Supplementary Material

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

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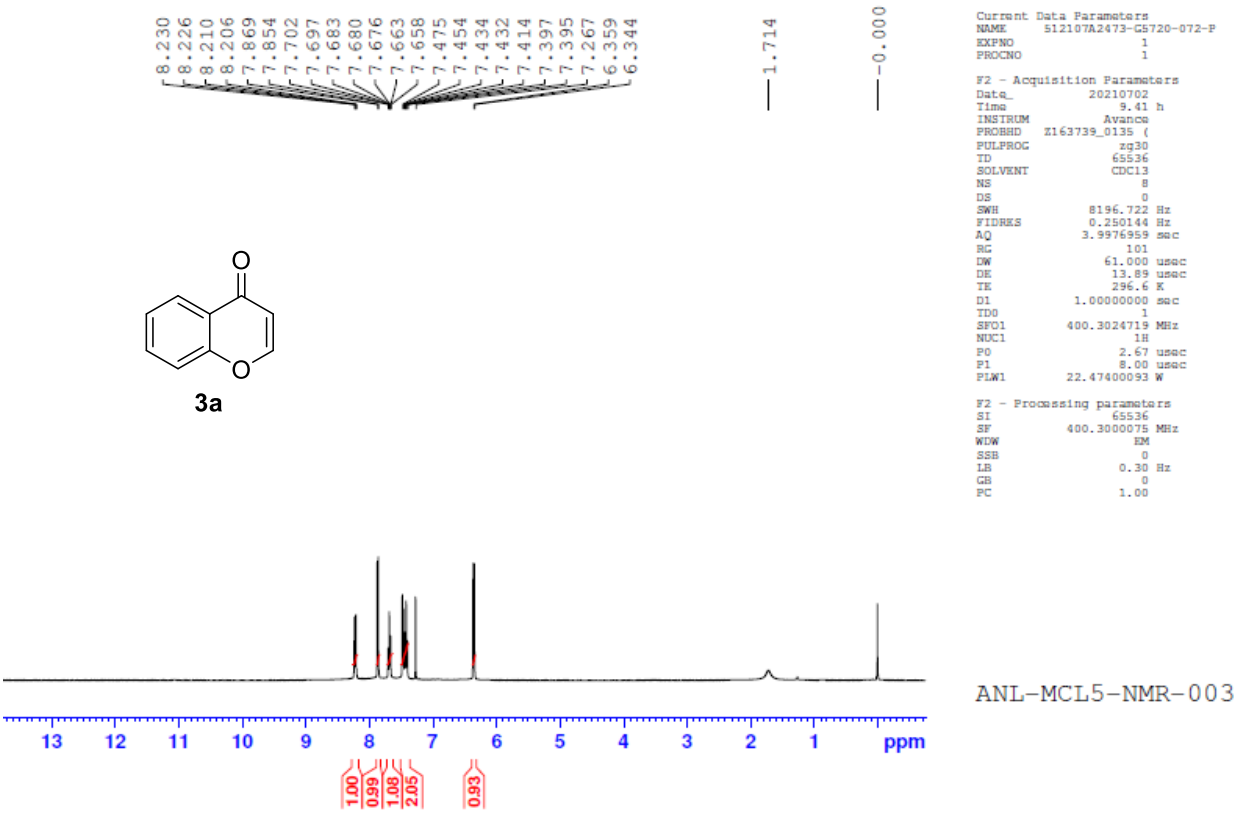
1. General

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 F_{254}. Silica gel column chromatography was performed on silica gel 60 (spherical 100-200 µm). IR spectrawere recorded on Perkin-Elmer FT/IR-4000 using ATR.^{1}H NMR spectra were recorded onVarian-400 (400 MHz) spectrometer. Chemical shifts of ^{1}H NMRspectra 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 to 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.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113.03
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O
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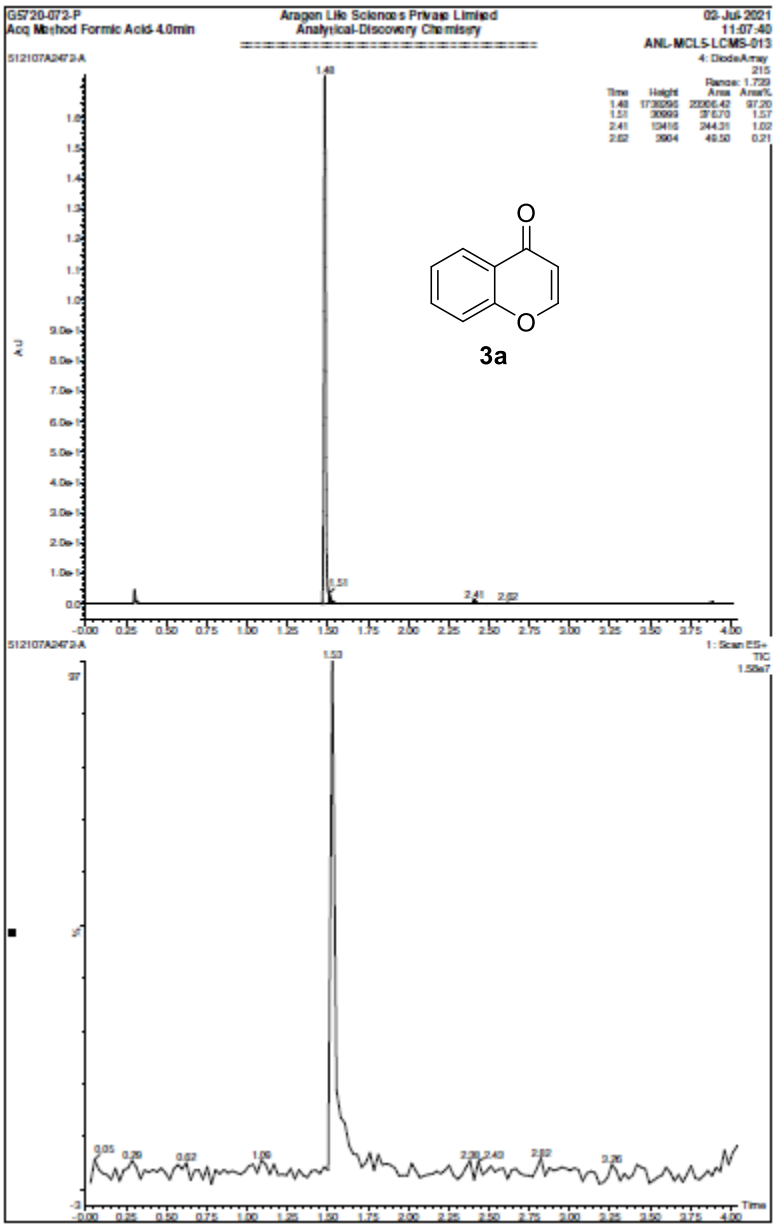
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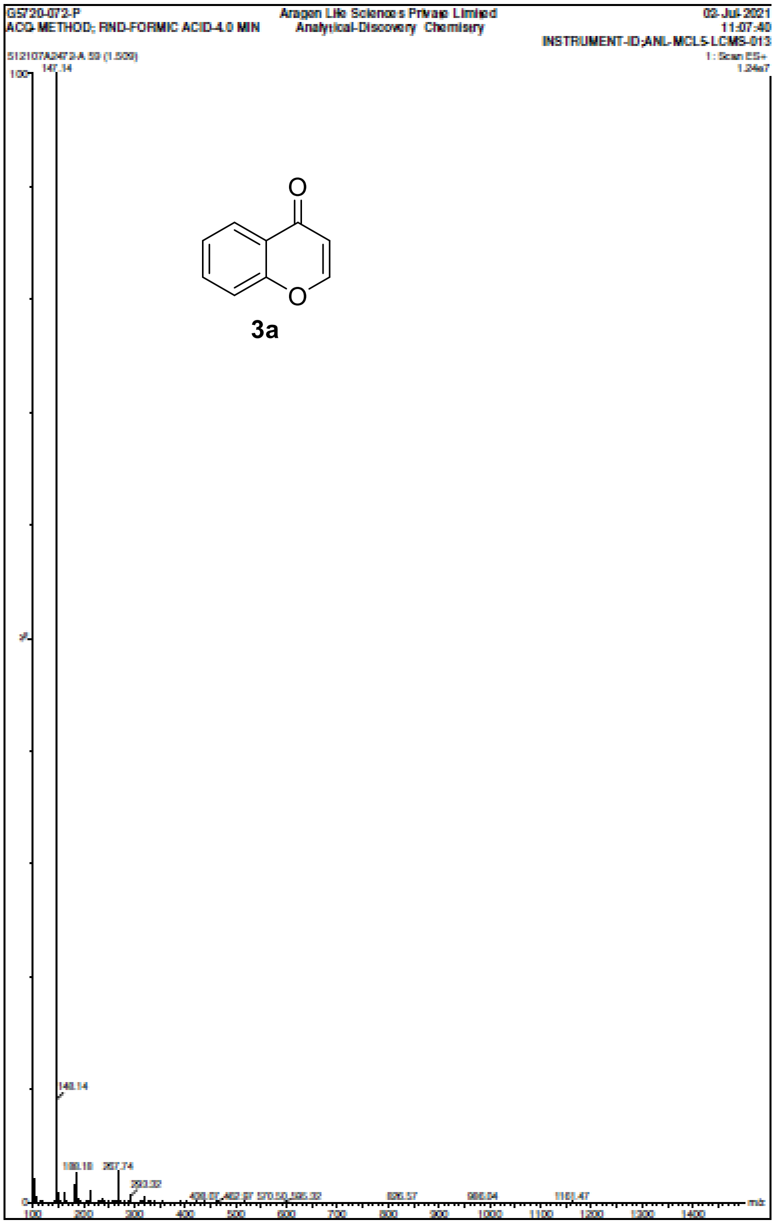
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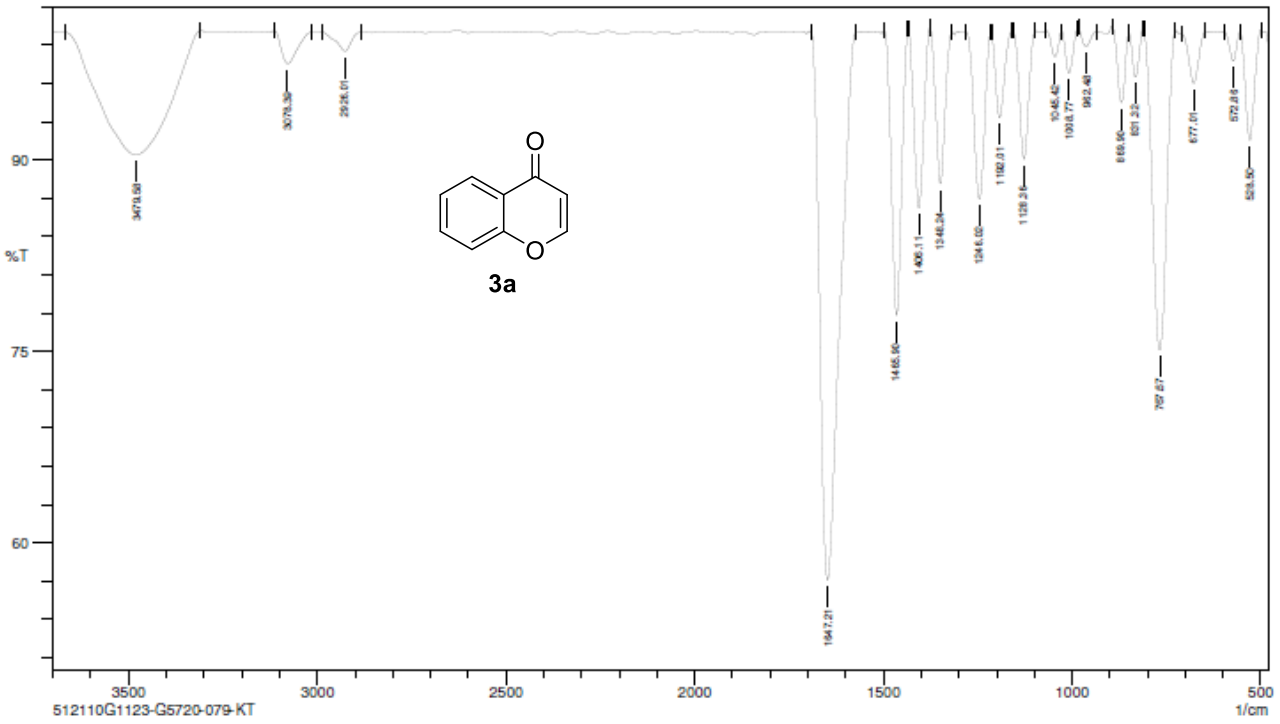

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User: Aragen

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Page 1

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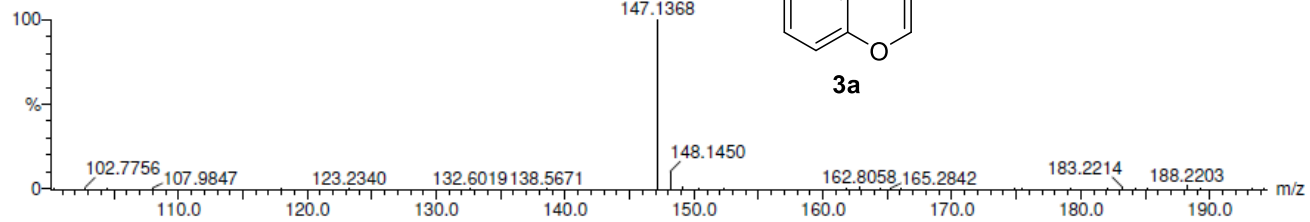

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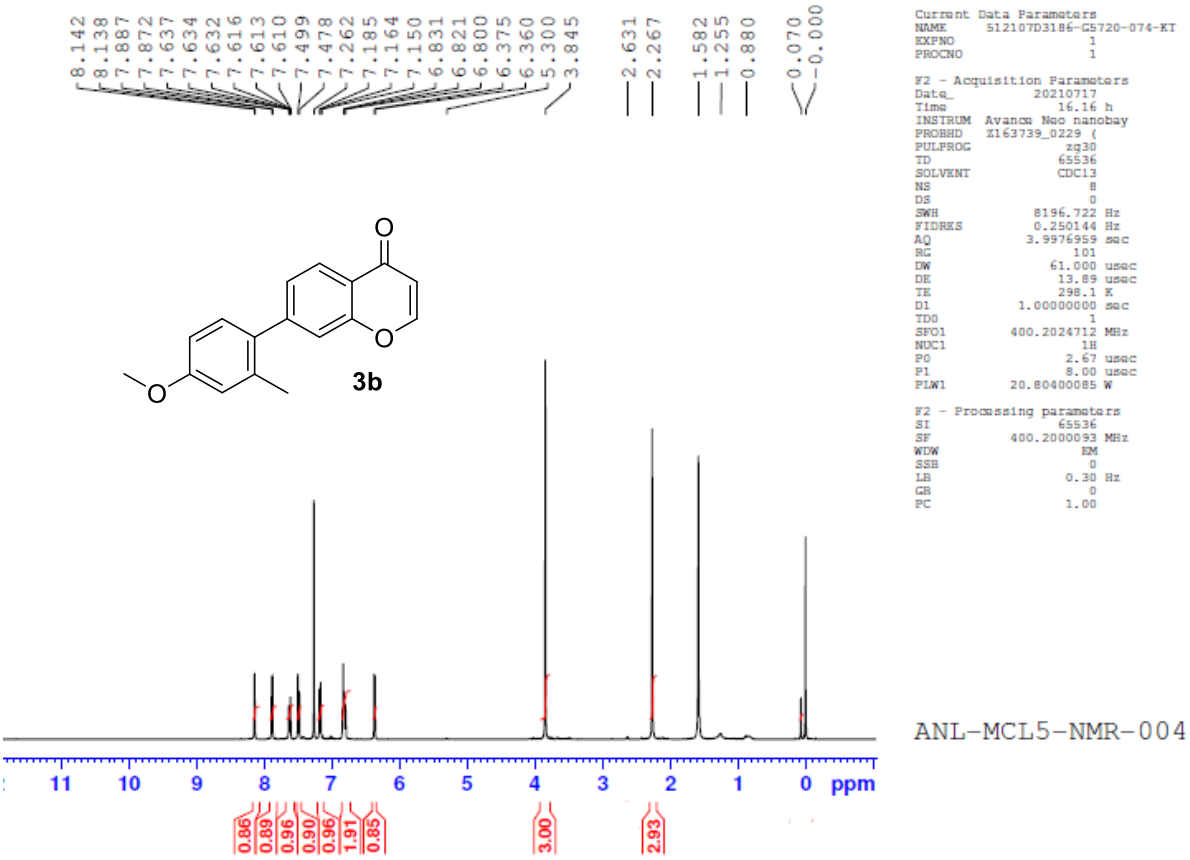
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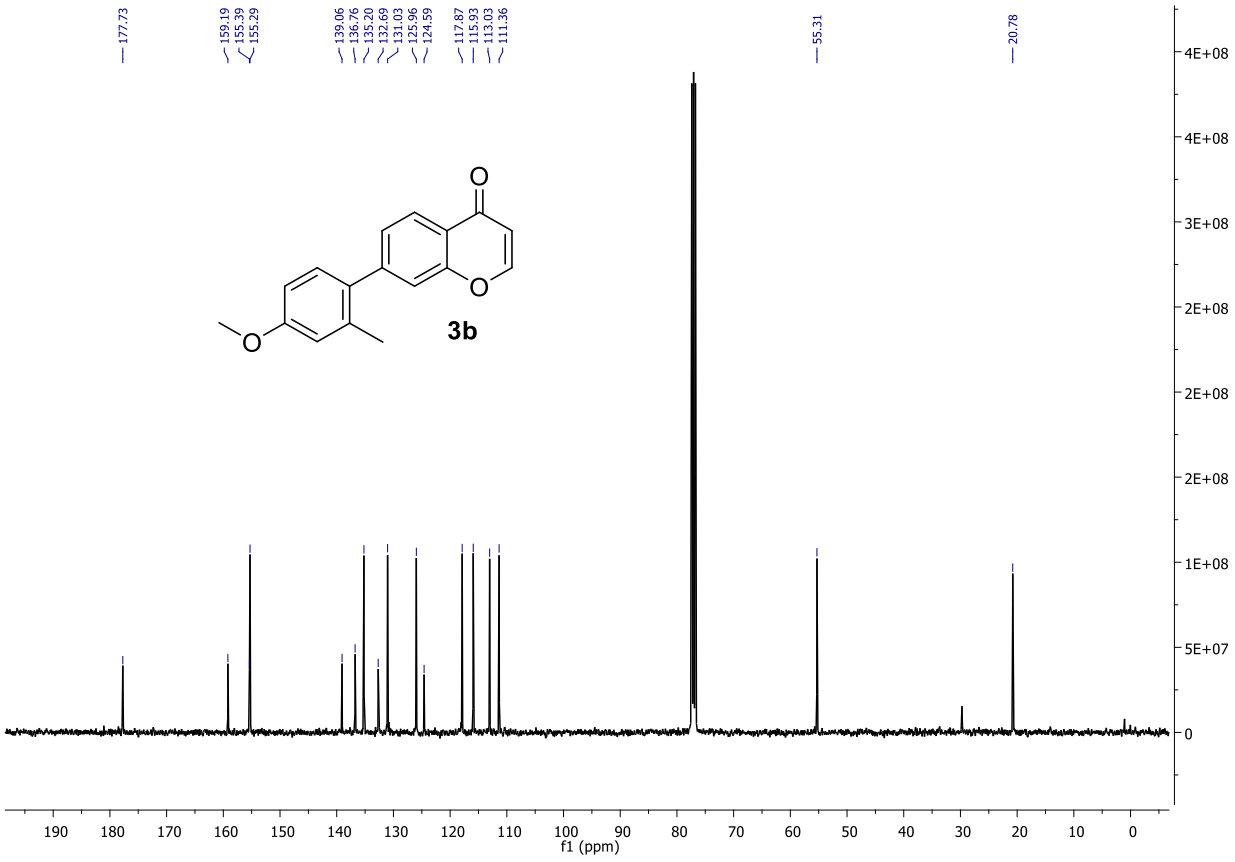
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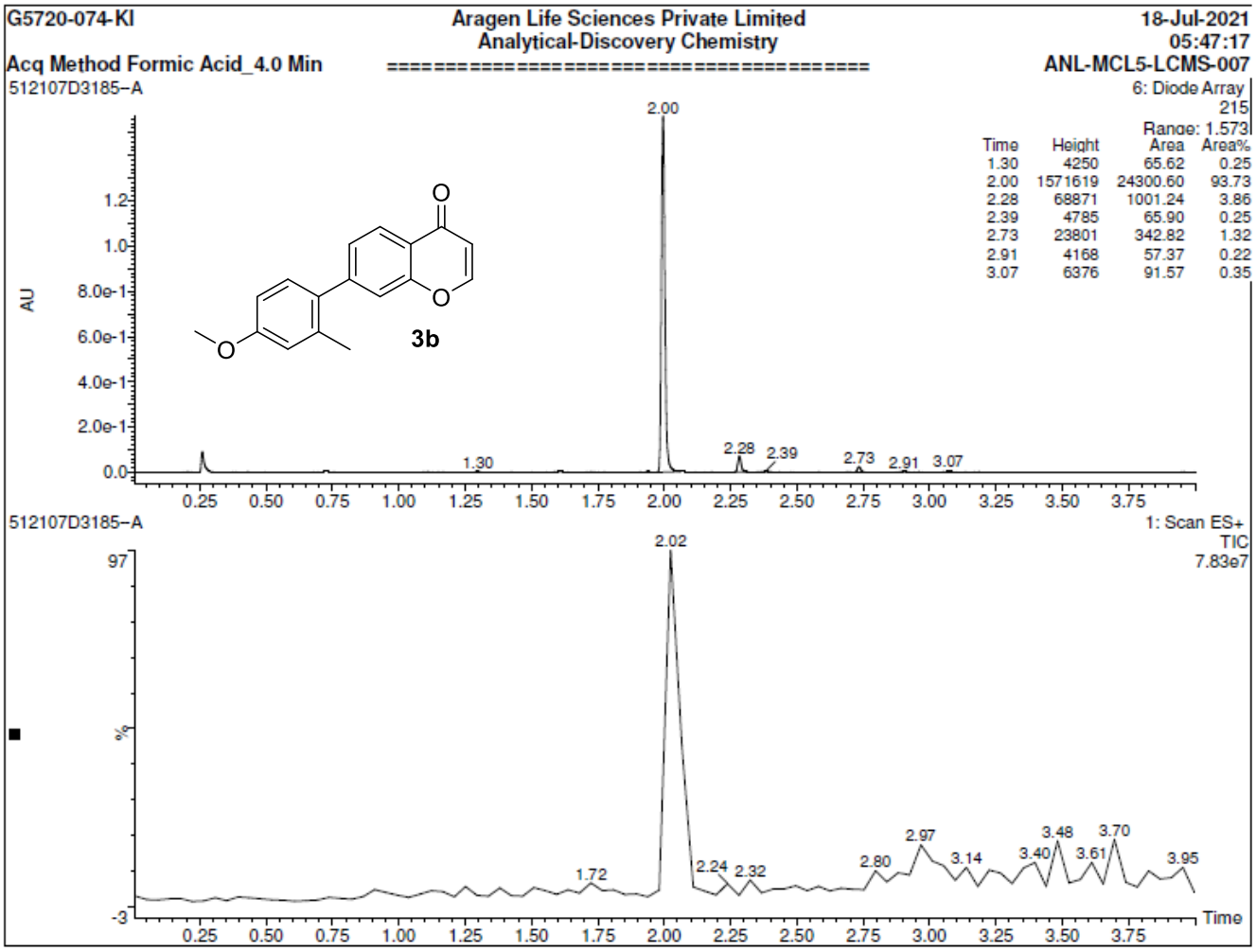
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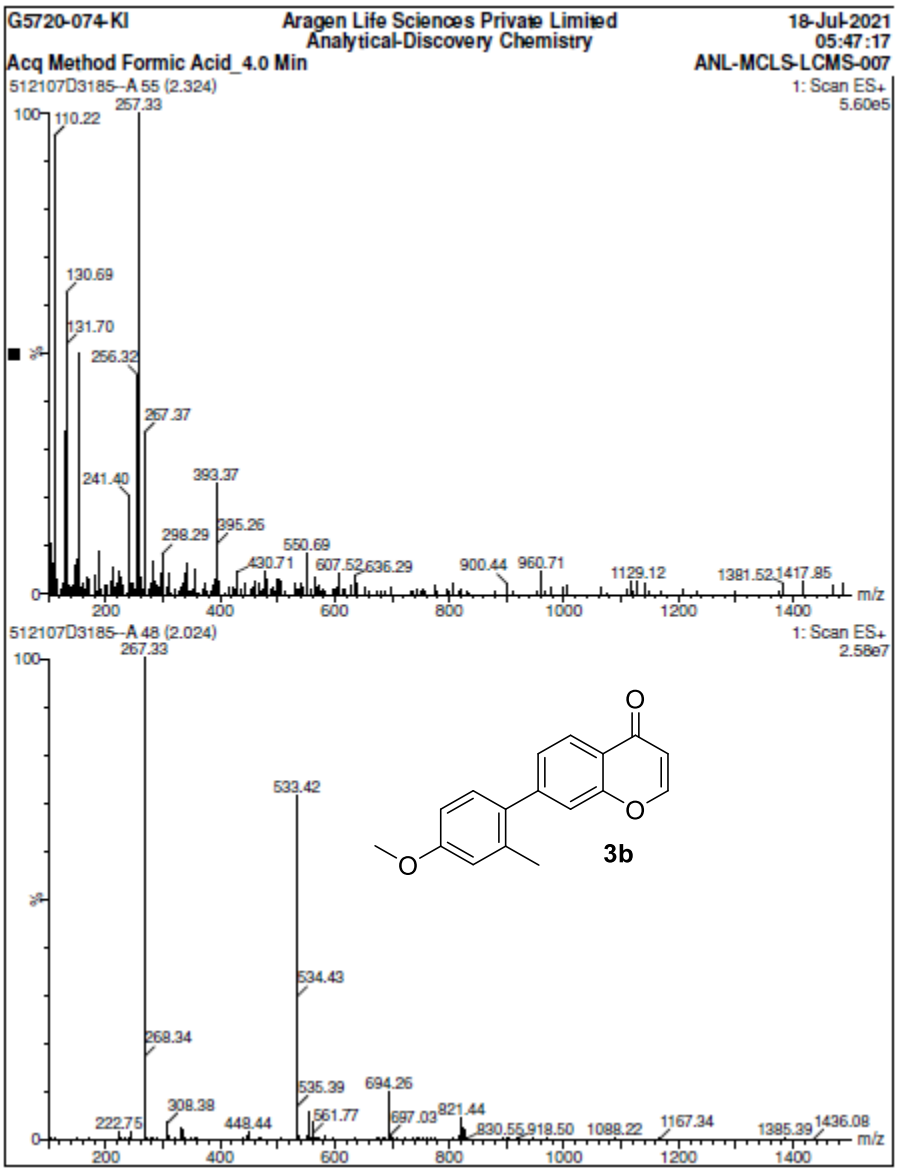
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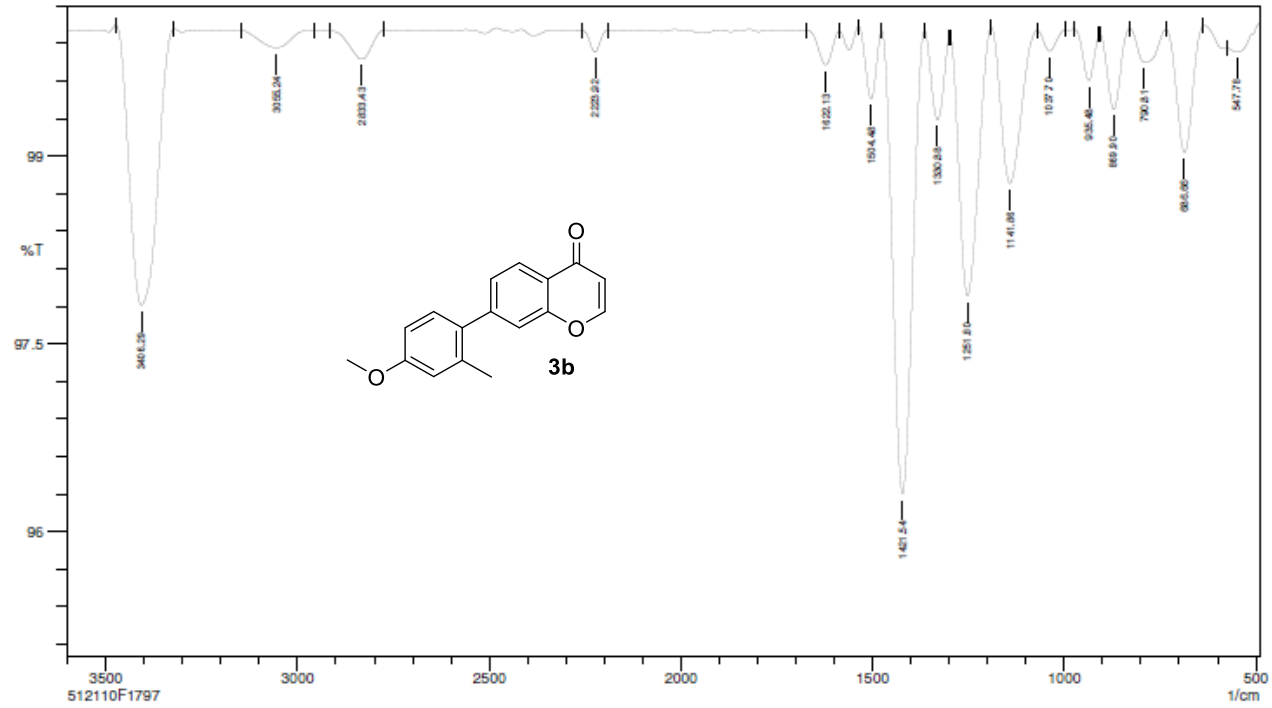
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry



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Elemental Composition Report

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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

Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry

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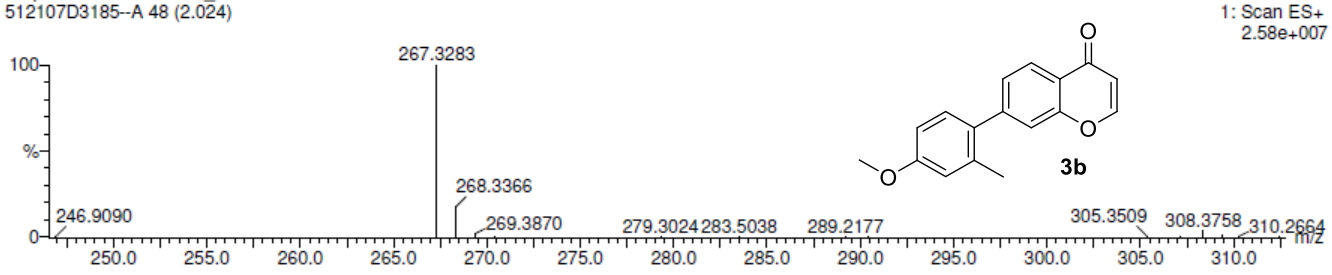

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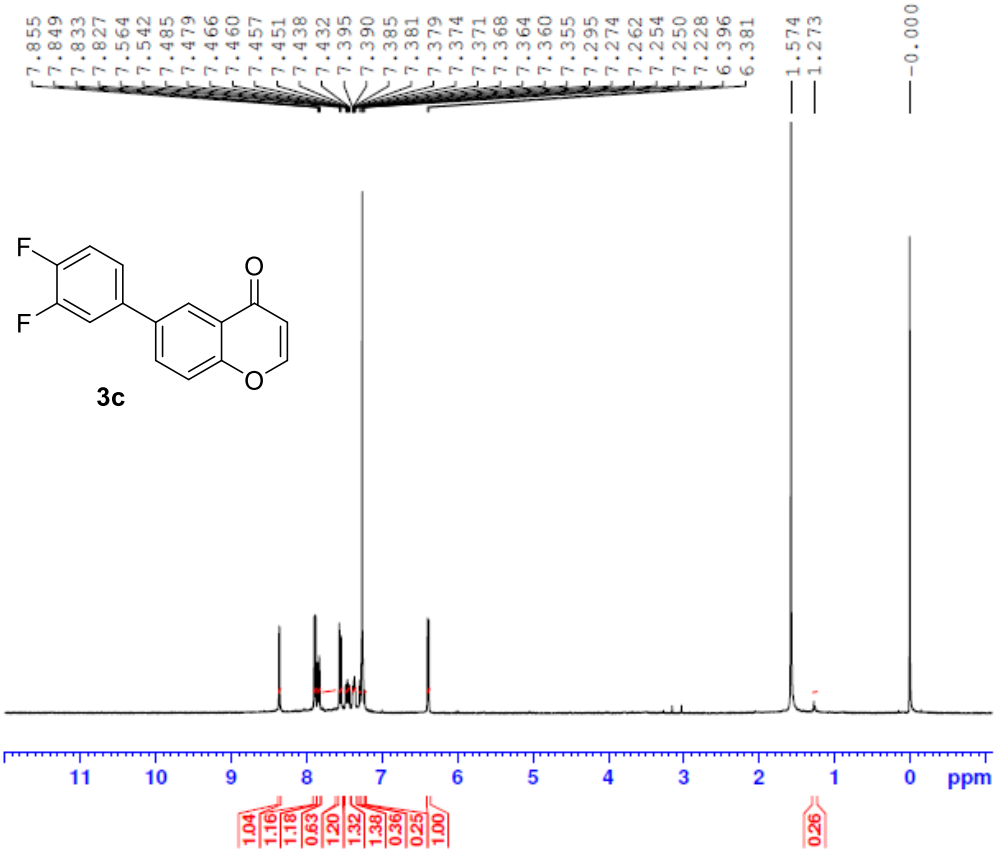


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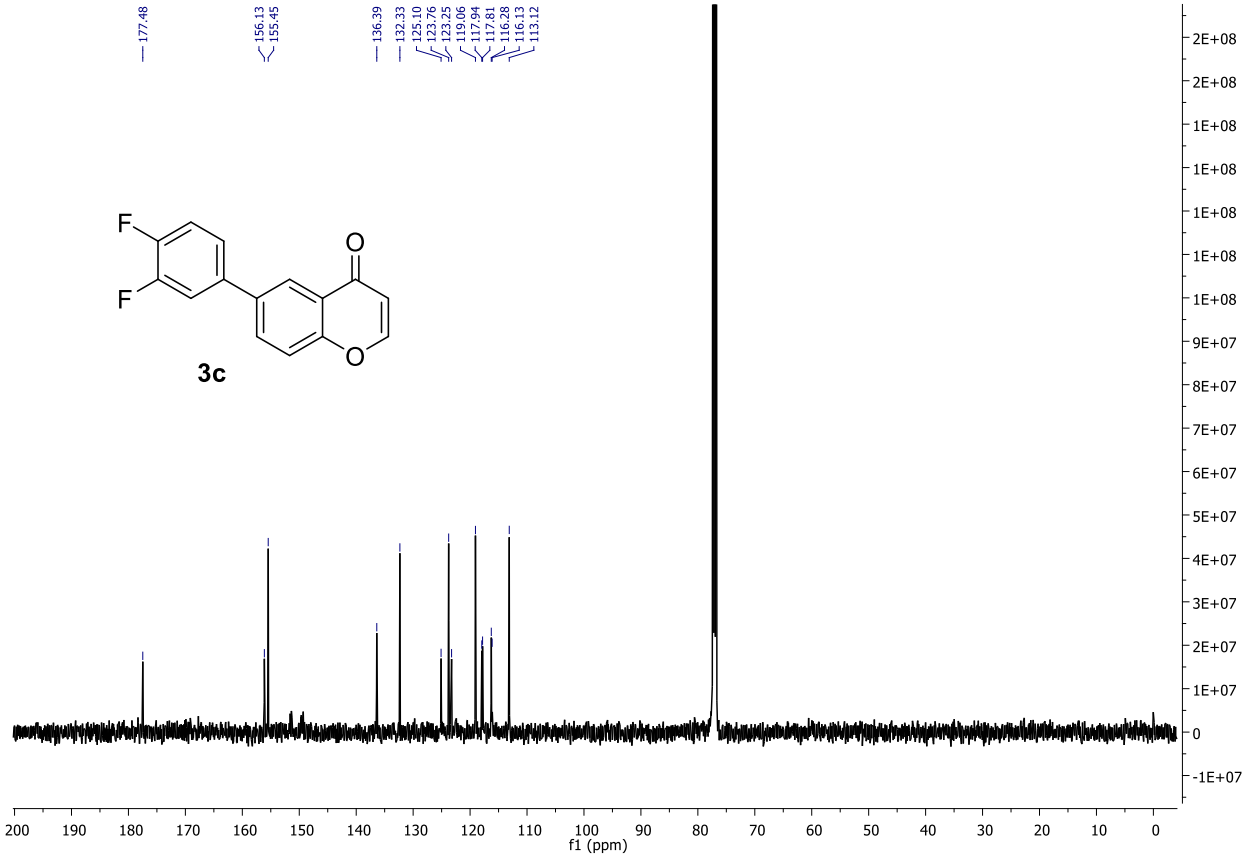

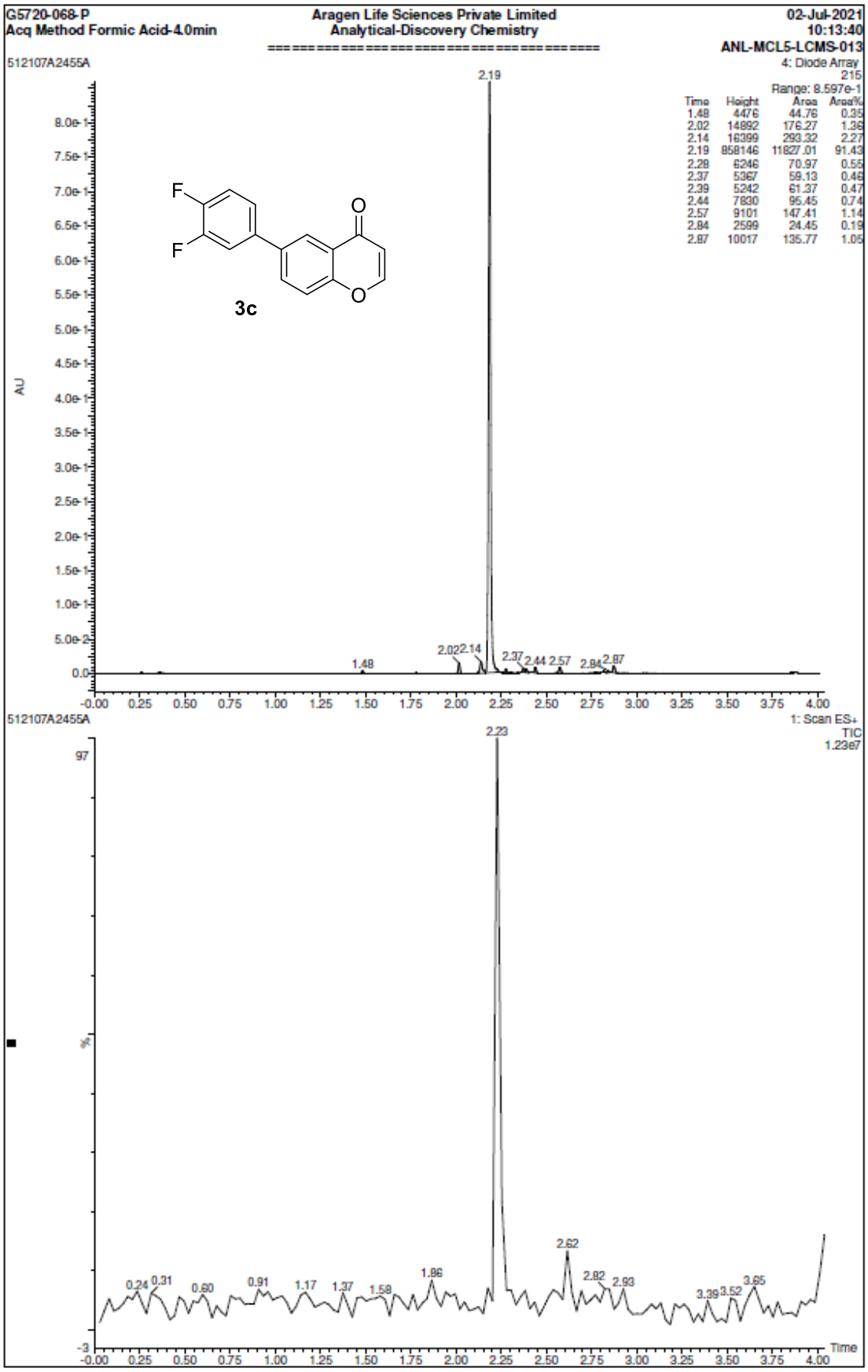
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F
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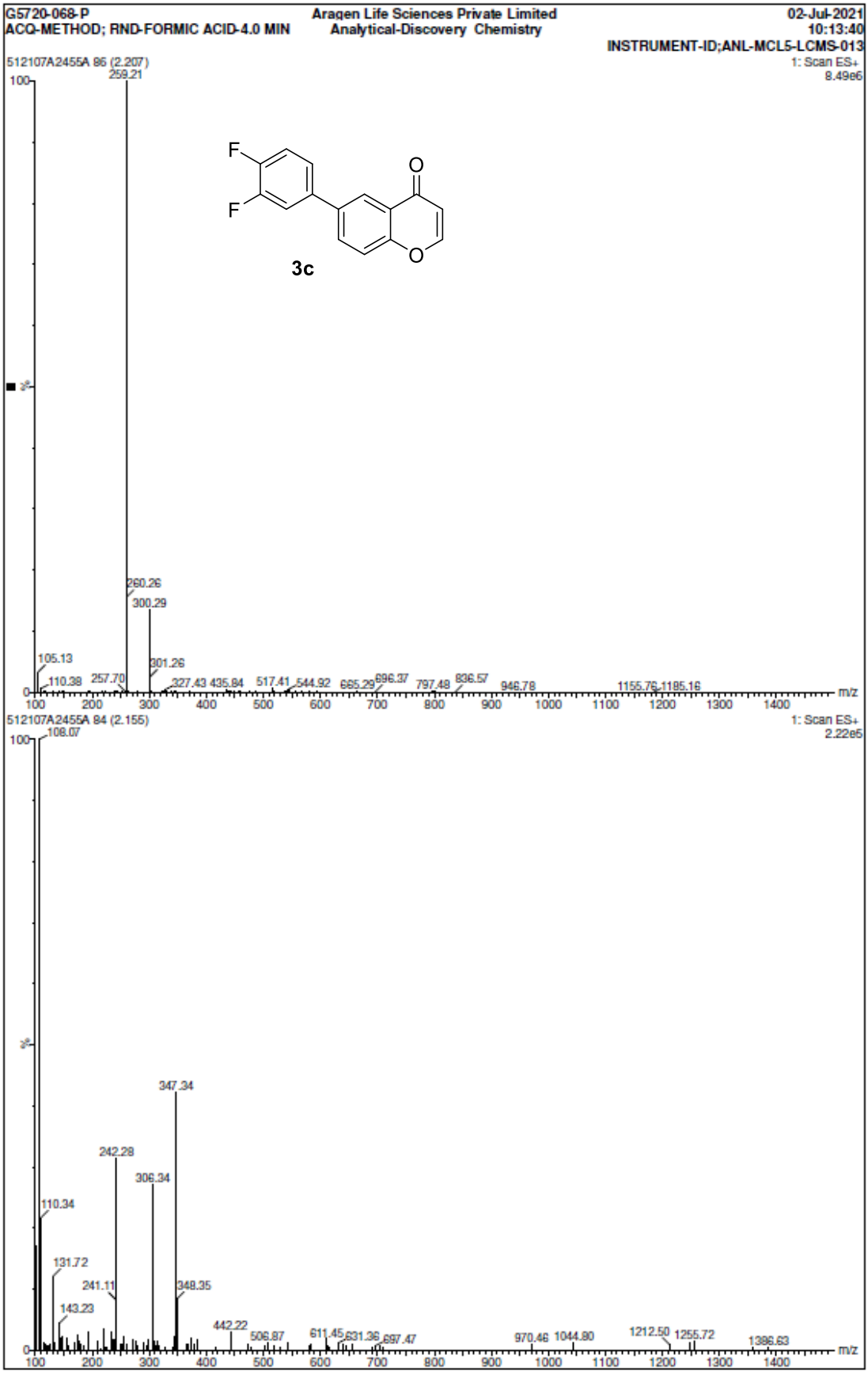
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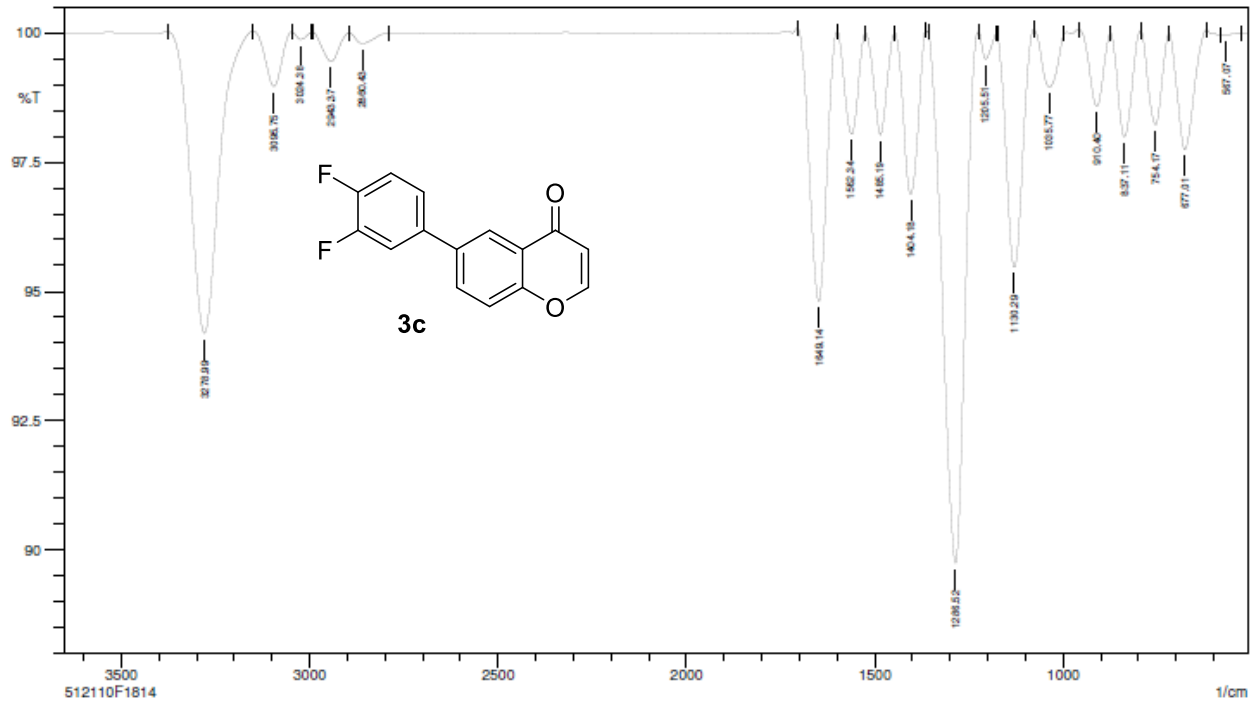
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry



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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

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G5720-068-P

02-07-2021
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02-Jul-2021
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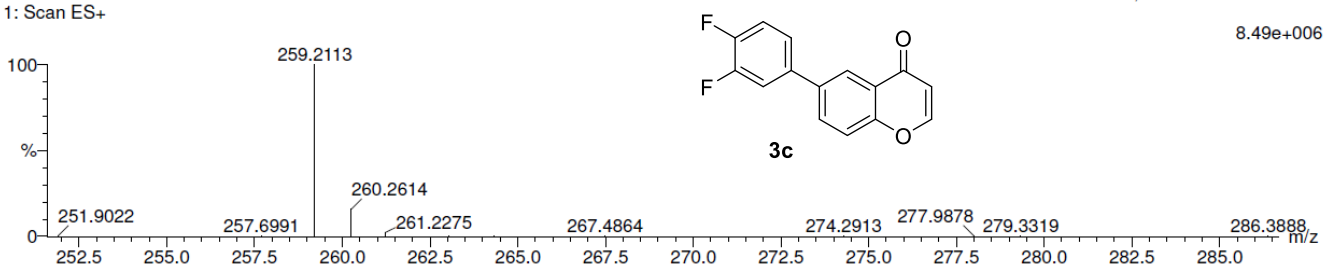

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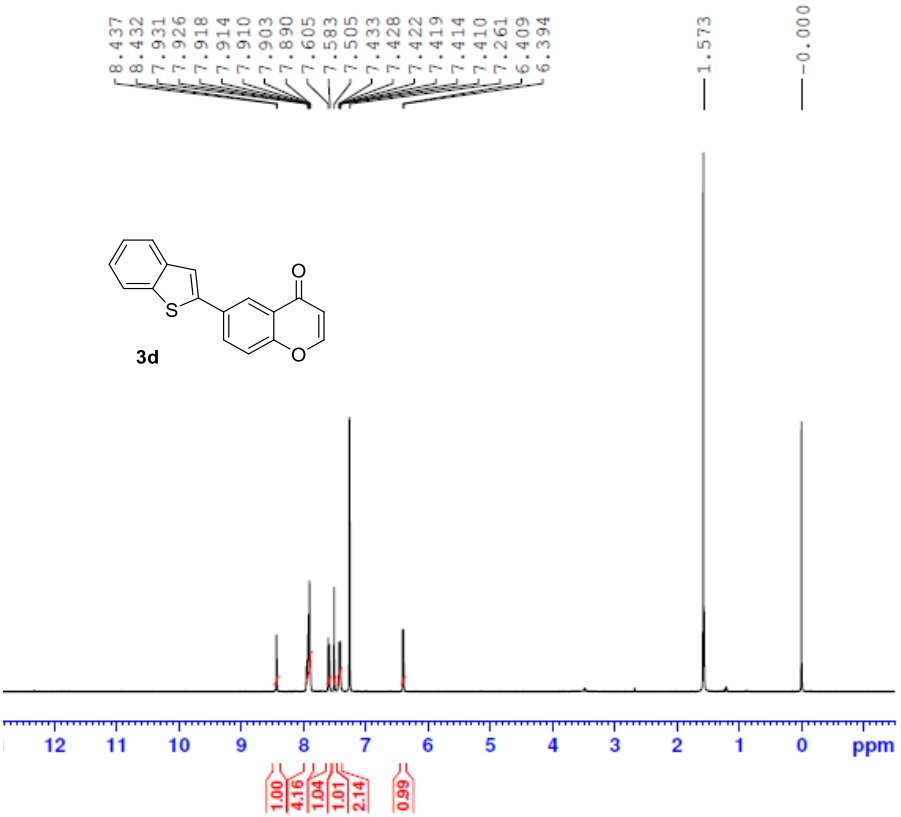


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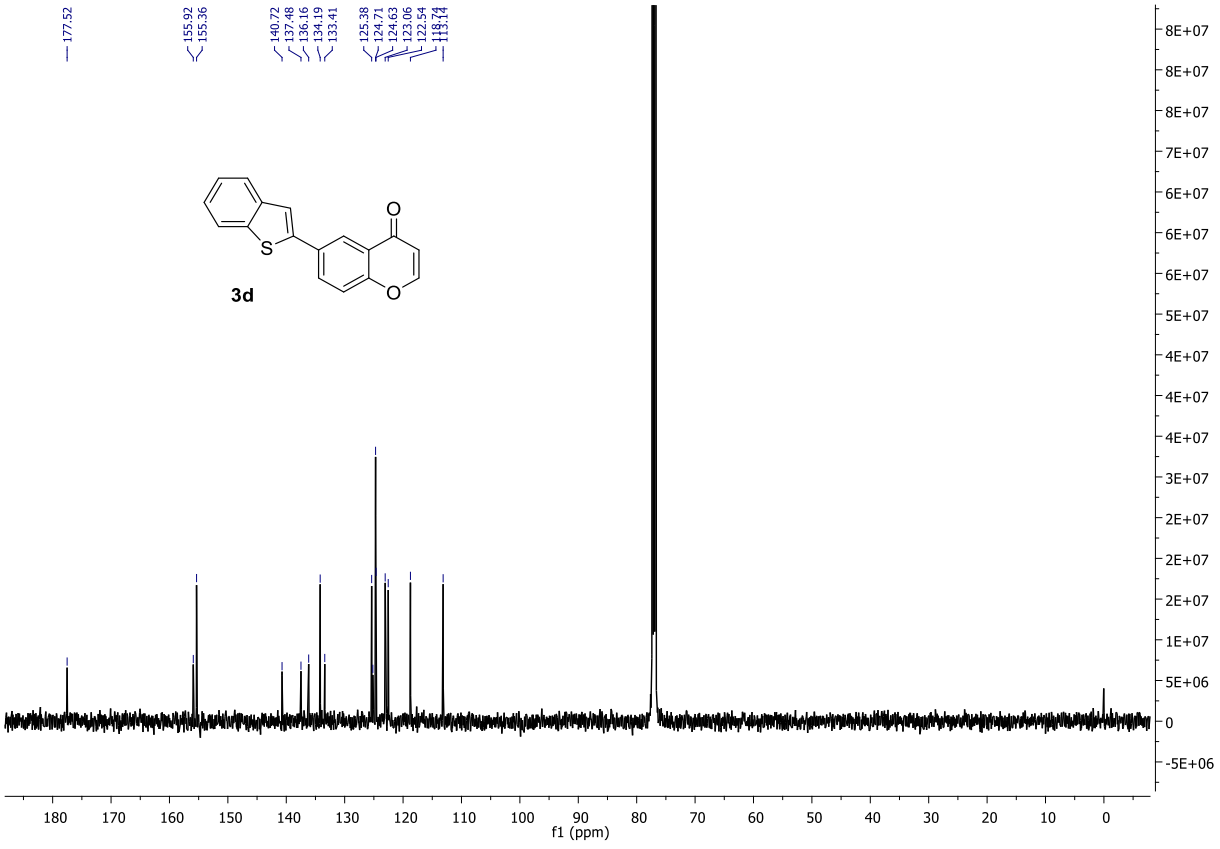

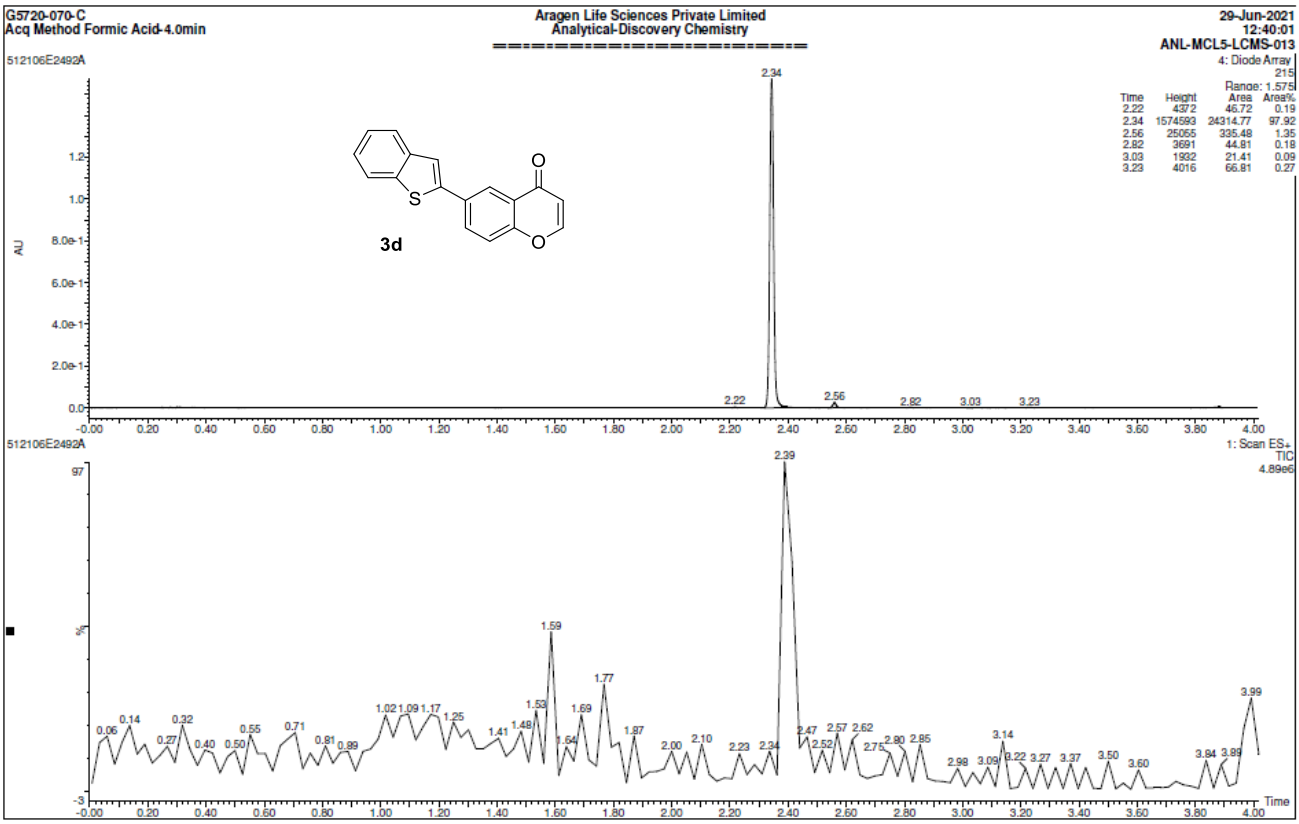
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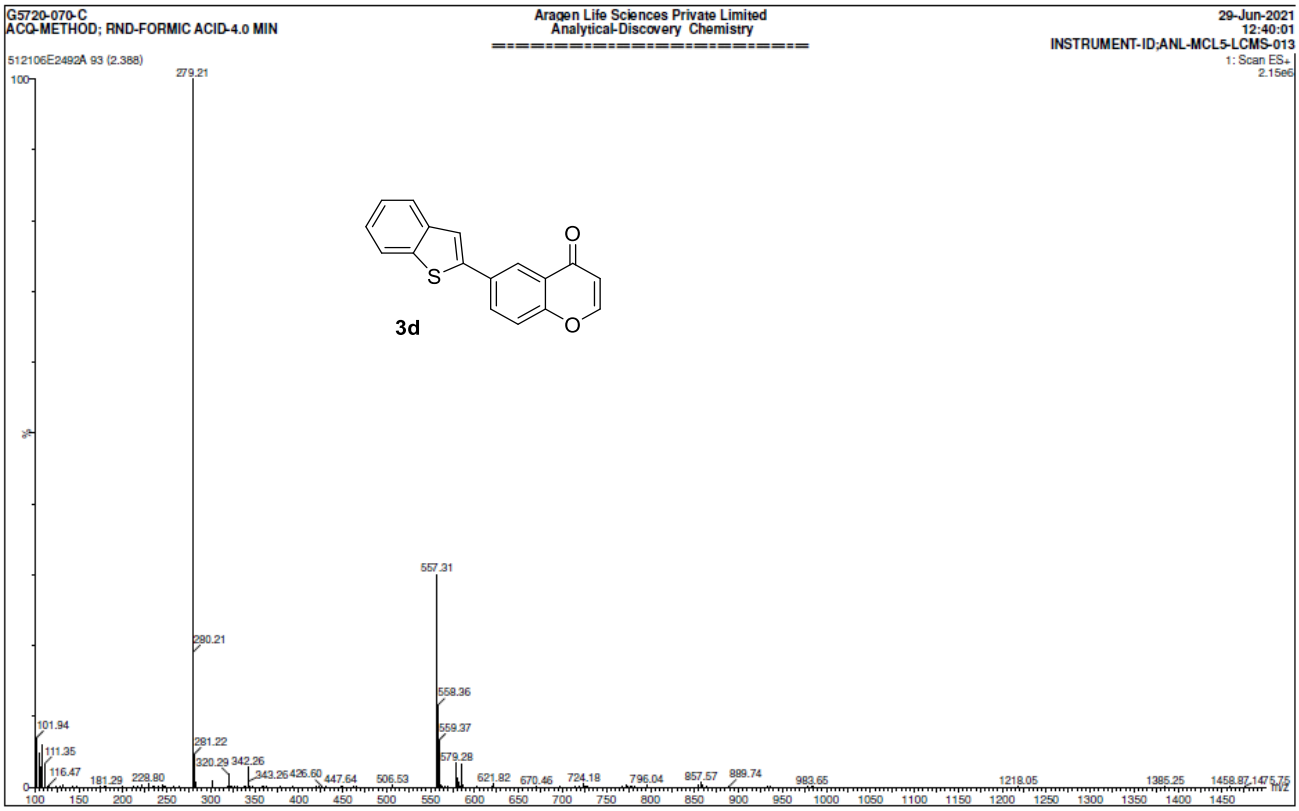
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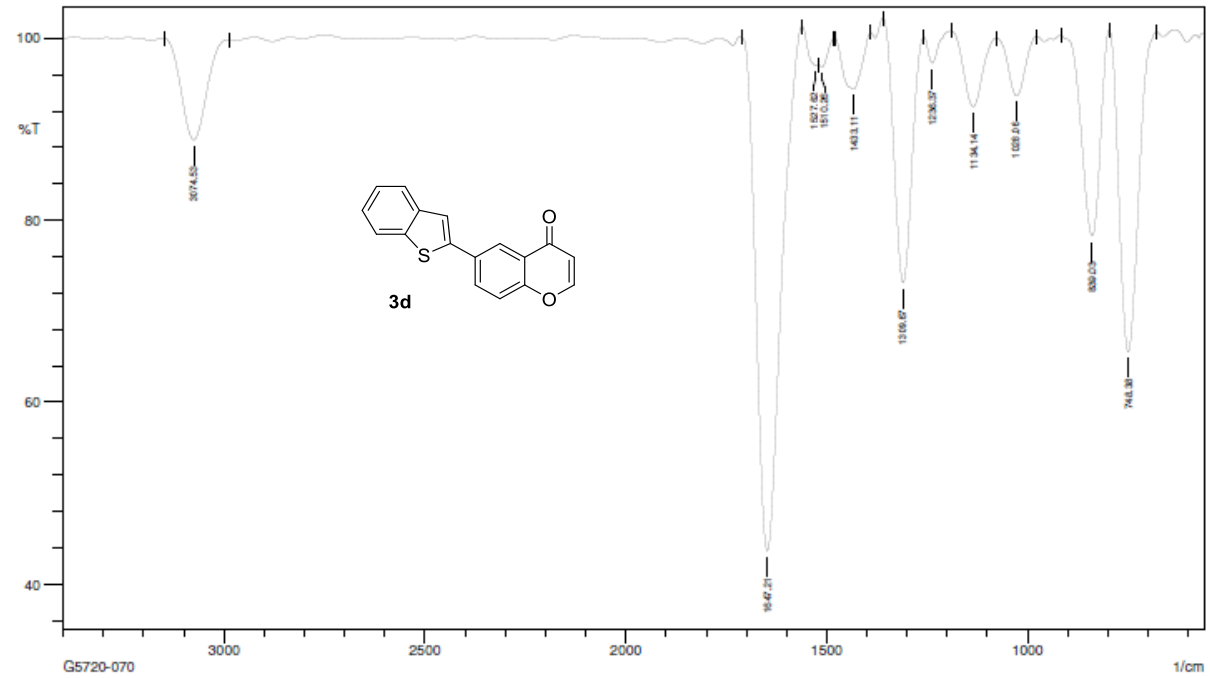
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry



Sample Name:
G5720-070

No. of Scans:

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

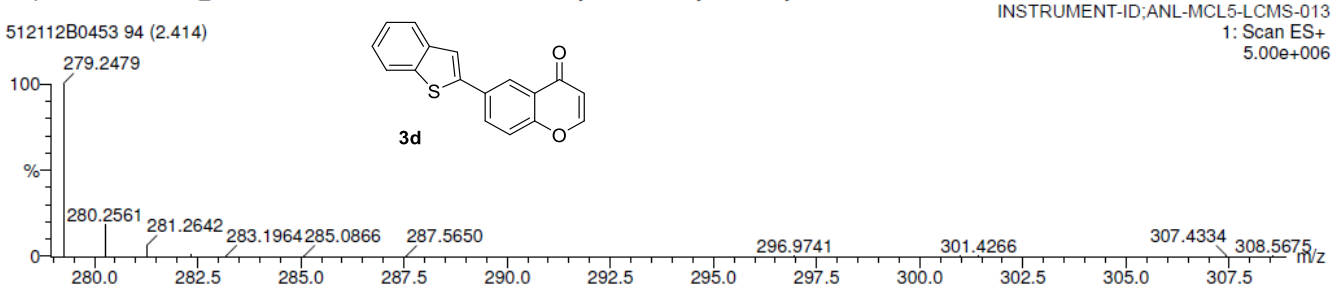
Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-17 H: 0-11 O: 0-2 S: 0-1

G5583-070-C
Acq.method formic acid_4min

Aragene Life sciences Private Limited
Analytical Discovery Chemistry

06-Dec-2021
08:08:58
INSTRUMENT-ID;ANL-MCL5-LCMS-013
1: Scan ES+
5.00e+006

512112B0453 94 (2.414)



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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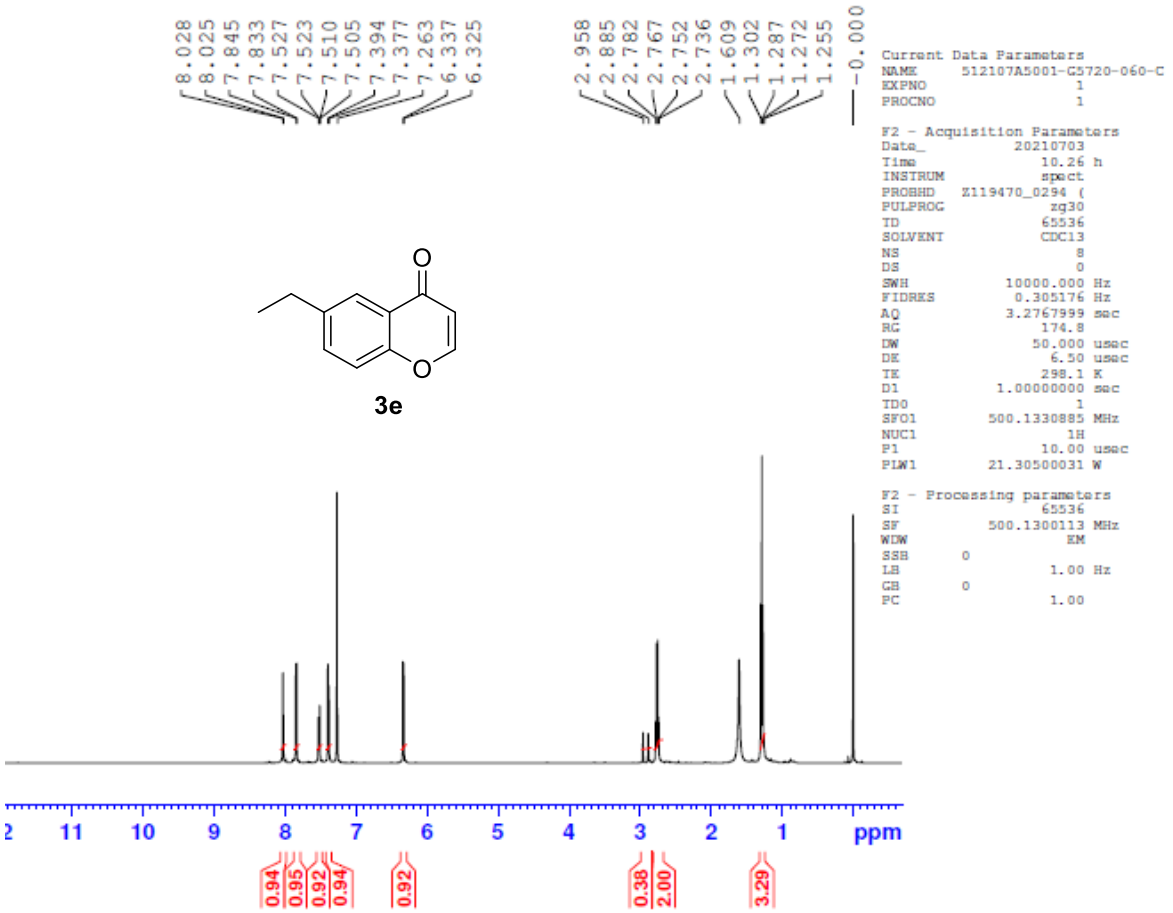
8.028
8.025
7.845
7.833
7.527
7.523
7.510
7.505
7.394
7.377
7.263
6.337
6.325
2.958
2.885
2.782
2.767
2.752
2.736
1.609
1.302
1.287
1.272
1.255
0.000
Current Data Parameters
NAME 512107A5001-G5720-060-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210703
Time 10.26 h
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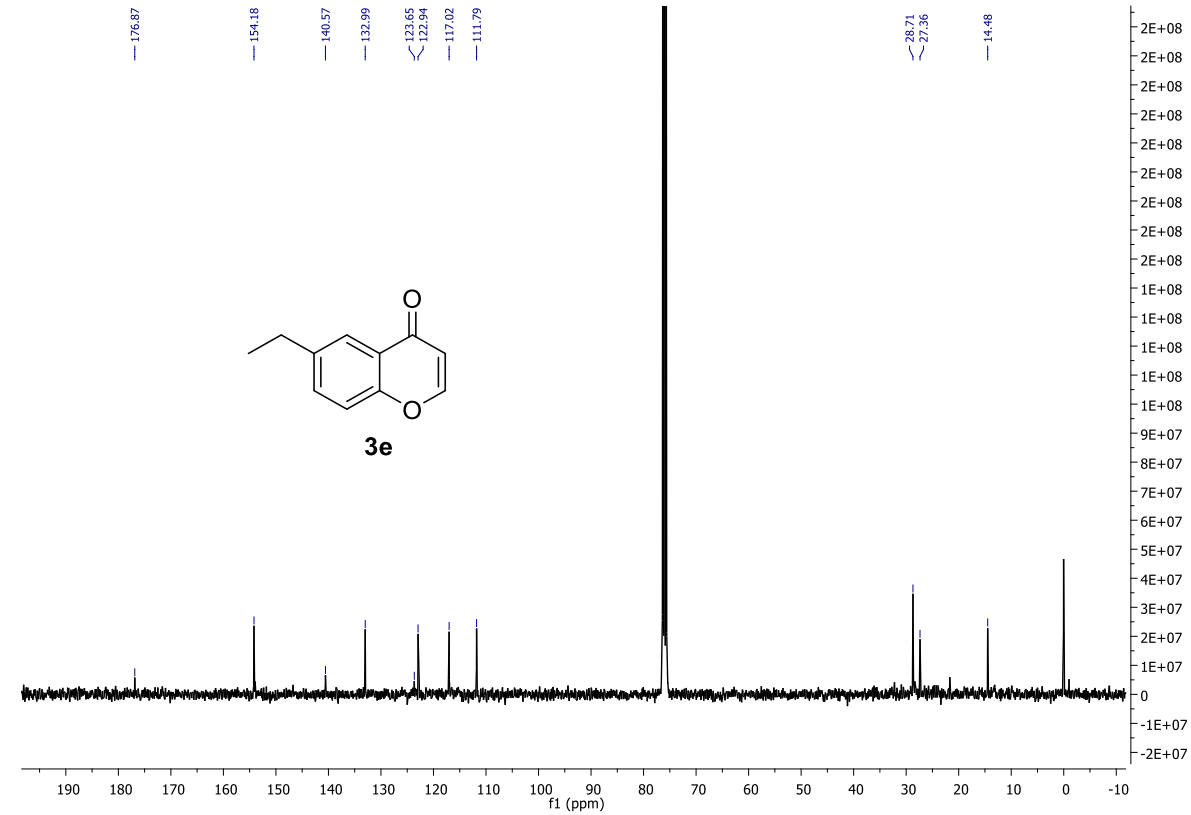
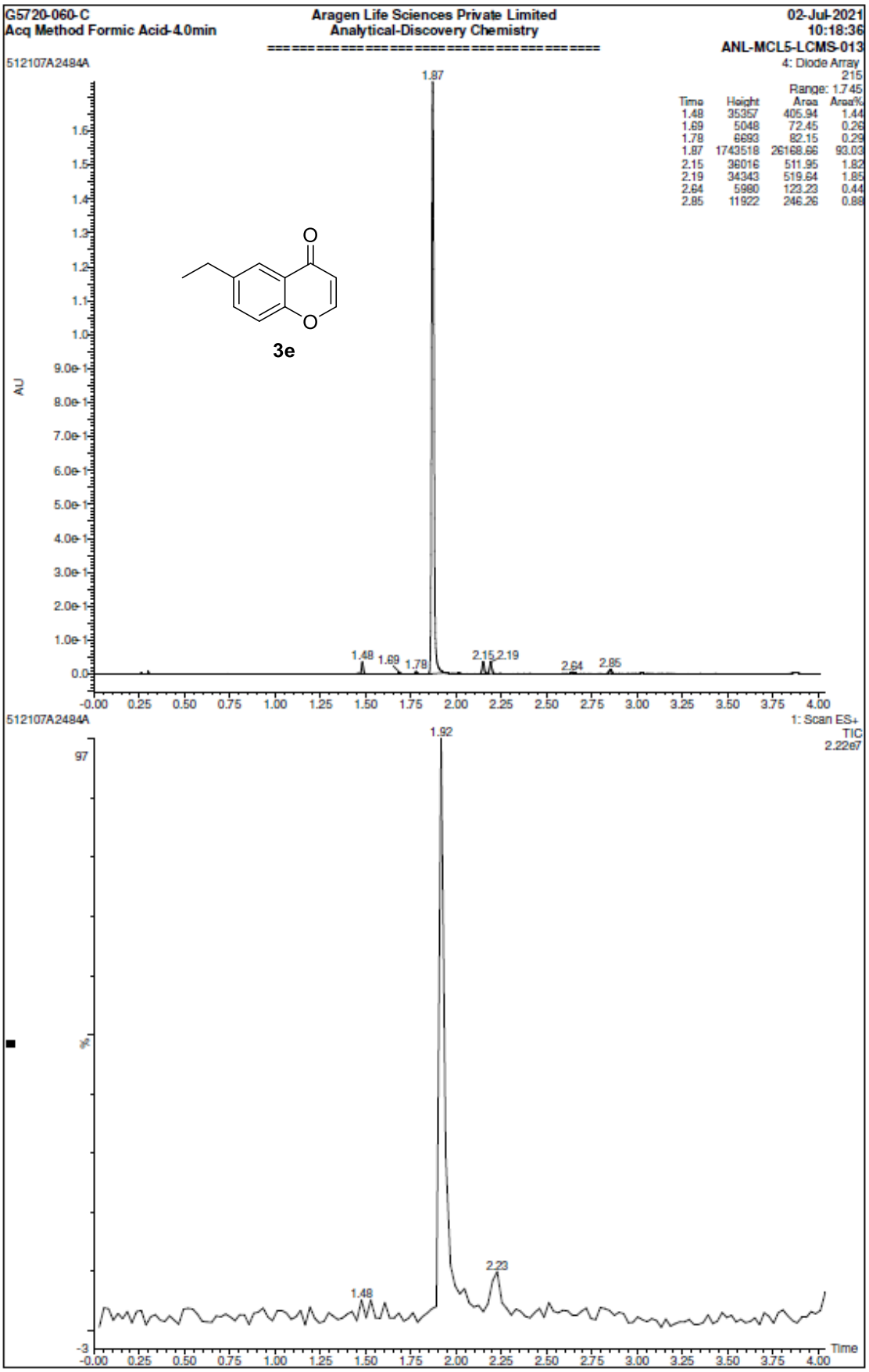
PROBHD Z119470_0294 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 174.8
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330885 MHz
NUC1 1H
P1 10.00 usec
PLW1 21.30500031 W
F2 - Processing parameters
SI 65536
SF 500.1300113 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
O
O
3e
2 11 10 9 8 7 6 5 4 3 2 1 ppm
0.94
0.95
0.92
0.94
0.92
0.38
2.00
3.29


176.87
154.18
140.57
132.99
123.65
122.94
117.02
111.79
28.71
27.36
14.48
O
O
3e
2E+08
1E+08
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
-1E+07
-2E+07
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


G5720-060-C
Acq Method Formic Acid-4.0min
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry
02-Jul-2021
10:18:36
ANL-MCL5-LCMS-013
512107A2484A
4: Diode Array
215
Range: 1.745
Time Height Area Area%
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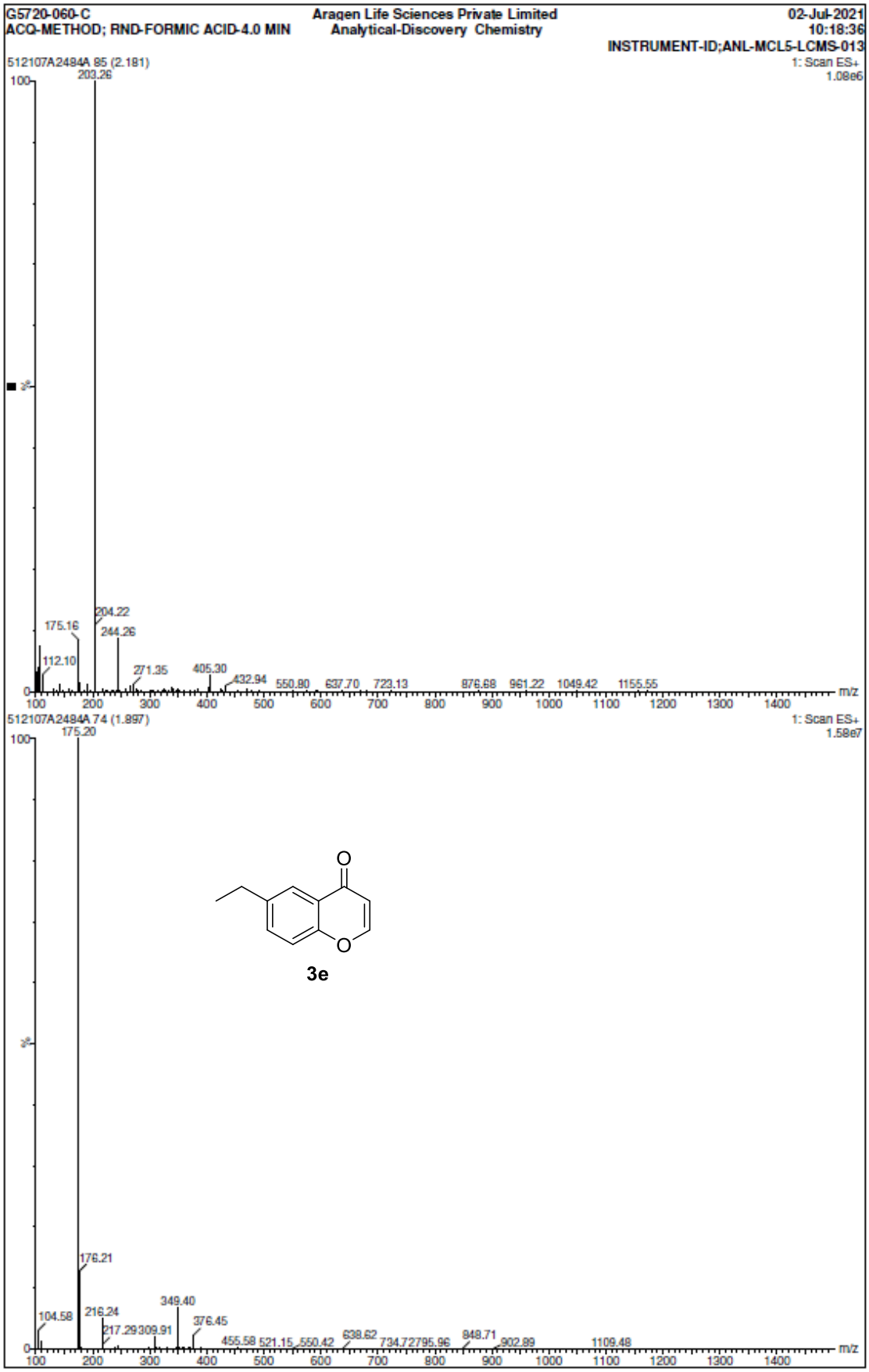
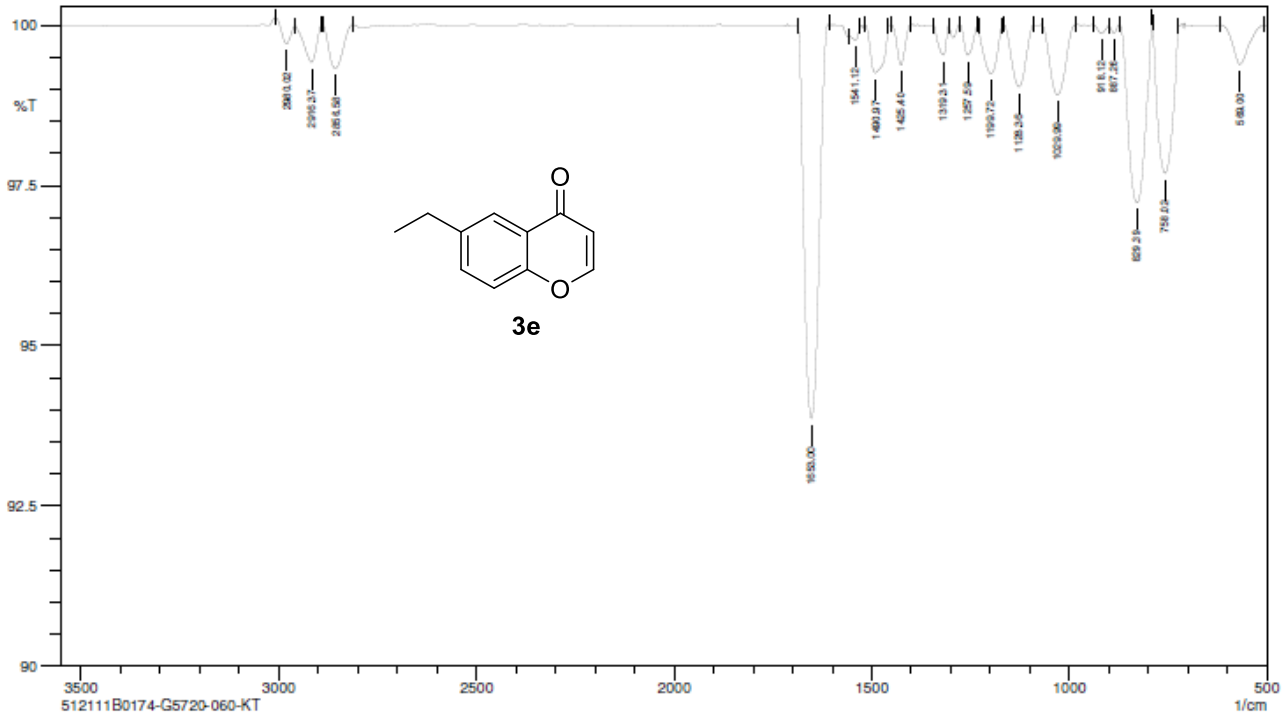
1.69 5048 72.45 0.26
1.78 6693 82.15 0.29
1.87 1743518 26168.66 93.03
2.15 36016 511.95 1.82
2.19 34343 519.64 1.85
2.64 5980 123.23 0.44
2.85 11922 246.26 0.88
1.87
1.48
1.69
1.78
2.15
2.19
2.64
2.85
AU
3e
512107A2484A
1: Scan ES+
TIC
2.22e7
1.92
2.23
1.48
%
Time


G5720-060-C
ACQ-METHOD; RND-FORMIC ACID-4.0 MIN
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry
02-Jul-2021
10:18:36
INSTRUMENT-ID;ANL-MCL5-LCMS-013
512107A2484A 85 (2.181)
1: Scan ES+
1.08e6
203.26
204.22
175.16
244.26
112.10
271.35
405.30
432.94
550.80
637.70
723.13
876.68
961.22
1049.42
1155.55
m/z
512107A2484A 74 (1.897)
1: Scan ES+
1.58e7
175.20
176.21
349.40
104.58
216.24
217.29
309.91
376.45
455.58
521.15
550.42
638.62
734.72
795.96
848.71
902.89
1109.48
m/z

3e

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

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

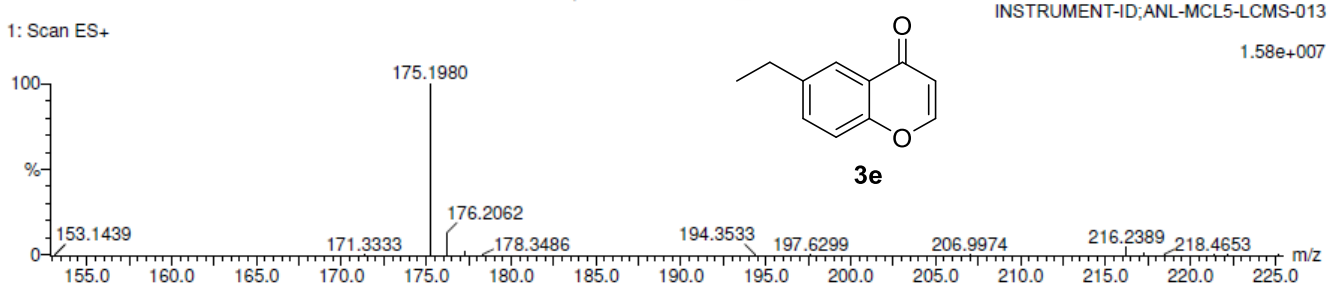
512107A2484A 74 (1.897)
G5720-060-C

02-07-2021
Acq.method formic acid_4min

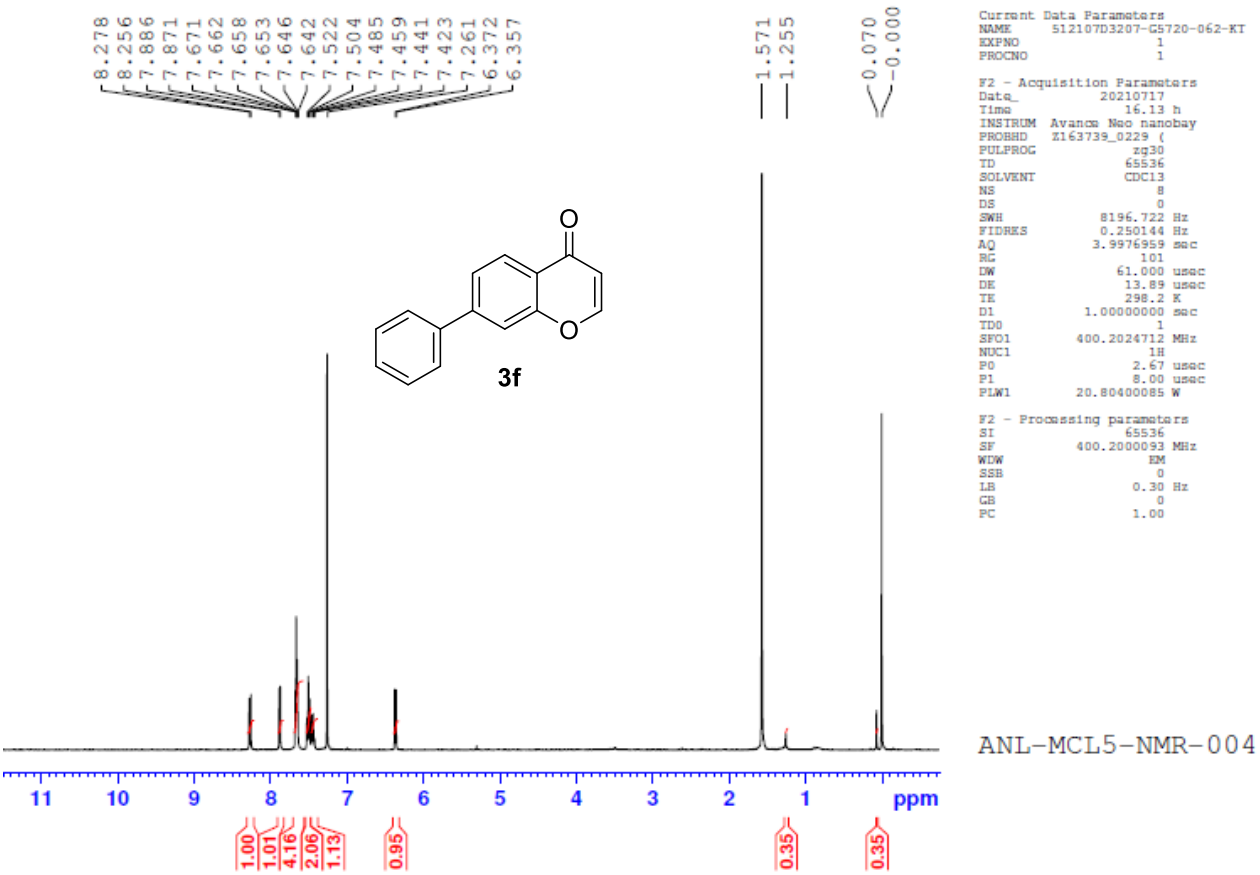
02-Jul-2021
10:18:36
INSTRUMENT-ID;ANL-MCL5-LCMS-013

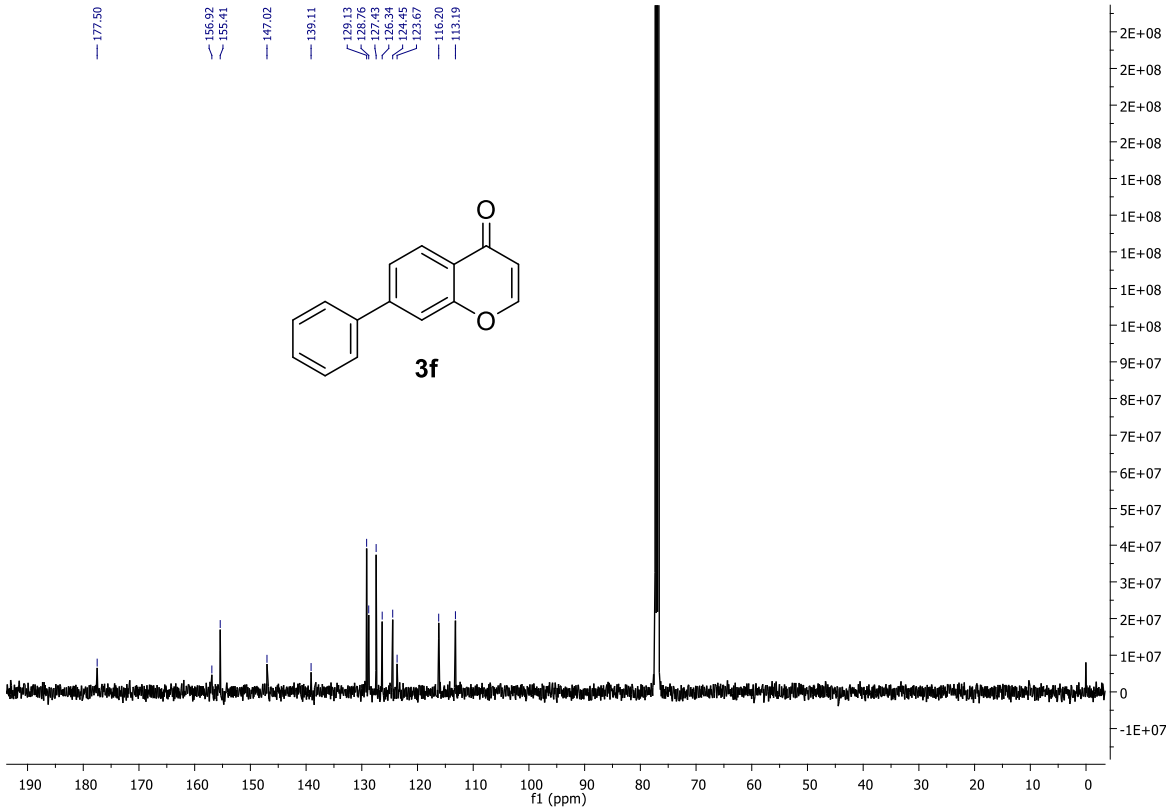
1: Scan ES+

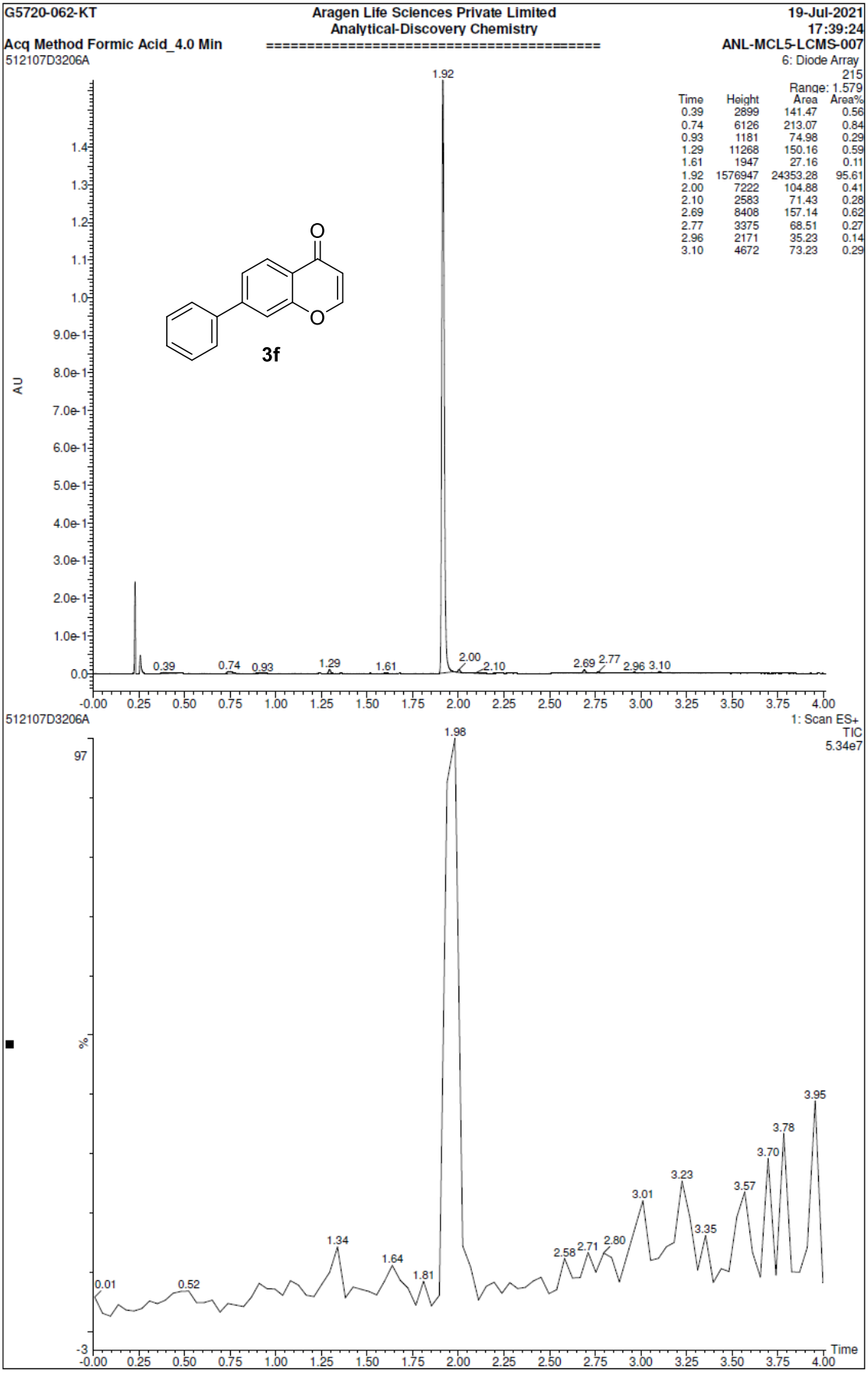
1.58e+007

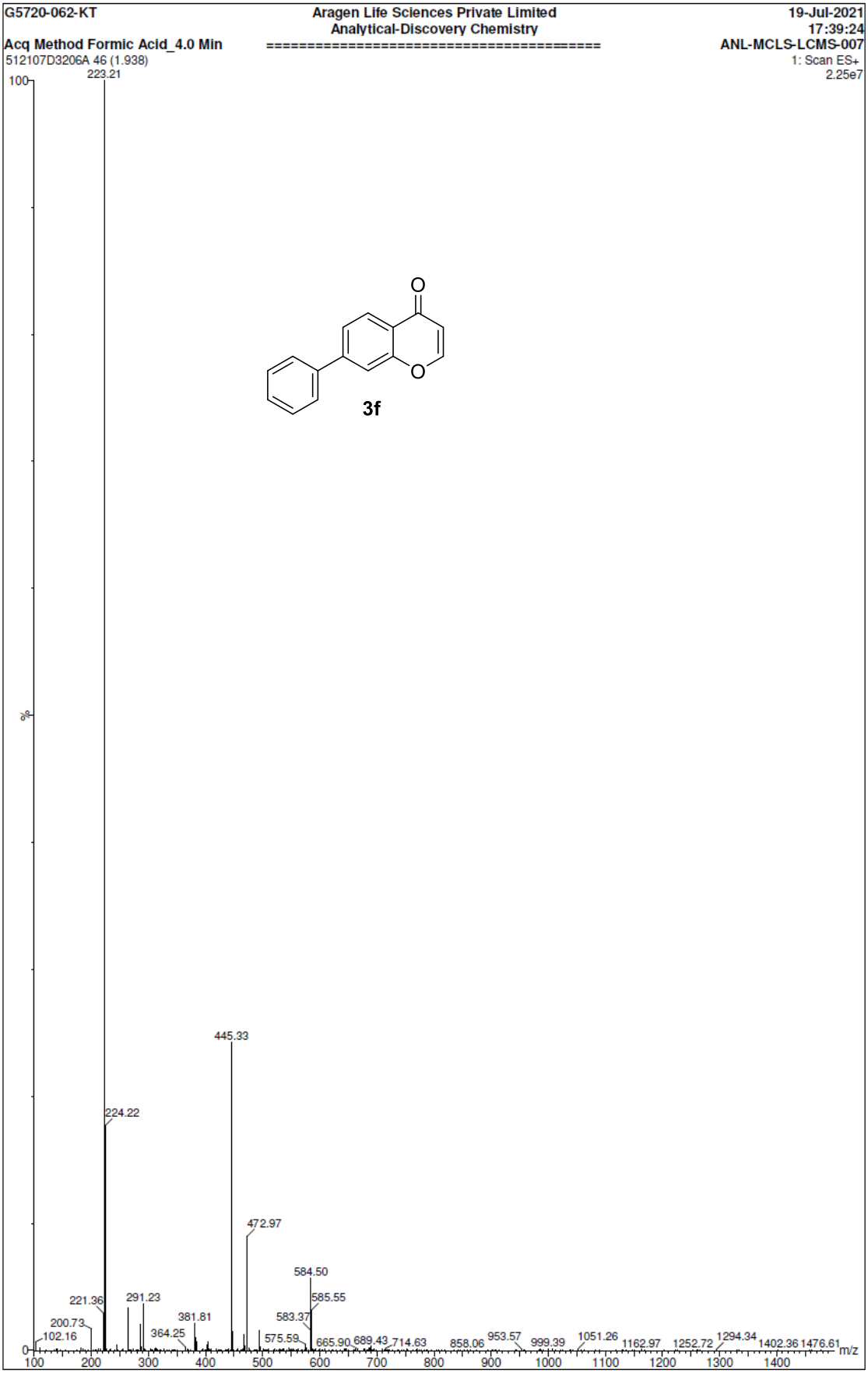


Minimum:				-1.5				
Maximum:		5.0	1000.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
175.0740	175.0759	-1.9	-10.9	6.5	41.4	n/a	n/a	C11 H11 O2

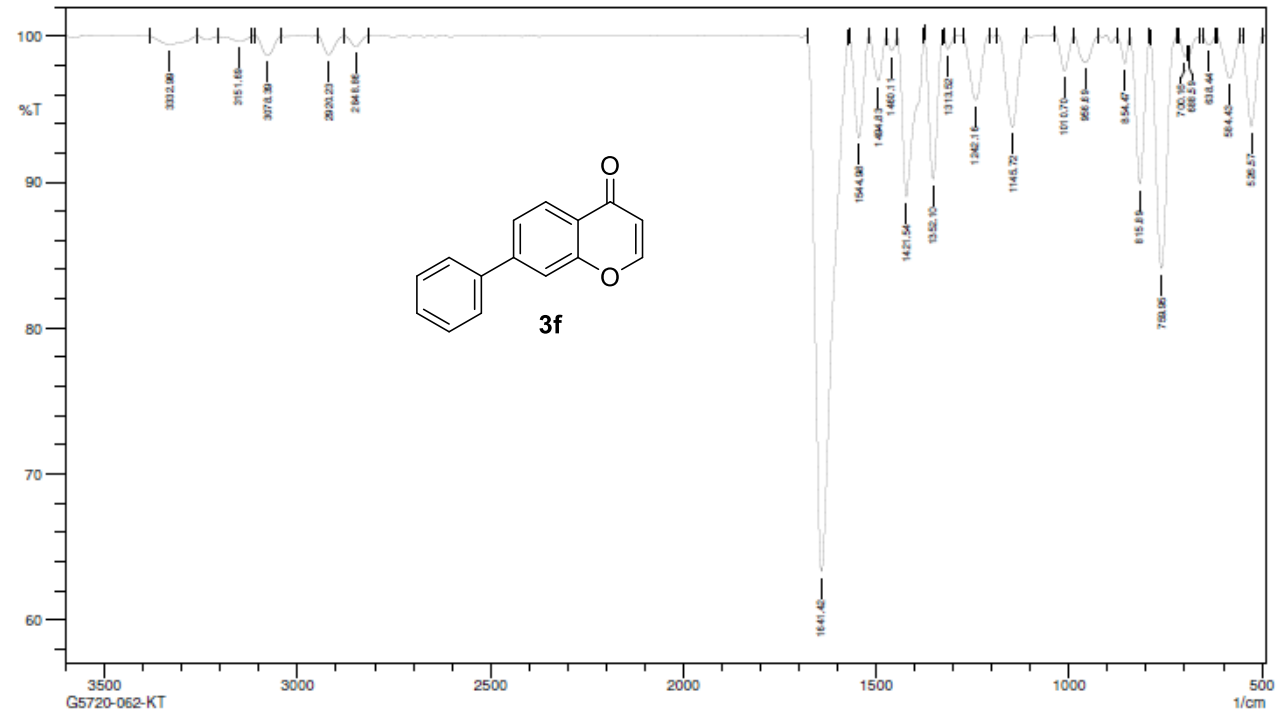

8.278
8.256
7.886
7.871
7.671
7.662
7.658
7.653
7.646
7.642
7.522
7.504
7.485
7.459
7.441
7.423
7.261
6.372
6.357
1.571
1.255
0.070
0.000
3f
Current Data Parameters
NAME 512107D3207-G5720-062-KT
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210717
Time 16.13 h
INSTRUM Avance Neo nanobay
PROBHD Z163739_0229 (
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
TD0 1
SFO1 400.2024712 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 20.80400085 W
F2 - Processing parameters
SI 65536
SF 400.2000093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ANL-MCL5-NMR-004
11 10 9 8 7 6 5 4 3 2 1 ppm
1.00 1.01 4.16 2.06 1.13 0.95 0.35 0.35


177.50
156.92
155.41
147.02
139.11
129.13
128.76
127.43
126.34
124.45
123.67
116.20
113.19
3f
2E+08
1E+08
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
-1E+07
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


G5720-062-KT
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry
19-Jul-2021
17:39:24
Acq Method Formic Acid_4.0 Min
ANL-MCL5-LCMS-007
512107D3206A
6: Diode Array
215
Range: 1.579
Time Height Area Area%
0.39 2899 141.47 0.56
0.74 6126 213.07 0.84
0.93 1181 74.98 0.29
1.29 11268 150.16 0.59
1.61 1947 27.16 0.11
1.92 1576947 24353.28 95.61
2.00 7222 104.88 0.41
2.10 2583 71.43 0.28
2.69 8408 157.14 0.62
2.77 3375 68.51 0.27
2.96 2171 35.23 0.14
3.10 4672 73.23 0.29
3f
AU
512107D3206A
1: Scan ES+
TIC
5.34e7
%
Time


G5720-062-KT
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry
19-Jul-2021
17:39:24
Acq Method Formic Acid_4.0 Min
ANL-MCLS-LCMS-007
512107D3206A 46 (1.938)
1: Scan ES+
2.25e7
100
%
0
223.21
445.33
224.22
472.97
584.50
585.55
221.36
291.23
583.37
381.81
200.73
102.16
364.25
575.59
665.90
689.43
714.63
858.06
953.57
999.39
1051.26
1162.97
1252.72
1294.34
1402.36
1476.61
m/z
100
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
O
O
3f

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

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

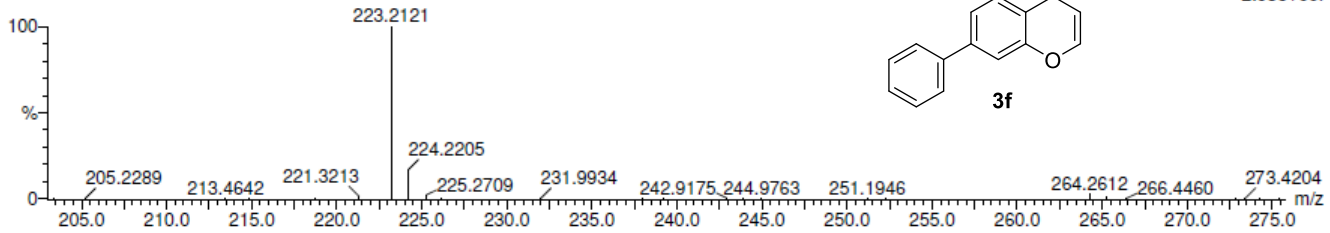
Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-15 H: 0-11 O: 0-2

G5720-062-KT

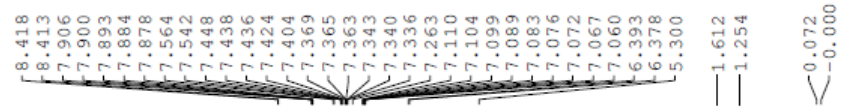
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry

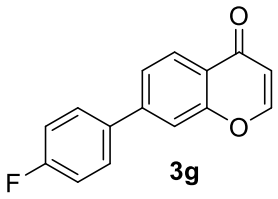
19-Jul-2021
17:39:24
ANL-MCL5-LCMS-007
1: Scan ES+
2.98e+007

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



Minimum:				-1.5				
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



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PROCNO               1

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Time               16.23 h
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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
TD0                    1
SFO1          400.2024712 MHz
NUC1                  1H
P0                 2.67 usec
P1                 8.00 usec
PLW1          20.80400085 W

F2 - Processing parameters
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SF            400.2000087 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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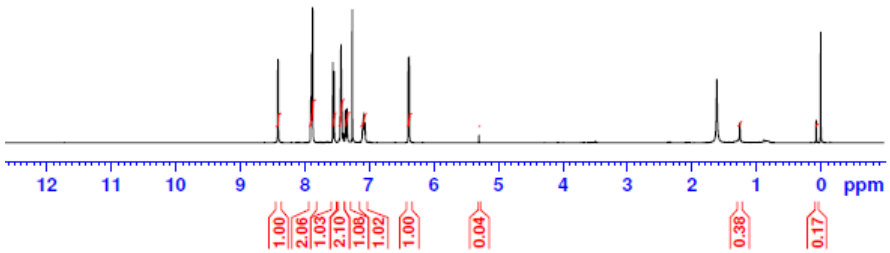
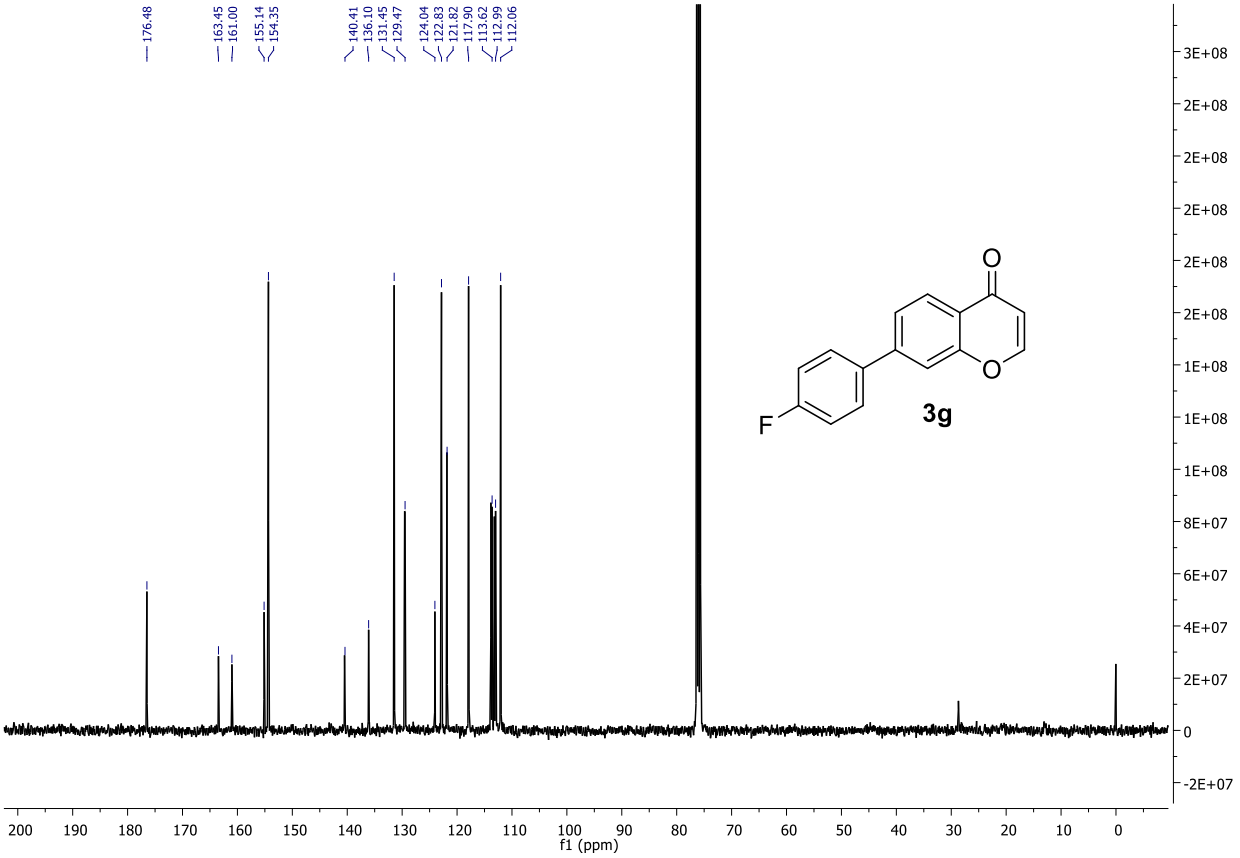
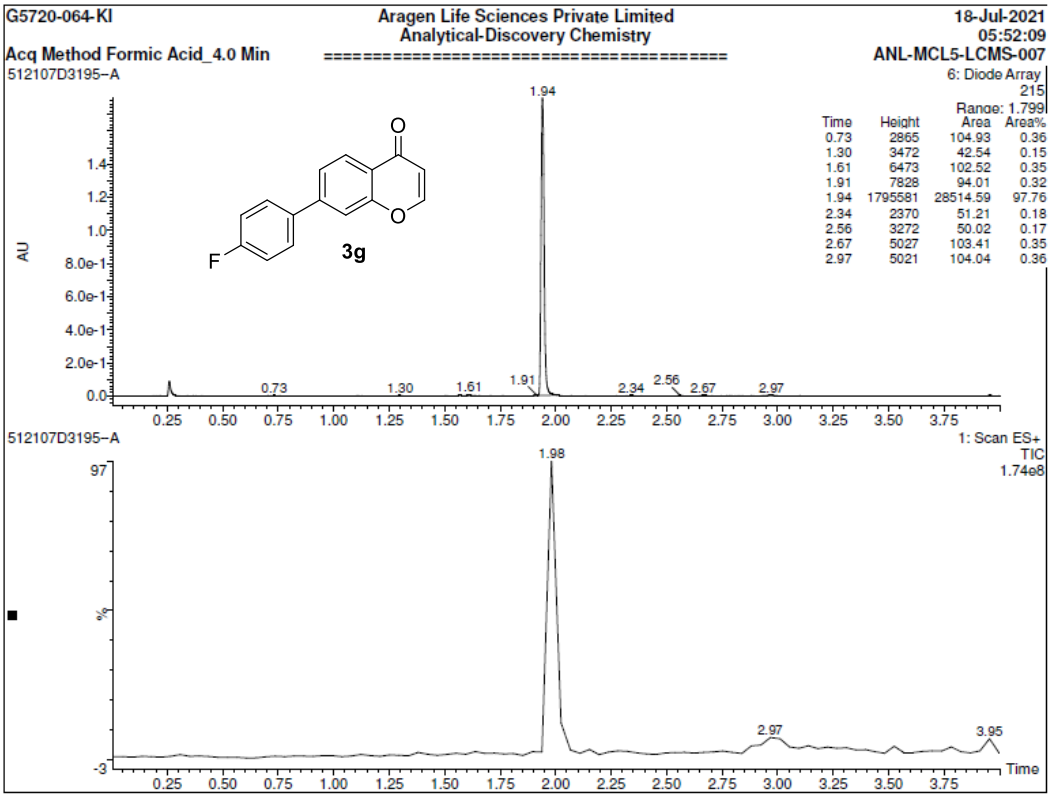


ANL-MCL5-NMR-004




G5720-064-KI
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry
18-Jul-2021
05:52:09
Acq Method Formic Acid_4.0 Min
ANL-MCL5-LCMS-007
512107D3195--A
6: Diode Array
215
Range: 1.799
Time Height Area Area%
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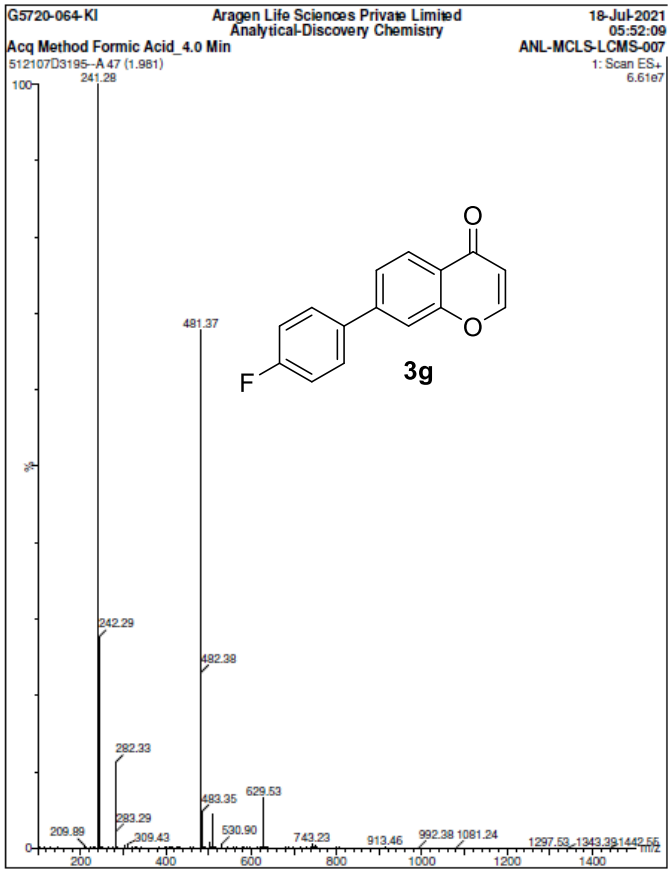
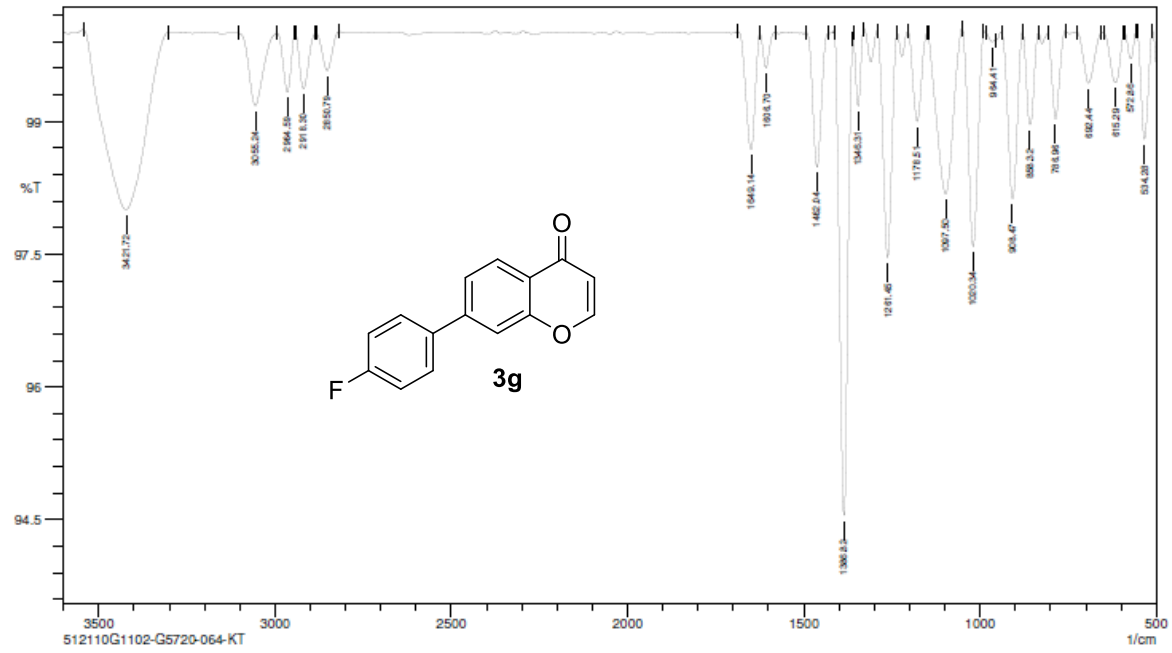
1.30 3472 42.54 0.15
1.61 6473 102.52 0.35
1.91 7828 94.01 0.32
1.94 1795581 28514.59 97.76
2.34 2370 51.21 0.18
2.56 3272 50.02 0.17
2.67 5027 103.41 0.35
2.97 5021 104.04 0.36
AU
1.94
0.73
1.30
1.61
1.91
2.34
2.56
2.67
2.97
3g
512107D3195--A
1: Scan ES+
TIC
1.74e8
1.98
2.97
3.95
Time


G5720-064-KI
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry
18-Jul-2021
05:52:09
Acq Method Formic Acid_4.0 Min
ANL-MCLS-LCMS-007
512107D3195--A 47 (1.981)
1: Scan ES+
6.61e7
241.28
481.37
242.29
482.38
282.33
483.35
629.53
293.29
209.89
309.43
530.90
743.23
913.46
992.38
1081.24
1297.53
1343.39
1442.55
m/z
3g

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

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

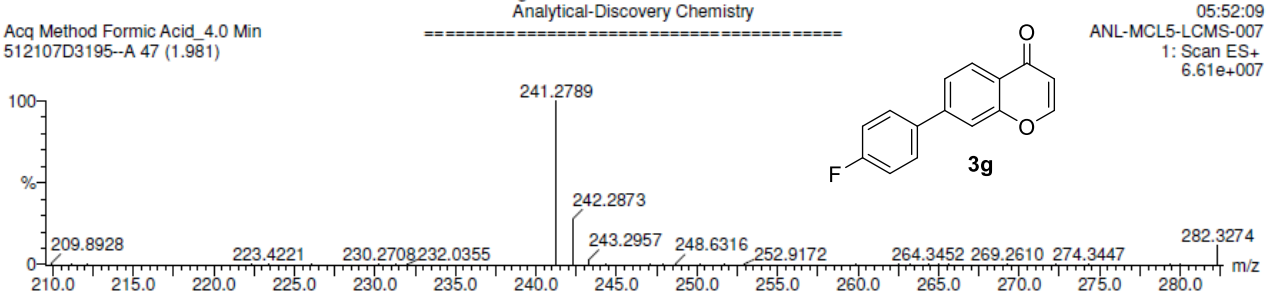
Monoisotopic Mass, Even Electron Ions
4 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-15 H: 0-10 O: 0-2 F: 0-1

G5720-064-KI

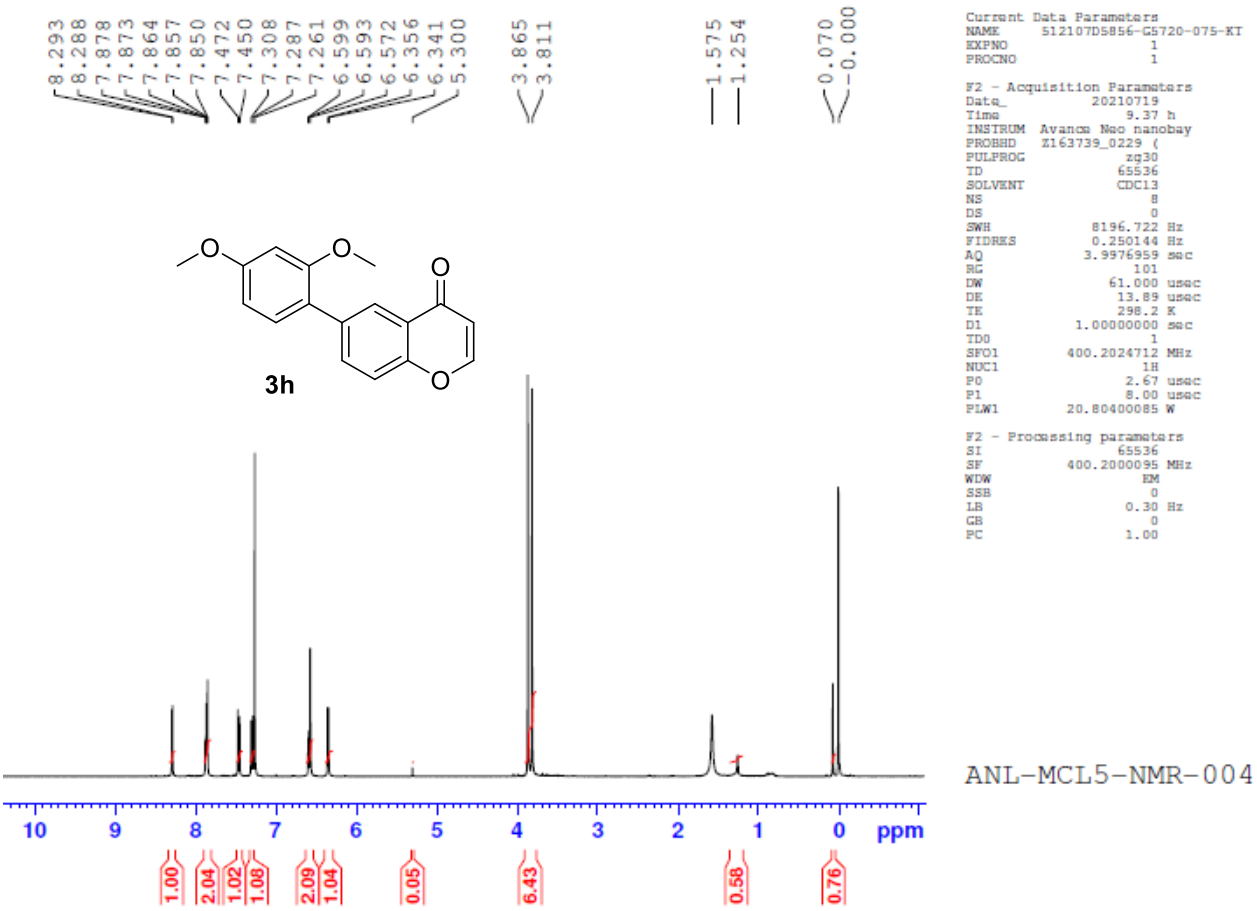
Acq Method Formic Acid_4.0 Min
512107D3195--A 47 (1.981)

Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry

18-Jul-2021
05:52:09
ANL-MCL5-LCMS-007
1: Scan ES+
6.61e+007



Minimum:				-1.5				
Maximum:		5.0	1000.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
241.2789	241.0665	212.4	880.3	10.5	50.3	n/a	n/a	C15 H10 O2 F

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PROCNO               1

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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
TD0                    1
SFO1          400.2024712 MHz
NUC1                  1H
P0                 2.67 usec
P1                 8.00 usec
PLW1          20.80400085 W

F2 - Processing parameters
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SF            400.2000095 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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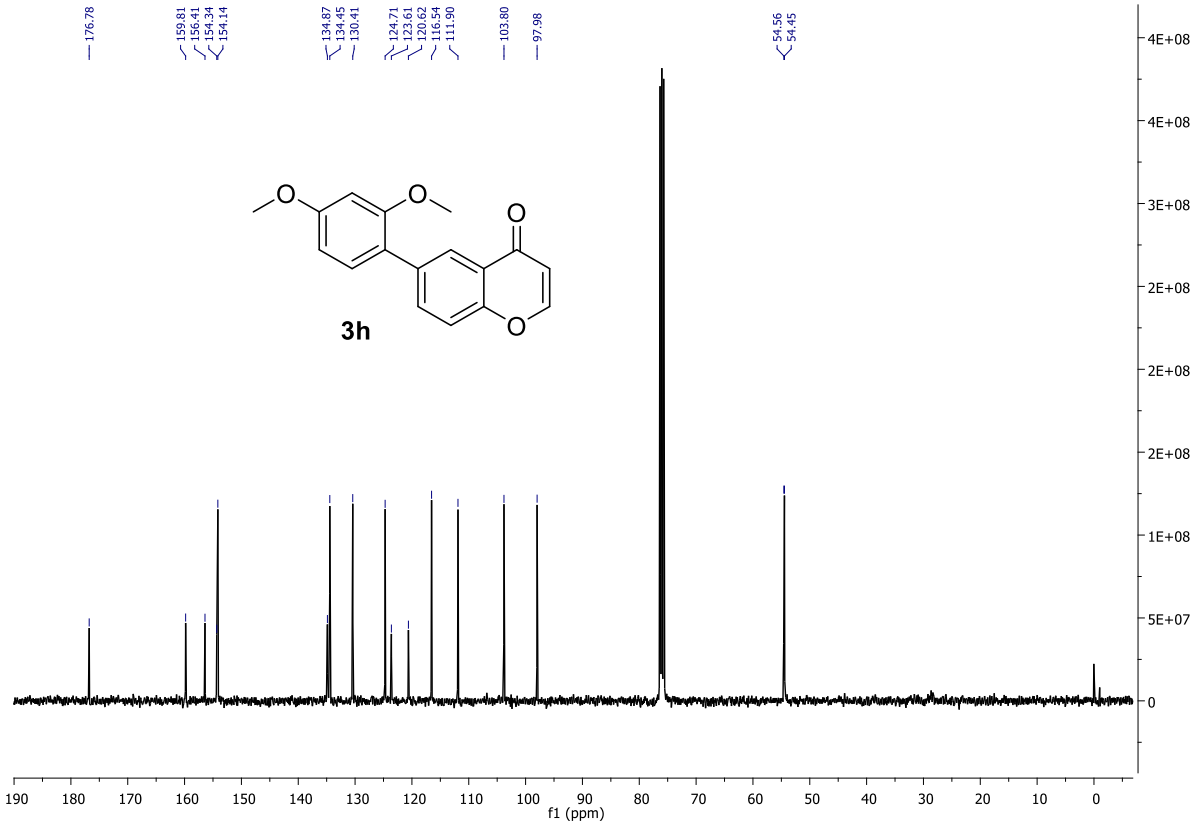
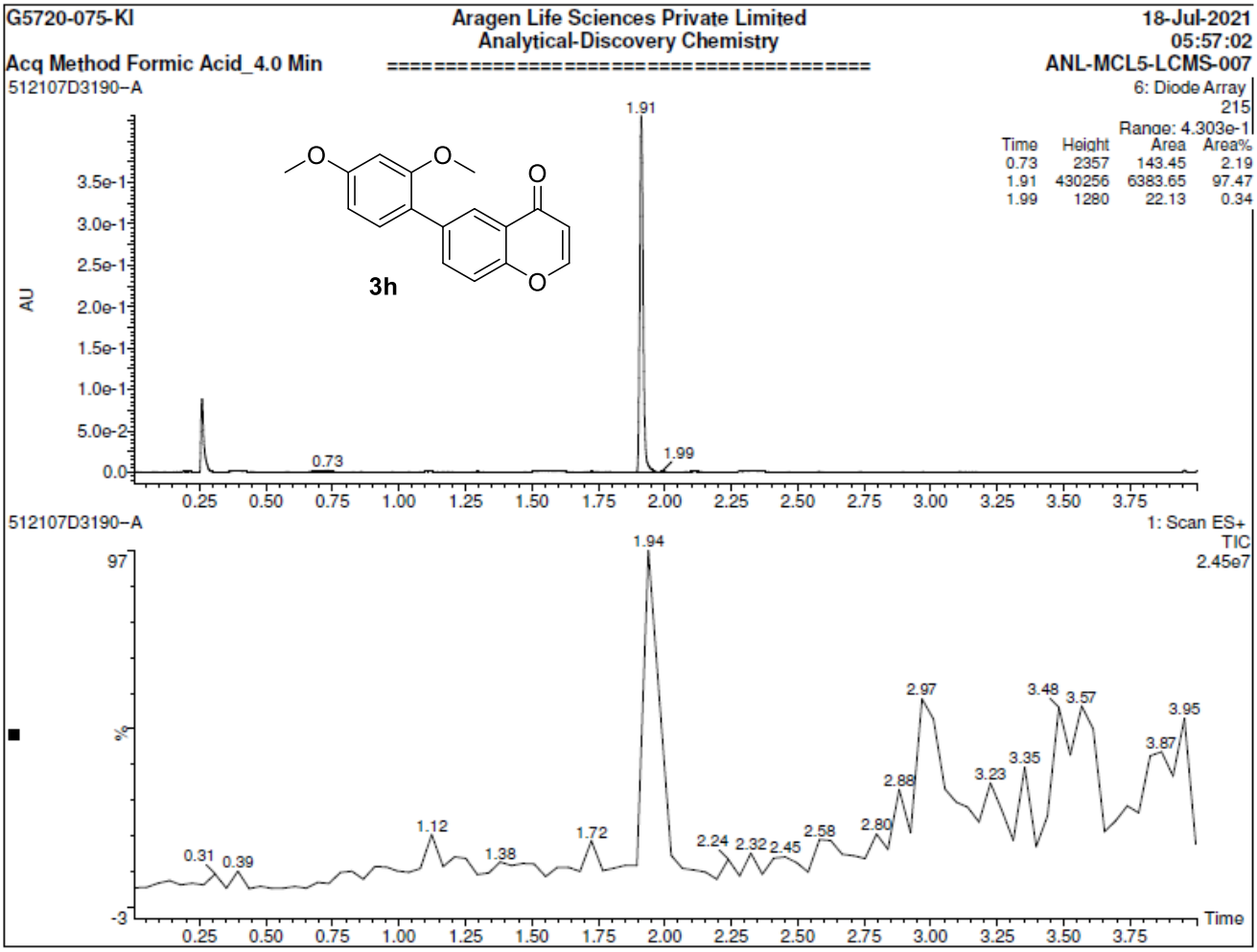
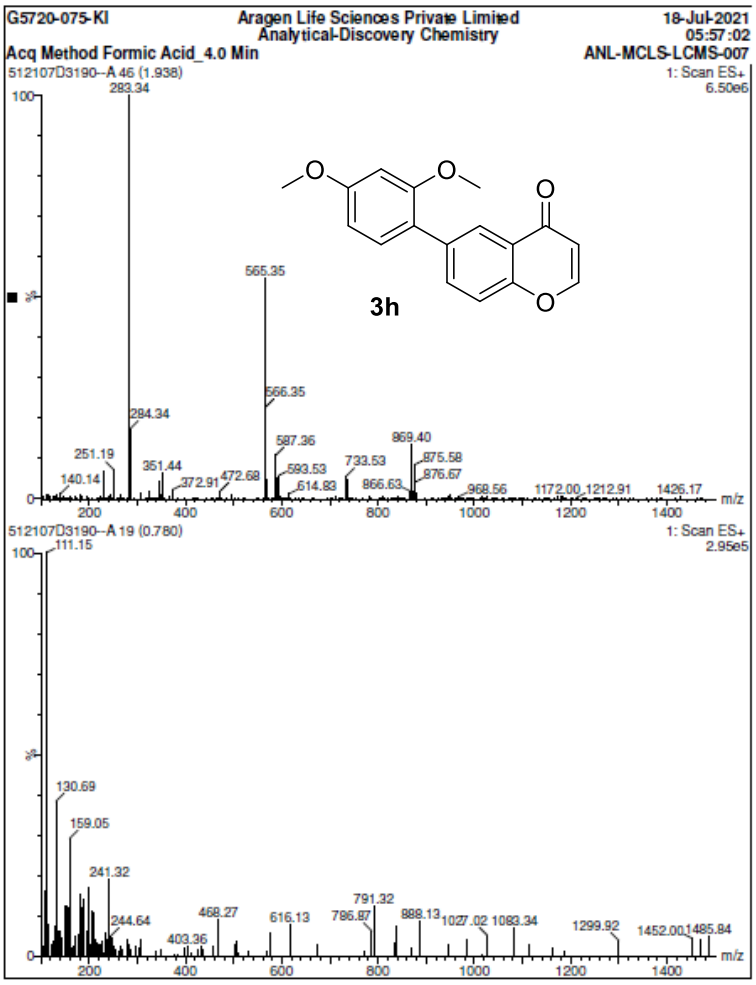
ANL-MCL5-NMR-004




G5720-075-KI
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry
18-Jul-2021
05:57:02
Acq Method Formic Acid_4.0 Min
ANL-MCL5-LCMS-007
512107D3190-A
6: Diode Array
215
Range: 4.303e-1
Time Height Area Area%
0.73 2357 143.45 2.19
1.91 430256 6383.65 97.47
1.99 1280 22.13 0.34
3h
AU
1.91
0.73
1.99
512107D3190-A
1: Scan ES+
TIC
2.45e7
%
1.94
0.31
0.39
1.12
1.38
1.72
2.24
2.32
2.45
2.58
2.80
2.88
2.97
3.23
3.35
3.48
3.57
3.87
3.95
Time



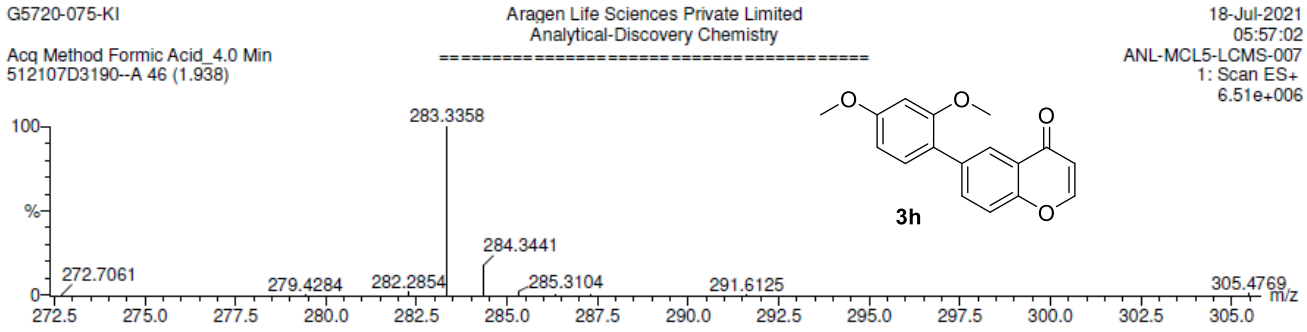
Elemental Composition Report

Page 1

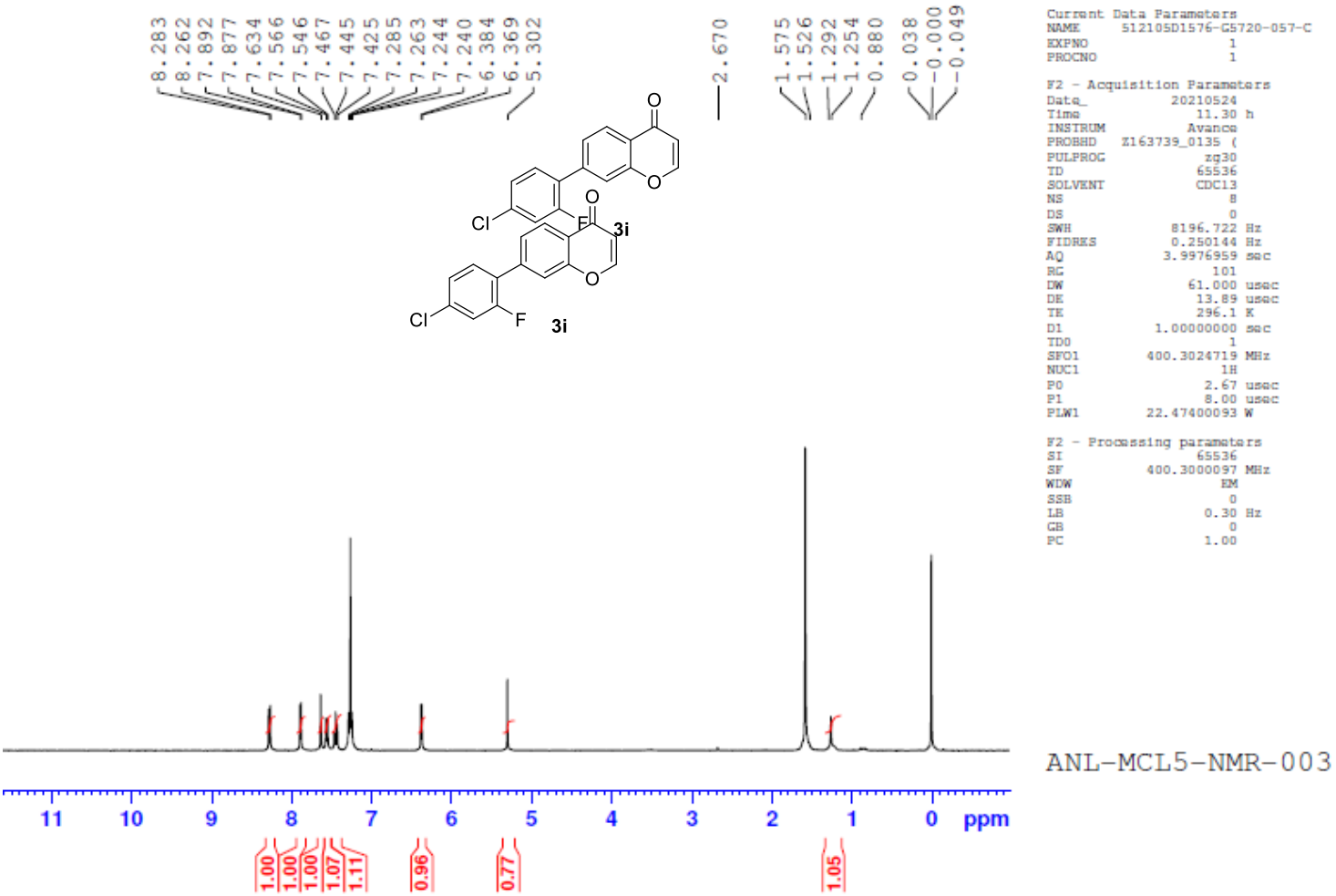
Single Mass Analysis

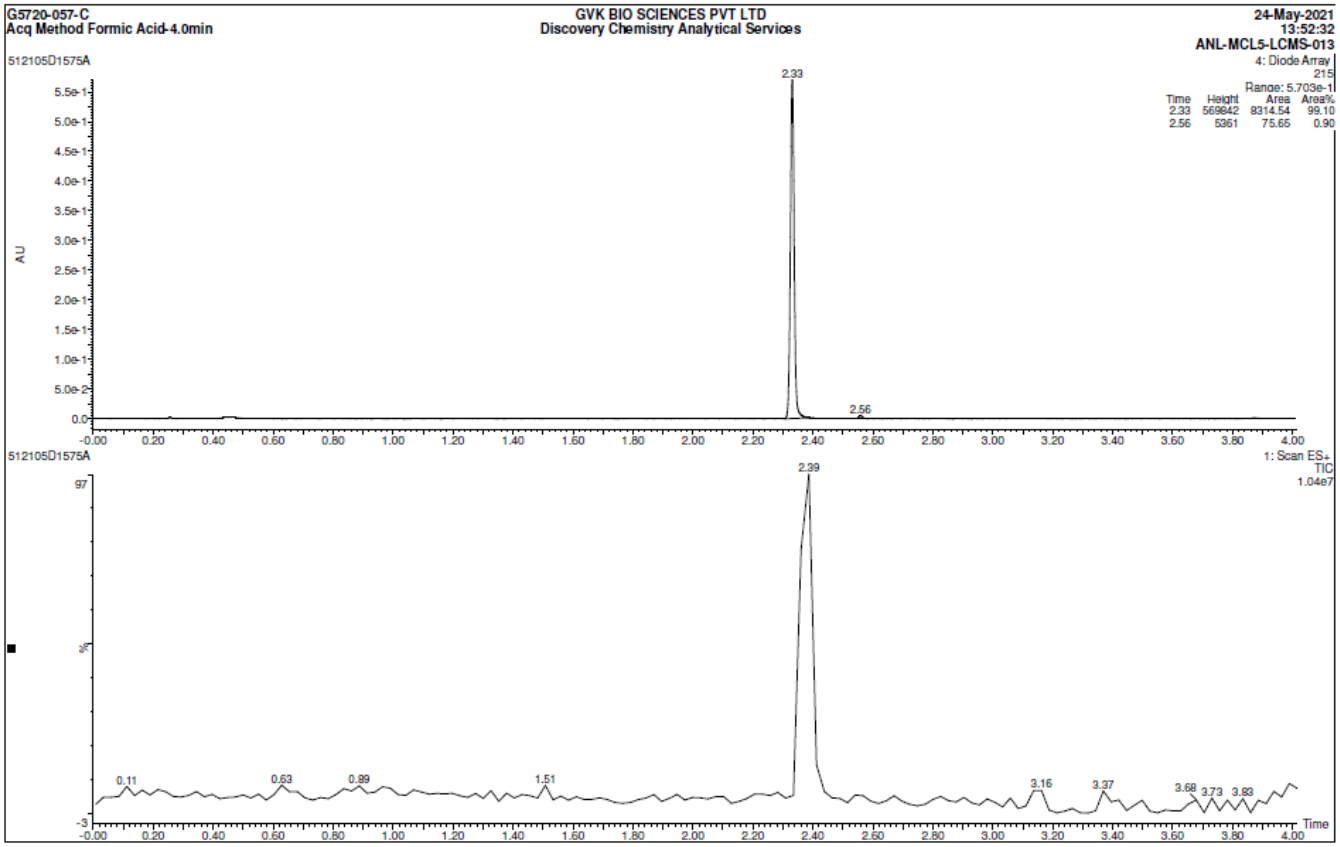
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

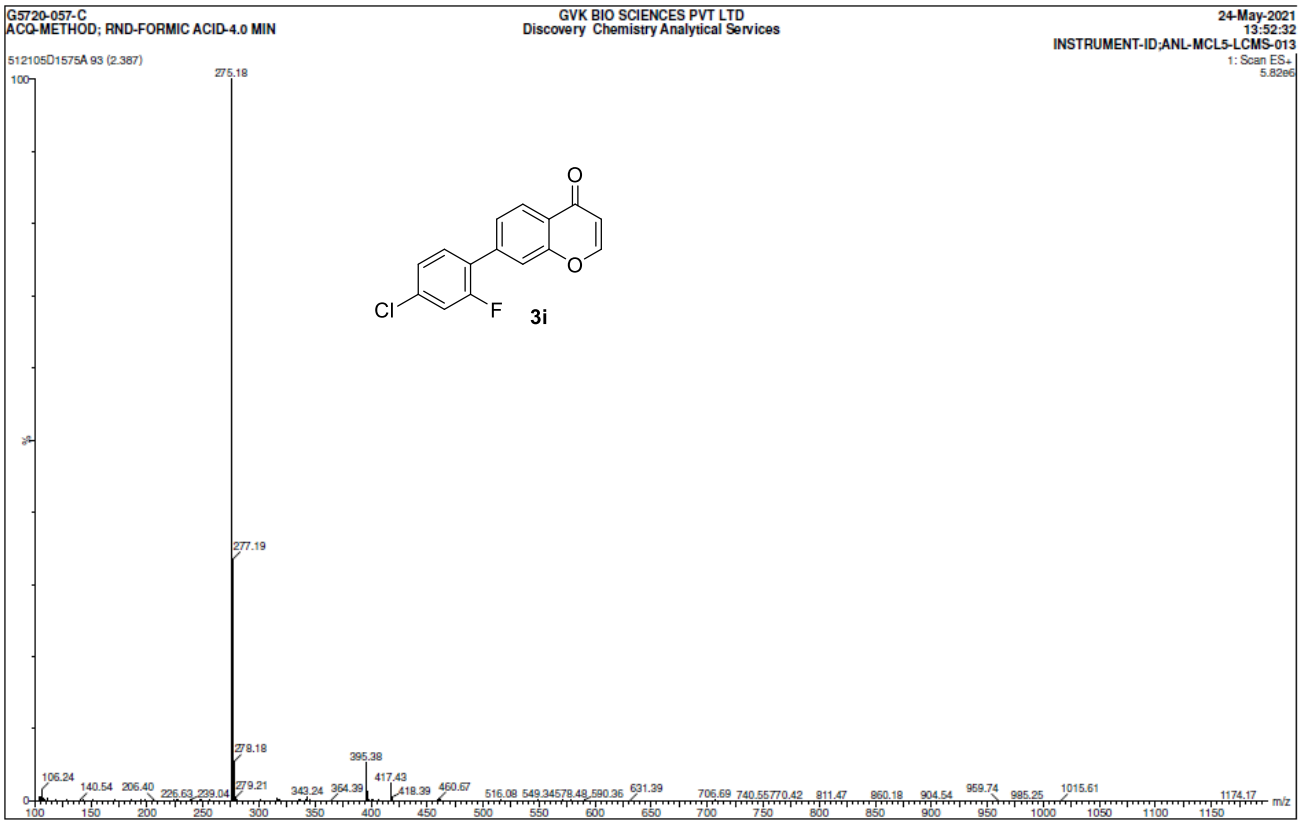
Monoisotopic Mass, Even Electron Ions
4 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-17 H: 0-15 O: 0-4

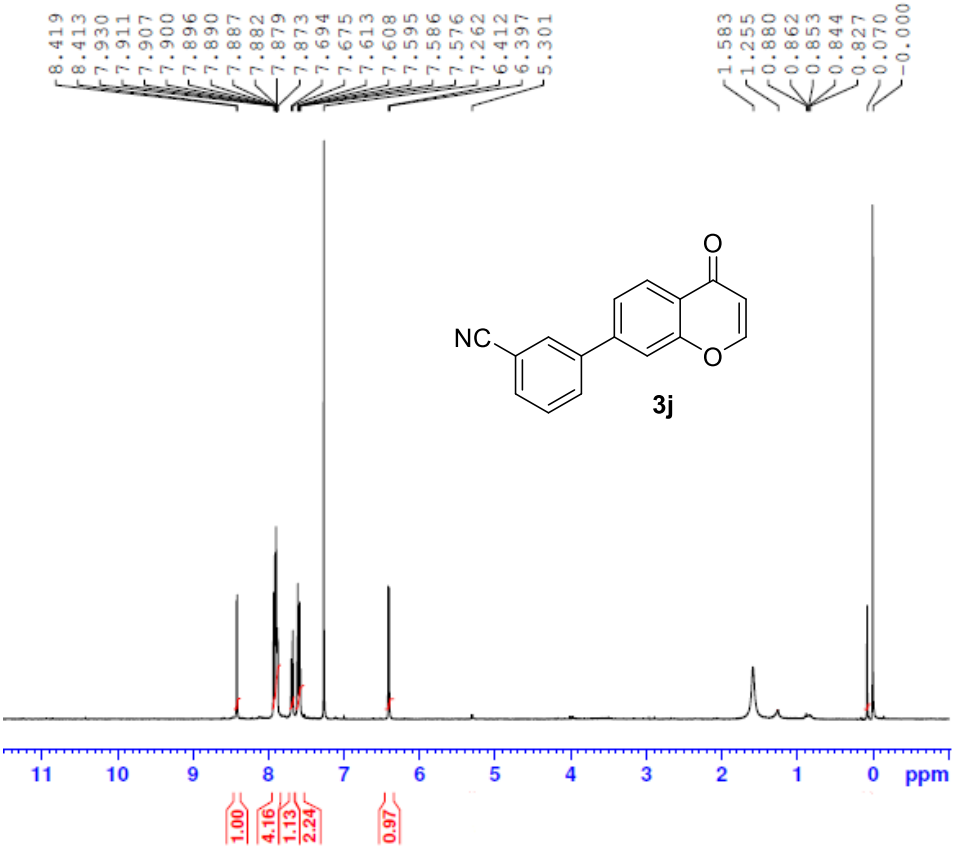


Minimum:				-1.5				
Maximum:		5.0	1000.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
283.0958	283.0970	-1.2	-4.2	10.5	39.4	n/a	n/a	C17 H15 O4


8.283
8.262
7.892
7.877
7.634
7.566
7.546
7.467
7.445
7.425
7.285
7.263
7.244
7.240
6.384
6.369
5.302
2.670
1.575
1.526
1.292
1.254
0.880
0.038
-0.000
-0.049
Cl
F
3i
Cl
F
3i
Current Data Parameters
NAME 512105D1576-G5720-057-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210524
Time 11.30 h
INSTRUM Avance
PROBHD Z163739_0135 (
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 296.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.3024719 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.47400093 W
F2 - Processing parameters
SI 65536
SF 400.3000097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ANL-MCL5-NMR-003
11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00 1.00 1.00 1.07 1.11 0.96 0.77 1.05


G5720-057-C
Acq Method Formic Acid-4.0min
GVK BIO SCIENCES PVT LTD
Discovery Chemistry Analytical Services
24-May-2021
13:52:32
ANL-MCL5-LCMS-013
512105D1575A
4: Diode Array
215
Range: 5.703e-1
Time Height Area Area%
2.33 569842 8314.54 99.10
2.56 5361 75.65 0.90
AU
2.33
2.56
512105D1575A
1: Scan ES+
TIC
1.04e7
%
2.39
0.11
0.63
0.89
1.51
3.16
3.37
3.68
3.73
3.93
Time



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EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
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Time                 9.34 h
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PROBHD   Z163739_0229 (
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
TD0                     1
SFO1           400.2024712 MHz
NUC1                   1H
P0                  2.67 usec
P1                  8.00 usec
PLW1           20.80400085 W

F2 - Processing parameters
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SF             400.2000089 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
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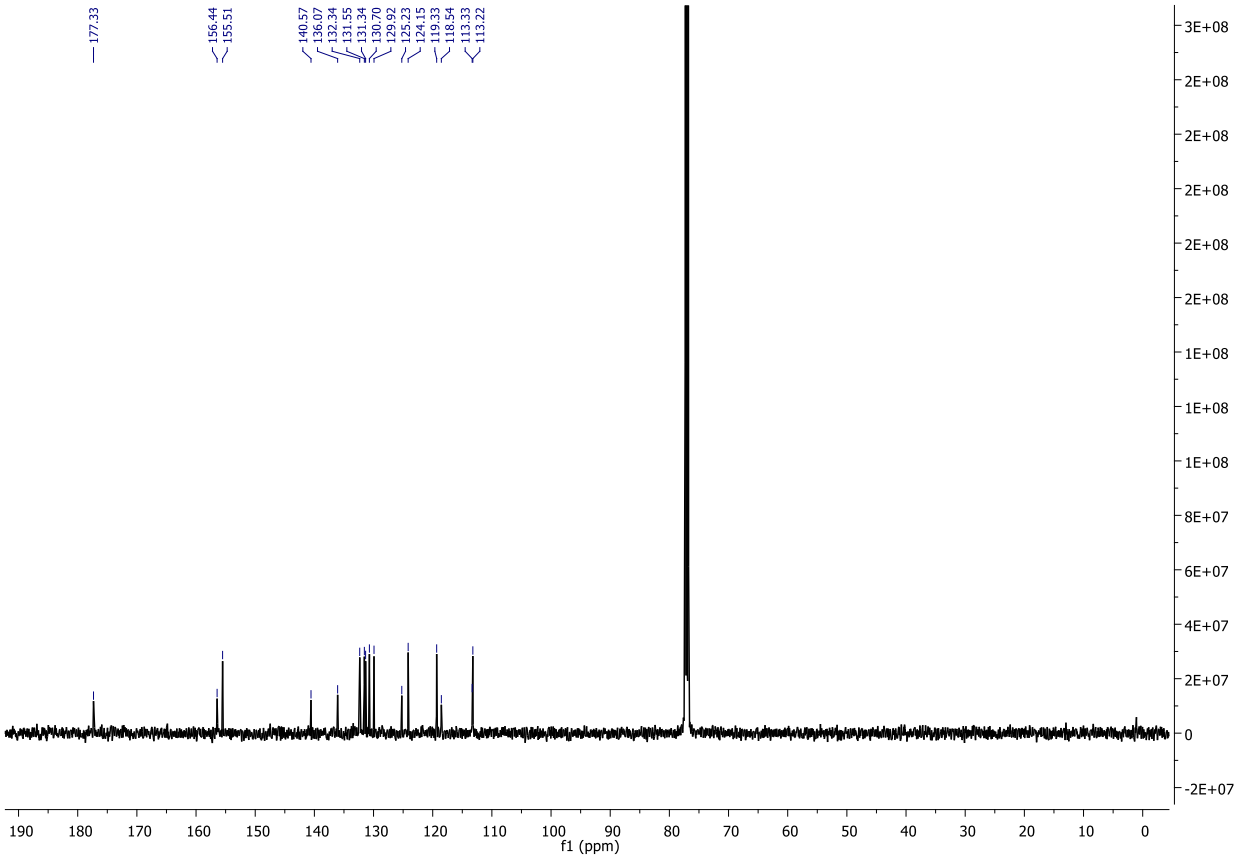
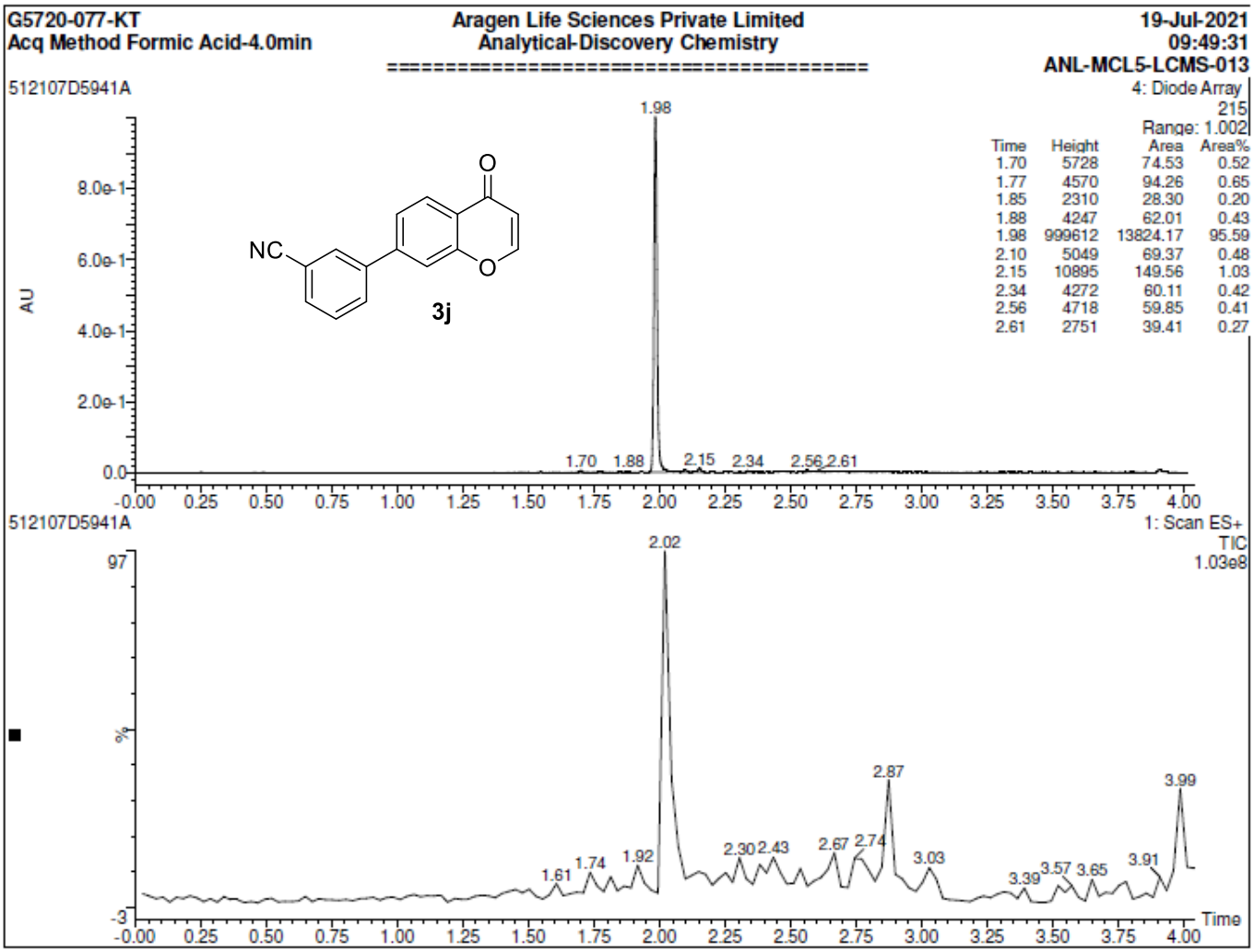
ANL-MCL5-NMR-004


177.33
156.44
155.51
140.57
136.07
132.34
131.55
131.34
130.70
129.92
125.23
124.15
119.33
118.54
113.33
113.22
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


G5720-077-KT
Acq Method Formic Acid-4.0min
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry
19-Jul-2021
09:49:31
ANL-MCL5-LCMS-013
512107D5941A
4: Diode Array
215
Range: 1.002
Time Height Area Area%
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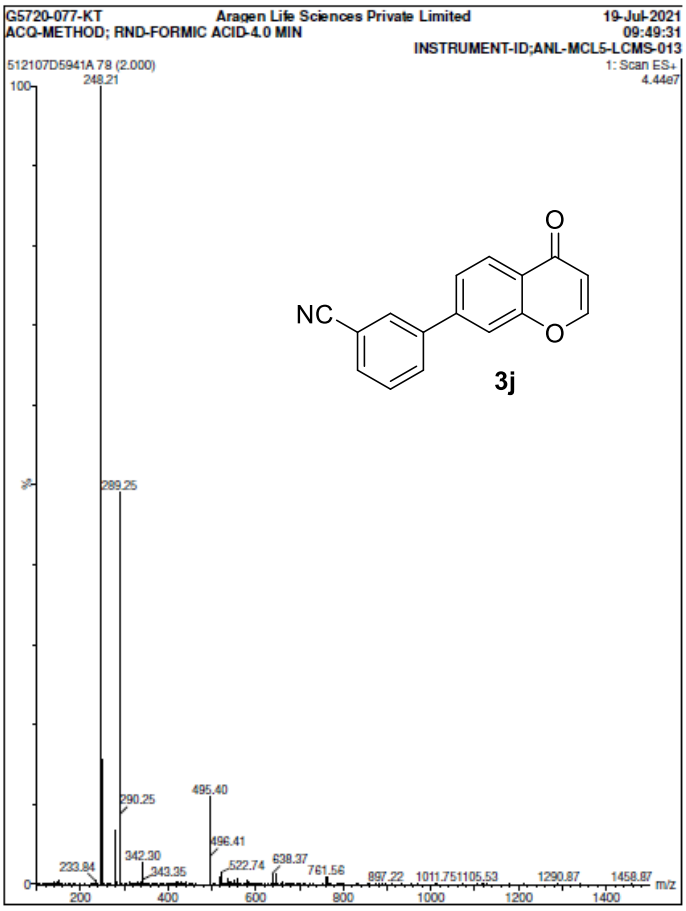
1.77 4570 94.26 0.65
1.85 2310 28.30 0.20
1.88 4247 62.01 0.43
1.98 999612 13824.17 95.59
2.10 5049 69.37 0.48
2.15 10895 149.56 1.03
2.34 4272 60.11 0.42
2.56 4718 59.85 0.41
2.61 2751 39.41 0.27
NC
O
O
3j
AU
1.98
1.70 1.88 2.15 2.34 2.56 2.61
512107D5941A
1: Scan ES+
TIC
1.03e8
%
2.02
1.61 1.74 1.92 2.30 2.43 2.67 2.74 2.87 3.03 3.39 3.57 3.65 3.91 3.99
Time



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

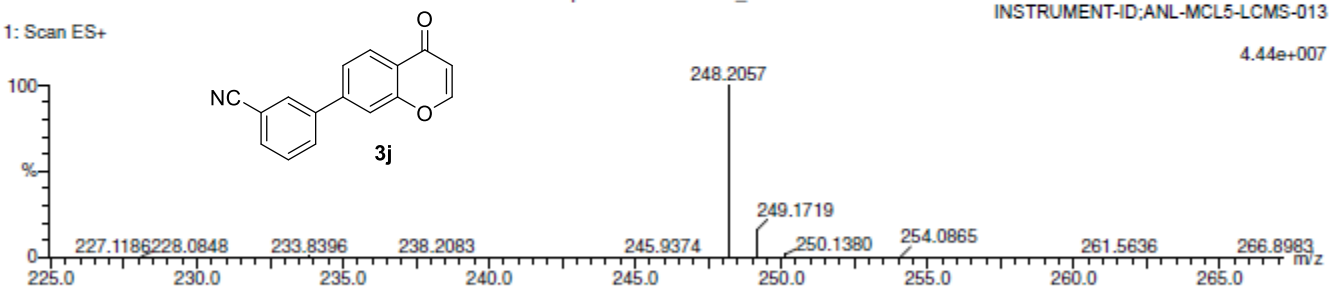
512107D5941A 78 (2.000)
G5720-077-KT

19-07-2021
Acq.method formic acid_4min

19-Jul-2021
09:49:31
INSTRUMENT-ID;ANL-MCL5-LCMS-013

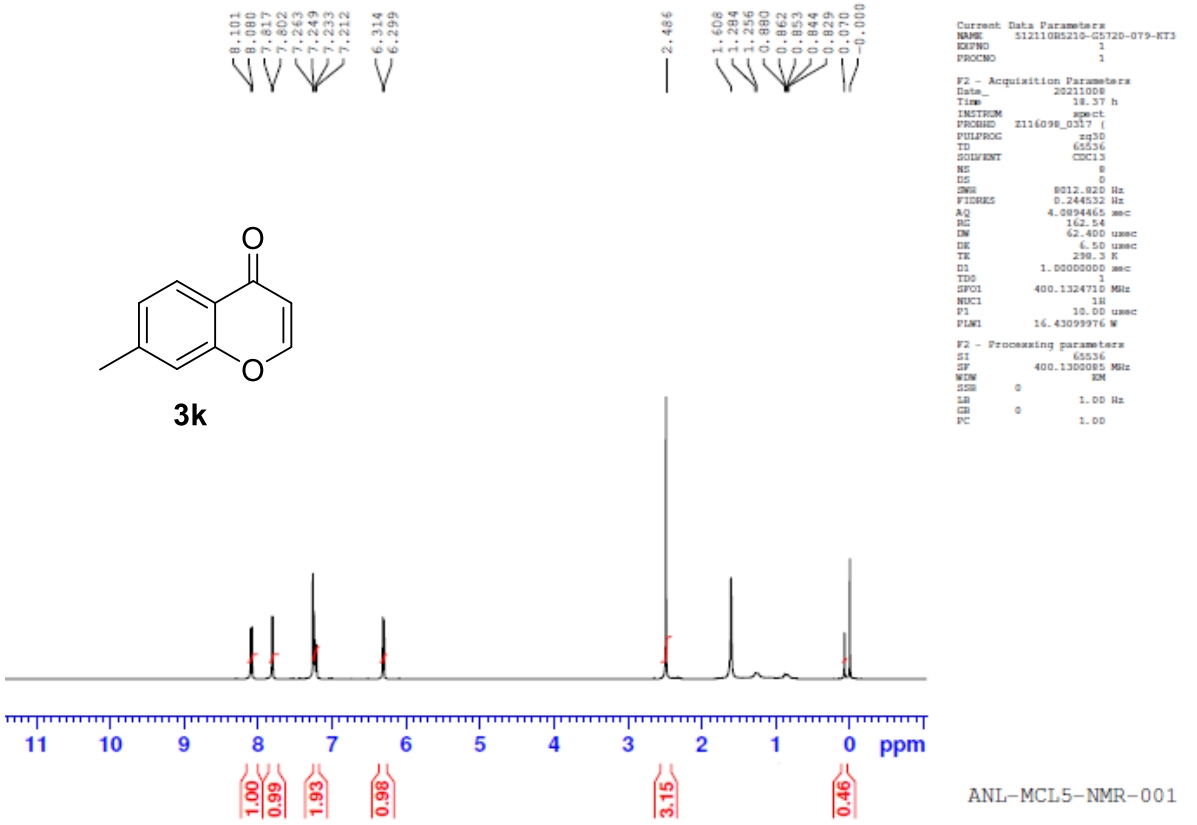
1: Scan ES+

4.44e+007



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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7.817
7.802
7.263
7.249
7.233
7.212
6.314
6.299
2.486
1.608
1.284
1.256
0.880
0.862
0.853
0.844
0.829
0.070
0.000
3k
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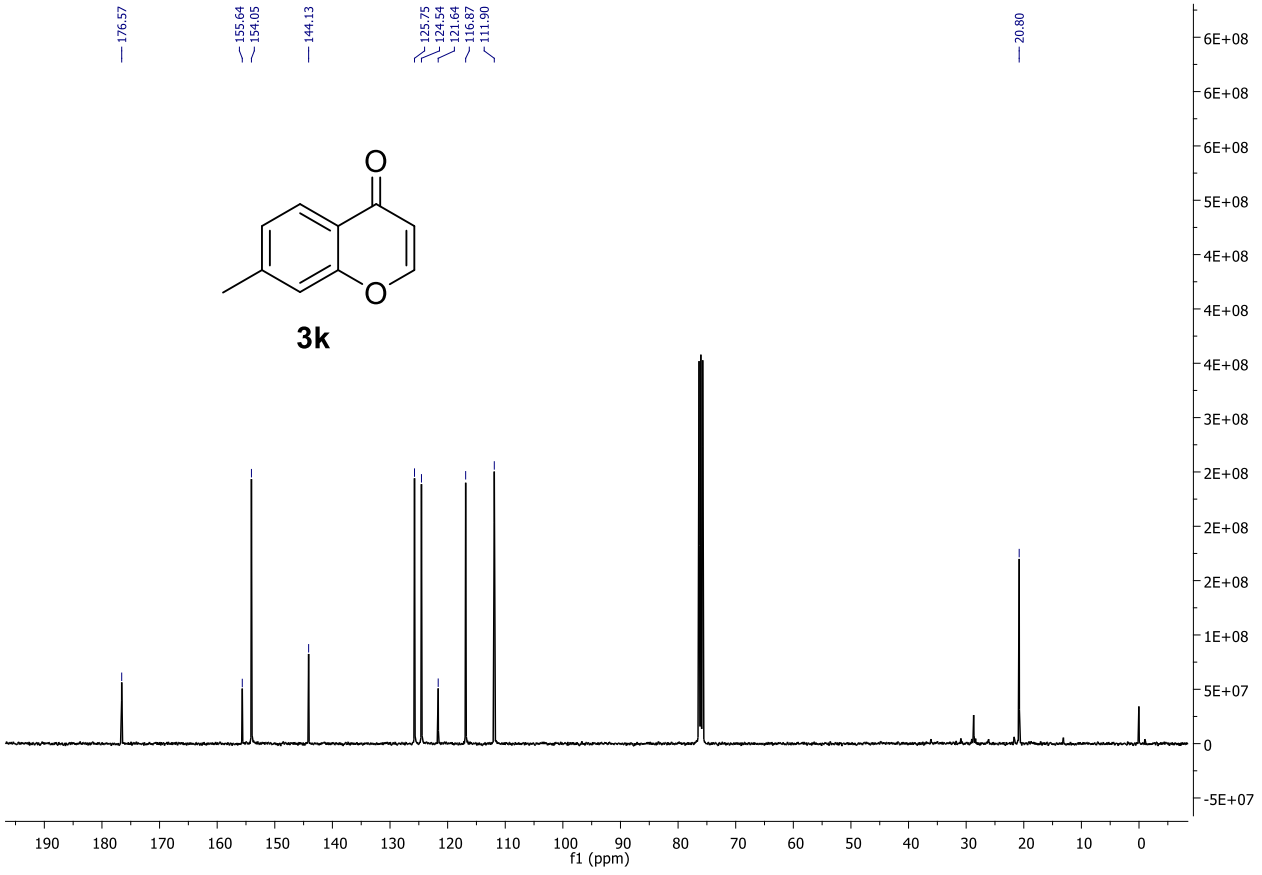
1.00
0.99
1.93
0.98
3.15
0.46
ANL-MCL5-NMR-001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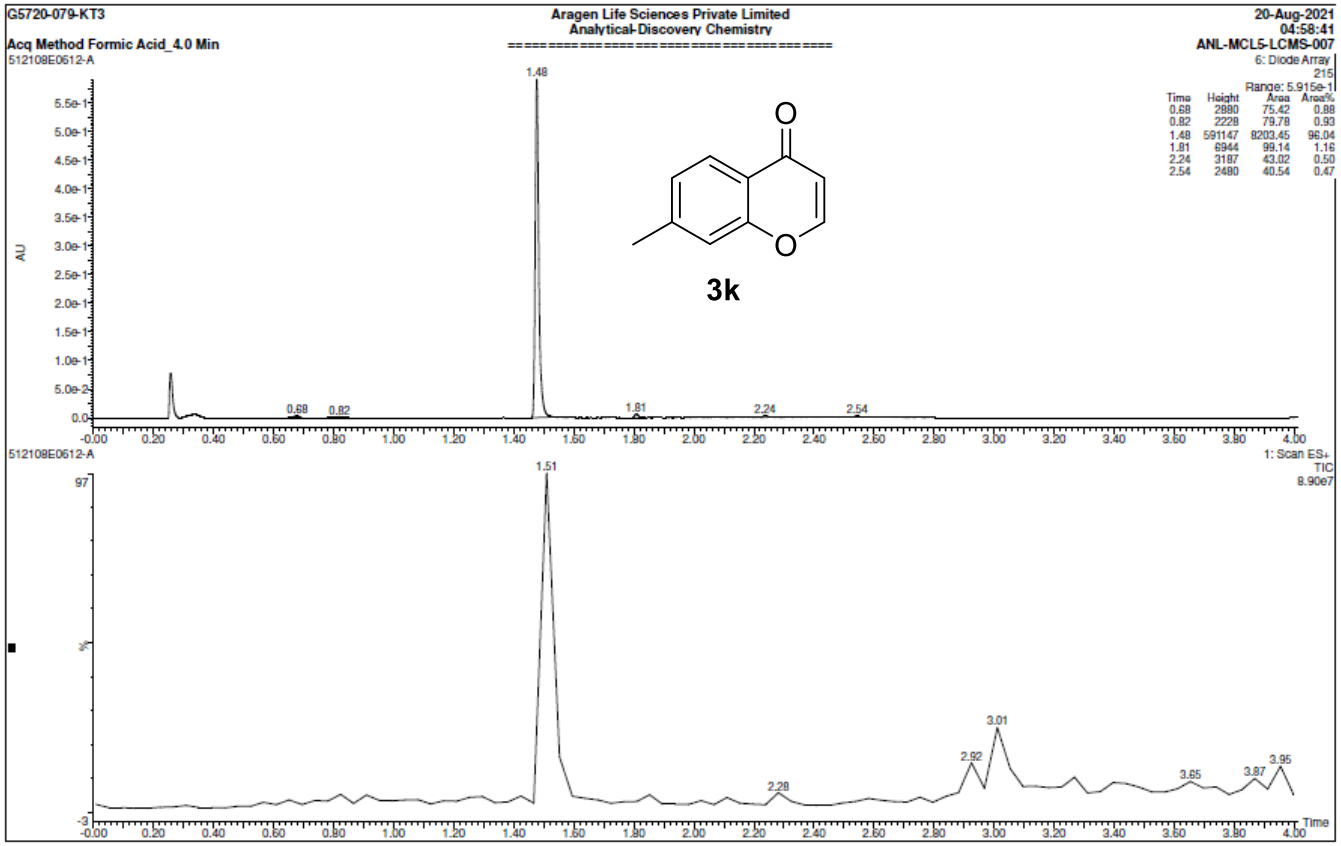
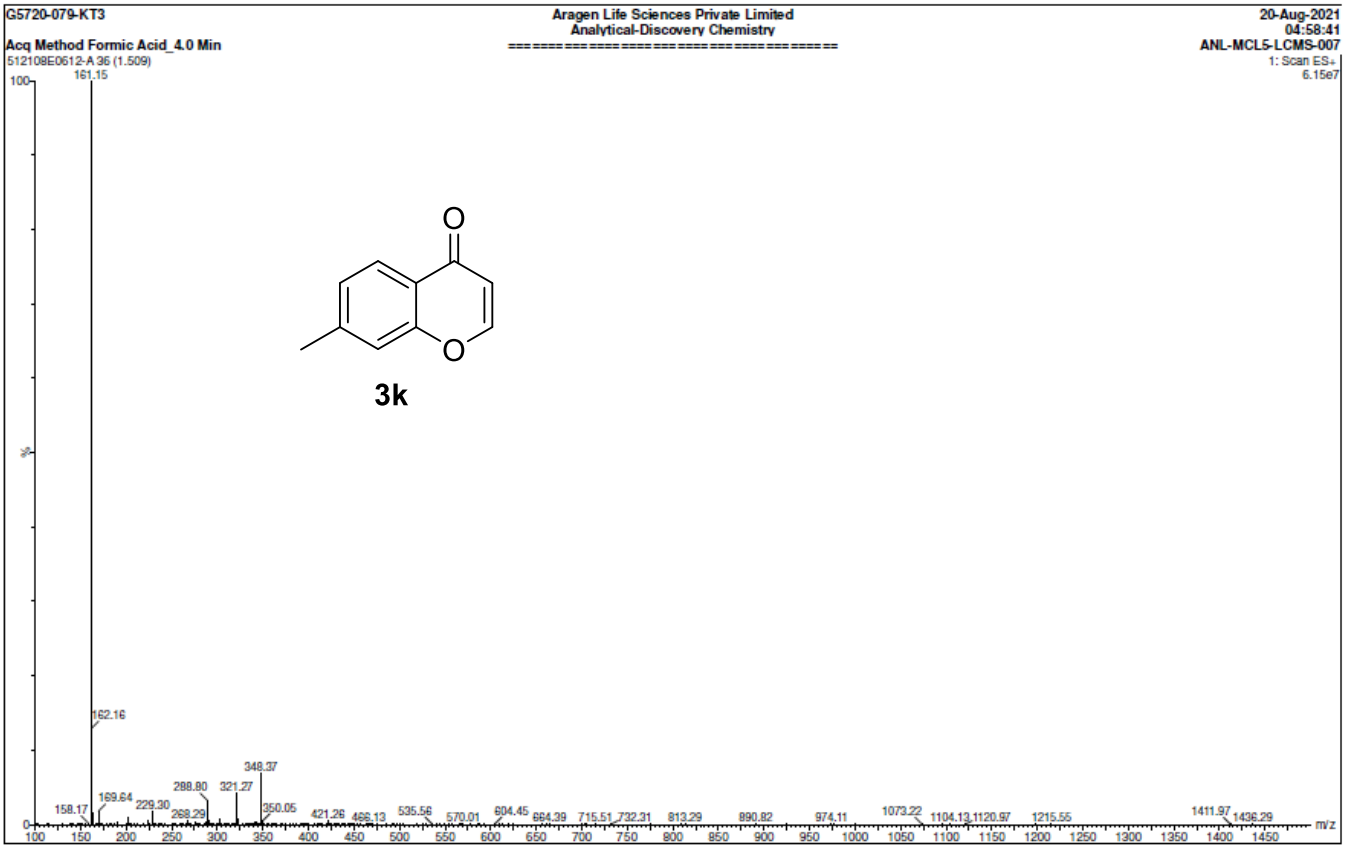
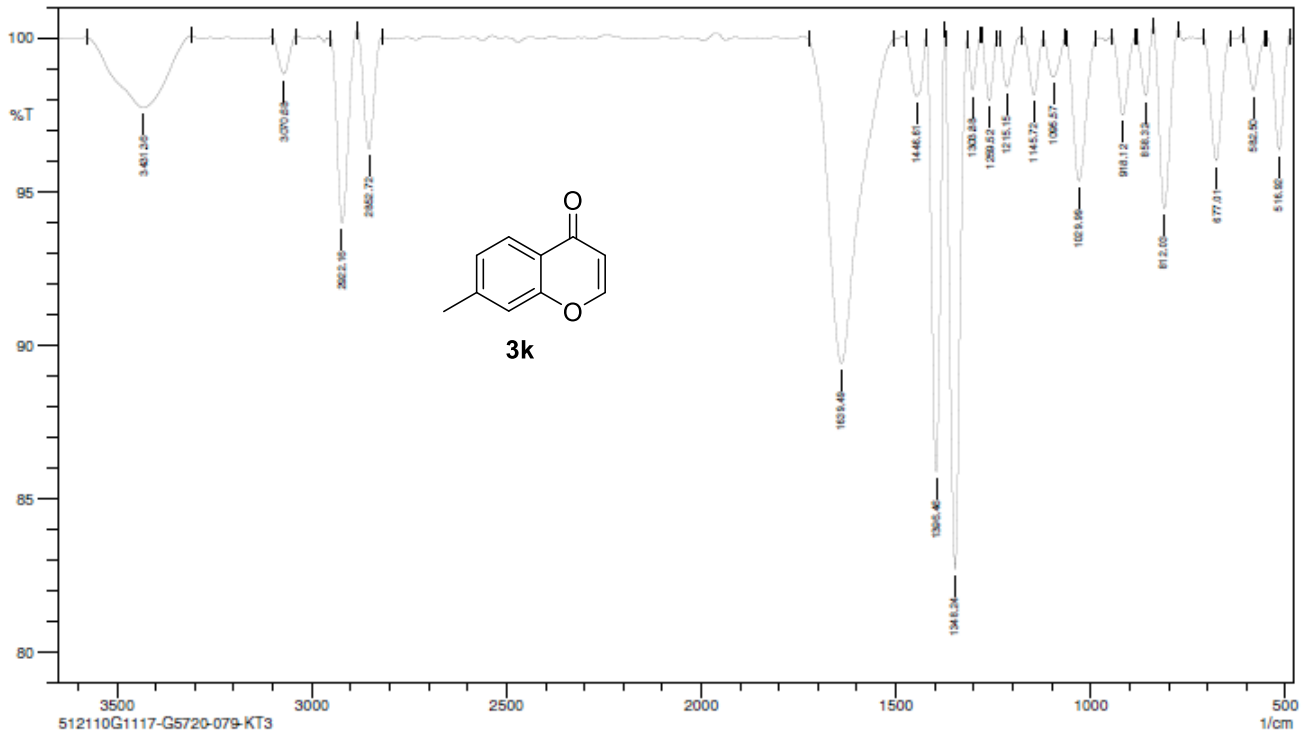
121.64
116.87
111.90
20.80
3k
f1 (ppm)


G5720-079-KT3
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry
20-Aug-2021
04:58:41
Acq Method Formic Acid_4.0 Min
ANL-MCLS-LCMS-007
512108E0612-A
6: Diode Array
215
Range: 5.915e-1
Time Height Area Area%
0.68 2880 75.42 0.88
0.82 2228 79.78 0.93
1.48 591147 8203.45 96.04
1.81 6944 99.14 1.16
2.24 3187 43.02 0.50
2.54 2480 40.54 0.47
AU
1.48
0.68
0.82
1.81
2.24
2.54
3k
512108E0612-A
1: Scan ES+
TIC
8.90e7
1.51
3.01
2.92
2.28
3.65
3.87
3.95
Time


G5720-079-KT3
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry
20-Aug-2021
04:58:41
Acq Method Formic Acid_4.0 Min
ANL-MCLS-LCMS-007
512108E0612-A 36 (1.509)
1: Scan ES+
6.15e7
161.15
162.16
348.37
288.80
321.27
169.64
229.30
158.17
268.29
350.05
3k
m/z

Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry



Sample Name:
512110G1117-G5720-079-KT3

No. of Scans:

Date/Time: 10/29/2021 7:48:10 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

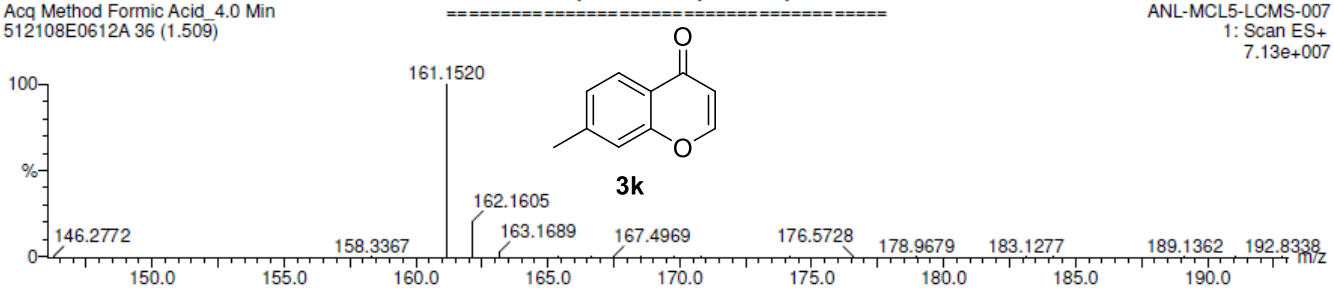
Monoisotopic Mass, Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-10 H: 0-9 O: 0-2

G5720-079-KT3

Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry

20-Aug-2021
02:02:33
ANL-MCL5-LCMS-007
1: Scan ES+
7.13e+007

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



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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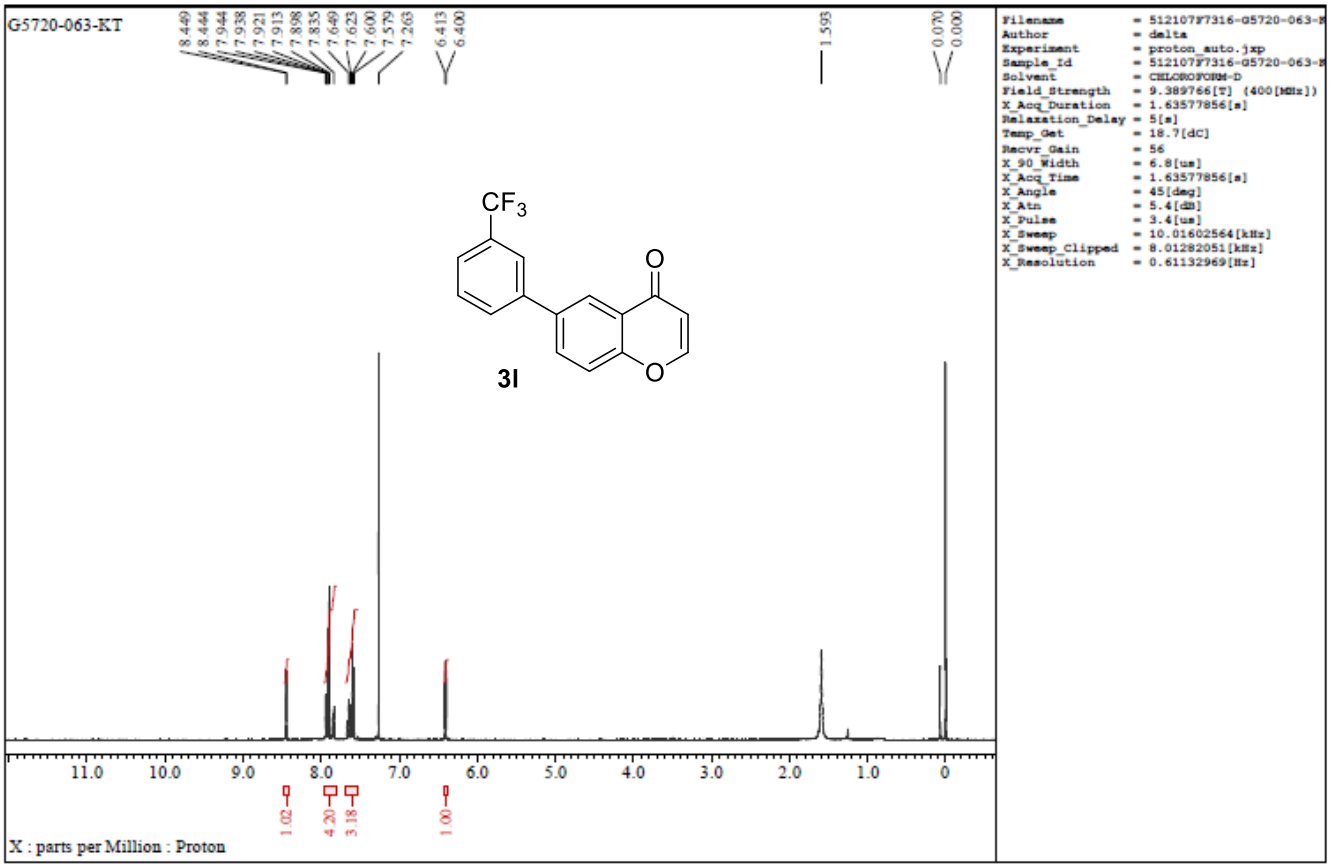
G5720-063-KT
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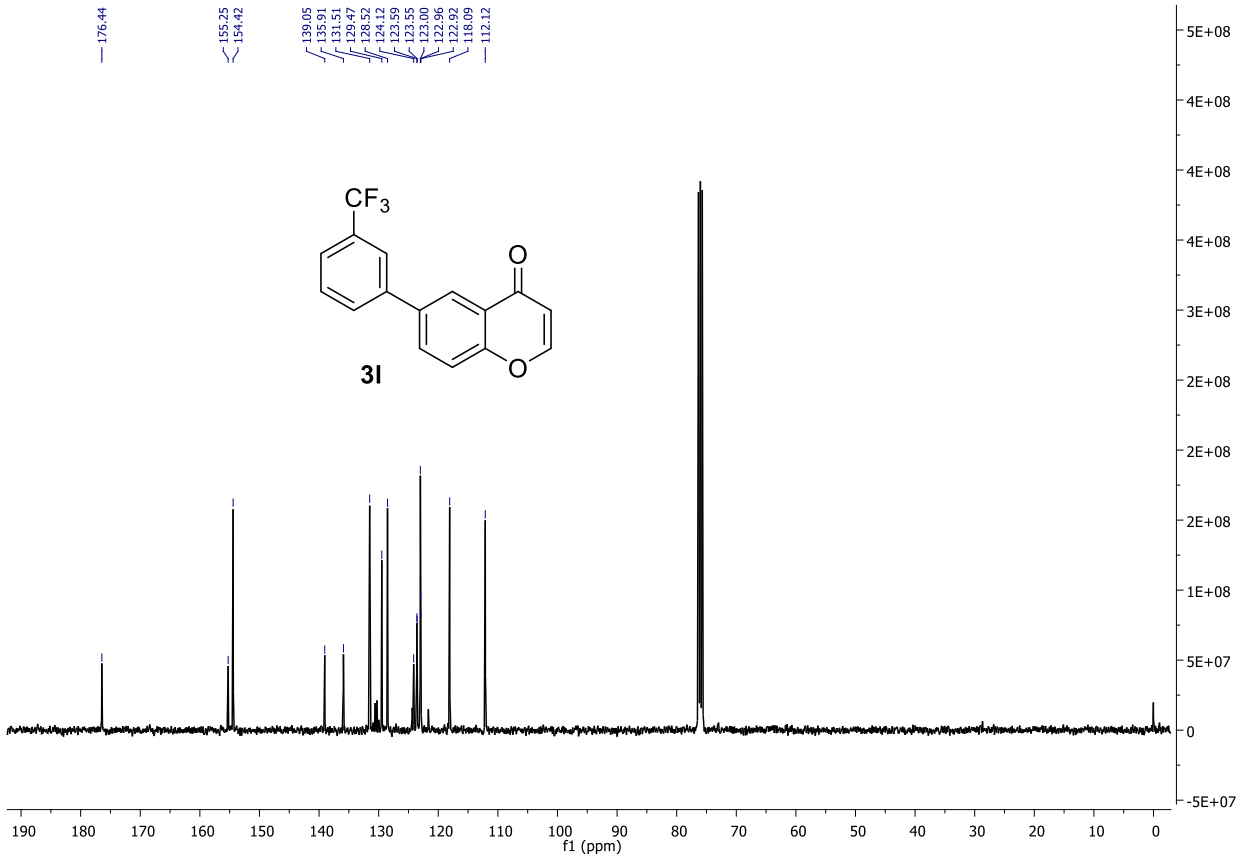
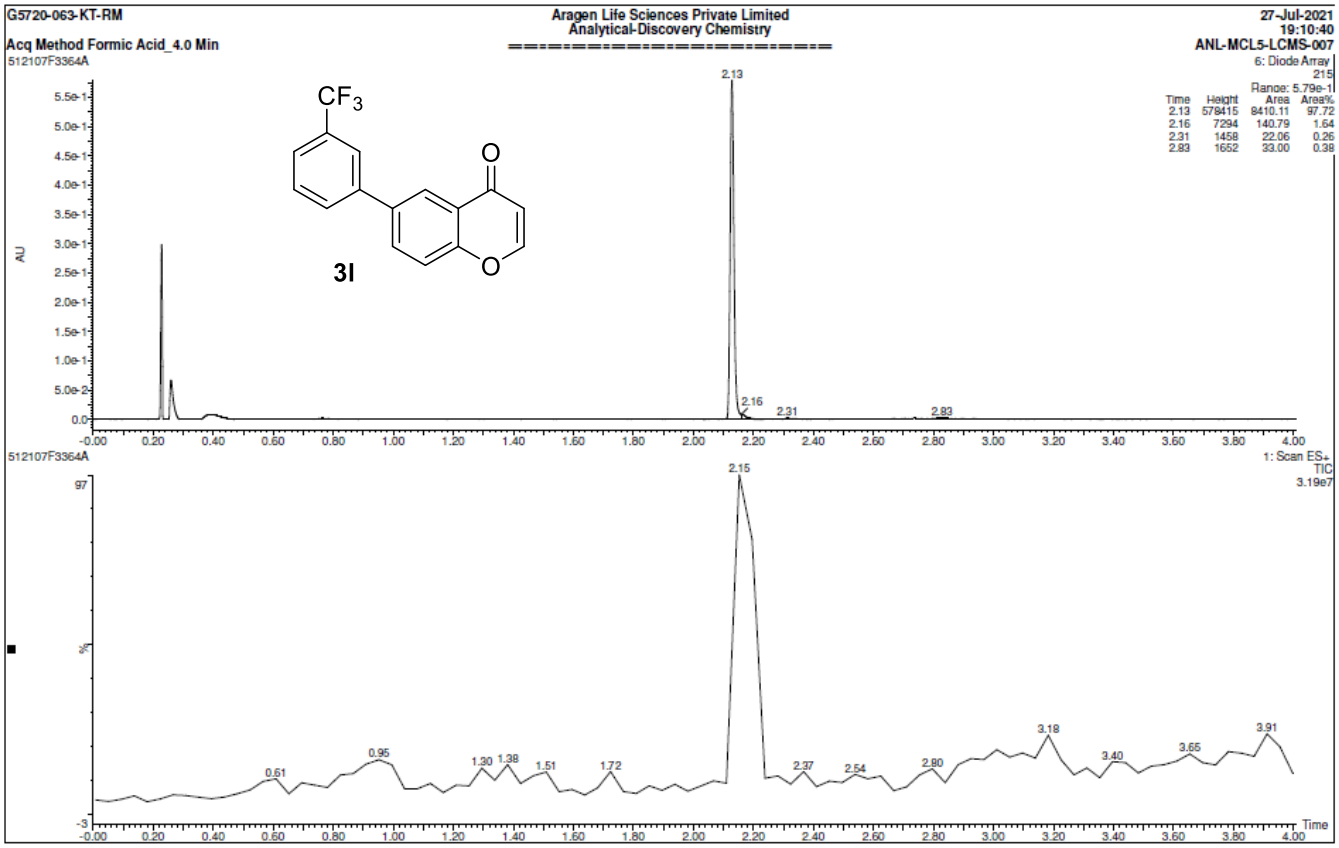
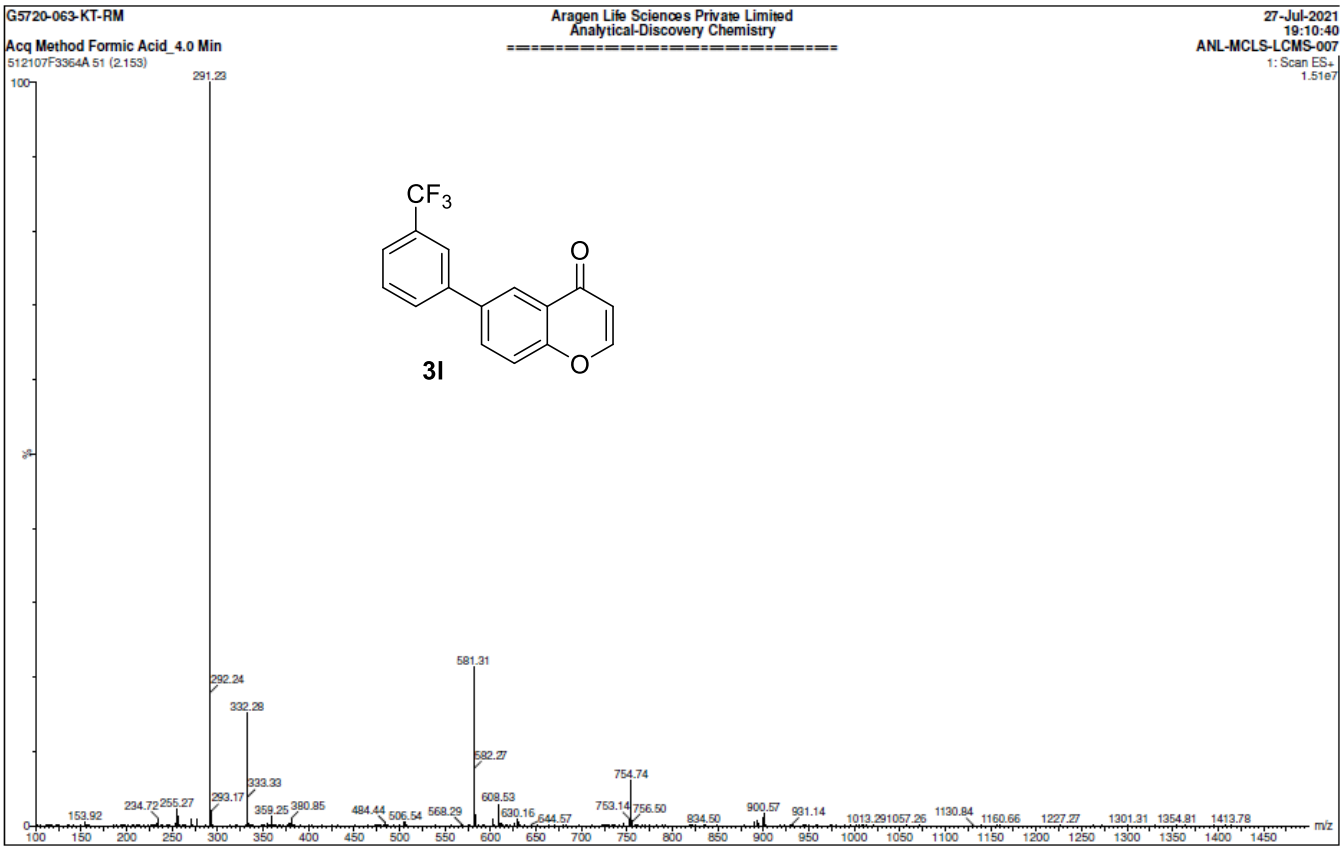
7.944
7.938
7.921
7.913
7.898
7.835
7.649
7.623
7.600
7.579
7.263
6.413
6.400
1.593
0.070
0.000
CF3
O
O
3l
Filename = 5121077316-G5720-063-K
Author = delta
Experiment = proton_auto.jxp
Sample_Id = 5121077316-G5720-063-K
Solvent = CHLOROFORM-D
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.63577856[s]
Relaxation_Delay = 5[s]
Temp_Get = 18.7[dC]
Recvr_Gain = 56
X_90_Width = 6.8[us]
X_Acq_Time = 1.63577856[s]
X_Angle = 45[deg]
X_Atn = 5.4[dB]
X_Pulse = 3.4[us]
X_Sweep = 10.01602564[kHz]
X_Sweep_Clipped = 8.01282051[kHz]
X_Resolution = 0.61132969[Hz]
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.02
4.20
3.18
1.00
X : parts per Million : Proton


176.44
155.25
154.42
139.05
135.91
131.51
129.47
128.52
124.12
123.59
123.55
123.00
122.96
122.92
118.09
112.12
CF3
O
O
3l
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


G5720-063-KT-RM
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry
27-Jul-2021
19:10:40
Acq Method Formic Acid_4.0 Min
ANL-MCL5-LCMS-007
512107F3364A
6: Diode Array
215
Range: 5.79e-1
Time Height Area Area%
2.13 578415 8410.11 97.72
2.16 7294 140.79 1.64
2.31 1458 22.06 0.26
2.83 1652 33.00 0.38
CF3
O
O
3l
AU
2.13
2.16
2.31
2.83
512107F3364A
1: Scan ES+
TIC
3.19e7
%
2.15
0.61
0.95
1.30
1.38
1.51
1.72
2.37
2.54
2.80
3.18
3.40
3.65
3.91
Time


G5720-063-KT-RM
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry
27-Jul-2021
19:10:40
Acq Method Formic Acid_4.0 Min
512107F3364A 51 (2.153)
ANL-MCLS-LCMS-007
1: Scan ES+
1.51e7
CF3
O
O
3l
%
291.23
581.31
292.24
332.28
582.27
754.74
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293.17
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234.72
255.27
359.25
380.85
484.44
506.54
568.29
630.16
644.57
753.14
756.50
834.50
900.57
931.14
1013.291057.26
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1160.66
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1301.31
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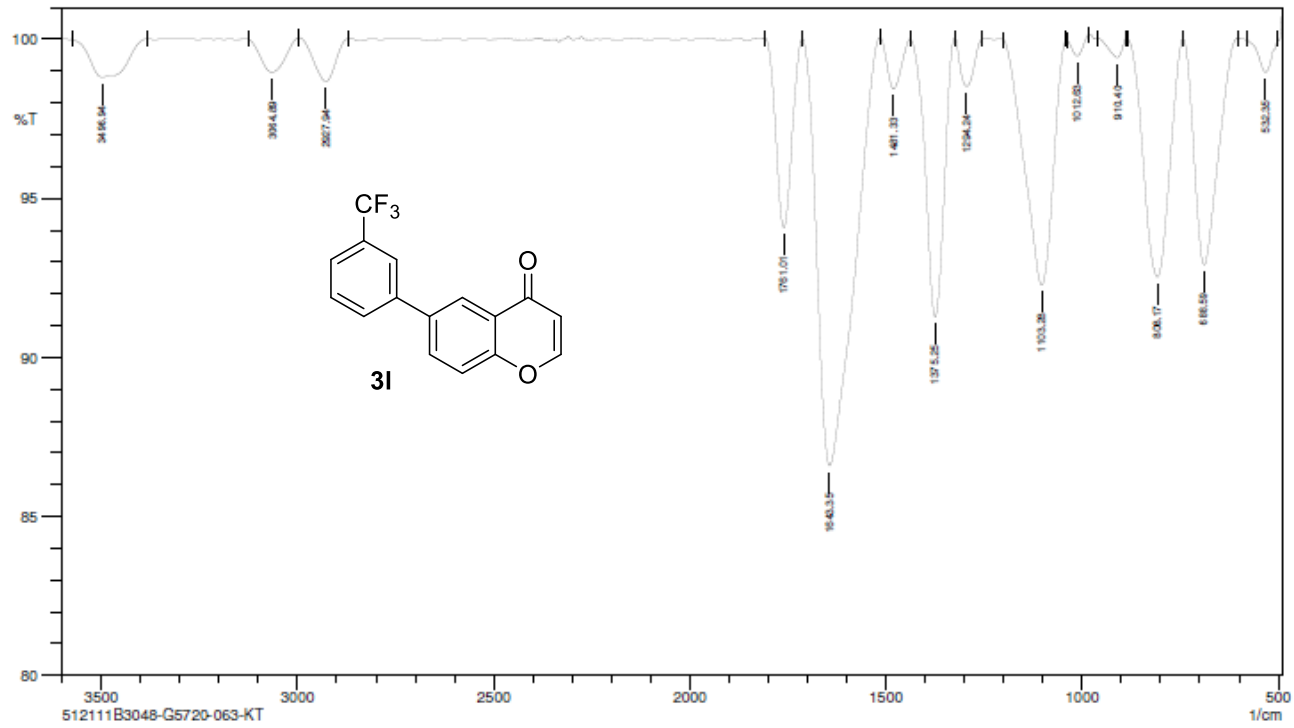
1413.78
153.92
m/z

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

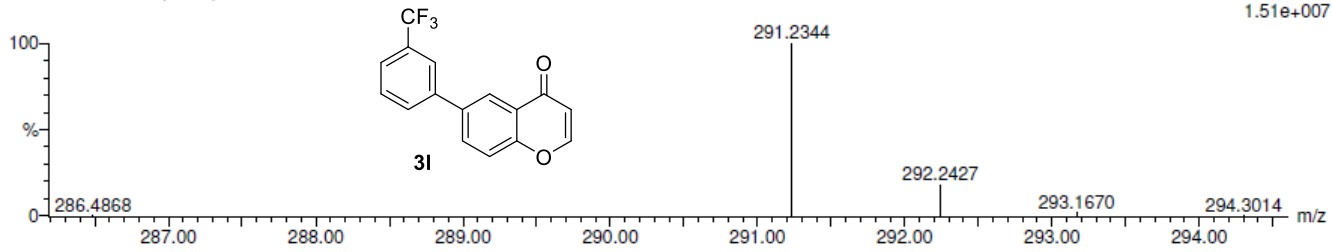
Monoisotopic Mass, Even Electron Ions
10 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-16 H: 0-10 O: 0-2 F: 0-3

G5720-063-KT-RM

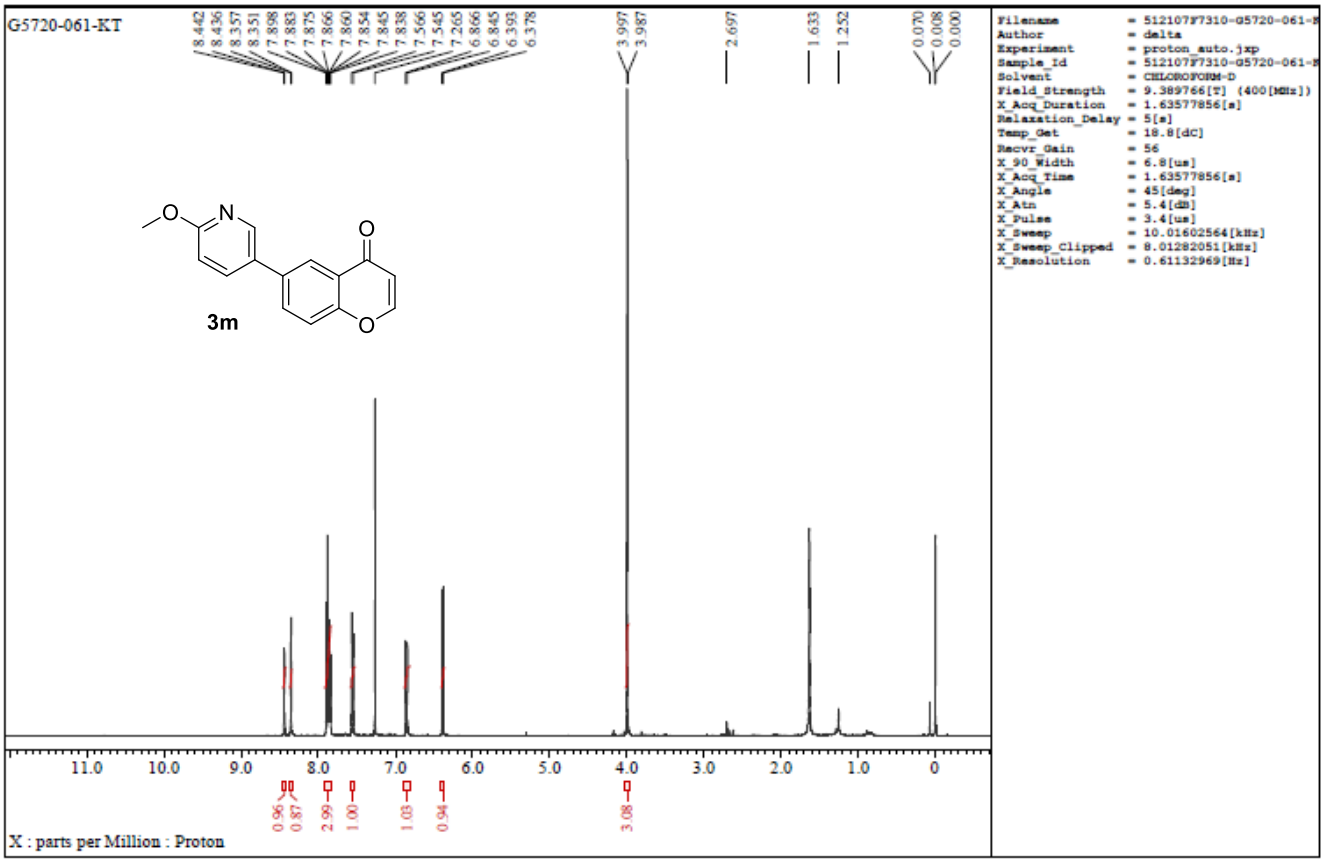
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry

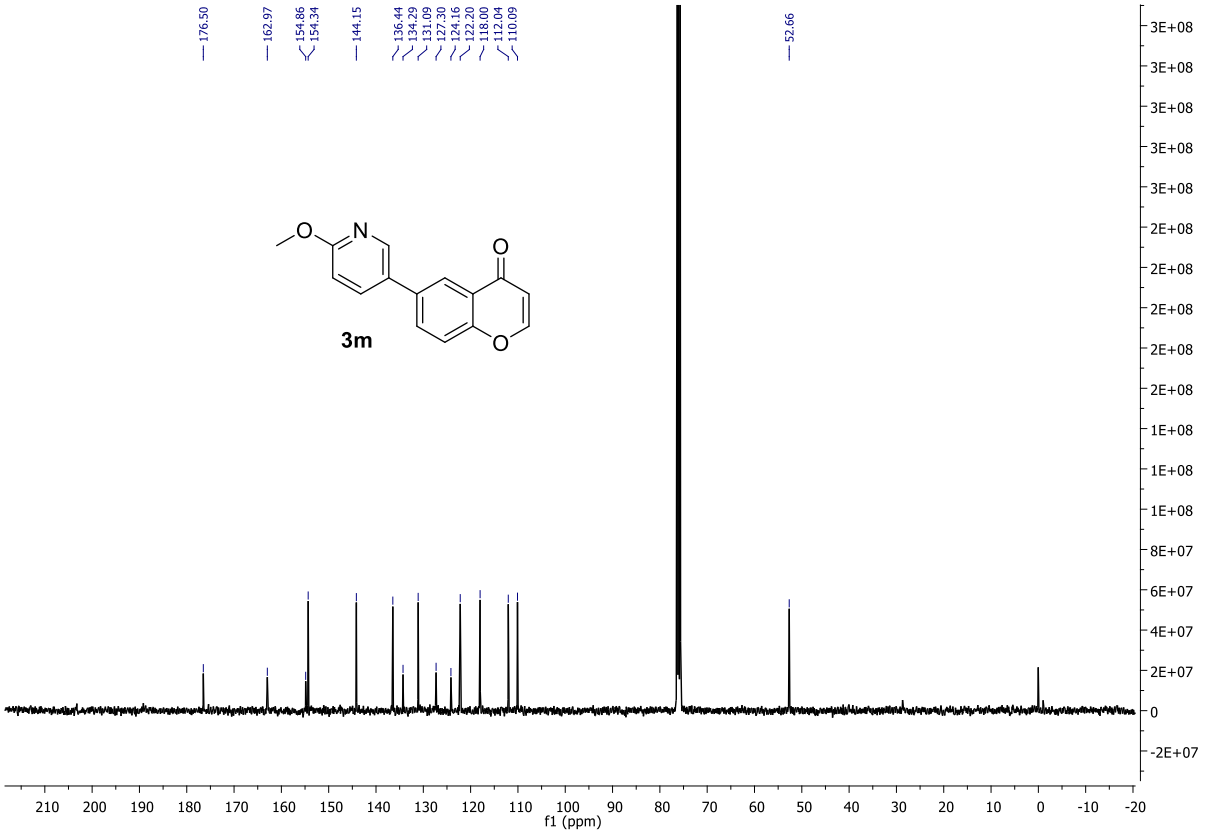
27-Jul-2021
19:10:40
ANL-MCL5-LCMS-007
1: Scan ES+
1.51e+007

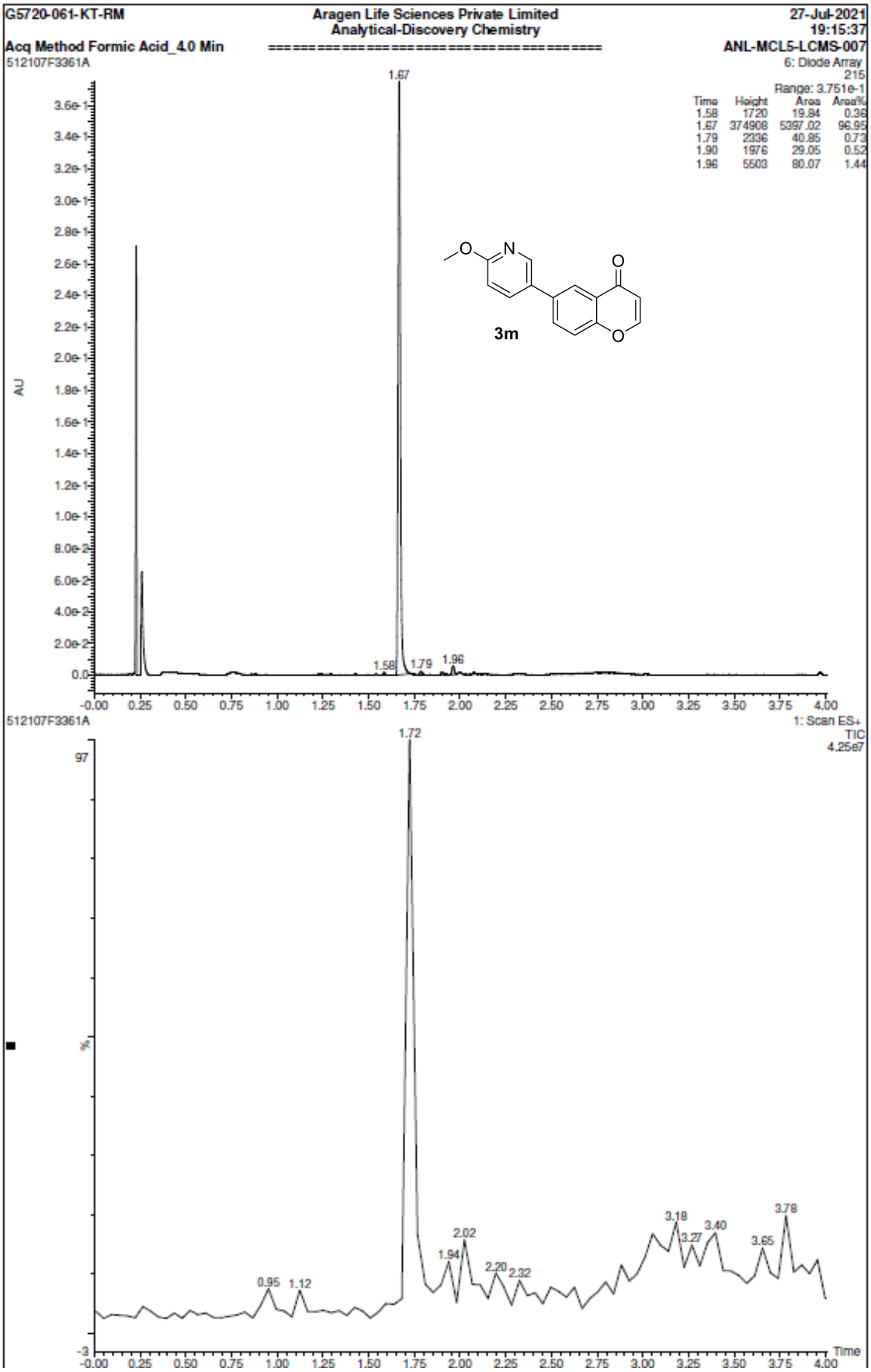
Acq Method Formic Acid_4.0 Min
512107F3364A 51 (2.153)

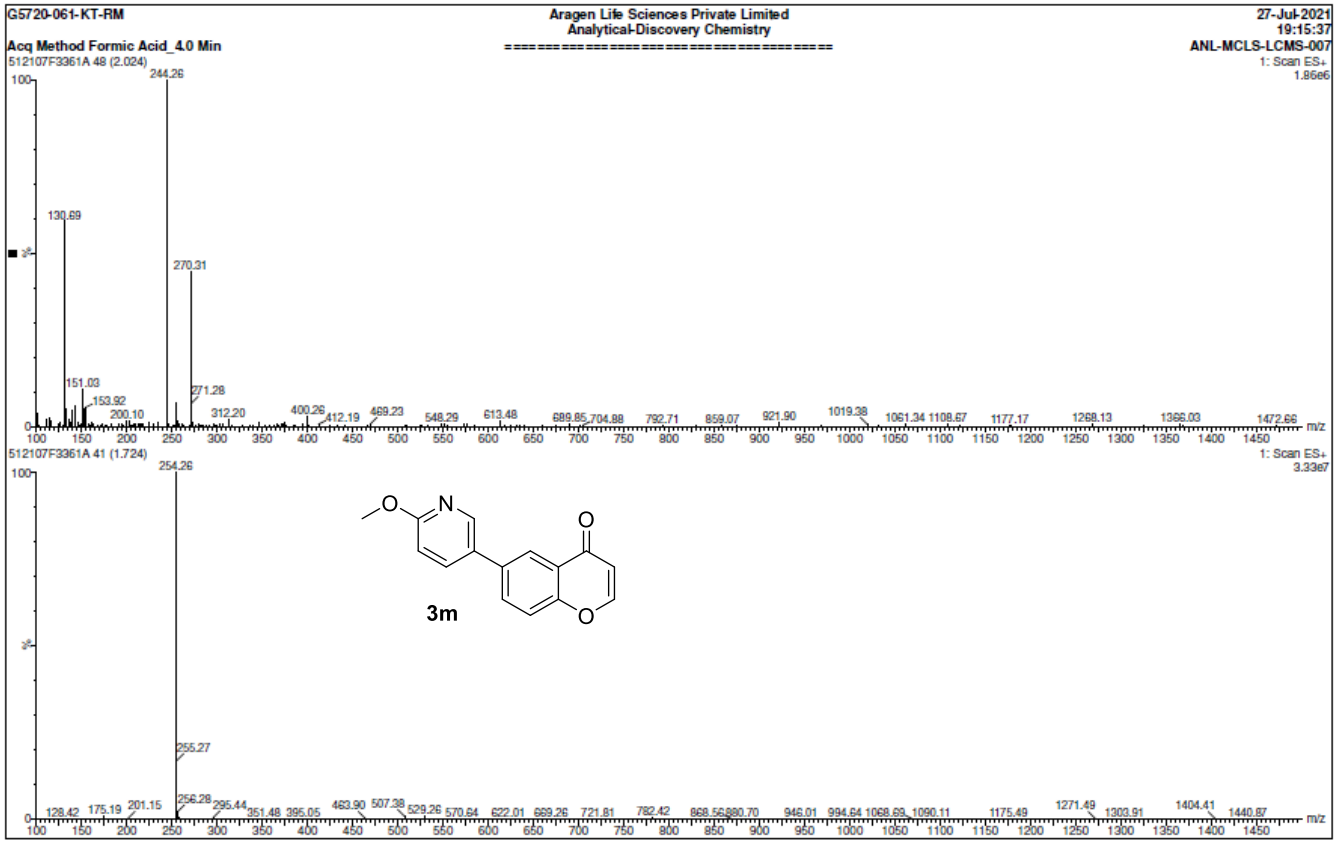


Minimum:				-1.5				
Maximum:		5.0	1000.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
291.0699	291.0633	6.6	22.7	10.5	40.3	n/a	n/a	C16 H10 O2 F3


G5720-061-KT
8.442
8.436
8.357
8.351
7.898
7.883
7.875
7.866
7.860
7.854
7.845
7.838
7.566
7.545
7.265
6.866
6.845
6.393
6.378
3.997
3.987
2.697
1.633
1.252
0.070
0.008
0.000
3m
Filename = 5121077310-G5720-061-K
Author = delta
Experiment = proton_auto.jxp
Sample_Id = 5121077310-G5720-061-K
Solvent = CHLOROFORM-D
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.63577856[s]
Relaxation_Delay = 5[s]
Temp_Get = 18.8[dC]
Recvr_Gain = 56
X_90_Width = 6.8[us]
X_Acq_Time = 1.63577856[s]
X_Angle = 45[deg]
X_Atn = 5.4[dB]
X_Pulse = 3.4[us]
X_Sweep = 10.01602564[kHz]
X_Sweep_Clipped = 8.01282051[kHz]
X_Resolution = 0.61132969[Hz]
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
0.96
0.87
2.99
1.00
1.03
0.94
3.08
X : parts per Million : Proton


176.50
162.97
154.86
154.34
144.15
136.44
134.29
131.09
127.30
124.16
122.20
118.00
112.04
110.09
52.66
3m
3E+08
3E+08
3E+08
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)


G5720-061-KT-RM
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry
27-Jul-2021
19:15:37
Acq Method Formic Acid_4.0 Min
ANL-MCL5-LCMS-007
512107F3361A
6: Diode Array
215
Range: 3.751e-1
Time Height Area Area%
1.58 1720 19.84 0.36
1.67 374908 5397.02 96.95
1.79 2336 40.85 0.73
1.90 1976 29.05 0.52
1.96 5503 80.07 1.44
1.67
1.58
1.79
1.96
AU
3m
512107F3361A
1: Scan ES+
TIC
4.25e7
1.72
0.95
1.12
1.94
2.02
2.20
2.32
3.18
3.27
3.40
3.65
3.78
%
Time



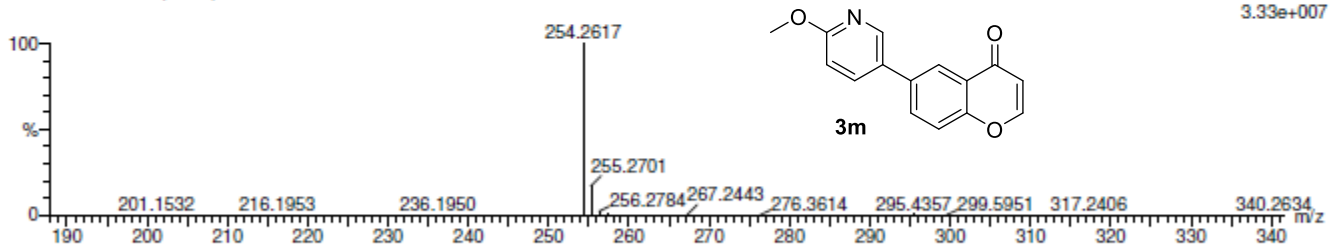
Elemental Composition Report

Single Mass Analysis

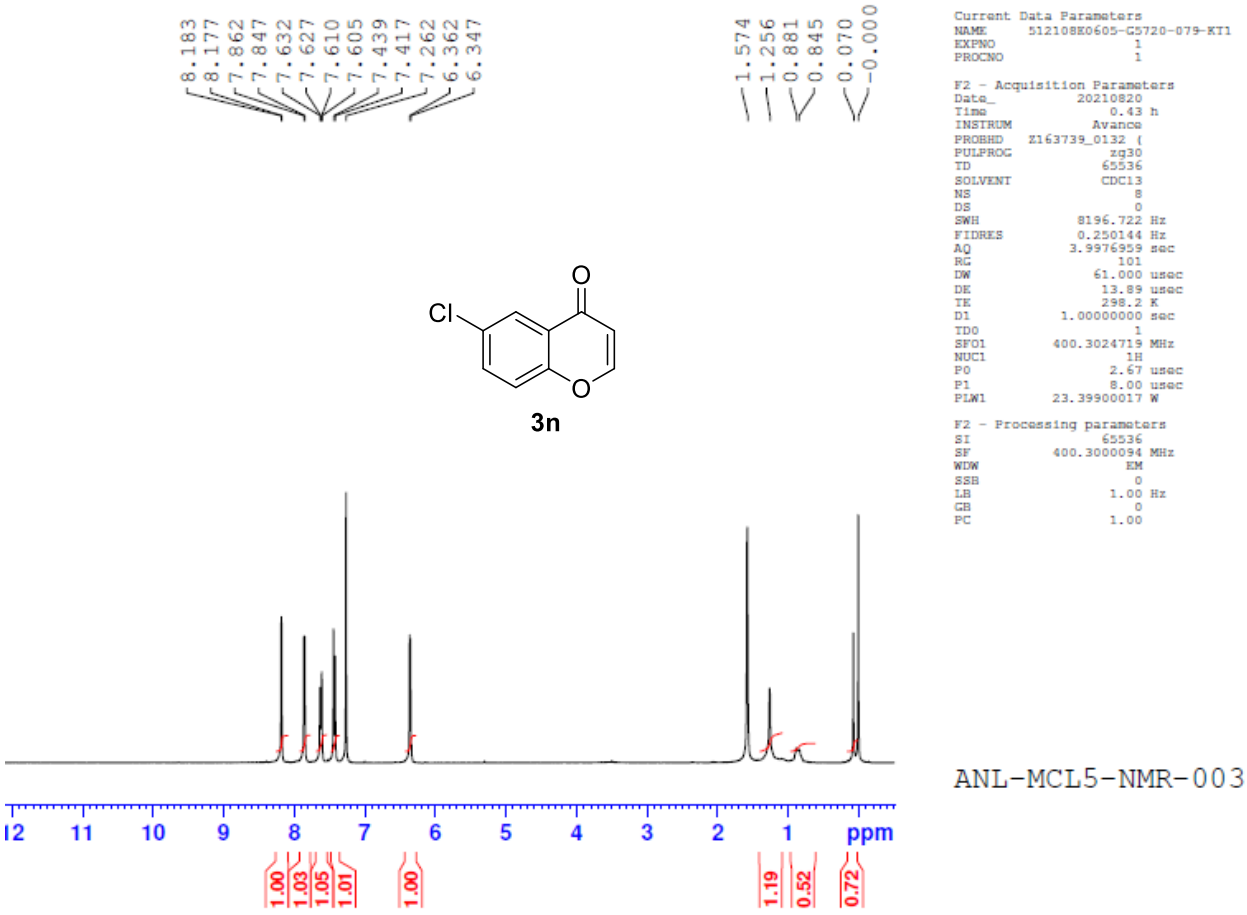
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

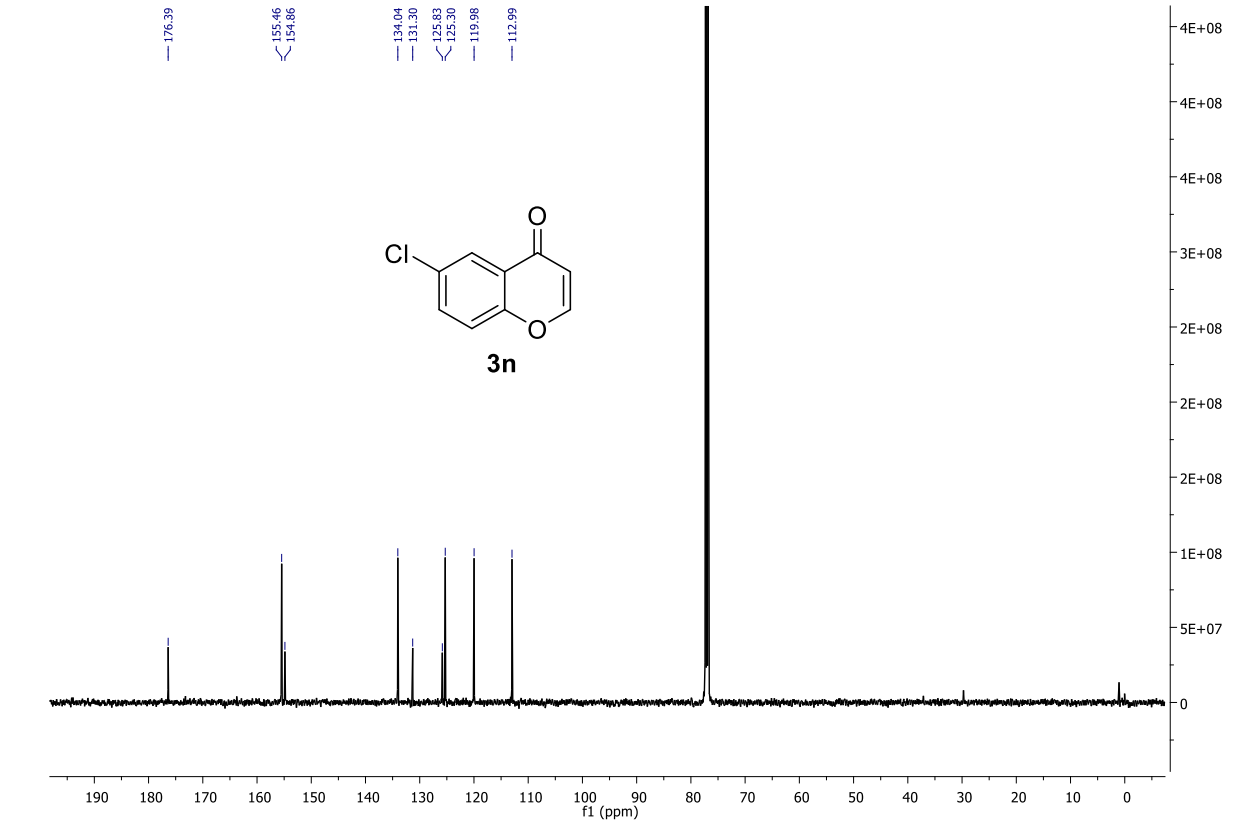
Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-15 H: 0-12 N: 0-1 O: 0-3

G5720-061-KT-RM
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry
27-Jul-2021
19:15:37
Acq Method Formic Acid_4.0 Min
ANL-MCLS-LCMS-007
512107F3361A 41 (1.724)
1: Scan ES+
3.33e+007

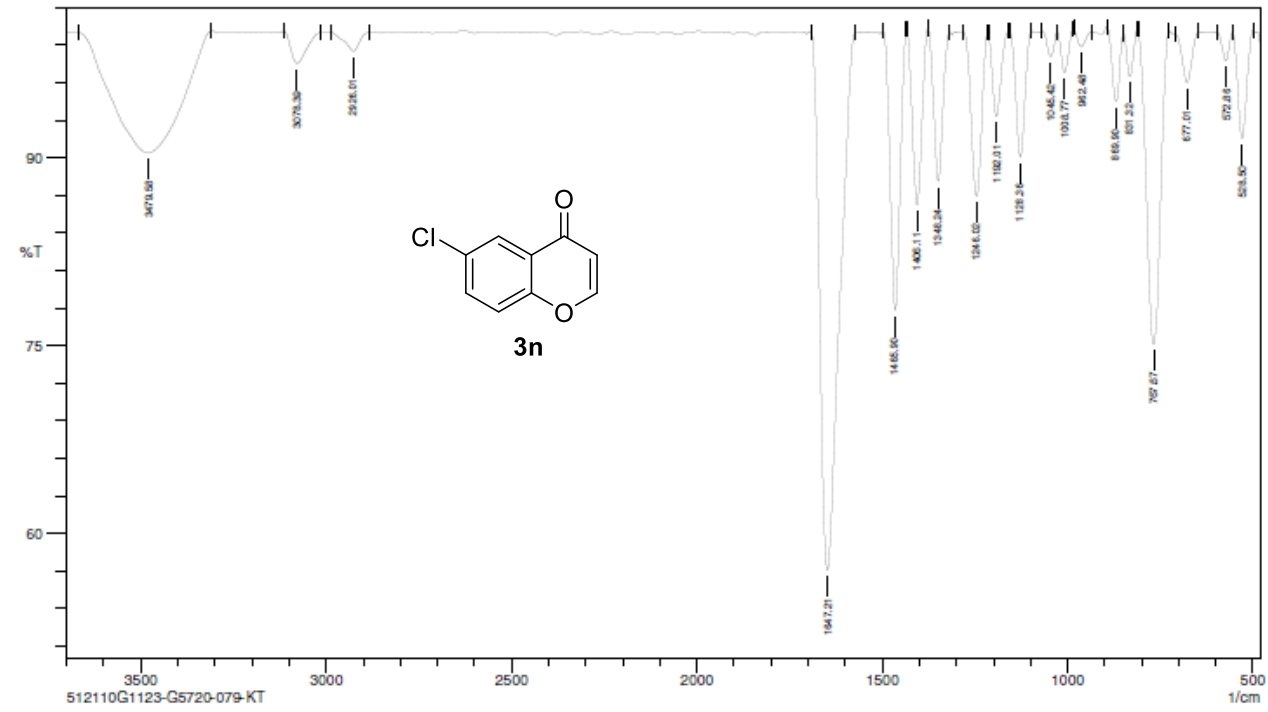


Minimum:				-1.5				
Maximum:		5.0	1000.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
254.0815	254.0817	-0.2	-0.8	10.5	33.8	n/a	n/a	C15 H12 N O3


8.183
8.177
7.862
7.847
7.632
7.627
7.610
7.605
7.439
7.417
7.262
6.362
6.347
1.574
1.256
0.881
0.845
0.070
-0.000
Cl
O
O
3n
Current Data Parameters
NAME 512108E0605-G5720-079-KT1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210820
Time 0.43 h
INSTRUM Avance
PROBHD Z163739_0132 (
PULPROG zg30
TD 65536
SOLVENT CDC13
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
TD0 1
SFO1 400.3024719 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 23.39900017 W
F2 - Processing parameters
SI 65536
SF 400.3000094 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
ANL-MCL5-NMR-003
12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.00
1.03
1.05
1.01
1.00
1.19
0.52
0.72


176.39
155.46
154.86
134.04
131.30
125.83
125.30
119.98
112.99
Cl
O
O
3n
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

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

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

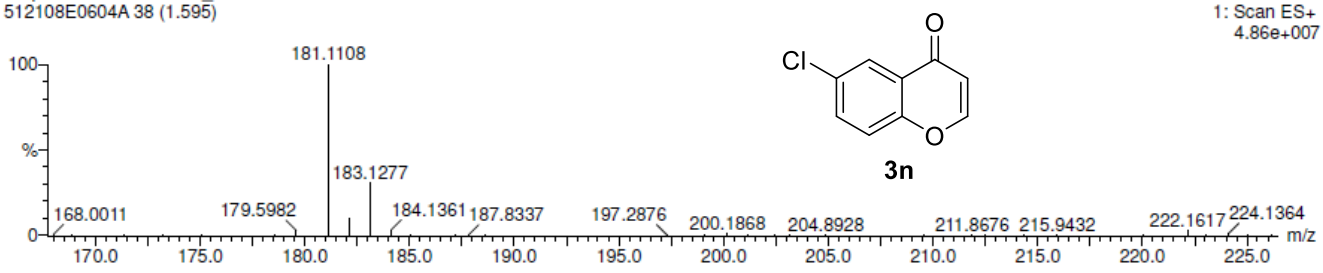
Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-9 H: 0-6 O: 0-2 Cl: 0-1

G5720-079-KT1

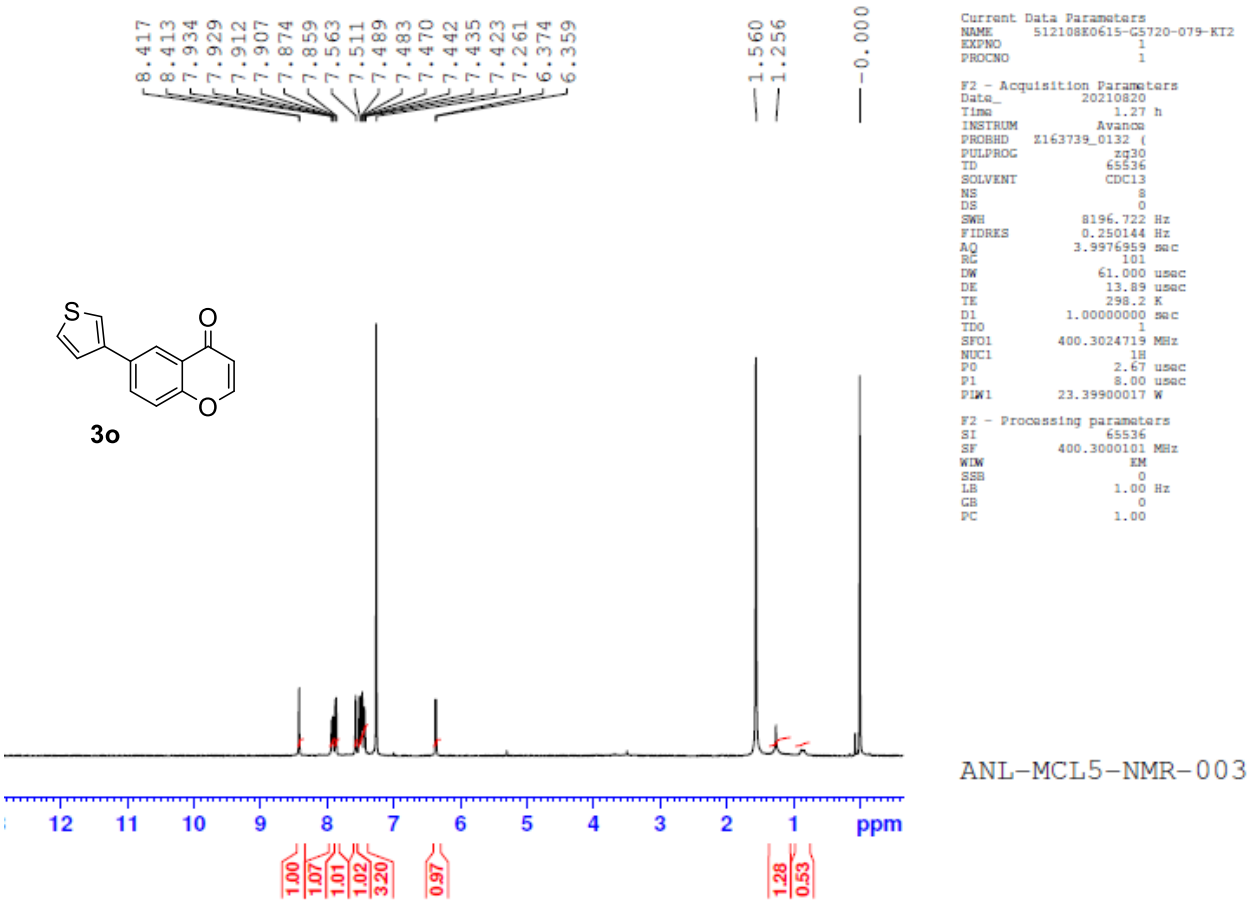
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry

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

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



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



Current Data Parameters
NAME 512108E0615-G5720-079-KT2
EXPNO 1
PROCNO 1

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Time 1.27 h
INSTRUM Avance
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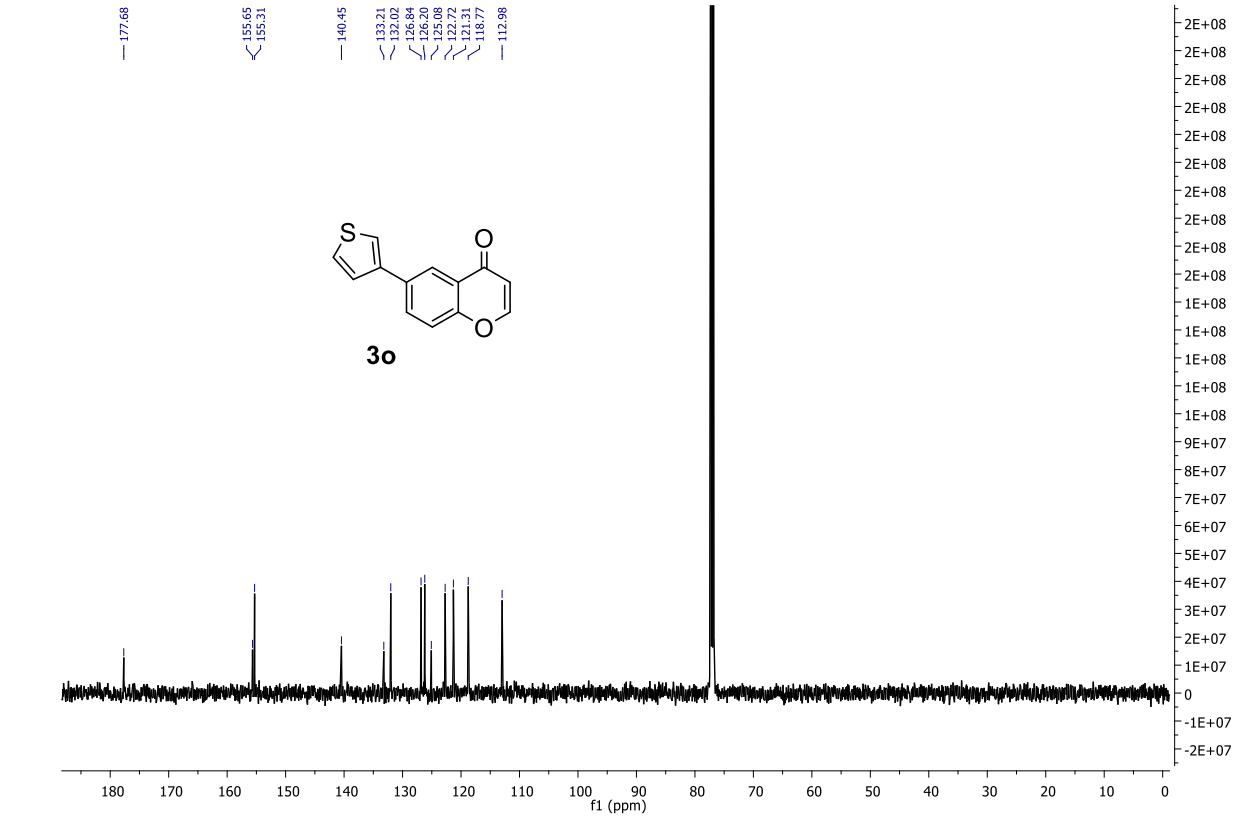
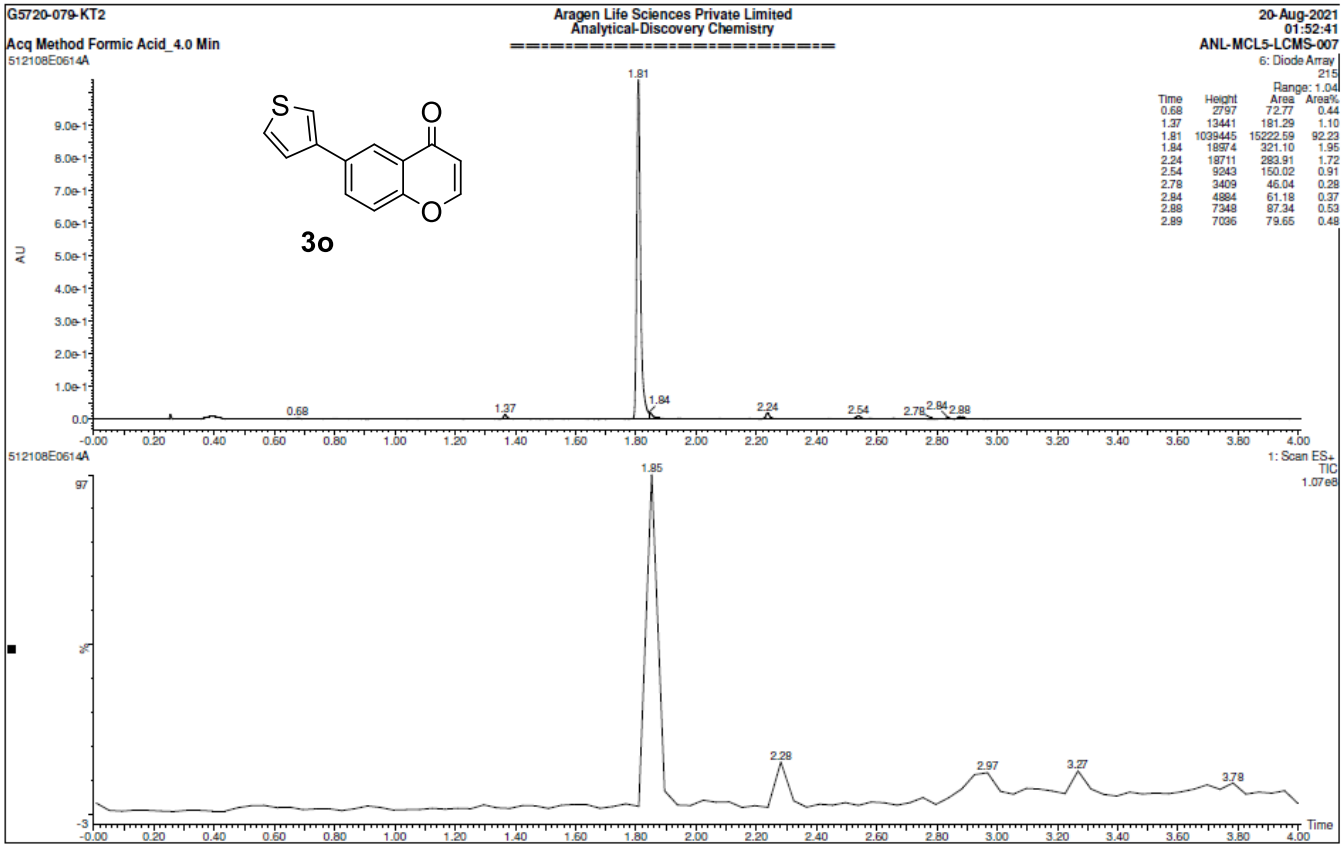
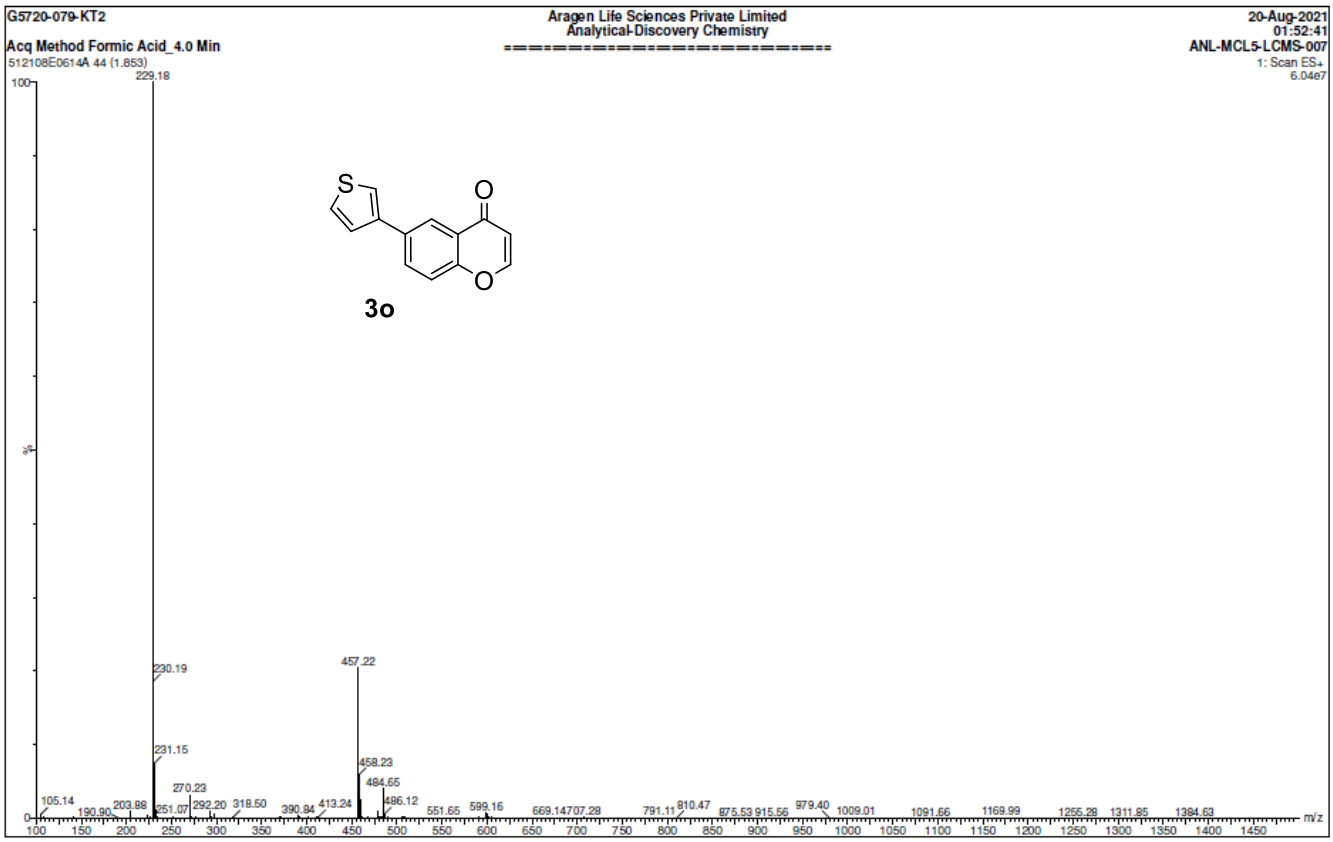
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.3024719 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 23.39900017 W

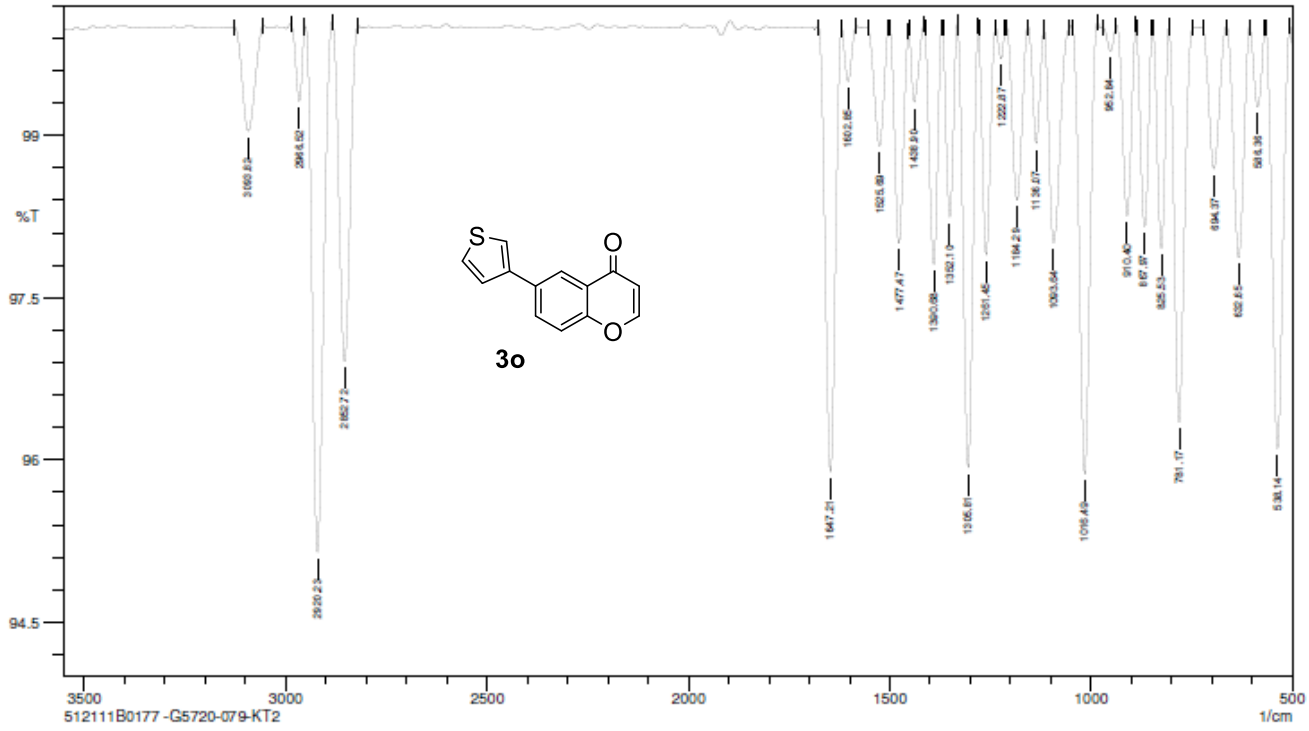
F2 - Processing parameters
SI 65536
SF 400.3000101 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00




G5720-079-KT2
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry
20-Aug-2021
01:52:41
Acq Method Formic Acid_4.0 Min
ANL-MCL5-LCMS-007
512108E0614A
6: Diode Array
215
Range: 1.04
Time Height Area Area%
0.68 2797 72.77 0.44
1.37 13441 181.29 1.10
1.81 1039445 15222.59 92.23
1.84 18974 321.10 1.95
2.24 18711 283.91 1.72
2.54 9243 150.02 0.91
2.78 3409 46.04 0.28
2.84 4884 61.18 0.37
2.88 7348 87.34 0.53
2.89 7036 79.65 0.48
AU
1.81
0.68
1.37
1.84
2.24
2.54
2.78
2.84
2.88
3o
512108E0614A
1: Scan ES+
TIC
1.07e8
1.85
2.28
2.97
3.27
3.78
%
Time


G5720-079-KT2
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry
20-Aug-2021
01:52:41
Acq Method Formic Acid_4.0 Min
ANL-MCL5-LCMS-007
512108E0614A 44 (1.853)
1: Scan ES+
6.04e7
229.18
230.19
231.15
457.22
458.23
484.65
486.12
3o
%
m/z

Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry



3o

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

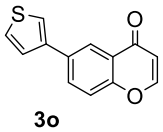
Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-13 H: 0-9 O: 0-2 S: 0-1

G5720-079-KT2

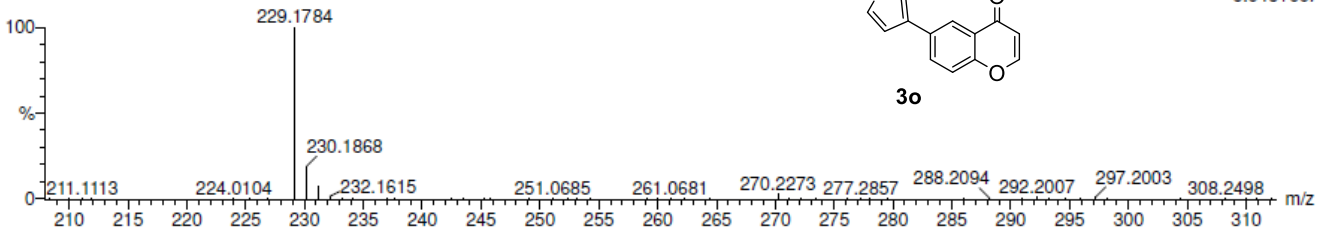
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry

20-Aug-2021
01:52:41
ANL-MCL5-LCMS-007
1: Scan ES+
6.04e+007

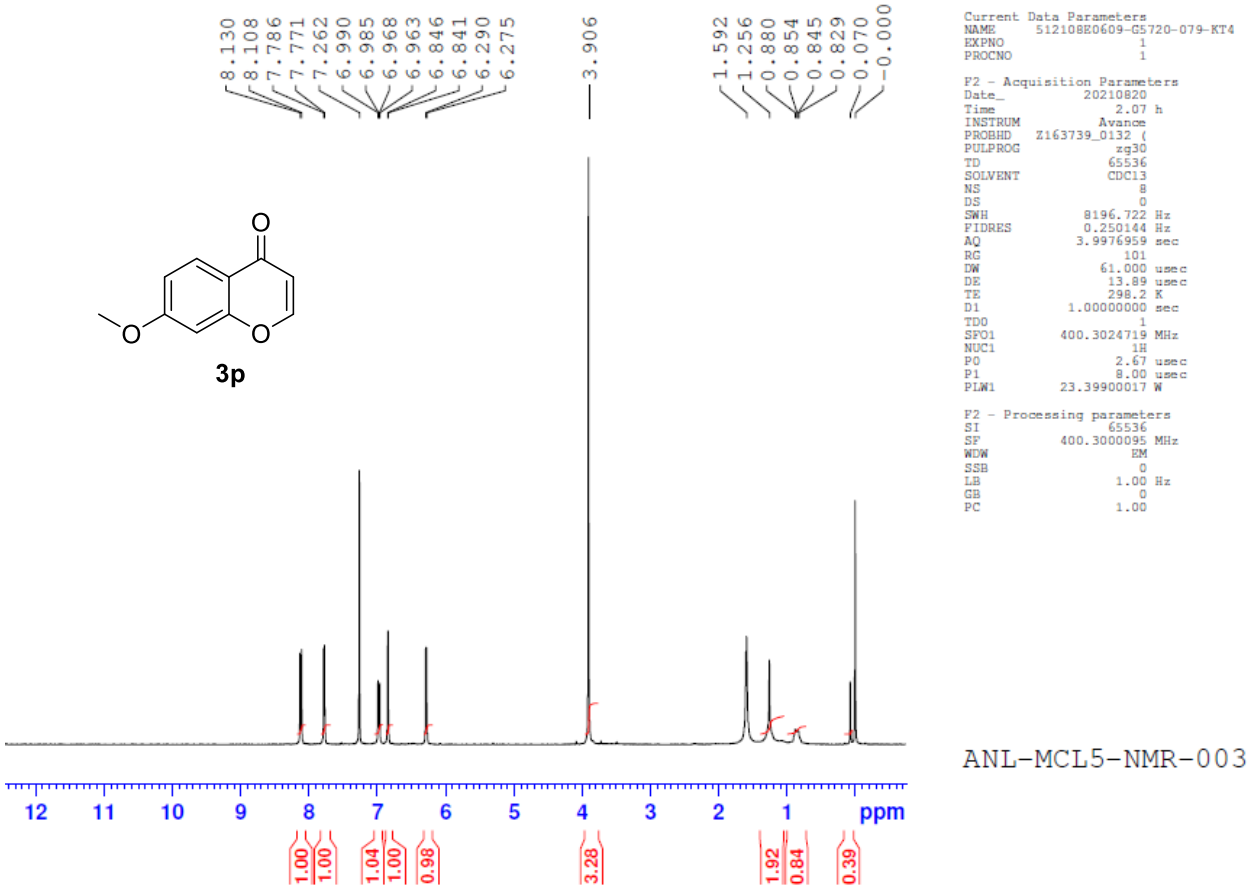
Acq Method Formic Acid_4.0 Min
512108E0614A 44 (1.853)



3o



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


8.130
8.108
7.786
7.771
7.262
6.990
6.985
6.968
6.963
6.846
6.841
6.290
6.275
3.906
1.592
1.256
0.880
0.854
0.845
0.829
0.070
-0.000
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NAME 512108E0609-G5720-079-KT4
EXPNO 1
PROCNO 1
P2 - Acquisition Parameters
Date_ 20210820
Time 2.07 h
INSTRUM Avance
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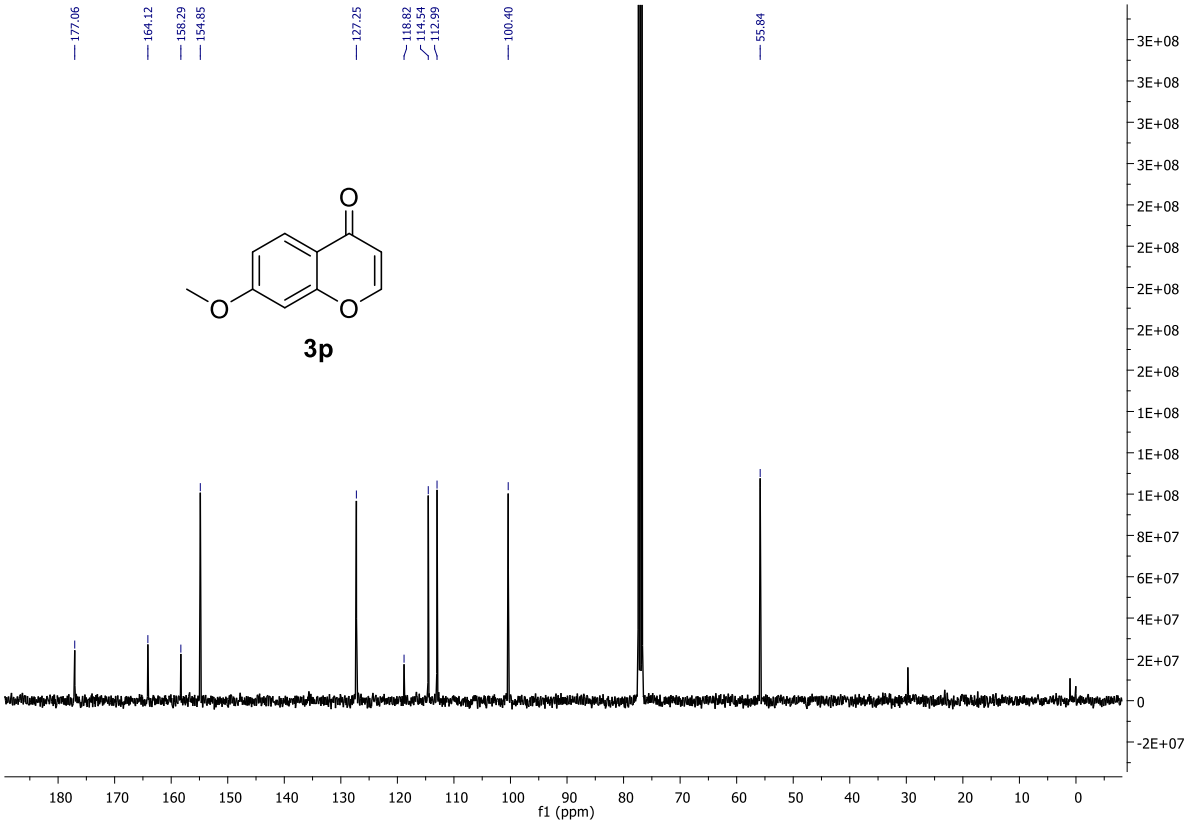
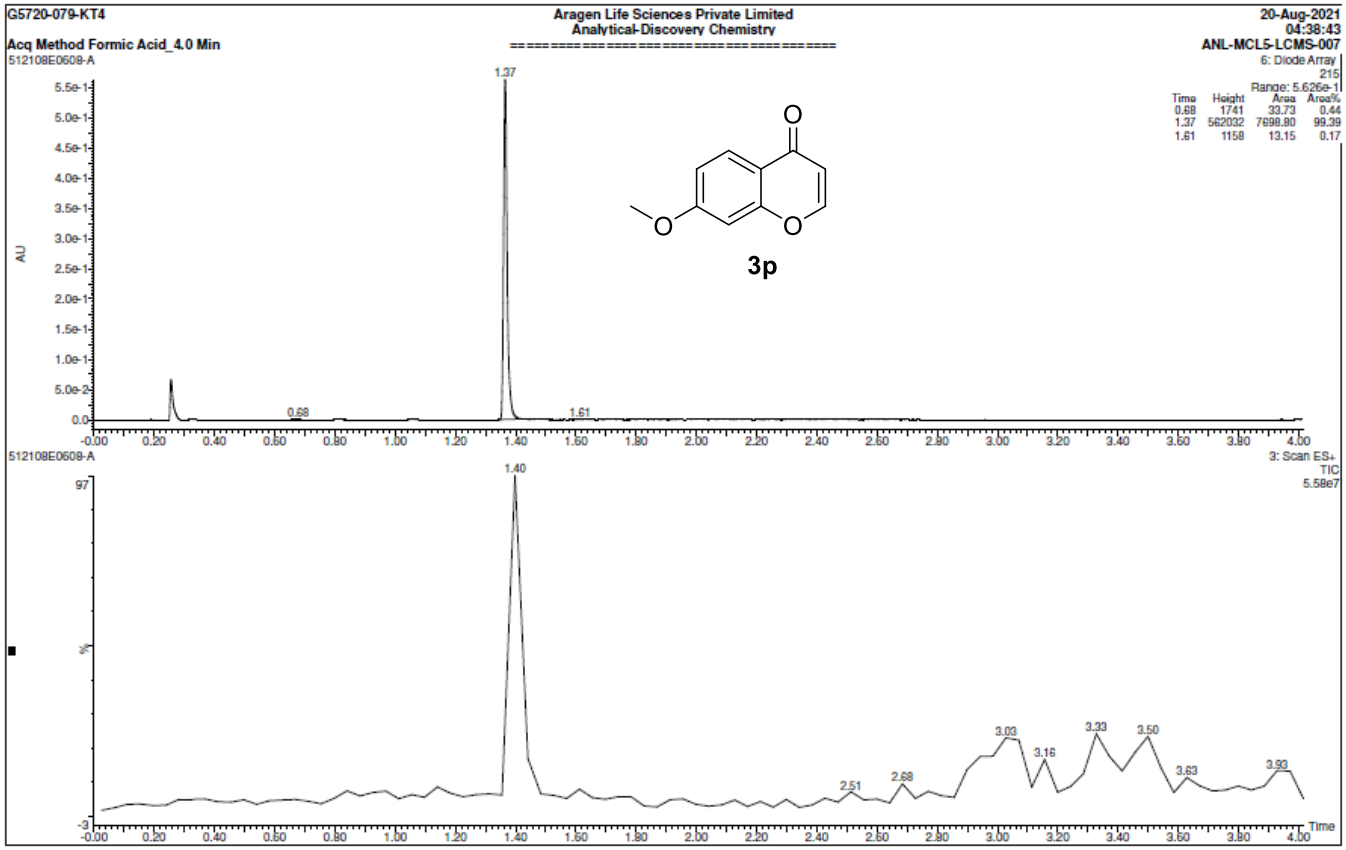
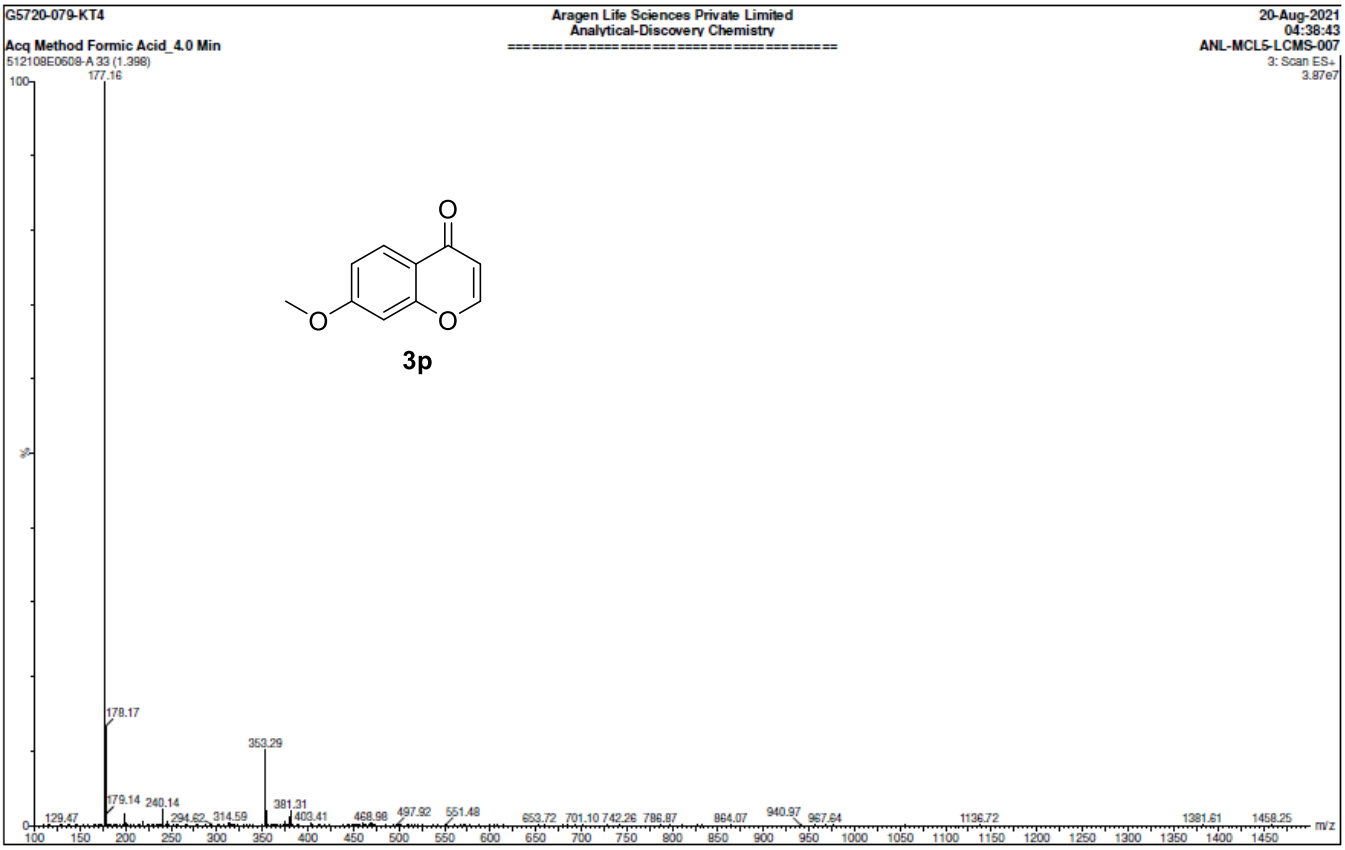
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 13.89 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.3024719 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 23.39900017 W
P2 - Processing parameters
SI 65536
SF 400.3000095 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
3p
ANL-MCL5-NMR-003
12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.00 1.00 1.04 1.00 0.98 3.28 1.92 0.84 0.39


177.06
164.12
158.29
154.85
127.25
118.82
114.54
112.99
100.40
55.84
3p
f1 (ppm)


G5720-079-KT4
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry
20-Aug-2021
04:38:43
Acq Method Formic Acid_4.0 Min
ANL-MCL5-LCMS-007
512108E0608-A
6: Diode Array
215
Range: 5.626e-1
Time Height Area Area%
0.68 1741 33.73 0.44
1.37 562032 7698.80 99.39
1.61 1158 13.15 0.17
1.37
0.68
1.61
AU
3p
512108E0608-A
3: Scan ES+
TIC
5.58e7
1.40
2.51
2.68
3.03
3.16
3.33
3.50
3.63
3.93
Time


G5720-079-KT4
Aragen Life Sciences Private Limited
Analytical-Discovery Chemistry
20-Aug-2021
04:38:43
Acq Method Formic Acid_4.0 Min
ANL-MCL5-LCMS-007
512108E0608-A 33 (1.398)
3: Scan ES+
3.87e7
177.16
178.17
353.29
179.14
240.14
381.31
3p
m/z

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

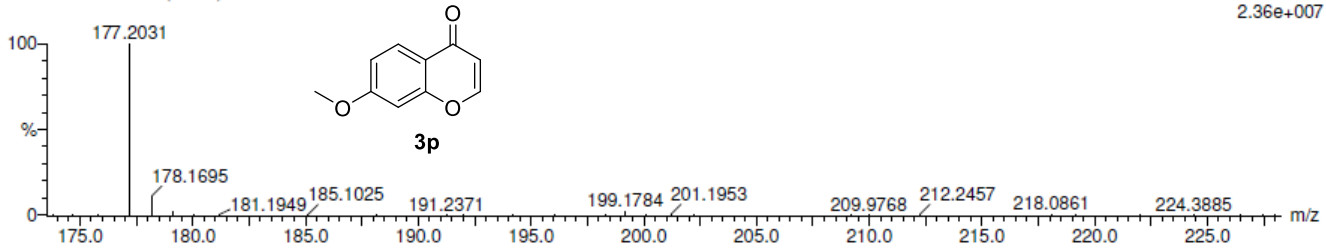
Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-10 H: 0-9 O: 0-3

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)



3p

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