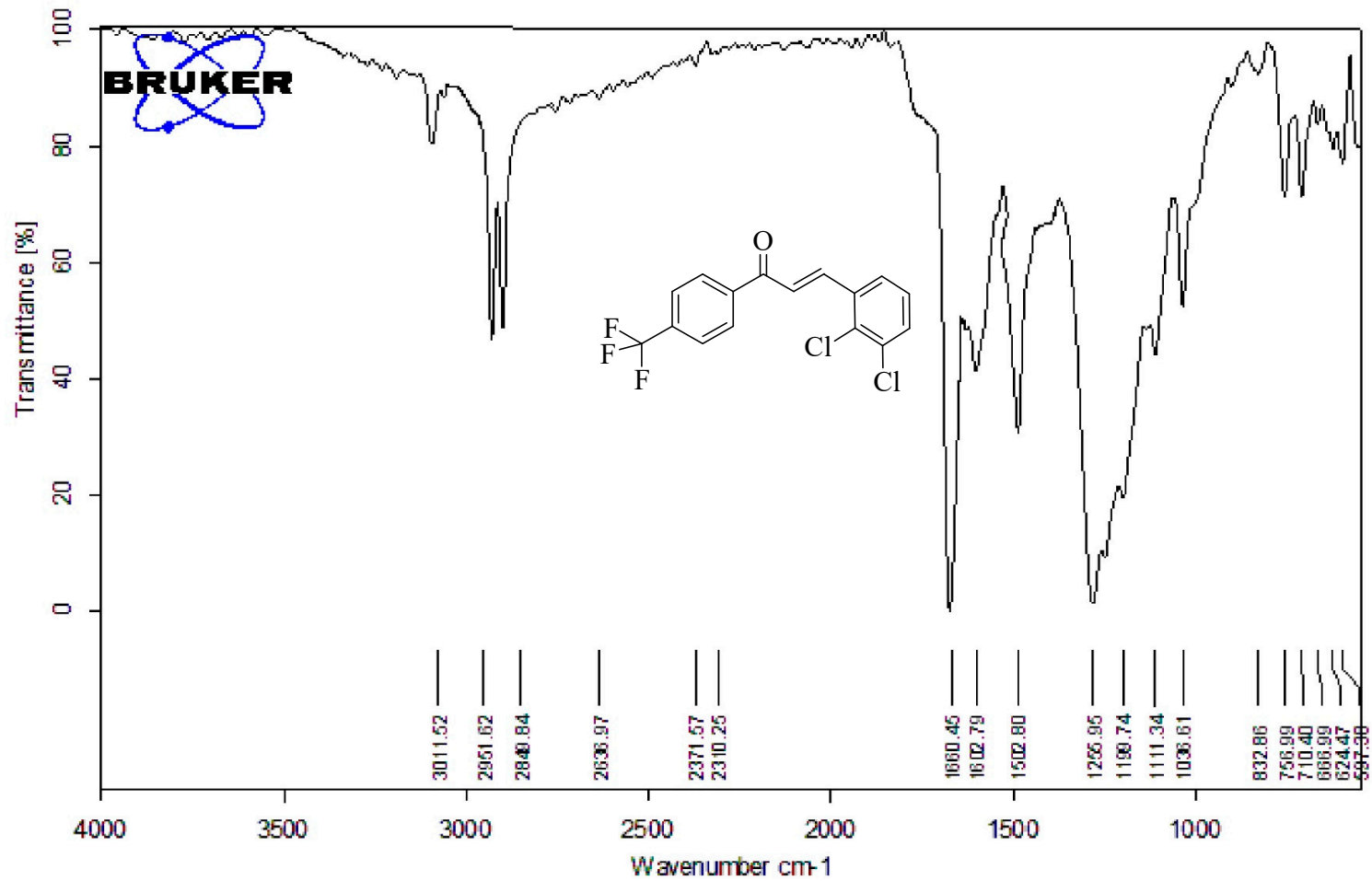


Supplementary Data

Design, synthesis, and antibacterial and antifungal activities of novel trifluoromethyl and trifluoromethoxy substituted chalcone derivatives

Lagu Surendra Babu^{1,*}, Yejella Rajendra Prasad², Richie R. Bhandare^{3,*} and Afzal B. Shaik^{4,*}

FT-IR, ¹H NMR, ¹³C NMR & MS



D:\FTIR DATA\2019 MARCH\SURENDRA1.0

A1

SOLID

3/19/2019

FT-IR Spectrum of (*E*)-3-(2'',3''-dichlorophenyl)-1-[4''-(trifluoromethyl)phenyl]prop-2-en-1-one (A1)

A1

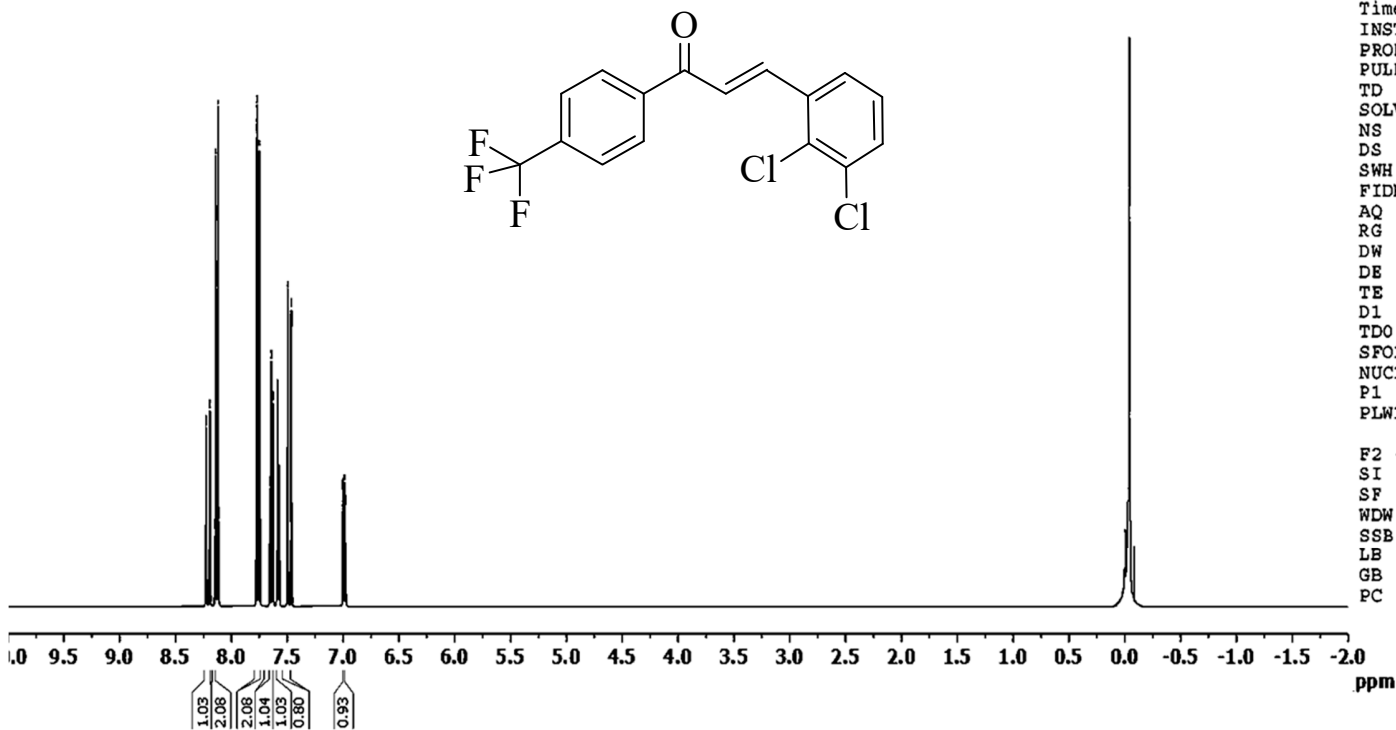
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8.2257
8.1949
8.1935
8.1444
8.1411
8.1385
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8.1195
8.1162
7.7738
7.7705
7.7676
7.7515
7.7489
7.7456
7.6566
7.6413
7.6254
7.5877
7.5852
7.5727
7.5702
7.4958
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6.9964
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6.9820
6.9798



Current Data Parameters
NAME 03042019
EXPNO 1
PROCNO 1

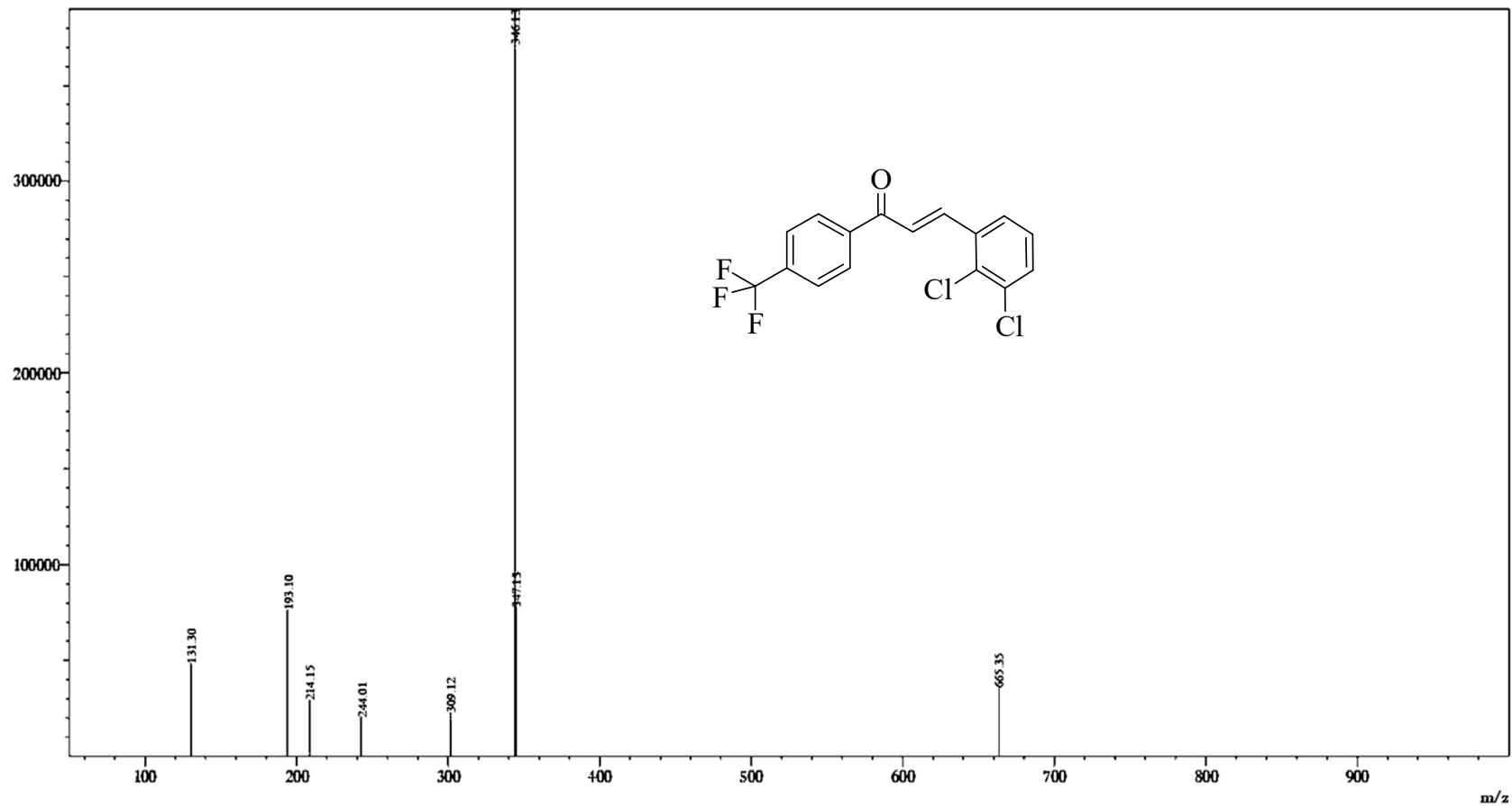
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 132.41
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1
SFO1 400.1324708 MHz
NUC1 1H
P1 15.00 usec
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F2 - Processing parameters
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PC 1.00

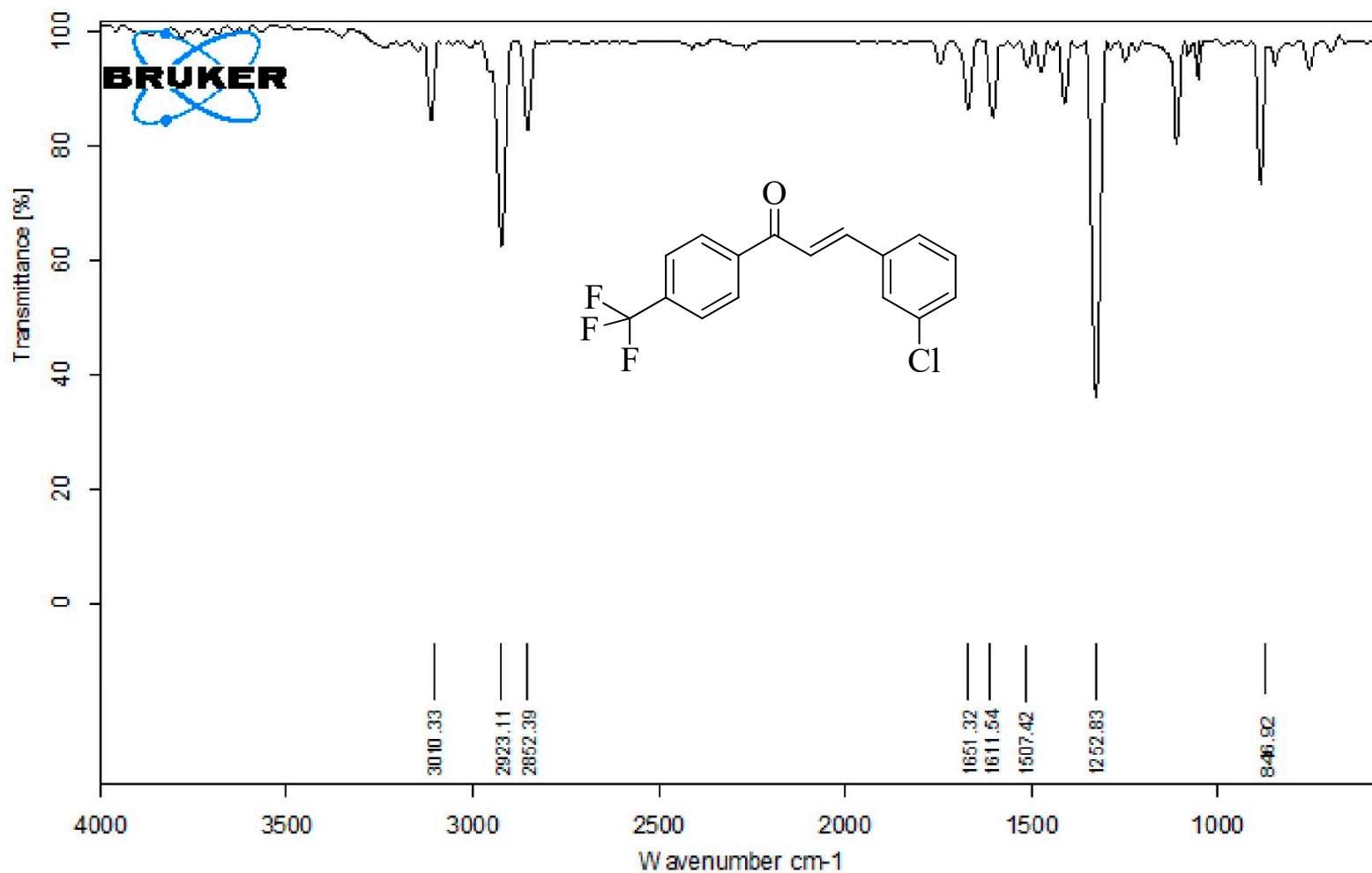


¹H NMR Spectrum of (*E*)-3-(2'',3''-dichlorophenyl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A1)

Averaged ESI Positive+
Spectrum Mode: Averaged 0.183-0.605(74-243)
[CPS]



Mass Spectrum of (*E*)-3-(2'',3''-dichlorophenyl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A1)

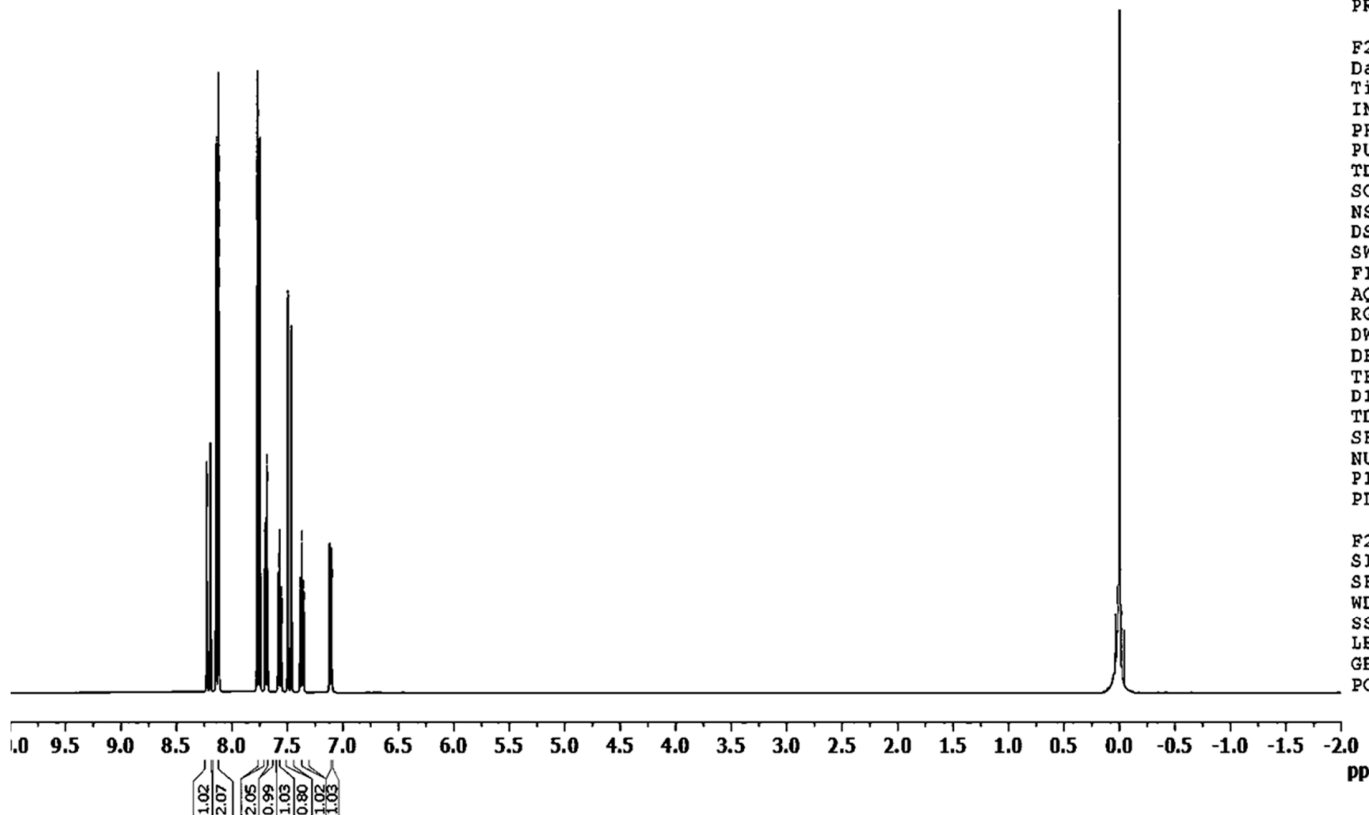


C:\Users\Lenovo\Documents\Bruker\OPUS_7.8.44\DATA\MEAS\DEMO.88	A2	SOLID	22-11-2019
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FT-IR Spectrum of *(E)*-3-(2''-chlorophenyl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A2)

A2

8.2272
8.2257
8.1949
8.1935
8.1444
8.1411
8.1385
8.1224
8.1195
8.1162
7.7738
7.7705
7.7676
7.7514
7.7489
7.7456
7.7001
7.6971
7.6840
7.6810
7.5863
7.5833
7.5723
7.5692
7.5672
7.5562
7.5530
7.4958
7.4636
7.3863
7.3834
7.3720
7.3706
7.3691
7.3677
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7.1197
7.1183
7.1166
7.1154
7.1042
7.1028
7.1010
7.0997



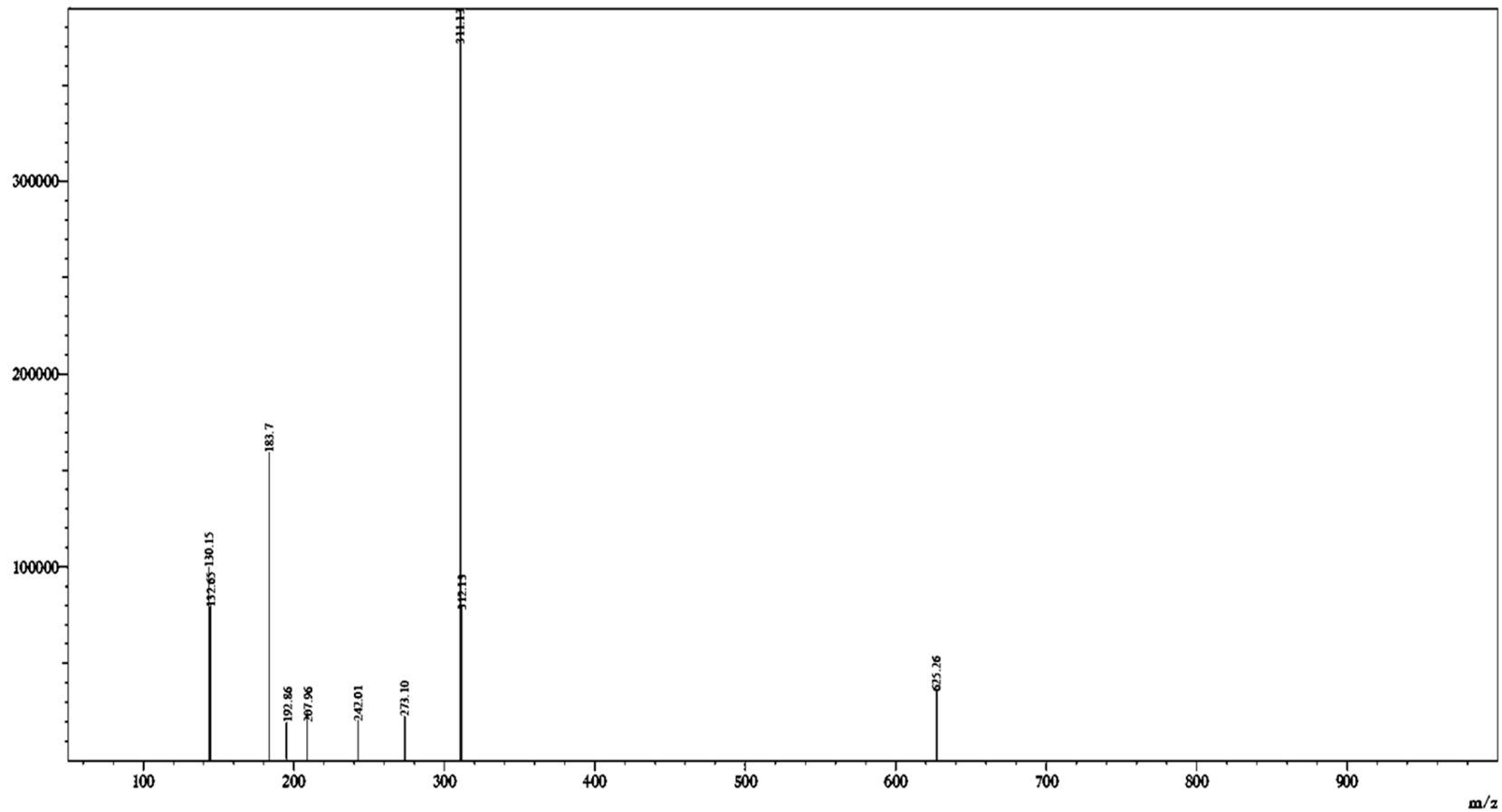
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PROCNO 1

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SOLVENT CDCl3
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FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 132.41
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
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TDO 1
SFO1 400.1324708 MHz
NUC1 1H
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PLW1 9.91339970 W

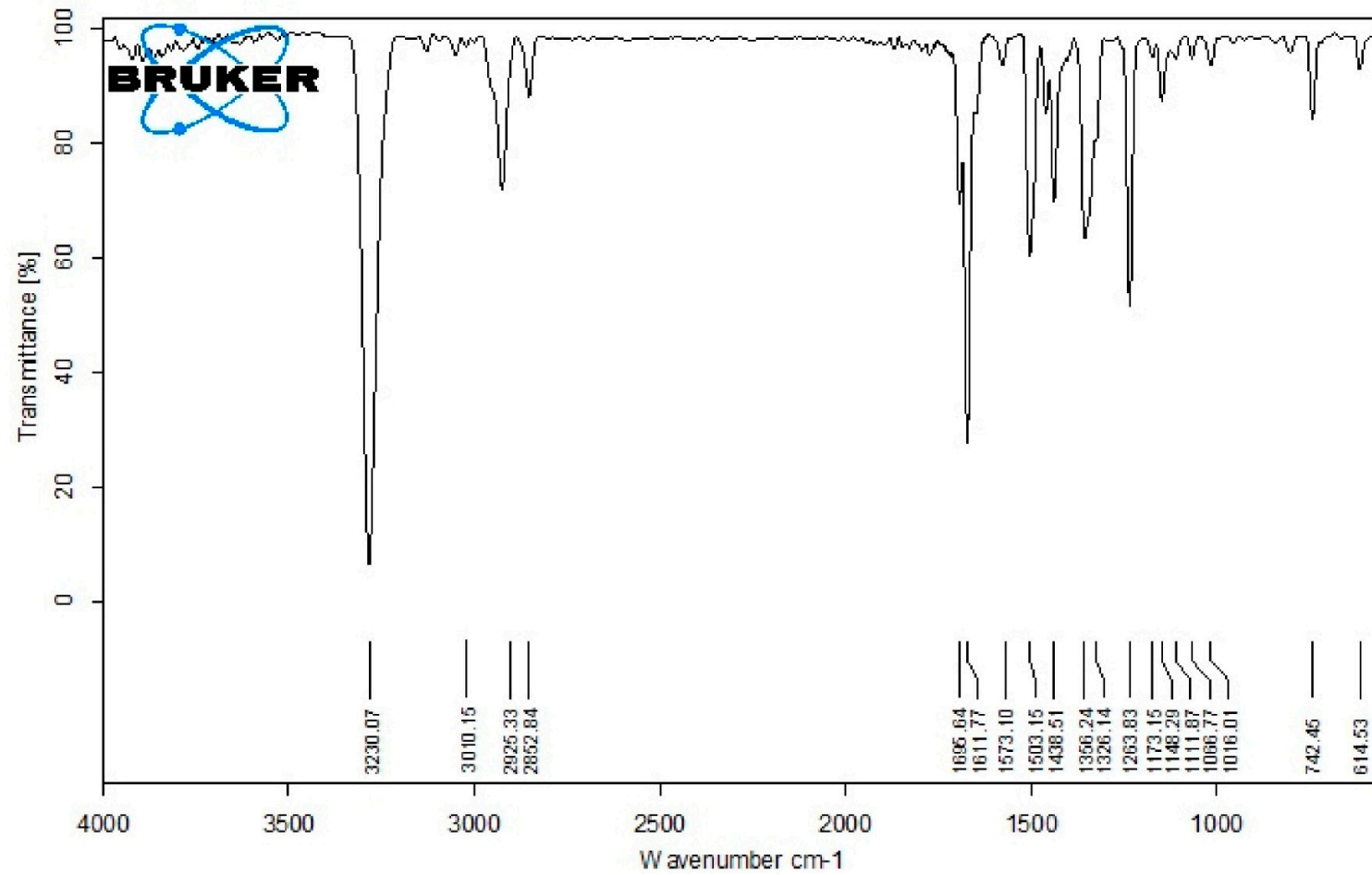
F2 - Processing parameters
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WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR Spectrum of (E)-3-(3''-chlorophenyl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A2)

Averaged ESI Positive+
Spectrum Mode: Averaged 0.183-0.605(74-243)
[CPS]



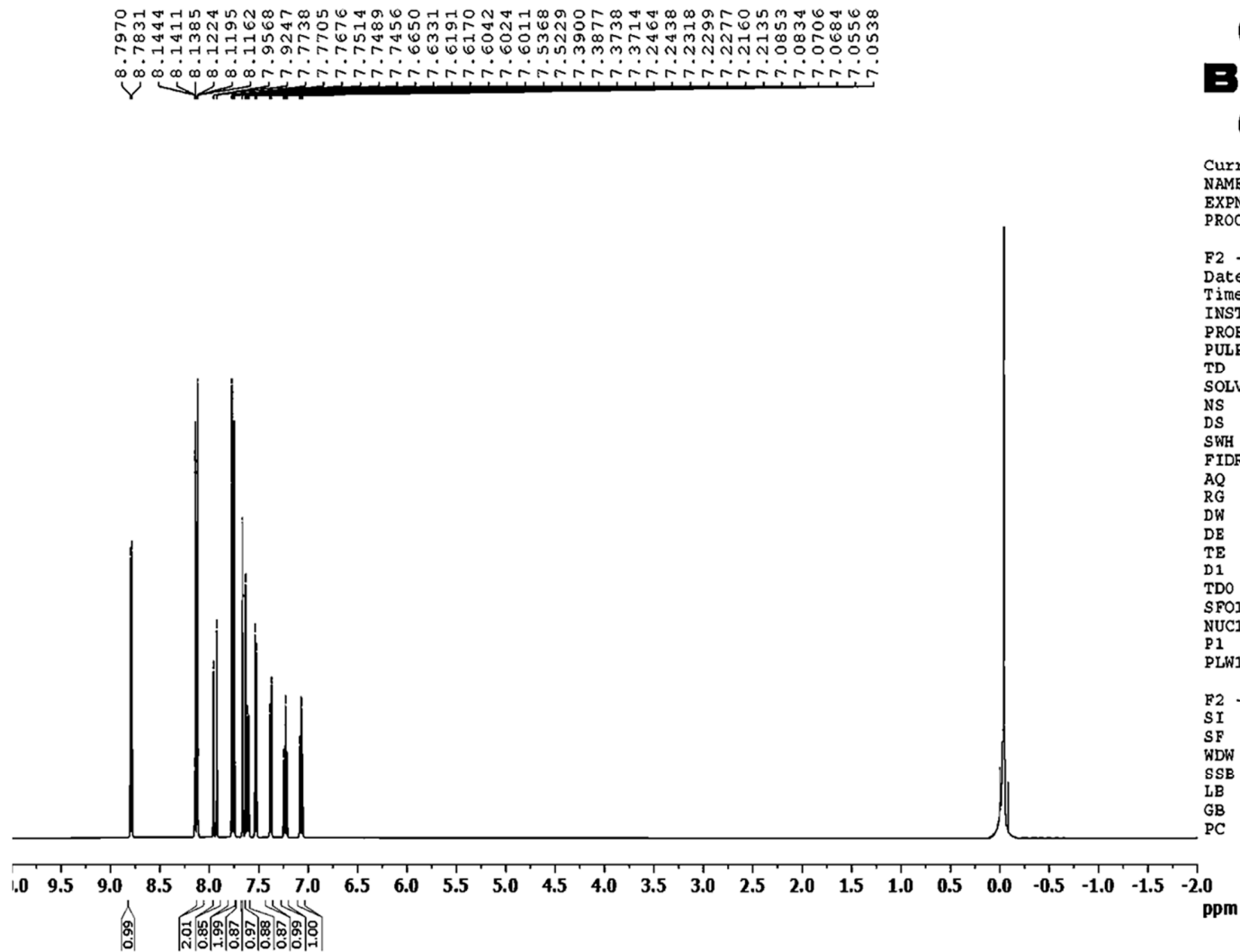
Mass Spectrum of (*E*)-3-(2''-chlorophenyl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A2)



C:\Users\Lenovo\Documents\Bruker\OPUS_7.8.44\Data\MEAS\ANURADHA.51	A3	SOLID	19-09-2019
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FT-IR Spectrum of (*E*)-3-(1''H-indol-3''-yl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A3)

A3



Current Data Parameters
 NAME 03042019
 EXPNO 3
 PROCNO 1

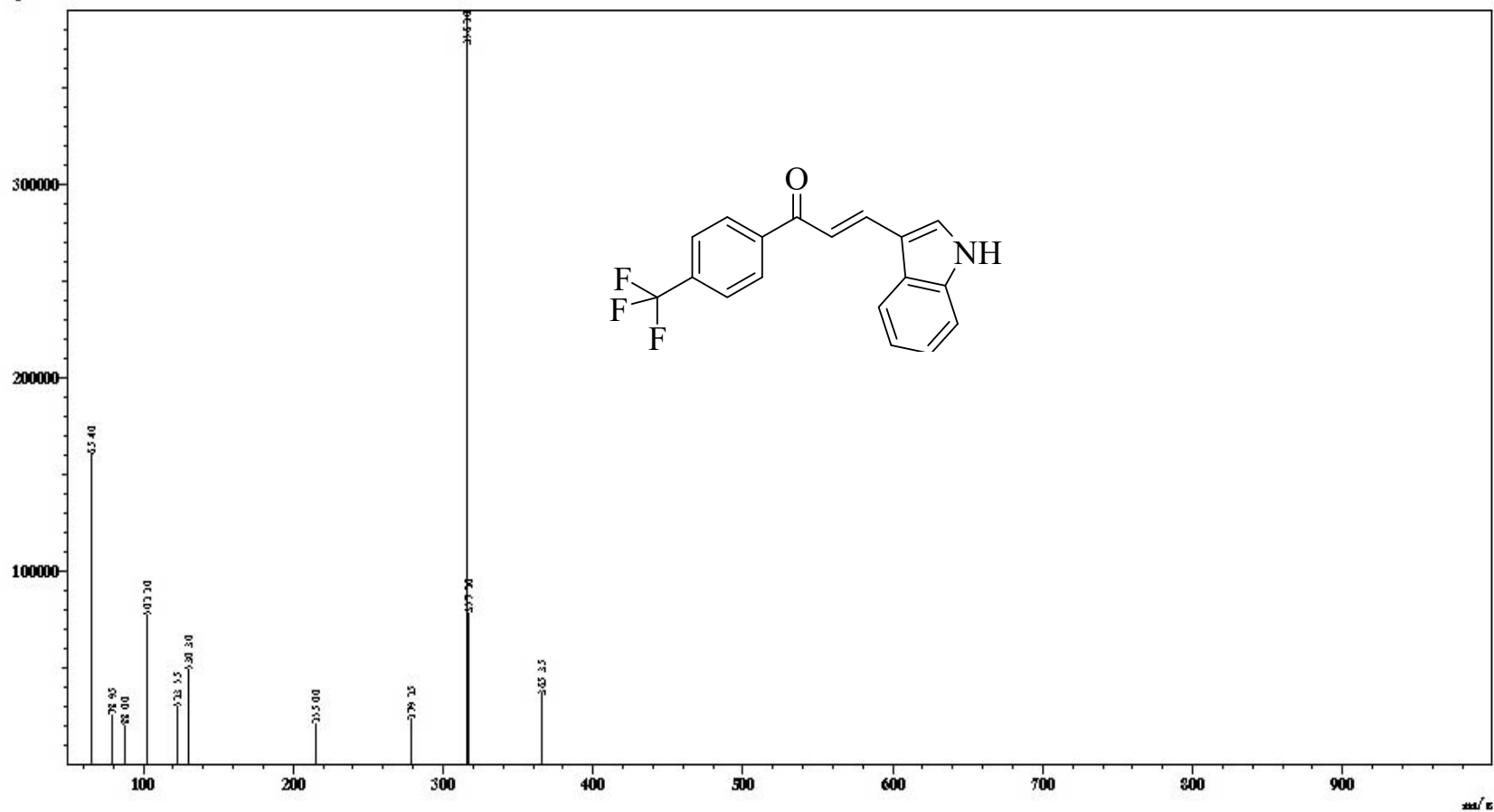
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 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 132.41
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1
 SFO1 400.1324708 MHz
 NUC1 1H
 P1 15.00 usec
 PLW1 9.91339970 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
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¹H NMR Spectrum of (E)-3-(1^H-indol-3'-yl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A3)

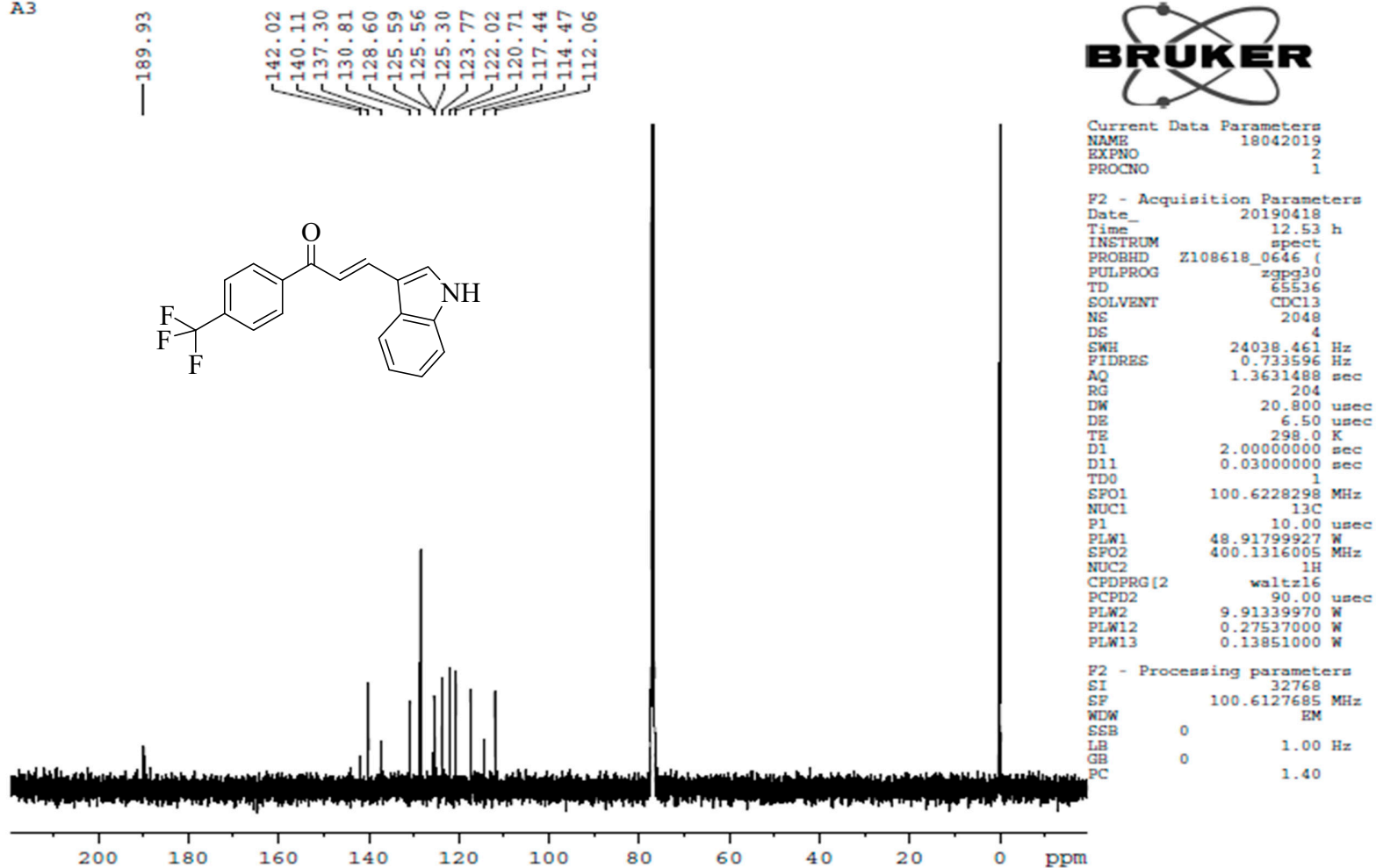
Averaged ESI Positive +
Spectrum Mode: Average of 0.133-0.605 (74-243)

[CPS]



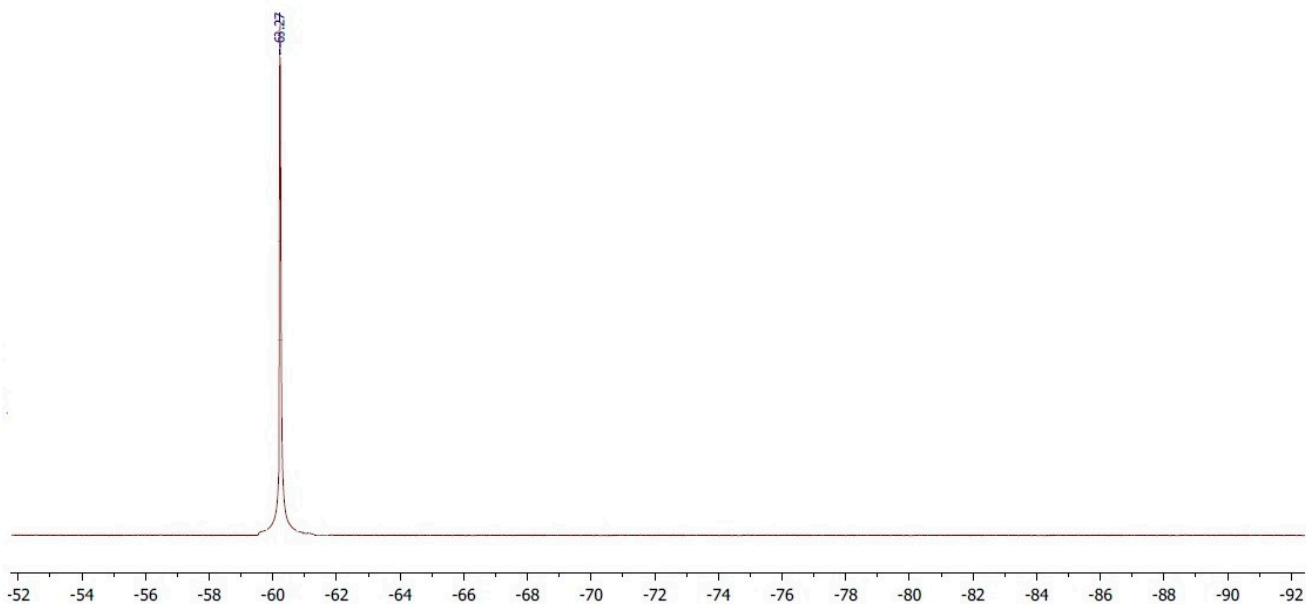
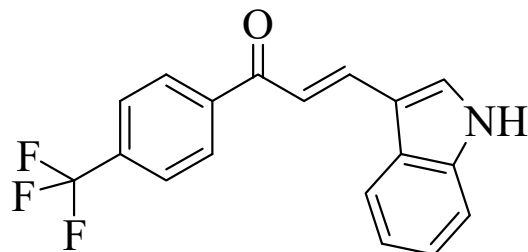
Mass Spectrum of (E)-3-(1''H-indol-3''-yl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A3)

A3



¹³C NMR Spectrum of (*E*)-3-(1''H-indol-3''-yl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A3)

FA3

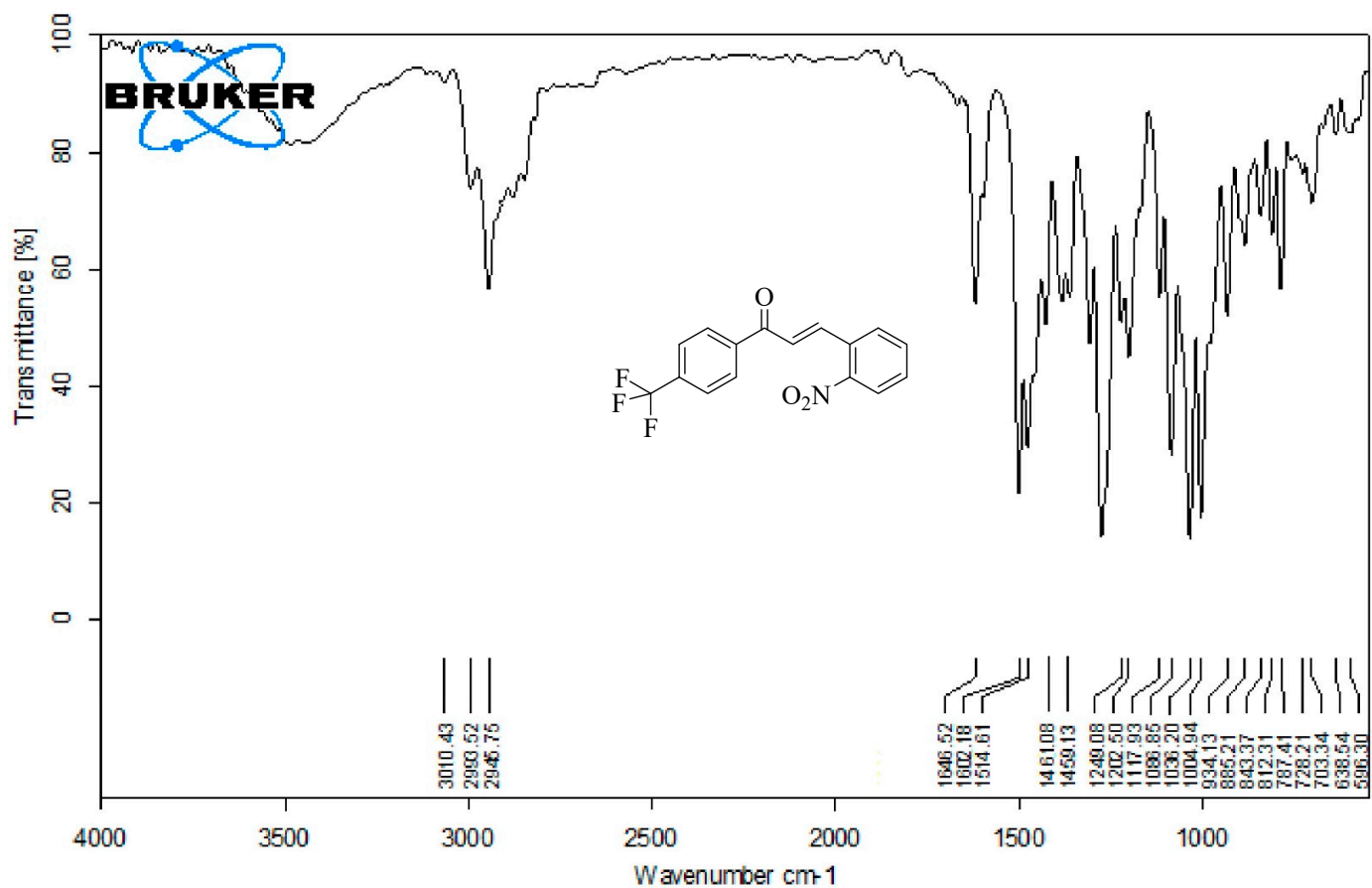


Current Data Parameters
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EXPNO 1
PROCNO 1

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TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 132.41
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 376.1524708 MHz
NUC1 1H
P1 15.00 usec
PLW1 9.91339970 W

F2 - Processing parameters
SI 65536
SF 376.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
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PC 1.00

¹⁰F NMR Spectrum of (*E*)-3-(1''H-indol-3''-yl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A3)

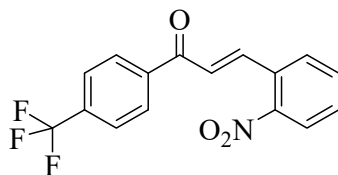


D:\FTIR DATA\2019 JAN\SURENDRA.23	A4	SOLID	1/23/2019
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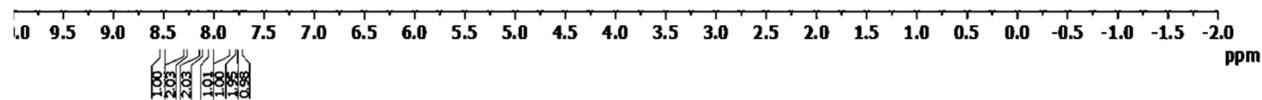
FT-IR Spectrum of (*E*)-3-(2''-nitrophenyl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A4)

A4

8.5172
8.5158
8.4850
8.4835
8.2901
8.2887
8.2868
8.2855
8.2805
8.2775
8.2750
8.2736
8.2718
8.2705
8.2630
8.2601
8.1444
8.1411
8.1385
8.1224
8.1195
8.1162
8.0169
8.0140
8.0017
7.9966
7.9862
7.9833
7.8576
7.8543
7.8419
7.8397
7.8368
7.8243
7.8214
7.7738
7.7705
7.7676
7.7514
7.7489
7.7456
7.7357
7.7035



¹H NMR Spectrum of (*E*)-3-(2''-nitrophenyl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A4)



¹H NMR Spectrum of (*E*)-3-(2''-nitrophenyl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A4)



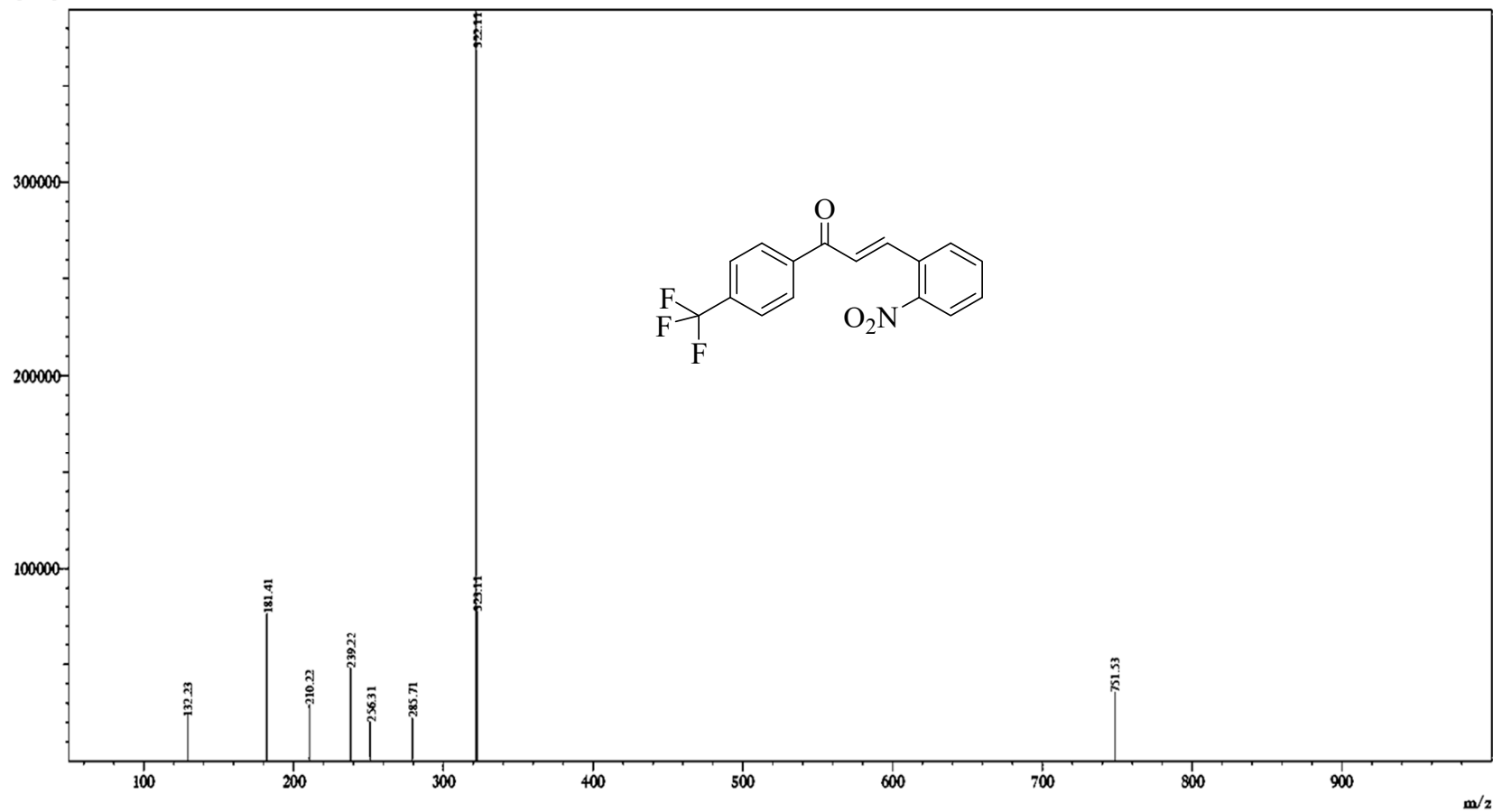
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EXPNO 4
PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 132.41
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1
SFO1 400.1324708 MHz
NUC1 1H
P1 15.00 usec
PLW1 9.91339970 W

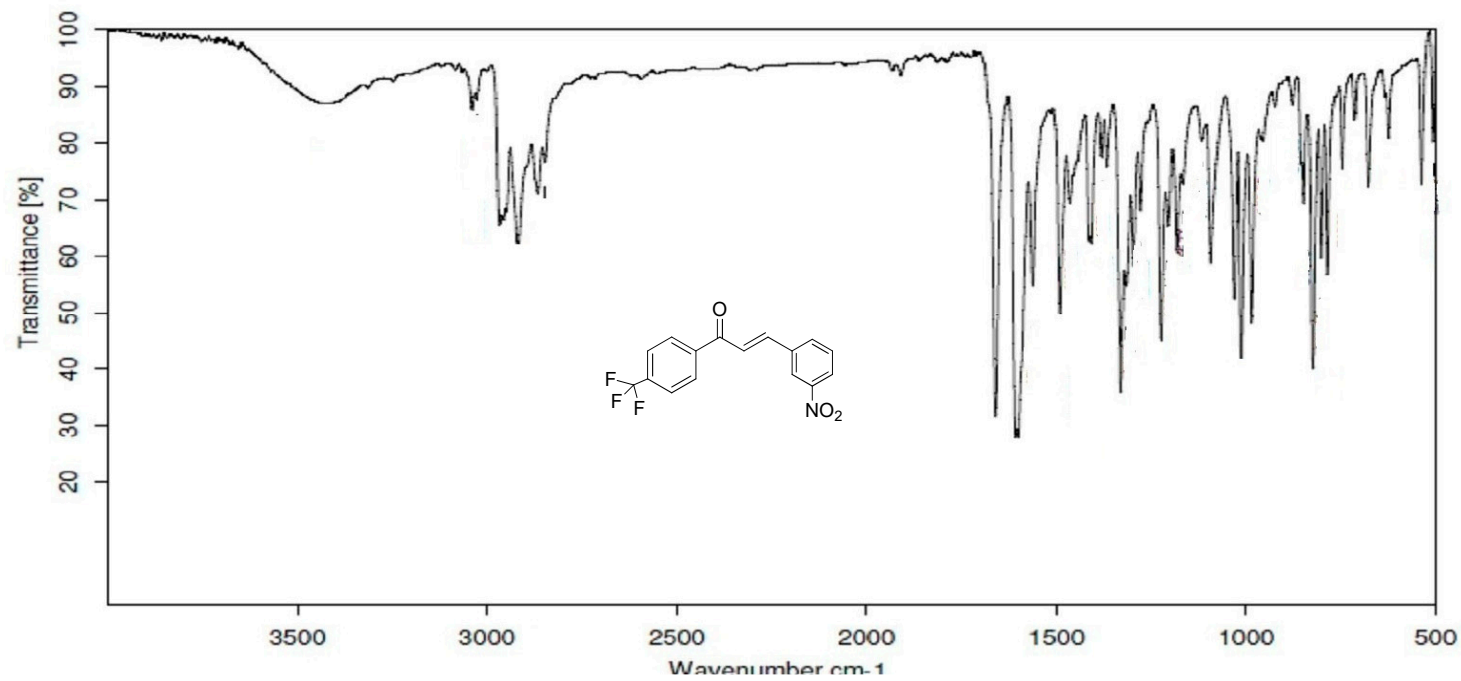
F2 - Processing parameters
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SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz

Averaged ESI Positive+
Spectrum Mode: Averaged 0.183-0.605(74-243)
[CPS]

MS Spectrum
D:\DATA\JULY-19\16072019.3.fcd



Mass Spectrum of (E)-3-(2''-nitrophenyl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A4)



FT-IR Spectrum of (*E*)-3-(3''-nitrophenyl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A5)

A5

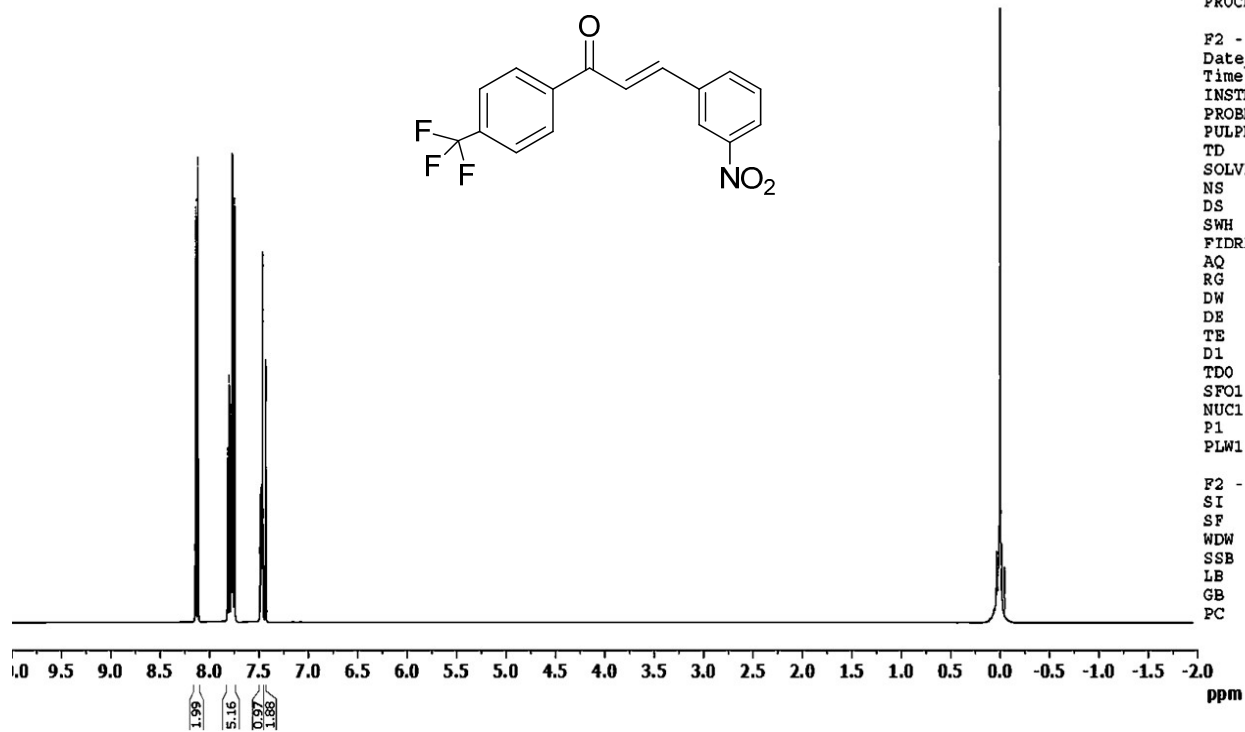
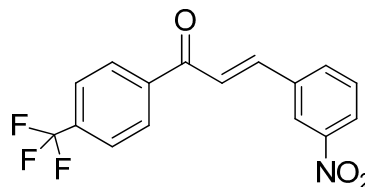
8.1444
8.1411
8.1385
8.1224
8.1195
8.1162
7.8163
7.8048
7.8010
7.7972
7.7849
7.7771
7.7738
7.7705
7.7675
7.7614
7.7514
7.7489
7.7456
7.7407
7.4881
7.4866
7.4845
7.4809
7.4776
7.4753
7.4732
7.4716
7.4691
7.4650
7.4614
7.4536



Current Data Parameters
NAME 05042019
EXPNO 7
PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 132.41
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1
SFO1 400.1324708 MHz
NUC1 1H
P1 15.00 usec
PLW1 9.91339970 W

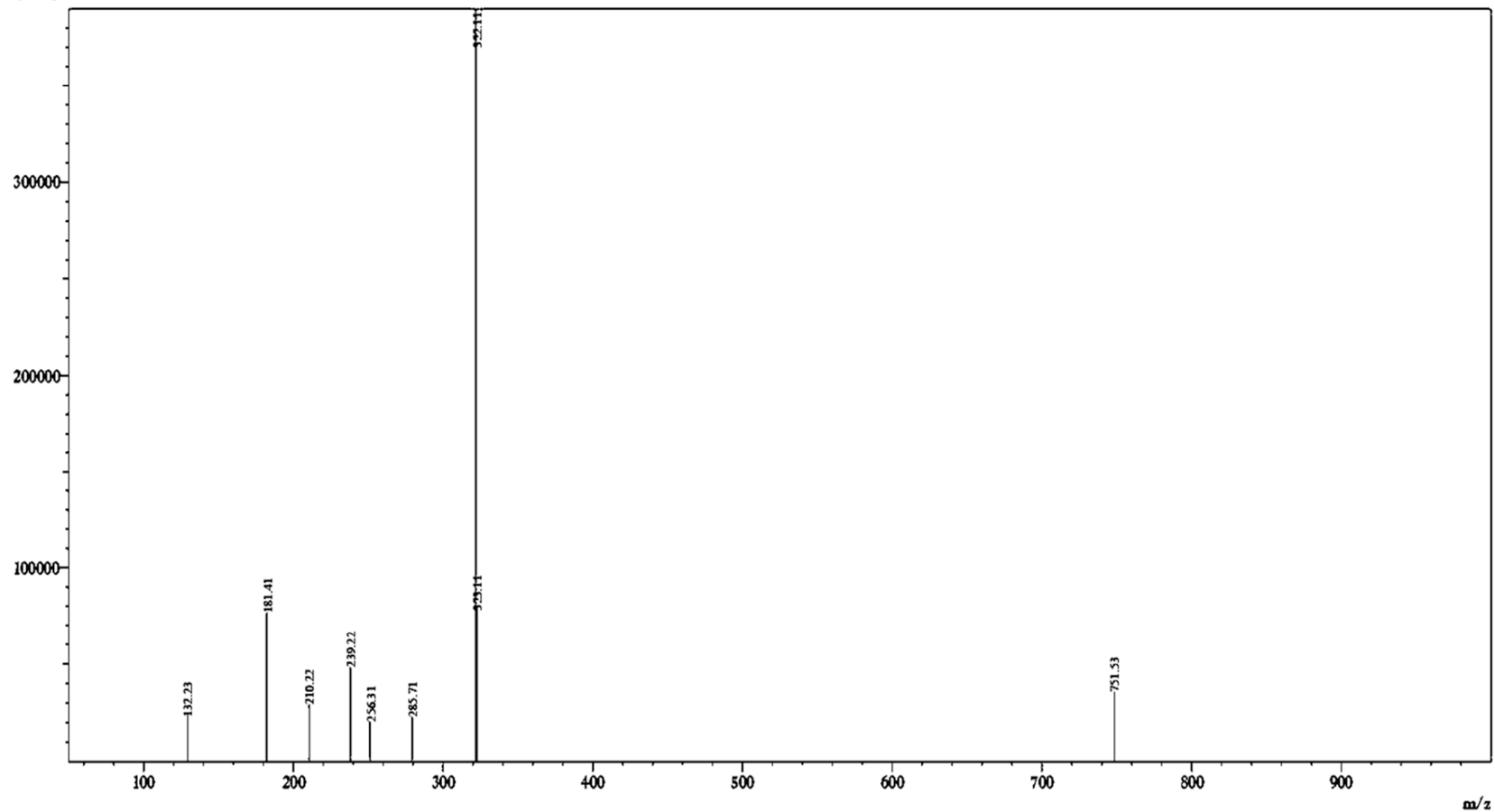
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SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1H NMR Spectrum of (*E*)-3-(3'-nitrophenyl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A5)

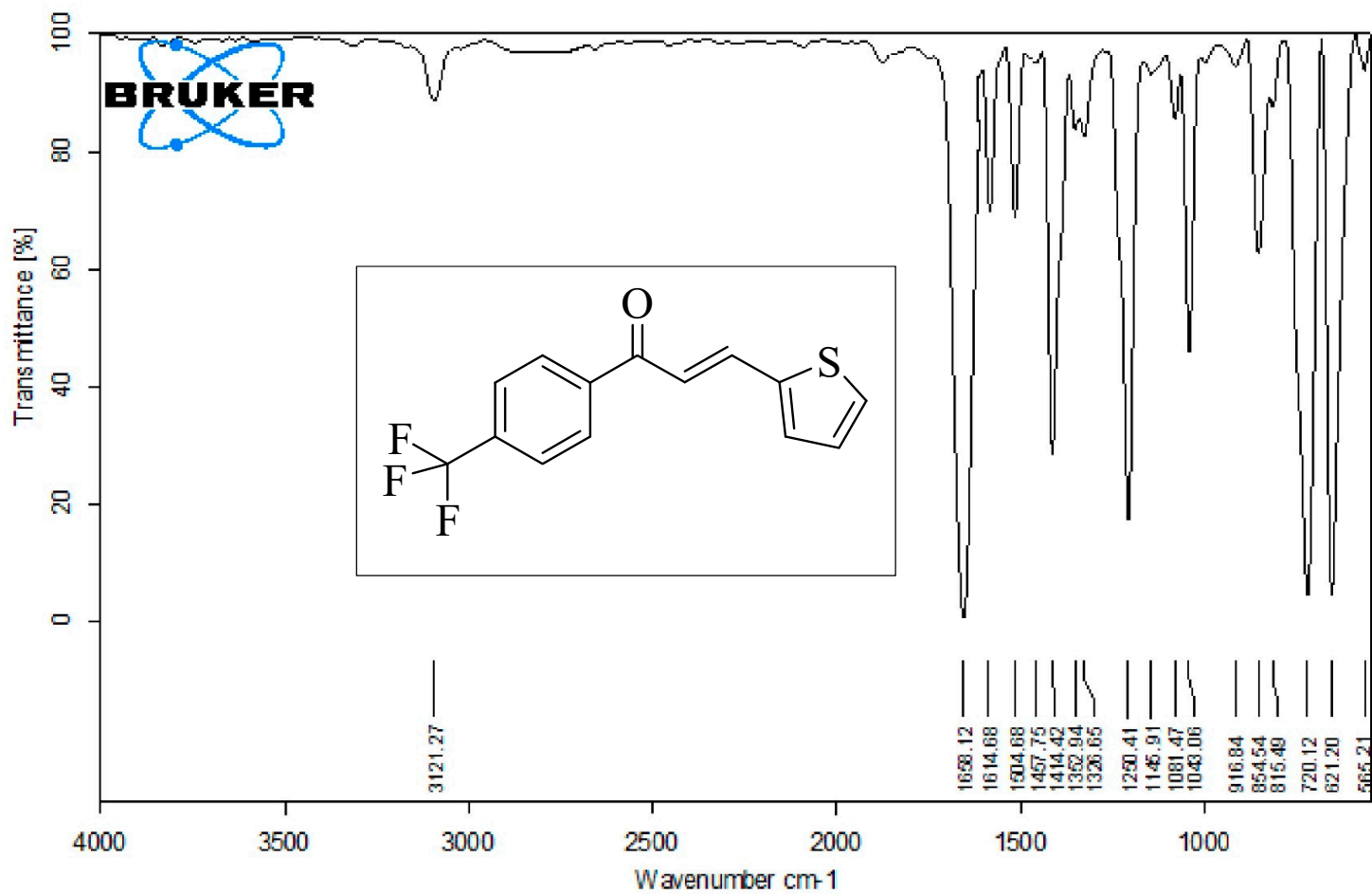
Averaged ESI Positive+
Spectrum Mode: Averaged 0.183-0.605(74-243)
[CPS]

MS Spectrum
D:\DATA\JULY-19\16072019.3.fcd



□

Mass Spectrum of (*E*)-3-(3''-nitrophenyl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A5)

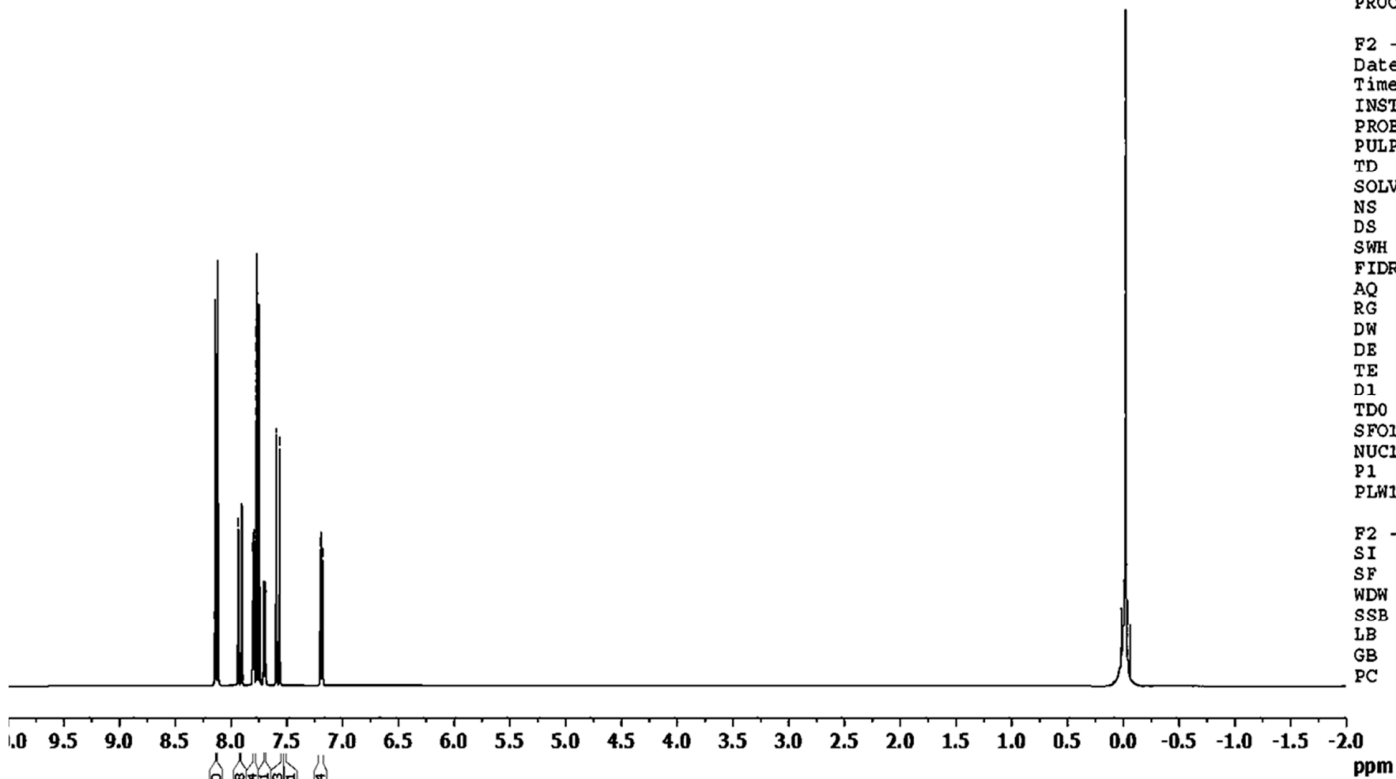


D:\FTIR DATA\2017 OCT\SURENDRA BABU	A6	SOLID	8/9/2018
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FT-IR Spectrum of (E)-3-(thiophen-2''-yl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A6)

A6

8.1444
8.1411
8.1385
8.1224
8.1195
8.1162
7.9363
7.9060
7.9045
7.8067
7.8034
7.7968
7.7935
7.7738
7.7705
7.7675
7.7515
7.7489
7.7456
7.7082
7.7049
7.6961
7.6946
7.6917
7.5947
7.5639
7.2010
7.1911
7.1886
7.1787



Current Data Parameters
NAME 03042019
EXPNO 6
PROCNO 1

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Time 11.53 h
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PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 132.41
DW 62.400 usec
DE 6.50 usec
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TD0 1
SFO1 400.1324708 MHz
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P1 15.00 usec
PLW1 9.91339970 W

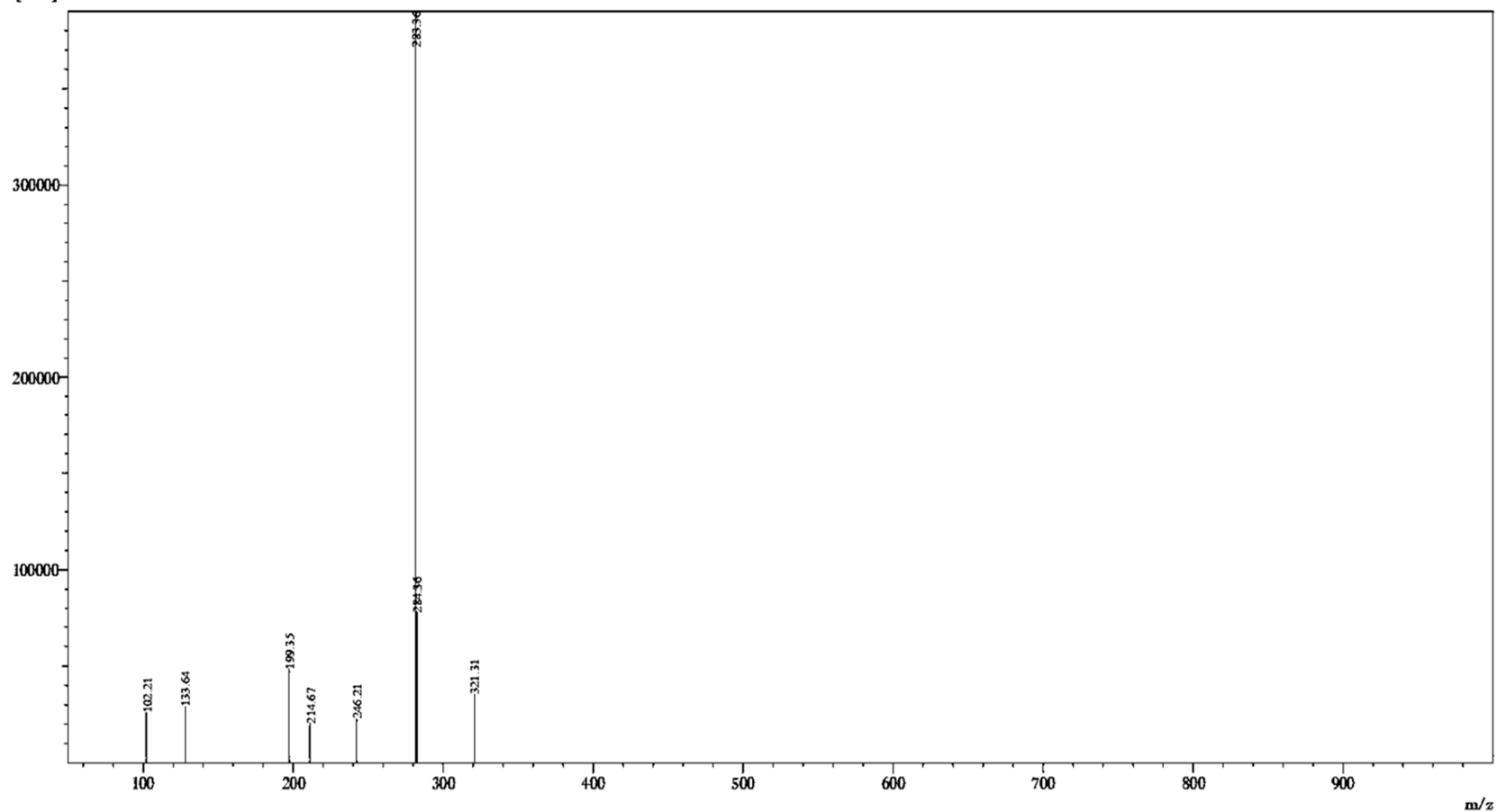
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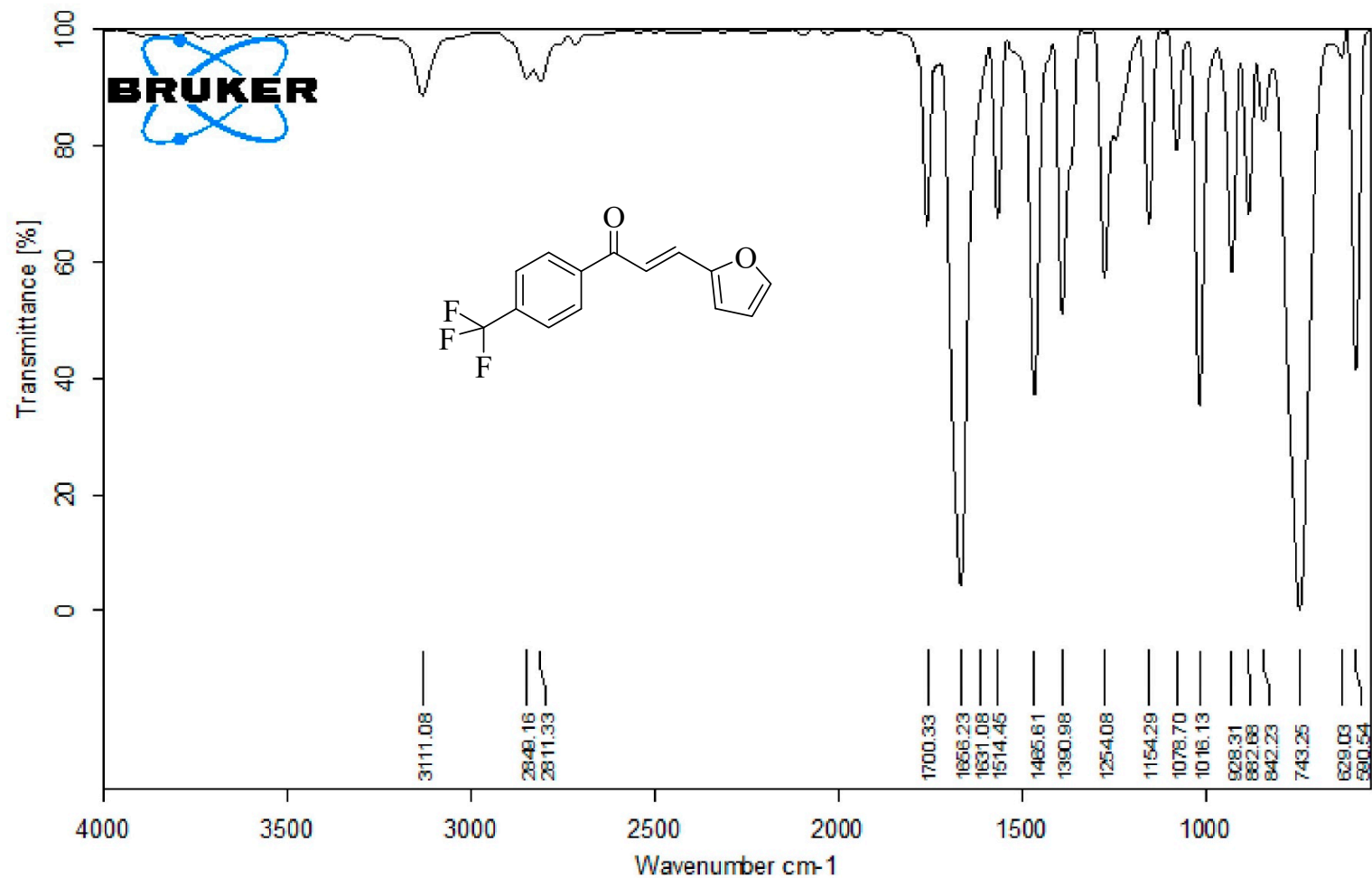
***1*H NMR Spectrum of (*E*)-3-(thiophen-2''-yl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A6)**

Sample Name : KSB-A6-282
Data File : 16072019.5.lcd
Date Acquired : 7/16/2019 10:52:00 AM
Batch File : 16072019.lcb

MS Spectrum
D:\DATA\JULY-19\16072019.5.lcd

AveragedESI Positive
Spectrum Mode:Averaged 0.183-0.605(74-243)
[CPS]





D:\FTIR DATA\2017 OCT\SURENDRA BABU.2

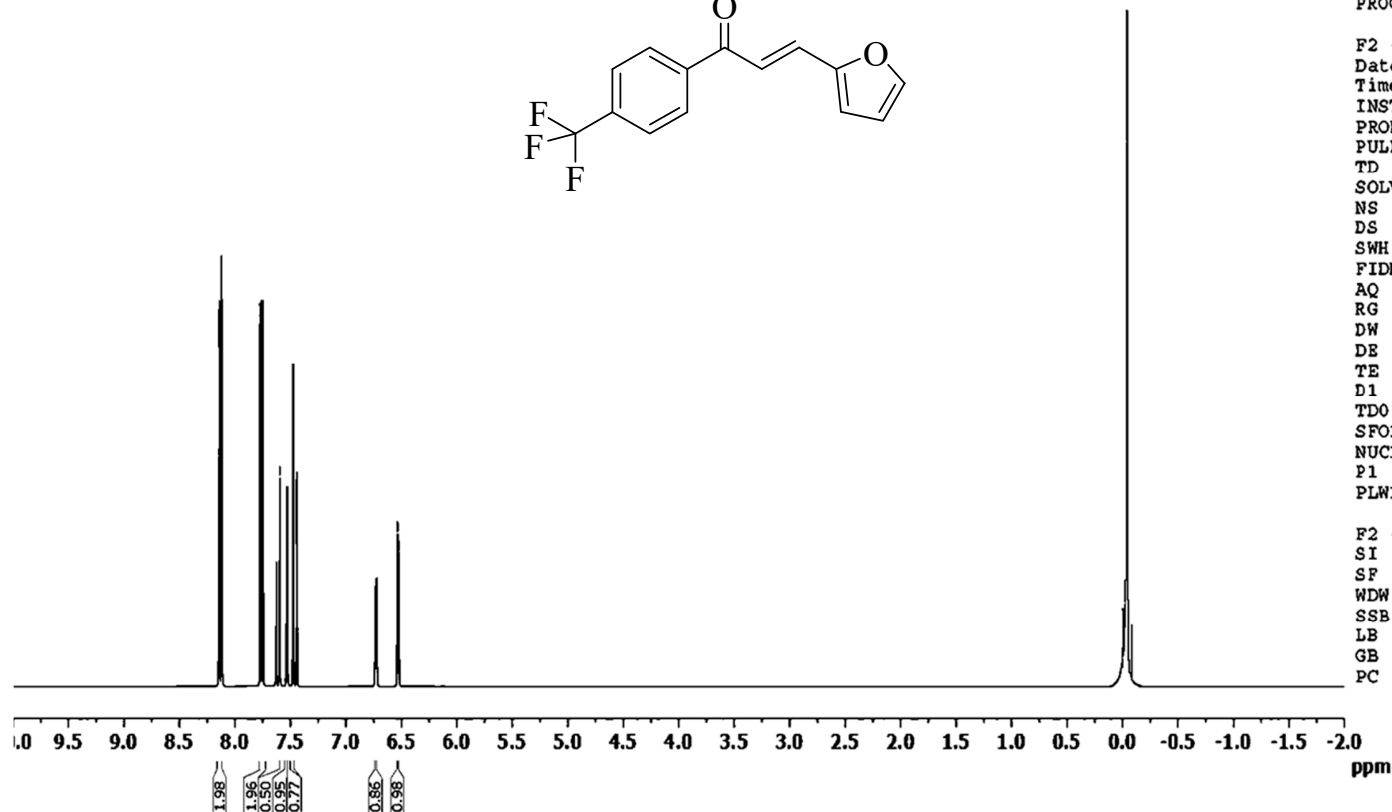
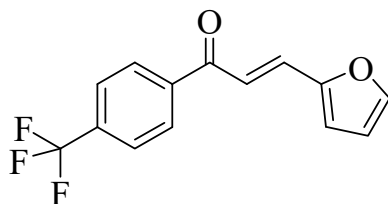
A7 LIQUID

8/9/2018

FT-IR Spectrum of (*E*)-3-(furan-2''-yl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A7)

A7

8.1411
8.1385
8.1224
8.1195
8.1162
7.7705
7.7676
7.7514
7.7489
7.5957
7.5328
7.5299
7.5270
7.4742
7.4424
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6.7231
6.5359
6.5337
6.5261
6.5235



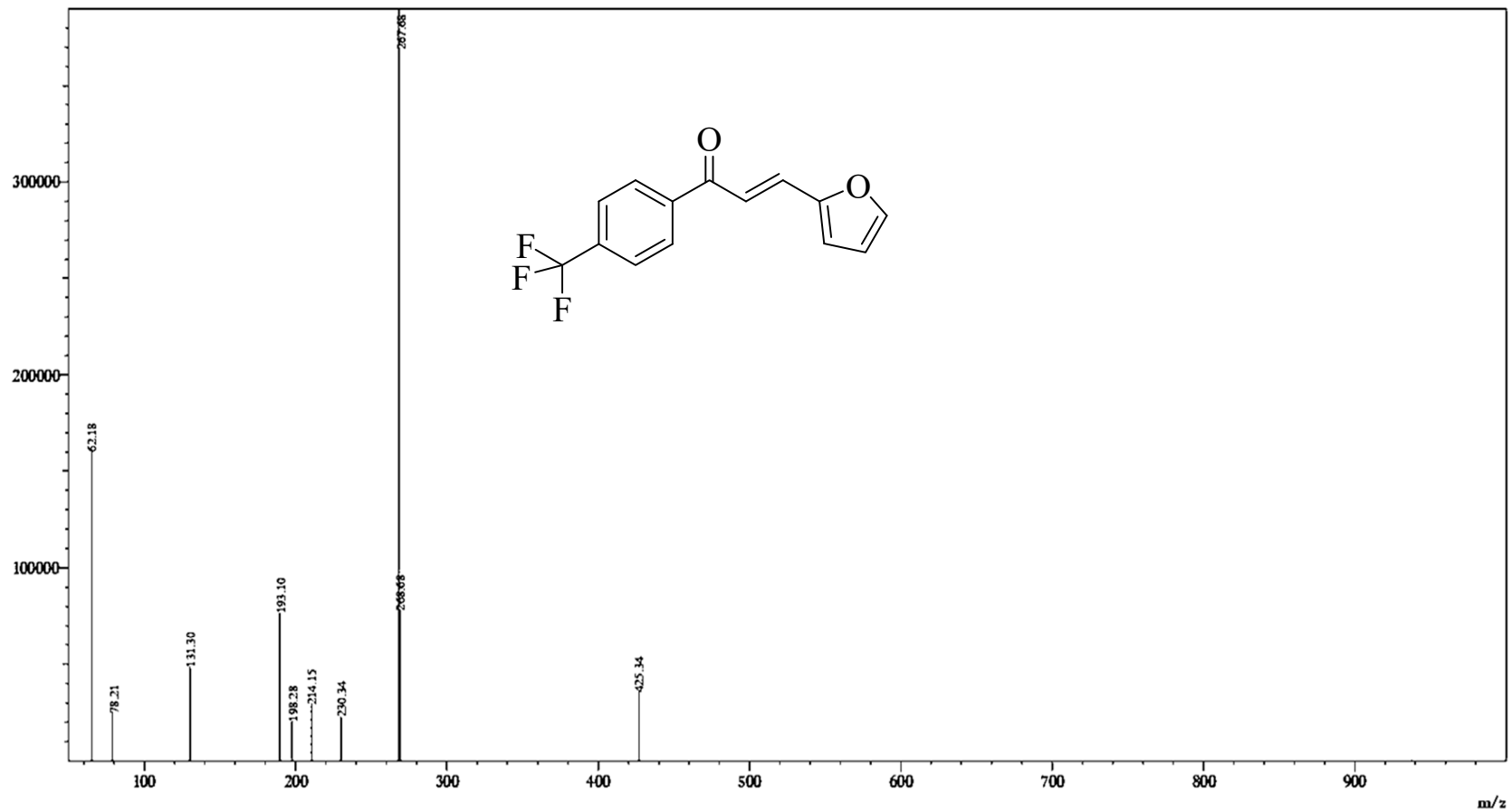
Current Data Parameters
NAME 03042019
EXPNO 7
PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 132.41
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1
SFO1 400.1324708 MHz
NUC1 1H
P1 15.00 usec
PLW1 9.91339970 W

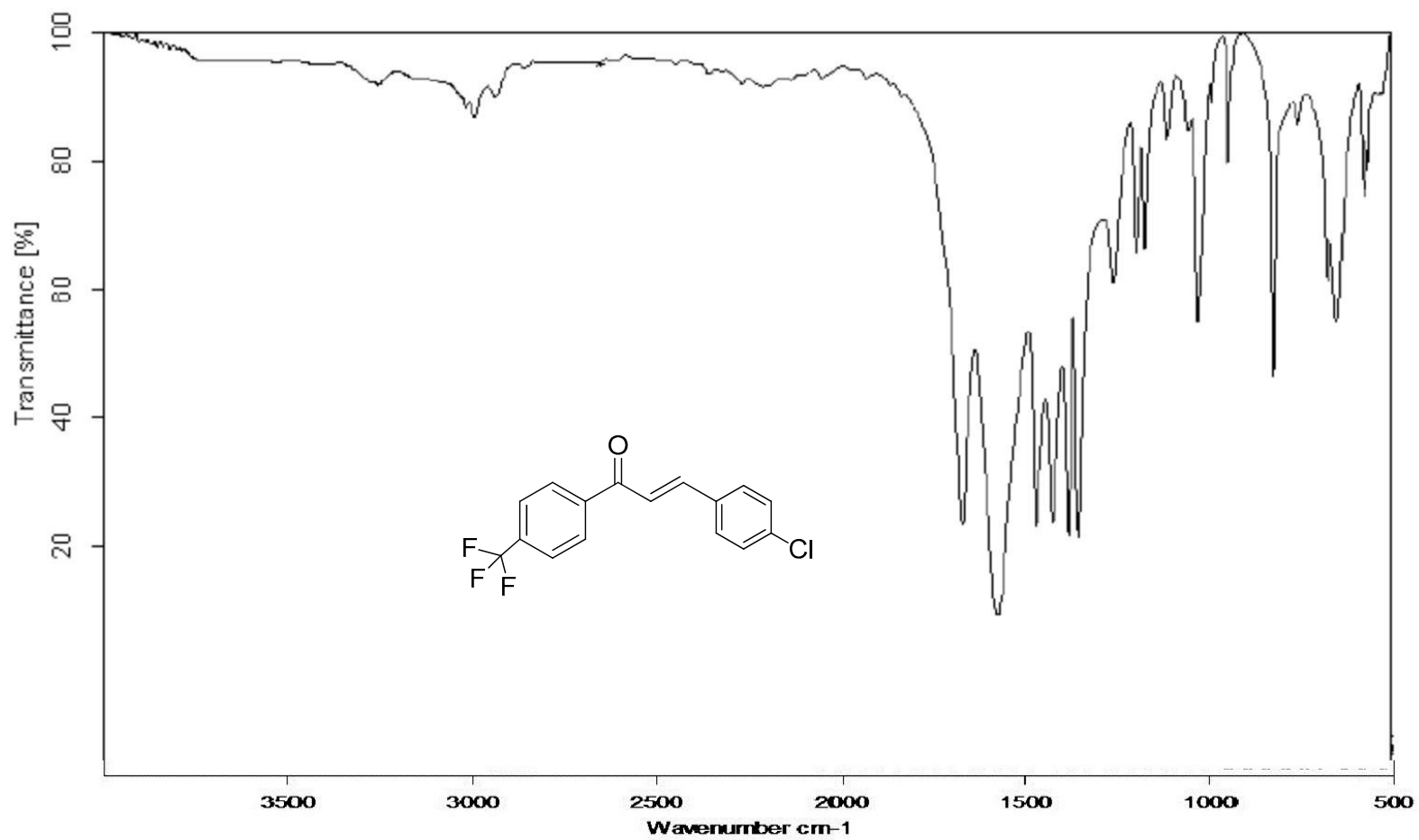
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
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¹H NMR Spectrum of (*E*)-3-(furan-2'-yl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A7)

Averaged ESI Positive
Spectrum Mode: Averaged 0.183-0.605(74-243)
[CPS]



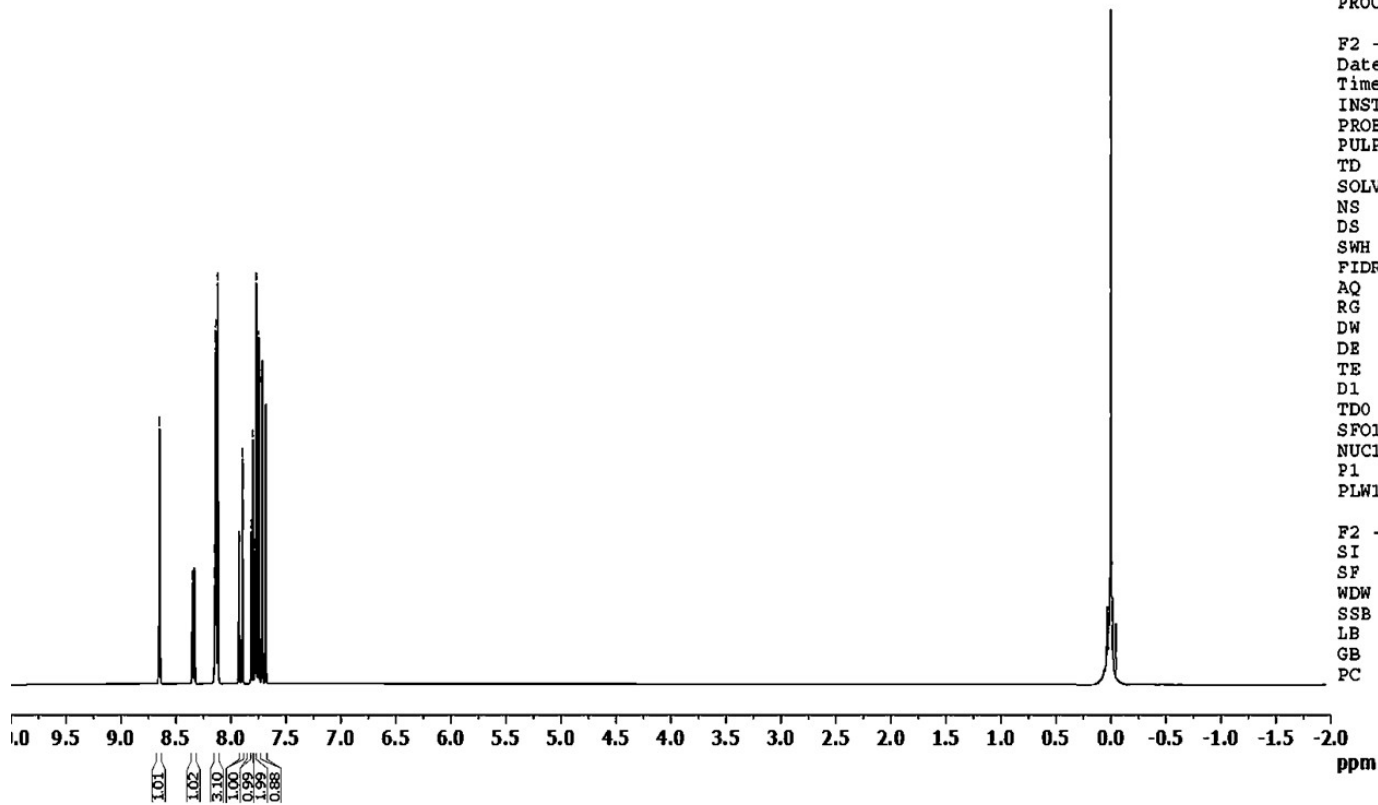
MASS Spectrum of (*E*)-3-(furan-2''-yl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A7)



FT-IR Spectrum of (*E*)-3-(4'-chlorophenyl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A8)

A8

8.638
8.650
8.646
8.317
8.349
8.347
8.345
8.348
8.326
8.330
8.386
8.121
8.150
8.148
8.146
8.144
8.141
8.138
8.135
8.139
8.134
8.132
8.130
8.128
8.124
8.119
8.116
7.927
7.926
7.896
7.895
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7.799
7.783
7.773
7.770
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7.751
7.748
7.745
7.714
7.689



Current Data Parameters
NAME 05042019
EXPNO 1
PROCNO 1

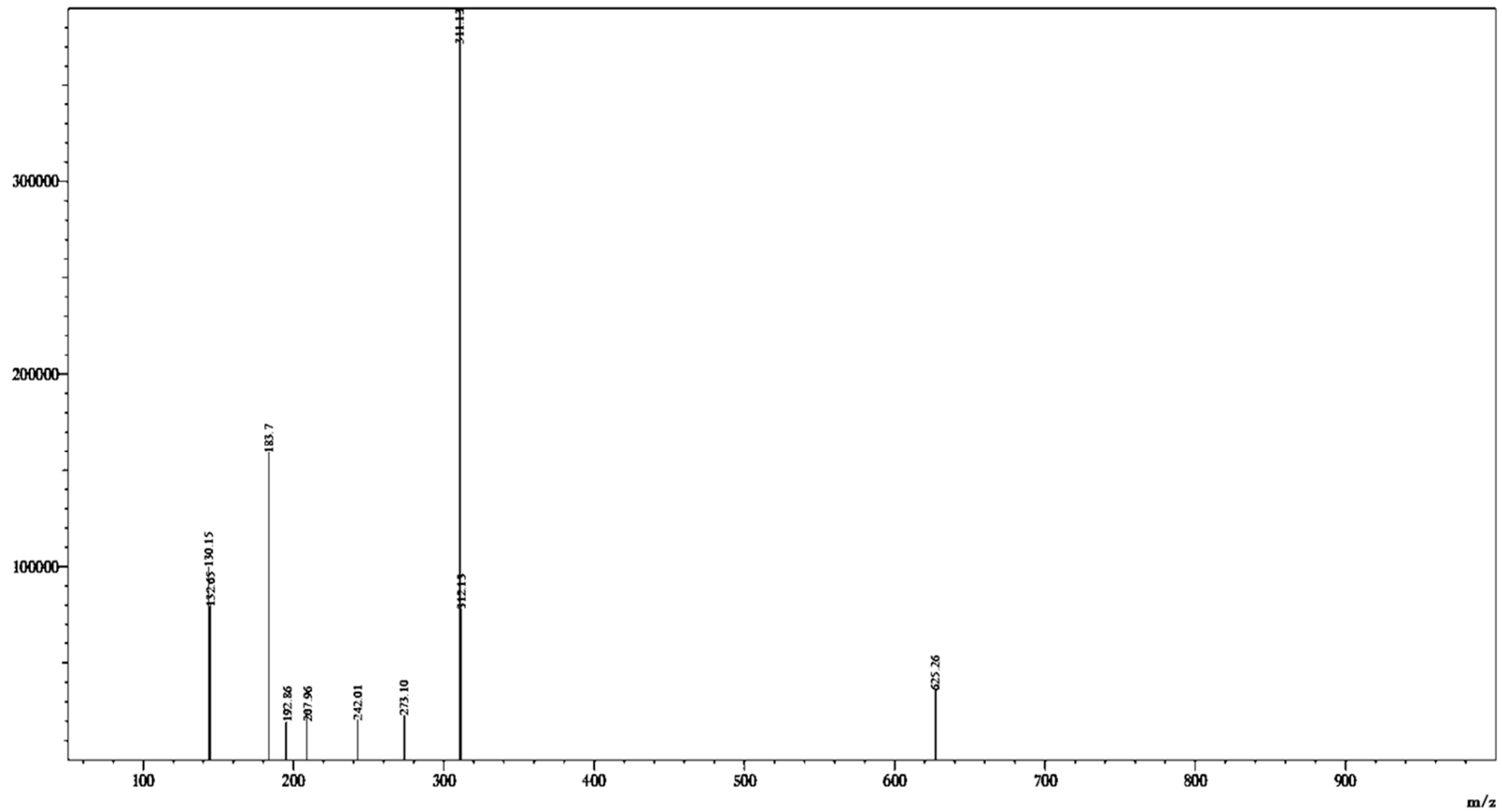
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PROBHD Z108618_0646 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 132.41
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1
SFO1 400.1324708 MHz
NUC1 1H
P1 15.00 usec
PLW1 9.91339970 W

F2 - Processing parameters
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SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

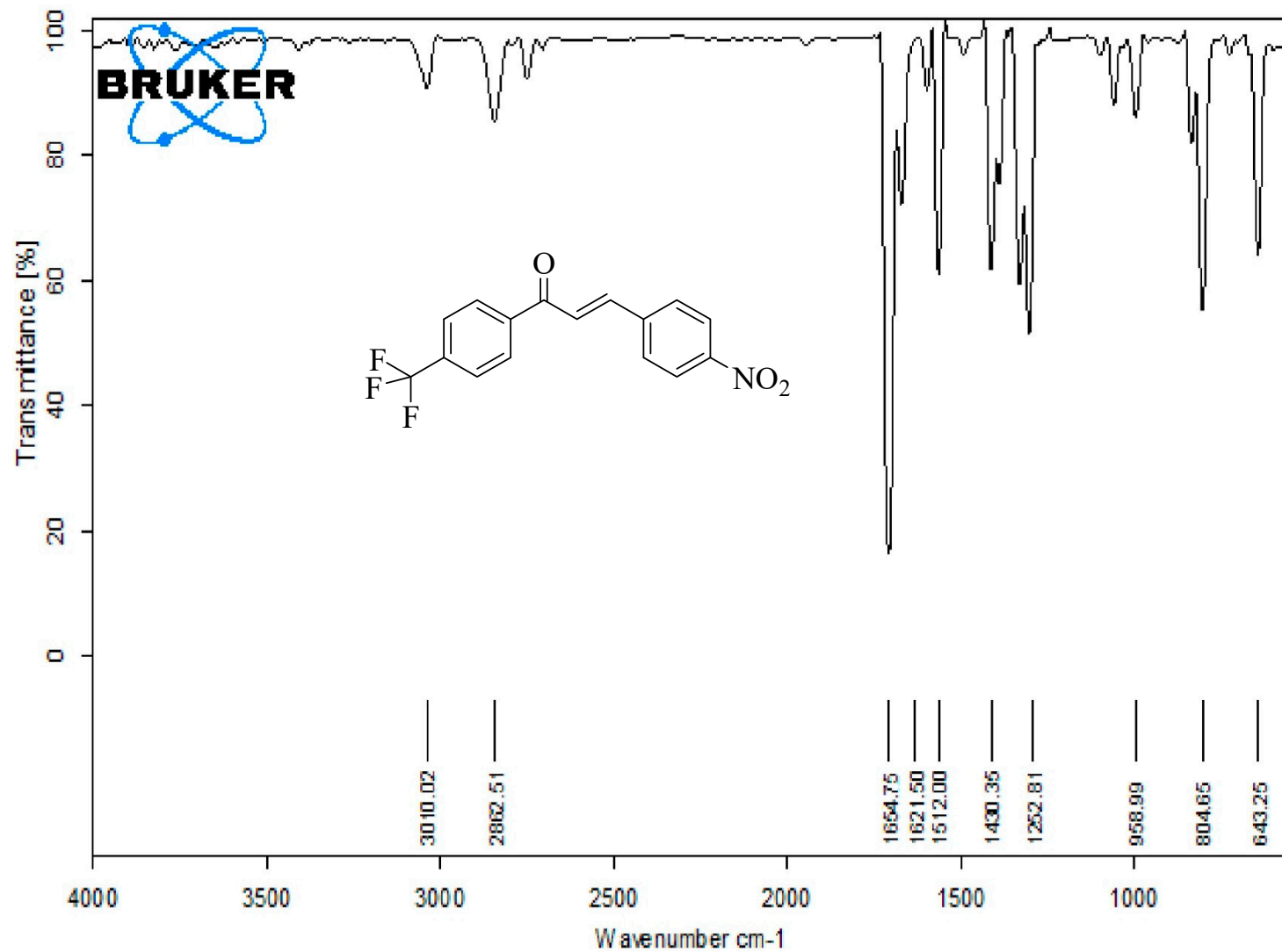
¹H NMR Spectrum of (*E*)-3-(4'-chlorophenyl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A8)

Averaged ESI Positive+
Spectrum Mode: Averaged 0.183-0.605(74-243)
[CPS]

MS Spectrum
D:\DATA\JULY-19\16072019.0.kcd



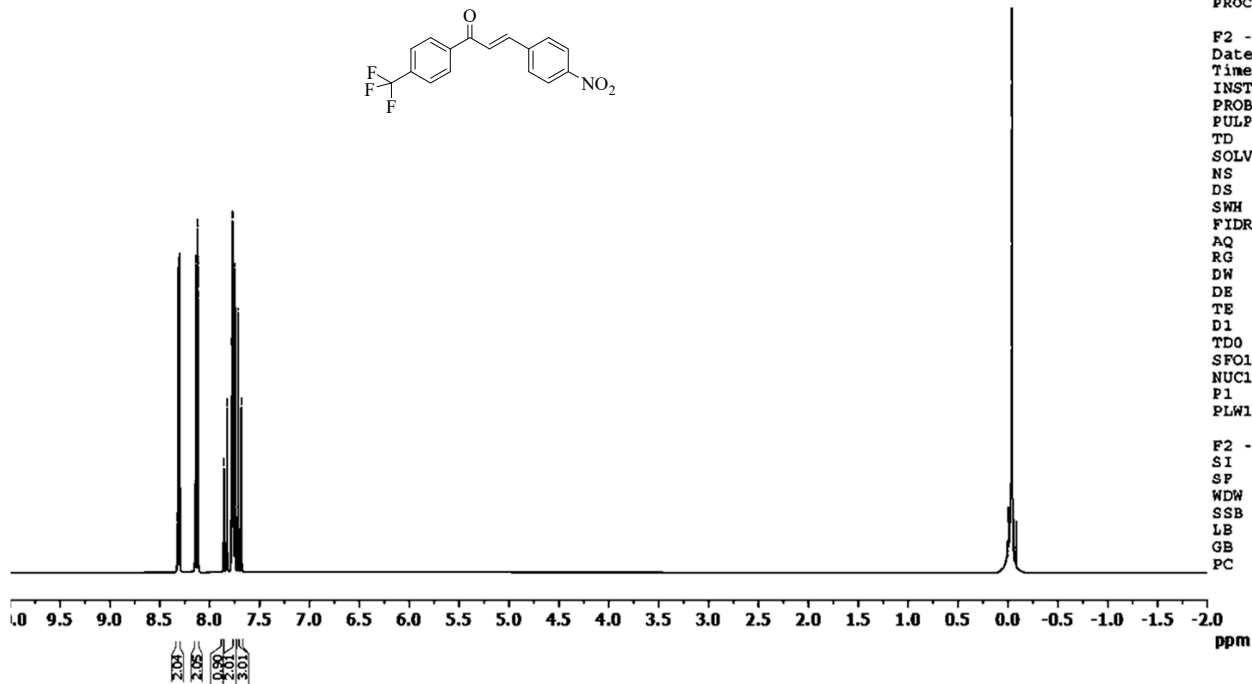
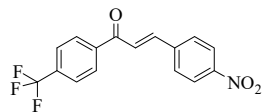
Mass Spectrum of (*E*)-3-(4'-chlorophenyl)-1-[4'-(trifluoromethyl)phenyl]prop-2-en-1-one (A8)



FI-IR Spectrum of 1-(4-(trifluoromethyl)phenyl)-3-(4-nitrophenyl)prop-2-en-1-one (A9)

A5

8.3220
8.3187
8.3162
8.3044
8.3016
8.2982
8.1444
8.1411
8.1385
8.1224
8.1195
8.1162
7.8595
7.8576
7.8276
7.8258
7.7821
7.7789
7.7775
7.7743
7.7705
7.7675
7.7645
7.7620
7.7606
7.7573
7.7514
7.7489
7.7456
7.7141
7.6822



Current Data Parameters
NAME 03042019
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
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PROBHD Z108618_0646 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 132.41
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1
SFO1 400.1324708 MHz
NUC1 1H
P1 15.00 usec
PLW1 9.91339970 W

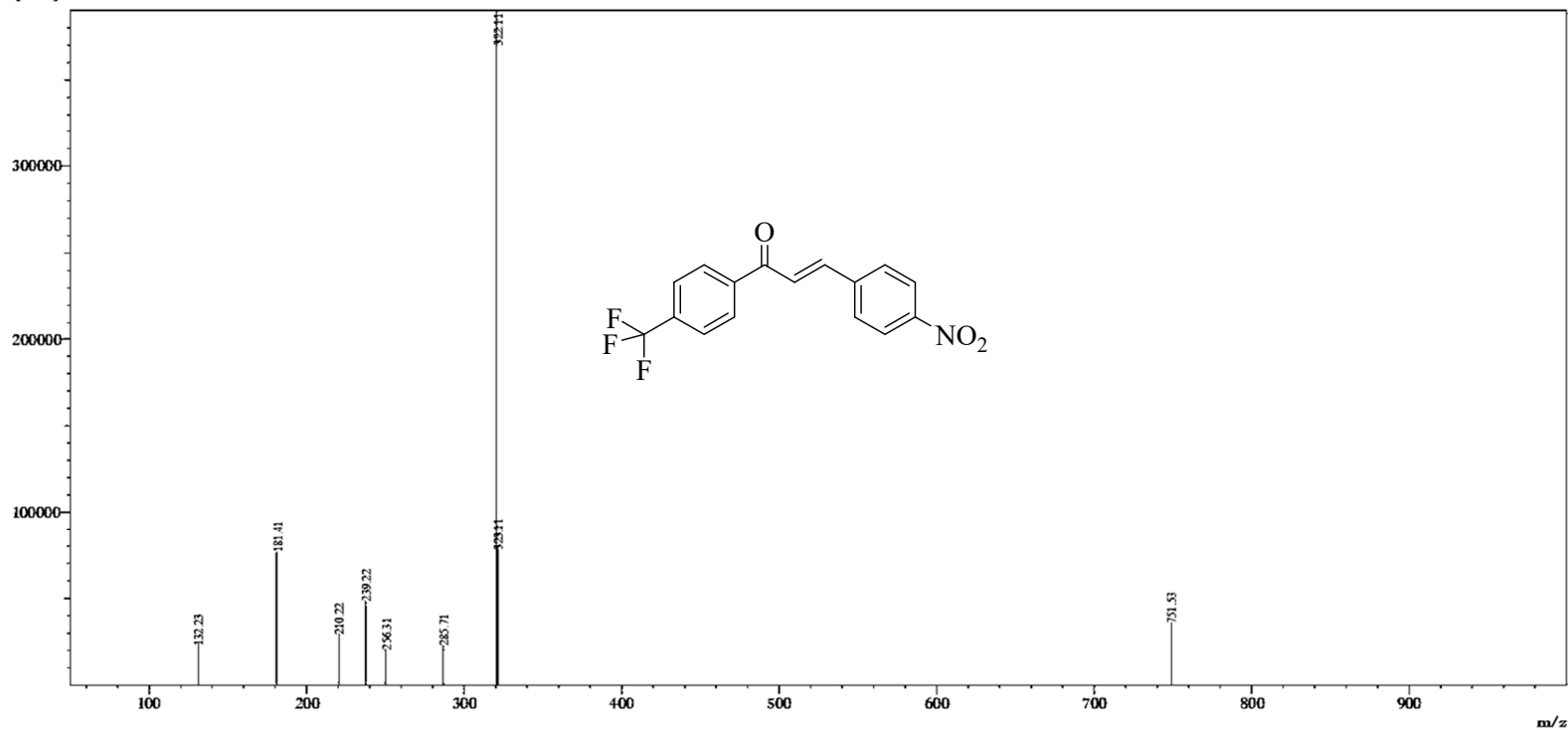
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1H NMR Spectrum of 1-(4-(trifluoromethyl)phenyl)-3-(4-nitrophenyl)prop-2-en-1-one (A9)

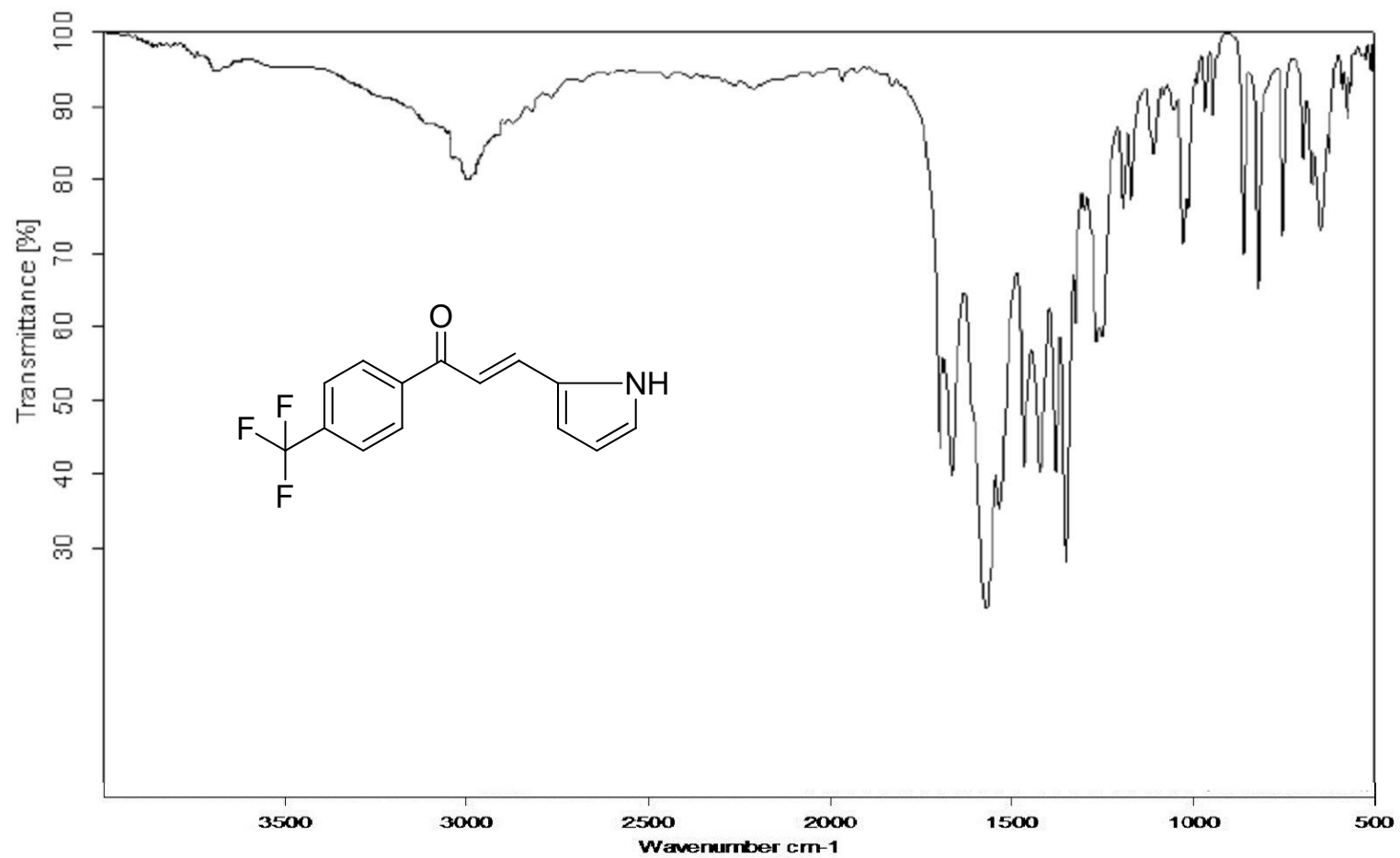
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Data File : 16072019.4.lcd
Date Acquired : 7/16/2019 10:30:43 AM
Batch File : 16072019.1cb

MS Spectrum
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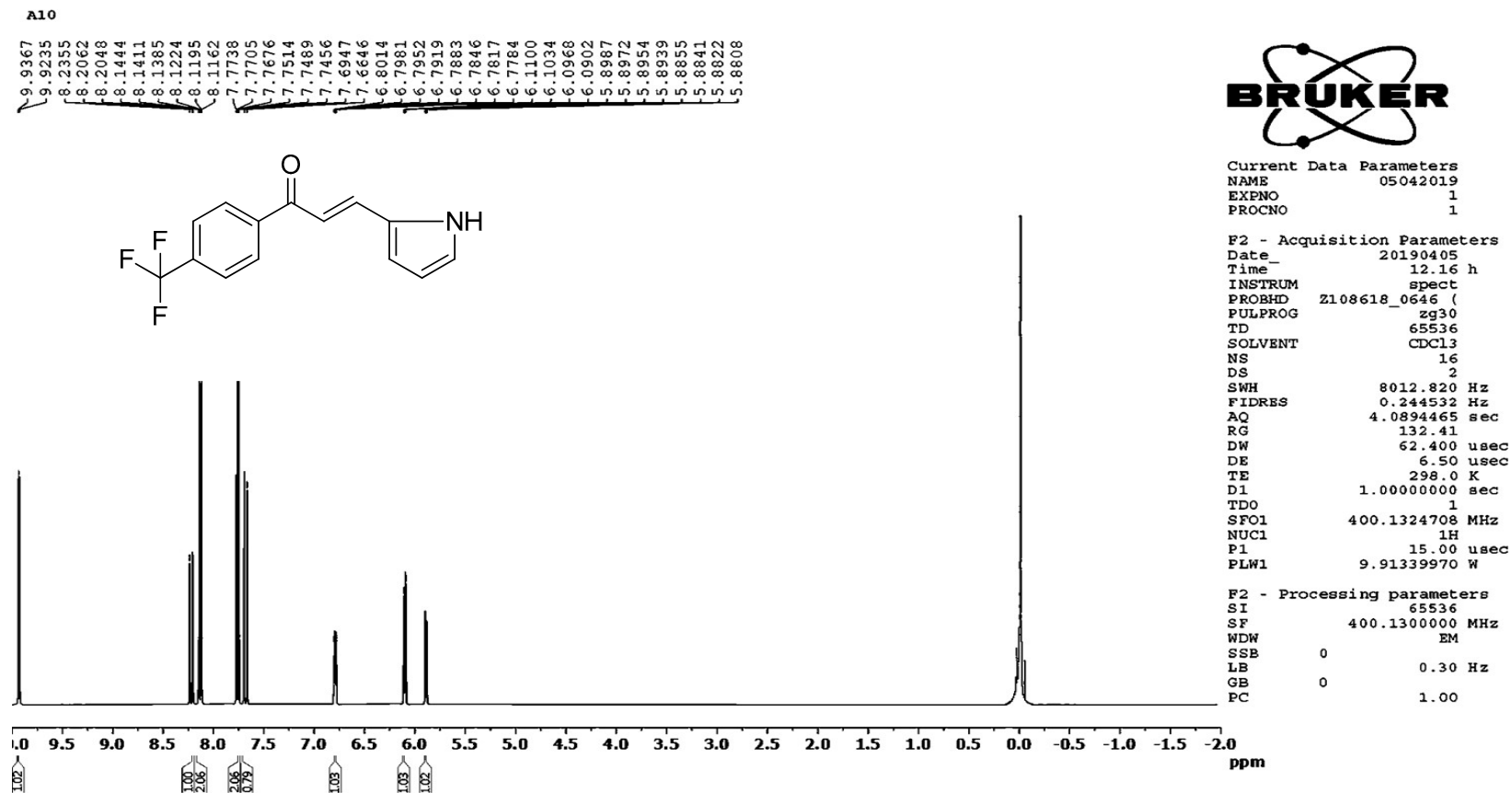
Averaged ESI Positive+
Spectrum Mode: Averaged 0.183-0.605(74-243)
[CPS]



Mass Spectrum of 1-(4-(trifluoromethyl)phenyl)-3-(4-nitrophenyl)prop-2-en-1-one (A9)

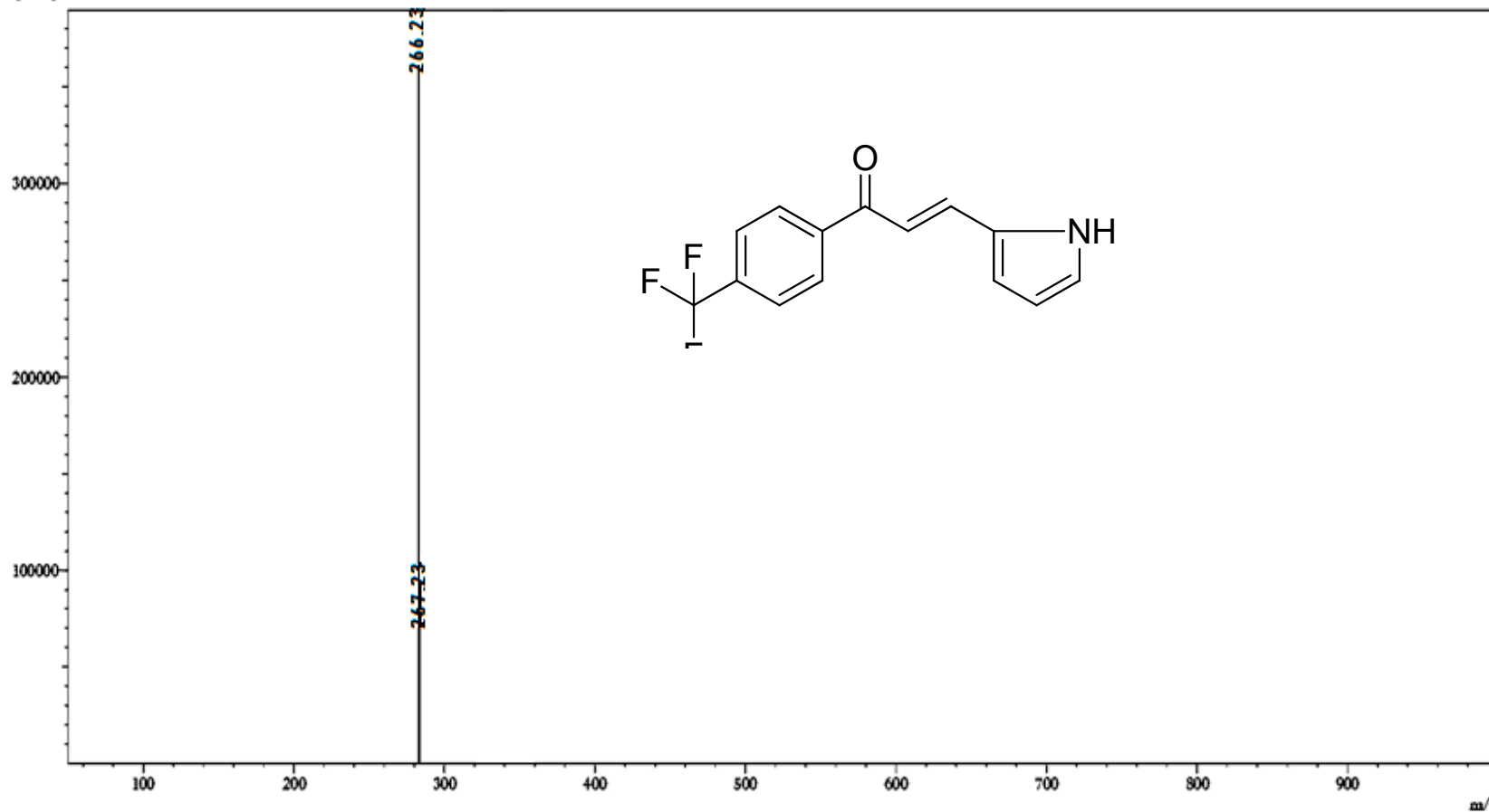


FT-IR Spectrum of (E)-3-(1H-pyrrol-2-yl)-1-(4-(trifluoromethyl)phenyl)prop-2-en-1-one (A10)

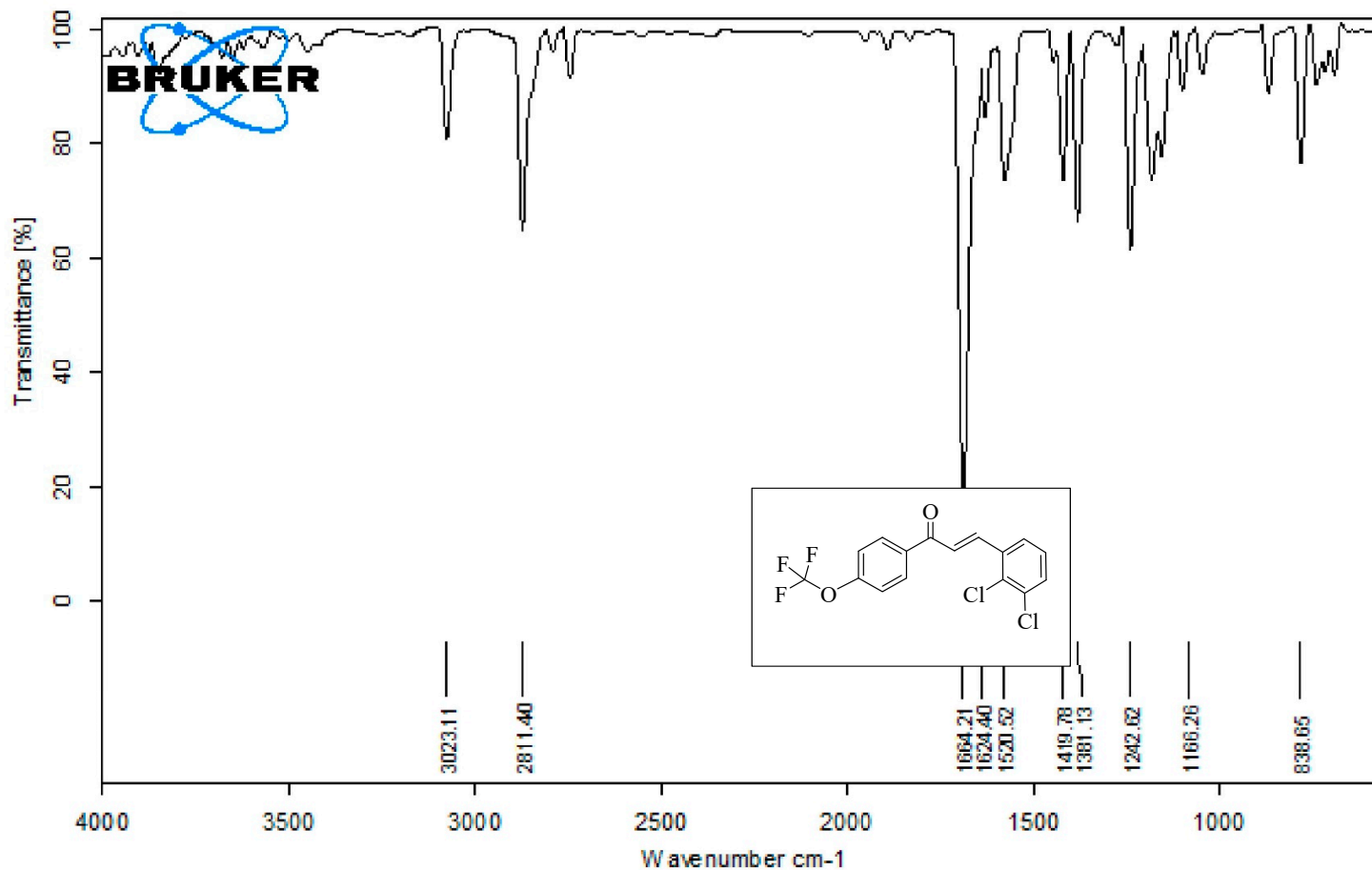


1H NMR Spectrum of (E)-3-(1H-pyrrol-2-yl)-1-(4-(trifluoromethyl)phenyl)prop-2-en-1-one (A10)

AveragedESI Positive
Spectrum Mode:Averaged 0.183-0.605(74-243)
[CPS]



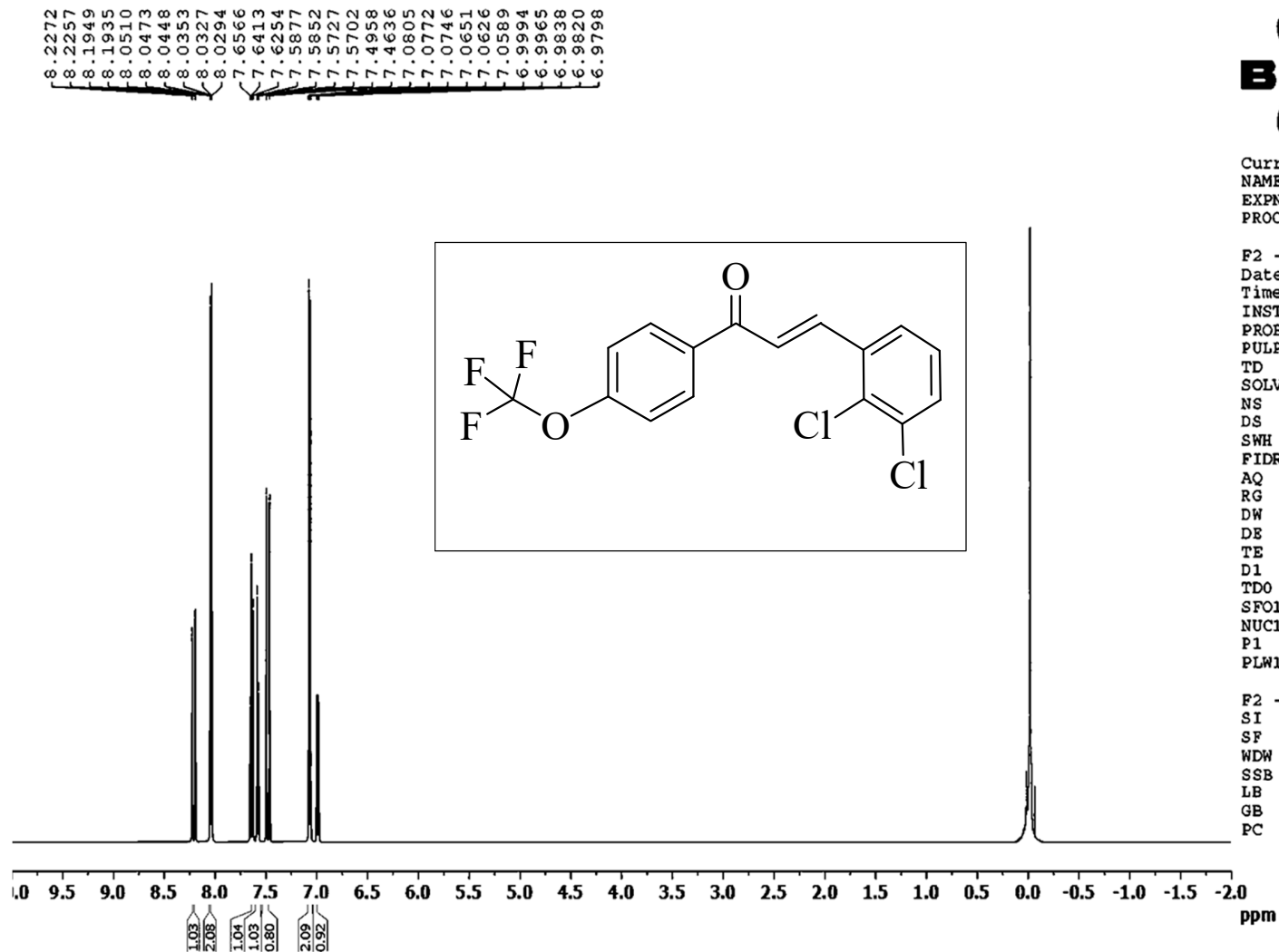
Mass Spectrum of (E)-3-(1H-pyrrol-2-yl)-1-(4-(trifluoromethyl)phenyl)prop-2-en-1-one (A10)



C:\Users\Lerov\Documents\Bruker\OPUS_7.8.44188	E1	SOLID	22-11-2019
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FT-IR Spectrum of (E)-3-(2'',3''-dichlorophenyl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B1)

B1



Current Data Parameters
NAME 03042019
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190403
Time 12.12 h
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 132.41
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1
SFO1 400.1324708 MHz
NUC1 1H
P1 15.00 usec
PLW1 9.91339970 W

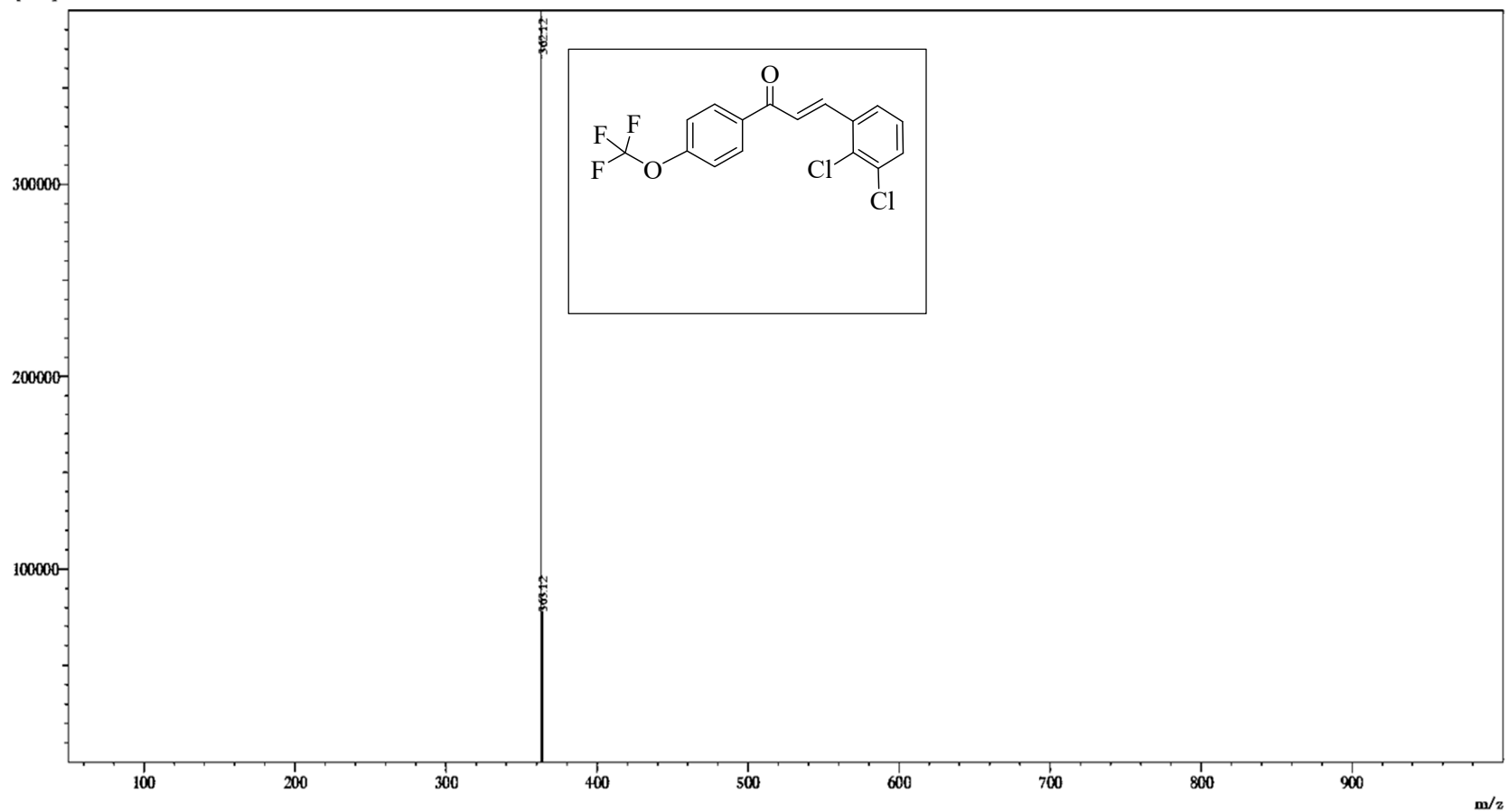
F2 - Processing parameters
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SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR Spectrum of 3-(2'',3''-dichlorophenyl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B1)

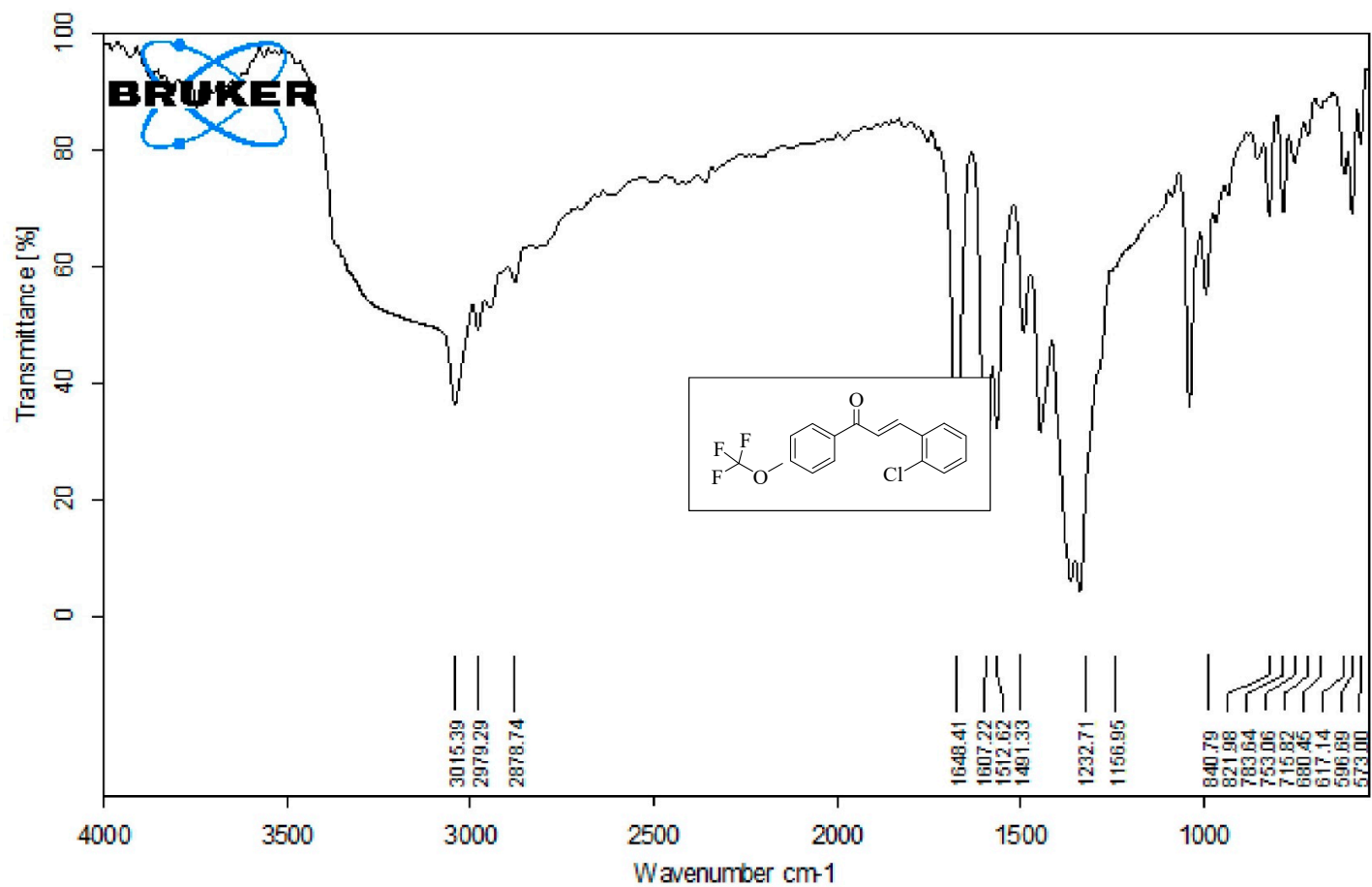
Sample Name : KSB-B1-361
Data File : 16072019.8.lcd
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Batch File : 16072019.1cb

MS Spectrum
D:\DATA\JULY-19\16072019.8.lcd

Averaged ESI Positive
Spectrum Mode: Averaged 0.183-0.605(74-243)
[CPS]



MASS Spectrum of 3-(2'',3''-dichlorophenyl)-1-[4''-(trifluoromethoxy)phenyl]prop-2-en-1-one (B1)



D:\FTIR DATA\2019 JAN\S URENDRA.2	B2	SOLID	1/22/2019
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FT-IR Spectrum of 3-(2'-chlorophenyl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B2)

B2

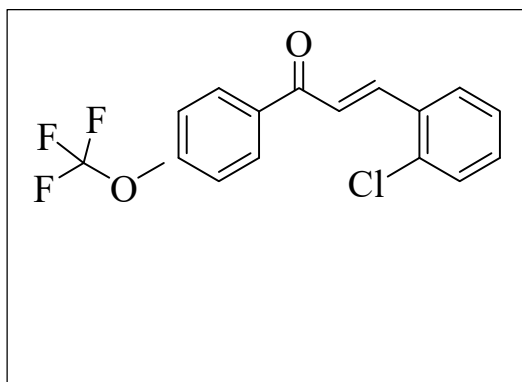
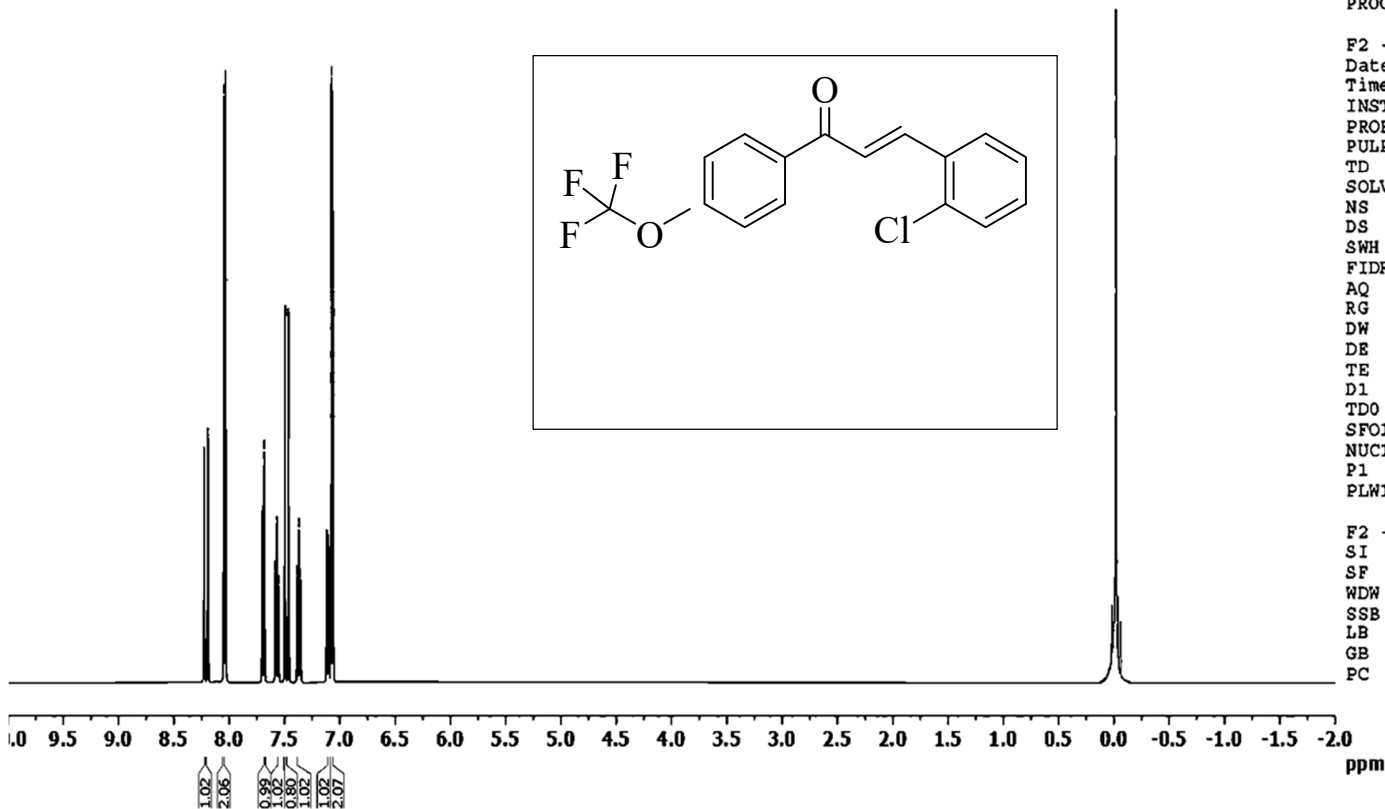
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8.1949
8.1935
8.0510
8.0473
8.0448
8.0353
8.0327
8.0294
7.7001
7.6971
7.6840
7.6810
7.5863
7.5833
7.5723
7.5692
7.5672
7.5562
7.5530
7.4958
7.4636
7.3863
7.3834
7.3720
7.3706
7.3691
7.3677
7.3566
7.3536
7.1197
7.1183
7.1167
7.1154
7.1043
7.1028
7.1010
7.0998
7.0805
7.0772
7.0746
7.0651
7.0626
7.0589



Current Data Parameters
NAME 03042019
EXPNO 9
PROCNO 1

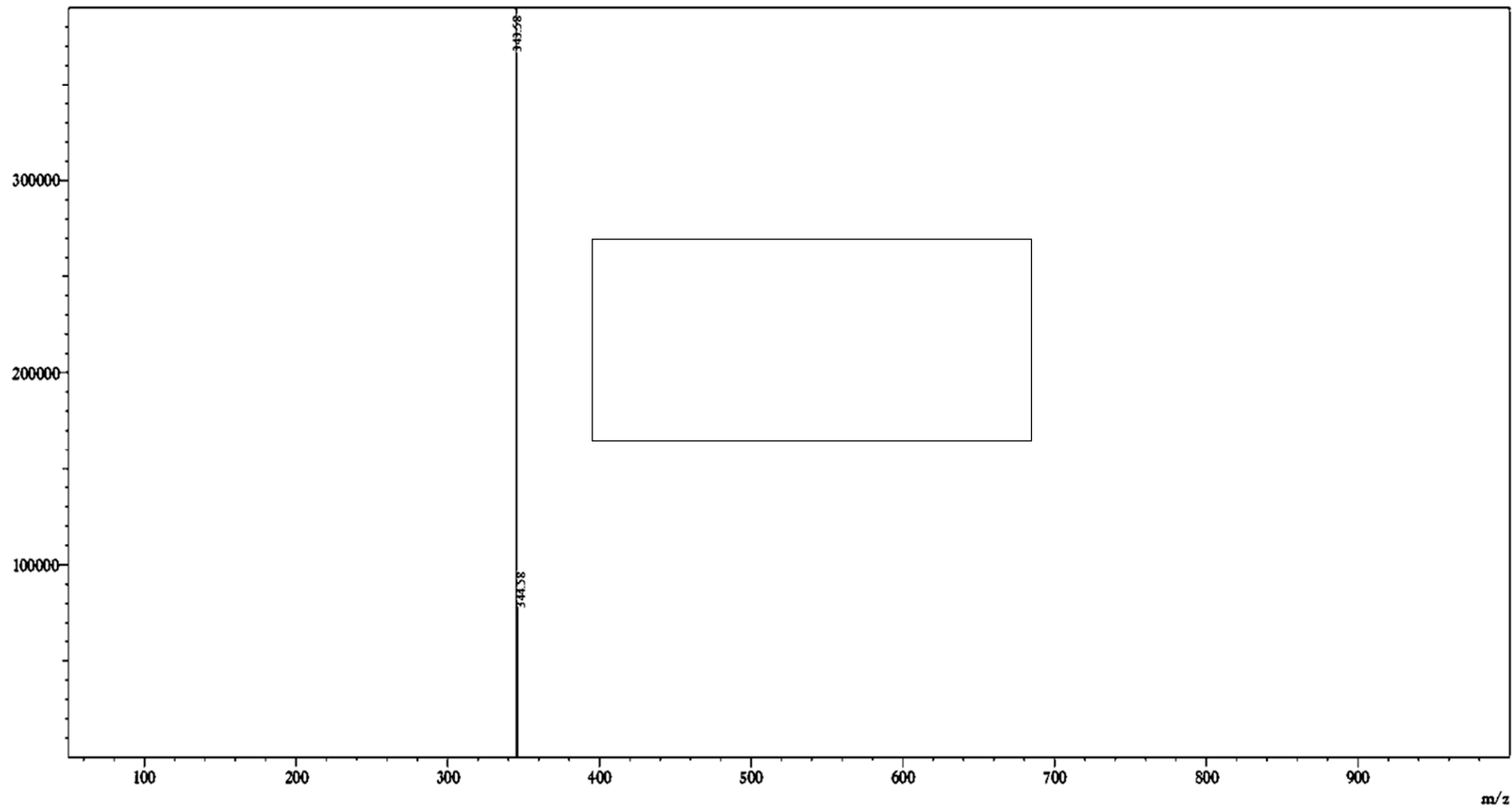
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TD 65536
SOLVENT CDCl3
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DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 132.41
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 15.00 usec
PLW1 9.91339970 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

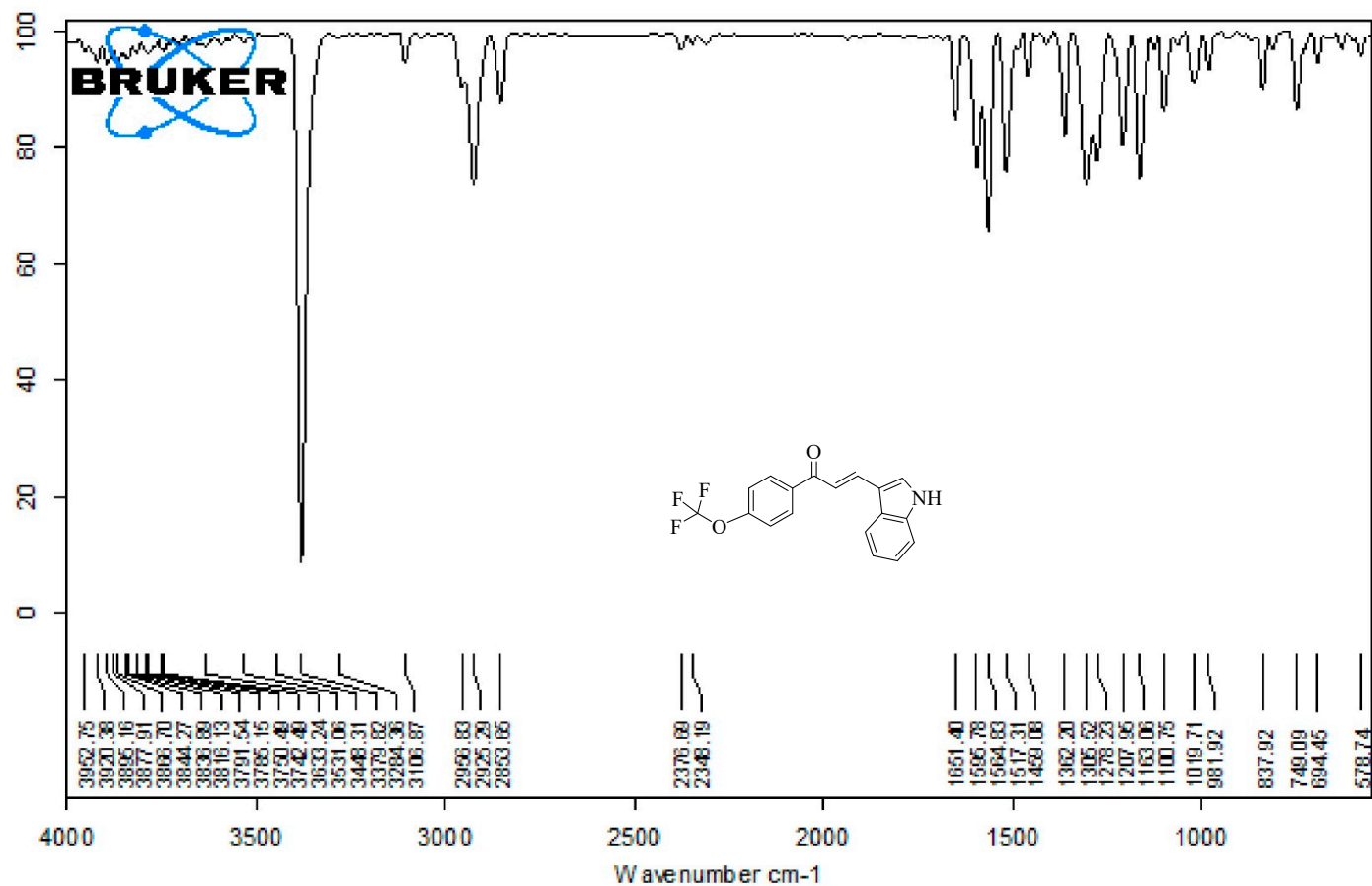


¹H NMR Spectrum of 3-(2''-chlorophenyl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B2)

Averaged ESI Positive+
Spectrum Mode: Averaged 0.183-0.605(74-243)
[CPS]



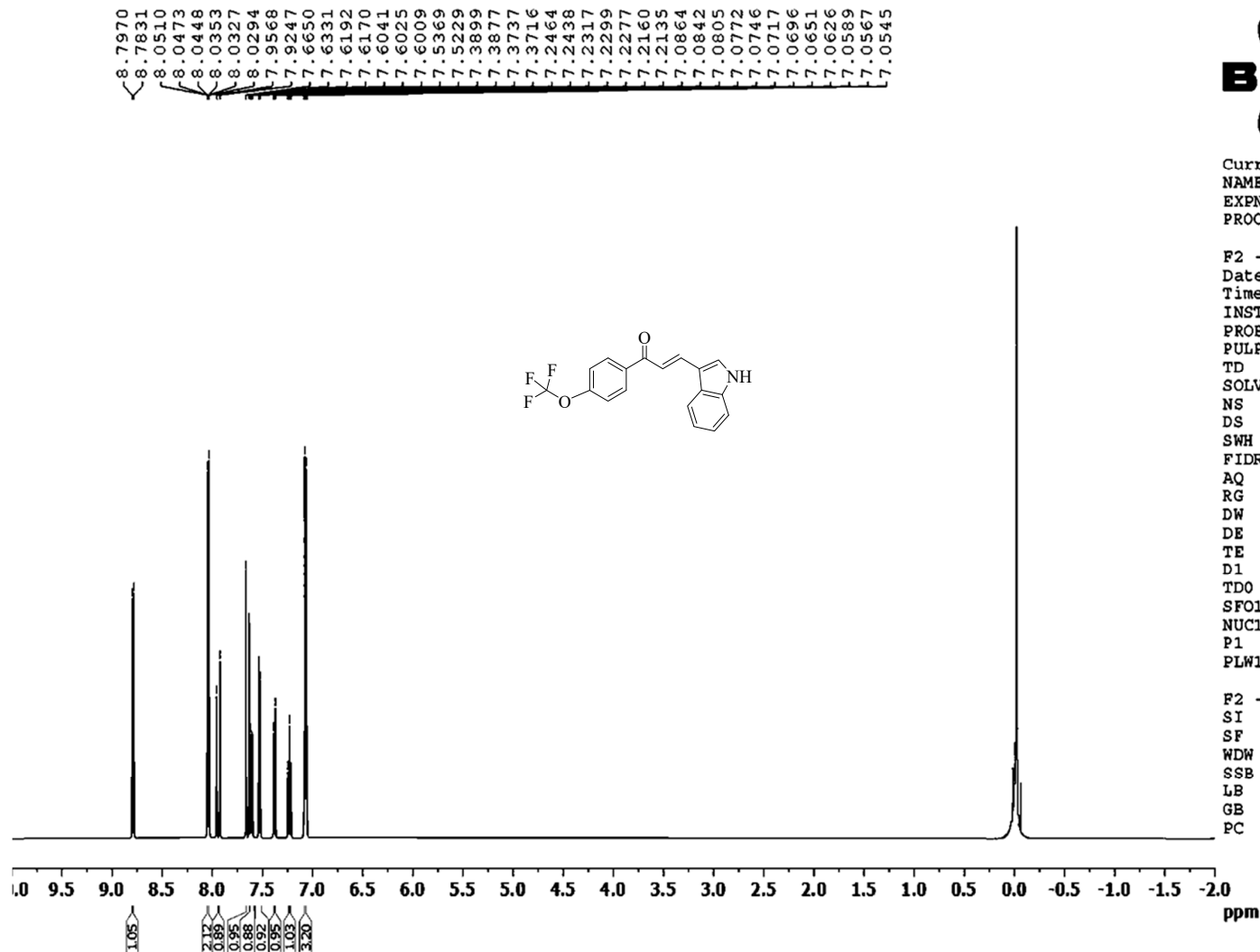
MASS Spectrum of 3-(2''-chlorophenyl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B2)



C:\Users\Lenovo\Documents\Bruker\OPUS_7.8.44\DATA\MEAS\ANURADHA.52	B3	SOLID	19-09-2019
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FT- IR Spectrum of (E)-3-(1''H-indol-3''-yl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B3)

B3



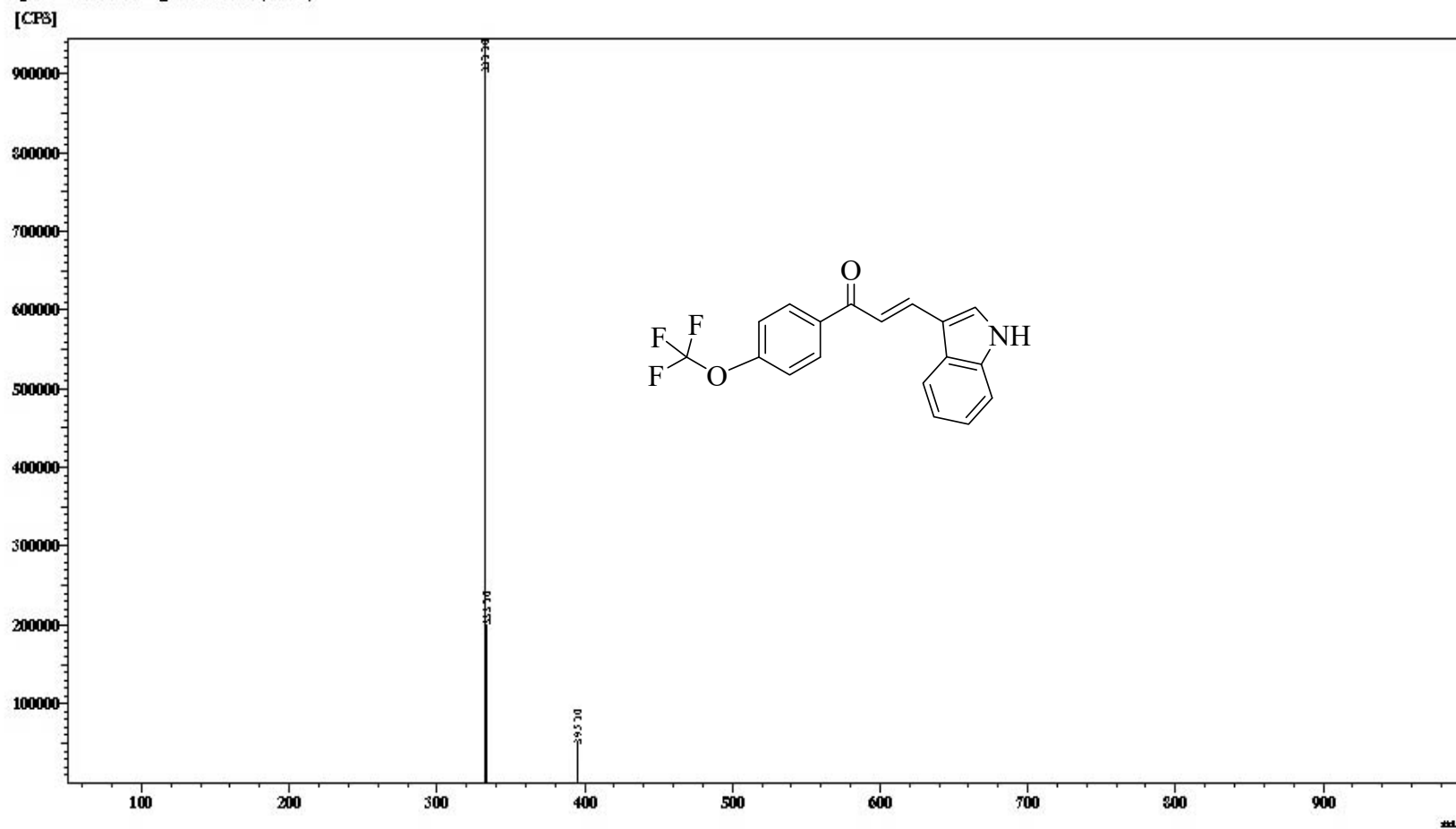
Current Data Parameters
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 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 132.41
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1
 SFO1 400.1324708 MHz
 NUCL 1H
 P1 15.00 usec
 PLW1 9.91339970 W

F2 - Processing parameters
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 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

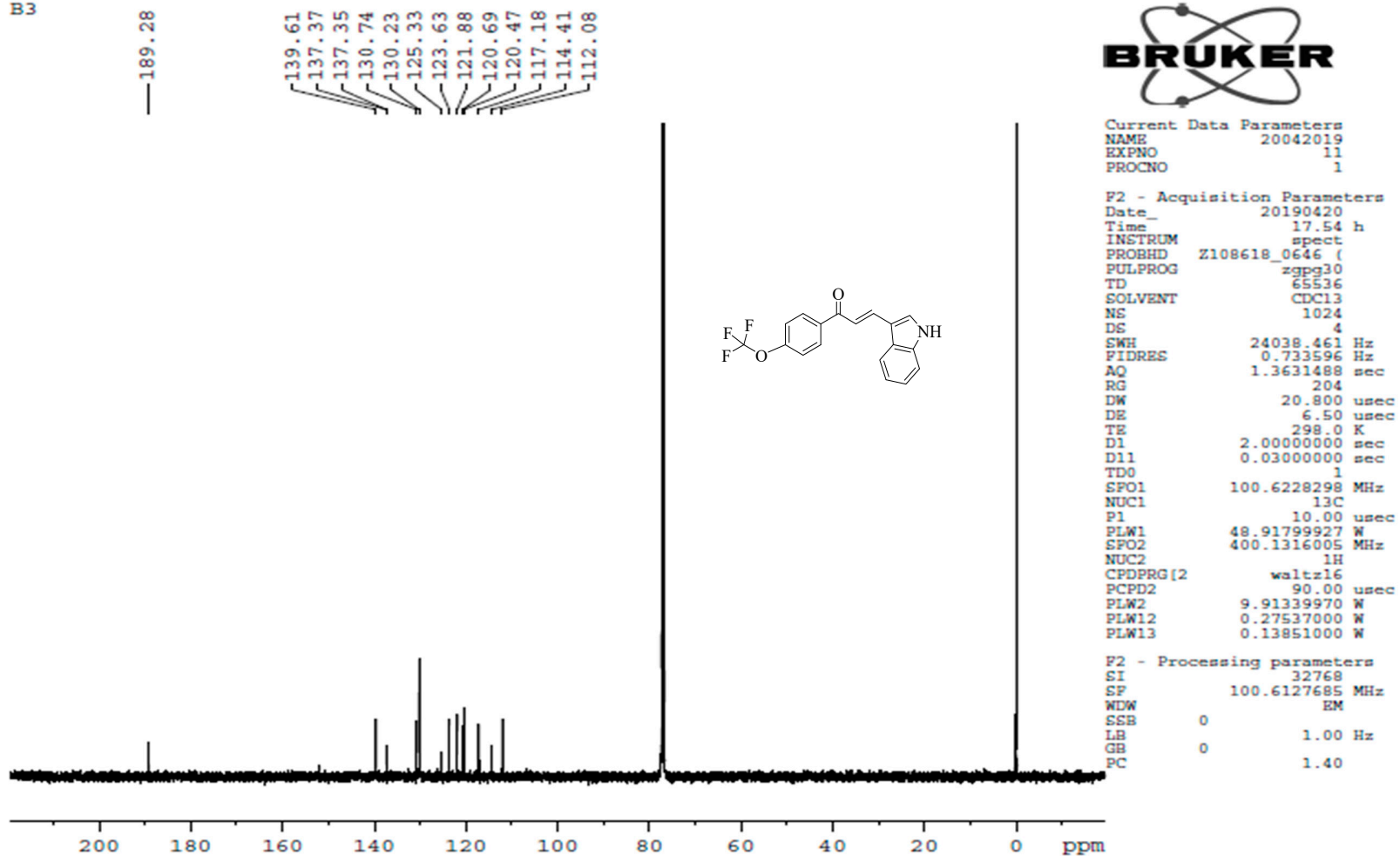
¹H NMR Spectrum of (E)-3-(1''H-indol-3''-yl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B3)

Average dEESI Positive+
Spectrum Model Averaged 0.163-0.553(66-224)



MASS Spectrum of (E)-3-(1''H-indol-3''-yl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B3)

B3



¹³C NMR Spectrum of (E)-3-(1''H-indol-3''-yl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B3)

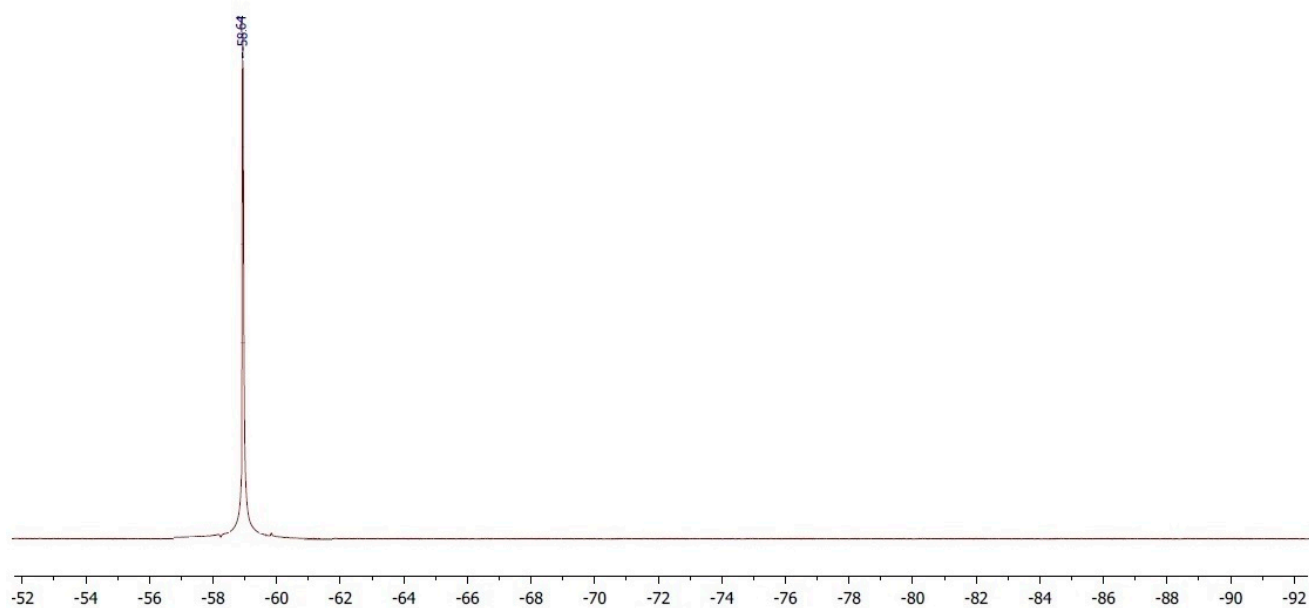
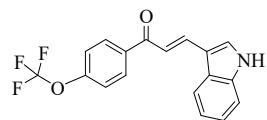
FB3



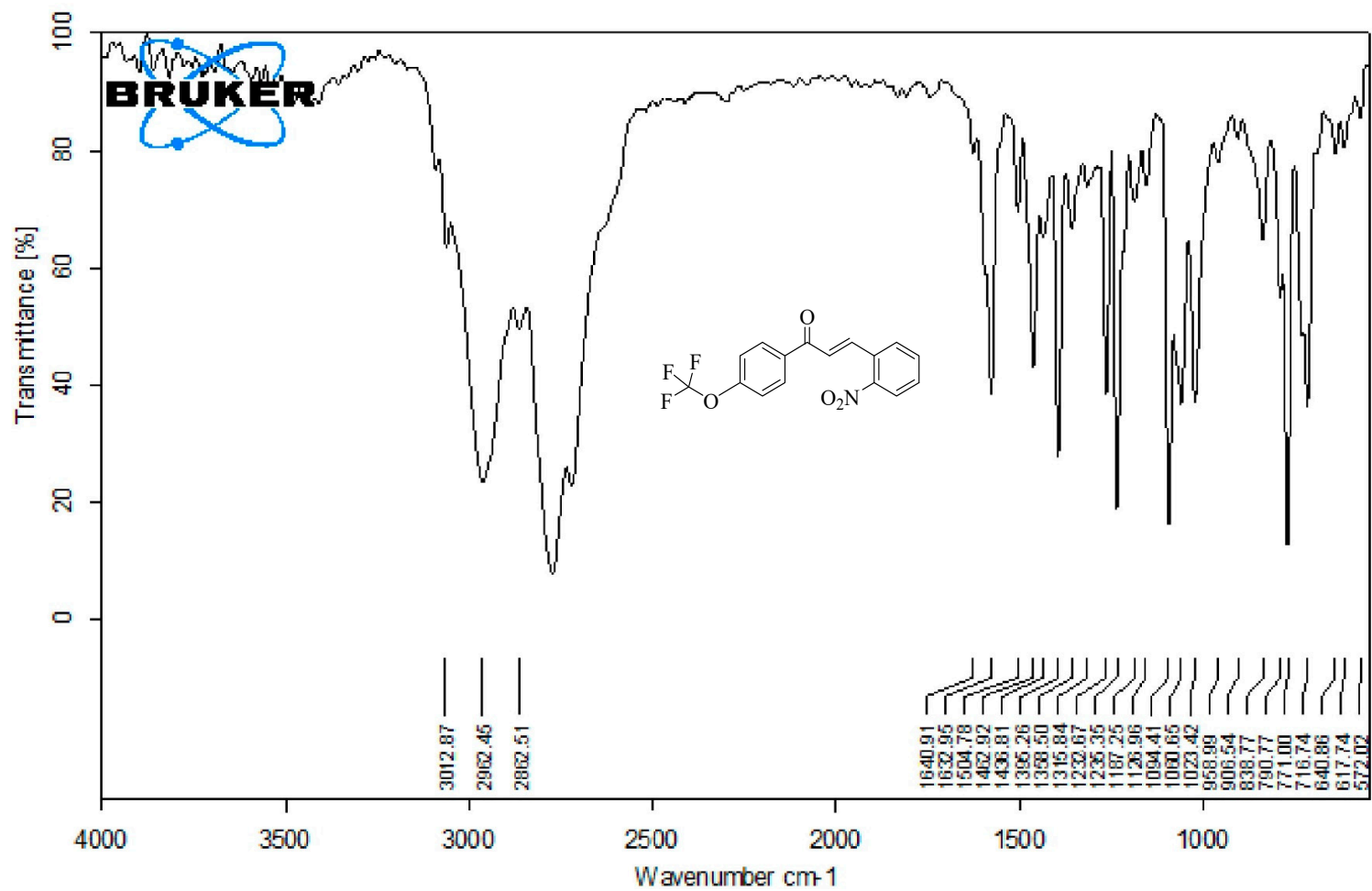
Current Data Parameters
NAME 24042019
EXPNO 1
PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
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DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 132.41
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1
SFO1 376.1524708 MHz
NUC1 1H
P1 15.00 usec
PLW1 9.91339970 W

F2 - Processing parameters
SI 65536
SF 376.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



¹⁰F Spectrum of (E)-3-(1''H-indol-3''-yl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B3)



D:\FTIR DATA\2019 JAN\SURENDRA.29	B4	SOLID	1/23/2019
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FT-IR Spectrum of (E)- 1-(4-(trifluoromethoxy)phenyl)-3-(2-nitrophenyl)prop-2-en-1-one (B4)

B4

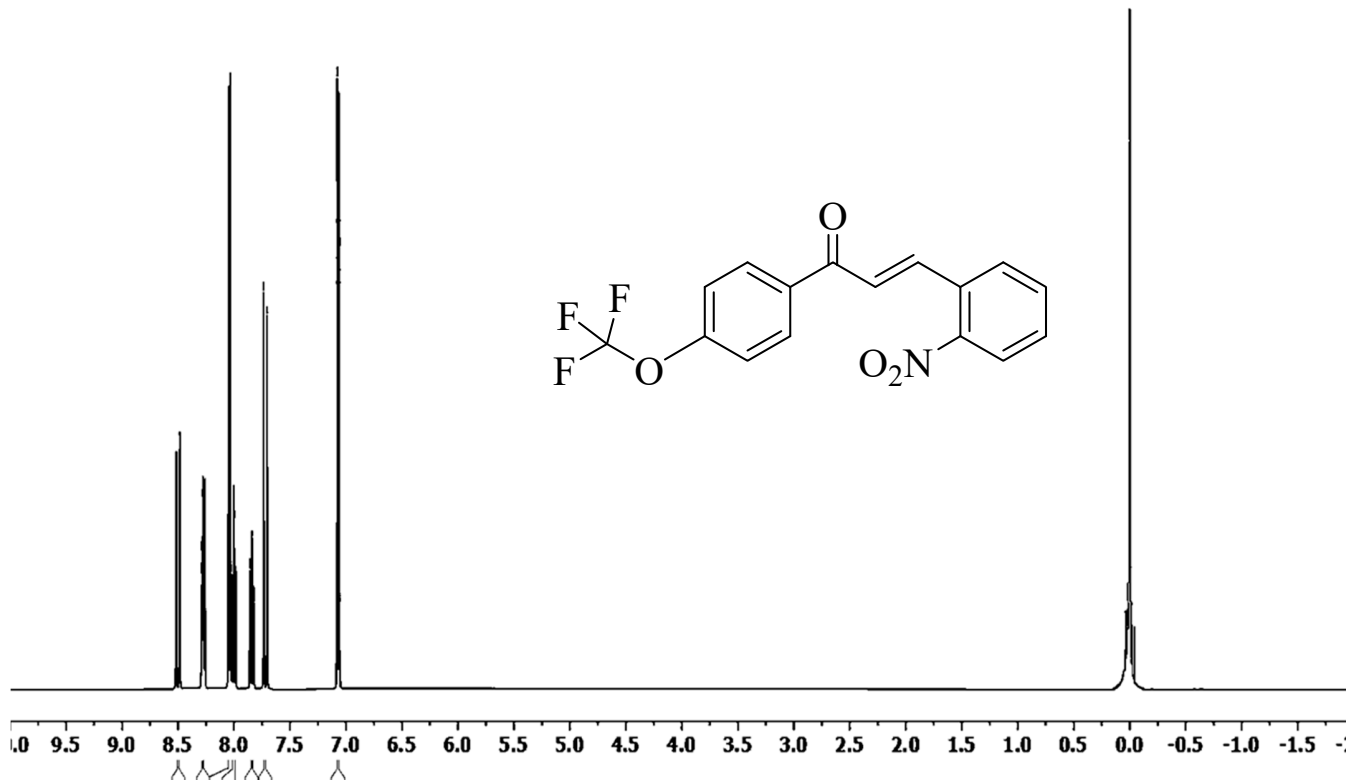
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8.2736
8.2718
8.2705
8.2630
8.2602
8.0510
8.0473
8.0448
8.0353
8.0327
8.0294
8.0169
8.0140
8.0017
7.9986
7.9862
7.9833
7.8576
7.8543
7.8419
7.8397
7.8368
7.8243
7.8214
7.7357
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7.0805
7.0772
7.0746
7.0651
7.0626
7.0589



Current Data Parameters
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EXPNO 11
PROCNO 1

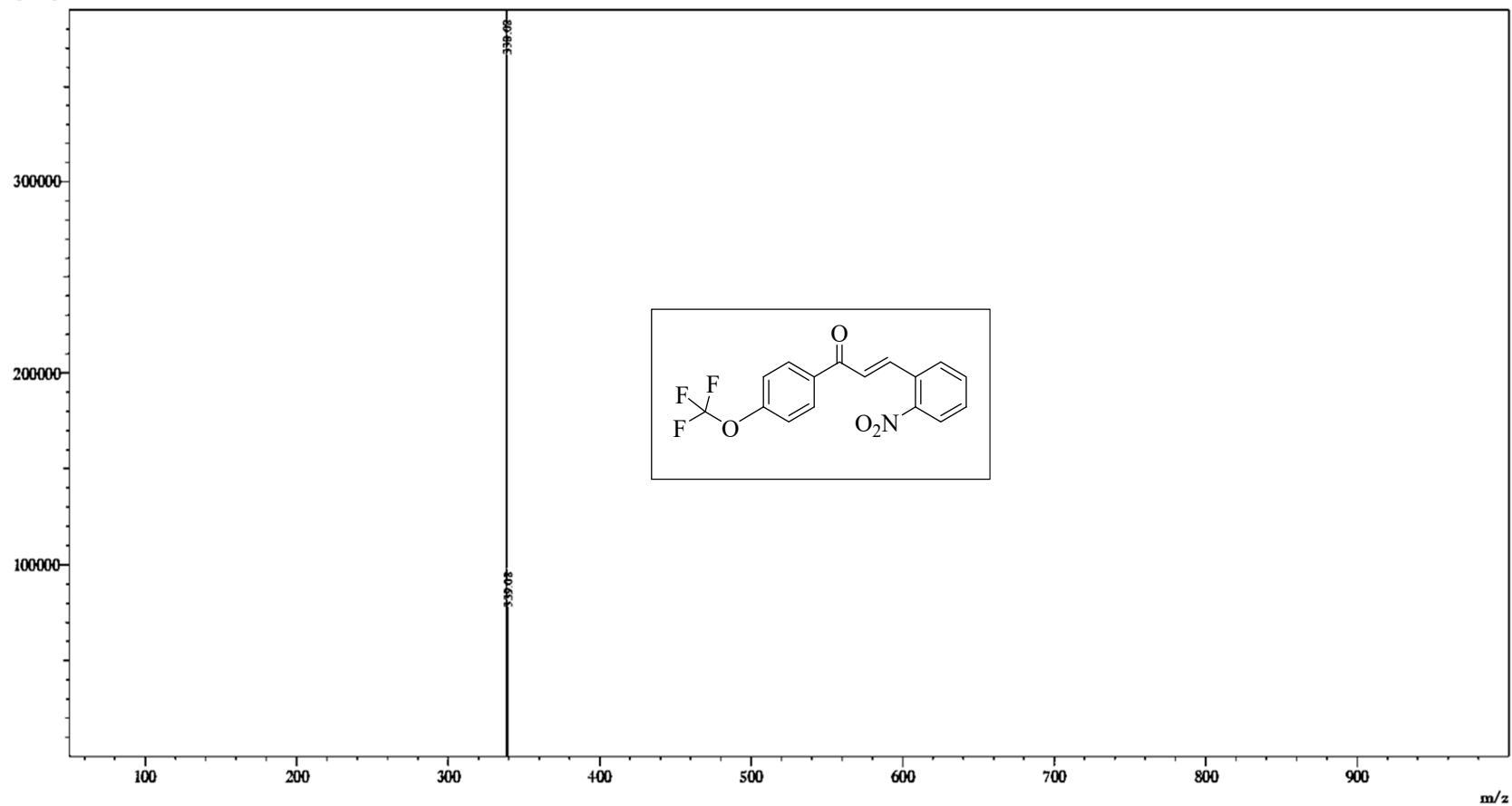
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TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 132.41
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 15.00 usec
PLW1 9.91339970 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

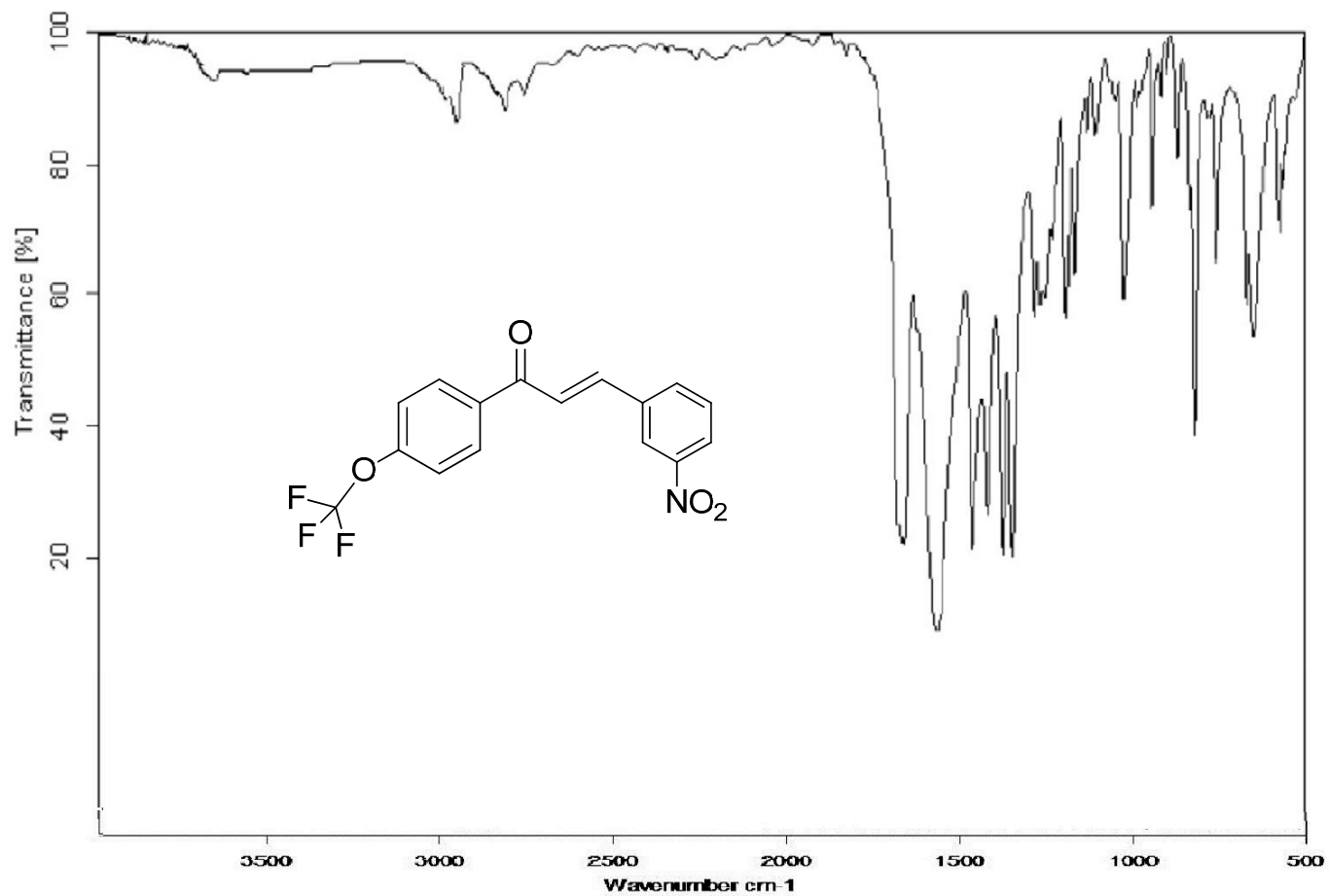


¹H NMR Spectrum of (E)-1-(4-(trifluoromethoxy)phenyl)-3-(2-nitrophenyl)prop-2-en-1-one (B4)

Averaged ESI Positive+
Spectrum Mode: Averaged 0.183-0.605(74-243)
[CPS]



MASS Spectrum of (E)-1-(4-(trifluoromethoxy)phenyl)-3-(2-nitrophenyl)prop-2-en-1-one (B4)



¹H NMR Spectrum of *(E)*-1-(4-(trifluoromethoxy)phenyl)-3-(3-nitrophenyl)prop-2-en-1-one (B5)

B5

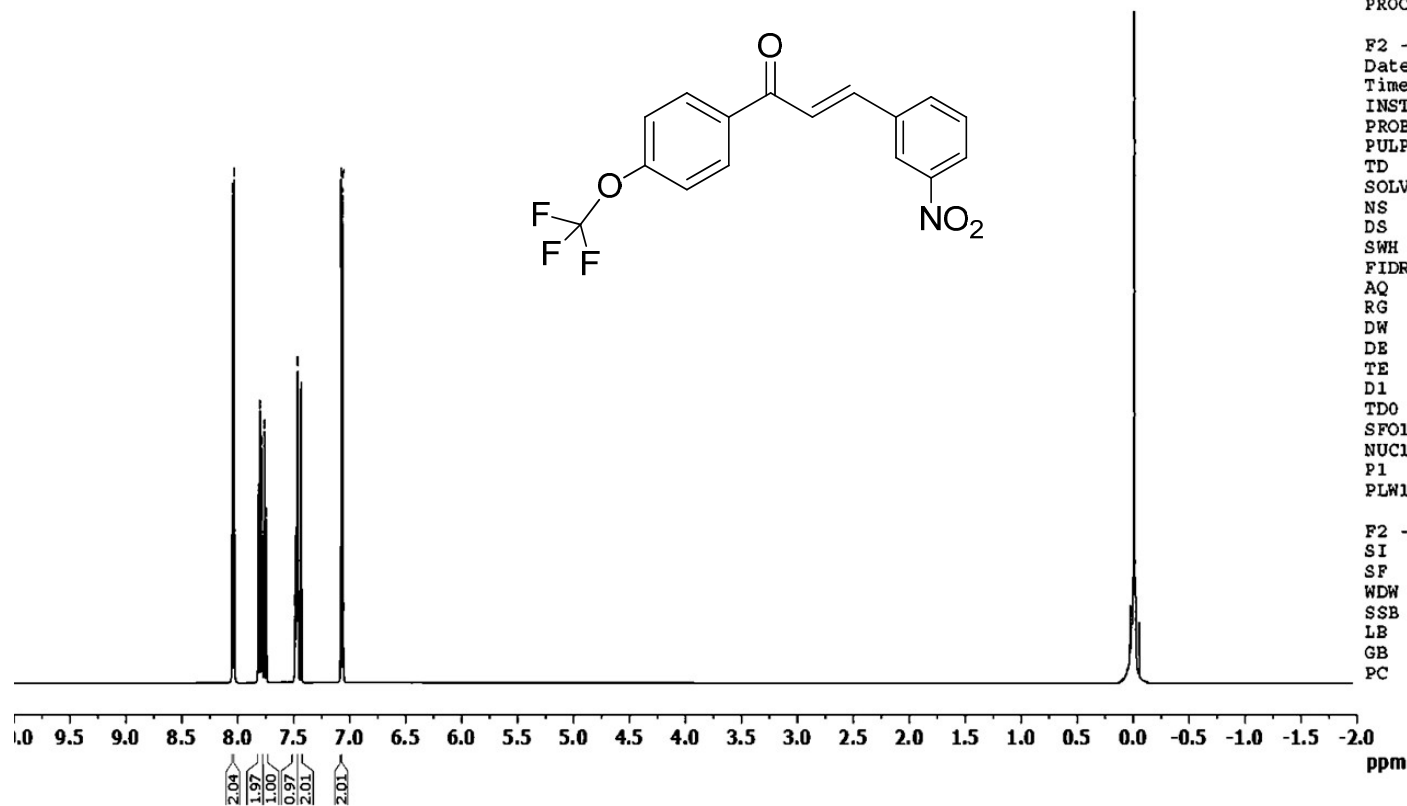
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8.0448
8.0353
8.0327
8.0294
7.8164
7.8048
7.8010
7.7972
7.7850
7.7762
7.7605
7.7447
7.4907
7.4881
7.4866
7.4844
7.4809
7.4775
7.4753
7.4732
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7.4615
7.4596
7.4578
7.4336
7.0805
7.0772
7.0746
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7.0626
7.0589



Current Data Parameters
NAME 05042019
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time 12.47 h
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 132.41
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1
SFO1 400.1324708 MHz
NUC1 1H
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PLW1 9.91339970 W

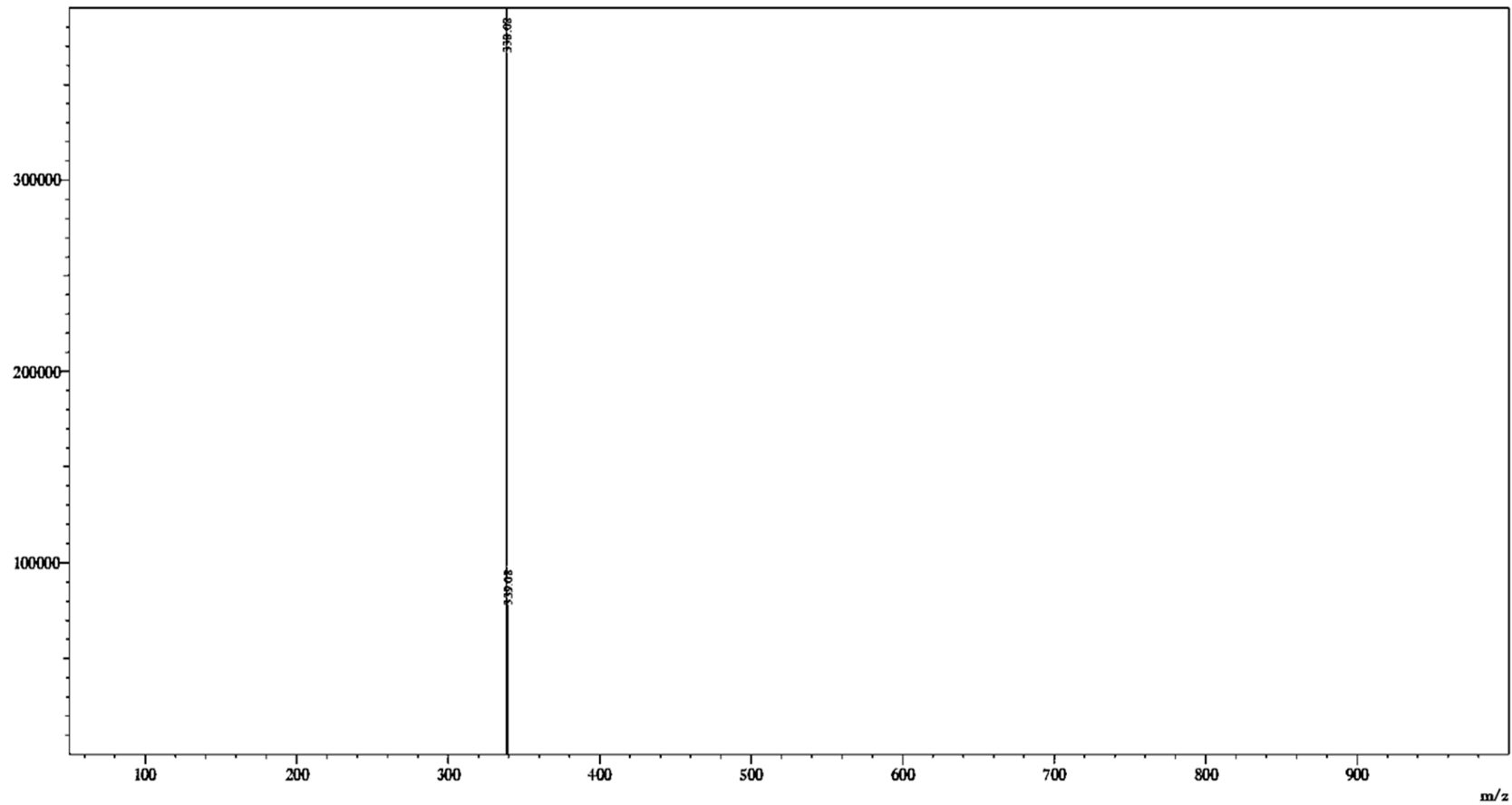
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SF 400.1300000 MHz
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SSB 0
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PC 1.00



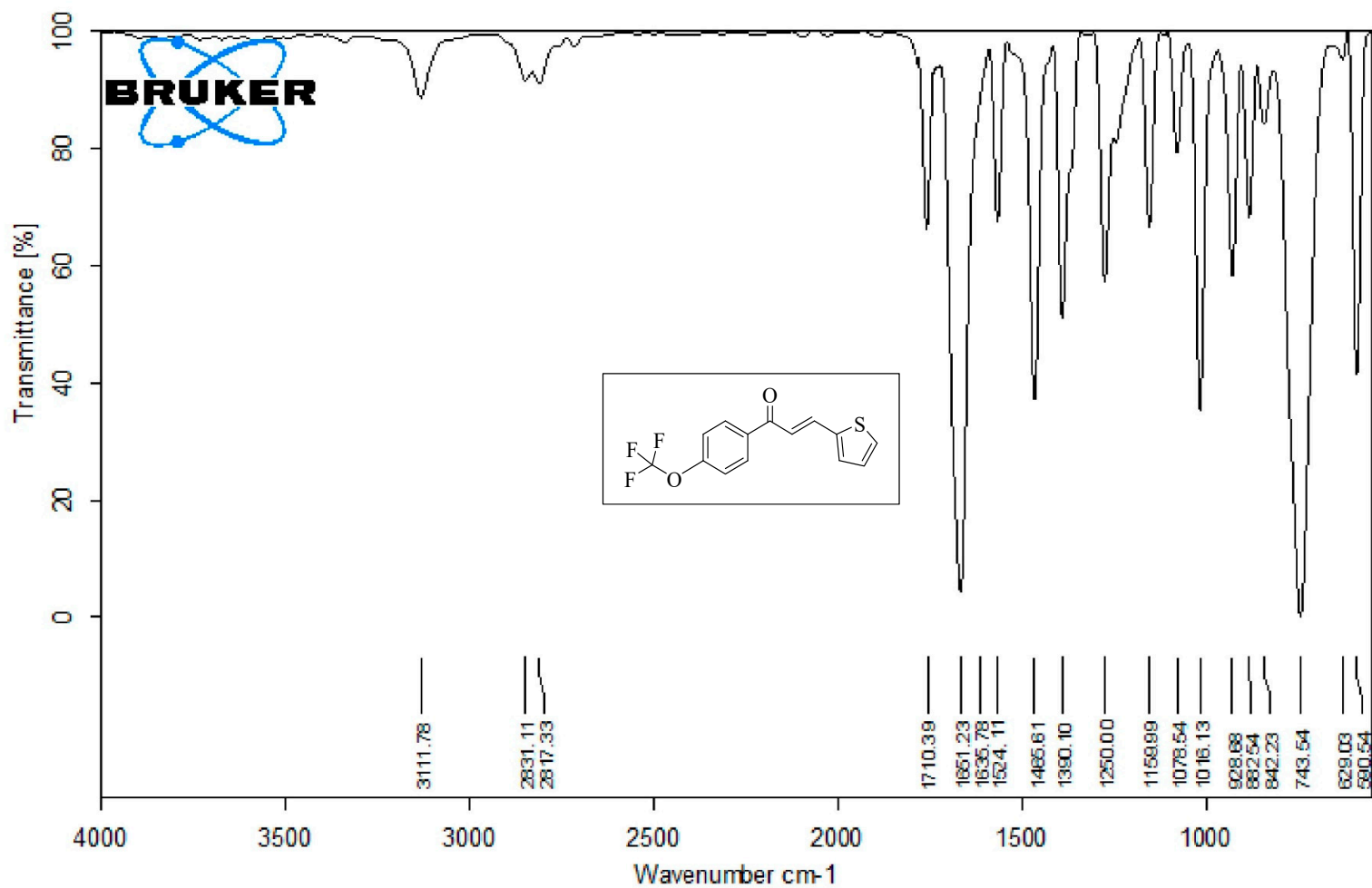
¹H NMR Spectrum of (E)- 1-(4-(trifluoromethoxy)phenyl)-3-(3-nitrophenyl)prop-2-en-1-one (B5)

Averaged ESI Positive+
Spectrum Mode: Averaged 0.183-0.605(74-243)
[CPS]

MS Spectrum
D:\DATA\JULY-19\16072019.3.lcd



MASS Spectrum of (E)- 1-(4-(trifluoromethoxy)phenyl)-3-(3-nitrophenyl)prop-2-en-1-one (B5)



D:\FTIR DATA\2017 OCT\SURENDRA BABU

B7

SOLID

8/9/2018

FT-IR Spectrum of (E)- 3-(thiophen-2''-yl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B6)

B6

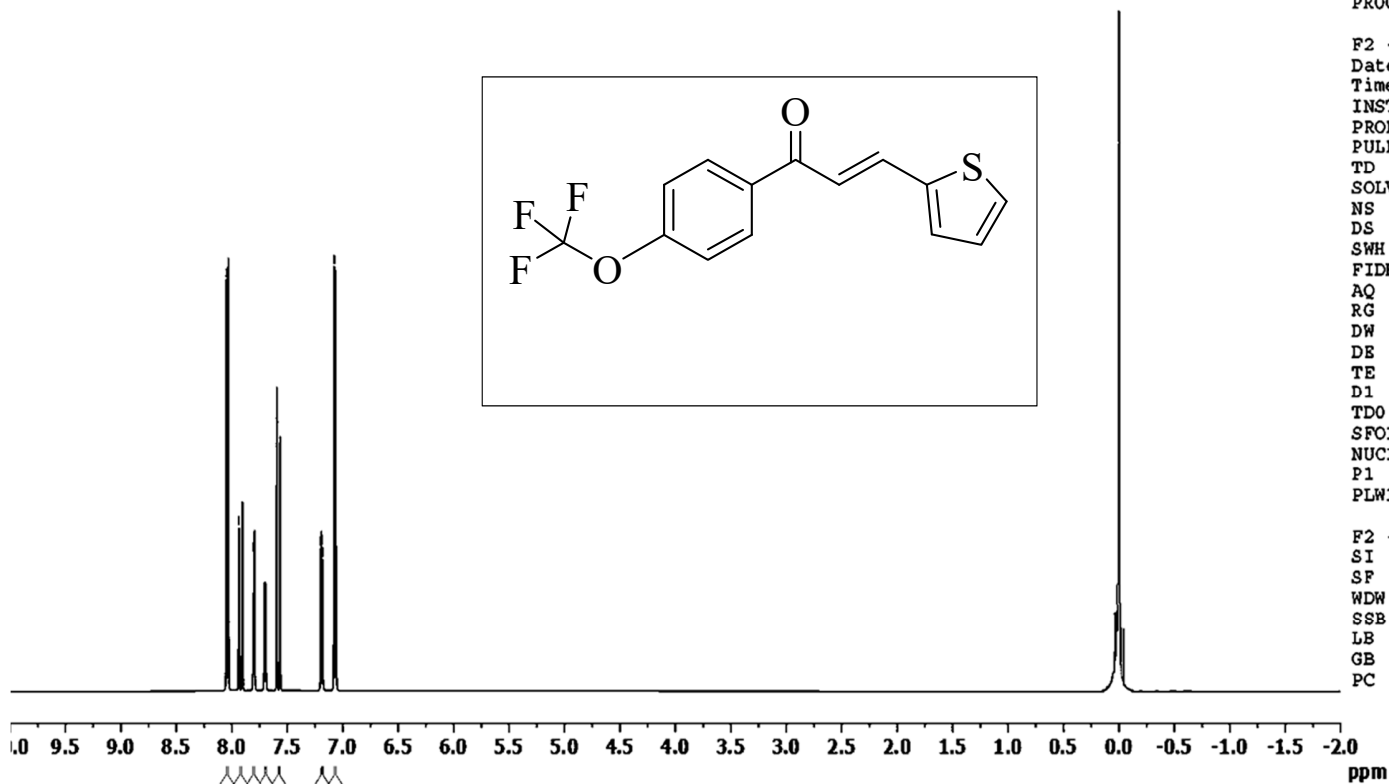
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8.0448
8.0353
8.0327
8.0294
7.9363
7.9059
7.9045
7.8067
7.8034
7.7968
7.7936
7.7082
7.7048
7.6961
7.6946
7.6917
7.5947
7.5640
7.2010
7.1911
7.1886
7.1787
7.0805
7.0772
7.0746
7.0651
7.0626
7.0589



Current Data Parameters
NAME 03042019
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
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Time_ 13.10 h
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 132.41
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1
SFO1 400.1324708 MHz
NUC1 1H
P1 15.00 usec
PLW1 9.91339970 W

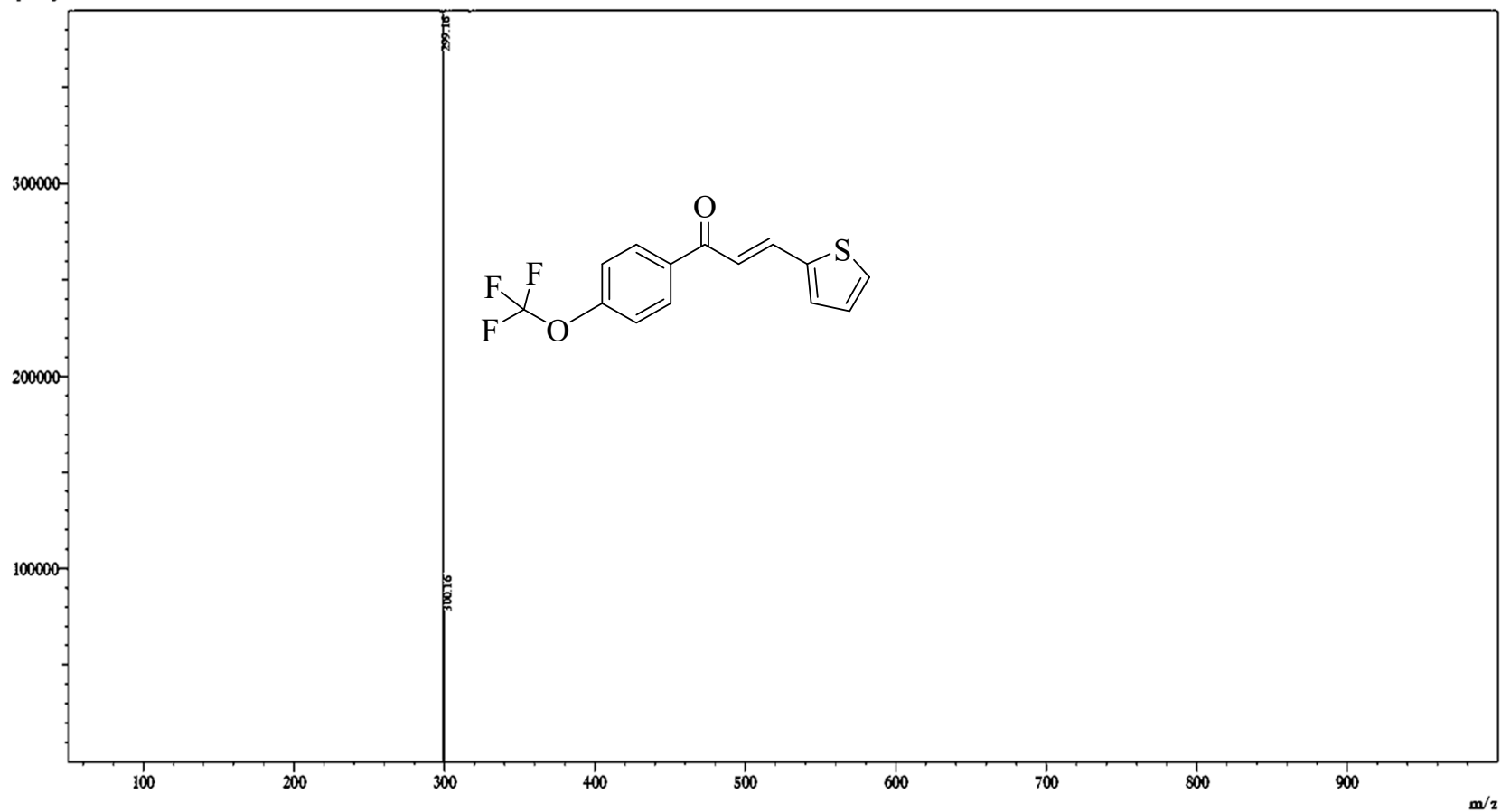
F2 - Processing parameters
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SF 400.1300000 MHz
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SSB 0
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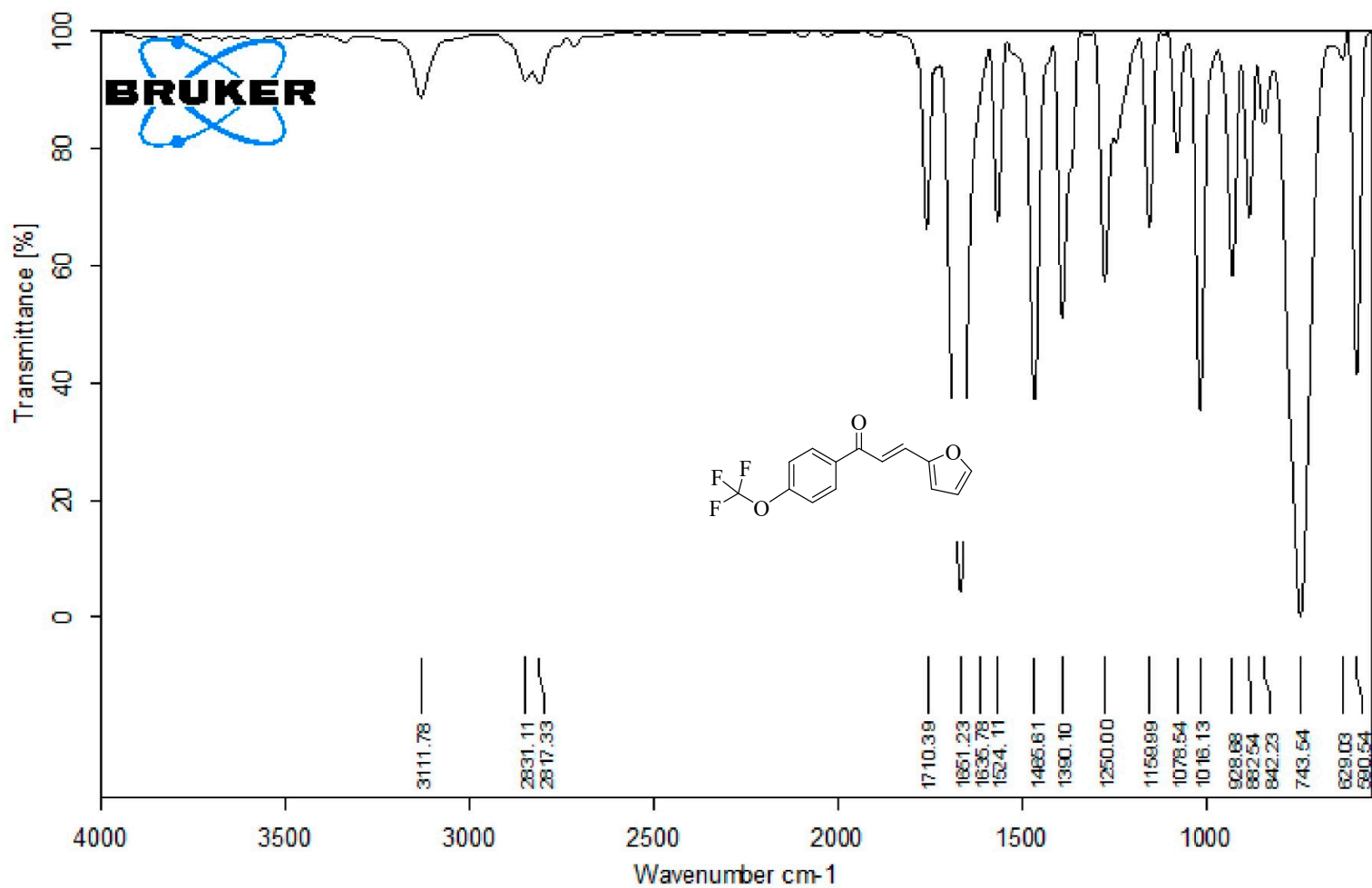
¹H NMR Spectrum of (E)- 3-(thiophen-2''-yl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B6)

Averaged ESI Positive
Spectrum Mode: Averaged 0.183-0.605(74-243)

[CPS]



MASS Spectrum of (E)- 3-(thiophen-2''-yl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B6)



D:\FTIR DATA\2017 OCT\SURENDRA BABU

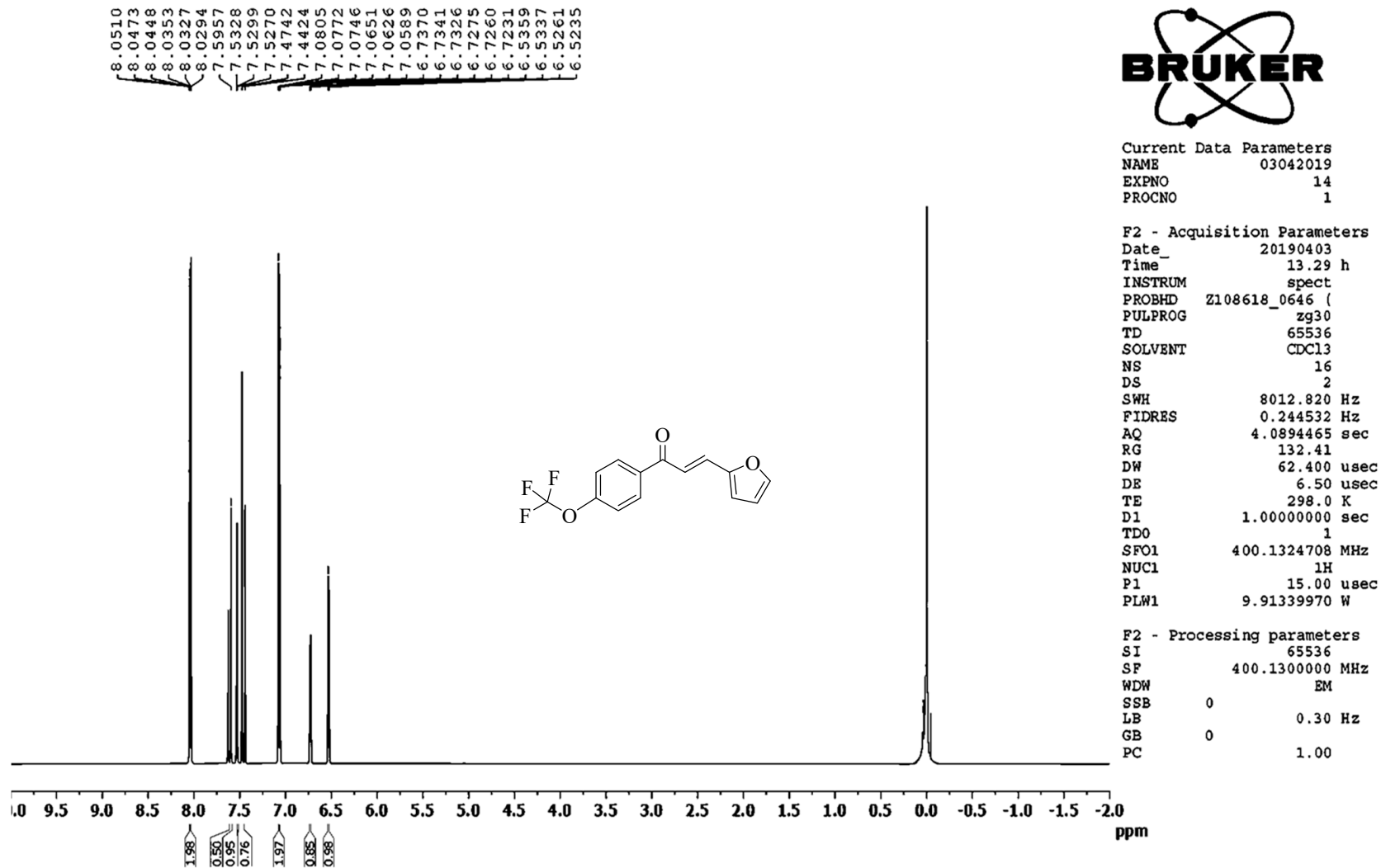
B7

SOLID

8/9/2018

FT-IR Spectrum of (E)-3-(furan-2''-yl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B7)

B7

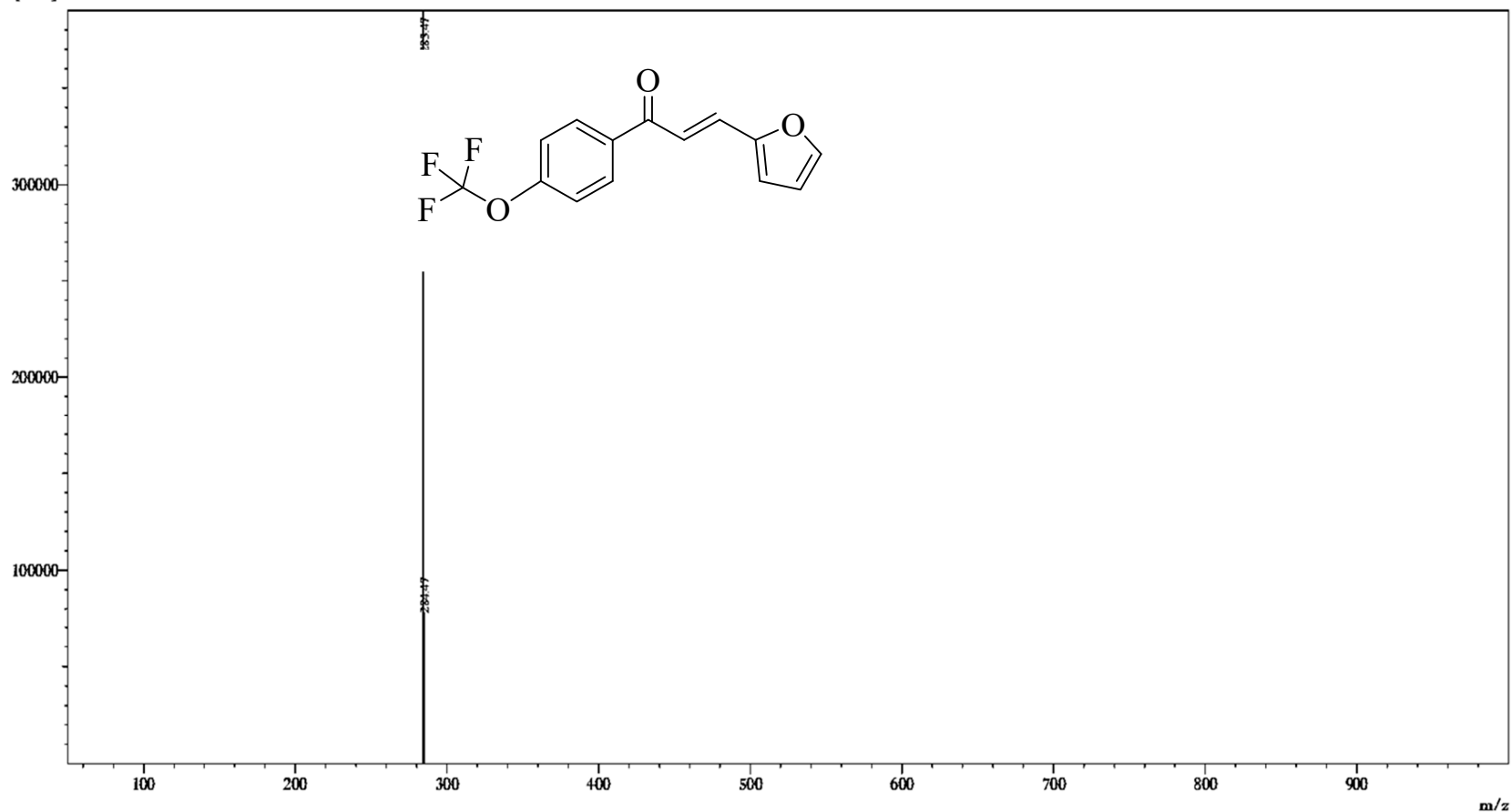


¹H NMR Spectrum of (E)-3-(furan-2''-yl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B7)

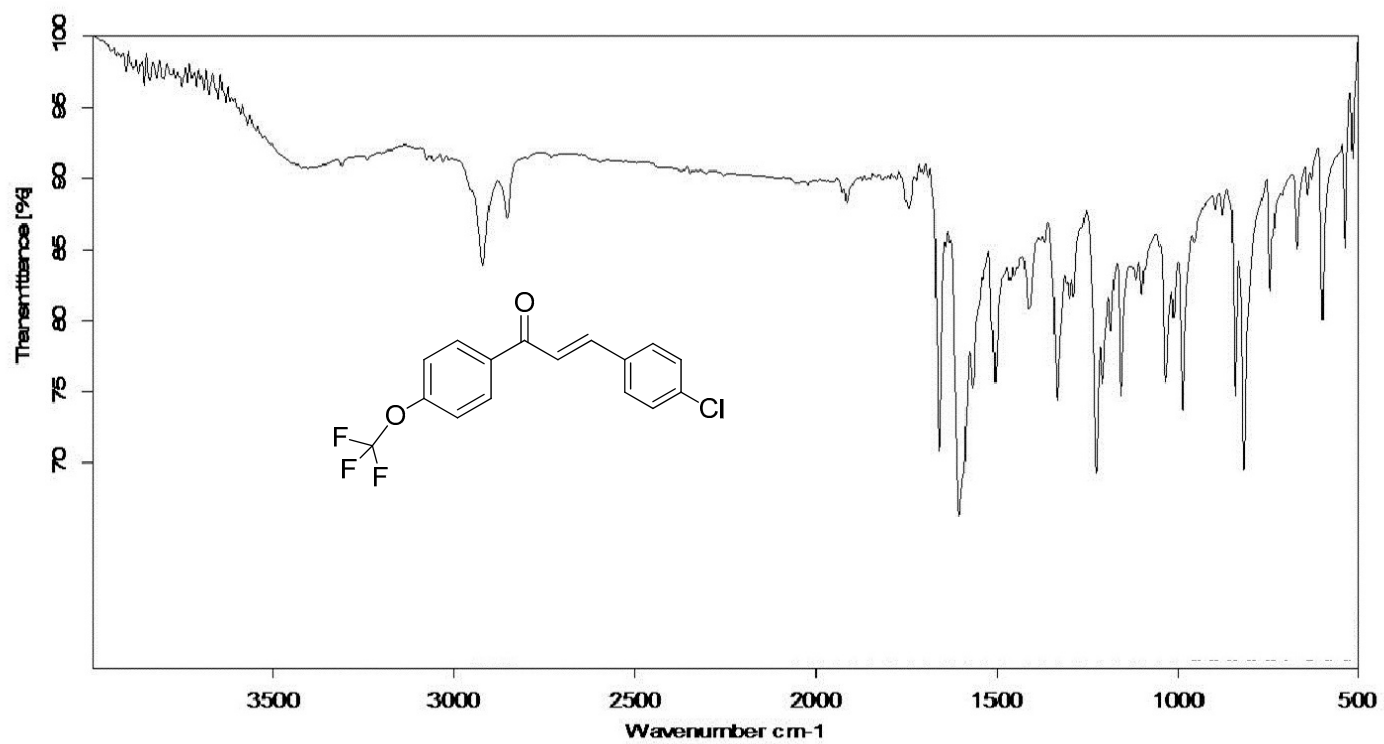
Sample Name : KSB-B7-282
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Date Acquired : 7/16/2019 10:11:00 AM
Batch File : 16072019.lcb

MS Spectrum
D:\DATA\JULY-19\16072019.9.lcd

Averaged ESI Positive+
Spectrum Mode: Averaged 0.183-0.605(74-243)
[CPS]



MASS Spectrum of (E)- 3-(furan-2''-yl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B7)



FT-IR Spectrum of (E)-3-(4''-chlorophenyl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B8)

B8

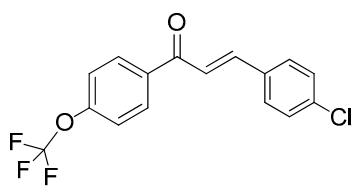
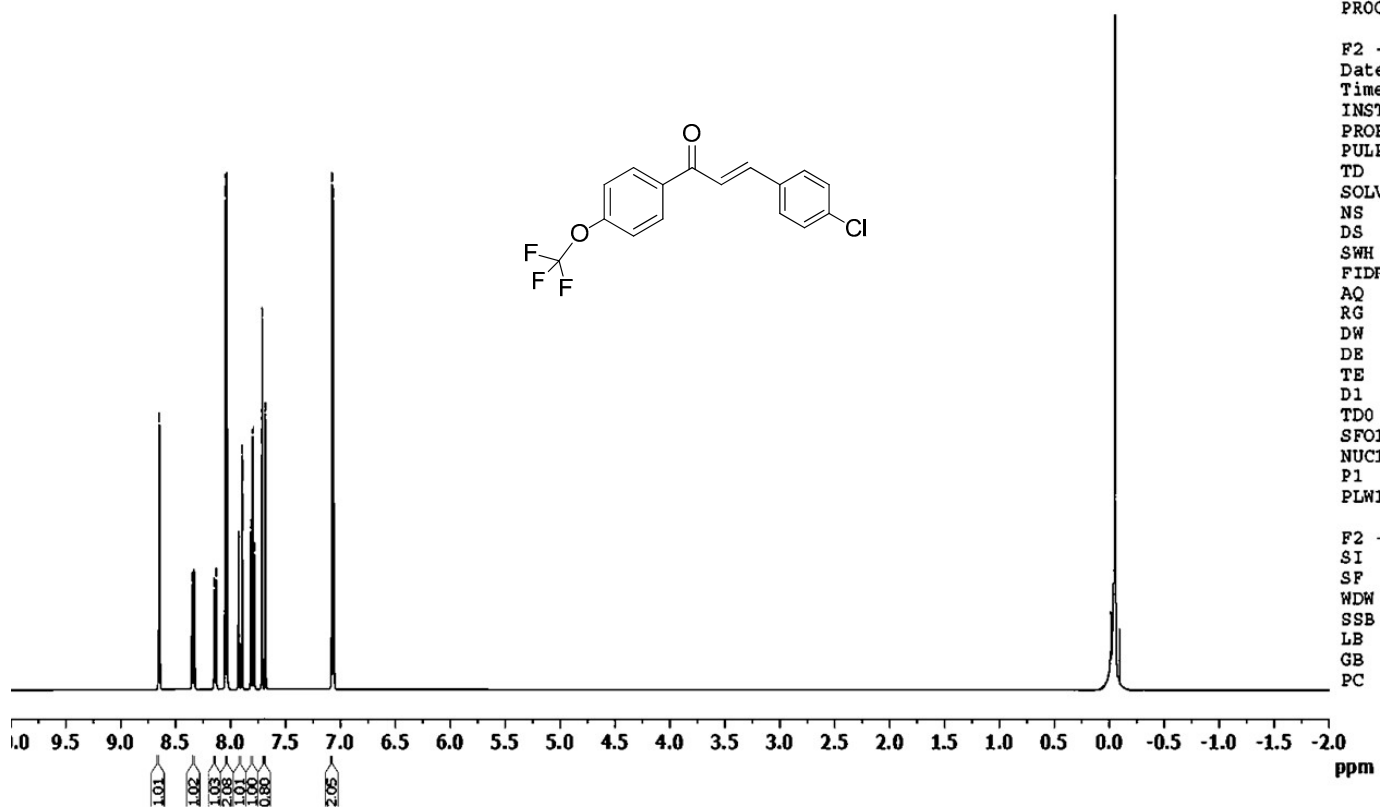
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8.3491
8.3476
8.3455
8.3348
8.3326
8.3308
8.3286
8.1520
8.1503
8.1483
8.1462
8.1444
8.1360
8.1341
8.1323
8.1305
8.1283
8.0510
8.0473
8.0448
8.0353
8.0327
8.0294
7.9276
7.9263
7.8961
7.8950
7.8161
7.7995
7.7831
7.7144
7.6829
7.0805
7.0772
7.0746
7.0652
7.0626
7.0589



Current Data Parameters
NAME 05042019
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time_ 12.32 h
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TD 65536
SOLVENT CDCl3
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DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 132.41
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1
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NUC1 1H
P1 15.00 usec
PLW1 9.91339970 W

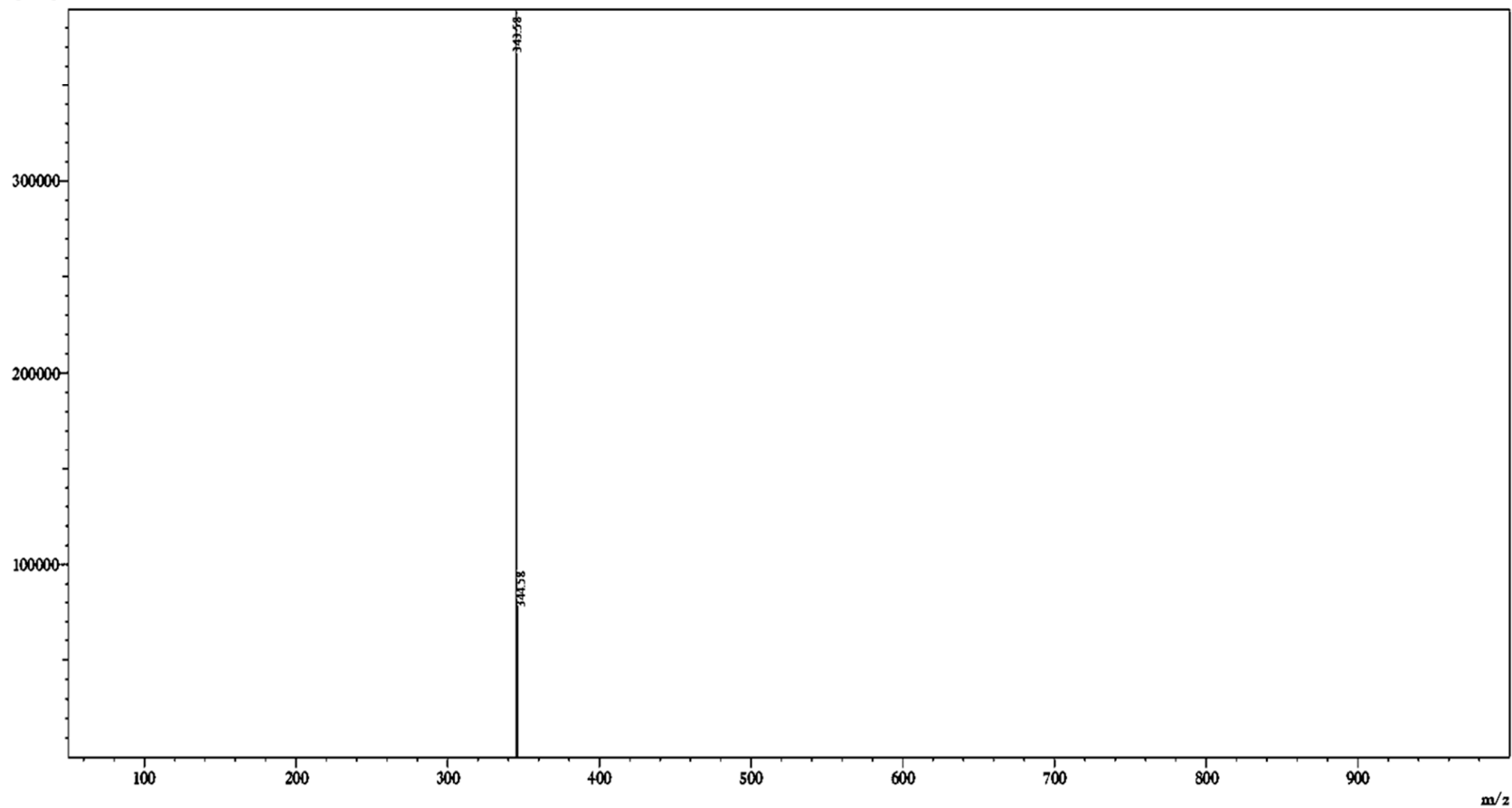
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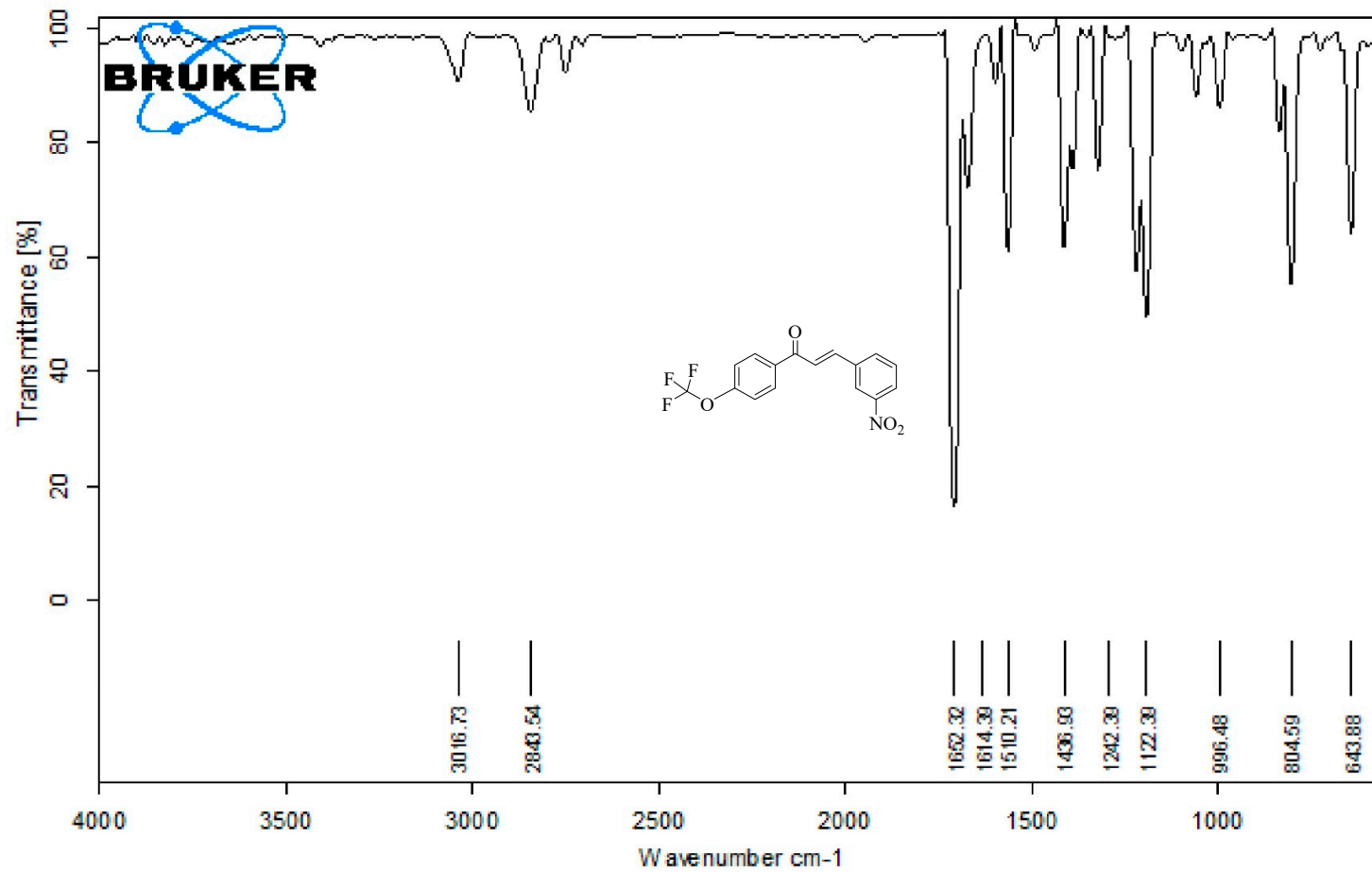
1H NMR Spectrum of (E)-3-(4'-chlorophenyl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B8)

Averaged ESI Positive+
Spectrum Mode: Averaged 0.183-0.605(74-243)
[CPS]

MS Spectrum
D:\DATA\JULY-19\16072019.9.lcd



Mass Spectrum of (E)-3-(4'-chlorophenyl)-1-[4'-(trifluoromethoxy)phenyl]prop-2-en-1-one (B8)



C:\Users\Lenovo\Documents\Bruker\OPUS_7.8.44\DATAWEAS\DEMO.90	B5	LIQUID	22-11-2019
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FT-IR Spectrum of (E)-1-(4-(trifluoromethoxy)phenyl)-3-(4-nitrophenyl)prop-2-en-1-one (B9)

B9

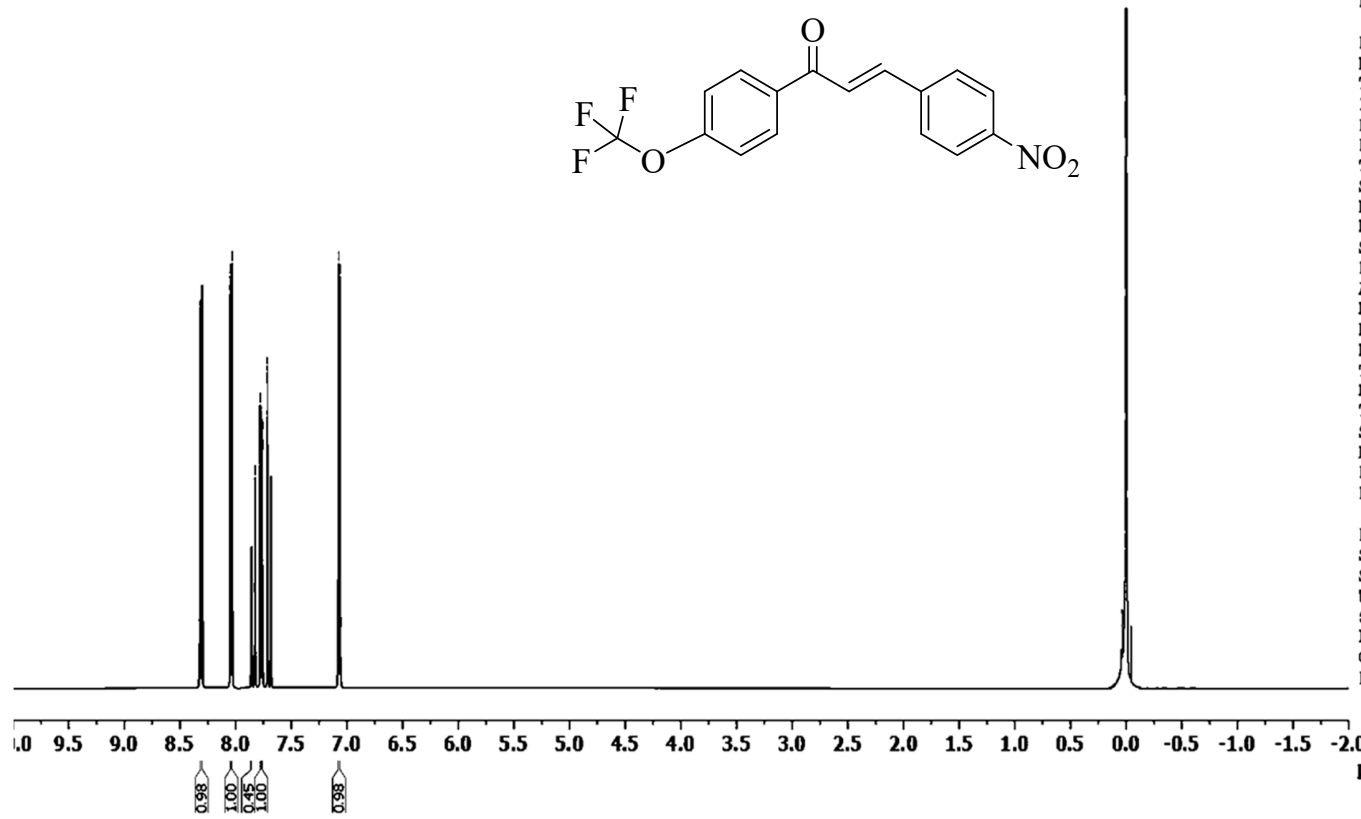
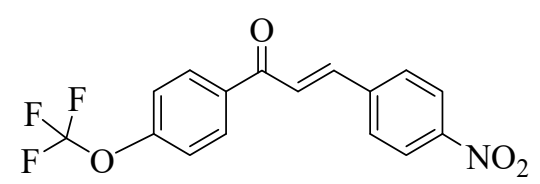
8.3220
8.3186
8.3161
8.3044
8.3016
8.2982
8.0510
8.0473
8.0448
8.0353
8.0327
8.0294
7.8595
7.8575
7.8276
7.8258
7.7820
7.7789
7.7776
7.7752
7.7645
7.7621
7.7607
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7.0772
7.0746
7.0652
7.0626
7.0589



Current Data Parameters
NAME 03042019
EXPNO 12
PROCNO 1

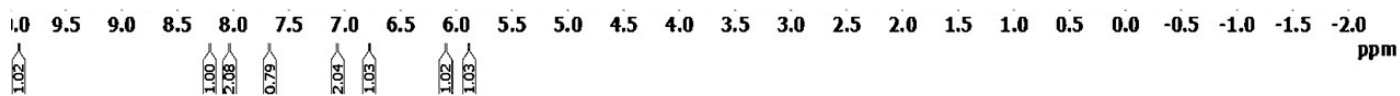
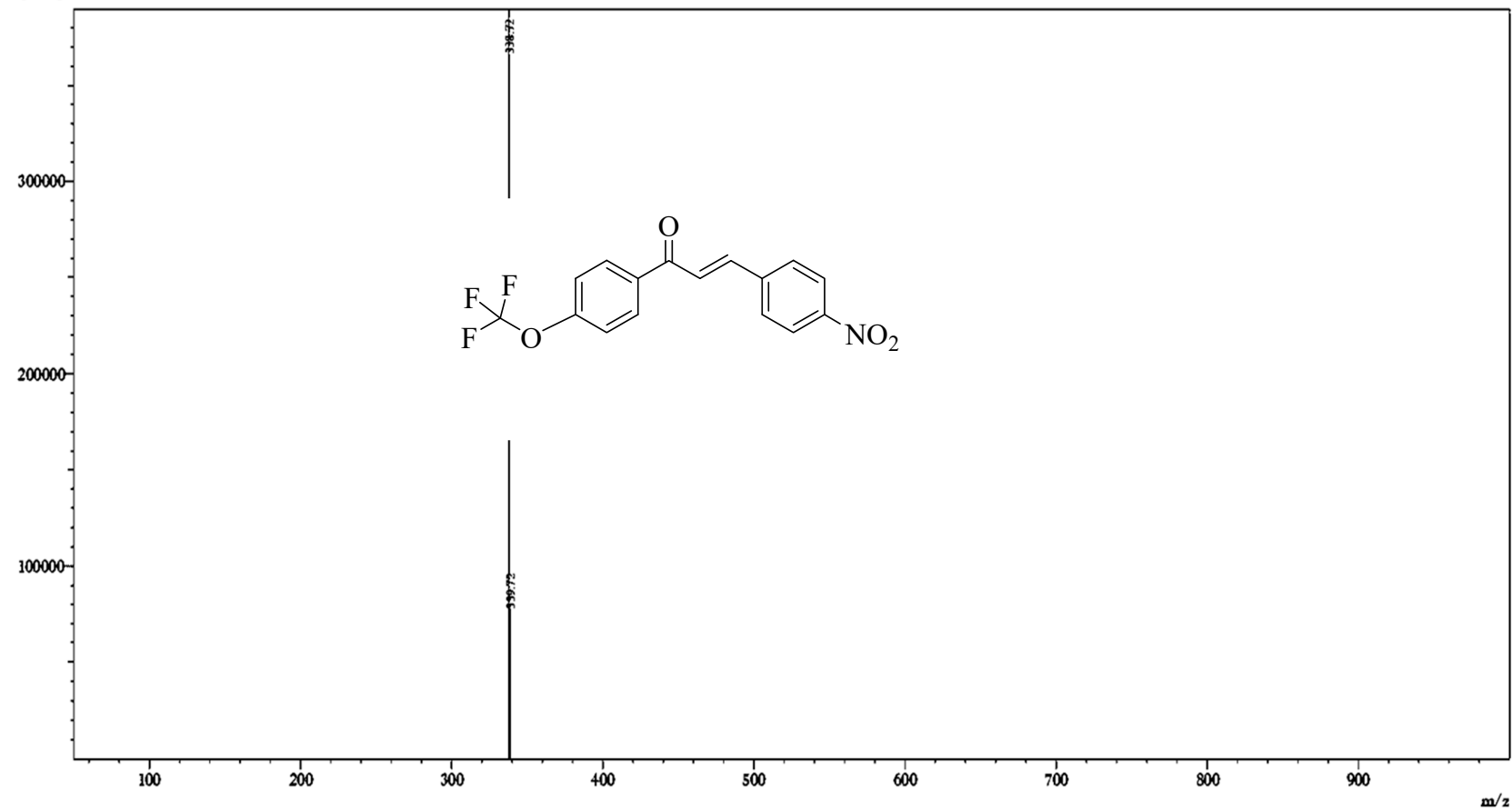
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 132.41
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SF01 400.1324708 MHz
NUC1 1H
P1 15.00 usec
PLW1 9.91339970 W

F2 - Processing parameters
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SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

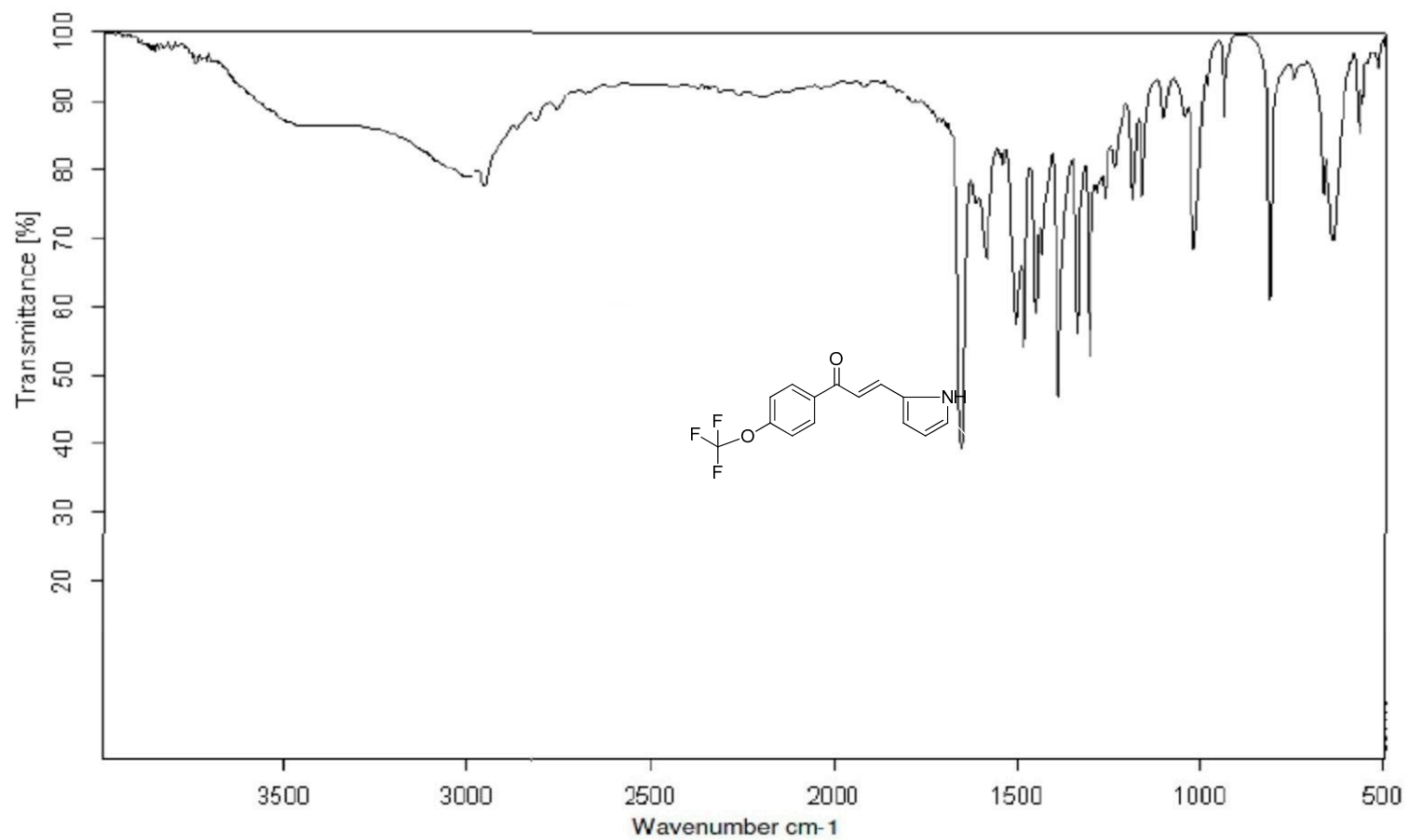


¹H NMR Spectrum of (E)-1-(4-(trifluoromethoxy)phenyl)-3-(4-nitrophenyl)prop-2-en-1-one (B9)

Averaged ESI Positive+
Spectrum Mode: Averaged 0.183-0.605(74-243)
[CPS]



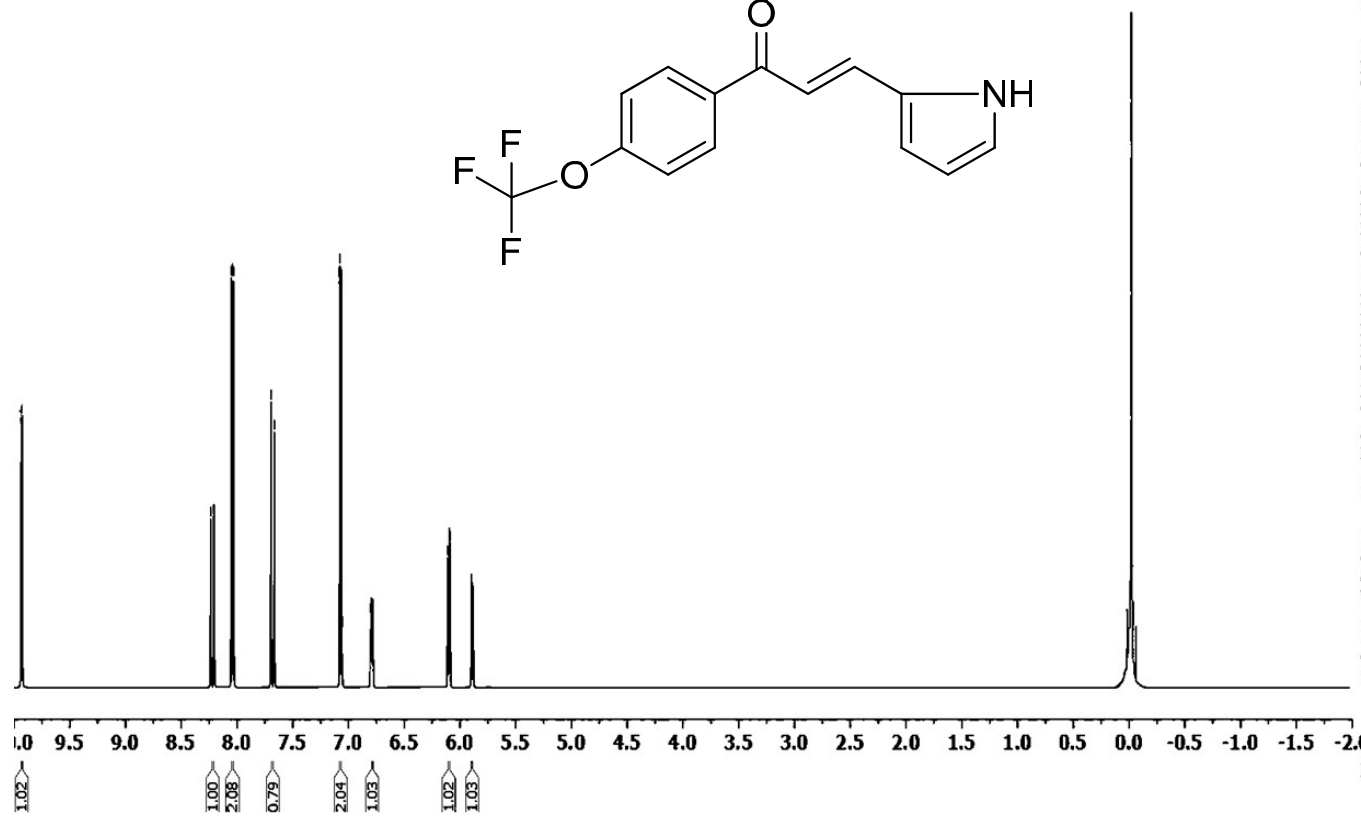
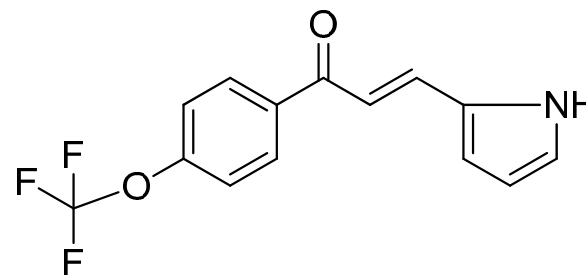
MASS Spectrum of 1-(4-(trifluoromethoxy)phenyl)-3-(4-nitrophenyl)prop-2-en-1-one (B9)



FT-IR spectrum of (E)-3-(1H-pyrrol-2-yl)-1-(4-(trifluoromethoxy)phenyl)prop-2-en-1-one (B10)

B10

9.9367
9.9235
8.2355
8.2062
8.2048
8.0510
8.0473
8.0448
8.0353
8.0327
8.0294
7.6947
7.6646
7.0805
7.0772
7.0746
7.0651
7.0626
7.0589
6.8014
6.7981
6.7952
6.7919
6.7883
6.7846
6.7817
6.7784
6.1100
6.1034
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5.8954
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5.8855
5.8840
5.8822
5.8808



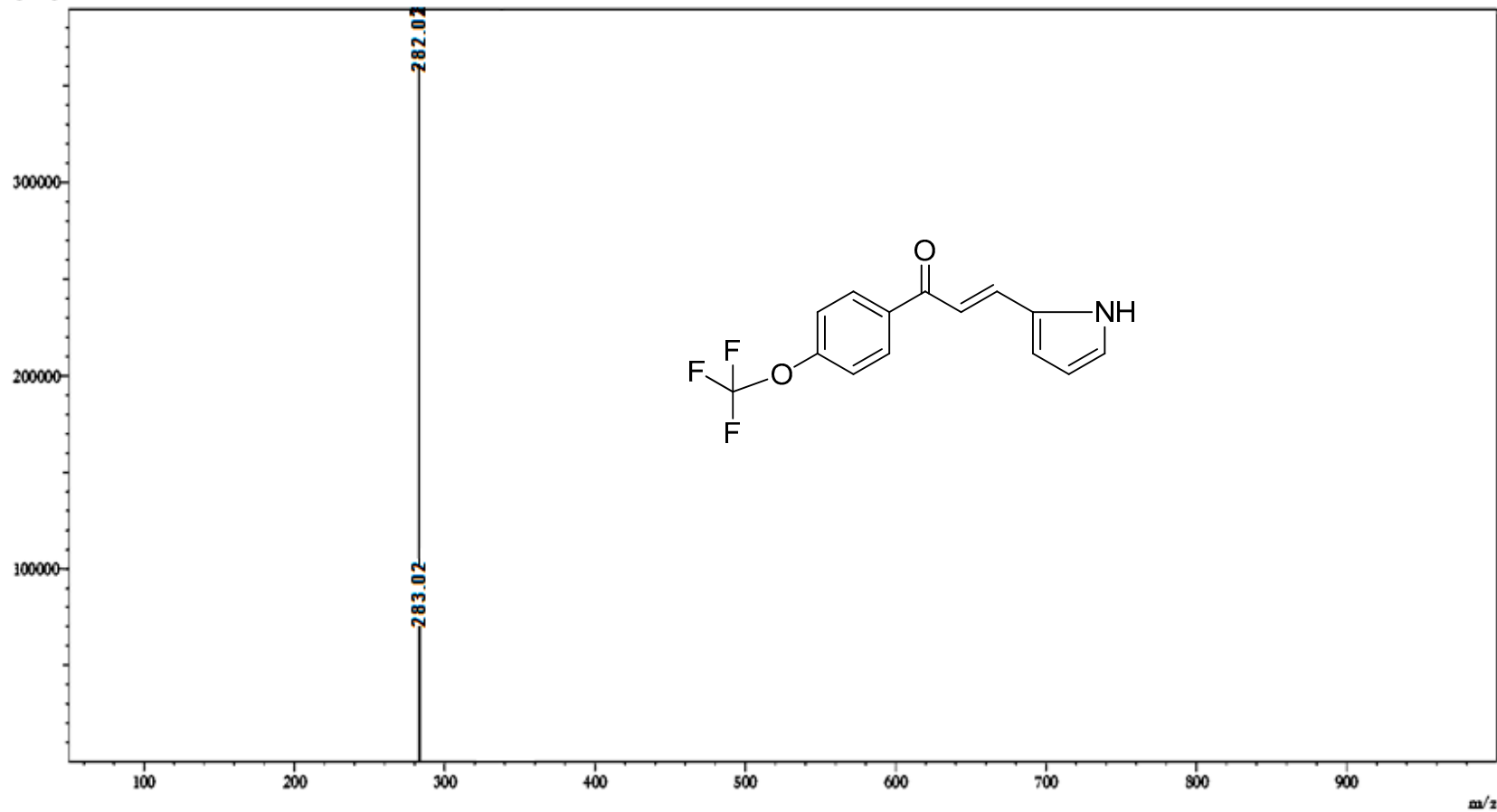
Current Data Parameters
NAME 05042019
EXPNO 1
PROCNO 1

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Time 12.24 h
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 132.41
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 15.00 usec
PLW1 9.91339970 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1H NMR spectrum of (E)-3-(1H-pyrrol-2-yl)-1-(4-(trifluoromethoxy)phenyl)prop-2-en-1-one (B10)

Averaged ESI Positive
Spectrum Mode: Averaged 0.183-0.605(74-243)
[CPS]



Mass spectrum of (E)-3-(1H-pyrrol-2-yl)-1-(4-(trifluoromethoxy)phenyl)prop-2-en-1-one (B10)