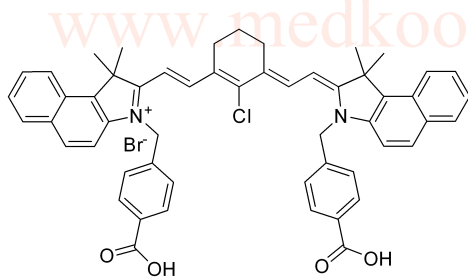


13.001  
12.999  
12.995

8.360 8.336 8.328 8.083 8.073 8.061 8.053 7.981 7.965 7.944 7.724 7.710 7.701 7.693 7.674 7.565 7.546 7.528 7.441 7.420 6.420 6.384 5.772 4.058 4.041 4.023 4.005 3.340 2.574 2.511 2.507 2.503 2.127 2.113 2.089 2.034 2.018 1.992 1.967 1.943 1.918 1.884 1.781 1.769 1.757 1.736

# IR-825 HNMR Analysis, Solvent = d6-DMSO



MedKoo Cat#: 530336  
Name: IR-825  
CAS#: 1558079-49-4  
Lot#: A8T03K18  
Chemical Formula: C<sub>54</sub>H<sub>48</sub>BrClN<sub>2</sub>O<sub>4</sub>  
Molecular Weight: 904.34

1.97

3.92  
10.10  
4.38  
8.01

1.89  
4.00

4.05  
13.01  
2.23

10.0

5.0

0.0

ppm (t1)

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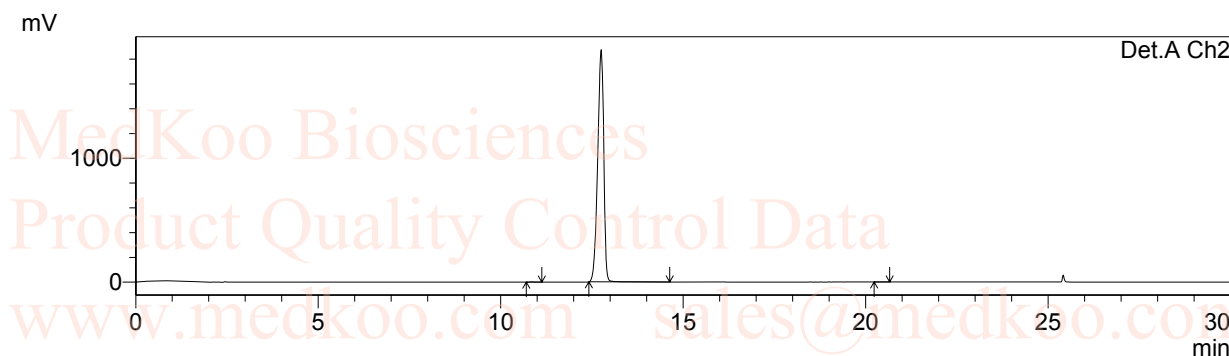
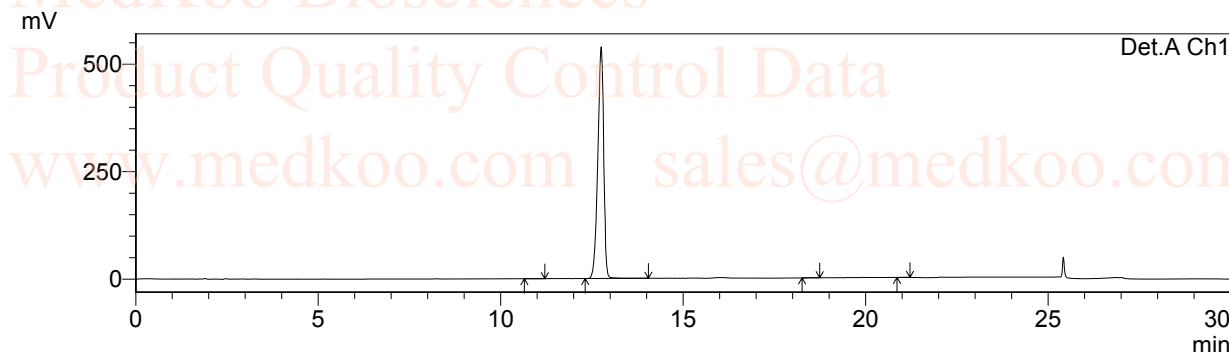
# IR-825 HPLC Analysis

Column : Inertil ODS-3, 5um 4.6\*150mm  
 Mobile phase : Solvent A: H2O(0.05%H3PO4) Solvent B:ACN(0.05%H3PO4)  
 Temperature : 40 °C  
 Flow rate : 1mL/min  
 Run time : 3min gradient(20%B), 12min gradient (20%-50%B), 5min gradient (50%-95%B),3 min(95%B),th  
 Detector : UV  
 Wavelength : 220/254 nm  
 User name : 1558079-49-4  
 Notebook page :  
 Sample description : 1558079-49-4  
 Injection Volume : 1558079-49-4

Data File Name : 1558079-49-4.lcd  
 Method File Name : 1558079-49-4.lcm

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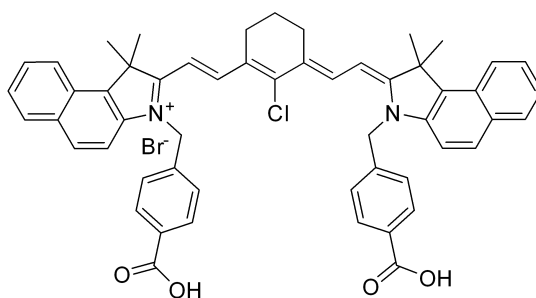


1Det.A Ch1/220nm  
2Det.A Ch2/254nm

PeakTable

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Area %	Theoretical Plate#
1	10.845	3640	0.060	40966.591
2	12.752	6051639	99.848	28516.052
3	18.490	1841	0.030	162547.793
4	21.059	3723	0.061	181999.789
Total		6060843	100.000	



PeakTable

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %	Theoretical Plate#
1	10.848	8629	0.040	51444.041
2	12.751	21682099	99.931	26920.836
3	20.473	6277	0.029	132958.216
Total		21697005	100.000	

MedKoo Cat#: 530336

Name: IR-825

CAS#: 1558079-49-4

Lot#: A8T03K18

Chemical Formula: C<sub>54</sub>H<sub>48</sub>BrClN<sub>2</sub>O<sub>4</sub>

Molecular Weight: 904.34

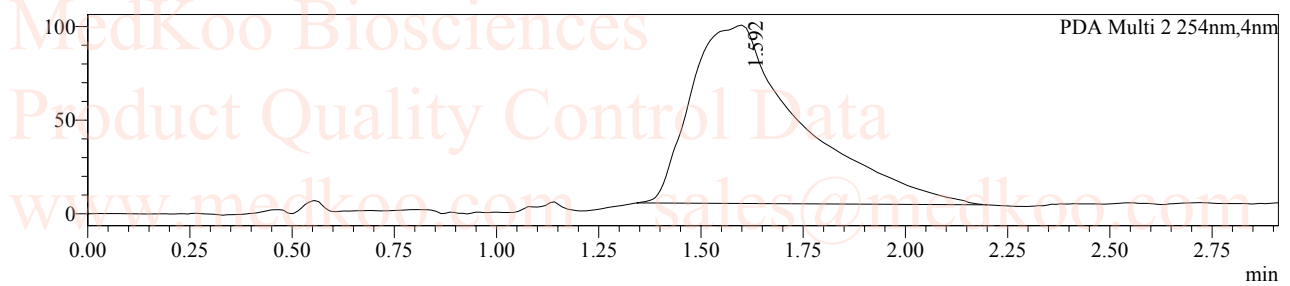
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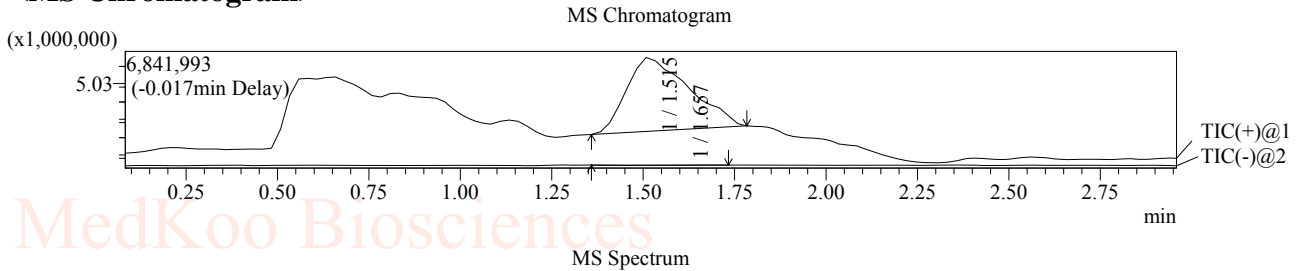
# IR-825 LC/MS Analysis

LC-MS condition  
Column : Chromolith SpeedROD ,RP-18e,50\*4.6mm LCMS-002  
Mobile Phase : A: H2O(0.05%FA)  
                  B: CH3CN  
Temperature : 35°C  
Flow rate : 2.5mL/min  
Run time : 0.1min@20%B,1.7min gradient(20-95% B), then0.7min@95% B,then0.4min@20% B  
Injection volume : 5 uL  
Detector : UV 220/254nm  
Mass range : 100-1000  
Scan : Postive/Negative  
User Name : 1558079-49-4  
Data Filename : 1558079-49-4.lcd

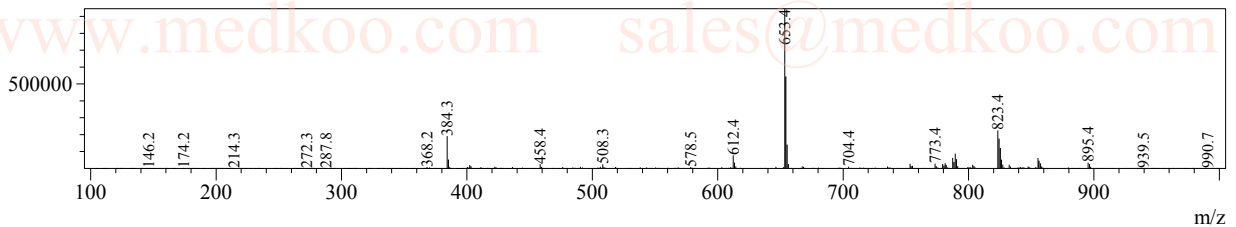
mAU



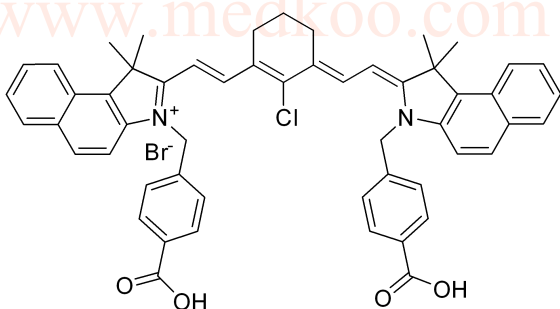
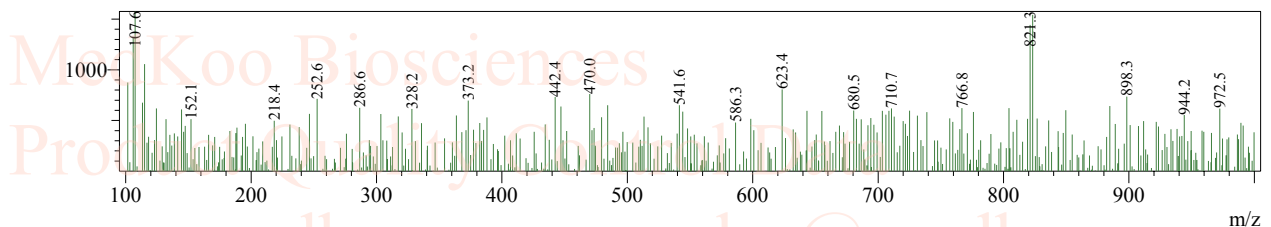
## <MS Chromatogram>



Peak#:1 R.Time:1.515(Scan#:115)  
MassPeaks:624  
Spectrum Mode:Averaged 1.483-1.533(113-117)  
BG Mode:Calc Segment 1 - Event 1



Peak#:1 R.Time:1.657(Scan#:126)  
MassPeaks:460  
Spectrum Mode:Averaged 1.617-1.667(124-128)  
BG Mode:Calc Segment 1 - Event 2



MedKoo Cat#: 530336

Name: IR-825

CAS#: 1558079-49-4

Lot#: A8T03K18

Chemical Formula: C54H48BrClN2O4

Molecular Weight: 904.342