

Supplementary Material

Greener route for the synthesis of chromone using Amberlyst®15 via enaminones

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^cDepartment of Chemistry, Faculty of Science of Technology, ICFI Foundation for Higher Education,
Dontanpally,

Hyderabad-501203, Telangana, India

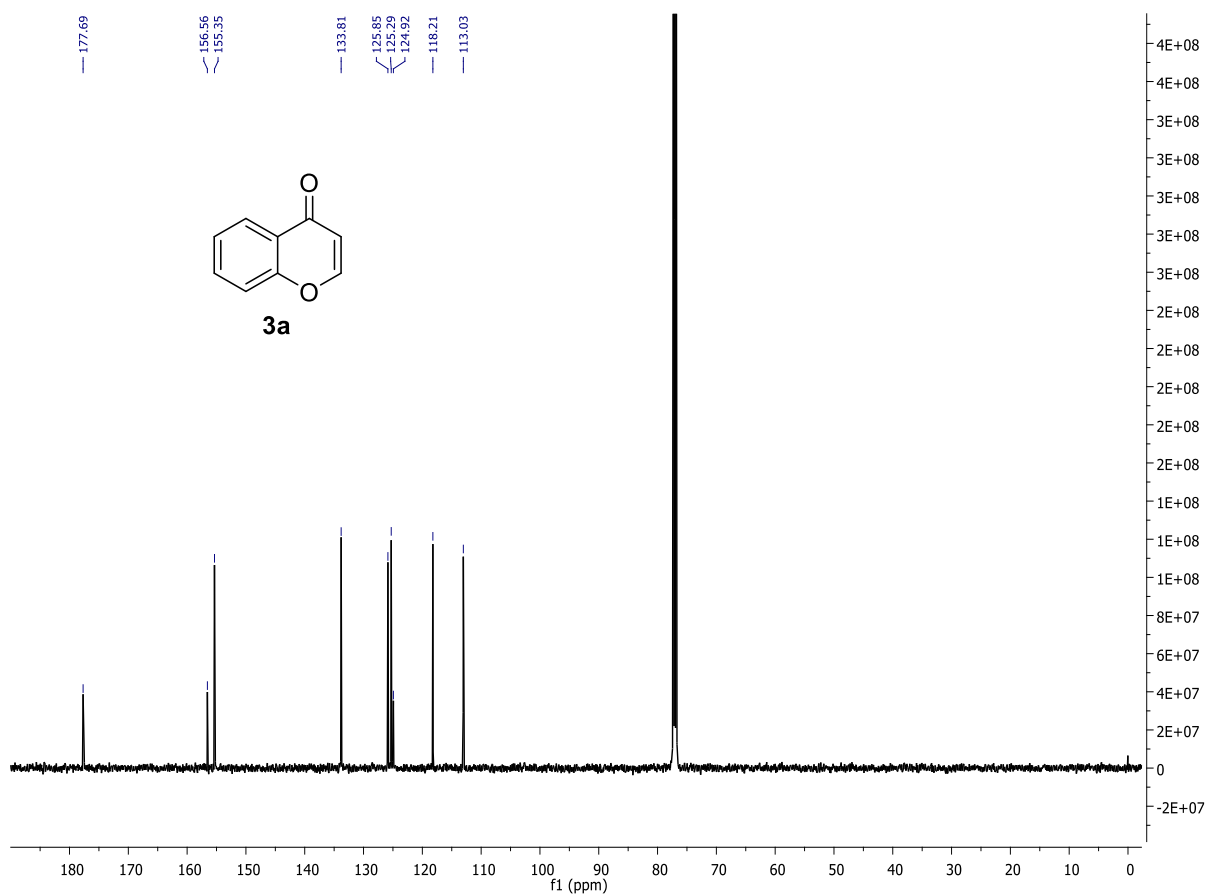
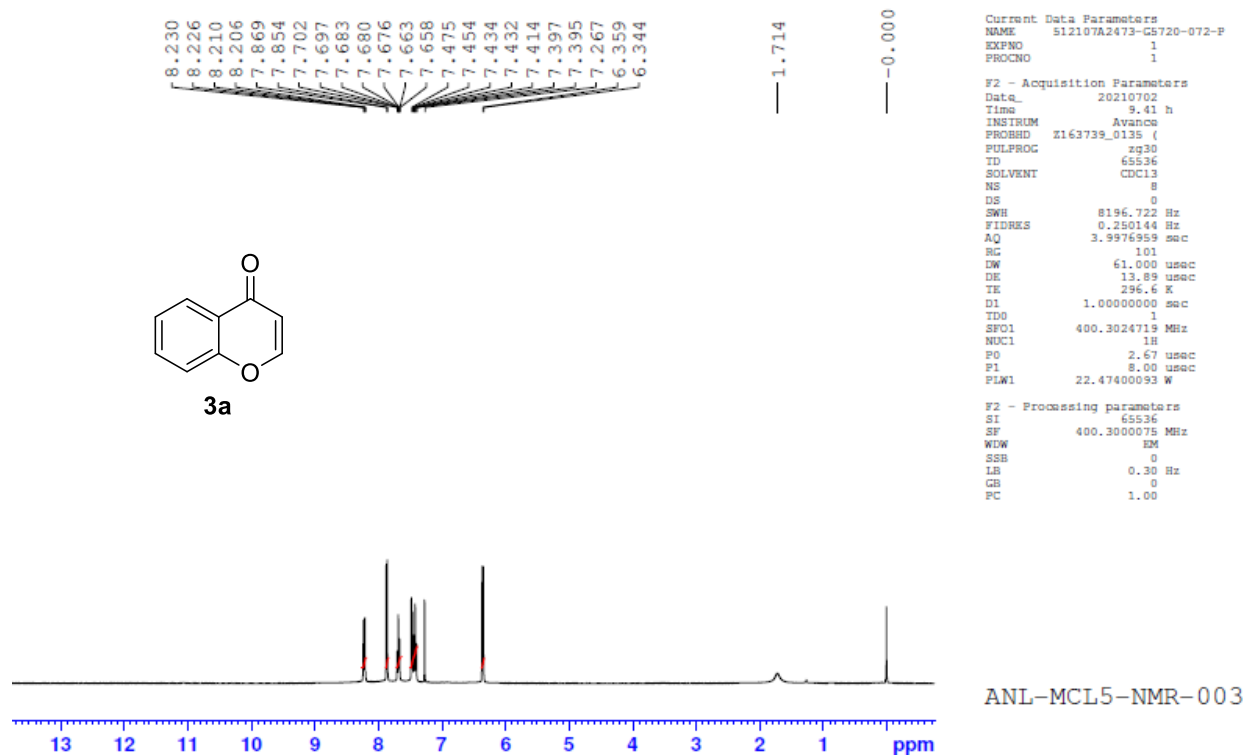
E-mail: Manoranjan.behera@aragen.com

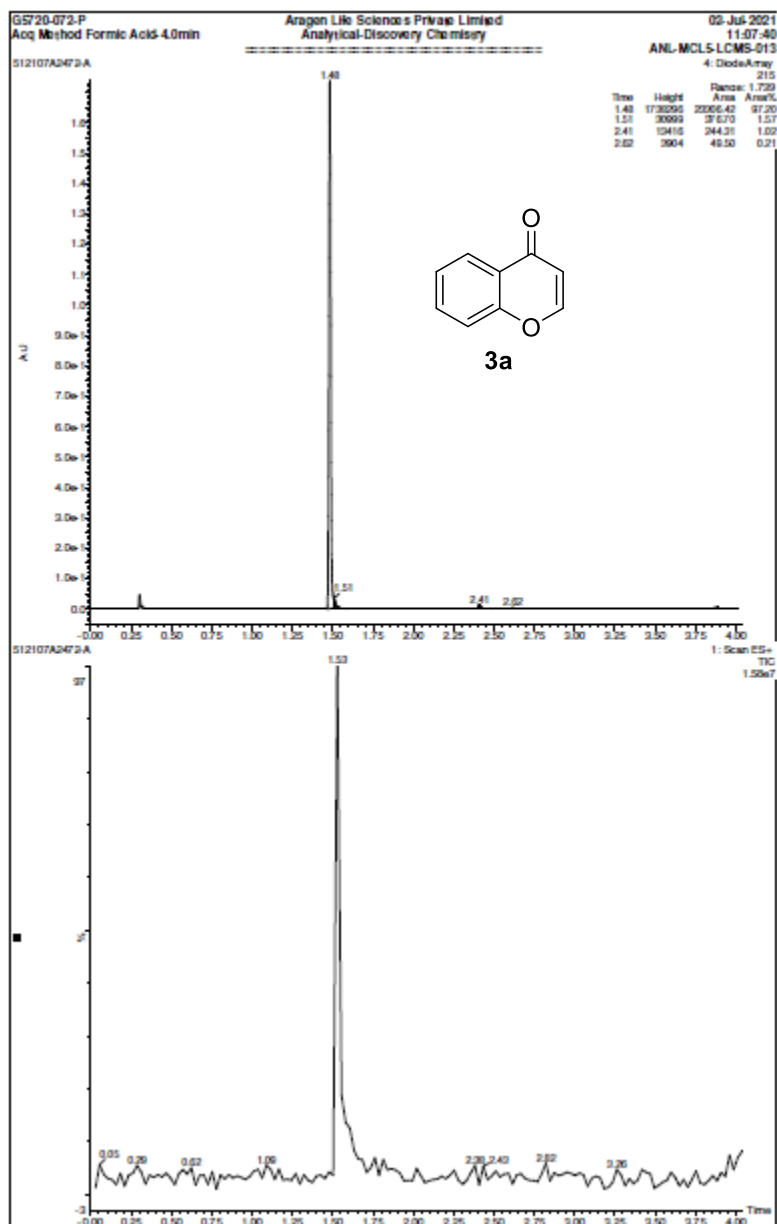
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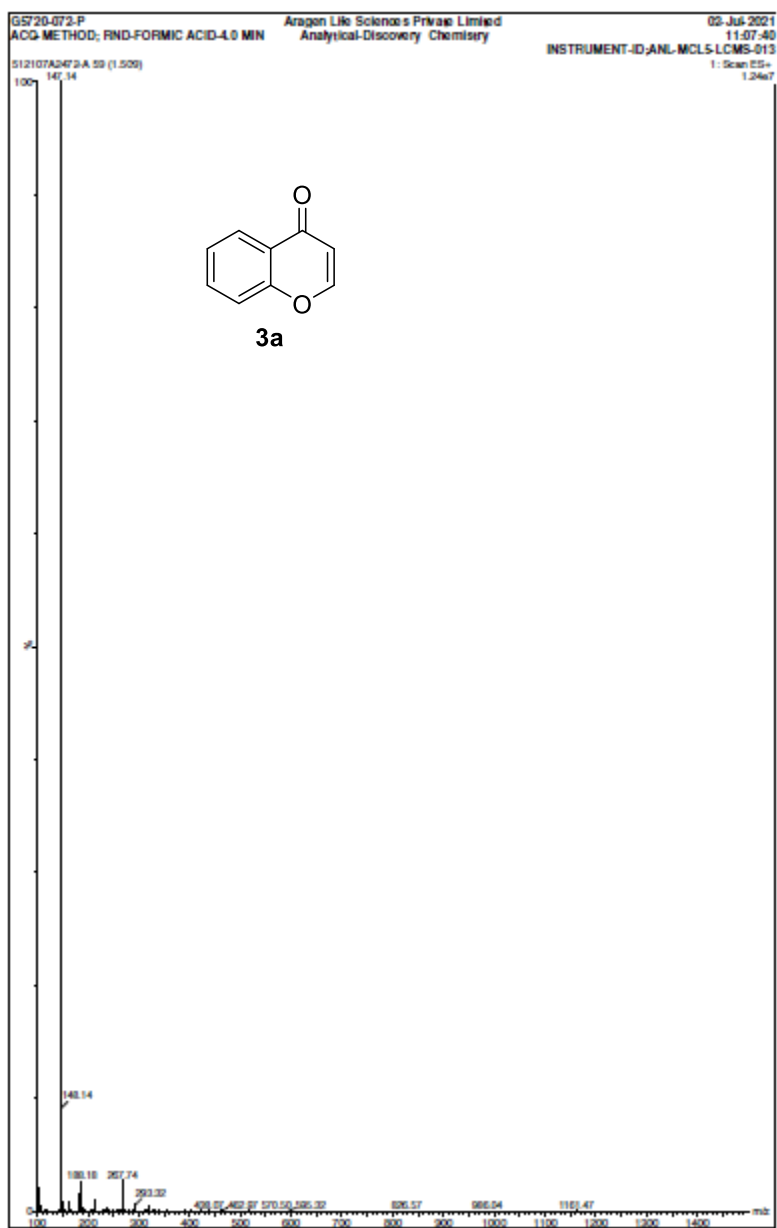
General.....	S2
Spectral data	S3

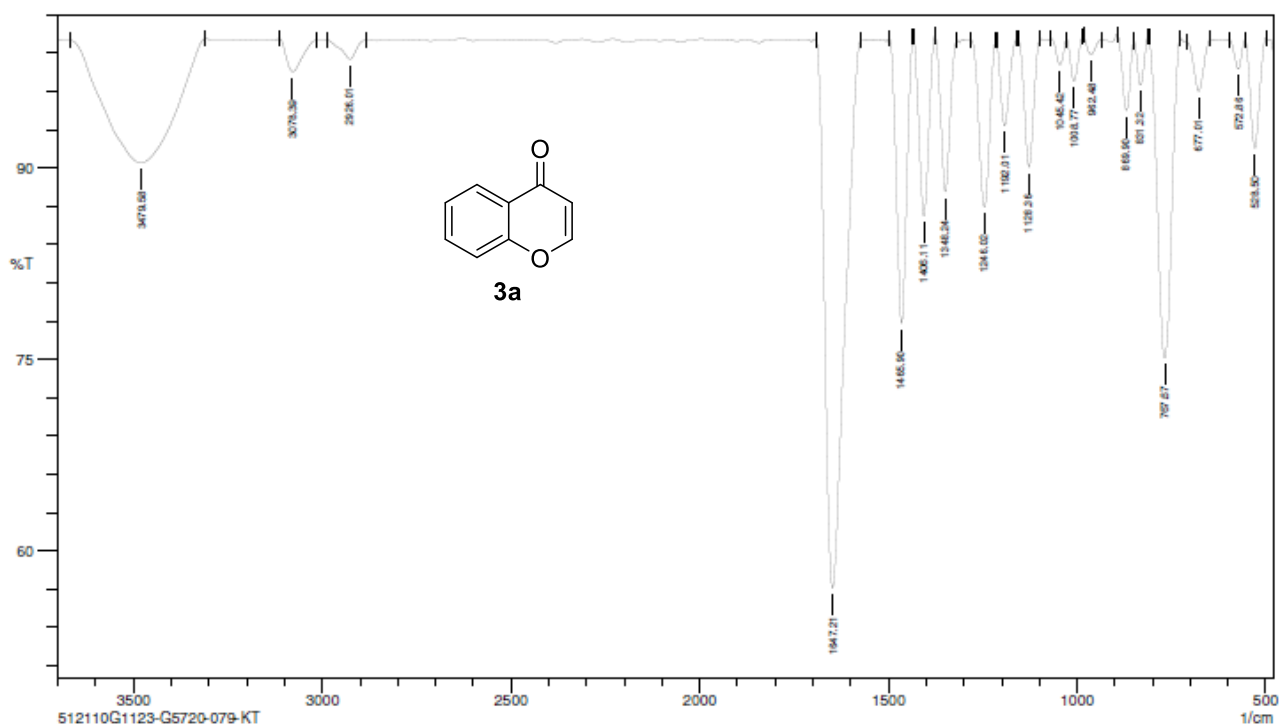
1. General

Dry solvents were purchased from chemical suppliers and used without further purification. Analytical thin-layer chromatography (TLC) was performed on commercially available Merck TLC Silica gel 60 F₂₅₄. Silica gel column chromatography was performed on silica gel 60 (spherical 100-200 μm). IR spectra were recorded on Perkin-Elmer FT/IR-4000 using ATR. ^1H NMR spectra were recorded on Varian-400 (400 MHz) spectrometer. Chemical shifts of ^1H NMR spectra were reported relative to tetramethylsilane (^{13}C NMR spectra were recorded on Varian-400 (100 MHz) spectrometer. Chemical shifts of ^{13}C NMR spectra were reported relative to CDCl_3 (77.16) and DMSO-d_6 (39.5). Splitting patterns were reported as s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; br, broad.









Sample Name: 512110G1123-G5720-079-KT

No. of Scans:

Date/Time: 10/29/2021 7:49:52 PM

User: Aragen

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-9 H: 0-7 O: 0-2

512107A2472A 59 (1.509)

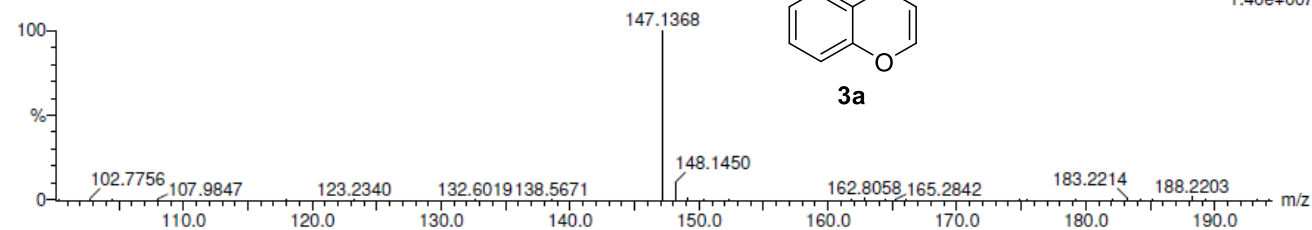
G5720-072-P

02-07-2021
Acq.method formic acid_4min

02-Jul-2021
10:08:29
INSTRUMENT-ID:ANL-MCL5-LCMS-013

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1.40e+007



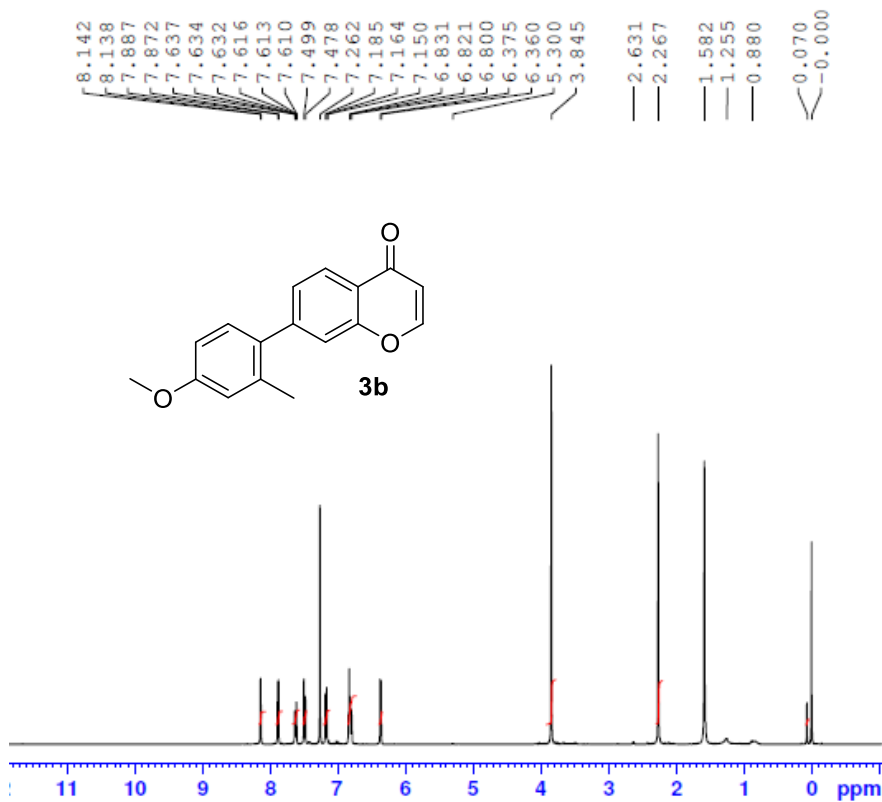
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5.0 1000.0 -1.5

Maximum:

-0.1 -0.7 6.5

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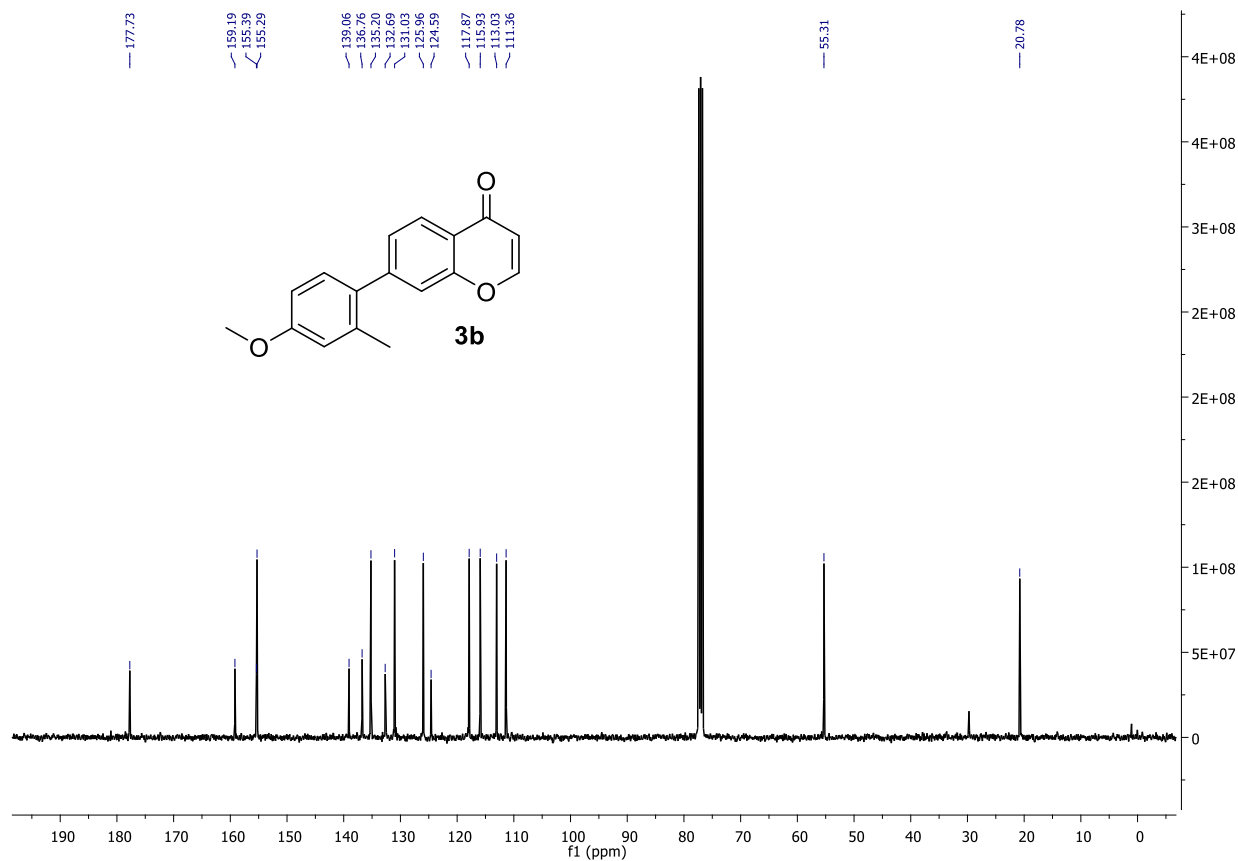
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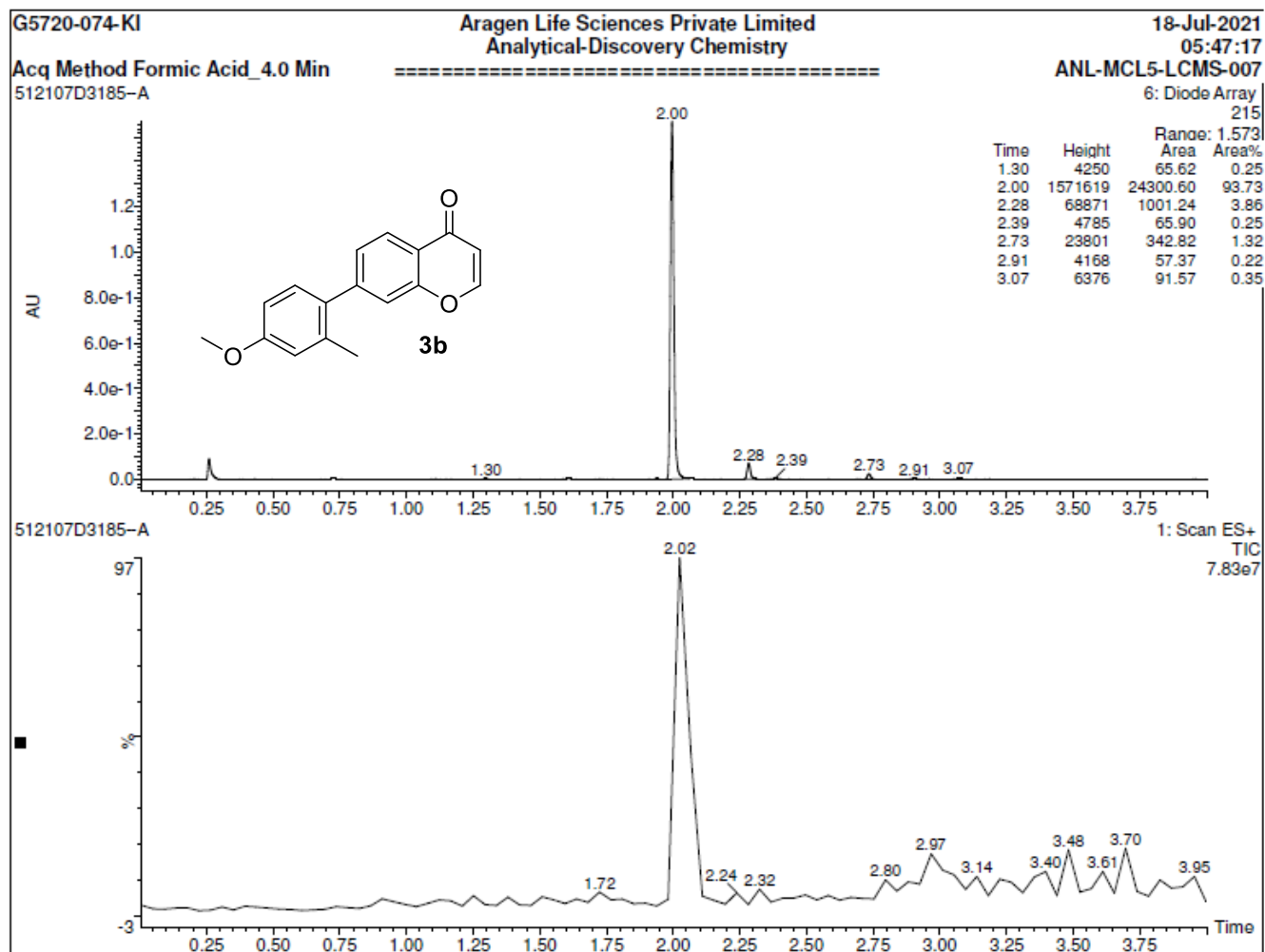
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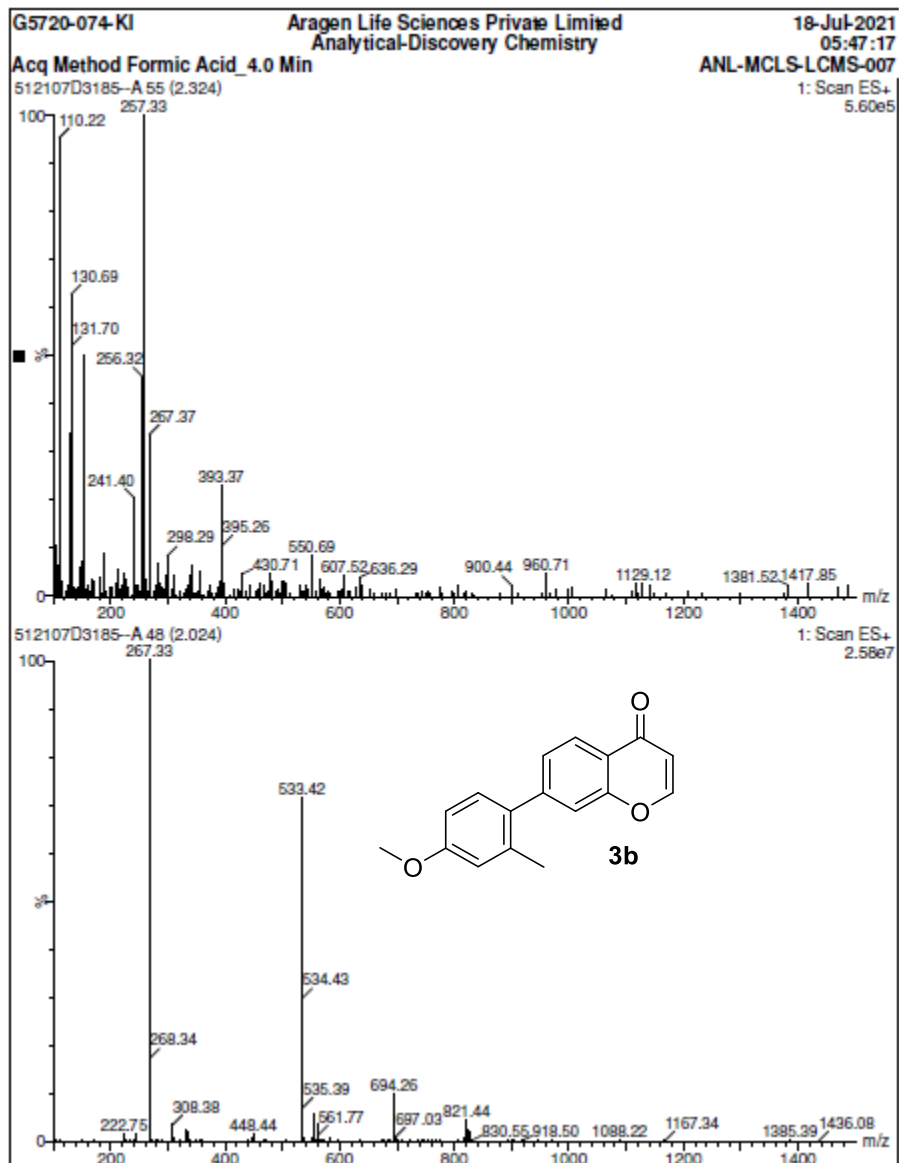
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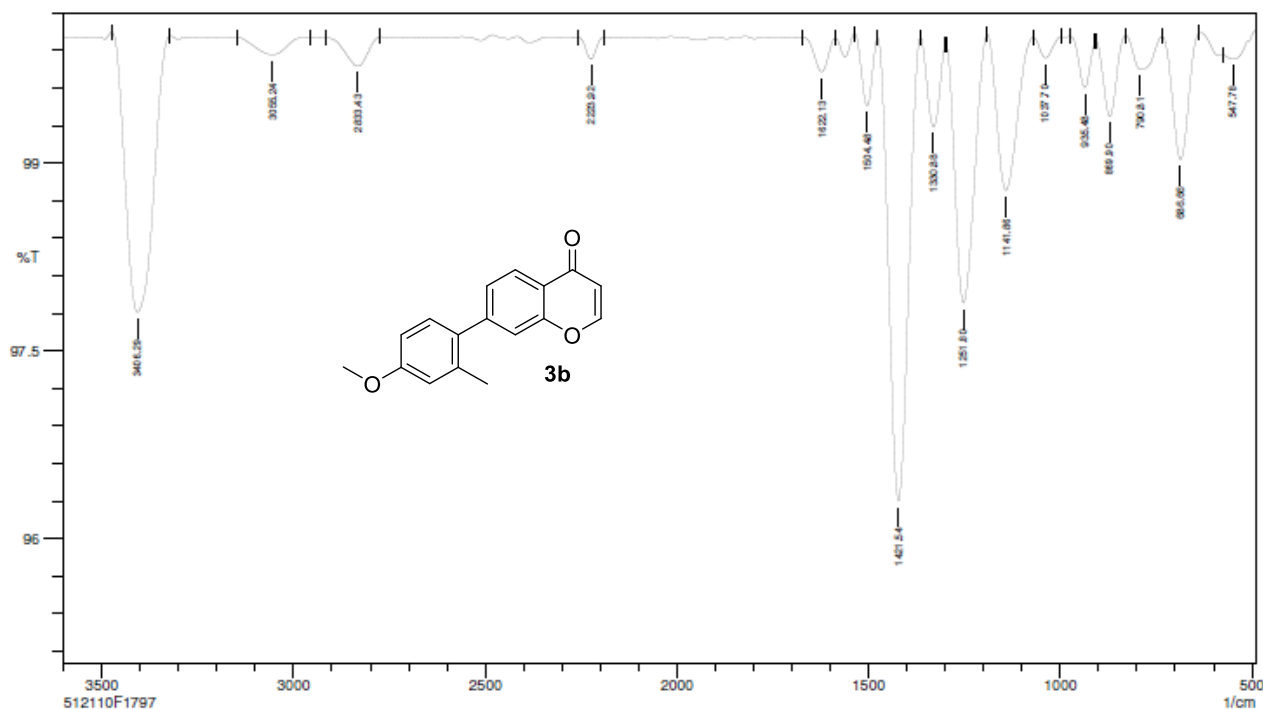
ANL-MCL5-NMR-004







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Analytical-Discovery Chemistry



Sample Name:
512110F1797

No. of Scans:

Date/Time: 10/26/2021 8:54:42 PM

User: Aragen

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

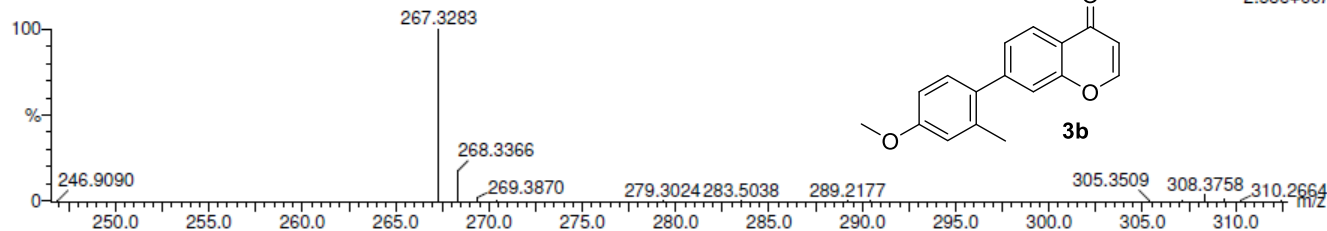
C: 0-17 H: 0-15 O: 0-3

G5720-074-KI

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512107D3185--A 48 (2.024)

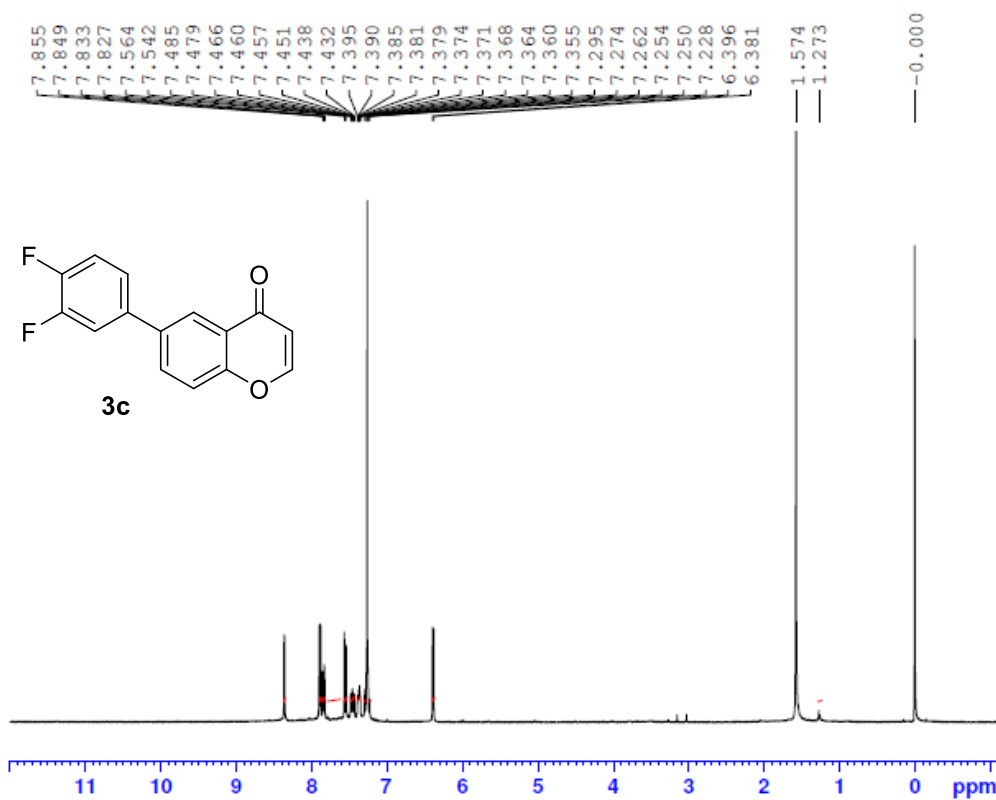
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry

18-Jul-2021
05:47:17
ANL-MCL5-LCMS-007
1: Scan ES+
2.58e+007



Minimum: -1.5
Maximum: 5.0 1000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
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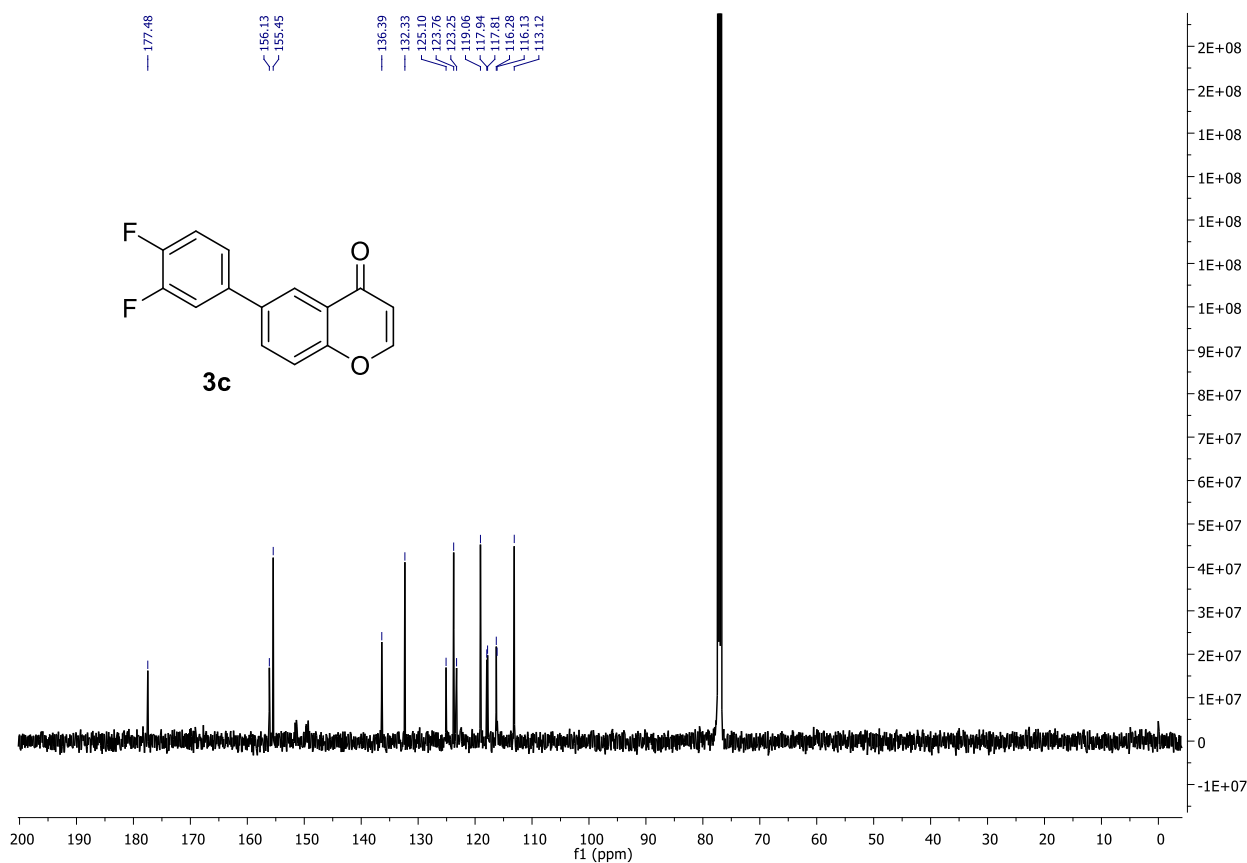
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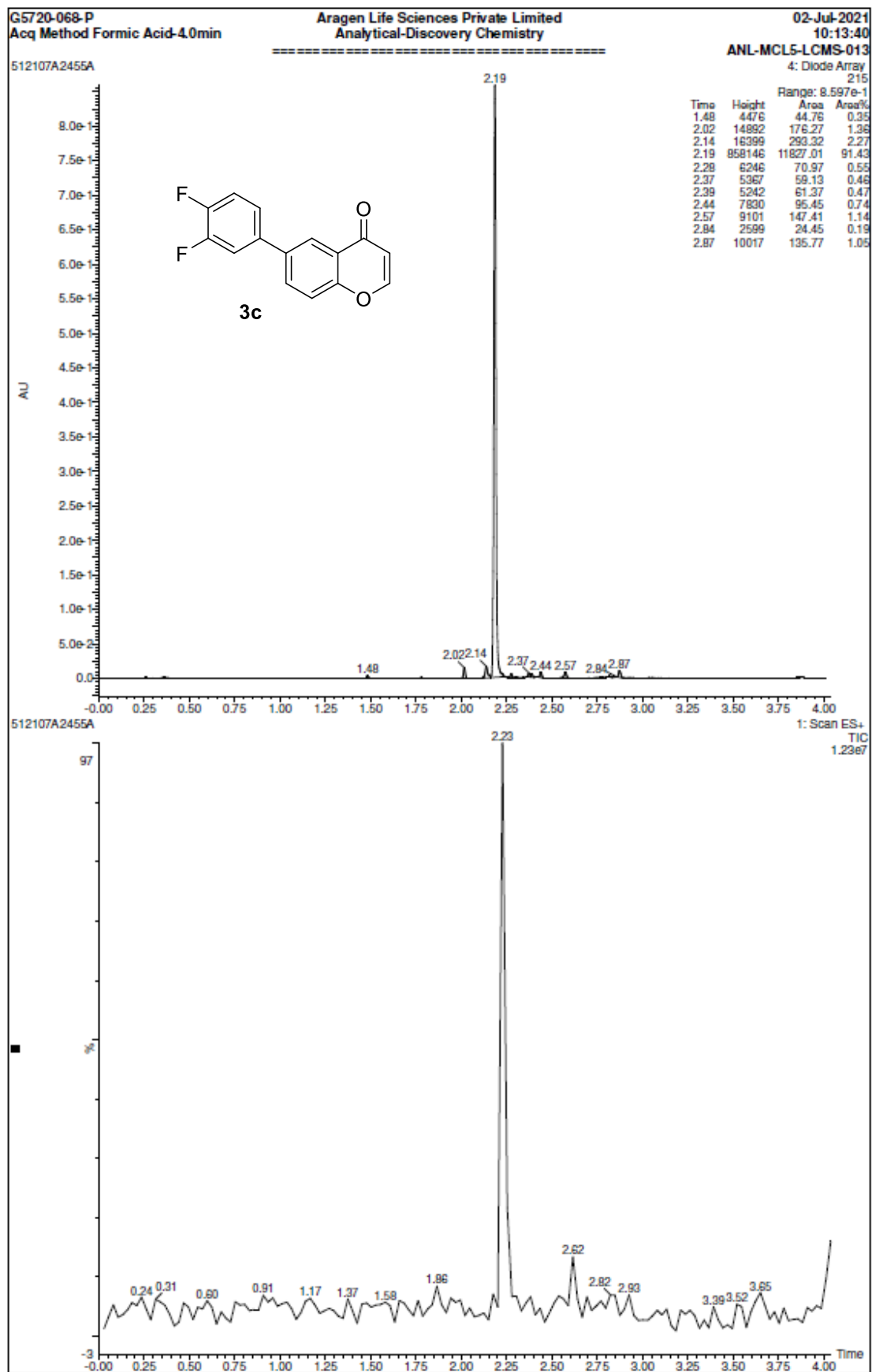
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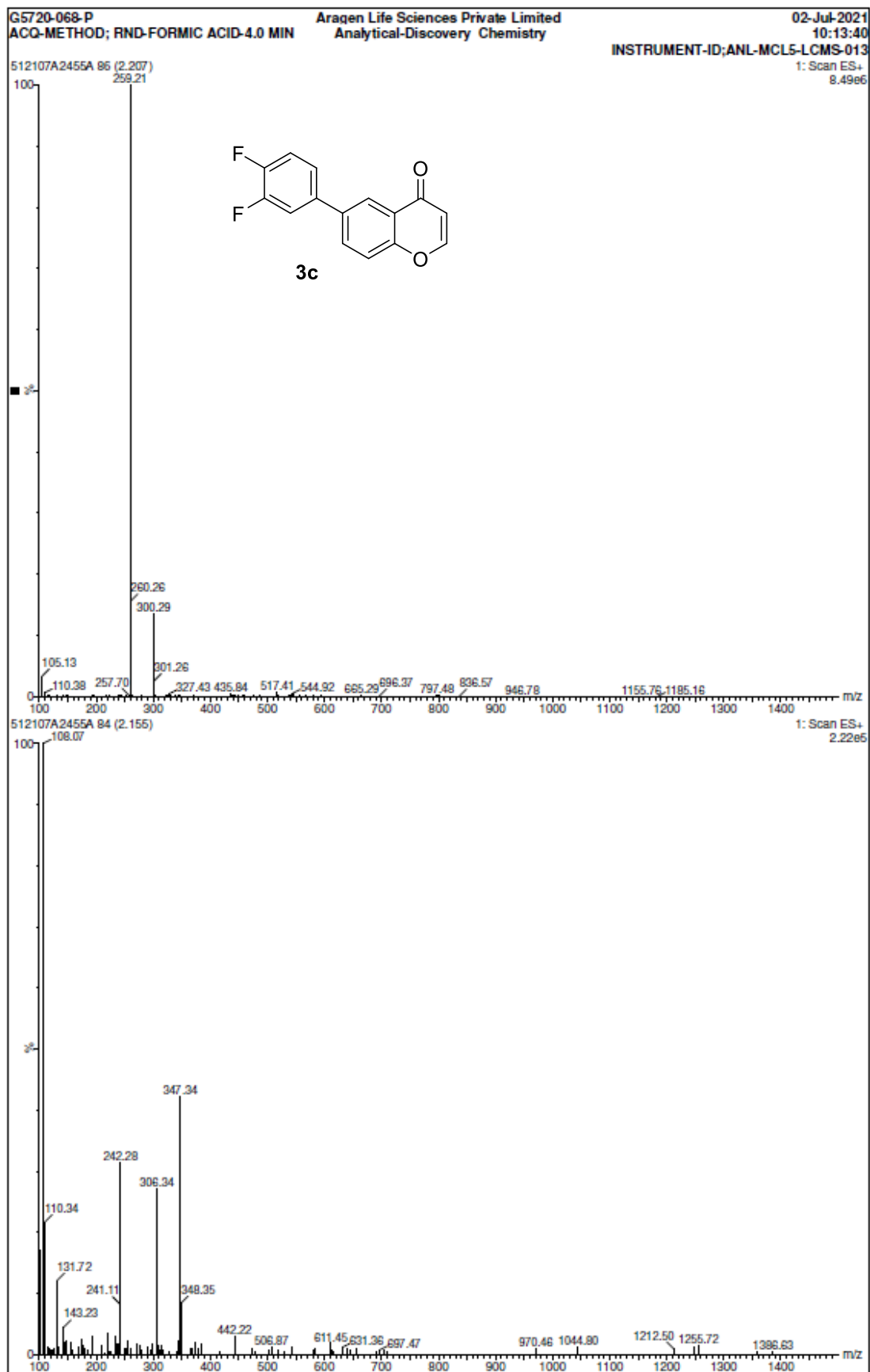
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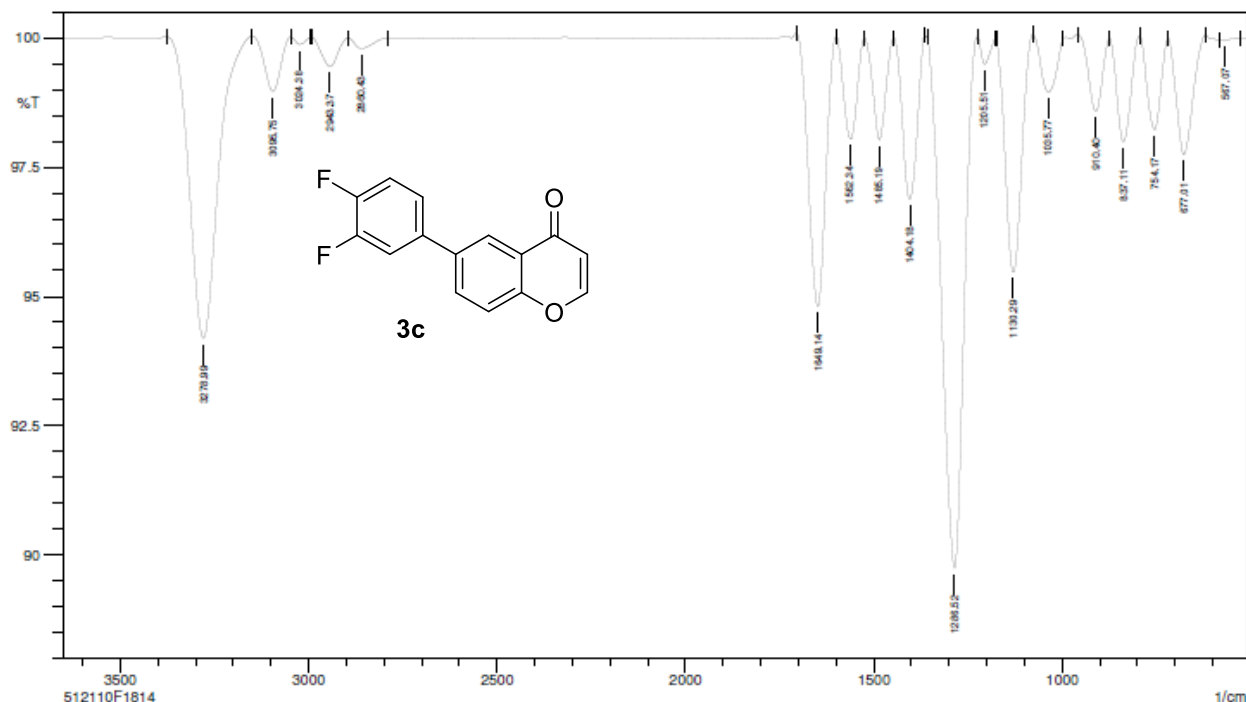
ANL-MCL5-NMR-003







Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry



Sample Name:
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No. of Scans:

Date/Time: 10/26/2021 9:20:09 PM

User: Aragen

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

7 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-15 H: 0-9 O: 0-2 F: 0-2

512107A2455A 86 (2.207)

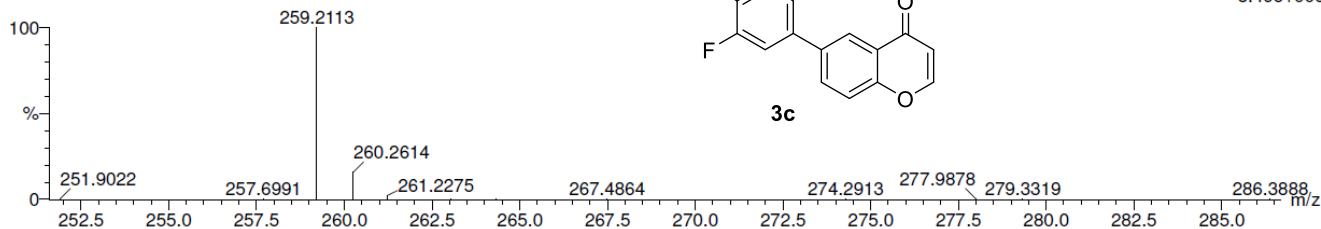
G5720-068-P

02-07-2021
Acq.method formic acid_4min

02-Jul-2021
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INSTRUMENT-ID;ANL-MCL5-LCMS-013

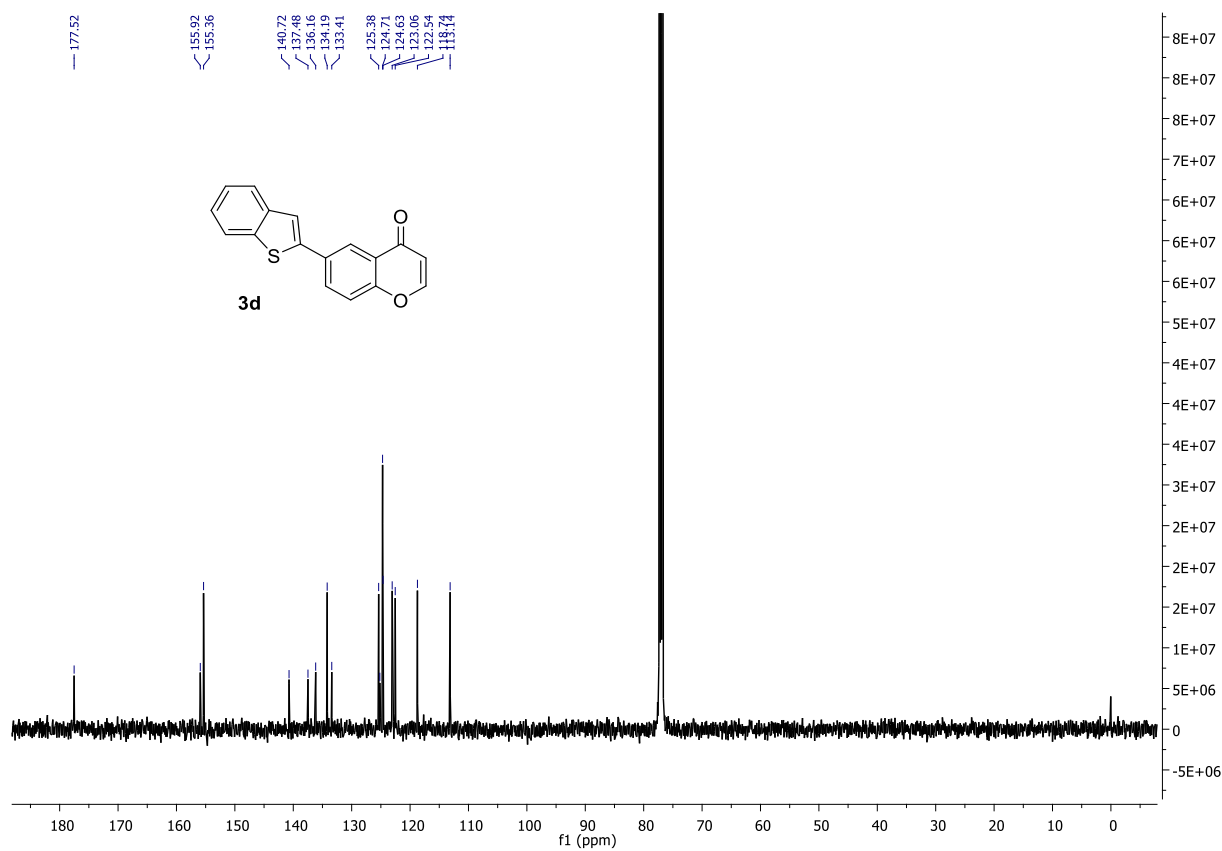
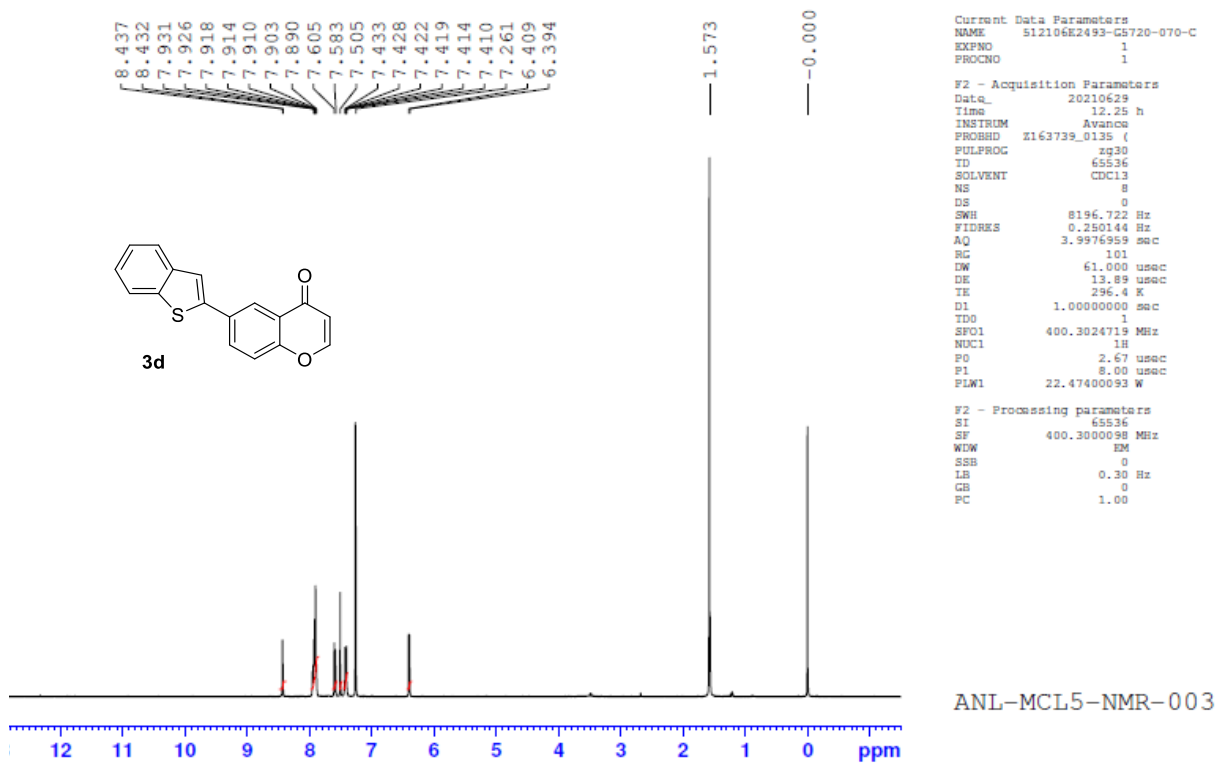
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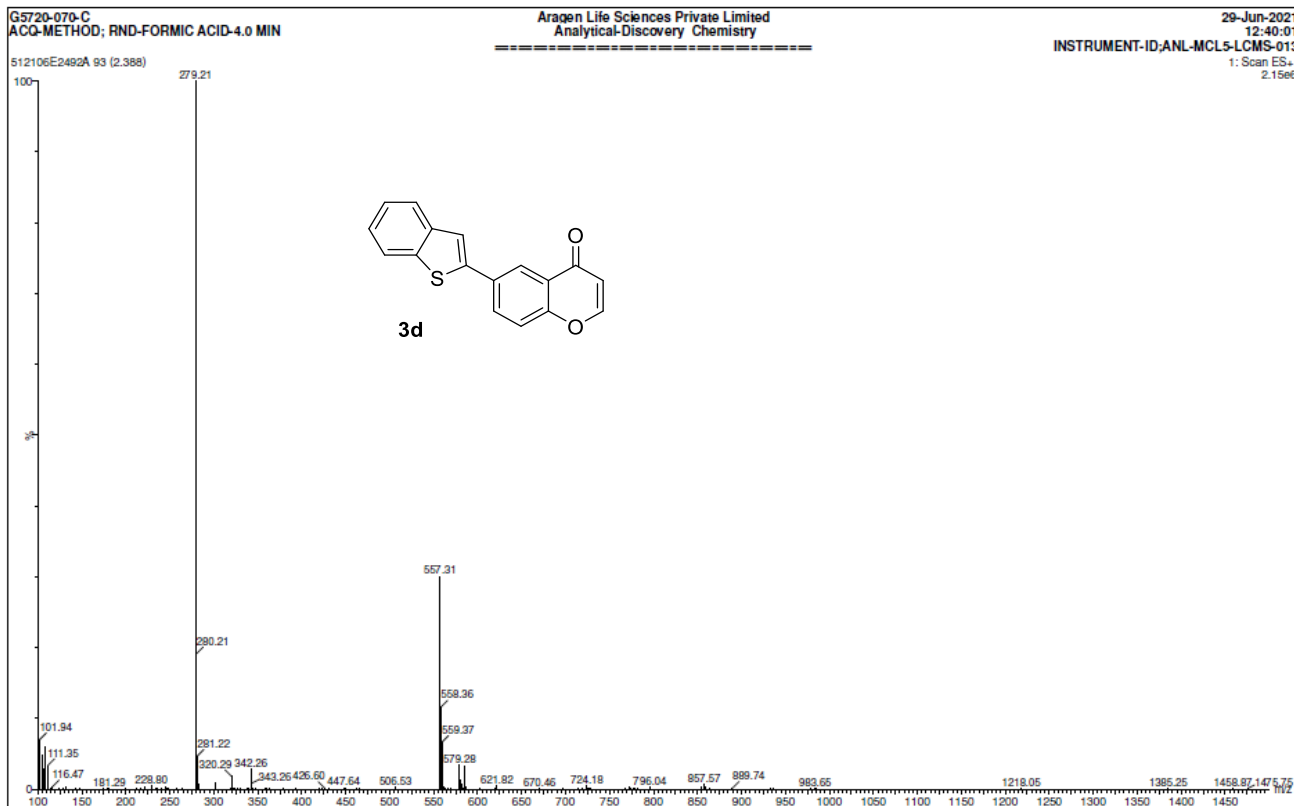
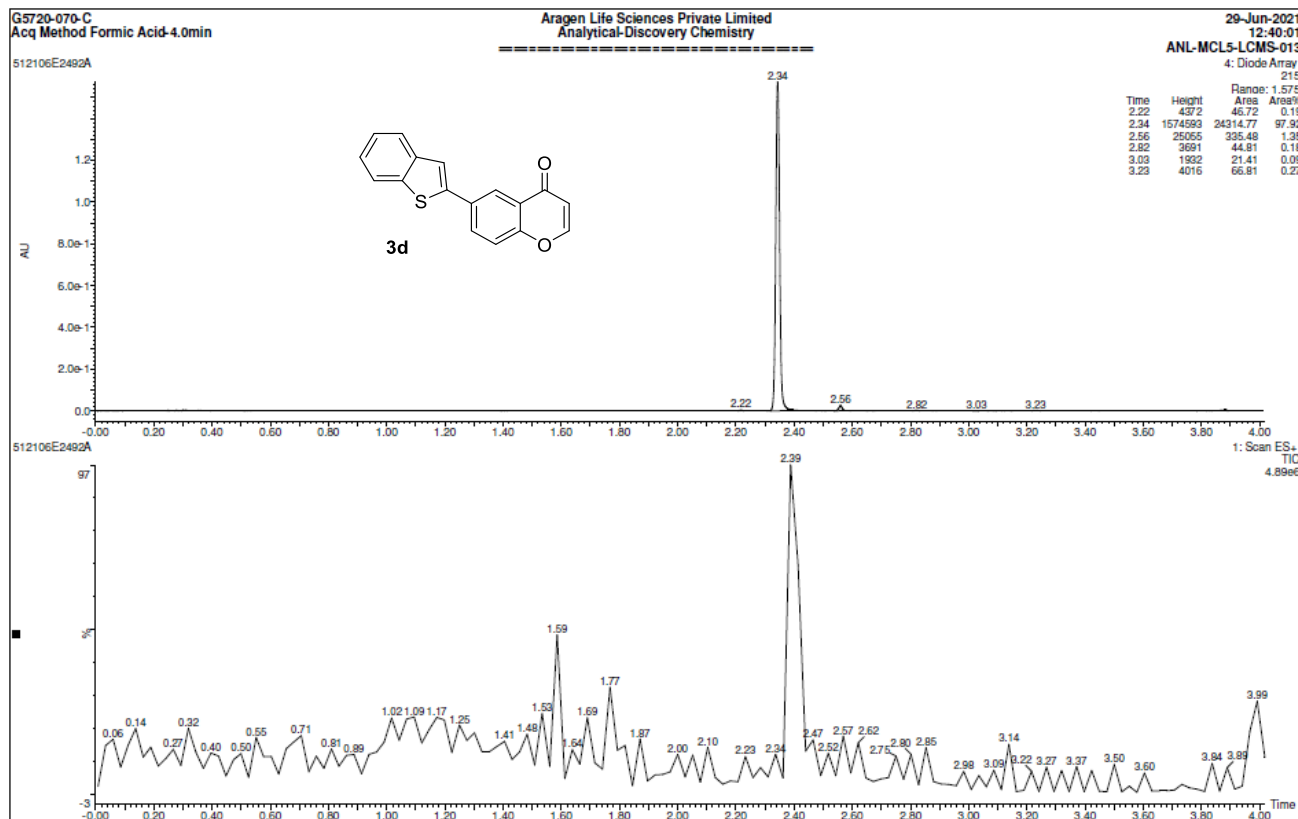
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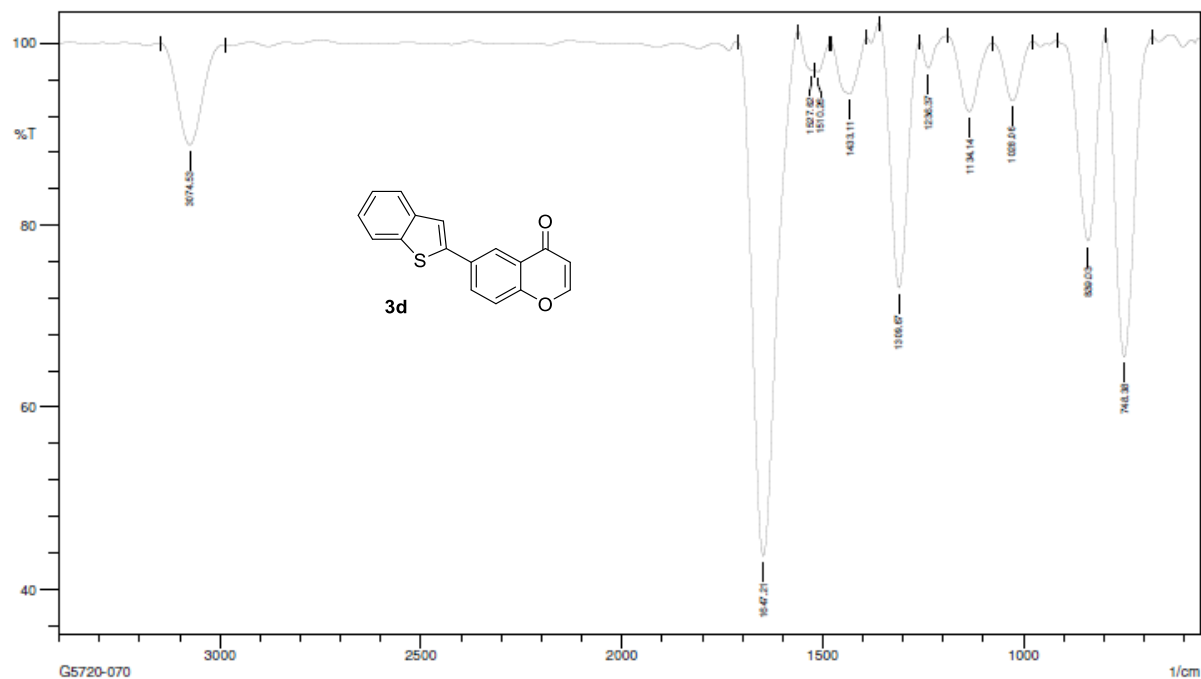


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
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Analytical-Discovery ChemistrySample Name:
G5720-070

No. of Scans:

Date/Time: 7/30/2021 3:15:43 PM

User: Aragen

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

3 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-17 H: 0-11 O: 0-2 S: 0-1

G5583-070-C

Acq.method formic acid_4min

Aragene Life sciences Private Limited
Analytical Discovery Chemistry

06-Dec-2021

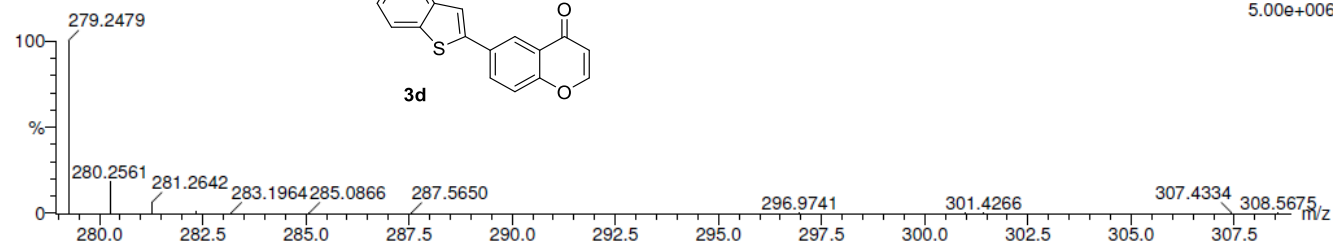
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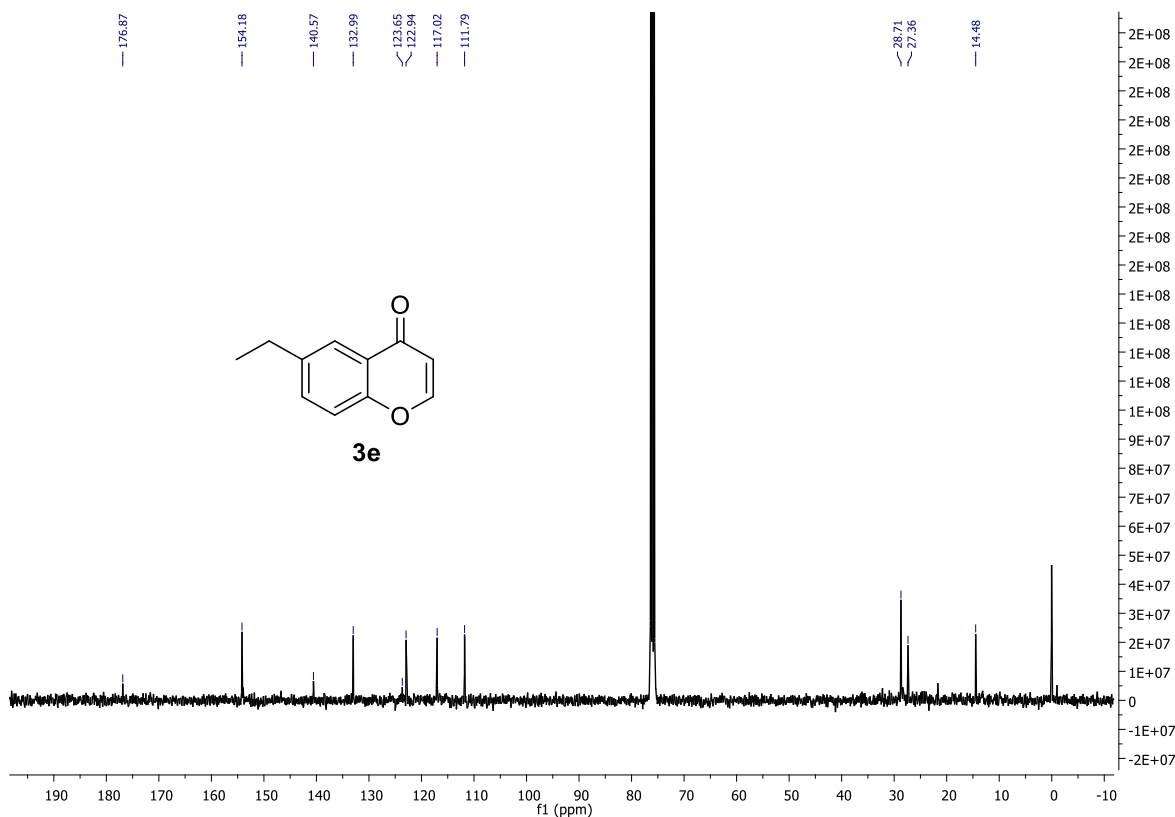
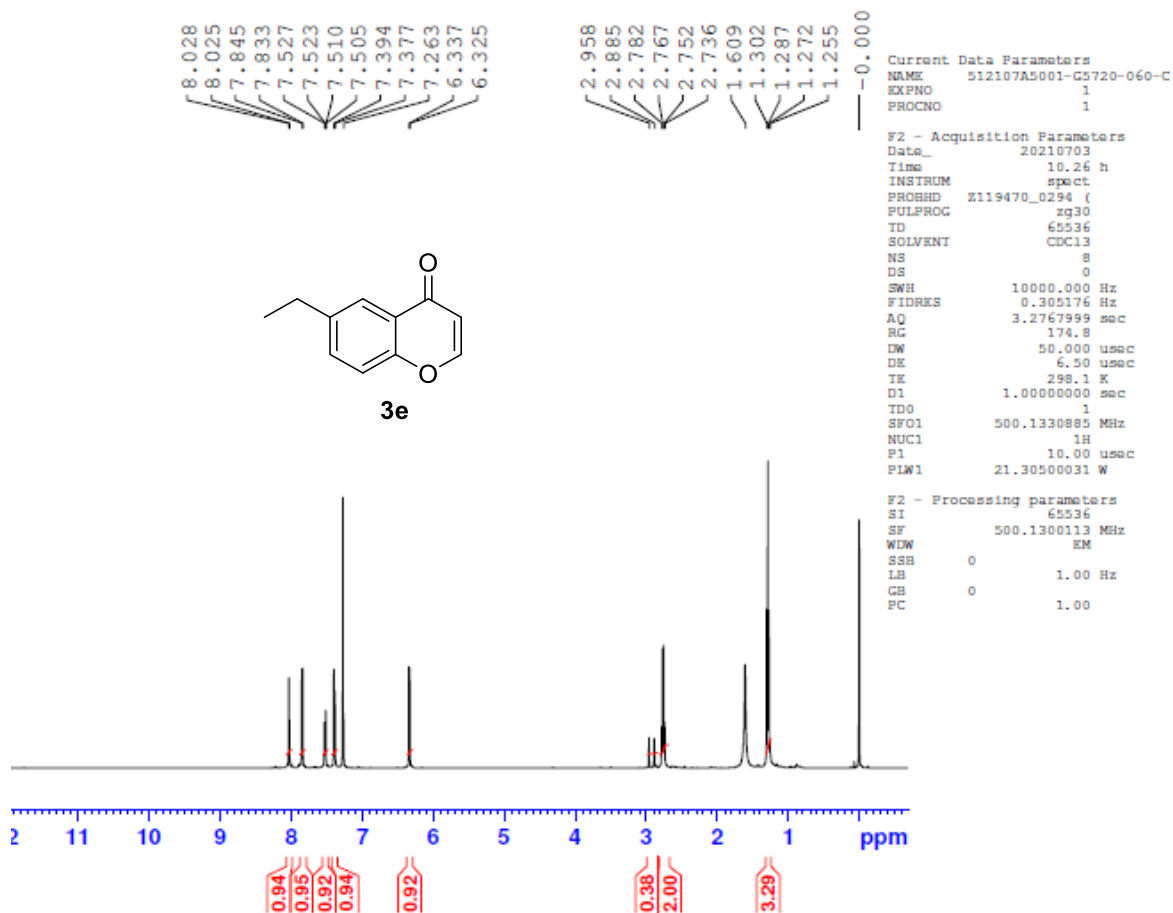
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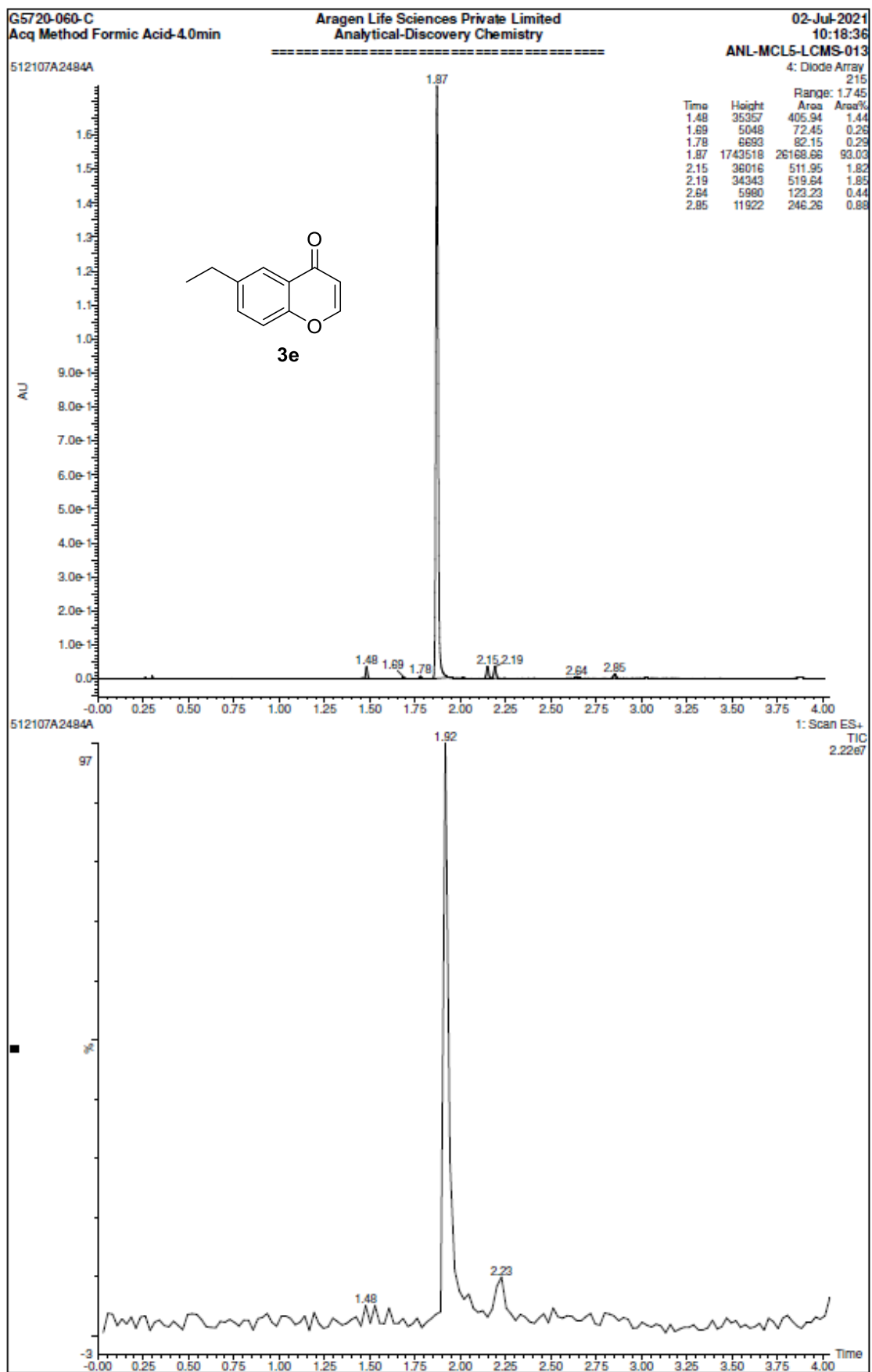
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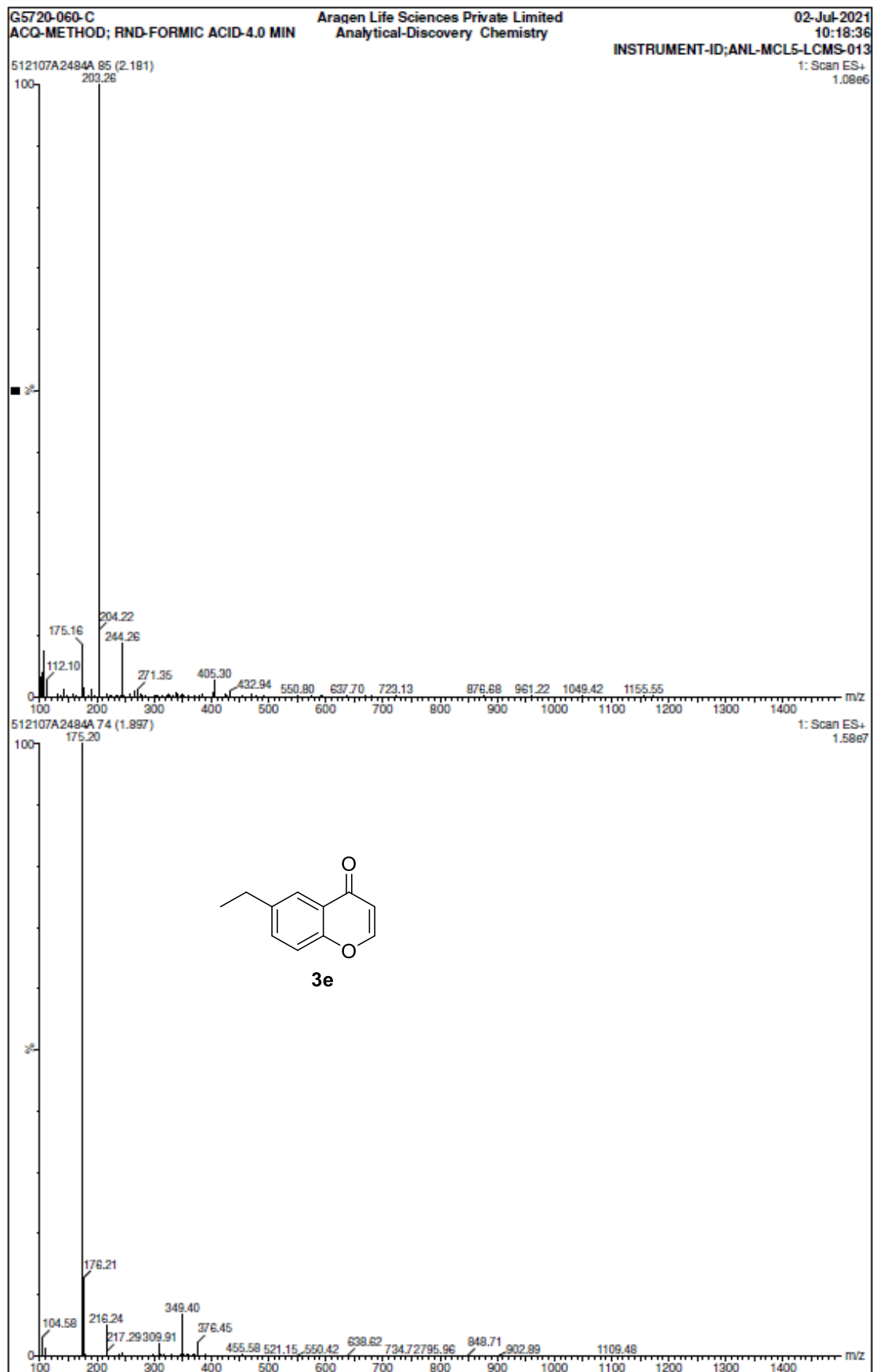
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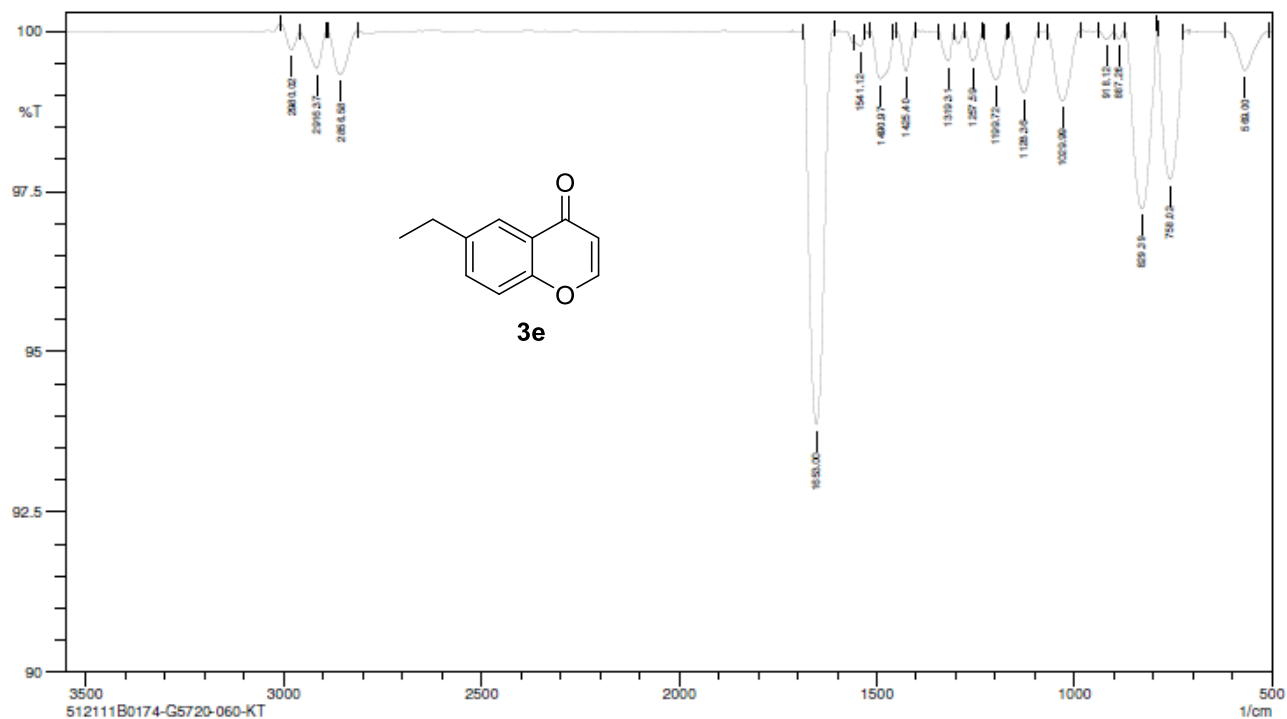
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Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry



Sample Name:
512111B0174-G5720-060-KT

No. of Scans:

Date/Time: 11/8/2021 6:43:06 PM

User: Aragen

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-11 H: 0-11 O: 0-2

512107A2484A 74 (1.897)

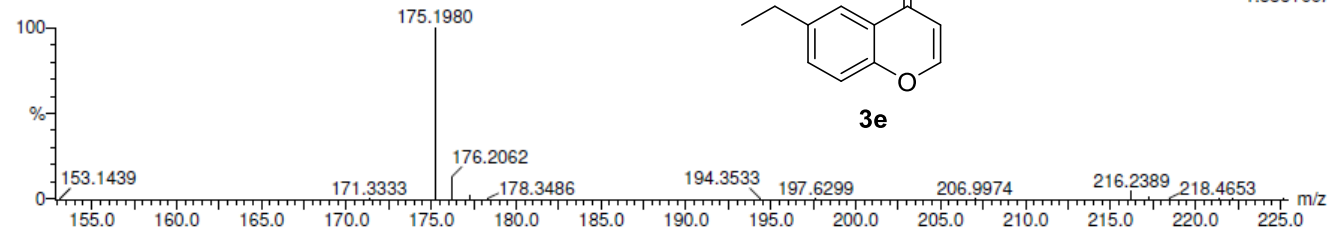
G5720-060-C

02-07-2021
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02-Jul-2021
10:18:36
INSTRUMENT-ID;ANL-MCL5-LCMS-013

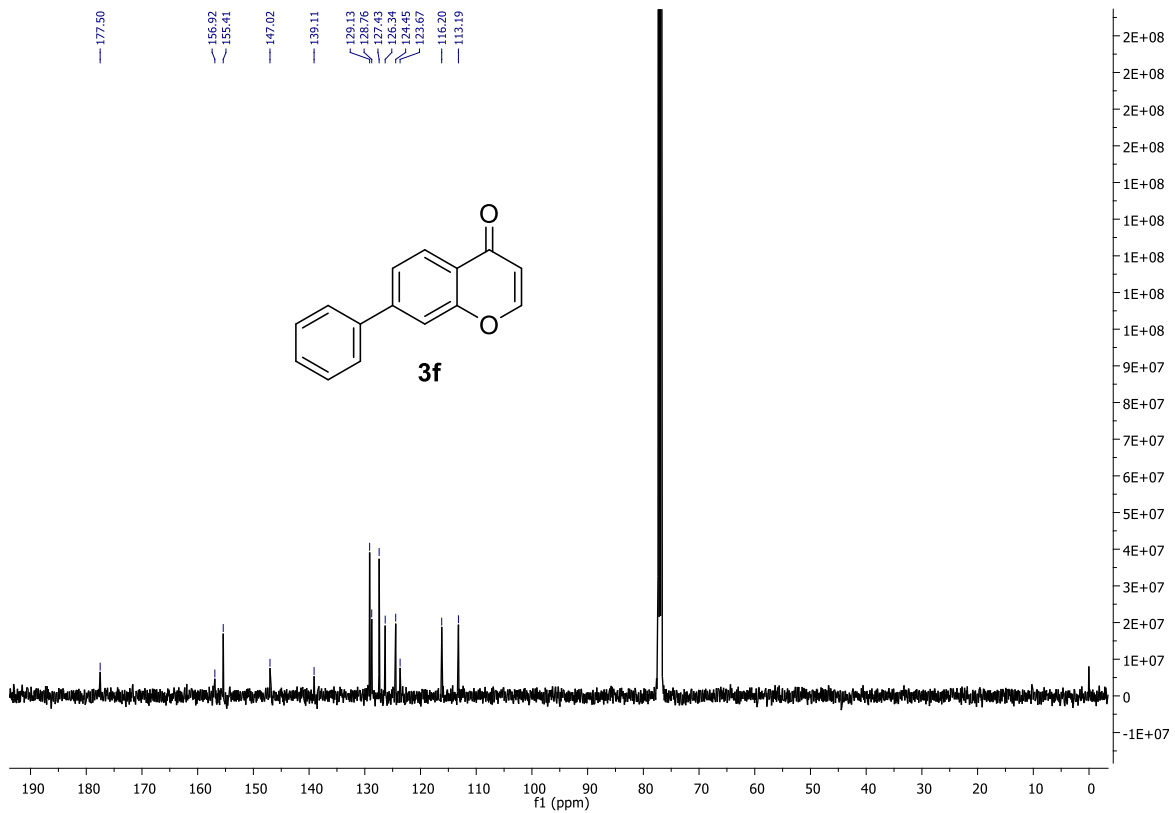
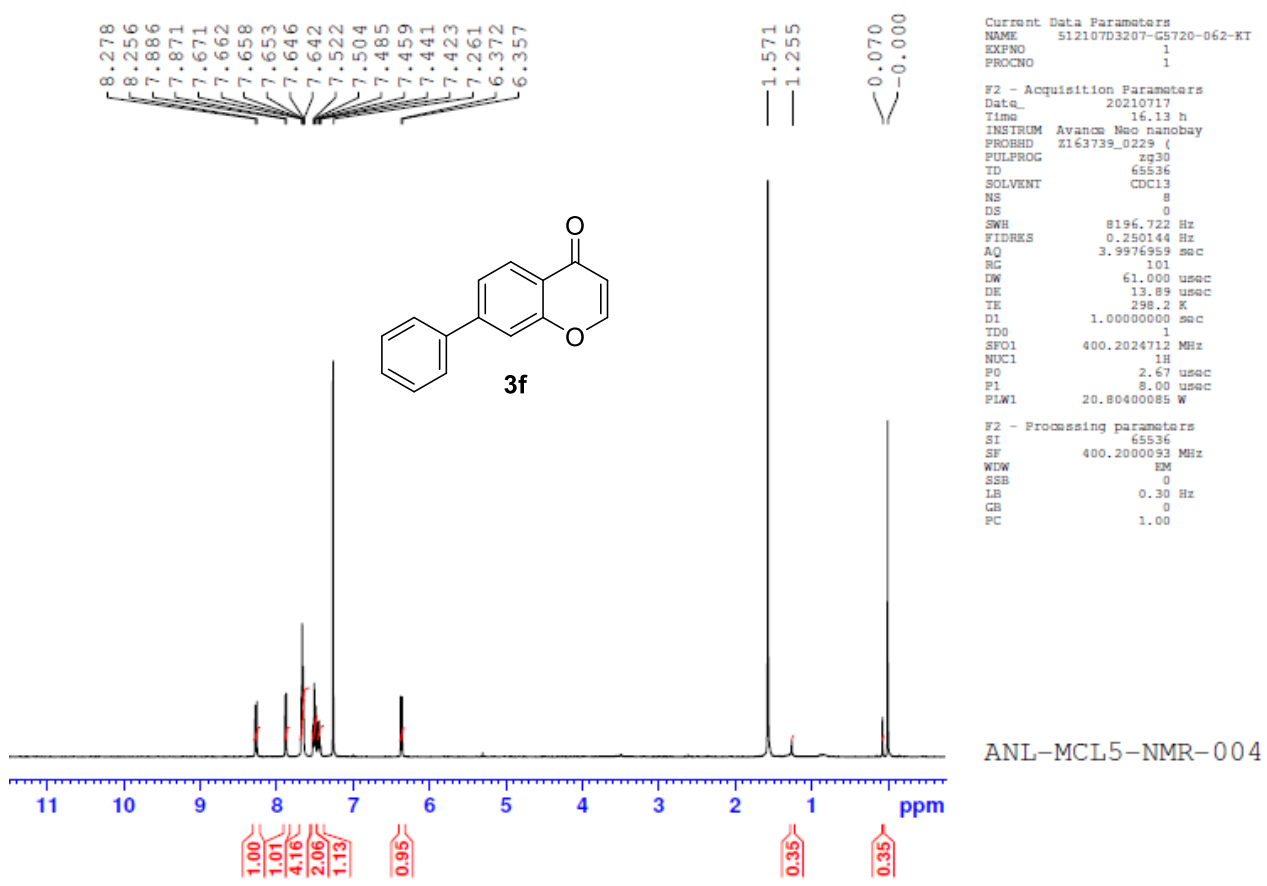
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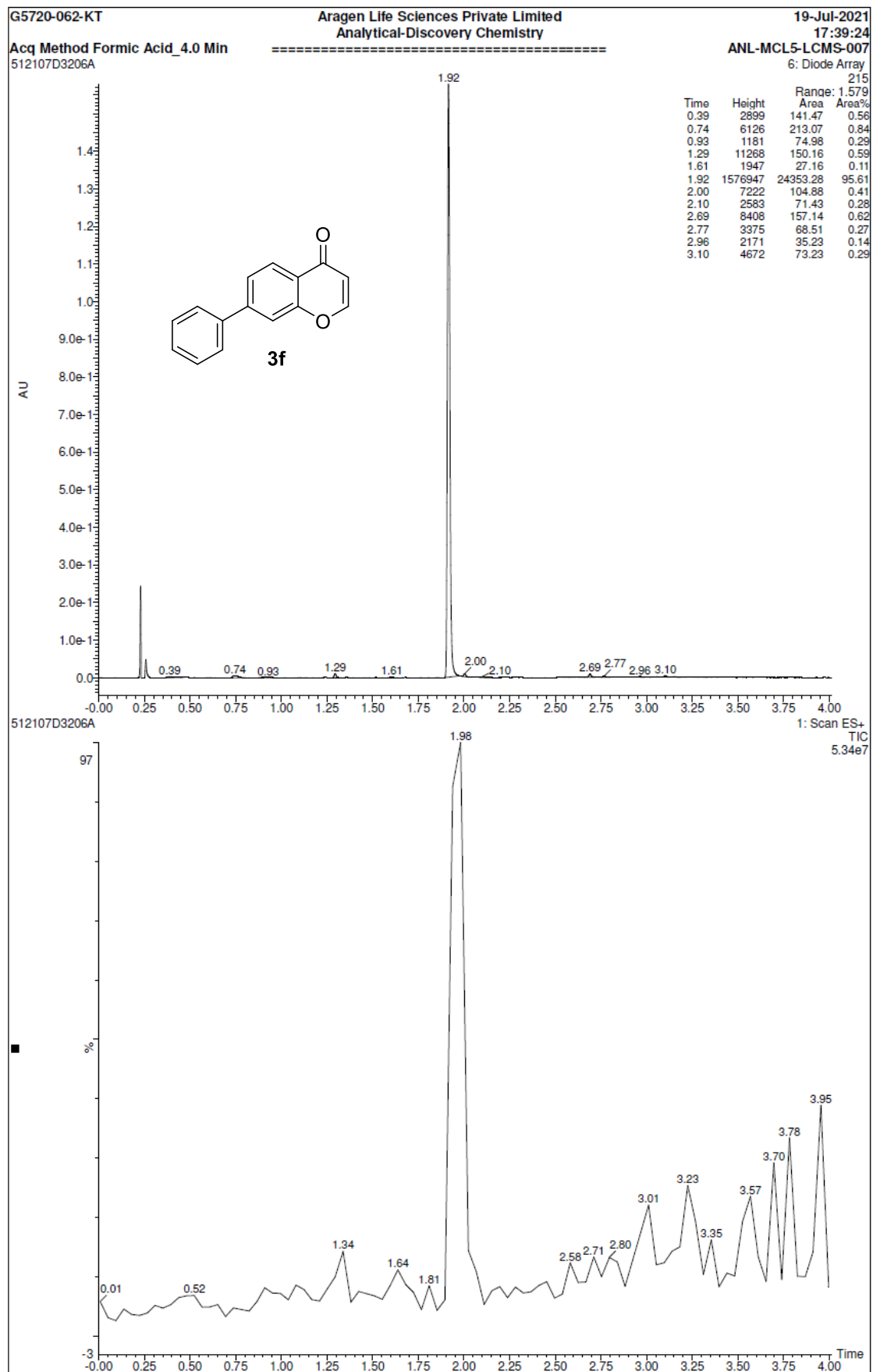
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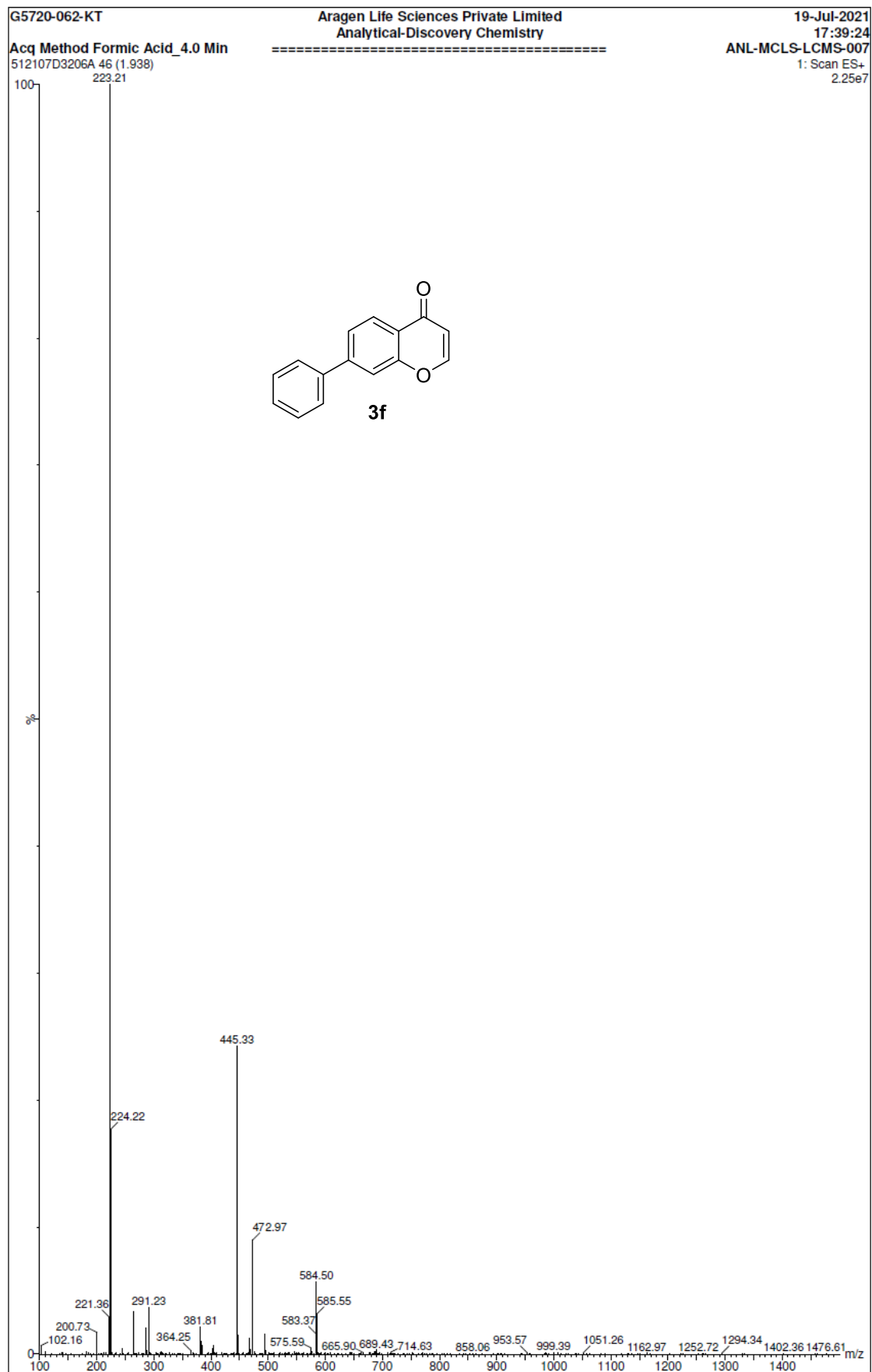


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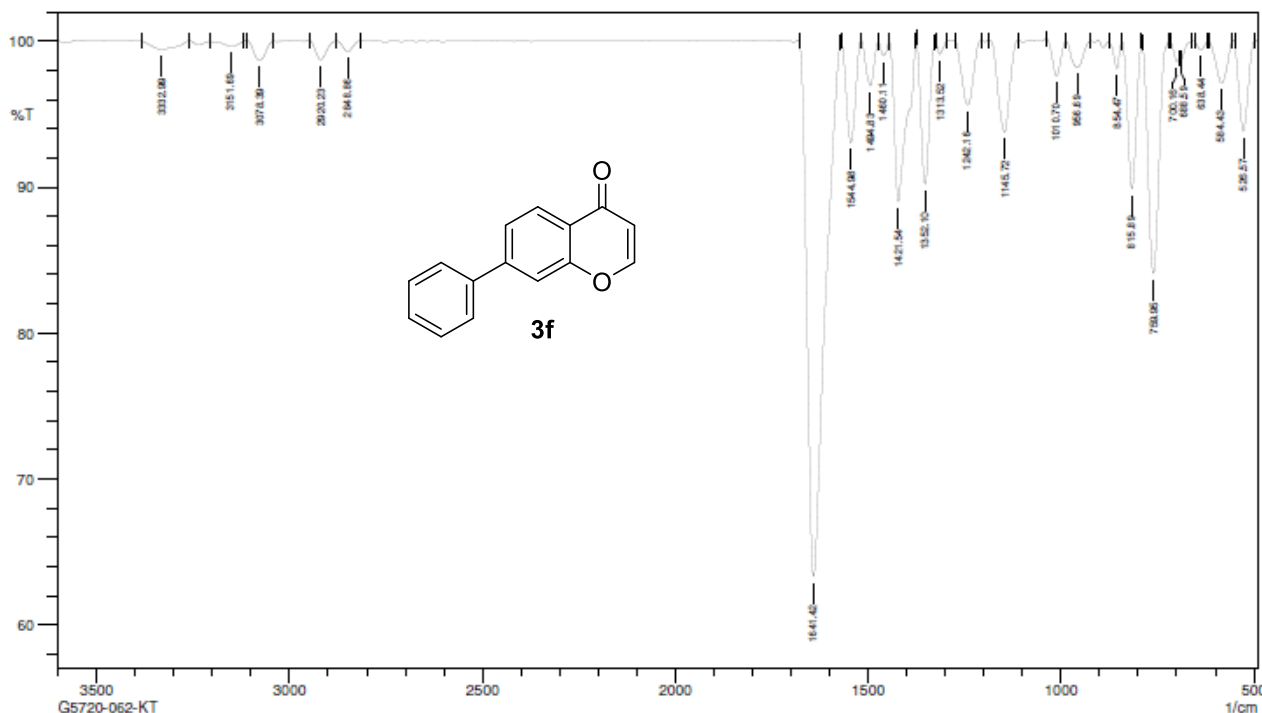
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
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Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry



Sample Name:
G5720-062-KT

No. of Scans:

Date/Time: 10/27/2021 8:51:44 PM

User: Aragen

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-15 H: 0-11 O: 0-2

G5720-062-KT

Acq Method Formic Acid_4.0 Min
512107D3206A 47 (1.981)

Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry

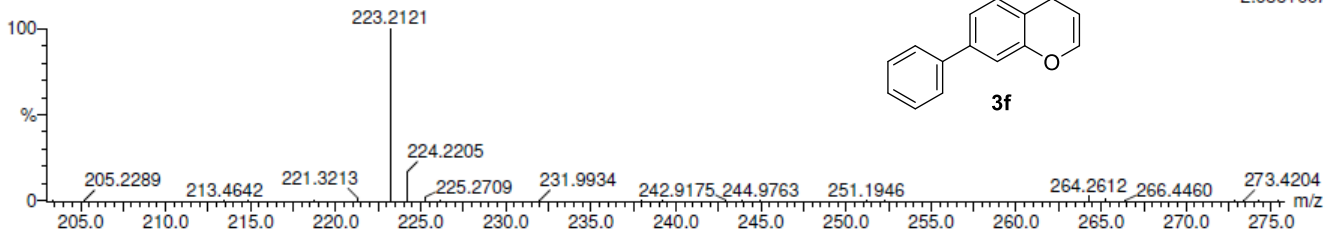
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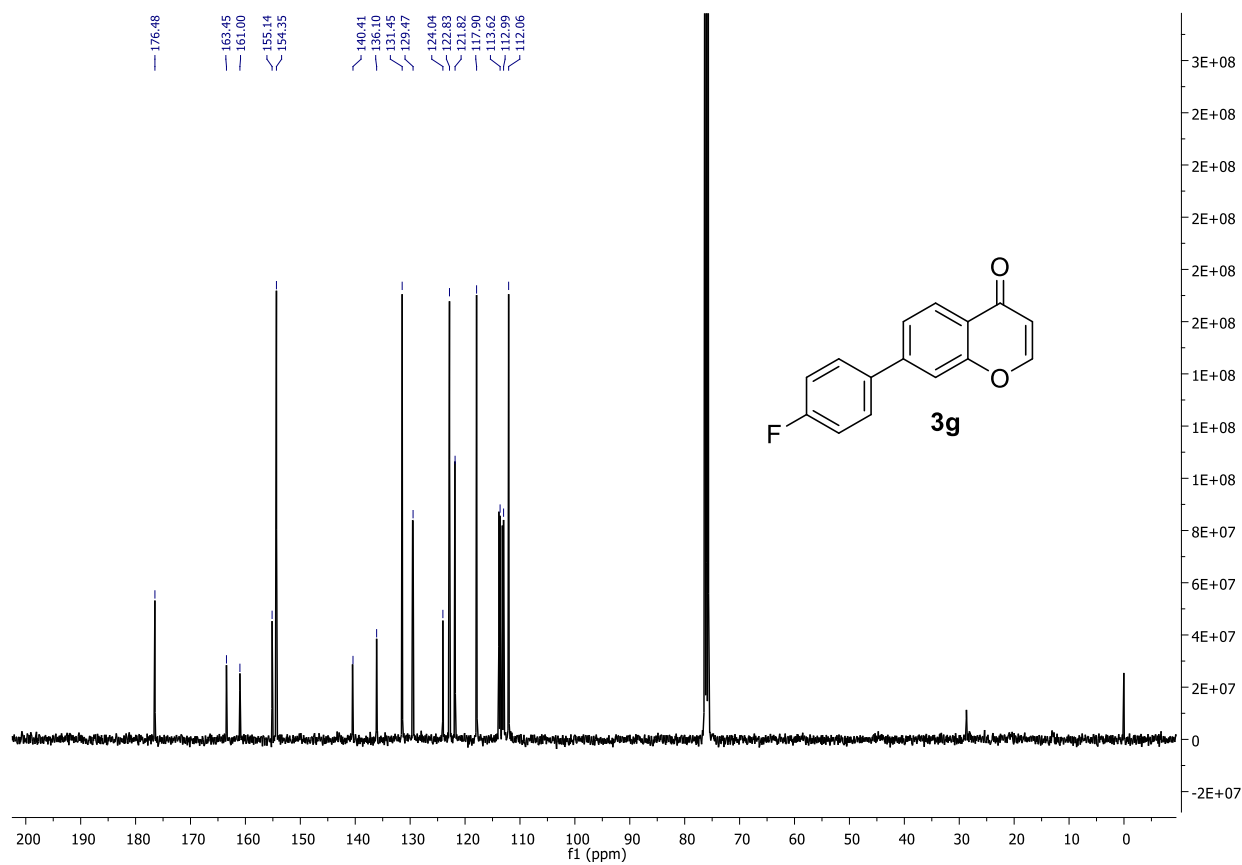
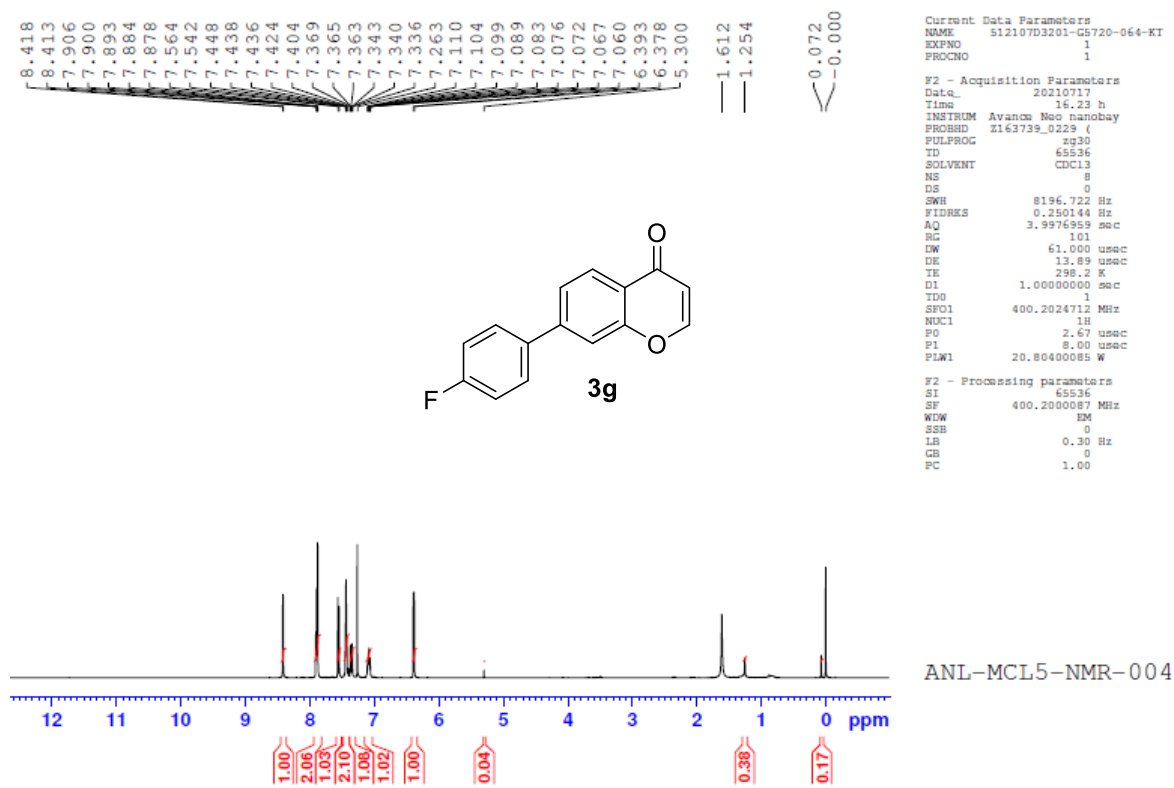
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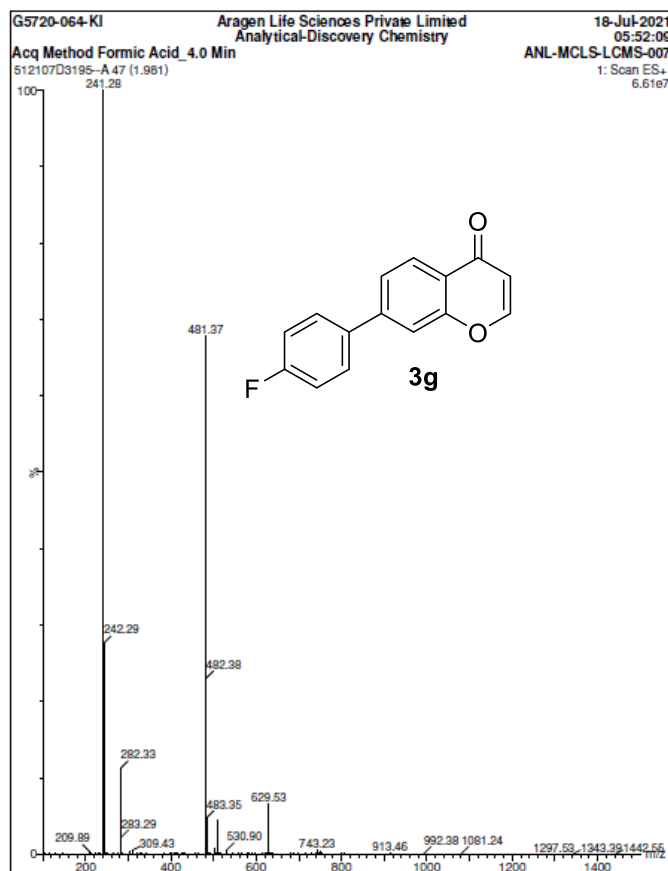
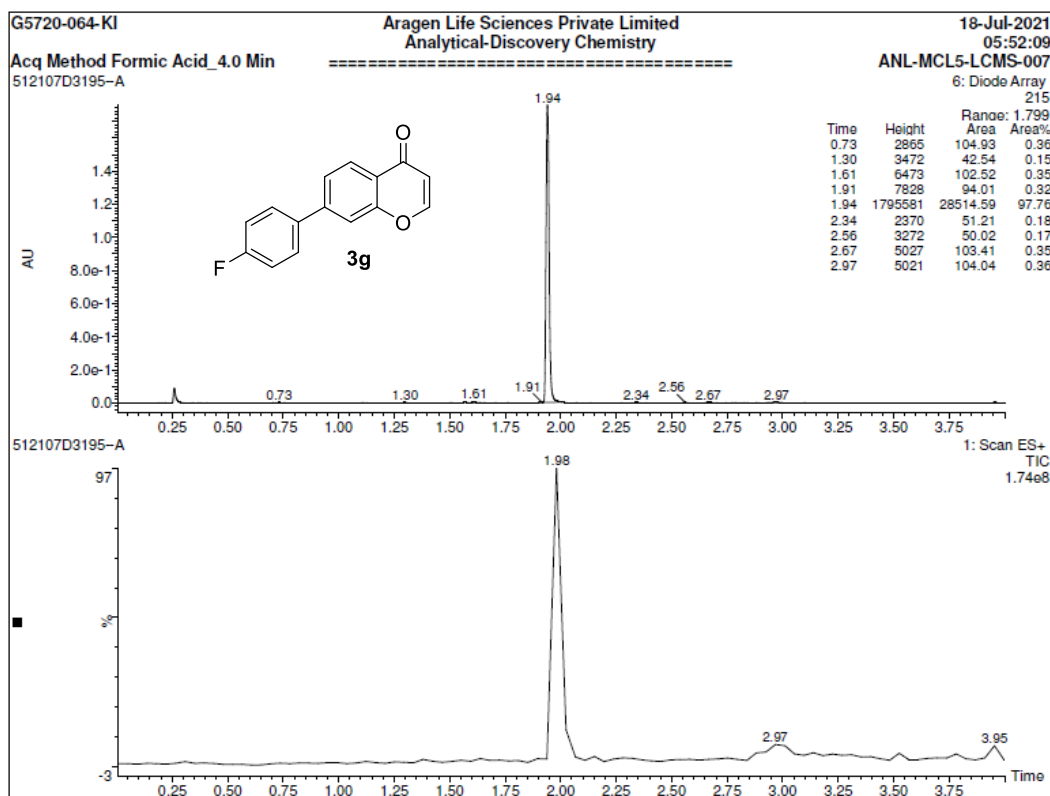
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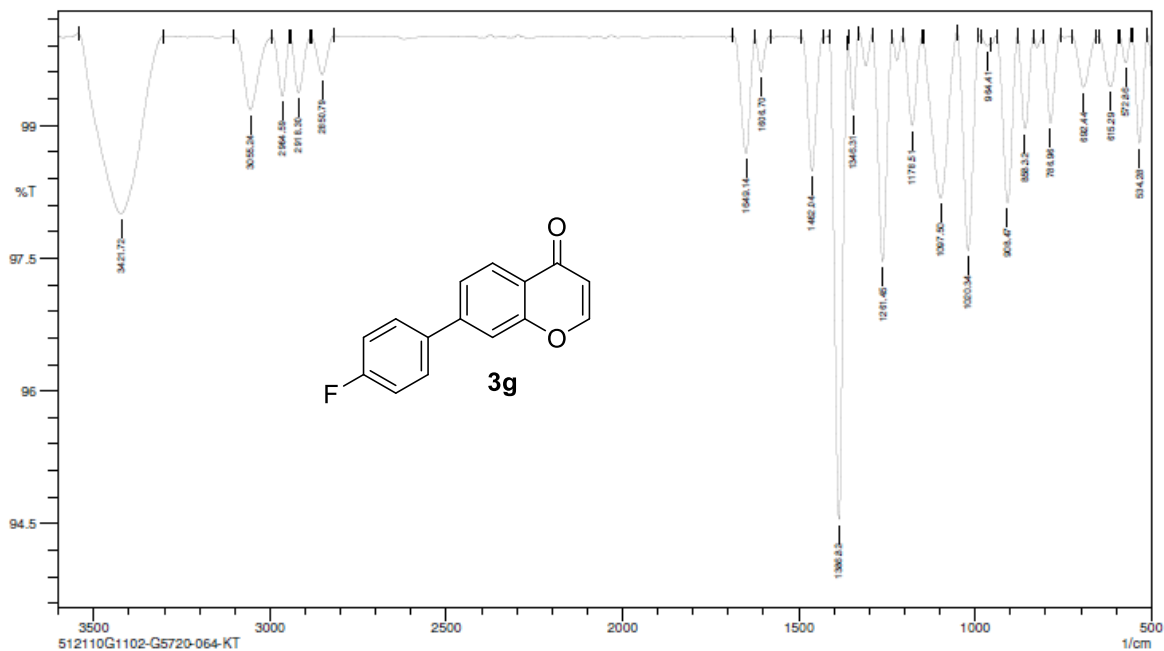
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Maximum: 5.0 1000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
223.2121	223.0759	136.2	610.2	10.5	42.5	n/a	n/a	C15 H11 O2





Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry



Sample Name:
512110G1102-G5720-064-KT

No. of Scans:

Date/Time: 10/29/2021 7:41:49 PM

User: Aragen

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

4 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

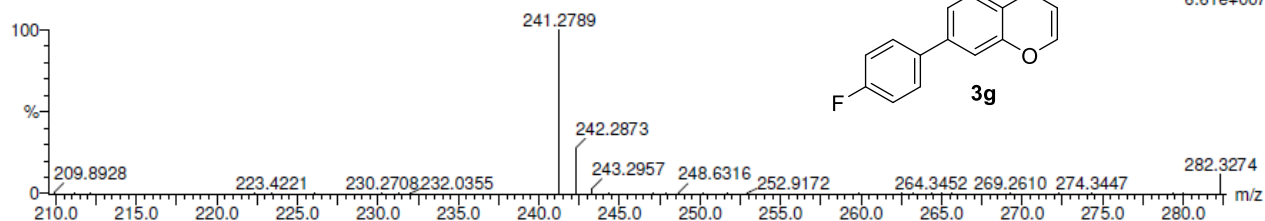
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G5720-064-KI

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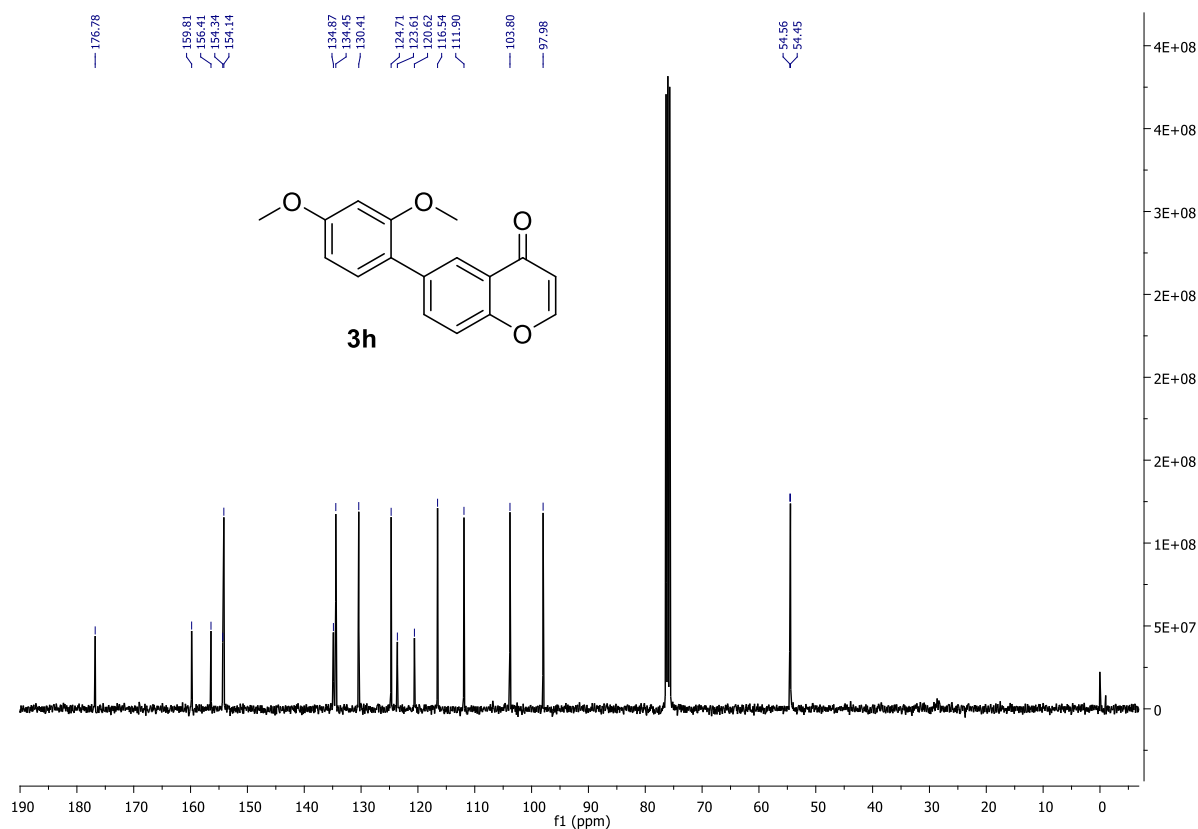
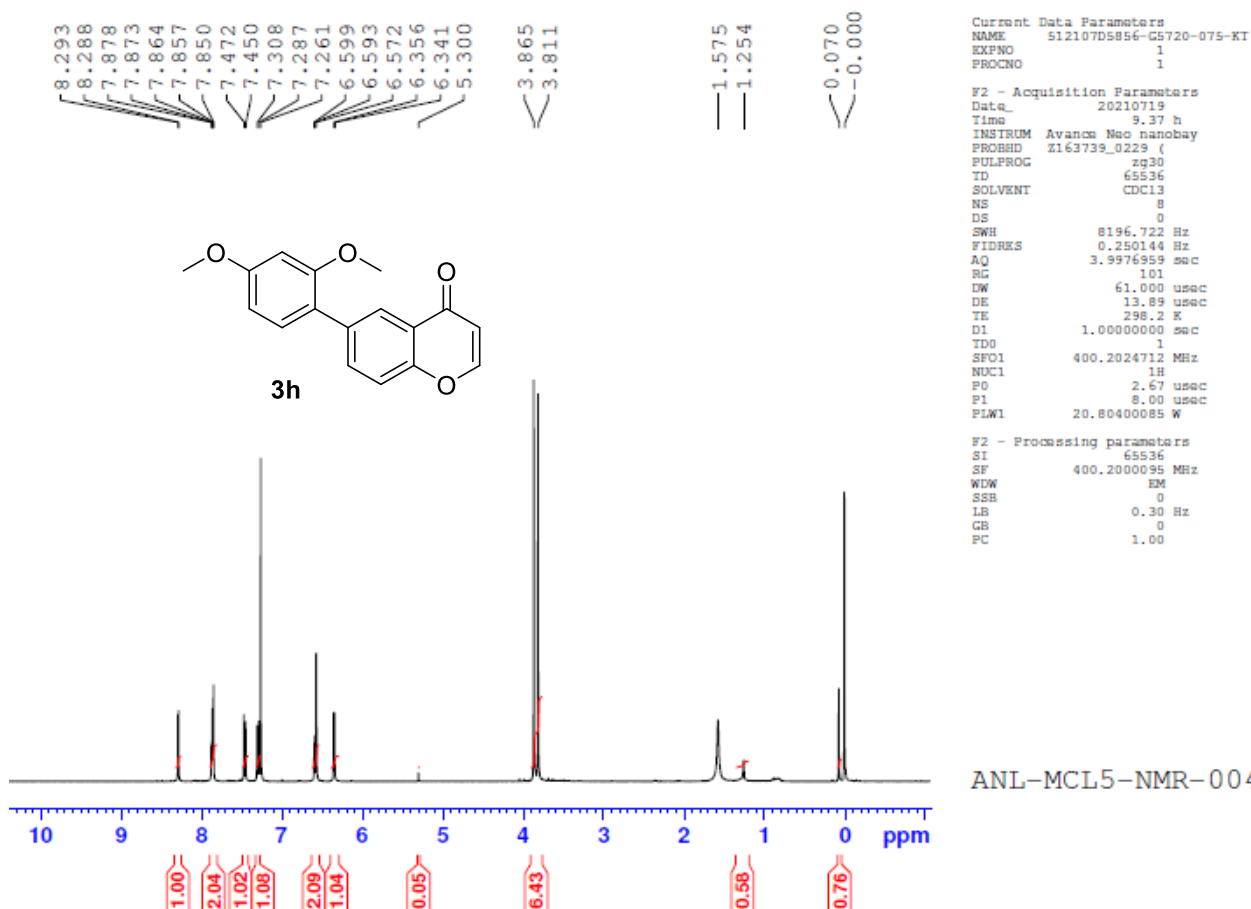
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry

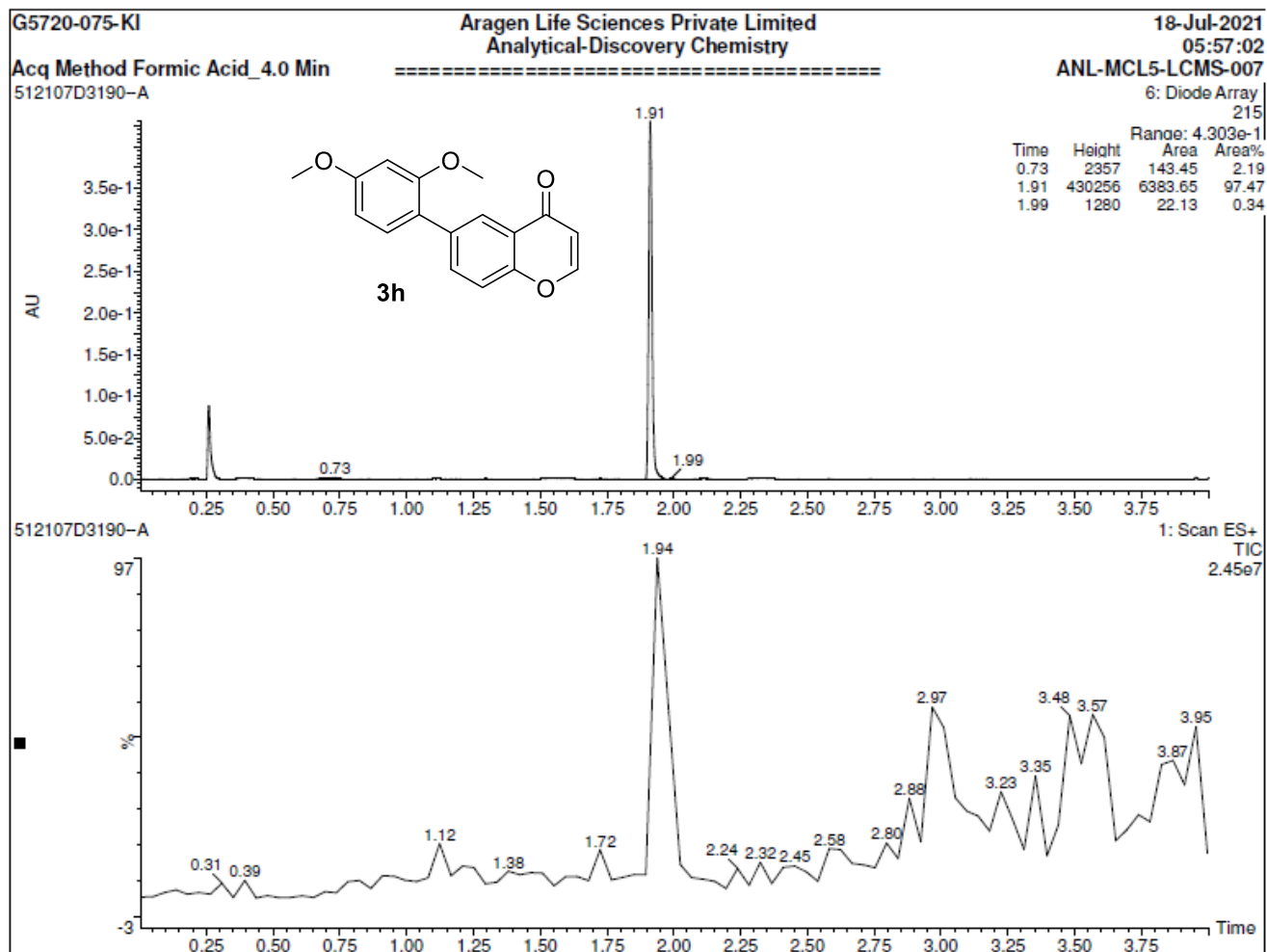
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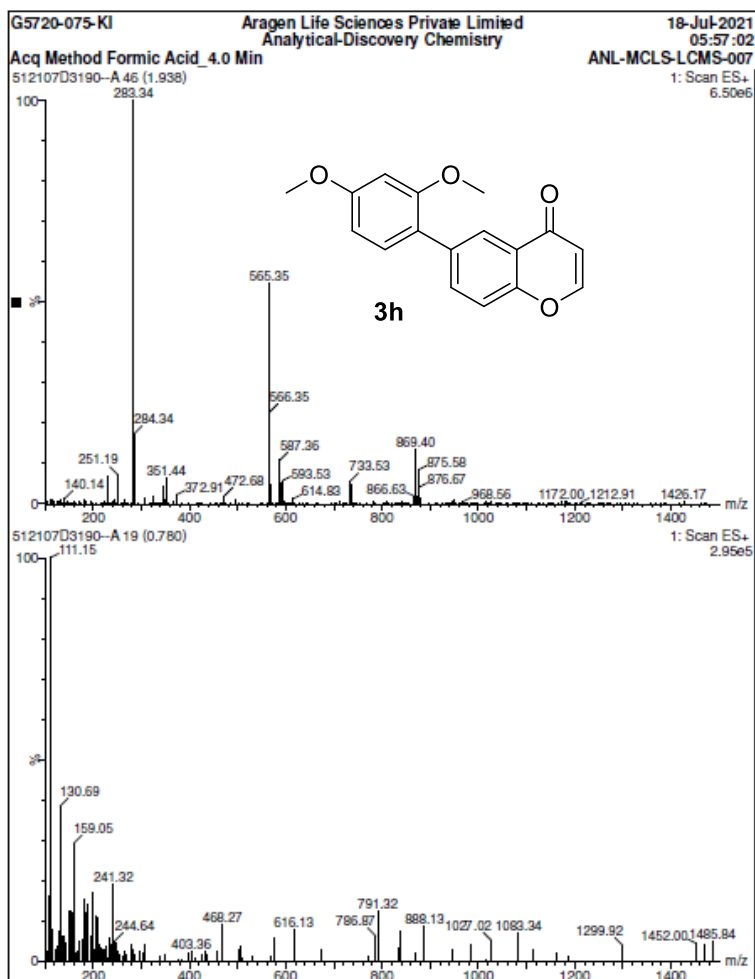


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
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Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

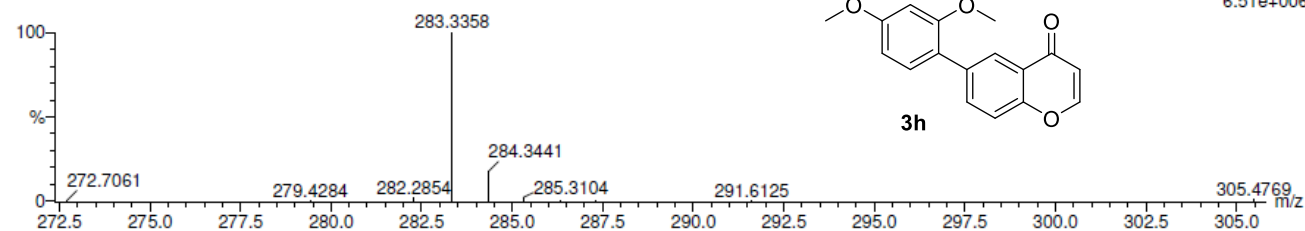
Monoisotopic Mass, Even Electron Ions

4 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

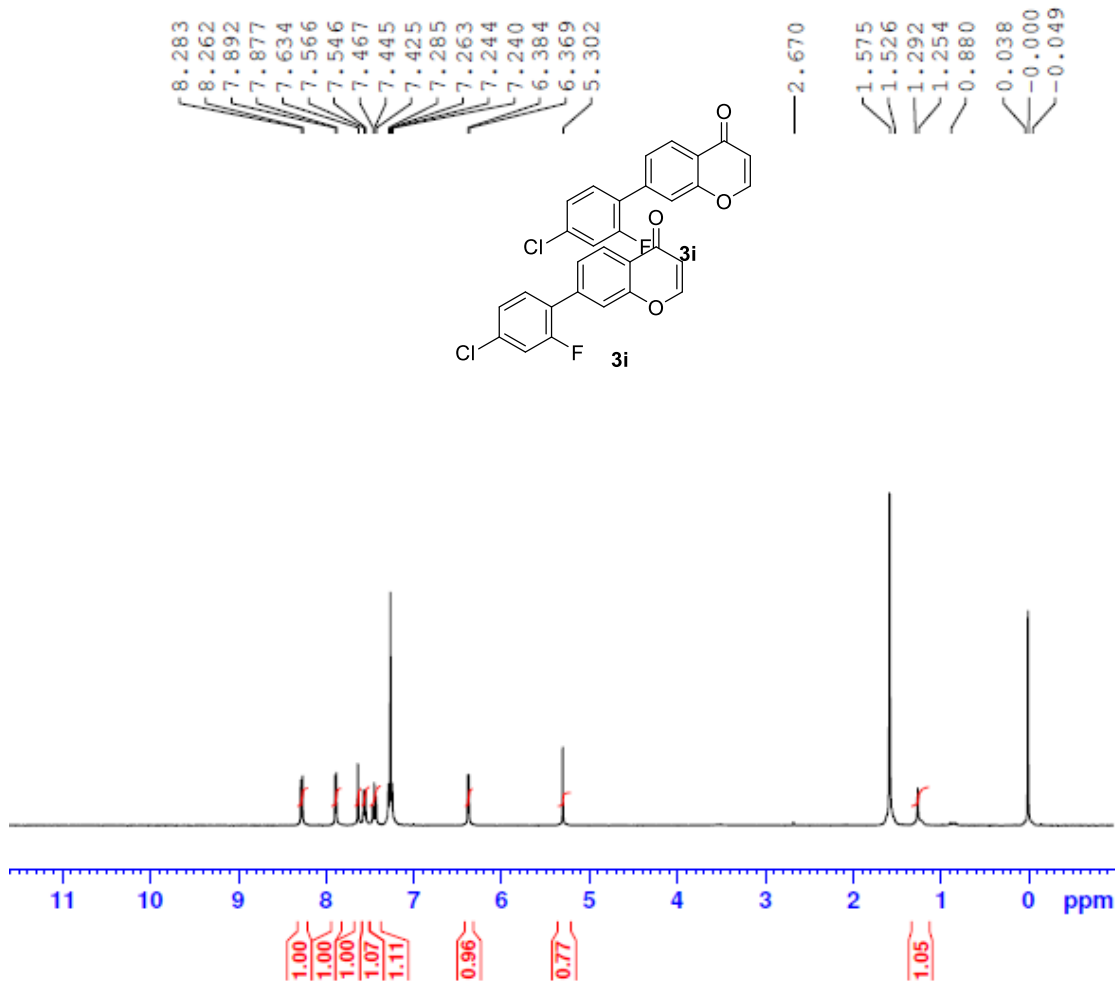
Elements Used:

C: 0-17 H: 0-15 O: 0-4

G5720-075-KI

Acq Method Formic Acid_4.0 Min
512107D3190-A 46 (1.938)Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry18-Jul-2021
05:57:02
ANL-MCLS-LCMS-007
1: Scan ES+
6.51e+006Minimum: -1.5
Maximum: 5.0 1000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
283.0958	283.0970	-1.2	-4.2	10.5	39.4	n/a	n/a	C17 H15 O4

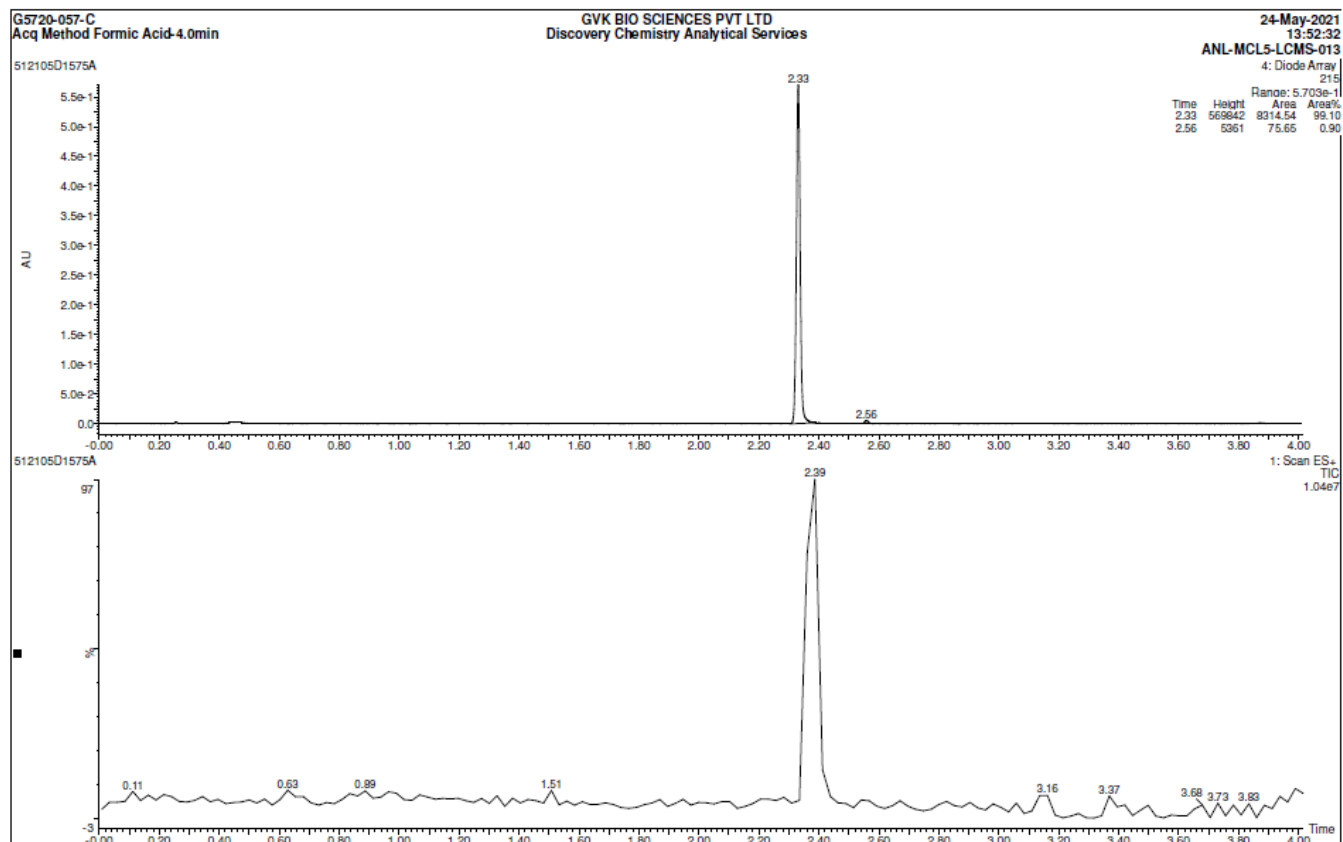


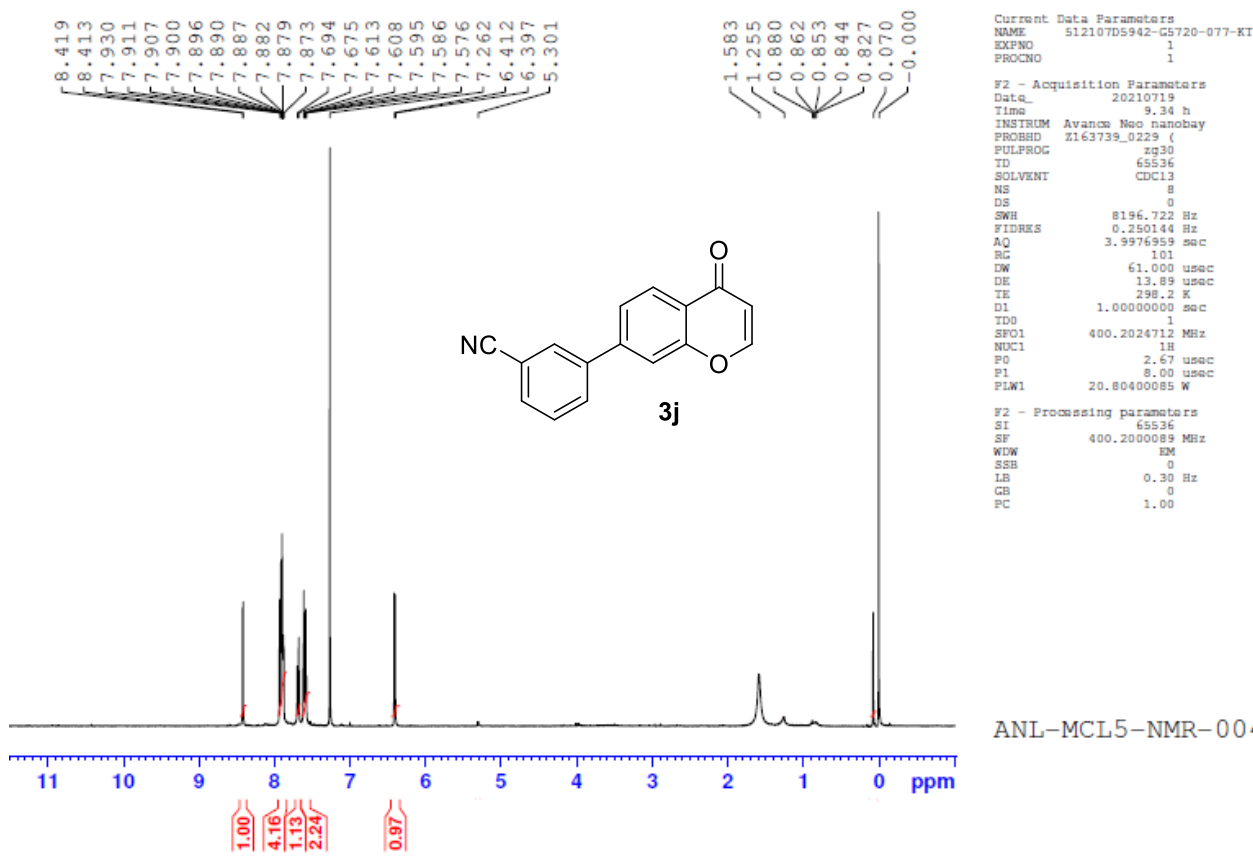
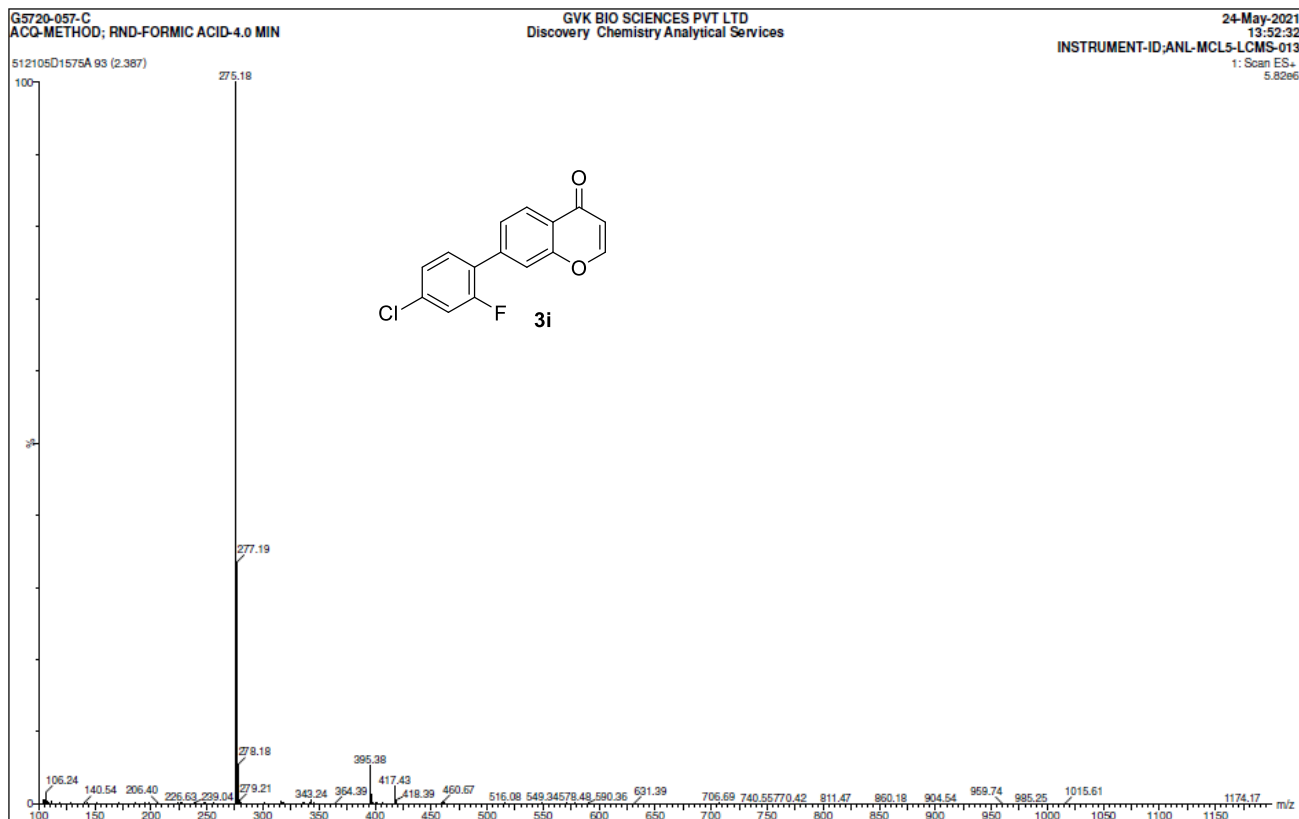
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 EXPNO 1
 PROCNO 1

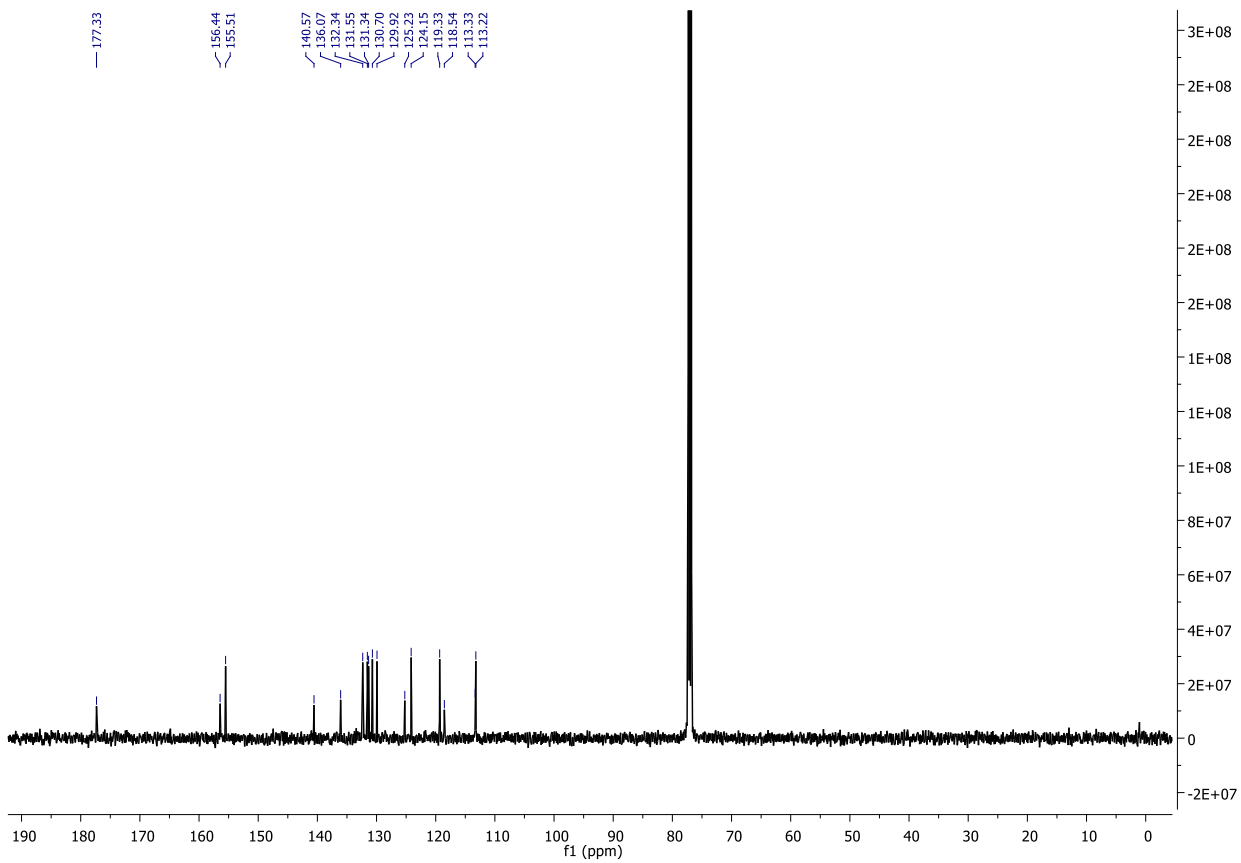
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 Time 11.30 h
 INSTRUM Avance
 PROBHD Z163739_0135 ()
 PULPROG zg30
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 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 8196.722 Hz
 FIDRES 0.250144 Hz
 AQ 3.9976959 sec
 RG 101
 DW 61.000 usec
 DE 13.89 usec
 TE 296.1 K
 D1 1.00000000 sec
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 SFO1 400.3024719 MHz
 NUC1 1H
 P0 2.67 usec
 P1 8.00 usec
 PLW1 22.47400093 W

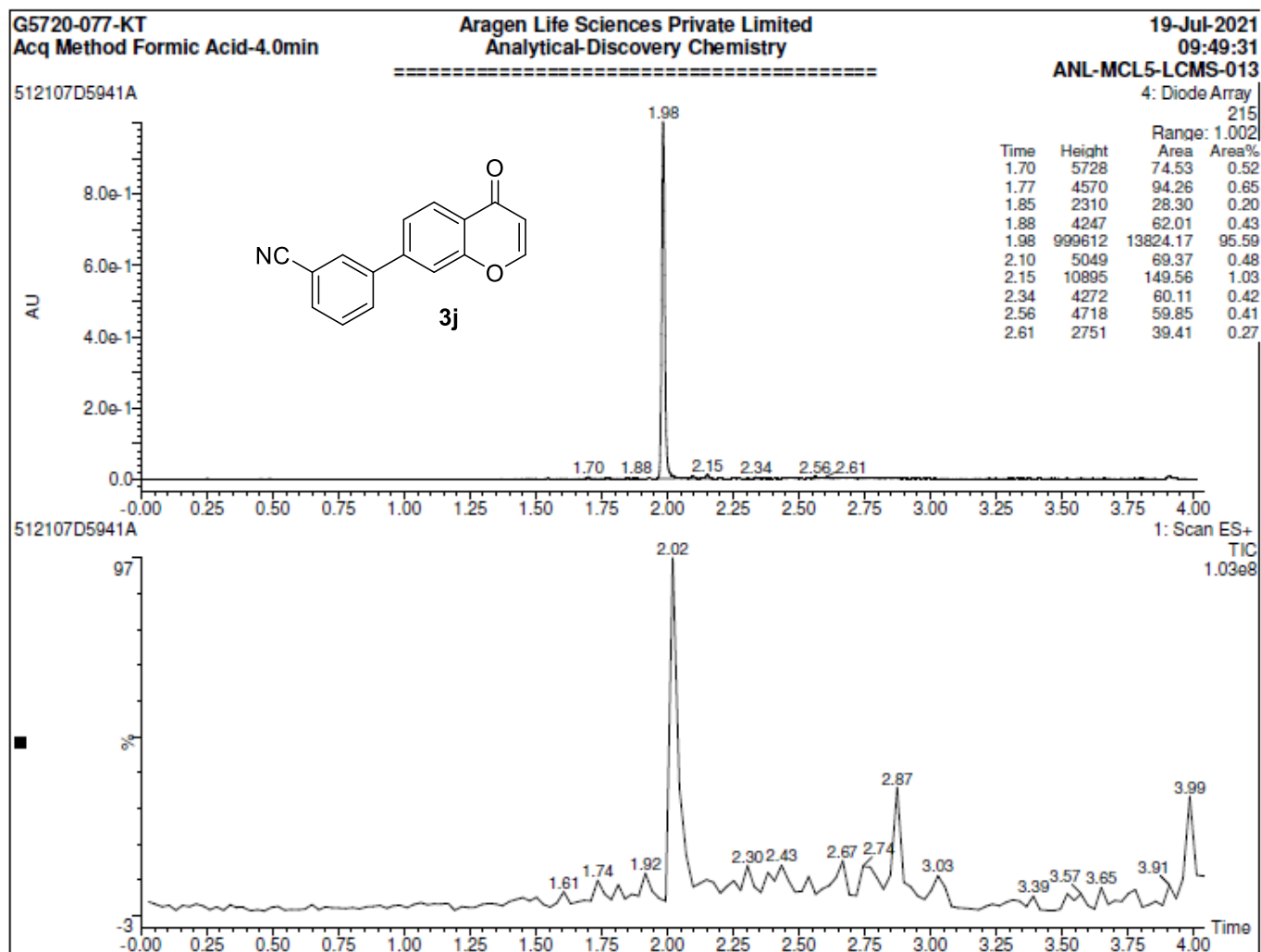
F2 - Processing parameters
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 SF 400.3000097 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

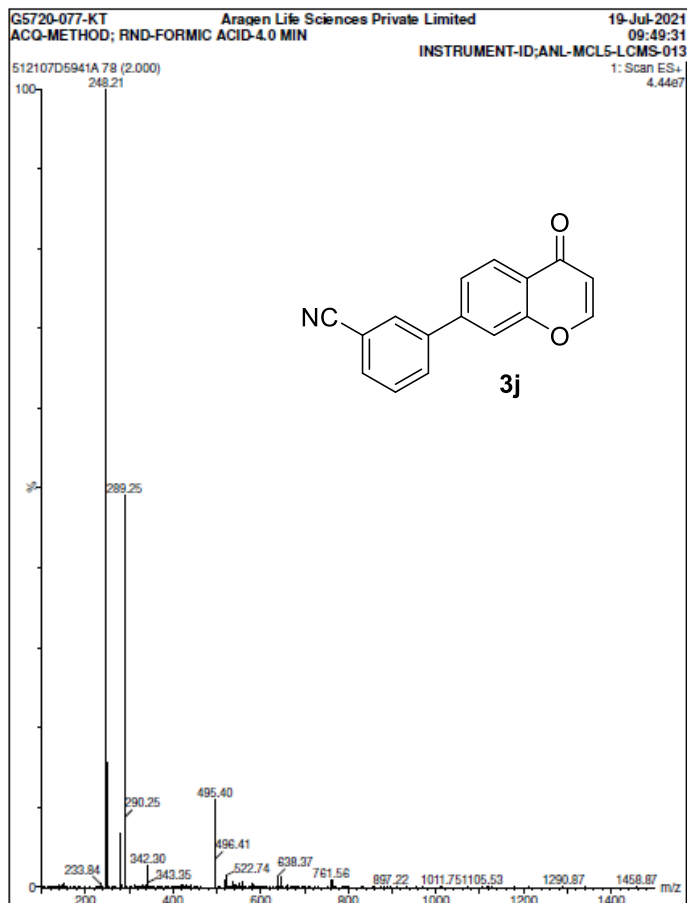
ANL-MCL5-NMR-003











Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-16 H: 0-10 N: 0-1 O: 0-2

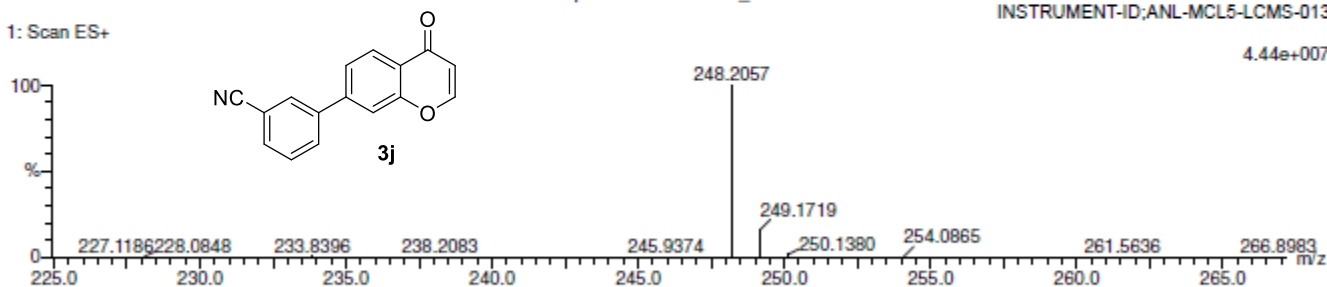
512107D5941A 78 (2.000)

G5720-077-KT

19-07-2021
Acq.method formic acid_4min19-Jul-2021
09:49:31
INSTRUMENT-ID;ANL-MCL5-LCMS-013

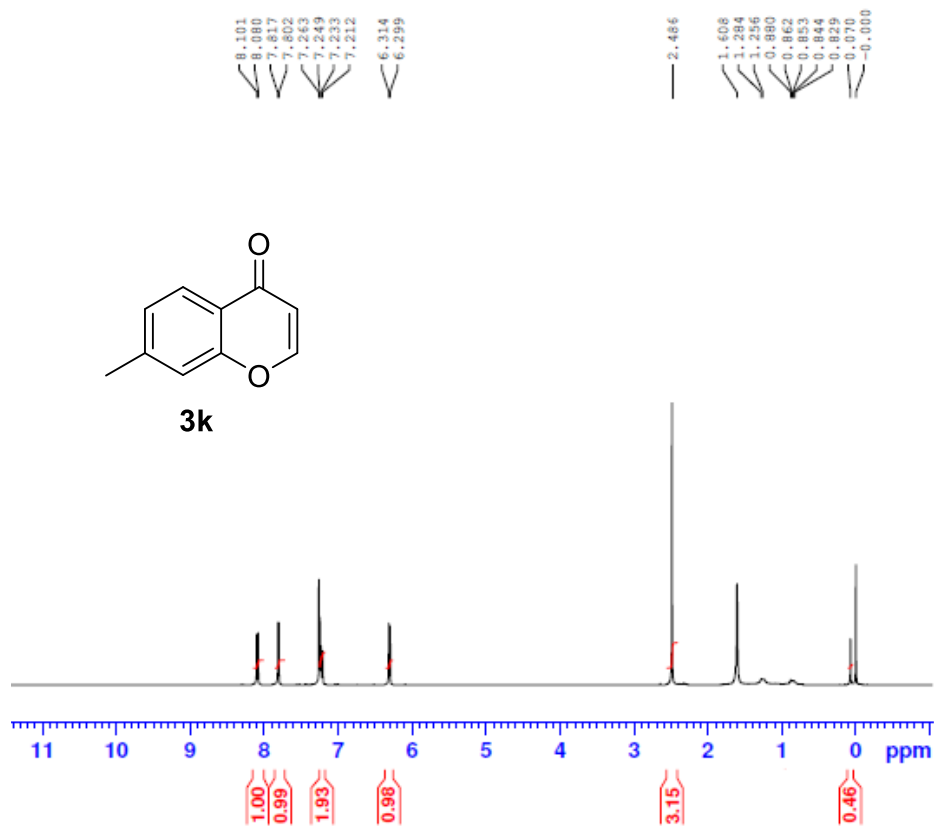
4.44e+007

1: Scan ES+

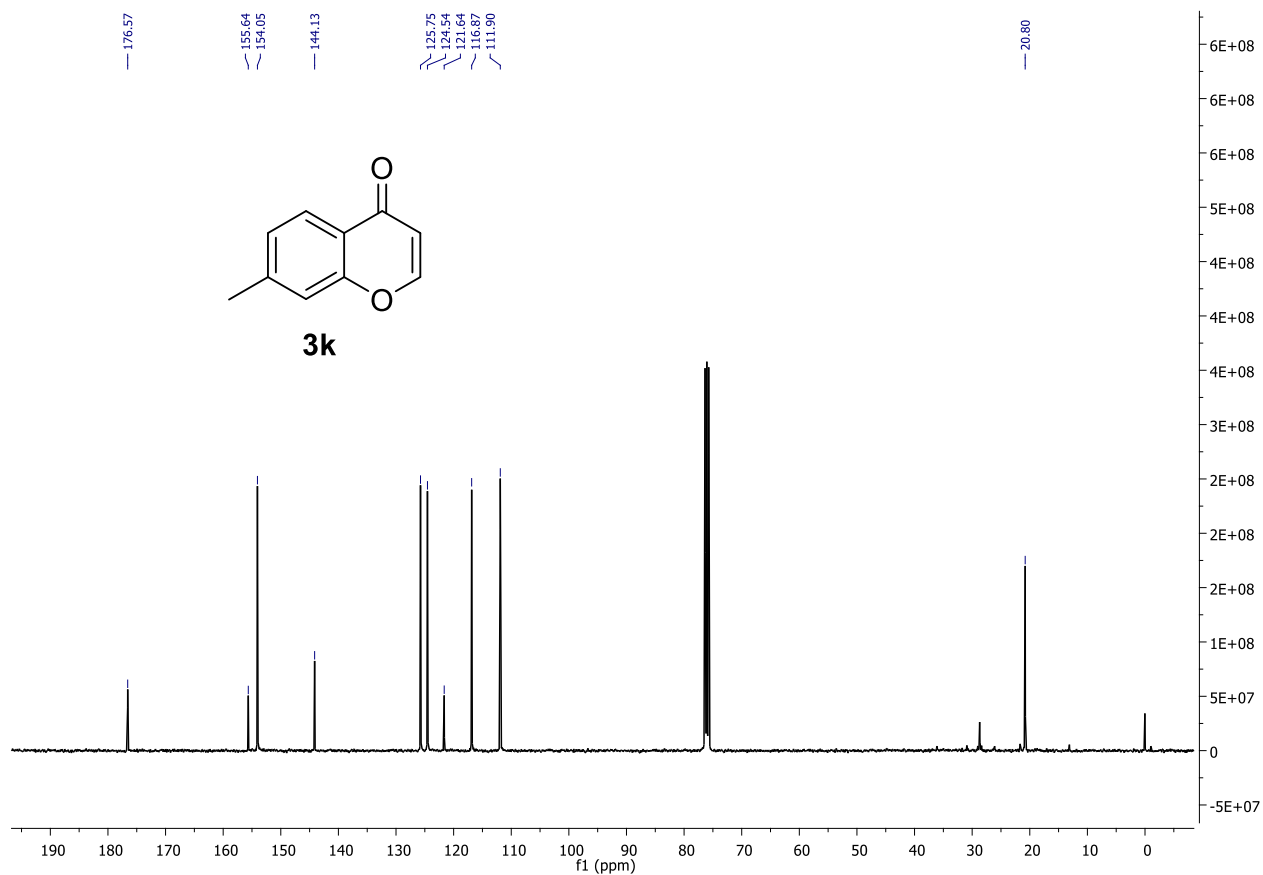


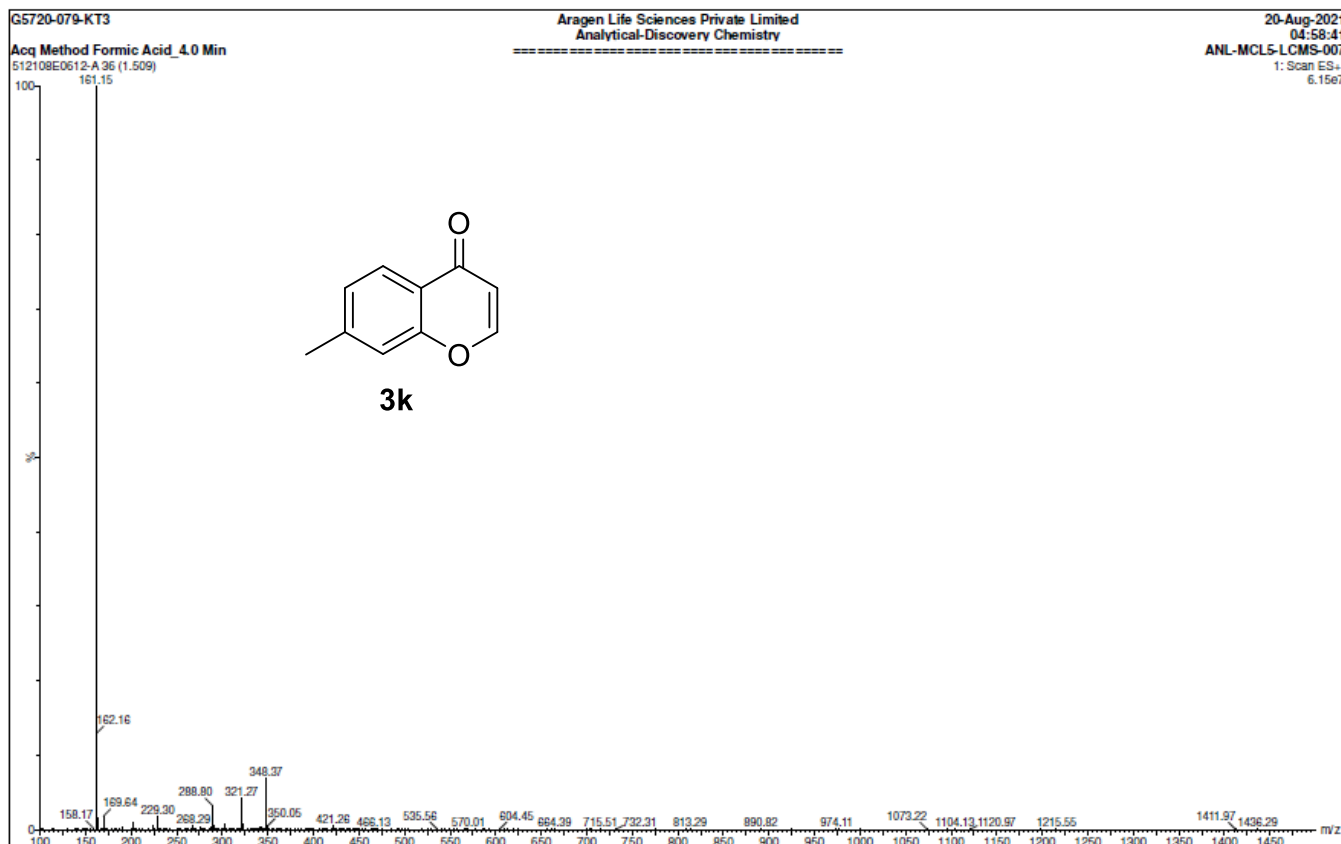
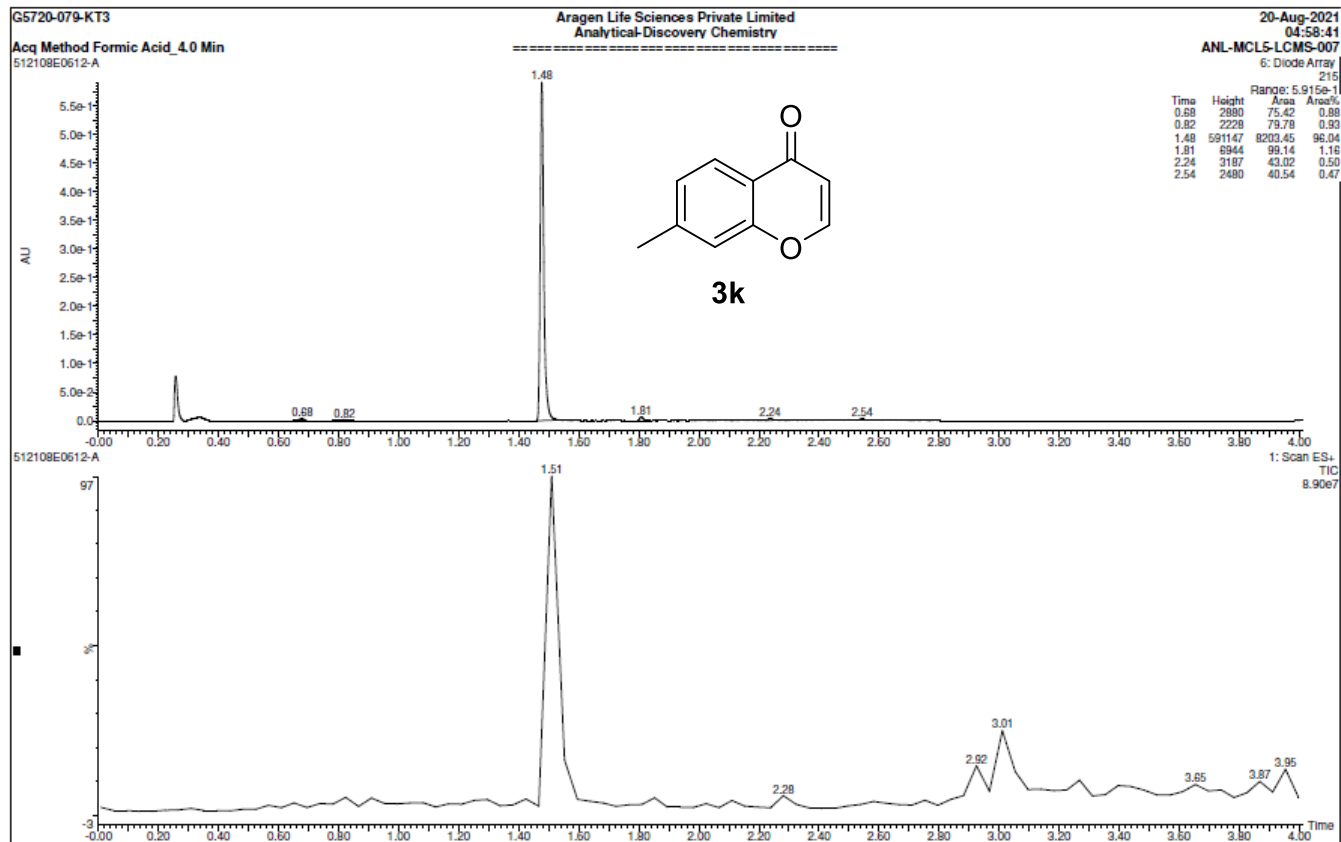
Minimum: -1.5
 Maximum: 5.0 1000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
248.0705	248.0712	-0.7	-2.8	12.5	51.4	n/a	n/a	C16 H10 N O2

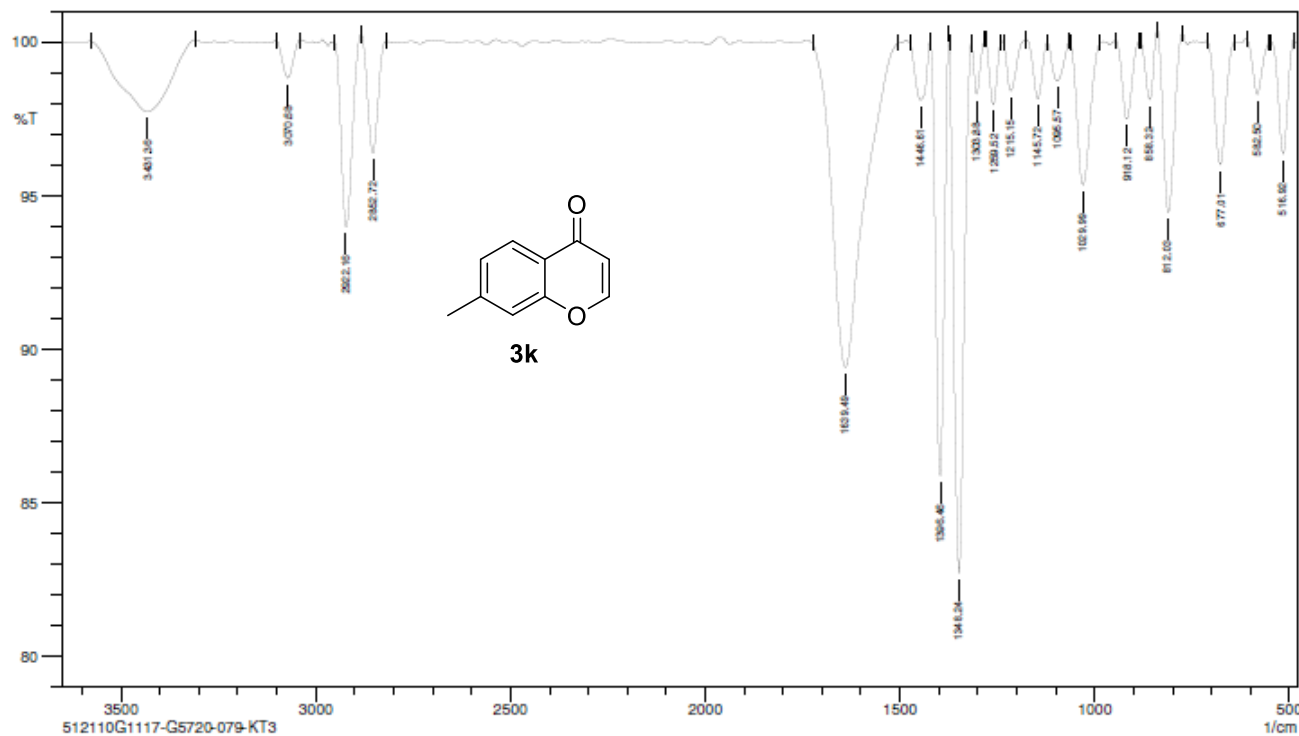


ANL-MCL5-NMR-001





Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry



Sample Name:
512110G1117-G5720-079-KT3

No. of Scans:

Date/Time: 10/29/2021 7:46:10 PM

User: Aragen

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-10 H: 0-9 O: 0-2

G5720-079-KT3

Acq Method Formic Acid_4.0 Min
512108E0612A 36 (1.509)

Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry

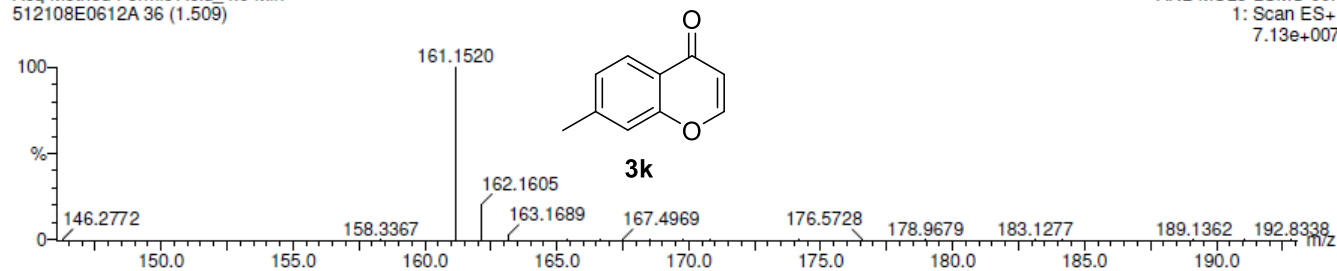
20-Aug-2021

02:02:33

ANL-MCL5-LCMS-007

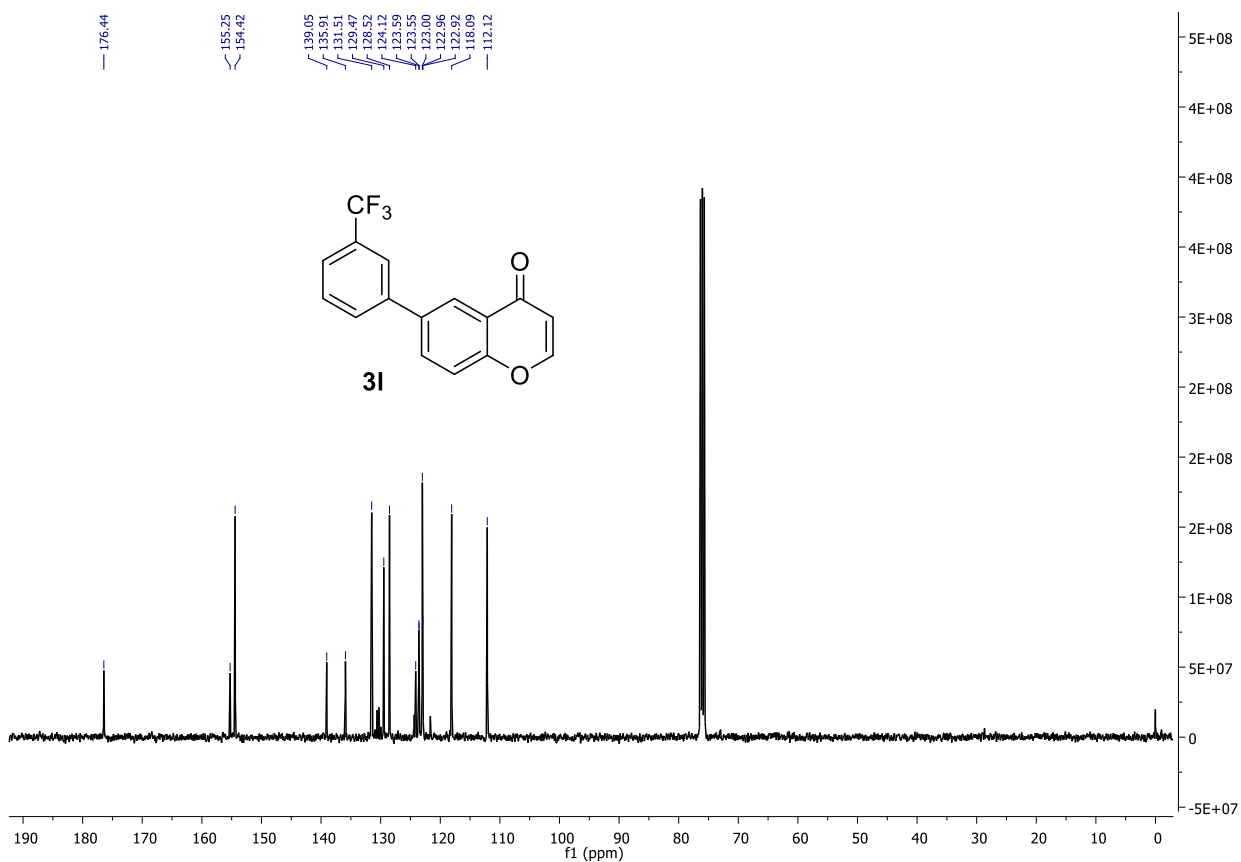
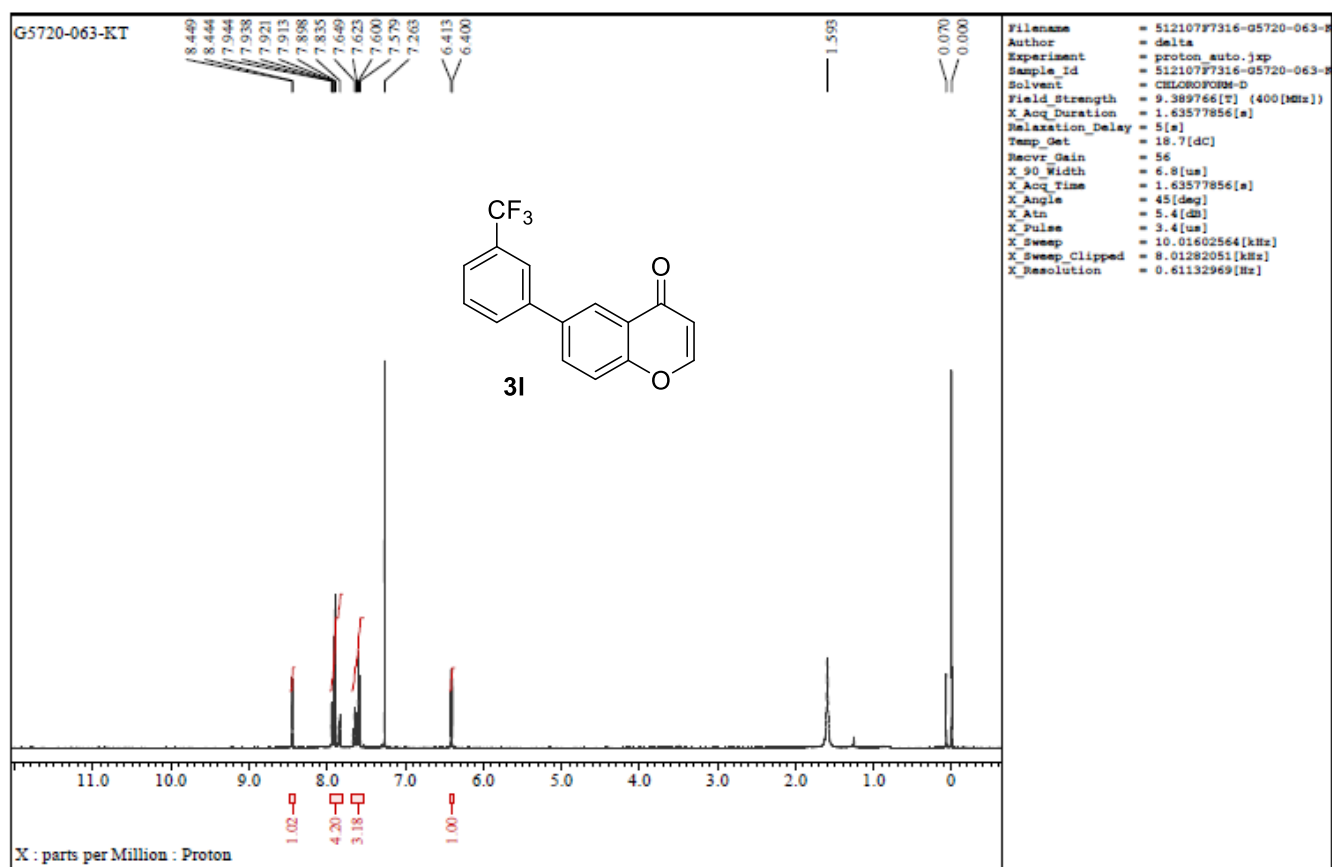
1: Scan ES+

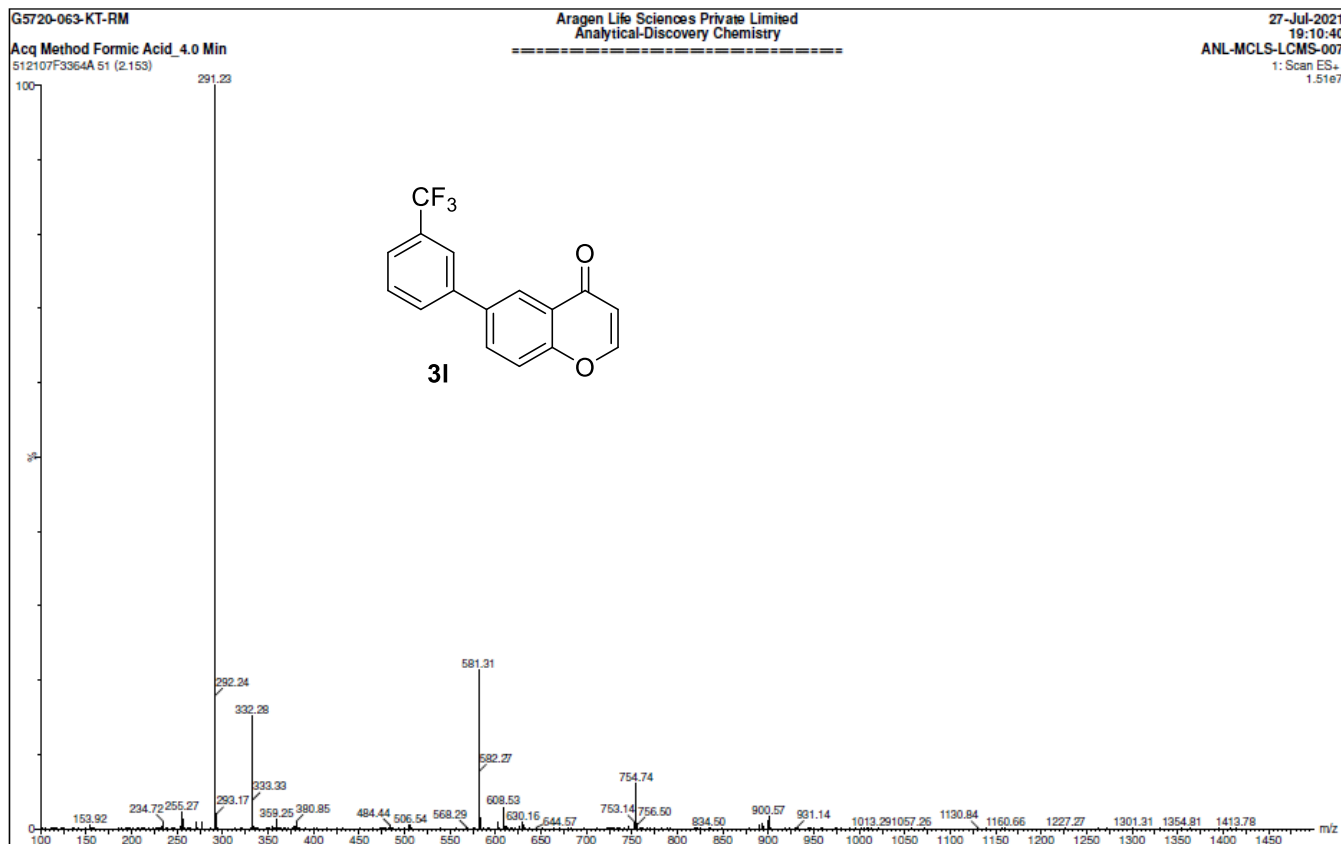
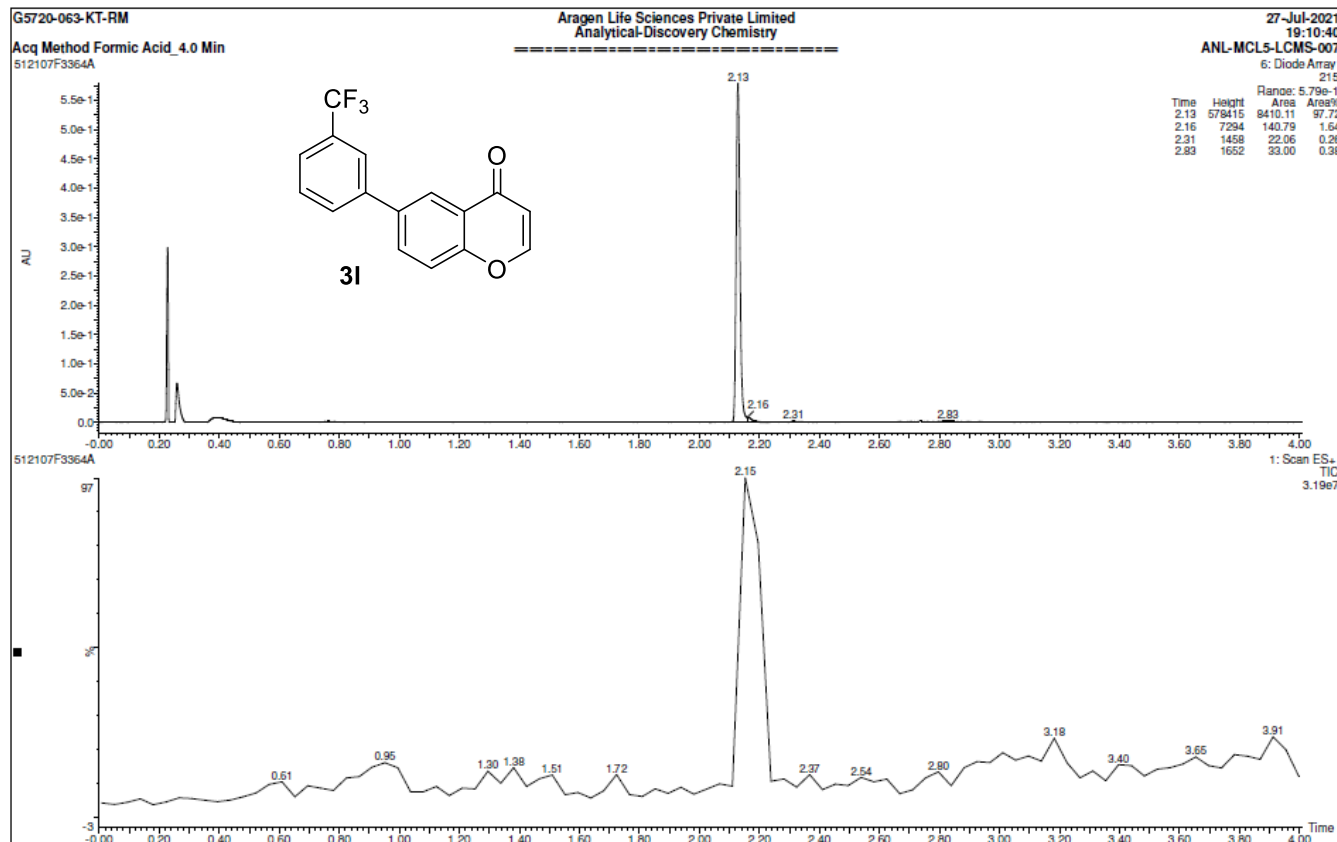
7.13e+007



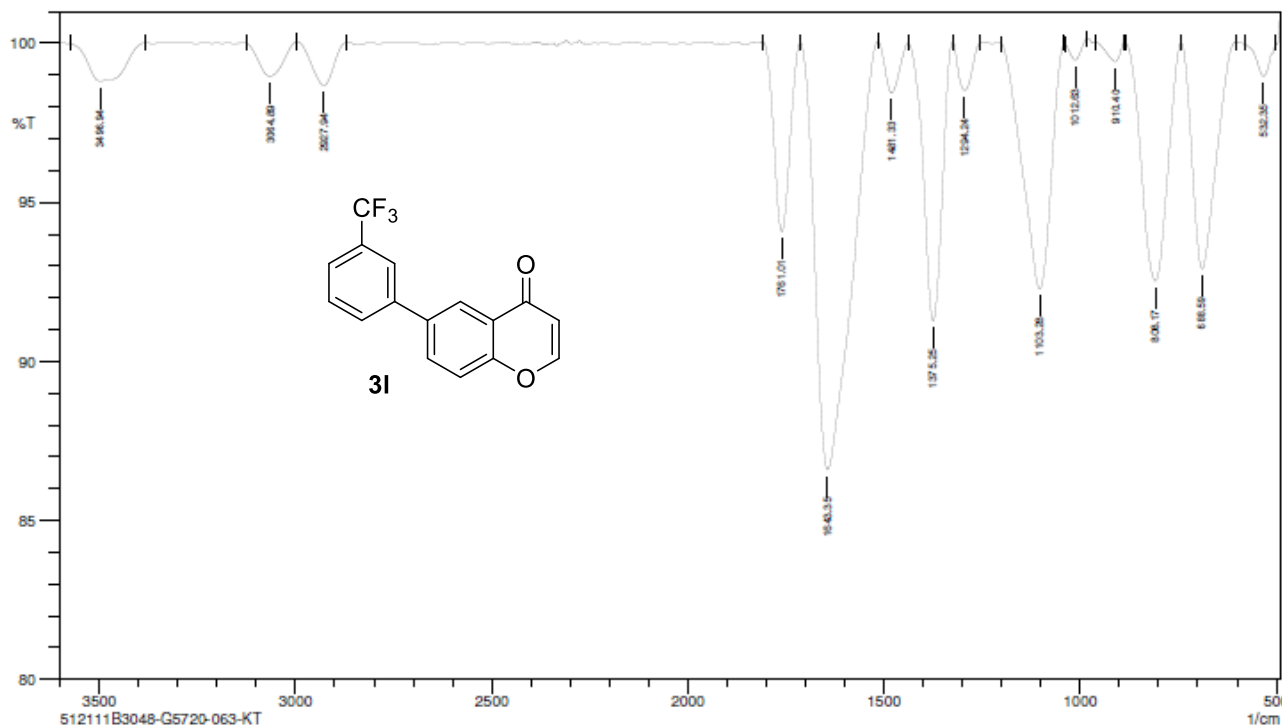
Minimum: -1.5
Maximum: 5.0 1000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
161.0512	161.0603	-9.1	-56.5	6.5	50.9	n/a	n/a	C10 H9 O2





Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry



Sample Name: 512111B3048-G5720-063-KT

No. of Scans:

Date/Time: 11/9/2021 8:58:37 PM

User: Aragen

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

10 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

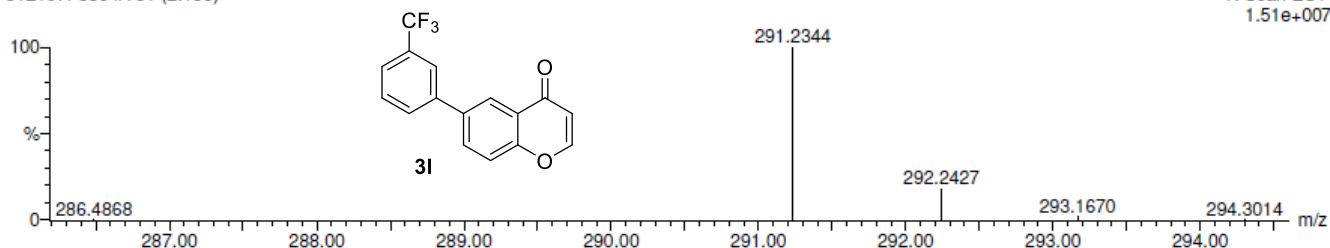
C: 0-16 H: 0-10 O: 0-2 F: 0-3

G5720-063-KT-RM

Acq Method Formic Acid_4.0 Min
512107F3364A 51 (2.153)

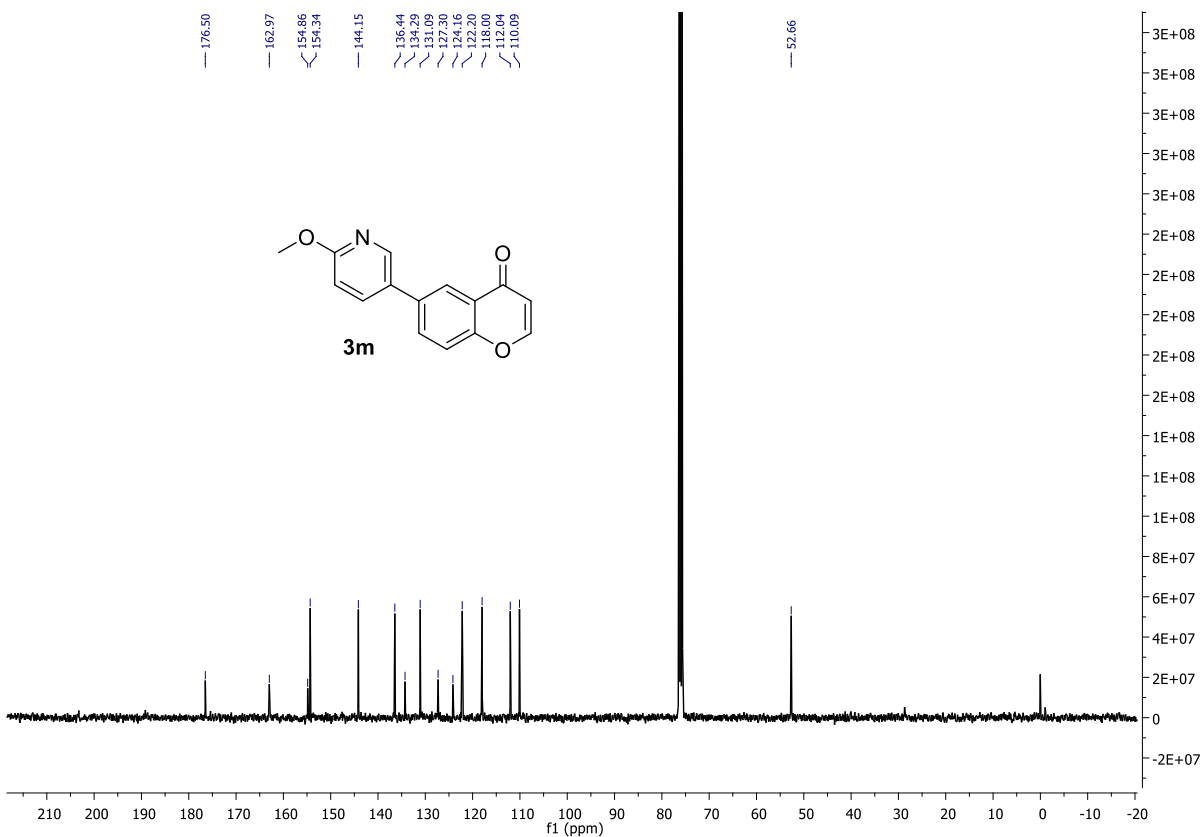
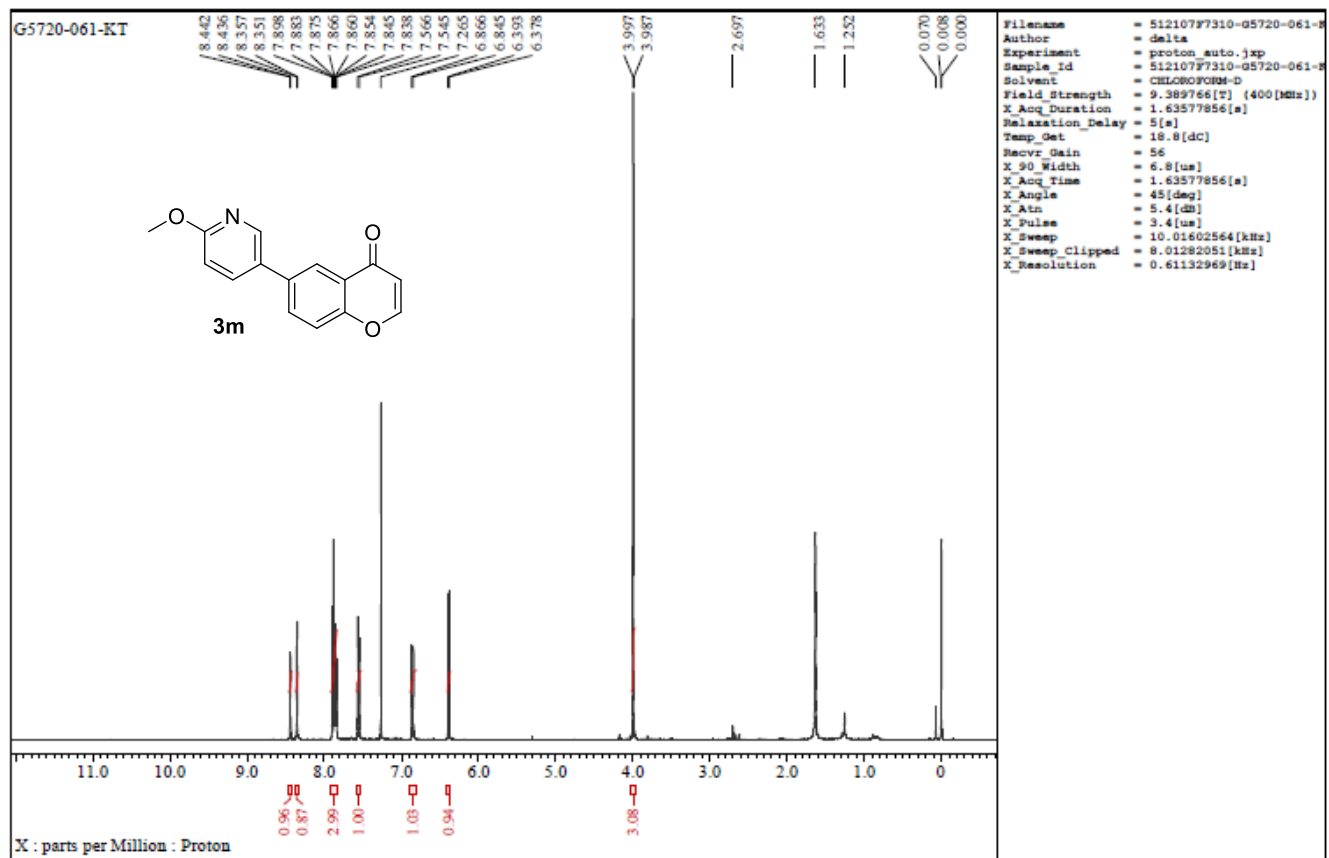
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry

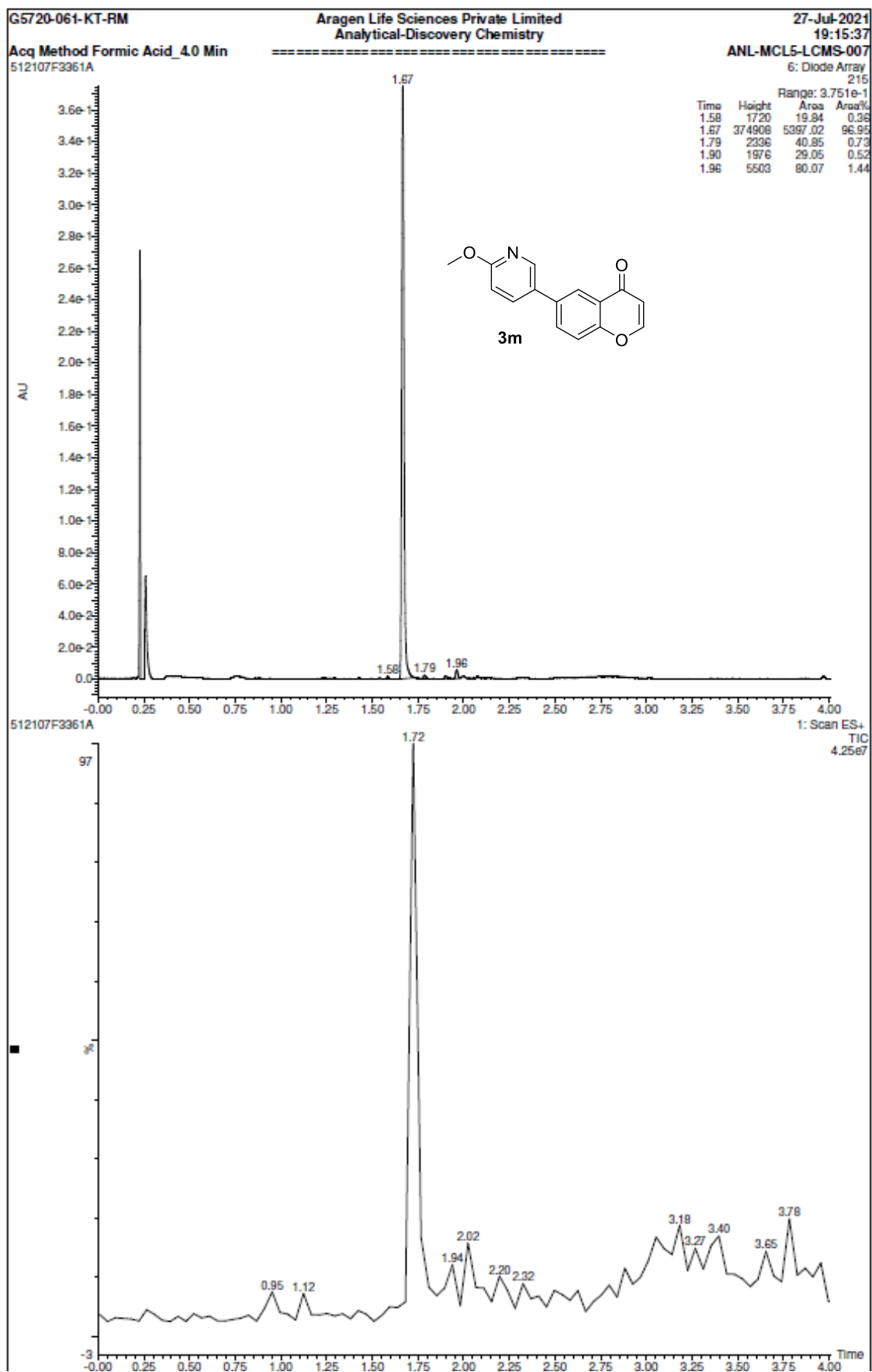
27-Jul-2021
19:10:40
ANL-MCL5-LCMS-007
1: Scan ES+
1.51e+007

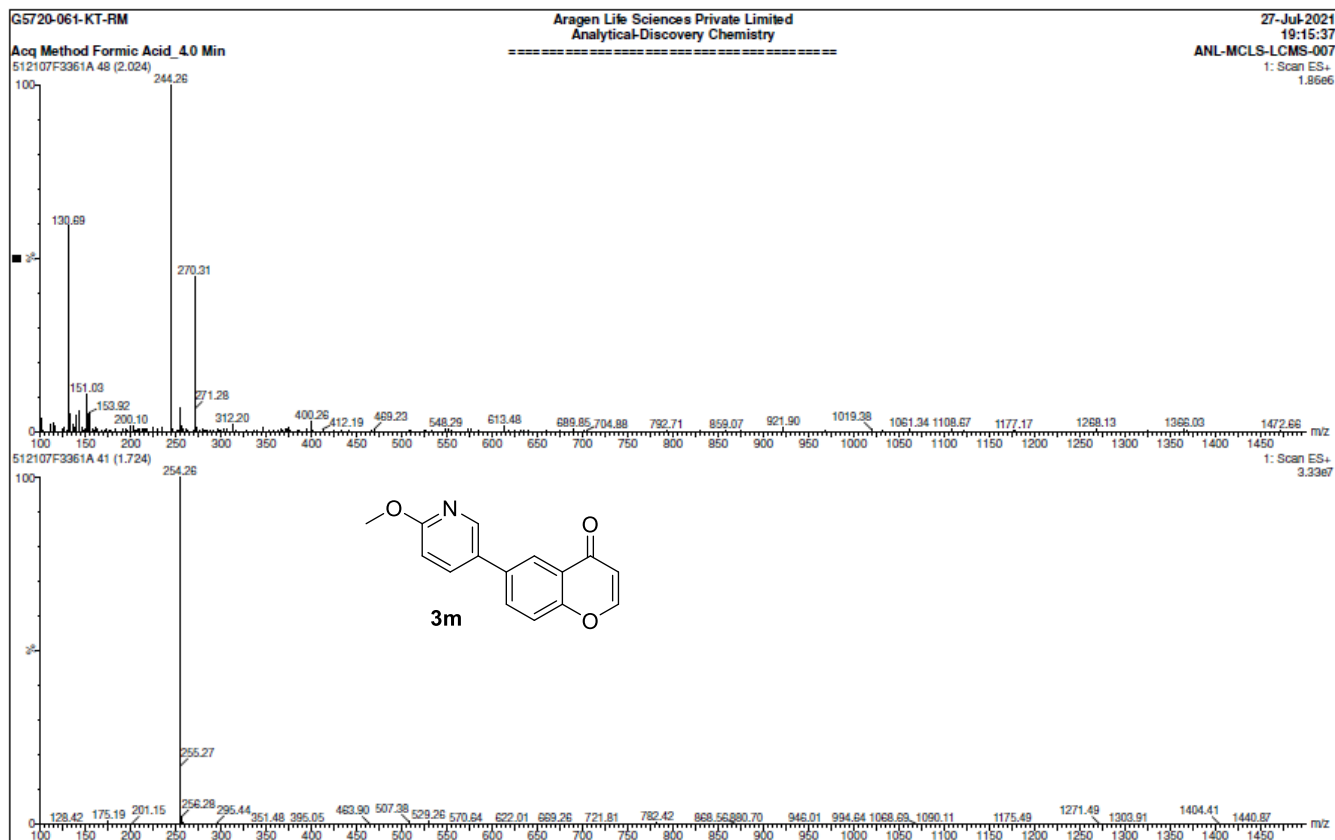


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
291.0699	291.0633	6.6	22.7	10.5	40.3	n/a	n/a	C16 H10 O2 F3







Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

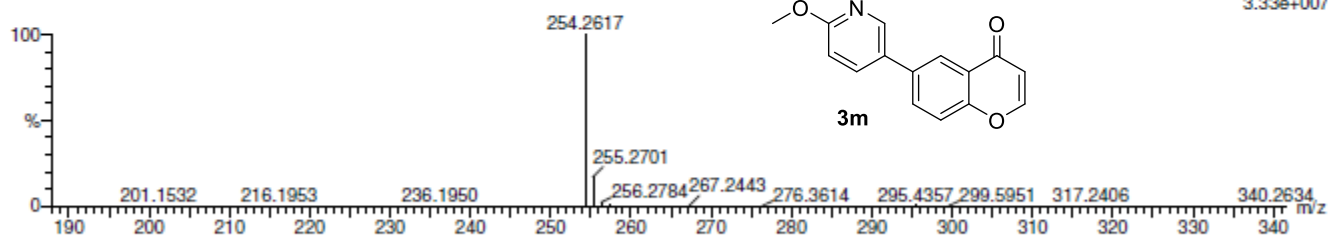
Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

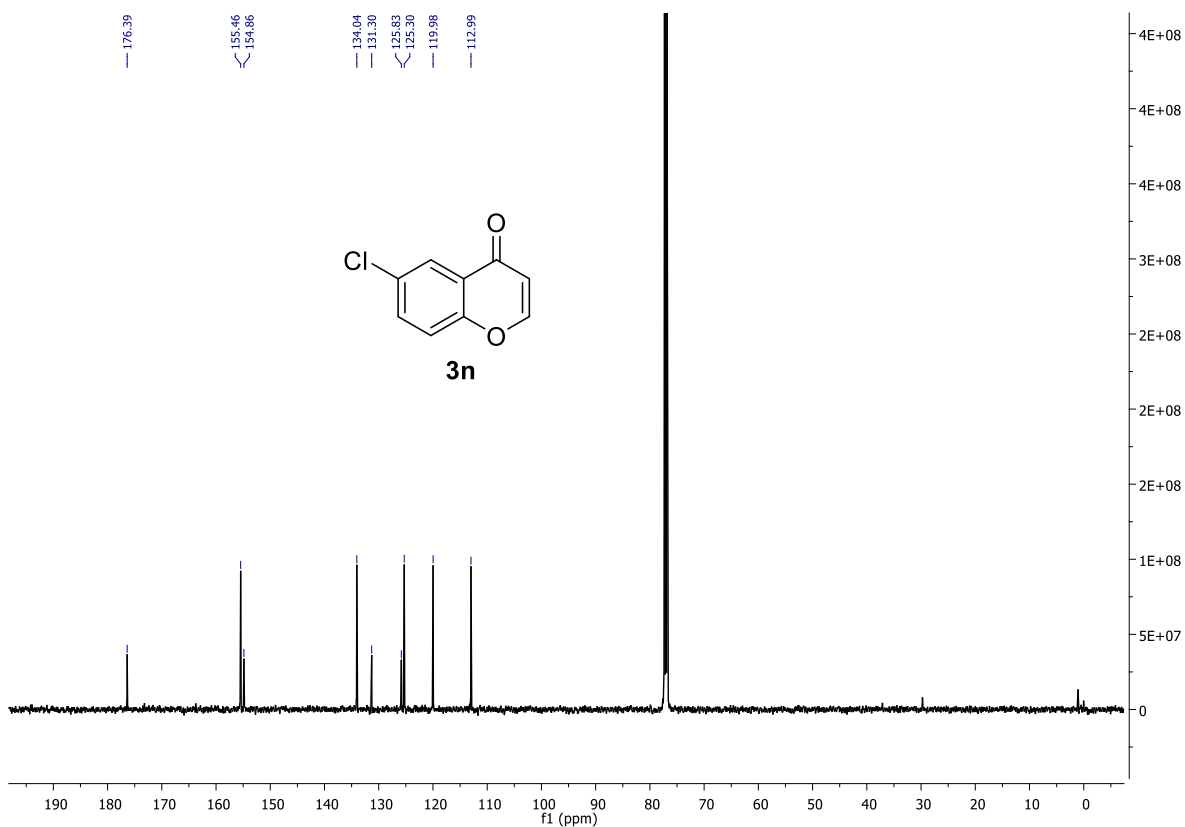
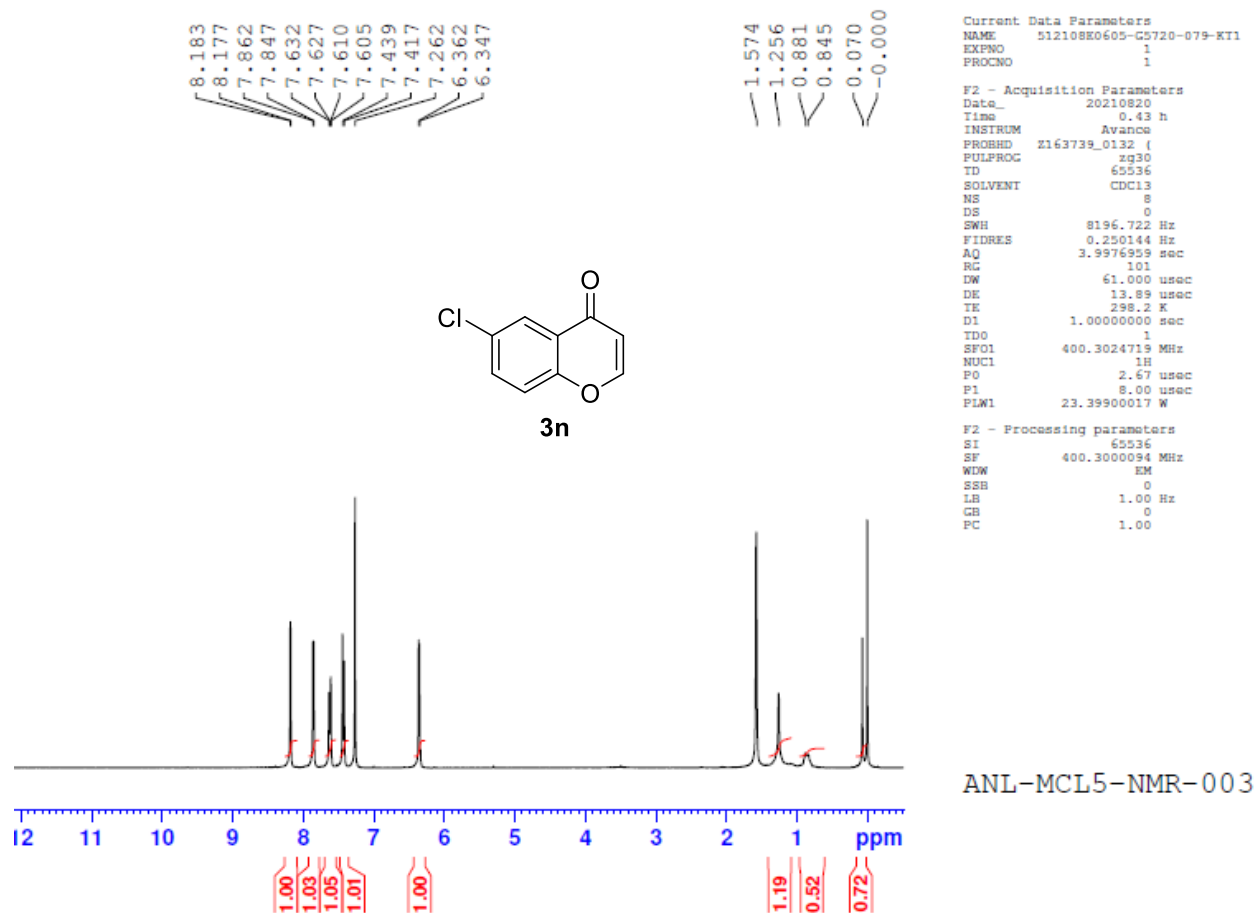
Elements Used:

C: 0-15 H: 0-12 N: 0-1 O: 0-3

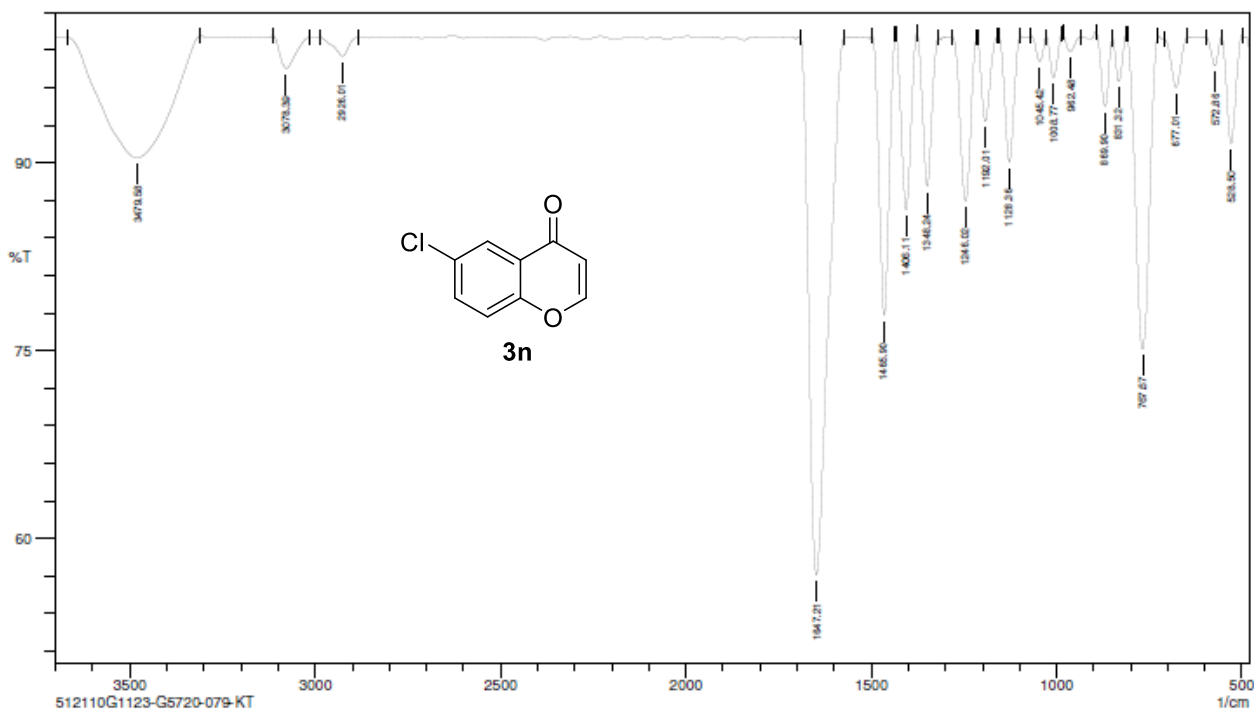
G5720-061-KT-RM

Acq Method Formic Acid_4.0 Min
512107F3361A 41 (1.724)Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry27-Jul-2021
19:15:37
ANL-MCLS-LCMS-007
1: Scan ES+
3.33e+007Minimum: -1.5
Maximum: 5.0 1000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
254.0815	254.0817	-0.2	-0.8	10.5	33.8	n/a	n/a	C15 H12 N O3



Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry



Sample Name:
512110G1123-G5720-079-KT

No. of Scans:

Date/Time: 10/29/2021 7:49:52 PM

User: Aragen

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

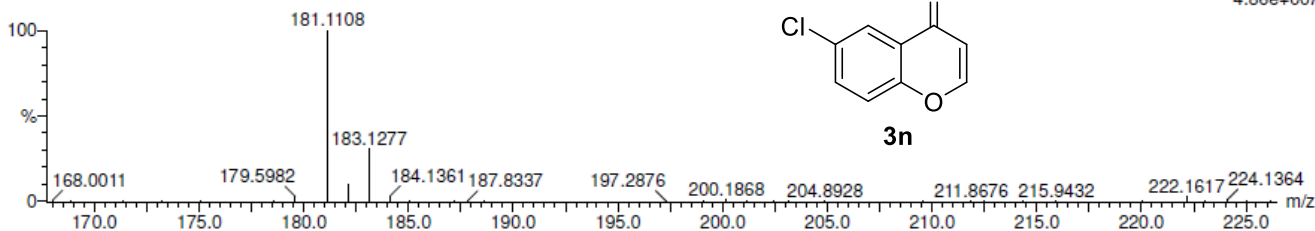
C: 0-9 H: 0-6 O: 0-2 Cl: 0-1

G5720-079-KT1

Acq Method Formic Acid_4.0 Min
512108E0604A 38 (1.595)

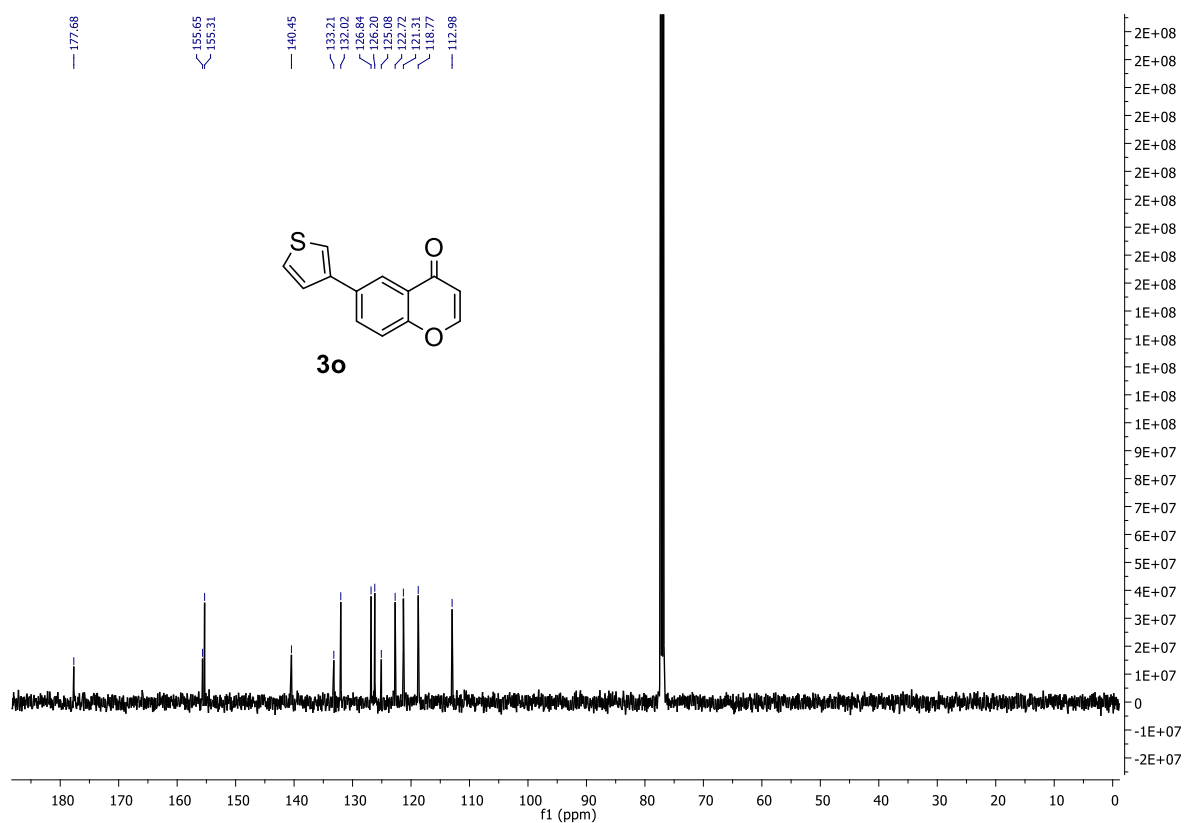
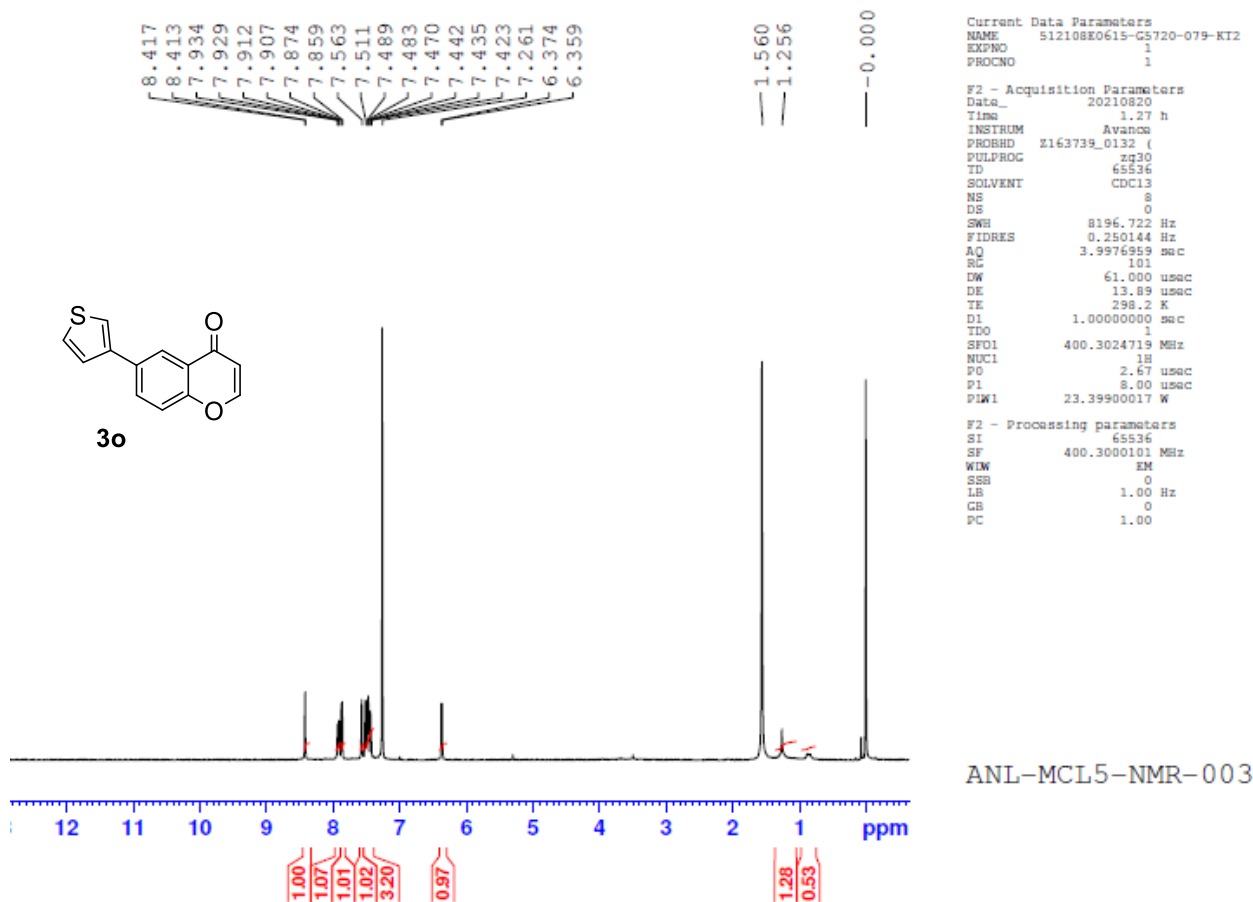
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry

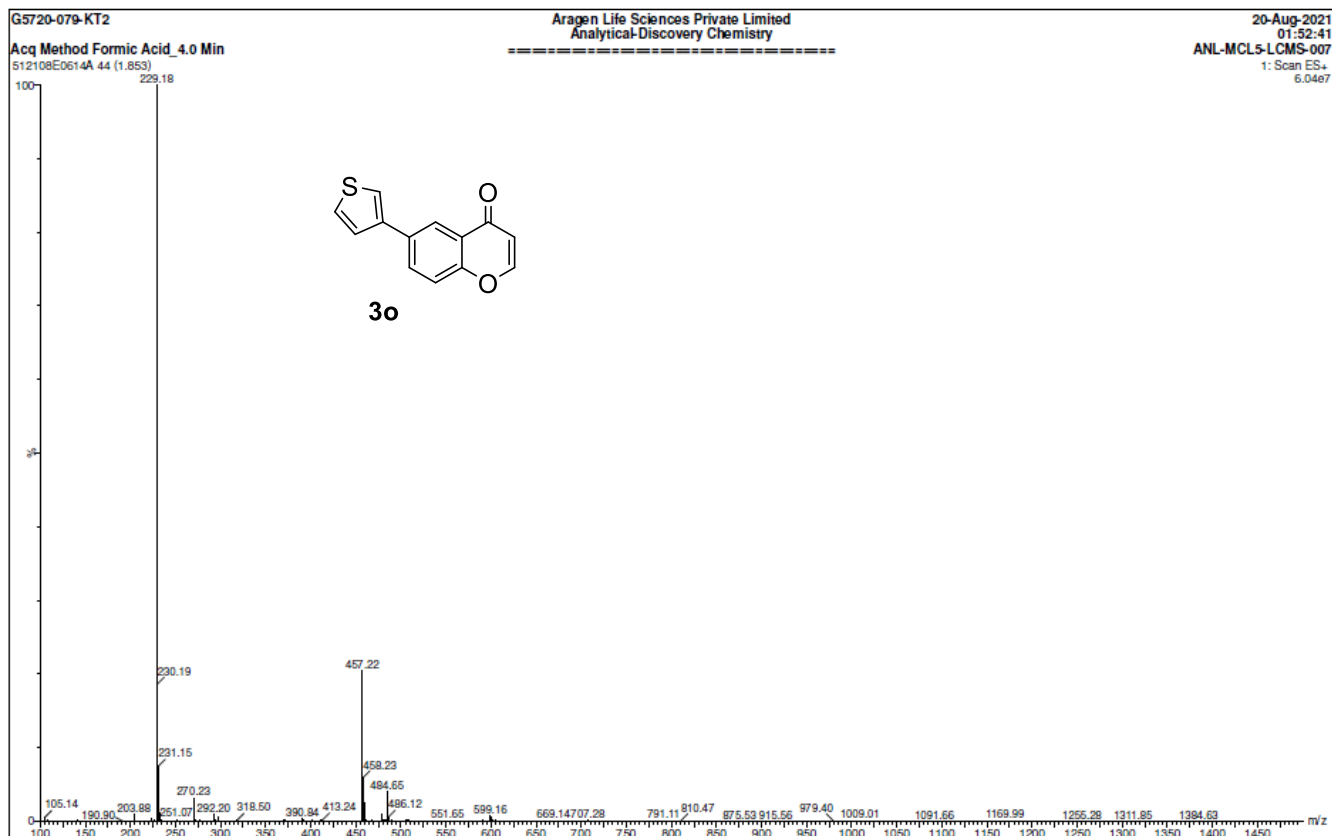
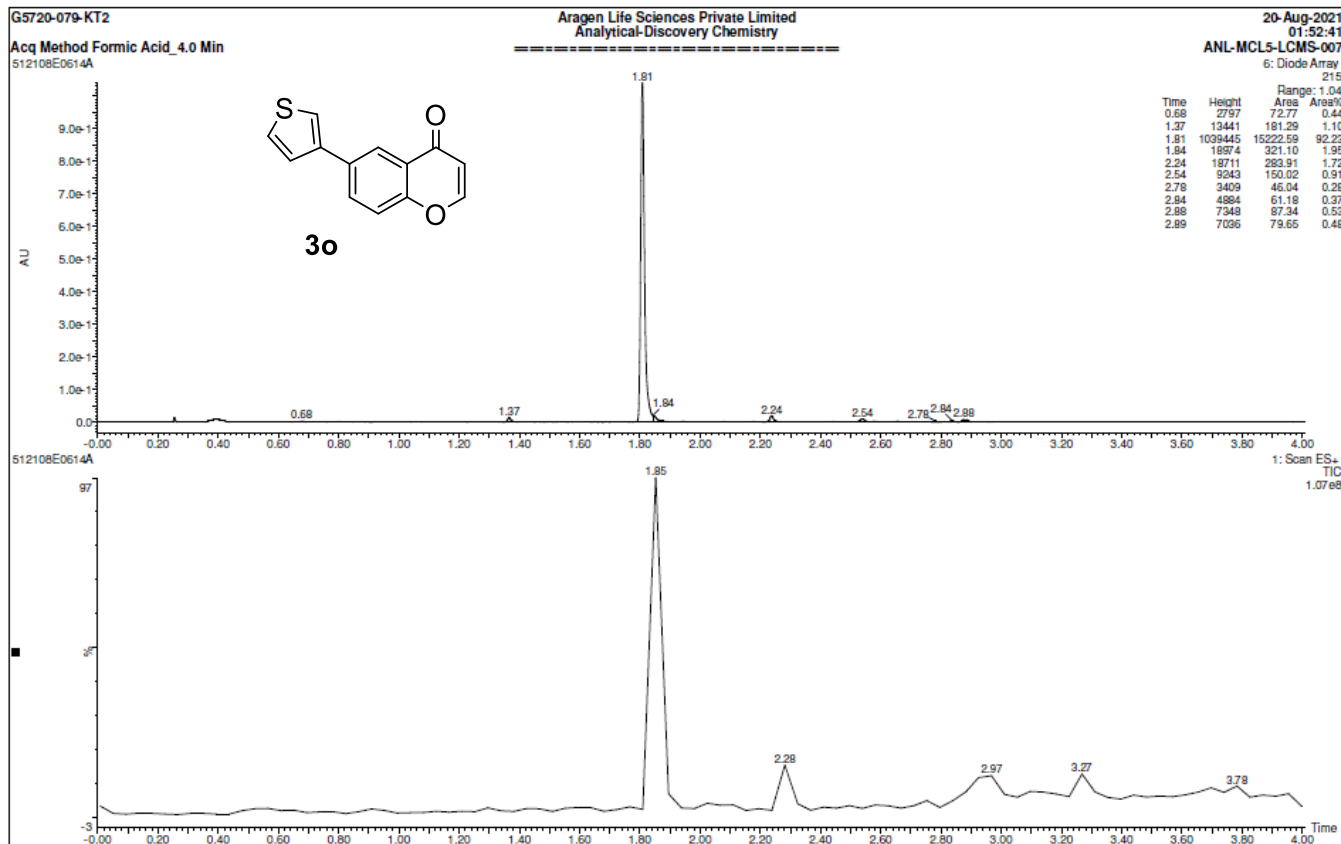
20-Aug-2021
01:57:37
ANL-MCL5-LCMS-007
1: Scan ES+
4.86e+007



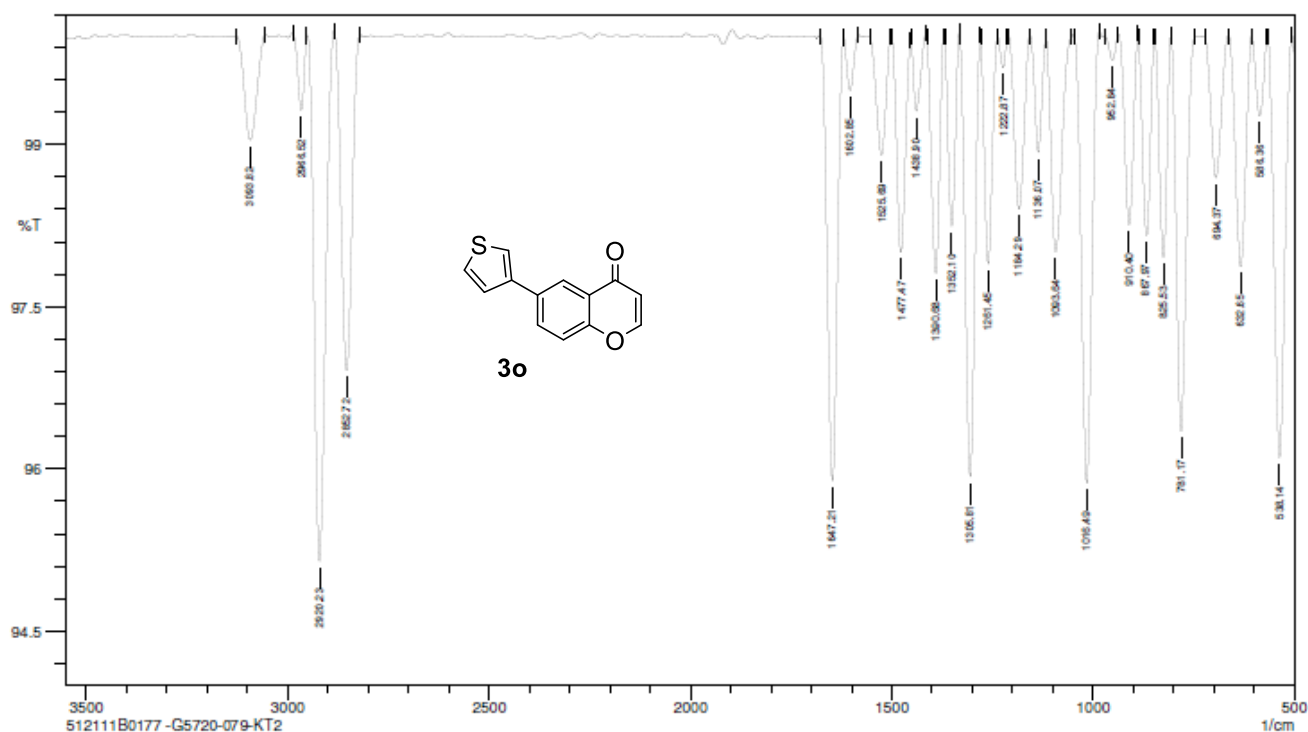
Minimum: -1.5
Maximum: 5.0 1000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
181.0112	181.0056	5.6	30.9	6.5	47.6	n/a	n/a	C9 H6 O2 Cl





Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry



Sample Name:
512111B0177 - G5720-079-KT2

No. of Scans:

Date/Time: 11/8/2021 6:56:07 PM

User: Aragen

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-13 H: 0-9 O: 0-2 S: 0-1

G5720-079-KT2

Acq Method Formic Acid_4.0 Min
512108E0614A 44 (1.853)

Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry

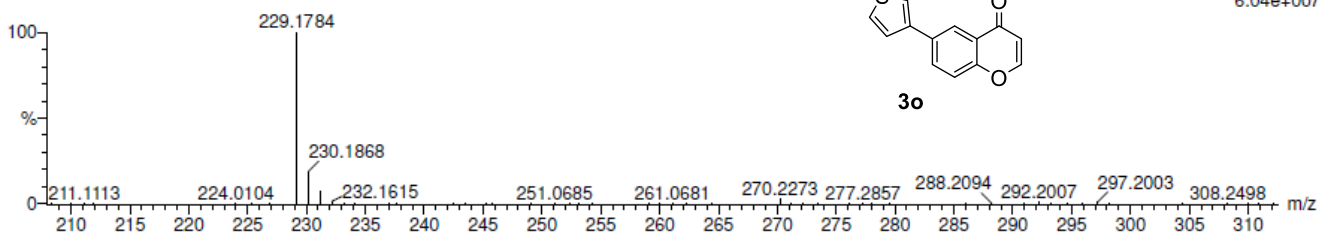
20-Aug-2021

01:52:41

ANL-MCL5-LCMS-007

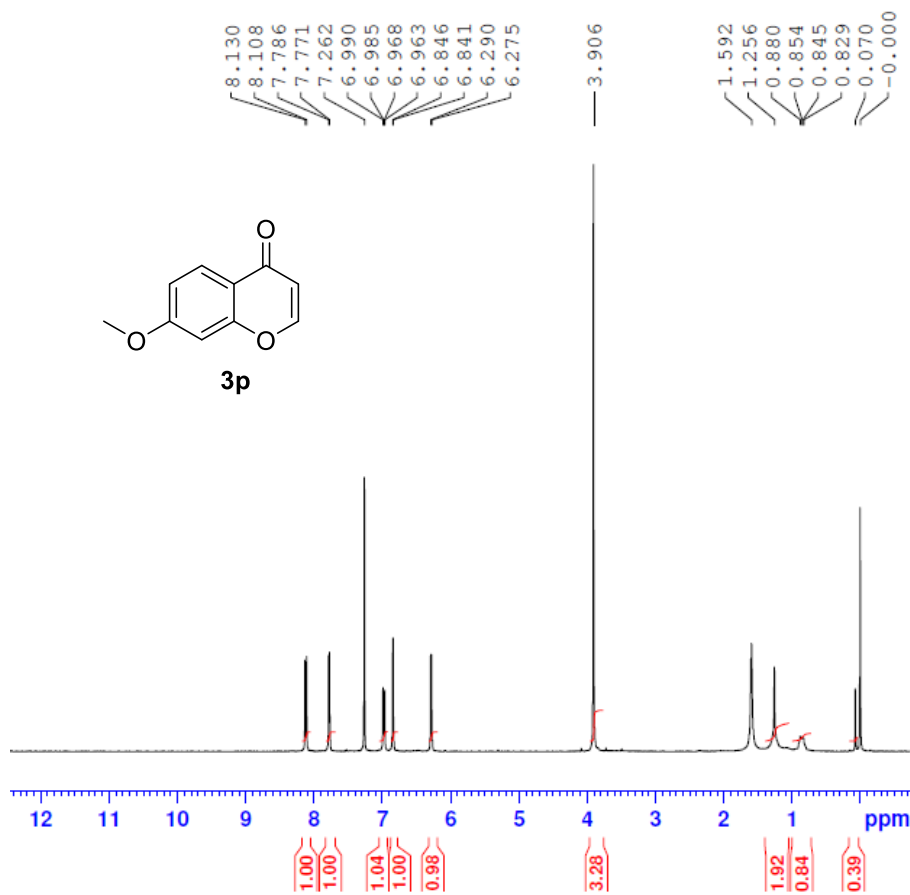
1: Scan ES+

6.04e+007



Minimum: -1.5
Maximum: 5.0 1000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
229.0245	229.0323	-7.8	-34.1	9.5	51.9	n/a	n/a	C13 H9 O2 S

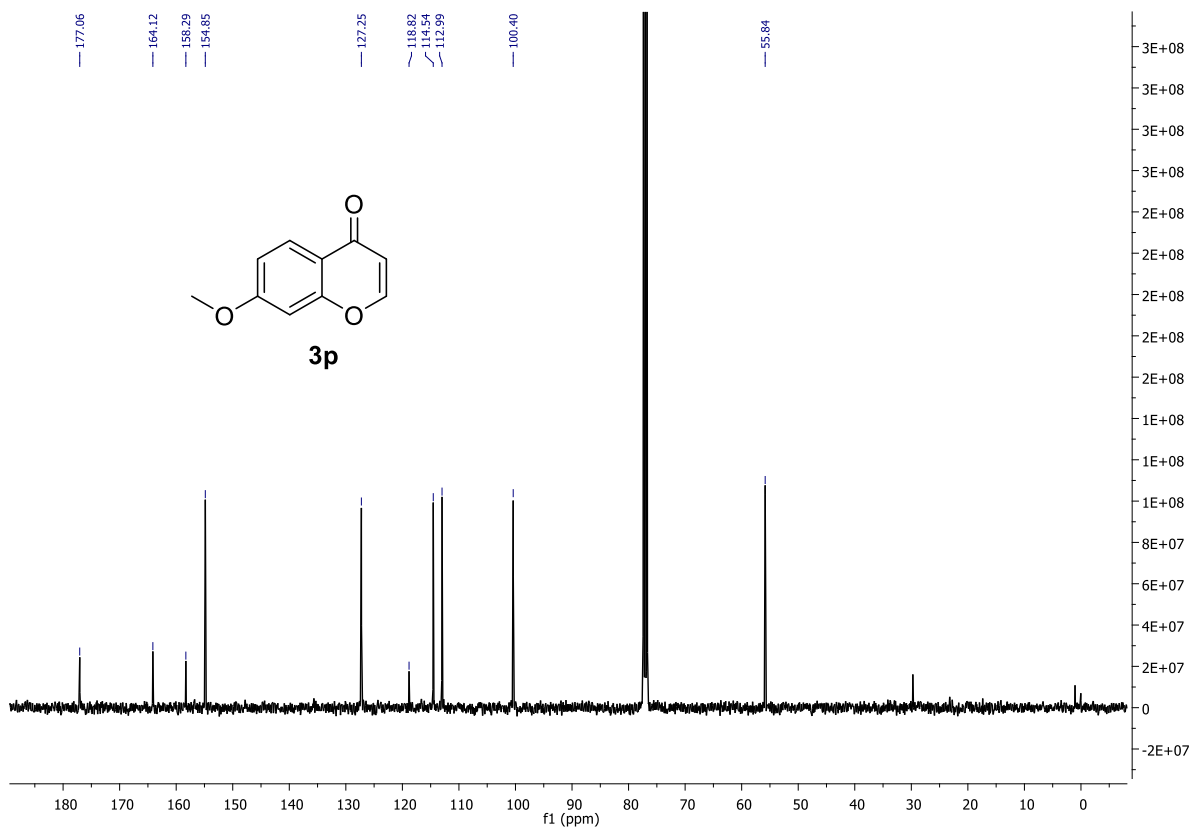


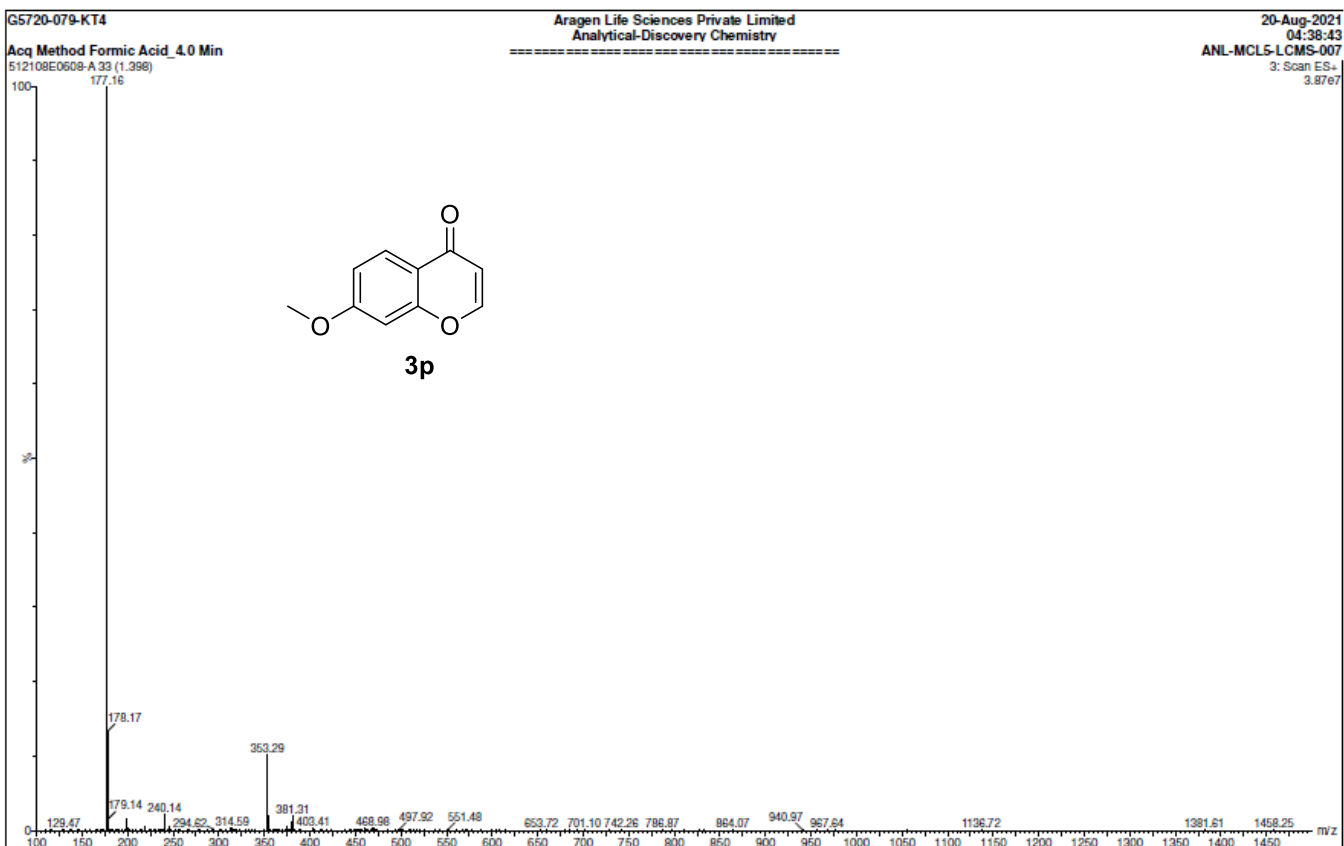
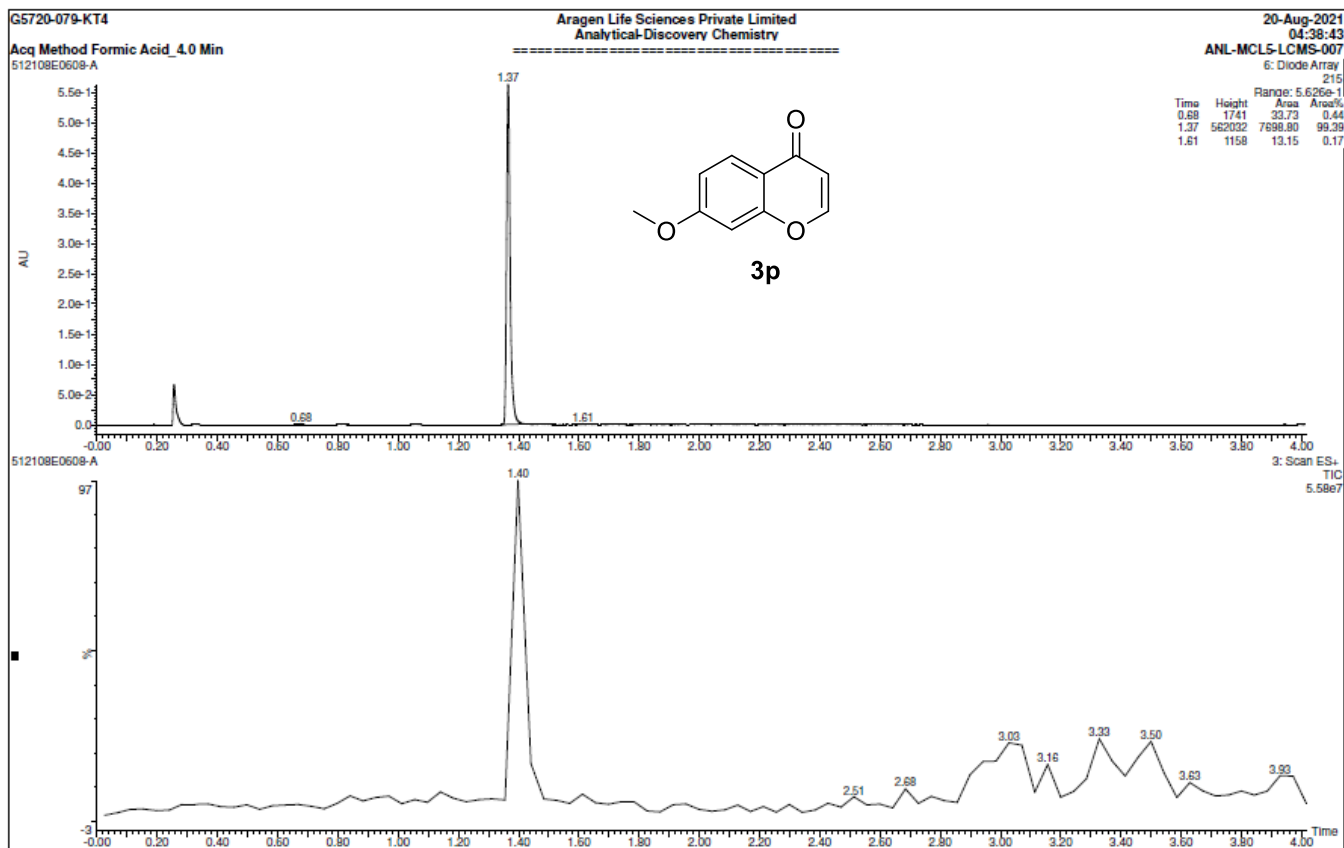
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 EXPNO 1
 PROCNO 1

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 Time 2.07 h
 INSTRUM Avance
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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 8196.722 Hz
 FIDRES 0.250144 Hz
 AQ 3.9976959 sec
 RG 101
 DW 61.000 usec
 DE 13.89 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1
 SFO1 400.3024719 MHz
 NUC1 1H
 PO 2.67 usec
 P1 8.00 usec
 PLW1 23.39900017 W

F2 - Processing parameters
 SI 65536
 SF 400.3000095 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

ANL-MCL5-NMR-003





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-10 H: 0-9 O: 0-3

G5720-079-KT4

Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry

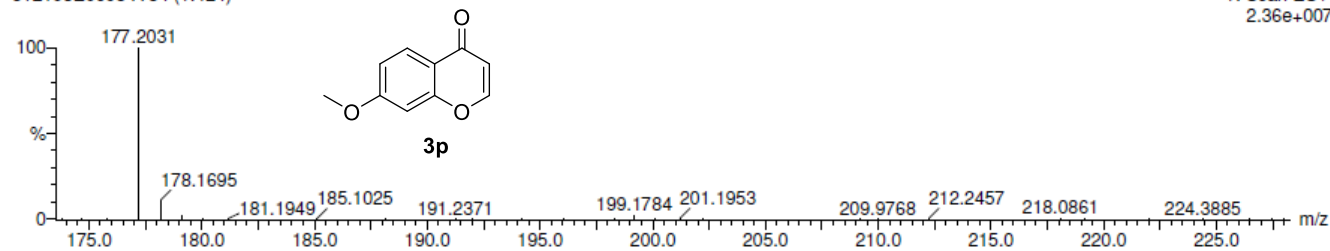
20-Aug-2021

04:38:43

ANL-MCL5-LCMS-007

1: Scan ES+

2.36e+007

Acq Method Formic Acid_4.0 Min
512108E0608-A 34 (1.424)

Minimum: -1.5
Maximum: 5.0 1000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
177.0552	177.0552	0.0	0.0	6.5	47.1	n/a	n/a	C10 H9 O3