

Supporting Information

Synthesis and anticancer studies of Michael adducts and Heck arylation products of sesquiterpene lactones, zaluzanin D and zaluzanin C from *Vernonia arborea*

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Table of Contents

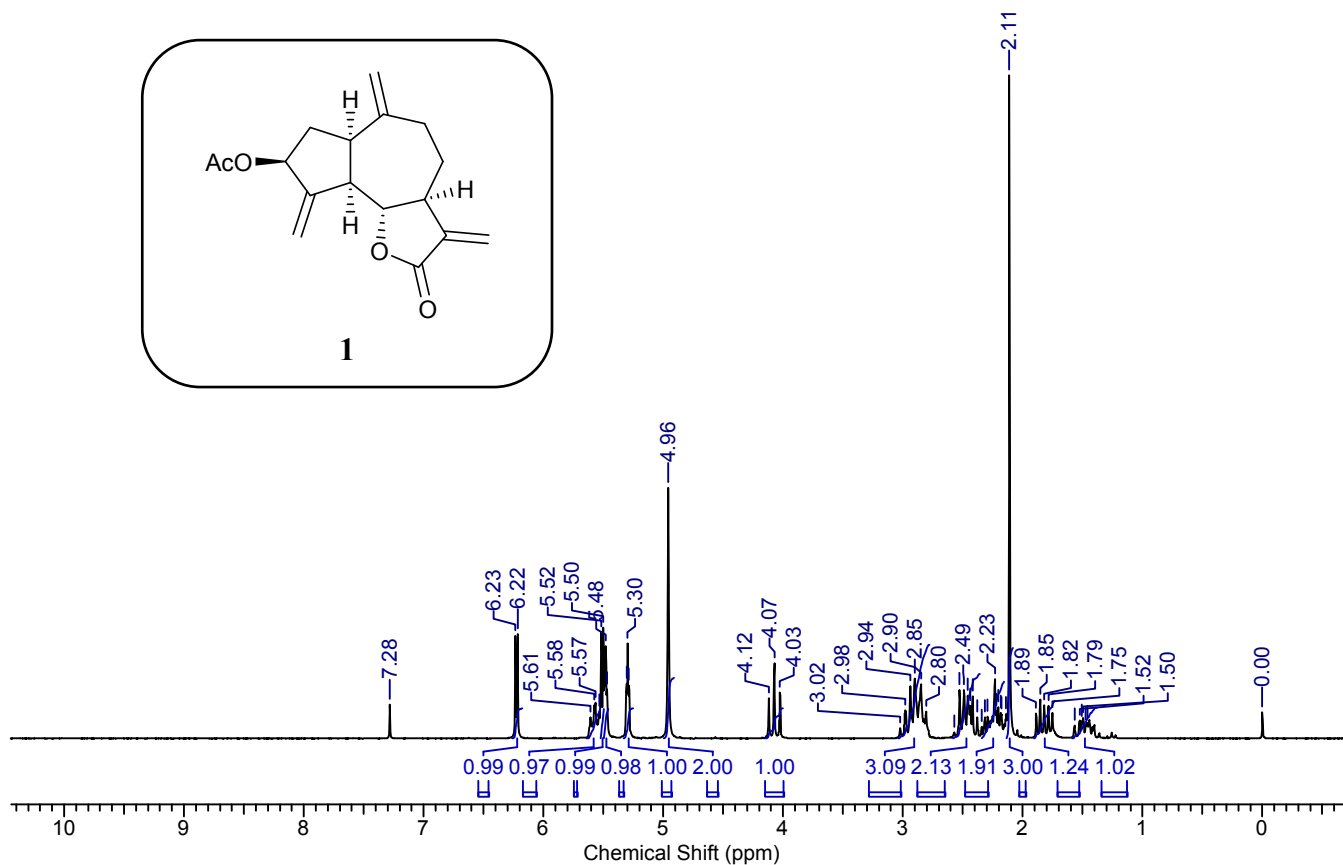
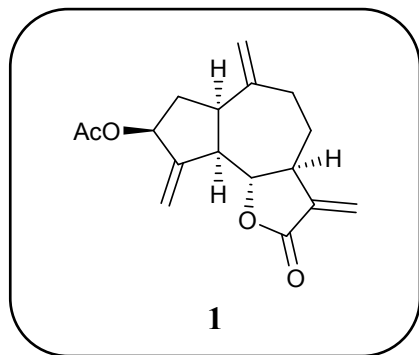
Copies of NMR and HRMS spectra of Michael adducts of zaluzanin D.....S2-S56

Copies of NMR and HRMS spectra of Heck analogs of zaluzanin D.....S56-S83

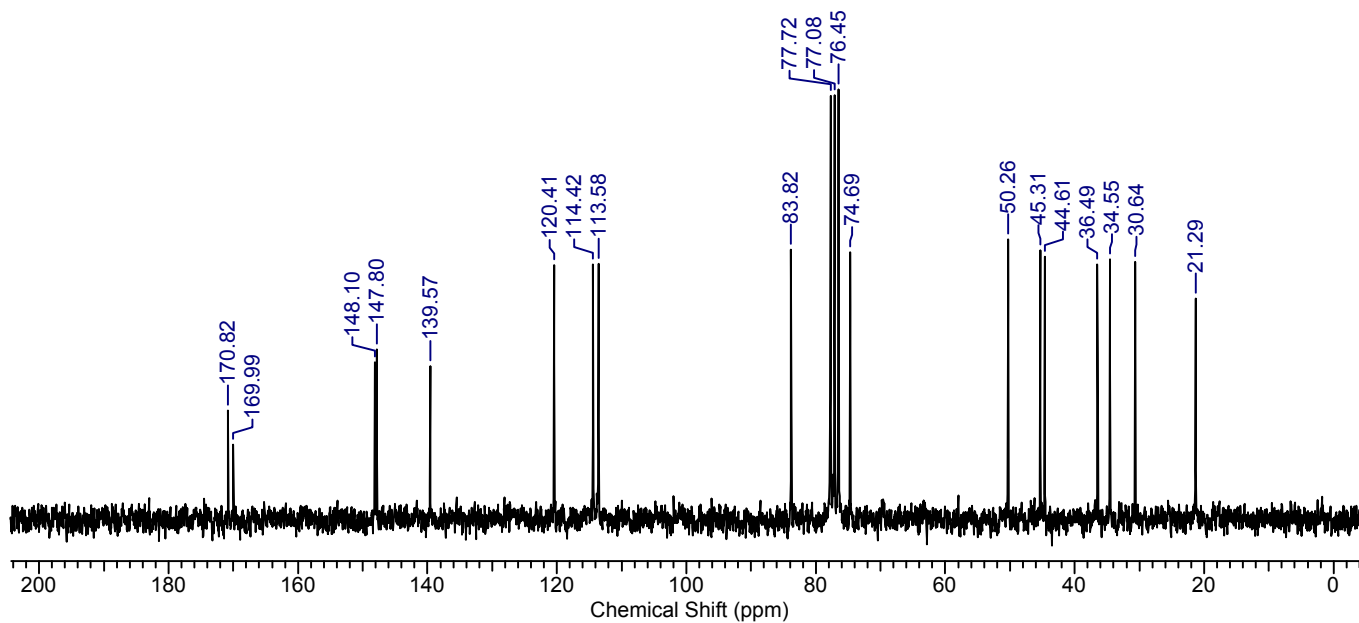
Experimental Section

General. All melting points were recorded on a Büchi melting point apparatus in open capillaries and are uncorrected. Commercially available reagents and solvents were used as such received. Dry MeOH was prepared following the standard procedures. All dry reactions were carried out under argon atmosphere and flash chromatography was performed with CombiFlash *Rf* 200*i* with UV/VIS and ELSD, Isco Teledyne Inc., USA using RediSep® column (SiO₂). ¹H NMR spectra were recorded on 400 or 200 MHz spectrometer and ¹³C NMR spectra were recorded at 100 or 50 MHz. Chemical shifts are reported as δ values (ppm) relative to internal standard tetramethylsilane in CDCl₃. HRMS (ESI) were recorded on an Orbitrap (quadrupole plus ion trap) and TOF mass analyser. FT-IR spectra were recorded on an FT-IR-8300 Shimadzu spectrometer. Optical rotations were recorded on a JASCO P-1020 polarimeter.

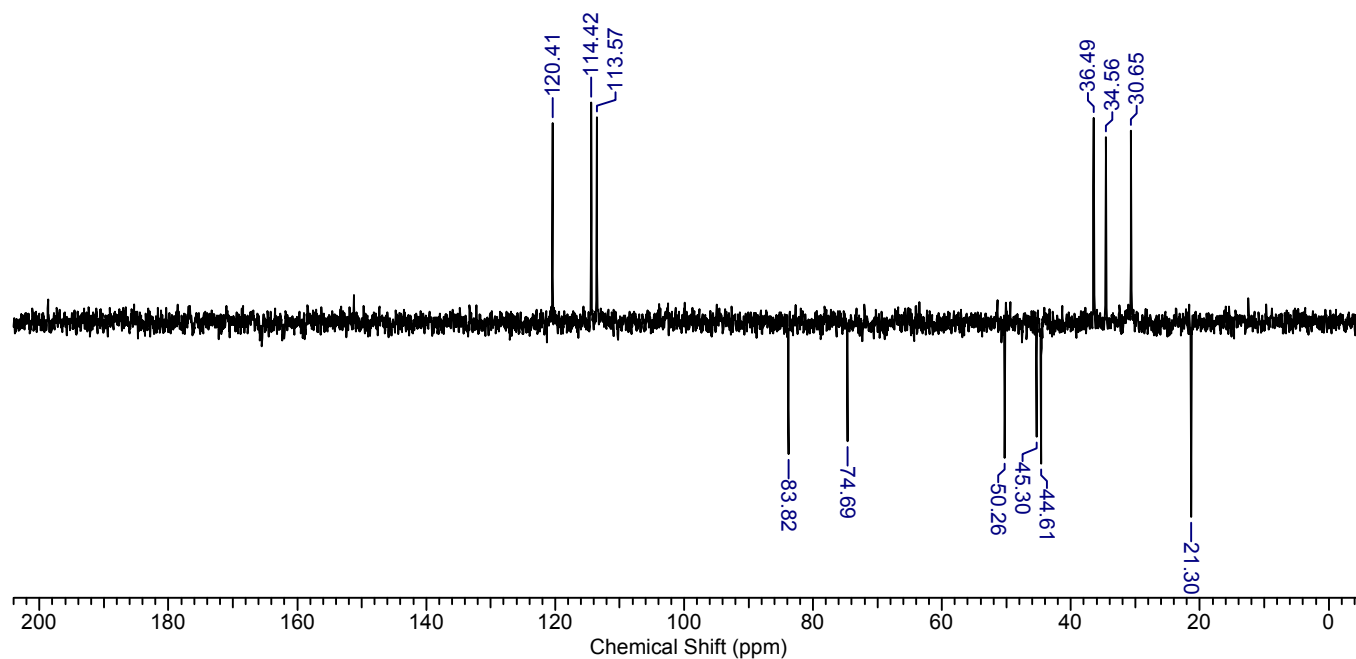
¹H NMR of Compound 1 (200 MHz, CDCl₃)



¹³C NMR of Compound 1 (50 MHz, CDCl₃)



DEPT of Compound 1 (50 MHz, CDCl₃)

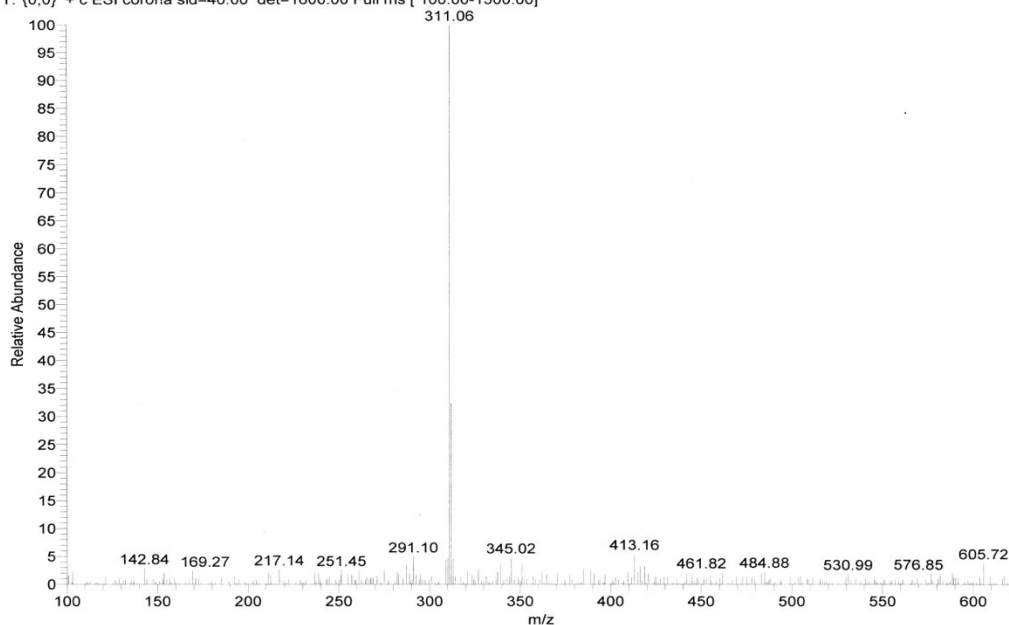


LC-MS of Compound 1

F:\DATA\Sept-2014\19\ZD_140919162231

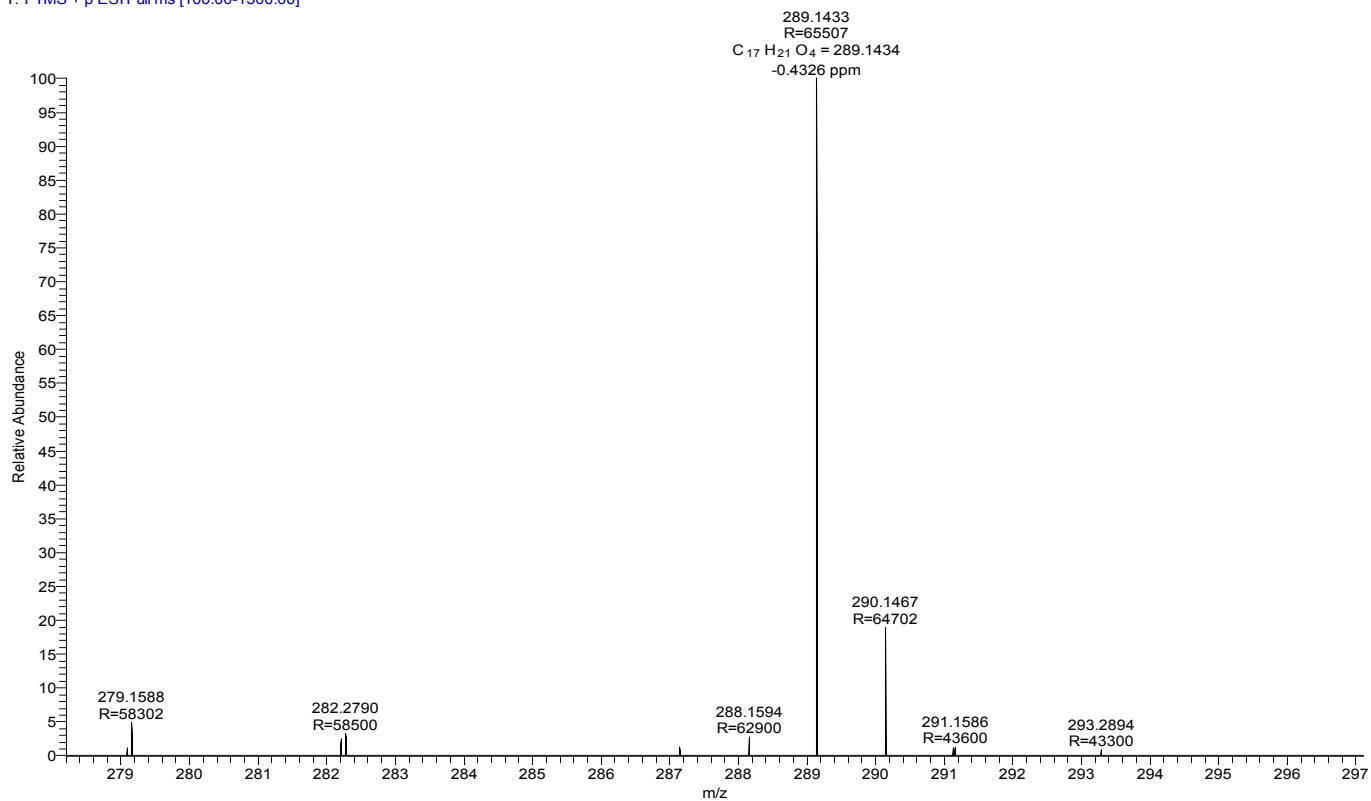
9/19/2014 4:22:31 PM

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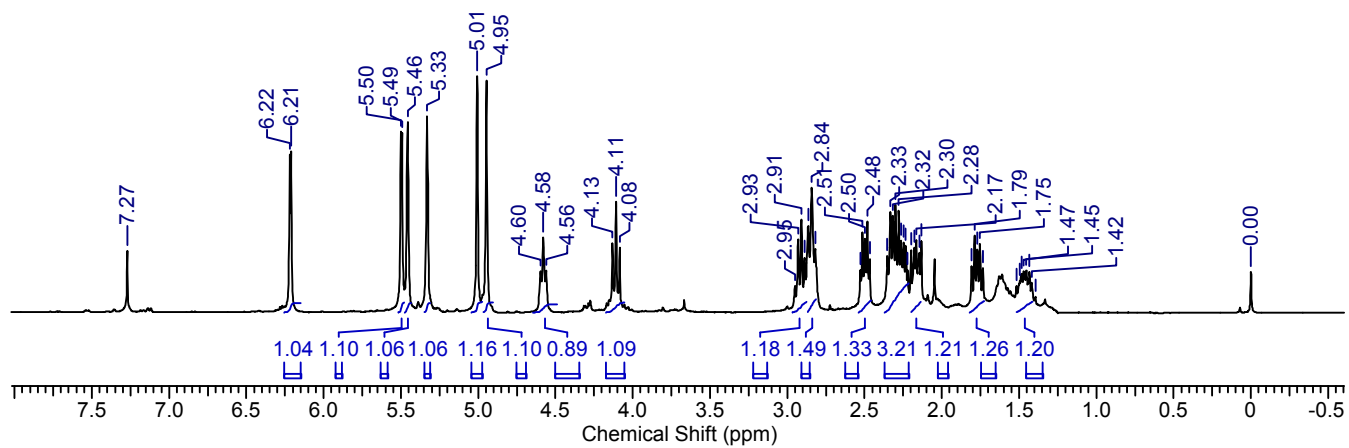
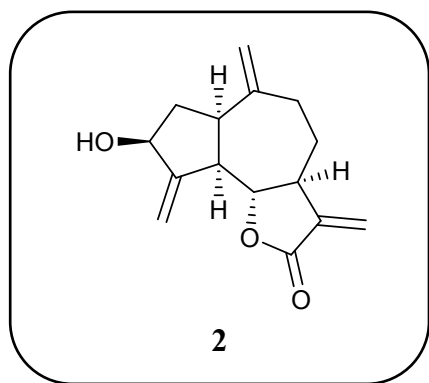


HR-MS of Compound 1

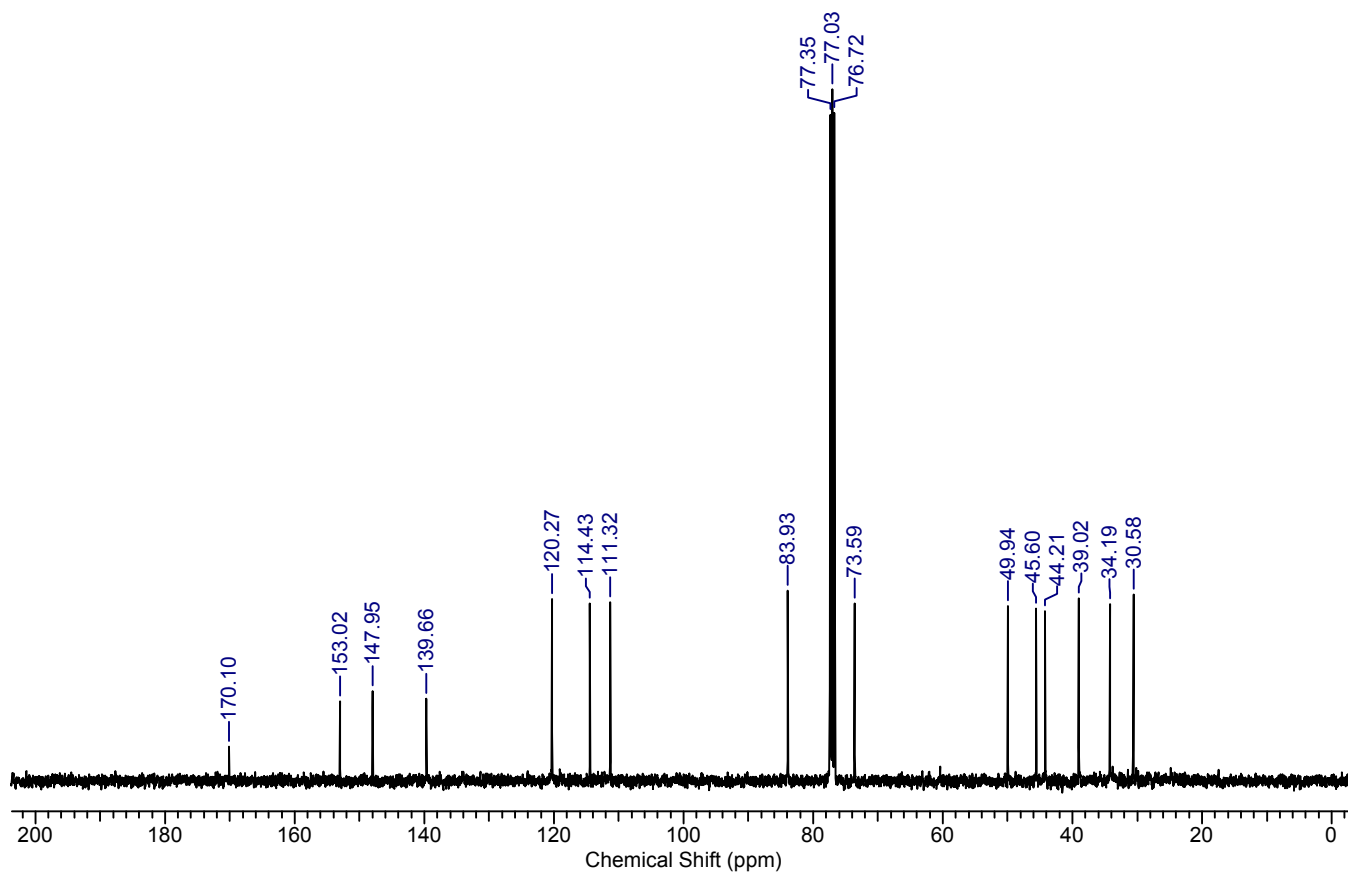
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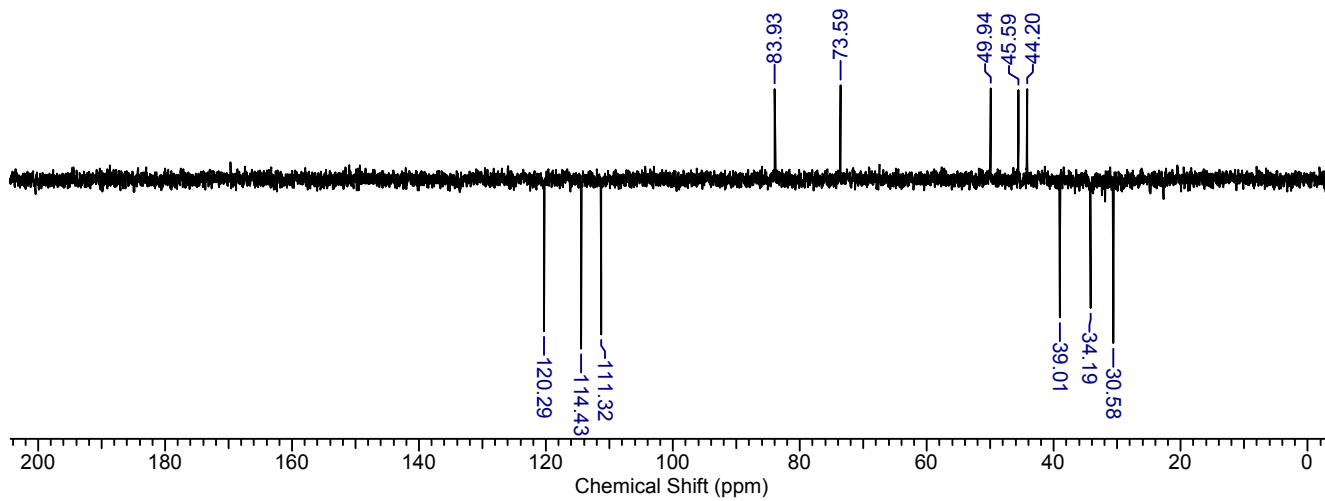
¹H NMR of Compound 2 (400 MHz, CDCl₃)



^{13}C NMR of Compound 2 (100 MHz, CDCl_3)

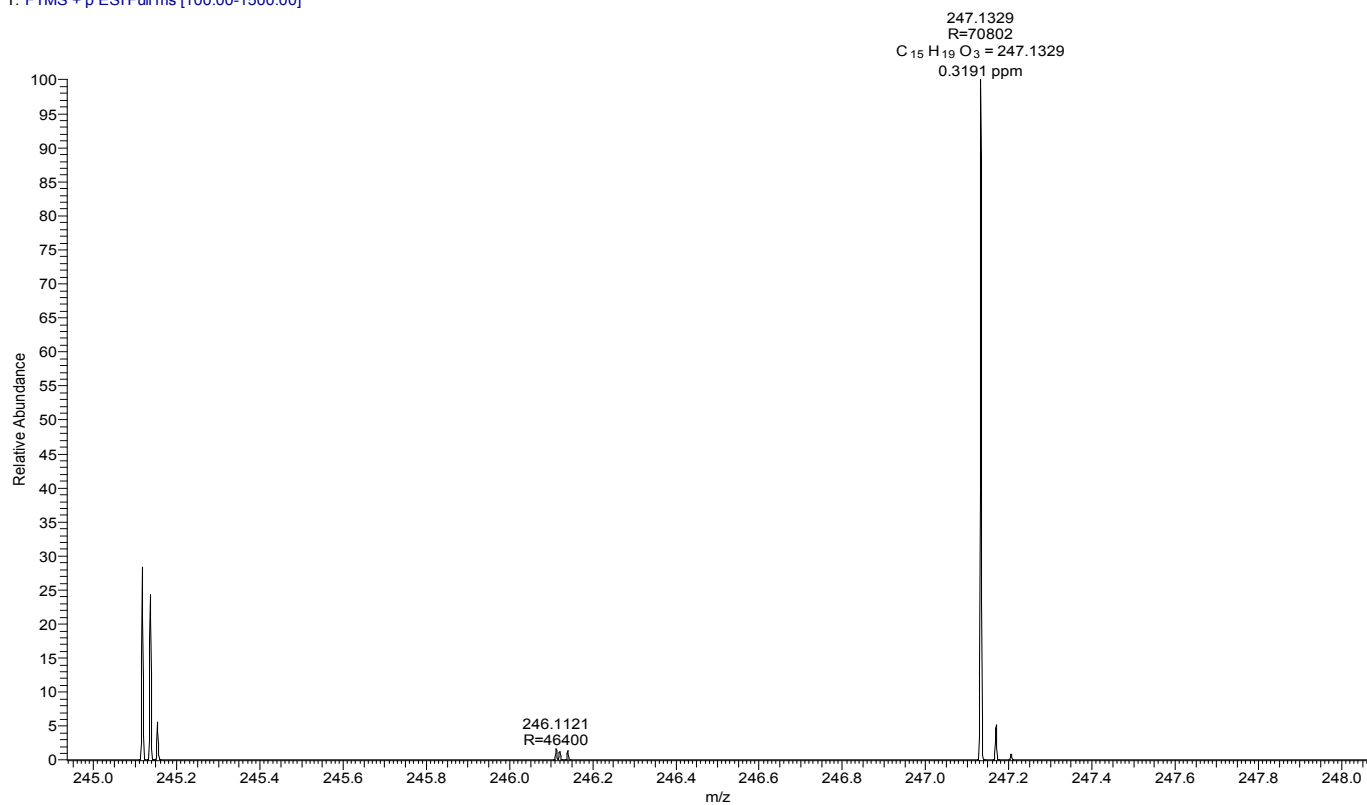


DEPT of Compound 2 (100 MHz, CDCl_3)

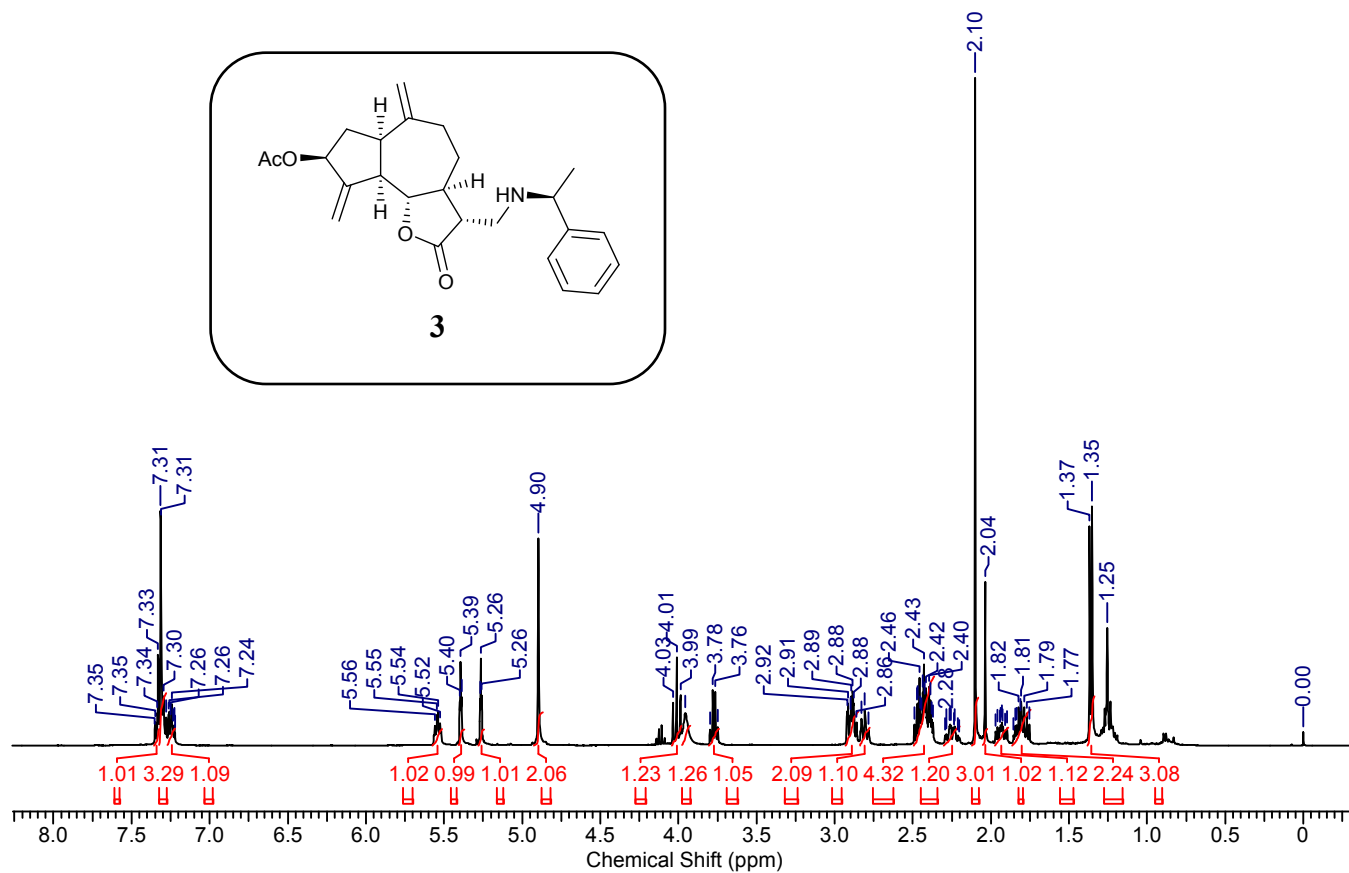
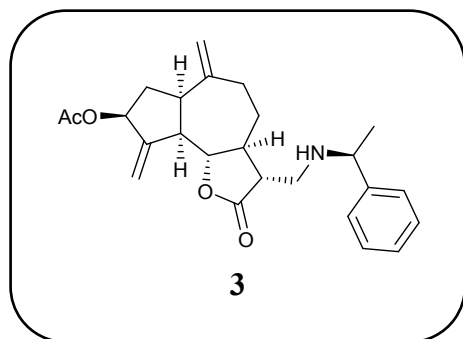


HR-MS of Compound 2

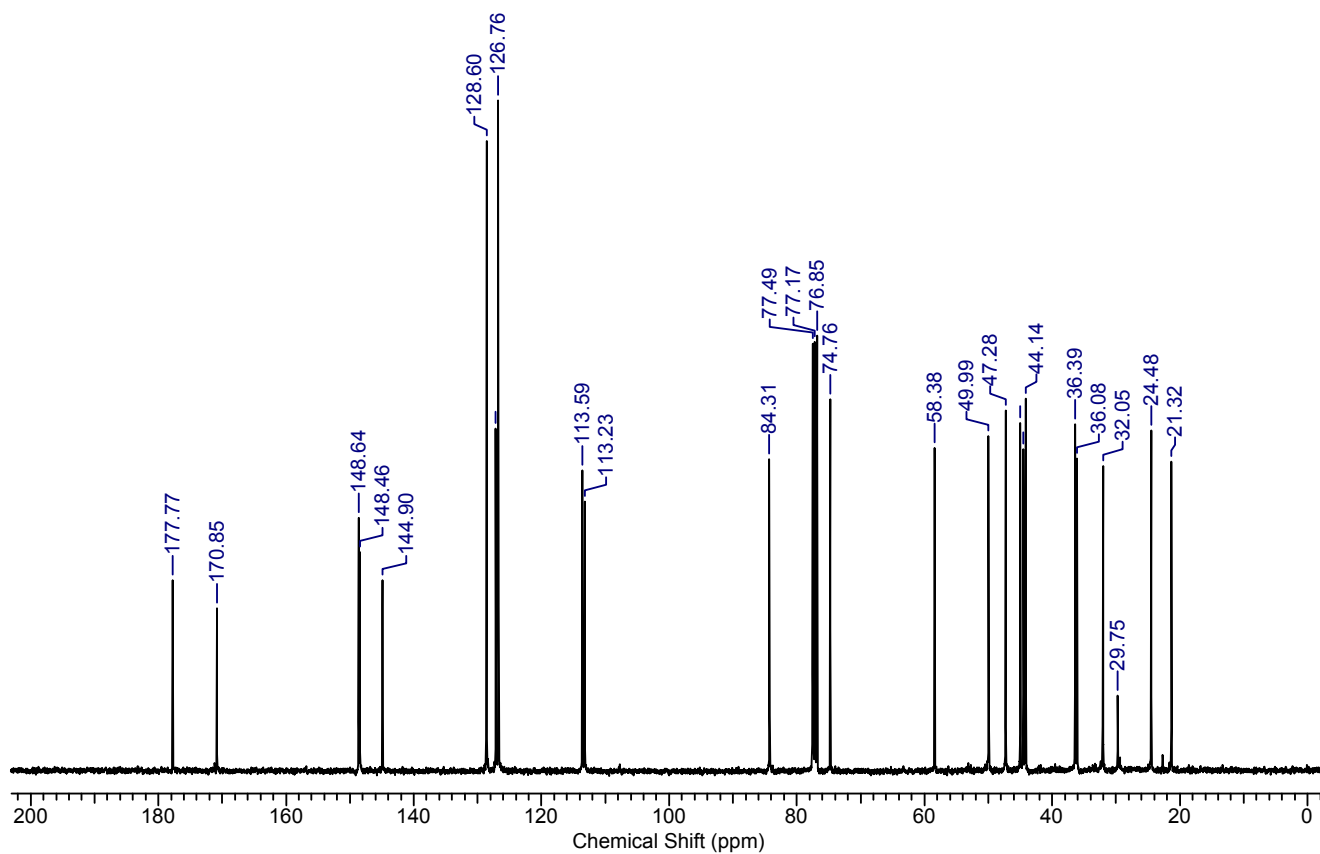
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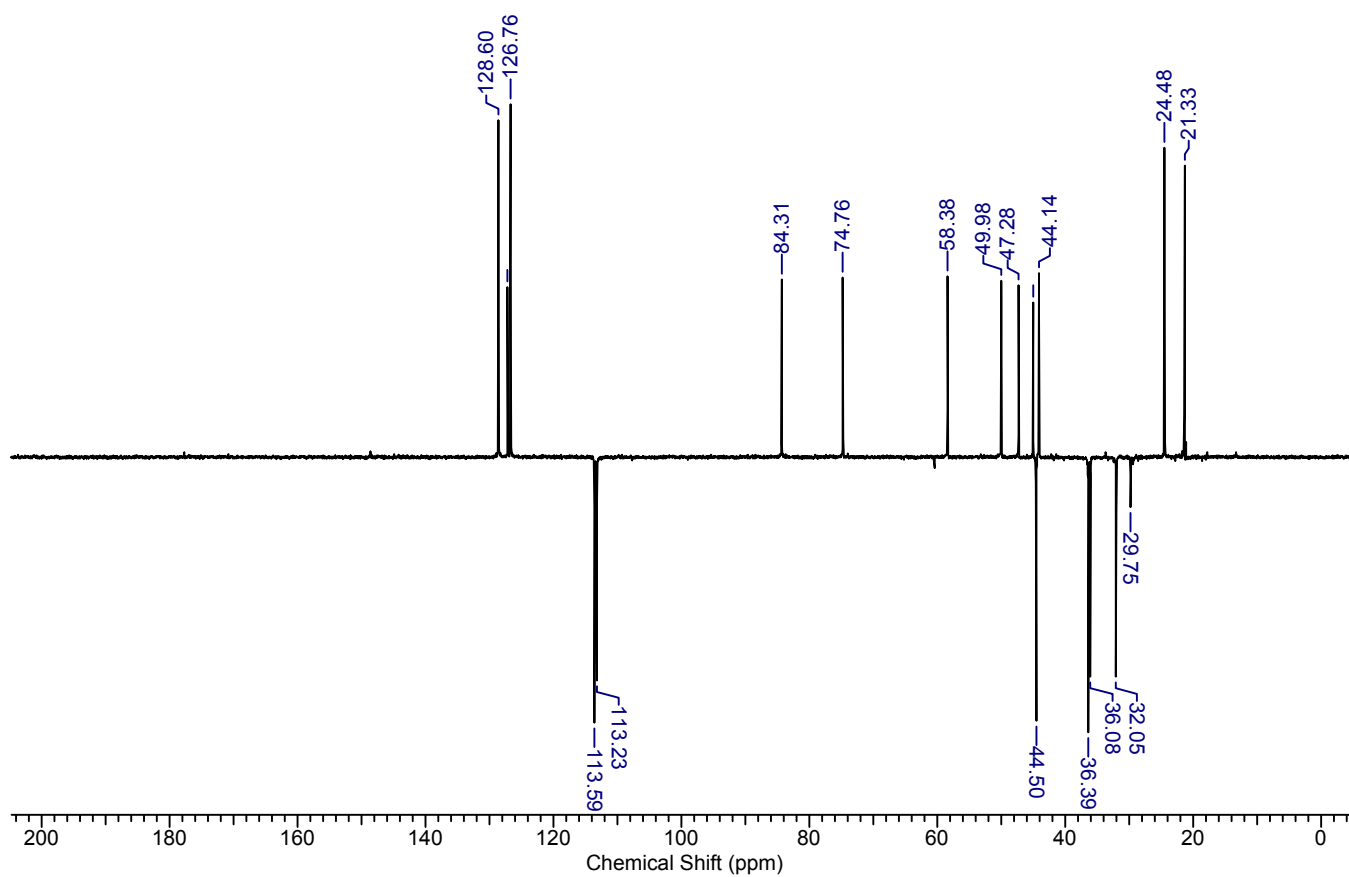
¹H NMR of Compound 3 (400 MHz, CDCl₃)



^{13}C NMR of Compound 3 (100 MHz, CDCl_3)



DEPT of Compound 3 (100 MHz, CDCl_3)

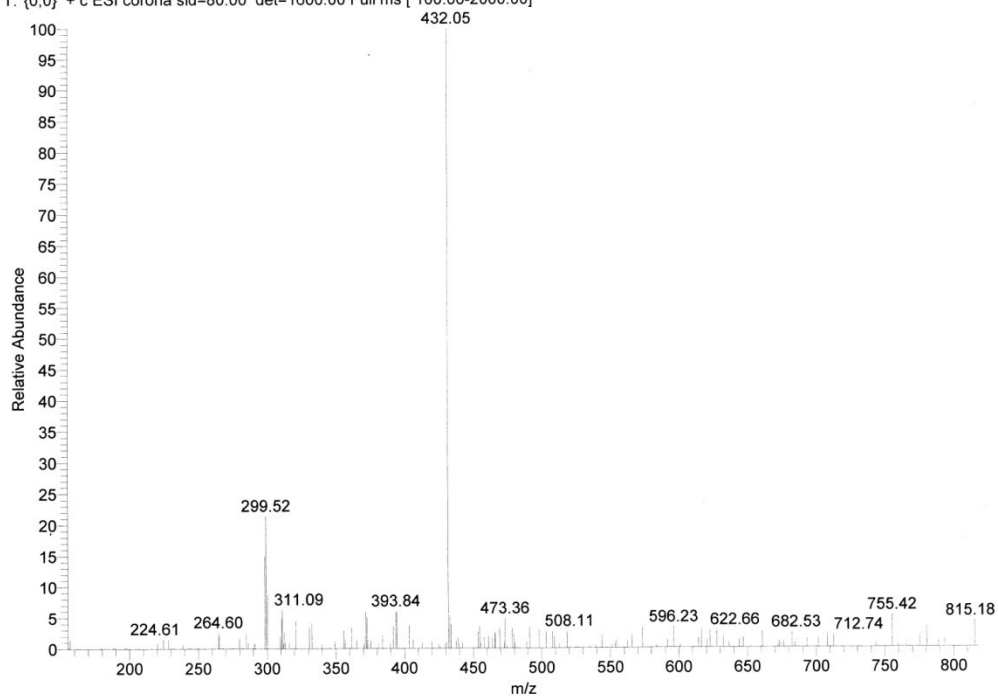


LC-MS of Compound 3

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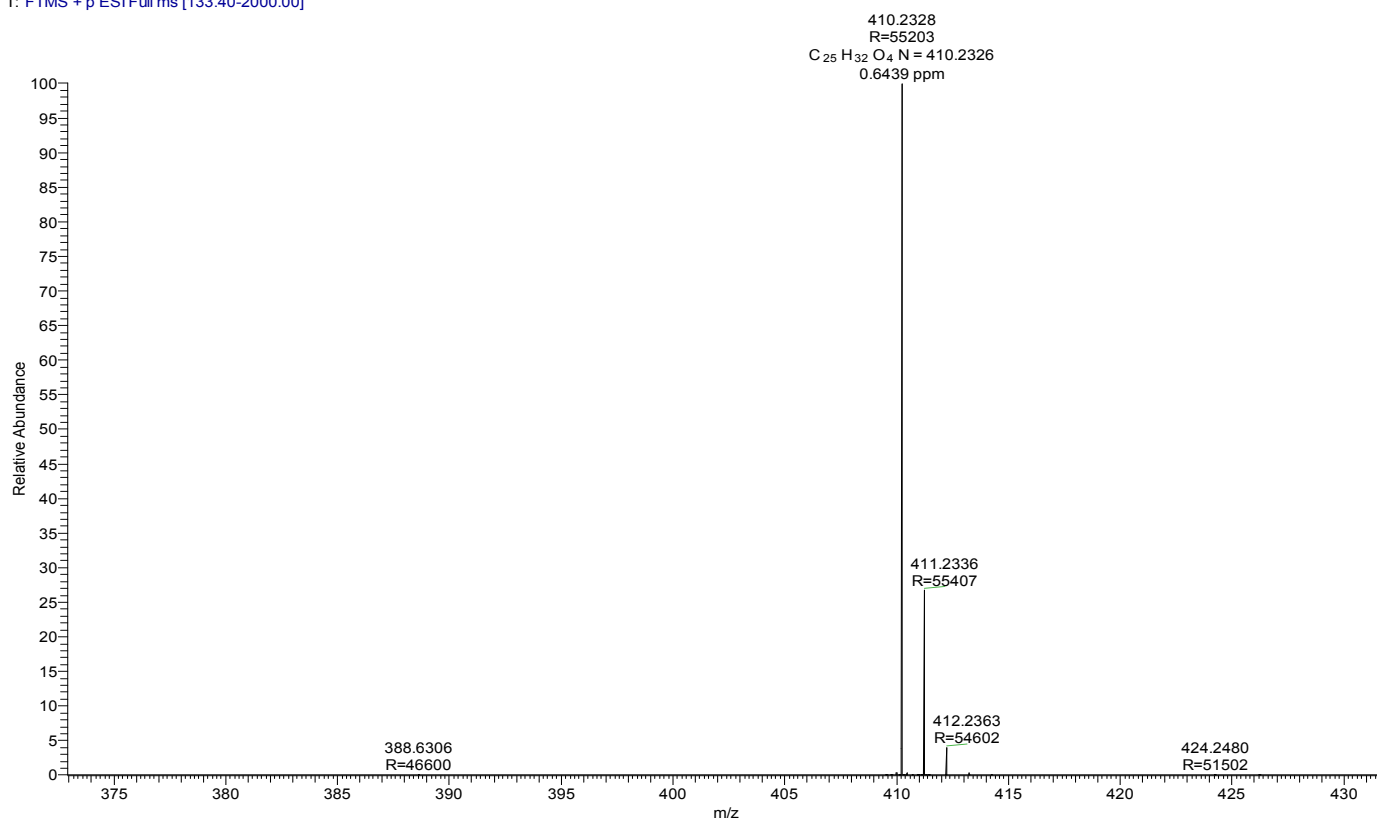
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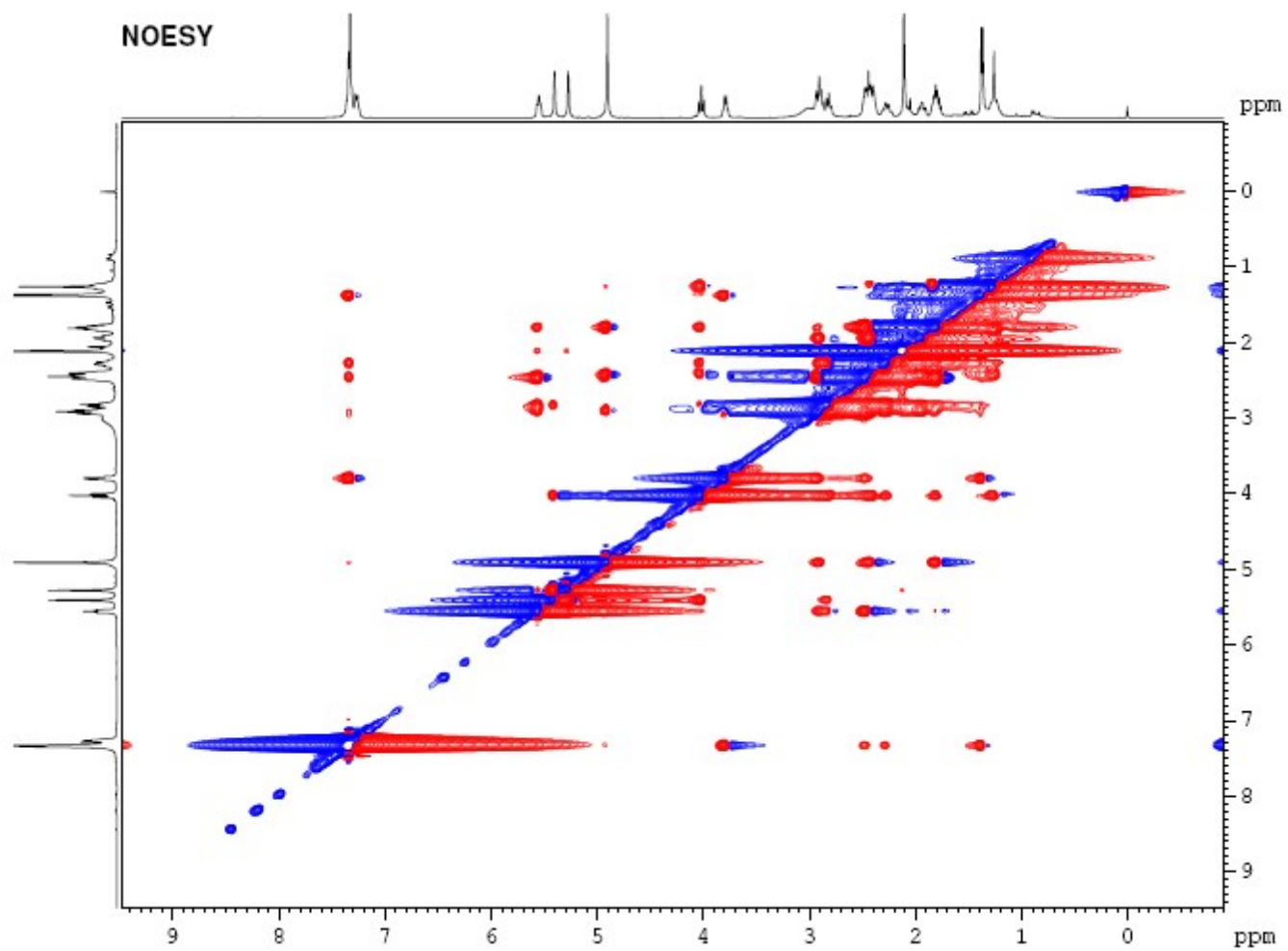


HR-MS of Compound 3

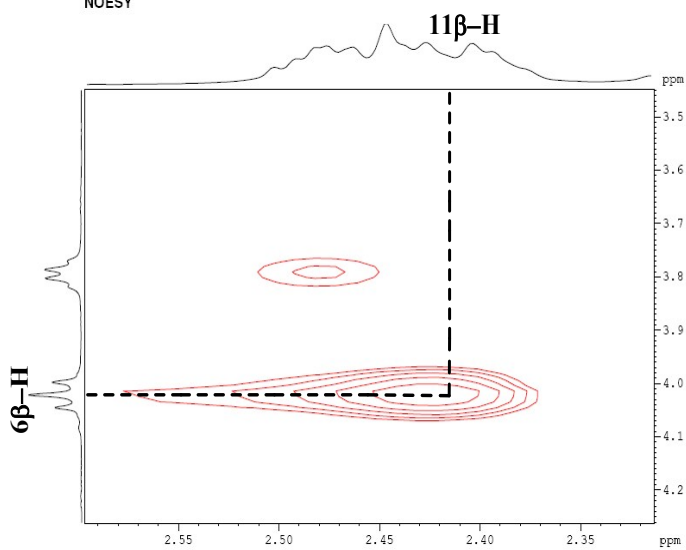
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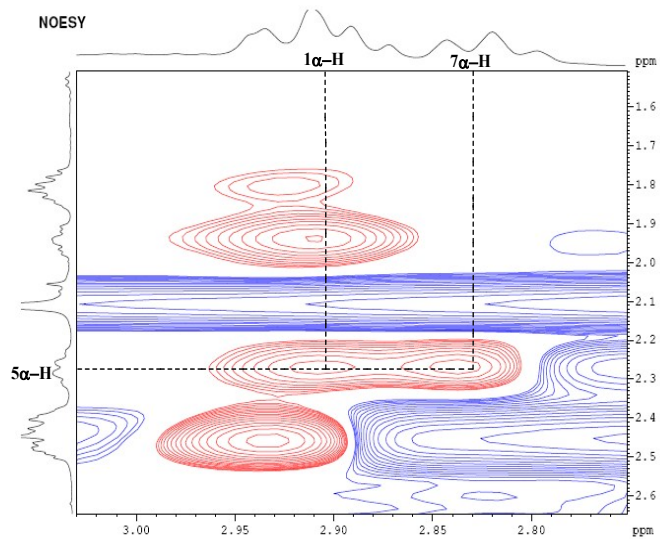
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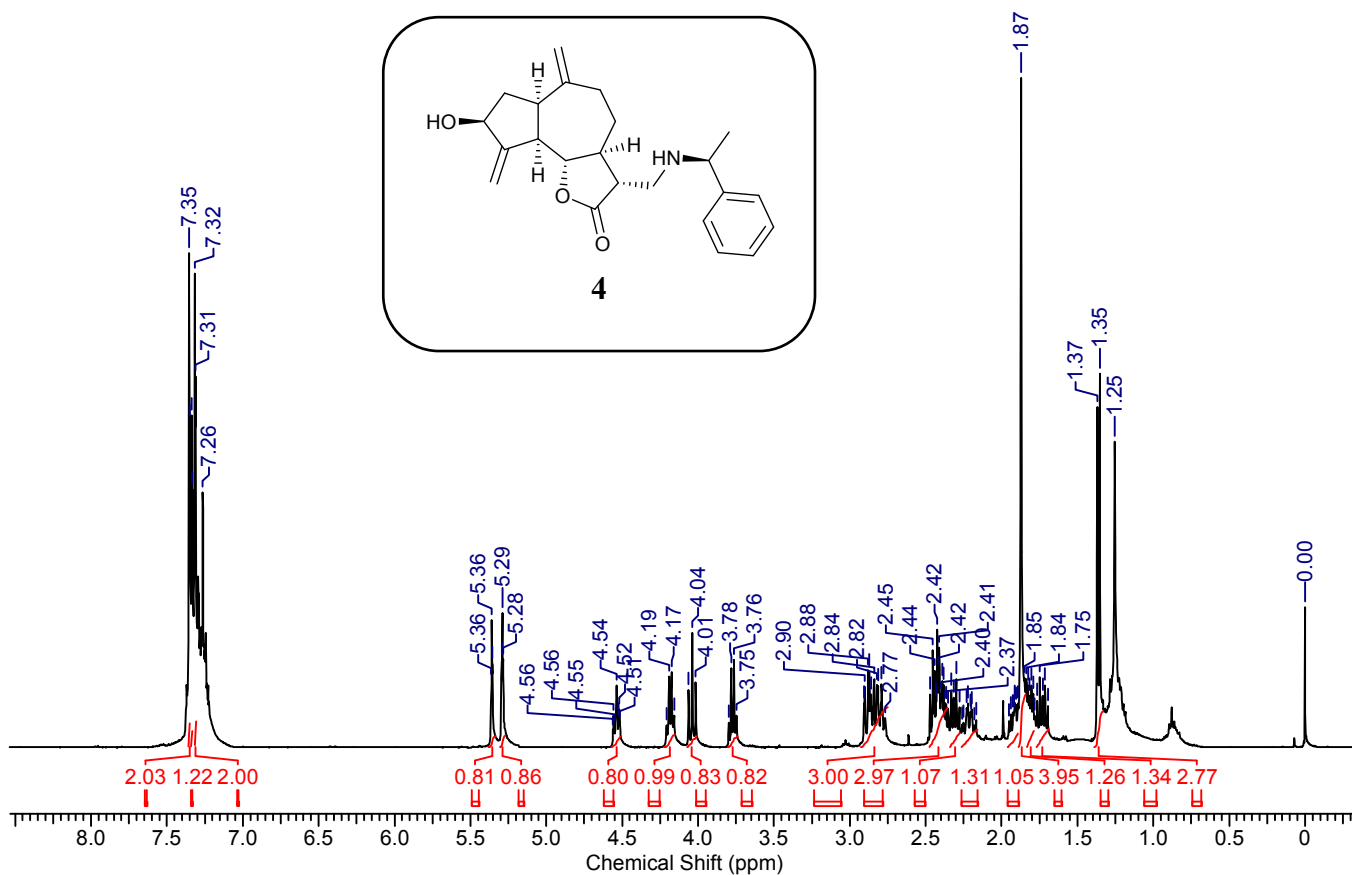
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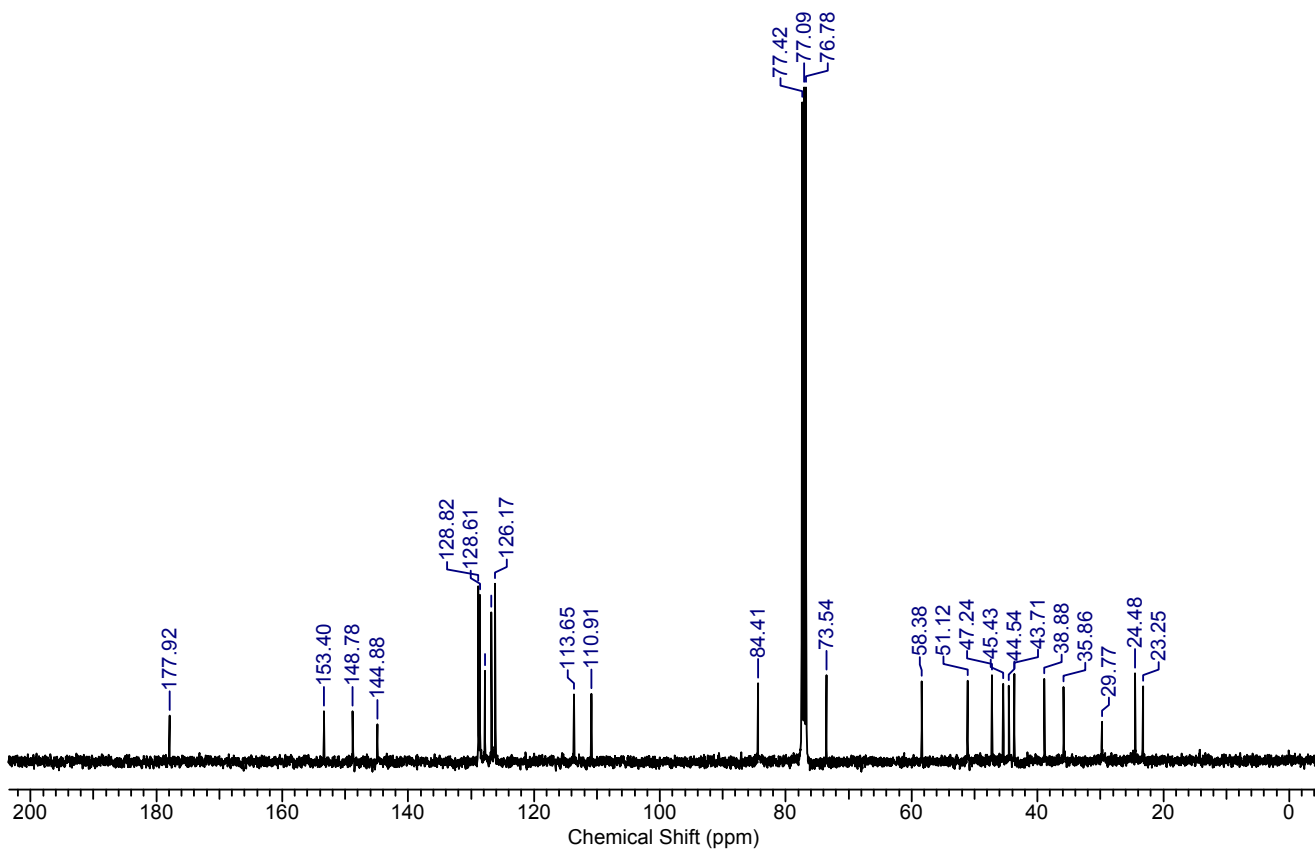
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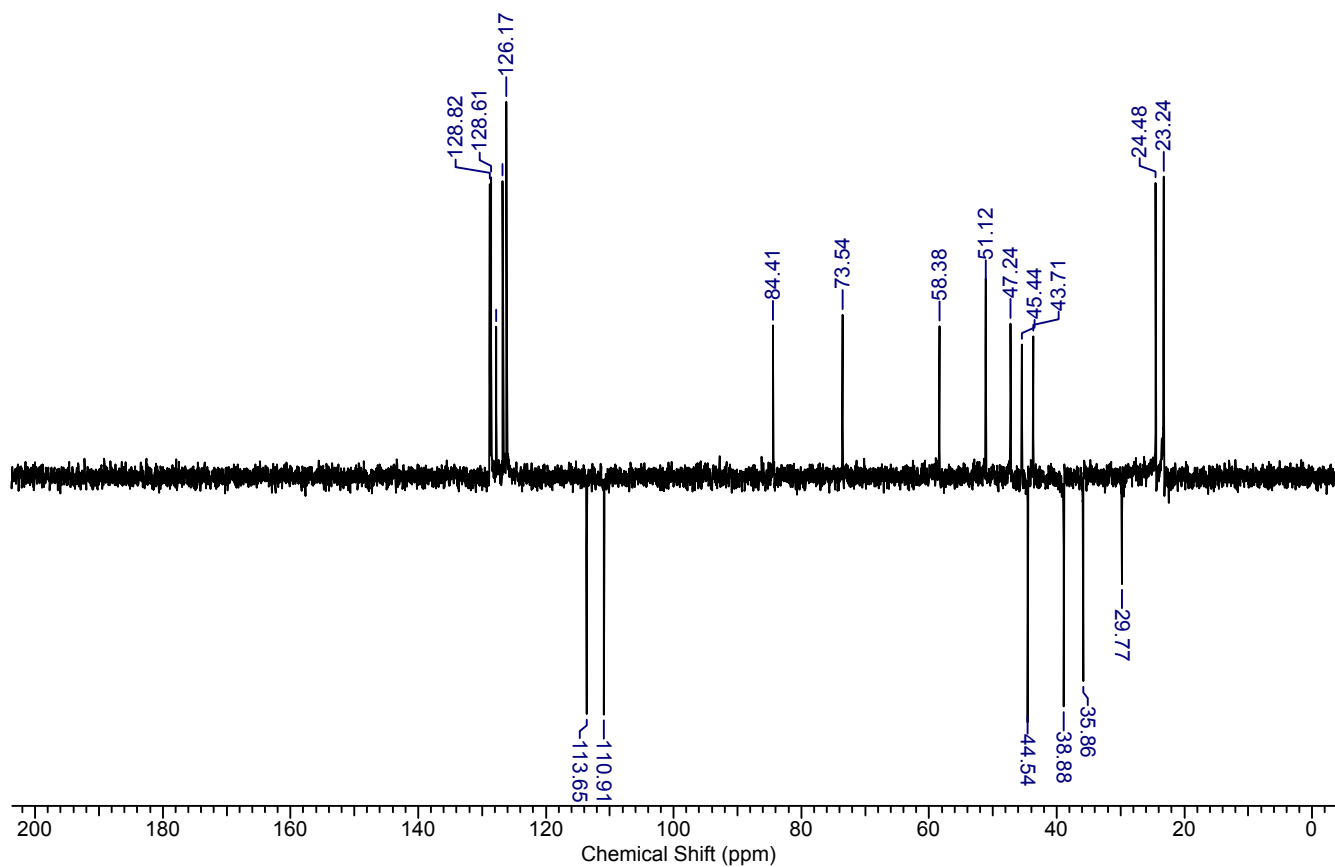
¹H NMR of Compound 4 (400 MHz, CDCl₃)



¹³C NMR of Compound 4 (100 MHz, CDCl₃)



DEPT of Compound 4 (100 MHz, CDCl₃)

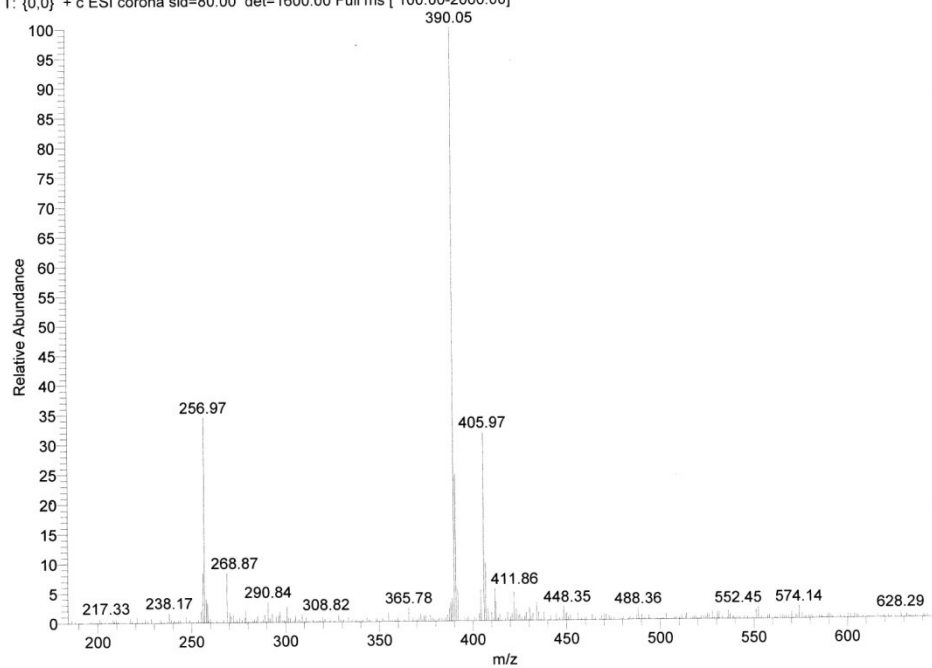


LC-MS of Compound 4

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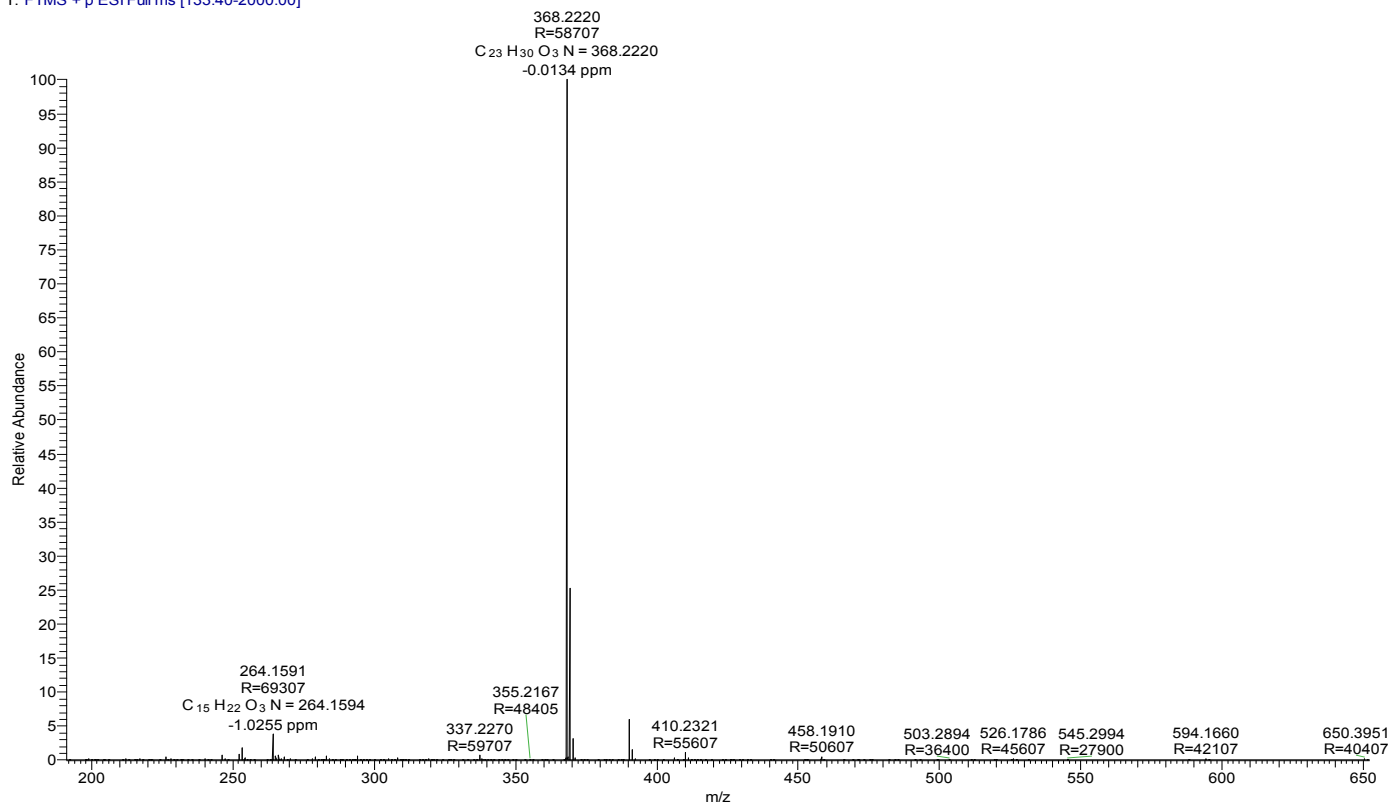
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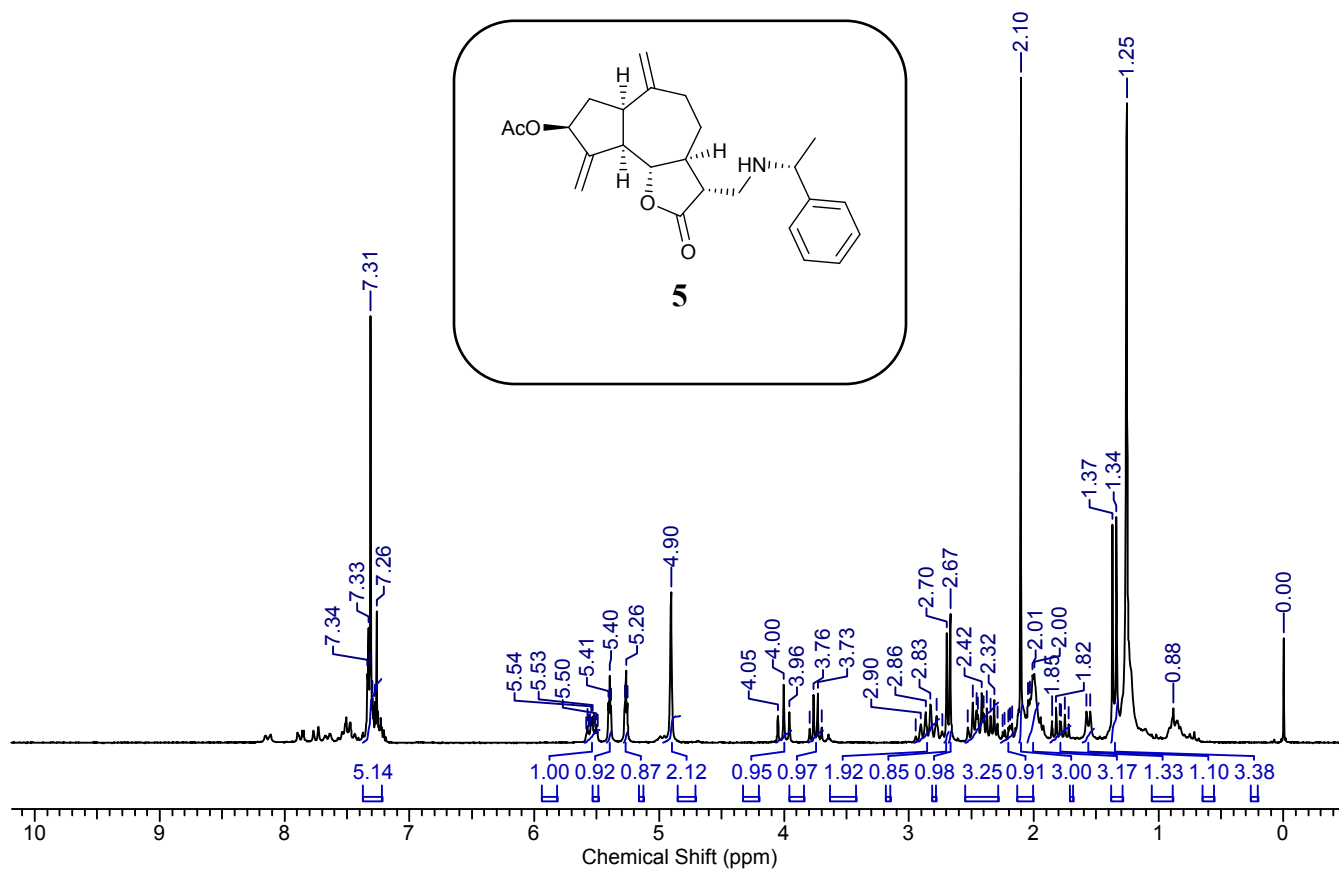


HR-MS of Compound 4

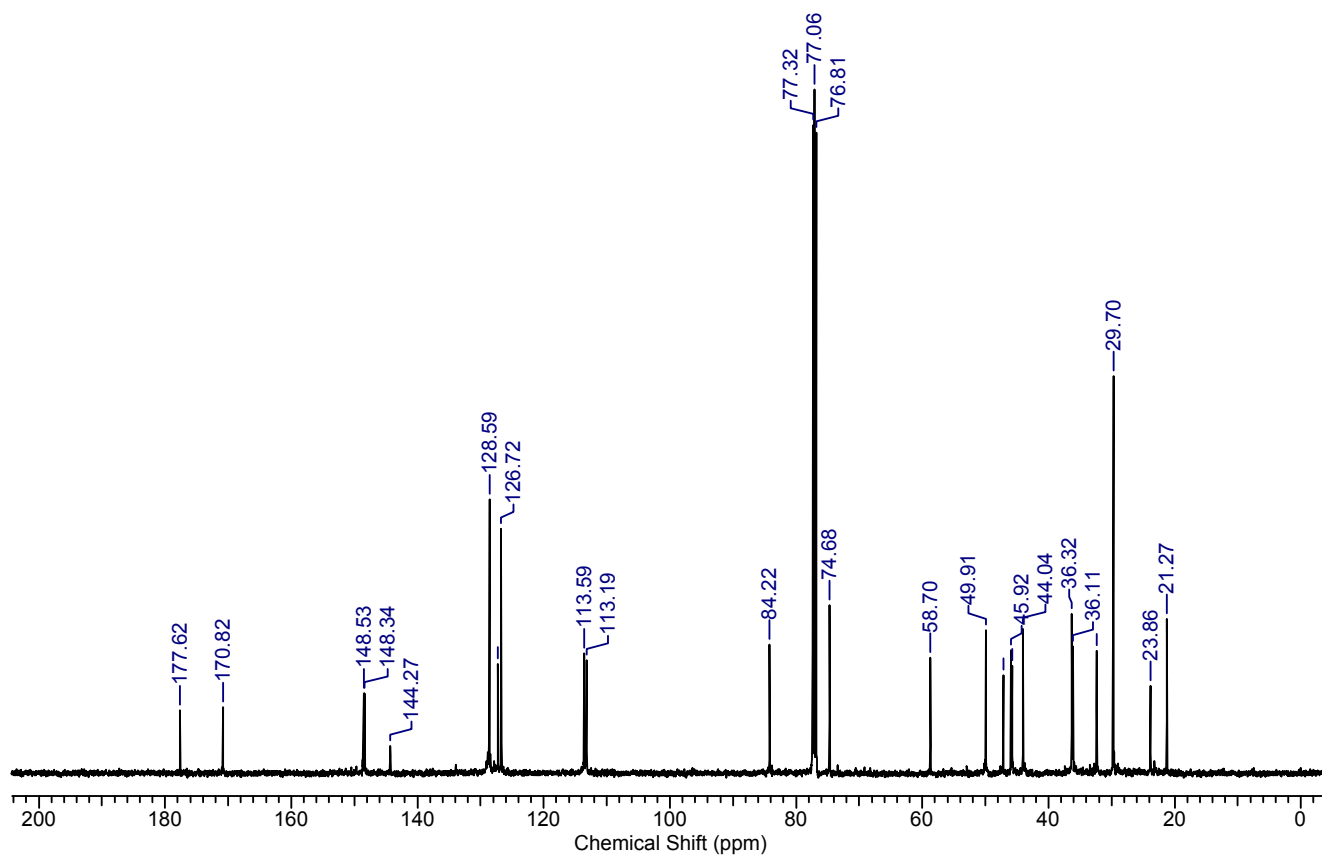
IS-295-B_160308160222 #86 RT: 0.38 AV: 1 NL: 5.63E9
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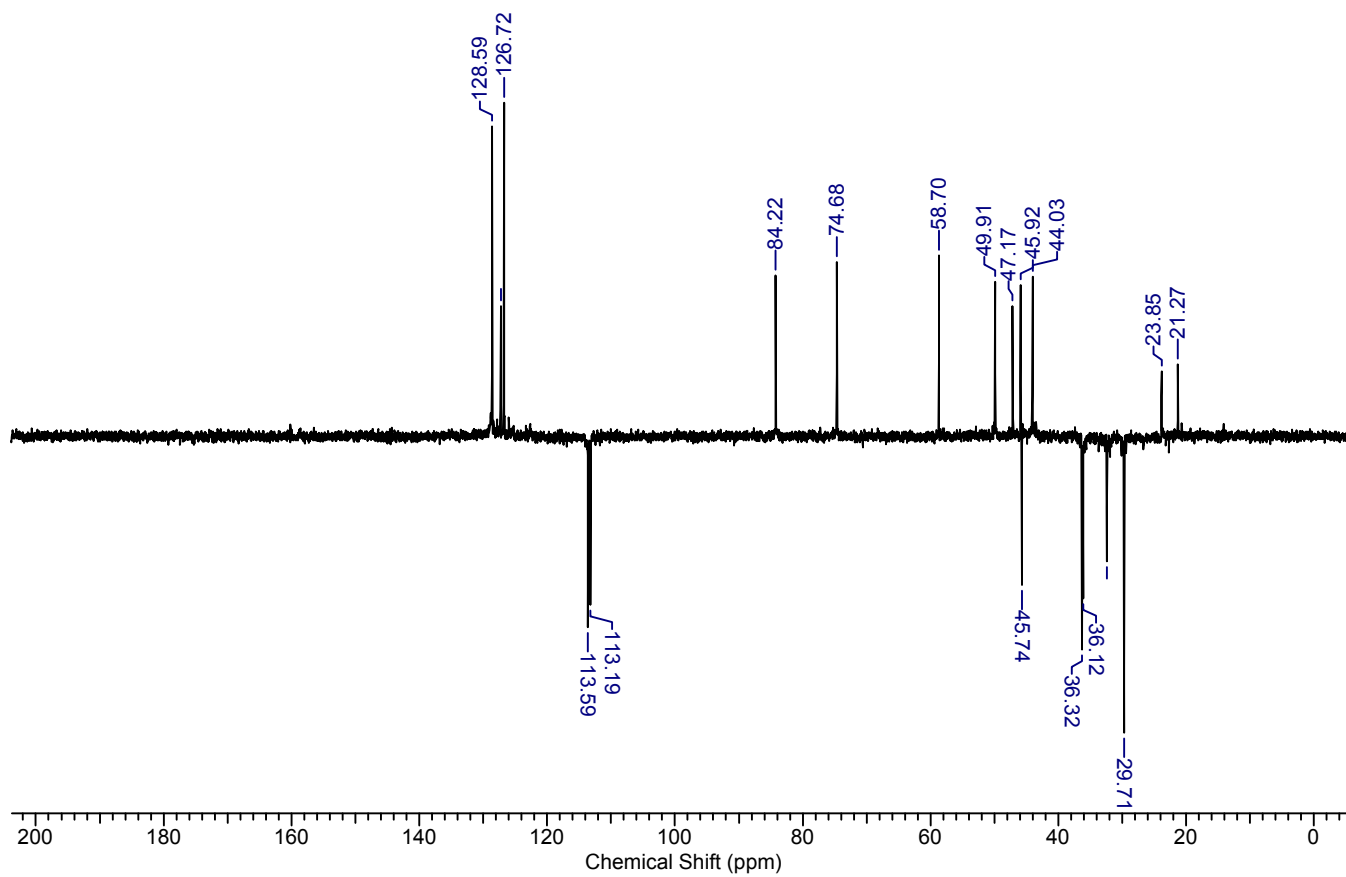
¹H NMR of Compound 5 (200 MHz, CDCl₃)



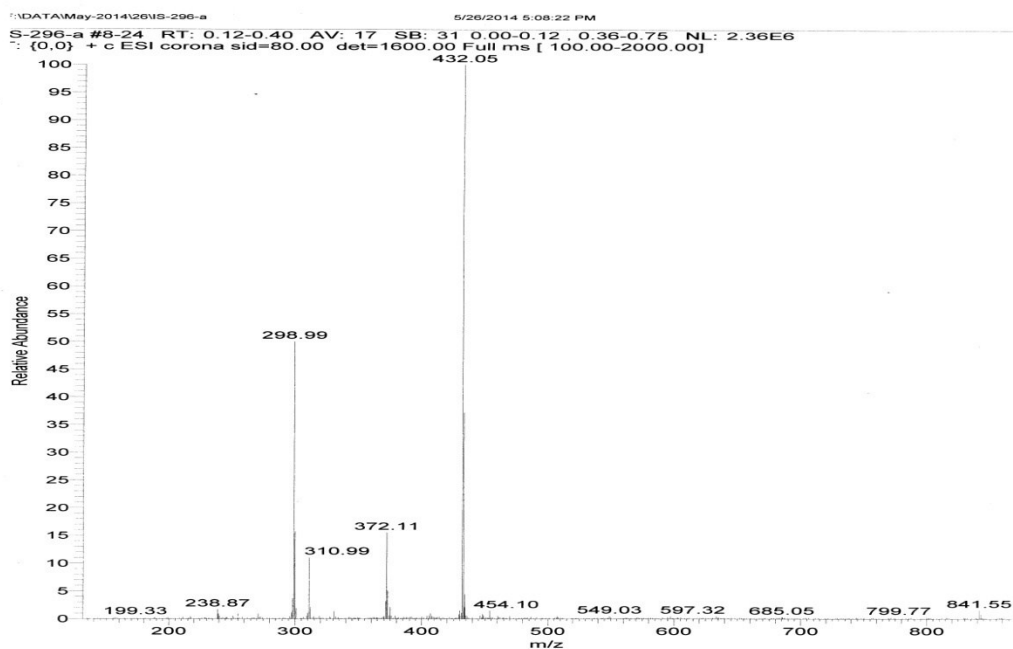
^{13}C NMR of Compound 5 (125 MHz, CDCl_3)



DEPT of Compound 5 (25 MHz, CDCl_3)

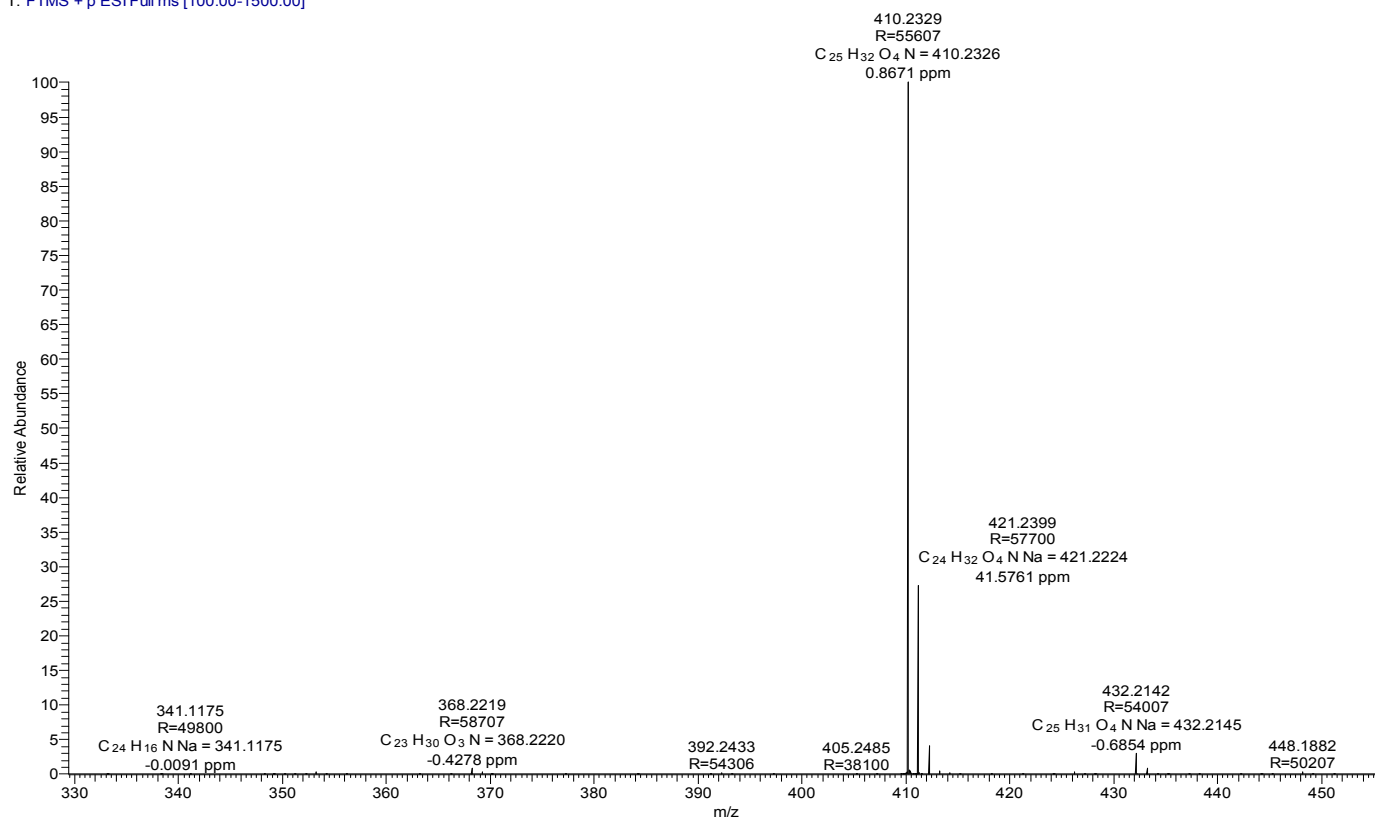


LC-MS of Compound 5

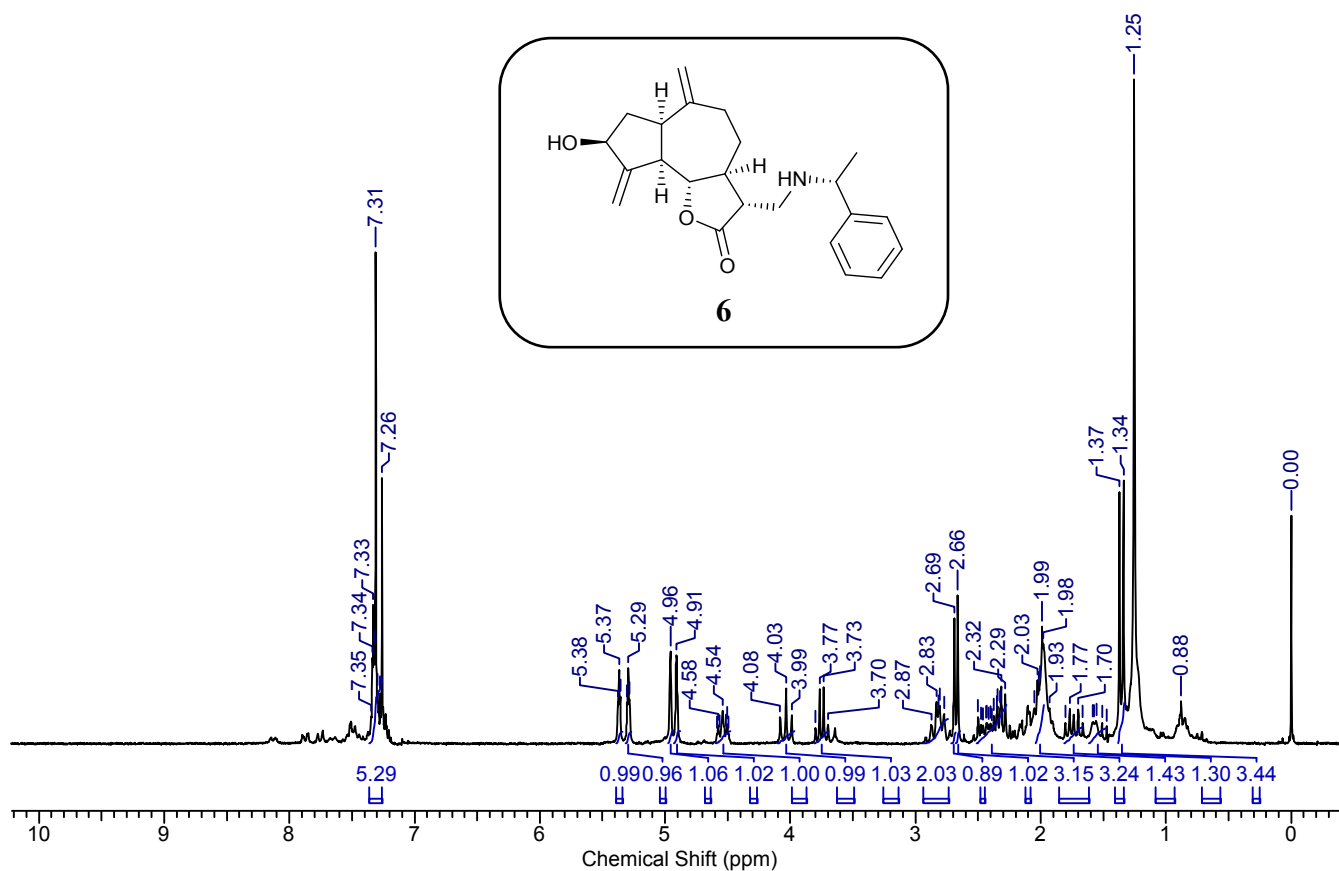


HR-MS of Compound 5

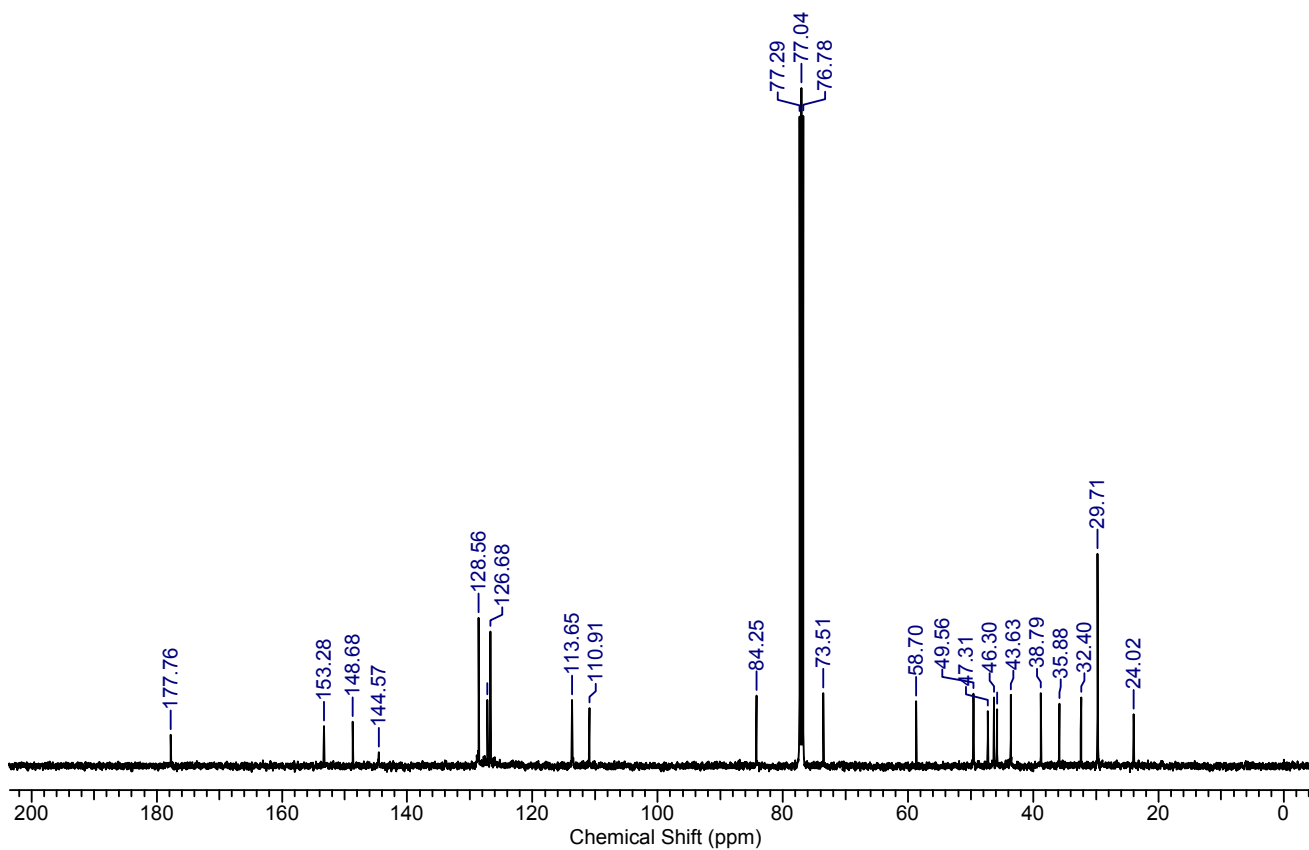
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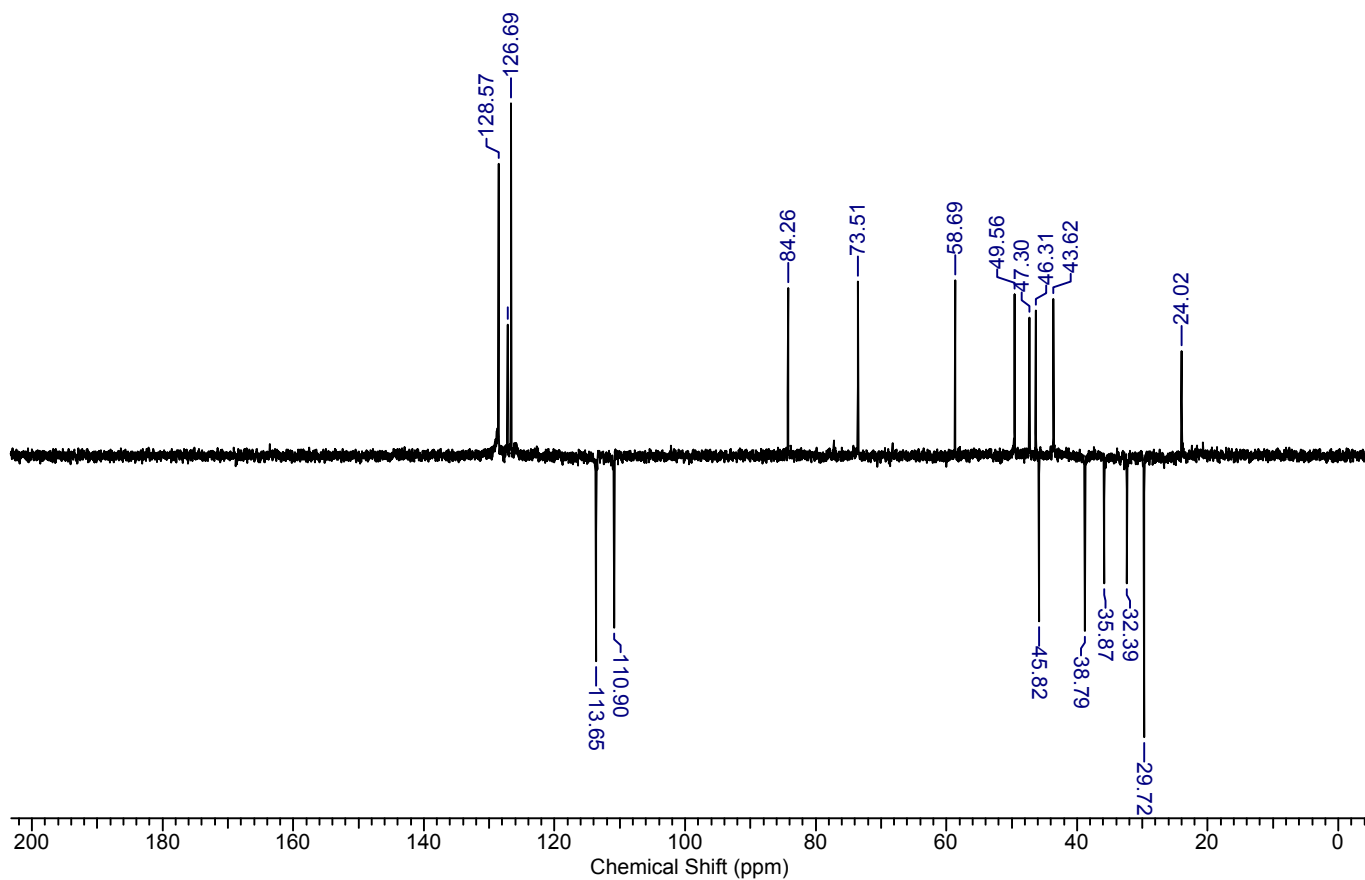
¹H NMR of Compound 6 (200 MHz, CDCl₃)



¹³C NMR of Compound 6 (125 MHz, CDCl₃)



DEPT of Compound 6 (125 MHz, CDCl₃)

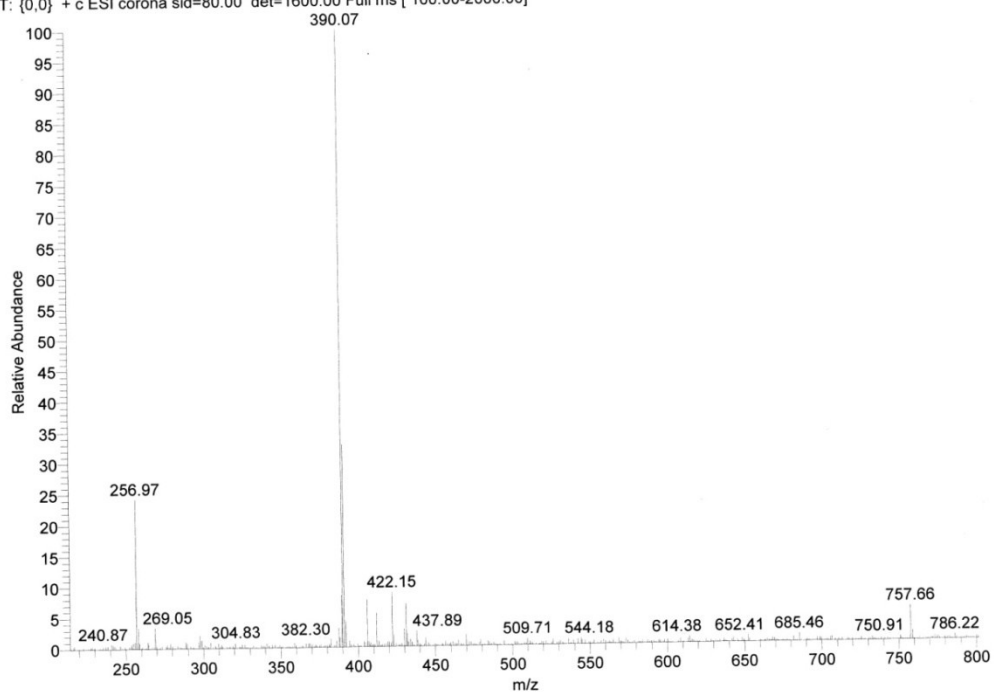


LC-MS of Compound 6

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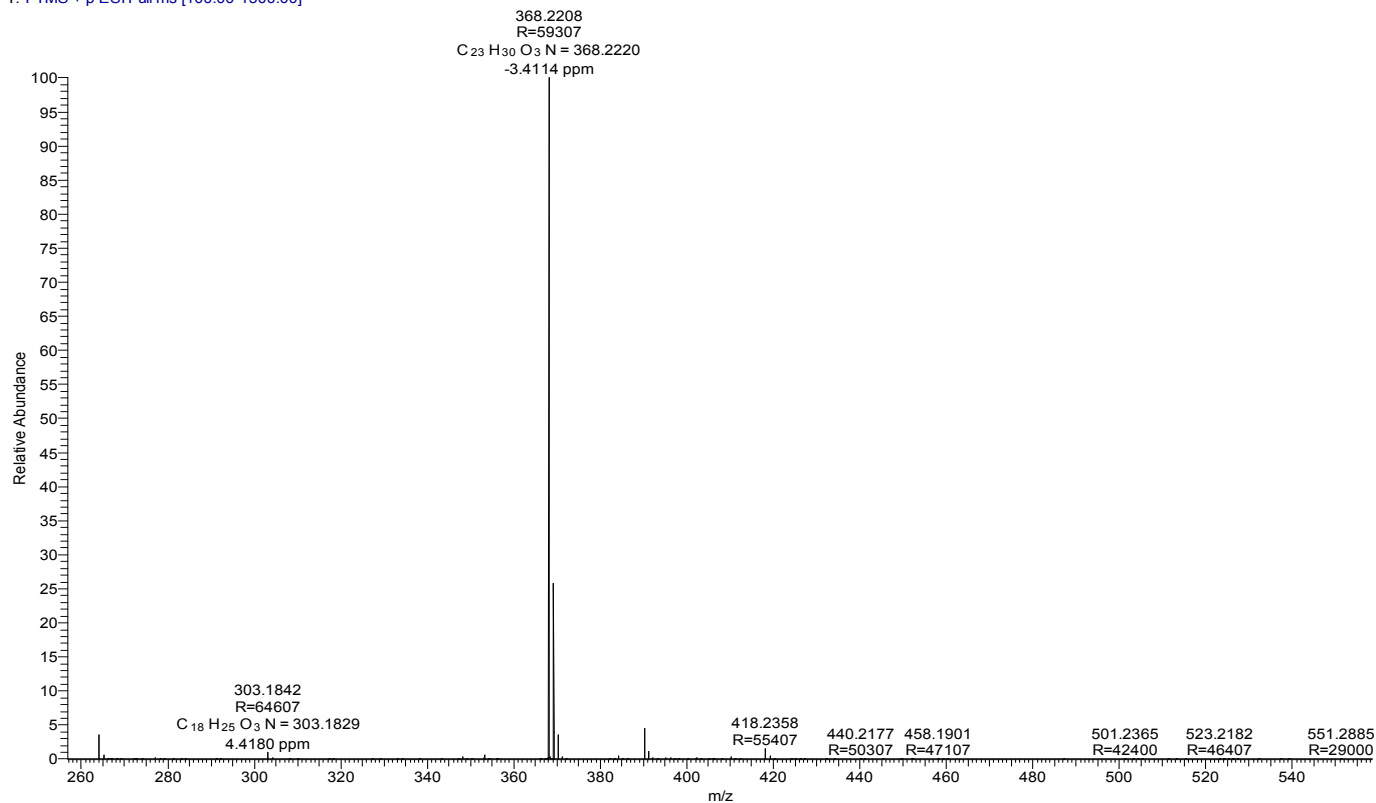
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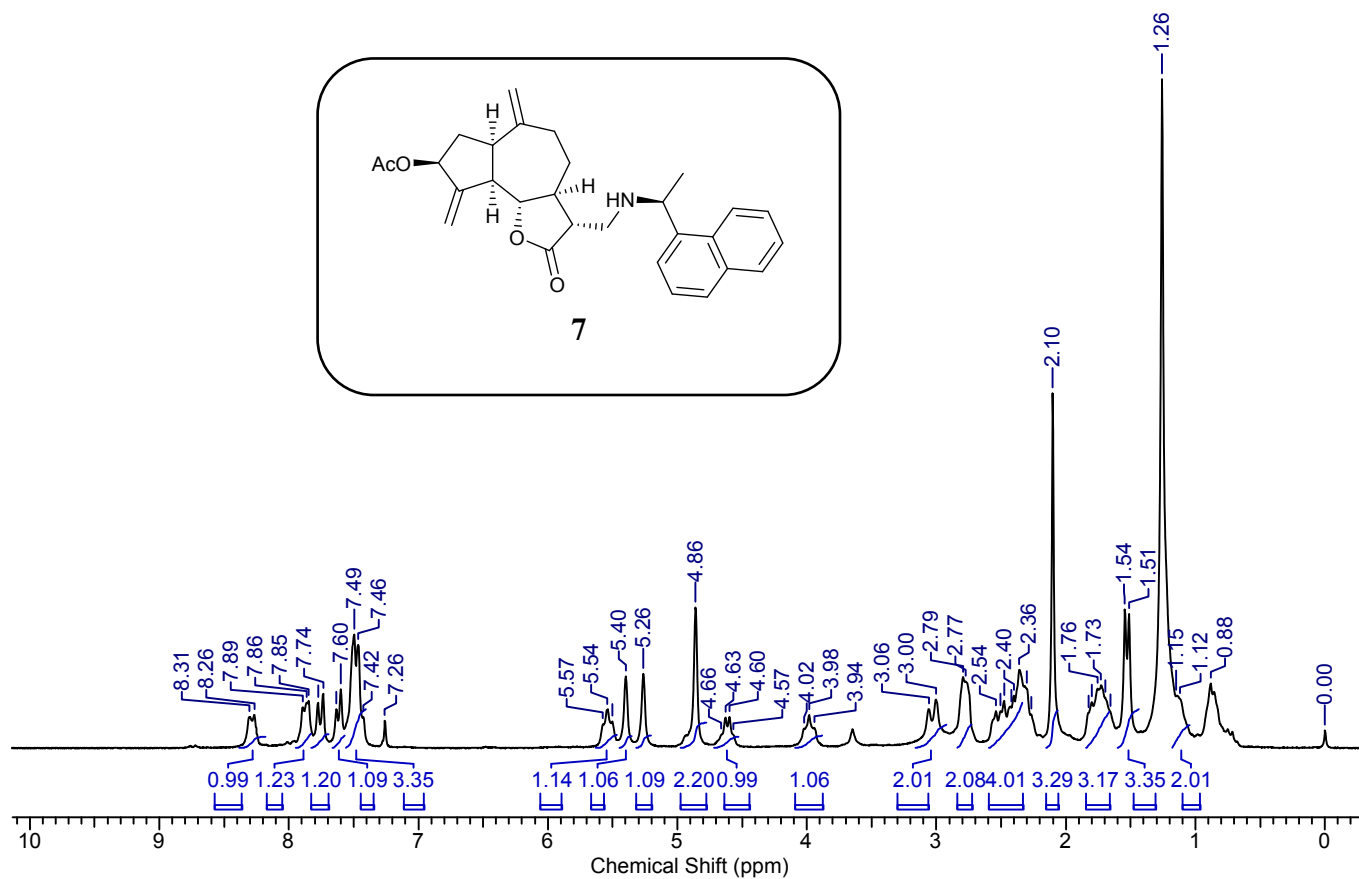
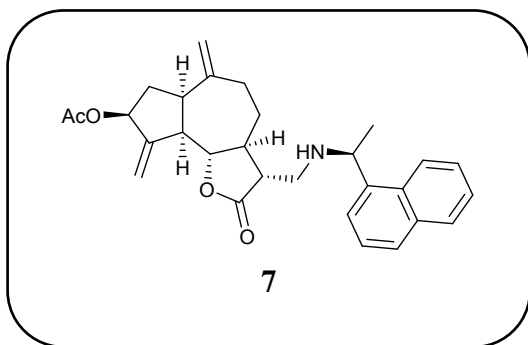


HR-MS of Compound 6

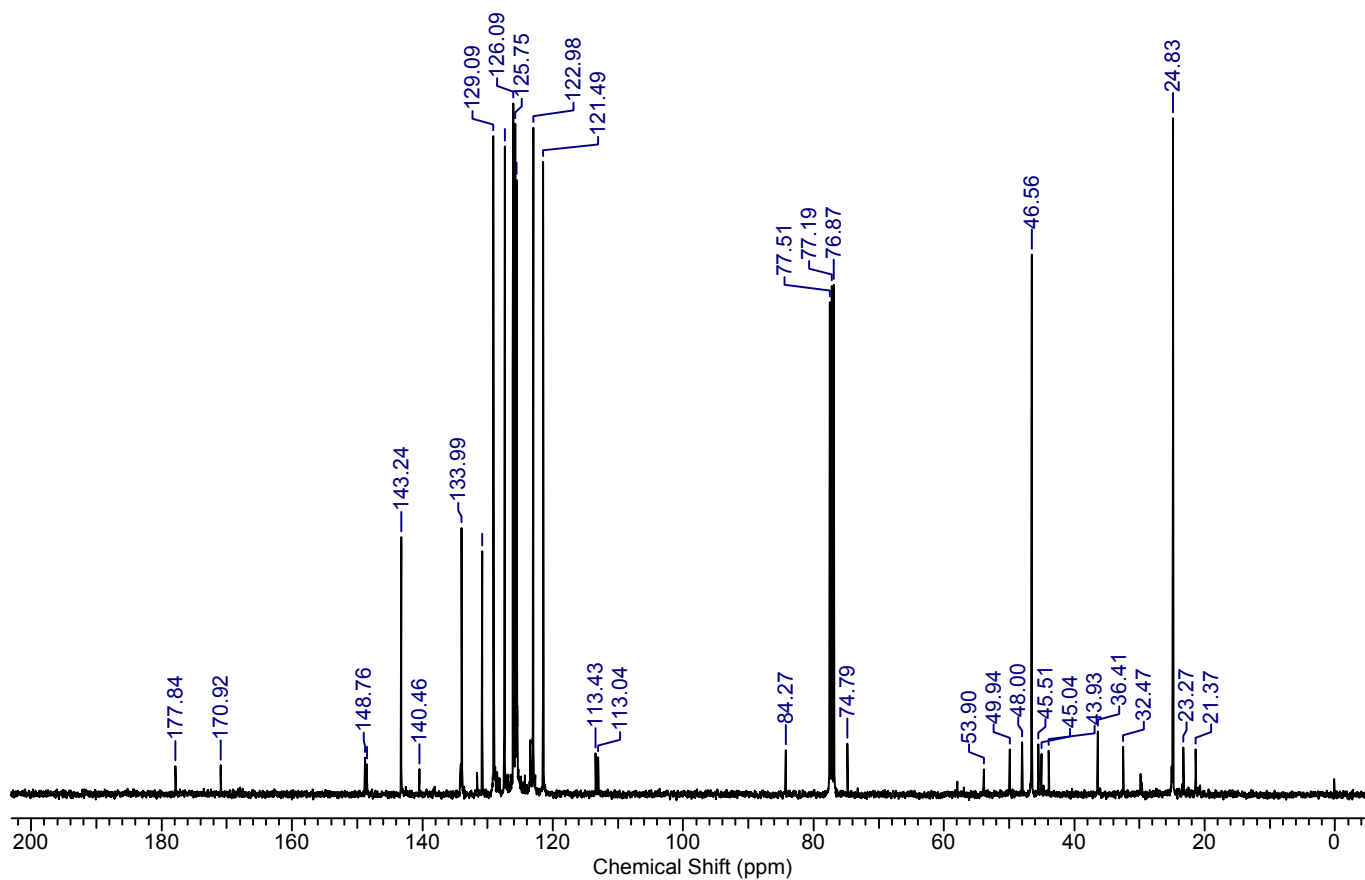
IS-296-B #79 RT: 0.35 AV: 1 NL: 8.77E9
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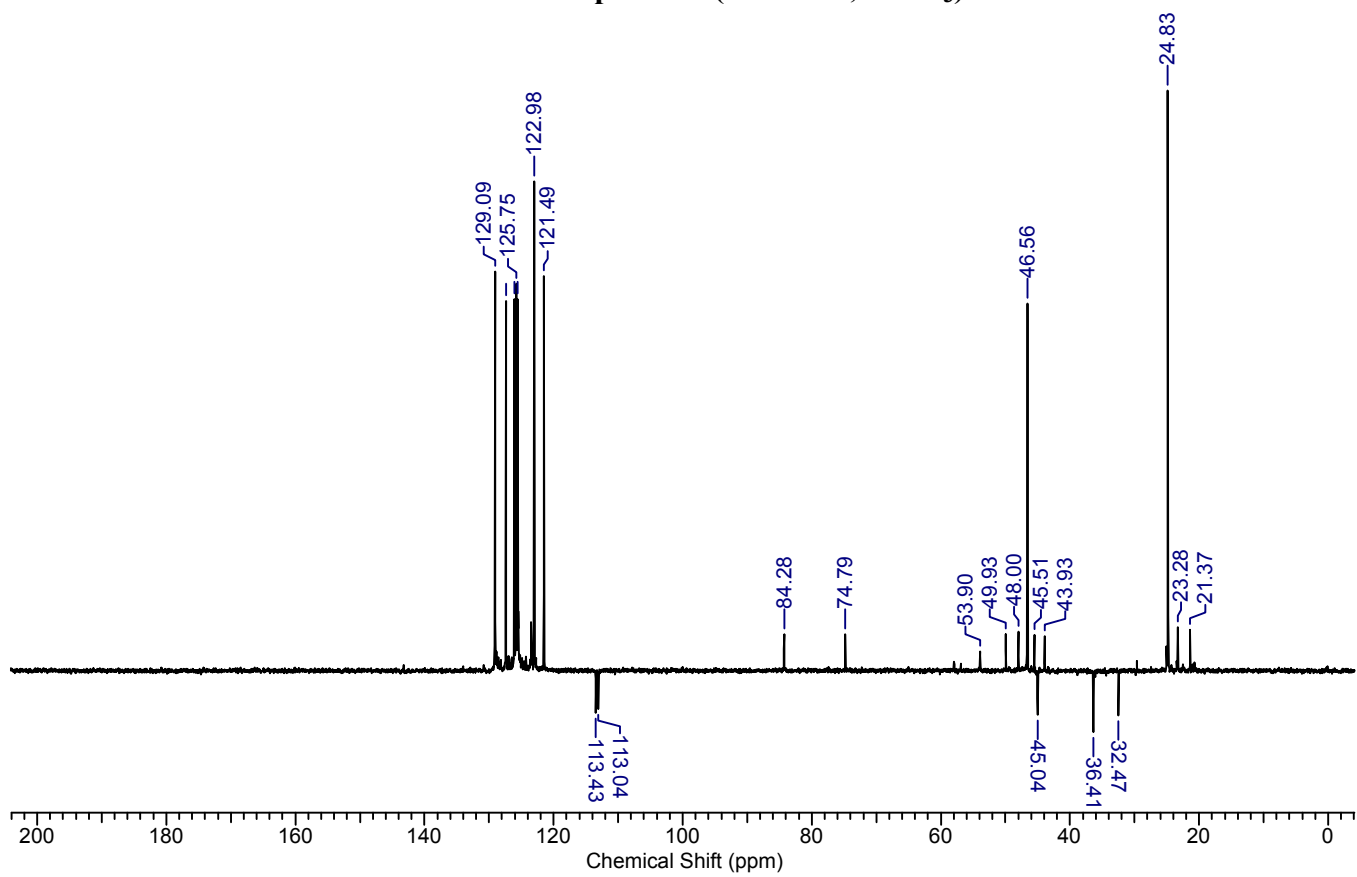
¹H NMR of Compound 7 (200 MHz, CDCl₃)



¹³C NMR of Compound 7 (100 MHz, CDCl₃)



DEPT of Compound 7 (100 MHz, CDCl₃)

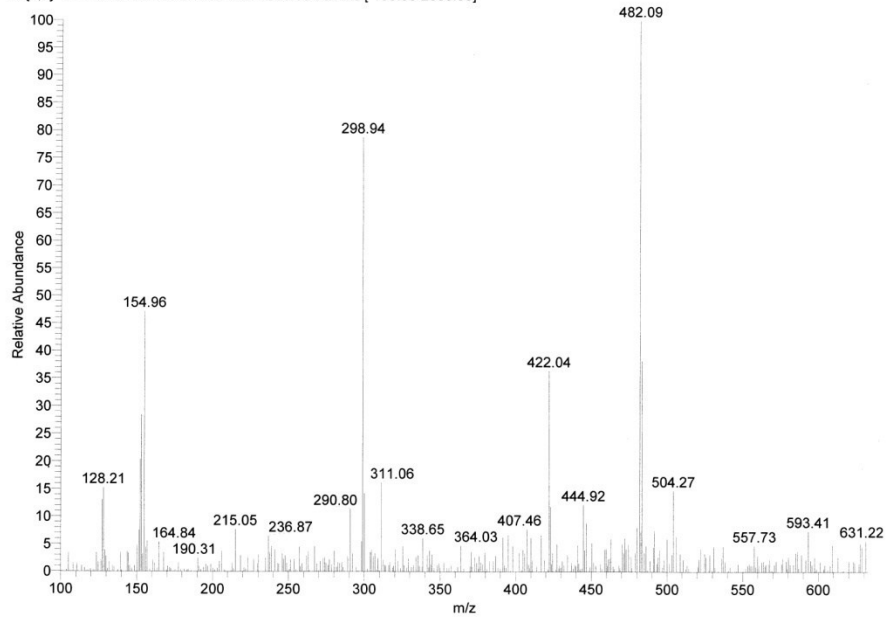


LC-MS of Compound 7

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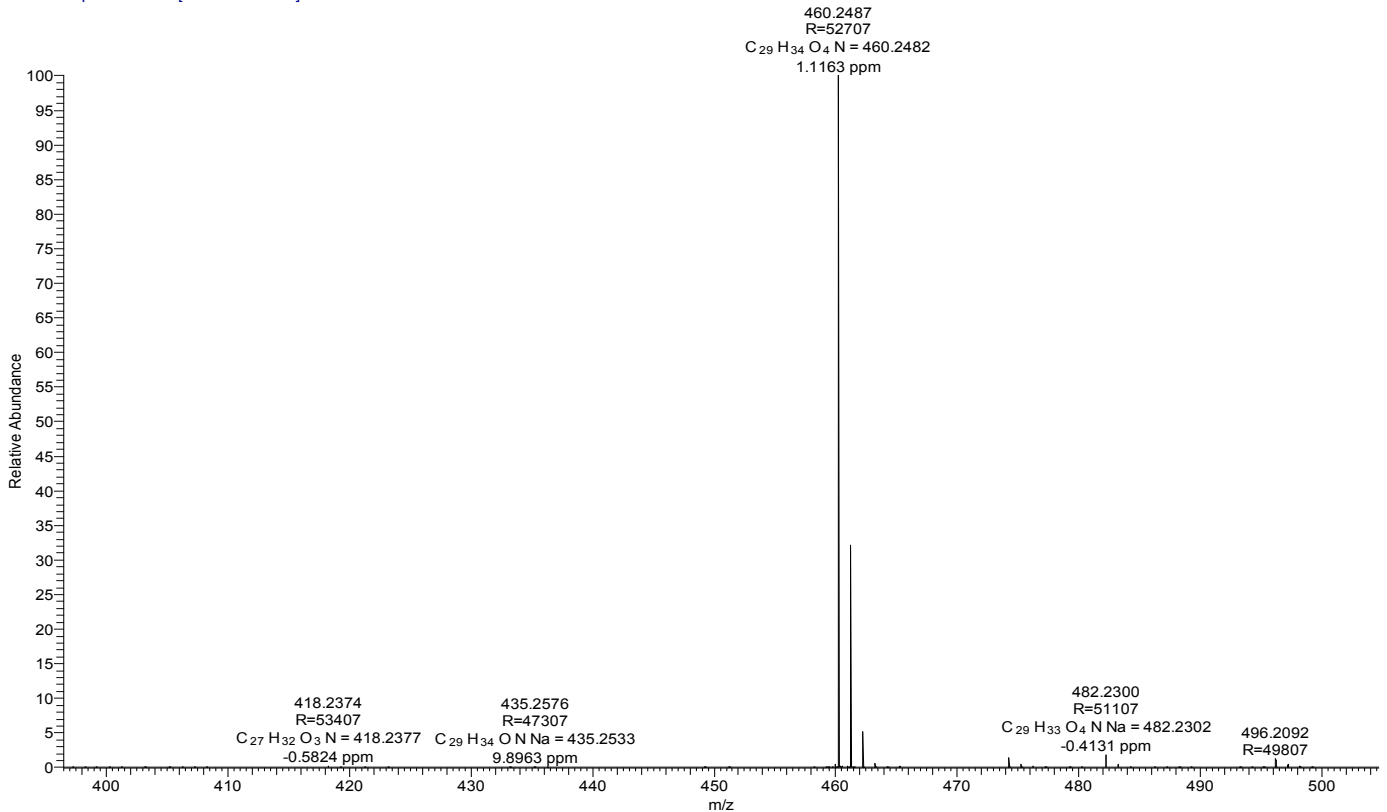
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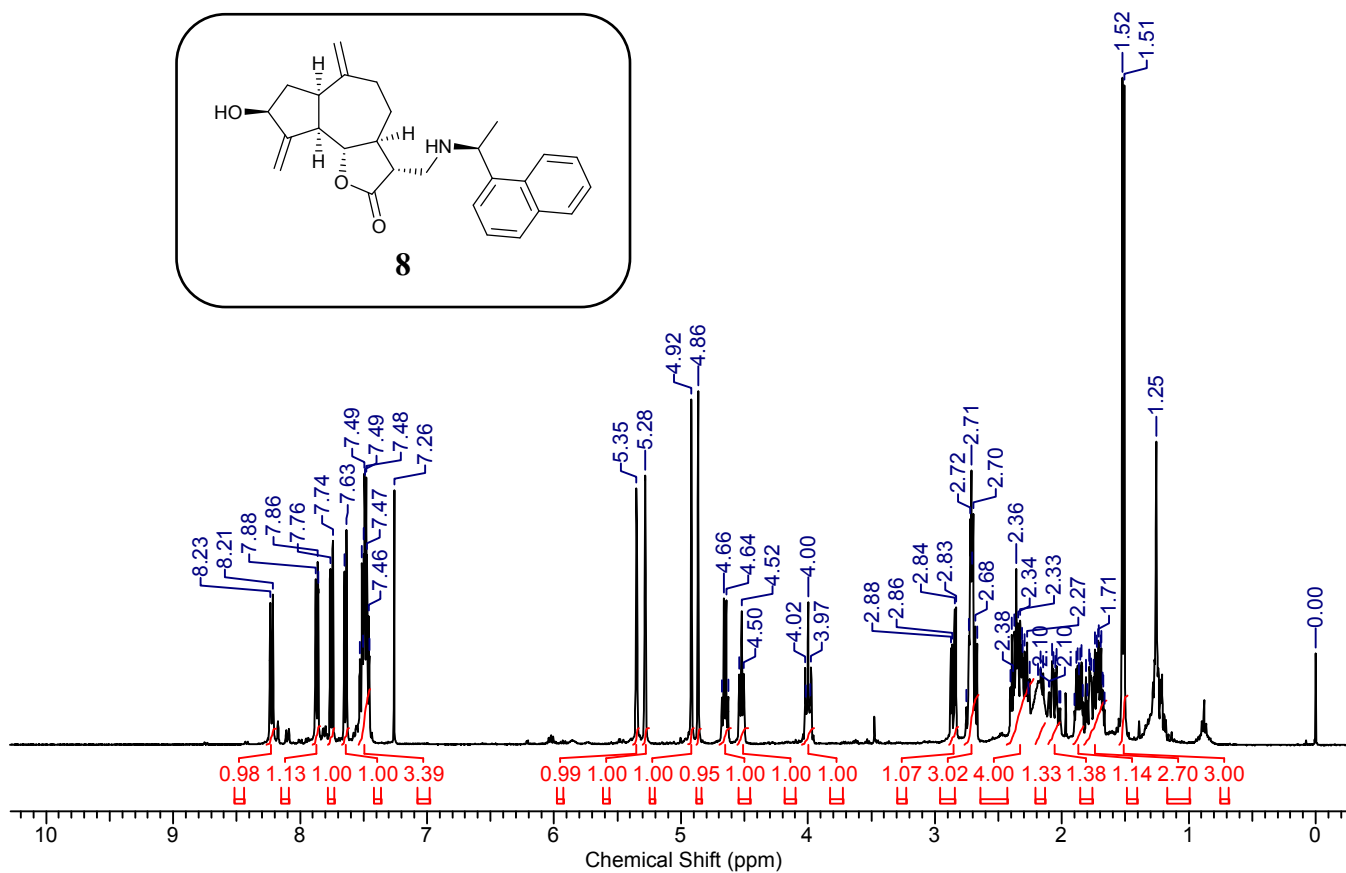
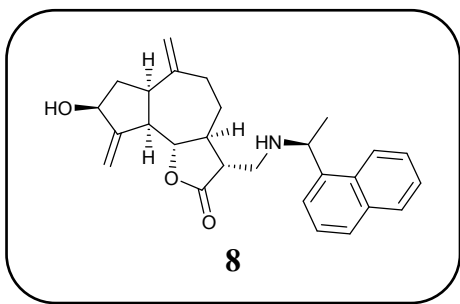


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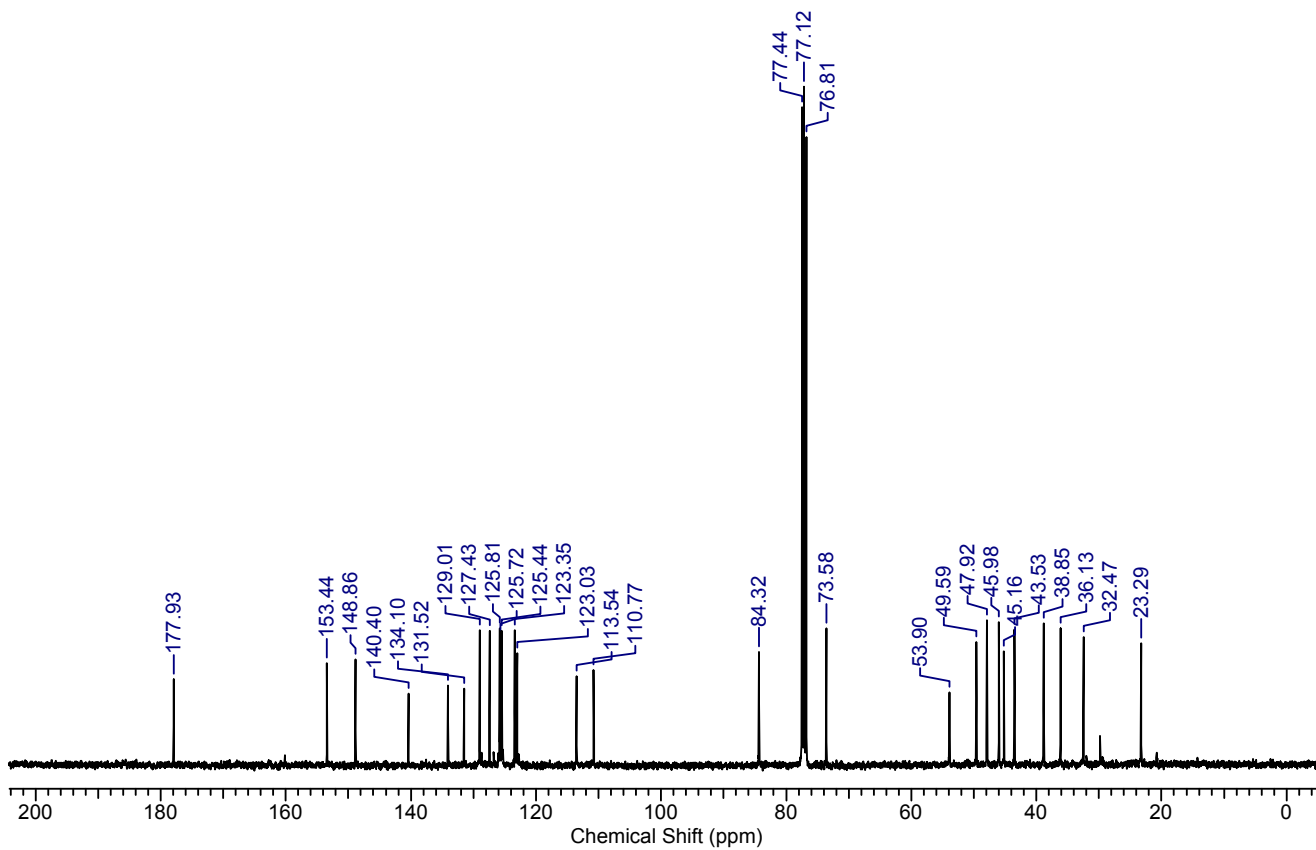
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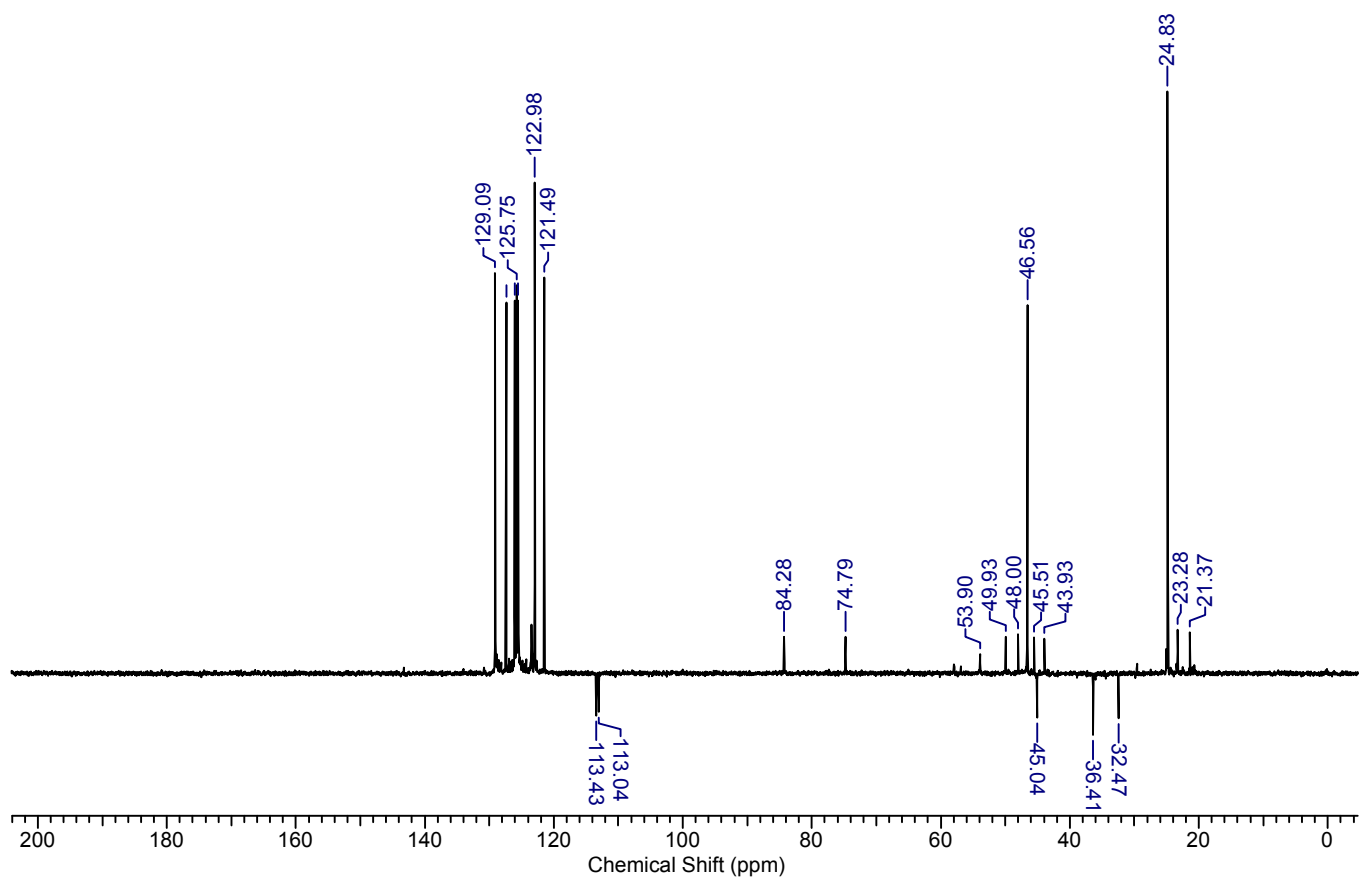
¹H NMR of Compound 8 (400 MHz, CDCl₃)



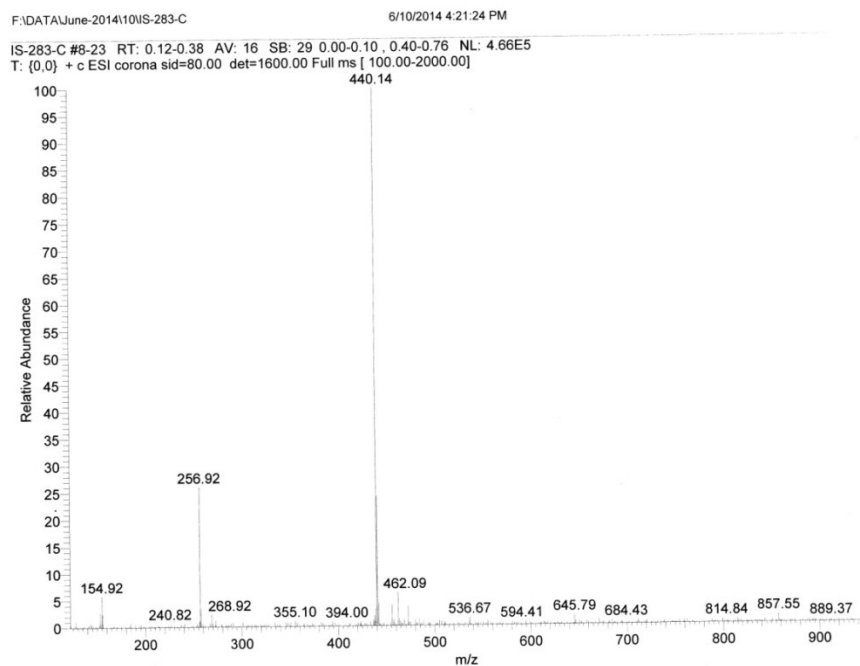
¹³C NMR of Compound 8 (100 MHz, CDCl₃)



DEPT of Compound 8 (100 MHz, CDCl₃)

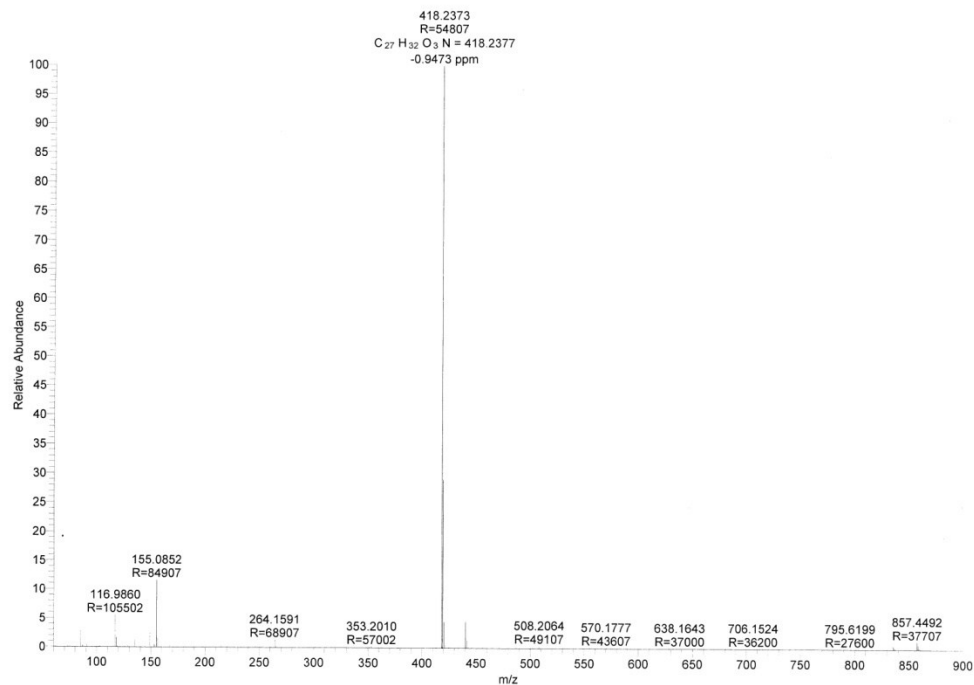


LC-MS of Compound 8

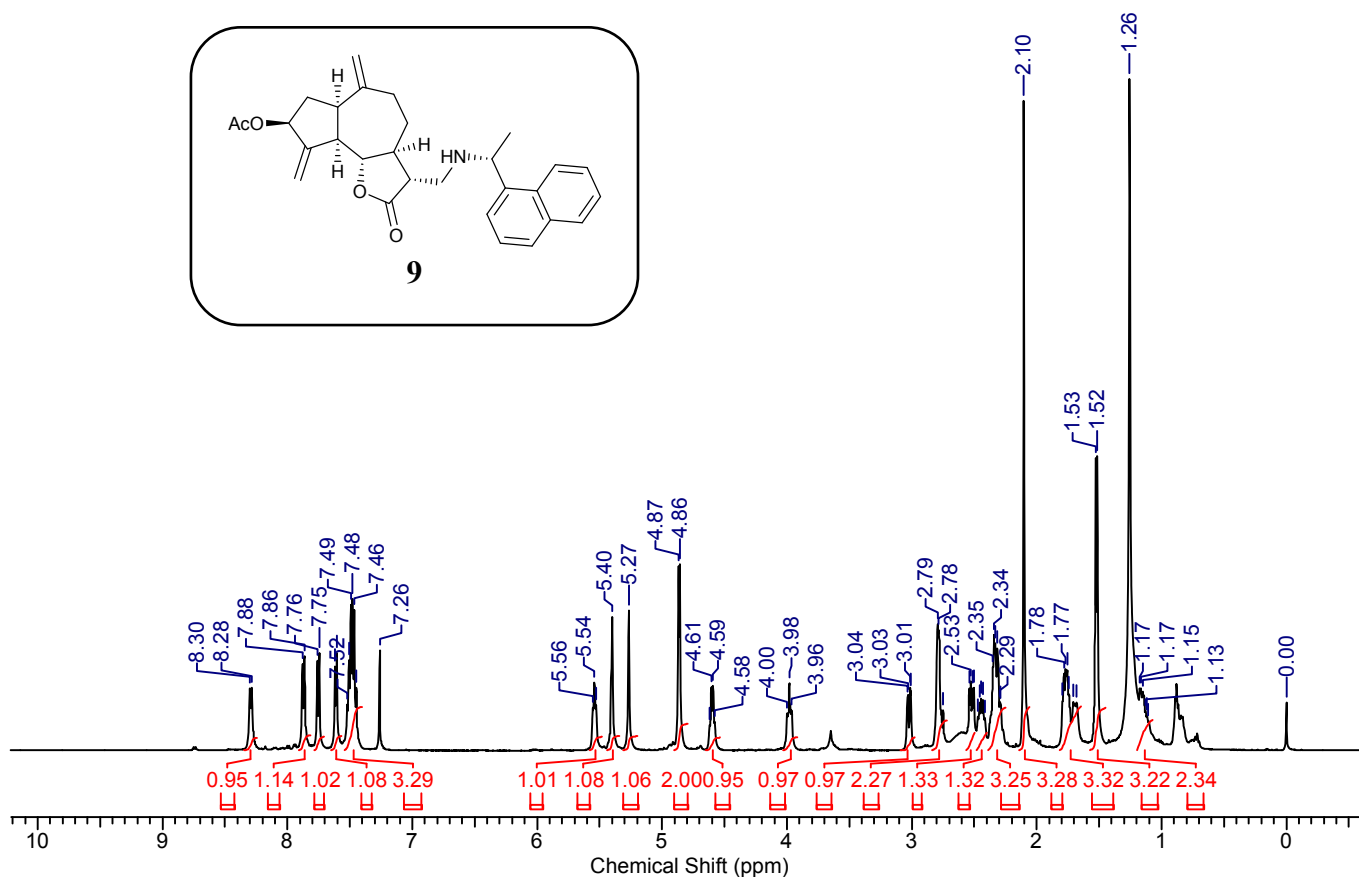
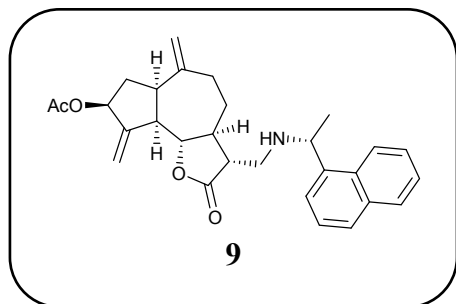


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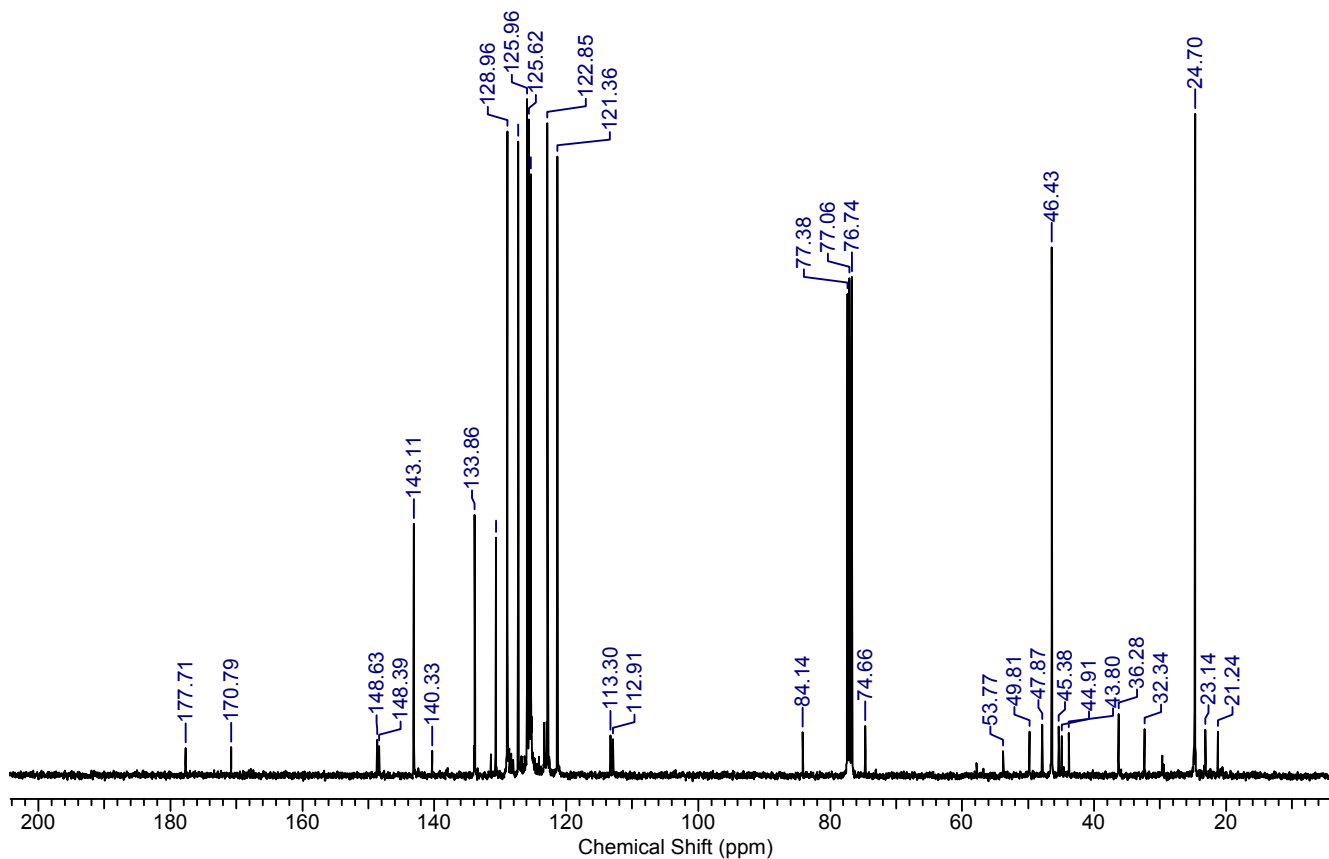
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¹H NMR of Compound 9 (400 MHz, CDCl₃)



¹³C NMR of Compound 9 (100 MHz, CDCl₃)

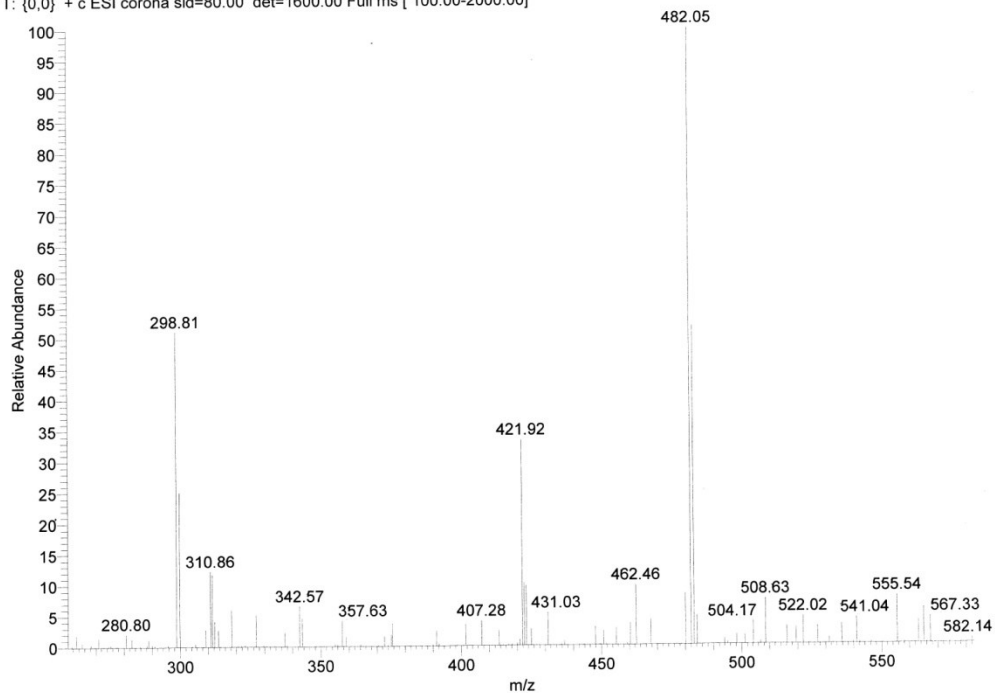


LC-MS of Compound 9

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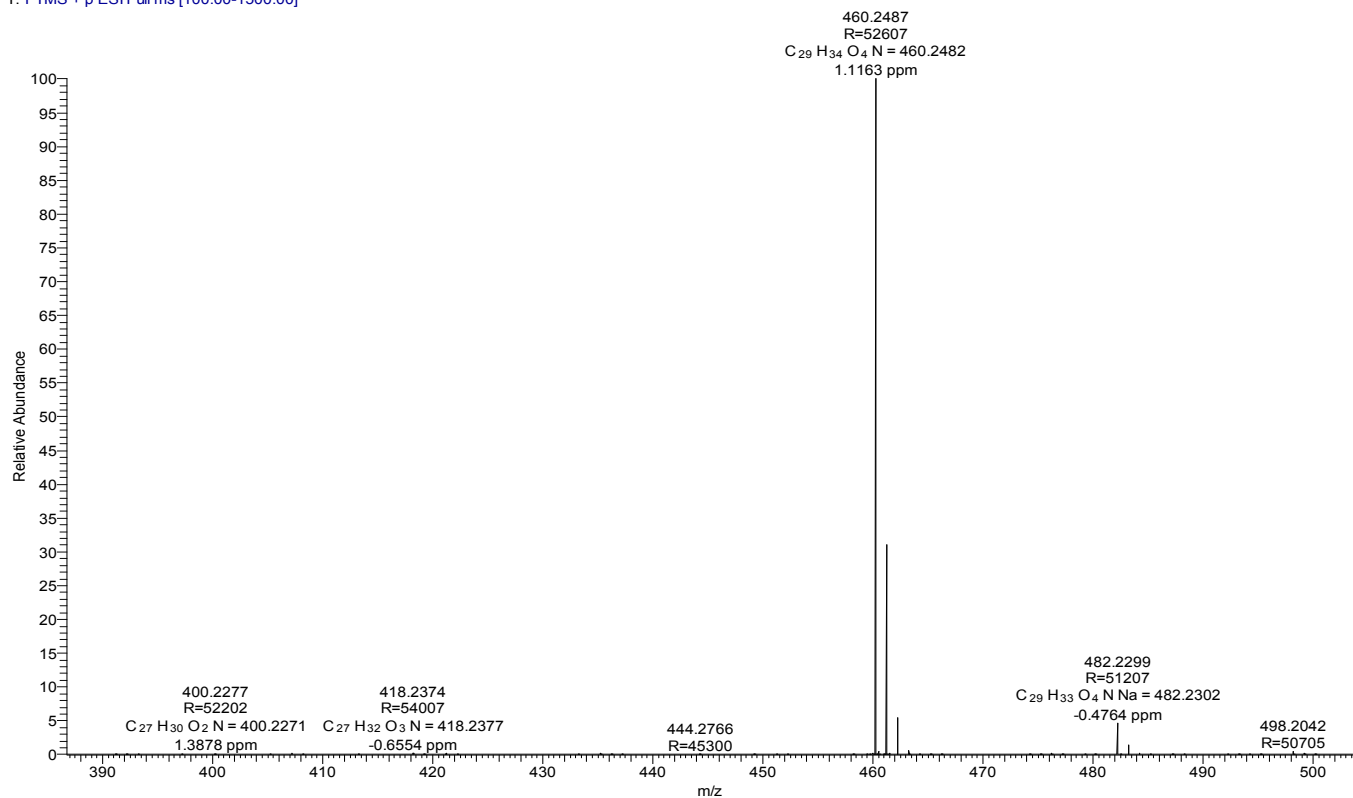
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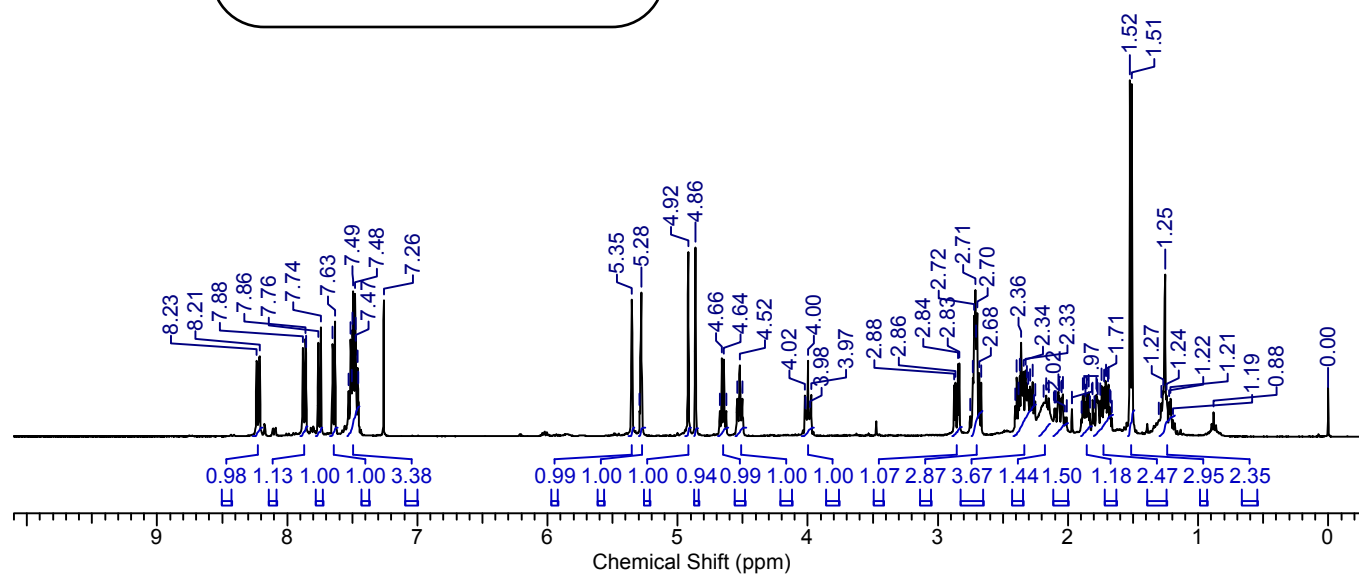
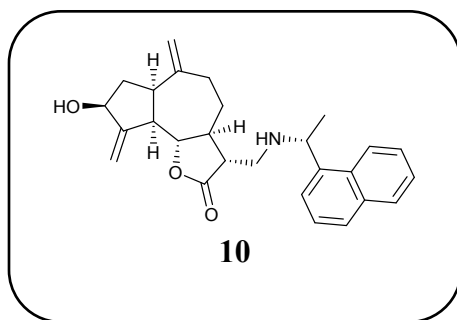


HR-MS of Compound 9

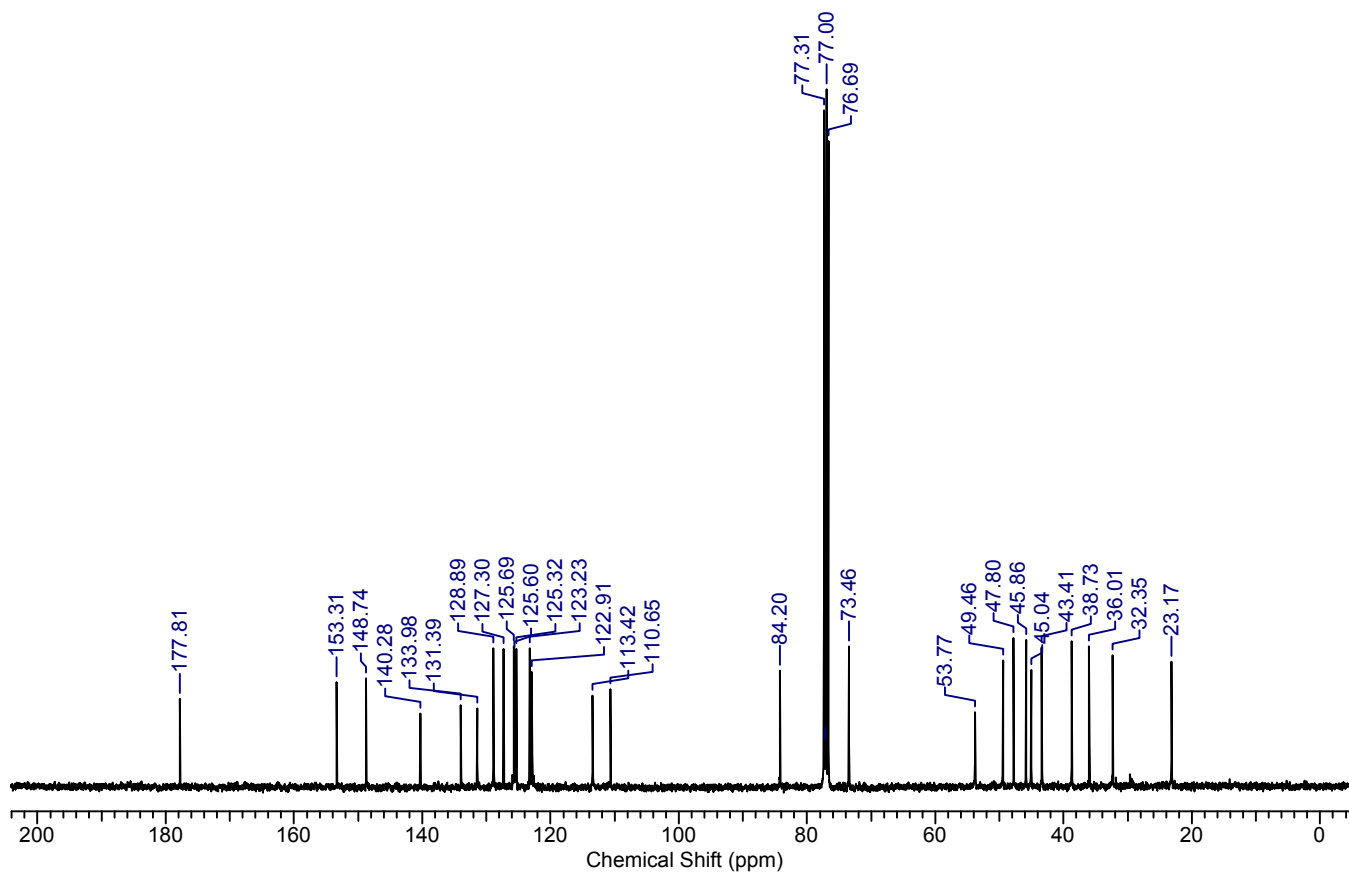
IS-293-A #89 RT: 0.39 AV: 1 NL: 6.82E9
T: FTMS + p ESI Full ms [100.00-1500.00]



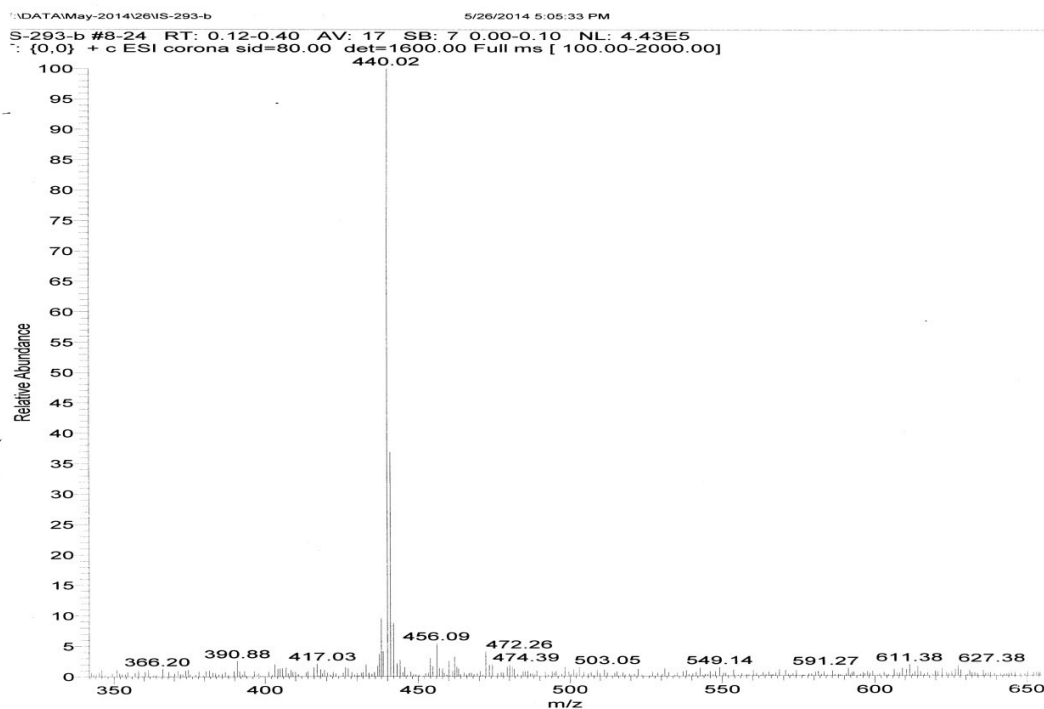
¹H NMR of Compound 10 (400 MHz, CDCl₃)



¹³C NMR of Compound 10 (100 MHz, CDCl₃)

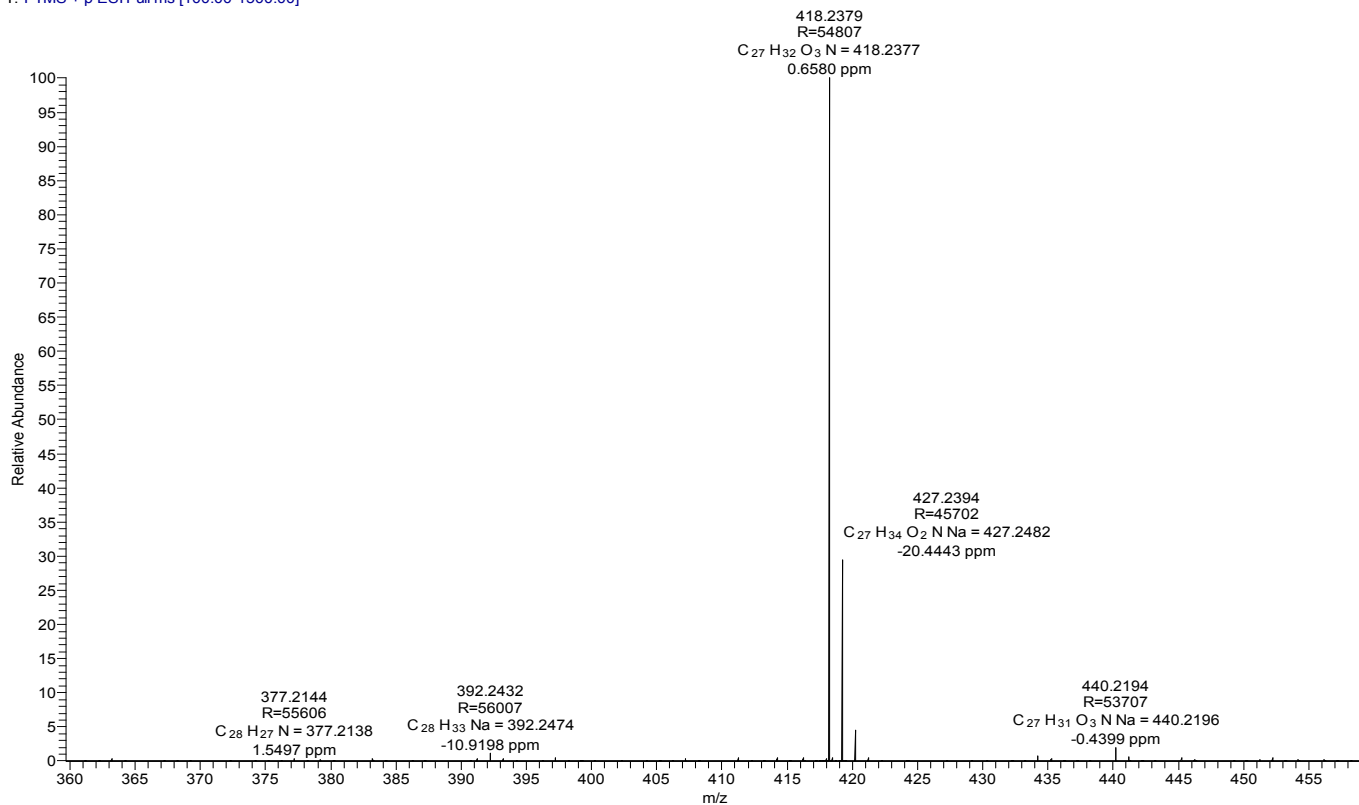


LC-MS of Compound 10

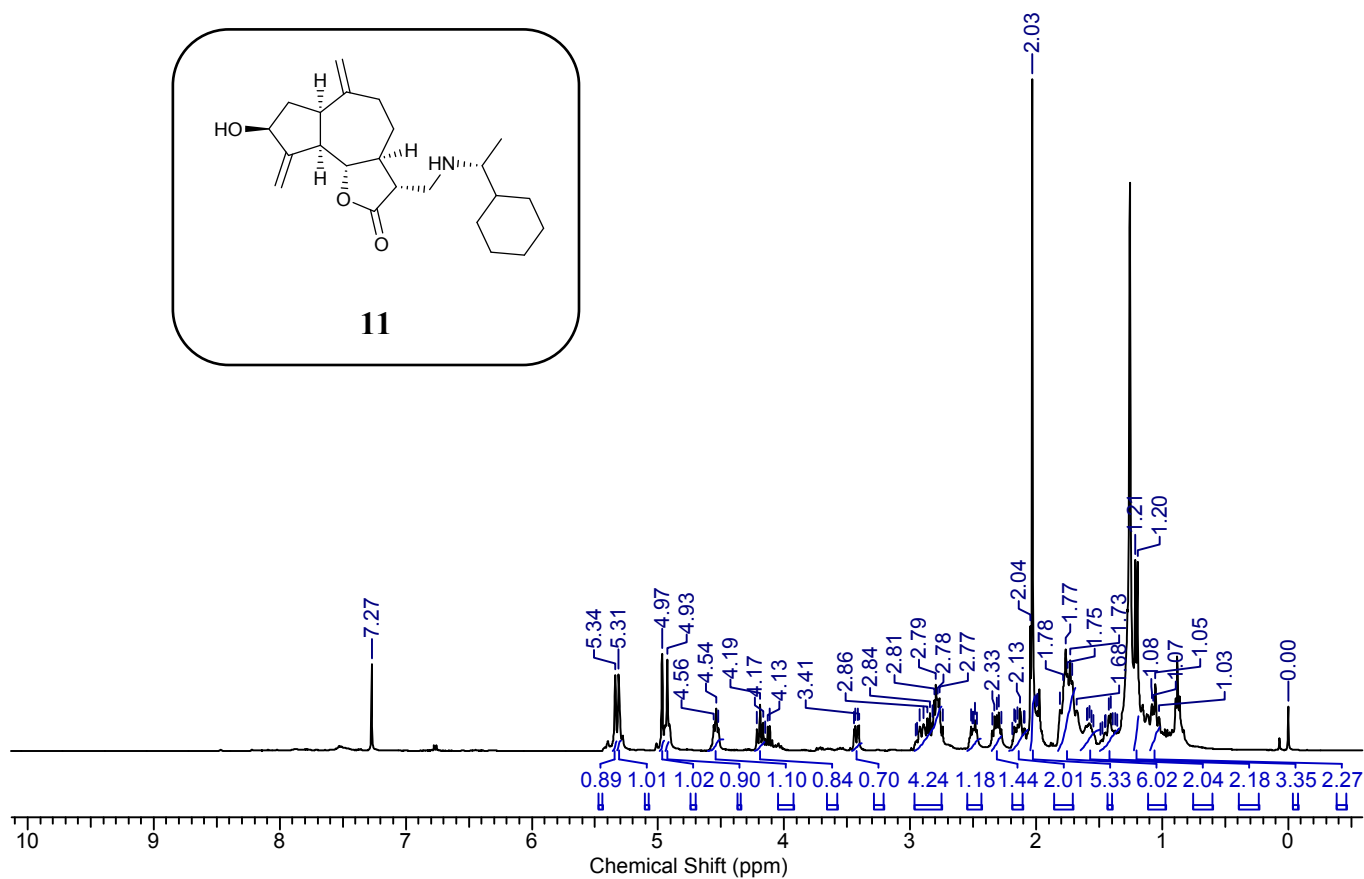
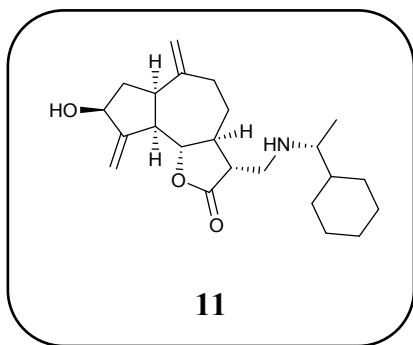


HR-MS of Compound 10

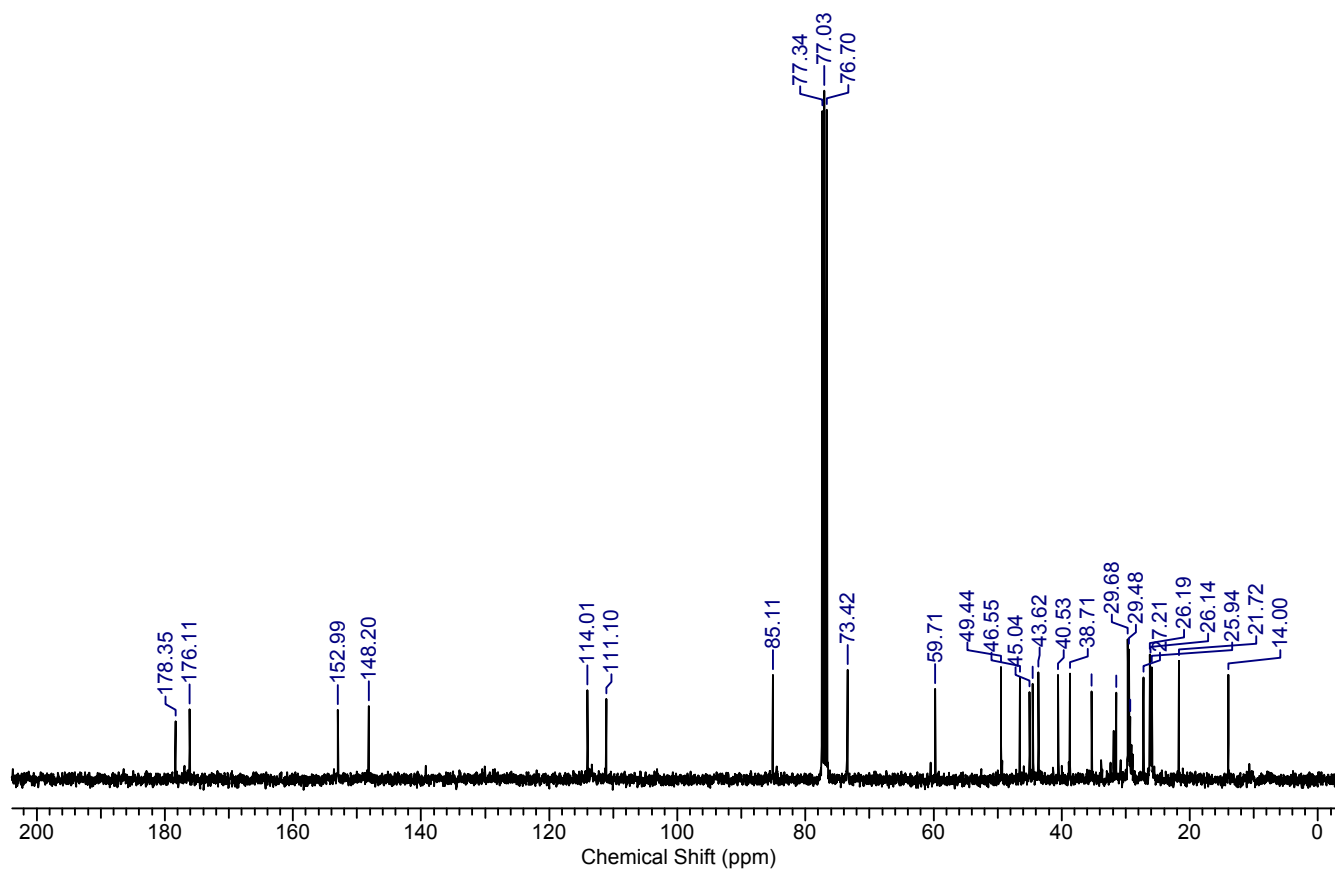
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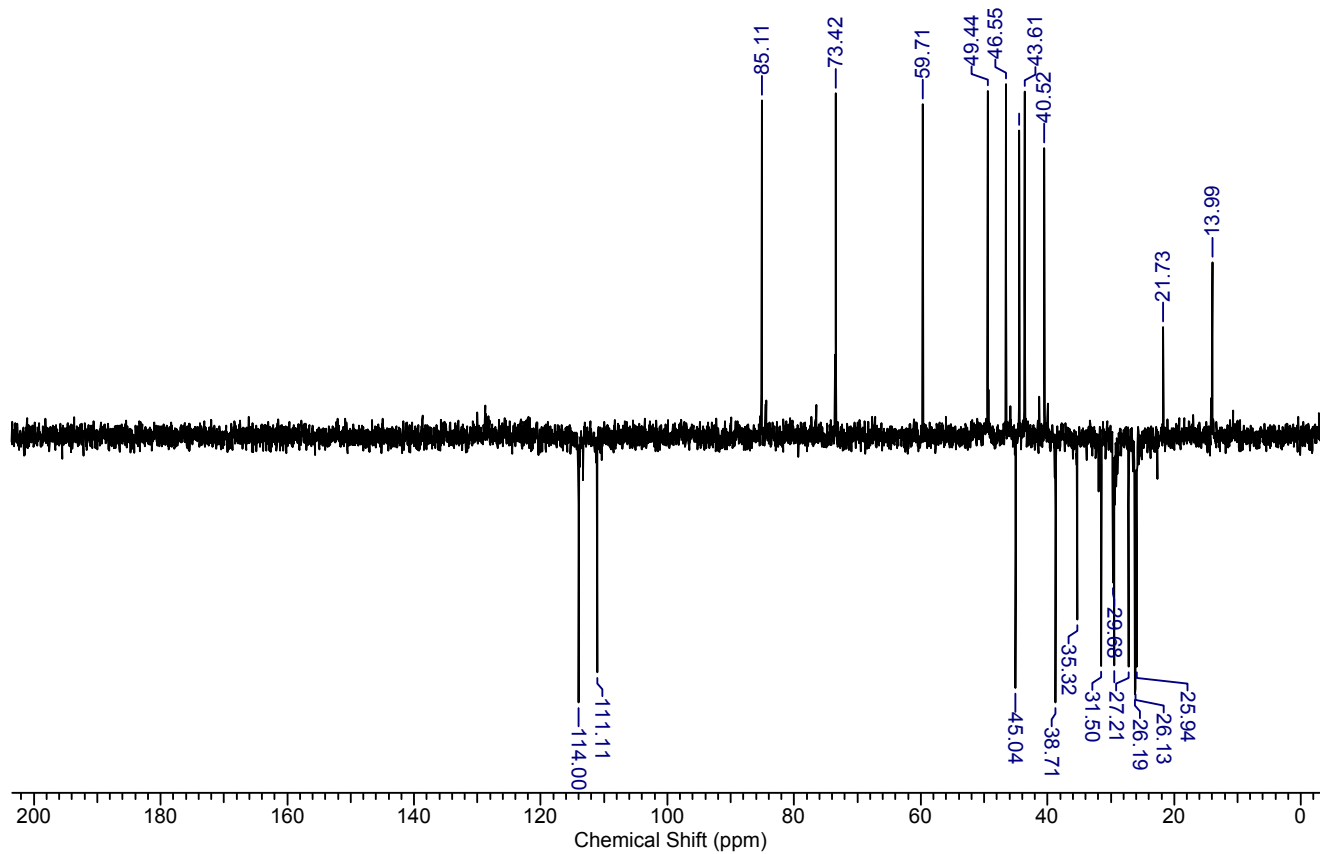
¹H NMR of Compound 11 (400 MHz, CDCl₃)



^{13}C NMR of Compound 11 (100 MHz, CDCl_3)



DEPT of Compound 11 (100 MHz, CDCl_3)

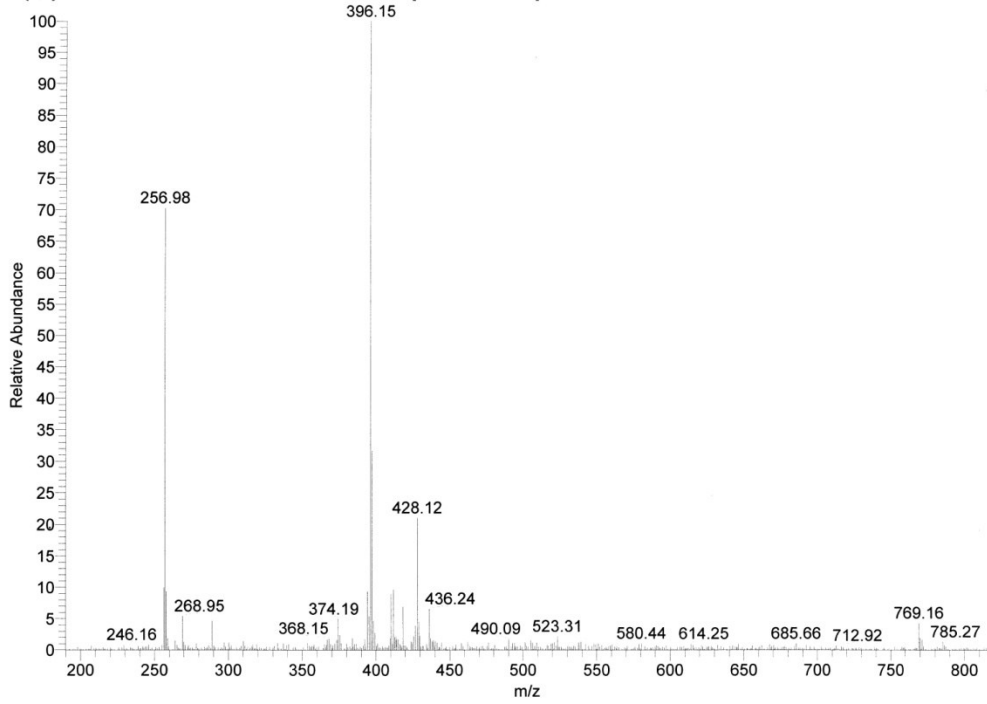


LC-MS of Compound 11

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6/10/2014 4:25:33 PM

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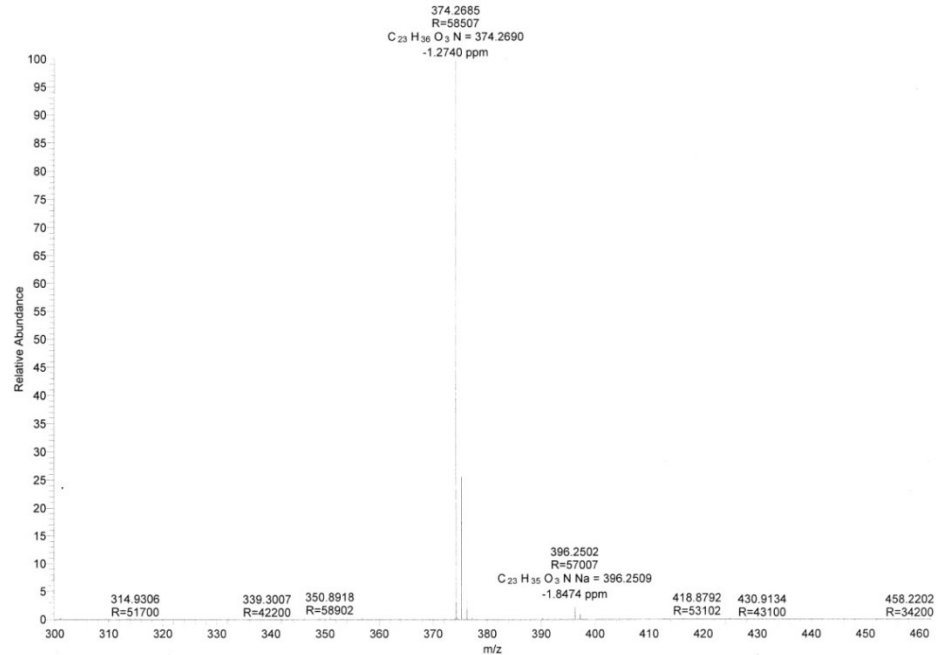


HR-MS of Compound 11

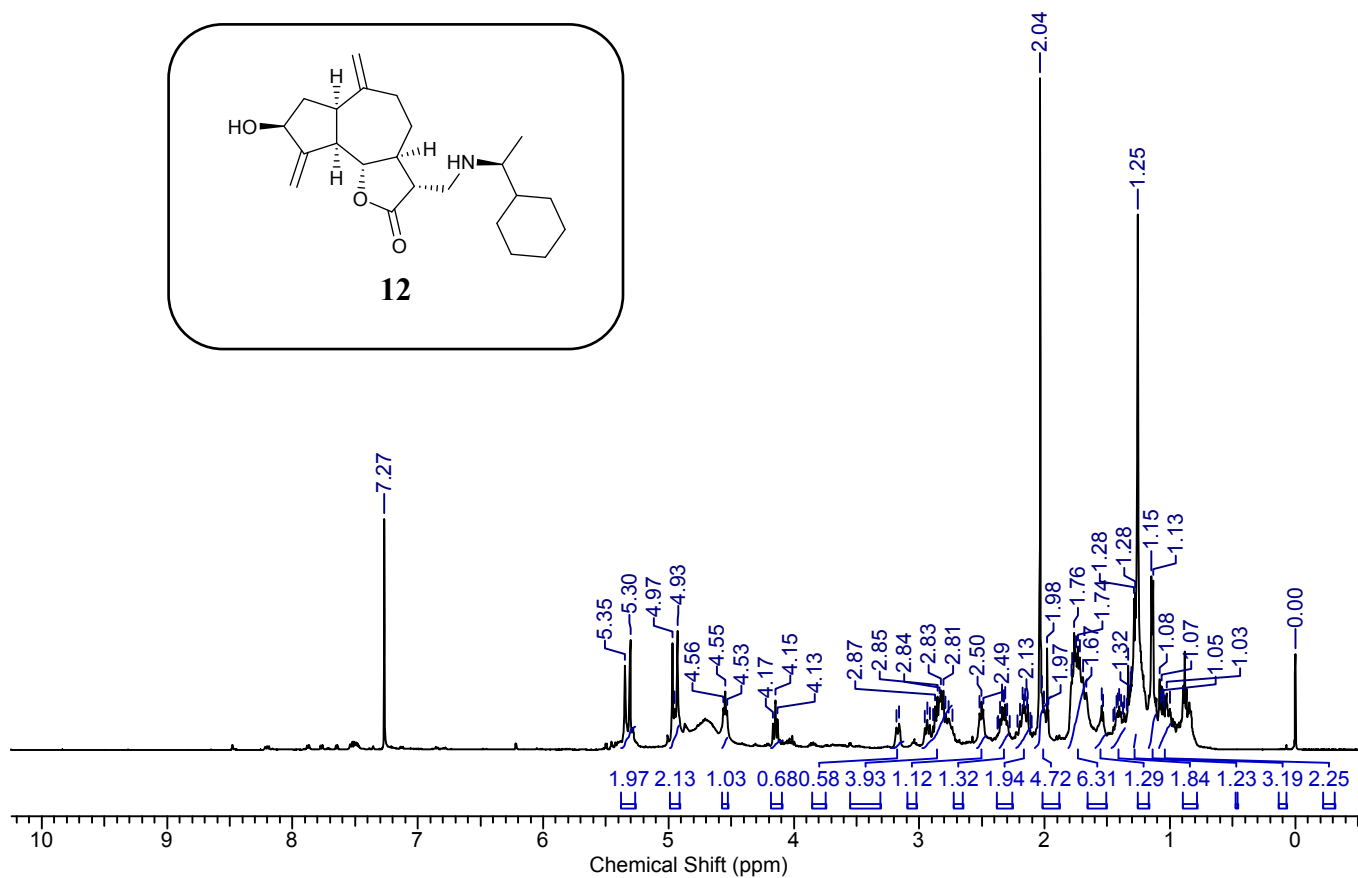
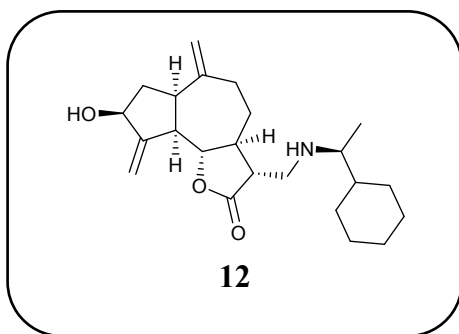
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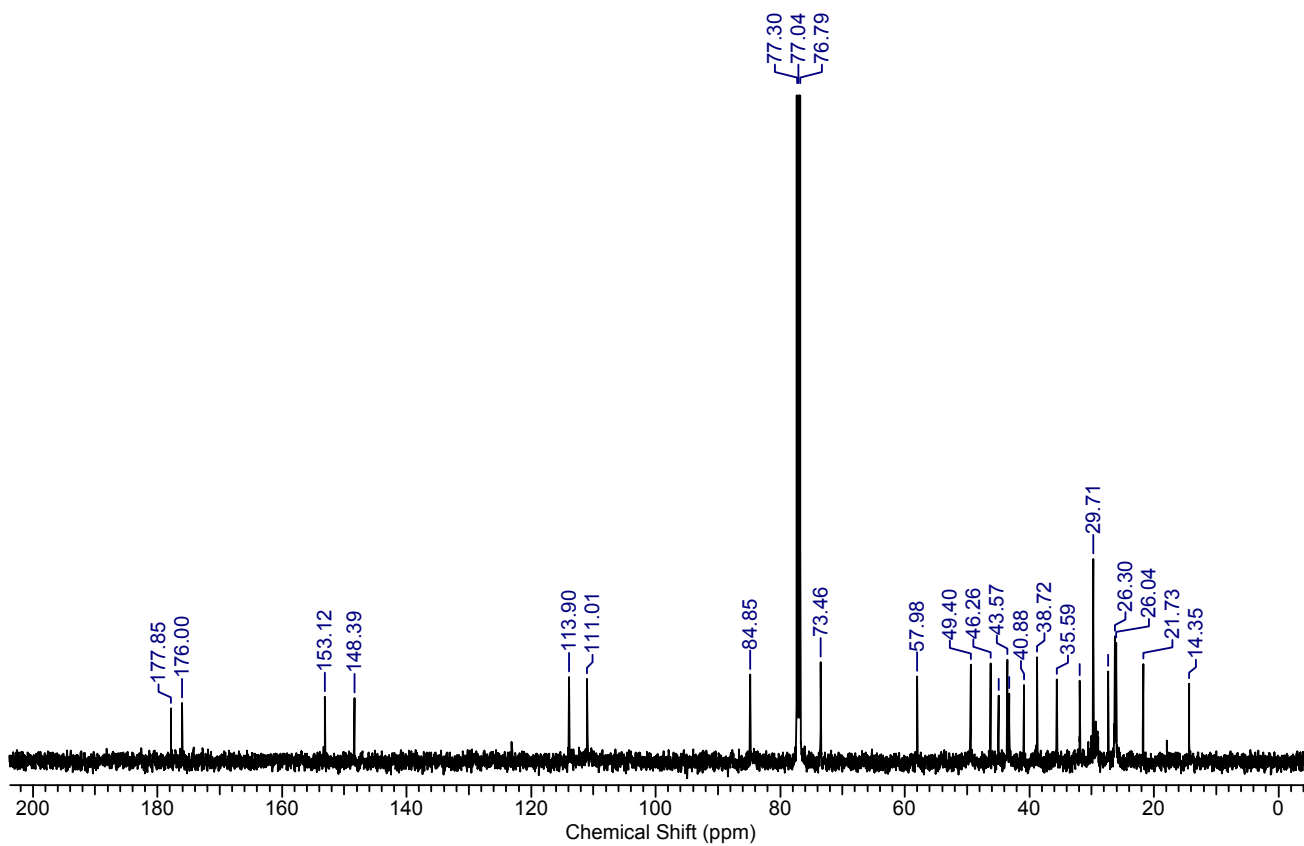
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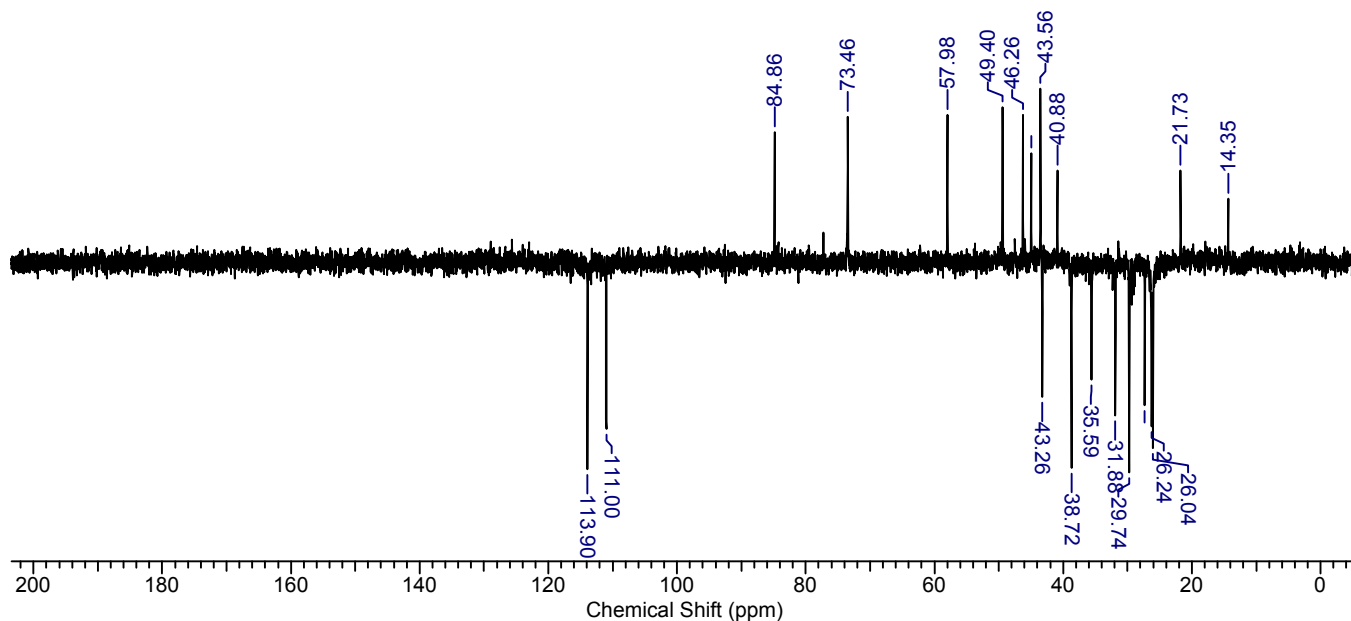
¹H NMR of Compound 12 (500 MHz, CDCl₃)



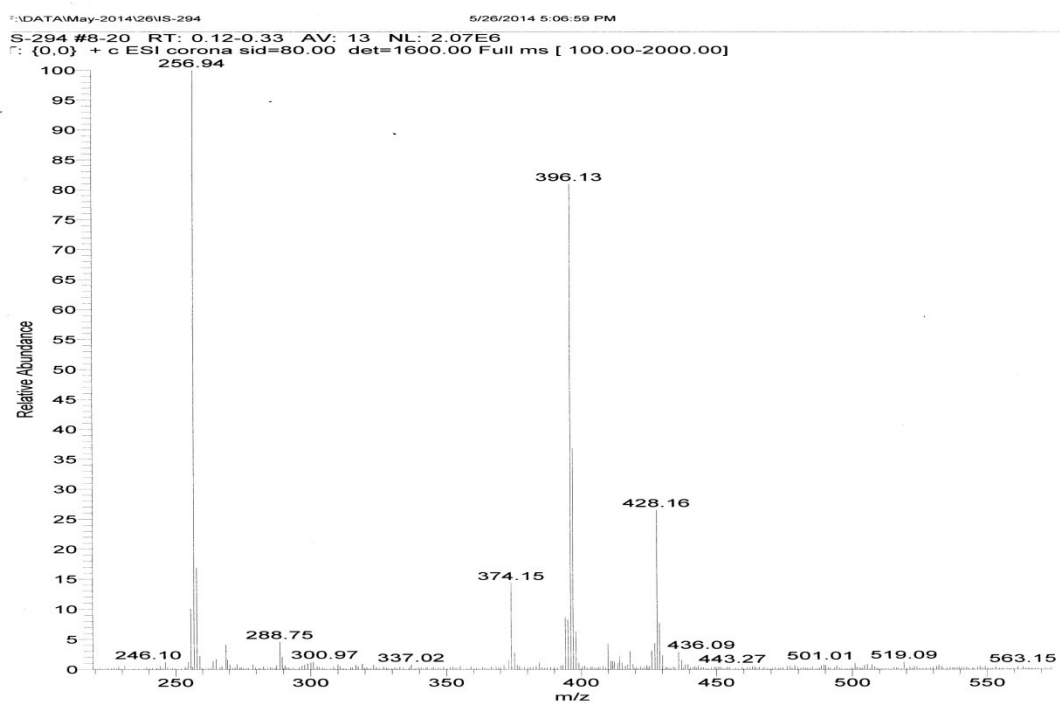
¹³C NMR of Compound 12 (125 MHz, CDCl₃)



DEPT of Compound 12 (125 MHz, CDCl₃)

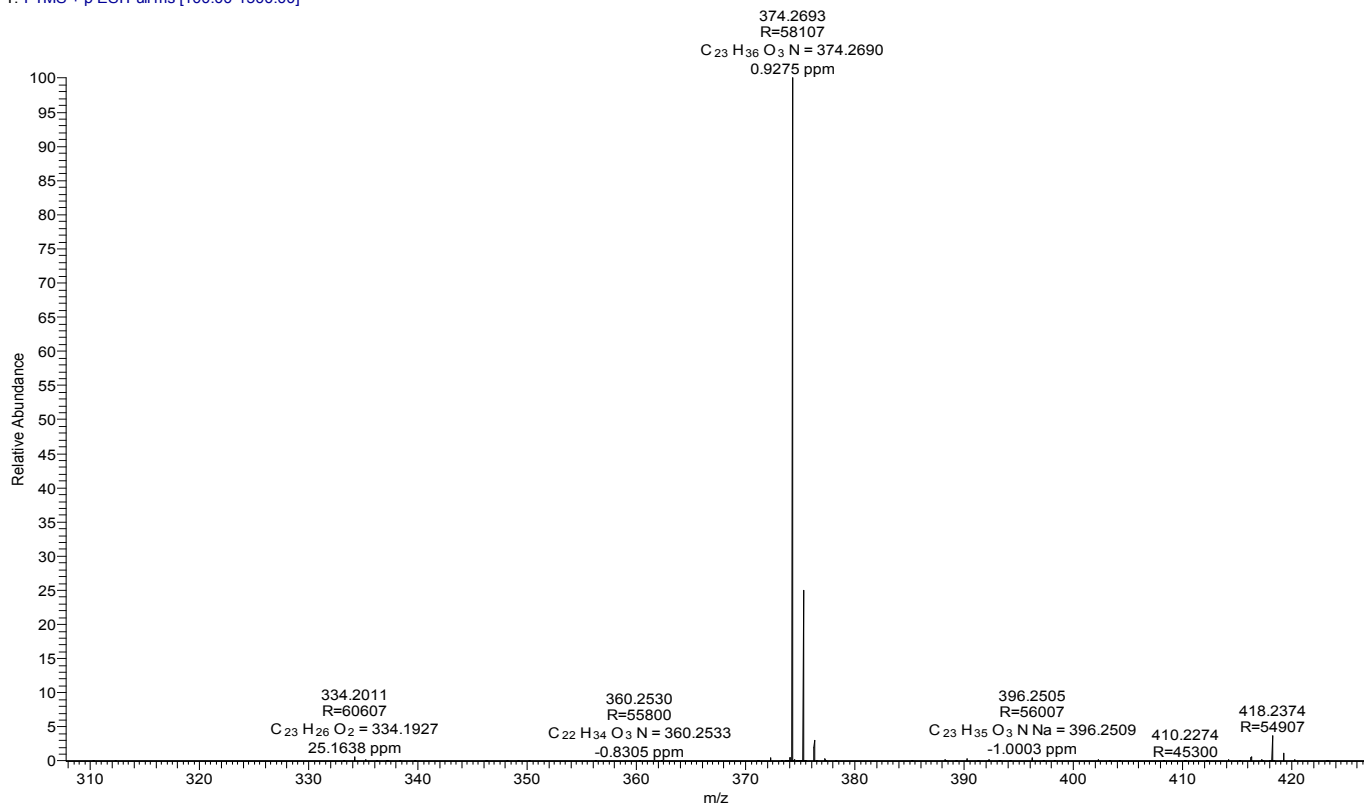


LC-MS of Compound 12

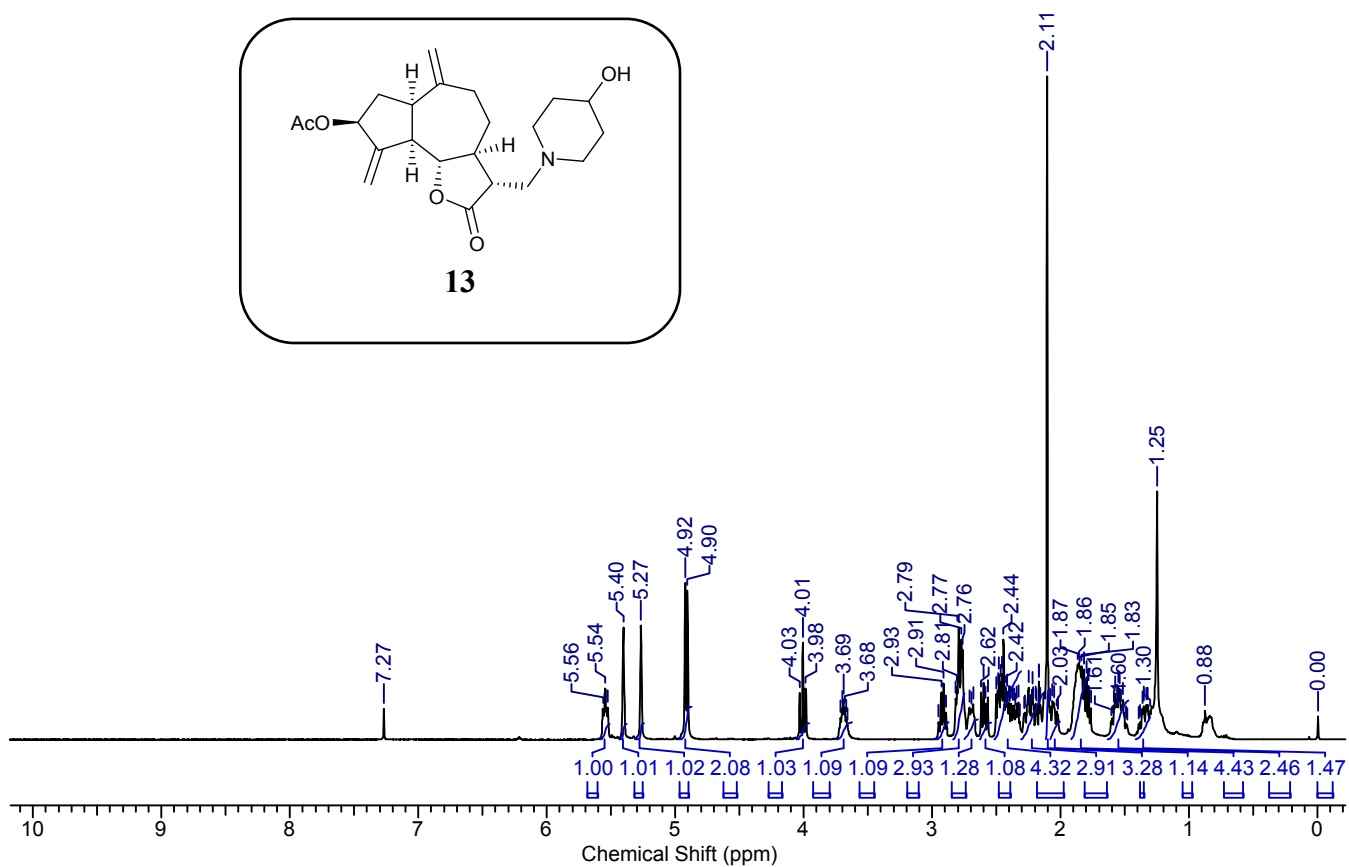
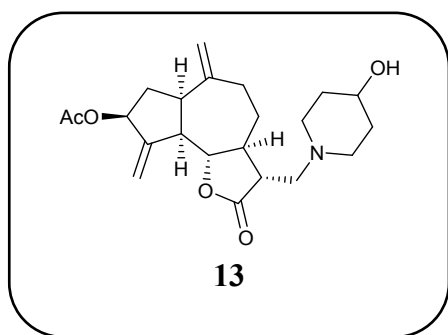


HR-MS of Compound 12

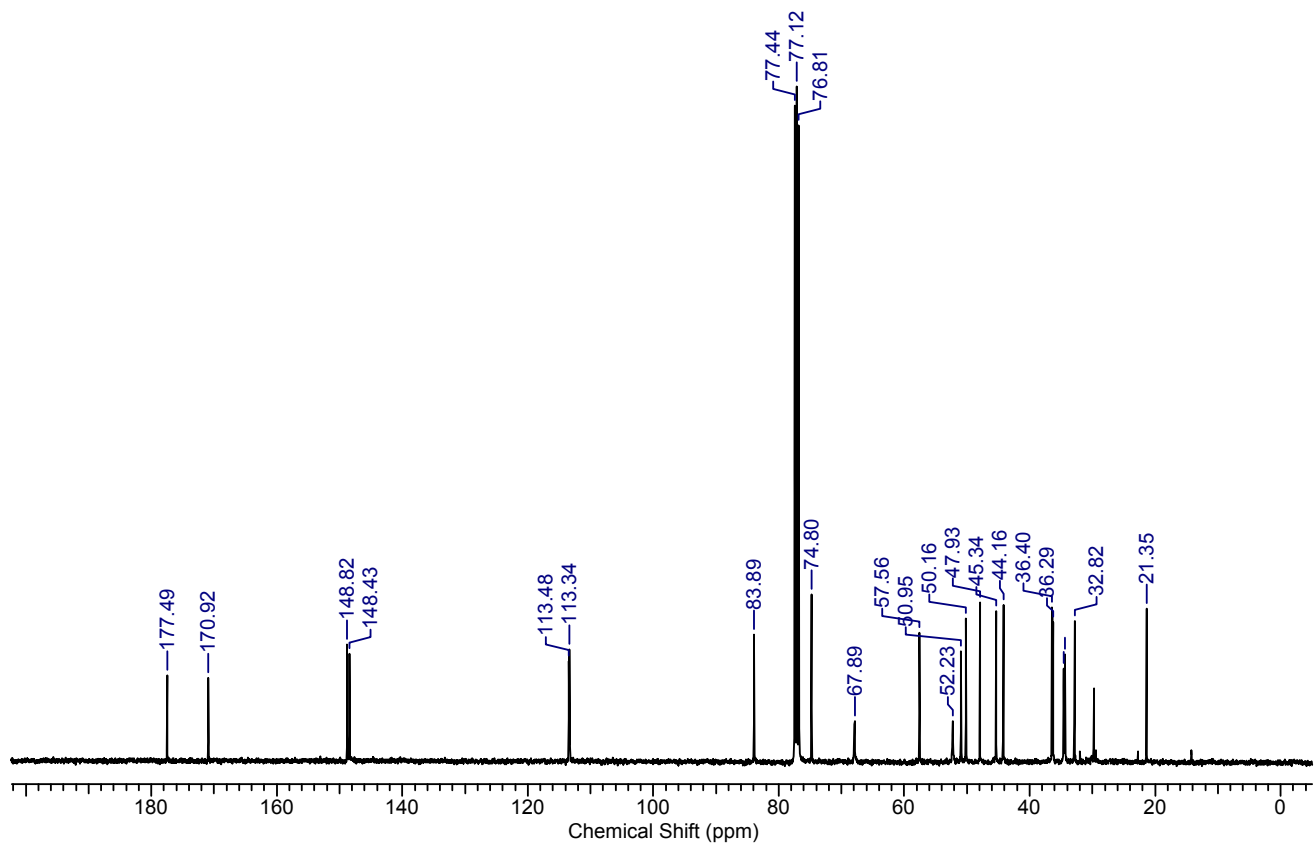
IS-294-A #87 RT: 0.38 AV: 1 NL: 7.63E9
T: FTMS + p ESI Full ms [100.00-1500.00]



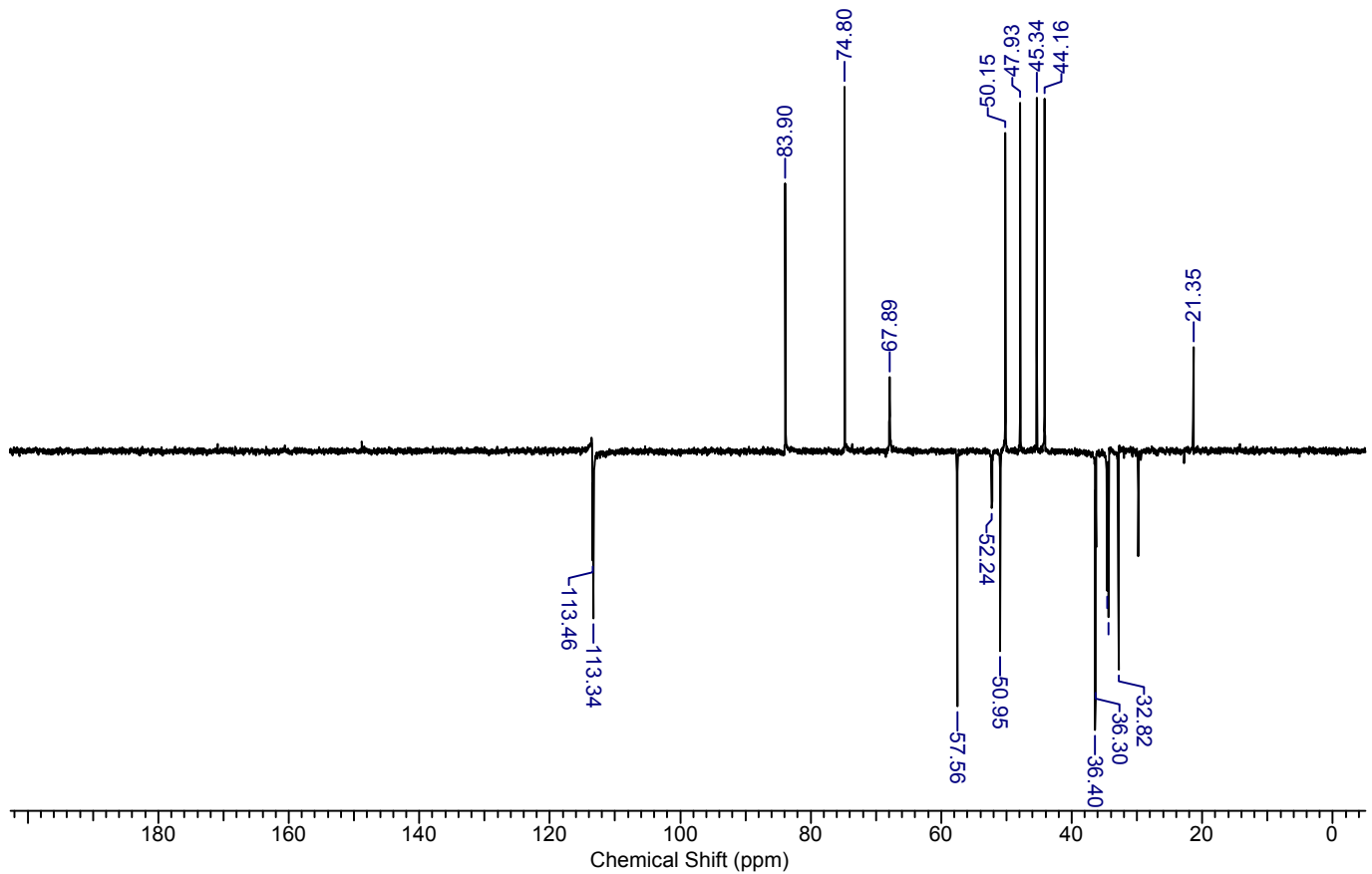
¹H NMR of Compound 13 (400 MHz, CDCl₃)



^{13}C NMR of Compound 13 (100 MHz, CDCl_3)



DEPT of Compound 13 (100 MHz, CDCl_3)

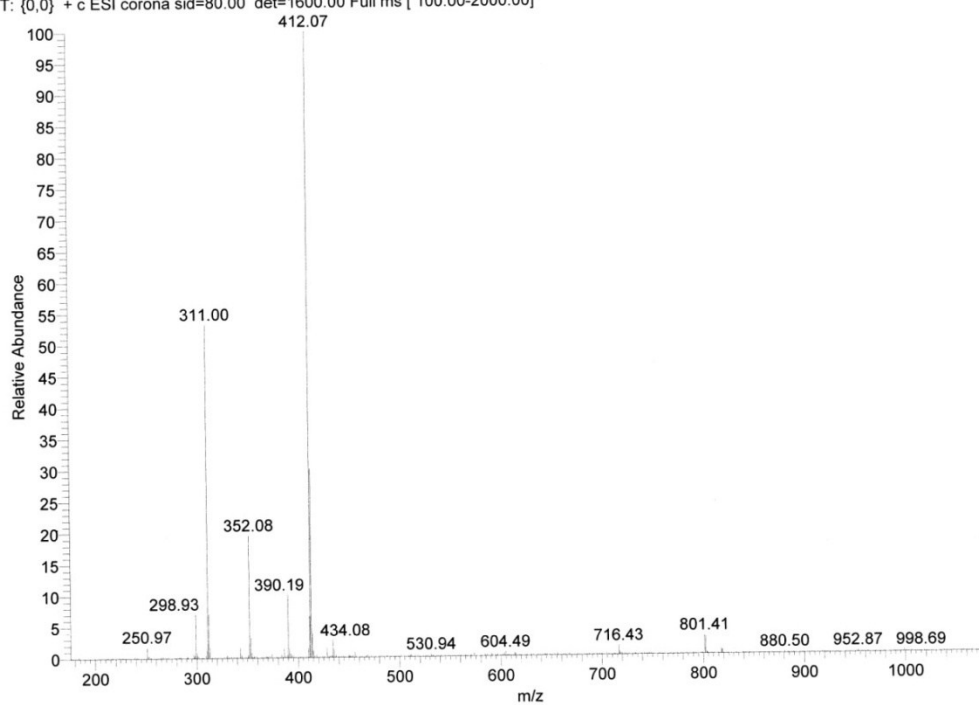


LC-MS of Compound 13

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6/10/2014 4:20:00 PM

IS-278-A #8-24 RT: 0.12-0.40 AV: 17 SB: 28 0.00-0.14 , 0.35-0.66 NL: 1.14E6
T: (0,0) + c ESI corona sid=80.00 det=1600.00 Full ms [100.00-2000.00]

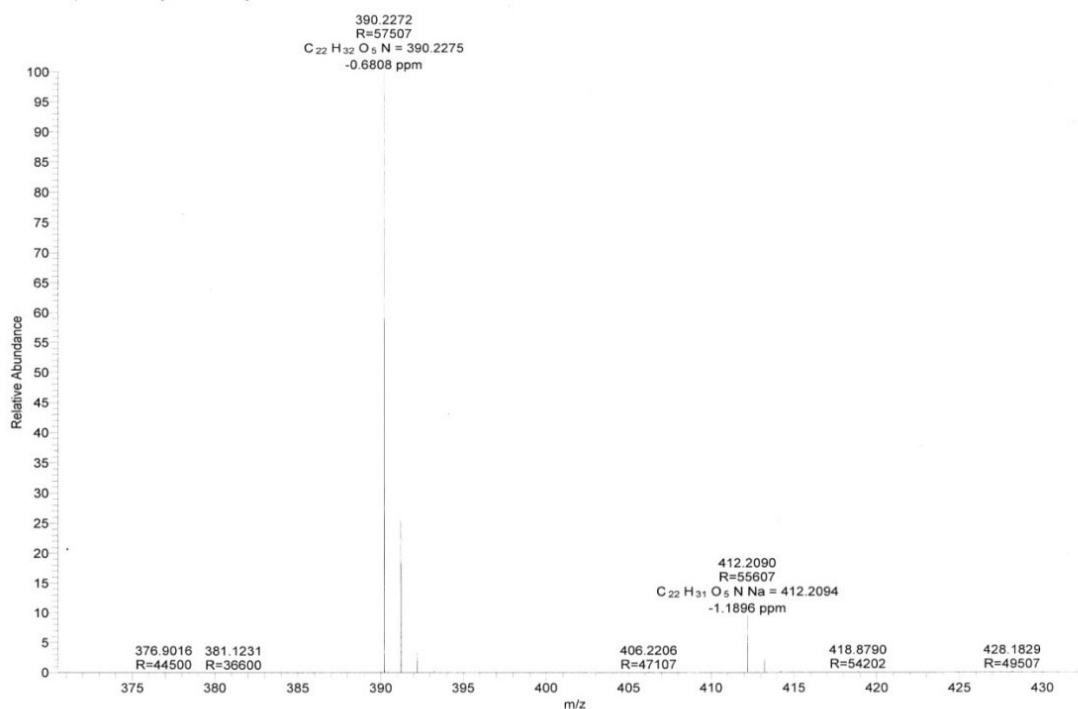


HR-MS of Compound 13

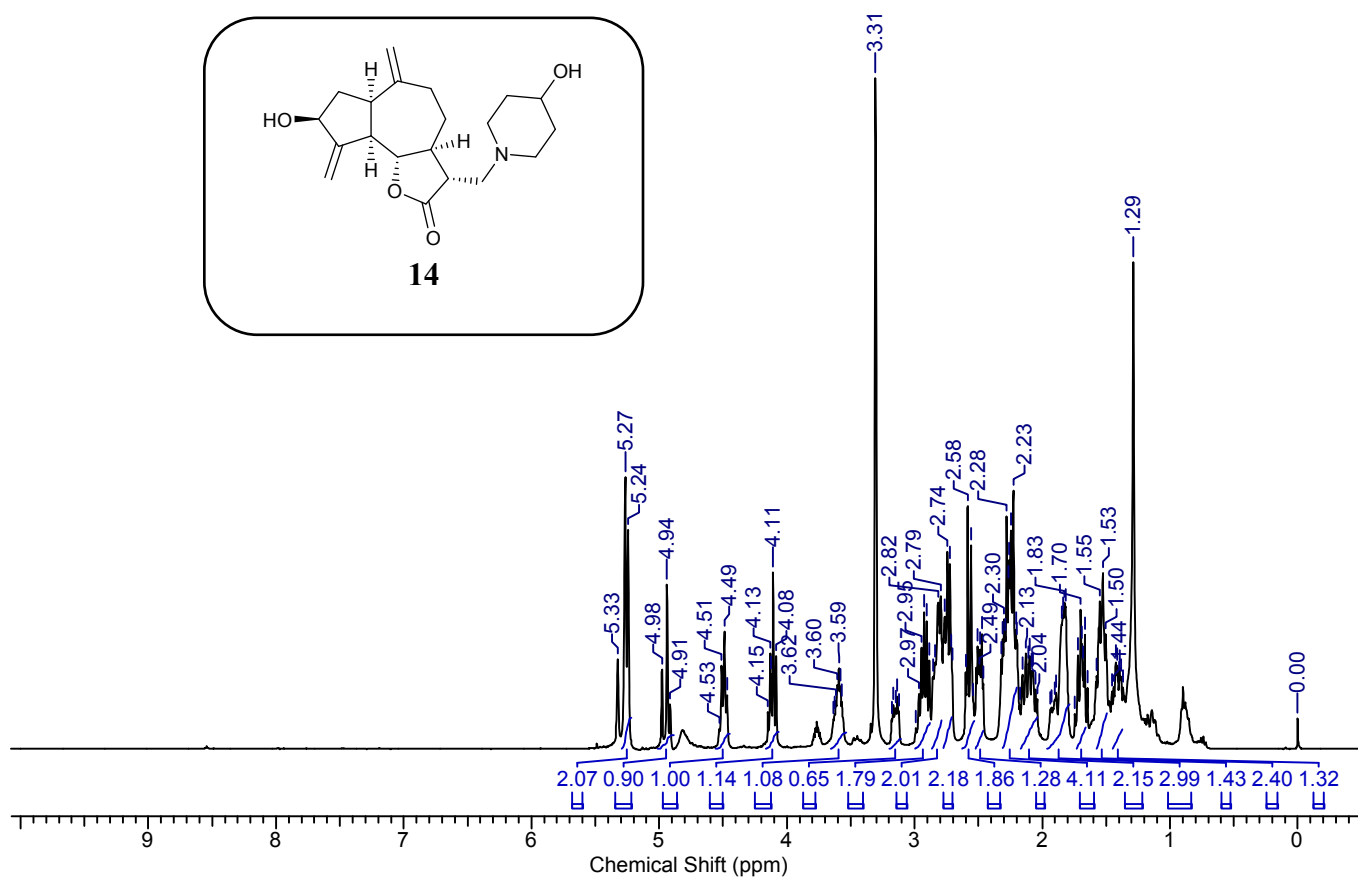
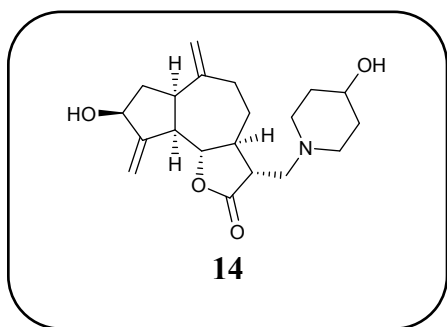
D:\Data\IS-278-A

8/14/2014 12:33:47 PM

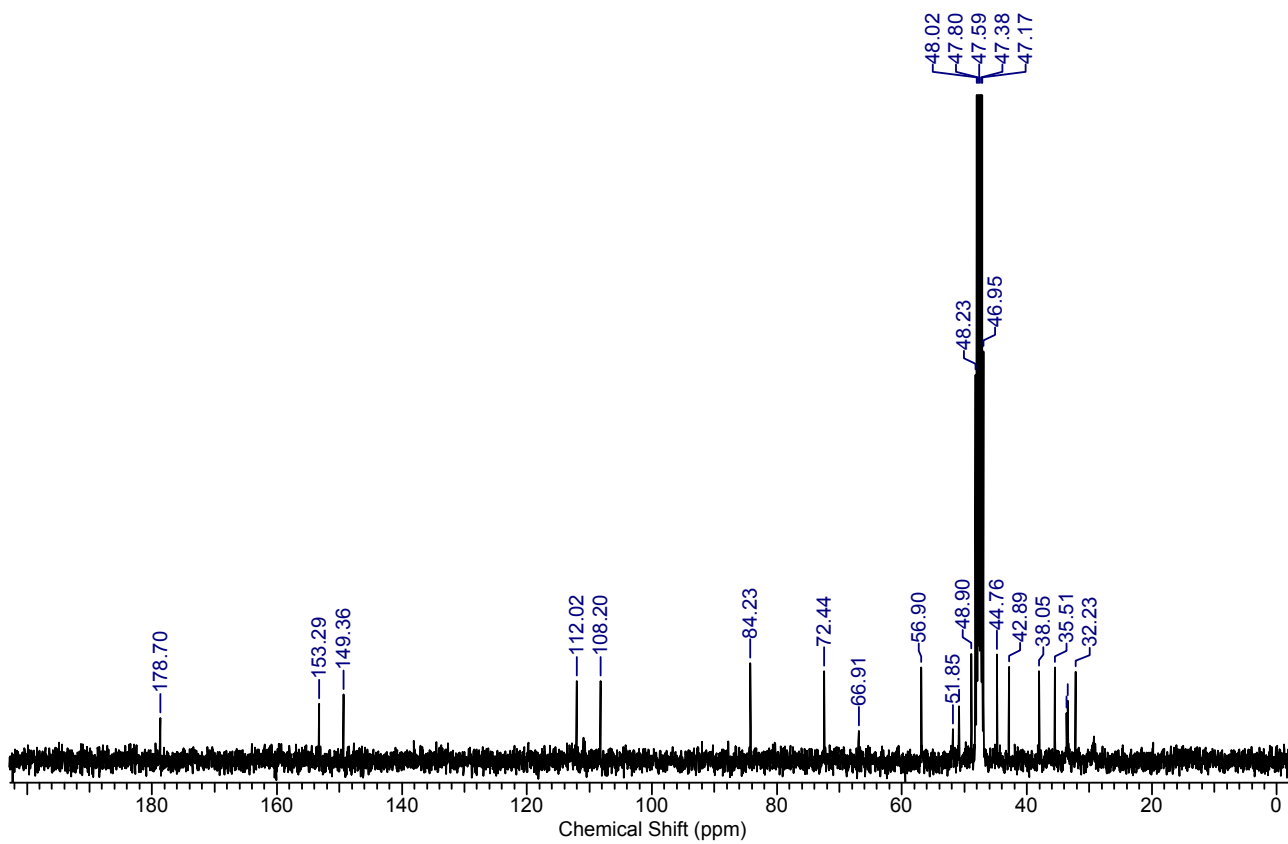
IS-278-A #469 RT: 2.09 AV: 1 NL: 1.34E9
T: FTMS + p ESI Full ms [60.00-900.00]



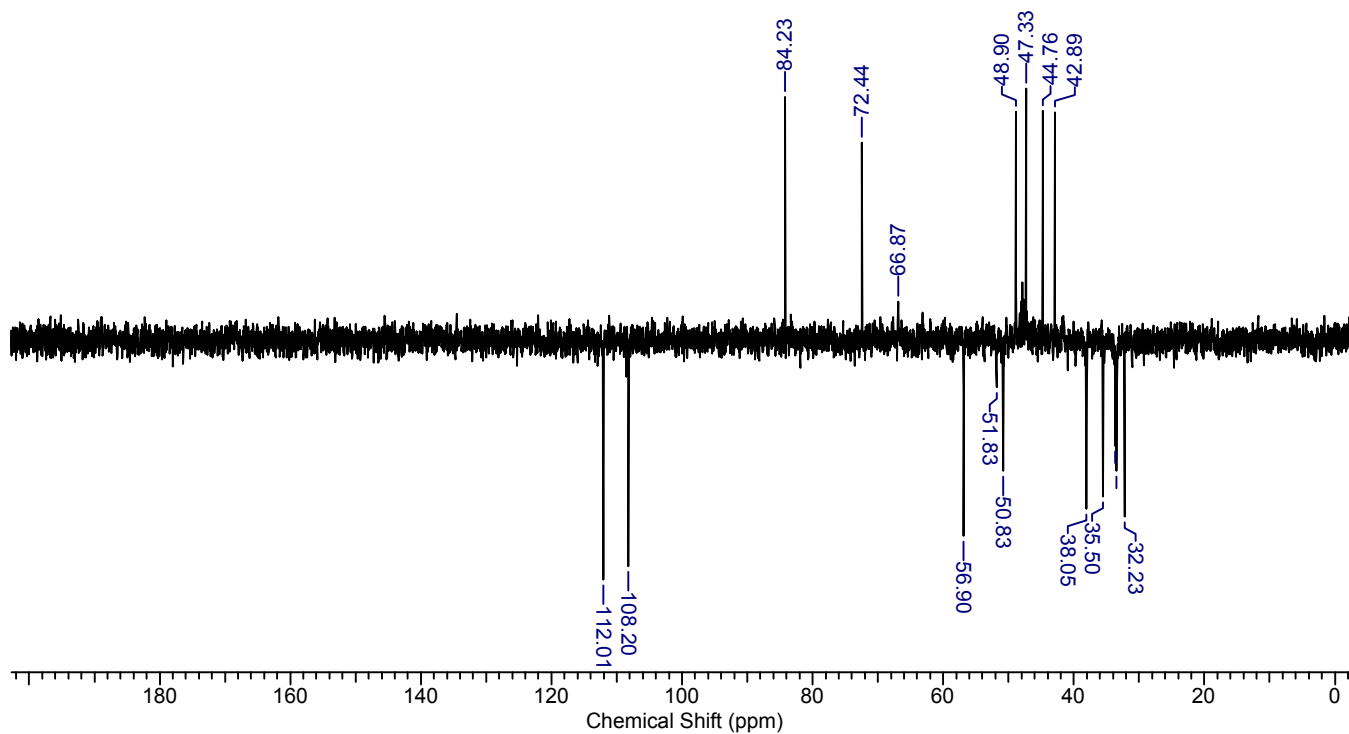
¹H NMR of Compound 14 (400 MHz, CDCl₃)



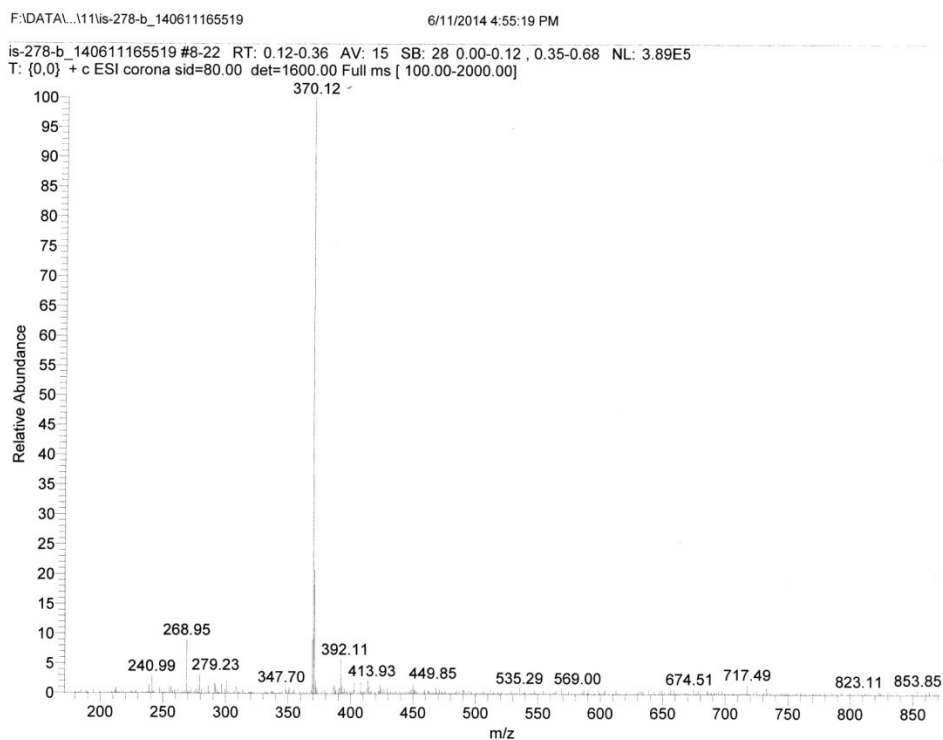
¹³C NMR of Compound 14 (100 MHz, CDCl₃)



DEPT of Compound 14 (100 MHz, CDCl₃)

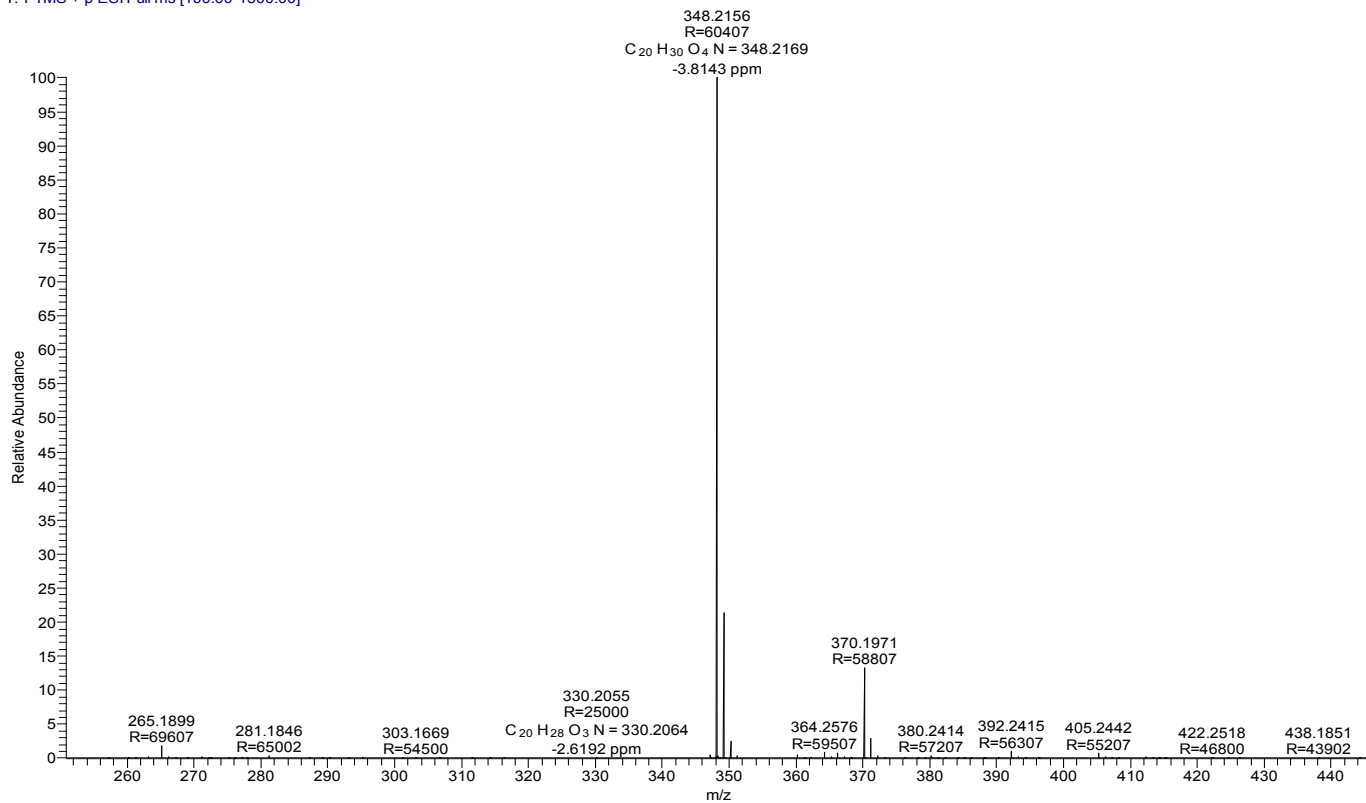


LC-MS of Compound 14

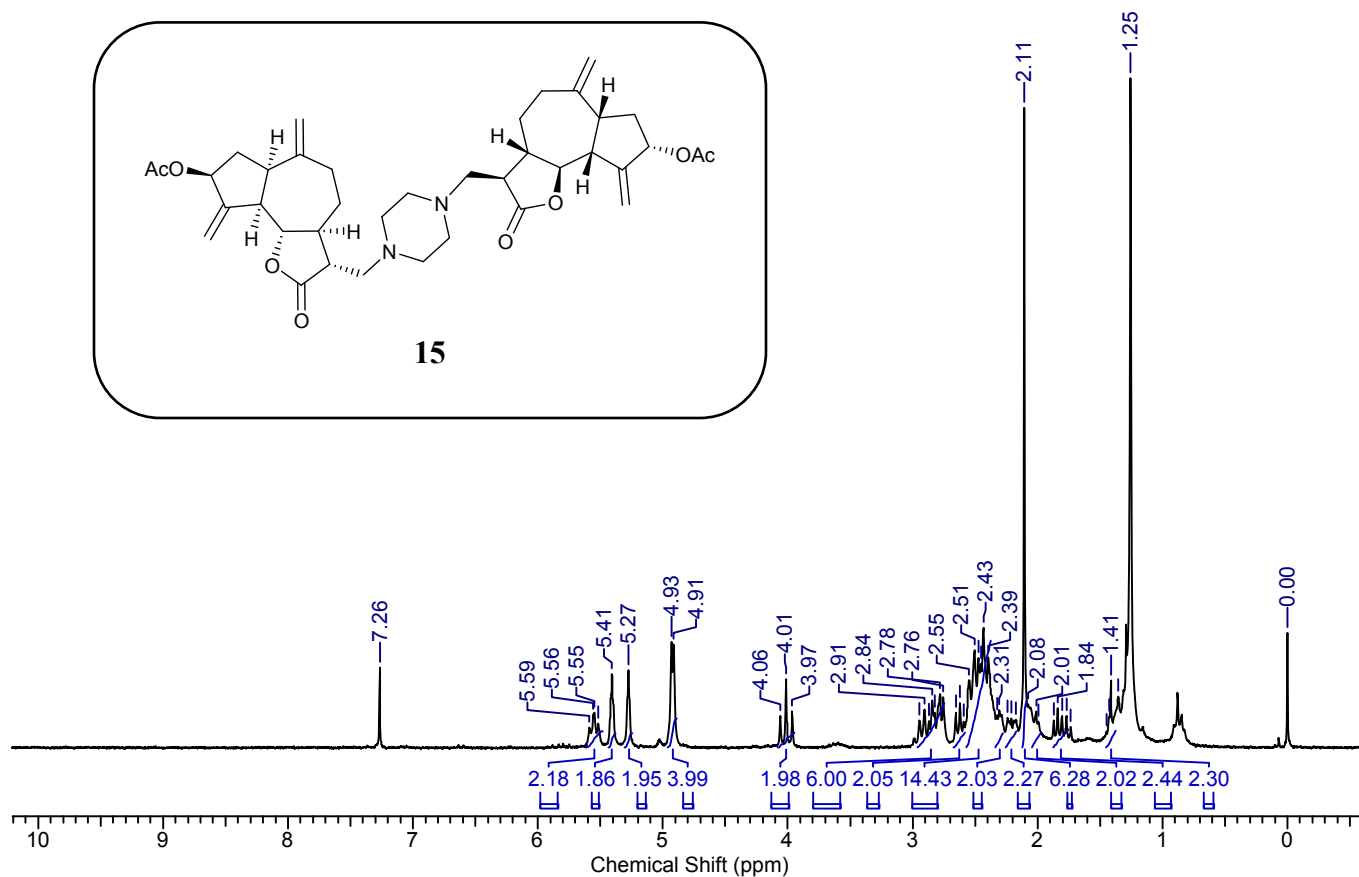
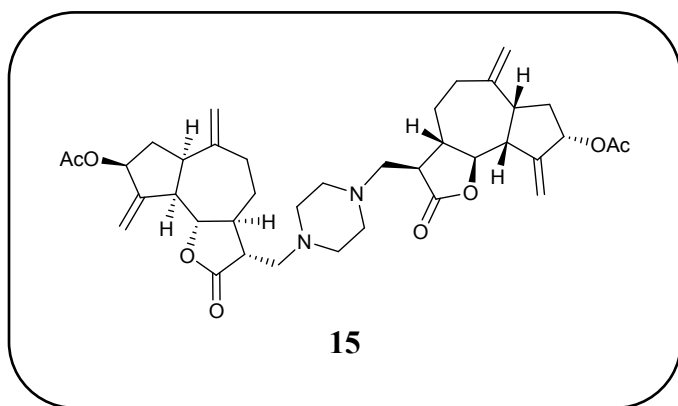


HR-MS of Compound 14

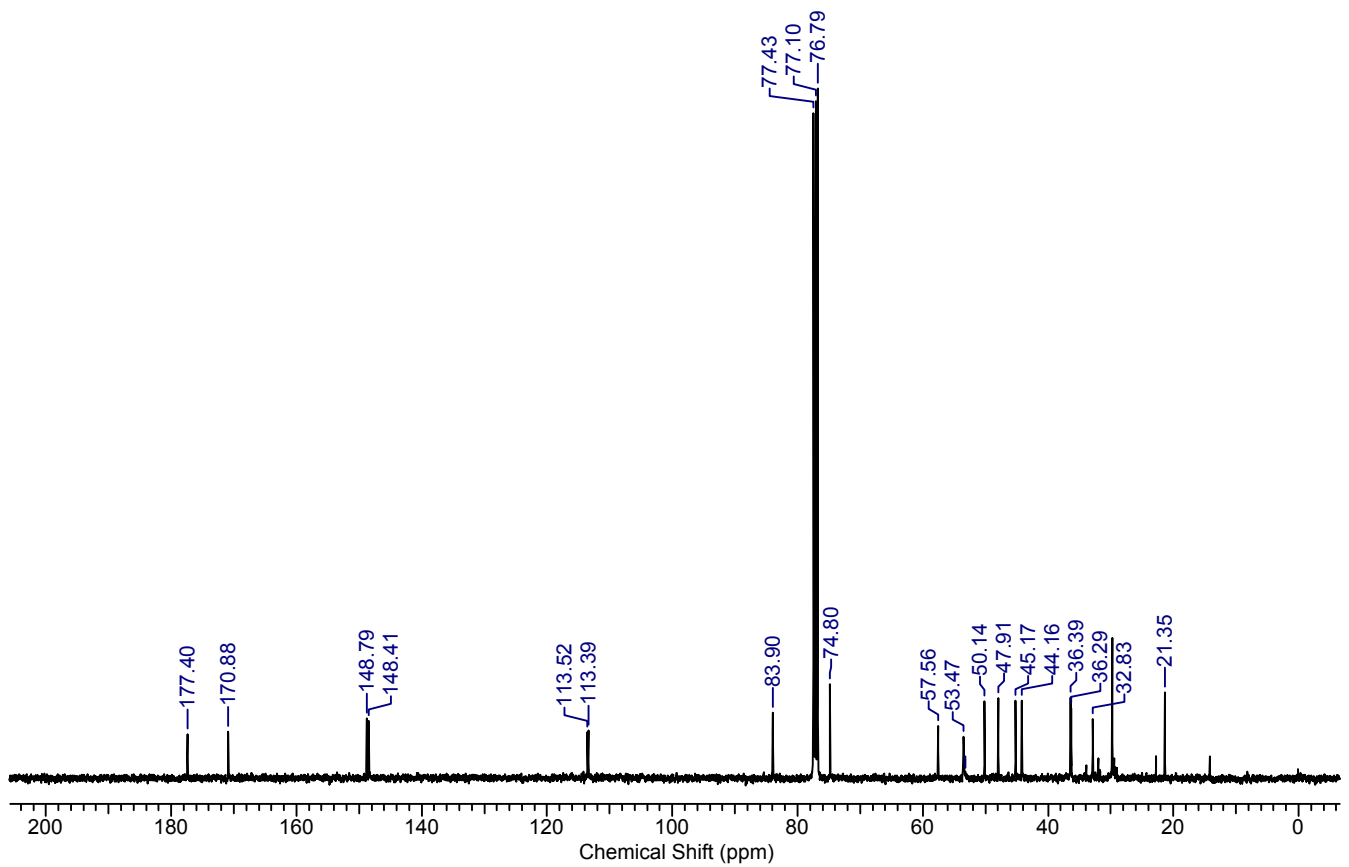
IS-278-B #89 RT: 0.39 AV: 1 NL: 9.00E9
T: FTMS + p ESI Full ms [100.00-1500.00]



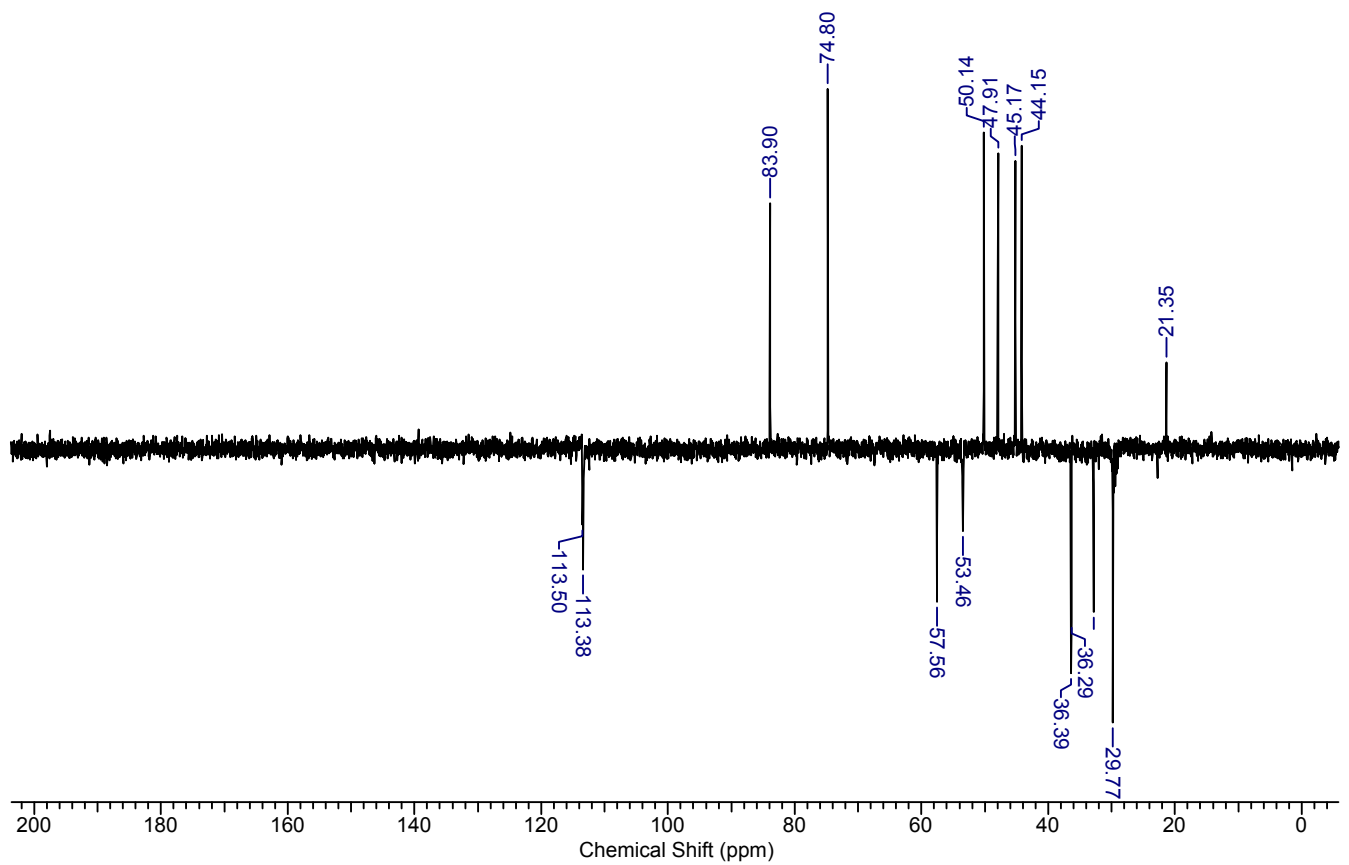
¹H NMR of Compound 15 (200 MHz, CDCl₃)



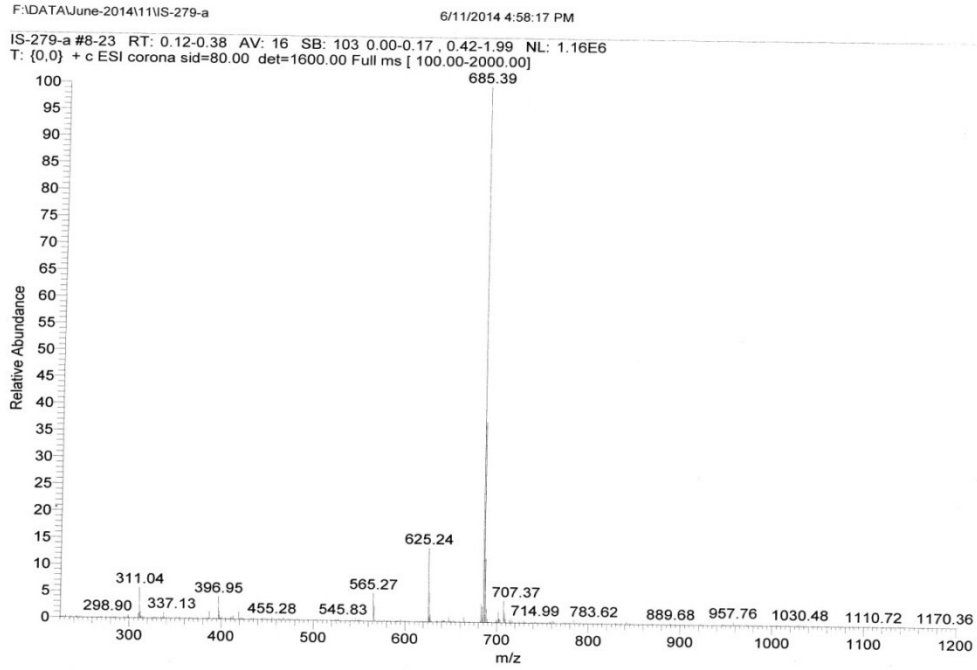
¹³C NMR of Compound 15 (100 MHz, CDCl₃)



DEPT of Compound 15 (100 MHz, CDCl₃)

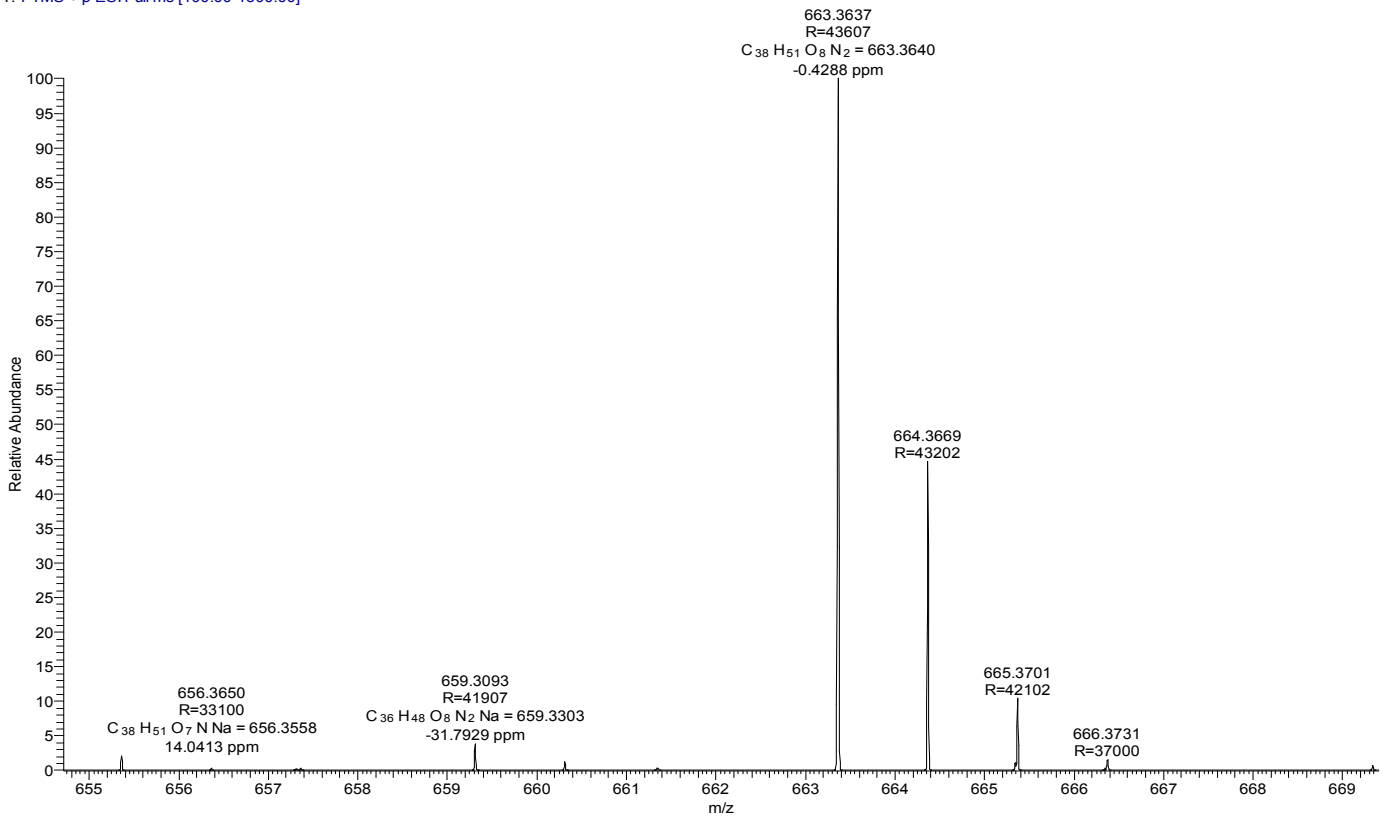


LC-MS of Compound 15

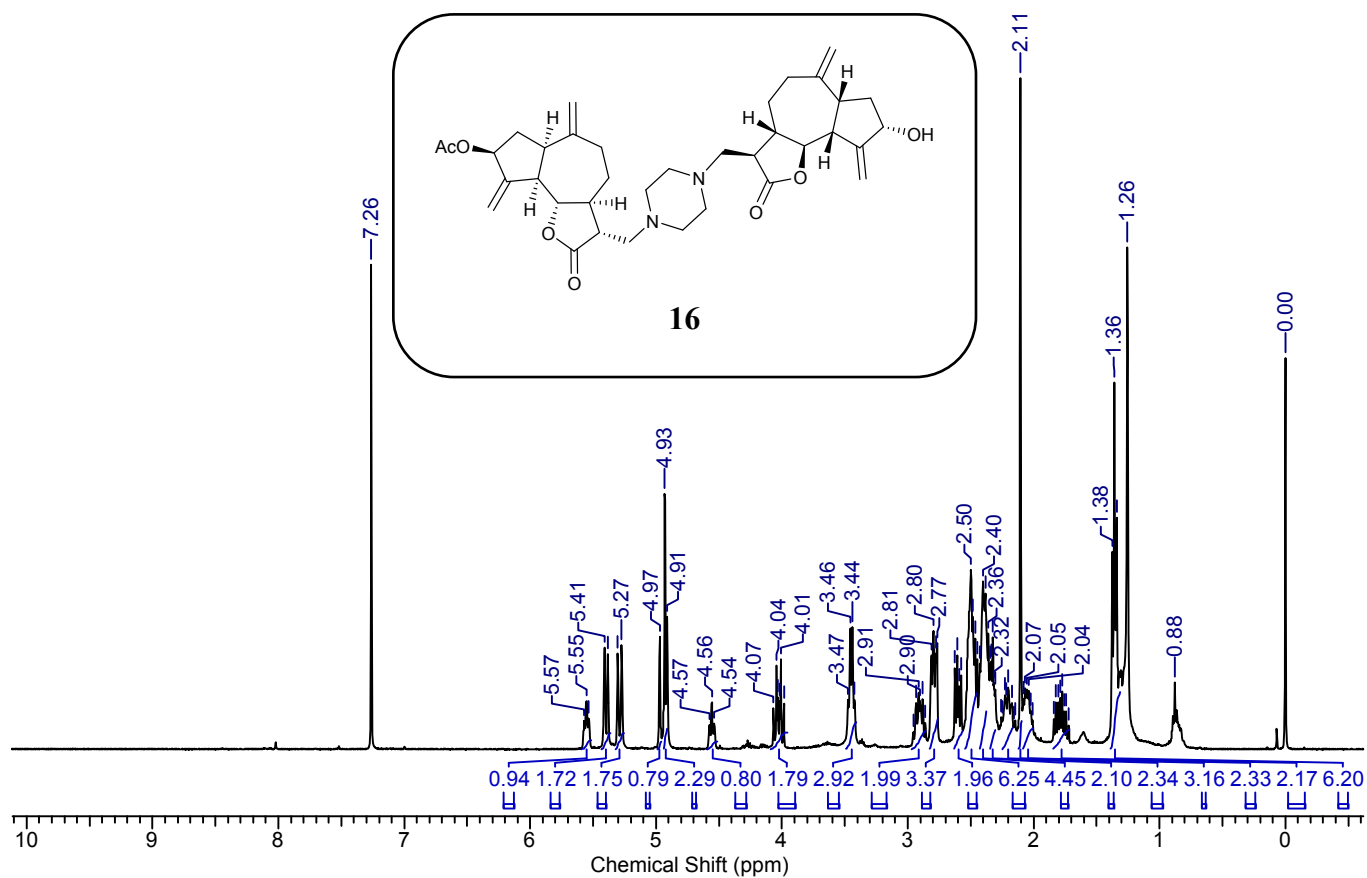


HR-MS of Compound 15

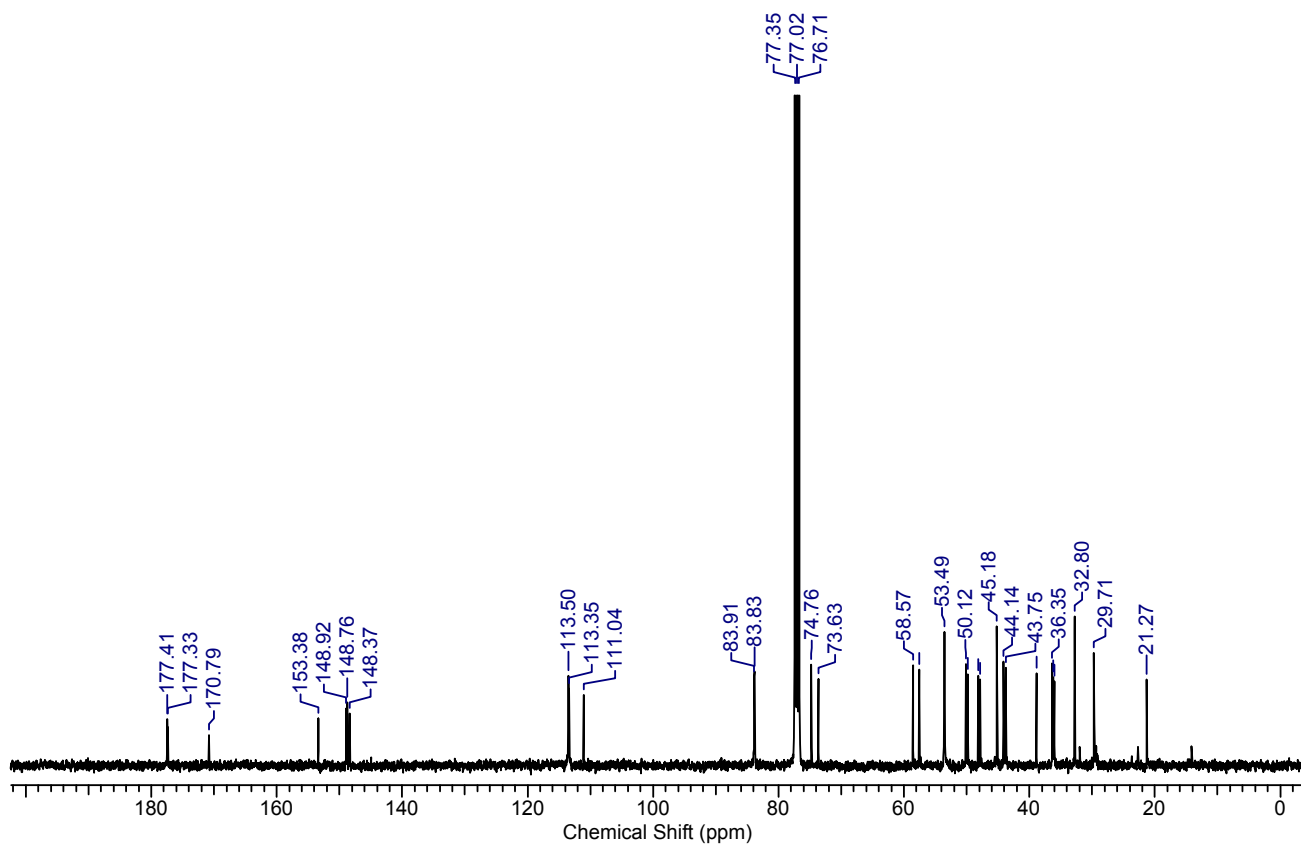
IS-279-B #86 RT: 0.38 AV: 1 NL: 1.01E8
T: FTMS + p ESI Full ms [100.00-1500.00]



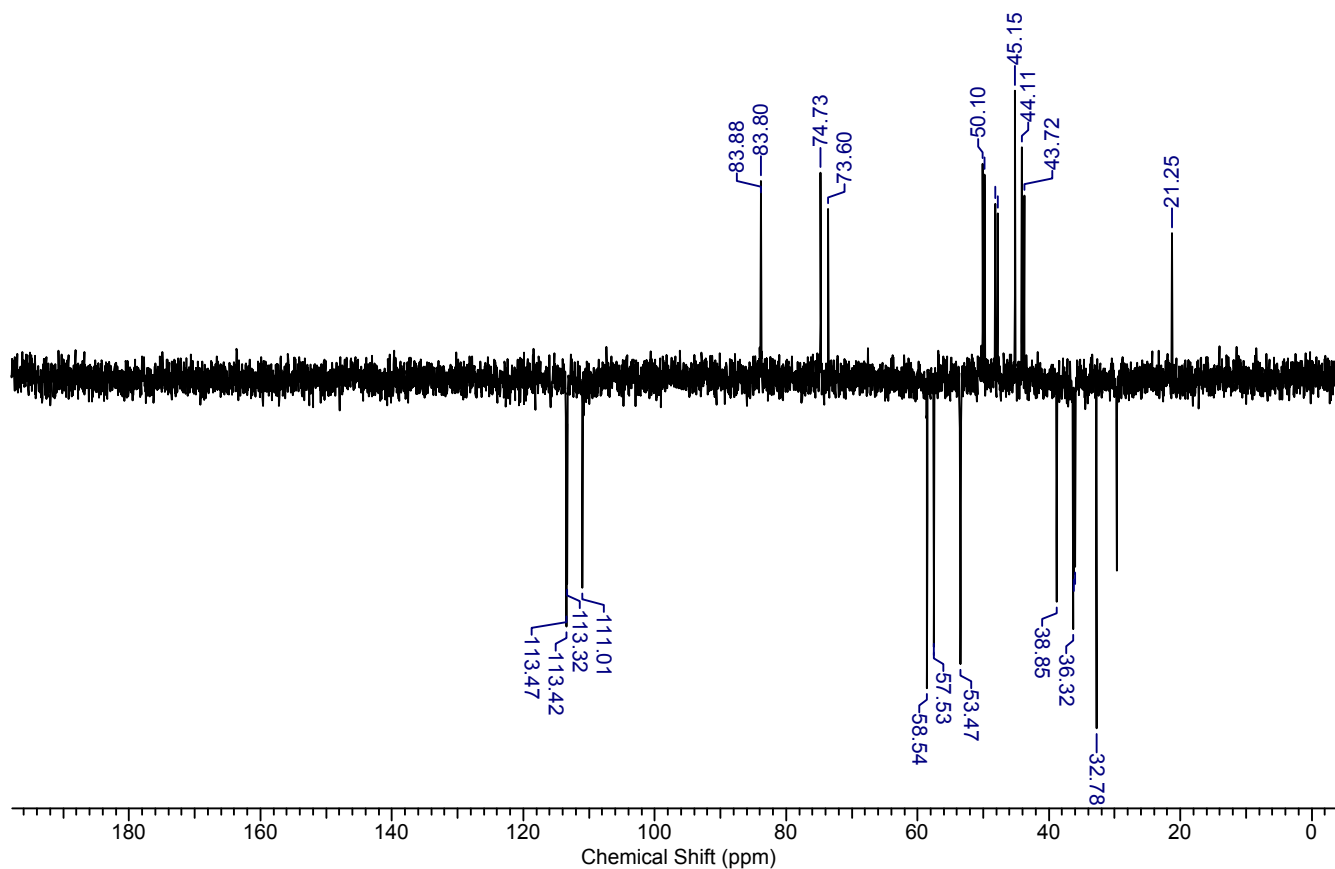
¹H NMR of Compound 16 (200 MHz, CDCl₃)



¹³C NMR of Compound 16 (100 MHz, CDCl₃)



DEPT of Compound 16 (100 MHz, CDCl₃)

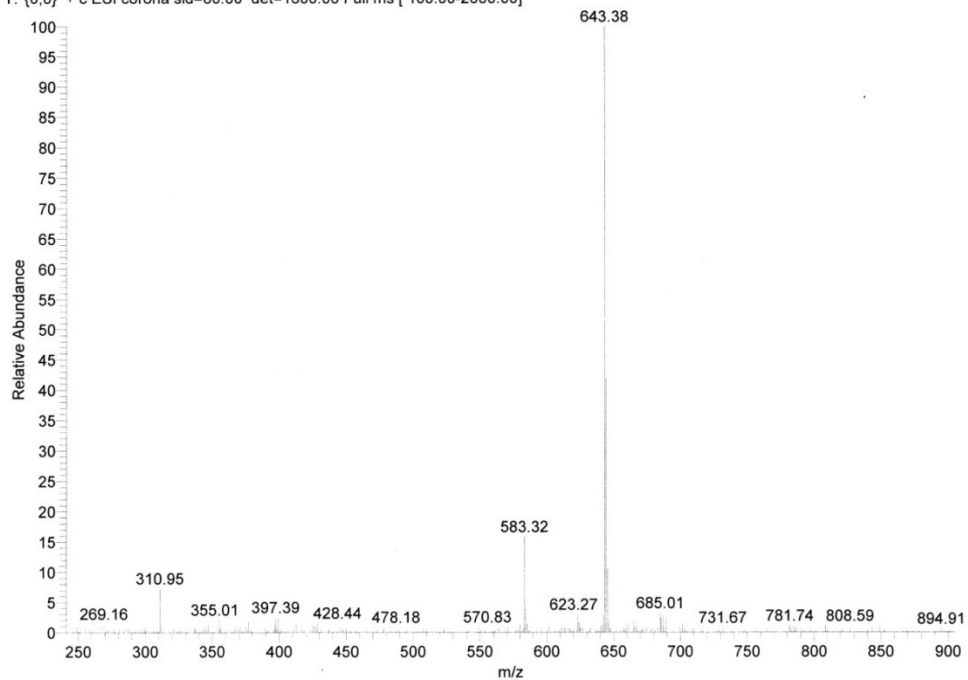


LC-MS of Compound 16

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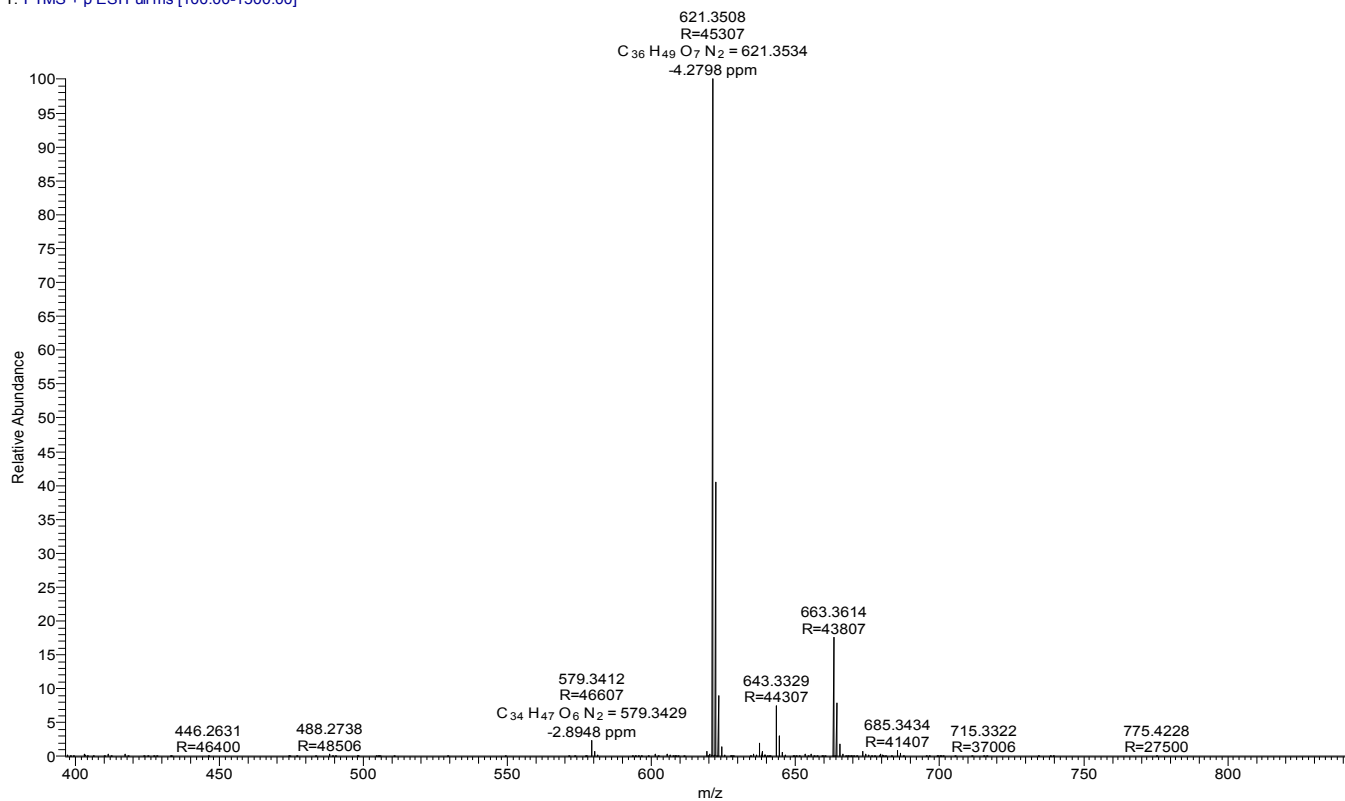
6/11/2014 5:00:54 PM

IS-279-B #7-22 RT: 0.10-0.36 AV: 16 SB: 61 0.00-0.19, 0.36-1.20 NL: 2.48E5
T: {0,0} +c ESI corona sid=80.00 det=1600.00 Full ms [100.00-2000.00]

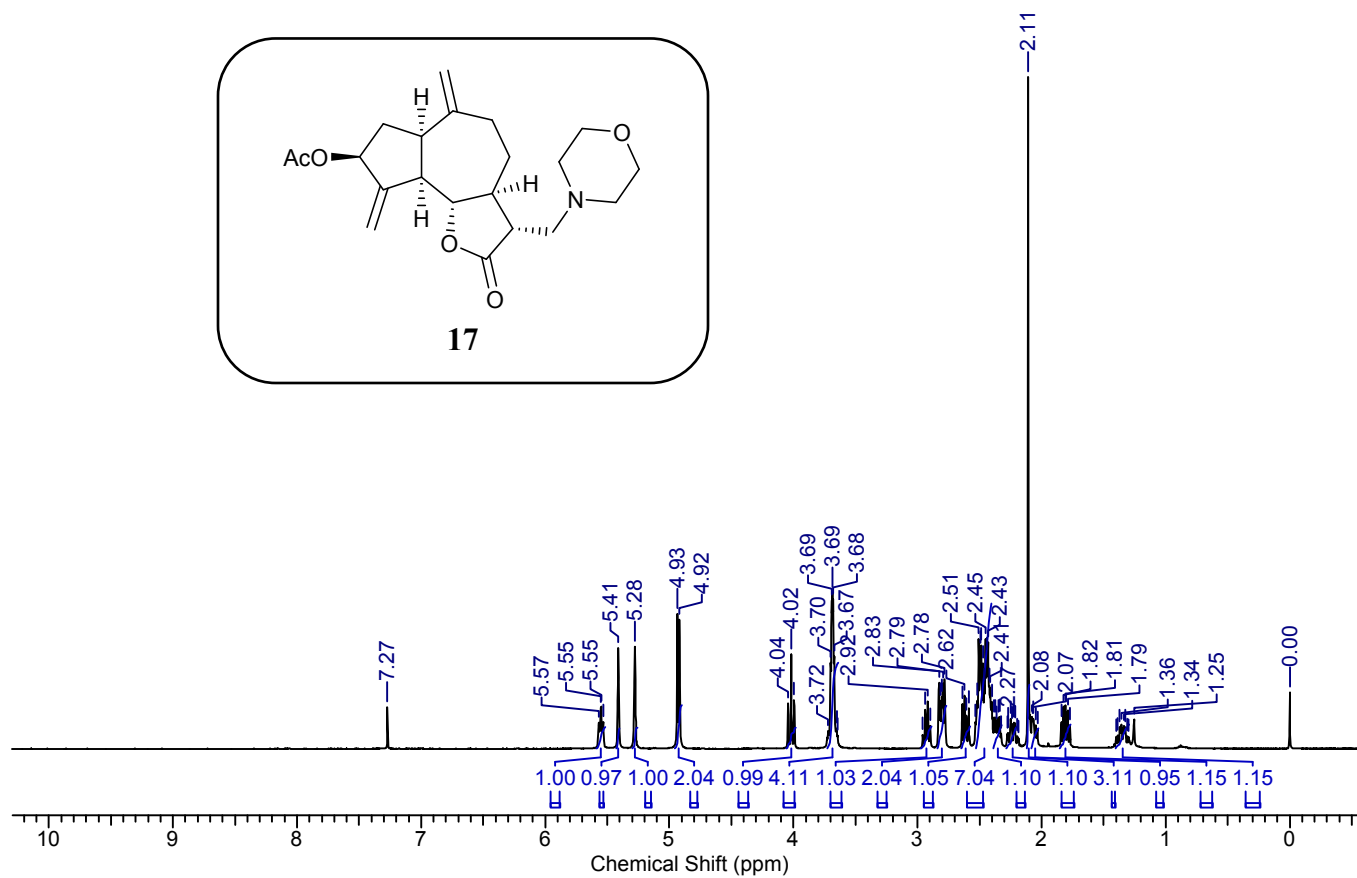
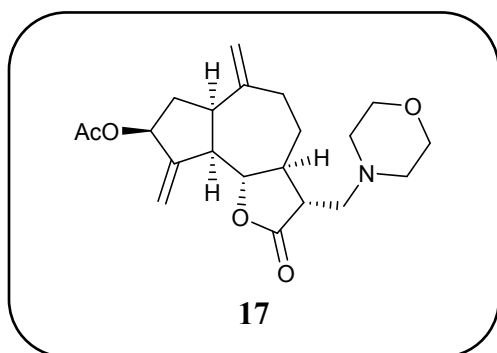


HR-MS of Compound 16

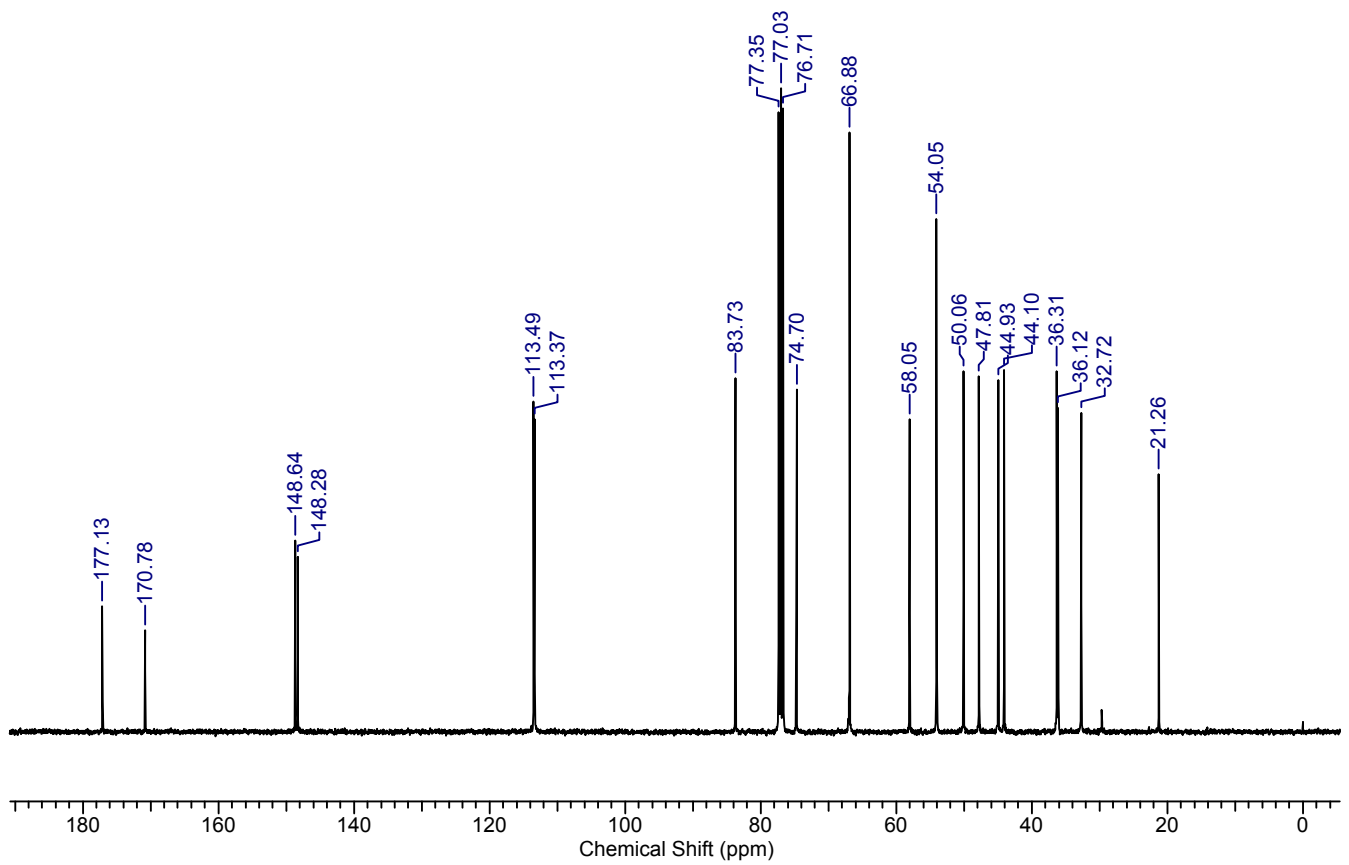
IS-279-B #80 RT: 0.35 AV: 1 NL: 2.42E9
T: FTMS + p ESI Full ms [100.00-1500.00]



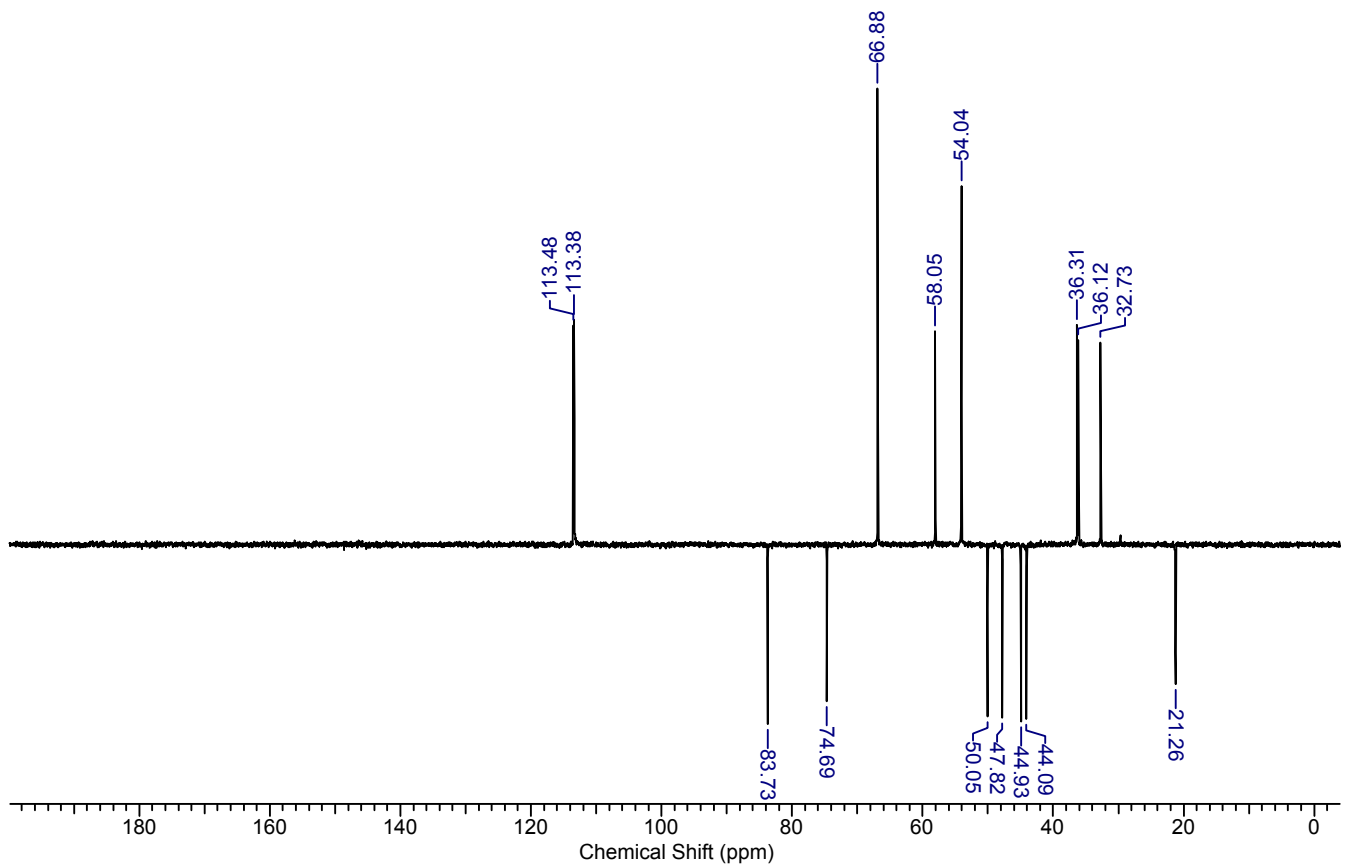
¹H NMR of Compound 17 (400 MHz, CDCl₃)



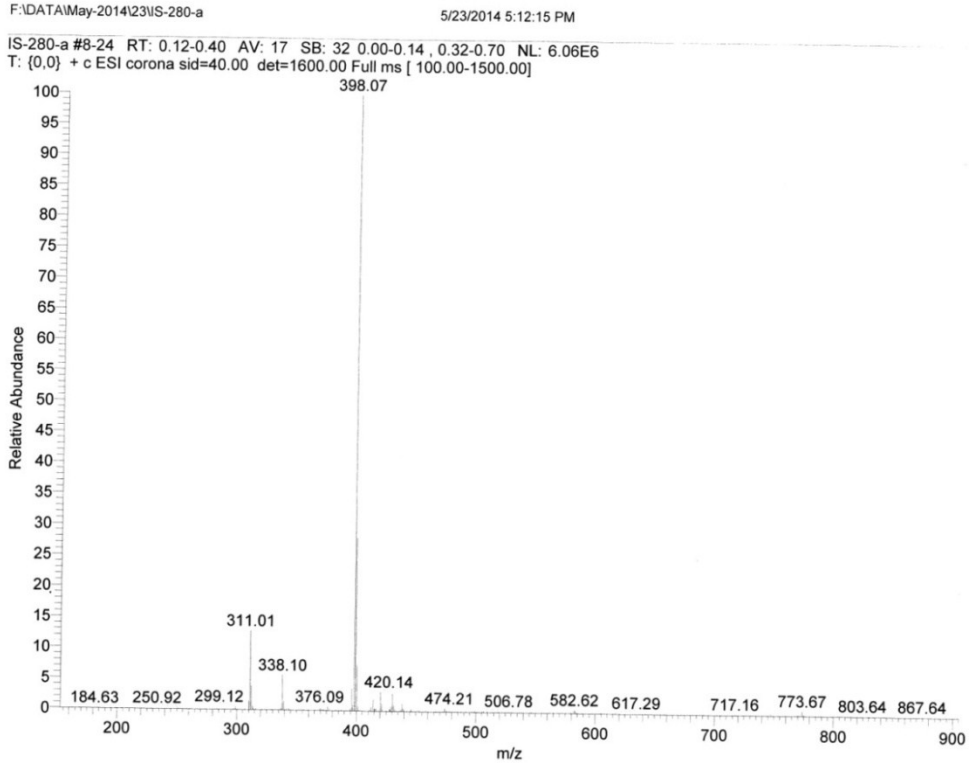
^{13}C NMR of Compound 17 (100 MHz, CDCl_3)



DEPT of Compound 17 (100 MHz, CDCl_3)

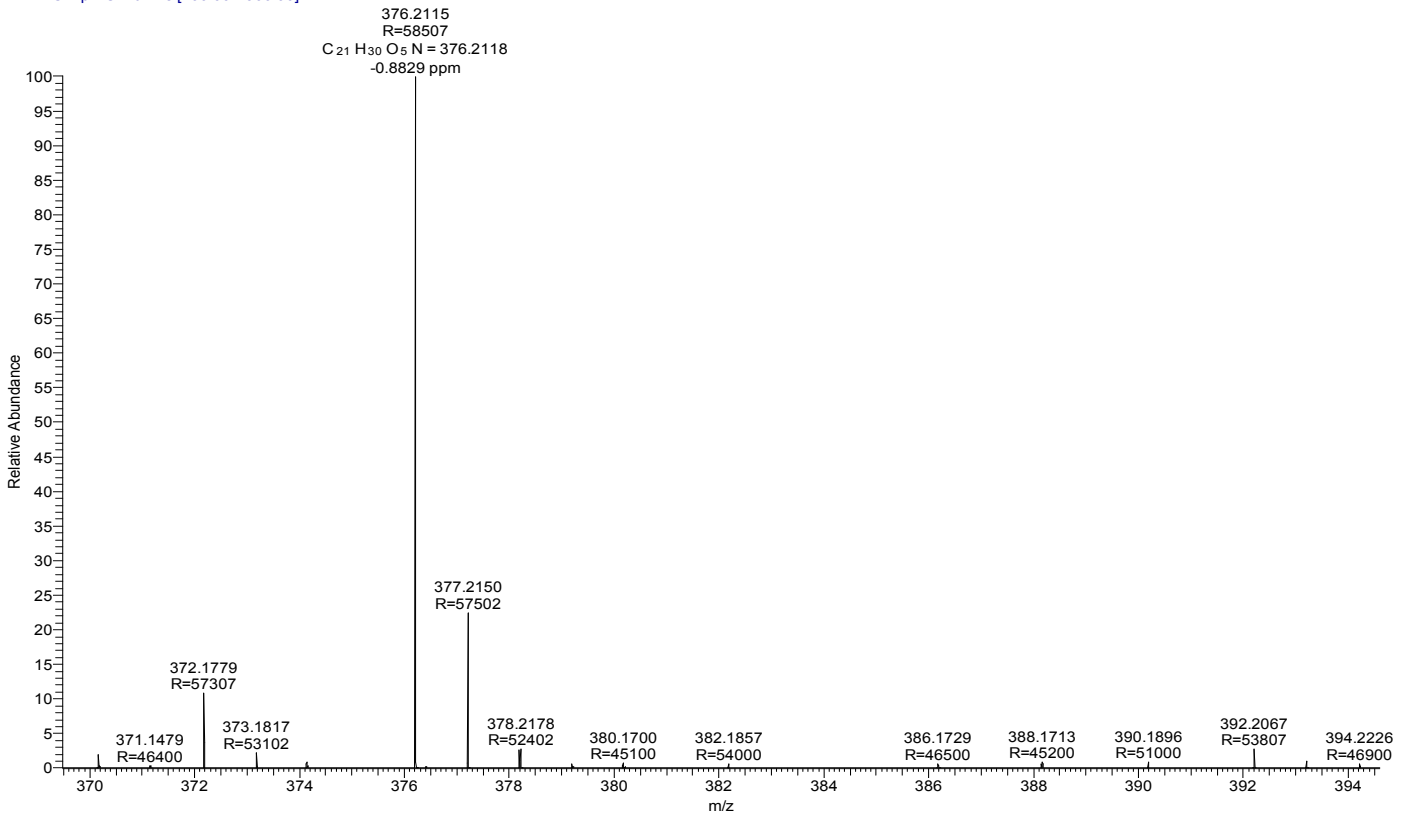


LC-MS of Compound 17

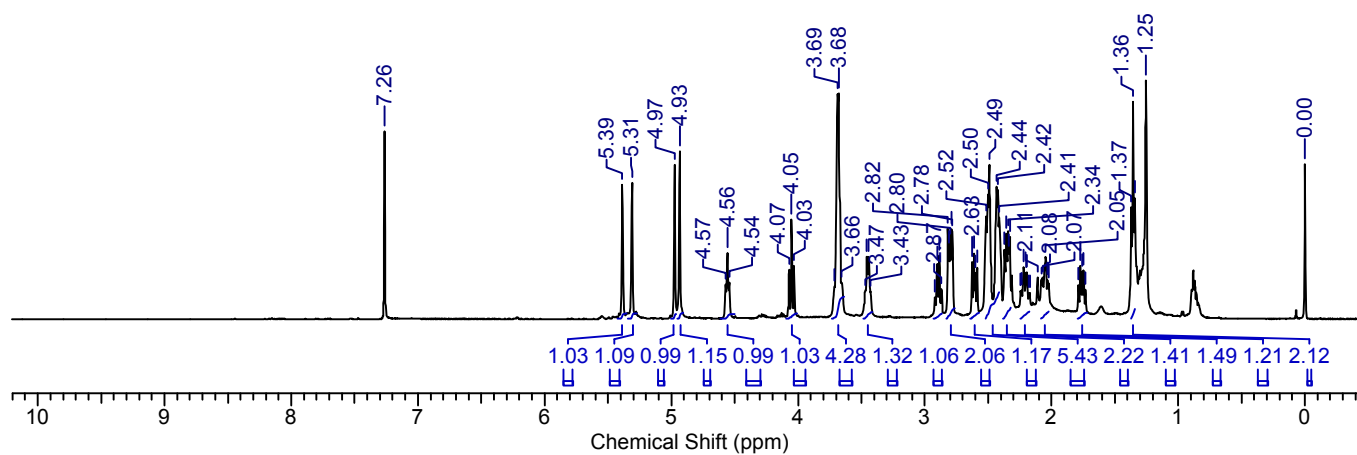
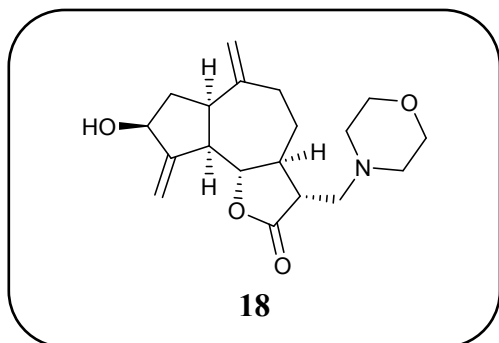


HR-MS of Compound 17

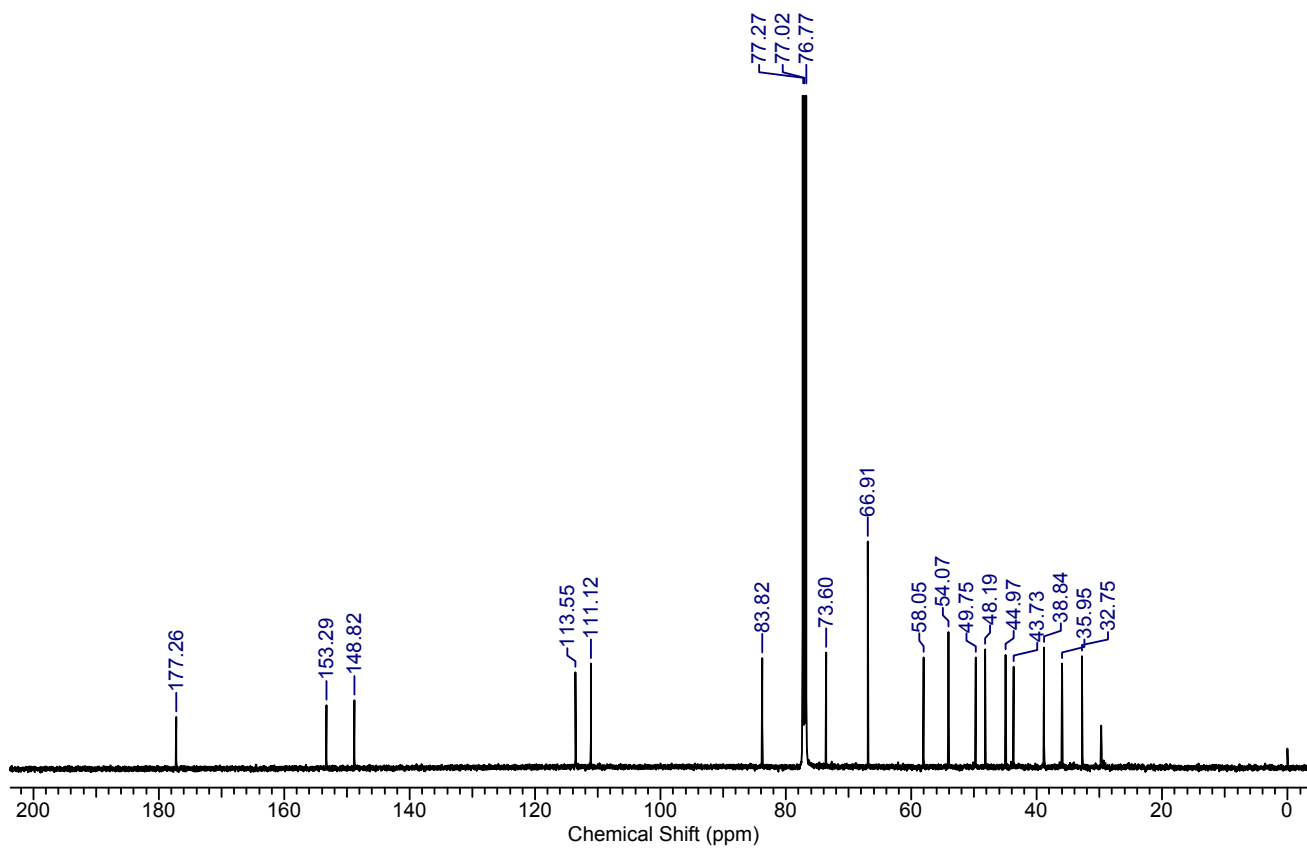
IS-280-B #87 RT: 0.38 AV: 1 NL: 1.64E8
T: FTMS + p ESI Full ms [100.00-1500.00]



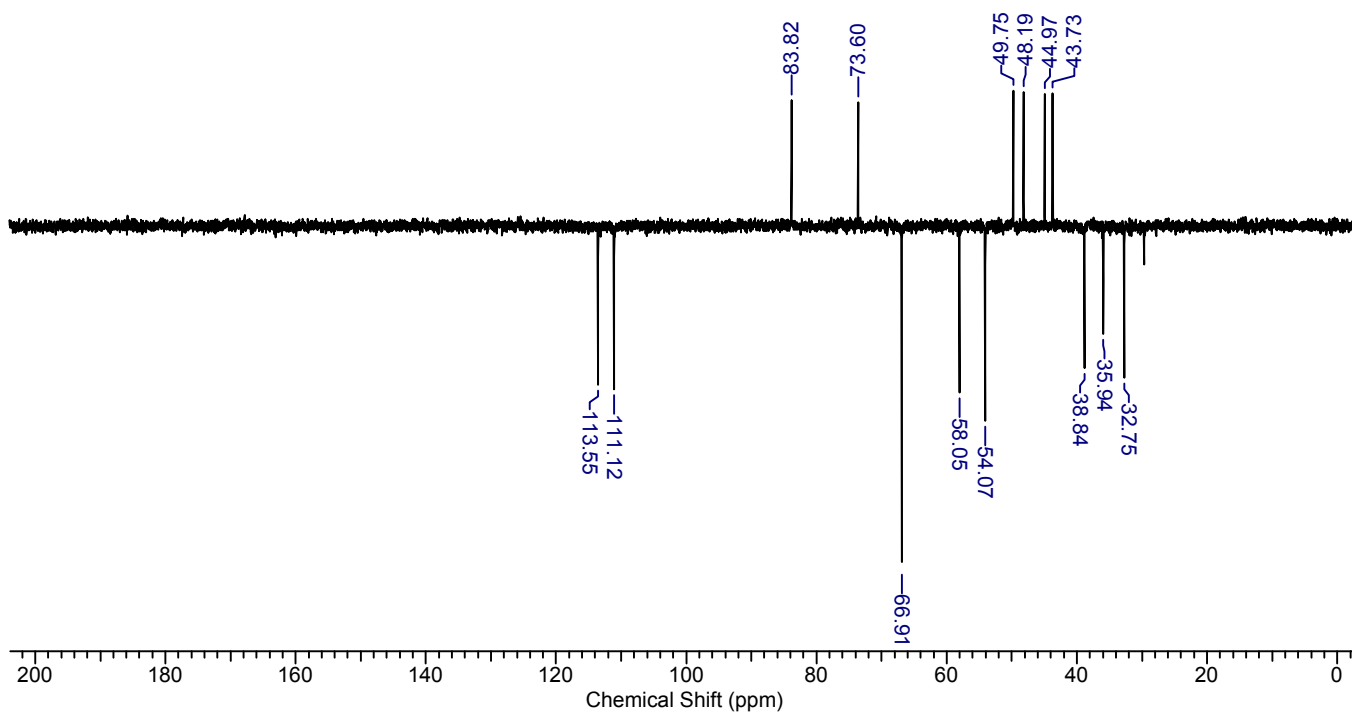
¹H NMR of Compound 18 (500 MHz, CDCl₃)



¹³C NMR of Compound 18 (125 MHz, CDCl₃)



DEPT of Compound 18 (125 MHz, CDCl₃)

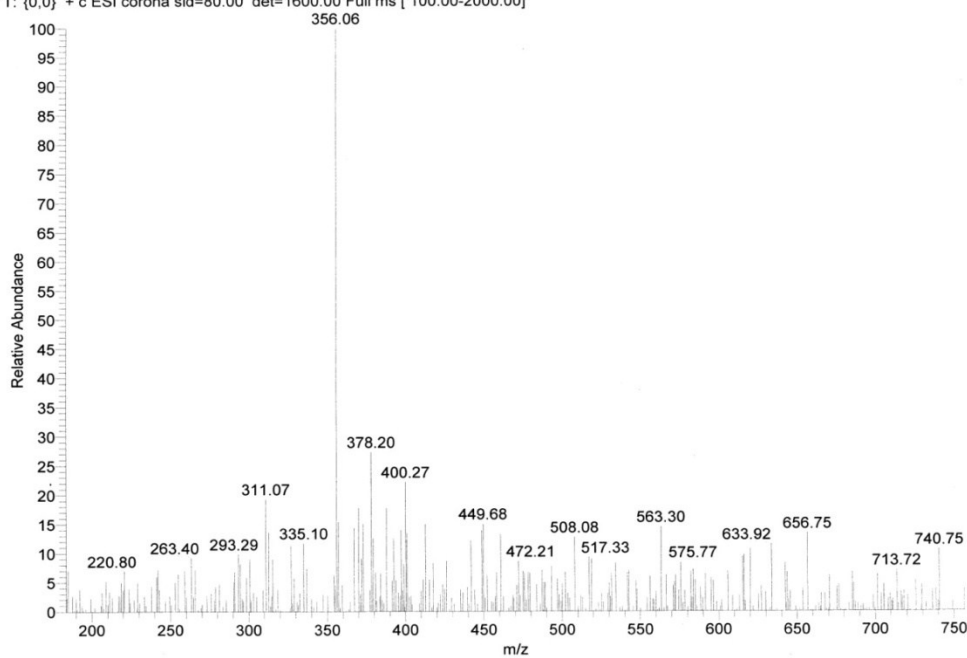


LC-MS of Compound 18

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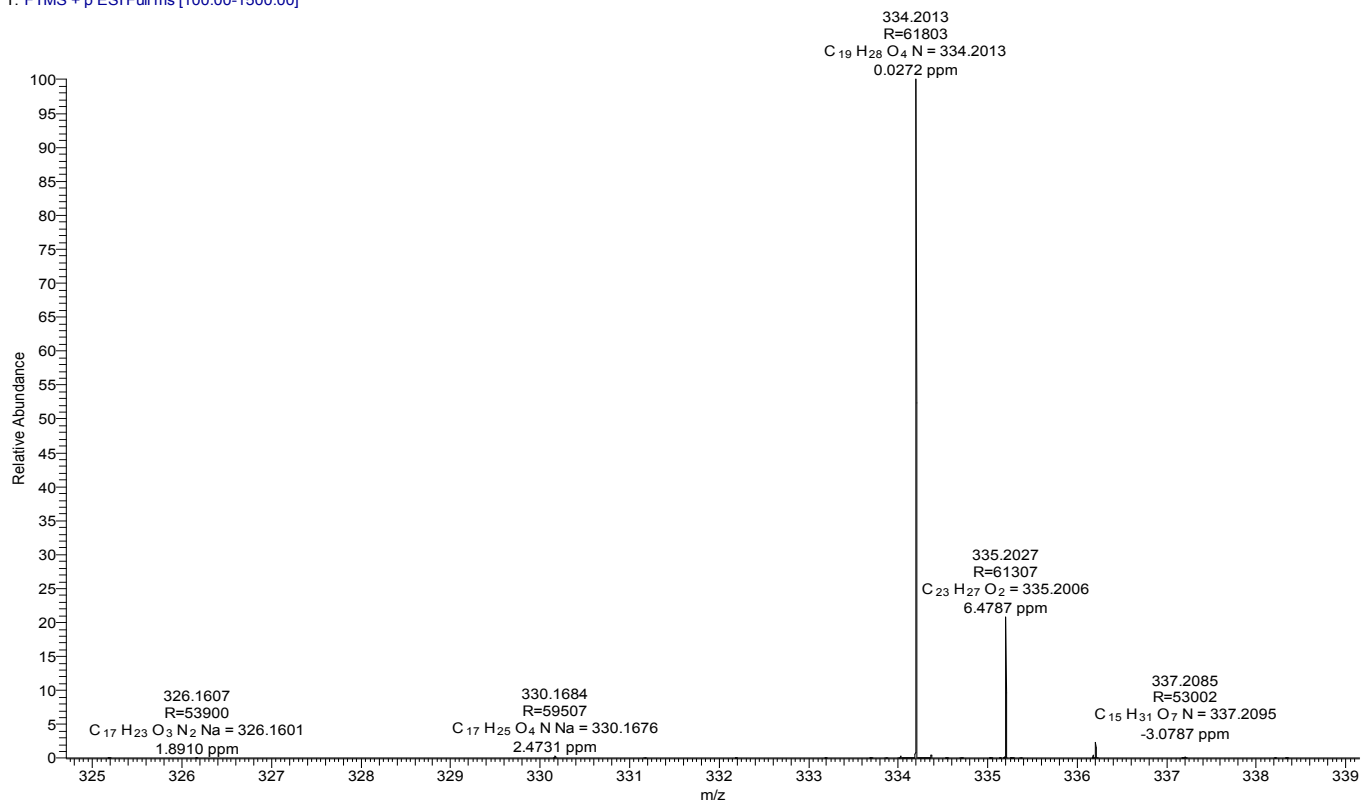
6/11/2014 5:02:42 PM

IS-280-b #10-17 RT: 0.16-0.28 AV: 8 SB: 43 0.00-0.17, 0.29-0.83 NL: 3.31E4
T: (0,0) + c ESI corona sid=80.00 det=1600.00 Full ms [100.00-2000.00]

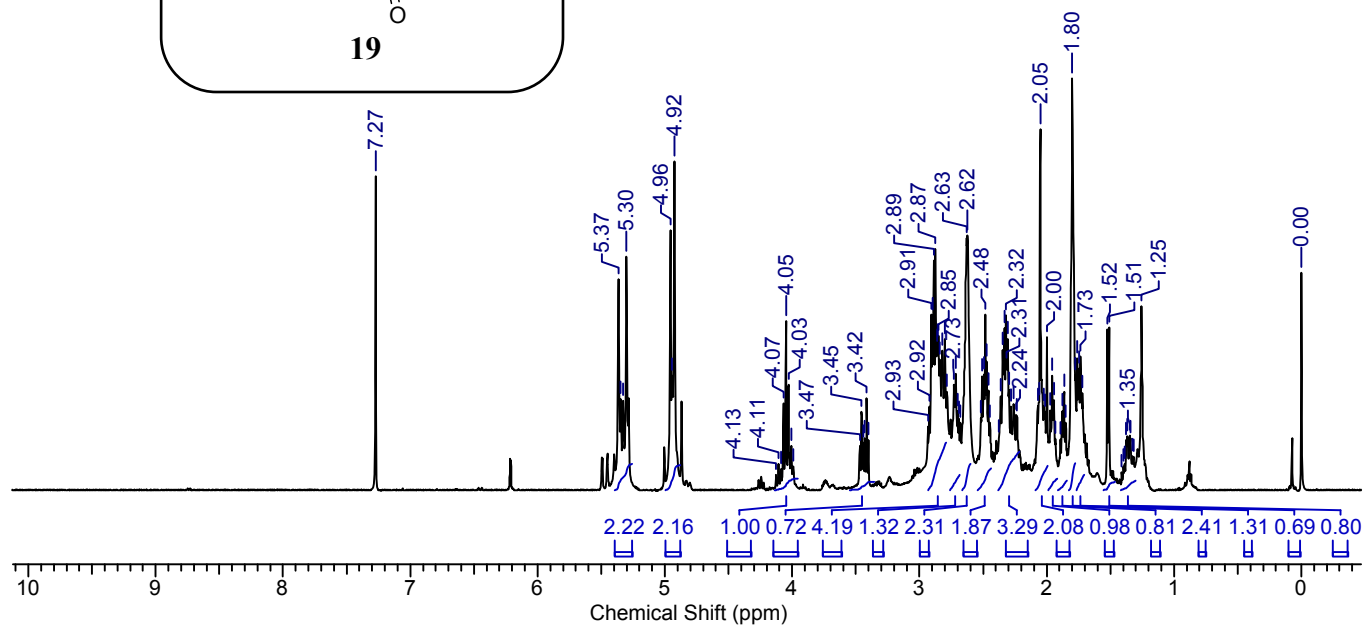
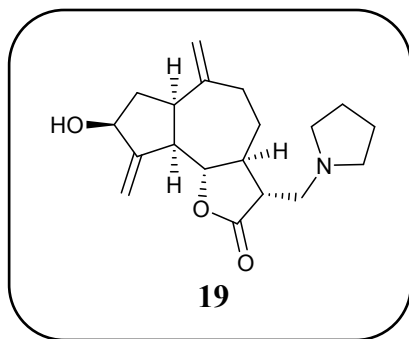


HR-MS of Compound 18

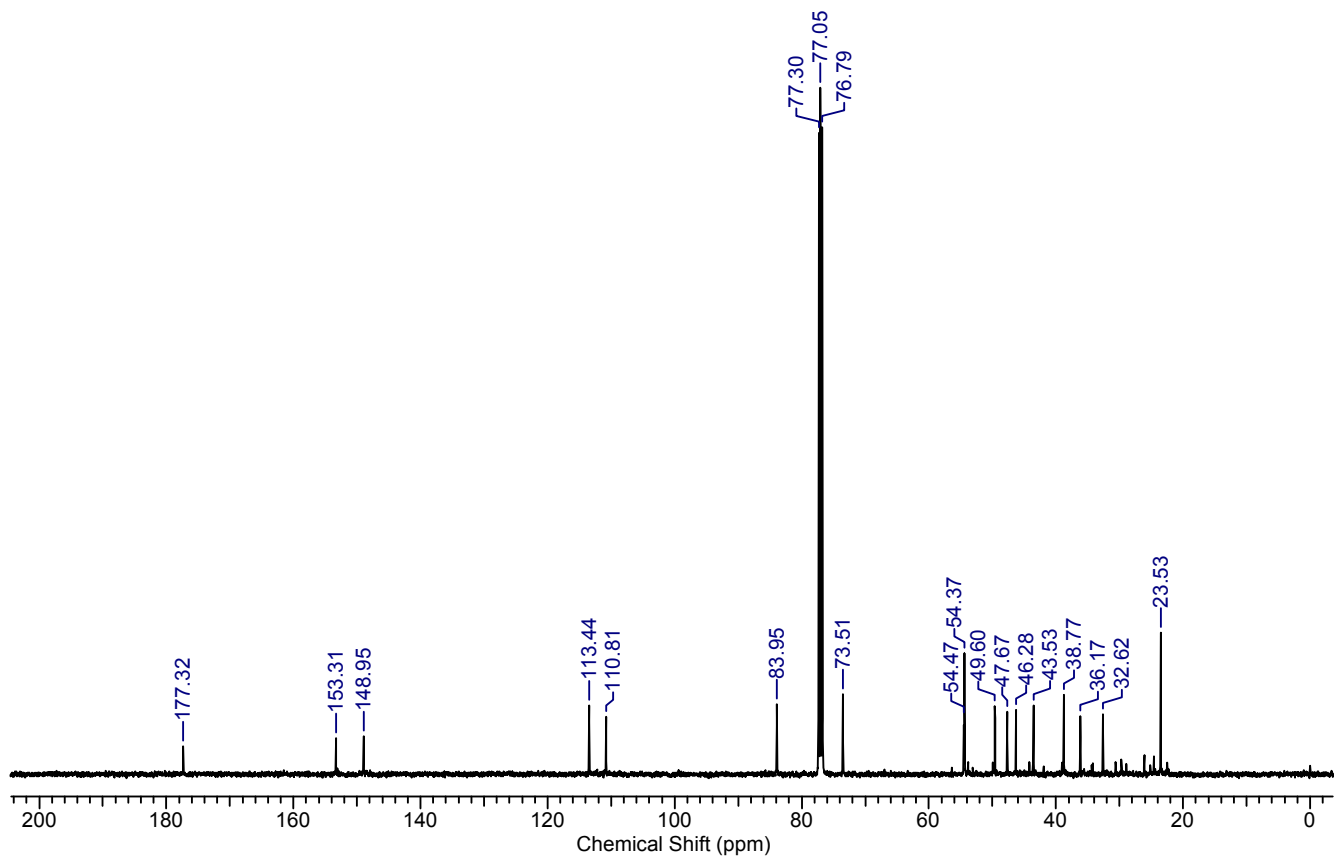
IS-280-B #86 RT: 0.38 AV: 1 NL: 3.27E9
T: FTMS + p ESI Full ms [100.00-1500.00]



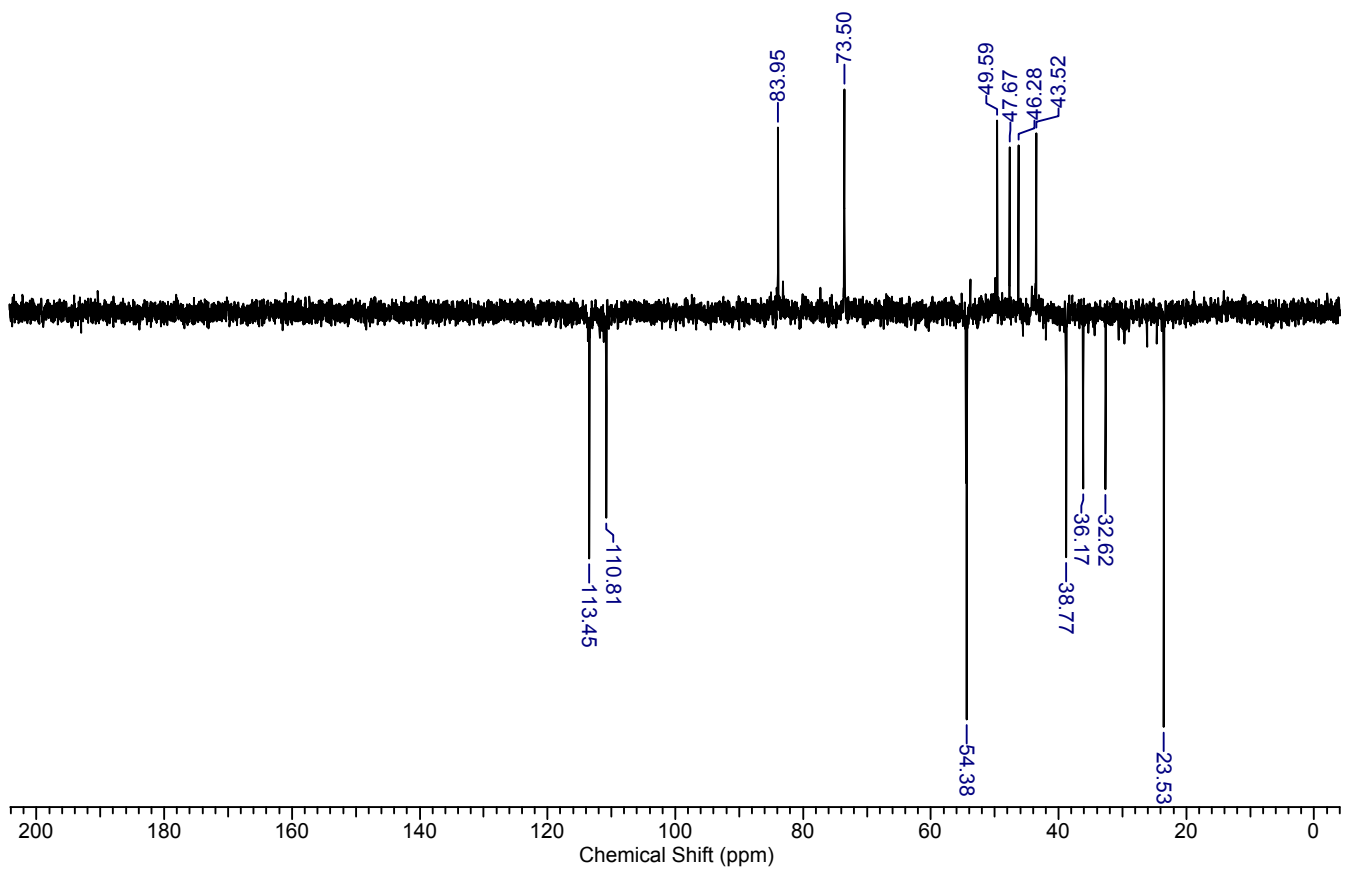
¹H NMR of Compound 19 (500 MHz, CDCl₃)



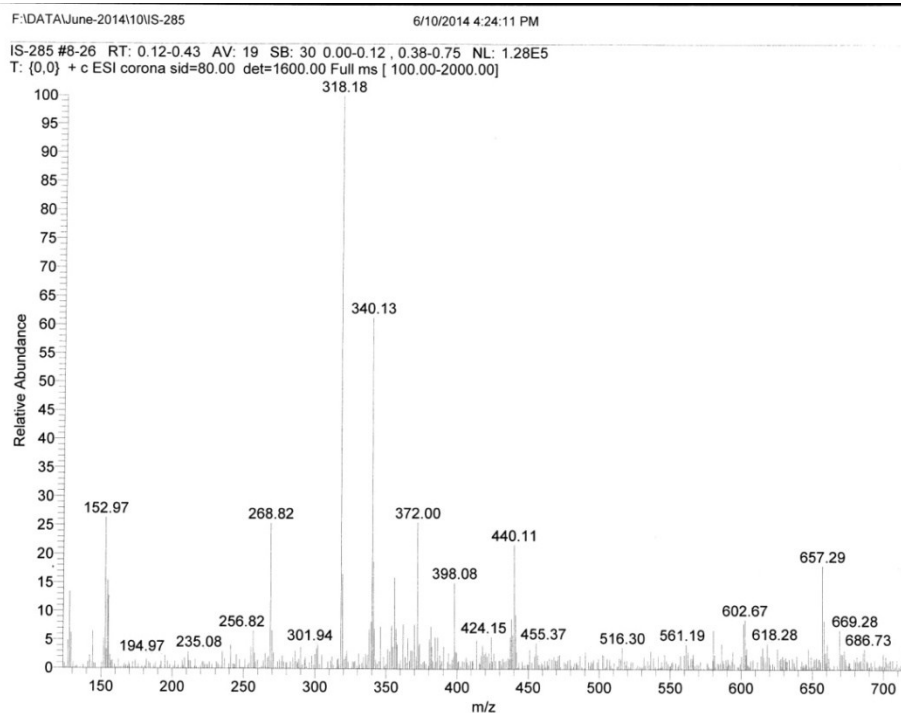
^{13}C NMR of Compound 19 (125 MHz, CDCl_3)



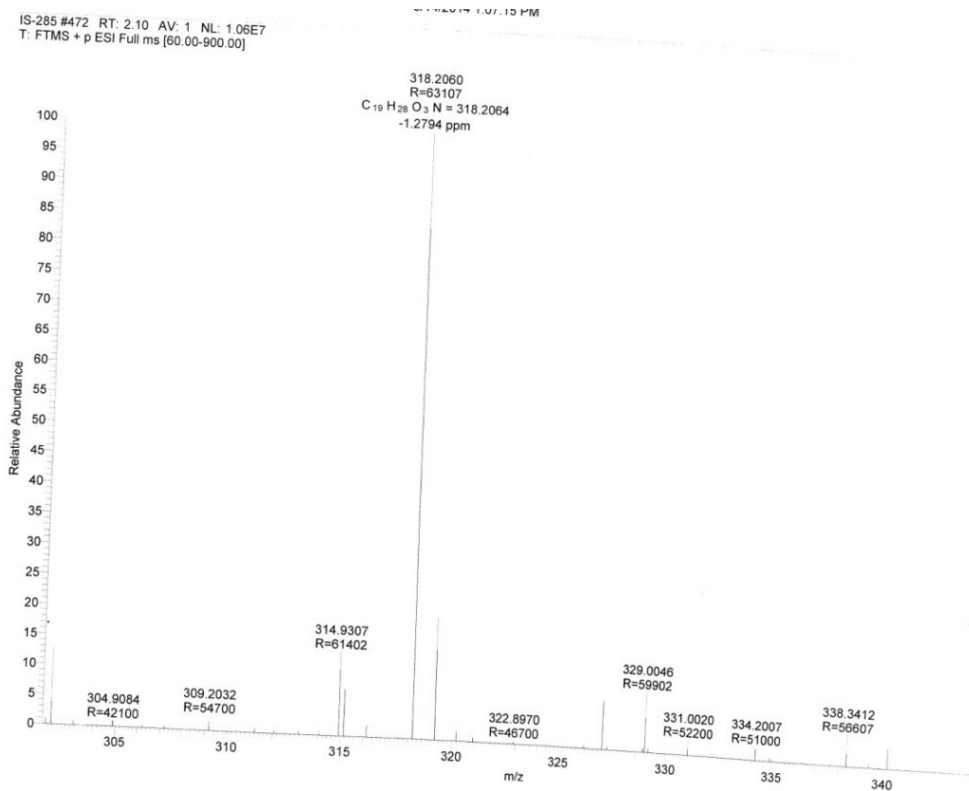
DEPT of Compound 19 (125 MHz, CDCl_3)



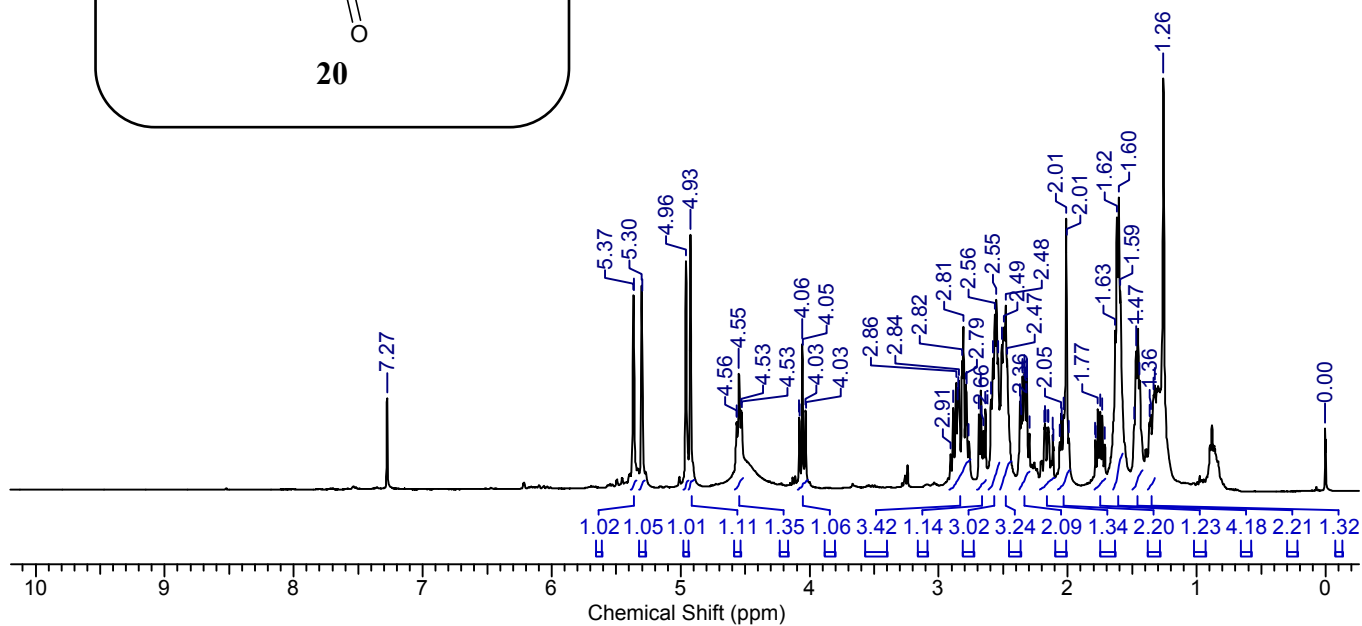
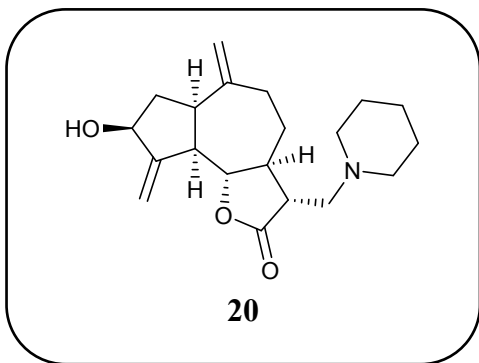
LC-MS of Compound 19



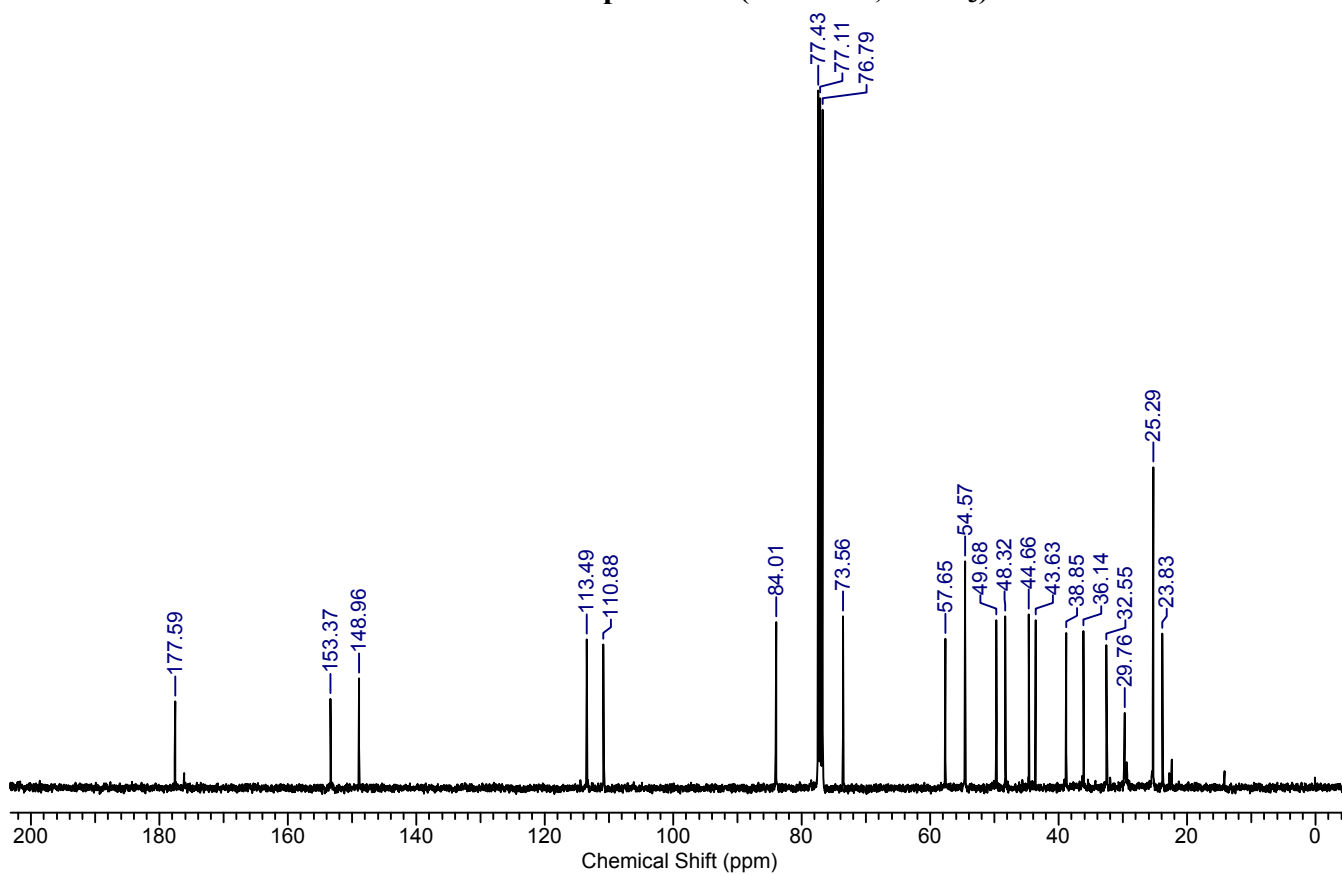
HR-MS of Compound 19



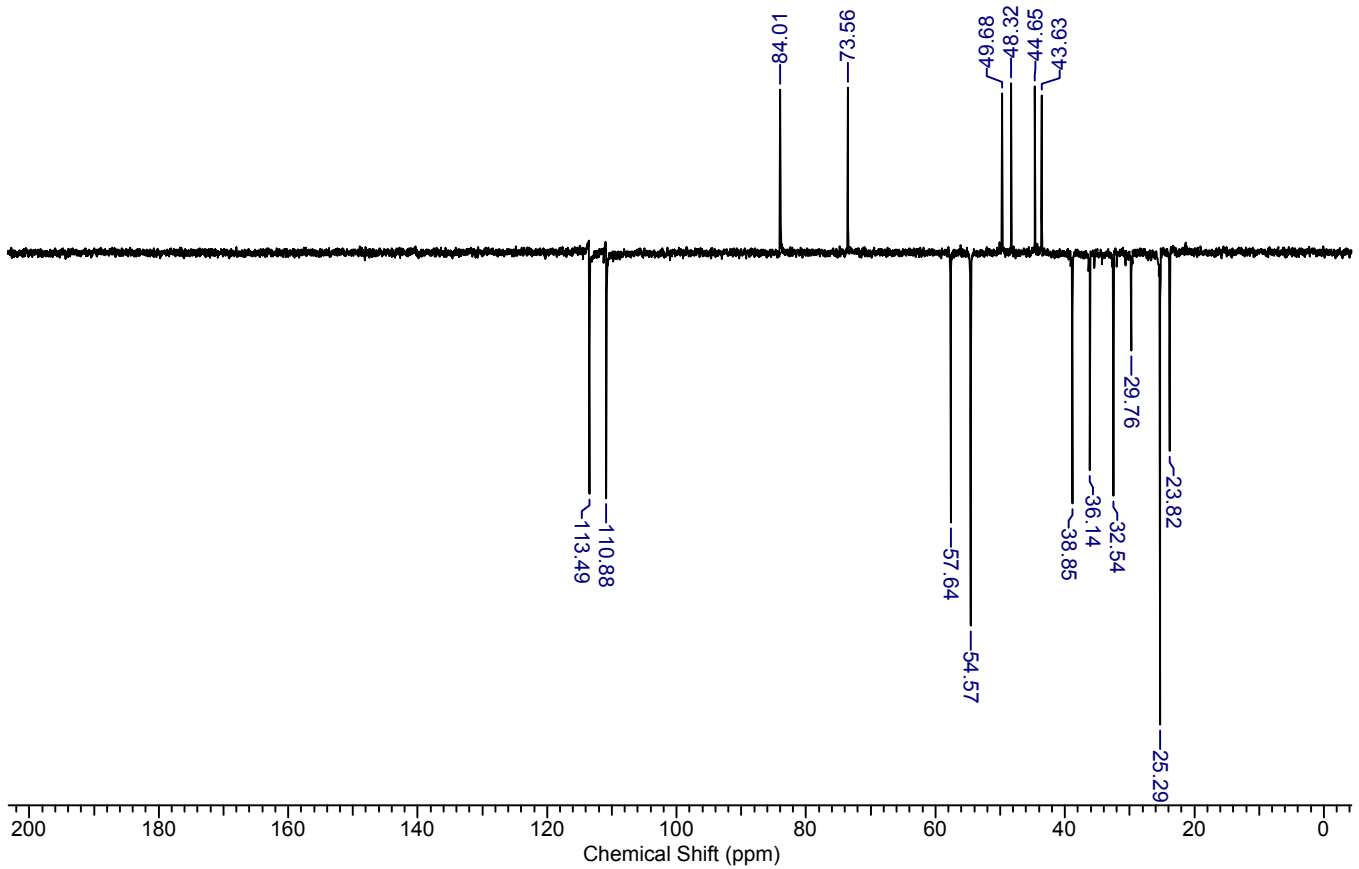
¹H NMR of Compound 20 (400 MHz, CDCl₃)



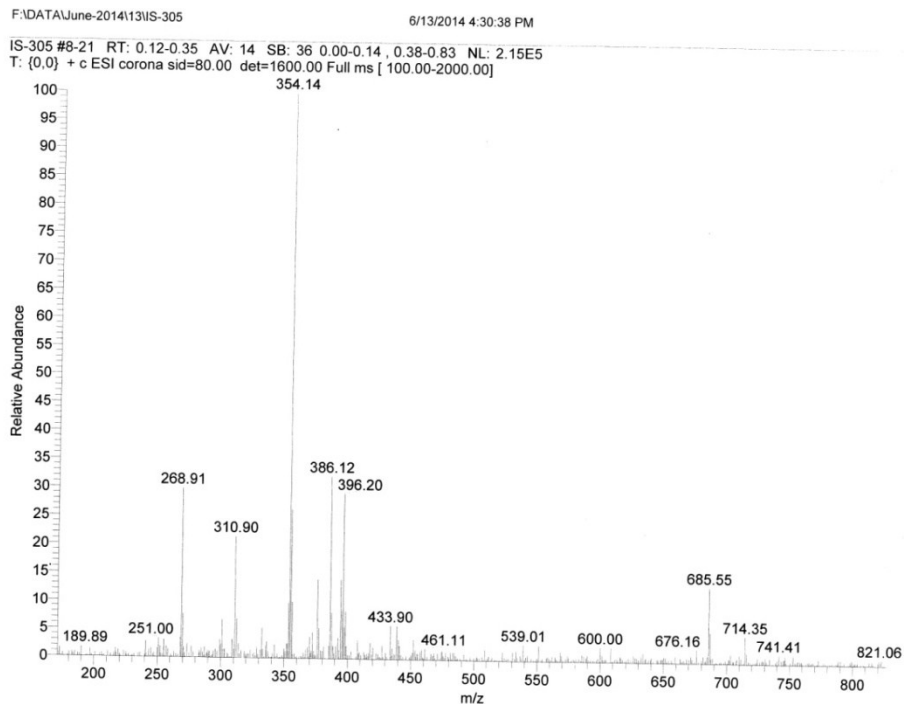
¹³C NMR of Compound 20 (100 MHz, CDCl₃)



DEPT of Compound 20 (100 MHz, CDCl₃)

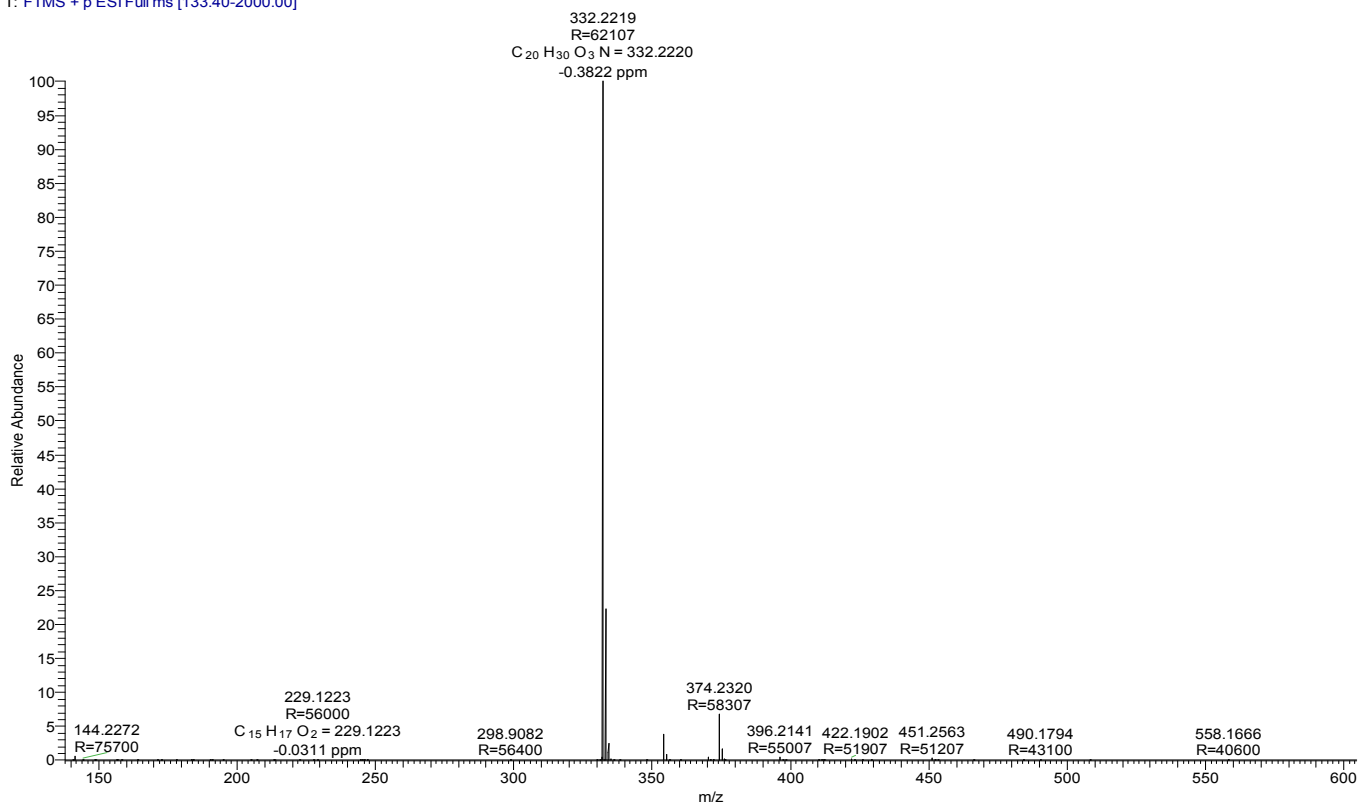


LC-MS of Compound 20

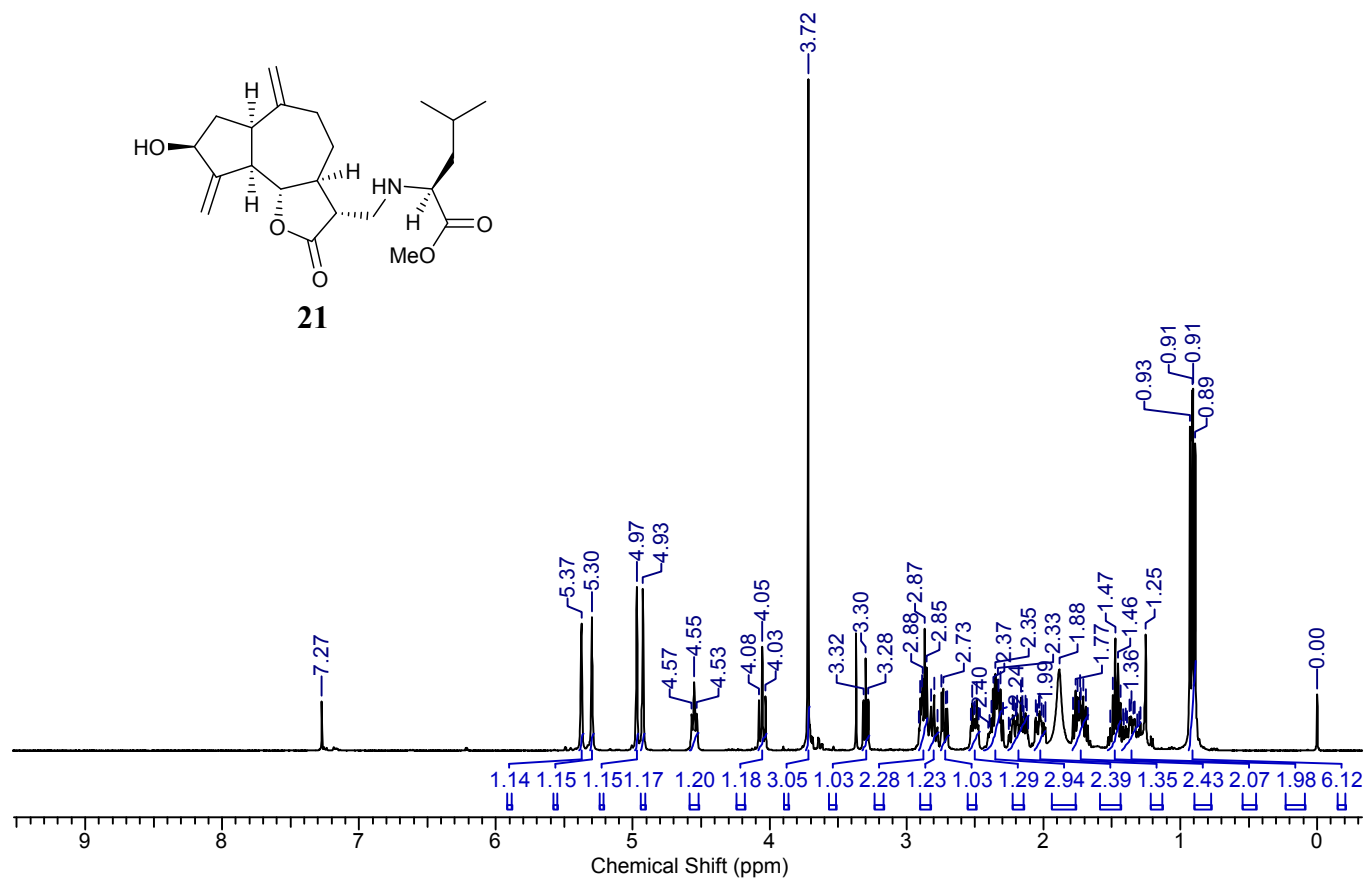
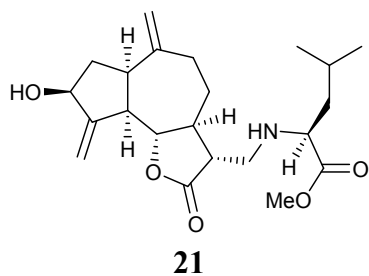


HR-MS of Compound 20

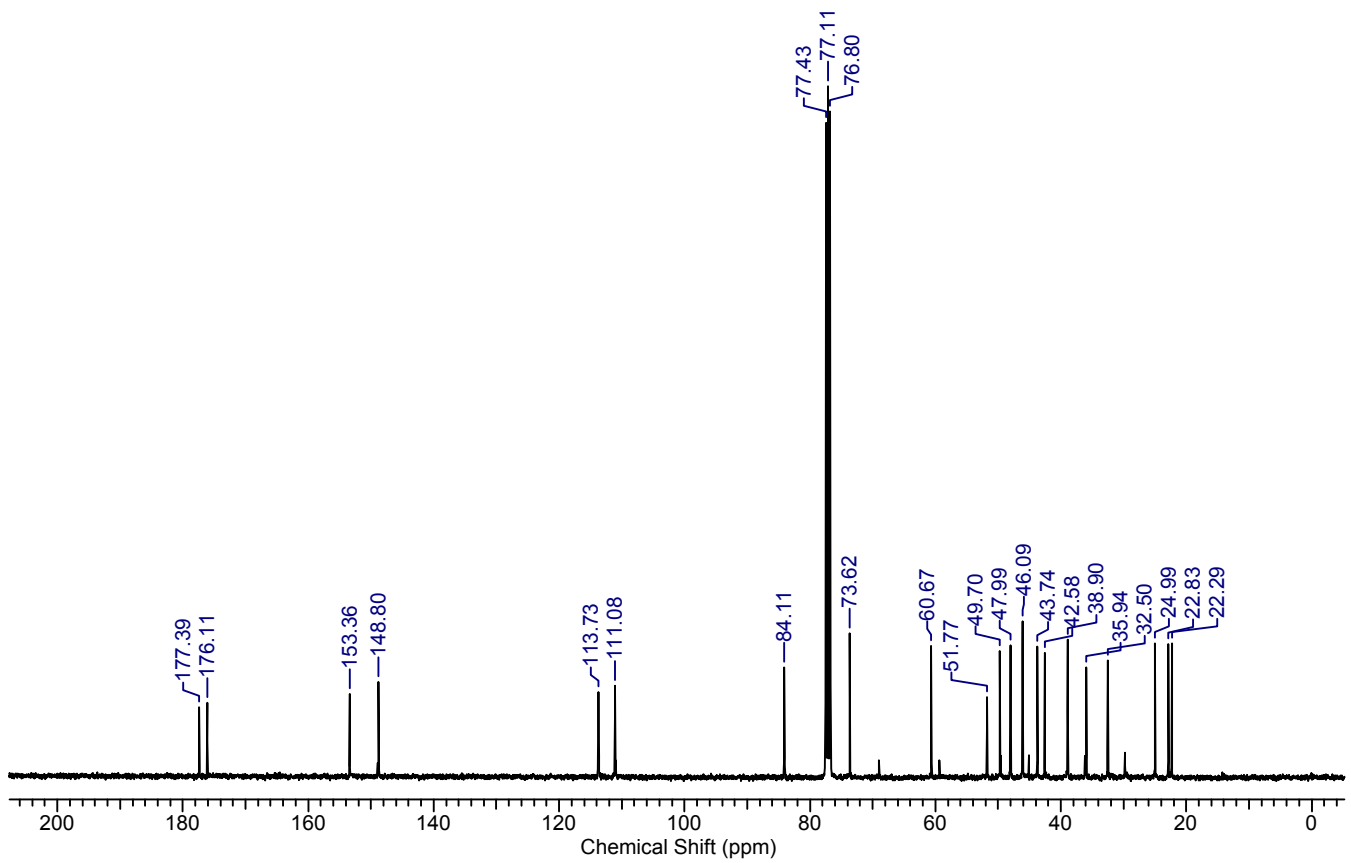
IS-305-B #83 RT: 0.37 AV: 1 NL: 8.76E9
T: FTMS + p ESI Full ms [133.40-2000.00]



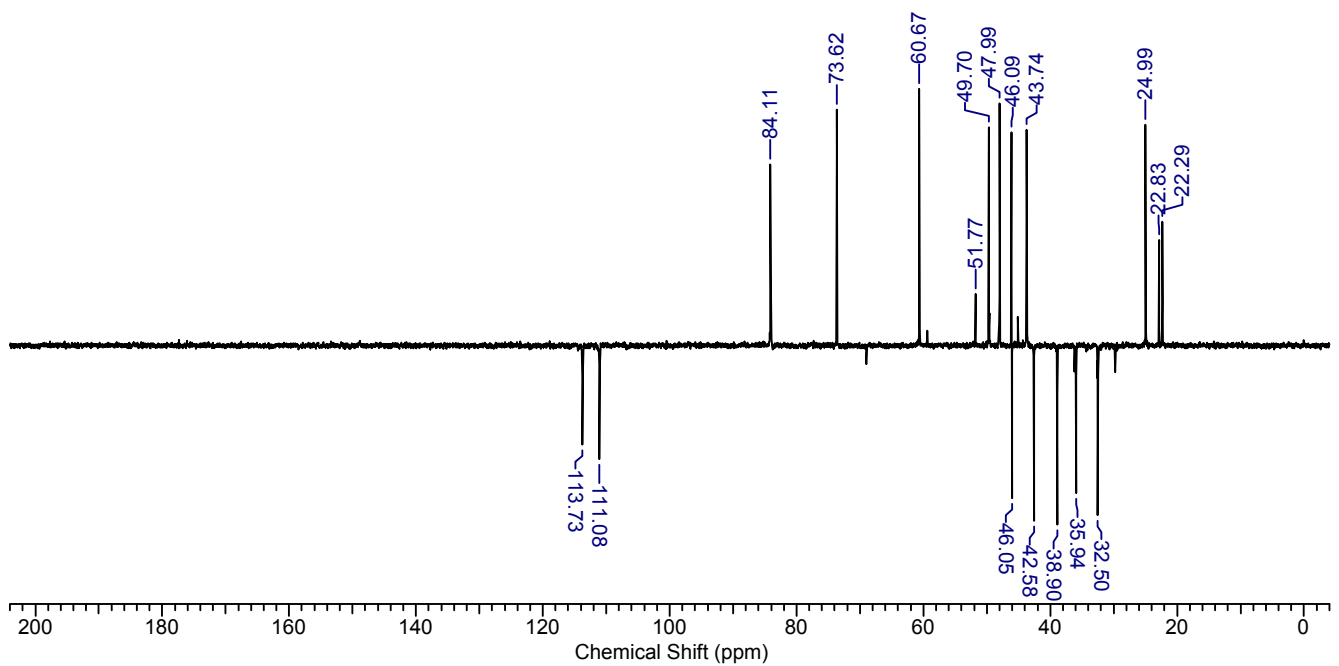
¹H NMR of Compound 21 (400 MHz, CDCl₃)



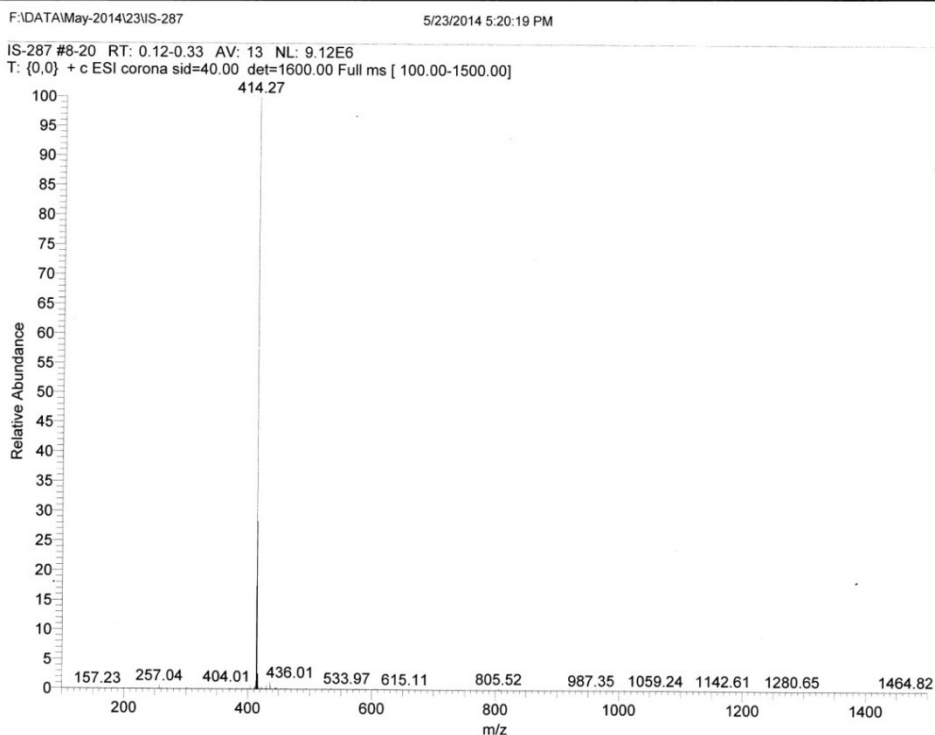
¹³C NMR of Compound 21 (100 MHz, CDCl₃)



DEPT of Compound 21 (100 MHz, CDCl₃)

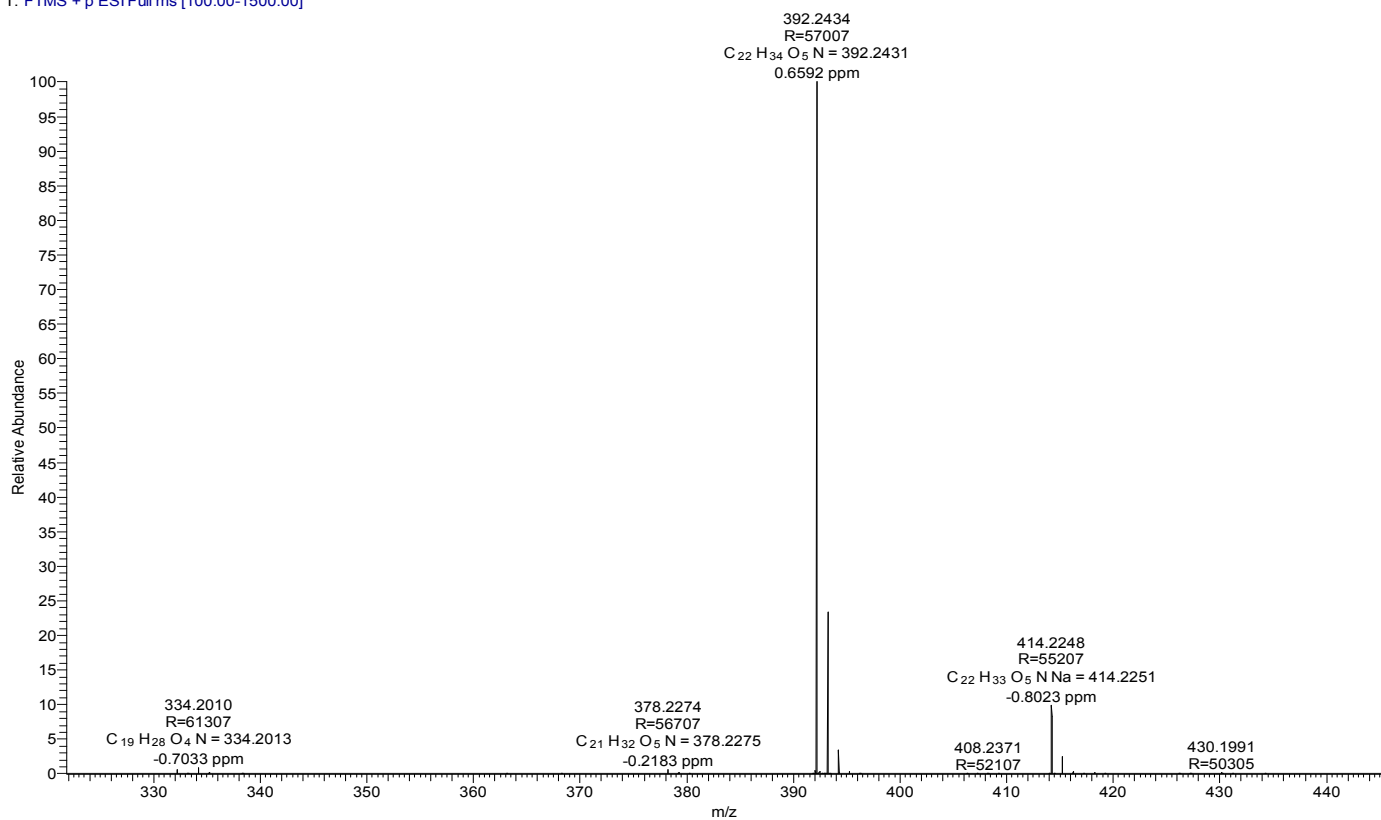


LC-MS of Compound 21

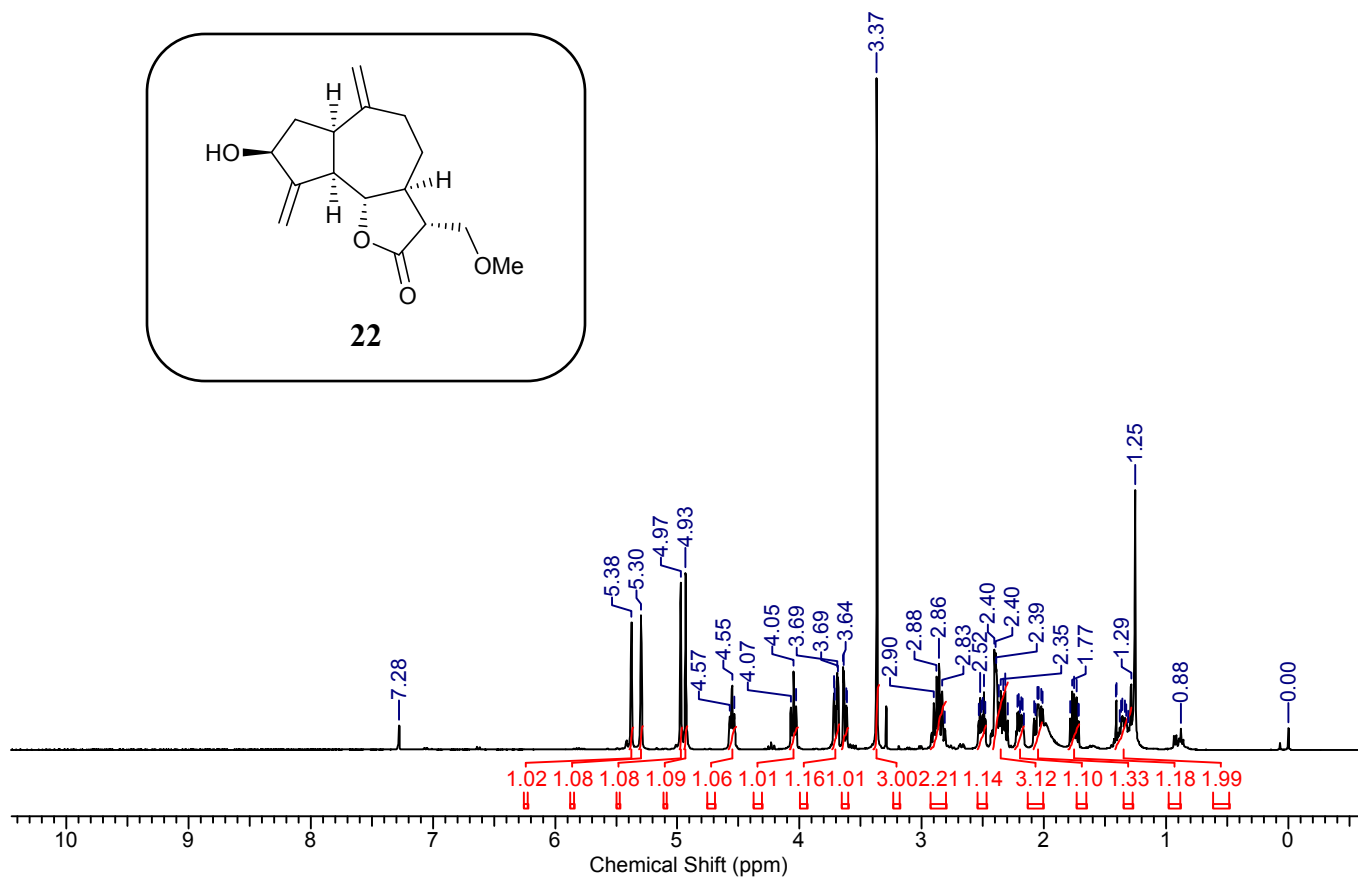
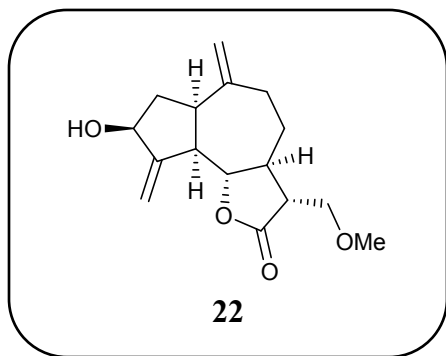


HR-MS of Compound 21

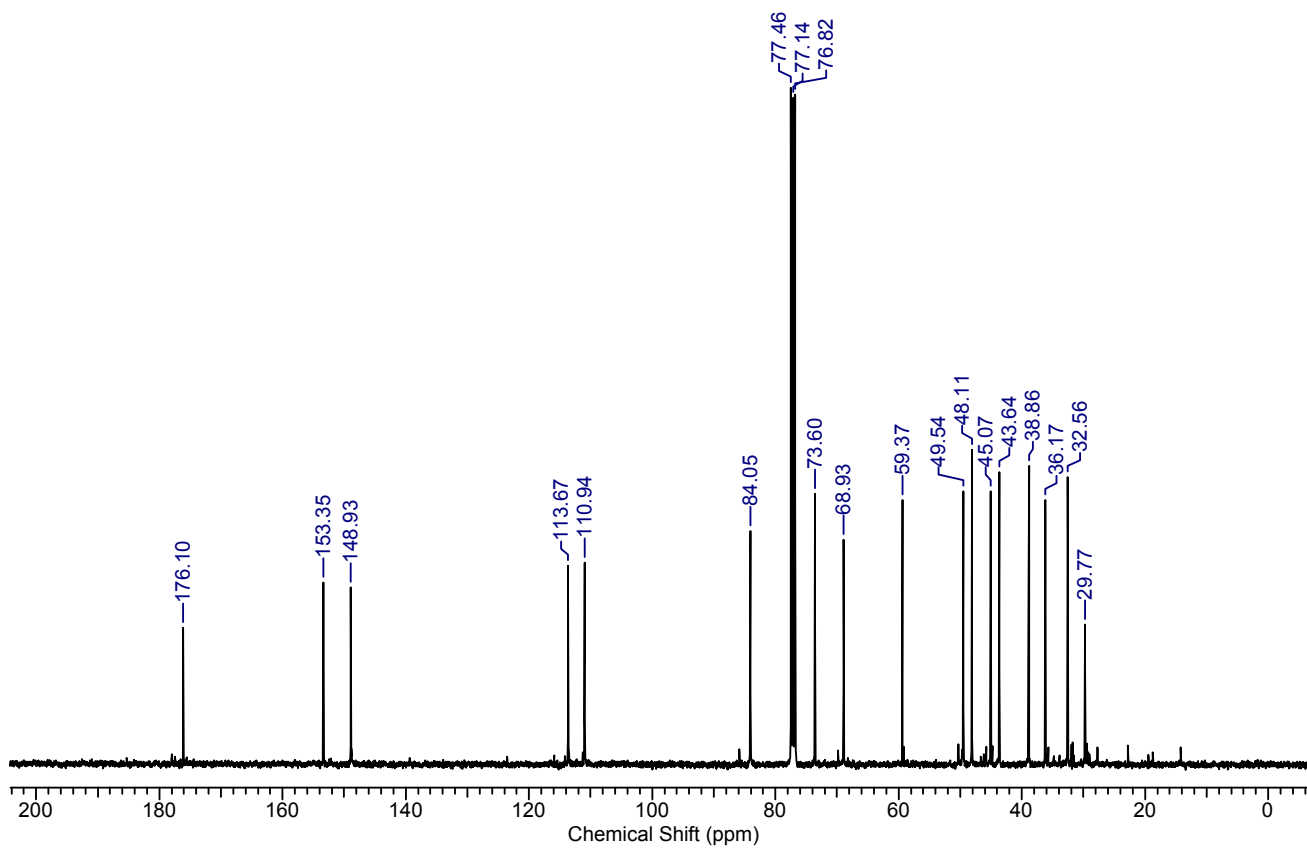
IS-287-A #89 RT: 0.39 AV: 1 NL: 9.40E9
T: FTMS + p ESI Full ms [100.00-1500.00]



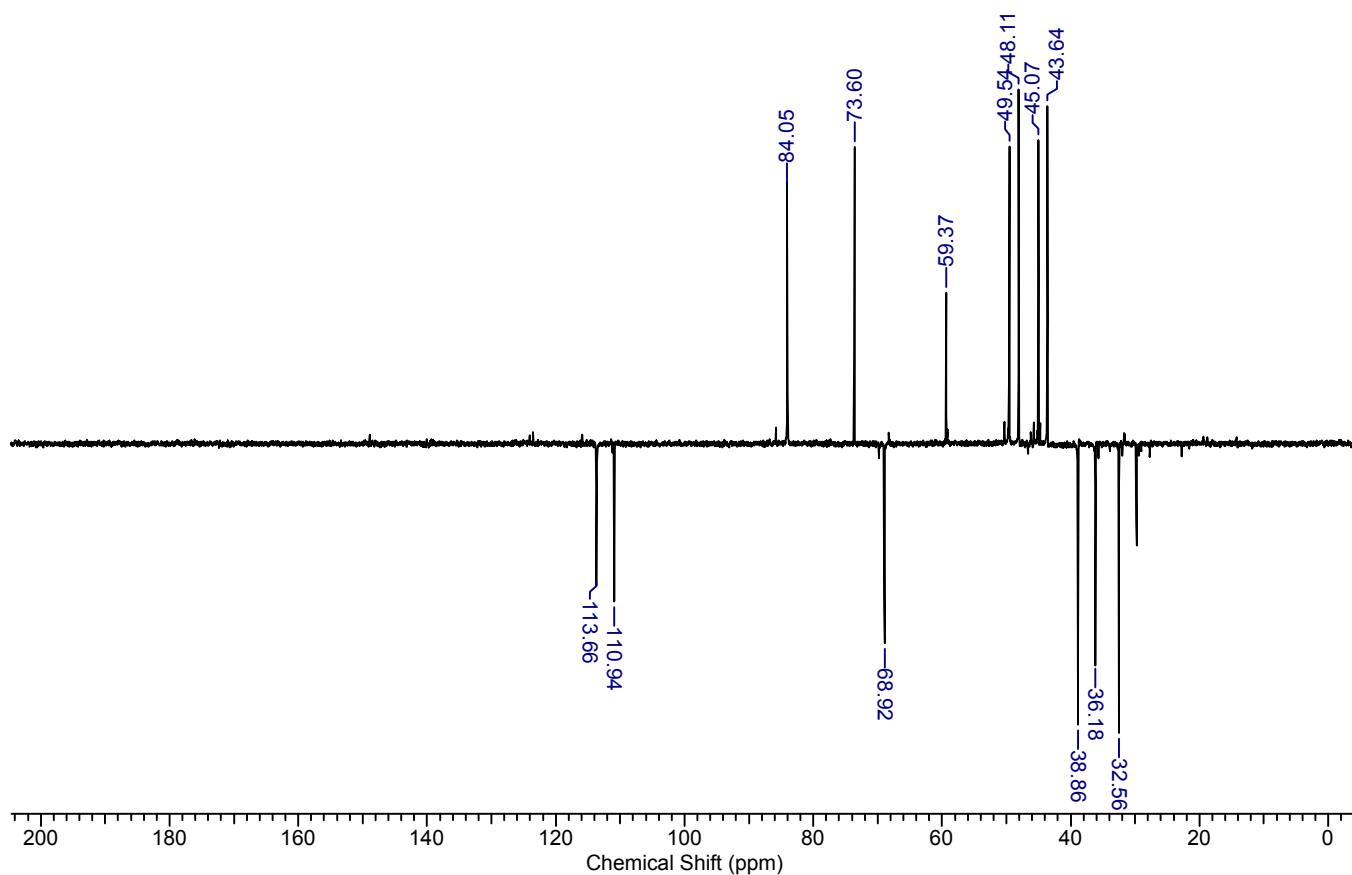
¹H NMR of Compound 22 (400 MHz, CDCl₃)



¹³C NMR of Compound 22 (100 MHz, CDCl₃)



DEPT of Compound 22 (100 MHz, CDCl₃)



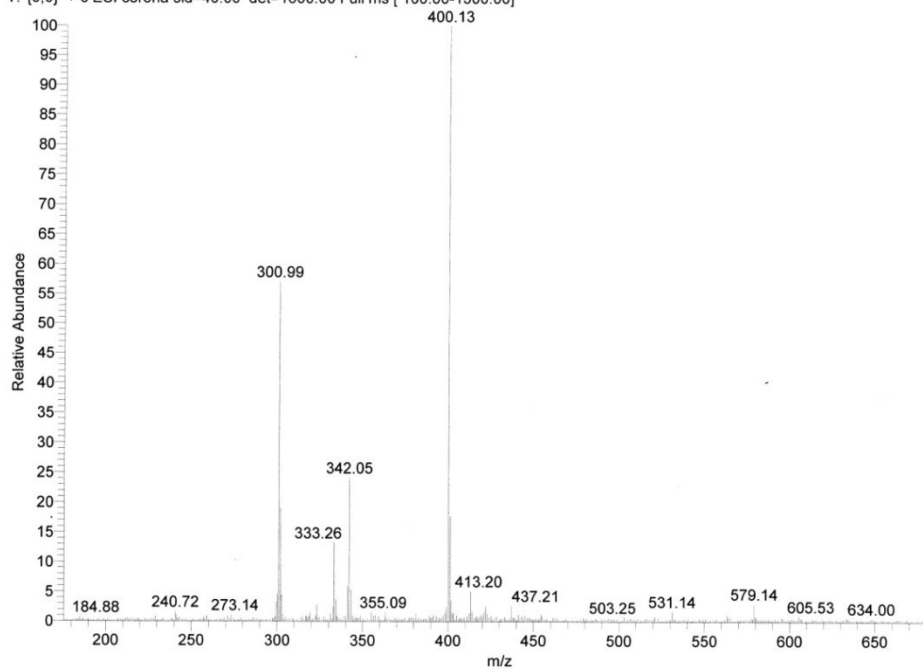
LC-MS of Compound 22

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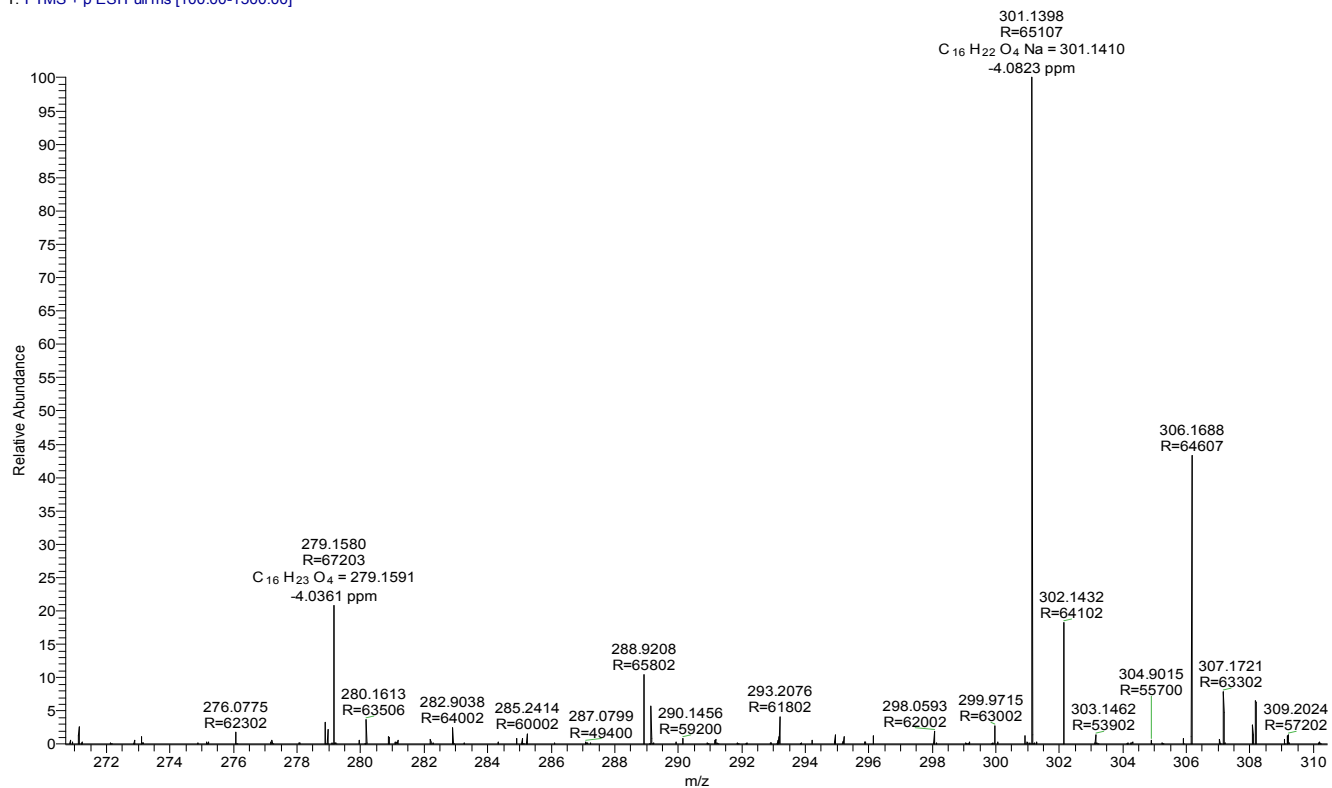
IS-292 #8-19 RT: 0.12-0.32 AV: 12 NL: 1.57E6

T: [0,0] + c ESI corona sid=40.00 det=1600.00 Full ms [100.00-1500.00]

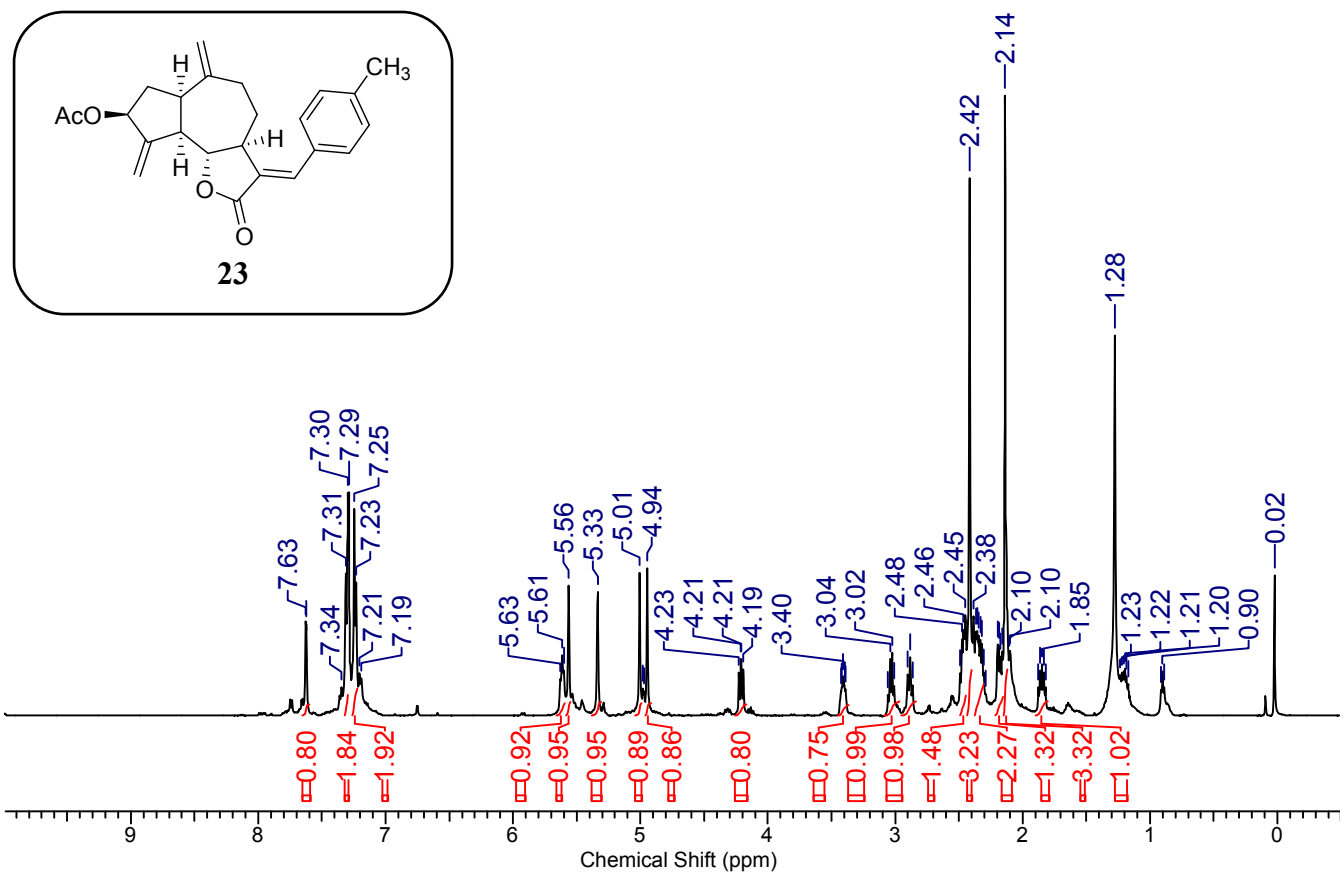


HR-MS of Compound 22

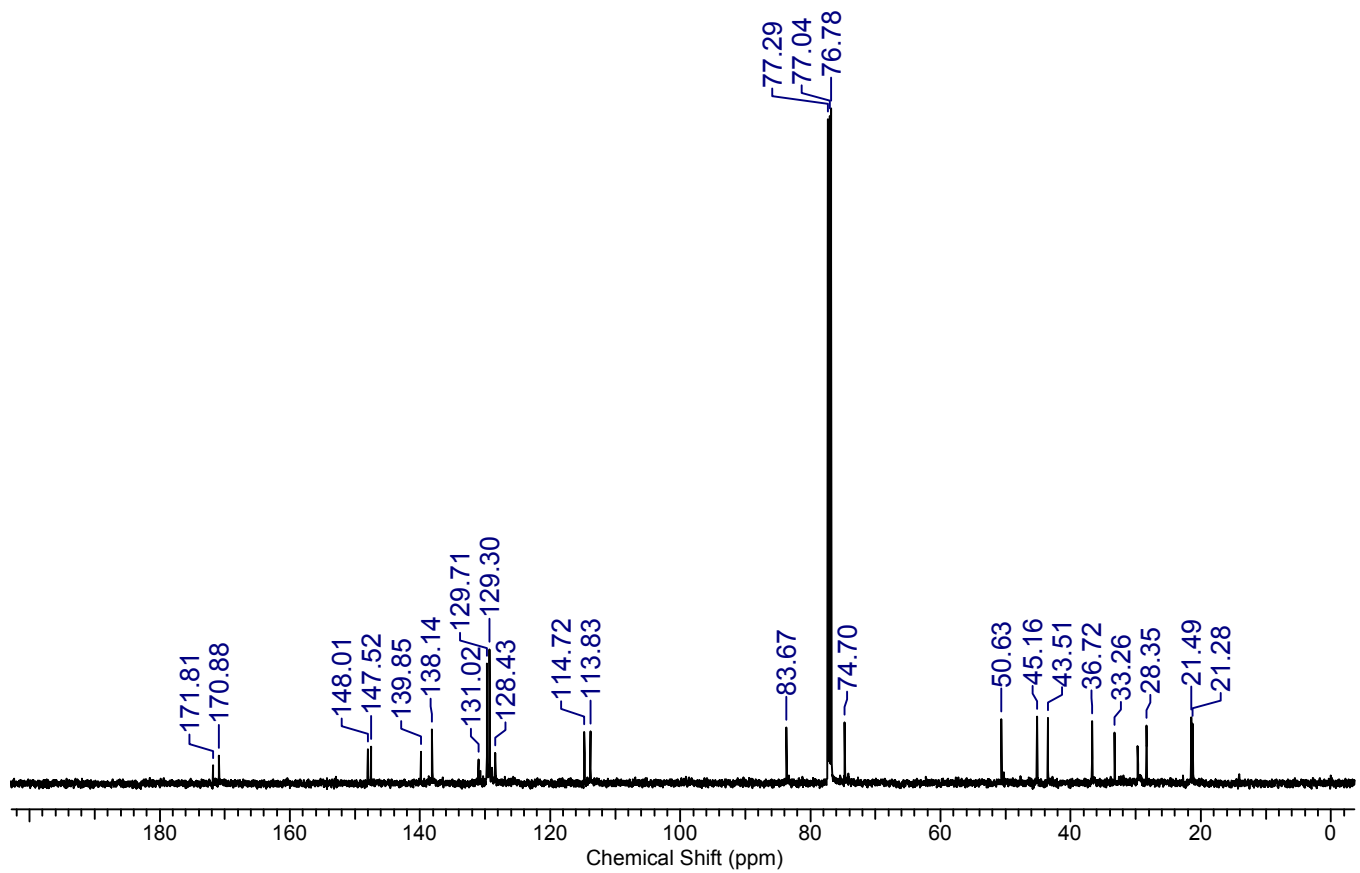
IS-292 #133 RT: 0.59 AV: 1 NL: 2.85E7
T: FTMS + p ESI Full ms [100.00-1500.00]



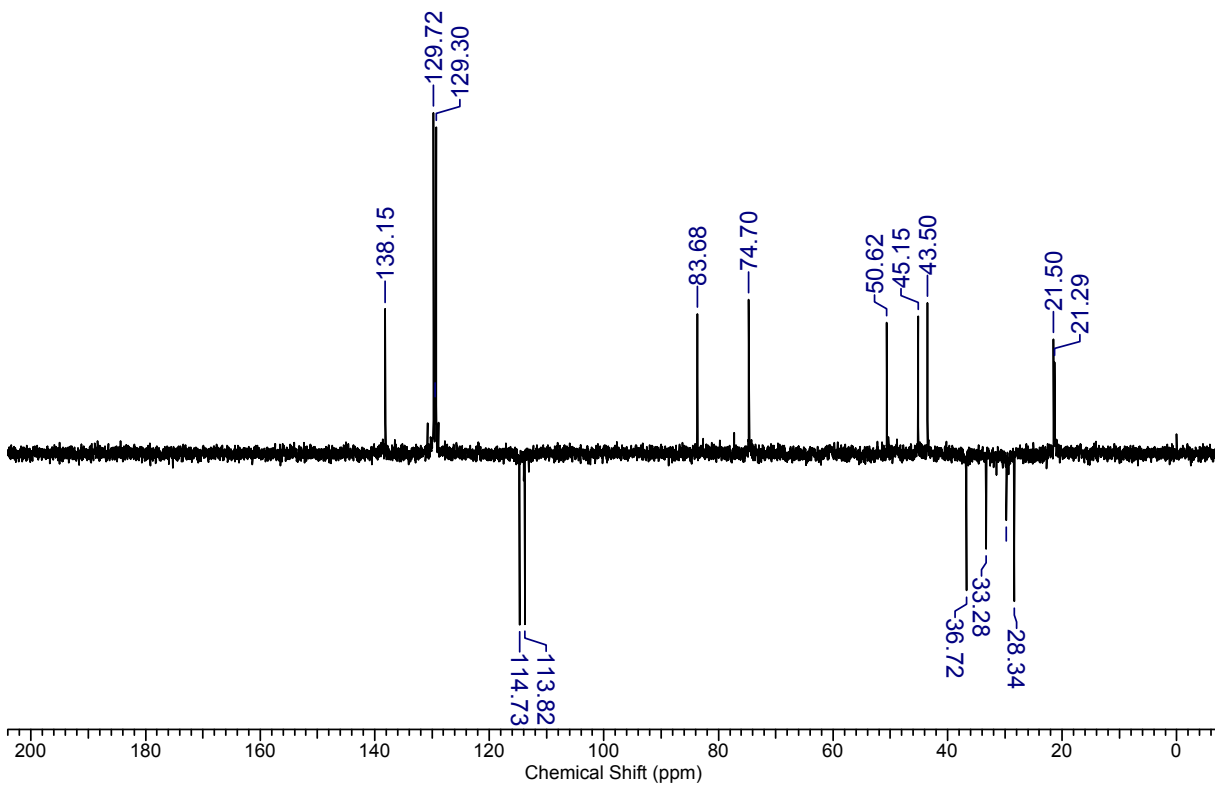
¹H NMR of Compound 23 (500 MHz, CDCl₃)



¹³C NMR of Compound 23 (125 MHz, CDCl₃)



DEPT of Compound 23 (125 MHz, CDCl₃)

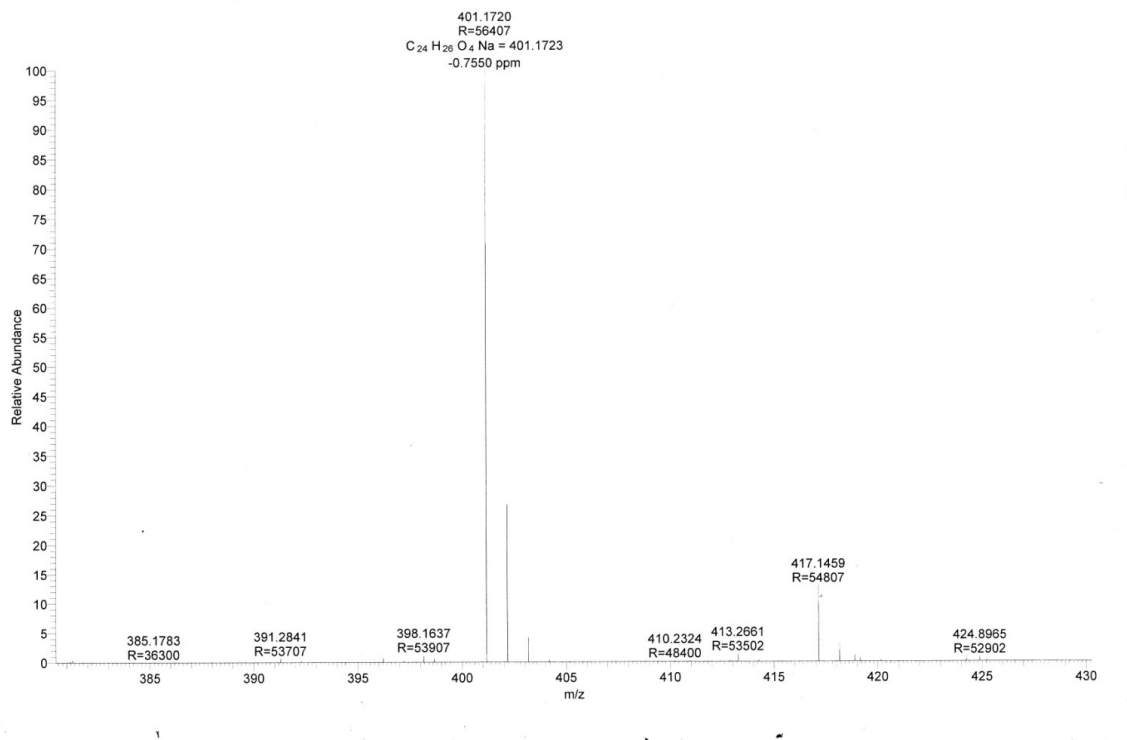


HR-MS of Compound 23

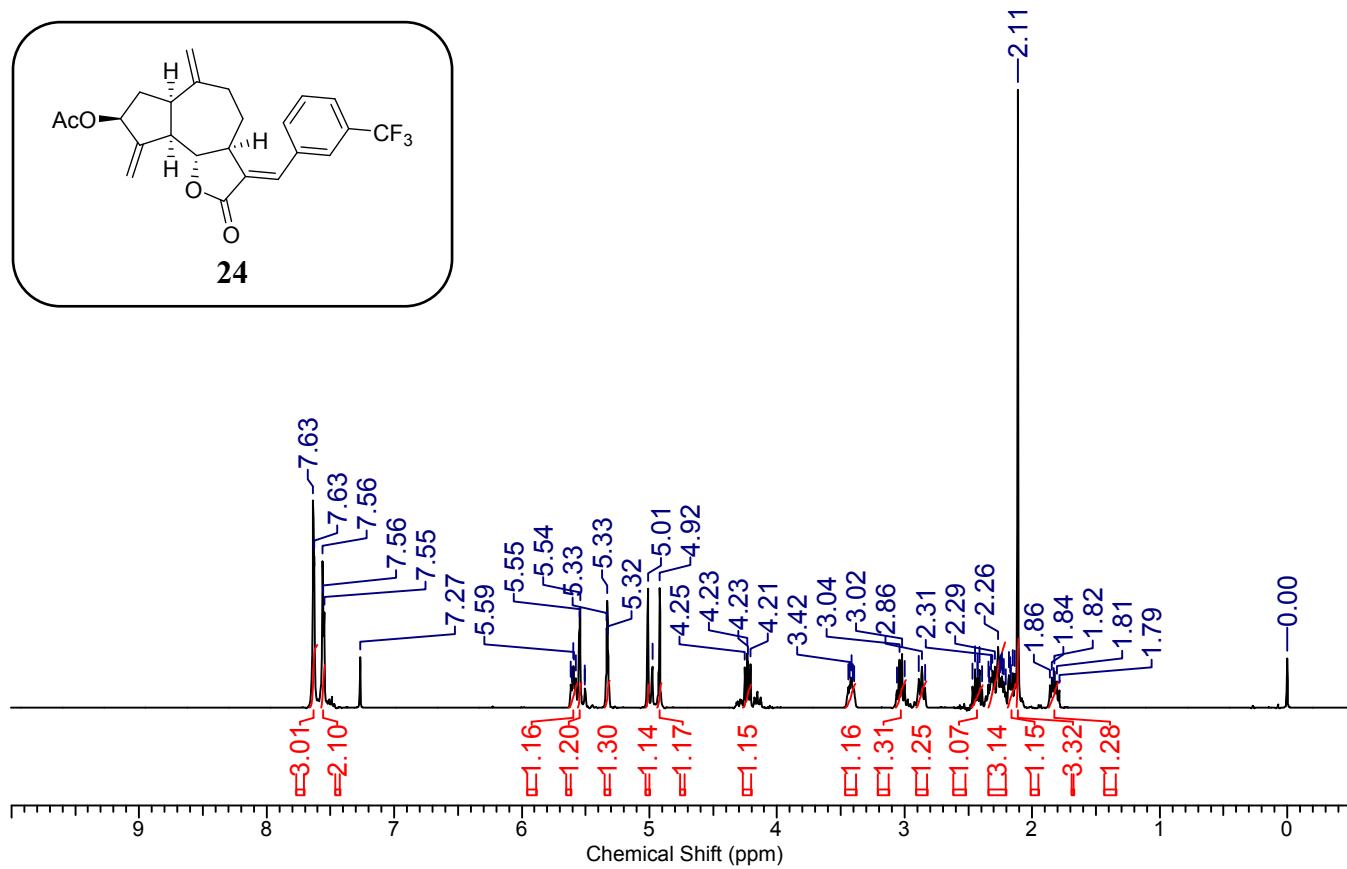
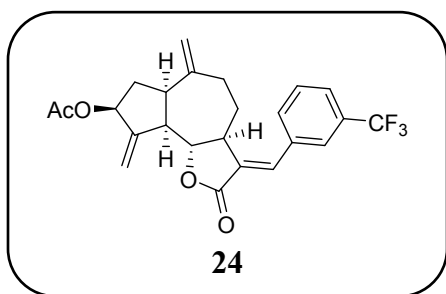
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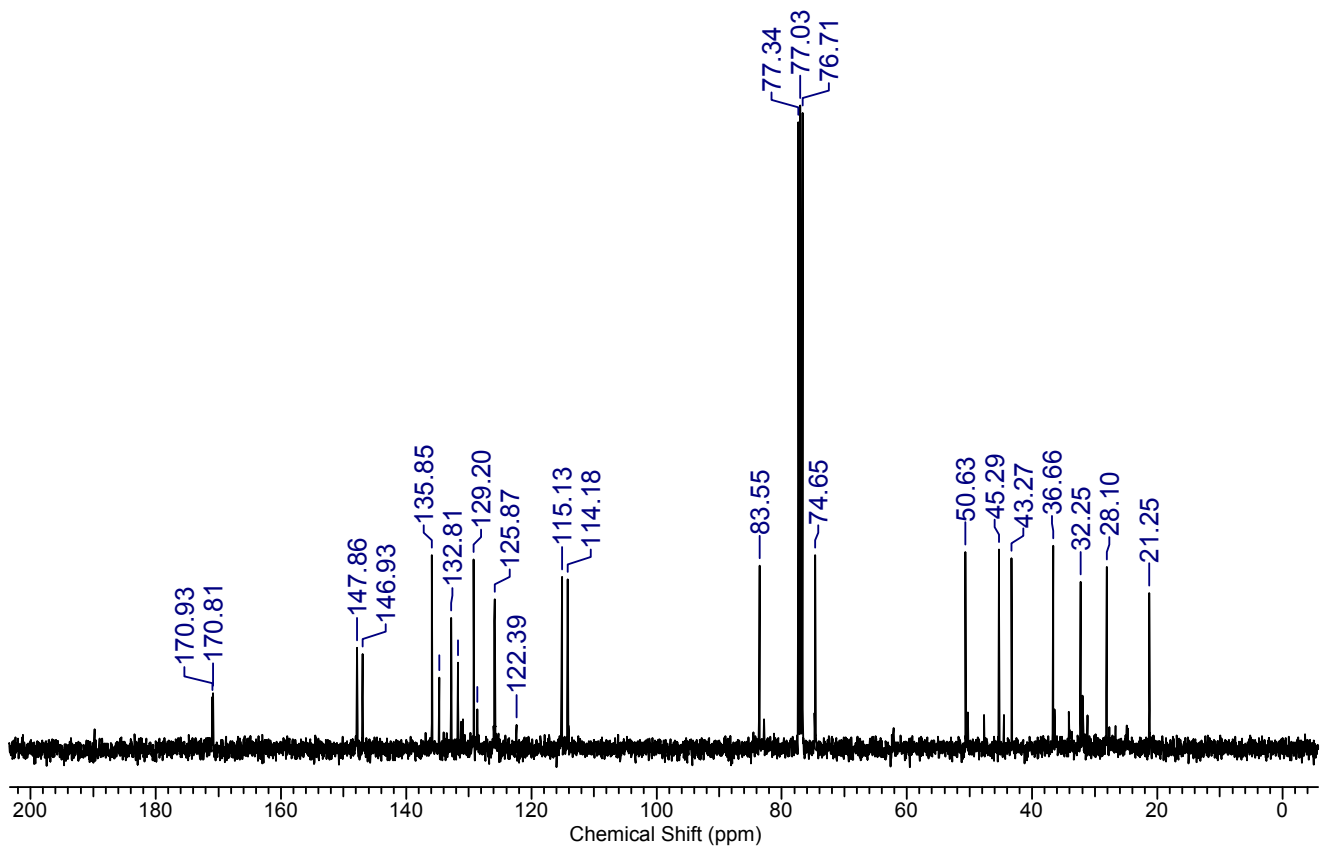
IS-341 #1150 RT: 5.12 AV: 1 NL: 9.63E7
T: FTMS + p ESI Full ms [66.70-1000.00]



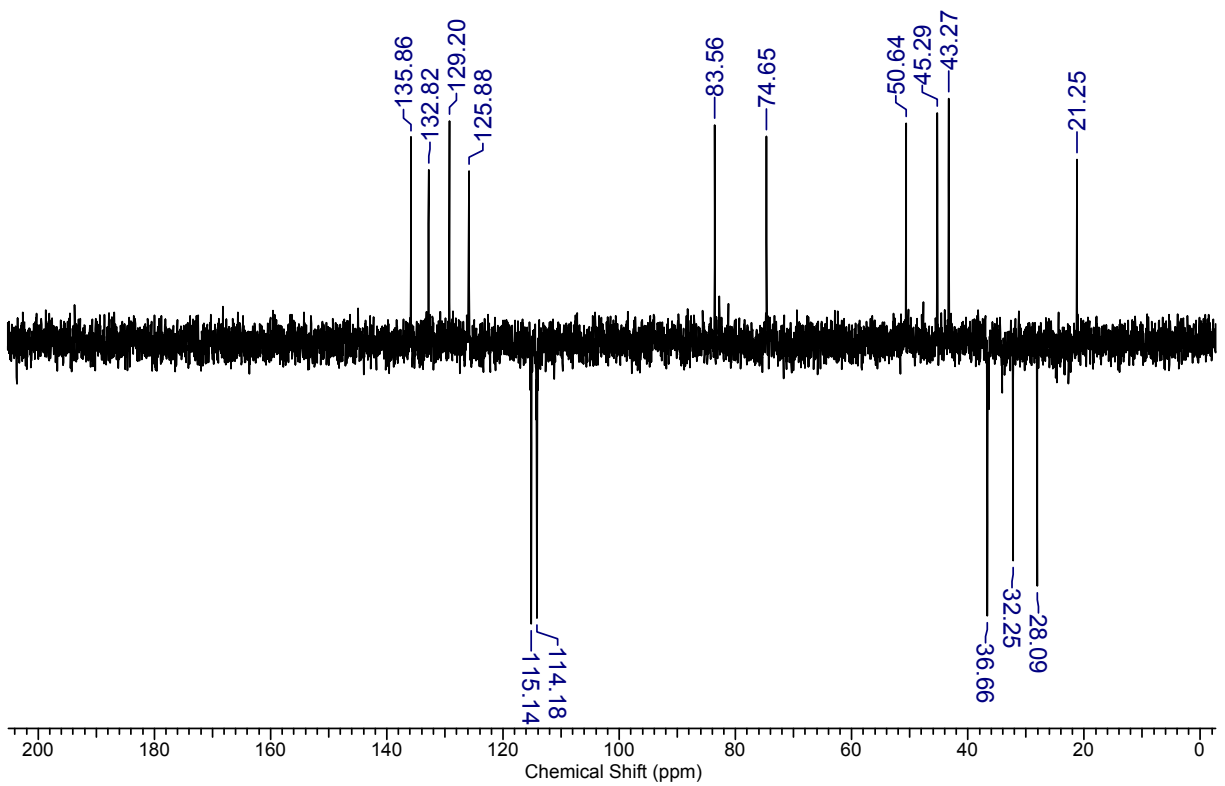
¹H NMR of Compound 24 (400 MHz, CDCl₃)



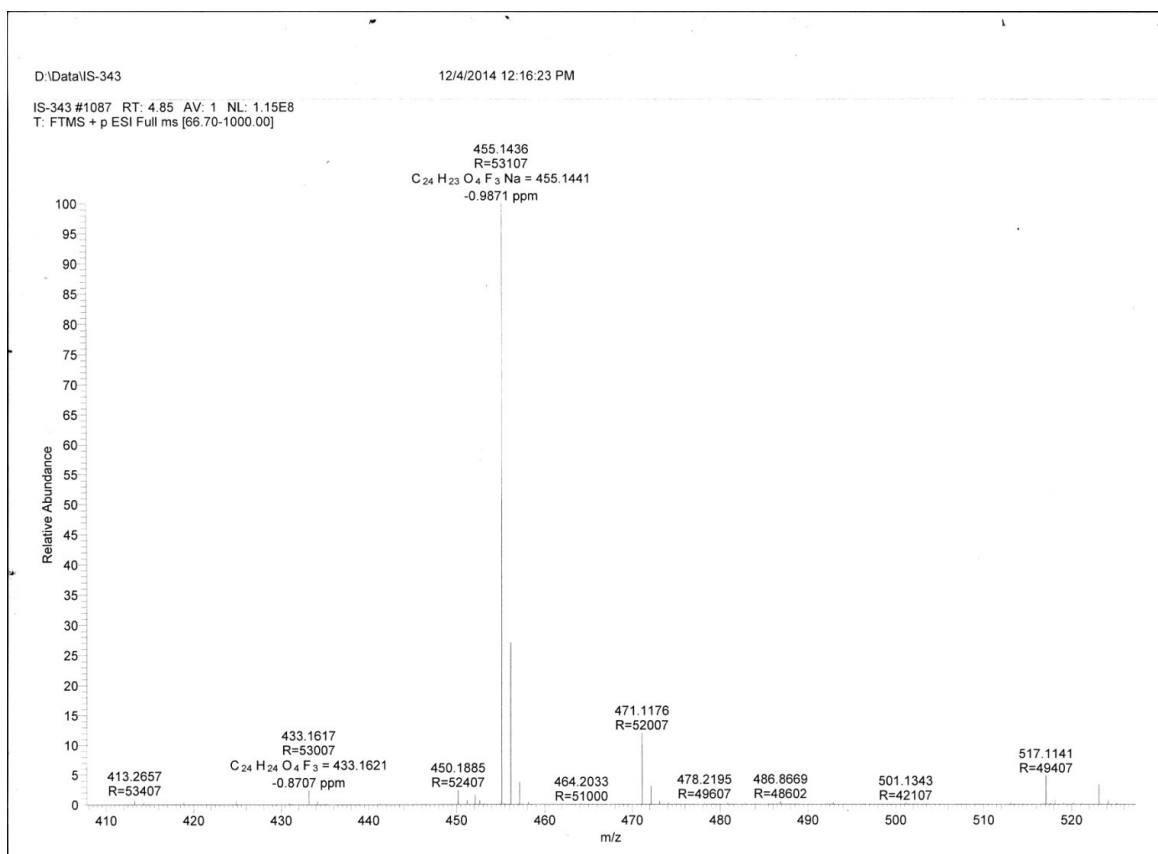
^{13}C NMR of Compound 24 (100 MHz, CDCl_3)



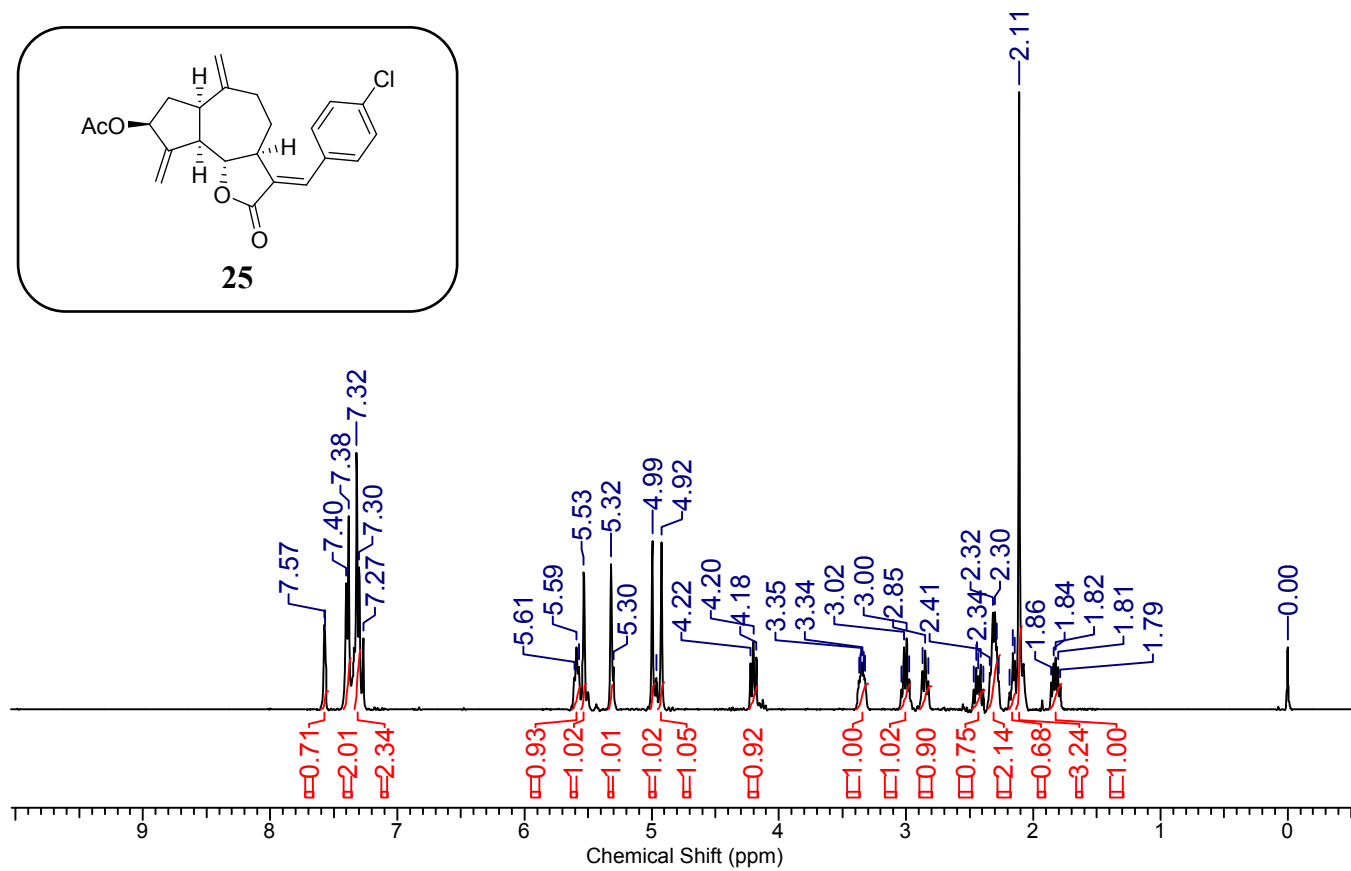
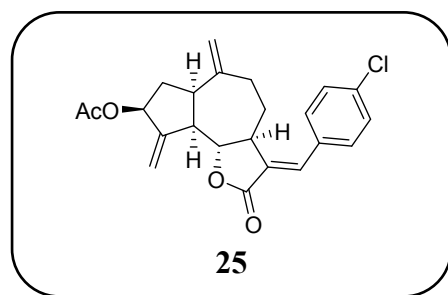
DEPT of Compound 24 (100 MHz, CDCl_3)



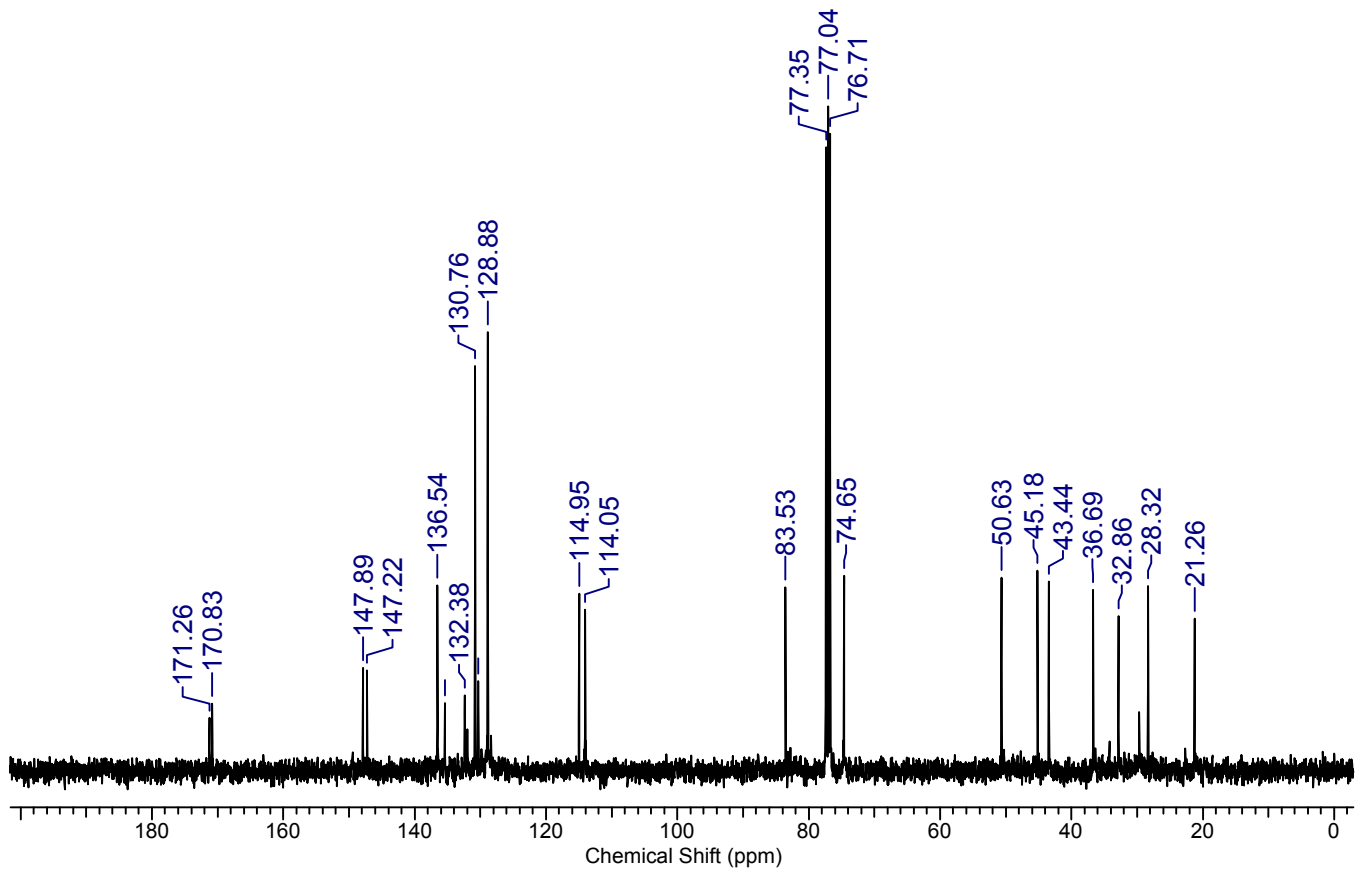
HR-MS of Compound 24



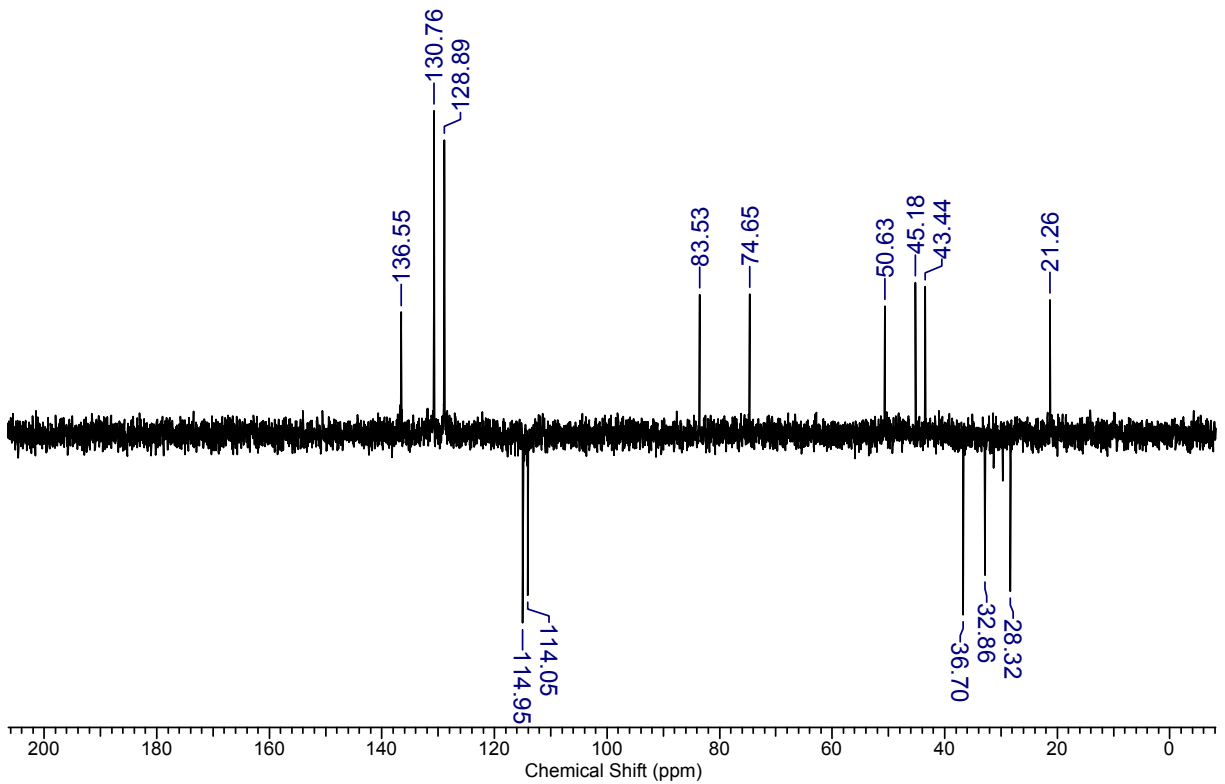
¹H NMR of Compound 25 (400 MHz, CDCl₃)



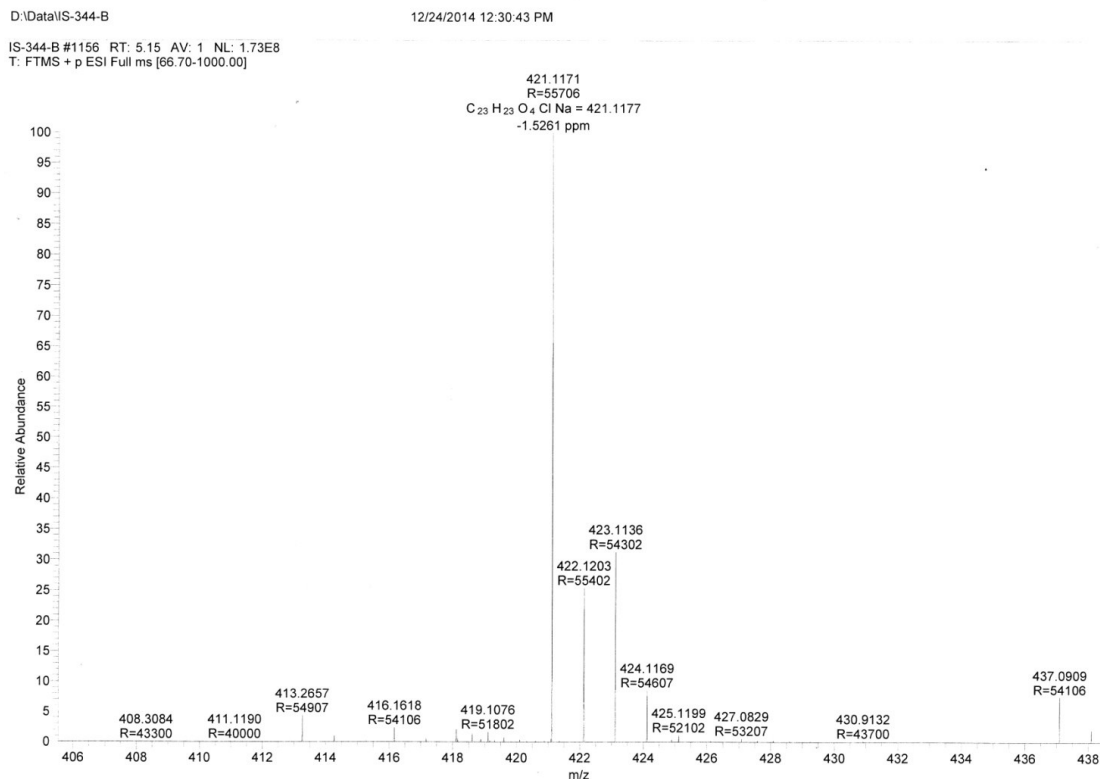
¹³C NMR of Compound 25 (100 MHz, CDCl₃)



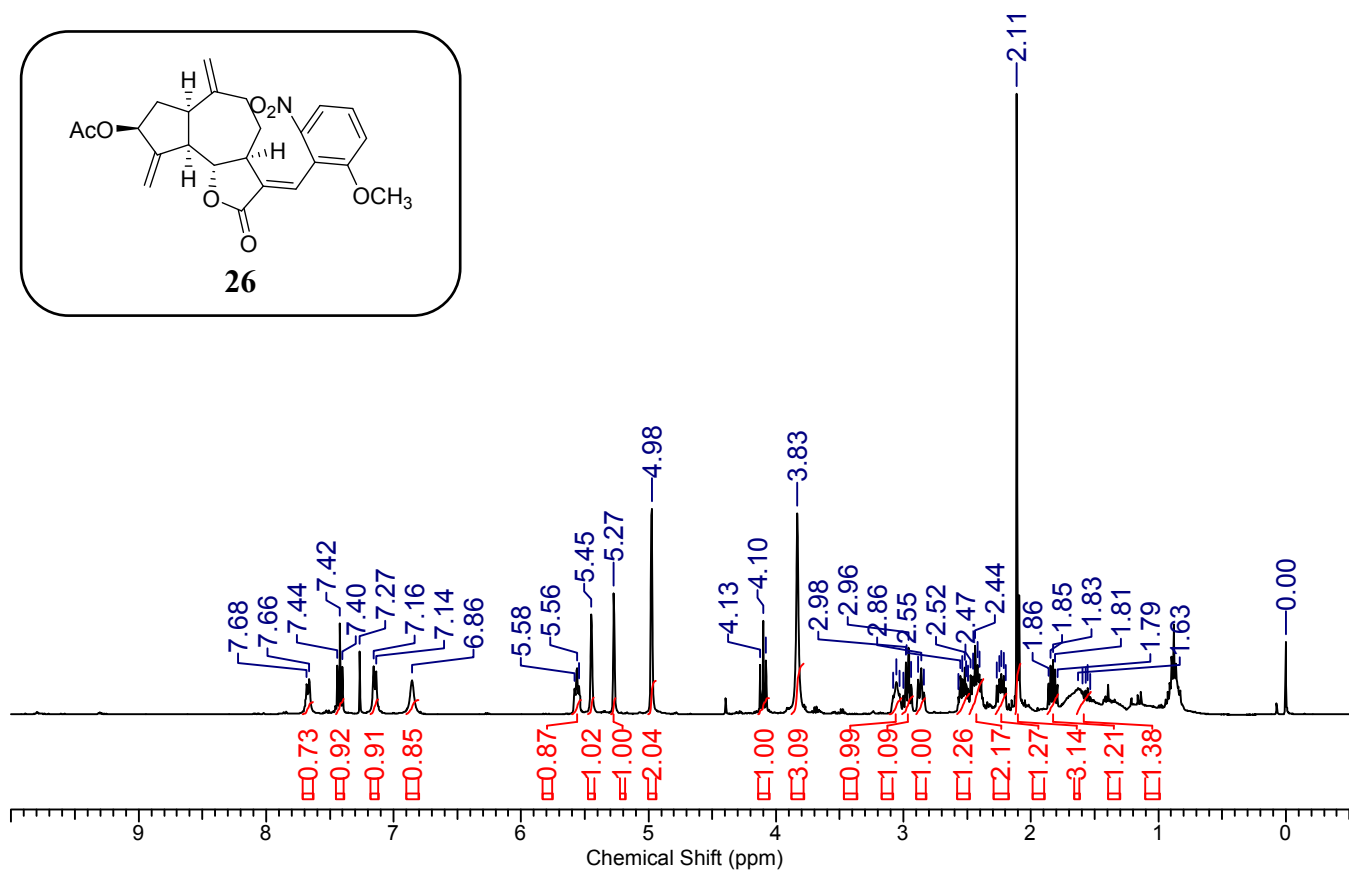
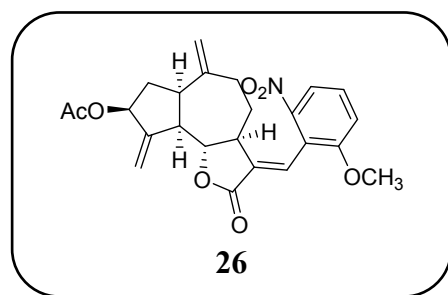
DEPT of Compound 25 (100 MHz, CDCl₃)



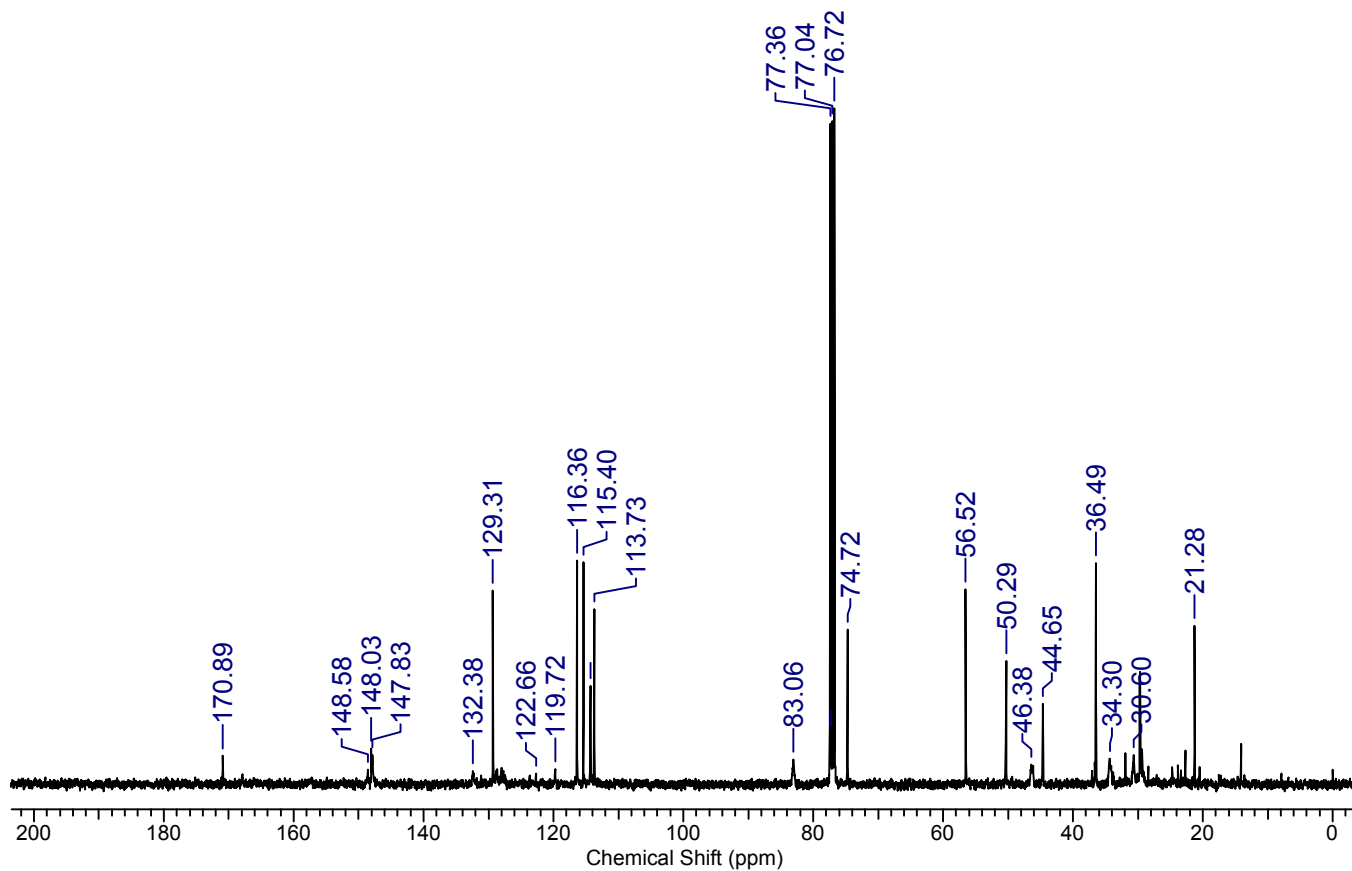
HR-MS of Compound 25



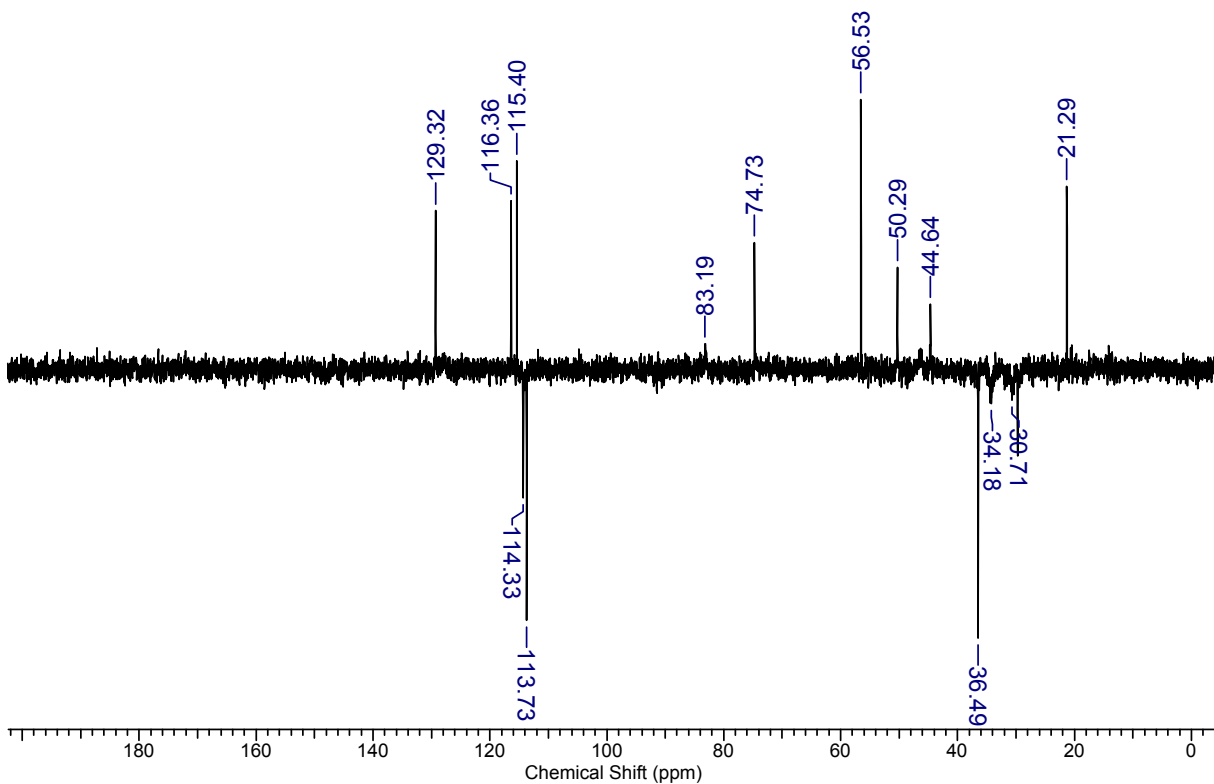
1H NMR of Compound 26 (400 MHz, $CDCl_3$)



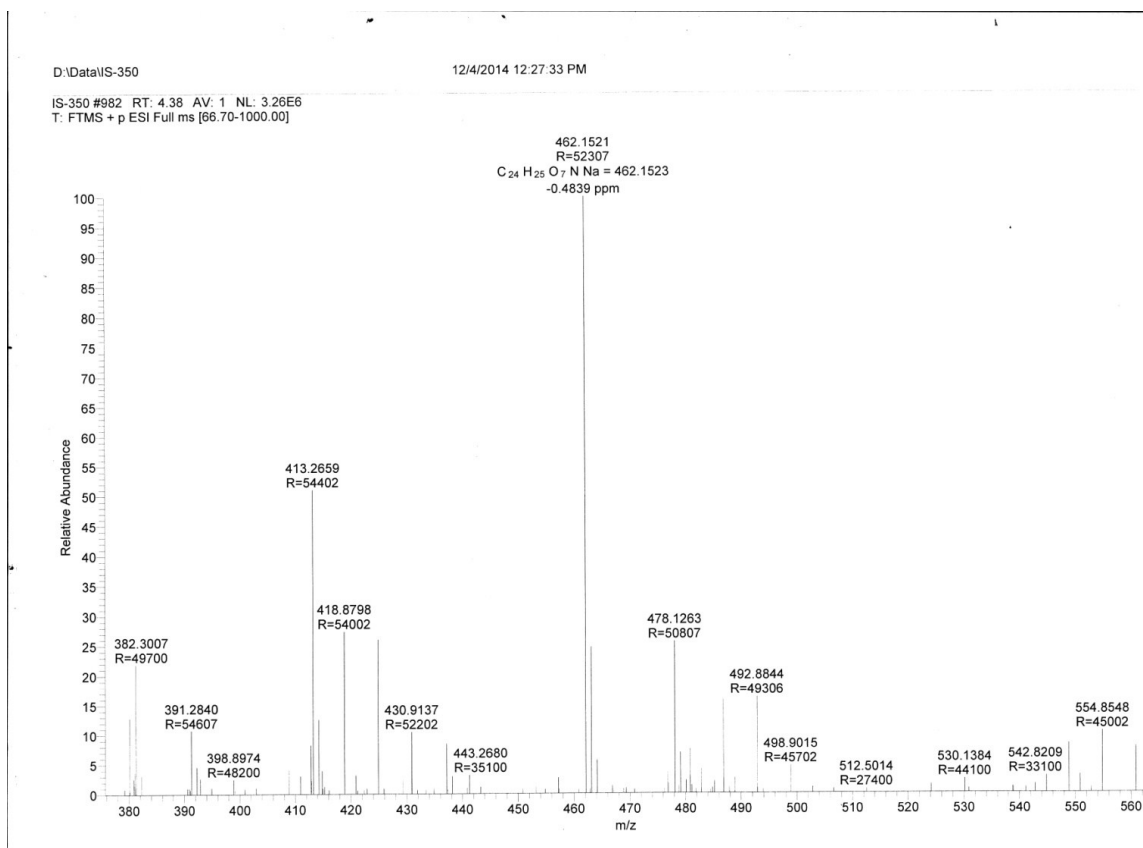
¹³C NMR of Compound 26 (100 MHz, CDCl₃)



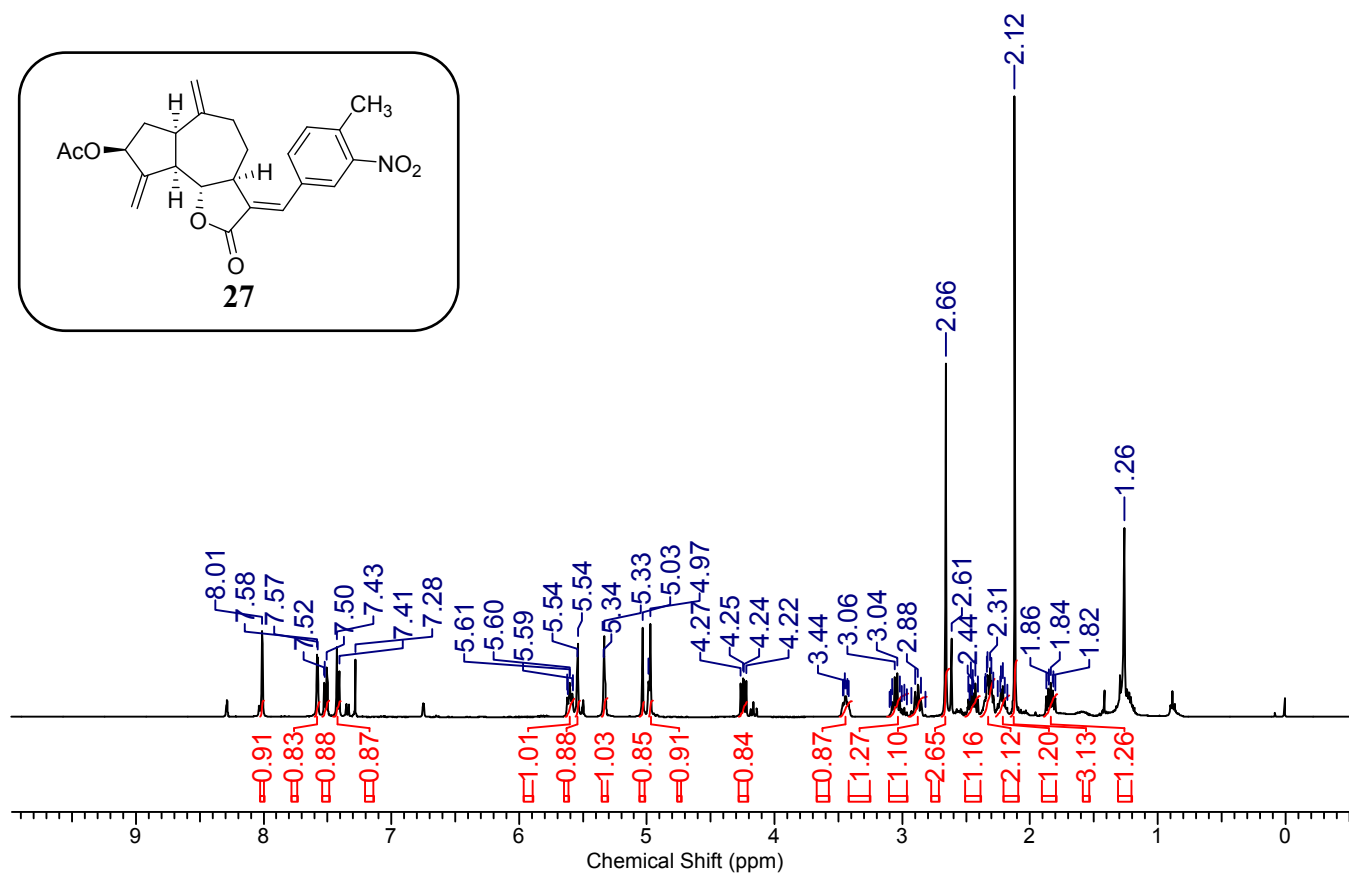
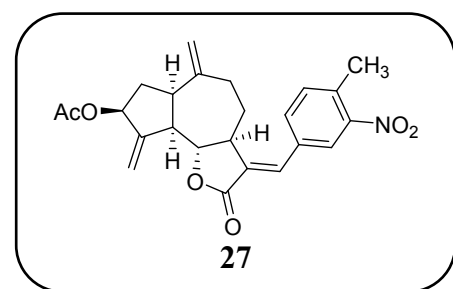
DEPT of Compound 26 (100 MHz, CDCl₃)



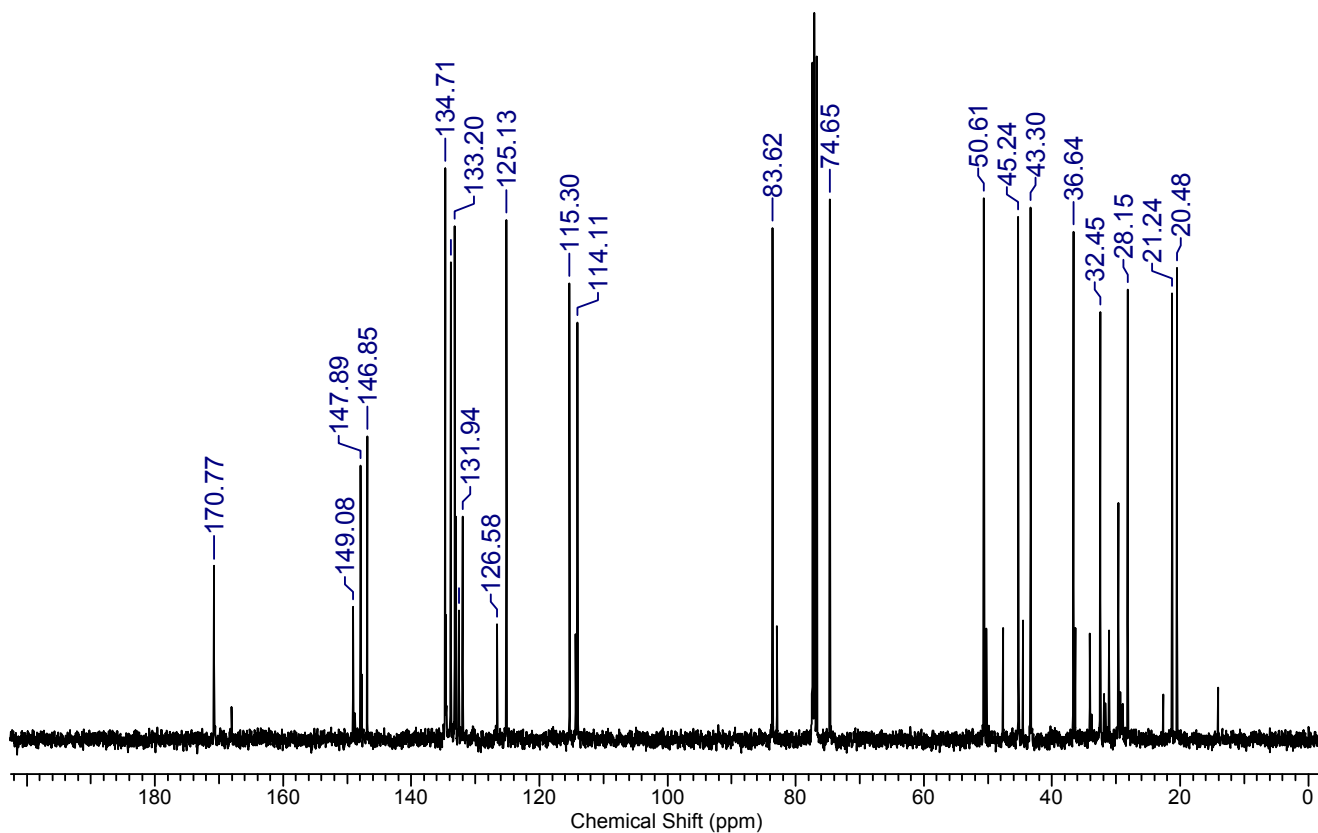
HR-MS of Compound 26



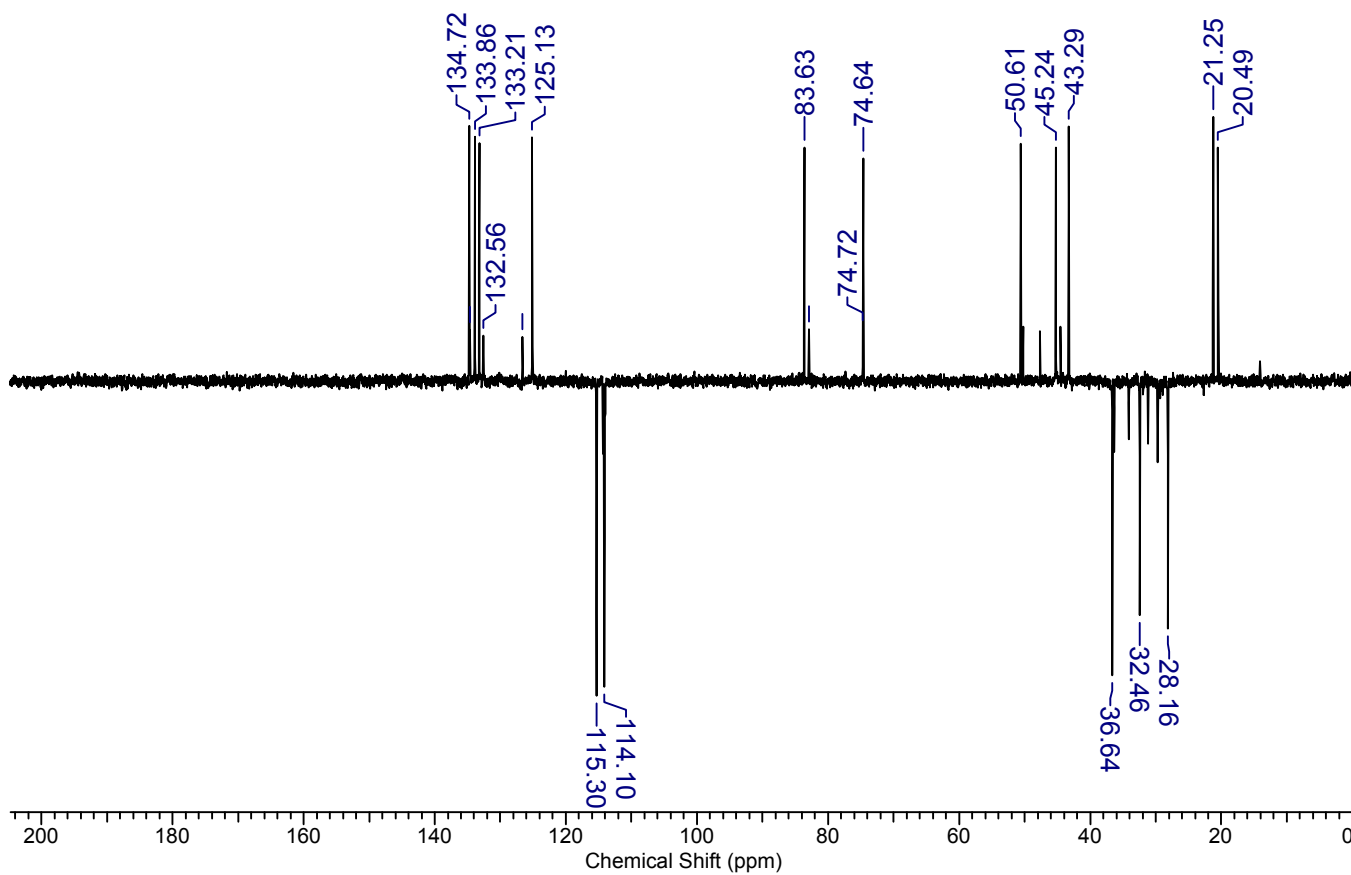
¹H NMR of Compound 27 (400 MHz, CDCl₃)



¹³C NMR of Compound 27 (100 MHz, CDCl₃)



DEPT of Compound 27 (100 MHz, CDCl₃)



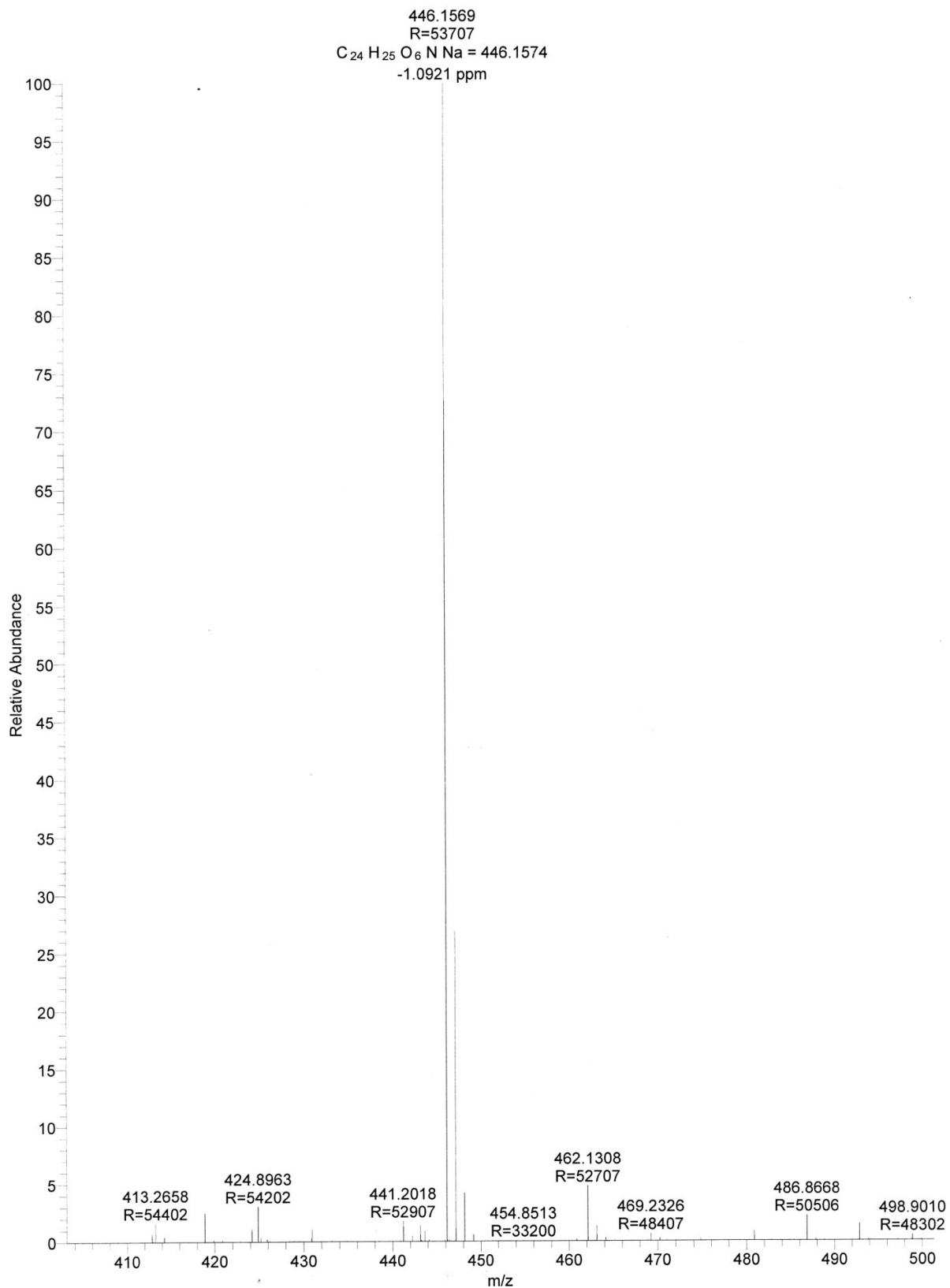
HR-MS of Compound 27

D:\Data\IS-352-A

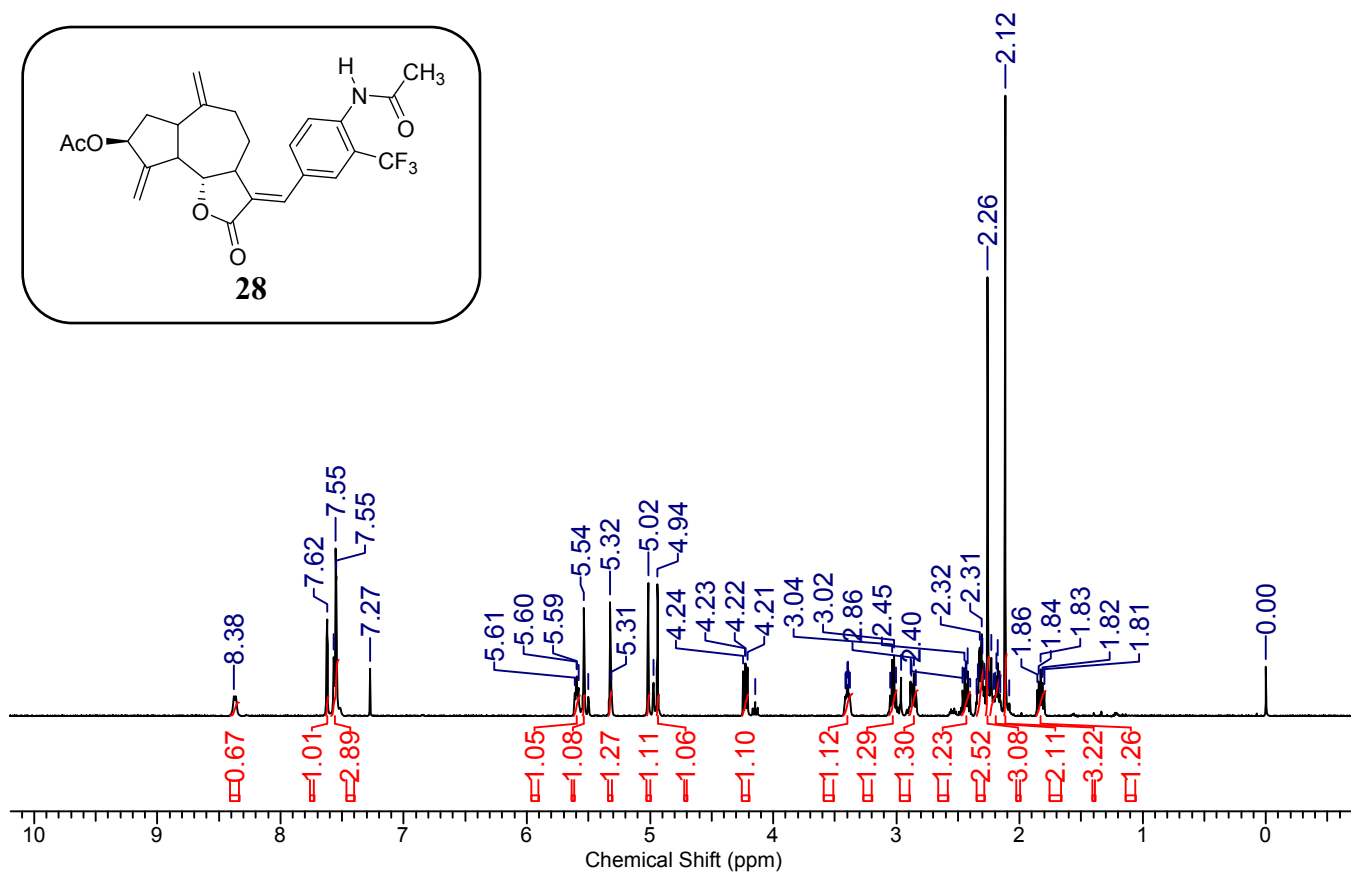
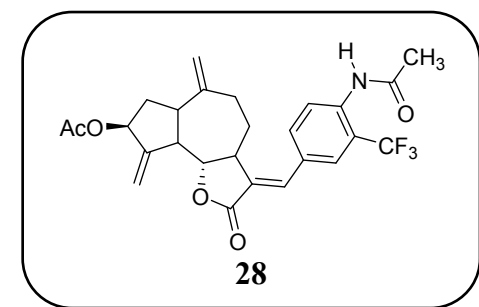
12/9/2014 12:36:52 PM

IS-352-A #1024 RT: 4.56 AV: 1 NL: 1.33E8

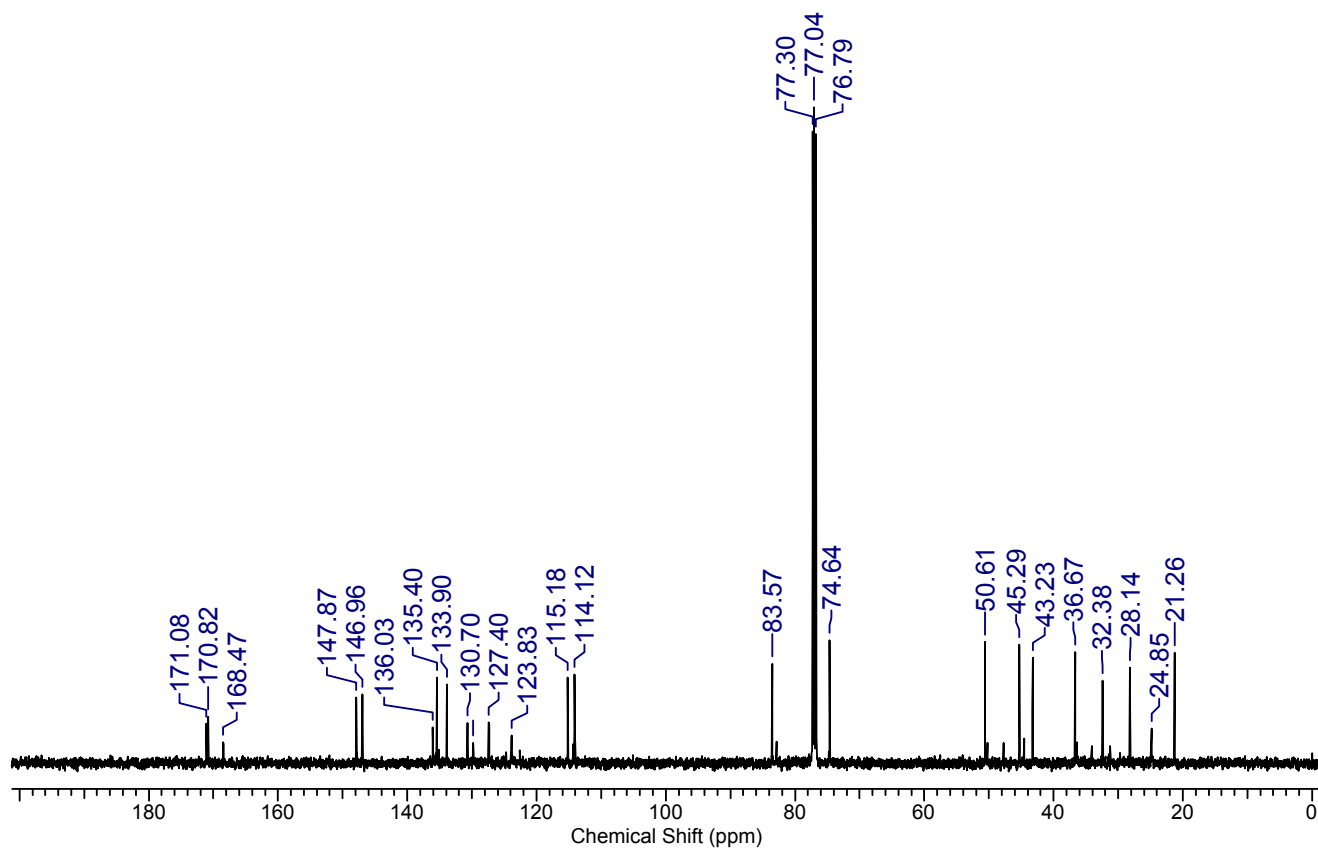
T: FTMS + p ESI Full ms [66.70-1000.00]



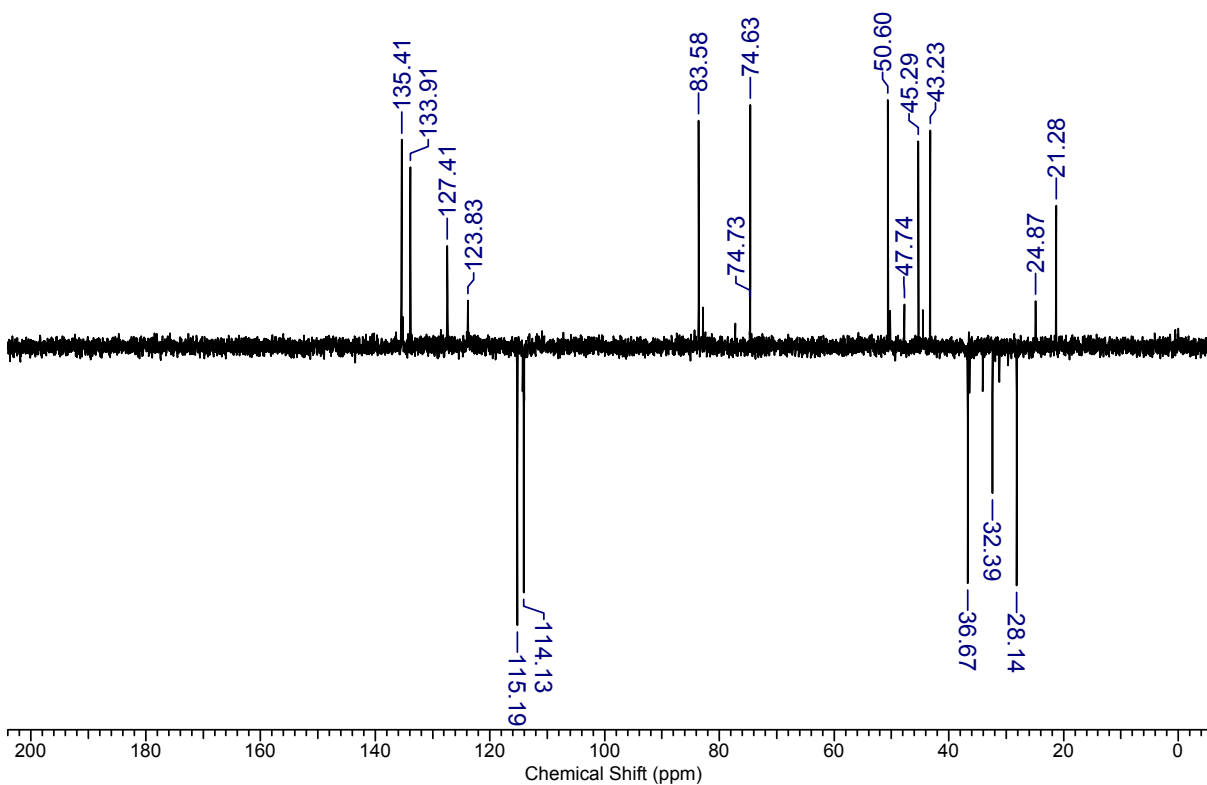
¹H NMR of Compound 28 (500 MHz, CDCl₃)



¹³C NMR of Compound 28 (125 MHz, CDCl₃)



DEPT of Compound 28 (125 MHz, CDCl₃)

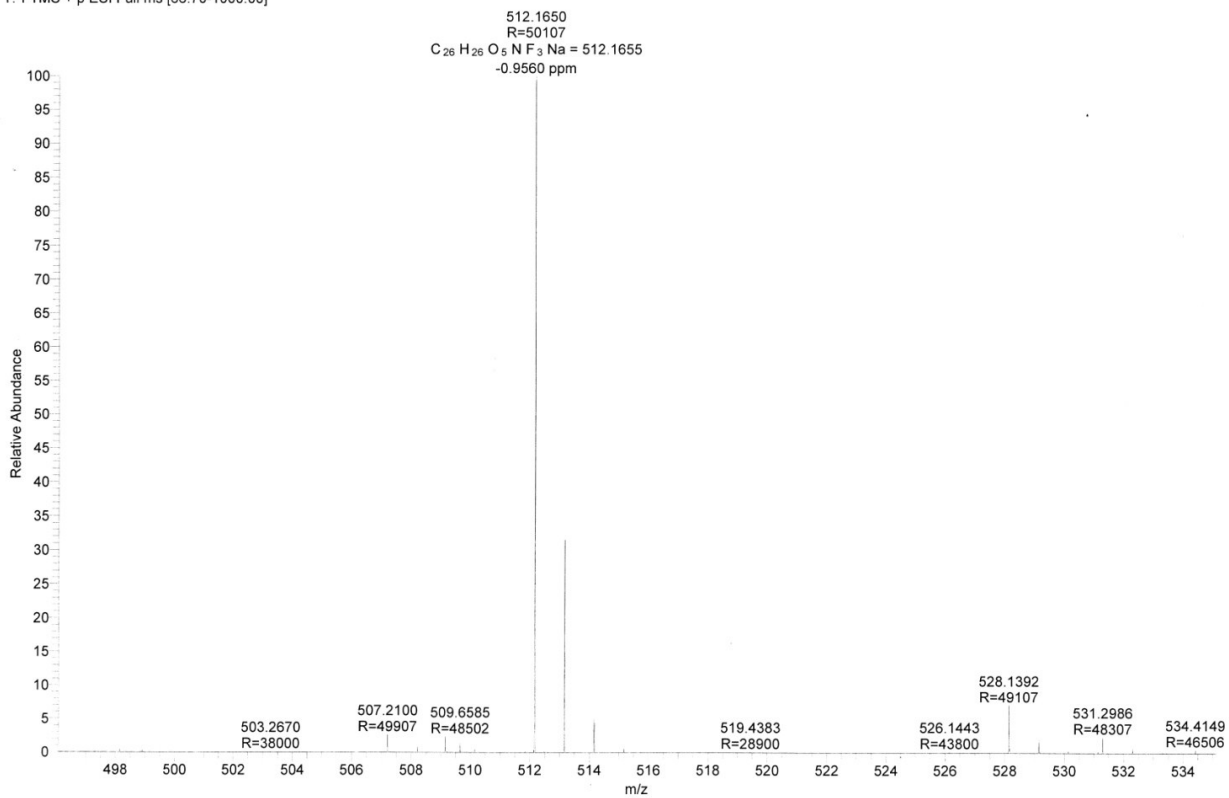


HR-MS of Compound 28

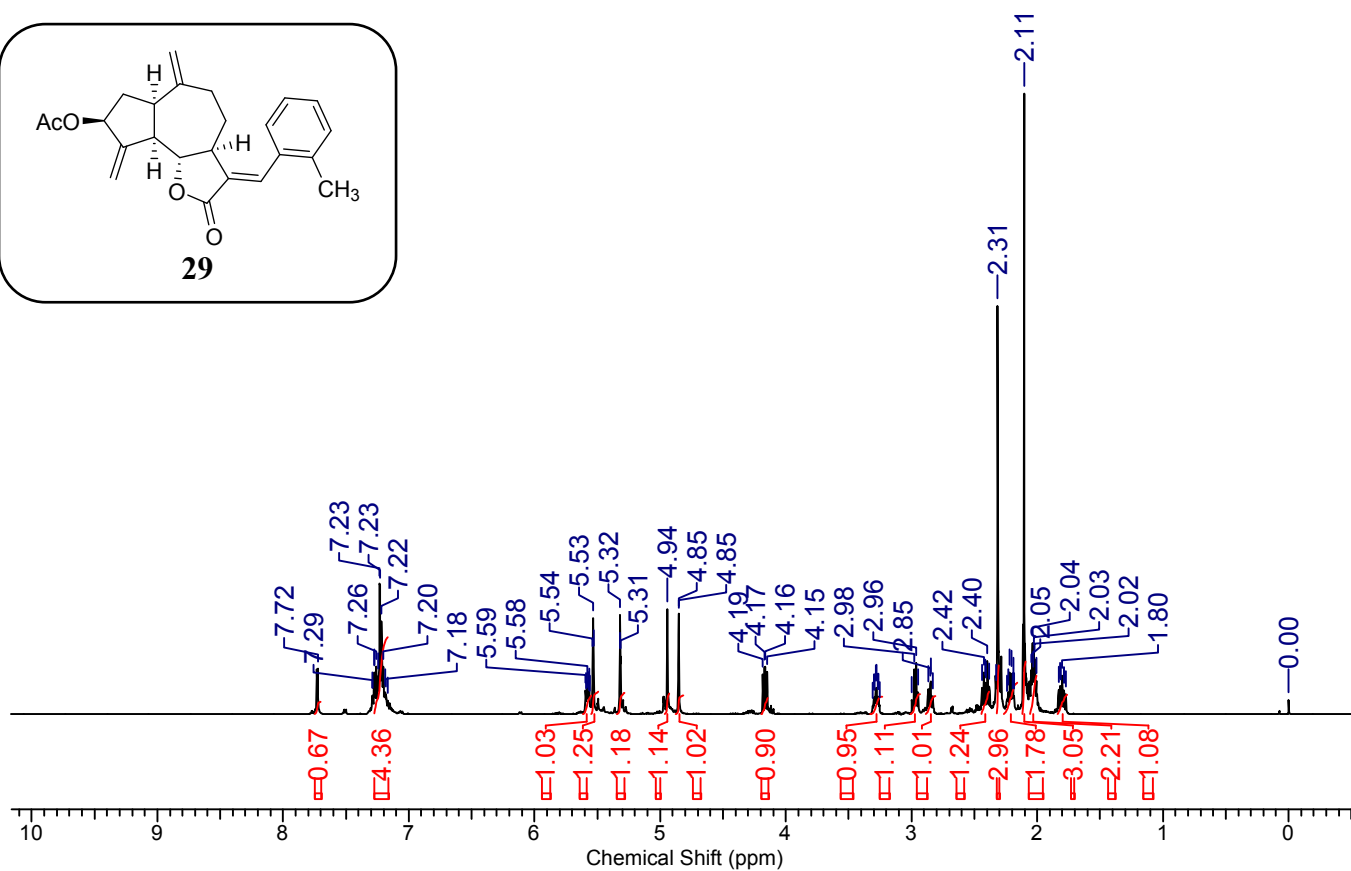
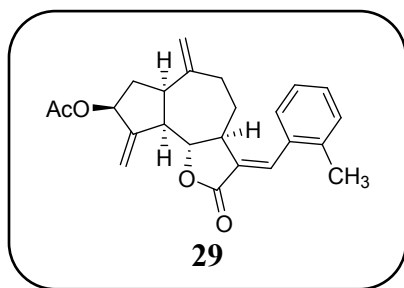
D:\Data\IS-365

12/24/2014 12:41:53 PM

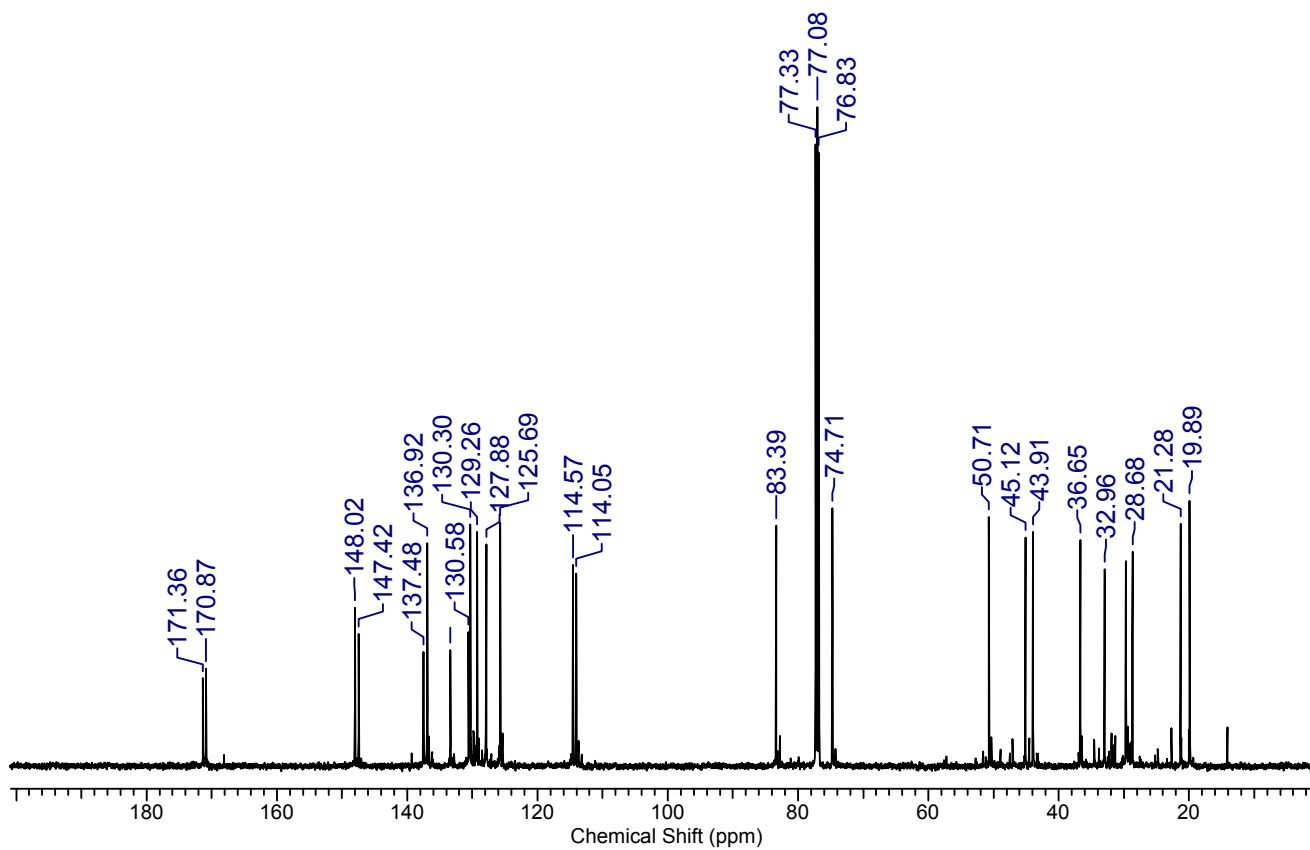
IS-365 #899 RT: 4.00 AV: 1 NL: 8.84E7
T: FTMS + p ESI Full ms [66.70-1000.00]



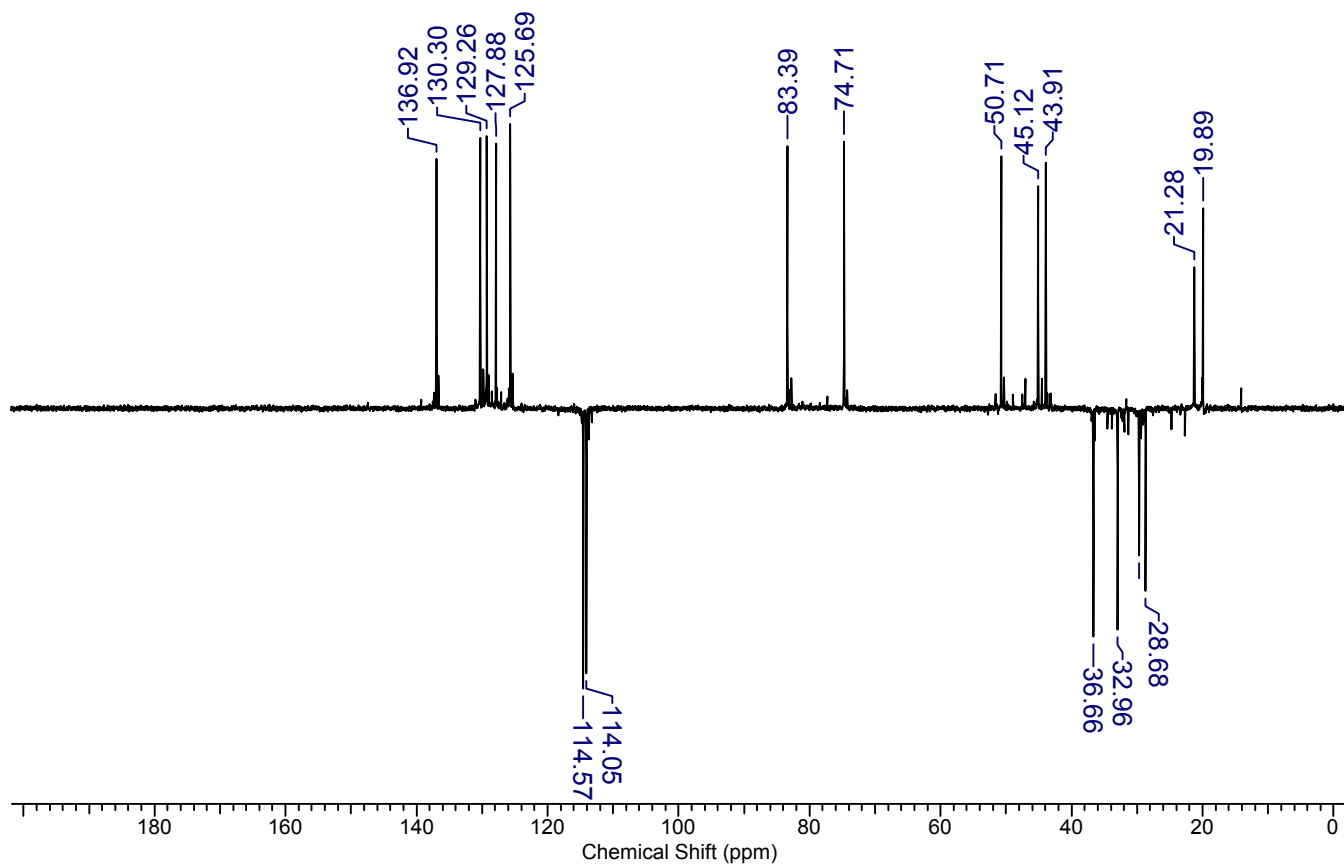
¹H NMR of Compound 29 (500 MHz, CDCl₃)



¹³C NMR of Compound 29 (125 MHz, CDCl₃)



DEPT of Compound 29 (125 MHz, CDCl₃)

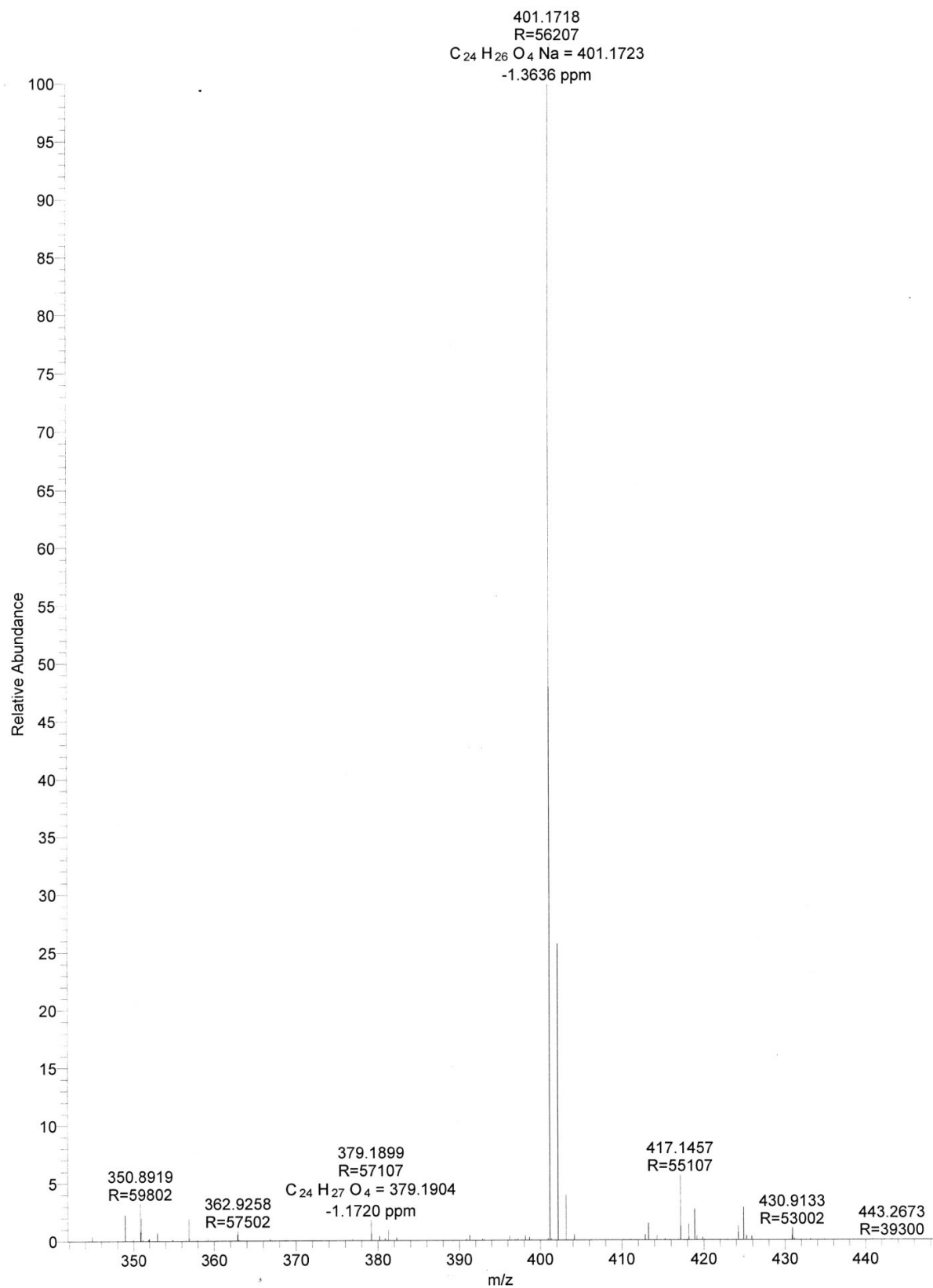


HR-MS of Compound 29

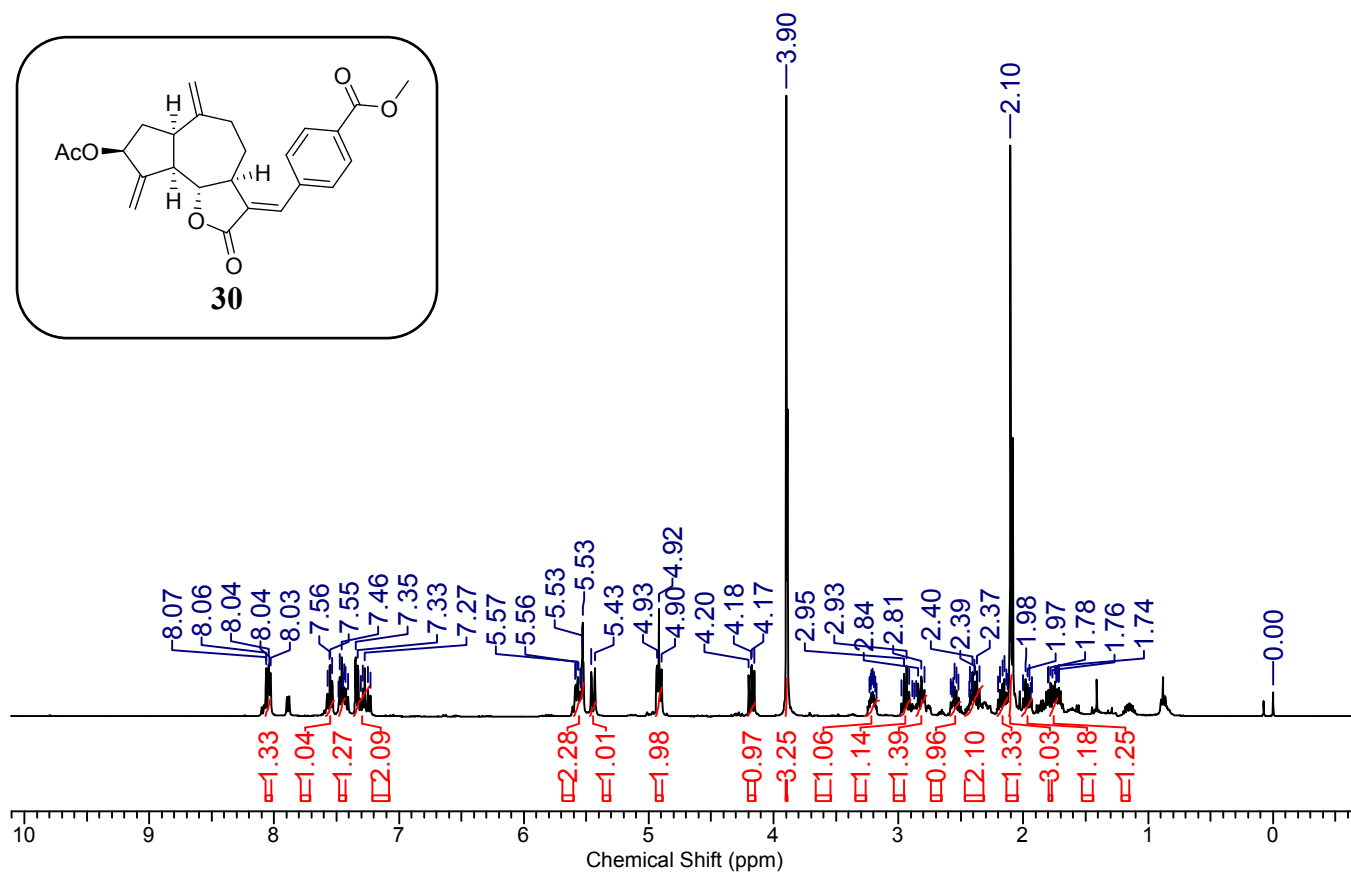
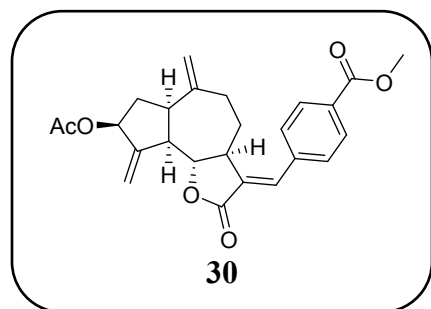
D:\Data\IS-366

12/9/2014 12:47:59 PM

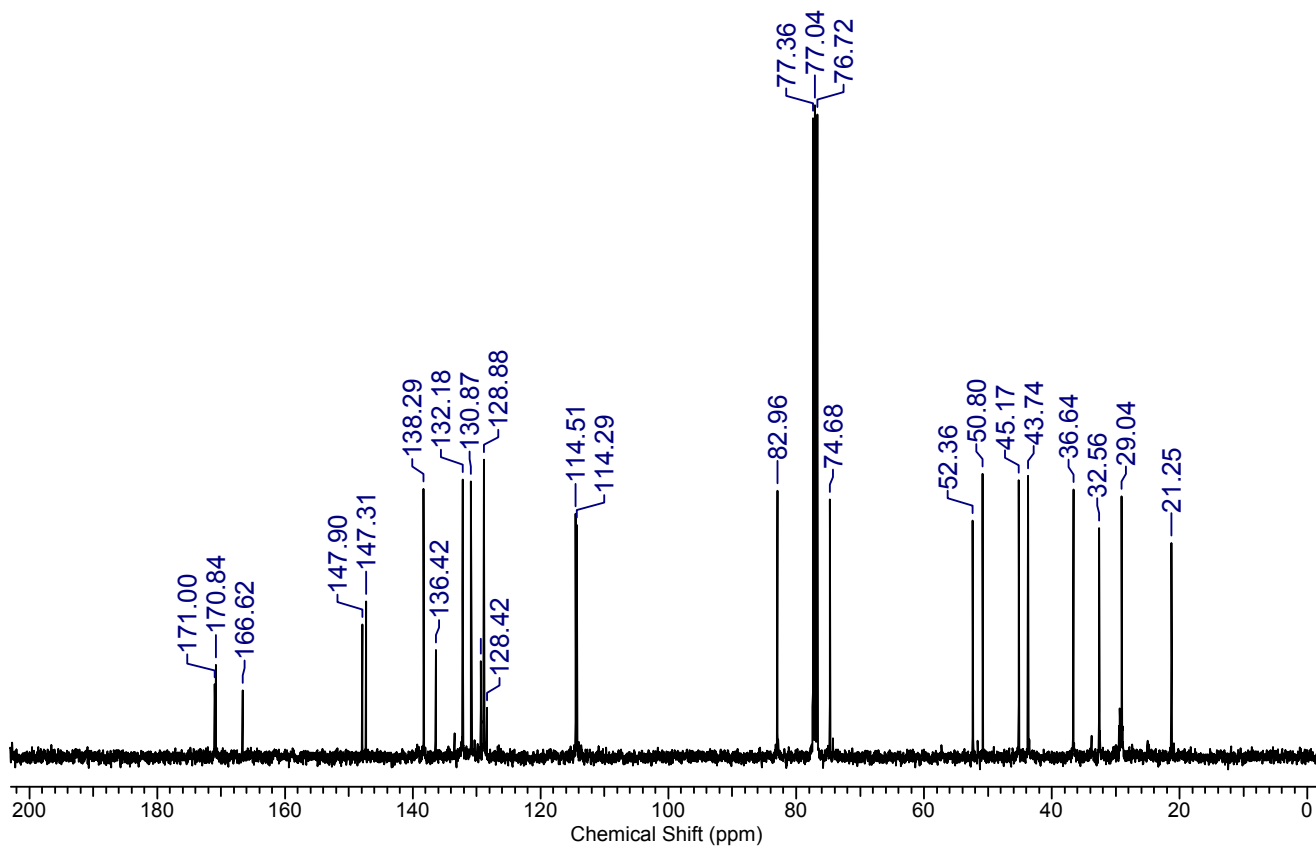
IS-366 #1092 RT: 4.86 AV: 1 NL: 1.47E8
T: FTMS + p ESI Full ms [66.70-1000.00]



¹H NMR of Compound 30 (400 MHz, CDCl₃)



¹³C NMR of Compound 30 (100 MHz, CDCl₃)

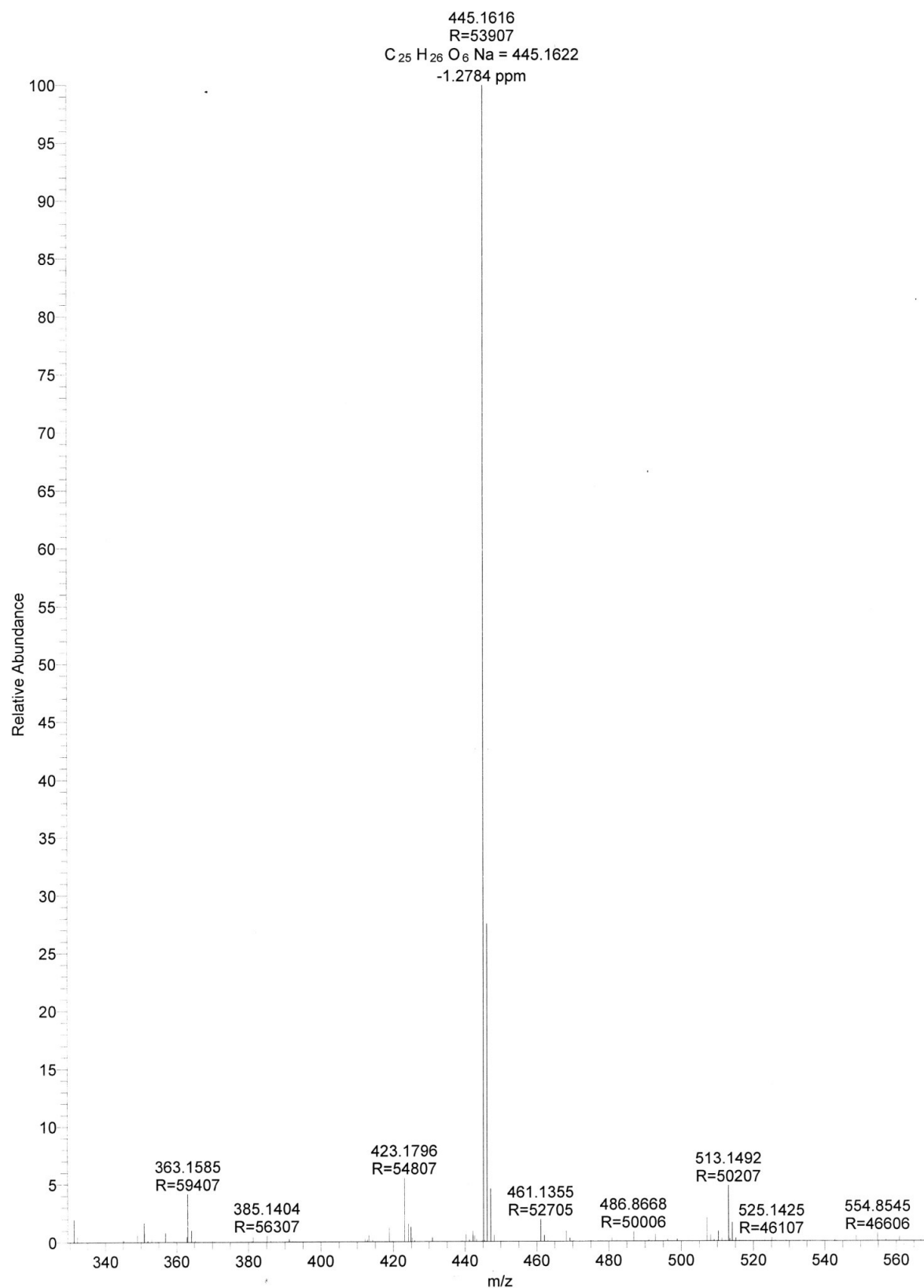


HR-MS of Compound 30

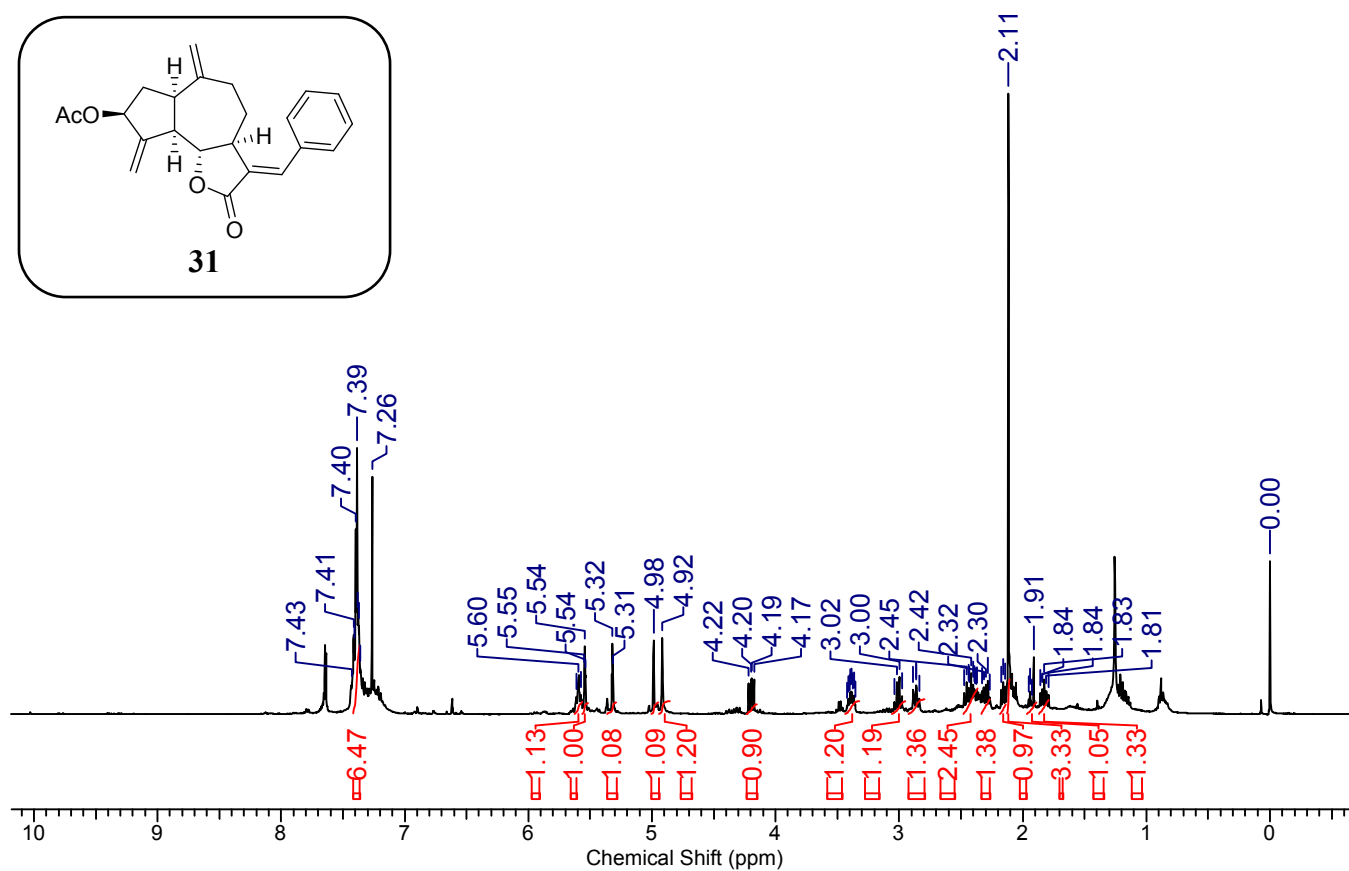
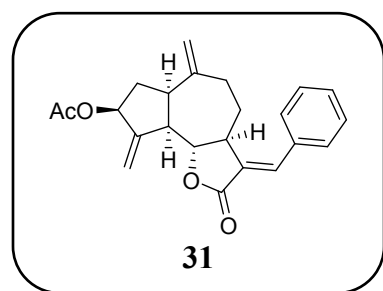
D:\Data\IS-367

12/9/2014 12:59:13 PM

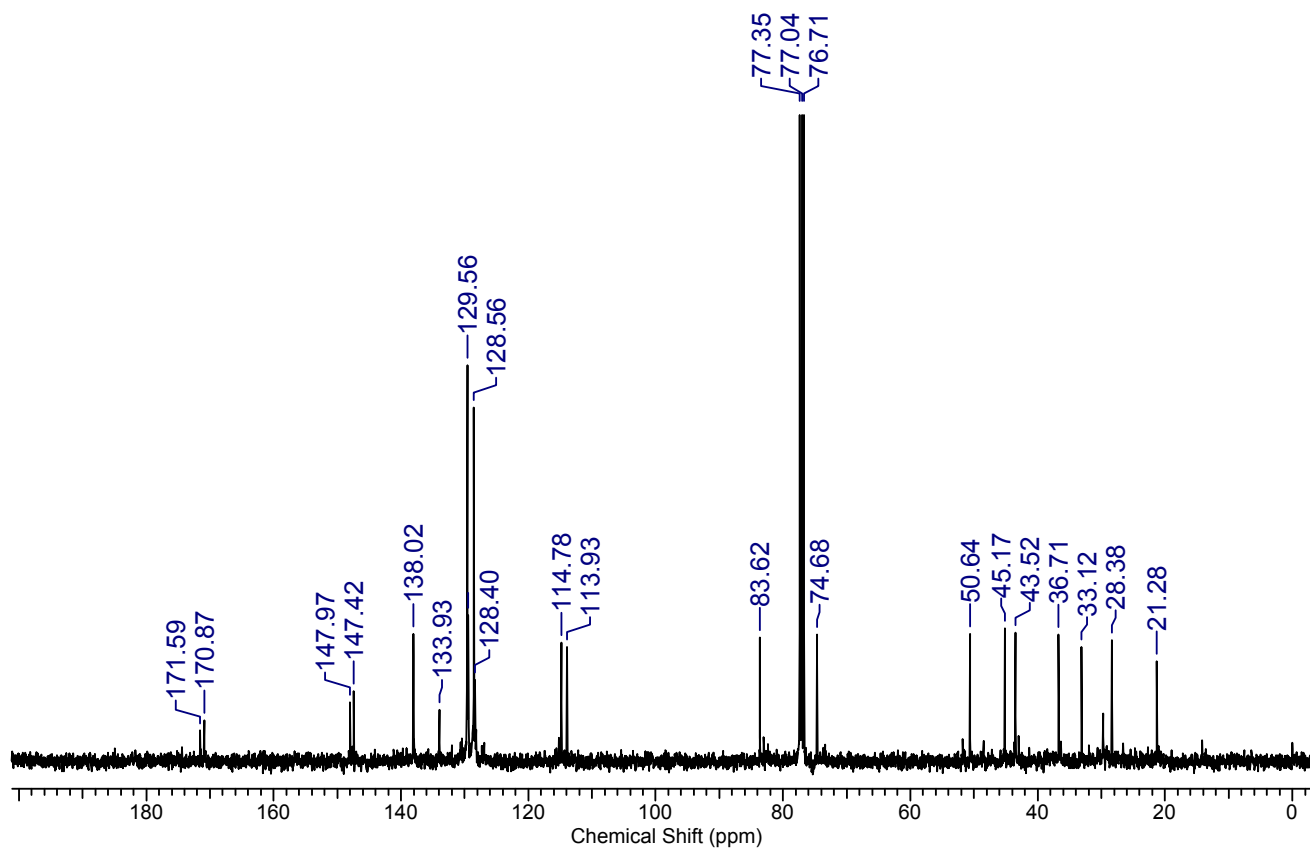
IS-367 #987 RT: 4.40 AV: 1 NL: 2.95E8
T: FTMS + p ESI Full ms [66.70-1000.00]



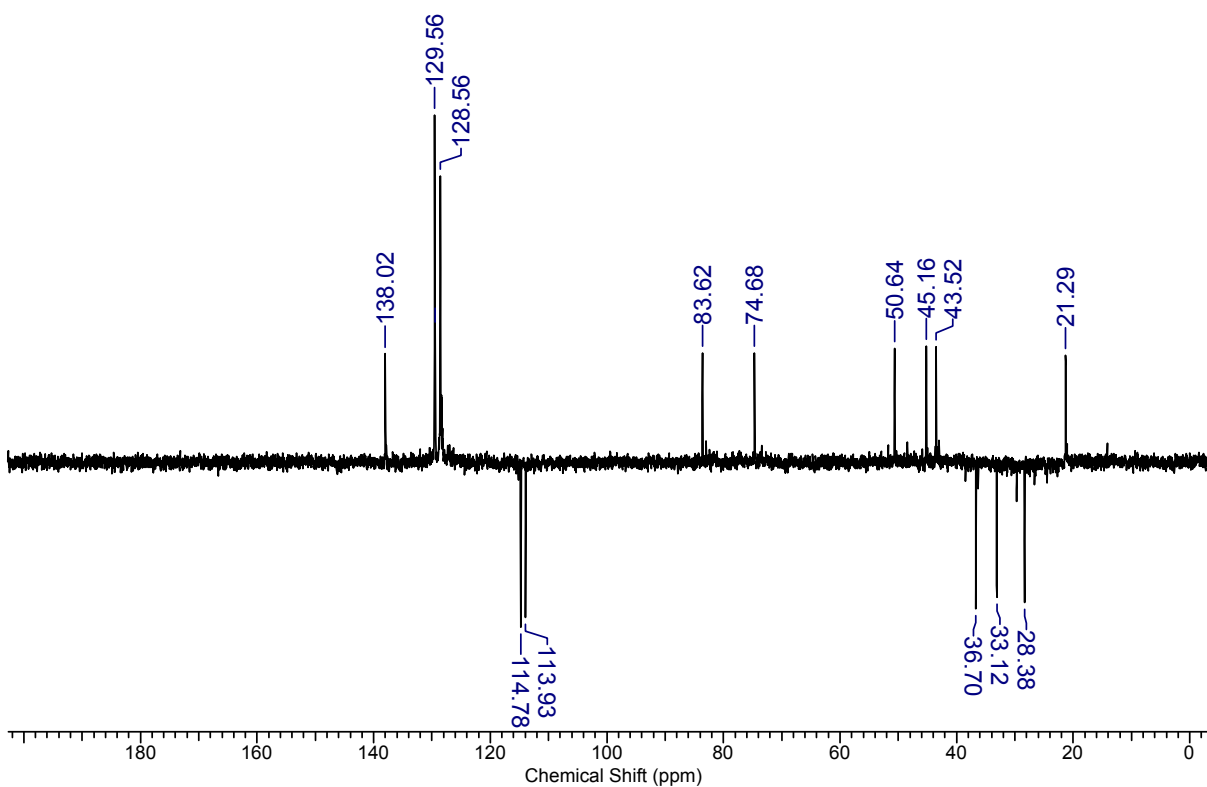
¹H NMR of Compound 31 (400 MHz, CDCl₃)



¹³C NMR of Compound 31 (100 MHz, CDCl₃)



DEPT of Compound 31 (100 MHz, CDCl₃)

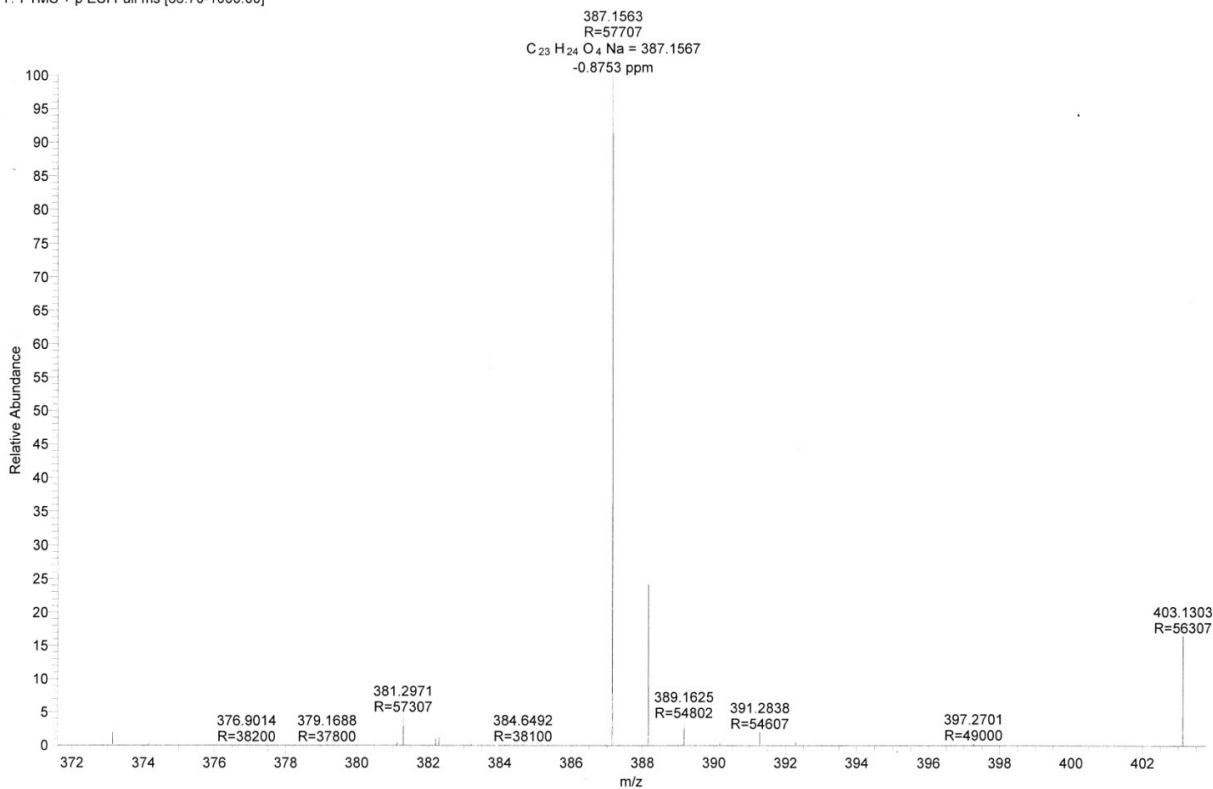


HR-MS of Compound 31

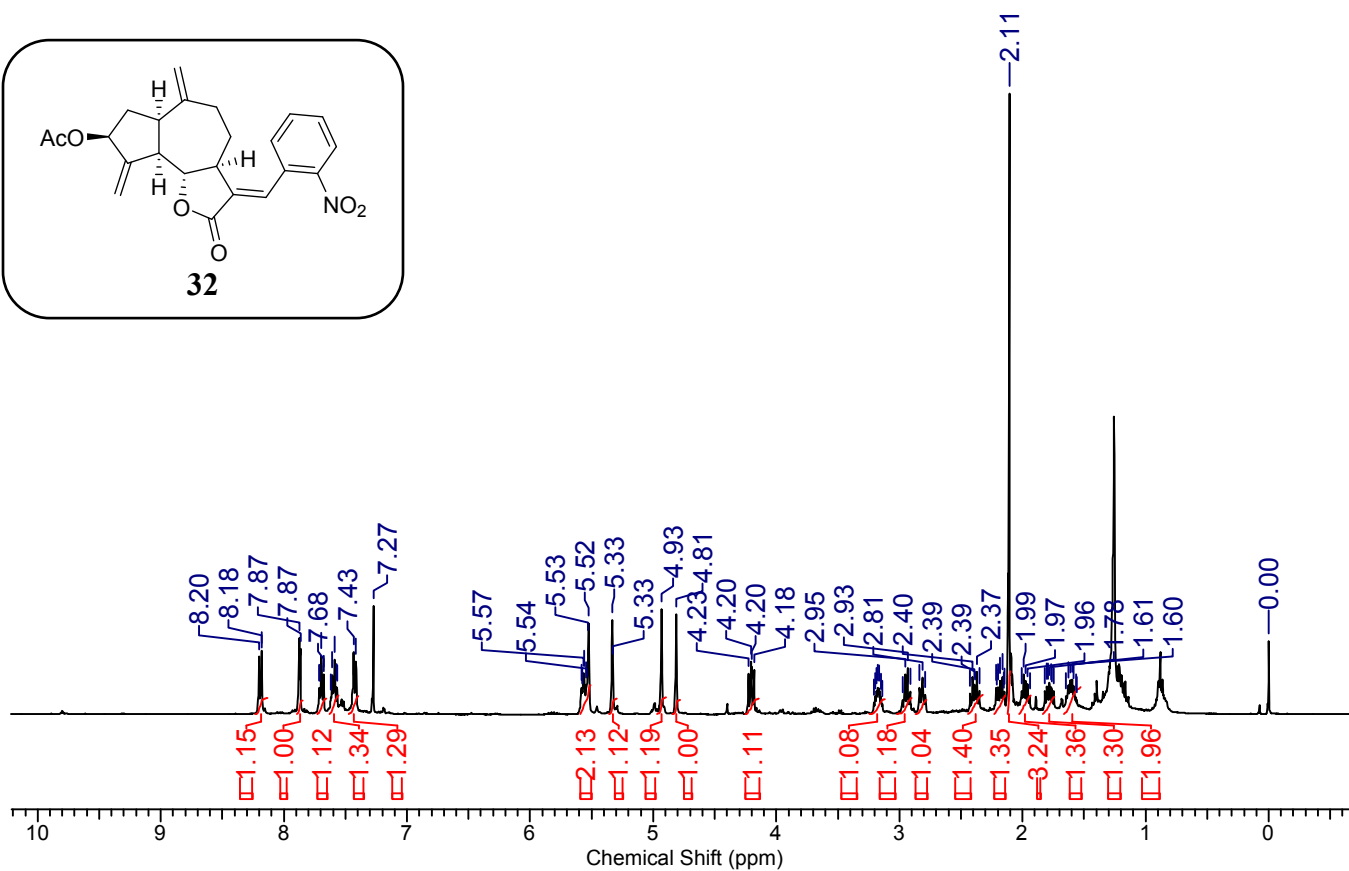
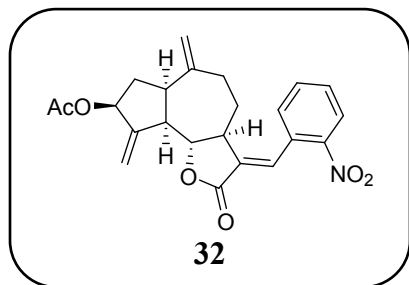
D:\Data\IS-369-B

12/24/2014 12:53:01 PM

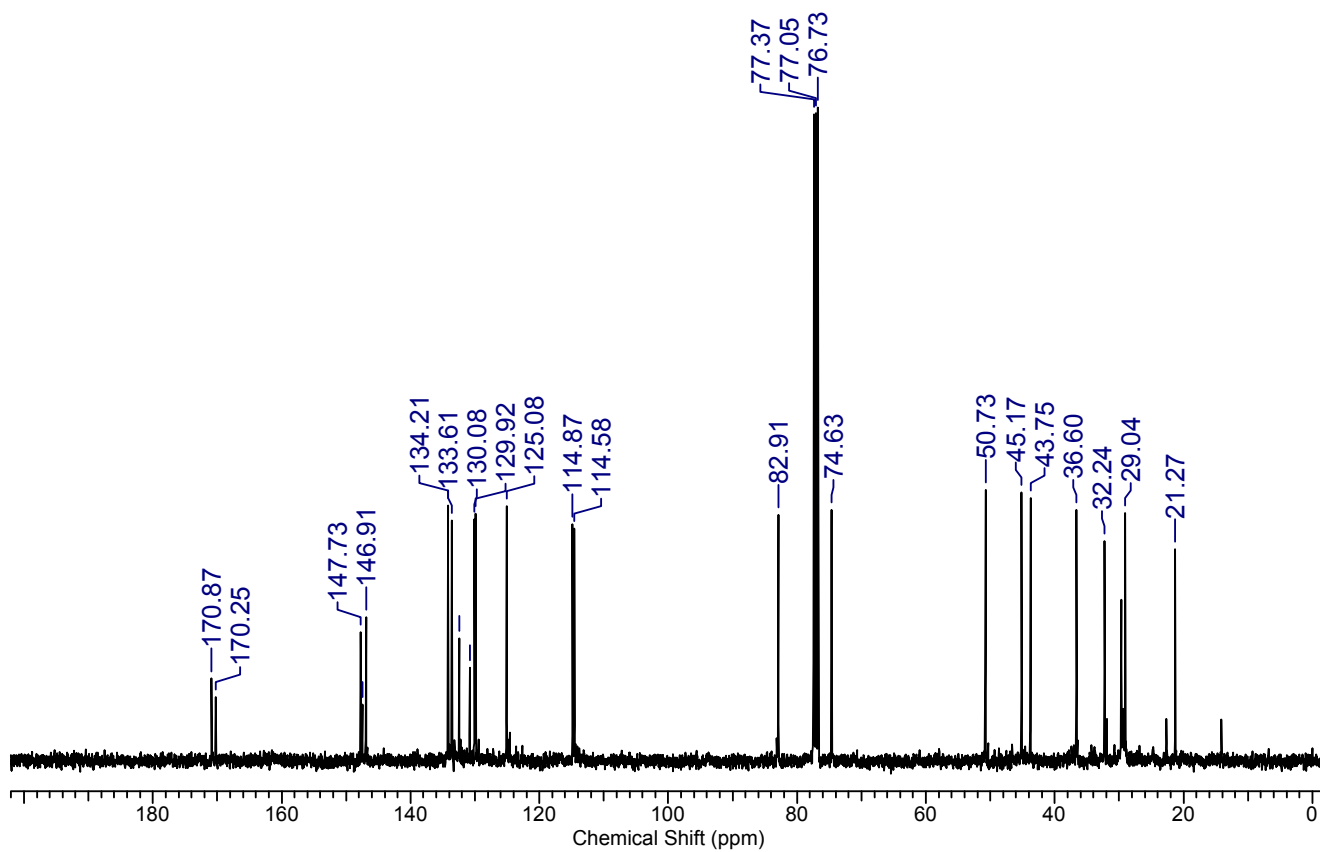
IS-369-B #1052 RT: 4.69 AV: 1 NL: 2.88E7
T: FTMS + p ESI Full ms [66.70-1000.00]



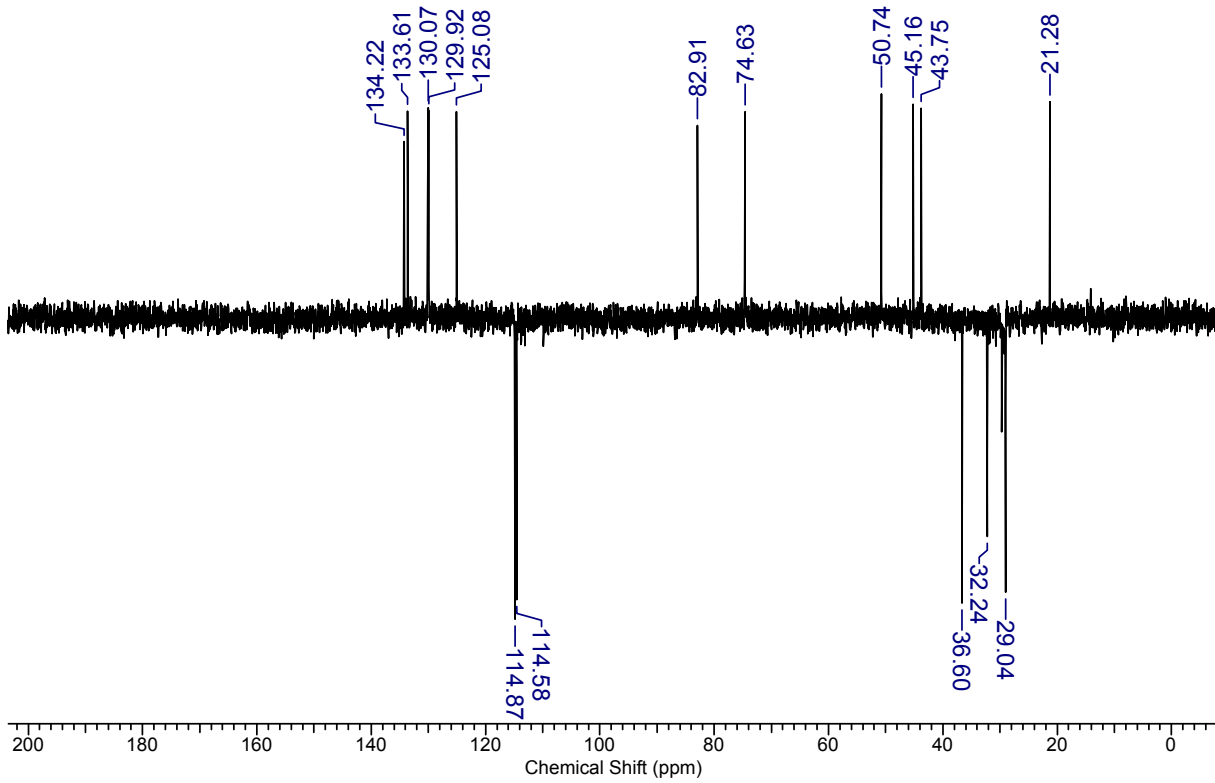
¹H NMR of Compound 32 (400 MHz, CDCl₃)



¹³C NMR of Compound 32 (100 MHz, CDCl₃)



DEPT of Compound 32 (100 MHz, CDCl₃)

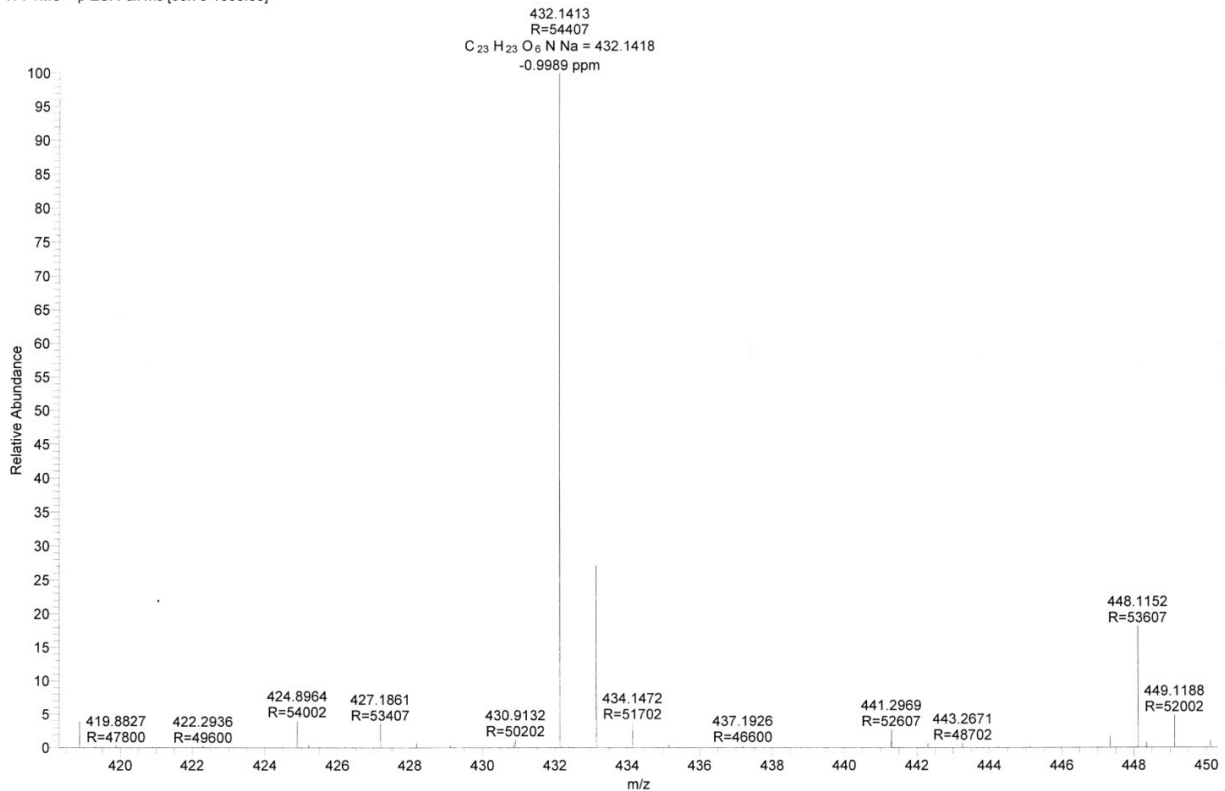


HR-MS of Compound 32

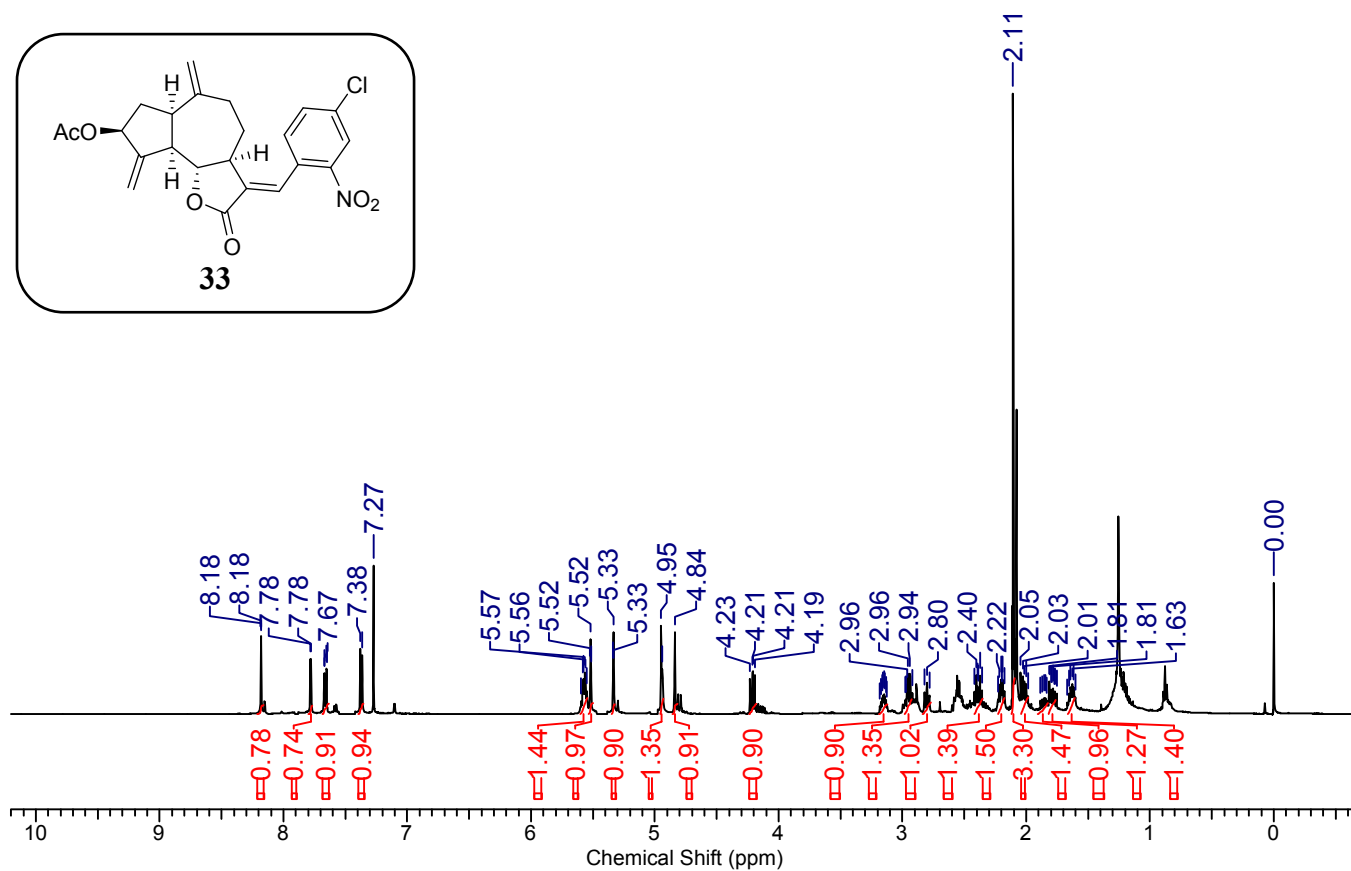
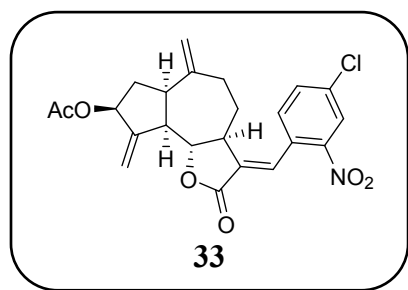
D:\Data\IS-370-C

12/24/2014 1:04:10 PM

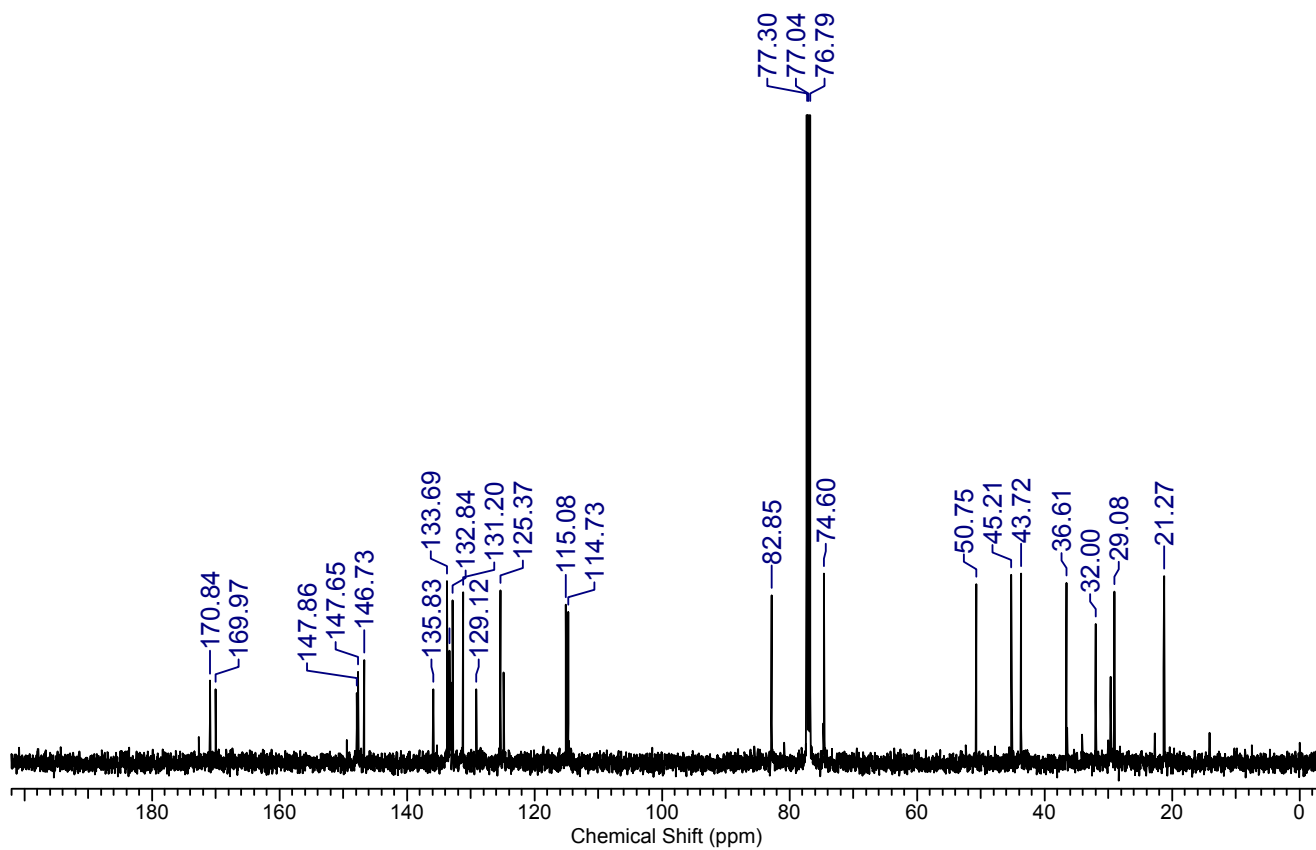
IS-370-C #977 RT: 4.35 AV: 1 NL: 3.18E7
T: FTMS + p ESI Full ms [66.70-1000.00]



¹H NMR of Compound 33 (500 MHz, CDCl₃)



¹³C NMR of Compound 33 (125 MHz, CDCl₃)

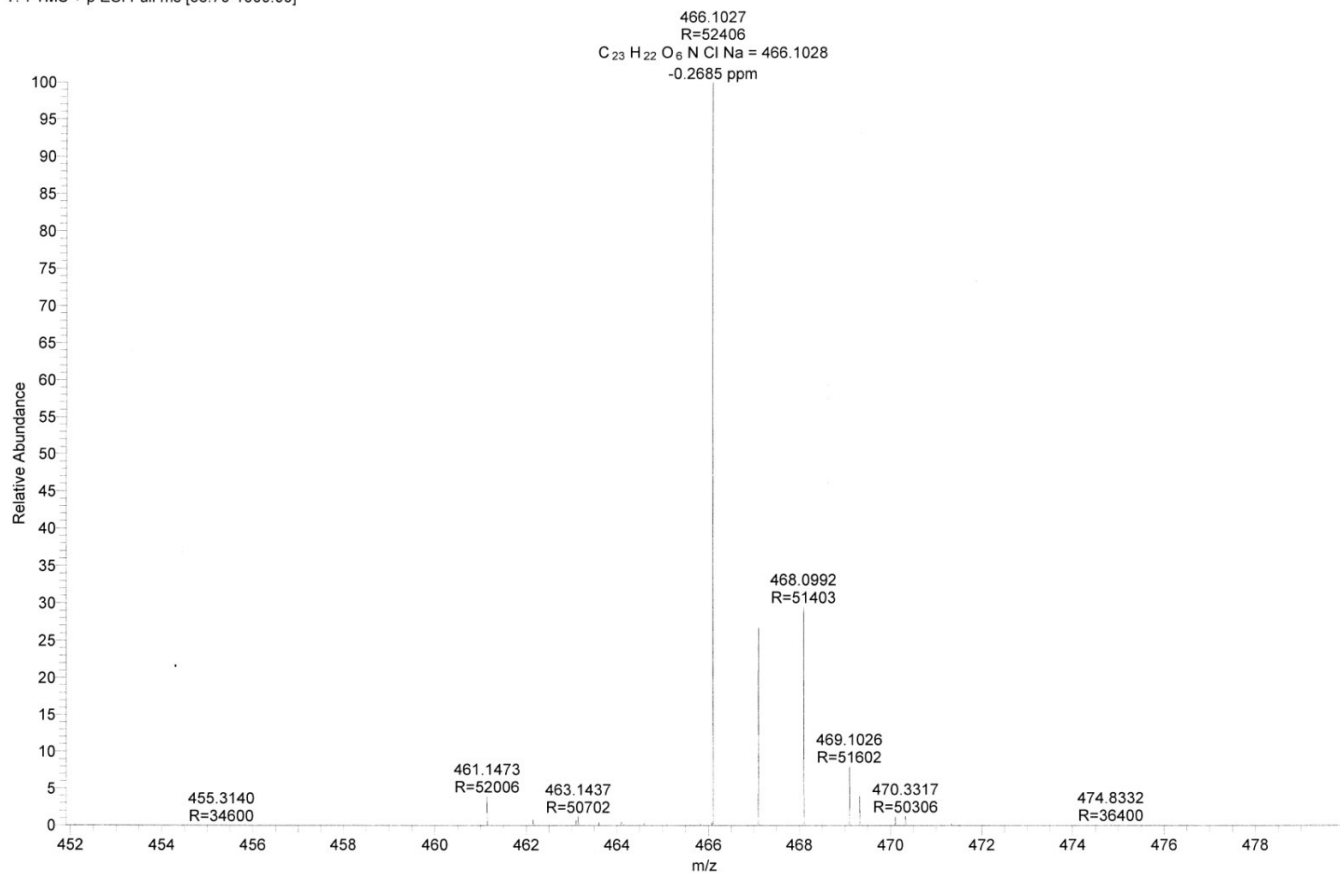


HR-MS of Compound 33

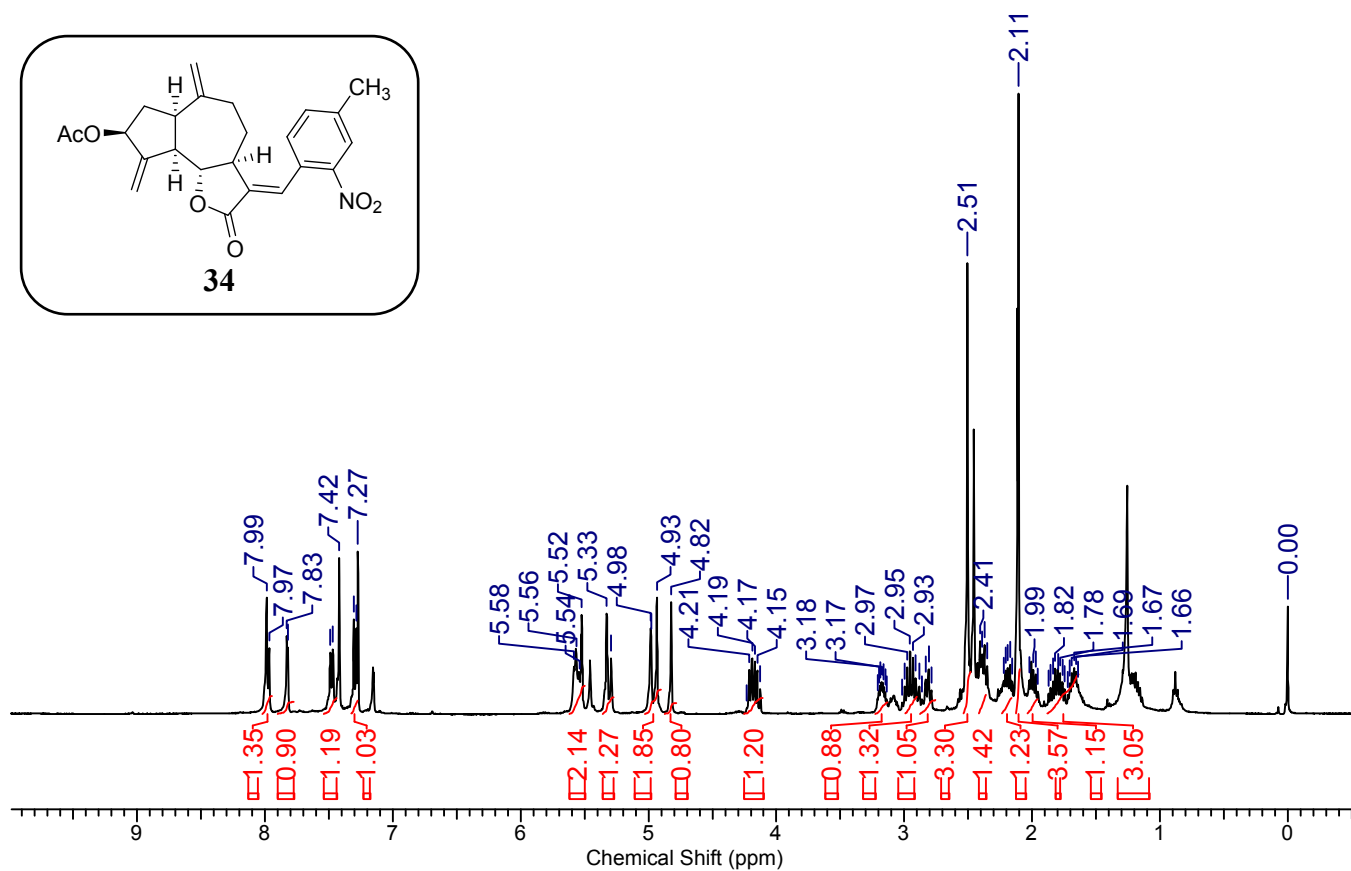
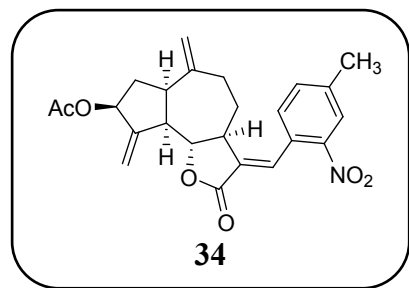
D:\Data\IS-371-B

12/24/2014 1:15:23 PM

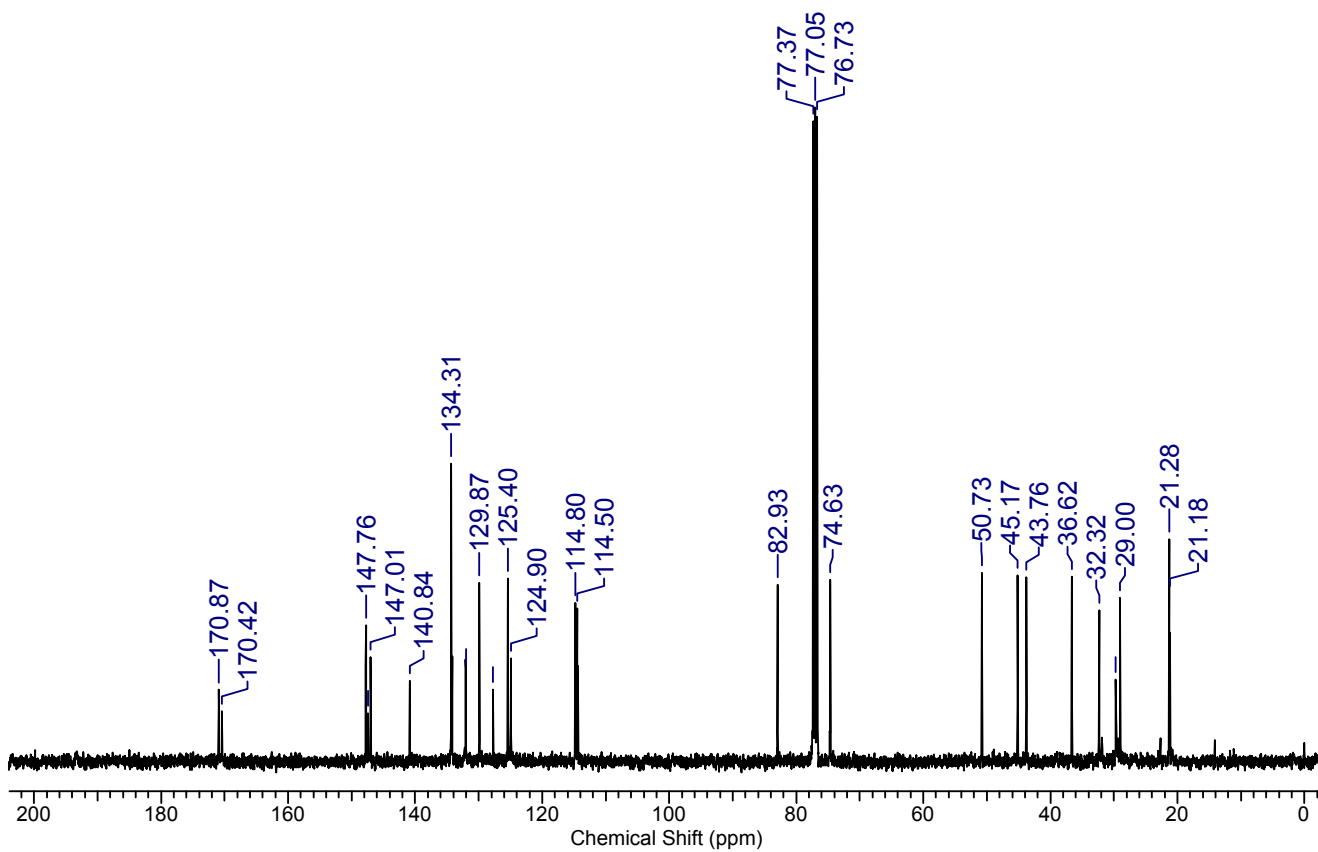
IS-371-B #1046 RT: 4.66 AV: 1 NL: 7.62E7
T: FTMS + p ESI Full ms [66.70-1000.00]



¹H NMR of Compound 34 (400 MHz, CDCl₃)



¹³C NMR of Compound 34 (100 MHz, CDCl₃)



HR-MS of Compound 34

D:\Data\IS-372-C

12/24/2014 1:37:44 PM

IS-372-C #1011 RT: 4.51 AV: 1 NL: 5.00E7
T: FTMS + p ESI Full ms [66.70-1000.00]

