

## Supplementary Material

### <sup>1</sup>H, <sup>13</sup>C NMR, & HRMS Spectra of Representative Compounds

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#### Spectras of representative compounds

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Table 1: R SQUARED VALUES

# Elemental Composition Report

## Single Mass Analysis

Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 18-18 H: 0-300 N: 0-4 O: 1-1

Sample Name : 280921\_AK-1

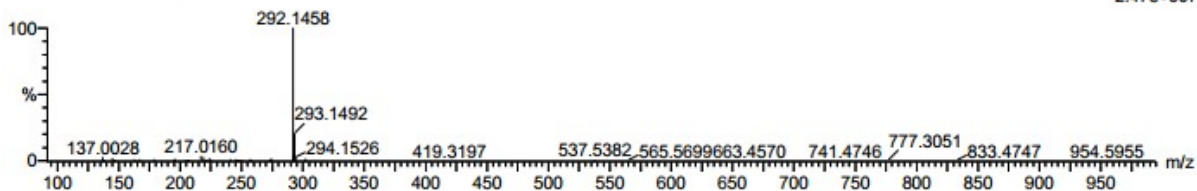
IITRPR

XEVO G2-XS QTOF

Test Name :

280921\_AK-1 20 (0.435)

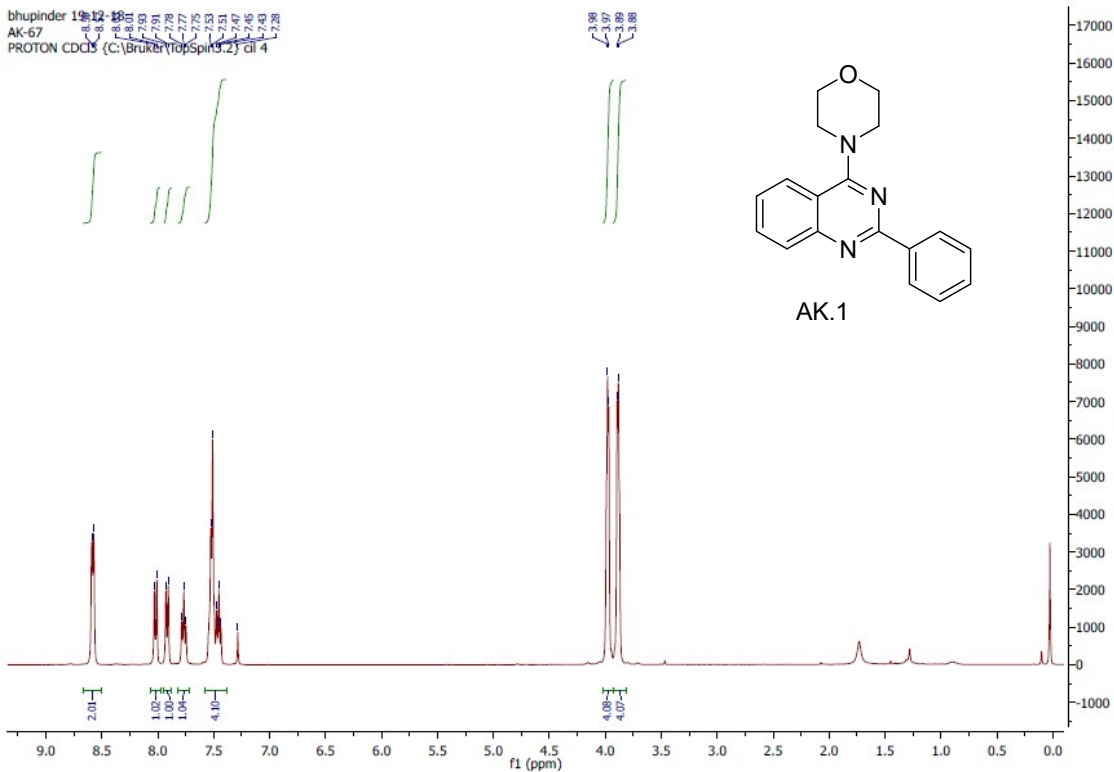
1: TOF MS ES+  
2.47e+007

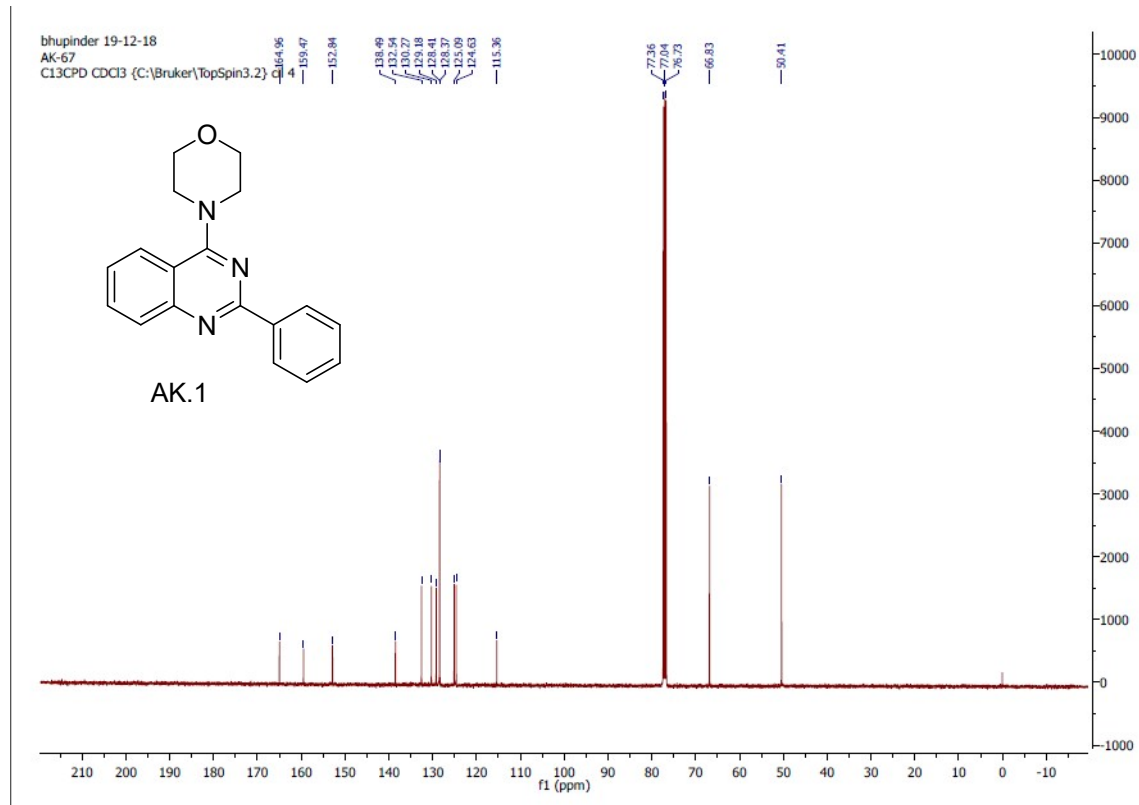


Minimum: -1.5  
Maximum: 2.0 300.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
292.1458	292.1450	0.8	2.7	11.5	1712.7	n/a	n/a	C18 H18 N3 O

bhupinder 19-12-20  
AK-67  
PROTON CDCl<sub>3</sub> (C: Bruker TopSpin 9.2) cil 4





**Figure 1.** Spectras of compound AK-1

## Elemental Composition Report

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### Single Mass Analysis

Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

10 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 19-19 H: 0-300 N: 0-4 O: 1-1 S: 0-1

Sample Name : 280921\_AK-2

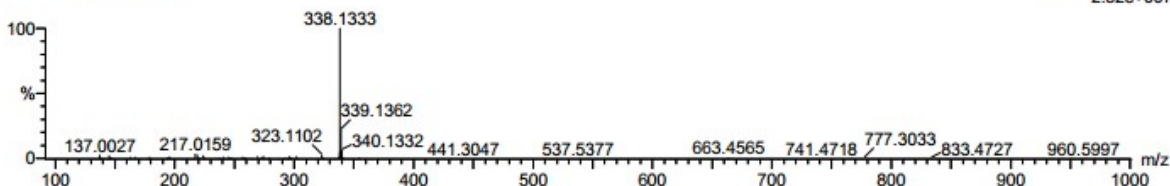
IITRPR

XEVO G2-XS QTOF

Test Name :

280921\_AK-2 21 (0.452)

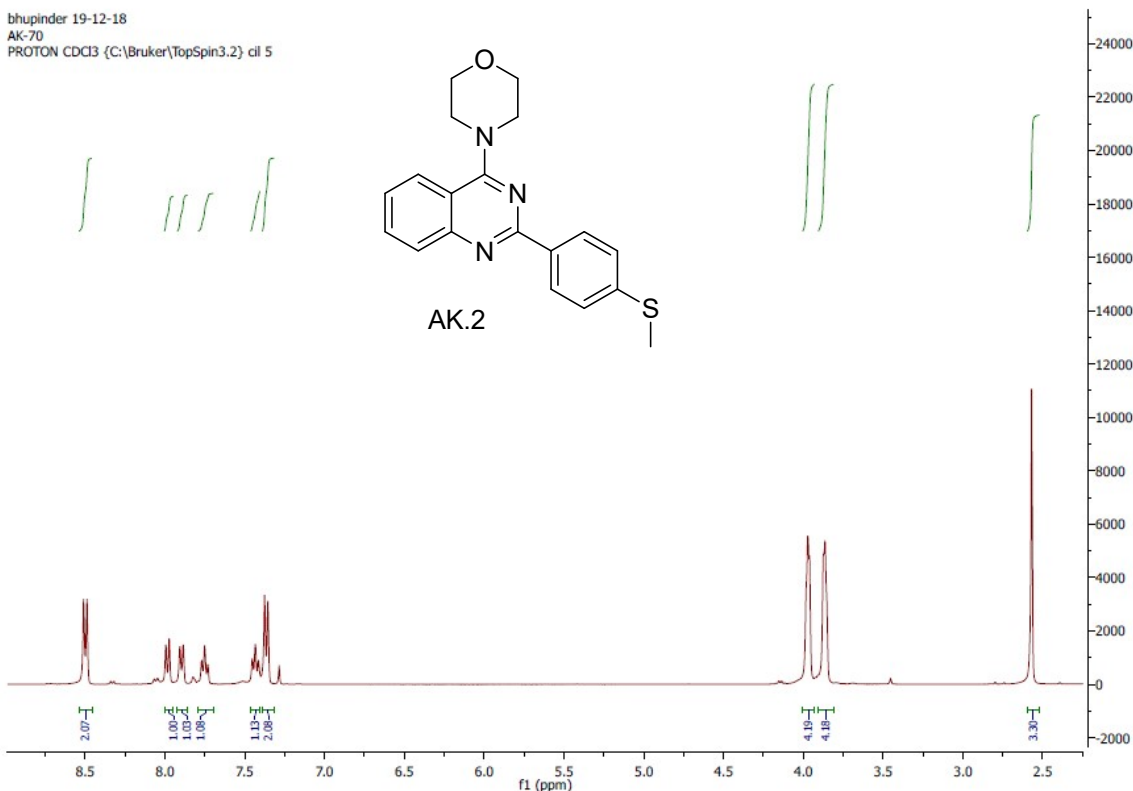
1: TOF MS ES+  
2.52e+007

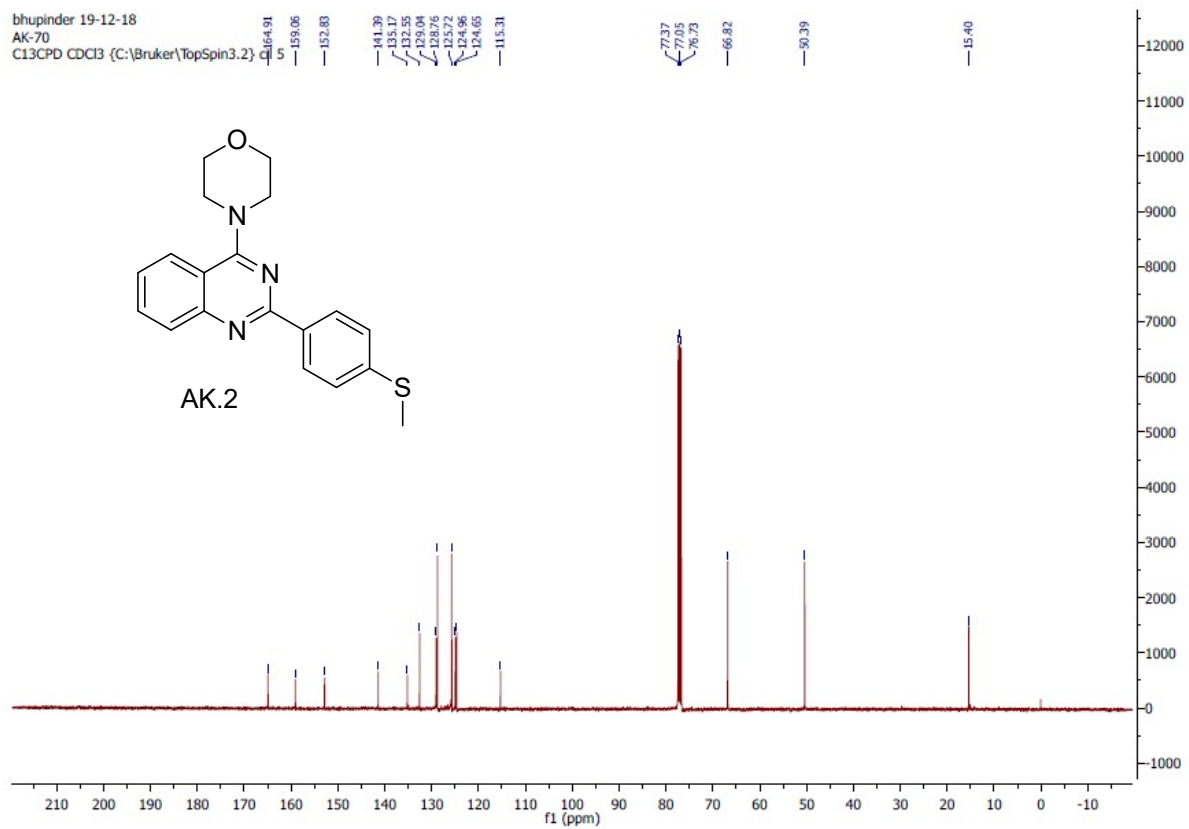


Minimum: -1.5  
Maximum: 2.0 300.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
338.1333	338.1327	0.6	1.8	11.5	1621.8	n/a	n/a	C19 H20 N3 O S

bhupinder 19-12-18  
AK-70  
PROTON CDCl3 (C:\Bruker\TopSpin3.2) cil 5





**Figure 2.** Spectras of compound AK-2

# Elemental Composition Report

## Single Mass Analysis

Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 0 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 18-18 H: 0-300 N: 0-4 O: 1-1 F: 6-6

Sample Name : 280921\_AK-3

IITRPR

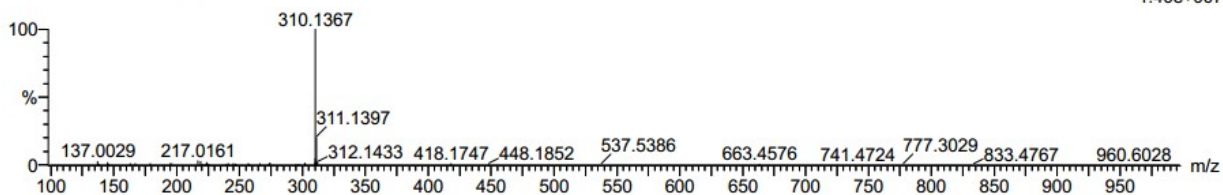
XEVO G2-XS QTOF

Test Name :

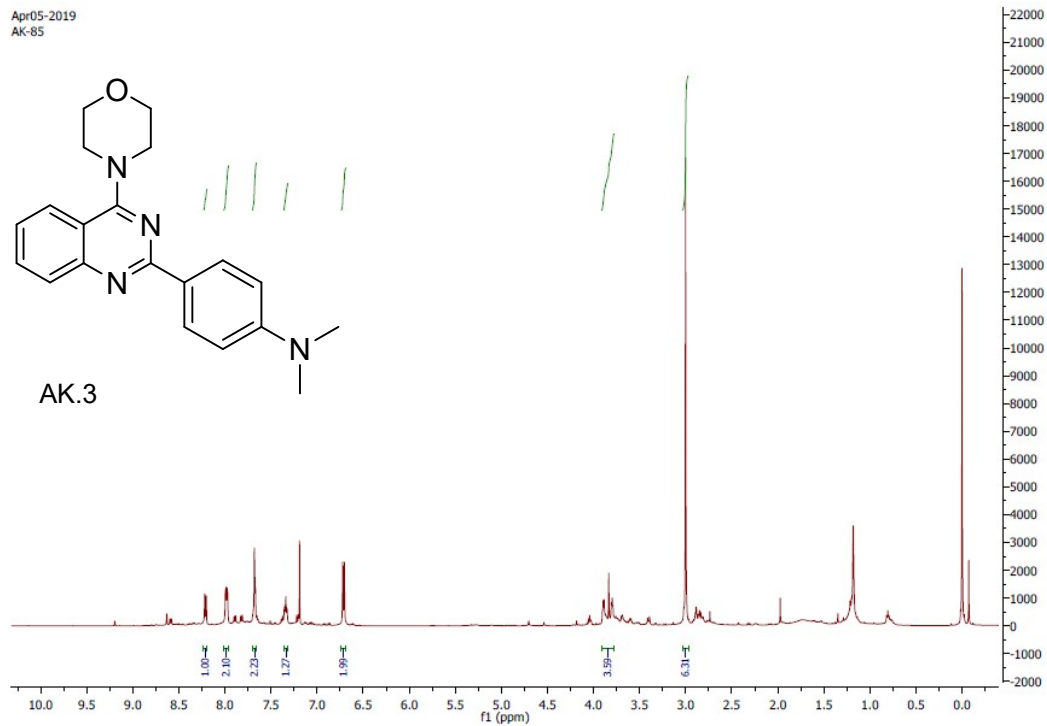
280921\_AK-3 23 (0.497)

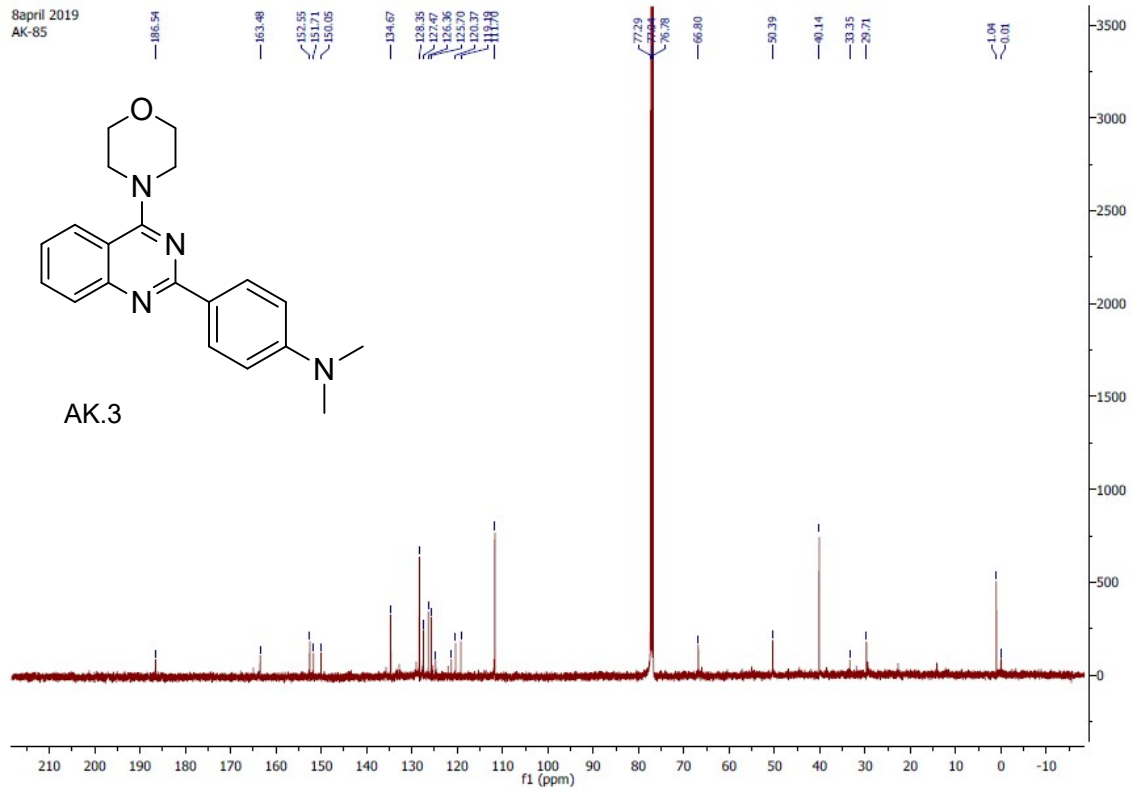
1: TOF MS ES+

1.40e+007



Apr05-2019  
AK-85





**Figure 3.** Spectras of compound AK-3

Elemental Composition Report

Single Mass Analysis

Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-20 H: 0-300 N: 0-4 O: 1-1

Sample Name : 280921\_AK-4

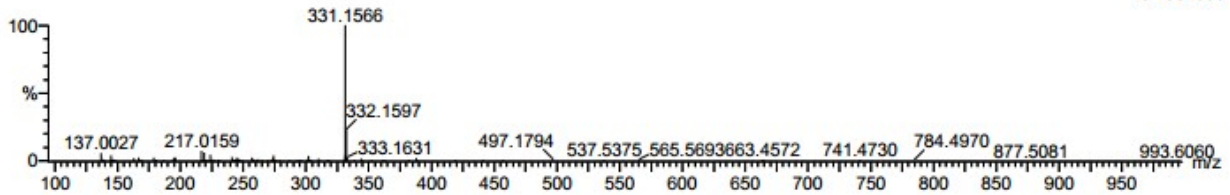
IITRPR

XEVO G2-XS QTOF

Test Name :

280921\_AK-4 22 (0.480)

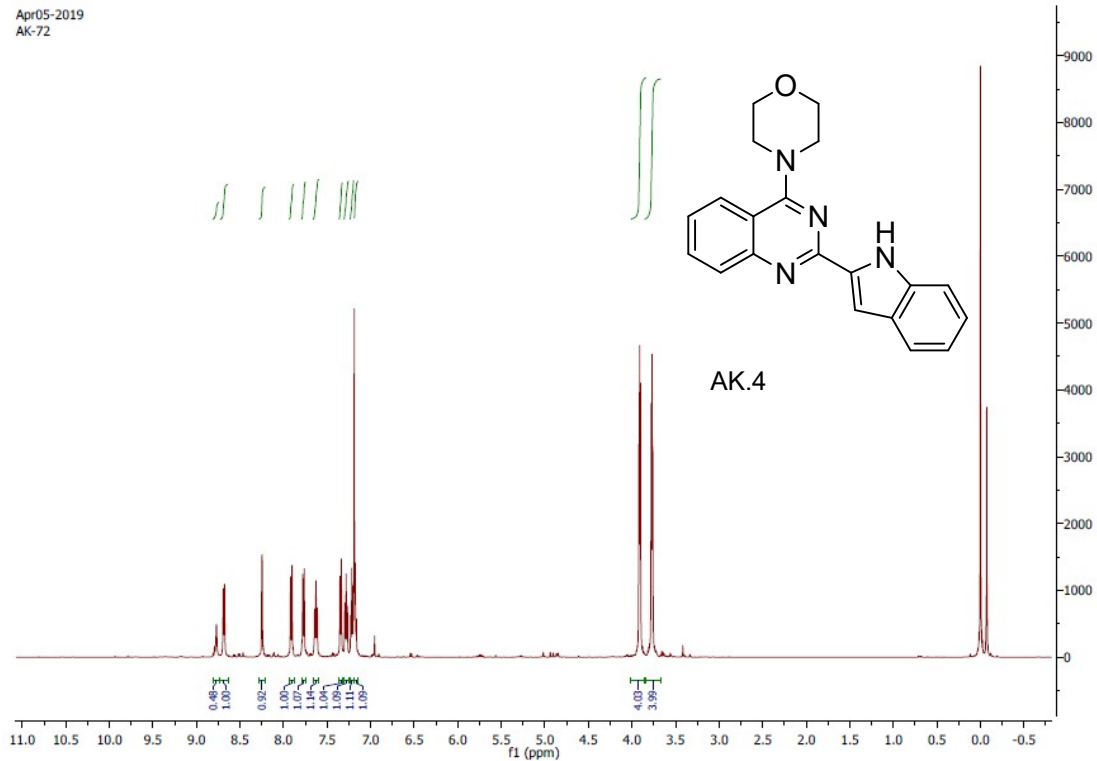
1: TOF MS ES+  
5.43e+006



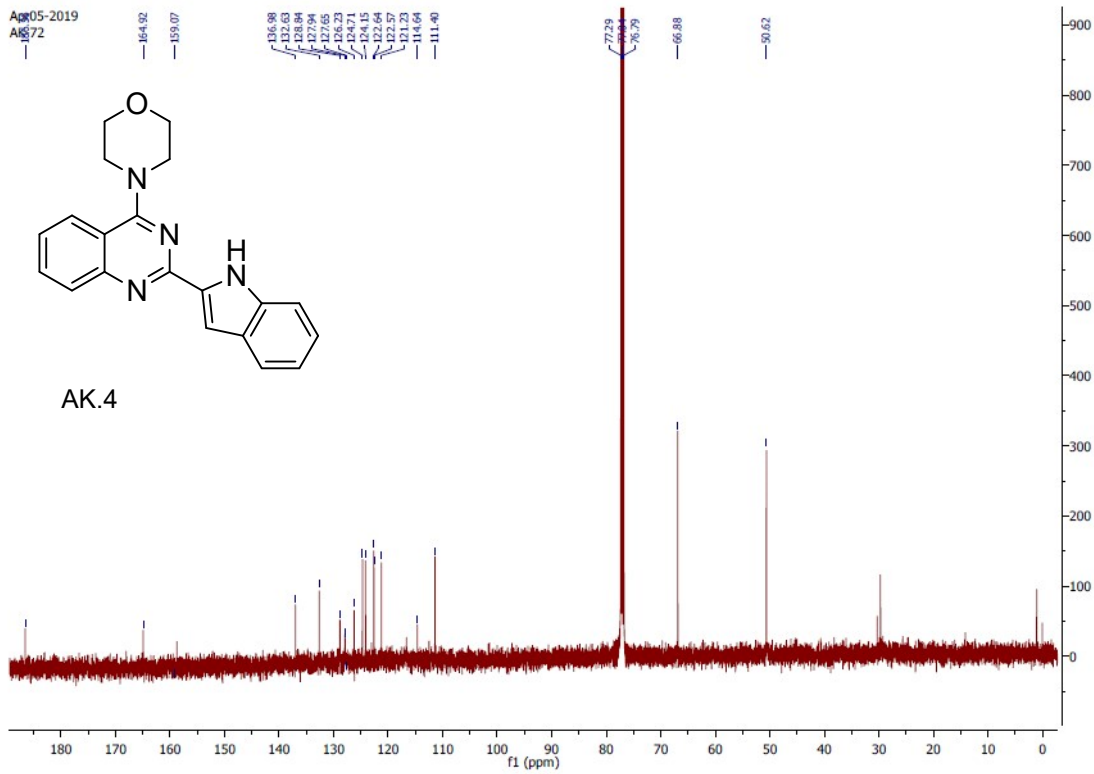
Minimum: -1.5  
Maximum: 2.0 300.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
331.1566	331.1559	0.7	2.1	13.5	1853.0	n/a	n/a	C20 H19 N4 O

Apr05-2019  
AK-72







**Figure 4.** Spectras of compound **AK-4**

Single Mass Analysis

Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

10 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 18-18 H: 0-300 N: 0-4 O: 1-2

Sample Name : 280921\_AK-5

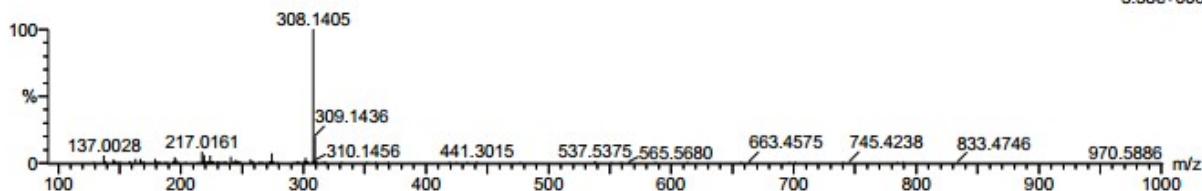
IITRPR

XEVO G2-XS QTOF

Test Name :

280921\_AK-5 34 (0.729)

1: TOF MS ES+  
3.38e+006



Minimum: -1.5  
Maximum: 2.0 300.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
308.1405	308.1399	0.6	1.9	11.5	1936.7	n/a	n/a	C18 H18 N3 O2

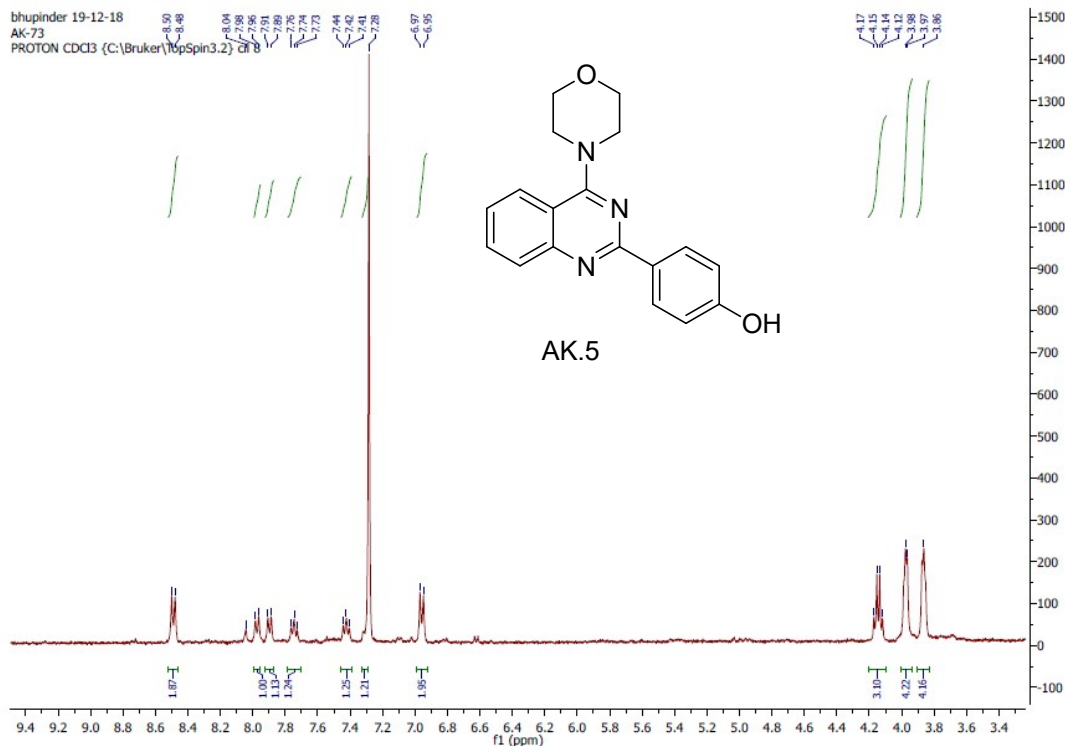


Figure 5. Spectras of compound AK-5

Single Mass Analysis

Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

3 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 19-19 H: 0-300 N: 4-4 O: 0-2

Sample Name : 280921\_AK-6

IITRPR

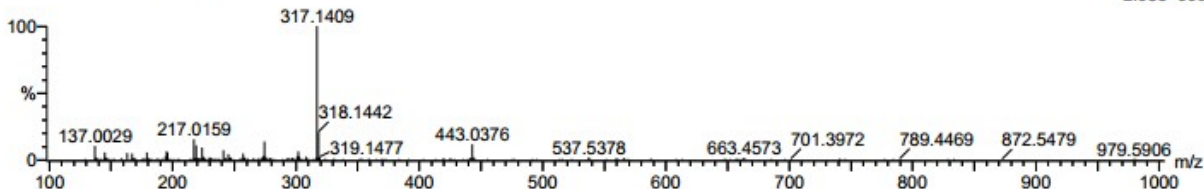
XEVO G2-XS QTOF

Test Name :

280921\_AK-6 32 (0.684)

1: TOF MS ES+

2.03e+006

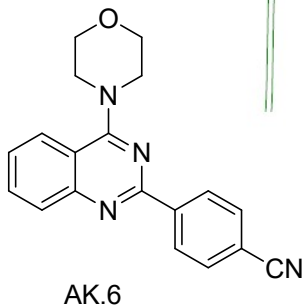
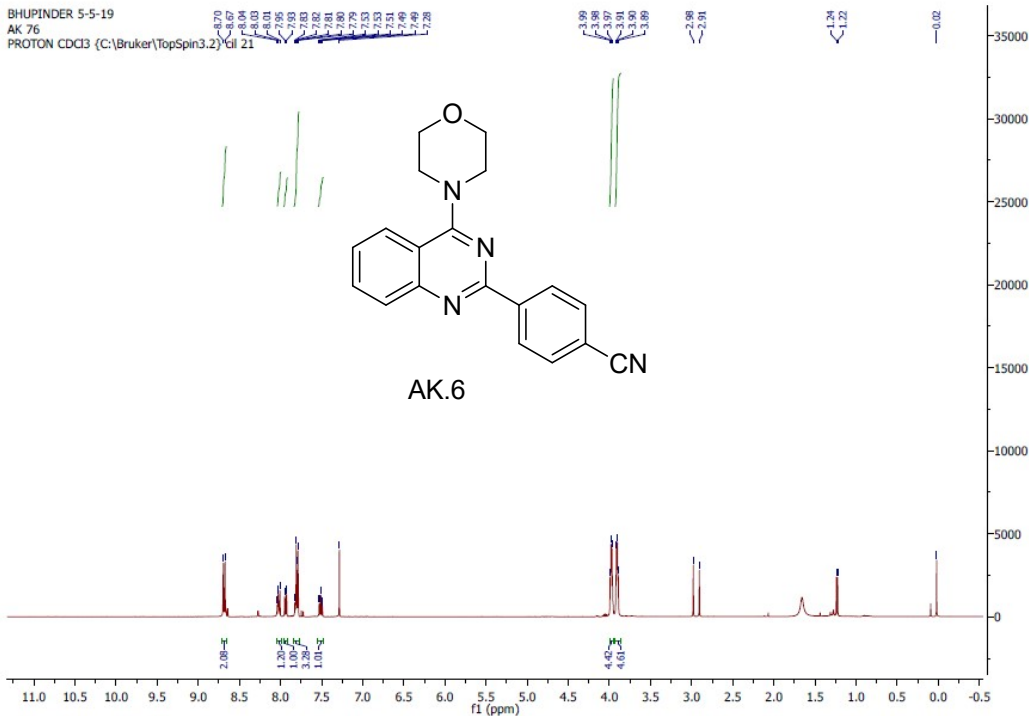


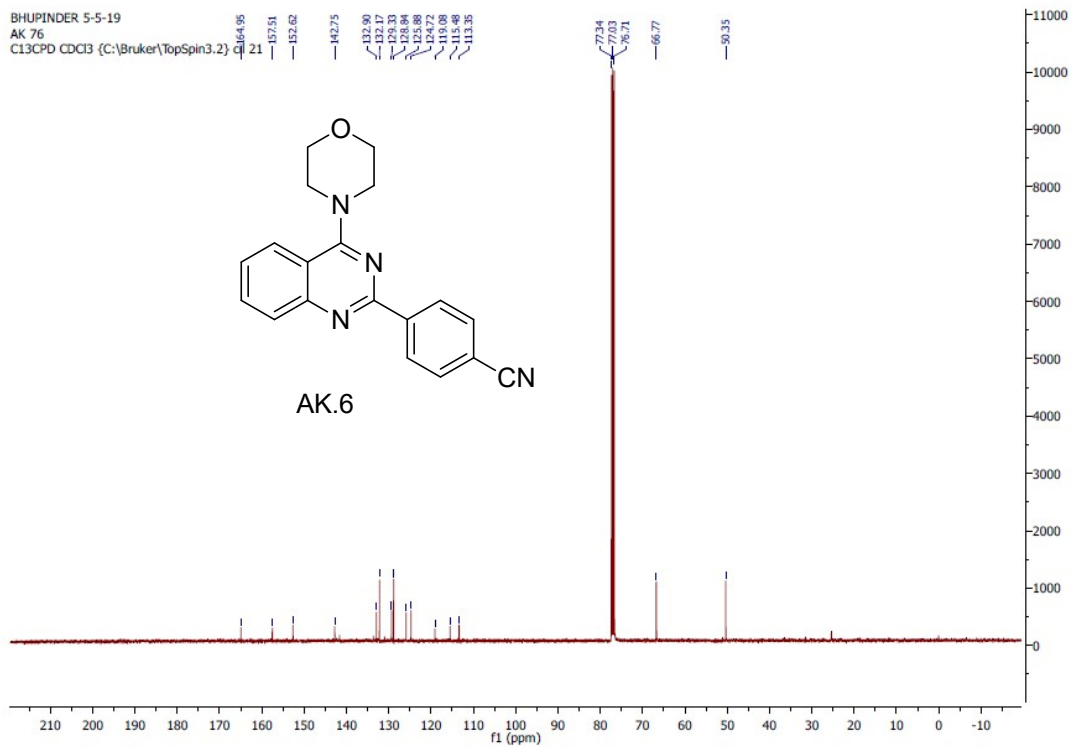
Minimum: -1.5  
Maximum: 2.0 300.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
317.1409	317.1402	0.7	2.2	13.5	1843.6	n/a	n/a	C19 H17 N4 O

BHUPINDER 5-5-19  
AK 76

PROTON CDCl3 (C:\Bruker\TopSpin3.2)\Gil 21





**Figure 6.** Spectras of compound AK-6

Elemental Composition Report

Single Mass Analysis

Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

25 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 21-21 H: 0-300 N: 0-4 O: 0-4

Sample Name : 280921\_AK-7

IITRRP

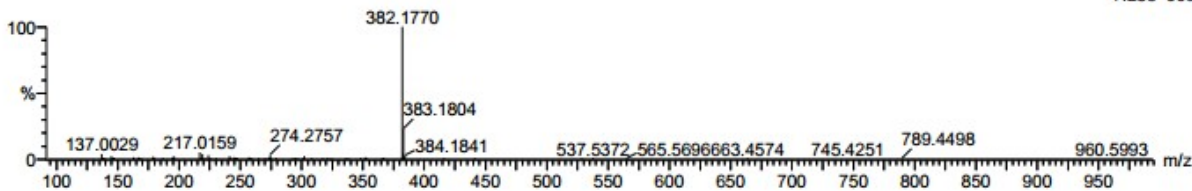
XEVO G2-XS QTOF

Test Name :

280921\_AK-7 27 (0.576)

1: TOF MS ES+

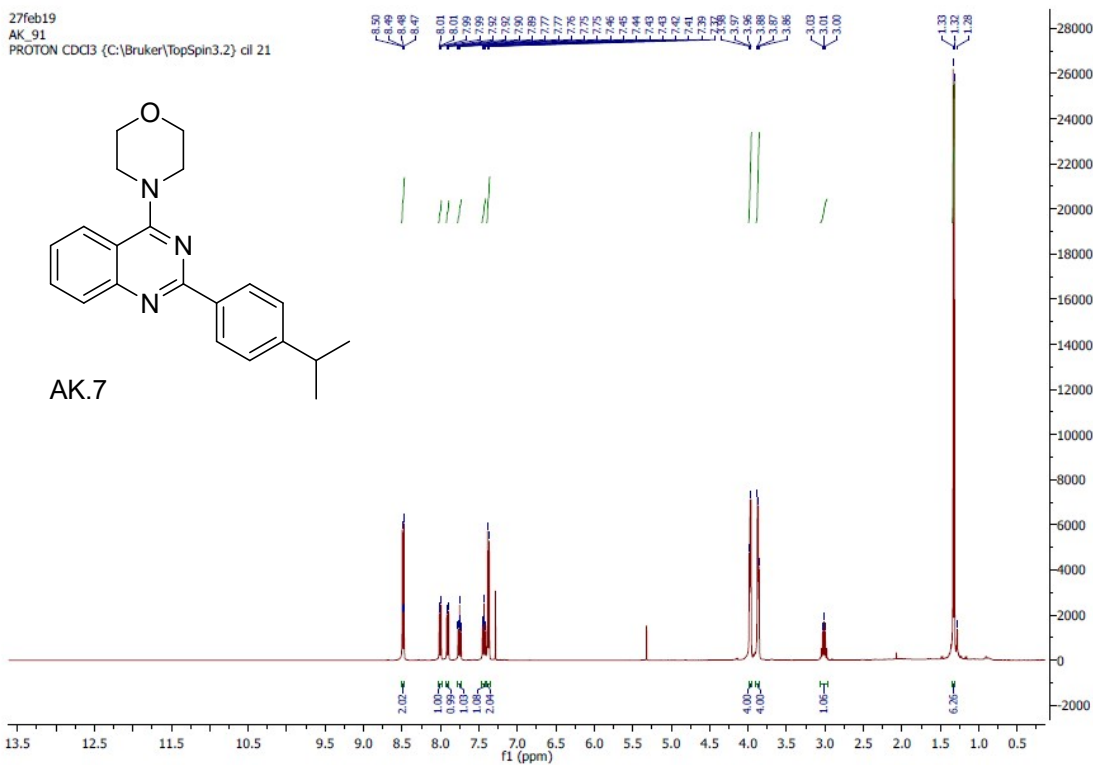
7.28e+006



Minimum: -1.5  
Maximum: 2.0 300.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
382.1770	382.1767	0.3	0.8	11.5	1420.1	n/a	n/a	C21 H24 N3 O4

27Feb19  
AK\_91  
PROTON CDCl3 (C:\Bruker\TopSpin3.2) cil 21



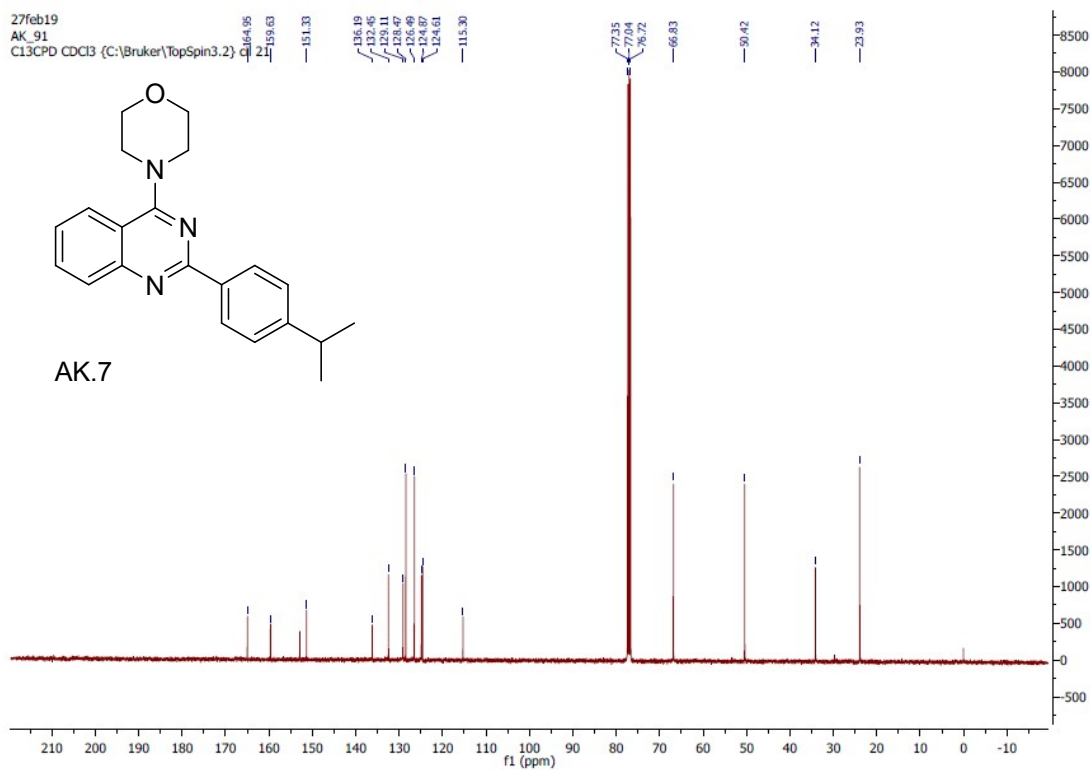


Figure 7. Spectras of compound AK-7

# Elemental Composition Report

## Single Mass Analysis

Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

15 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 19-19 H: 0-300 N: 0-4 O: 0-2

Sample Name : 280921\_AK-8

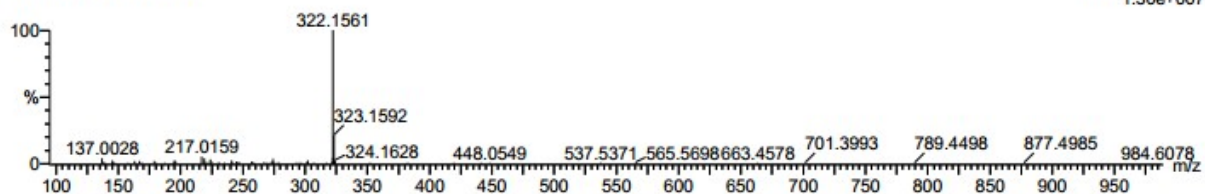
IITRPR

XEVO G2-XS QTOF

Test Name :

280921\_AK-8 29 (0.622)

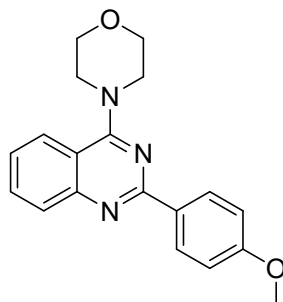
1: TOF MS ES+  
1.30e+007



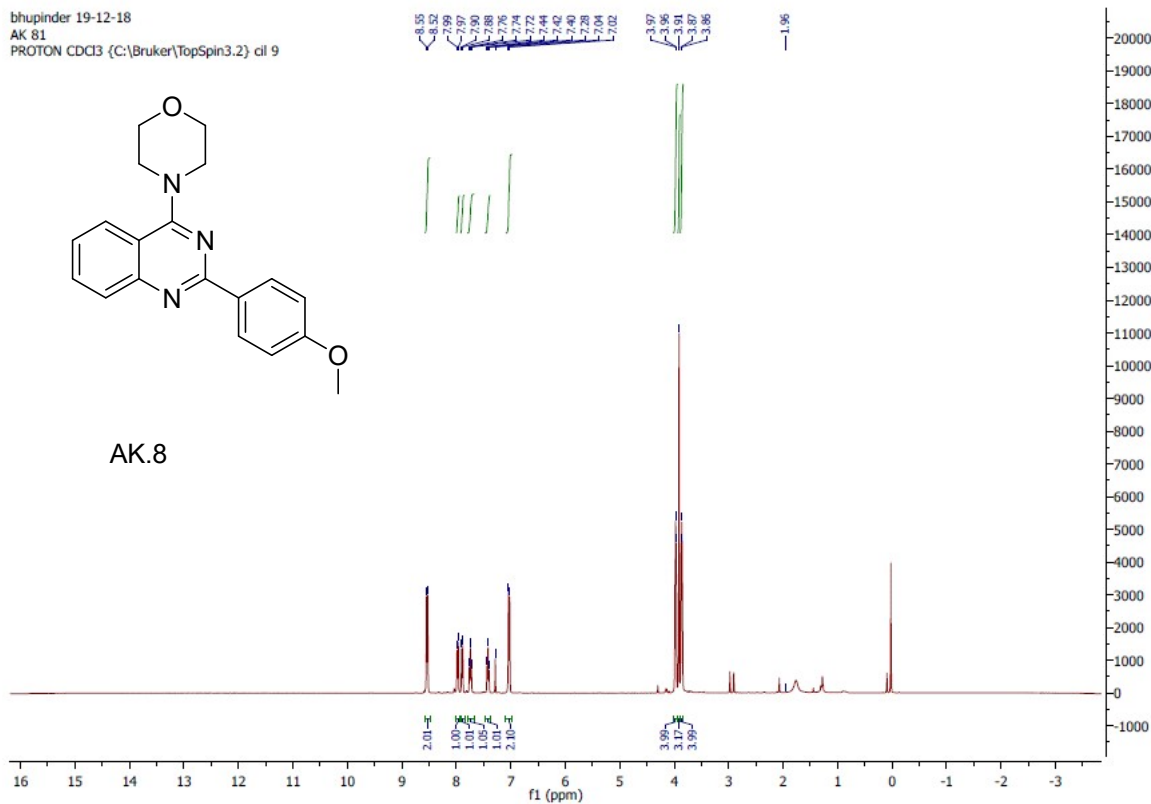
Minimum: -1.5  
Maximum: 2.0 300.0 50.0

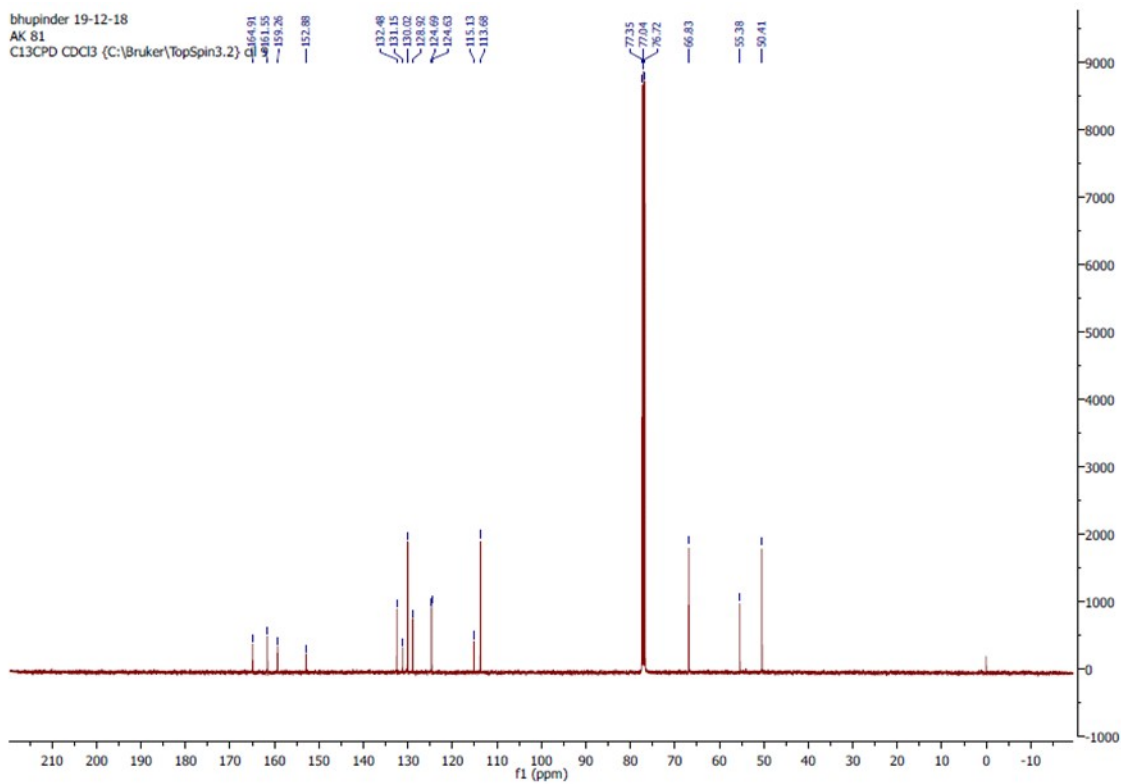
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
322.1561	322.1556	0.5	1.6	11.5	1507.9	n/a	n/a	C19 H20 N3 O2

bhupinder 19-12-18  
AK 81  
PROTON CDCl3 (C:\Bruker\TopSpin3.2) cil 9



AK.8





**Figure 8.** Spectras of compound AK-8



# Elemental Composition Report

## Single Mass Analysis

Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

15 formula(e) evaluated with 0 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-20 H: 0-300 N: 0-4 O: 0-2

Sample Name : 280921\_AK-9

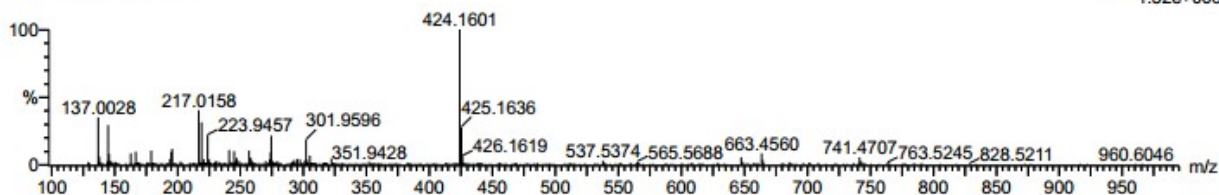
IITRPR

XEVO G2-XS QTOF

Test Name :

280921\_AK-9 13 (0.294)

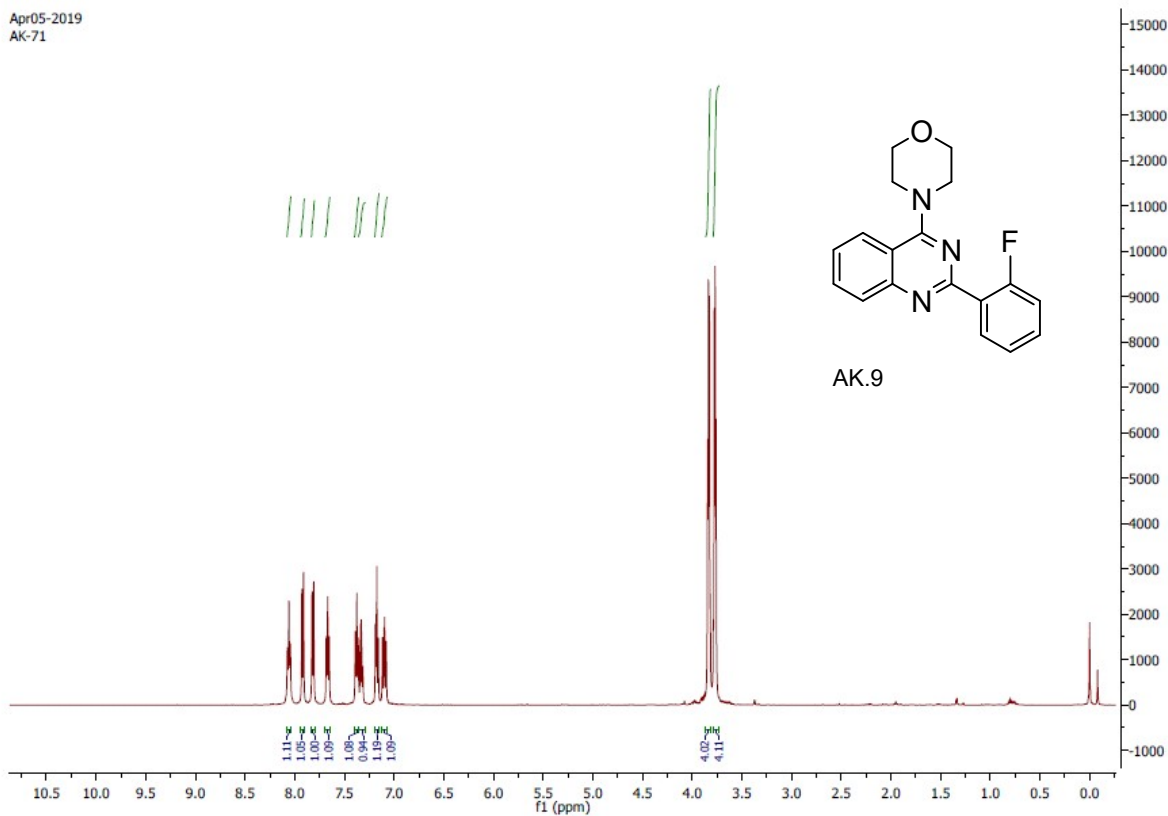
1: TOF MS ES+  
1.32e+006



Minimum: -1.5  
Maximum: 2.0 300.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
424.1601	---							

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AK-71



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AK-71

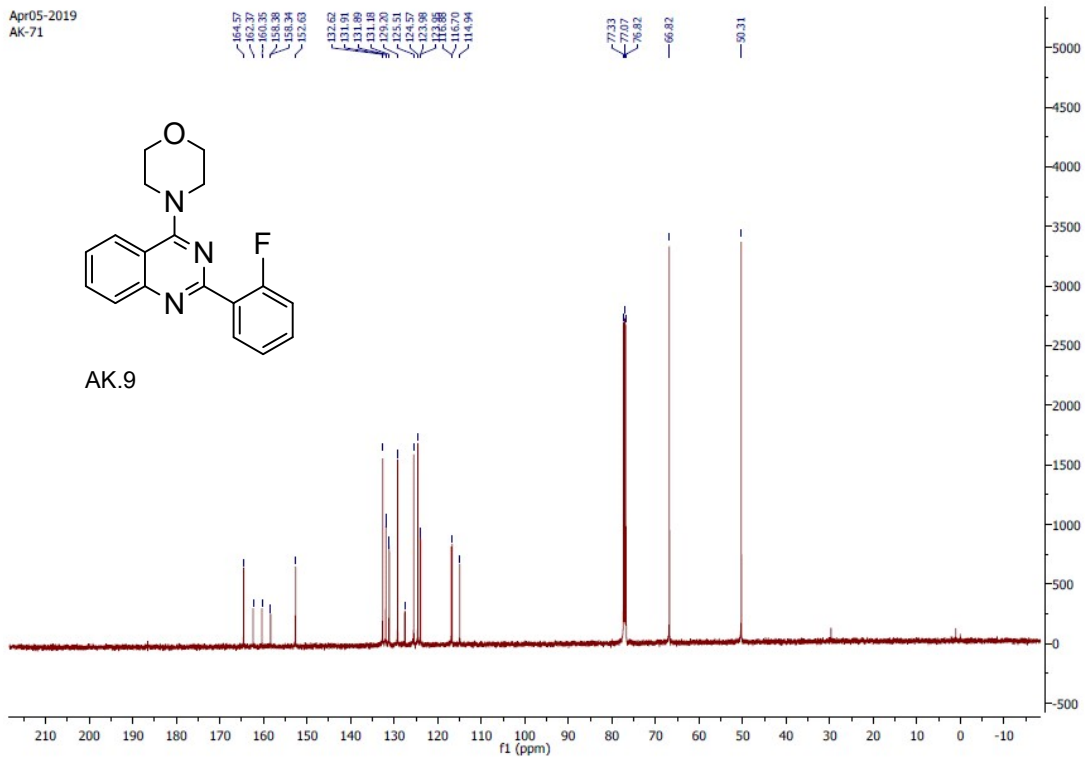


Figure 9. Spectras of compound AK-9

Single Mass Analysis

Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

21 formula(e) evaluated with 6 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 20-21 H: 0-300 N: 0-4 O: 0-2

Sample Name : 280921\_AK-10

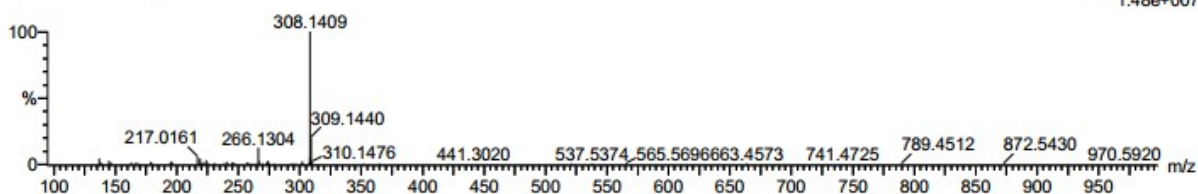
IITRPR

XEVO G2-XS QTOF

Test Name :

280921\_AK-10 20 (0.435)

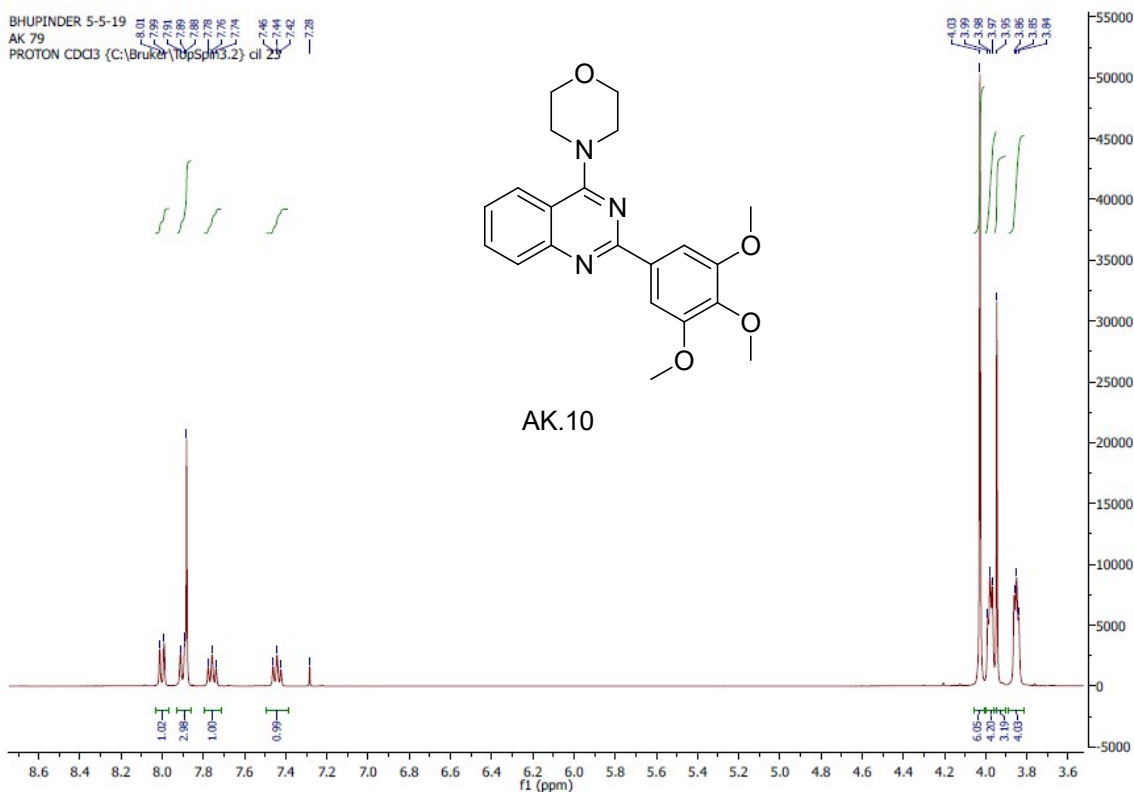
1: TOF MS ES+  
1.48e+007

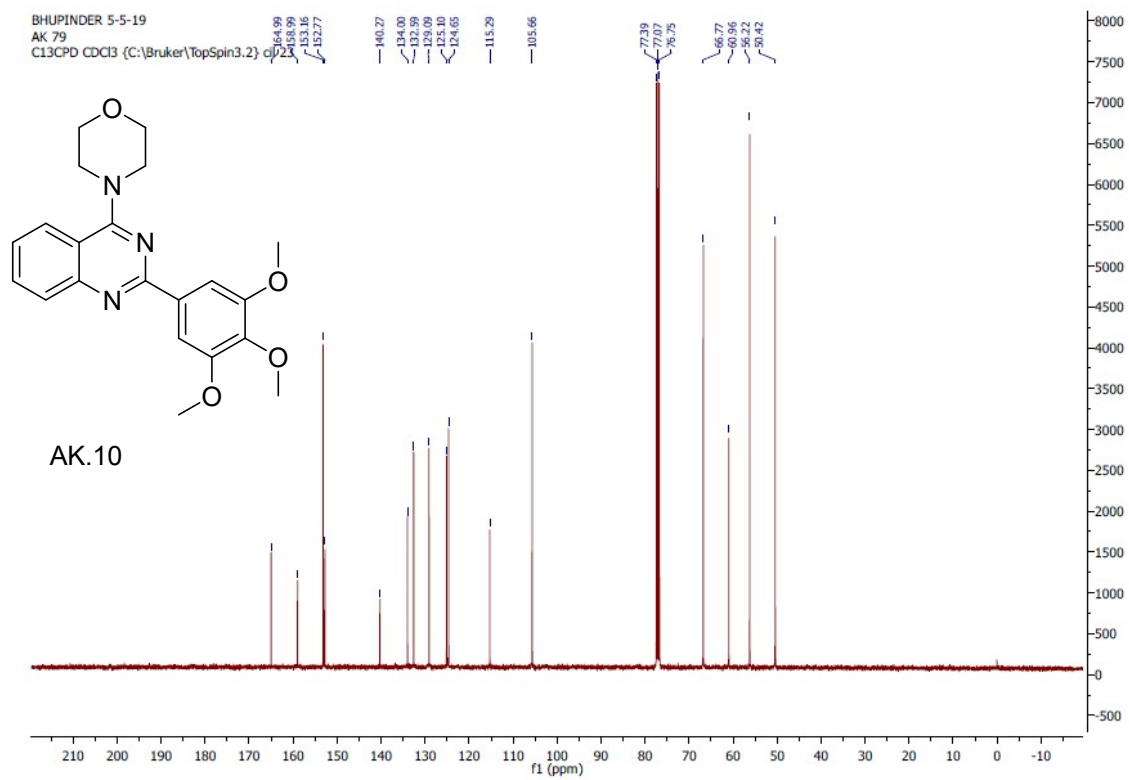


Minimum: -1.5  
 Maximum: 2.0 300.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
308.1409	308.1188	22.1	71.7	16.5	1567.9	2.578	7.60	C21 H14 N3
	308.1651	-24.2	-78.5	10.5	1566.7	1.401	24.65	C20 H22 N O2
	308.0824	58.5	189.8	17.5	1566.7	1.427	24.00	C20 H10 N3 O
	308.2014	-60.5	-196.3	9.5	1567.6	2.309	9.94	C21 H26 N O
	308.0712	69.7	226.2	17.5	1568.1	2.829	5.91	C21 H10 N O2

BHUPINDER 5-5-19  
 AK 79  
 PROTON CDCl3 (C:\Bruker\TopSpin3.2) d1 25





**Figure 10.** Spectras of compound AK-10

Elemental Composition Report

Single Mass Analysis

Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

40 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 18-18 H: 0-300 N: 0-4 O: 0-1 Cl: 0-1 F: 0-1

Sample Name : 280921\_AK-11

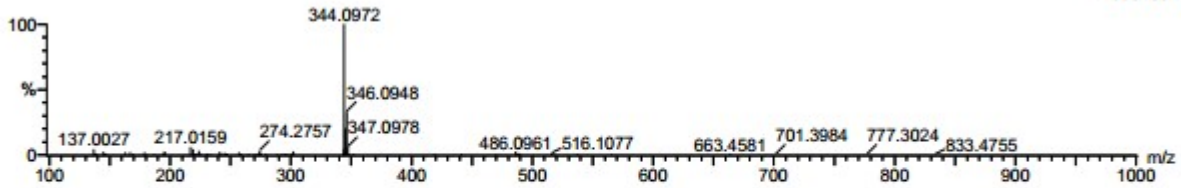
IITRPR

XEVO G2-XS QTOF

Test Name :

280921\_AK-11 22 (0.480)

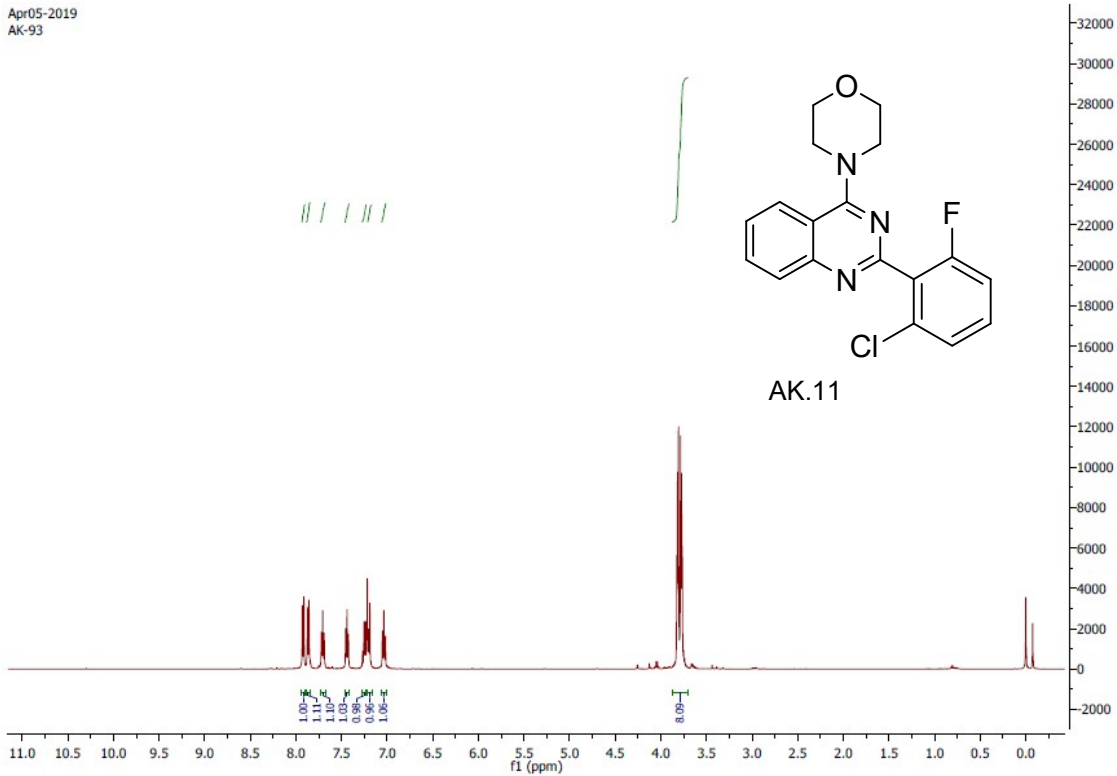
1: TOF MS ES+  
1.33e+007

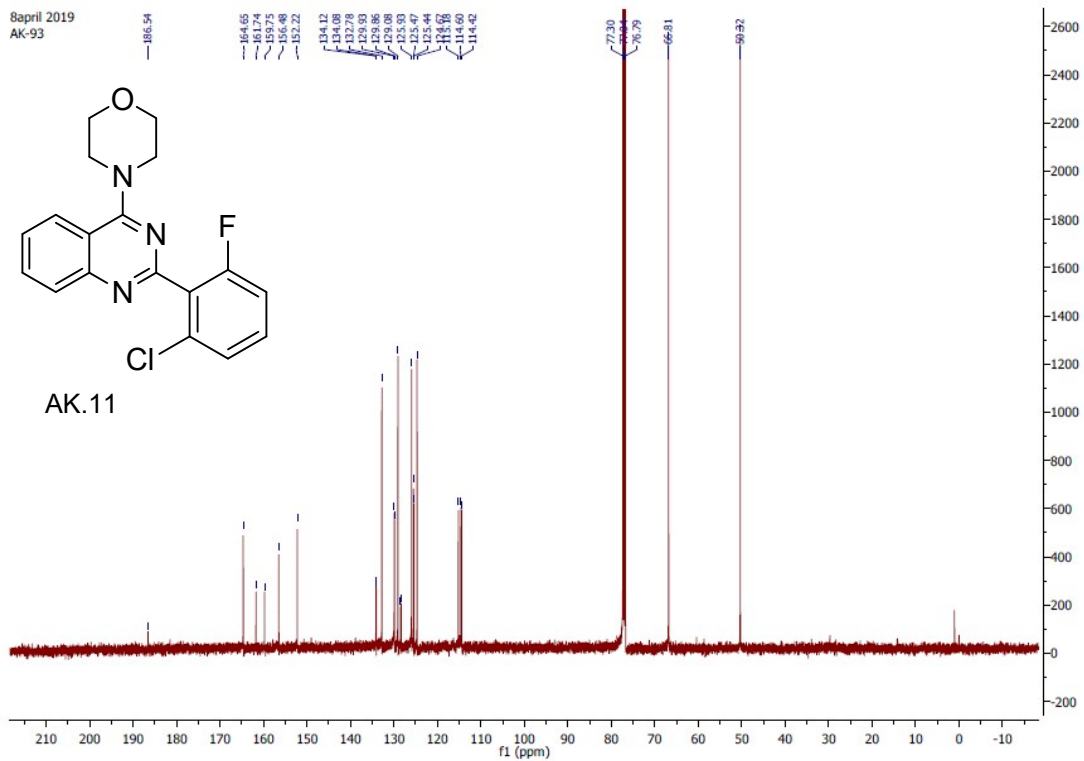


Minimum: -1.5  
Maximum: 2.0 300.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
344.0972	344.0966	0.6	1.7	11.5	1547.3	n/a	n/a	C18 H16 N3 O Cl F

Apr05-2019  
AK-93





**Figure 11.** Spectras of compound AK-11

# Elemental Composition Report

## Single Mass Analysis

Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

10 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 19-19 H: 0-300 N: 0-4 O: 0-1

Sample Name : 280921\_AK-12

IITRPR

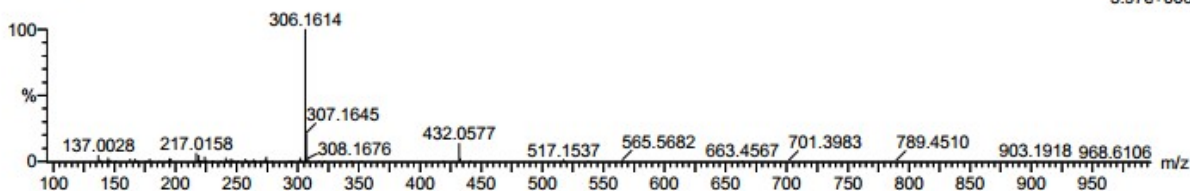
XEVO G2-XS QTOF

Test Name :

280921\_AK-12 22 (0.480)

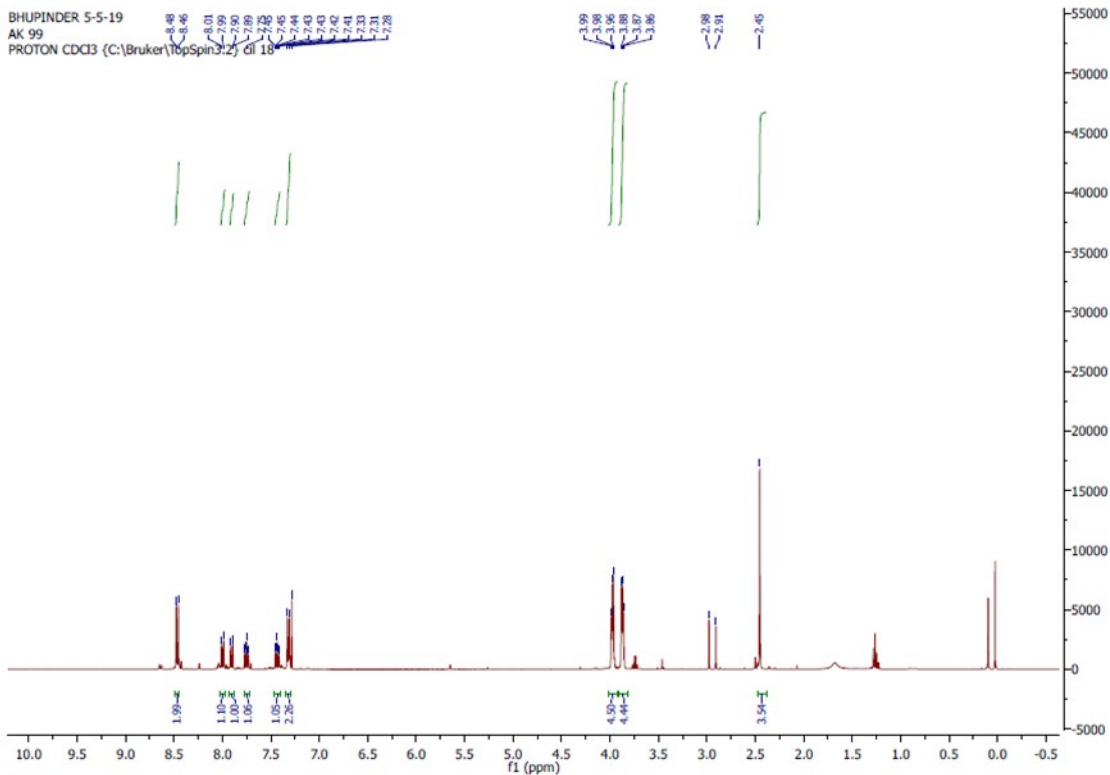
1: TOF MS ES+

5.97e+006



Minimum: -1.5  
Maximum: 2.0 300.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
306.1614	306.1606	0.8	2.6	11.5	1385.2	n/a	n/a	C19 H20 N3 O



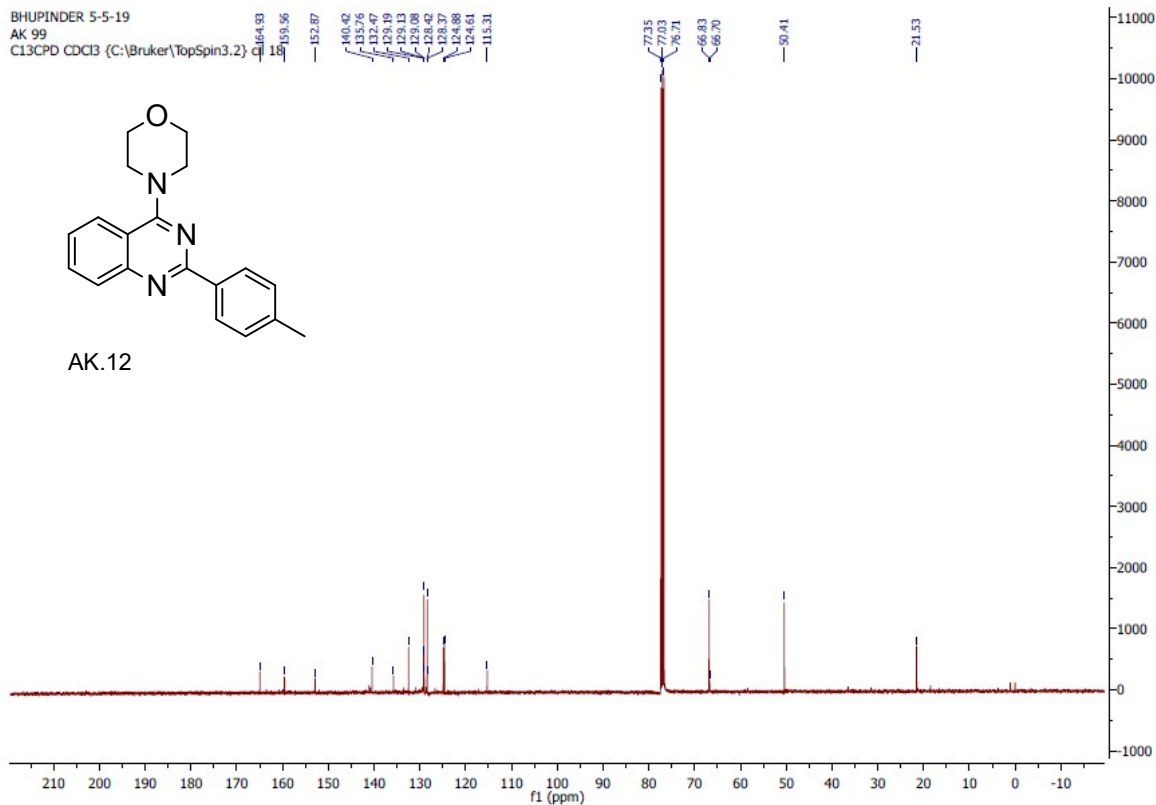


Figure 12. Spectras of compound AK-12

Elemental Composition Report

Single Mass Analysis

Tolerance = 300.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

32 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 19-19 H: 0-300 N: 0-3 O: 0-1 F: 0-3

Sample Name : 280921\_AK-13

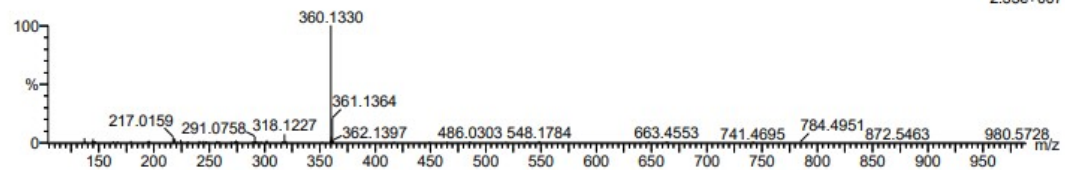
IITRPR

XEVO G2-XS QTOF

Test Name :

280921\_AK-13 15 (0.328)

1: TOF MS ES+  
2.35e+007



Minimum: -1.5  
Maximum: 2.0 300.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
360.1330	360.1324	0.6	1.7	11.5	1624.3	n/a	n/a	C19 H17 N3 O F3



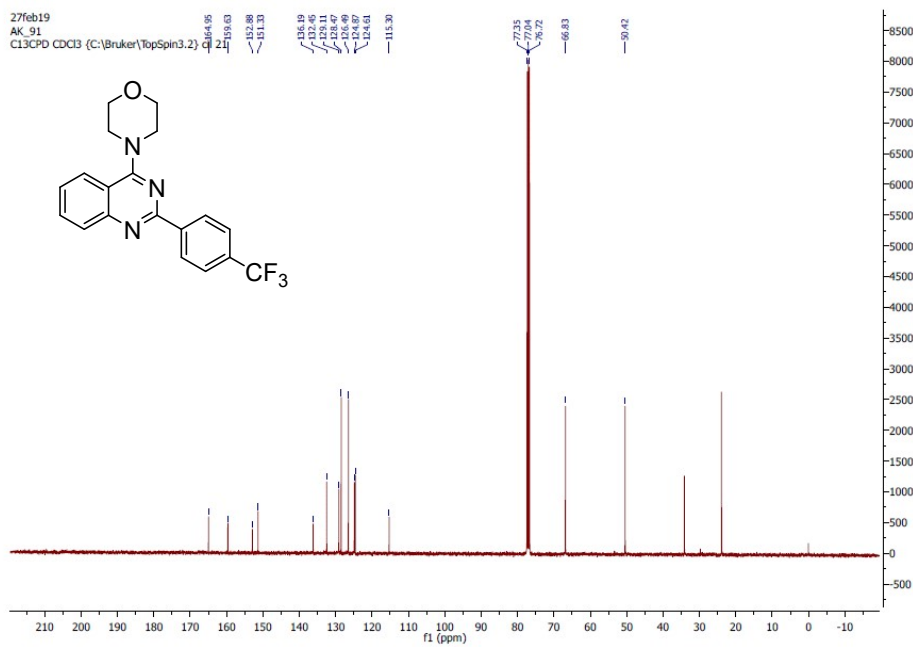
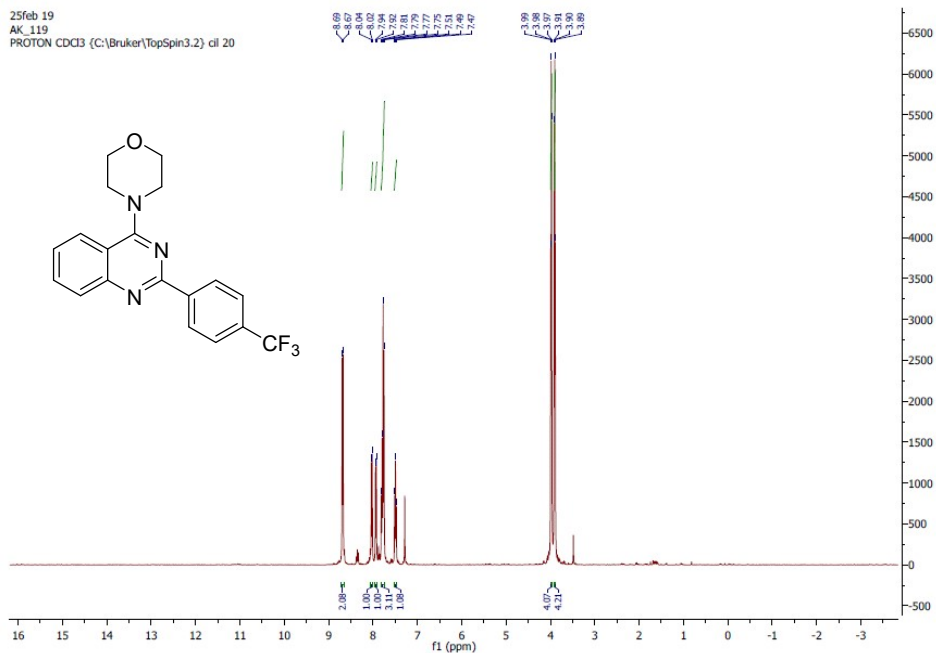


Figure 13. Spectras of compound AK-13

## DOCKING

**CDK-4**- PDB-ID: - 2W96

Coordinates for 2W96 binding site:  $x = -3.12, y = -3.92, z = 85.1$

No docking poses were generated.

**BAX**- PDB-ID: - 4S00

Coordinates for 2W96 binding site:  $x = 11.89, y = 7.0, z = 31.62$

Sr. No.	Compound	Docking score
1	AK-10	-2.380
2	AK-3	-1.207

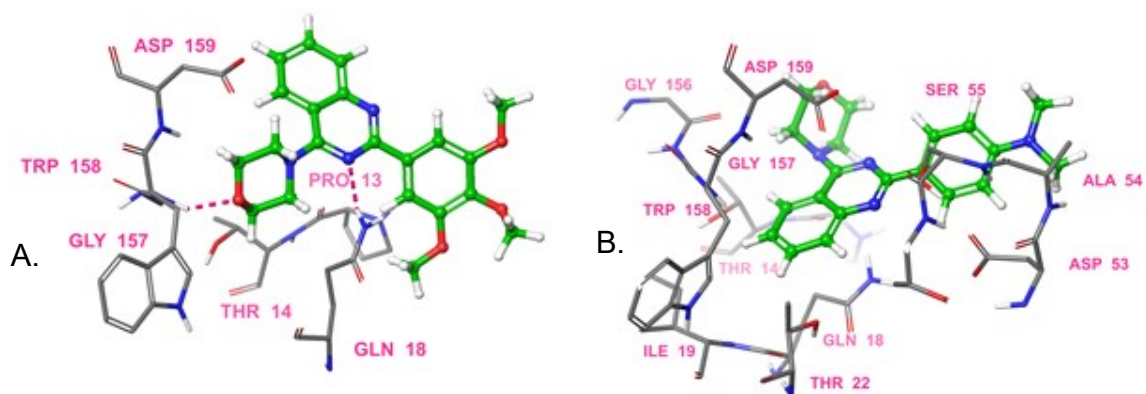


Figure 14: Docking pose of AK-3 (A) and AK-10 (B) with **BAX**- PDB-ID: 4S00

**BCL-XL**- PDB-ID: - 6VWC

Coordinates for 2W96 binding site:  $x = 1.78, y = -4.03, z = 10.8$

Sr. No.	Compound	Docking score
1	AK-3	-7.042
2	AK-10	-6.965

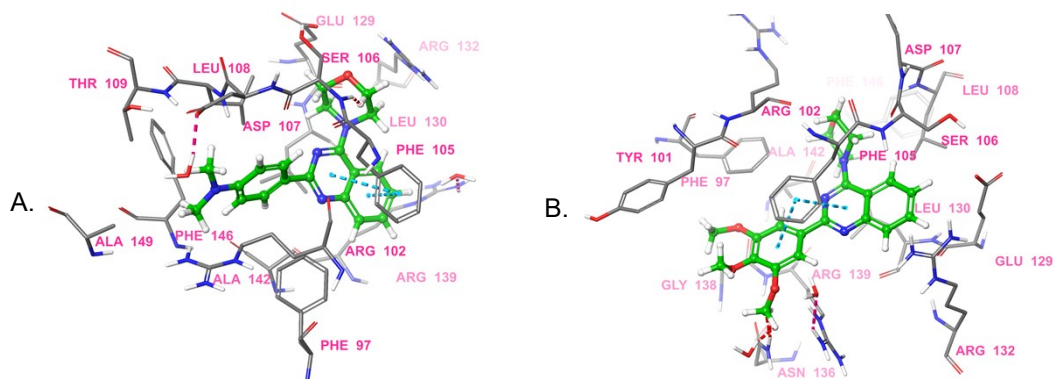


Figure 15: Docking pose of AK-3 (A) and AK-10 (B) with **BCL-XL**- PDB-ID: 6VWC

**Table 1: R SQUARED VALUES**

Compound	R <sup>2</sup>			
	A549	MCF7	SHSY	HEK
AK-1	0.9797	0.9335	1	NA
AK-2	1	0.9279	0.9941	NA
AK-3	0.8641	0.952	0.8162	0.785
AK-4	1	0.9273	0.9762	NA
AK-5	0.9619	0.9934	0.9478	0.9692
AK-6	0.9918	0.945	0.9063	NA
AK-7	0.9975	0.9816	0.9273	NA
AK-8	0.9661	0.964	0.2599	NA
AK-9	0.9771	0.9362	0.705	0.899
AK-10	0.9862	0.9821	0.9978	0.9781
AK-11	0.9761	0.9074	0.945	NA
AK-12	0.9856	0.9696	0.9613	NA
AK-13	0.994	0.9842	0.9974	0.8906
COLCHICINE	0.9887	0.9753	0.9999	0.9097

