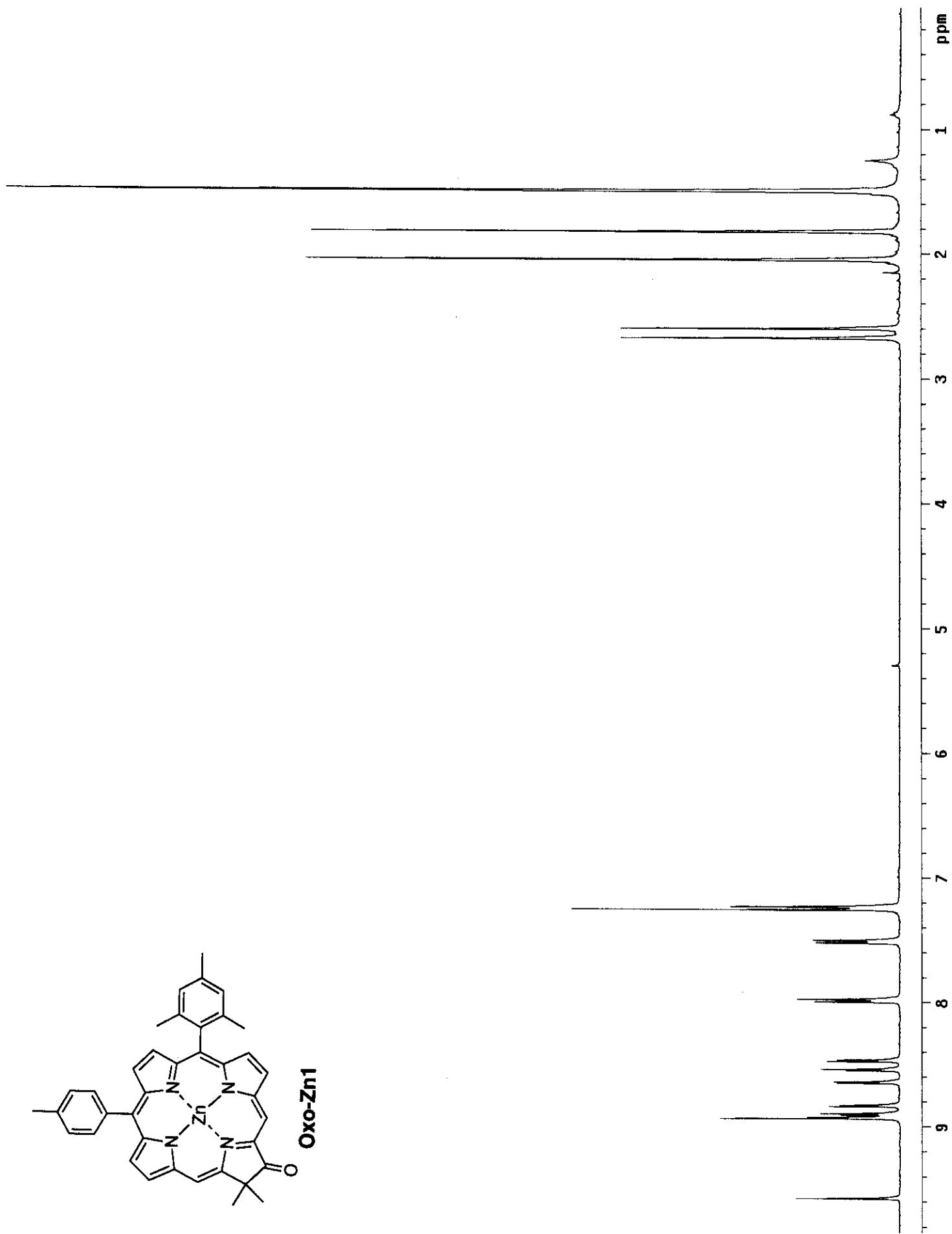
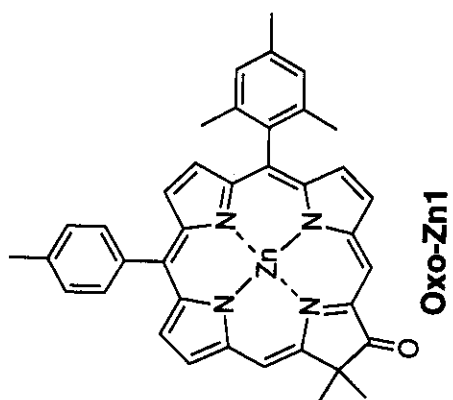


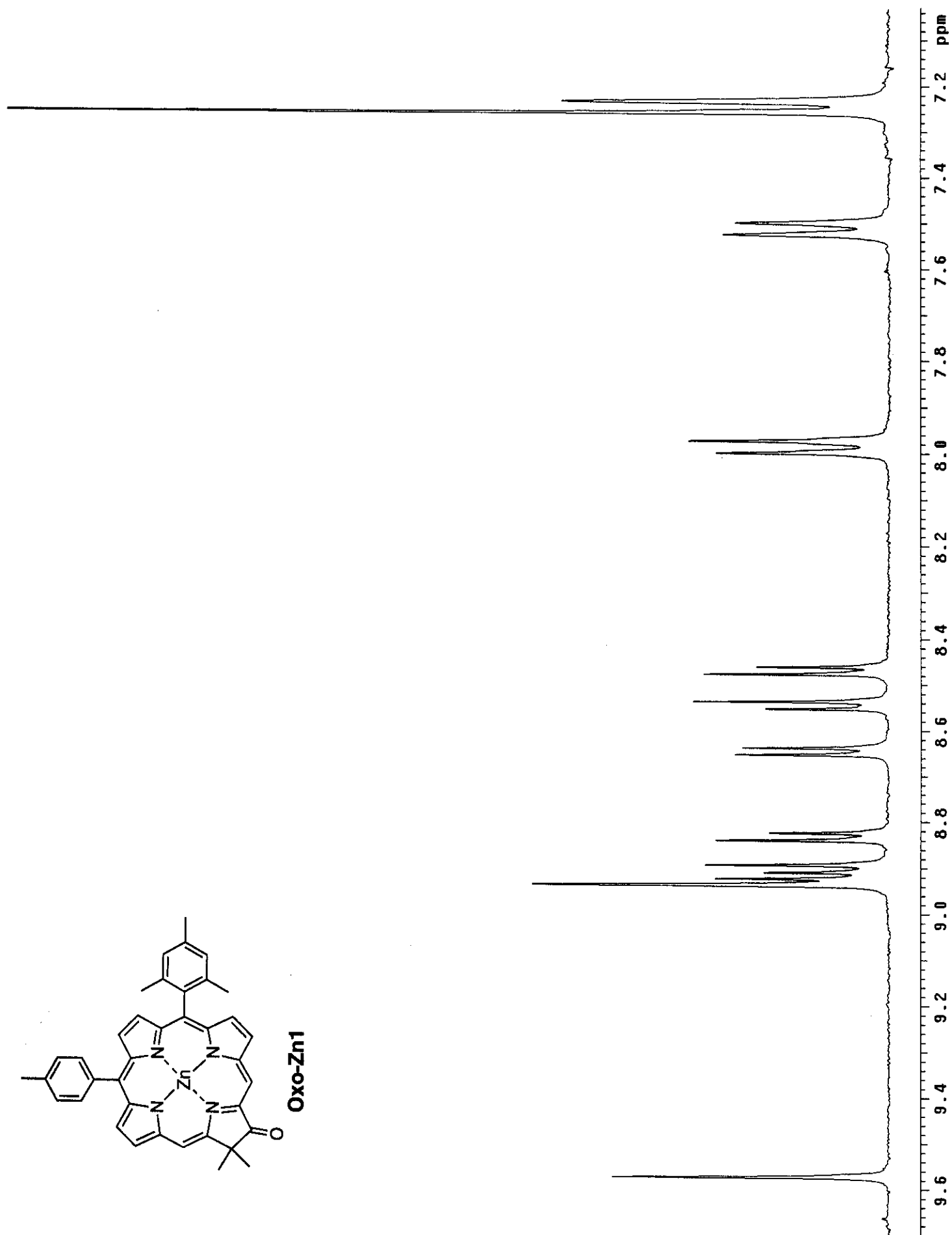
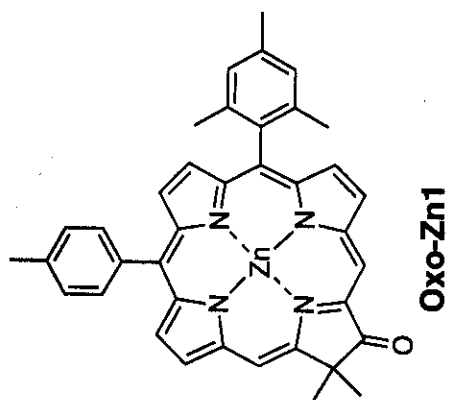
Supporting Information for:
Synthesis and Electronic Properties of Regioisomerically Pure Oxochlorins

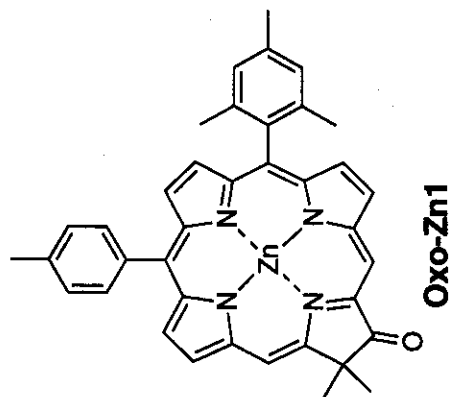
Masahiko Taniguchi, Han-Je Kim, Doyoung Ra,
Jennifer K. Schwartz, Christine Kirmaier, Eve Hindin, James R. Diers,
Sreedharan Prathapan, David F. Bocian, Dewey Holten, and Jonathan S. Lindsey

Table of contents:

Experimental data for all new chlorins and oxochlorins.



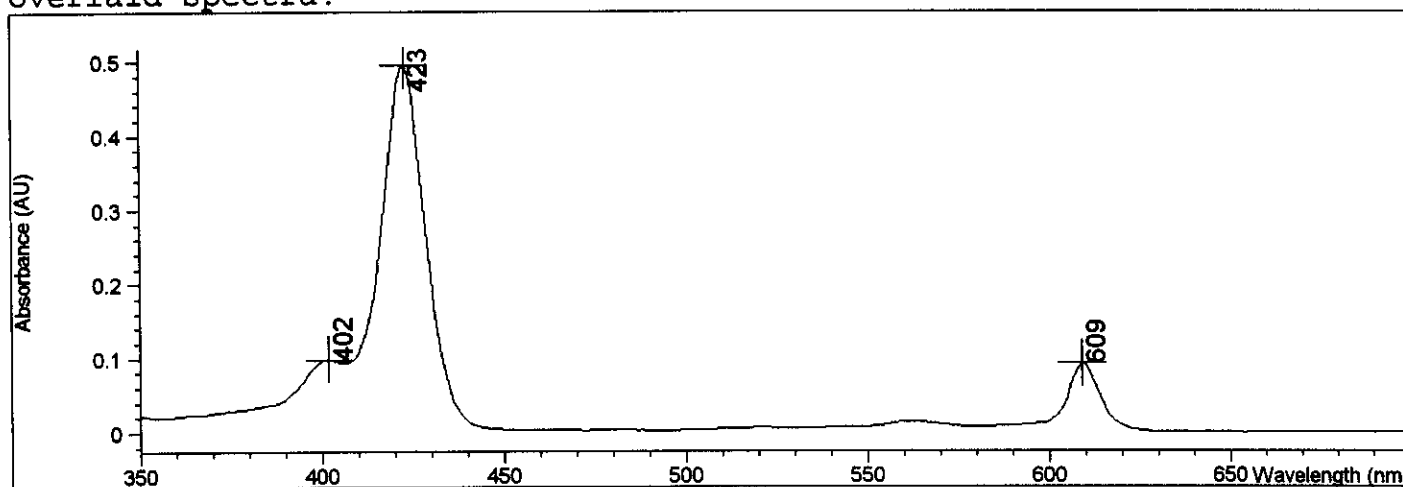




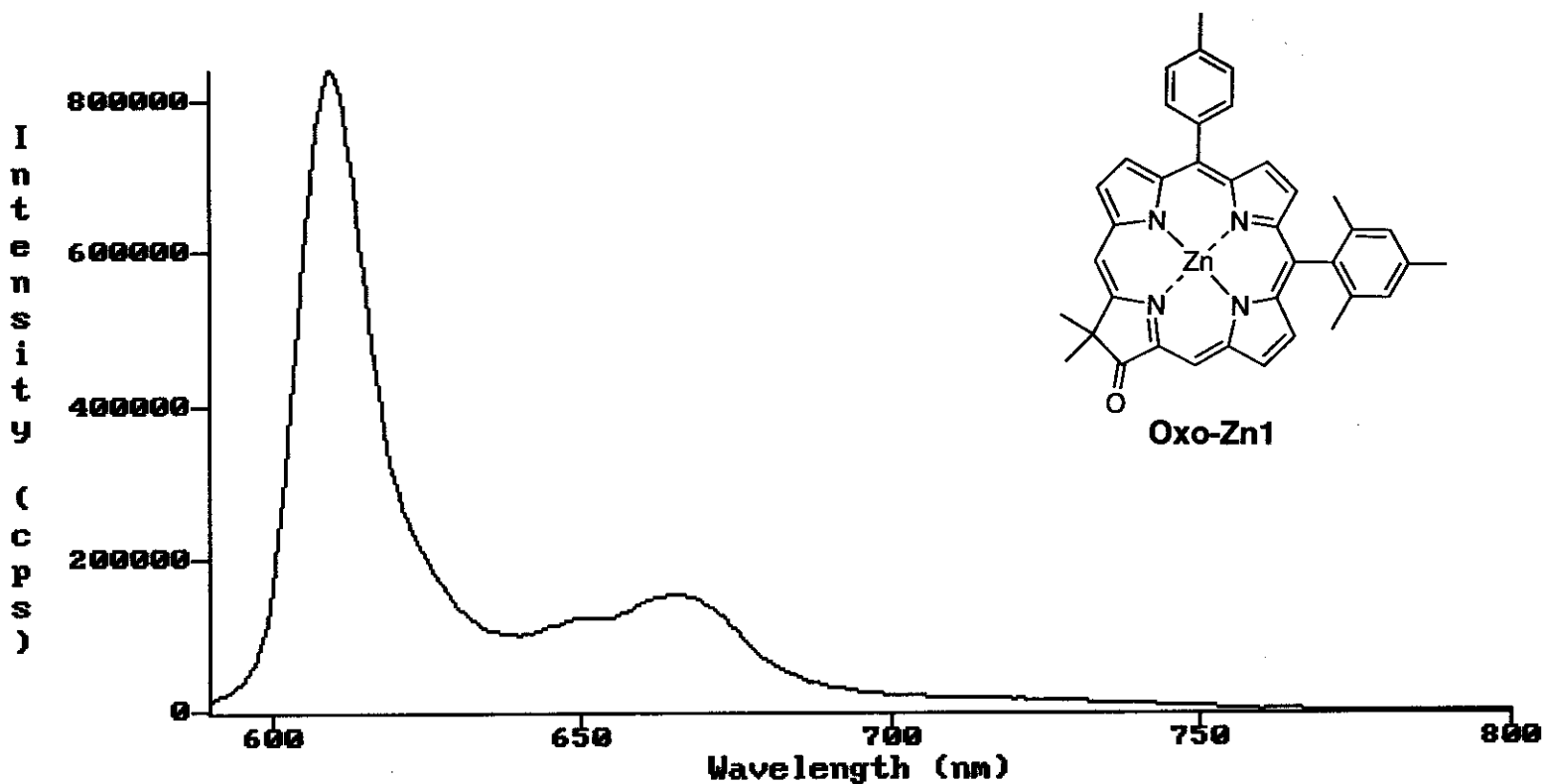
INSTRUM	TOP
OpId	Unknown
SNNAMN	0148160
EXP_DATE	Wed Mar 14 15:37:20 2001
PATN	/data/chemistry/LINOSSET/PRAITHAPAN
DATA	FOCUS
Aperture	Reflector
ApMag	30000
TID	NOSHOTS
	50
SHOMON	0
SNOWTS1	0
SNOWTS2	0
SNOWTS3	0
DW	1.00 [ms]
DELAY	0 [ms]
U1s1	20.00 [KV]
U1s2	18.50 [KV]
U1s3	17.00 [KV]
U1s4	7.50 [KV]
UB1smax	10.00 [KV]
UB1smaxF	0.00 [KV]
UB1smaxFull	0.00 [KV]
UB1sacc	1.55 [KV]
UB1sR	9.00 [KV]
UB1sG	9.00 [KV]
REPZ1	1.00 [Hz]
AUTZEN	30.0
M1	2067510.748
M2	353.368
	0.000
HITURNO	no
GDOWN	Yes
CURELY	short
DEFTURN	no
RANSRD	no
U1S2RD	no
UPCAL1	510.84
DPAPASS	200.00 [Da]
LREMOVAL	0.38
LRANDVAL	0.23
LRANDNOV	0.31
CMT2	

Method file : <untitled>
 Information : Default Method
 Data File : C:\RSLSPE~1\04220102.SD Created : 4/22/01
 17:47:51

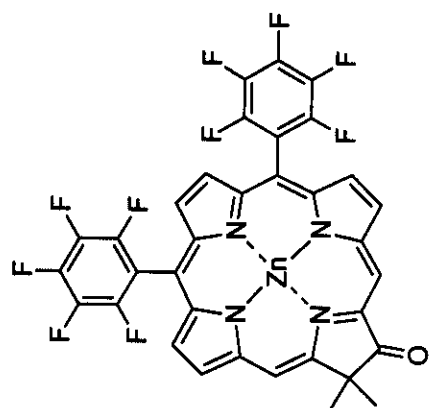
Overlaid Spectra:



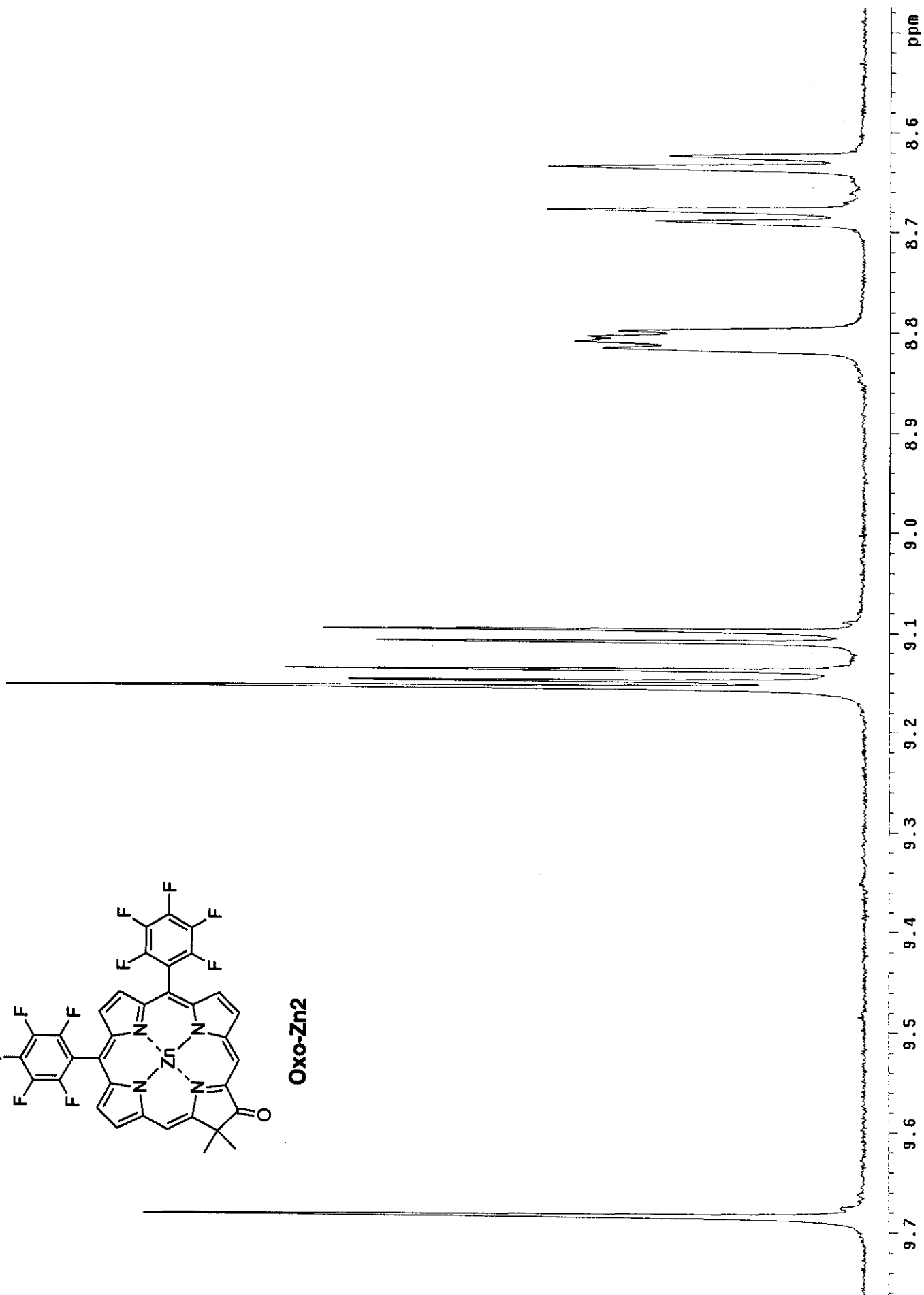
#	Name	Peaks (nm)	Abs (AU)
1	Mes-Tol-Zn-Oxo	423.0	0.49478
		402.0	9.8378E-2
		609.0	9.2124E-2

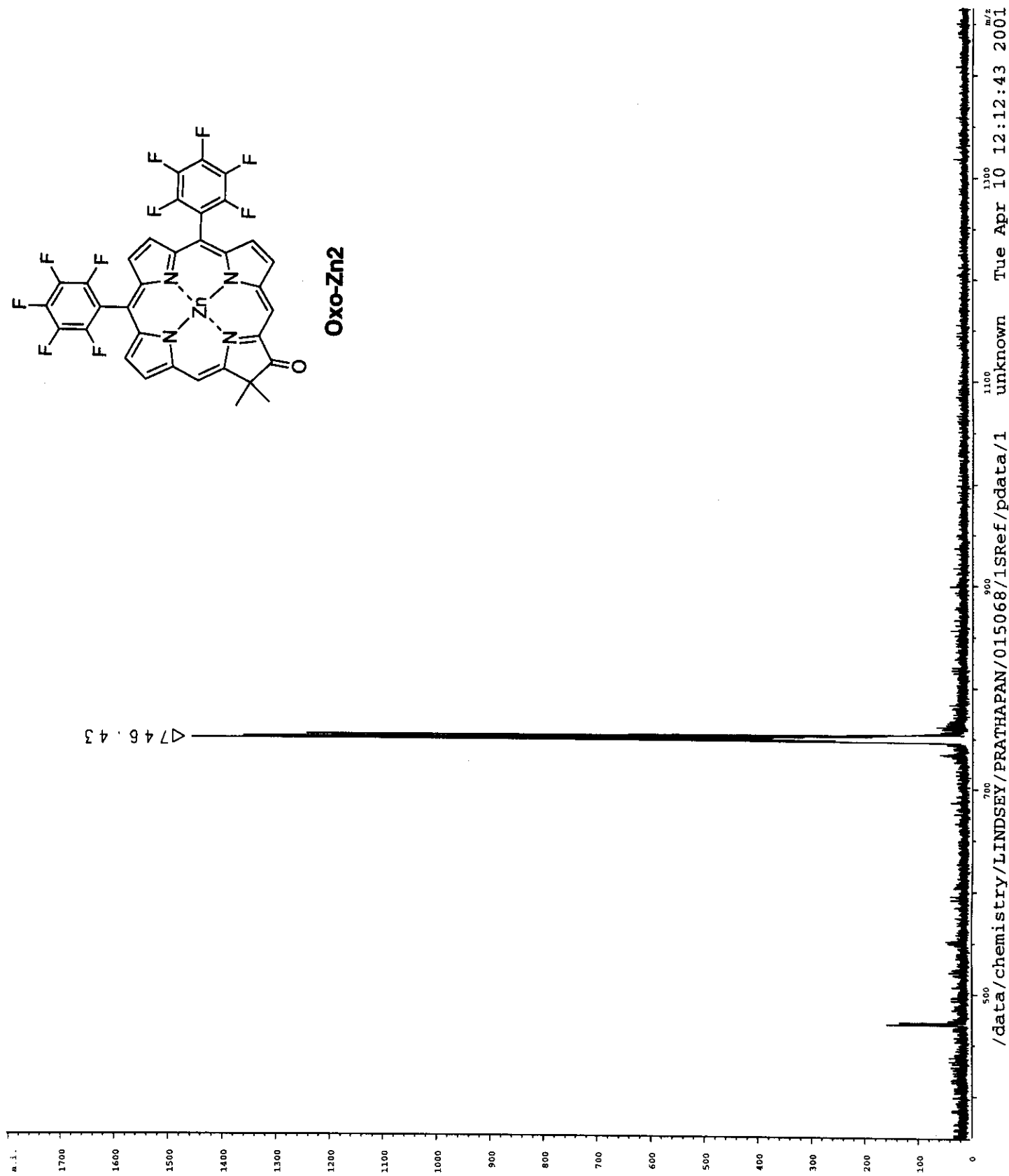






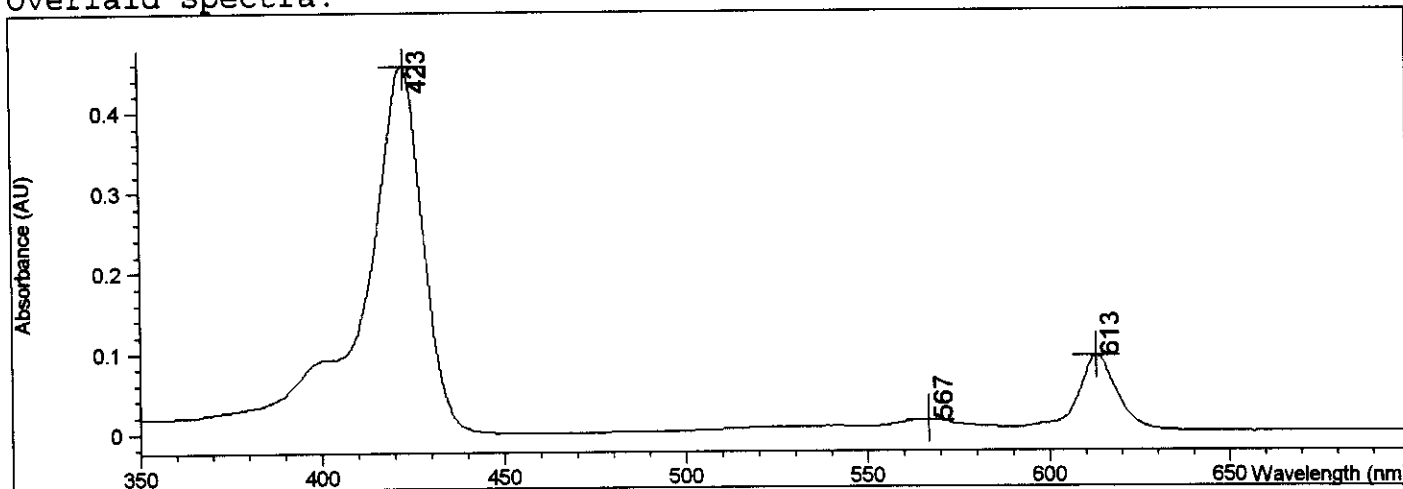
Oxo-Zn2





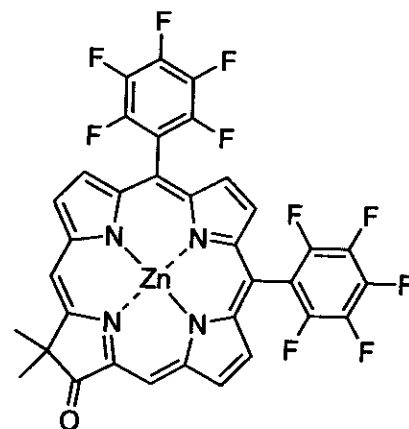
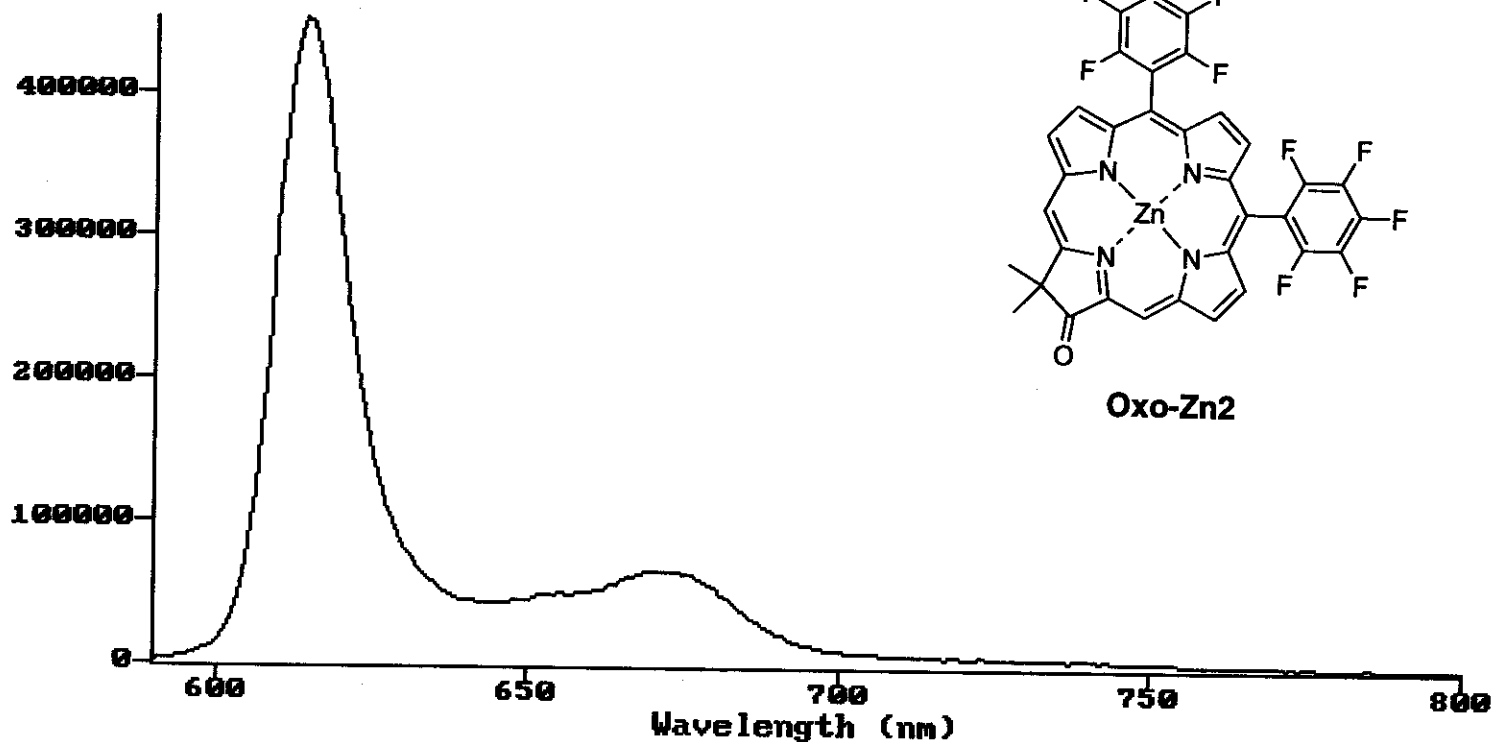
Method file : <untitled>
 Information : Default Method
 Data File : C:\RSLSPE~1\04220104.SD Created : 4/22/01
 19:11:23

Overlaid Spectra:

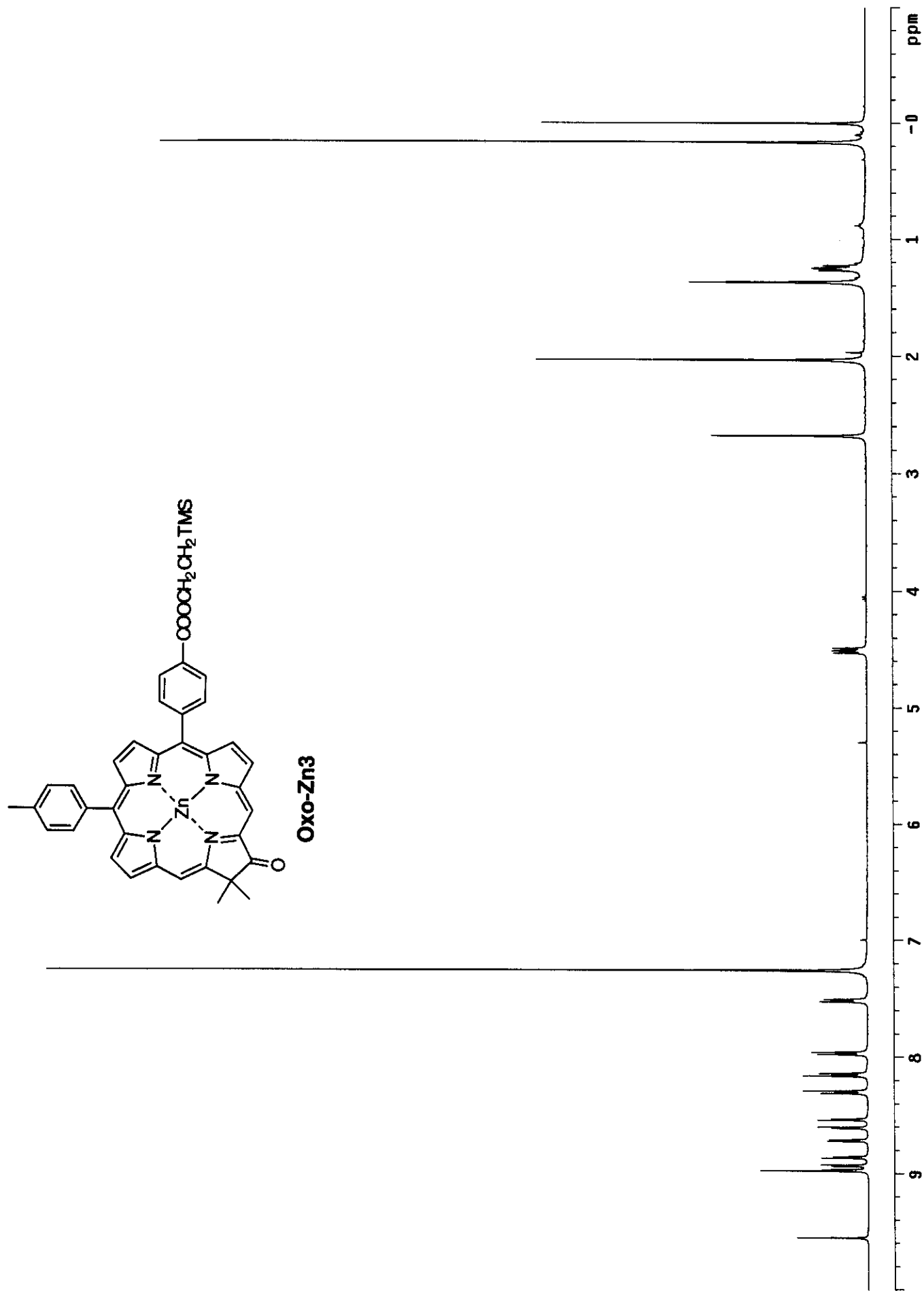


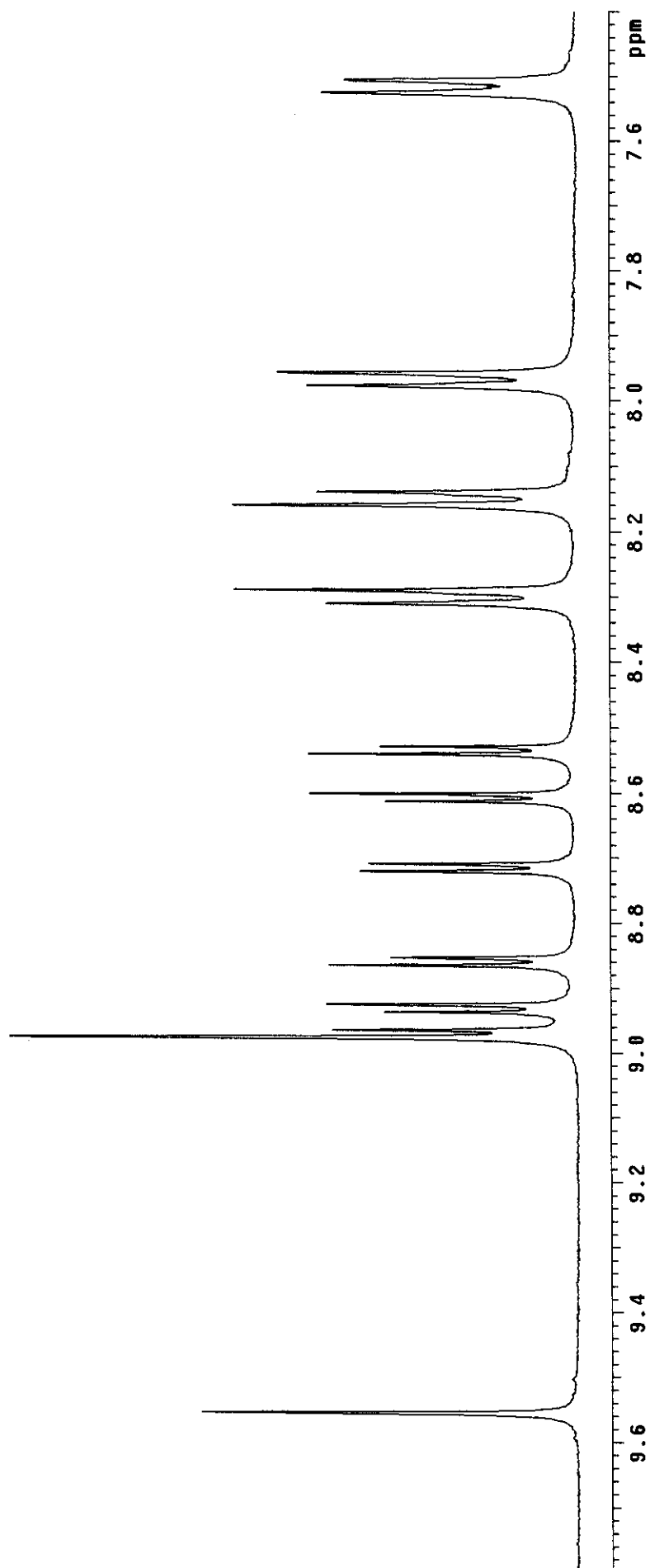
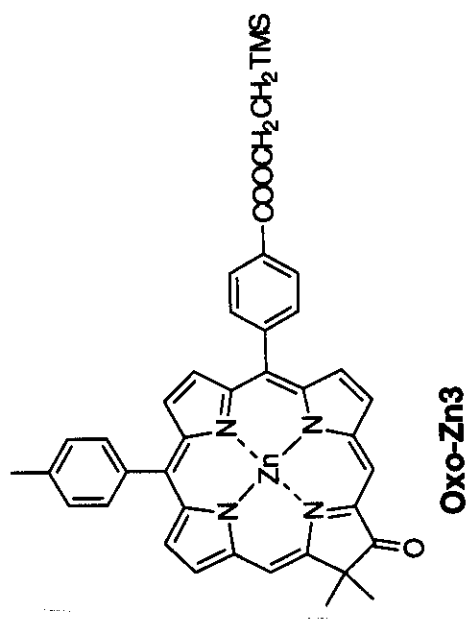
#	Name	Peaks (nm)	Abs (AU)
1	F5-Zn-Oxo	423.0	0.45626
1		613.0	9.2612E-2
1		567.0	1.4304E-2

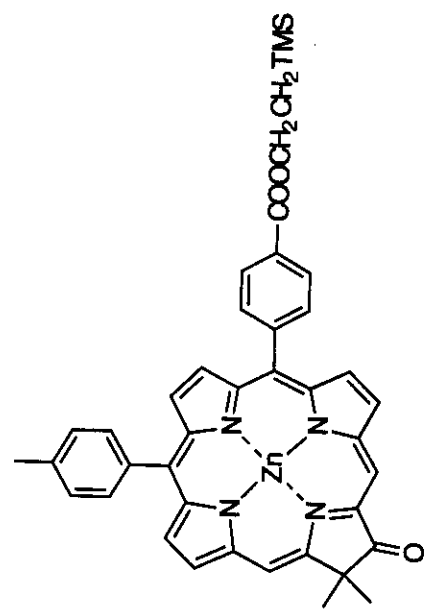
Intensity (cps)



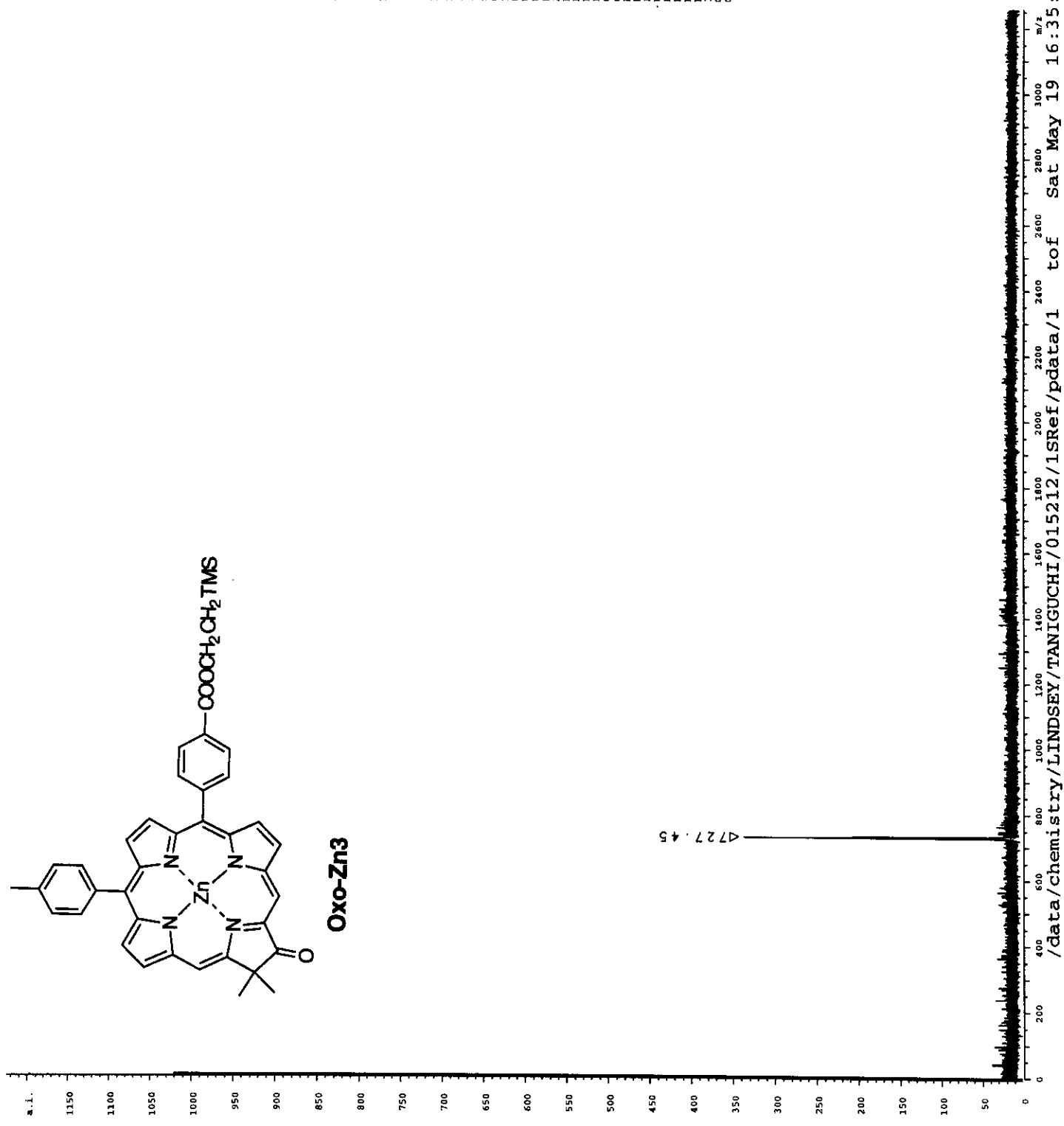
Oxo-Zn2



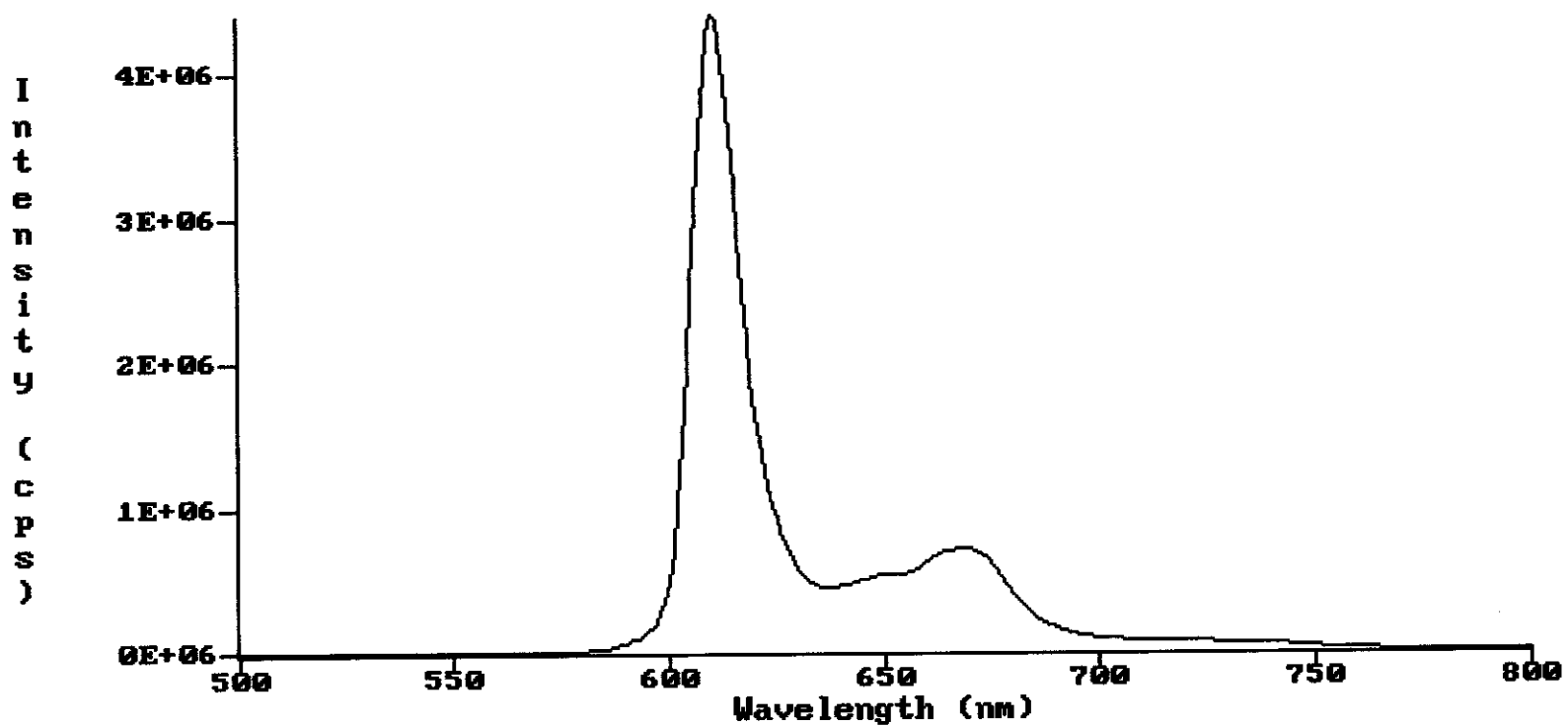
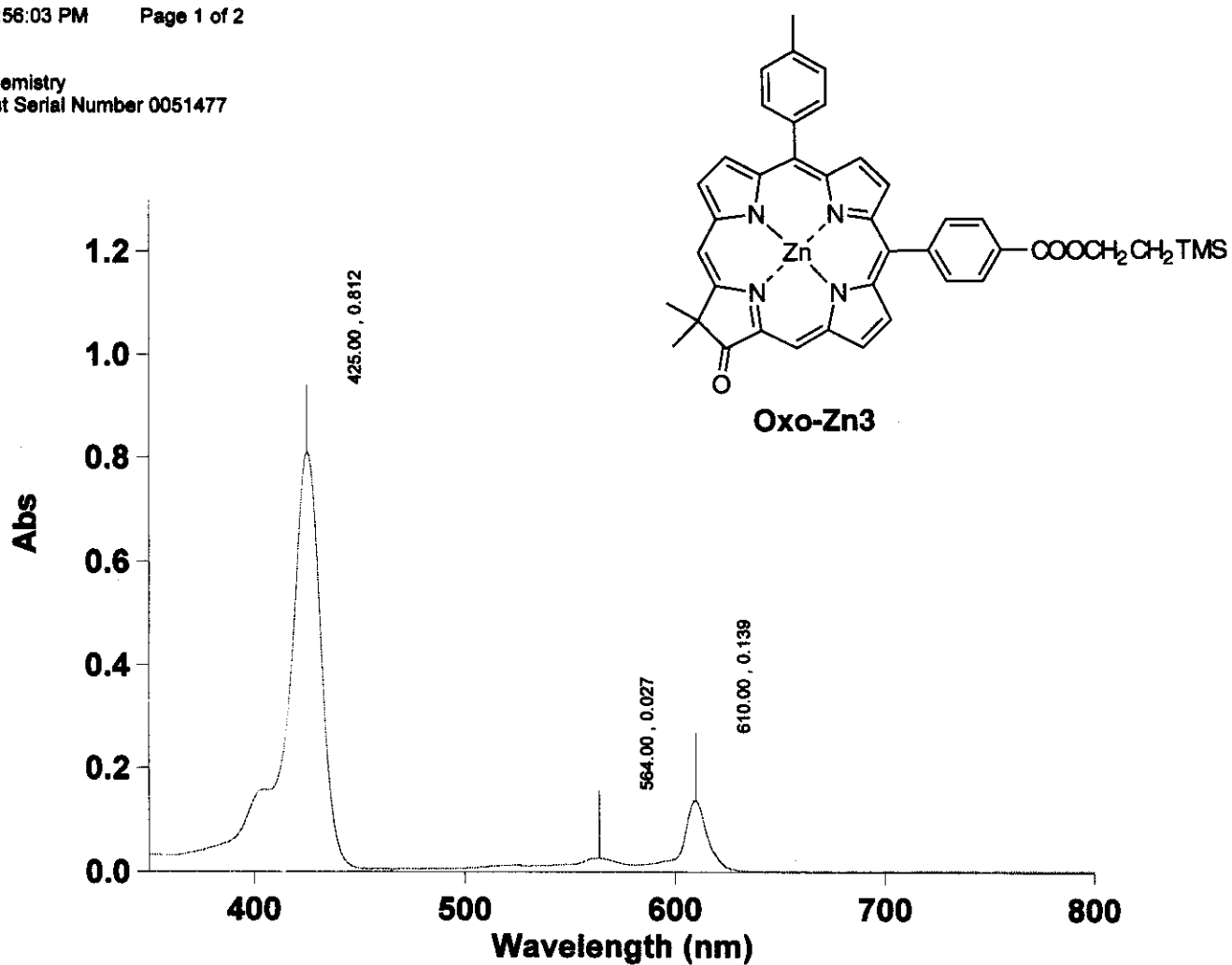


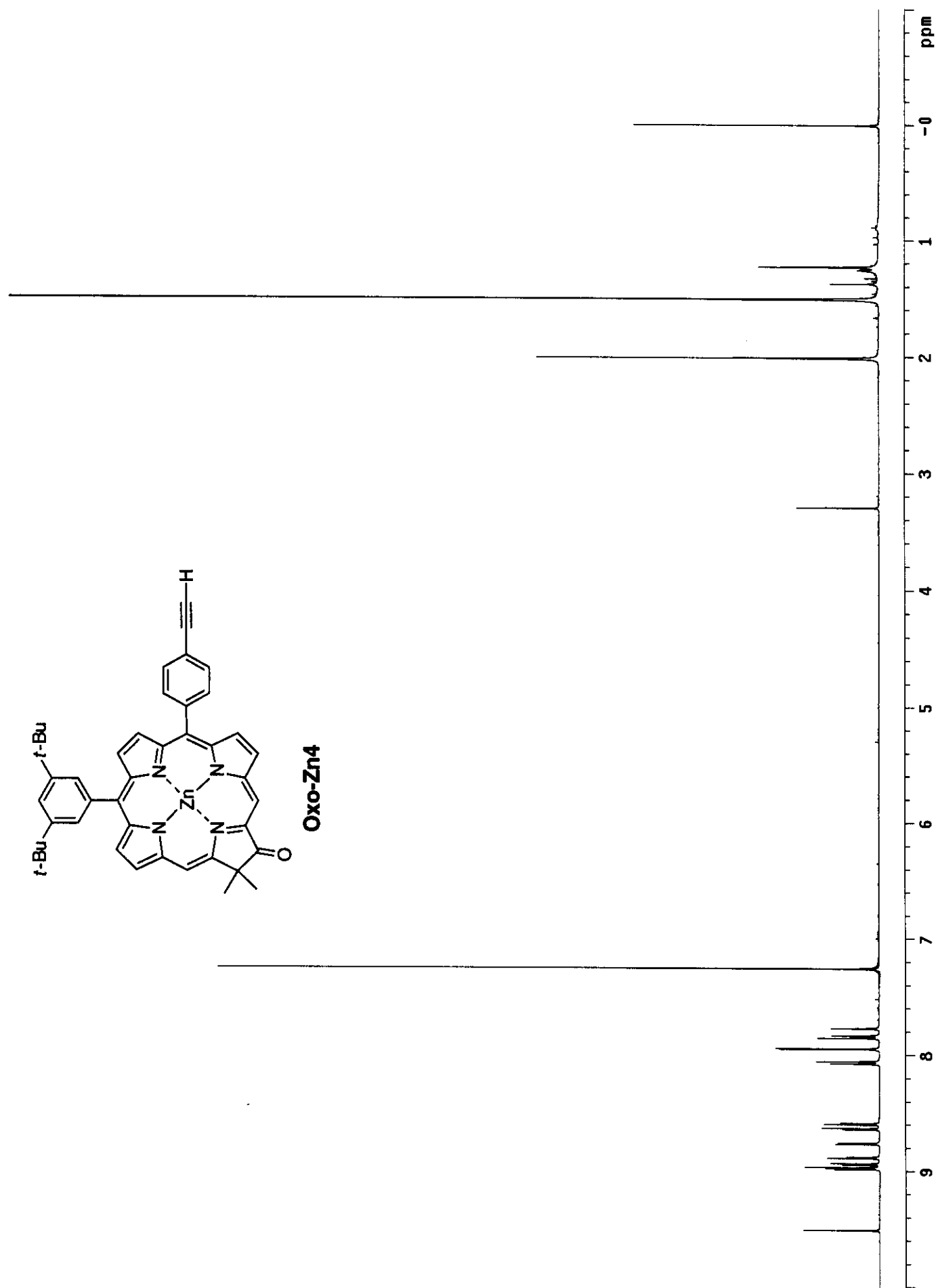


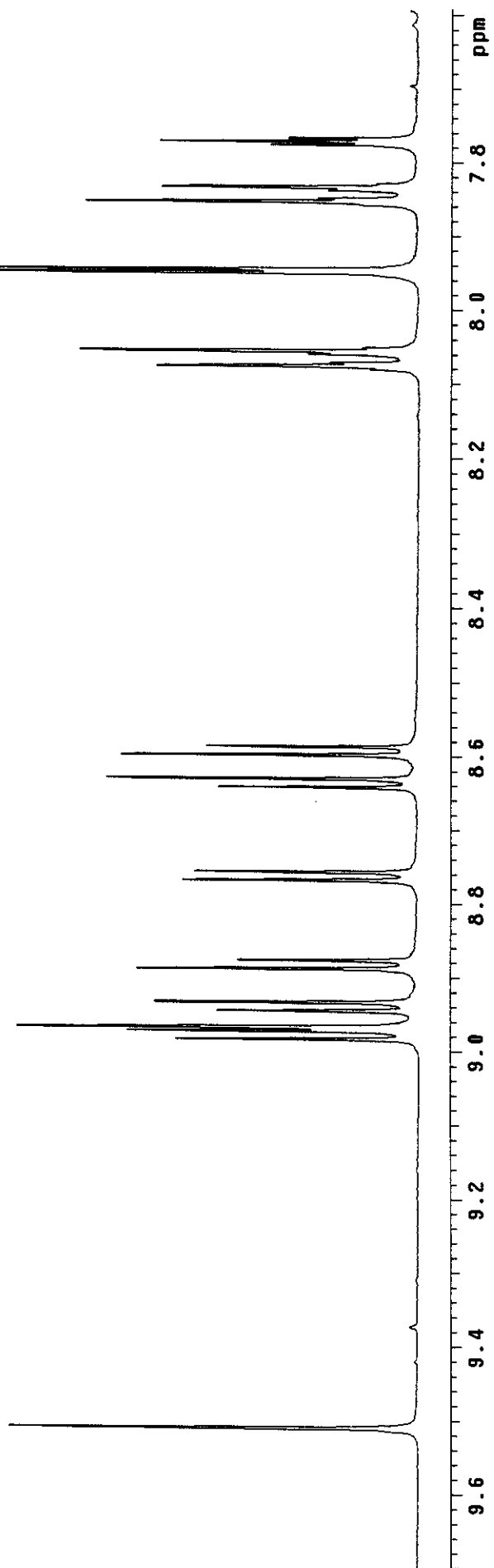
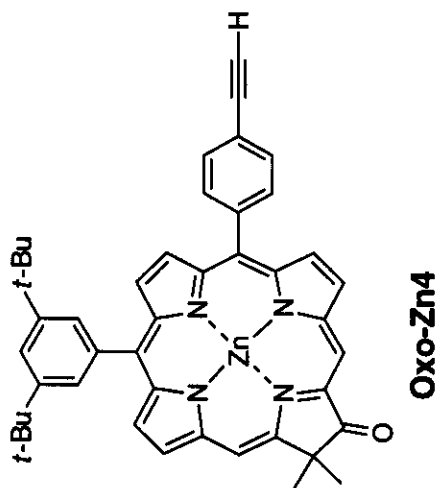
Oxo-Zn3

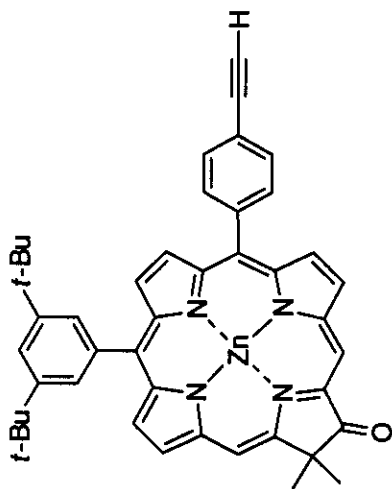


INSTRUM TOF
 OpId N. Srinivasan
 SMPNAM 015212
 ACQDATE Sat May 19 16:34:54 2001
 DATA /data/chemistry/LINDSEY/TANIGUCHI
 POLARI POS
 AQOP m Reflector
 TD 40000
 NC SHOTS 35
 SMOXUM 0
 SHOTS1 0
 SHOTS2 0
 SHOTS3 0
 DM 1.00 [ns]
 DELAY 0 [ns]
 Uis1 20.00 [KV]
 Uis2 18.70 [KV]
 Uref1 0.00 [KV]
 Uref2 7.00 [KV]
 Uisens 10.00 [KV]
 Uisense 10.00 [KV]
 RefPull 0.00 [KV]
 UdetL 1.50 [KV]
 UdetR 0.60 [KV]
 Udef1 2.00 [KV]
 REPH2 1.00 [Hz]
 MTEN 207110.891
 ML1 123.058
 ML2 0.000
 HITURBO no
 GDEON yes
 GDELY short
 REFEND no
 RLSSEND no
 LANSEND no
 UIS2END no
 DFCALI 510.84
 DPMASS 700.00 [Da]
 REMOVAL 0.33
 IS2ENDV 0.91
 CMT1 Zn-Oxo-CH1-COOCTWS
 CMT2 Att=39, 35shots

NCSU Chemistry
Instrument Serial Number 0051477

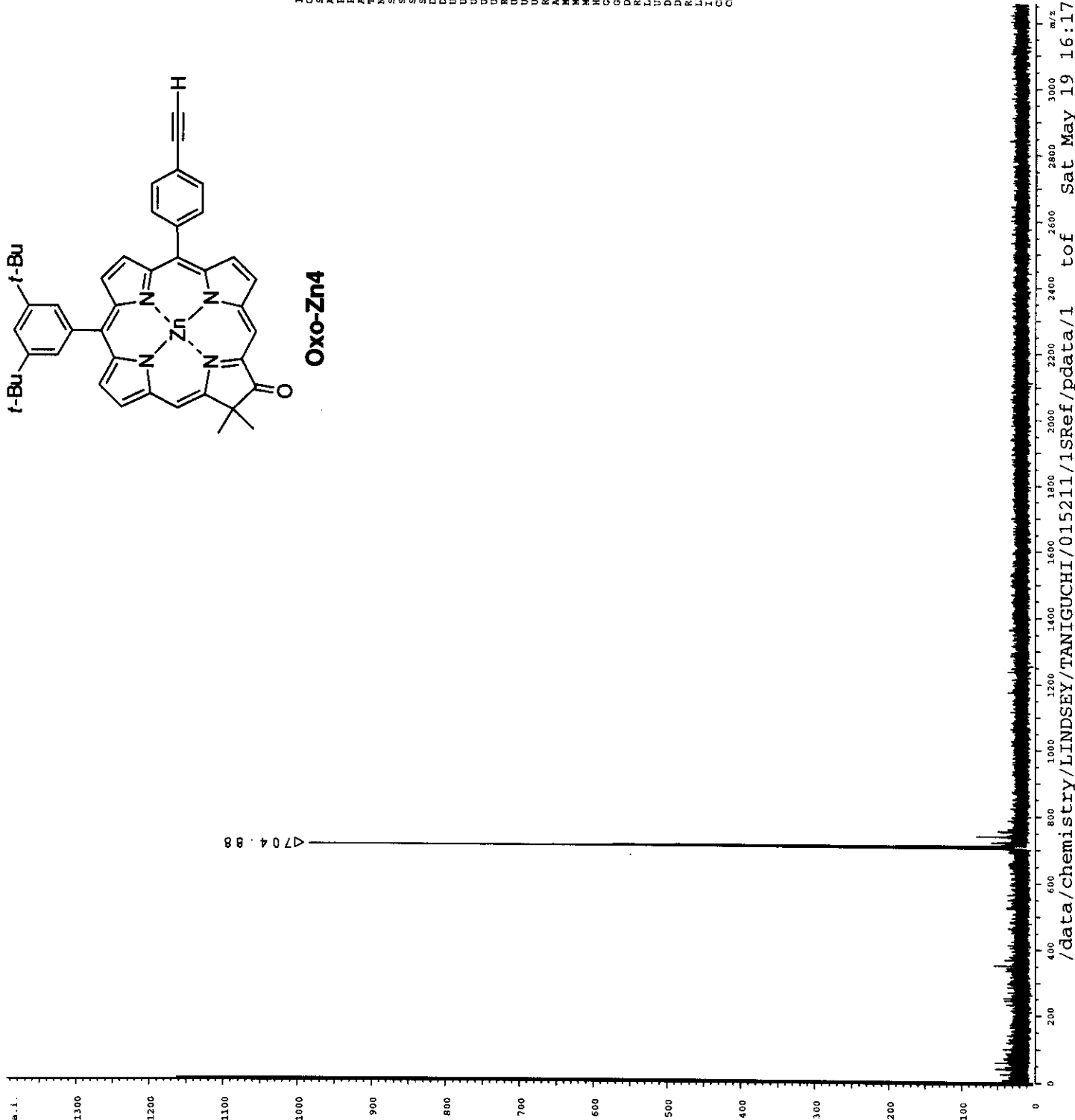




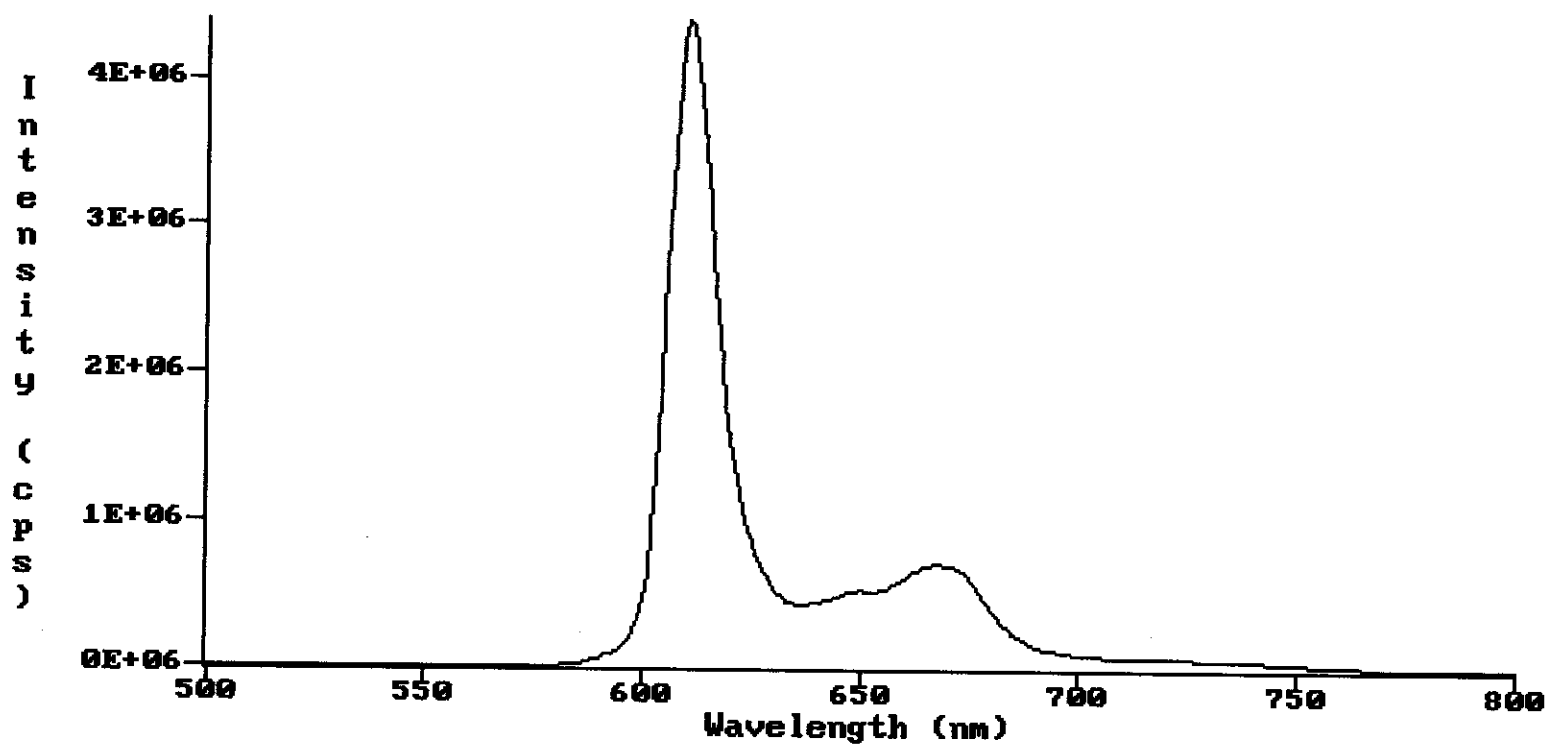
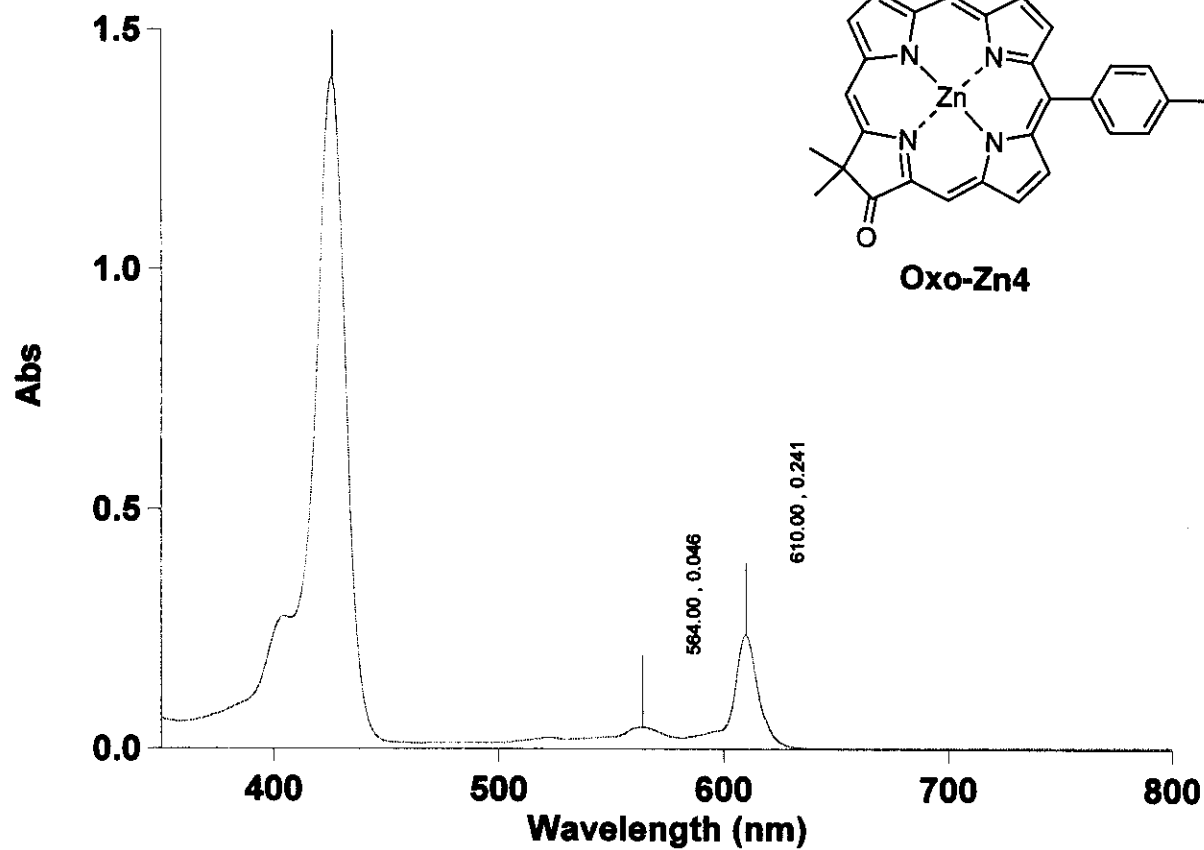


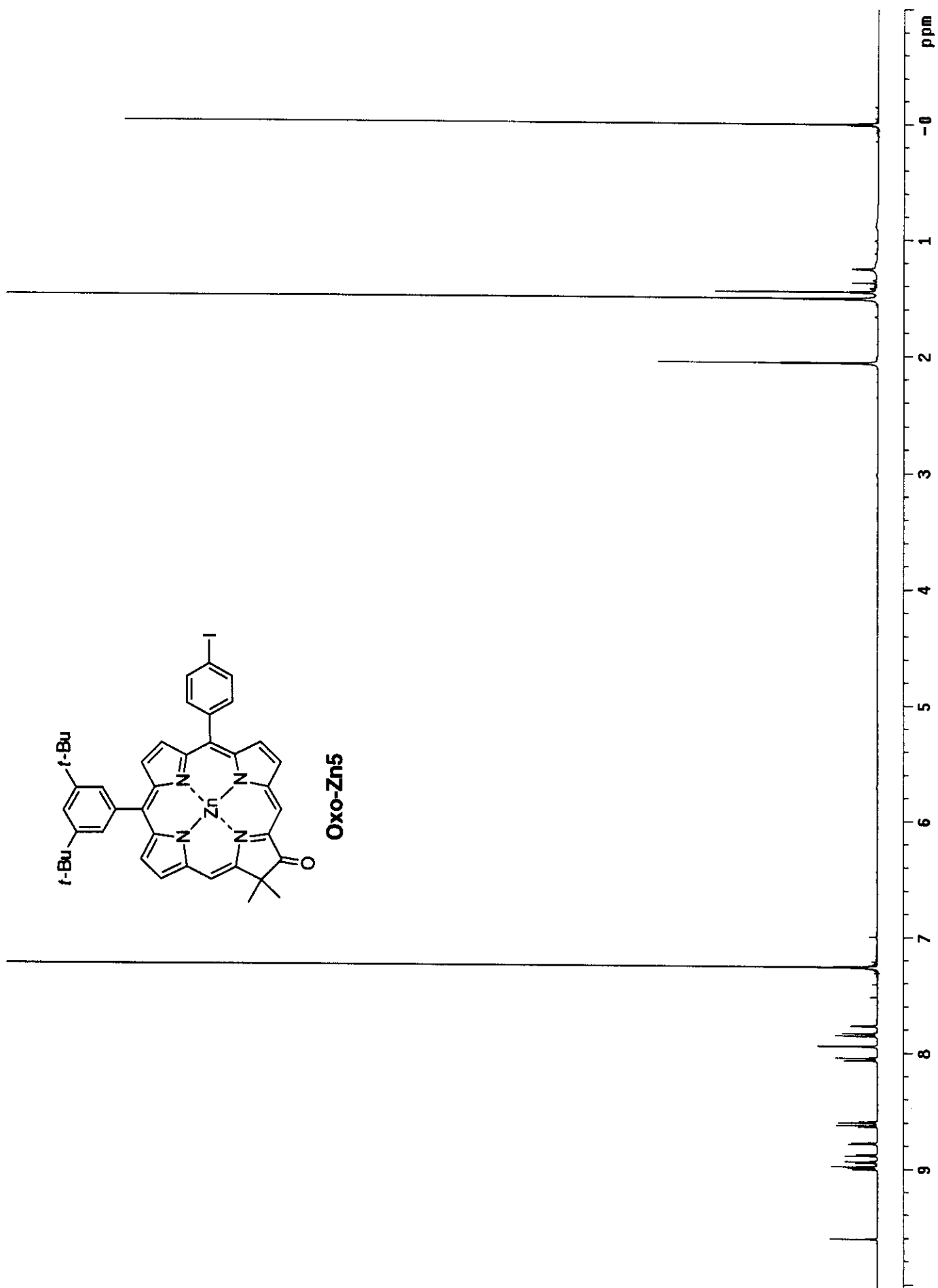
Oxo-Zn4

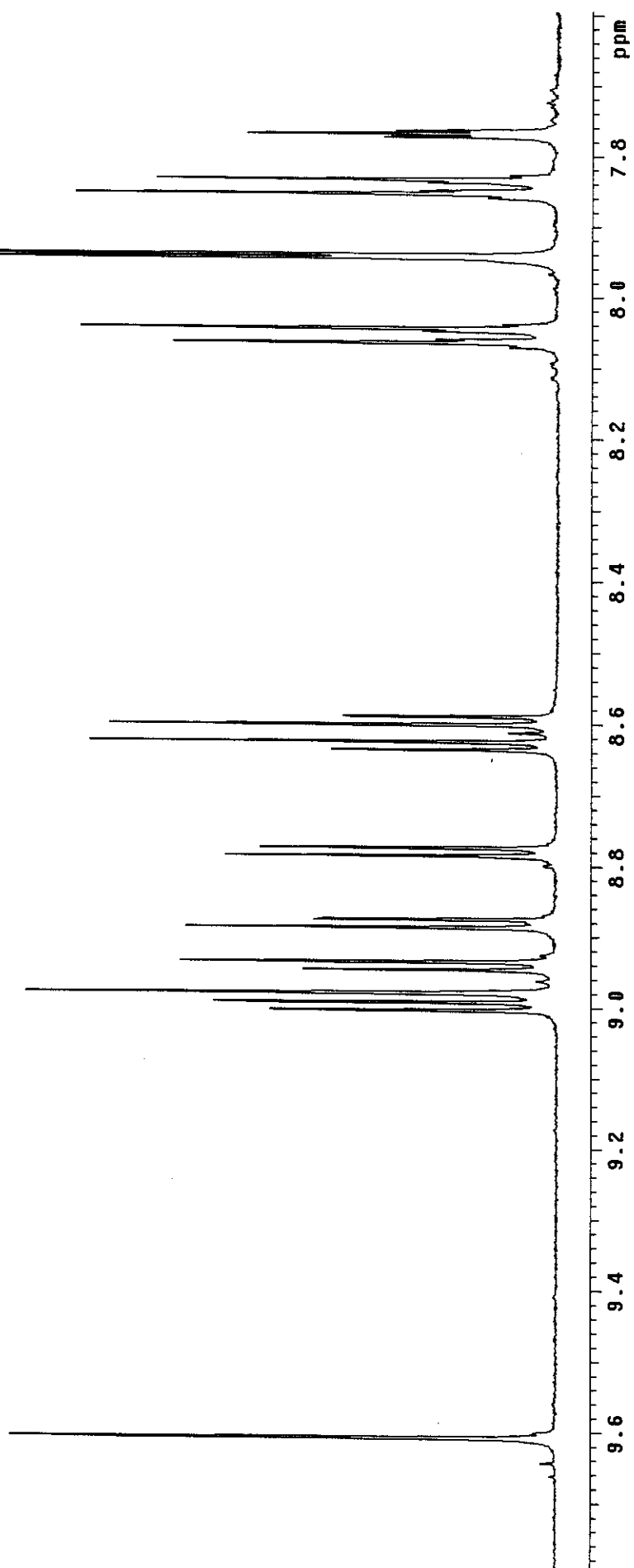
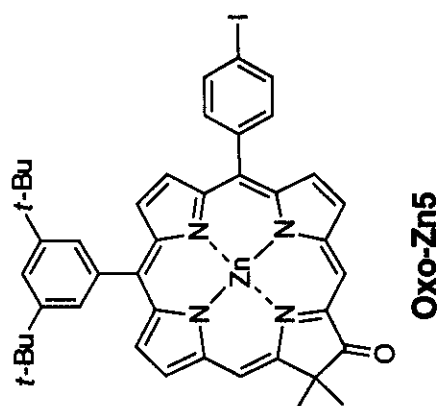
INSTRUM TOF
 OPID M 0152111
 DATE Sat May 19 16:16:41 2001
 PATH /data/chemistry/LINDSEY/TANIGUCHI
 POLARI POS
 AQP J Reflector
 TD 40000
 ACQUIS 51
 SMOPT1 0
 SMOPT2 0
 SMOPT3 0
 DW 1.00 [ns]
 DELAY 0 [ns]
 U1s1 20.00 [kV]
 U1s2 18.00 [kV]
 U1s3 7.50 [kV]
 U1s4 10.00 [kV]
 U1s5 10.00 [kV]
 U1s6 10.00 [kV]
 U1s7 1.50 [kV]
 U1s8 0.00 [kV]
 U1s9 2.00 [kV]
 U1s10 1.00 [kV]
 U1s11 35.0 [ns]
 ML1 2071110.891
 ML2 323.058
 ML3 0.000
 HITURBO no
 GEDLY short
 DEPLON no
 RLNSND no
 LINSND no
 U1S2RND no
 DECALI 510.84 [Da]
 PRNSI 700.33
 RESOL 0.28
 LENDVAL 0.91
 IS2BNDV 0.91
 CMT1 Zn-Oxo-Chl-CCl
 CMT2 Att=35, 100shots

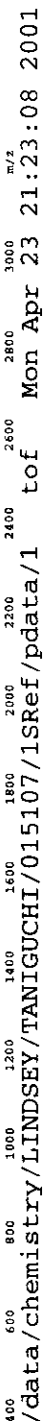


NCSU Chemistry
Instrument Serial Number 0051477





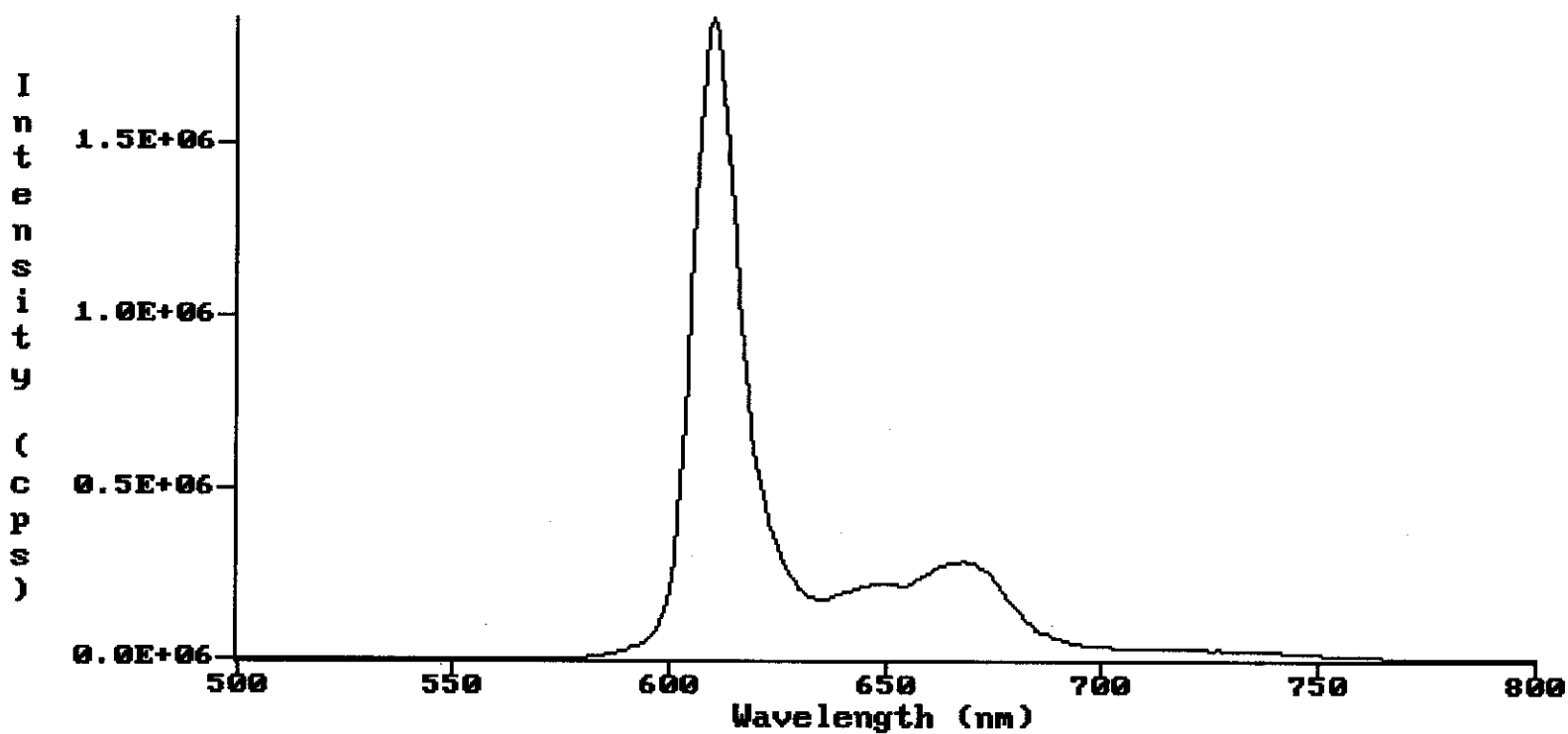
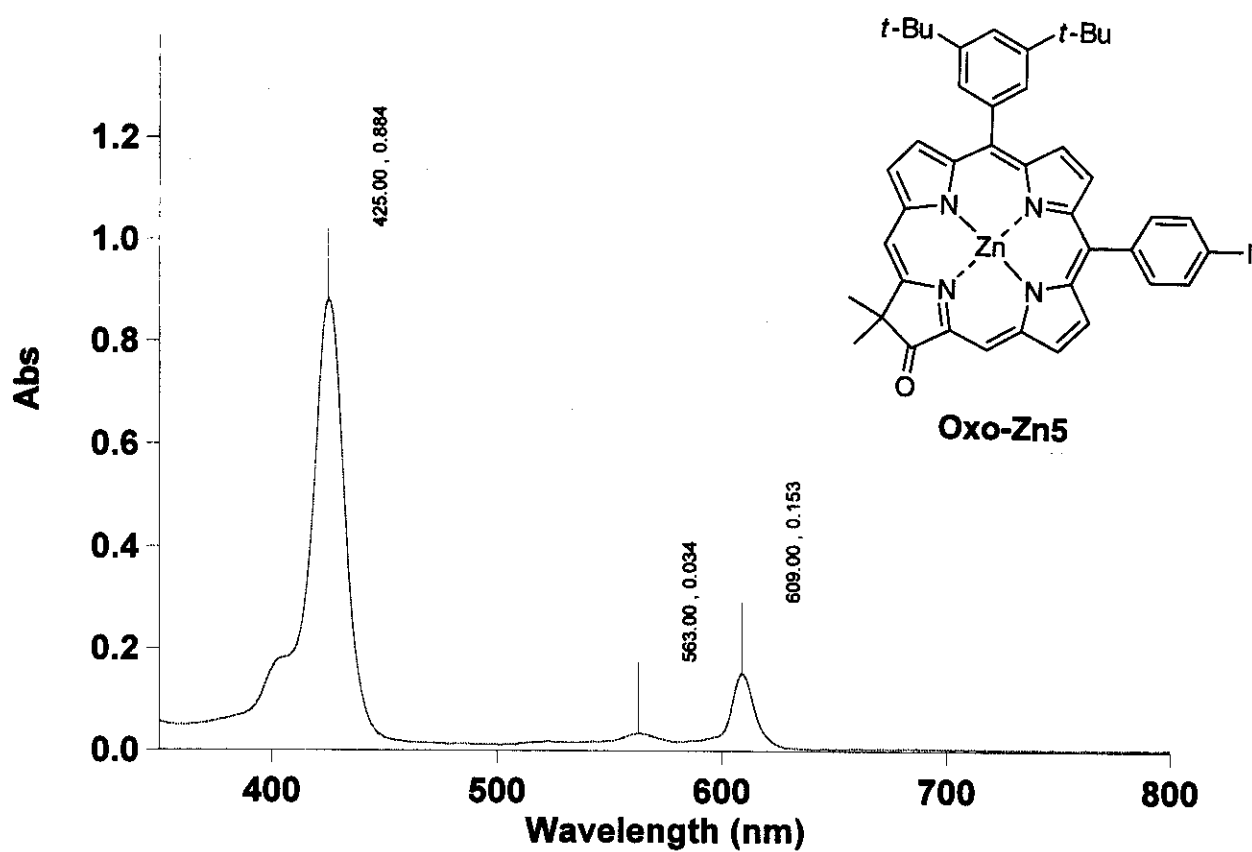


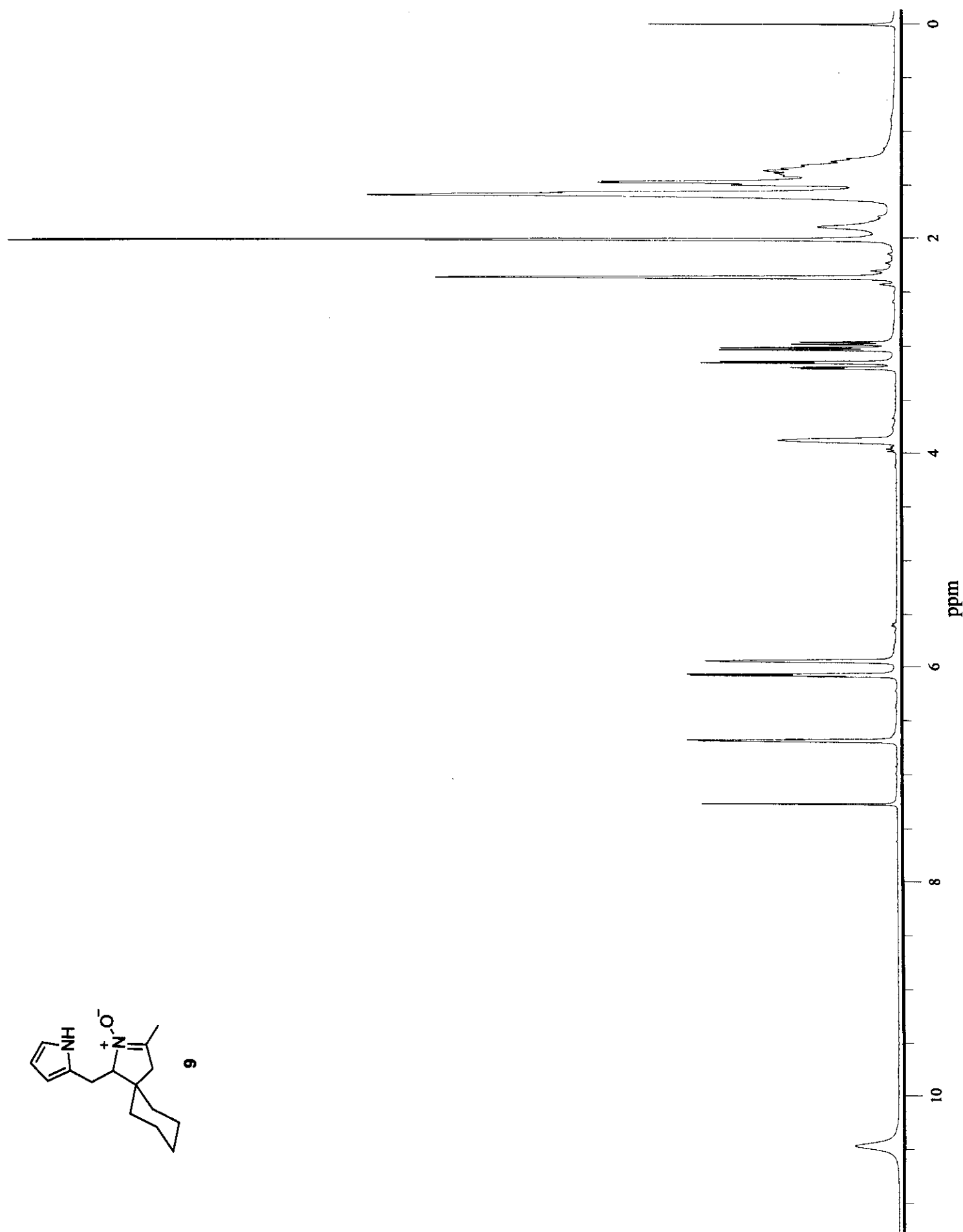


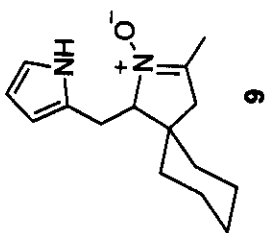
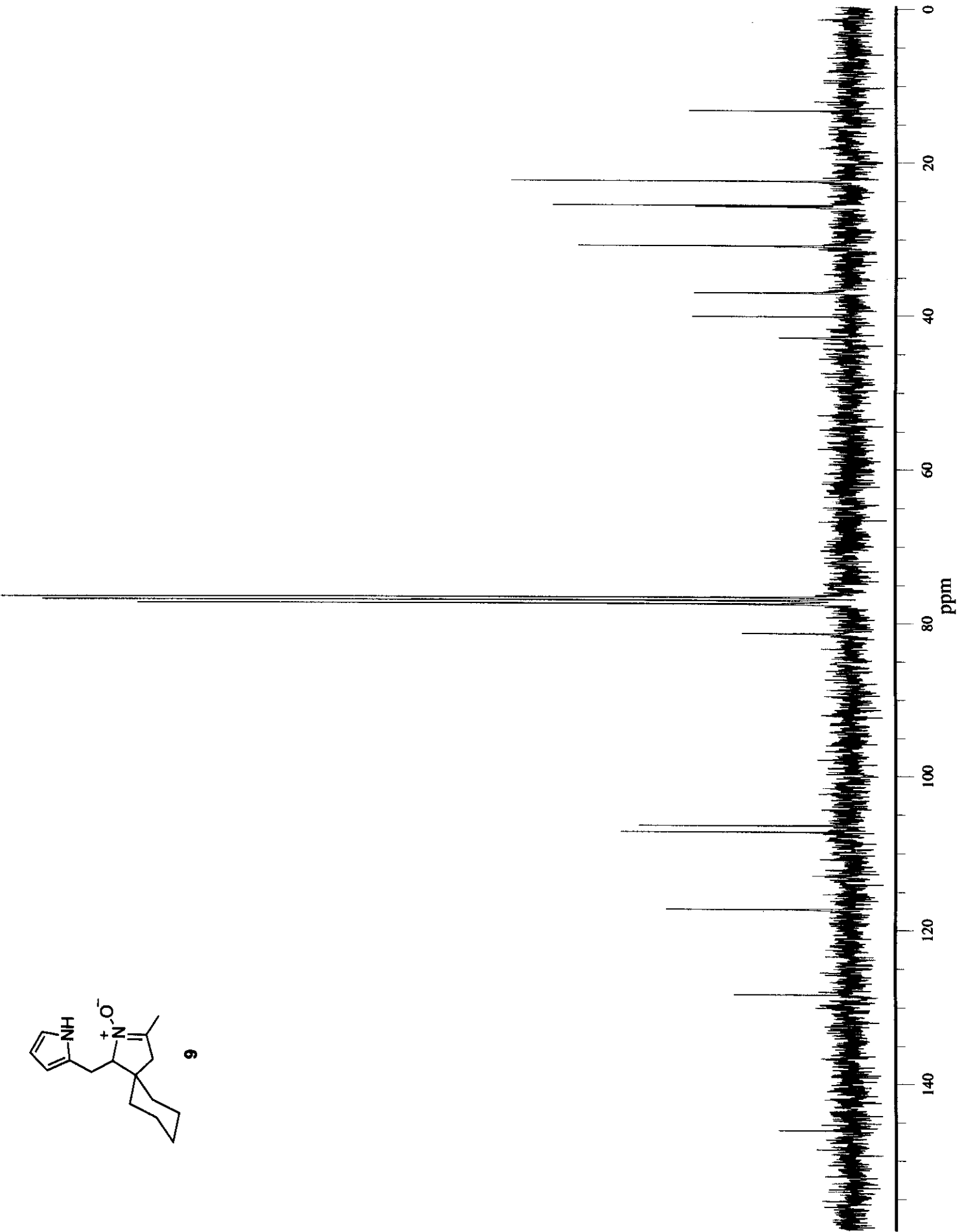
Oxo-Zn5

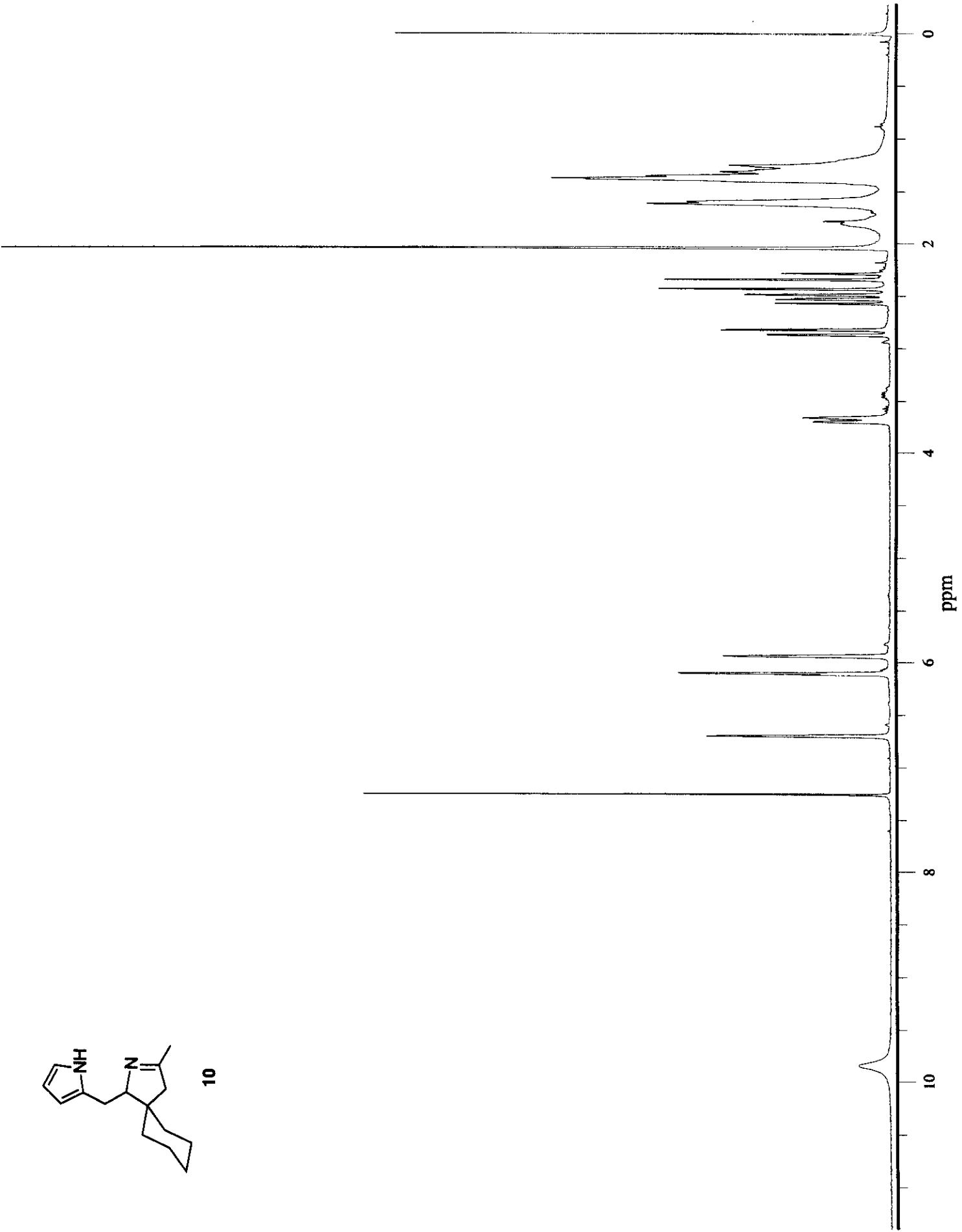
[illegible]

NCSU Chemistry
Instrument Serial Number 0051477





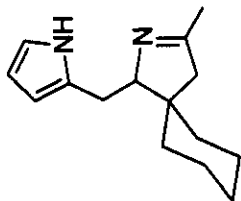




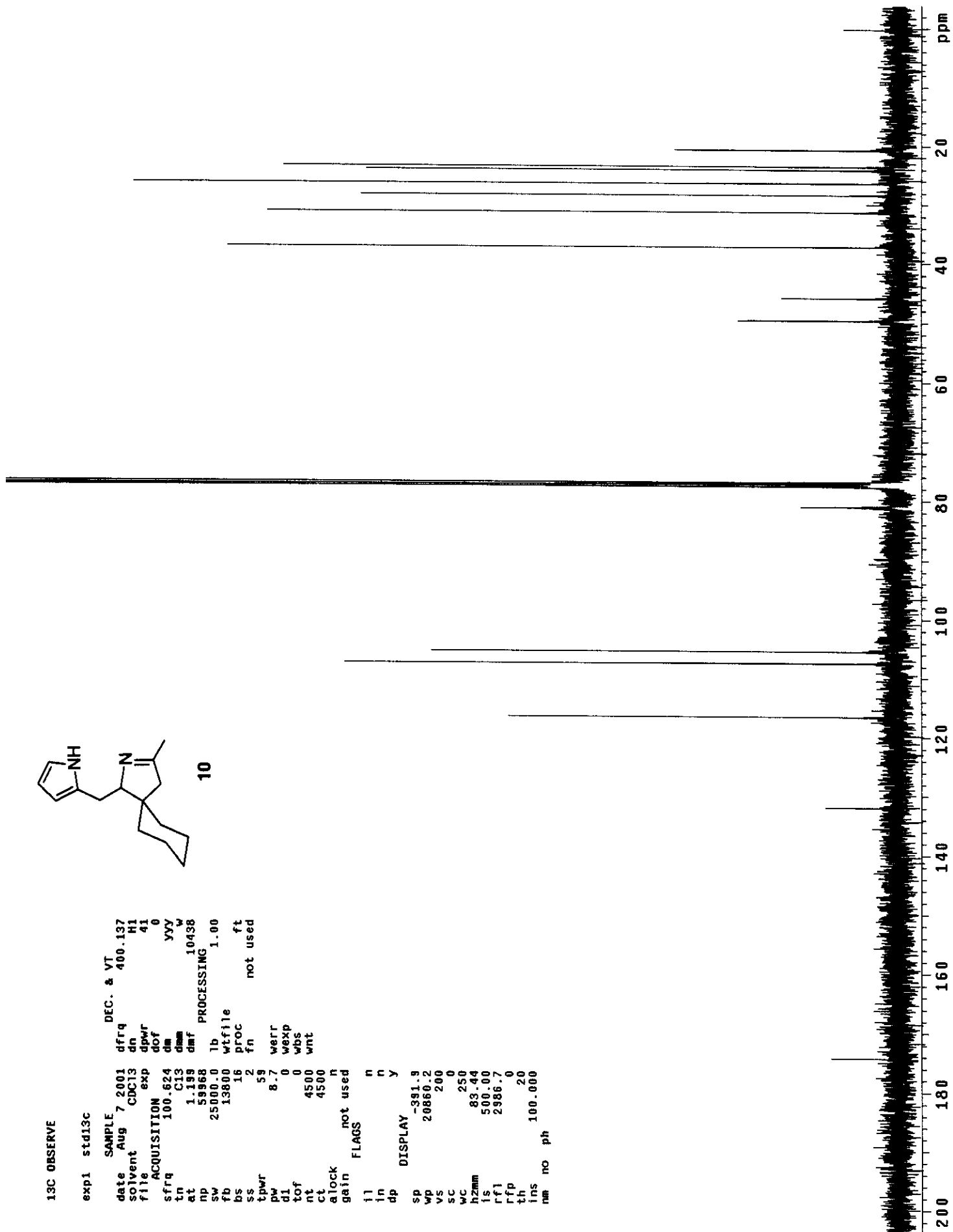
13C OBSERVE

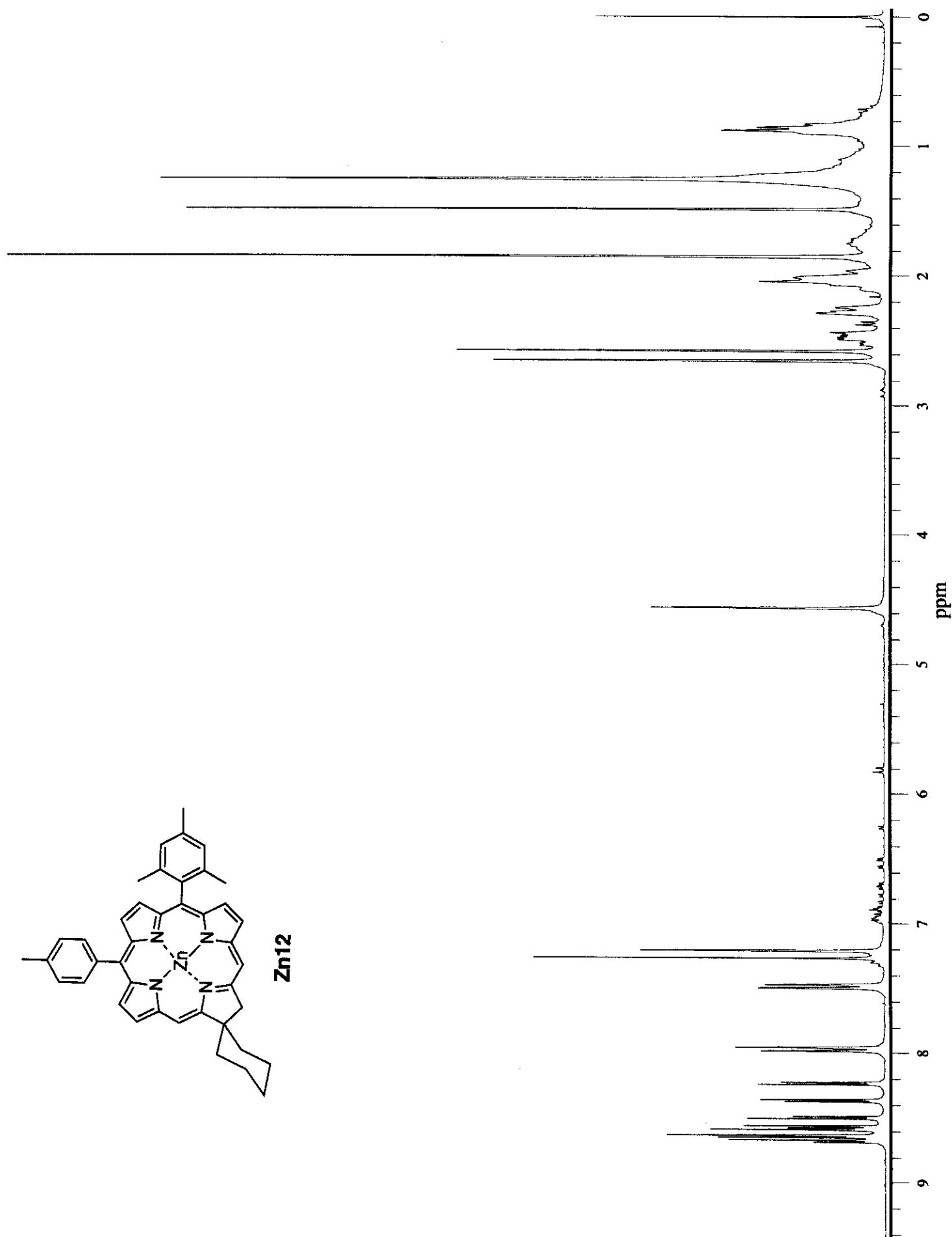
exp1 std13c

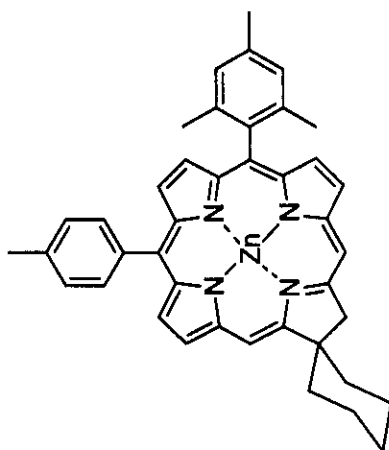
SAMPLE		DEC. & VT	
date	Aug 7 2001	dfrq	400.137
solvent	CDC13	dn	H1
file	exp	dpwr	41
ACQUISITION		dof	0
sfrq	100.624	dm	yyv
tn	C13	dmf	w
at	1.199	dmf	10438
np	59968	PROCESSING	
sw	25000.0	lb	1.00
fb	13800	wtfile	ft
bs	16	proc	not used
ss	12	fn	
tpwr	59		
pw	8.7	werr	
dl	0	wexp	
tof	0	wbs	
nt	4500	wnt	
ct	4500		
alock	not used		
gain	not used		
FLAGS			
ll	n		
ln	n		
dp	y		
DISPLAY			
sp	-391.9		
wp	20860.2		
vs	200		
sc	0		
wc	250		
hzmm	83.44		
ls	500.00		
rfl	2986.7		
rff	0		
th	20		
ins	100.000		
nm	no	ph	



10

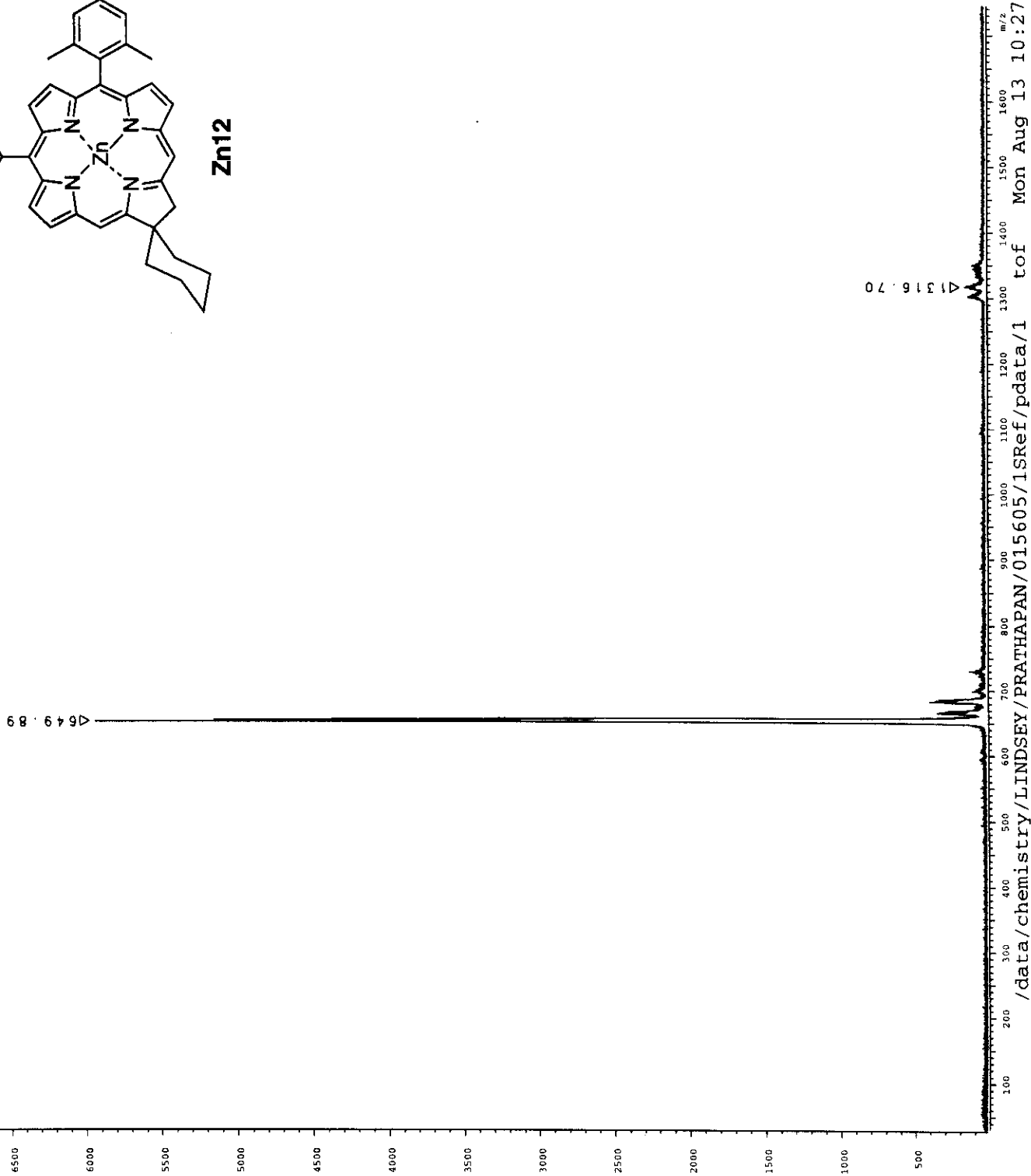






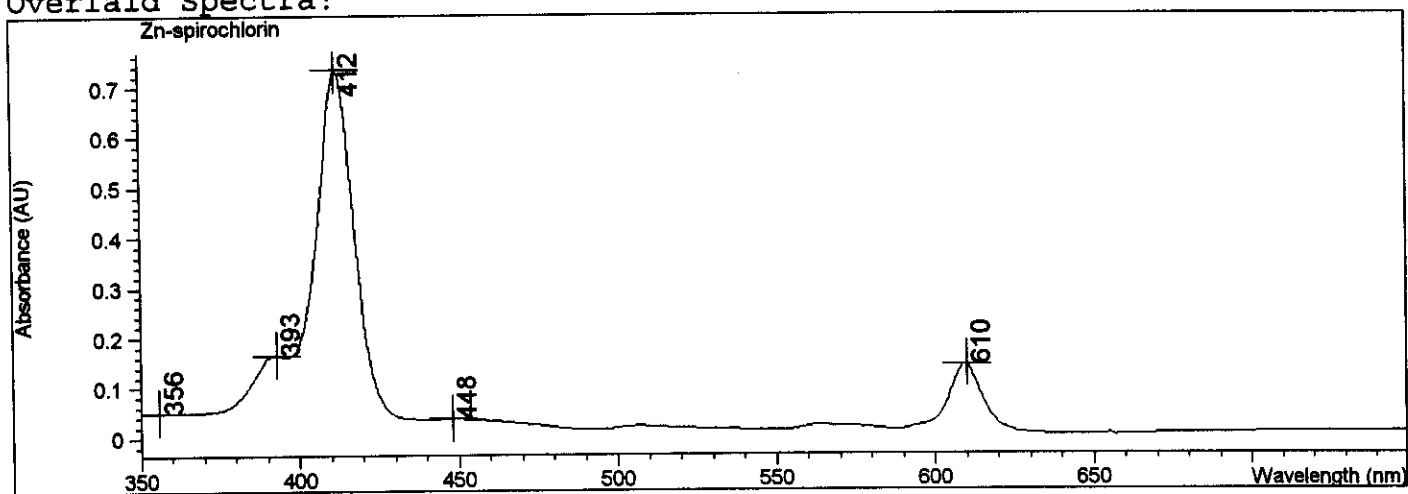
Zn12

INSTRUM TOP
 OpId N_Srinivasan
 SPMNAM 015605
 AC DATE Mon Aug 13 10:25:01 2001
 PATH /data/chemistry/LINDSEY/PRATHAPAN
 PLOT1 POS
 ACQ1 m Reflector
 TD 40000
 NSLOTS 100
 SMOBUM 0
 SMOPTS1 0
 SMOPTS2 0
 SMOPTS3 0
 DM 1.00 [ns]
 DELAY 0 [ns]
 Uis1 20.00 [kV]
 Uis2 18.70 [kV]
 Uref1 0.00 [kV]
 Uisens 7.00 [kV]
 Uref2 0.00 [kV]
 RefPull 0.00 [kV]
 Udet1 1.50 [kV]
 Udet2 0.00 [kV]
 Udef1 2.00 [kV]
 REPHZ 1.00 [Hz]
 ATEN 2047122 193
 ML1 333.982
 ML2 0.000
 ML3
 HITURE no
 GDBON yes
 GDBLY short
 REFON no
 REFEND no
 LINSND no
 LIS2END no
 DFCAL1 510.84
 DPMAS1 700.00 [Da]
 REMVAL 0.33
 RESVAL 0.42
 IS2END 0
 CMT1 Zn-spirochlorin
 CMT2 atn =15, shot =100

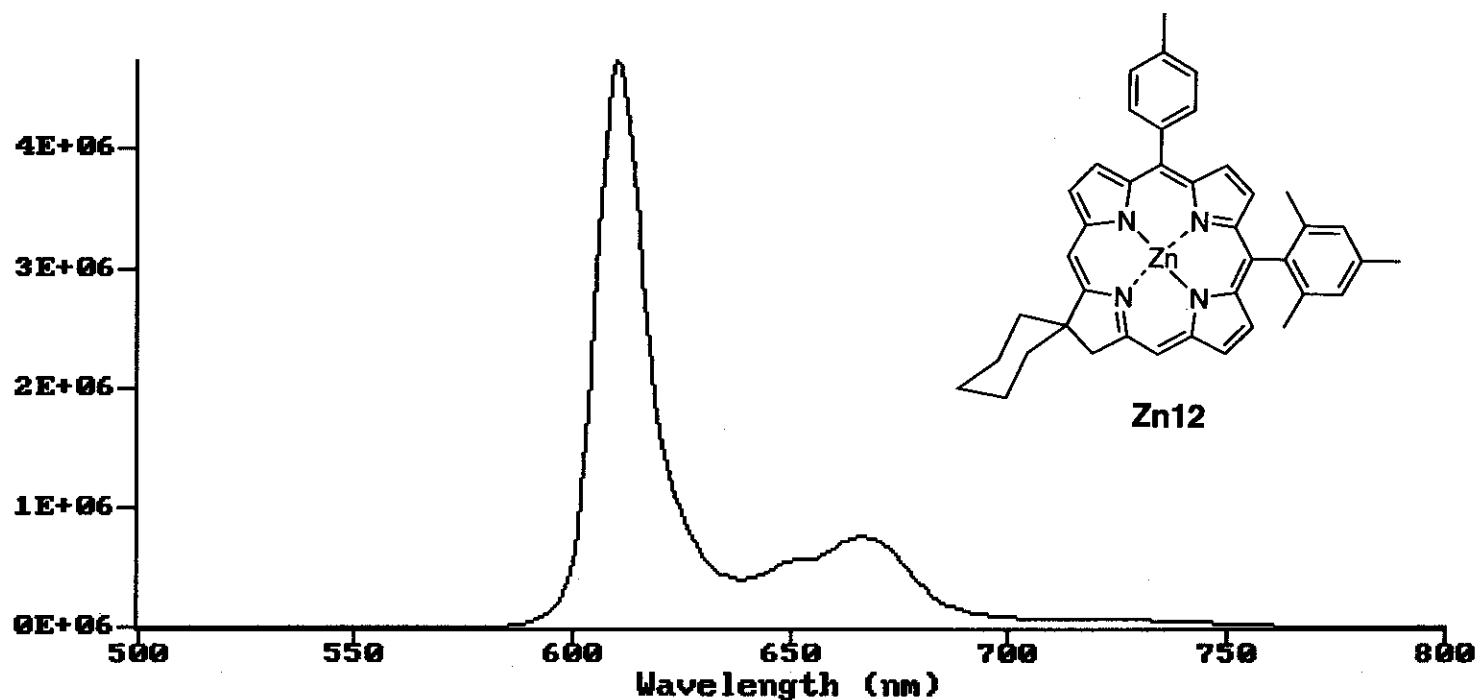


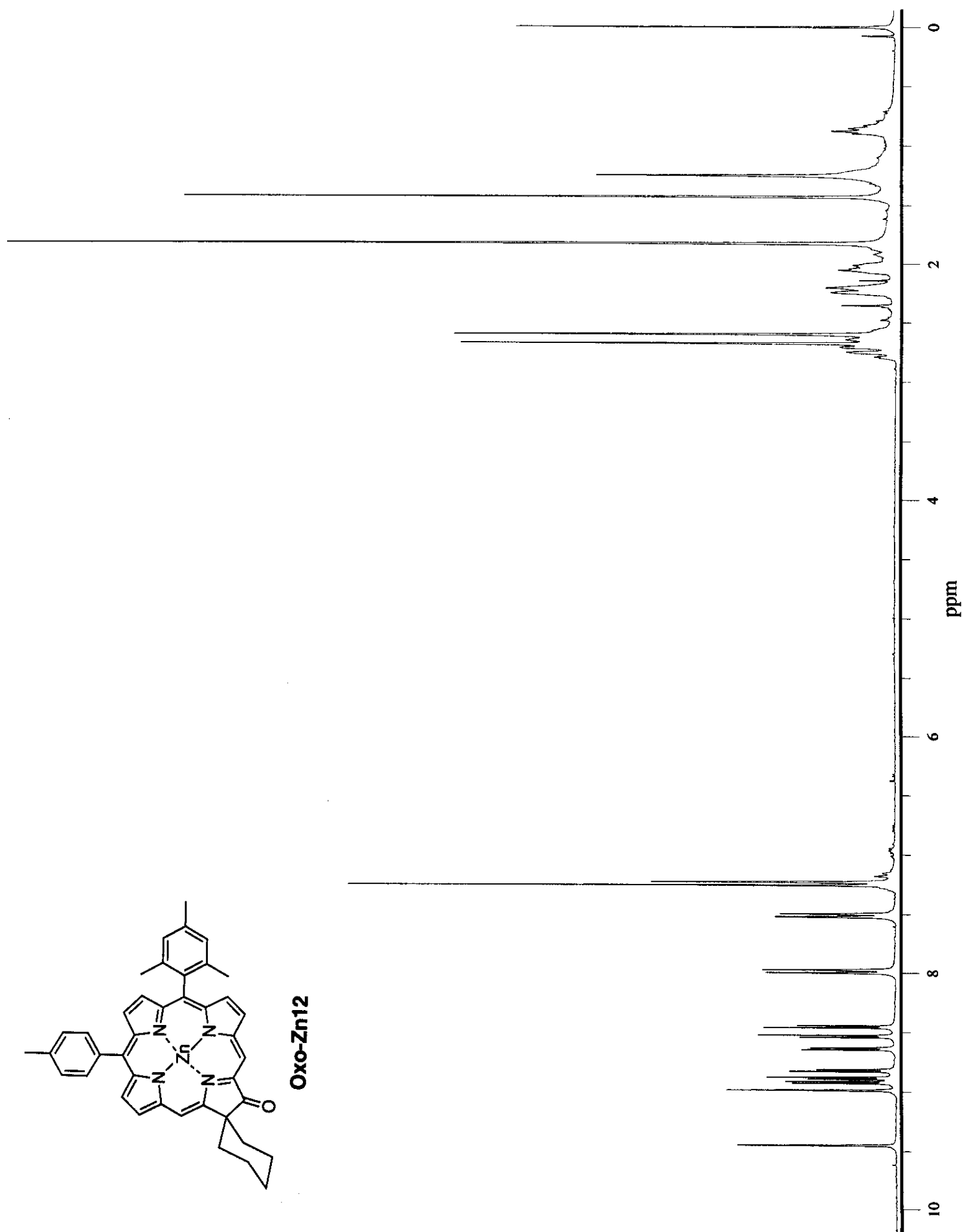
Method file : <untitled>
 Information : Default Method
 Data File : <untitled>

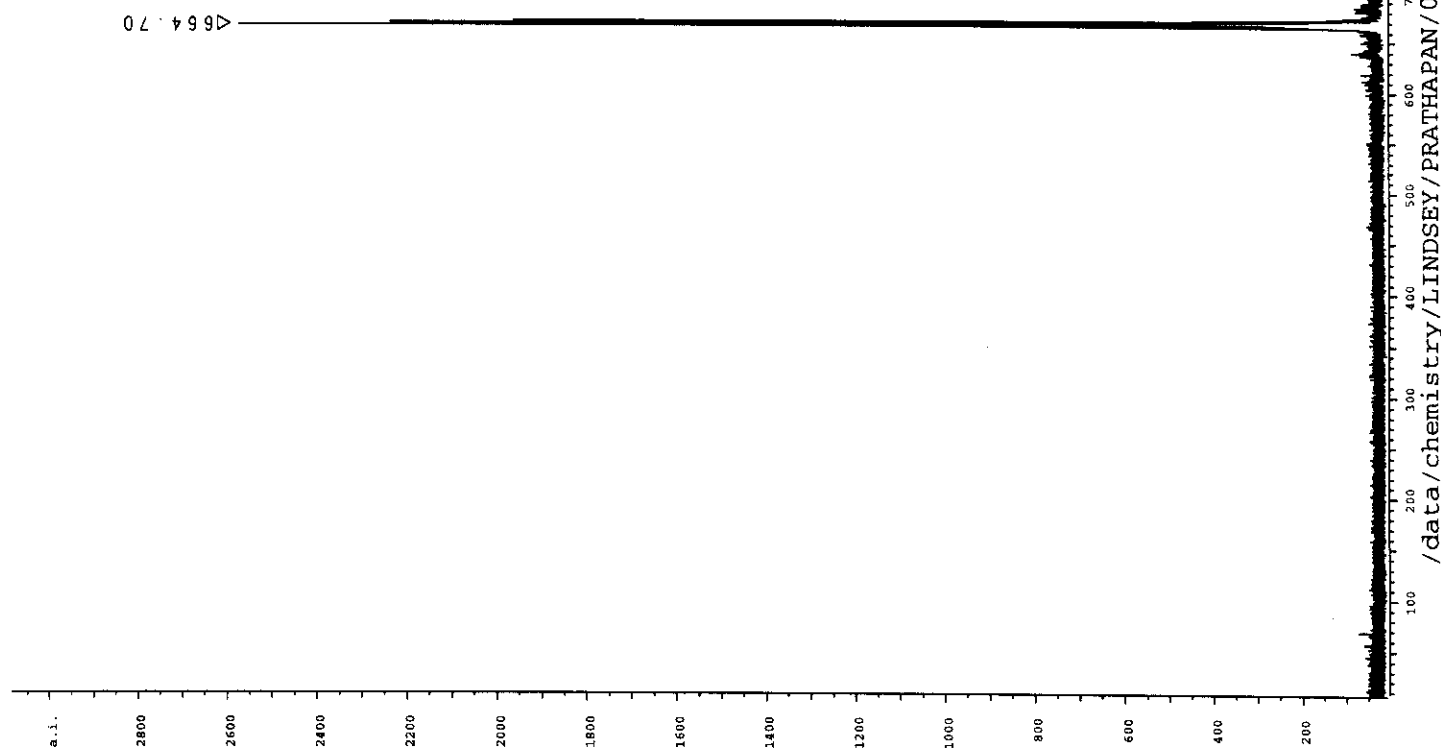
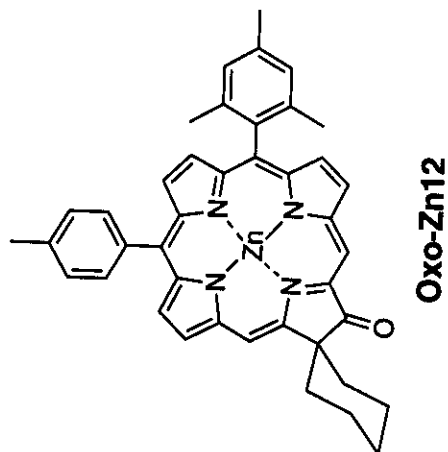
Overlaid Spectra:



#	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

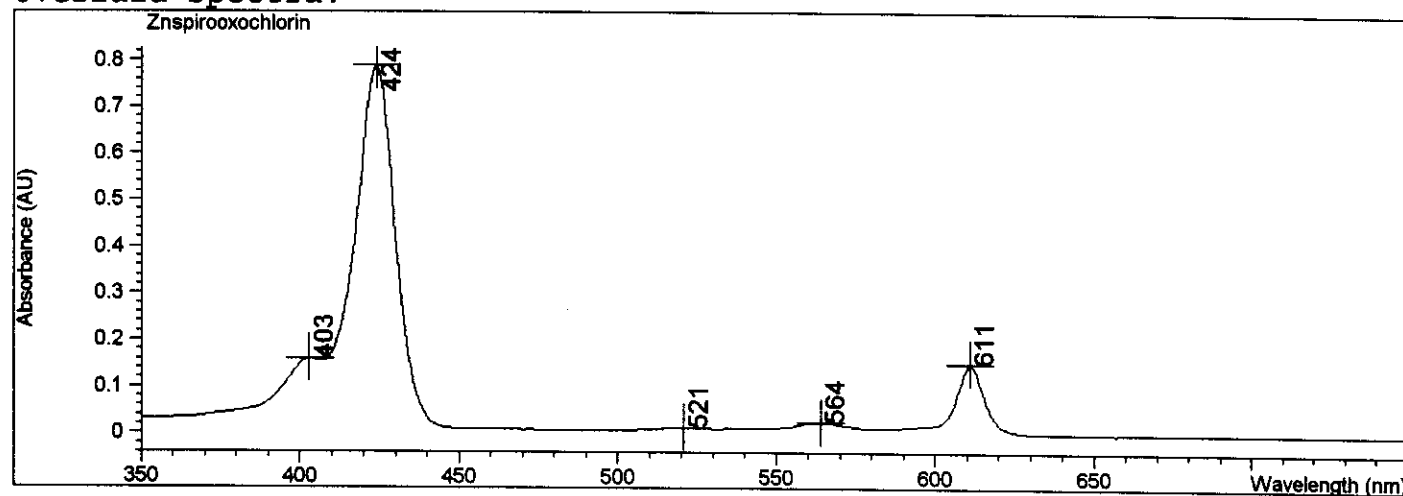






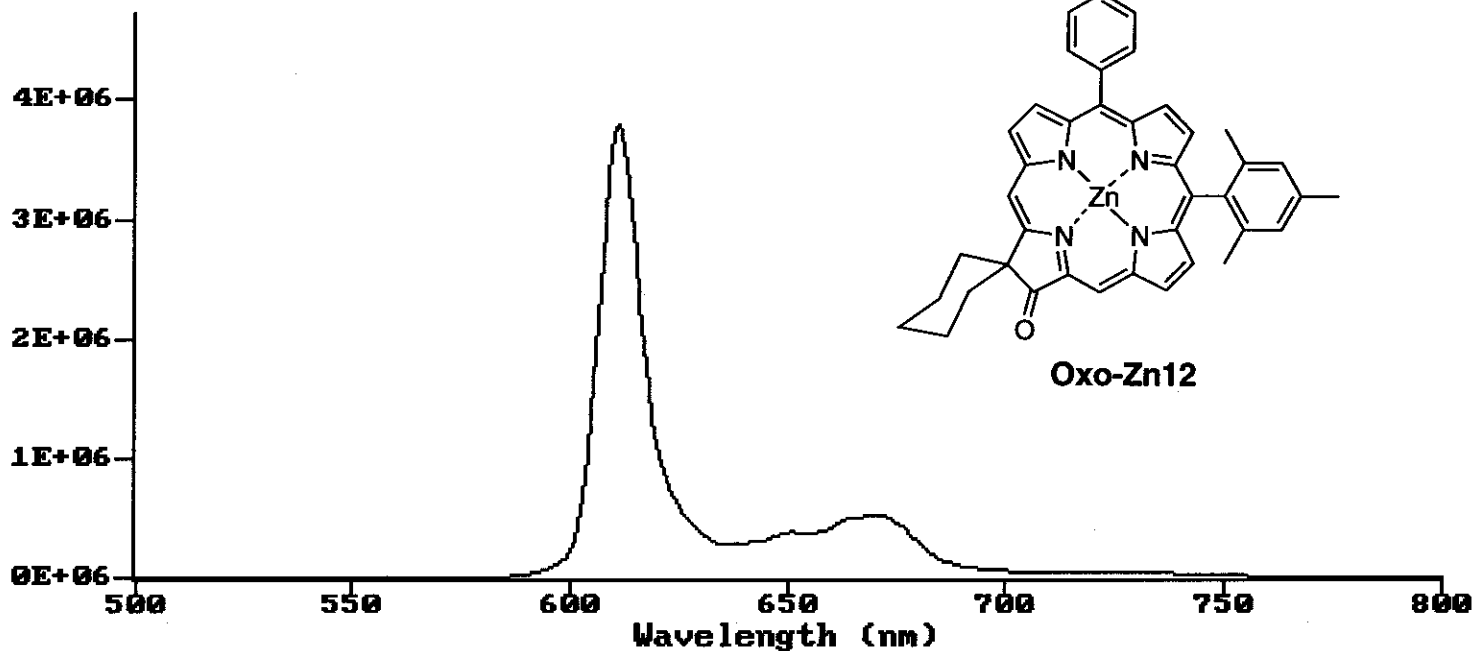
Method file : <untitled>
 Information : Default Method
 Data File : <untitled>

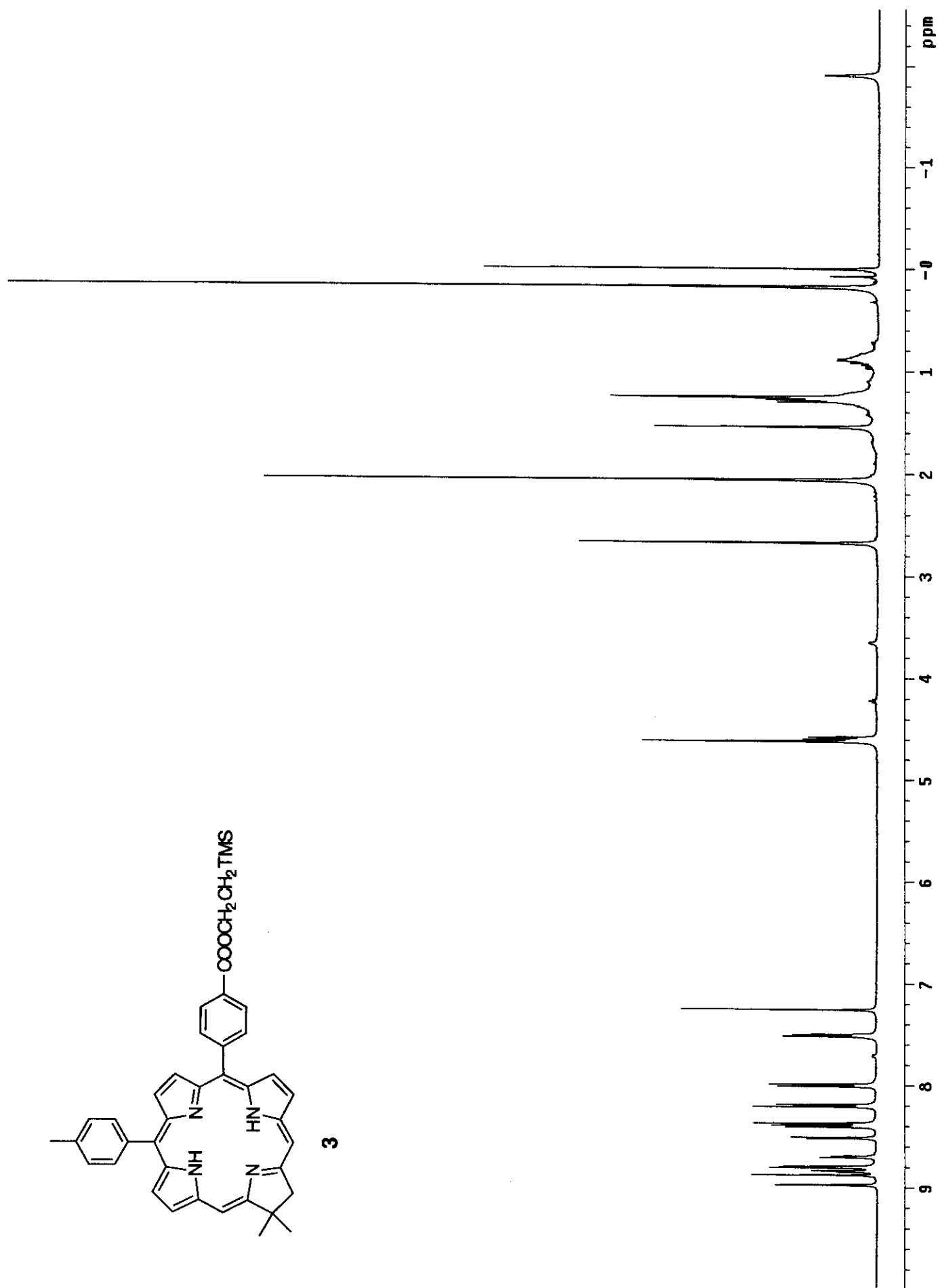
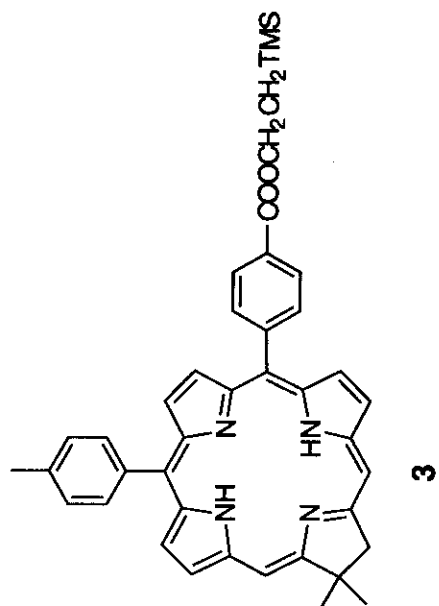
Overlaid Spectra:

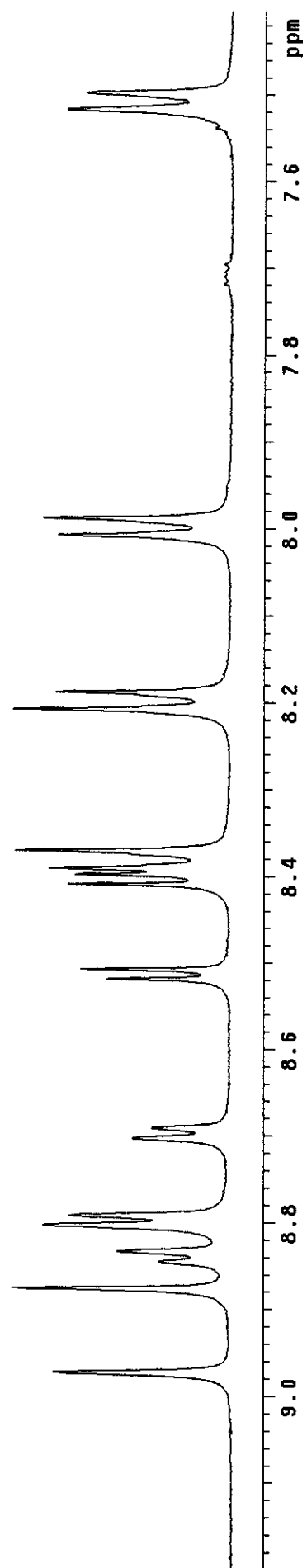
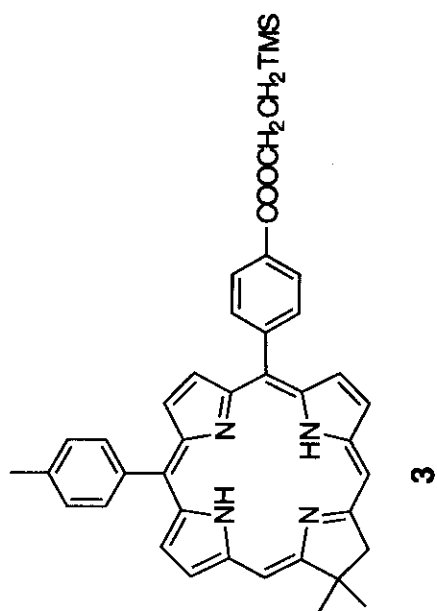


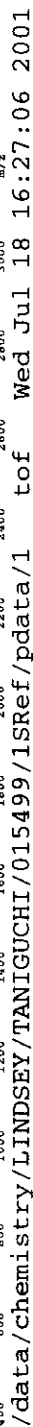
#	Name	Peaks (nm)	Abs (AU)
1	Znspiroporphyrin	424.0	0.78796
1		403.0	0.15892
1		611.0	0.15093
1		564.0	2.3799E-2
1		521.0	1.1910E-2

I
n
t
e
n
s
i
t
y
(
c
p
s
)





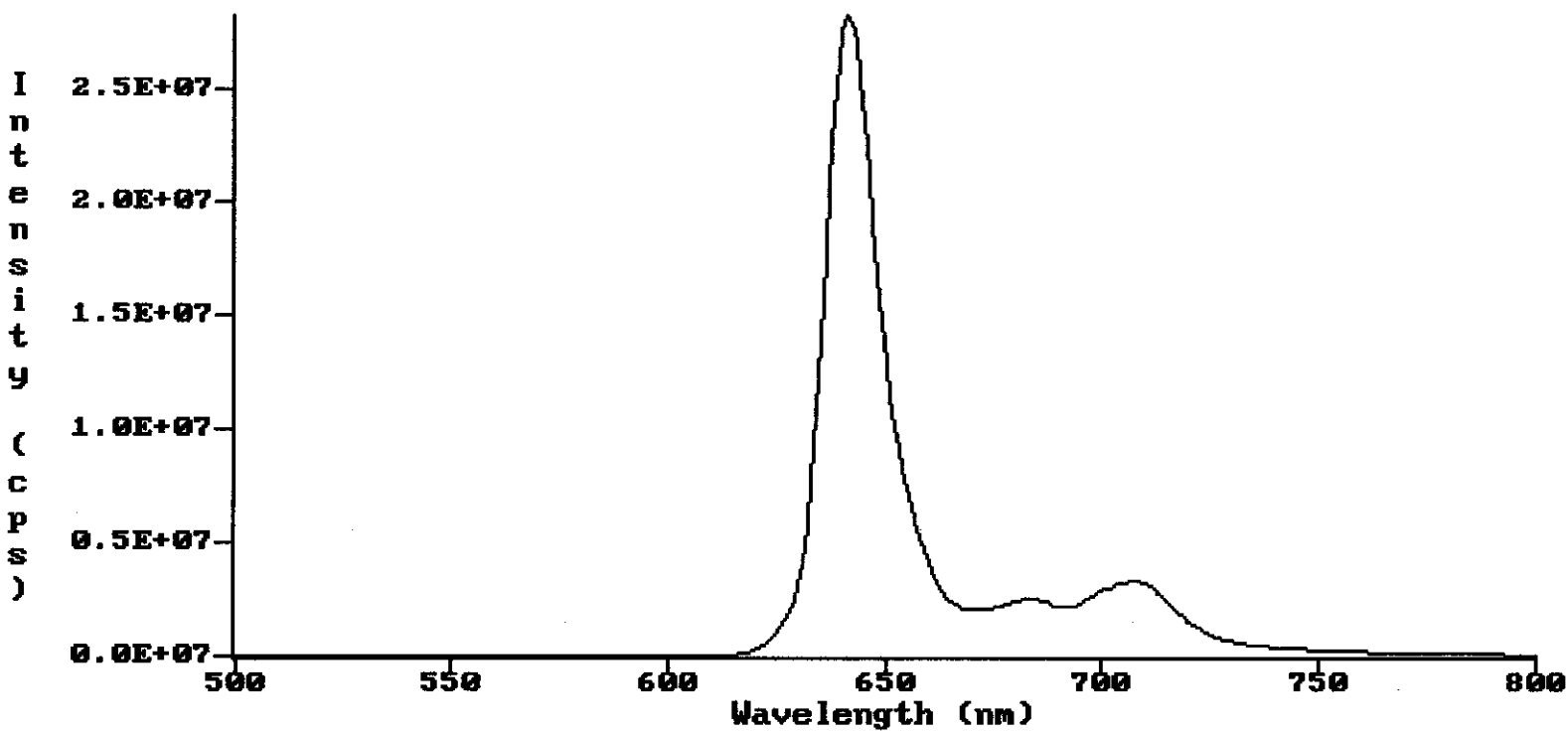
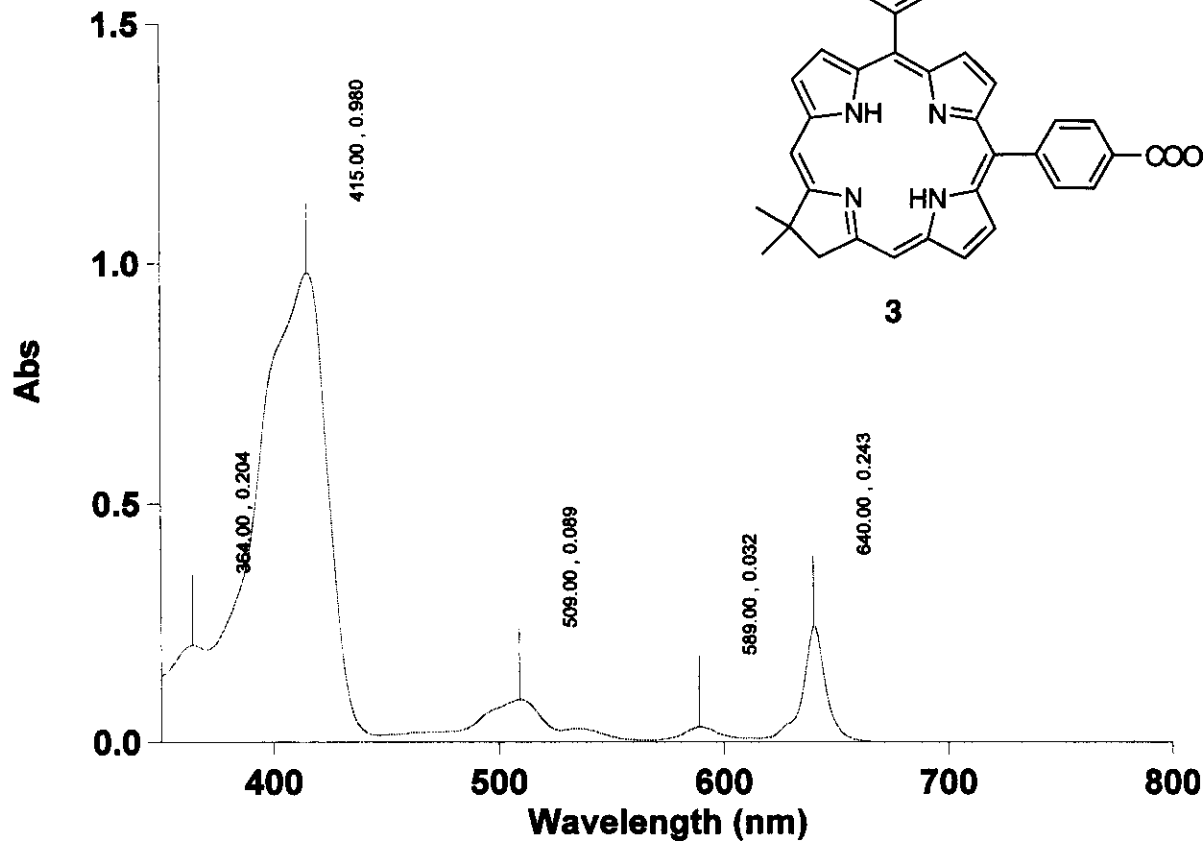


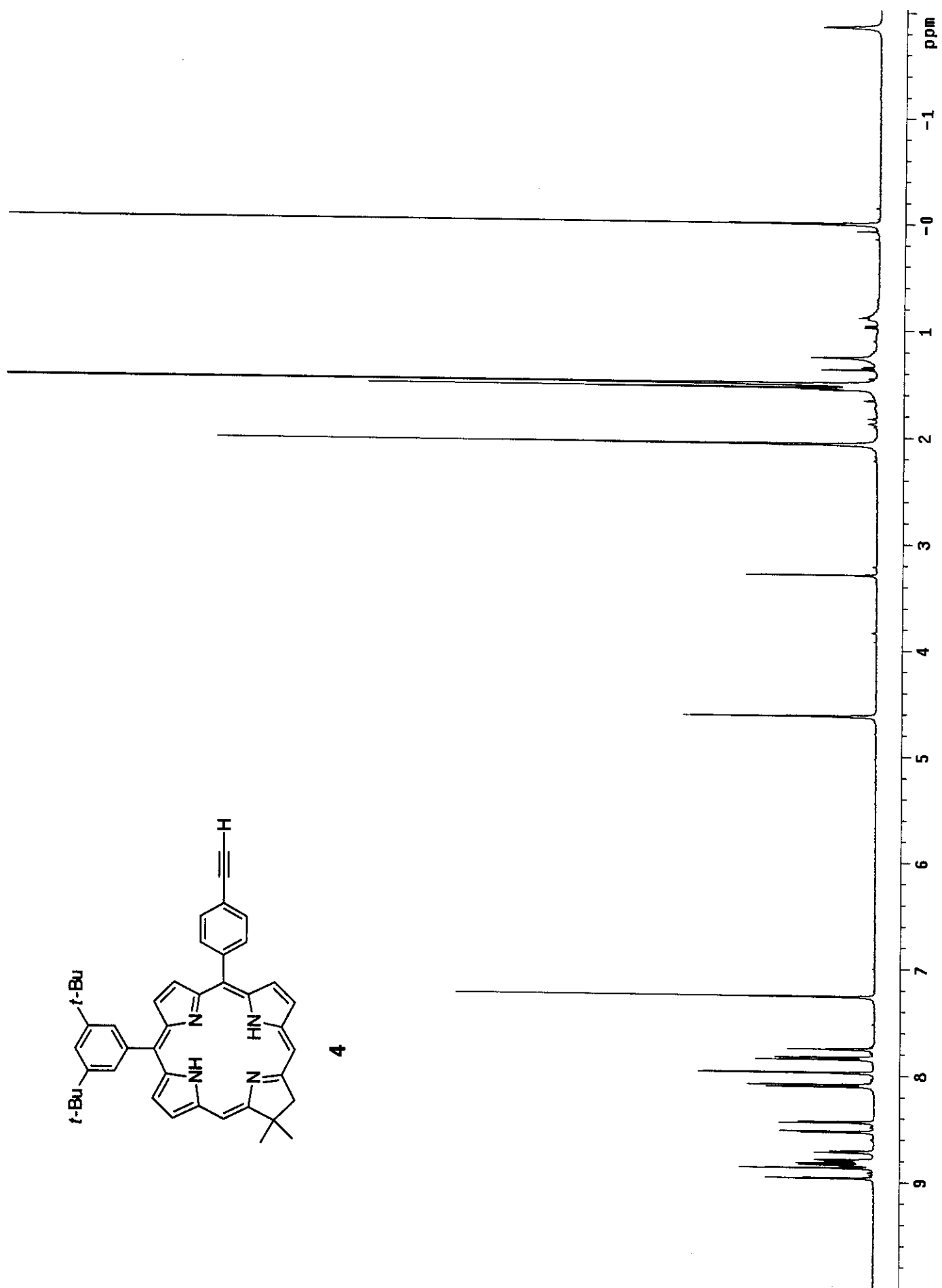


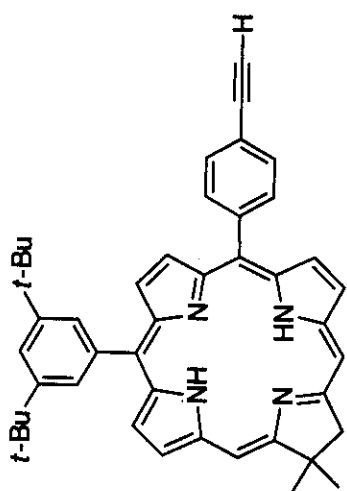
Chemical structure of compound 3, a phthalocyanine derivative. It features a central macrocyclic ring with four nitrogen atoms (NH). Substituents include a 4-(trimethylsilyl)ethoxyphenyl group at the top and a 4-methylphenyl group at the left. The structure is labeled with a large '3' on the right.

INSTRUM TOP	Q101	N. Srinivasan
SNRPMAN	015499	
ACQ DATE	Wed Jul 18 16:25:41 2001	
DATA PATH	/data/chemistry/LINDSEY/TANIGUCHI	
POLARITY	POS	
WAVELENGTH	40000	
TE	40000	
NO. SHOTS	100	
SNORMON	0	
SNORPTS1	0	
SNORPTS2	0	
SNORPTS3	0	
DM	1.00	[ms]
DELAY	0	[ms]
U1s1	20.00	[KV]
U1s2	18.70	[KV]
U1s3	17.40	[KV]
U1s4	7.50	[KV]
U1s5	10.00	[KV]
U1s6	10.00	[KV]
U1s7	1.50	[KV]
U1s8	2.00	[KV]
U1s9	2.00	[KV]
REPRTZ	1.00	[Hz]
ATTEN	40.0	
MC1	2065947.190	
MC2	327.134	
MC3	0.000	
HITURBO	no	
GUEON	yes	
GOODLY	short	
DEFION	no	
NO	no	
NO	no	
ILLANSND	no	
U132RND	no	
DPCCAL1	510.84	
DPCCAL2	700.00	[Da]
DPCCAL3	0.33	
RENDVAL	0.33	
RENDVAL2	0.91	
RENSNDV	0.00	
CMW1	PD-CHL-COCCUTMS	
CMW2	att 40_shot1500	

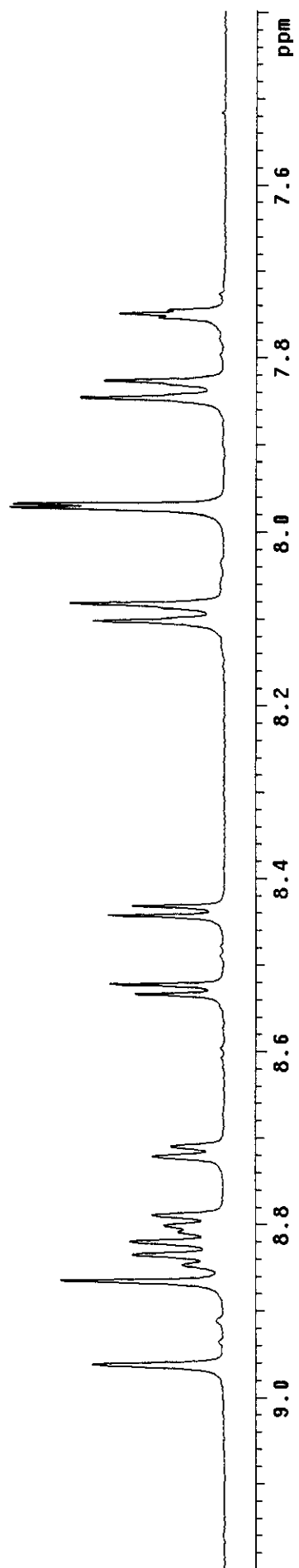
NCSU Chemistry
Instrument Serial Number 0051477

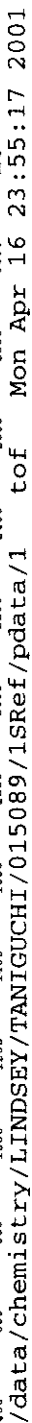






4

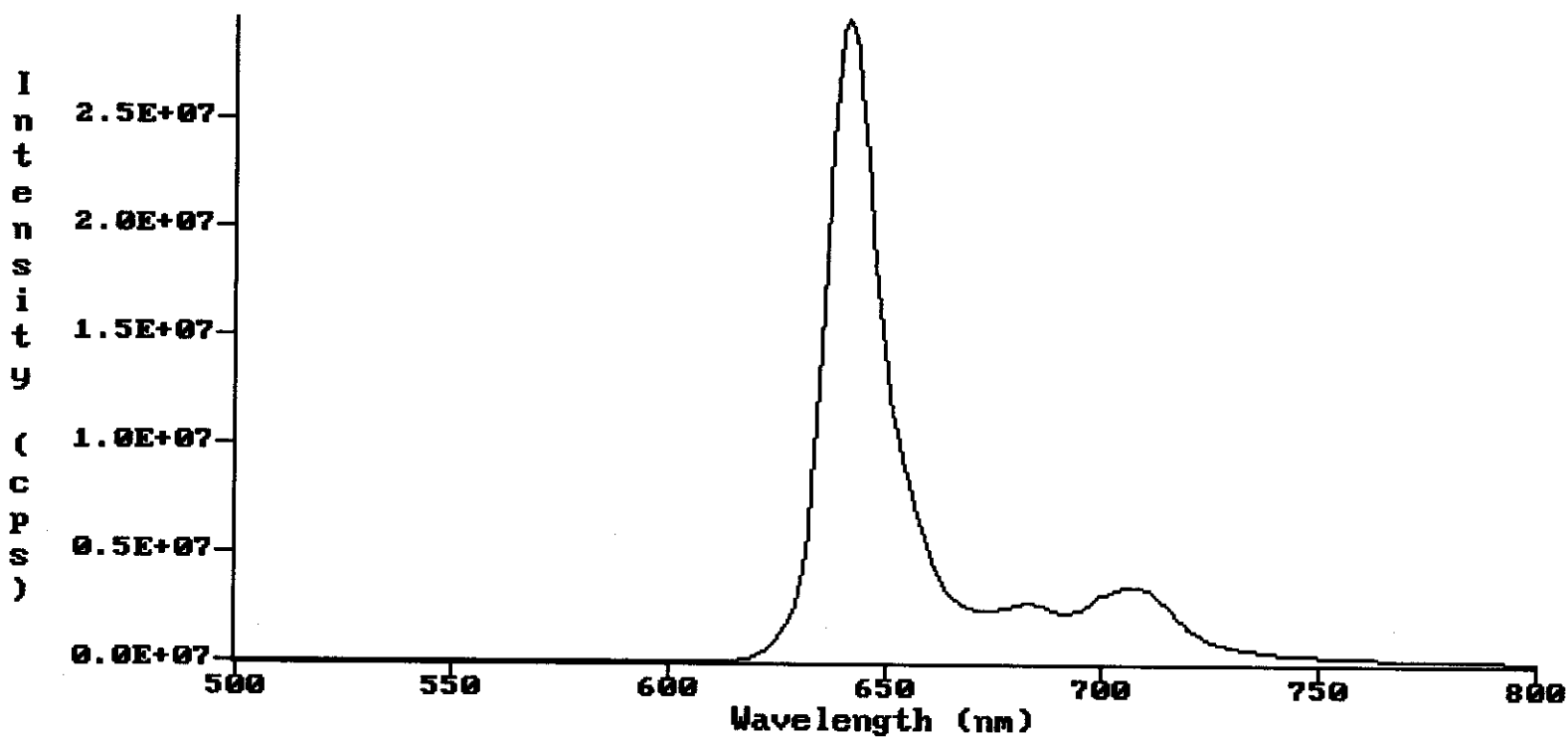
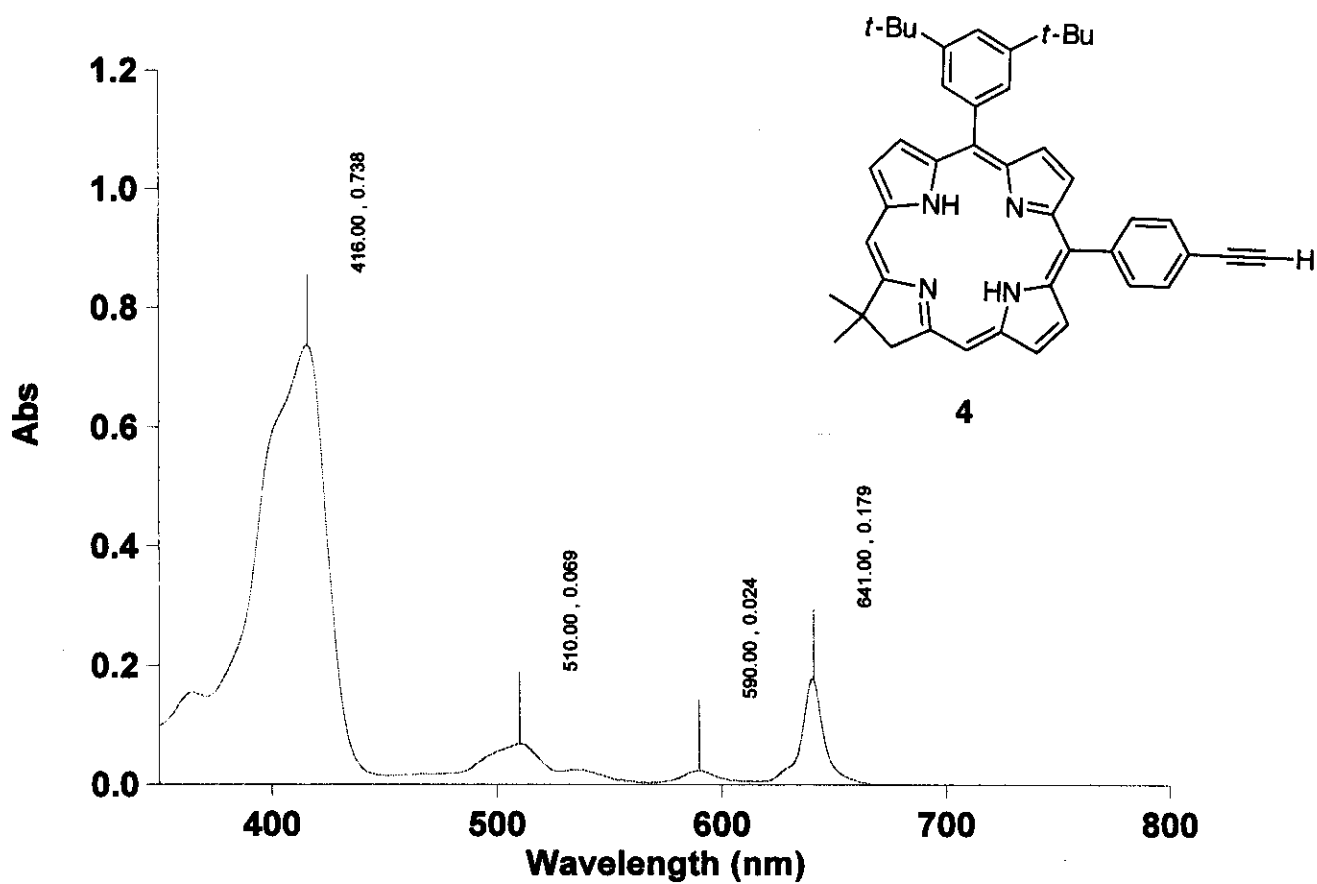


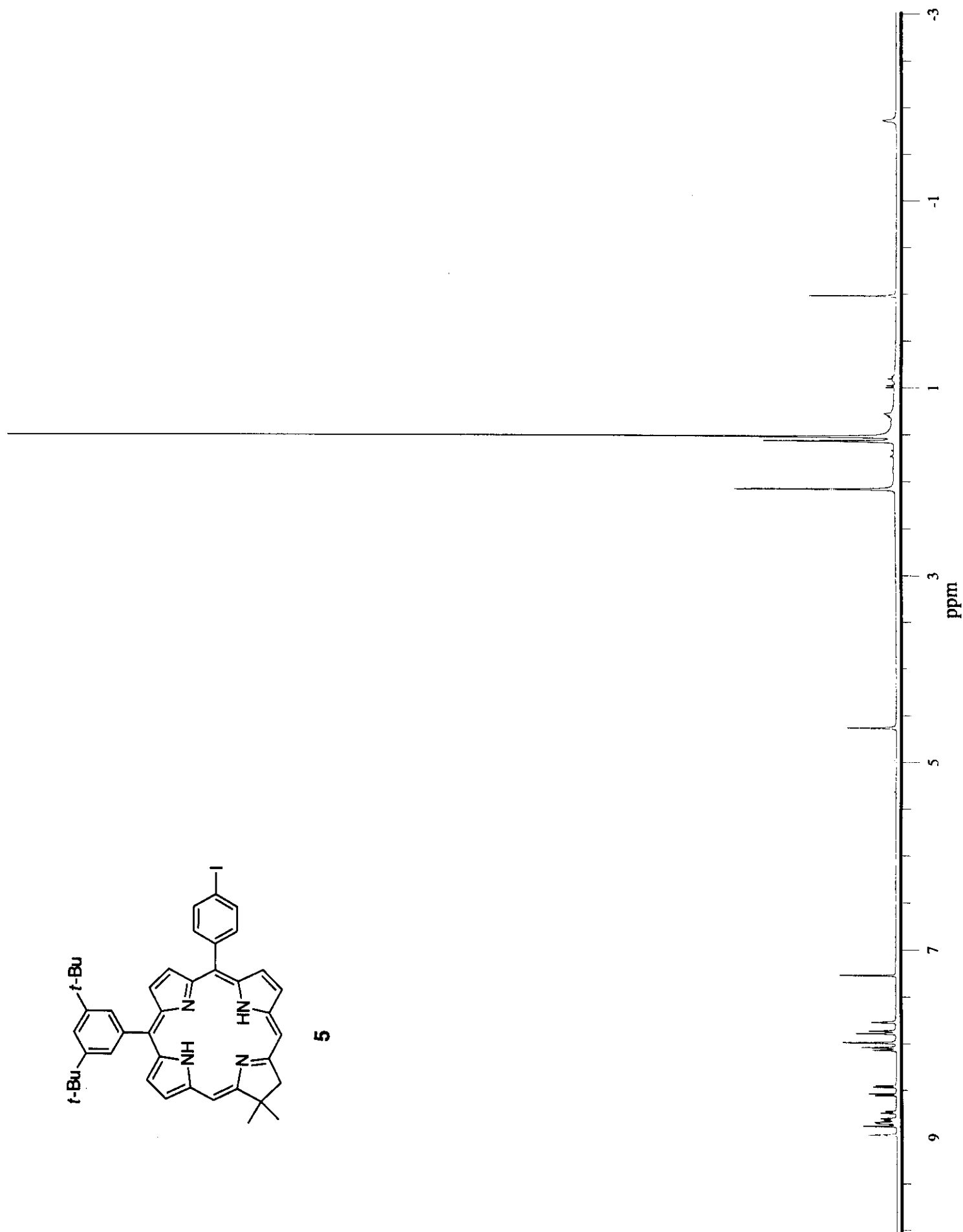


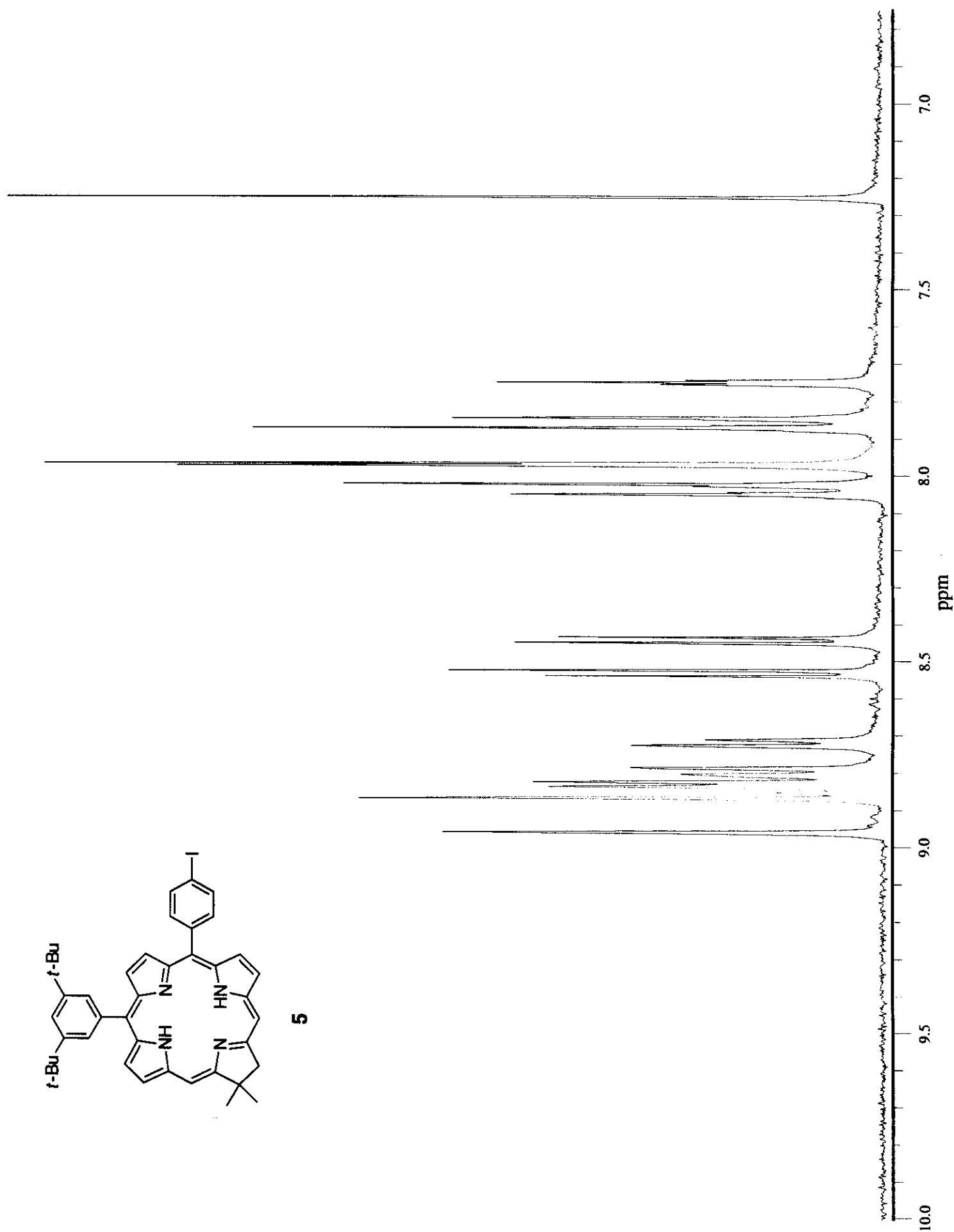
4

INSTRUM TOP	N. Srinivasan
Opid	015089
SERIALNUM	Mon Apr 16 23:51:51 2001
ACQ DATE	data/chemistry/LINSEY/TANIGUCHI
PATH	
APPROX	
APCOP	Reflector
TID	40000
NoSHOTS	100
SNOWM	0
SNOWPTS1	0
SNOWPTS2	0
SNOWPTS3	0
DW	1.00 [ms]
DELAY	0 [ms]
U1s1	20.00 [KV]
U1s2	18.70 [KV]
U1s3	18.70 [KV]
U1s4	7.50 [KV]
U1s5	7.50 [KV]
U1s6	10.00 [KV]
U1s7	10.00 [KV]
U1s8	0.00 [KV]
U1s9	1.50 [KV]
U1s10	0.00 [KV]
U1s11	0.00 [KV]
U1s12	0.00 [KV]
REPZ	1.00 [Hz]
ATTEN	24.0
M1	2074469.941
M2	355.586
NUBRO	0.000
NUBRO no	
UDRON Yes	
DEEPLY short	
DEPLEN no	
SENSEND no	
SENSEND no	
SENSEND no	
SENSEND no	
SENSEND no	
POPCALL	510.84
PMASS	700.00 [Da]
BENDVAL	0.33
BENDVAL	0.28
BENDVAL	0.31
PH CHL CCH	
ATTEN 27	atten 26, shots 100

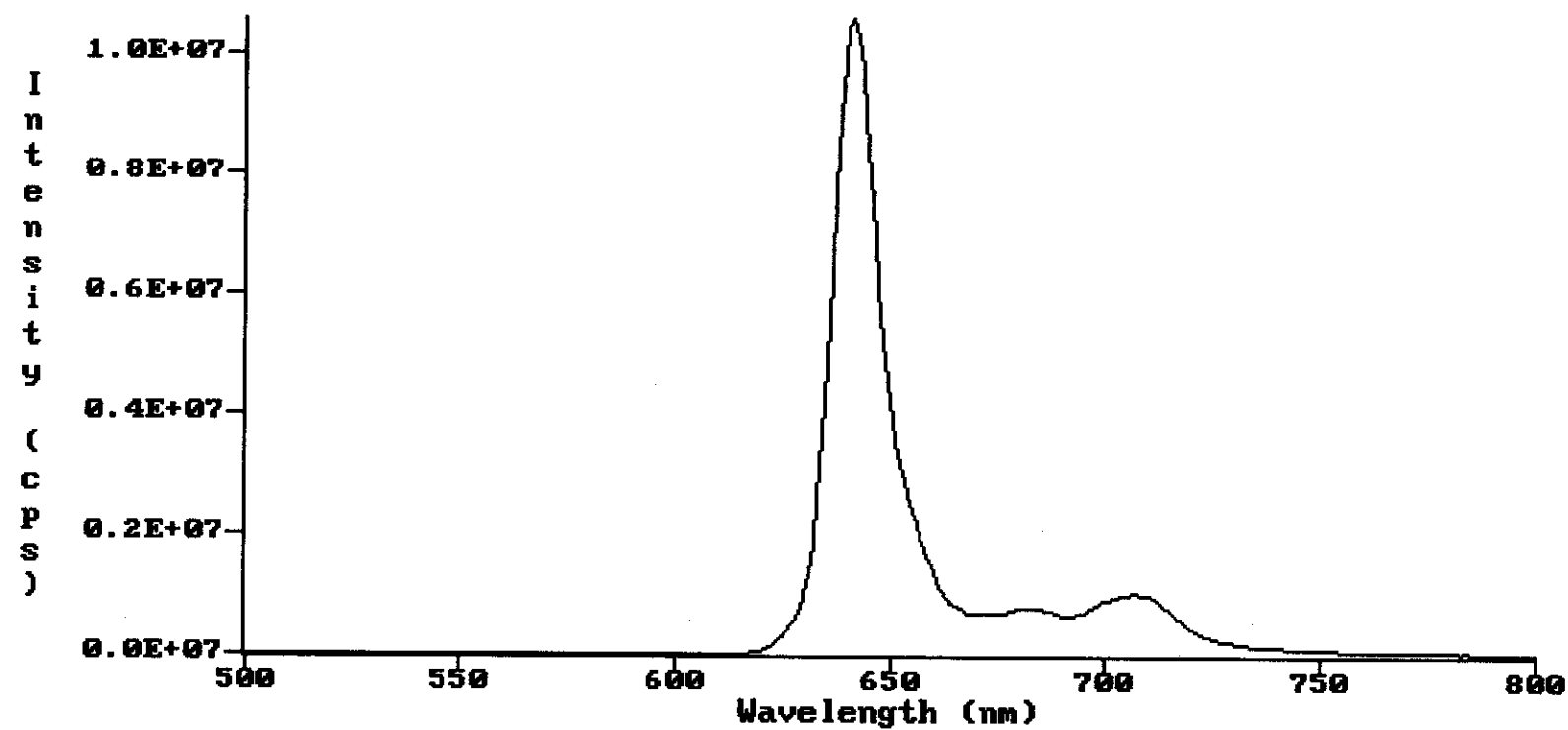
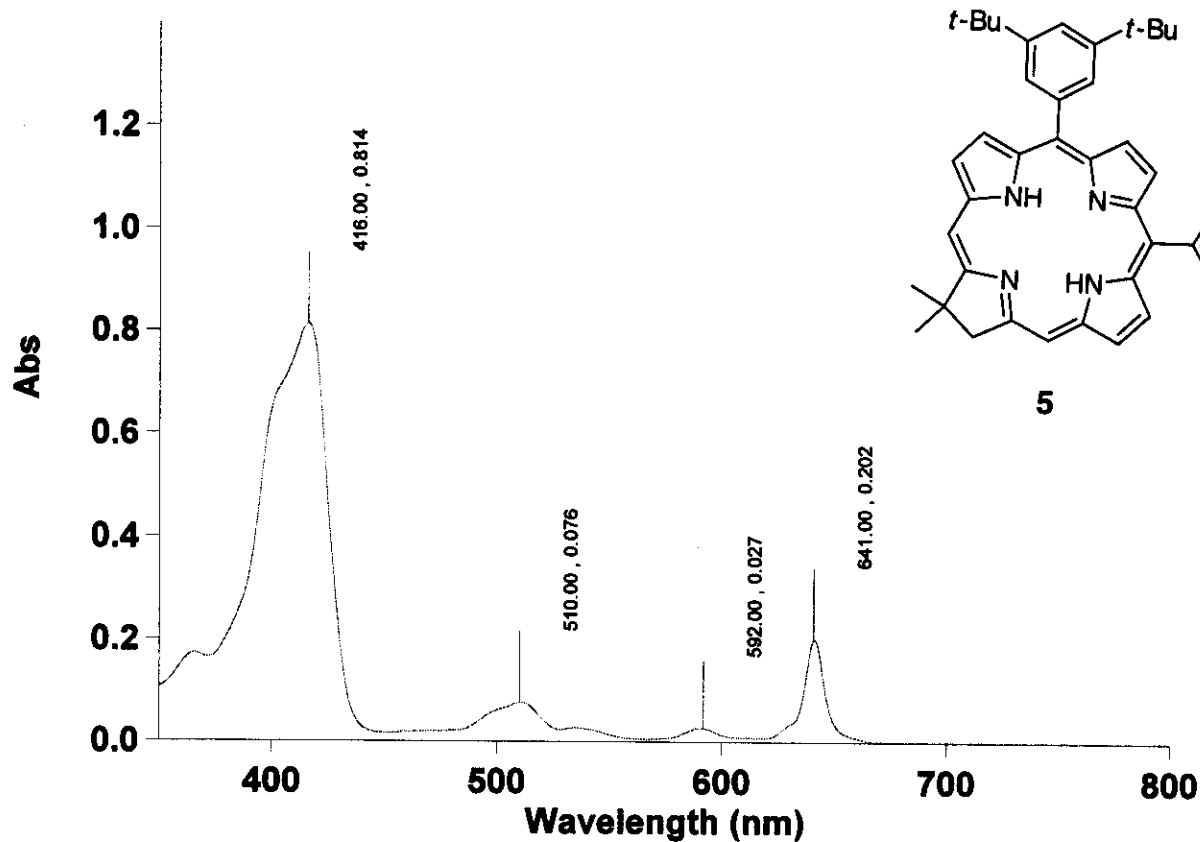
NCSU Chemistry
Instrument Serial Number 0051477



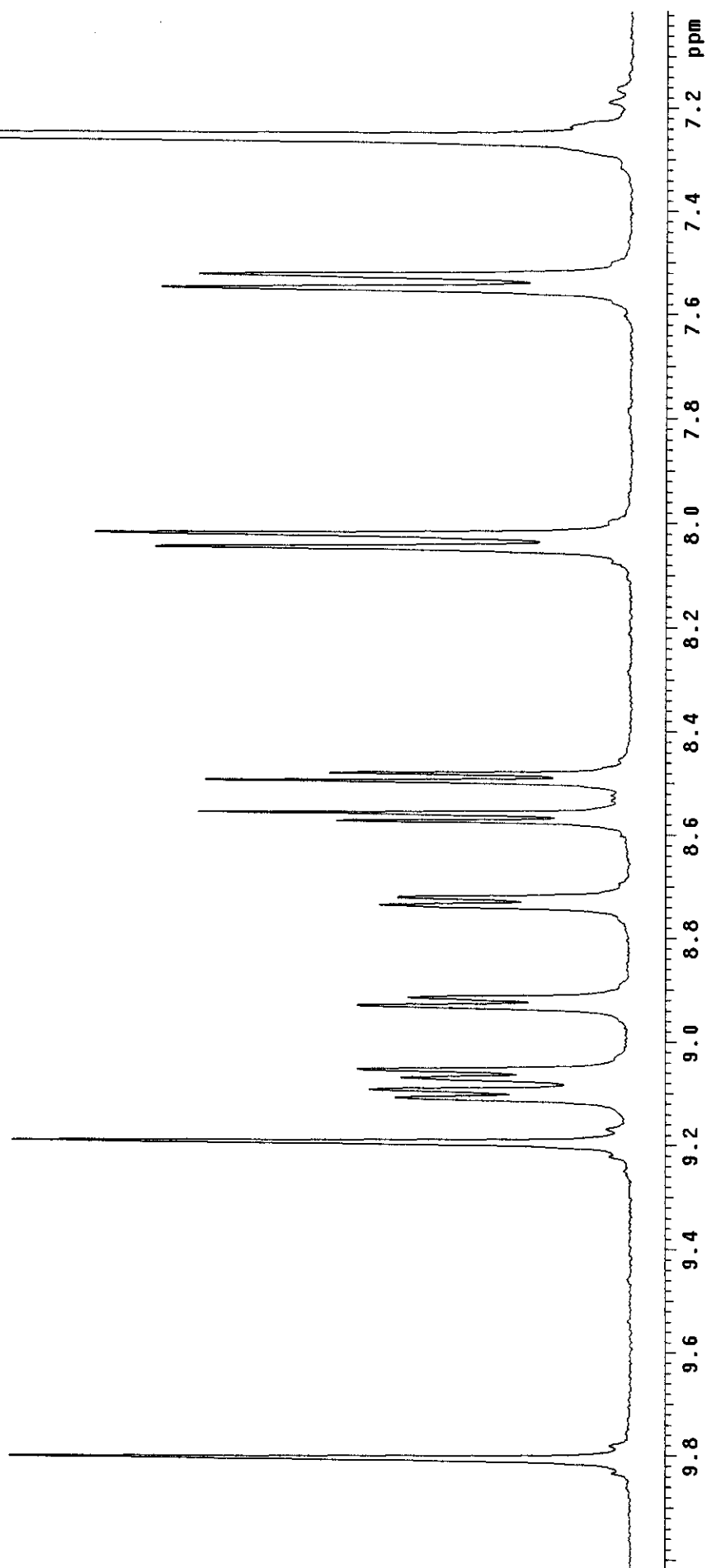
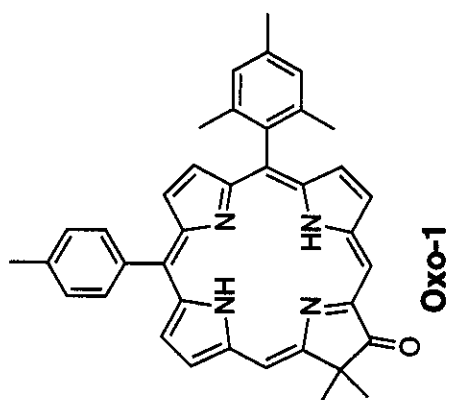


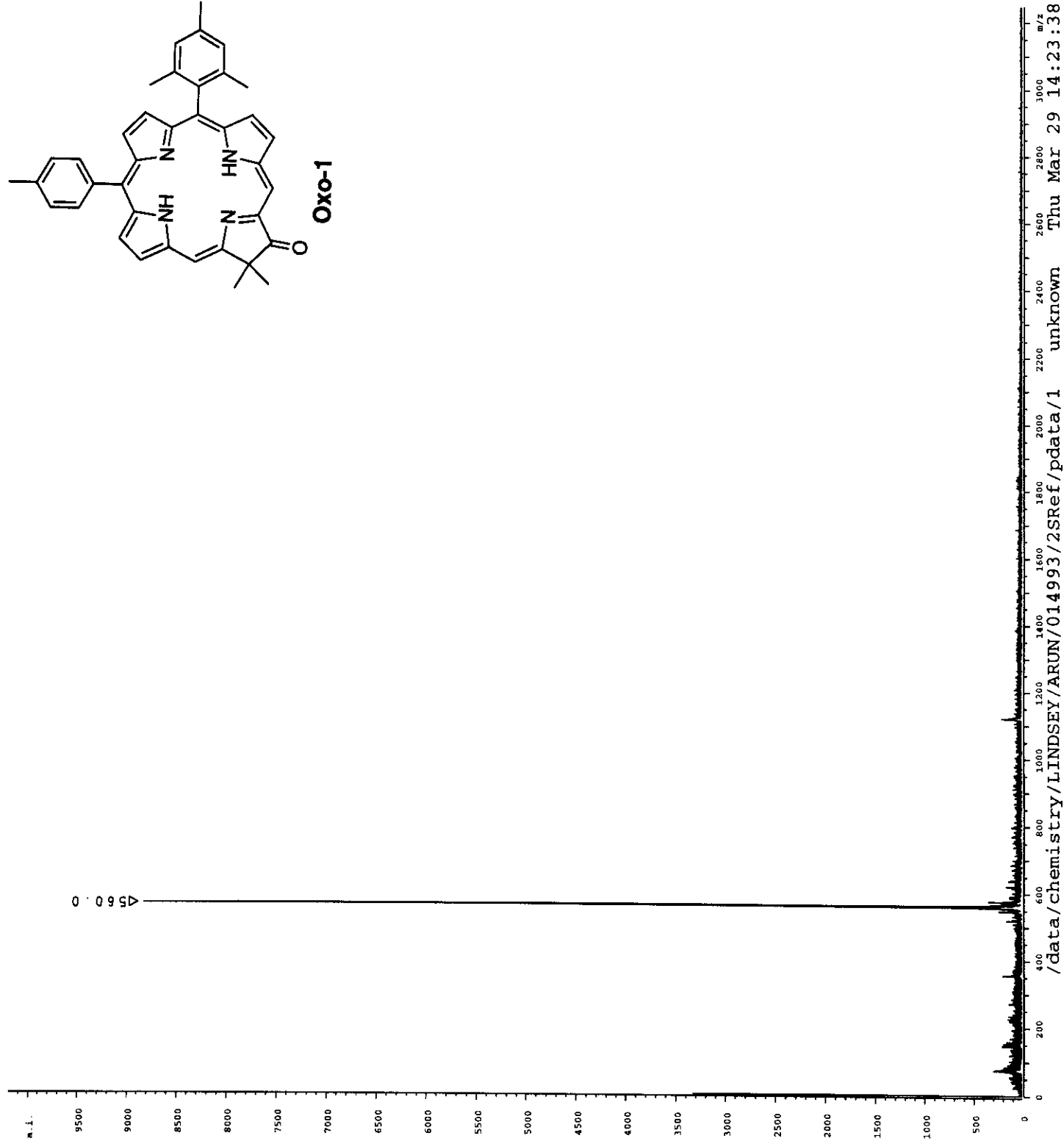
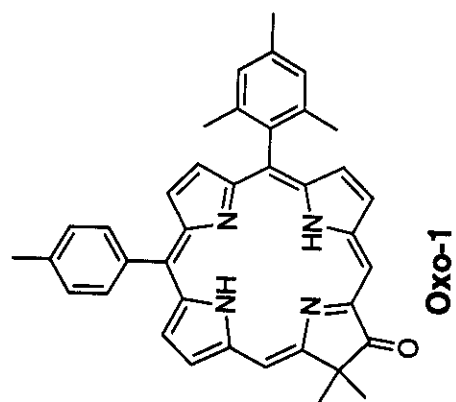


NCSU Chemistry
Instrument Serial Number 0051477



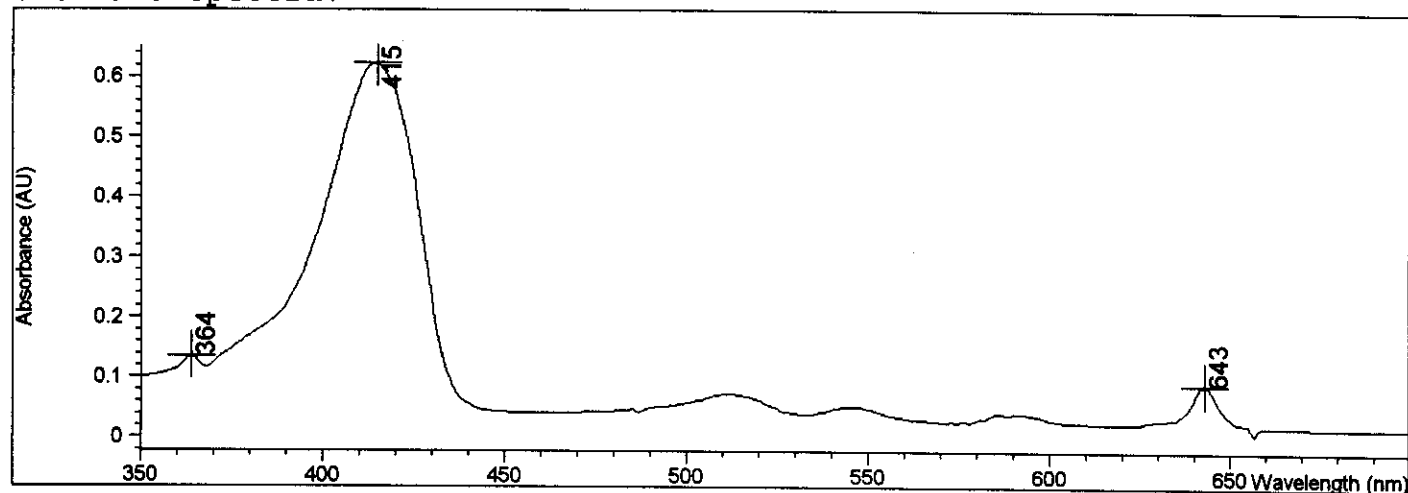




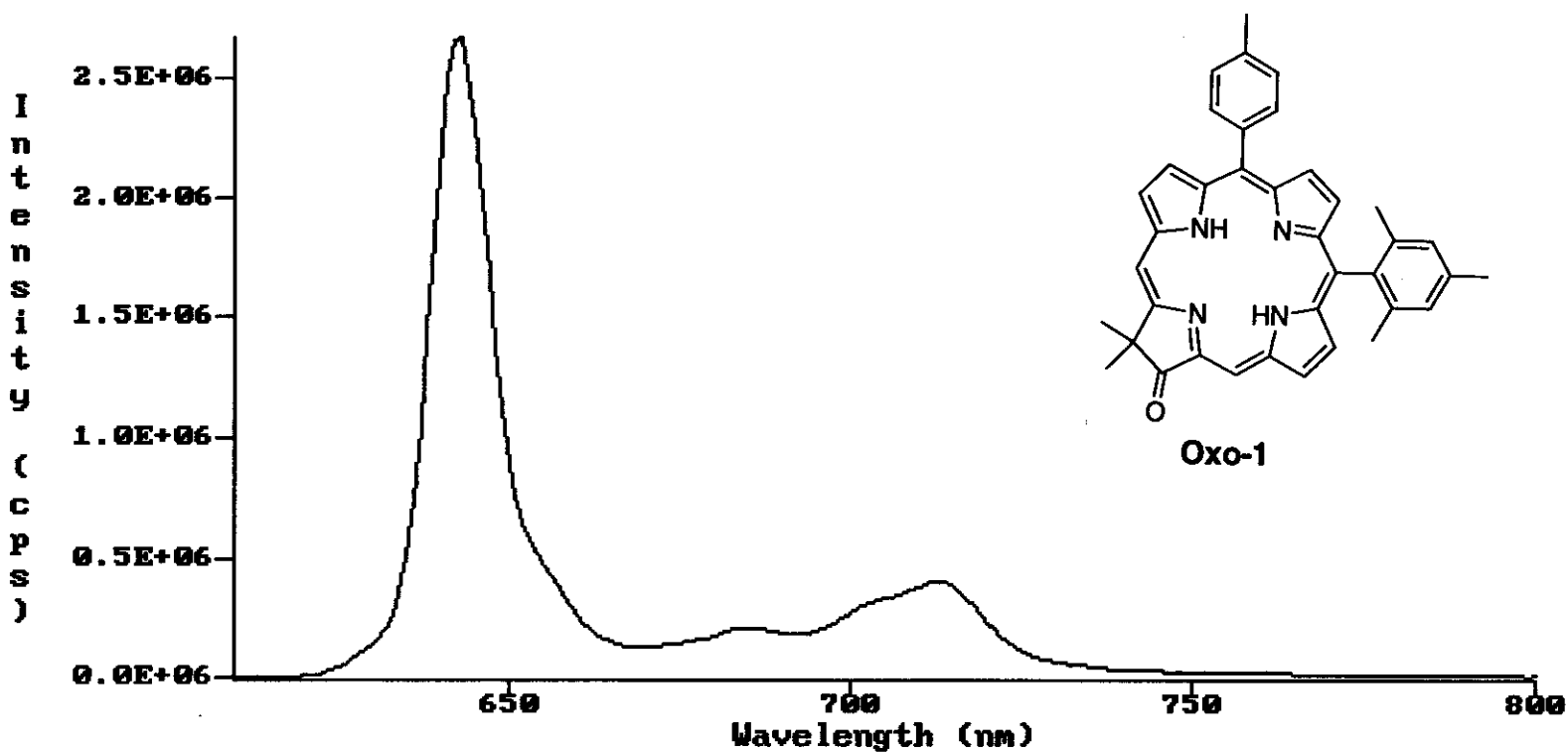


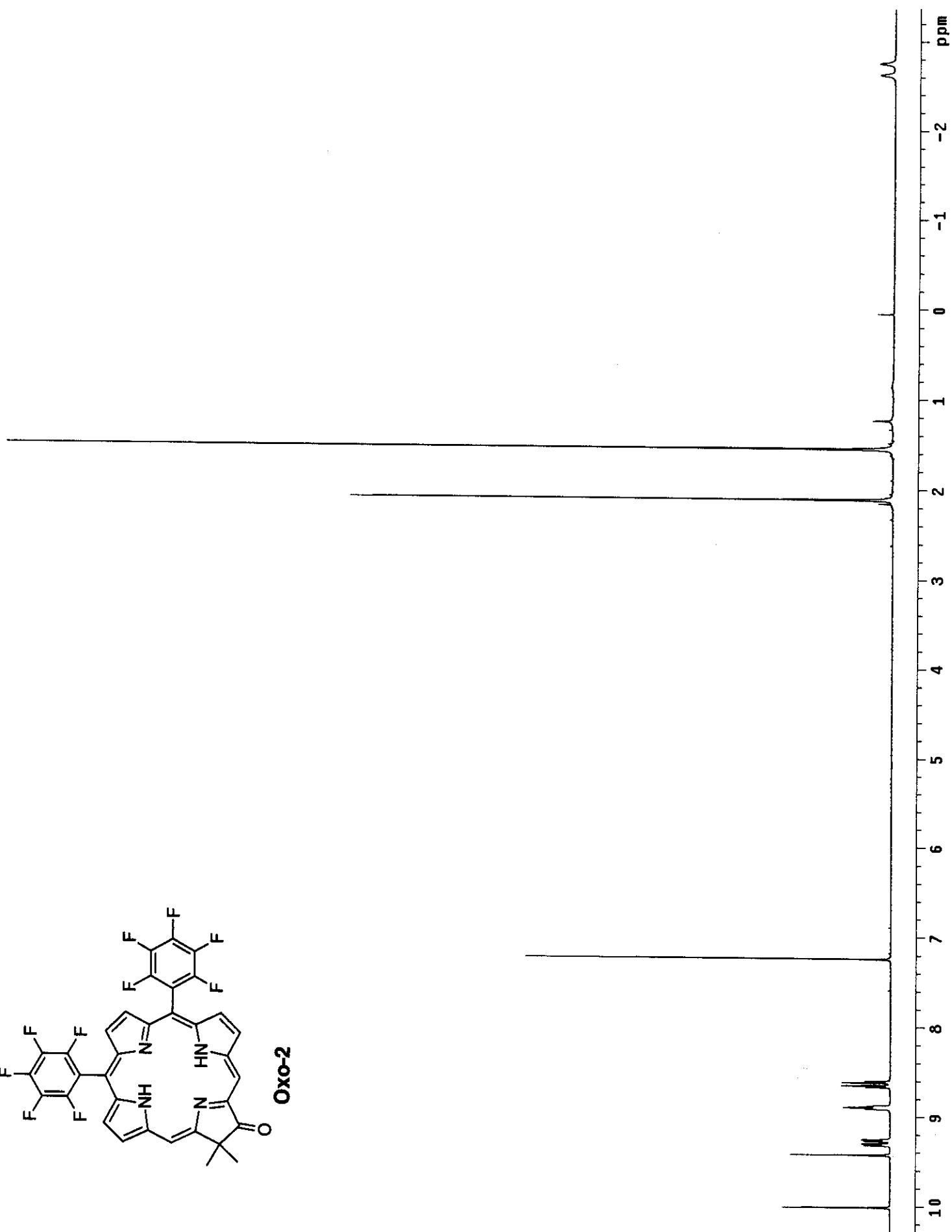
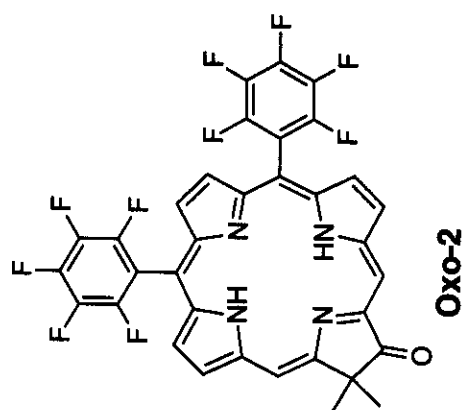
Method file : <untitled>
 Information : Default Method
 Data File : C:\RSLSP\1\04230102.SD Created : 4/23/01
 17:36:37

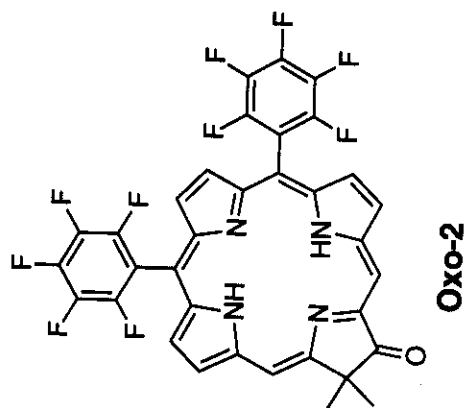
Overlaid Spectra:

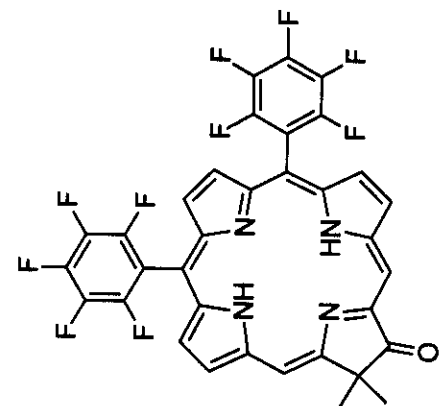


#	Name	Peaks (nm)	Abs (AU)
1	Mes-Fb-Oxo	415.0	0.62237
1		364.0	0.13570
1		643.0	8.9929E-2





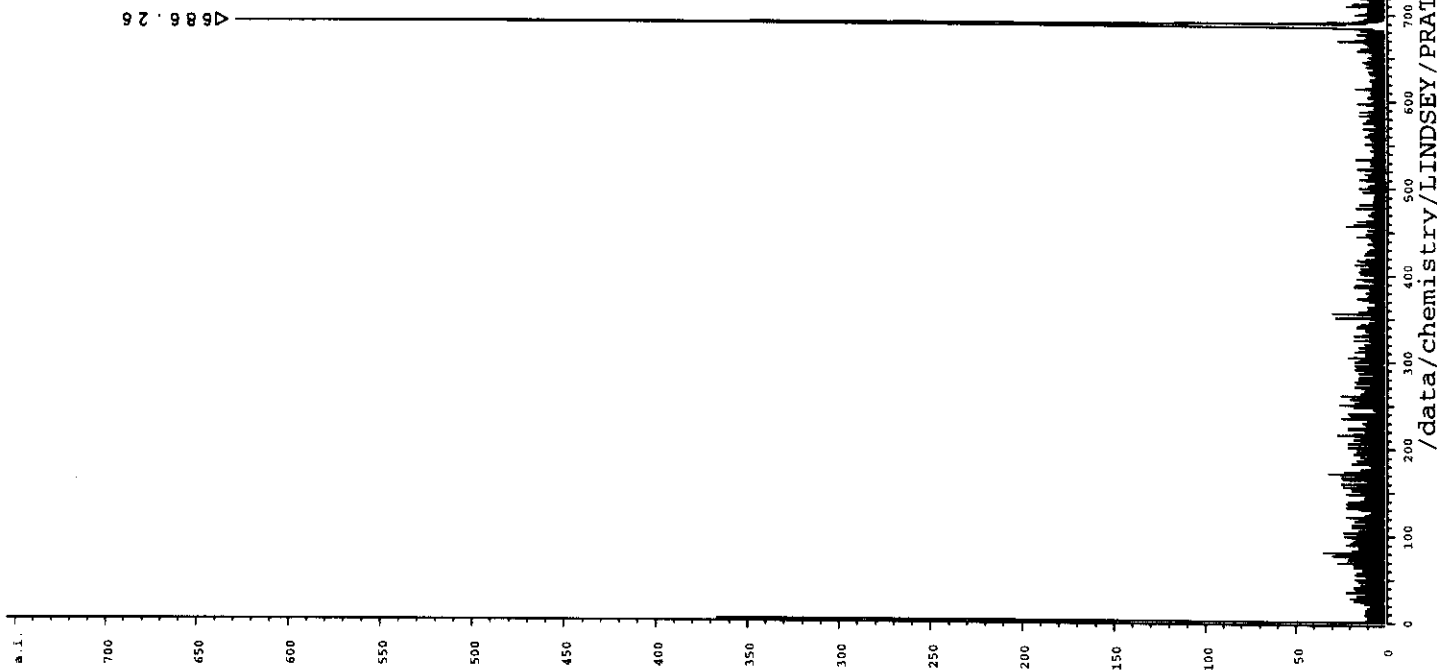




Oxo-2

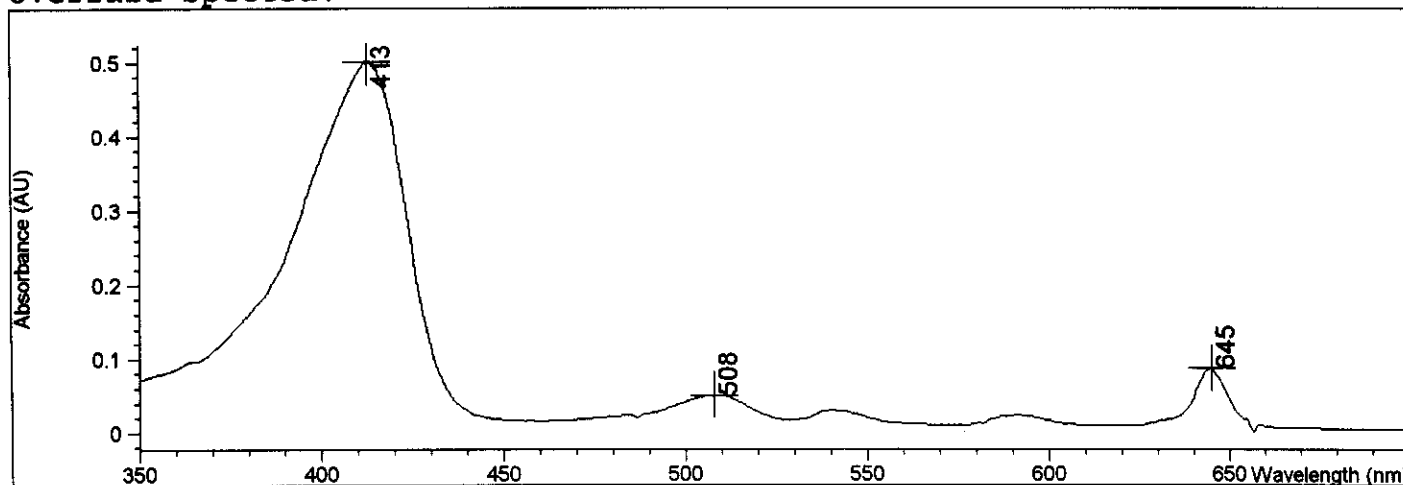
INSTRUM TOP
OPID N. Srinivasan
PATNAM 015034
DATE 4 11:26:08 2001
PATH /data/chemistry/LINDSEY/PRATHAPAN
POLARI POS
AQOP_m Reflector
TO 40000
NGSHOTS 20
SHOOTN 0
SHOOTST 0
SHOOTSD 0
SHOOTTS 0
DM 1.00 [ns]
DELAY 0 [ns]
U1s1 20.00 [KV]
U1s2 18.70 [KV]
U1e1 0.00 [KV]
U1e2 7.50 [KV]
U1mass 10.00 [KV]
RefFull 0.00 [KV]
UdetL 1.50 [KV]
UdetR 0.00 [KV]
Udef1 2.00 [KV]
Udef2 1.00 [KV]
ATTEN 33.0 [Hz]
ML1 2067125.193
ML2 333.982
ML3 0.000
HITURBO no
GOODN yes
GOODT short
DEFLON no
BLASND no
LANSND no
LANSND ac
LANSND nc
DPCAL 510.84 [Da]
DPMAS 700.00
PRVAL 0.33
LUNDVAL 0.28
LSDNDV 0.91
CMT1 (PPP)2PbChlorin
CMT2 atcn 33, shots 20

Δ686.26

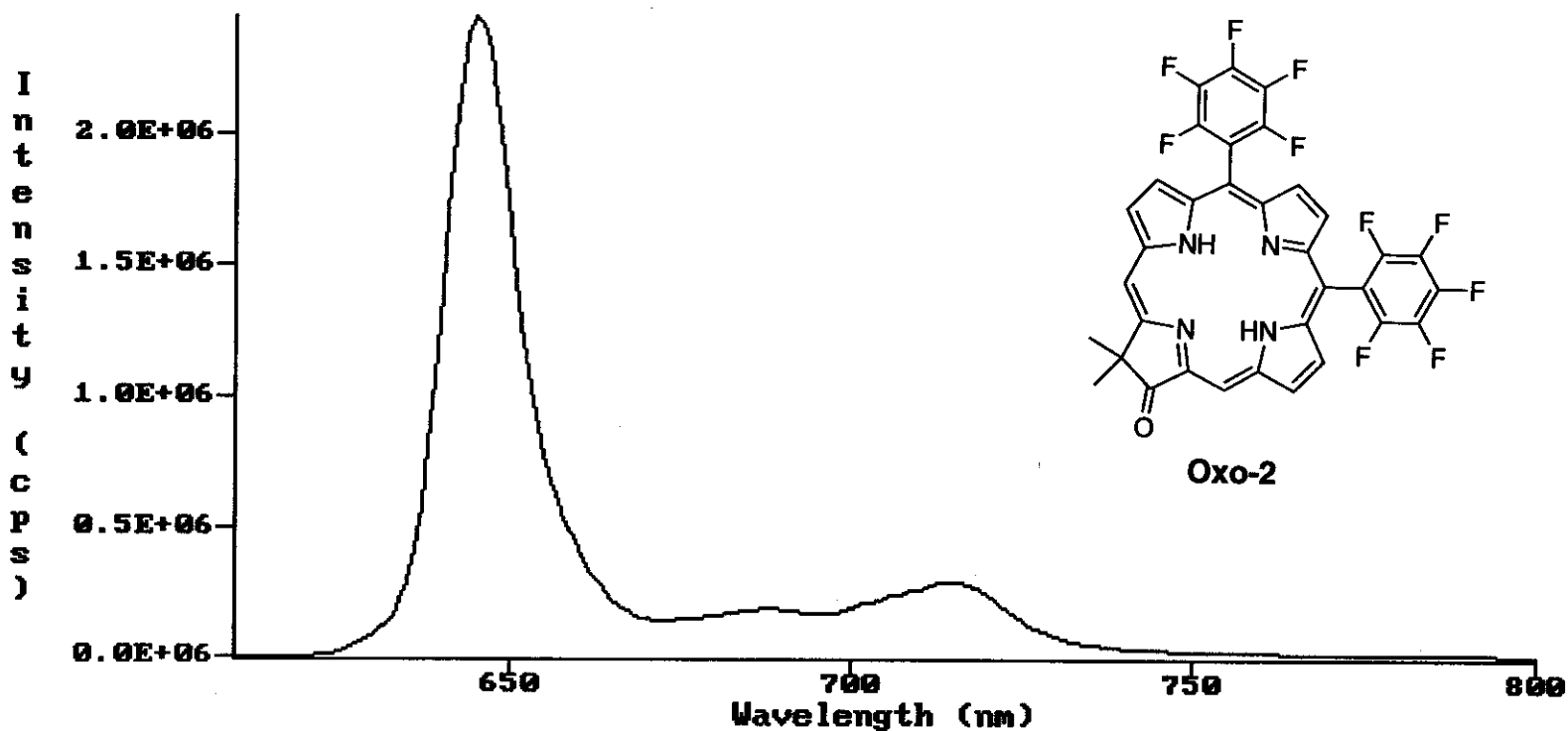


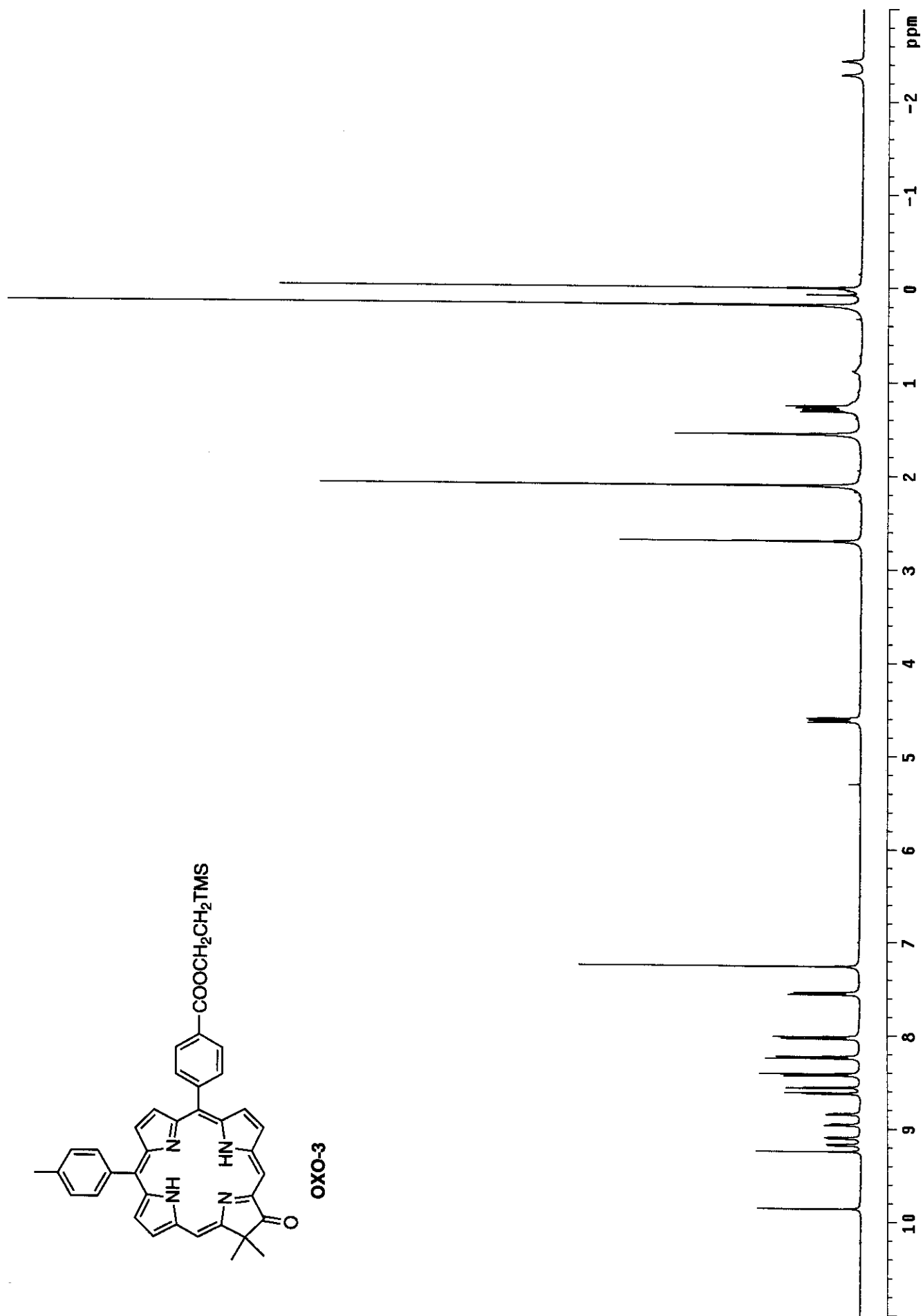
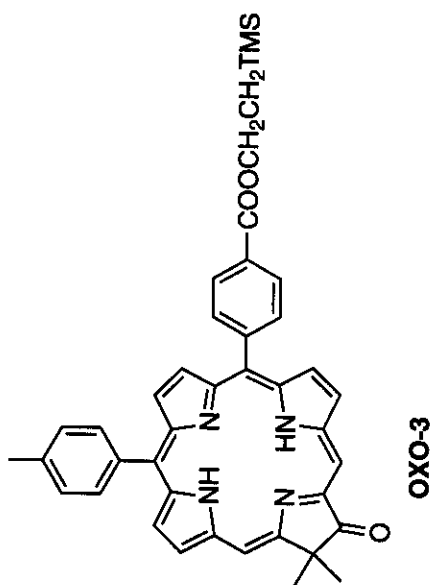
Method file : <untitled>
 Information : Default Method
 Data File : C:\RSLSP\1\04230103.SD Created : 4/23/01
 18:02:39

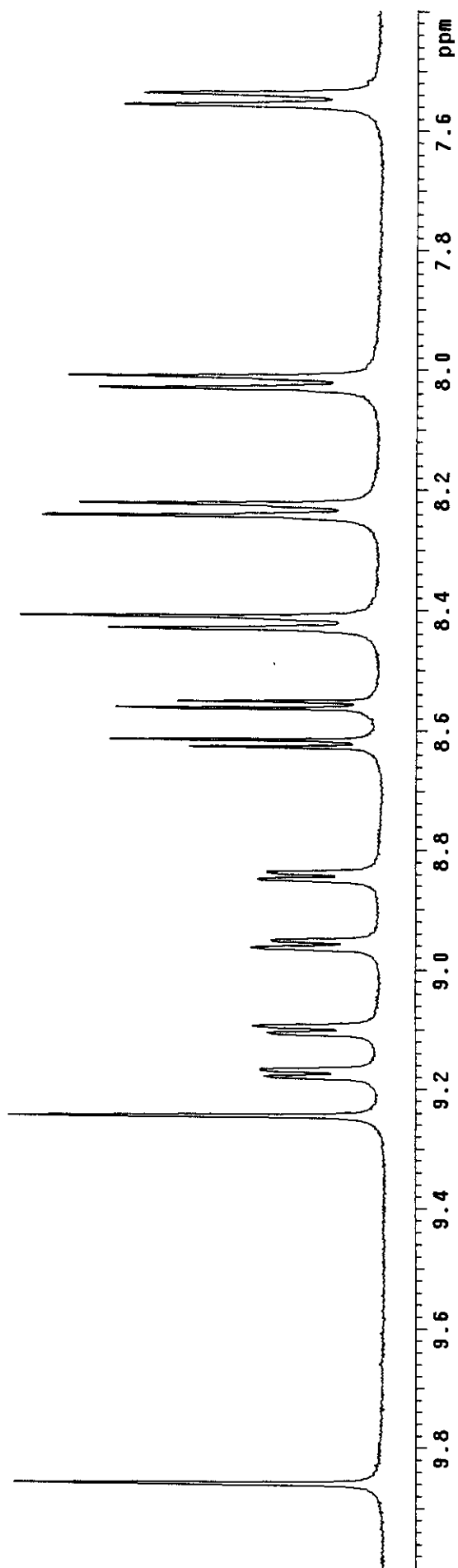
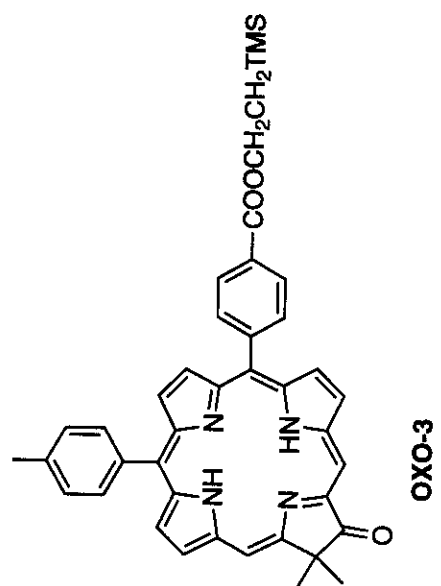
Overlaid Spectra:

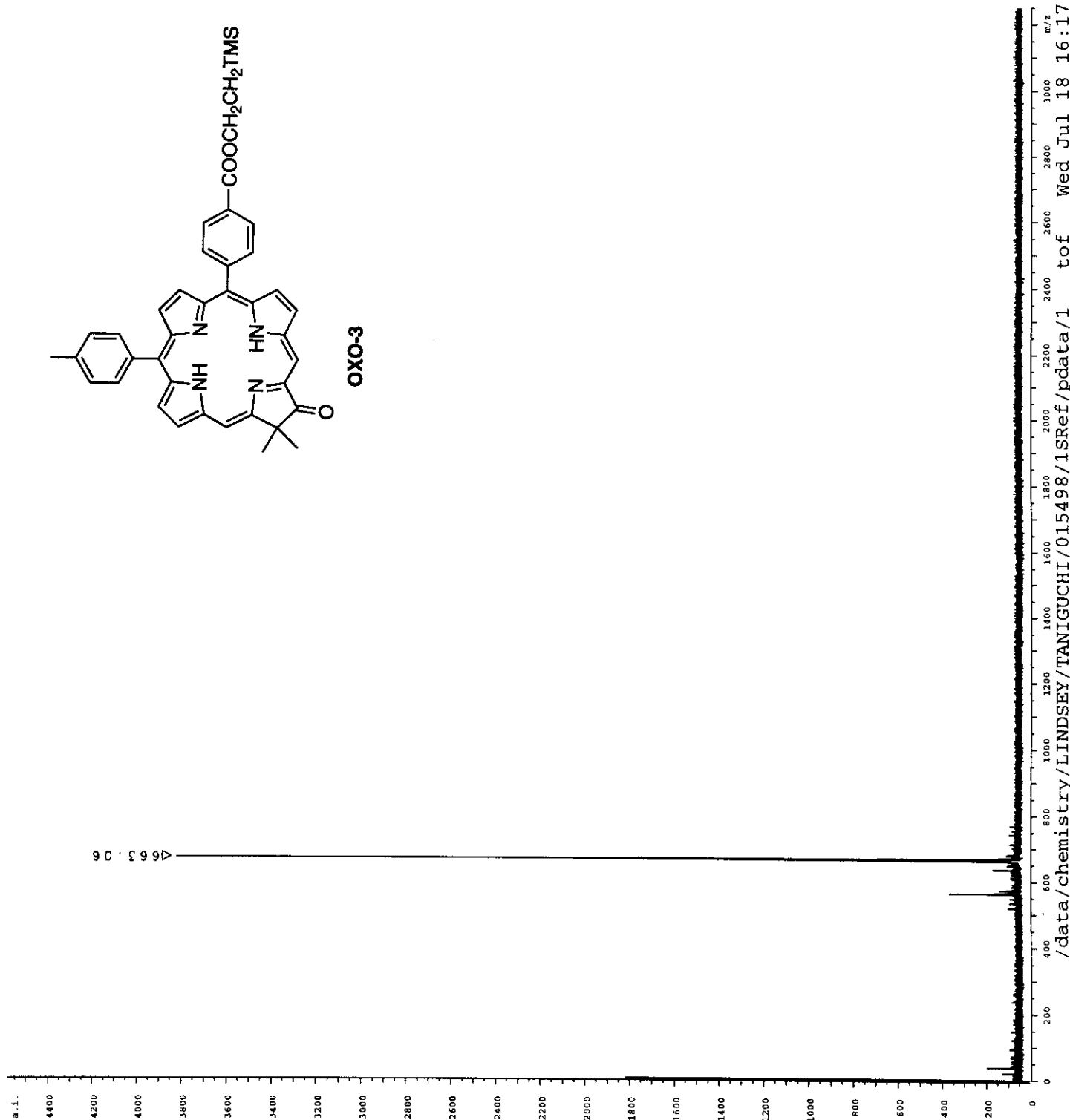


#	Name	Peaks (nm)	Abs (AU)
1	F5-Fb-Oxo	413.0	0.50016
1		645.0	8.6864E-2
1		508.0	5.0235E-2

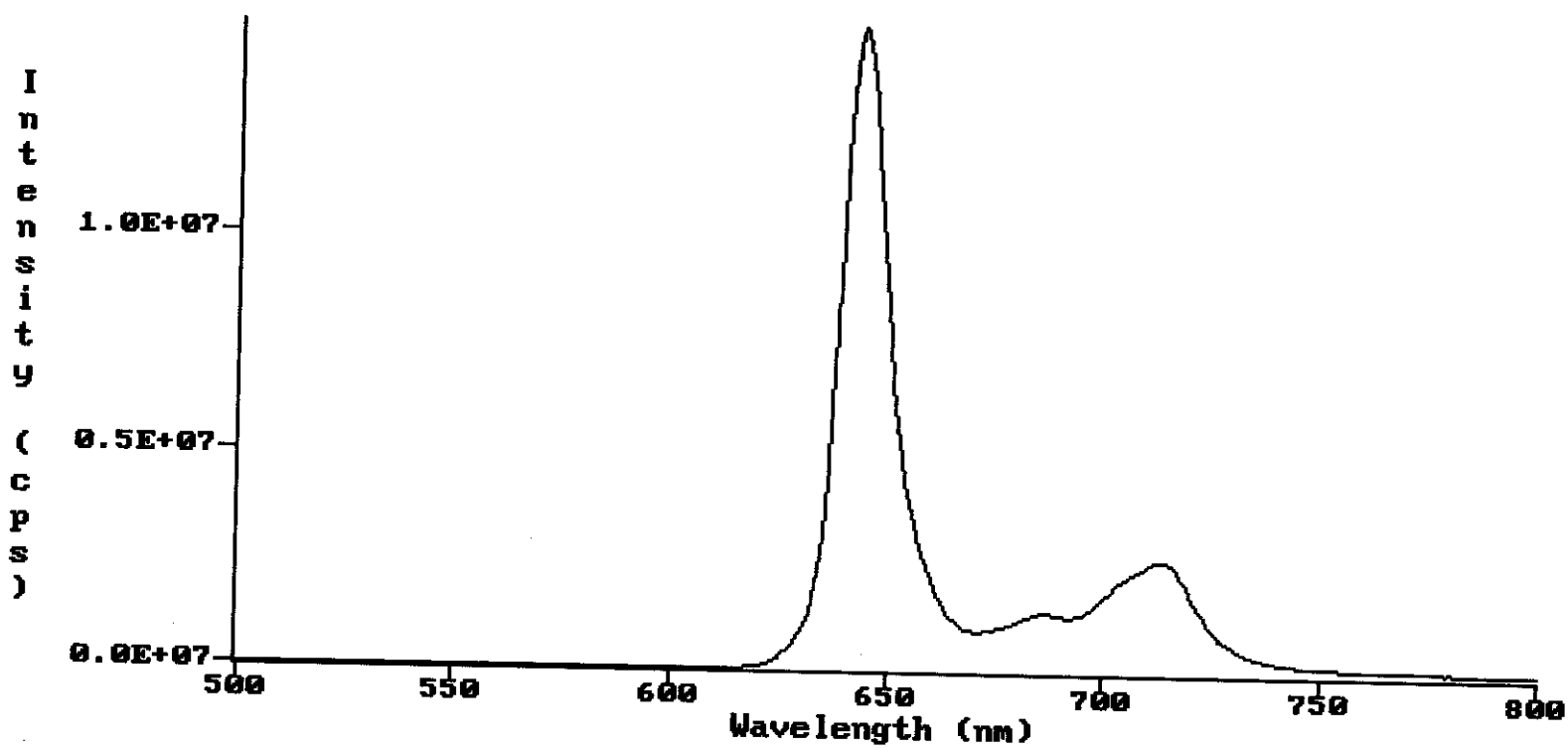
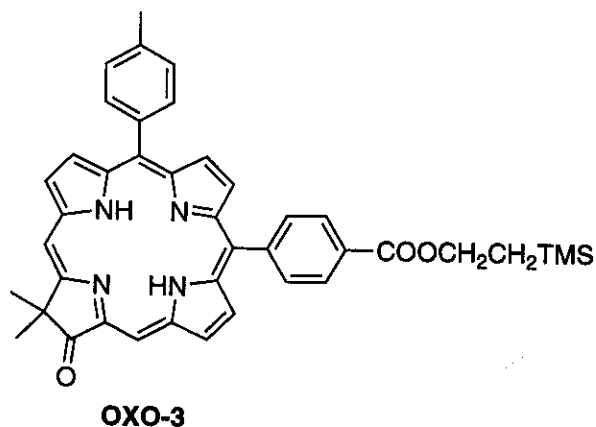


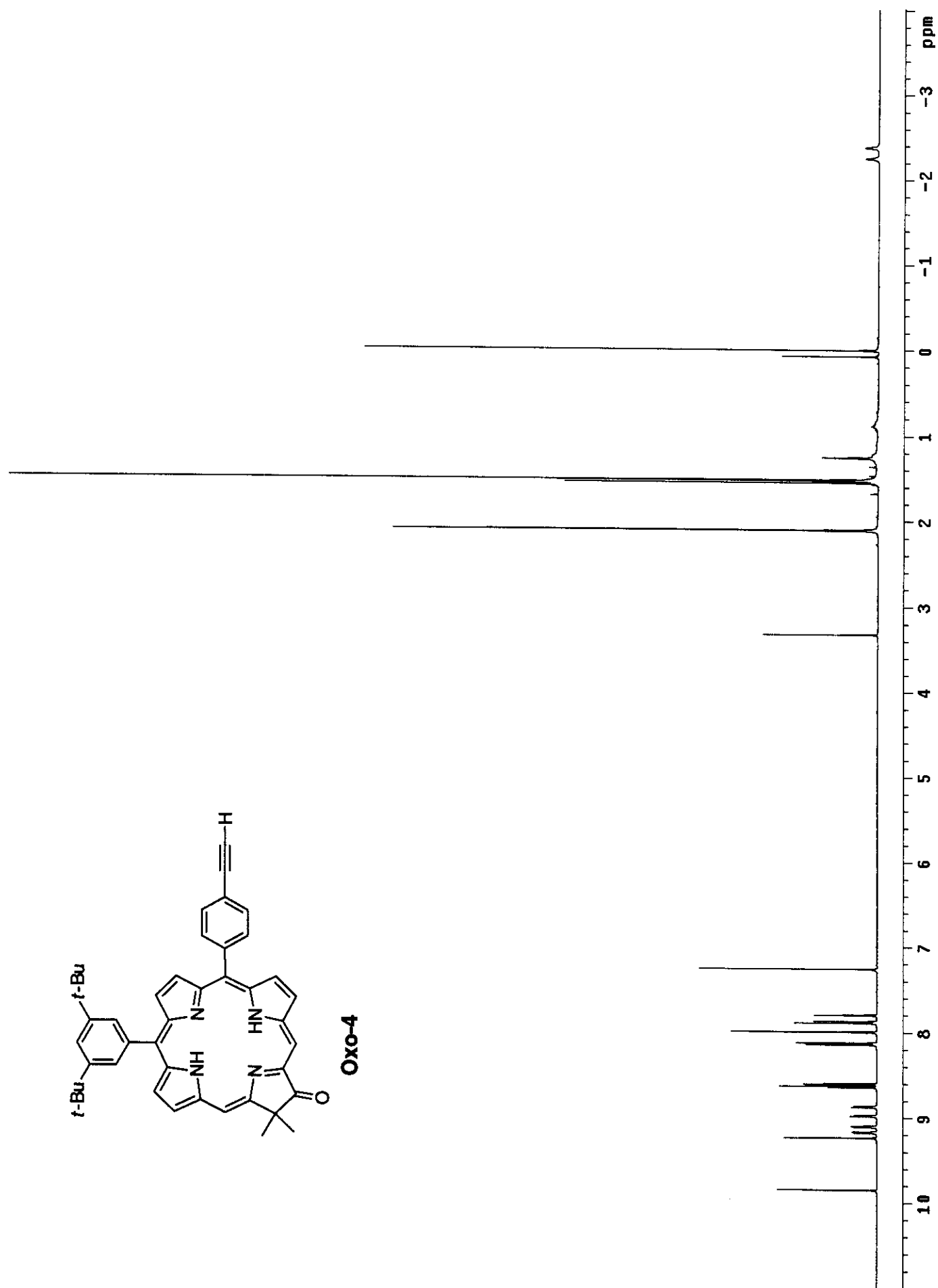


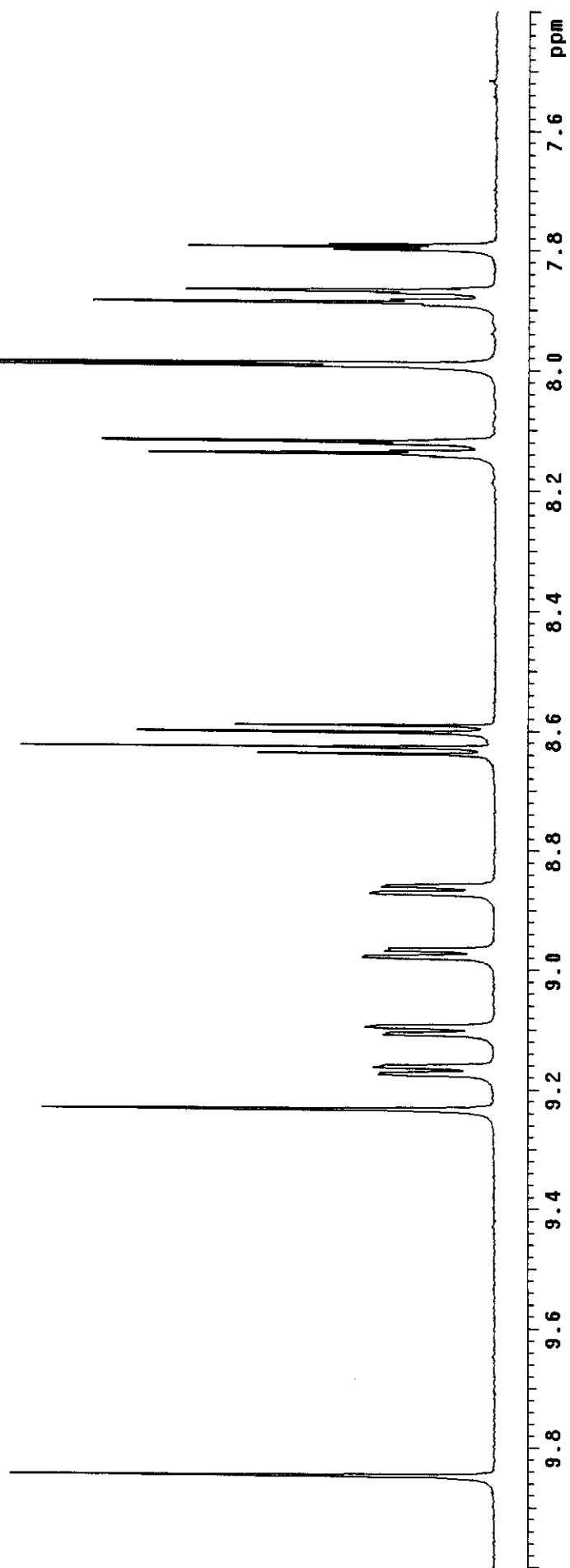
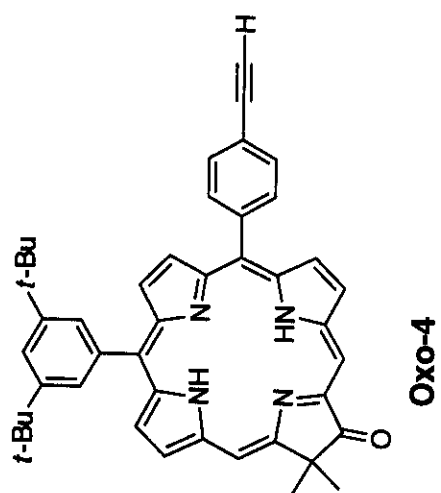


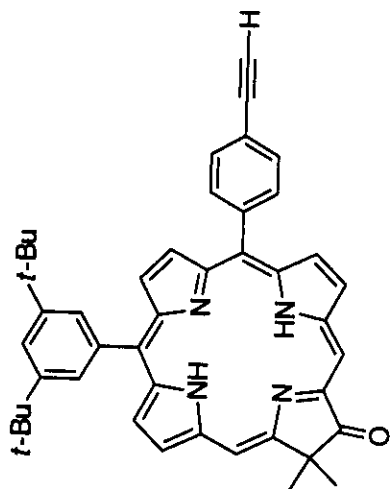
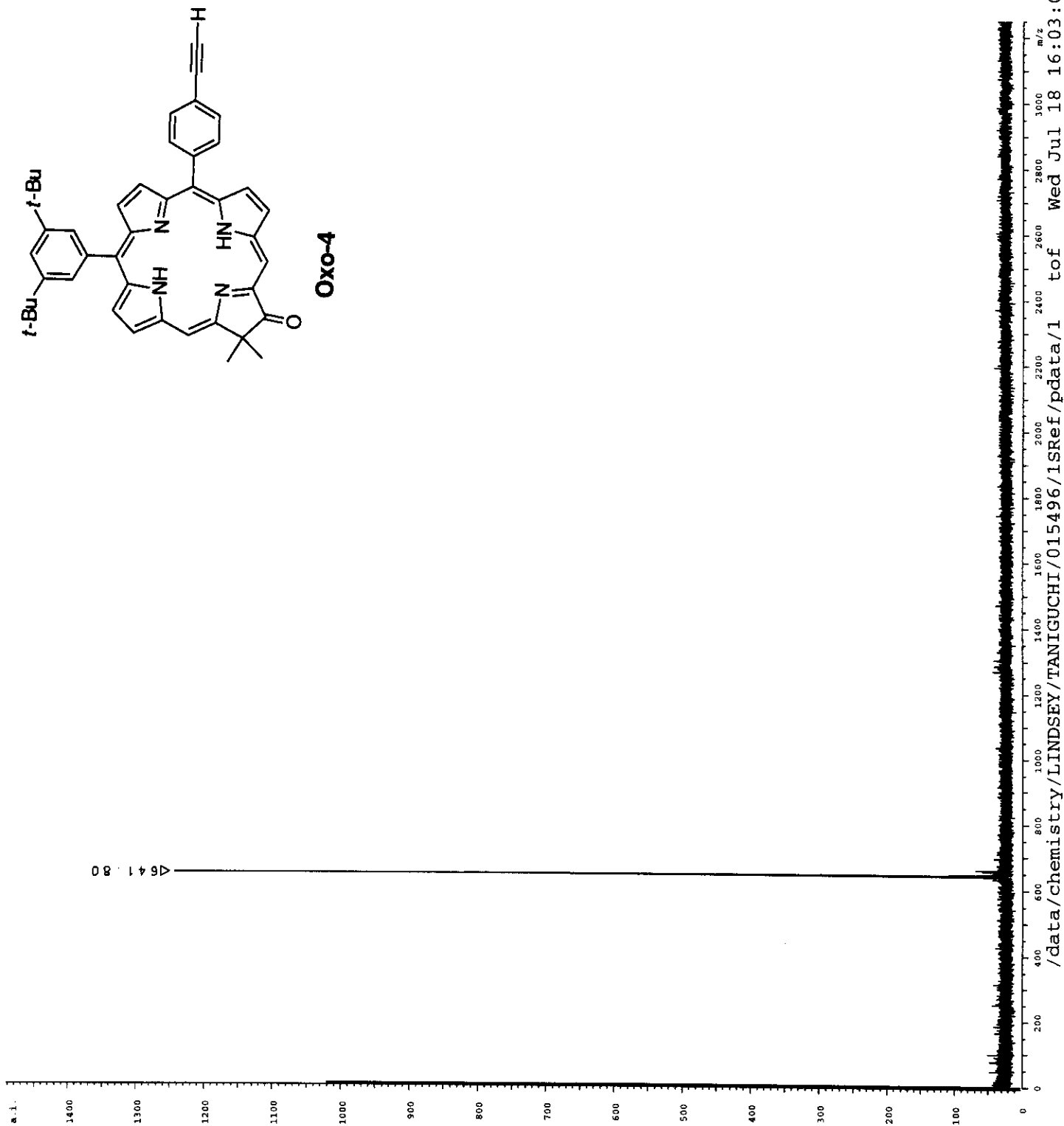


INSTRUM TOP
OBJID N. Srinivasan
EXPNO 11446
DATE_ 941703 18 16:14:40 2001
PATH /data/chemistry/LINDSEY/TANIGUCHI
POLARI POS
AQOP_m Reflector
TD 40000
RSHOTS 100
SAMPN 0
SMTS1 0
SMTS2 0
SMTS3 0
DW 1.00 [ns]
DELAY 0 [ns]
U1s1 20.00 [KV]
U1s2 18.70 [KV]
U1s3 0.50 [KV]
U1s4 7.50 [KV]
U1s5 10.00 [KV]
U1mass 0.00 [KV]
RefPull 1.50 [KV]
UdetL 0.00 [KV]
UdetR 0.00 [KV]
UdetS 2.00 [KV]
U1s5 1.00 [Hz]
ML1 2065947.190
ML2 327.134
ML3 0.000
HITURBO no
GUESS yes
GUESS short
DEFLON no
RLSND no
LINSND no
UISZND no
DPGALL 510.84 [Da]
DPMAS 700.00
SERVAL 0.25
LUNVAL 0.28
TS2BNV 0.91
CMT1 PL-OK-COCCINS
CMT2 att 44 shots#50



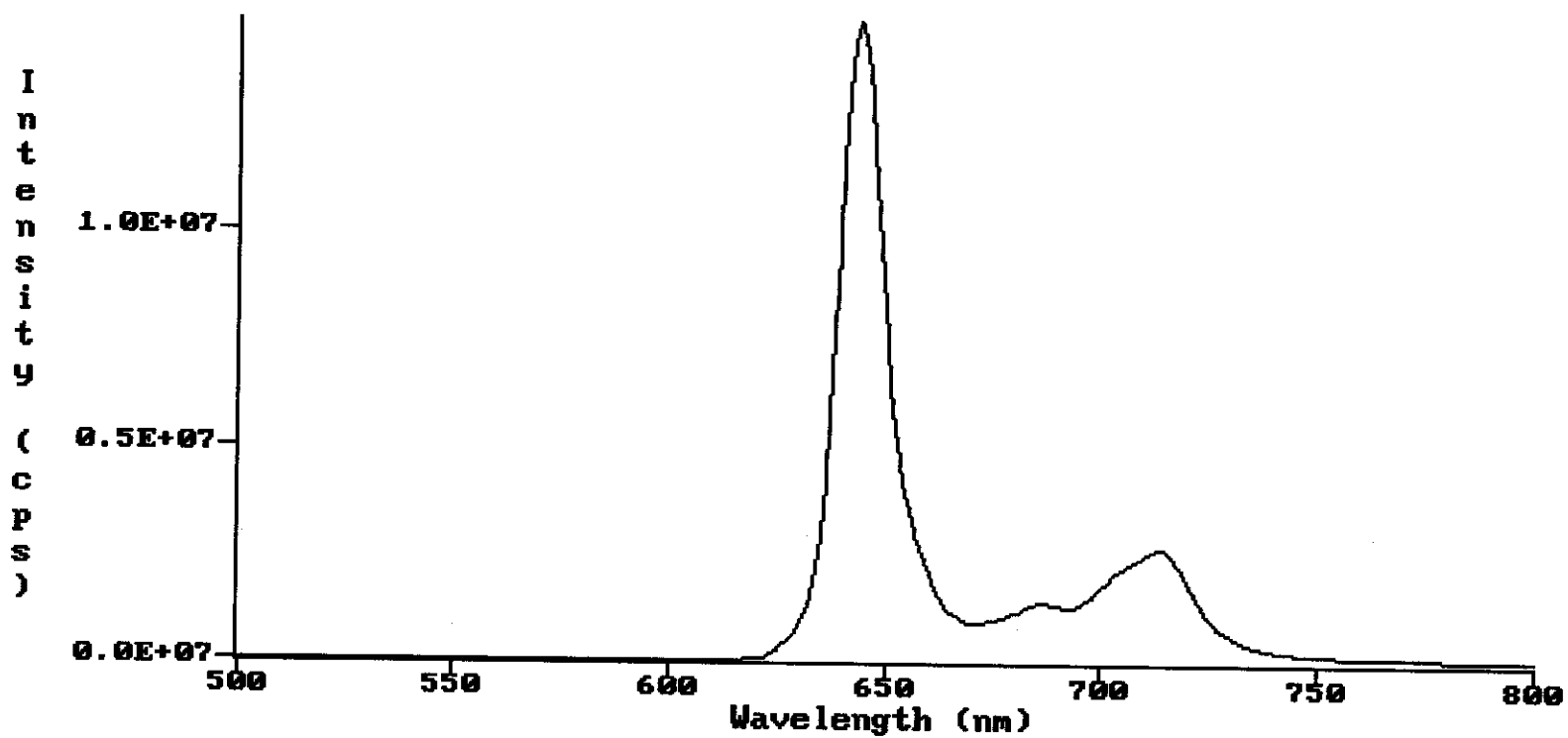
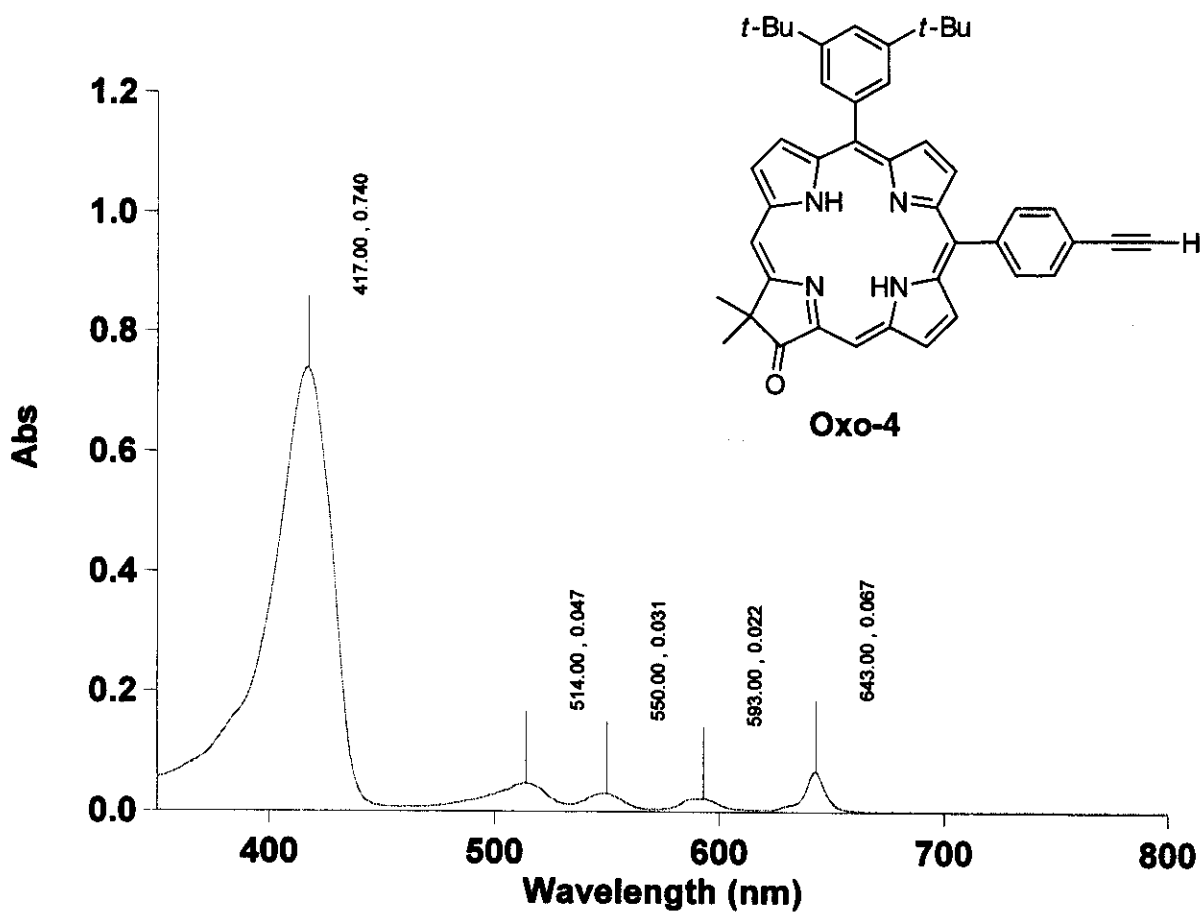


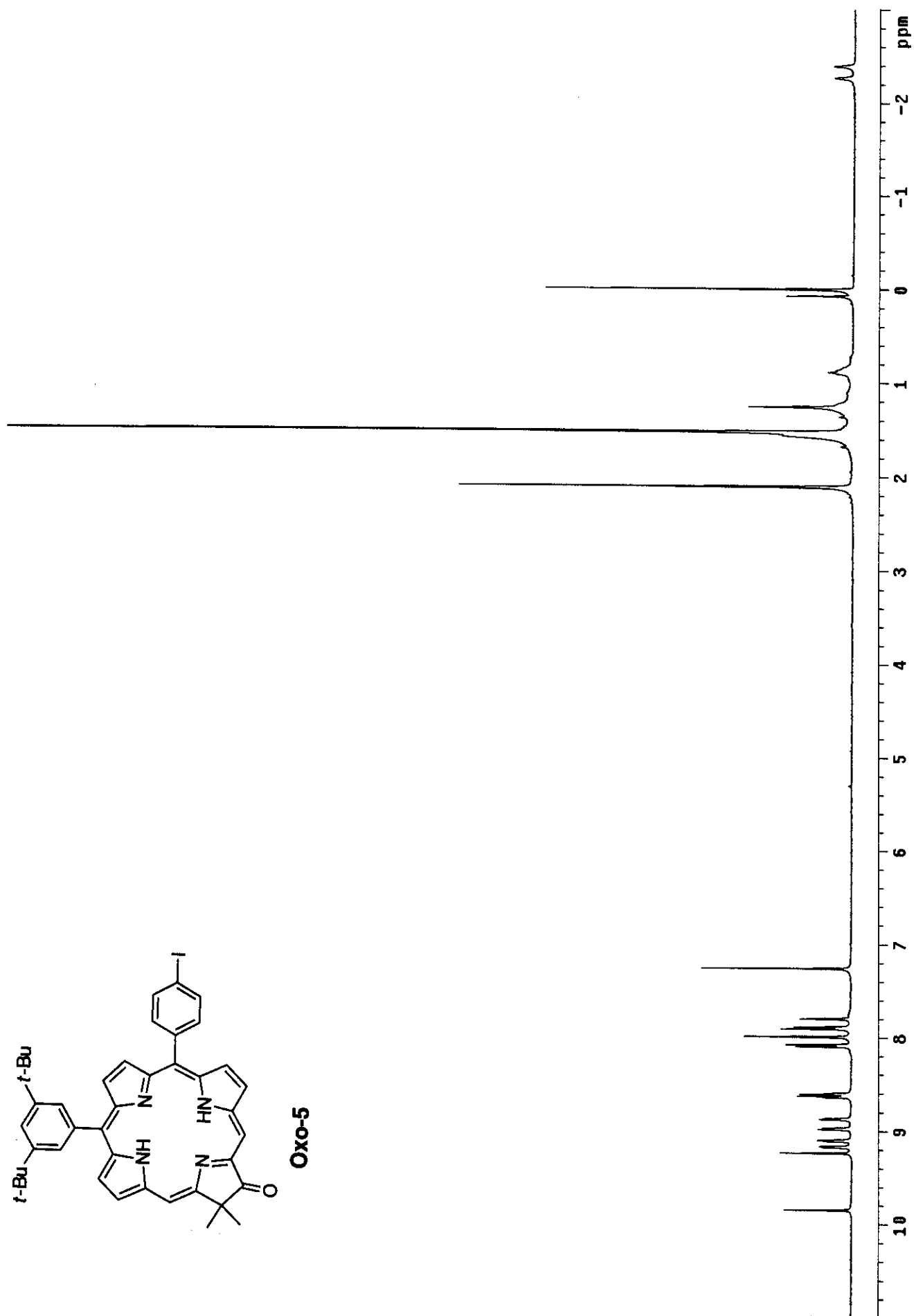
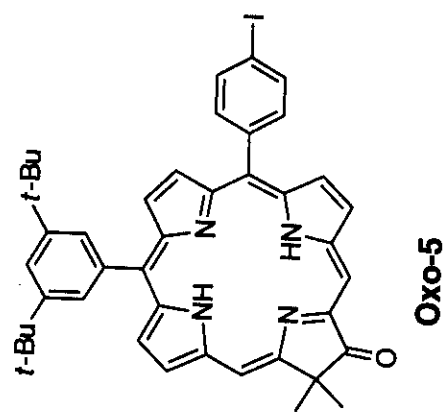


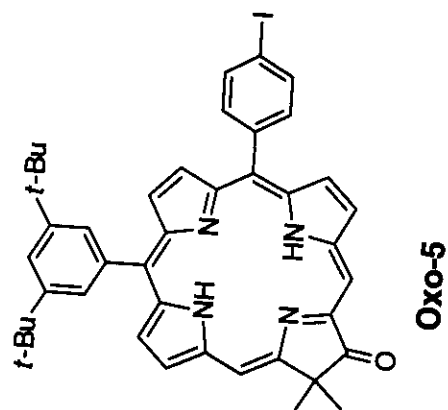


Oxo-4

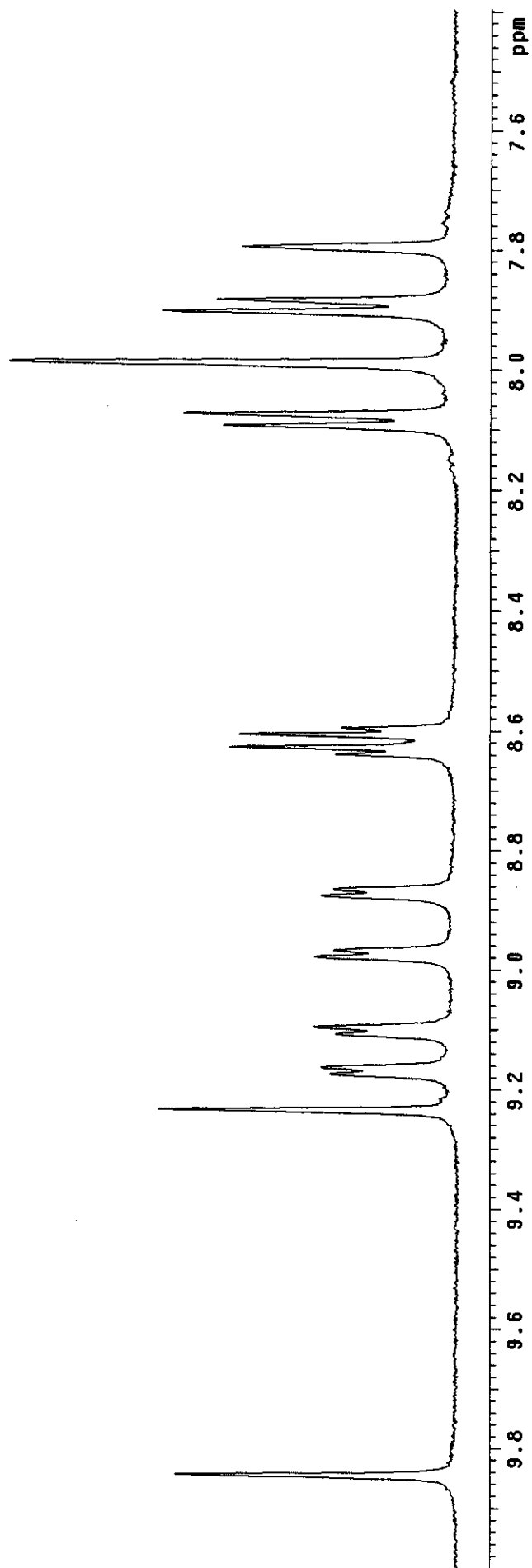
INSTRUM TOF
 OpId N. Srinivasan
 SMPNAM 015496
 ACQ DATE Wed Jul 18 16:02:07 2001
 DATA /data/chemistry/LINDSEY/TANIGUCHI
 POLARI POS
 ACOP m Reflector
 TD 40000
 RGSOTS 50
 SMOBUM 0
 SMOPTS1 0
 SMOPTS2 0
 SMOPTS3 0
 DM 1.00 (ns)
 DELAY 0 (ns)
 Uis1 20.00 (KV)
 Uis2 18.70 (KV)
 Uref1 0.00 (KV)
 Uisens 7.00 (KV)
 RefPull 10.00 (KV)
 Udet1 0.00 (KV)
 UdetL 1.50 (KV)
 UdetR 0.00 (KV)
 Udef1 2.00 (KV)
 REPHZ 1.00 (Hz)
 MTEN 42
 ML1 2067125.193
 ML2 333.982
 ML3 0.000
 HITURBO no
 GDEON yes
 GDELY short
 REFEND no
 LENSND no
 LINSND no
 U152END no
 DPCALI 510.84
 DPMAS 700.00 (Da)
 REMVAL 0.33
 REMVAL 0.33
 152ENDV 0
 CMF1 Pb-OXO-CCH
 CMF2 att 42, shot#50

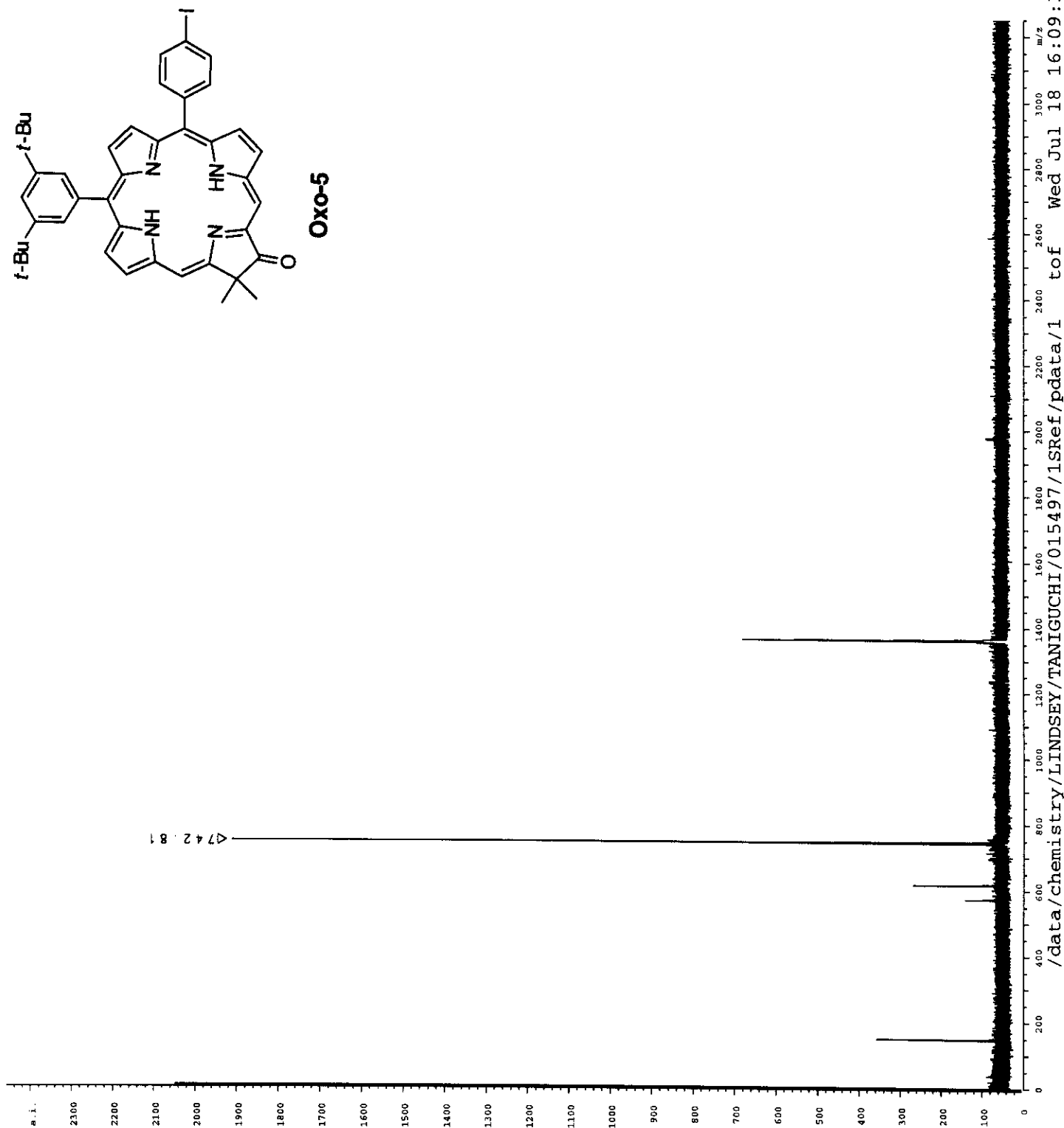
NCSU Chemistry
Instrument Serial Number 0051477





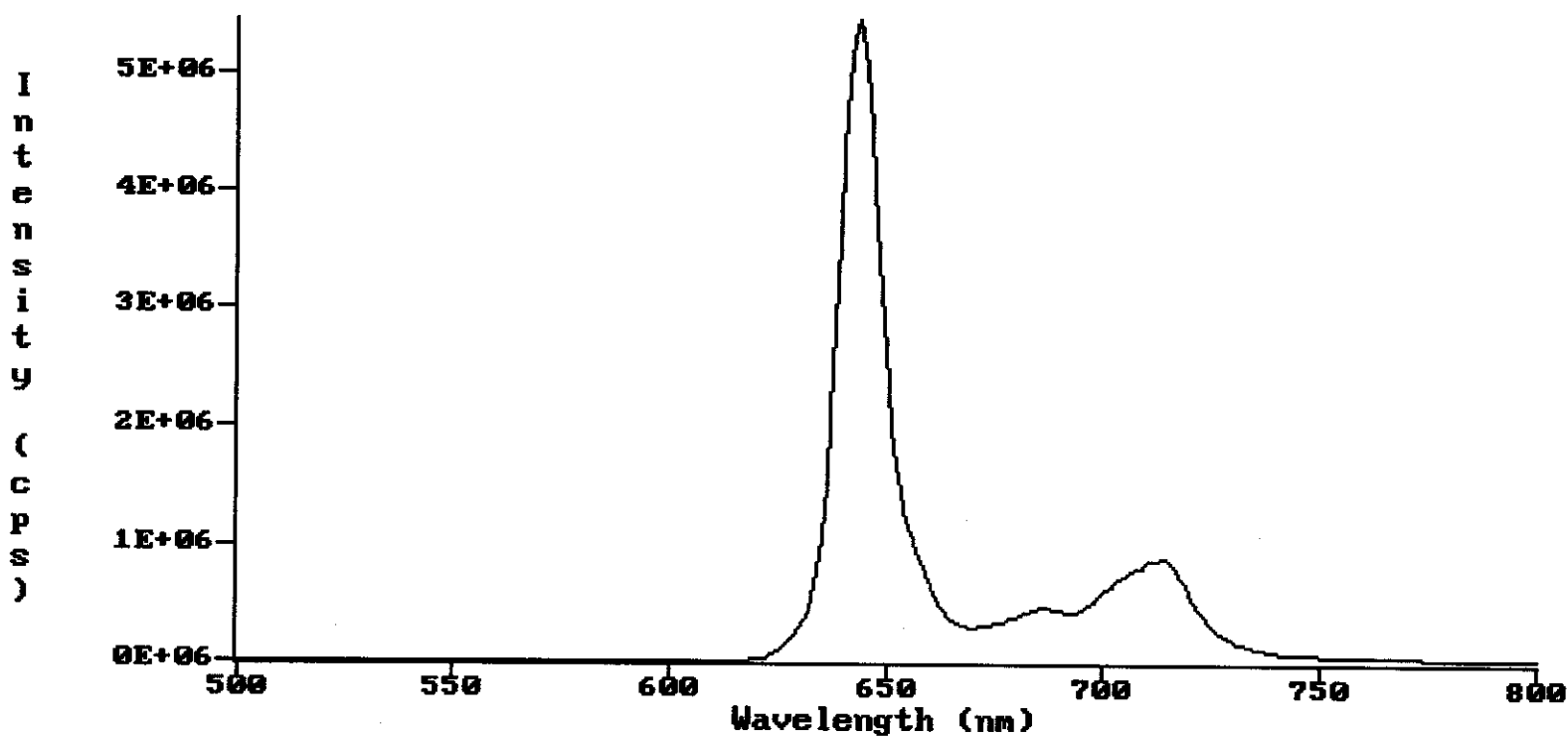
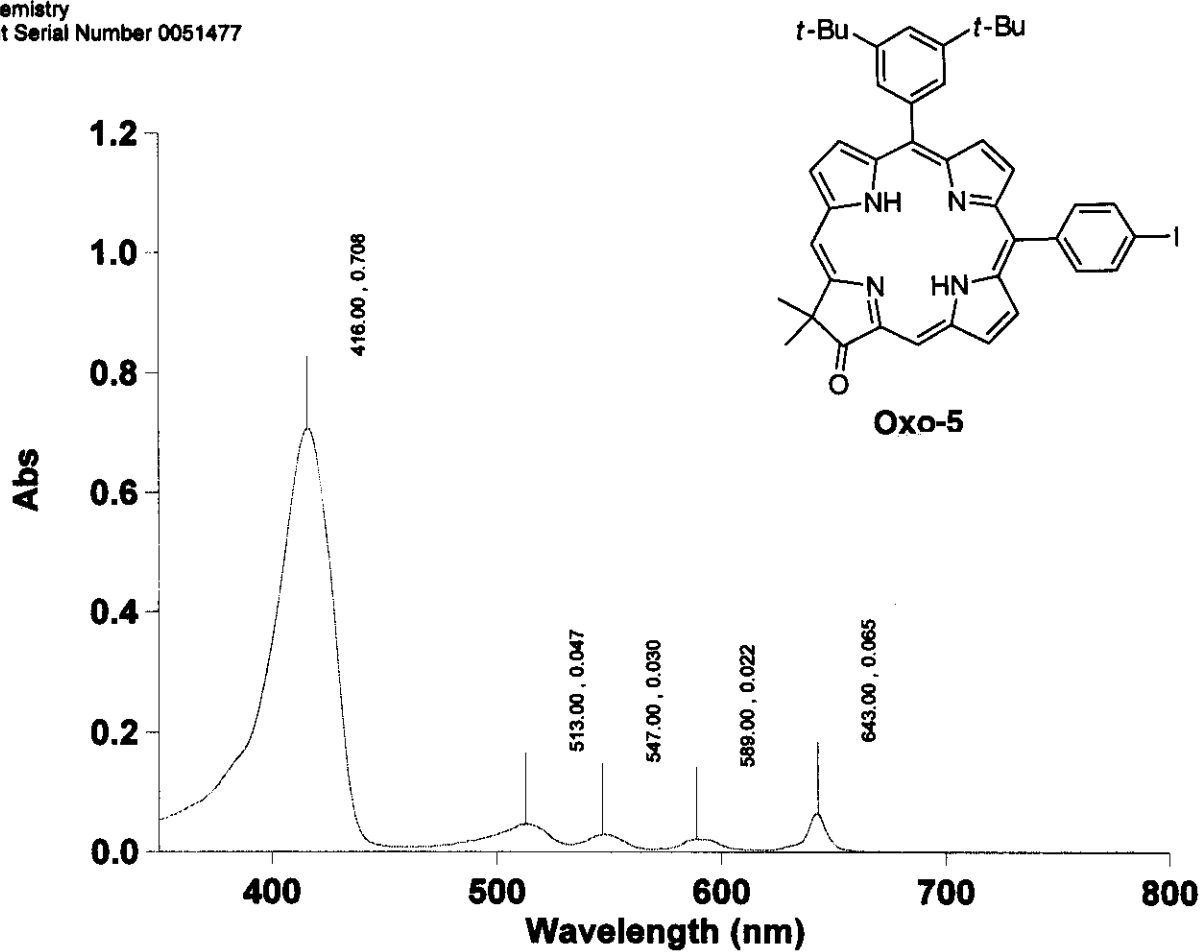
Oxo-5

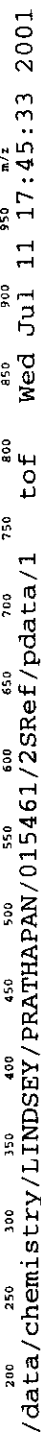




INSTRUM TOP
 OpId N Srinivasan
 SMPNAM 015497
 AC DATE Wed Jul 18 16:08:40 2001
 DATA /data/chemistry/LINDSEY/TANIGUCHI
 POLAR NO
 ACOP_m Reflector
 TO 40000
 NoSHOTS 100
 SMOHUM 0
 SMOPTSI 0
 SMOPTSI2 0
 SMOPTSI3 0
 DM 1.00 [ns]
 DELAY 0 [ns]
 Uis1 20.00 [kV]
 Uis2 18.70 [kV]
 Uref1 0.00 [kV]
 Uref2 0.00 [kV]
 Uisens 7.00 [kV]
 Uisens2 10.00 [kV]
 RefPull 0.00 [kV]
 UdetL 1.50 [kV]
 UdetR 0.00 [kV]
 Udef1 2.00 [kV]
 REPWZ 1.00 [Hz]
 ATTEN 43
 ML1 2067121.93
 ML2 333.982
 ML3 0.000
 HITURO no
 GIBSON yes
 GIBLY short
 REFNO no
 REFNO2 no
 RESEND no
 LINSBND no
 U152BND no
 DPCAL1 510.84
 DPMAS 700.00 [Da]
 REMVAL 0.33
 RESCAL 0.28
 152BNDV 0.91
 CMT1 Pb-OXO-PRI
 CMT2 att 43,shots100

NCSU Chemistry
Instrument Serial Number 0051477



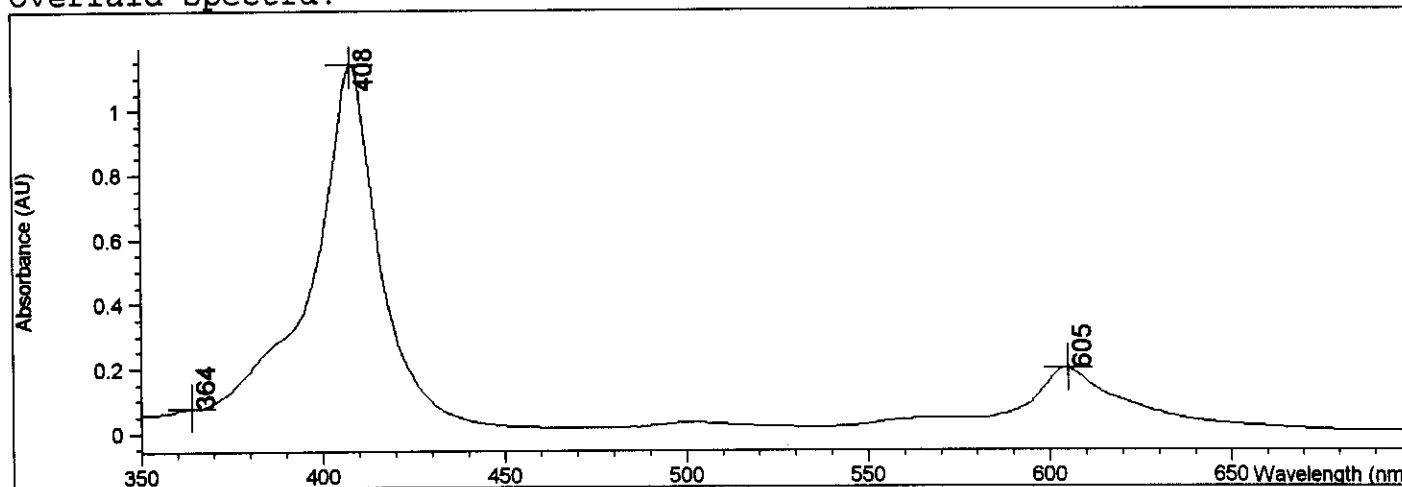


Cu1

[illegible]

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

Overlaid Spectra:

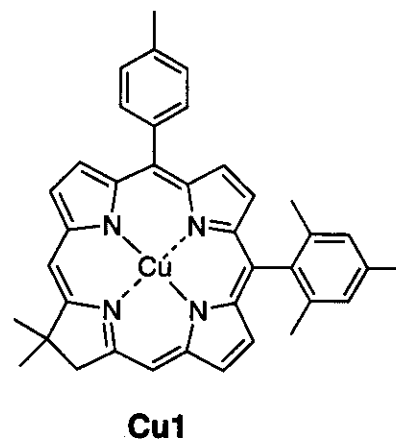


#	Name	Peaks (nm)	Abs (AU)
1	Mes-Cu-Chl	408.0	1.14090
1		605.0	0.19516
1		364.0	7.9418E-2

Report generated by :

Signature:

*** End Spectrum/Peak Report ***

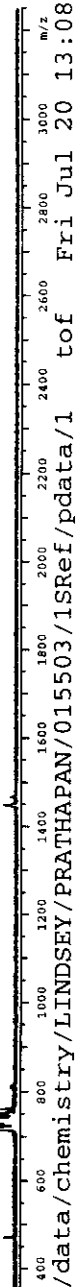


The chemical structure shows a central copper atom (Cu) coordinated by four nitrogen atoms in a square planar geometry, forming a macrocyclic ligand. Two pentafluorophenyl groups are attached to the macrocycle at the 10 and 20 positions. The copper atom is also coordinated by two additional ligands, represented by dashed lines, likely water or hydroxide groups, to complete its coordination sphere.

Cu2

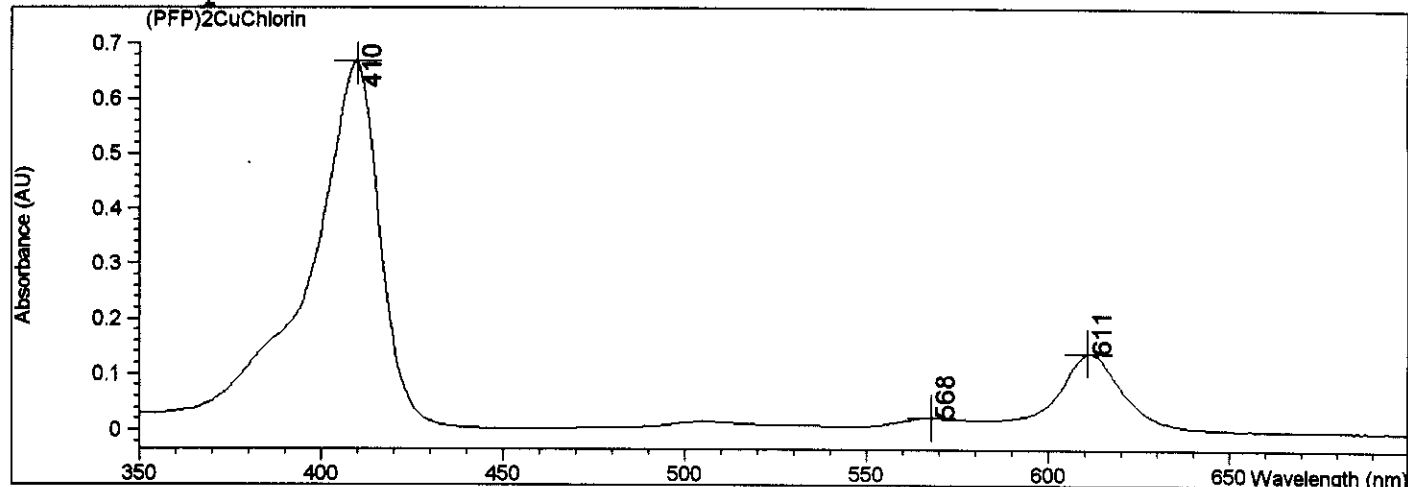
INSTRUM	TOP	Opid	N	Scintivasean
SRPMAN	015503			
AD DATE	Fri Jul 20 13:07:01 2001			
DATA PATH	/data/chemistry/LINSEY/PRATHAPAN			
FOSS				
ACQPGM	Reflector			
TO	40000			
NGSHOTS	100			
SNORM0	0			
SNORM1	0			
SNORM2	0			
SNORM3	0			
DM	1.00	[ms]		
DELAY	0	[ms]		
U1s1	20.00	[KV]		
U1s2	18.50	[KV]		
U1s3	17.50	[KV]		
U1s4	7.50	[KV]		
U1s5	10.00	[KV]		
U1s6	10.00	[KV]		
U1s7	1.50	[KV]		
U1s8	1.50	[KV]		
U1s9	2.00	[KV]		
U1s10	2.00	[KV]		
REPZ1	1.00	[Hz]		
REPZ2	35.0			
ATTEN	2065947.190			
M1	327.134			
M2	0.000			
HITURBO	no			
GIBSON	yes			
DEPLEN	short			
DEPLEN	no			
DEPLEN	no			
DEPLEN	no			
DEPLEN	no			
U1S2BNO	no			
OPCAL1	510.84			
OPCAL2	700.00	[Da]		
OPCAL3	0.33			
PERDVAL	0.33			
PERDVAL	0.33			
LEADENY	0.67			
LEADENY	0.67			
PP2	25Cchlorin			
ATTN3	shots100			
CM2				

4733.07



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

Overlaid Spectra:

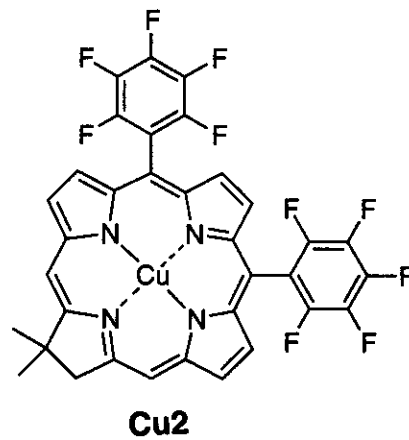


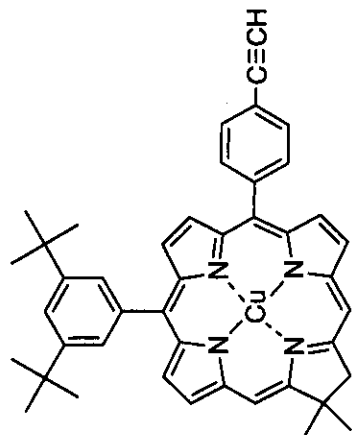
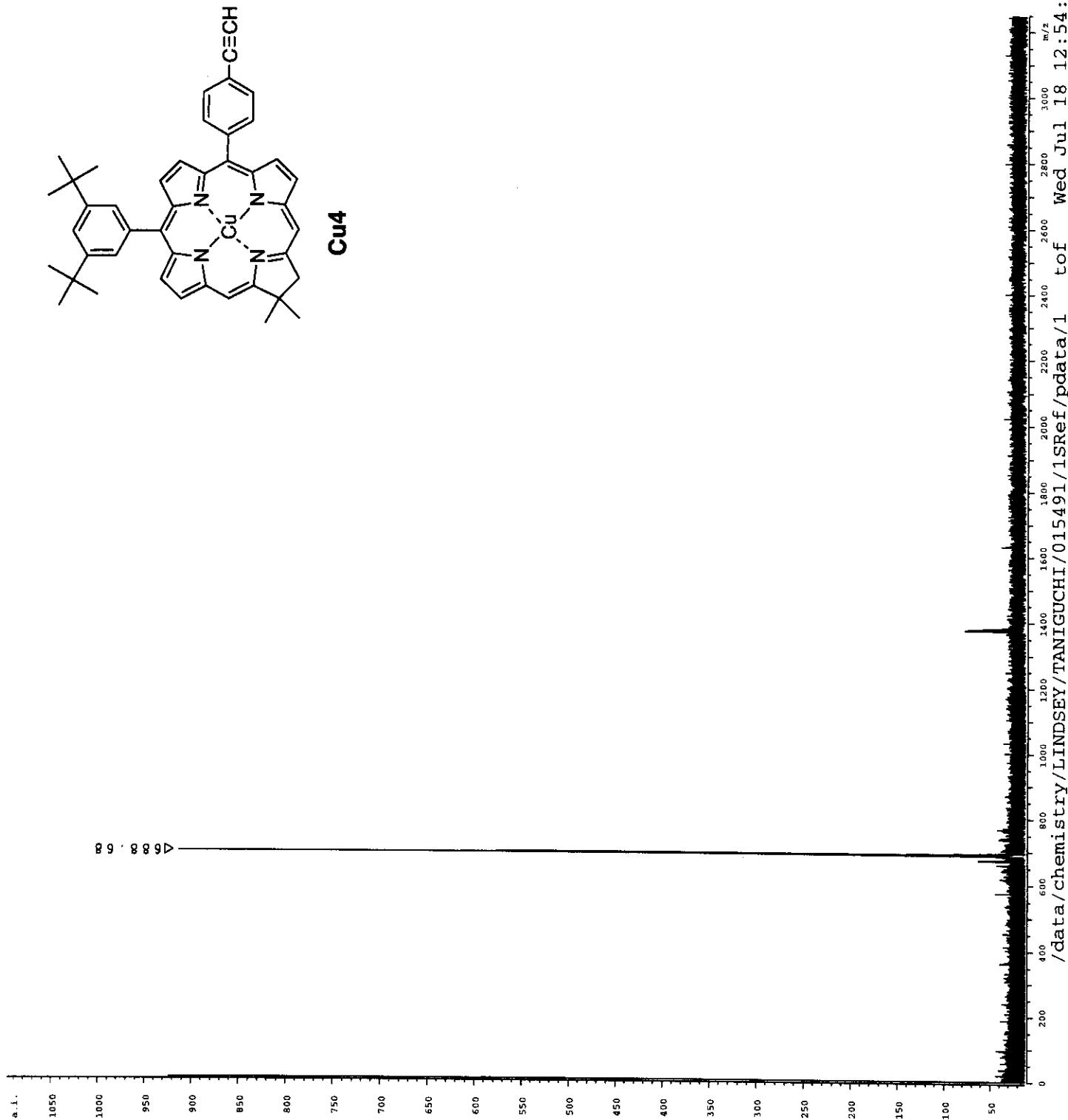
#	Name	Peaks (nm)	Abs (AU)
1	(PFP)2CuChlorin	410.0	0.66764
1		611.0	0.13924
1		568.0	2.2439E-2

Report generated by :

Signature:

*** End Spectrum/Peak Report ***

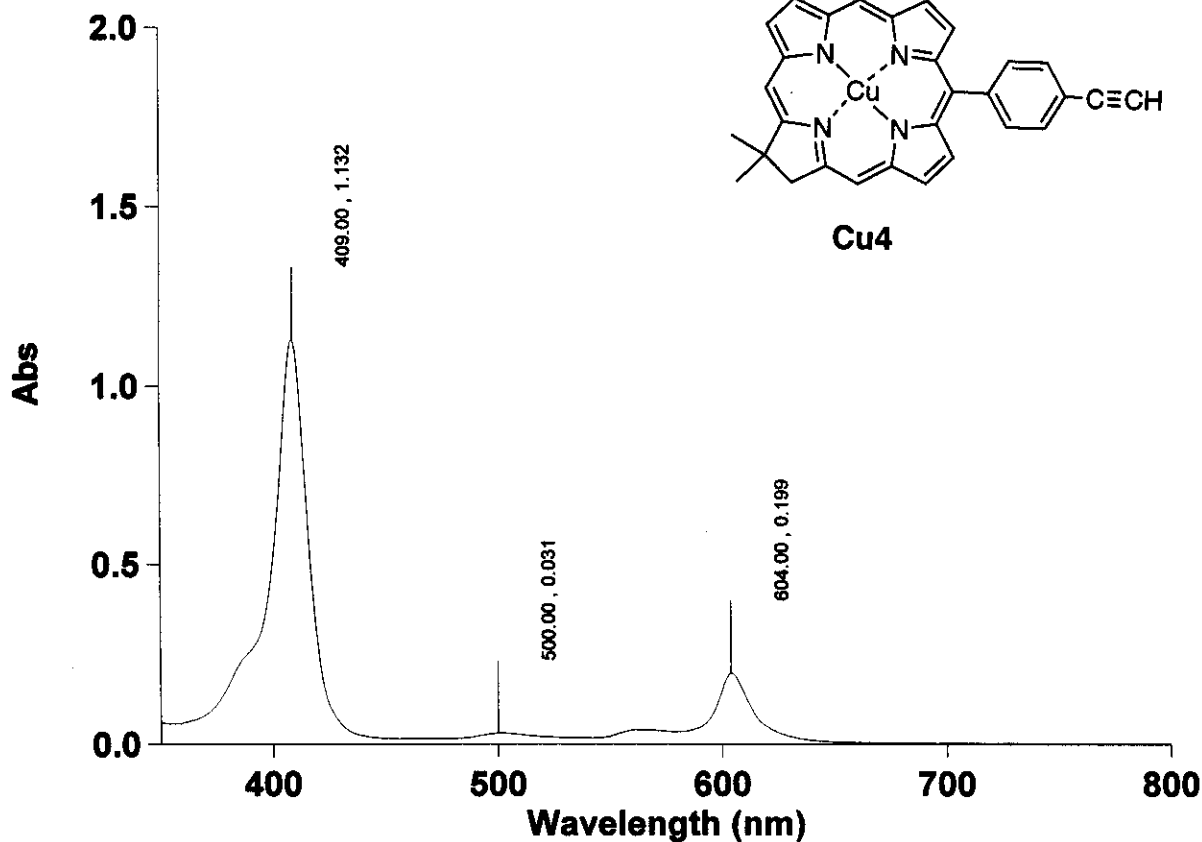




Cu4

INSTRUM TOP
OpId N. Srinivasan
SMPNAM 015491
AC_DATE Wed Jul 18 12:28:16 2001
ANALYST /data/chemistry/LINDSEY/TANIGUCHI
POLAR1 posCa/chemistry/LINDSEY/TANIGUCHI
ACQF_m Reflector
TD 40000
NGSHOTS 50
SNGNUM 0
SNGPTS1 0
SNGPTS2 0
SNGPTS3 0
DM 1.00 [ns]
DELAY 0 [ns]
Uls1 20.00 [kV]
Uls2 18.70 [kV]
Uref1 0.00 [kV]
Uref2 7.50 [kV]
Uens 10.00 [kV]
Ubeam 0.00 [kV]
RefPull 1.50 [kV]
UdetL 0.00 [kV]
UdetR 0.00 [kV]
Udef1 2.00 [kV]
REPH2 1.00 [Hz]
ATTEN 206712.93
ML1 333.982
ML2 0.000
ML3 0.000
HITURBO no
GDECN yes
GDELY short
EPCEN no
EPCND no
PLASND no
LANSND no
UIS2END no
DPCAL1 510.84
DPMAS 700.00 [Da]
REMOVAL 0.33
REPAIR 0.28
TSPRNDV 0.91
CMT1 Cu-Chl-CCH
CMT2 at 42,shots50

NCSU Chemistry
Instrument Serial Number 0051477



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

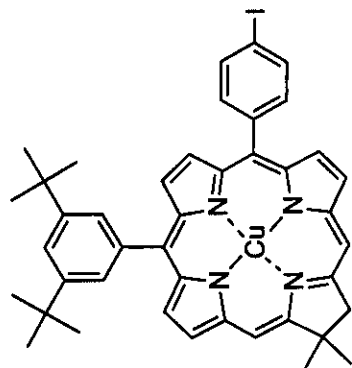
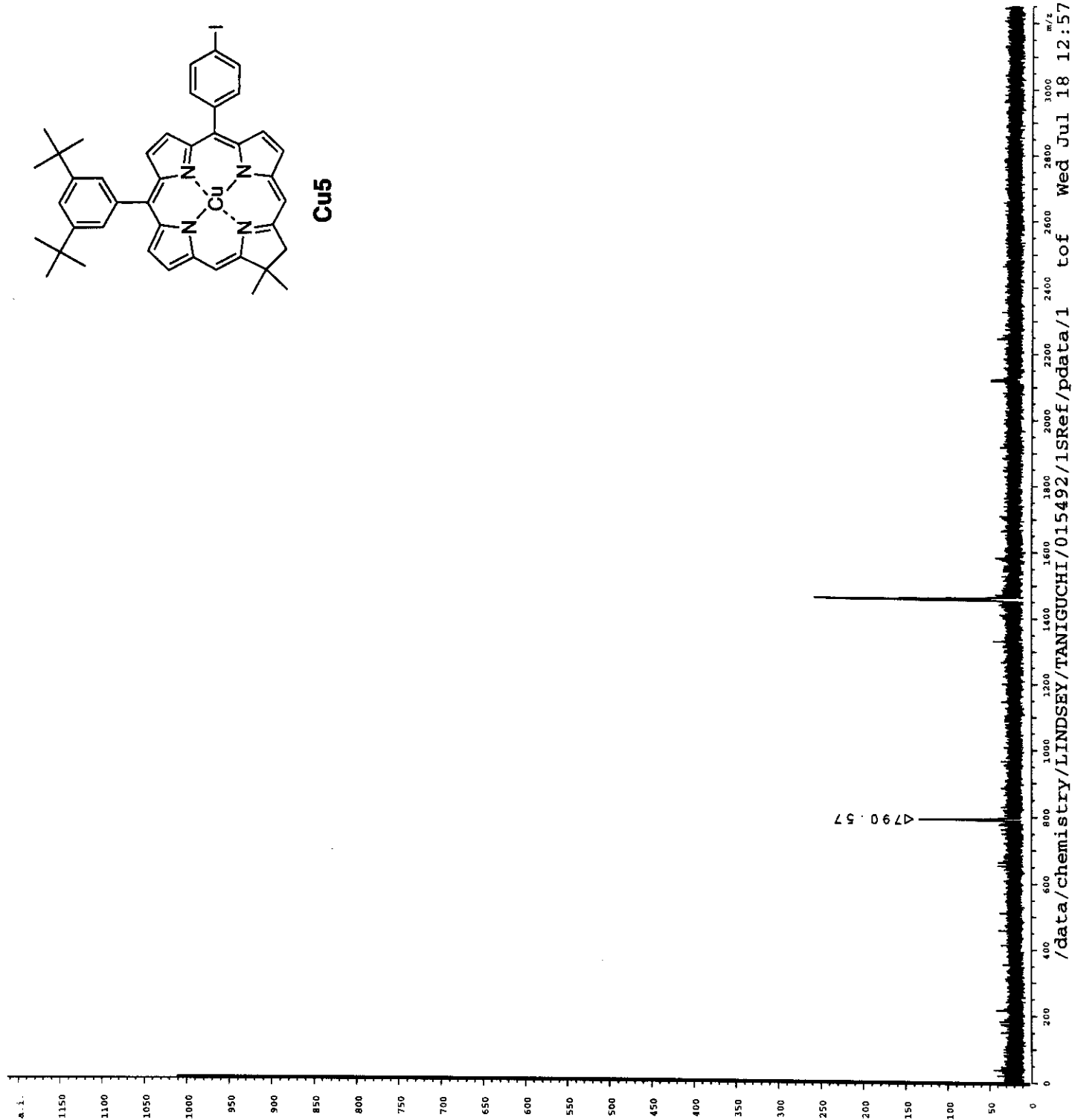
Scan Analysis Report

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

Sample Name: cu-chl-cch

Collection Time

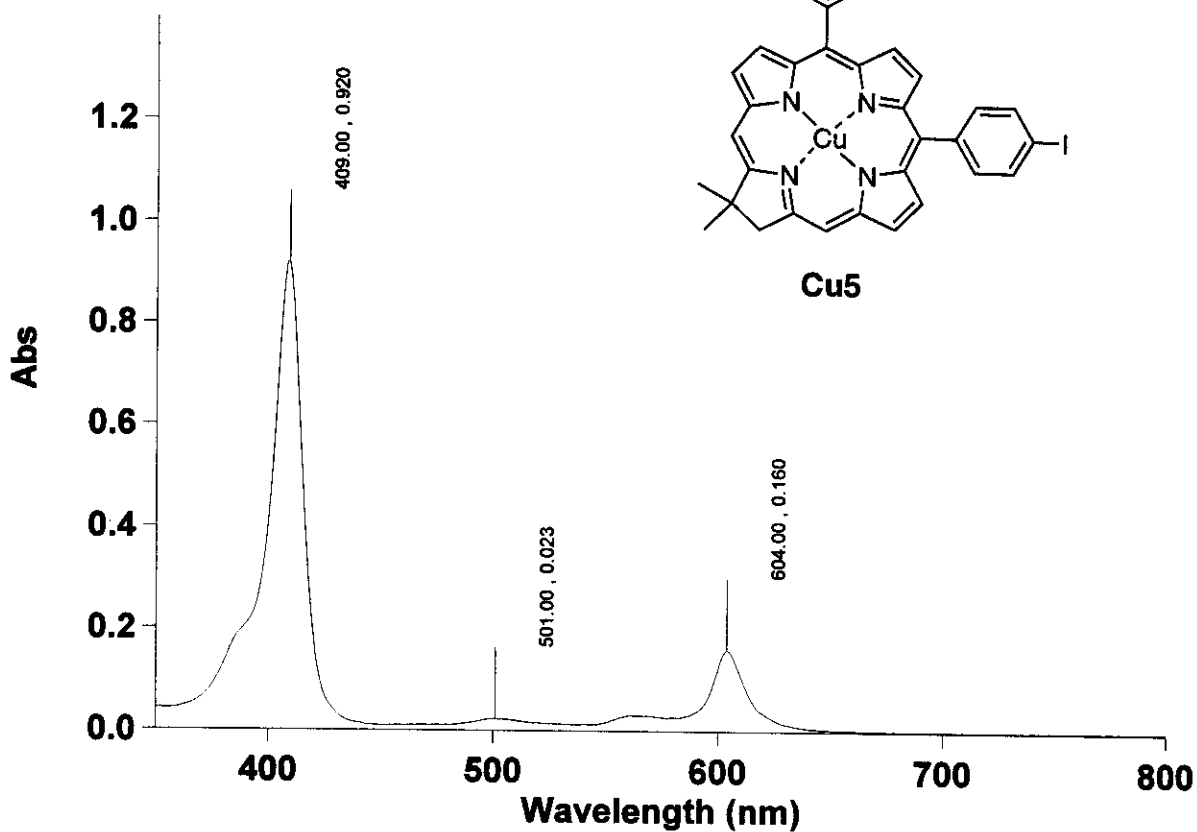
7/16/01 1:44:45 PM



Cu5

INSTRUM TOP
OpId N. Srinivasan
SEPNAM 015492
AC DATE Wed Jul 18 12:36:19 2001
DATA /data/chemistry/LINDSEY/TANIGUCHI
POLARI POS
AQOP_m Reflector
TD 40000
RGSHOTS 50
SMONUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DM 1.00 [ms]
DELAY 0 [ms]
Uis1 20.00 [kV]
Uis2 18.70 [kV]
Uref1 0.00 [kV]
Uis1as 7.00 [kV]
Uis2as 10.00 [kV]
RefPull 0.00 [kV]
UdetL 1.50 [kV]
UdetR 0.00 [kV]
Udef1 2.00 [kV]
REPHIZ 1.00 [Hz]
REFREN 43
ML1 2067125.593
ML2 333.582
ML3 0.000
HITREO no
GDEON yes
GDEULY short
REFREN no
RELAND no
RELAND no
UIS2END no
UIS2END no
DPCALI 510.84 [Da]
DPMALSS 700.00
RENDVAL 0.33
RENDVAL 0.33
IS2ENDV 0.91
CMT1 Cu-Chl-PhI
CMT2 att 43.shots50

NCSU Chemistry
Instrument Serial Number 0051477



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-chi-cch

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



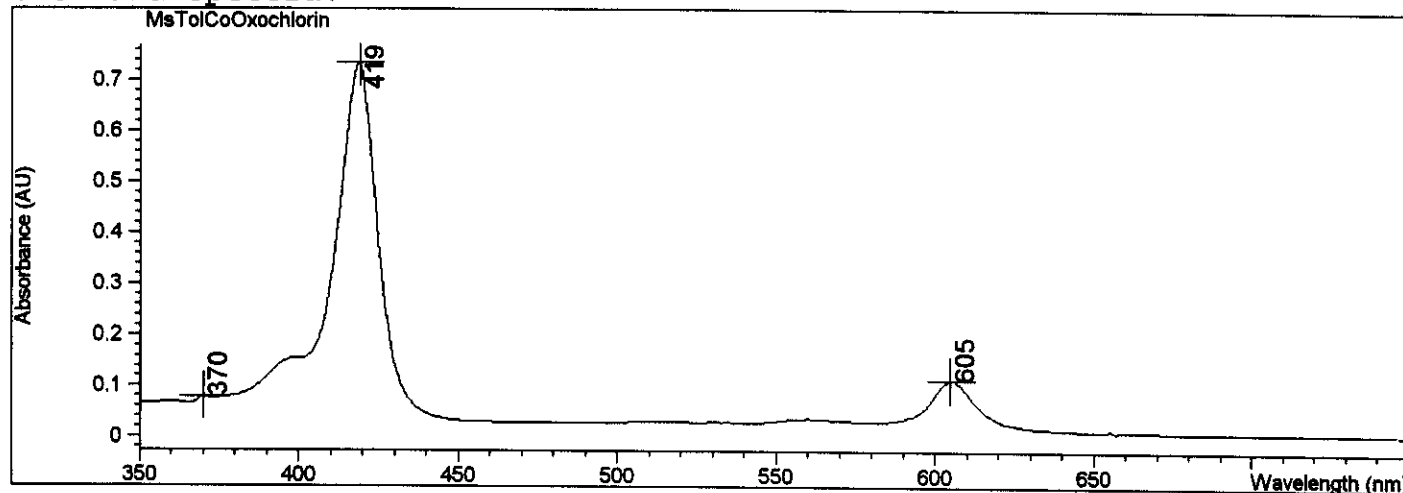
▷ 623,00

m/z	900	1000	1100	1200	1300
100					
200					
300					
400					
500					
600					
700					
800					
900					
1000					
1100					
1200					
1300					

200	300	400	500	600	700	800	900	1000	1100	1200	1300	m/z	
/data/chemistry/LINDSEY/PRATHAPAN/015548/1SRef/pdata/1												tof	Thu Jul 26 10:54:13 2001

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

Overlaid Spectra:

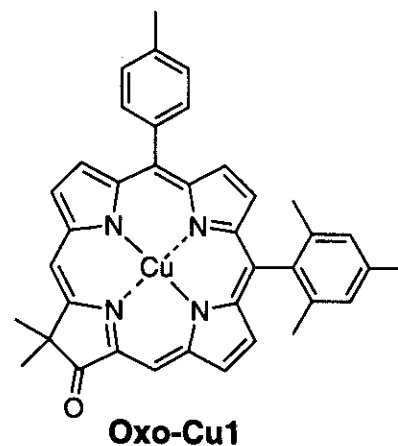


#	Name	Peaks (nm)	Abs (AU)
1	MsTolCoOxochlori	419.0	0.73345
1		605.0	0.11356
1		370.0	7.9889E-2

Report generated by :

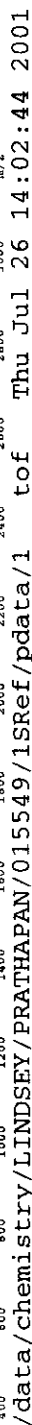
Signature:

*** End Spectrum/Peak Report ***



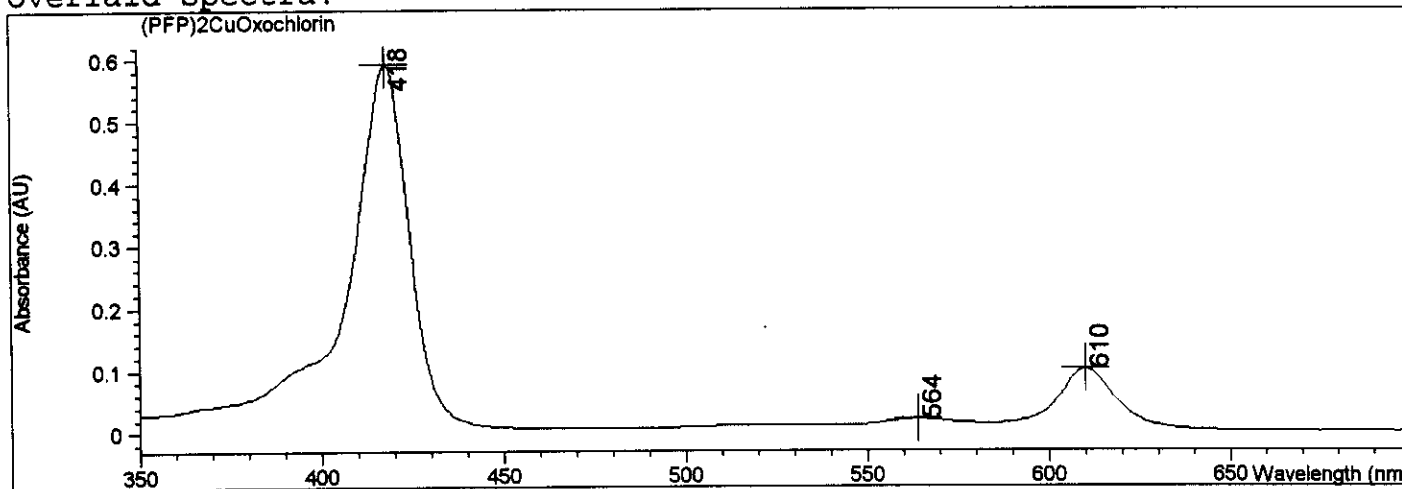


INSTRUM TOP		Unknown	
OPID	SNPMAN	015549	
ACQ_DATE	TUE JUL 26 14:01:33 2001		
PATN	/data/chemistry/LINDSEY/PRAITHIPAN		
EXPNO	1		
PROCNO	1		
ADQ_AOP	Reflector		
TD	40000		
NGSHOTS	100		
SNOBND	0		
SNOPTS1	0		
SNOPTS2	0		
SNOPTS3	0		
DW	1.00 [ms]		
DELAY	0 [ms]		
U1s1	20.00 [KV]		
U1s2	18.50 [KV]		
U1s3	17.00 [KV]		
U1s4	7.50 [KV]		
U1s5	10.00 [KV]		
U1smax	10.00 [KV]		
U1sfull	0.00 [KV]		
U1sbetcl	1.55 [KV]		
U1sbetcr	9.00 [KV]		
U1sbetphz	9.00 [KV]		
BREPHZ	1.00 [Hz]		
ATTEN	40.0		
MU1	2067510.748		
MU2	353.368		
NUC	0.000		
HITRNG	no		
GDRON	yes		
CORFLY	short		
DEFTUN	no		
RANSRD	no		
UIESRD	no		
UPKCAL1		510.84	
DPMSAS		200.00 [Ds]	
RETRVAL		0.33	
LENDVAL		0.28	
SCAND		0.000	
PPF2CHOCORLIN			
attn_40_shots	100		
CMT1			



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

Overlaid Spectra:

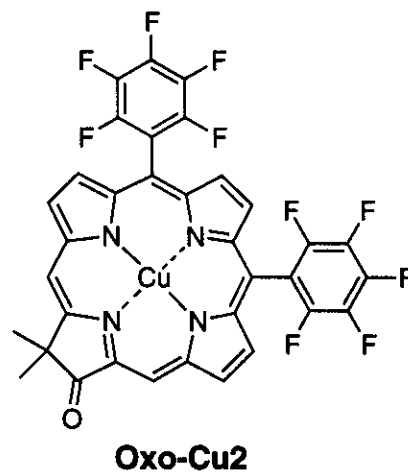


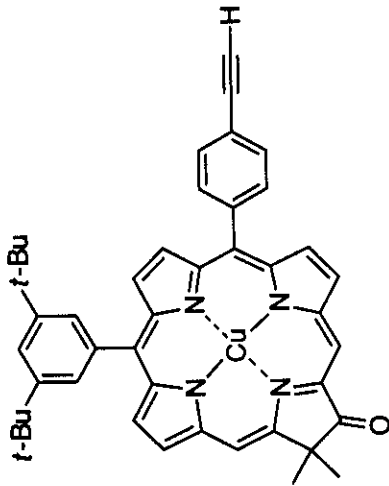
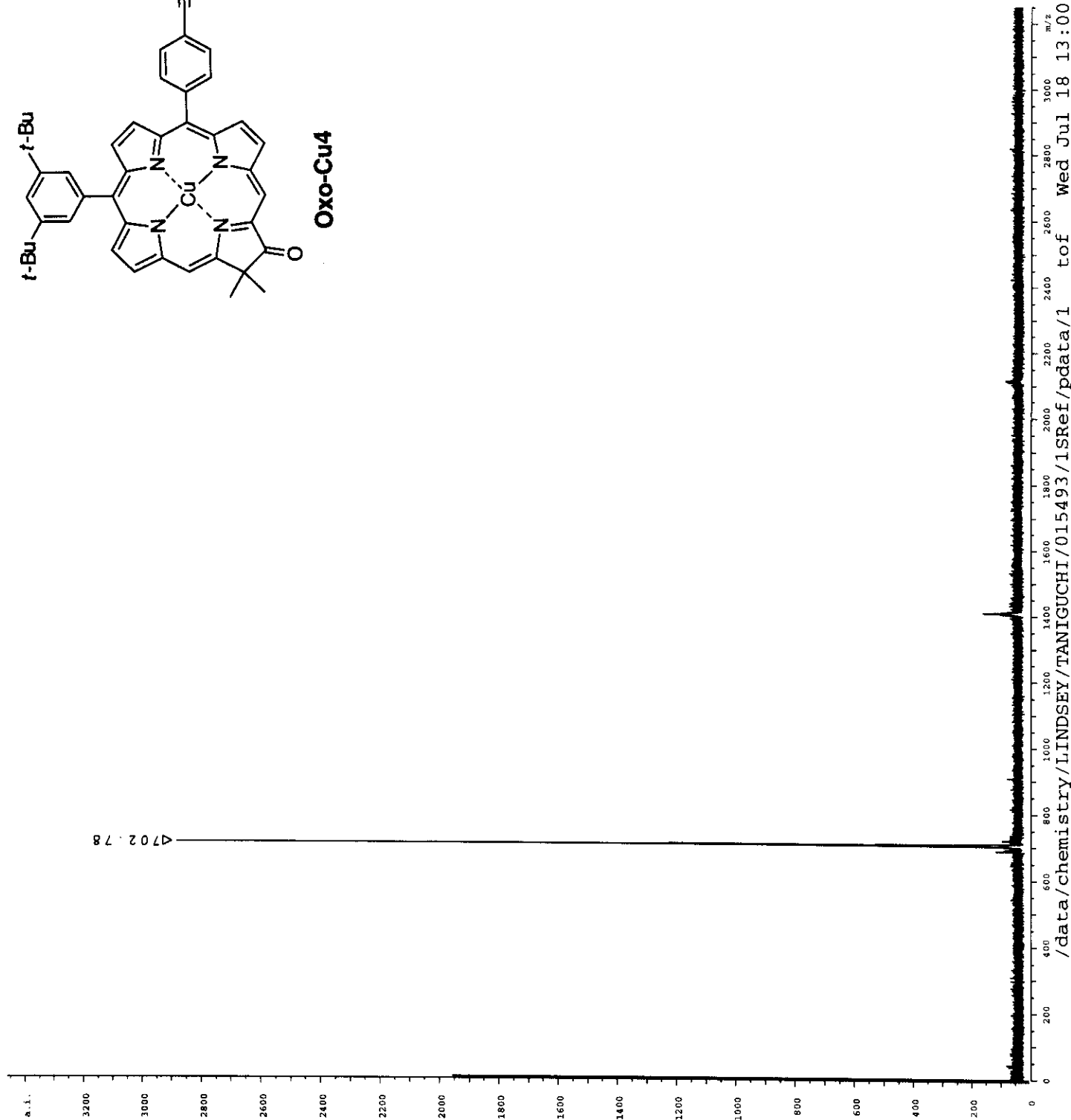
#	Name	Peaks (nm)	Abs (AU)
1	(PFP)2CuOxochlor	418.0	0.59165
1		610.0	0.10066
1		564.0	2.0638E-2

Report generated by :

Signature:

*** End Spectrum/Peak Report ***



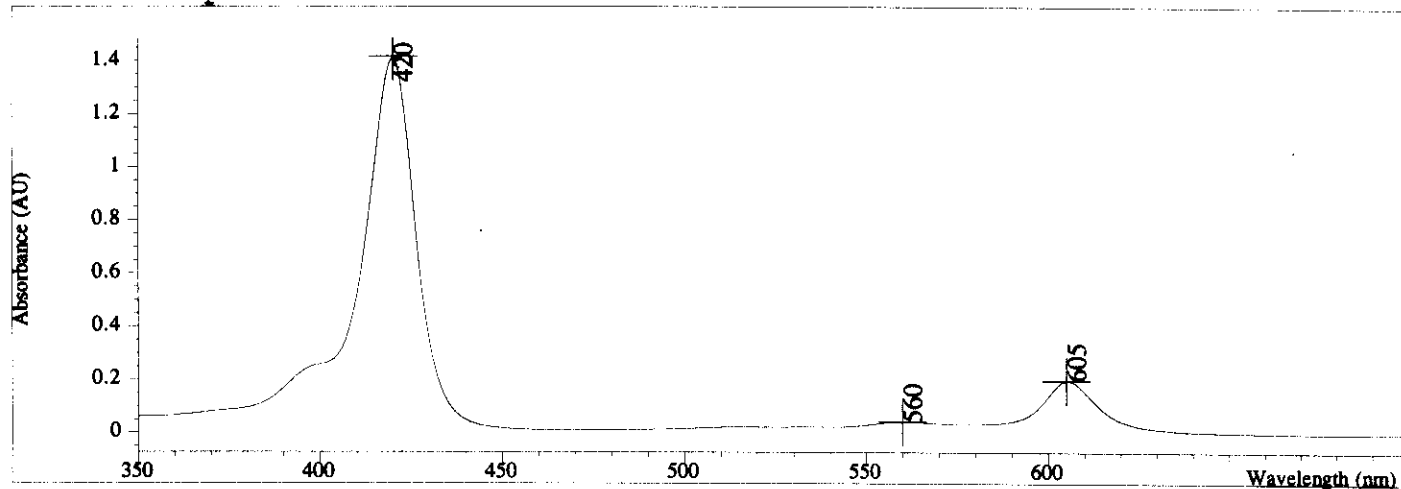


Oxo-Cu4

INSTRUM TOP
 OpId N. Srinivasan
 SKPM 015493
 DATE 18 Jul 18 12:39:45 2001
 PATH /data/chemistry/LINDSEY/TANIGUCHI
 POLARI POS /data/chemistry/LINDSEY/TANIGUCHI
 AQOP_m Reflector
 TD 40000
 NSHOTS 100
 SHOTNO 0
 SMOPT32 0
 SMOPT33 0
 DM 1.00 [ns]
 DELAY 0 [ns]
 Uls1 20.00 [KV]
 Uls2 18.70 [KV]
 Uls3 18.70 [KV]
 Uls4 7.50 [KV]
 Uls5 10.00 [KV]
 Uls6 10.00 [KV]
 Uls7 1.50 [KV]
 Uls8 0.00 [KV]
 Uls9 0.00 [KV]
 Uls10 2.00 [KV]
 Uls11 2.00 [KV]
 Uls12 4.00 [KV]
 Uls13 4.00 [KV]
 Uls14 2067125.193
 ML1 333.982
 ML2 0.000
 ML3 0.000
 HITURBO no
 GDSN yes
 GDSN1 short
 GDSN2 short
 DEFLON no
 ELANDND no
 ELANDND no
 ULS2END no
 ULS2END no
 DPICALI 510.84 [Da]
 DPICALI 700.00 [Da]
 DPICALI 0.31
 DPICALI 0.28
 DPICALI 0.91
 CWT1 CU-OXO-CCH
 CWT2 att 46.shots100

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

Overlaid Spectra:

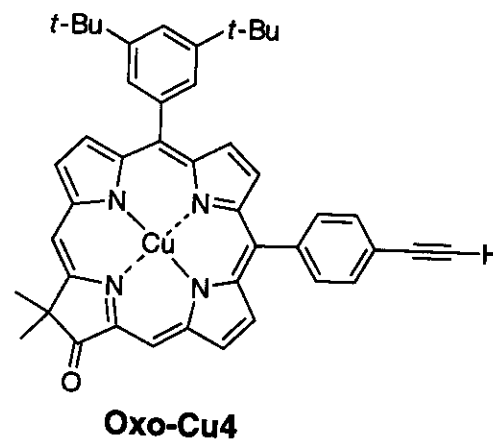


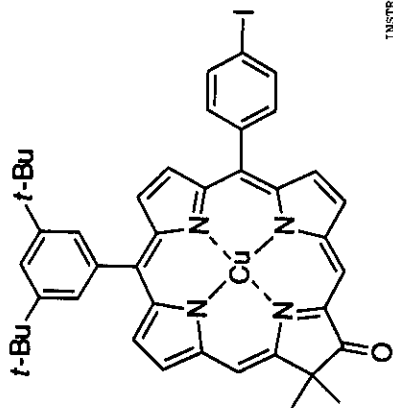
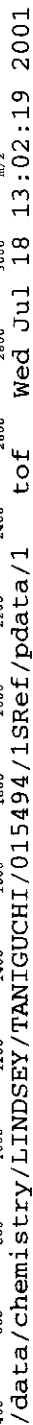
#	Name	Peaks (nm)	Abs (AU)
1		420.0	1.41610
1		605.0	0.19806
1		560.0	4.2498E-2

Report generated by :

Signature:

*** End Spectrum/Peak Report ***



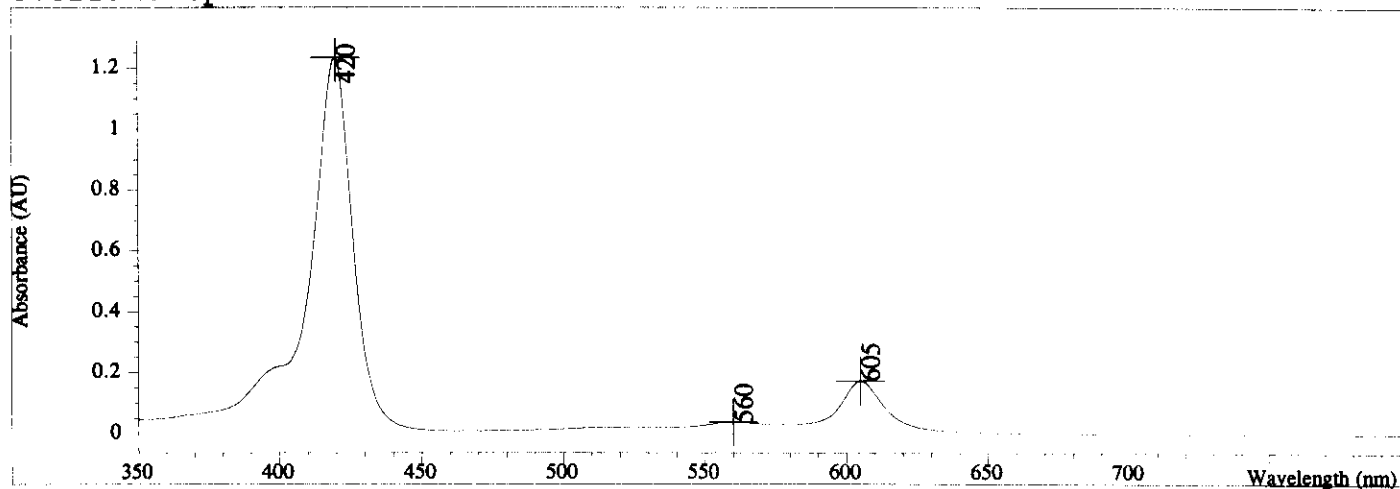


Oxo-Cu5

```
INSTRUM TOP      INSTRUM TOP
Opid   N_Srinivasan
SKNPNR    015494
ACQDATE Wed Jul 18 12:47:55 2001
DATA PATH /data/chemistry/LINOSSE/TANIGUCHI
FOR       Reflector
RGDGM     4000
TD         150
NSHOT5    0
SHOTS1    0
SNOUTS1   0
SNOUTS2   0
SNOUTS3   0
          0
          0
          1.00 [ms]
          0 [ms]
DELAY      20.00 [kV]
U1s1       18.70 [kV]
U1s2       18.70 [kV]
U1s3       7.50 [kV]
U1s4       7.50 [kV]
UHmass     10.00 [kV]
KohMass    10.00 [kV]
tubedelt   1.50 [kV]
tubetemp   0.00 [kV]
tubepress  0.00 [kV]
REPZ       1.00 [Hz]
ATTEN      44.0
          2067125.193
M.C1       333.982
M.L2       0.000
HITURBO no
HIDRON yes
DECELLEN short
CELELY no
KLASND no
KLASND no
KLASND no
KLASBMD no
OPPCAL1    510.84
REMOVAL    700.00 [Da]
REMOVAL    0.33
REMOVAL    0.28
REMOVAL    0.01
CUT1       31.4
Cu-OXO-Phi Cu-OXO-Phi
CMT2       44 shot=100
```

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

Overlaid Spectra:

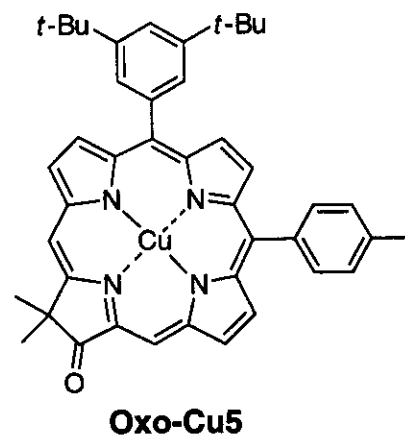


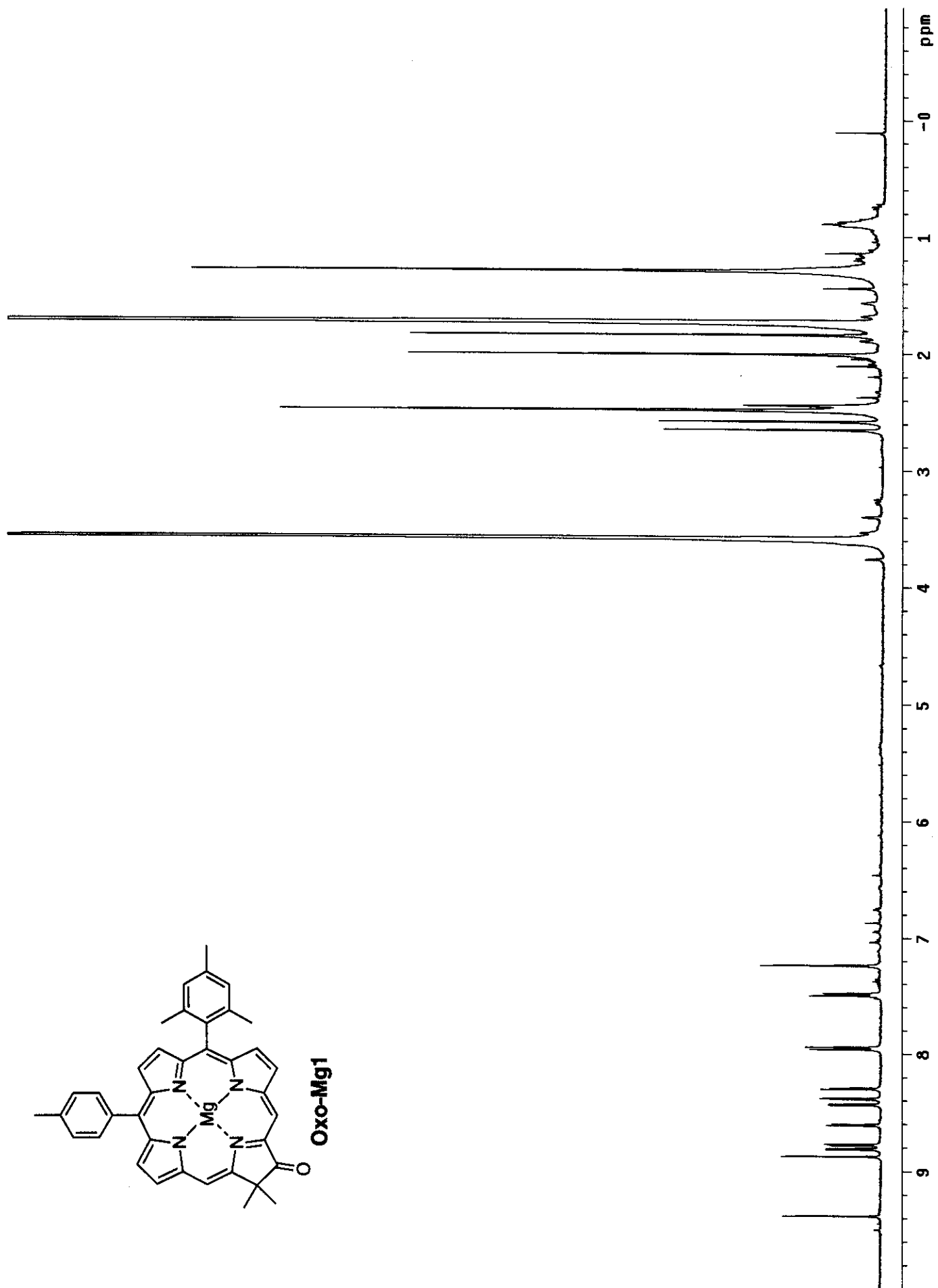
#	Name	Peaks (nm)	Abs (AU)
1		420.0	1.23490
1		605.0	0.17264
1		560.0	3.7736E-2

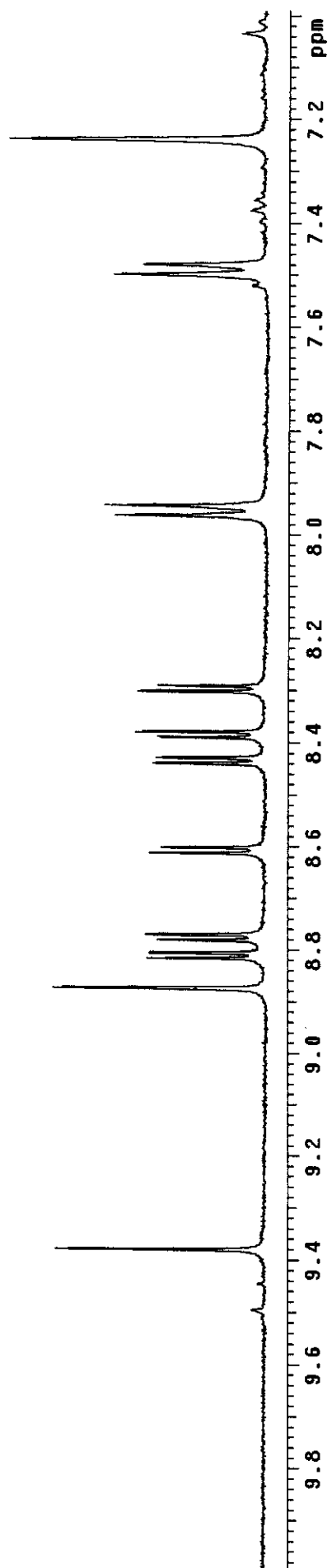
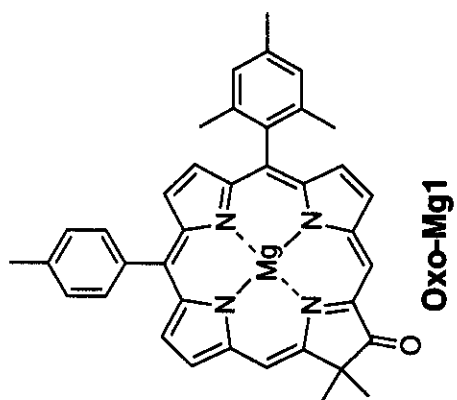
Report generated by :

Signature:

*** End Spectrum/Peak Report ***





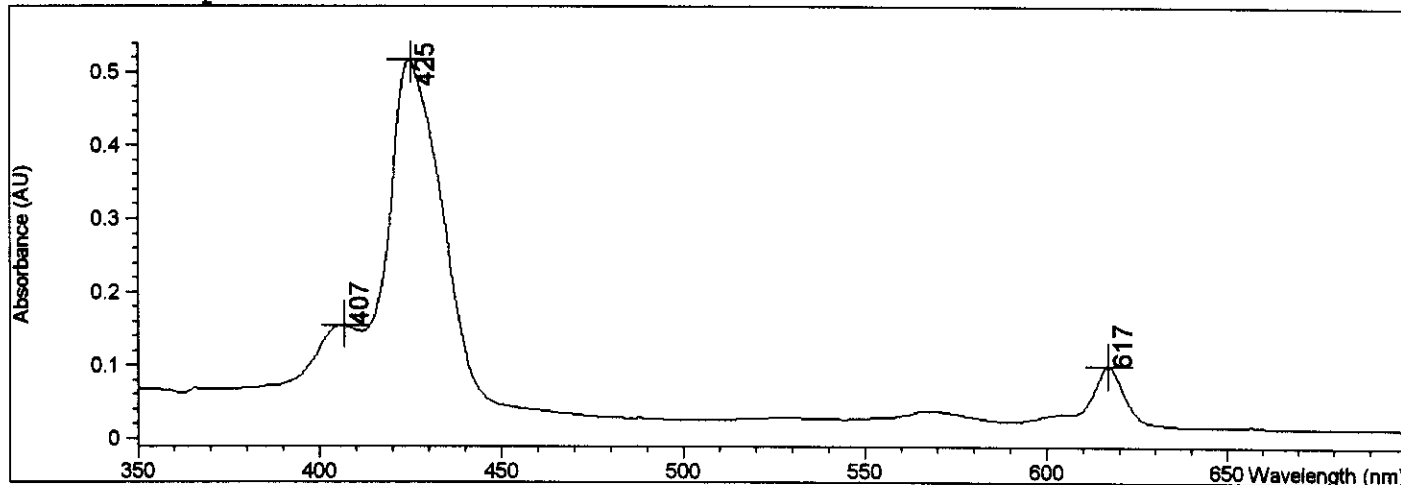




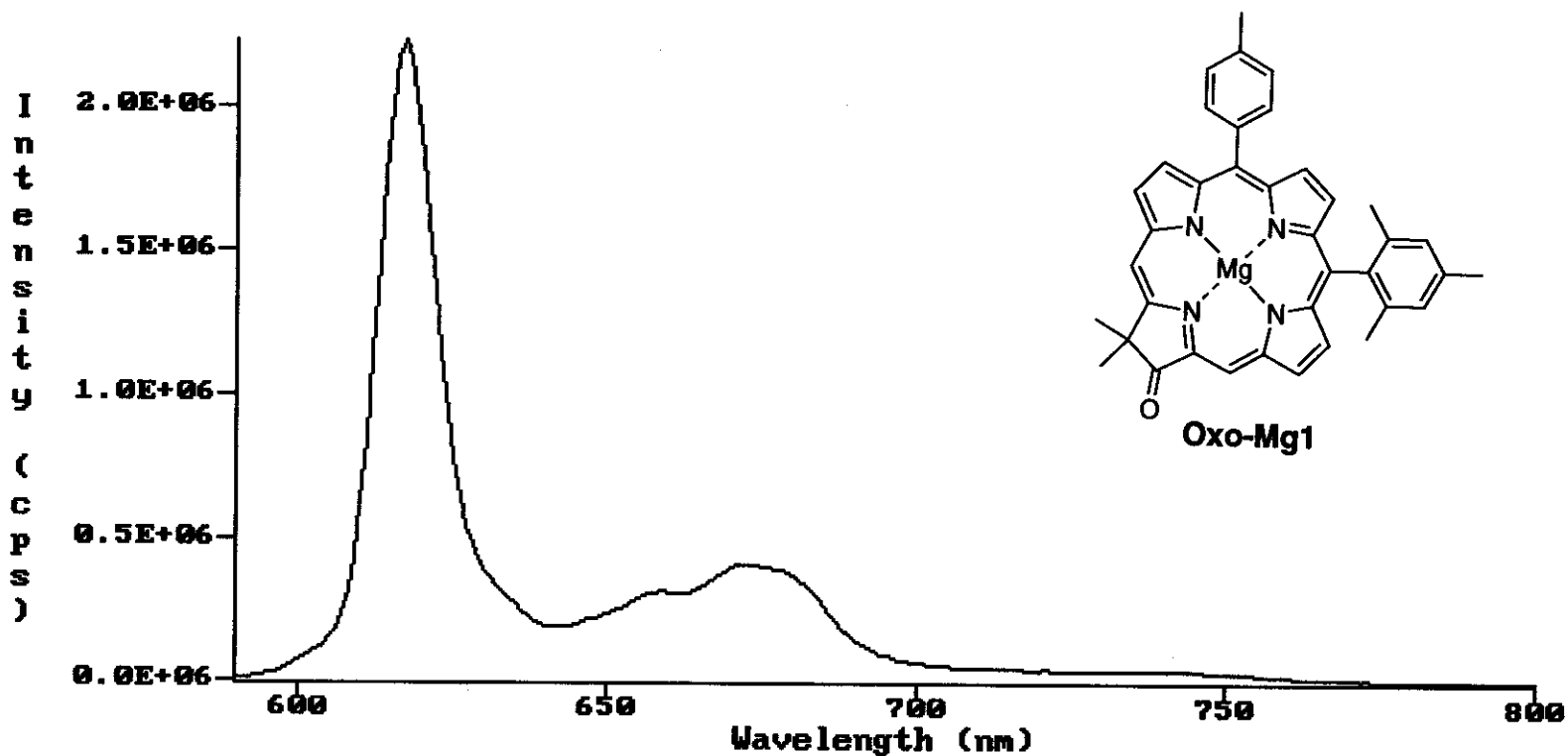
INSTRUM TOP
 OPERM N. Srinivasan
 DATE 020181
 POLDATE 7 15:53:36 2002
 PATH /data/chemistry/LINDSEY/TANIGUCHI
 POLARI POS
 AOPF_m Reflector
 TD 50000
 NGSHOTS 50
 MAGN 0
 SNOPTS1 0
 SNOPTS2 0
 SNOPTS3 0
 DM 1.00 [ns]
 DELAY 0 [ns]
 U1a1 20.00 [KV]
 U1a2 18.70 [KV]
 U1a3 0.00 [KV]
 U1a4 7.50 [KV]
 U1a5 10.00 [KV]
 U1a6 0.00 [KV]
 RefFull 1.50 [KV]
 UdetL 0.00 [KV]
 UdetR 0.00 [KV]
 UdetL 2.00 [KV]
 UdetR 2.00 [KV]
 ATTEN 56.0
 ML1 2067125.193
 ML2 333.982
 ML3 0.000
 HITURBO no
 GDEON yes
 GDEON short
 DIEZON no
 PLASBND no
 LANSBND no
 U1S2BND no
 DPCAL1 510.84 [Da]
 DPMAS1 700.00 [Da]
 FWHM1 0.31
 FWHM2 0.28
 FWHM3 0.91
 IS2BNDV
 CMT1 Oxo-Mg-1b
 CMT2 Att=56, shots = 50

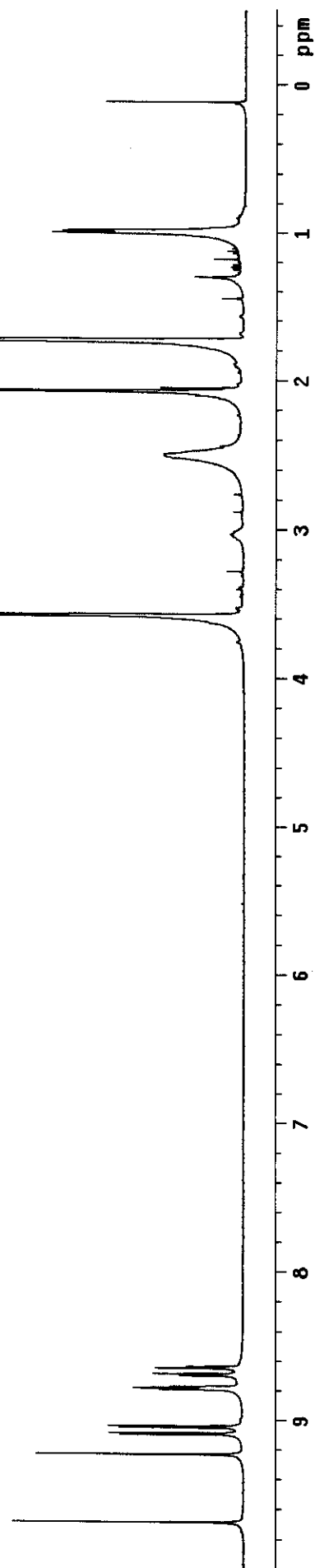
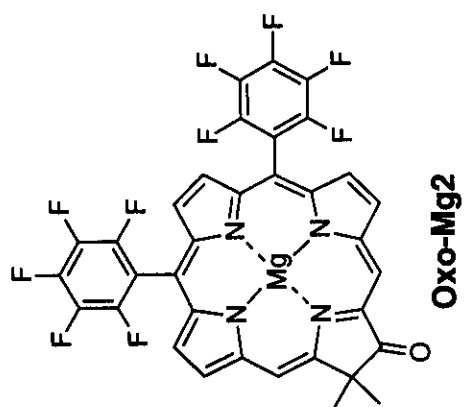
Method file : <untitled>
 Information : Default Method
 Data File : C:\RSLSP\1\04220103.SD Created : 4/22/01
 18:10:37

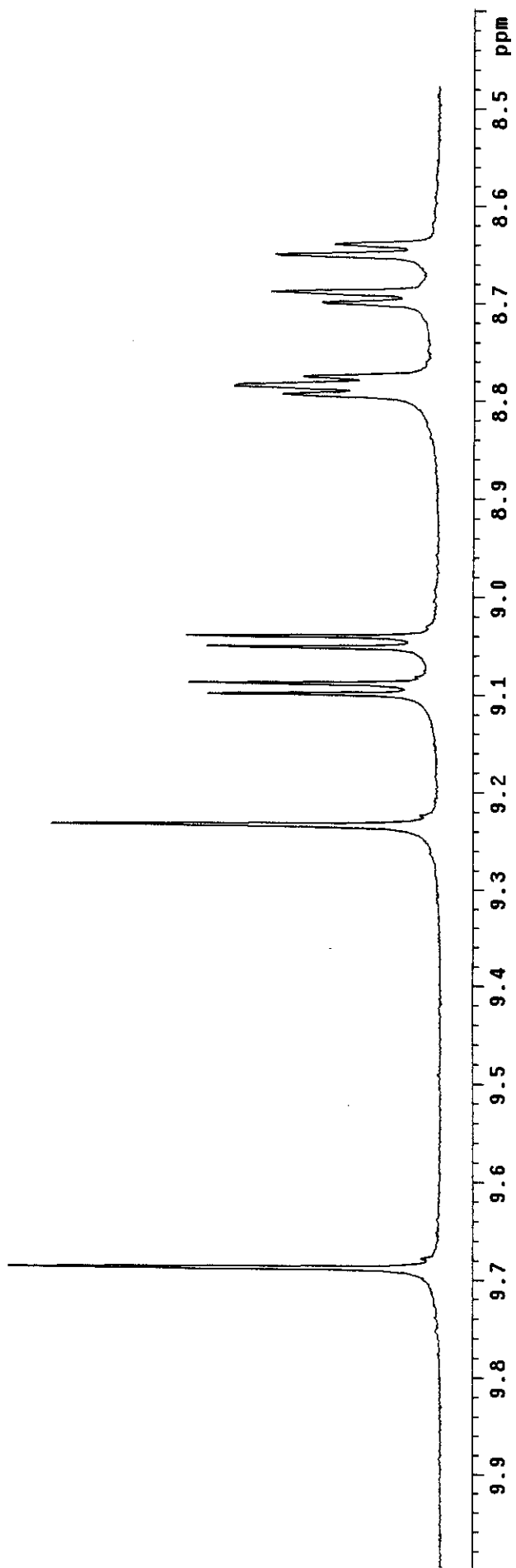
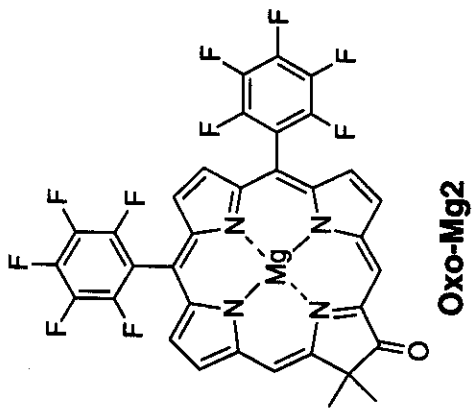
Overlaid Spectra:

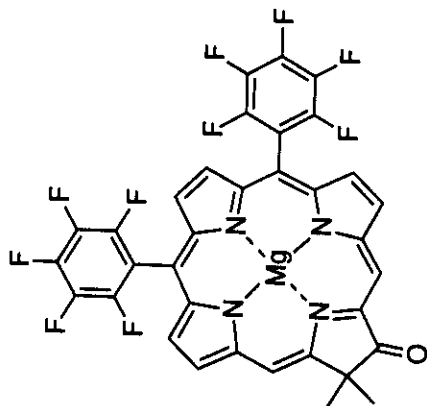


#	Name	Peaks (nm)	Abs (AU)
1	Mes-Tol-Mg-Oxo	425.0	0.51621
1		407.0	0.15494
1		617.0	9.9904E-2

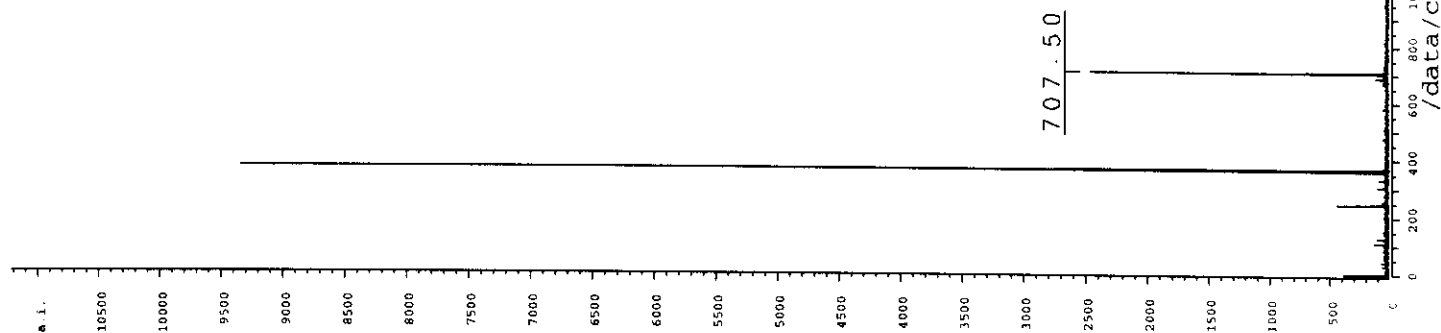








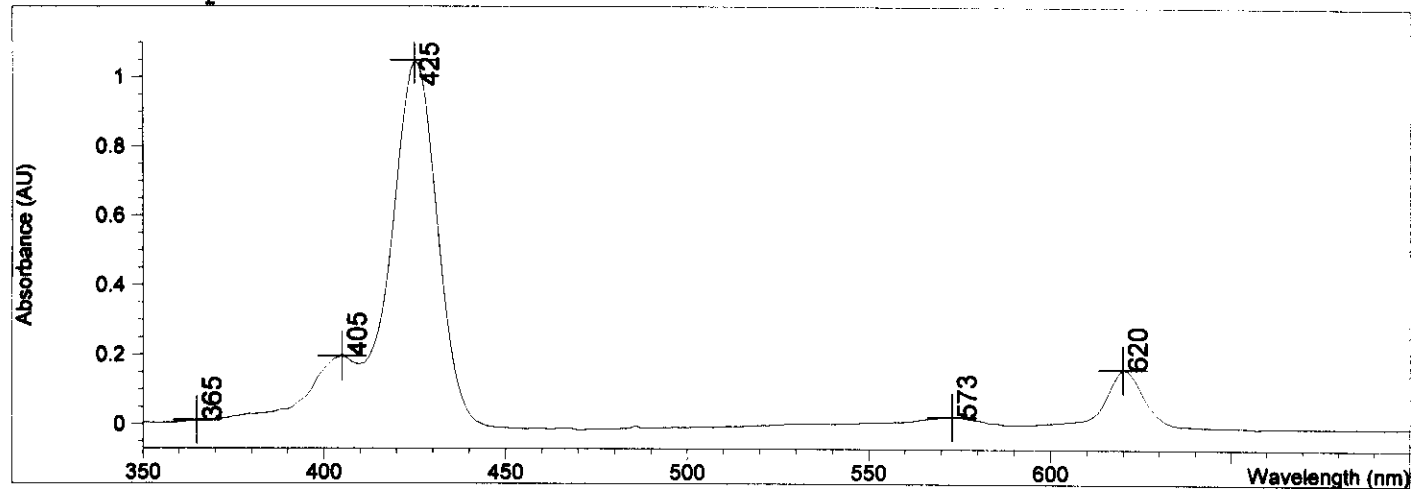
Oxo-Mg2



INSTRUM TOP
OpId N. Stinivasan
SRNAM 020180
ANALYTE Thu Mar 7 15:52:03 2002
PATH /data/chemistry/LINDSEY/TANIGUCHI
POLARI POS
ACQ m Reflector
TD 50000
NO SHOTS 50
SNOBOM 0
SNOBPS1 0
SNOBPS2 0
SNOBPS3 0
DM 1.00 [ns]
DELAY 0 [ns]
U1s1 20.00 [KV]
U1s2 18.70 [KV]
U1s3 0.00 [KV]
U1s4 7.50 [KV]
U1s5 10.00 [KV]
U1s6 0.00 [KV]
RefFull 1.50 [KV]
UdetL 0.00 [KV]
UdetR 2.00 [KV]
U1s7 1.00 [KV]
U1s8 1.00 [Hz]
ML1 2067125.193
ML2 333.982
ML3 0.000
HITURBO no
CHRON yes
CHRON short
CHRON no
CHRON no
CLASSNO no
CLASSNO no
CLASSNO no
U1S2END no
U1S2END no
DPCALI 510.84
DPMASS 700.00 [Da]
FINDVAL 0.13
FINDVAL 0.23
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

