 7/16/01 1:39:59 PM

Scan Analysis Report

Report Time : Mon 16 Jul 01:44:37 PM 2001
Batch:
Software version: 02.00(25)
Operator:

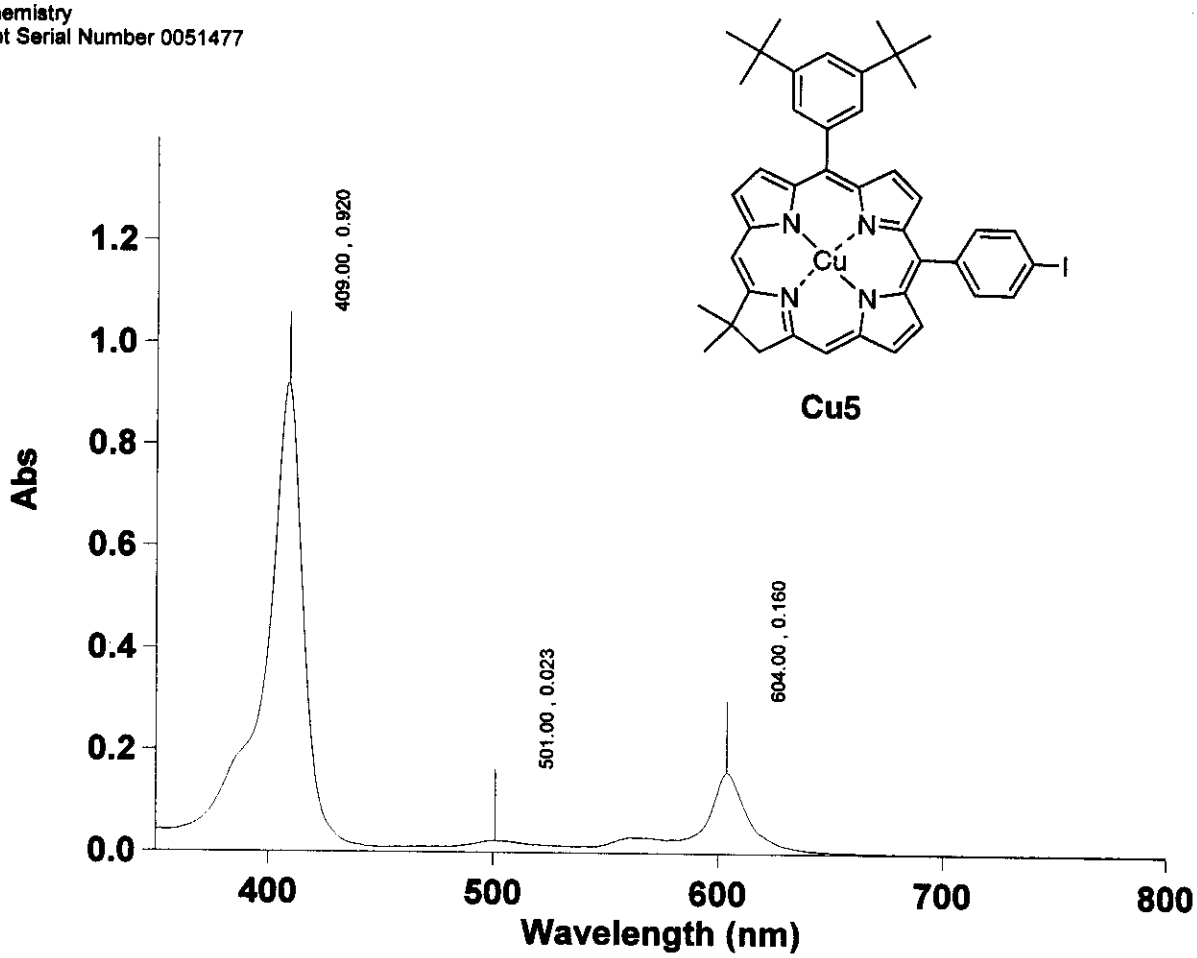
Sample Name: cu-chl-cch
Collection Time 7/16/01 1:44:45 PM



Cu5

```
INSTRUM TOF
OpId    N. Srinivasan
SMPNAM  015492
AQ_DATE Wed Jul 18 12:36:19 2001
PATH    /data/chemistry/LINDSEY/TANIGUCHI
POLARI  POS
AQOP_m  Reflector
TD              40000
NoSHOTS            50
SMONUM              0
SMOPTS1             0
SMOPTS2             0
SMOPTS3             0
DW                  1.00  [ns]
DELAY               0 [ns]
Uis1               20.00  [kV]
Uis2               18.70  [kV]
Urefl               0.00  [kV]
Ulens               7.50  [kV]
Uhimass            10.00  [kV]
RefFull             0.00  [kV]
UdetL               1.50  [kV]
UdetR               0.00  [kV]
Udefl               2.00  [kV]
REPHZ               1.00  [Hz]
ATTEN               43.0
ML1           2067125.193
ML2               333.982
ML3                 0.000
HITURBO no
GDBON   yes
GDEDLY  short
DEFLON  no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1            510.84
DPMASS            700.00  [Da]
RBNDVAL             0.33
LBNDVAL             0.28
IS2BNDV             0.91
CMT1    Cu-Chl-PhI
CMT2    att 43,shots50
```

NCSU Chemistry
Instrument Serial Number 0051477



Cu5

Scan Analysis Report

Report Time : Mon 16 Jul 01:39:56 PM 2001
Batch:
Software version: 02.00(25)
Operator:

Sample Name: sample1

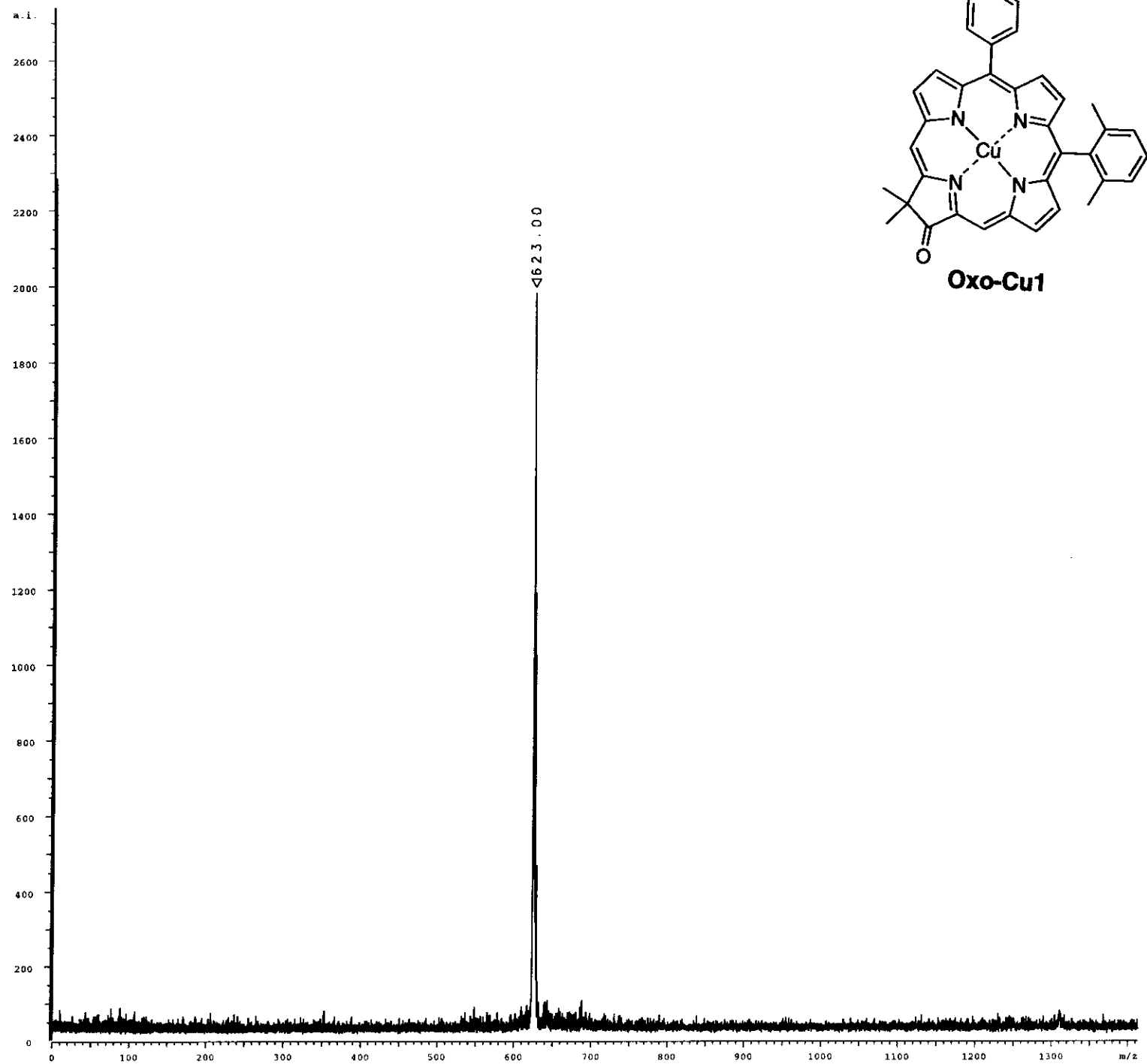
Collection Time 7/16/01 1:39:59 PM

Scan Analysis Report

Report Time : Mon 16 Jul 01:44:37 PM 2001
Batch:
Software version: 02.00(25)
Operator:

Sample Name: cu-chl-cch

Collection Time 7/16/01 1:44:45 PM



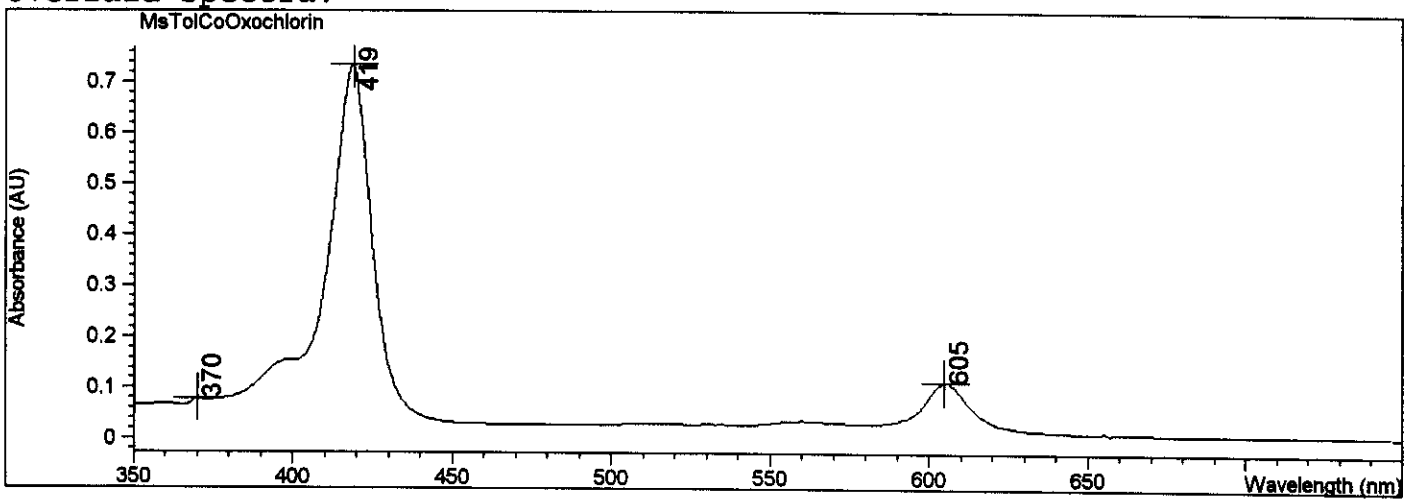
Oxo-Cu1

```
INSTRUM TOF
OpId    Unknown
SMPNAM  015548
AQ_DATE Thu Jul 26 10:52:45 2001
PATH    /data/chemistry/LINDSEY/PRATHAPAN
POLARI  POS
AQQP_m  Reflector
TD              40000
NoSHOTS           100
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]
Ulens               7.50  [kV]
Uhimass            10.00  [kV]
RefPul1             0.00  [kV]
UdetL               1.55  [kV]
UdetR               0.00  [kV]
Udef1               2.00  [kV]
REPHZ               1.00  [Hz]
ATTEN              36.0
ML1          2065514.657
ML2              327.231
ML3                0.000
HITURBO no
GDEON   yes
GDEDLY  short
DEFLON  no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1           510.84
DPMASS           200.00  [Da]
RBNDVAL            0.33
LBNDVAL            0.28
IS2BNDV            0.91
CMT1    MsTolCuOxochlorin
CMT2    attn:35, shots 100
```

Spectrum/Peak Report Date 07/24/01 Time 17:52:02 Page 1 of 1

Method file : <untitled>
Information : Default Method
Data File : <untitled>

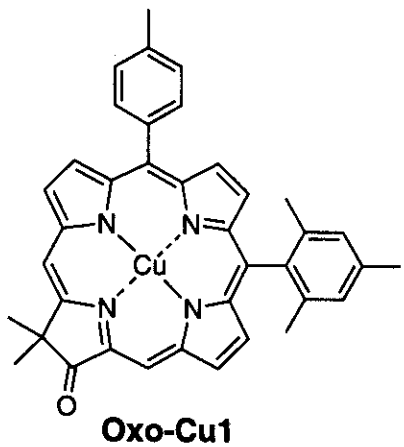
Overlaid Spectra:



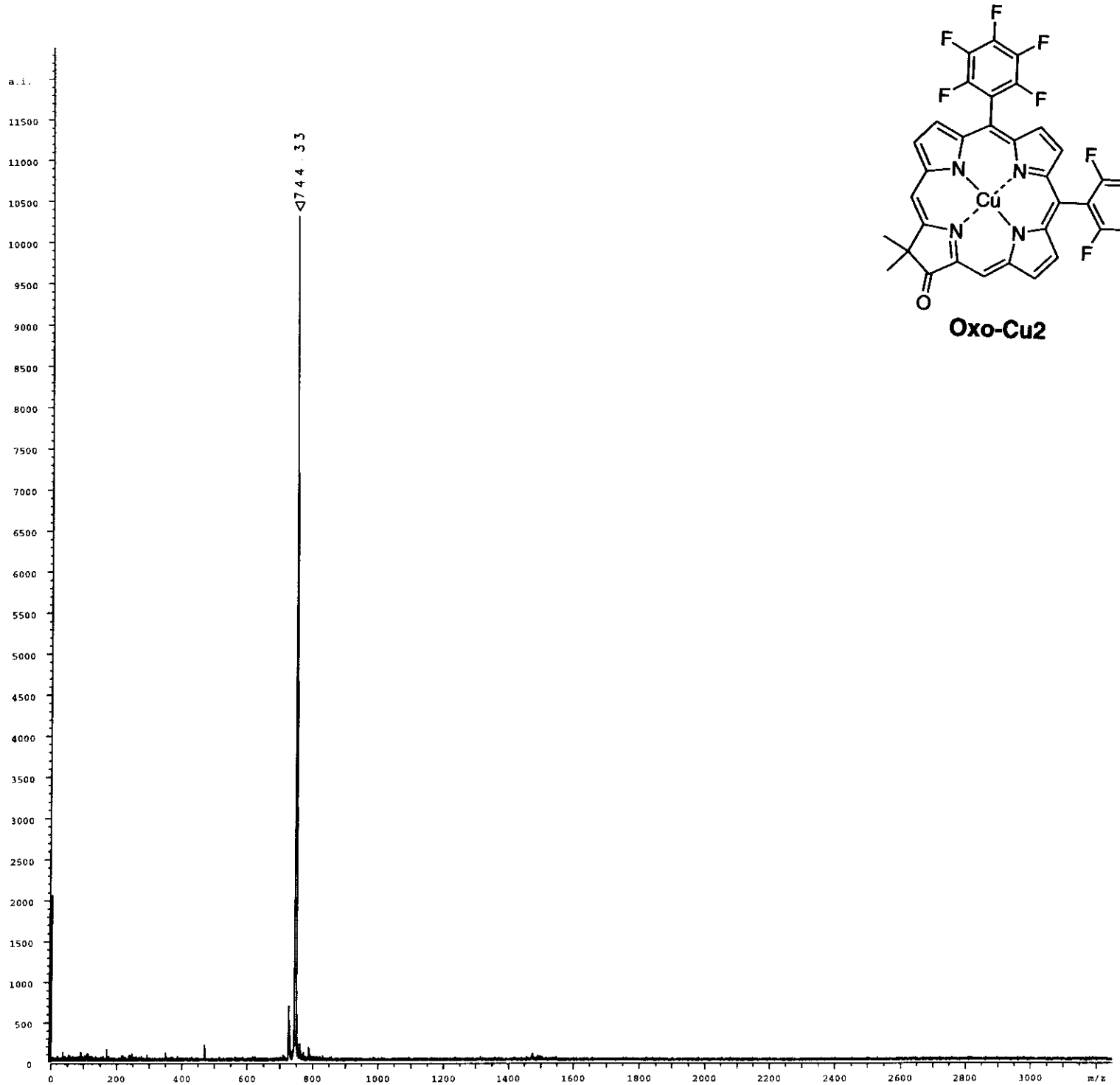
#	Name	Peaks(nm)	Abs(AU)
1	MsTolCoOxochlori	419.0	0.73345
1		605.0	0.11356
1		370.0	7.9889E-2

Report generated by : Signature: .....

*** End Spectrum/Peak Report ***



Oxo-Cu1



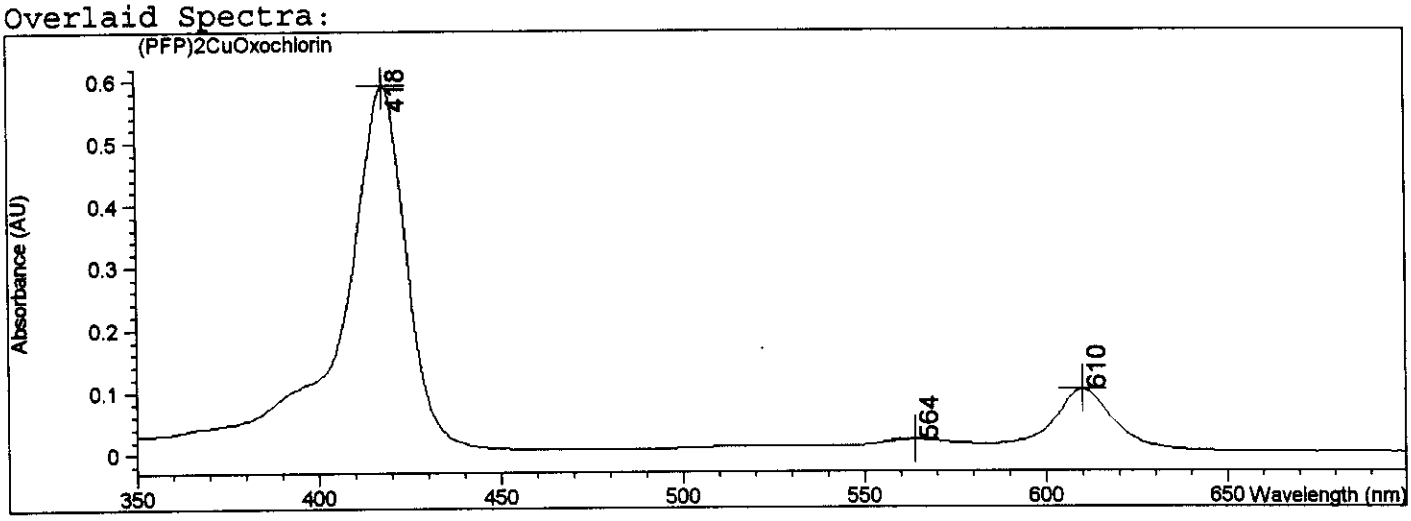
Oxo-Cu2

INSTRUM	TOF	
OpId	Unknown	
SMPNAM	015549	
AQ_DATE	Thu Jul 26 14:01:33 2001	
PATH	/data/chemistry/LINDSEY/PRATHAPAN	
POLARI	POS	
AQOP_m	Reflector	
TD	40000	
NoSHOTS	100	
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]
Ulens	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	40.0	
ML1	2067510.748	
ML2	353.368	
ML3	0.000	
HITURBO	no	
GDEON	yes	
GDEDLY	short	
DEFLON	no	
RLNSBND	no	
LLNSBND	no	
UIS2BND	no	
DPCAL1	510.84	
DPMASS	200.00	[Da]
RBNDVAL	0.33	
LBNDVAL	0.28	
IS2BNDV	0.91	
CMT1	(PFP)2CuOxochlorin	
CMT2	attn:40, shots 100	

Spectrum/Peak Report Date 08/27/01 Time 18:46:46 Page 1 of 1

Method file : <untitled>
Information : Default Method
Data File : C:\HPCHEM\1\DATA\MASA\07240102.SD Created : 7/24/01 17:41:01

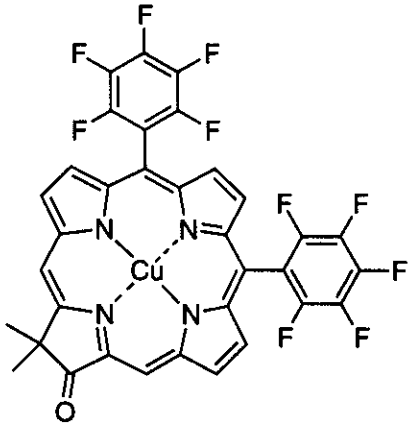
Overlaid Spectra:



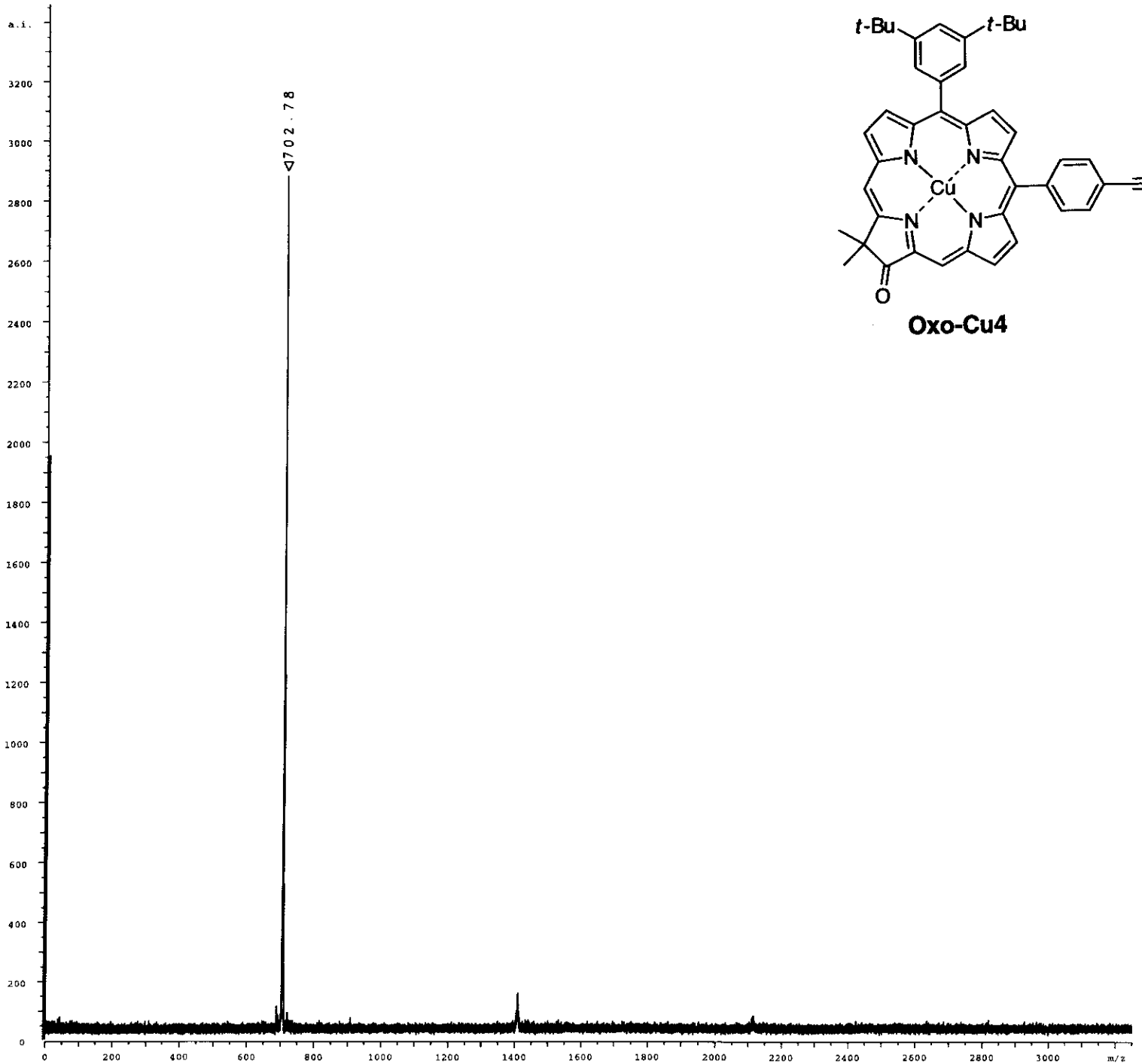
#	Name	Peaks (nm)	Abs (AU)
1	(PFP)2CuOxochlor	418.0	0.59165
1		610.0	0.10066
1		564.0	2.0638E-2

Report generated by : Signature: .....

*** End Spectrum/Peak Report ***



Oxo-Cu2



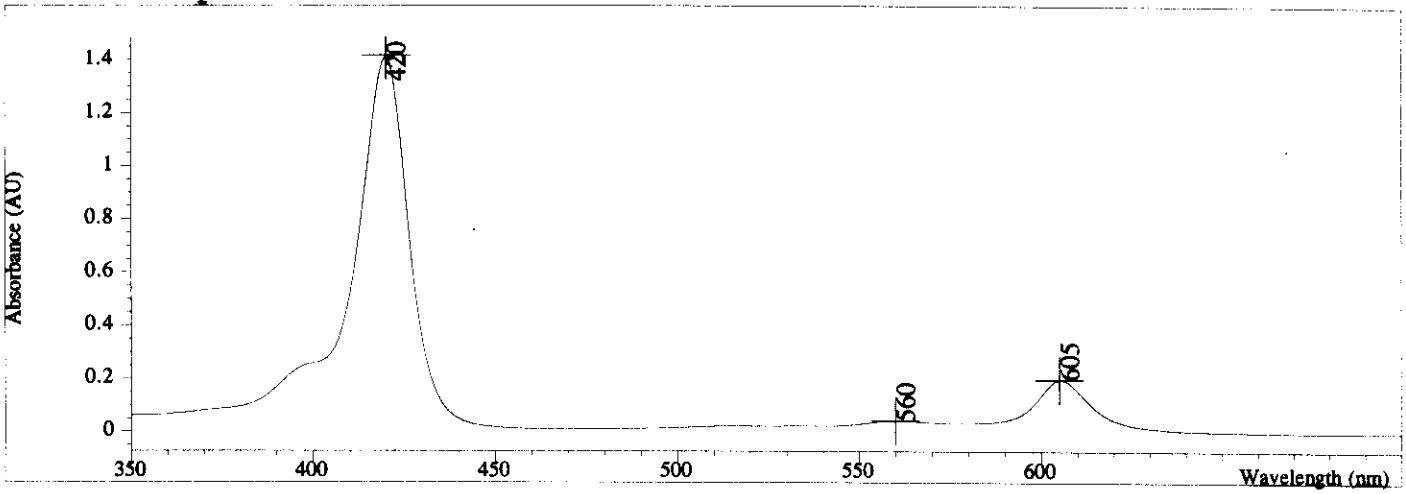
Oxo-Cu4

```
INSTRUM TOF
OpId    N. Srinivasan
SMPNAM  015493
AQ_DATE Wed Jul 18 12:39:45 2001
PATH    /data/chemistry/LINDSEY/TANIGUCHI
POLARI  POS
AQOP_m  Reflector
TD          40000
NoSHOTS       100
SMONUM          0
SMOPTS1         0
SMOPTS2         0
SMOPTS3         0
DW              1.00  [ns]
DELAY           0 [ns]
Uis1           20.00  [kV]
Uis2           18.70  [kV]
Urefl           0.00  [kV]
Ulens           7.50  [kV]
Uhimass        10.00  [kV]
RefFull         0.00  [kV]
UdetL           1.50  [kV]
UdetR           0.00  [kV]
Udefl           2.00  [kV]
REPH2           1.00  [Hz]
ATTEN           46.0
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
DPMASS         700.00  [Da]
RBNDVAL          0.33
LBNDVAL          0.28
IS2BNDV          0.91
CMT1    Cu-OXO-CCH
CMT2    att 46,shots100
```

Spectrum/Peak Report Date 07/17/01 Time 16:21:50 Page 1 of 1

Method file : <untitled>
Information : Default Method
Data File : C:\HPCHEM\1\DATA\MASA\CUOXOCCH.SD Created : 7/17/01 16:21:13

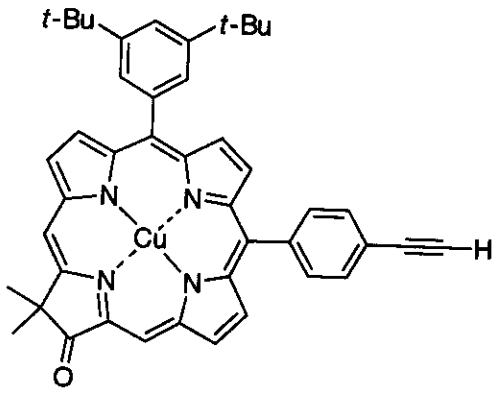
Overlaid Spectra:



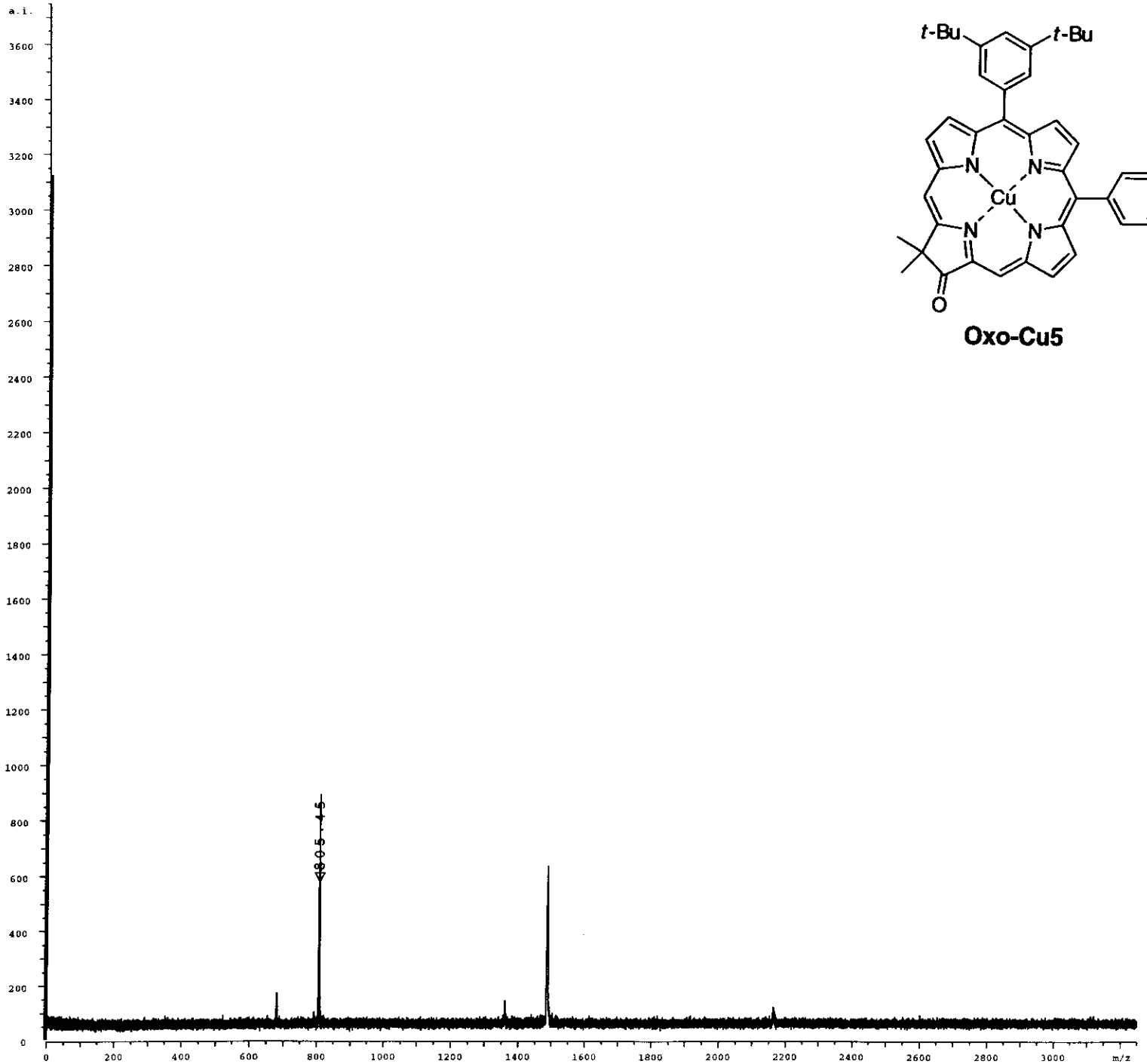
#	Name	Peaks(nm)	Abs(AU)
1		420.0	1.41610
1		605.0	0.19806
1		560.0	4.2498E-2

Report generated by : Signature: .....

*** End Spectrum/Peak Report ***



Oxo-Cu4



Oxo-Cu5

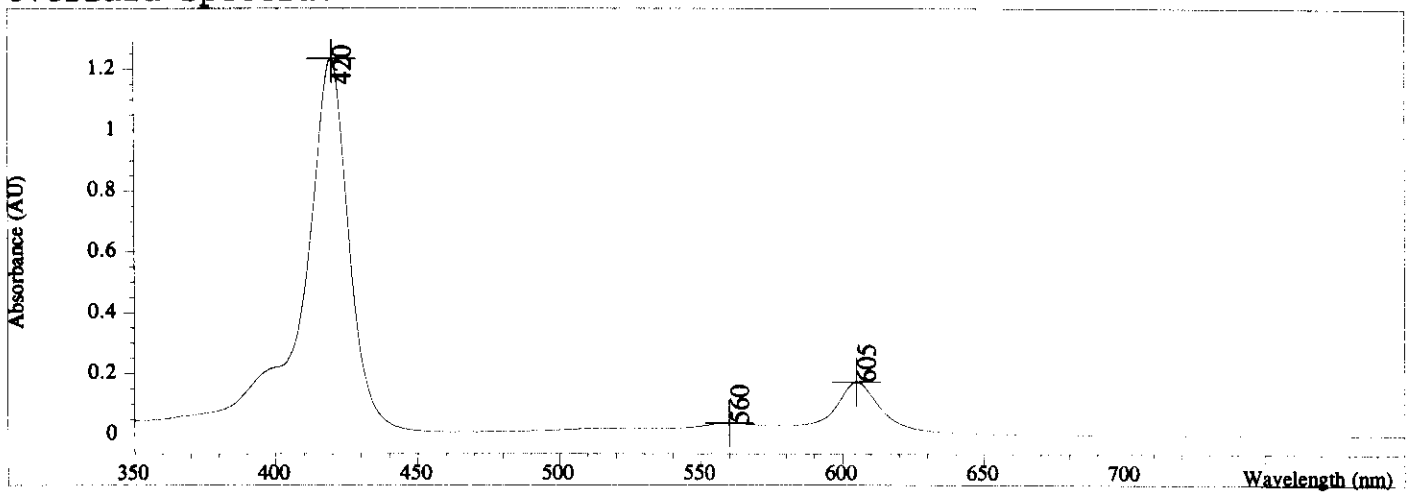
```
INSTRUM TOF
OpId    N. Srinivasan
SMPNAM  015494
AQ_DATE Wed Jul 18 12:47:55 2001
PATH    /data/chemistry/LINDSEY/TANIGUCHI
POLARI  POS
AQOP_m  Reflector
TD              40000
NoSHOTS           150
SMONUM              0
SMOPTS1             0
SMOPTS2             0
SMOPTS3             0
DW                  1.00  [ns]
DELAY               0 [ns]
Uis1               20.00  [kV]
Uis2               18.70  [kV]
Uref1               0.00  [kV]
Ulens               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               44.0
ML1          2067125.193
ML2              333.982
ML3                0.000
HITURBO no
GDEON   yes
GDEDLY  short
DEFLON  no
RLNSBND no
LLNSBND no
ULS2BND no
DPCAL1           510.84
DPMASS           700.00  [Da]
RBNDVAL            0.33
LBNDVAL            0.28
IS2BNDV            0.91
CMT1    Cu-OXO-PhI
CMT2    att 44,shots100
```

/data/chemistry/LINDSEY/TANIGUCHI/015494/1SRef/pdata/1 tof Wed Jul 18 13:02:19 2001

Spectrum/Peak Report Date 07/17/01 Time 18:43:22 Page 1 of 1

Method file : <untitled>
Information : Default Method
Data File : <untitled>

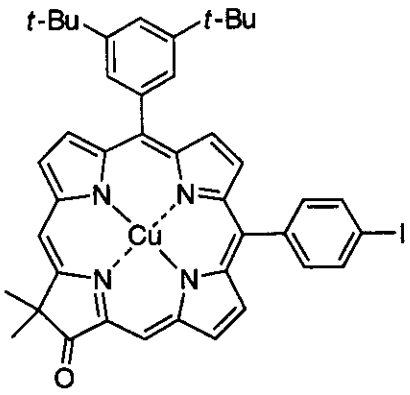
Overlaid Spectra:



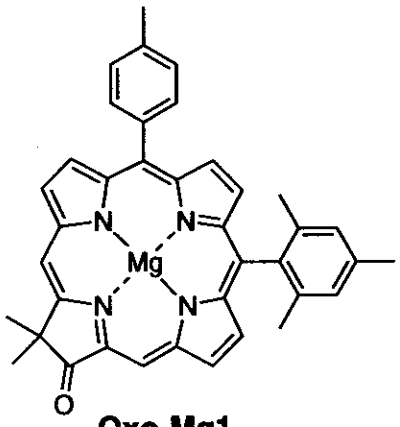
#	Name	Peaks(nm)	Abs(AU)
1		420.0	1.23490
1		605.0	0.17264
1		560.0	3.7736E-2

Report generated by : Signature: .....

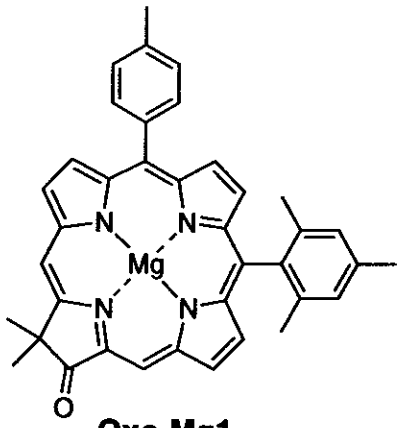
*** End Spectrum/Peak Report ***



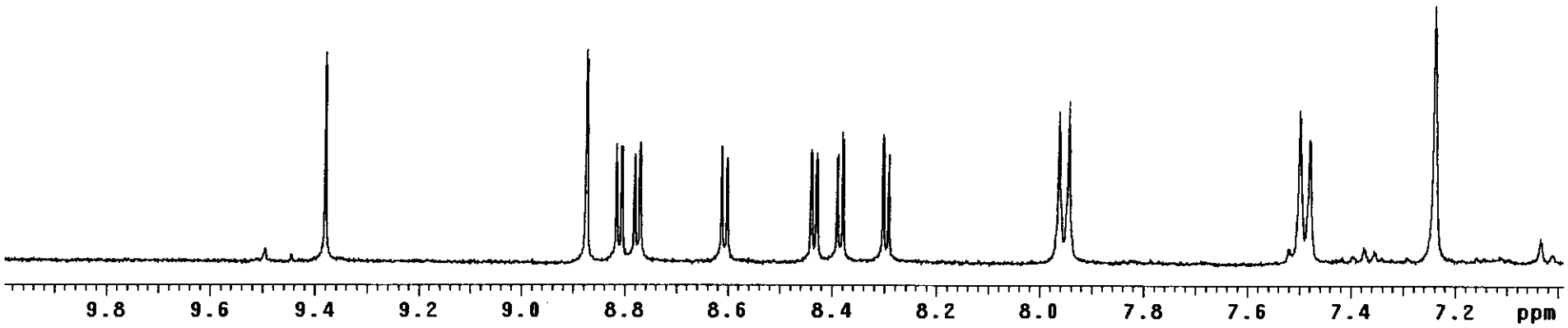
Oxo-Cu5

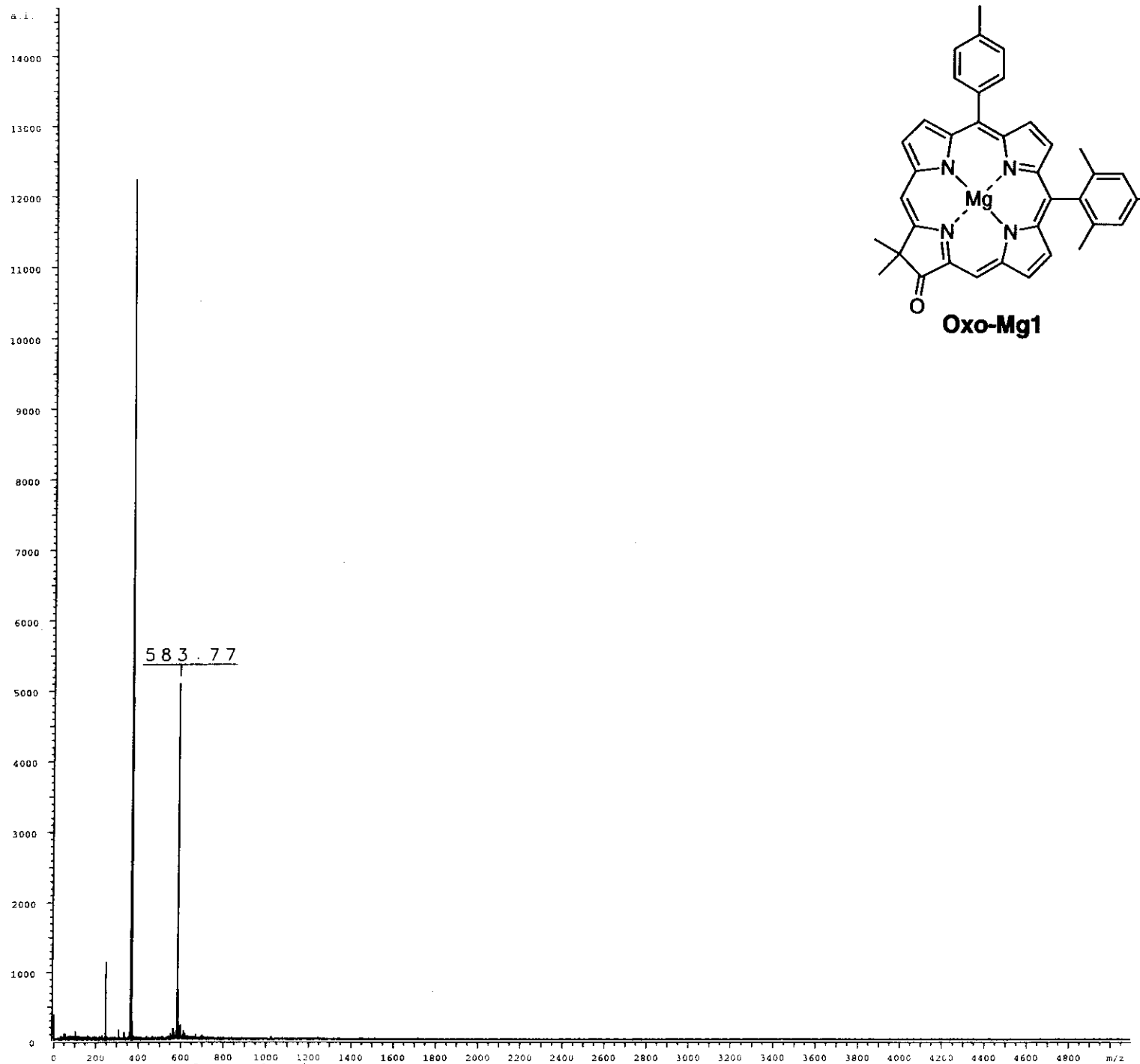


Oxo-Mg1



Oxo-Mg1



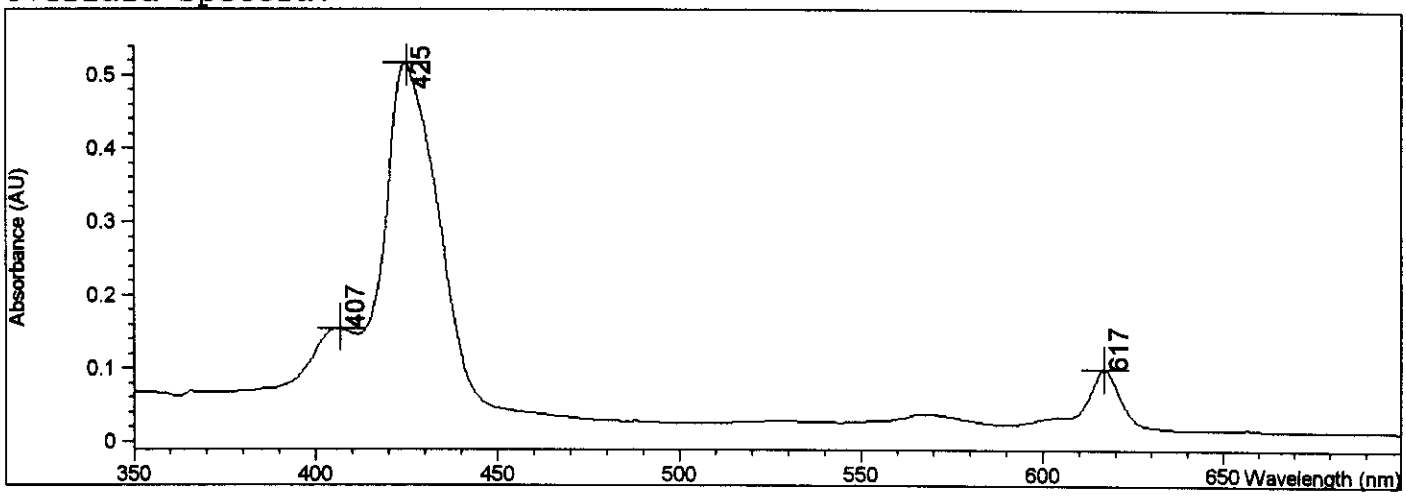


Oxo-Mg1

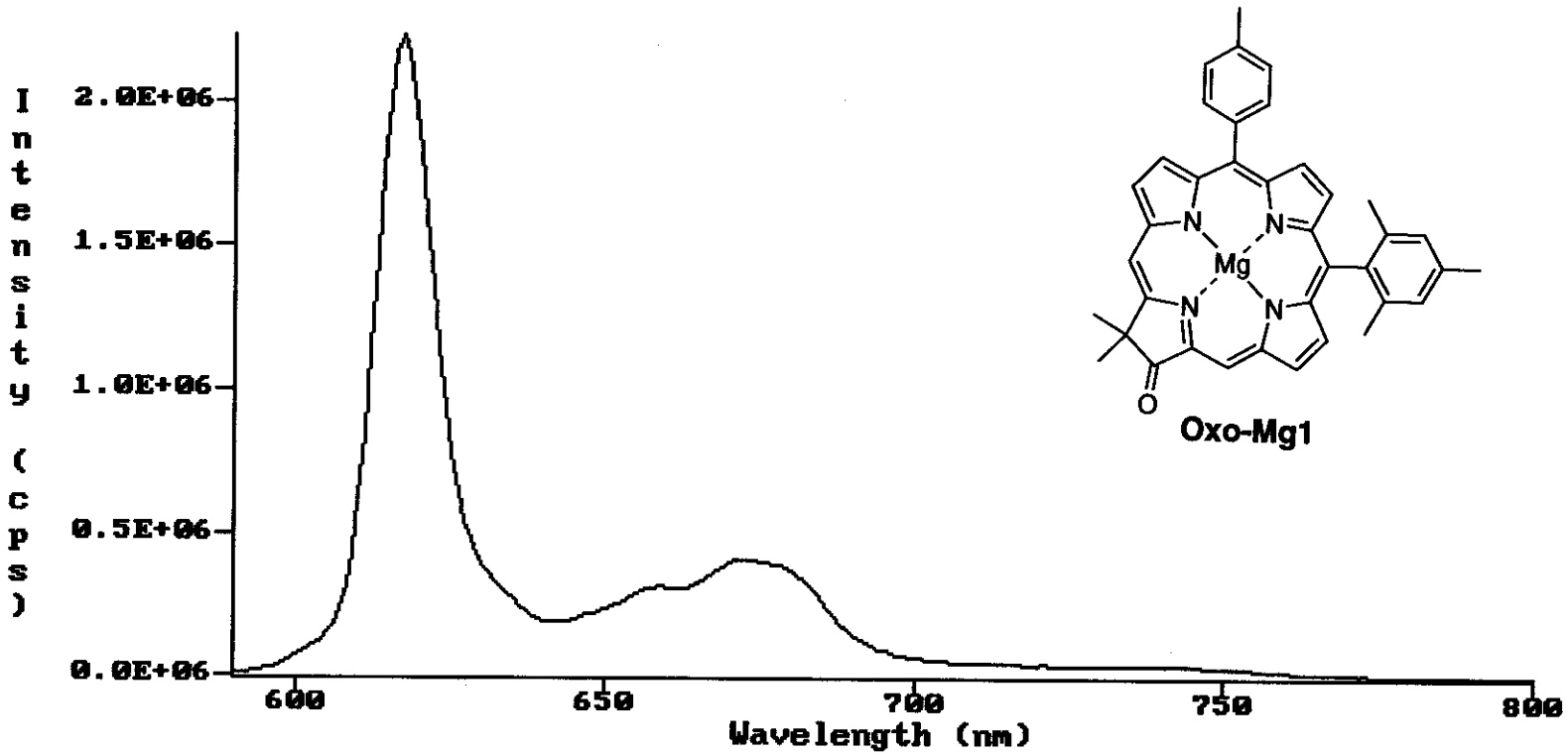
```
INSTRUM TOF
OpId    N. Srinivasan
SMPNAM  020181
AQ_DATE Thu Mar  7 15:53:36 2002
PATH    /data/chemistry/LINDSEY/TANIGUCHI
POLARI  POS
AQOP_m  Reflector
TD          50000
NoSHOTS        50
SMONUM          0
SMOPTS1         0
SMOPTS2         0
SMOPTS3         0
DW              1.00  [ns]
DELAY           0 [ns]
Uis1           20.00  [kV]
Uis2           18.70  [kV]
Urefl           0.00  [kV]
Ulens           7.50  [kV]
Uhimass        10.00  [kV]
RefFull         0.00  [kV]
UdetL           1.50  [kV]
UdetR           0.00  [kV]
Udefl           2.00  [kV]
REPHZ           1.00  [Hz]
ATTEN           56.0
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
DPMASS        700.00  [Da]
RBNDVAL         0.33
LBNDVAL         0.28
IS2BNDV         0.91
CMT1    Oxo-Mg-1b
CMT2    Attn=56, shots = 50
```

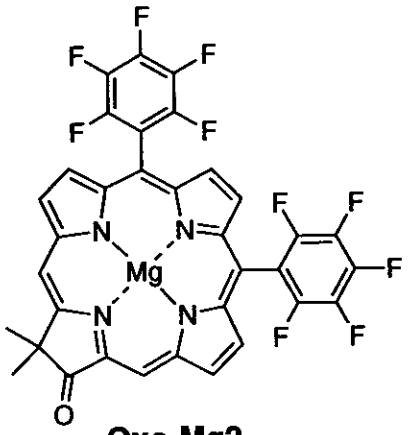
Method file : <untitled>
Information : Default Method
Data File : C:\RSLSPE~1\04220103.SD Created : 4/22/01 18:10:37

Overlaid Spectra:

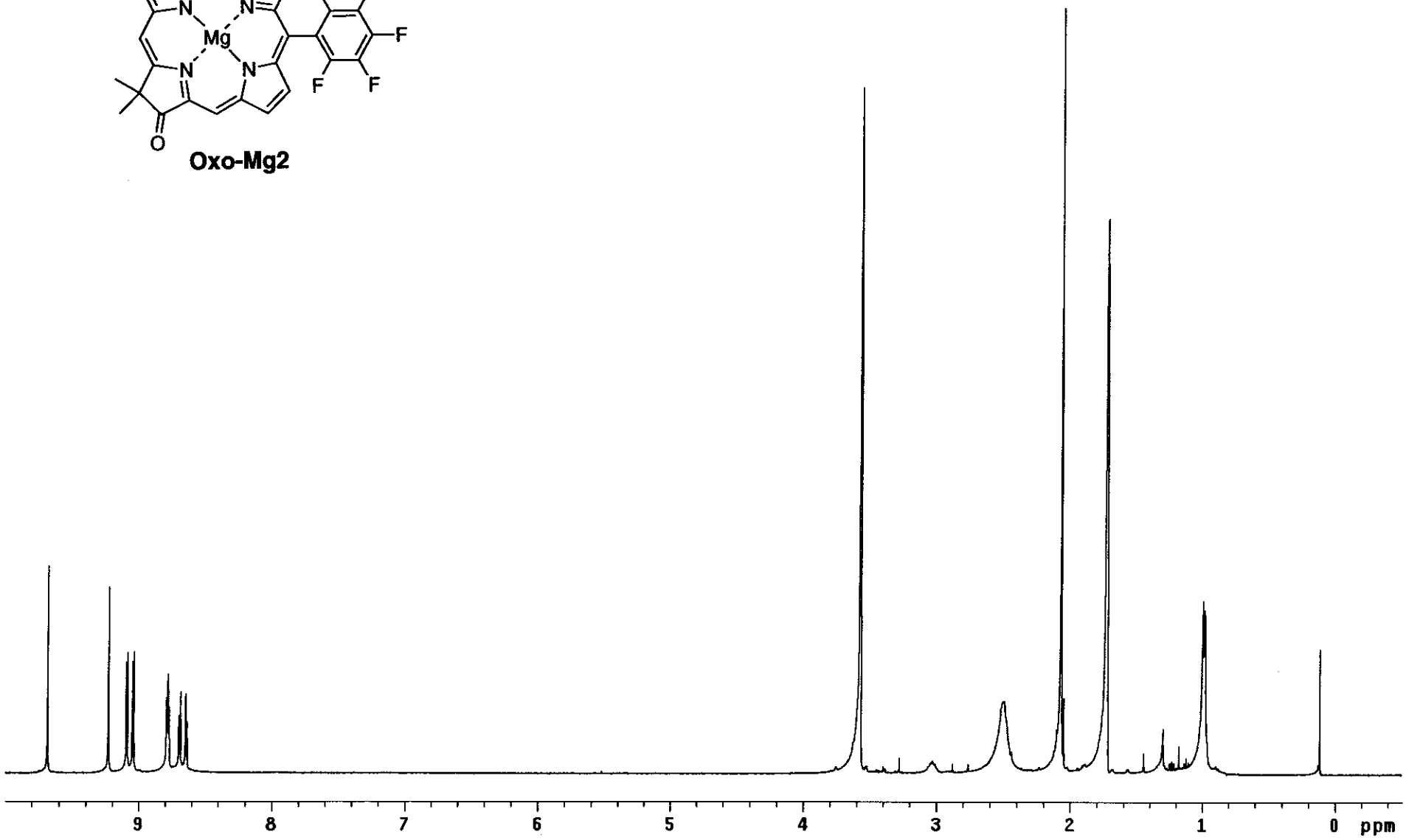


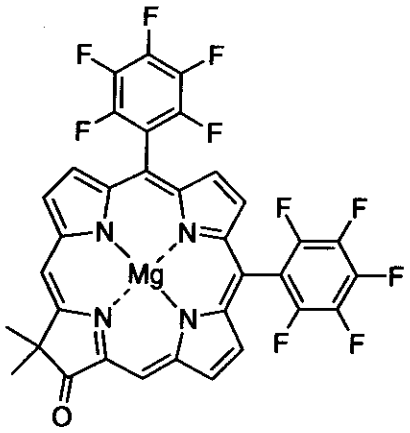
#	Name	Peaks(nm)	Abs(AU)
1	Mes-Tol-Mg-Oxo	425.0	0.51621
1		407.0	0.15494
1		617.0	9.9904E-2



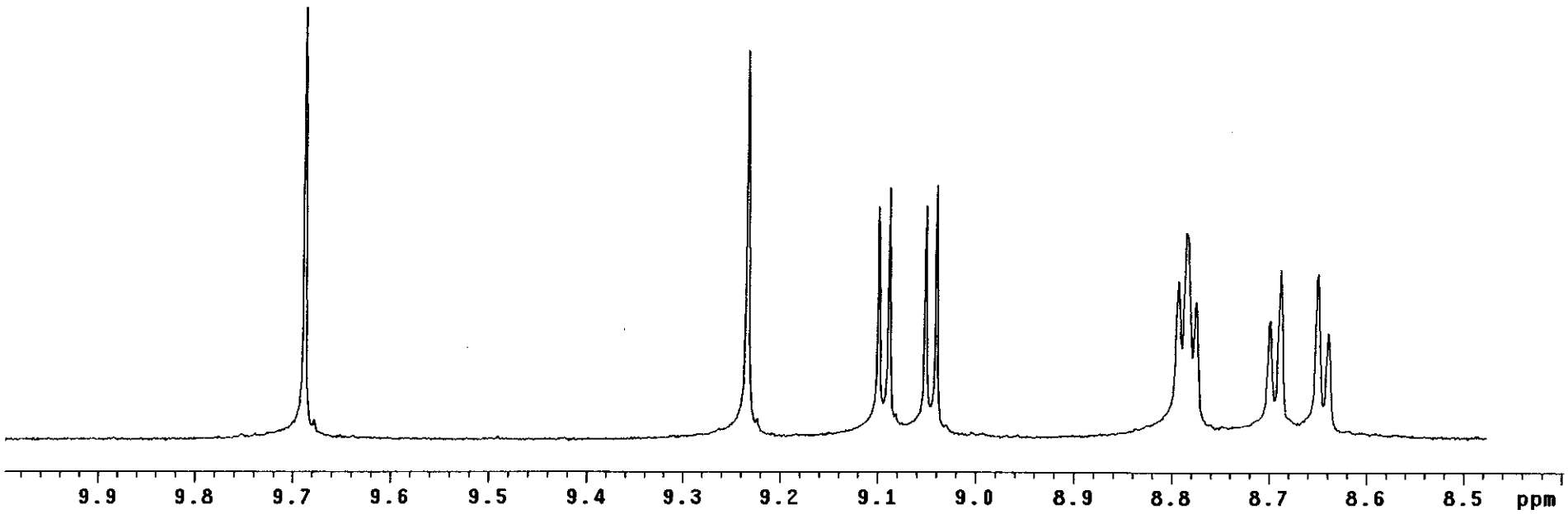


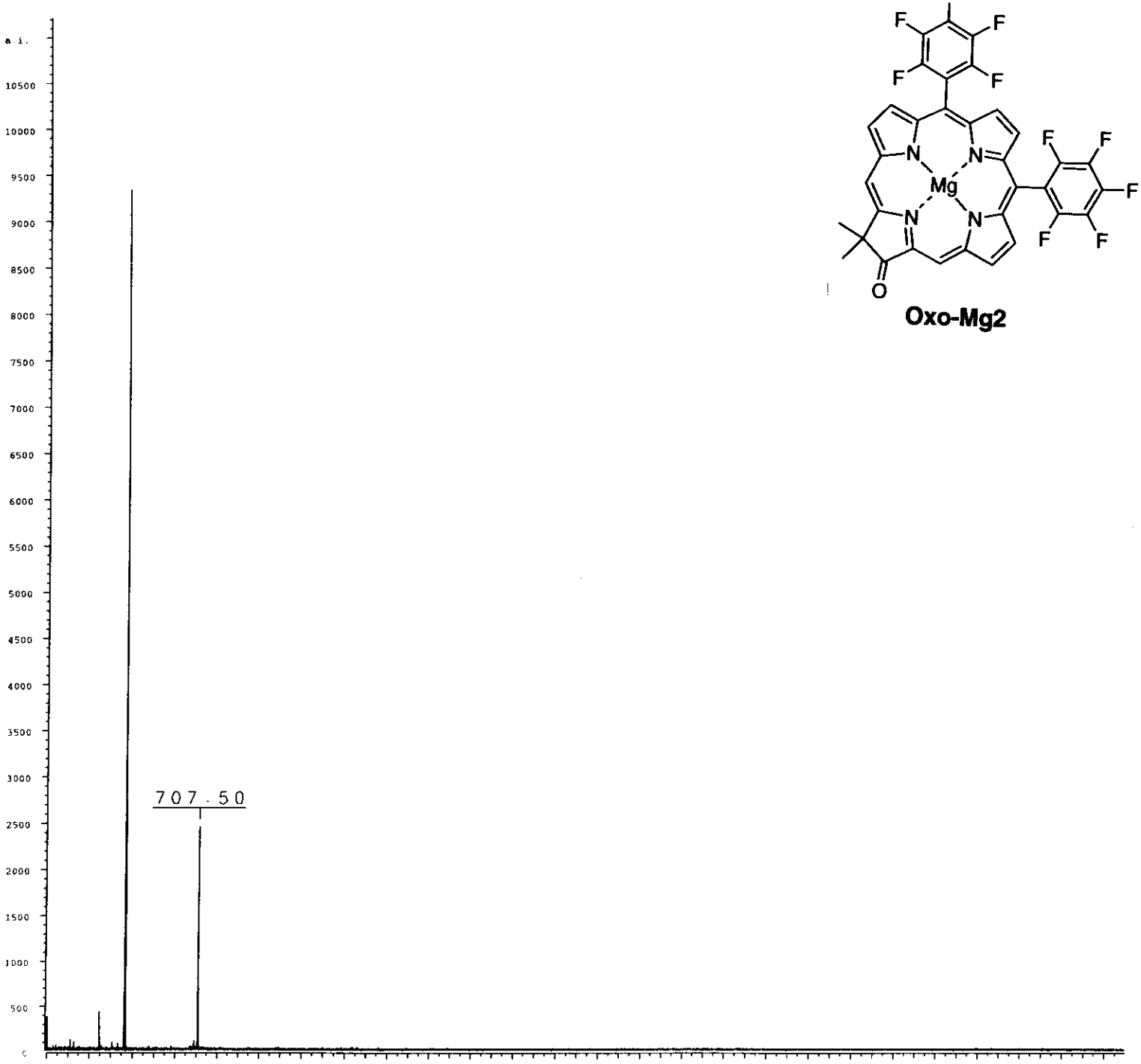
Oxo-Mg2




F
F
F
F
F
N
N
Mg
N
N
F
F
F
F
F
O

Oxo-Mg2


9.9
9.8
9.7
9.6
9.5
9.4
9.3
9.2
9.1
9.0
8.9
8.8
8.7
8.6
8.5
ppm

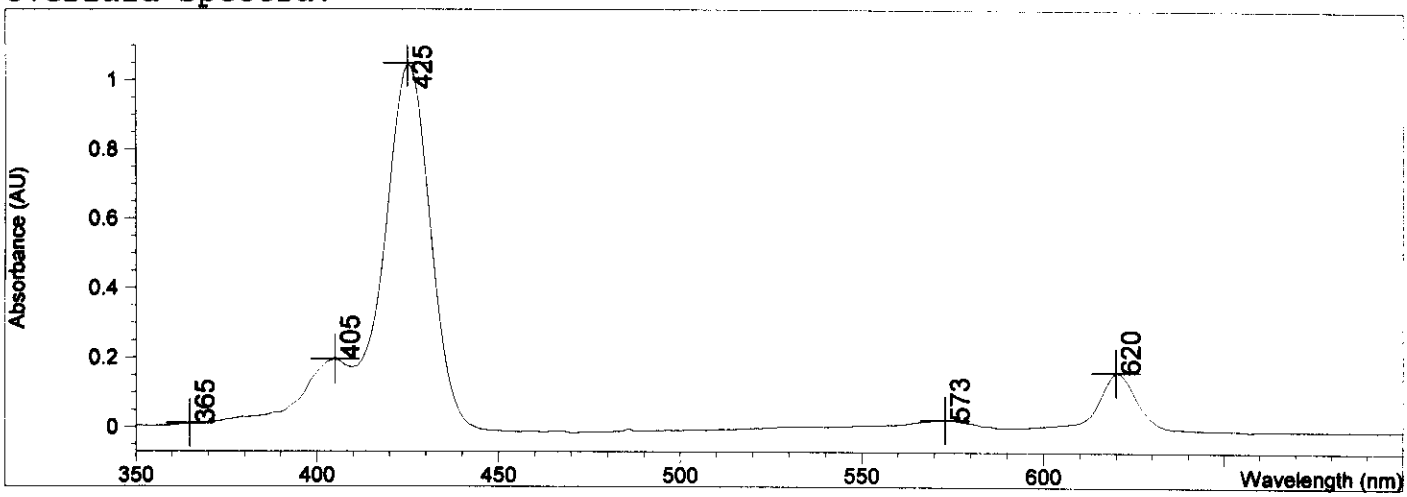


Oxo-Mg2

```
INSTRUM TOF
OpId    N. Srinivasan
SMPNAM  020180
AQ_DATE Thu Mar  7 15:52:03 2002
PATH    /data/chemistry/LINDSEY/TANIGUCHI
POLARI  POS
AQOP_m  Reflector
TD          50000
NoSHOTS        50
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]
Ulens           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           56.0
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
DPMASS         700.00  [Da]
RBNDVAL          0.33
LBNDVAL          0.28
IS2BNDV          0.91
CMT1    Oxo-Mg-1b
CMT2    Attn=56, shots = 50
```

Method file : <untitled>
Information : Default Method
Data File : C:\HPCHEM\1\DATA\MASA\OXMG1B.SD Created : 3/14/02 15:47:31

Overlaid Spectra:



#	Name	Peaks(nm)	Abs(AU)
1		425.0	1.04920
1		405.0	0.19552
1		620.0	0.16023
1		573.0	2.2091E-2
1		365.0	1.1292E-2