

## Supporting Information

# **Synthesis and biological evaluation of 1,3-dideazapurine-like 7-amino-5-hydroxymethyl-benzimidazole ribonucleoside analogues as aminoacyl-tRNA synthetase inhibitors**

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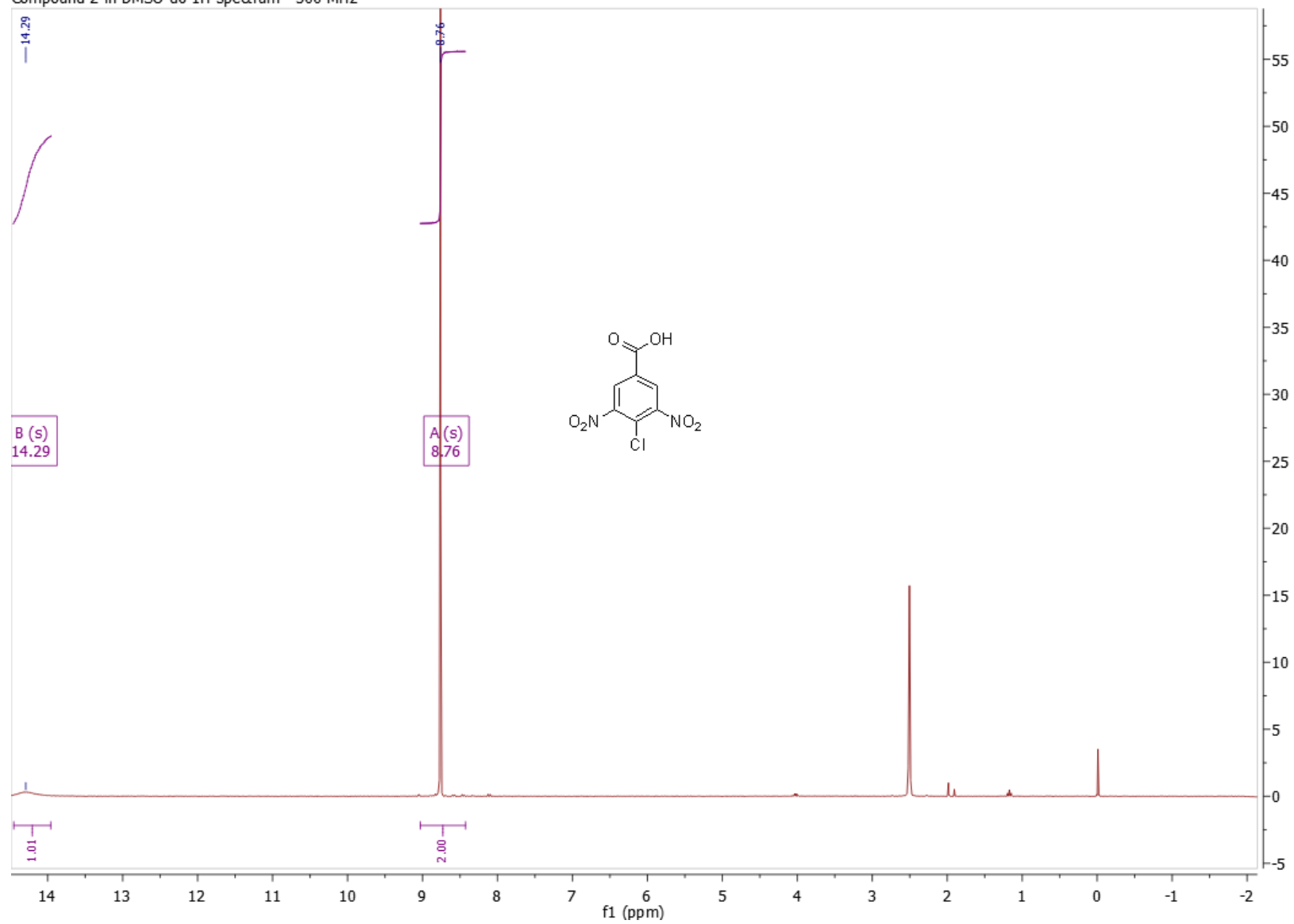
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<sup>§</sup> Present address: Hybio Medicine Park, No.37 Keji C, Str. 2nd, Shenzhen Hi-Tech Industrial Park ,P. R. China

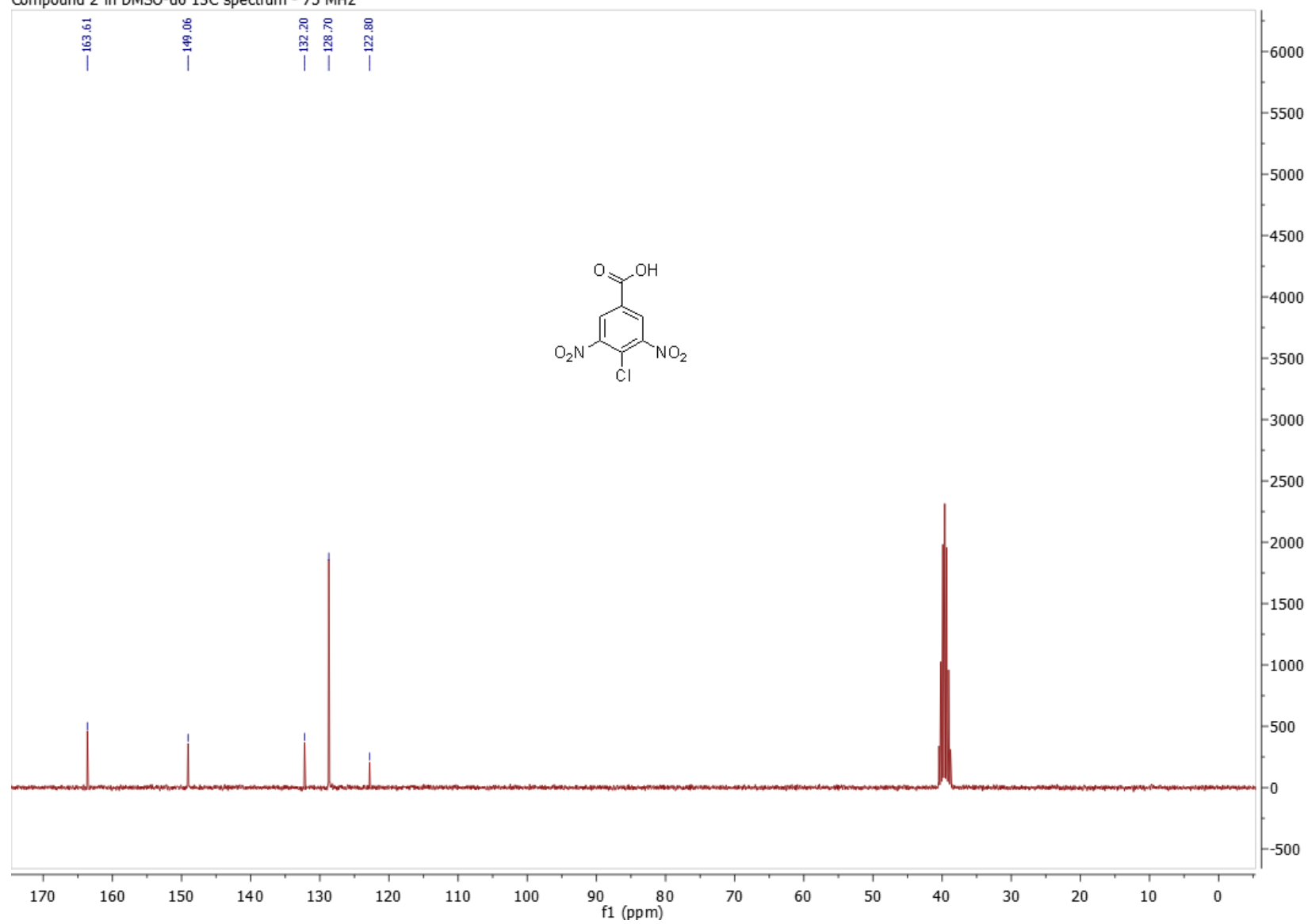
<sup>¥</sup> Present address: OrthogonX, Gaston Geenslaan 1, 3001 Leuven, Belgium

\* Corresponding author: [Arthur.Vanaerschot@kuleuven.be](mailto:Arthur.Vanaerschot@kuleuven.be)

Compound 2 in DMSO-d6 1H spectrum - 300 MHz



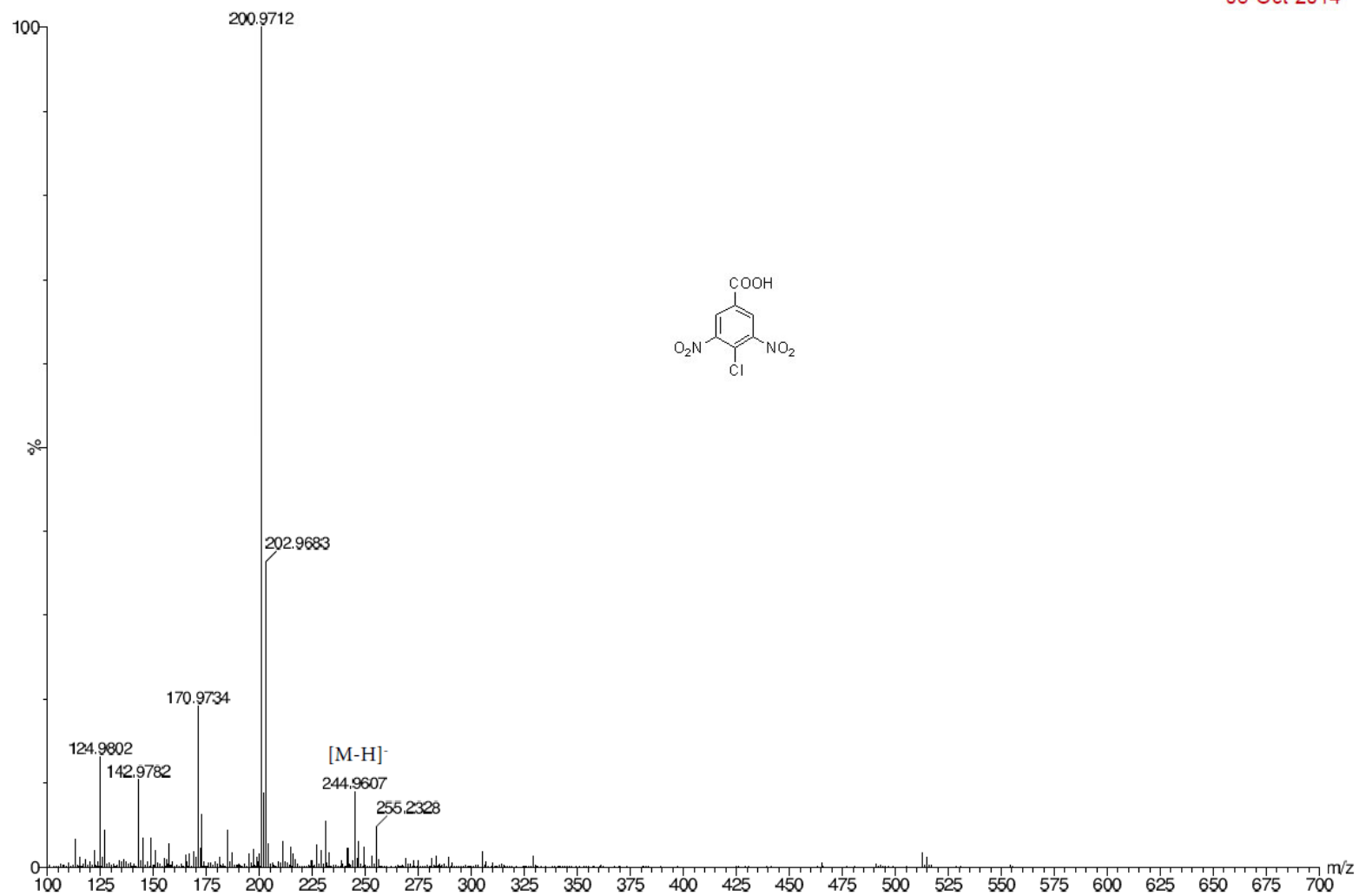
Compound 2 in DMSO-d6 13C spectrum - 75 MHz



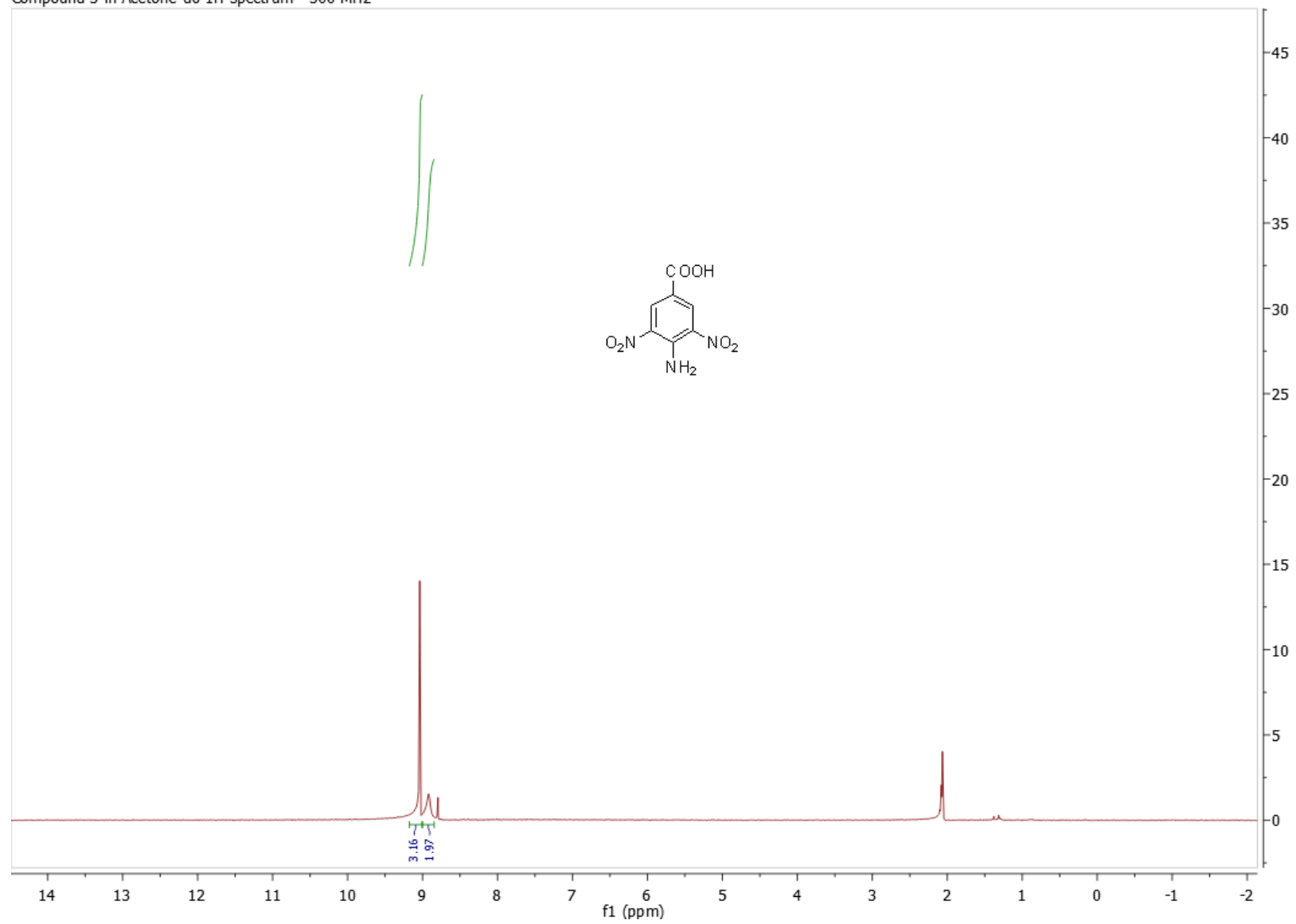
compound 2

accurate mass

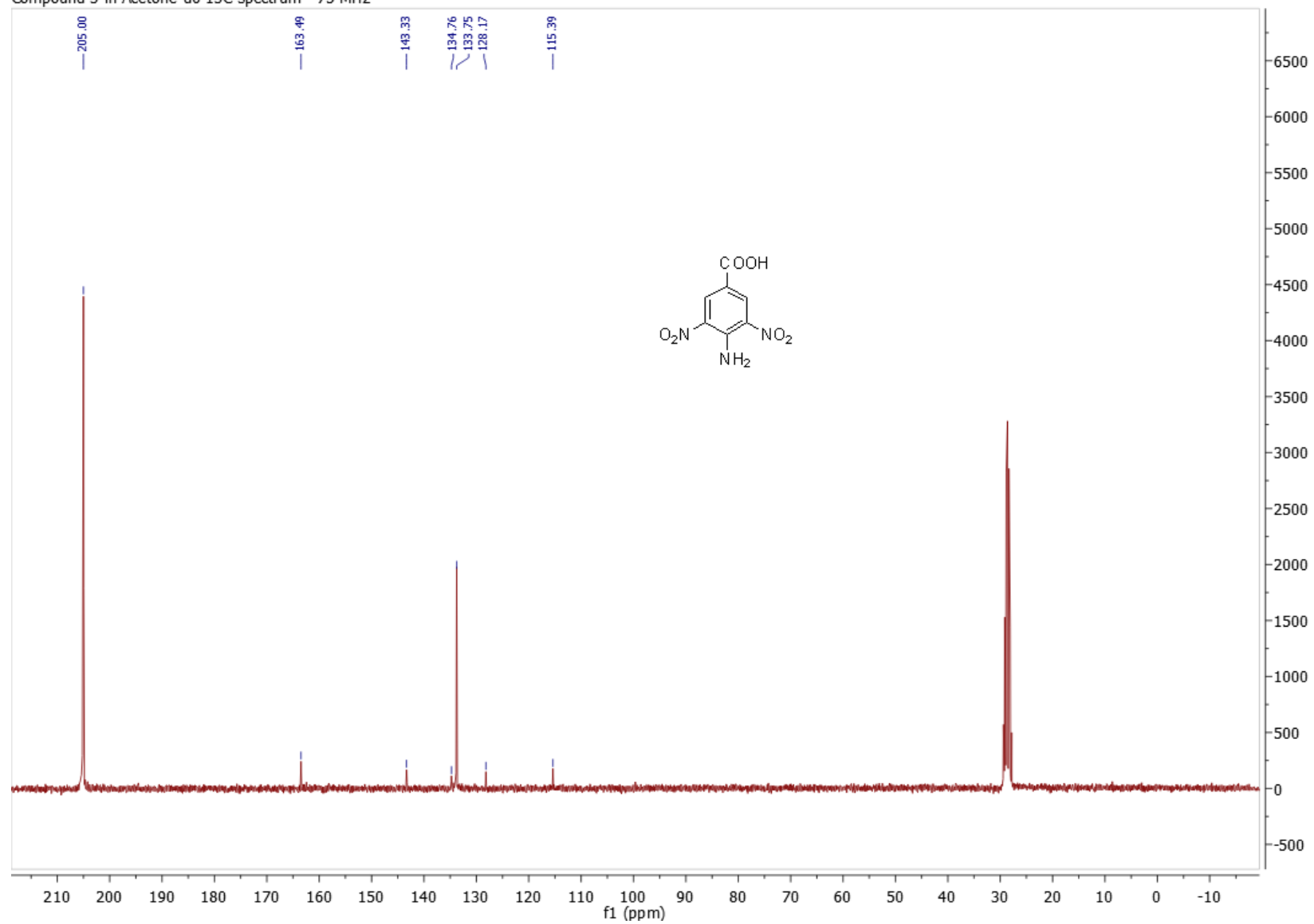
ES-  
08-Oct-2014



Compound 3 in Acetone-d6 1H spectrum - 300 MHz



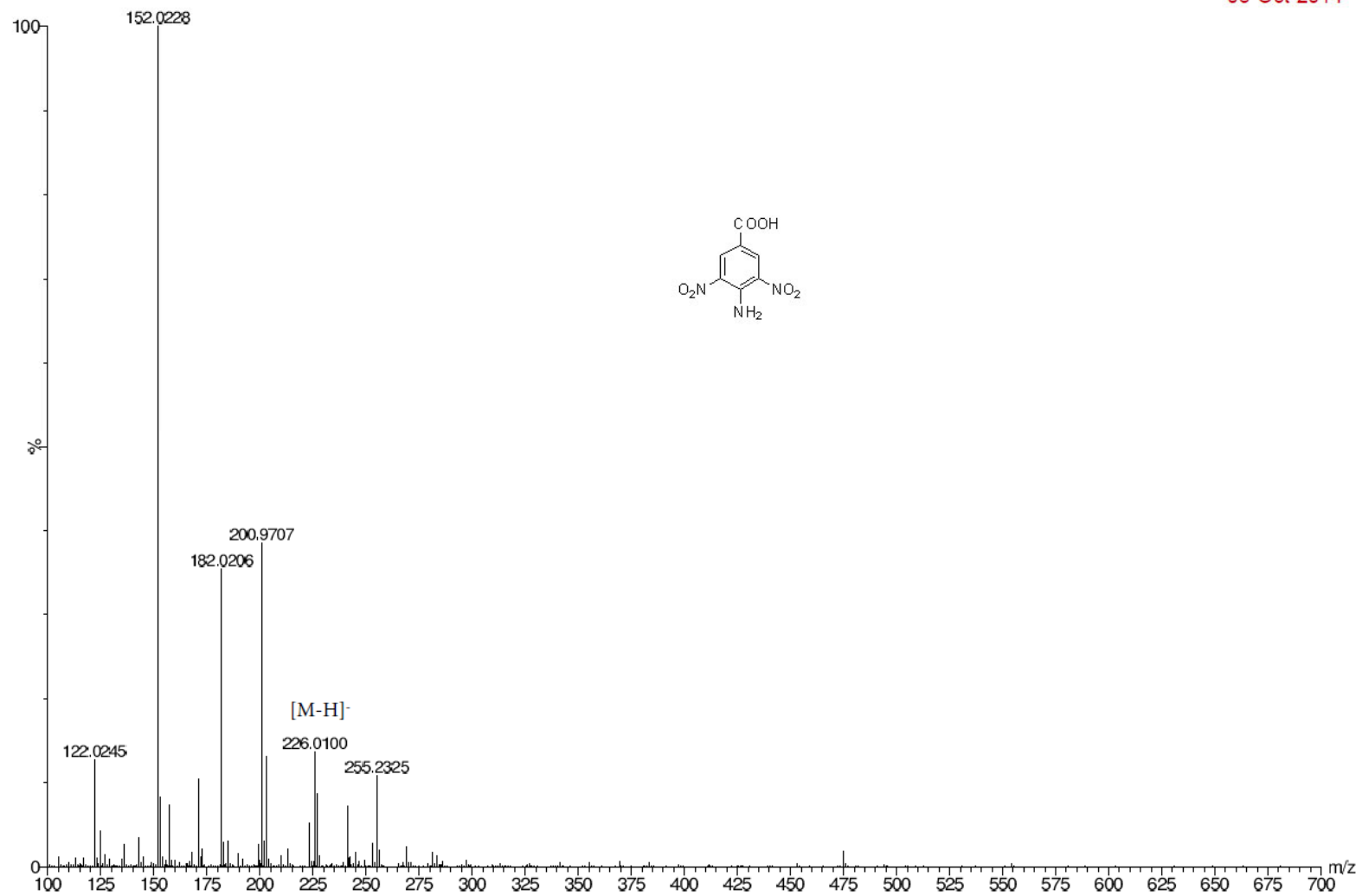
Compound 3 in Acetone-d6 13C spectrum - 75 MHz



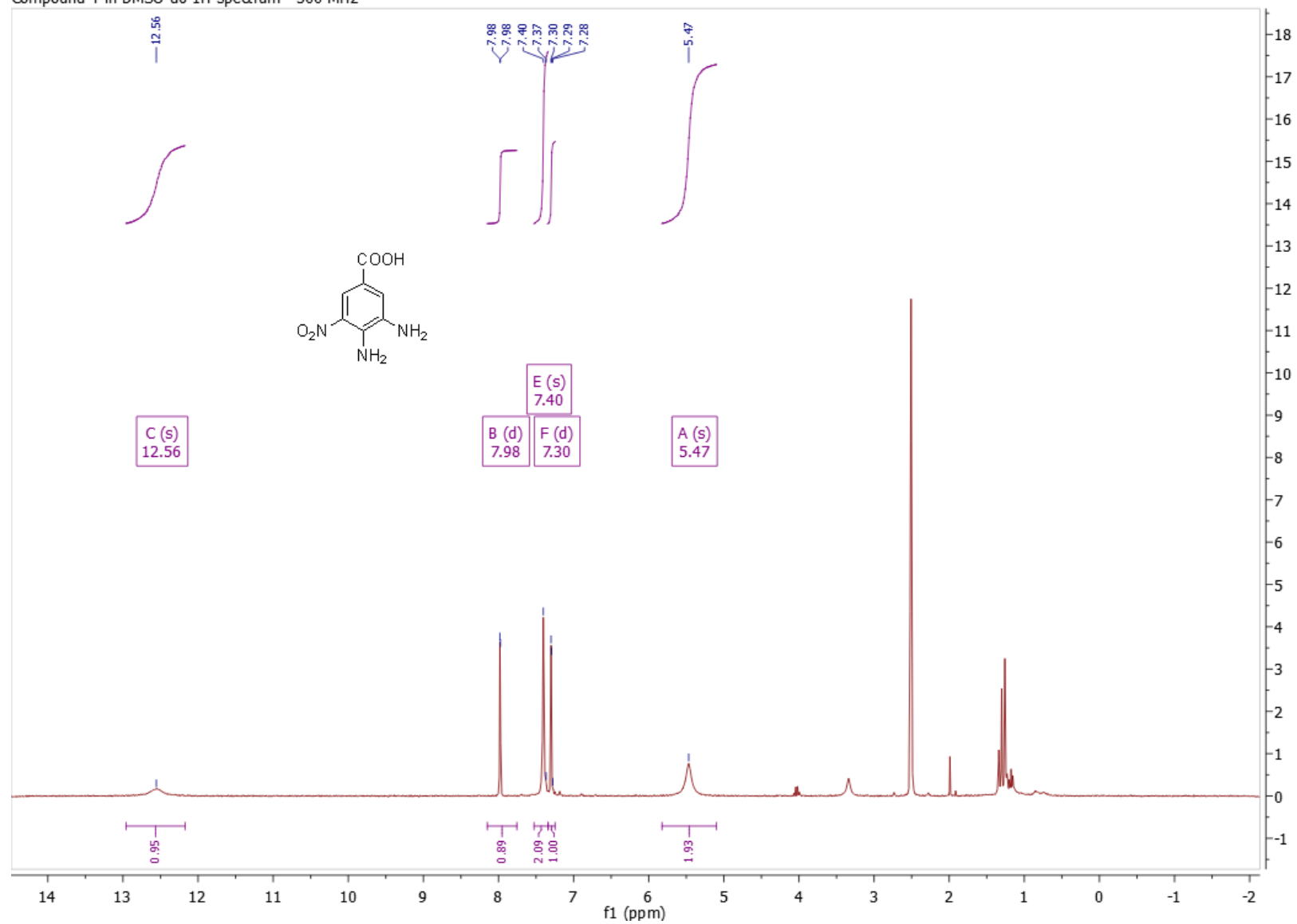
compound 3

accurate mass

ES-  
08-Oct-2014

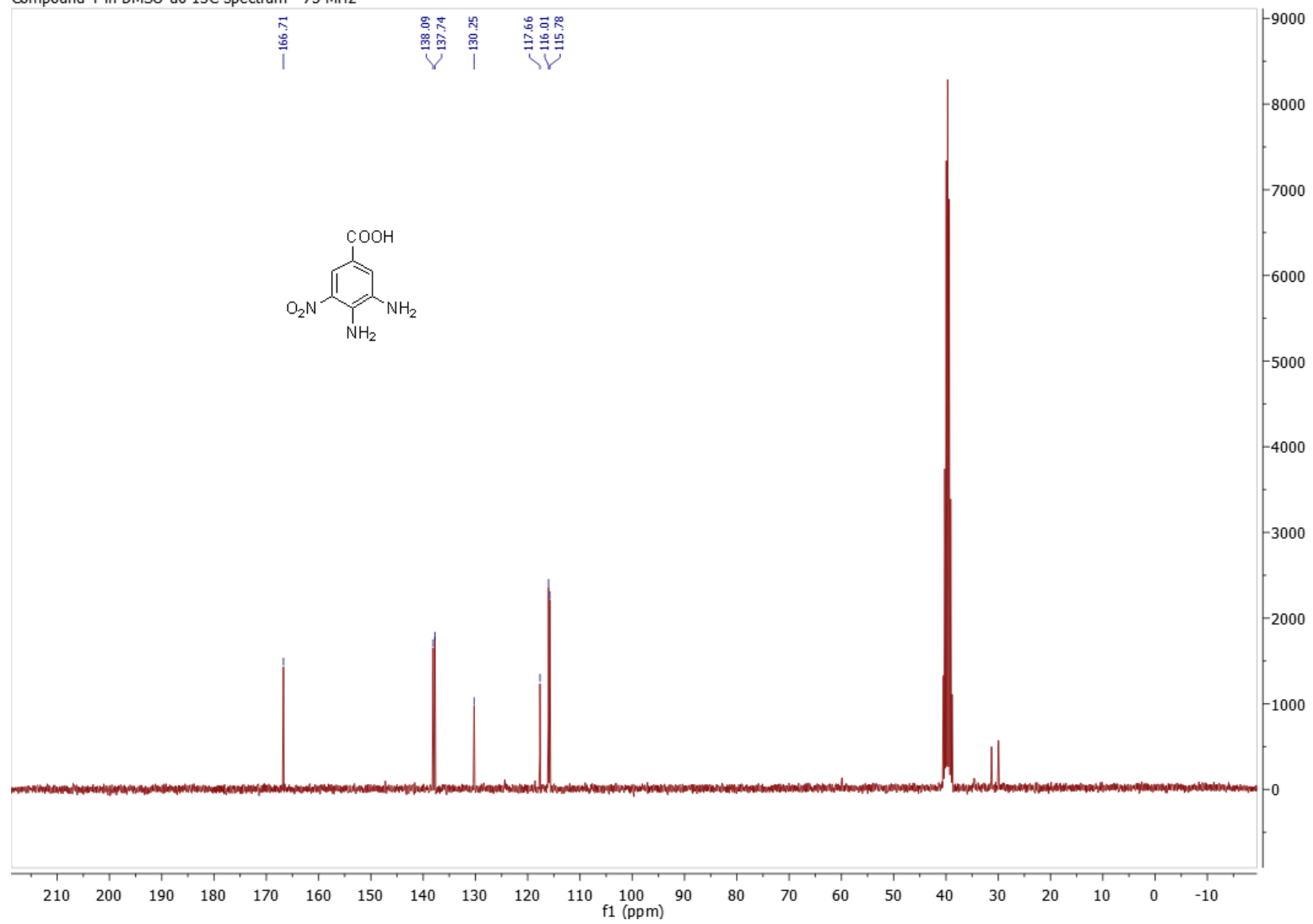


Compound 4 in DMSO-d6 1H spectrum - 300 MHz





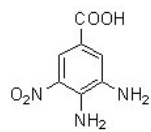
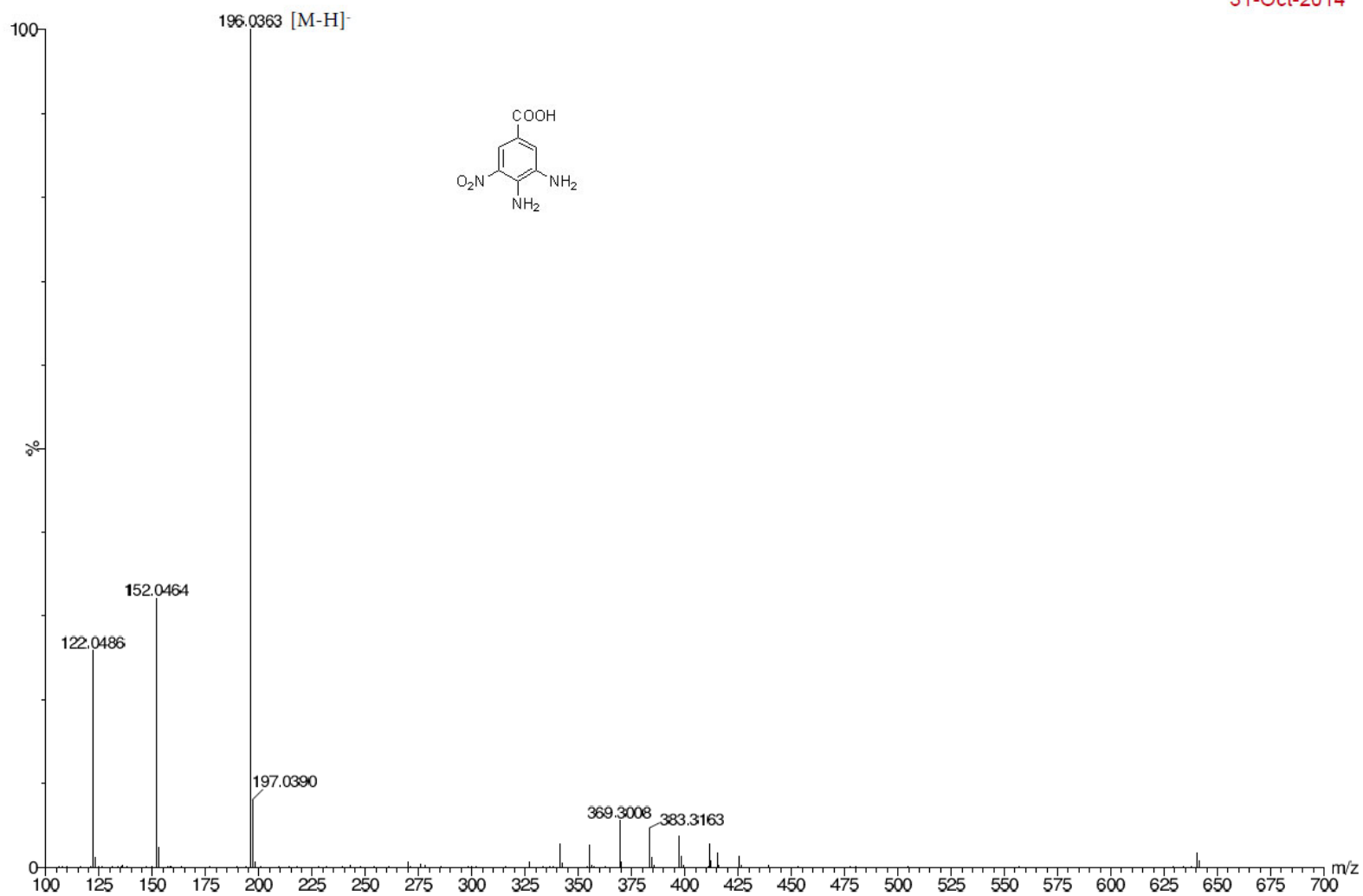
Compound 4 in DMSO-d6 13C spectrum - 75 MHz



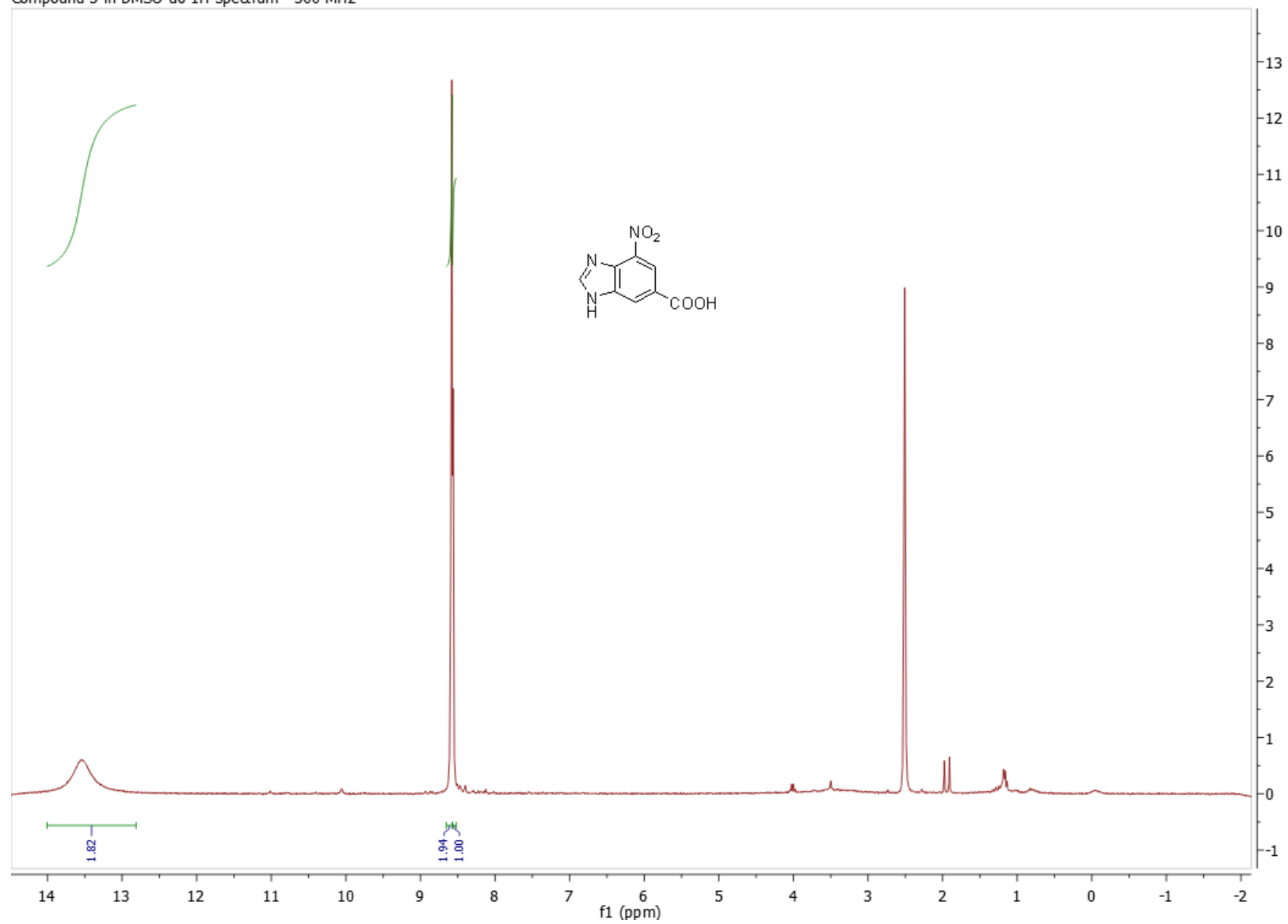
compound 4

accurate mass

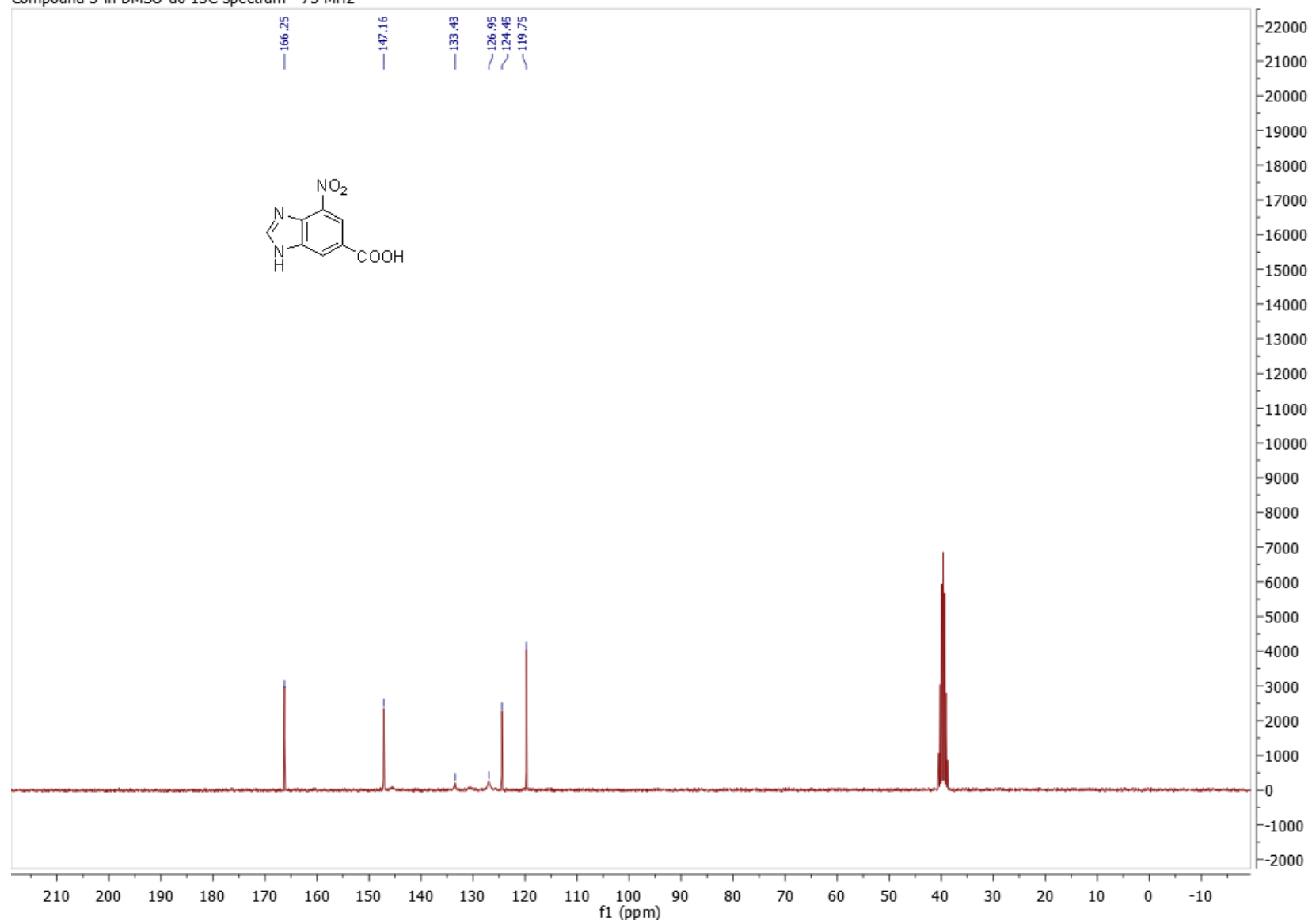
ES-  
31-Oct-2014



Compound 5 in DMSO-d6 1H spectrum - 300 MHz



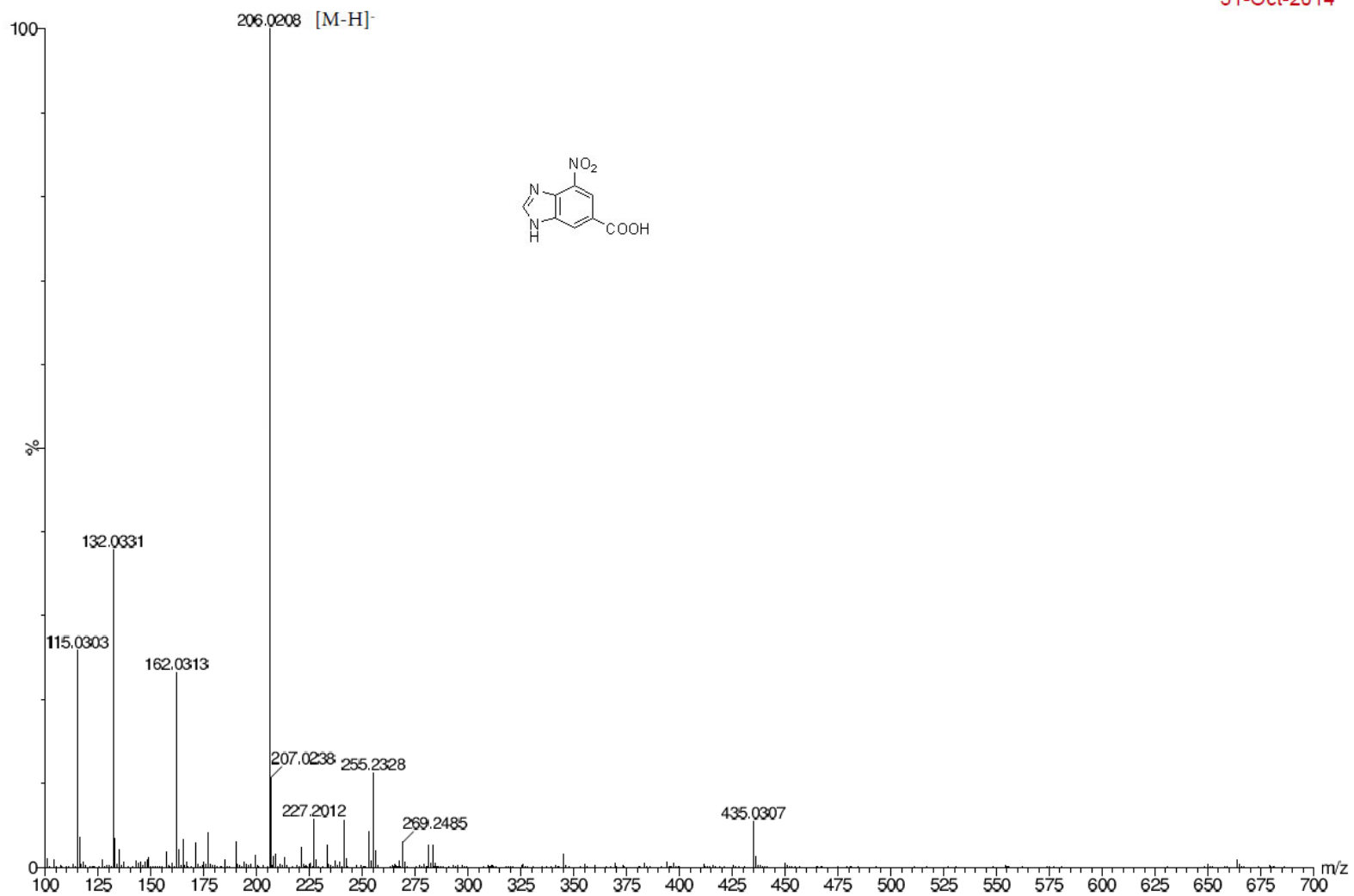
Compound 5 in DMSO-d6 13C spectrum - 75 MHz



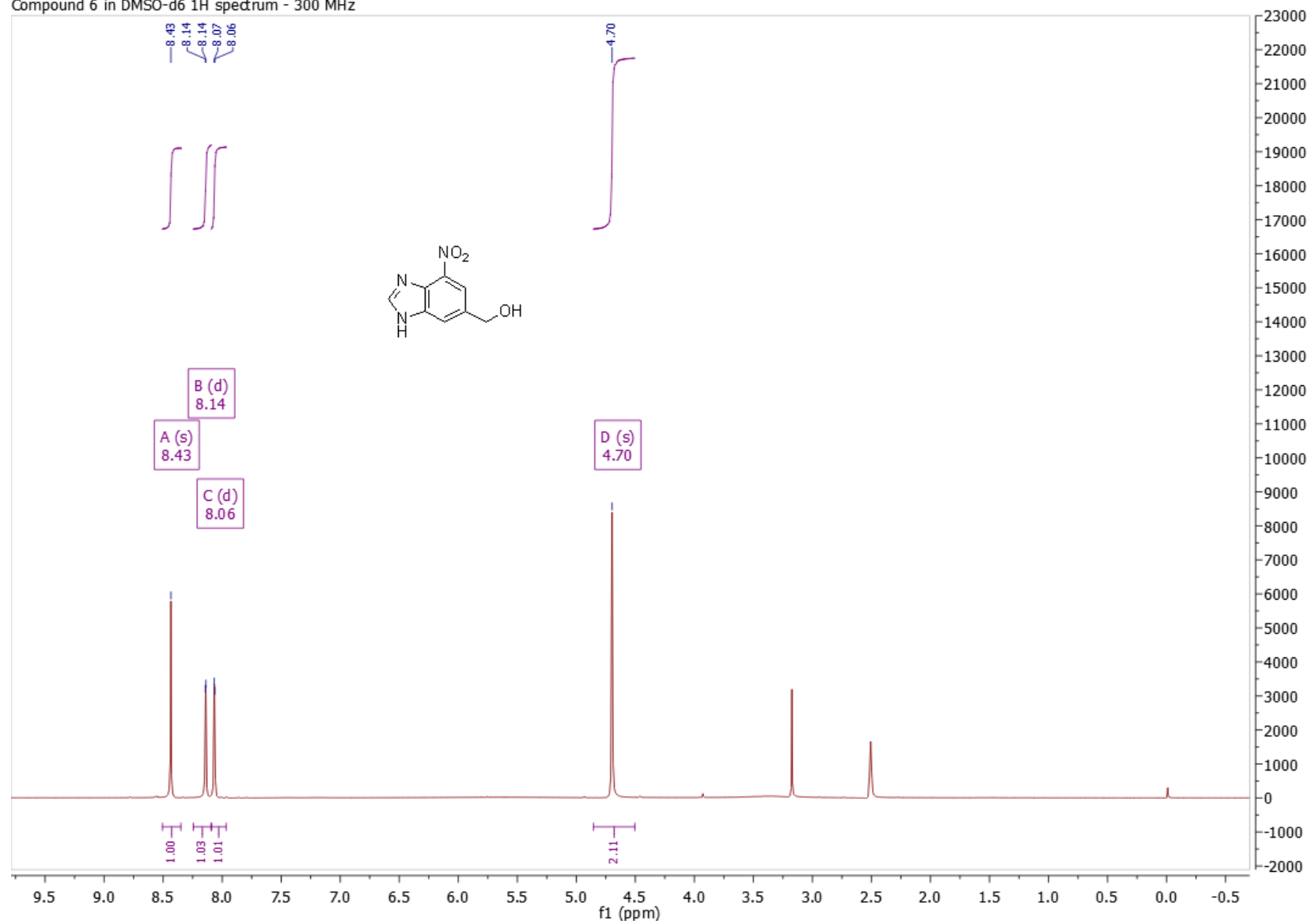
compound 5

accurate mass

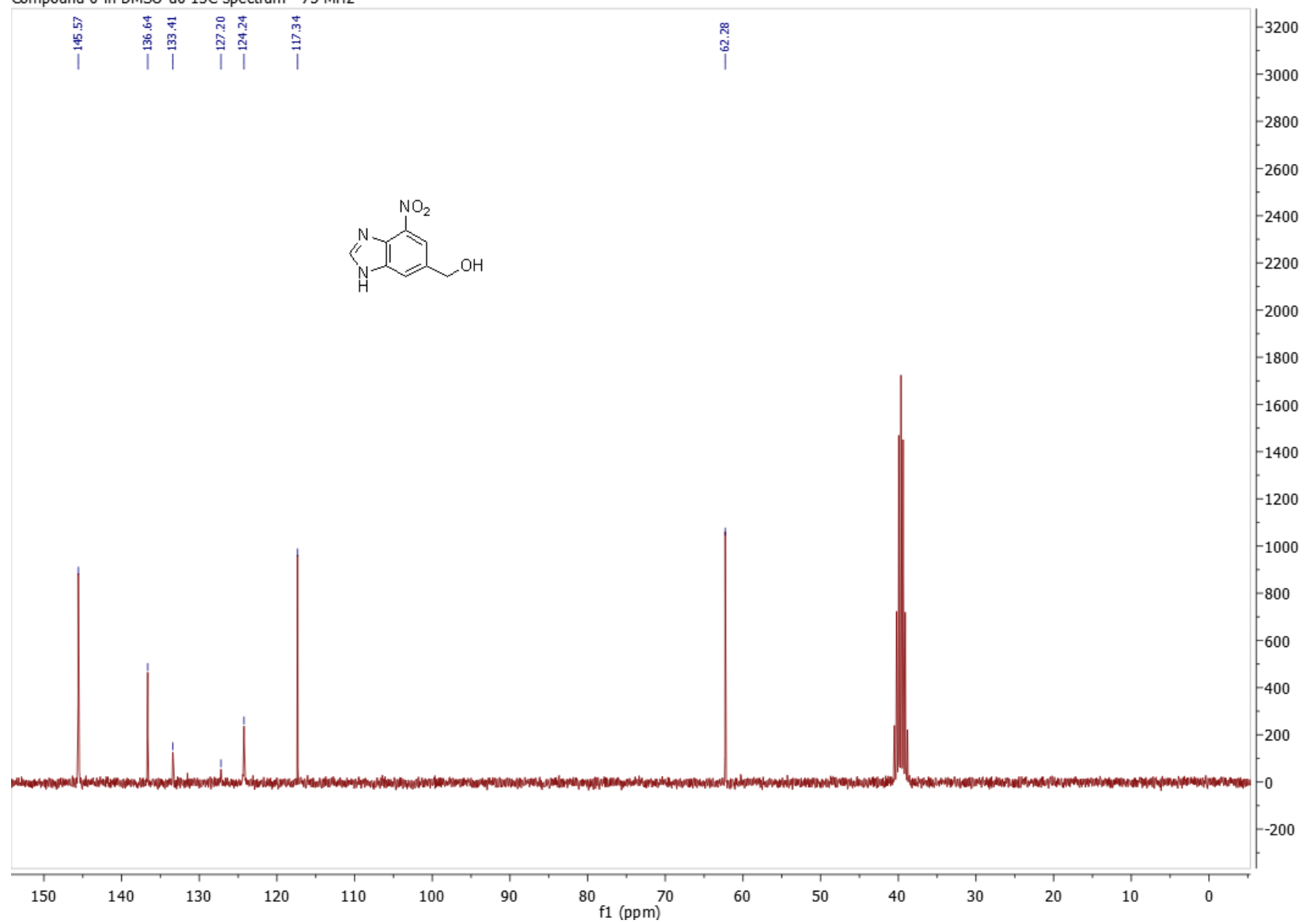
ES-  
31-Oct-2014



Compound 6 in DMSO-d6 1H spectrum - 300 MHz



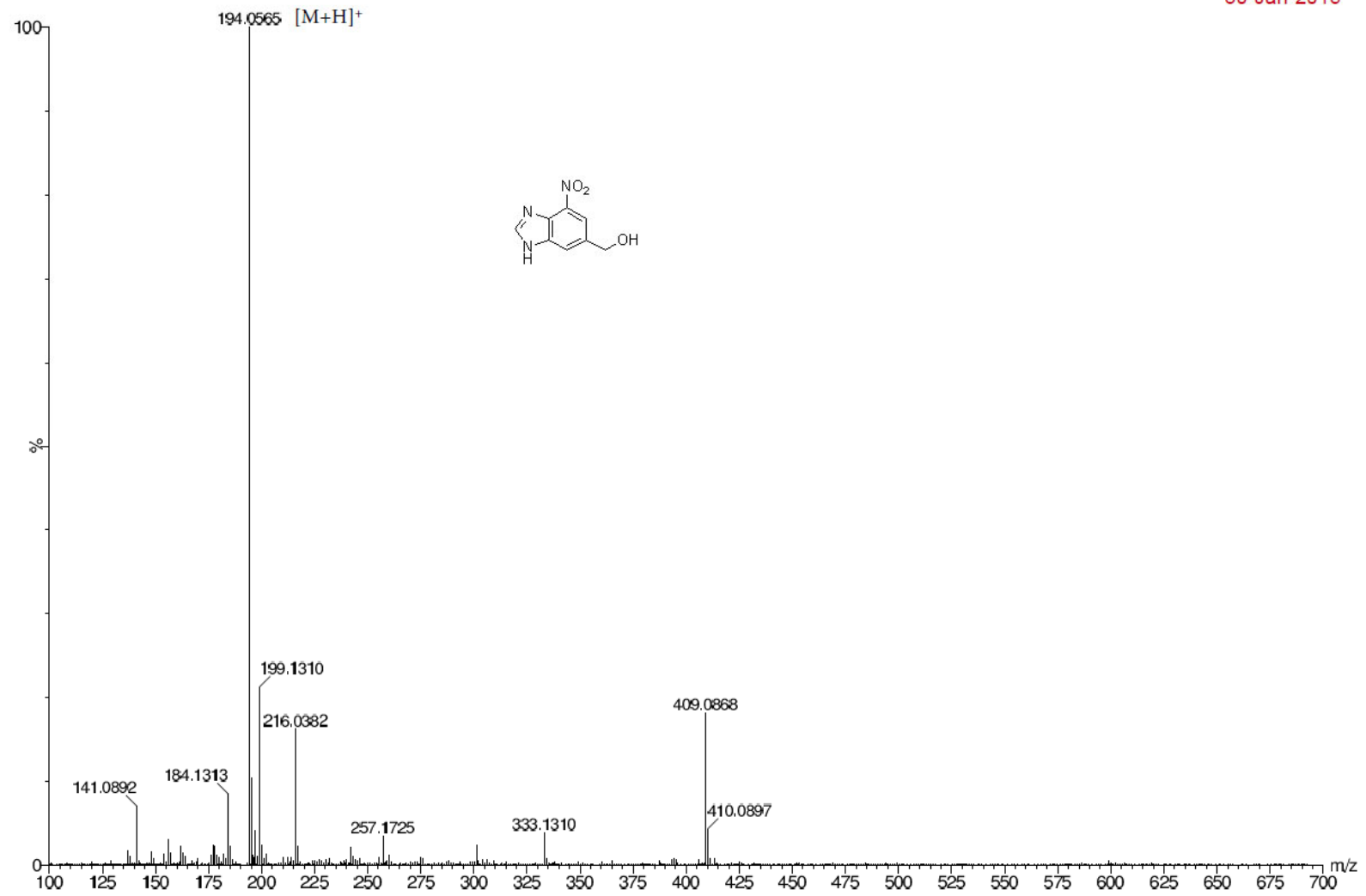
Compound 6 in DMSO-d6 13C spectrum - 75 MHz



compound 6

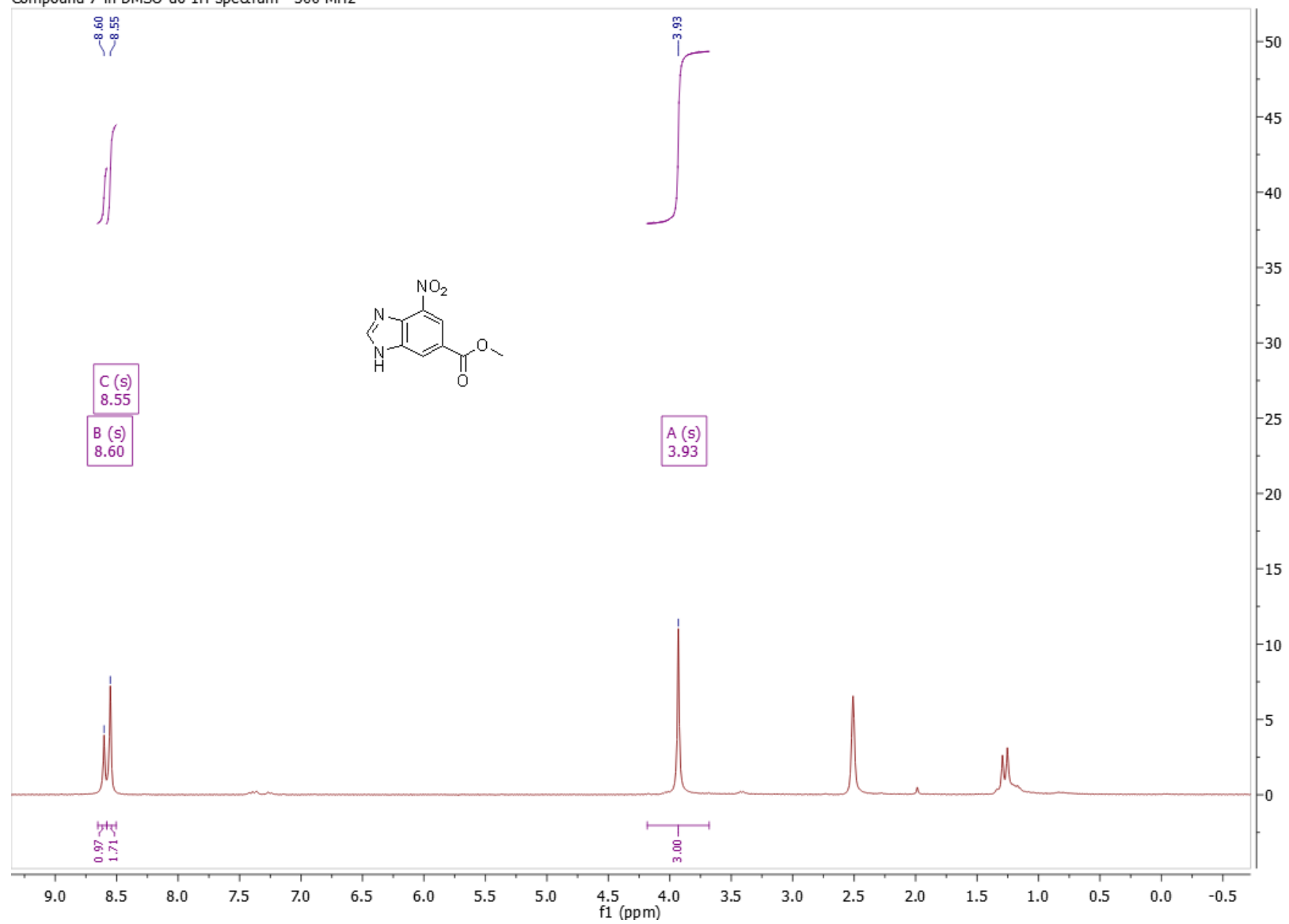
accurate mass

ES+  
30-Jan-2015

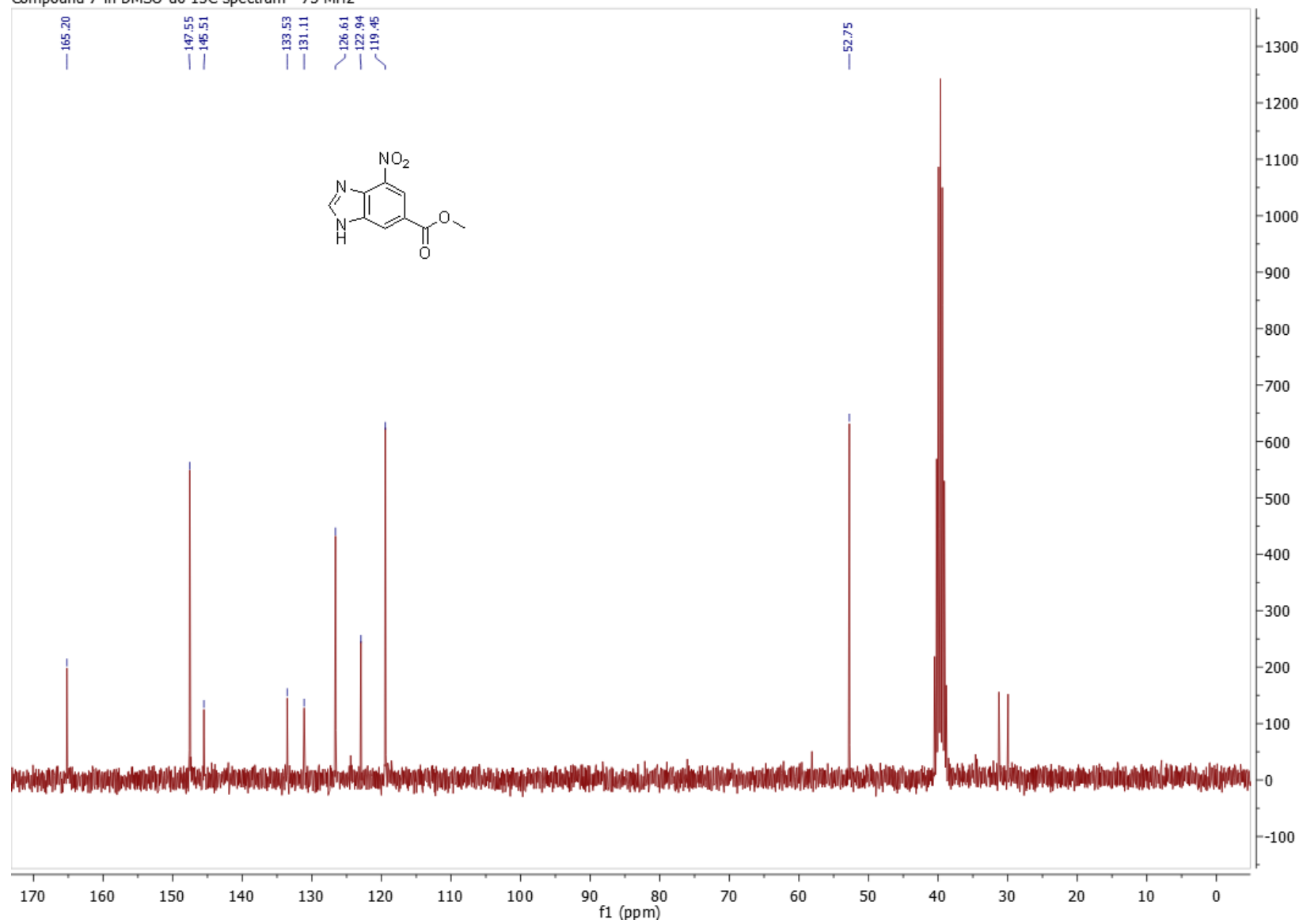




Compound 7 in DMSO-d6 1H spectrum - 300 MHz



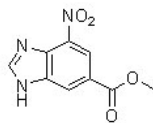
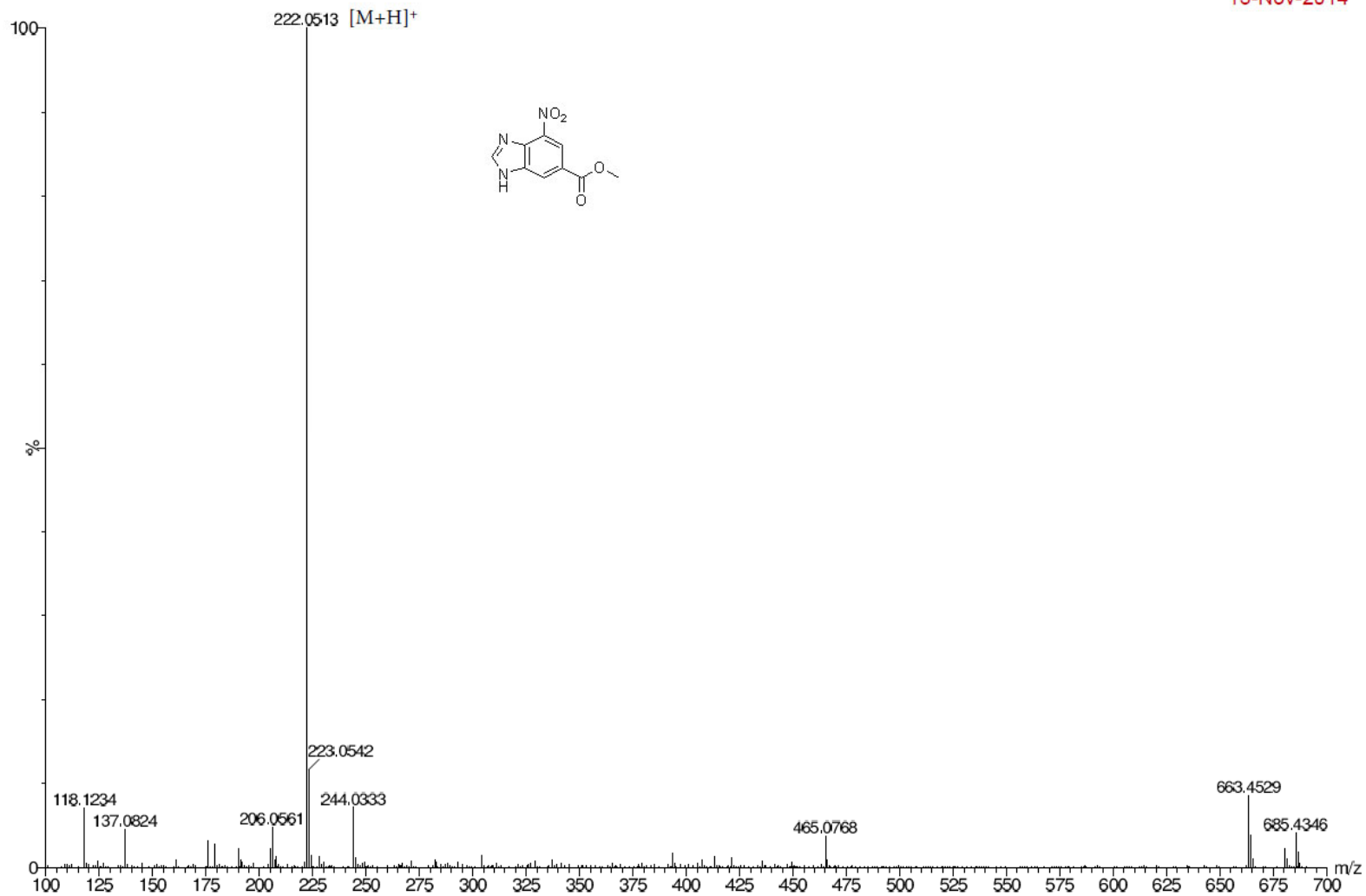
Compound 7 in DMSO-d6 13C spectrum - 75 MHz



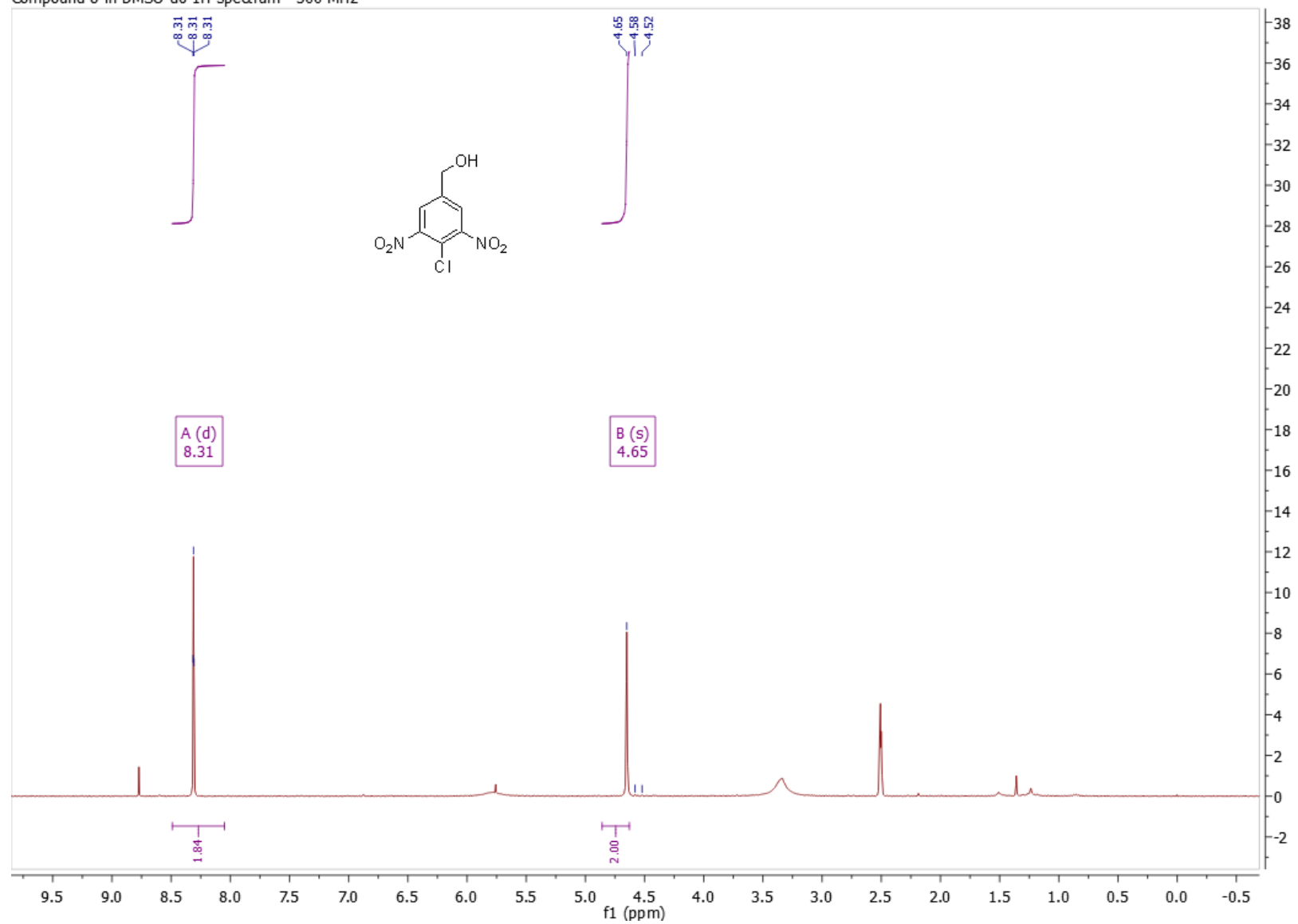
compound 7

accurate mass

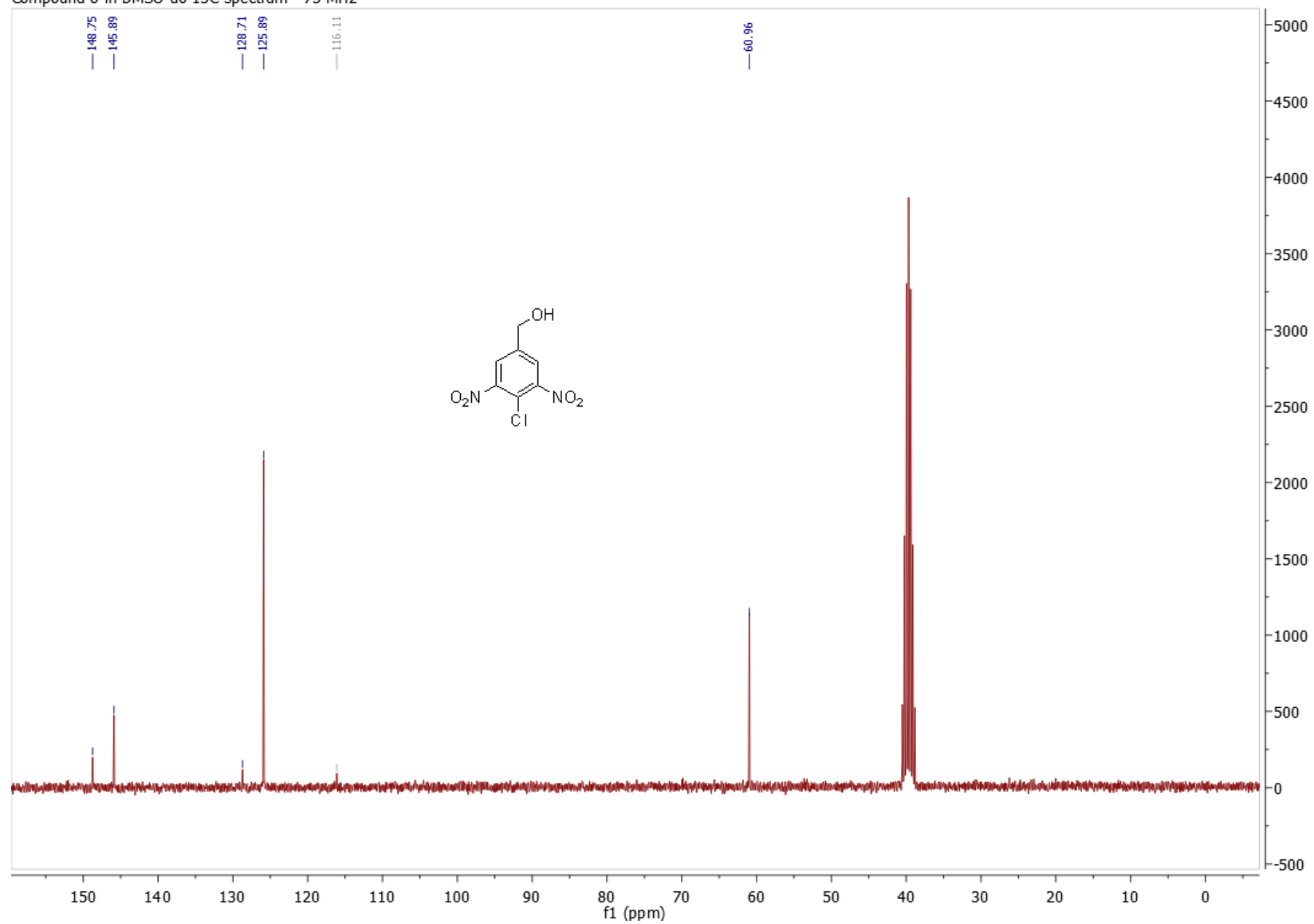
ES+  
13-Nov-2014



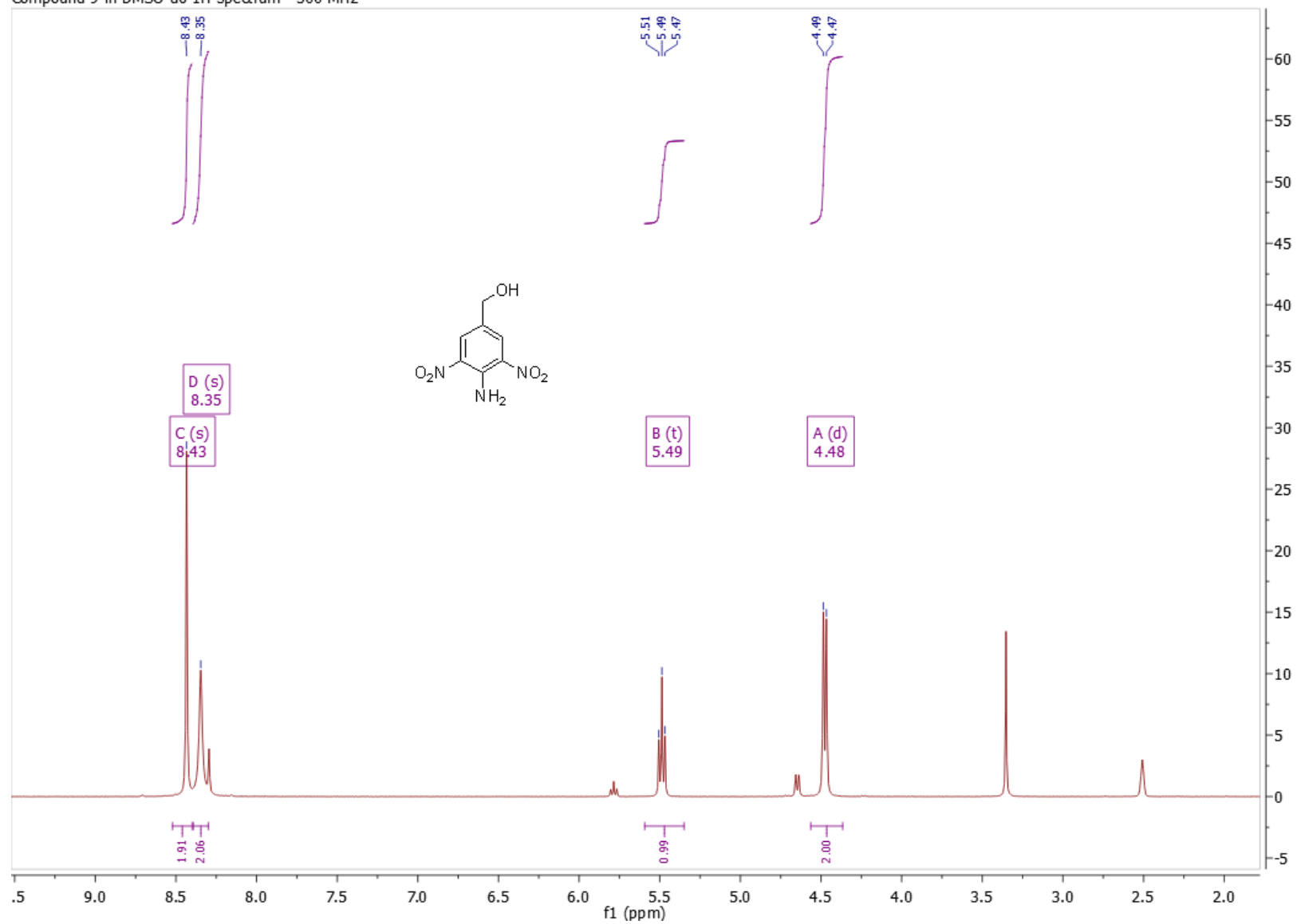
Compound 8 in DMSO-d6 1H spectrum - 300 MHz



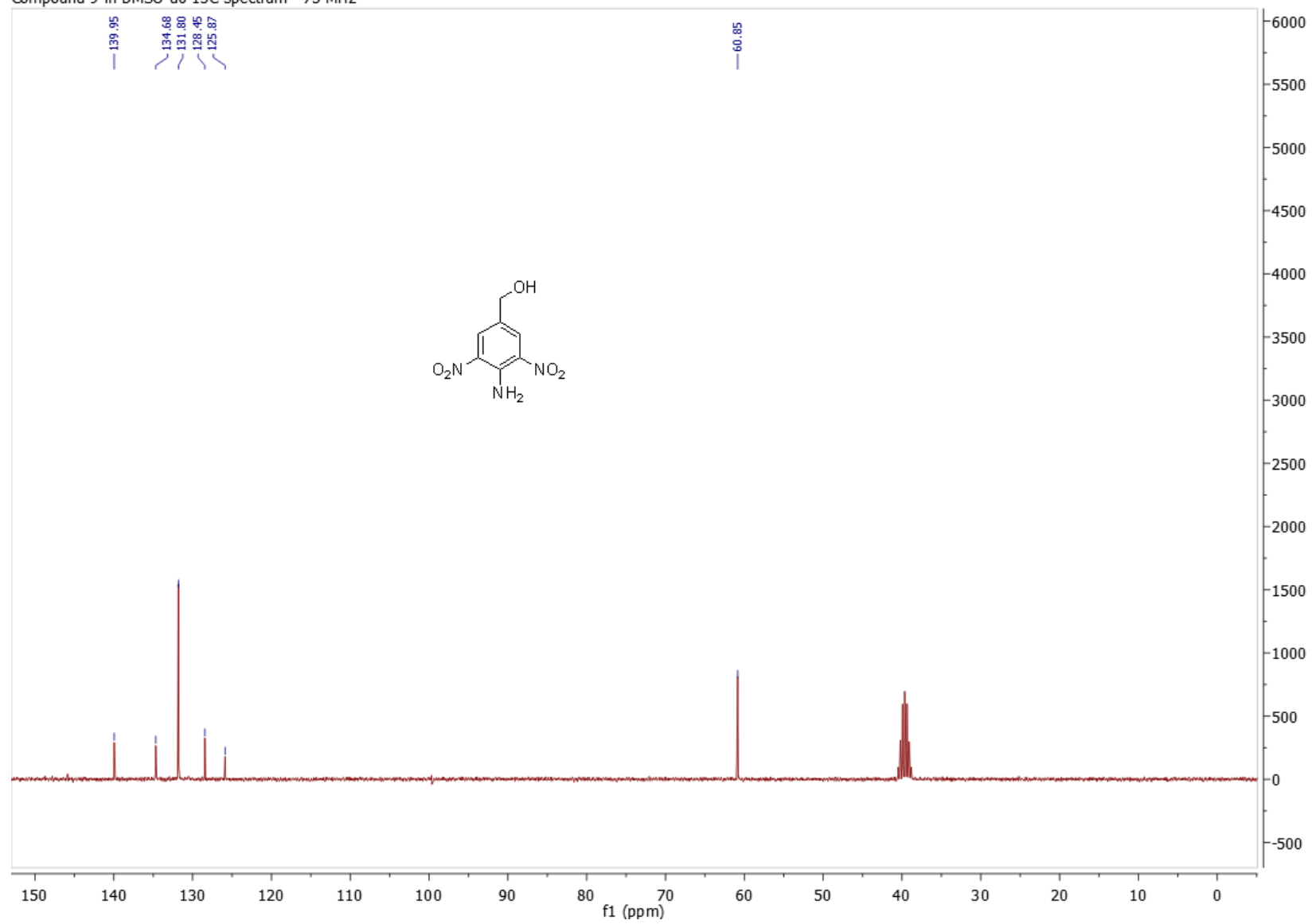
Compound 8 in DMSO-d6 13C spectrum - 75 MHz



Compound 9 in DMSO-d6 1H spectrum - 300 MHz



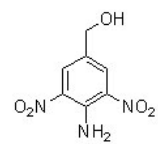
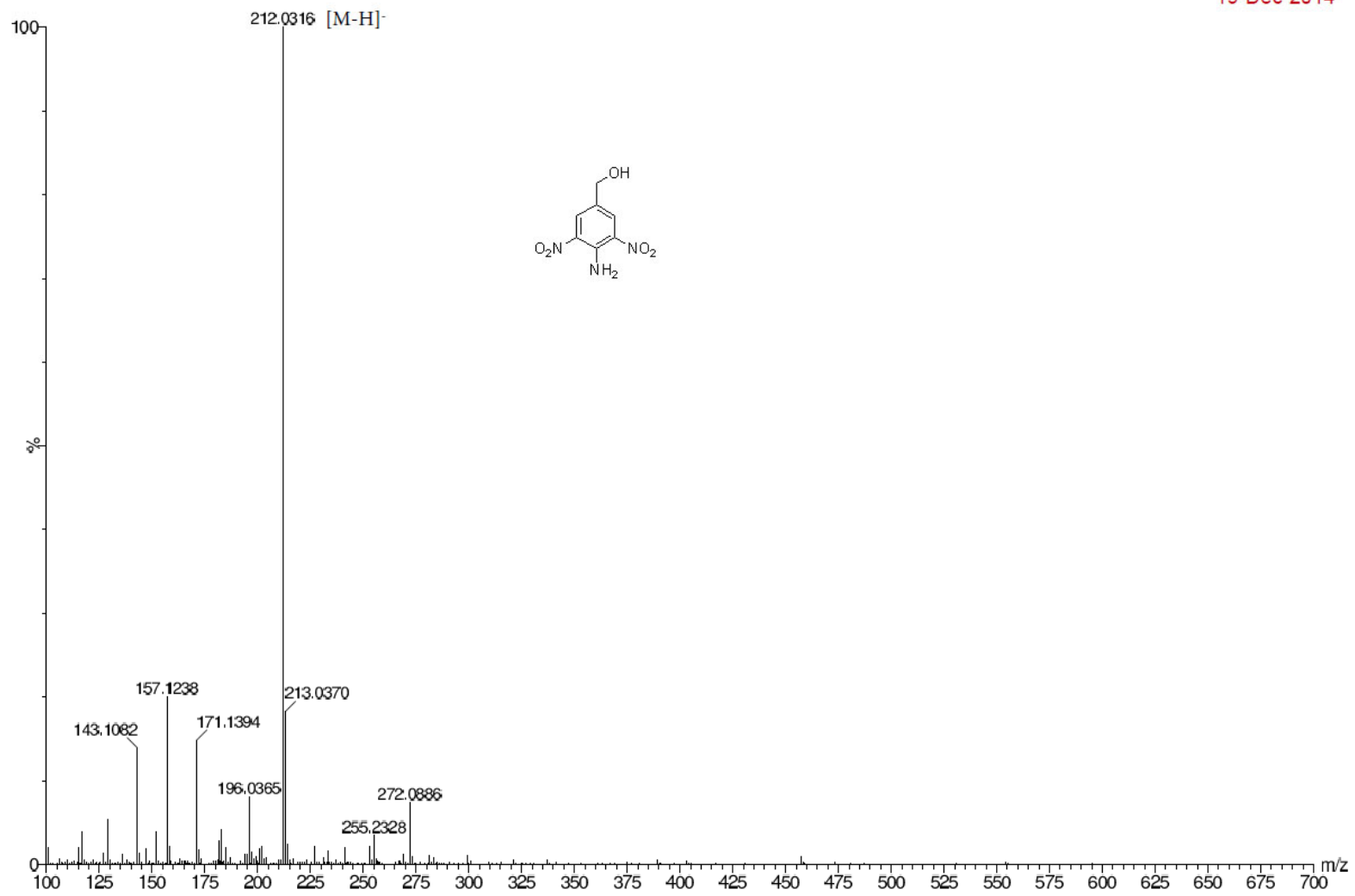
Compound 9 in DMSO-d6 13C spectrum - 75 MHz



compound 9

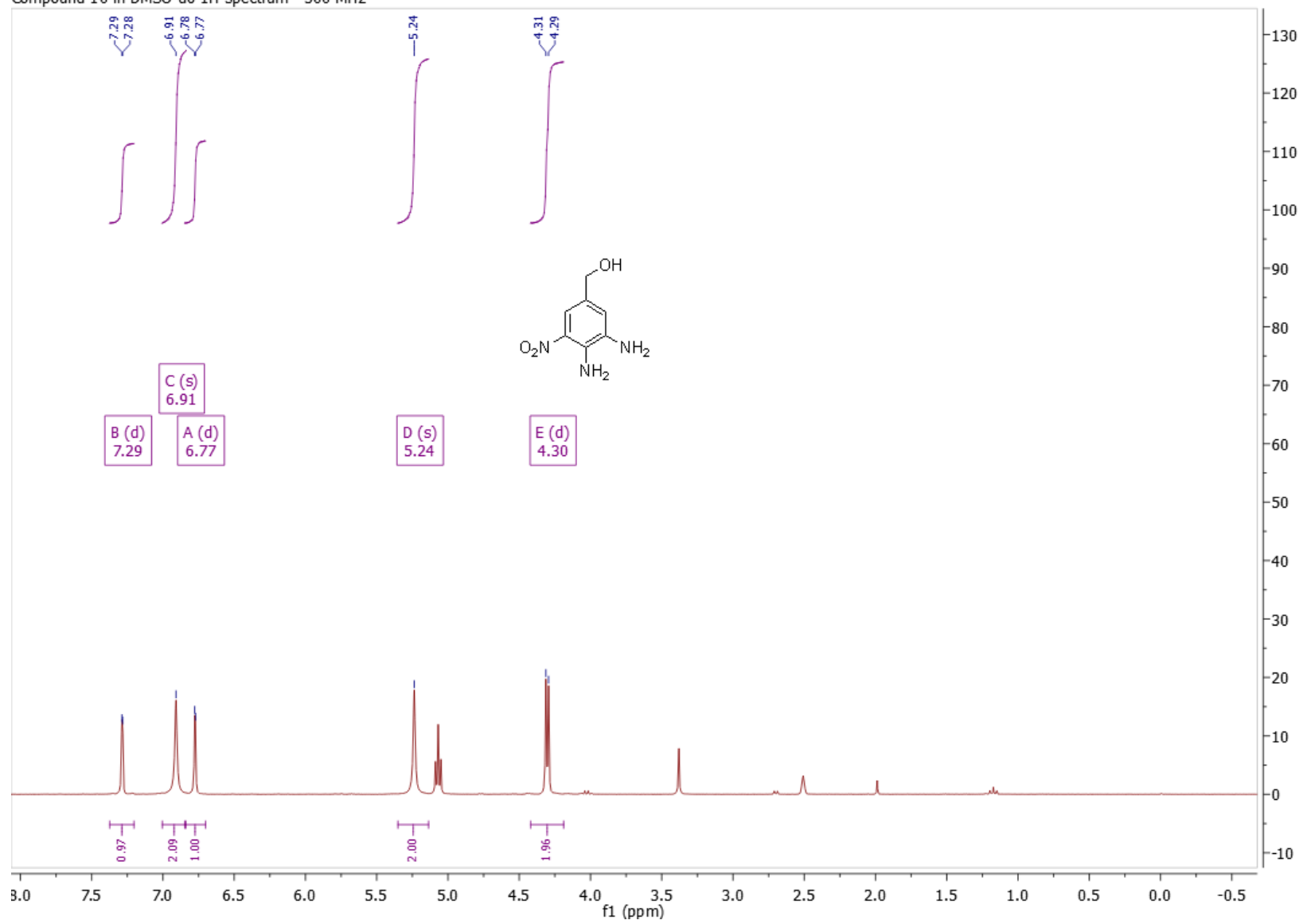
accurate mass

ES-  
19-Dec-2014

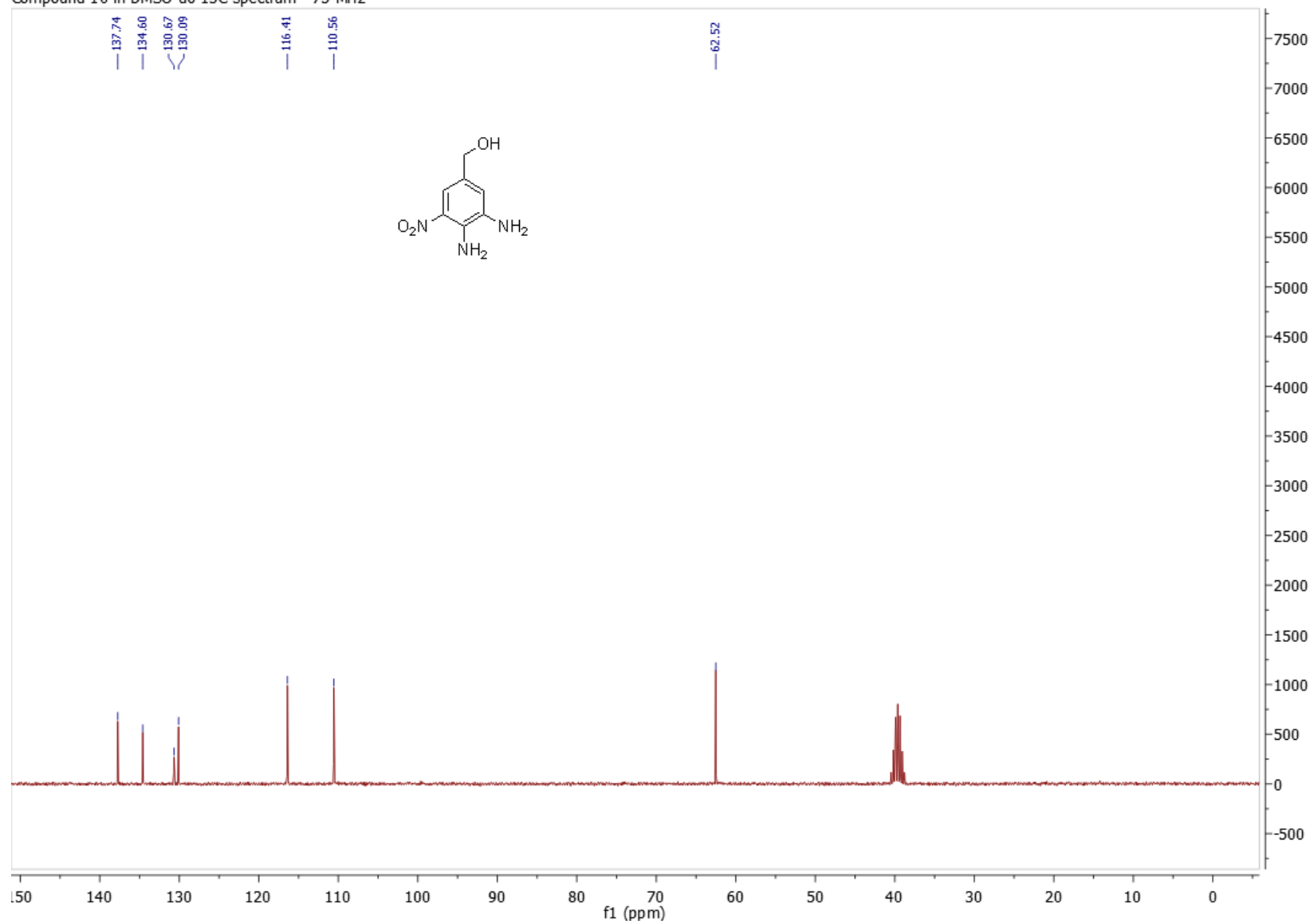




Compound 10 in DMSO-d6 1H spectrum - 300 MHz



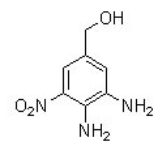
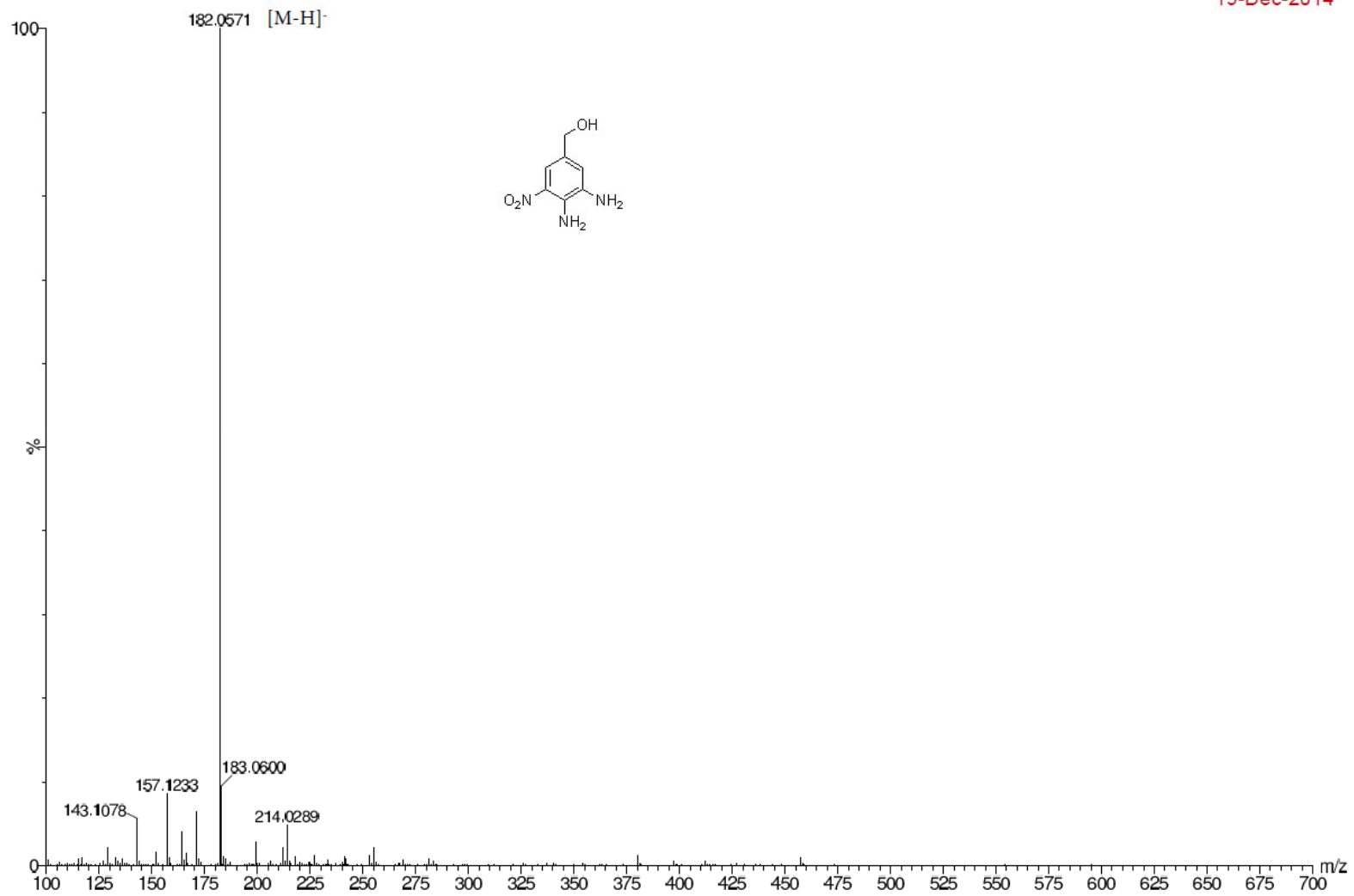
Compound 10 in DMSO-d6 13C spectrum - 75 MHz



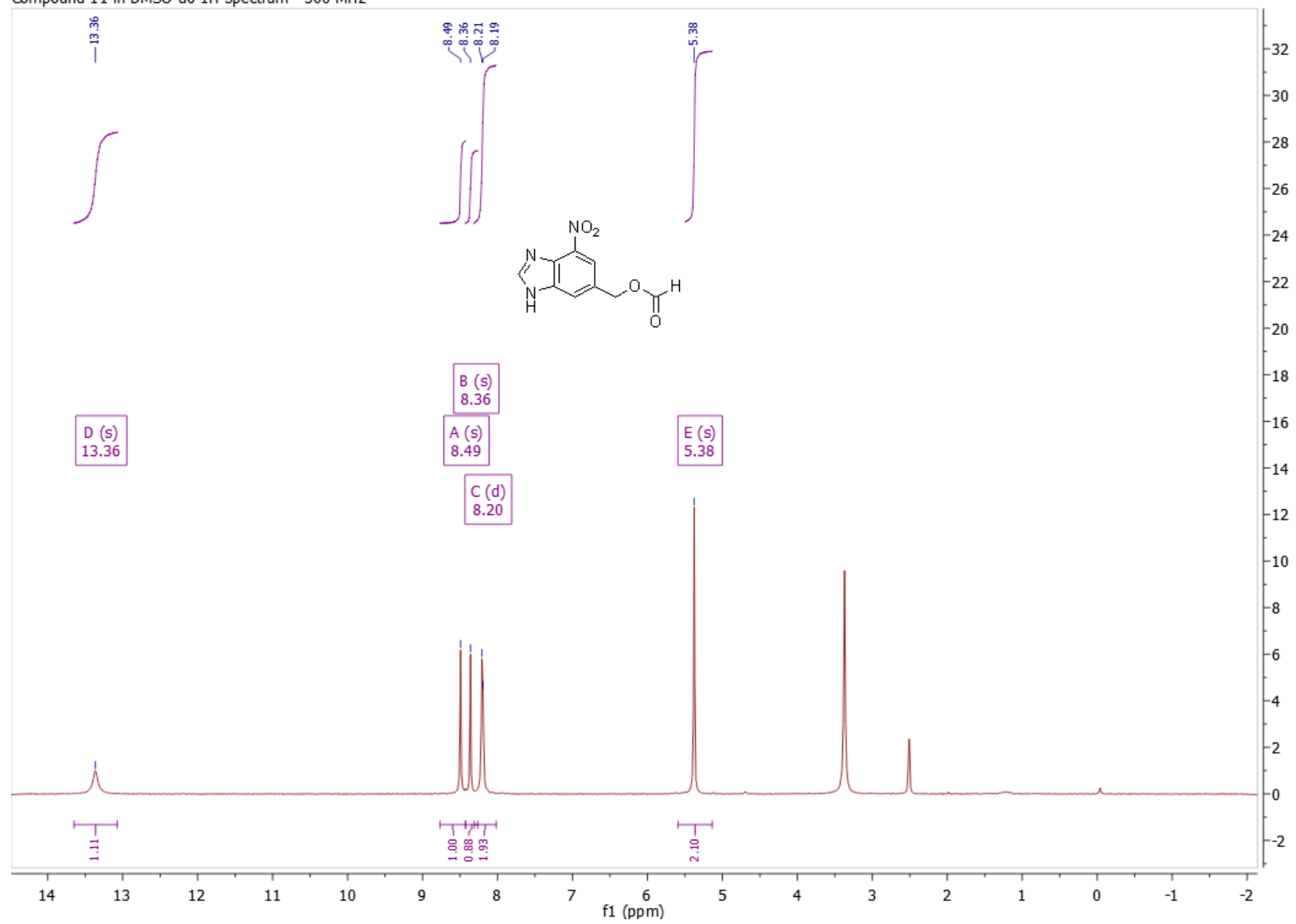
compound 10

accurate mass

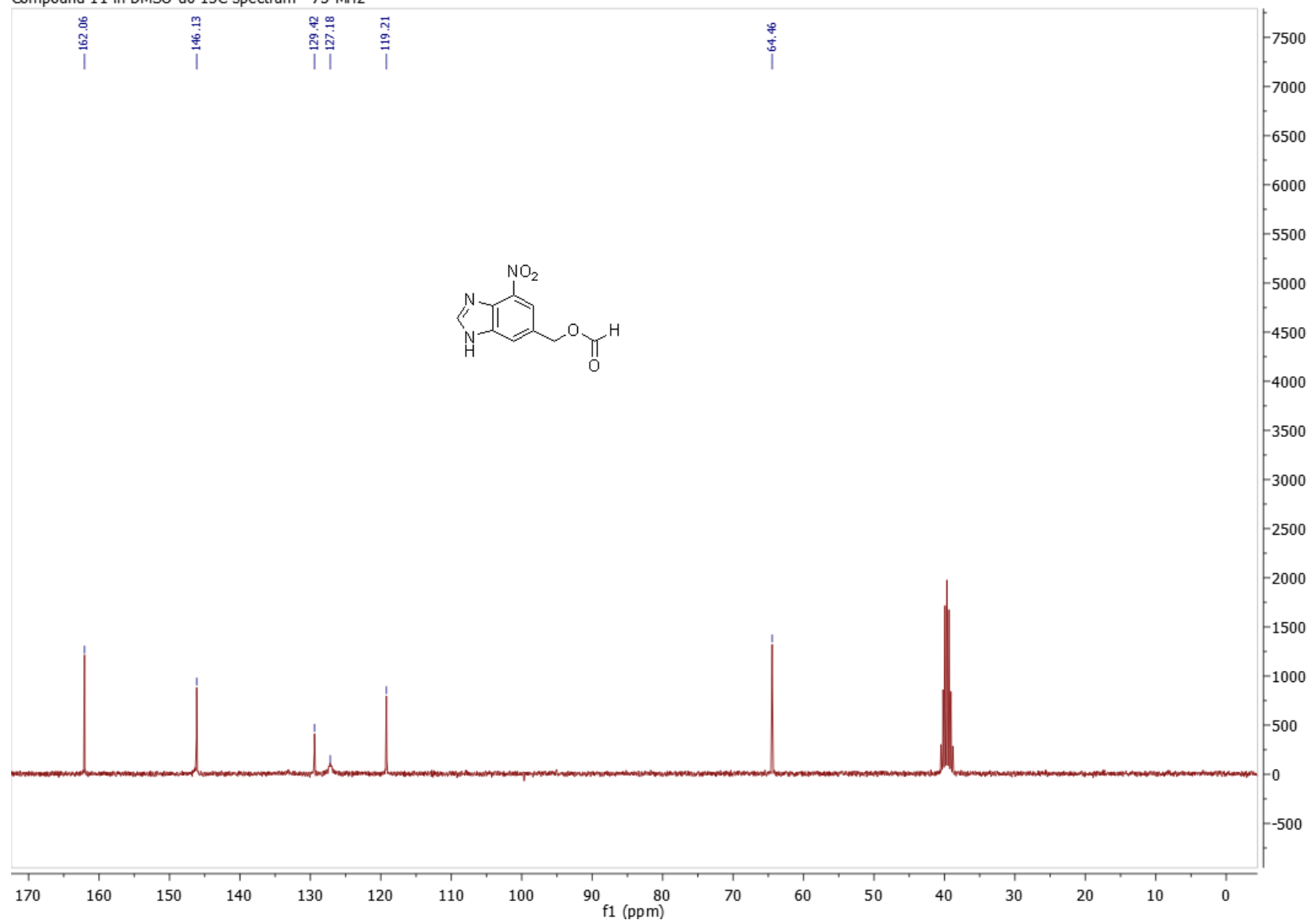
ES-  
19-Dec-2014



Compound 11 in DMSO-d6 1H spectrum - 300 MHz



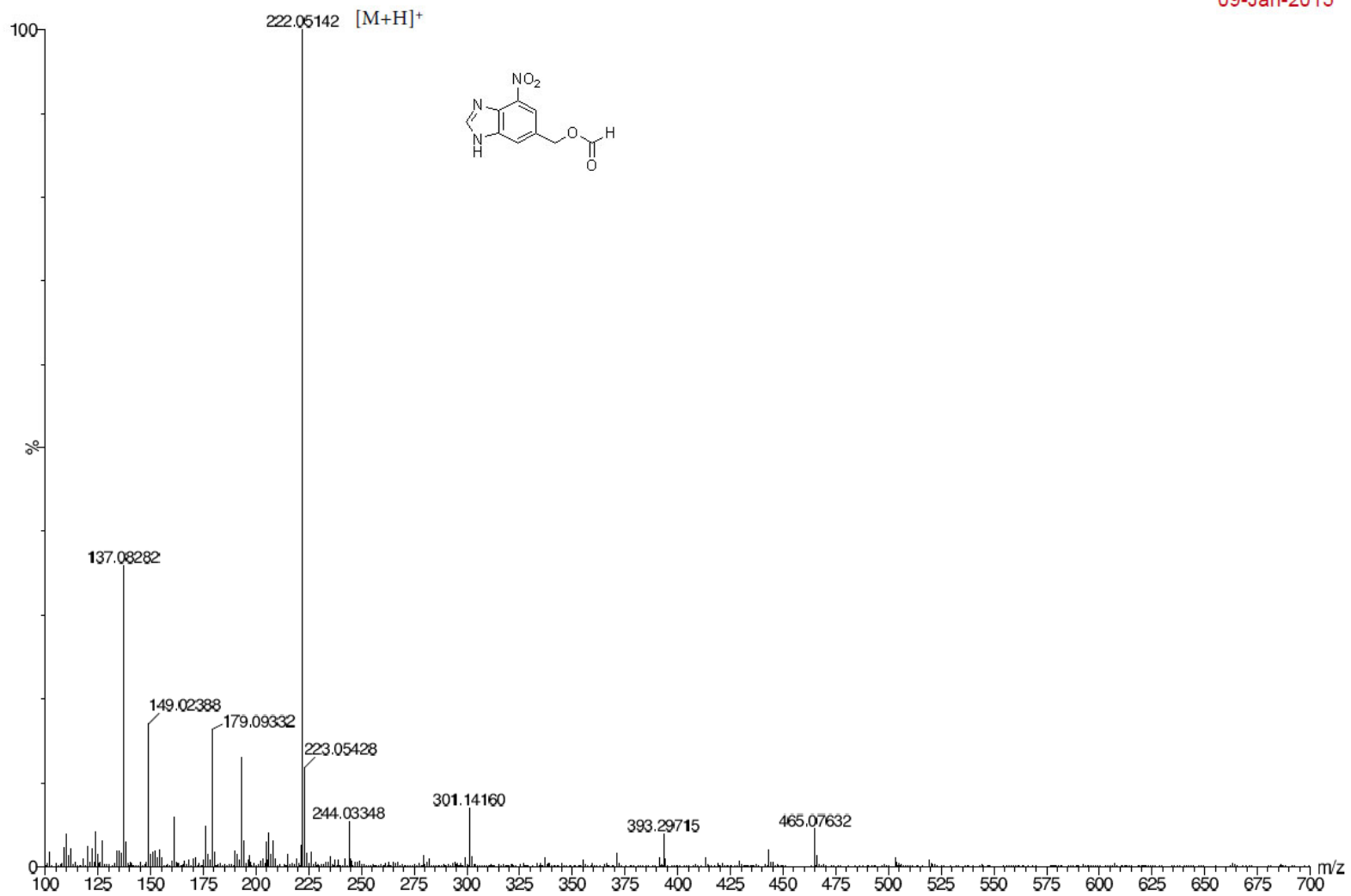
Compound 11 in DMSO-d6 13C spectrum - 75 MHz



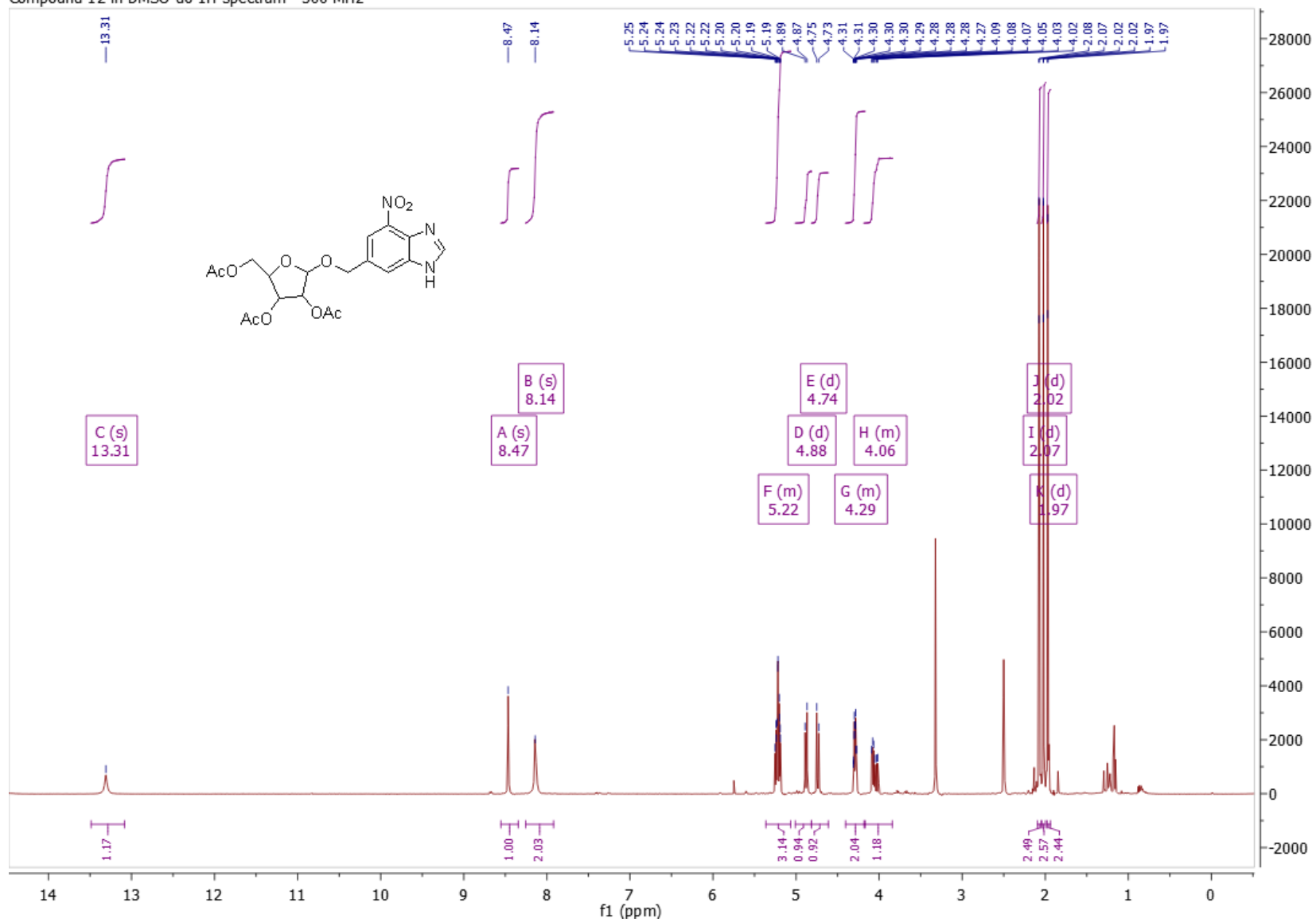
compound 11

accurate mass

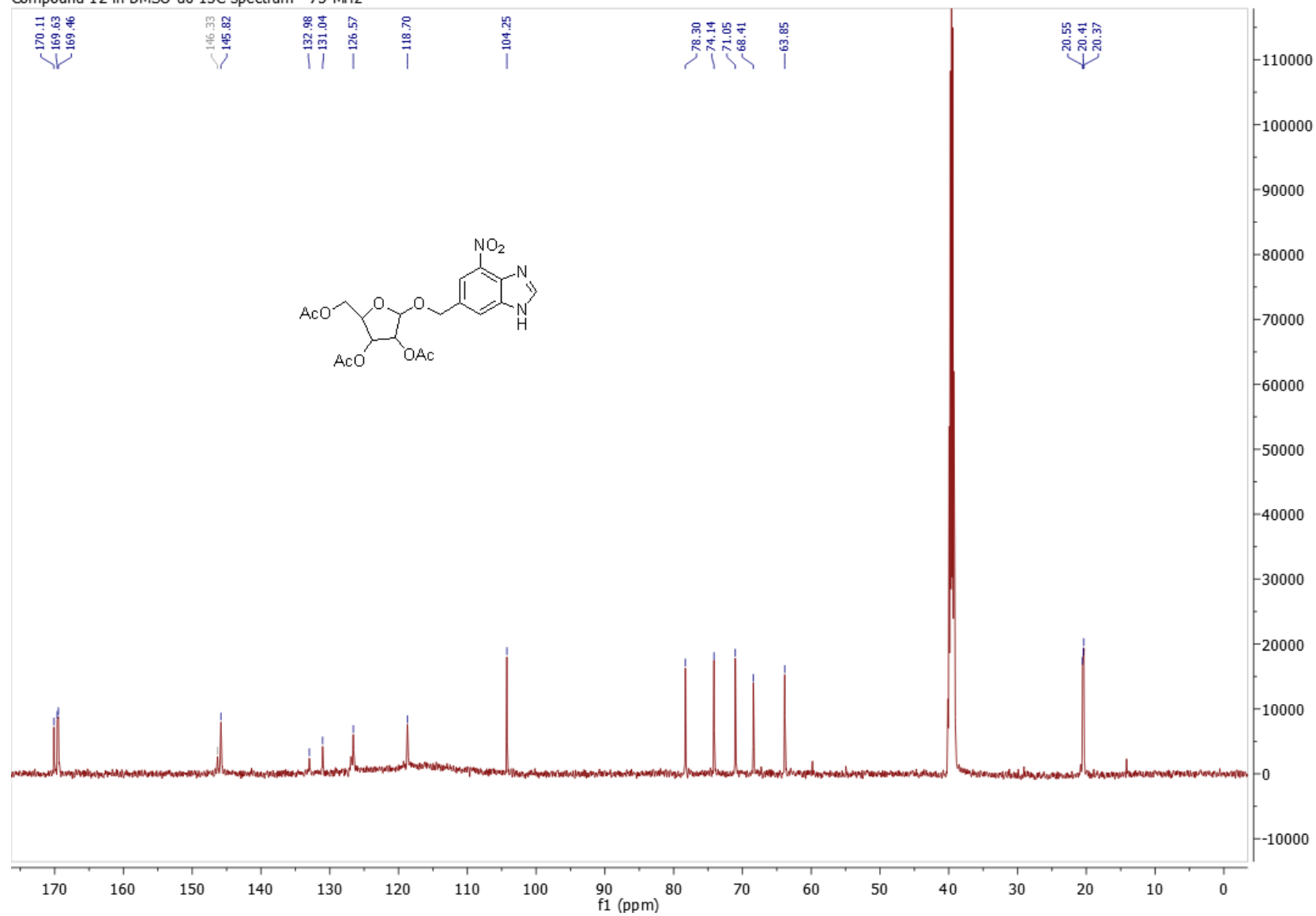
ES+  
09-Jan-2015



Compound 12 in DMSO-d6 1H spectrum - 300 MHz



Compound 12 in DMSO-d6 13C spectrum - 75 MHz

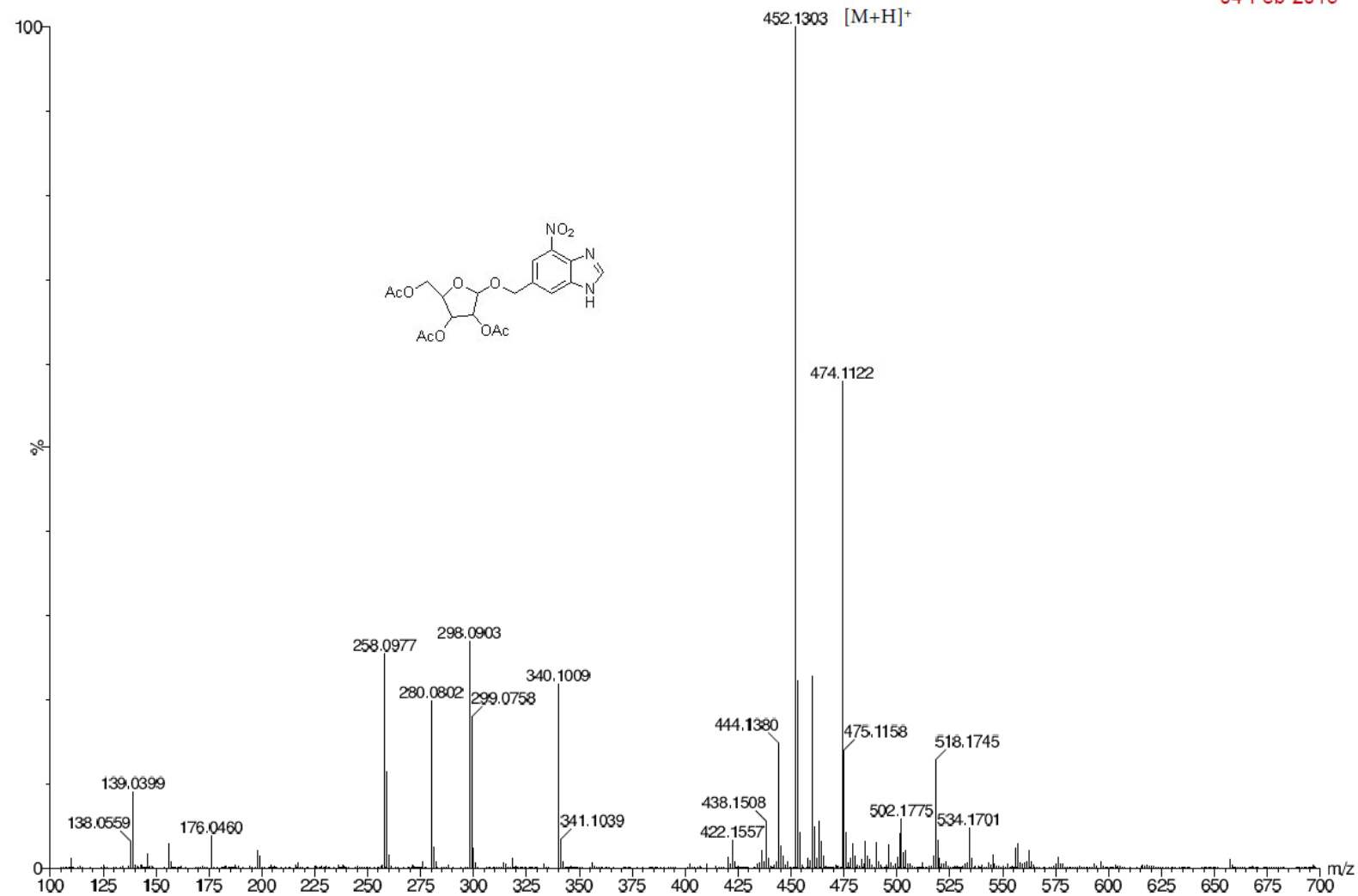




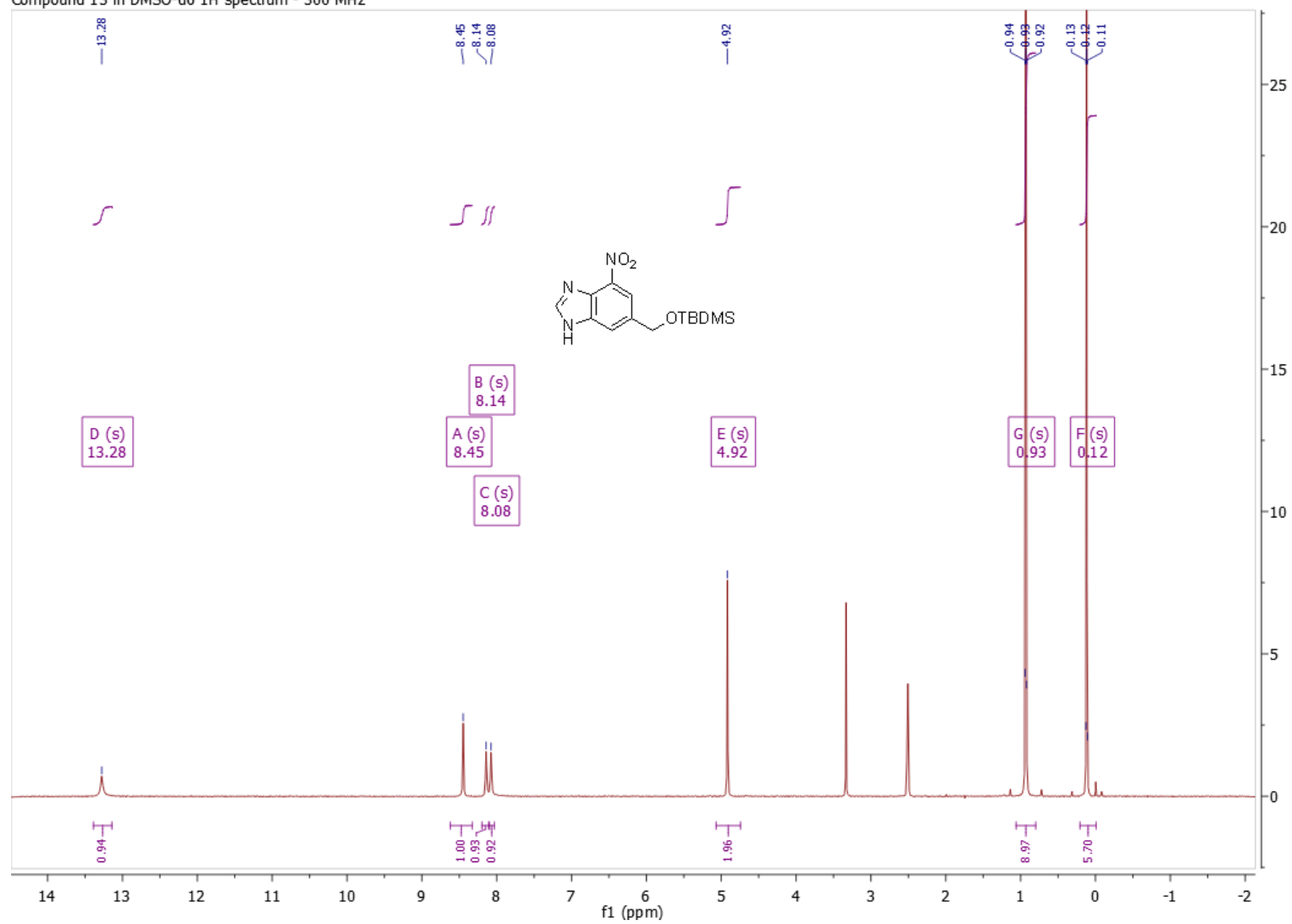
compound 12

accurate mass

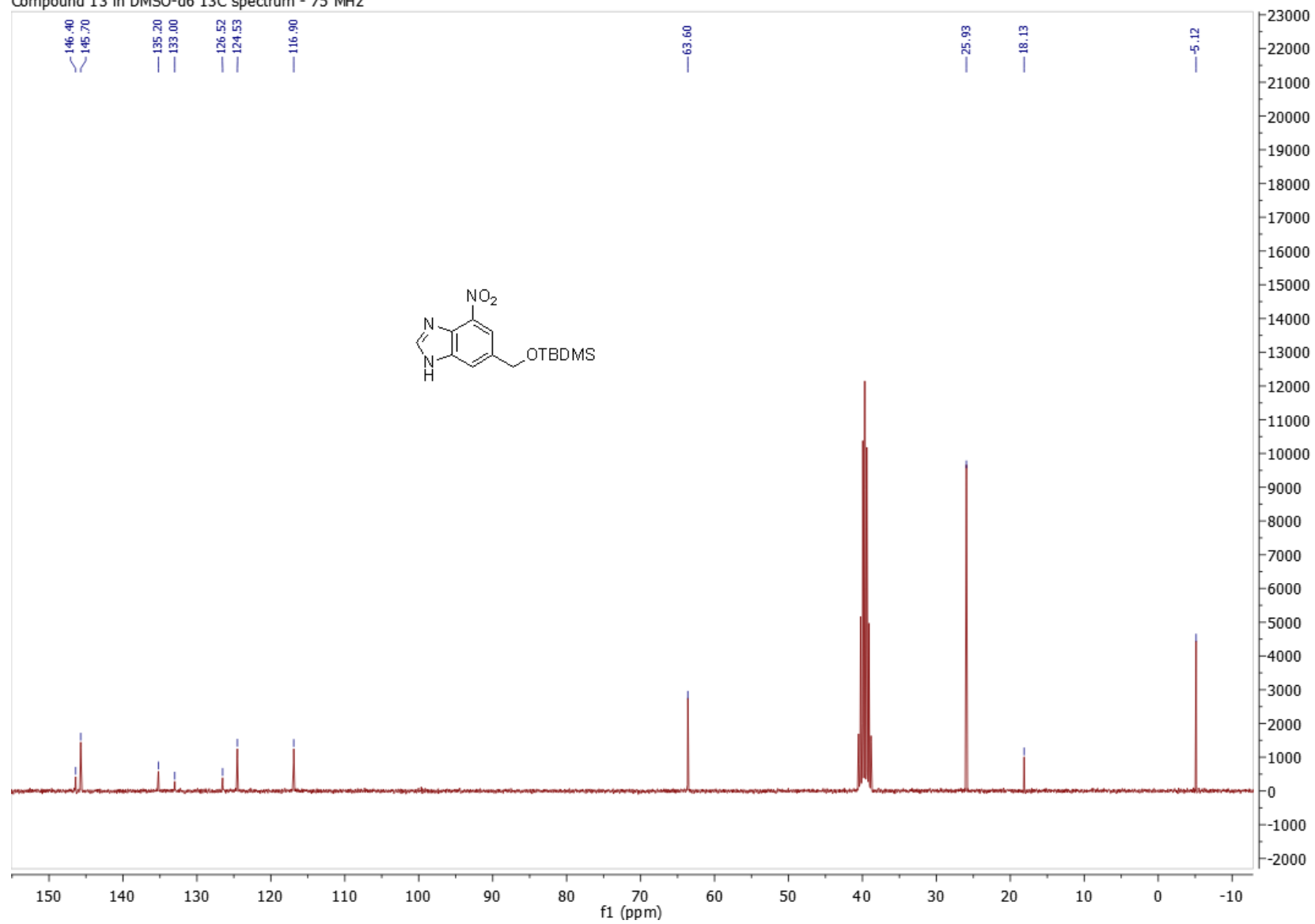
ES+  
04-Feb-2015



Compound 13 in DMSO-d6 1H spectrum - 300 MHz



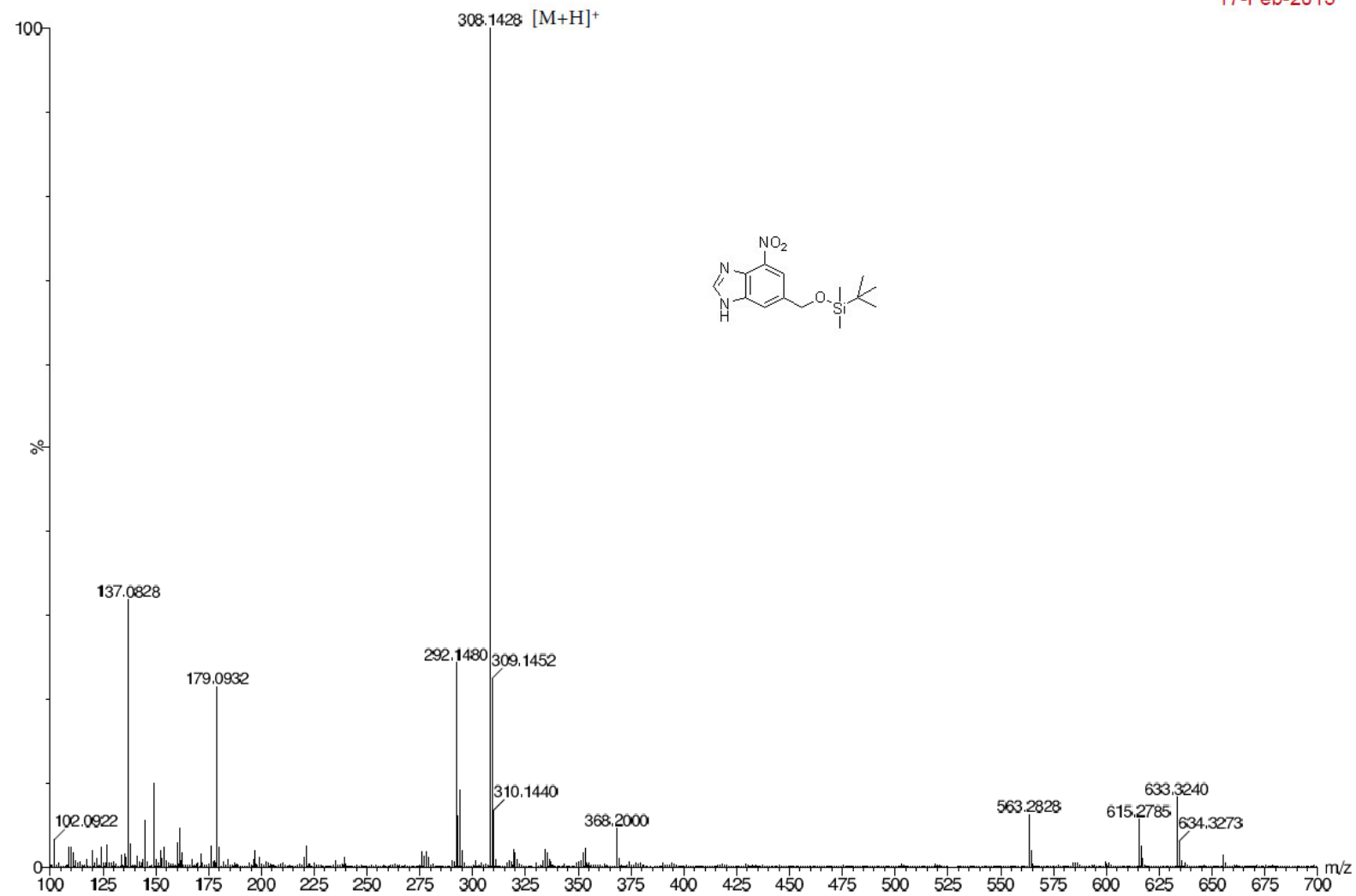
Compound 13 in DMSO-d6 13C spectrum - 75 MHz



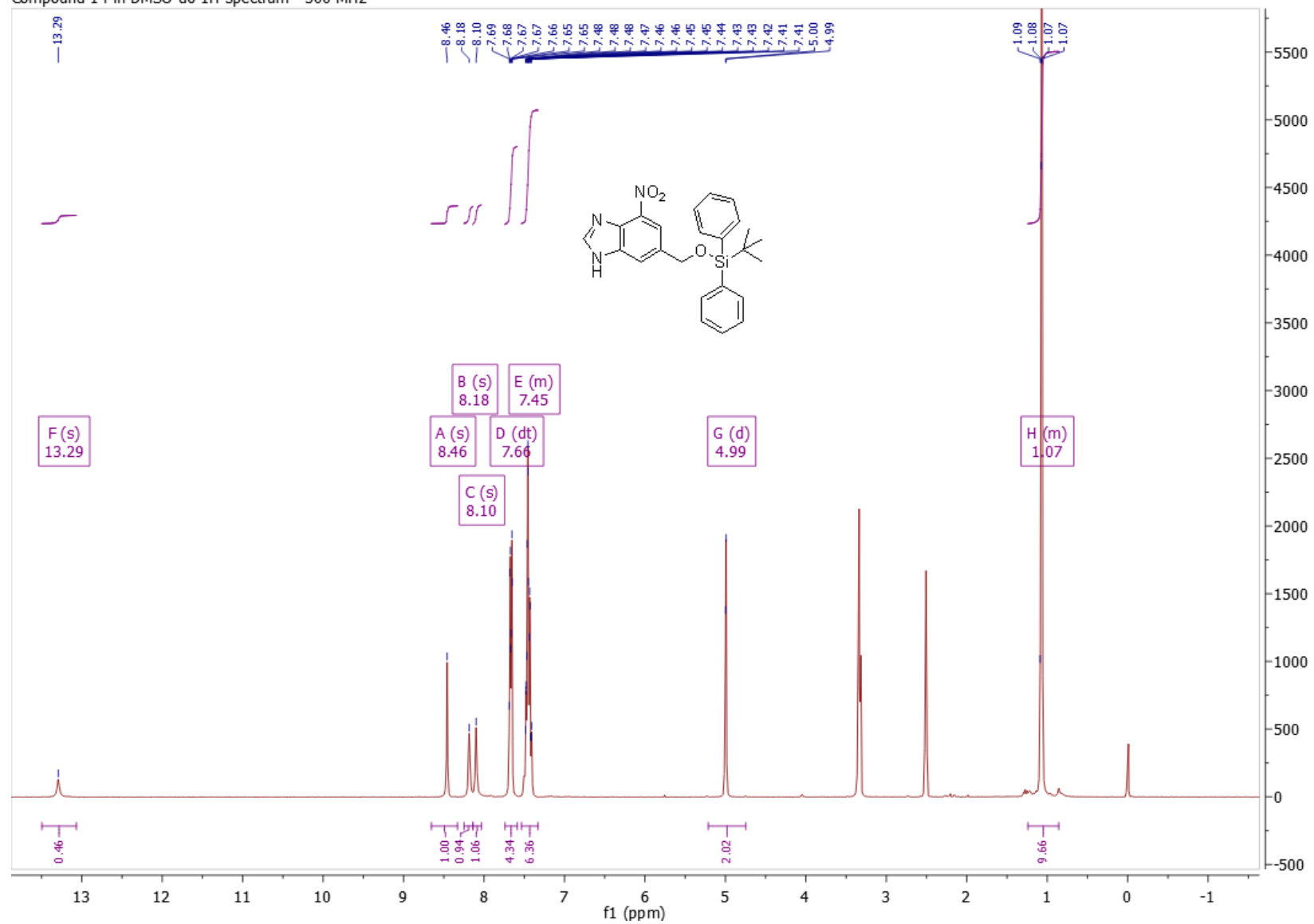
compound 13

accurate mass

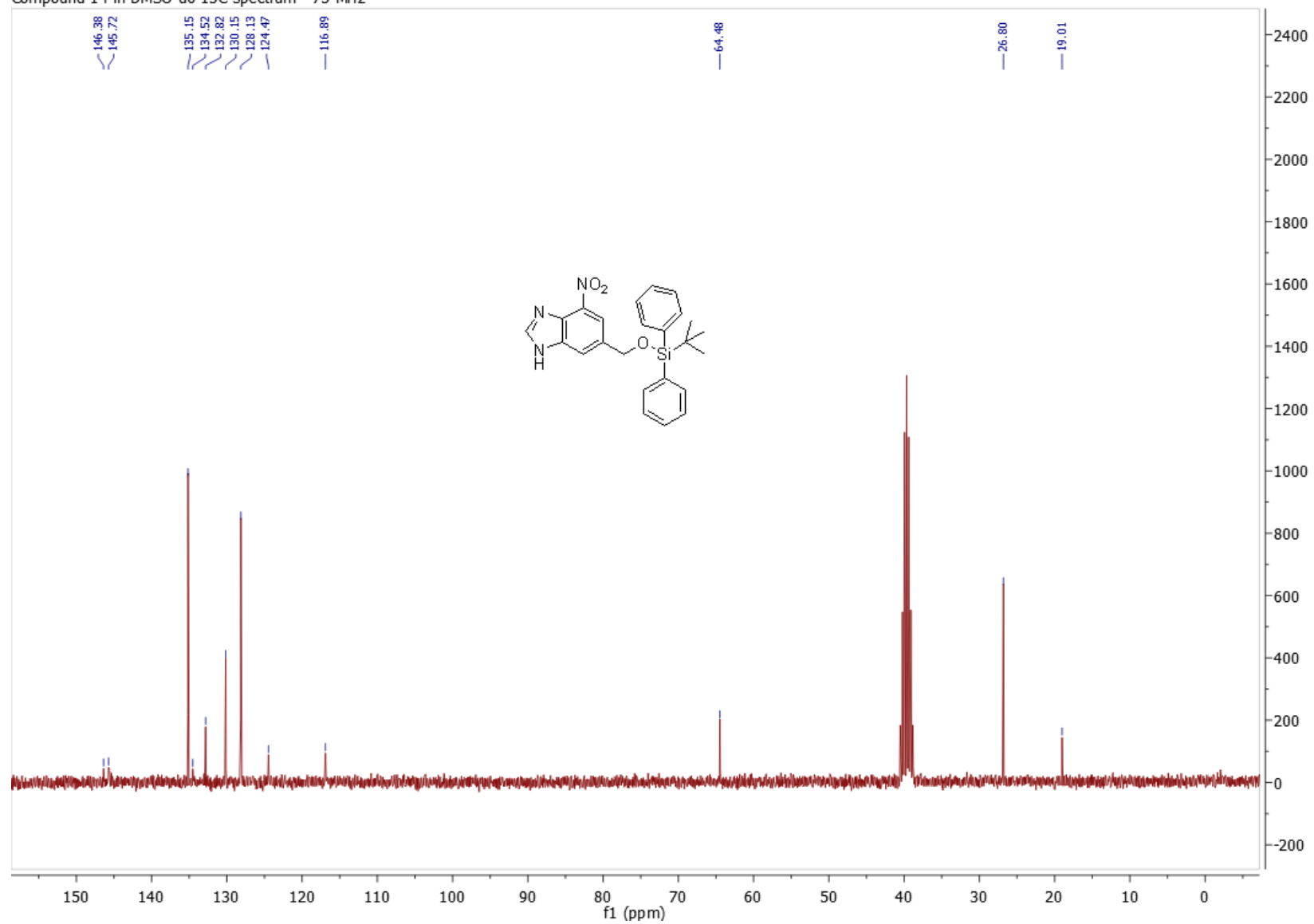
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17-Feb-2015



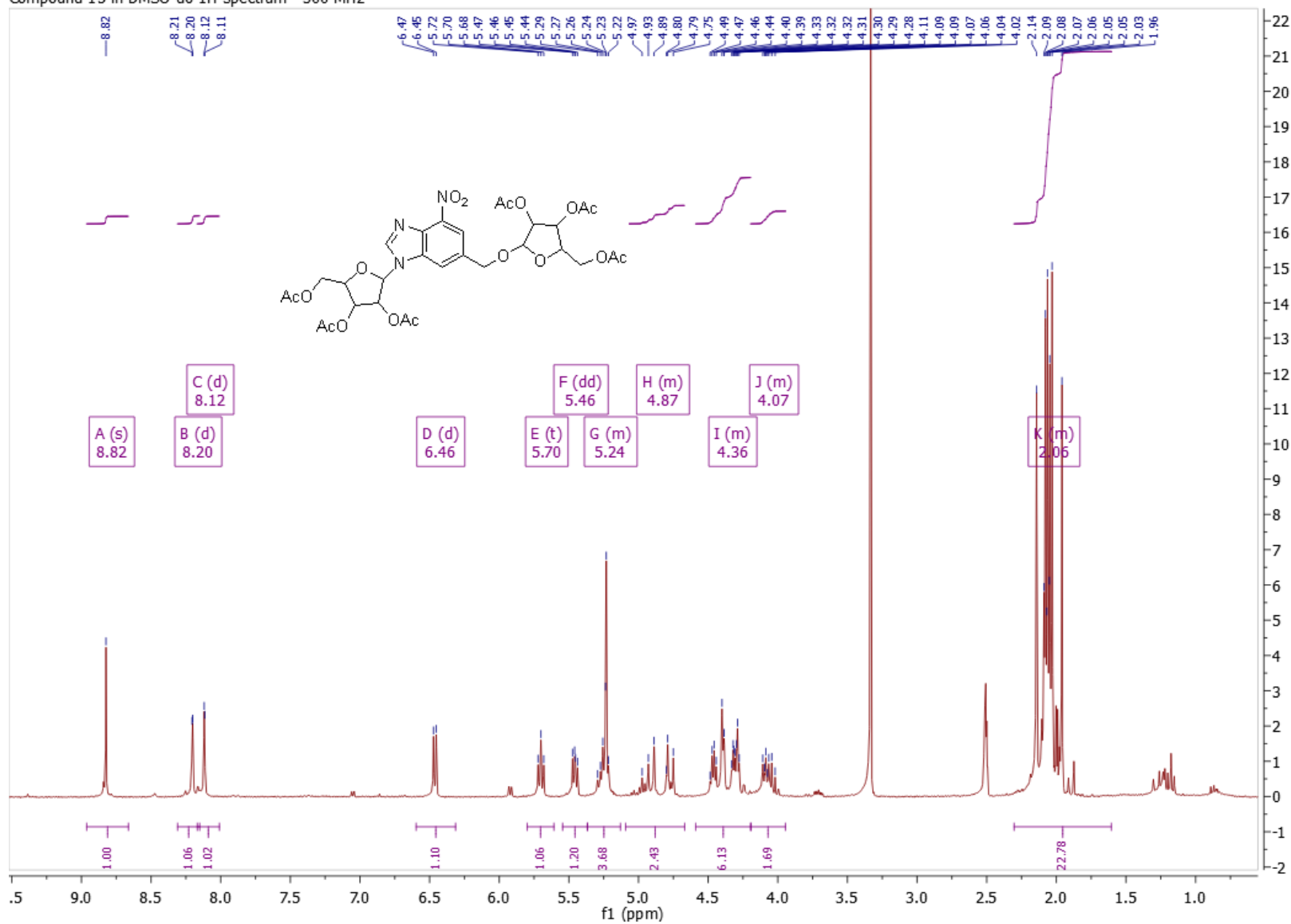
Compound 14 in DMSO-d6 1H spectrum - 300 MHz



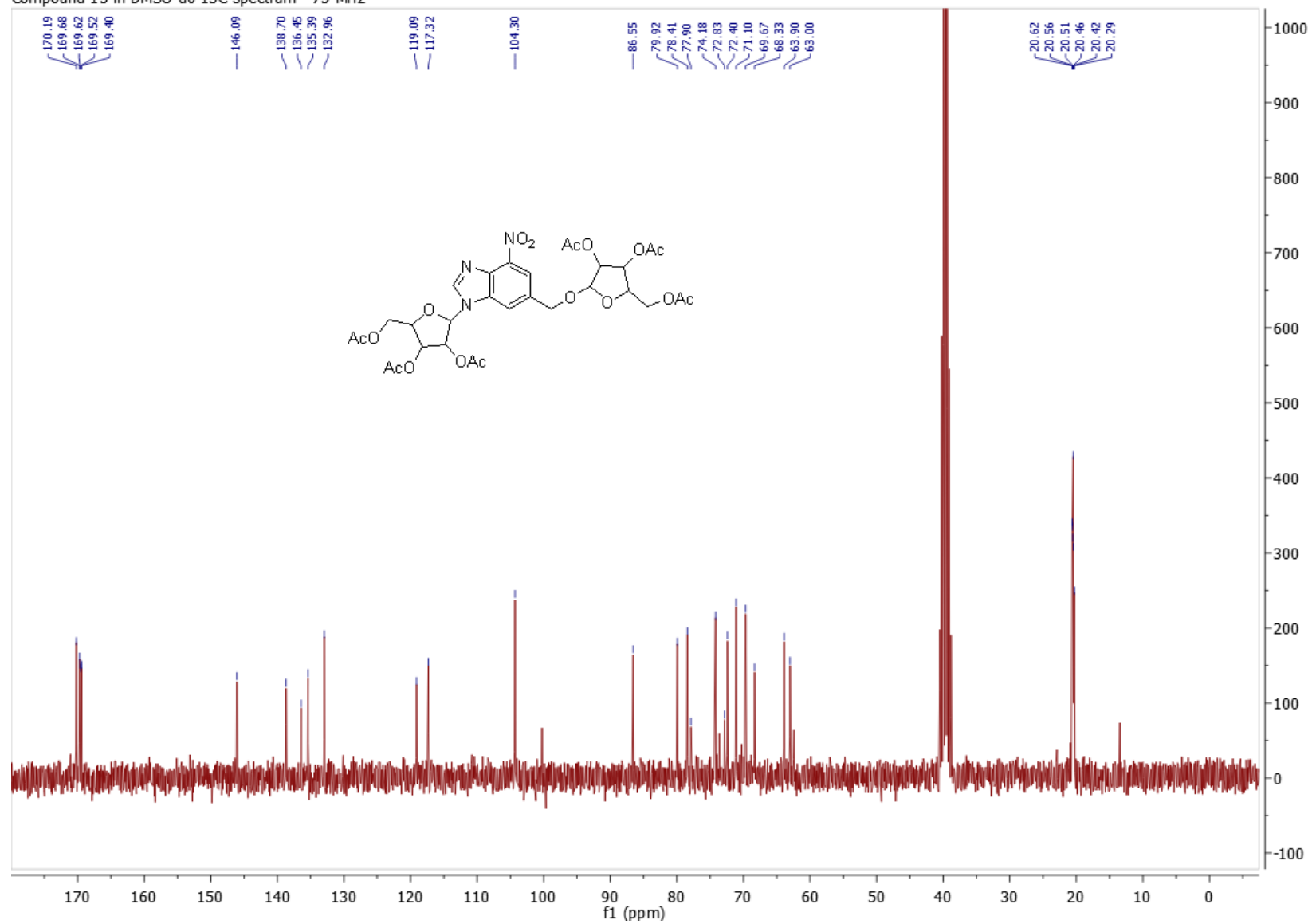
Compound 14 in DMSO-d6 13C spectrum - 75 MHz



Compound 15 in DMSO-d6 1H spectrum - 300 MHz

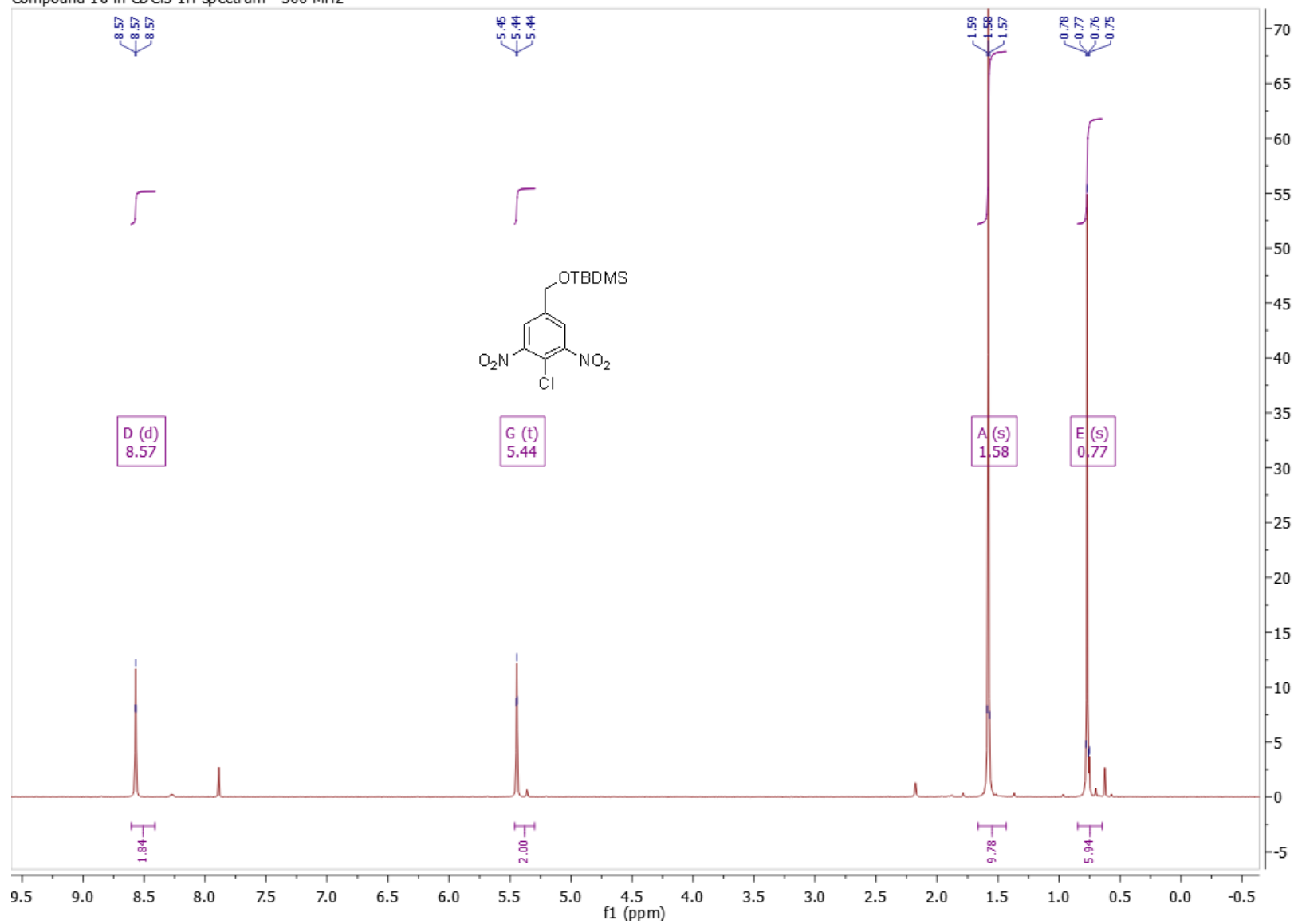


Compound 15 in DMSO-d6 13C spectrum - 75 MHz

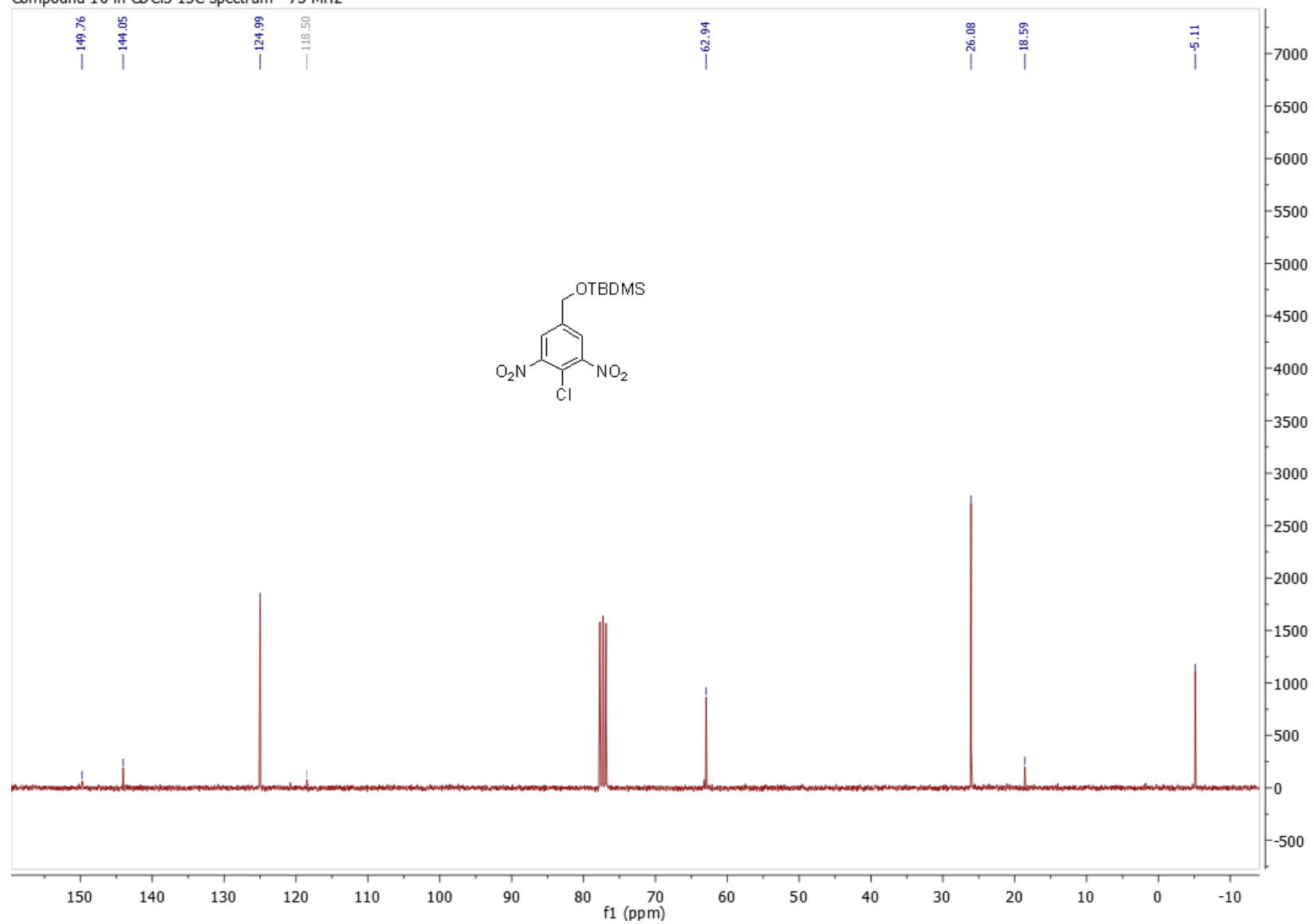




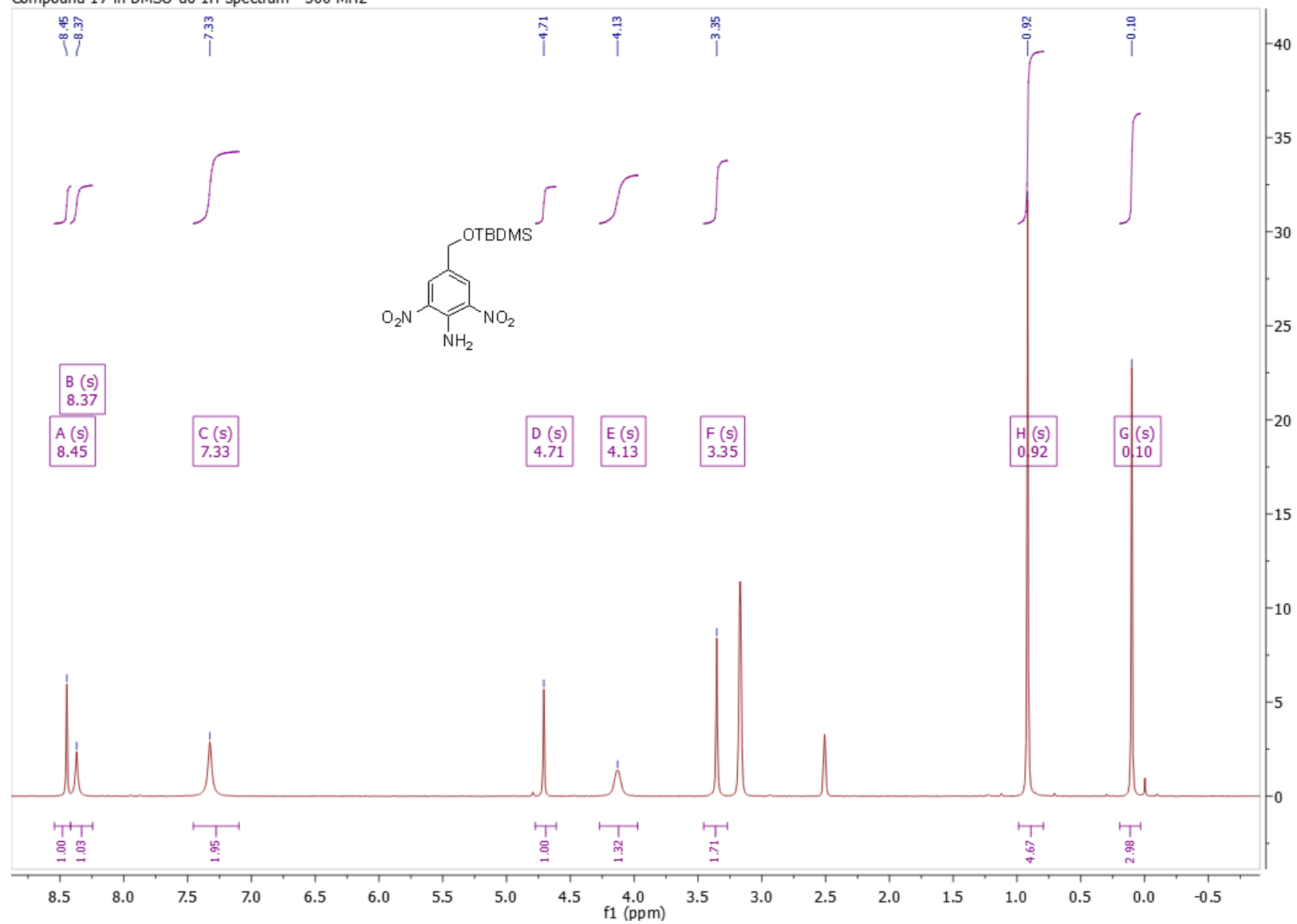
Compound 16 in CDCl<sub>3</sub> 1H spectrum - 300 MHz



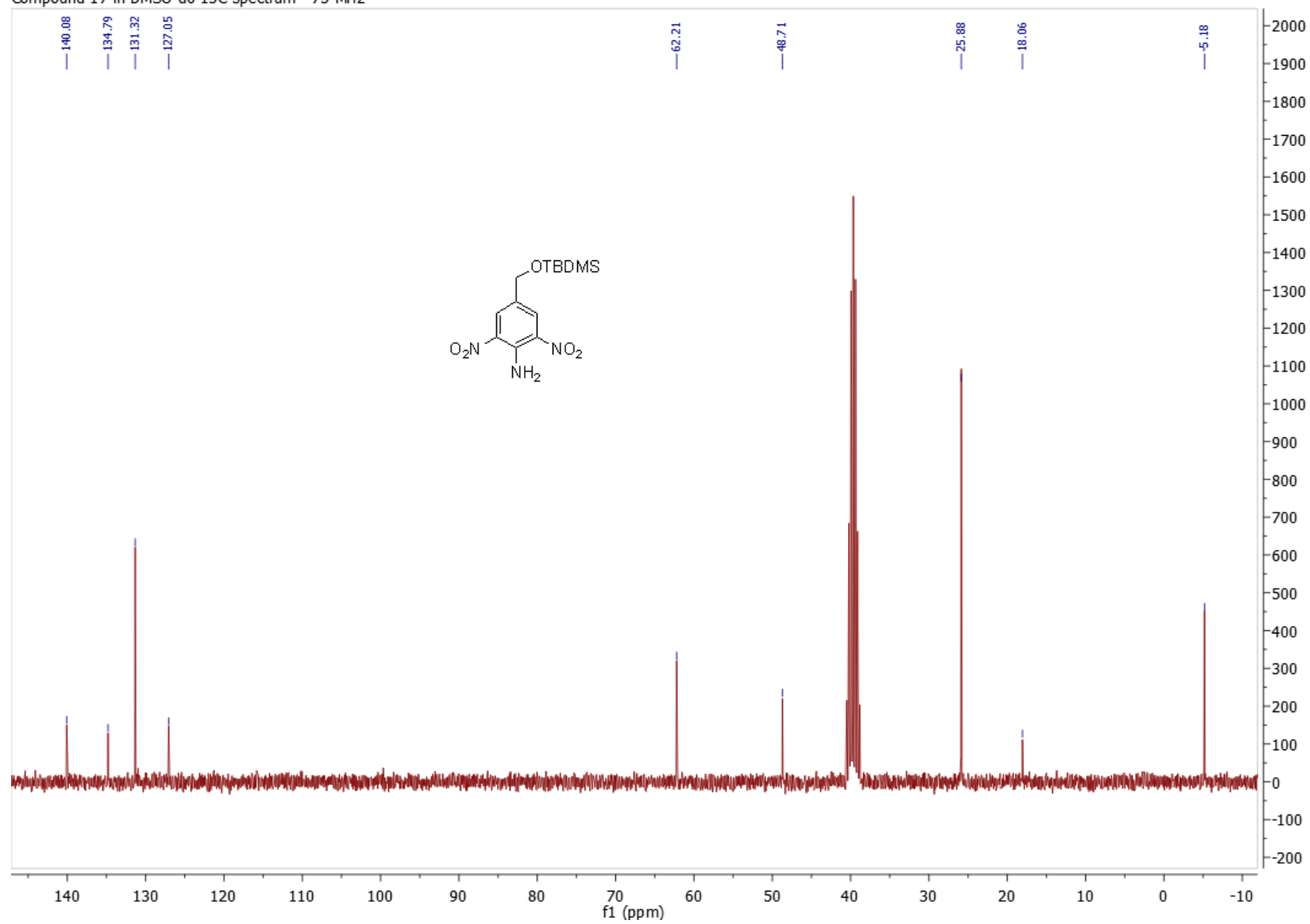
Compound 16 in CDCl<sub>3</sub> 13C spectrum - 75 MHz



Compound 17 in DMSO-d6 1H spectrum - 300 MHz



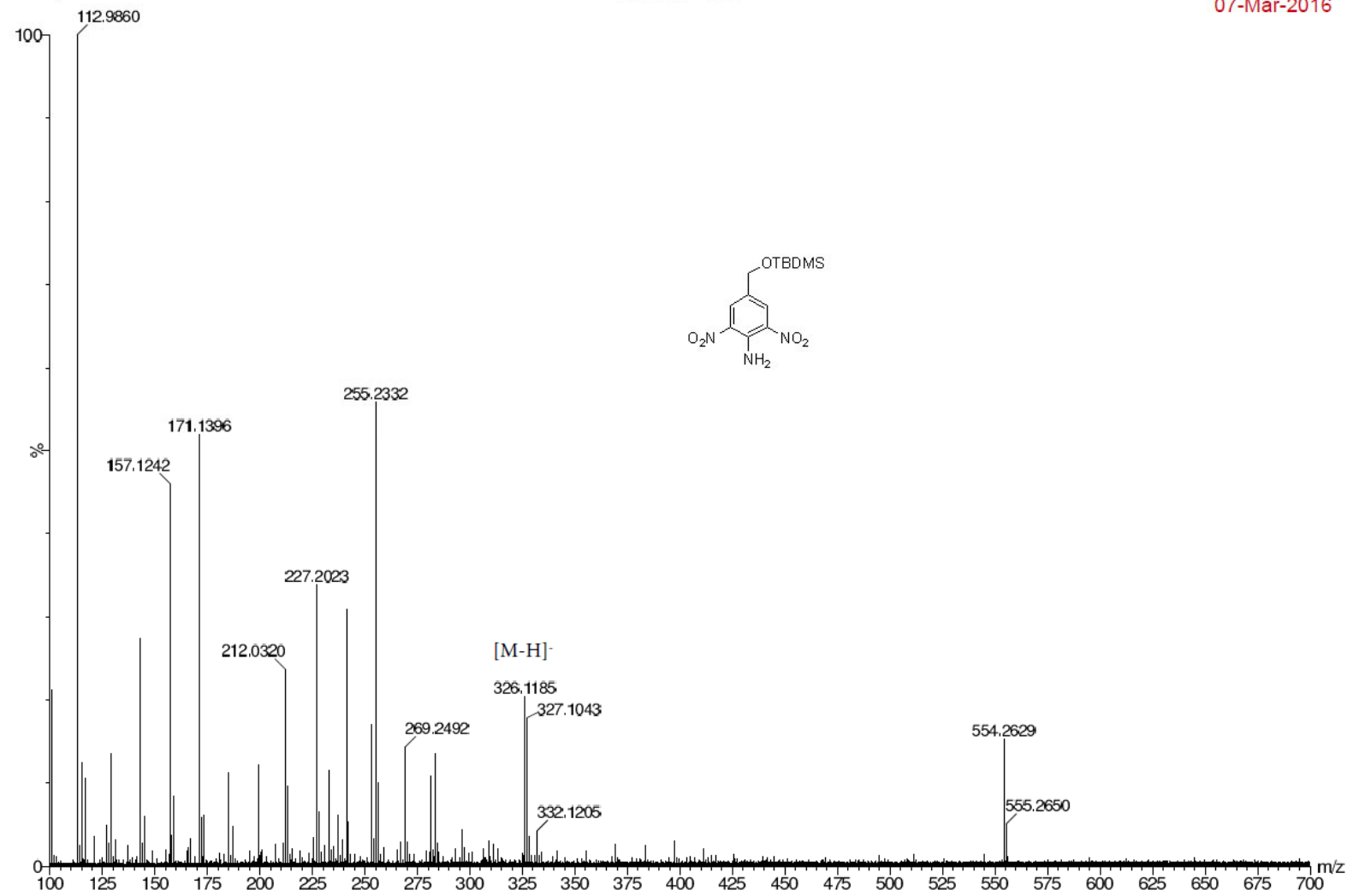
Compound 17 in DMSO-d6 13C spectrum - 75 MHz



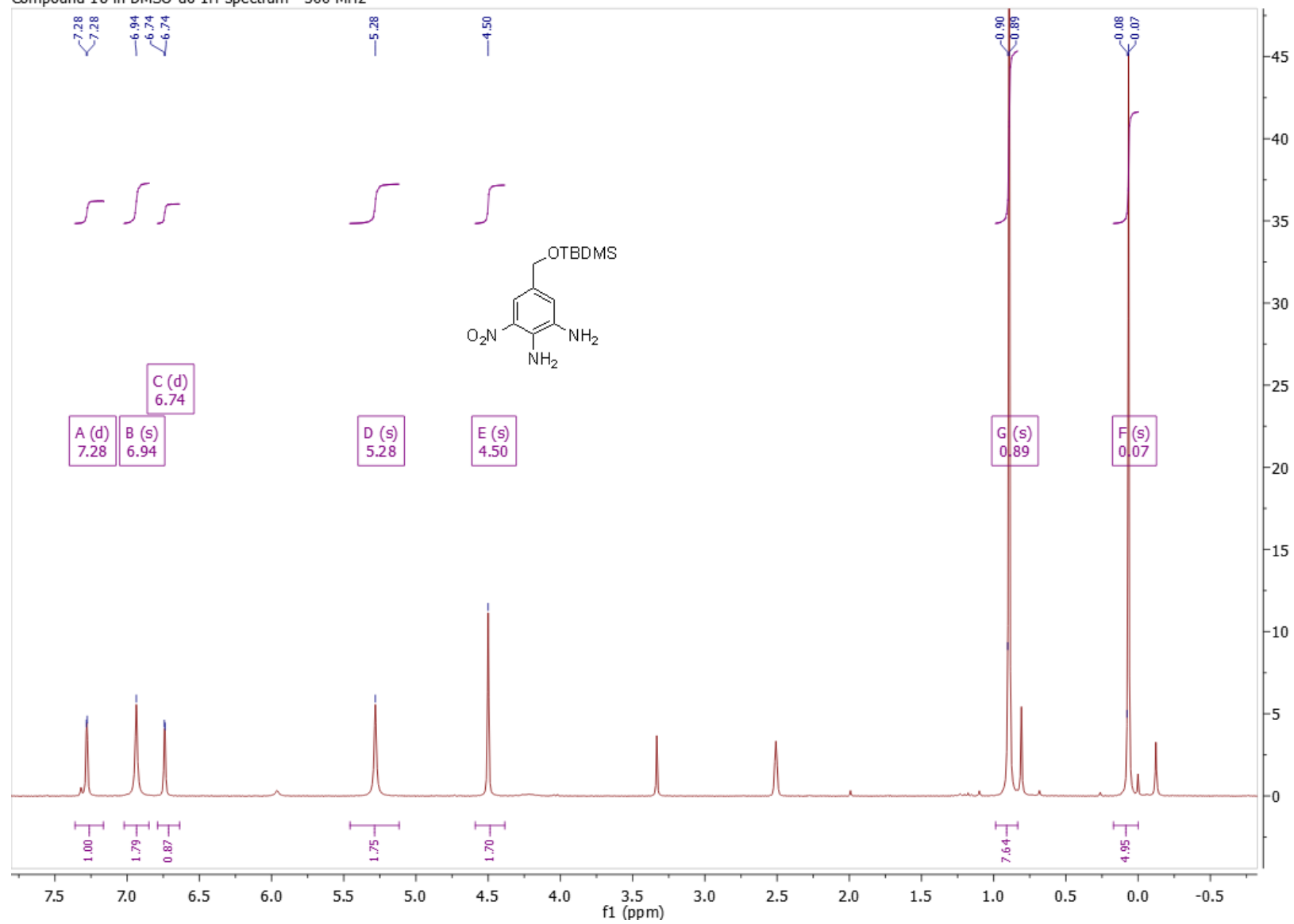
compound 17

accurate mass

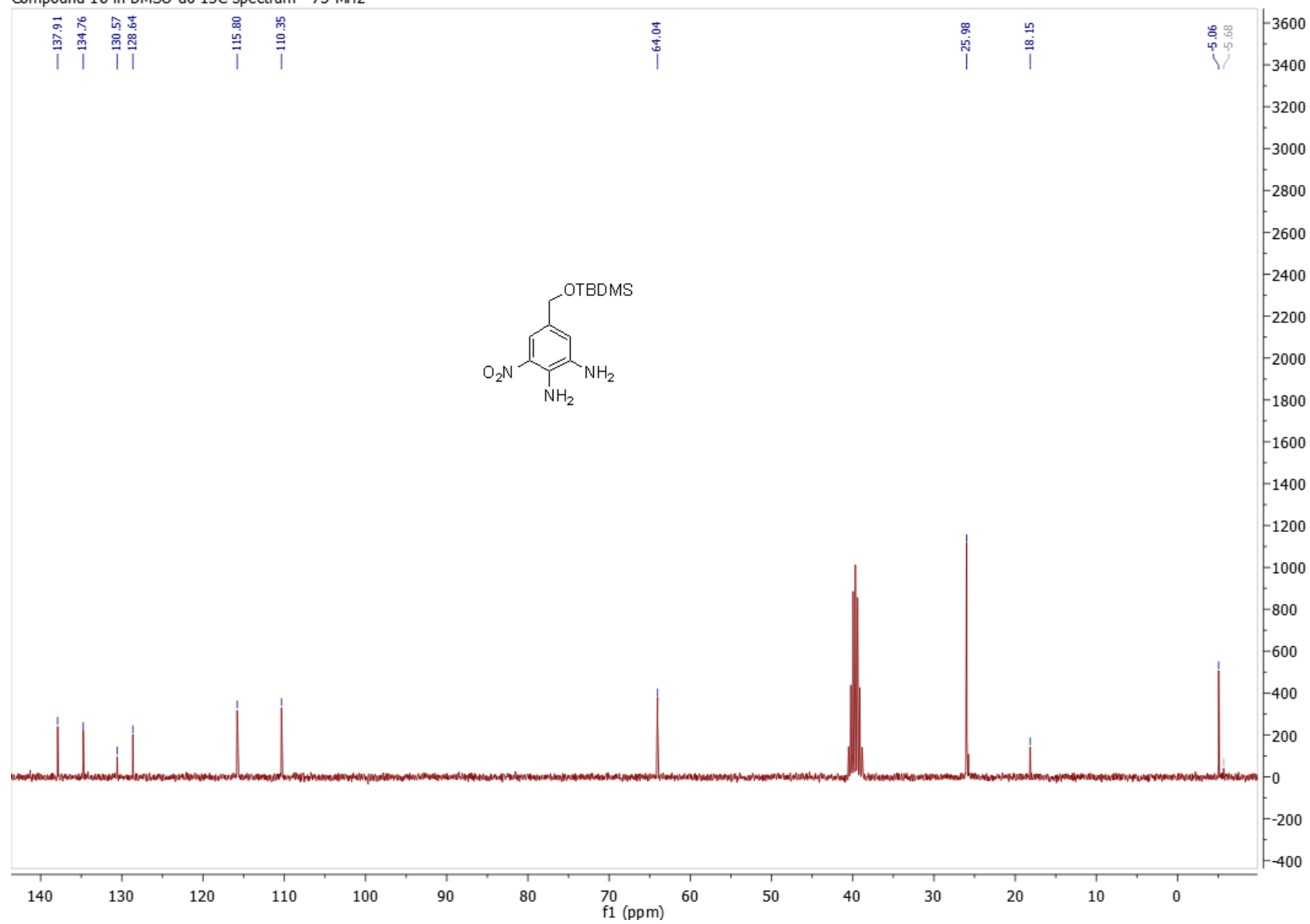
ES-  
07-Mar-2016



Compound 18 in DMSO-d6 1H spectrum - 300 MHz



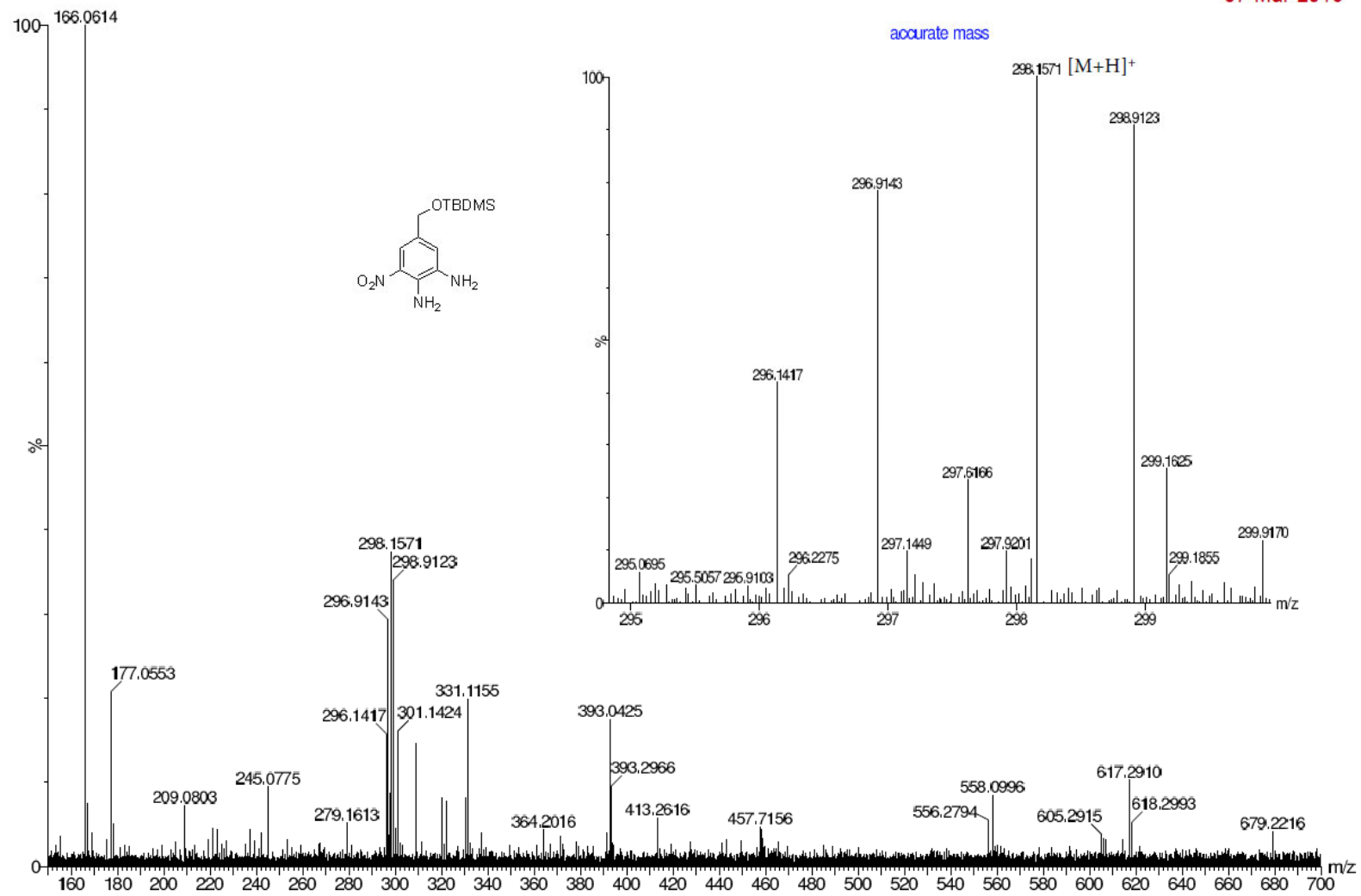
Compound 18 in DMSO-d6 13C spectrum - 75 MHz



compound 18

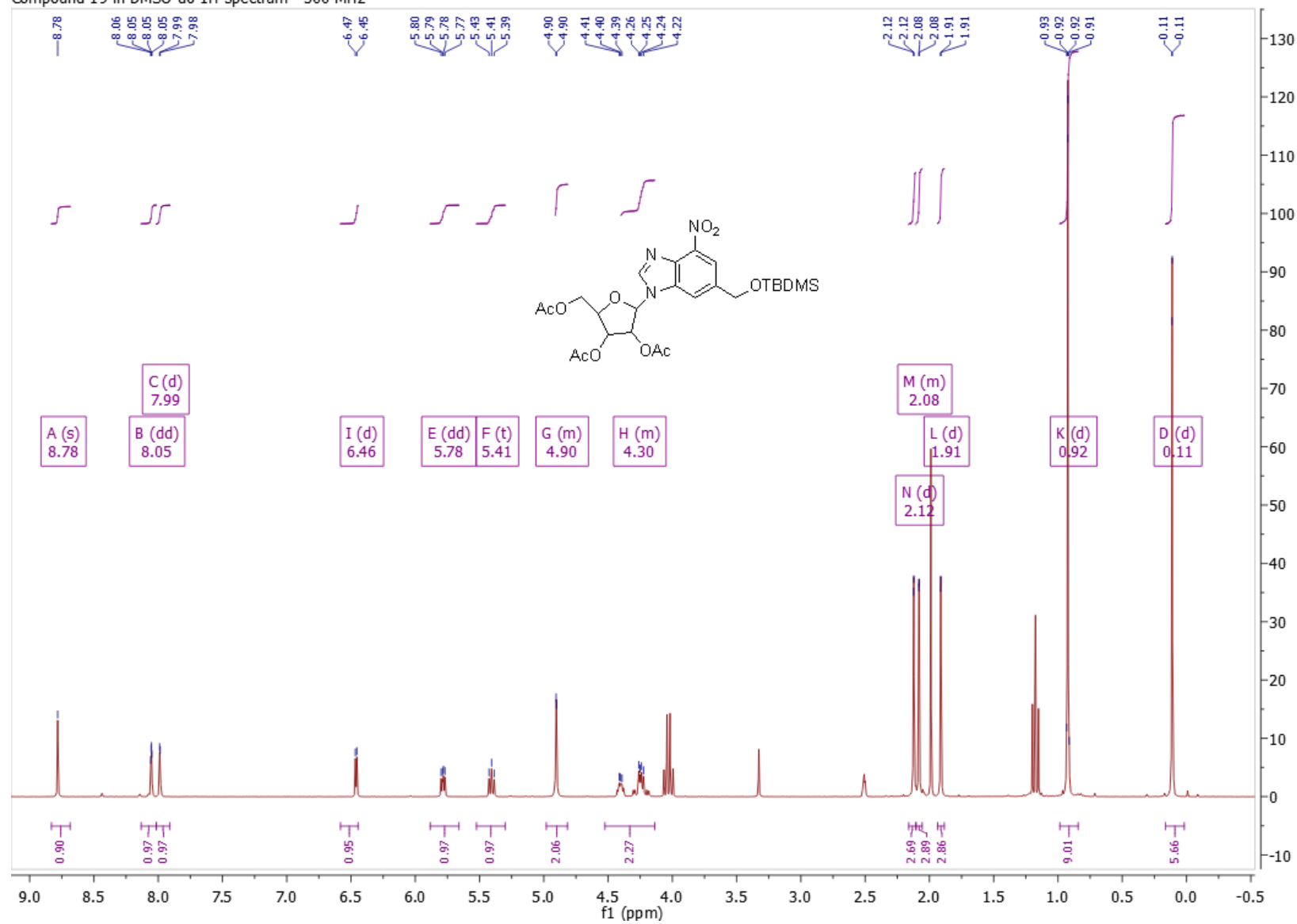
accurate mass

ES+  
07-Mar-2016

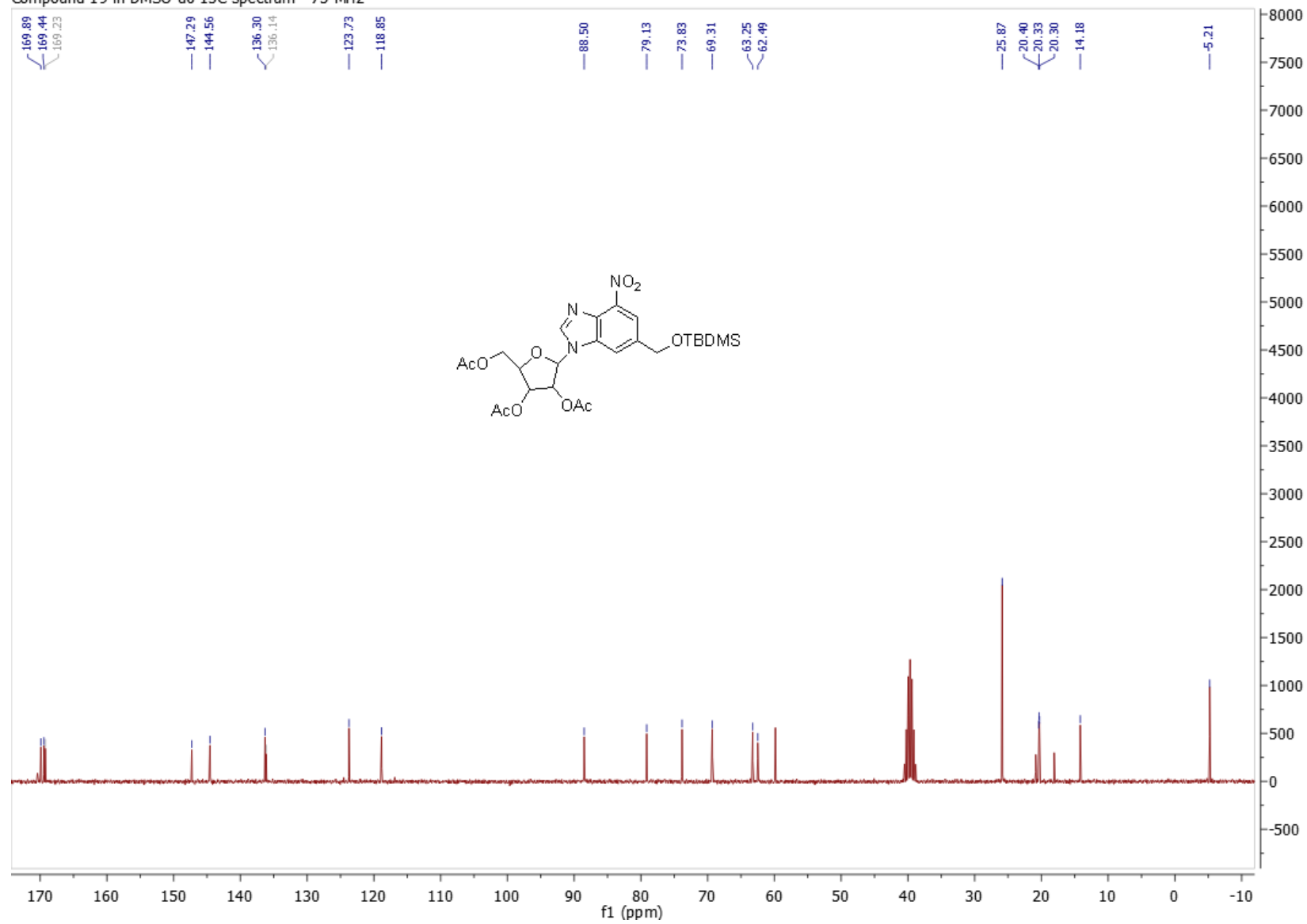




Compound 19 in DMSO-d6 1H spectrum - 300 MHz



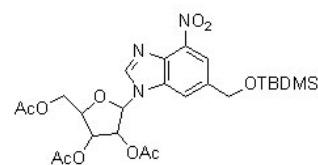
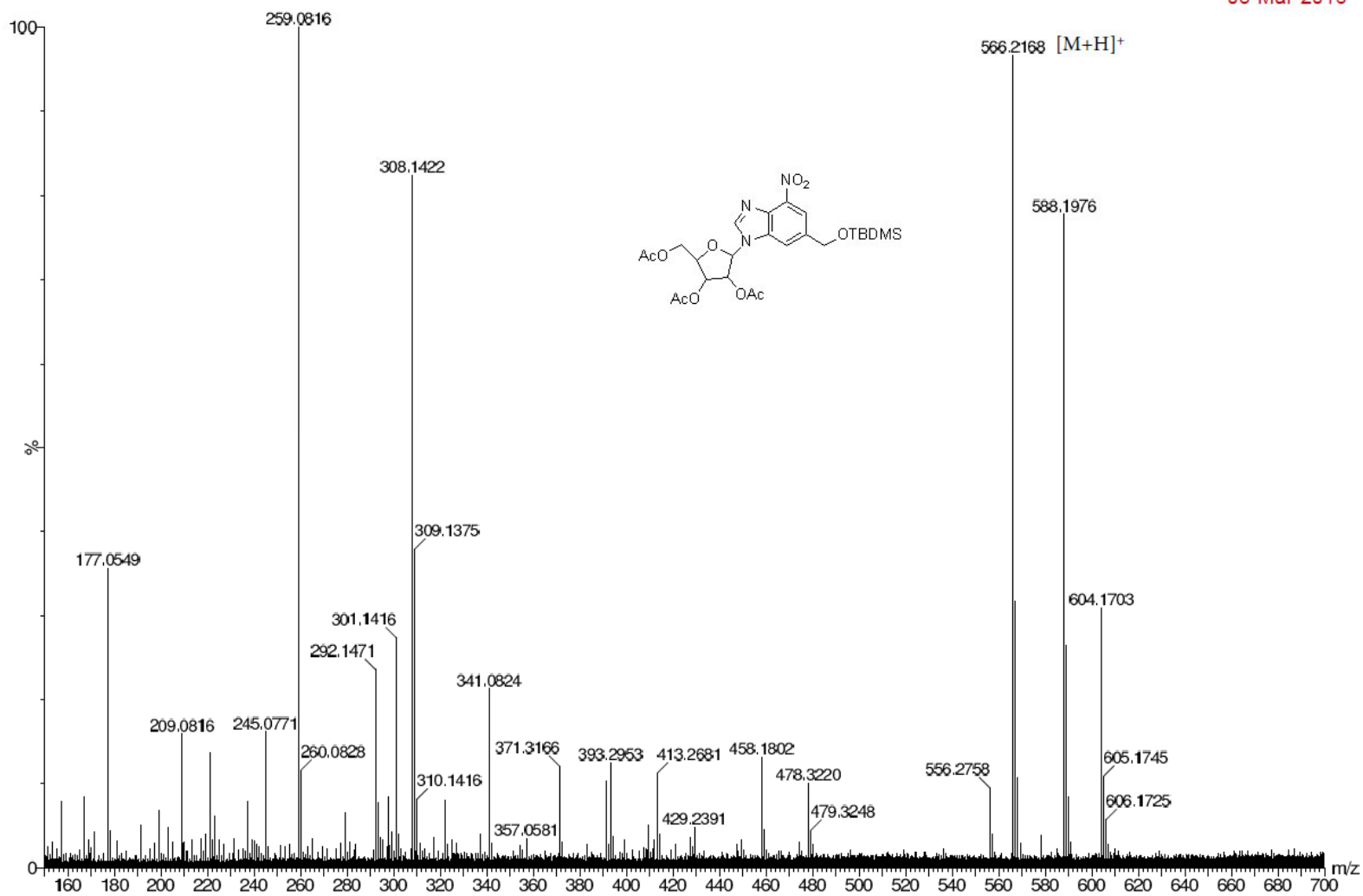
Compound 19 in DMSO-d6 13C spectrum - 75 MHz



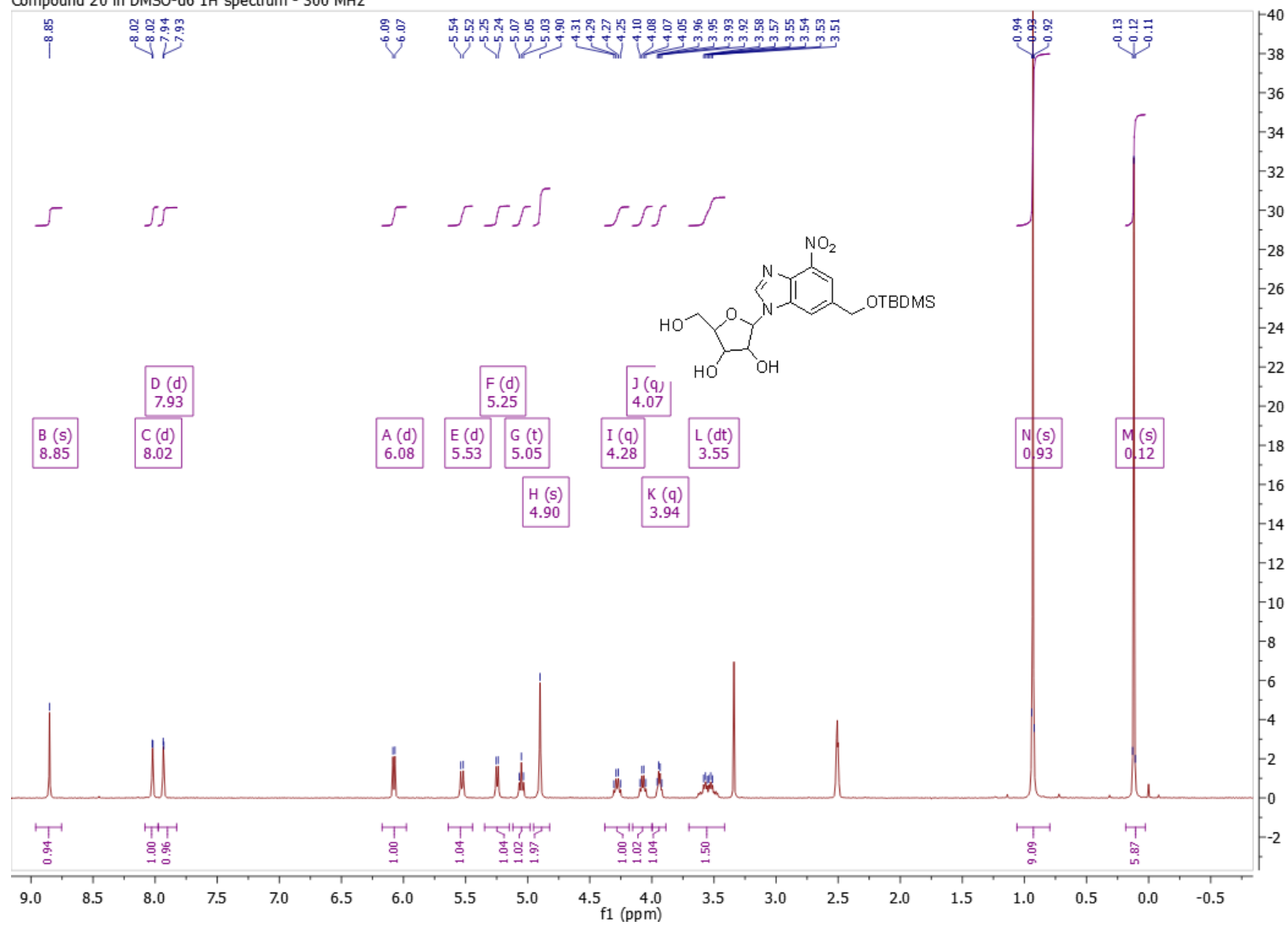
compound 19

accurate mass

ES+  
08-Mar-2016



Compound 20 in DMSO-d6 1H spectrum - 300 MHz

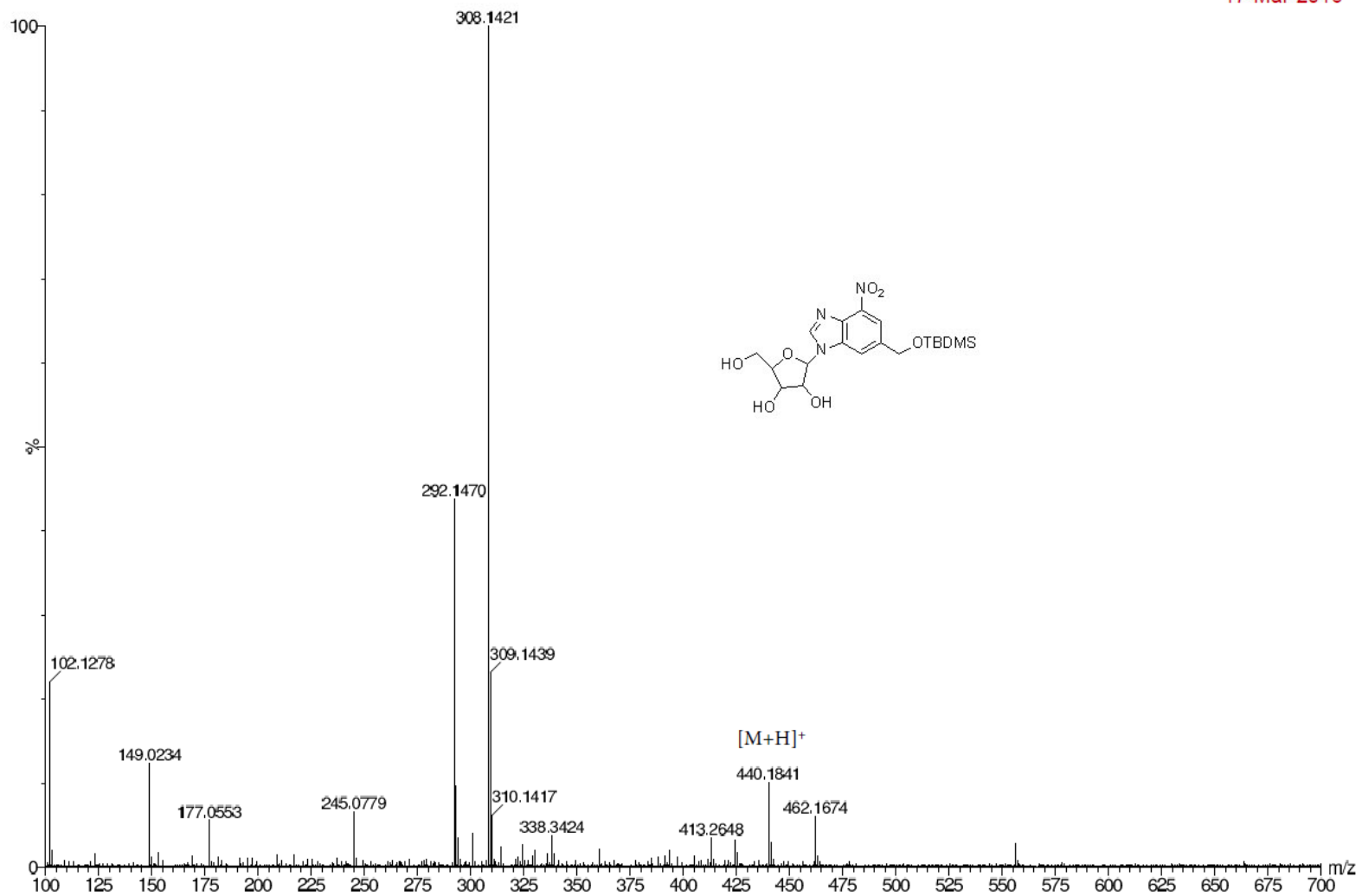




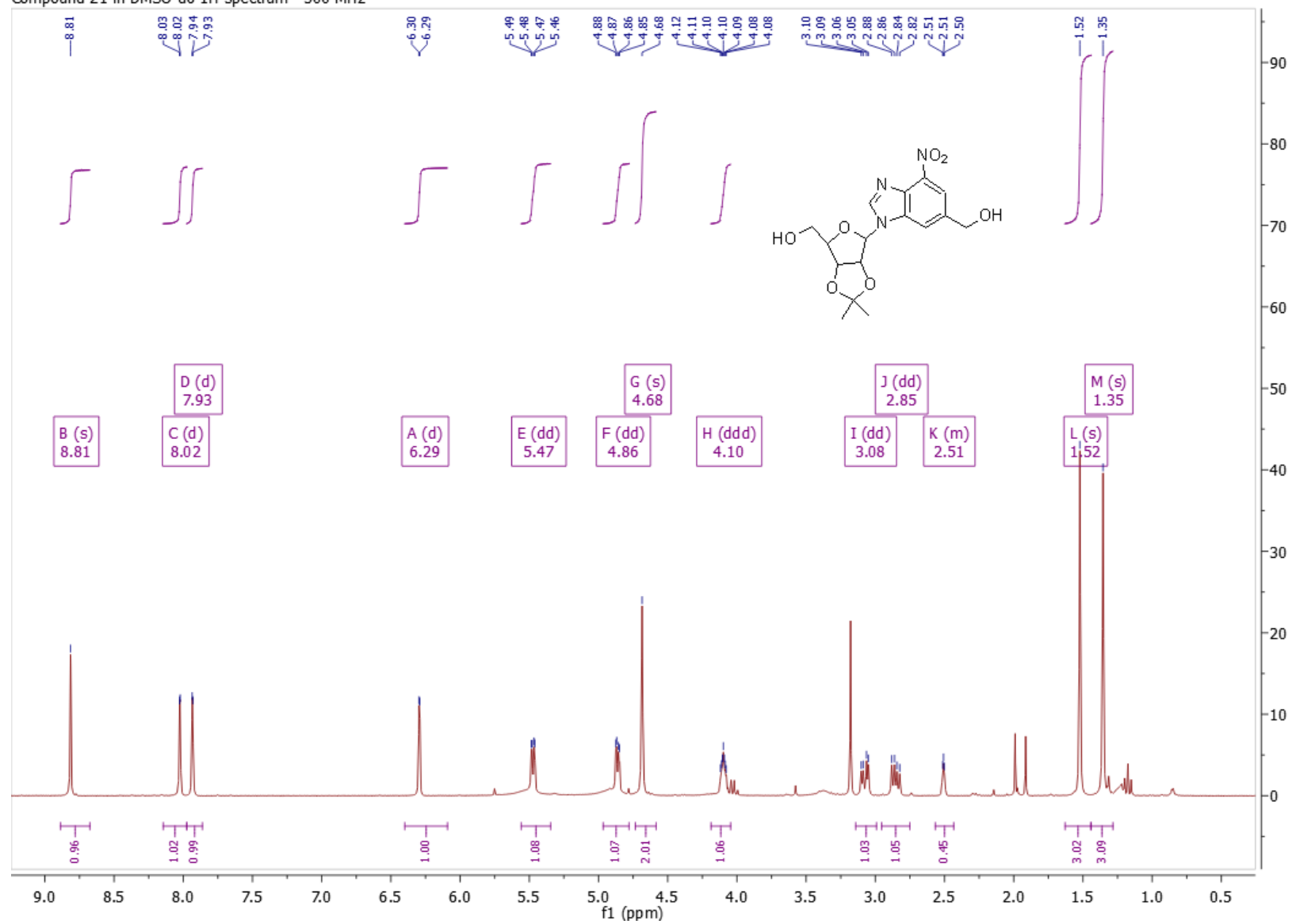
compound 20

accurate mass

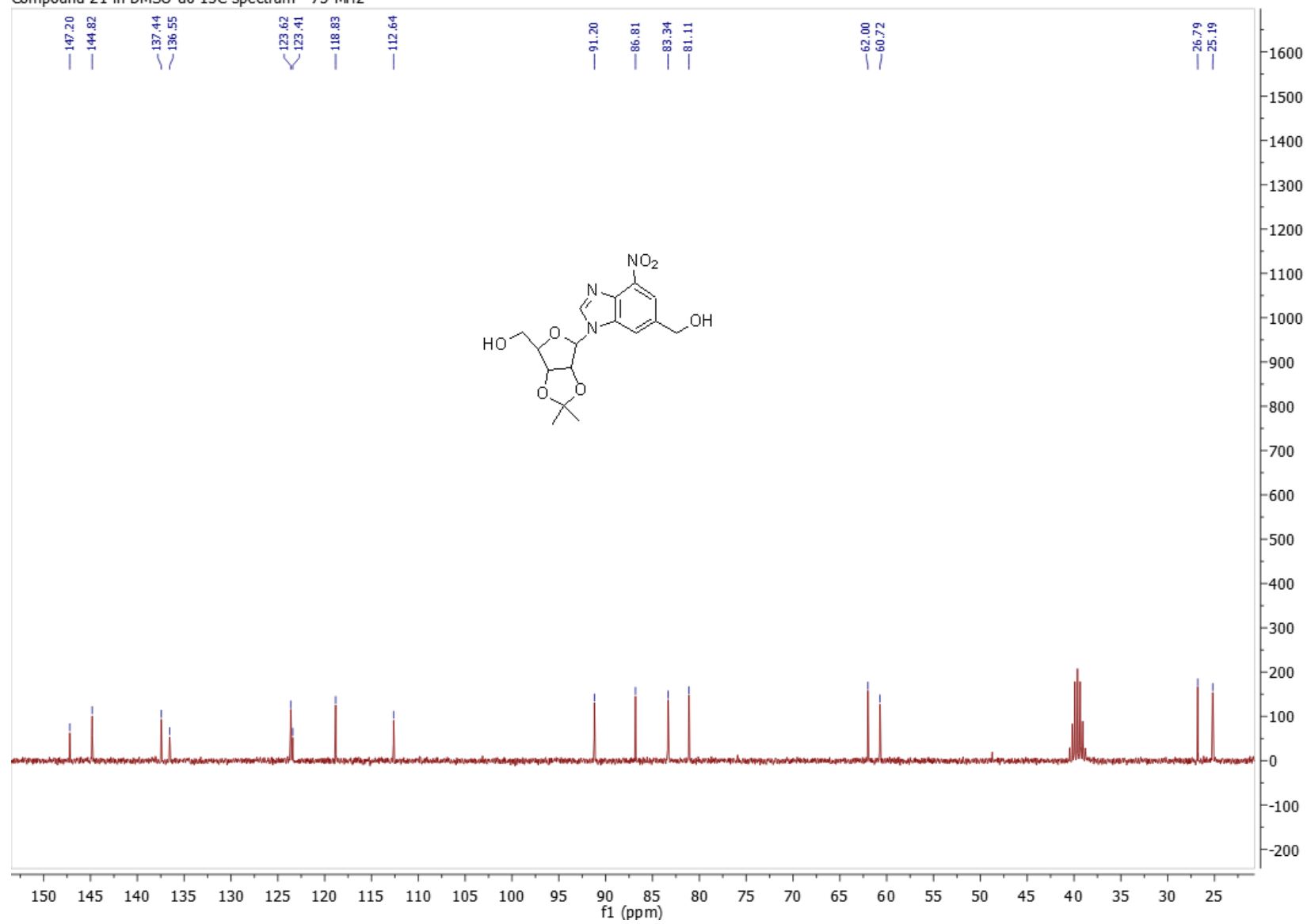
ES+  
17-Mar-2016



Compound 21 in DMSO-d6 1H spectrum - 300 MHz



Compound 21 in DMSO-d6 13C spectrum - 75 MHz

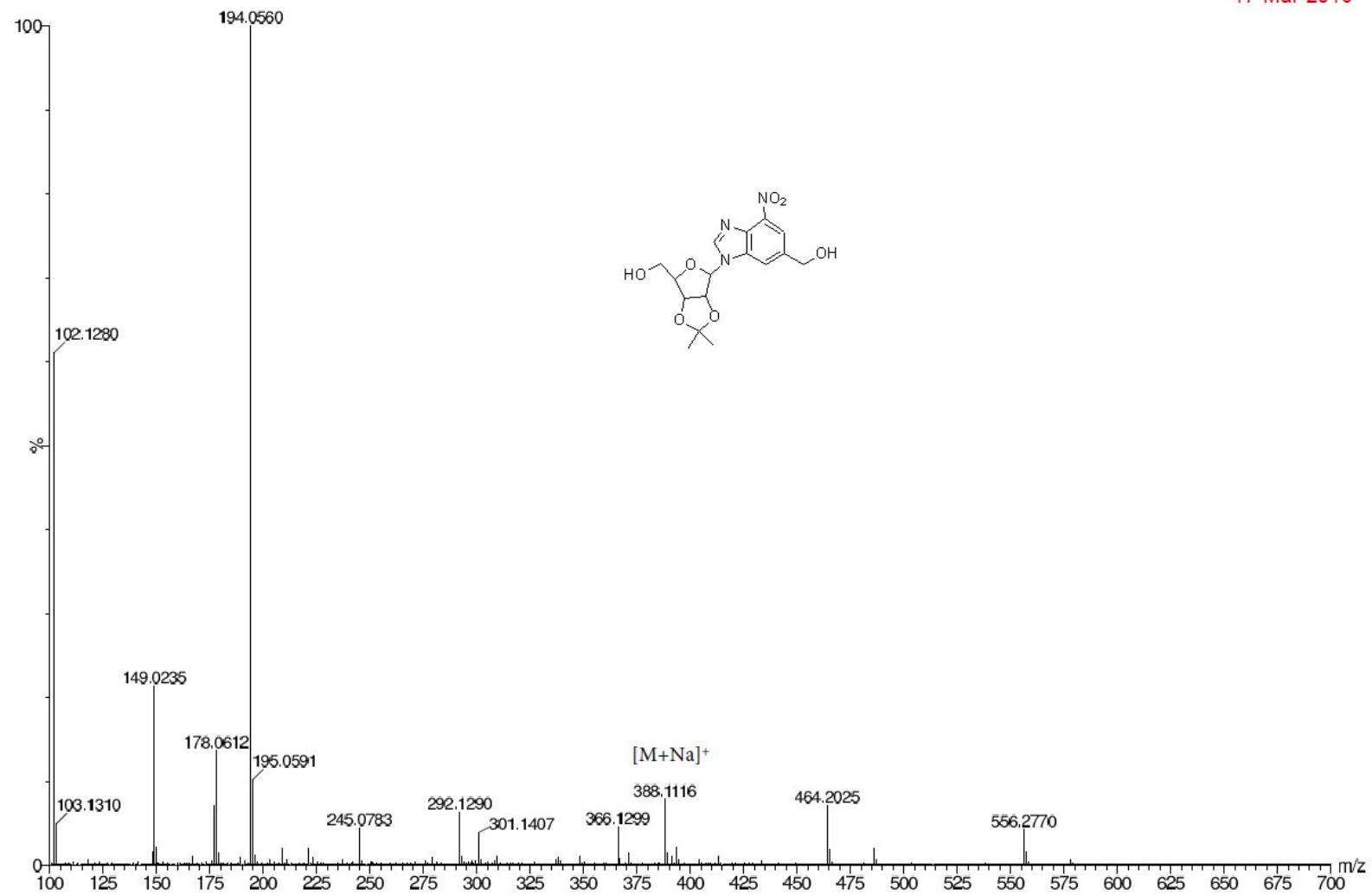




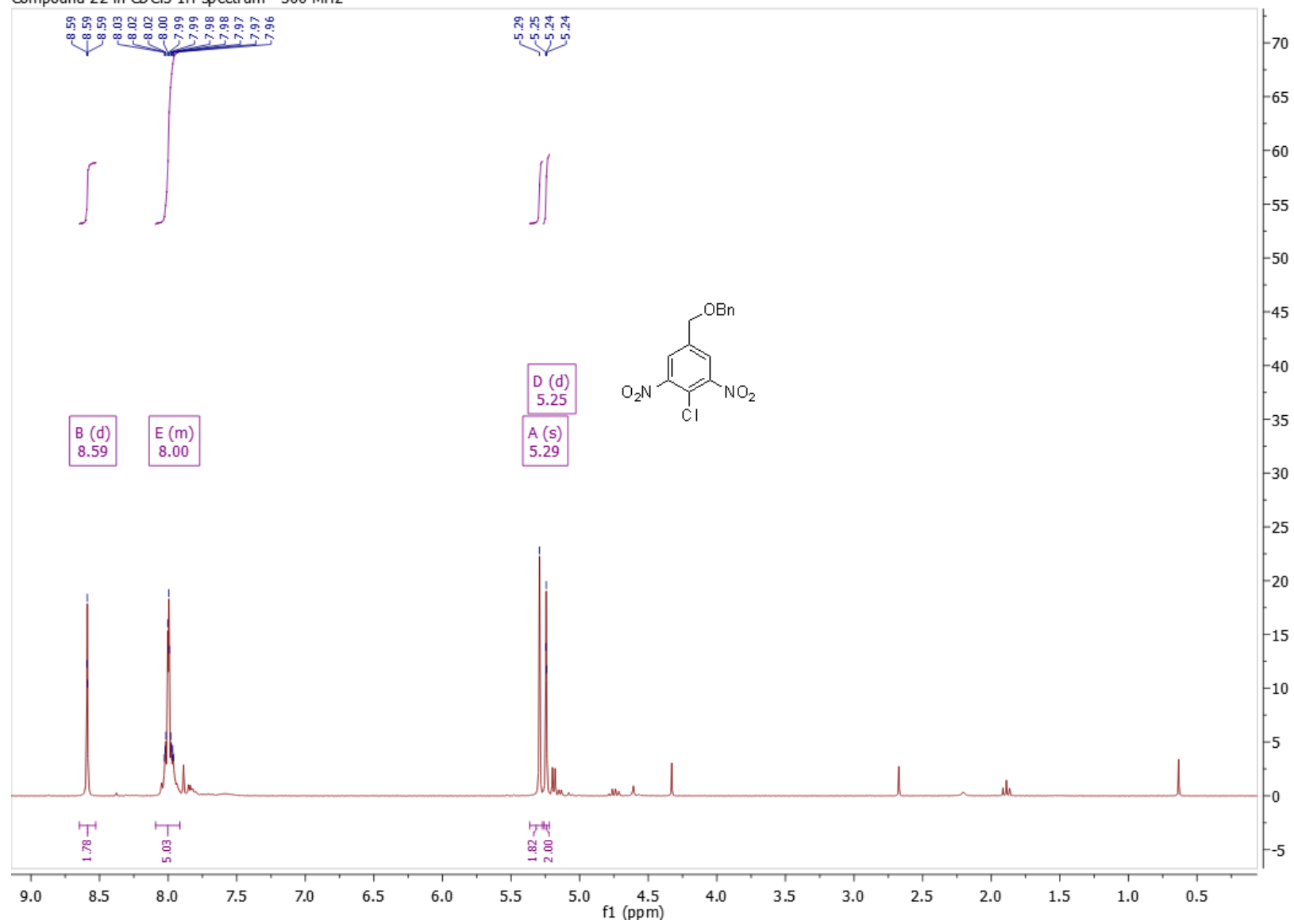
compound 21

accurate mass

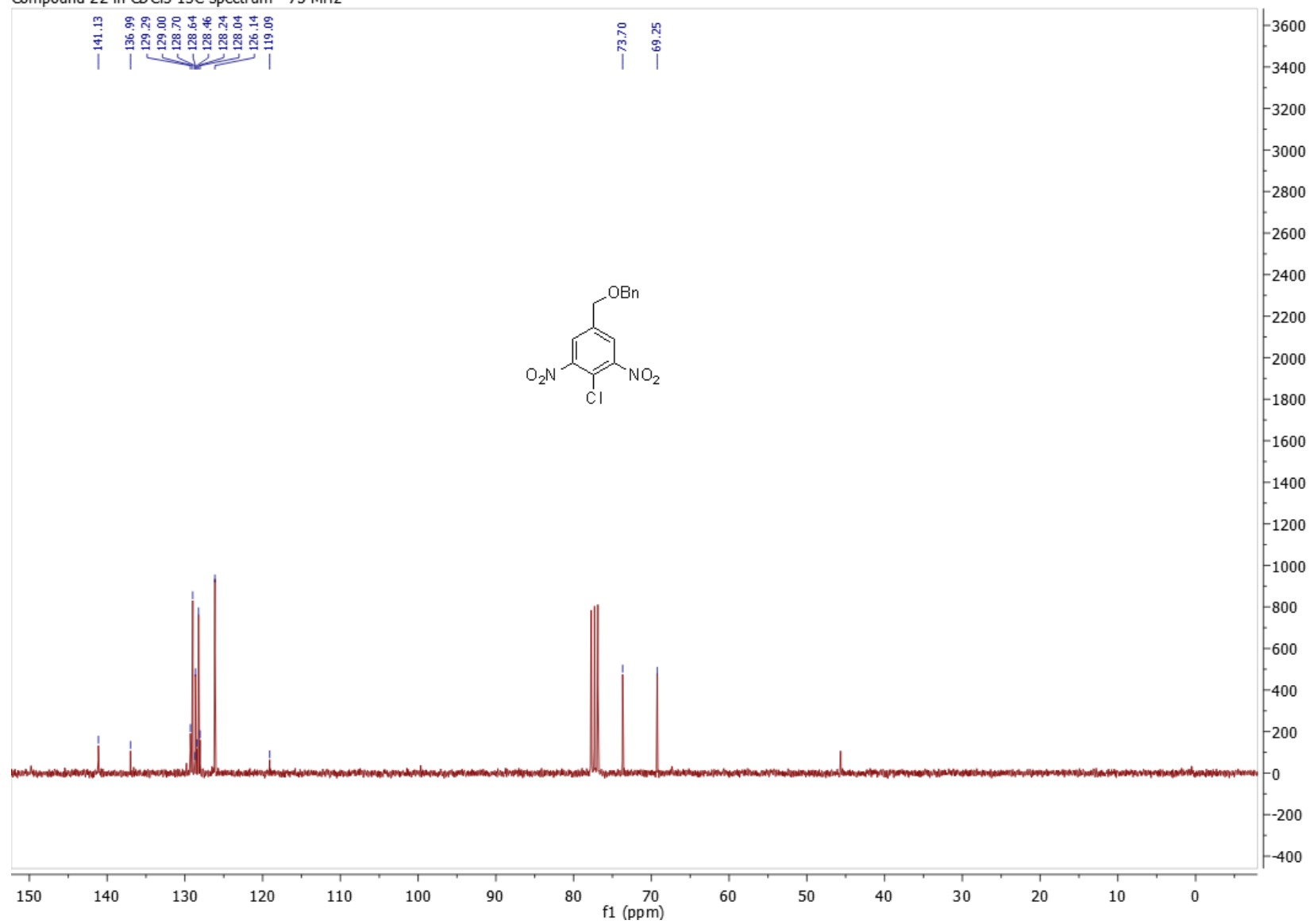
ES+  
17-Mar-2016



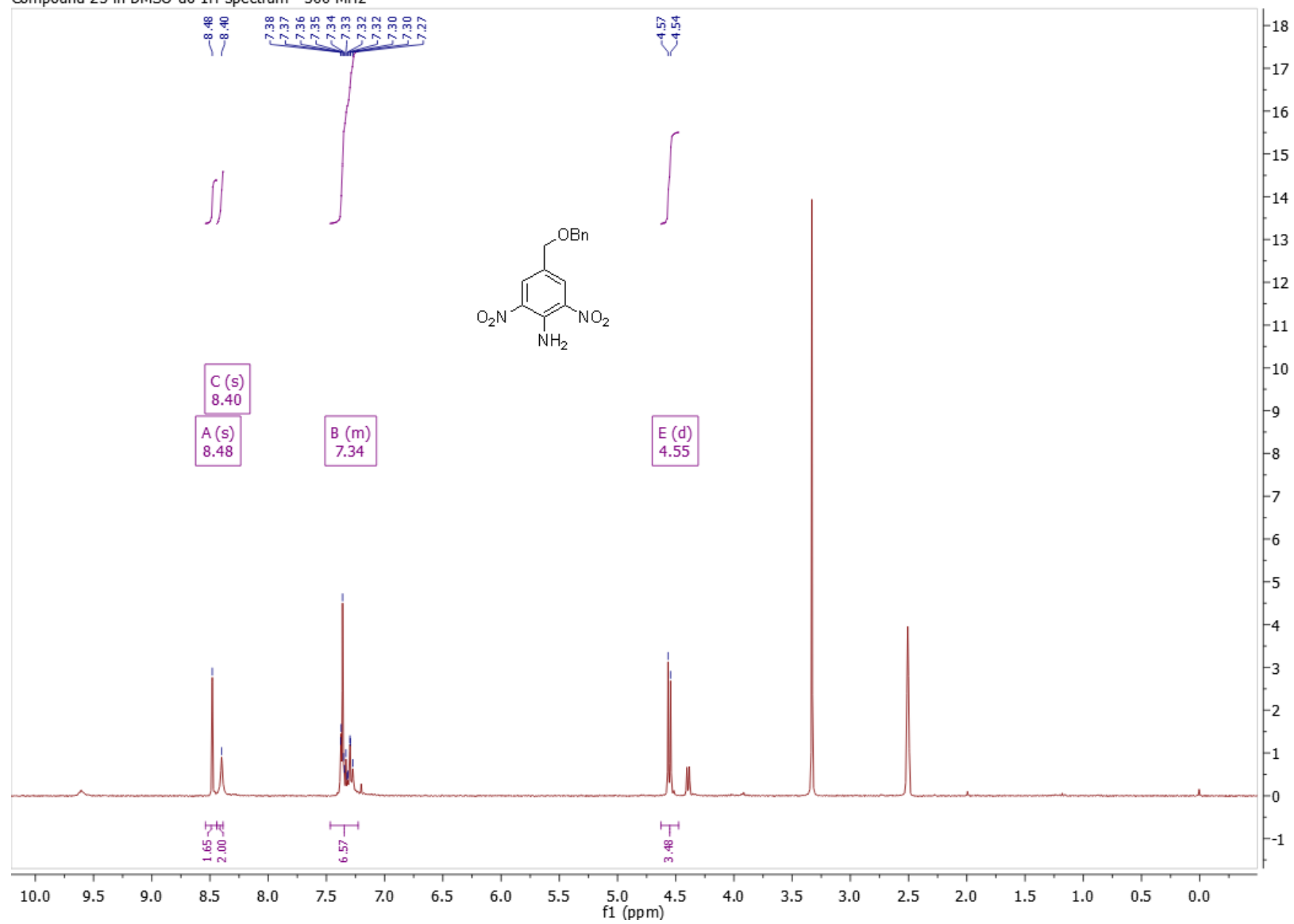
Compound 22 in CDCl<sub>3</sub> 1H spectrum - 300 MHz



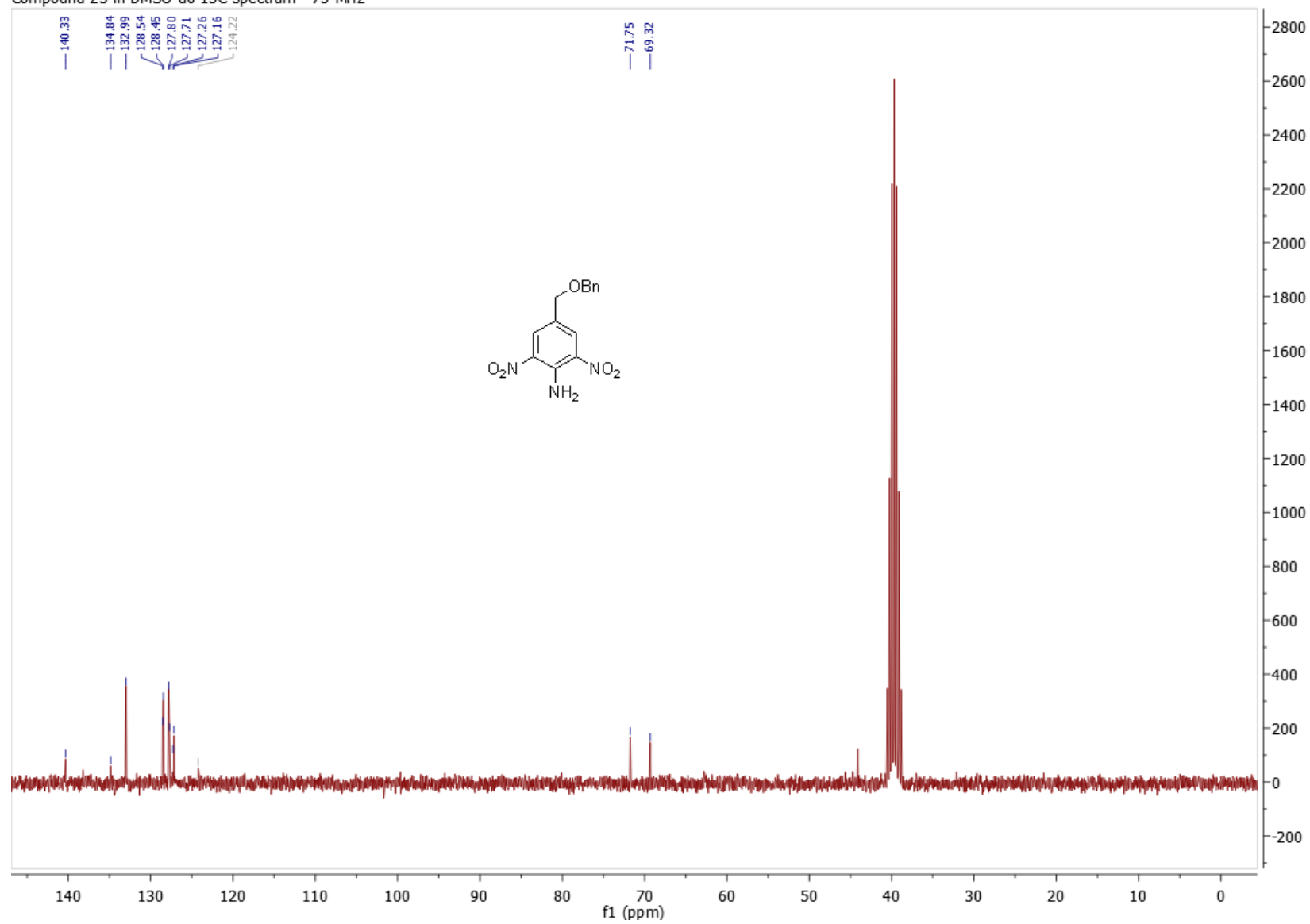
Compound 22 in CDCl<sub>3</sub> 13C spectrum - 75 MHz



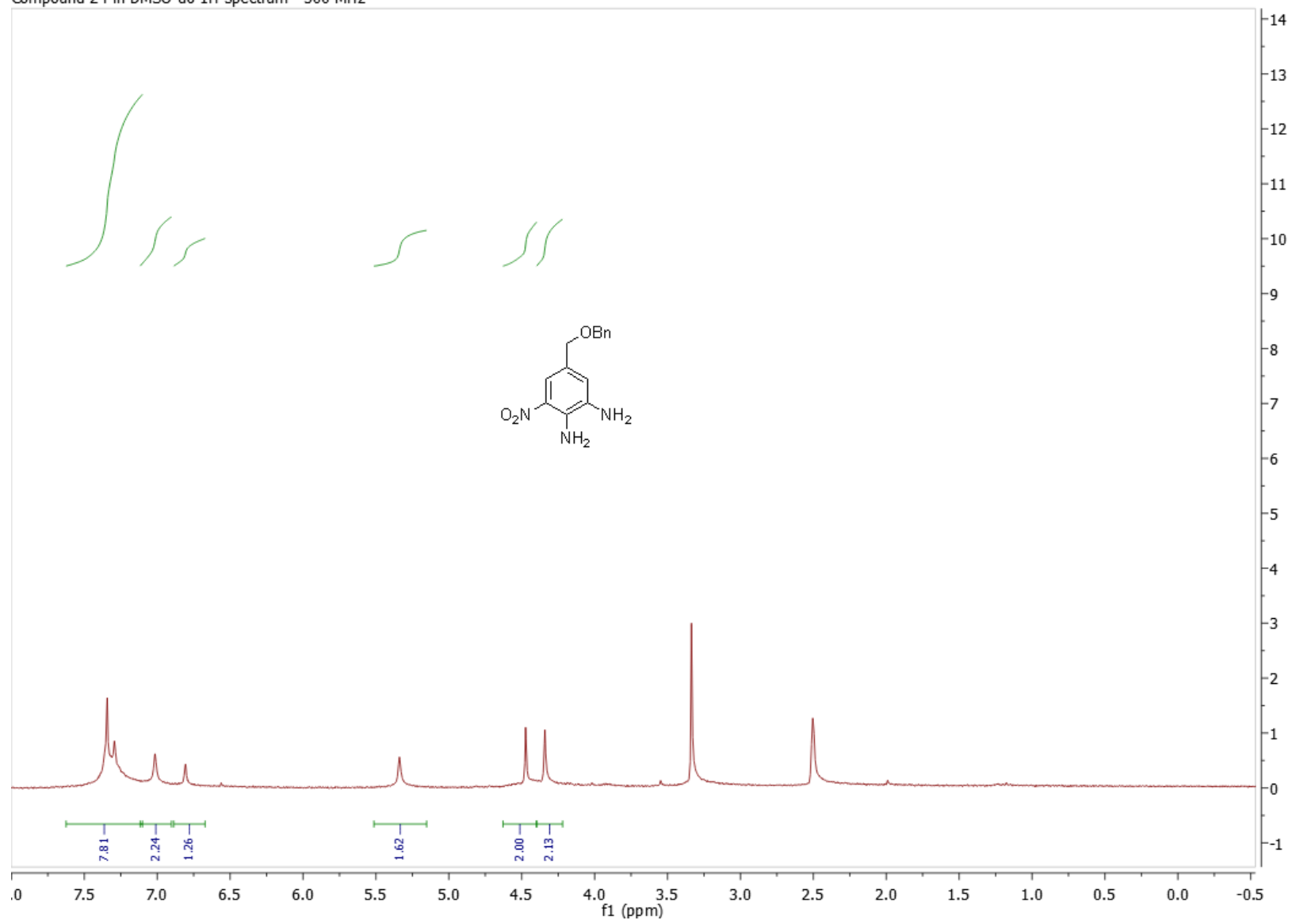
Compound 23 in DMSO-d6 1H spectrum - 300 MHz



Compound 23 in DMSO-d6 13C spectrum - 75 MHz



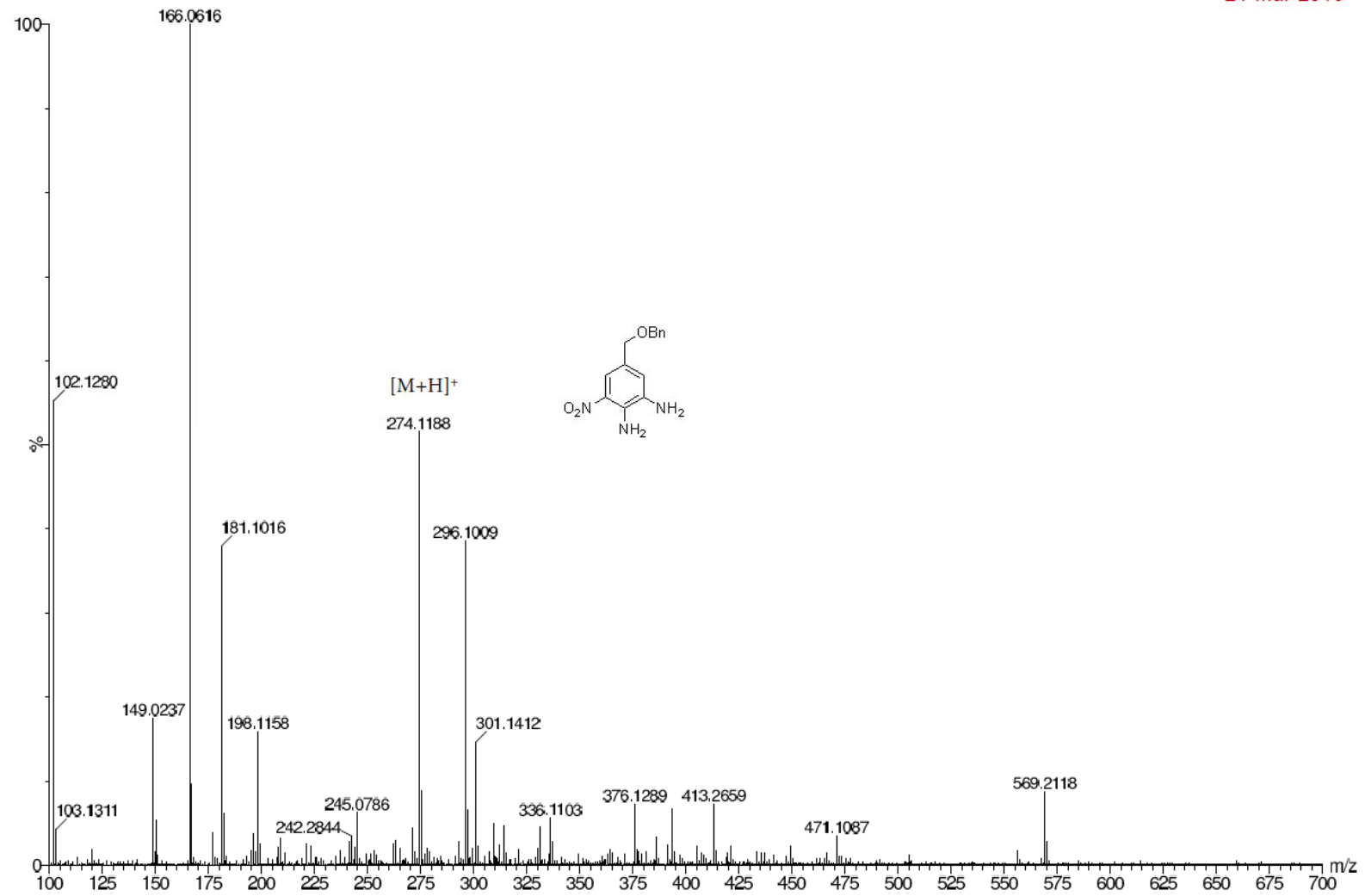
Compound 24 in DMSO-d6 1H spectrum - 300 MHz



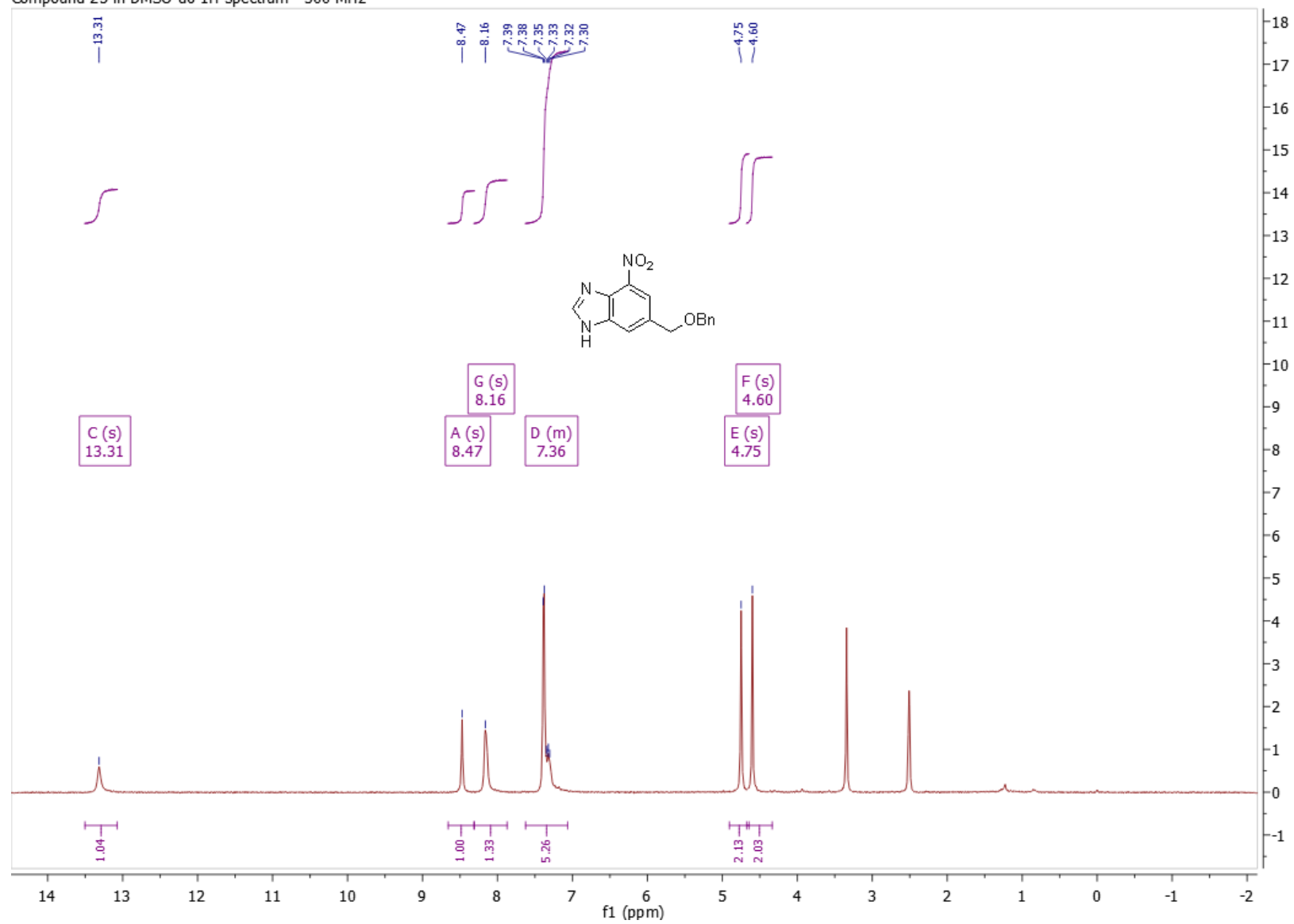
compound 24

accurate mass

ES+  
21-Mar-2016

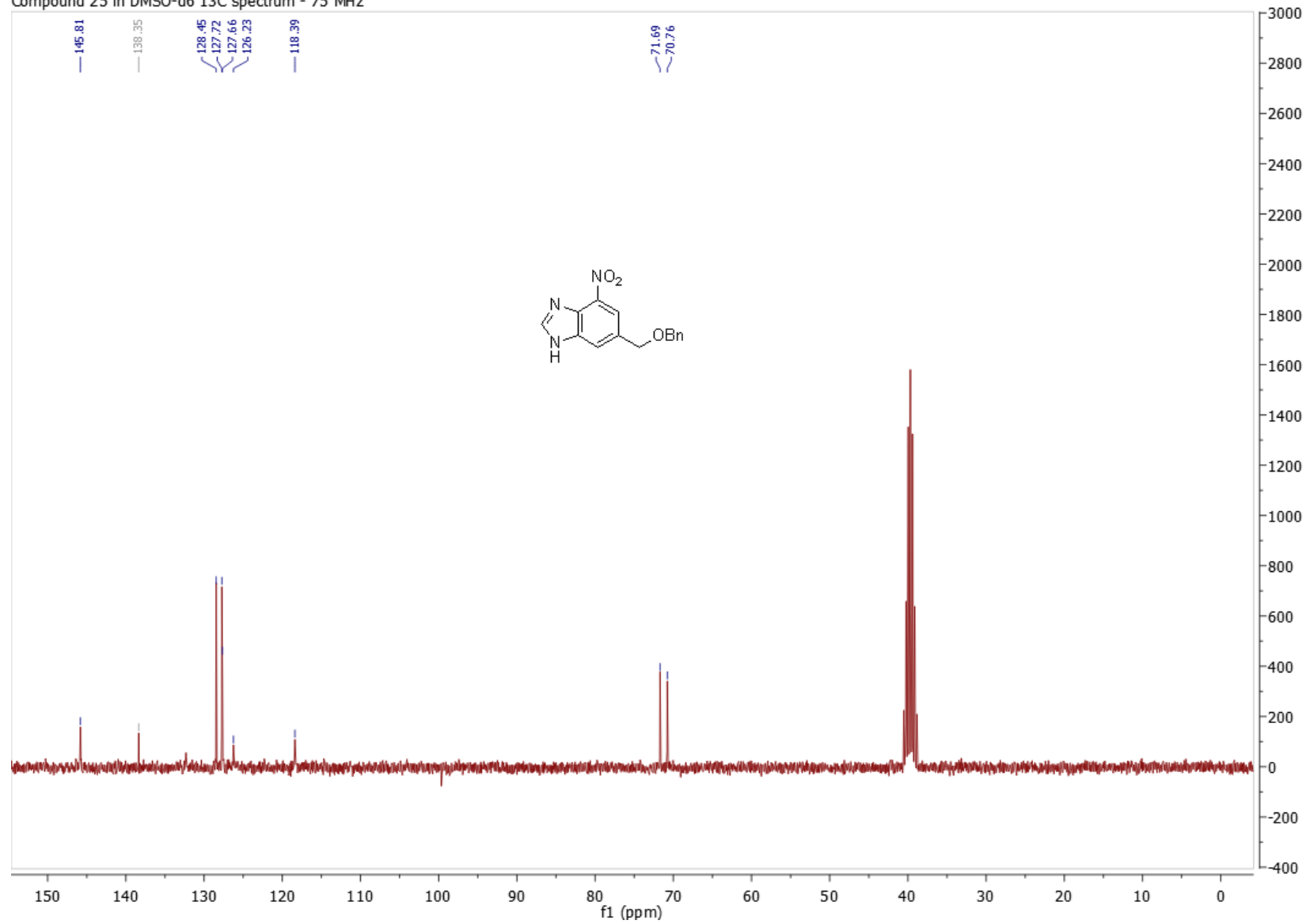


Compound 25 in DMSO-d6 1H spectrum - 300 MHz





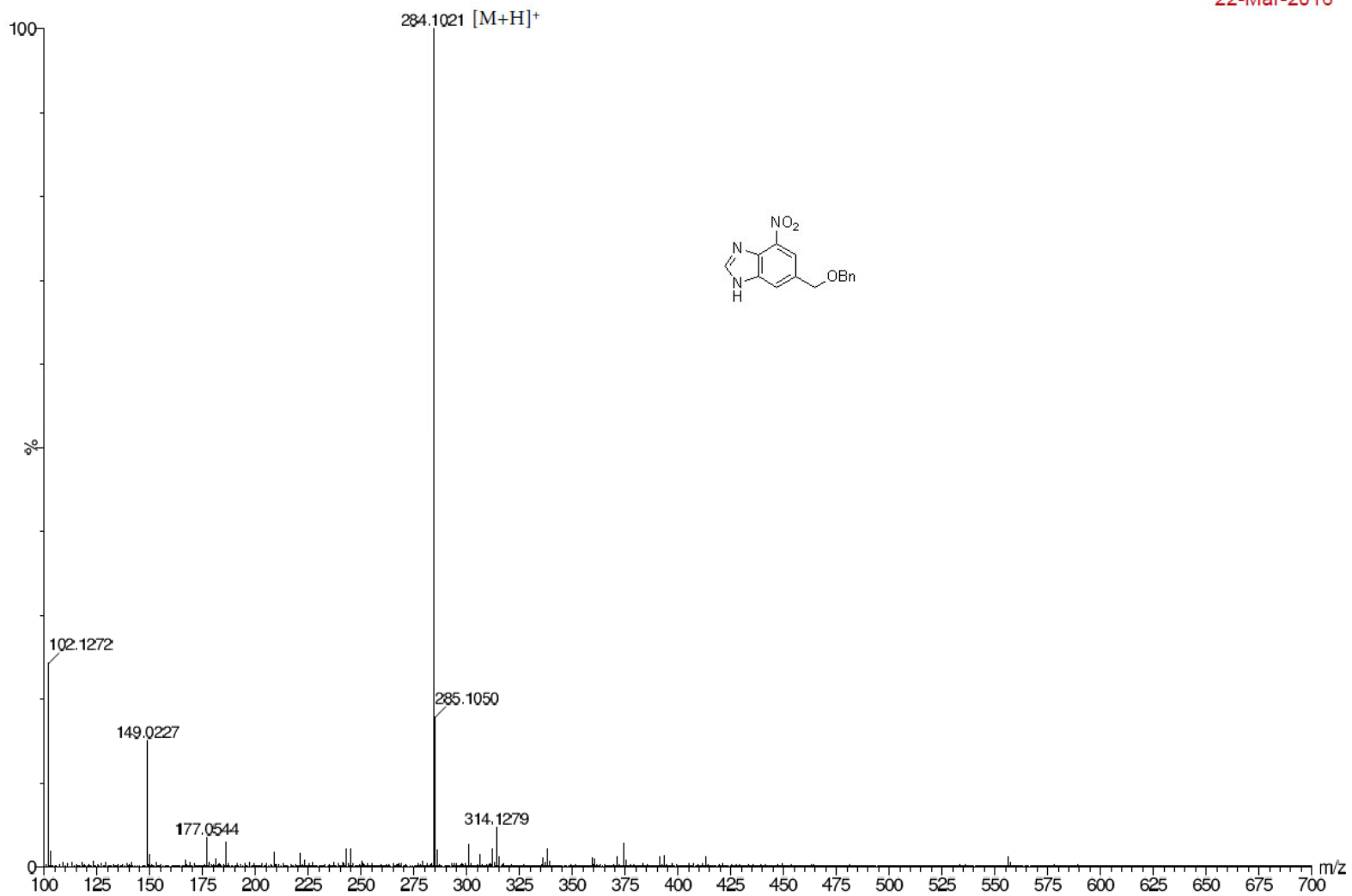
Compound 25 in DMSO-d6 13C spectrum - 75 MHz



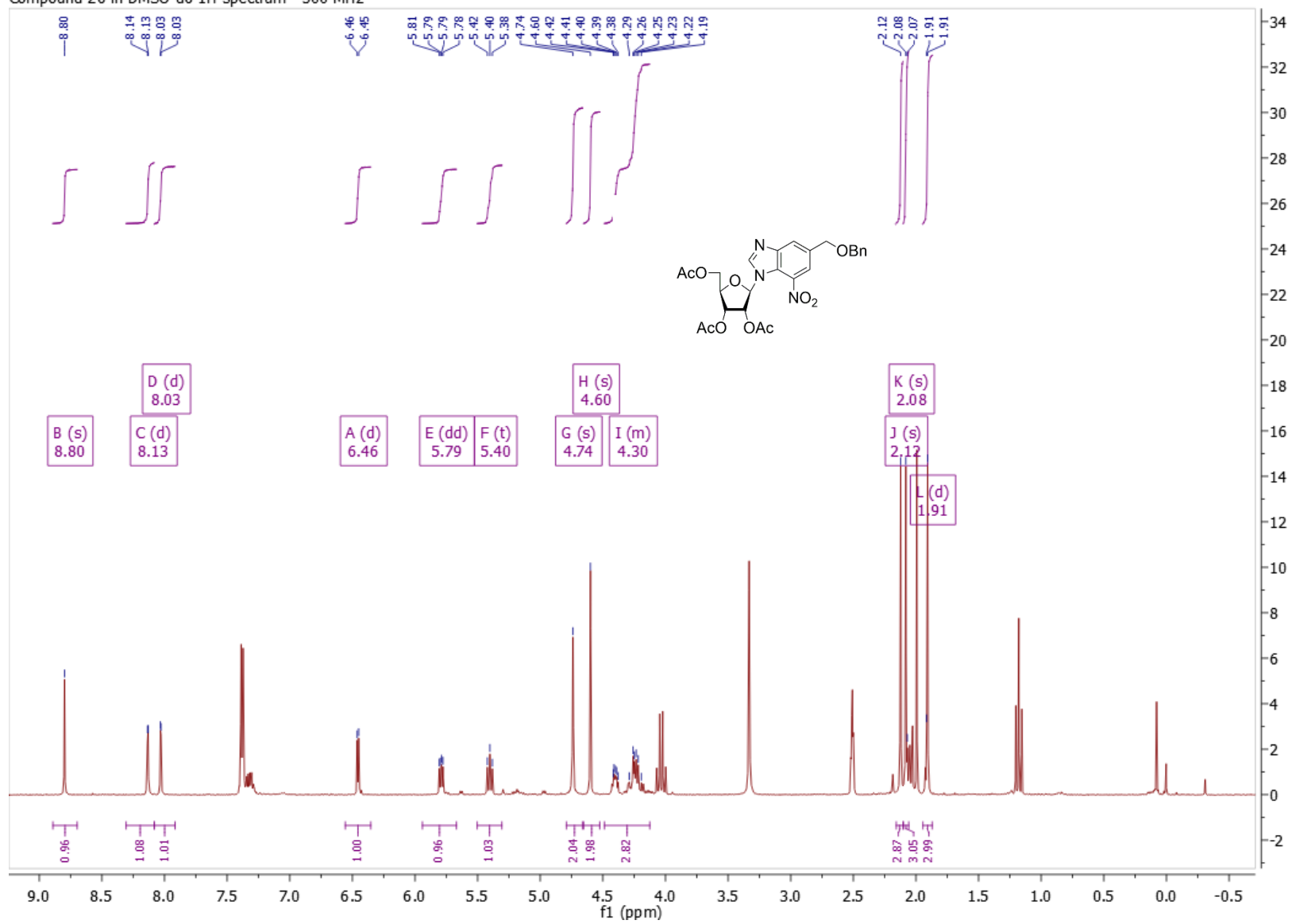
compound 25

accurate mass

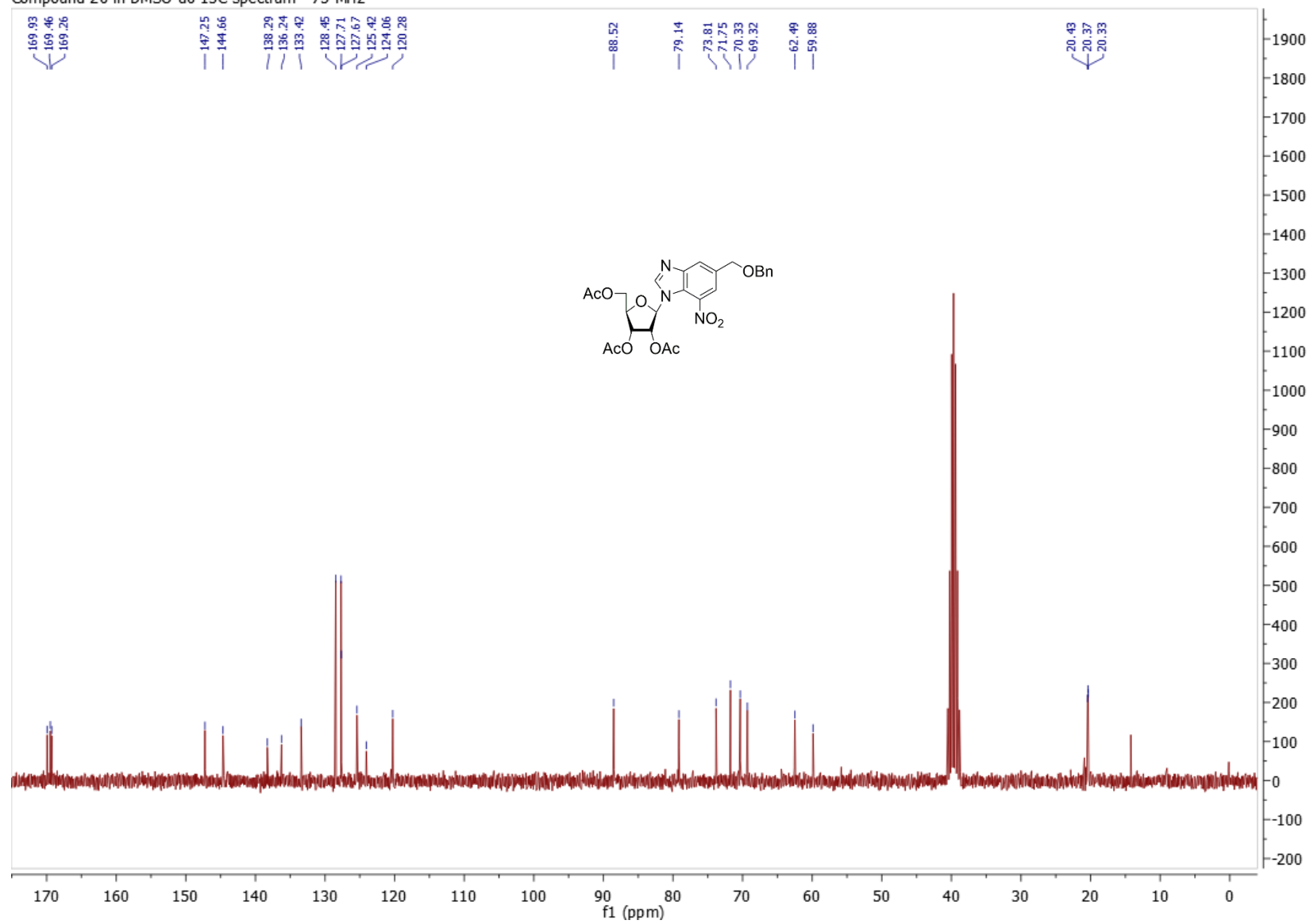
ES+  
22-Mar-2016



Compound 26 in DMSO-d6 1H spectrum - 300 MHz



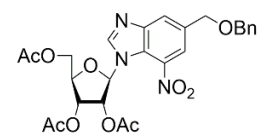
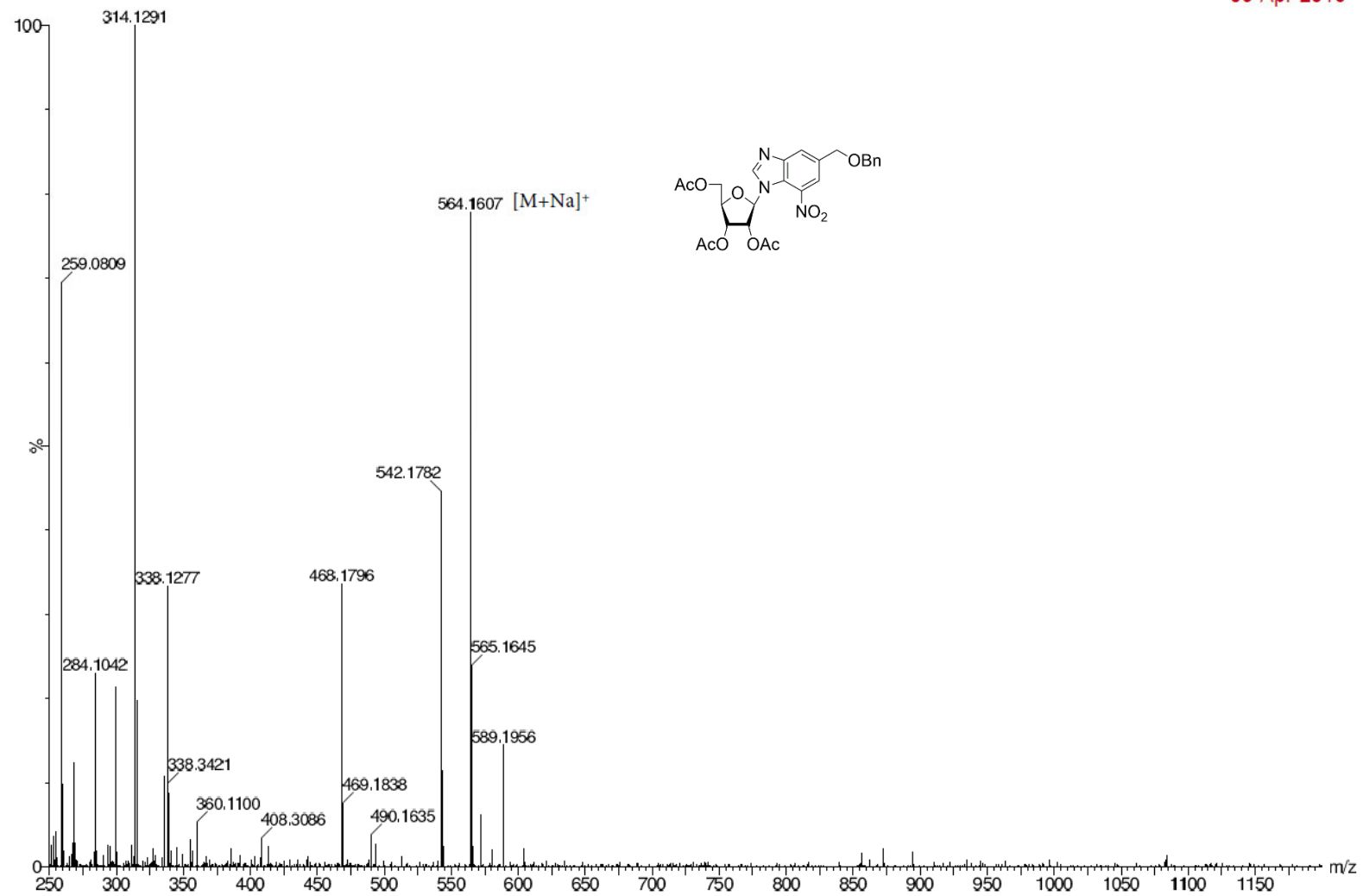
Compound 26 in DMSO-d6 13C spectrum - 75 MHz



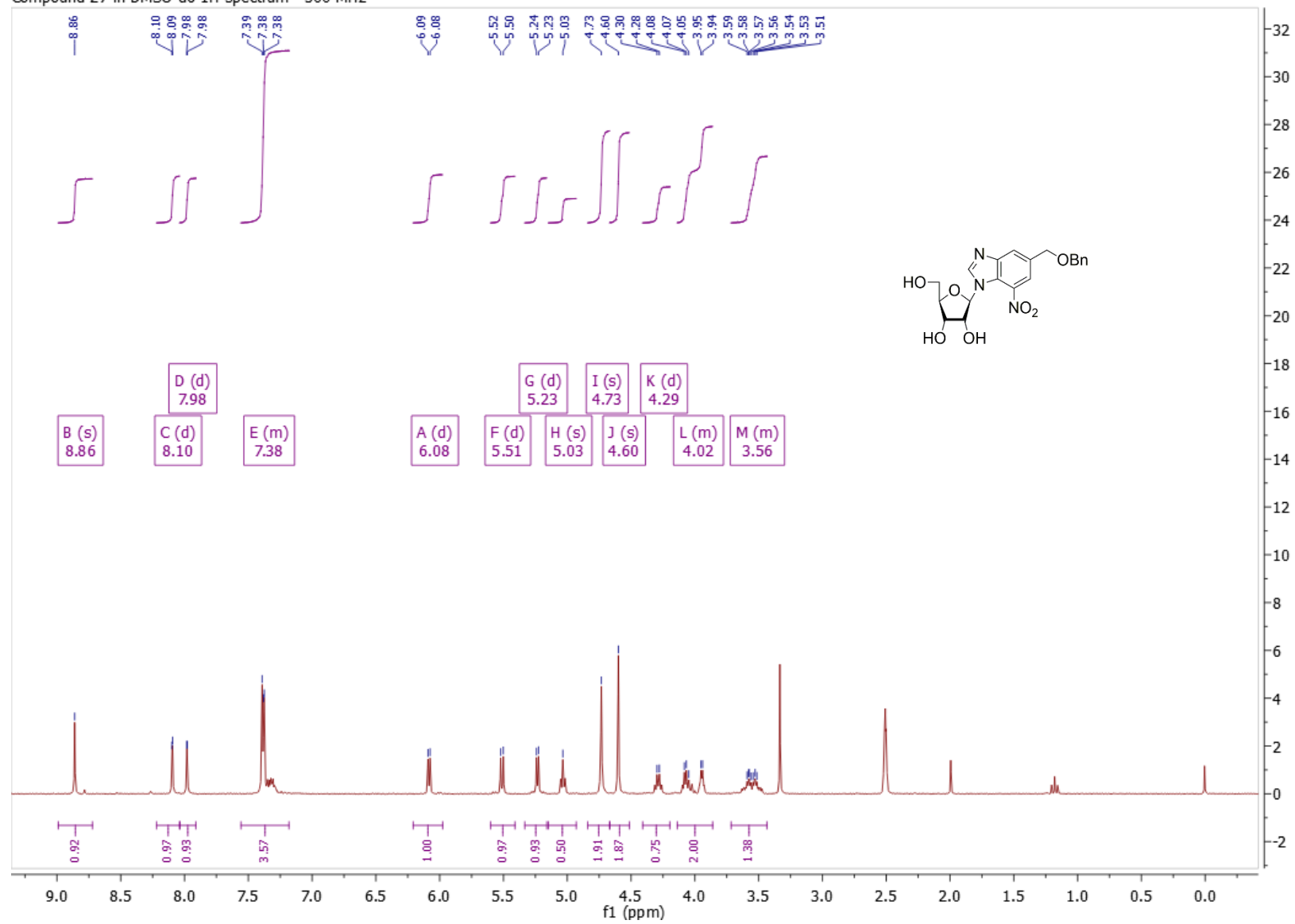
compound 26

accurate mass

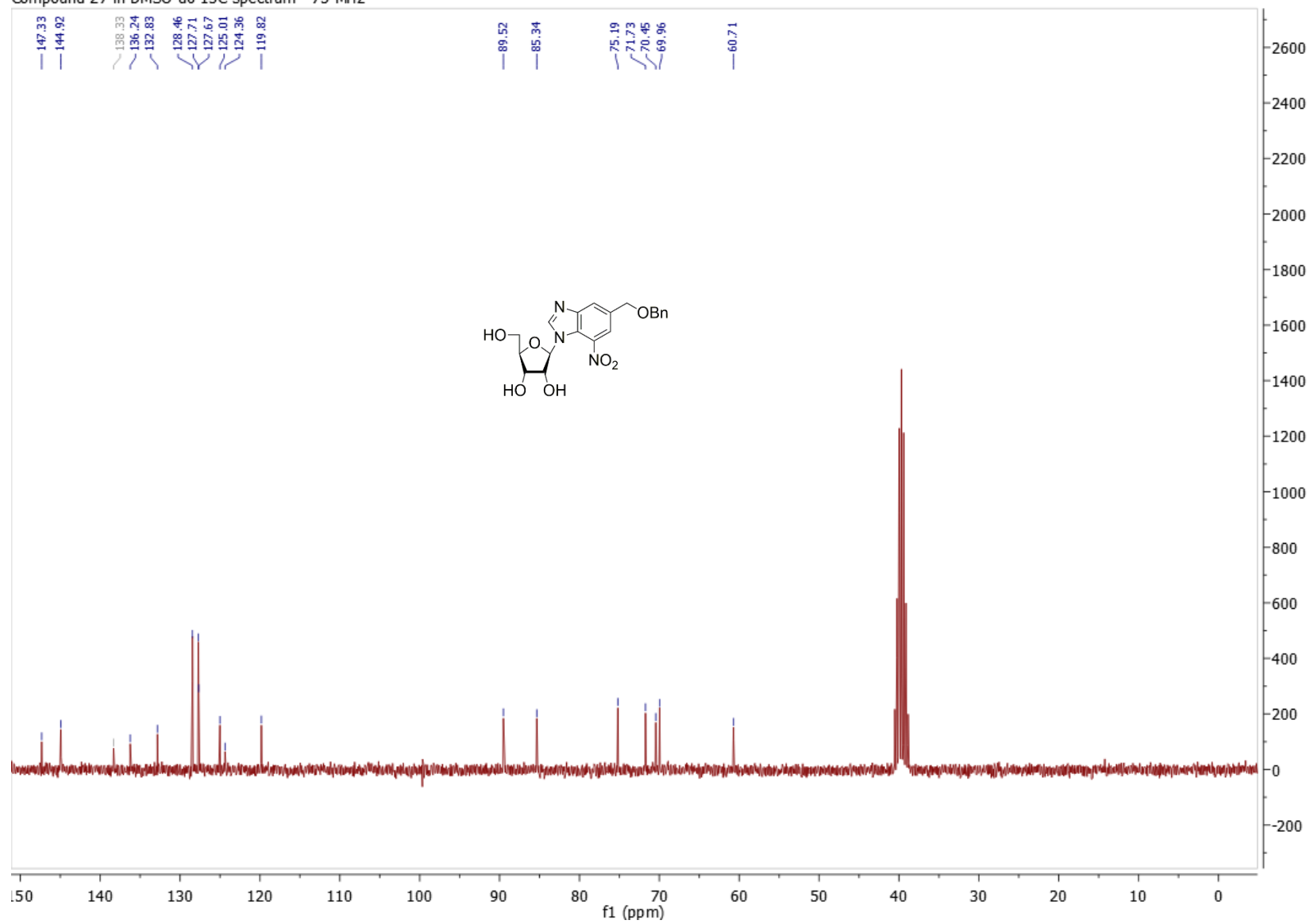
ES+  
05-Apr-2016



Compound 27 in DMSO-d6 1H spectrum - 300 MHz



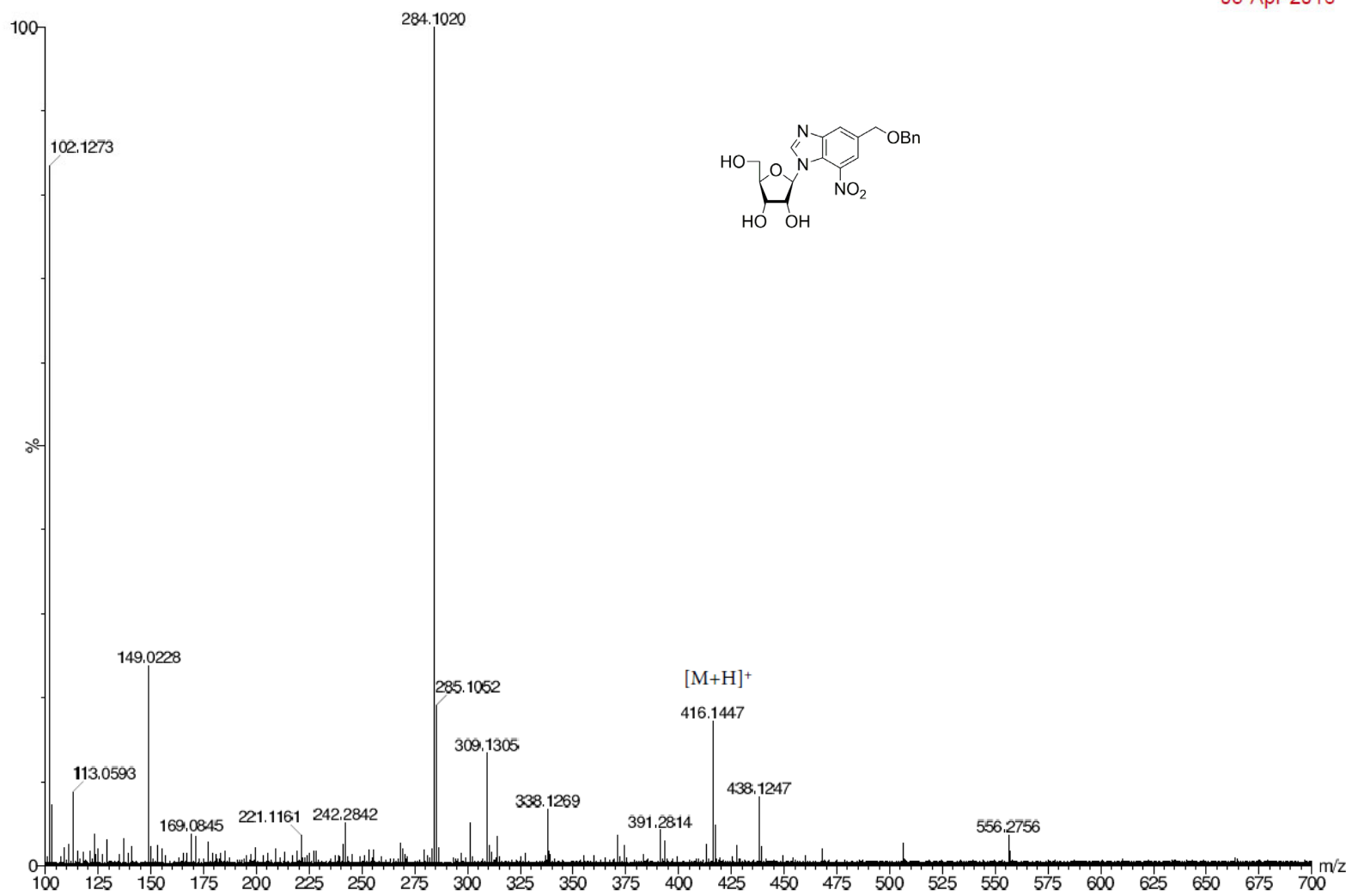
Compound 27 in DMSO-d6 13C spectrum - 75 MHz



compound 27

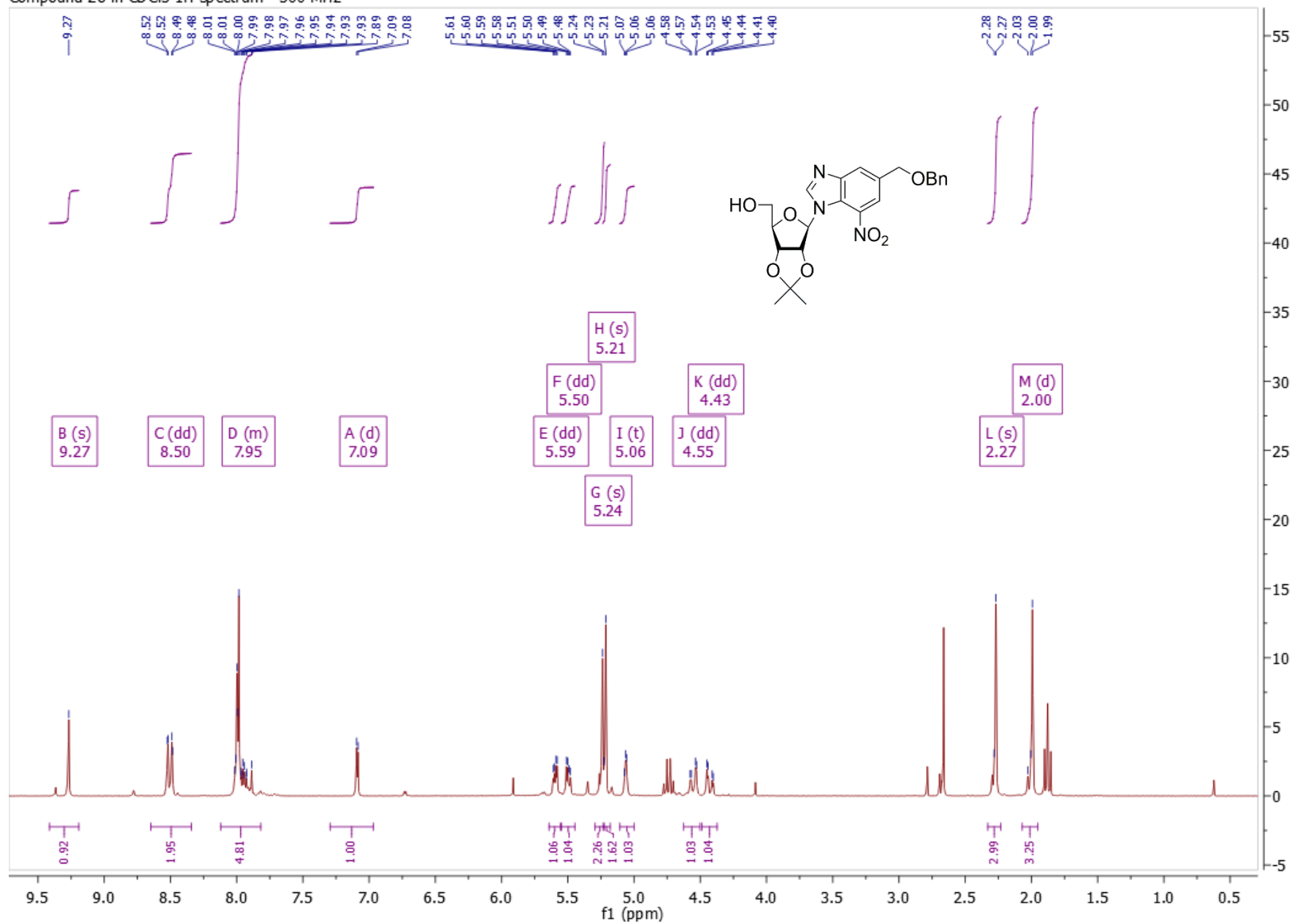
accurate mass

ES+  
05-Apr-2016

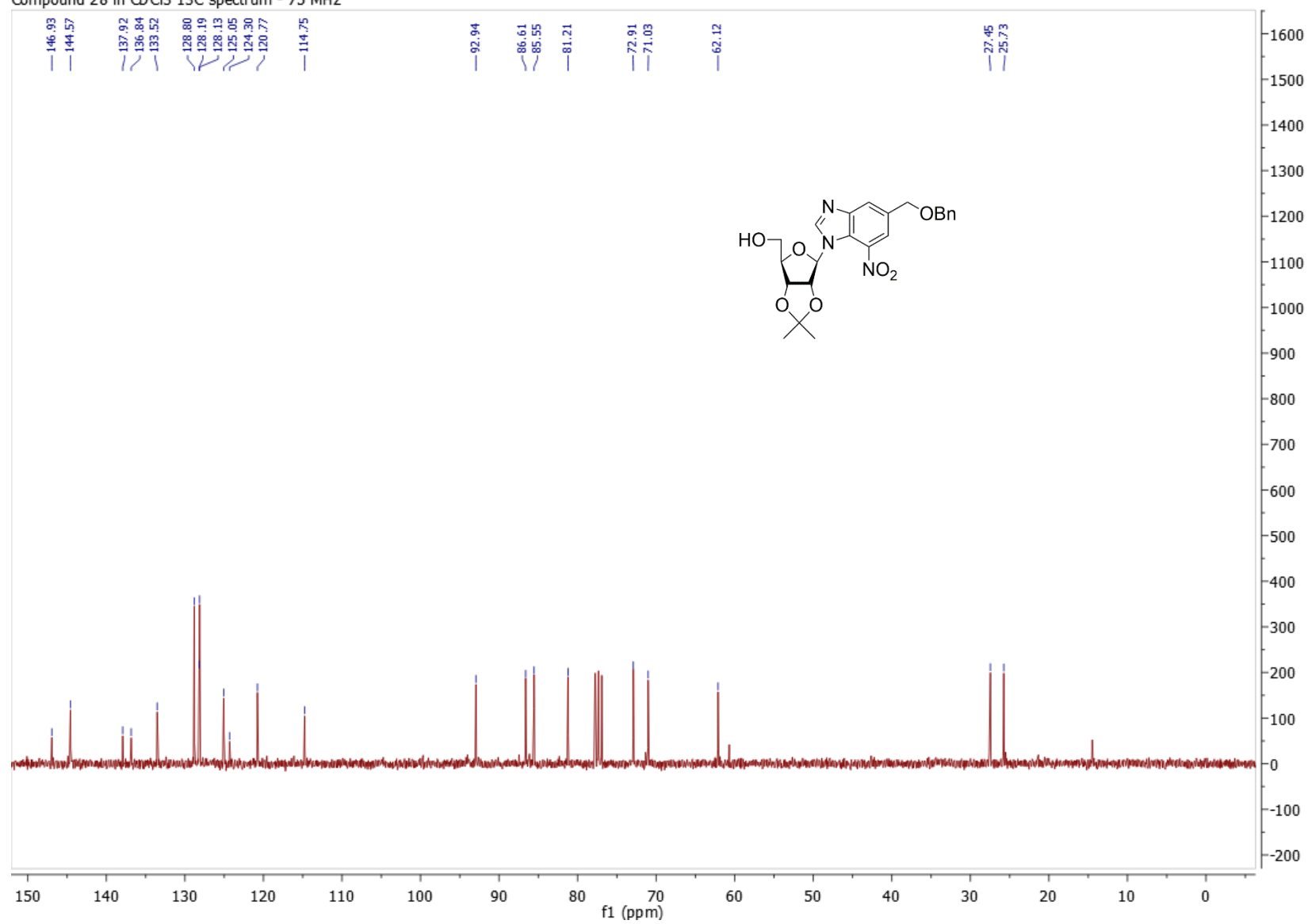




Compound 28 in CDCl<sub>3</sub> 1H spectrum - 300 MHz



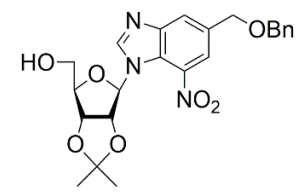
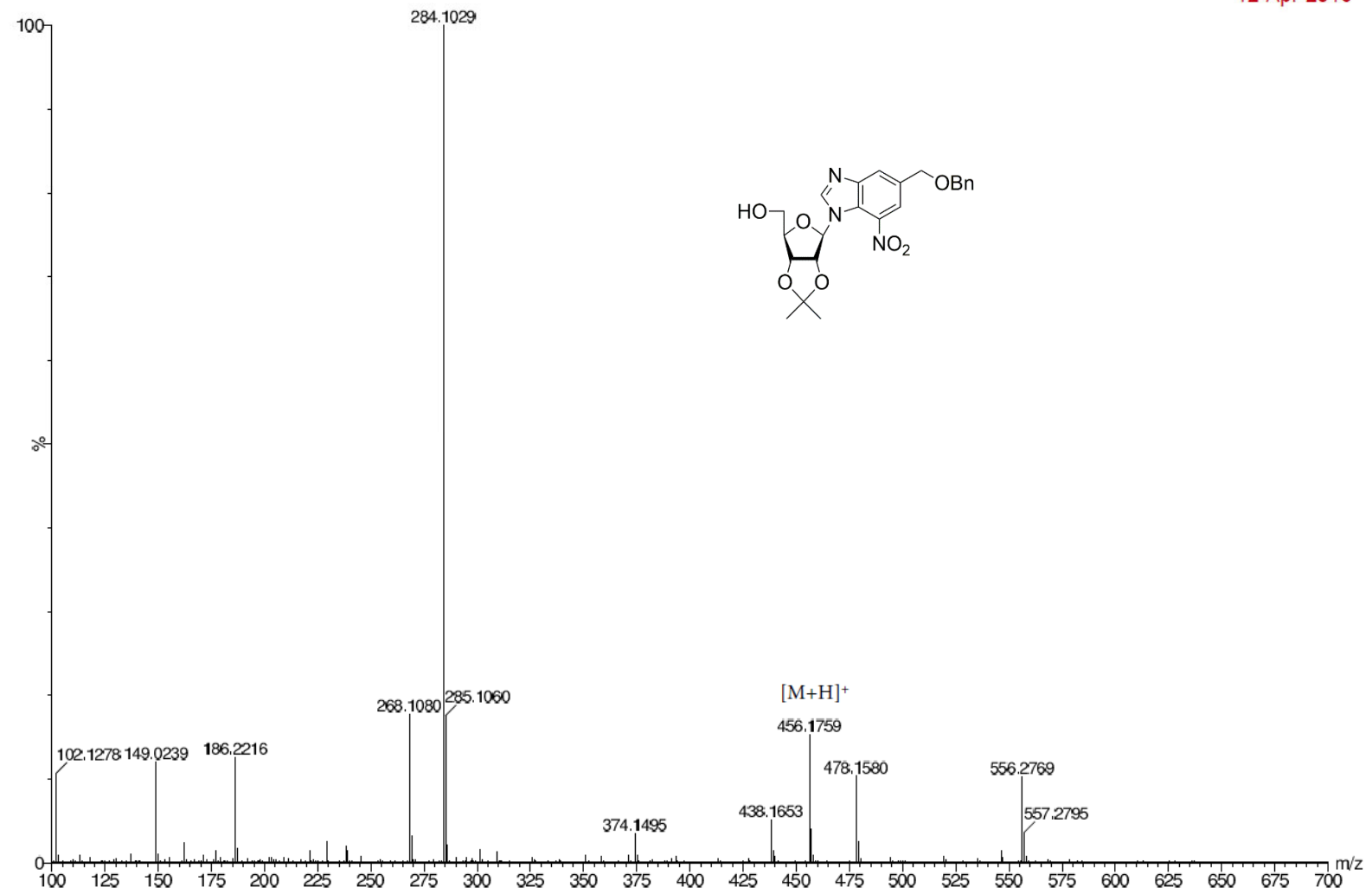
Compound 28 in CDCl<sub>3</sub> 13C spectrum - 75 MHz



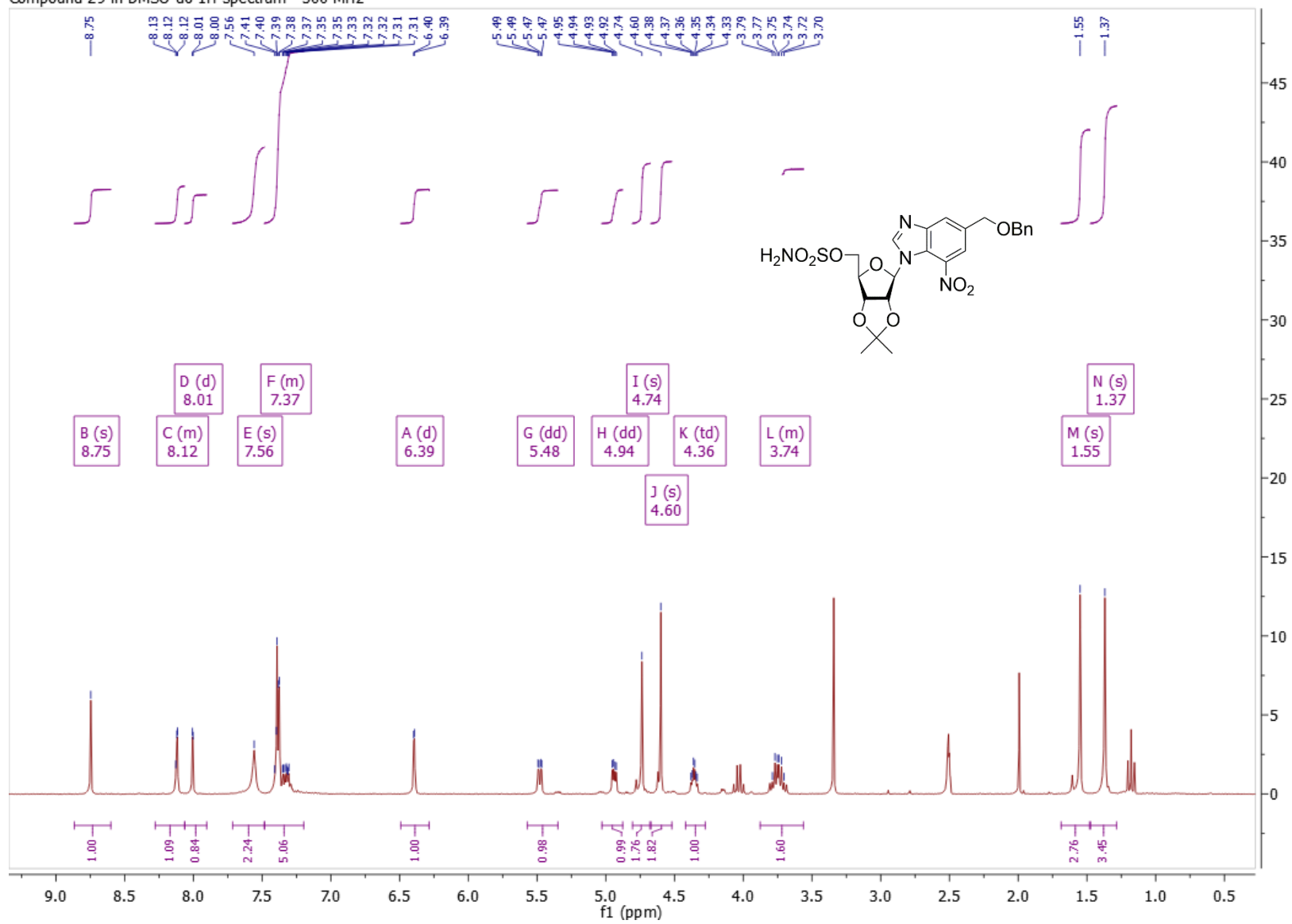
compound 28

accurate mass

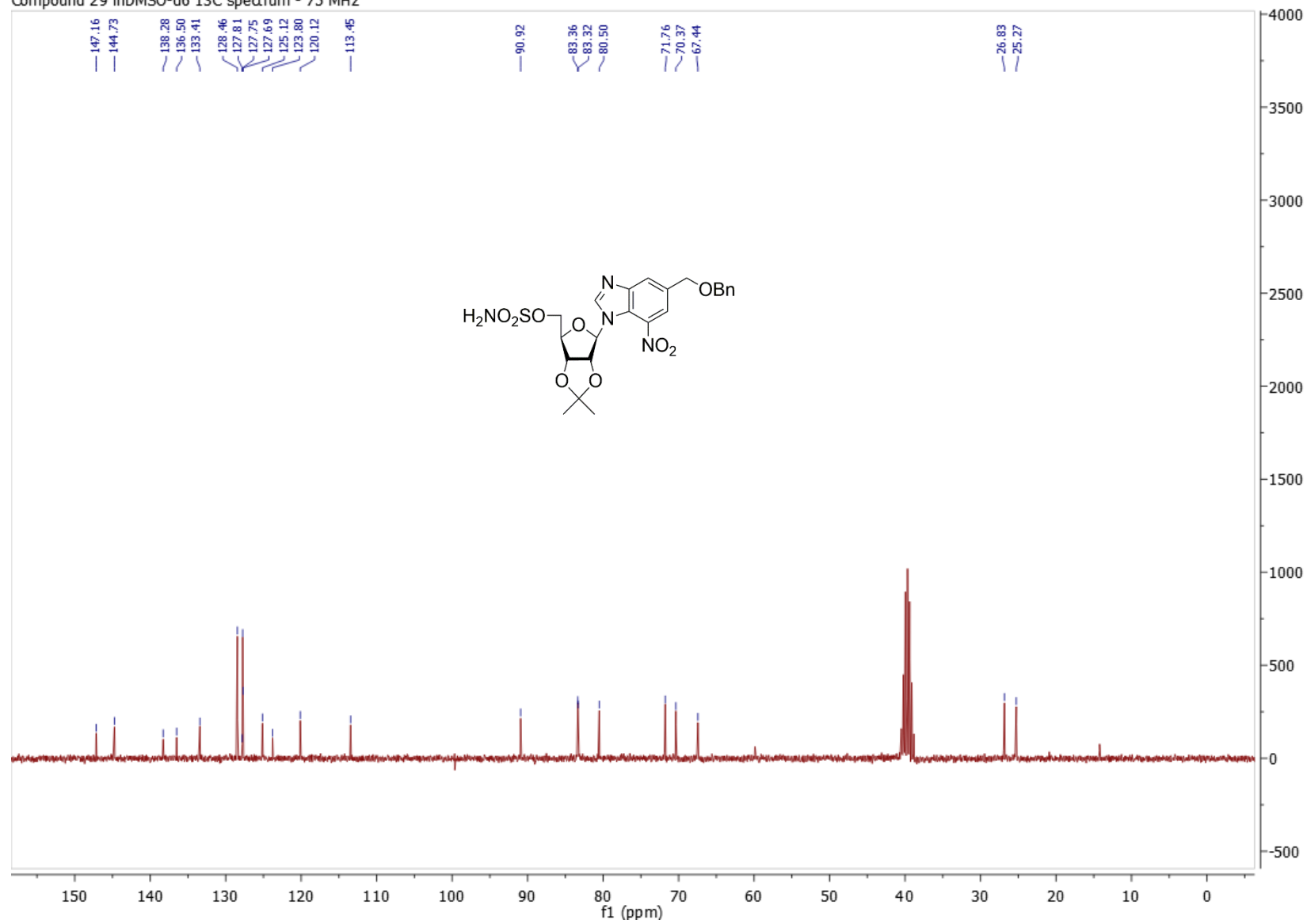
ES+  
12-Apr-2016



Compound 29 in DMSO-d6 1H spectrum - 300 MHz



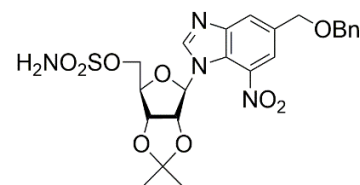
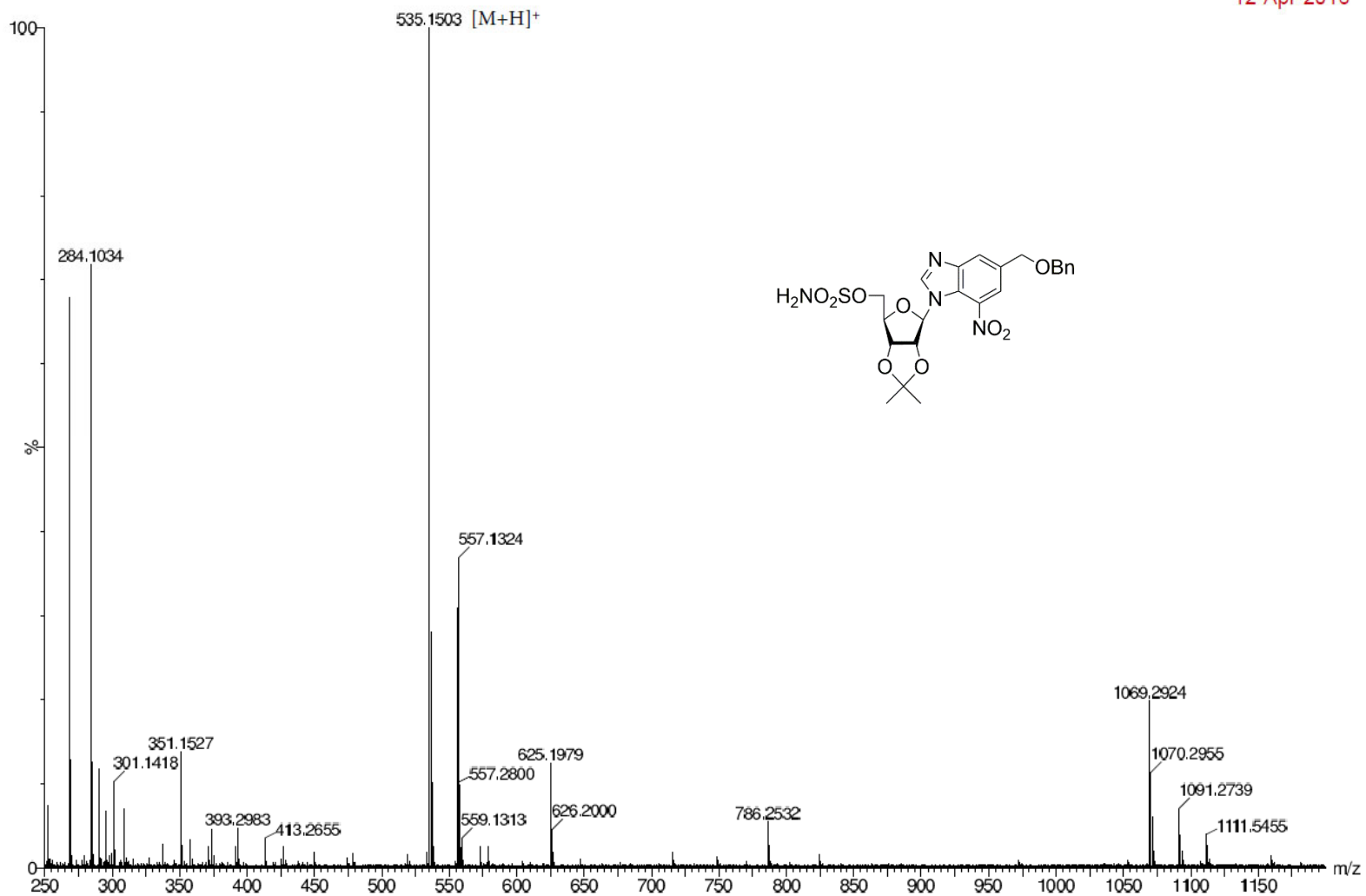
Compound 29 in DMSO-d6 13C spectrum - 75 MHz



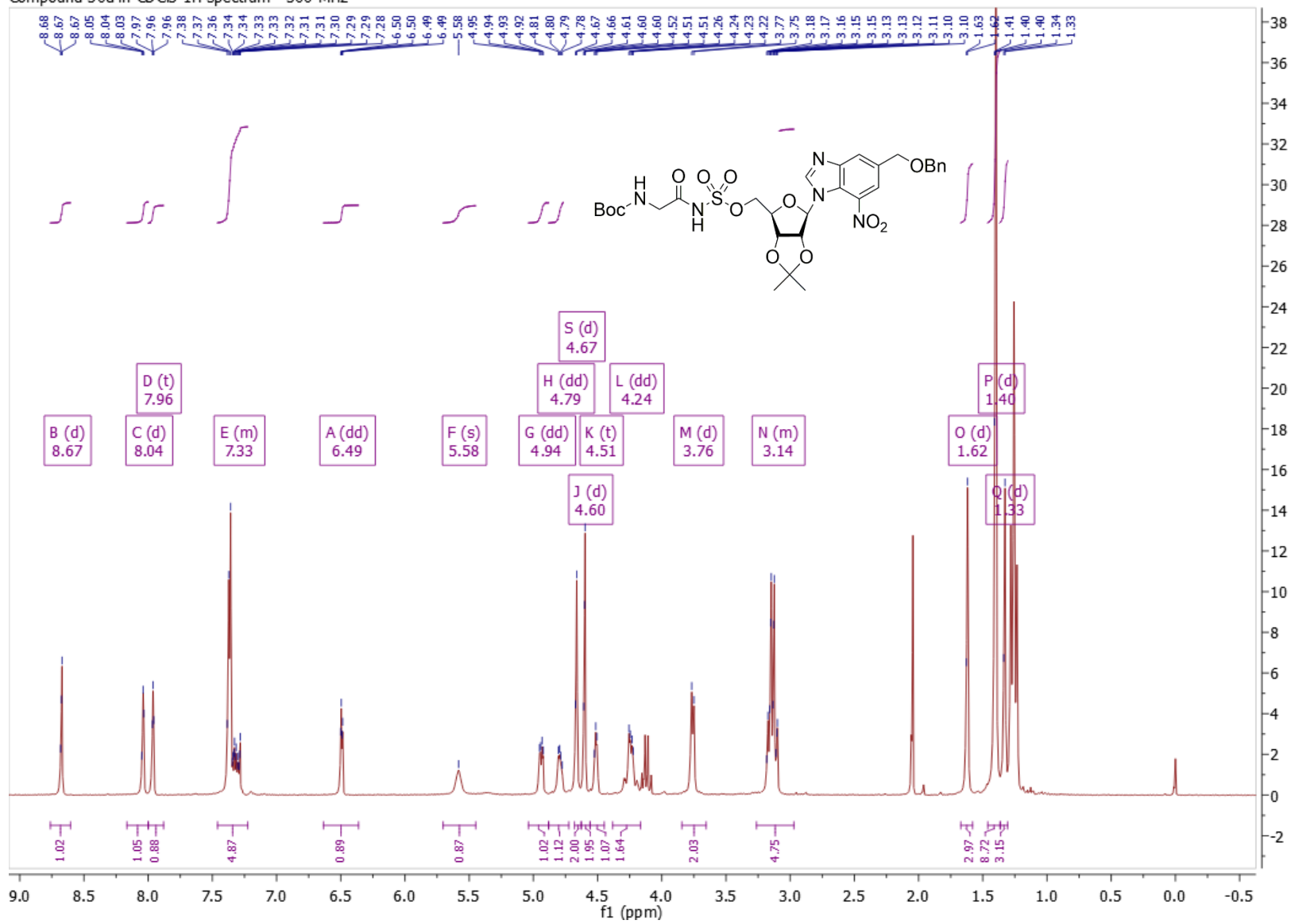
compound 29

accurate mass

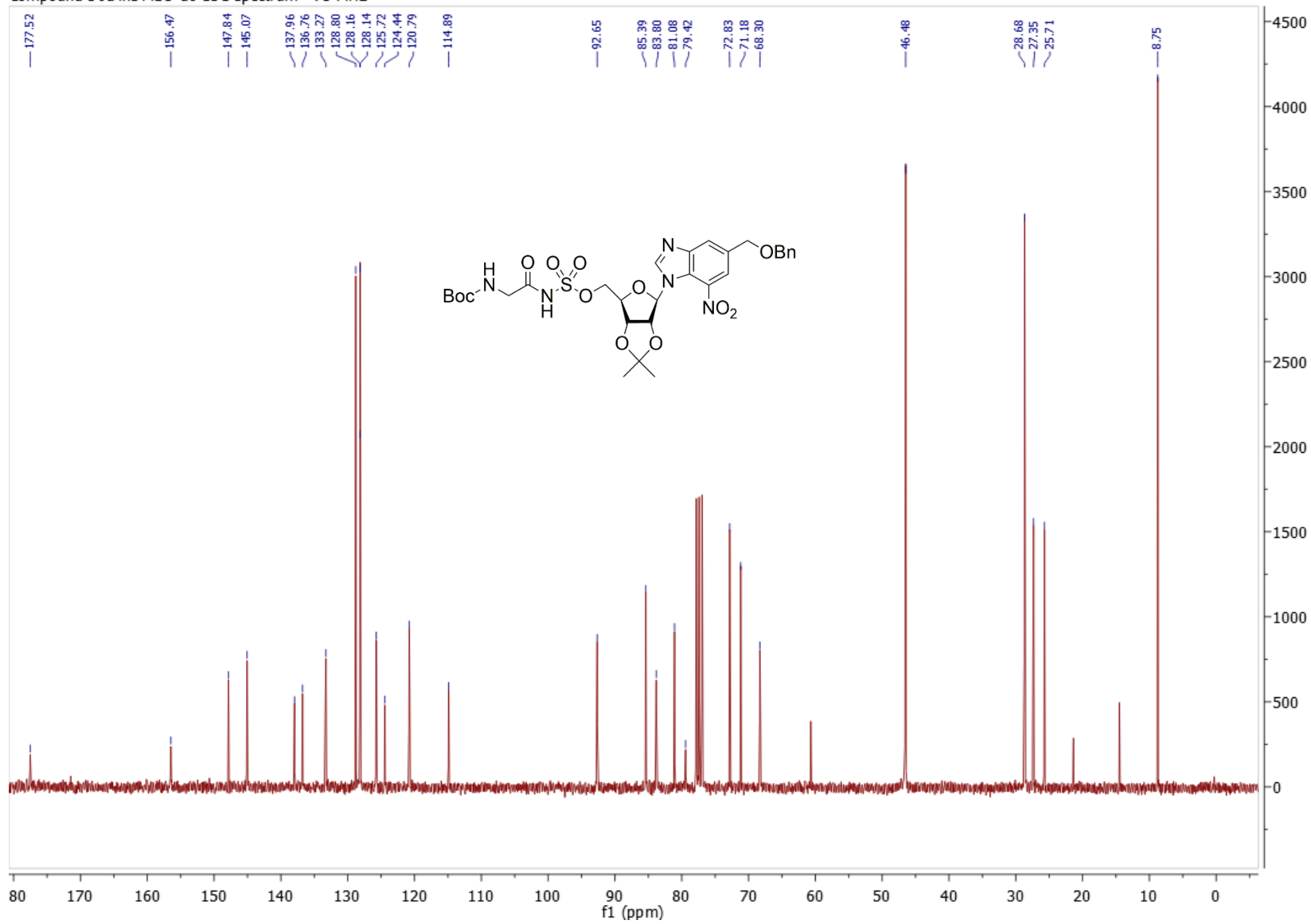
ES+  
12-Apr-2016



Compound 30a in CDCl<sub>3</sub> 1H spectrum - 300 MHz



Compound 30a in DMSO-d6 13C spectrum - 75 MHz

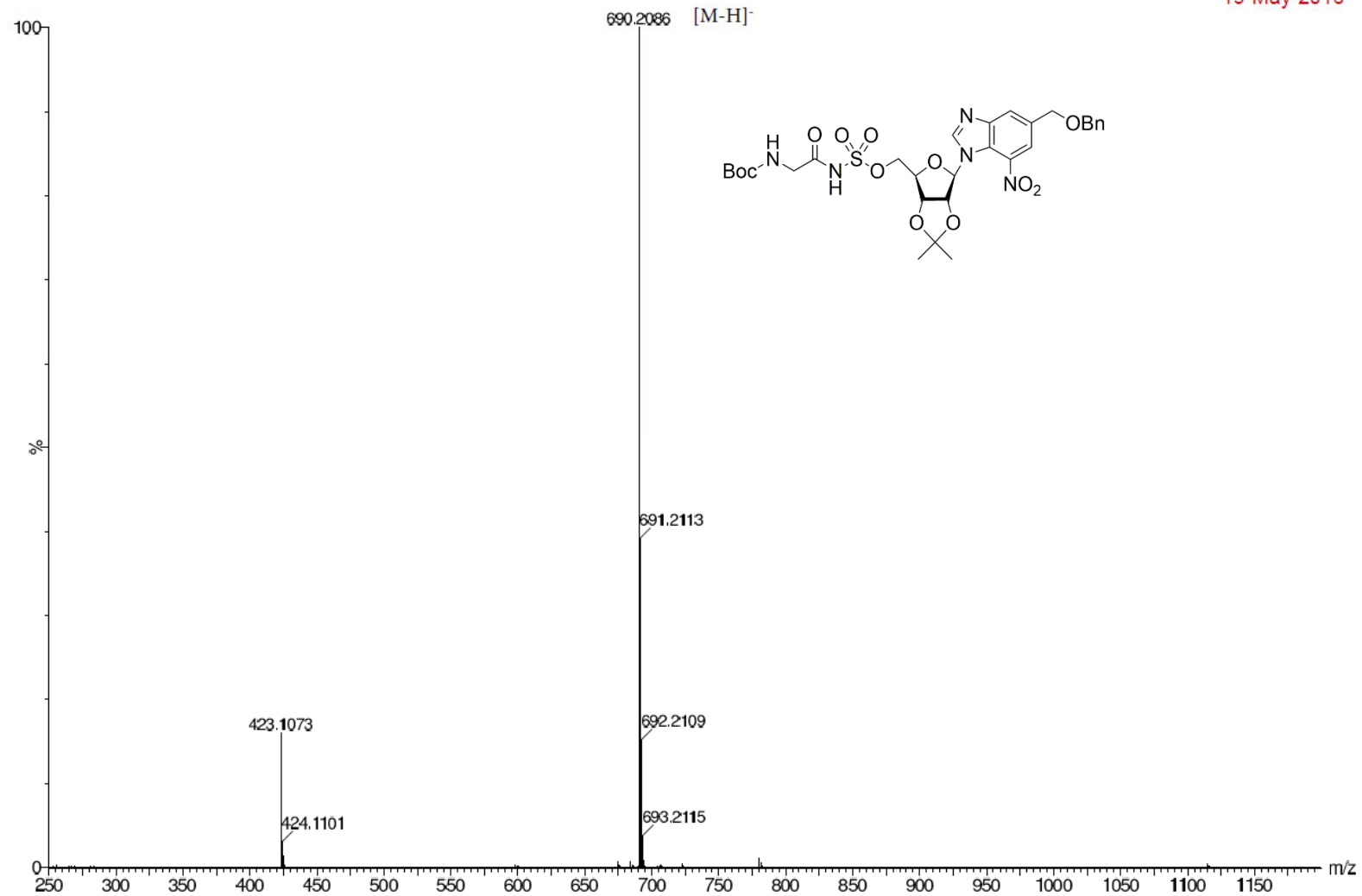




compound 30a

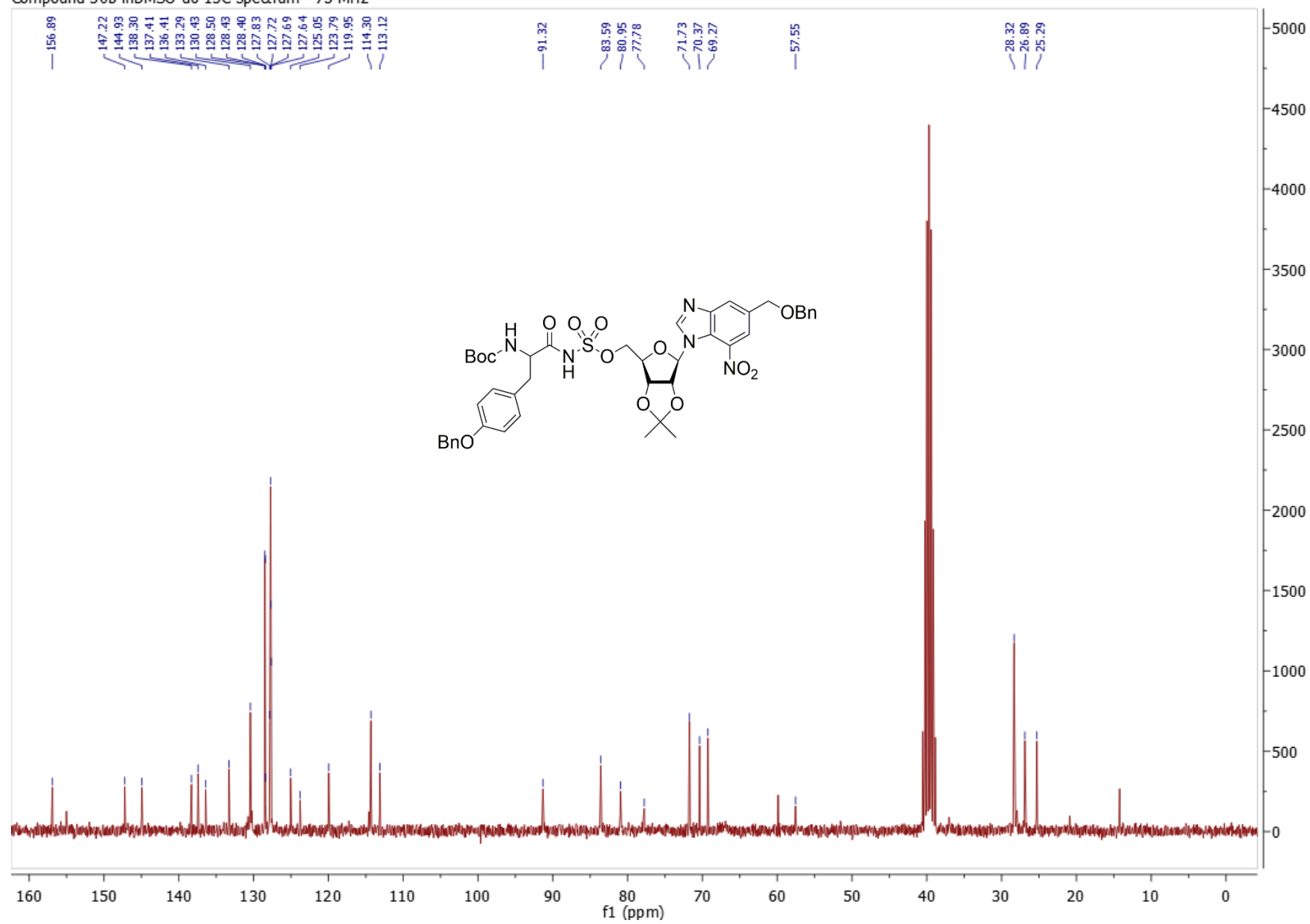
accurate mass

ES-  
19-May-2016



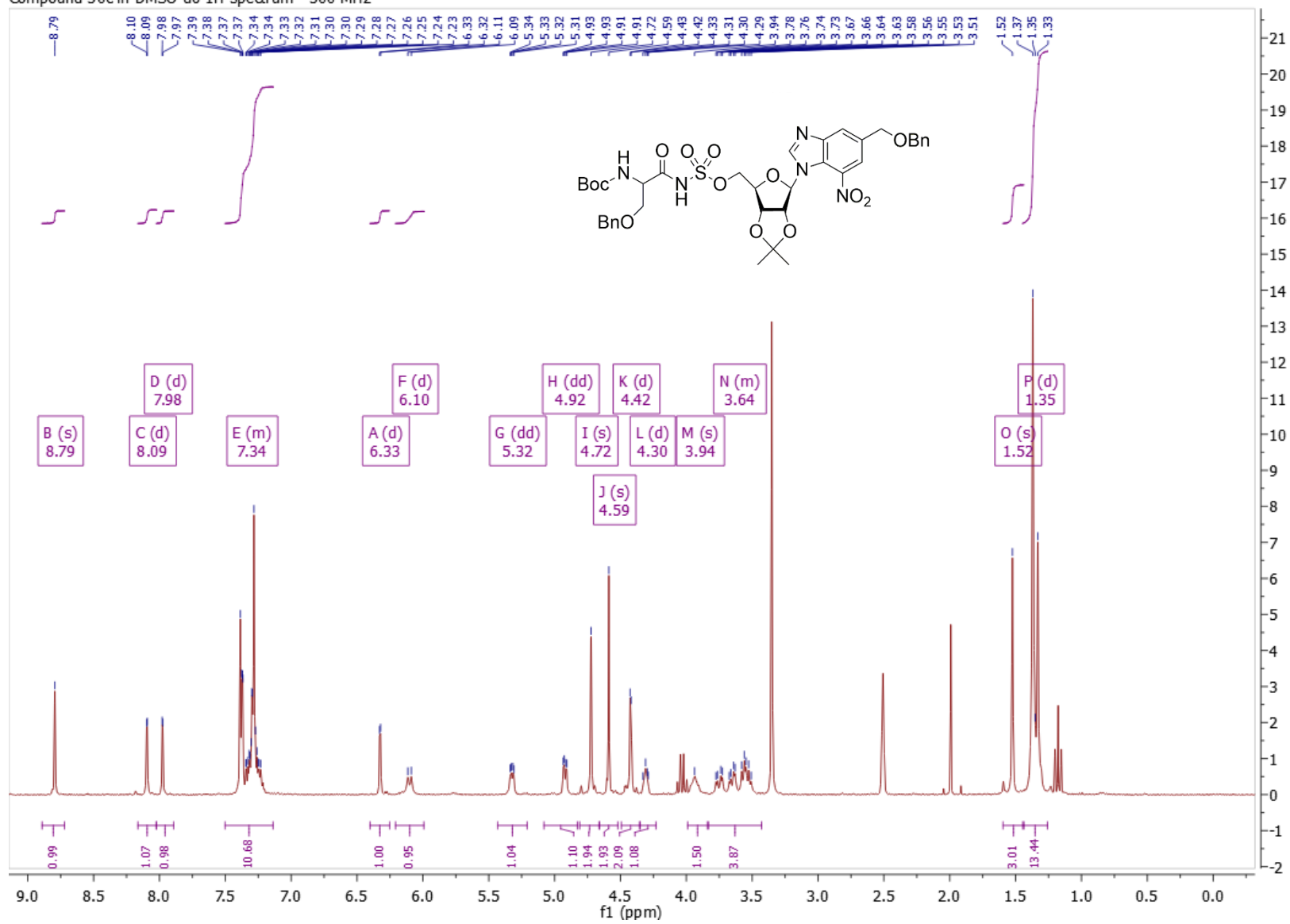


Compound 30b in DMSO-d6 13C spectrum - 75 MHz





Compound 30c in DMSO-d6 1H spectrum - 300 MHz

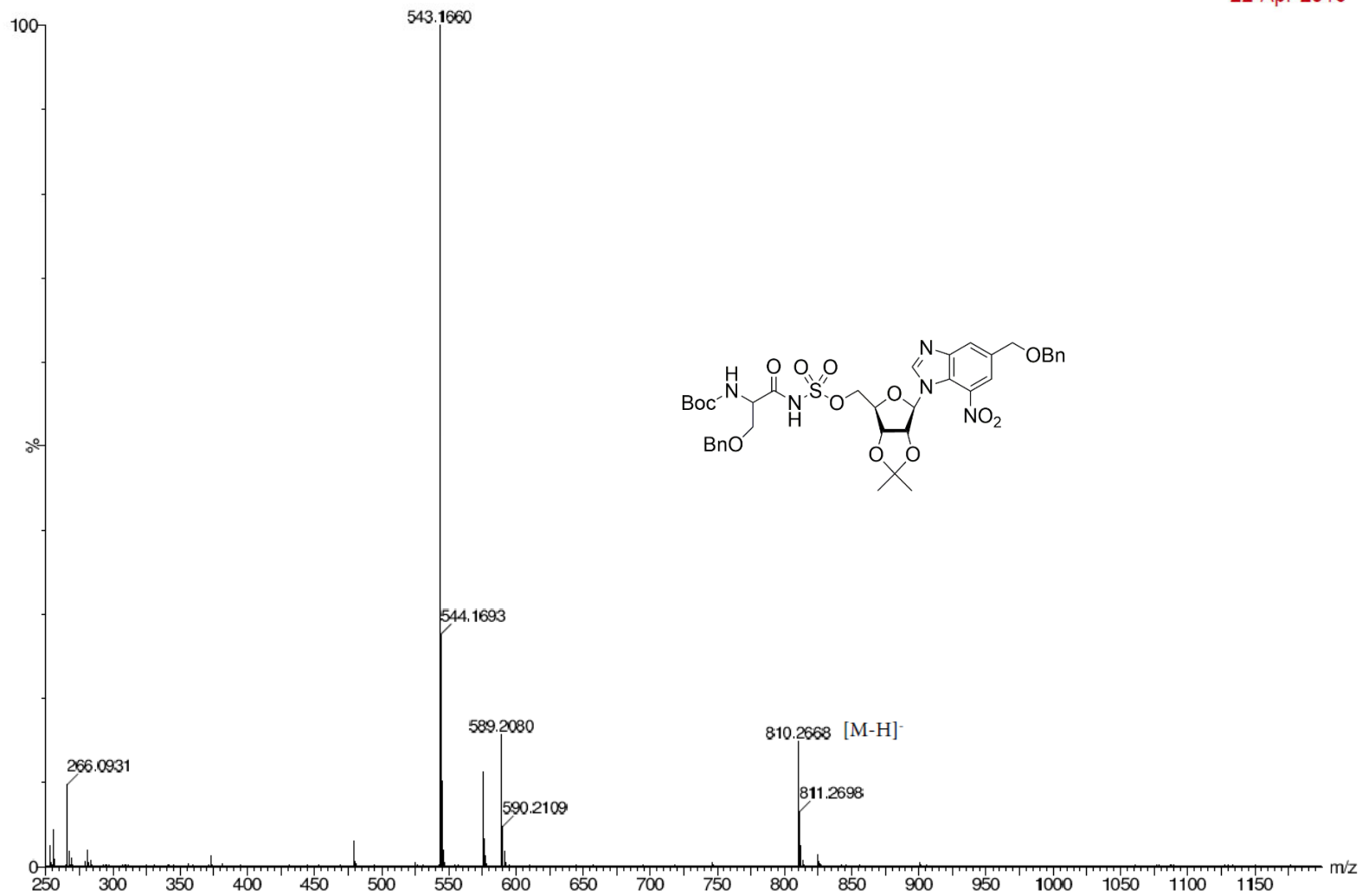




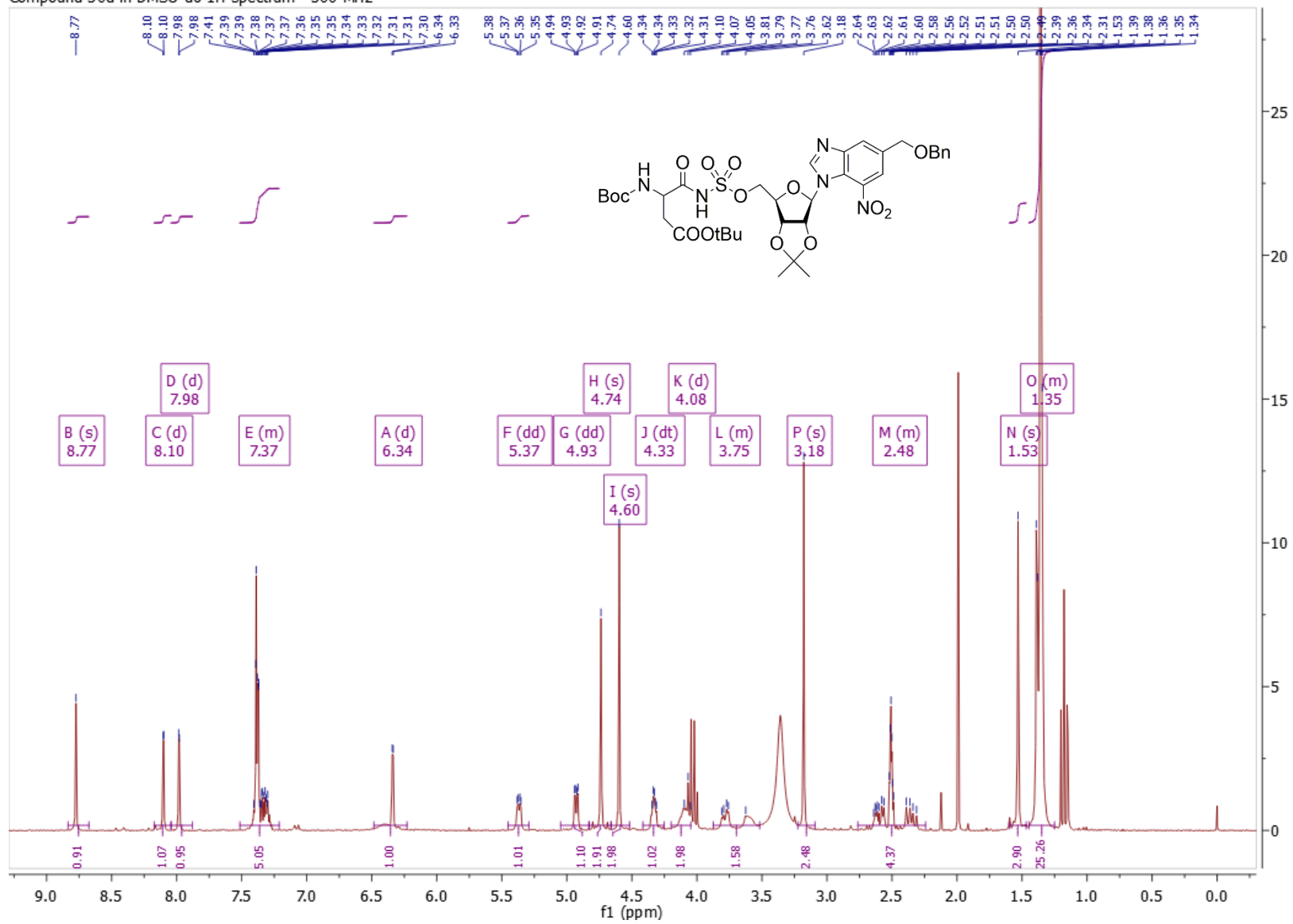
compound 30c

accurate mass

ES-  
22-Apr-2016

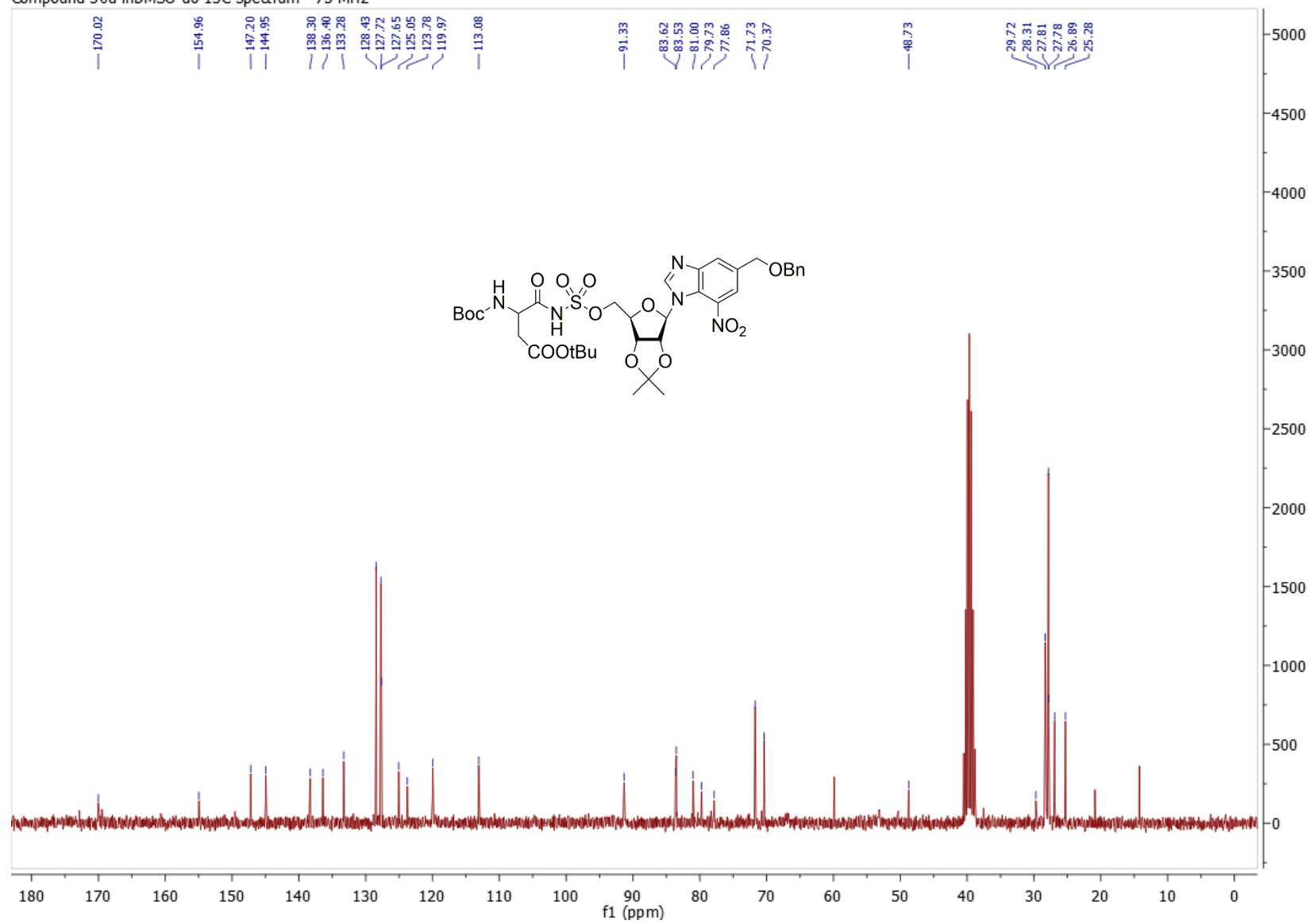


Compound 30d in DMSO-d6 1H spectrum - 300 MHz





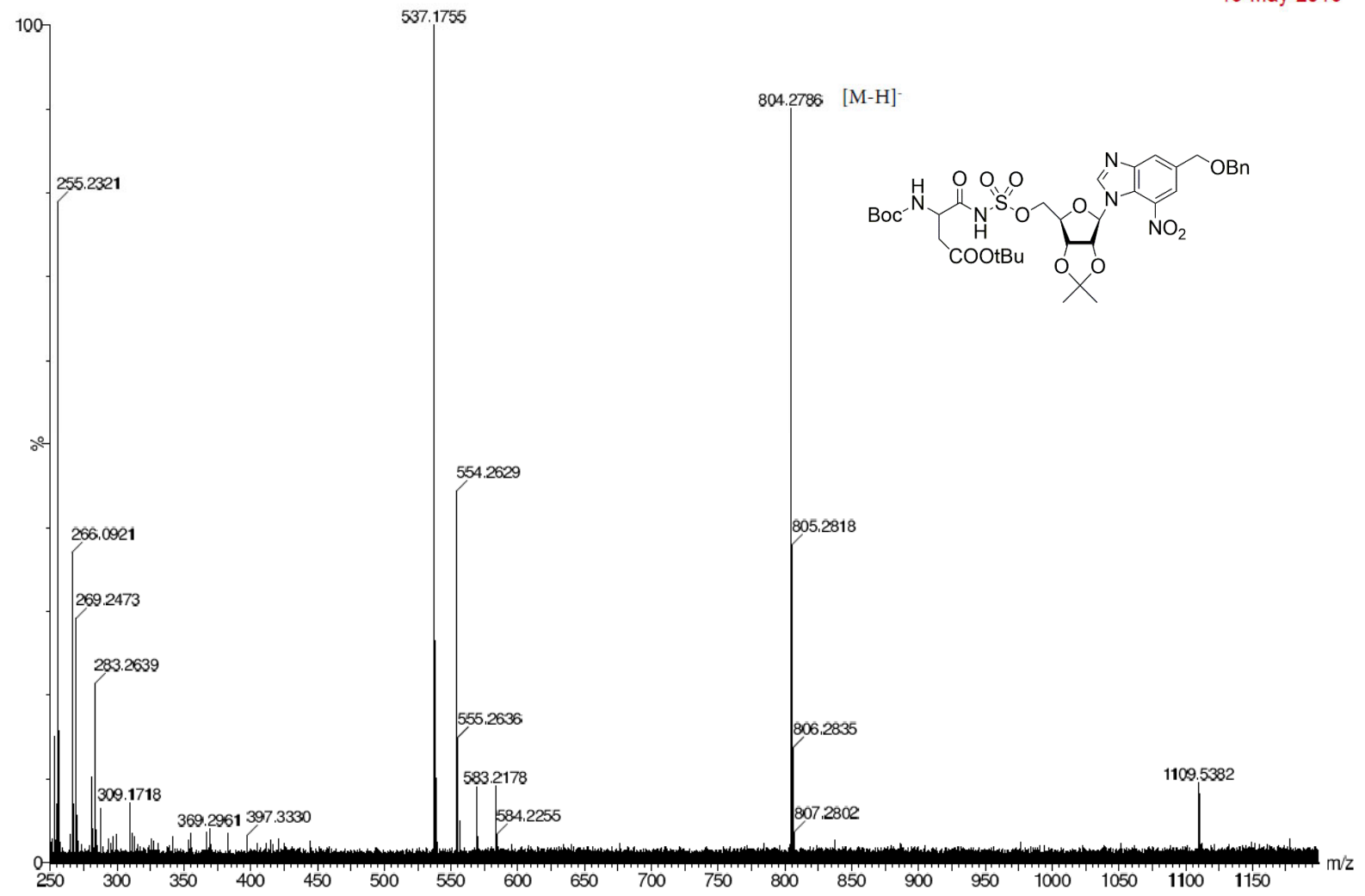
Compound 30d in DMSO-d6 13C spectrum - 75 MHz



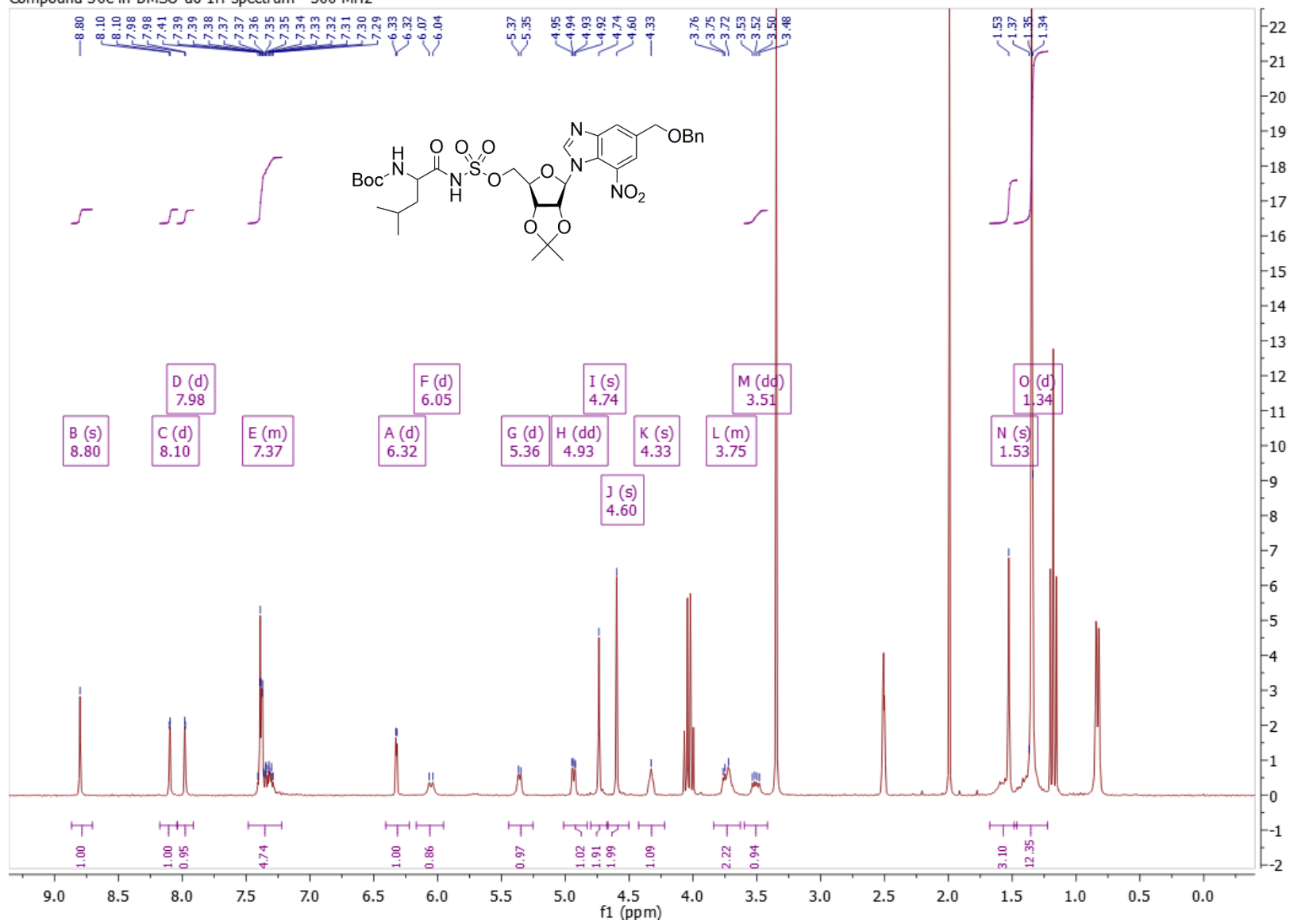
compound 30d

accurate mass

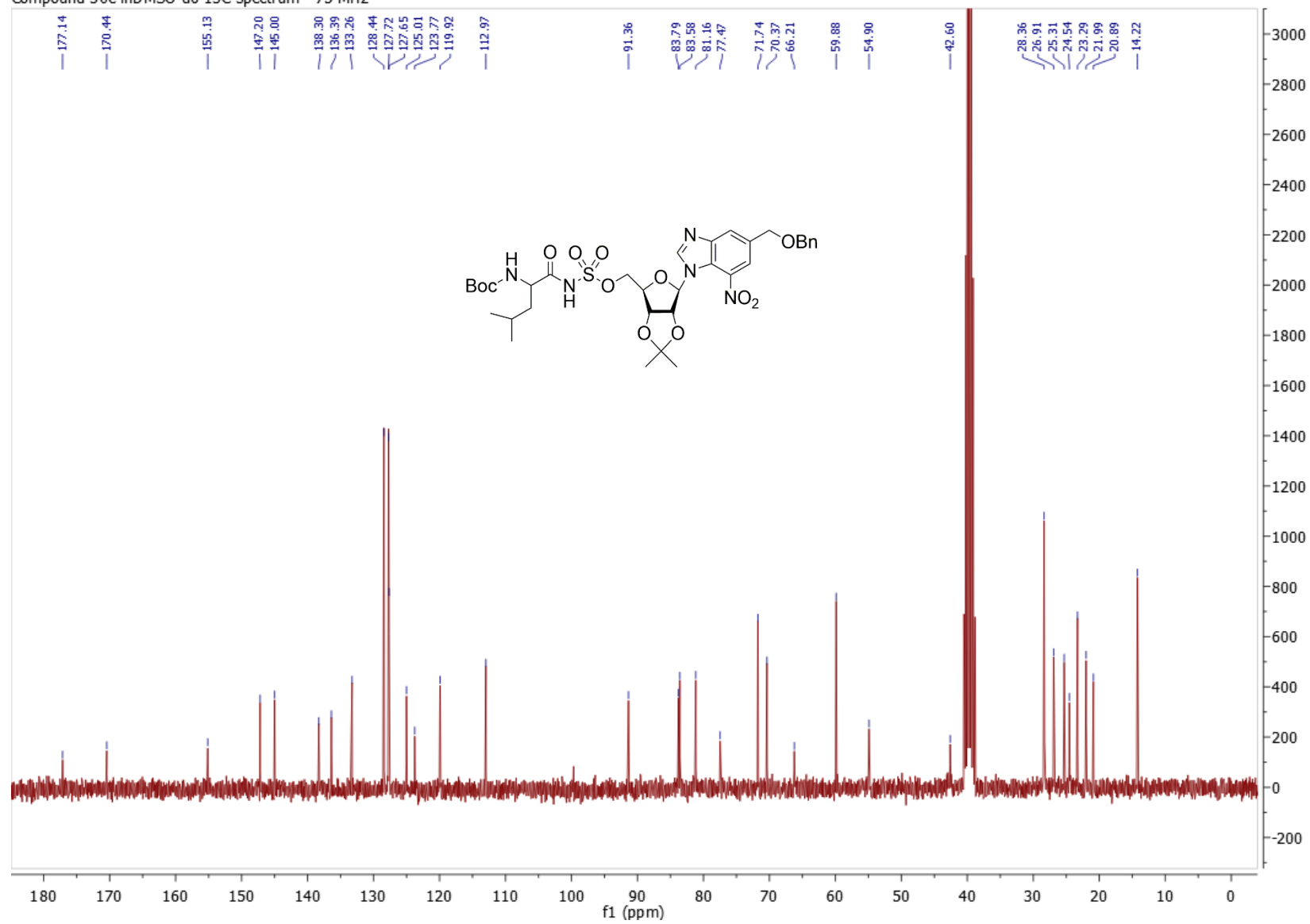
ES-  
19-May-2016



Compound 30e in DMSO-d6 1H spectrum - 300 MHz



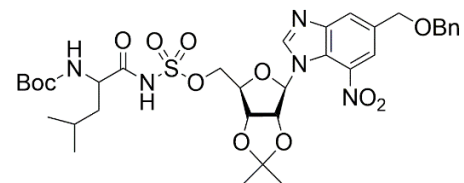
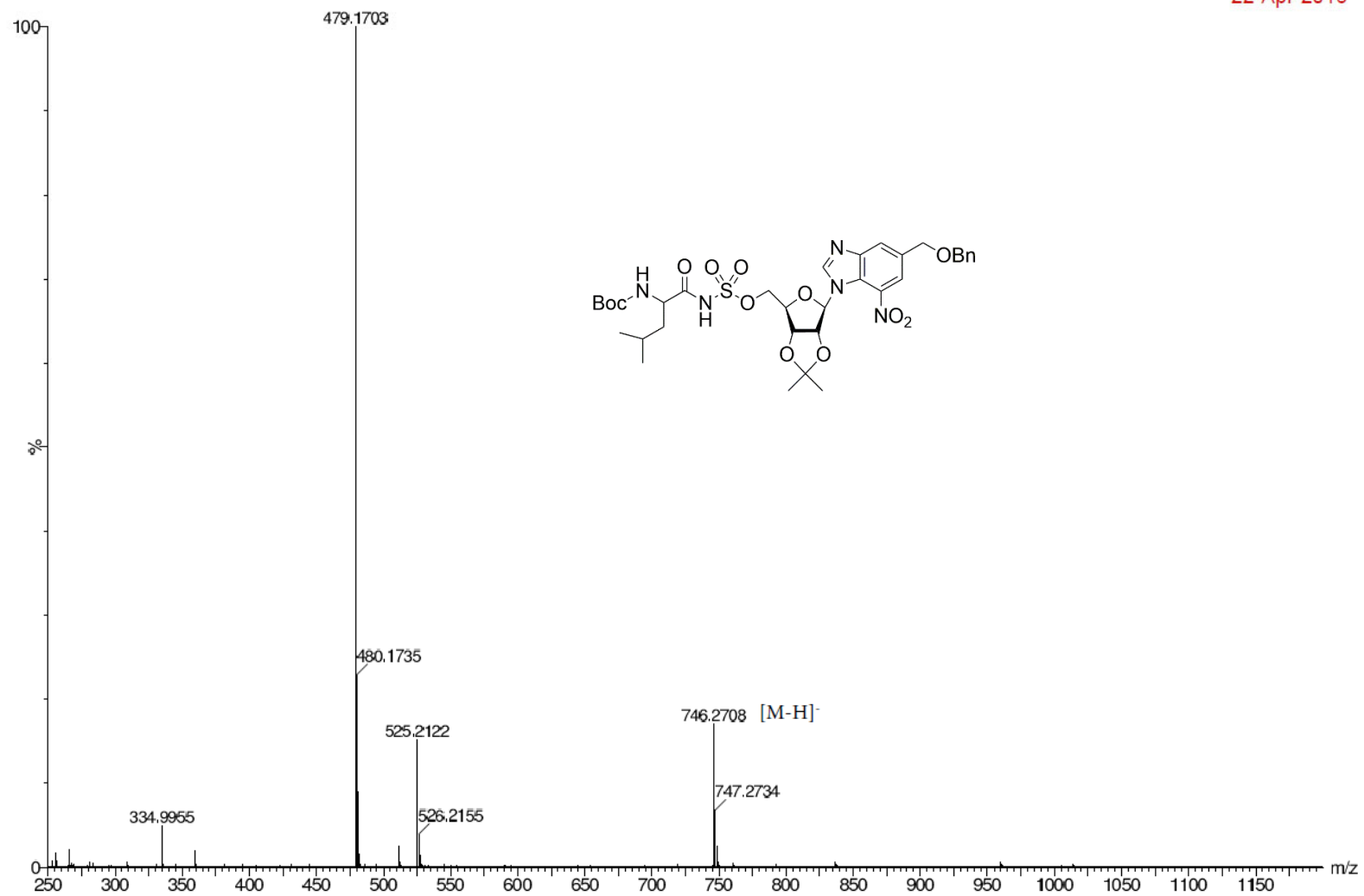
Compound 30e in DMSO-d6 13C spectrum - 75 MHz



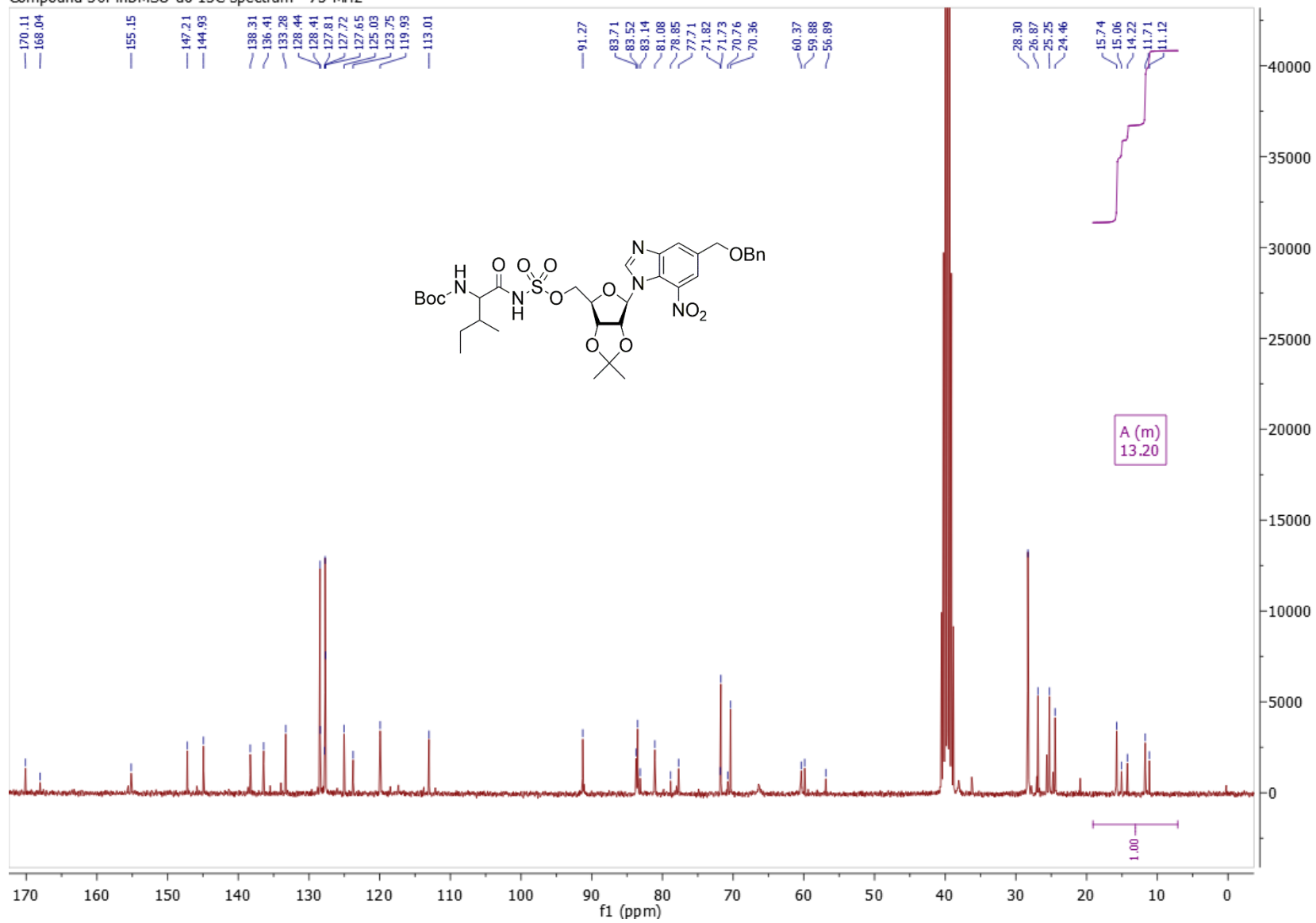
compound 30e

accurate mass

ES-  
22-Apr-2016



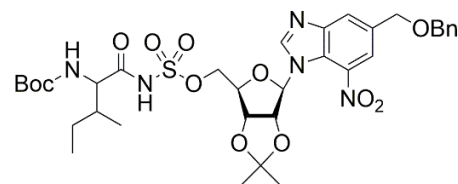
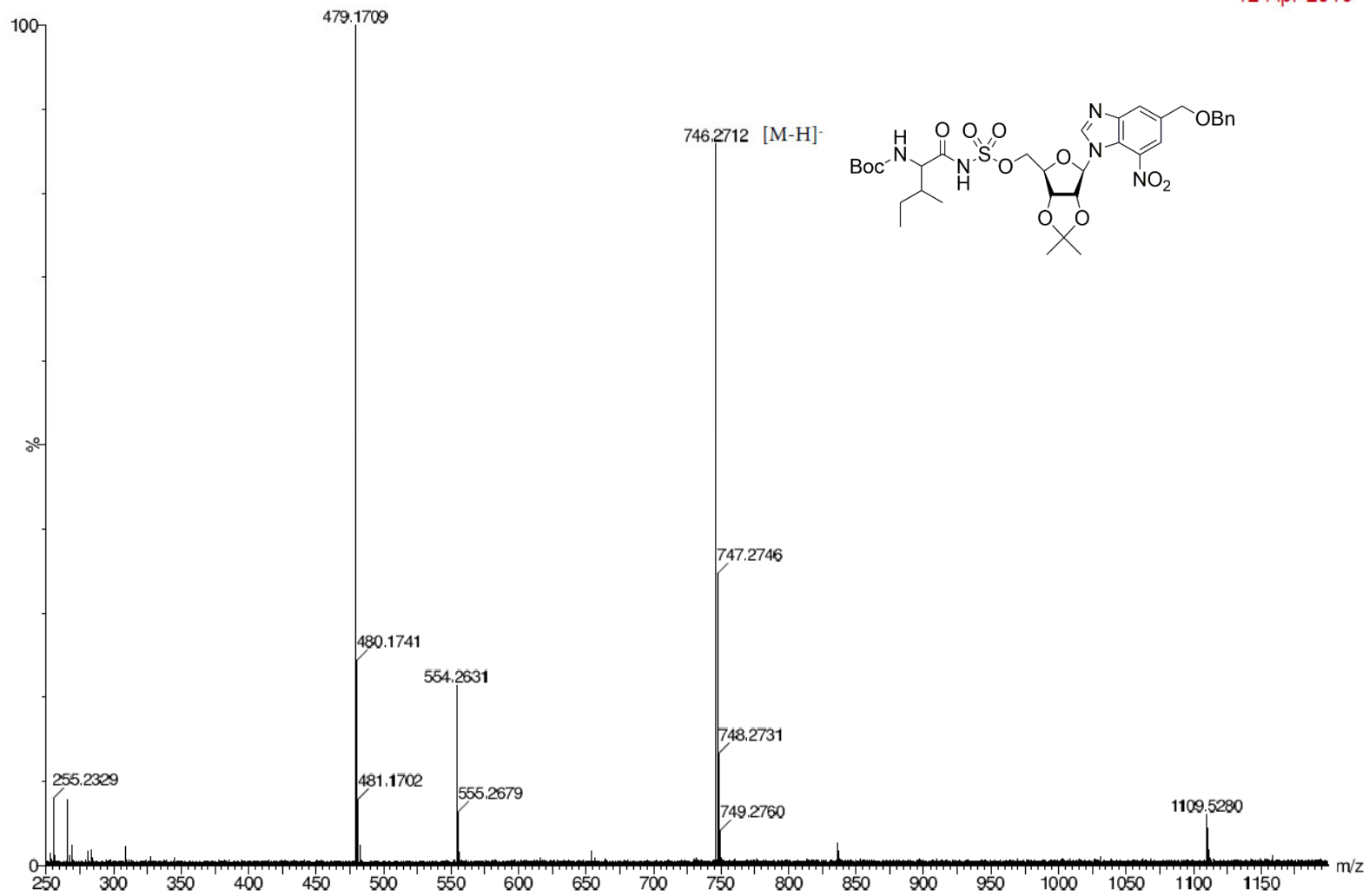
Compound 30f in DMSO-d6 13C spectrum - 75 MHz



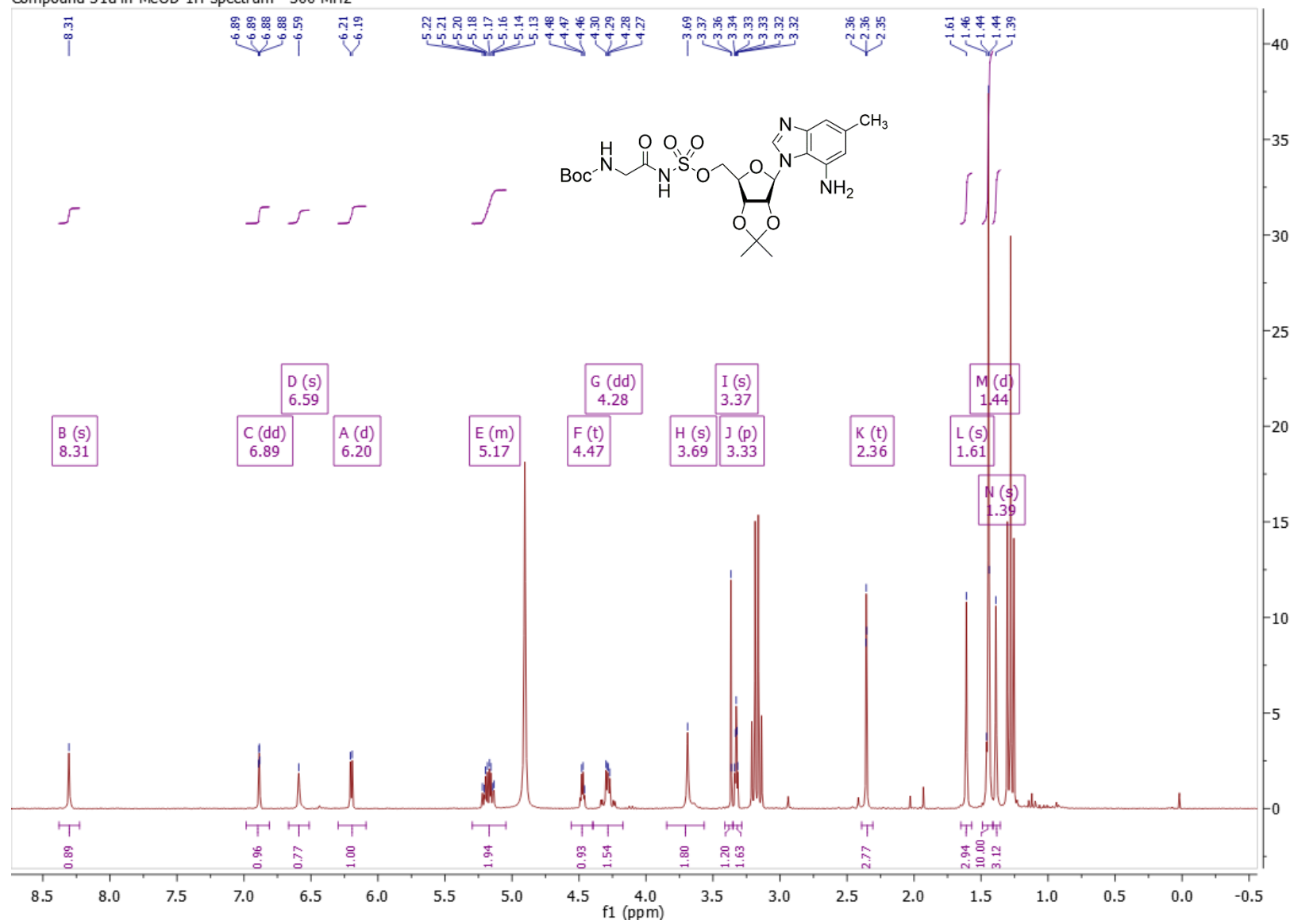
compound 30f

accurate mass

ES-  
12-Apr-2016

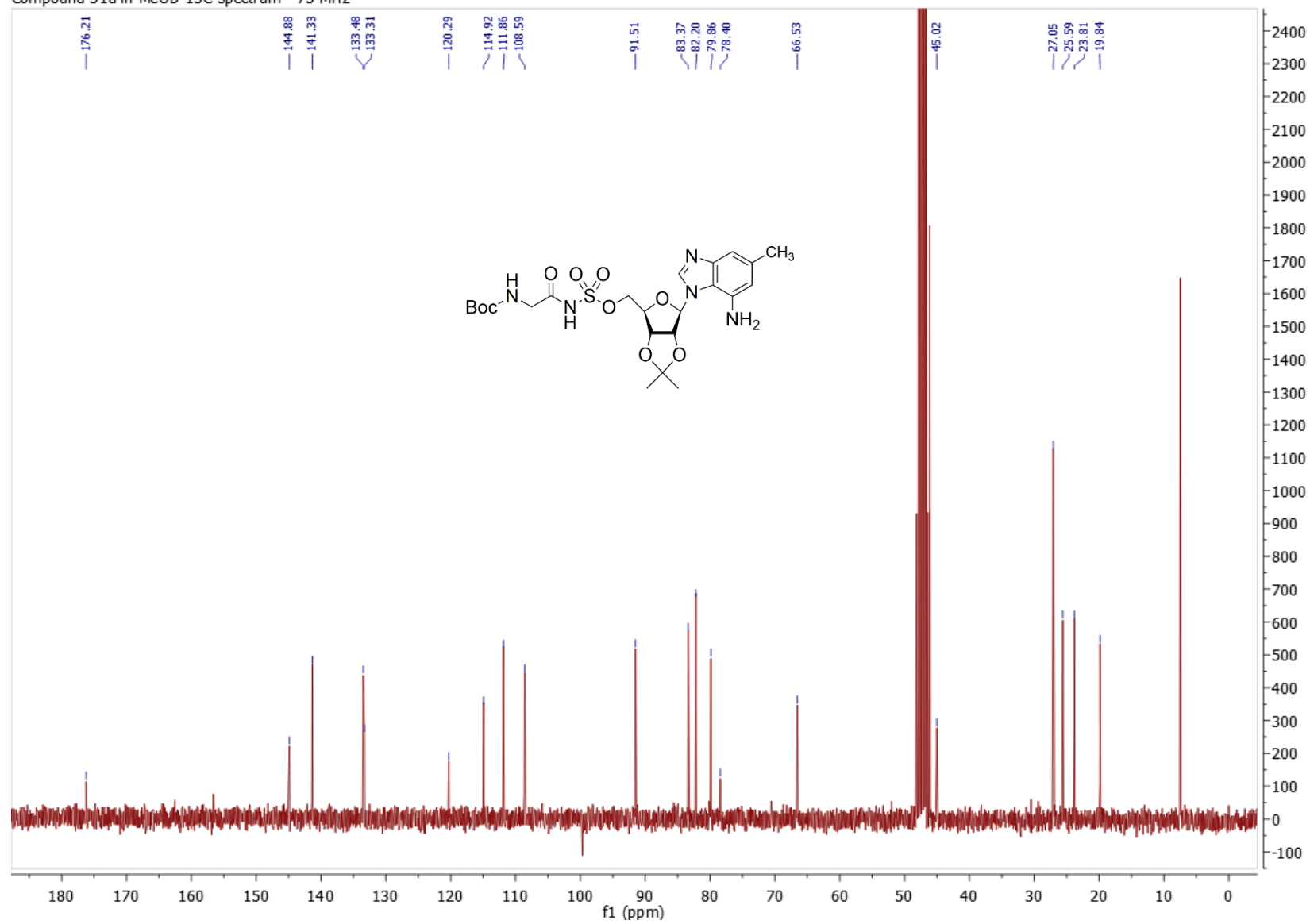


Compound 31a in MeOD 1H spectrum - 300 MHz





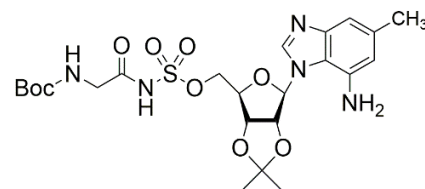
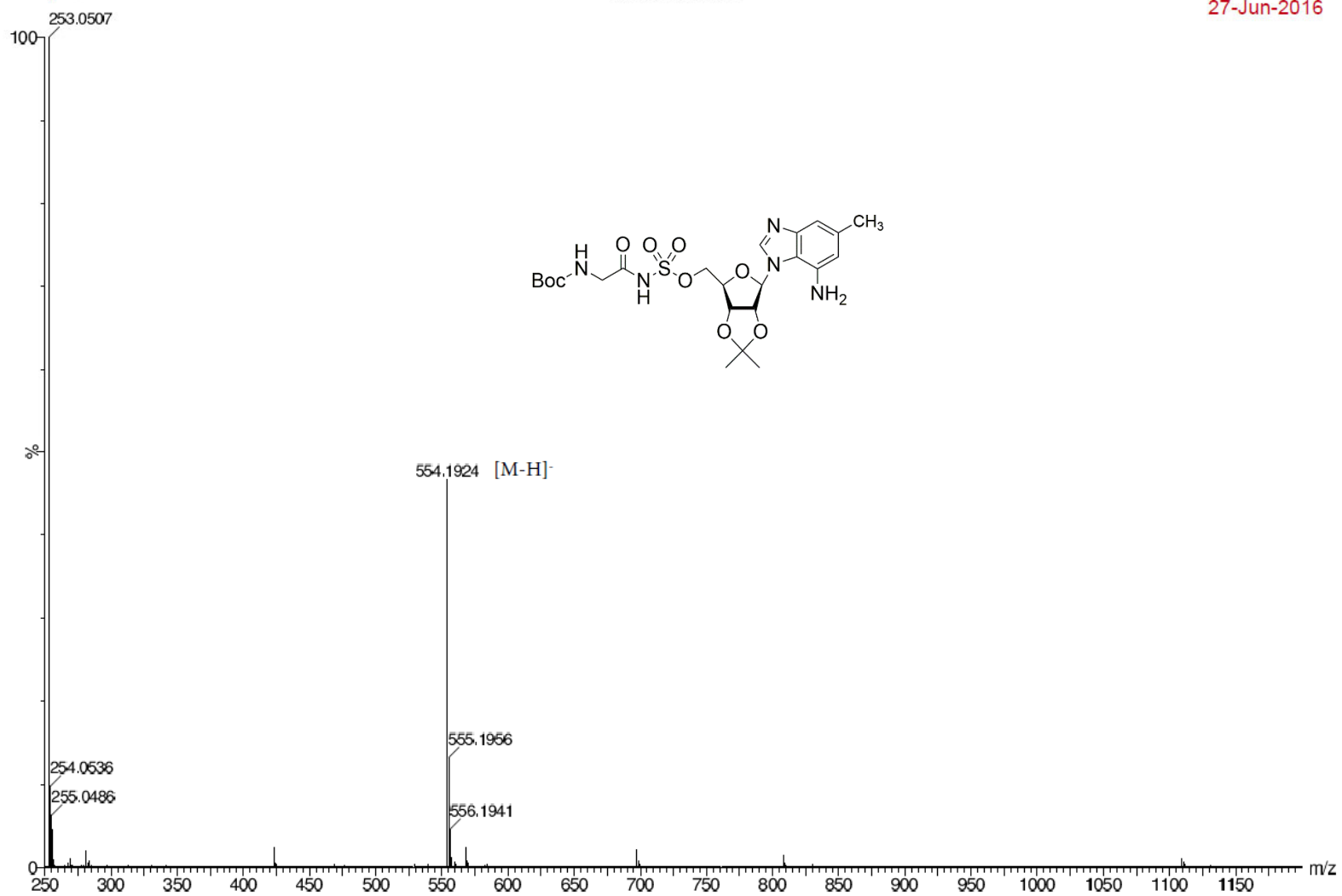
Compound 31a in MeOD 13C spectrum - 75 MHz



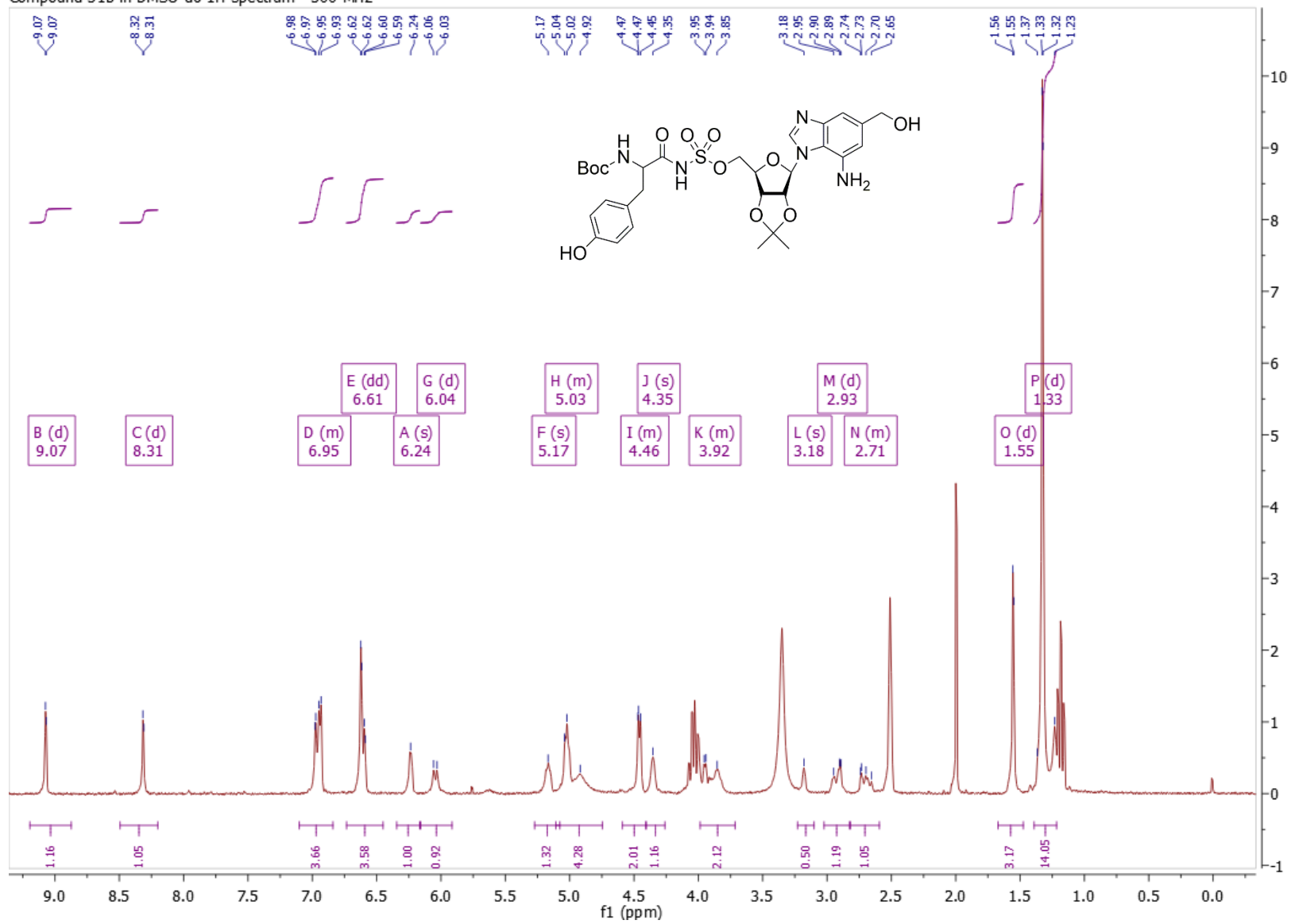
compound 31a

accurate mass

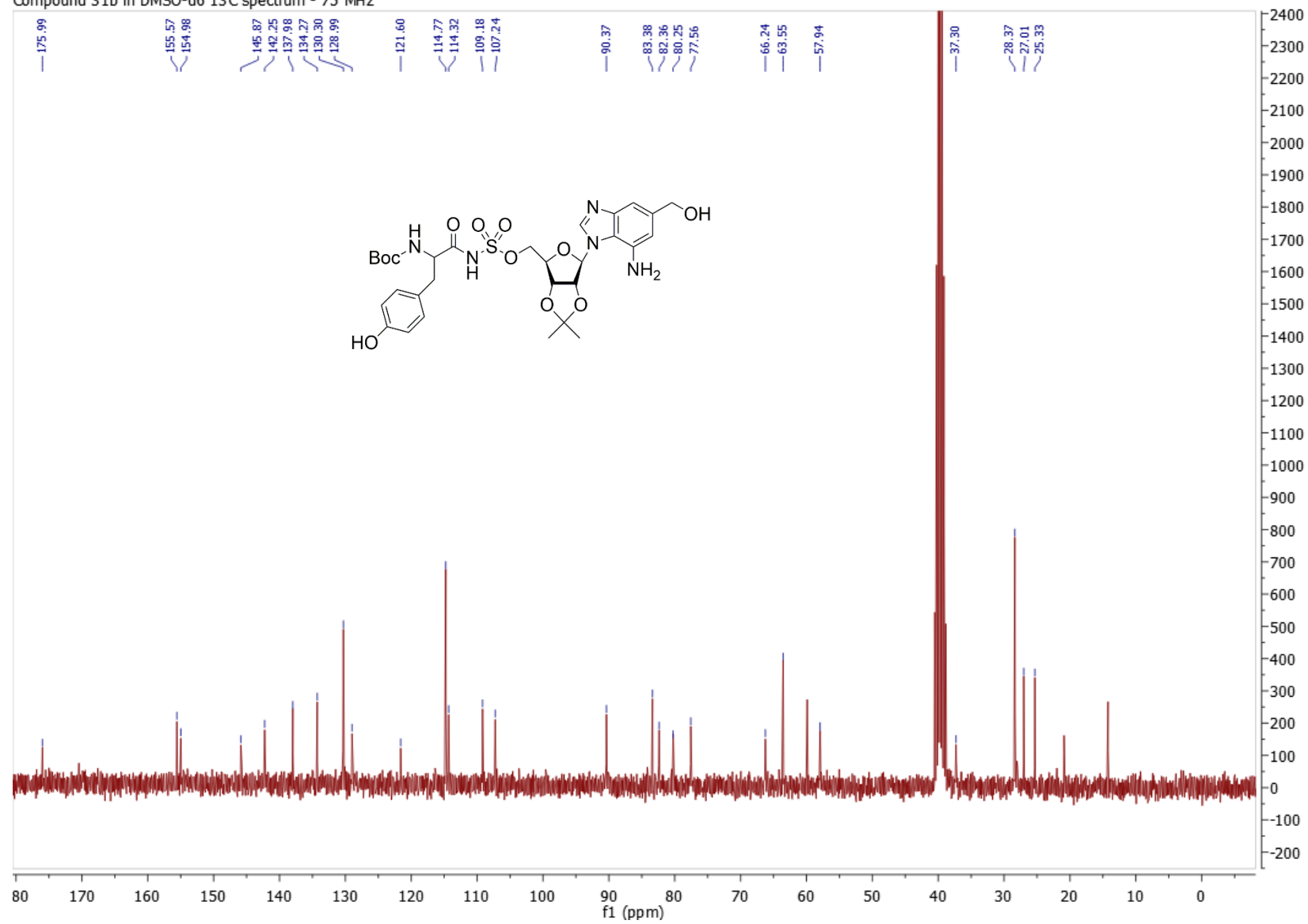
ES-  
27-Jun-2016



Compound 31b in DMSO-d6 1H spectrum - 300 MHz



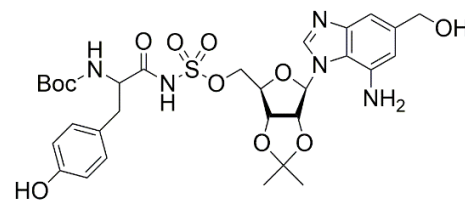
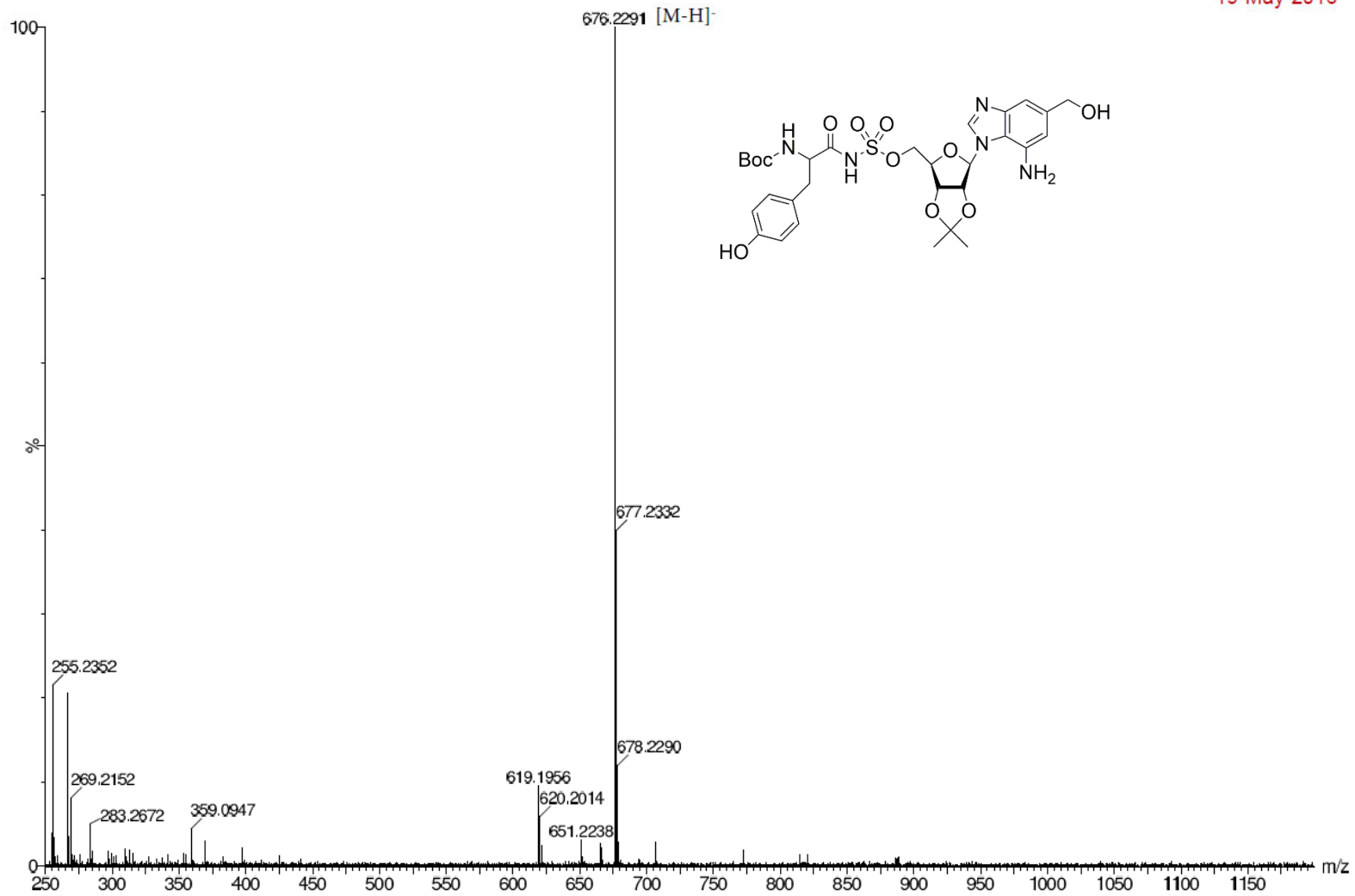
Compound 31b in DMSO-d6 13C spectrum - 75 MHz



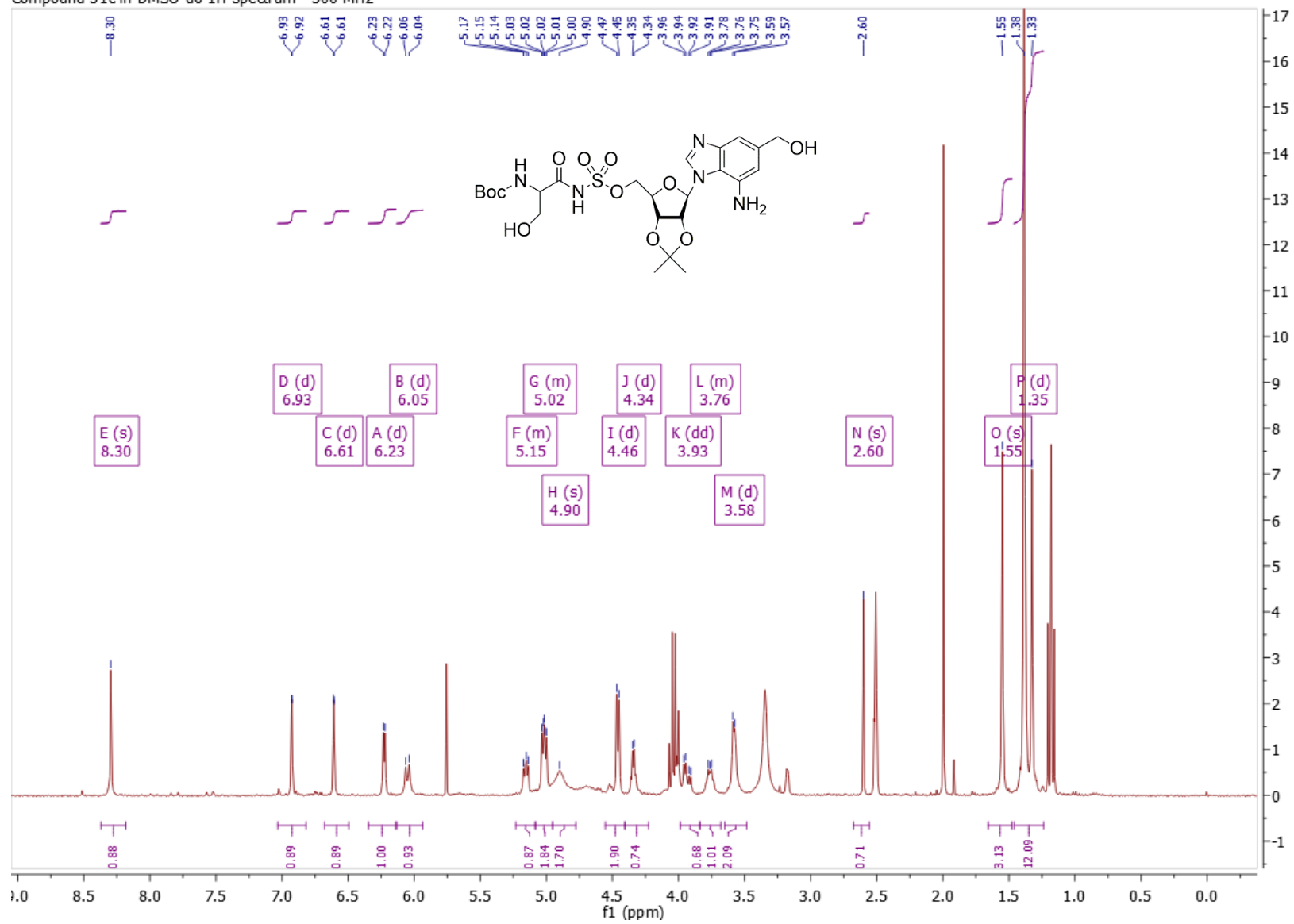
compound 31b

accurate mass

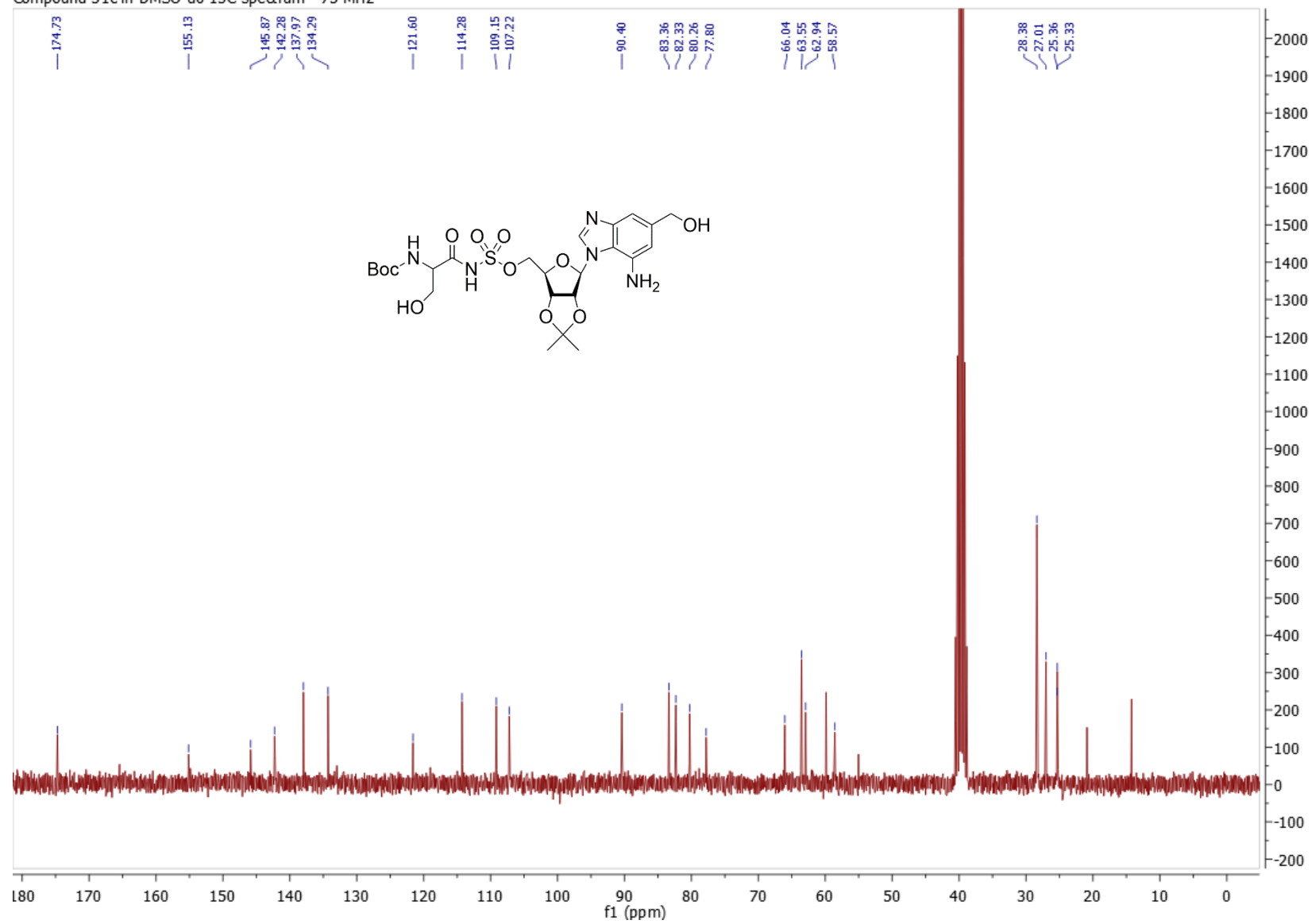
ES-  
19-May-2016



Compound 31c in DMSO-d6 1H spectrum - 300 MHz



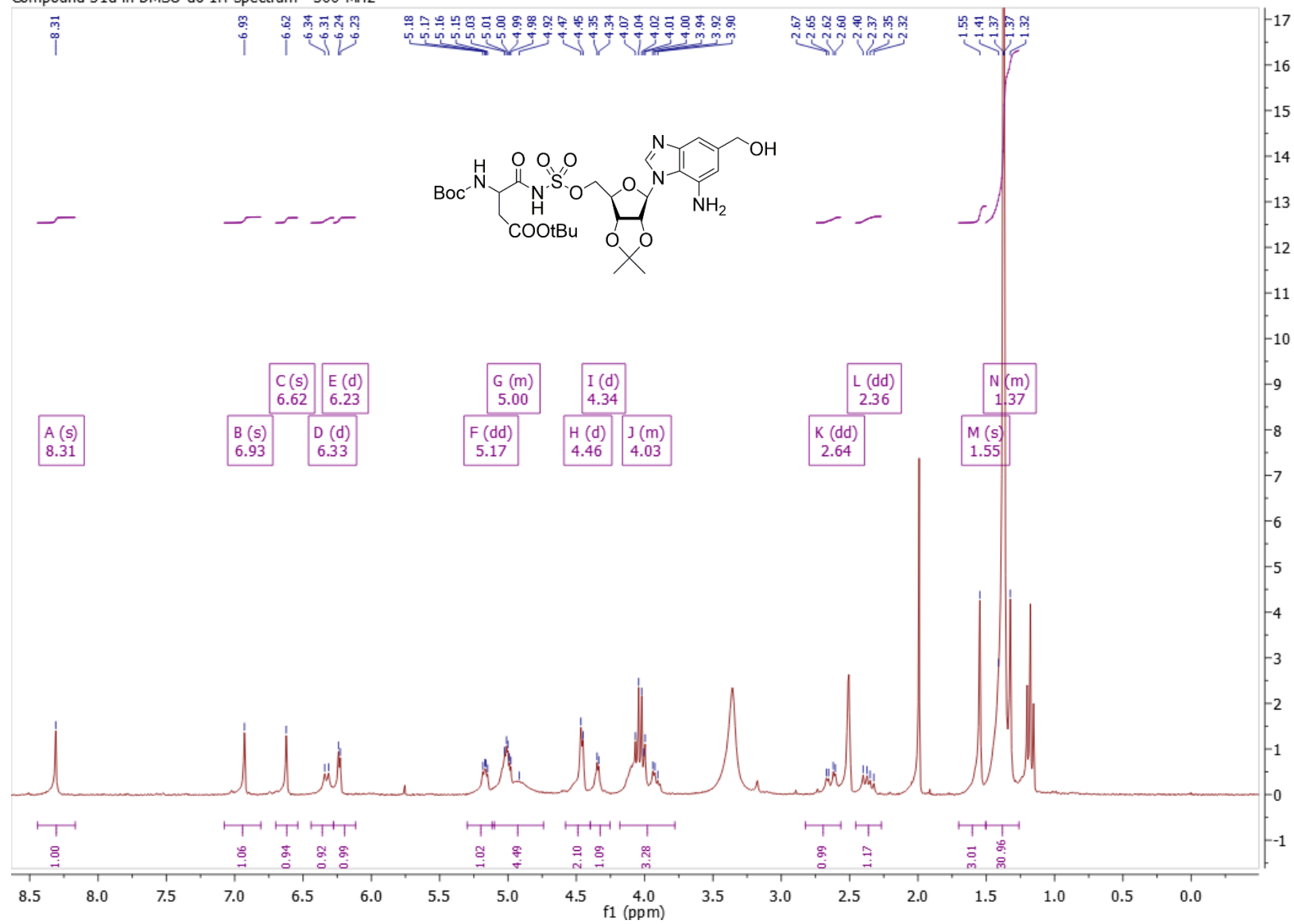
Compound 31c in DMSO-d6 13C spectrum - 75 MHz



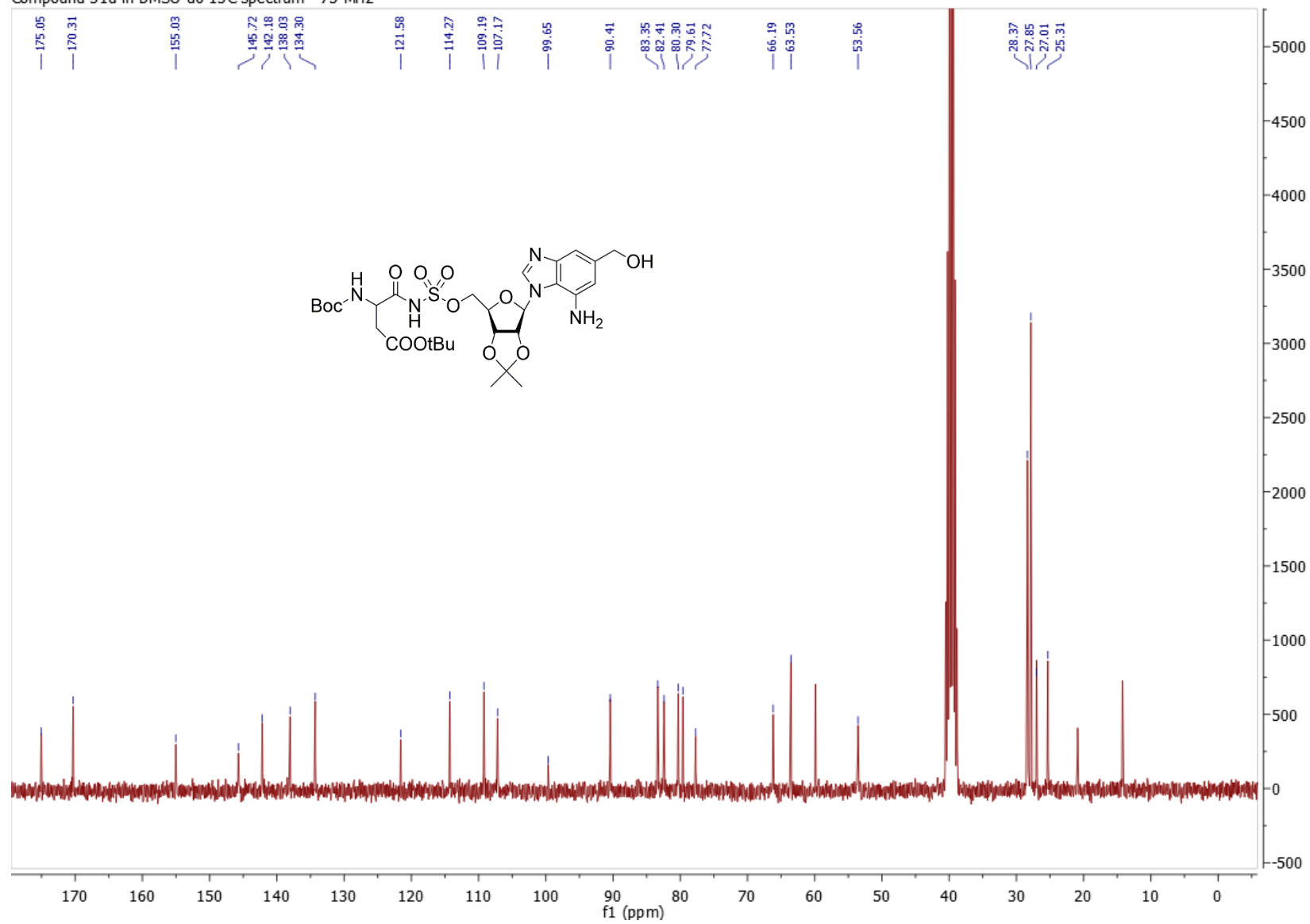




Compound 31d in DMSO-d6 1H spectrum - 300 MHz



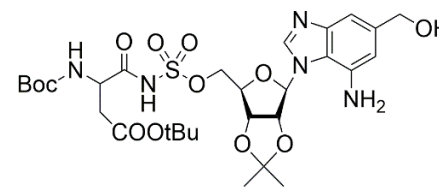
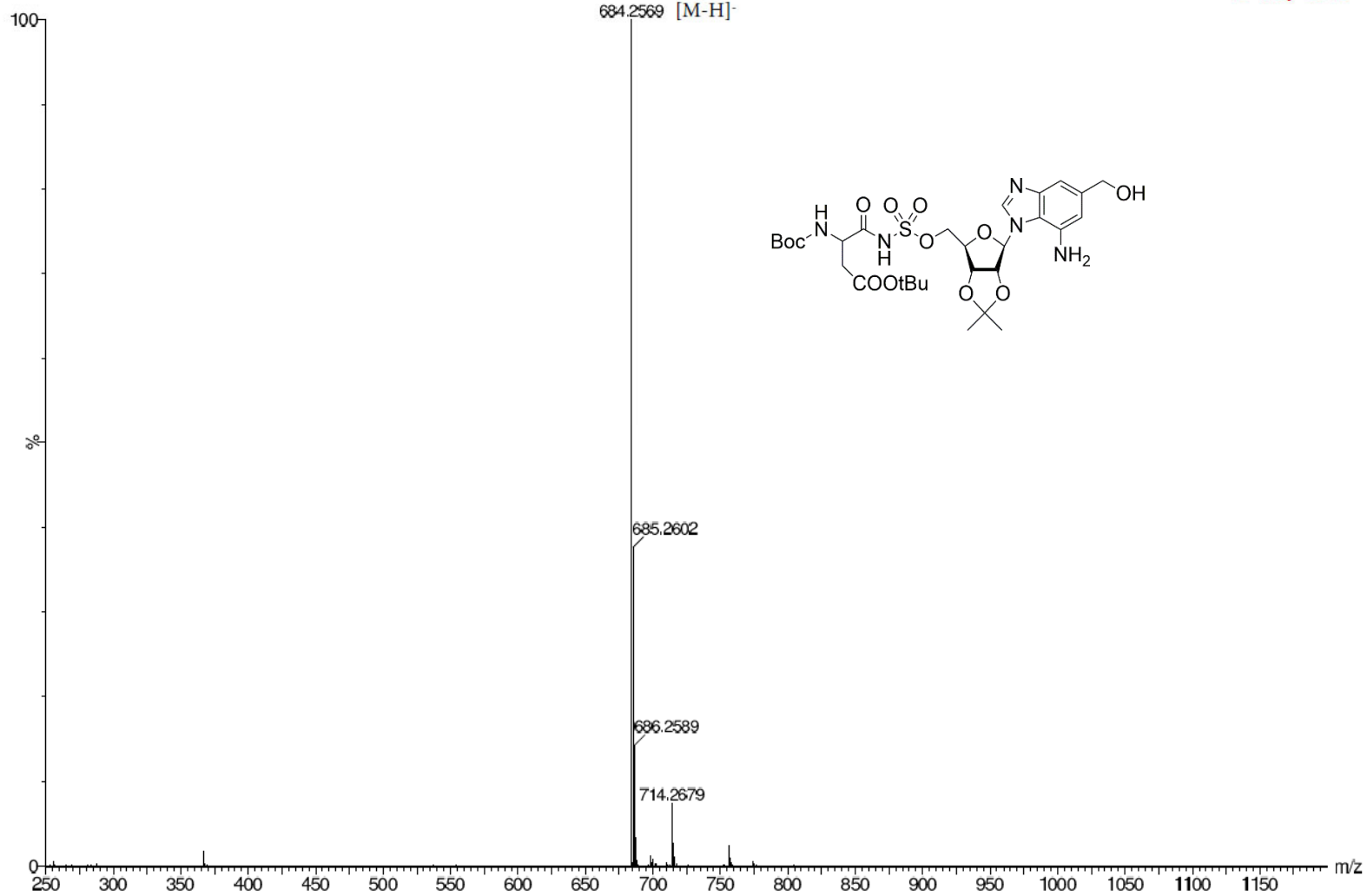
Compound 31d in DMSO-d6 13C spectrum - 75 MHz



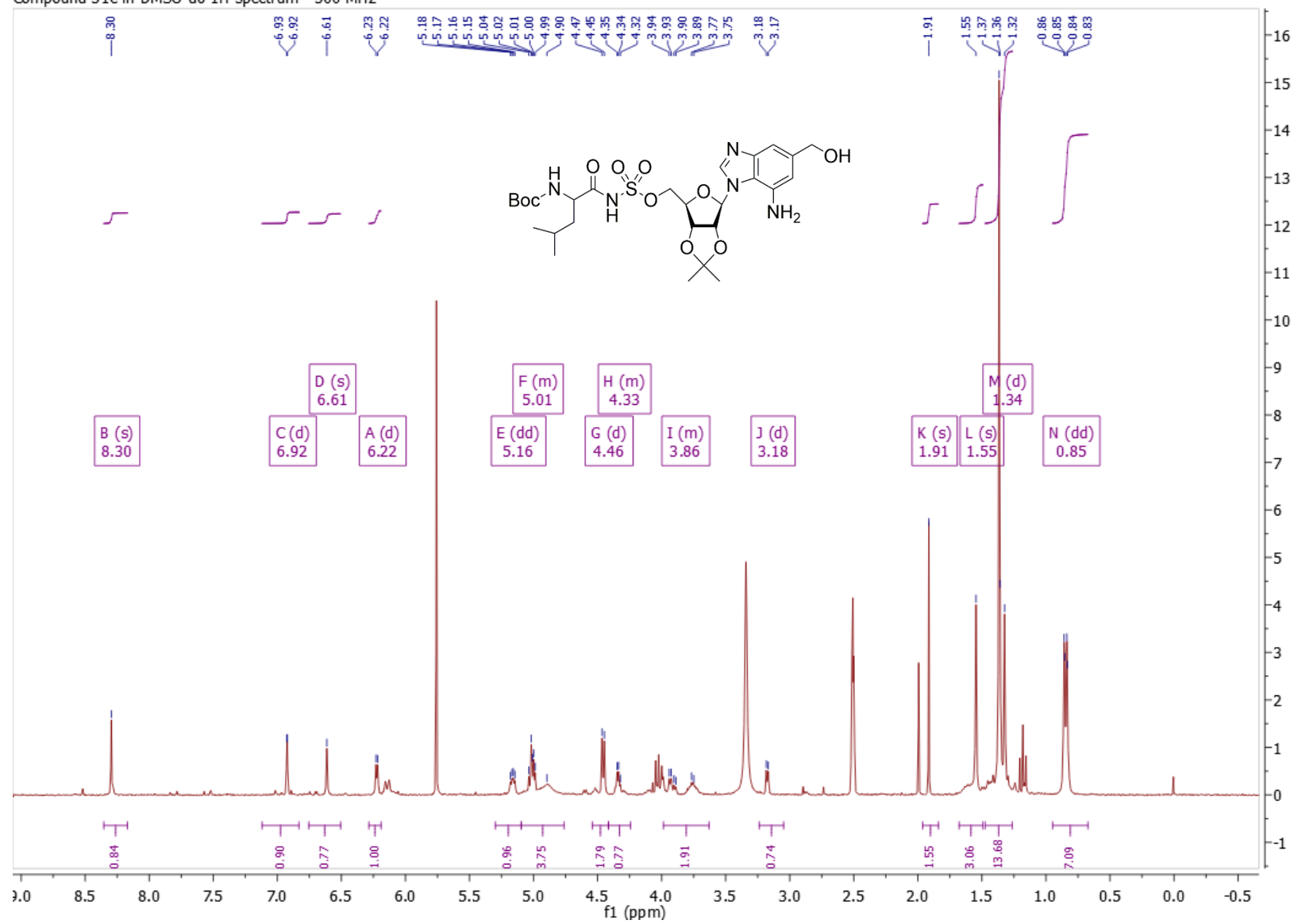
compound 31d

accurate mass

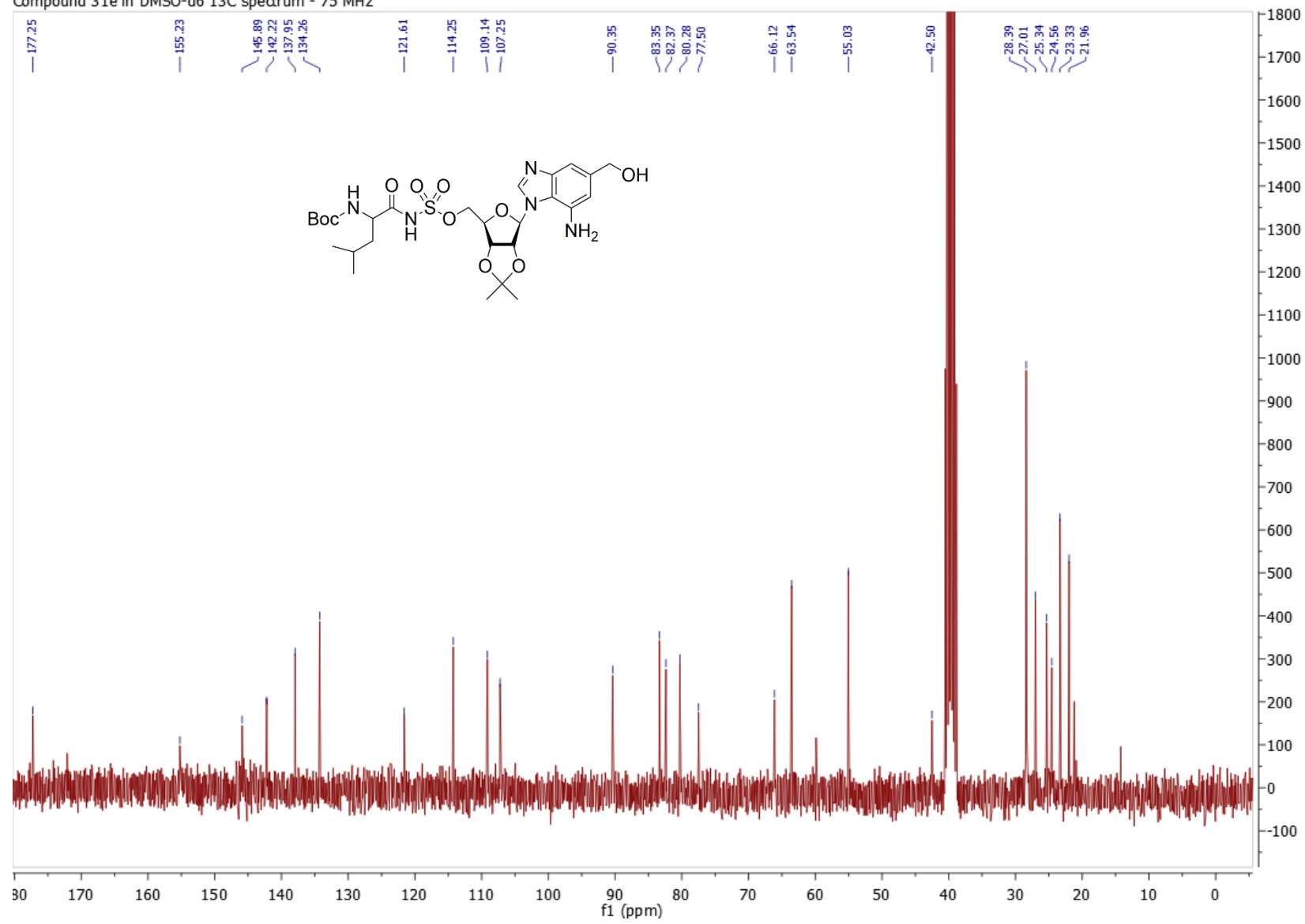
ES-  
19-May-2016



Compound 31e in DMSO-d6 1H spectrum - 300 MHz



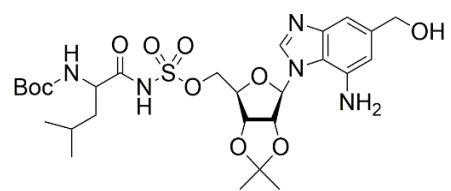
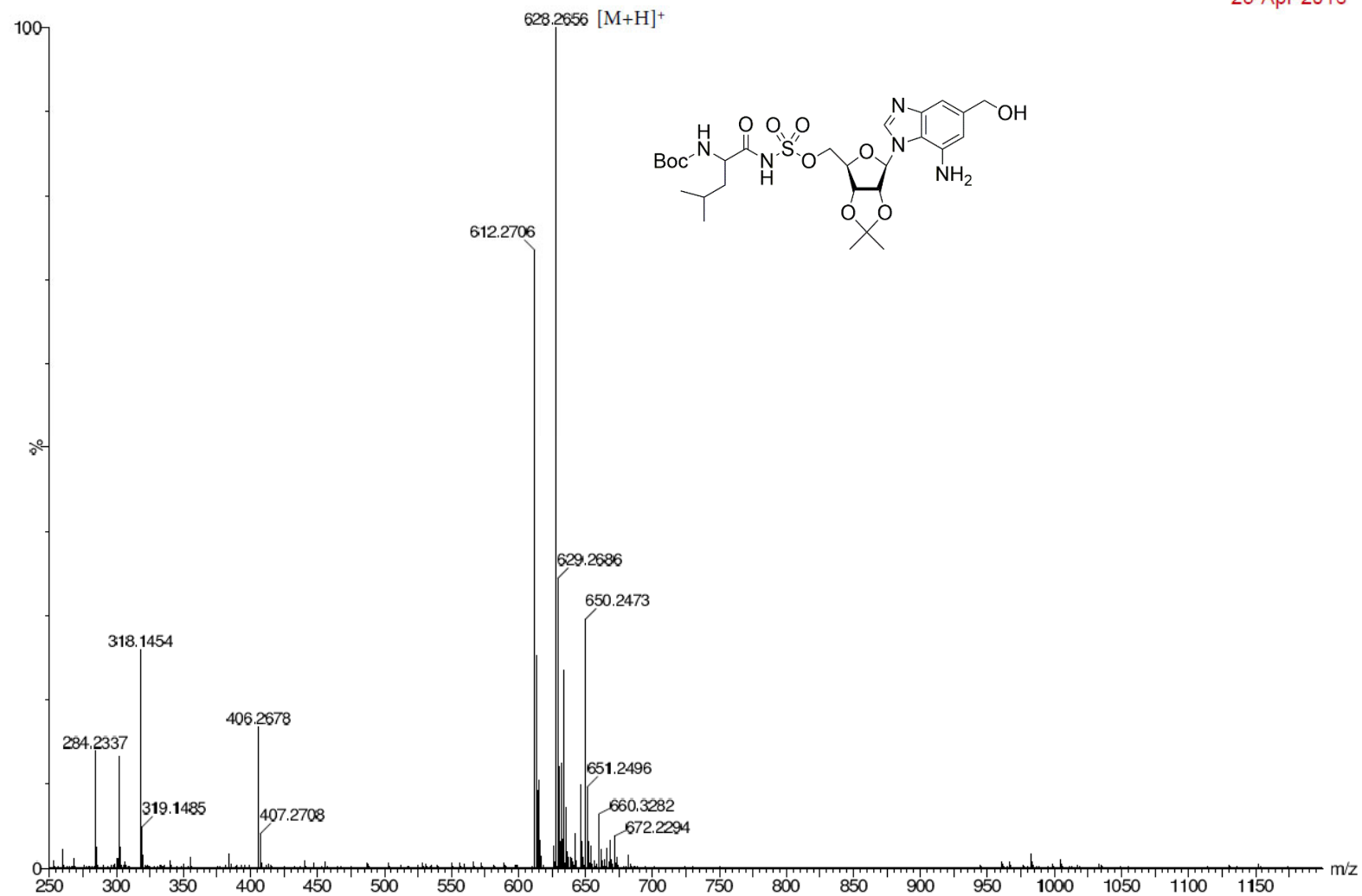
Compound 31e in DMSO-d6 13C spectrum - 75 MHz



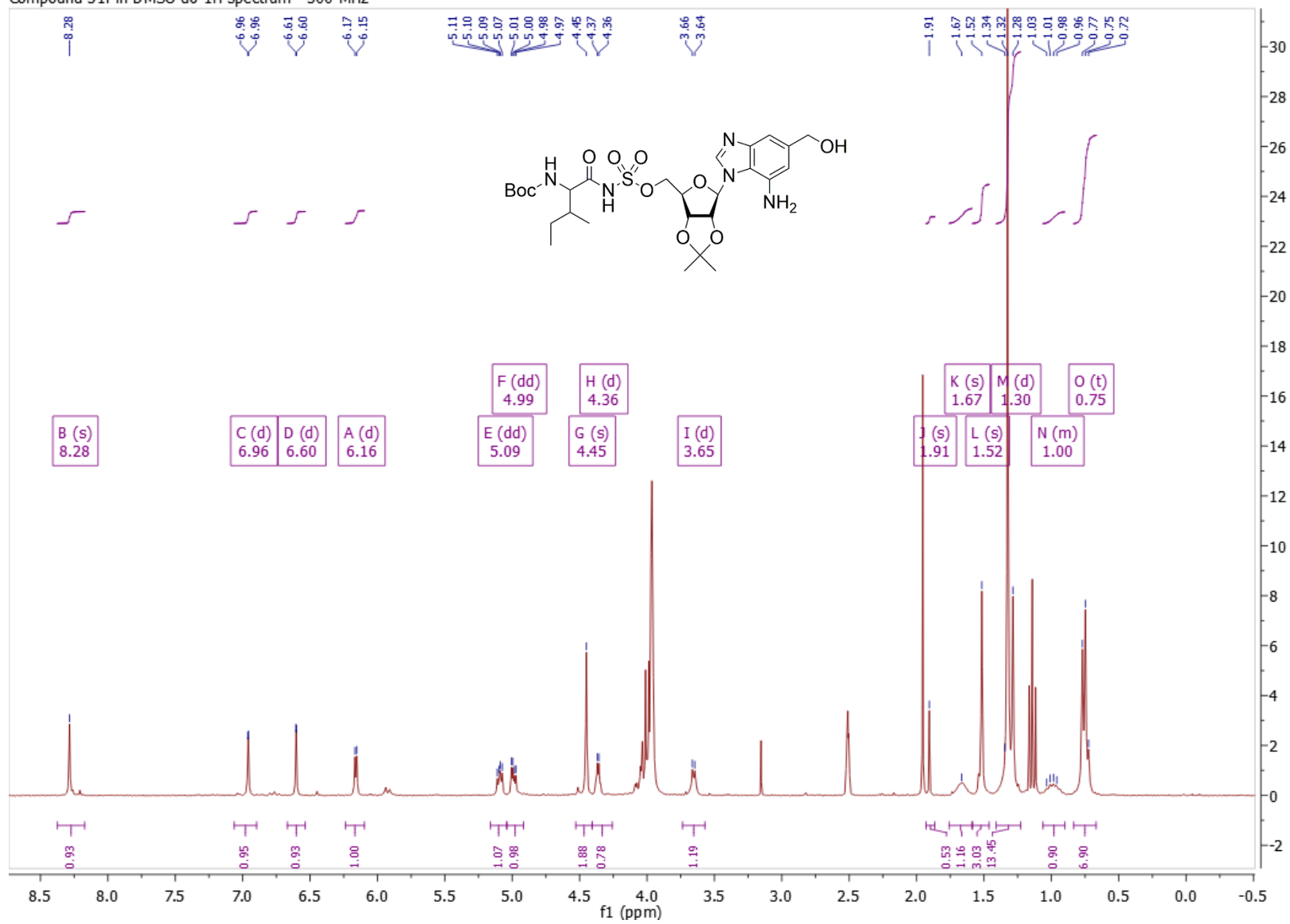
compound 31e

accurate mass

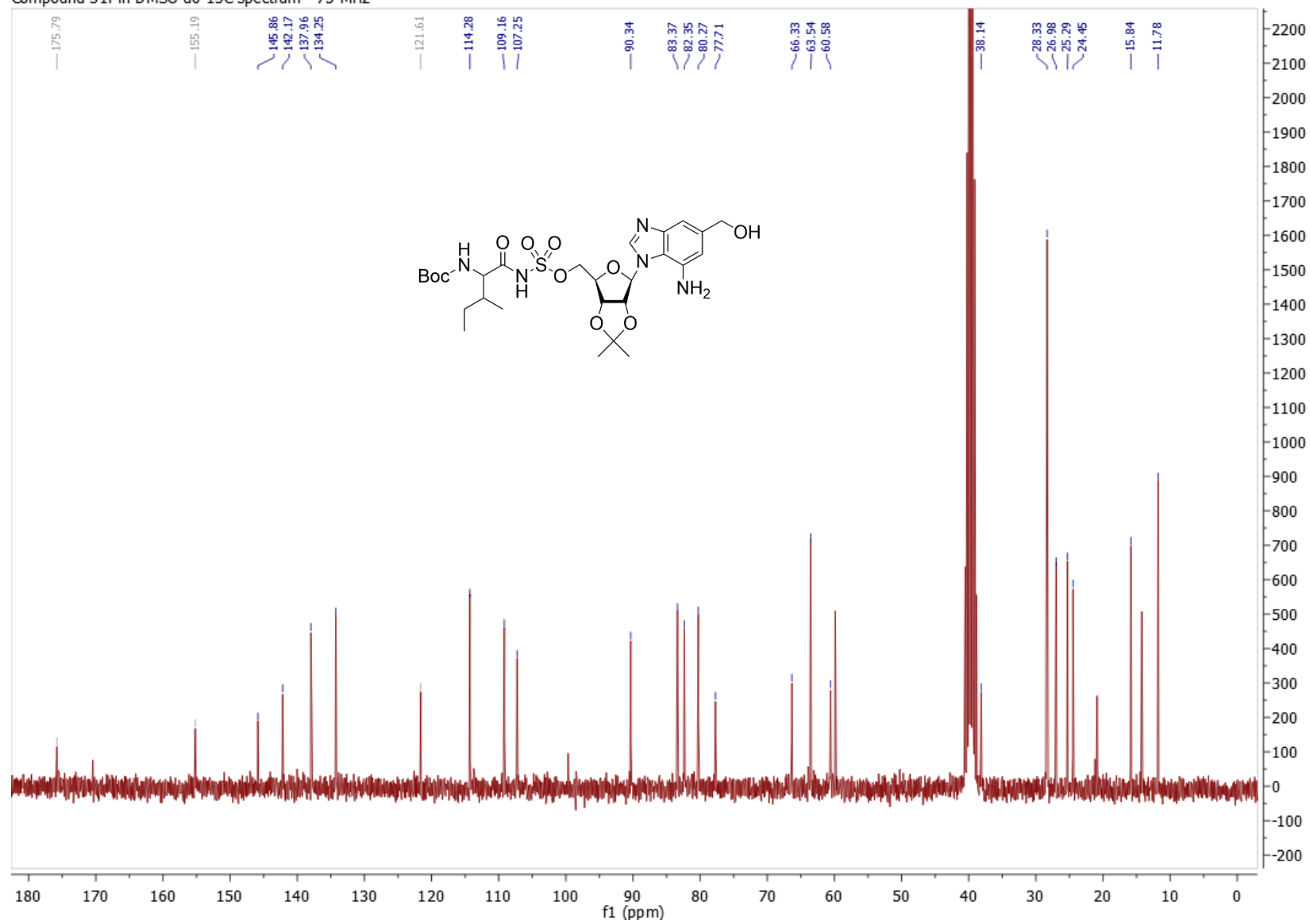
ES+  
25-Apr-2016



Compound 31f in DMSO-d6 1H spectrum - 300 MHz



Compound 31f in DMSO-d6 13C spectrum - 75 MHz

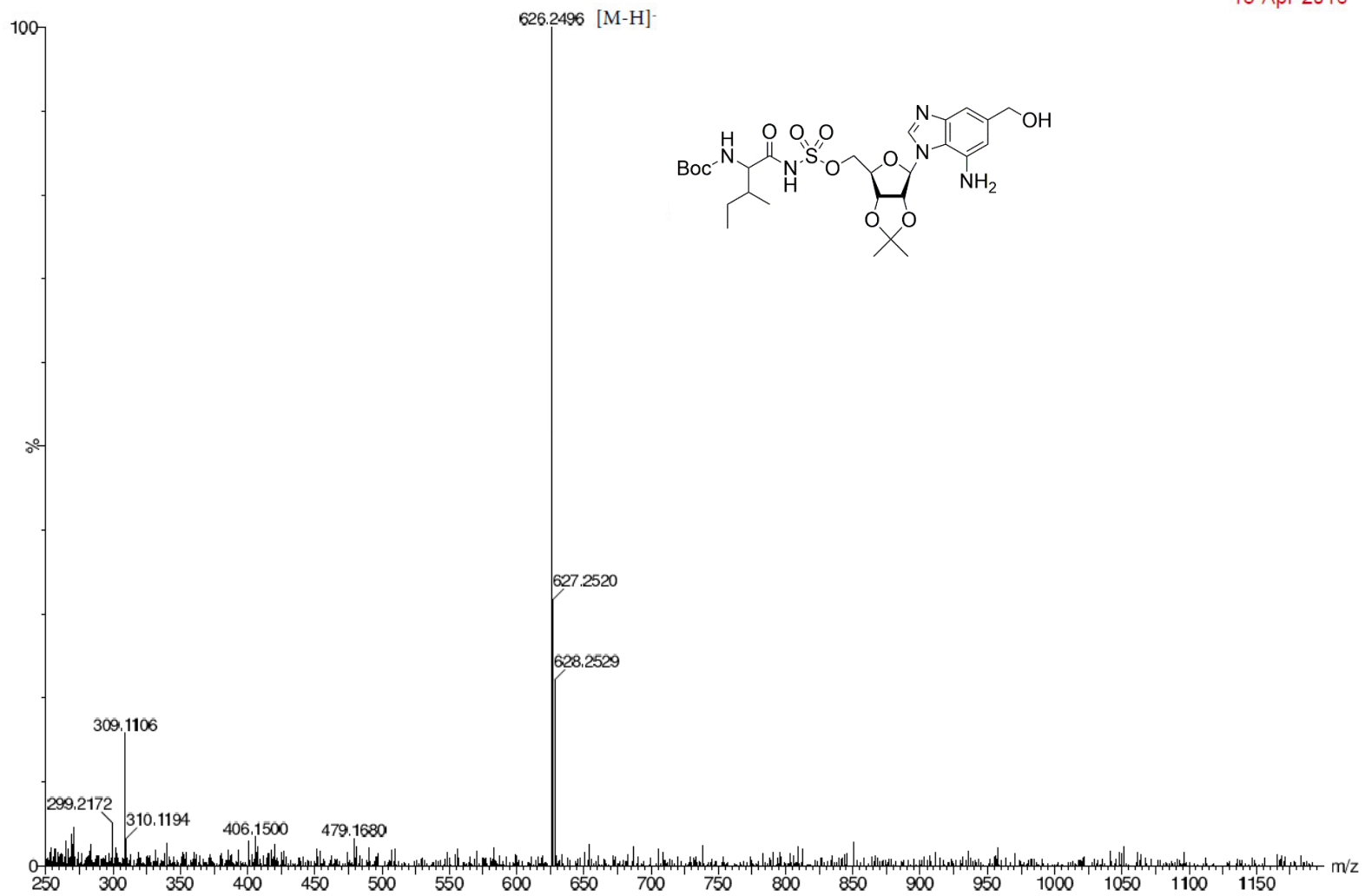




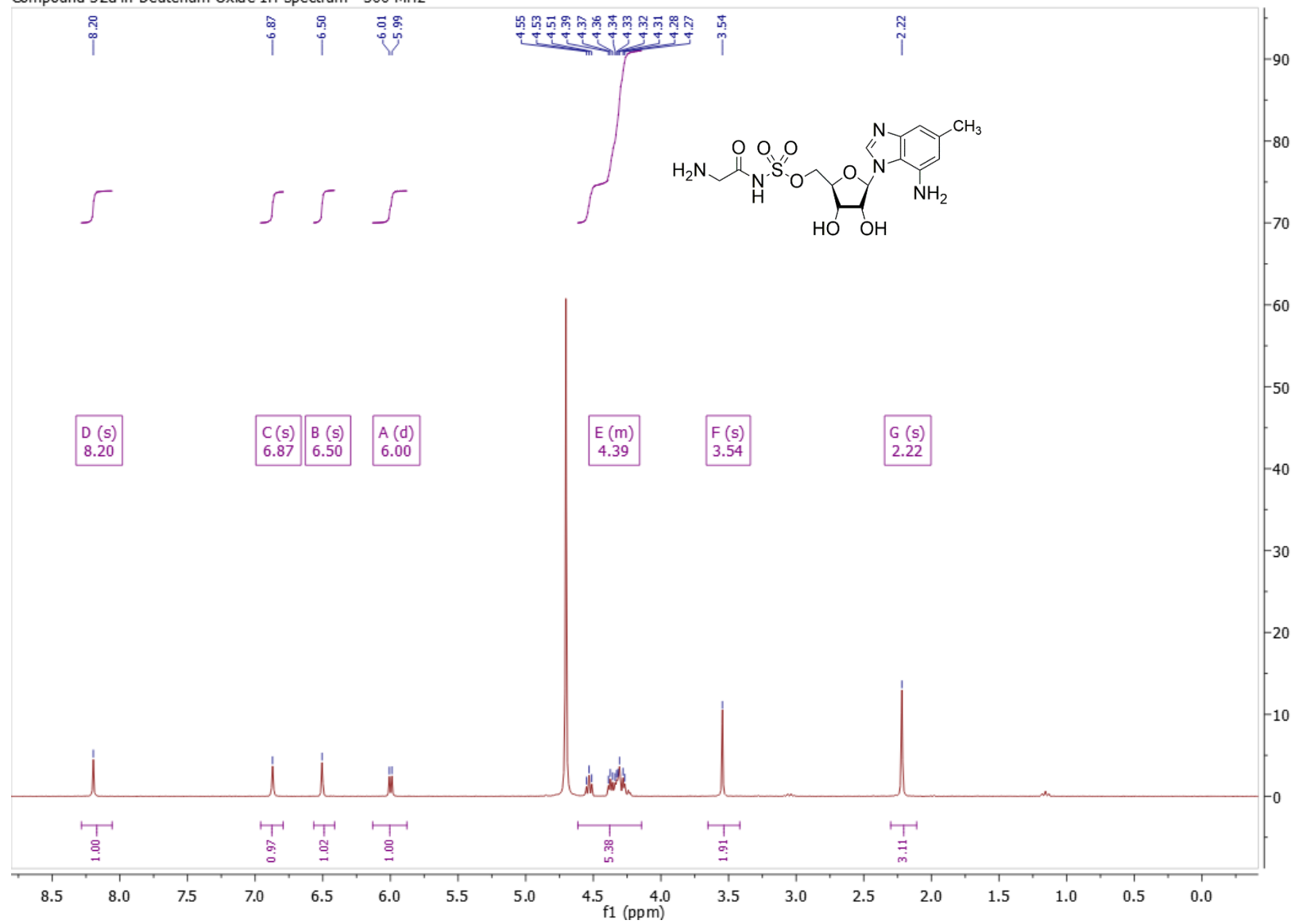
compound 31f

accurate mass

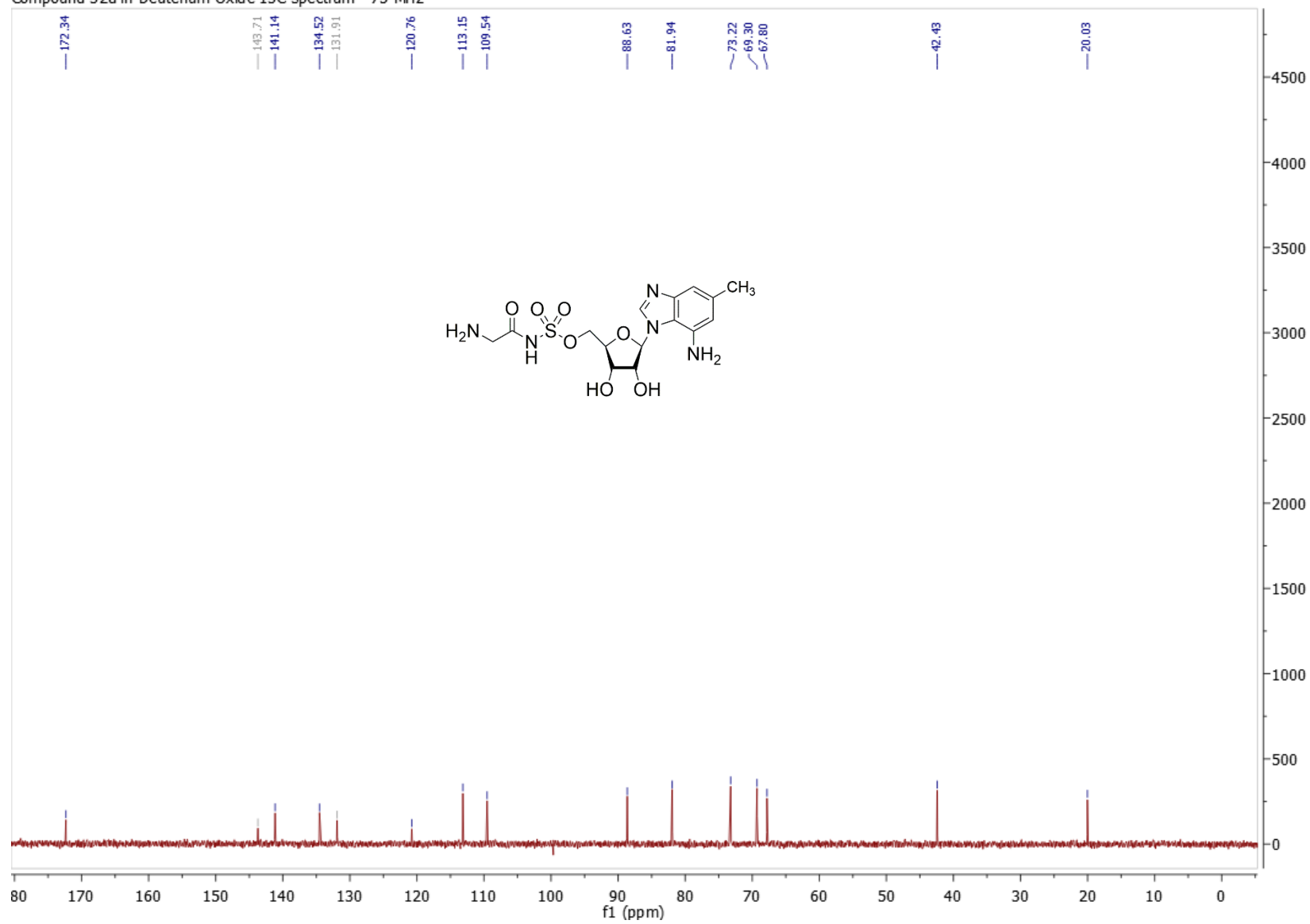
ES-  
13-Apr-2016



Compound 32a in Deuterium Oxide 1H spectrum - 300 MHz



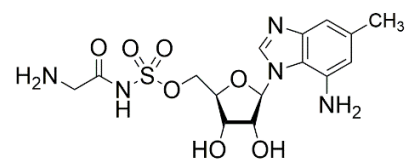
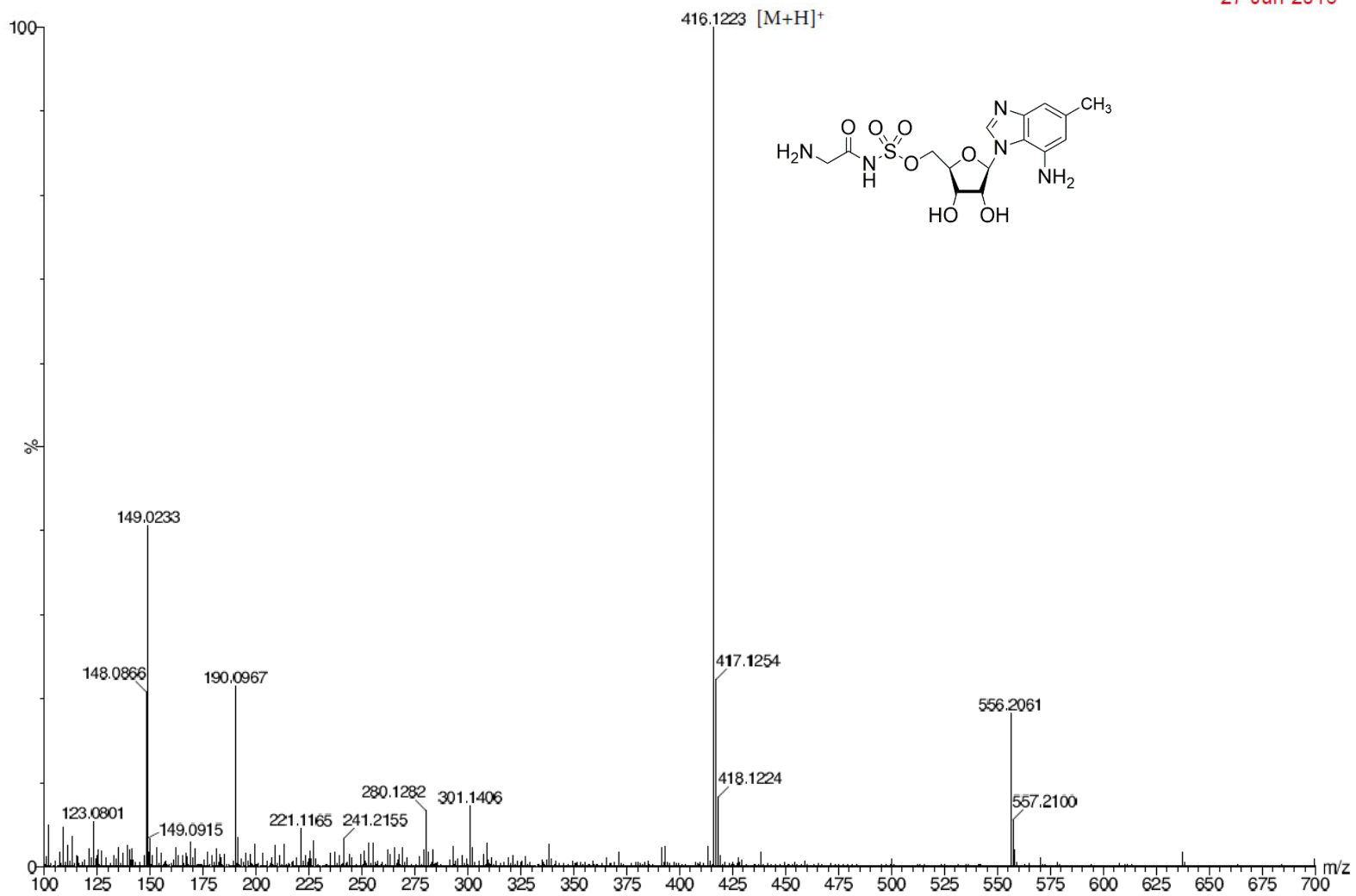
Compound 32a in Deuterium Oxide 13C spectrum - 75 MHz



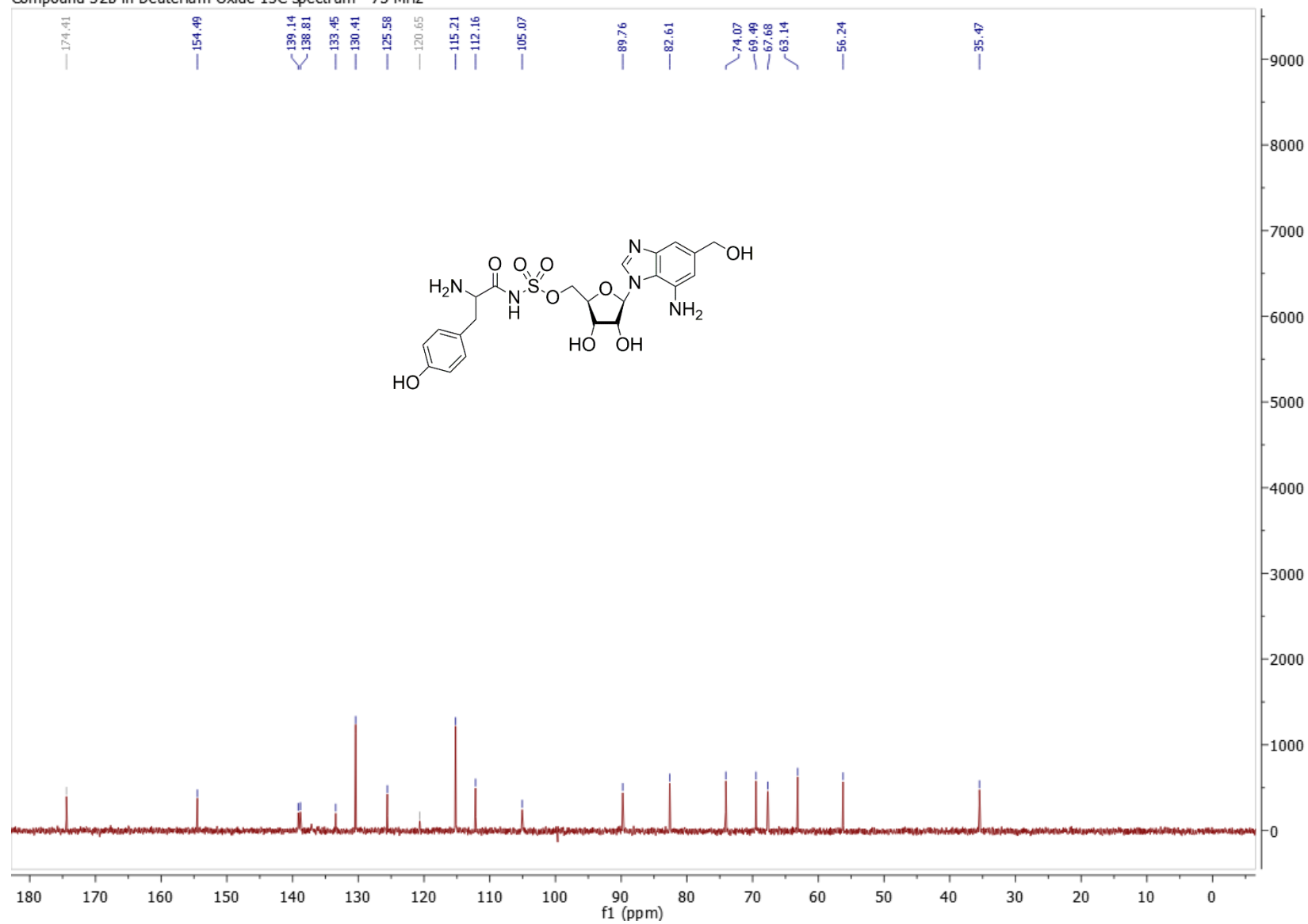
compound 32a

accurate mass

ES+  
27-Jun-2016



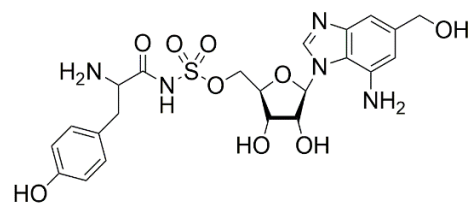
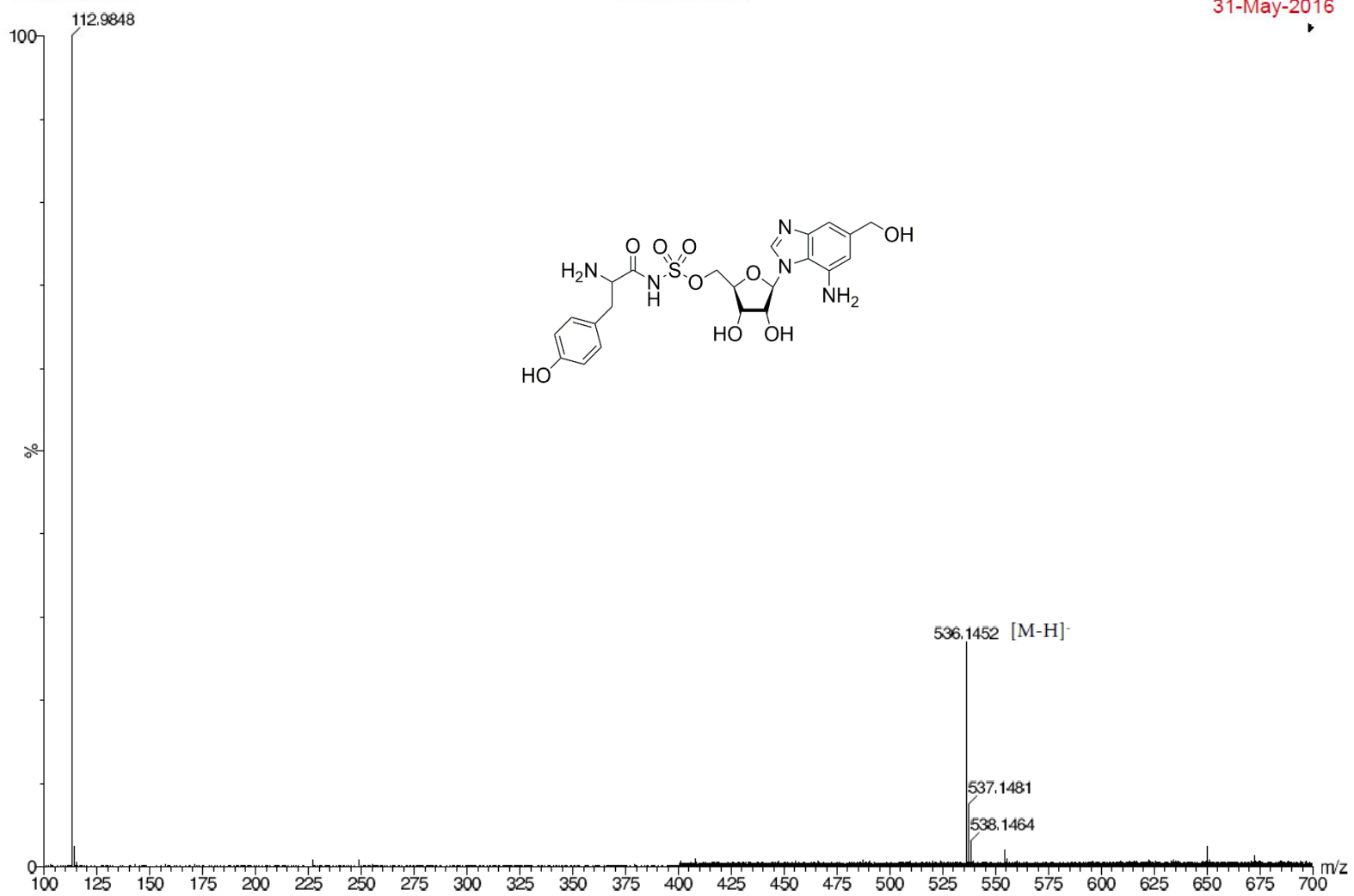
Compound 32b in Deuterium Oxide <sup>13</sup>C spectrum - 75 MHz



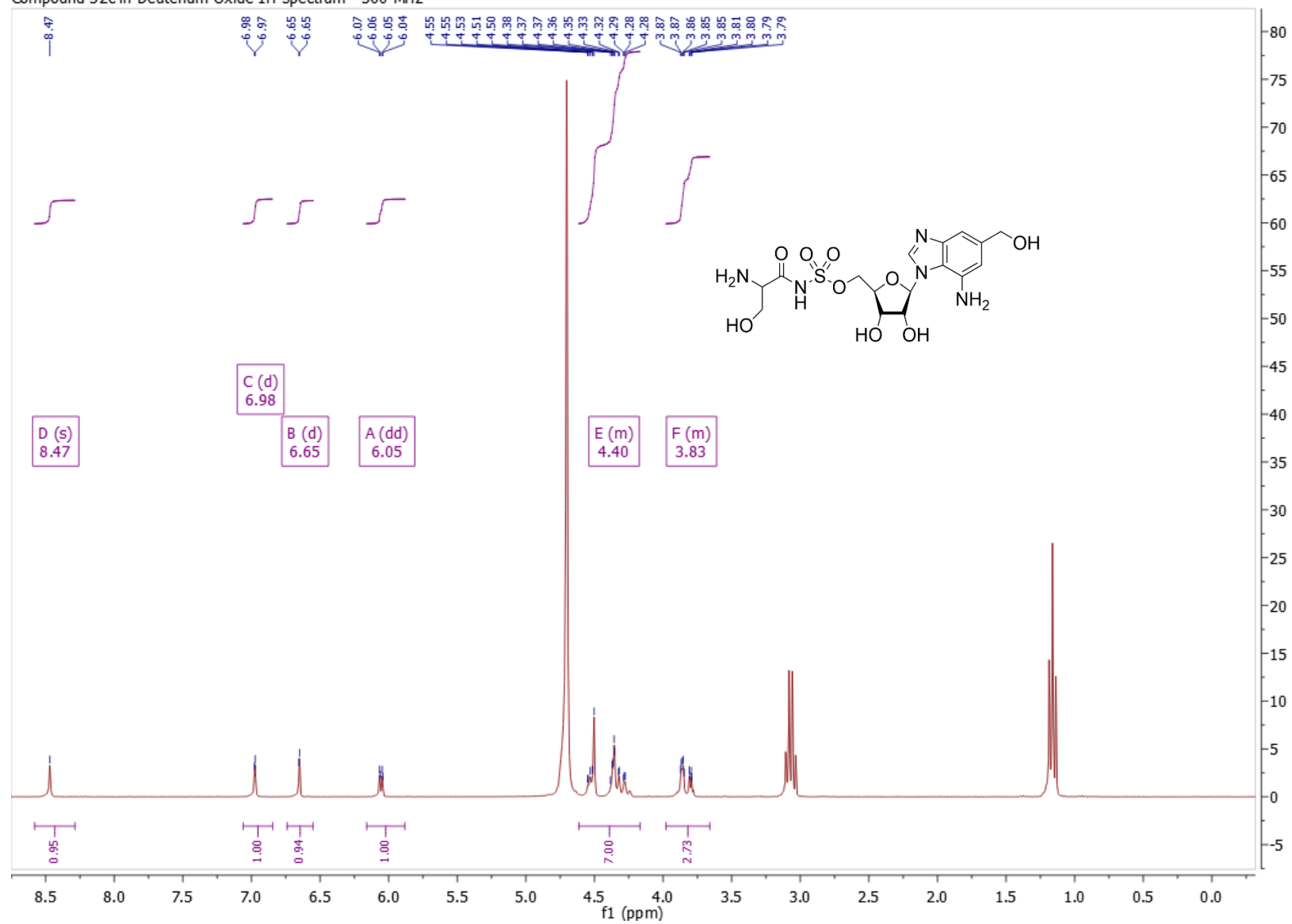
compound 32b

accurate mass

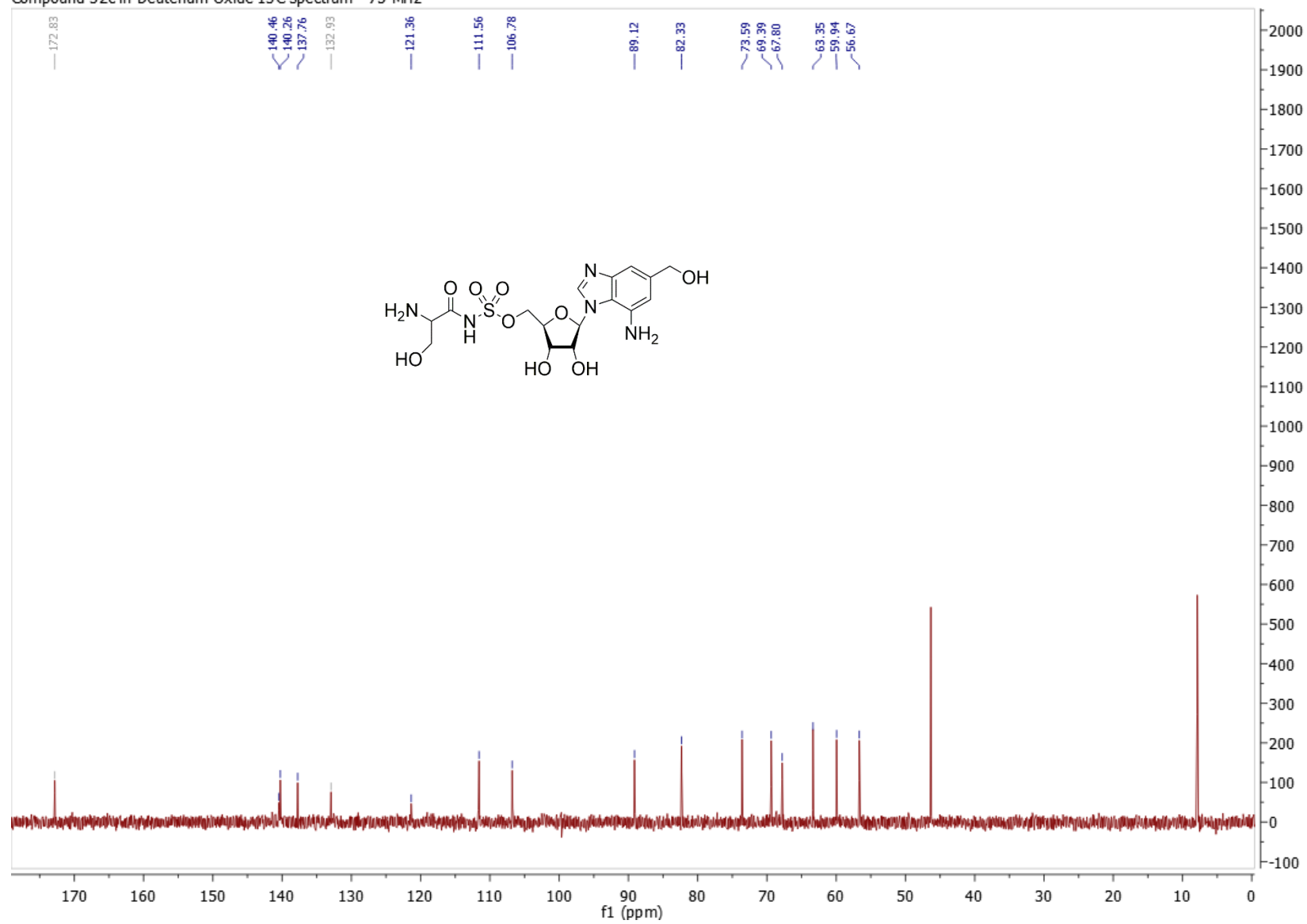
ES-  
31-May-2016



Compound 32c in Deuterium Oxide 1H spectrum - 300 MHz



Compound 32c in Deuterium Oxide <sup>13</sup>C spectrum - 75 MHz

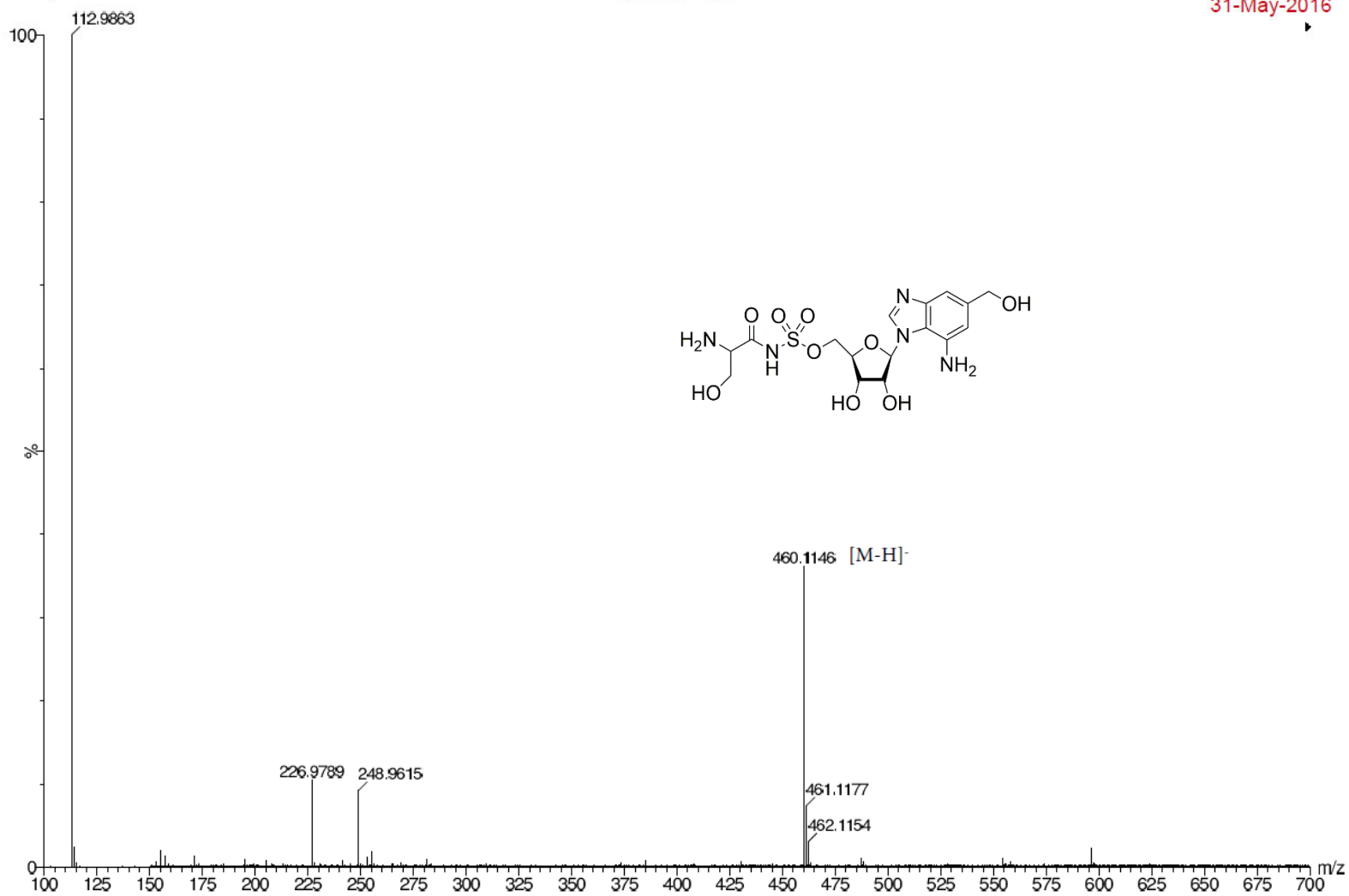




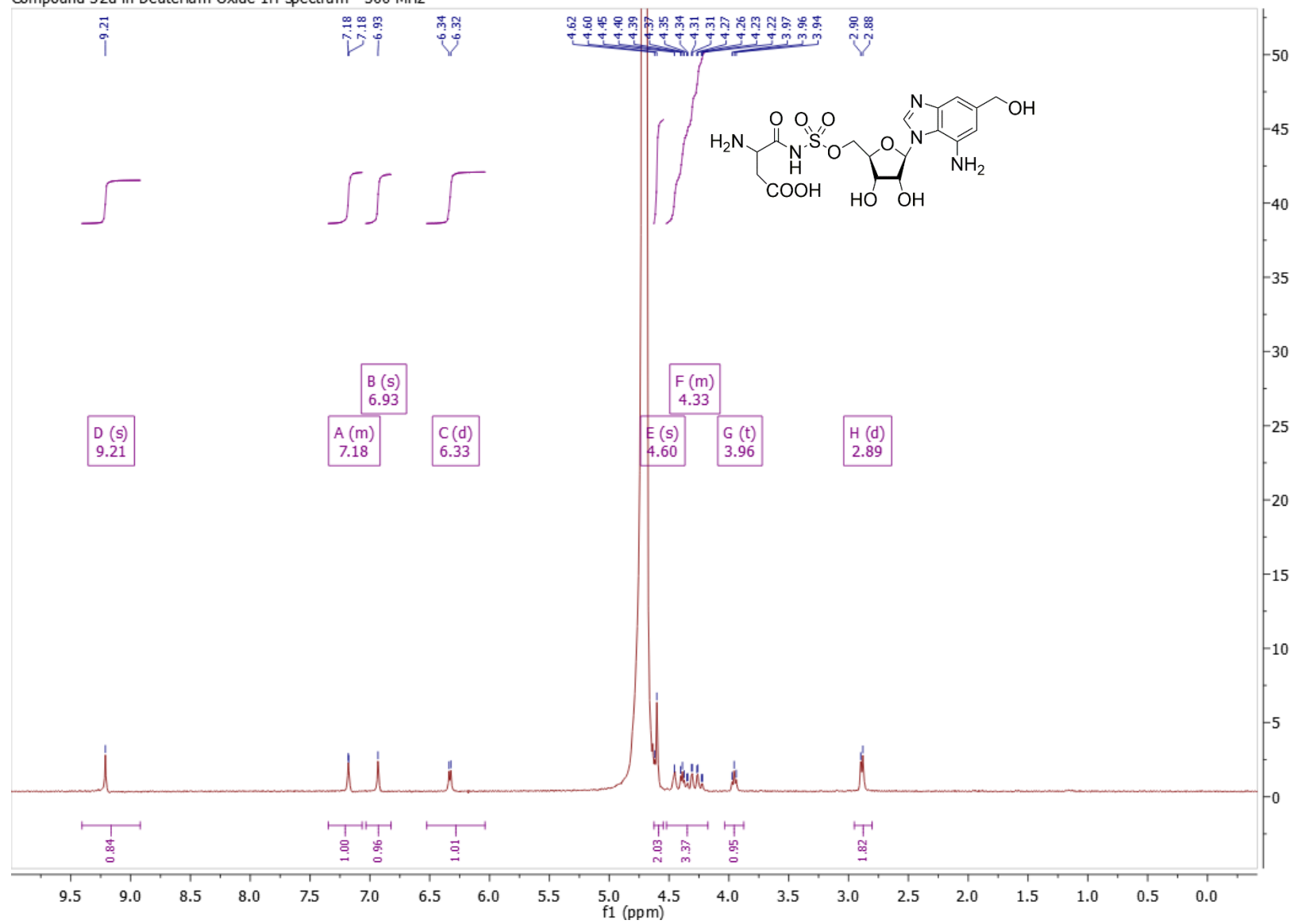
compound 32c

accurate mass

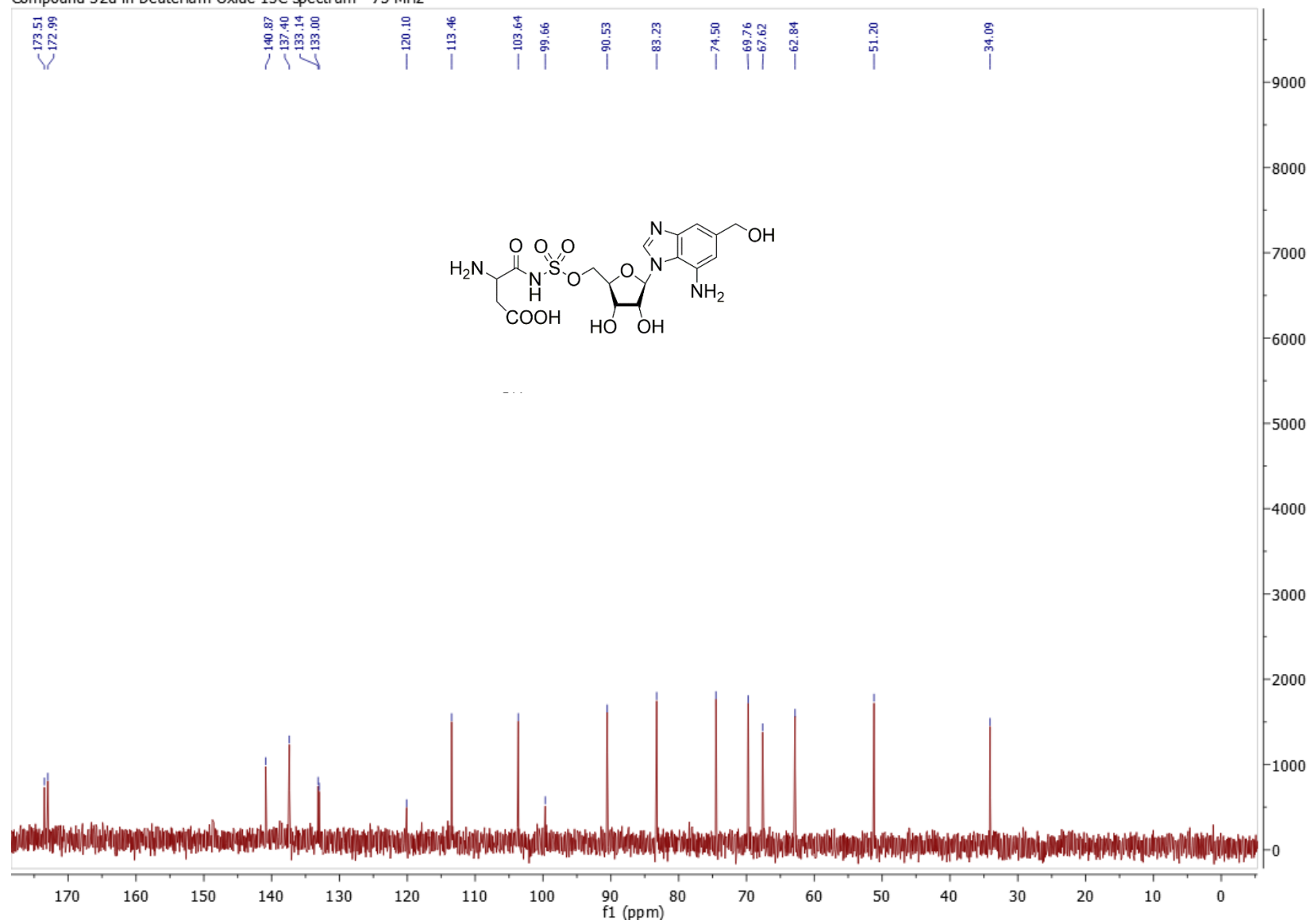
ES-  
31-May-2016



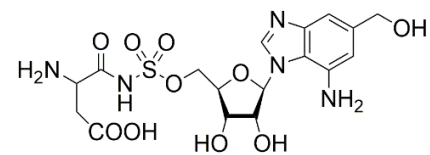
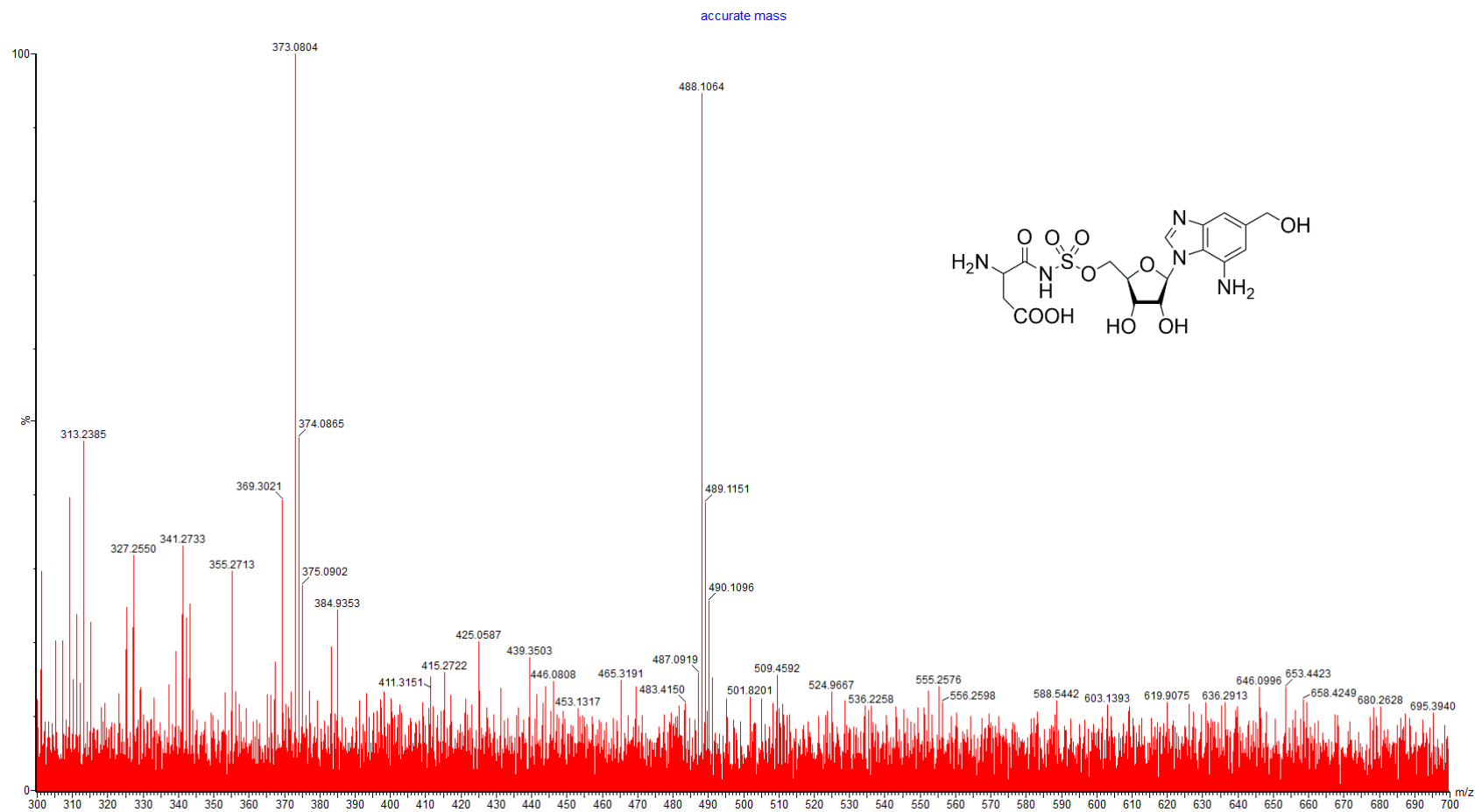
Compound 32d in Deuterium Oxide 1H spectrum - 300 MHz



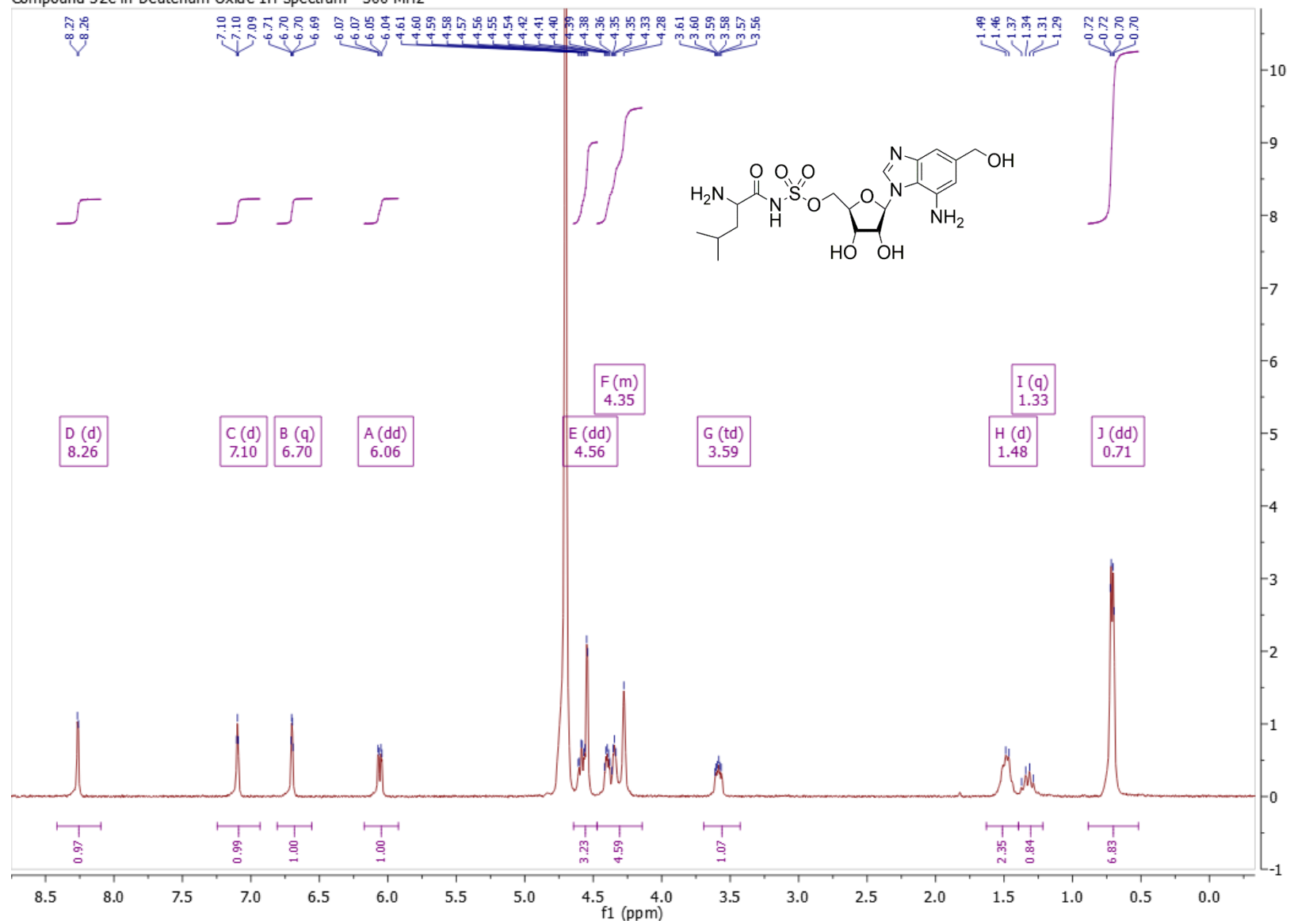
Compound 32d in Deuterium Oxide 13C spectrum - 75 MHz



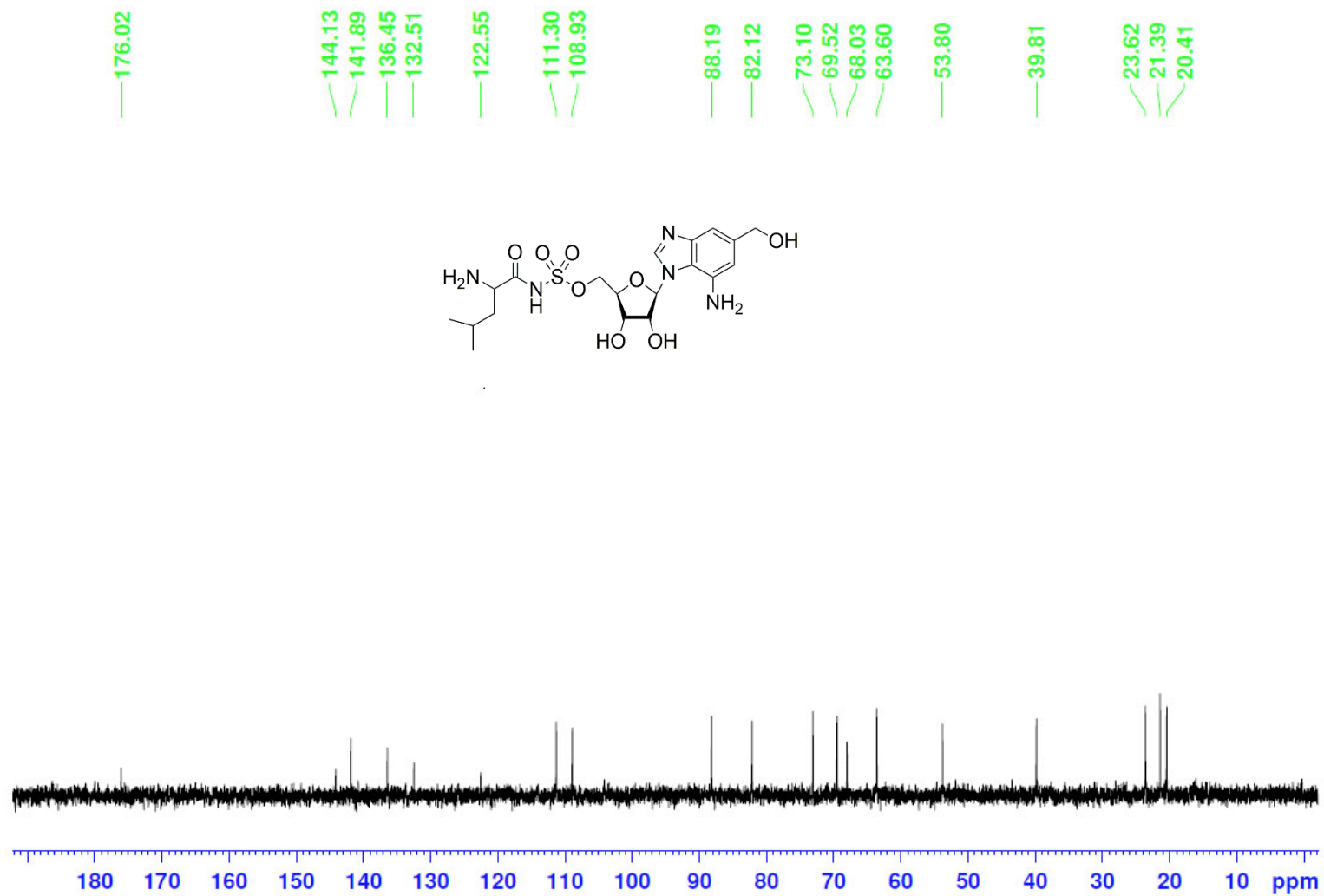
# Compound 32d



Compound 32e in Deuterium Oxide 1H spectrum - 300 MHz



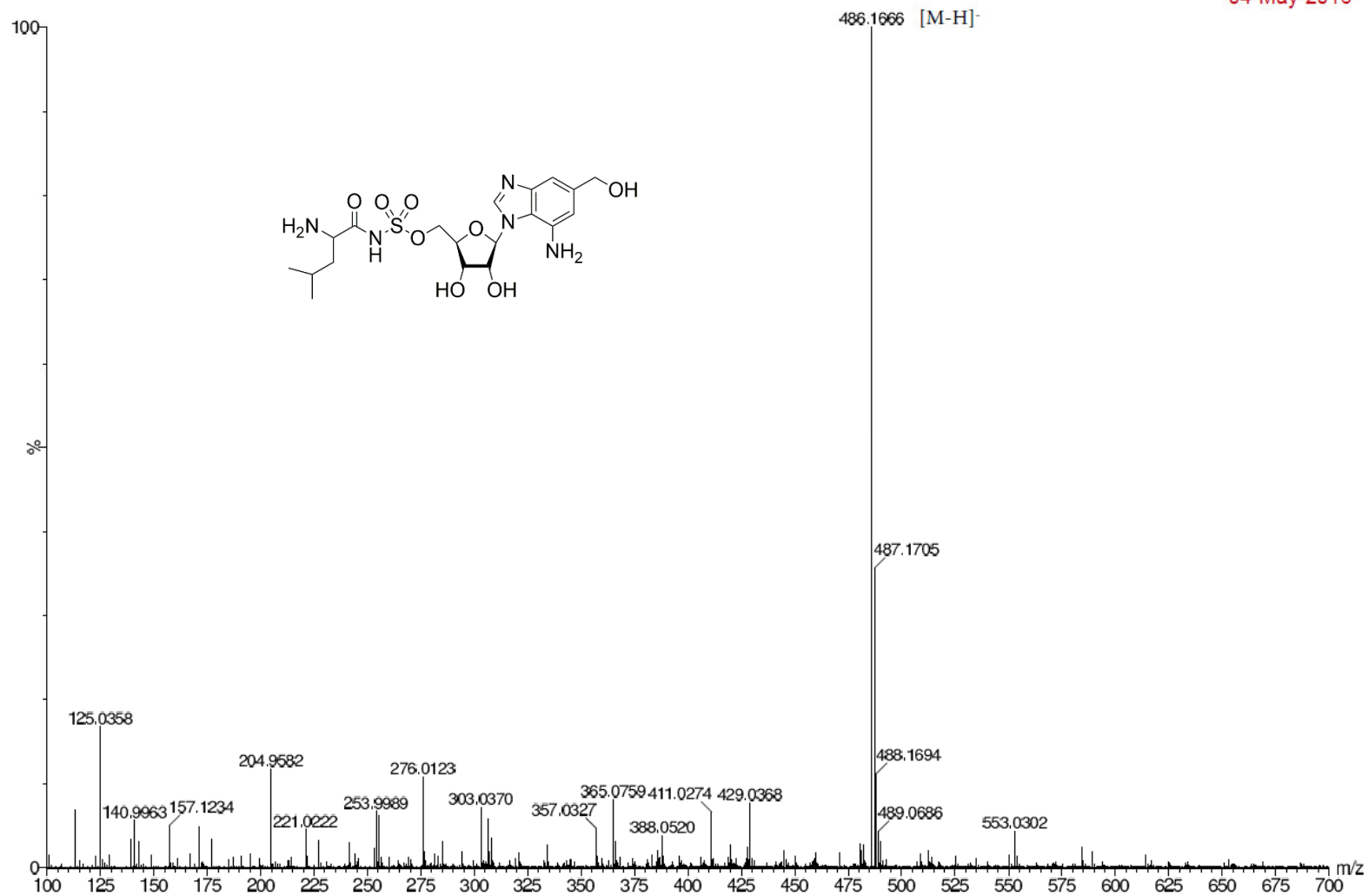
Compound 32e in Deuterium Oxide  $^{13}\text{C}$  spectrum - 75 MHz



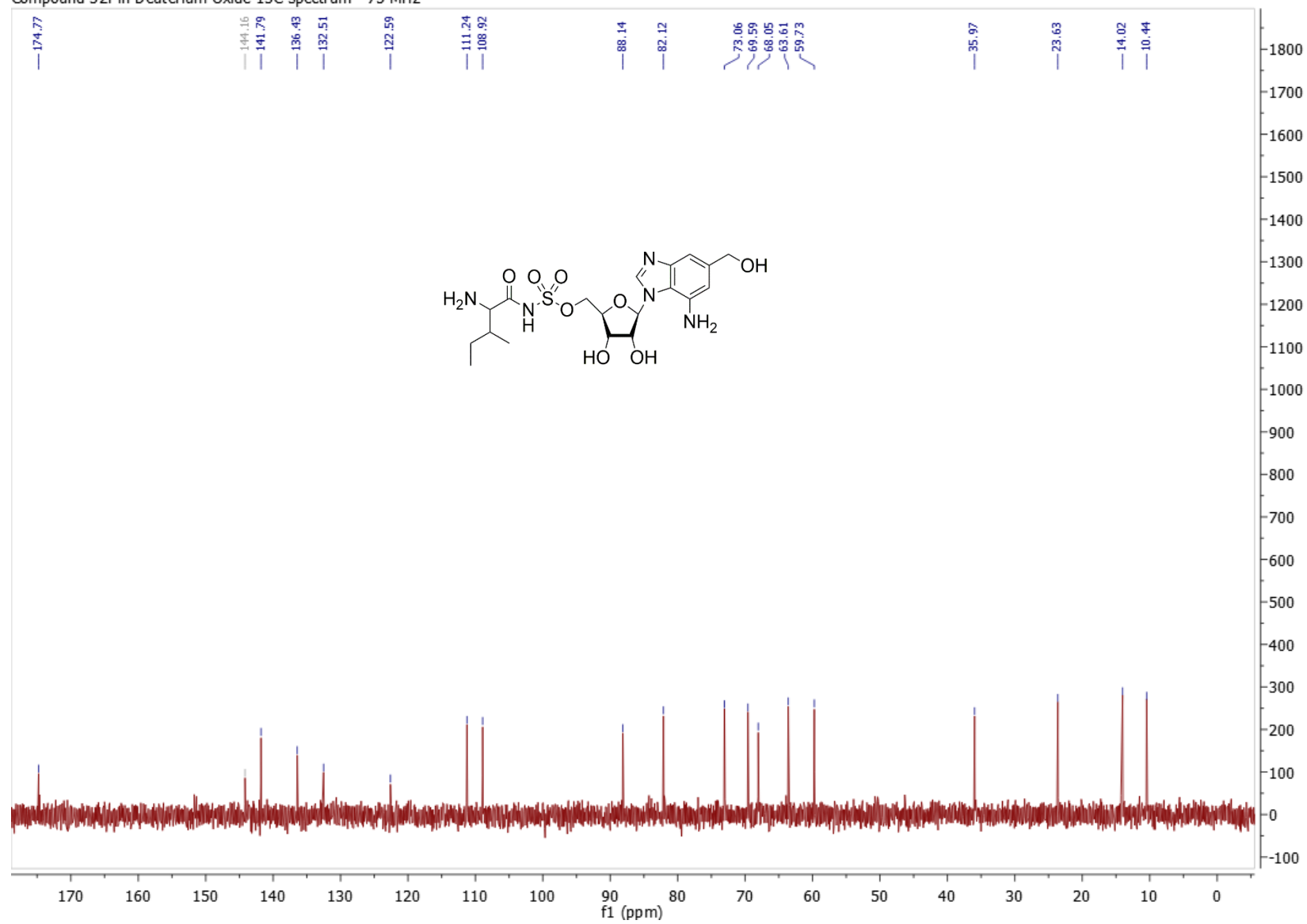
compound 32e

accurate mass

ES-  
04-May-2016



Compound 32f in Deuterium Oxide <sup>13</sup>C spectrum - 75 MHz





compound 32f

accurate mass

ES-  
22-Apr-2016

