

Electronic Supplementary Information

Construction of the Quinobenzoxazine Core *via* Gold-Catalyzed Dual Annulation of Azide-Tethered Alkynones with Anthranil

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General information:

The reactions were carried out in anhydrous solvents under argon atmosphere in oven-dried glassware. All anhydrous solvents were distilled prior to use. Commercial reagents were used without any purification. Column chromatography was carried out by using silica gel (60–120, 100–200, 230–400 mesh). ^1H and ^{13}C NMR chemical shifts are reported relative to chloroform-d ($\delta = 7.27$) or TMS, and coupling constants (J) are reported in hertz (Hz). The following abbreviations have been used to designate signal multiplicity: s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, sxt = sextet, sept = septet, m = multiplet, b = broad. High-resolution mass spectra (HRMS) were recorded on a Q Exactive Hybrid Quadrupole Orbitrap mass spectrometer, where the mass analyzer used for analysis is orbitrap & some compounds on electrospray ionization time-of-flight (ESI-TOF). Infra-red (IR) spectra were measured in cm^{-1} using FT-IR spectrophotometer. All *o*-azidoacetylenic ketones¹⁻³ & anthranil⁴ substrates were prepared by the known literature procedures.

Crystallographic data for the structural analysis of compound 7

Good quality single crystals were hand-picked under polarized optical microscopy and then mounted in the diffractometer. The data collection was done at 100-150 K. X-ray intensity data measurements of **7** was carried out on a Bruker SMART APEX II CCD diffractometer with graphite-monochromatized ($\text{MoK}\alpha = 0.71073 \text{ \AA}$) radiation. The X-ray generator was operated at 50 kV and 30 mA. A preliminary set of cell constants and an orientation matrix were calculated from three sets of 36 frames. Data were collected with ω scan width of 0.5° at different settings of φ and 2θ keeping the sample-to-detector distance fixed at 5.00 cm. The X-ray data collection was monitored by APEX2 program (Bruker, 2006).⁵ All the data were corrected for Lorentzian, polarization, and absorption effects using SAINT and SADABS programs (Bruker, 2006). SHELX-97 was used for structure solution and full matrix least-squares refinement on F^2 .⁶ All the hydrogen atoms were placed in geometrically idealized position and constrained to ride on their parent atoms. An *ORTEP* view of **7** was drawn with 50% probability displacement ellipsoids and H atoms omitted for clarity.⁷

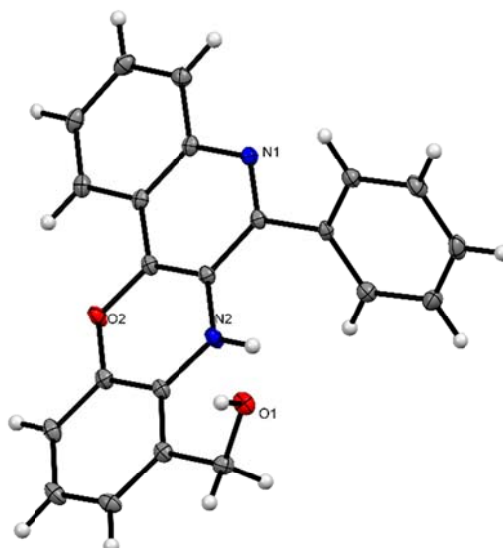


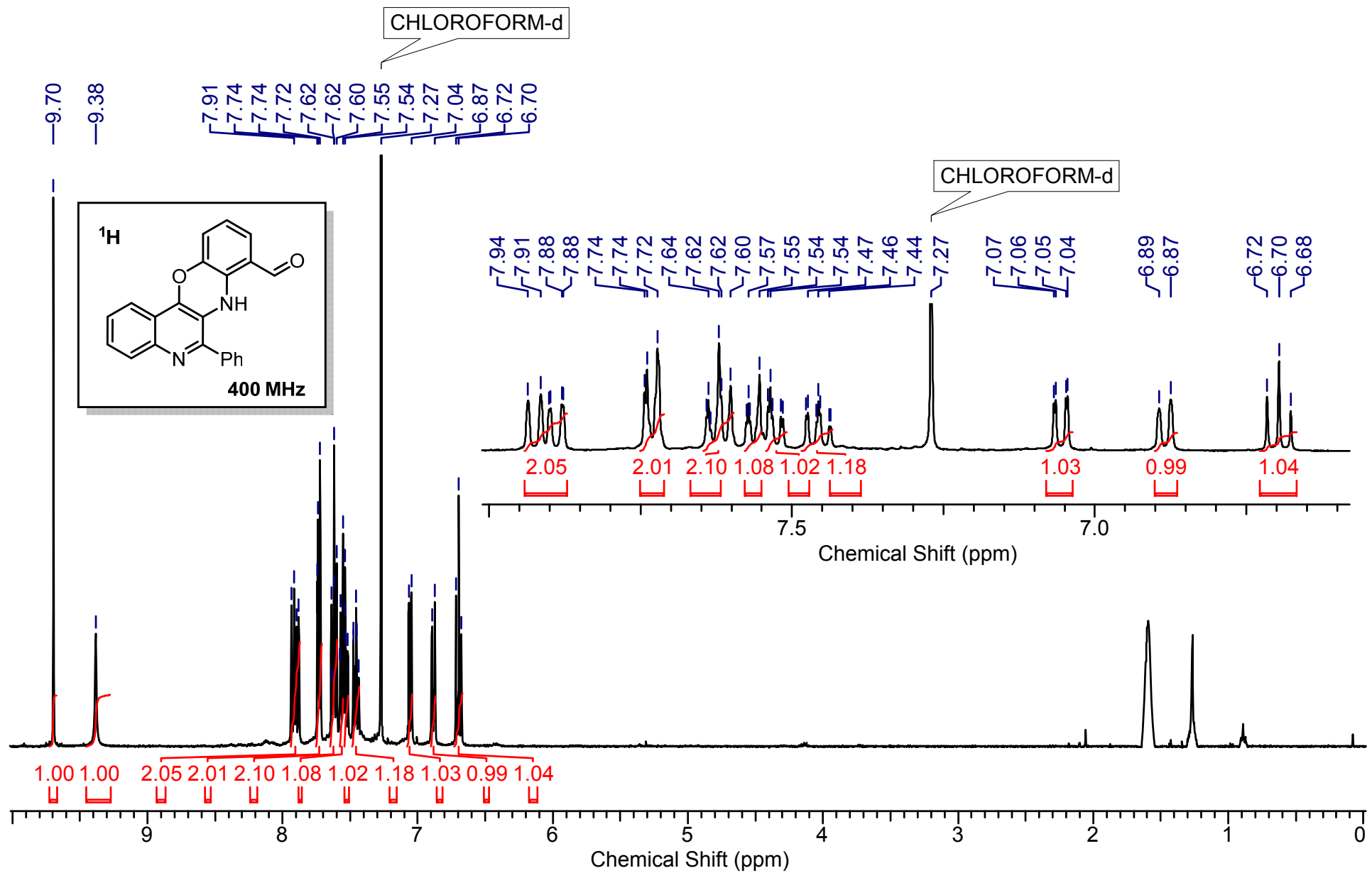
Figure S1: ORTEP diagram of Compound 7.
(Thermal ellipsoids are shown at 50% probability level.)]

Single Crystal Data of Compound 7	
Empirical Formula	C ₂₂ H ₁₆ N ₂ O ₂
Formula Weight	340.38
Crystal System	Monoclinic
Space Group	P2 ₁ /n
T (K)	100
<i>a</i> (Å)	9.4049(9)
<i>b</i> (Å)	13.3896(12)
<i>c</i> (Å)	12.7634(13)
α (°)	90
β (°)	91.507(4)
γ (°)	90
<i>V</i> (Å ³)	1606.7(3)
<i>D</i> _{calc} (g cm ⁻³)	1.407
<i>Z</i>	4
<i>R</i> ₁ (<i>I</i> > 2σ(<i>I</i>))	0.0455
<i>R</i> _{int}	0.0430
<i>wR</i> ₂ (all)	0.1209
Measured reflections	45851
Independent Reflections	4126
Reflections with <i>I</i> > 2σ(<i>I</i>)	3780
Goodness of Fit (<i>S</i>)	1.057
X-Ray Diffractometer	Bruker
CCDC Number	2193978

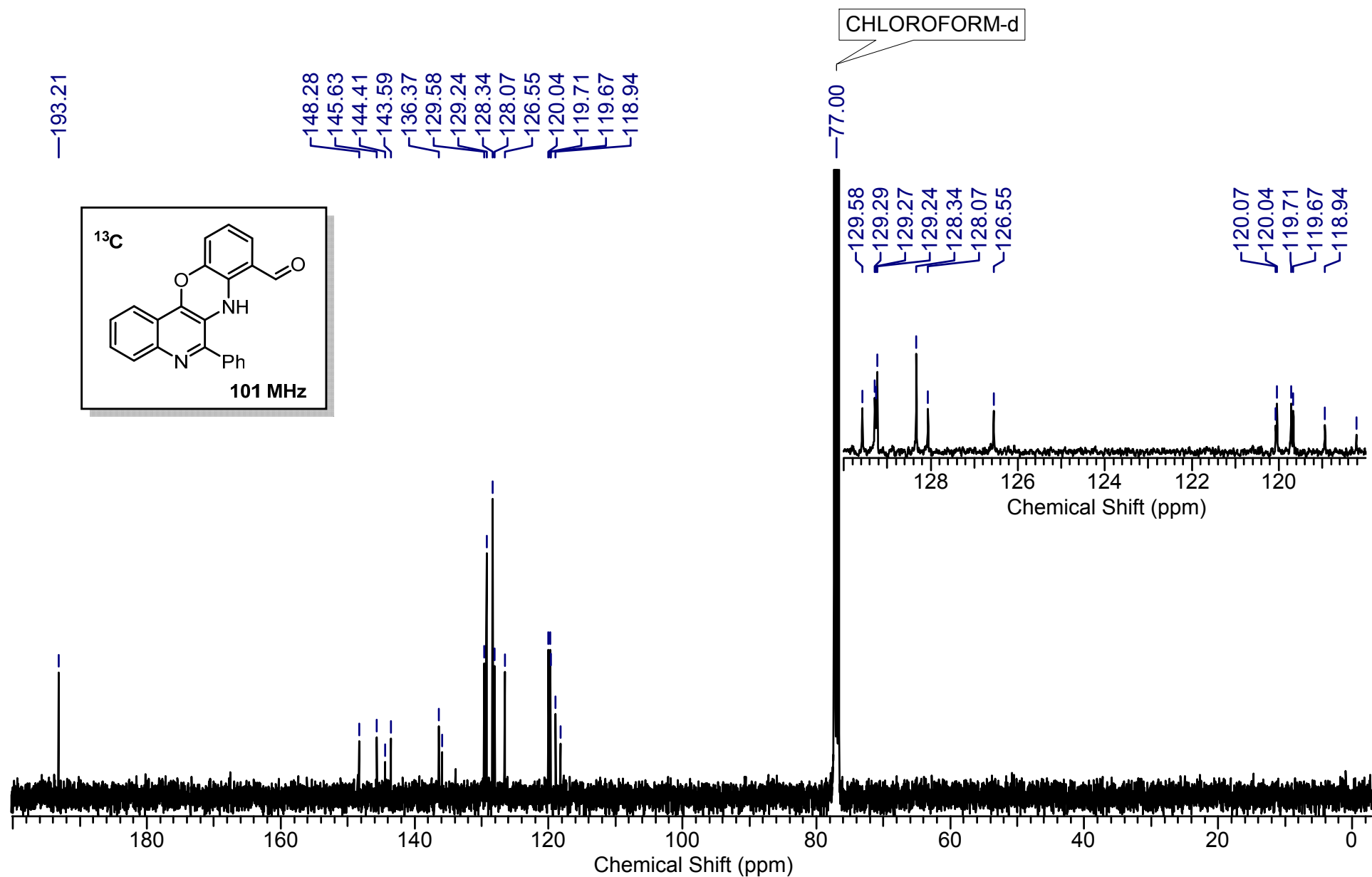
References:

1. H. Su, M. Bao, C. Pei, W. Hu, L. Qiu and X. Xu, *Org. Chem. Front.*, 2019, **6**, 2404–2409.
2. X. Wu, L. L. Zheng, L. P. Zhao, C. F. Zhu and Y. G. Li, *Chem. Commun.*, 2019, **55**, 14769–14772.
3. J. Huang, H. Su, M. Bao, L. Qiu, Y. Zhang and X. Xu, *Org. Biomol. Chem.*, 2020, **18**, 3888–3892.
4. J. Chauhan and S. Fletcher, *Tetrahedron Letters*, 2012, **53**, 4951–4954.
5. Bruker (2006). APEX2, SAINT and SADABS. Bruker AXS Inc. Madison, Wisconsin, USA.
6. G. M. Sheldrick, *Acta Cryst.*, 2008, **A64**, 112–122.
7. L. J. Farrugia, *J. Appl. Cryst.*, 1997, **30**, 565.

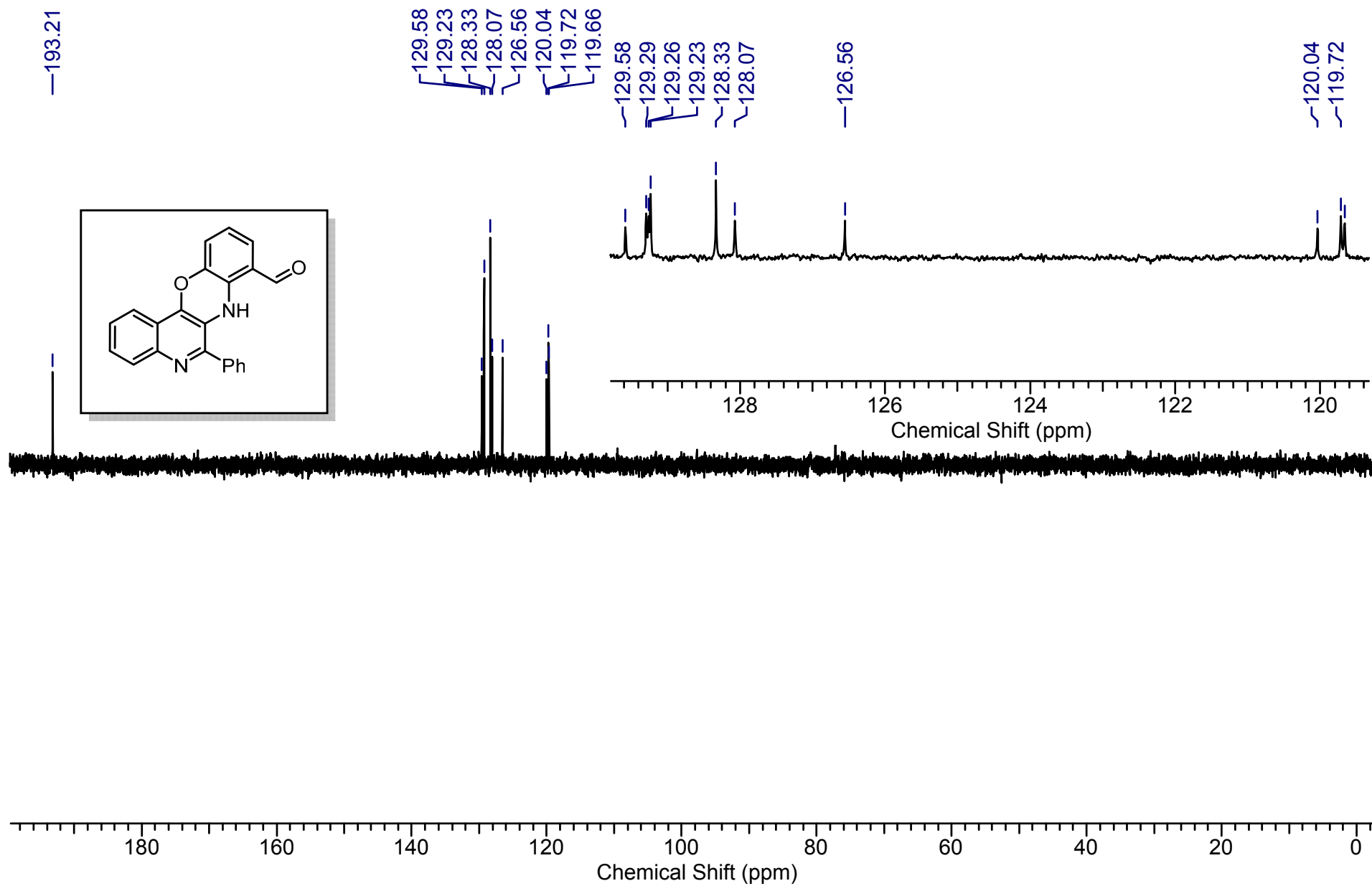
3aa



3aa

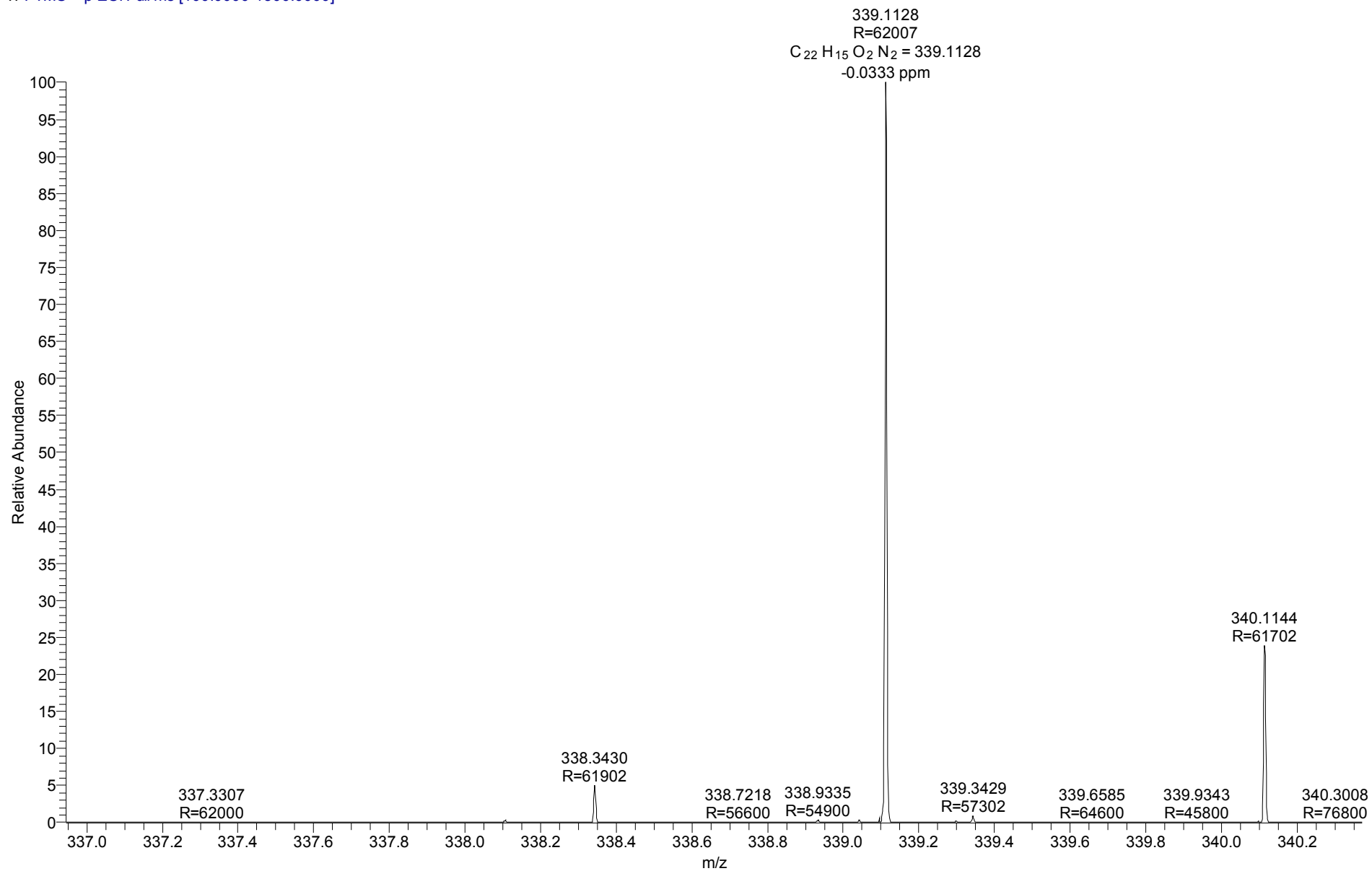


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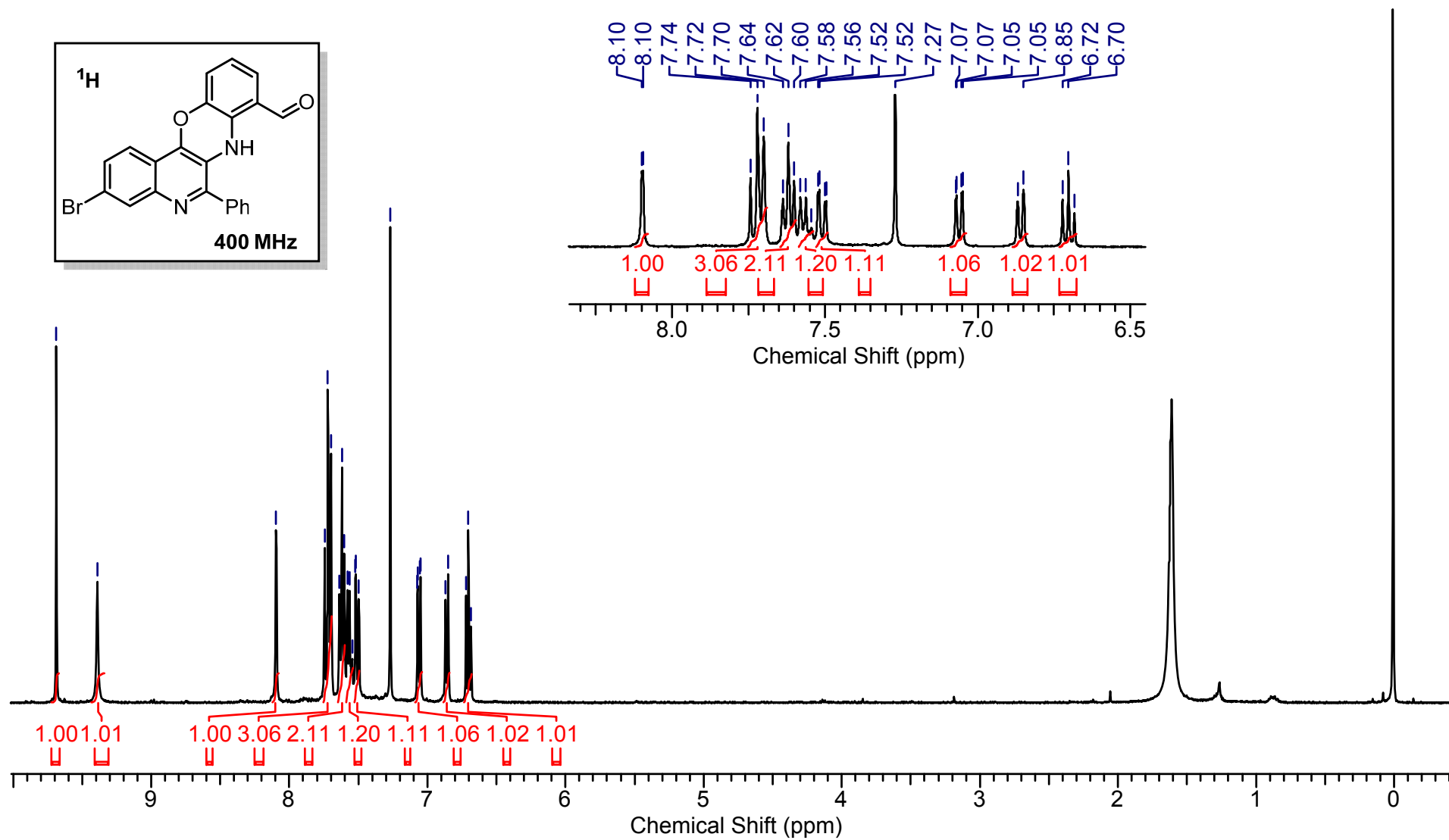
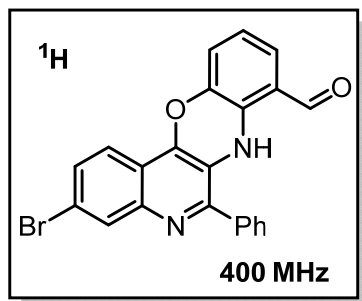
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Main-Substrate #613 RT: 2.73 AV: 1 NL: 3.32E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



3ba

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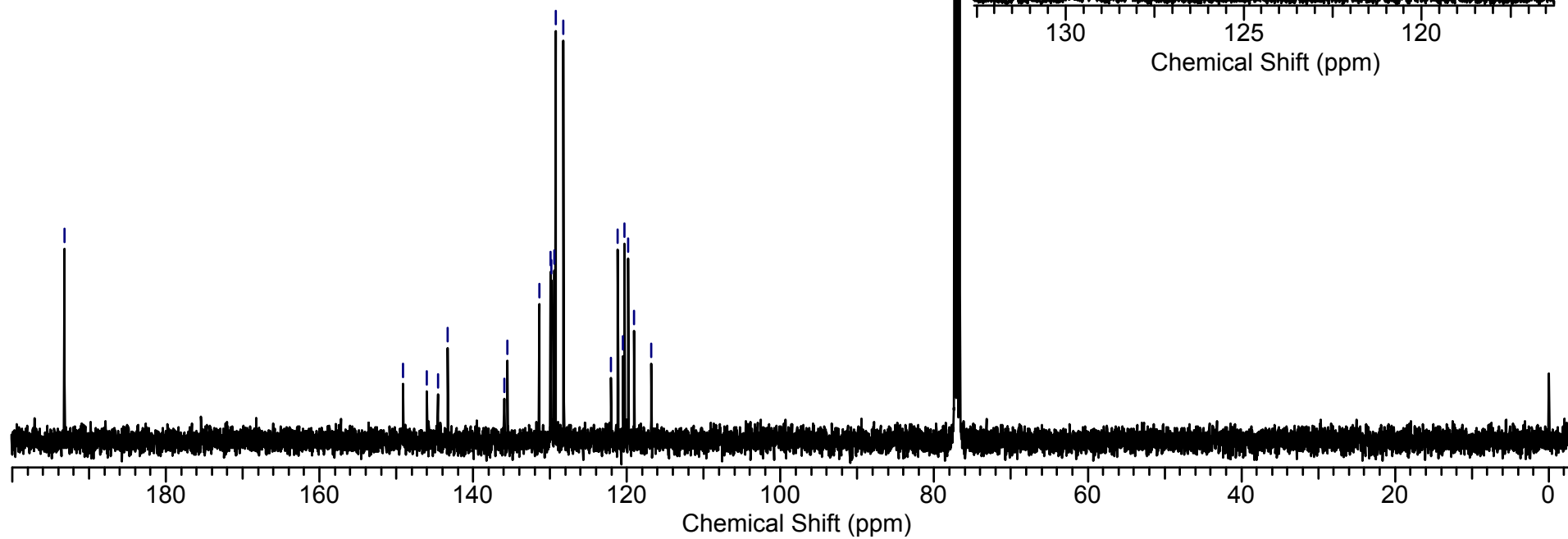
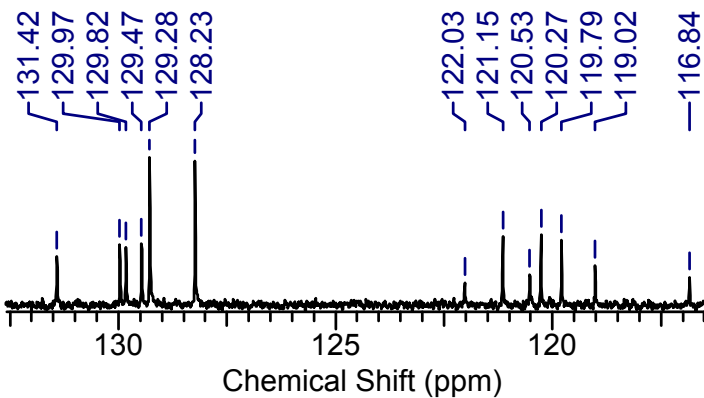
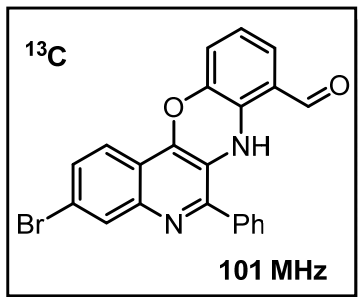


3ba

193.23

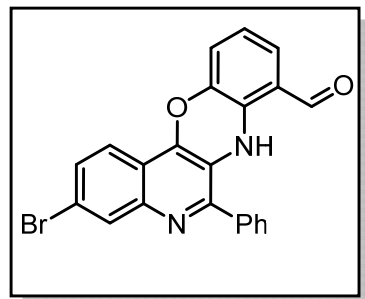
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119.02

77.31
77.00
76.68



3ba

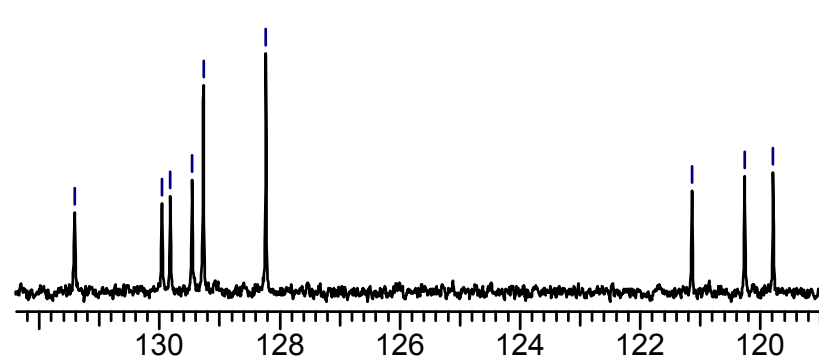
—193.23



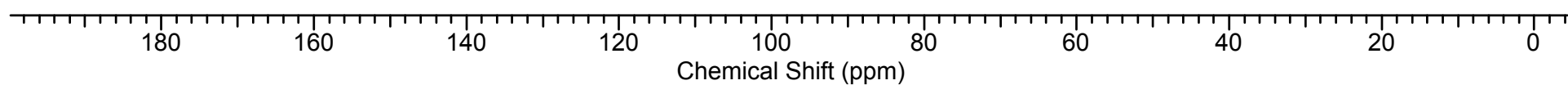
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129.46
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128.23

121.14
120.27
119.79

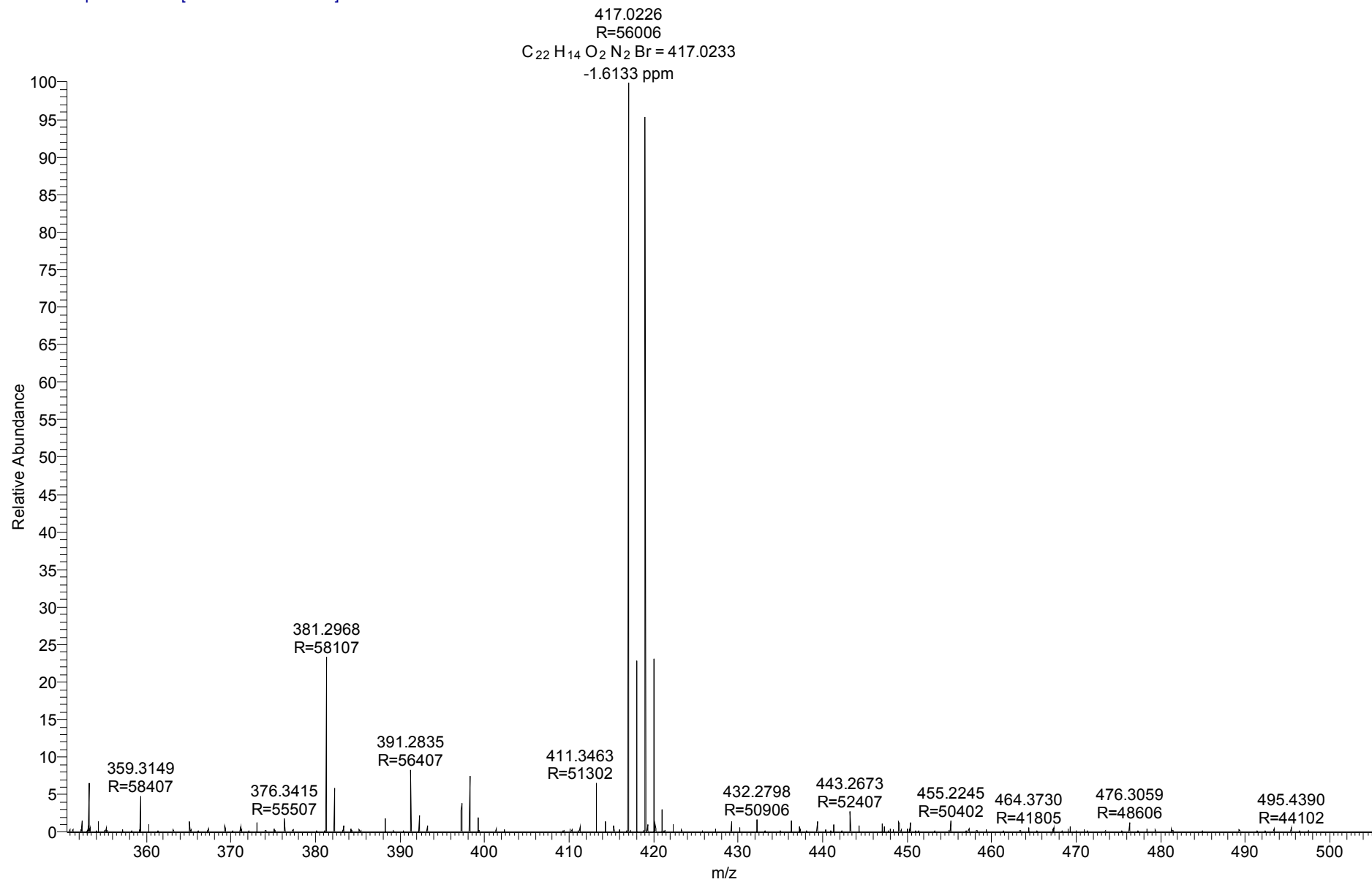


Chemical Shift (ppm)



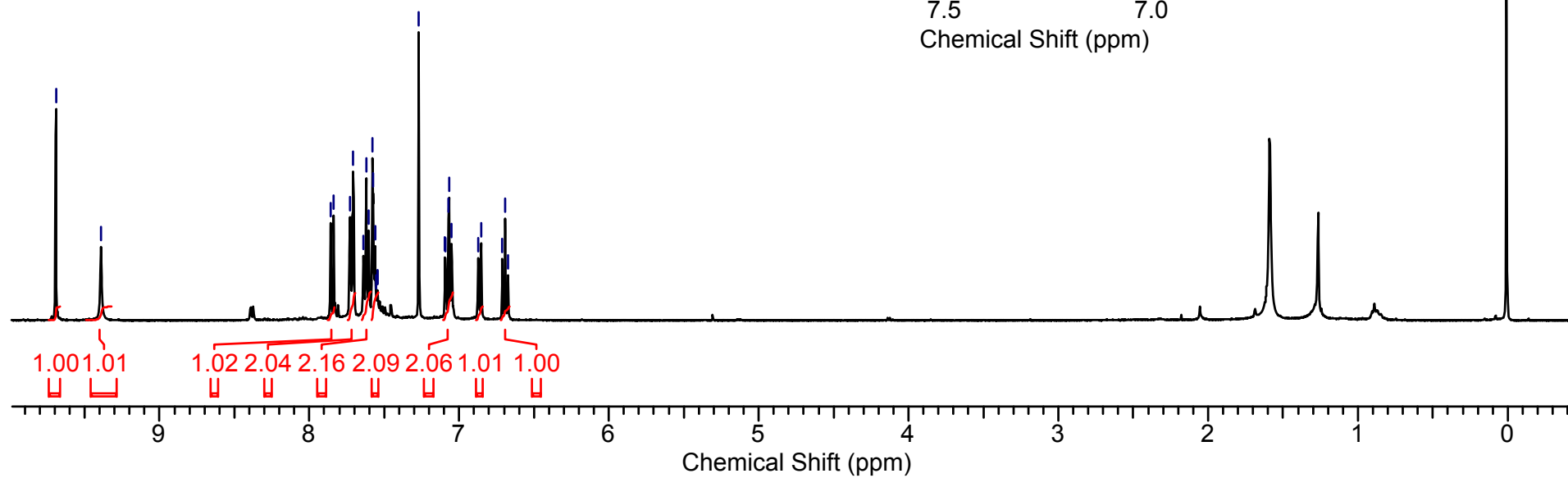
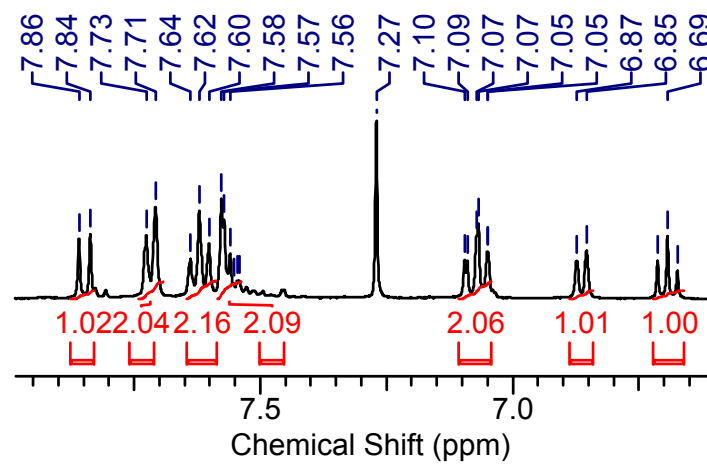
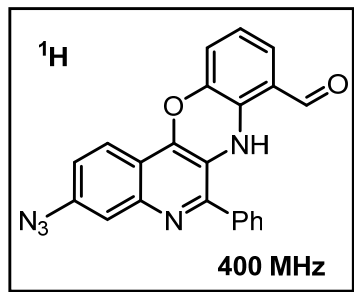
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3ca

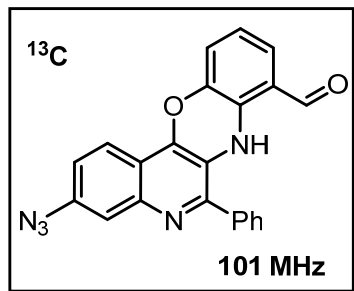
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9.39
7.86
7.84
7.73
7.71
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7.57
7.27
7.07
7.07
7.05
6.85
6.69



3ca

—193.19

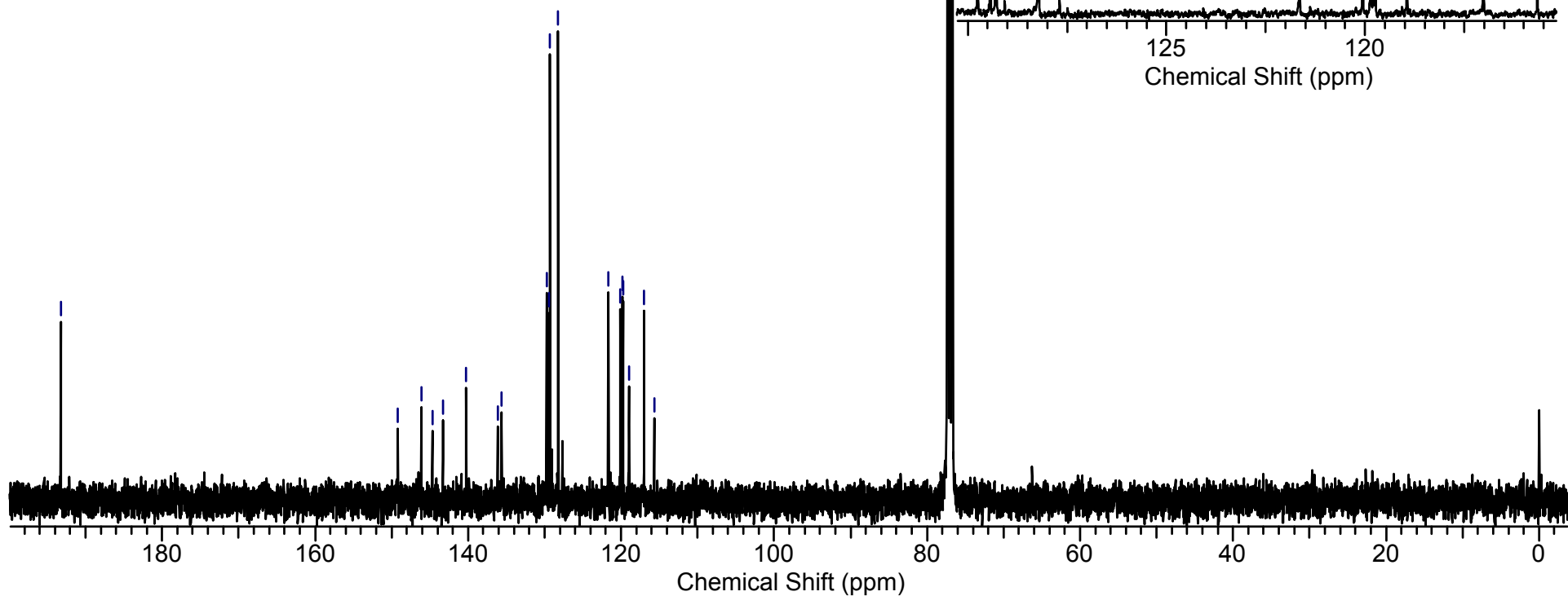
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146.12
144.68
140.23
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120.06
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119.74
118.94
117.02



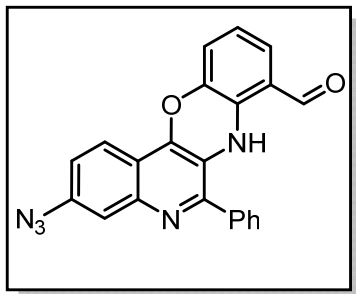
77.32
129.75
77.00
129.43
76.68
129.28
128.22

121.65
120.06
119.85
119.80
119.74
118.94
117.02
115.66

125
120
Chemical Shift (ppm)



3ca



193.19

129.75
129.43
129.28
128.21
121.65
120.06
119.85
119.73
117.02

129.75
129.43
129.28

128.21

121.65

120.06
119.85
119.73

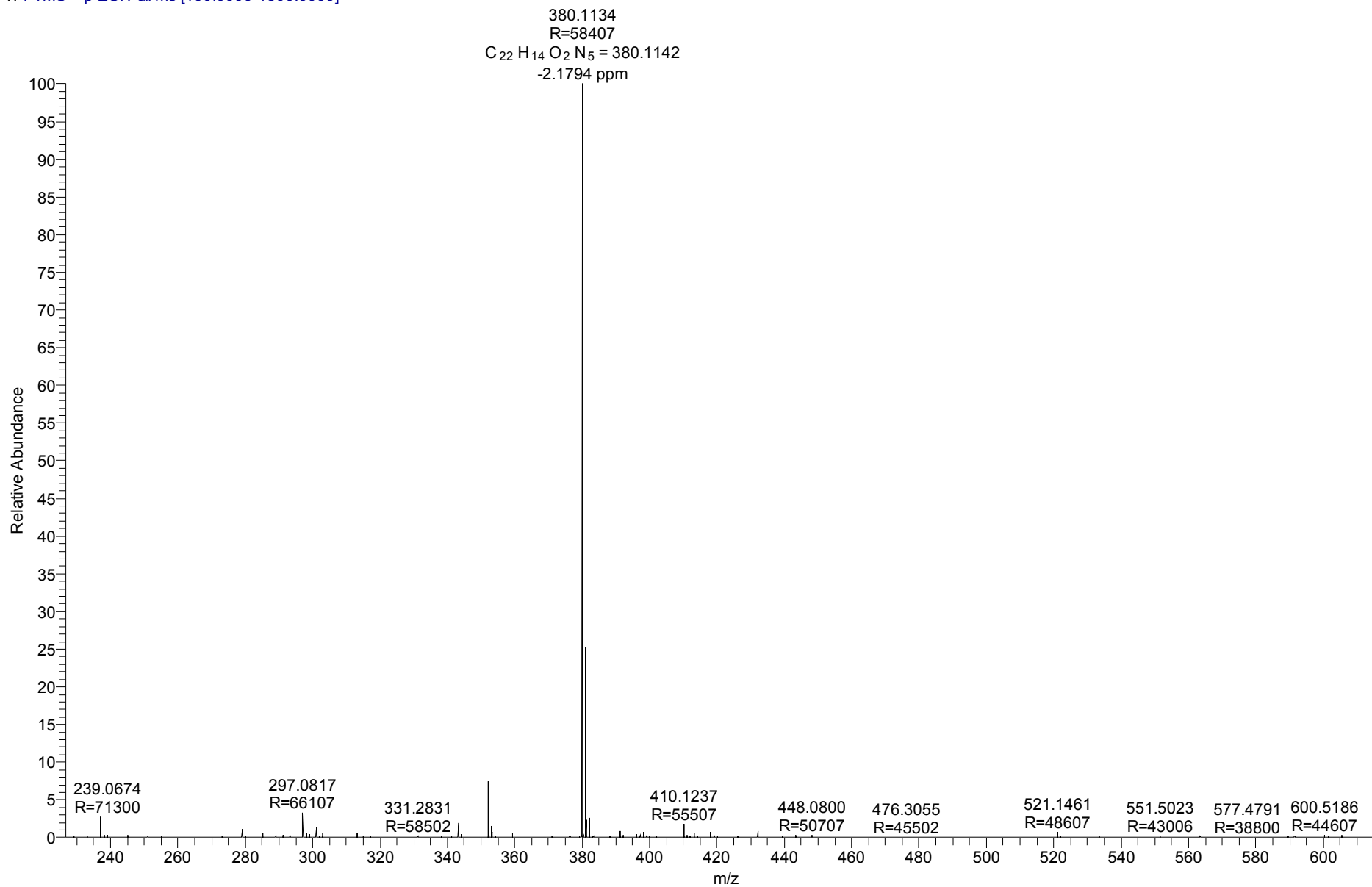
117.02

130 128 126 124 122 120 118
Chemical Shift (ppm)

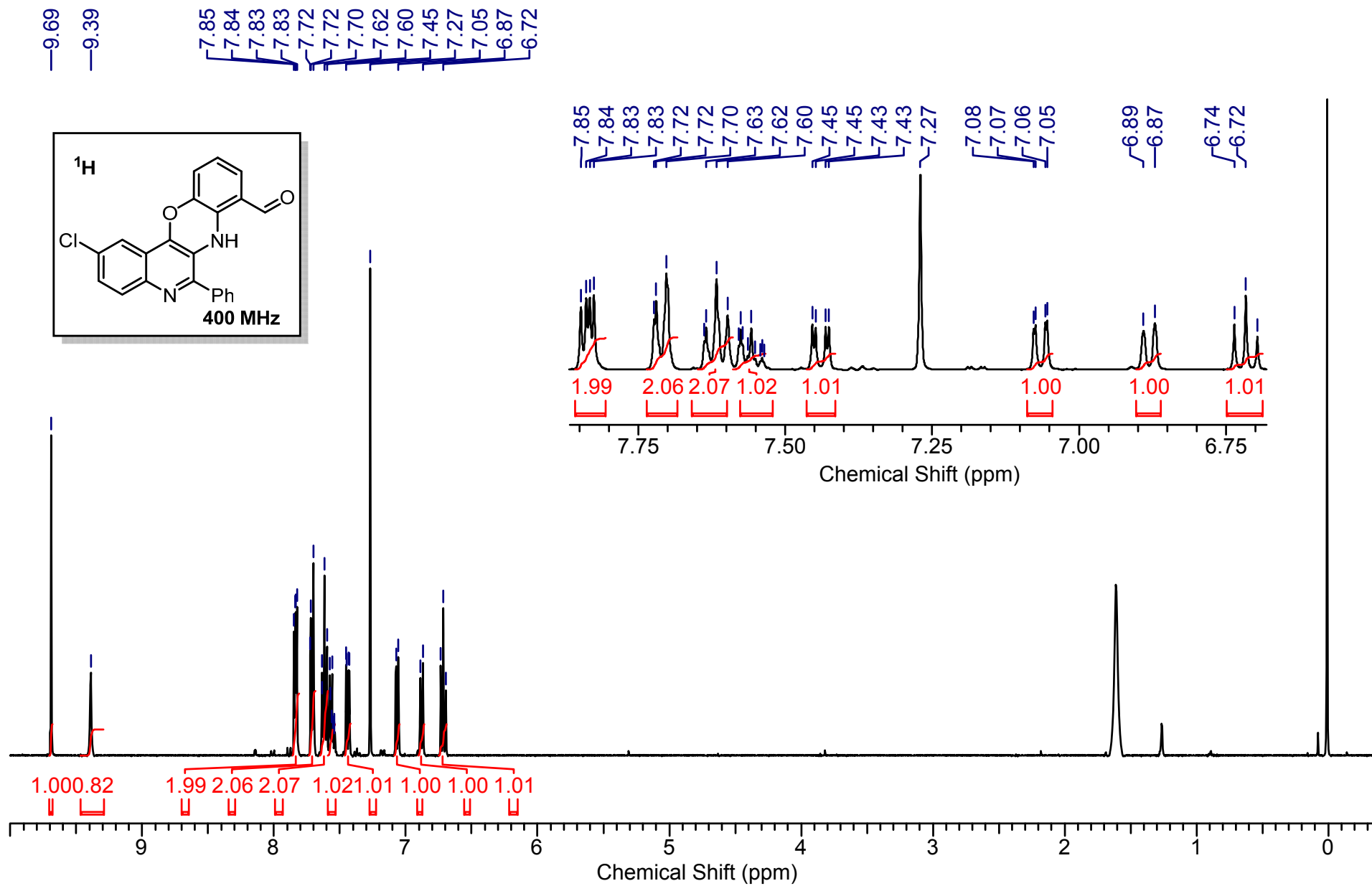
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Chemical Shift (ppm)

3ca

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3da

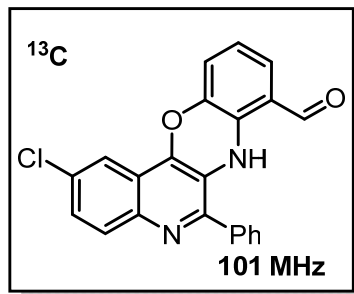


3da

193.27

148.43
143.84
143.38
136.00
132.58
130.88
129.76
129.44
129.28
128.95
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120.40
119.84
119.07
118.64

77.31
77.00
76.68



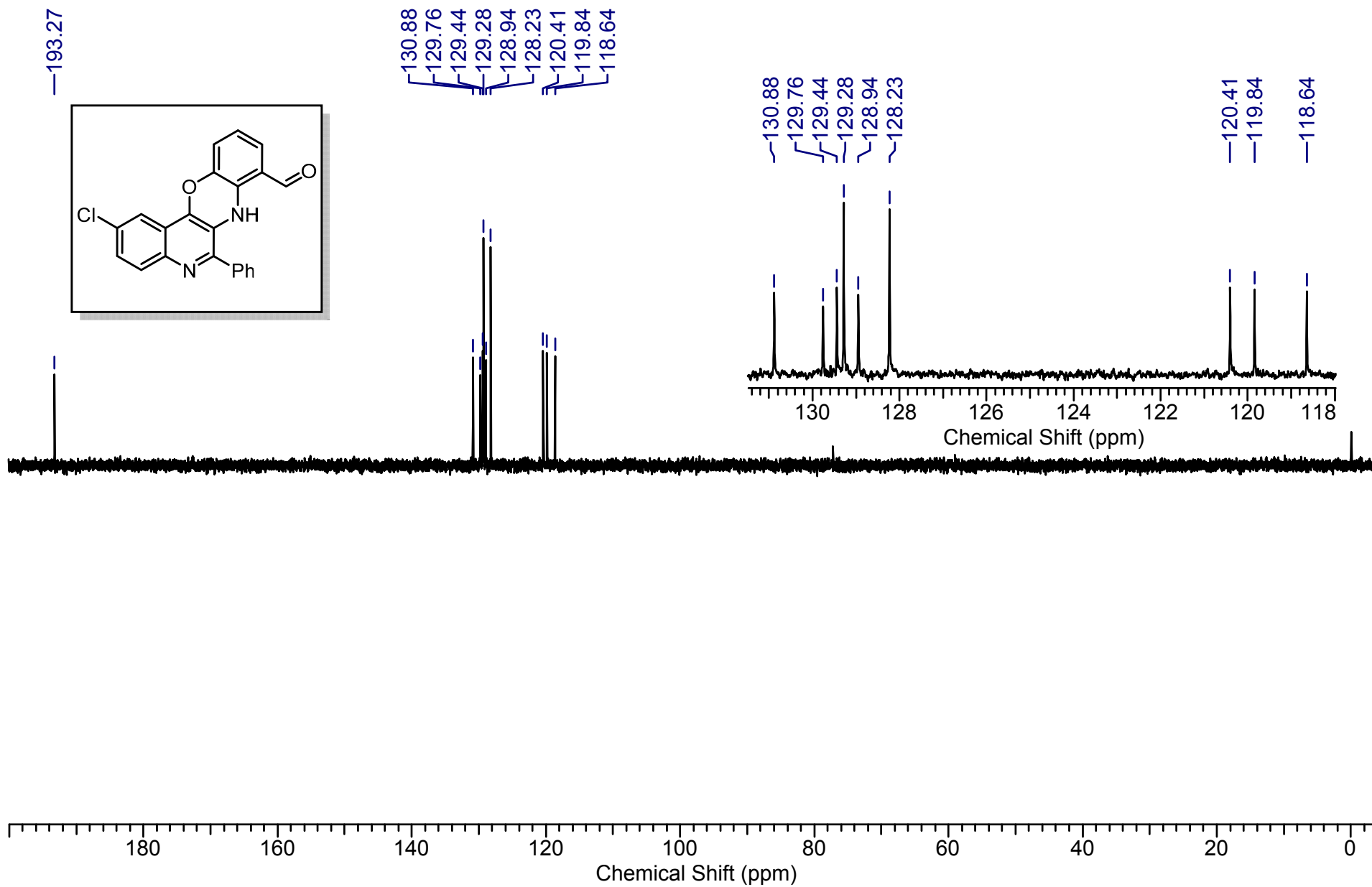
130.88
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128.95
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120.93
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119.07
118.80
118.64

Chemical Shift (ppm)

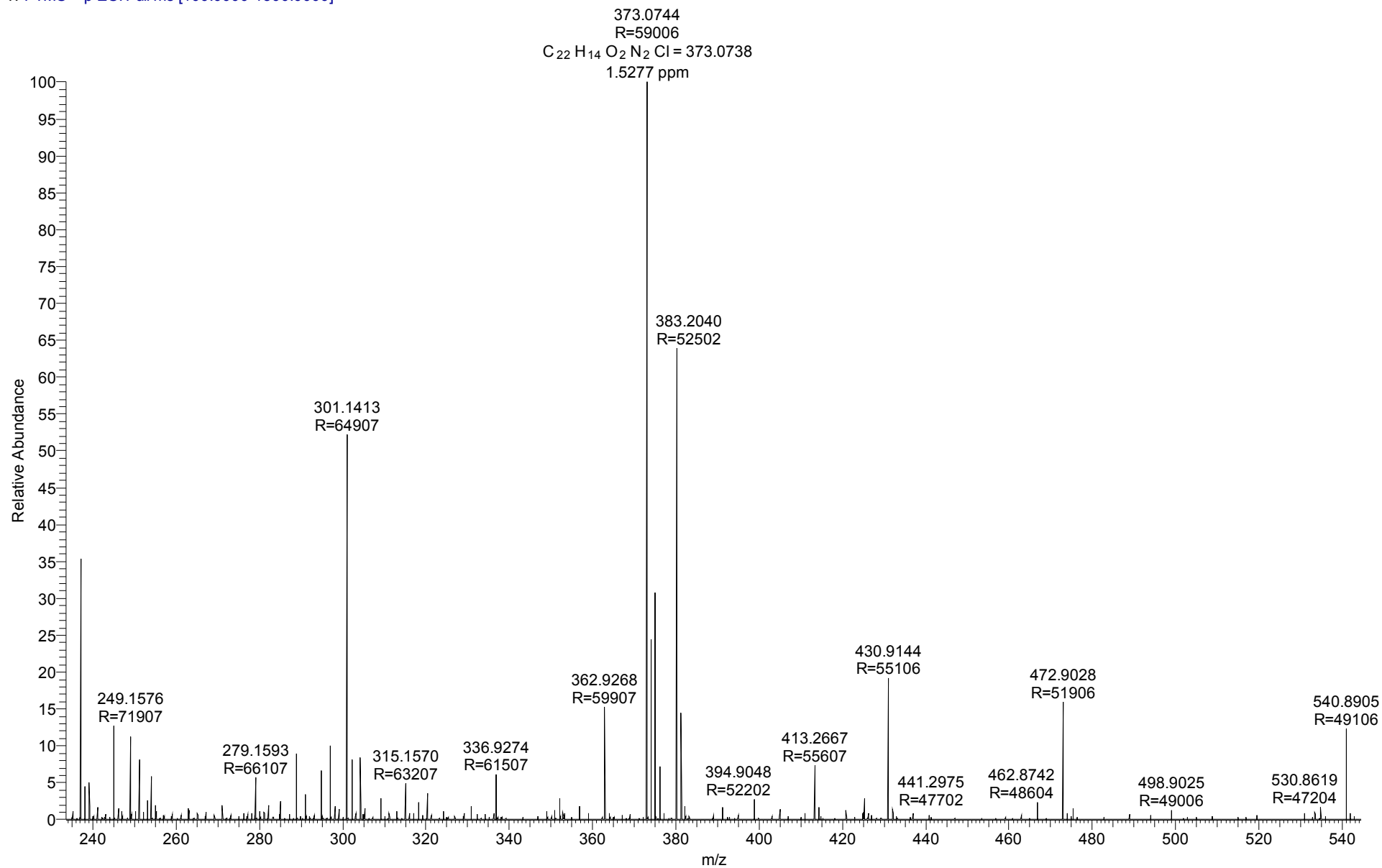
Chemical Shift (ppm)

3da

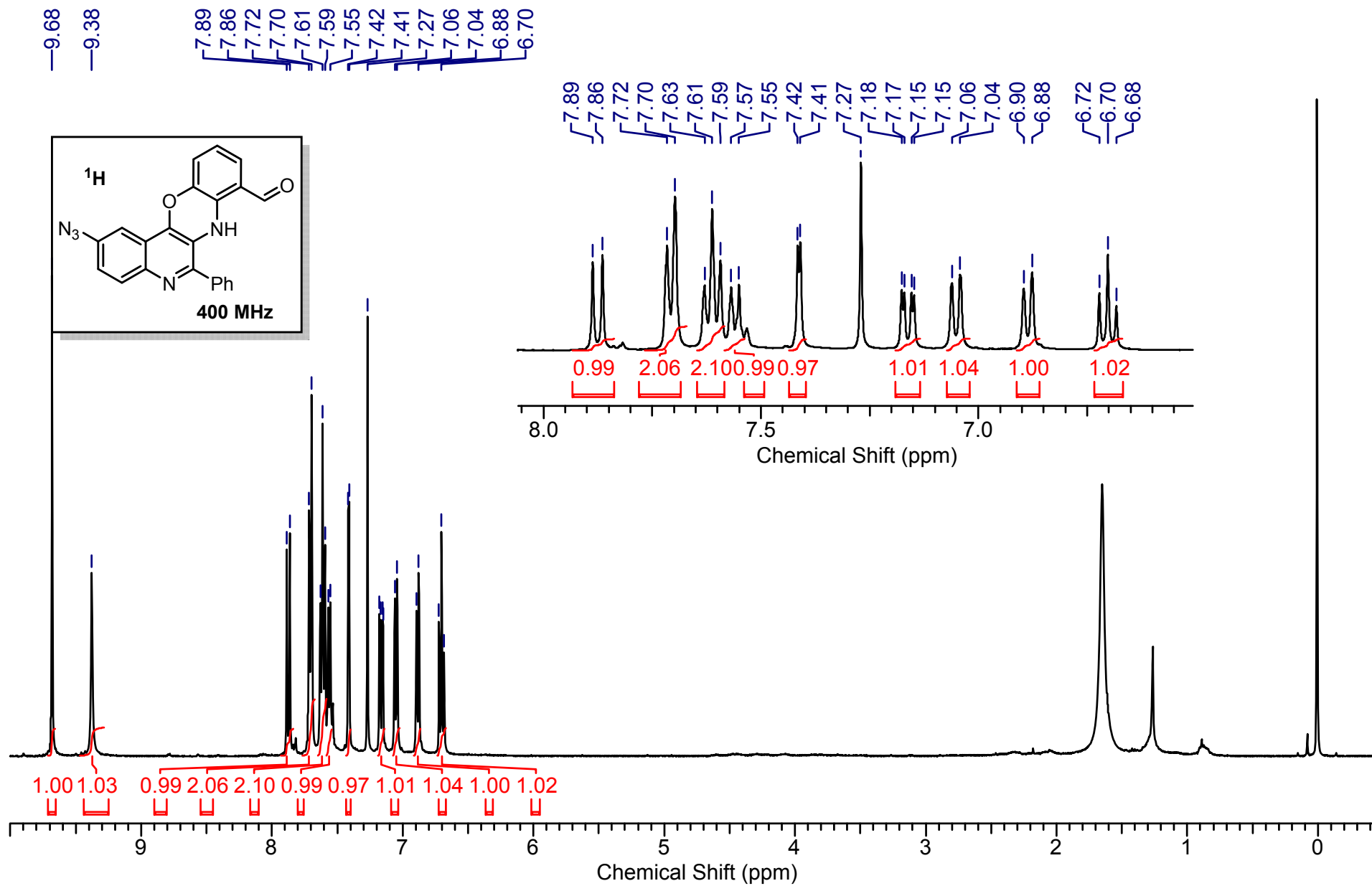


3da

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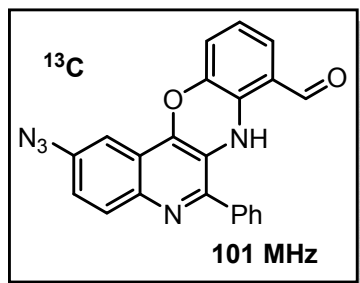
3ea



3ea

193.25

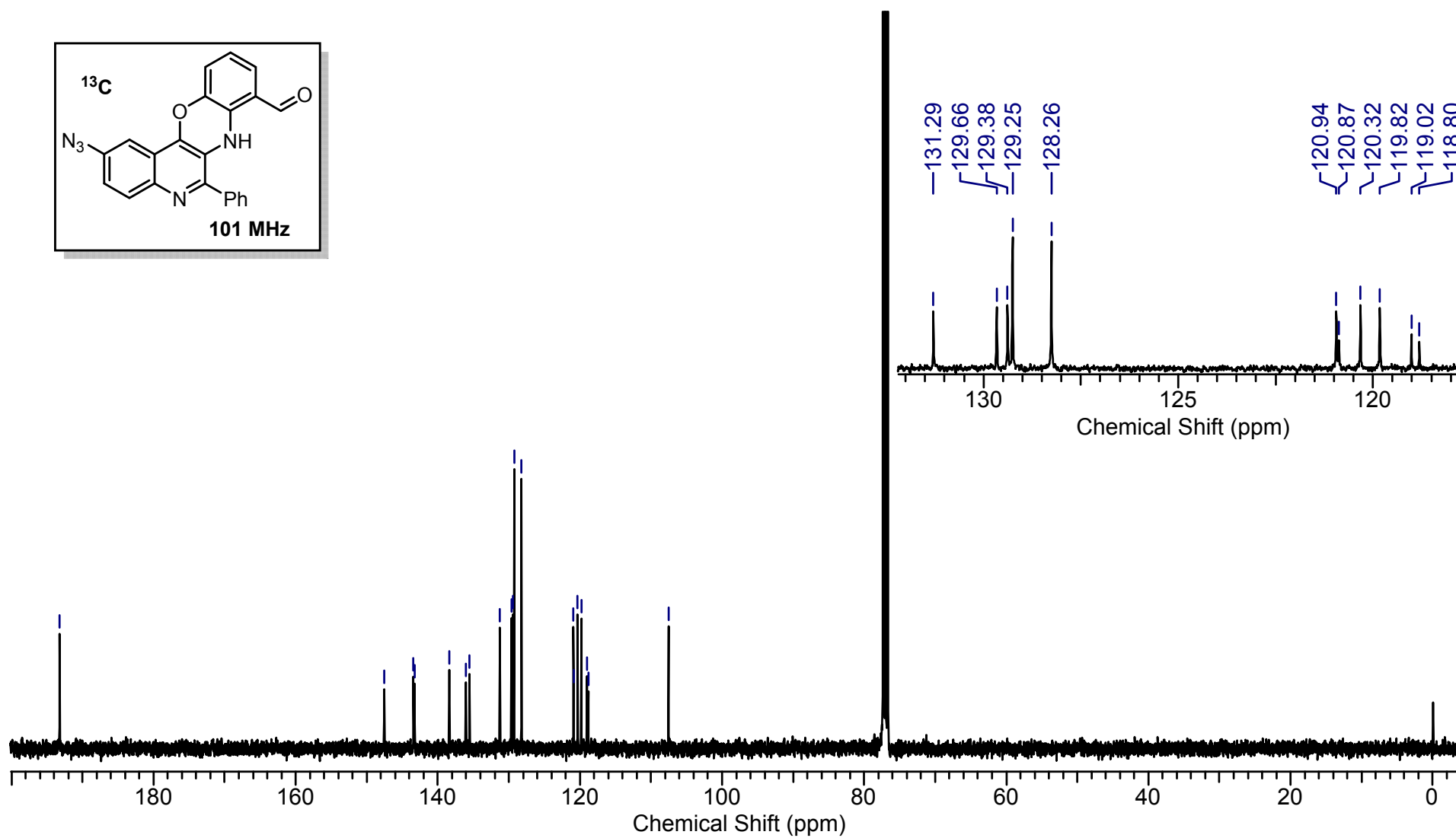
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119.02
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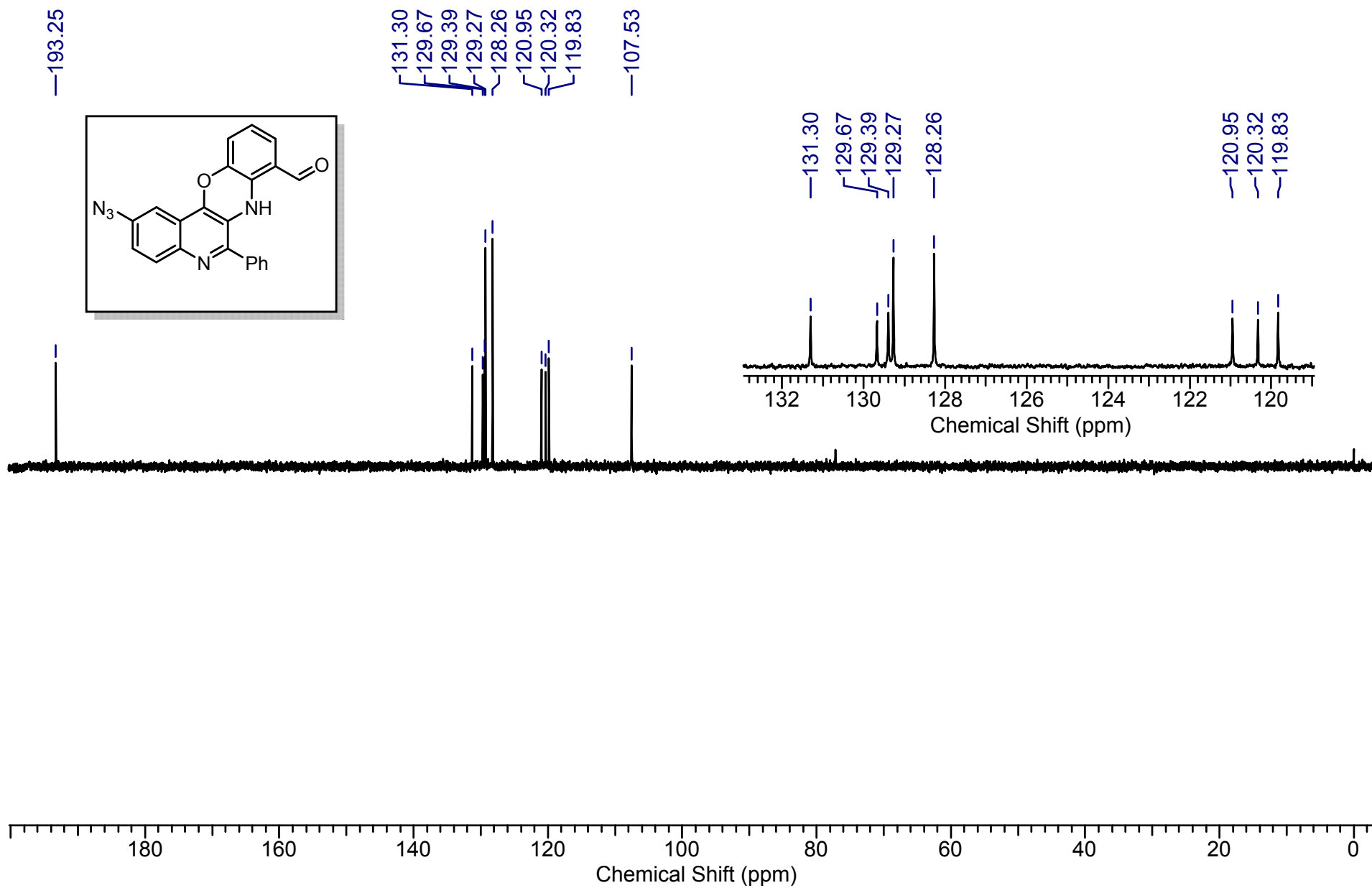


77.32
77.00
76.68

131.29
129.66
129.38
129.25
128.26

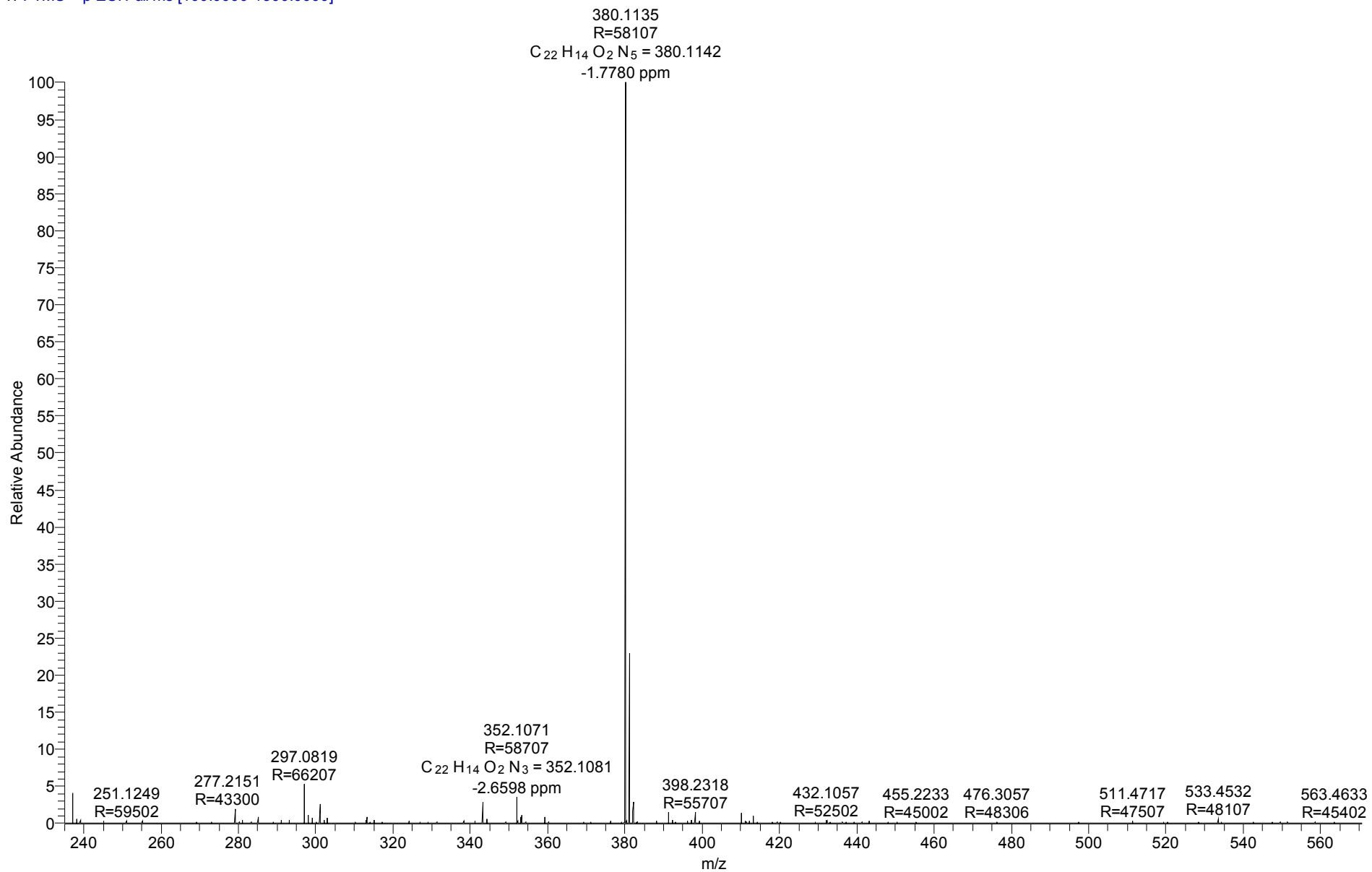
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120.87
120.32
119.82
119.02
118.80



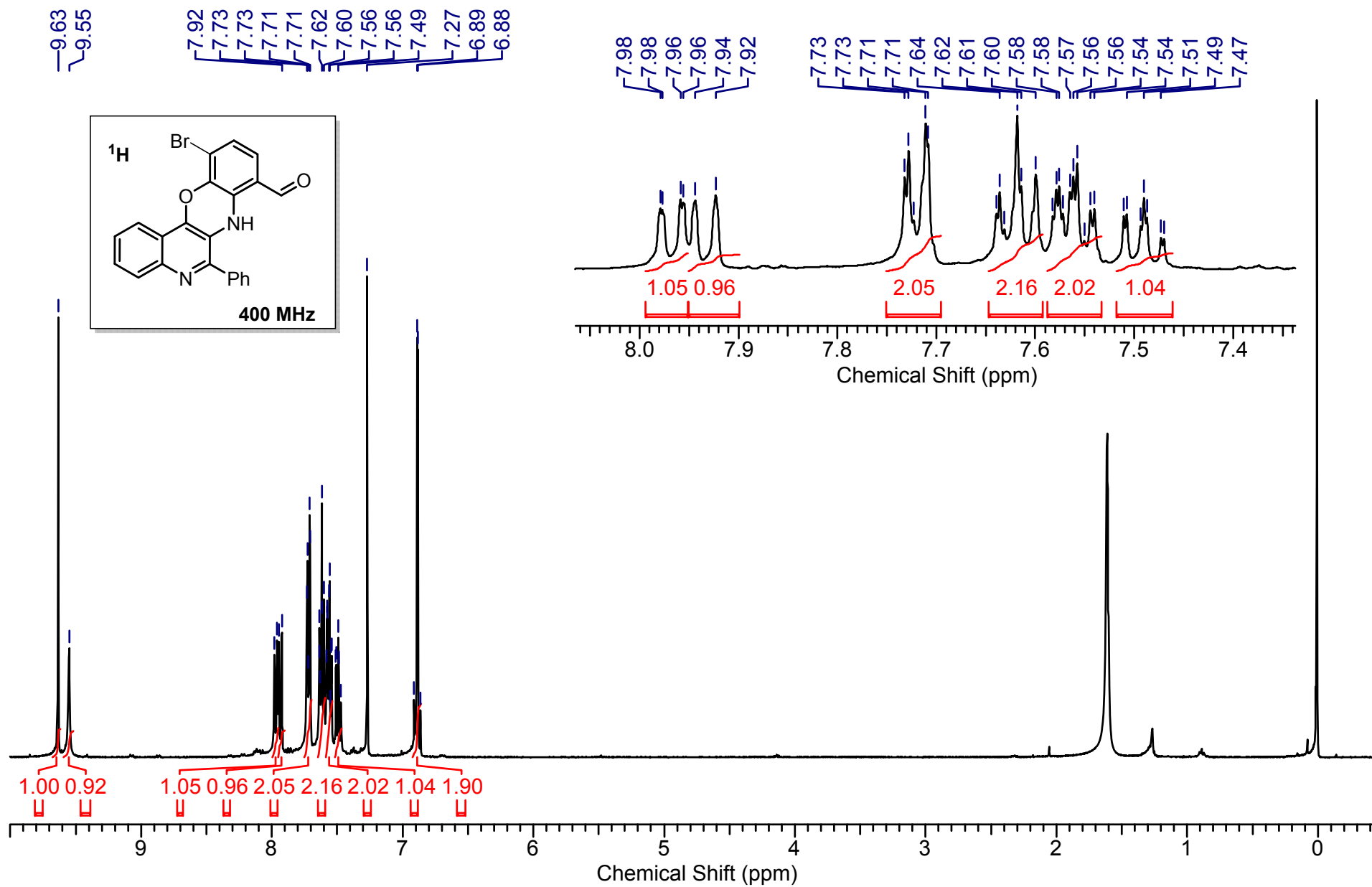


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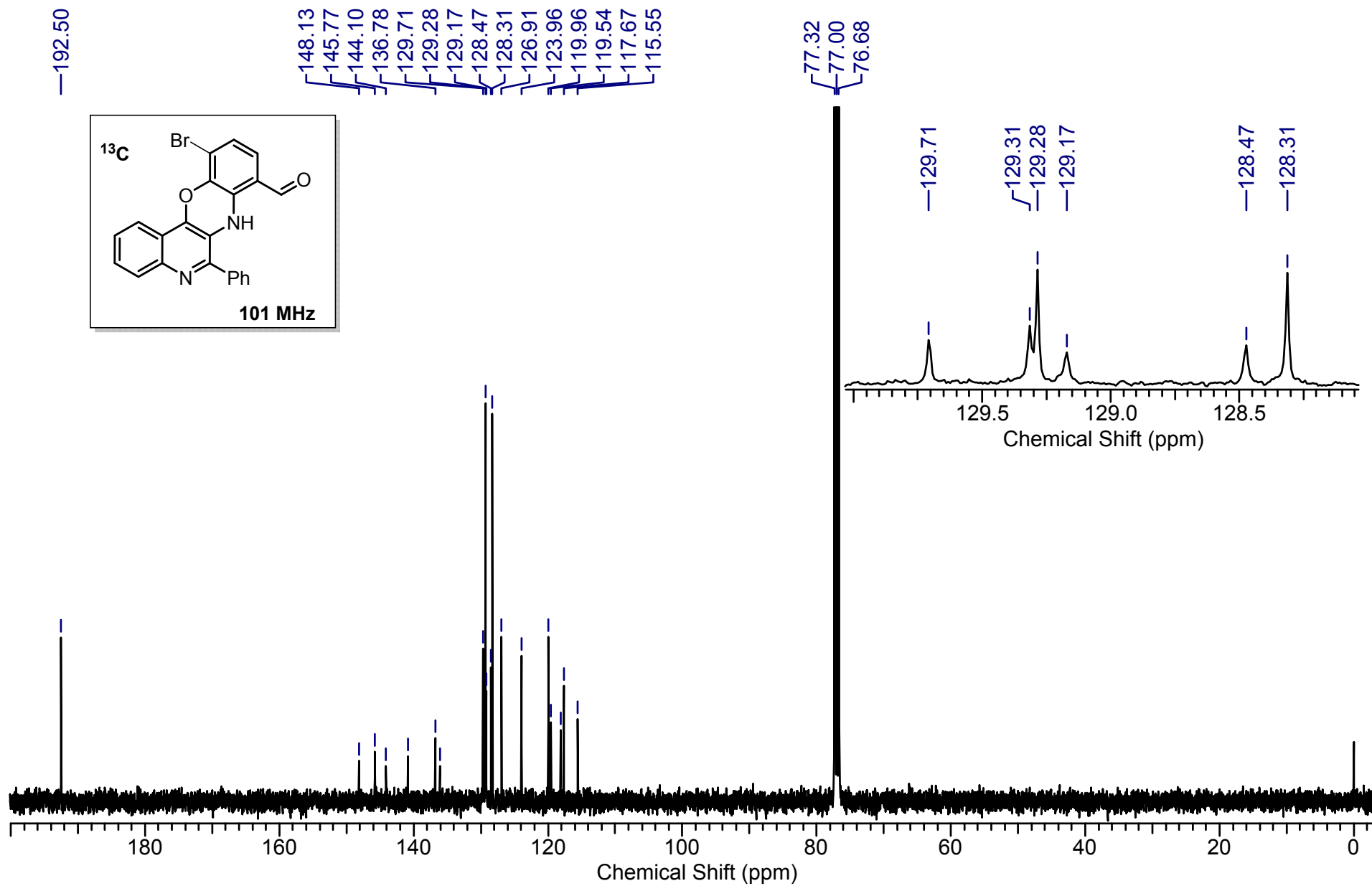
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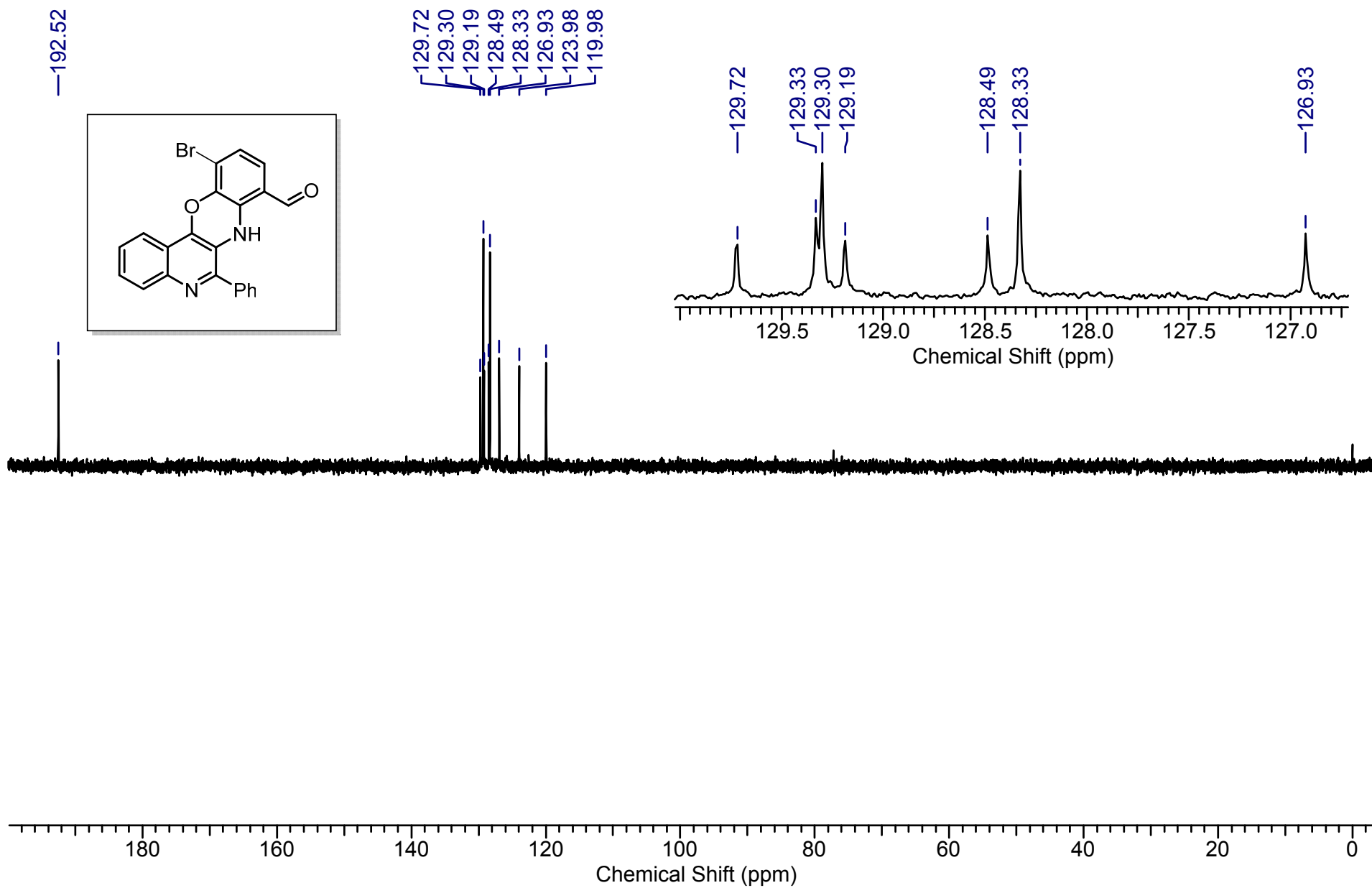
3ab



3ab

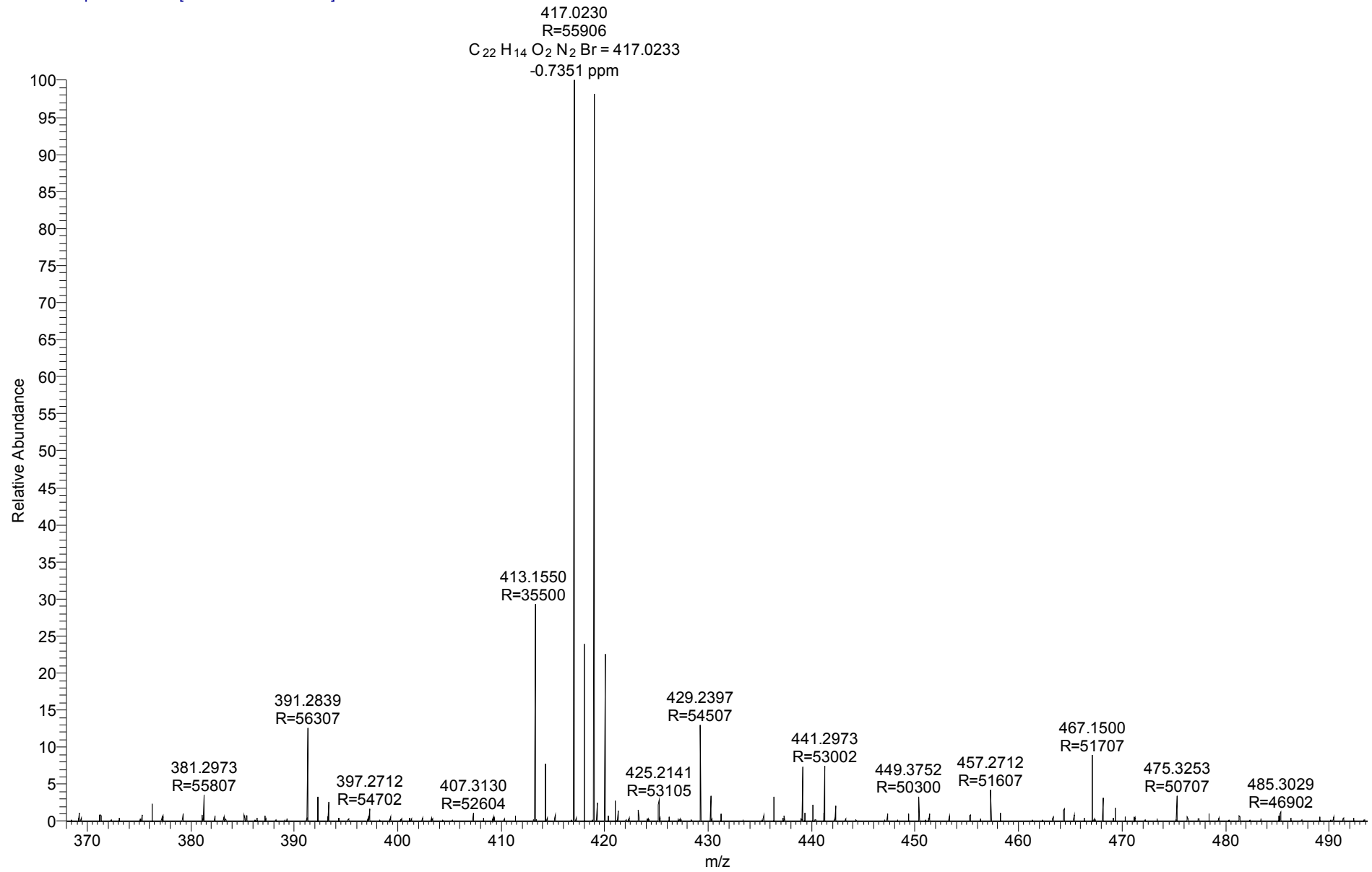


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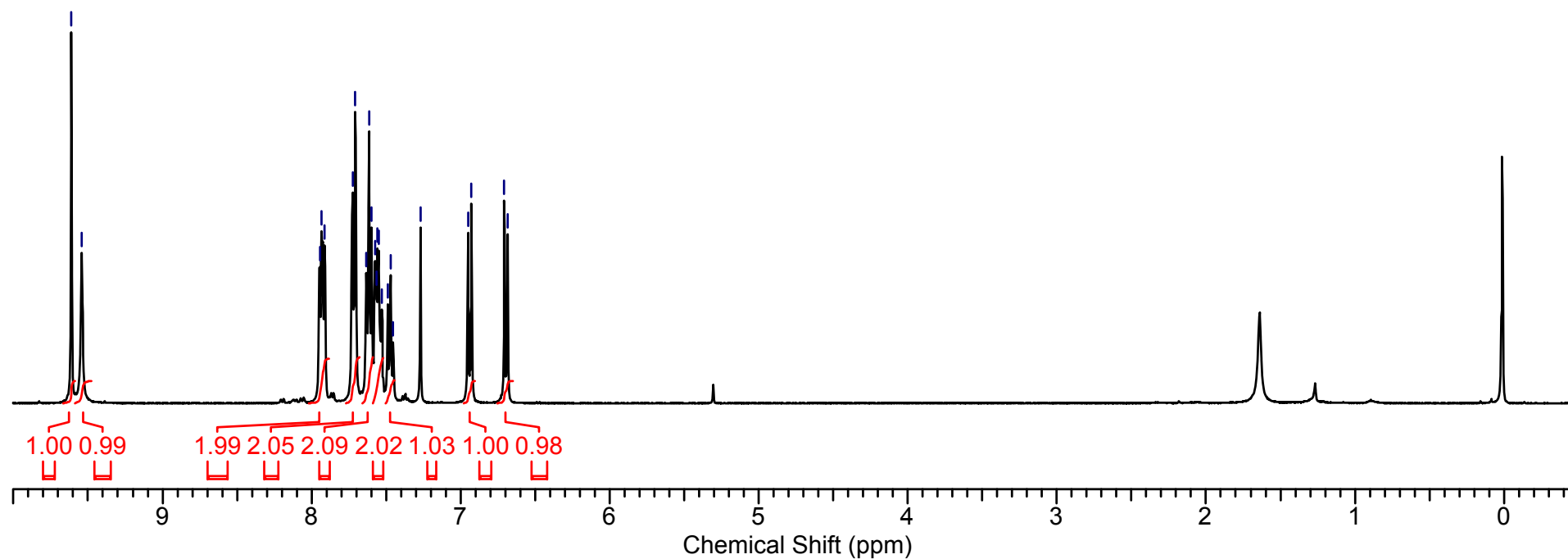
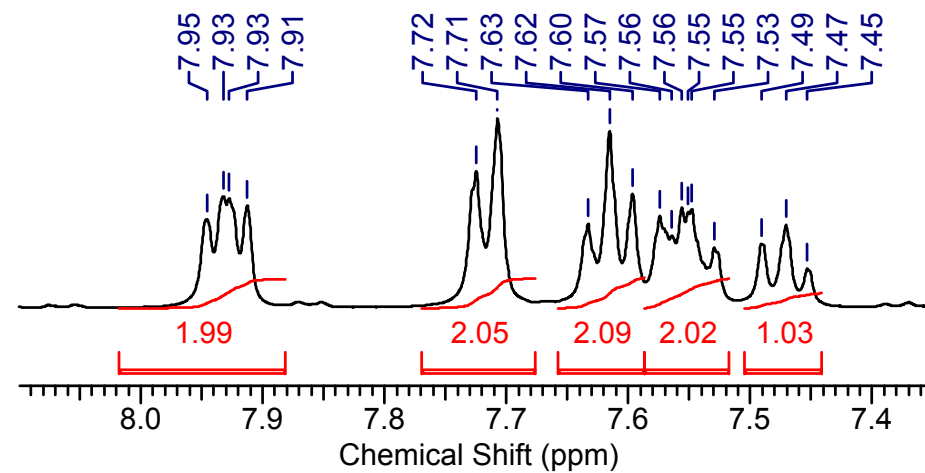
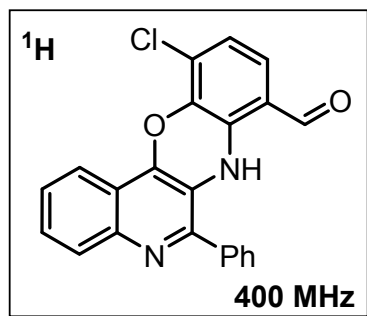
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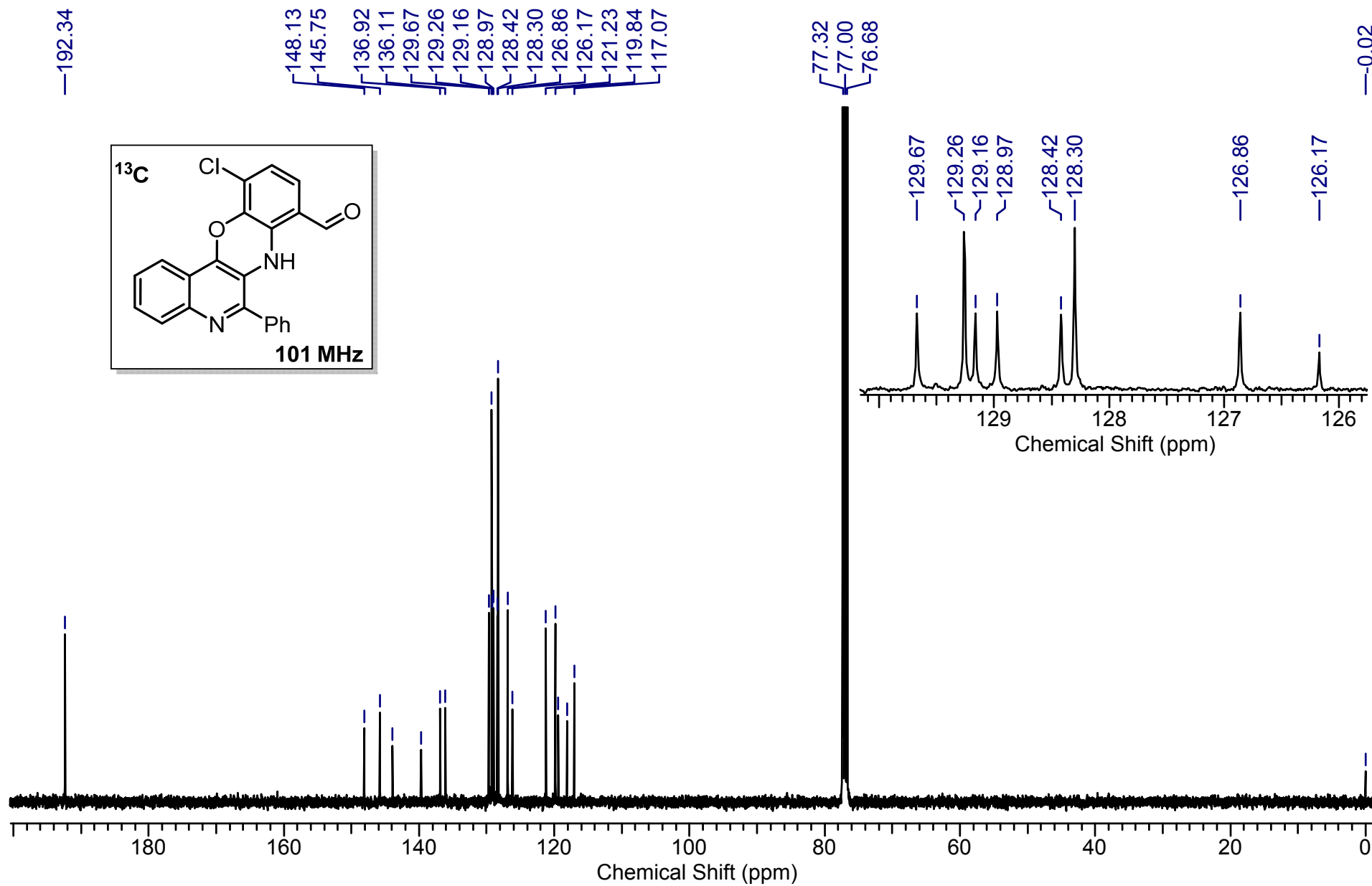


3ac

9.61
9.54
7.93
7.91
7.72
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7.57
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7.55
7.27
6.95
6.93
6.71
6.69

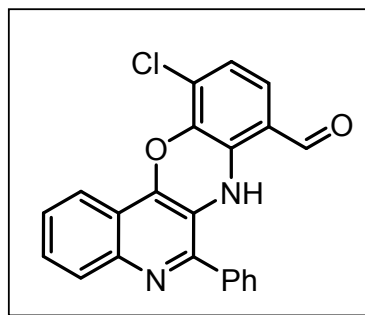


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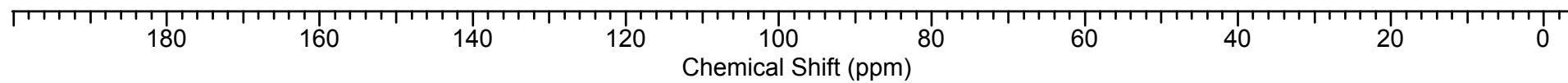
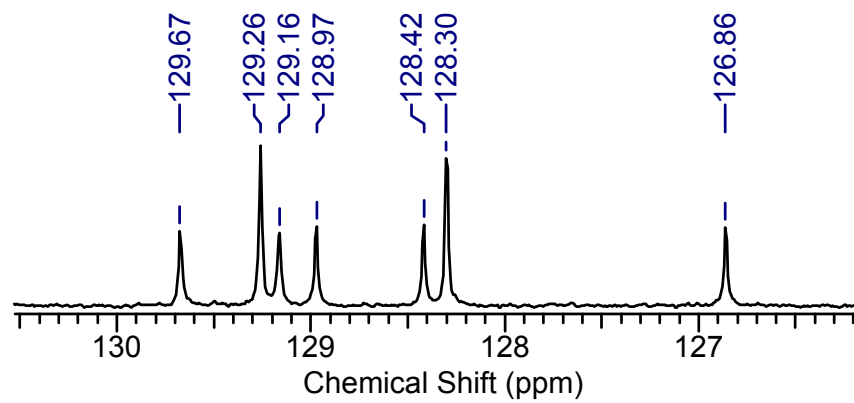


3ac

—192.34

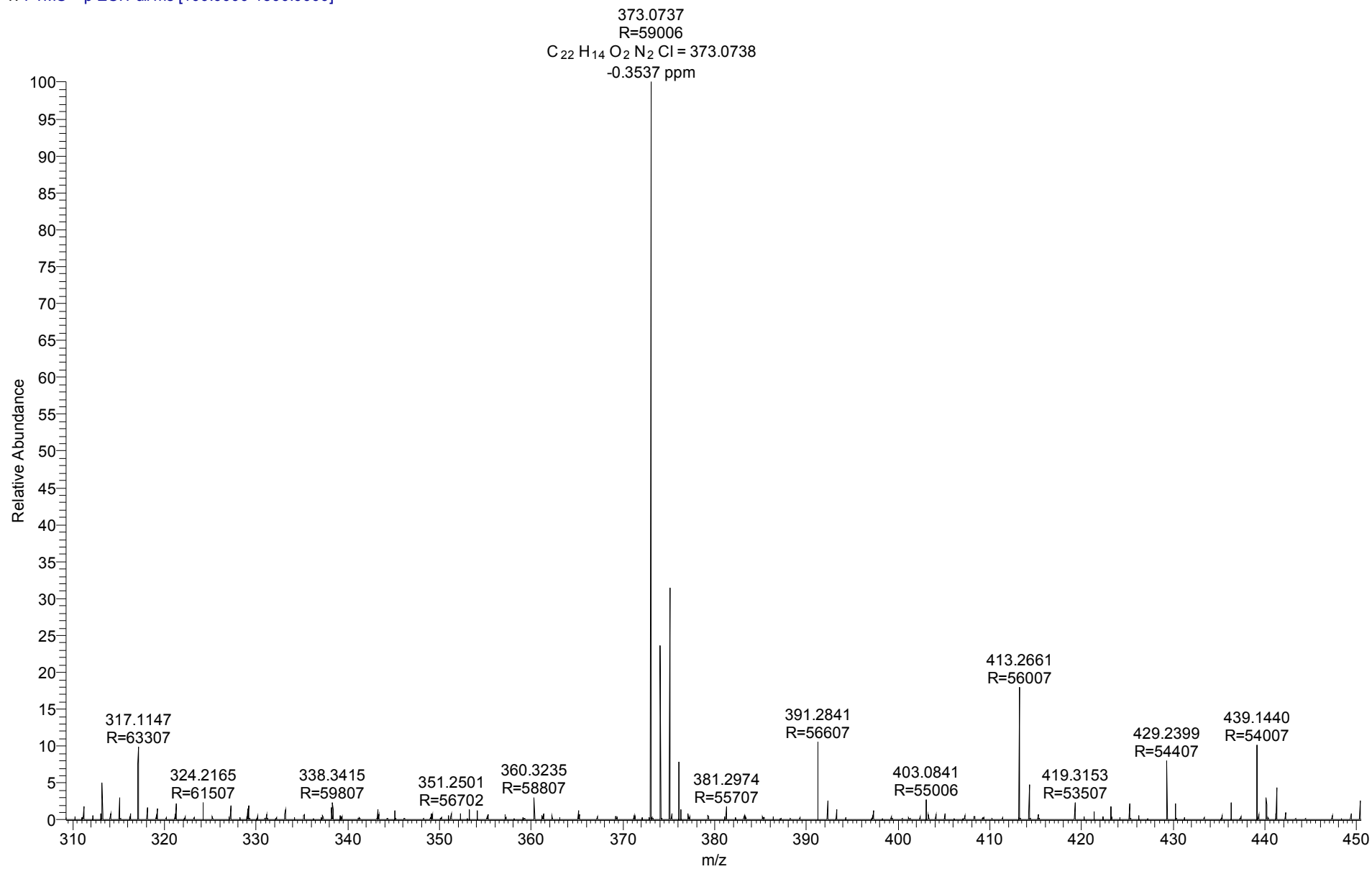


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—129.26
—129.16
—128.97
—128.42
—128.30
—126.86
—121.23
—119.83

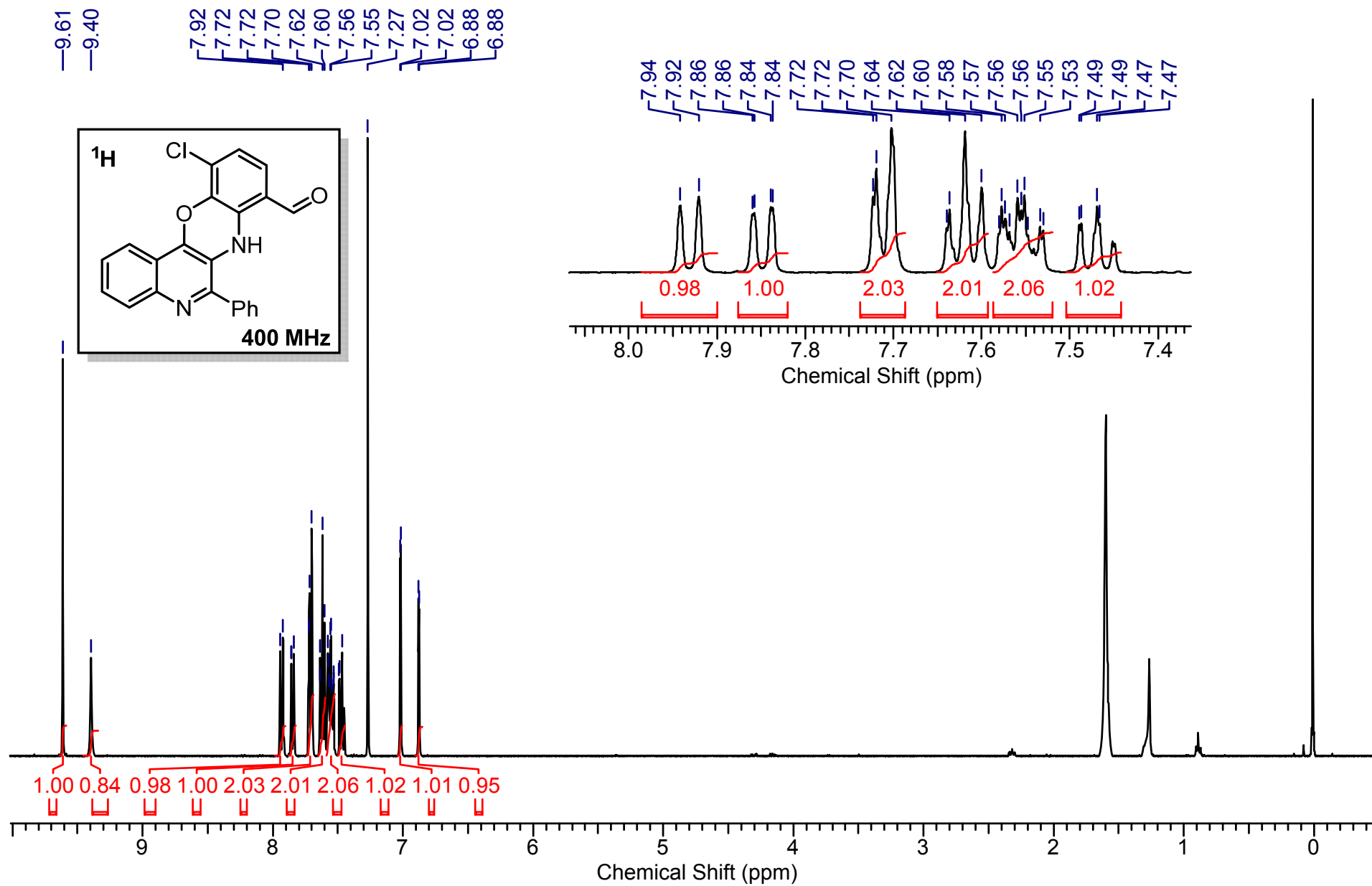


3ac

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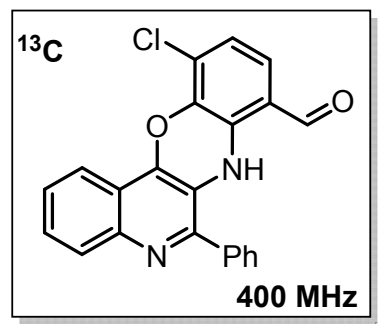


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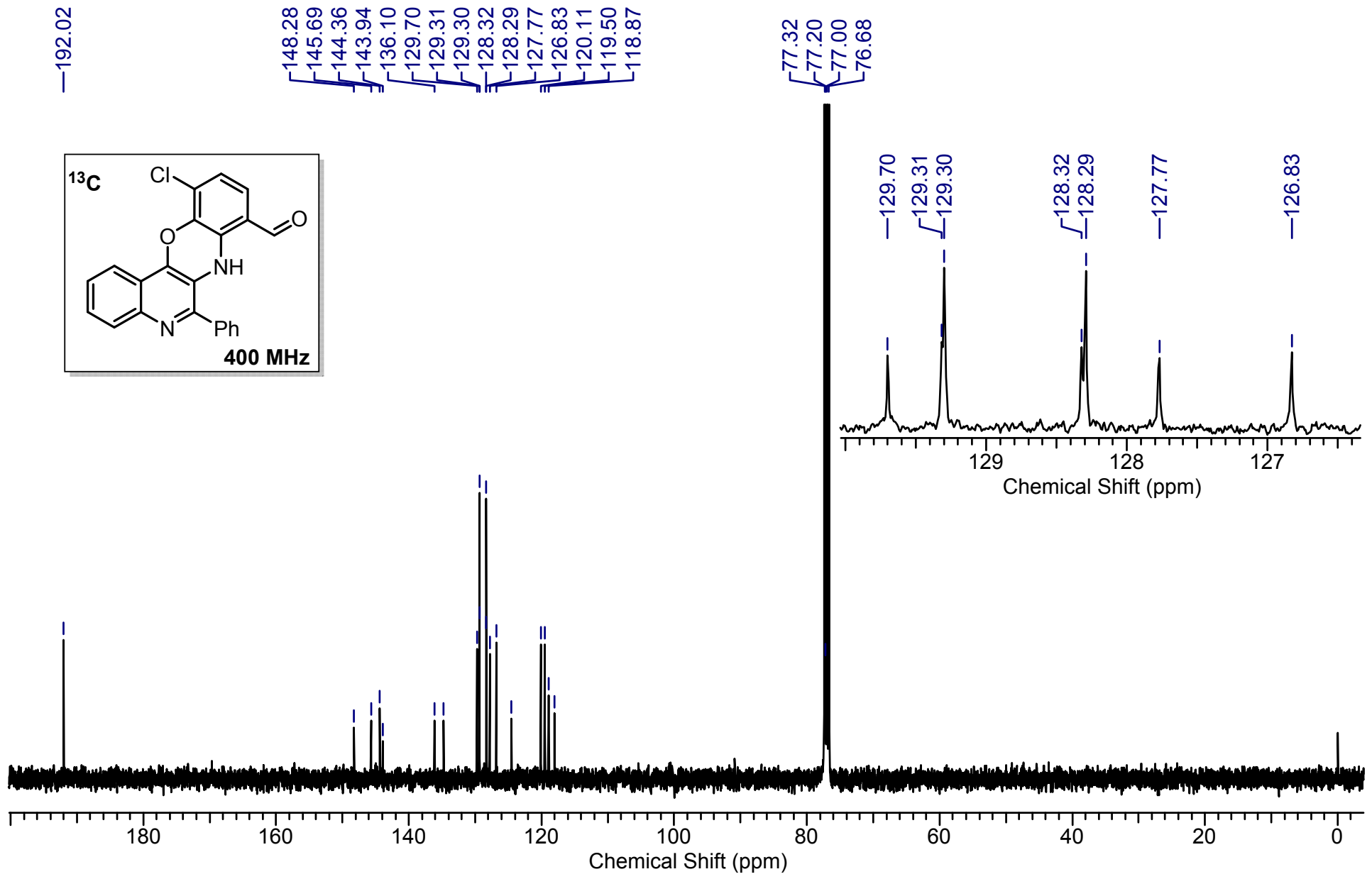
192.02

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144.36
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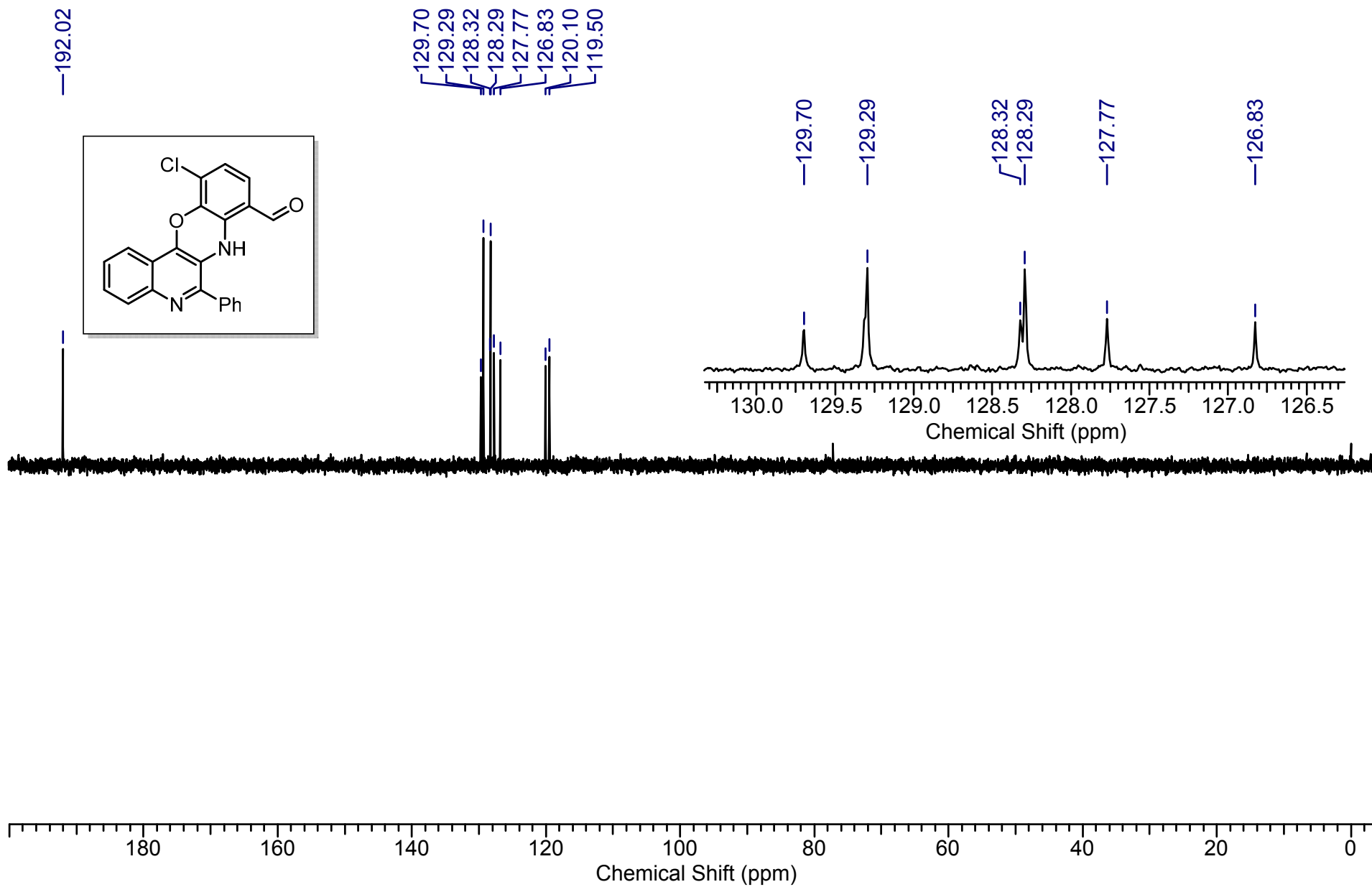
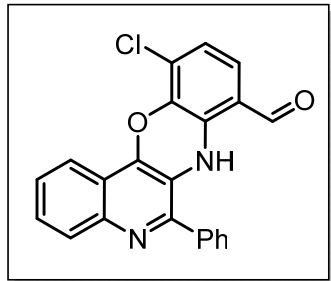
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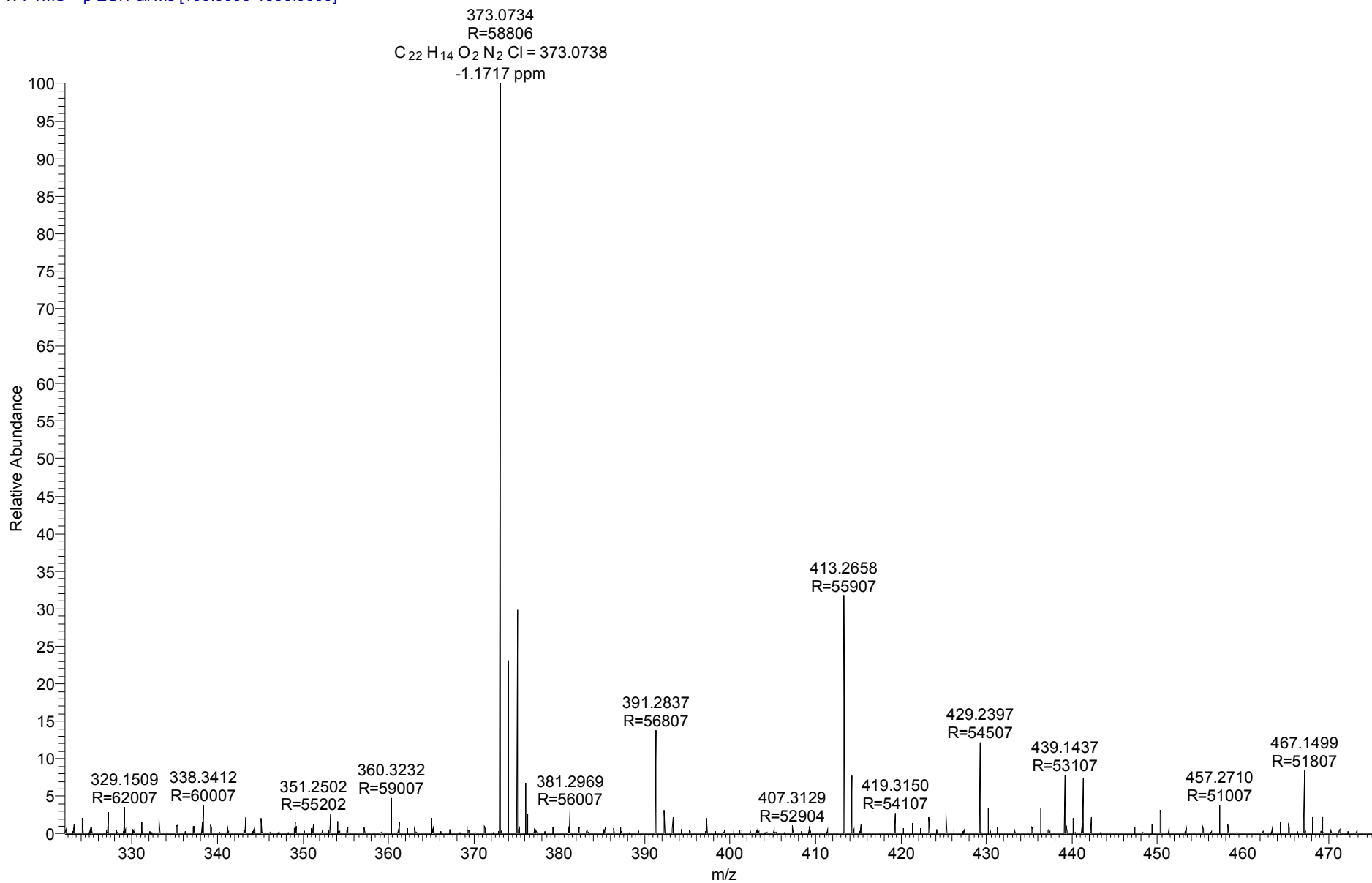


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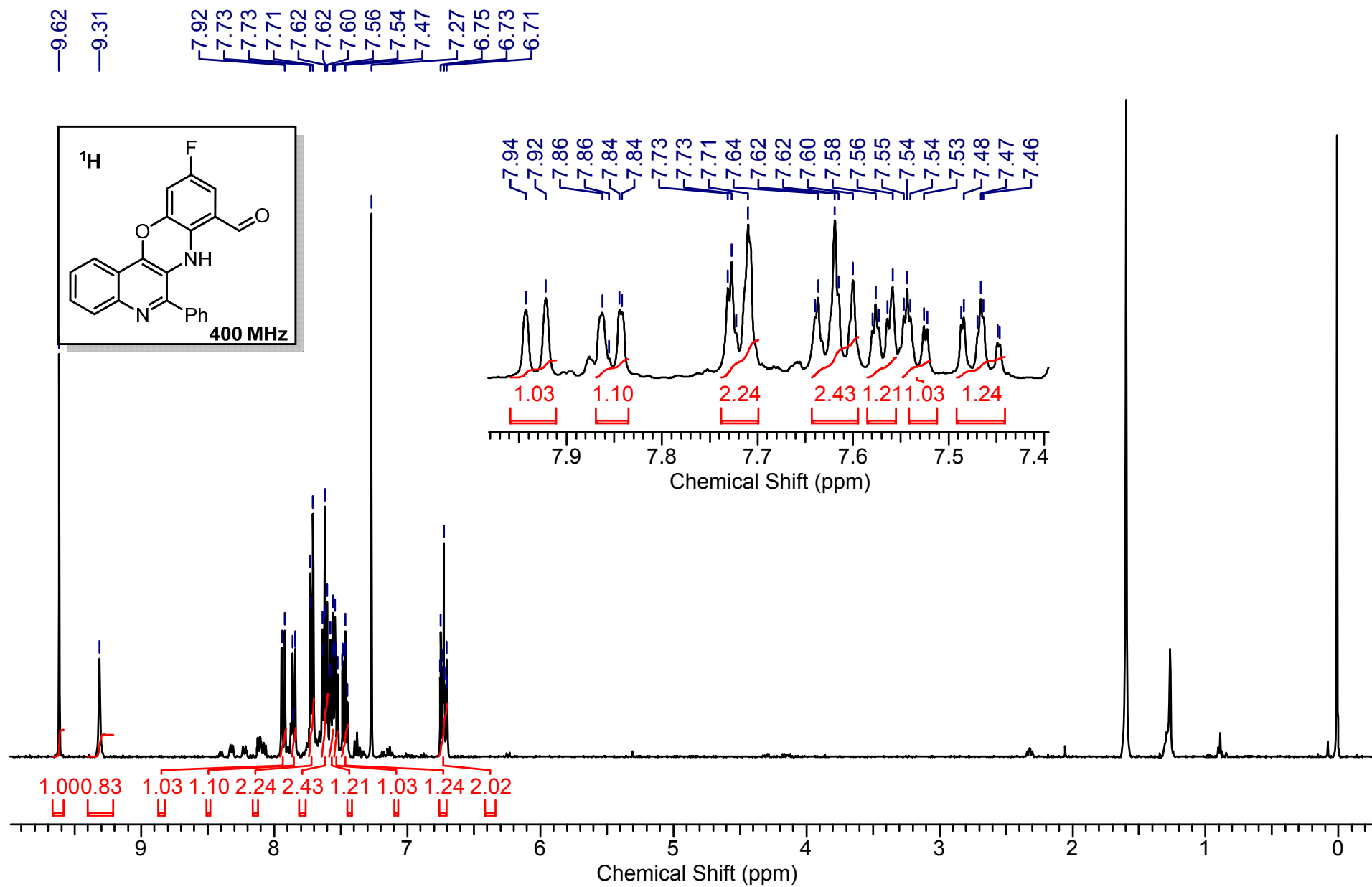


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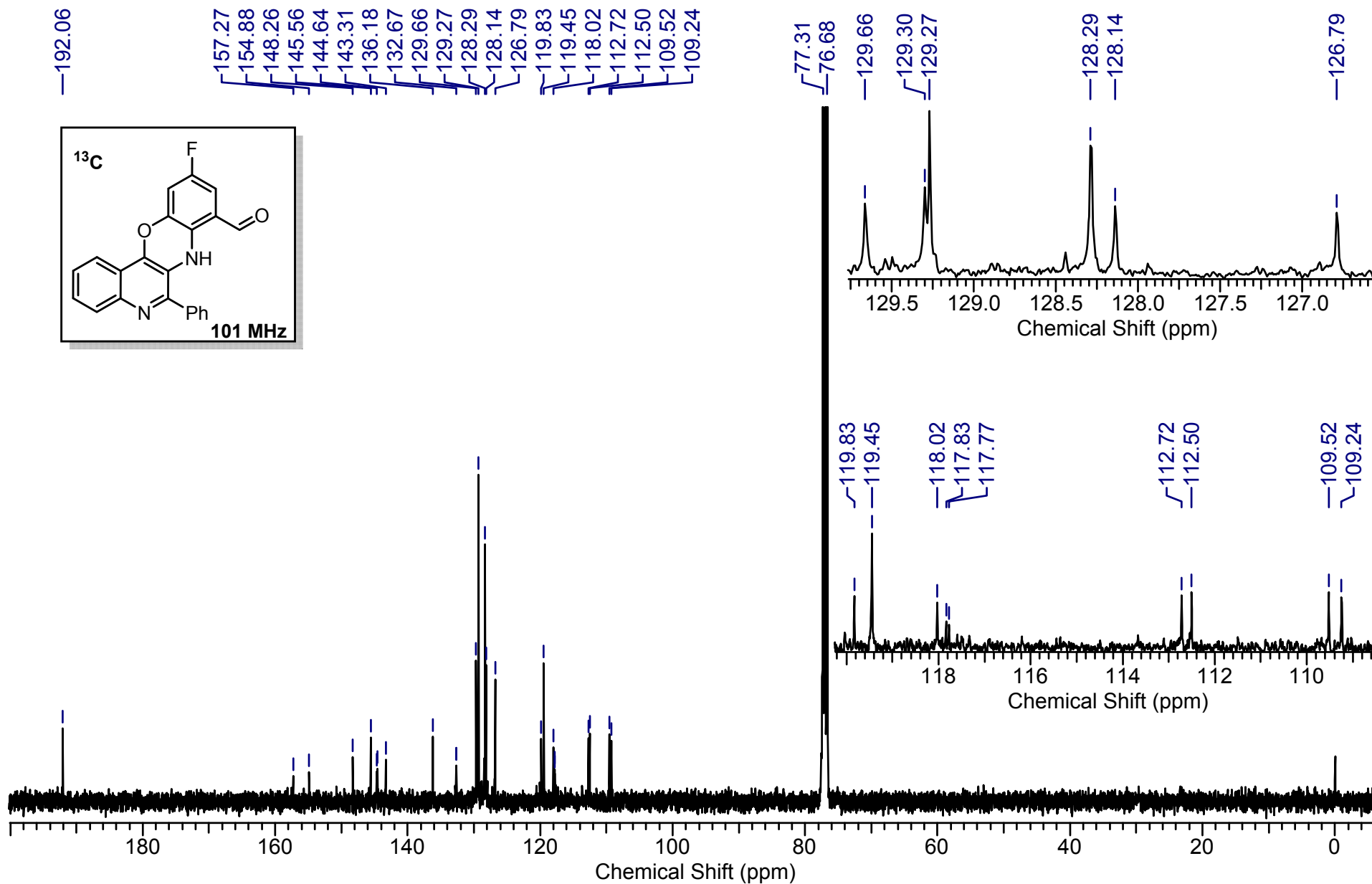
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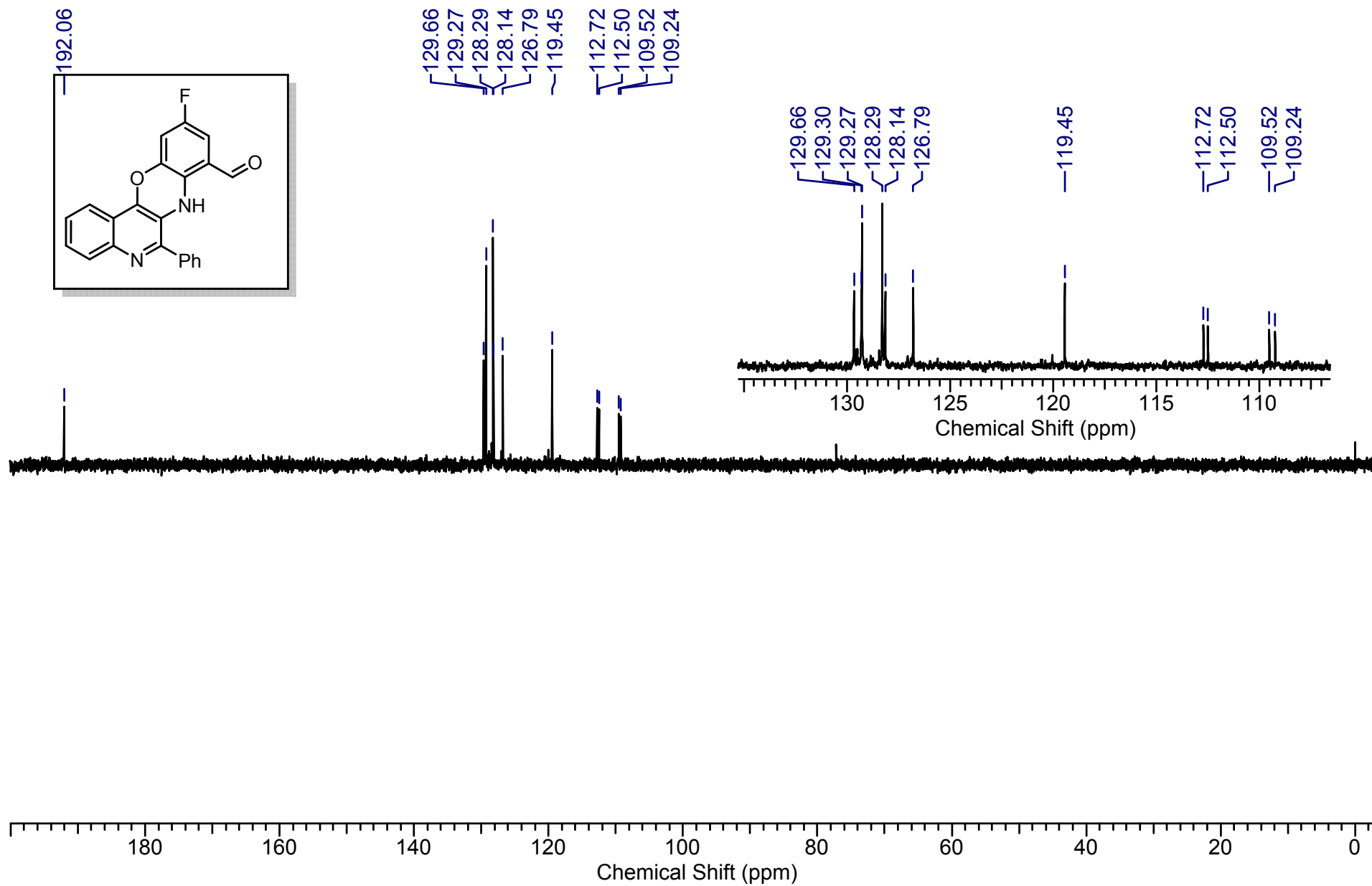
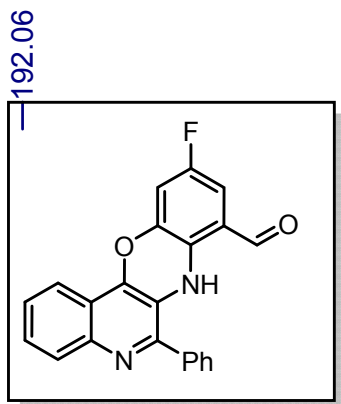
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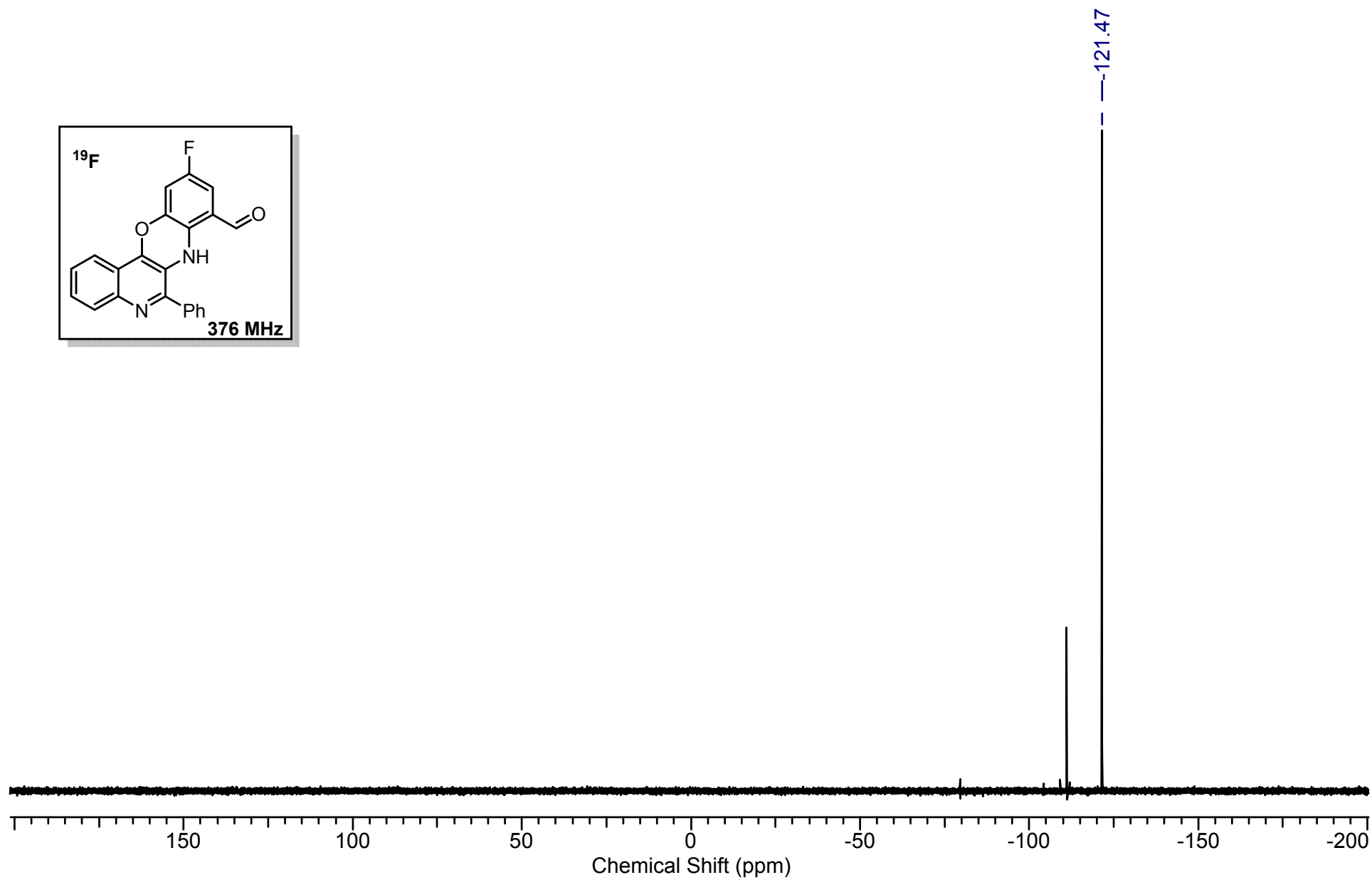
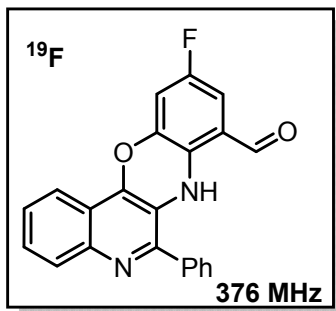
3ae



3ae

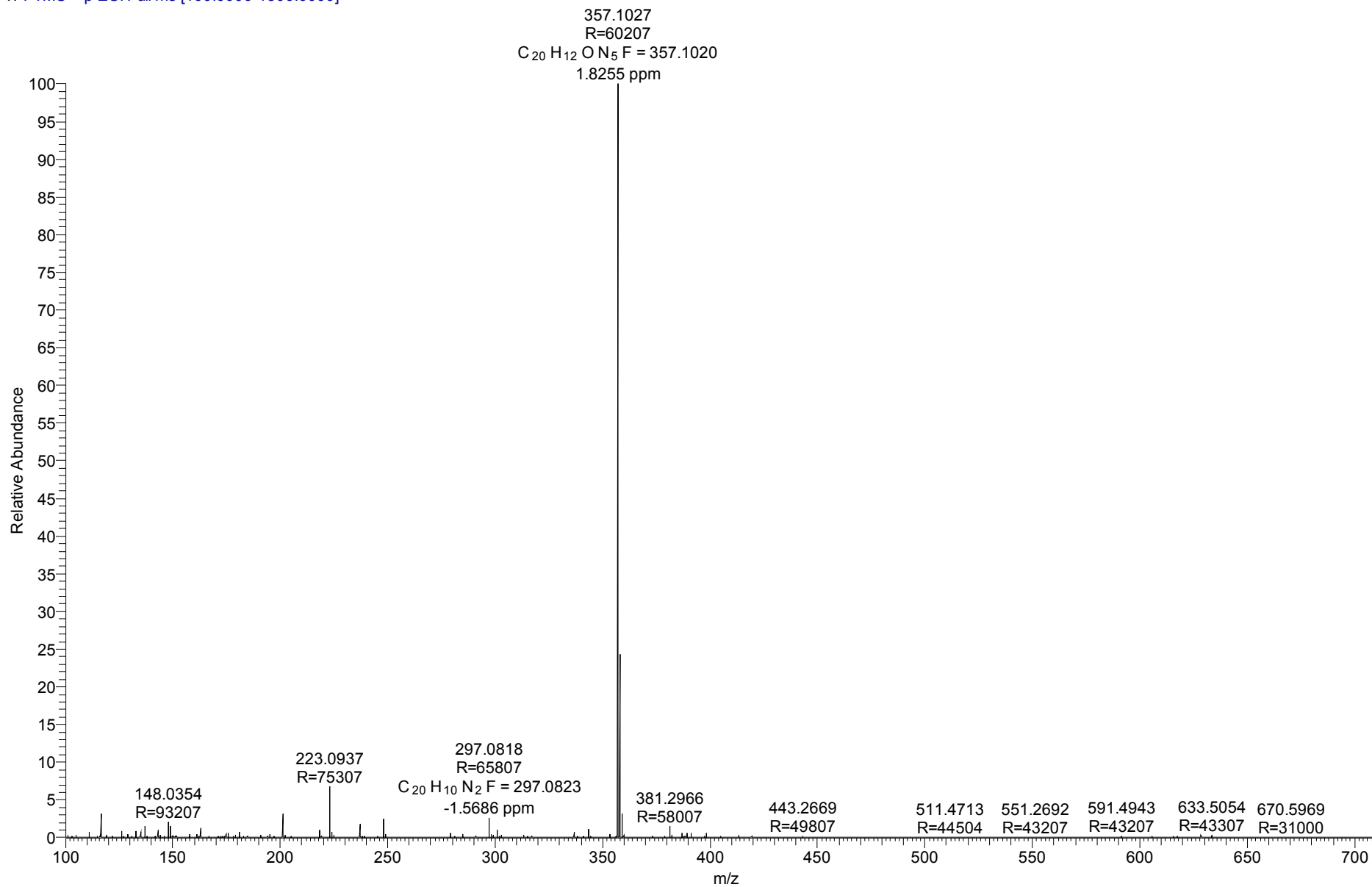


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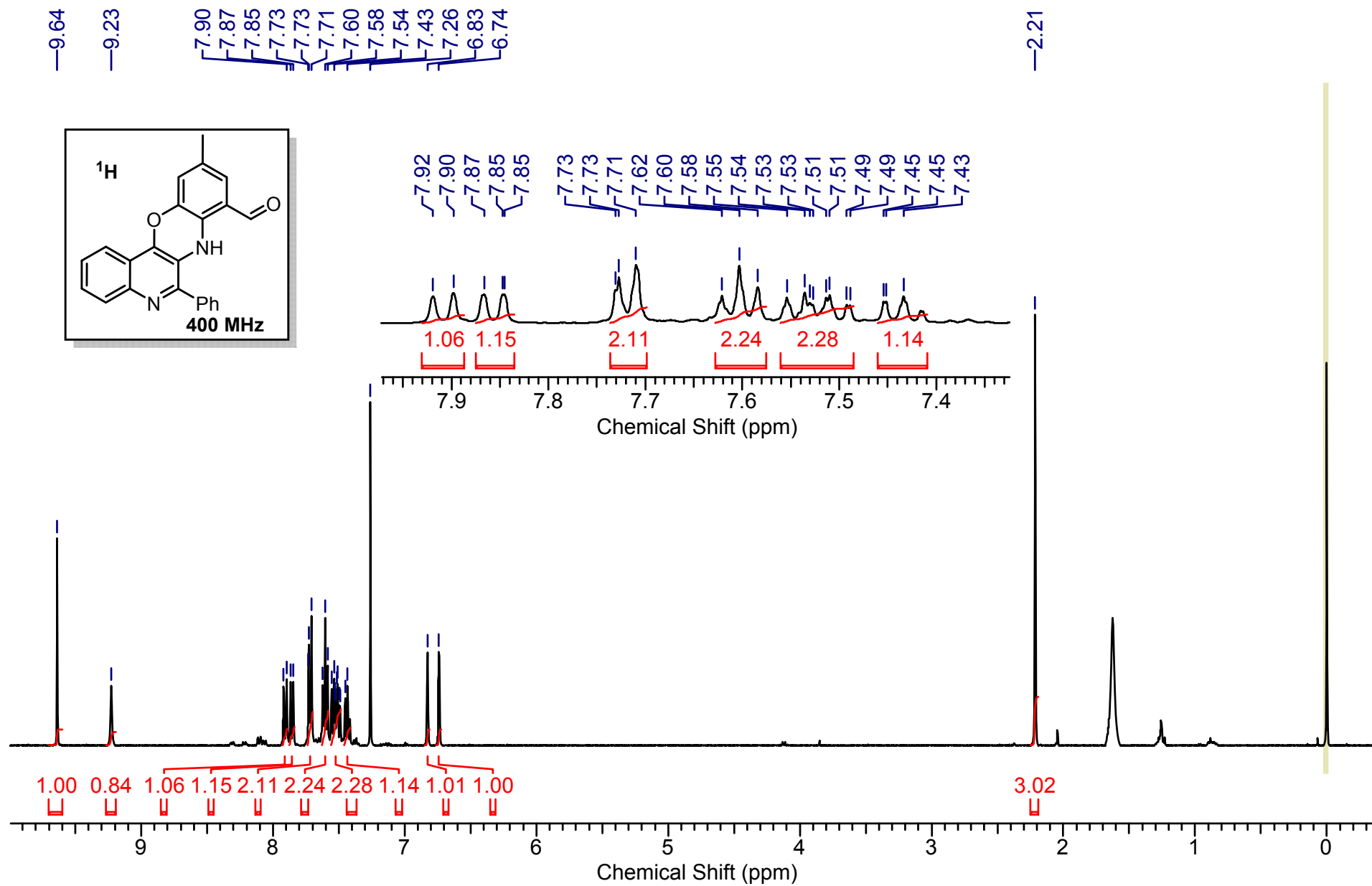


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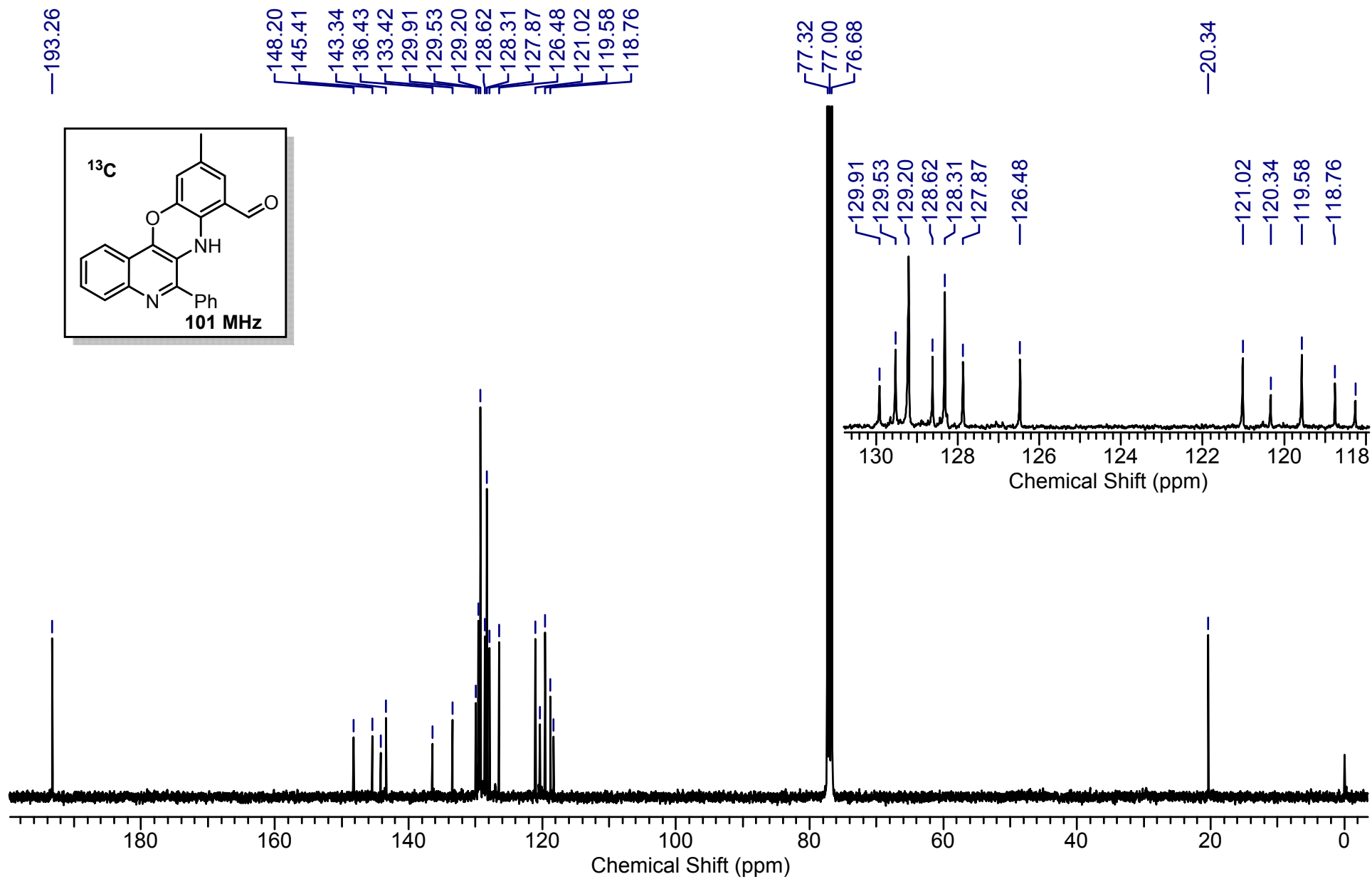
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3af



3af

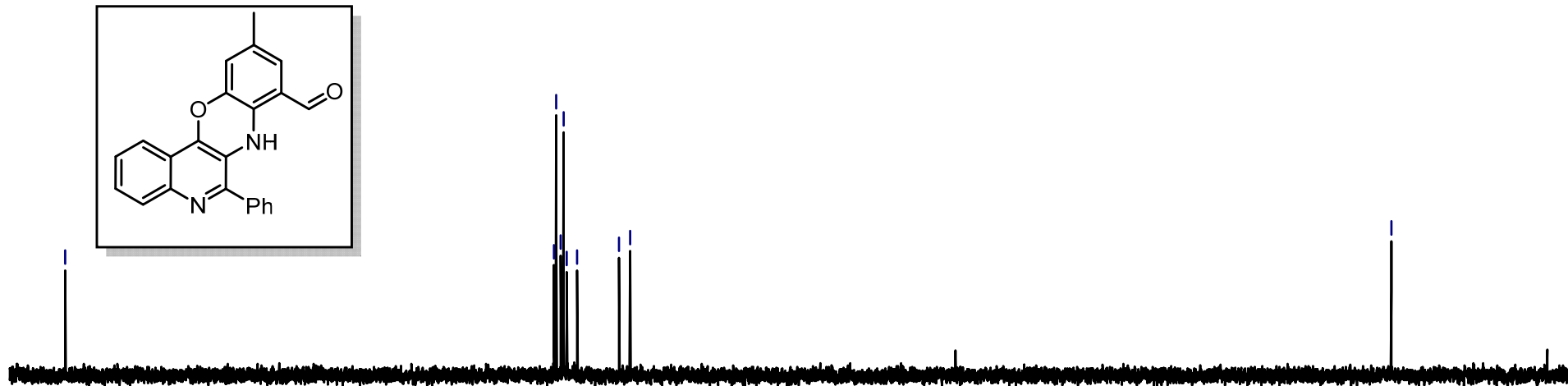
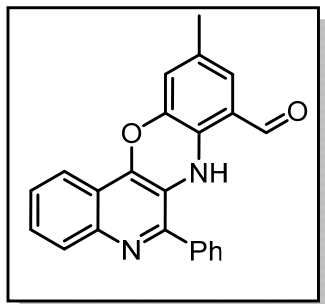


3af

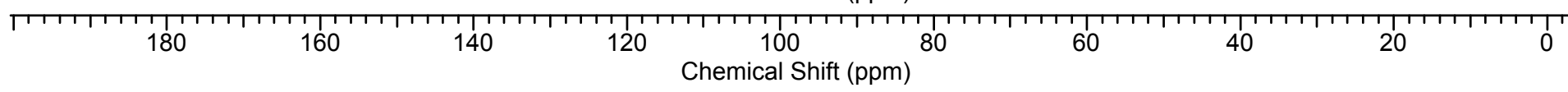
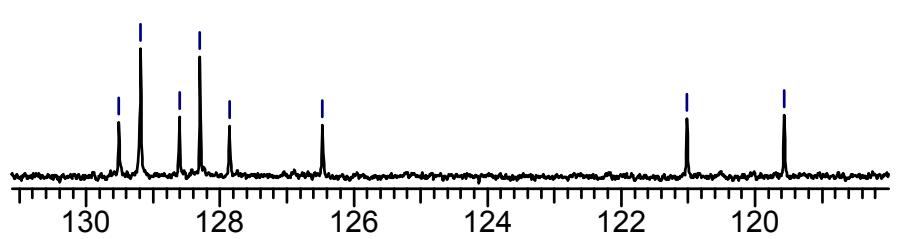
—193.26

129.51
129.18
128.61
128.30
127.86
126.46
121.02
119.56

—20.32

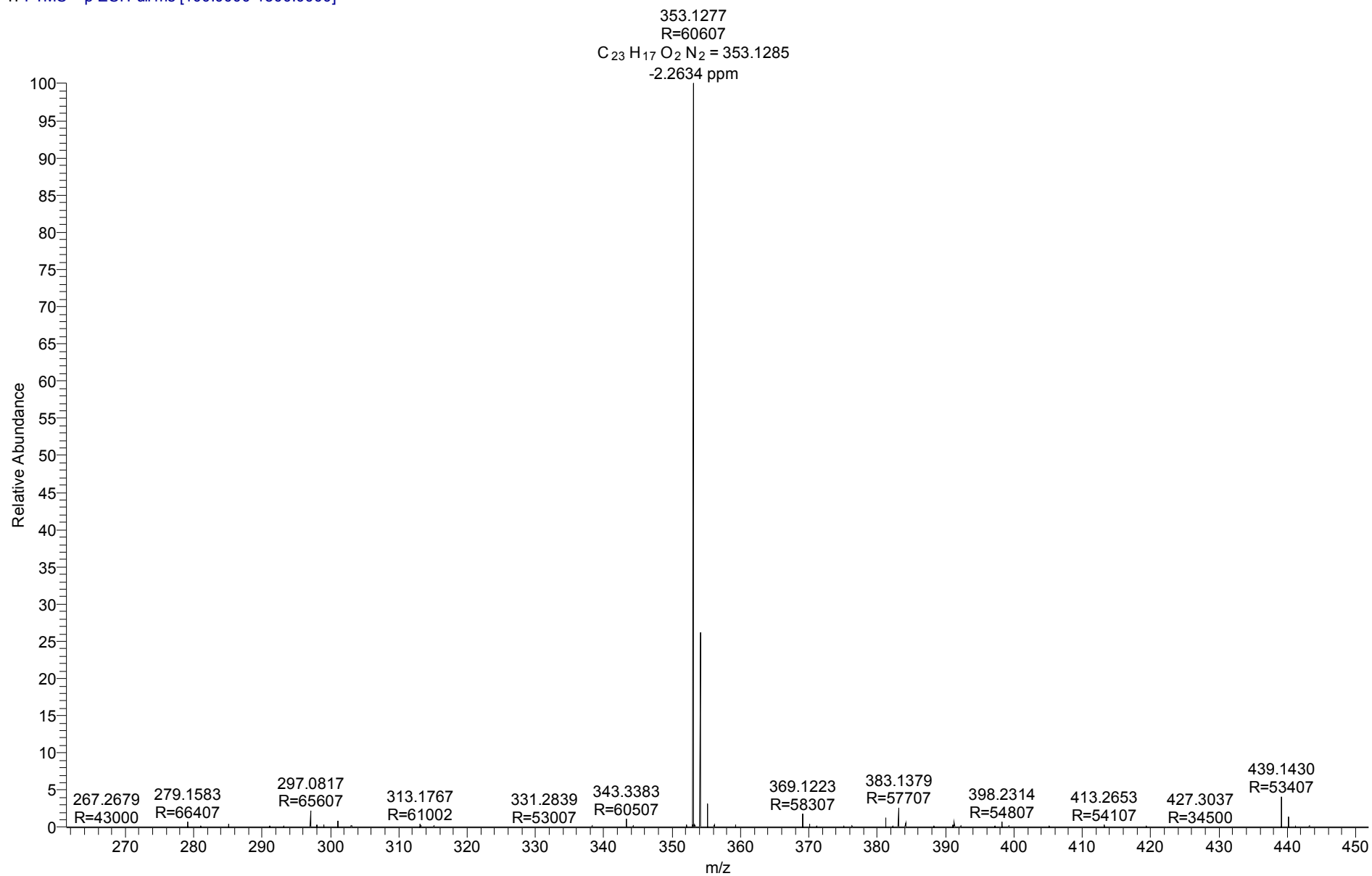


129.51
129.18
128.61
128.30
127.86
126.46
121.02
119.56



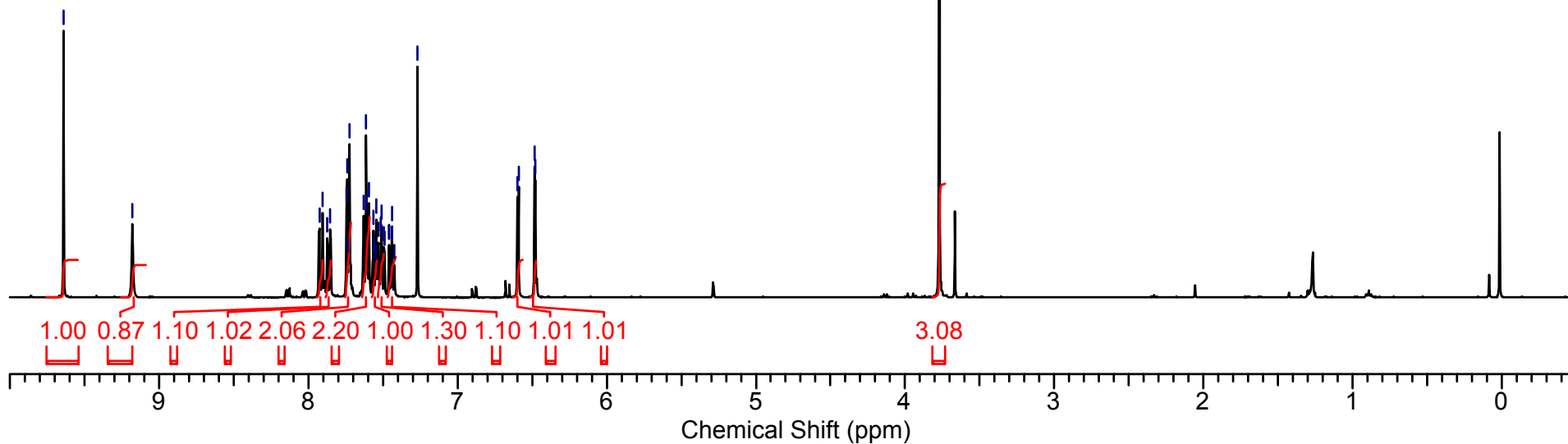
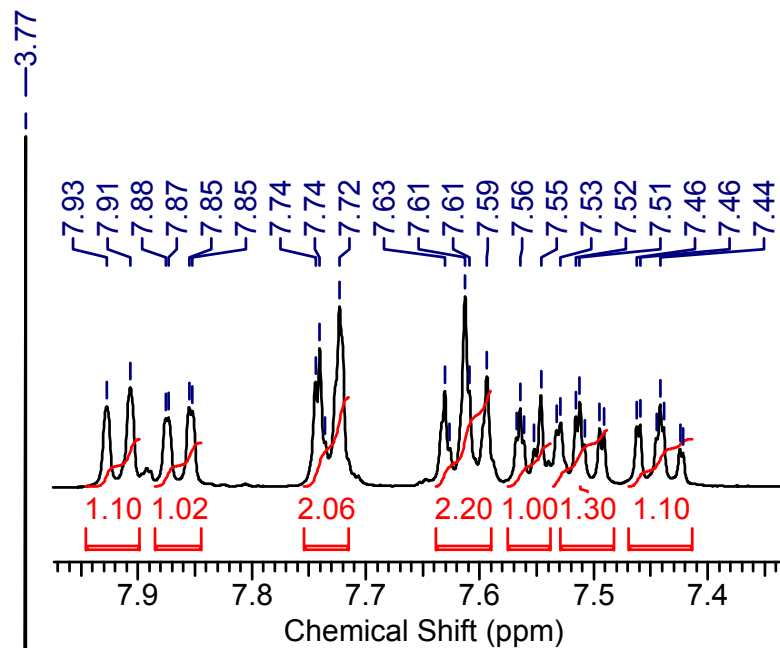
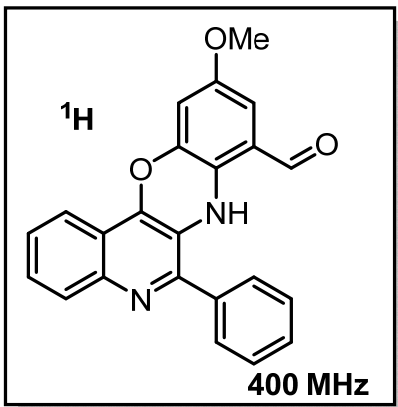
3af

SVH-665 #704 RT: 3.14 AV: 1 NL: 2.69E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



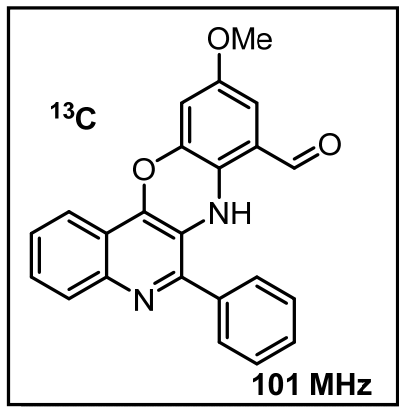
3ag

9.64 9.18 7.91 7.74 7.74 7.72 7.63 7.61 7.61 7.59 7.55 7.44 7.27 6.60 6.59 6.49 6.48



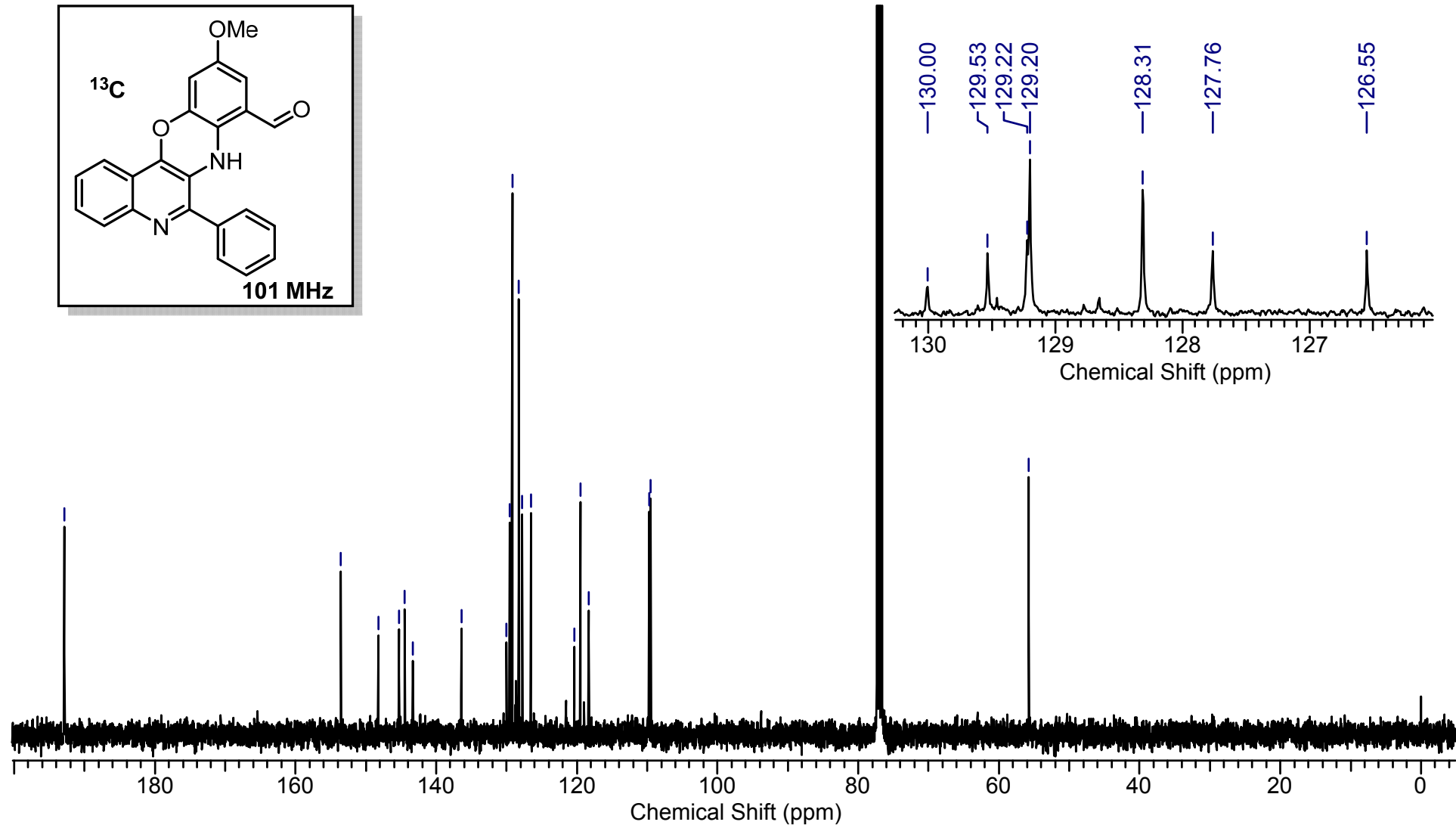
3ag

192.88
153.54
148.22
145.26
144.45
143.34
136.43
130.00
129.53
129.20
128.31
127.76
126.55
120.39
119.51
118.30
109.73
109.52

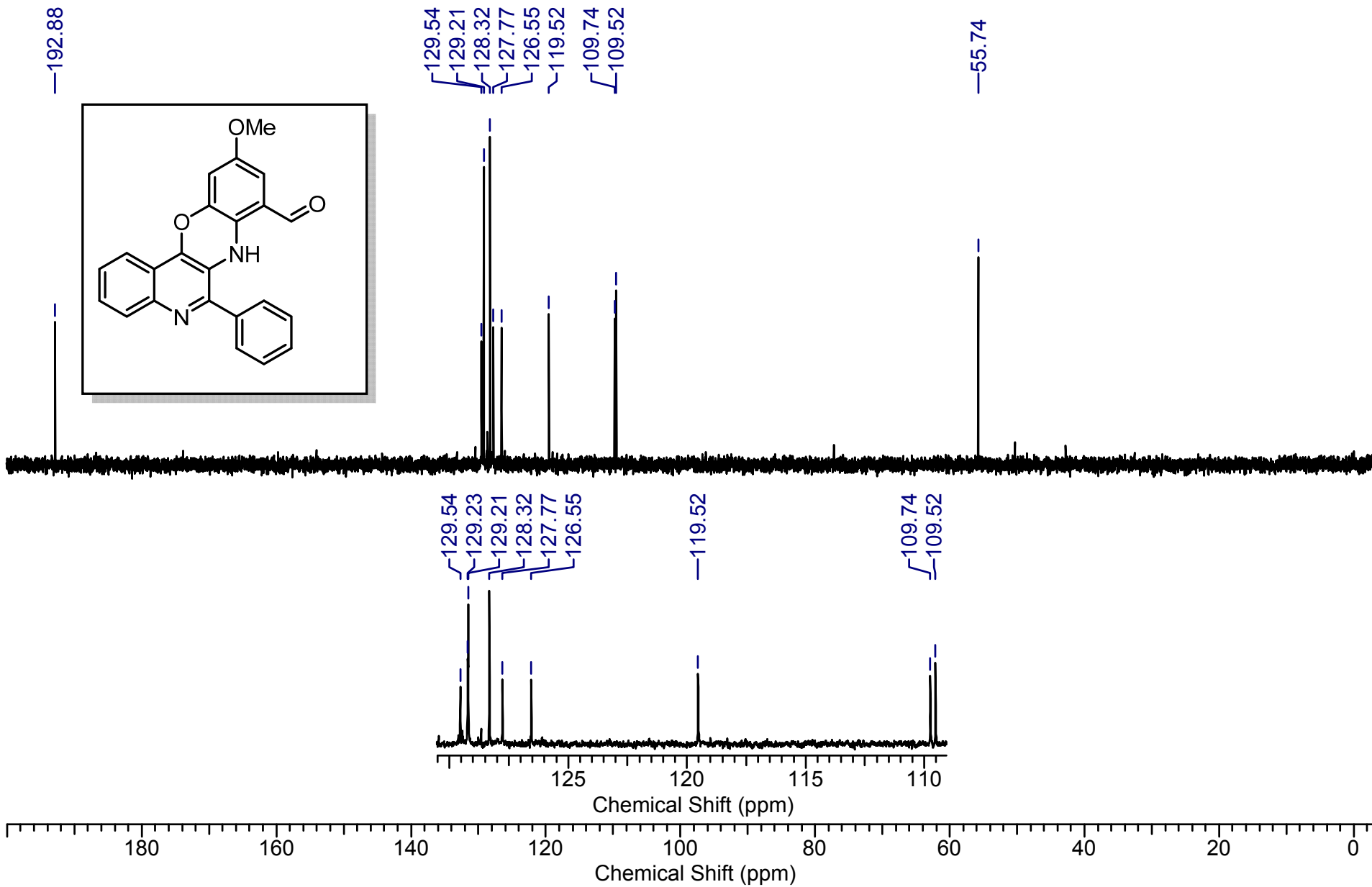
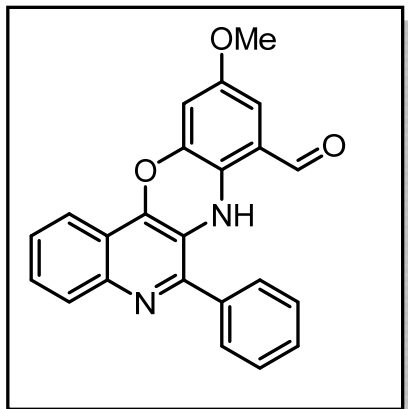


77.32
77.00
76.68

130.00
129.53
129.22
129.20
128.31
127.76
126.55

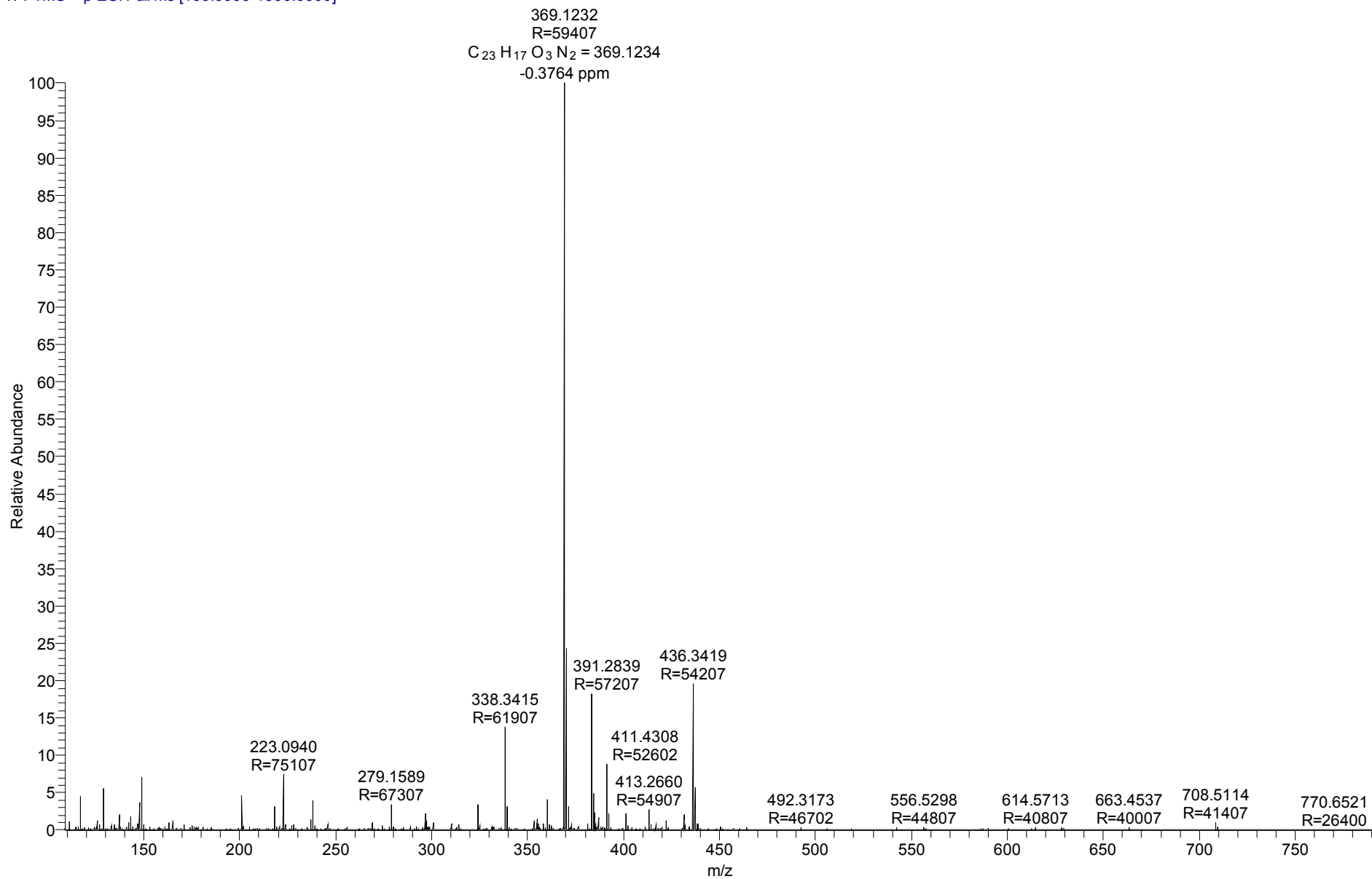


3ag

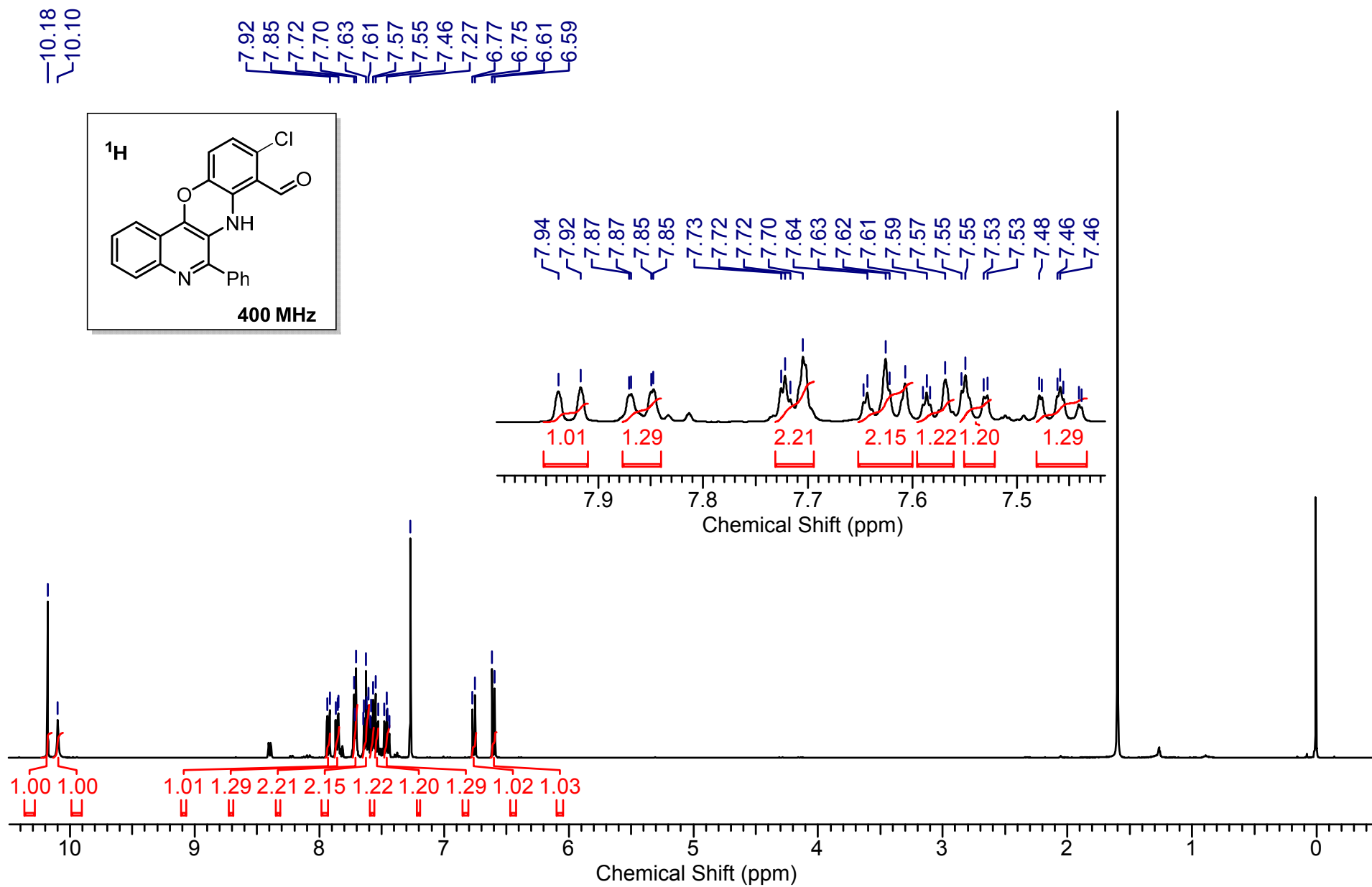


3ag

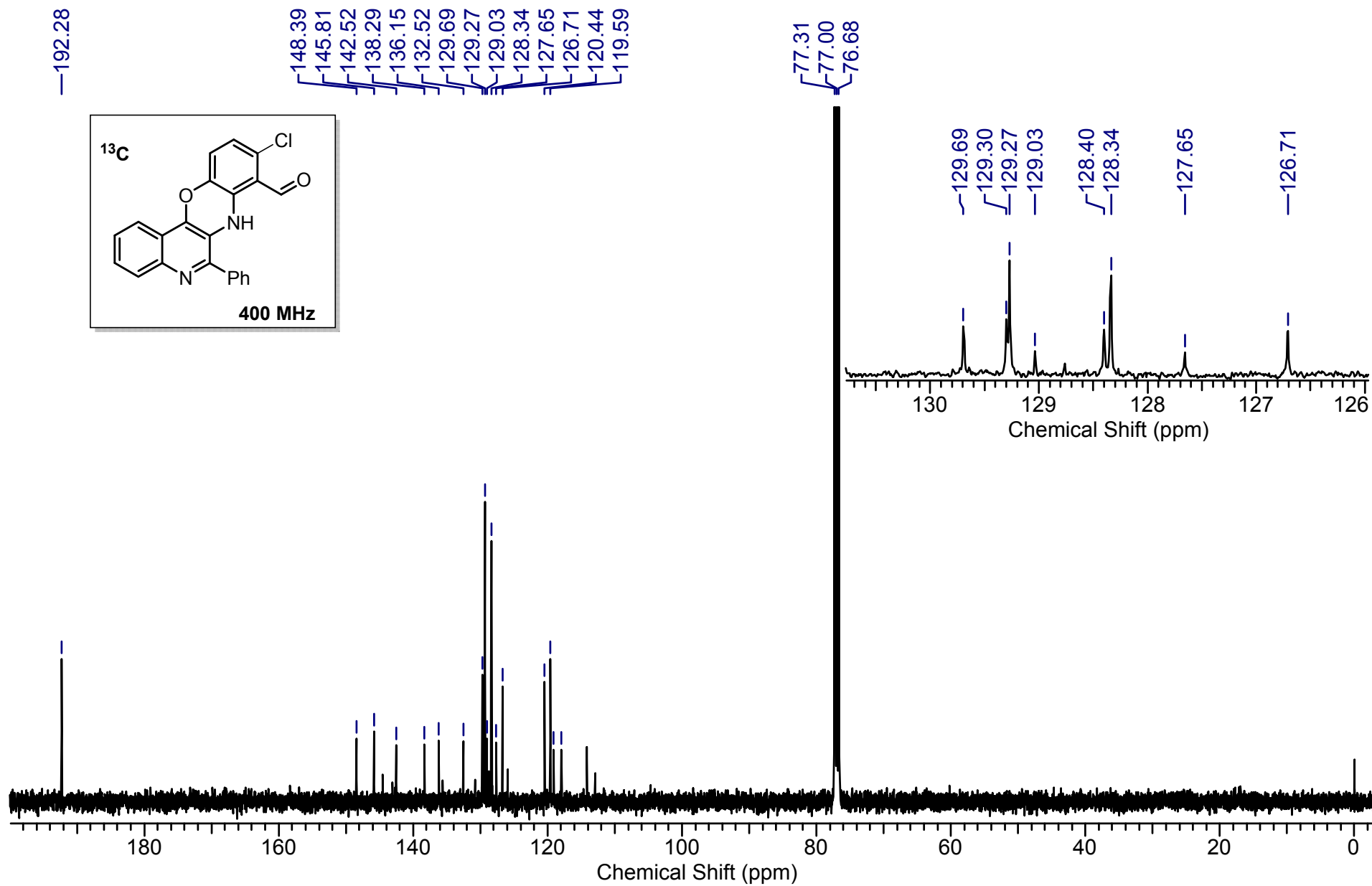
SVH-842 #399 RT: 1.78 AV: 1 NL: 8.00E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



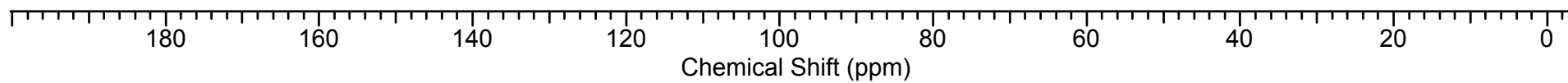
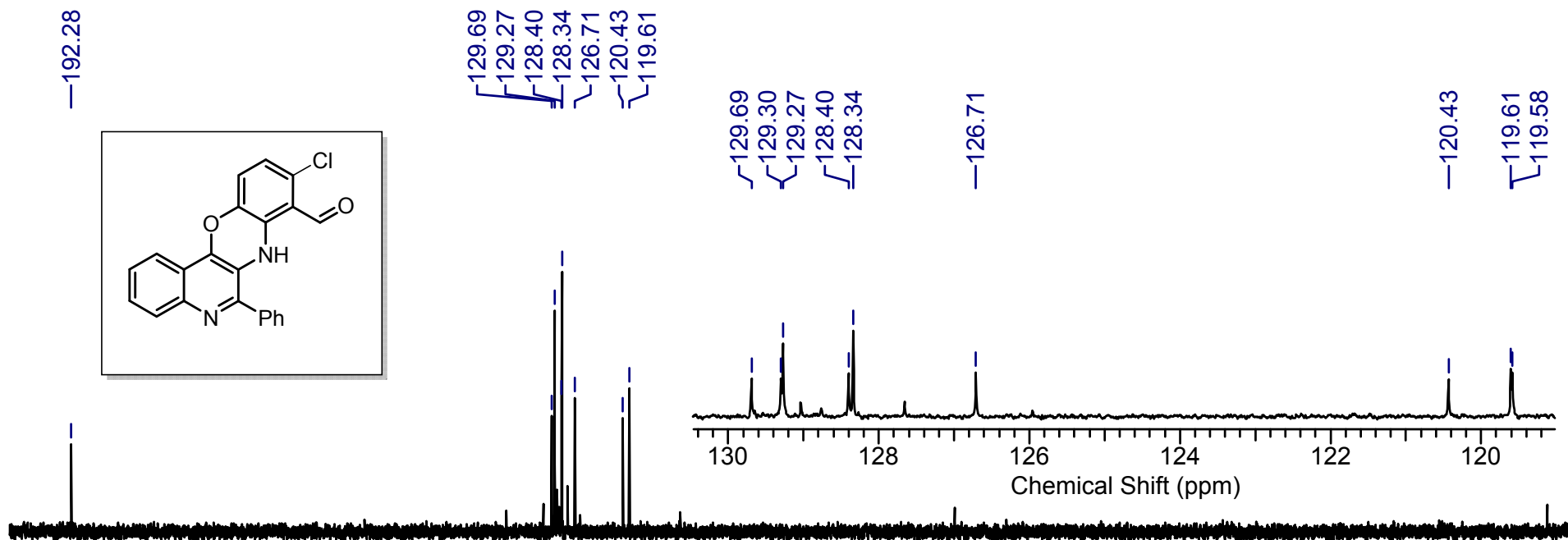
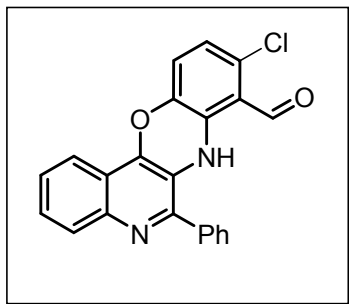
3ah



3ah

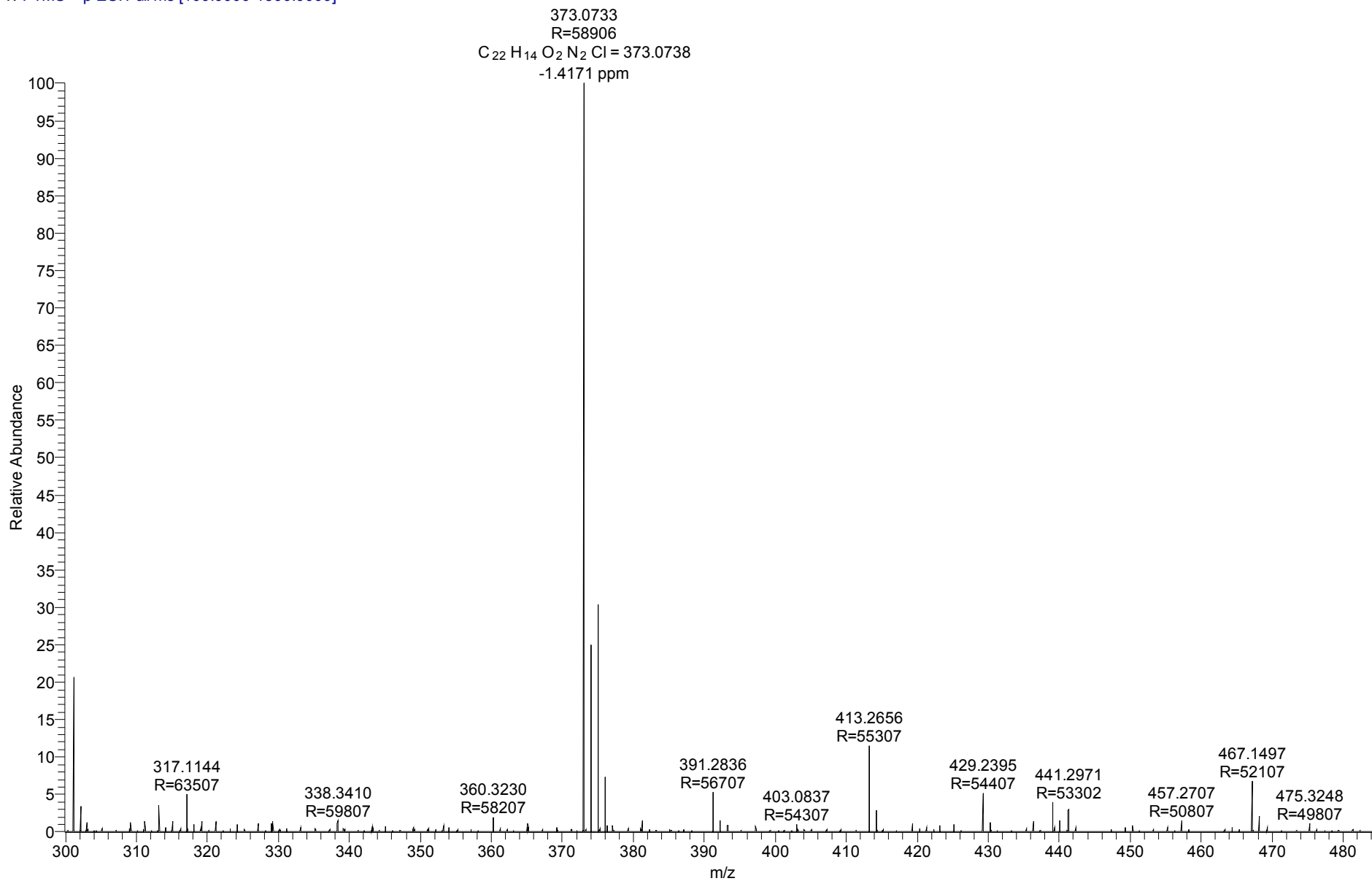


3ah

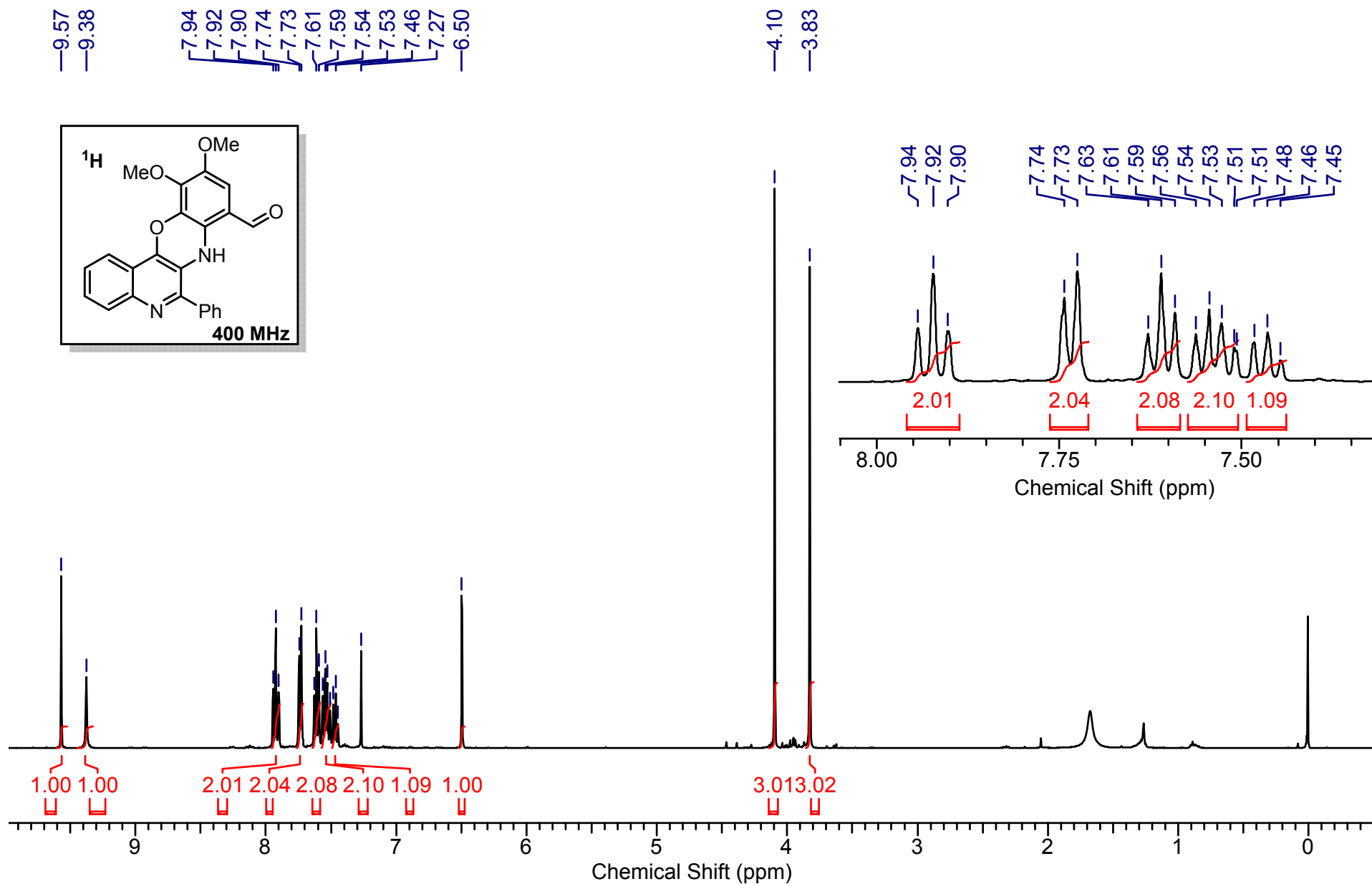


3ah

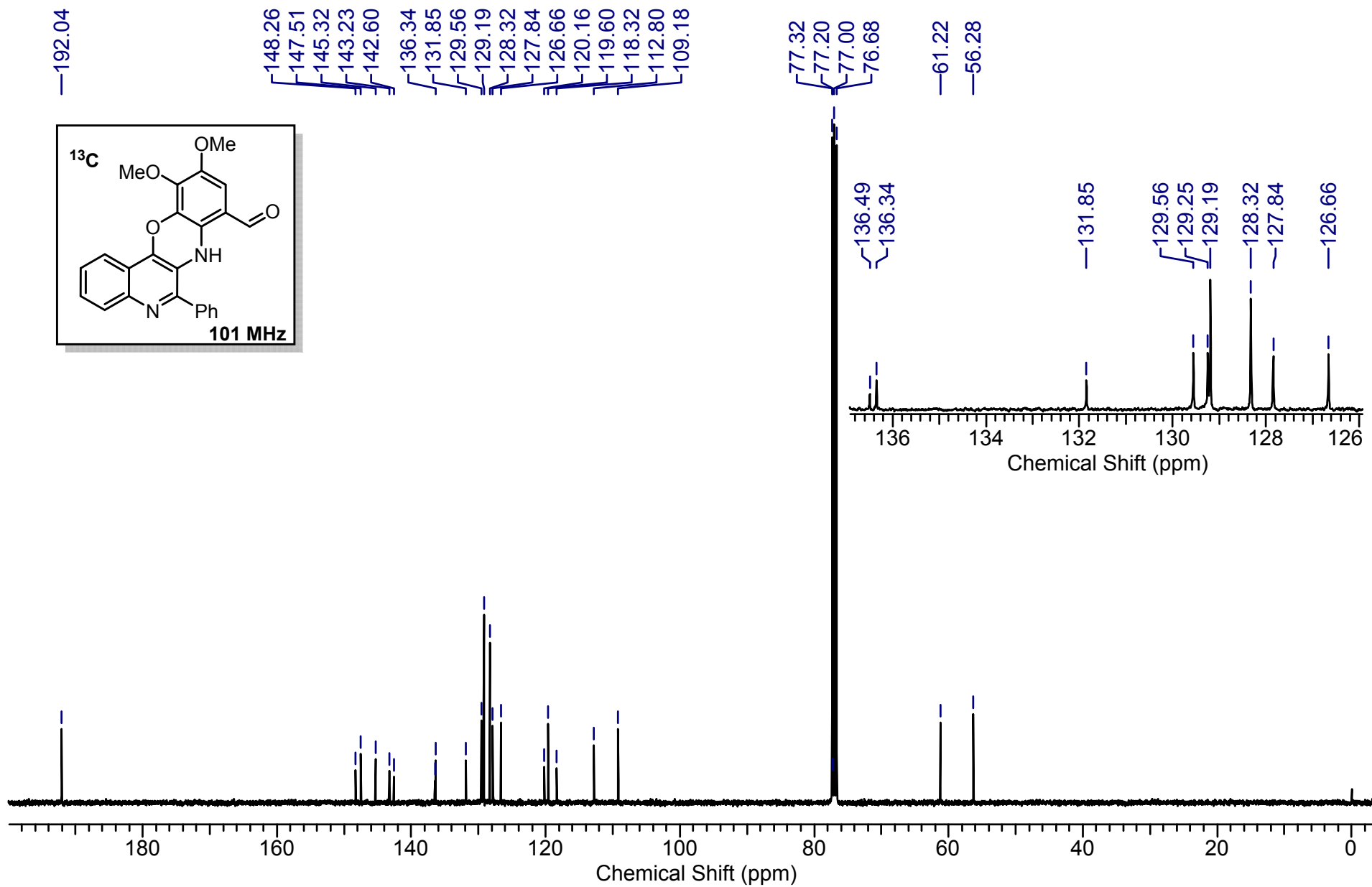
SH-610 #483 RT: 2.56 AV: 1 NL: 5.76E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



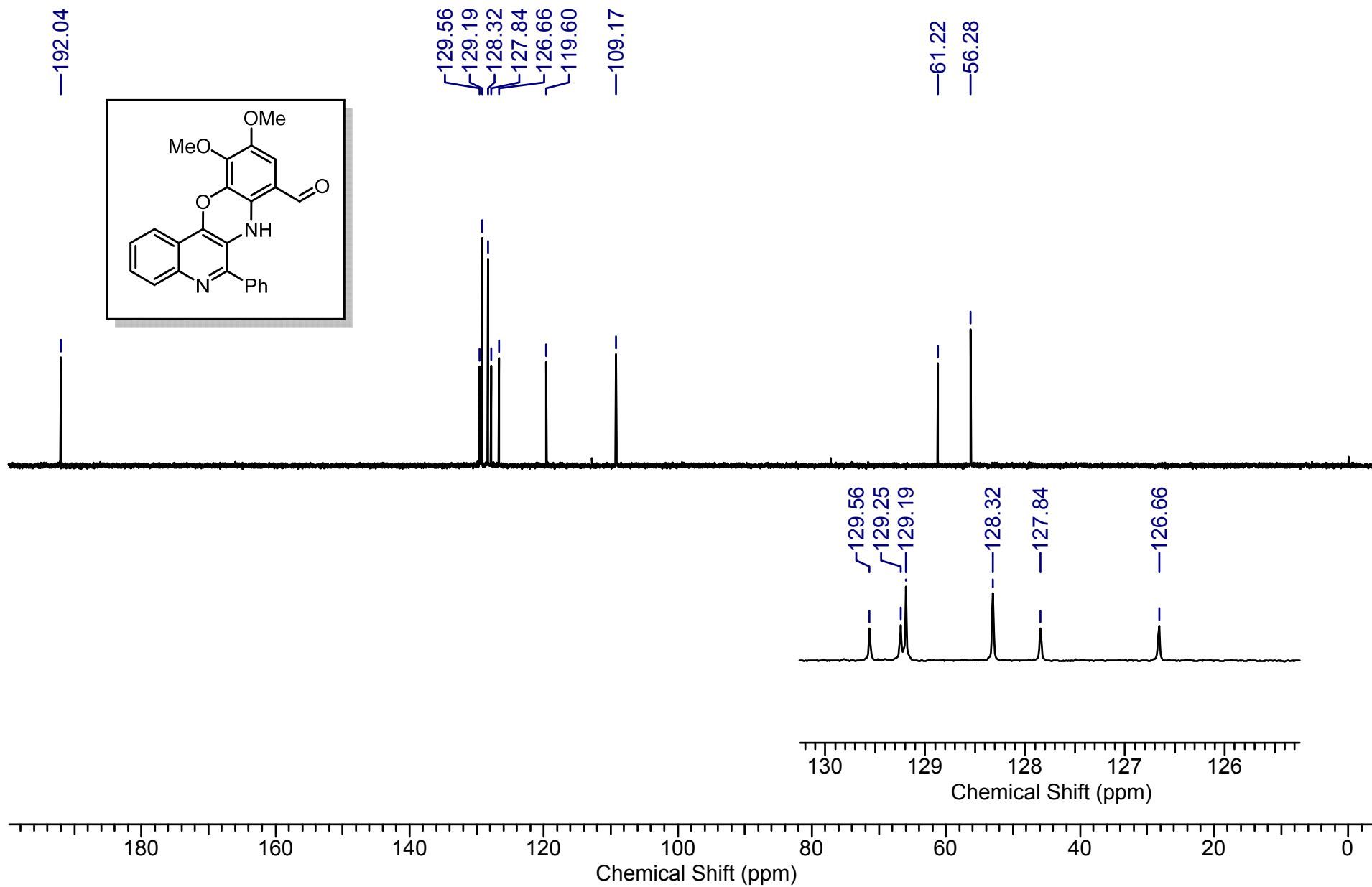
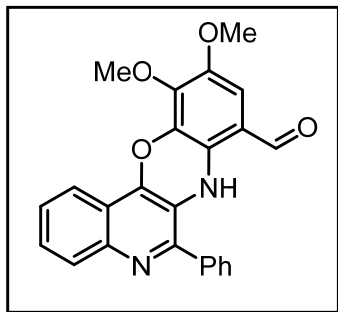
3ai



3ai

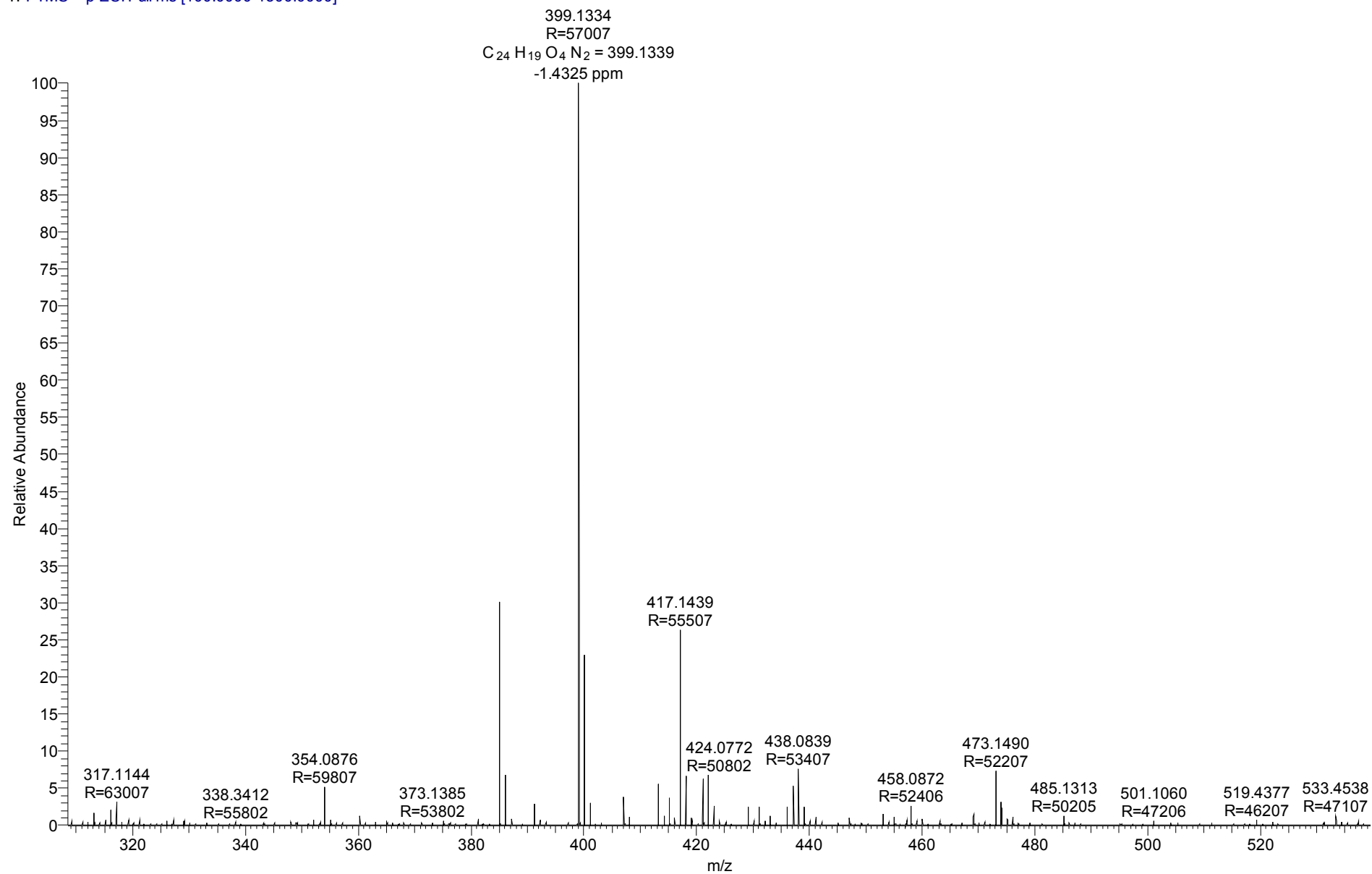


3ai

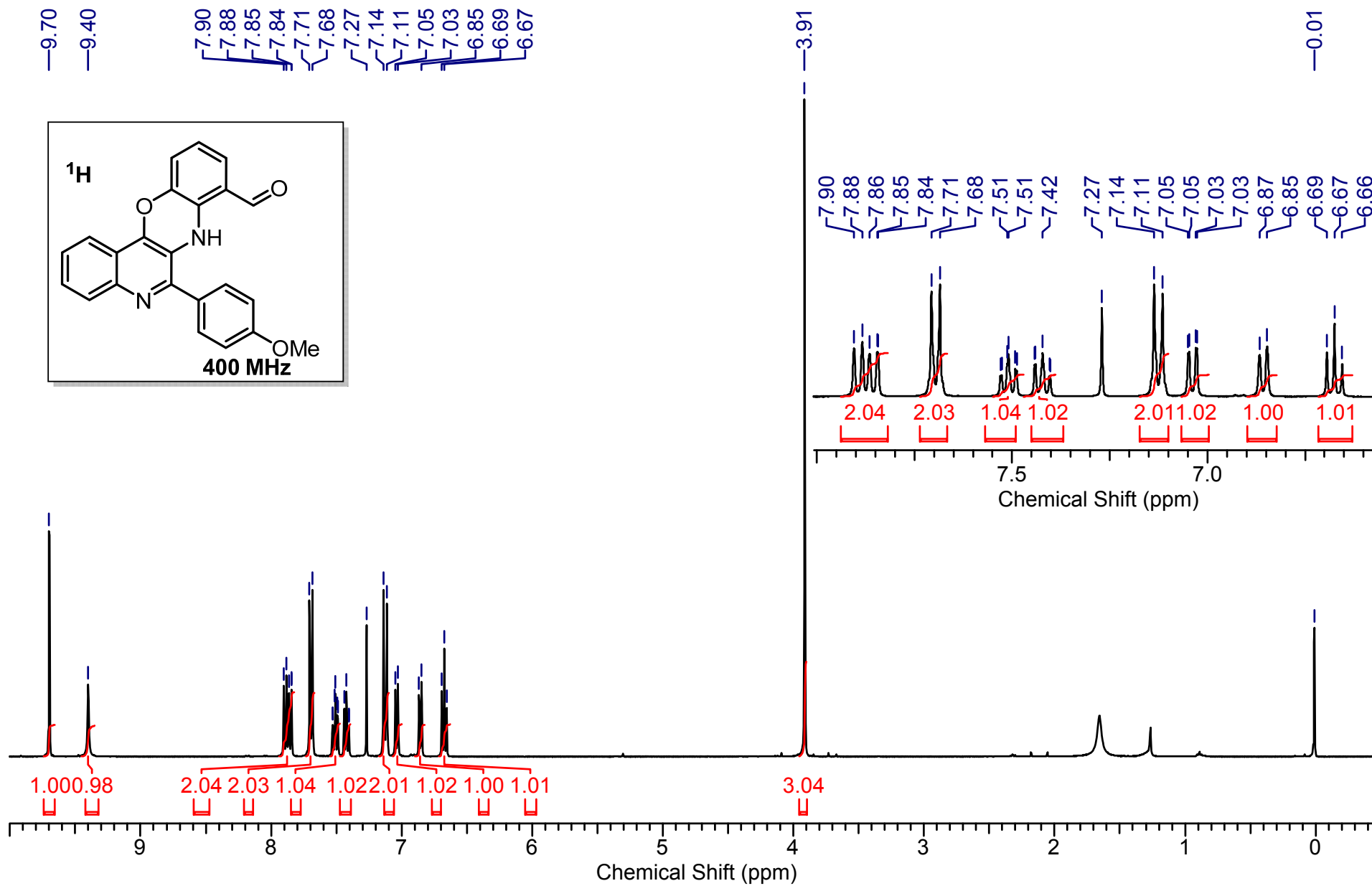


3ai

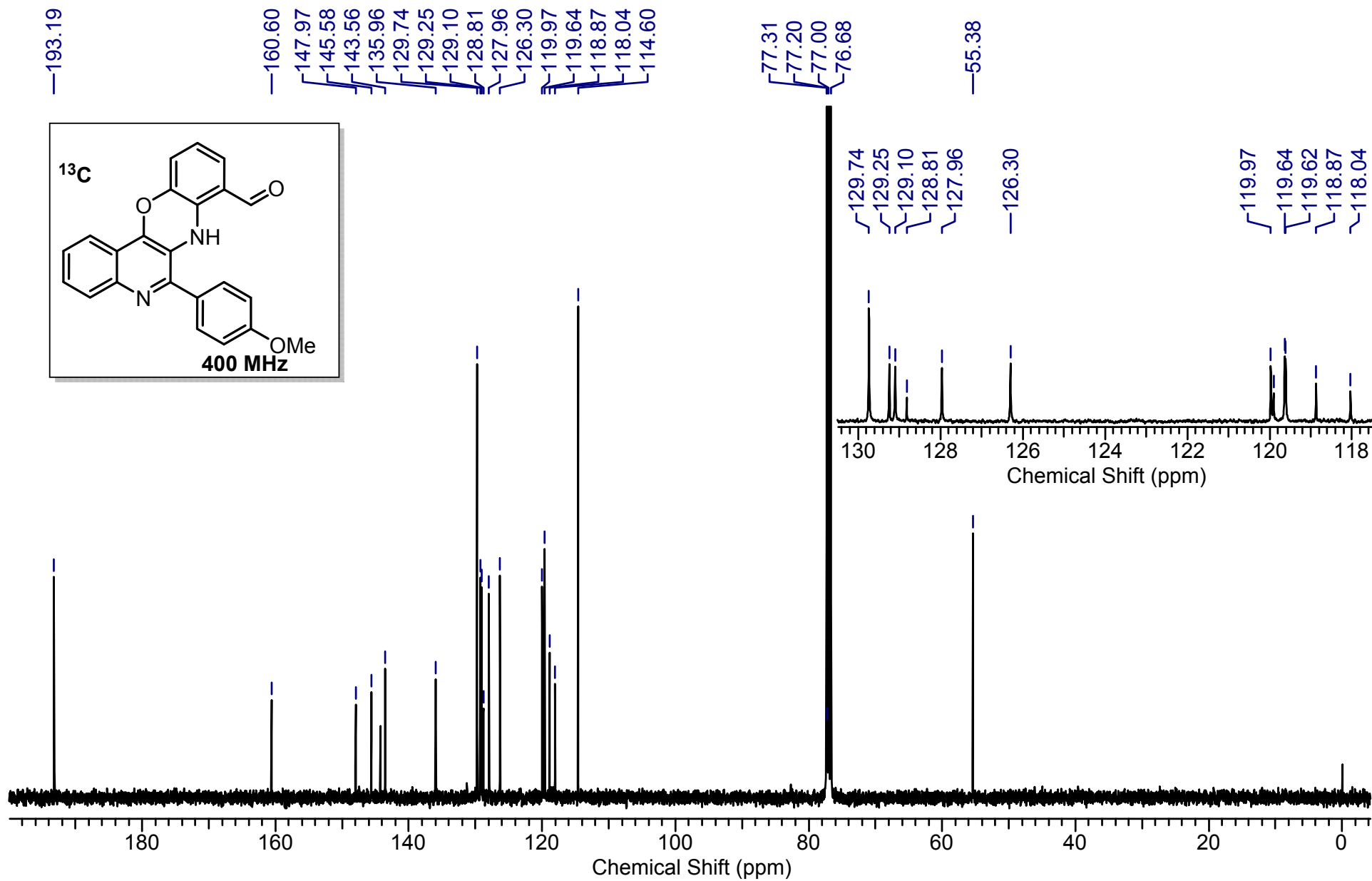
SH-607 #264 RT: 1.40 AV: 1 NL: 9.75E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



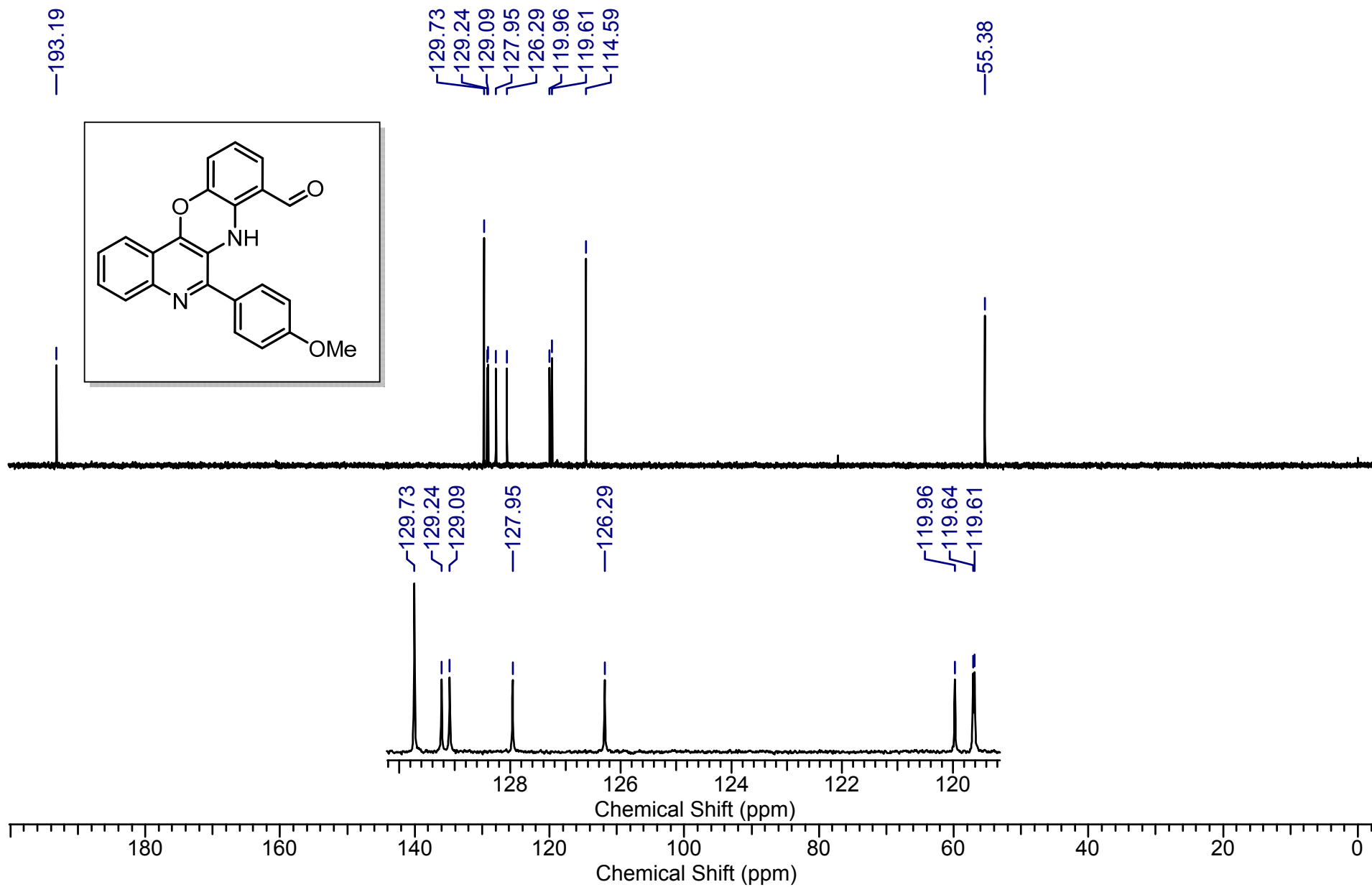
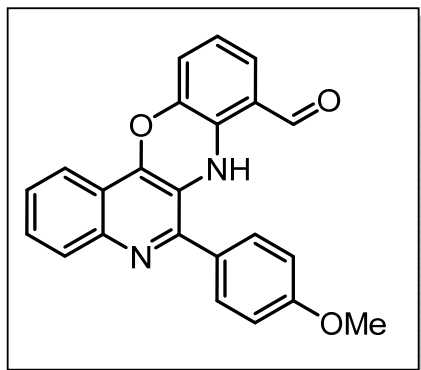
3fa



3fa

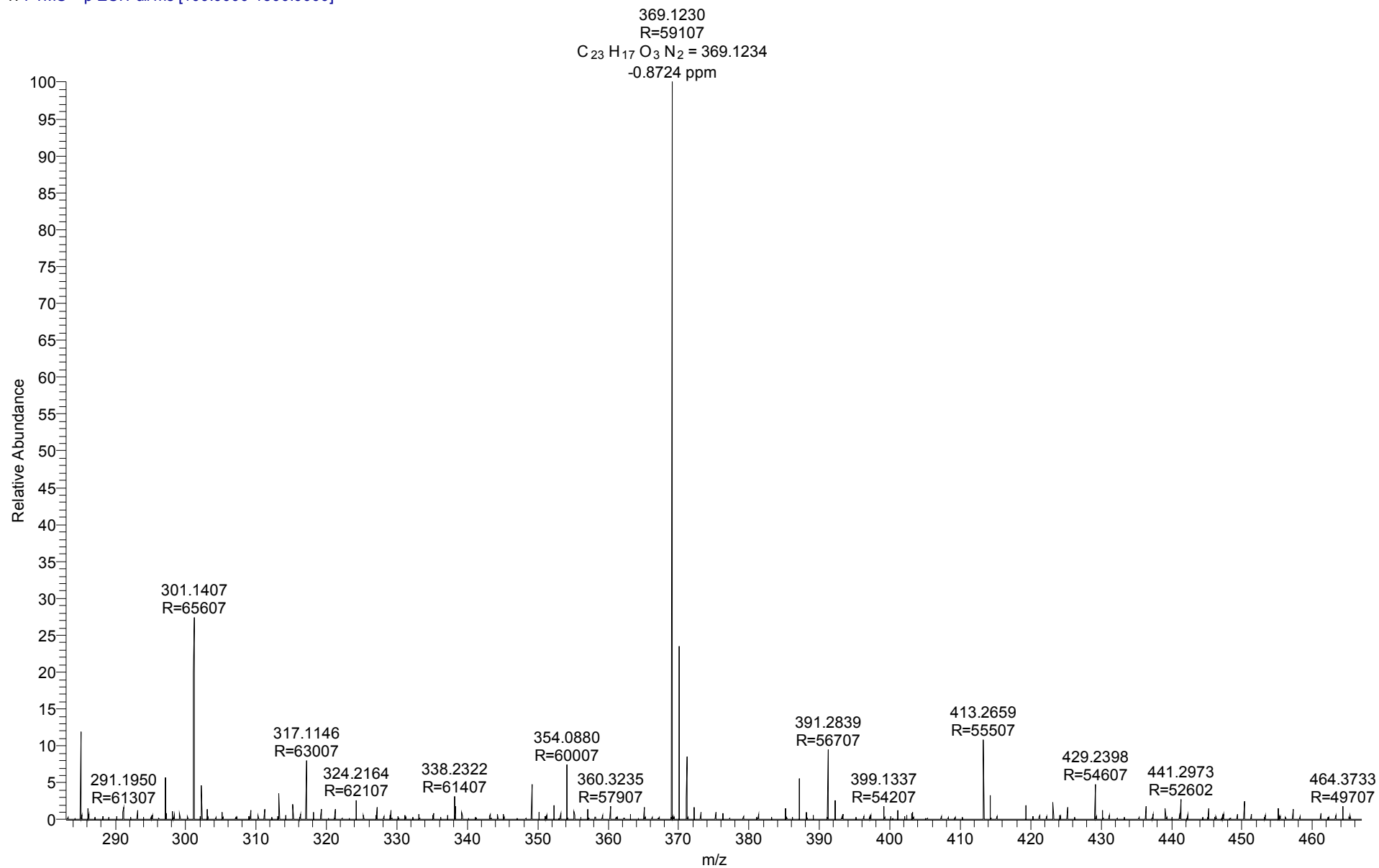


3fa



3fa

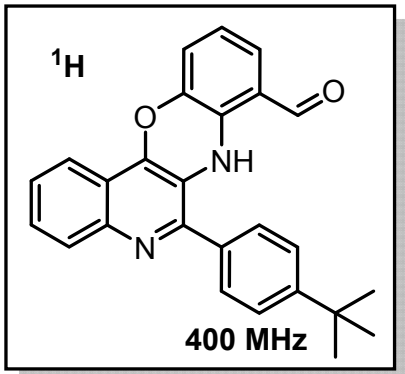
SH-618 #377 RT: 1.99 AV: 1 NL: 5.54E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



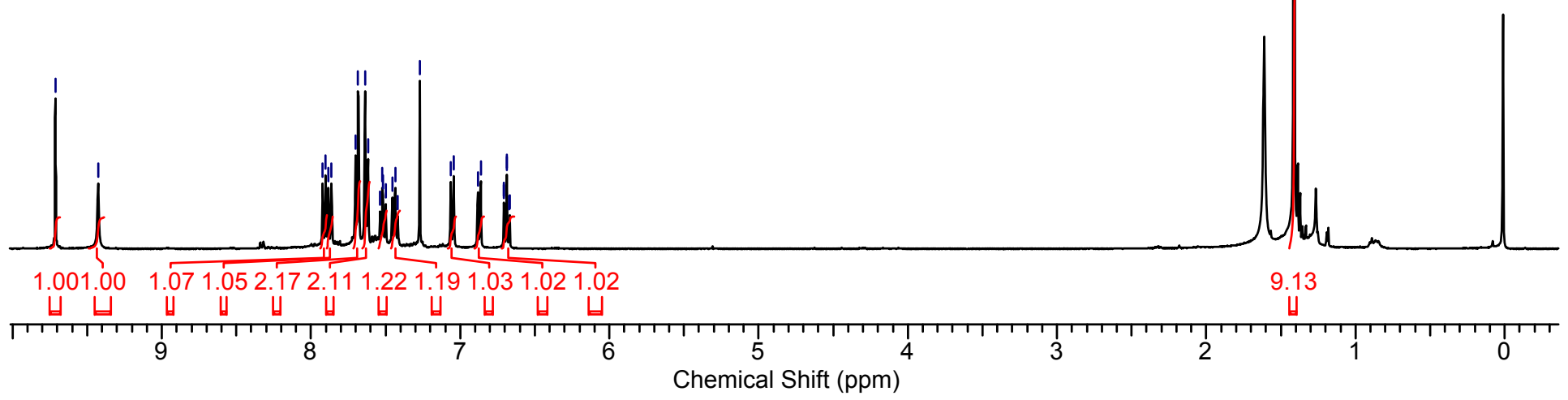
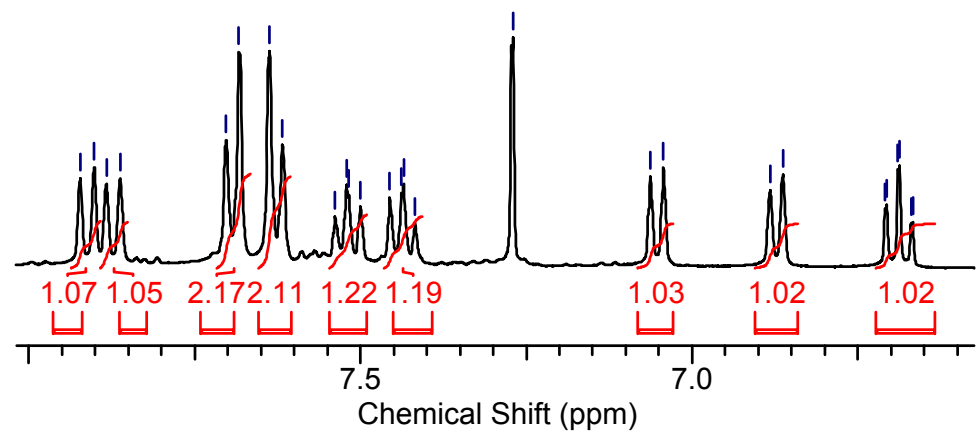
3ga

9.71
9.43

7.92
7.90
7.86
7.70
7.68
7.64
7.62
7.44
7.27
7.06
7.04
6.86
6.69
6.69



7.92
7.90
7.88
7.86
7.70
7.68
7.64
7.62
7.52
7.52
7.50
7.46
7.44
7.44
7.42
7.27
7.06
7.04
6.88
6.86
6.71
6.71
6.69
6.69
6.67



3ga

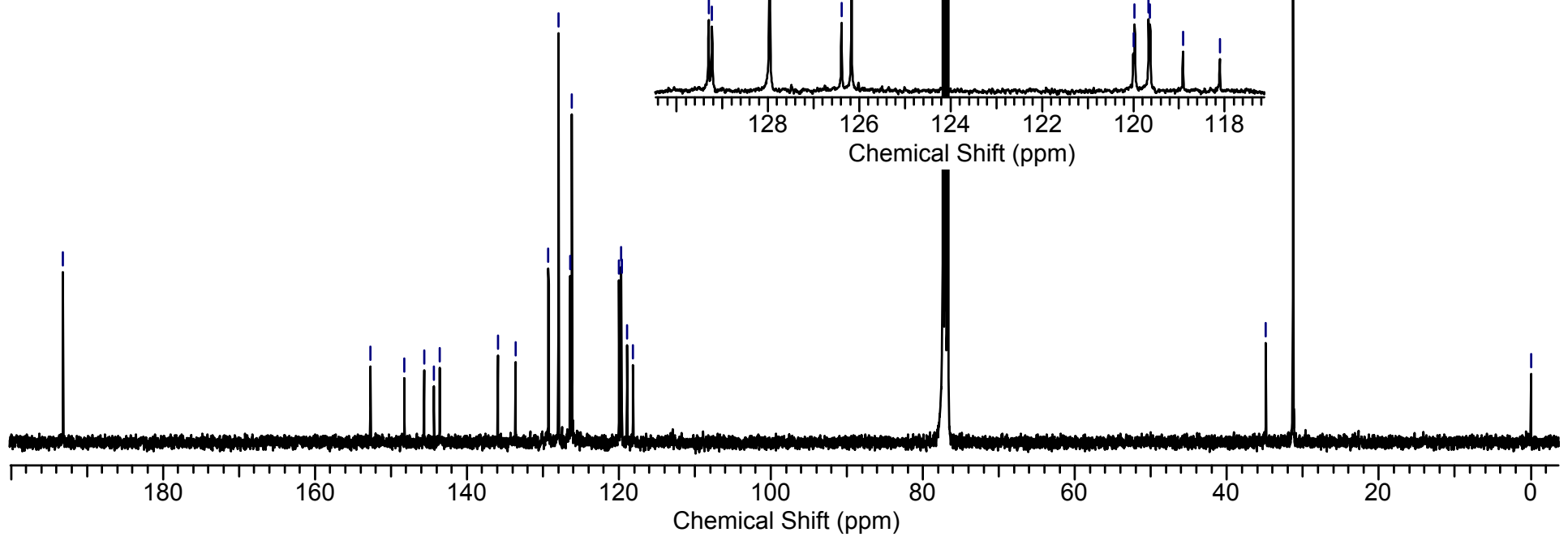
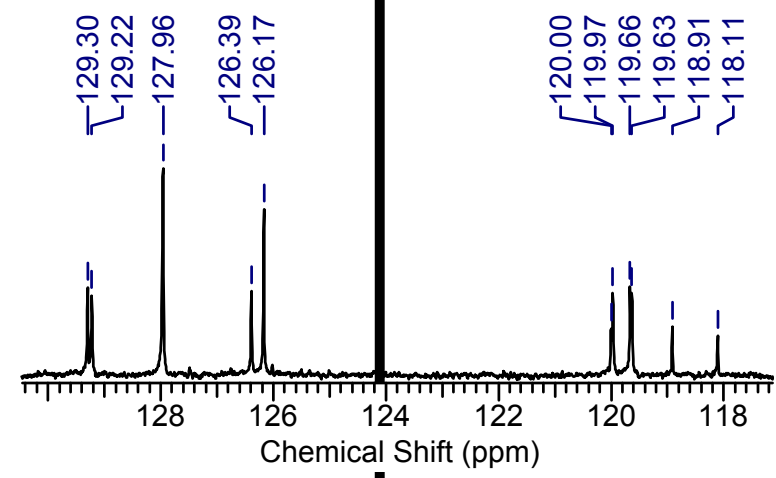
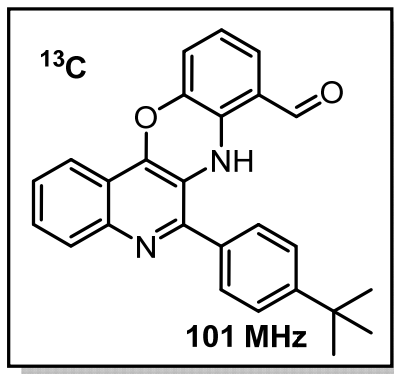
—193.16

—152.67
—148.20
—145.64
—143.59
—135.95
—133.58
—129.30
—127.96
—126.39
—126.17
—119.97
—119.66
—119.63
—118.91

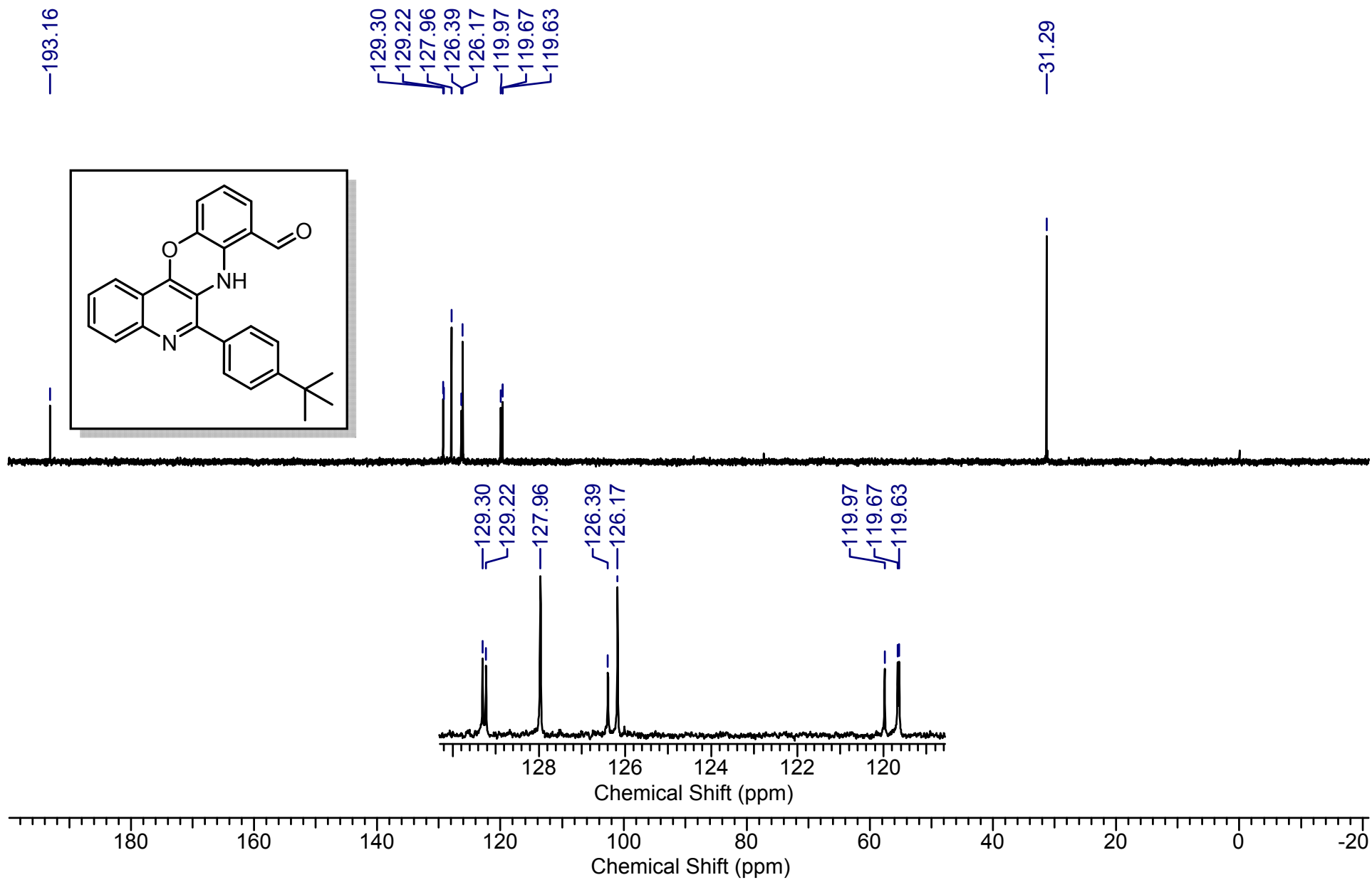
—77.32
—77.00
—76.68

—34.85
—31.29

—0.02

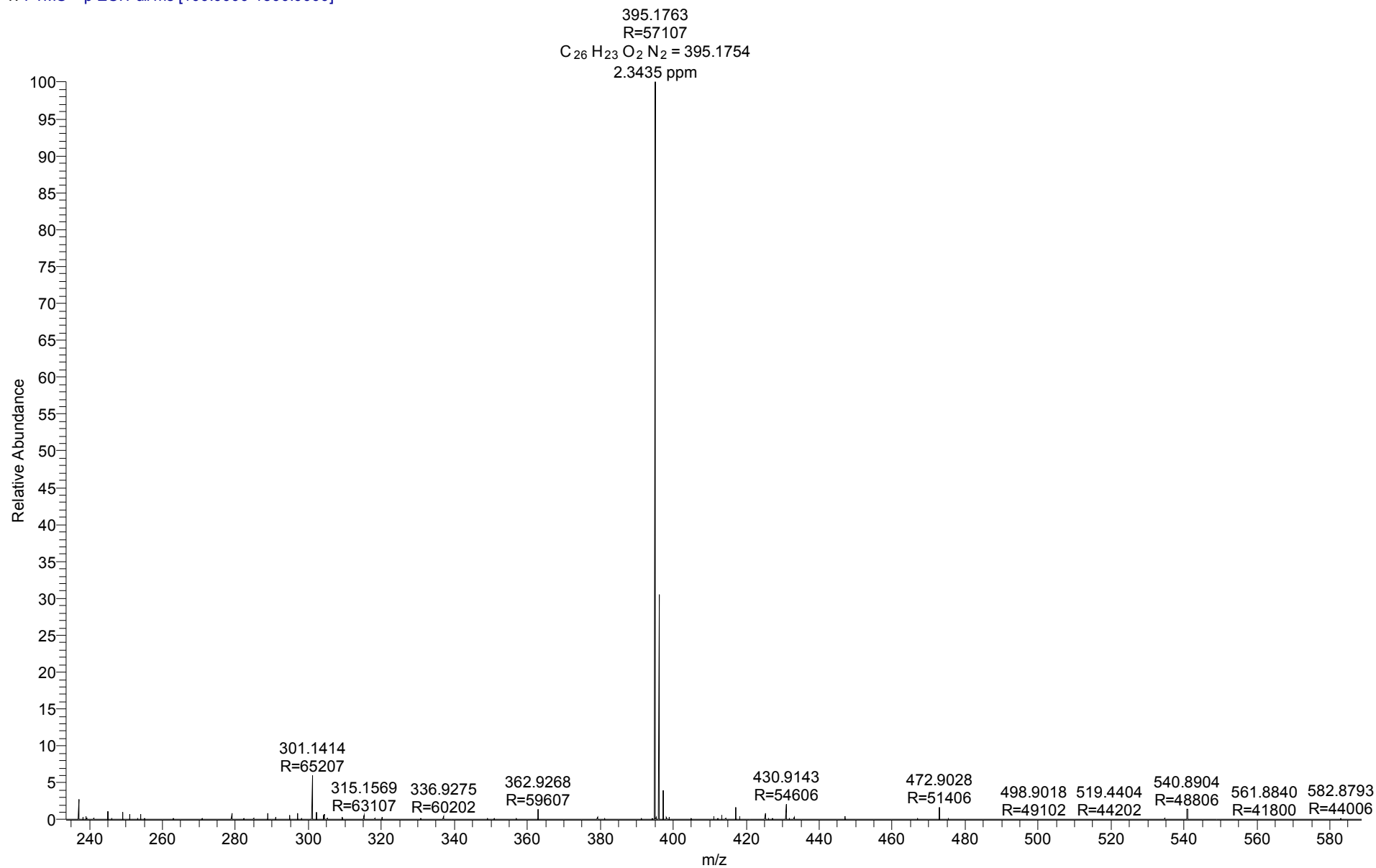


3ga

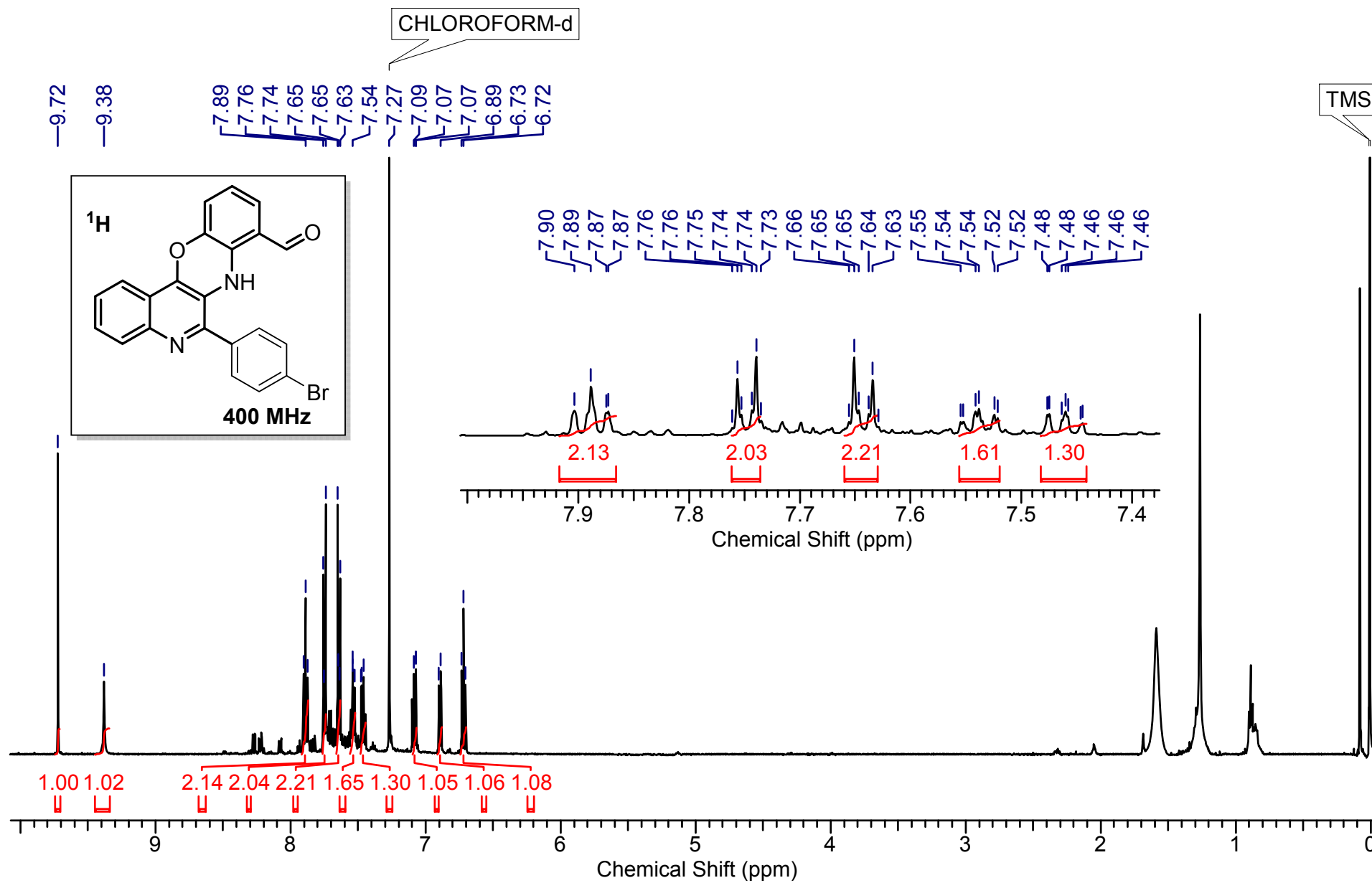


3ga

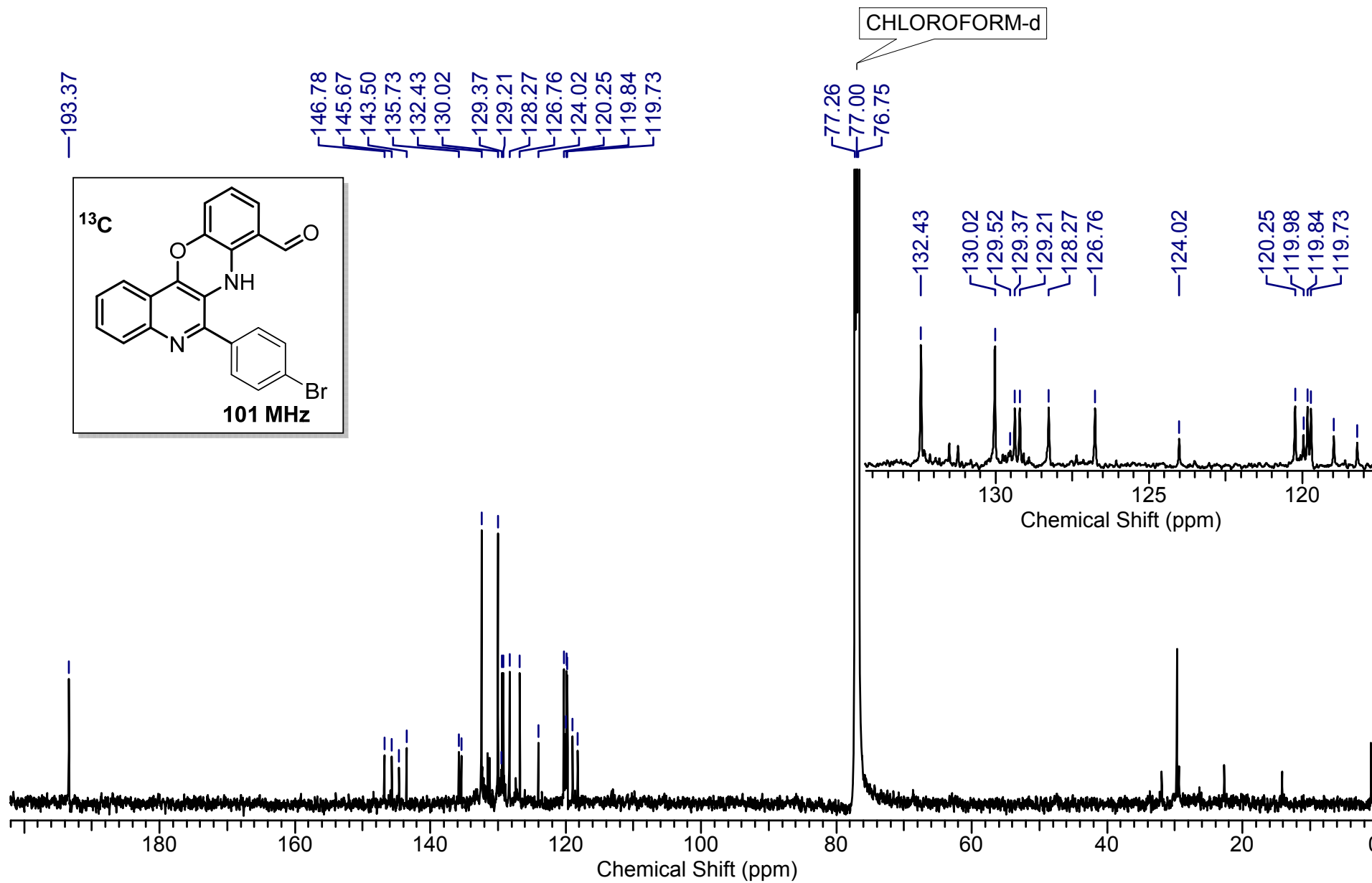
SH-634 #489 RT: 2.63 AV: 1 NL: 3.15E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



3ha

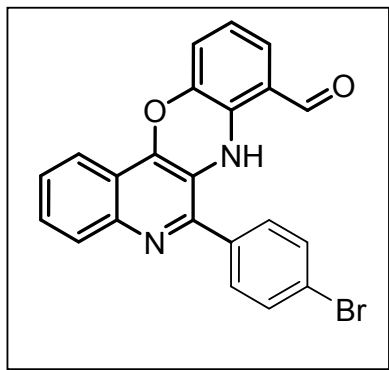


3ha

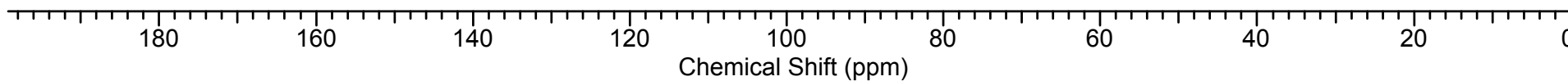
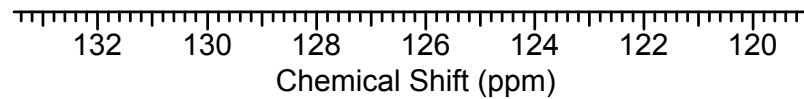
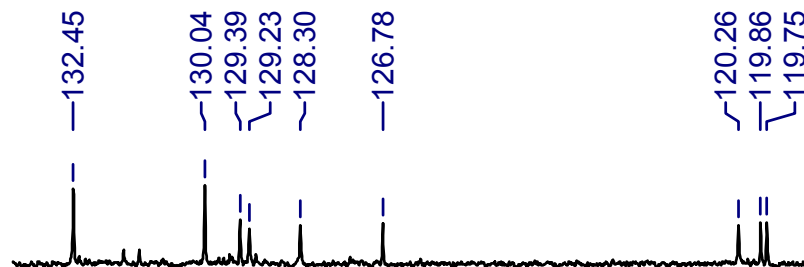


3ha

193.39

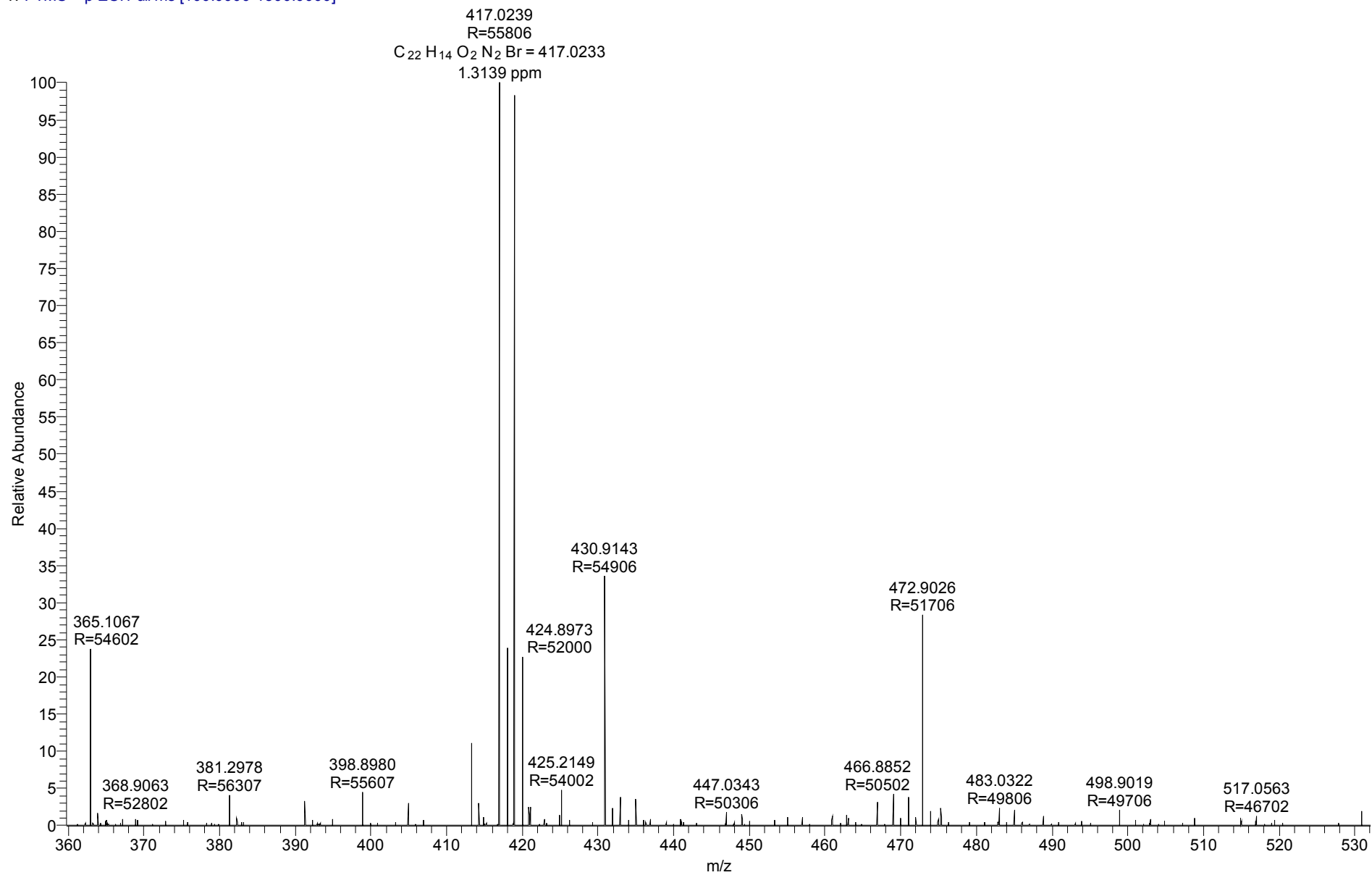


132.45
130.04
129.39
129.23
128.30
126.78
120.26
119.86
119.75



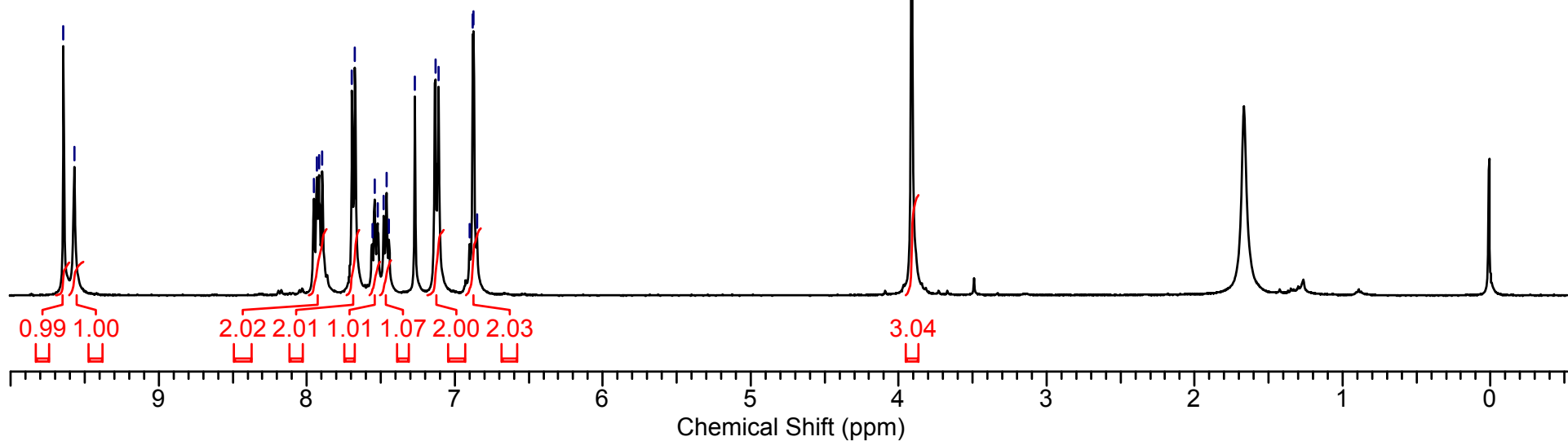
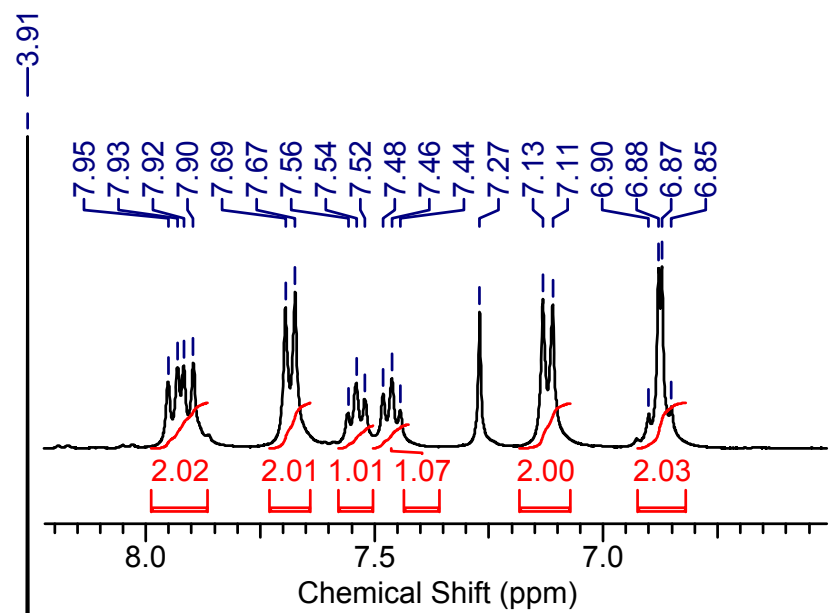
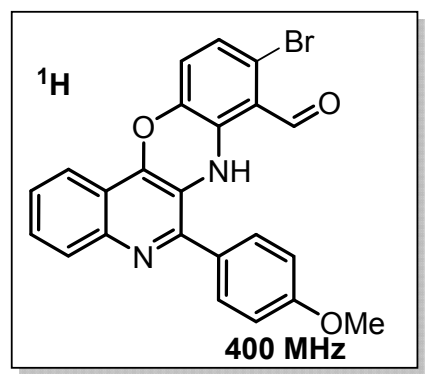
3ha

SH-653 #438 RT: 2.35 AV: 1 NL: 2.04E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

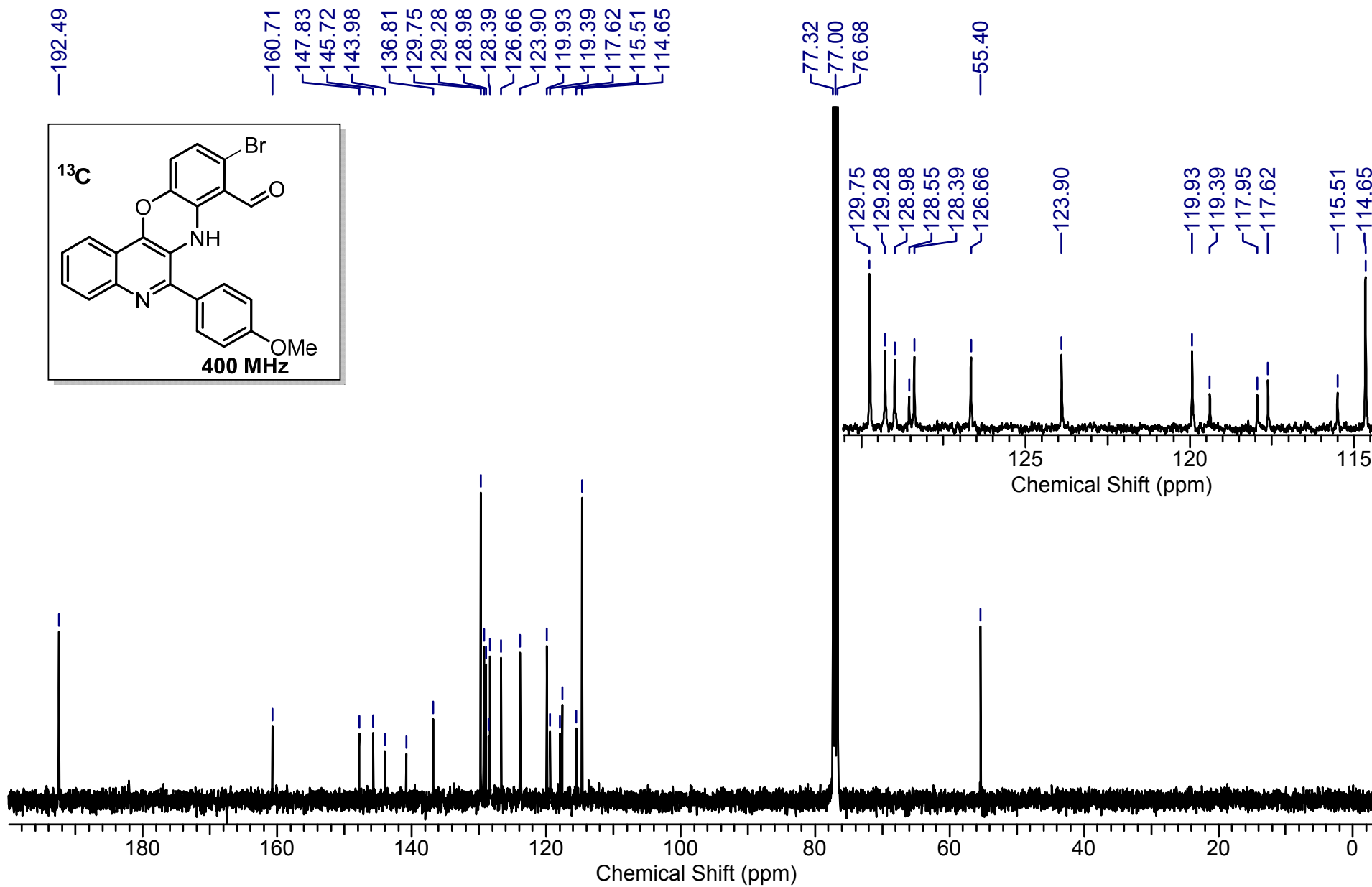


3fb

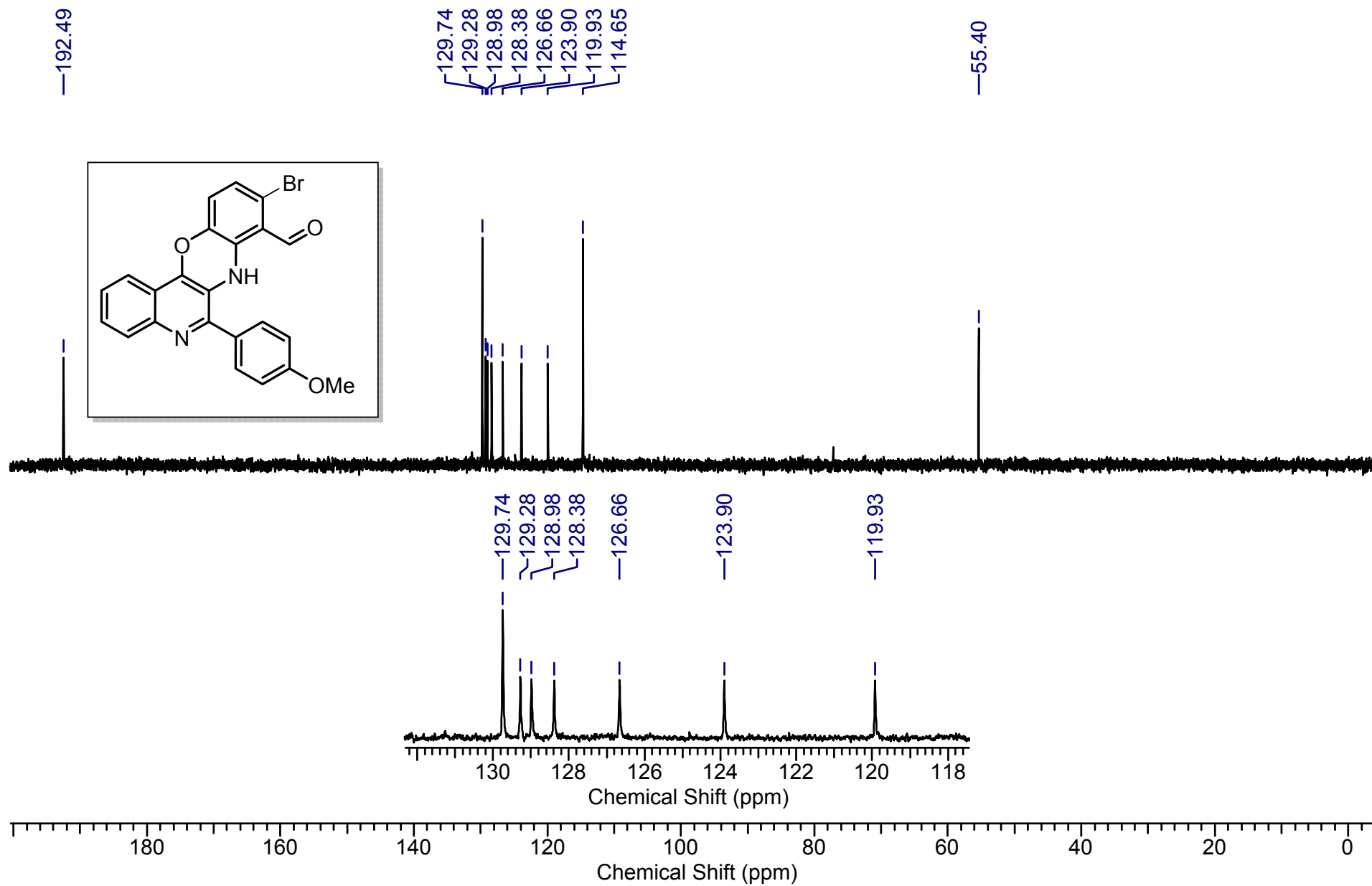
9.64
9.57
7.95
7.93
7.92
7.90
7.69
7.67
7.54
7.46
7.27
7.13
7.11
6.88
6.87



3fb

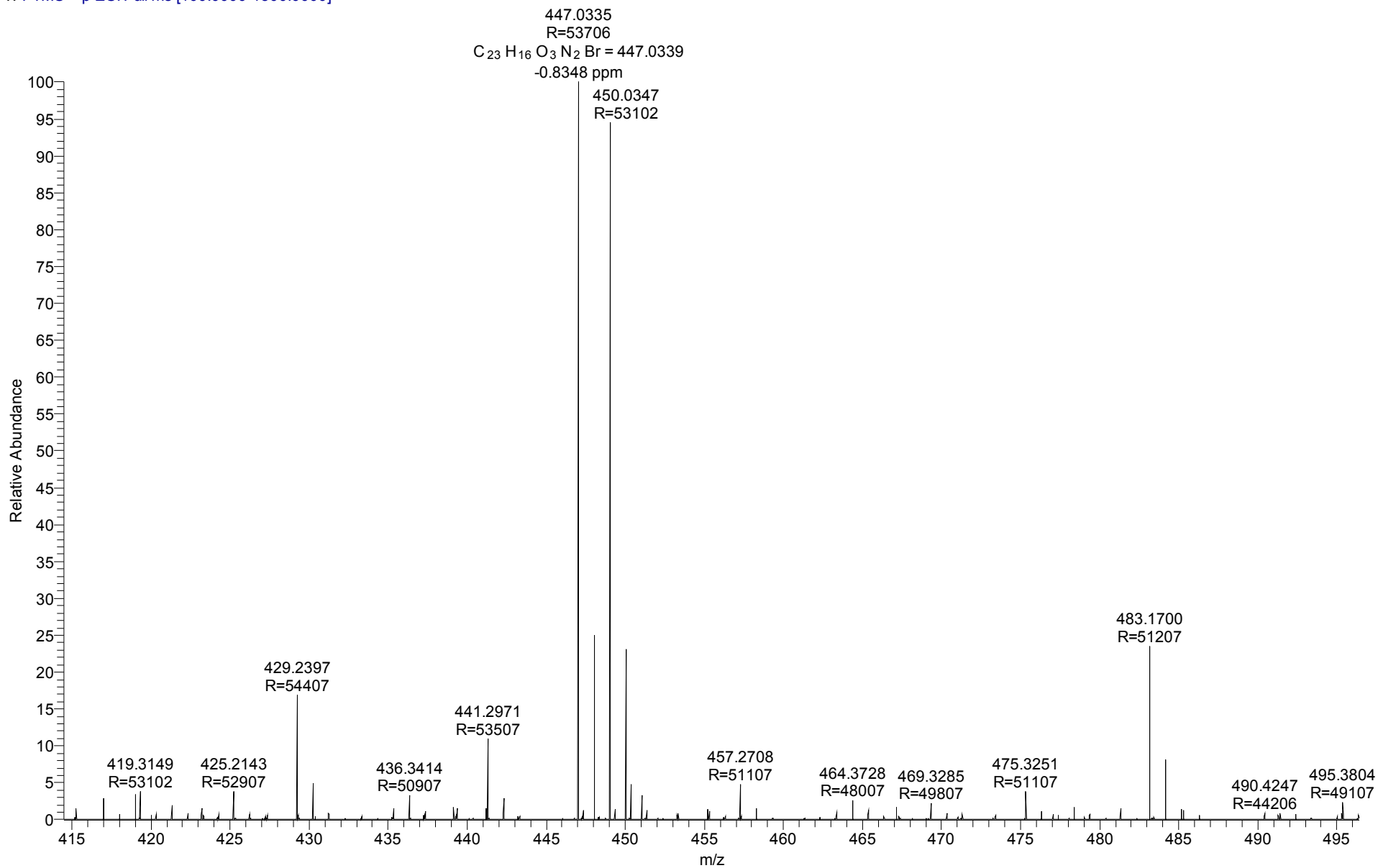


3fb



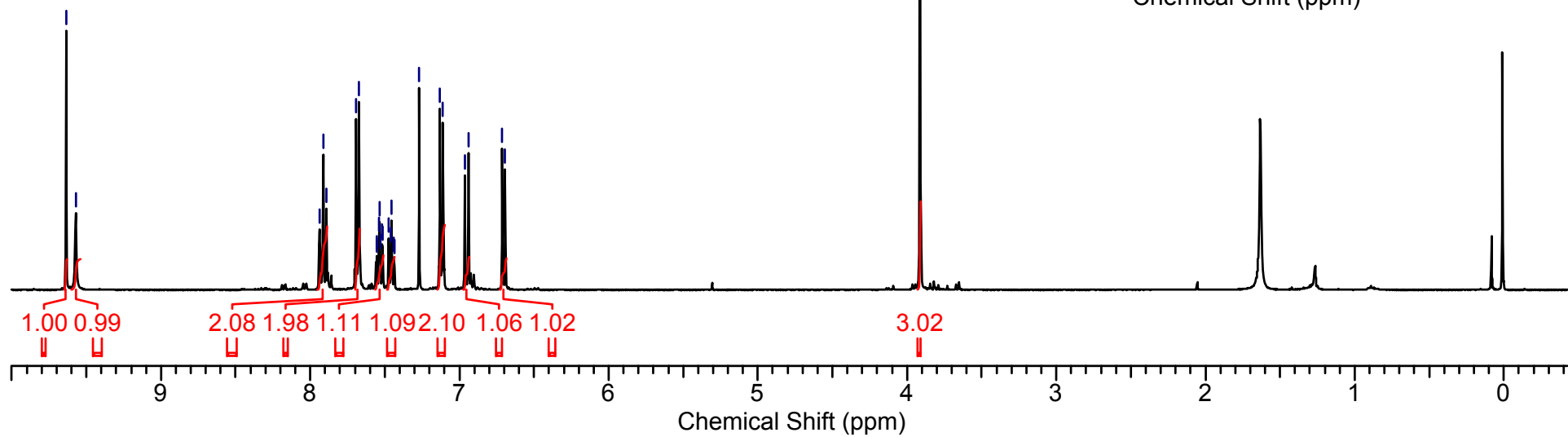
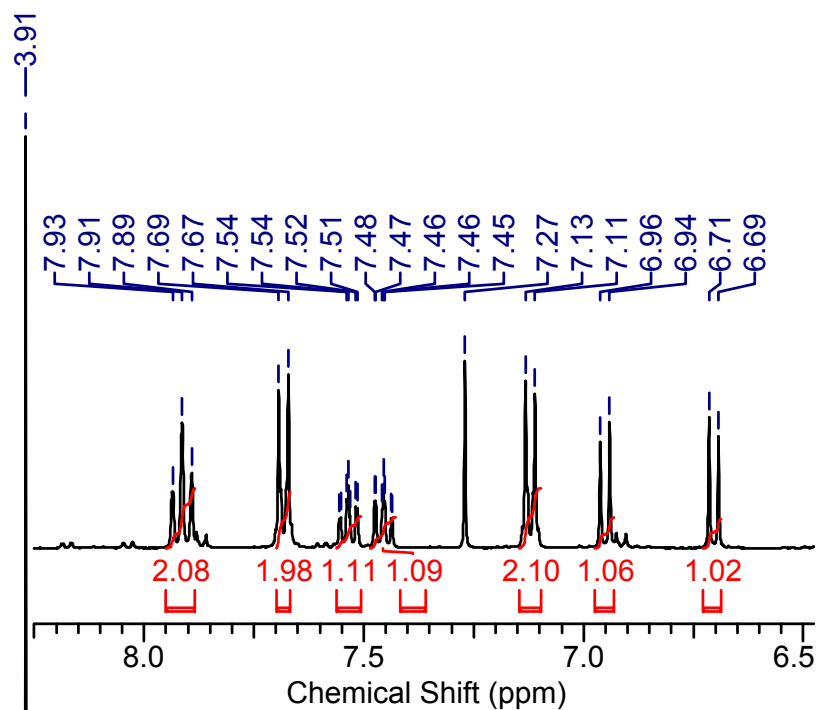
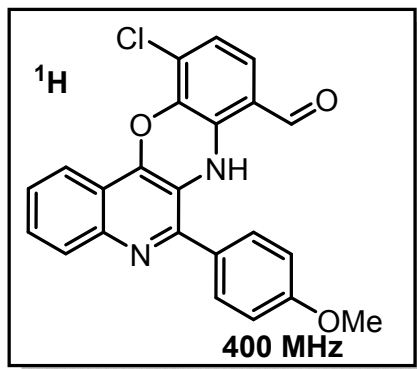
3fb

SH-614 #483 RT: 2.56 AV: 1 NL: 1.87E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

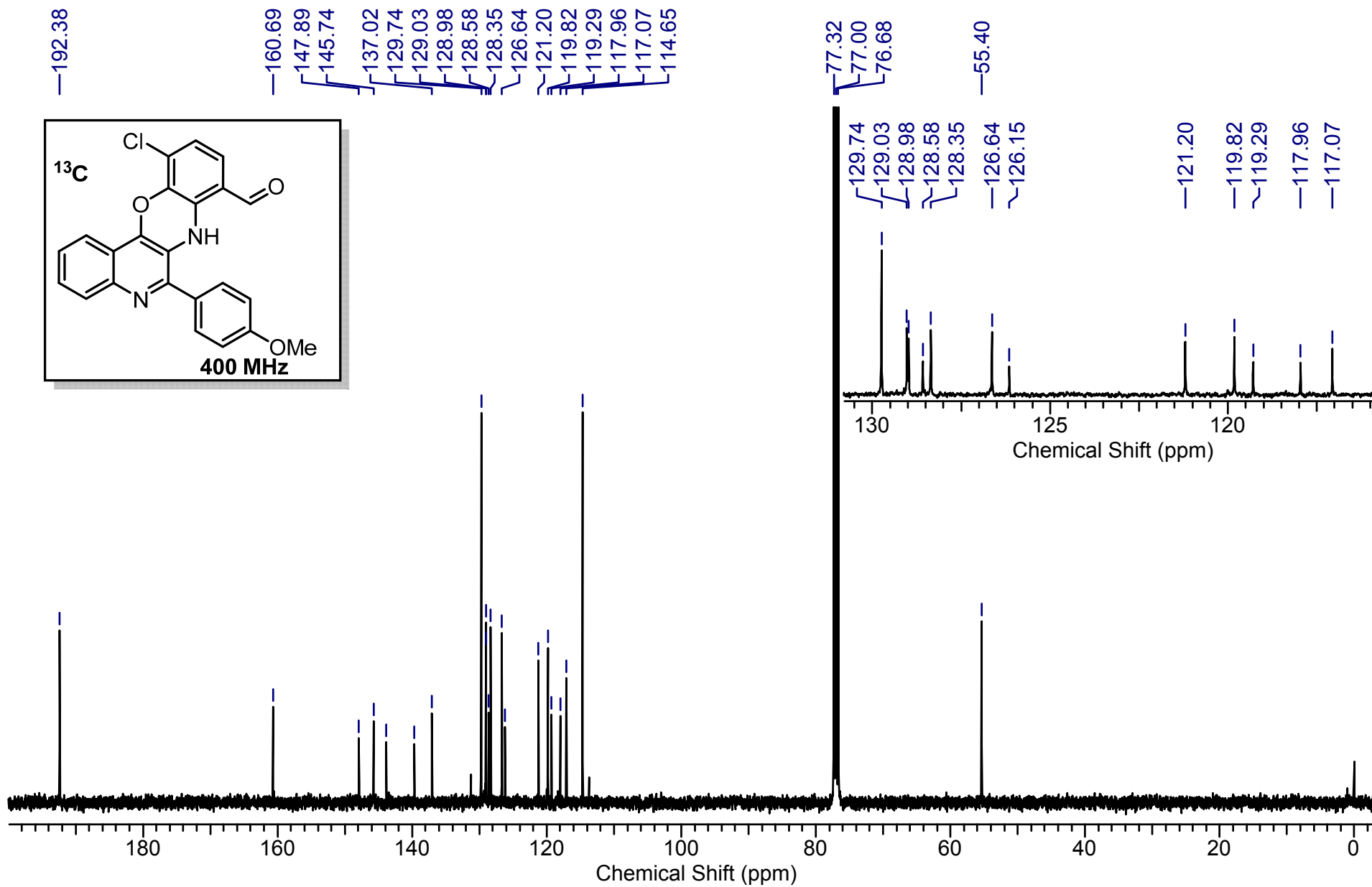
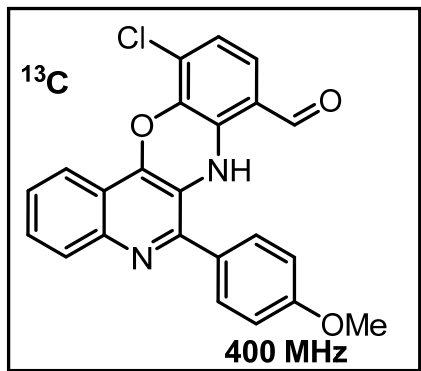


3fc

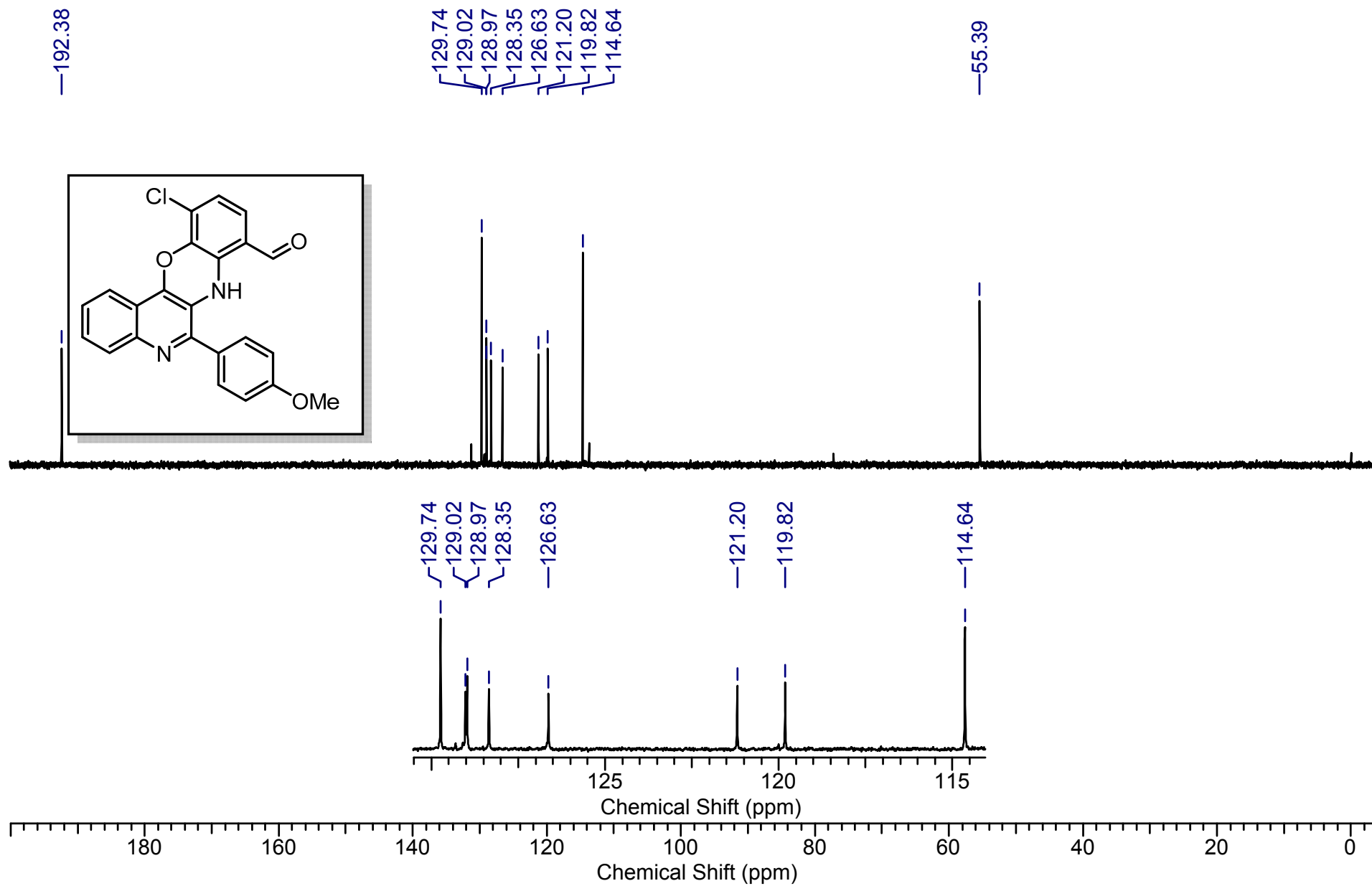
9.64
9.57
7.93
7.91
7.89
7.69
7.67
7.54
7.46
7.27
7.13
7.11
6.96
6.94
6.71
6.69



3fc

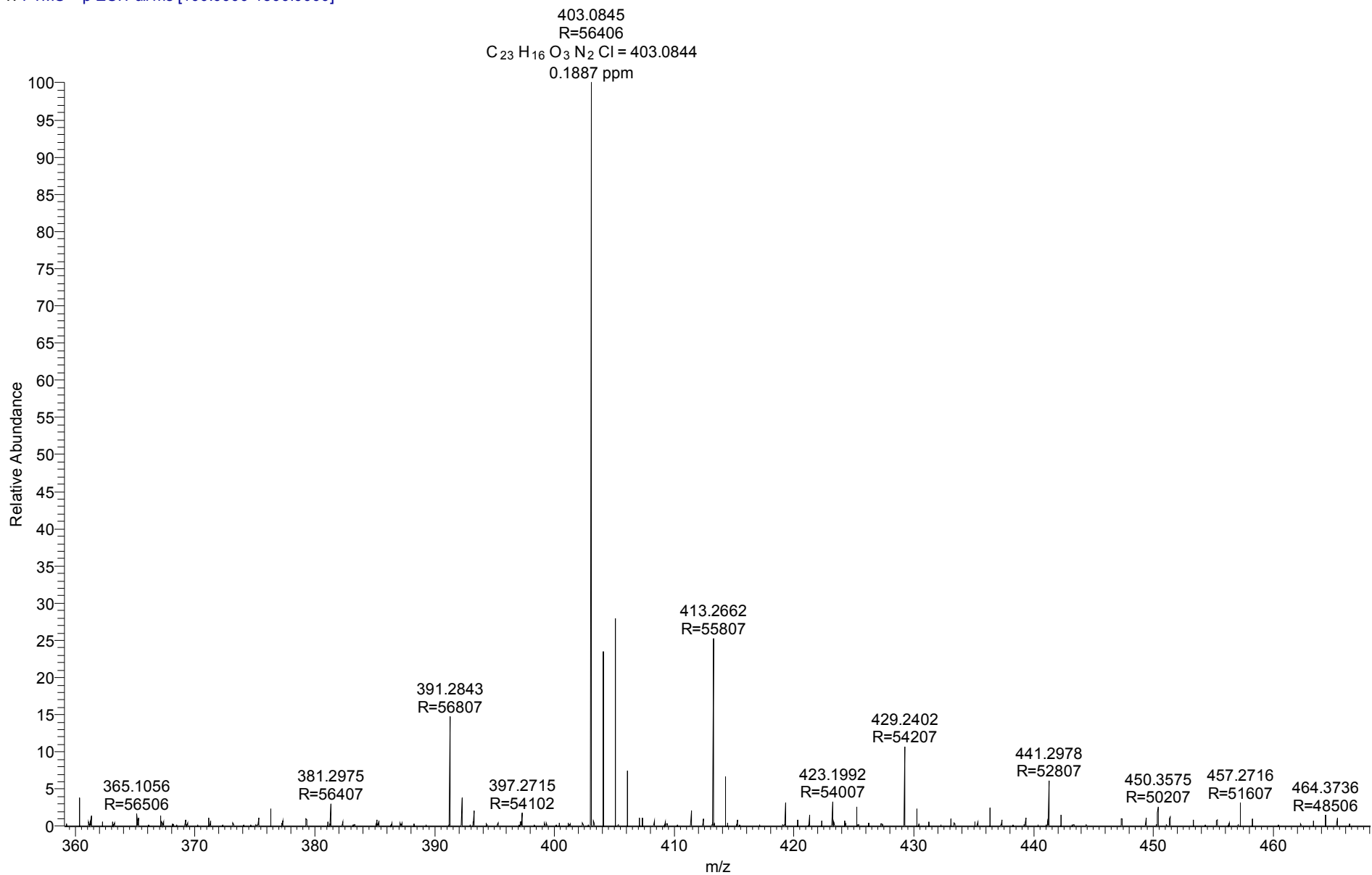


3fc

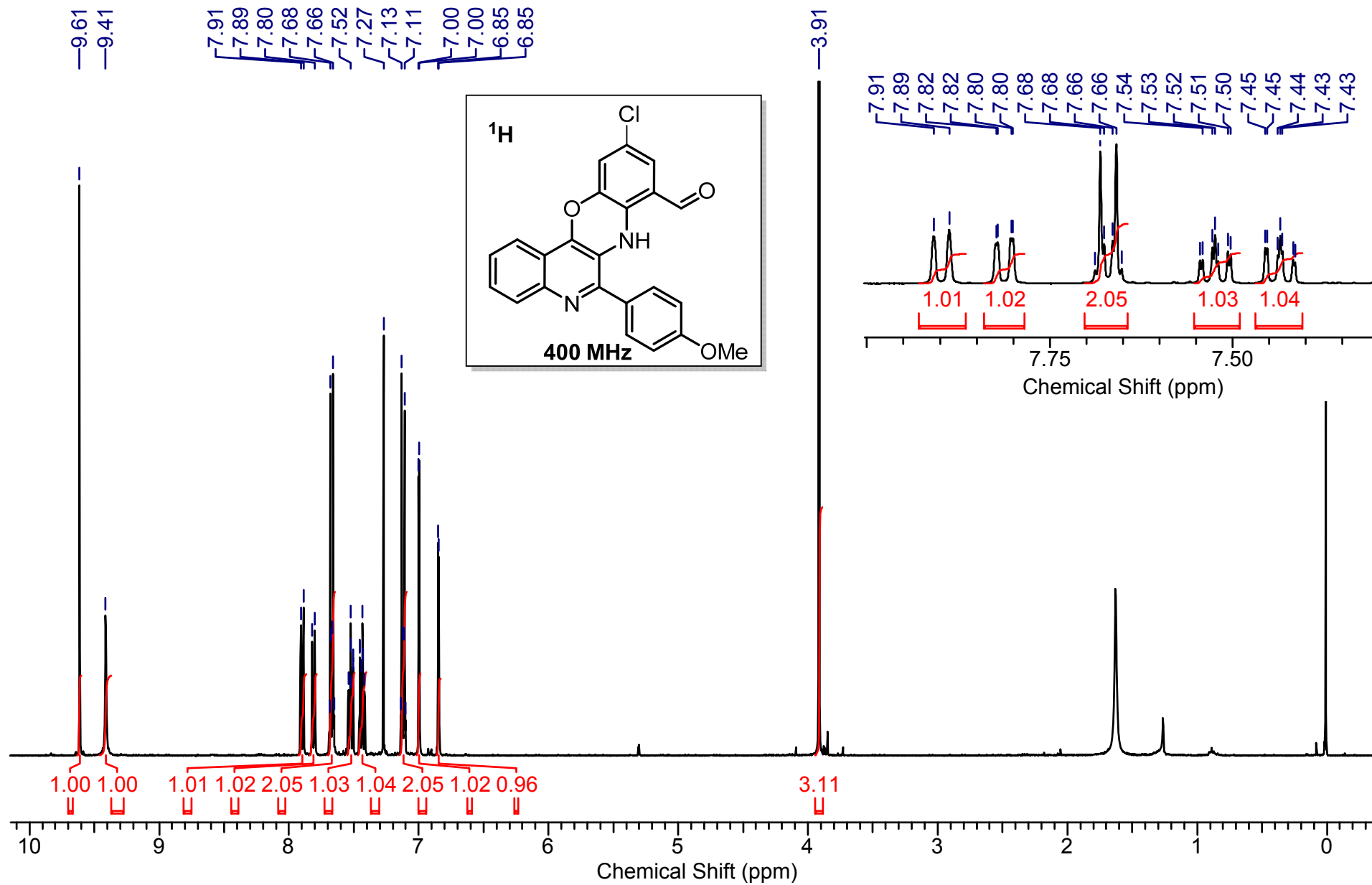


3fc

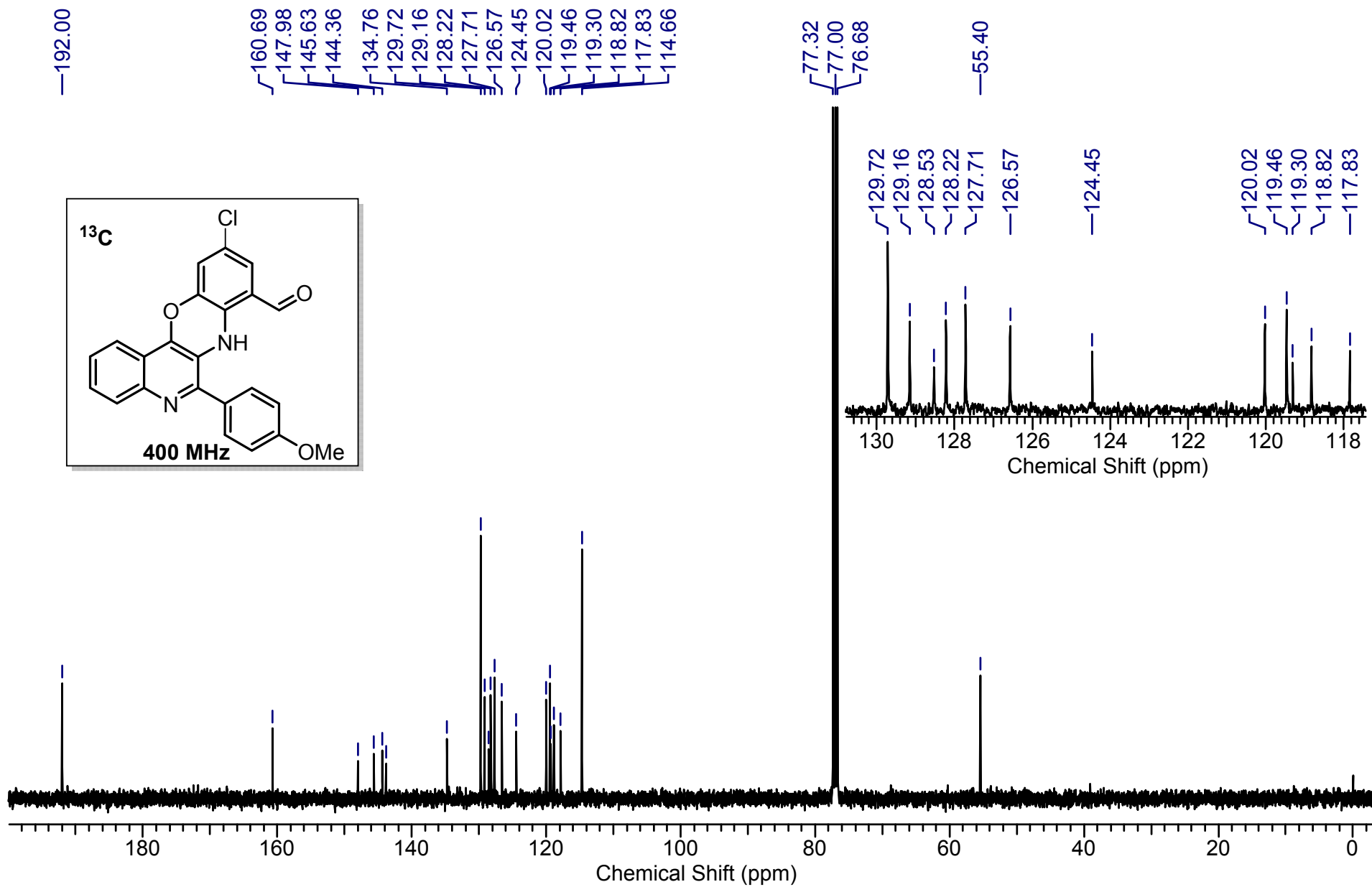
SH-613 #477 RT: 2.53 AV: 1 NL: 2.51E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



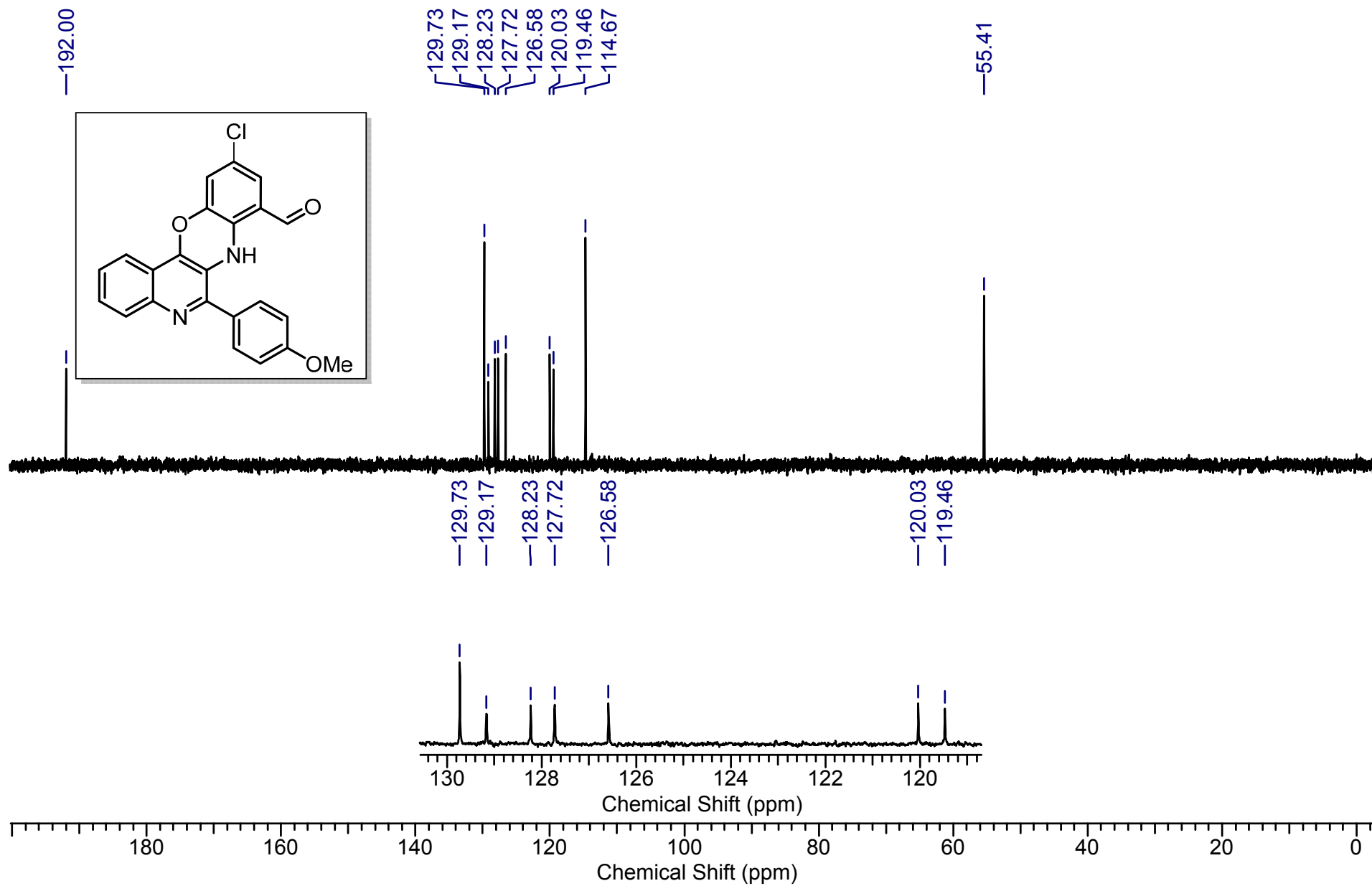
3fd



3fd

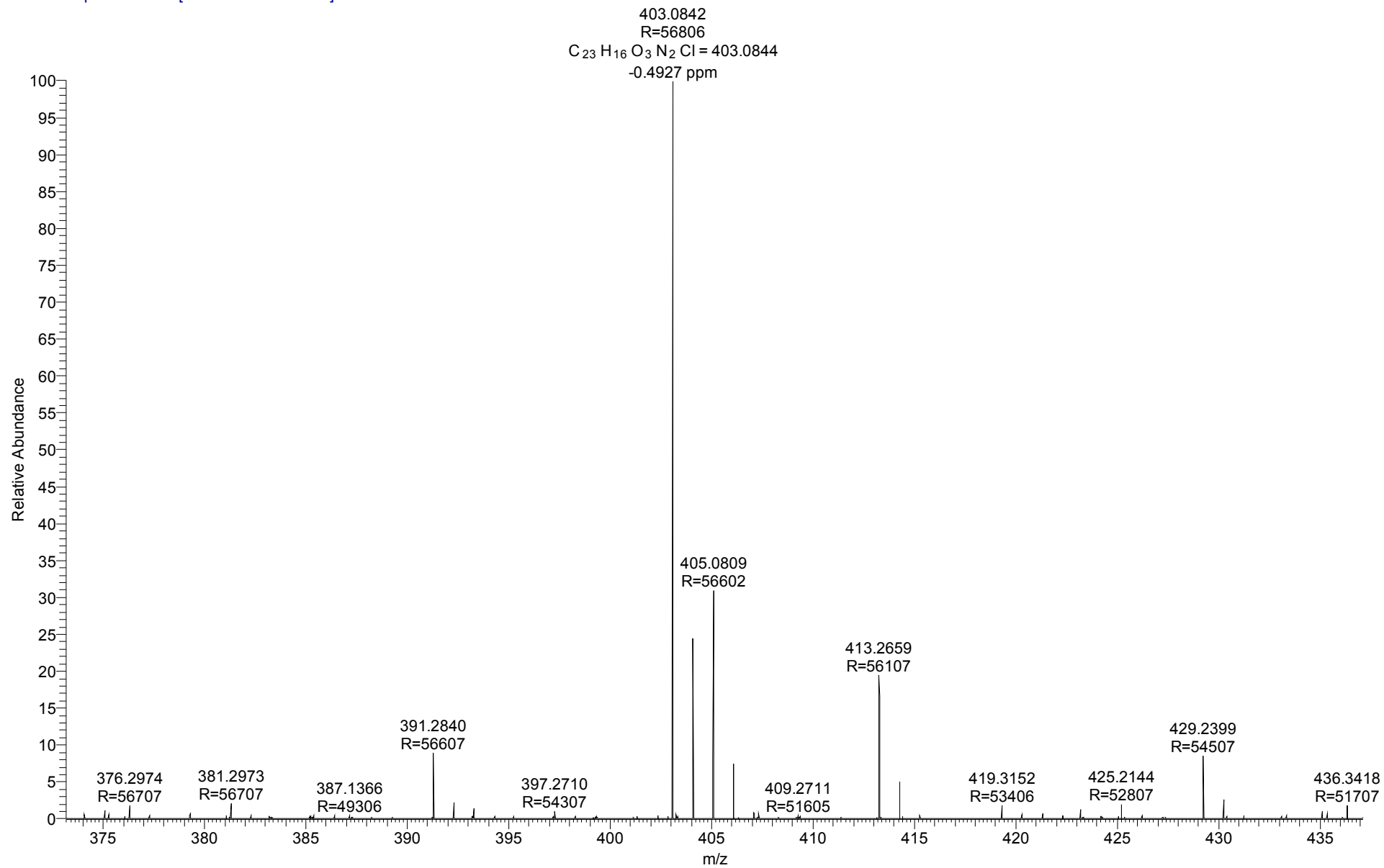


3fd

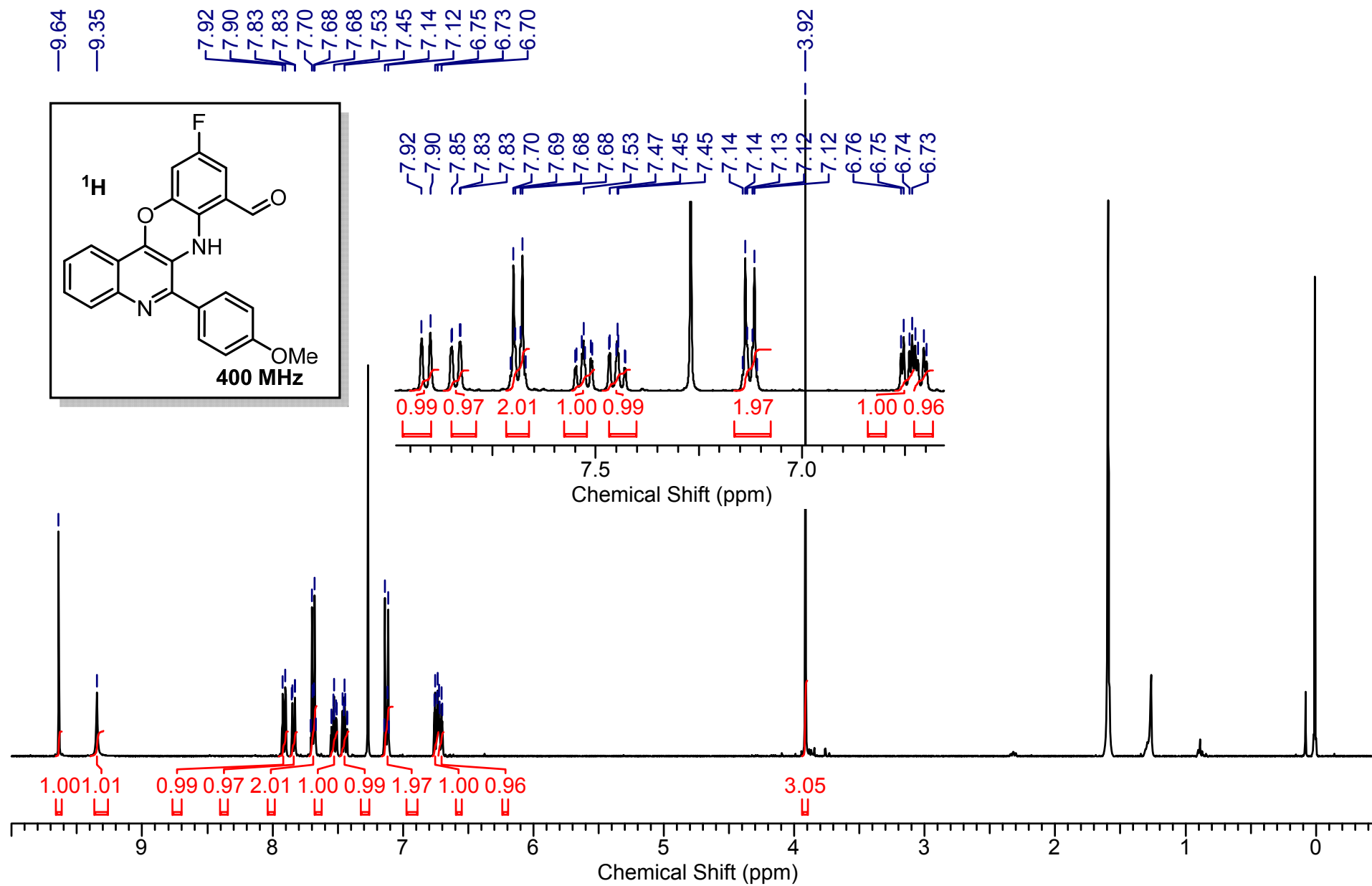


3fd

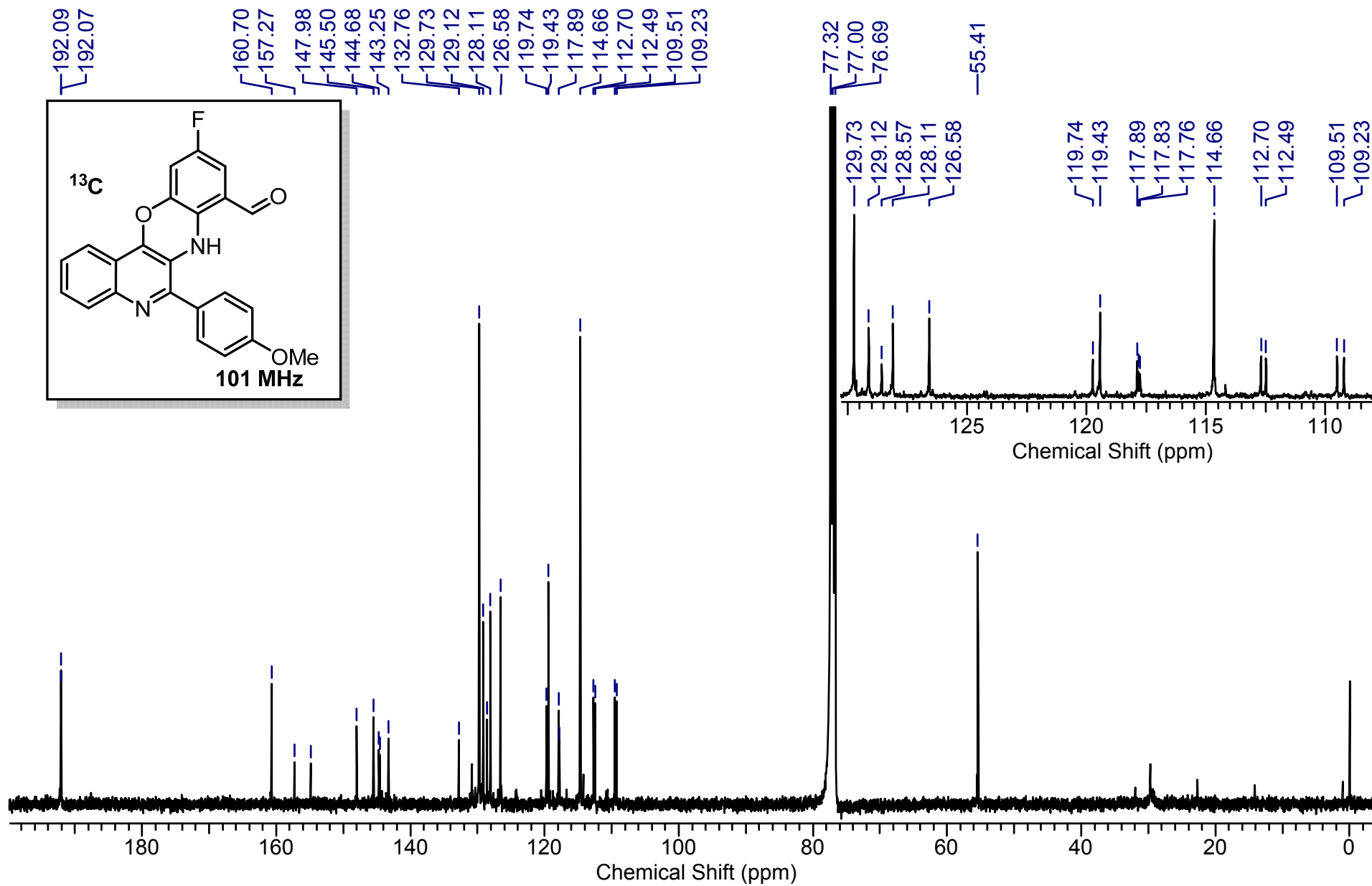
SH-615 #473 RT: 2.50 AV: 1 NL: 4.46E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



3fe

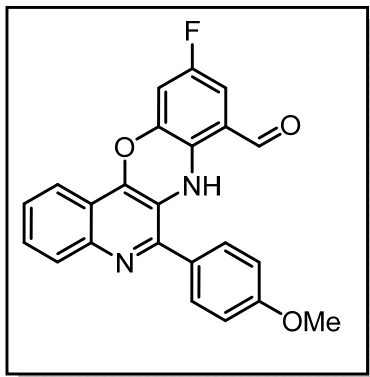


3fe



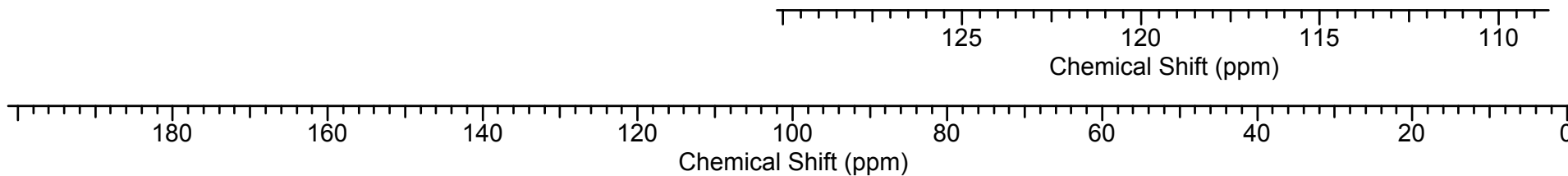
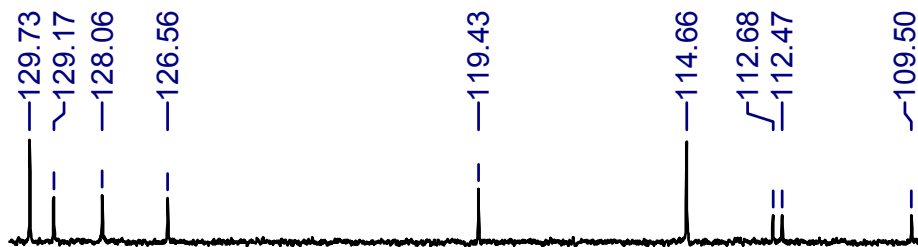
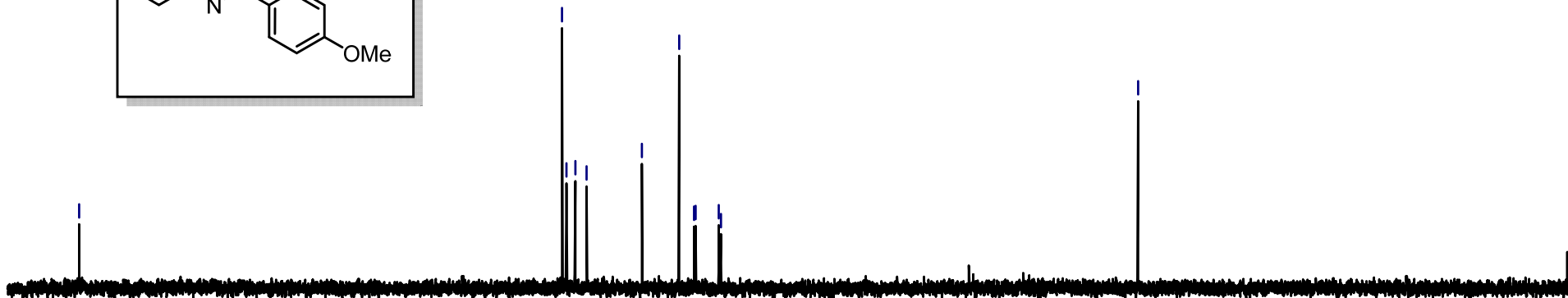
3fe

—192.09

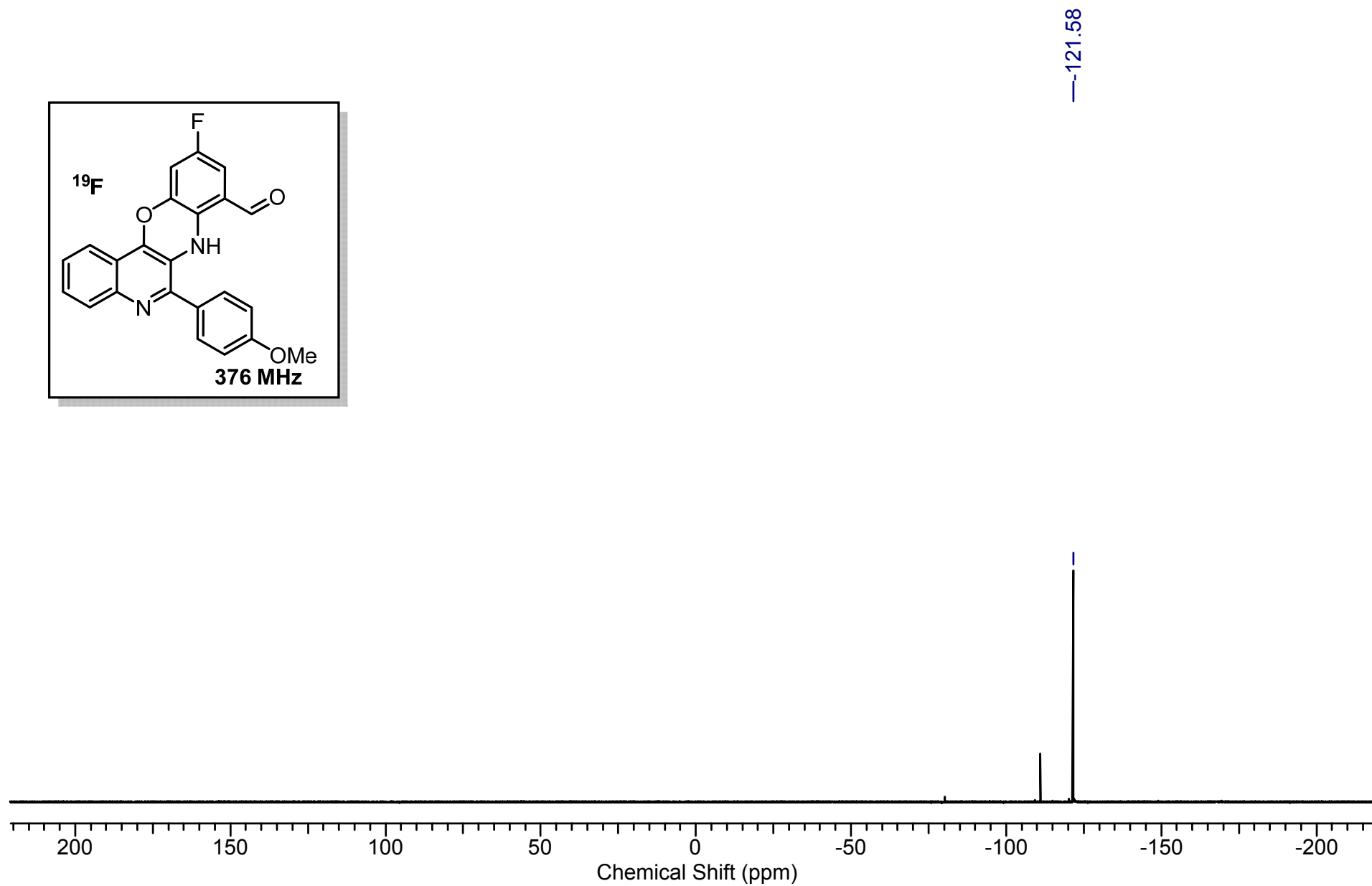
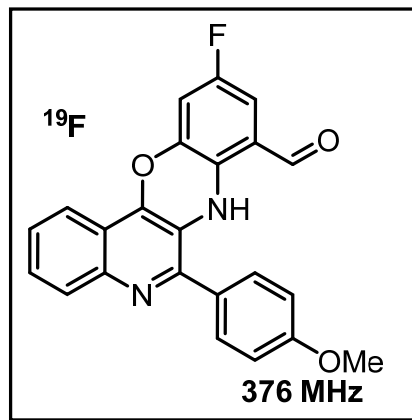


129.73
129.17
128.06
126.56
119.43
114.66
112.68
112.47
109.50
109.22

—55.41

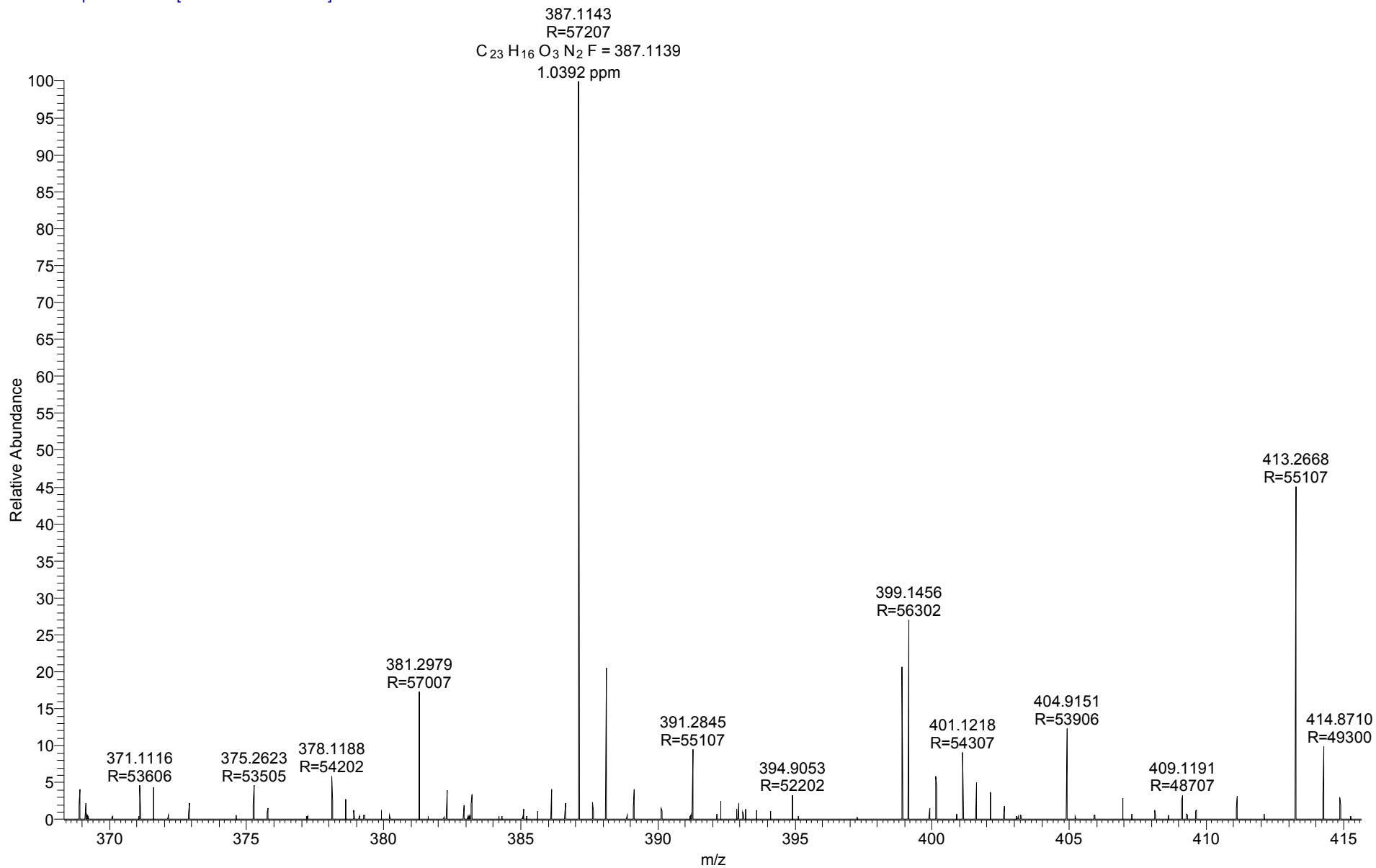


3fe

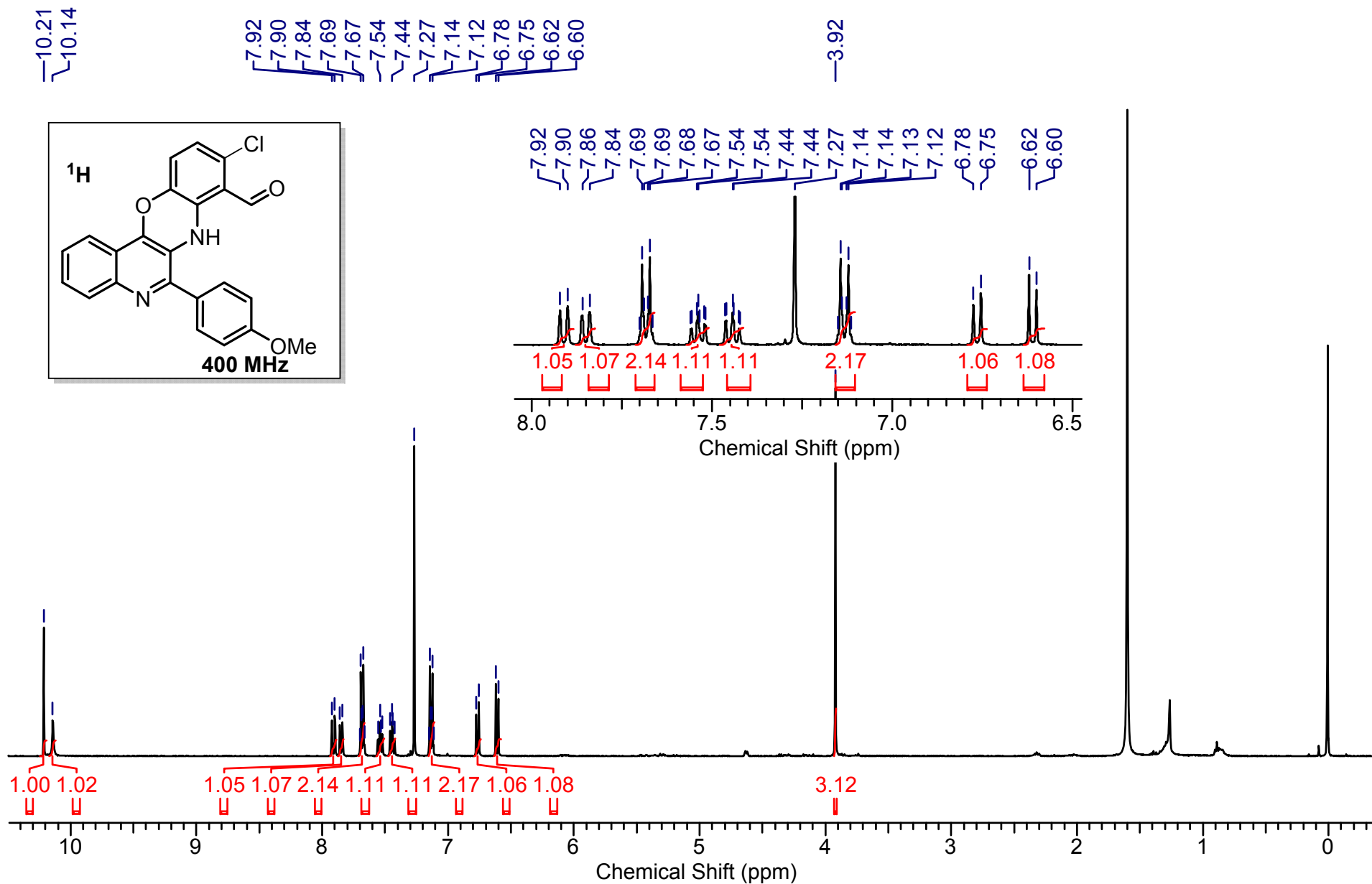


3fe

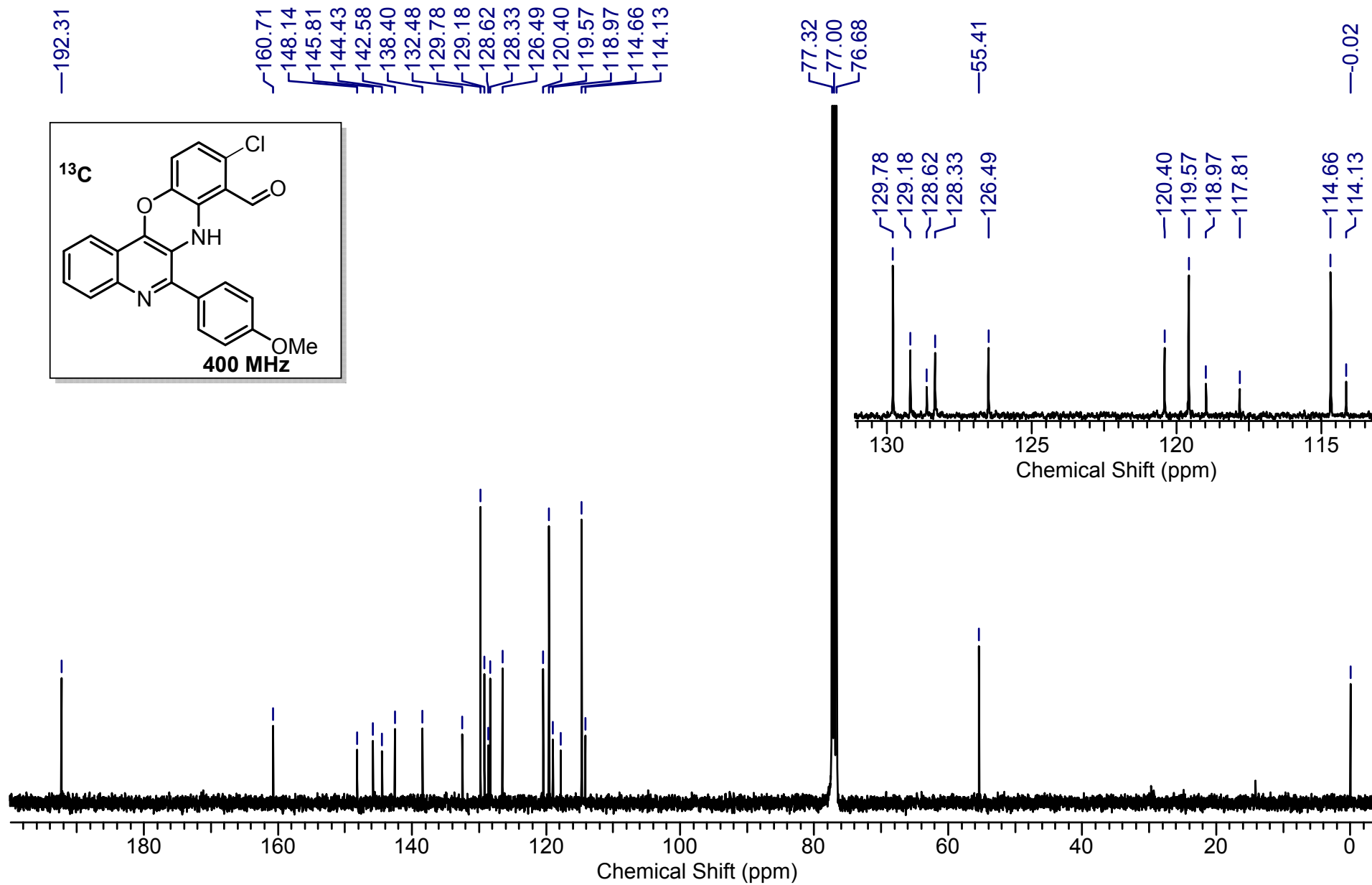
SH-624 #368 RT: 1.98 AV: 1 NL: 4.05E6
T: FTMS + p ESI Full ms [100.0000-1500.0000]



3fh



3fh

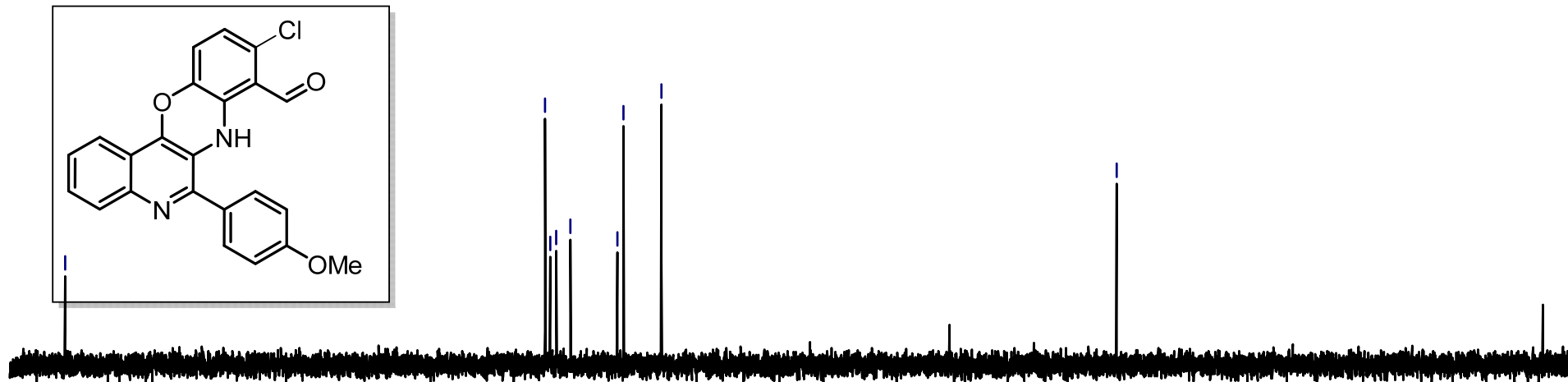
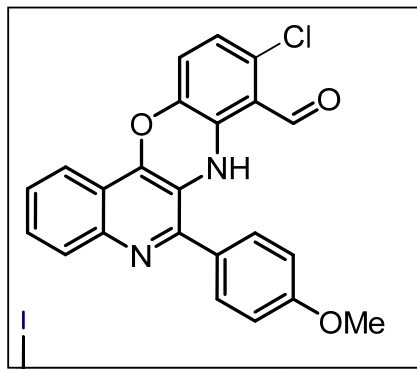


3fh

—192.31

129.78
129.17
128.33
126.49
120.41
119.57
114.66

—55.42



~129.78

~129.17

~128.33

—126.49

~120.41

—119.57

—114.66

130

Chemical Shift (ppm)

125

120

115

180

160

140

Chemical Shift (ppm)

100

80

60

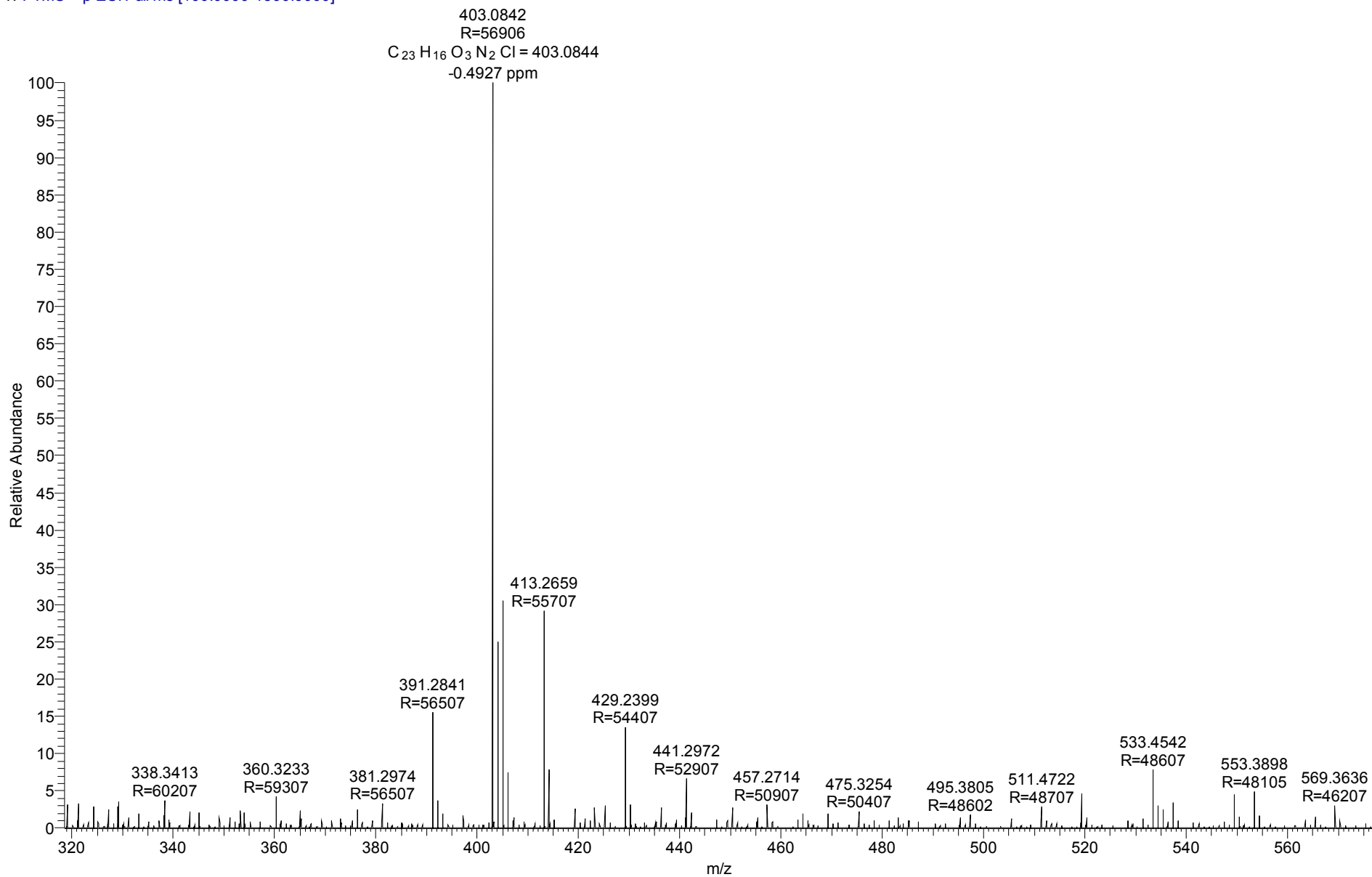
40

20

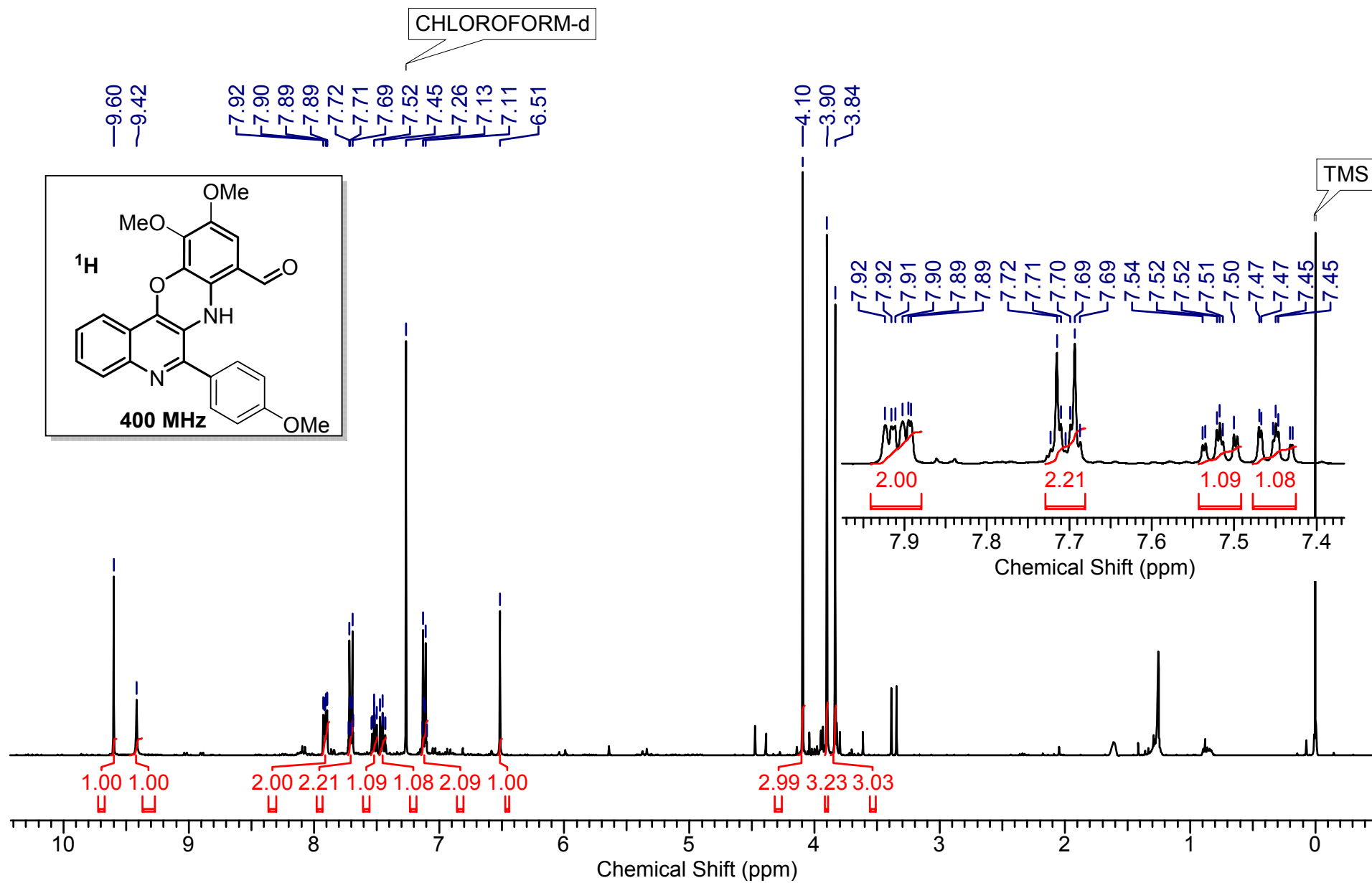
0

3fh

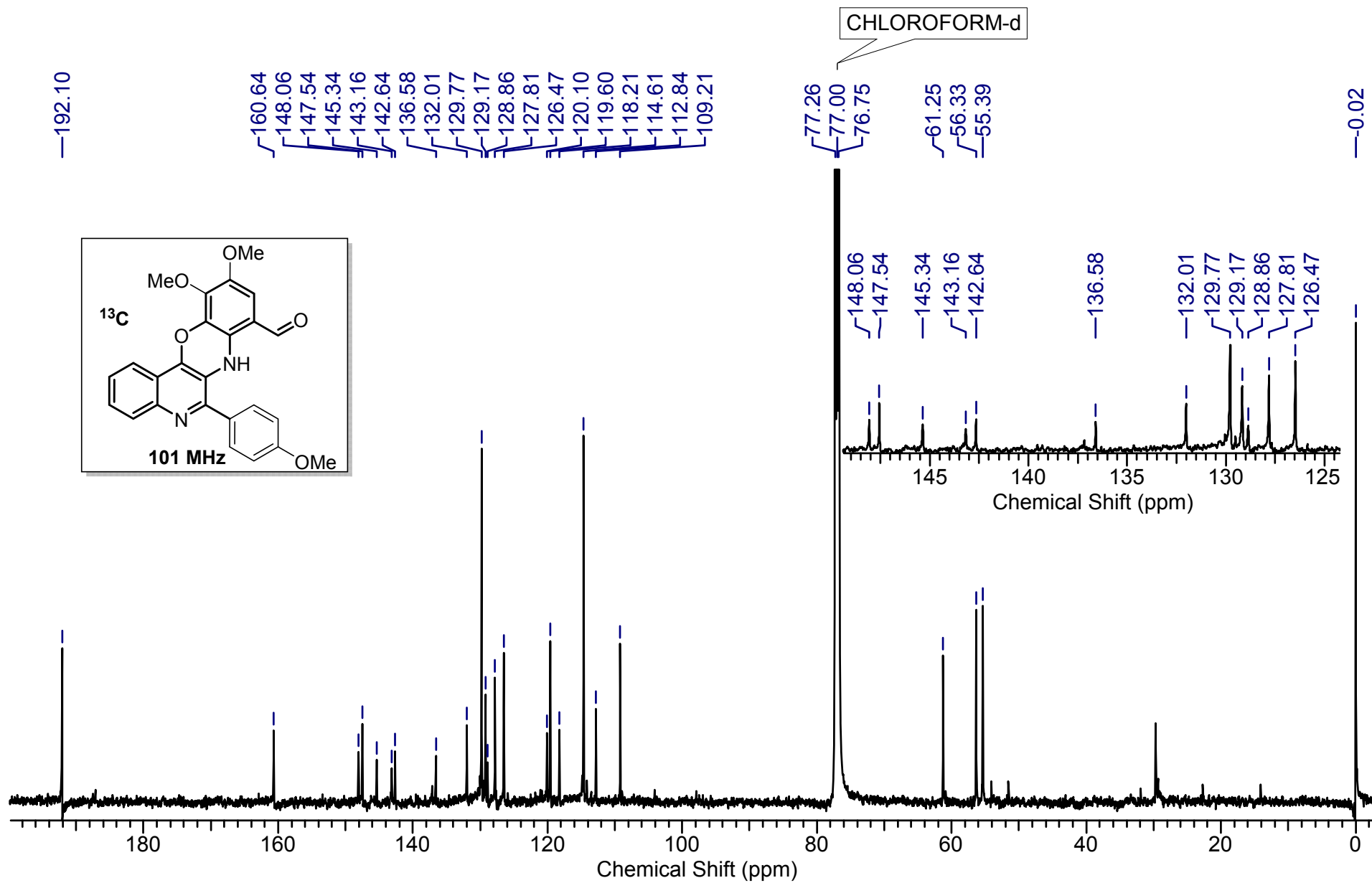
SH-616 #473 RT: 2.51 AV: 1 NL: 2.46E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



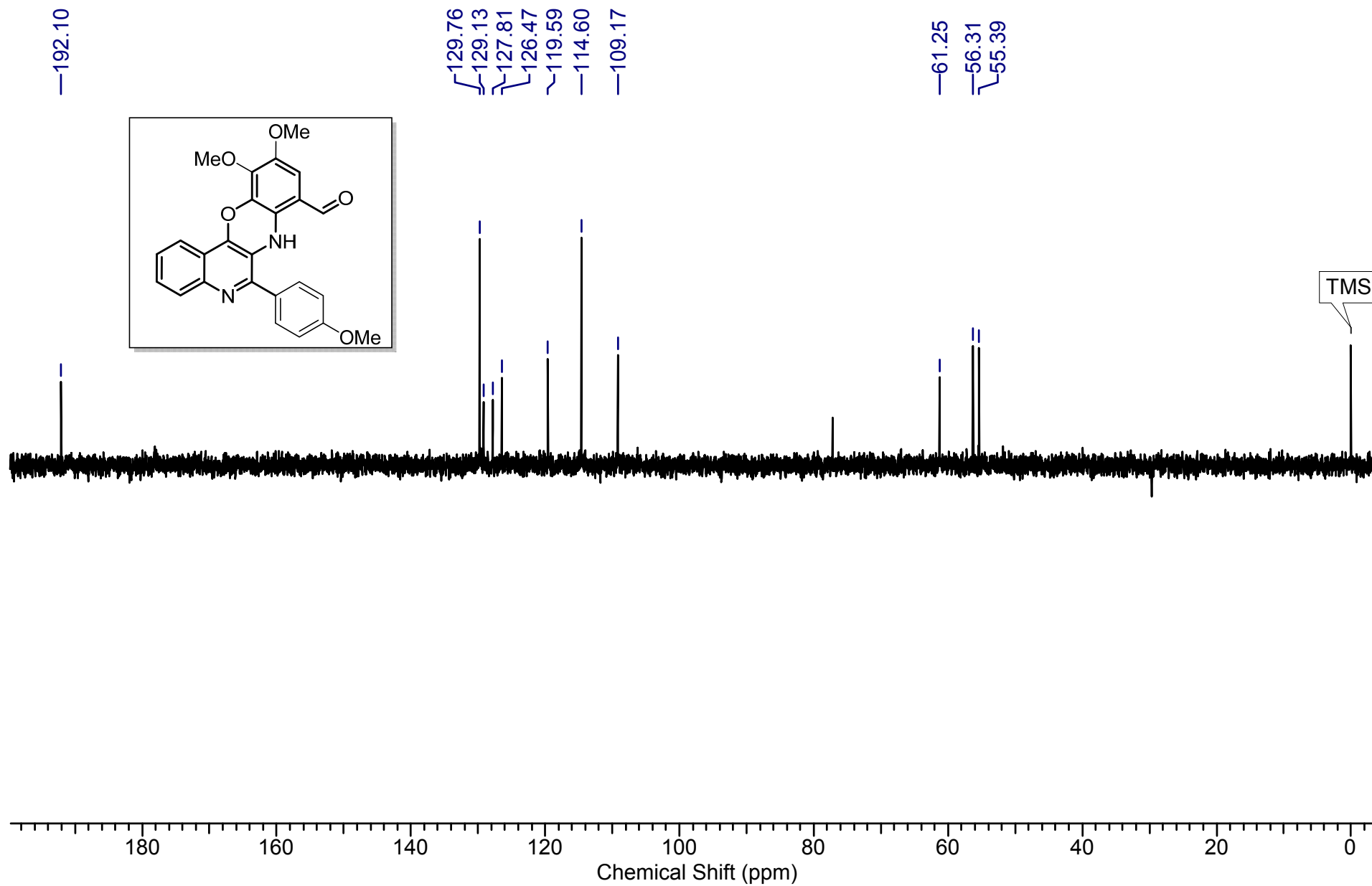
3fi



3fi

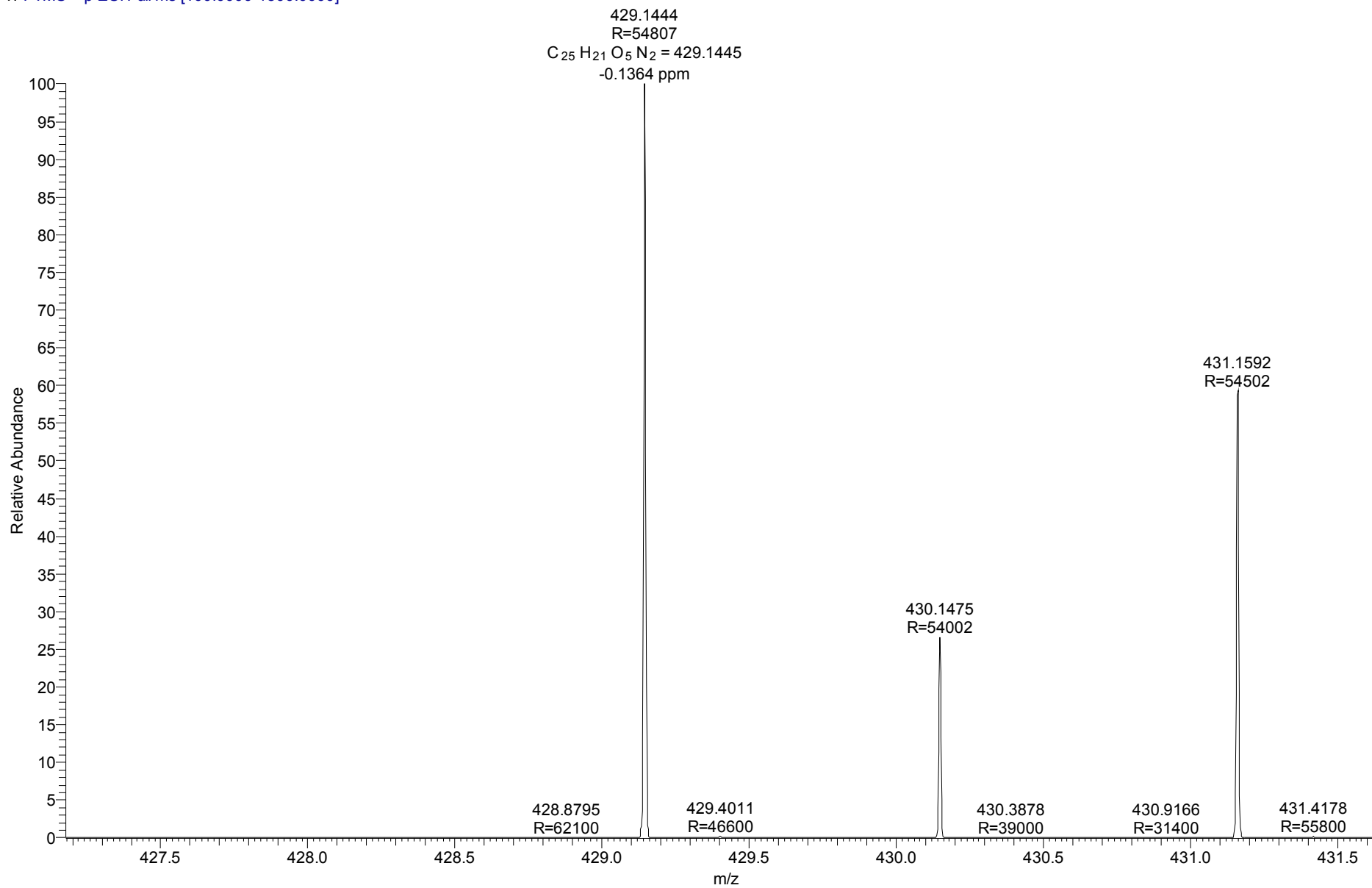


3fi



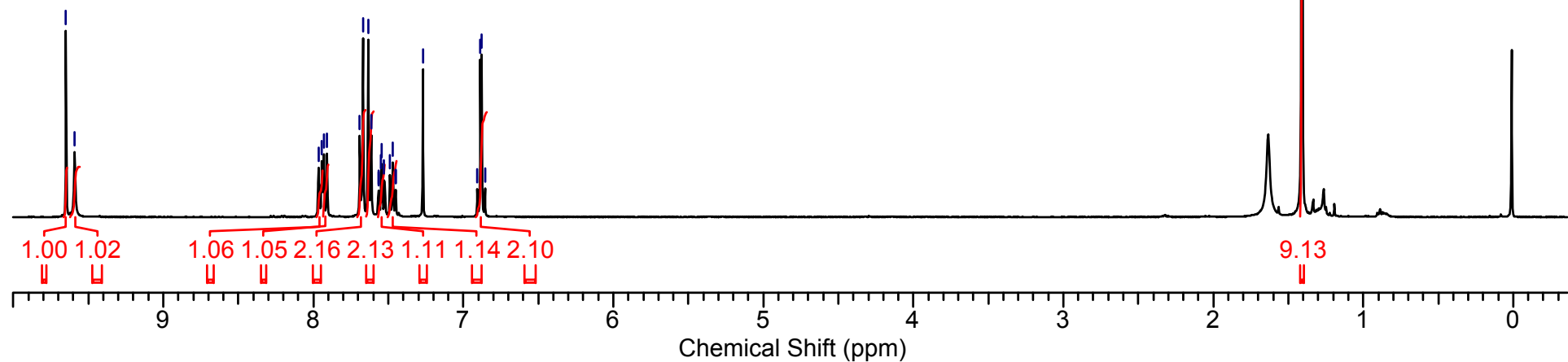
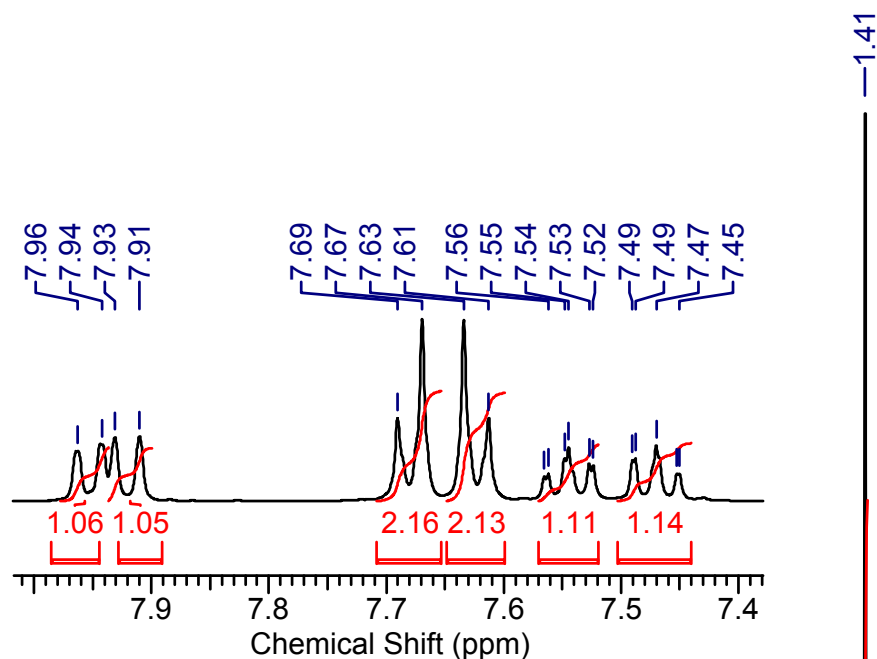
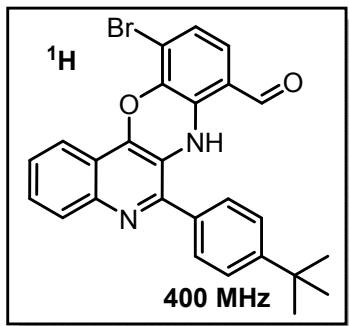
3fi

TRIMETHOXY#356 RT: 1.62 AV: 1 NL: 2.11E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

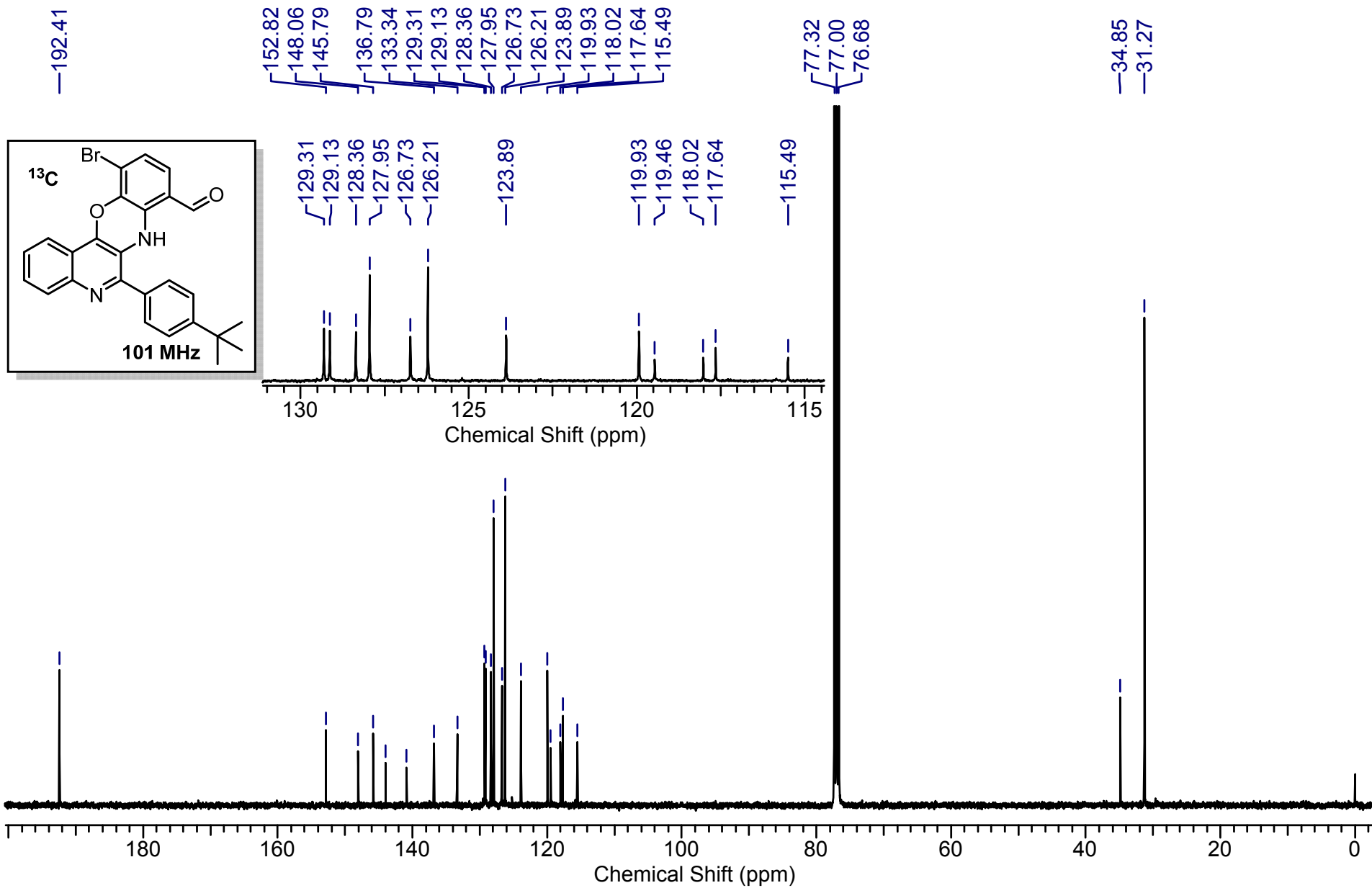


3gb

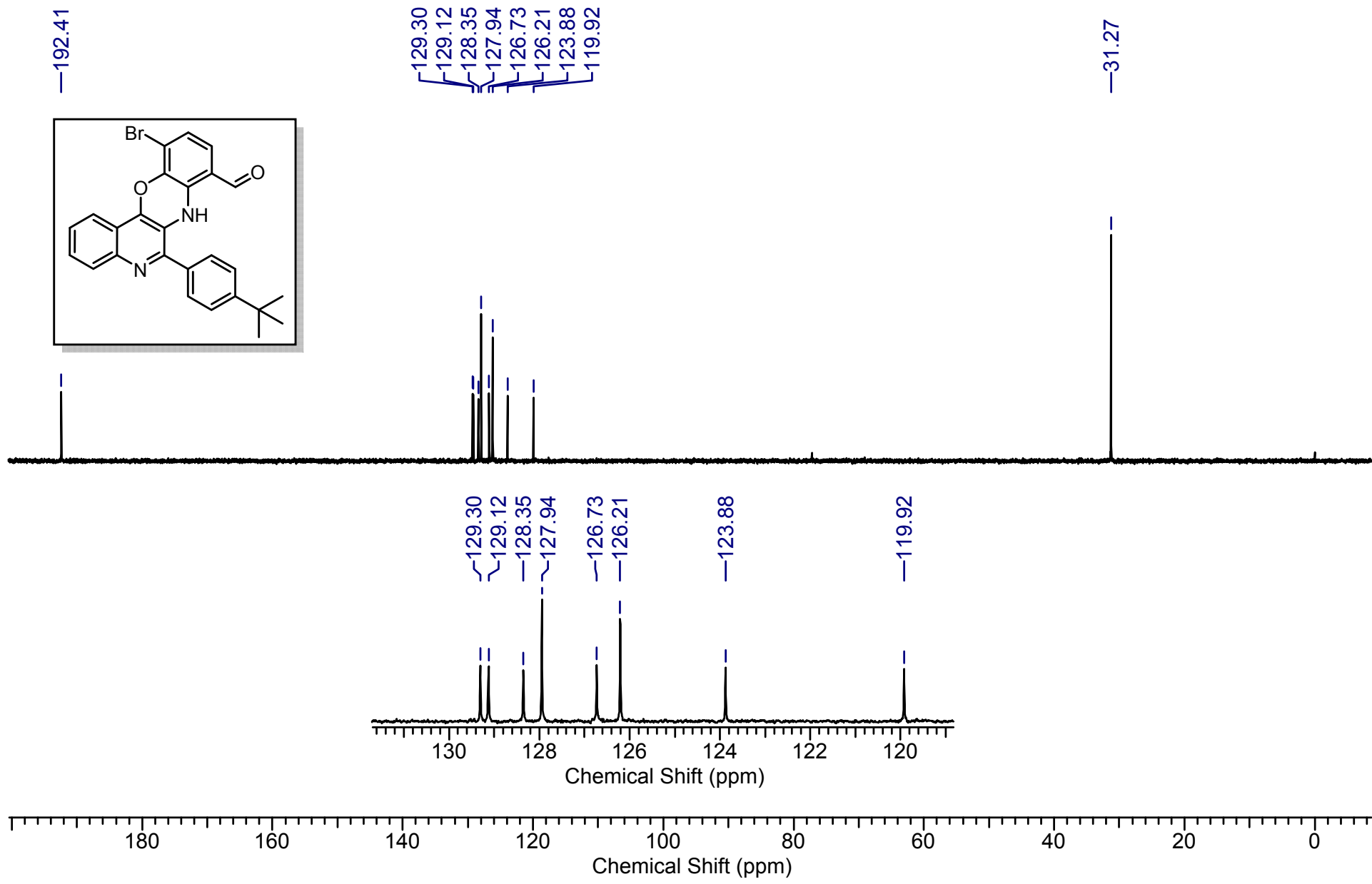
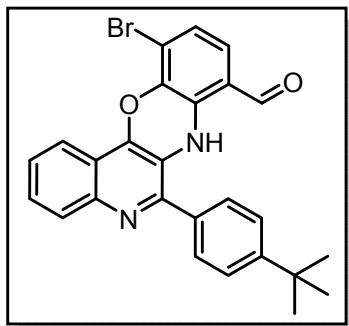
9.65
9.59
7.96
7.94
7.93
7.91
7.69
7.67
7.63
7.61
7.54
7.47
7.27
6.89
6.88



3gb

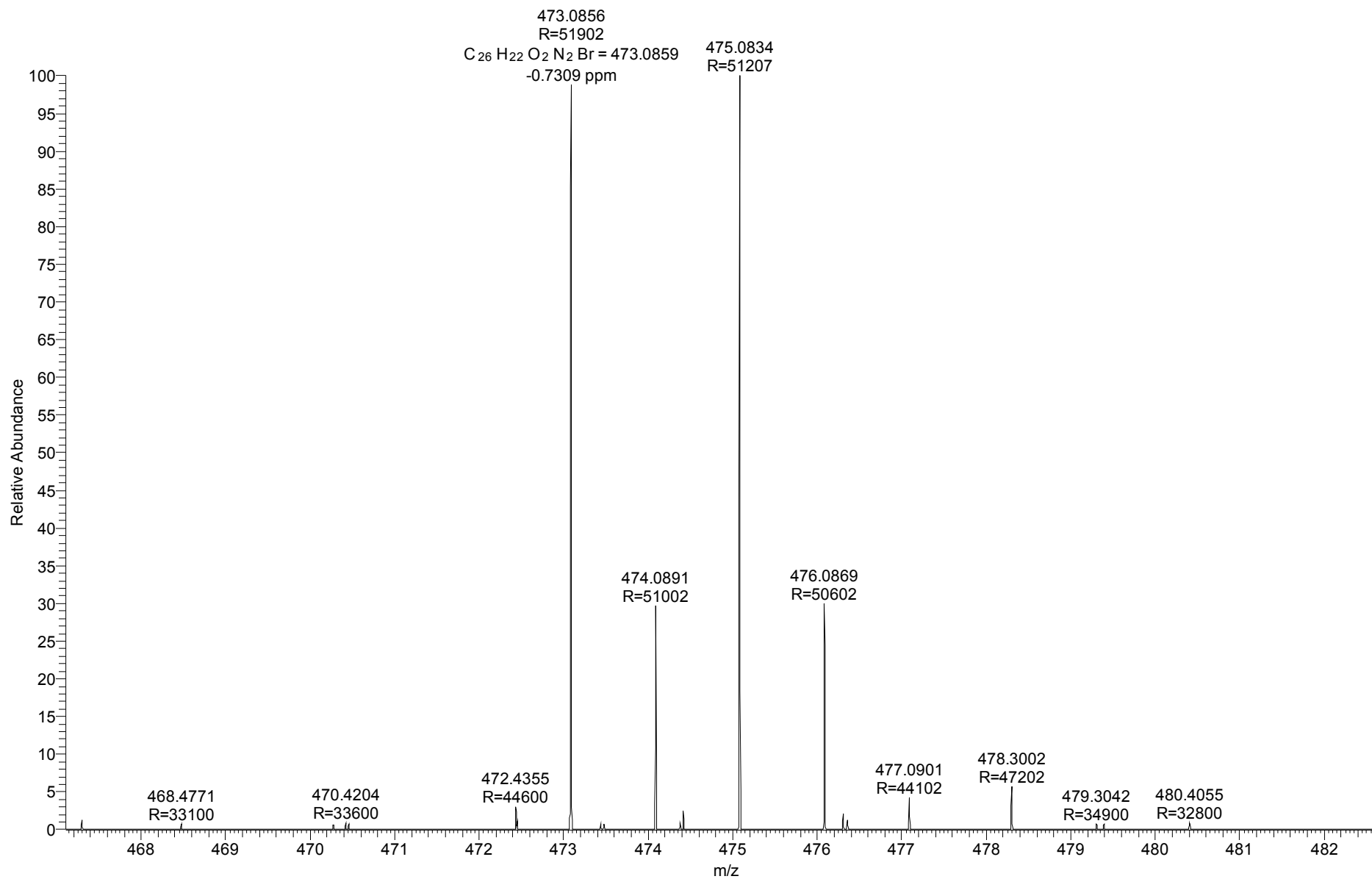


3gb



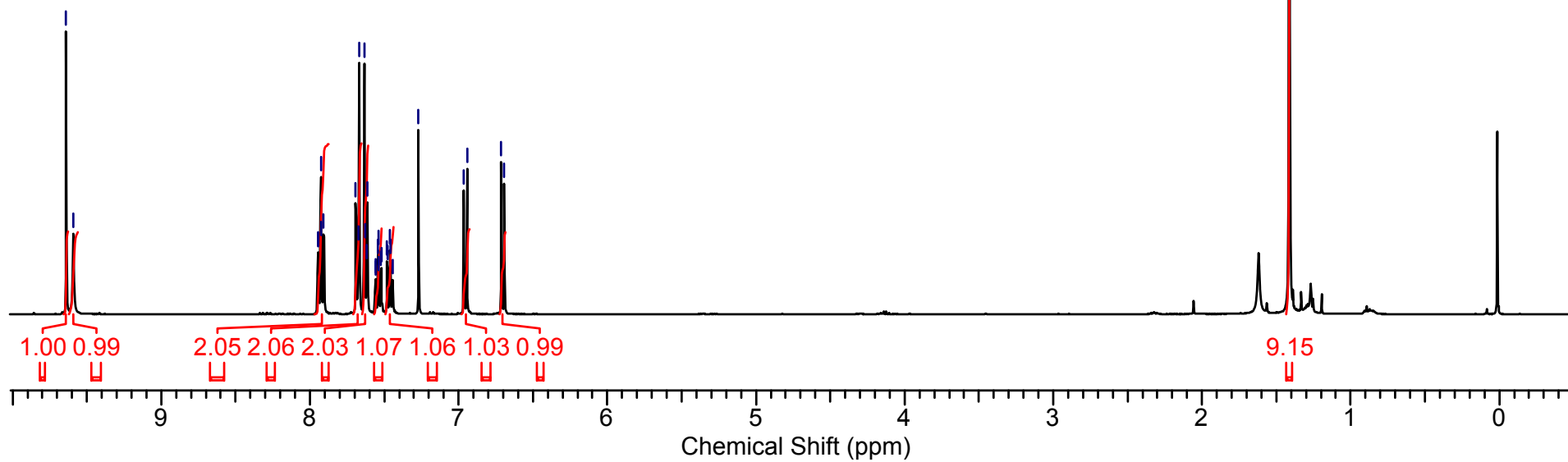
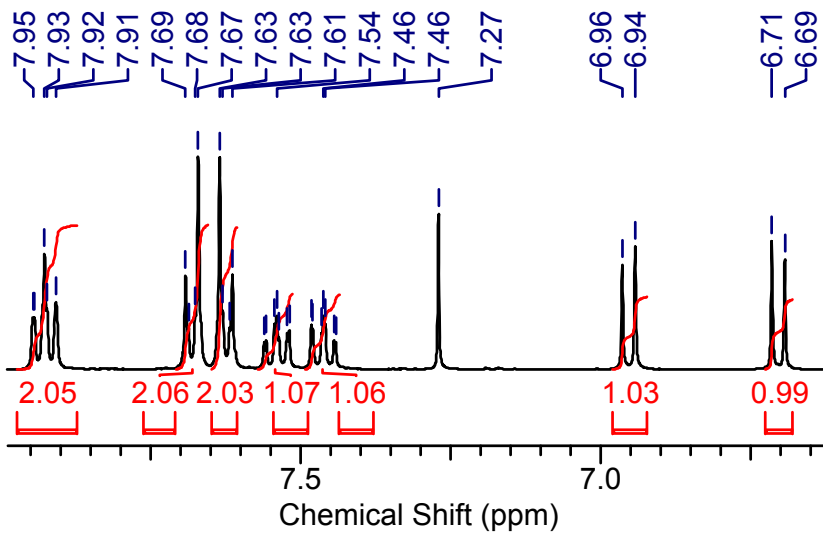
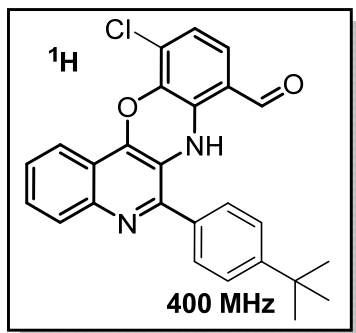
3gb

635 #1091 RT: 4.95 AV: 1 NL: 4.86E5
T: FTMS + p ESI Full ms [100.0000-1500.0000]



3gc

9.64
9.59
7.95
7.93
7.92
7.91
7.69
7.67
7.63
7.63
7.61
7.27
6.96
6.94
6.71
6.69



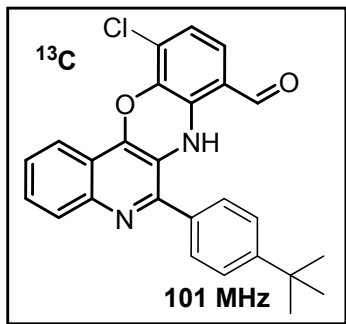
3gc

192.30

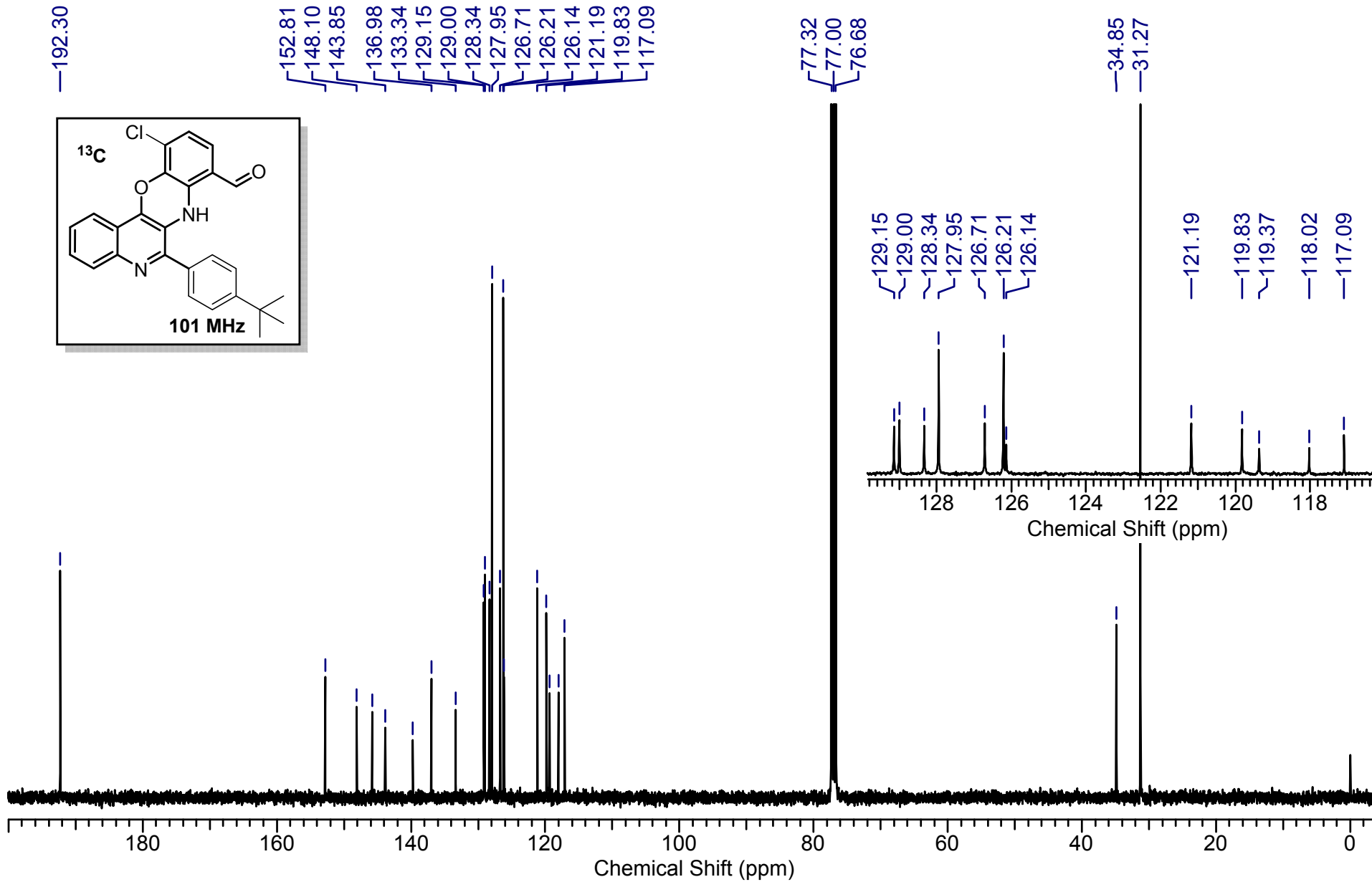
152.81
148.10
143.85
136.98
133.34
129.15
129.00
128.34
127.95
126.71
126.21
126.14
121.19
119.83
117.09

77.32
77.00
76.68

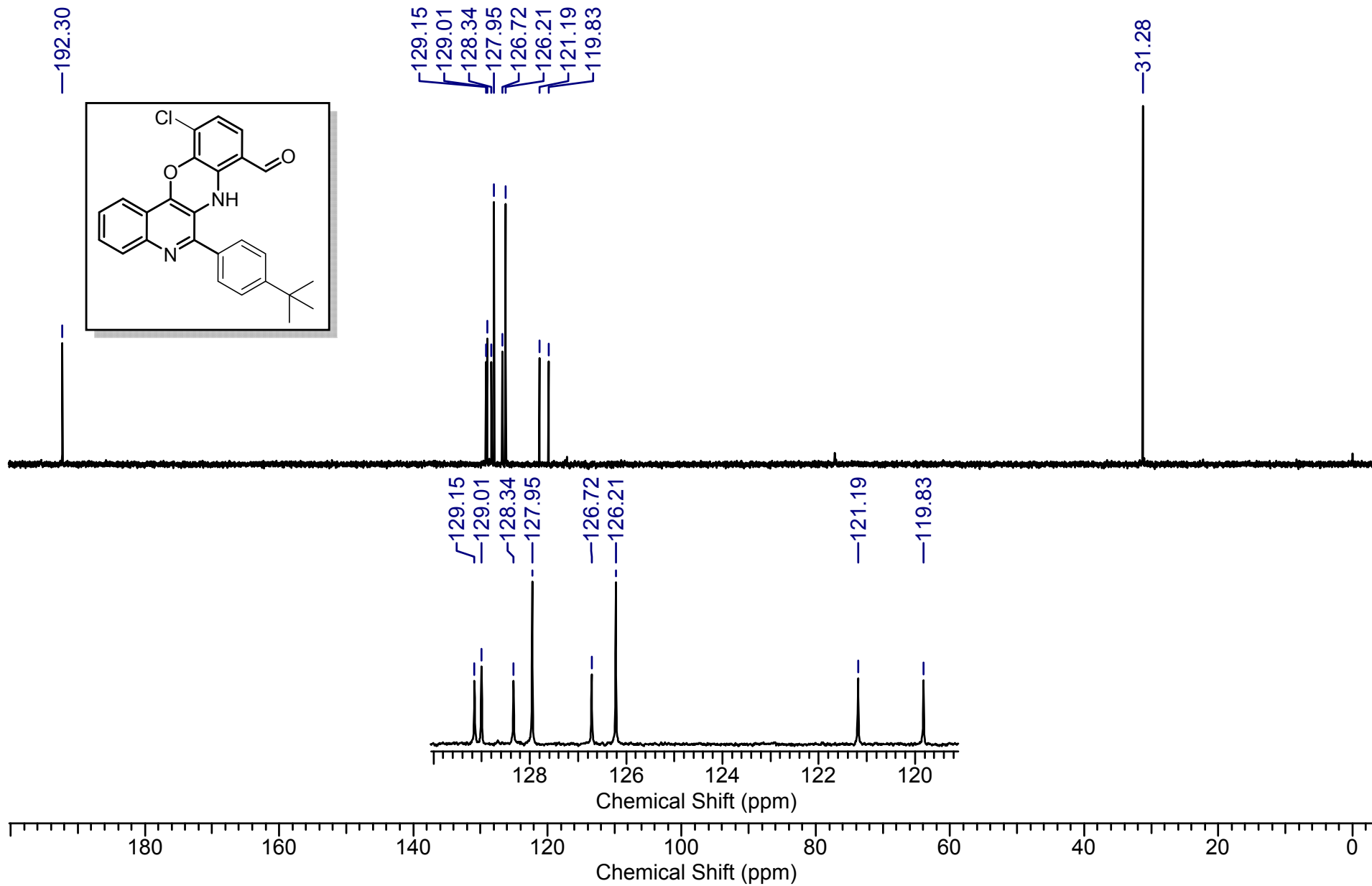
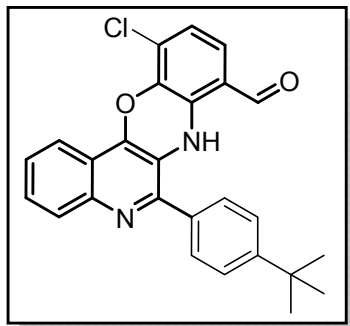
34.85
31.27



129.15
129.00
128.34
127.95
126.71
126.21
126.14
121.19
119.83
119.37
118.02
117.09

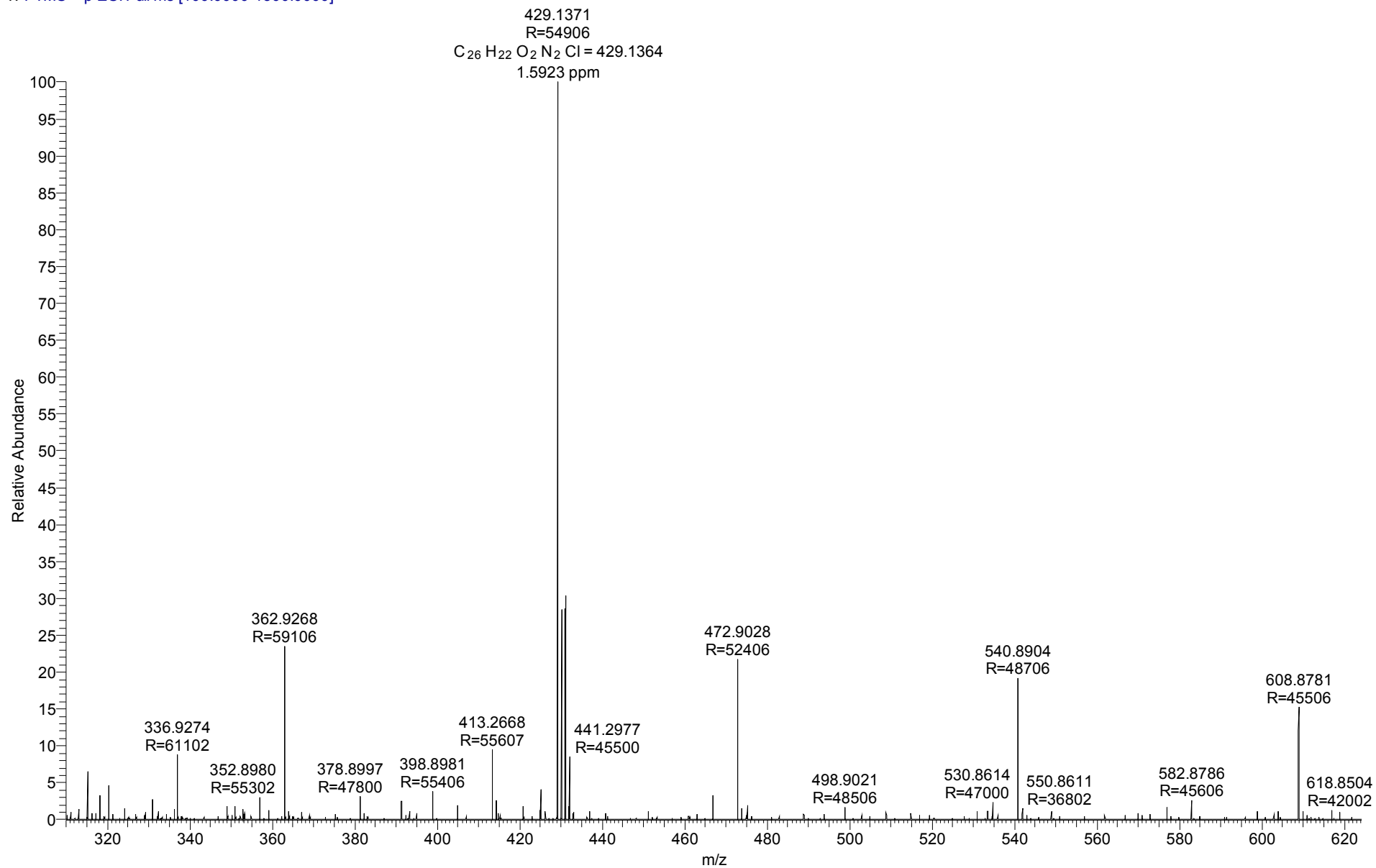


3gc



3gc

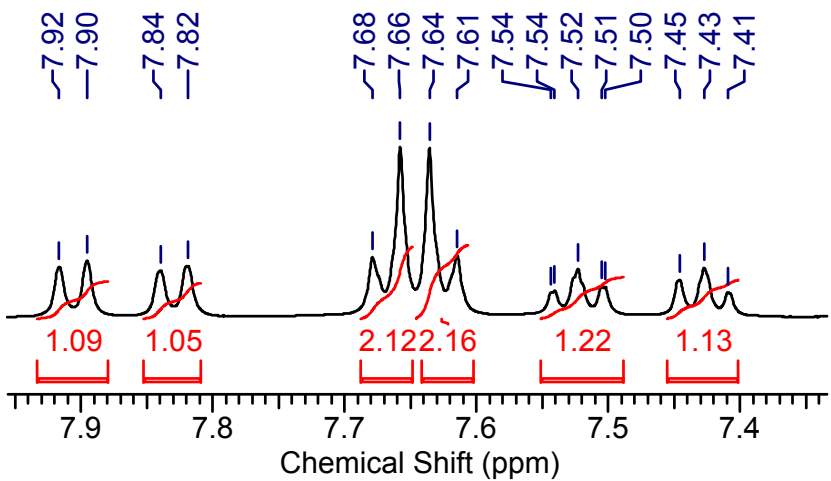
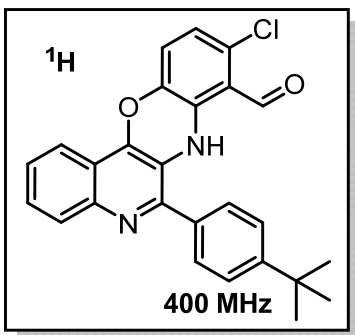
SH-636 #660 RT: 3.55 AV: 1 NL: 2.06E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



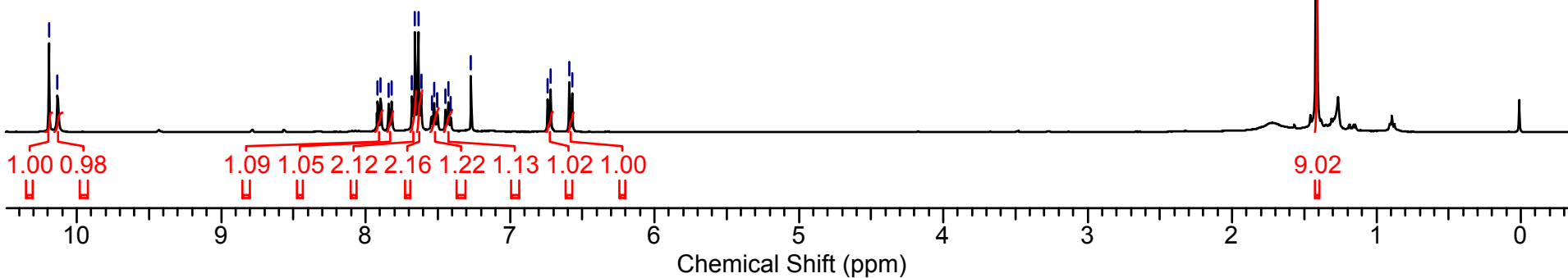
3gd

10.19
10.13

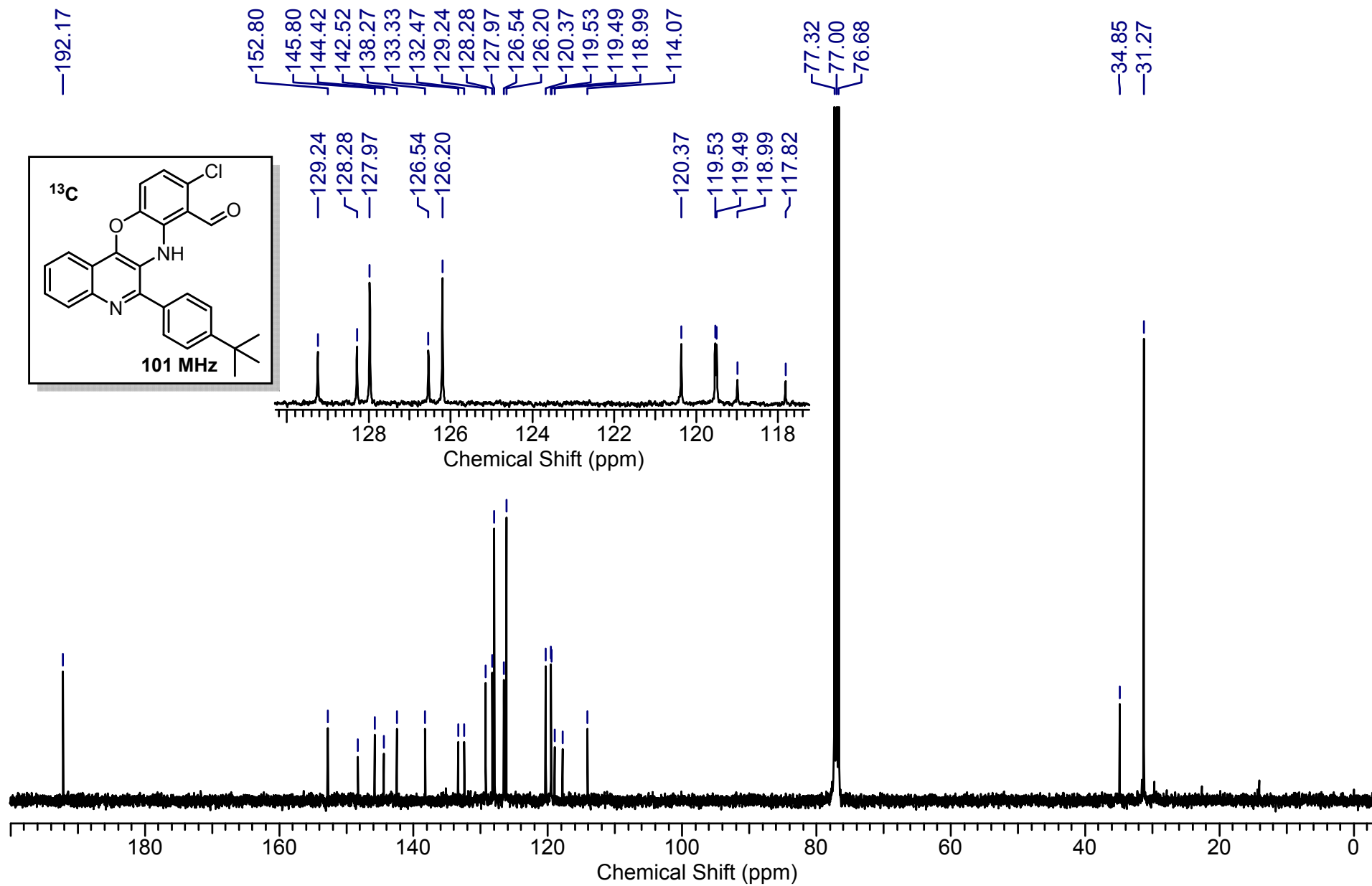
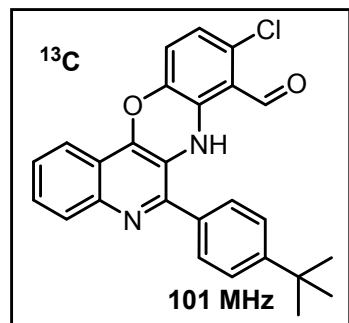
7.92
7.90
7.82
7.68
7.66
7.64
7.61
7.52
7.43
7.27
6.74
6.72
6.59
6.57



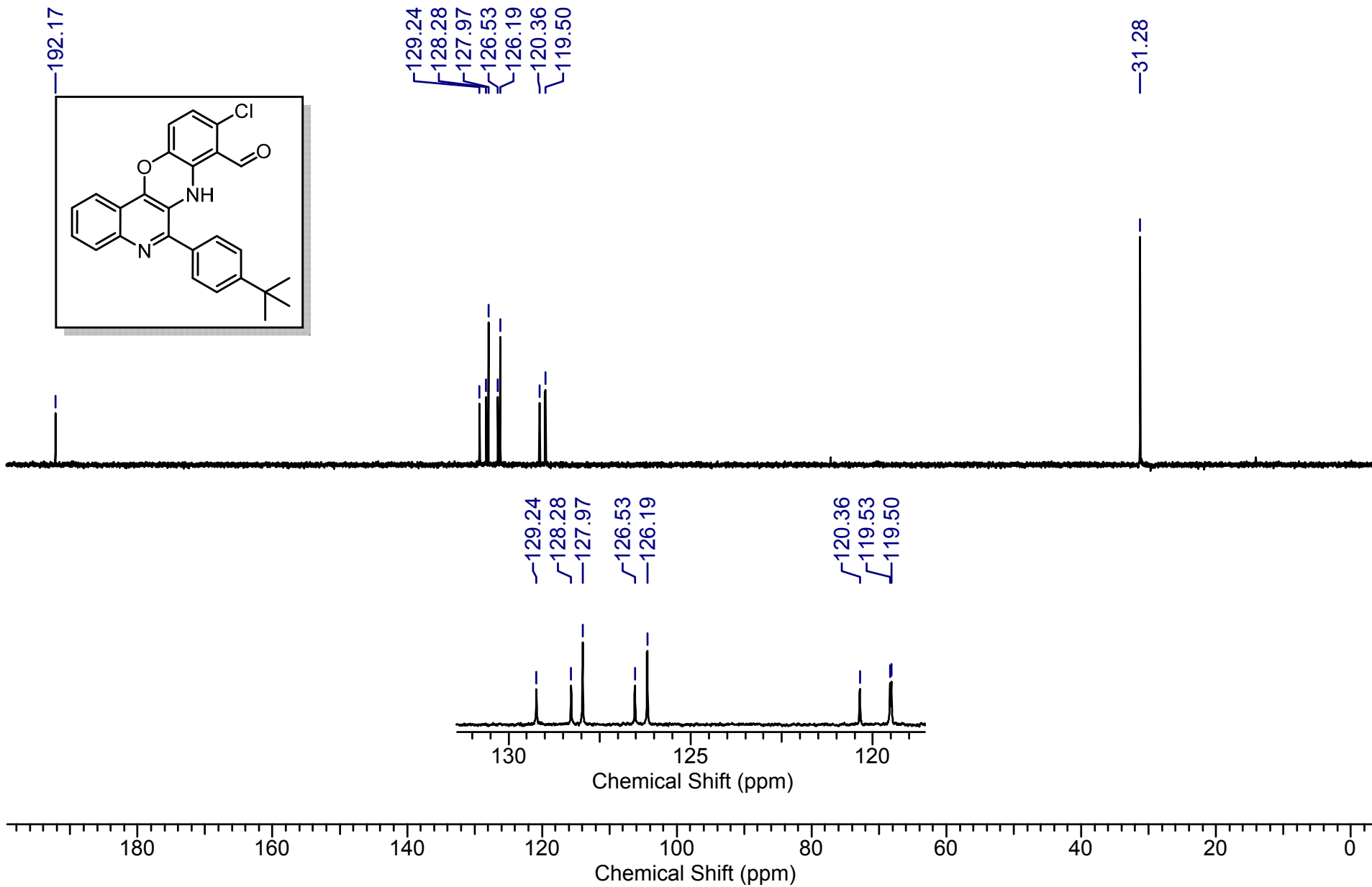
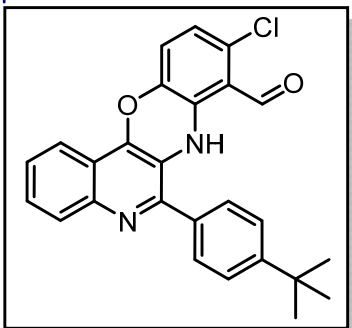
1.41



3gd

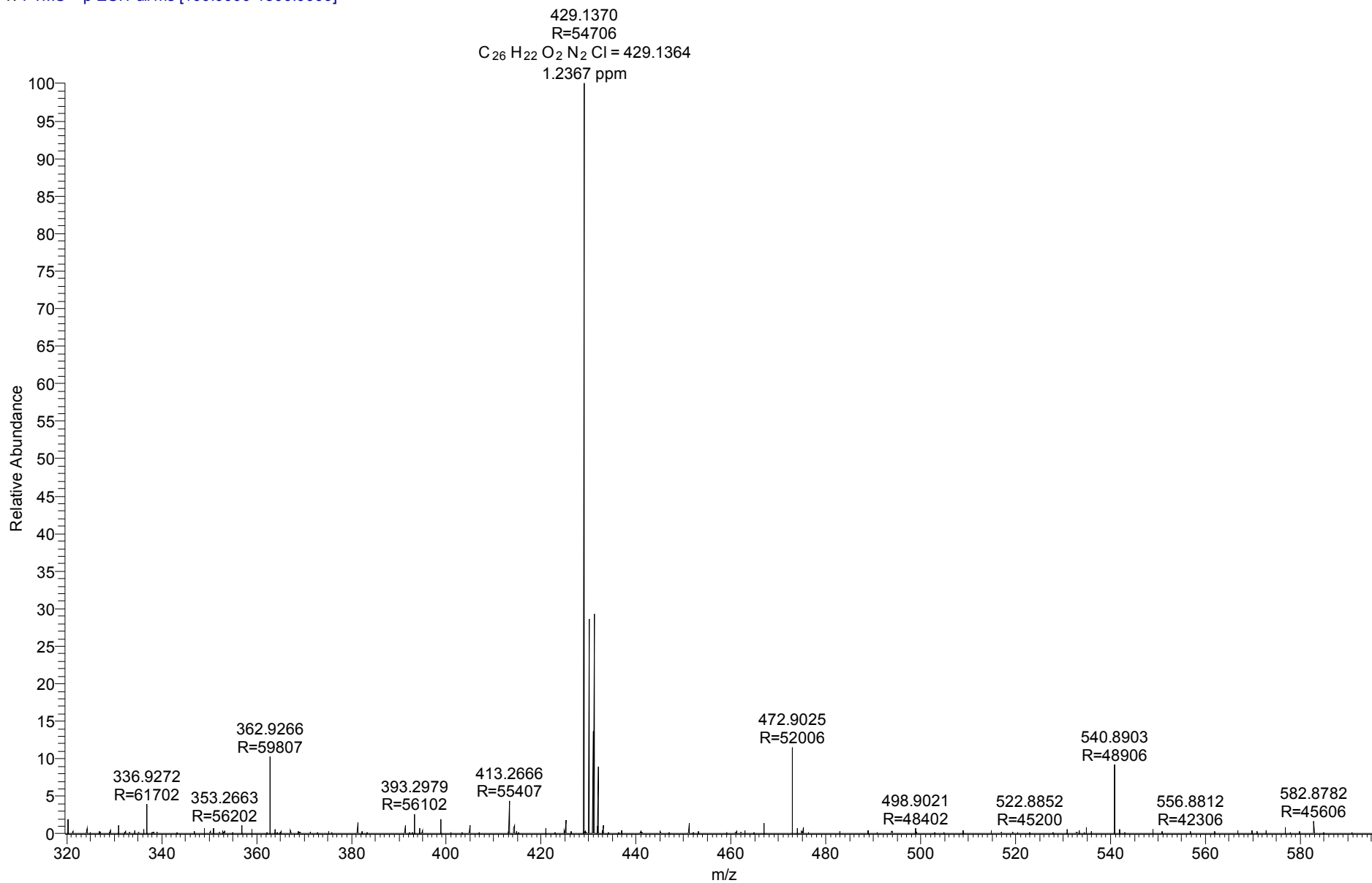


3gd



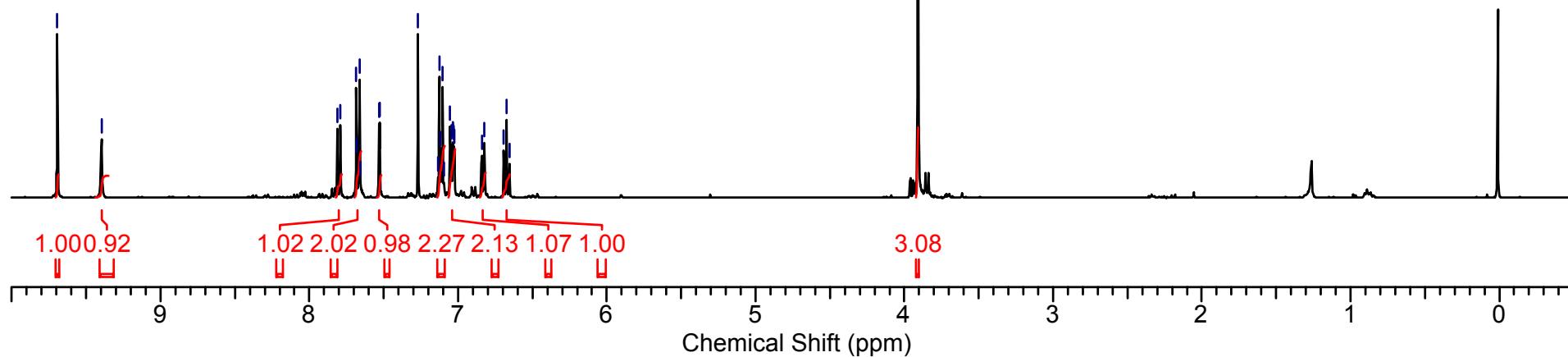
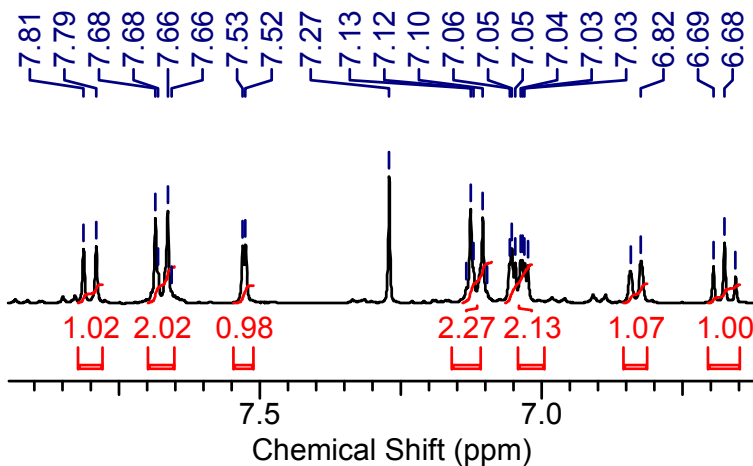
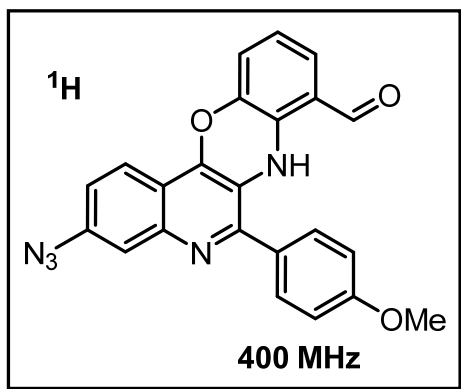
3gd

SH-639 #698 RT: 3.75 AV: 1 NL: 4.80E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

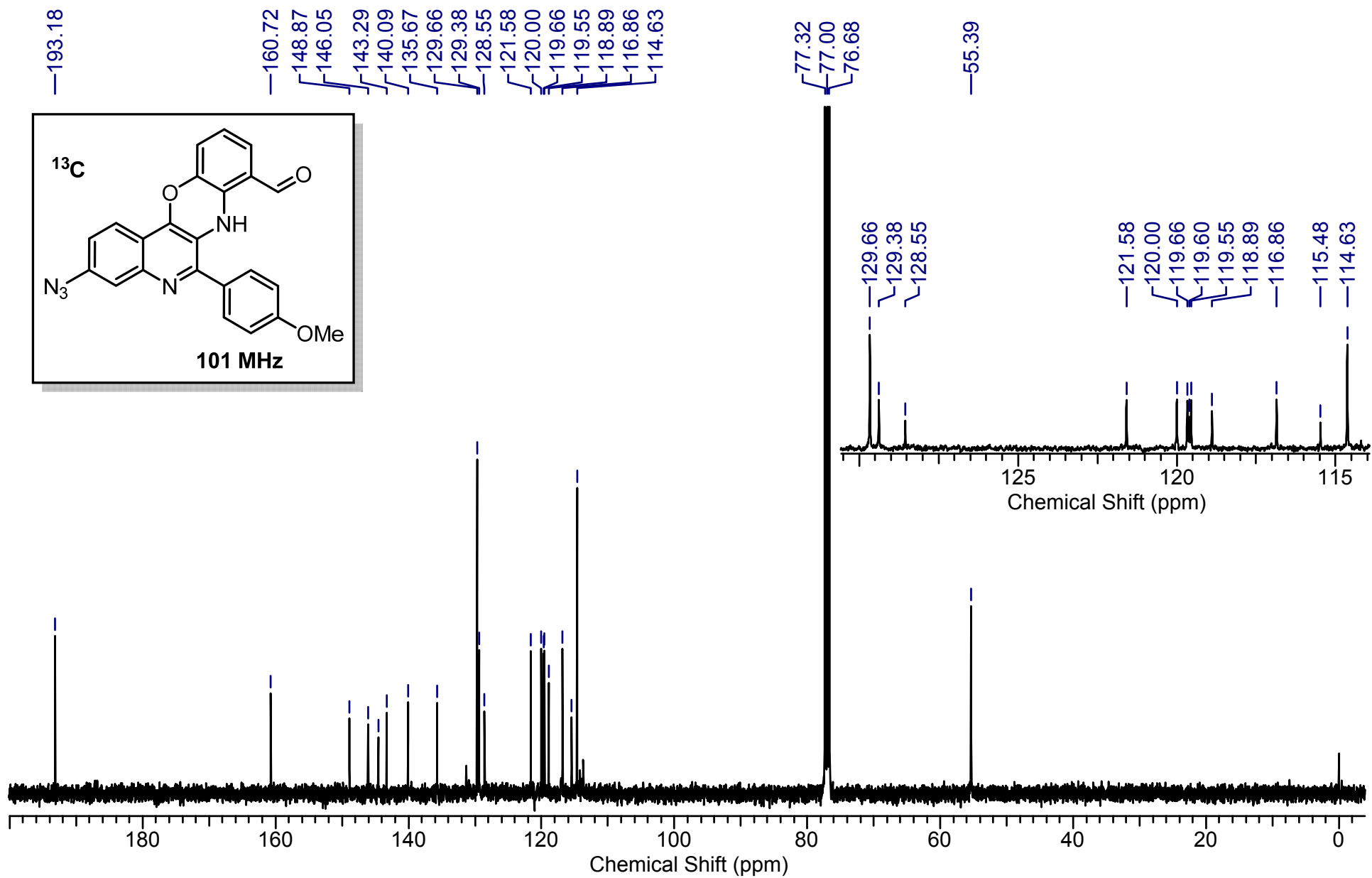


3ia

9.69
9.40
7.81
7.79
7.68
7.66
7.53
7.52
7.27
7.13
7.10
7.05
7.03
6.82
6.68
3.91

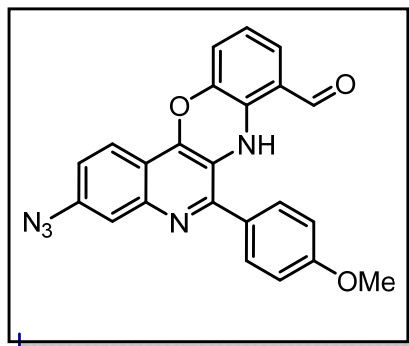


3ia



3ia

—193.18



129.66
129.38
121.58
120.00
119.66
119.54
116.85
114.63

—55.39



129.66
129.38

121.58
120.00
119.66
119.54

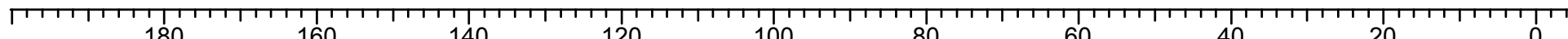
—116.85

—114.63



130
125
120
115

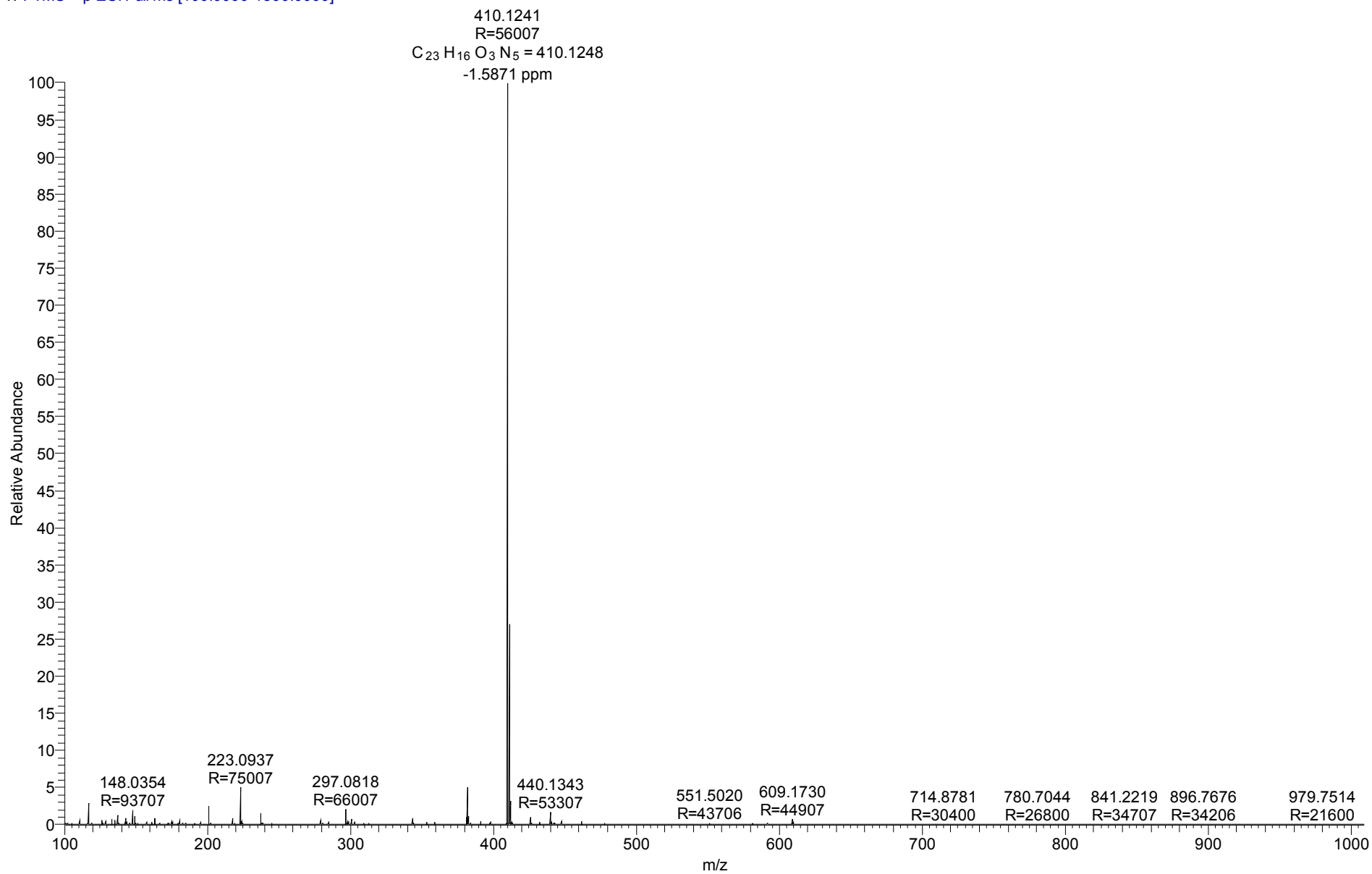
Chemical Shift (ppm)



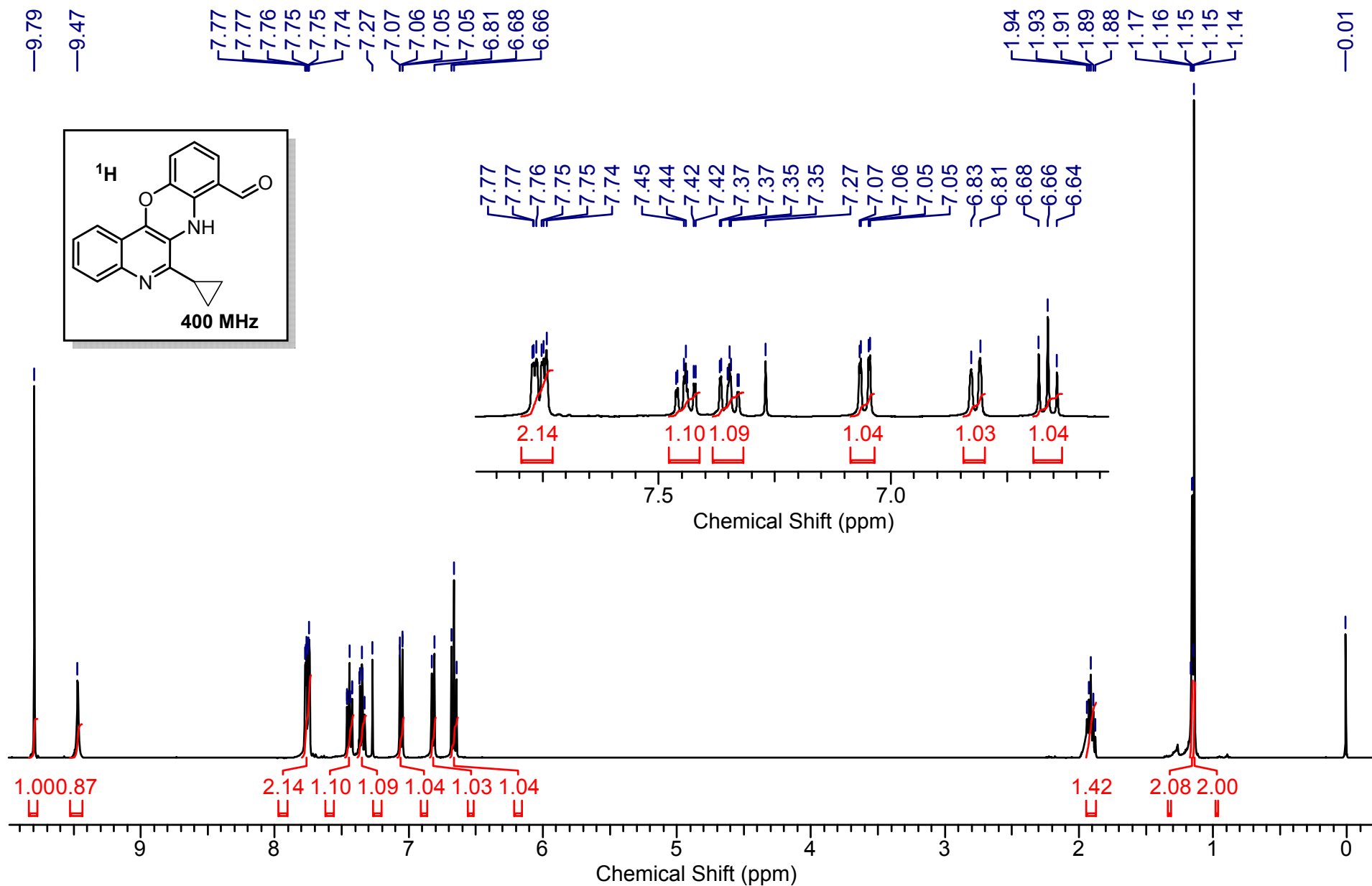
Chemical Shift (ppm)

3ia

SVH-764 #726 RT: 3.23 AV: 1 NL: 3.12E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



3ja



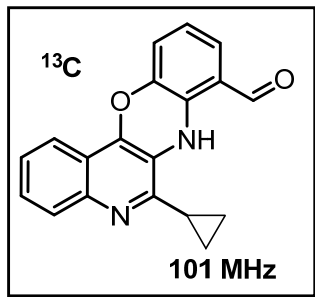
3ja

193.63

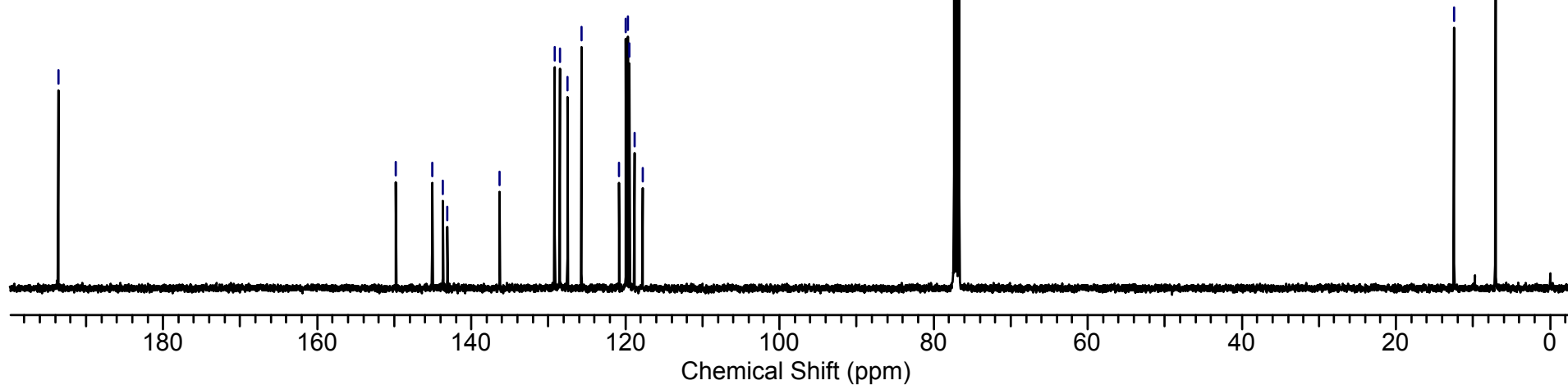
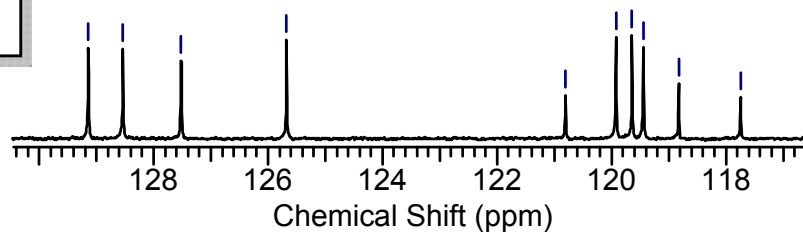
149.75
145.03
143.70
136.33
129.14
128.53
127.52
125.67
120.80
119.92
119.64
119.44
118.83

77.32
77.00
76.68

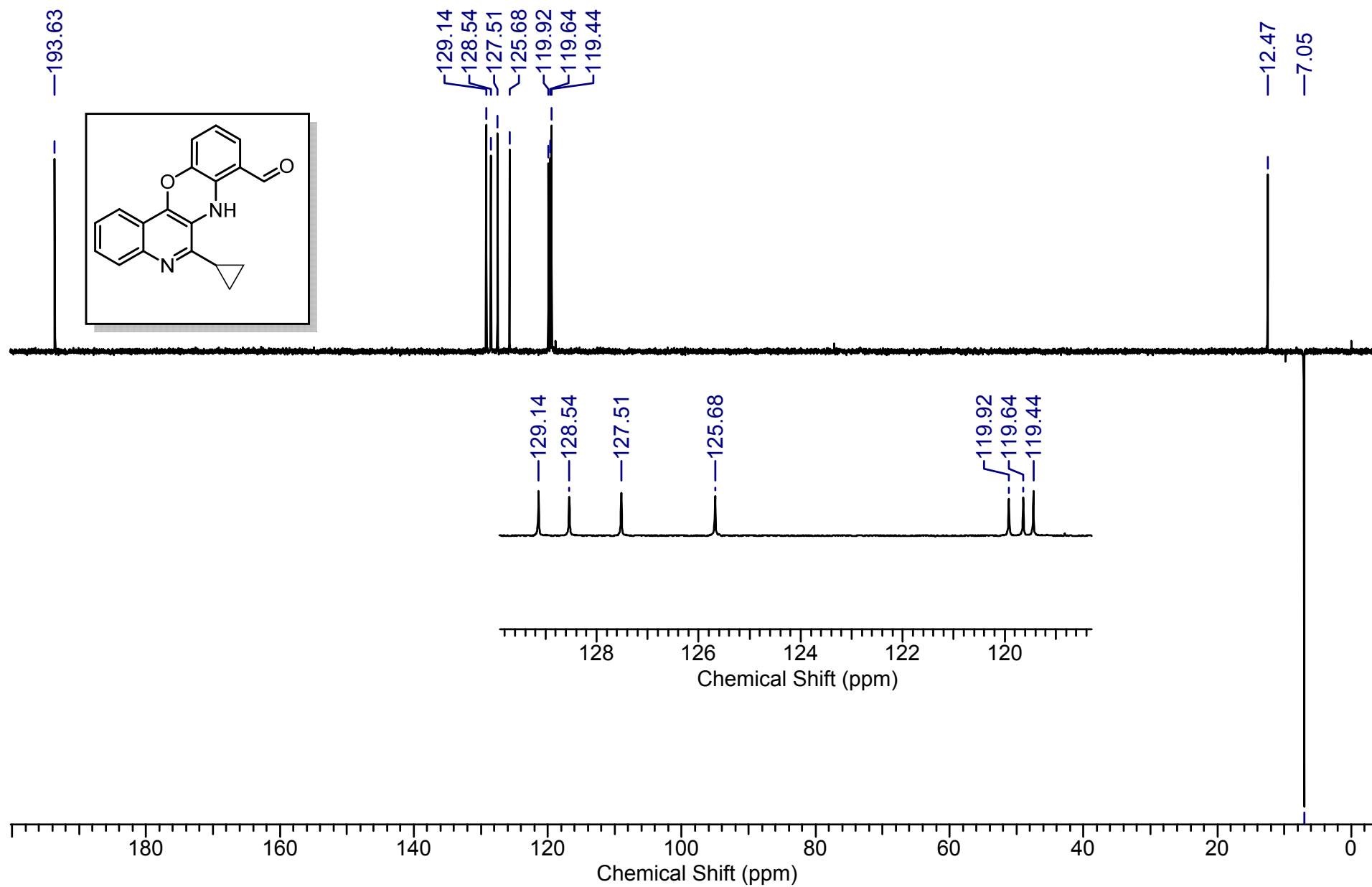
12.48
7.05



129.14
128.53
127.52
125.67
120.80
119.92
119.64
119.44
118.83
117.74

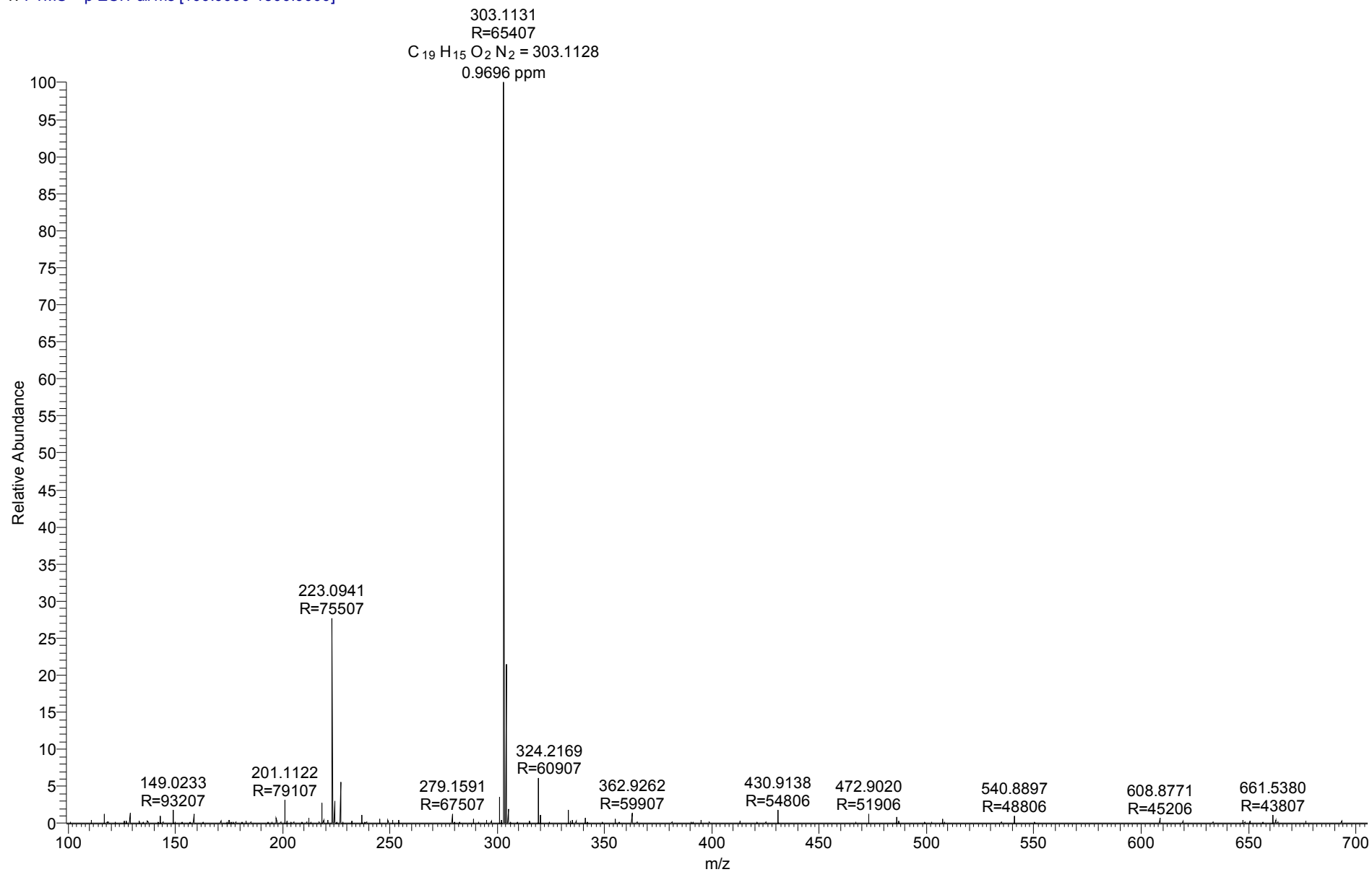


3ja

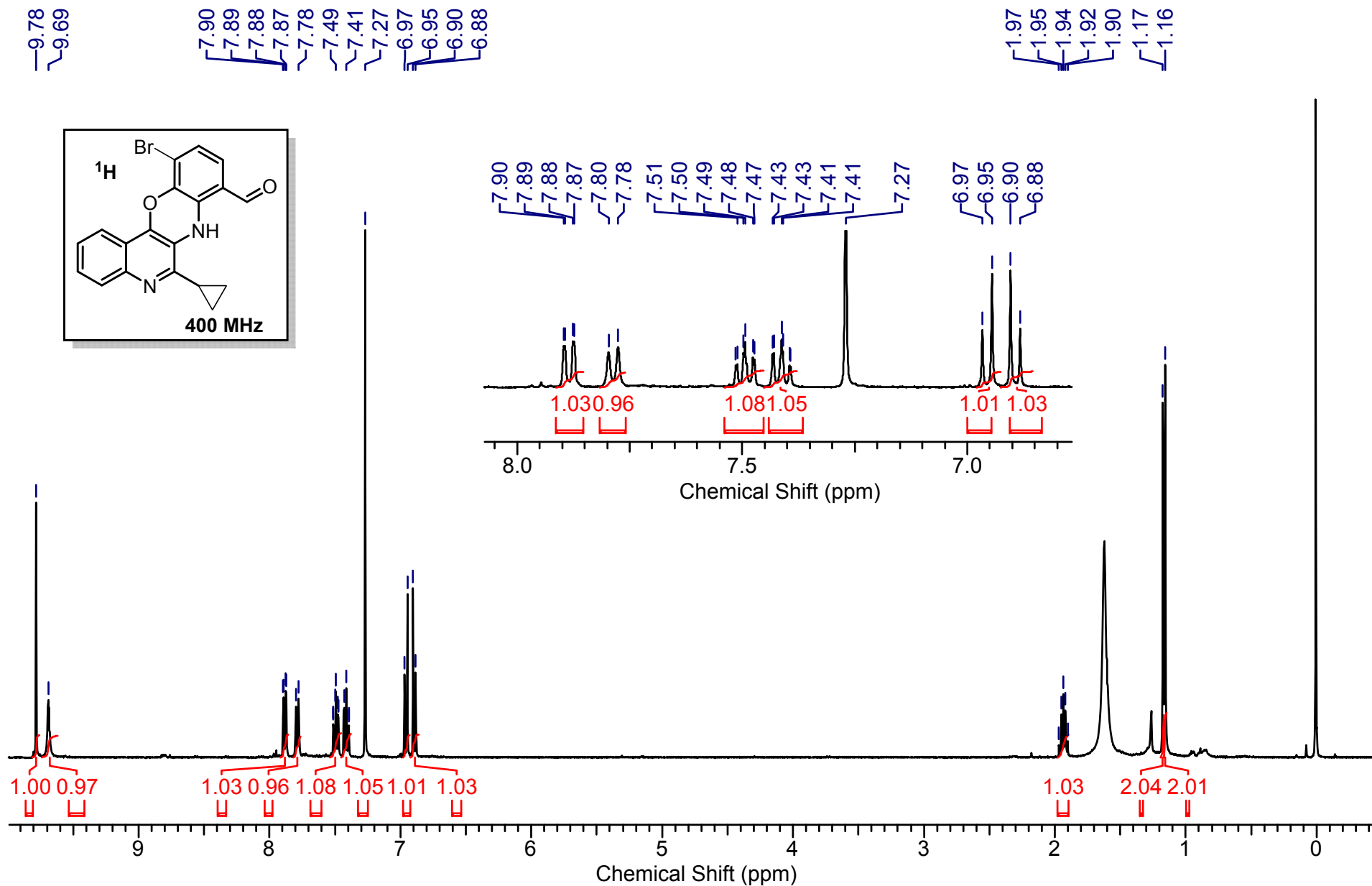


3ja

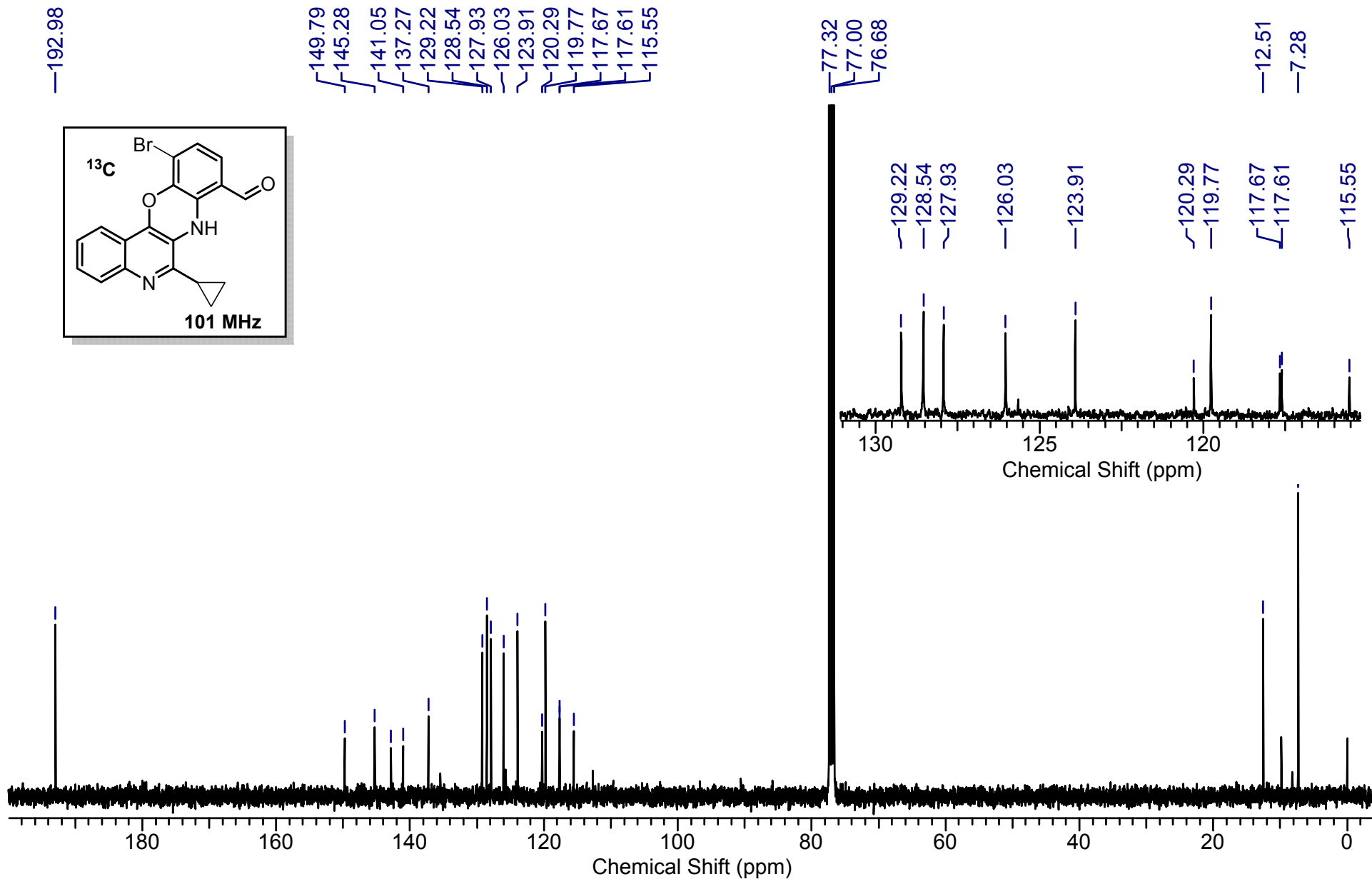
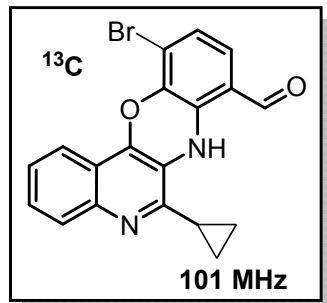
SH-660 #364 RT: 1.96 AV: 1 NL: 4.30E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



3jb

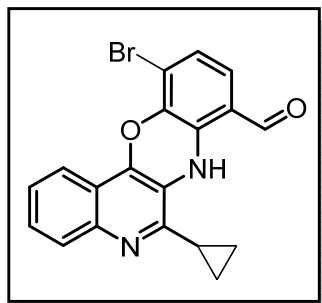


3jb

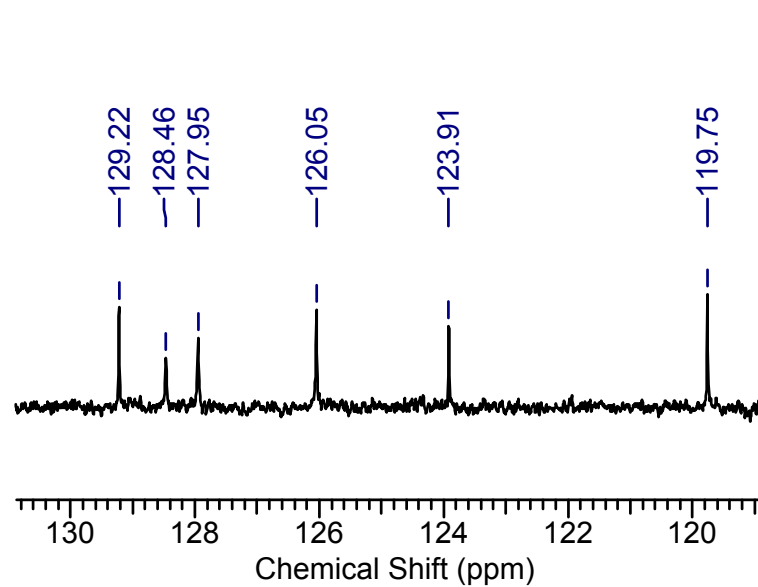


3jb

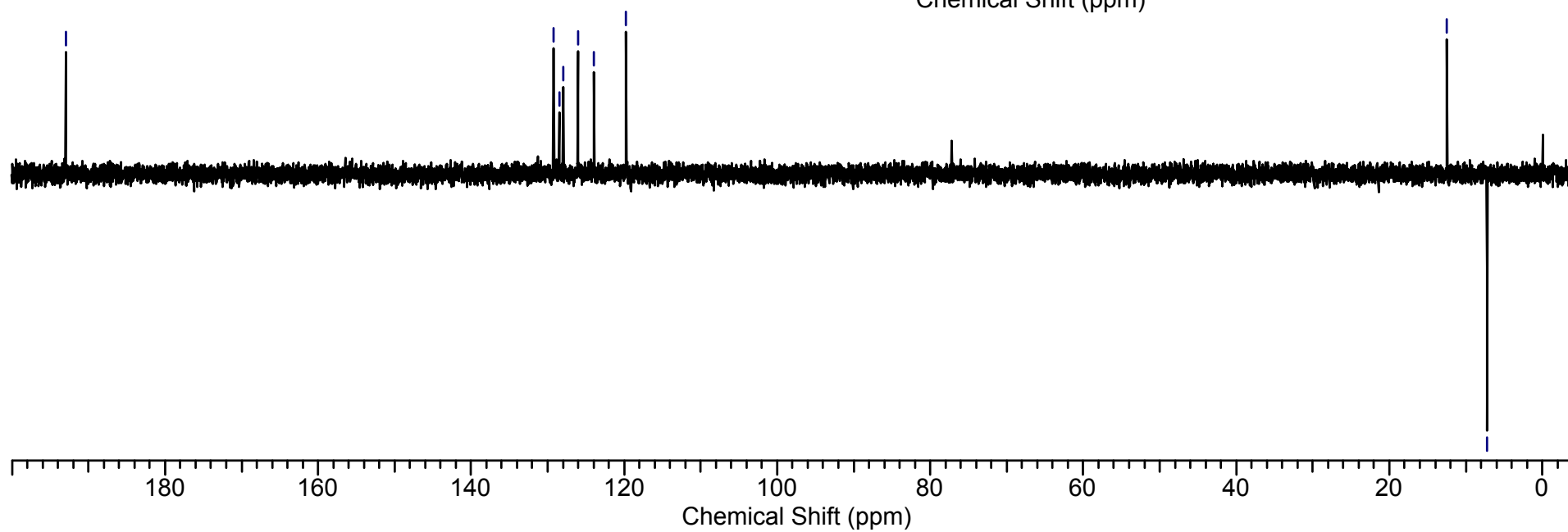
—192.98



129.22
128.46
127.95
126.05
123.91
119.75

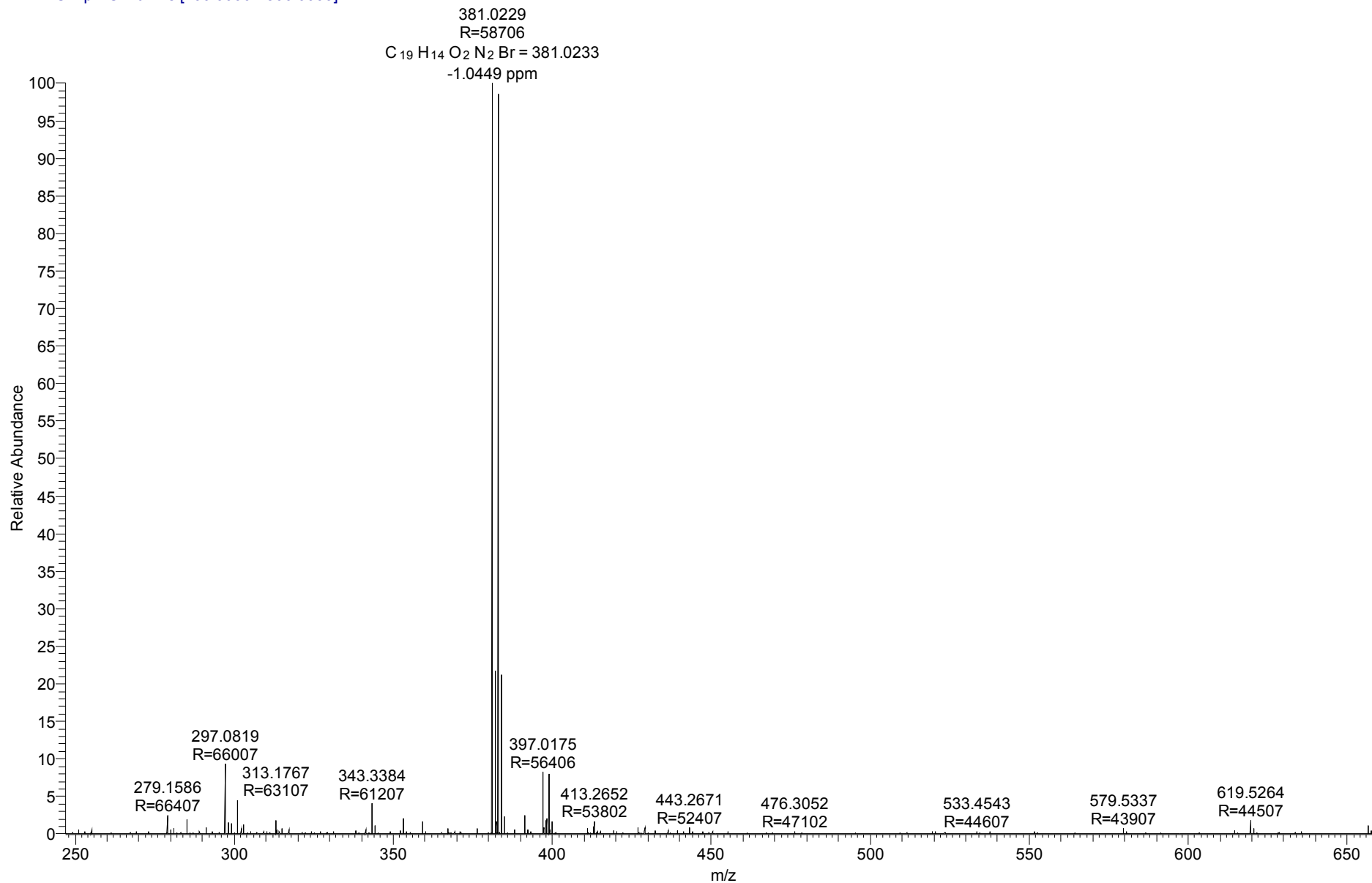


—12.49
—7.22

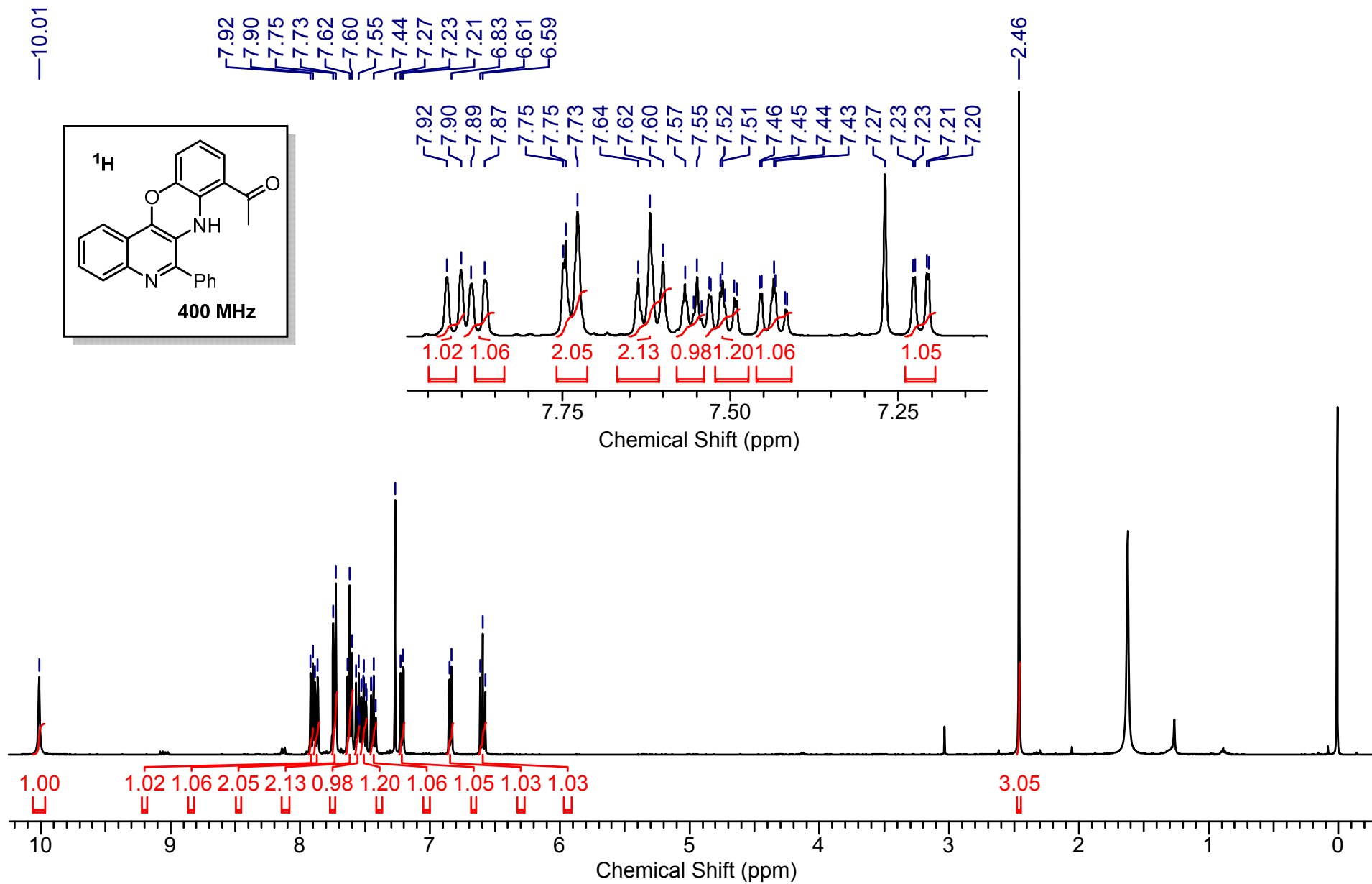


3jb

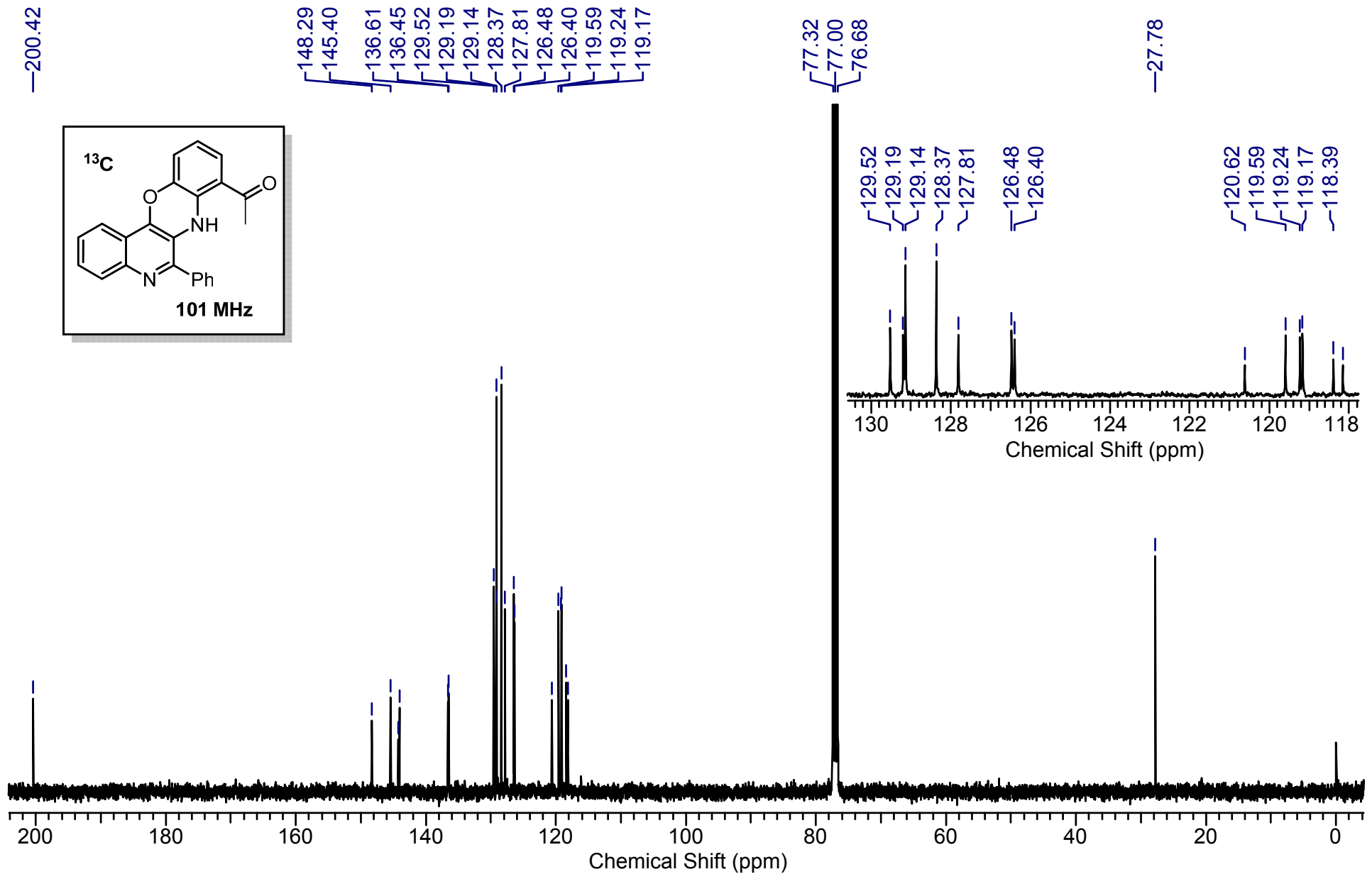
SVH-661 #904 RT: 4.03 AV: 1 NL: 5.87E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



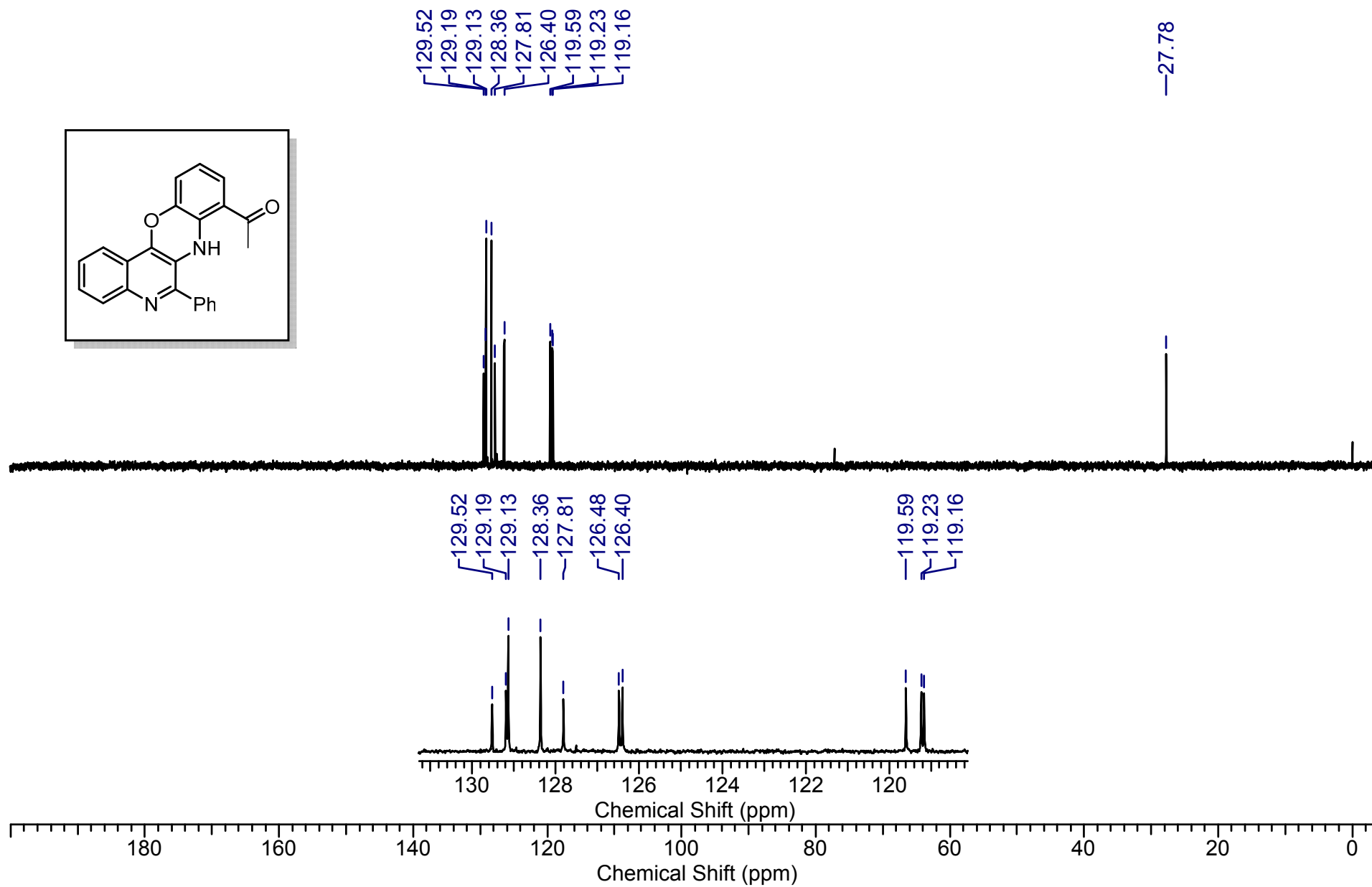
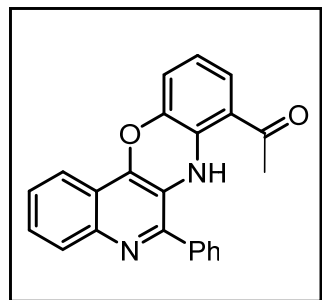
3aj



3aj

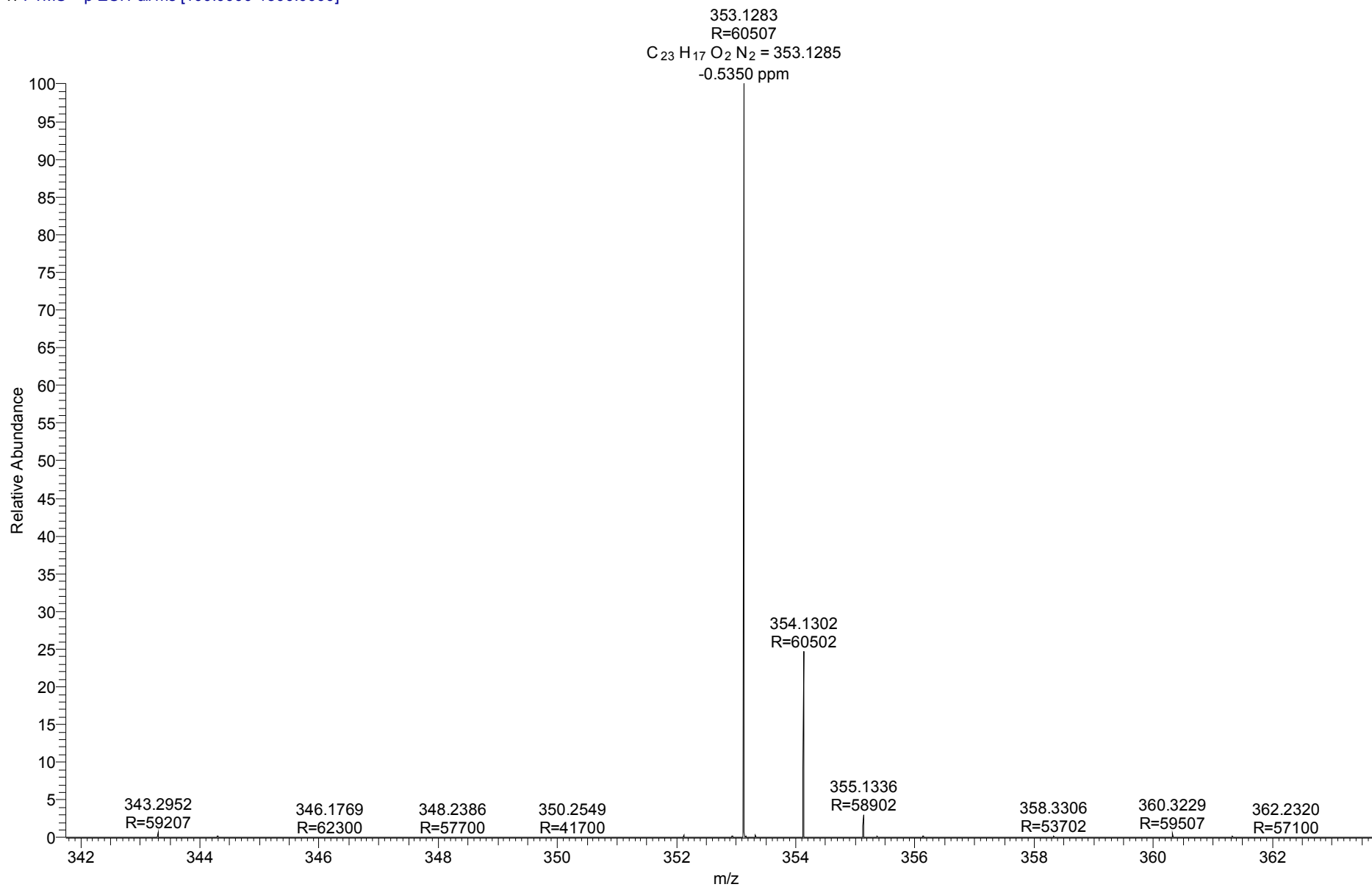


3aj

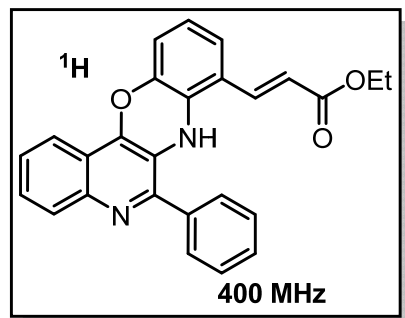


3aj

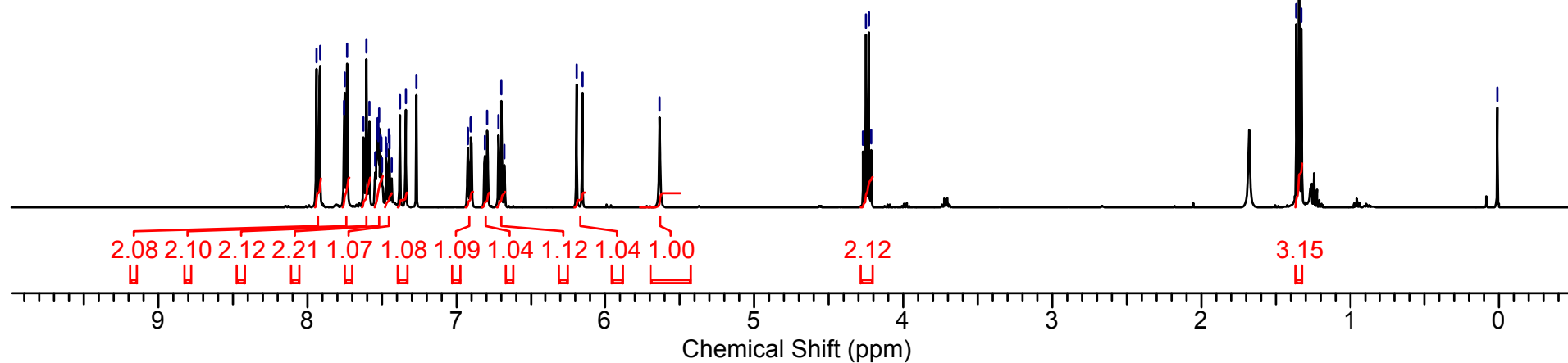
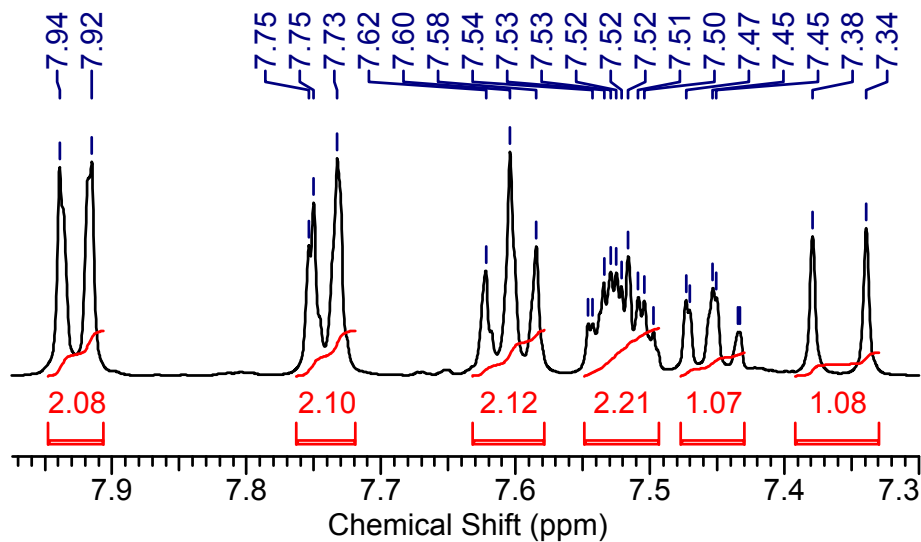
652 #574 RT: 2.60 AV: 1 NL: 2.55E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



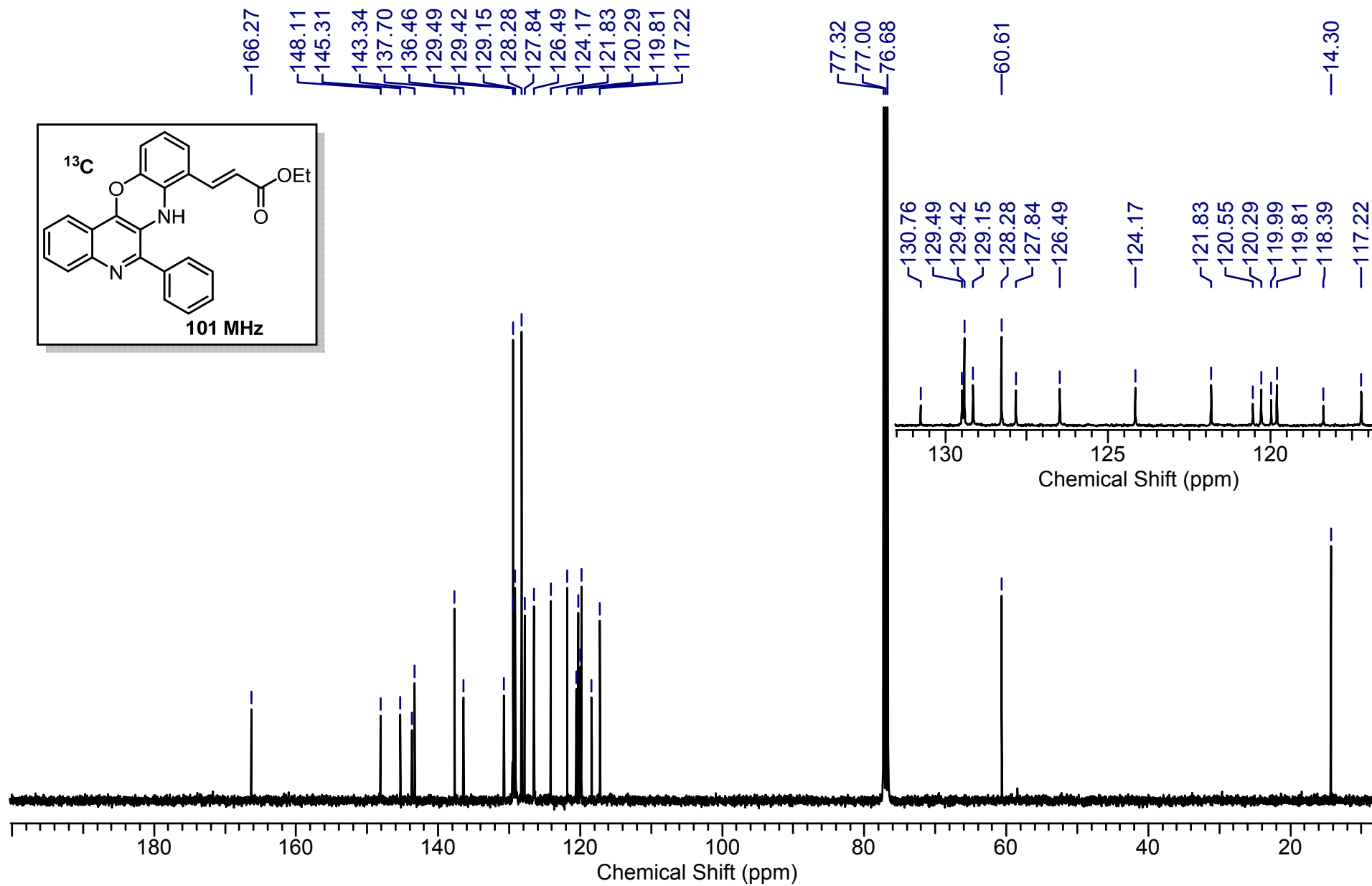
5



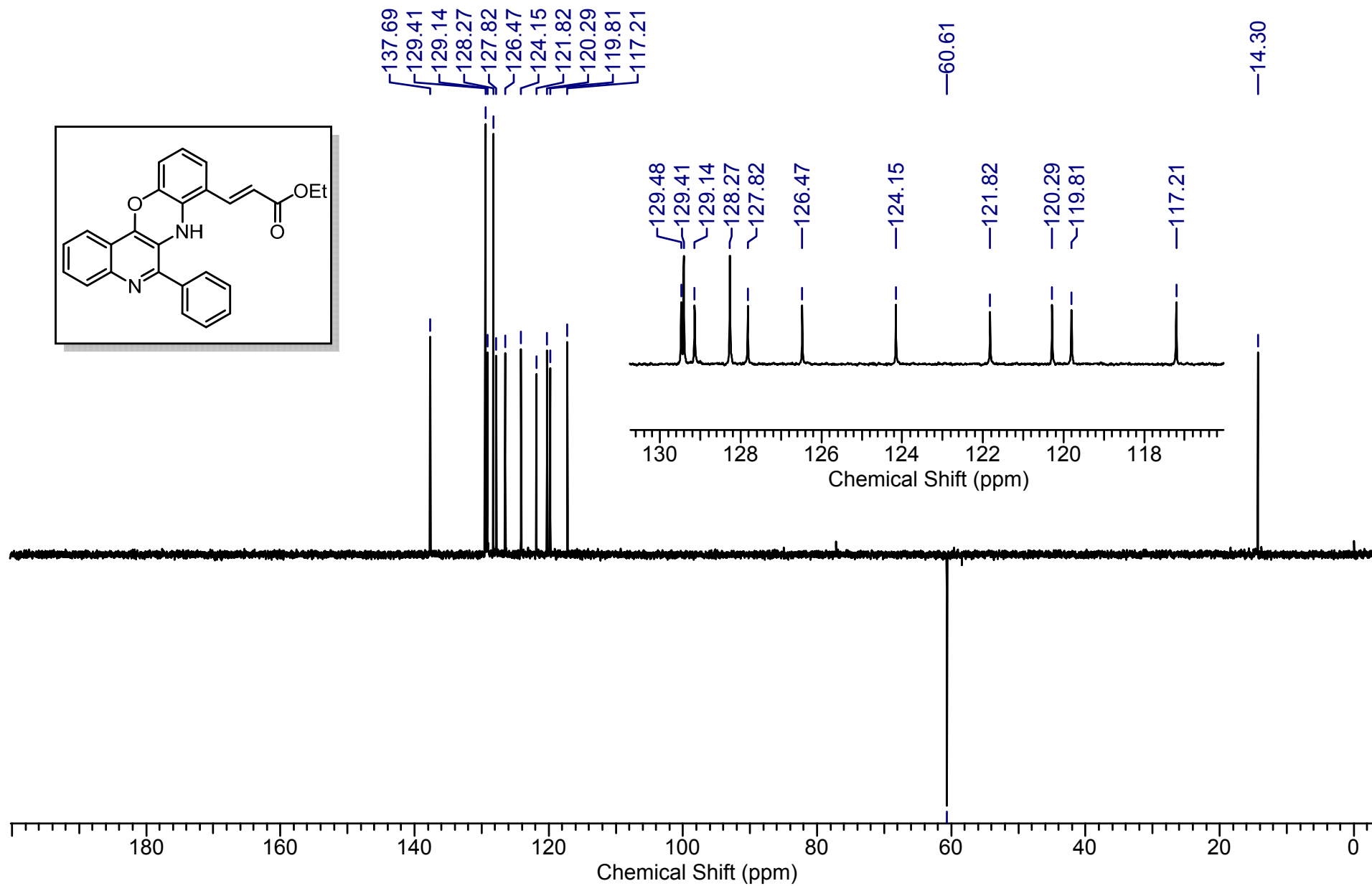
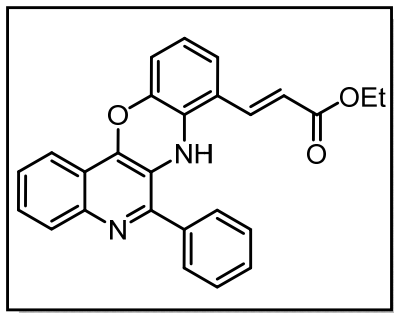
7.94
7.92
7.75
7.75
7.73
7.60
7.58
7.52
7.38
7.34
7.27
6.79
6.72
6.70
6.19
6.15
5.64
4.27
4.25
4.23
4.22
1.36
1.35
1.33
0.01



5

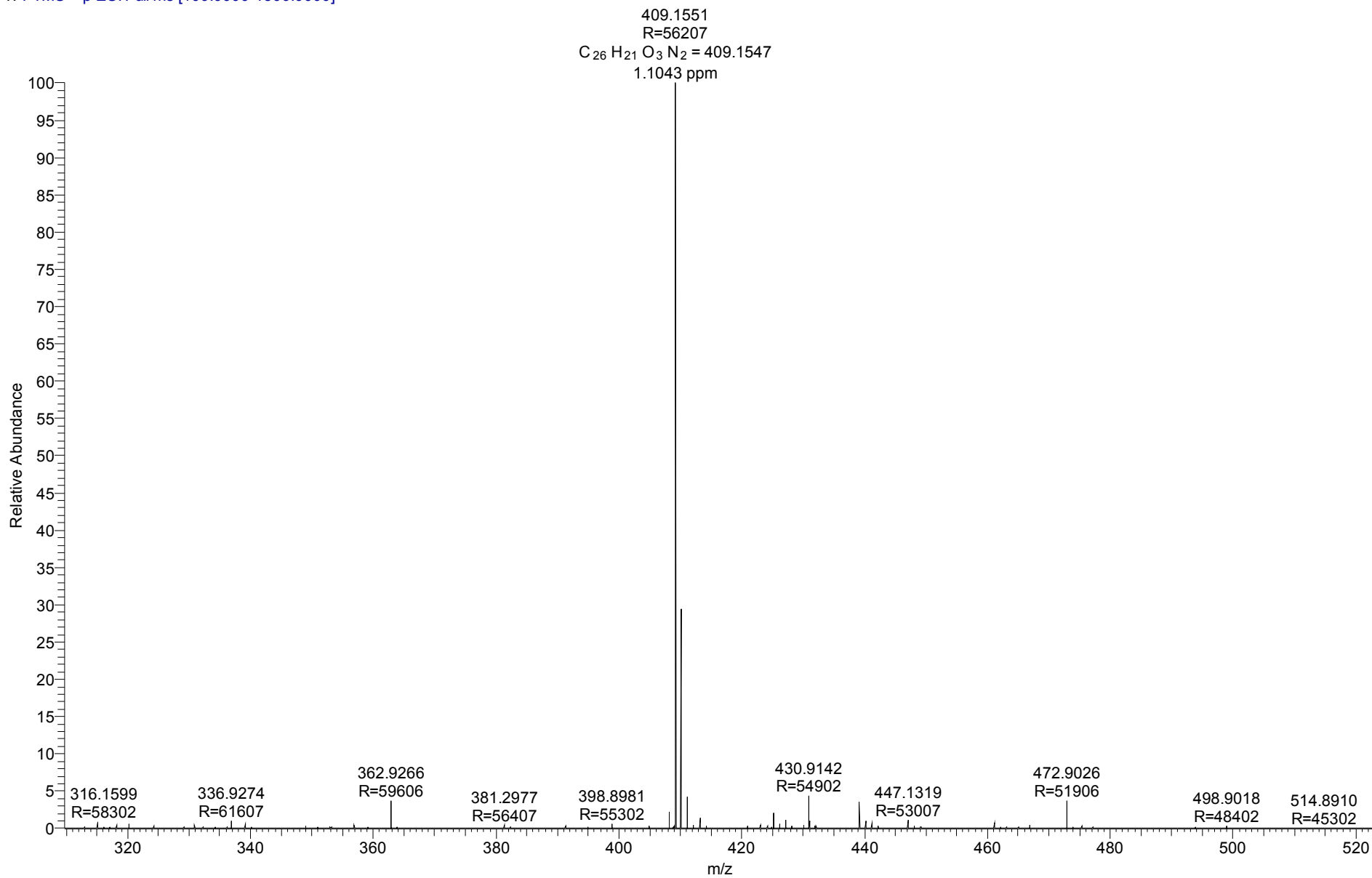


5

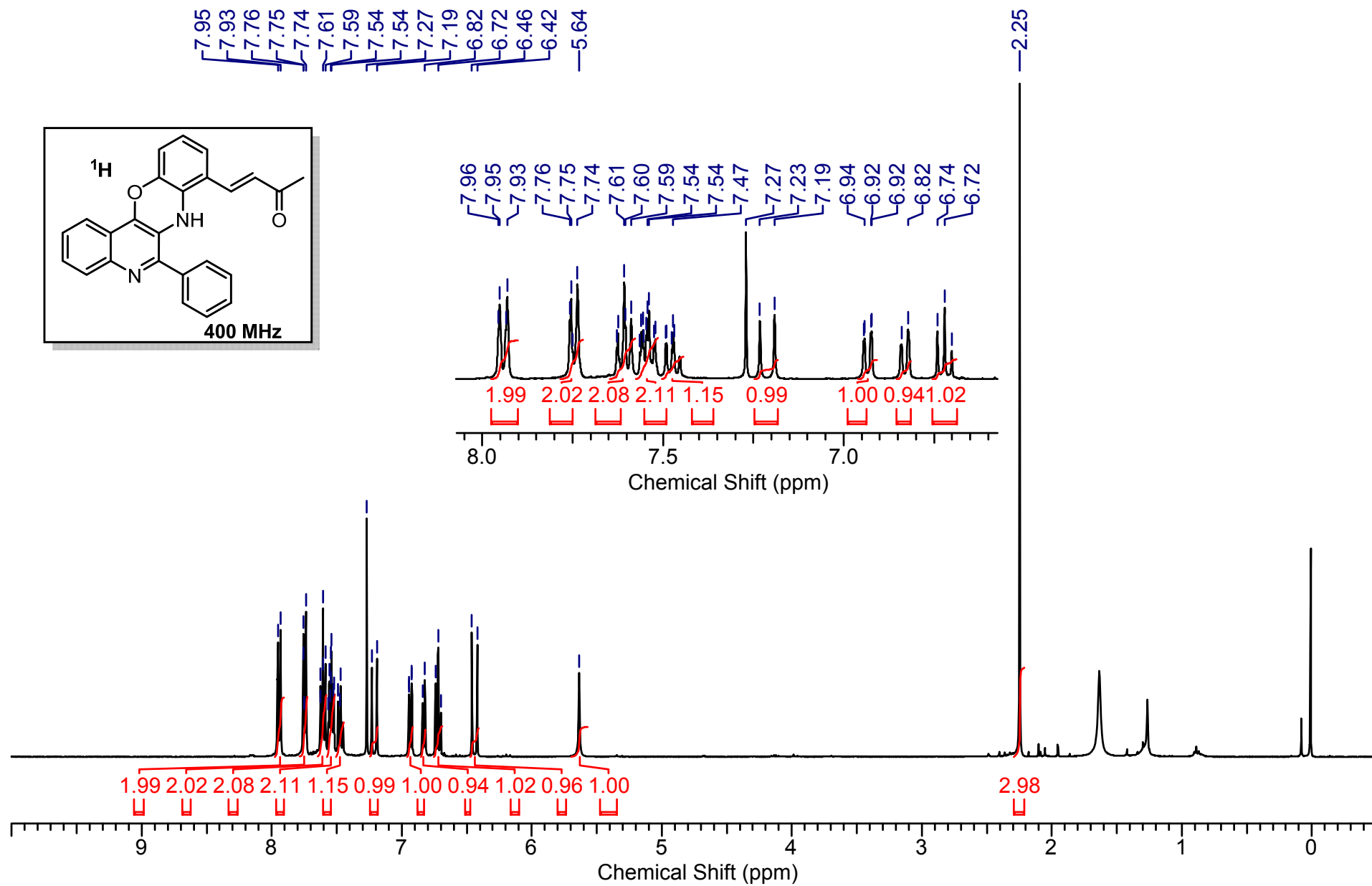


5

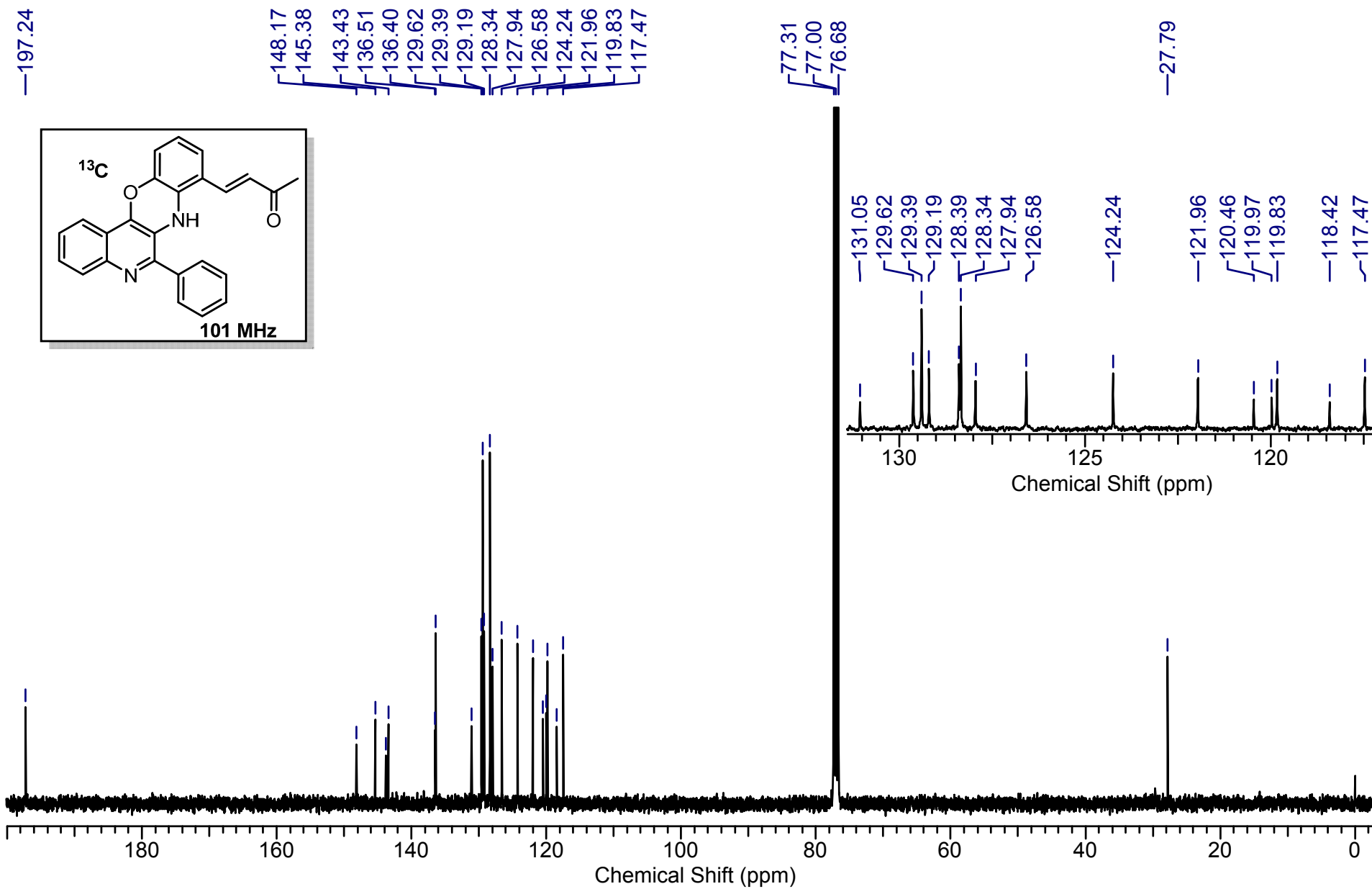
SH-685 #394 RT: 2.11 AV: 1 NL: 1.31E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



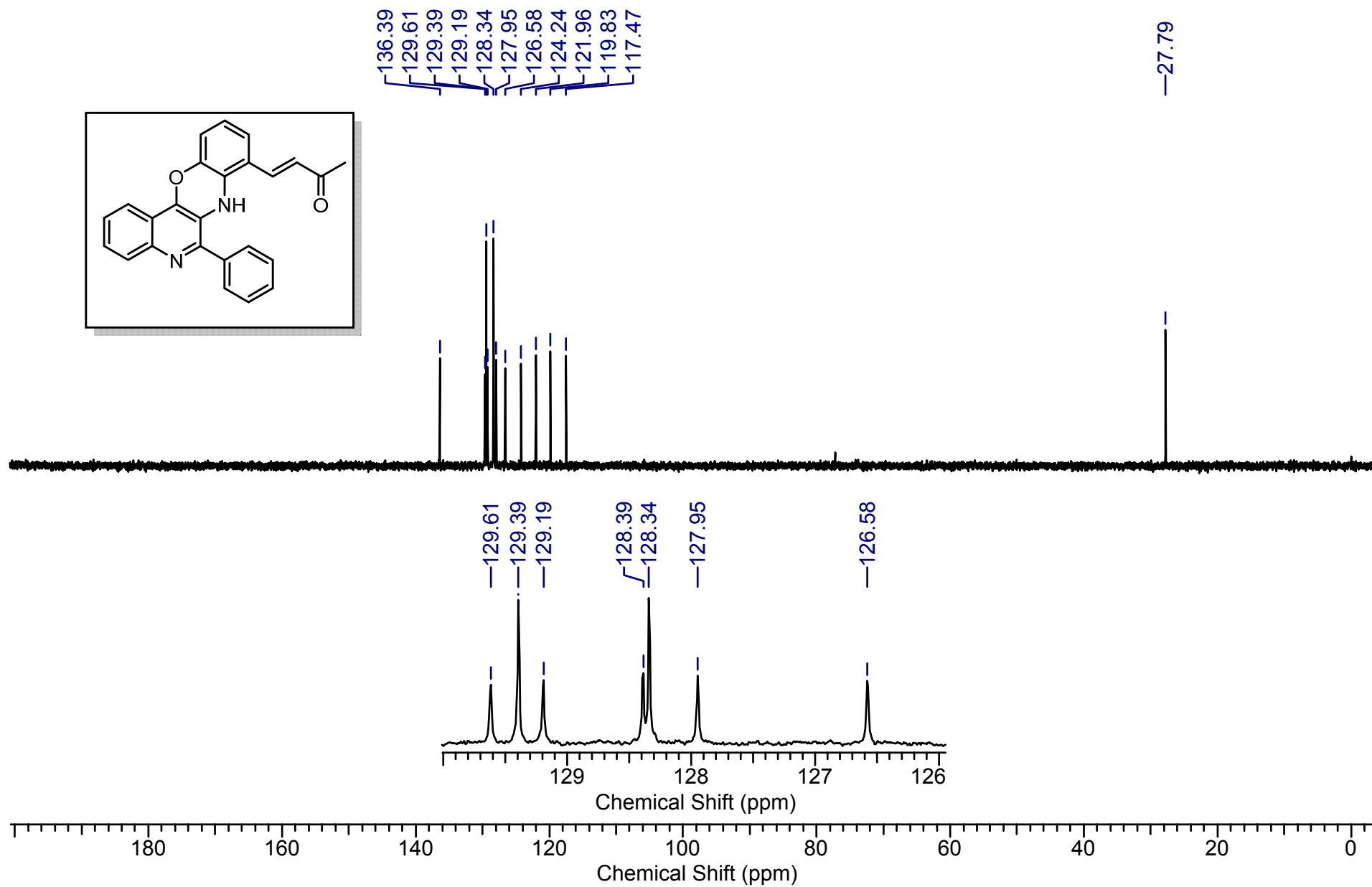
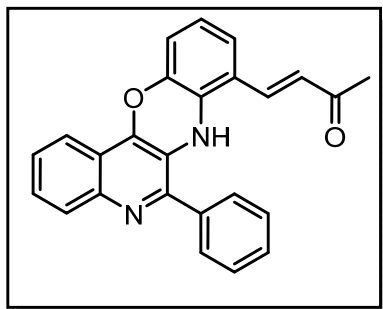
6



6

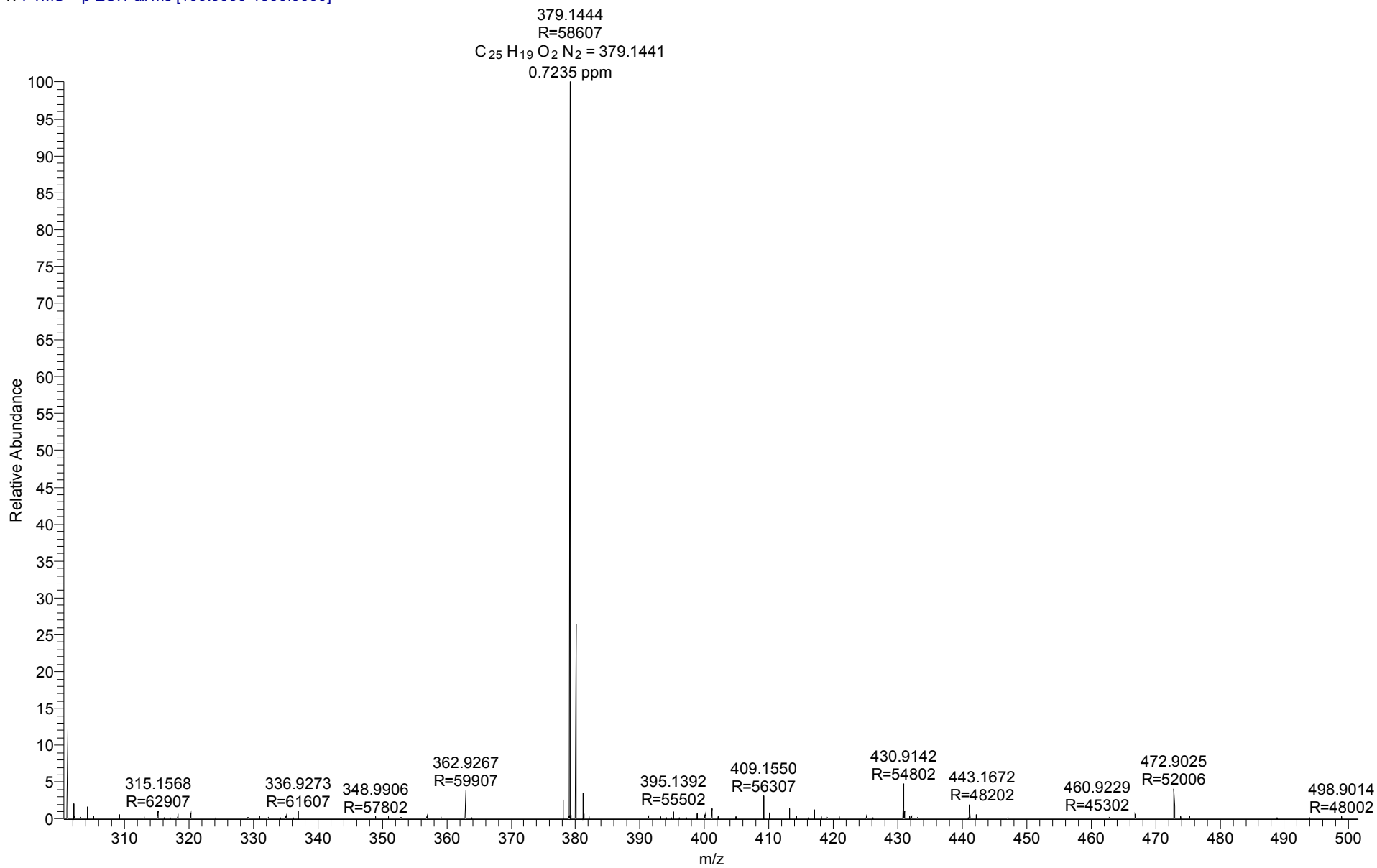


6

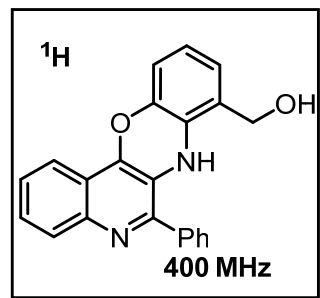


6

SH-684 #334 RT: 1.79 AV: 1 NL: 1.40E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

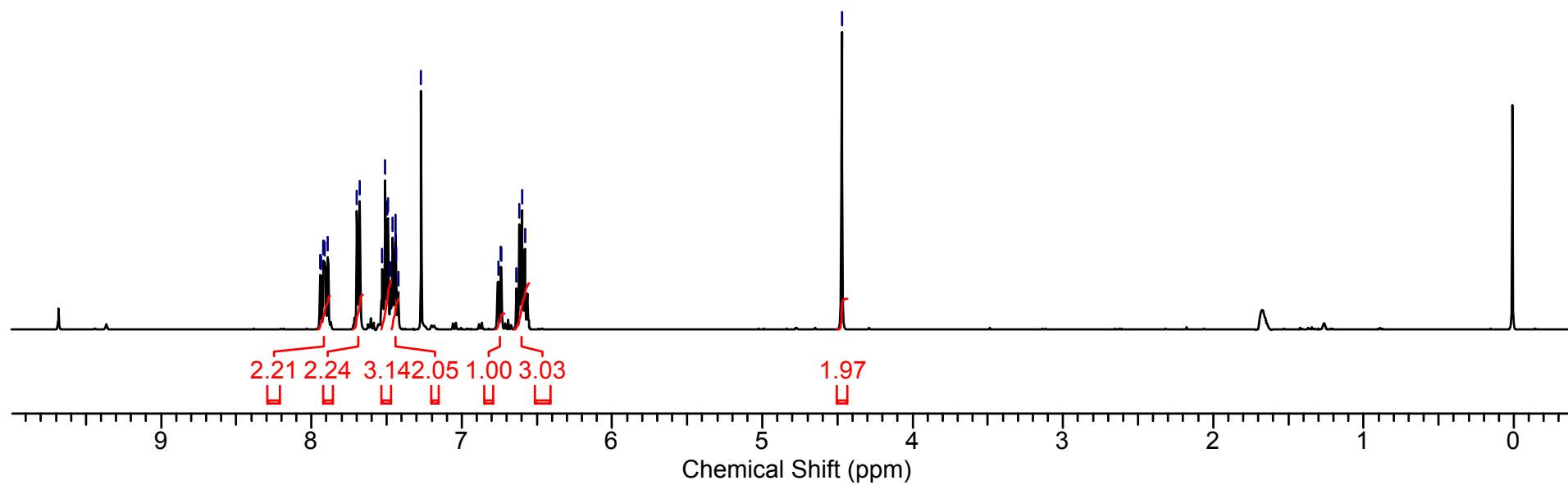
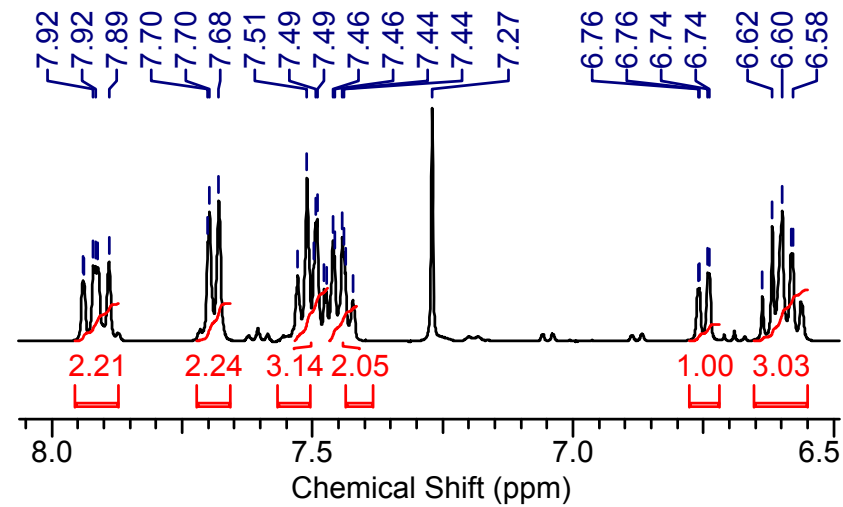


7

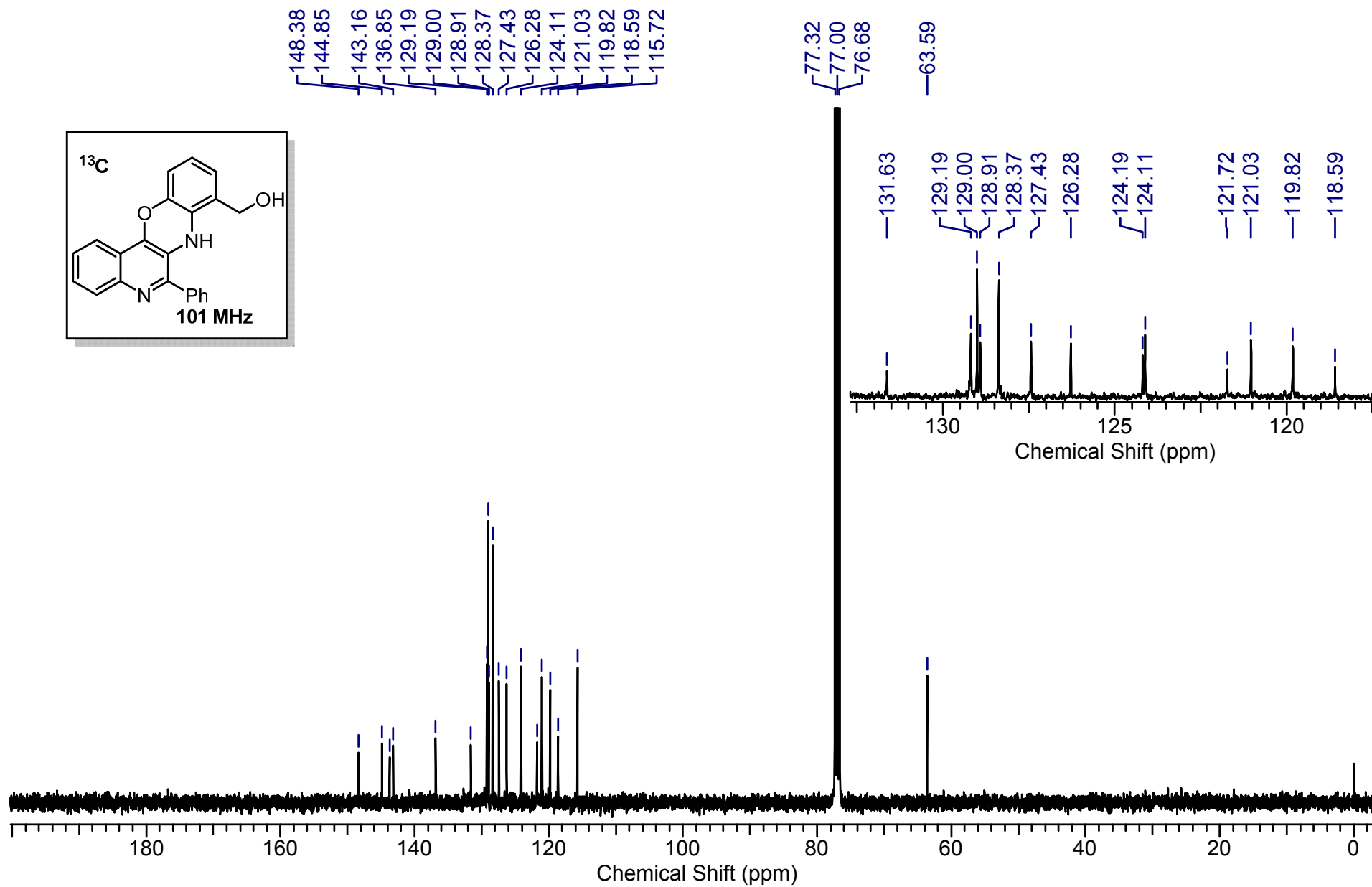


7.92
7.89
7.70
7.68
7.51
7.49
7.49
7.46
7.44
7.44
7.27
6.74
6.62
6.60
6.58

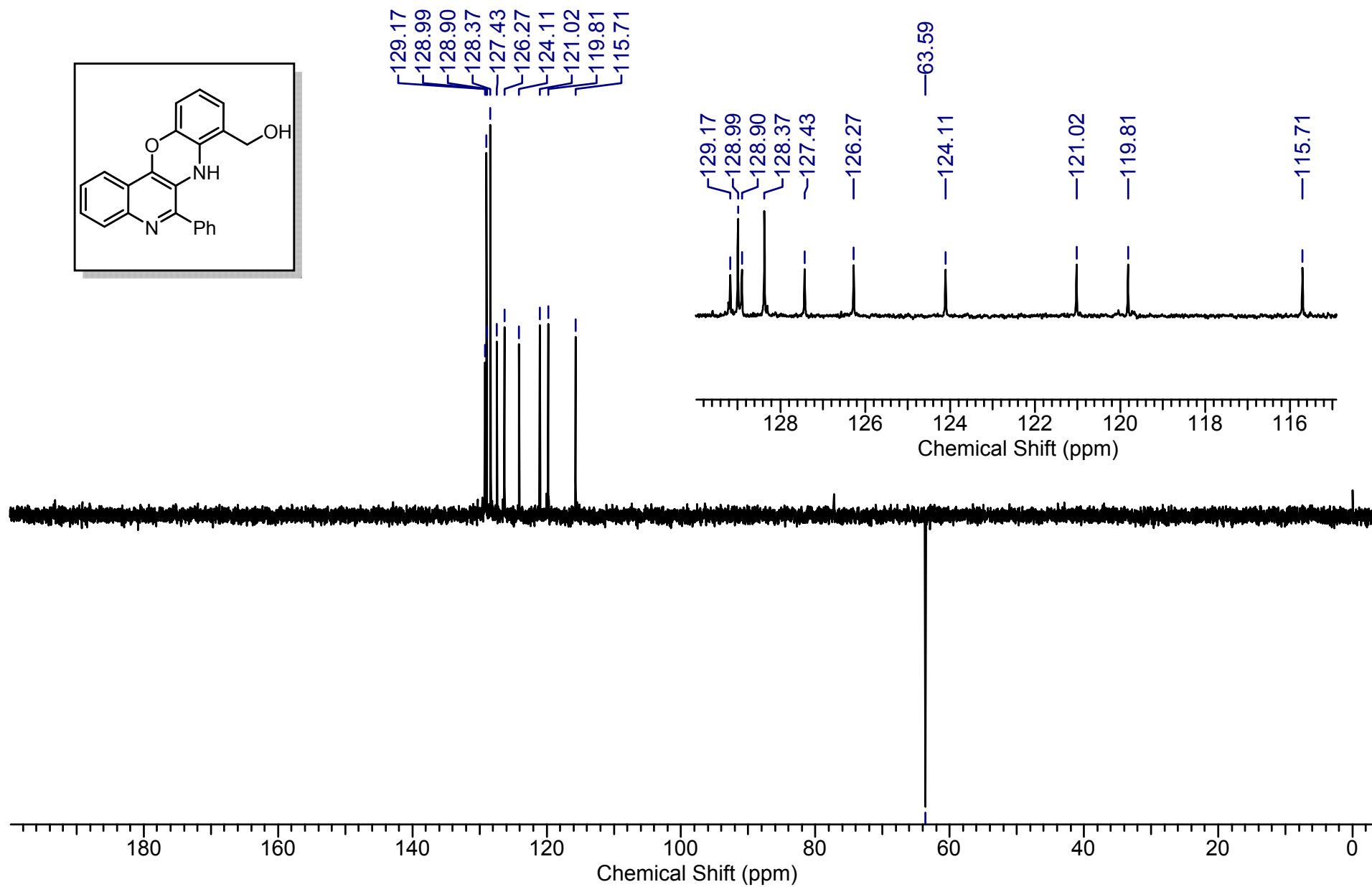
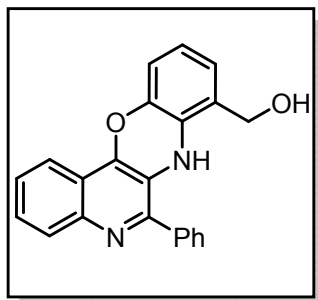
4.47



7

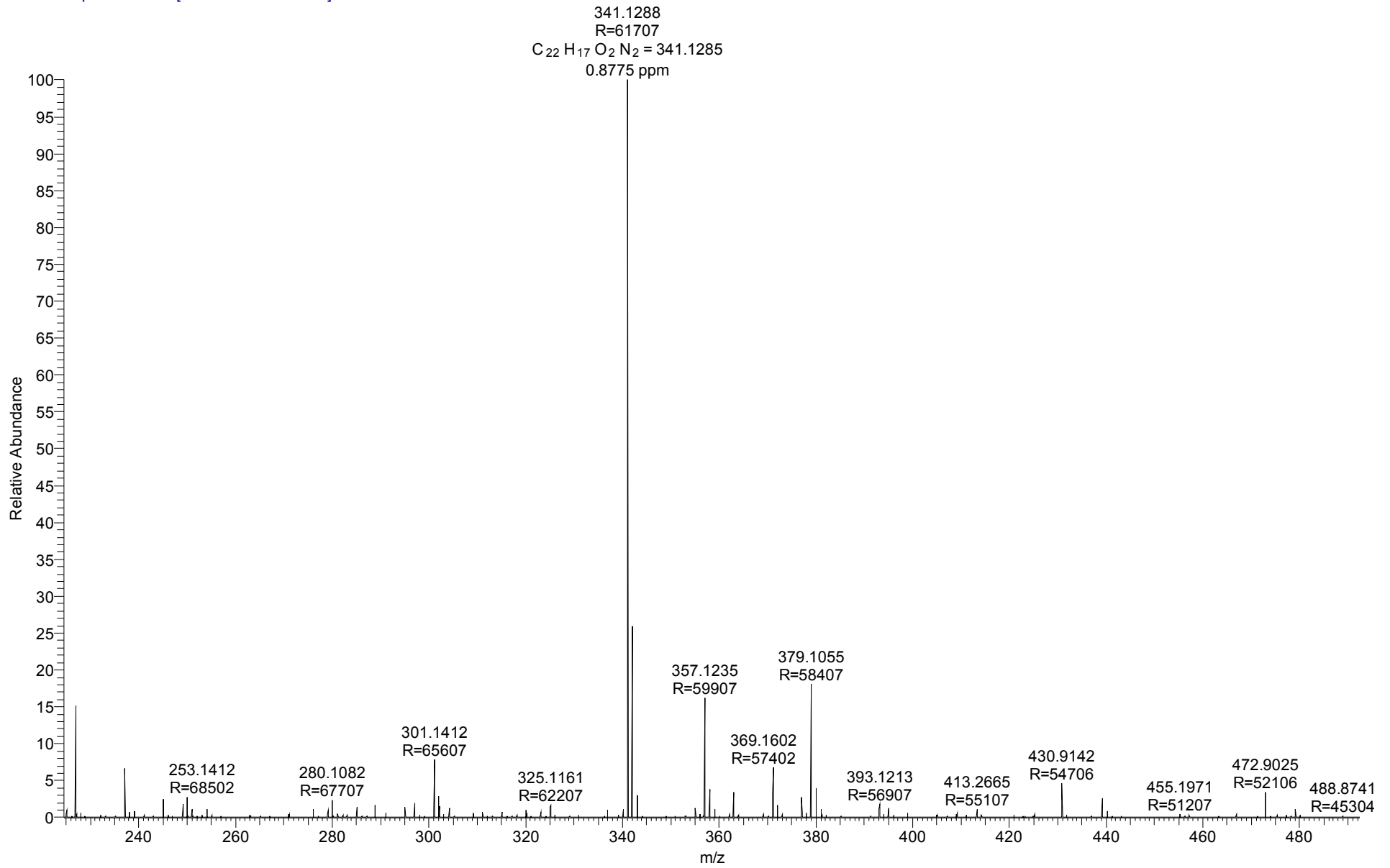


7

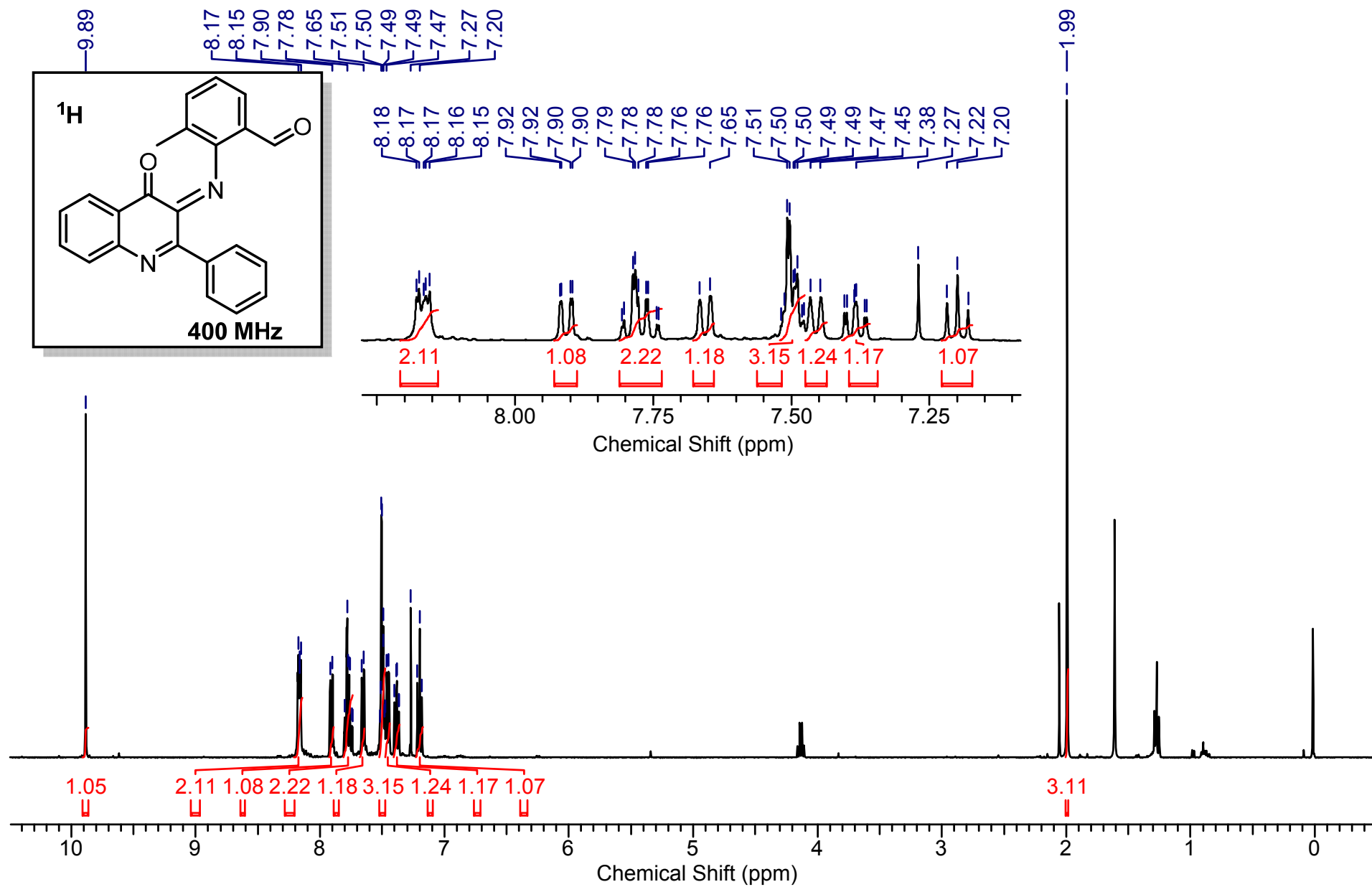


7

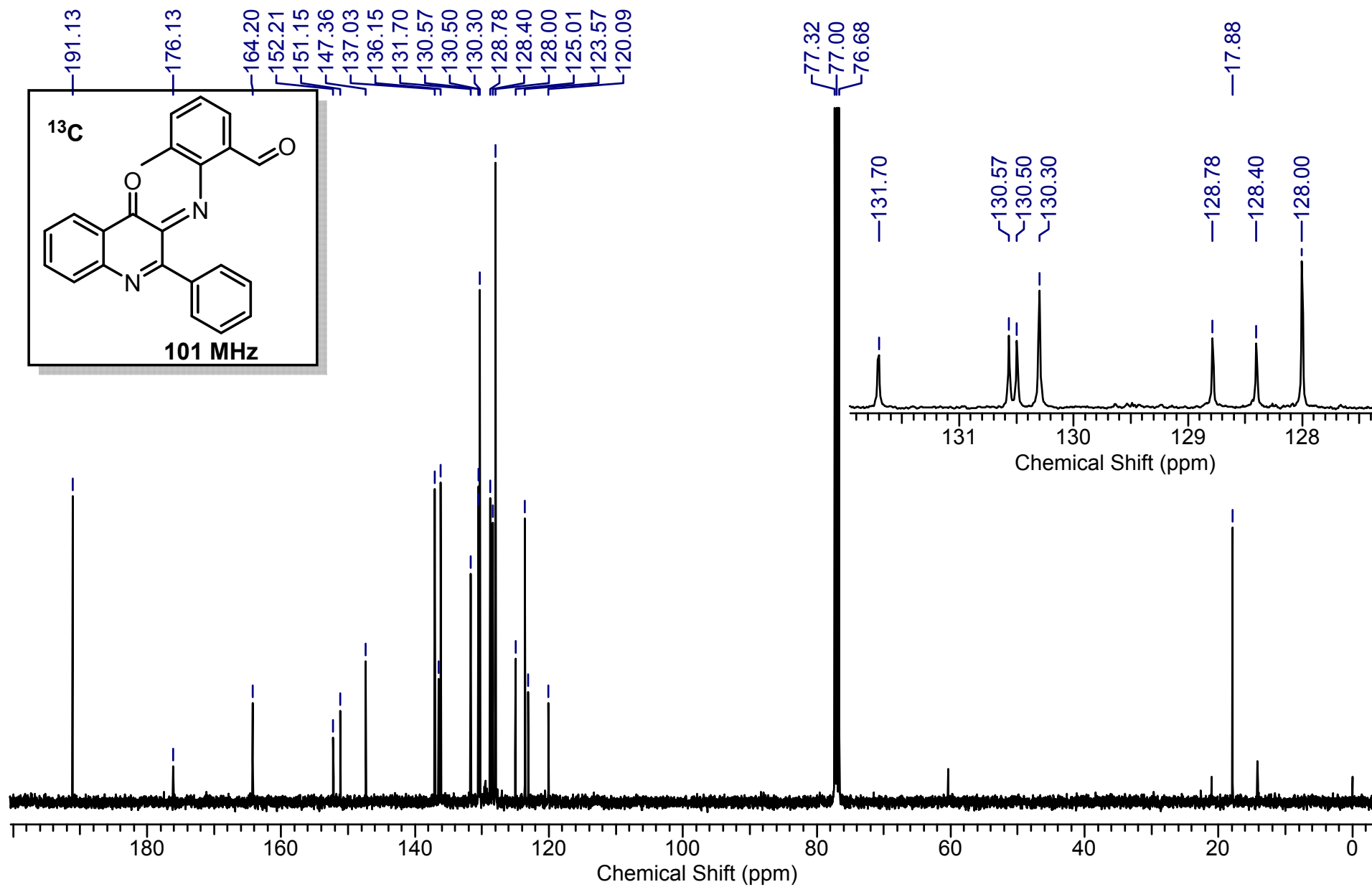
SH-701 #268 RT: 1.44 AV: 1 NL: 1.46E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



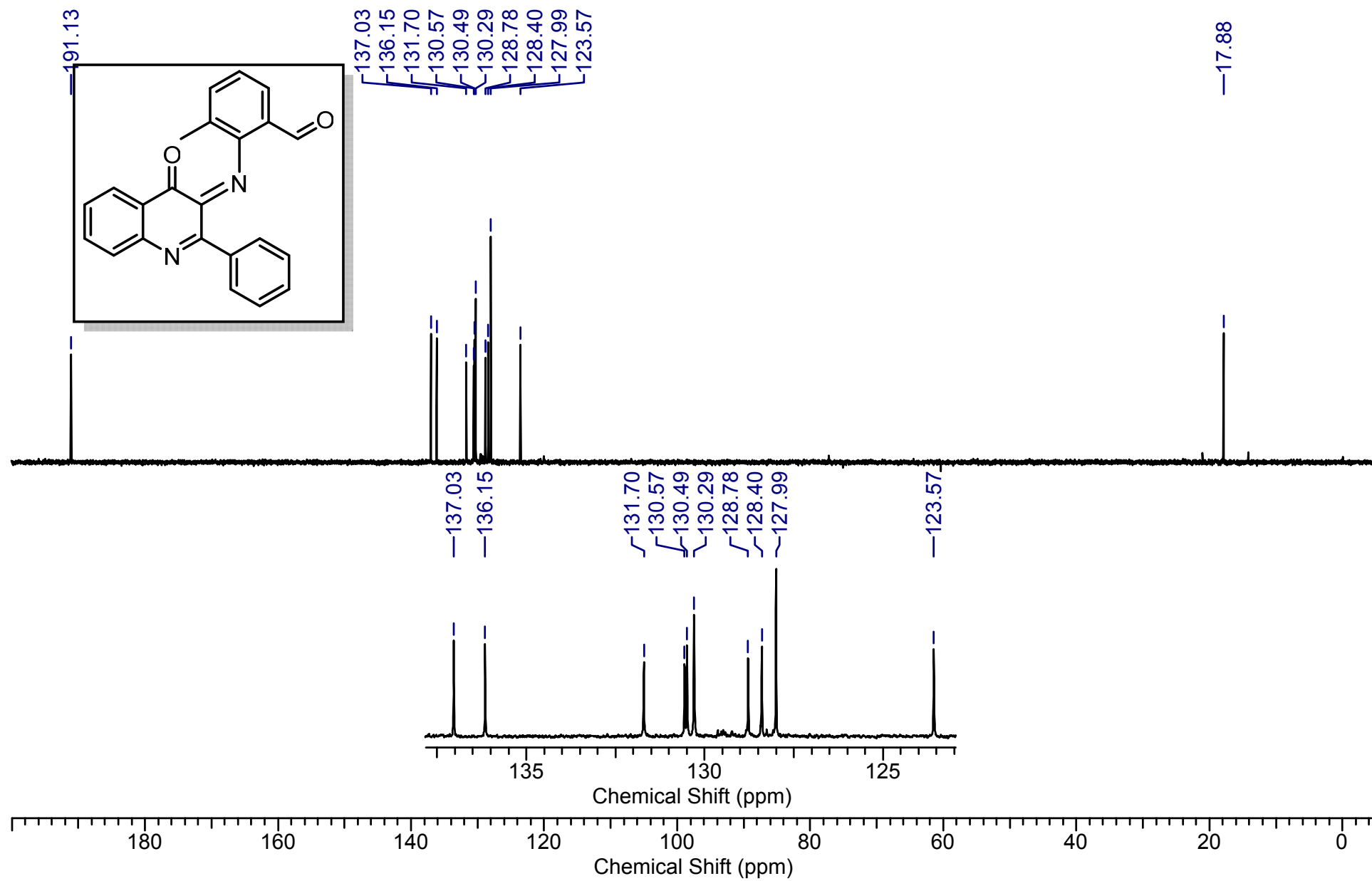
8



8

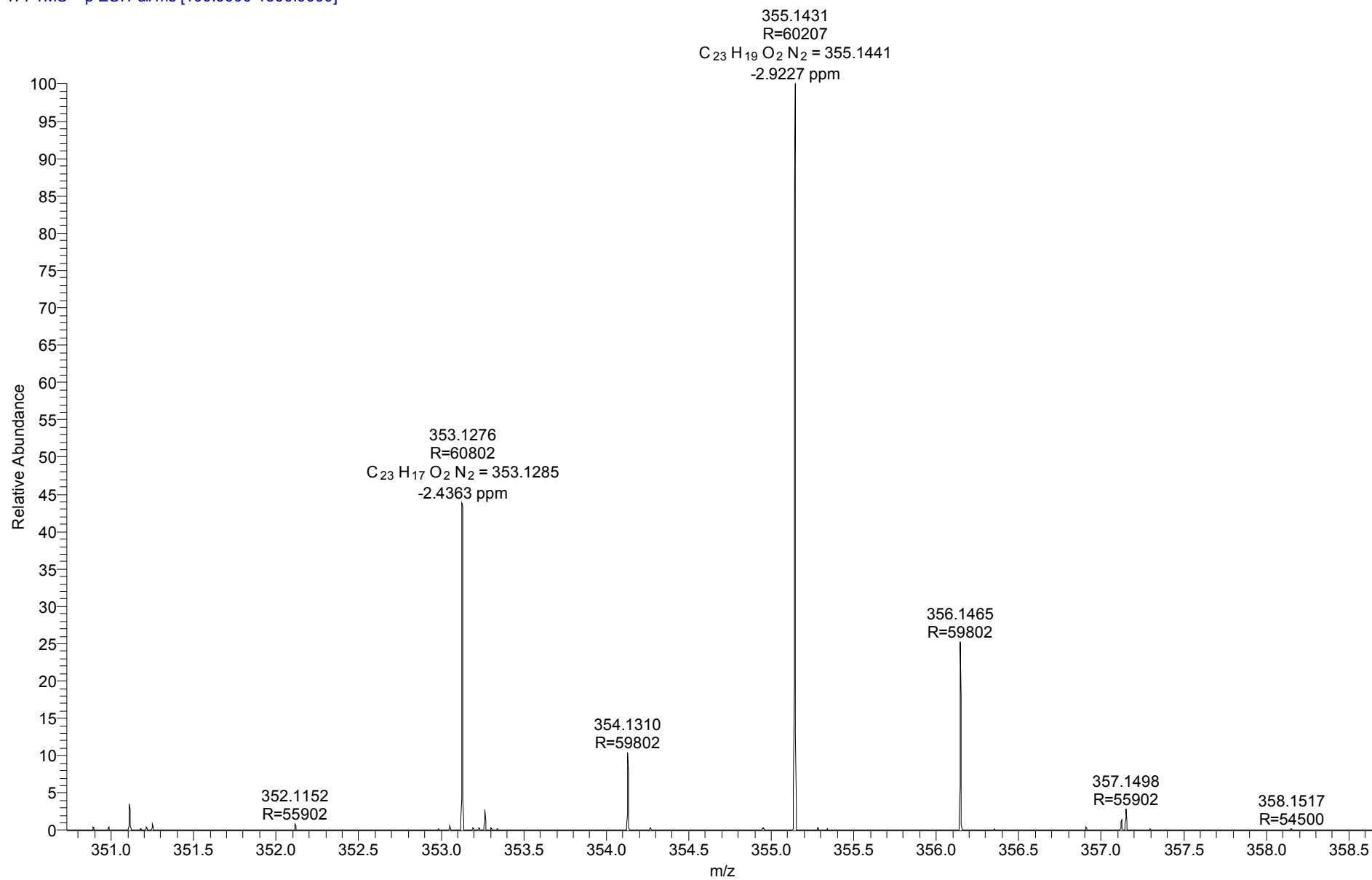


8

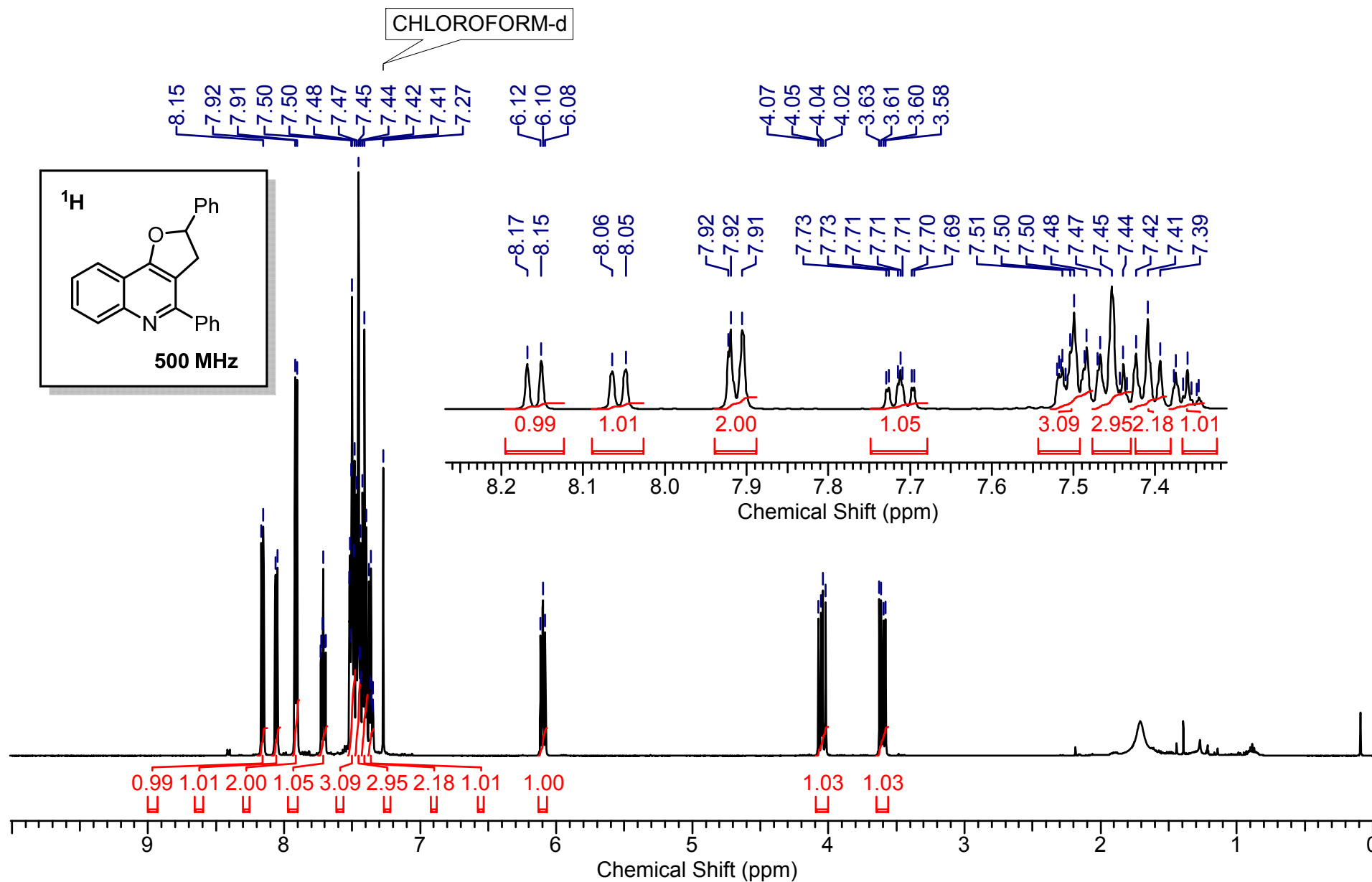


8

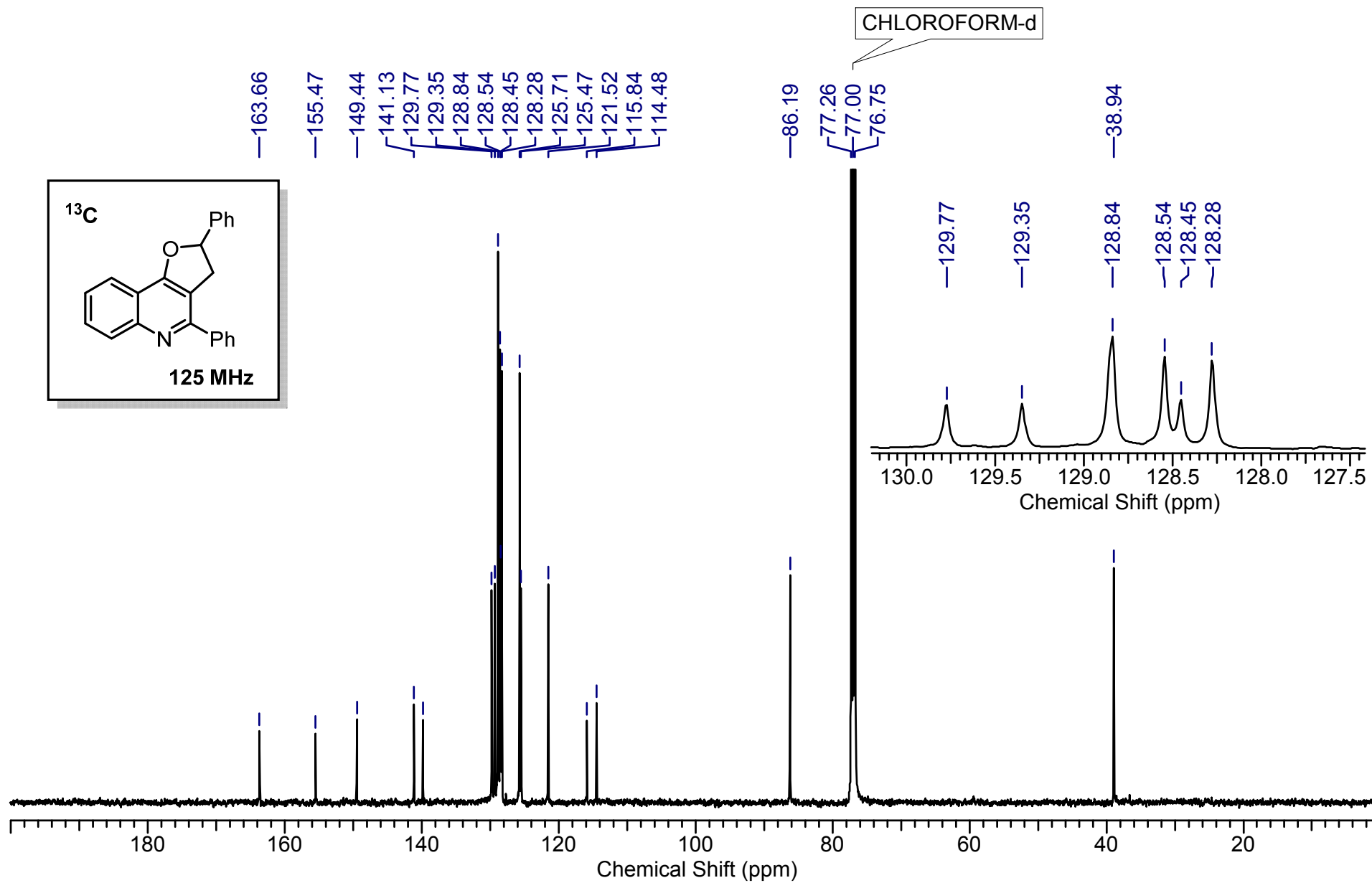
SVH-840 #530 RT: 2.86 AV: 1 NL: 1.87E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



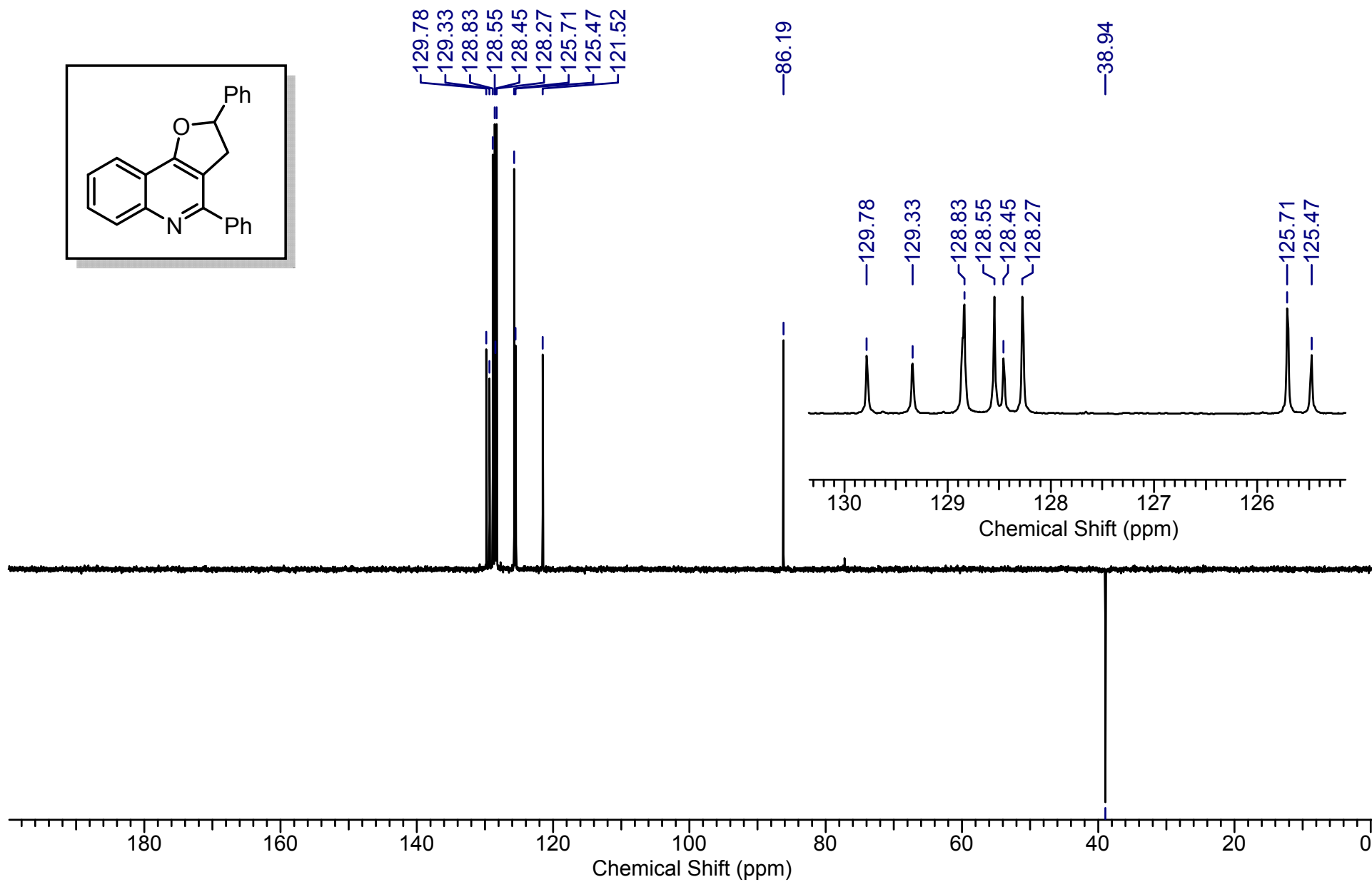
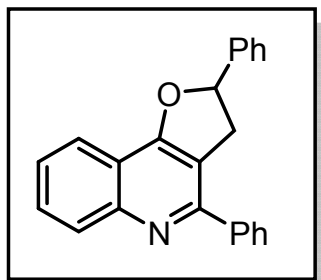
10



10



10



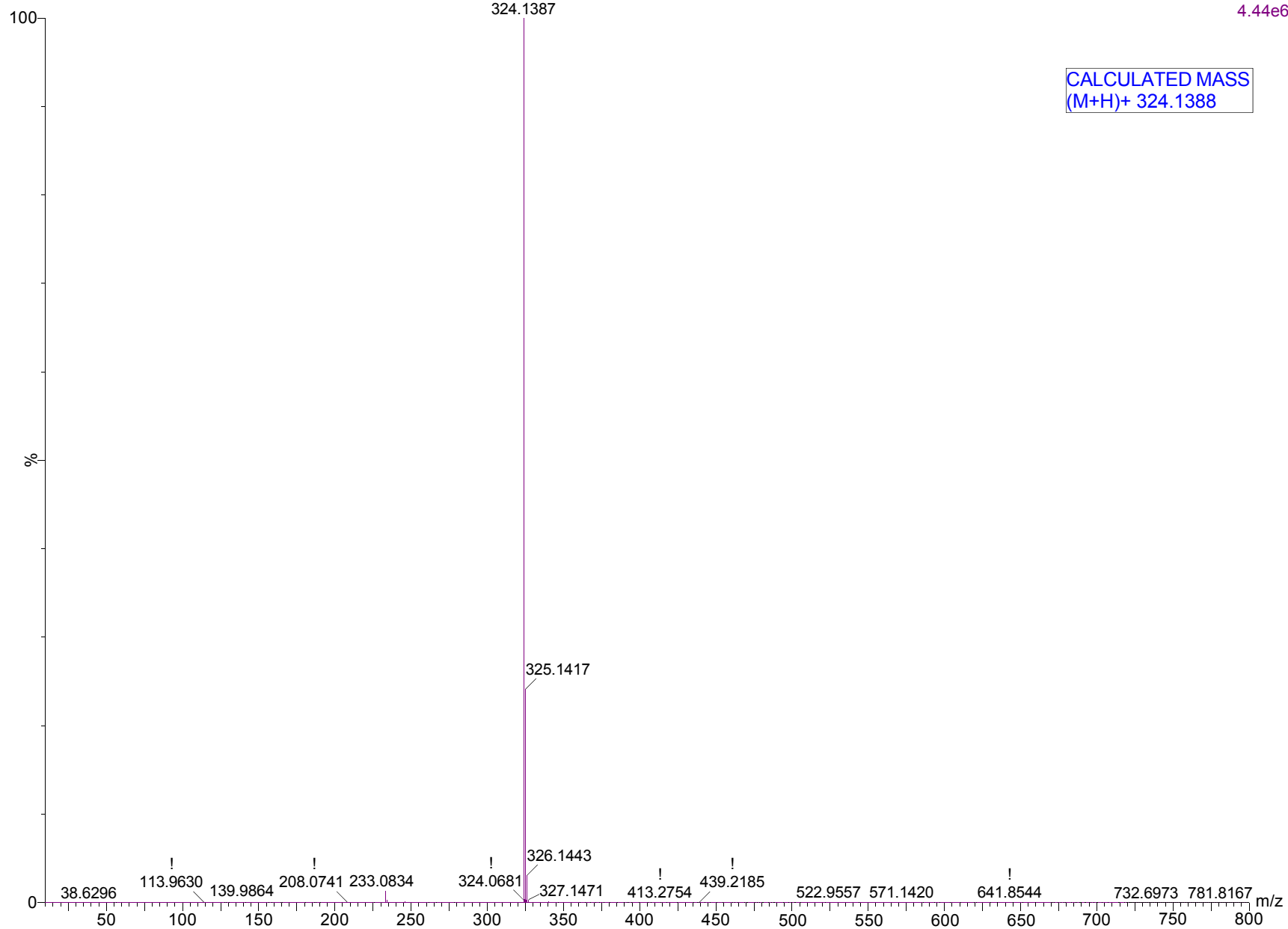
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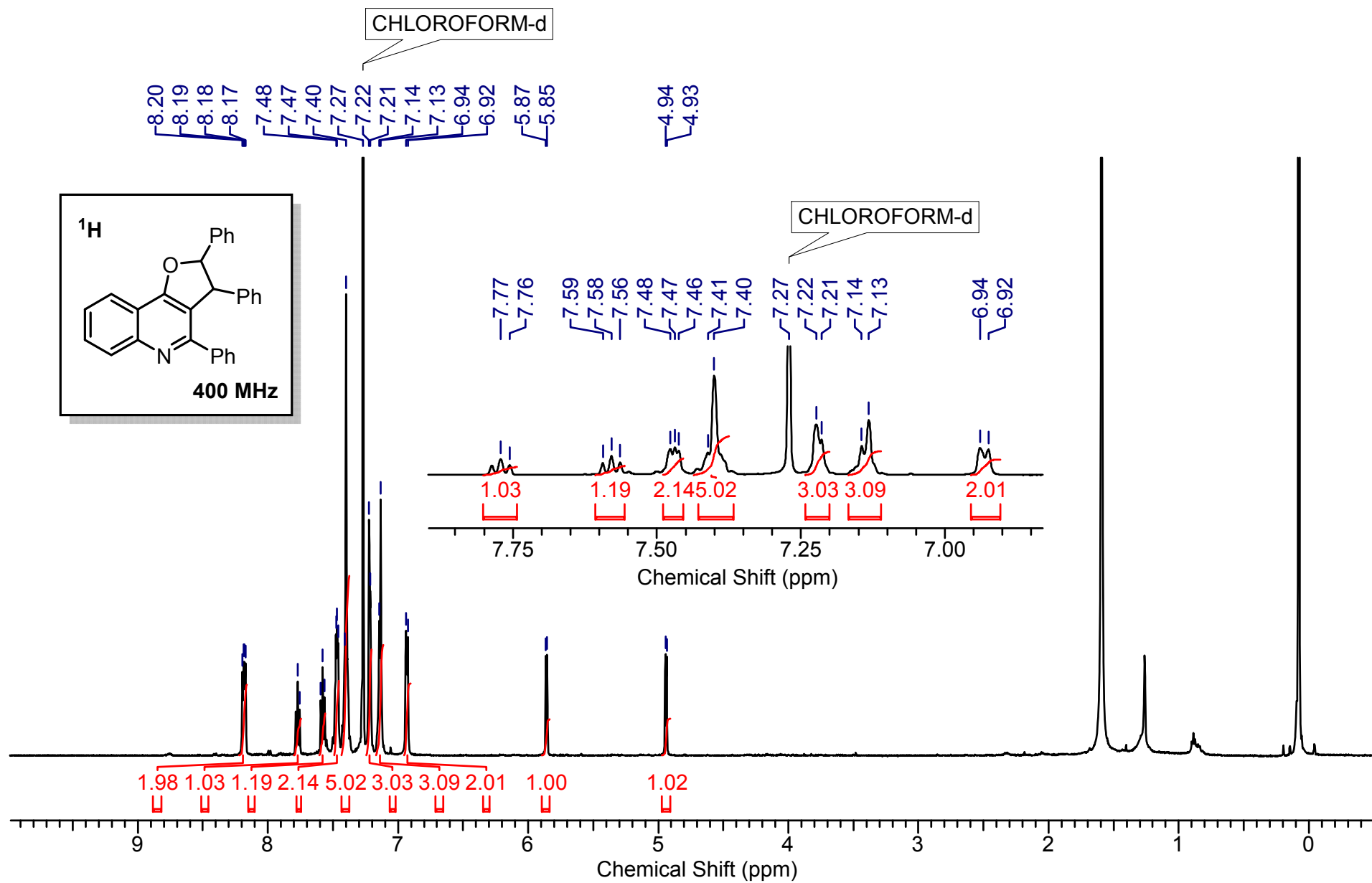
NK 1

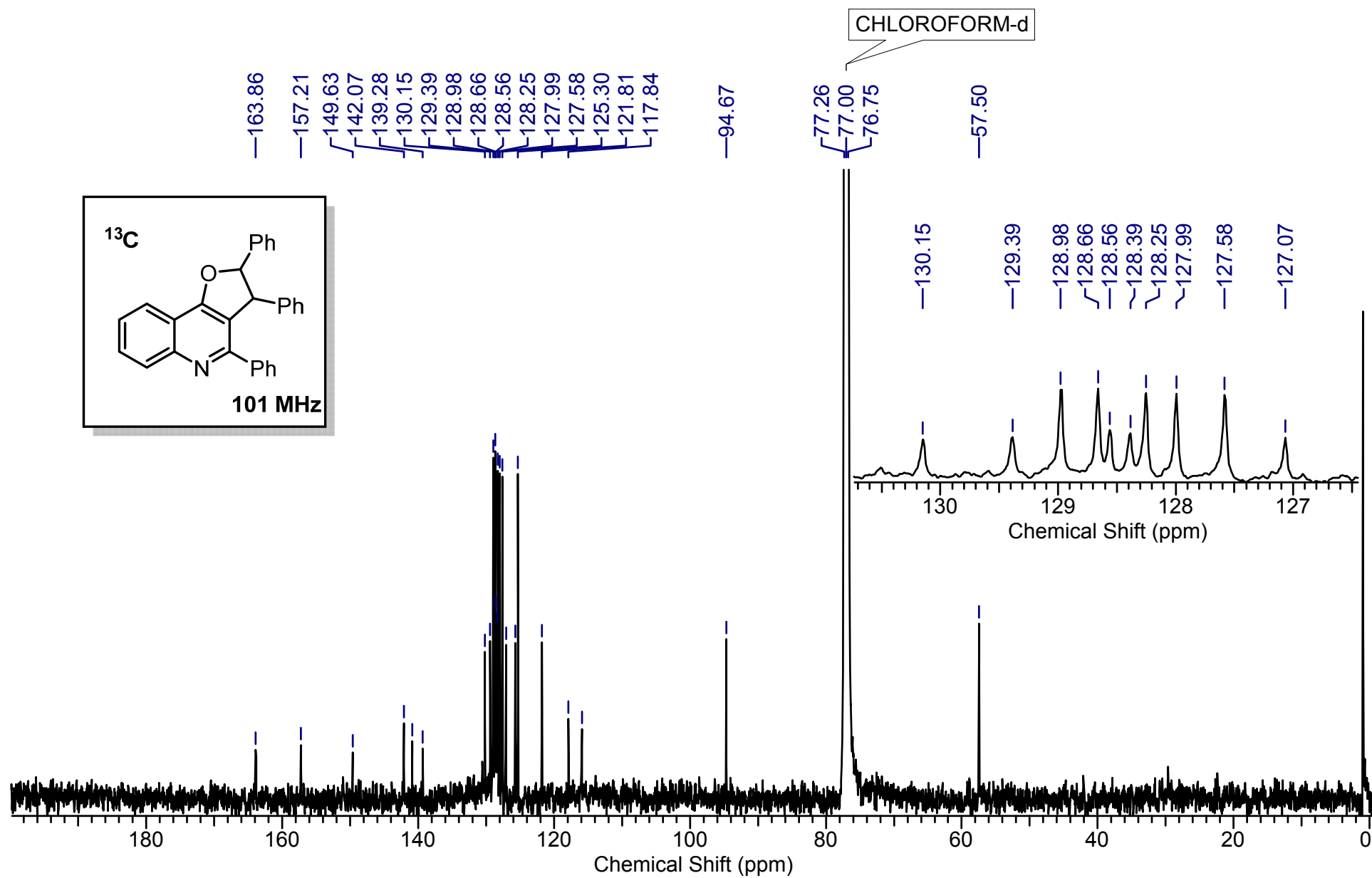
IISER PUNE

NK 1 87 (1.599) AM2 (Ar,20000.0,556.28,0.00,LS 3); Sm (SG, 3x1.00)

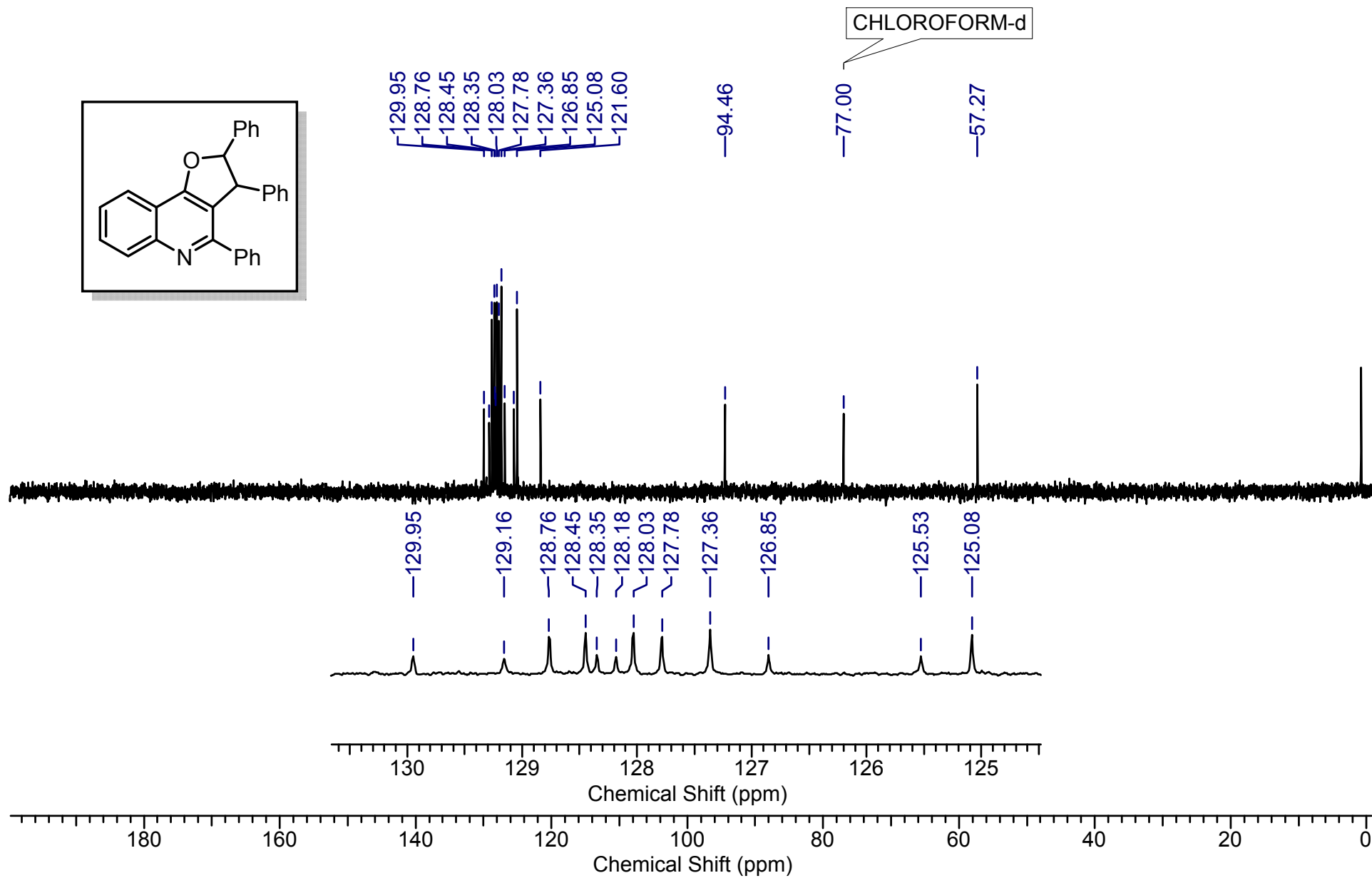
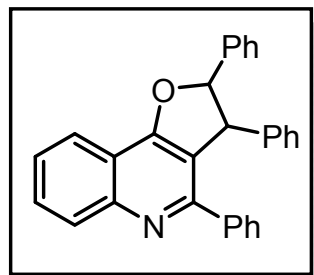
1: TOF MS ES+
4.44e6







11



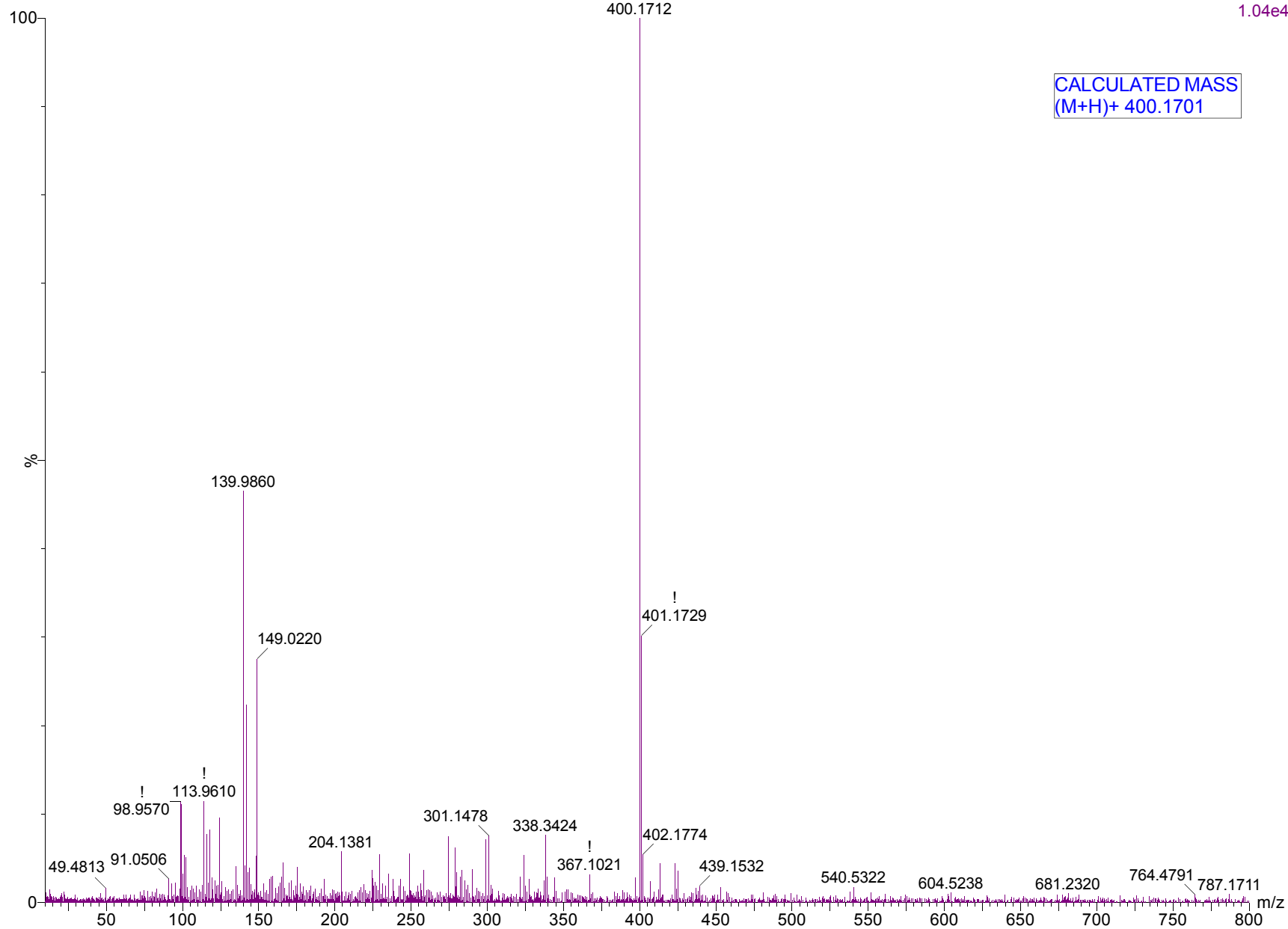
11

NK 2

NK 2 105 (1.926) AM2 (Ar,20000.0,556.28,0.00,LS 3); Sm (SG, 3x1.00)

IISER PUNE

1: TOF MS ES+
1.04e4



CALCULATED MASS
(M+H)+ 400.1701