LCMS Analysis Report

Acquired by	: System Administrator
Sample Name	: LCMS93-PH-ABI-D010-015-0-1(0724-WXH01)1T
Injection Volume	: 1
Data File	: LCMS93-PH-ABI-D010-015-0-1(0724-WXH01)1T.lcd
Method File	: ACN-Water-0.05%TFA-5%B-1.5-2.0MIN(90-900).lcm
Report Format File	: LCMS2020-PDA+ELSD+MS.lsr
Date Acquired	: 2018/7/24 8:45:24
Comment	: Mobile phase A:Water/0.05%TFA Mobile phase B:Acetonitrile/0.05%TFA

Instrument Name:Shimadzu LCMS-2020

<<Pump>>

Mode	: Binary gradient
Pump A	: LC-20ADXR
Pump B	: LC-20ADXR
Total Flow	: 1.5000 mL/min
B Conc.	: 5.0 %

<<Oven>>

Oven Temperature	: 40 C

<<PDA>>

PDA Model	: SPD-M20A
Lamp	: D2
Start Wavelength	: 190 nm
End Wavelength	: 400 nm

<<Interface>>

Interface	:ESI
DL Temperature	:250 C
Nebulizing Gas Frow	:1.50 L/min
Heat Block	:300 C
Drying Gas	:On
	15.00 L/min

<<MS Parameter>>

Initial Valve Position	:-
--Segment 1 Event 1--	
Start Time	:0.00 min
End Time	:2.00 min
Acquisition Mode	:Scan
Polarity	:Positive
Event Time	:0.50 sec
Detector Voltage	:+0.80 kV
Threshold	:20
Start m/z	:90.00
End m/z	:900.00
Scan Speed	:1667 u/sec
Interface Volt.	:Use the Data in the Tuning File
DL Volt.	:Use the Data in the Tuning File
Qarray DC Voltage	:Use the Data in the Tuning File
Qarray DC Voltage	:Use the Data in the Tuning File

System Configuration

<<Column>>

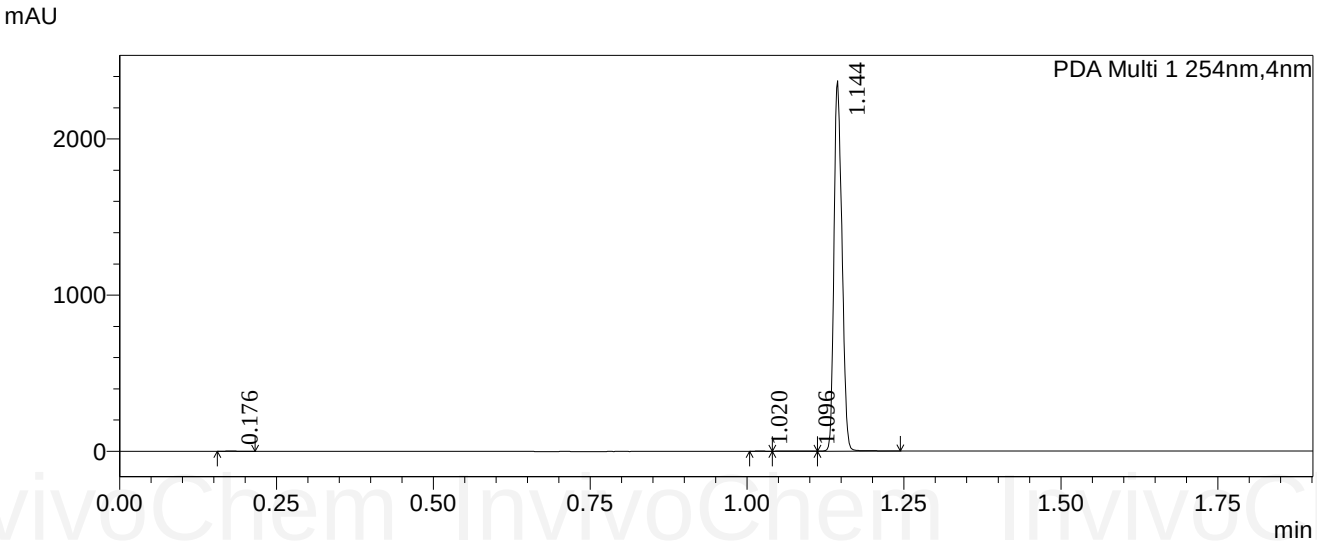
Column Name	: Ascentis Express C18
Length	: 50 mm
Internal Diameter	: 3.0 mm
Description	: 2.7um

<<LC Time Program>>

Time	Module	Command	Value
0.01	Pumps	Pump B Conc.	5
1.10	Pumps	Pump B Conc.	95
1.80	Pumps	Pump B Conc.	95
1.90	Pumps	Pump B Conc.	5
2.00	Controller	Stop	

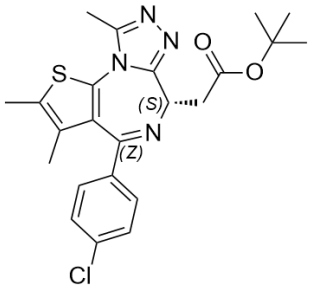
LCMS Analysis for (+)-JQ1

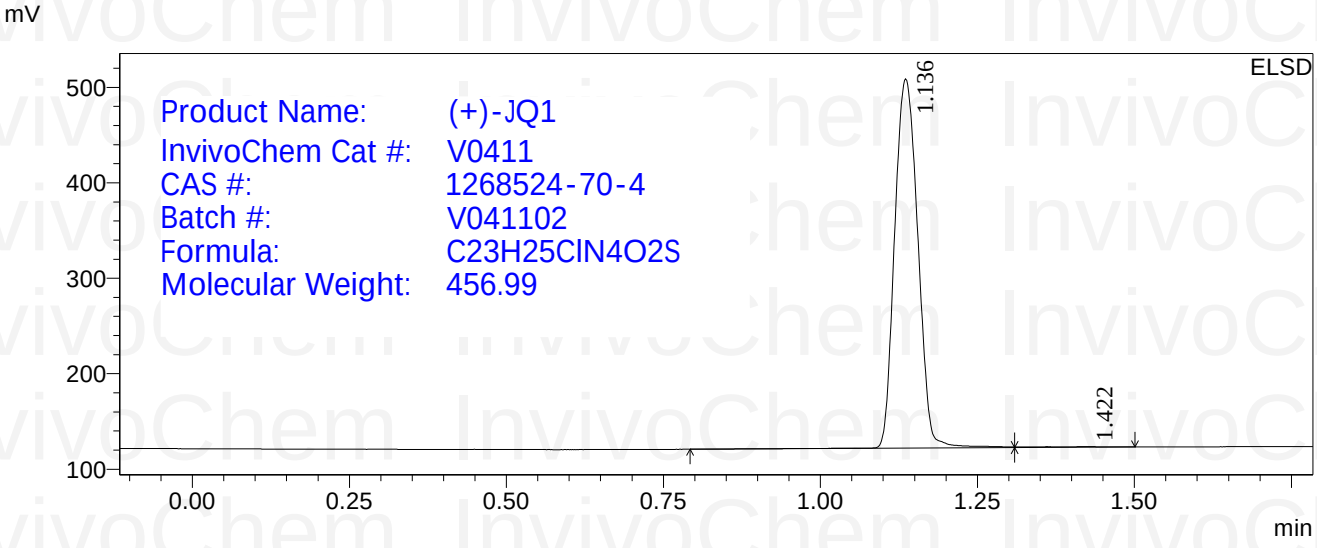
<Chromatogram>



Peak Table
PDA Ch1 254nm

Peak#	Ret. Time	Height	Height%	Area	Area%
1	0.176	2089	0.091	3277	0.154
2	1.020	1492	0.065	1656	0.078
3	1.096	1844	0.081	5480	0.258
4	1.144	2278851	99.763	2114366	99.510
Total		2284275	100.000	2124780	100.000





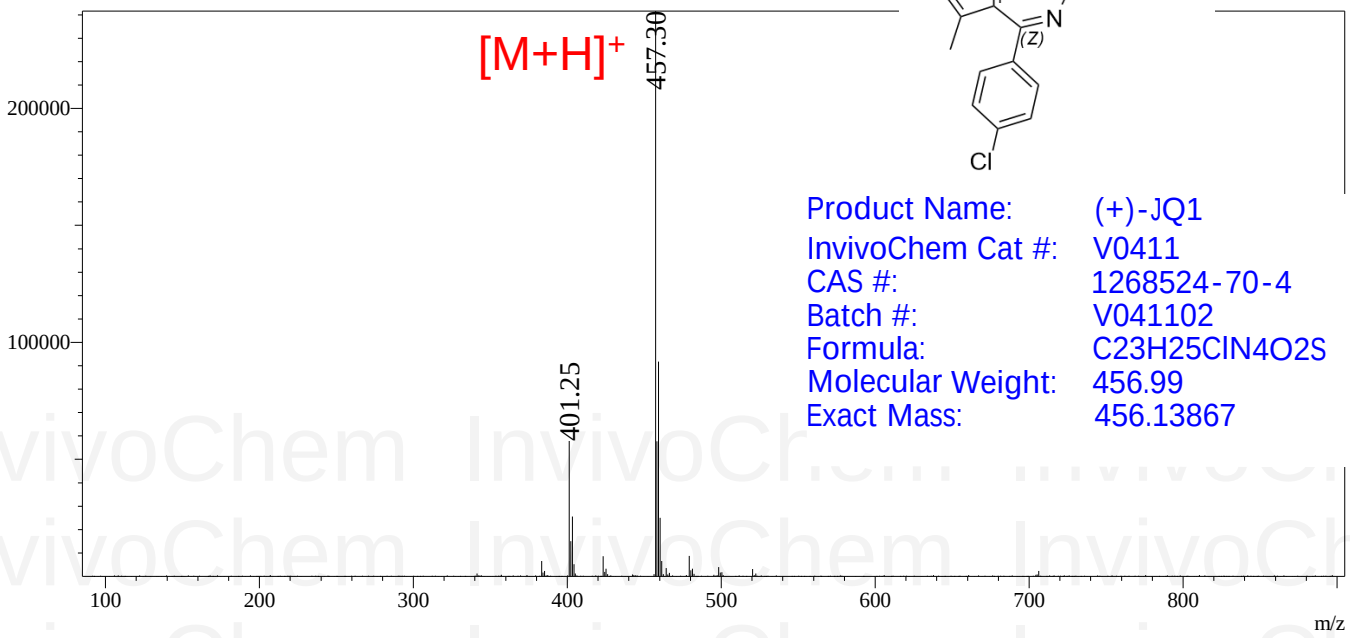
Peak Table
ELSD

Peak#	Ret. Time	Height	Height%	Area	Area%
1	1.136	377430	99.844	996857	99.520
2	1.422	591	0.156	4812	0.480
Total		378021	100.000	1001669	100.000

LCMS Analysis for (+)-JQ1

MS Spectrum

Retention time: 1.140
Spectrum Mode:Averaged 1.132-1.148(141-143) Base Peak:457.30(241576)
BG Mode:Calc Segment 1 - Event 1



Product Name:	(+)-JQ1
InvivoChem Cat #:	V0411
CAS #:	1268524-70-4
Batch #:	V041102
Formula:	C23H25ClN4O2S
Molecular Weight:	456.99
Exact Mass:	456.13867