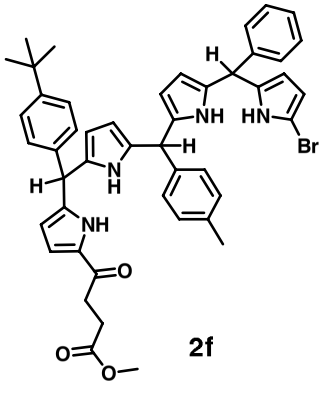
Supporting Information for:

Investigation of the Scope of a New Route to ABCD-Bilanes and ABCD-Porphyrins

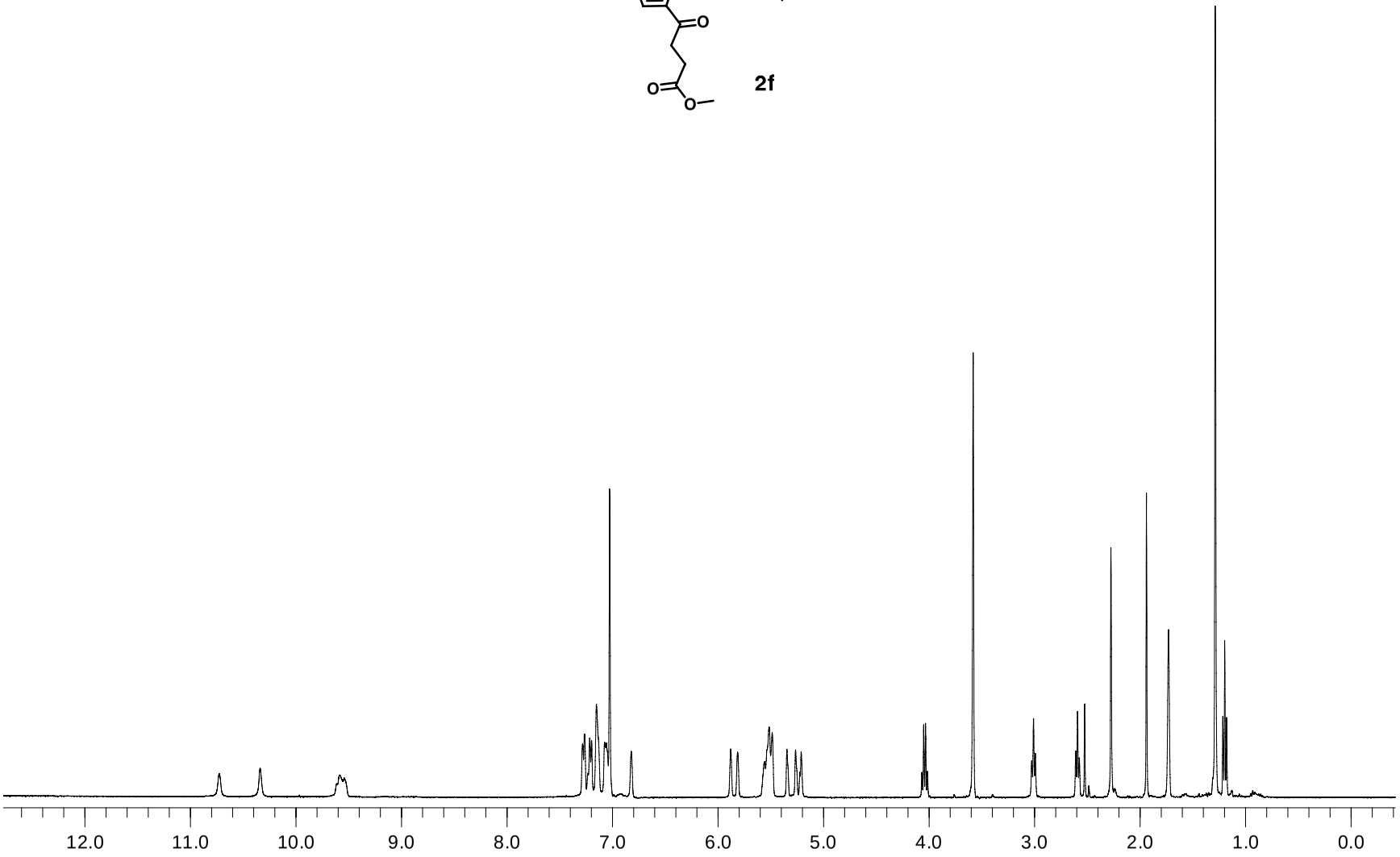
Dilek Kiper Dogutan and Jonathan S. Lindsey

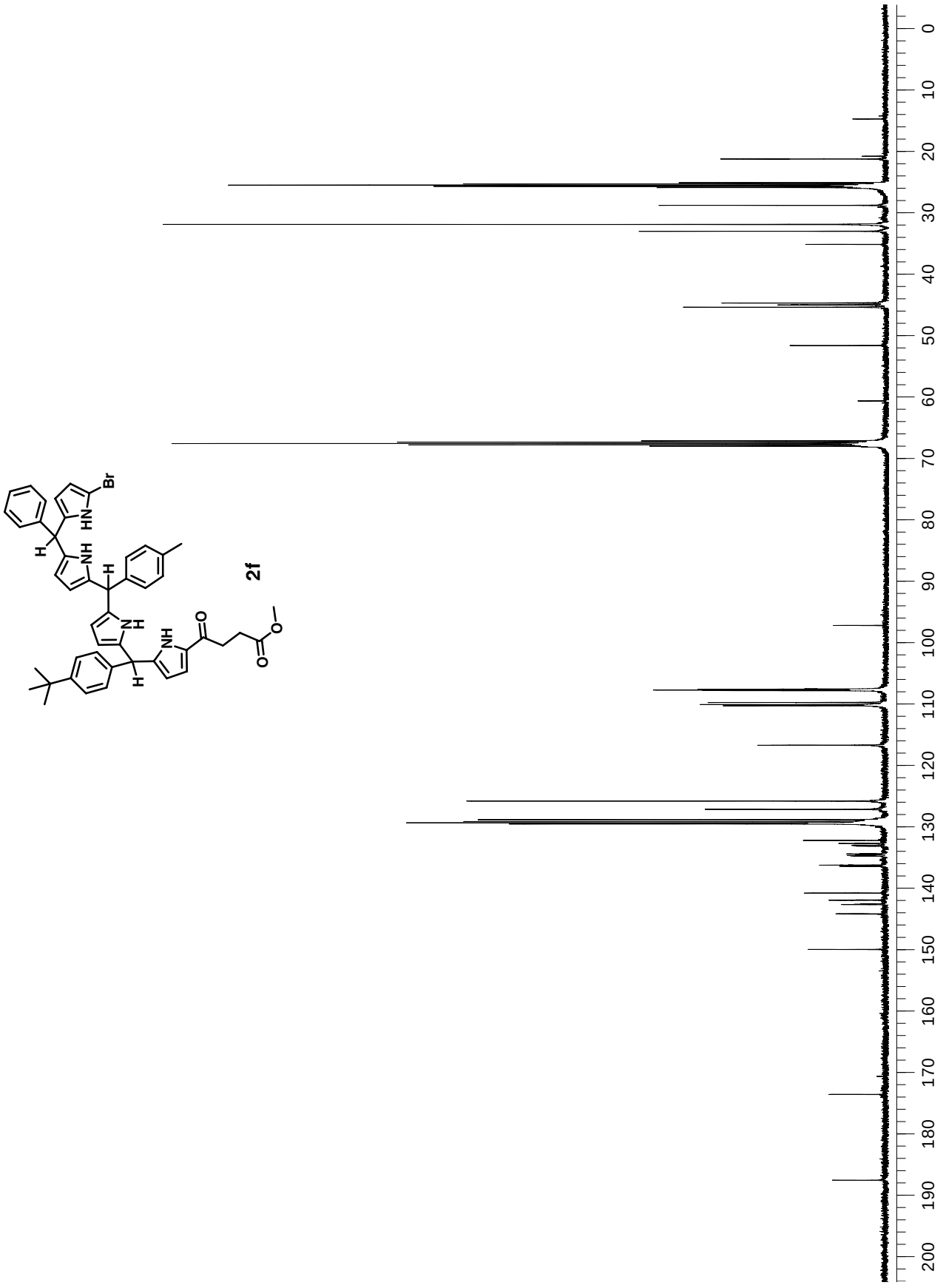
Table of Contents (Section 4)

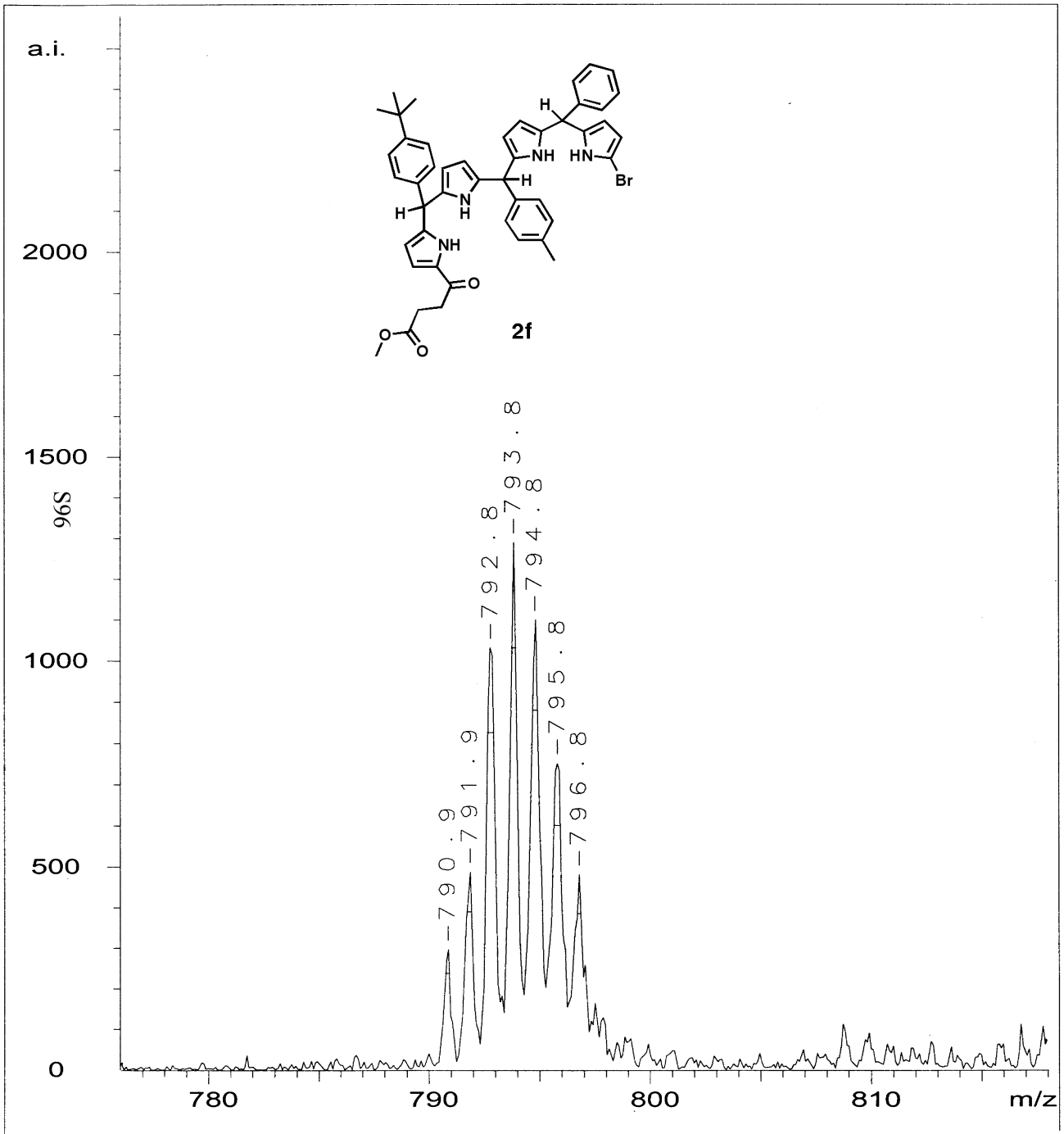
I.	Cover page	S93
II.	Spectral data for new compounds **2f-h**, **12a-f**, **MgP-1b-e**, and **MgP-2b**	S94-S132



2f

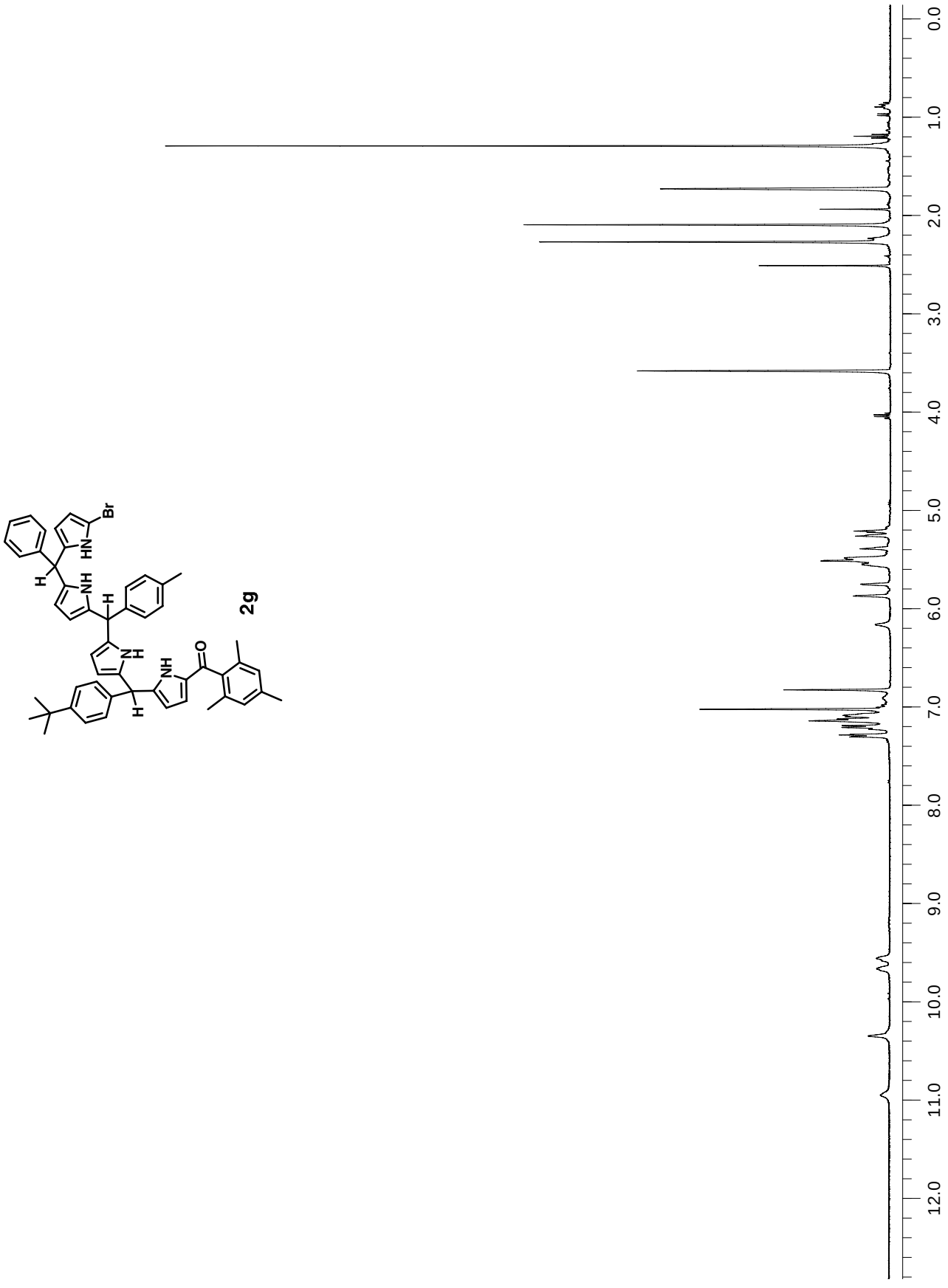


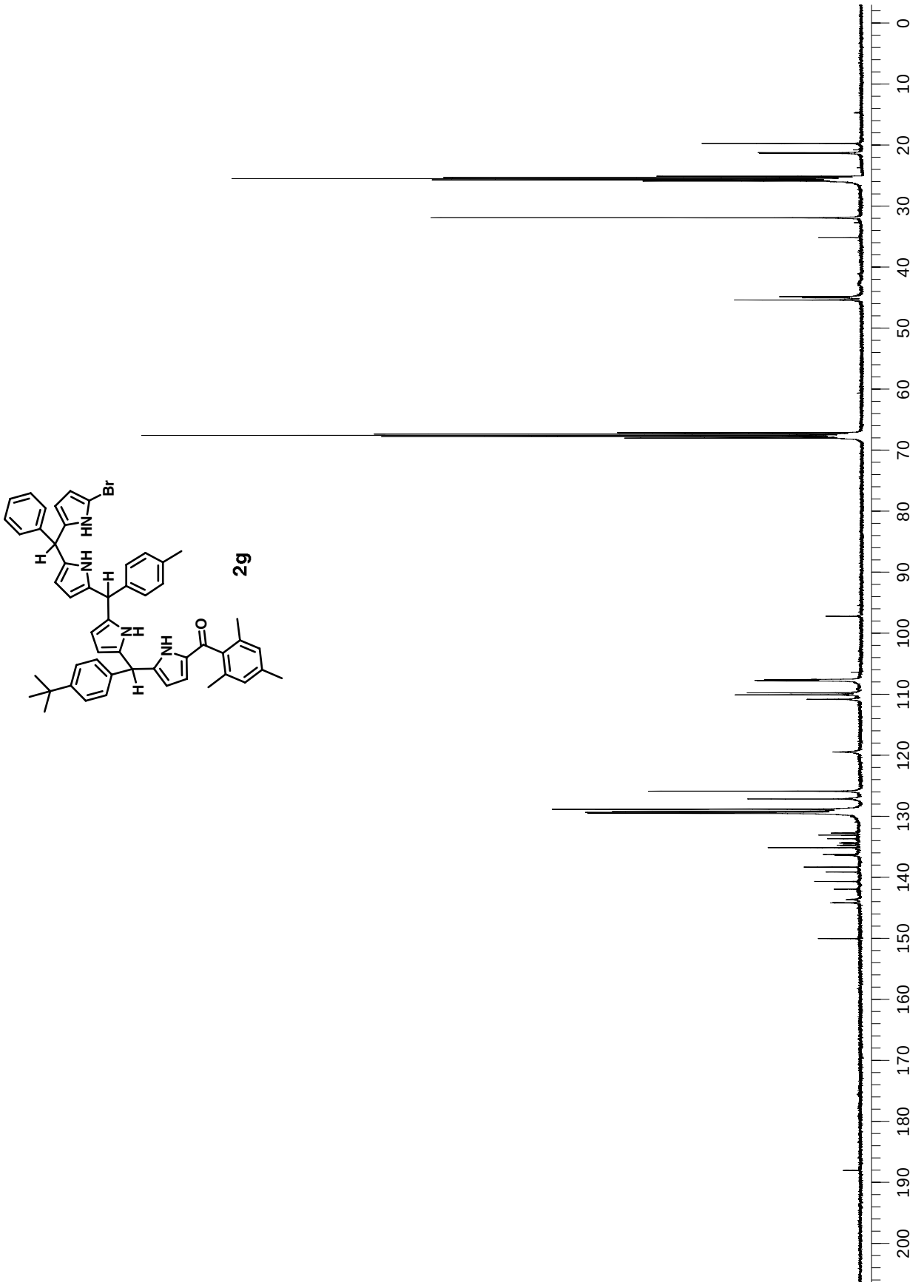

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H
H
N
H
NH
O
O
O
2f
0
10
20
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150
160
170
180
190
200

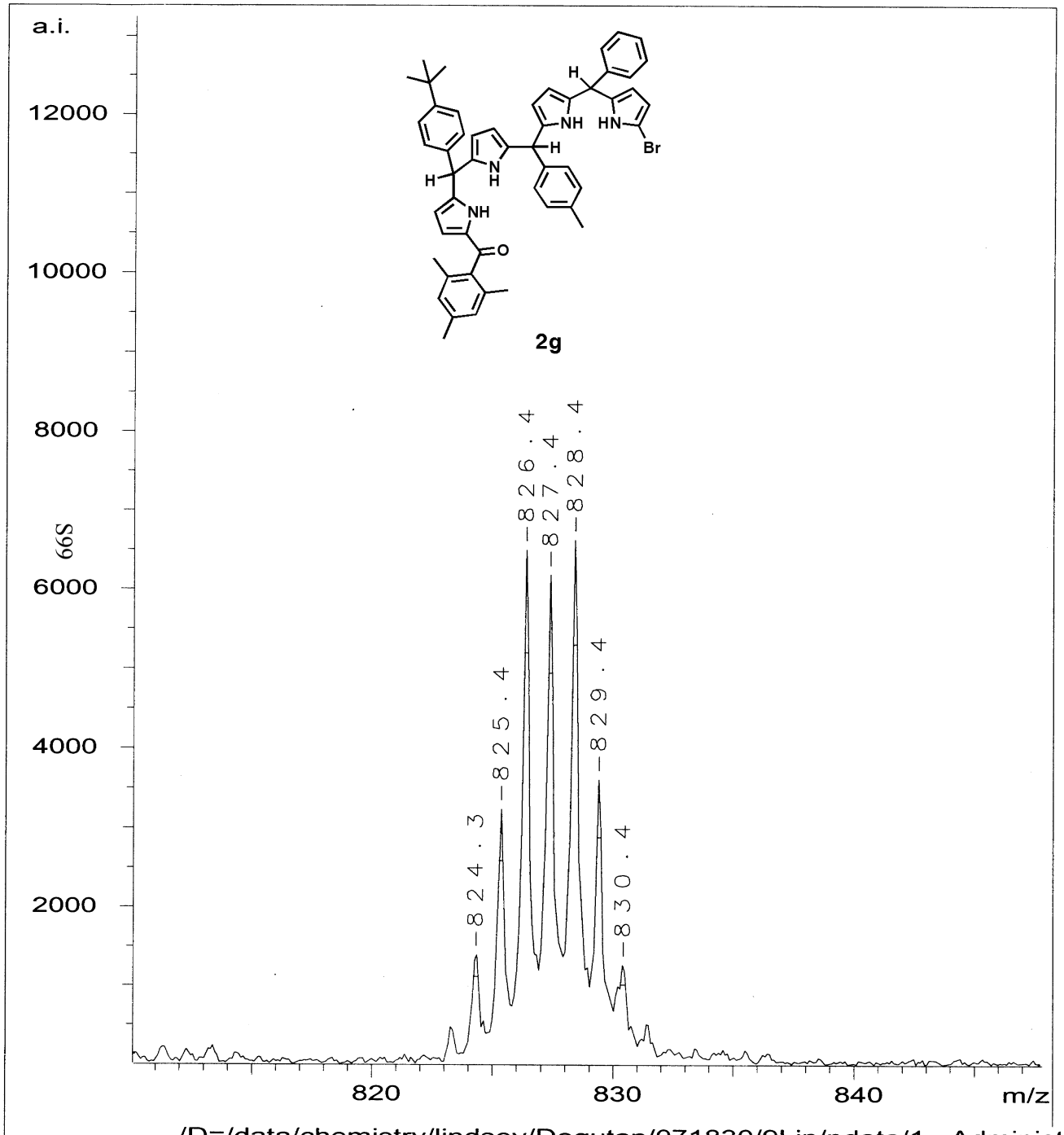


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TD 23334
NoSHOTS 200
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SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 5184 [ns]
Uis1 19.00 [kV]
Uis2 17.50 [kV]
Urefl 0.00 [kV]
Ulens 9.70 [kV]
Uhimass 0.00 [kV]
RefFull 0.00 [kV]
UdetL 1.62 [kV]
UdetR 0.00 [kV]
Udefl 0.00 [kV]
REPHZ 3.00 [Hz]
ATTEN 34.0
ML1 2514172.733
ML2 317.834
ML3 0.000
HITURBO no
GDEON yes
GDEDLY short
DEFLON no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 0.38
DPMASS 1000.00 [Da]
RBNDVAL 0.00
LBNDVAL 0.00
IS2BNDV 0.00
CMT1 EXP382 20ester bilane
CMT2

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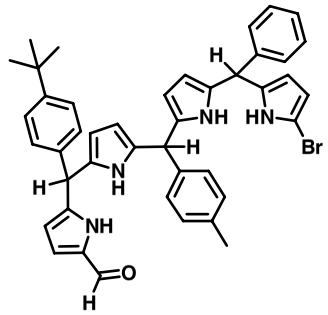

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H
H
N
H
NH
O
H
2g
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1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0


Br
HN
NH
H
H
NH
NH
O
2g
0
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130
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180
190
200

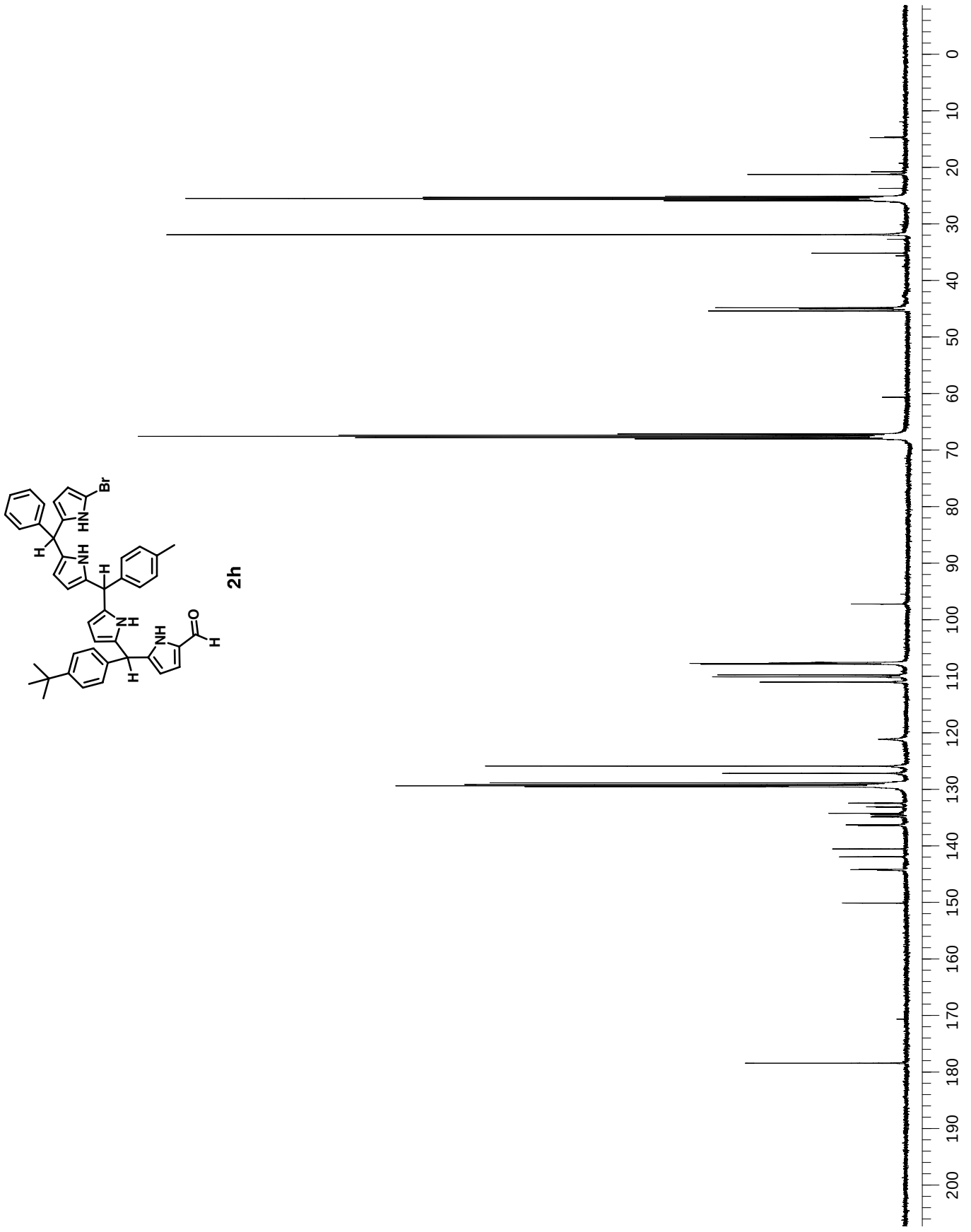


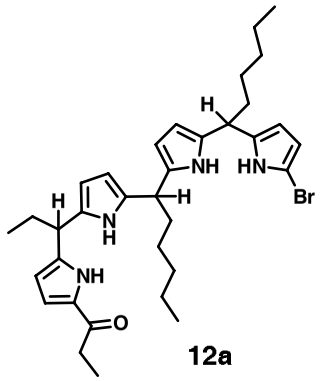
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TD 23334
NoSHOTS 200
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SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 5184 [ns]
Uis1 19.00 [kV]
Uis2 17.50 [kV]
Urefl 0.00 [kV]
Ulens 9.70 [kV]
Uhimass 0.00 [kV]
RefFull 0.00 [kV]
UdetL 1.62 [kV]
UdetR 0.00 [kV]
Udefl 0.00 [kV]
REPHZ 3.00 [Hz]
ATTEN 10.0
ML1 2513554.247
ML2 314.237
ML3 0.000
HITURBO no
GDEON yes
GDEDLY short
DEFLON no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 0.38
DPMASS 1000.00 [Da]
RBNDVAL 0.00
LBNDVAL 0.00
IS2BNDV 0.00
CMT1 EXP390
CMT2 20mesitylbilane

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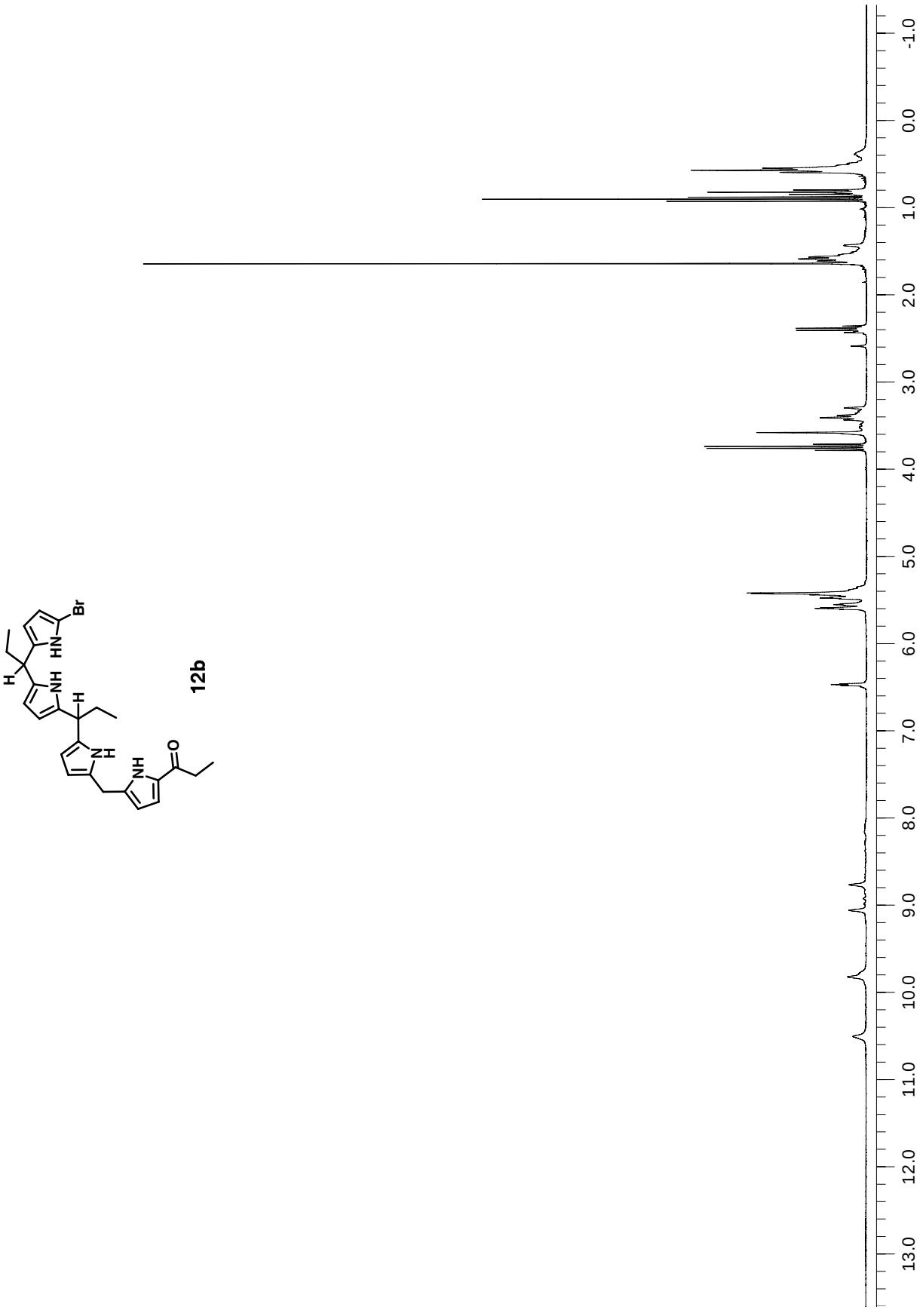


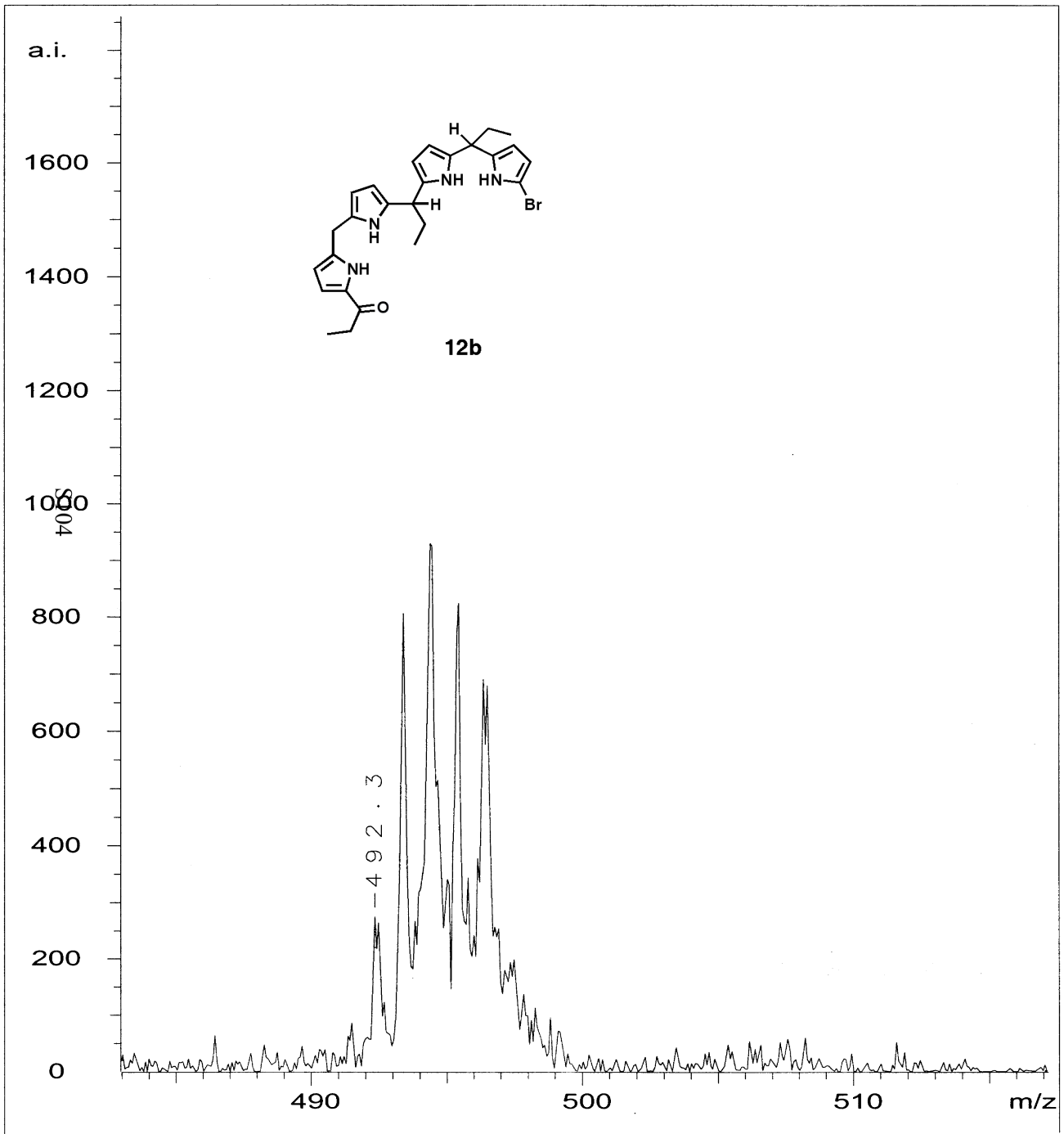
2h


Br
NH
NH
H
H
N
H
NH
O
H
H
2h
0
10
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170
180
190
200



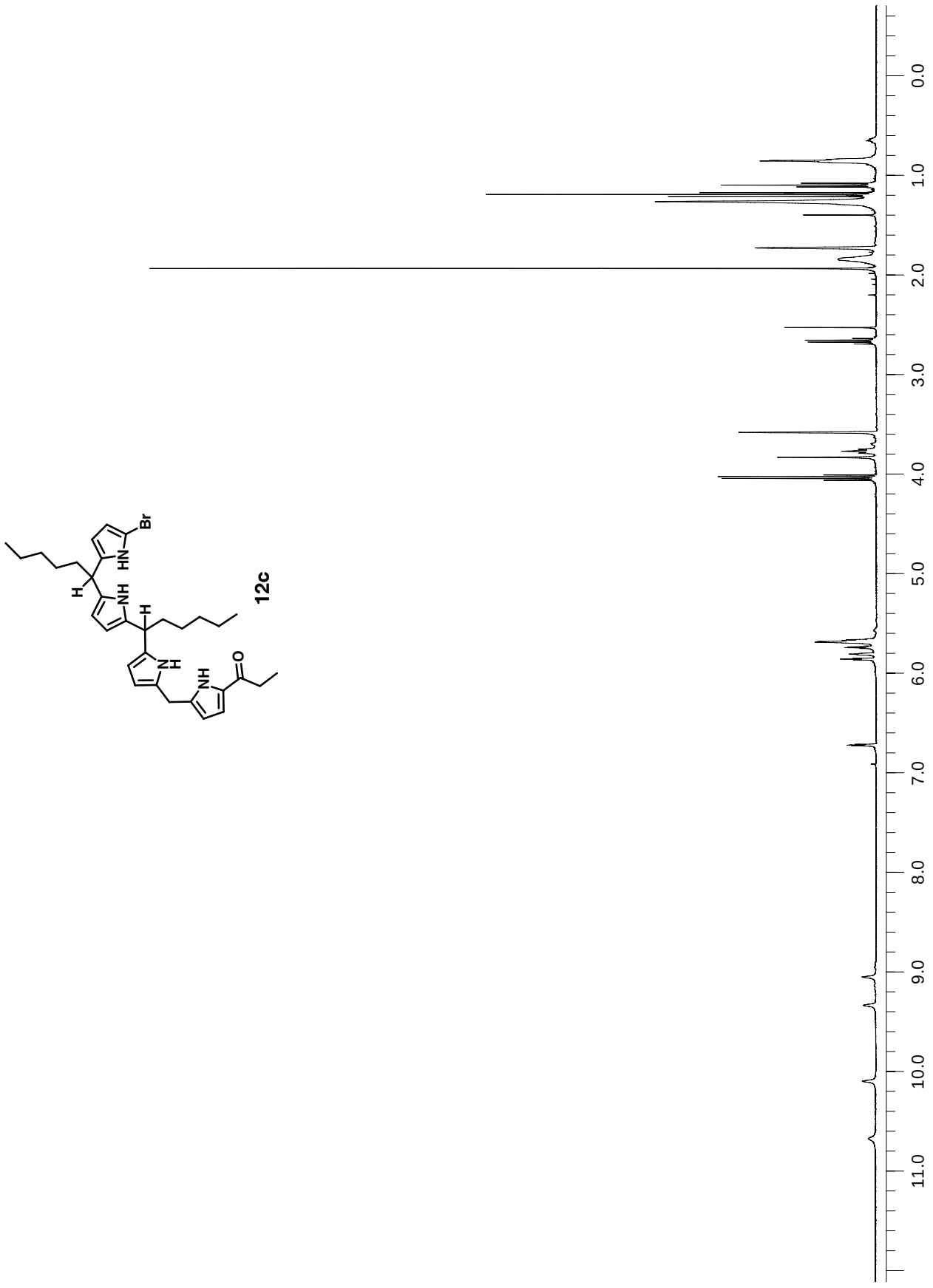
12a

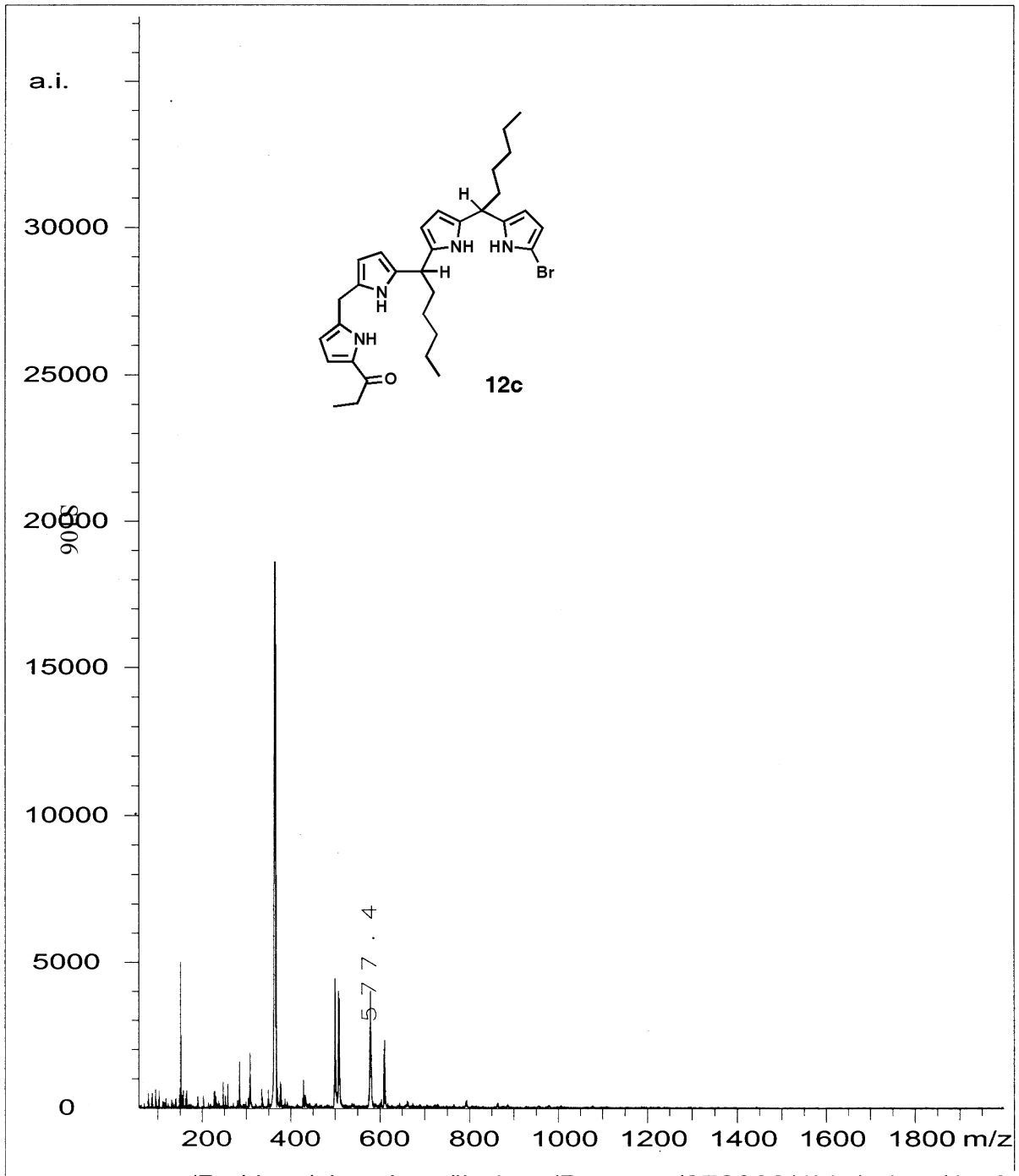

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H
NH
O
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12.0
11.0
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8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0



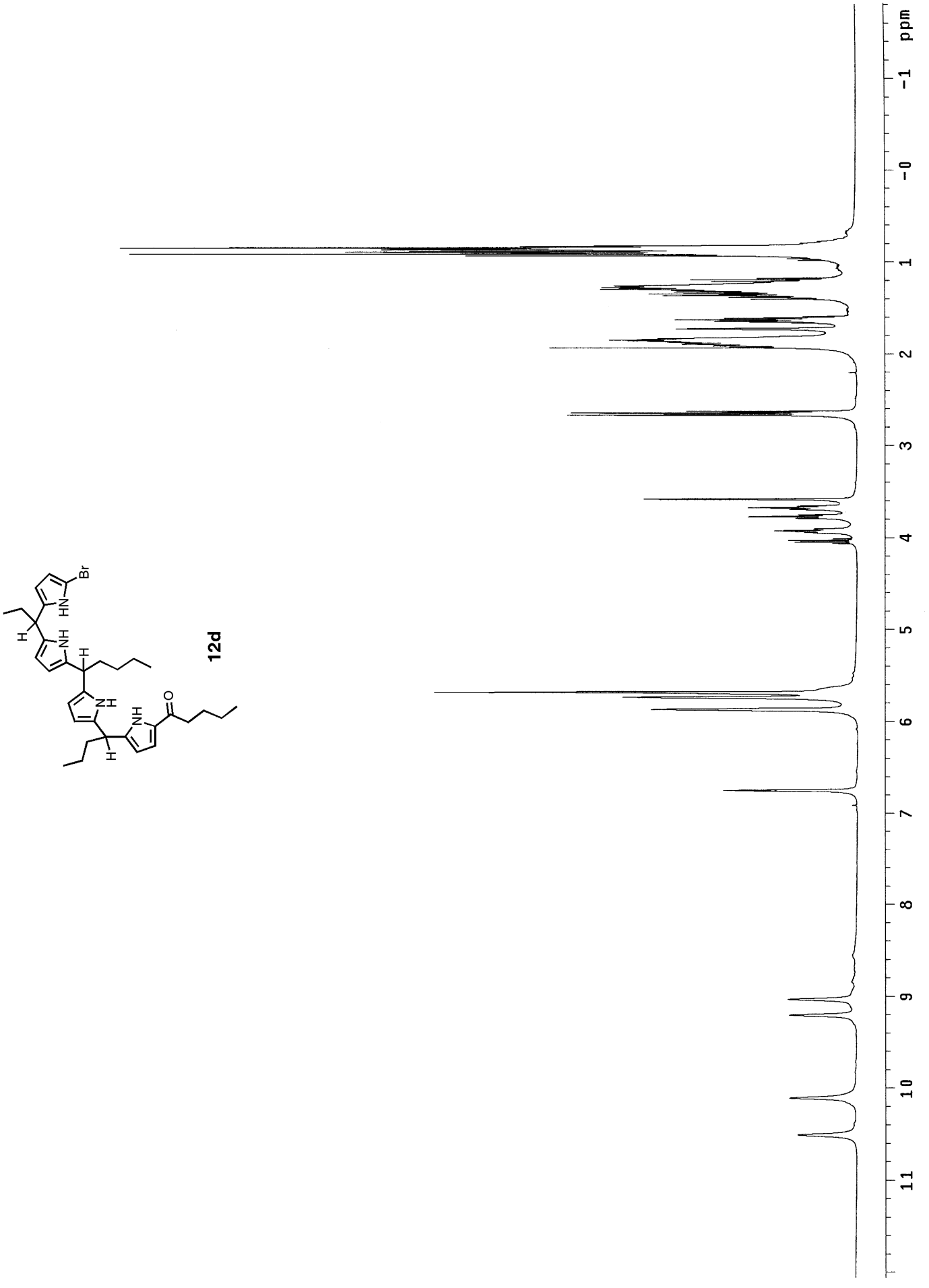
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SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
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DELAY 5184 [ns]
Uis1 19.00 [kV]
Uis2 17.50 [kV]
Urefl 0.00 [kV]
Ulens 9.70 [kV]
Uhimass 0.00 [kV]
RefFull 0.00 [kV]
UdetL 1.62 [kV]
UdetR 0.00 [kV]
Udefl 0.00 [kV]
REPHZ 3.00 [Hz]
ATTEN 27.0
ML1 2513737.301
ML2 314.106
ML3 0.000
HITURBO no
GDEON yes
GDEDLY short
DEFLON no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 0.38
DPMASS 1000.00 [Da]
RBNDVAL 0.00
LBNDVAL 0.00
IS2BNDV 0.00
CMT1 Exp 420
CMT2 5-10-20ethyl bilane

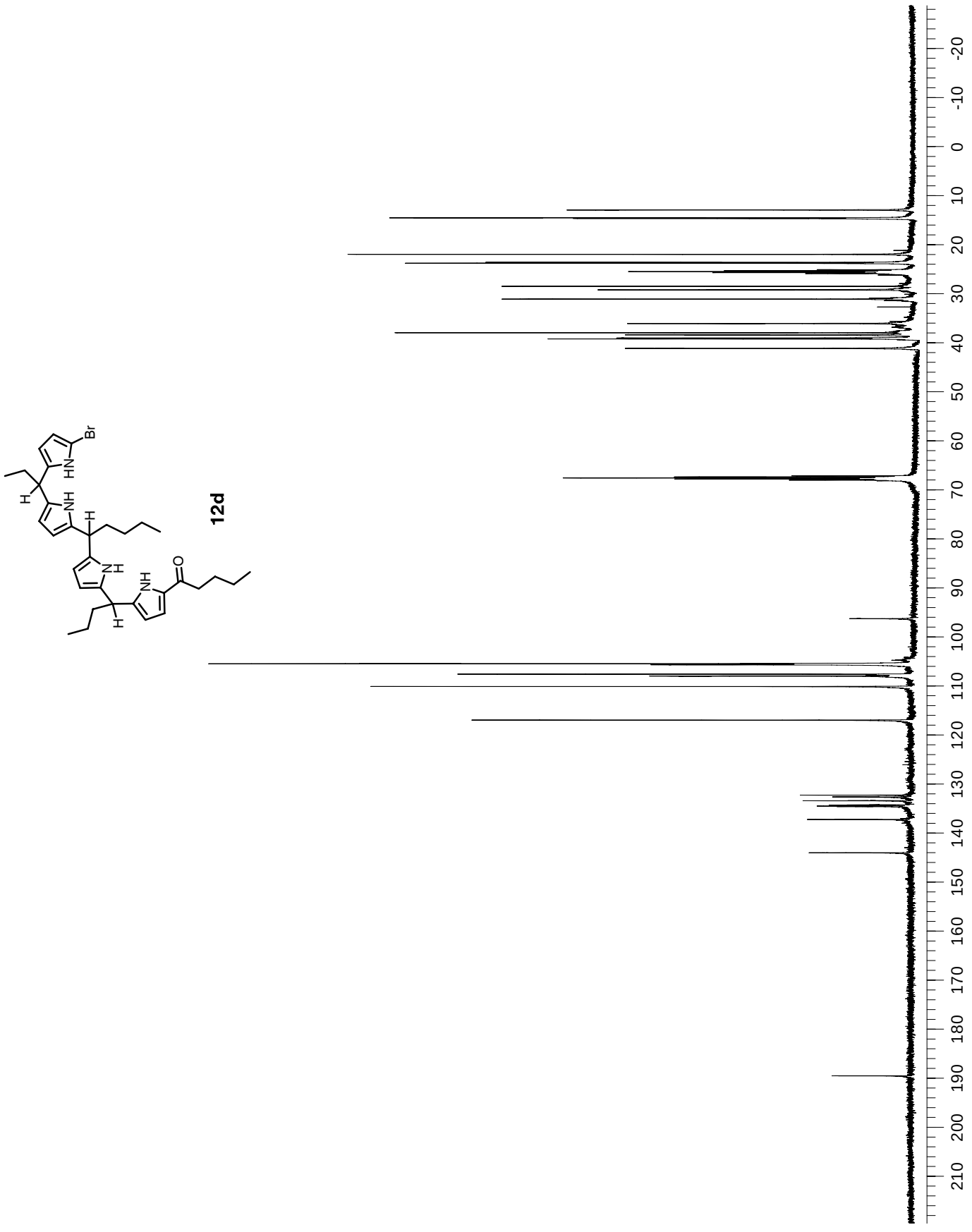
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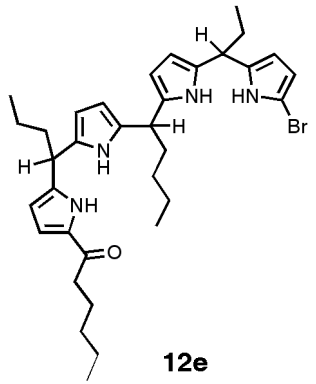

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NH
H
H
NH
NH
O
12c
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10.0
11.0



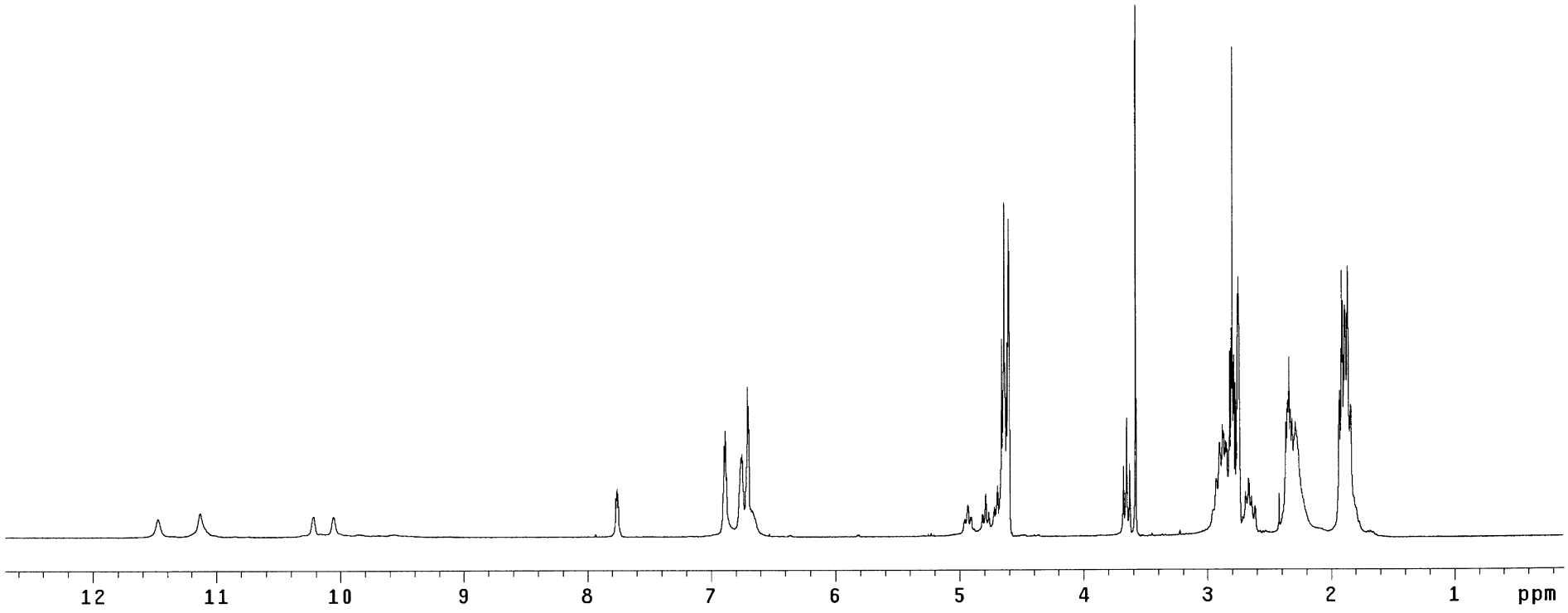
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SMOPTS2 0
SMOPTS3 0
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DELAY 5184 [ns]
Uis1 19.00 [kV]
Uis2 17.50 [kV]
Urefl 0.00 [kV]
Ulens 9.70 [kV]
Uhimass 0.00 [kV]
RefFull 0.00 [kV]
UdetL 1.62 [kV]
UdetR 0.00 [kV]
Udefl 0.00 [kV]
REPHZ 3.00 [Hz]
ATTEN 28.0
ML1 2513859.468
ML2 314.891
ML3 0.000
HITURBO no
GDEON yes
GDEDLY short
DEFLON no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 0.38
DPMASS 1000.00 [Da]
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LBNDVAL 0.00
IS2BNDV 0.00
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CMT2 5,10-pentyl-15unbstituted-20ethylbilane

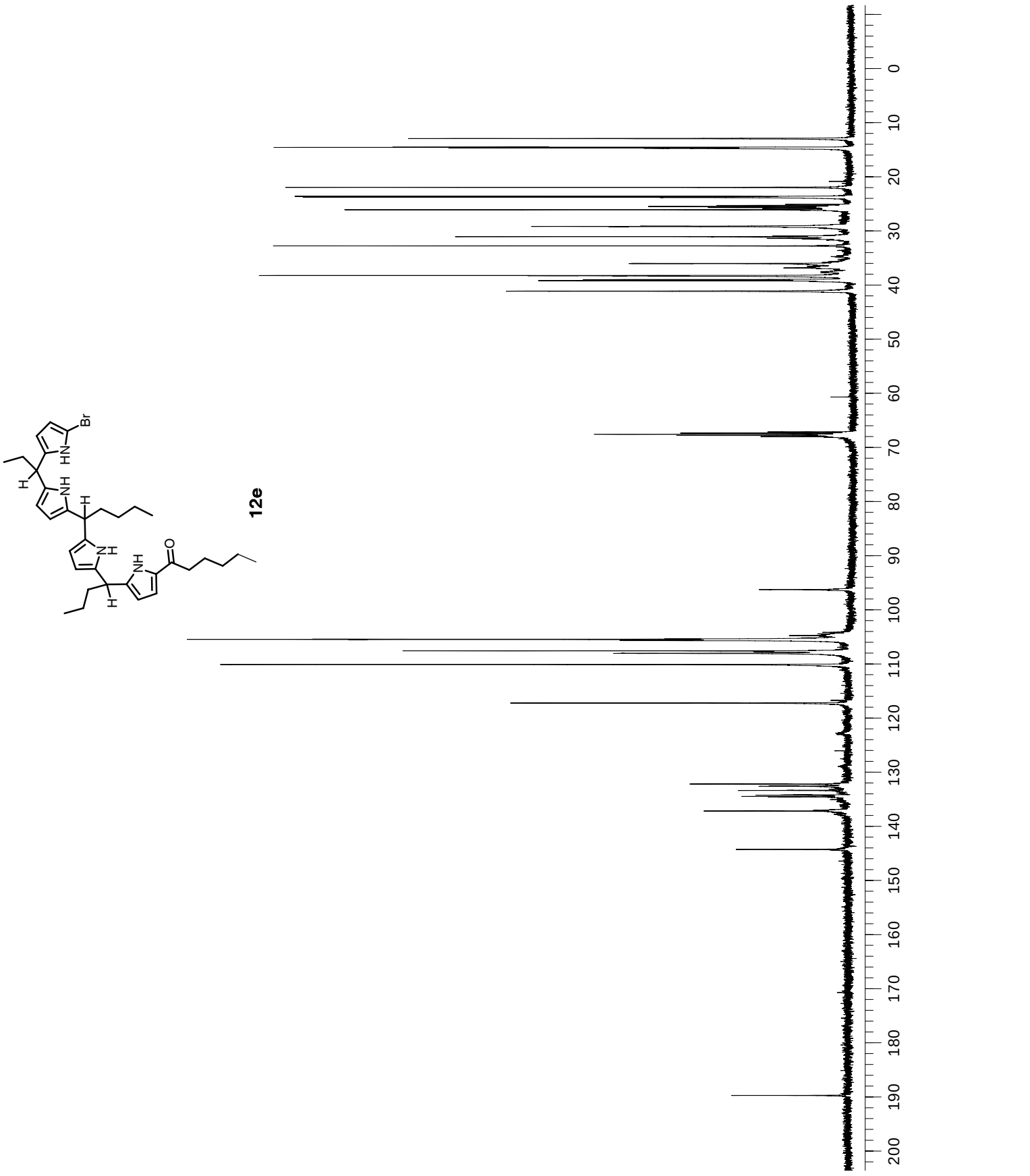

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NH
H
NH
O
NH
H
12d
ppm
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-0
1
2
3
4
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8
9
10
11

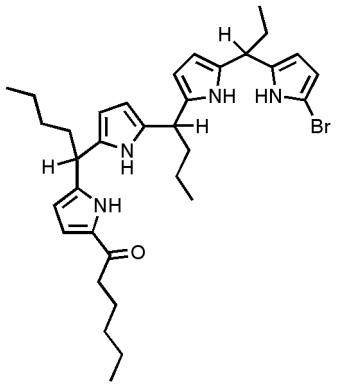

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NH
NH
NH
O
H
H
H
210
200
190
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-10
-20



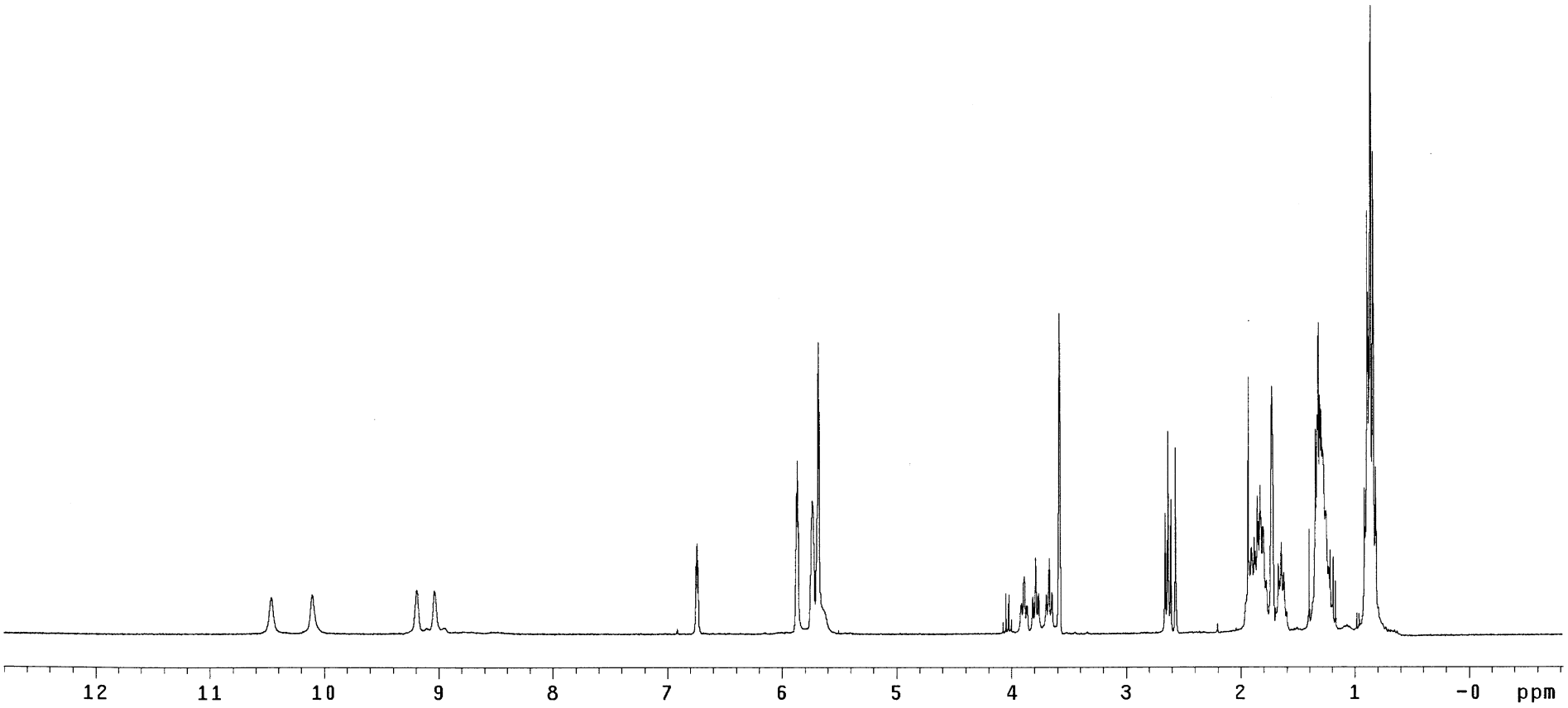
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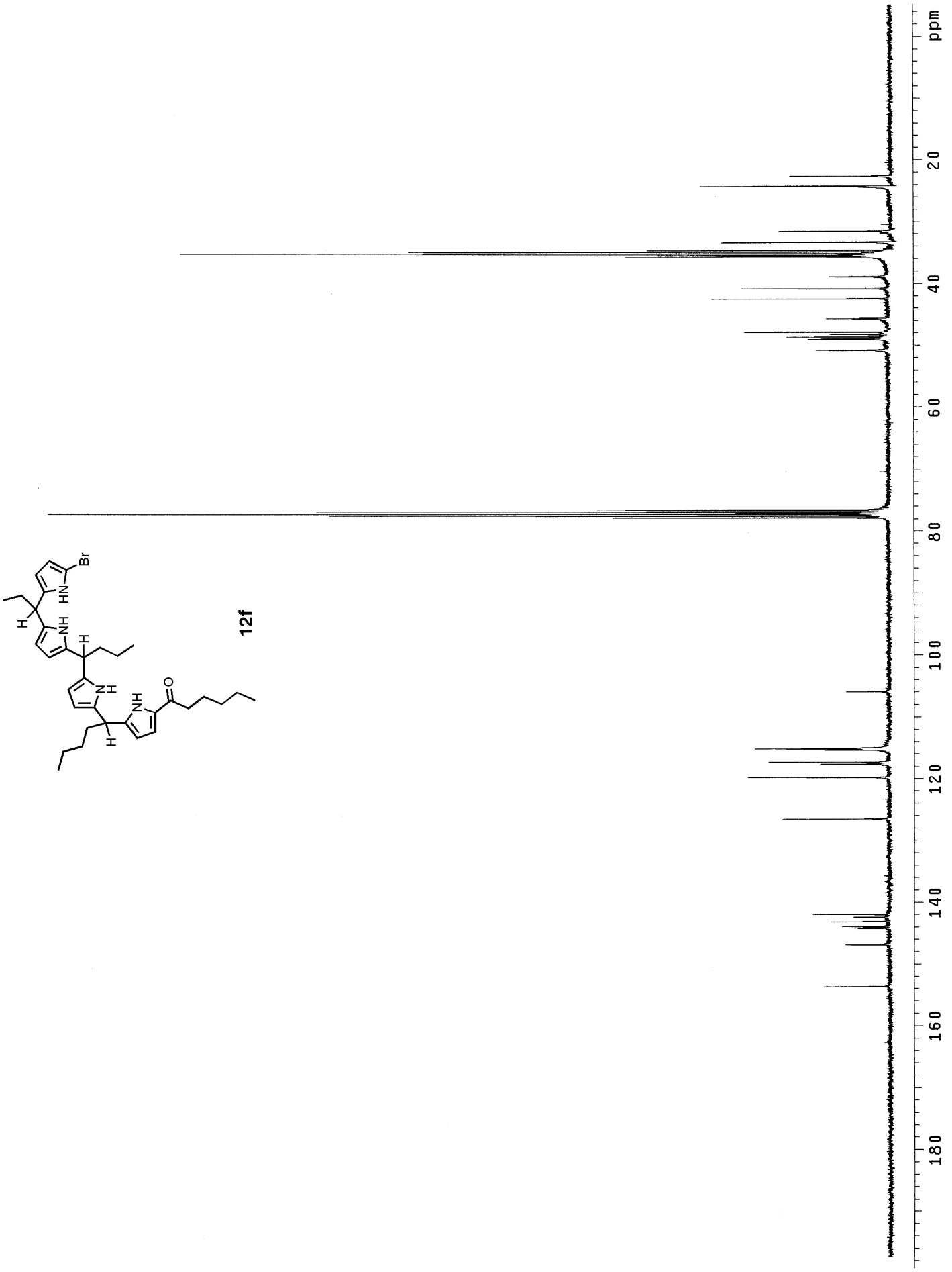


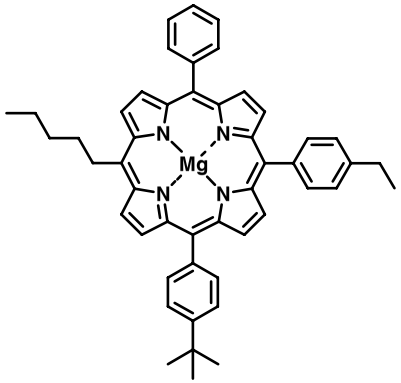

Br
HN
NH
H
H
N
H
NH
O
H
12e
0
10
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190
200



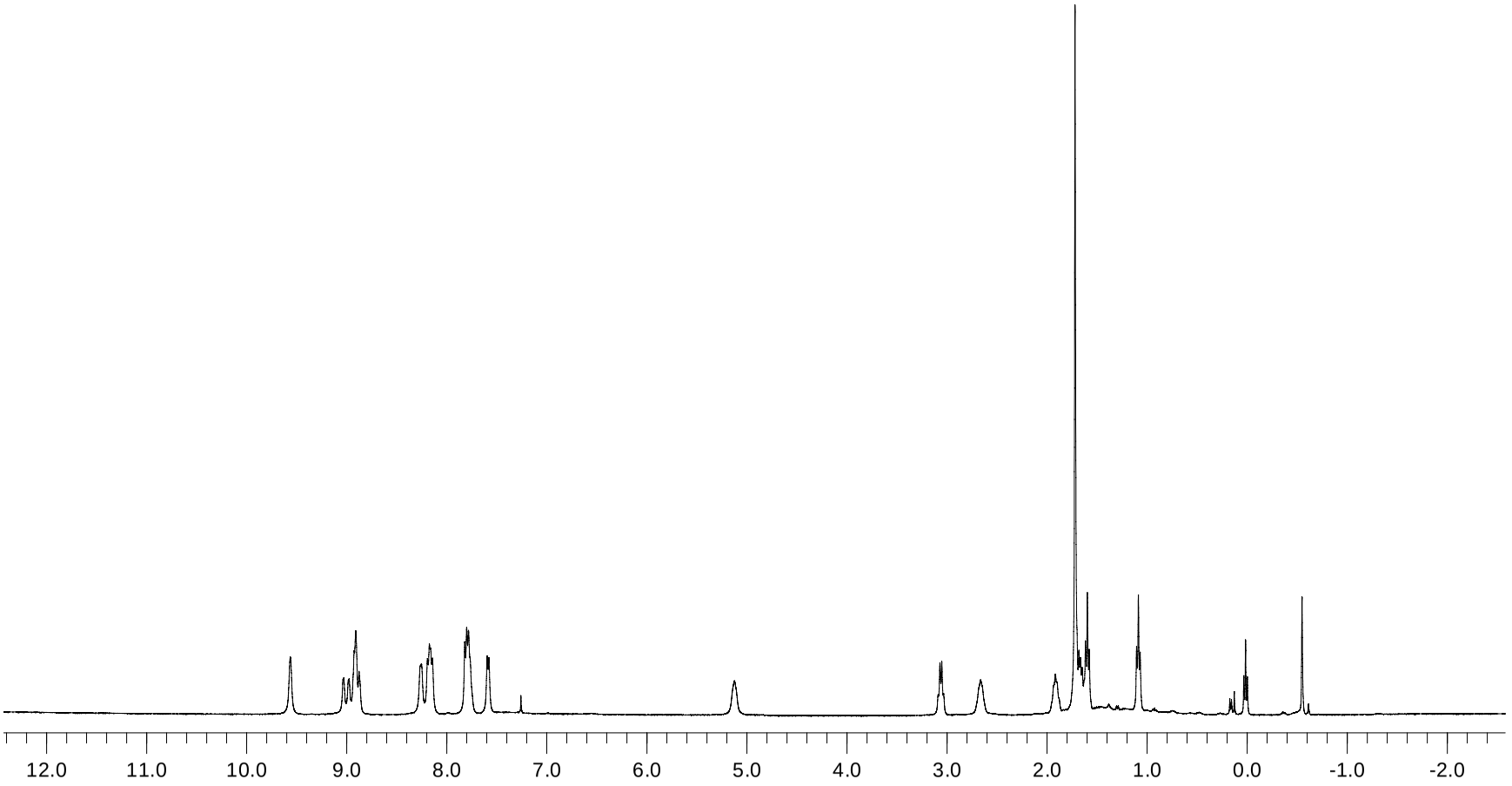
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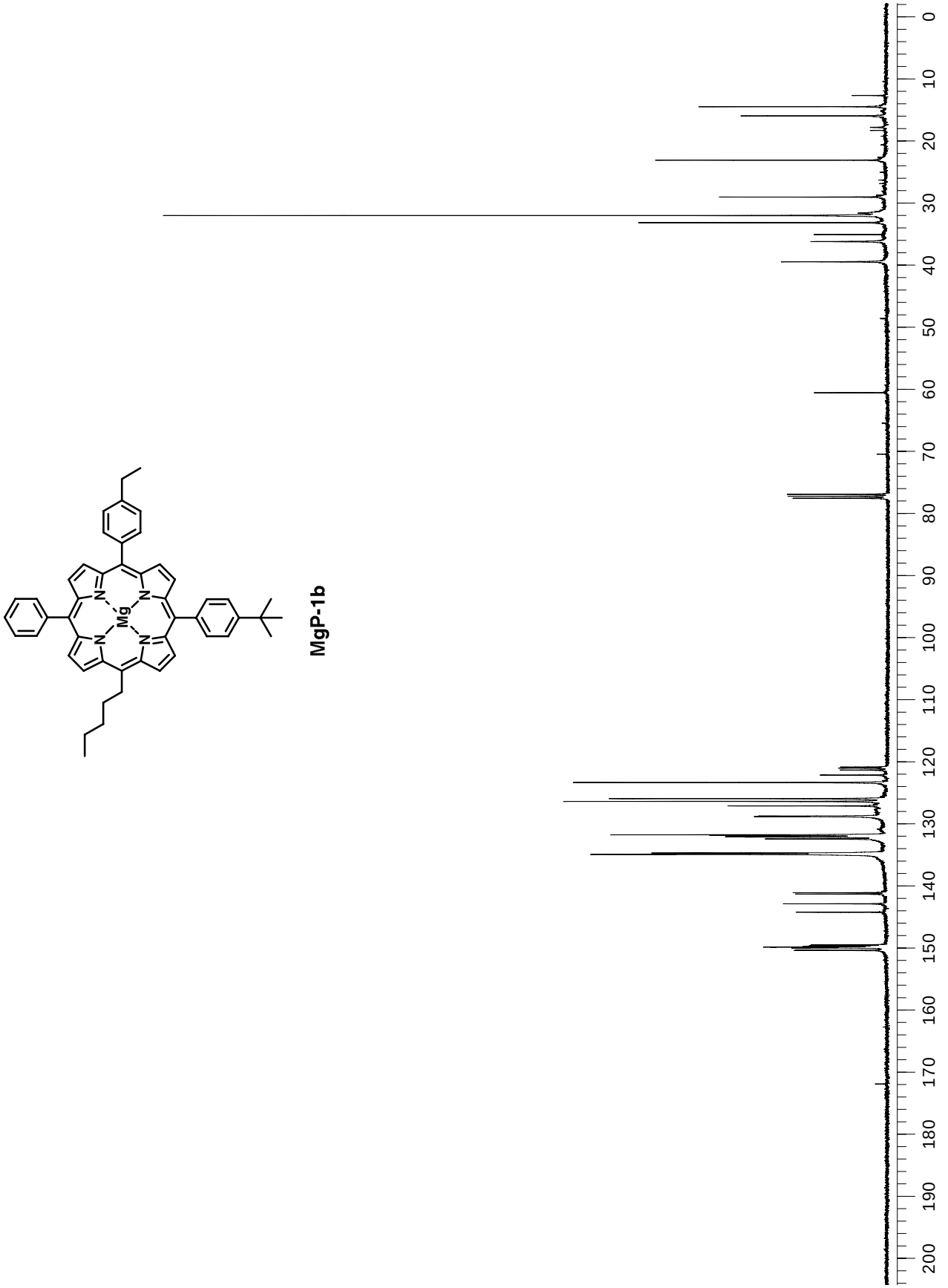


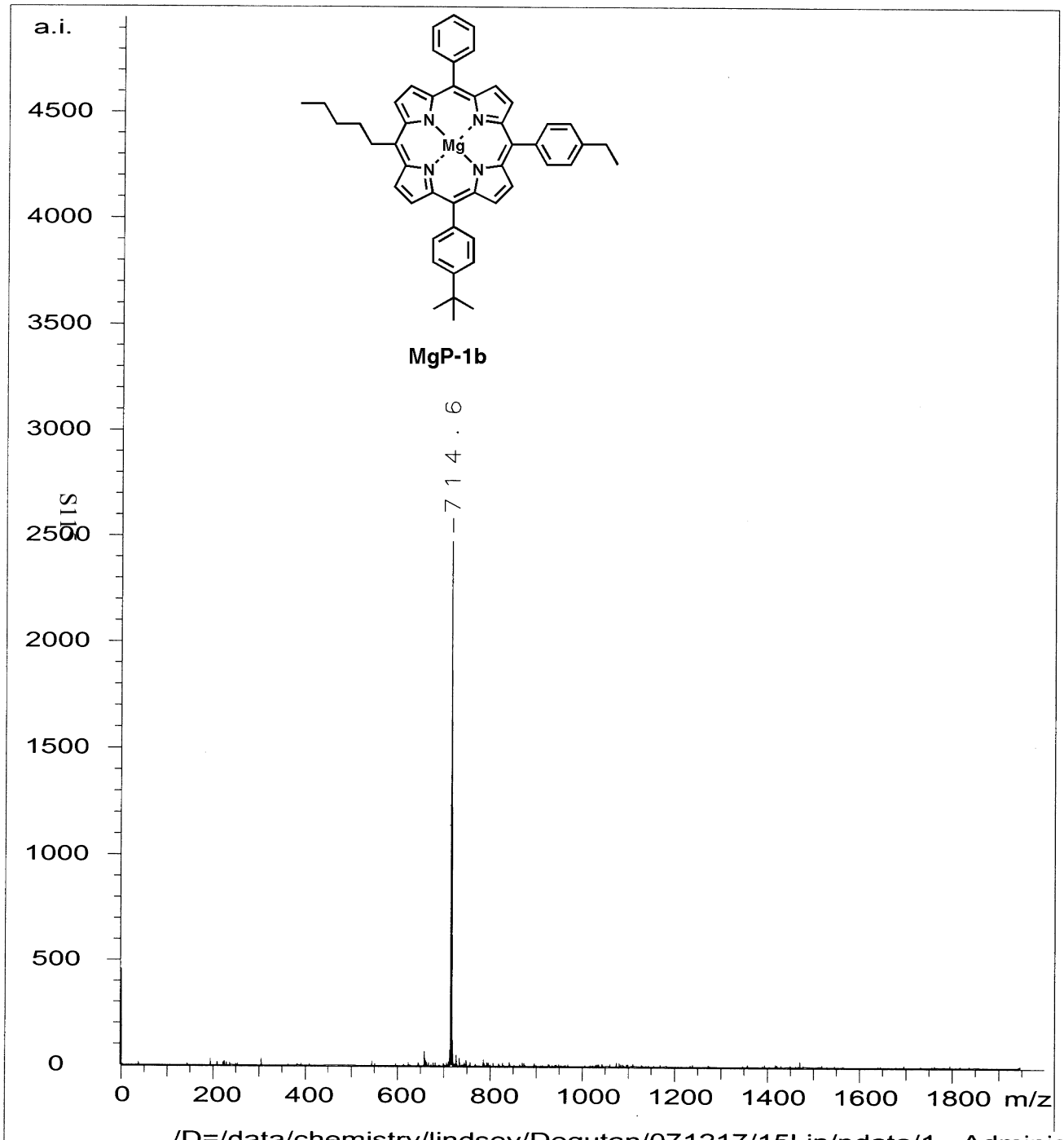

Br
HN
NH
H
NH
H
NH
O
H
12f
ppm
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40
60
80
100
120
140
160
180



MgP-1b



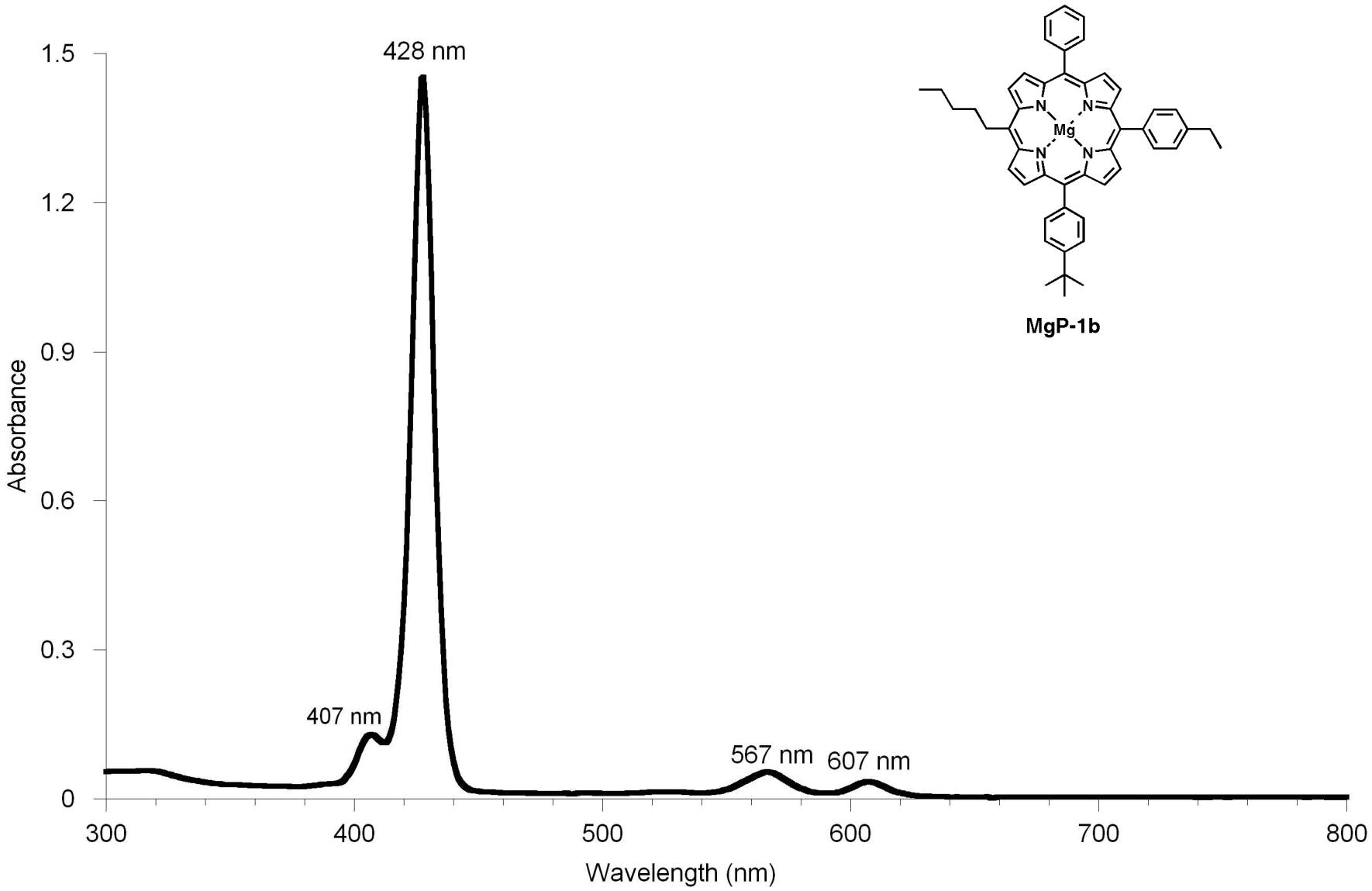

MgP-1b
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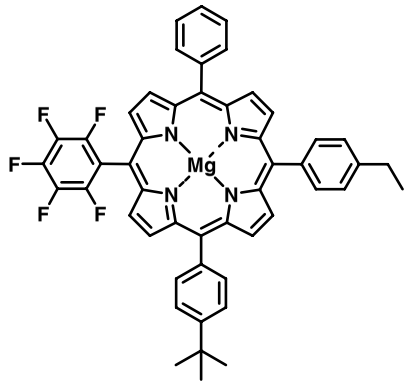


MgP-1b

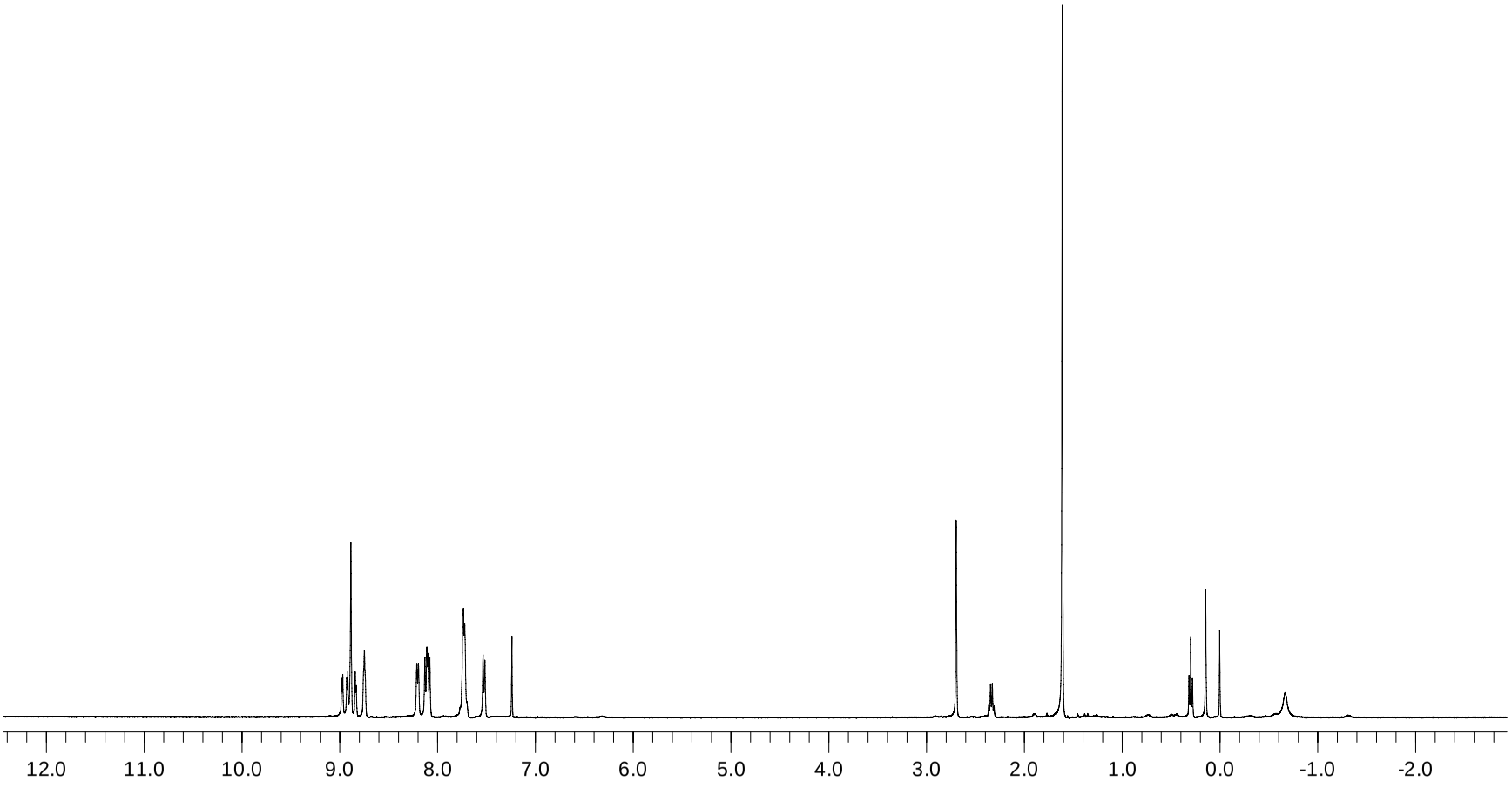
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SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 294 [ns]
Uis1 19.00 [kV]
Uis2 17.60 [kV]
Urefl 0.00 [kV]
Ulens 9.70 [kV]
Uhimass 0.00 [kV]
RefFull 0.00 [kV]
UdetL 1.62 [kV]
UdetR 0.00 [kV]
Udefl 0.00 [kV]
REPHZ 3.00 [Hz]
ATTEN 35.0
ML1 2510030.964
ML2 302.246
ML3 0.000
HITURBO no
GDEON yes
GDEDLY short
DEFLON no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 0.38
DPMASS 500.00 [Da]
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LBNDVAL 0.00
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CMT1 I-A pentyl porphyrin
CMT2

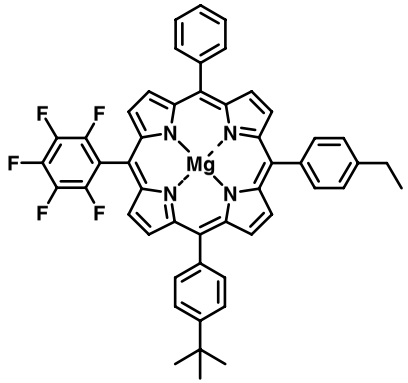
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428 nm
407 nm
567 nm
607 nm
Absorbance
Wavelength (nm)
1.5
1.2
0.9
0.6
0.3
0
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400
500
600
700
800
N
N
Mg
N
N
MgP-1b

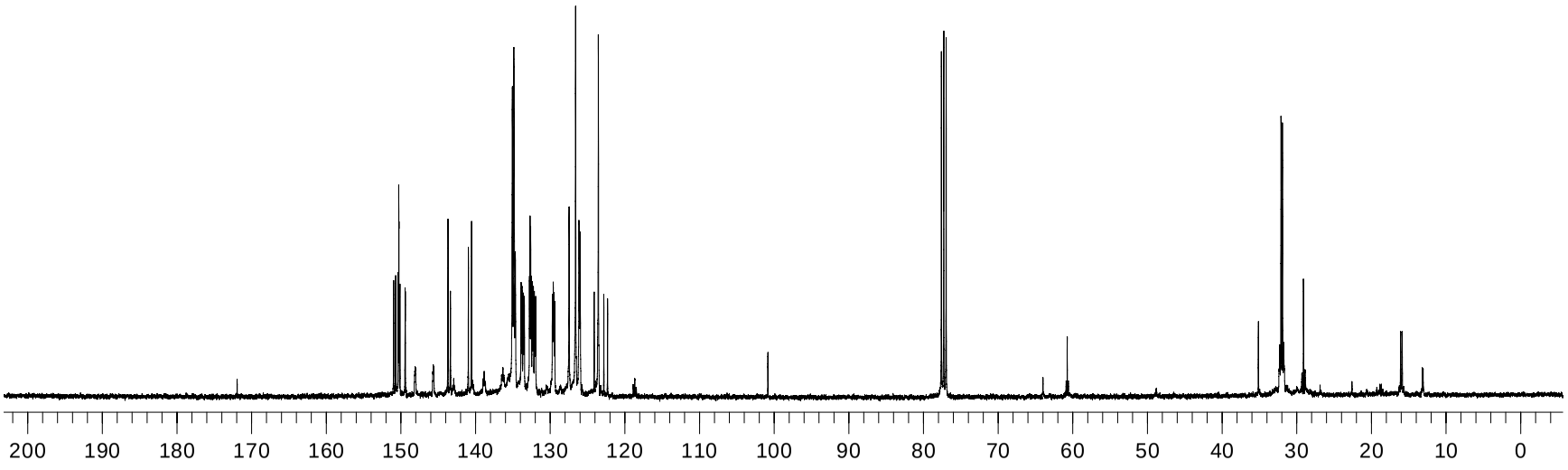


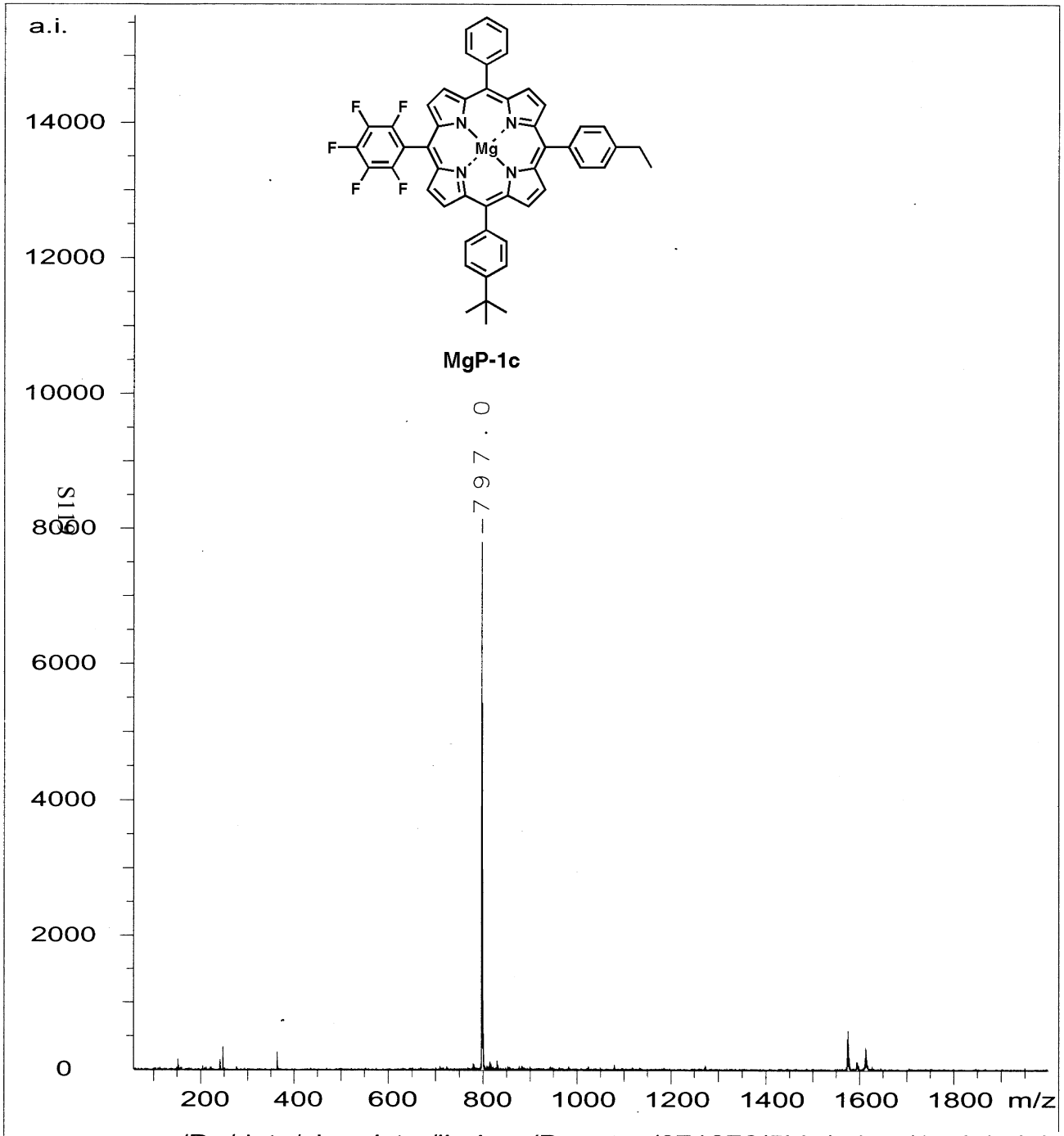
MgP-1c




F
F
F
F
F
N
N
Mg
N
N

MgP-1c

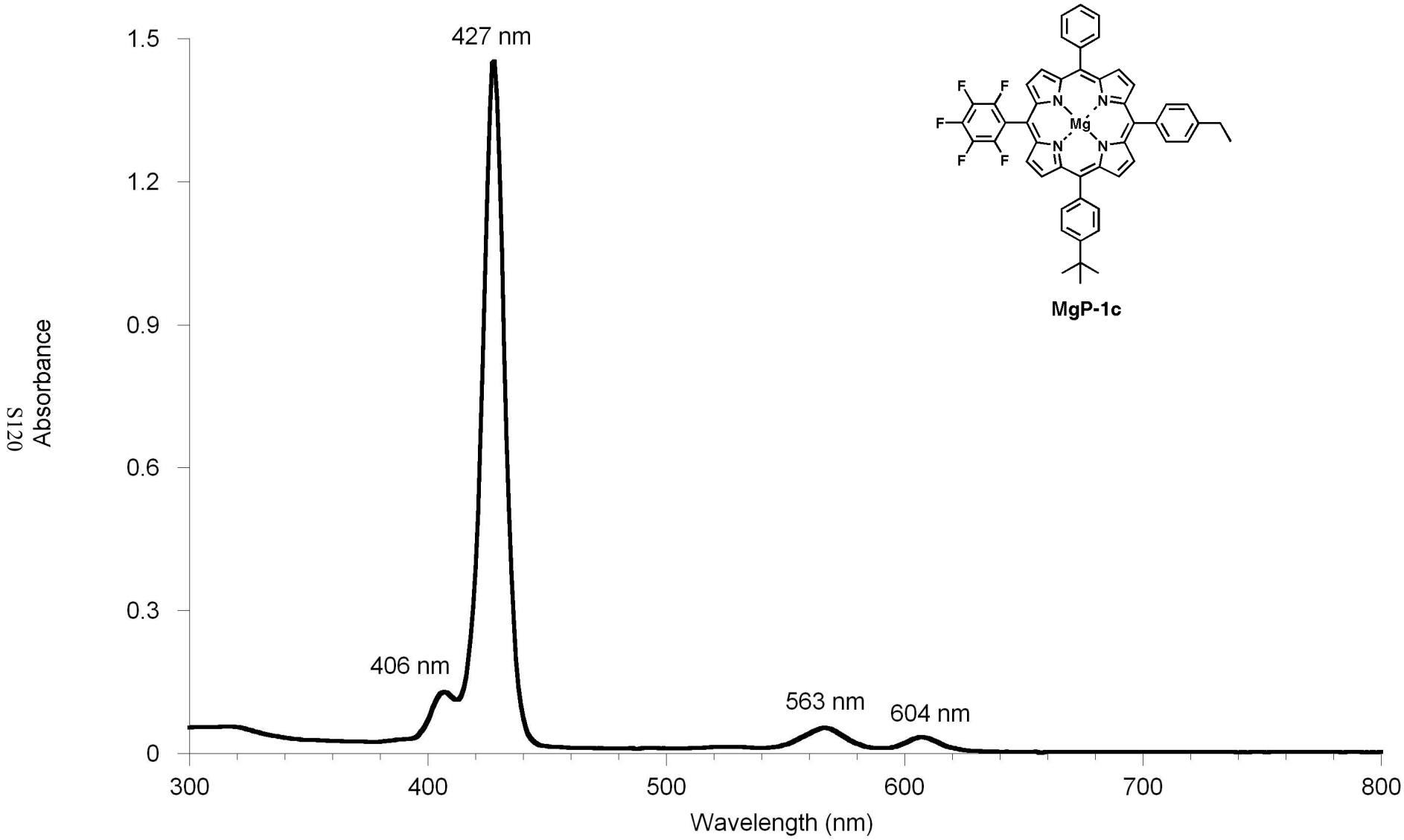

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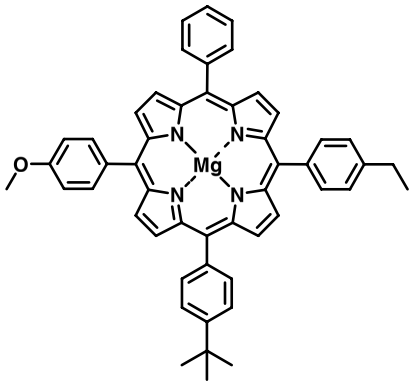


MgP-1c

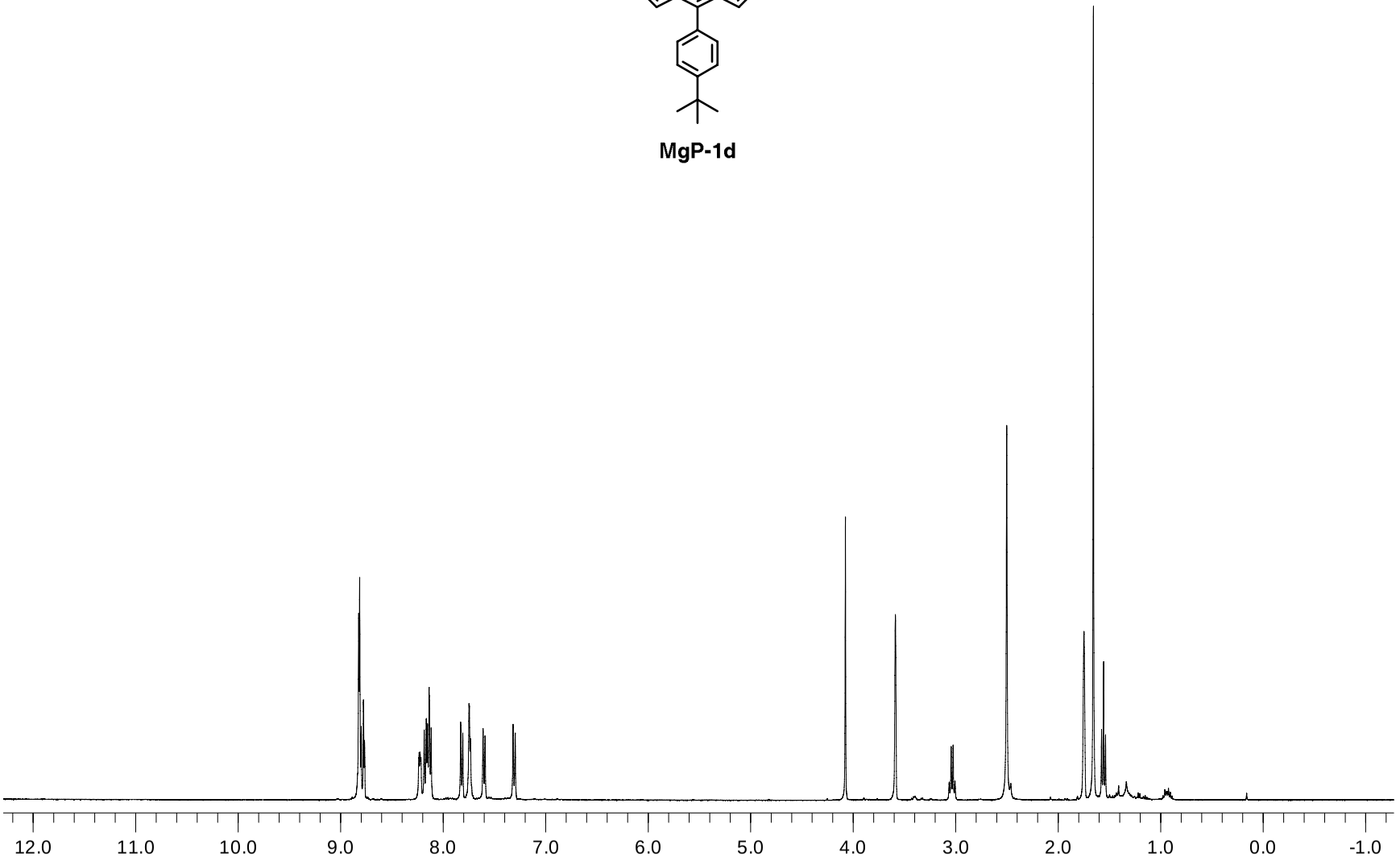
INSTRUM MASSDEC
OpId tof
SMPNAM 071876
AQ_DATE 2007-10-29 18:04:00
PATH D:\data\Chemistry\Lindsey\Dogutan
POLARI POS
AQOP_m Reflector
TD 23334
NoSHOTS 200
SMONUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 5184 [ns]
Uis1 19.00 [kV]
Uis2 17.50 [kV]
Urefl 0.00 [kV]
Ulens 9.70 [kV]
Uhimass 0.00 [kV]
RefFull 0.00 [kV]
UdetL 1.62 [kV]
UdetR 0.00 [kV]
Udefl 0.00 [kV]
REPHZ 3.00 [Hz]
ATTEN 36.0
ML1 2513830.874
ML2 314.250
ML3 0.000
HITURBO no
GDEON yes
GDEDLY short
DEFLON no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 0.38
DPMASS 1000.00 [Da]
RBNDVAL 0.00
LBNDVAL 0.00
IS2BNDV 0.00
CMT1 ref
CMT2 10pentafloro Mg Porphyrin

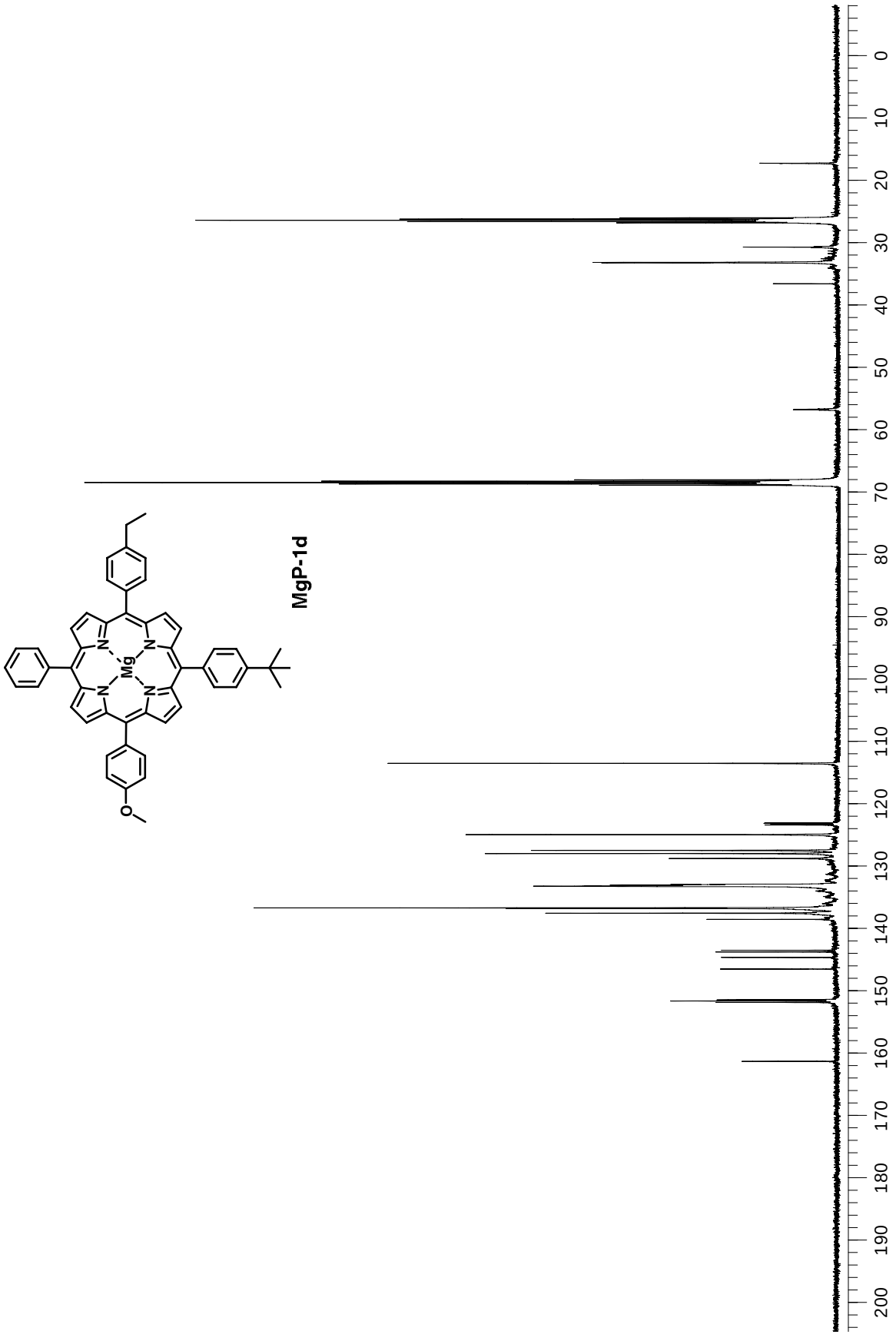
/D=/data/chemistry/lindsey/Dogutan/071876/5Lin/pdata/1 Administrator Mon Oct 29 18:20:52 2007

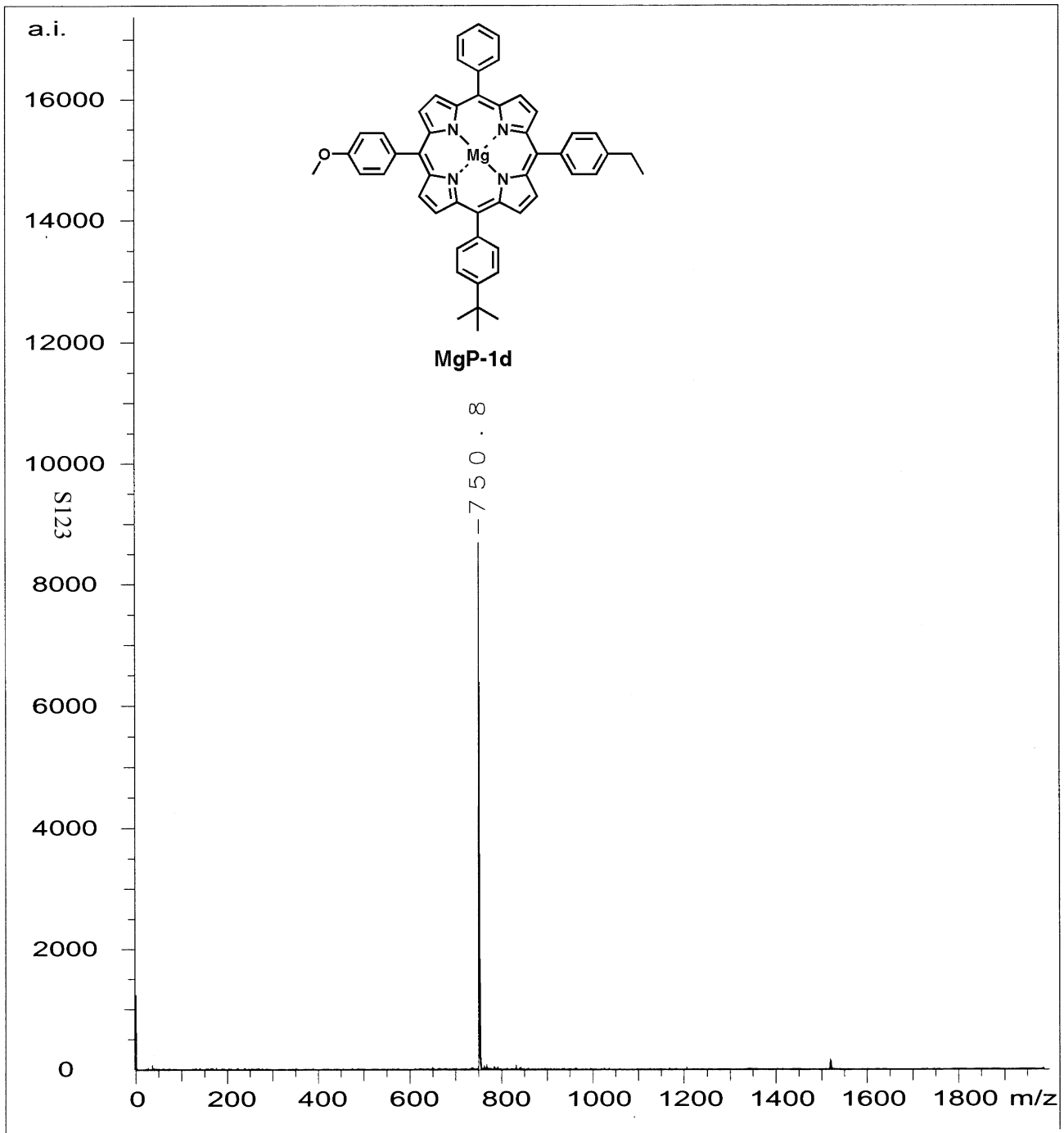

427 nm
406 nm
563 nm
604 nm
1.5
1.2
0.9
0.6
0.3
0
300
400
500
600
700
800
Absorbance
Wavelength (nm)
F
F
F
F
F
N
N
Mg
N
N
MgP-1c



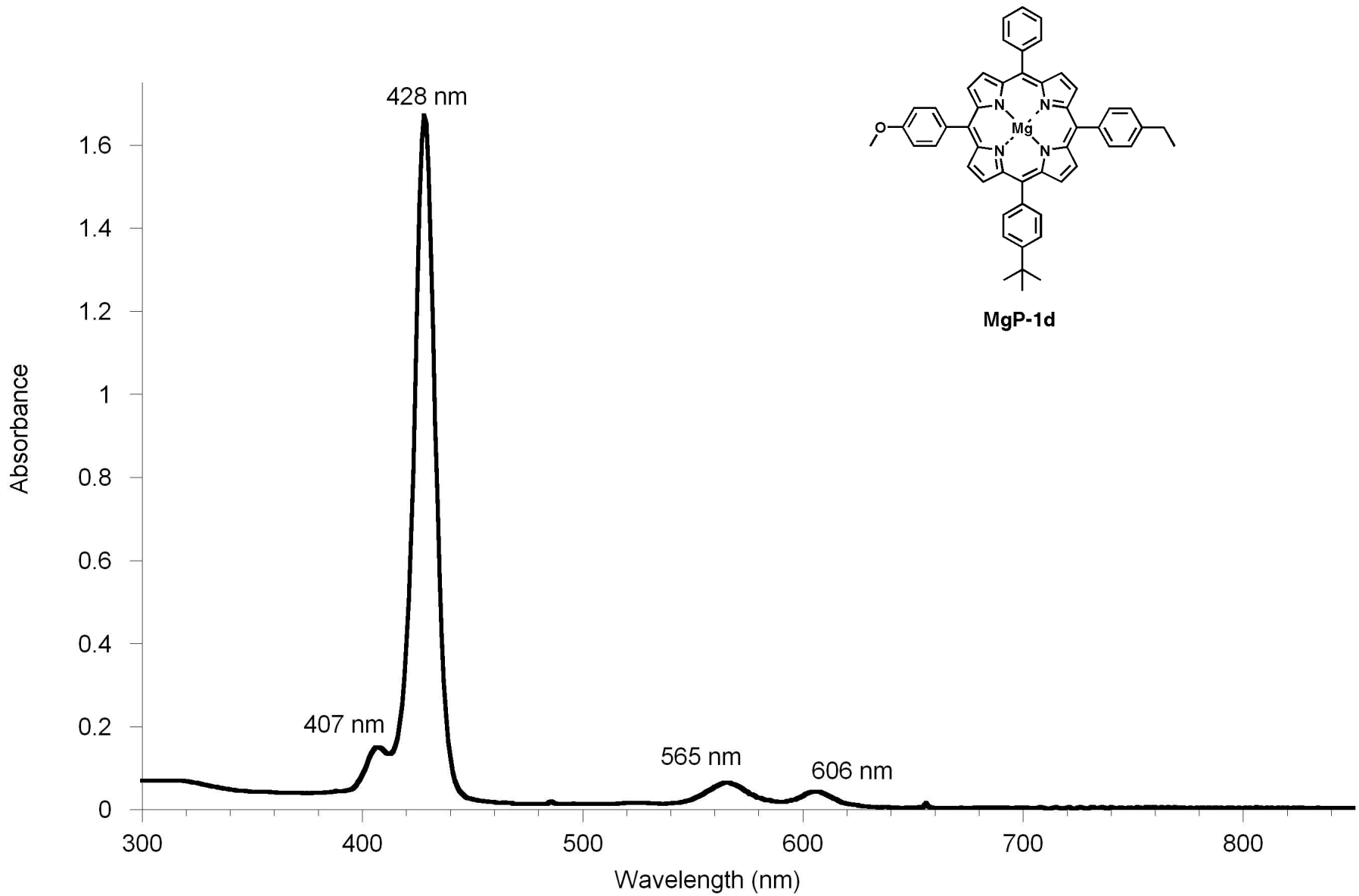
MgP-1d



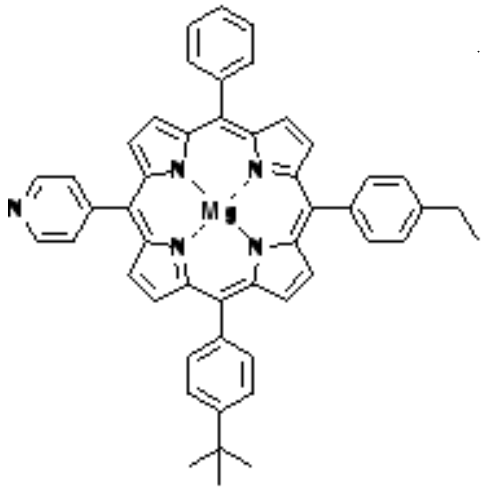

MgP-1d
Mg
N
O
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200



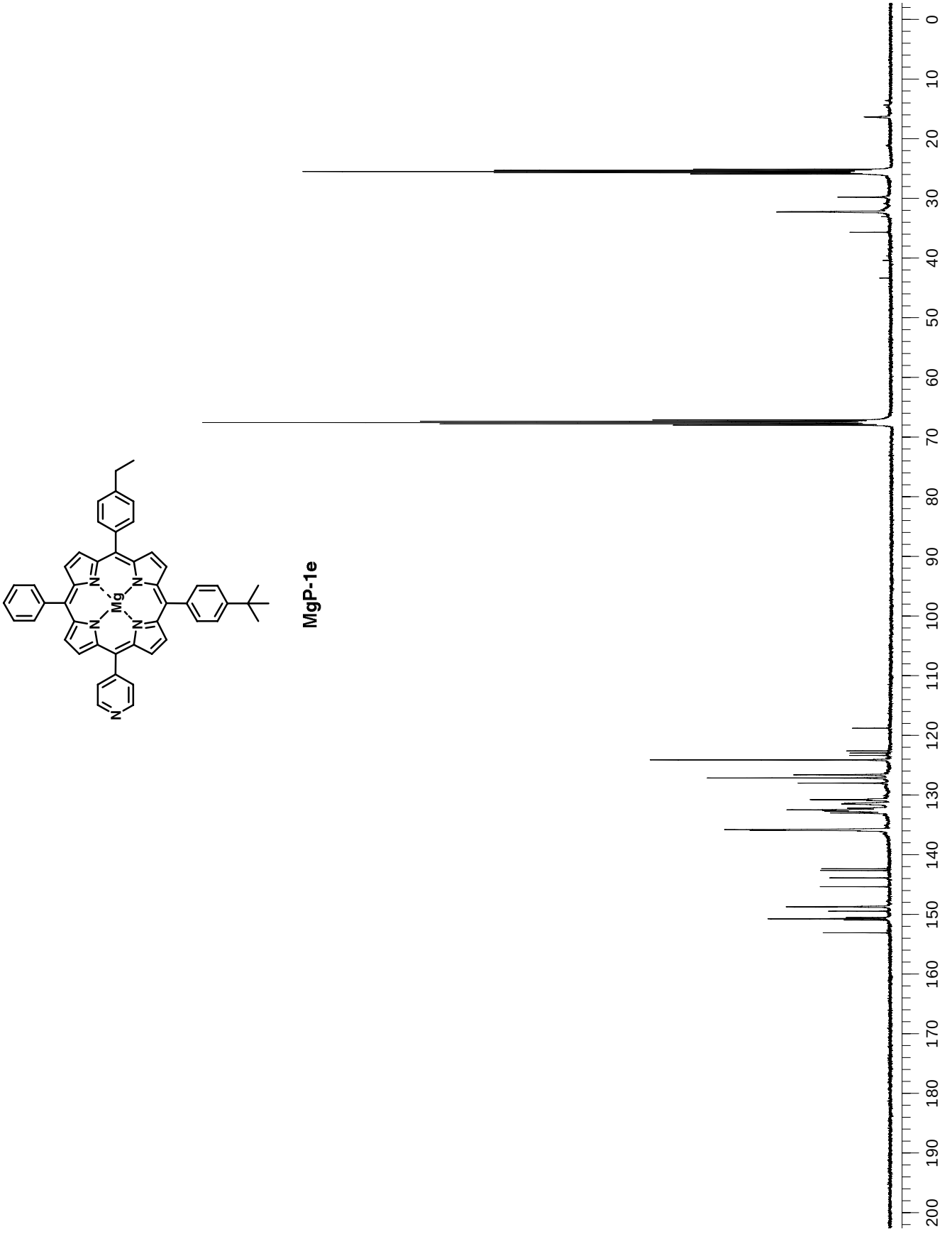
INSTRUM MASSDEC
OpId tof
SMPNAM 071351
AQ_DATE 2007-08-06 18:17:13
PATH D:\data\Chemistry\Lindsey\Dogutan
POLARI POS
AQOP_m Reflector
TD 28224
NoSHOTS 200
SMONUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 294 [ns]
Uis1 19.00 [kV]
Uis2 17.60 [kV]
Urefl 0.00 [kV]
Ulens 9.70 [kV]
Uhimass 0.00 [kV]
RefFull 0.00 [kV]
UdetL 1.62 [kV]
UdetR 0.00 [kV]
Udefl 0.00 [kV]
REPHZ 3.00 [Hz]
ATTEN 32.0
ML1 2510212.749
ML2 304.087
ML3 0.000
HITURBO no
GDEON yes
GDEDLY short
DEFLON no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 0.38
DPMASS 500.00 [Da]
RBNDVAL 0.00
LBNDVAL 0.00
IS2BNDV 0.00
CMT1 EXP354
CMT2

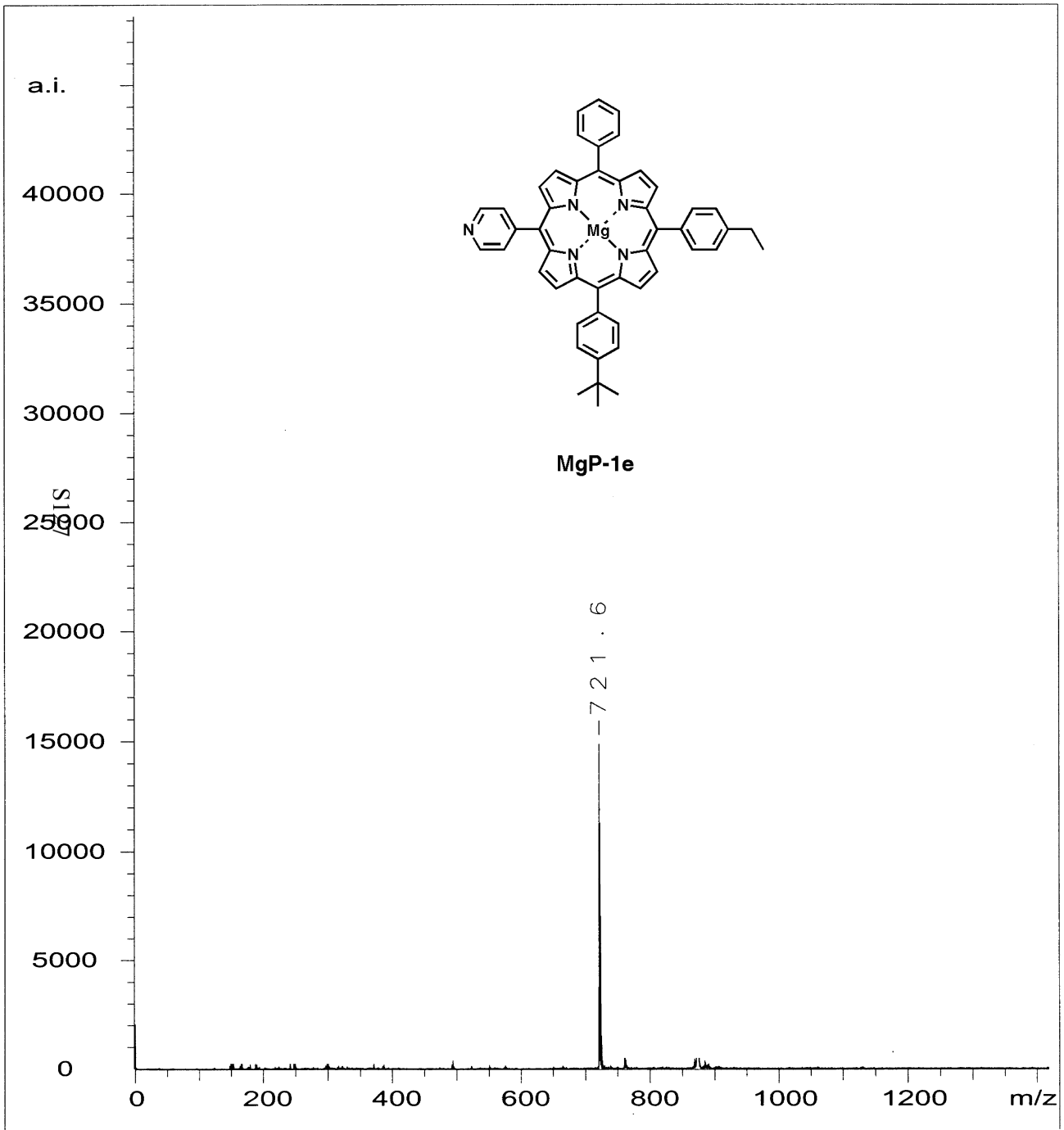

428 nm
407 nm
565 nm
606 nm
Absorbance
Wavelength (nm)
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
300
400
500
600
700
800
O
N
N
Mg
N
N

MgP-1d

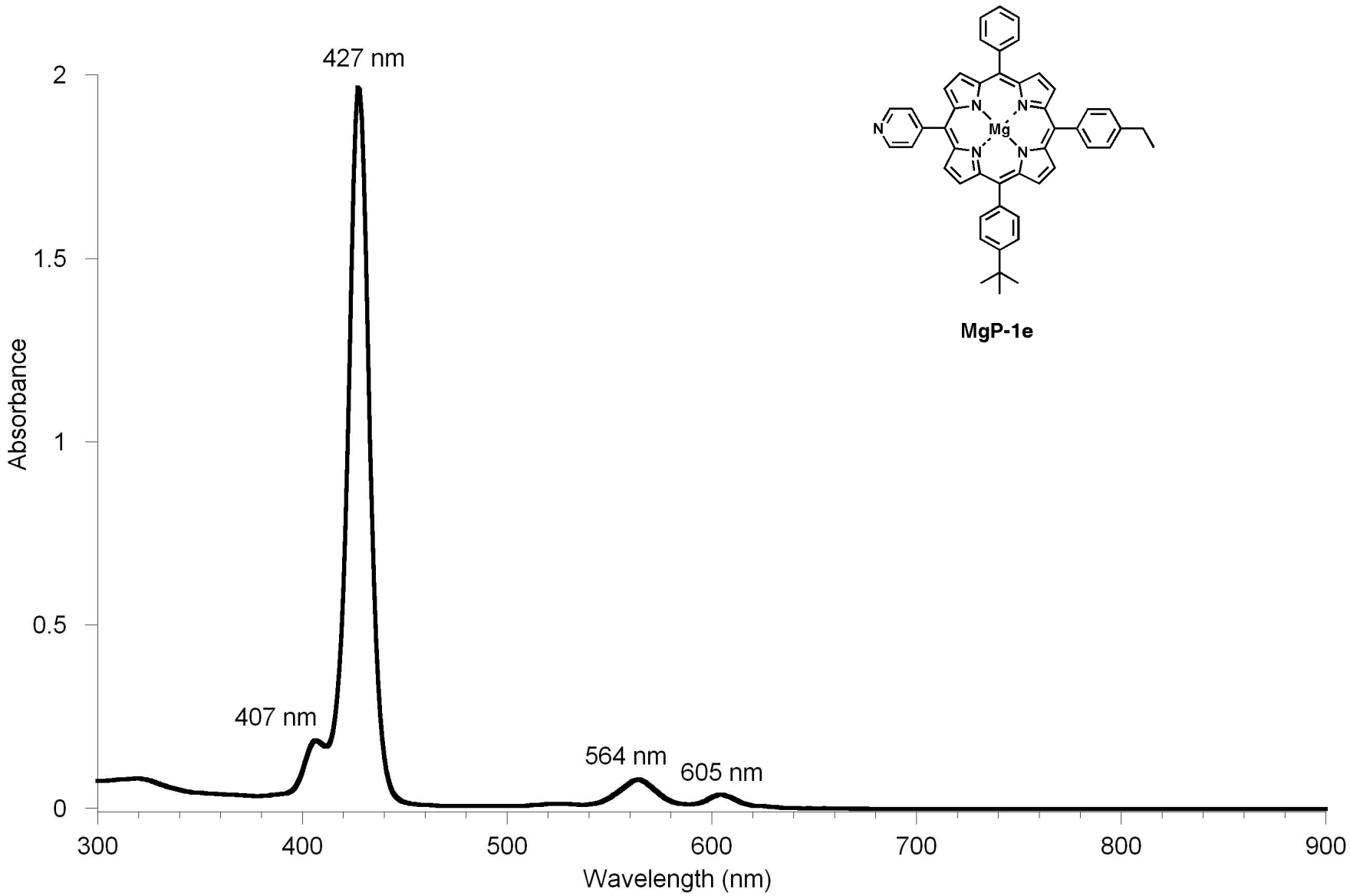


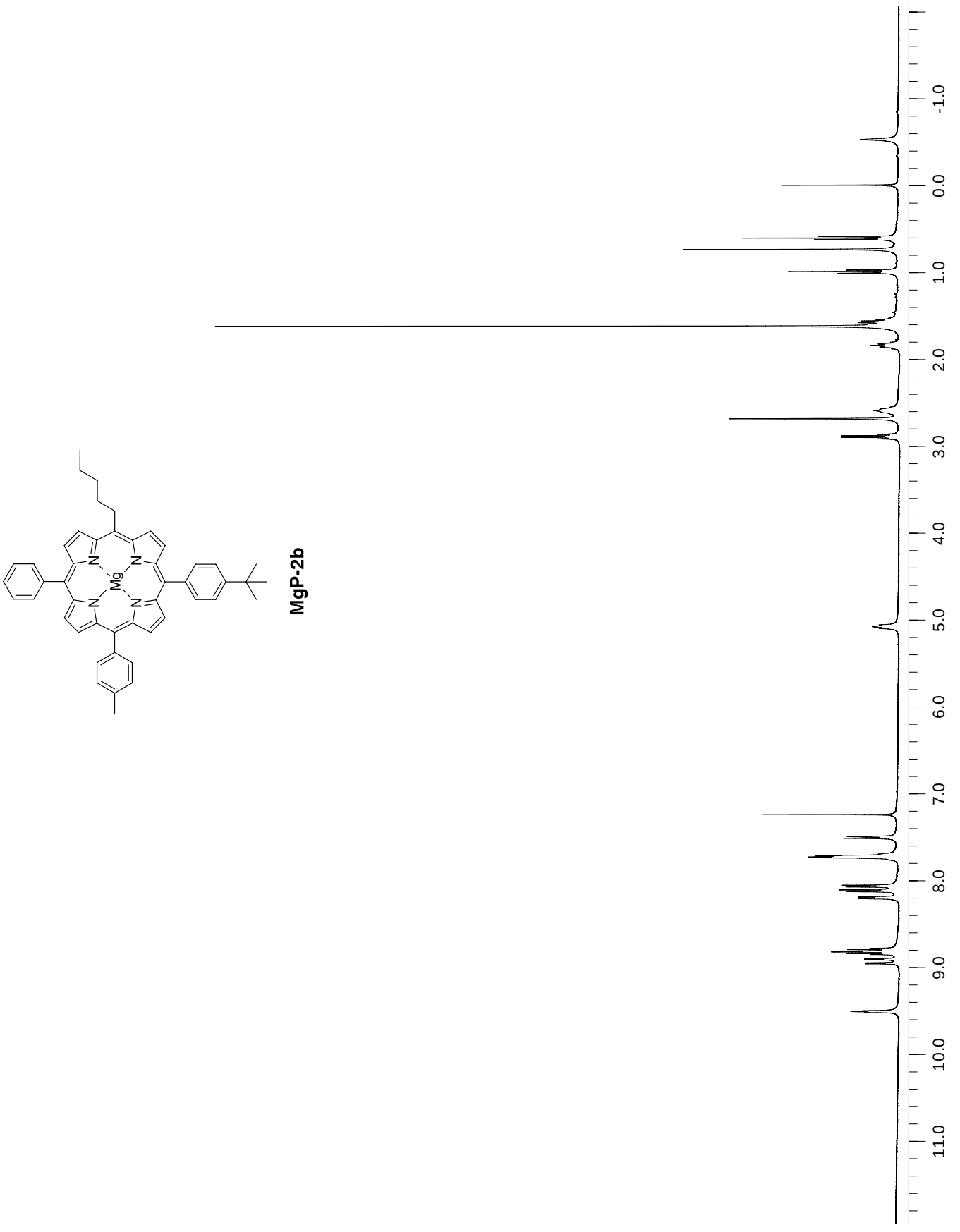
MgP-1e

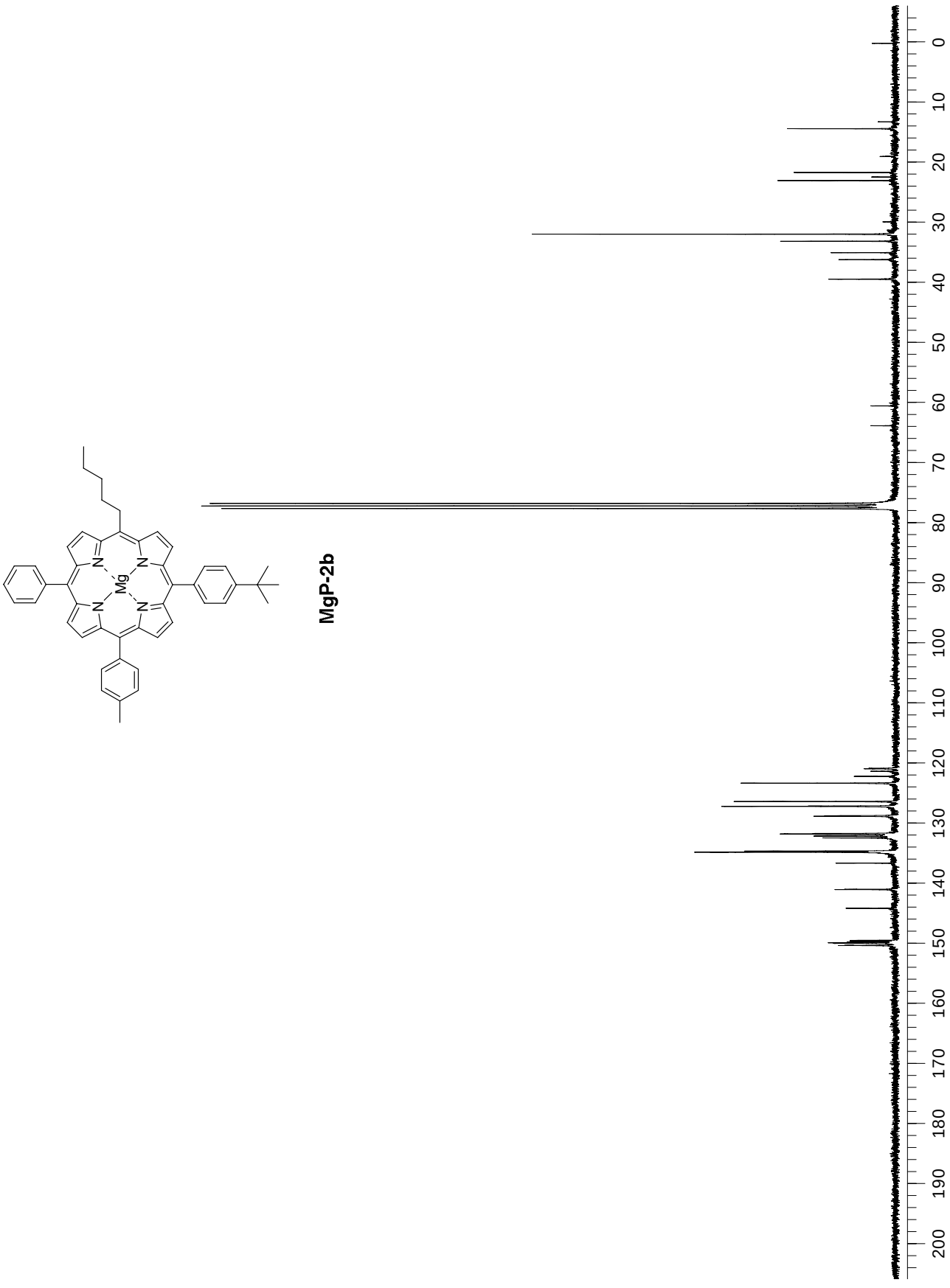

MgP-1e
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200

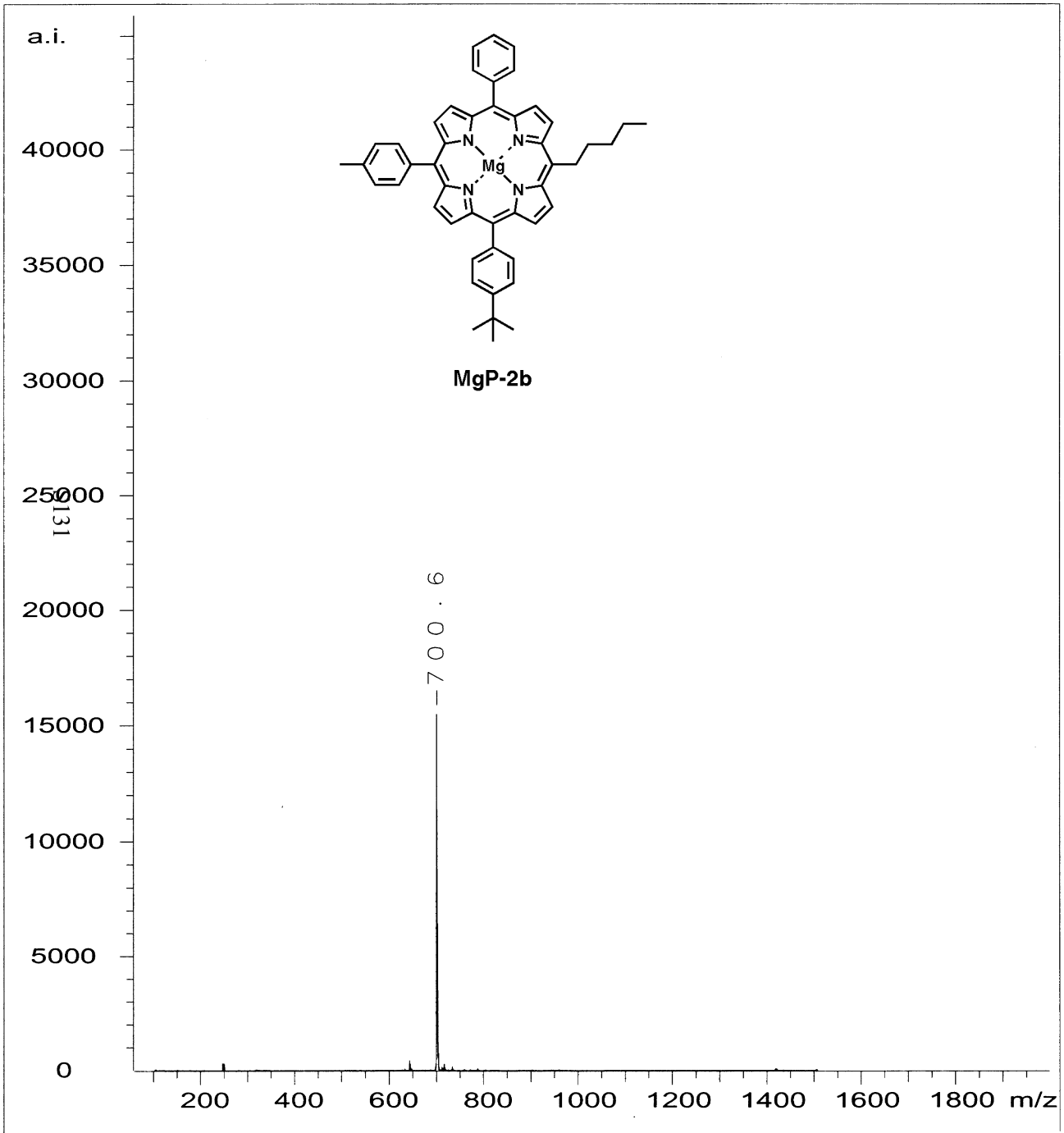


INSTRUM MASSDEC
OpId tof
SMPNAM 071434
AQ_DATE 2007-09-06 18:13:56
PATH D:\data\Chemistry\Lindsey\Dogutan
POLARI POS
AQOP_m Reflector
TD 23784
NoSHOTS 200
SMONUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 294 [ns]
Uis1 19.00 [kV]
Uis2 17.60 [kV]
Urefl 0.00 [kV]
Ulens 9.70 [kV]
Uhimass 0.00 [kV]
RefFull 0.00 [kV]
UdetL 1.62 [kV]
UdetR 0.00 [kV]
Udefl 0.00 [kV]
REPHZ 3.00 [Hz]
ATTEN 28.0
ML1 2510245.292
ML2 303.237
ML3 0.000
HITURBO no
GDEON yes
GDEDLY short
DEFLON no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 0.38
DPMASS 500.00 [Da]
RBNDVAL 0.00
LBNDVAL 0.00
IS2BNDV 0.00
CMT1 EXP366
CMT2 20pyridyl-Mgporphyrin


427 nm
407 nm
564 nm
605 nm
Absorbance
Wavelength (nm)
2
1.5
1
0.5
0
300
400
500
600
700
800
900
N
N
N
N
Mg
N
MgP-1e

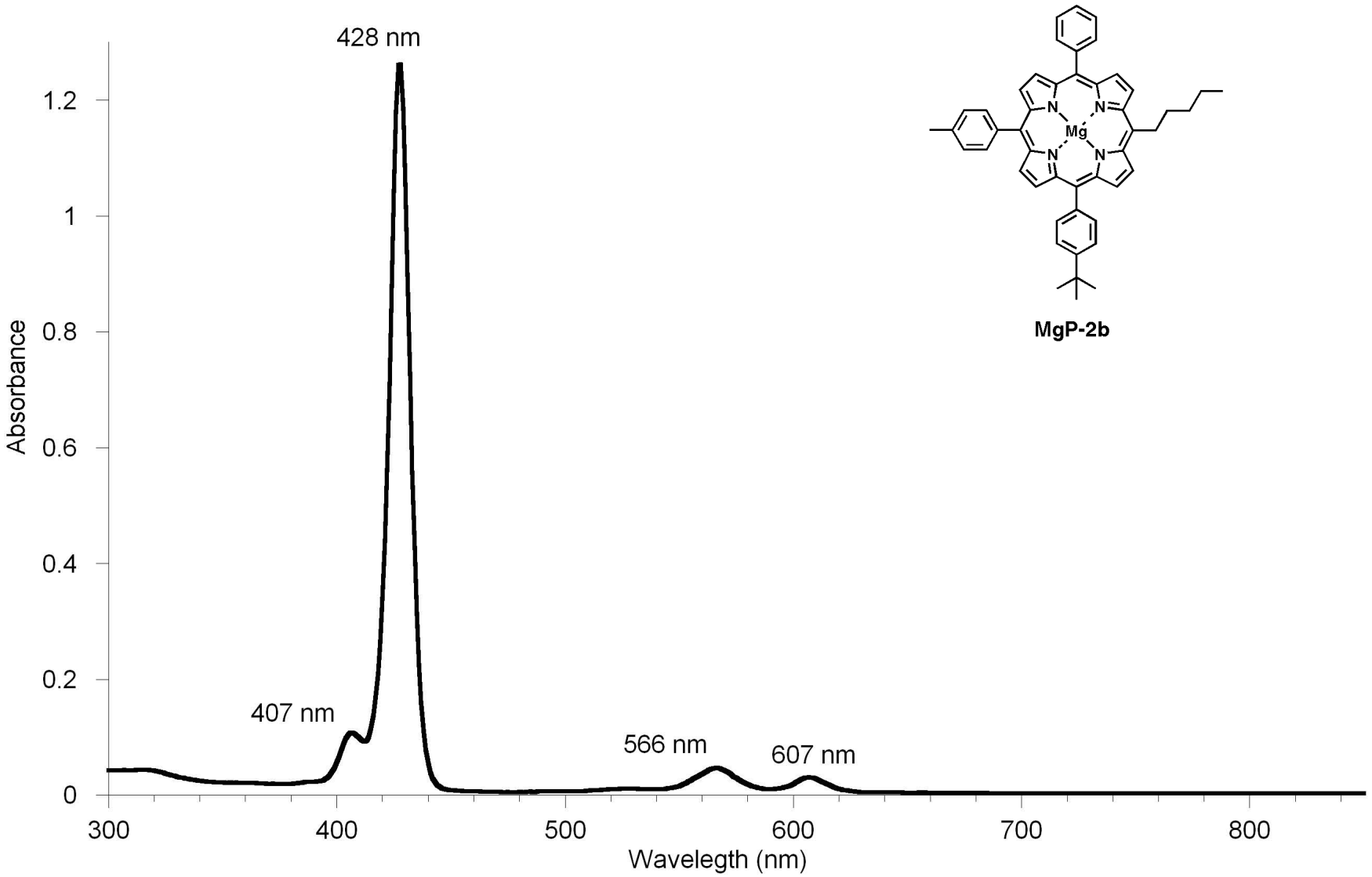

MgP-2b
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0


MgP-2b
N
N
N
N
Mg
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200



MgP-2b

INSTRUM MASSDEC
OpId tof
SMPNAM 071535
AQ_DATE 2007-09-25 15:36:14
PATH D:\data\Chemistry\Lindsey\Dogutan
POLARI POS
AQOP_m Reflector
TD 23334
NoSHOTS 200
SMONUM 0
SMOPTS1 0
SMOPTS2 0
SMOPTS3 0
DW 1.00 [ns]
DELAY 5184 [ns]
Uis1 19.00 [kV]
Uis2 17.50 [kV]
Urefl 0.00 [kV]
Ulens 9.70 [kV]
Uhimass 0.00 [kV]
RefFull 0.00 [kV]
UdetL 1.62 [kV]
UdetR 0.00 [kV]
Udefl 0.00 [kV]
REPHZ 3.00 [Hz]
ATTEN 31.0
ML1 2513708.122
ML2 317.440
ML3 0.000
HITURBO no
GDEON yes
GDEDLY short
DEFLON no
RLNSBND no
LLNSBND no
UIS2BND no
DPCAL1 0.38
DPMASS 1000.00 [Da]
RBNDVAL 0.00
LBNDVAL 0.00
IS2BNDV 0.00
CMT1 20pentyl-Mgporphyrin
CMT2 EXP377


428 nm
407 nm
566 nm
607 nm
Absorbance
Wavelegth (nm)
0
0.2
0.4
0.6
0.8
1
1.2
300
400
500
600
700
800
N
N
Mg
N
N

MgP-2b