

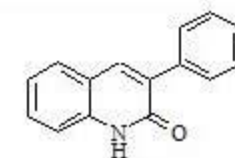
Metal-Free ANRORC Reaction of Indoles with Nitroalkenes: a Simple, Modular Approach to 3-Substituted 2-Quinolones

Alexander V. Aksenov,^{*a} Alexander N. Smirnov,^a Nicolai A. Aksenov,^a

Inna V. Aksenova,^a Jonathon P. Matheny,^b and Michael Rubin^{*a,b}

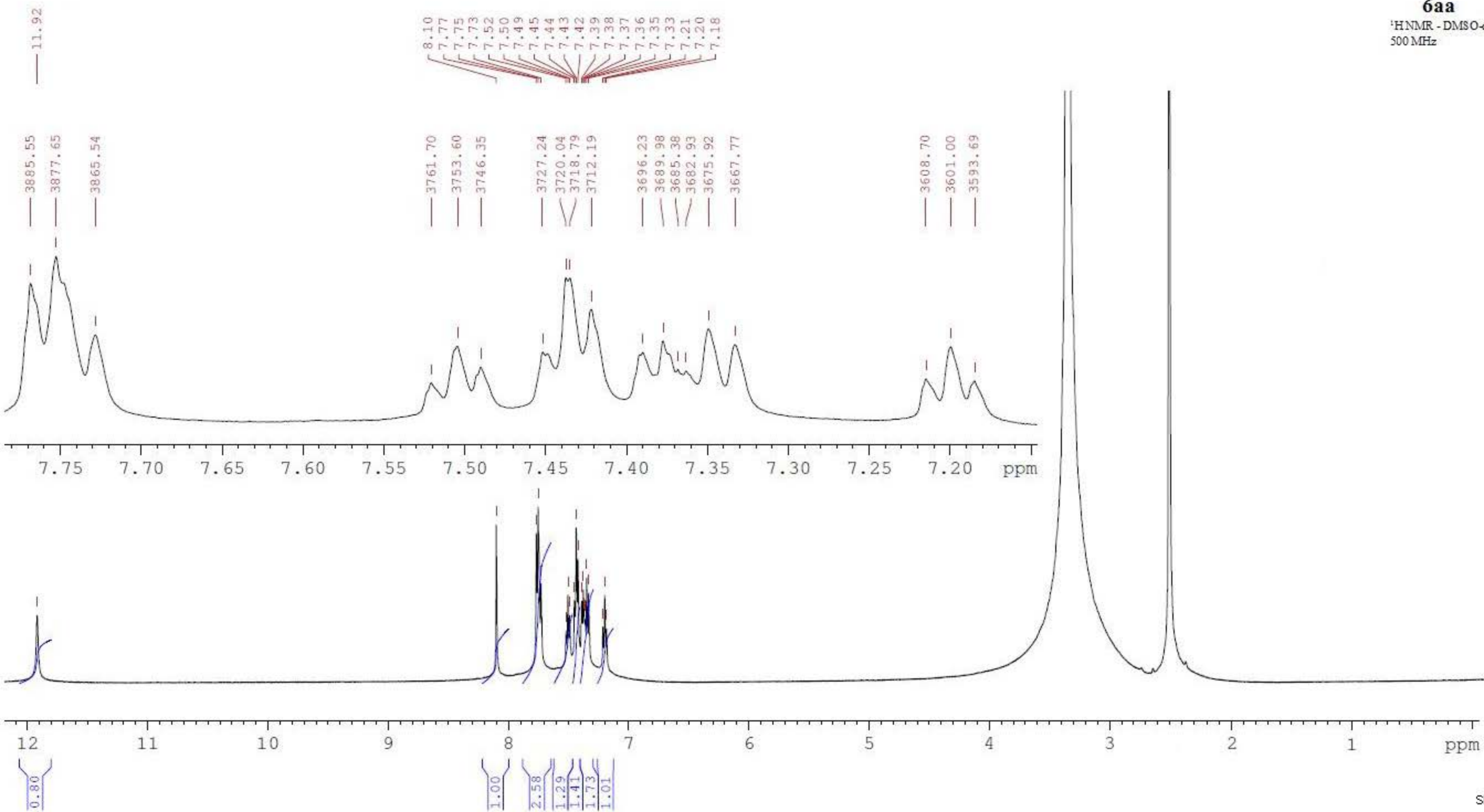
Supporting Information

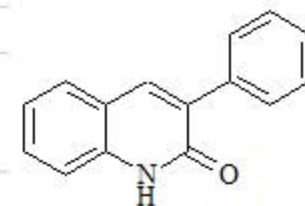
210409
10.05.2012



6aa

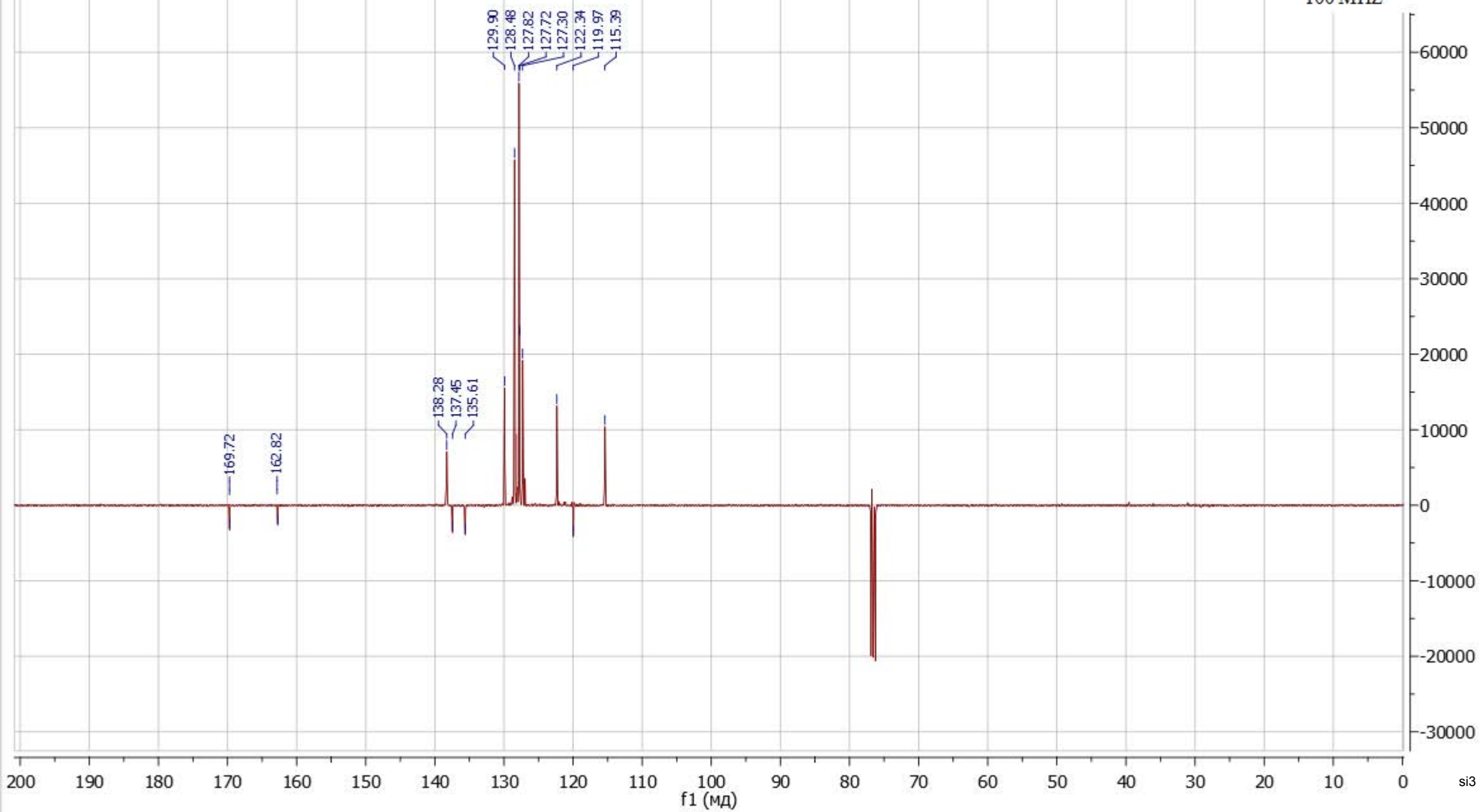
¹H NMR - DMSO-d₆
500 MHz

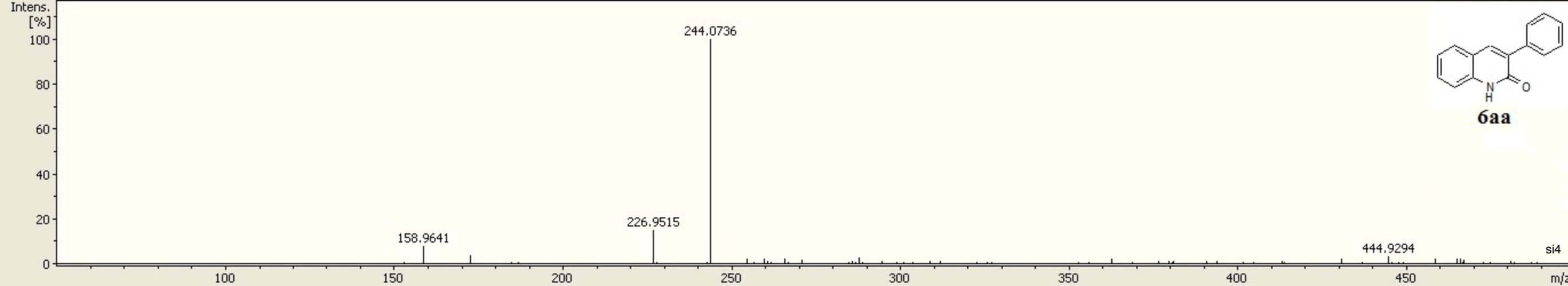


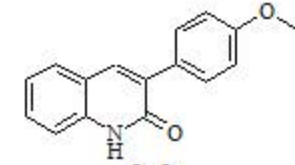


6aa

^{13}C NMR - CDCl_3
100 MHz

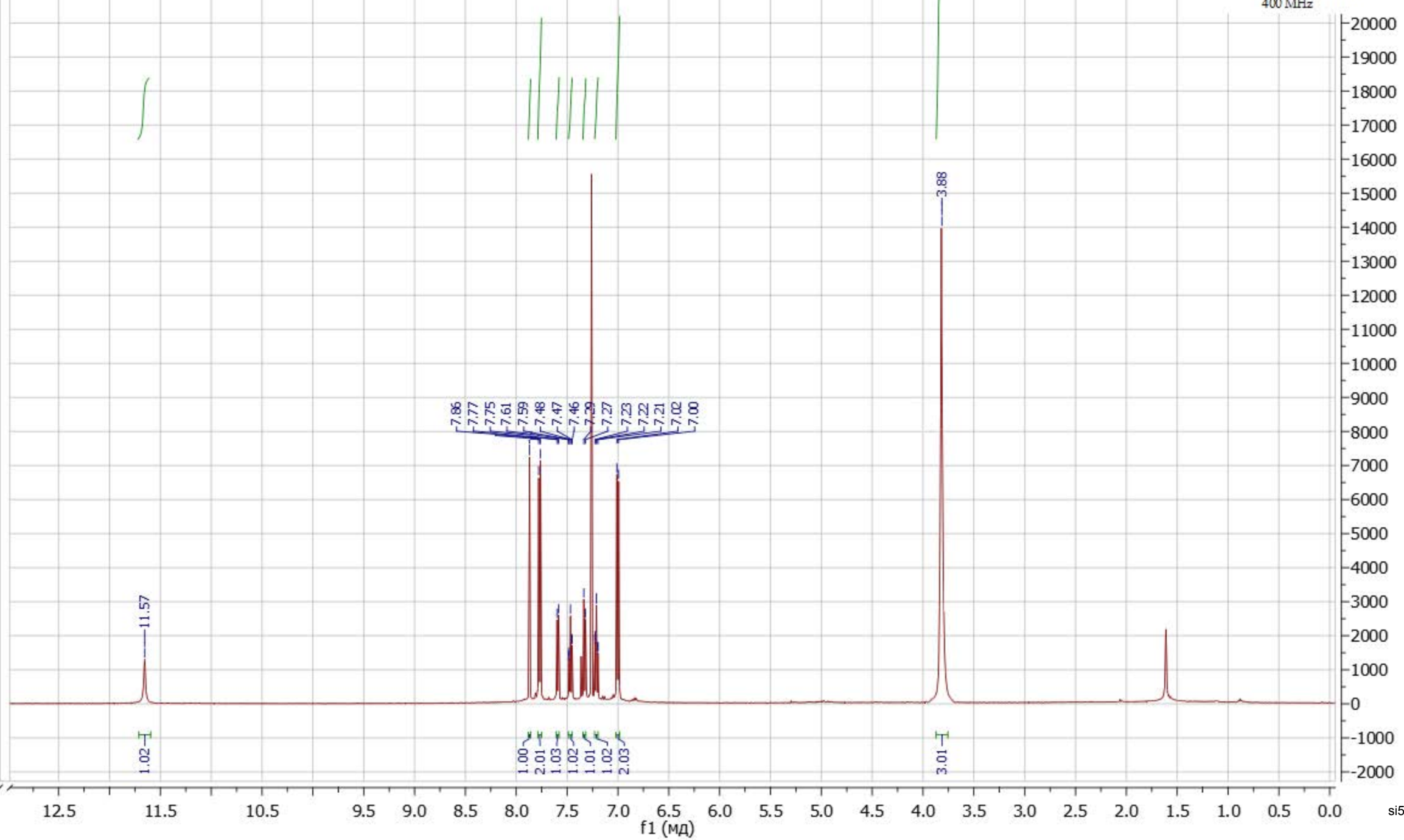






6ab

¹H NMR - CDCl₃
400 MHz



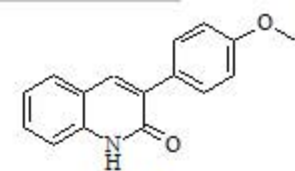
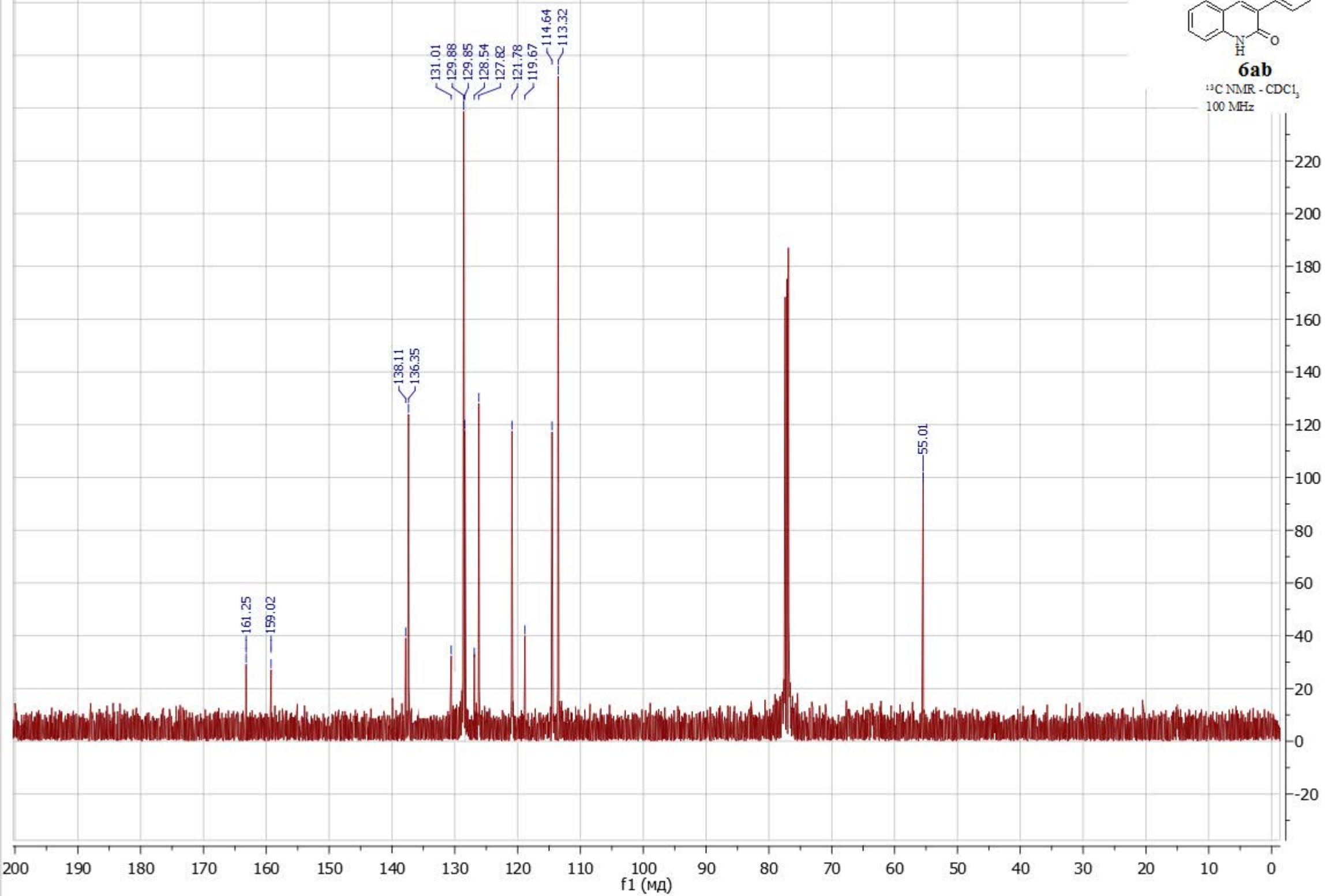
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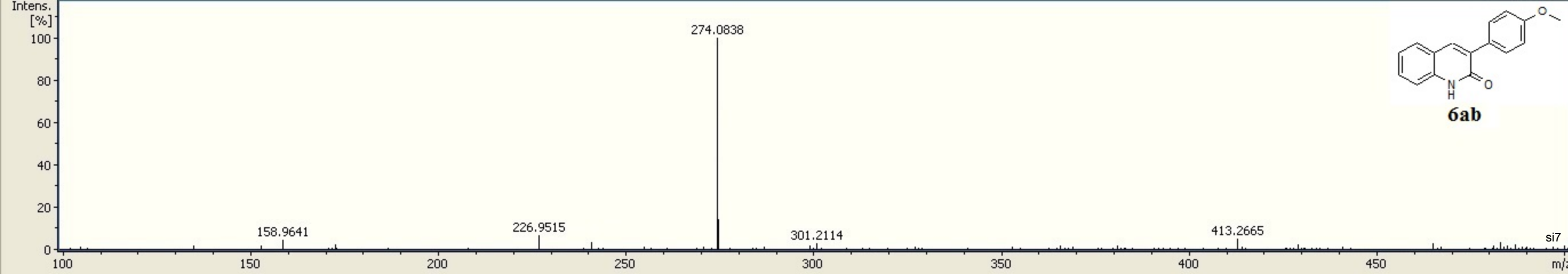
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7.77
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7.00

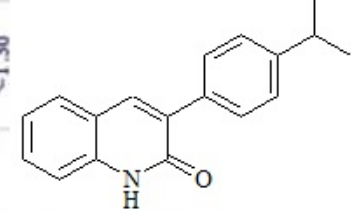
1.00
2.01
1.03
1.02
1.01
1.02
2.03

3.88
3.01

12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 f1 (ppm) si5

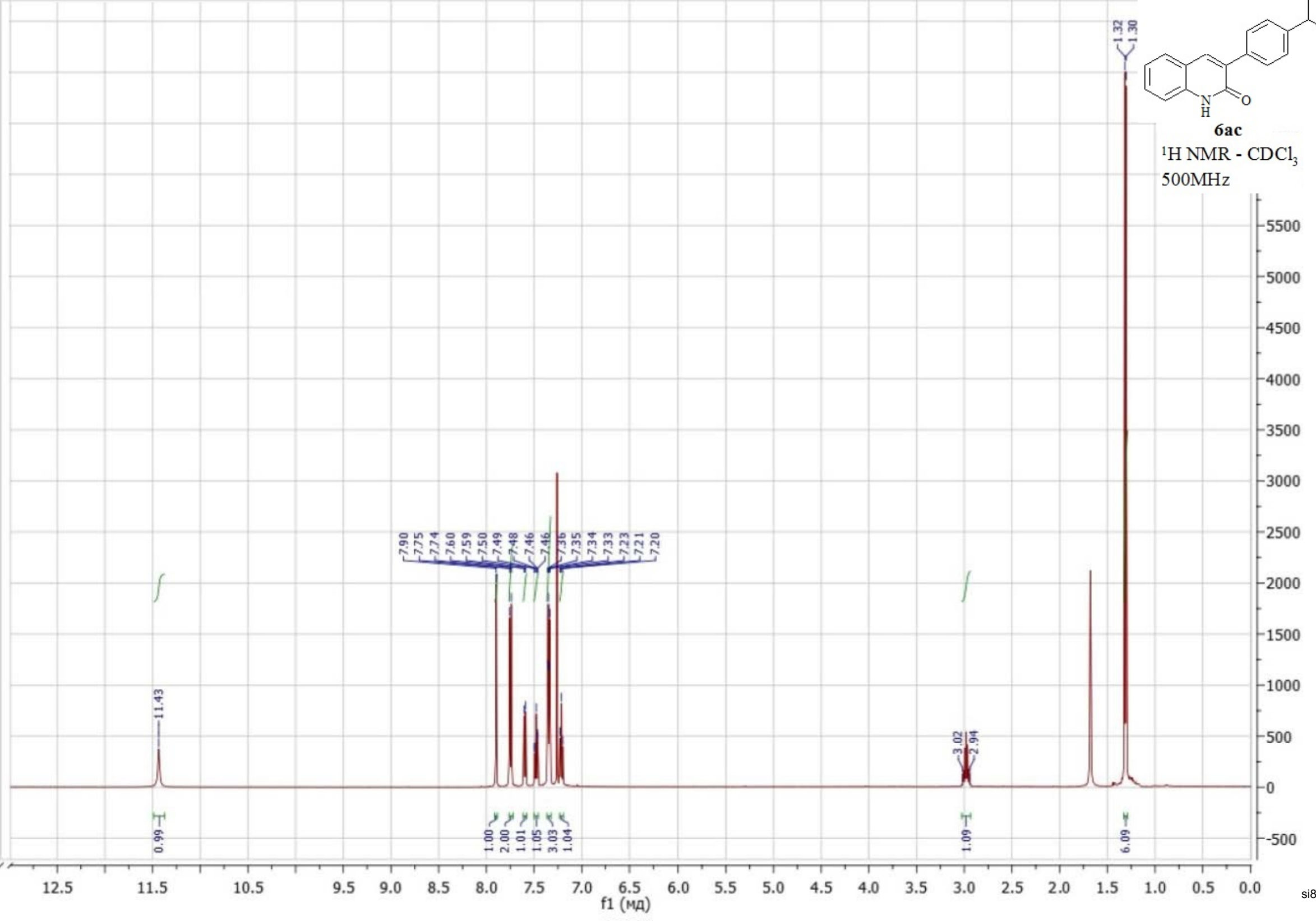
**6ab**¹³C NMR - CDCl₃
100 MHz

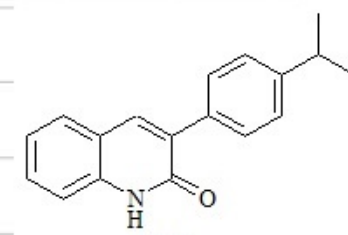




6ac

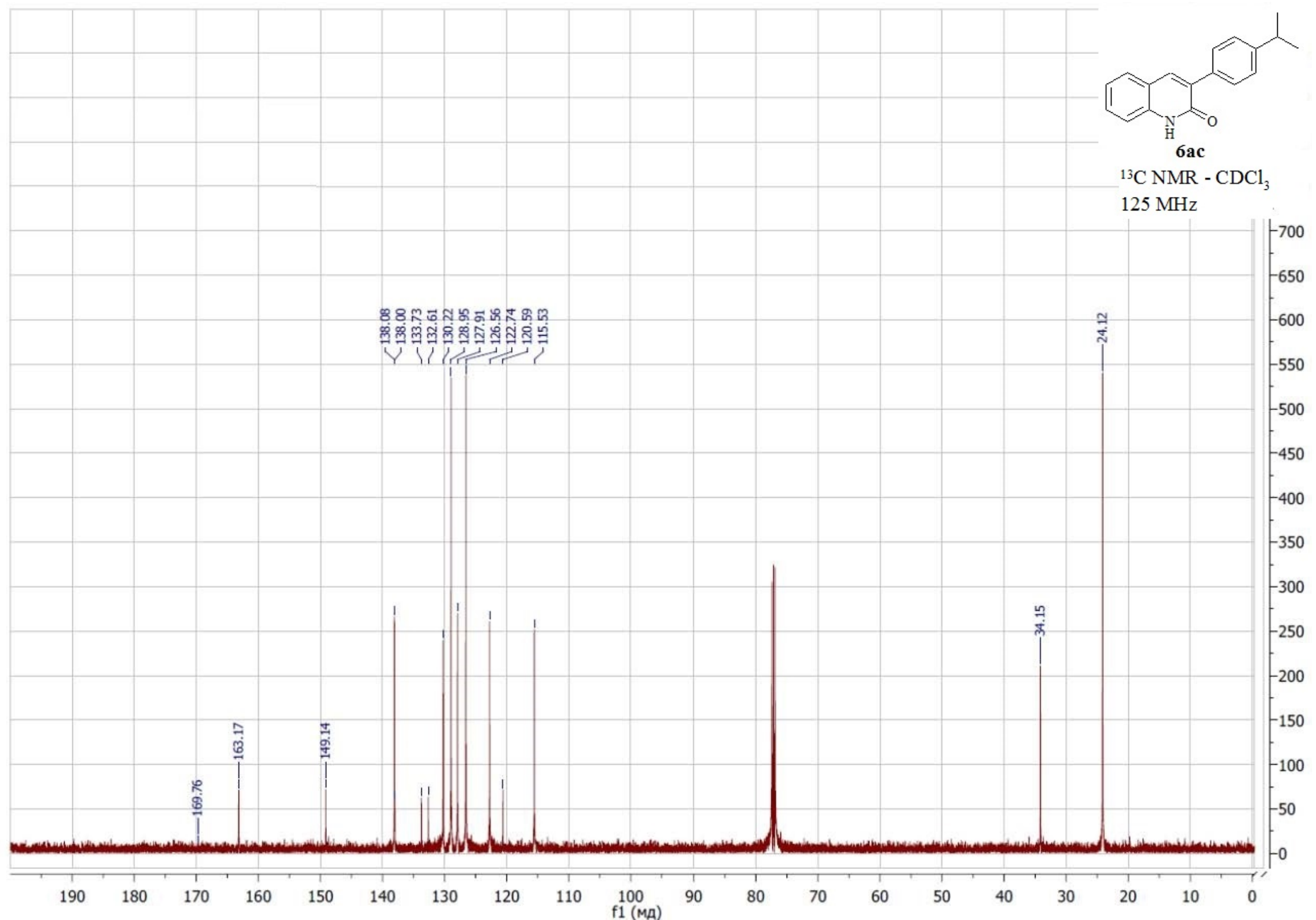
¹H NMR - CDCl₃
500MHz

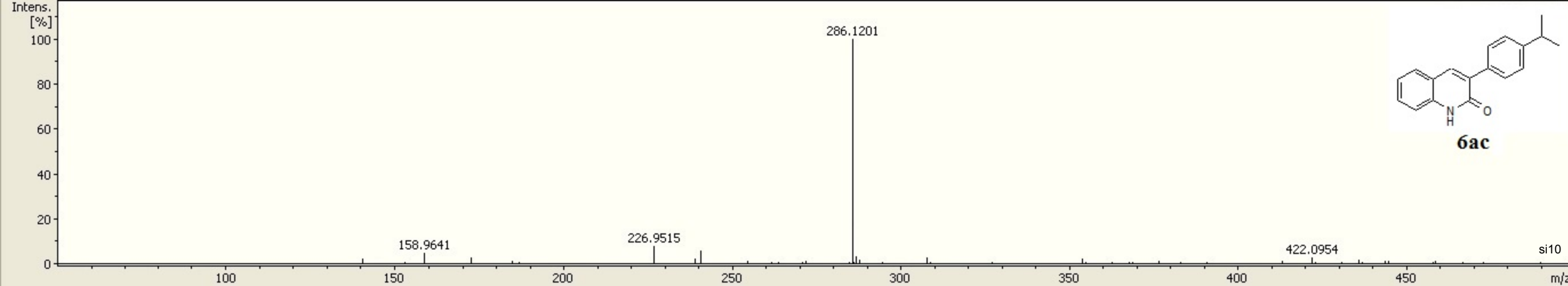


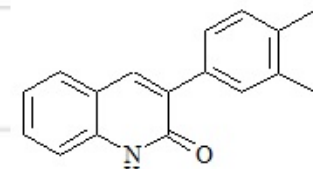


6ac

¹³C NMR - CDCl₃
125 MHz

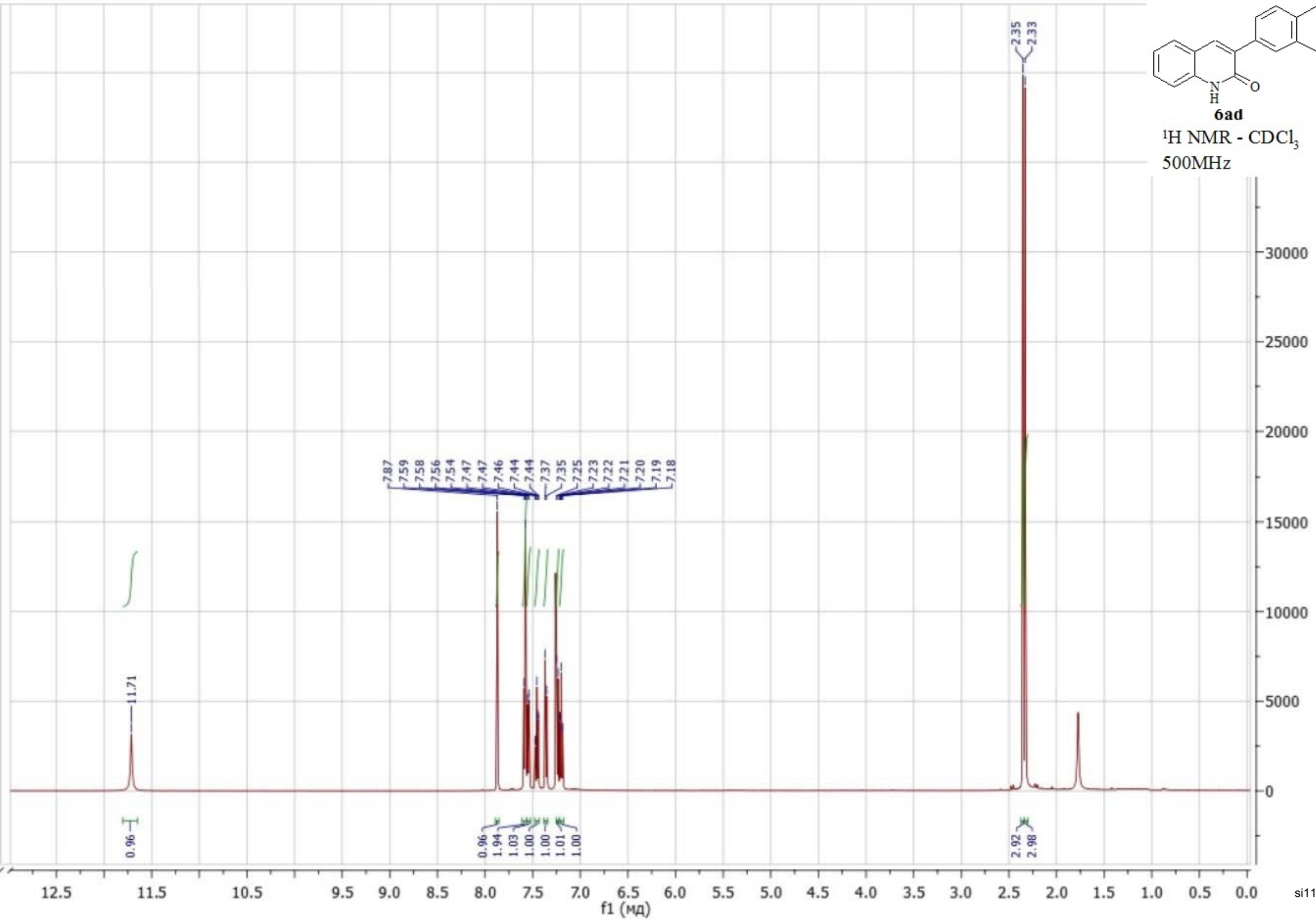


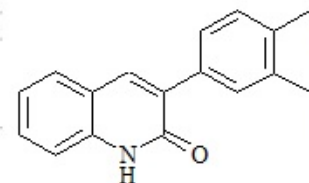




6ad

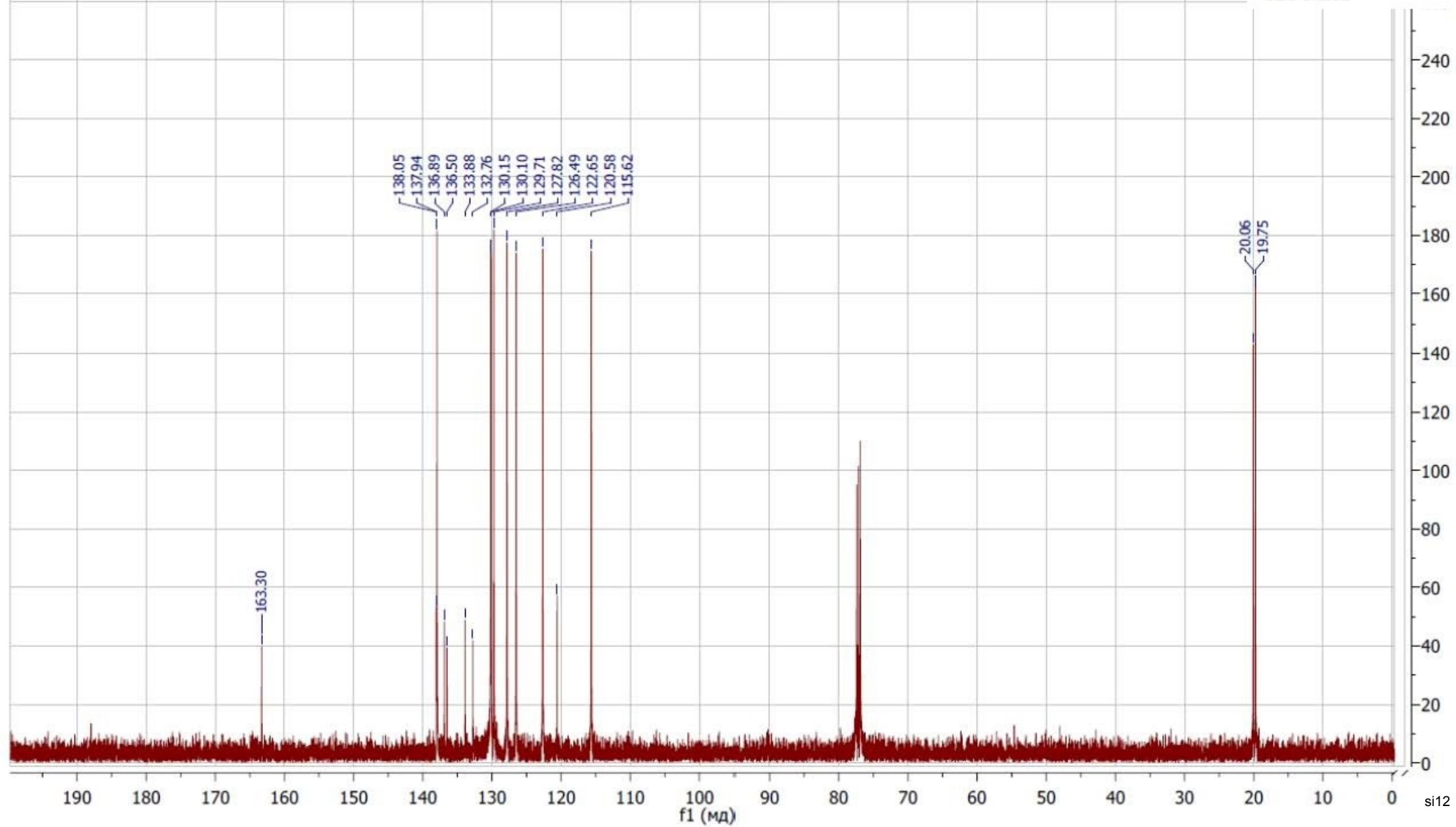
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500MHz

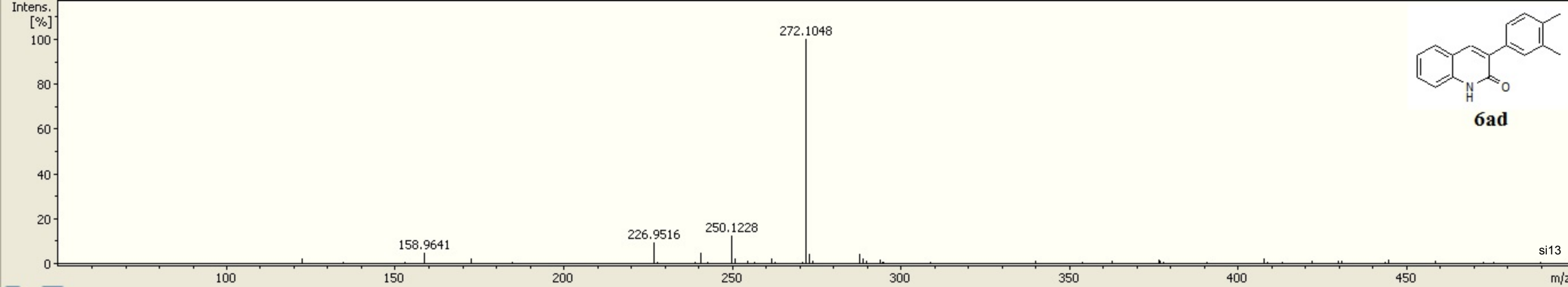


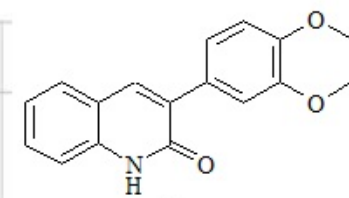


6ad

^{13}C NMR - CDCl_3
125 MHz



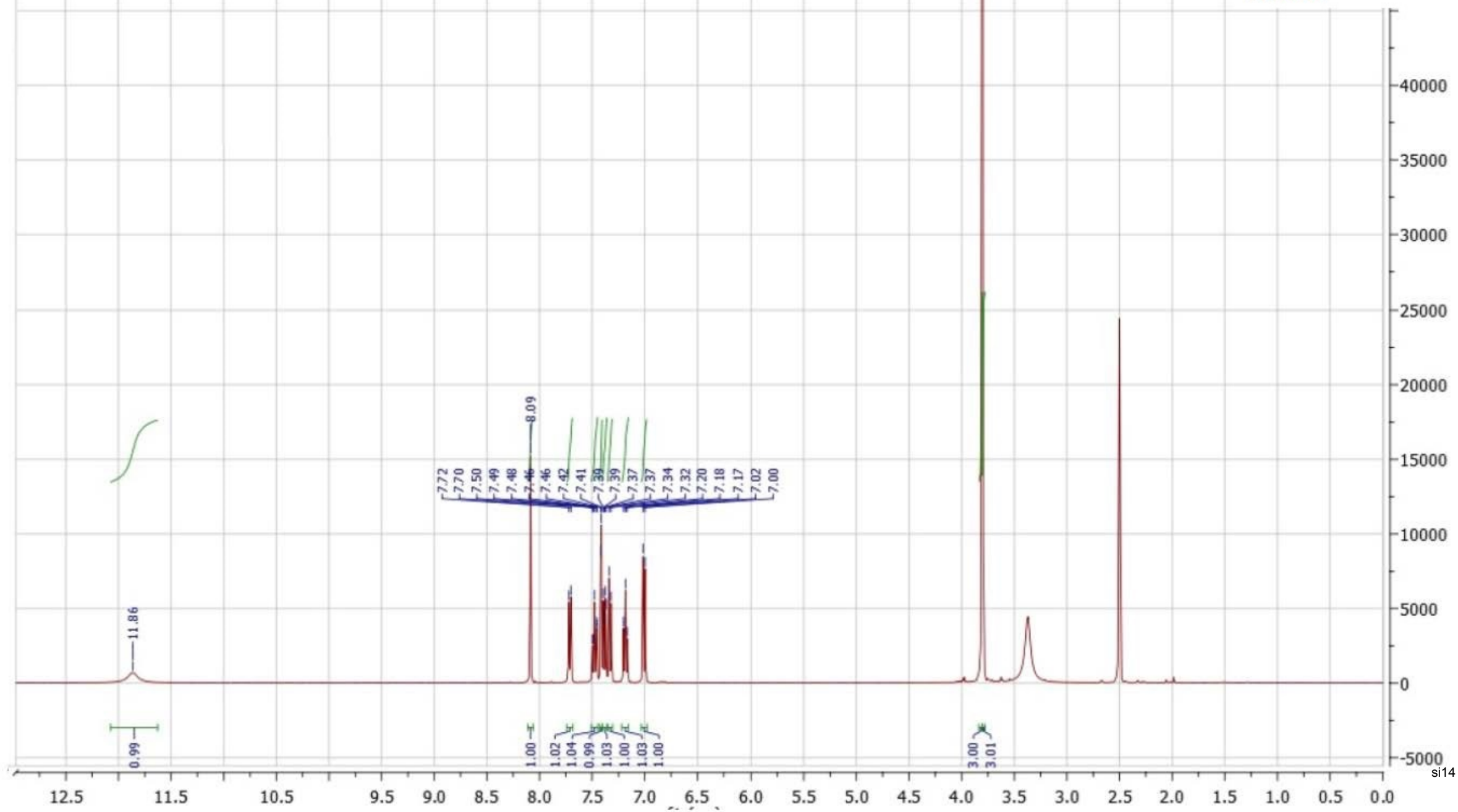


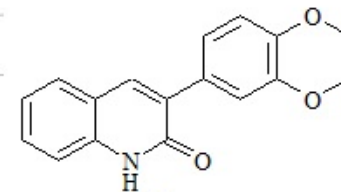


6ae

^1H NMR - DMSO-d_6

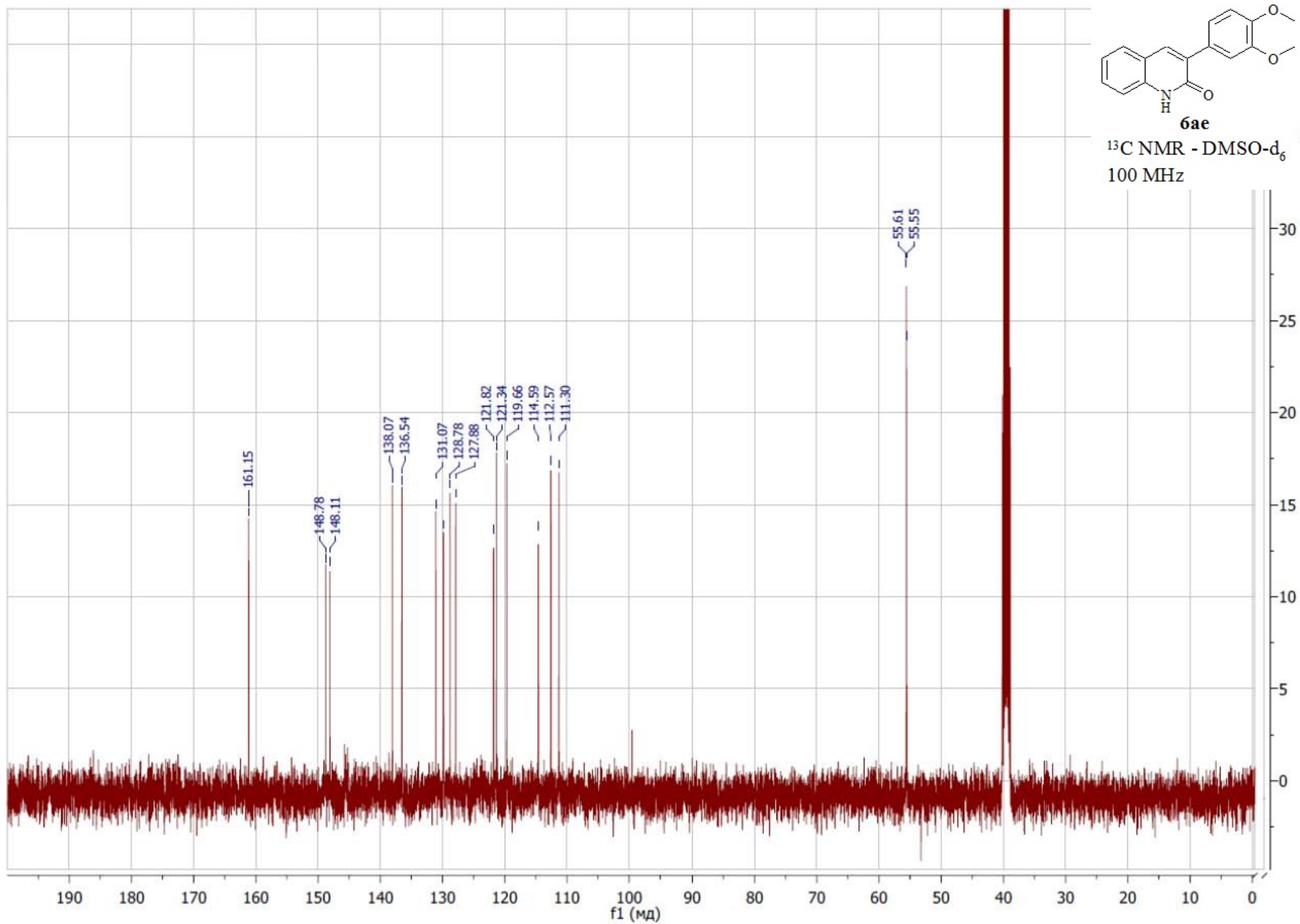
400MHz

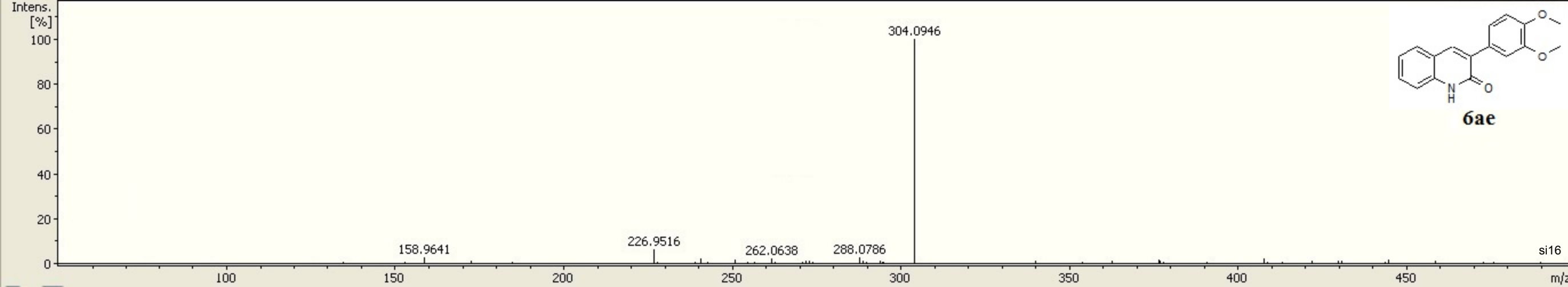


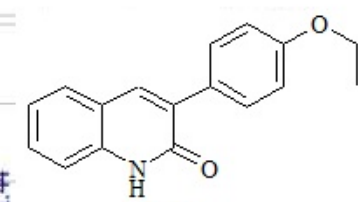


6ae

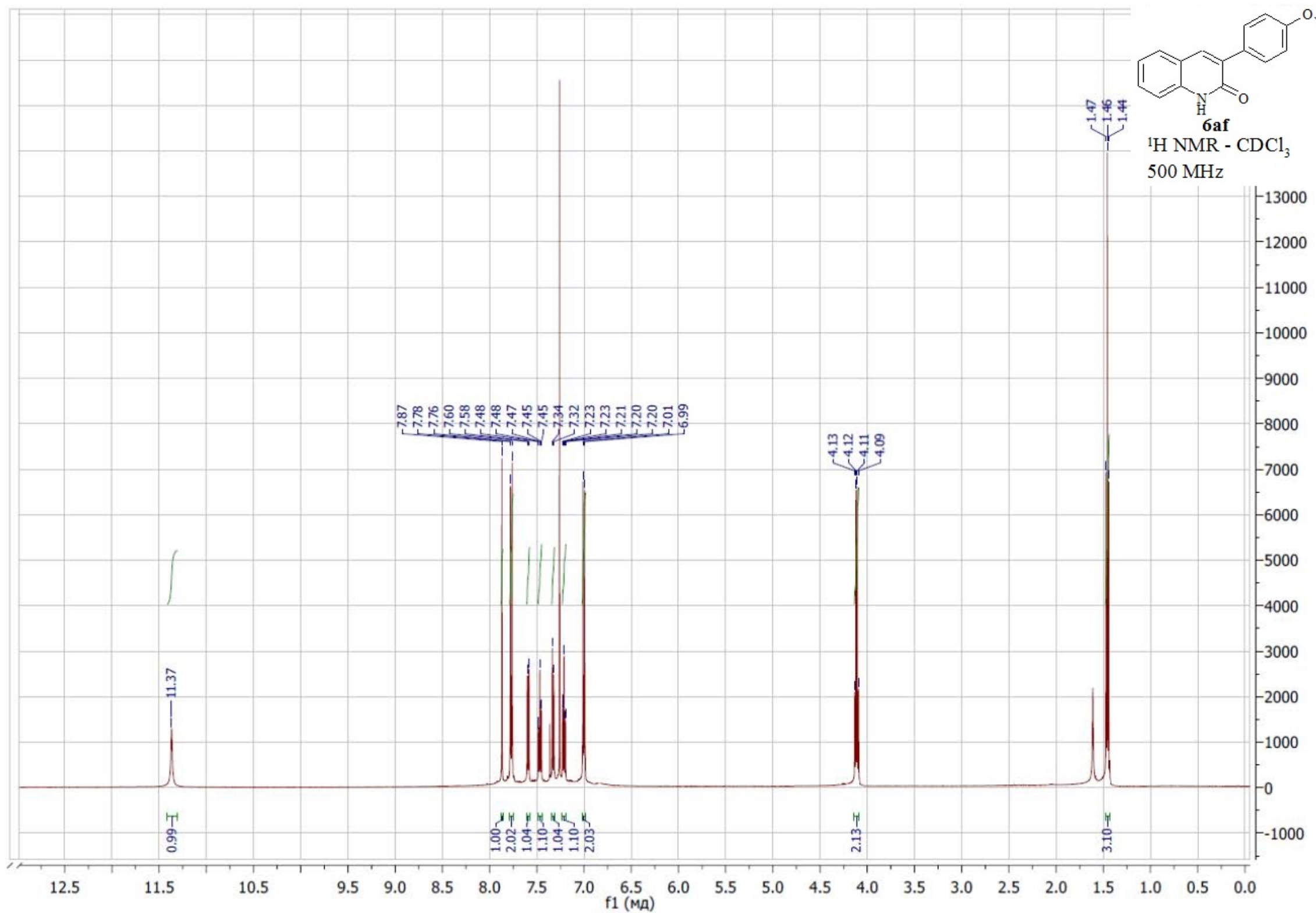
^{13}C NMR - DMSO- d_6
100 MHz

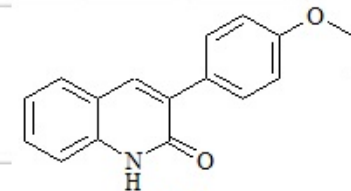






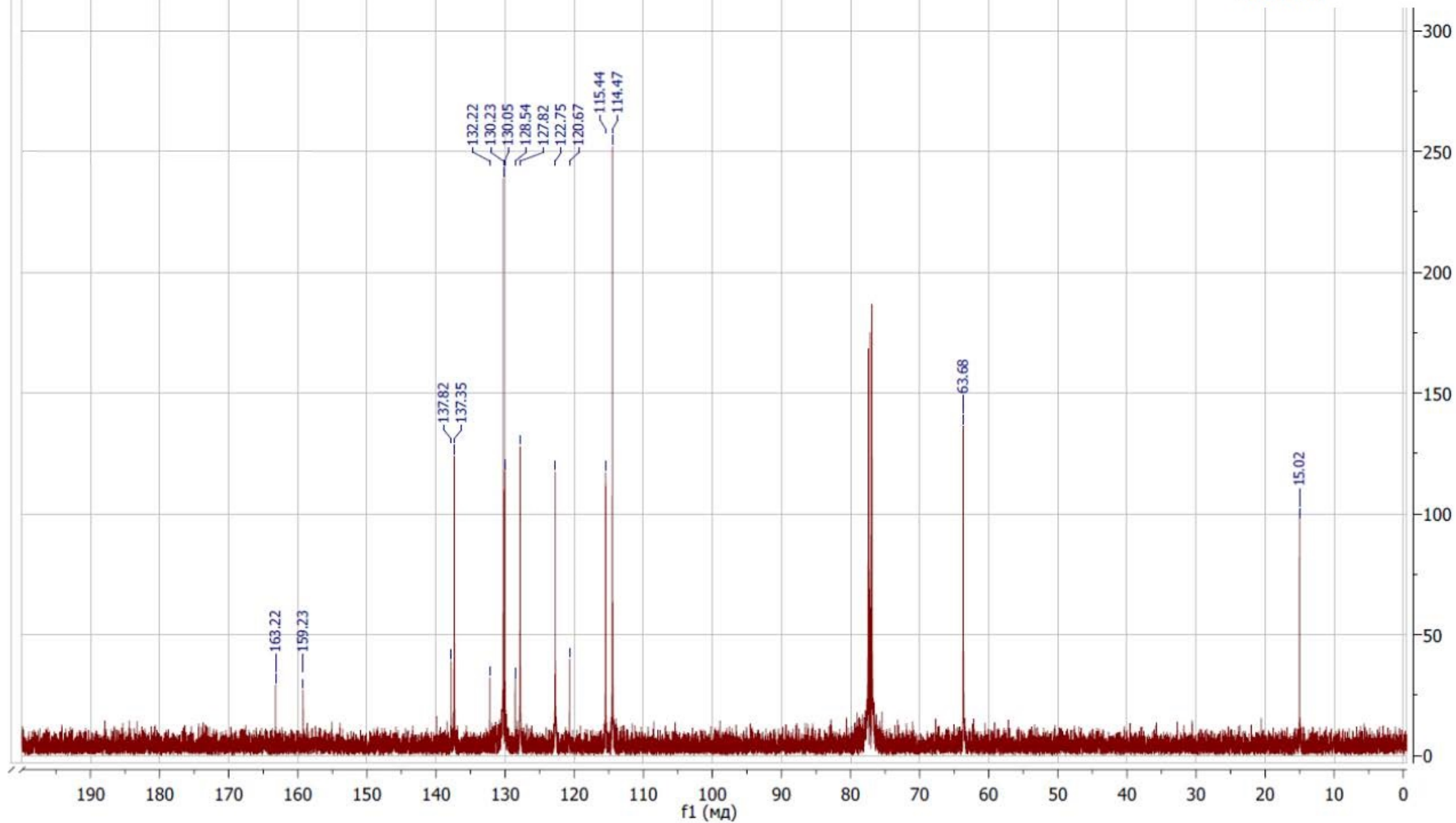
6af
¹H NMR - CDCl₃
500 MHz

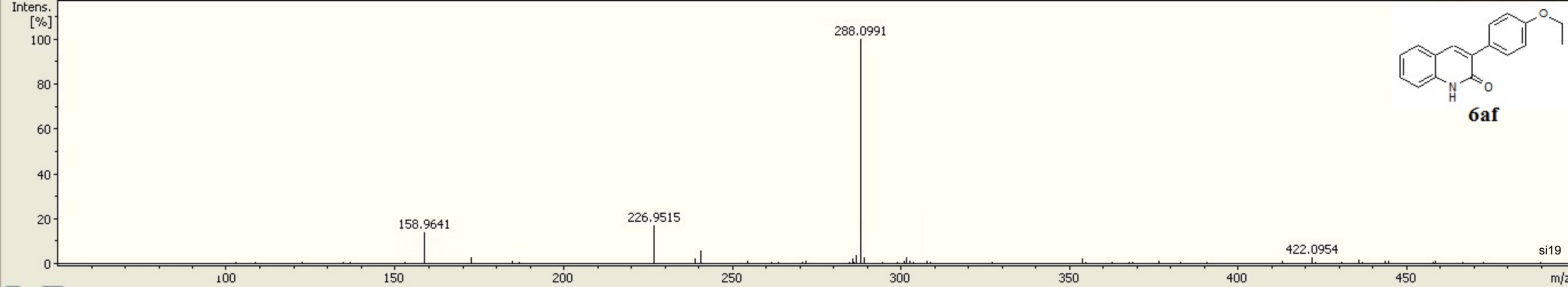


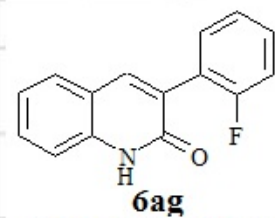


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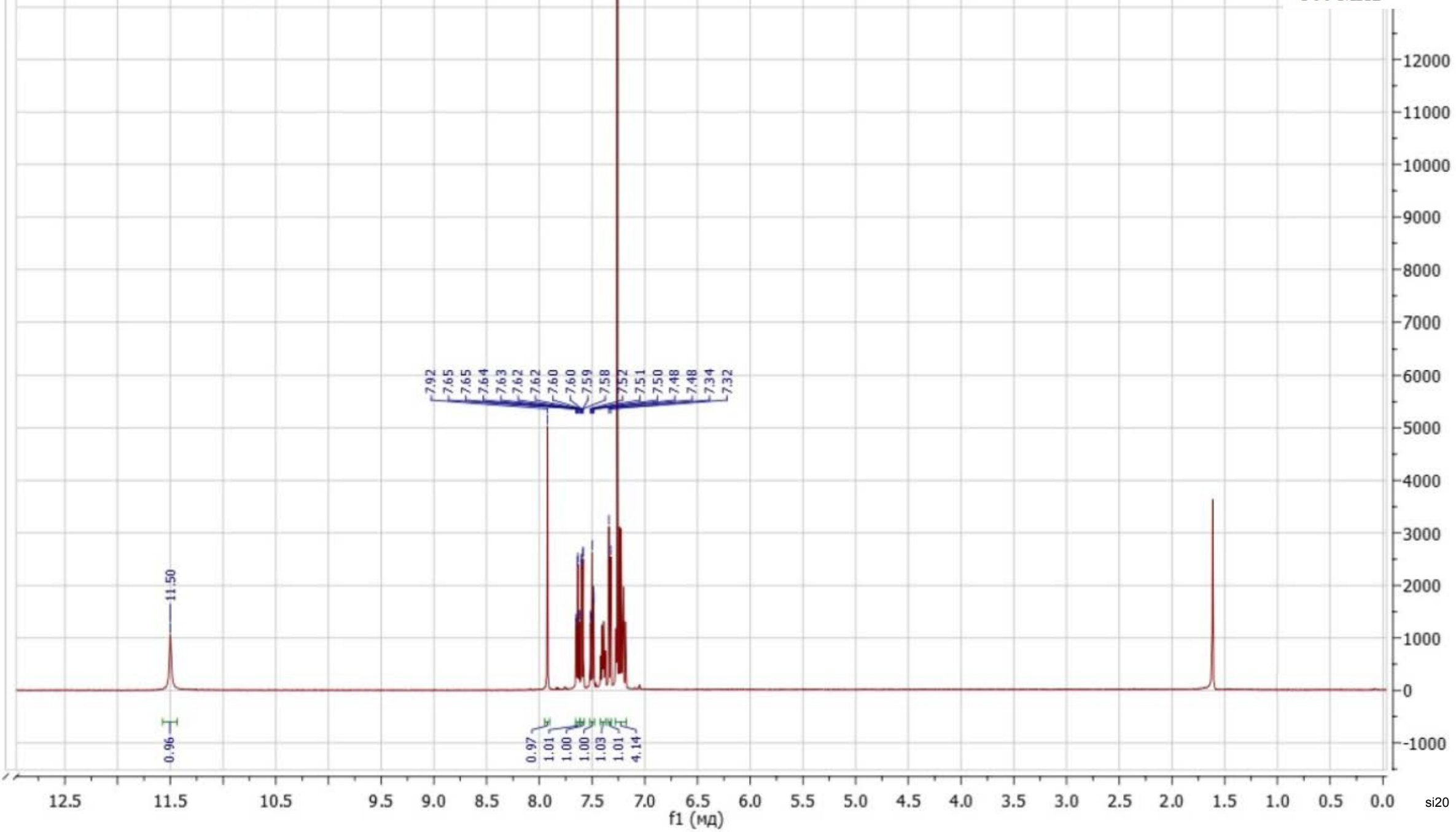
^{13}C NMR - CDCl_3
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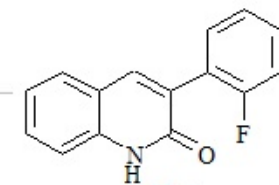






^1H NMR - CDCl_3
500 MHz

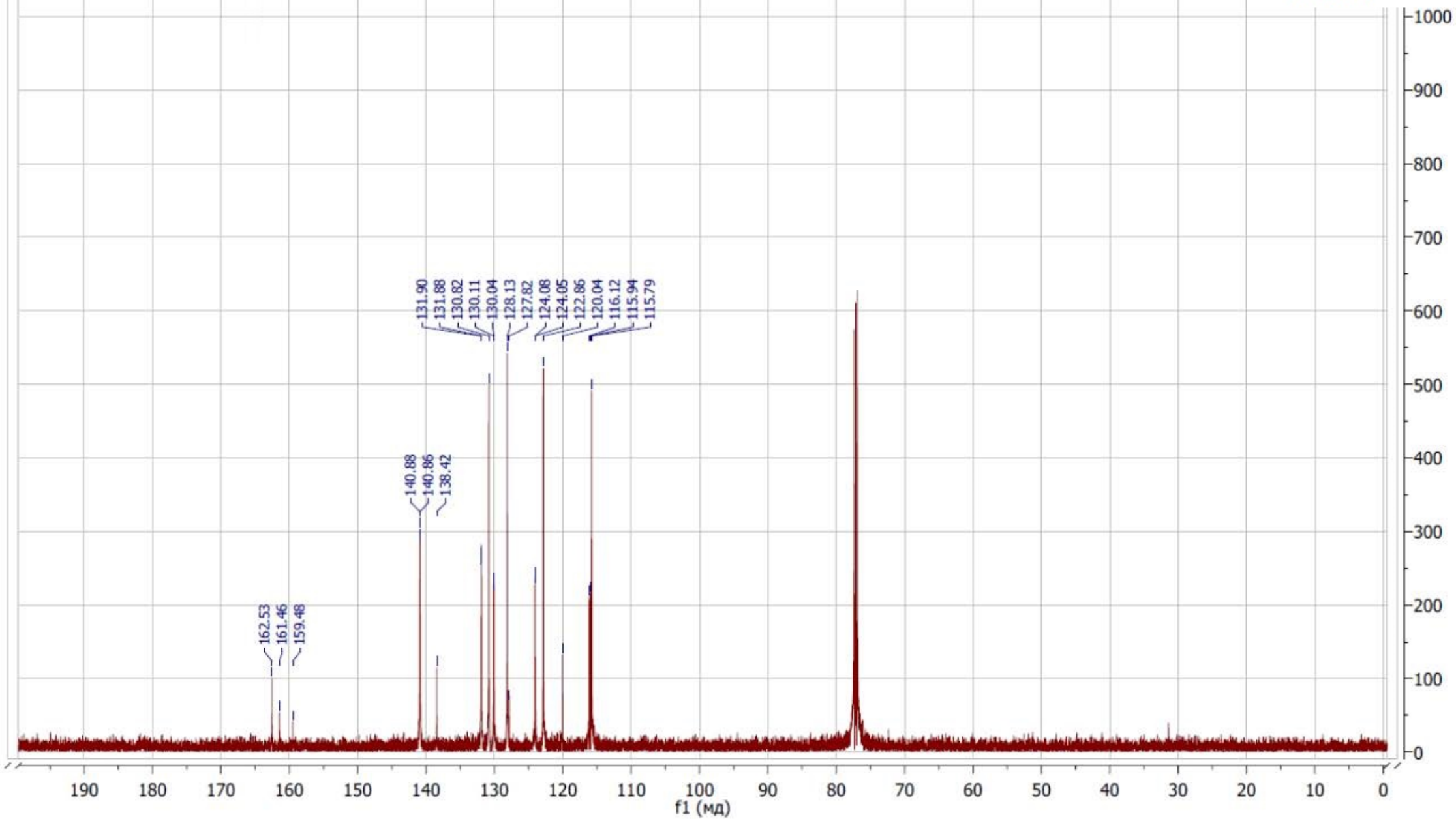


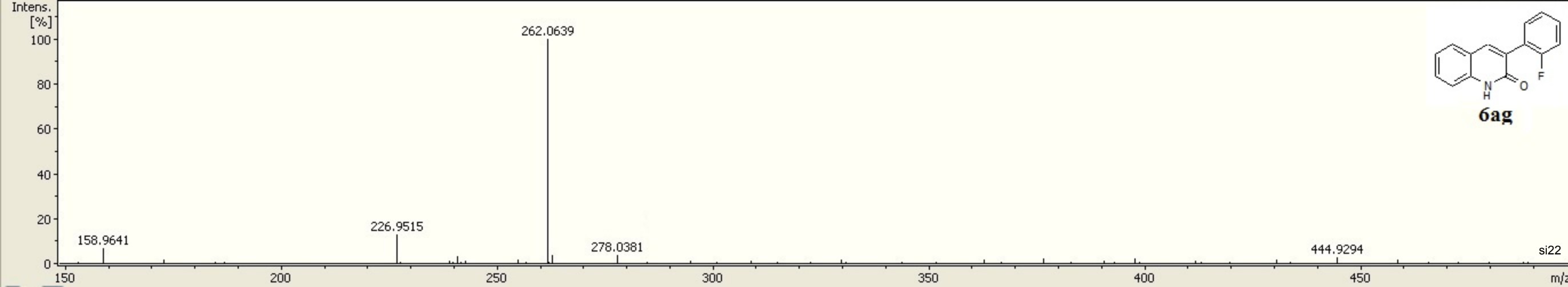


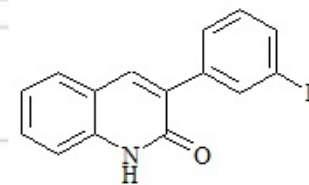
6ag

^{13}C NMR - CDCl_3

125 MHz



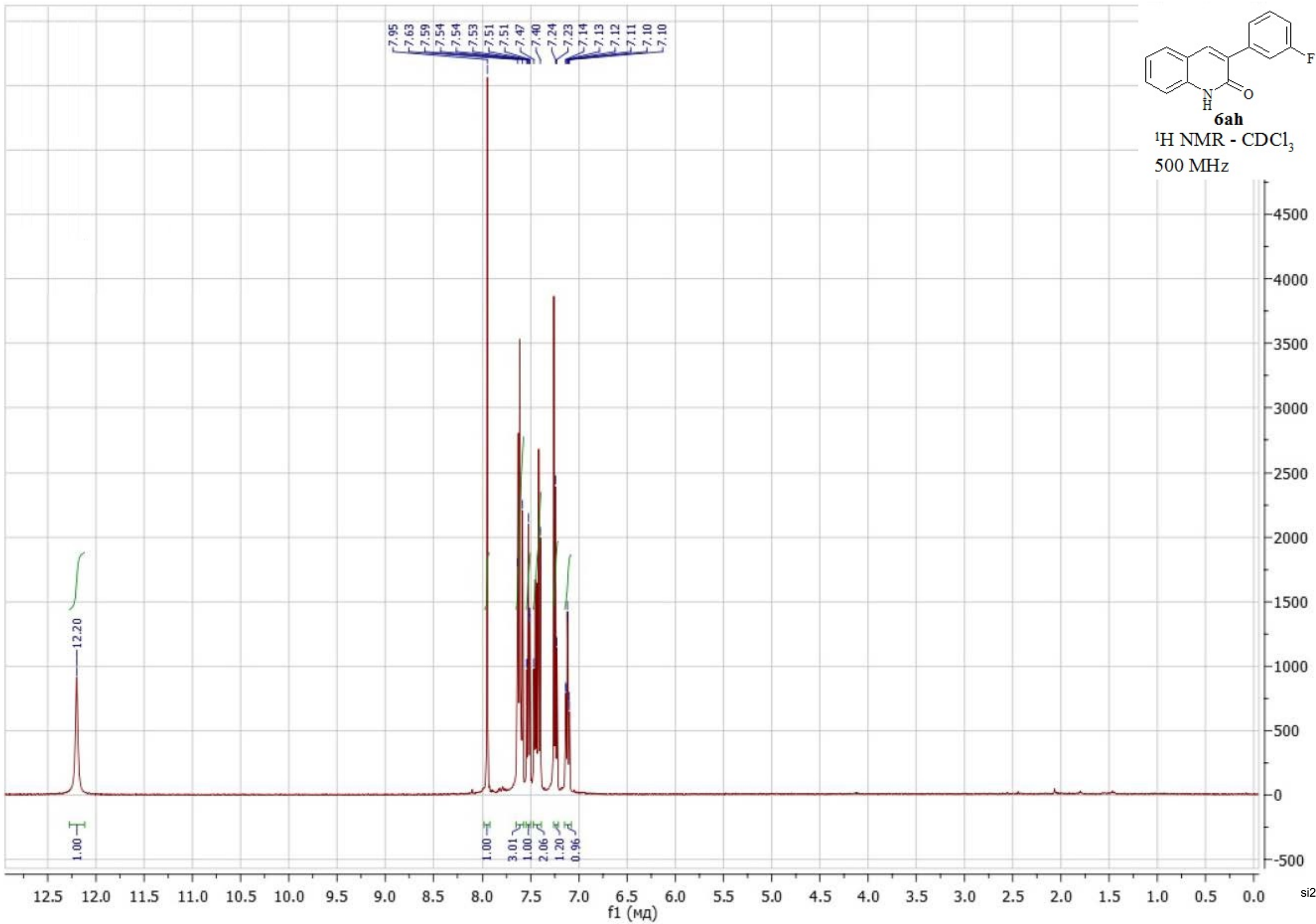


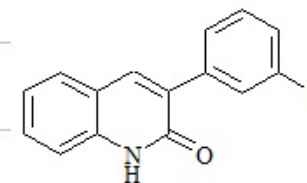


6ah

¹H NMR - CDCl₃

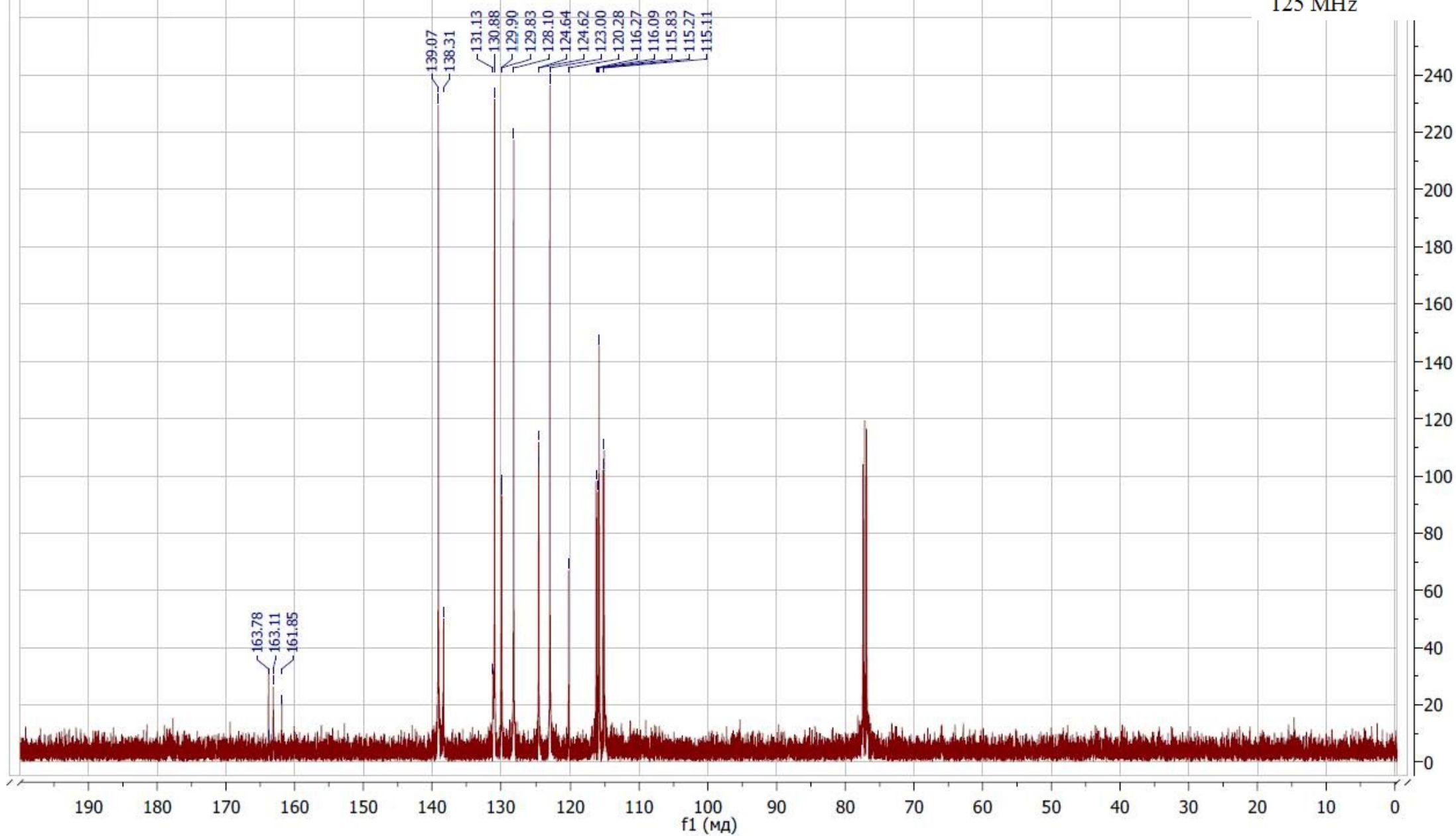
500 MHz

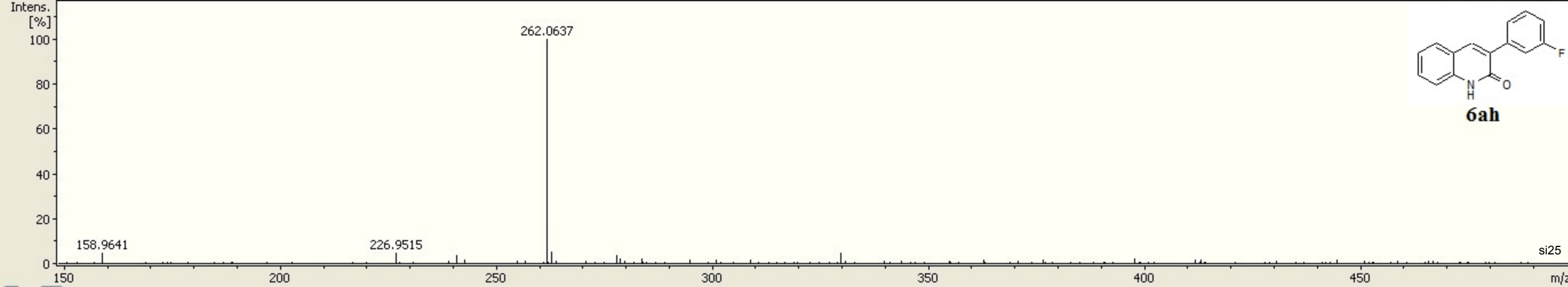


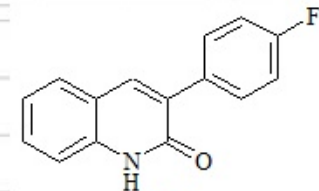


6ah

^{13}C NMR - CDCl_3
125 MHz

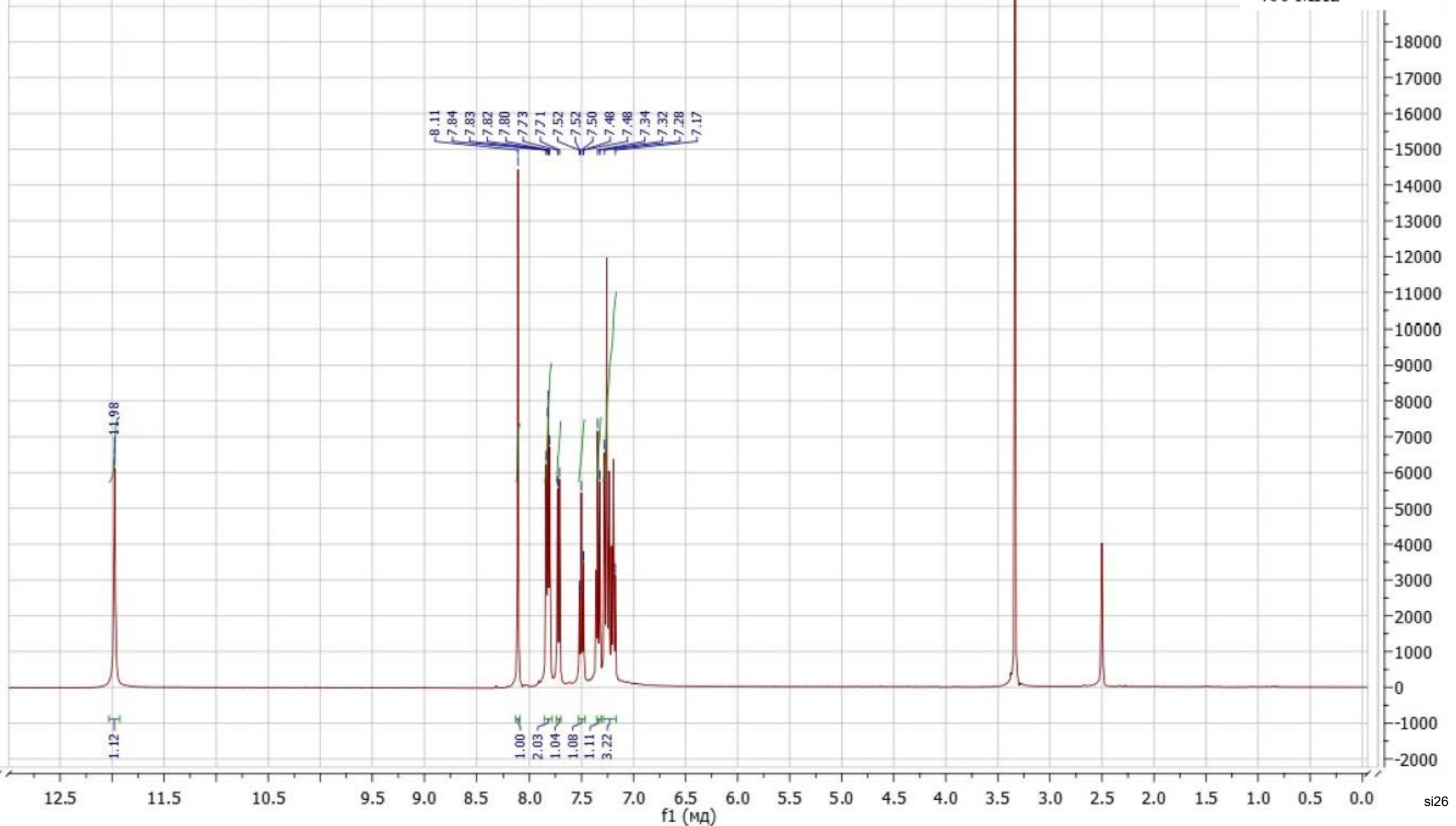


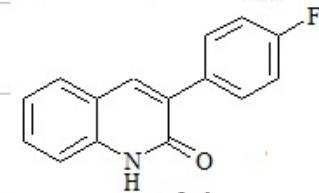




6ai

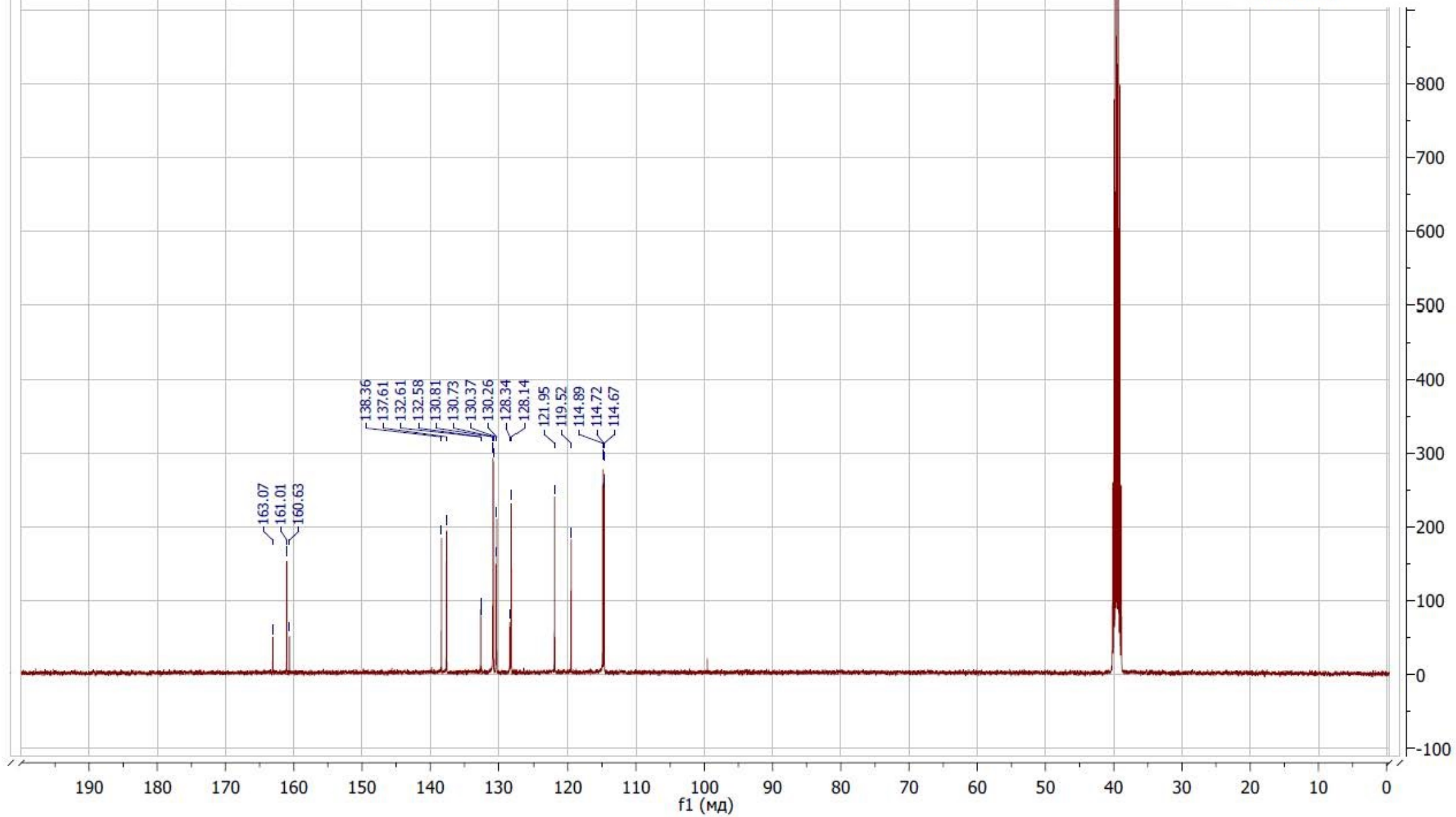
¹H NMR - DMSO-d₆
400 MHz

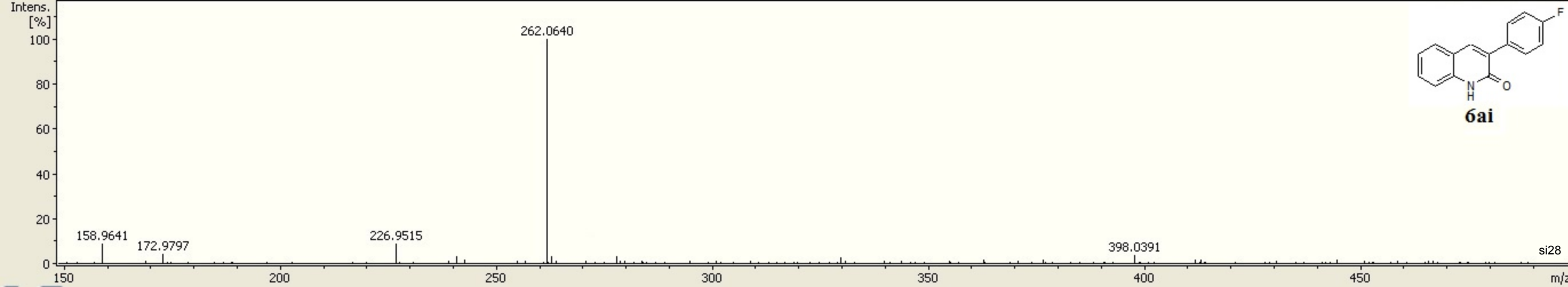


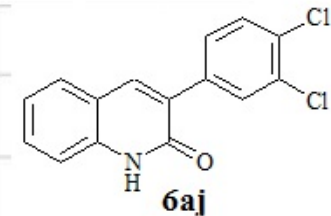


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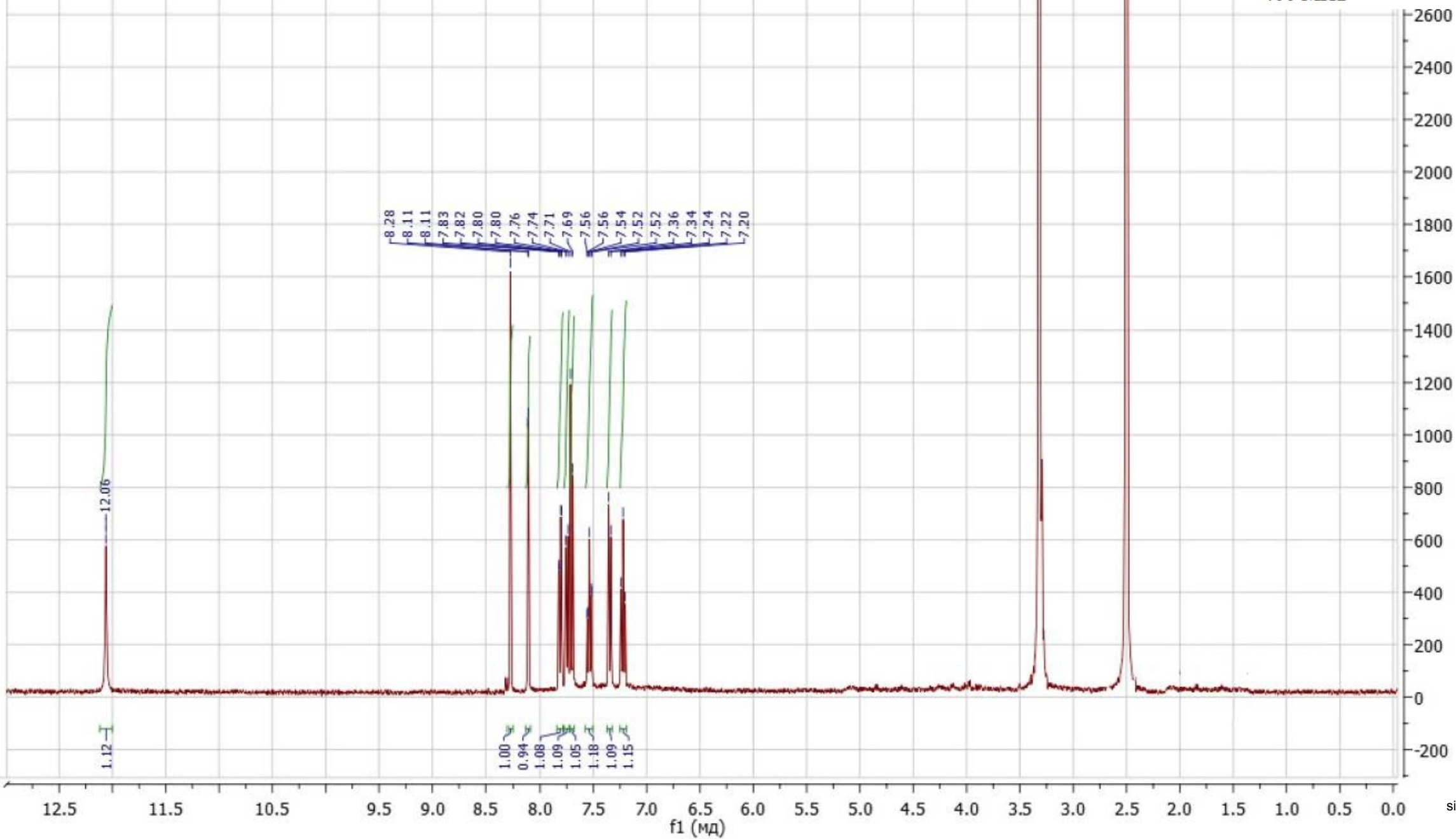
^{13}C NMR - DMSO- d_6
100 MHz

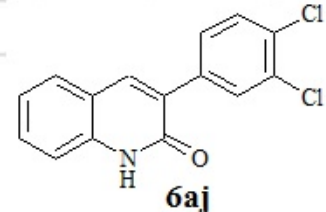






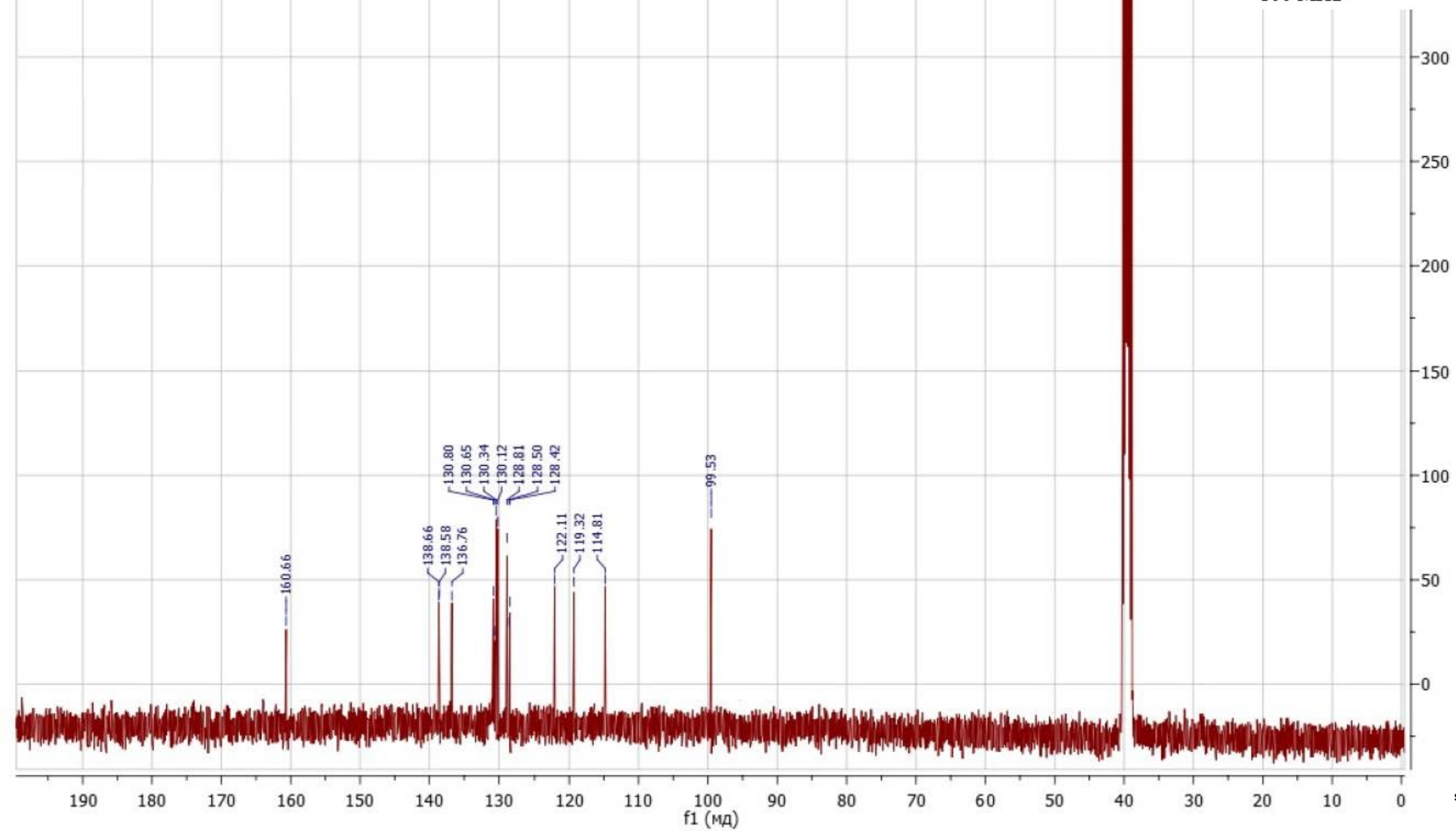
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400 MHz

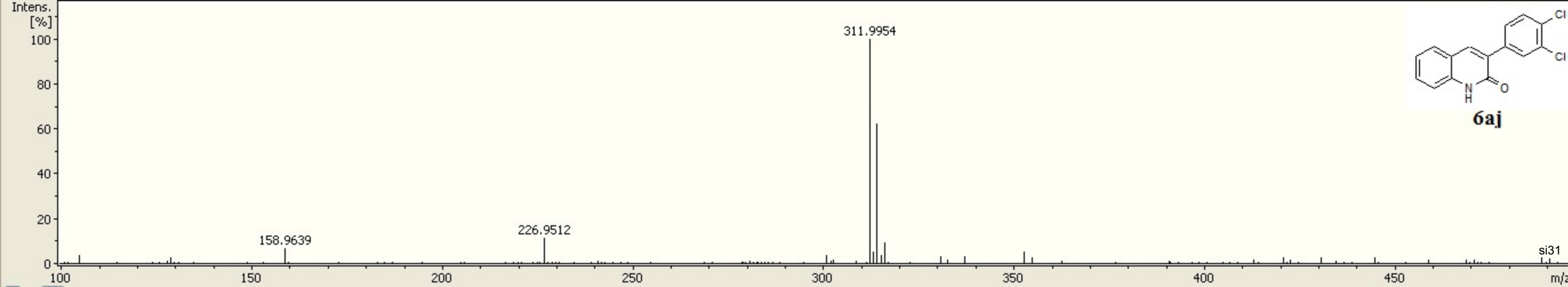


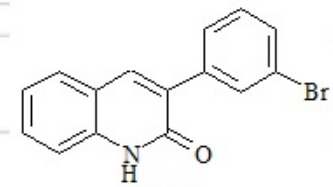


6aj

¹³C NMR - DMSO-d₆
100 MHz

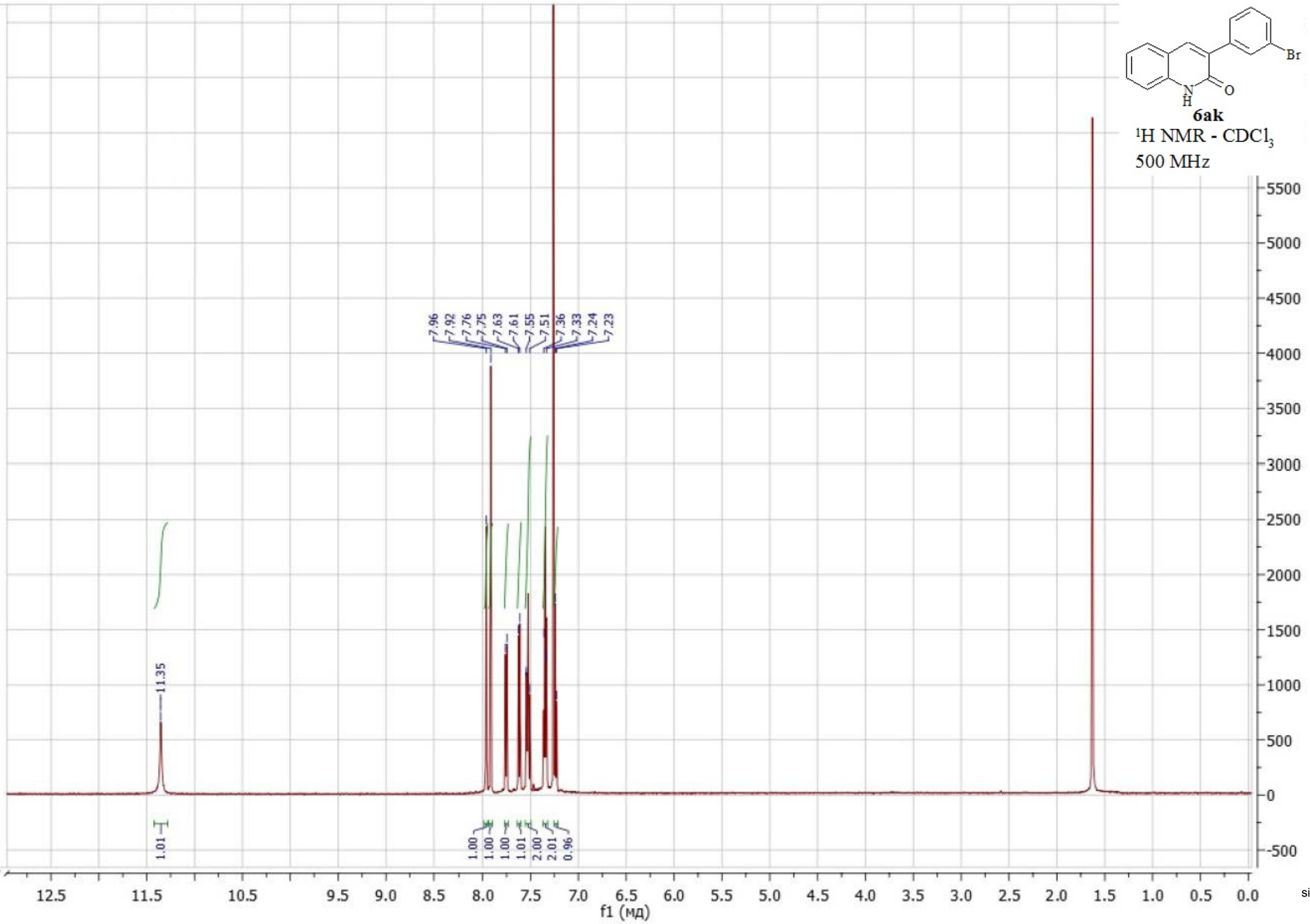


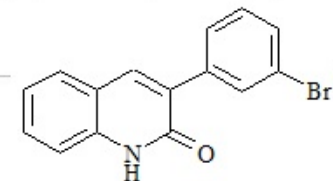




6ak

¹H NMR - CDCl₃
500 MHz

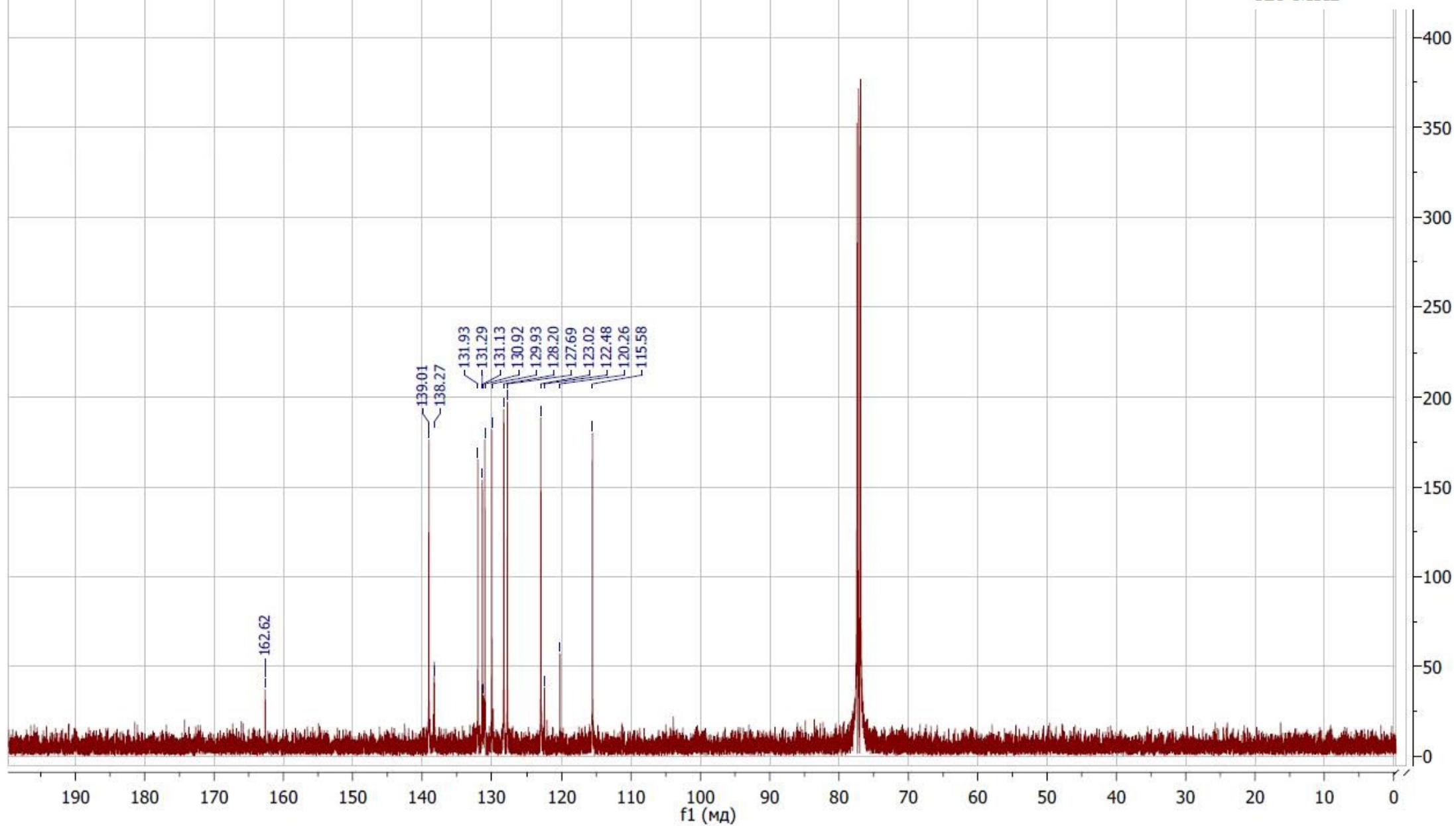


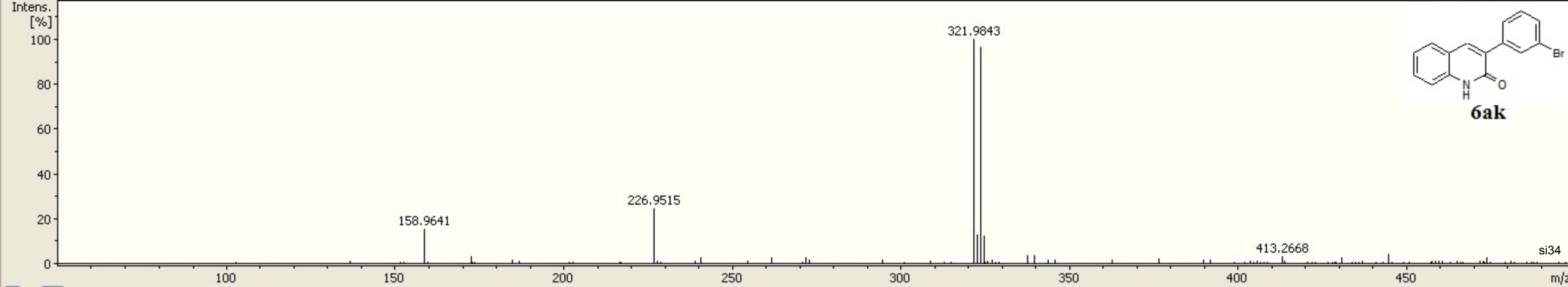


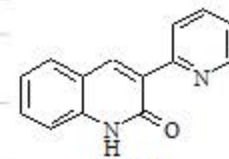
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^{13}C NMR - CDCl_3

125 MHz

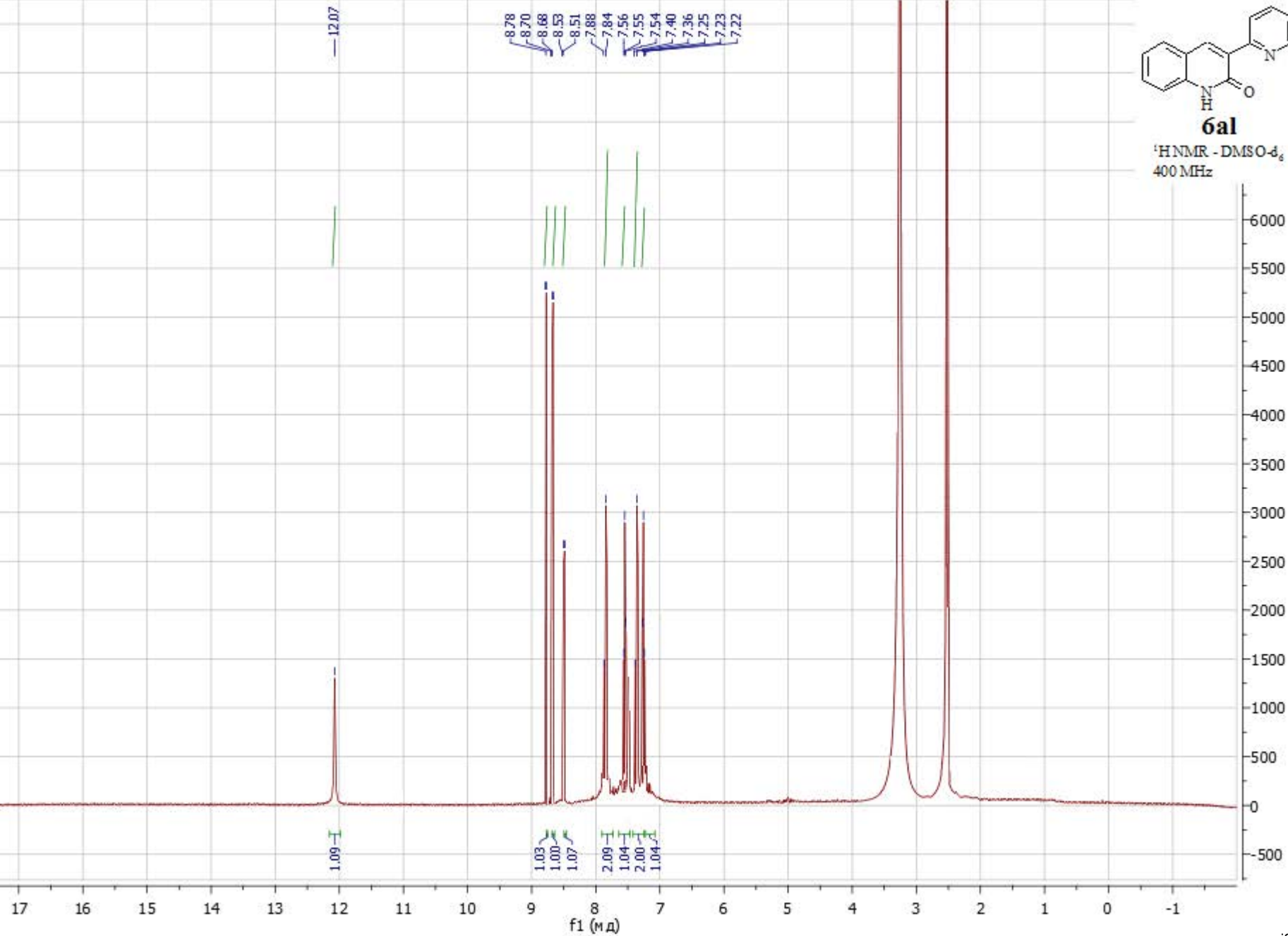


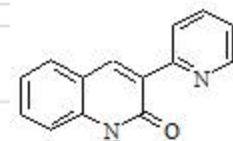




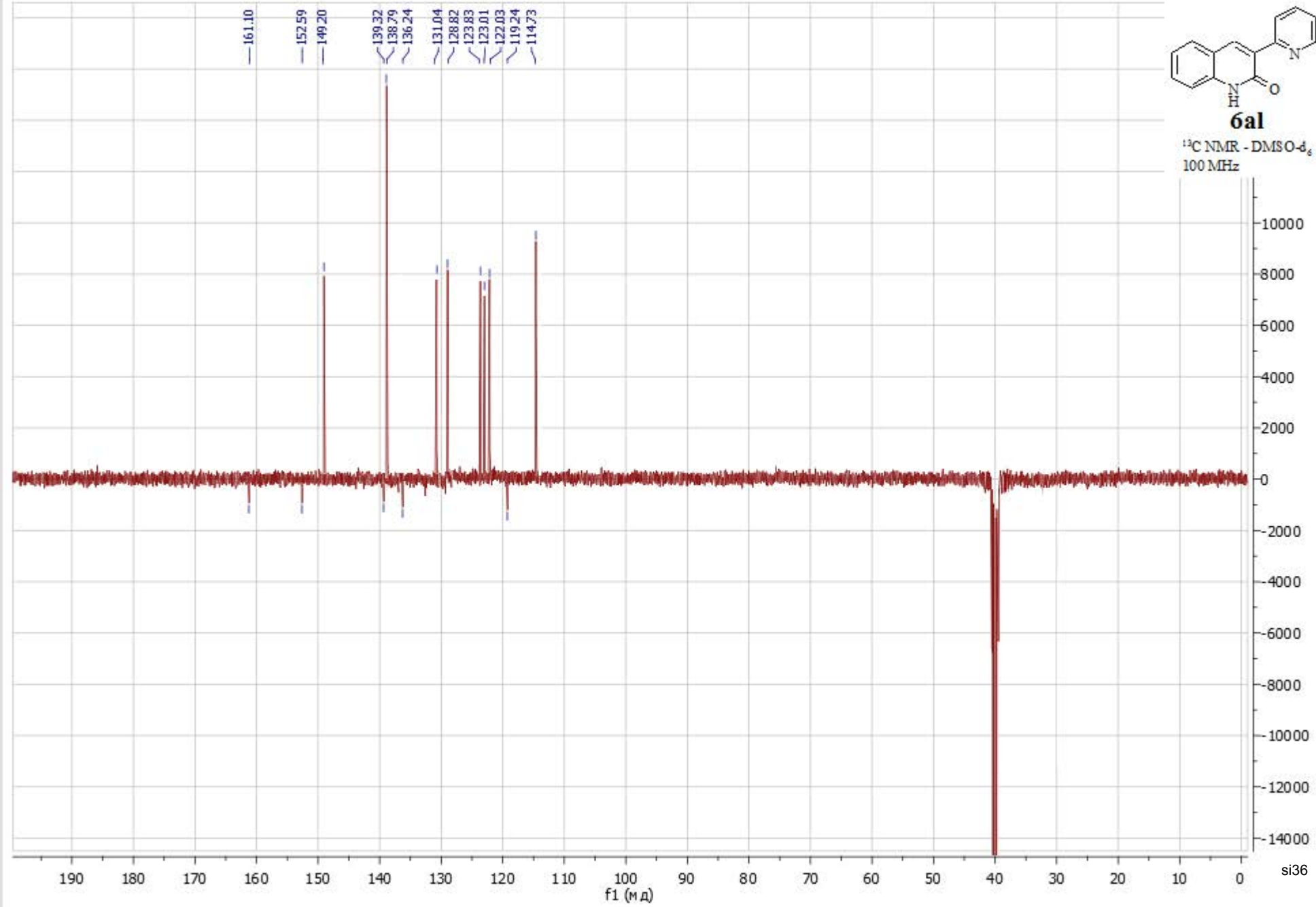
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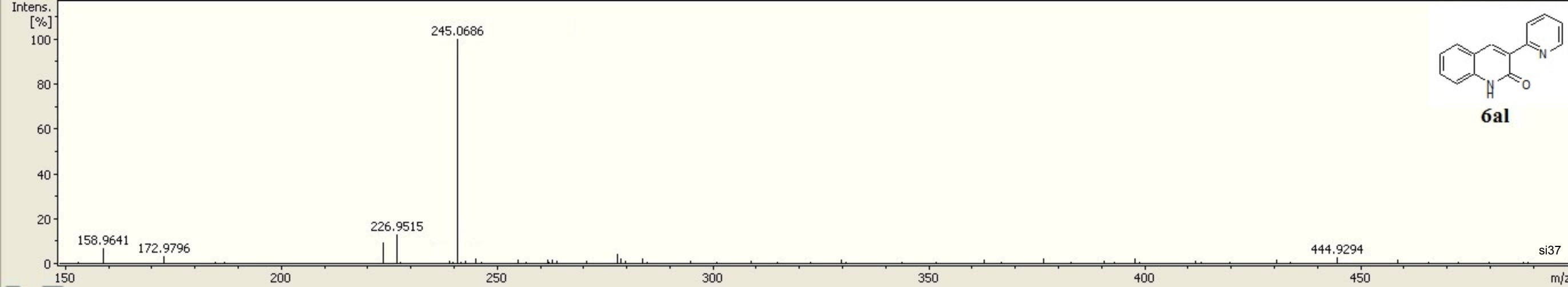
¹H NMR - DMSO-d₆
400 MHz

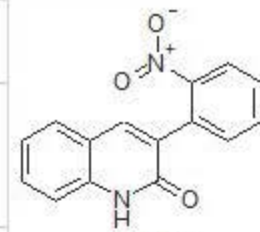


**6al**

¹³C NMR - DMSO-d₆
100 MHz

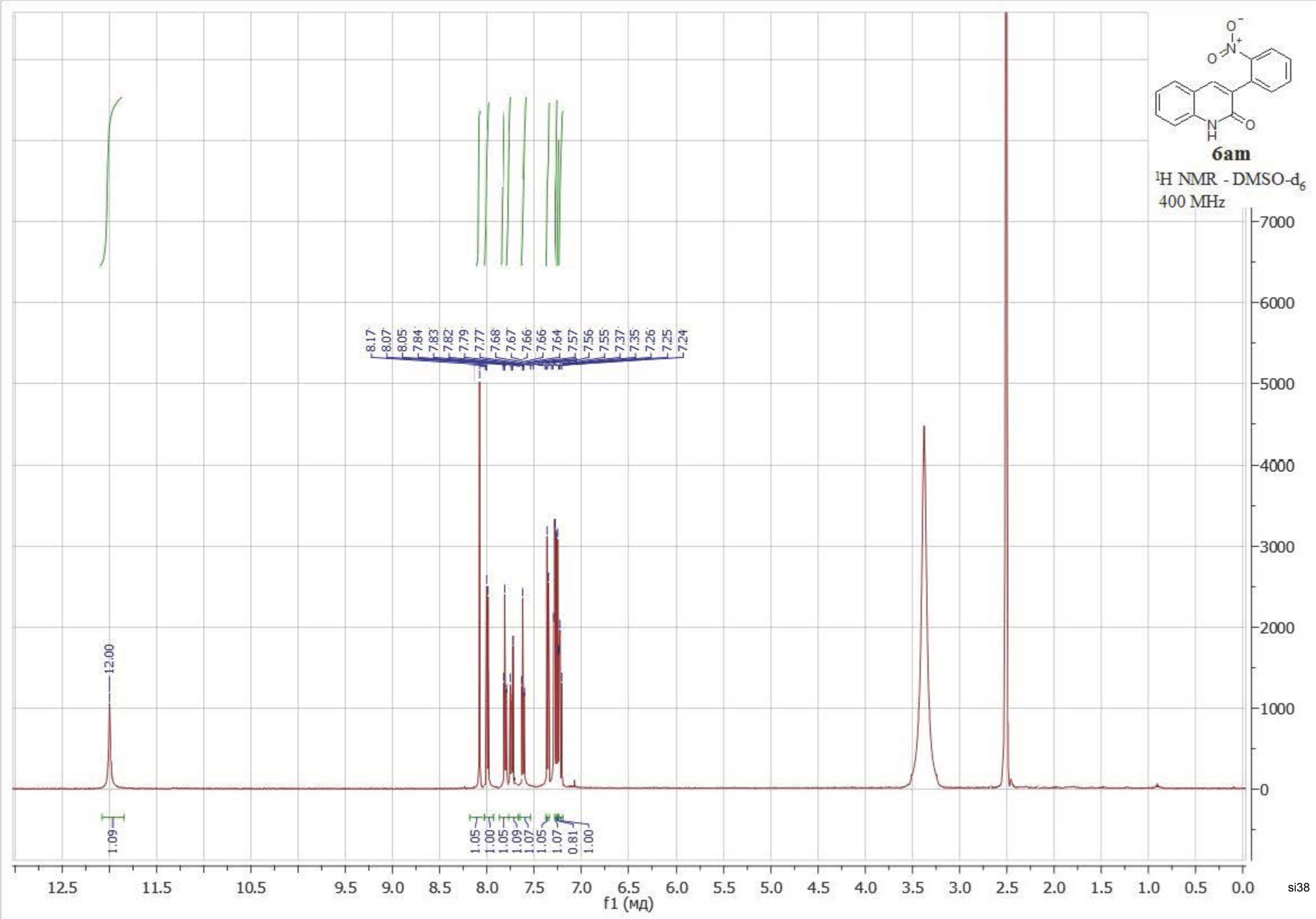


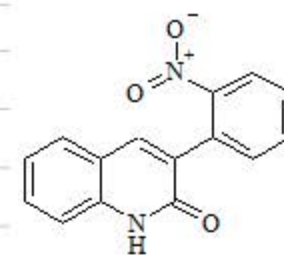




6am

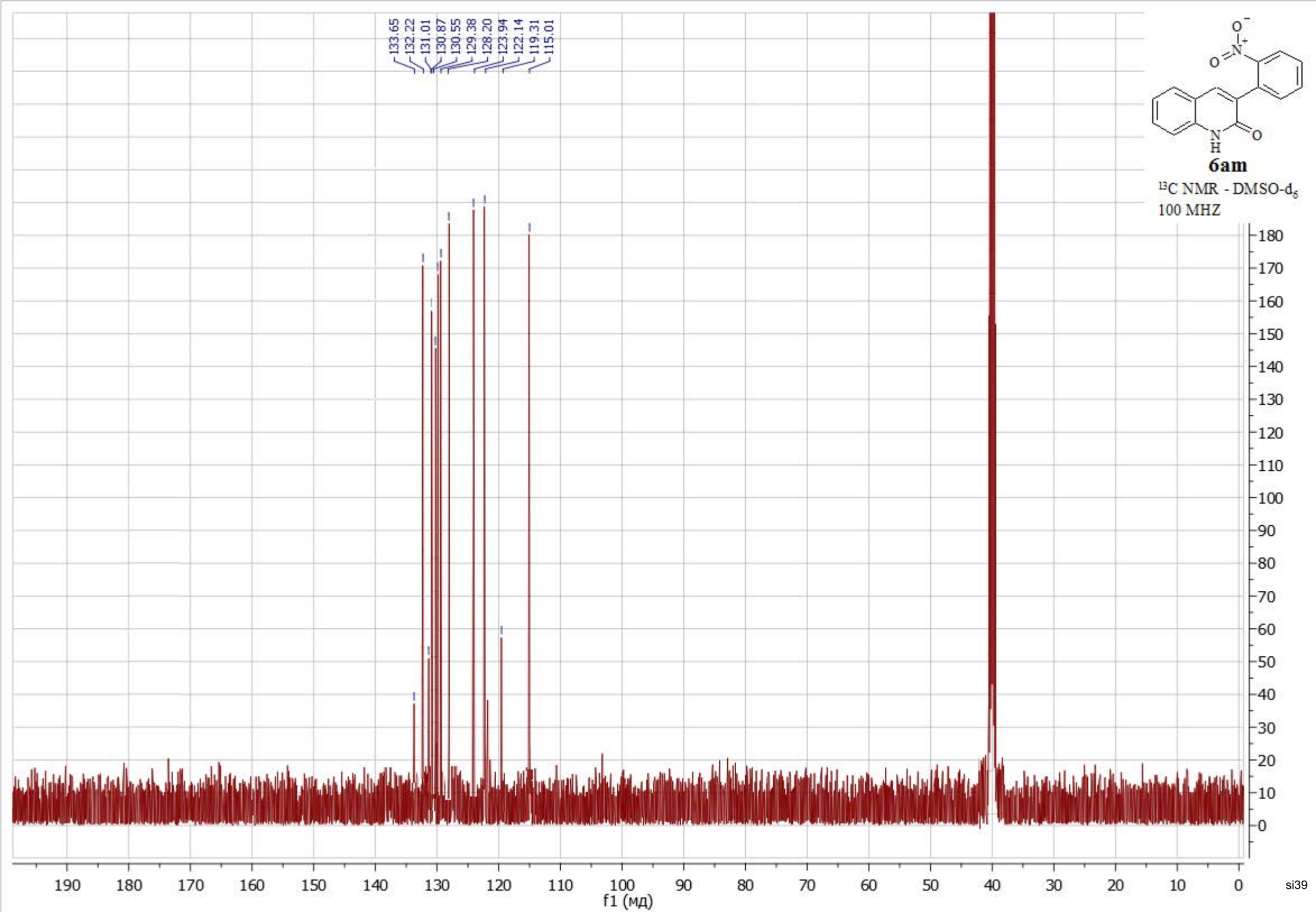
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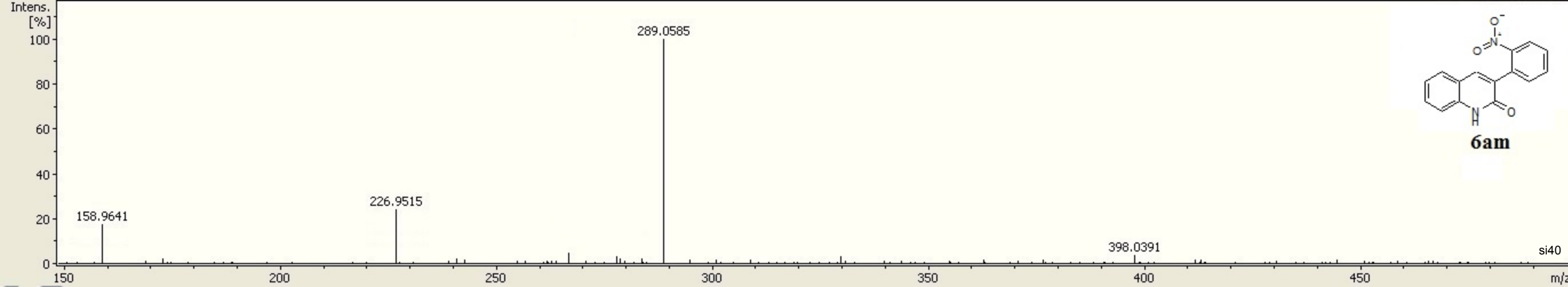


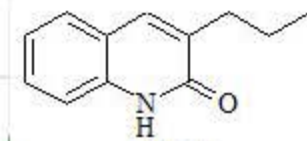


6am

^{13}C NMR - DMSO- d_6
100 MHz

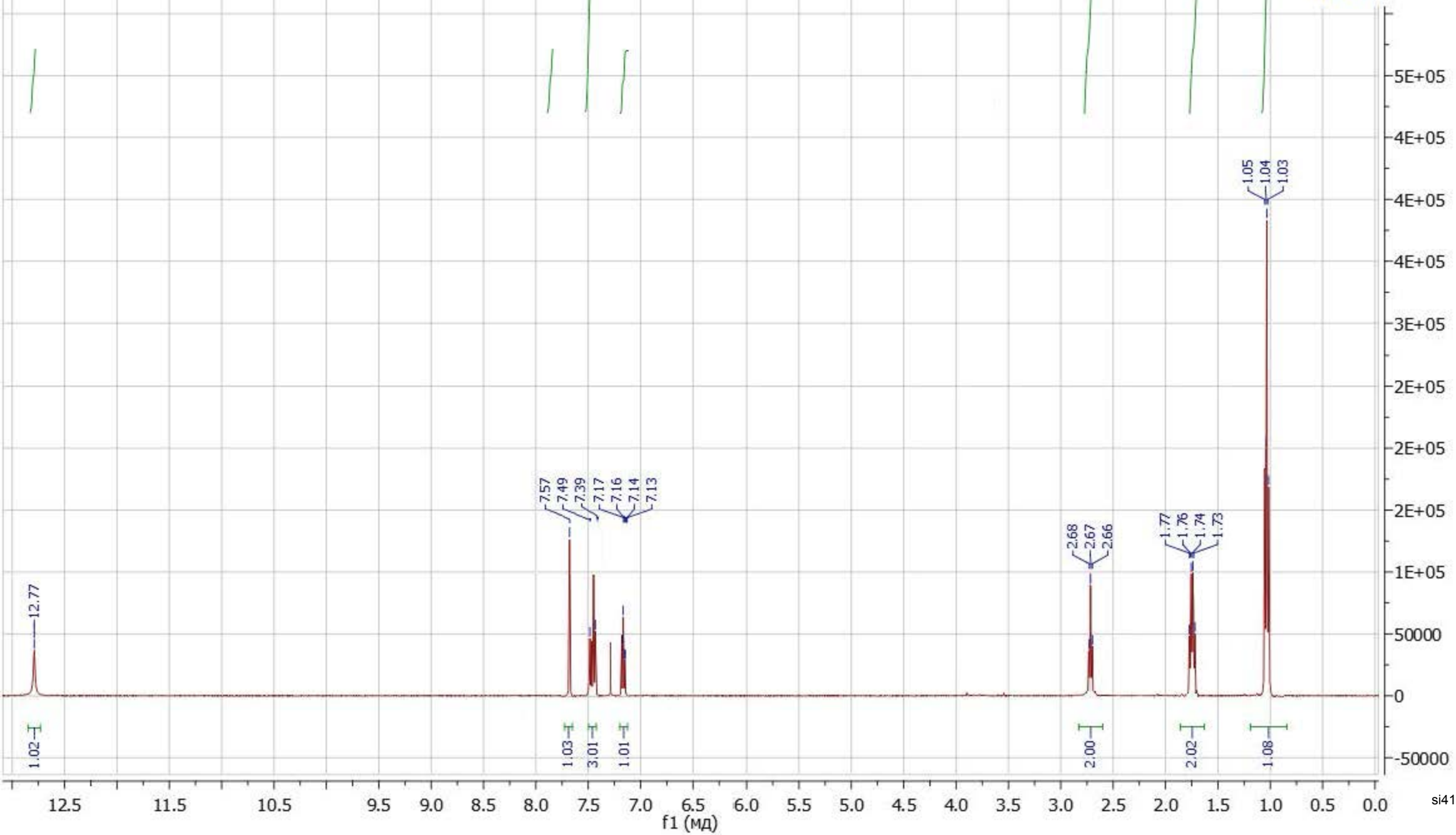


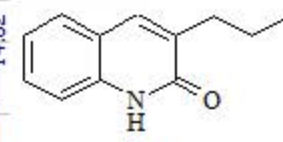




6ap

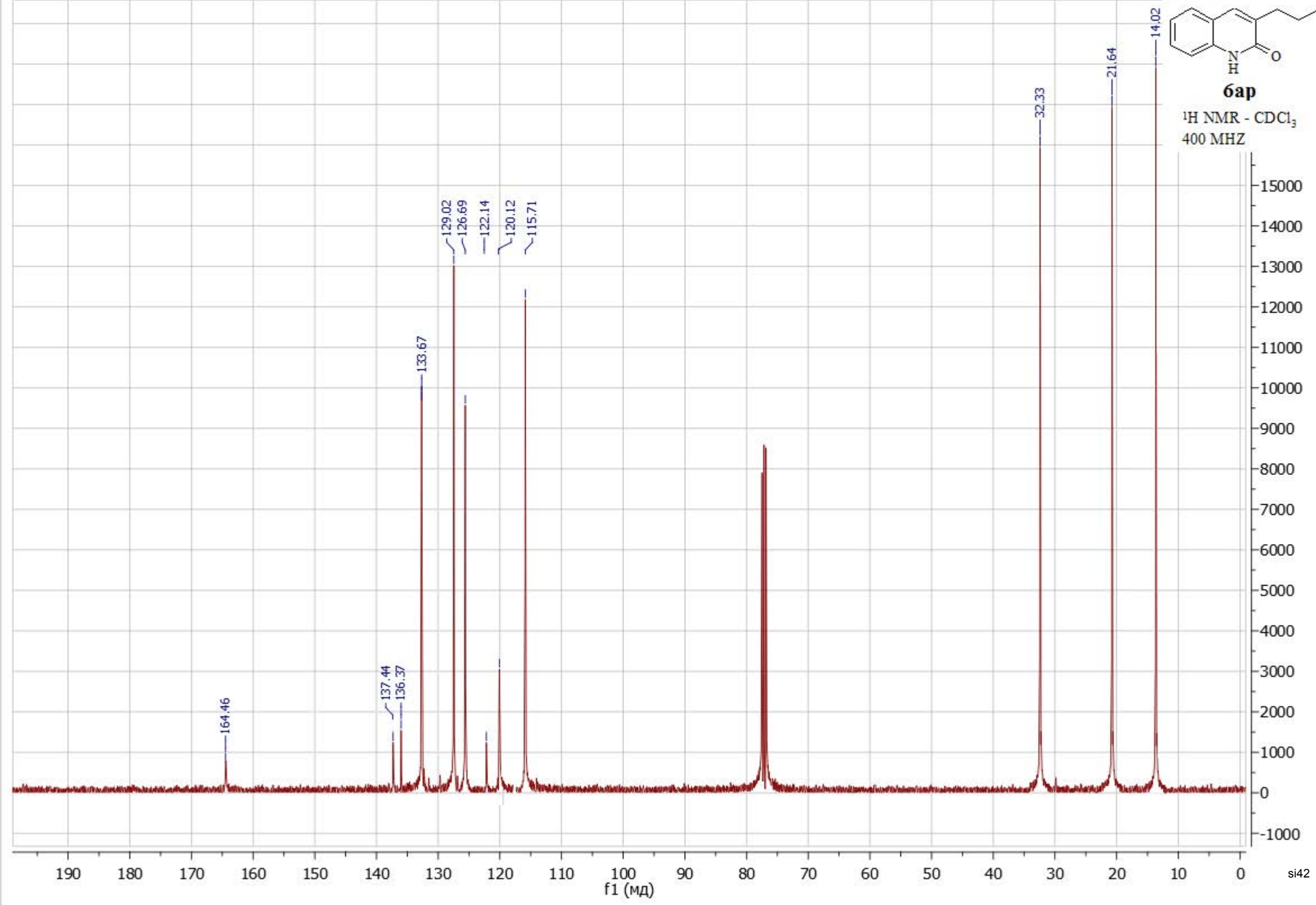
¹H NMR - CDCl₃
400 MHz





6ap

¹H NMR - CDCl₃
400 MHz



Intens.

[%]

100

80

60

40

20

0

100

150

200

250

300

350

400

450

m/z

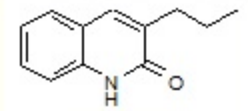
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226.9515

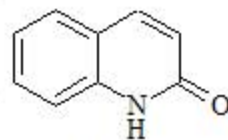
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si43

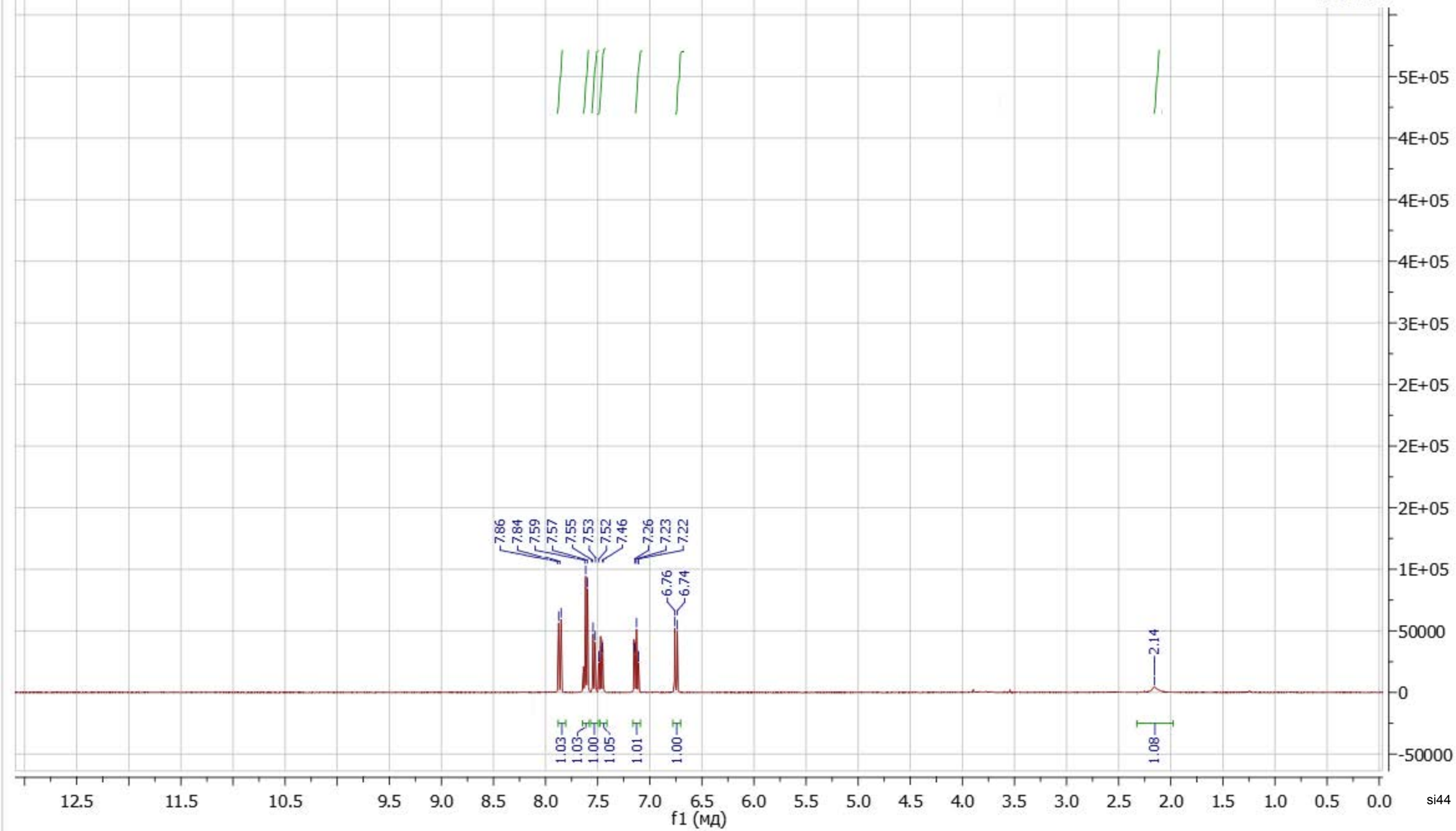


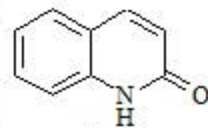
6ap



6aq

¹H NMR - CDCl₃
400 MHz

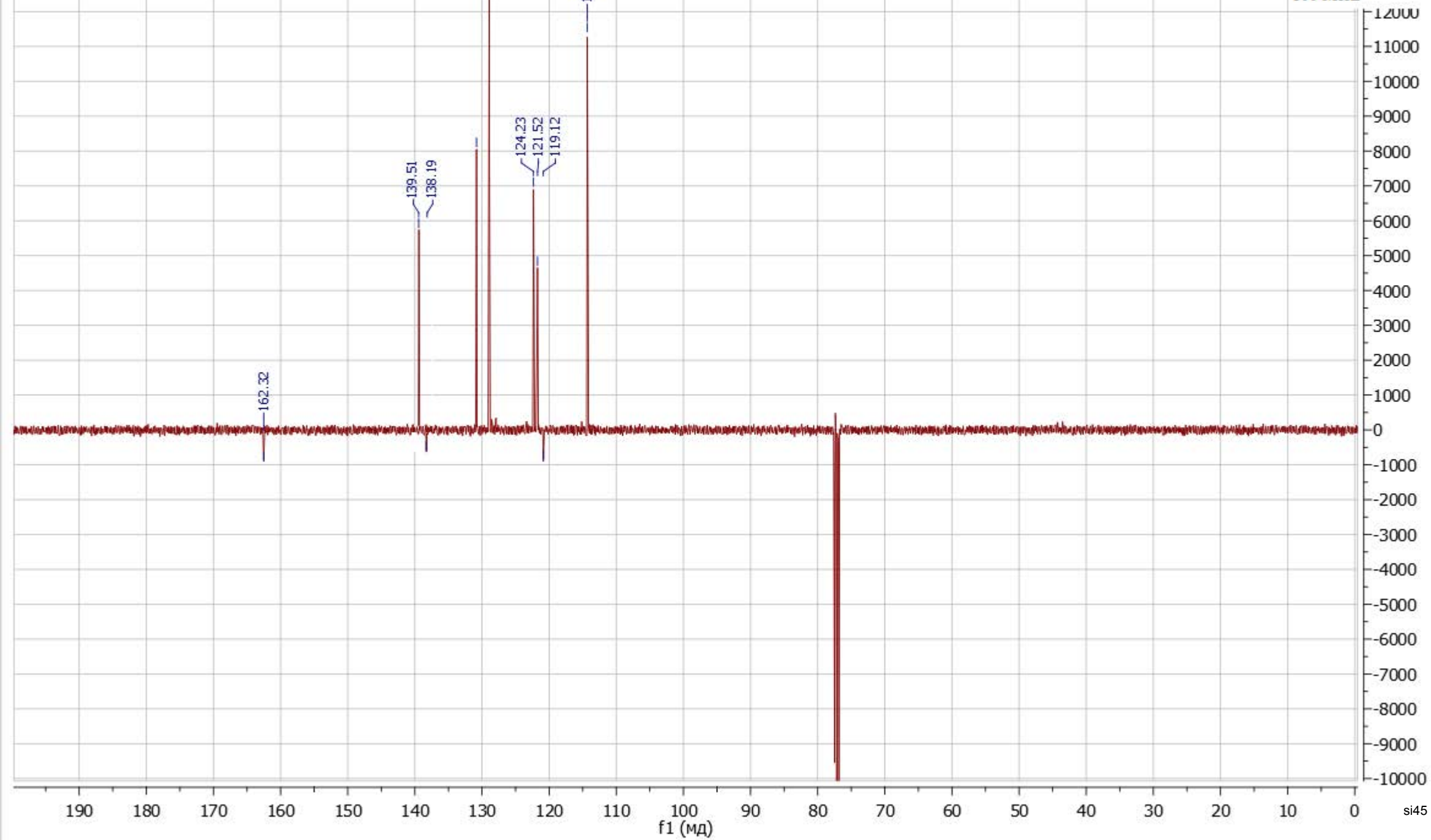




6aq

^{13}C NMR - CDCl_3

100 MHz



Intens.

[%]

100

80

60

40

20

0

100

150

200

250

300

350

400

450

m/z

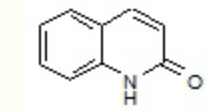
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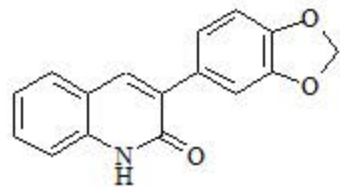
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226.9515

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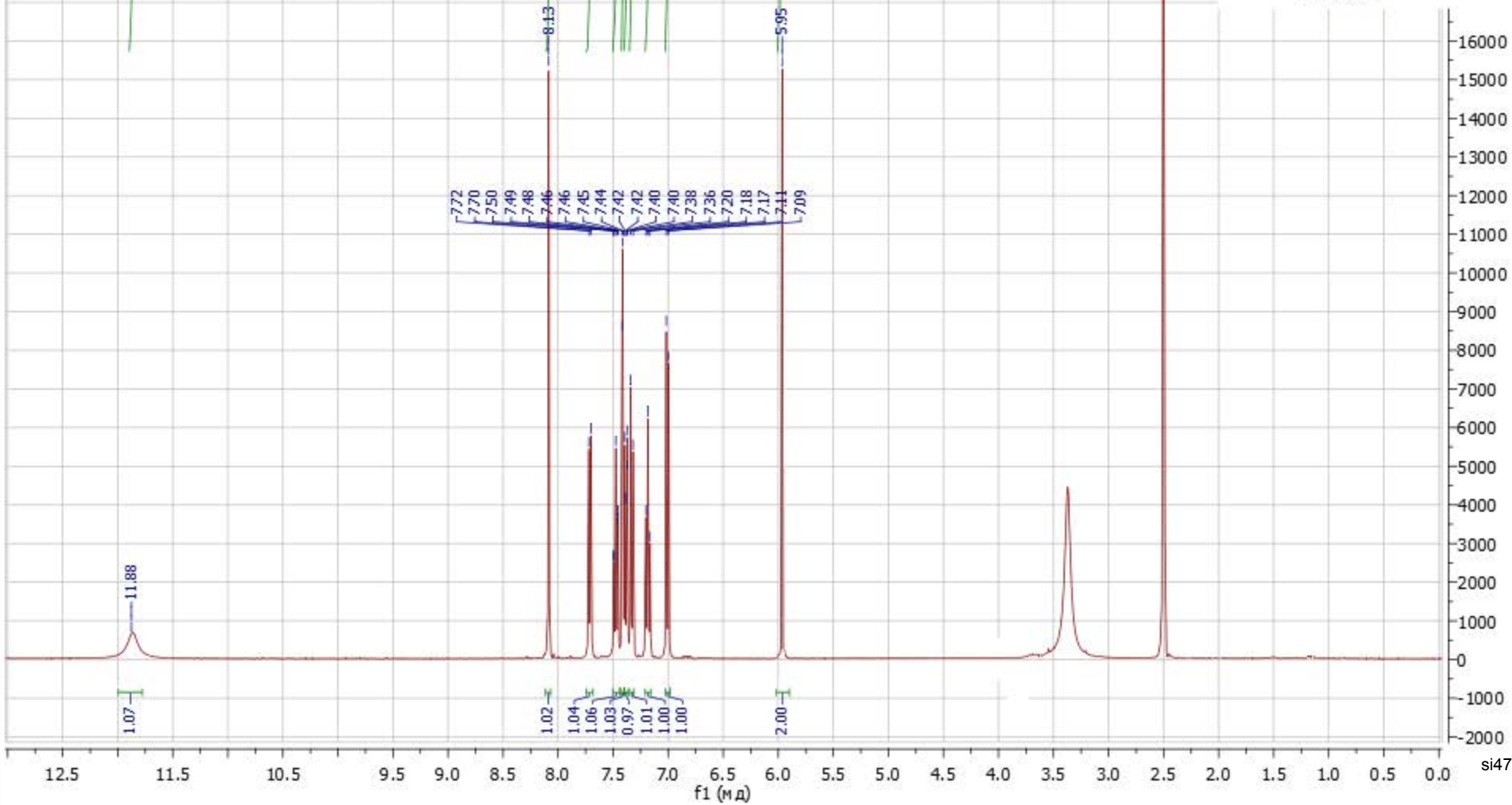
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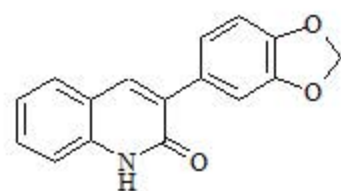




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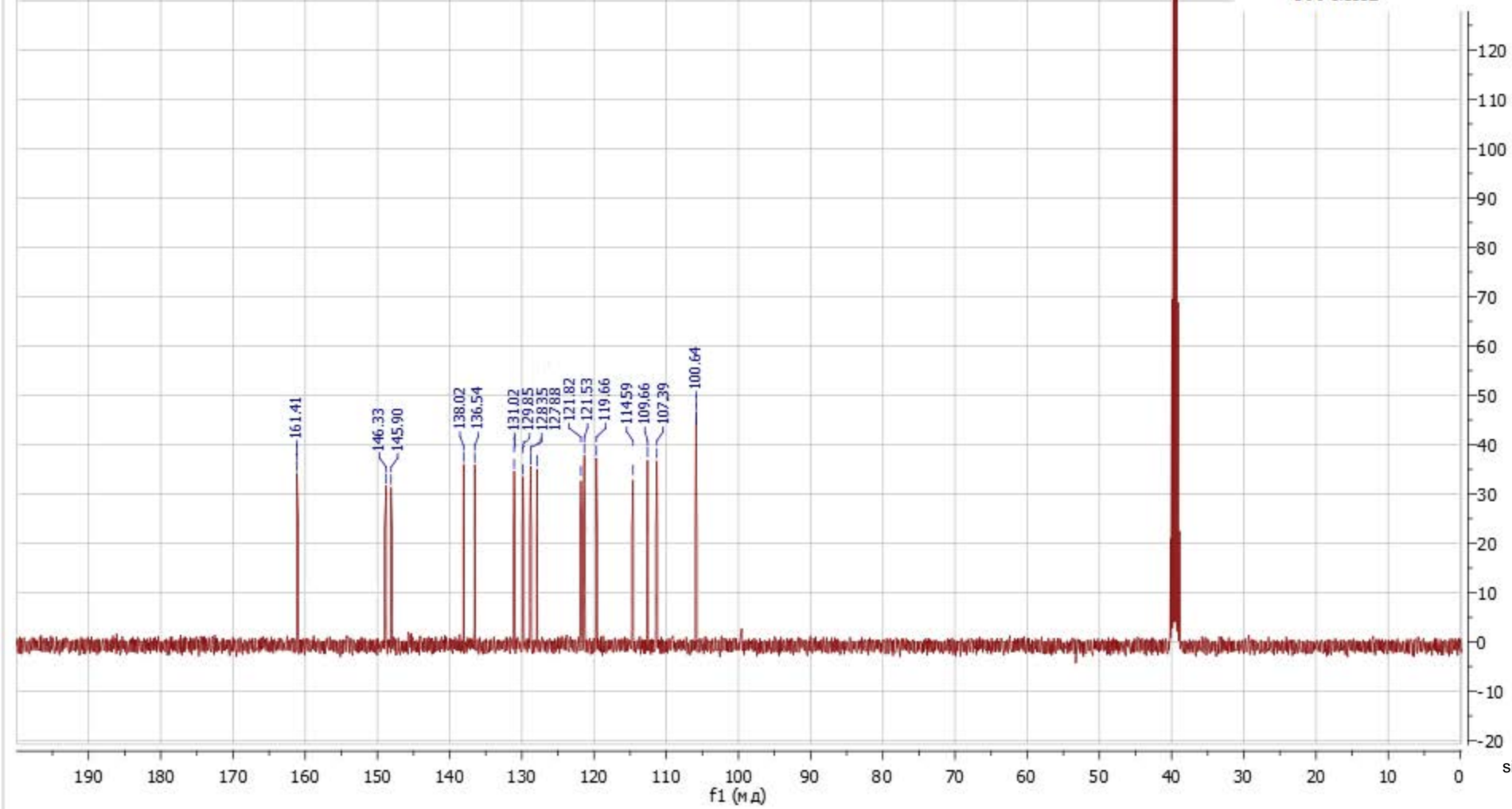
^1H NMR - DMSO- d_6
400 MHz

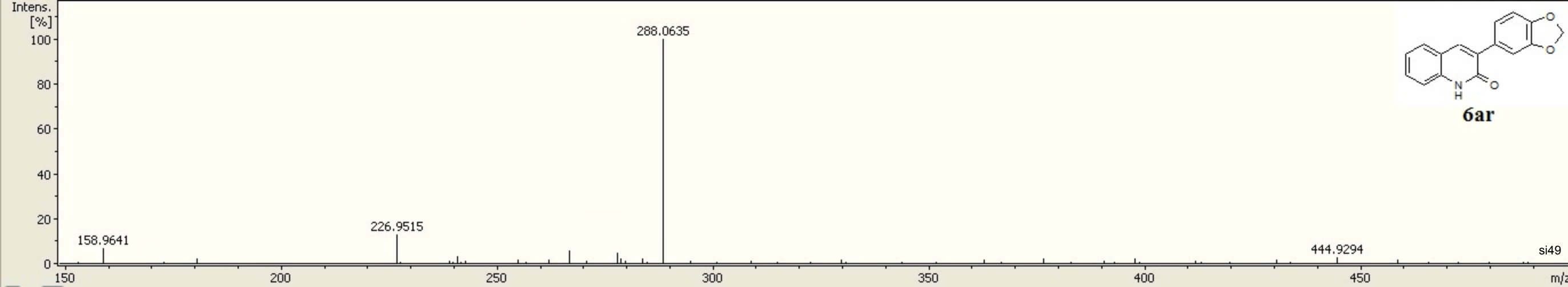


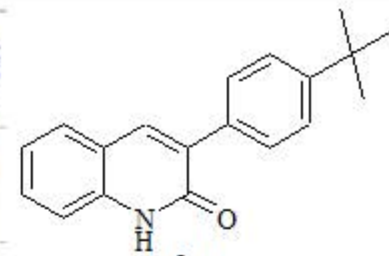


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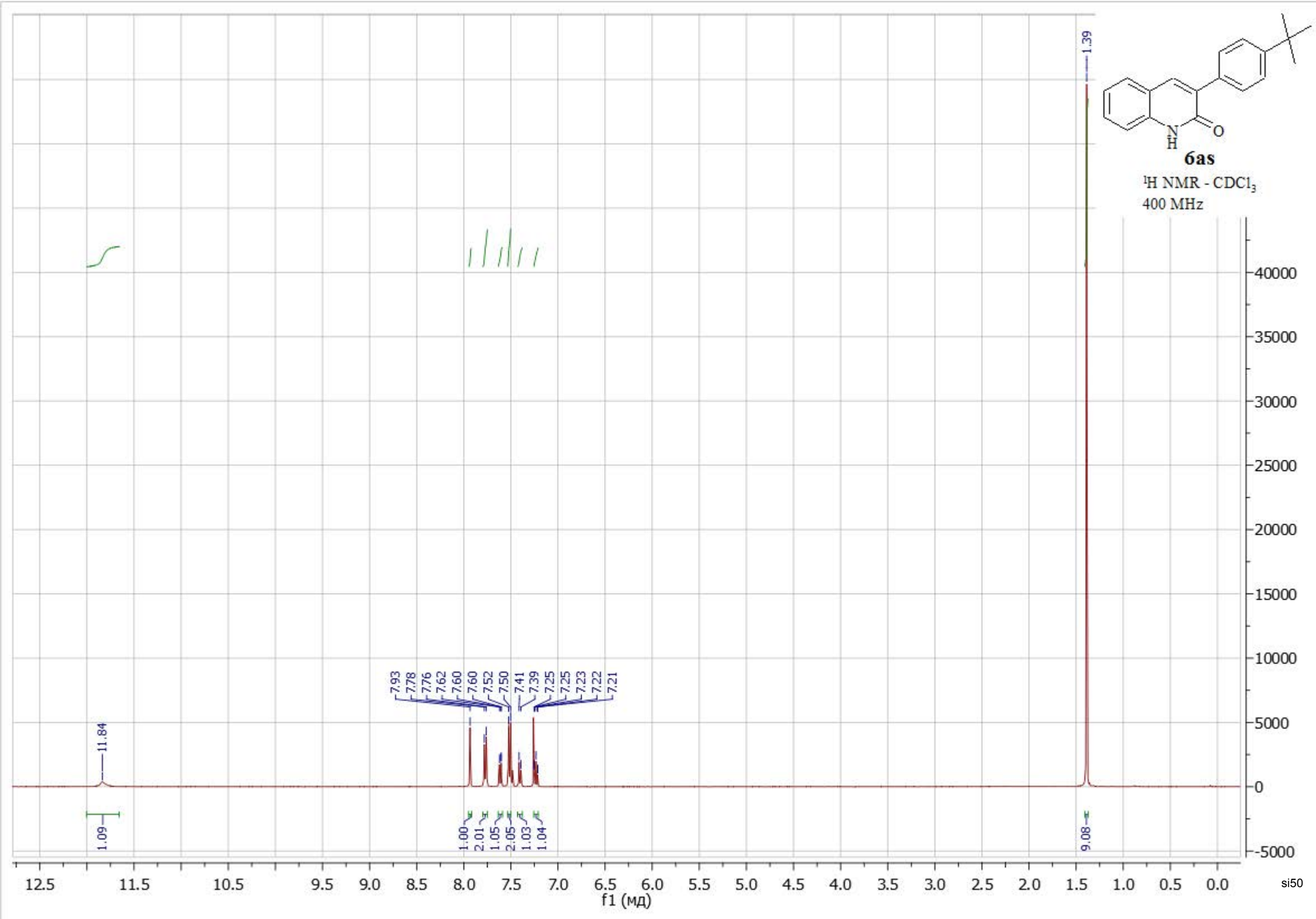
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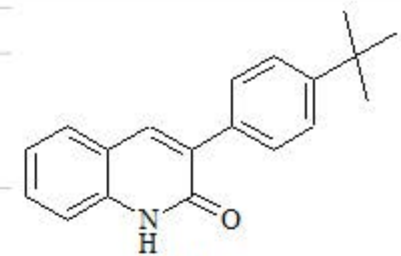




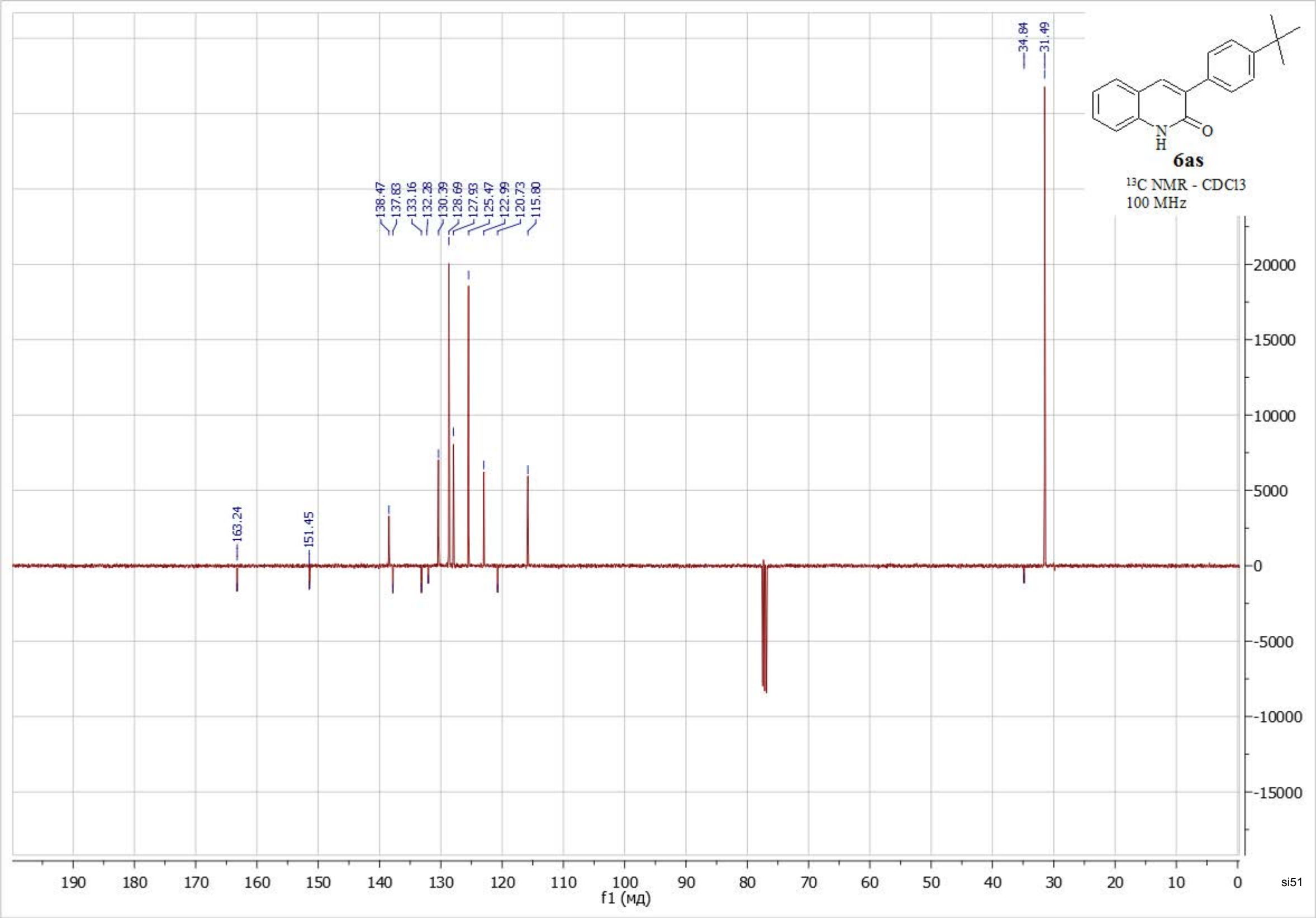


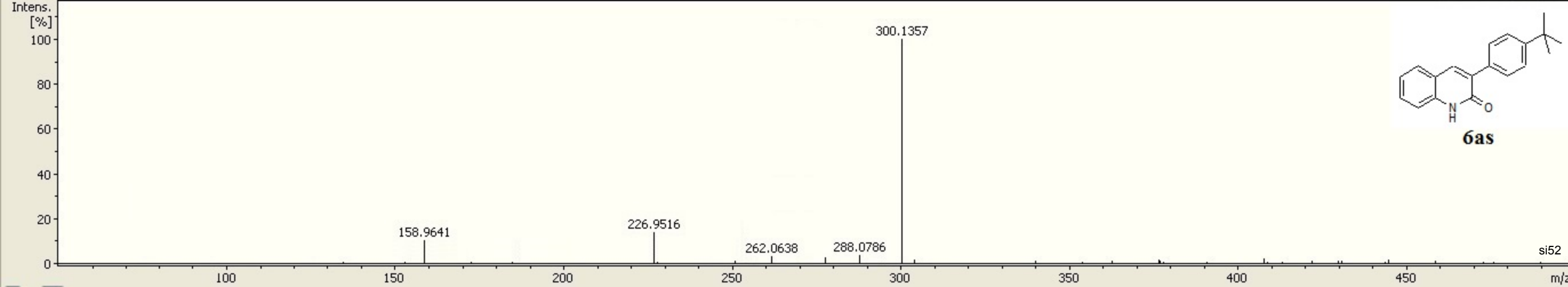
¹H NMR - CDCl₃
400 MHz

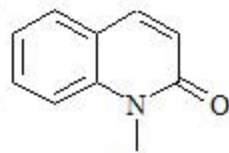




¹³C NMR - CDCl₃
100 MHz

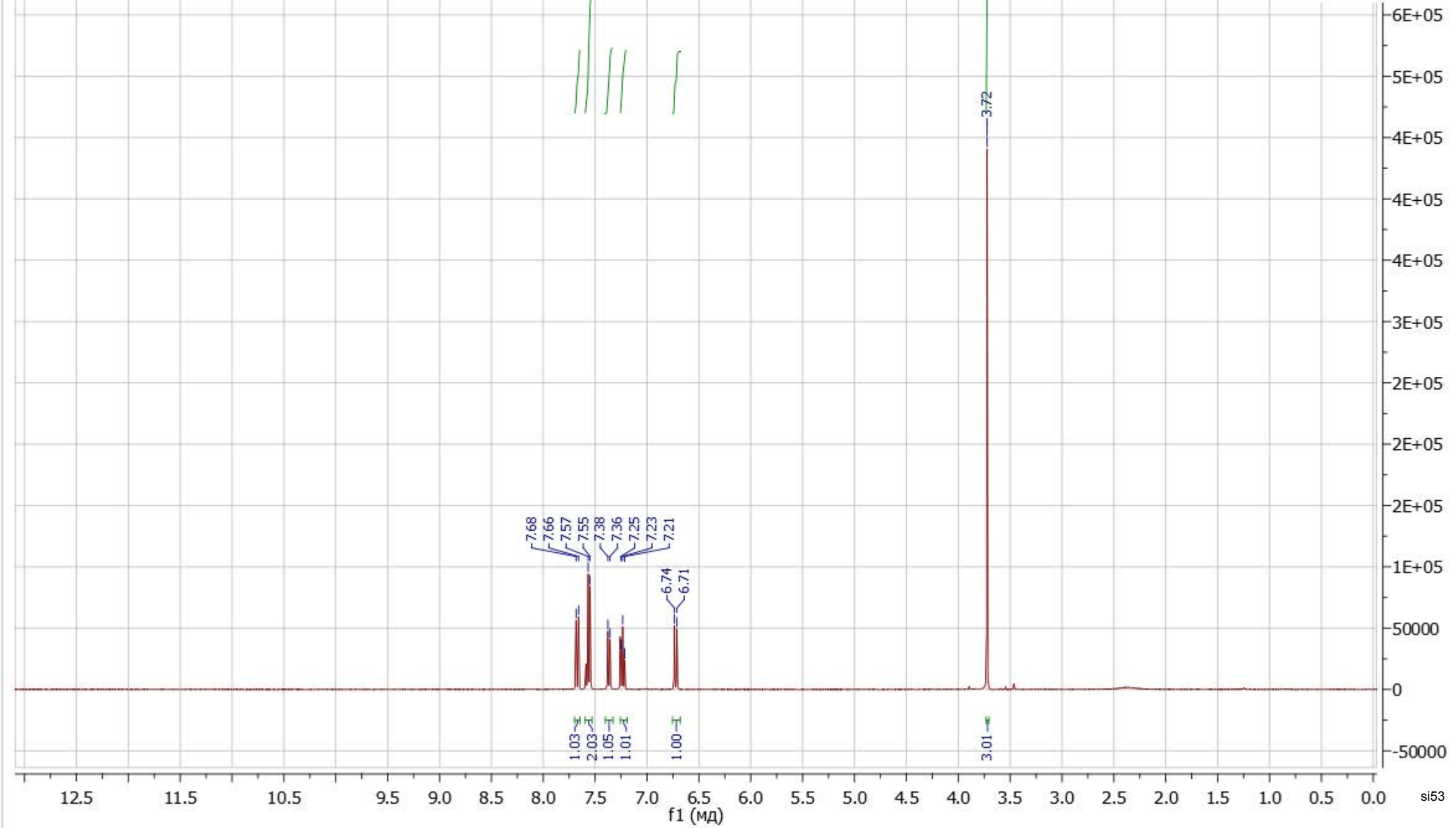


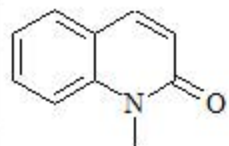




6cq

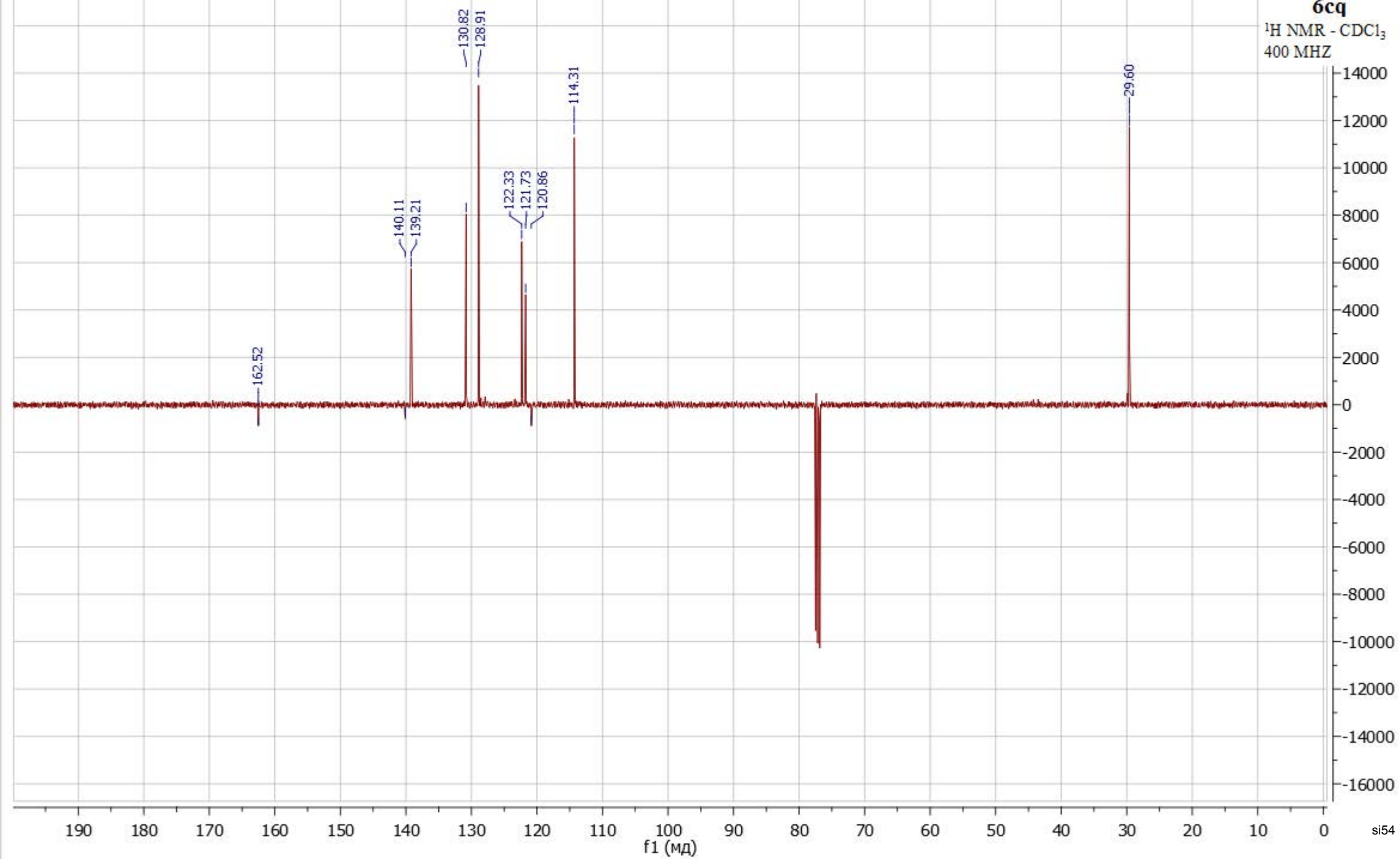
¹H NMR - CDCl₃
400 MHz





6cq

^1H NMR - CDCl_3
400 MHz



Intens.

[%]

100

80

60

40

20

0

100

150

200

250

300

350

400

450

m/z

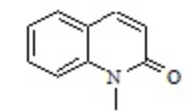
182.0577

158.9641

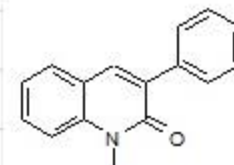
226.9515

302.0943

si55

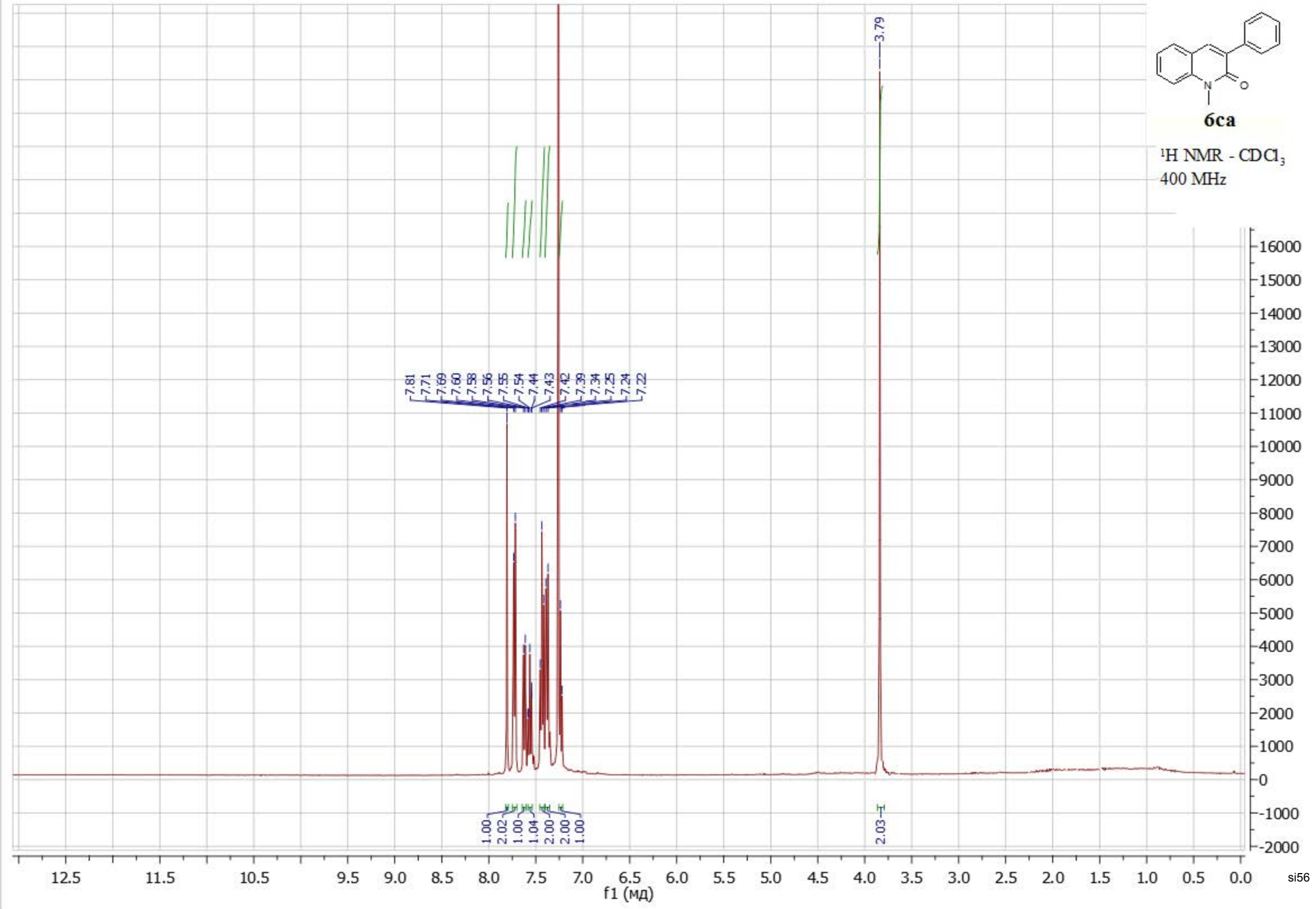


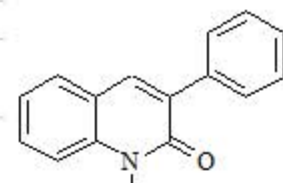
6cq



6ca

¹H NMR - CDCl₃
400 MHz

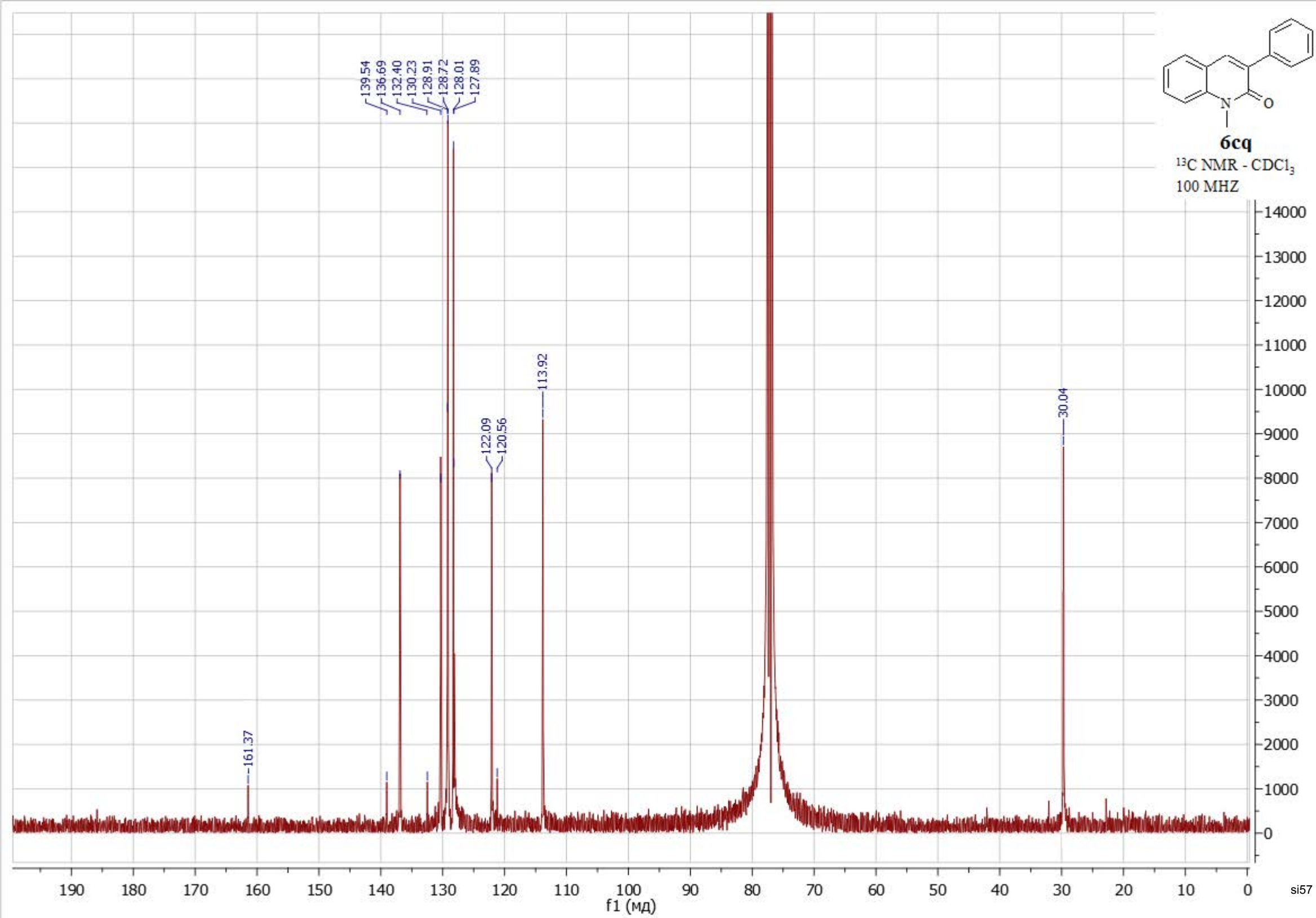


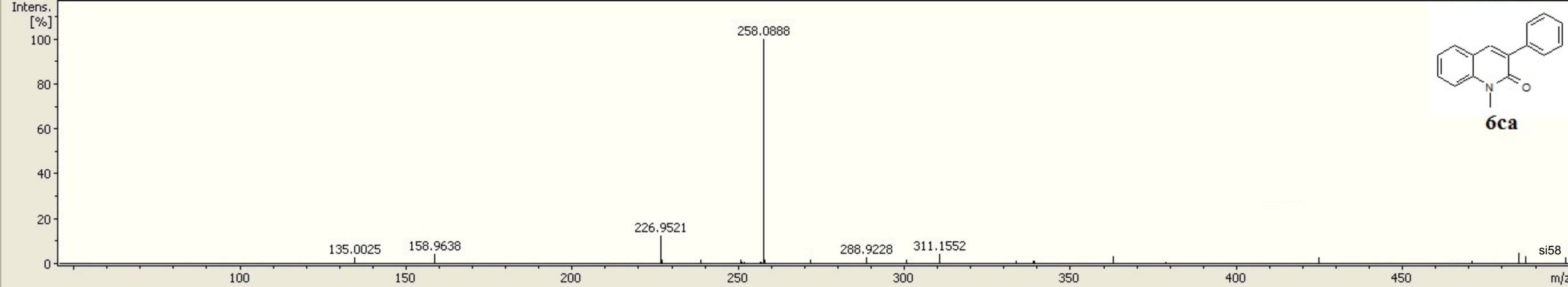


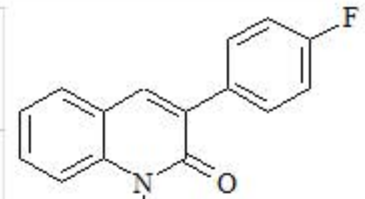
6cq

^{13}C NMR - CDCl_3

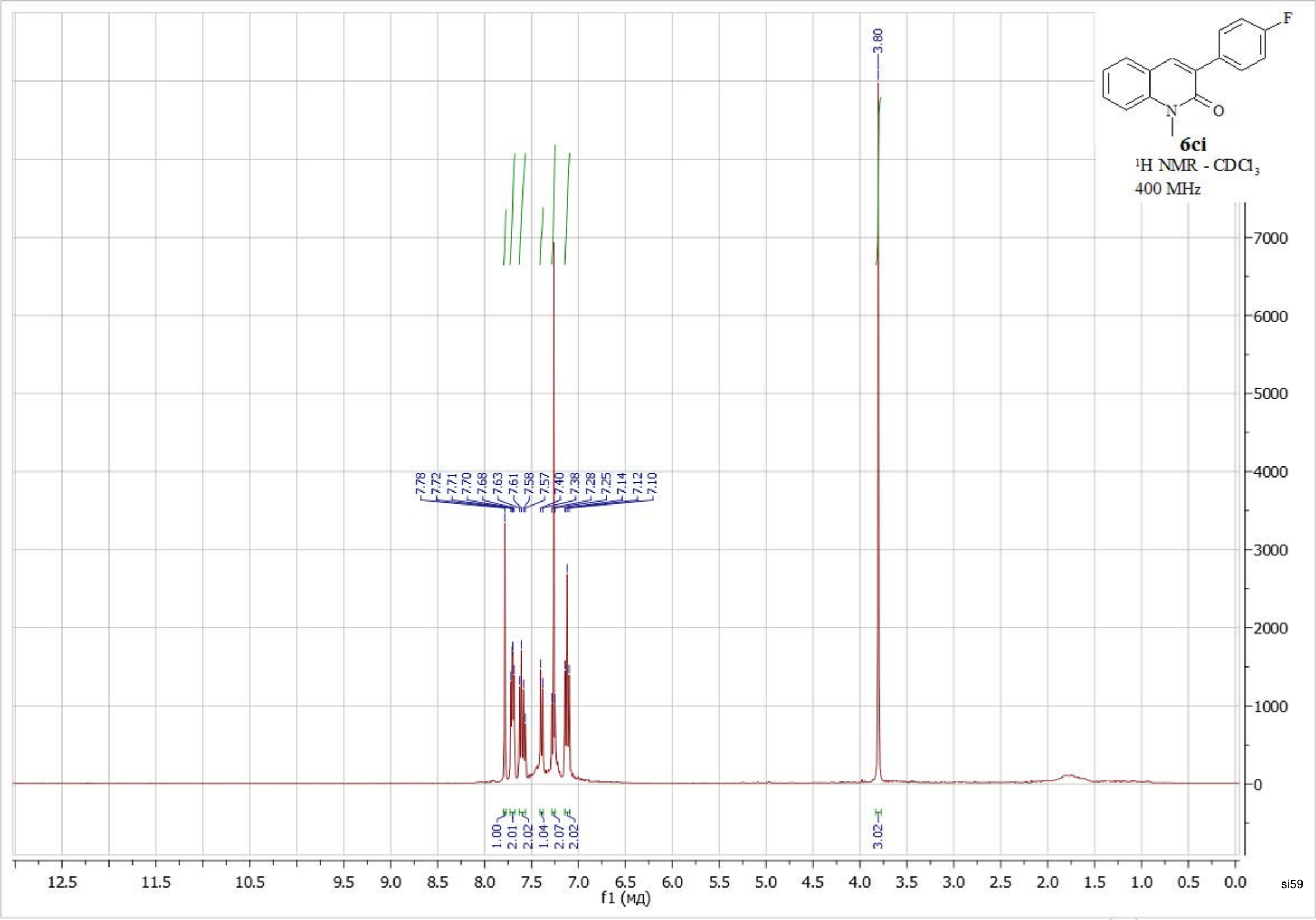
100 MHz

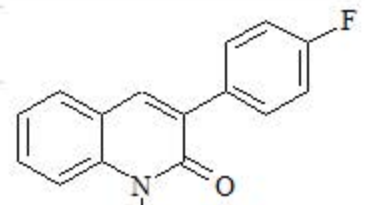




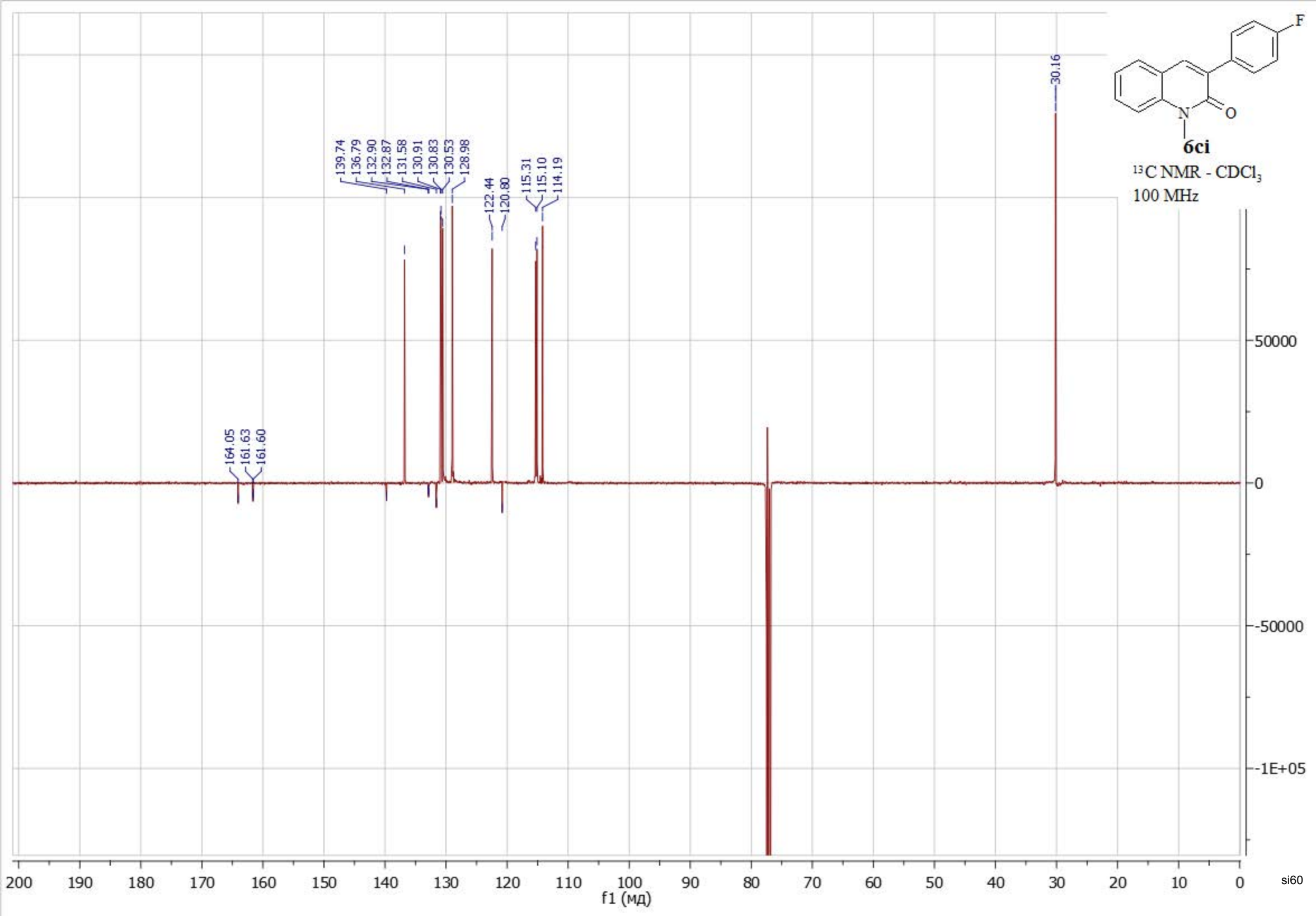


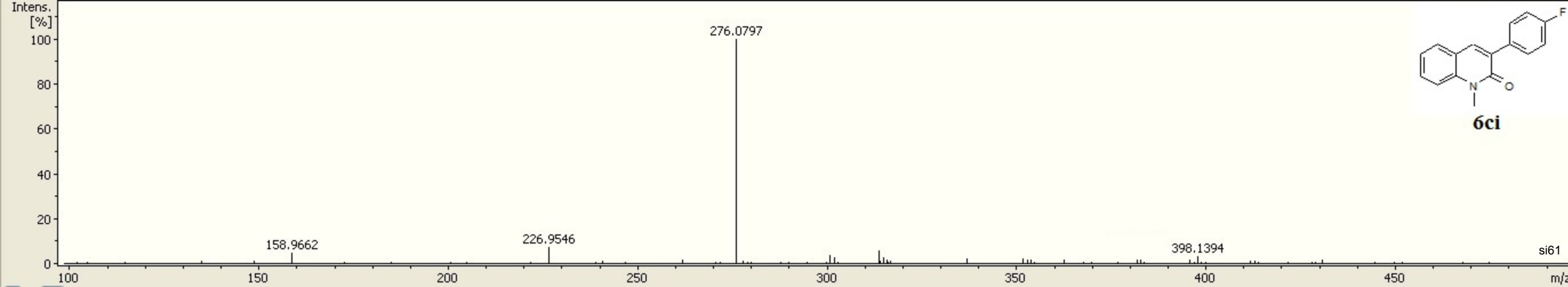
6ci
¹H NMR - CDCl₃
400 MHz

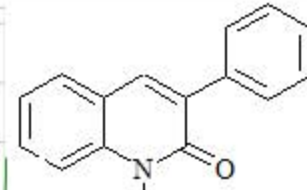




¹³C NMR - CDCl₃
100 MHz

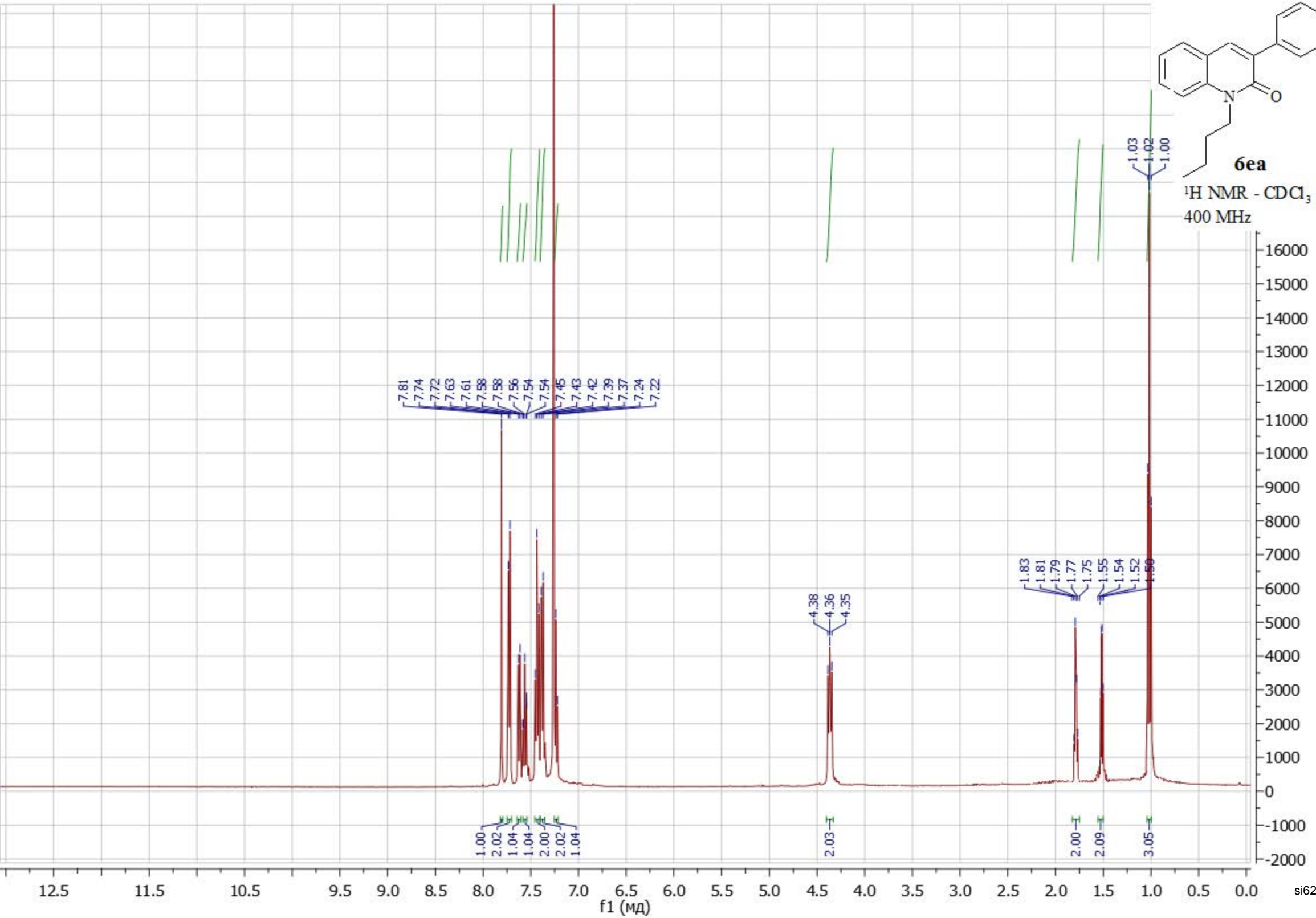


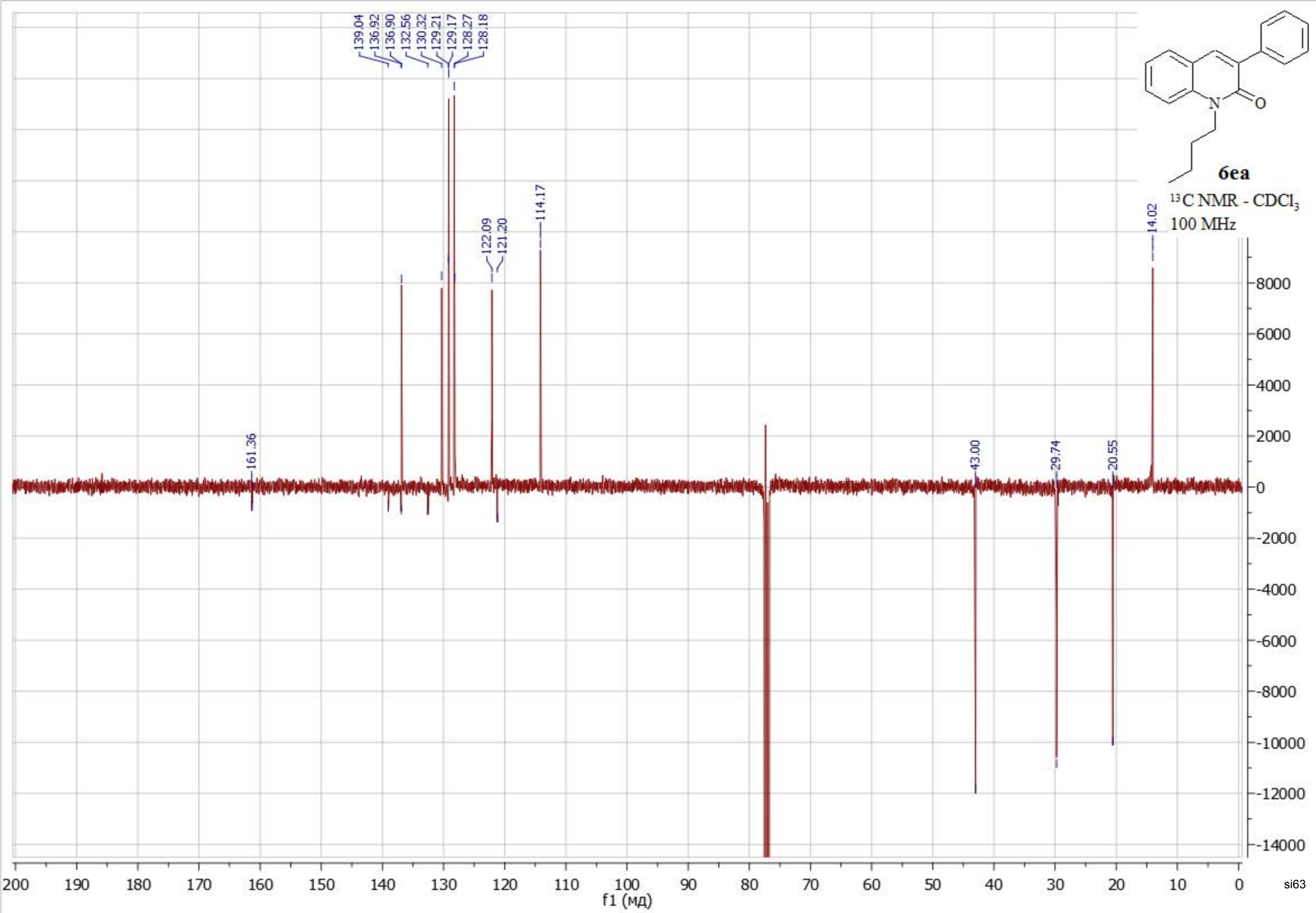


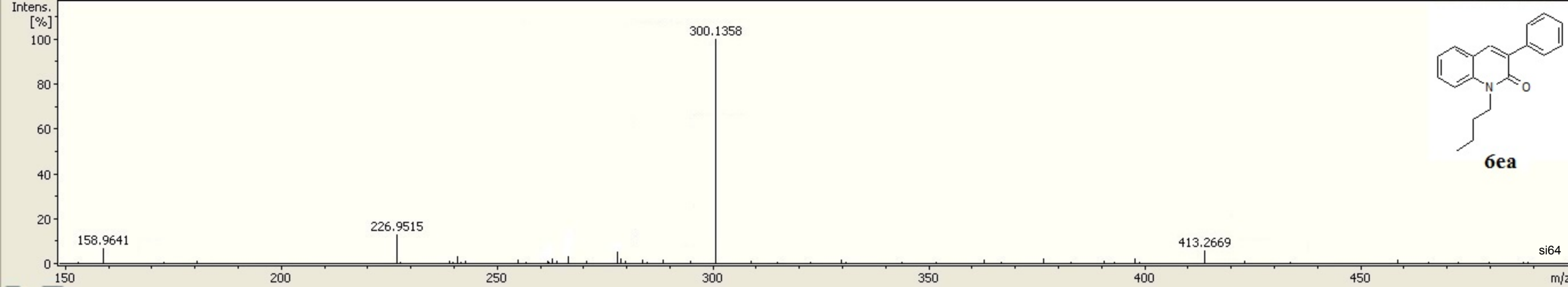


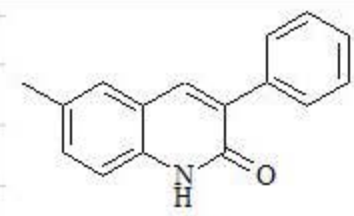
6ea

¹H NMR - CDCl₃
400 MHz



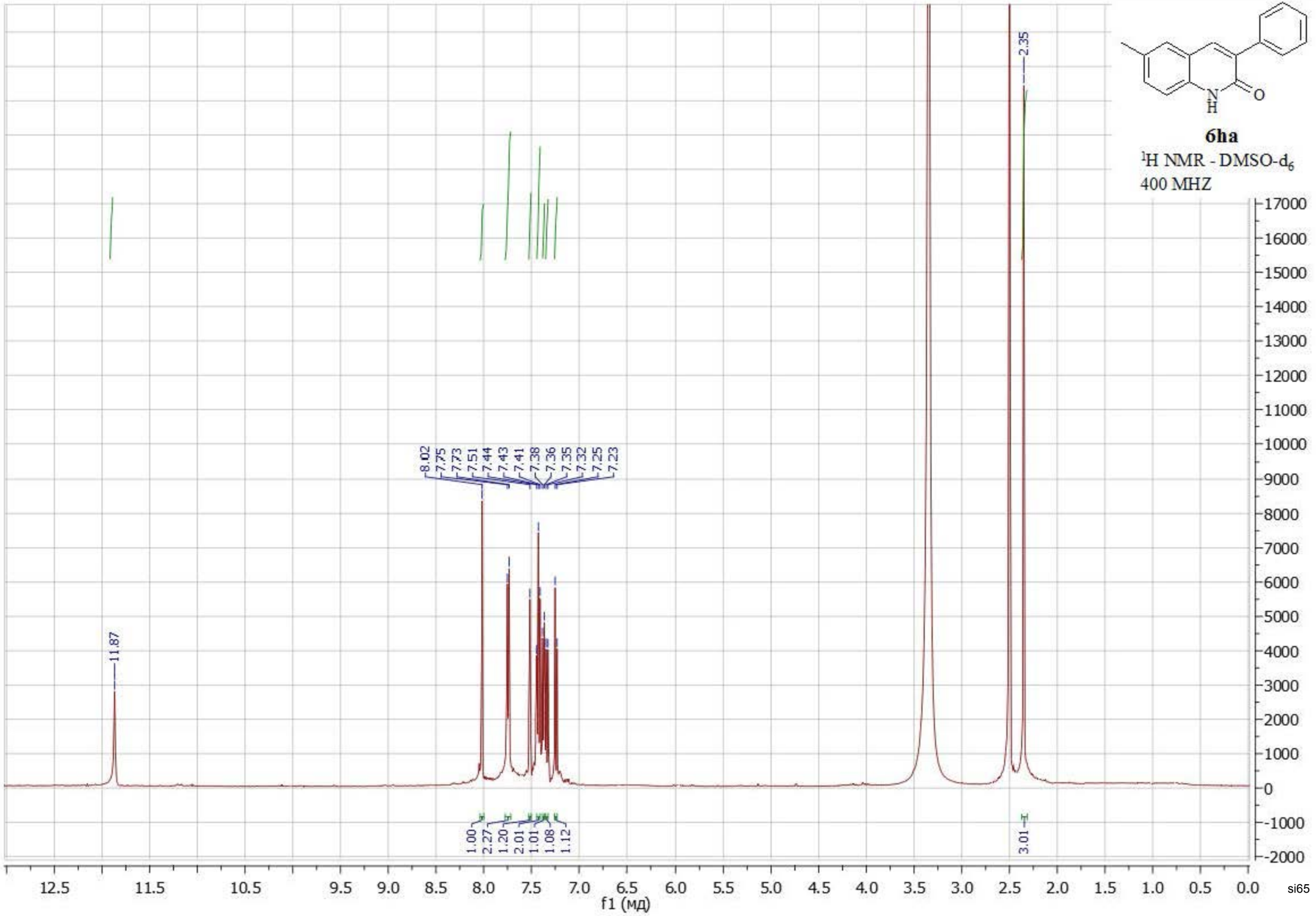


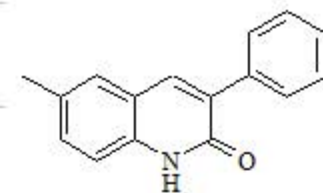




6ha

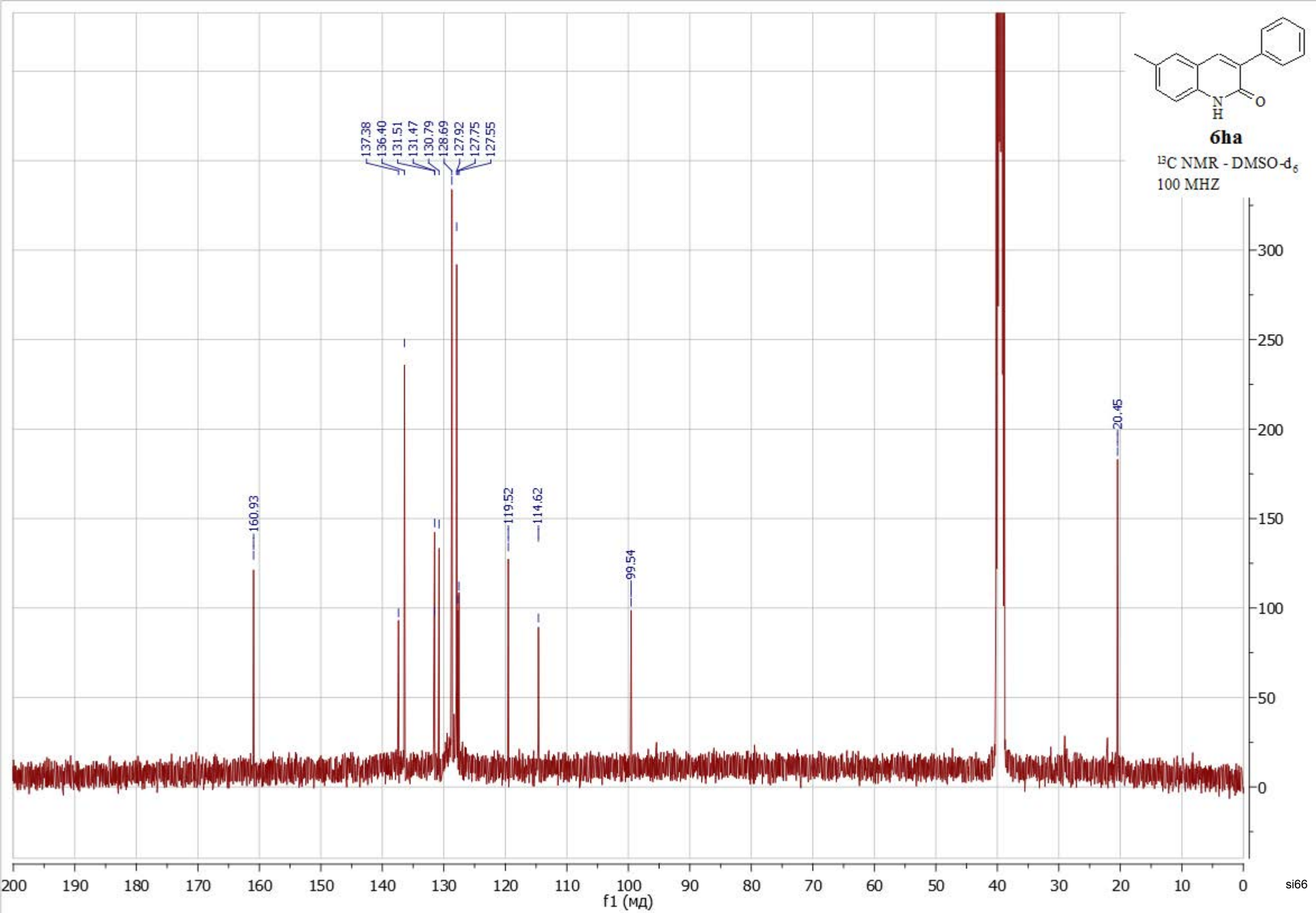
^1H NMR - DMSO- d_6
400 MHz

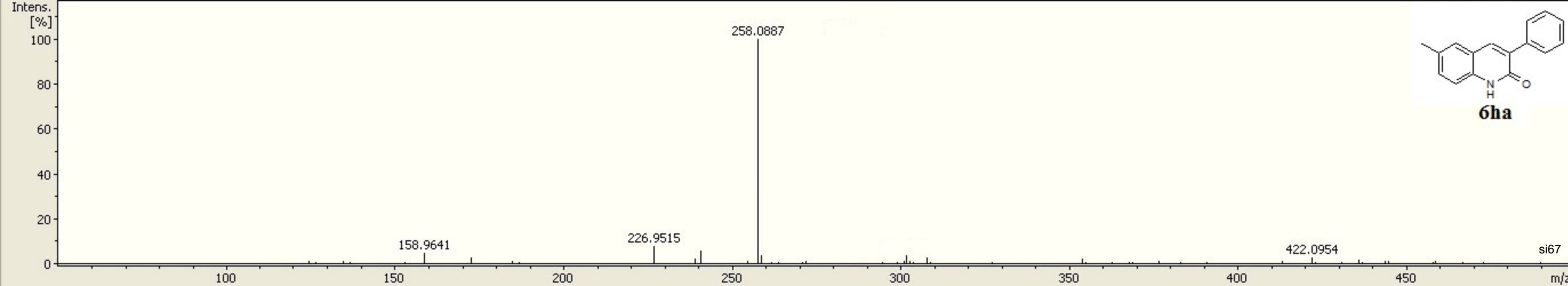


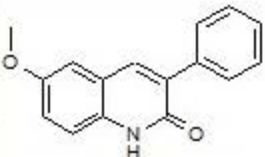


6ha

^{13}C NMR - DMSO-d_6
100 MHz

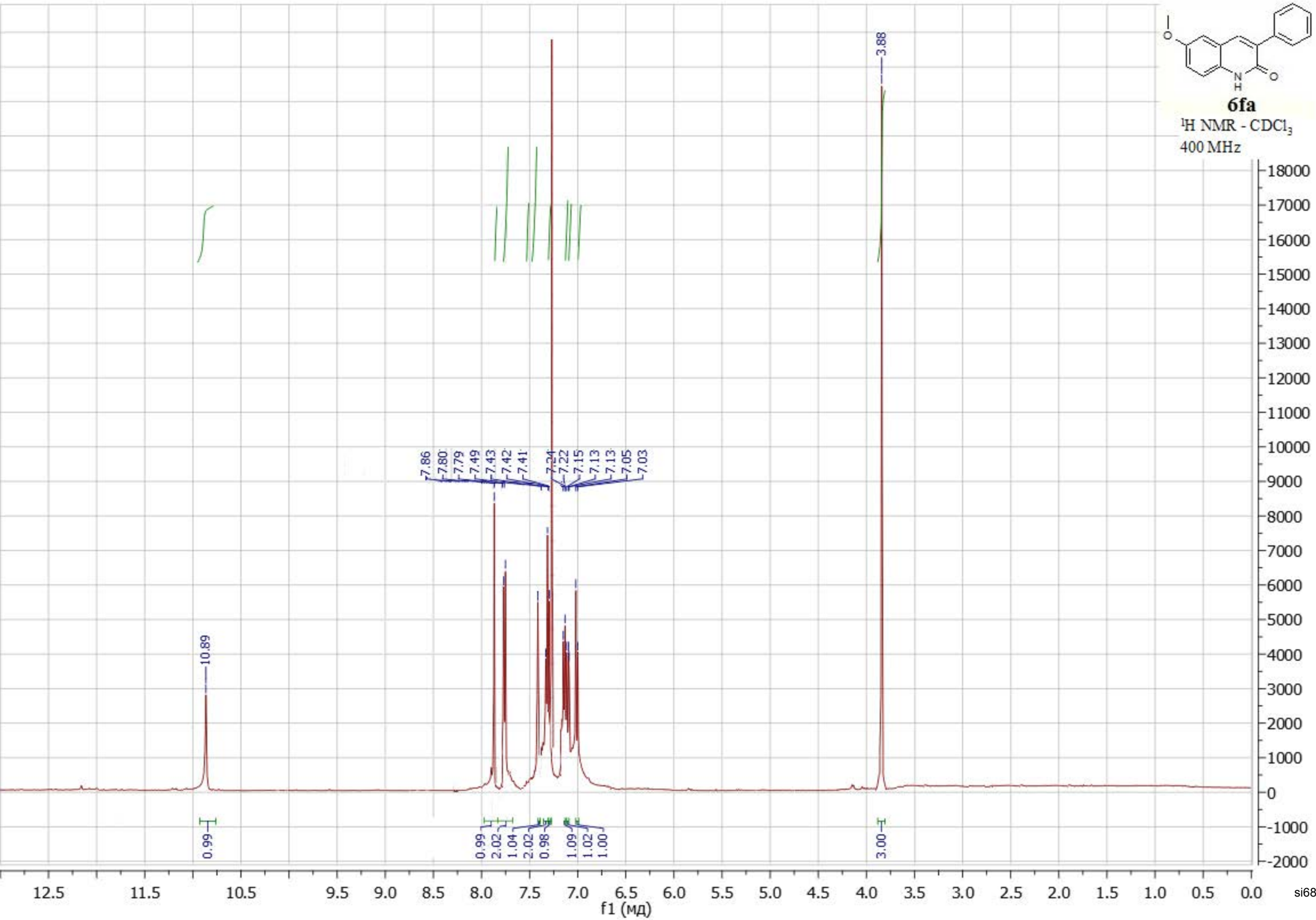


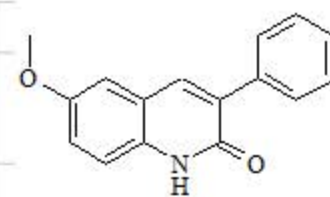




6fa

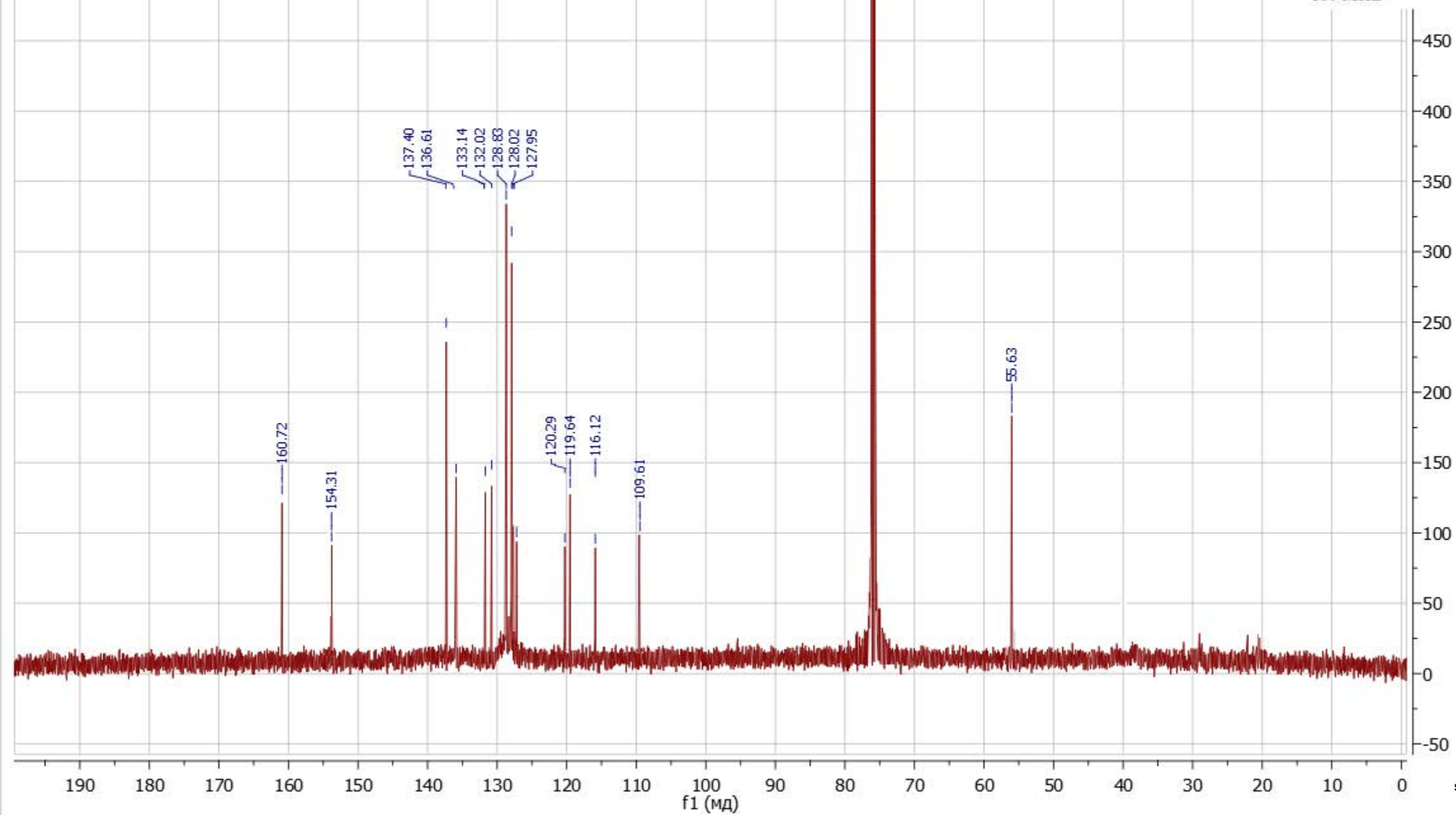
¹H NMR - CDCl₃
400 MHz

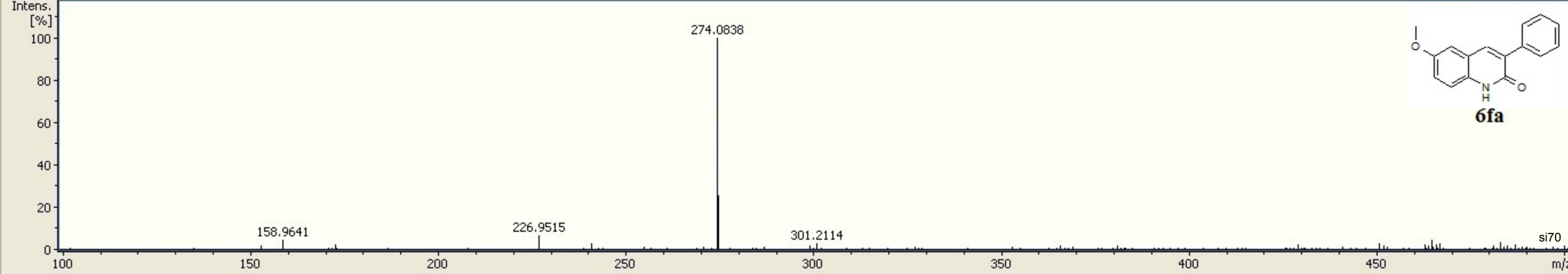


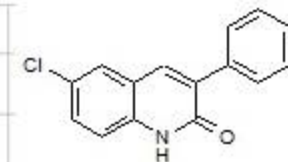


6fa

^{13}C NMR - $\text{DMSO-}d_6$
100 MHz

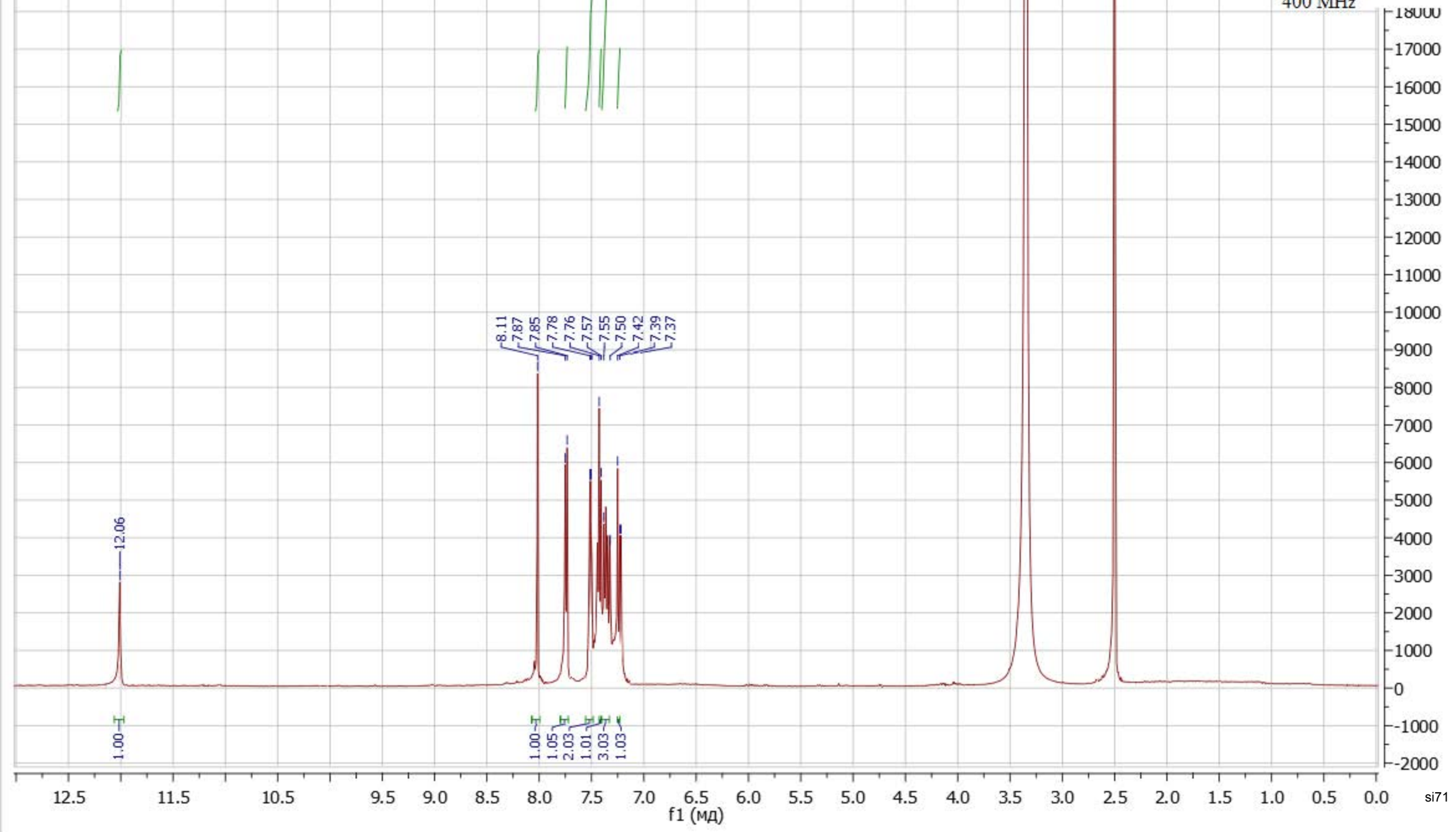


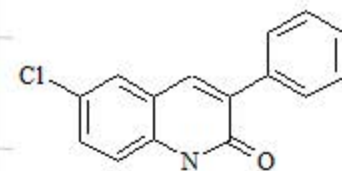




6ga

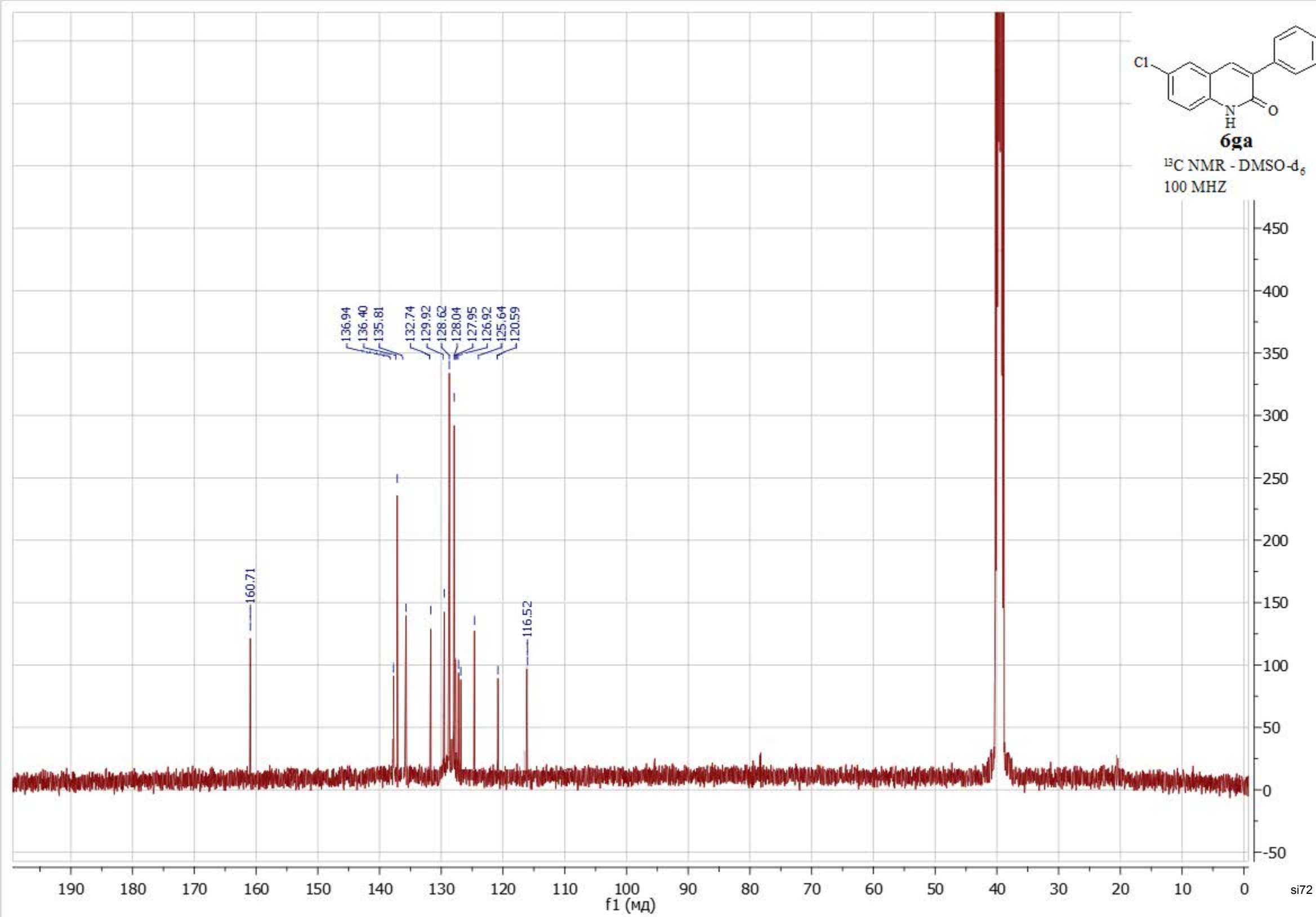
¹H NMR - DMSO-d₆
400 MHz

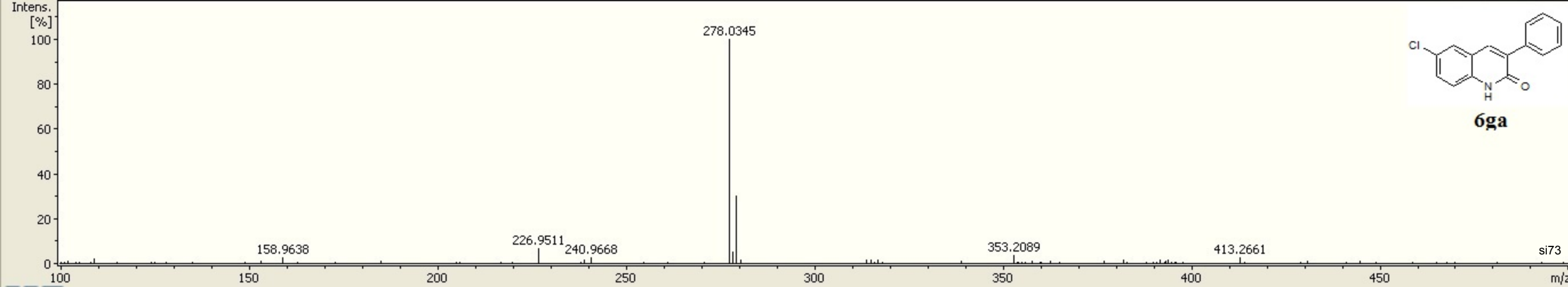


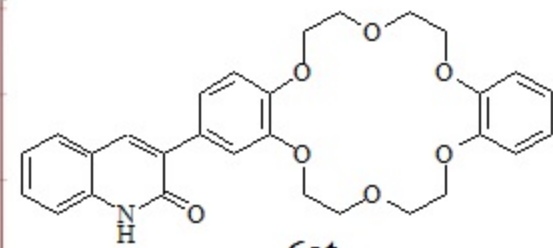


6ga

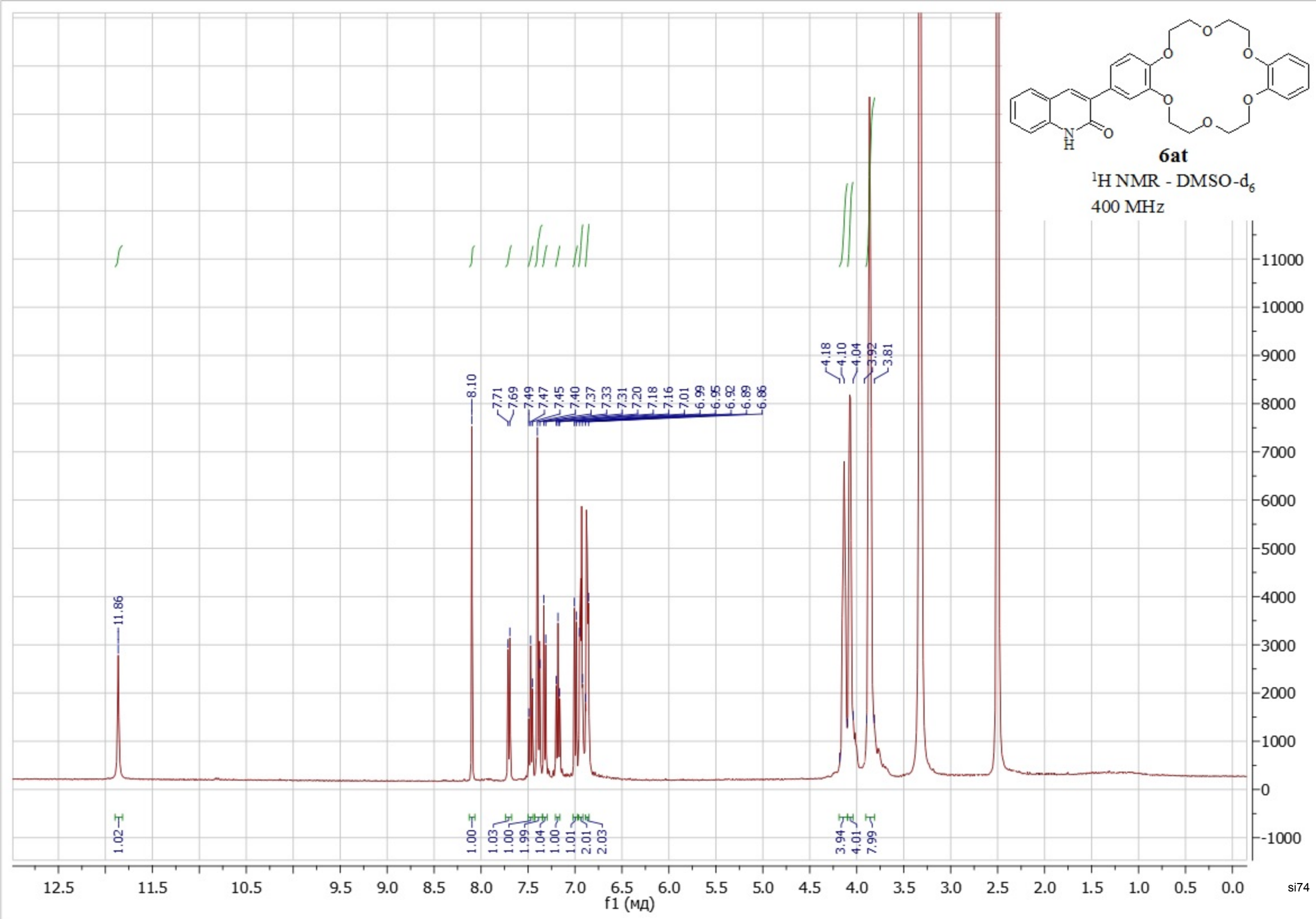
^{13}C NMR - $\text{DMSO-}d_6$
100 MHz

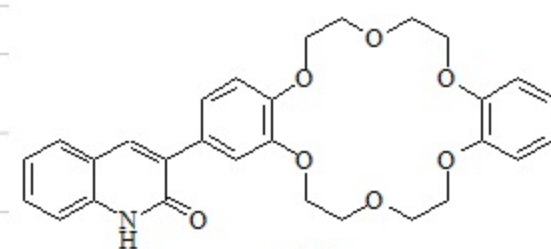






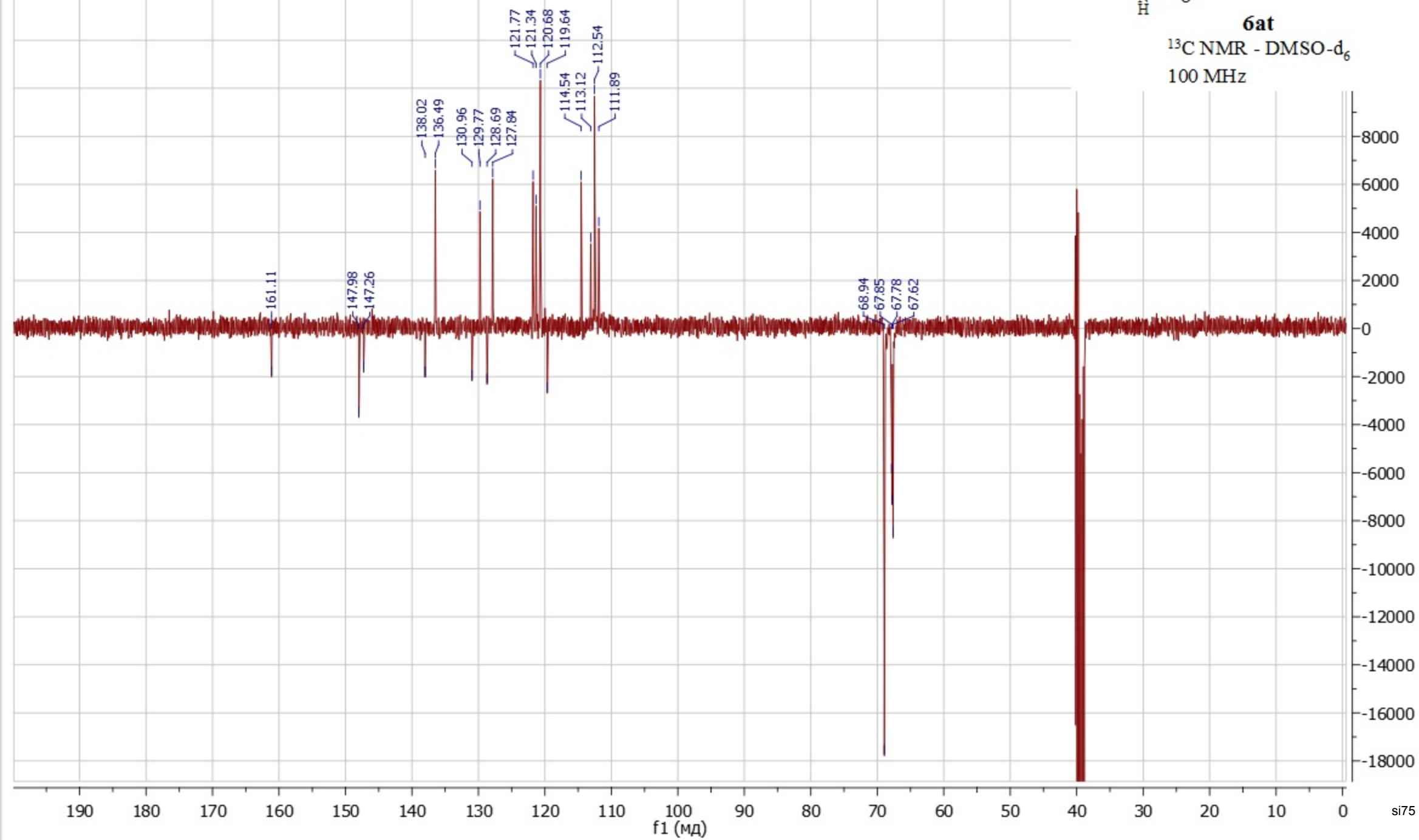
¹H NMR - DMSO-d₆
400 MHz

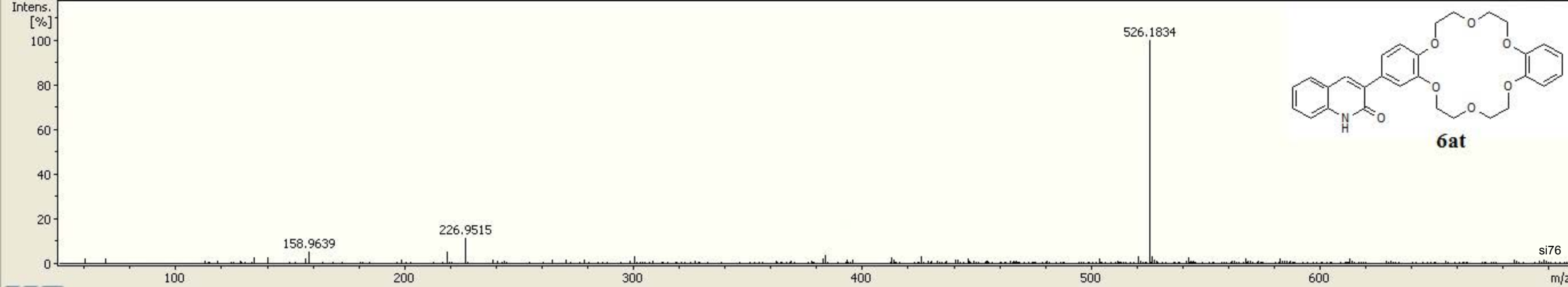


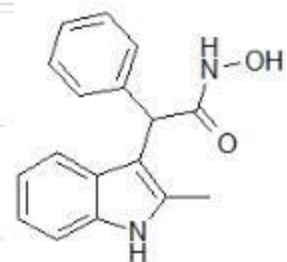


6at

^{13}C NMR - DMSO-d_6
100 MHz

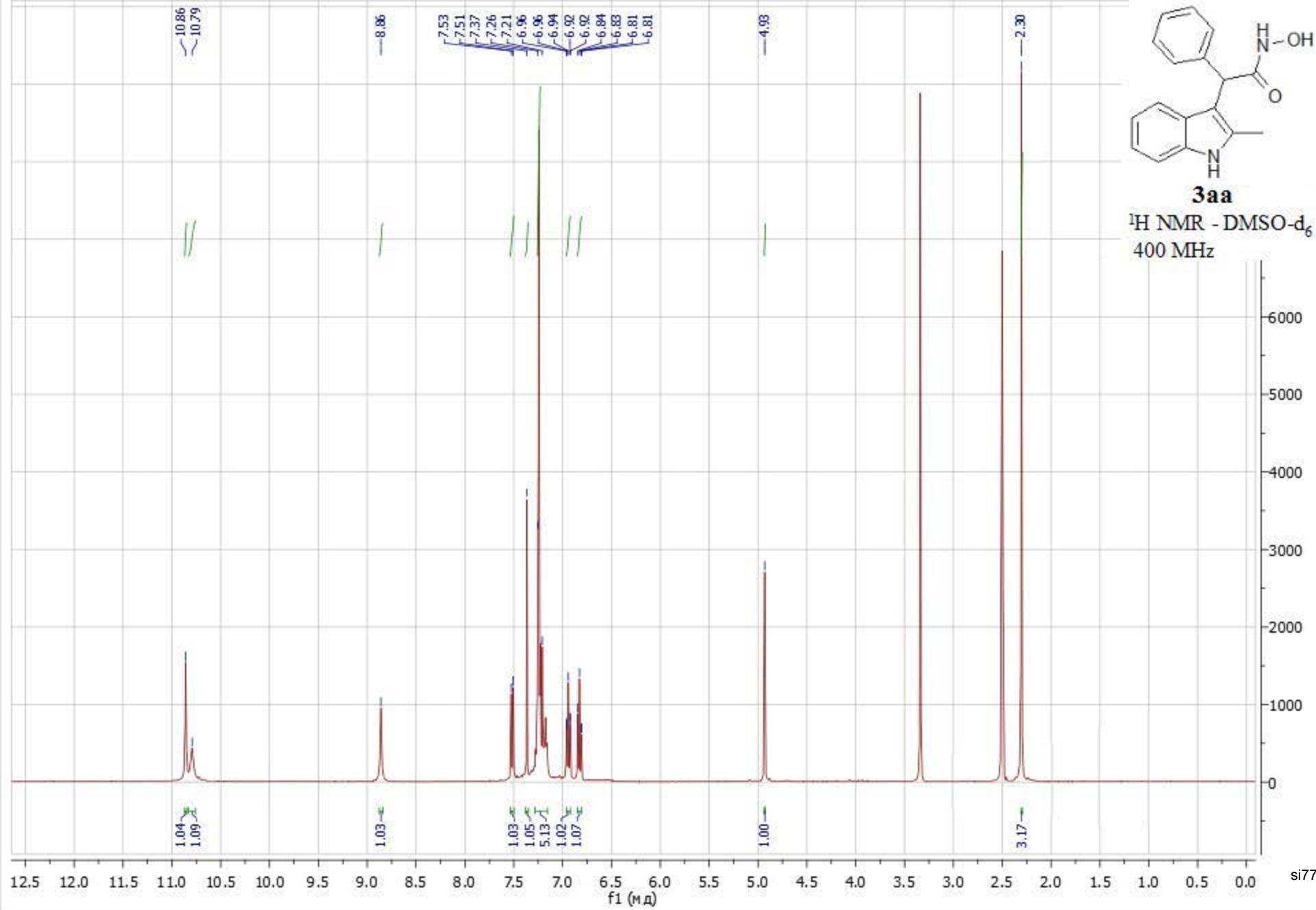


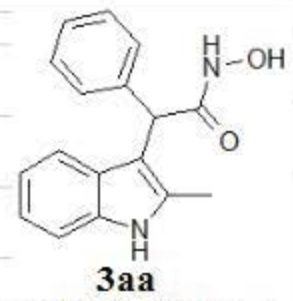




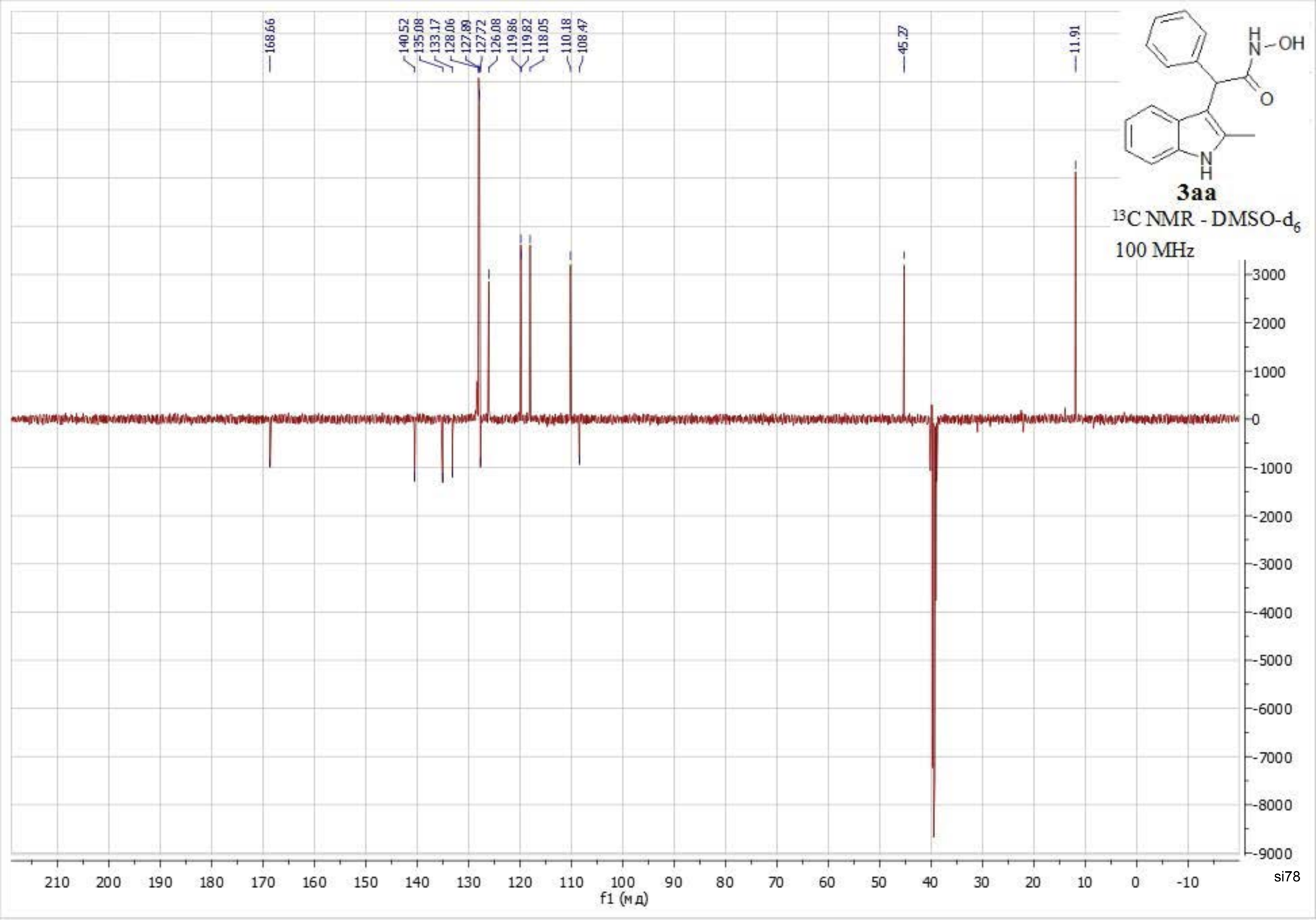
3aa

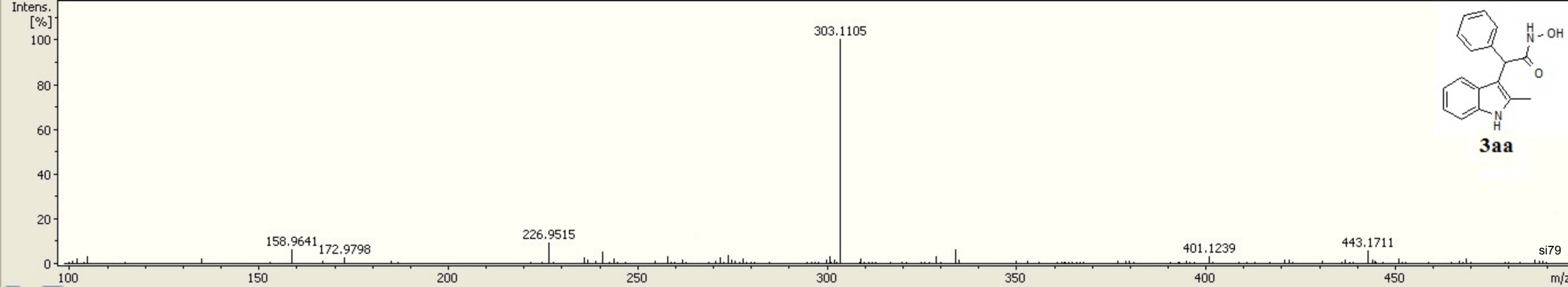
^1H NMR - DMSO- d_6
400 MHz

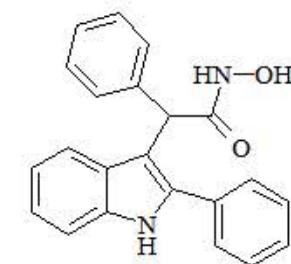




¹³C NMR - DMSO-d₆
100 MHz

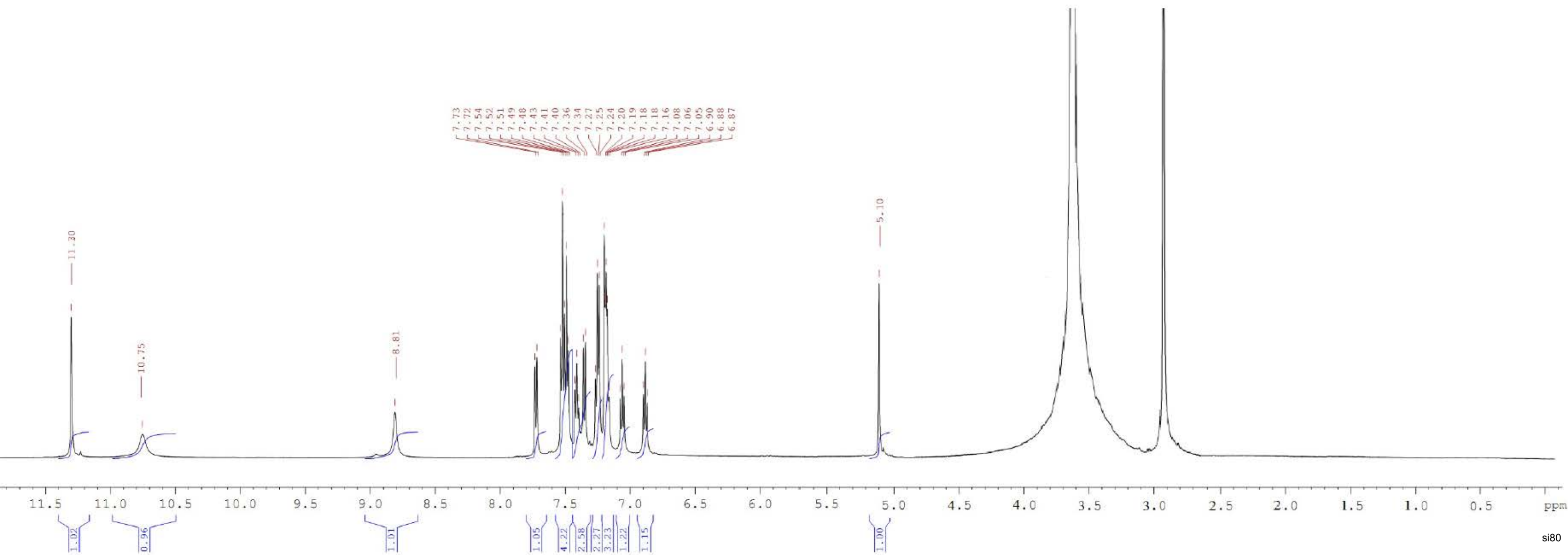


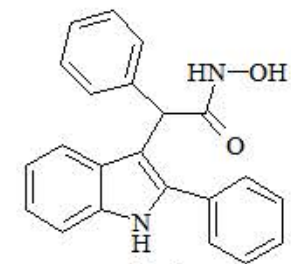




3ab

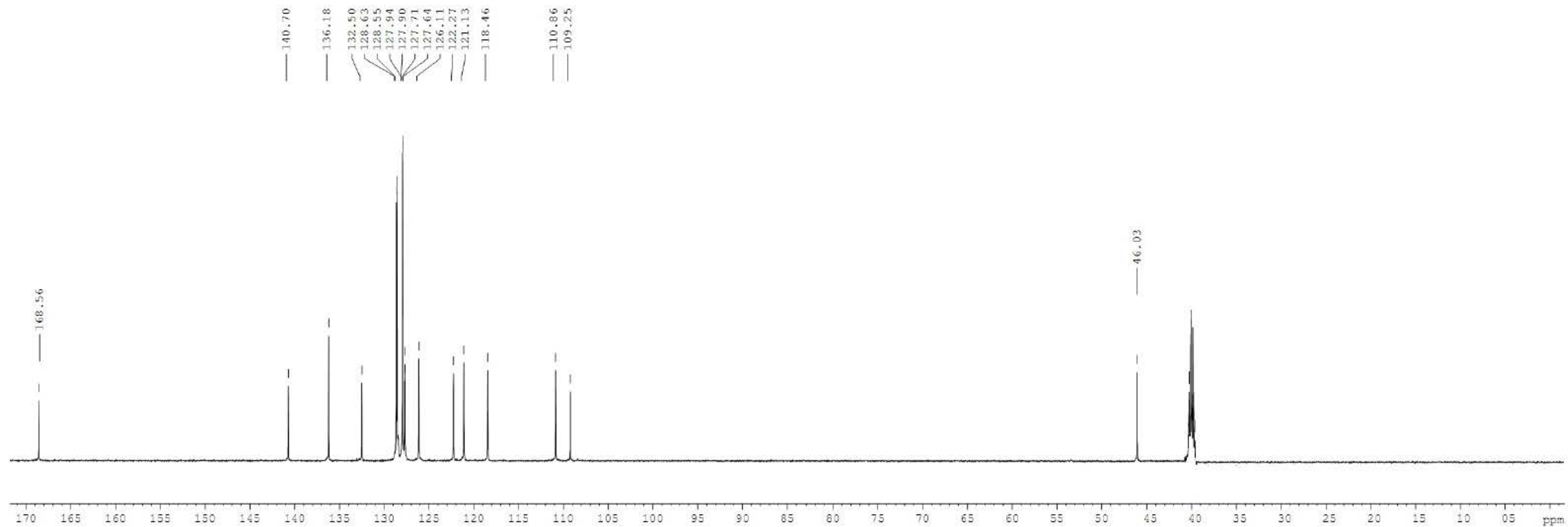
¹H NMR - DMSO-d₆
500 MHz

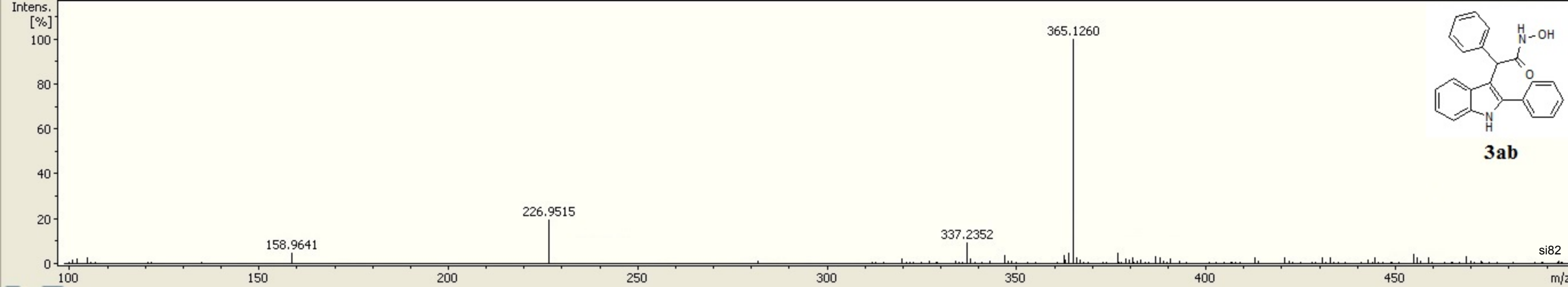


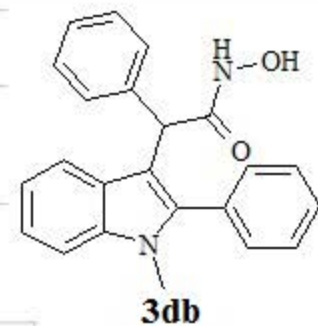


3ab

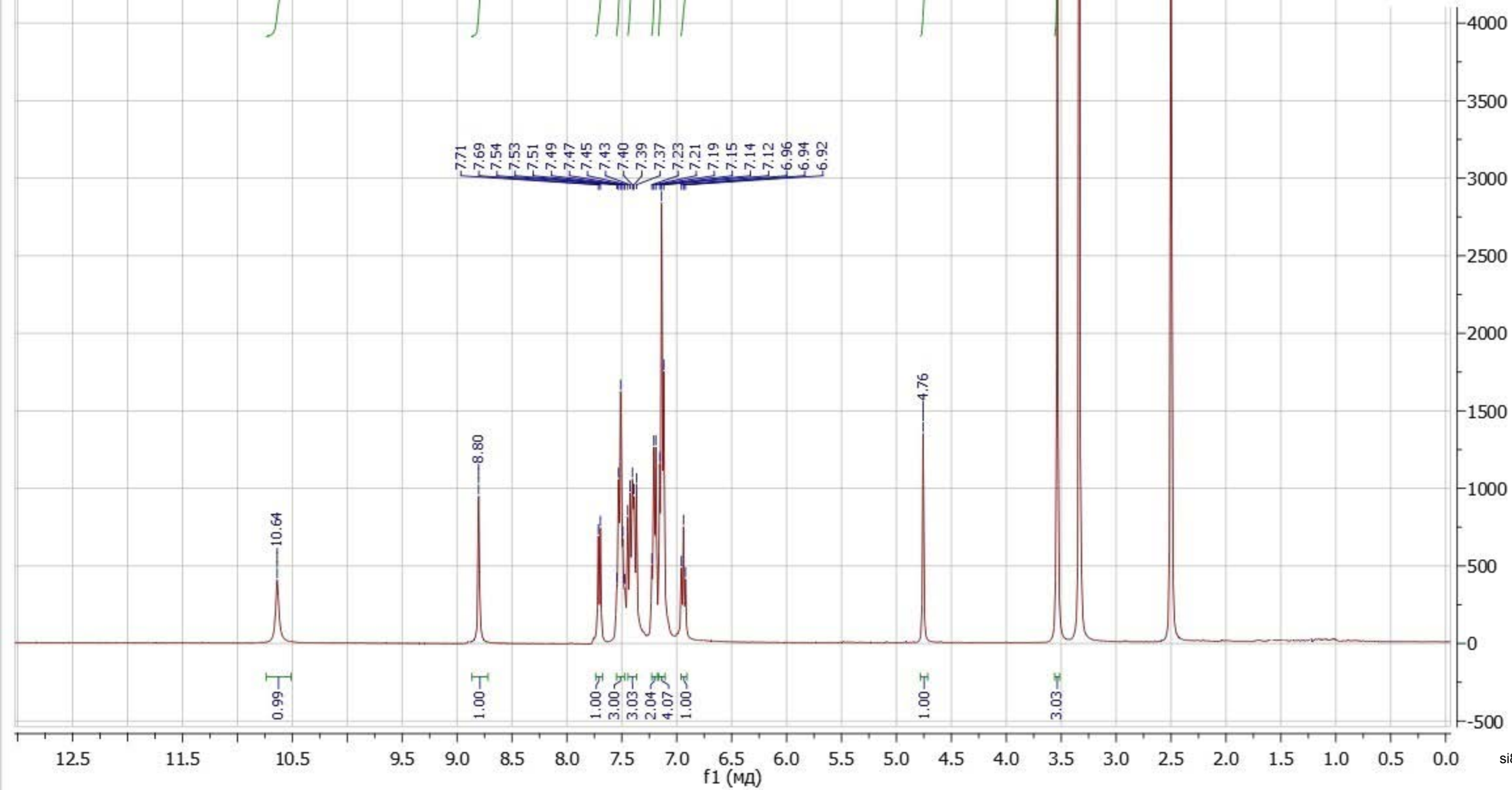
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125 MHz

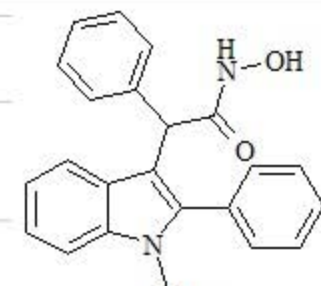






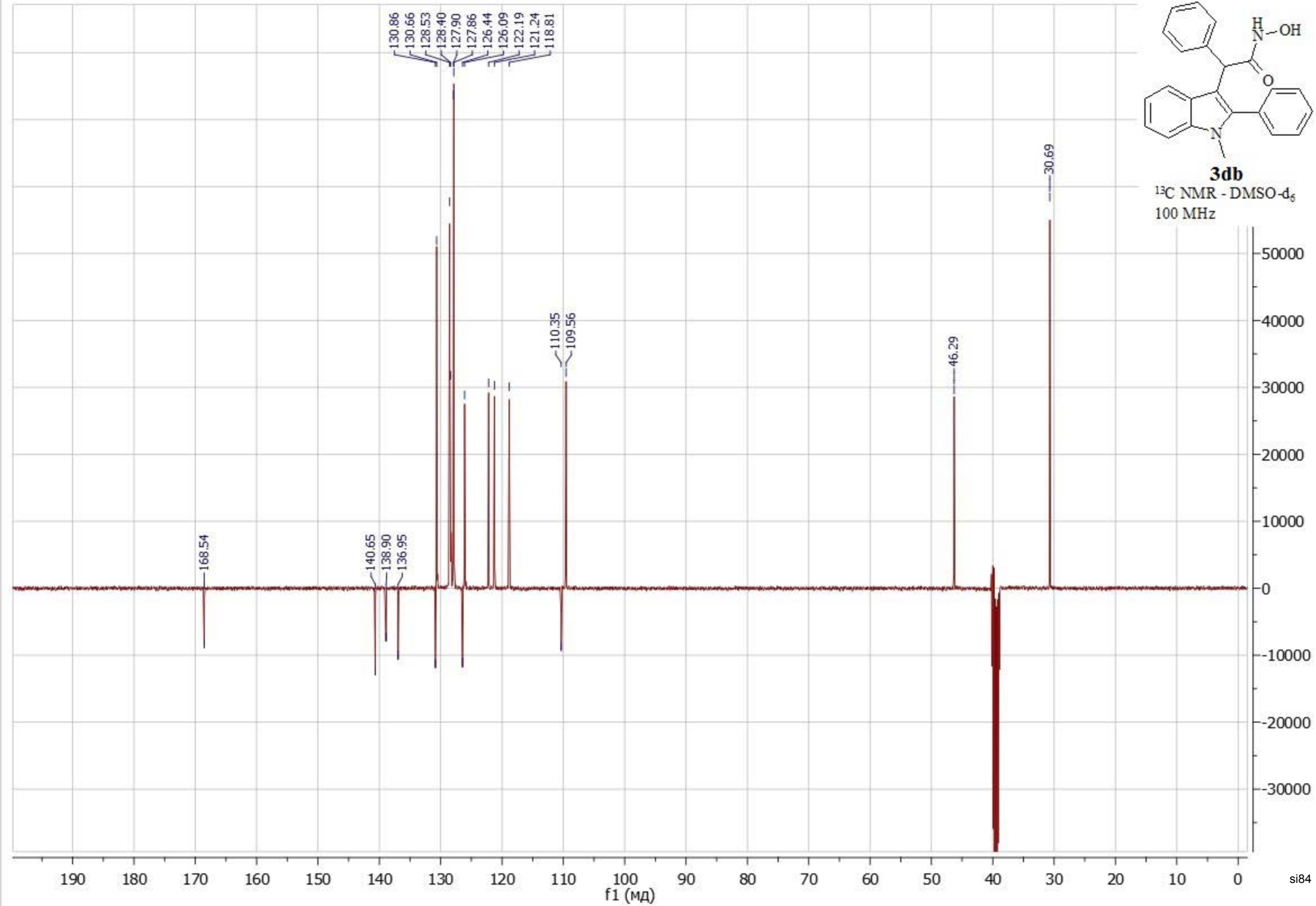
¹H NMR - DMSO-d₆
400 MHz

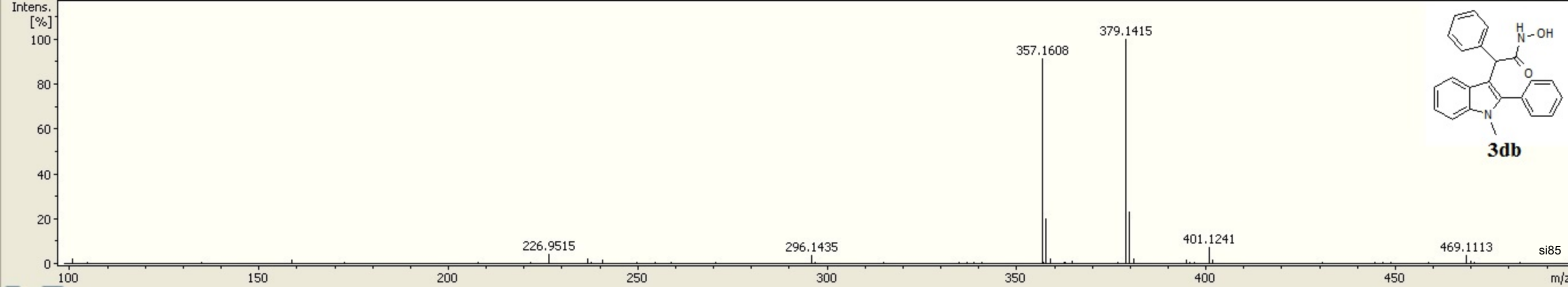


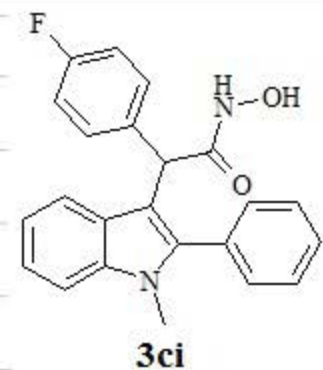


3db

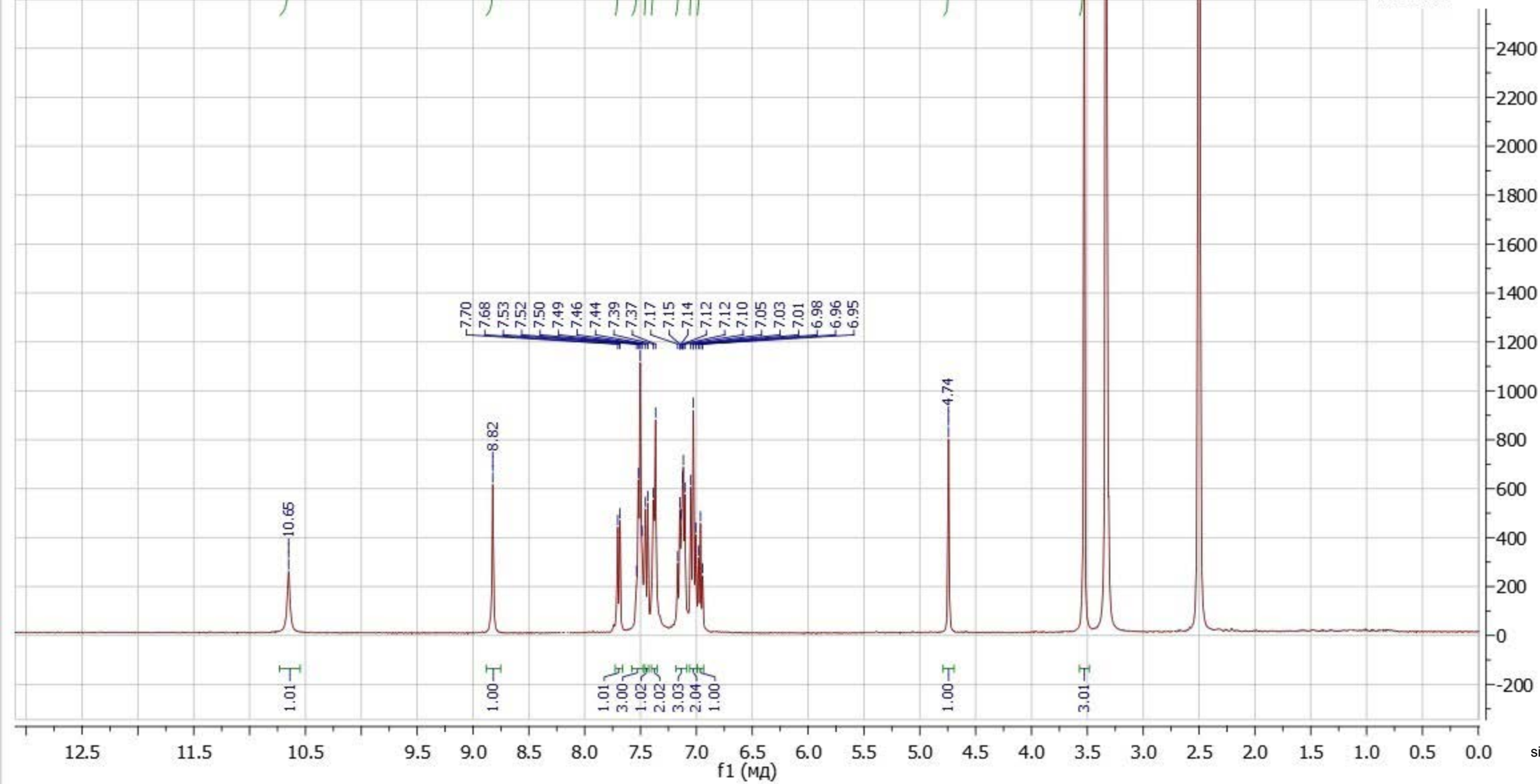
^{13}C NMR - DMSO- d_6
100 MHz

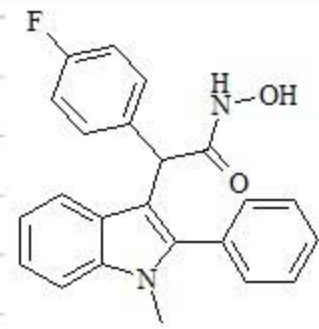




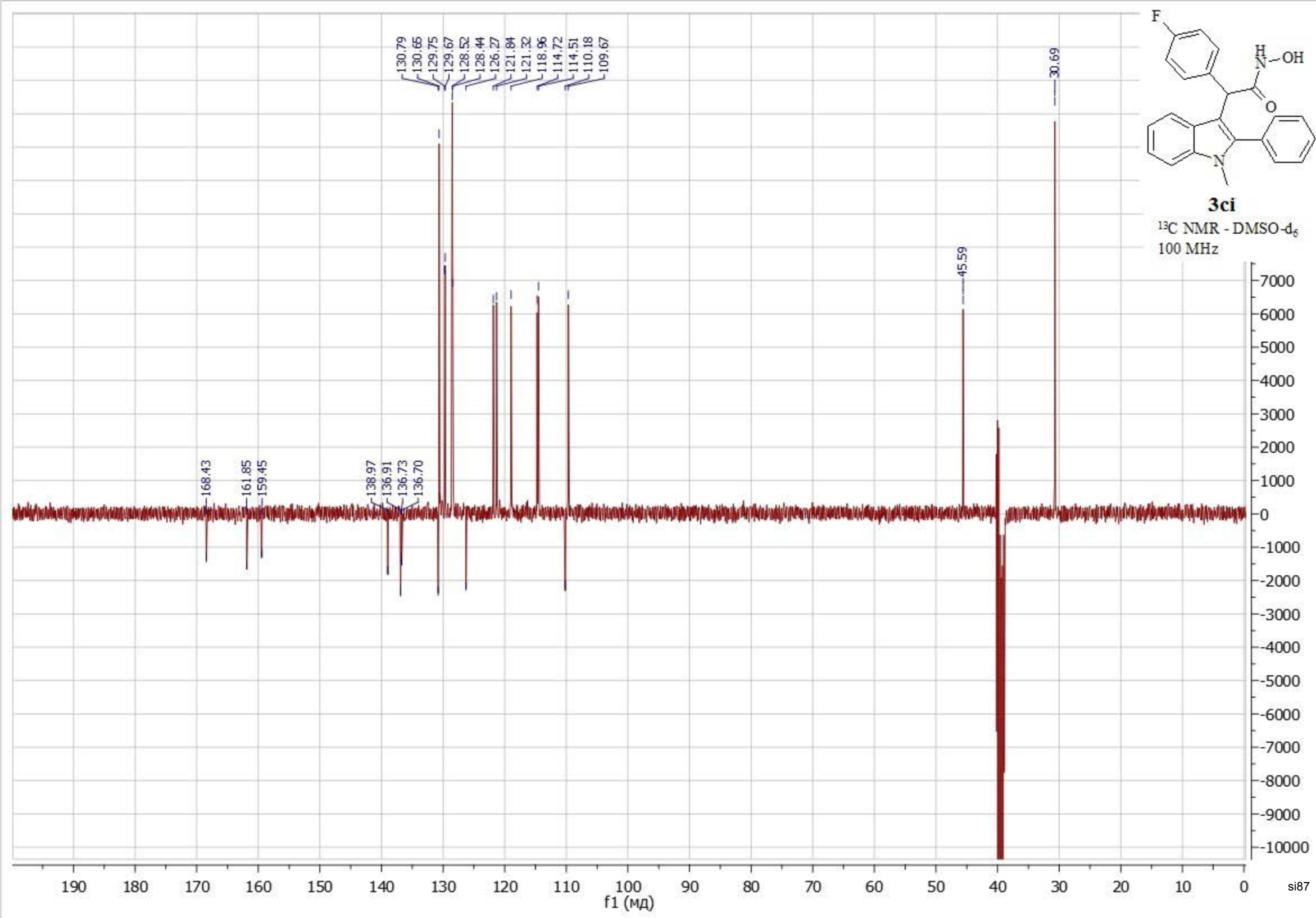


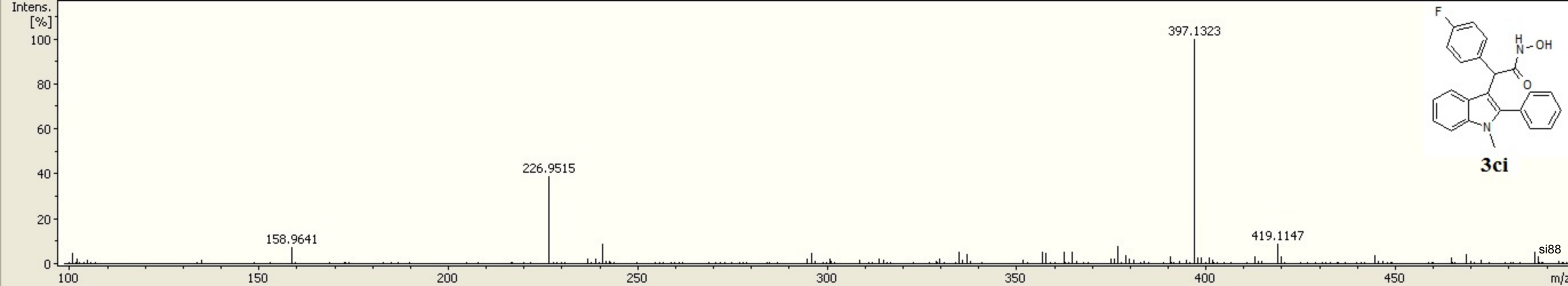
¹H NMR - DMSO-d₆
400 MHz

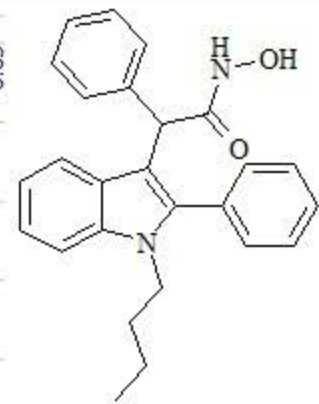




¹³C NMR - DMSO-d₆
100 MHz







3ea

¹H NMR - DMSO-d₆
400 MHz

