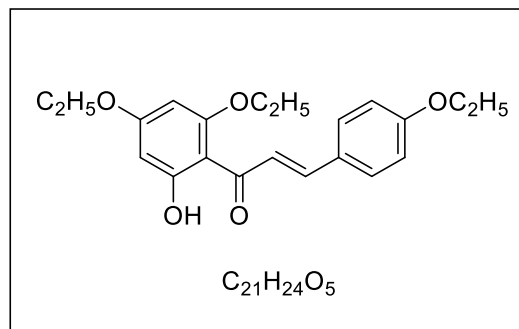
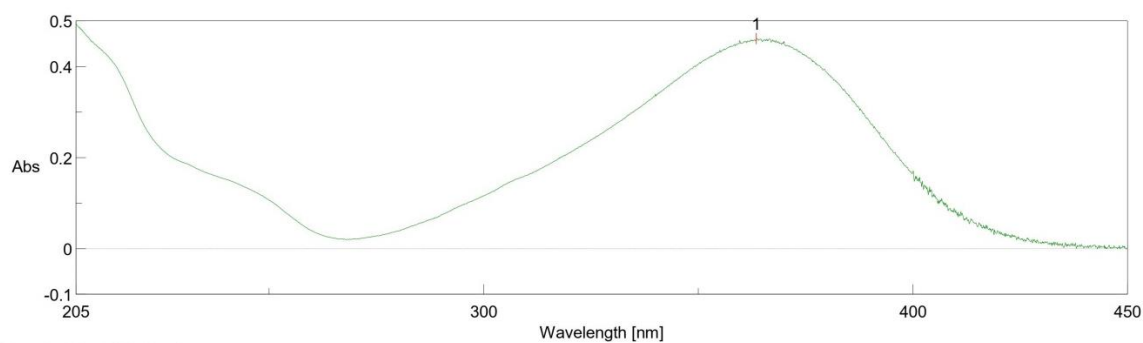


**Table S4. Spectral data of compound 4**



## UV



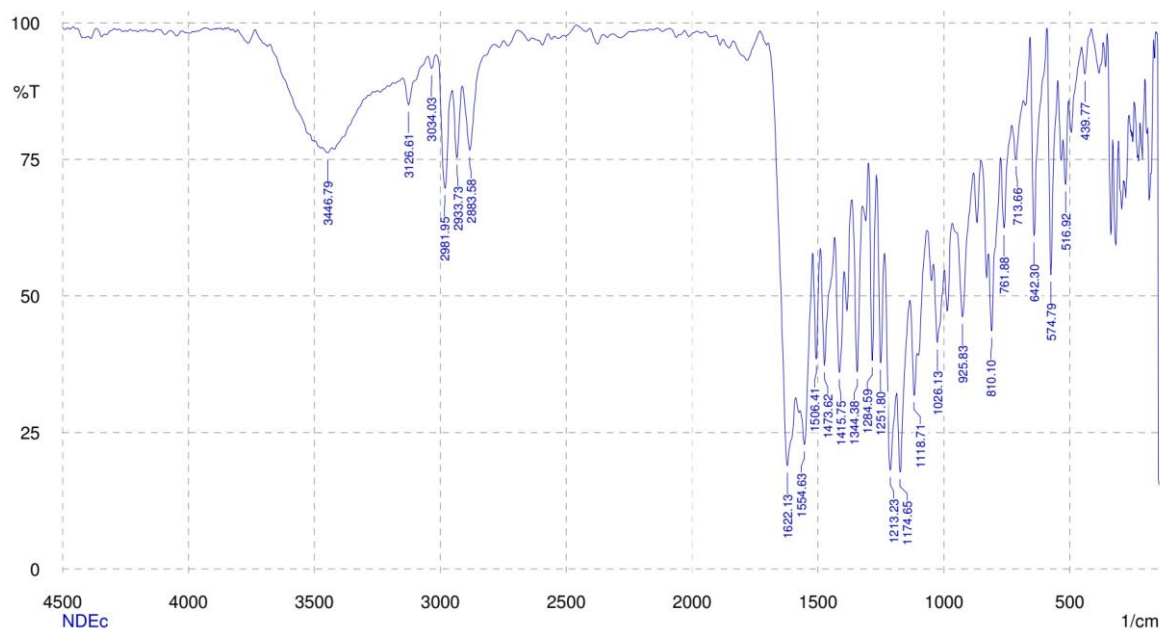
[ Result of Peak Picking ]

No.	Position	Intensity
1	363.5	0.461398

No.	Position	Intensity
-----	----------	-----------

No.	Position	Intensity
-----	----------	-----------

## IR



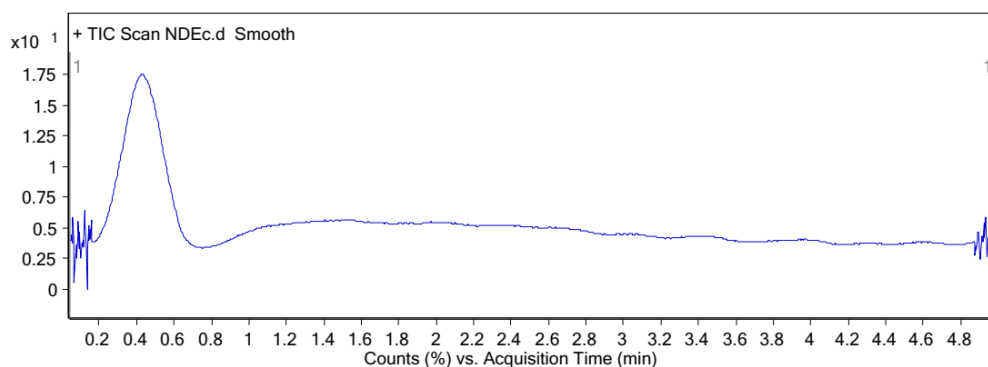
# HR-MS

## Qualitative Analysis Report

Data File	NDEc.d	Sample Name	NDEc
Sample Type	Sample	Position	P1-A4
Instrument Name	Instrument 1	User Name	
Acq Method	Cot ngan - MSMS_Pos.m	Acquired Time	01/07/2021 3:17:40 PM
IRM Calibration Status	Success	DA Method	COTNGAN.M.m
Comment		Info.	
Sample Group		Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)
Stream Name	LC 1		

## User Chromatograms

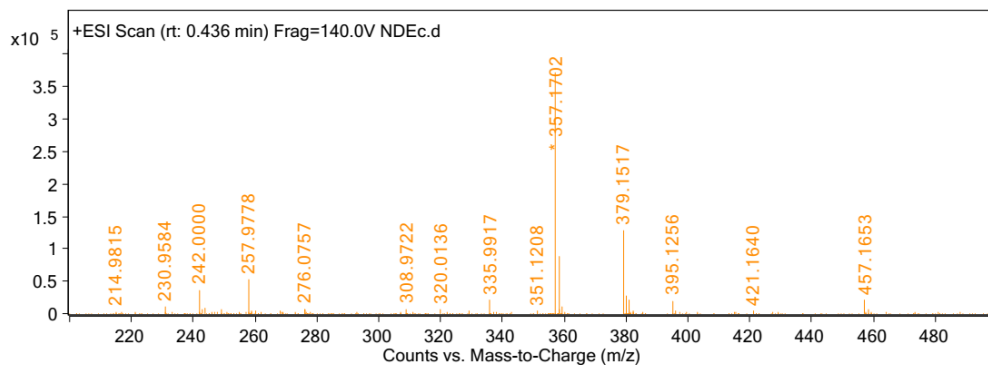
Fragmentor Voltage 140 Collision Energy 0 Ionization Mode ESI



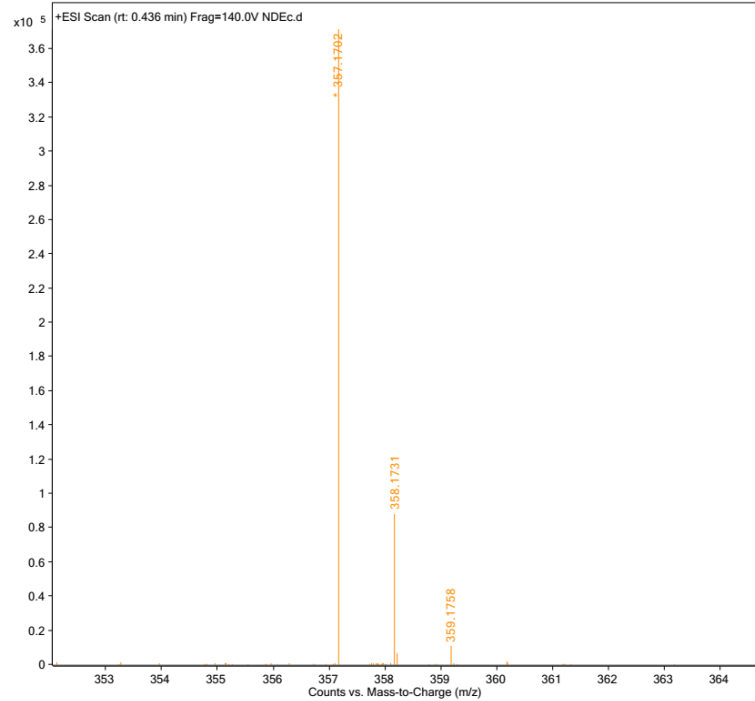
## Qualitative Analysis Report

## User Spectra

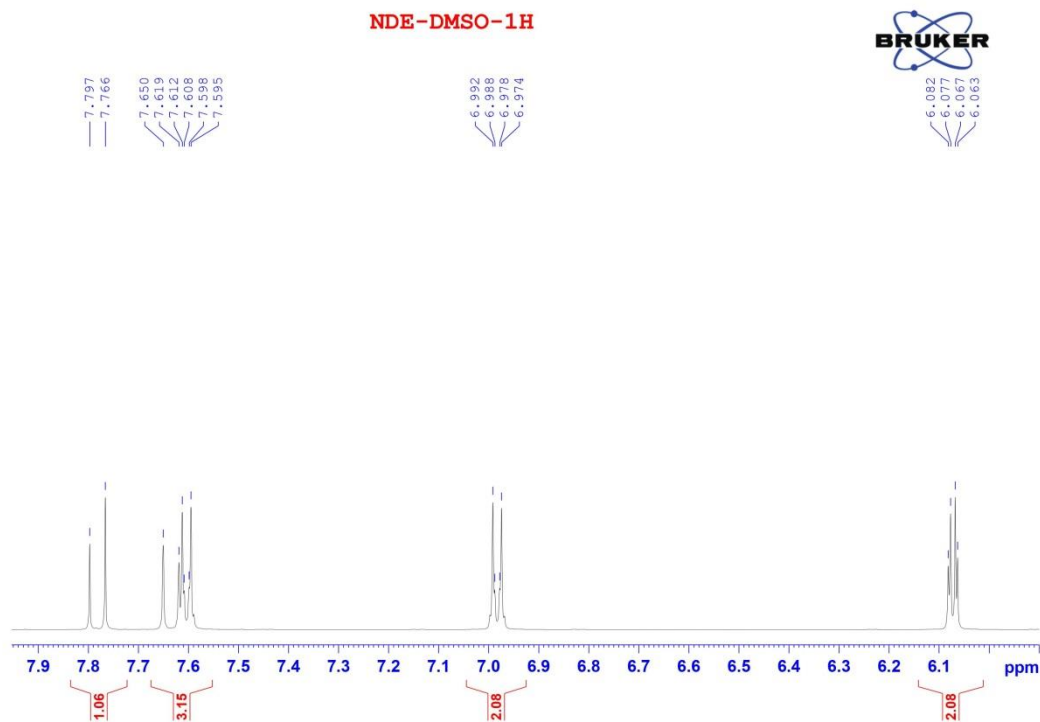
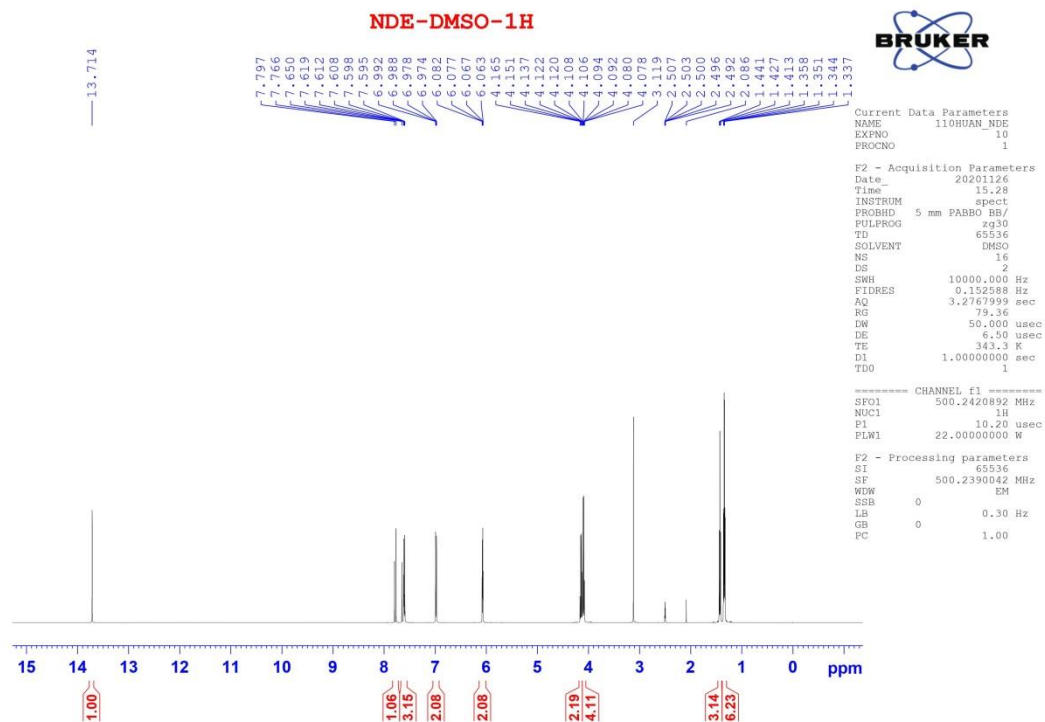
Fragmentor Voltage 140 Collision Energy 0 Ionization Mode ESI



Sample Name	NDEc	Position	P1-A4	Instrument Name	Instrument 1
User Name		Inj Vol	2	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	NDEc.d
ACQ Method	Cot ngan - MSMS_Pos.m	Comment		Acquired Time	01/07/2021 3:17:40 PM

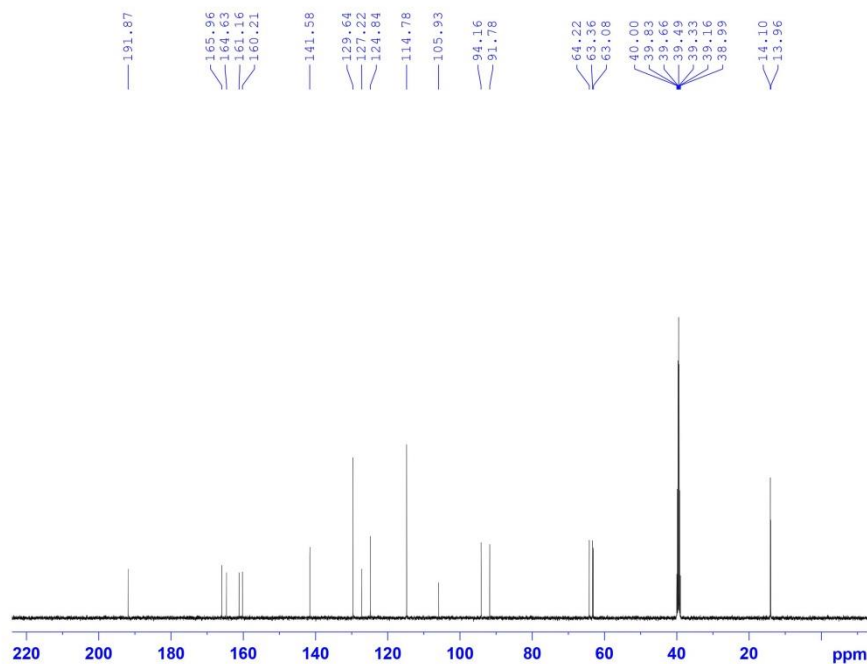


# $^1\text{H}$ -NMR



# $^{13}\text{C}$ -NMR

NDE-DMSO-C13CPD



Current Data Parameters  
NAME 11GHUAN\_NDE  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20201126  
Time 15.38  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 128  
DS 4  
SWH 31250.000 Hz  
FIDRES 0.476837 Hz  
AQ 1.0485760 sec  
RG 198.57  
DM 16.000 usec  
DE 6.50 usec  
TE 343.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 125.7990330 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 88.00000000 W

===== CHANNEL f2 =====  
SFO2 500.2410010 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLM2 22.00000000 W  
PLM12 0.35764000 W  
PLM13 0.17989001 W

F2 - Processing parameters  
SI 32768  
SF 125.7853020 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

NDE-DMSO-C13CPD

