

Supplimentary information for

Synthesis, *in vitro* COX-1/COX-2 inhibition testing and molecular docking study of novel 1,4-benzoxazine derivatives

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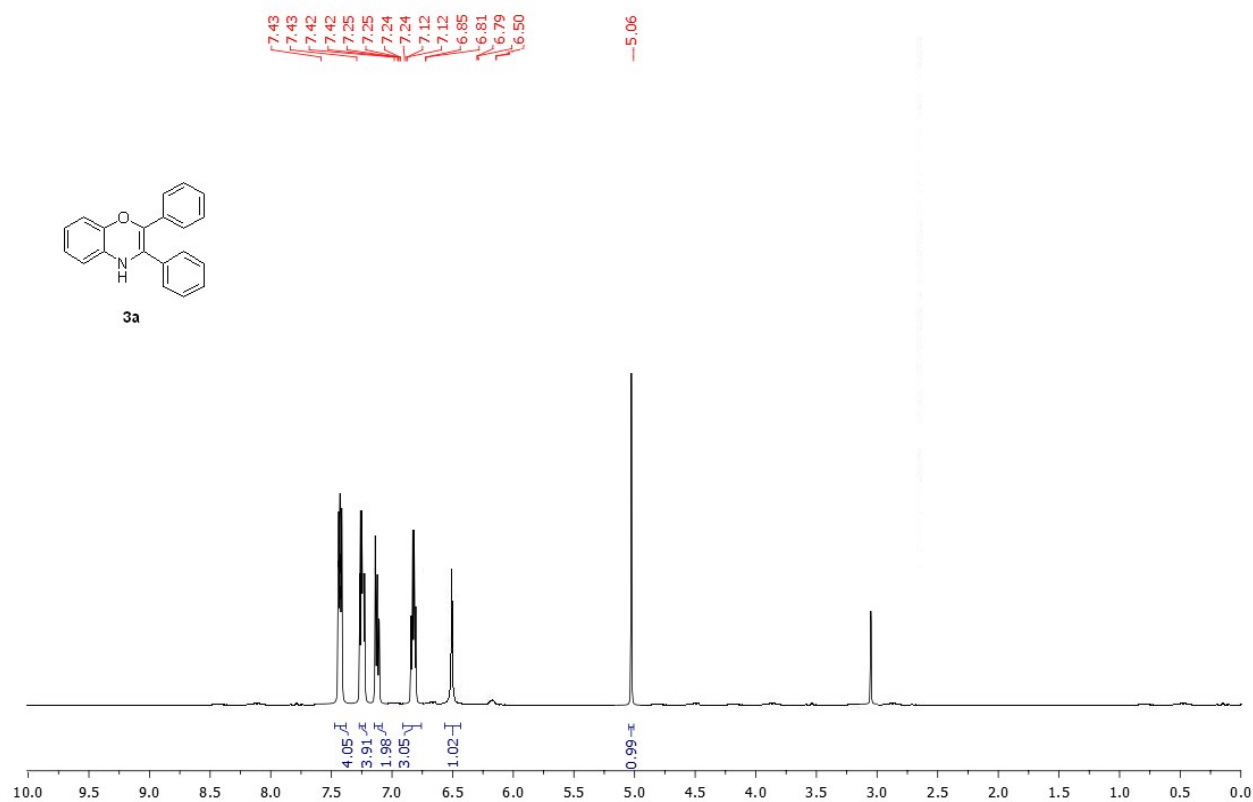
²Division of Biological and Life Sciences, Ahmedabad University, Ahmedabad, Gujarat, India.

*Department of Chemistry, Veer Narmad South Gujarat University, Surat, Gujarat, India.

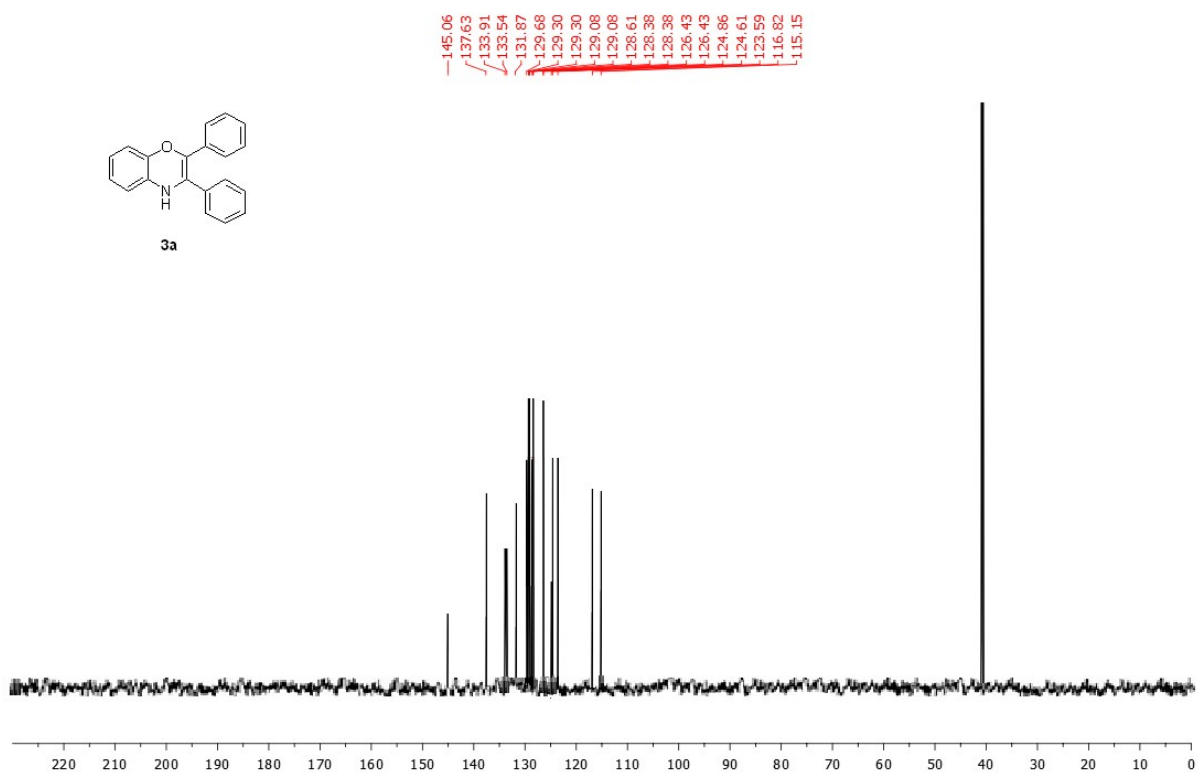
1. ¹ H and ¹³ C NMR and HRMS Spectra.....	2
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1. ^1H and ^{13}C NMR spectra:

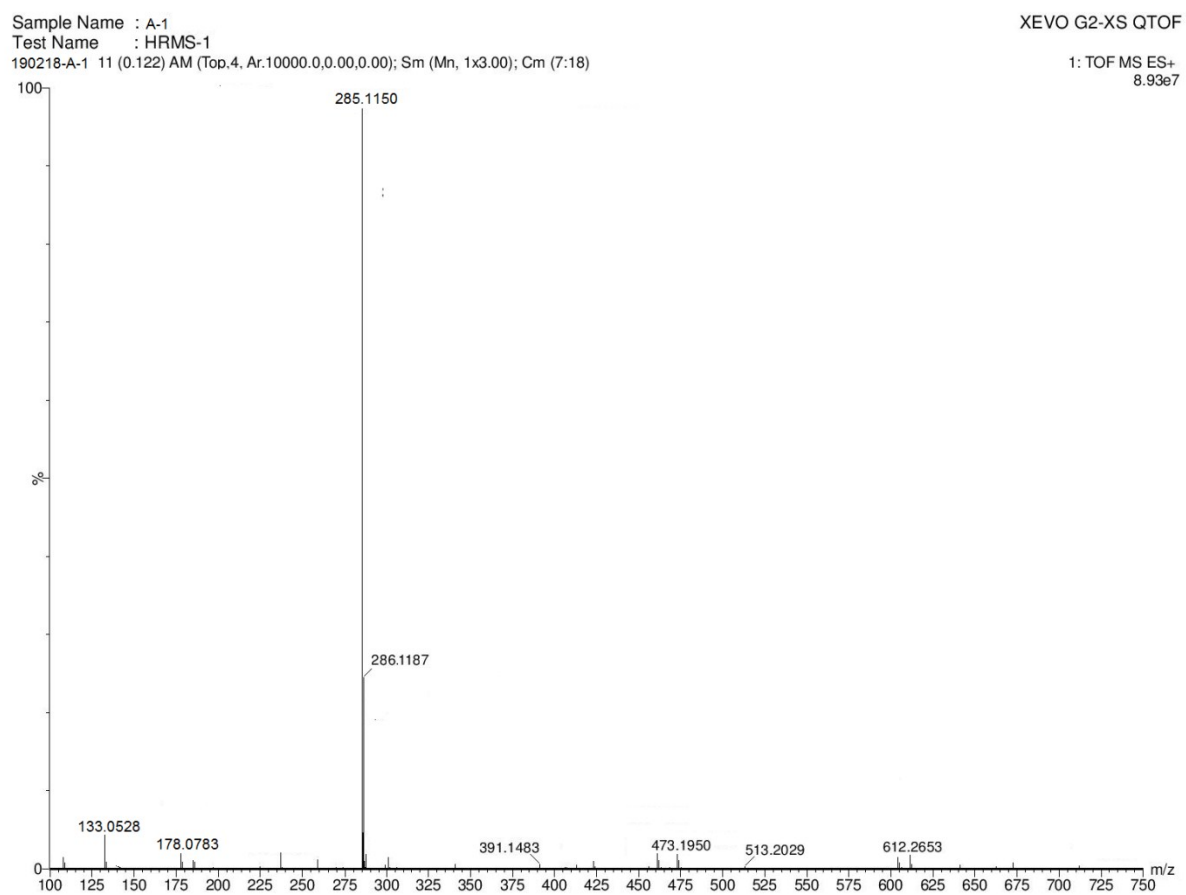
^1H NMR spectrum of 3a



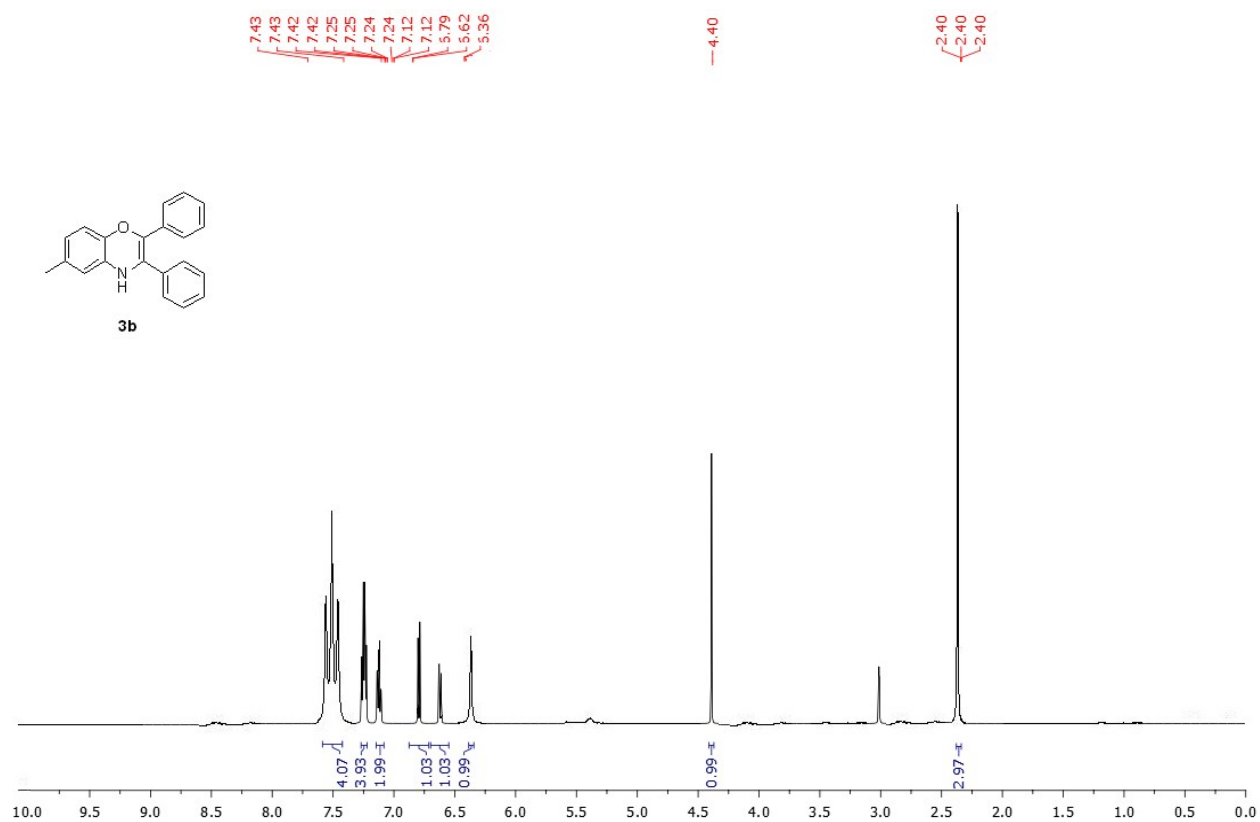
^{13}C NMR spectrum of 3a



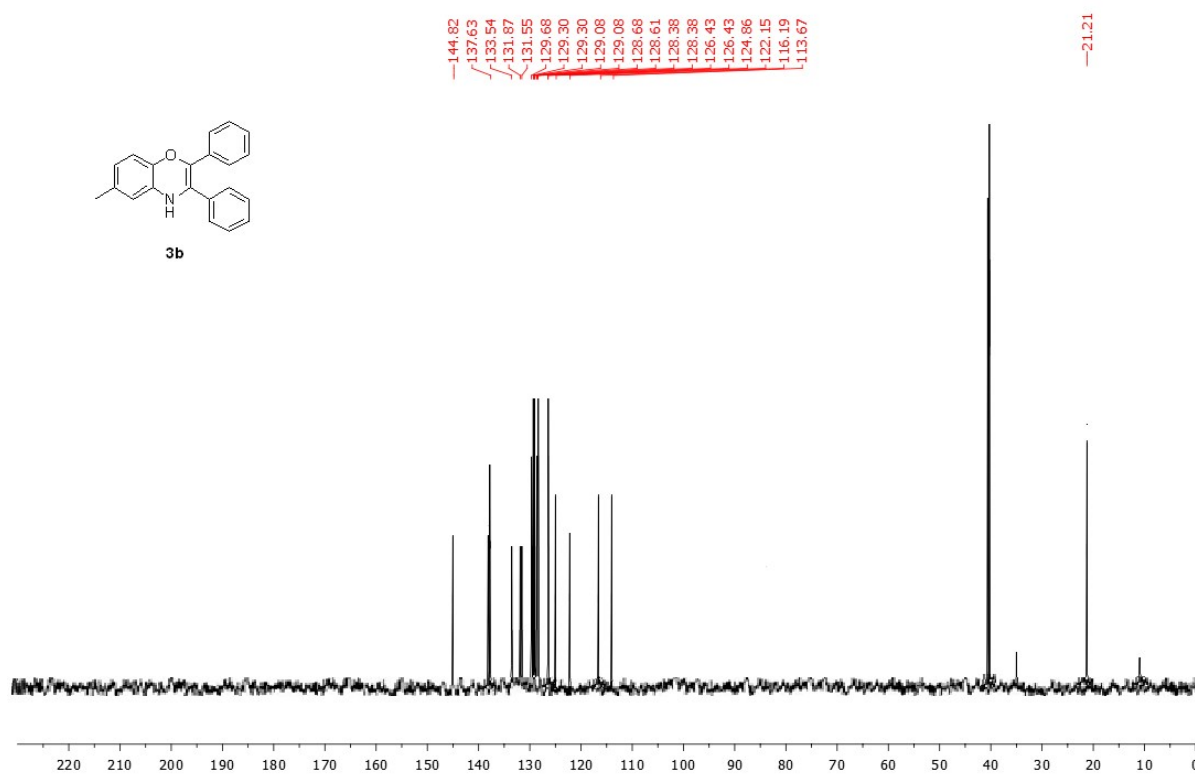
HRMS spectrum of 3a:



^1H NMR spectrum of 3b



¹³C NMR spectrum of 3b

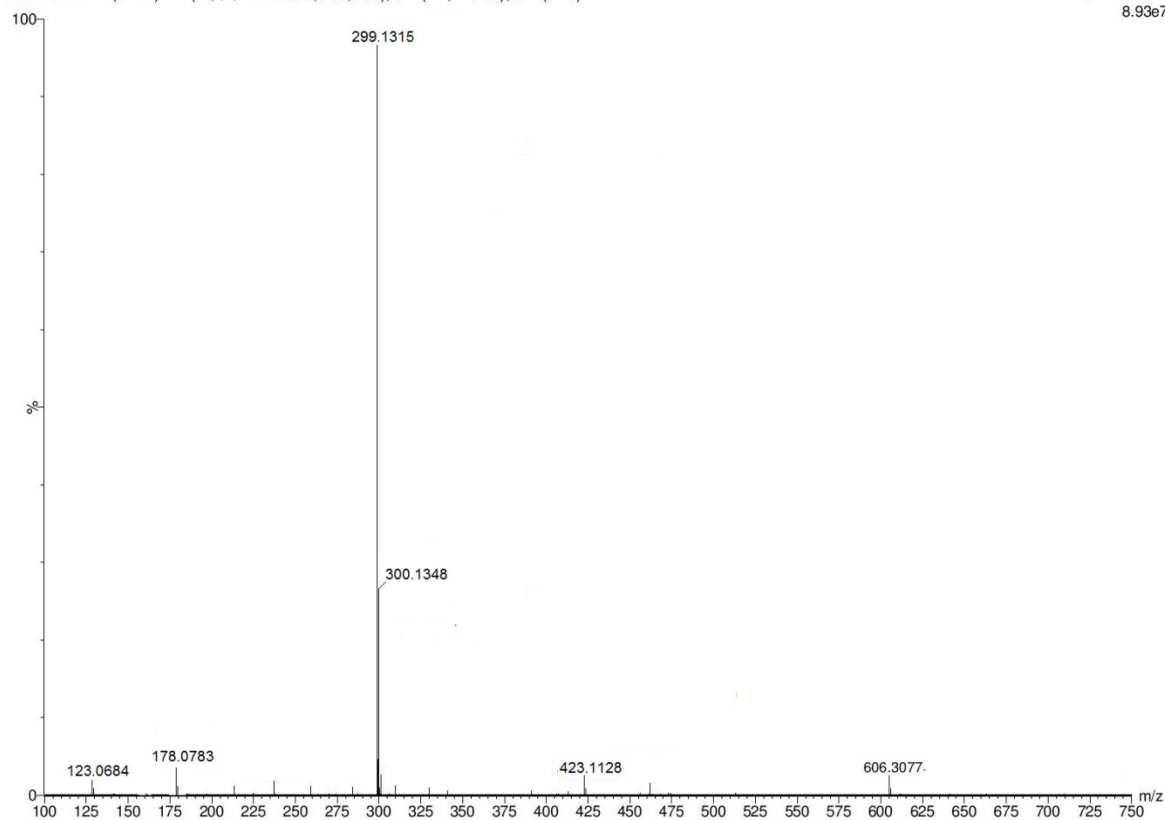


HRMS spectrum of 3b:

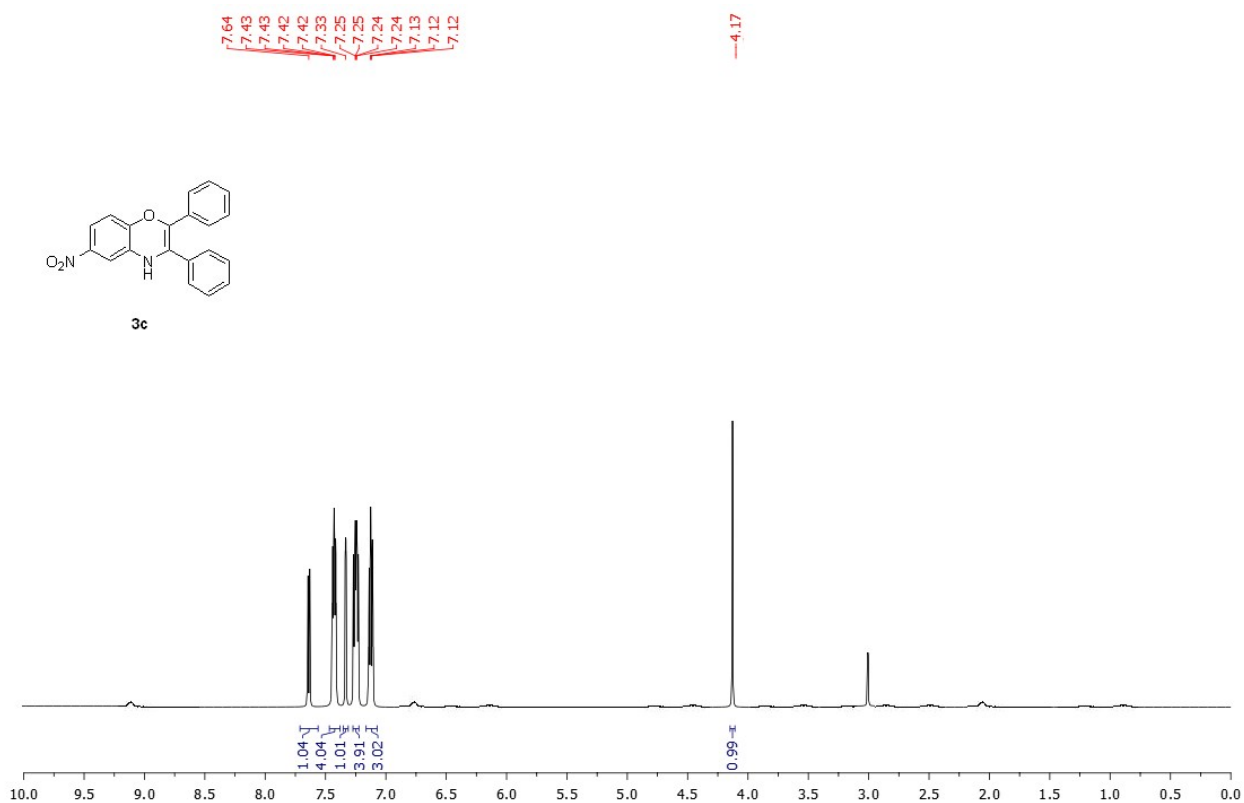
Sample Name : A-2
 Test Name : HRMS-1
 200218-A-2 11 (0.112) AM (Top,4, Ar.10000.0,0.00,0.00); Sm (Mn, 1x3.00); Cm (7:18)

XEVO G2-XS QTOF

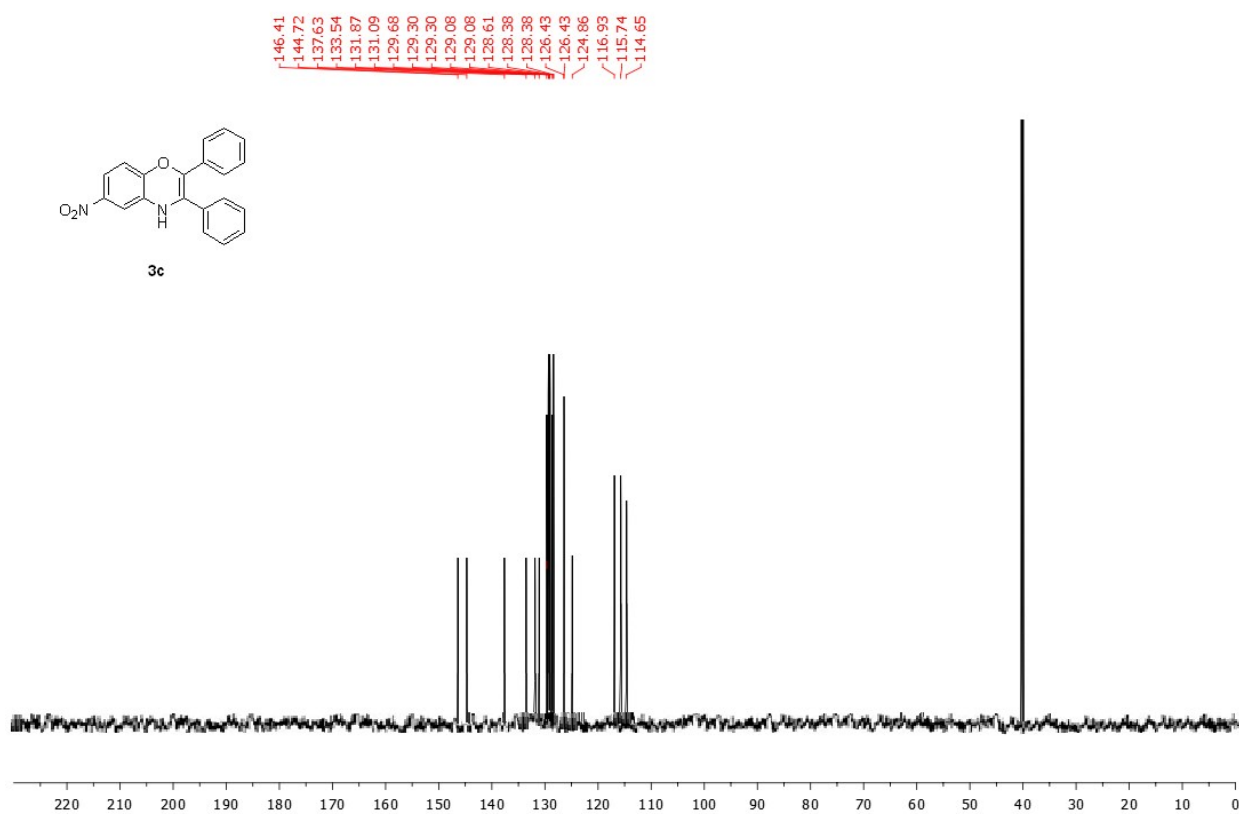
1: TOF MS ES+
 8.93e7



^1H NMR spectrum of 3c



^{13}C NMR spectrum of 3c

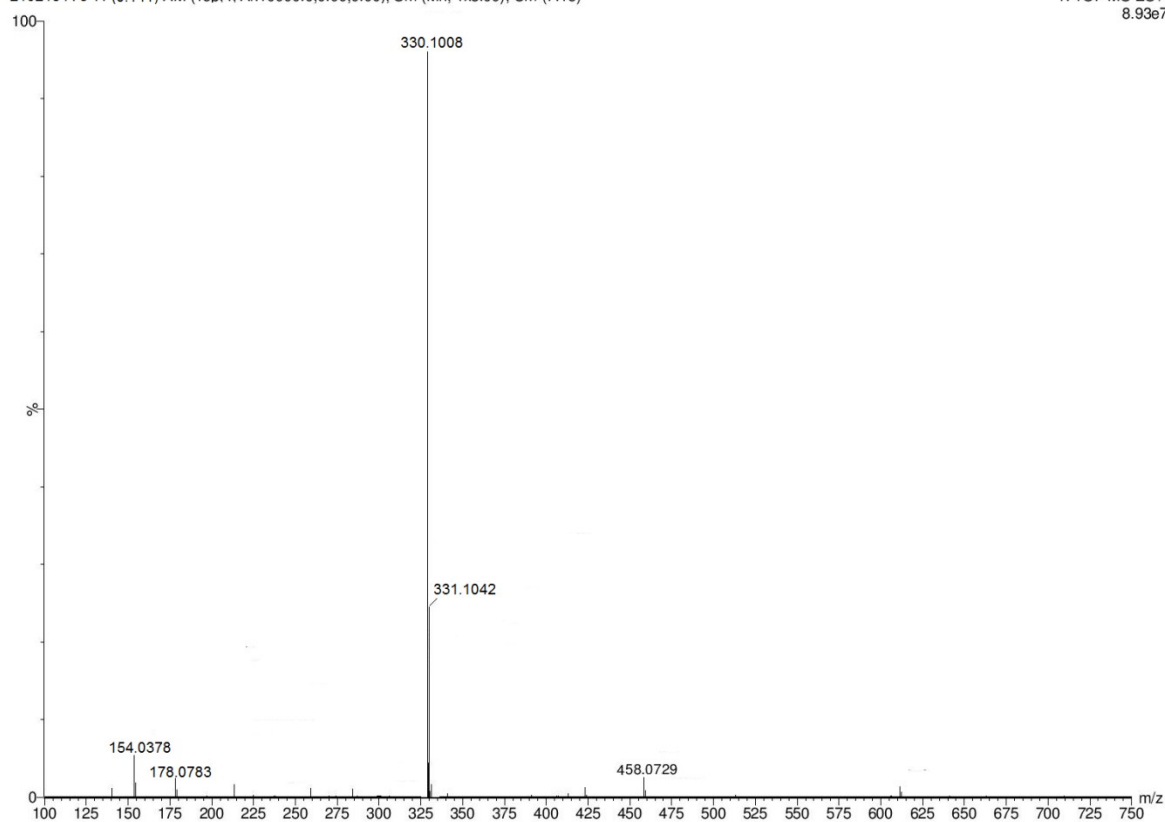


HRMS spectrum of **3c**:

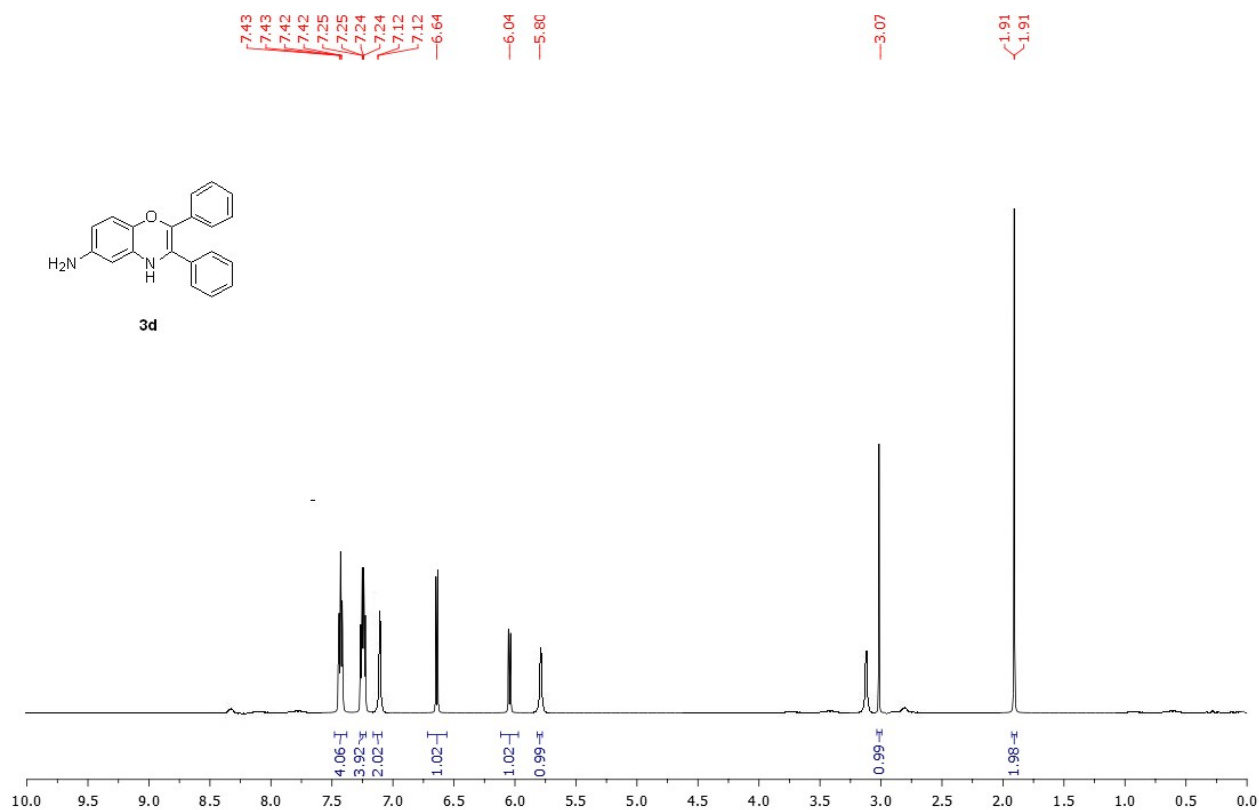
Sample Name : A-3
 Test Name : HRMS-1
 210218-A-3 11 (0.141) AM (Top,4, Ar:10000.0,0.00,0.00); Sm (Mn, 1x3.00); Cm (7:18)

XEVO G2-XS QTOF

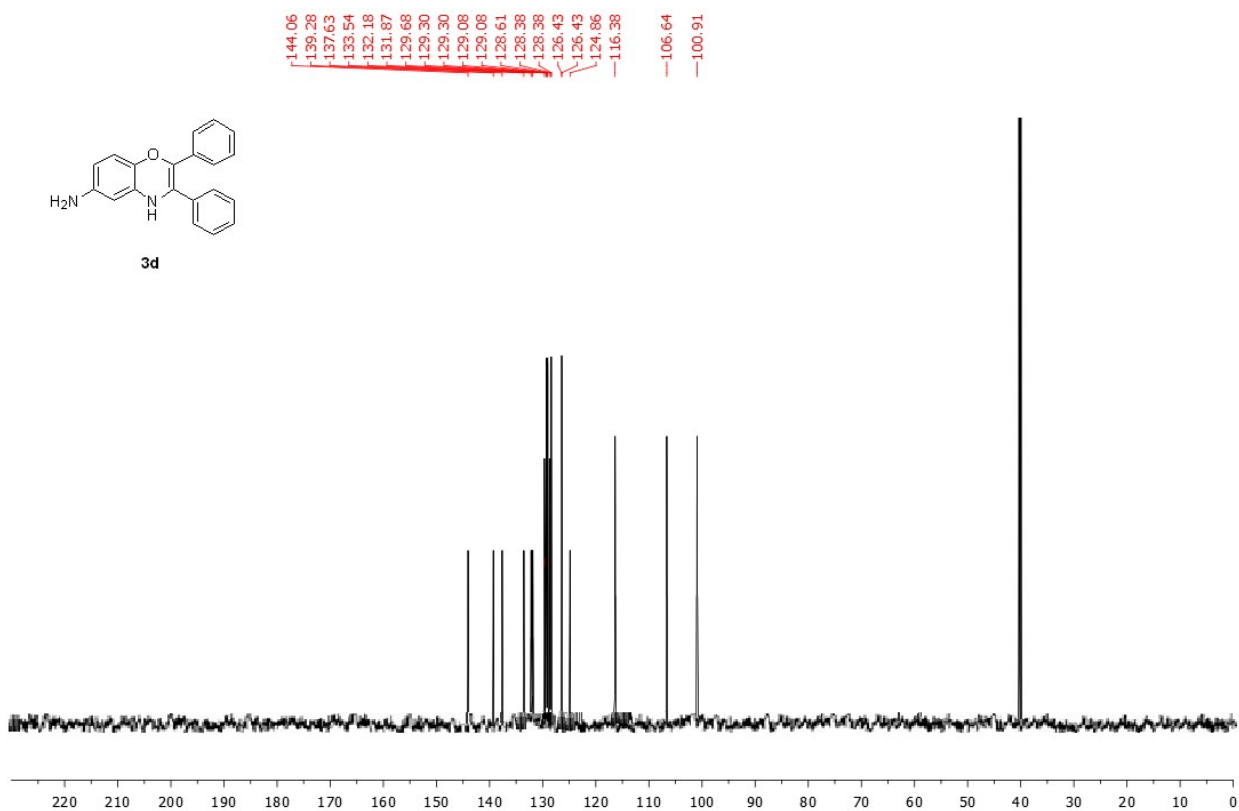
1: TOF MS ES+
 8.93e7



^1H NMR spectrum of 3d



^{13}C NMR spectrum of 3d

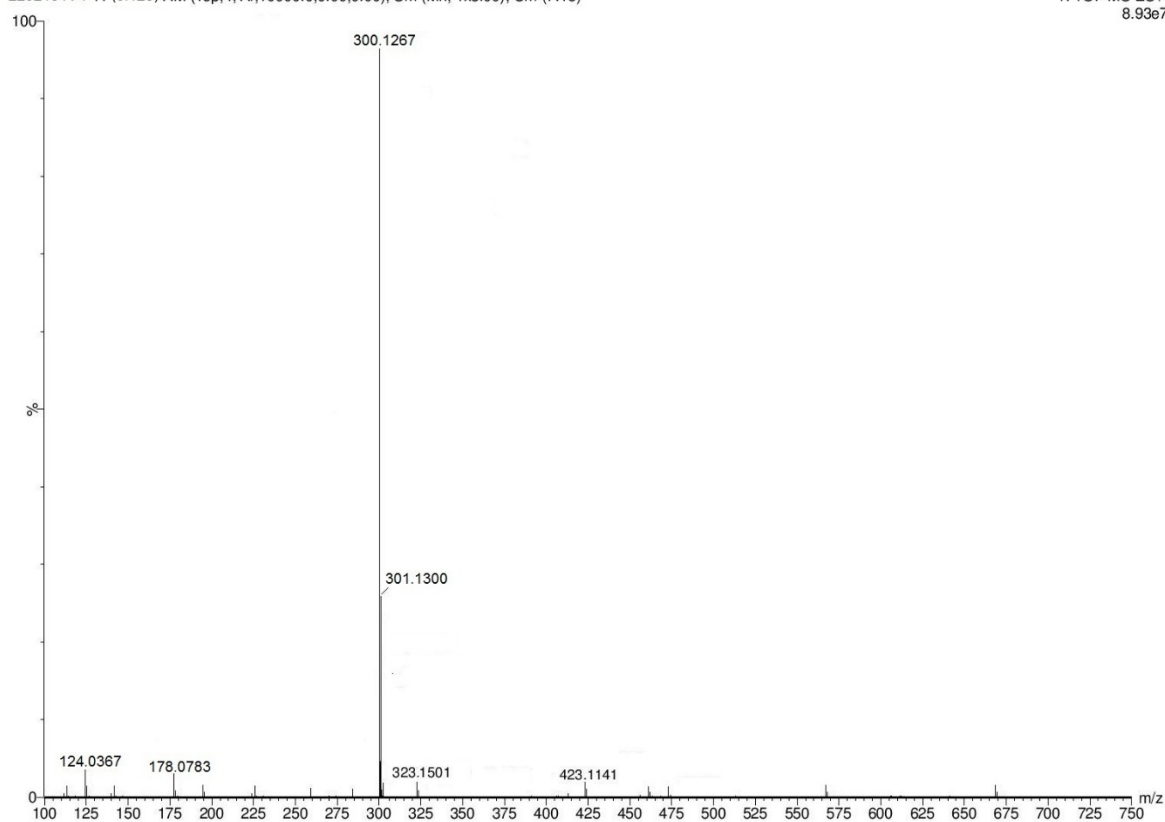


HRMS spectrum of **3d**:

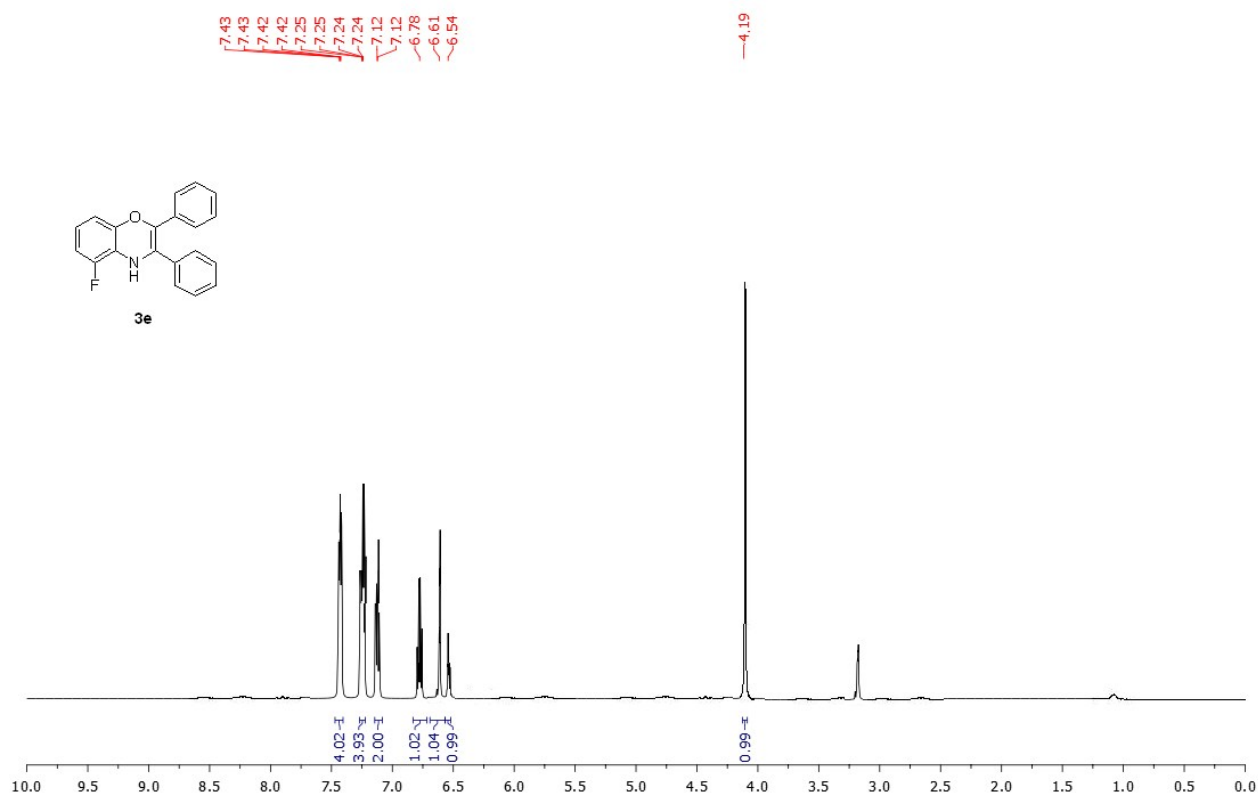
Sample Name : A-4
 Test Name : HRMS-1
 220218-A-4 11 (0.125) AM (Top,4, Ar,10000.0,0.00,0.00); Sm (Mn, 1x3.00); Cm (7:18)

XEVO G2-XS QTOF

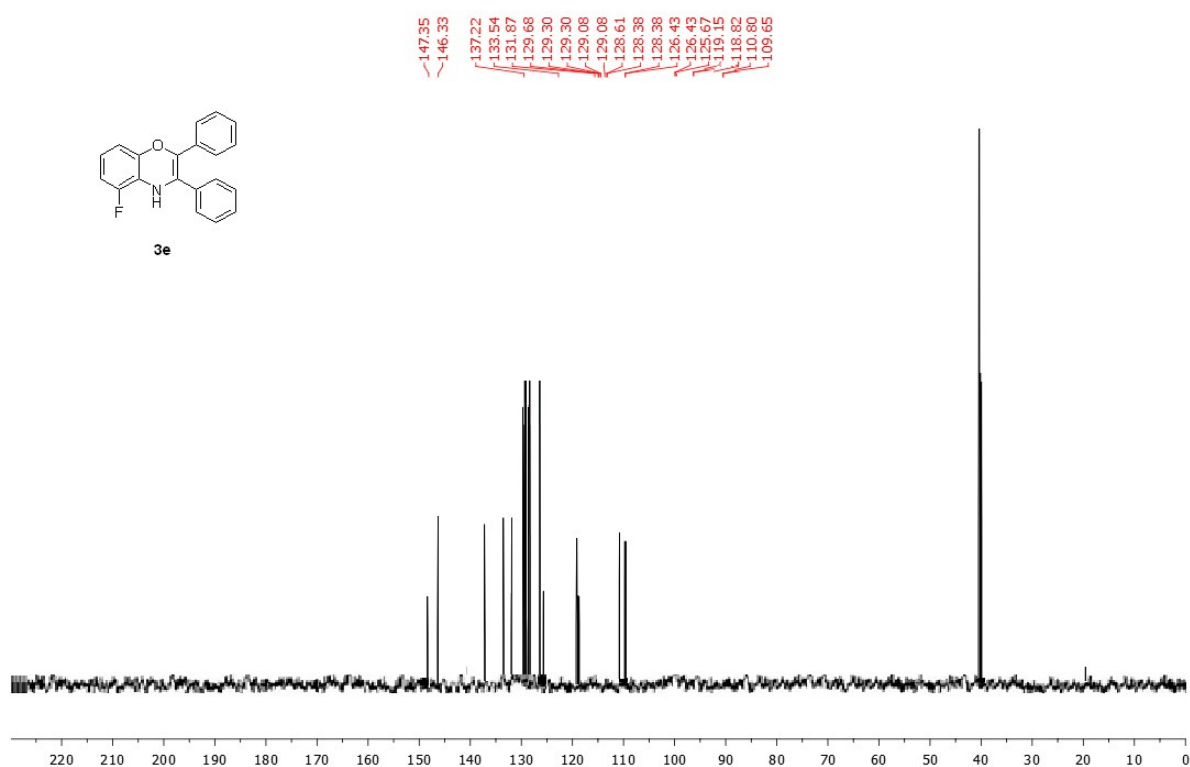
1: TOF MS ES+
 8.93e7



^1H NMR spectrum of 3e



^{13}C NMR spectrum of 3e

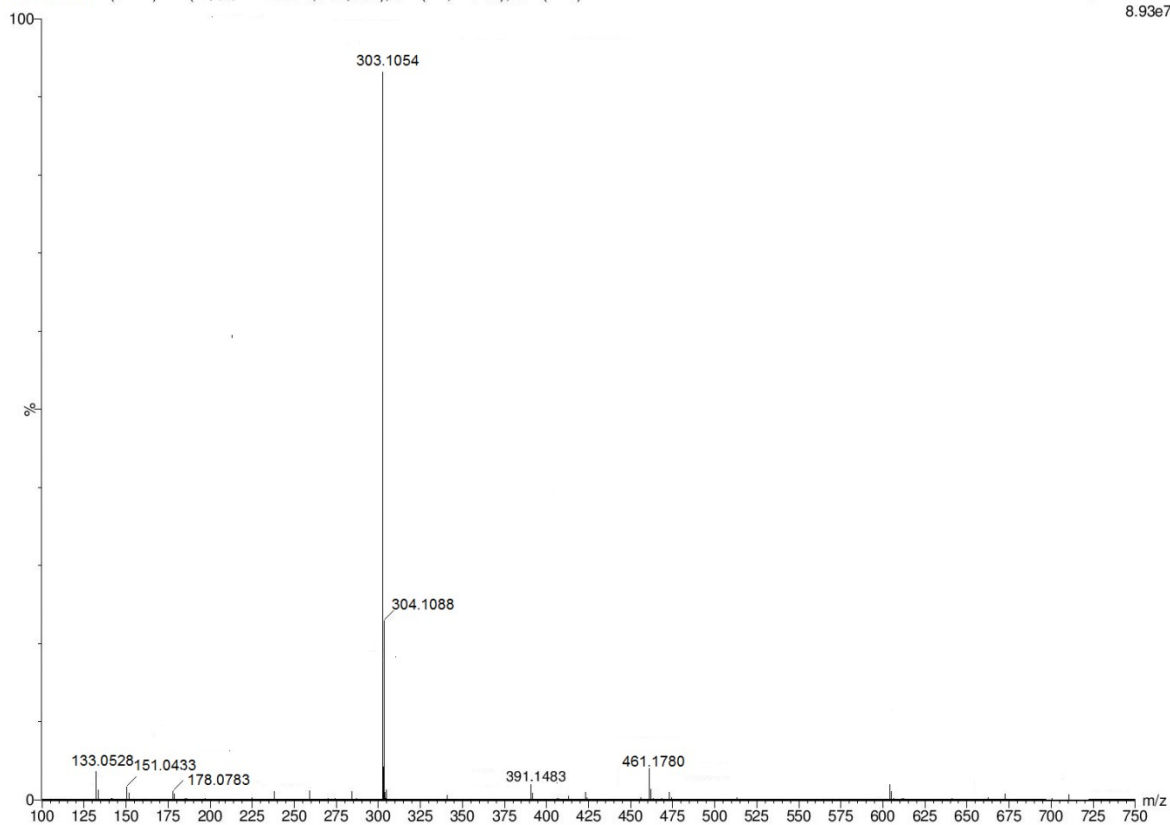


HRMS spectrum of 3e:

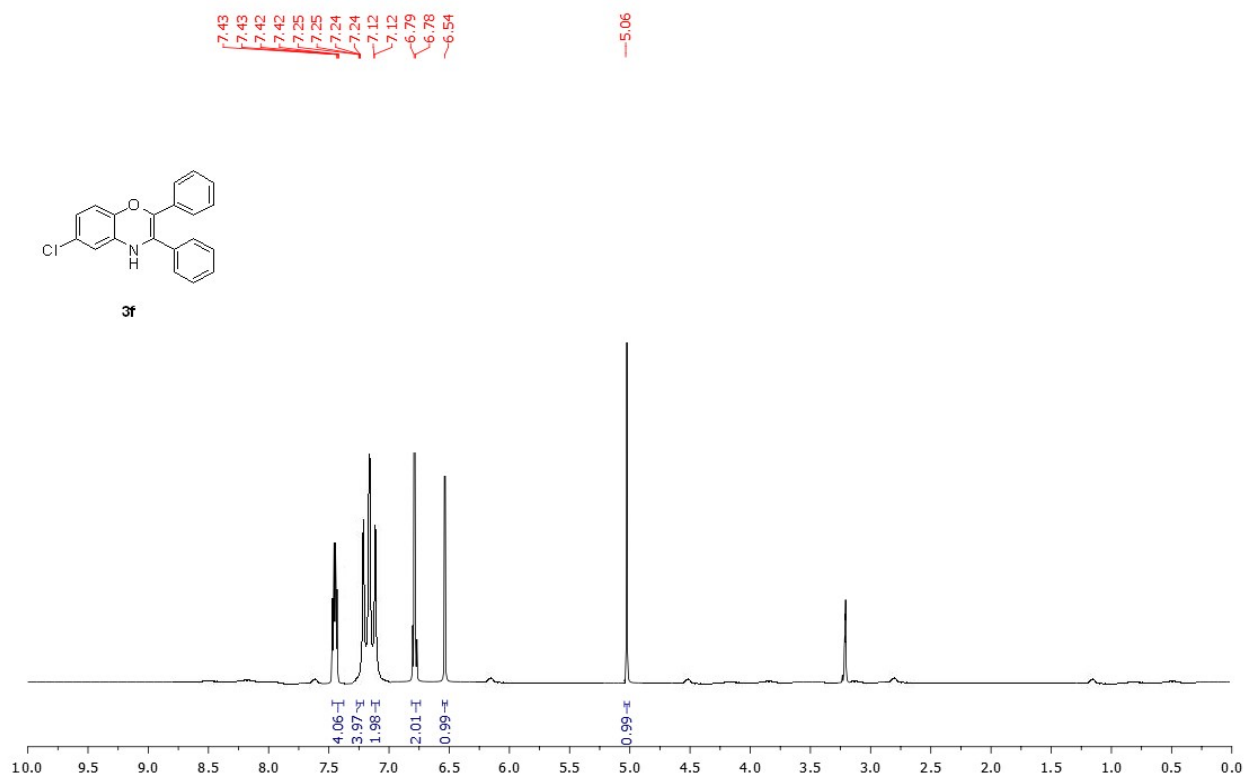
Sample Name : A-5
 Test Name : HRMS-1
 100218-A-5 11 (0.122) AM (Top.4, Ar.10000.0,0.00,0.00); Sm (Mn, 1x3.00); Cm (7:18)

XEVO G2-XS QTOF

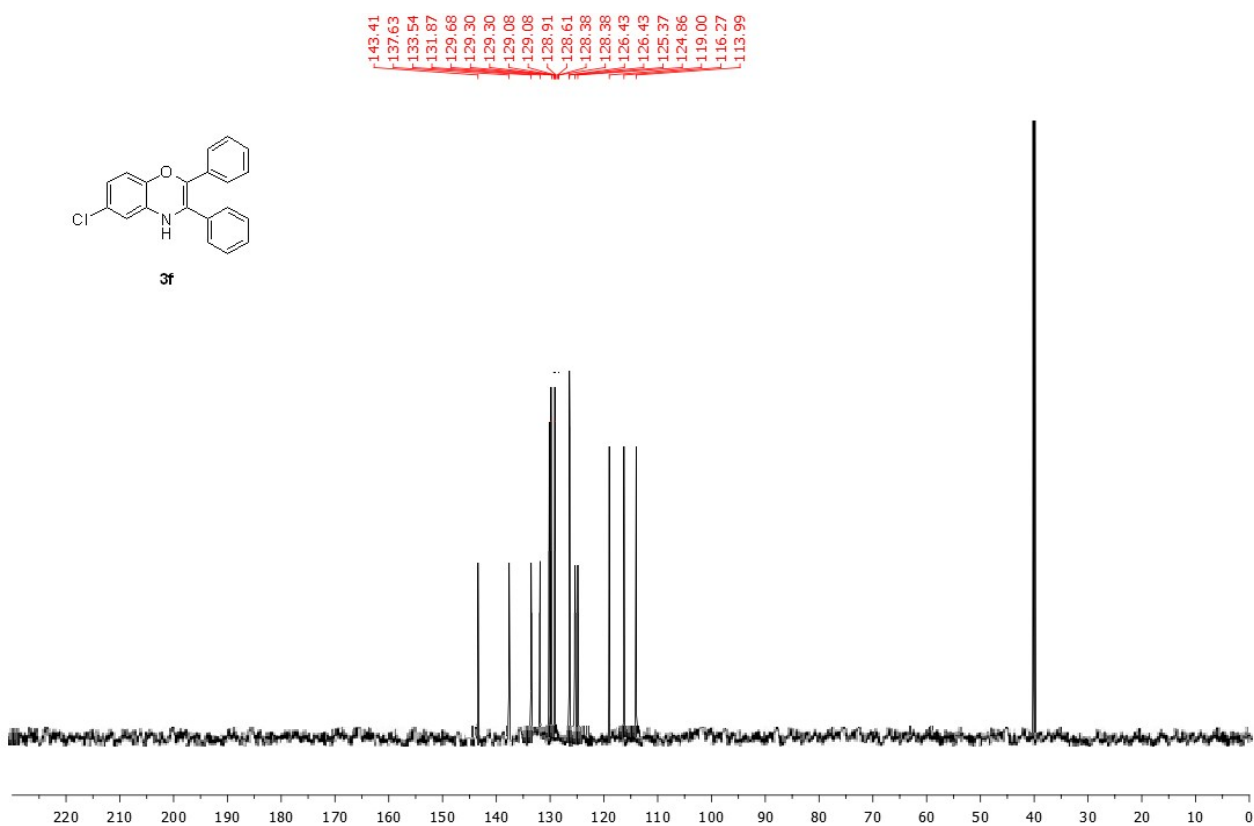
1: TOF MS ES+
 8.93e7



¹H NMR spectrum of 3f



¹³C NMR spectrum of 3f

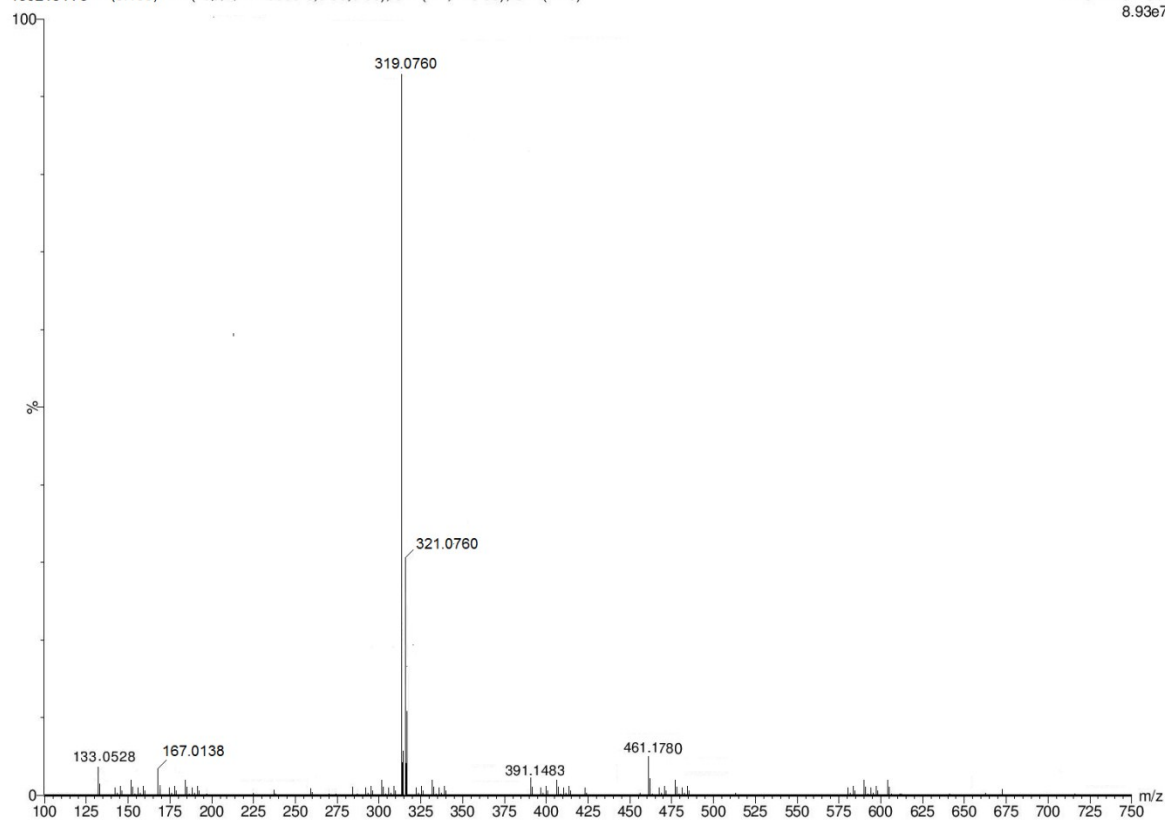


HRMS spectrum 3f:

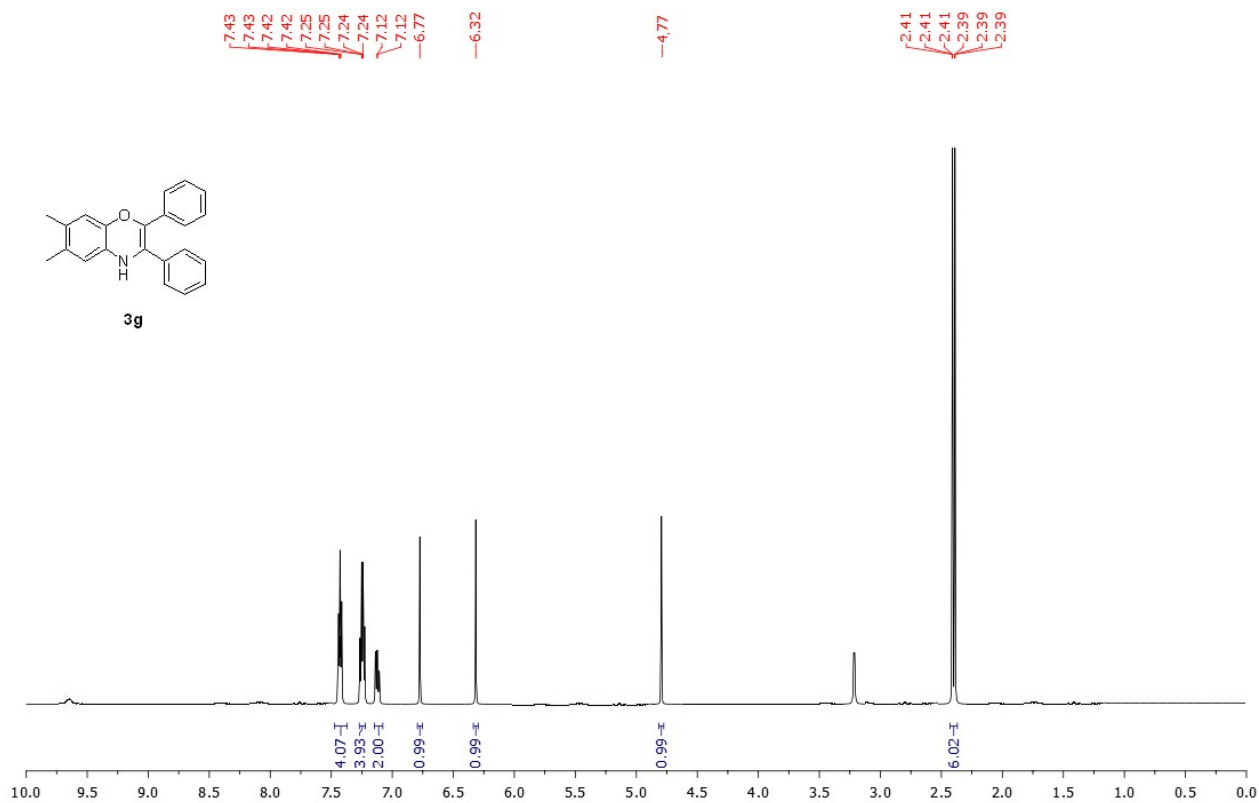
Sample Name : A-6
 Test Name : HRMS-1
 130218-A-6 11 (0.130) AM (Top,4, Ar:10000.0,0.00,0.00); Sm (Mn, 1x3.00); Cm (7:18)

XEVO G2-XS QTOF

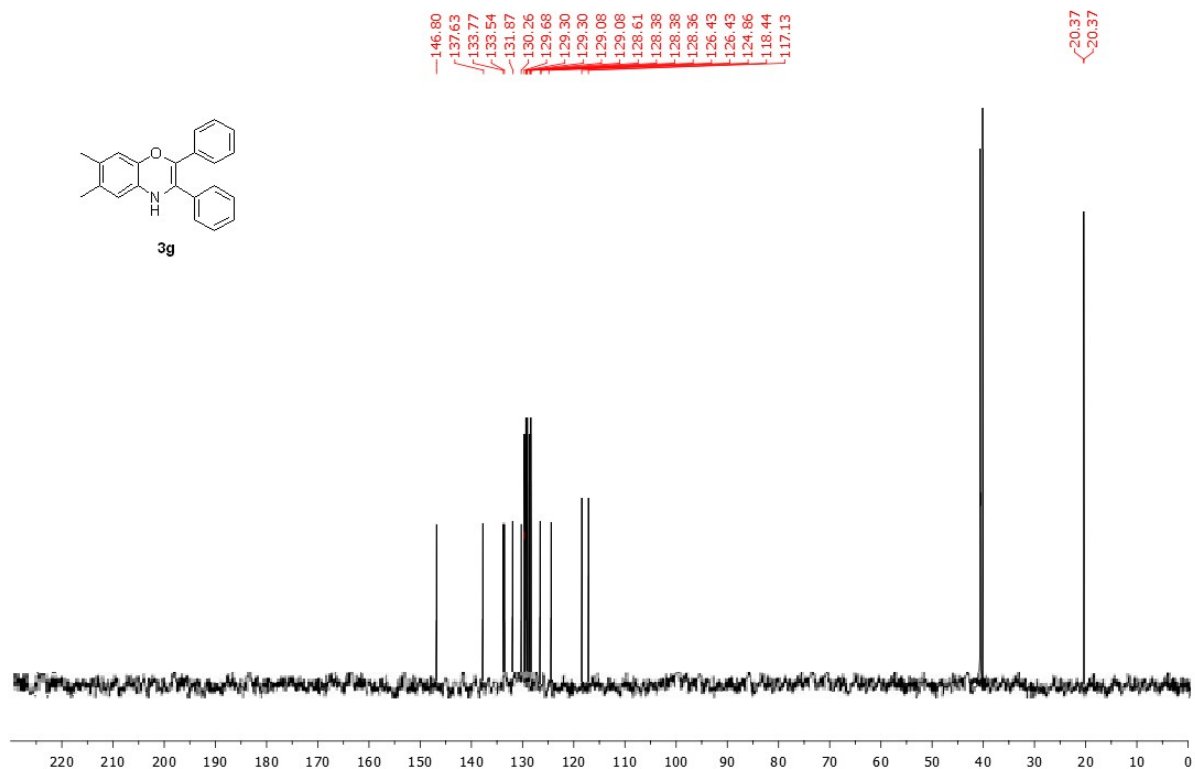
1: TOF MS ES+
 8.93e7



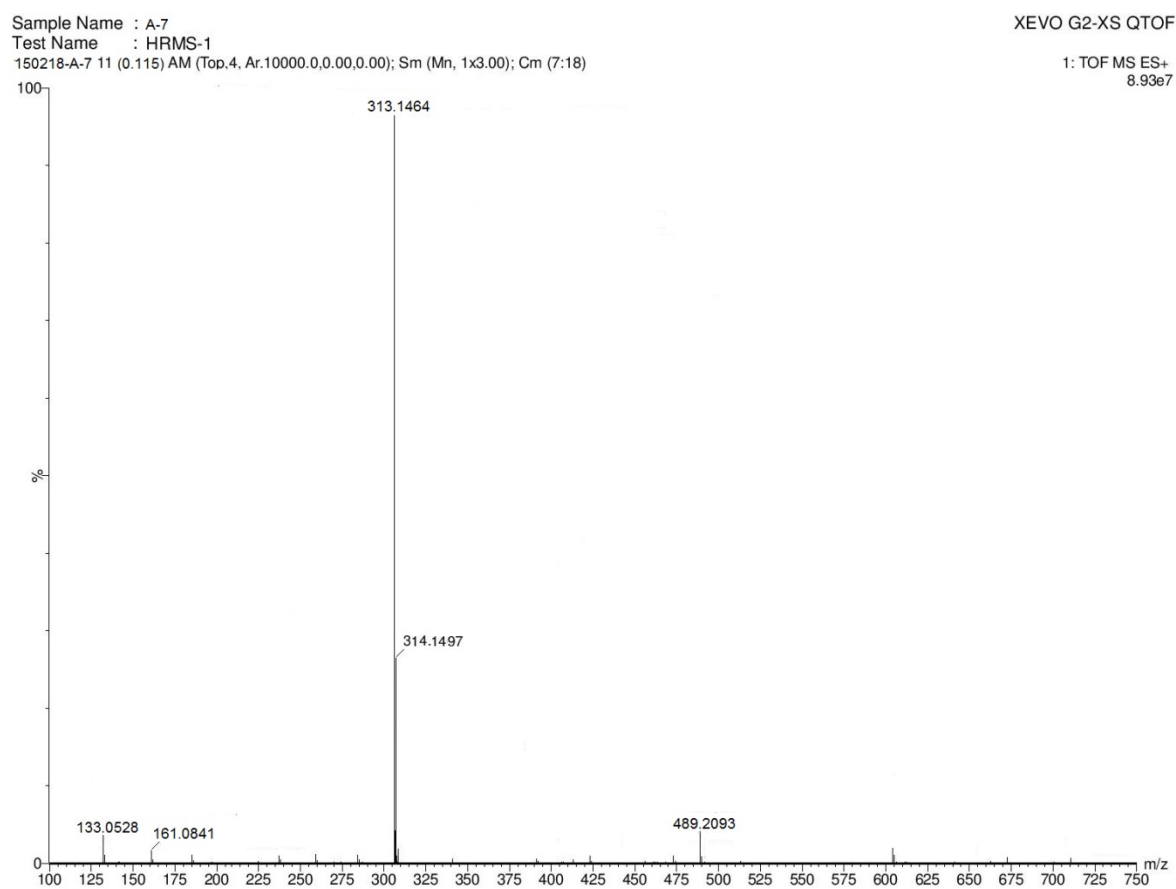
^1H NMR spectrum of 3g



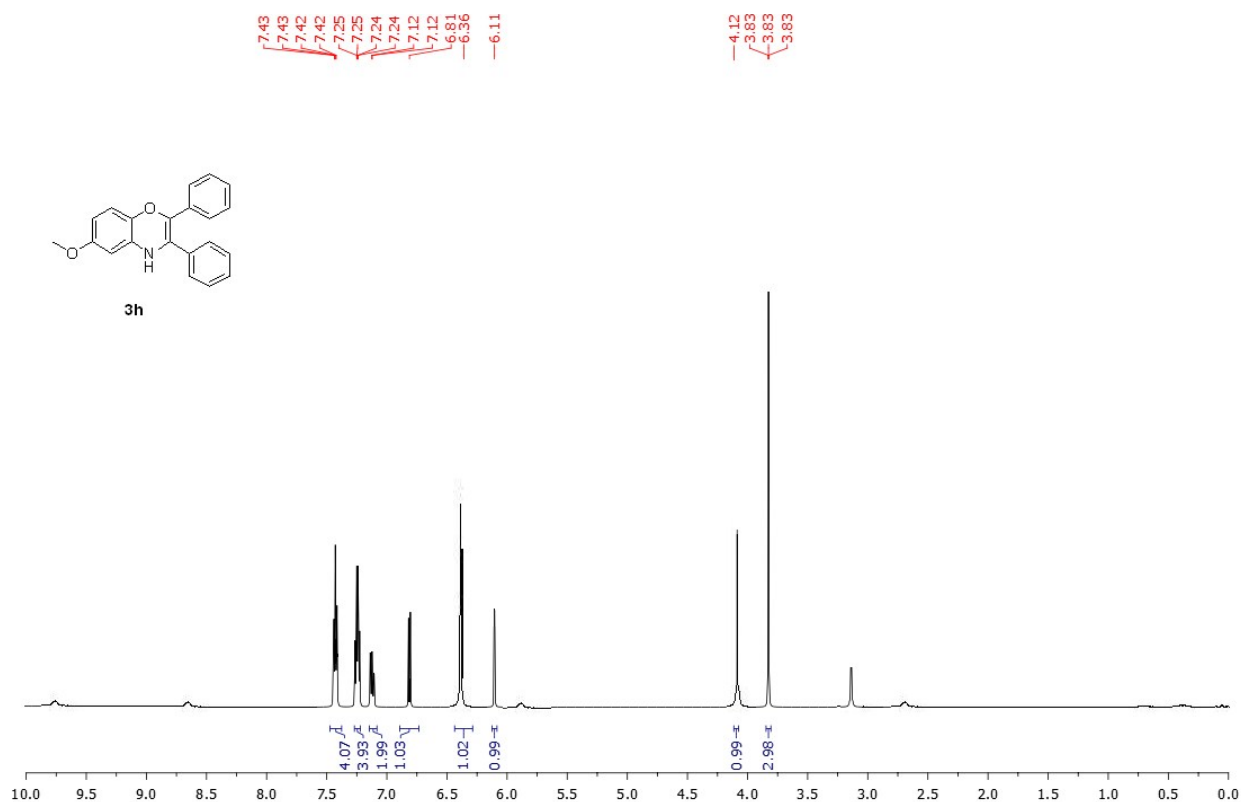
^{13}C NMR spectrum of 3g



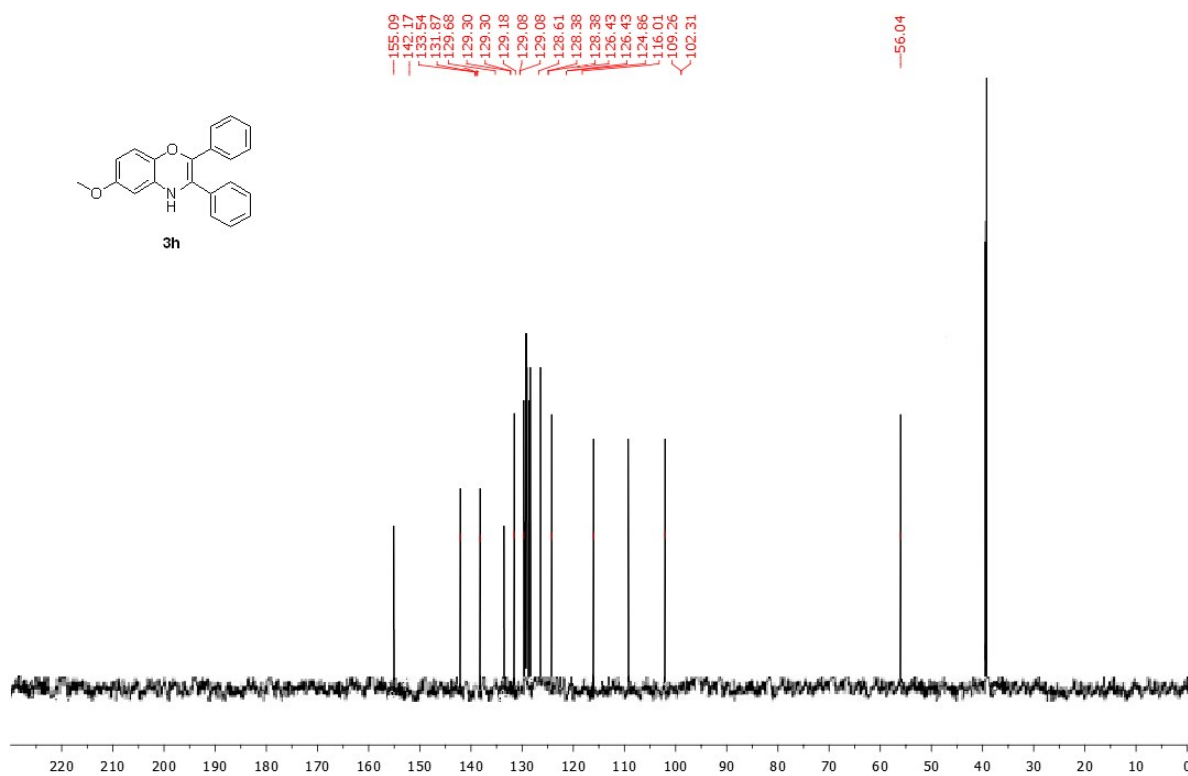
HRMS spectrum 3g:



¹H NMR spectrum of 3h



¹³C NMR spectrum of 3h

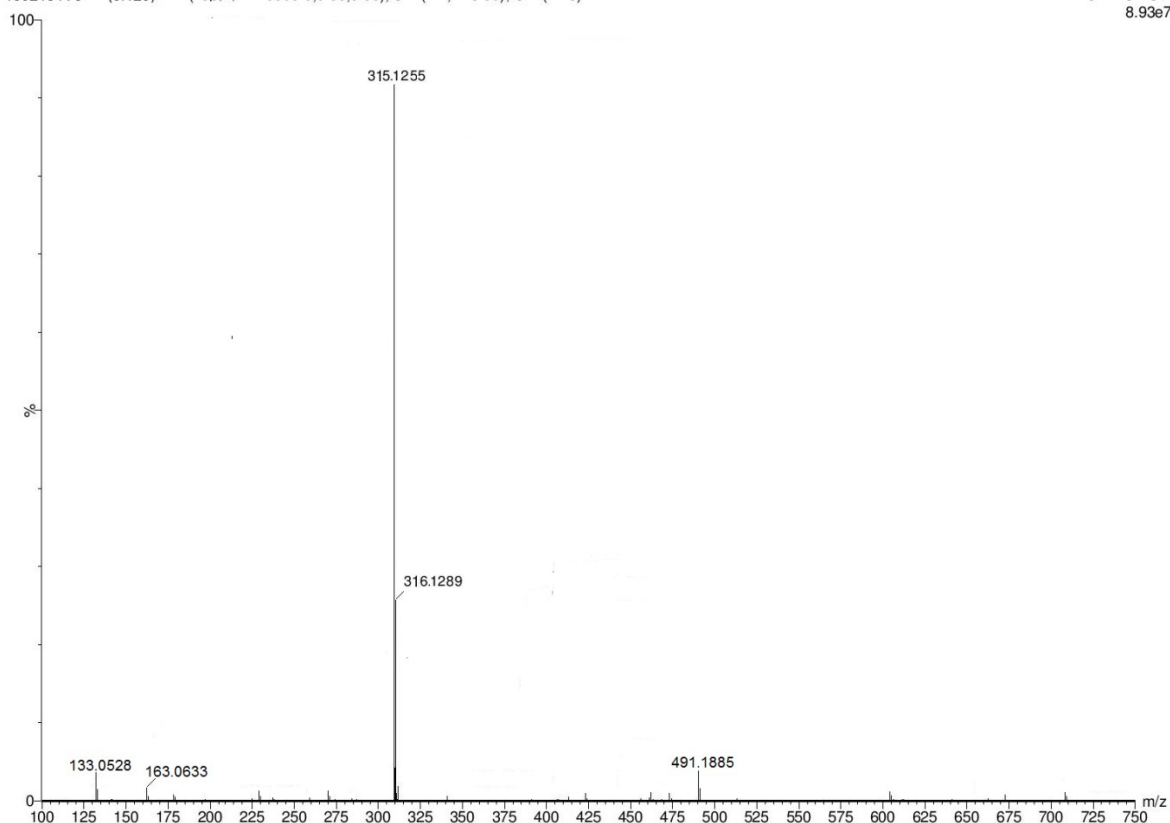


HRMS spectrum of 3h:

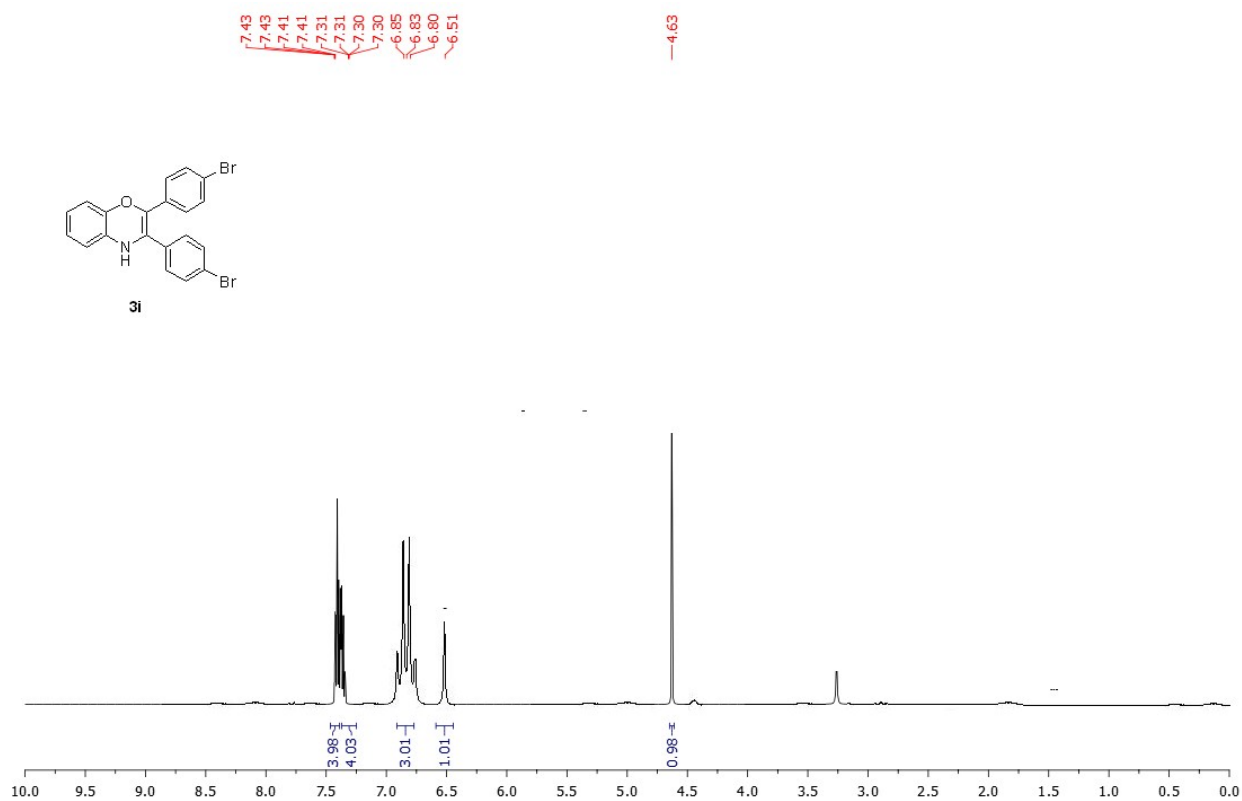
Sample Name : A-8
 Test Name : HRMS-1
 160218-A-8 11 (0.120) AM (Top.4, Ar.10000.0,0.00,0.00); Sm (Mn, 1x3.00); Cm (7:18)

XEVO G2-XS QTOF

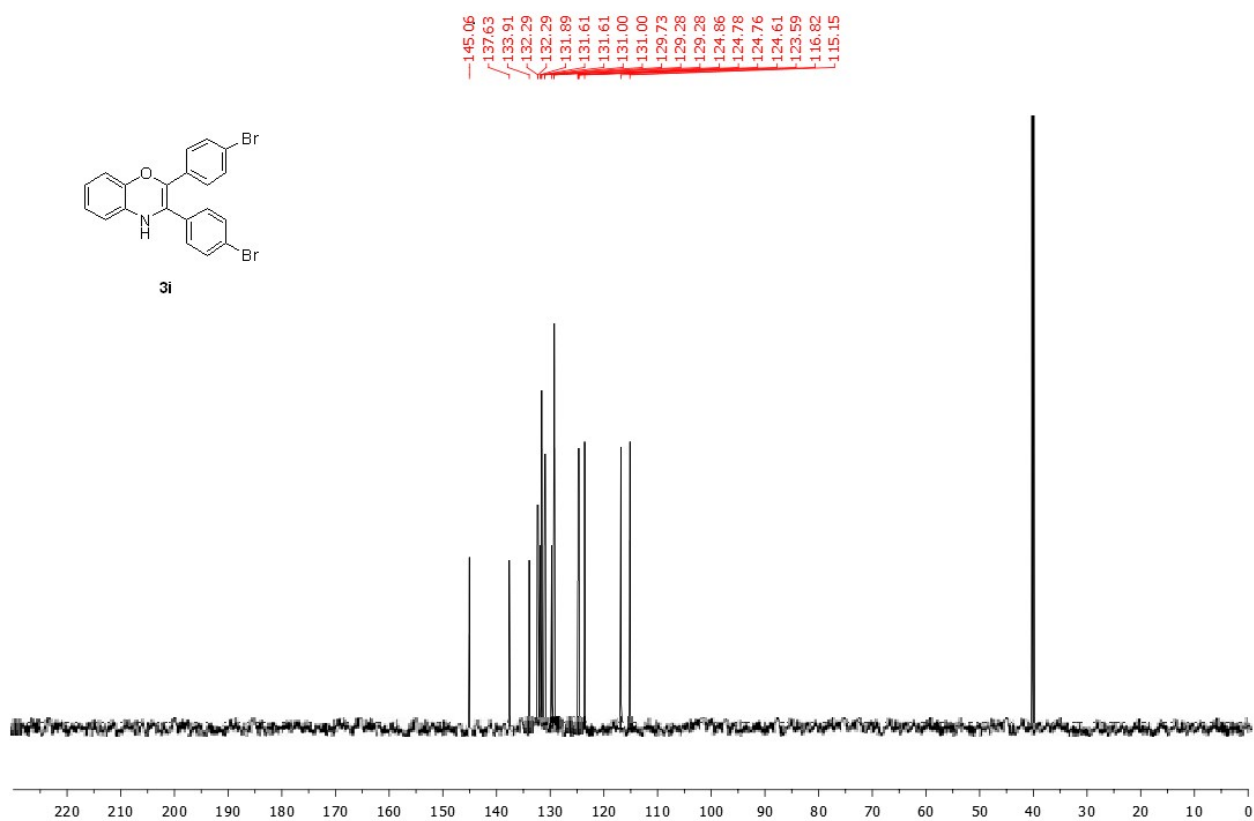
1: TOF MS ES+
 8.93e7



^1H NMR spectrum of 3i



^{13}C NMR spectrum of 3i

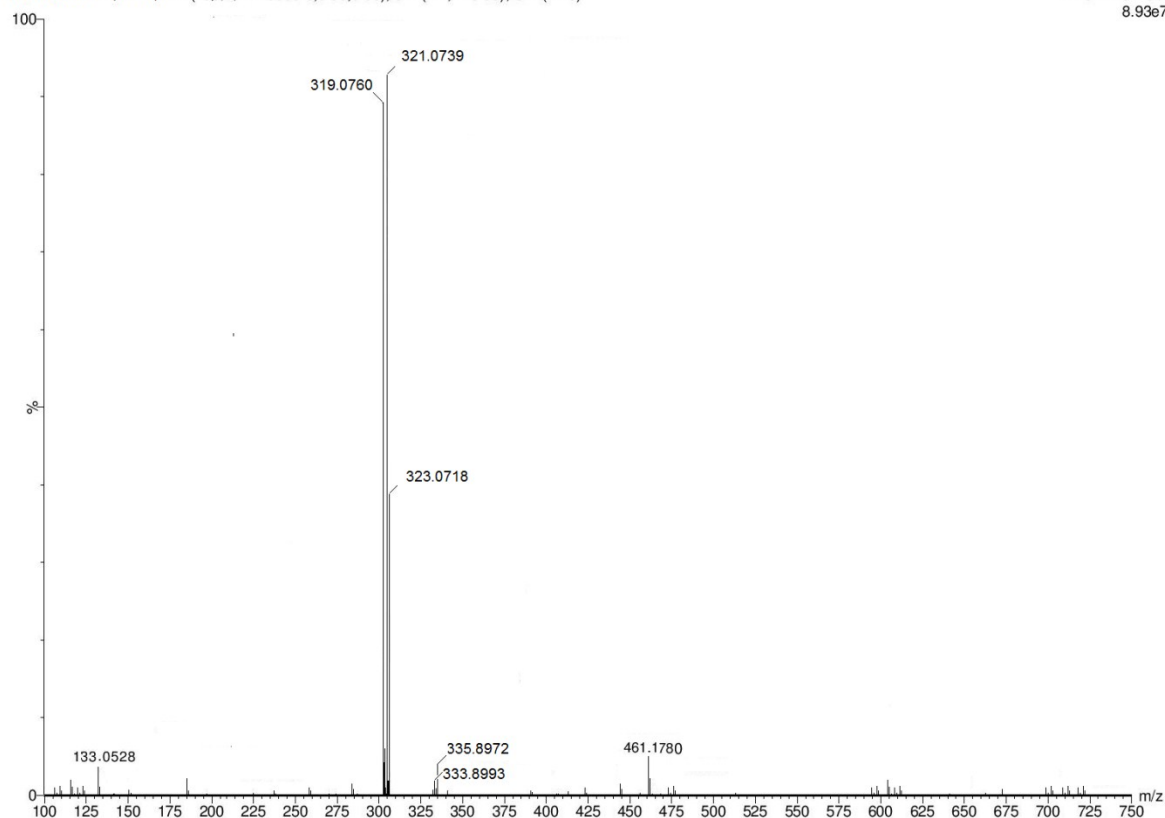


HRMS spectrum of **3i**:

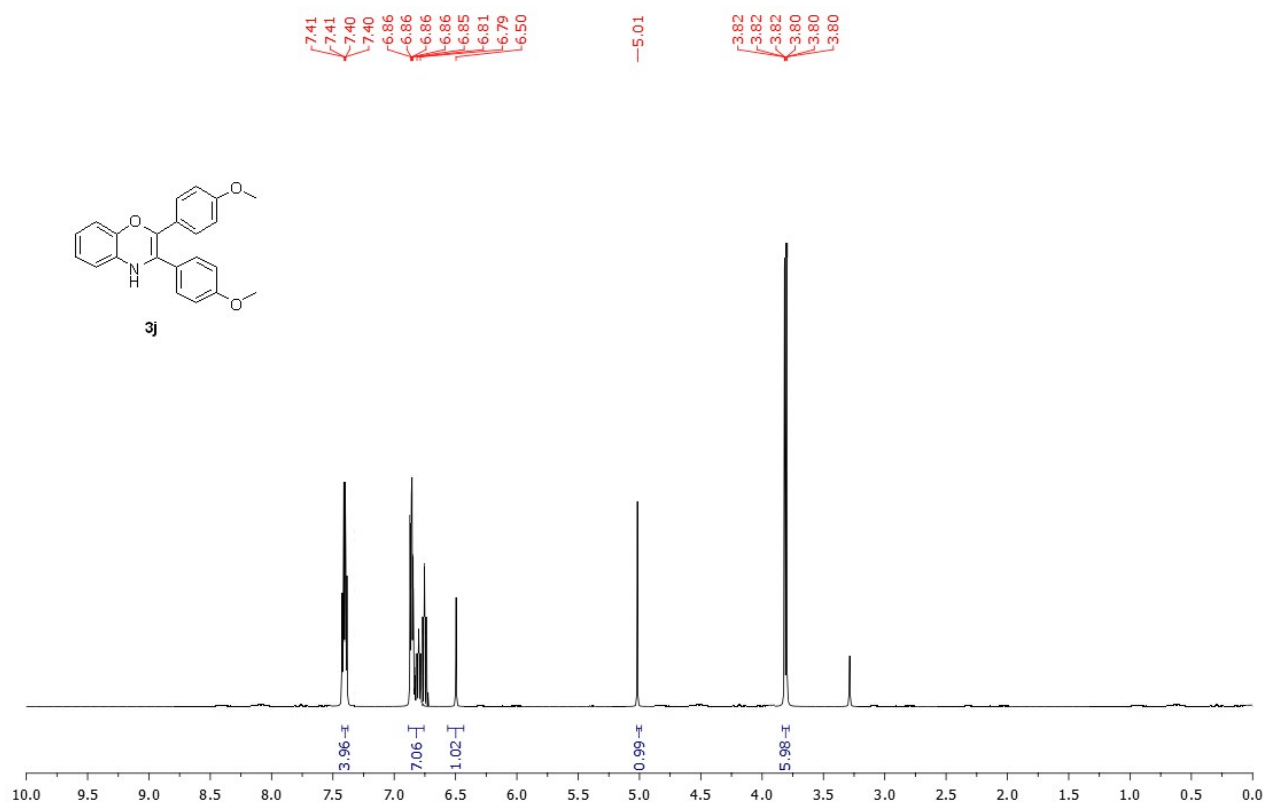
Sample Name : A-9
 Test Name : HRMS-1
 170218-A-9 11 (0.110) AM (Top,4, Ar:10000.0,0.00,0.00); Sm (Mn, 1x3.00); Cm (7:18)

XEVO G2-XS QTOF

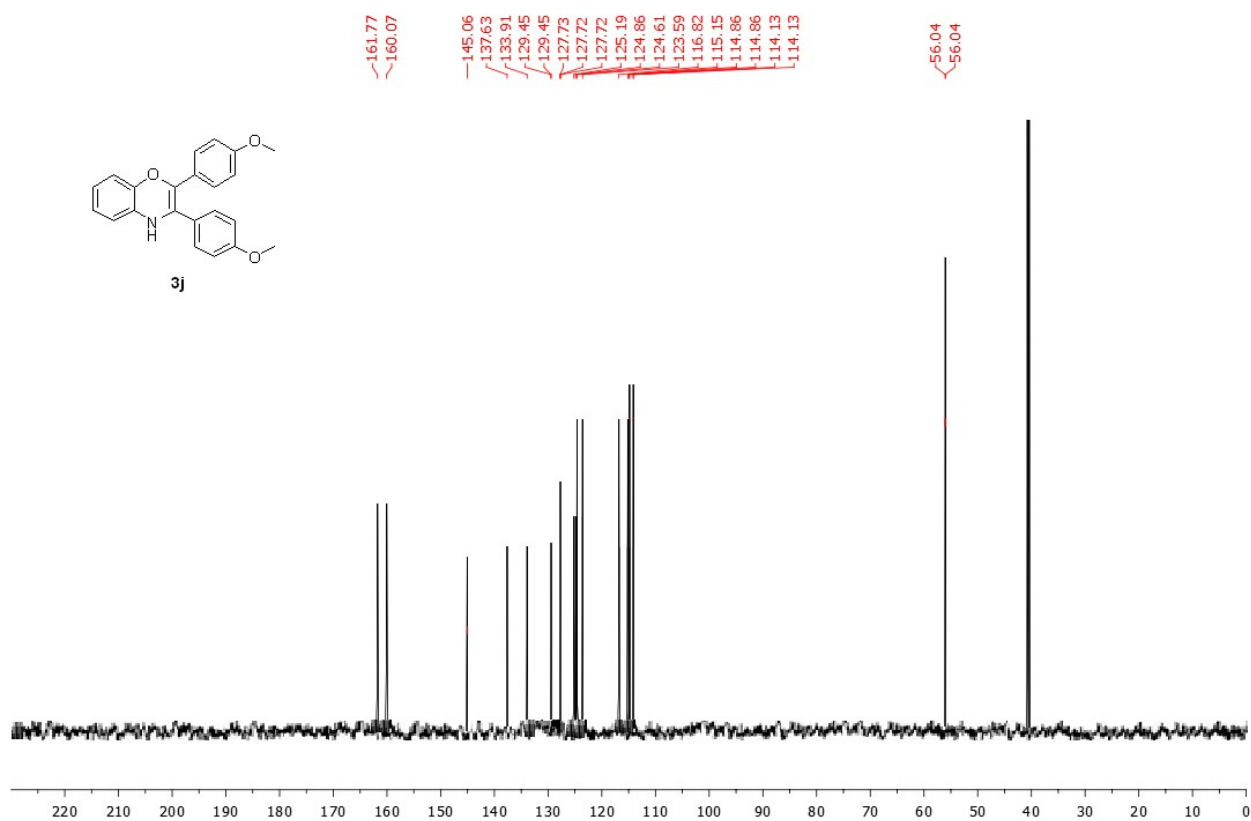
1: TOF MS ES+
 8.93e7



^1H NMR spectrum of 3j



^{13}C NMR spectrum of 3j

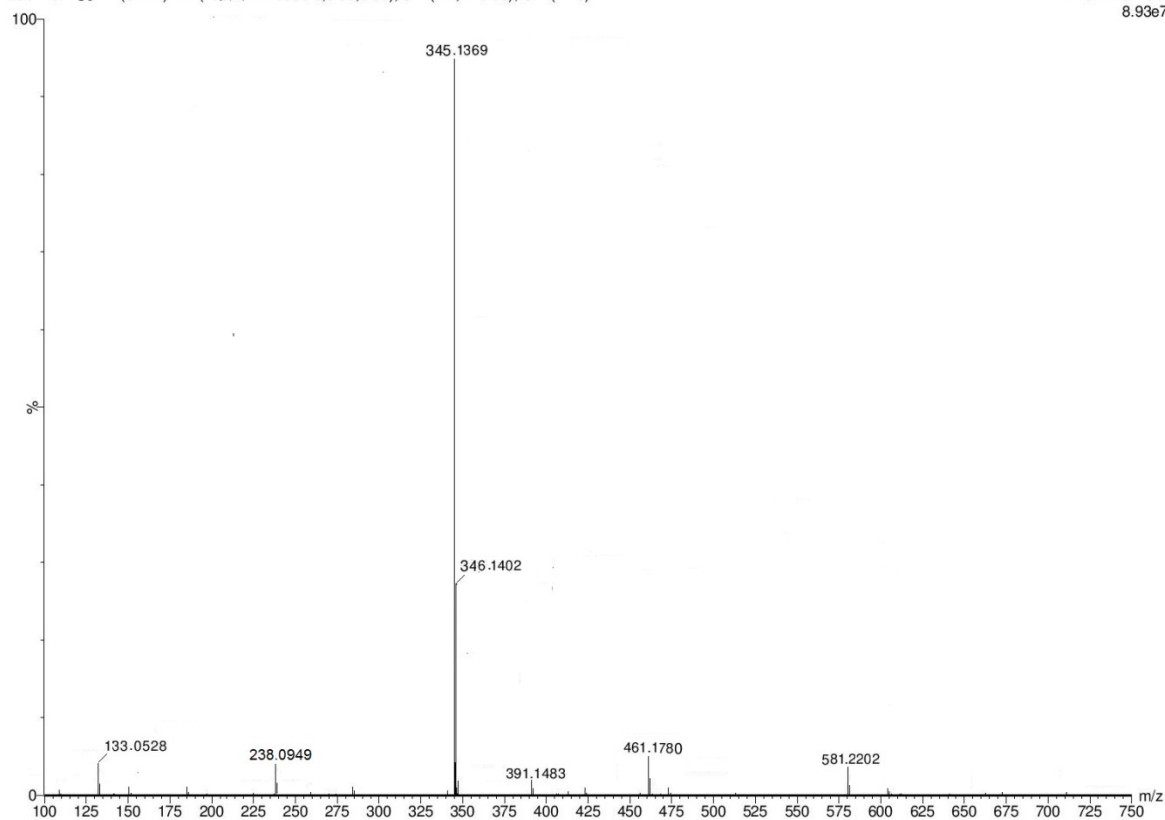


HRMS spectrum of 3j:

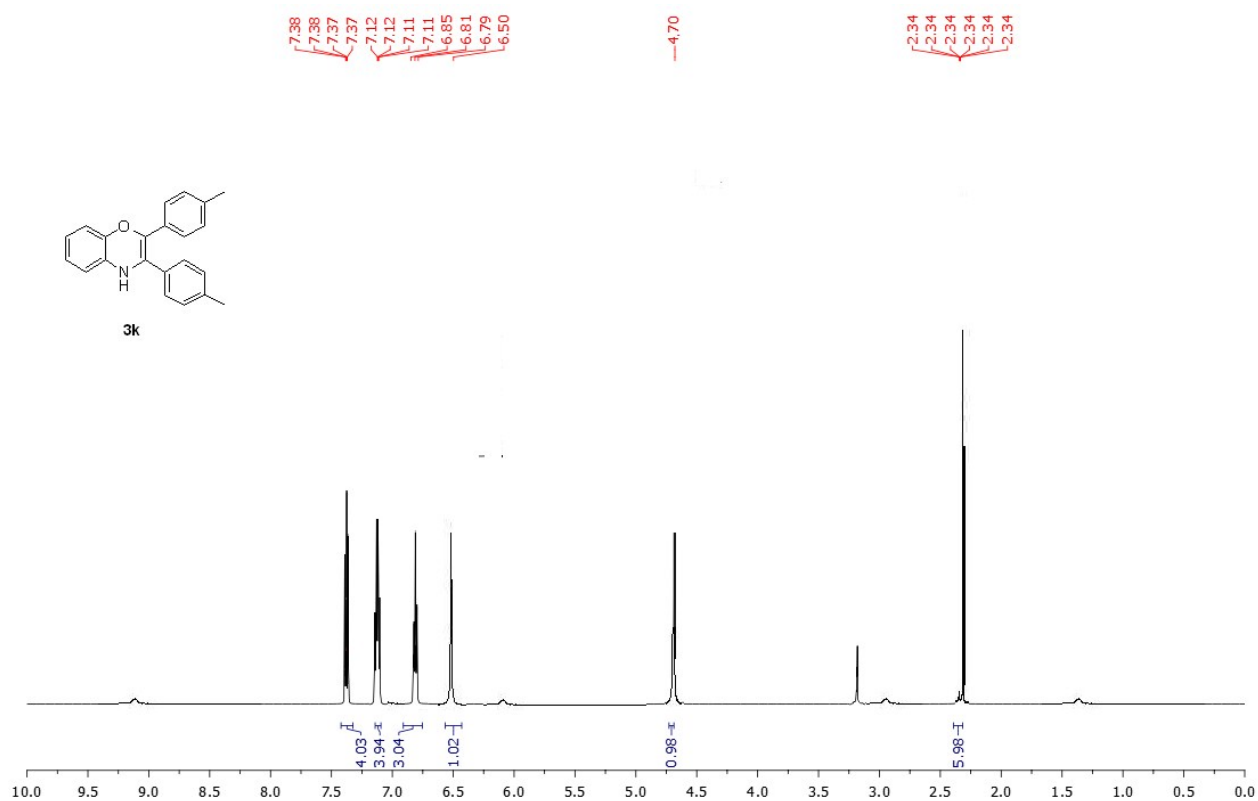
Sample Name : A-10
 Test Name : HRMS-1
 200218-A-10 11 (0.122) AM (Top, 4, Ar.10000.0,0.00,0.00); Sm (Mn, 1x3.00); Cm (7:18)

XEVO G2-XS QTOF

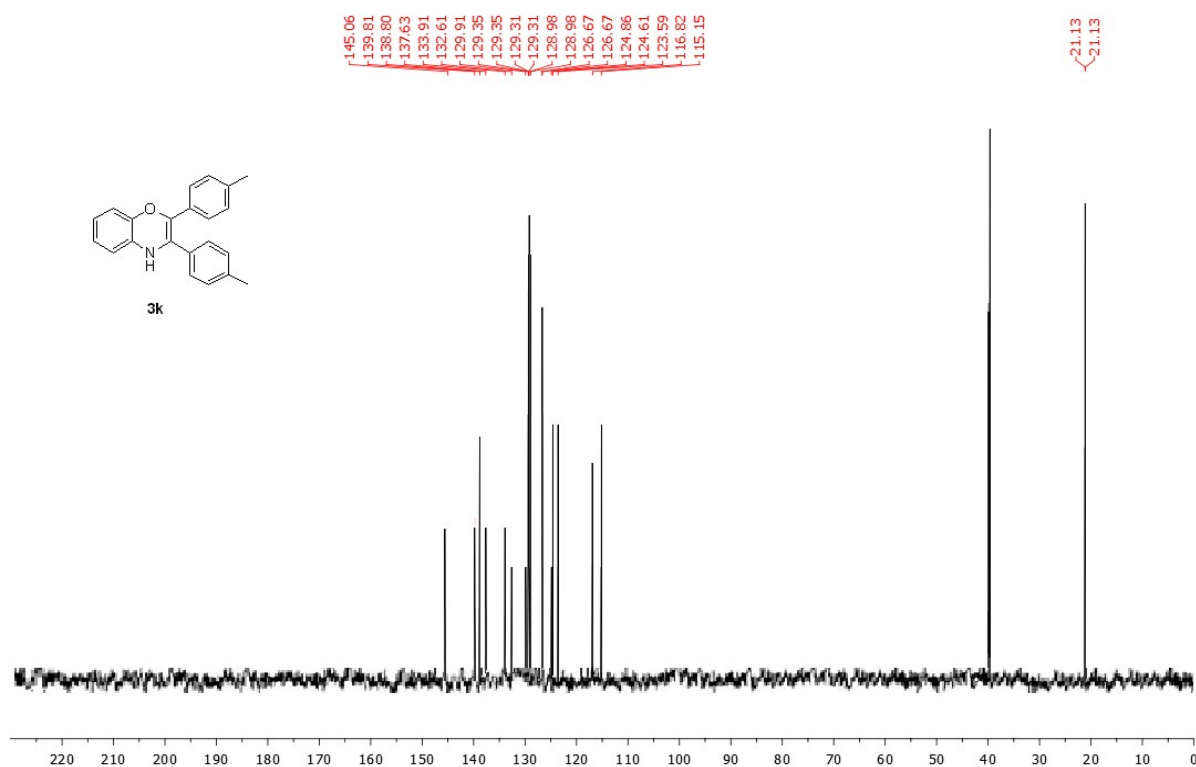
1: TOF MS ES+
 8.93e7



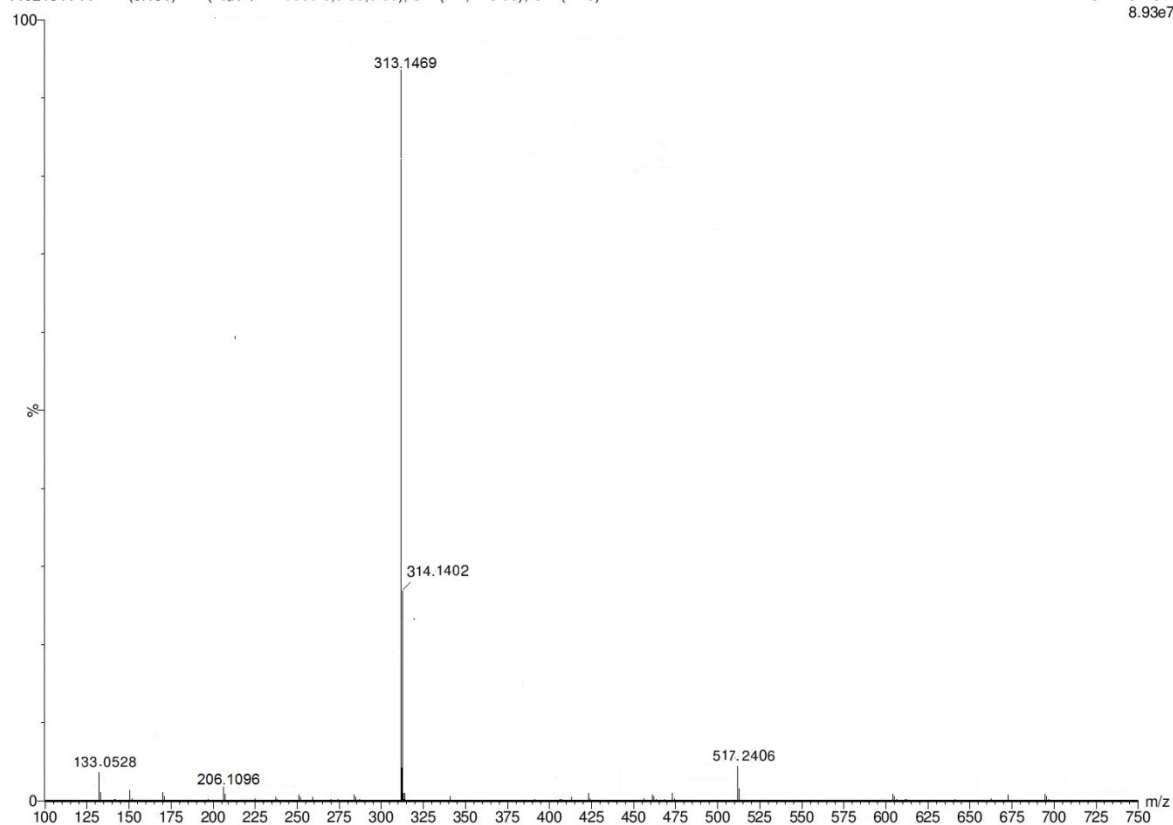
^1H NMR spectrum of 3k



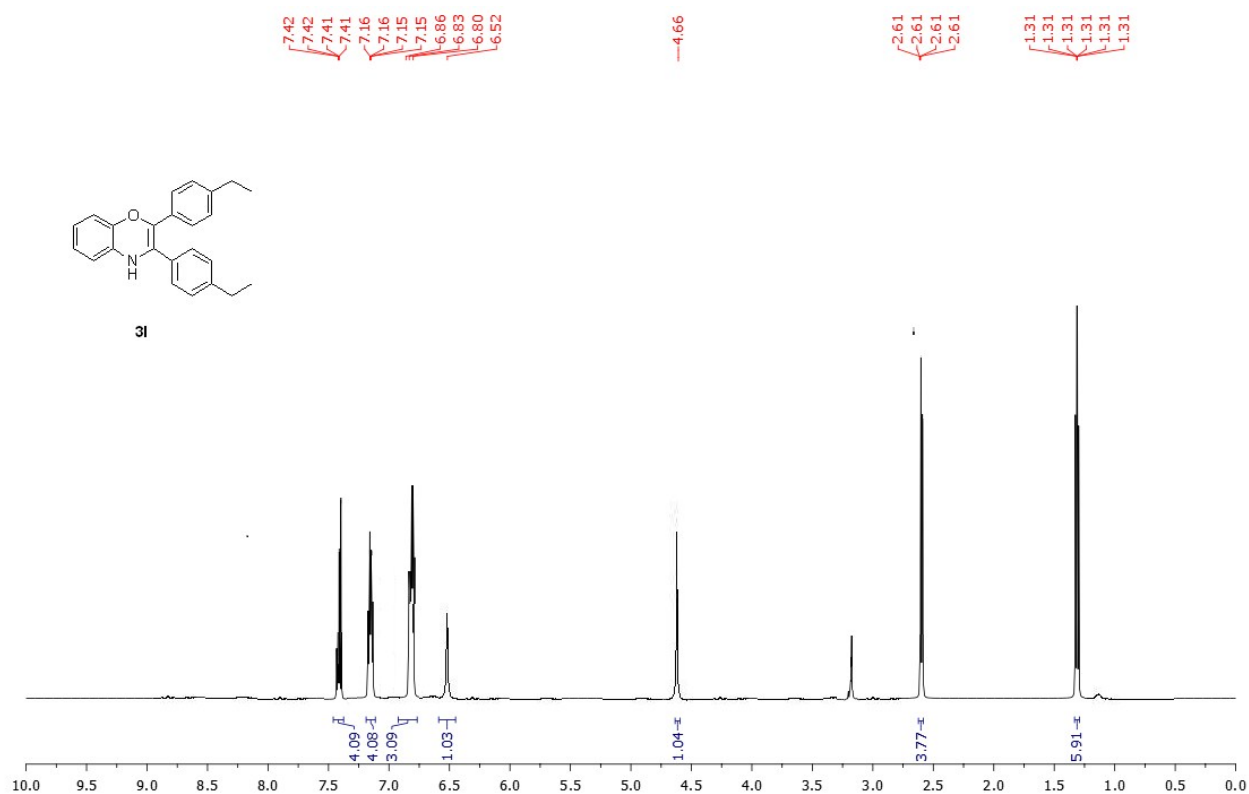
^{13}C NMR spectrum of 3k



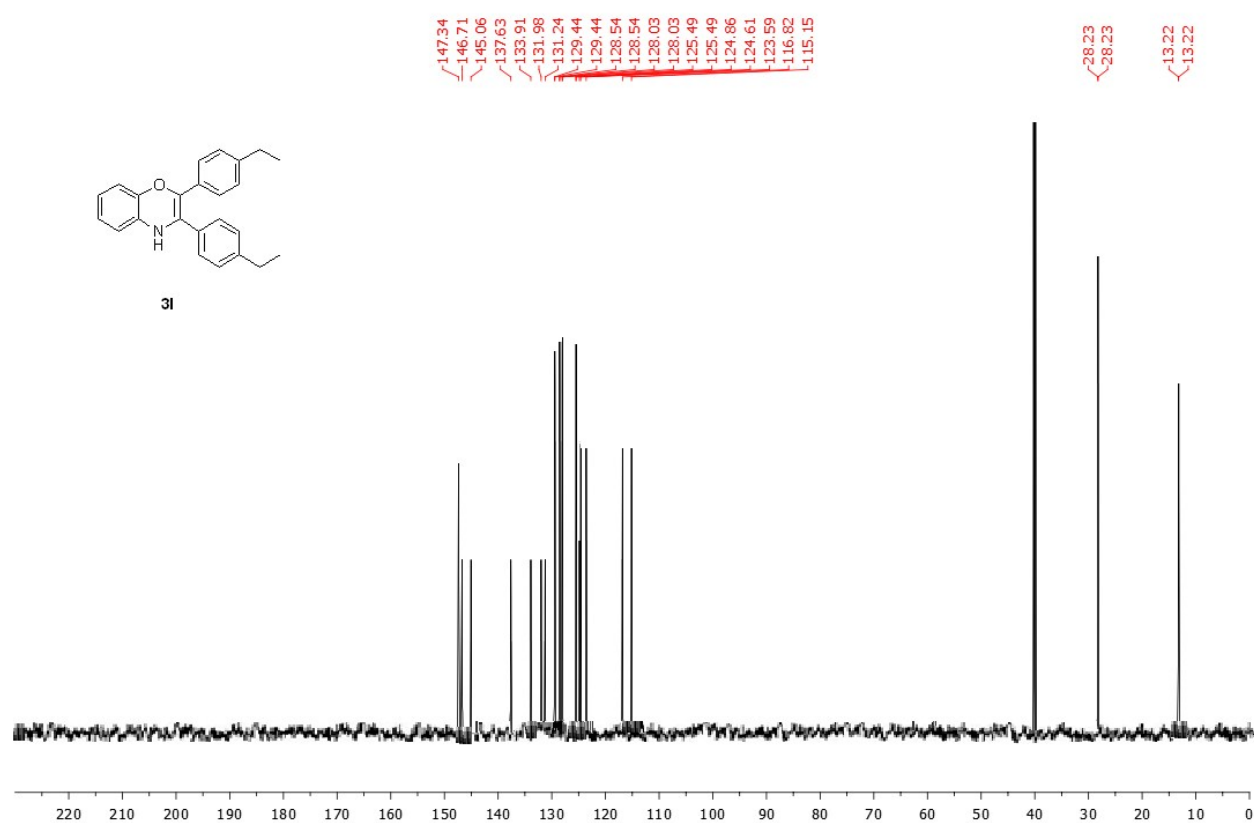
HRMS spectrum of 3k:



^1H NMR spectrum of 31



^{13}C NMR spectrum of 31

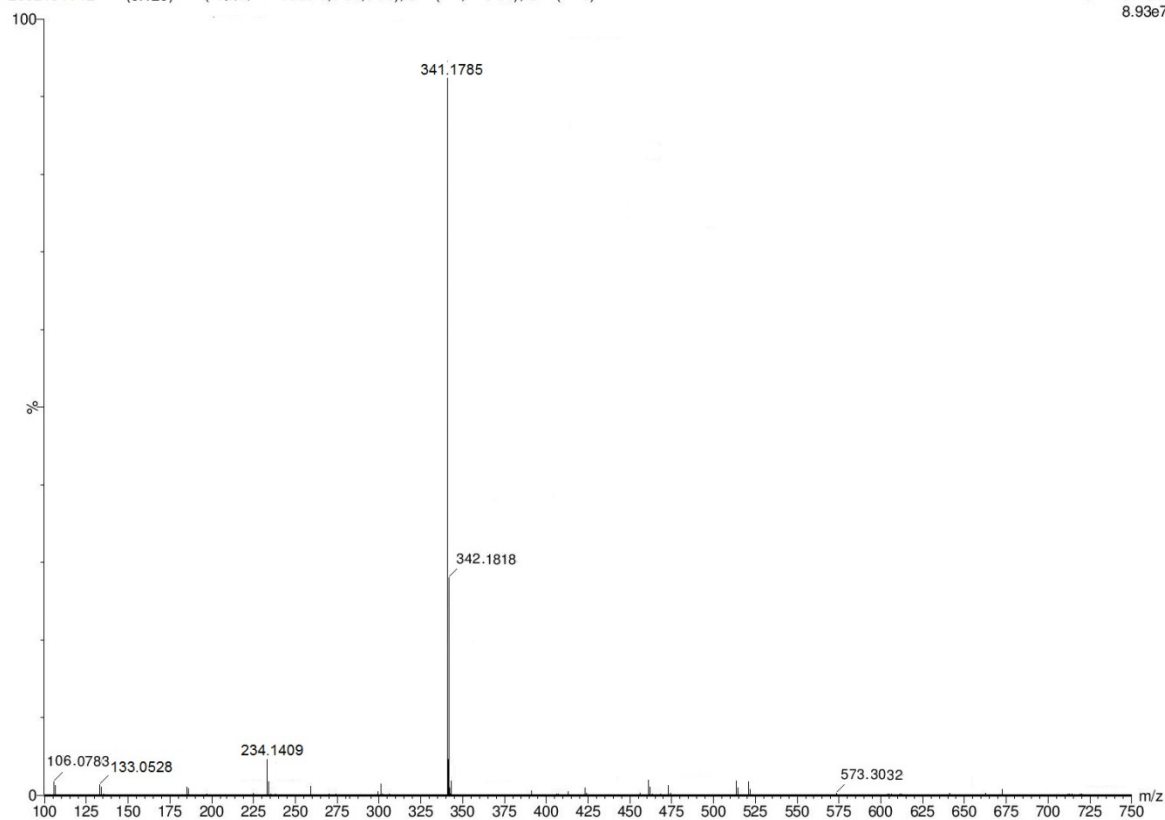


HRMS spectrum of 3l:

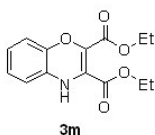
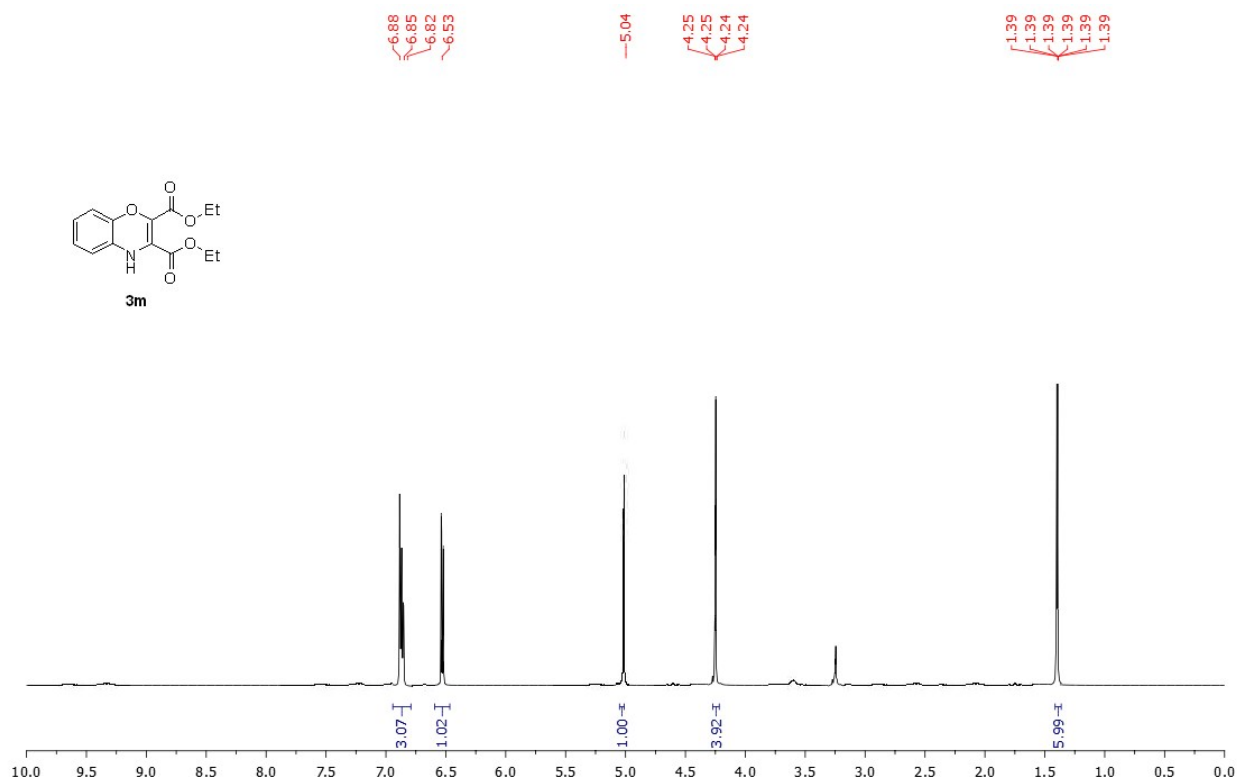
Sample Name : A-12
 Test Name : HRMS-1
 280218-A-12 11 (0.120) AM (Top.4, Ar.10000.0,0.00,0.00); Sm (Mn, 1x3.00); Cm (7:18)

XEVO G2-XS QTOF

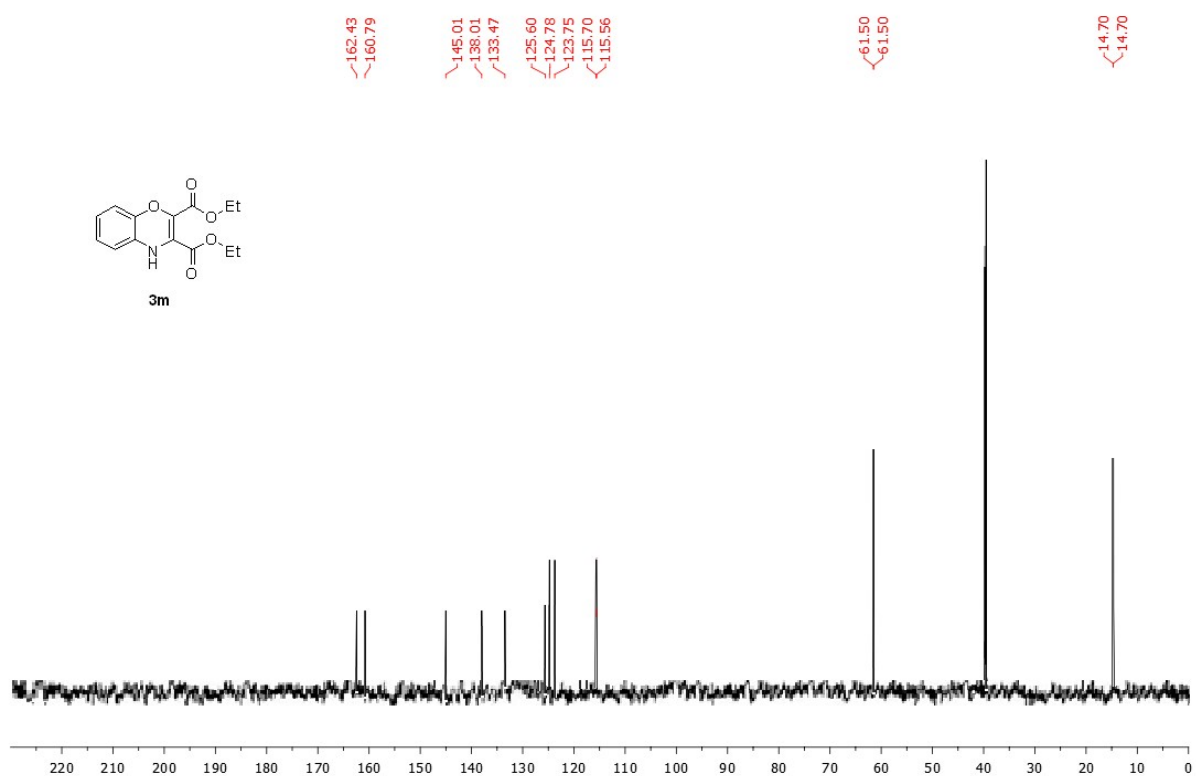
1: TOF MS ES+
 8.93e7



^1H NMR spectrum of 3m



^{13}C NMR spectrum of 3m

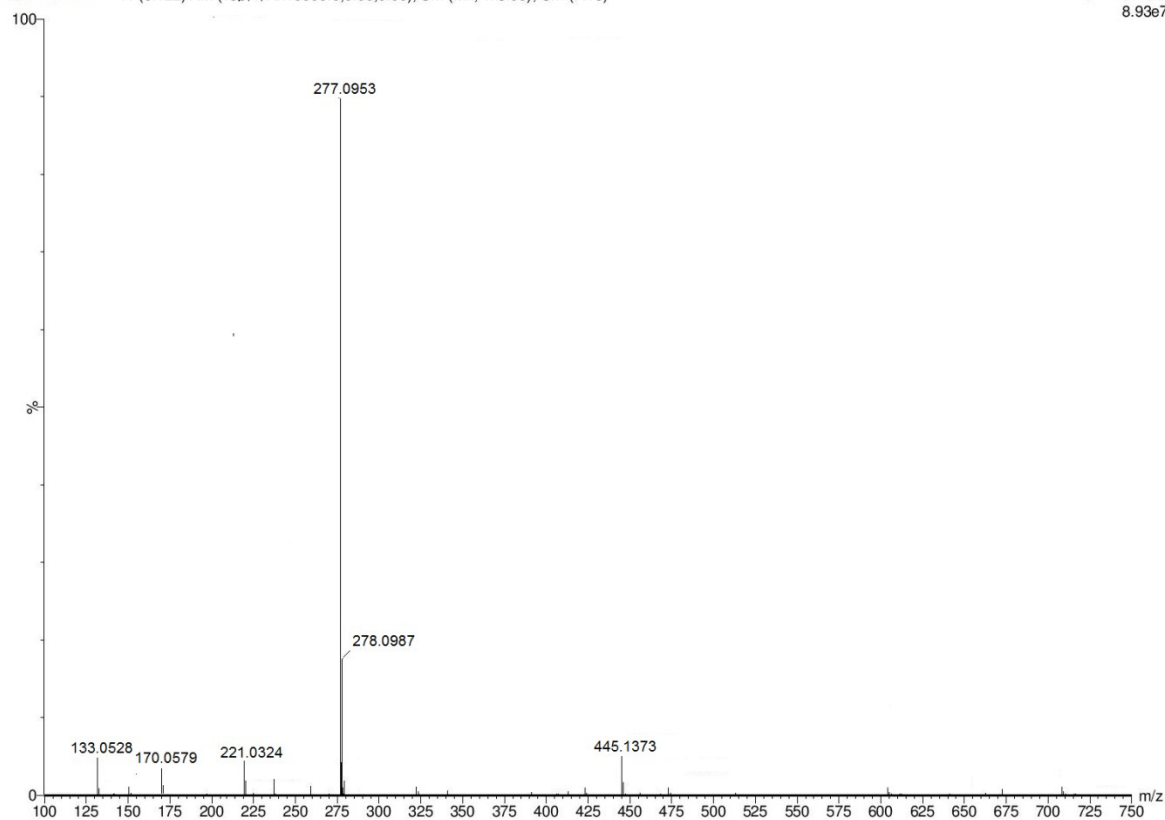


HRMS spectrum of 3m:

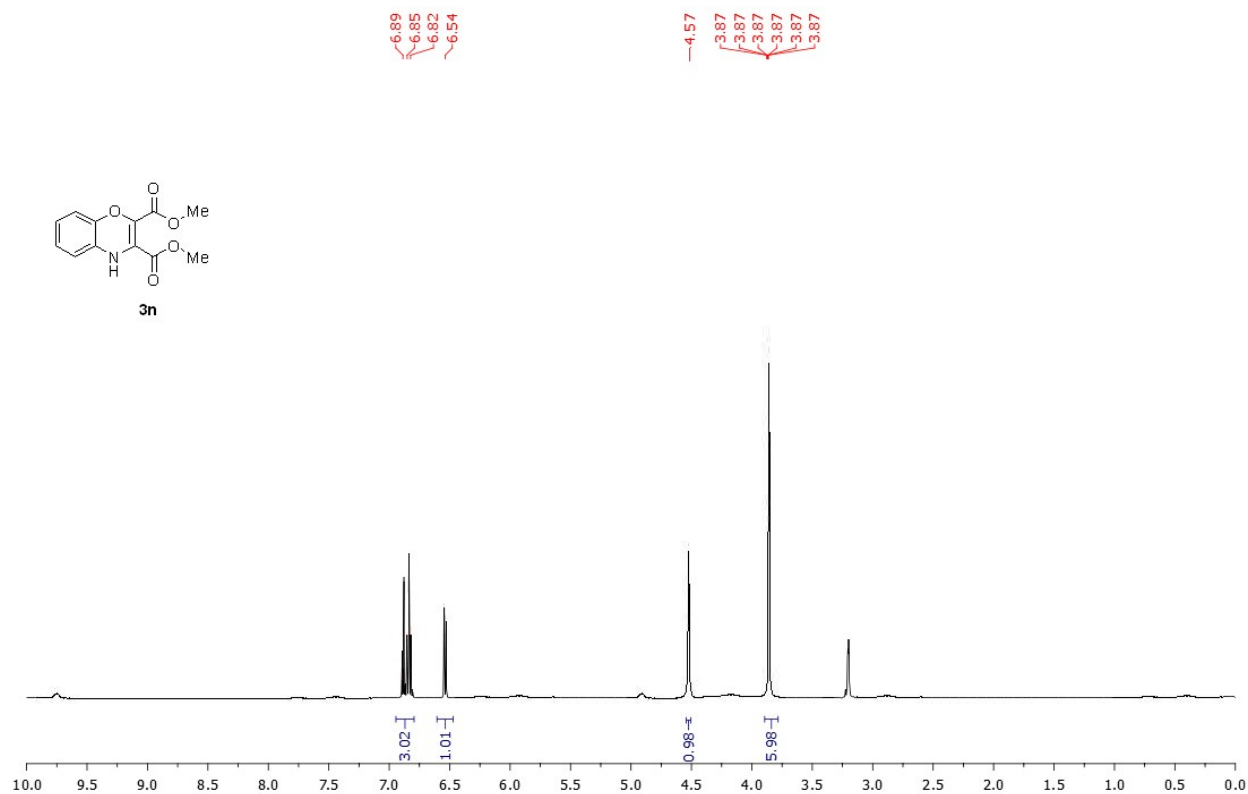
Sample Name : A-13
 Test Name : HRMS-1
 270218-A-13 11 (0.122) AM (Top.4, Ar.10000.0,0.00,0.00); Sm (Mn, 1x3.00); Cm (7:18)

XEVO G2-XS QTOF

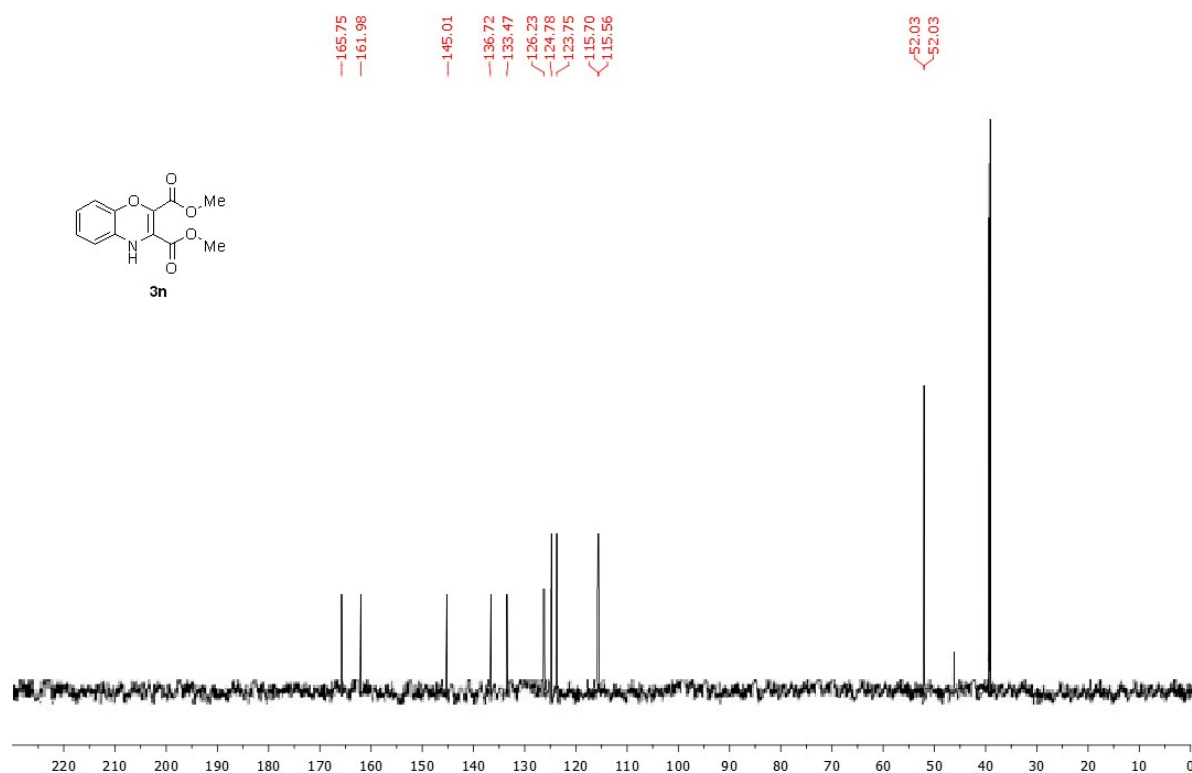
1: TOF MS ES+
 8.93e7



^1H NMR spectrum of 3n



^{13}C NMR spectrum of 3n

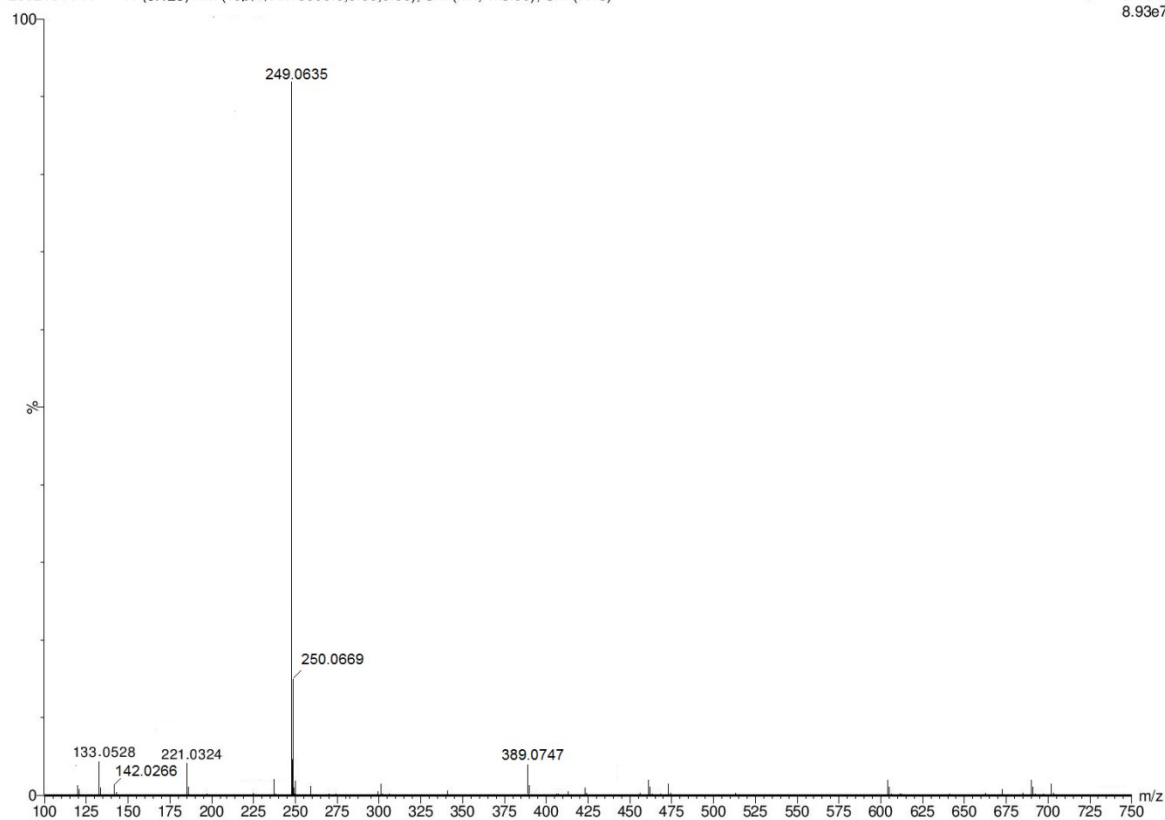


HRMS spectrum of 3n:

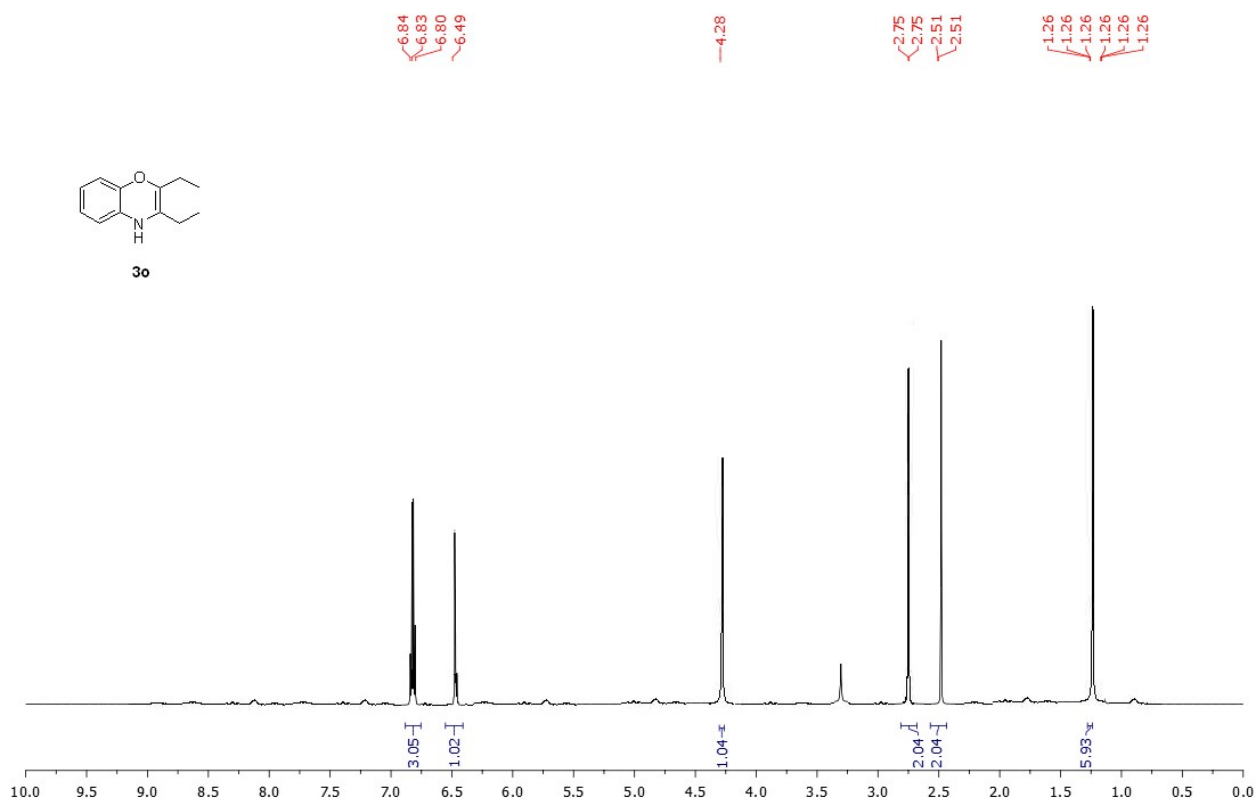
Sample Name : A-14
 Test Name : HRMS-1
 250218-A-14 11 (0.125) AM (Top.4, Ar.10000.0,0.00,0.00); Sm (Mn, 1x3.00); Cm (7:18)

XEVO G2-XS QTOF

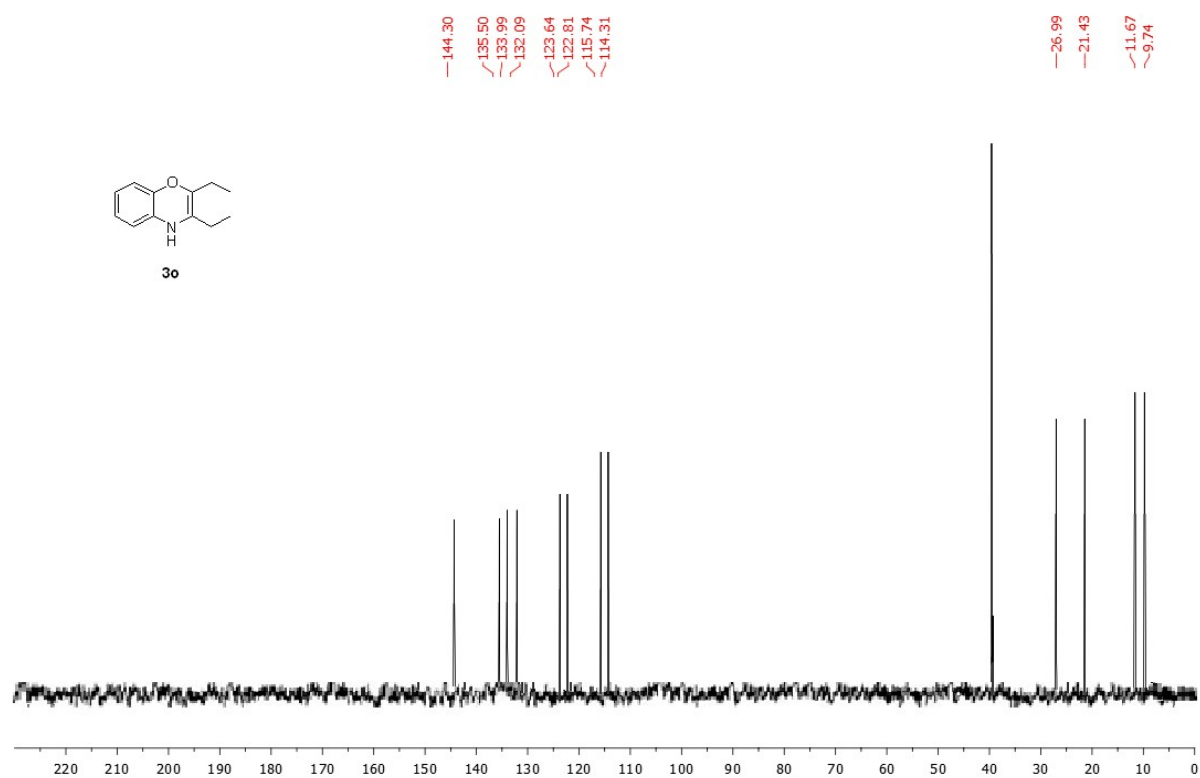
1: TOF MS ES+
 8.93e7



^1H NMR spectrum of 3o



^{13}C NMR spectrum of 3o

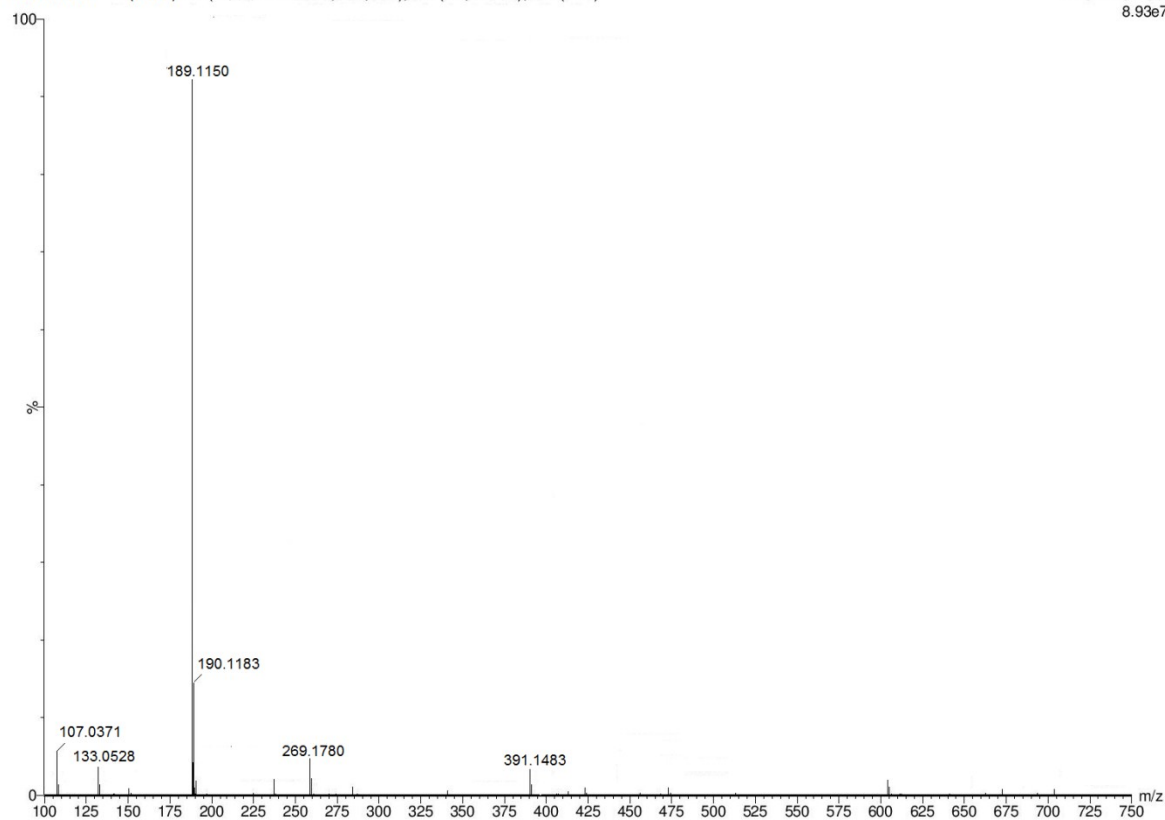


HRMS spectrum of 3o:

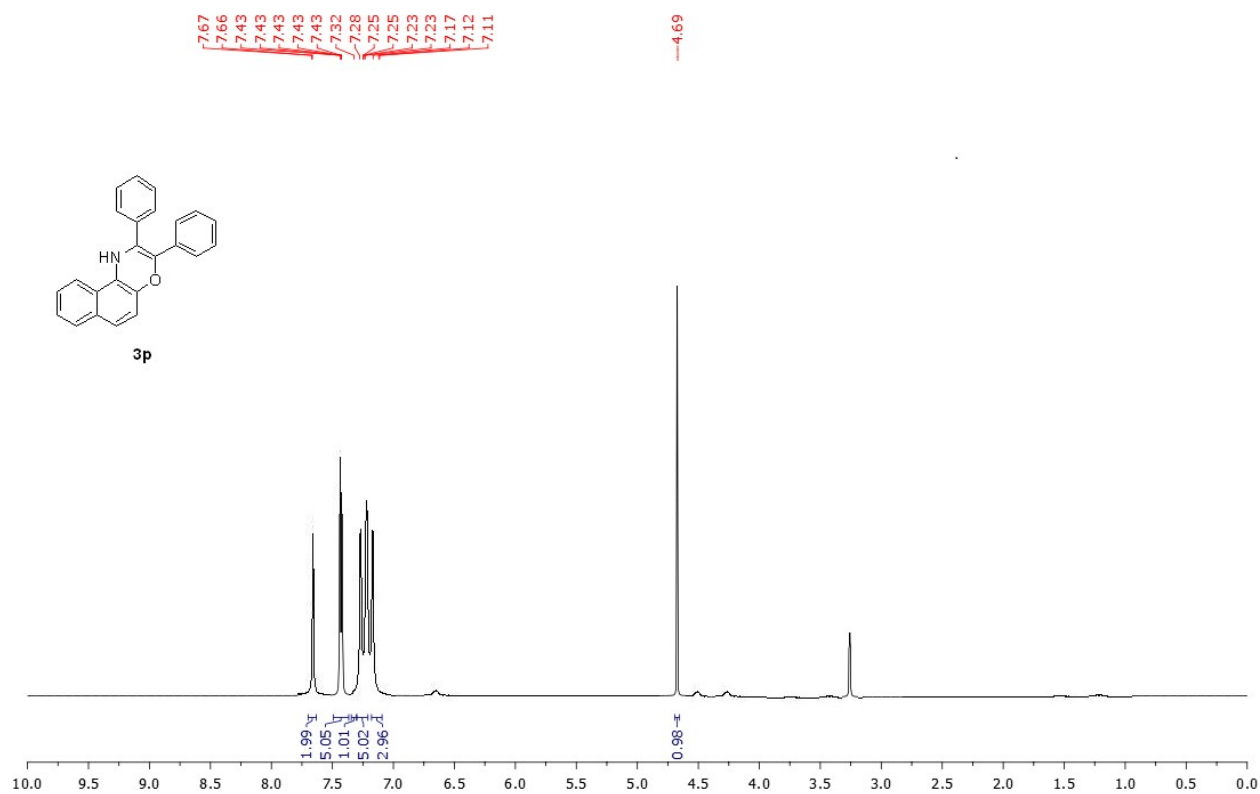
Sample Name : A-15
 Test Name : HRMS-1
 260218-A-15 11 (0.128) AM (Top, 4, Ar.10000.0,0.00,0.00); Sm (Mn, 1x3.00); Cm (7:18)

XEVO G2-XS QTOF

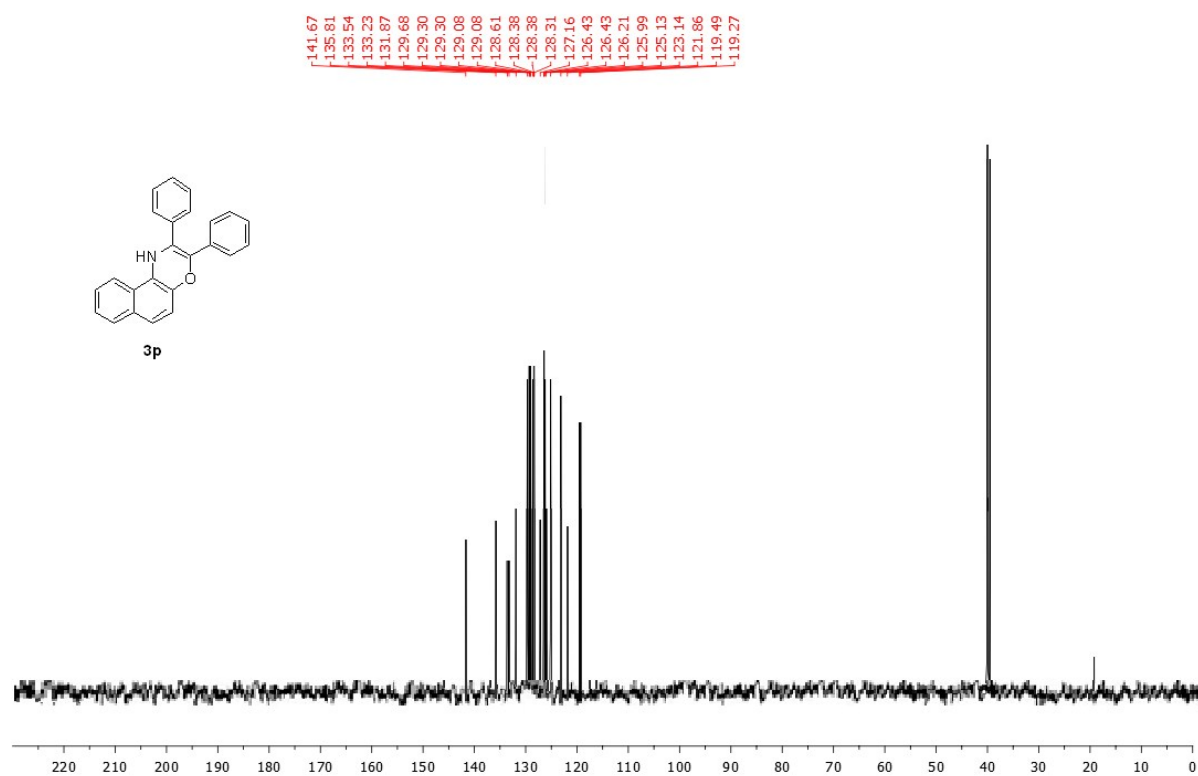
1: TOF MS ES+
 8.93e7



^1H NMR spectrum of 3p



^{13}C NMR spectrum of 3p

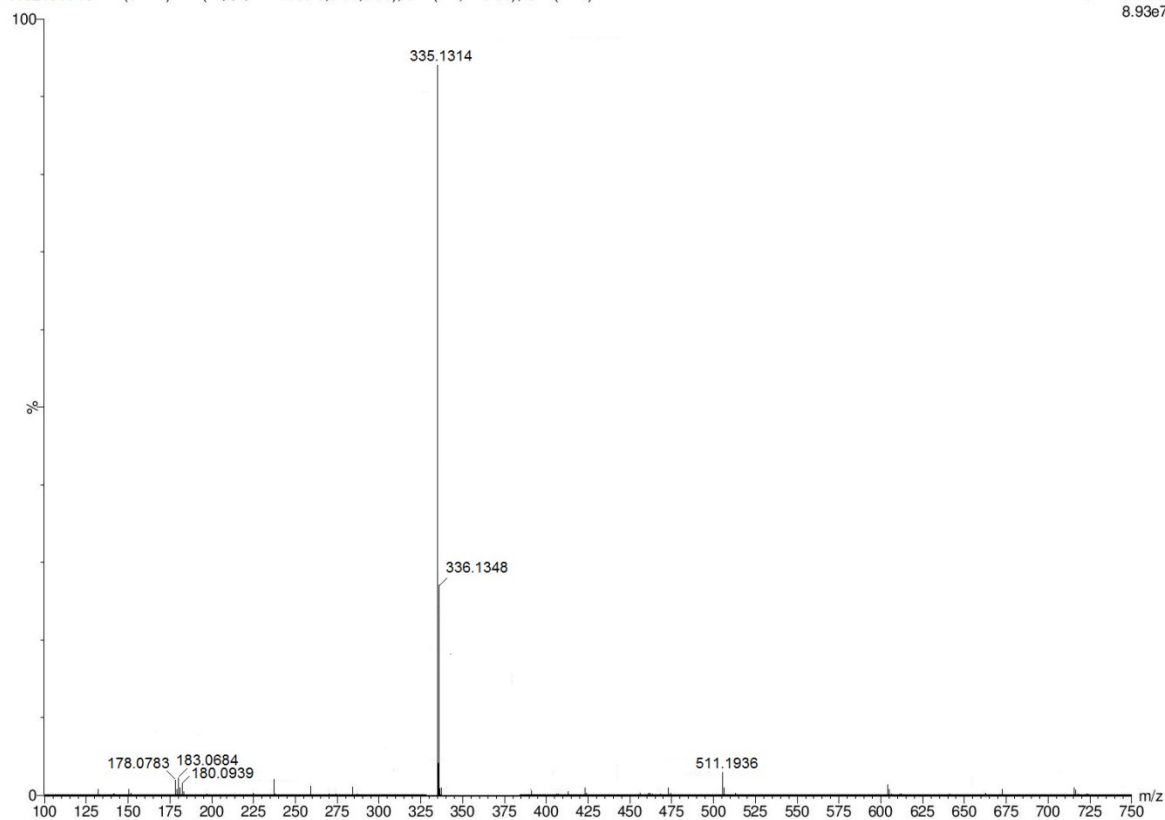


HRMS spectrum of 3p:

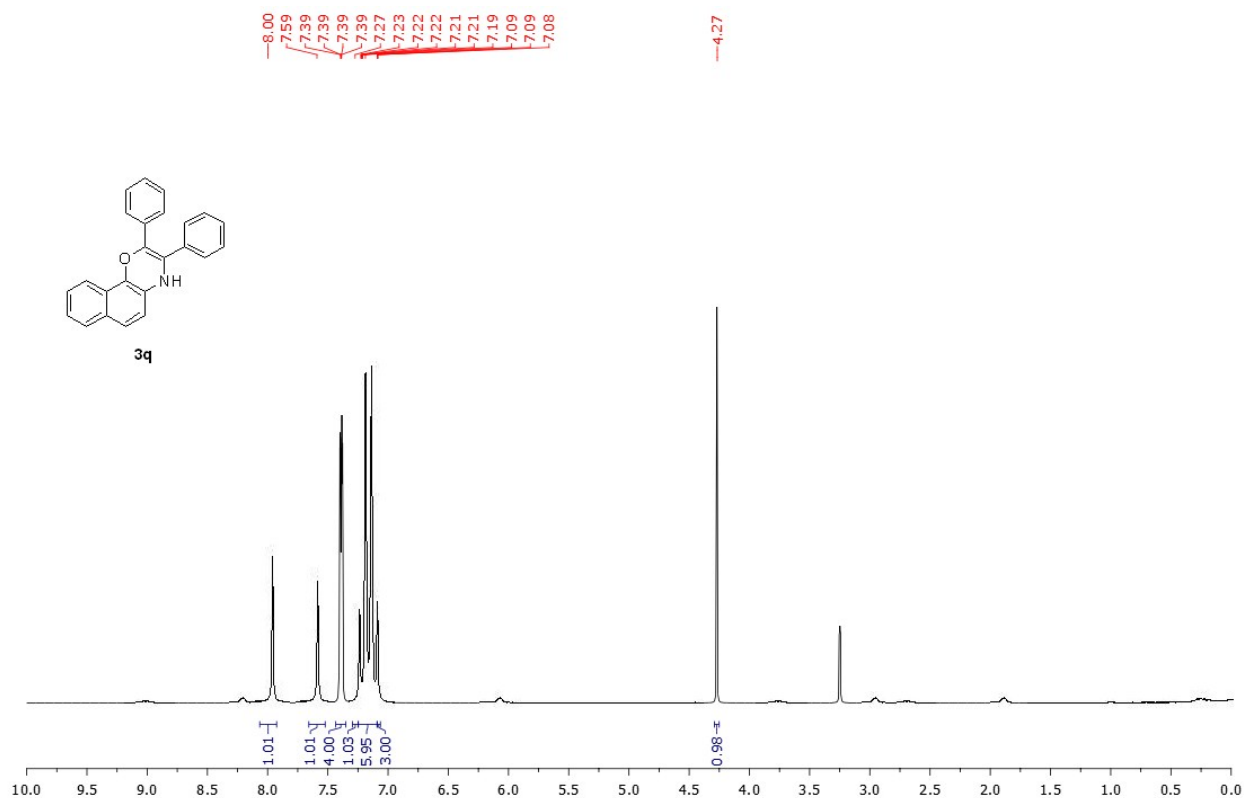
Sample Name : A-16
 Test Name : HRMS-1
 110218-A-16 11 (0.122) AM (Top.4, Ar.10000.0,0.00,0.00); Sm (Mn, 1x3.00); Cm (7:18)

XEVO G2-XS QTOF

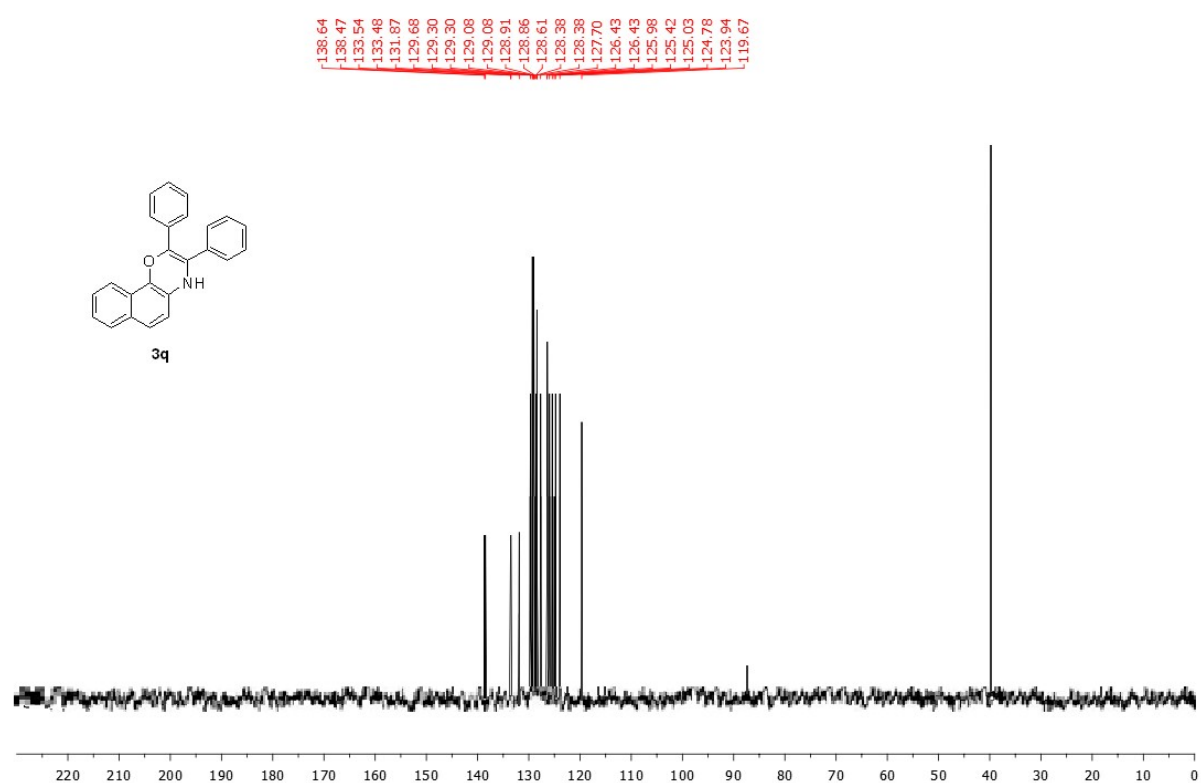
1: TOF MS ES+
 8.93e7



^1H NMR spectrum of 3q



^{13}C NMR spectrum of 3q

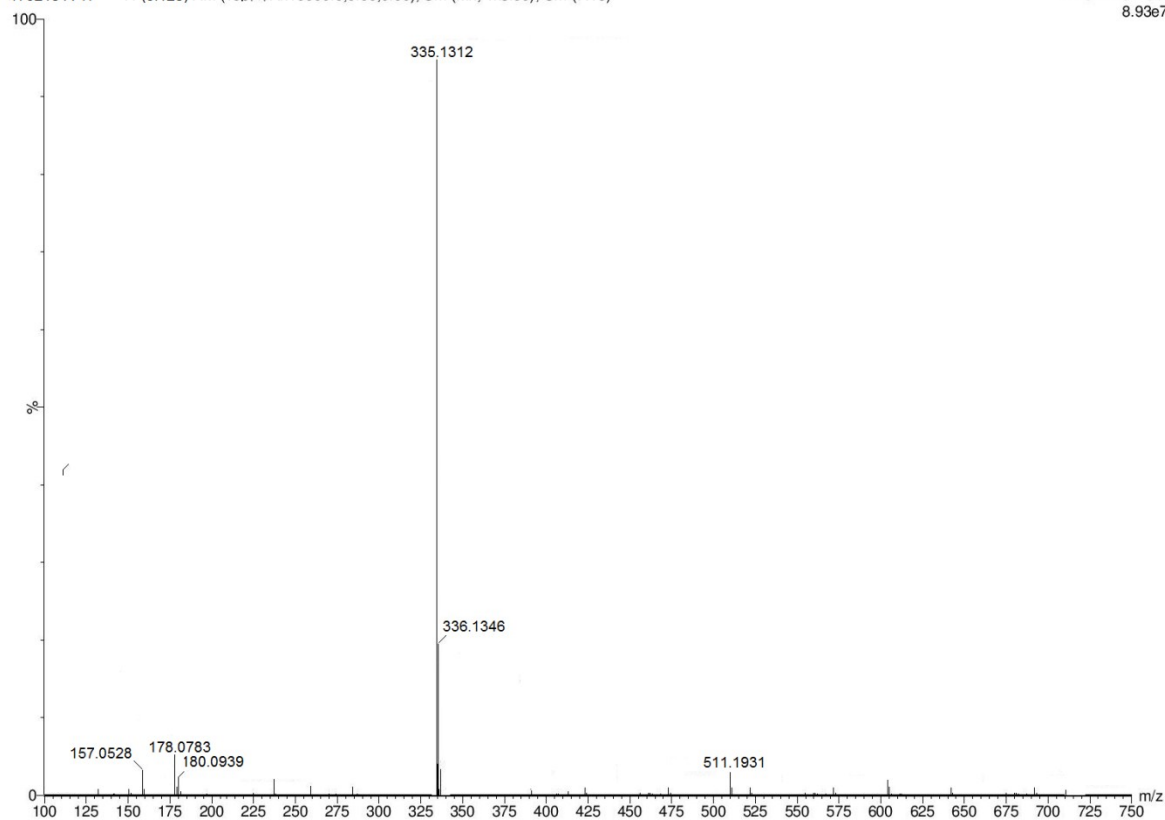


HRMS spectrum of 3q:

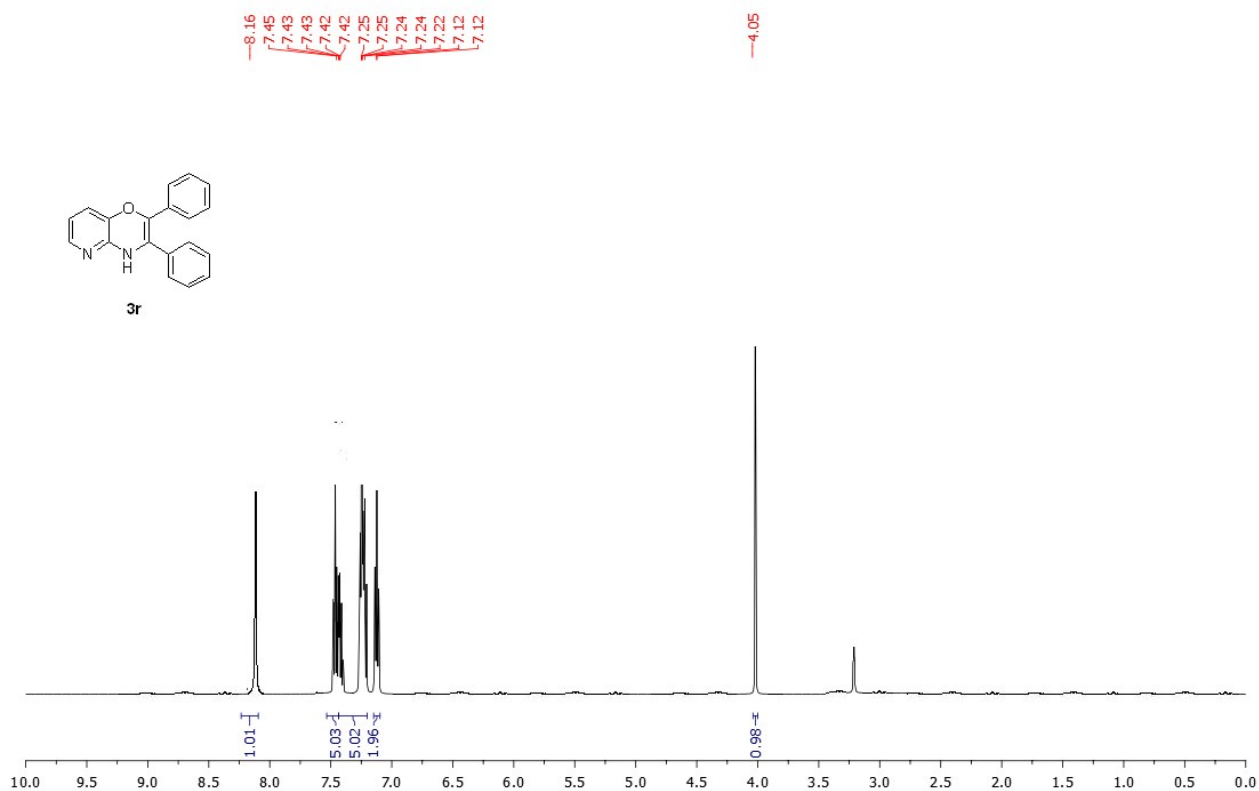
Sample Name : A-17
 Test Name : HRMS-1
 170218-A-17 11 (0.125) AM (Top.4, Ar.10000.0,0.00,0.00); Sm (Mn, 1x3.00); Cm (7:18)

XEVO G2-XS QTOF

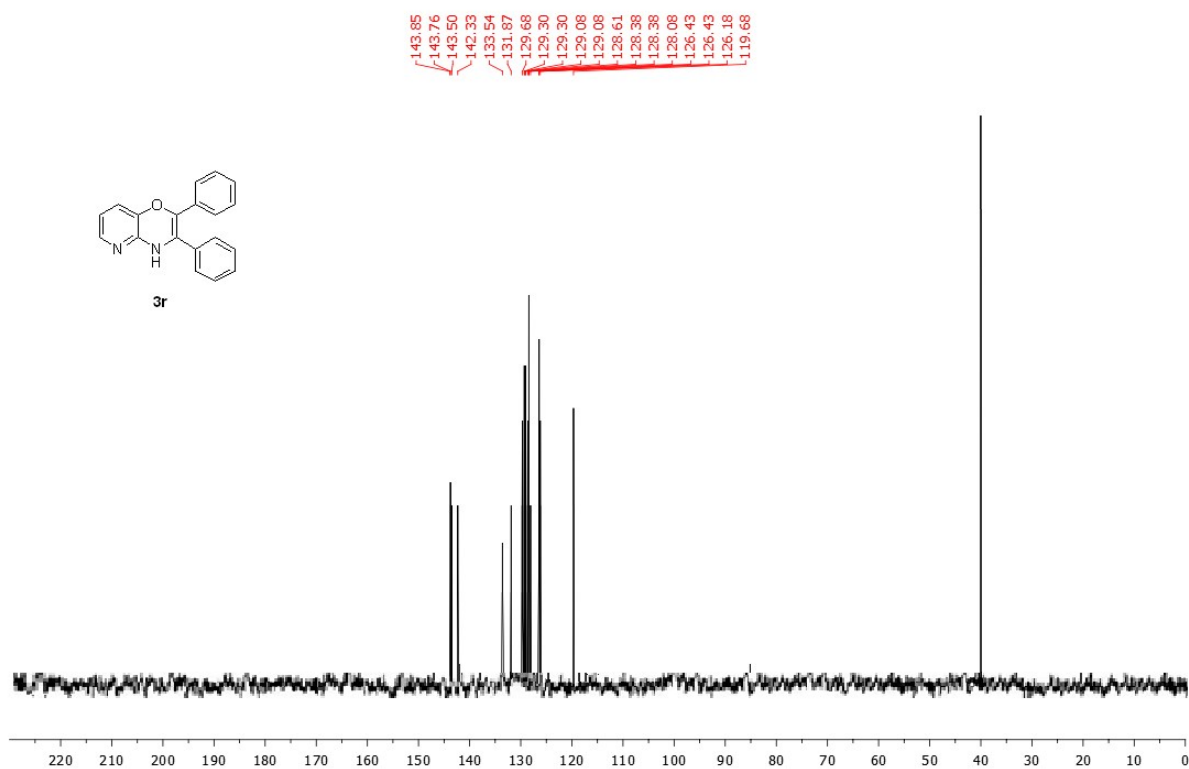
1: TOF MS ES+
 8.93e7



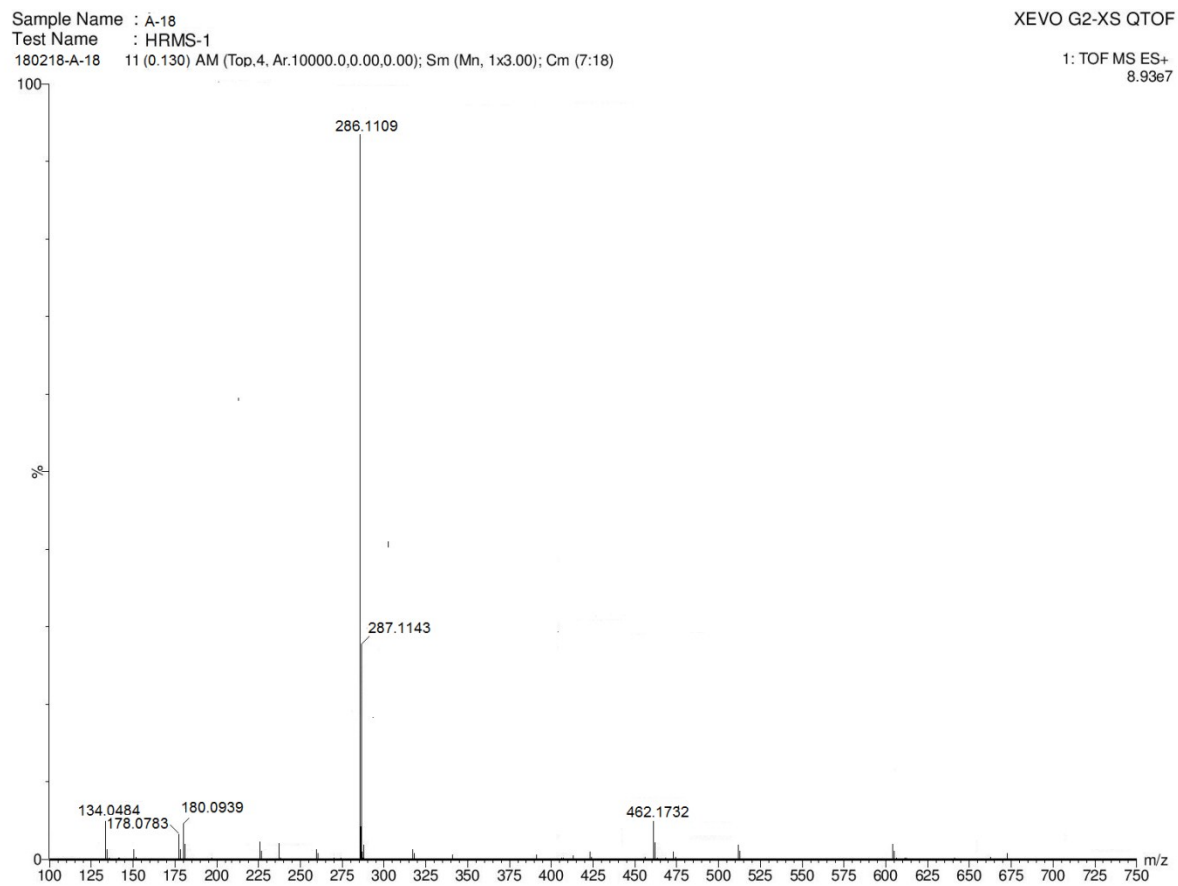
^1H NMR spectrum of 3r



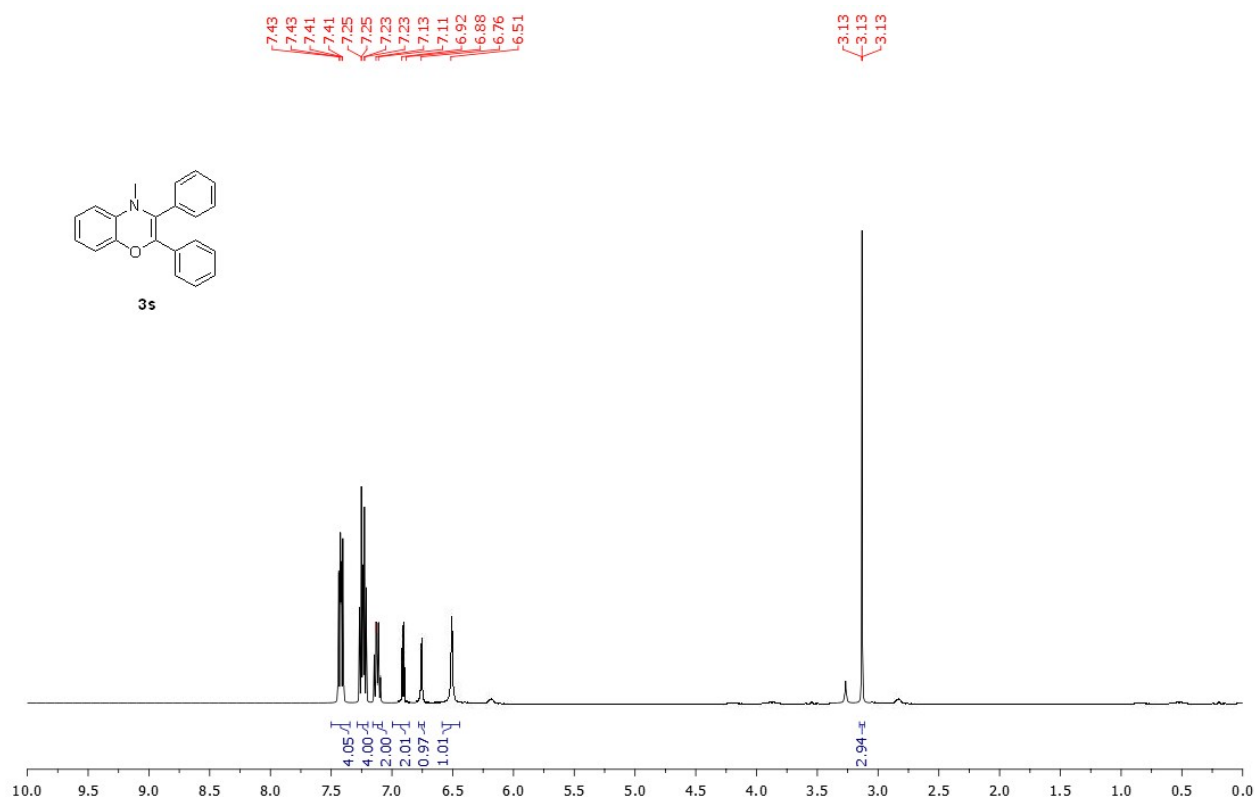
^{13}C NMR spectrum of 3r



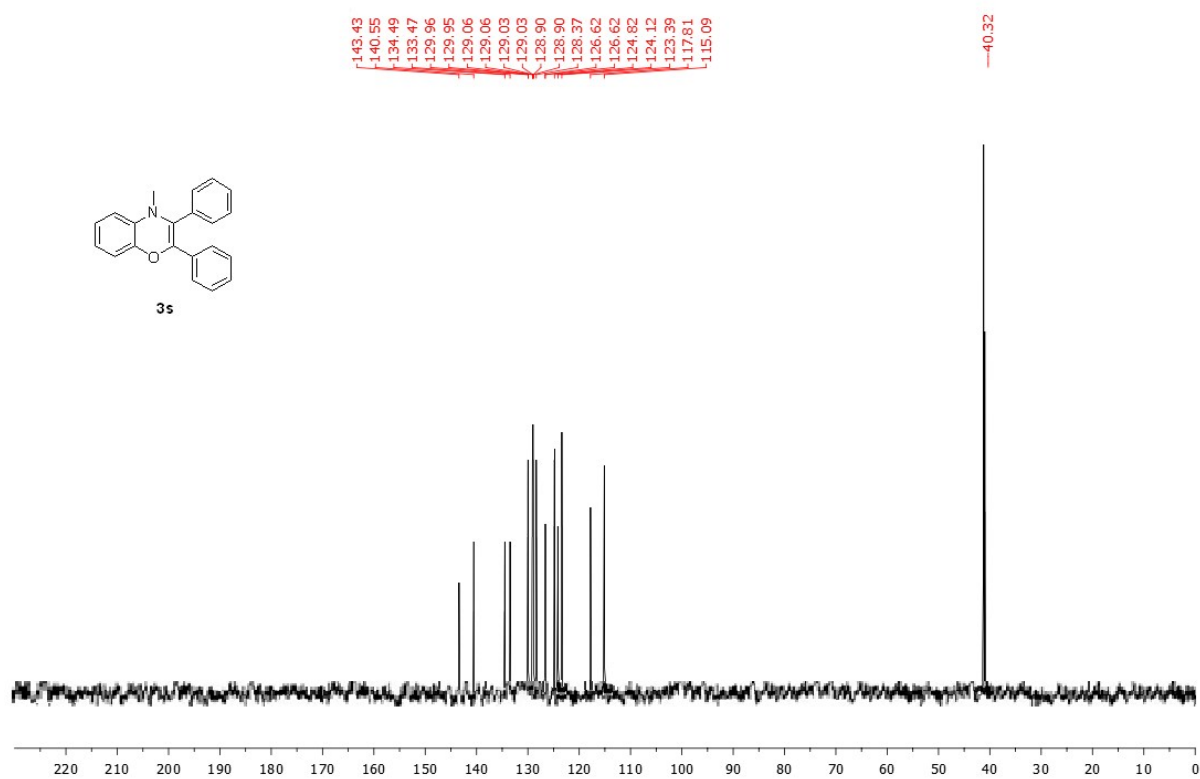
HRMS spectrum of **3r**:



¹H NMR spectrum of 3s



¹³C NMR spectrum of 3s

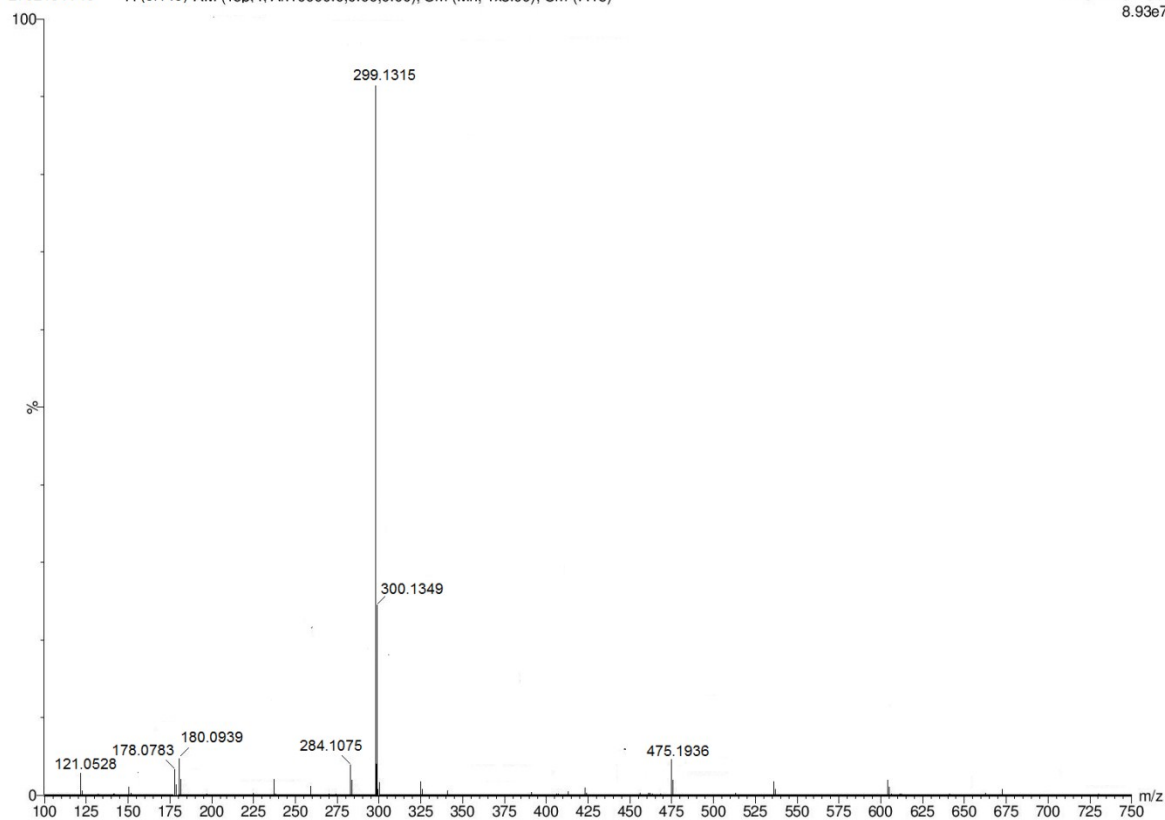


HRMS spectrum of 3s:

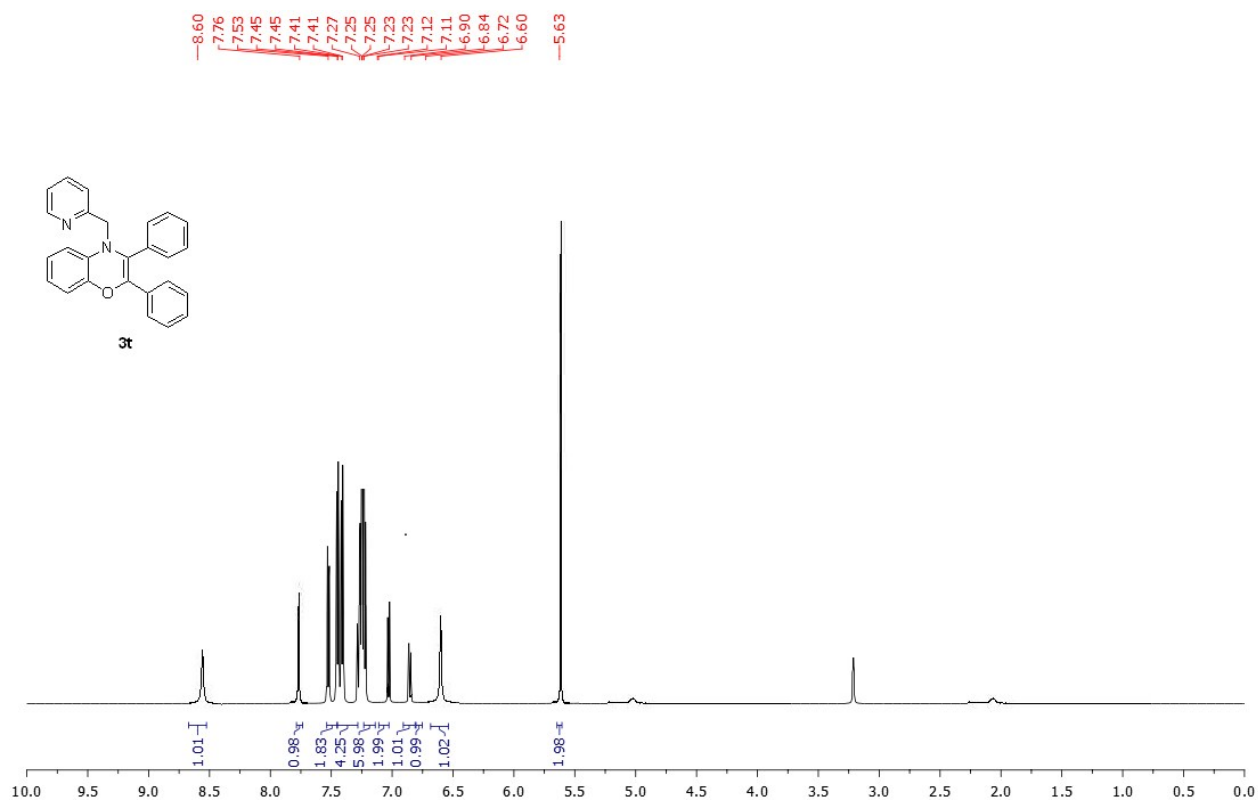
Sample Name : A-19
 Test Name : HRMS-1
 270218-A-19 11 (0.140) AM (Top,4, Ar.10000.0,0.00,0.00); Sm (Mn, 1x3.00); Cm (7:18)

XEVO G2-XS QTOF

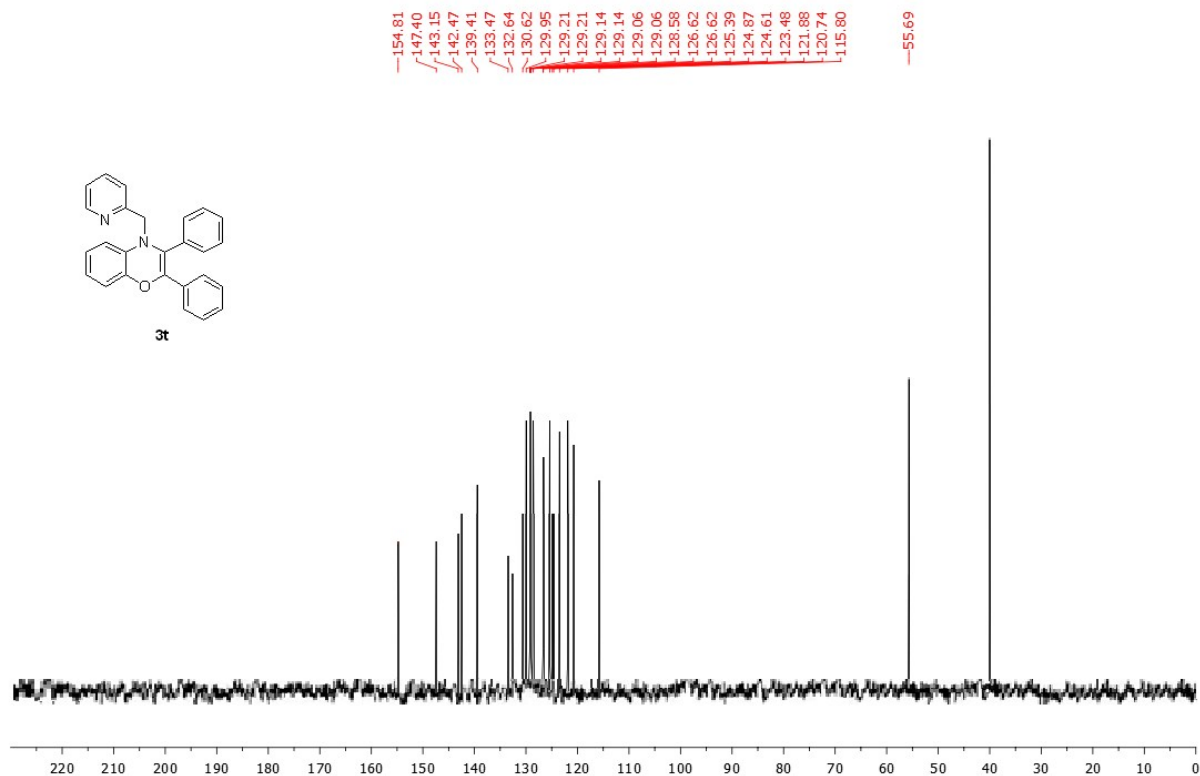
1: TOF MS ES+
 8.93e7



^1H NMR spectrum of 3t



^{13}C NMR spectrum of 3t



HRMS spectrum of 3t:

