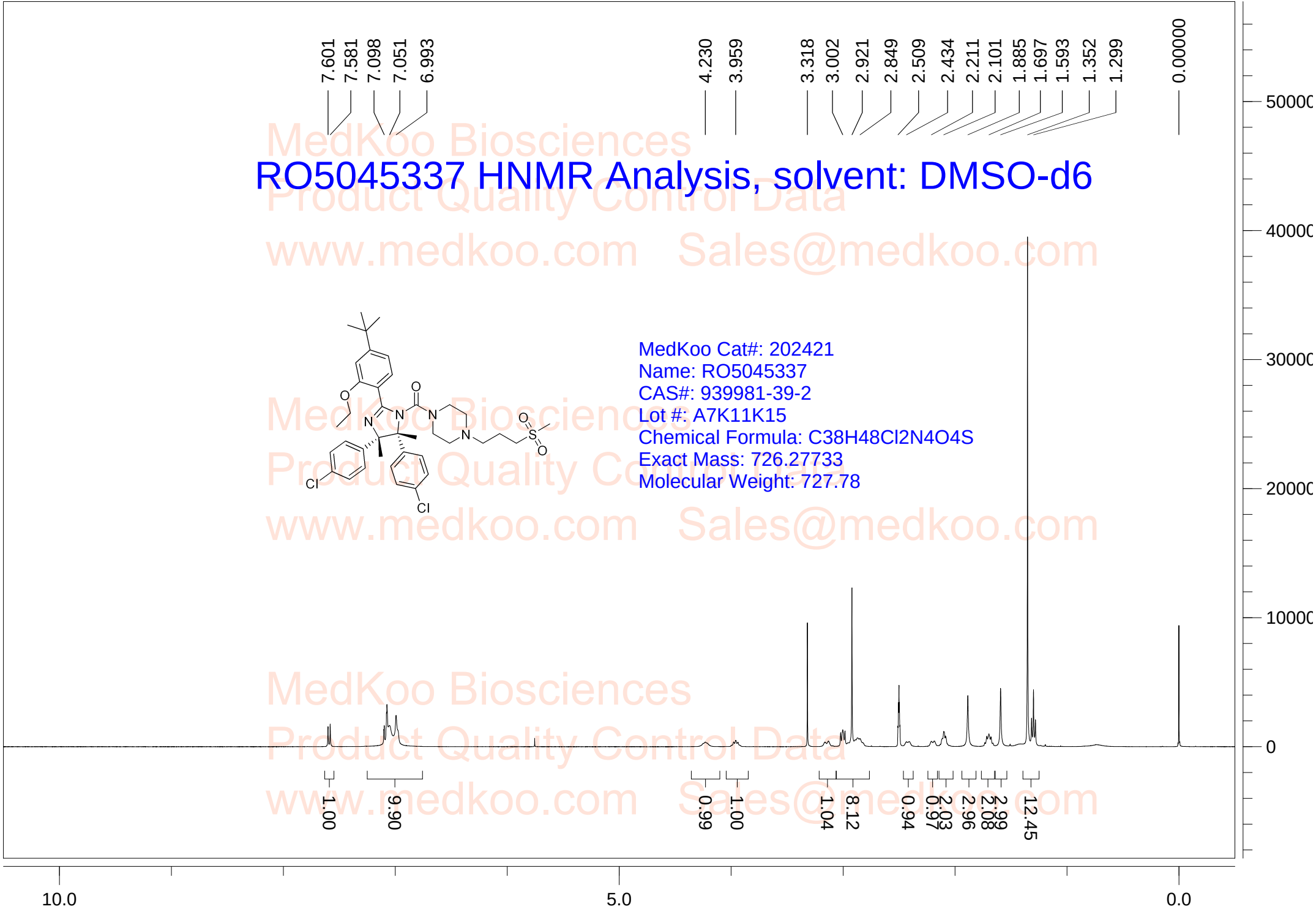
RO5045337 HNMR Analysis, solvent: DMSO-d6



MedKoo Cat#: 202421
Name: RO5045337
CAS#: 939981-39-2
Lot #: A7K11K15
Chemical Formula: C38H48Cl2N4O4S
Exact Mass: 726.27733
Molecular Weight: 727.78

MedKoo Biosciences
Product Quality Control Data
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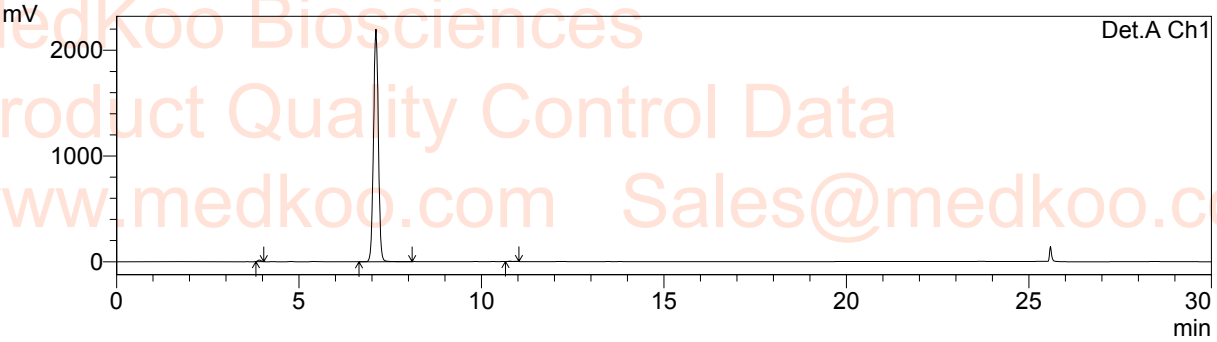
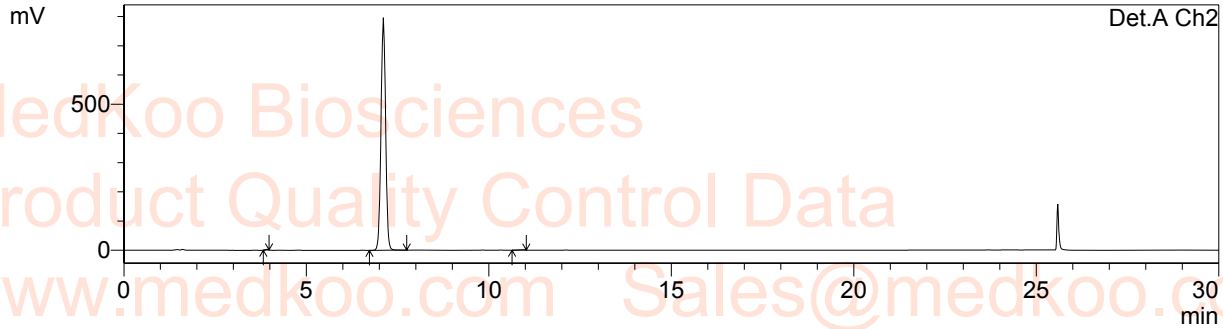
RO5045337 HPLC Analysis

Column : Inertil ODS-3，5um 4.6*150mm
Mobile phase : Solvent A: H2O(0.05%H3PO4) Solvent B:ACN(0.05%H3PO4)
Temperature : 40 ℃
Flow rate : 1mL/min
Run time : 3min gradient(30%B), 15min gradient (30%-70%B),5 min(70%B),then 7min @(30%B)
Detector : UV
Wavelenth : 220/254 nm
User name : PC E-005
Notebook page :
Sample description : in ACN
Injection Volume : 1 uL

Data File Name : 939981-39-2.lcd
Method File Name : 939981-39-2.lc





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

PeakTable

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Area %	Theoretical Plate#
1	3.906	95112	0.463	7582.276
2	7.104	20413958	99.355	12694.552
3	10.772	37483	0.182	44238.503
Total		20546554	100.000	

Detector A Ch2 254nm

Peak#	Ret. Time	Area	Area %	Theoretical Plate#
1	3.905	12379	0.174	11385.356
2	7.104	7072753	99.588	13683.686
3	10.942	16880	0.238	54395.993
Total		7102012	100.000	

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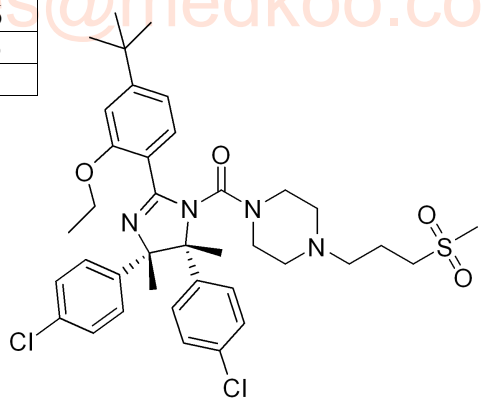

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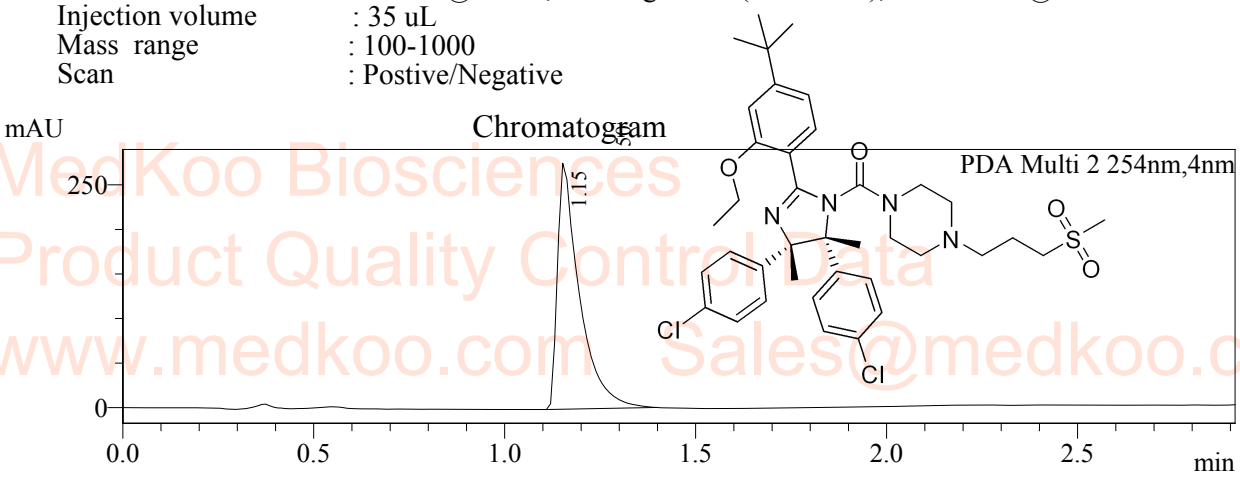
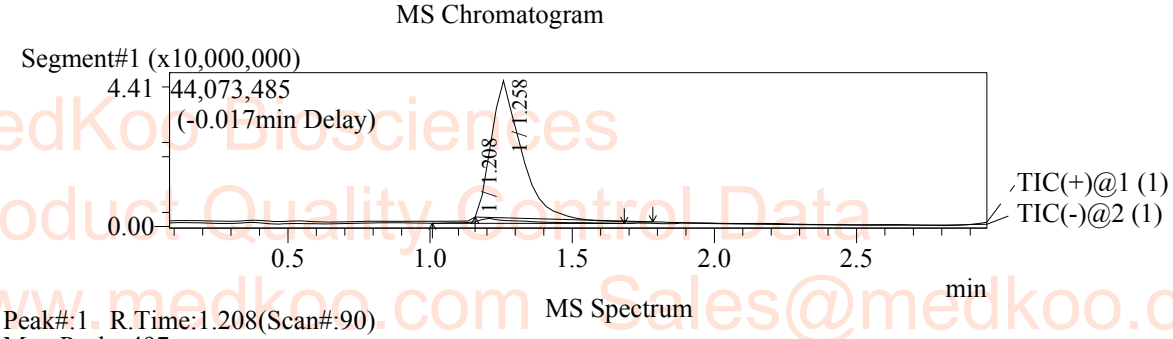
RO5045337 LC/MS Analysis

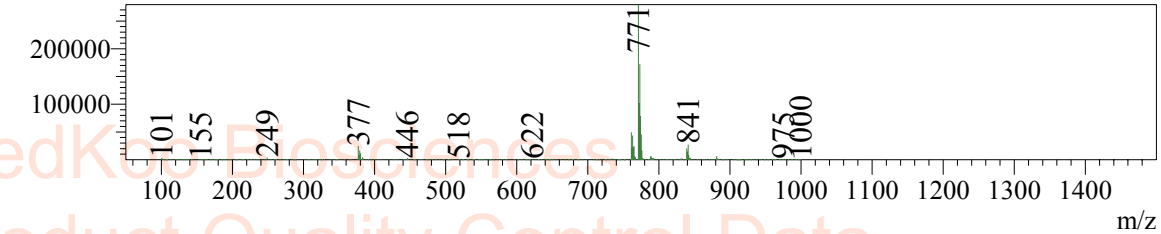
LC-MS condition

Column	: Chromolith SpeedROD ,RP-18e,50*4.6mm
Mobile Phase	: A: H2O/CH3CN/FA=90/10/0.05； B: CH3CN/H2O/FA=90/10/0.05
Temperature	: 35℃
Flow rate	: 3mL/min
Run time	: 0.4min@20%B,1.4min gradient(20-95% B), then0.4min@95% B
Injection volume	: 35 uL
Mass range	: 100-1000
Scan	: Postive/Negative





Peak#:1 R.Time:1.208(Scan#:90)
MassPeaks:497
Spectrum Mode:Averaged 1.167-1.217(88-92)
BG Mode:Calc Segment 1 - Event 2



Peak#:1 R.Time:1.258(Scan#:93)
MassPeaks:460
Spectrum Mode:Averaged 1.208-1.258(91-95)
BG Mode:Calc Segment 1 - Event 1

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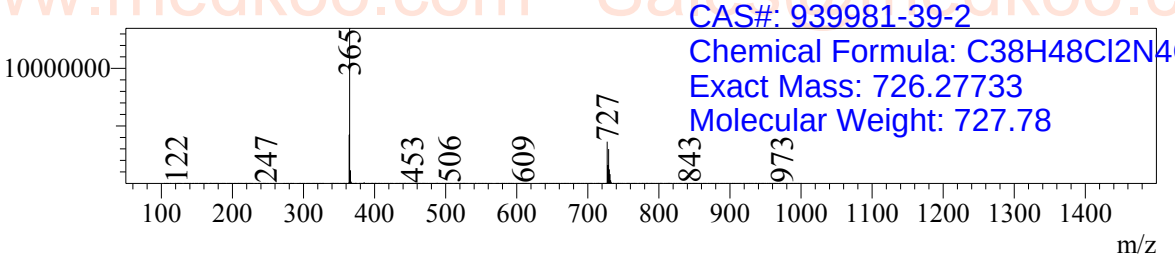

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