

Chemical Formula: C₂₁H₁₈FN₅O₃S
Molecular Weight: 471.46

10.351

8.707
8.691
8.679
8.664
8.638
7.923
7.916
7.892
7.395
7.389
7.378
7.349
7.337
7.325
7.295
7.290
7.274
7.268
6.988
6.978
6.835

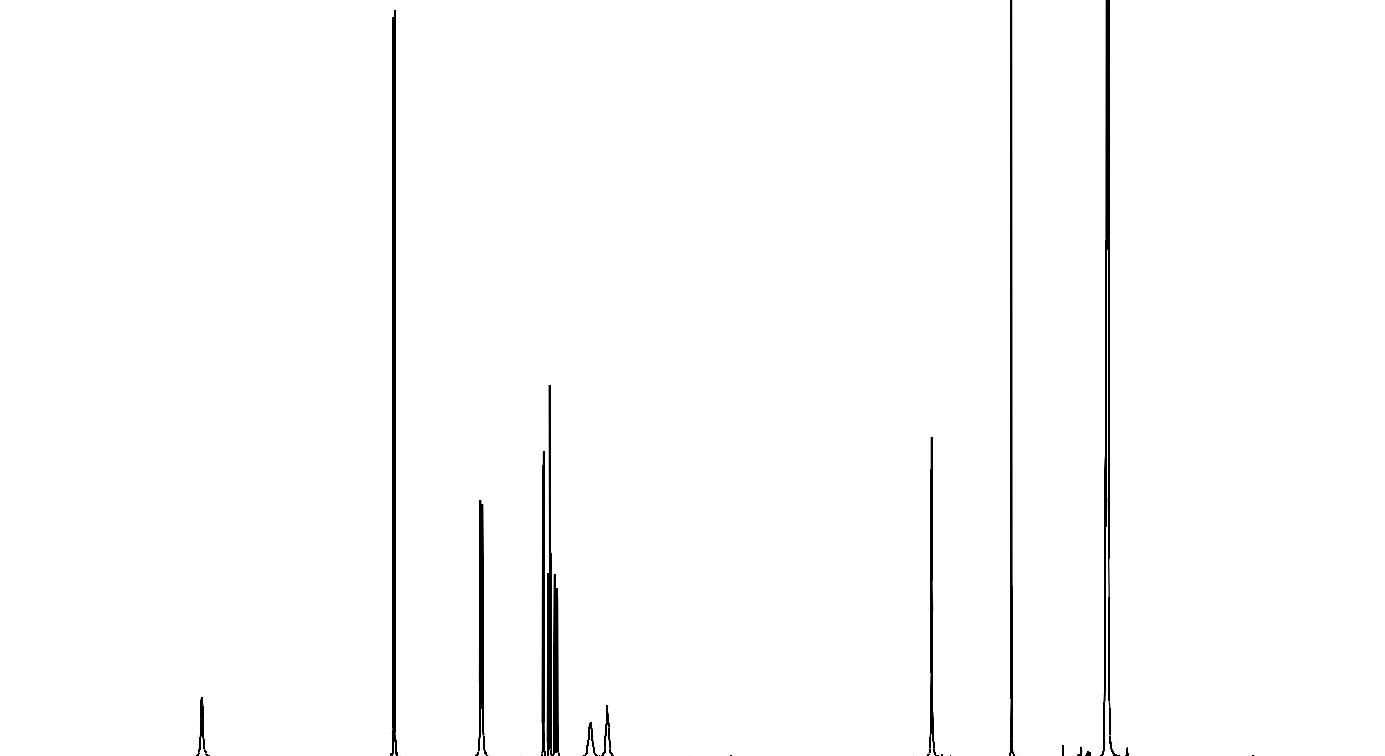
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3.332
2.888
2.728
2.727
2.673
2.669
2.664
2.650
2.516
2.509
2.504
2.500
2.495
2.491
2.466
2.450
2.441
2.327
2.322



Current Data Parameters
NAME NSC-758248-Q1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221027
Time 12.25 h
INSTRUM spect
PROBHD Z104450_0348 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 128
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 3.9845889 sec
RG 80.6
DW 60.800 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324710 MHz
NUC1 1H
P0 4.99 usec
P1 14.96 usec
PLW1 9.92000008 W

F2 - Processing parameters
SI 32768
SF 400.1300032 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



11 10 9 8 7 6 5 4 3 2 1 ppm

8.707
8.691
8.679
8.664

7.938
7.923
7.916
7.892

7.395
7.389
7.378
7.349
7.337
7.325
7.295
7.290
7.274
7.268

6.988
6.978

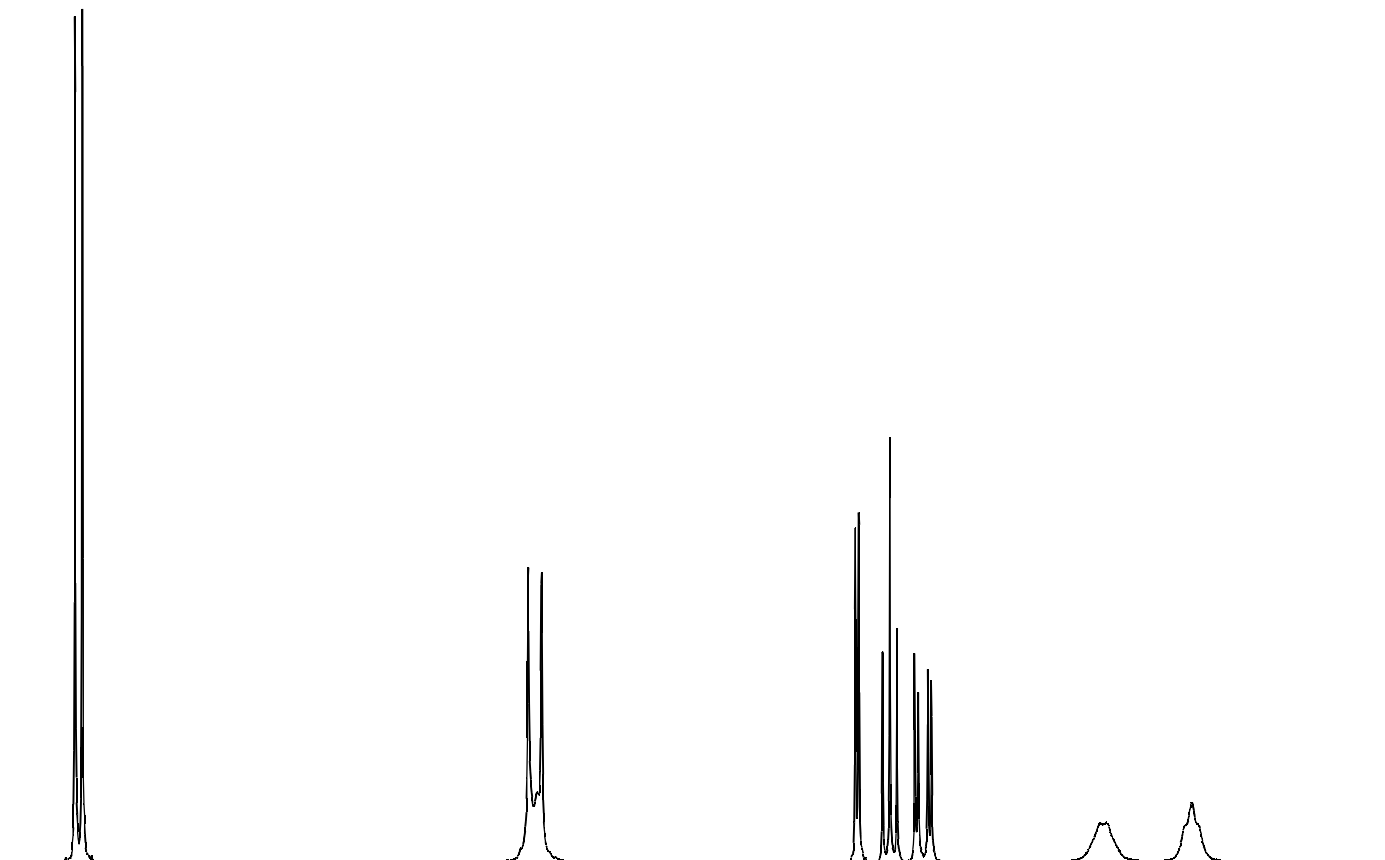
6.835



Current Data Parameters
NAME NSC-758248-Q1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221027
Time 12.25 h
INSTRUM spect
PROBHD Z104450_0348 (
PULPROG zg30
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F2 - Processing parameters
SI 32768
SF 400.1300032 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 ppm

2.0185

2.0398

3.0237

1.0023

1.0352

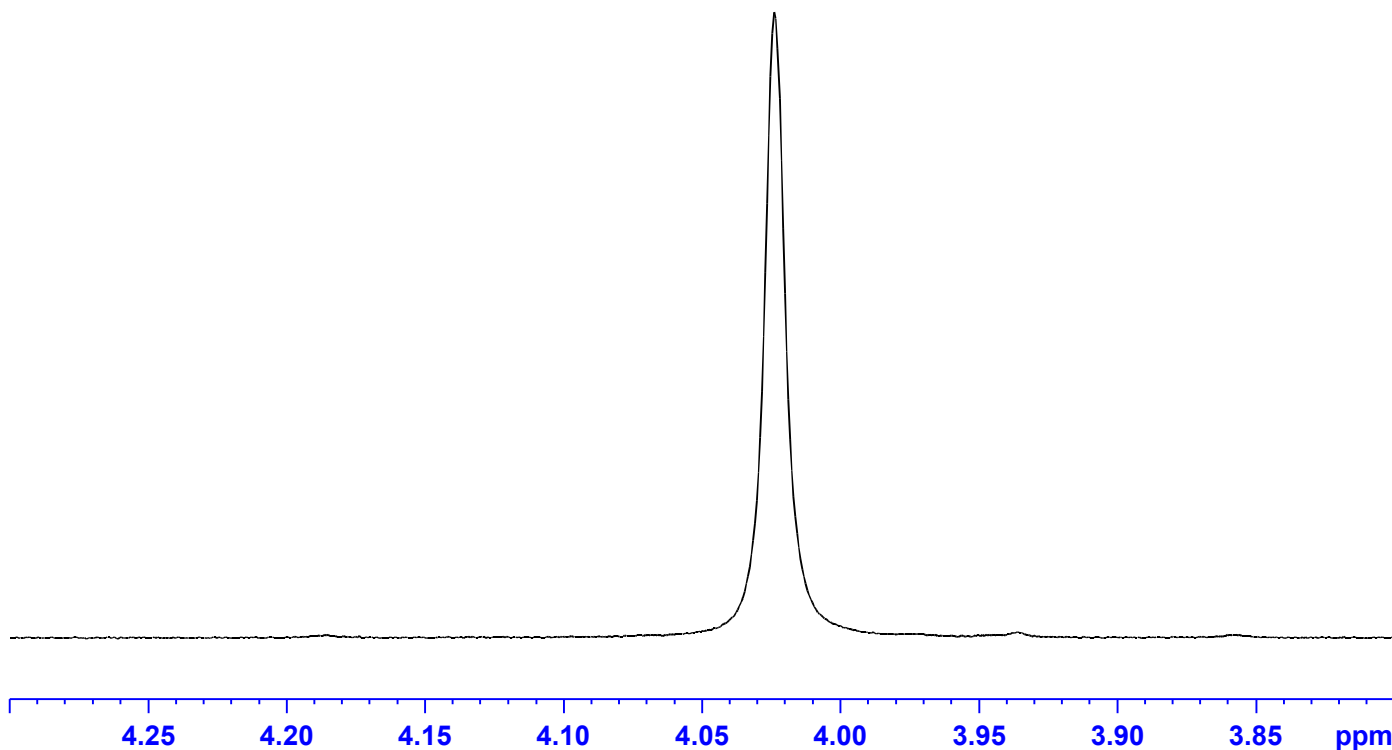
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Current Data Parameters
NAME NSC-758248-Q1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221027
Time 12.25 h
INSTRUM spect
PROBHD Z104450_0348 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 128
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 3.9845889 sec
RG 80.6
DW 60.800 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324710 MHz
NUC1 1H
P0 4.99 usec
P1 14.96 usec
PLW1 9.92000008 W

F2 - Processing parameters
SI 32768
SF 400.1300032 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



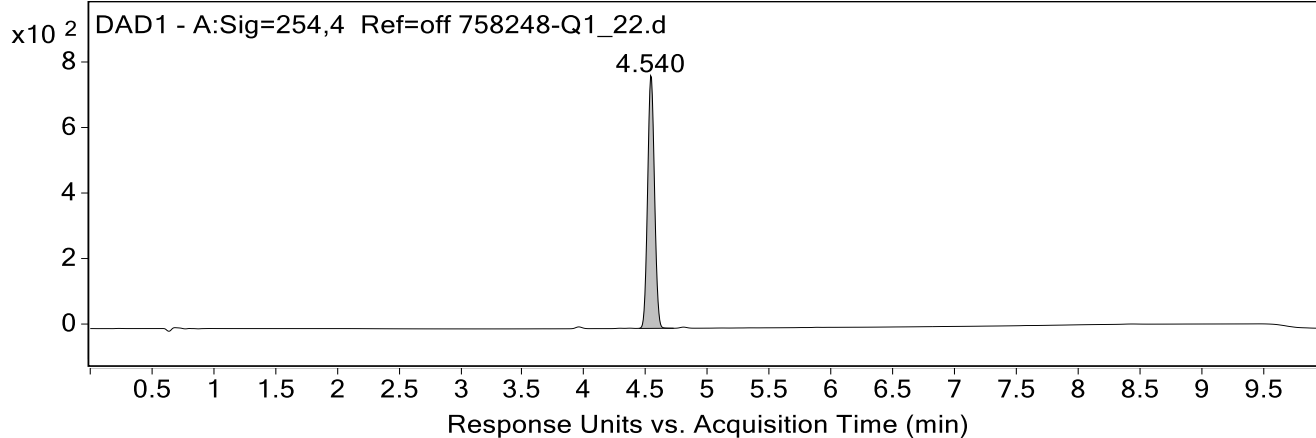
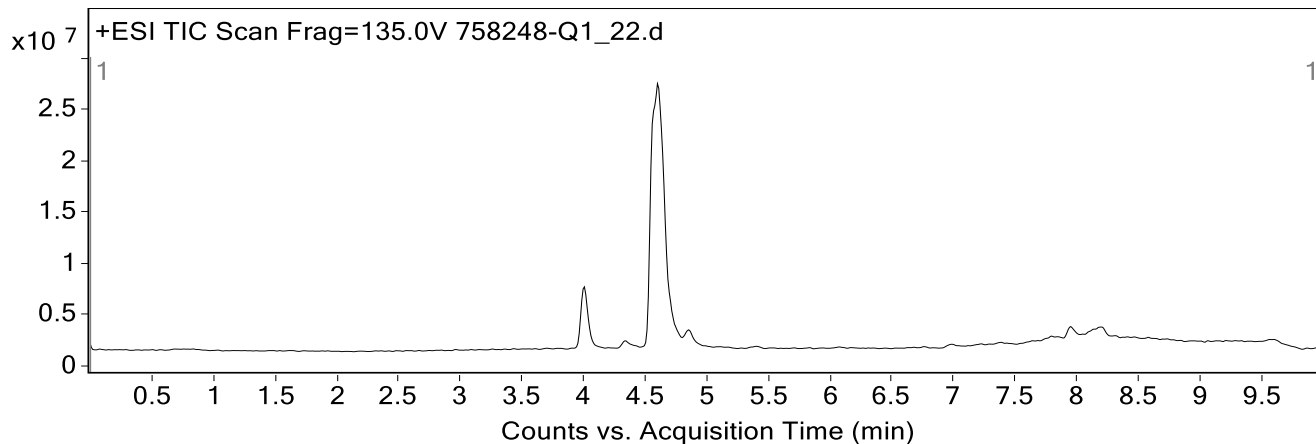
Qualitative Analysis Report

Data Filename 758248-Q1_22.d **Sample Name** 758248-Q1
Sample Type Sample **Position** P1-C1
Instrument Name Instrument 1 **User Name**
Acq Method 5-95_10min_pos.m **Acquired Time** 10/24/2022 6:08:11 PM (UTC-07:00)
IRM Calibration Status Not Applicable **DA Method** Default.m
Comment

Sample Group
Stream Name LC 1 **Info.**
Acquisition Time (Local) 10/24/2022 6:08:11 PM (UTC-07:00)
Acquisition SW Version 6400 Series Triple
Quadrupole
B.08.02 (B8260.0)

Chromatograms

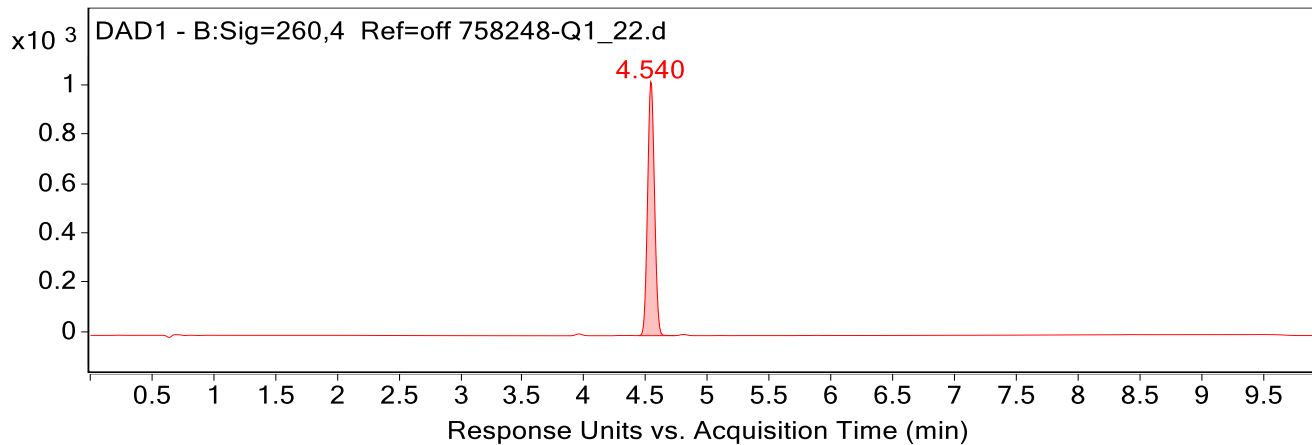
Fragmentor Voltage 135 **Collision Energy** 0 **Ionization Mode** ESI



Integration Peak List

Peak	Start	RT	End	Height	Area	Area Sum %
1	4.447	4.540	4.727	769.4	2994.2	100.0

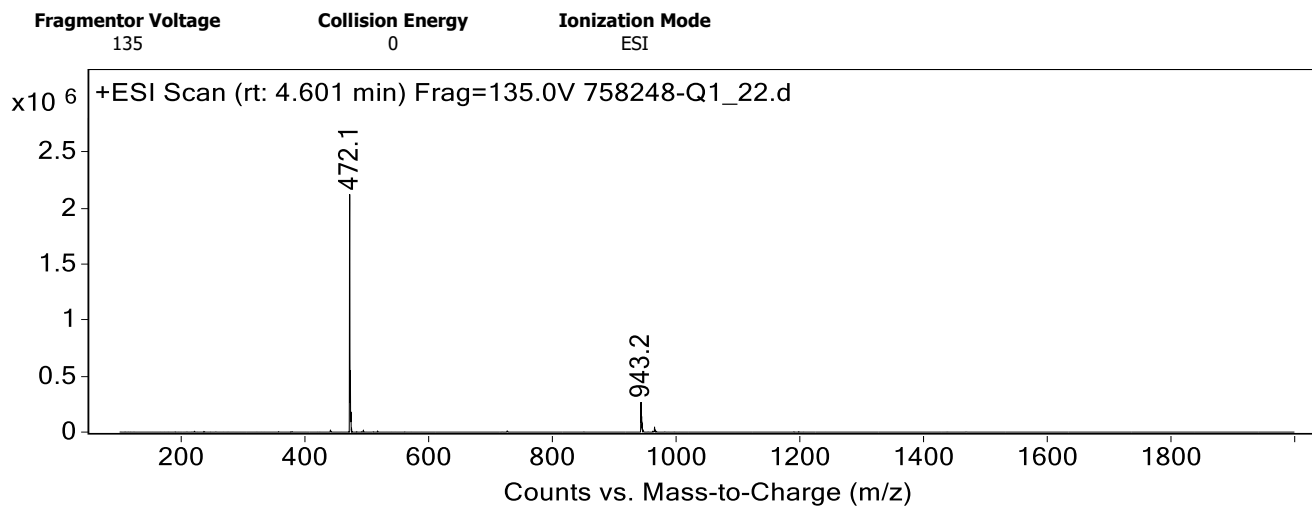
Qualitative Analysis Report



Integration Peak List

Peak	Start	RT	End	Height	Area	Area Sum %
1	4.447	4.540	4.733	1027.9	4006.8	100.0

Spectra

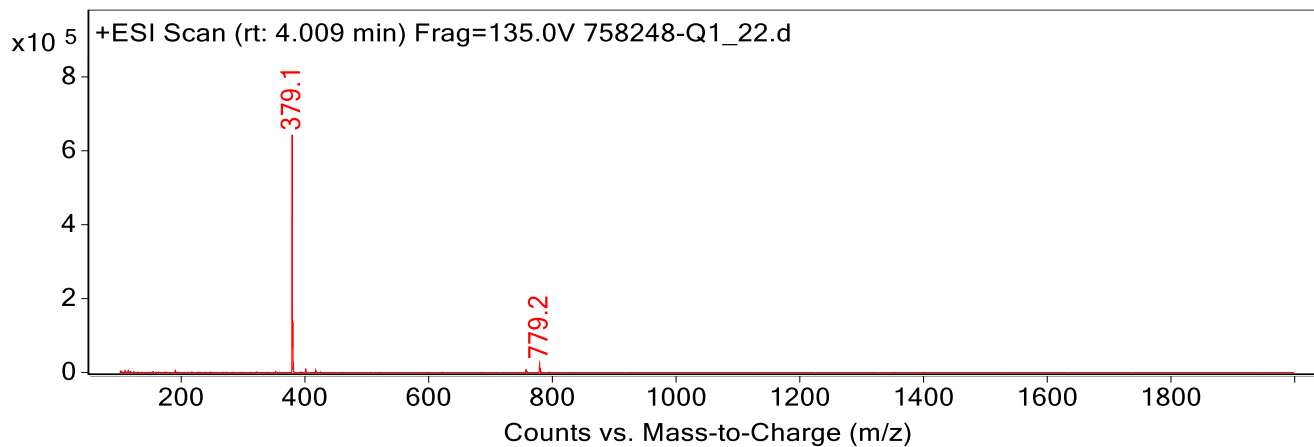


Peak List

m/z	z	Abund
472.1	1	2124263
473.1	1	552318
474.1	1	181031
475.1	1	30200
943.2	1	268233
944.2	1	139611
945.3	1	64060
946.3	1	21381
965.2		40487

Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI

Qualitative Analysis Report



Peak List

<i>m/z</i>	<i>z</i>	Abund
379.1	1	644812
380.1	1	137897
381.1	1	20093
401.1		9665
757.2		7429
779.2	1	24984
780.3	1	9909

--- End Of Report ---