

Supplementary Material

An alternative synthetic strategy to construct apixaban analogues

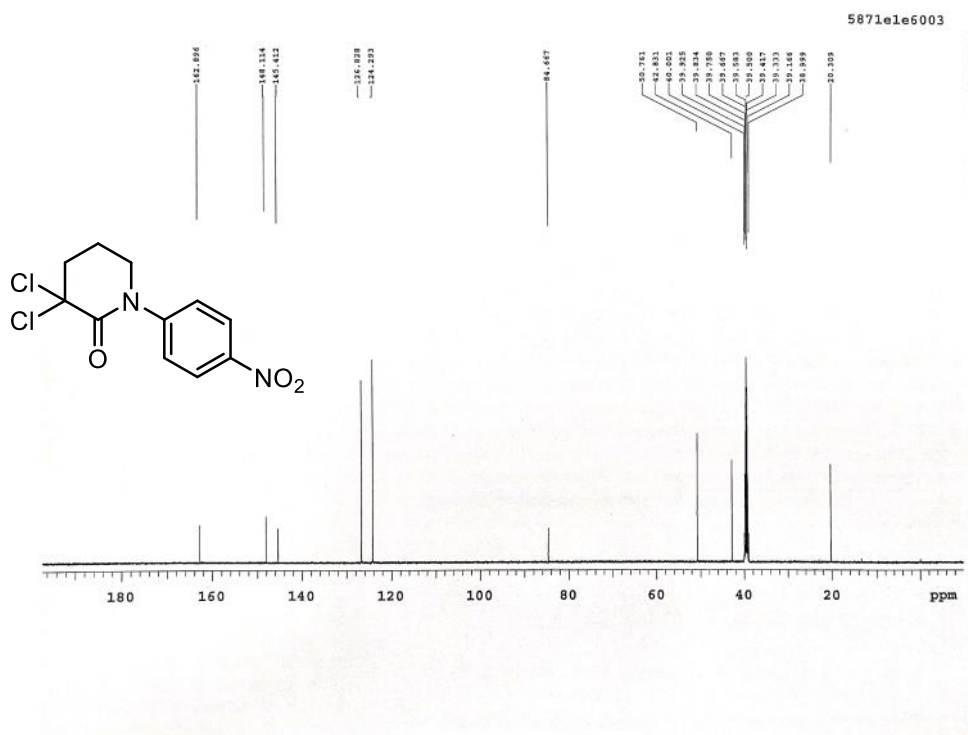
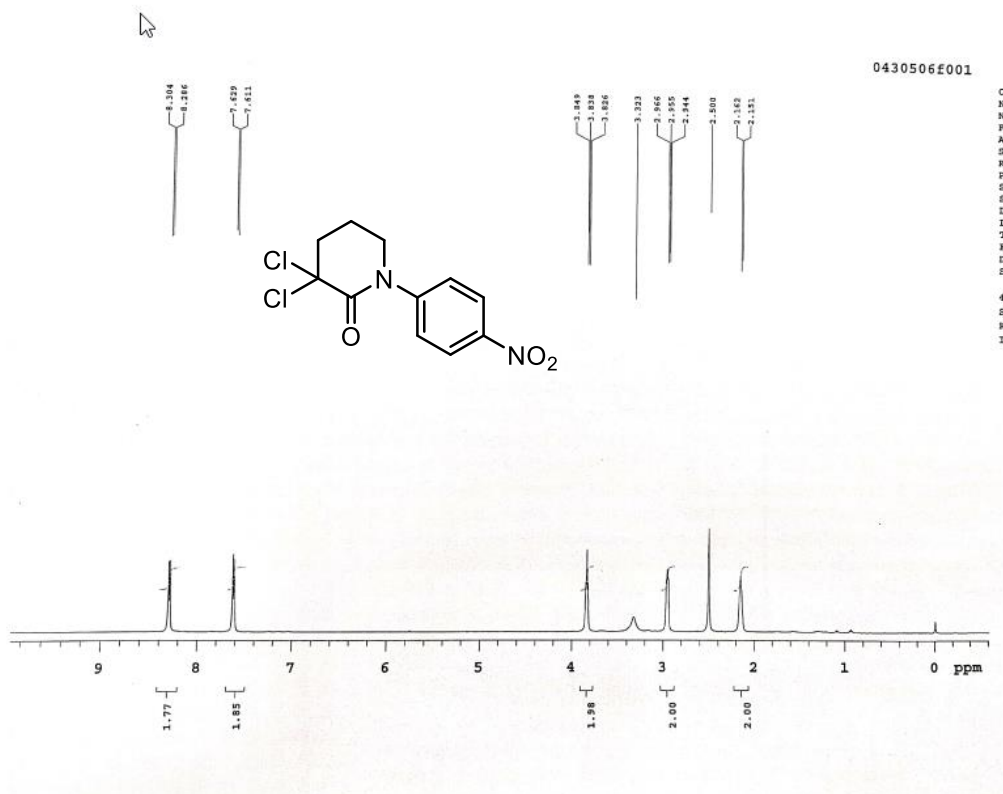
Dattatray Gaikwad,^a Rana Chatterjee,^b Sujeet Gaware,^b Achyuta Nanda Acharya,^{*a} Rambabu Dandela^{*b}

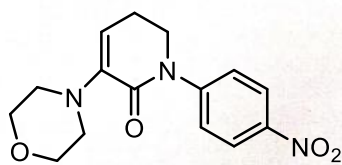
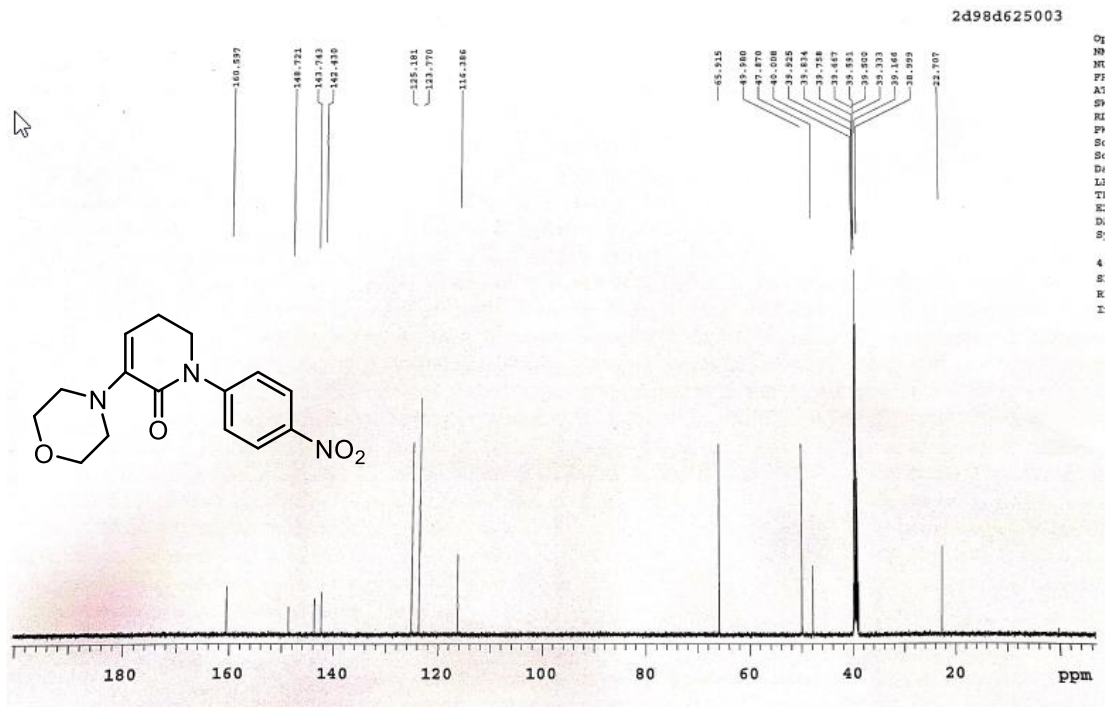
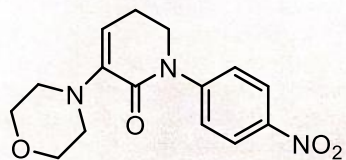
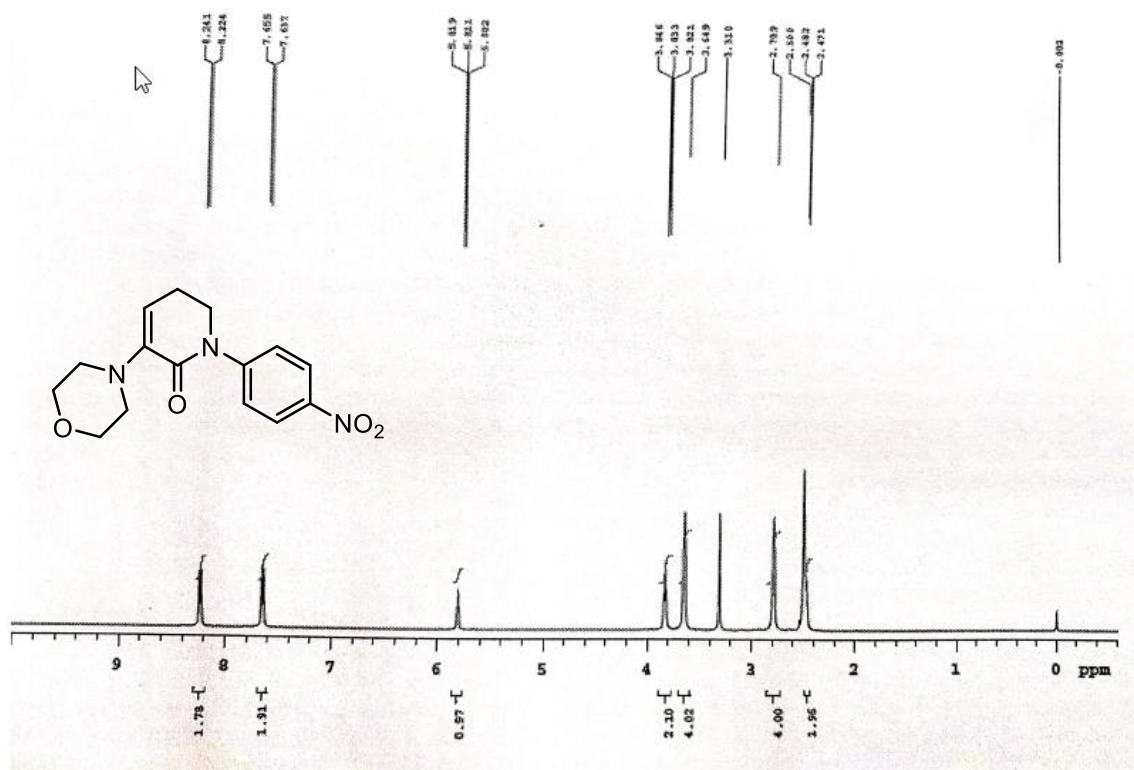
^a Department of Chemistry, Odisha University of Technology and Research (OUTR), Kalinga Nagar, Bhubaneswar-751003, Odisha, India

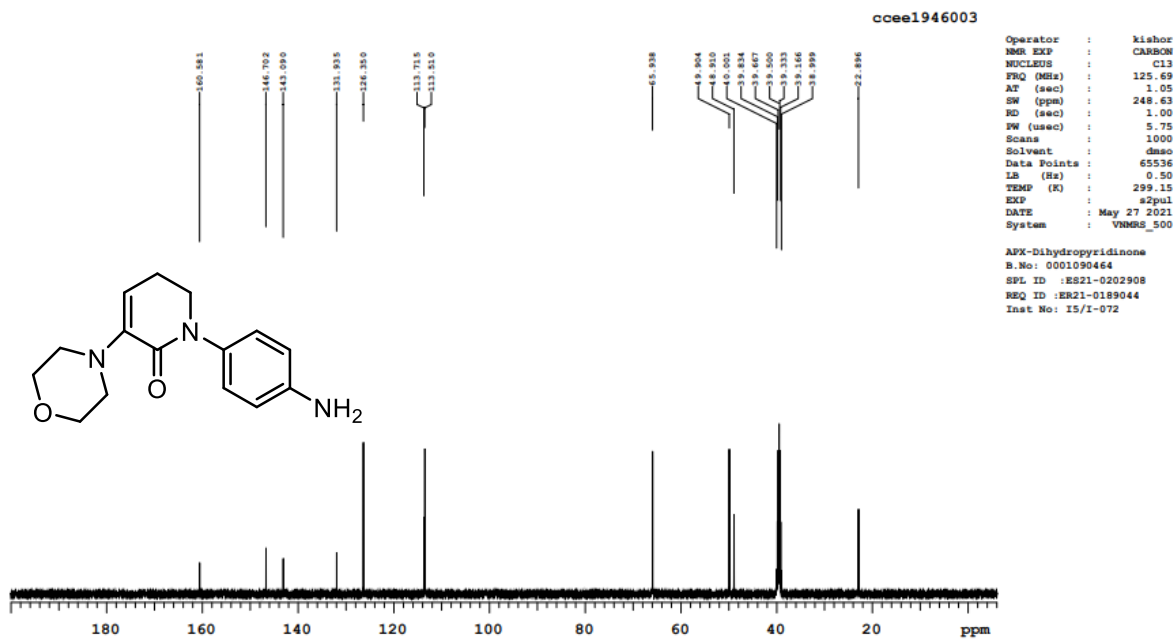
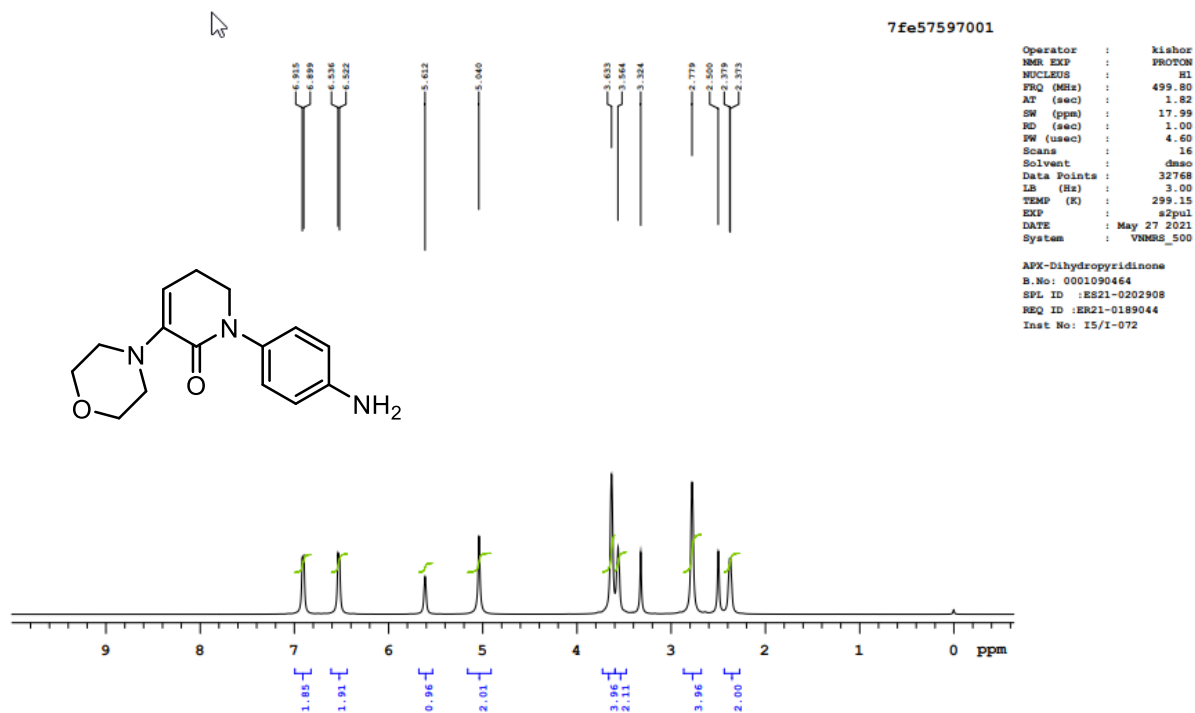
^b Department of Chemistry, Institute of Chemical Technology-Indian Oil Odisha Campus, IIT Kharagpur Extension Centre, Mouza Samantpuri, Bhubaneswar, Odisha-751013, India
Email: r.dandela@iocb.ictmumbai.edu.in

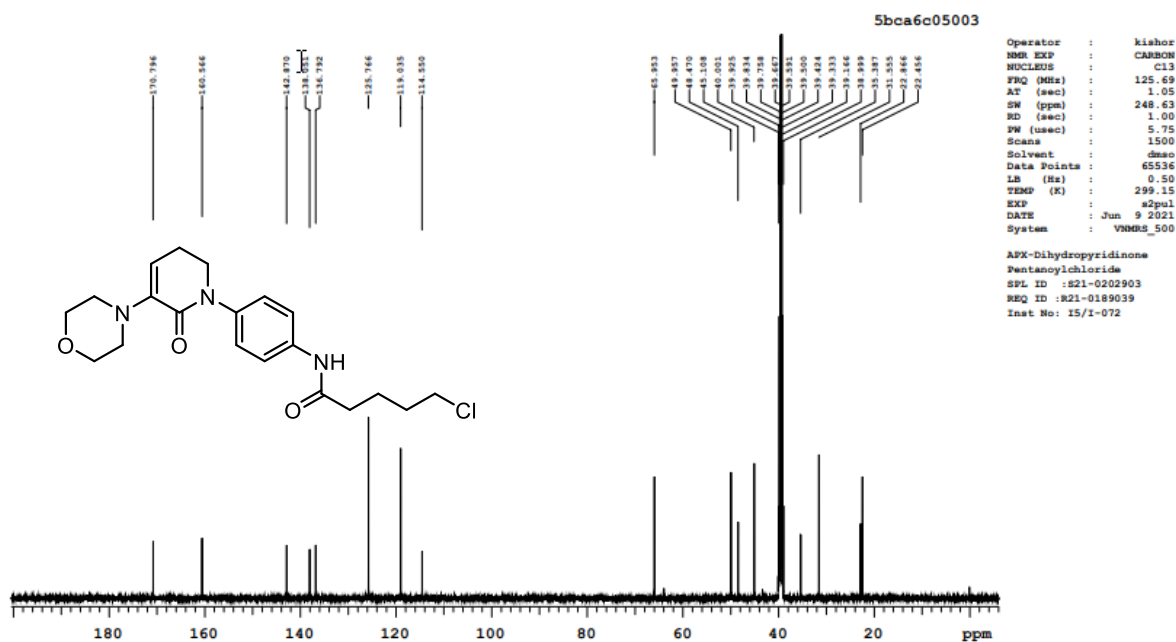
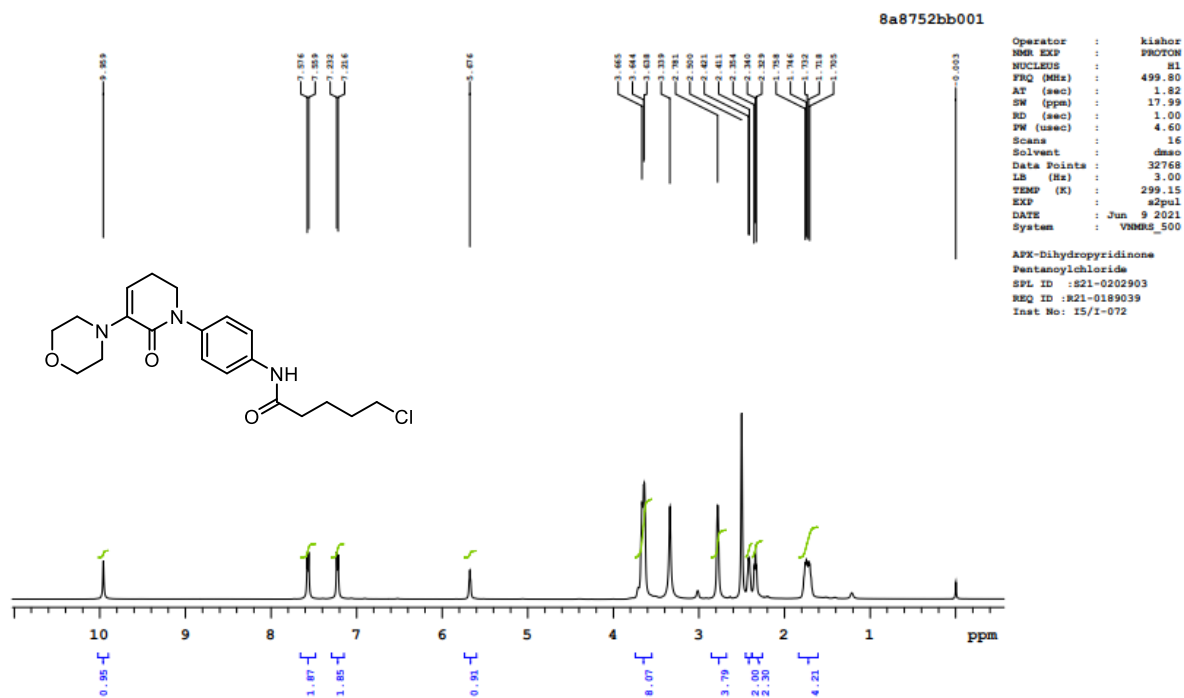
Table of Contents

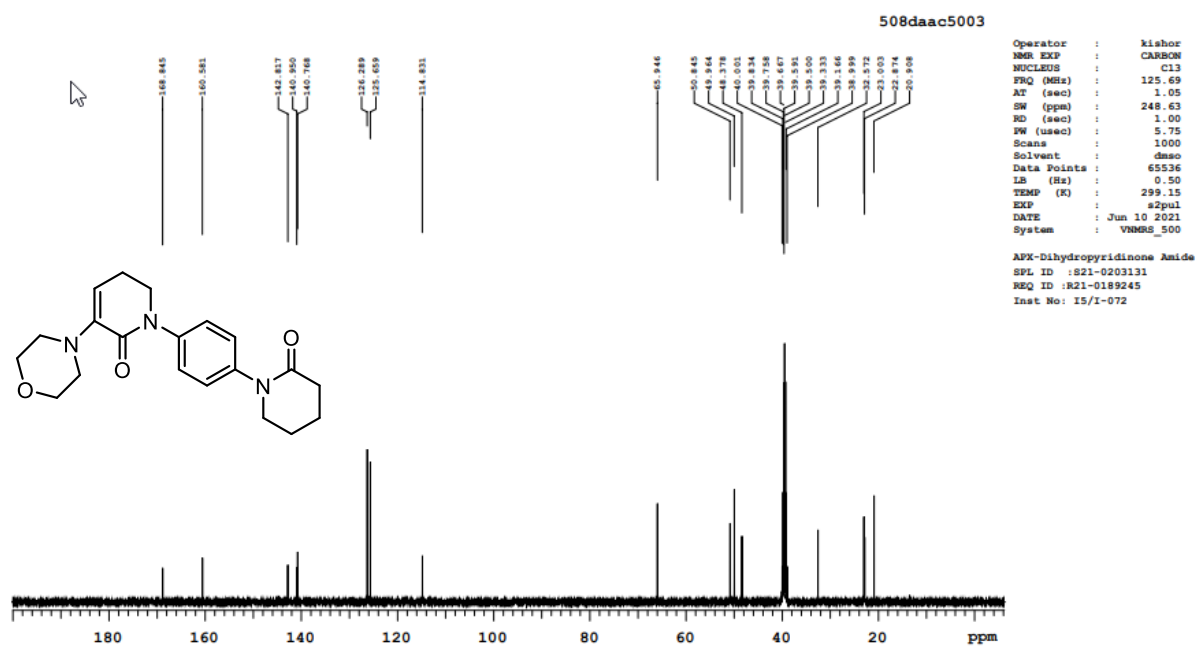
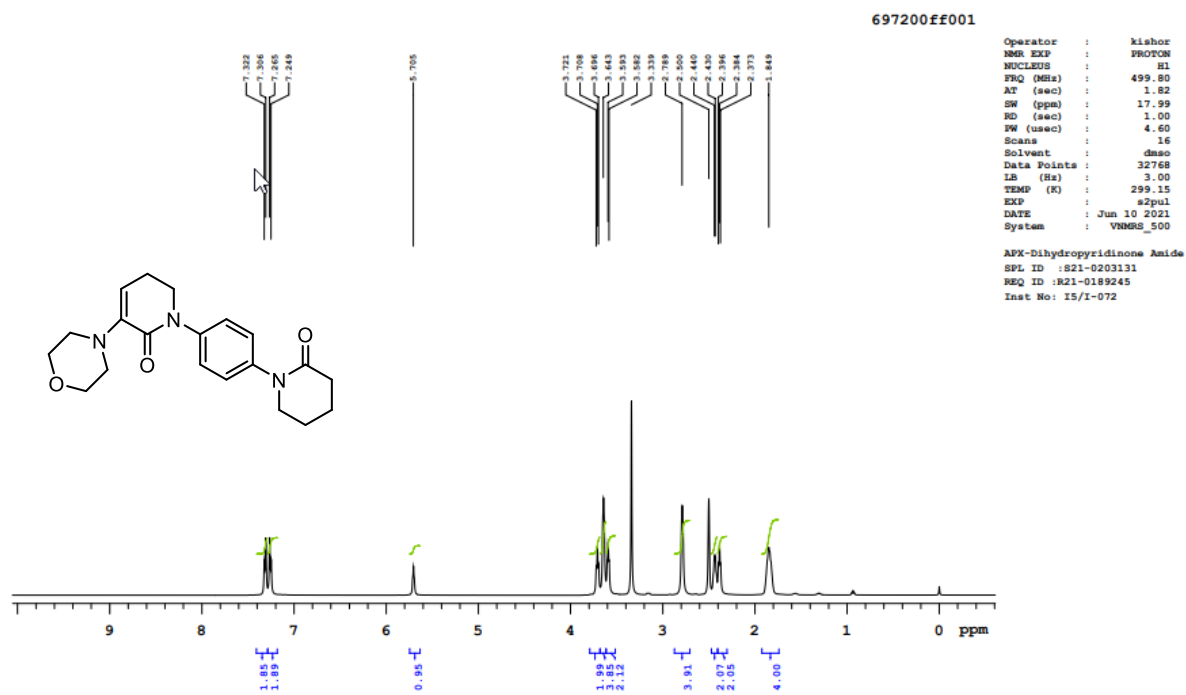
¹ H and ¹³ C NMR spectra of compounds.....	S2
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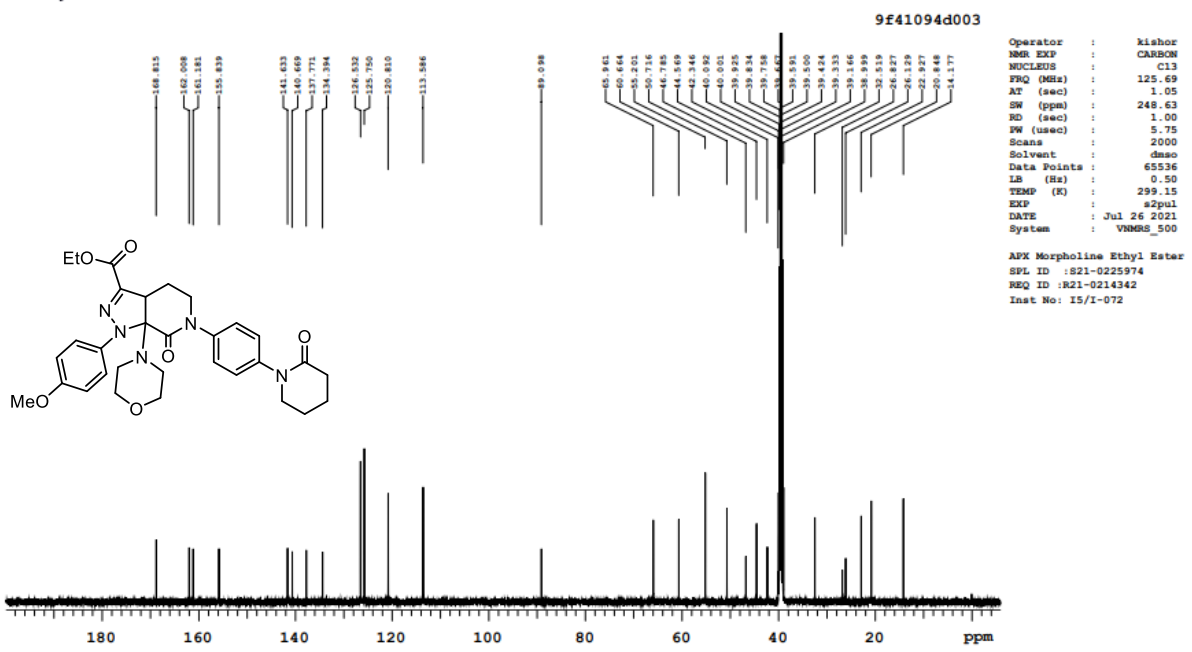
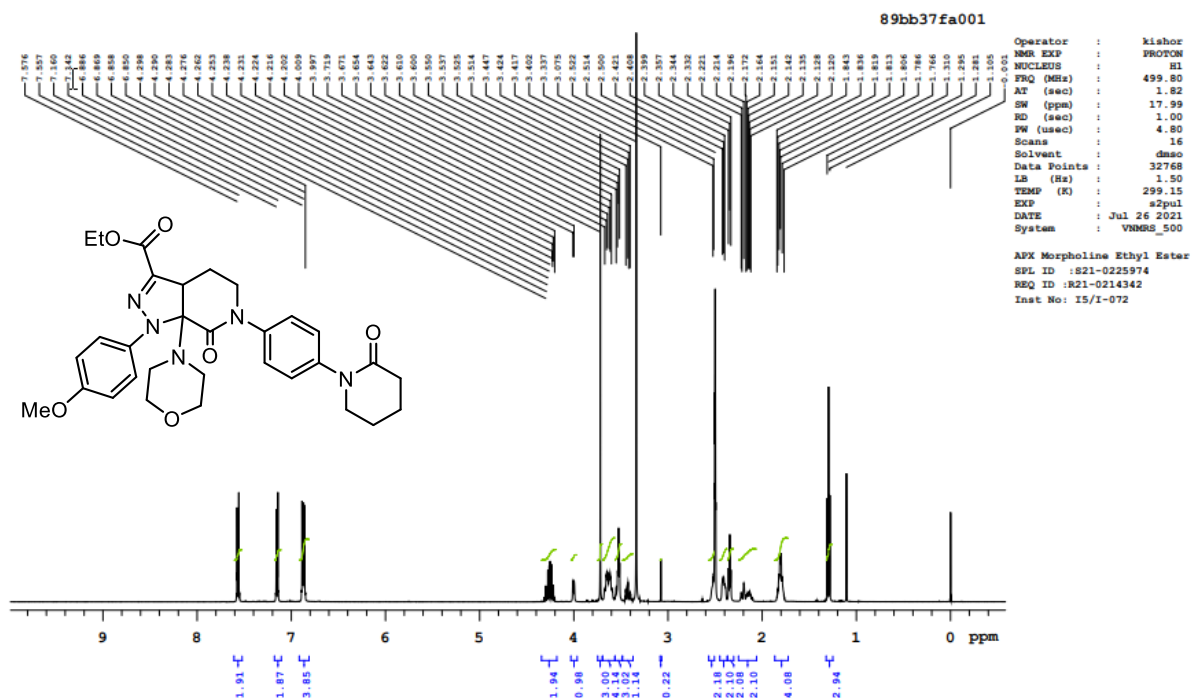


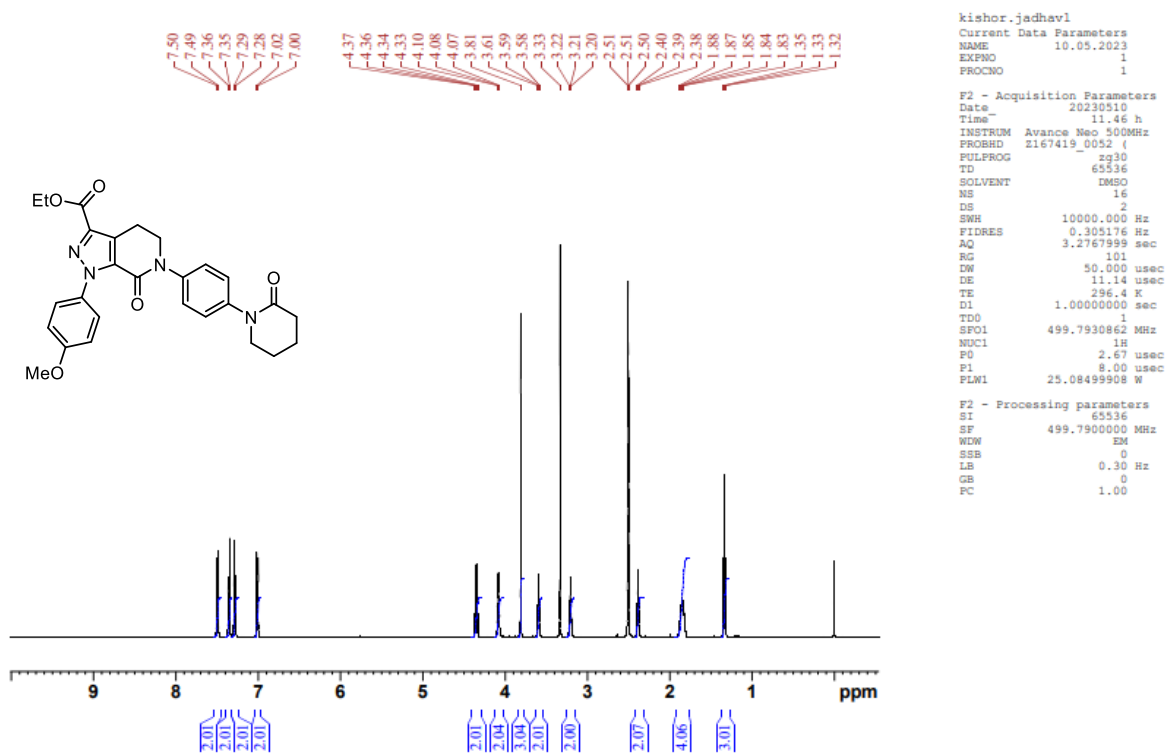








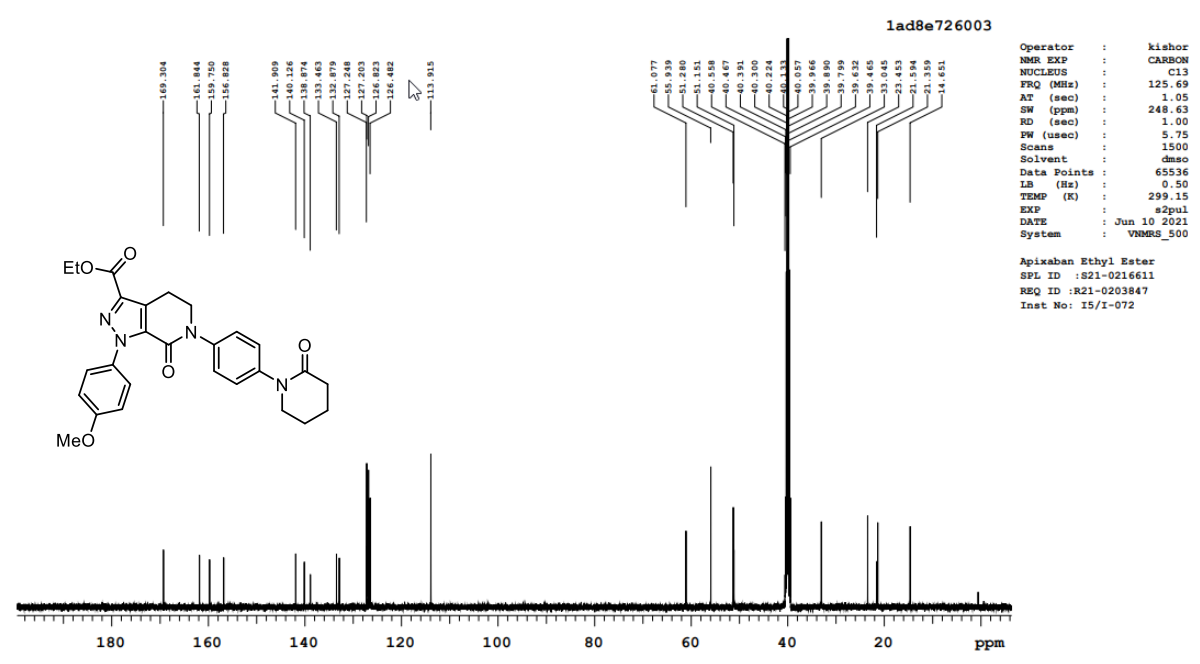




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 PROCNO 1

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 SOLVENT DMSO
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 DS 2
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 FIDRES 0.305176 Hz
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 RG 101
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 DE 11.14 usec
 TE 296.4 K
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 NUC1 1H
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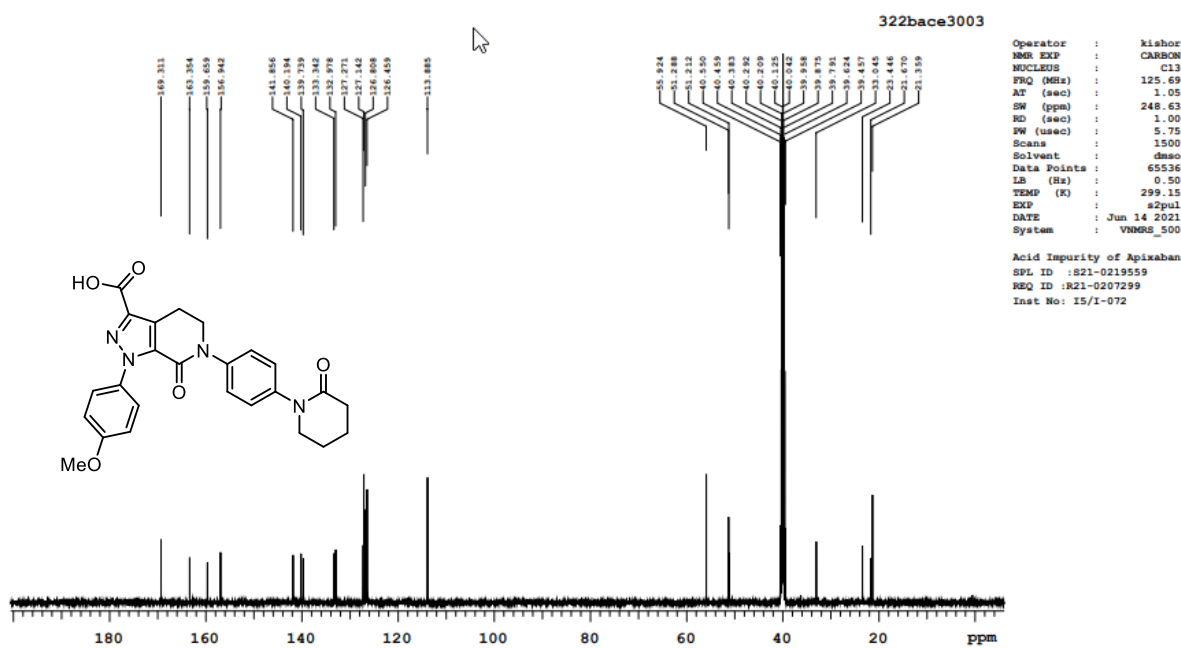
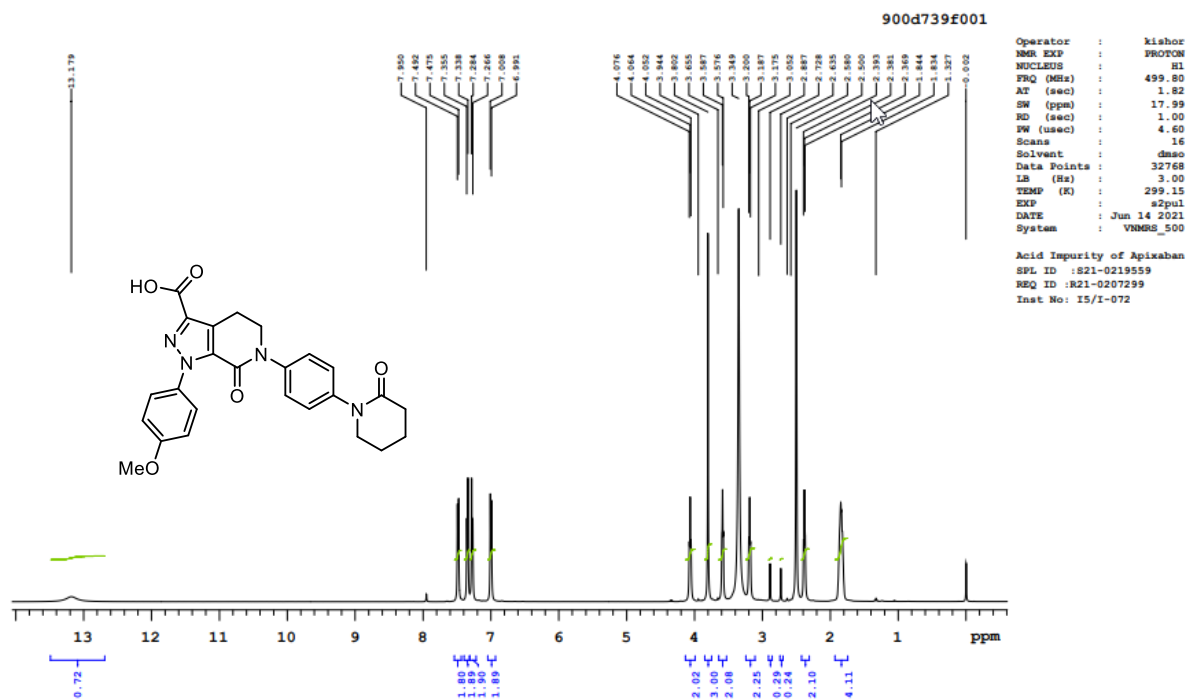
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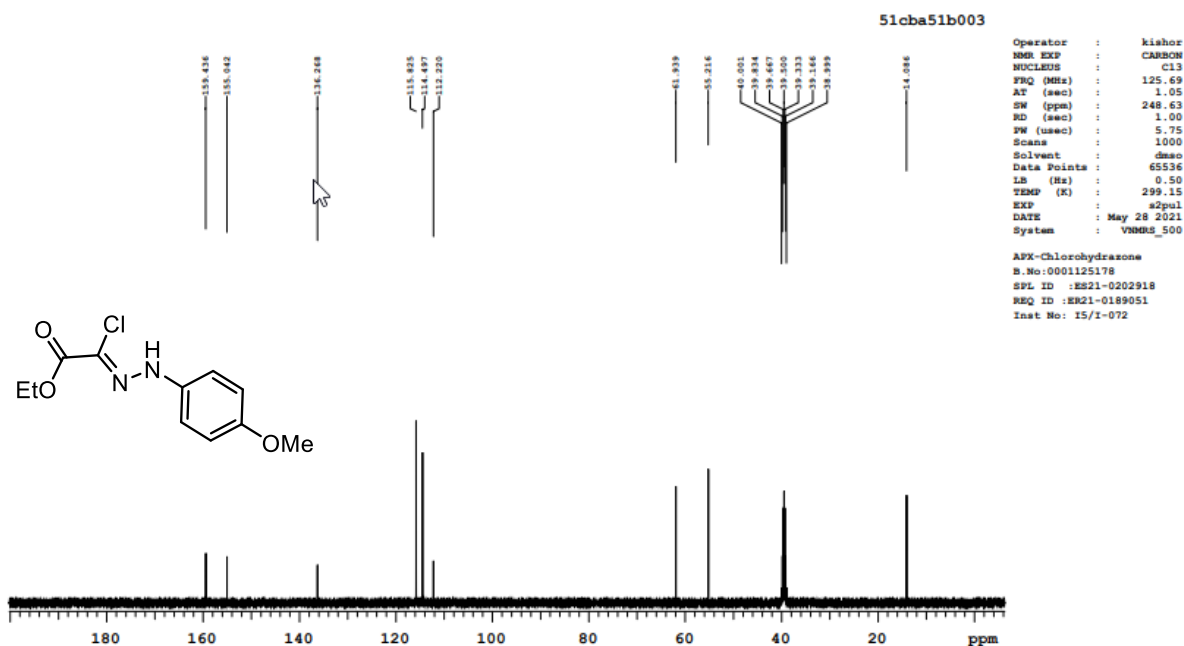
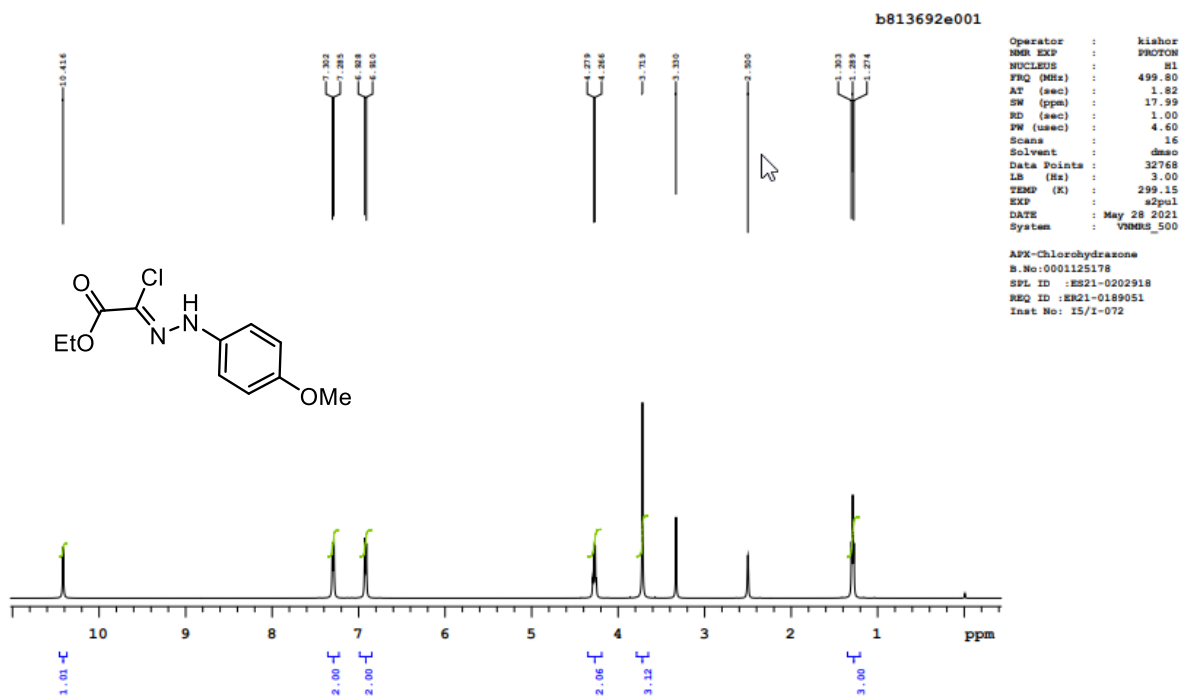


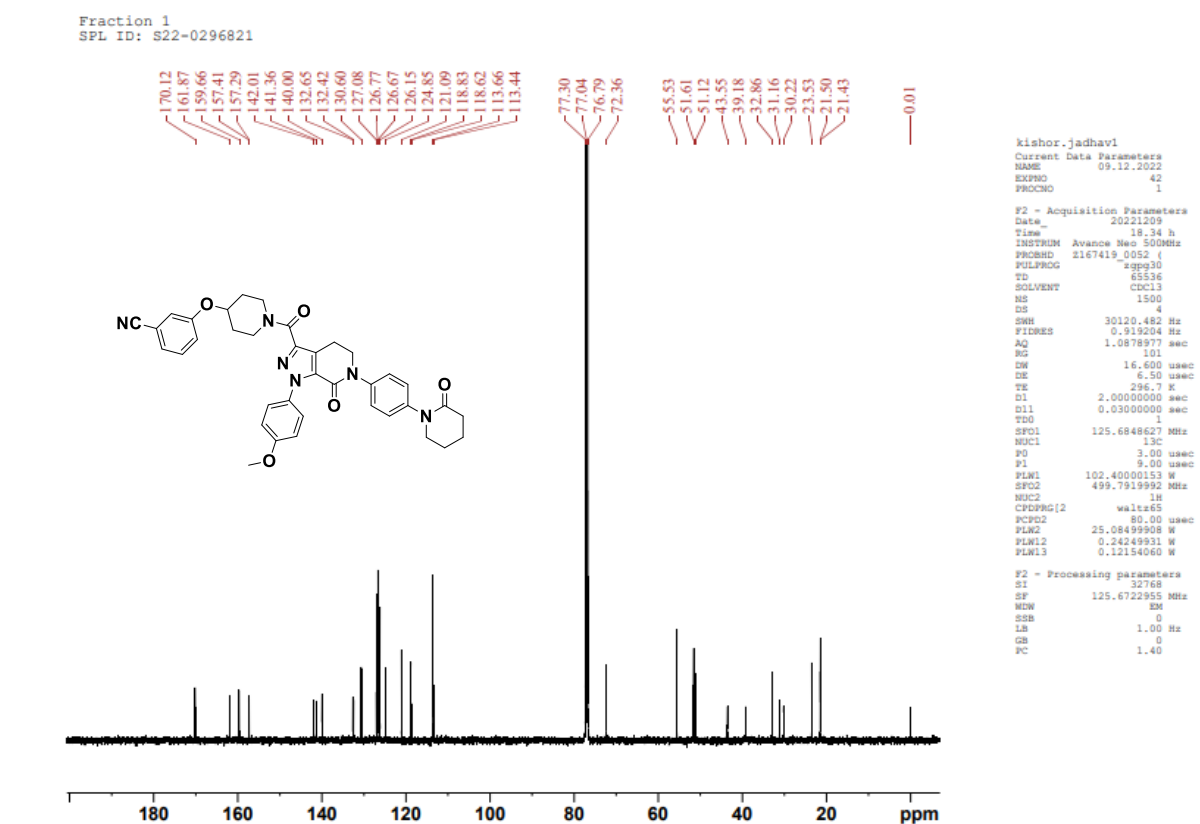
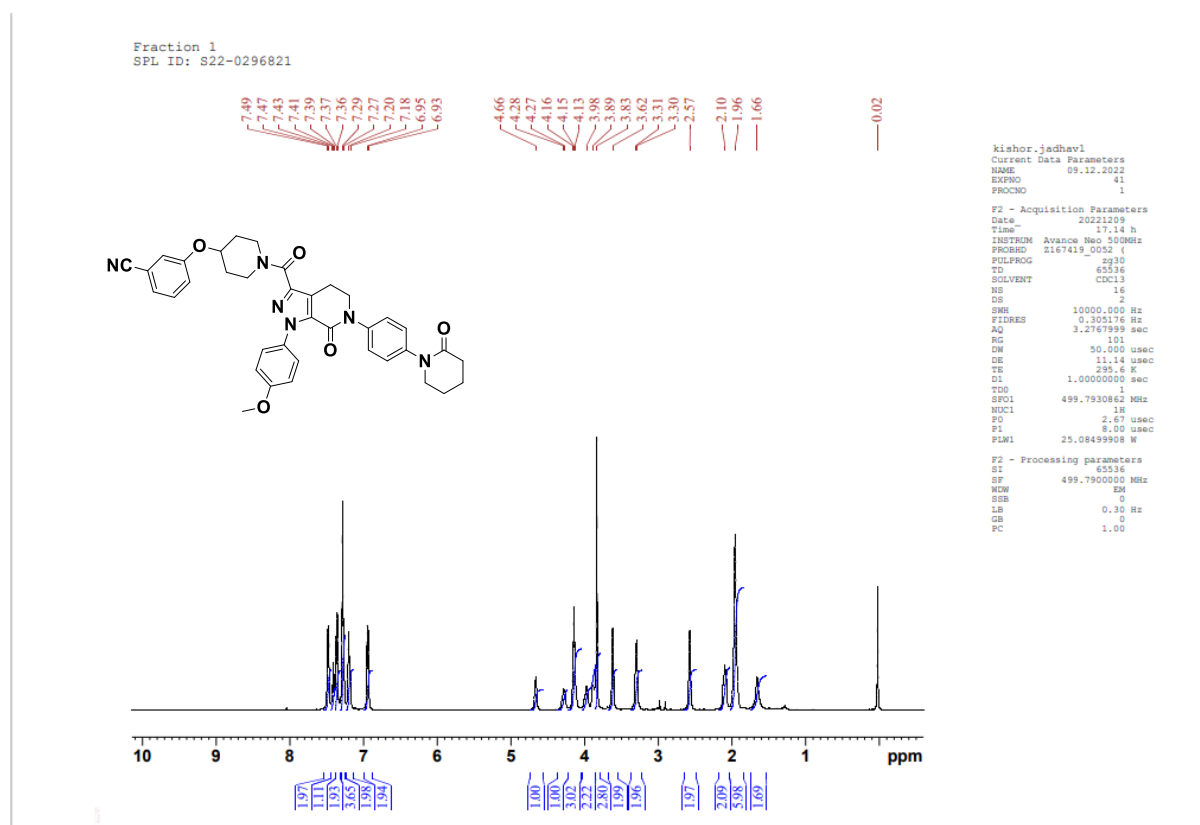
1ad8e726003

Operator : kishor
 NMR EXP : CARBON
 NUCLEUS : C13
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 AT (sec) : 1.05
 SW (ppm) : 248.63
 RD (sec) : 1.00
 PW (usec) : 5.75
 Scans : 1500
 Solvent : dmsd
 Data Points : 65536
 LB (Hz) : 0.50
 TEMP (K) : 299.15
 EXP : s2pul
 DATE : Jun 10 2021
 System : VNMR5_500

Apixaban Ethyl Ester
 SPL ID : S21-0216611
 REQ ID : R21-0203847
 Inst No: I5/I-072

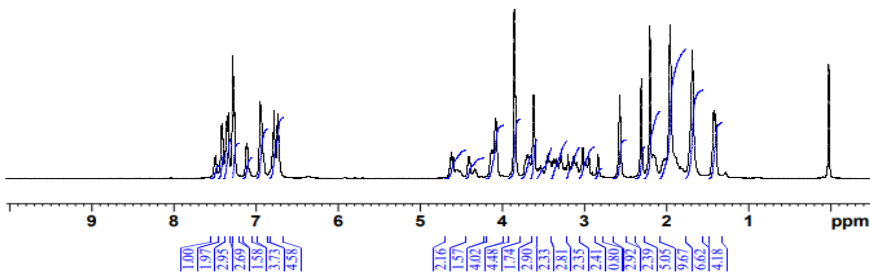
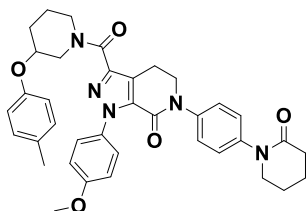






Fraction 2
SPL ID: S22-0296826

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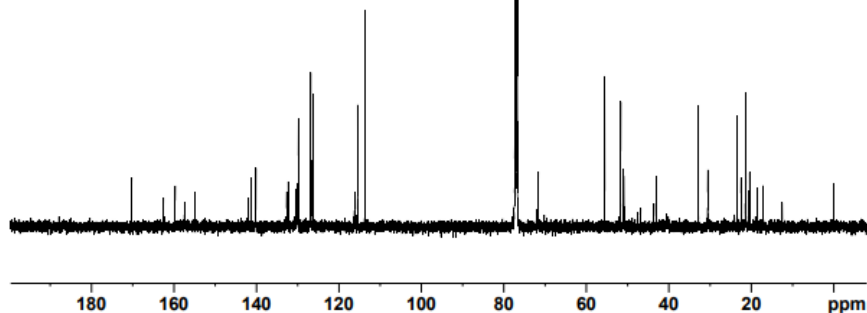
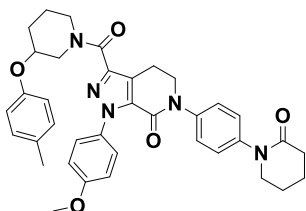
kishor.jadhav1
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EXPNO 51
PROCNO 1

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TD 65536
SOLVENT CDCl3
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DS 2
SWH 10000.000 Hz
FIDRES 0.303176 Hz
AQ 3.2767999 sec
RG 101
DM 50.000 usec
DE 11.14 usec
TE 295.6 K
D1 1.00000000 sec
TDO 1
SFO1 499.7930662 MHz
NUC1 1H
PO 2.67 usec
PI 8.00 usec
PLW1 25.08499908 W

F2 - Processing parameters
SI 65536
SF 499.7900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
    
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Fraction 2
SPL ID: S22-0296826

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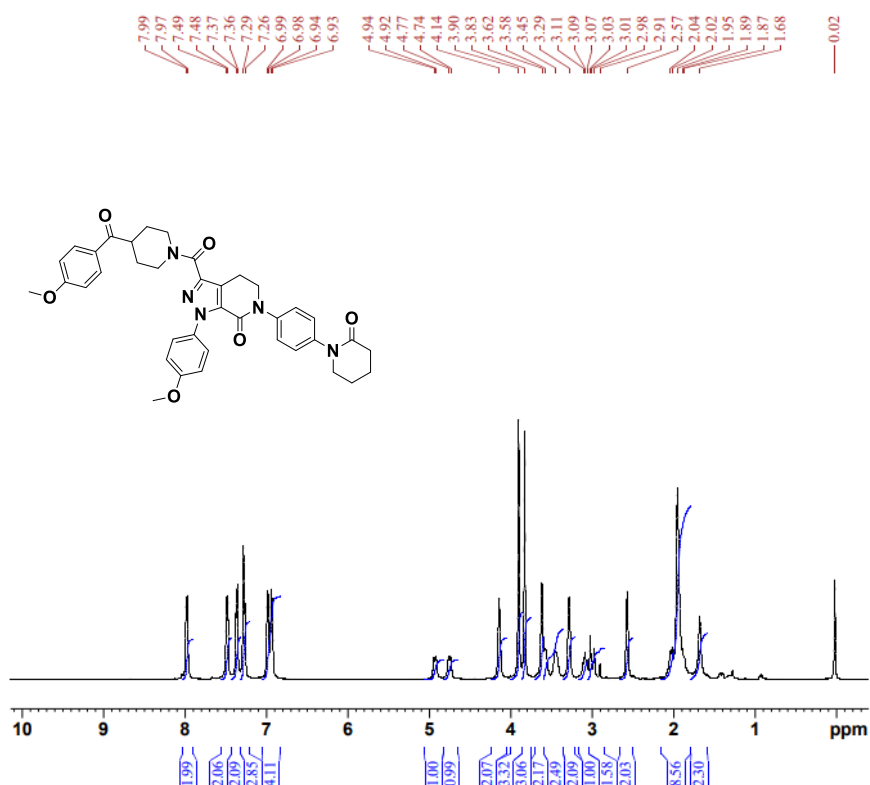
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kishor.jadhav1
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EXPNO 52
PROCNO 1

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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1500
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DM 16.600 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
SFO1 125.6848627 MHz
NUC1 13C
PO 3.00 usec
PI 9.00 usec
PLW1 102.40000153 W
SFO2 499.7919992 MHz
SFO2 499.7919992 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 25.08499908 W
PLW12 0.24249931 W
PLW13 0.12154060 W

F2 - Processing parameters
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SSB 0
LB 1.00 Hz
GB 0
PC 1.40
    
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Fraction 3
SPL ID: S22-0296827



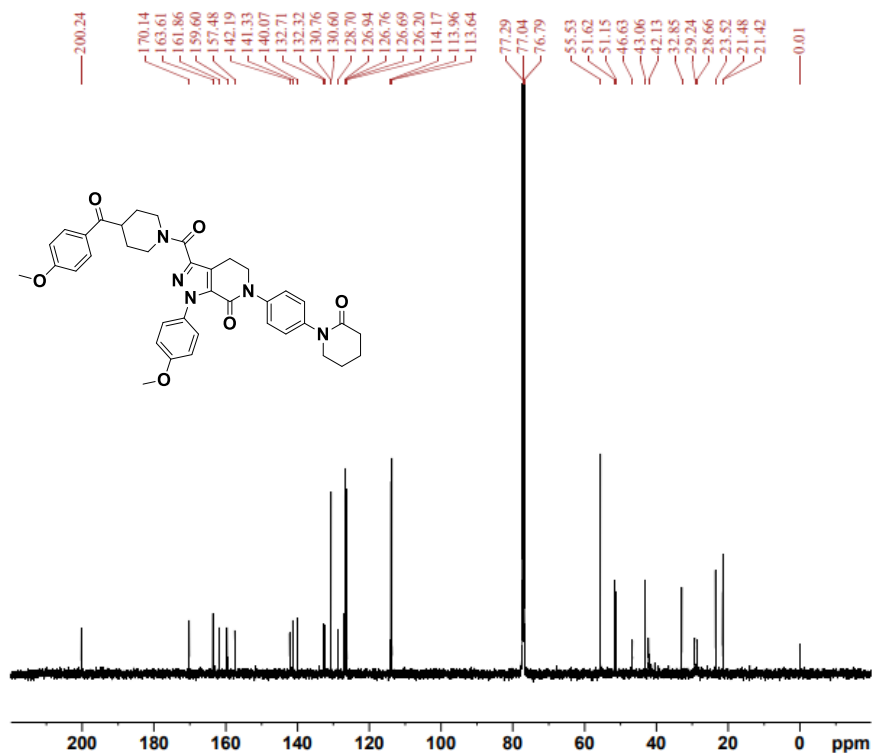
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kishor-jadhavi
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EXPNO    61
PROCNO   1

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PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       10000.000 Hz
FIDRES    0.305176 Hz
AQ        3.276799 sec
RG        101
DN        50.000 usec
DE        11.14 usec
TE        295.8 K
D1        1.00000000 sec
SFO1     499.7930862 MHz
NUC1      1H
PC        2.67 usec
P1        8.00 usec
PLW1     25.08499908 W

F2 - Processing parameters
SI        65536
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SSB       0
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GB        0
PC        1.00
    
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Fraction 3
SPL ID: S22-0296827

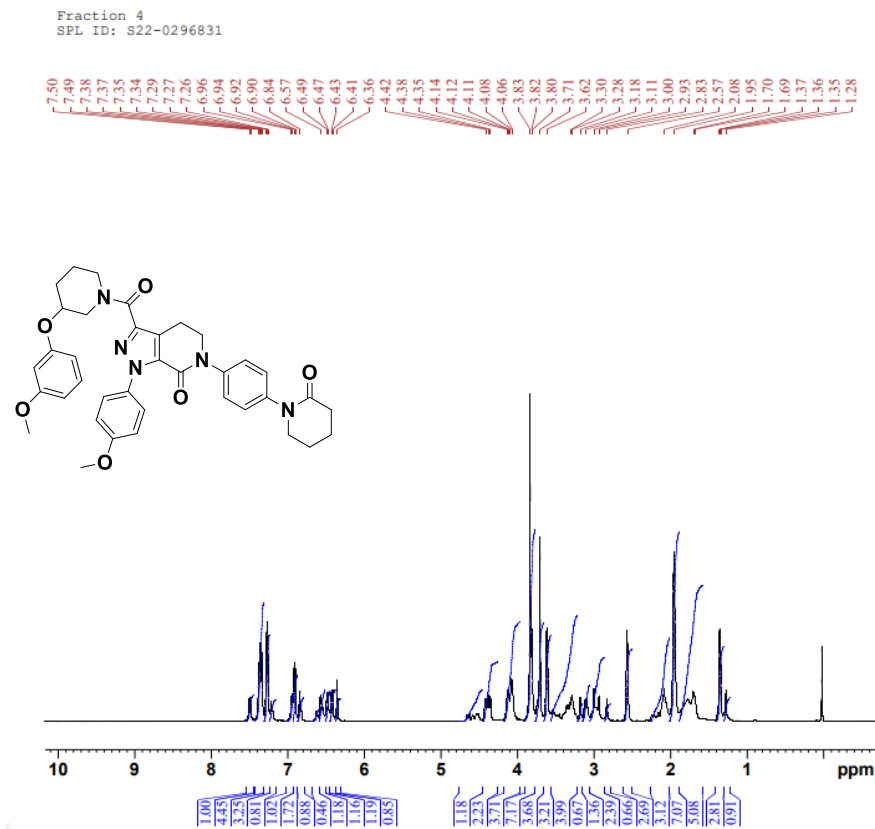


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kishor-jadhavi
Current Data Parameters
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EXPNO    62
PROCNO   1

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INSTRUM  Avance Neo 500MHz
PROBHD   2167419_0052 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        1500
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FIDRES    0.919204 Hz
AQ        1.0878977 sec
RG        101
DN        16.600 usec
DE        6.50 usec
TE        298.1 K
D1        2.00000000 sec
D11       0.03000000 sec
SFO1     125.6848627 MHz
NUC1      13C
PC        3.00 usec
P1        9.00 usec
PLW1     102.40000153 W
SFO2     499.7919994 MHz
NUC2      1H
CPDPRG2  waltz65
PCPD2    80.00 usec
PLW2     25.08499908 W
PLW12    0.24249931 W
PLW13    0.12154068 W

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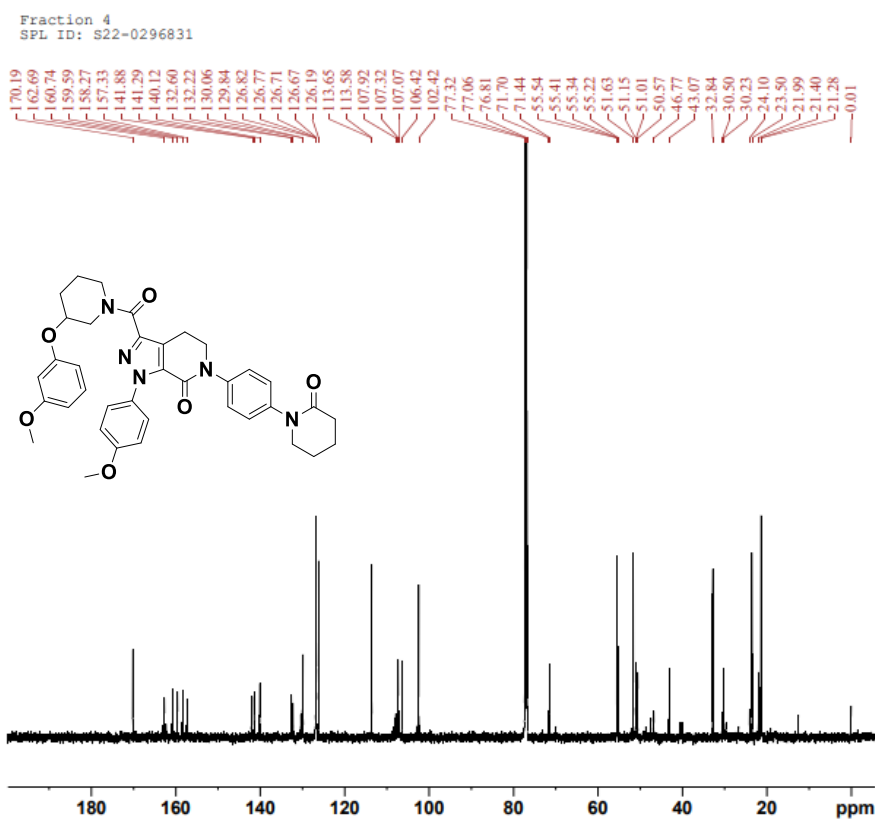


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kishor.jadhavi
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EXPNO    71
PROCNO   1

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Time     21.32 h
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PROBHD   2167419_0052 (
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      10000.000 Hz
FIDRES   0.305176 Hz
AQ       3.2767999 sec
RG       101
DN       50.000 usec
DE       11.14 usec
TE       297.0 K
D1       1.0000000 sec
TDO      1
SFO1     499.7930862 MHz
NUC1     1H
PC       2.67 usec
PI       8.00 usec
PLW1     25.08499908 W

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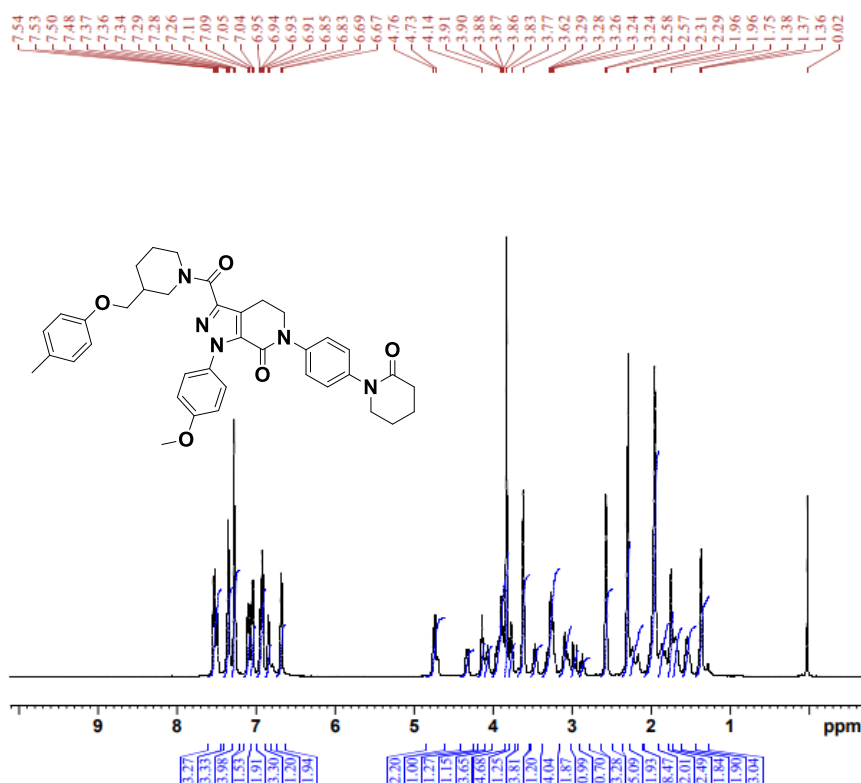
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kishor.jadhavi
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EXPNO    72
PROCNO   1

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Time     22.52 h
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PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       1500
DS       4
SWH      30120.482 Hz
FIDRES   0.919204 Hz
AQ       1.0878977 sec
RG       101
DN       16.600 usec
DE       6.50 usec
TE       297.0 K
D1       2.0000000 sec
D11      0.0300000 sec
TDO      1
SFO1     125.6848627 MHz
NUC1     13C
PC       3.00 usec
PI       3.00 usec
PLW1     102.4000153 W
SFO2     499.7919992 MHz
NUC2     1H
CPDPRG2  waltz65
PCPD2    80.00 usec
PLW2     25.08499908 W
PLW12    0.2424931 W
PLW13    0.12154060 W

F2 - Processing parameters
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Fraction 5
SPL ID: S22-0296832



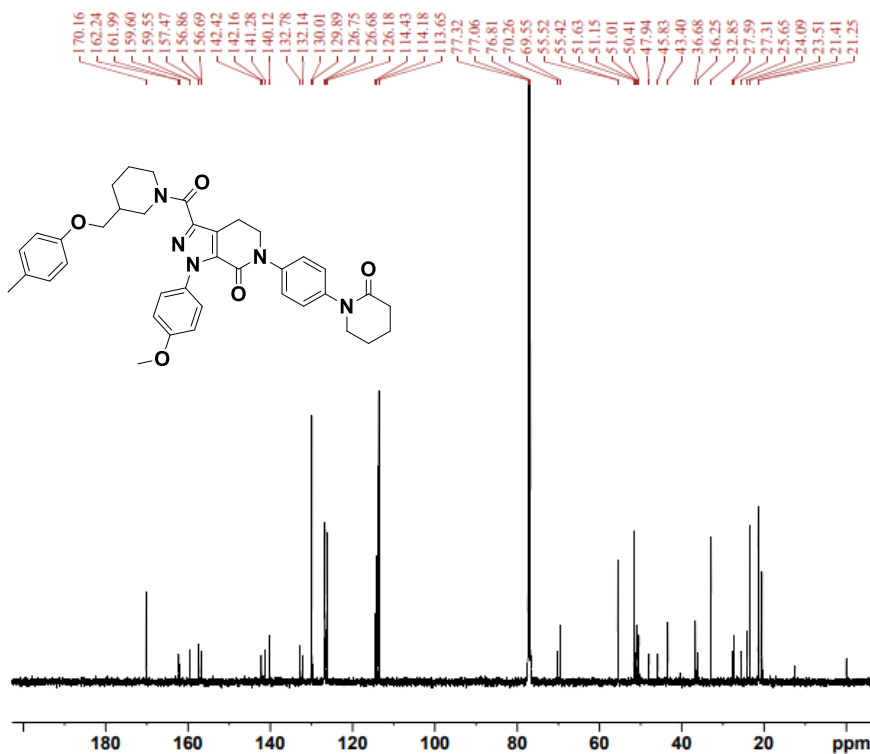
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kishor.jadhavi
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EXPNO    81
PROCNO   1

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SOLVENT  CDCl3
NS        16
DS        2
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FIDRES    0.305176 Hz
AQ         3.2767999 sec
RG         101
DE         50.000 usec
TE         11.14 usec
TE        296.0 K
D1         1.00000000 sec
TDO        1
SFO1      499.7930862 MHz
NUC1       1H
PC         2.67 usec
PL         8.00 usec
PLW1      25.08499908 W

F2 - Processing parameters
SI         65536
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Fraction 5
SPL ID: S22-0296832



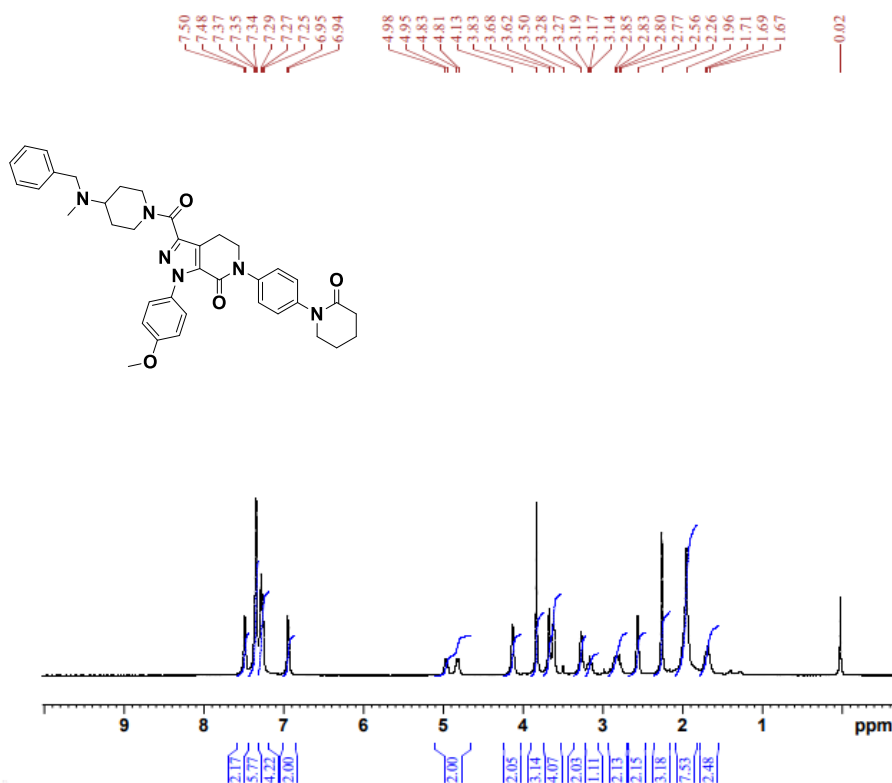
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kishor.jadhavi
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EXPNO    82
PROCNO   1

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SOLVENT  CDCl3
NS        1500
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FIDRES    0.319204 Hz
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RG         101
DE         16.600 usec
TE         6.50 usec
TE        297.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1
SFO1      125.6848627 MHz
NUC1       13C
PC         3.00 usec
PL         9.00 usec
PLW1      102.40000153 W
SFO2      499.7919992 MHz
NUC2       1H
CPCPPRG2  waltz65
PCPD2     80.00 usec
PLM2      25.08499908 W
PLW2      0.24249931 W
PLW12     0.24249931 W
PLW13     0.12154060 W

F2 - Processing parameters
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Fraction 6
SPL ID: S22-0296833



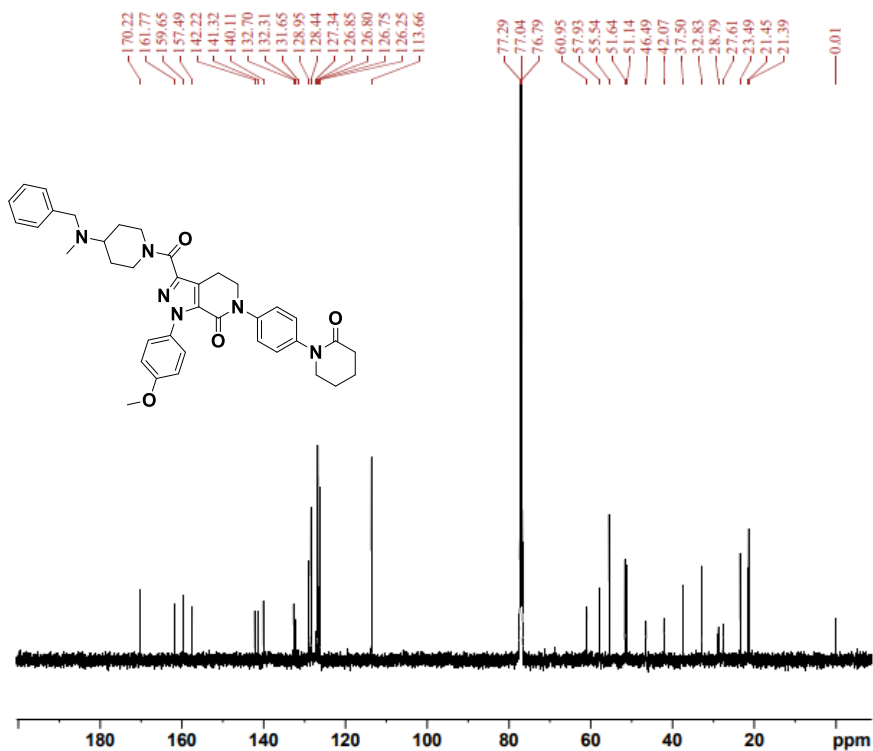
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PULPROG   zg30
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SOLVENT   CDCl3
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FIDRES     0.305176 Hz
AQ         3.2767999 sec
RG         101
DW         50.000 usec
DE         11.14 usec
TE         295.7 K
D1         1.00000000 sec
TDO        1
SFO1       499.7930862 MHz
NUC1       1H
PQ         2.67 usec
P1         8.00 usec
PLW1       25.08499908 W

F2 - Processing parameters
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Fraction 6
SPL ID: S22-0296833



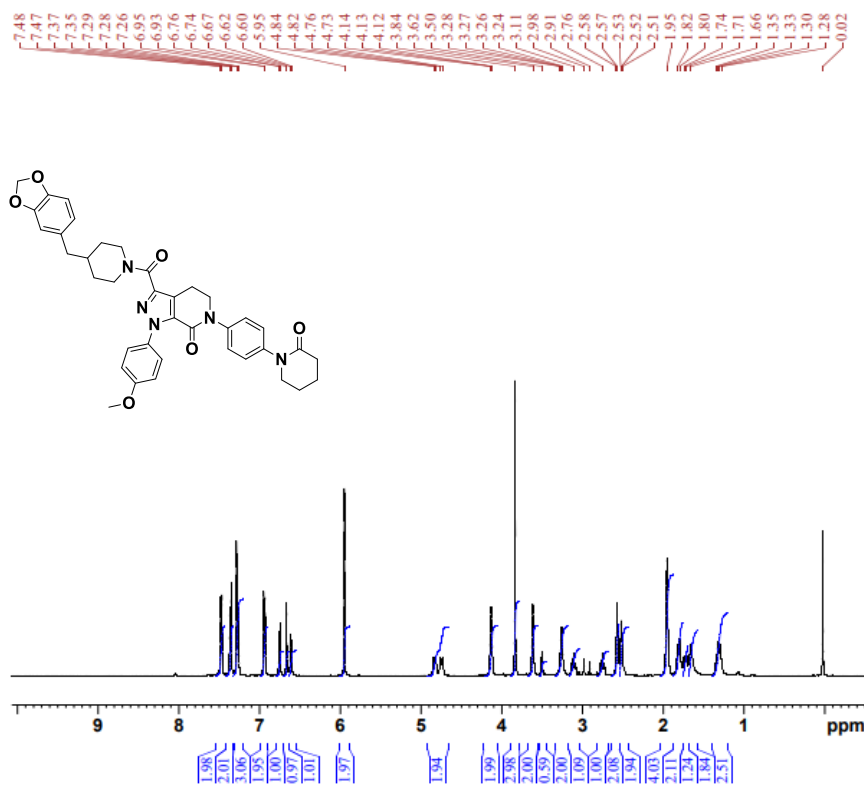
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PROCNO    1

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PULPROG   zgpg30
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SOLVENT   CDCl3
NS         1500
DS         4
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FIDRES     0.919204 Hz
AQ         1.0878977 sec
RG         101
DW         16.600 usec
DE         6.50 usec
TE         296.8 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1
SFO1       125.6848627 MHz
NUC1       13C
PQ         3.00 usec
P1         9.00 usec
PLW1       102.4000153 W
SFO2       499.7919992 MHz
NUC2       1H
CPDPRG2   waltz65
PCPG2     80.00 usec
PLW2       25.08499908 W
PLW12     0.24249931 W
PLW13     0.12154060 W

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Fraction 7
SPL ID: S22-0296834

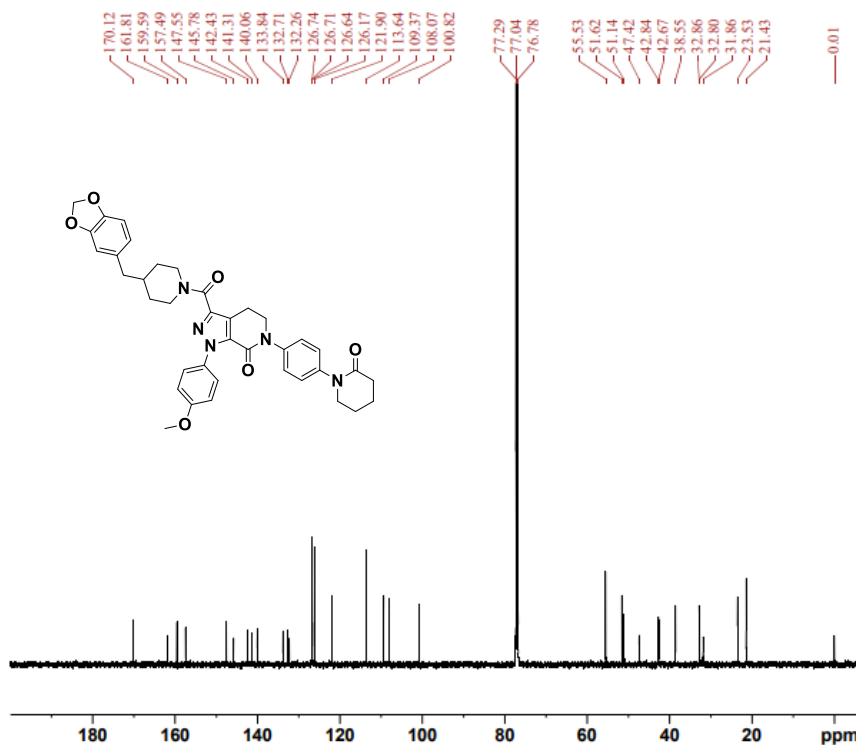


Kishor.jadhavi
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EXPNO 21
PROCNO 1

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SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DW 50.000 usec
DE 11.14 usec
TE 295.7 K
D1 1.0000000 sec
TDO 1
SFO1 499.7930862 MHz
NUC1 1H
PQ 2.67 usec
P1 8.00 usec
PLW1 25.08499908 W

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PC 1.00

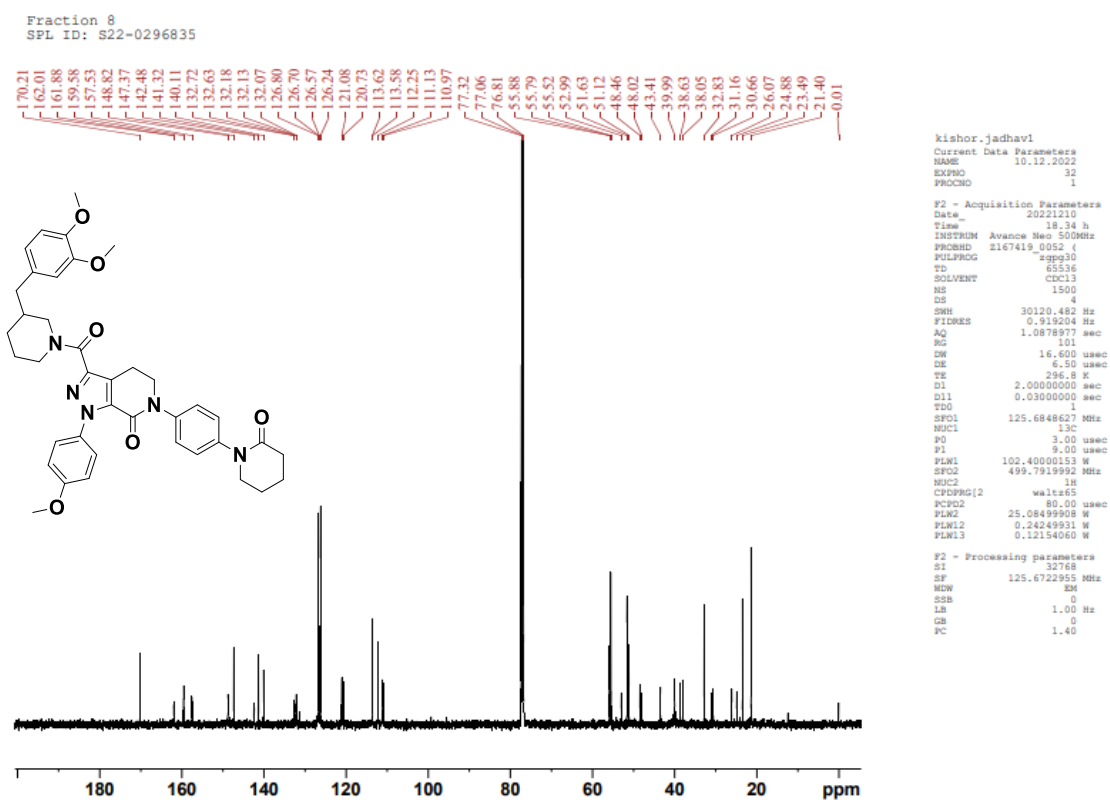
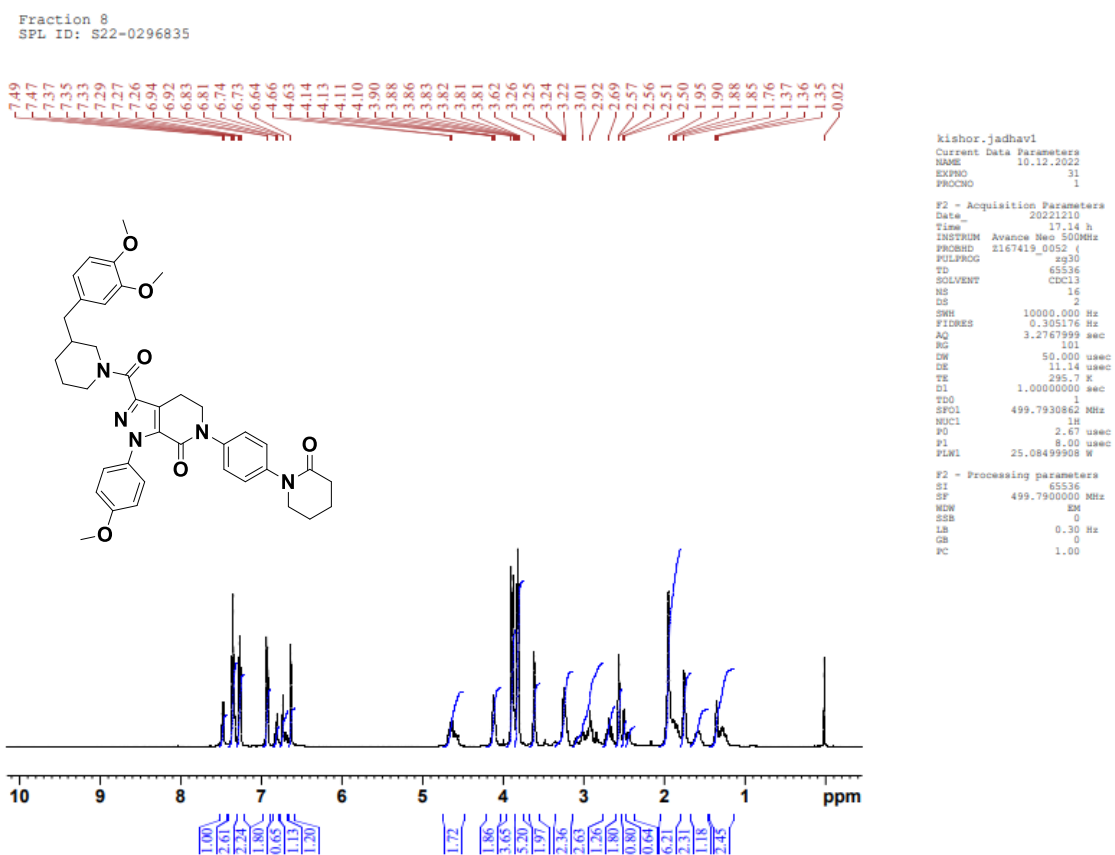
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SPL ID: S22-0296834



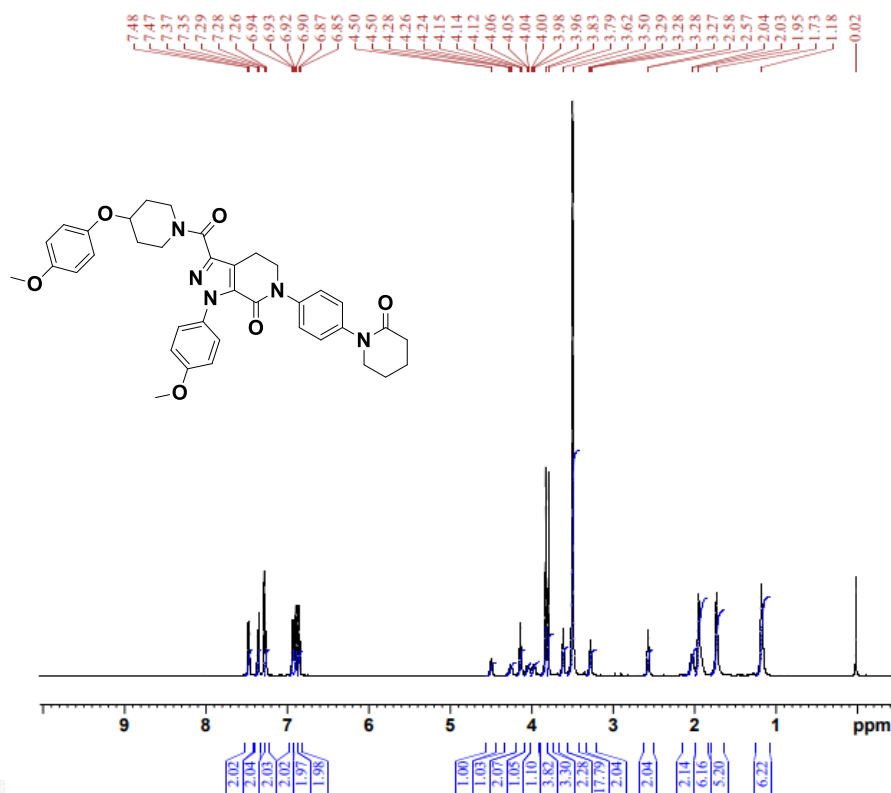
Kishor.jadhavi
Current Data Parameters
NAME 10.12.2022
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221210
Time 21.20 h
INSTRUM Avance Neo 500MHz
PROCNO 2167419_0052 ()
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1500
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DW 16.600 usec
DE 6.50 usec
TE 297.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1
SFO1 125.6848627 MHz
NUC1 13C
PQ 3.00 usec
P1 9.00 usec
PLW1 102.40000153 W
SFO2 499.7919992 MHz
NUC2 1H
CPCPRG2 waltz165
PCPD2 80.00 usec
PLW2 25.08499908 W
PLW12 0.24249931 W
PLW13 0.12154060 W

F2 - Processing parameters
SI 32768
SF 125.6722955 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Fraction 9
SPL ID: S22-0296836

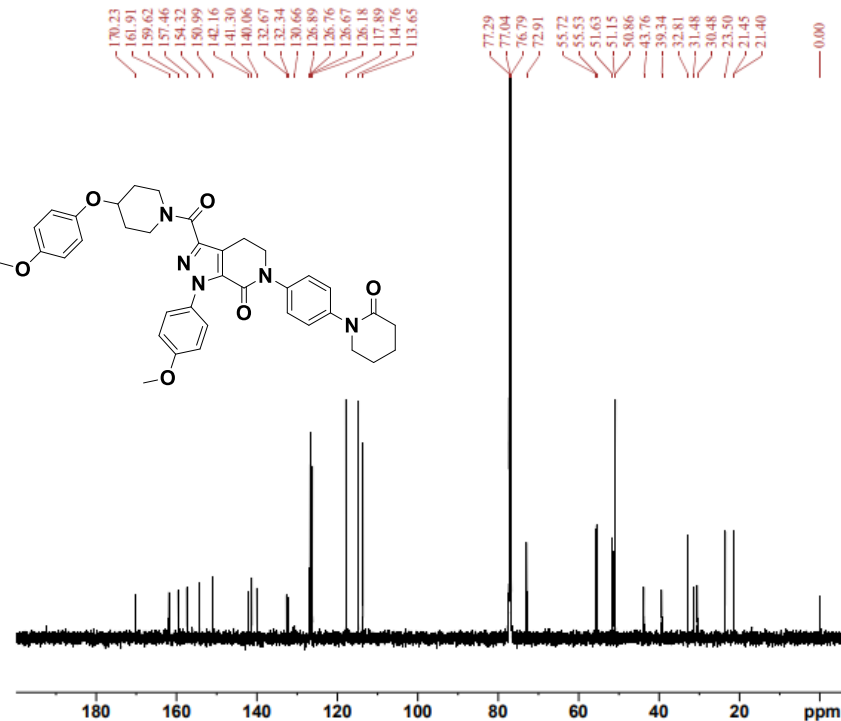


kishor.jadhavi
Current Data Parameters
NAME 10.12.2022
EXPNO 41
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221210
Time_ 21.25 h
INSTRUM Avance Neo 500MHz
PROBHD z167419_0052 (z
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DW 50.000 usec
DE 11.14 usec
TE 295.9 K
D1 1.00000000 sec
TD0 1
SFO1 499.7930862 MHz
NUC1 1H
P0 2.87 usec
P1 8.00 usec
PLW1 25.08499908 W

F2 - Processing parameters
SI 65536
SF 499.7900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fraction 9
SPL ID: S22-0296836

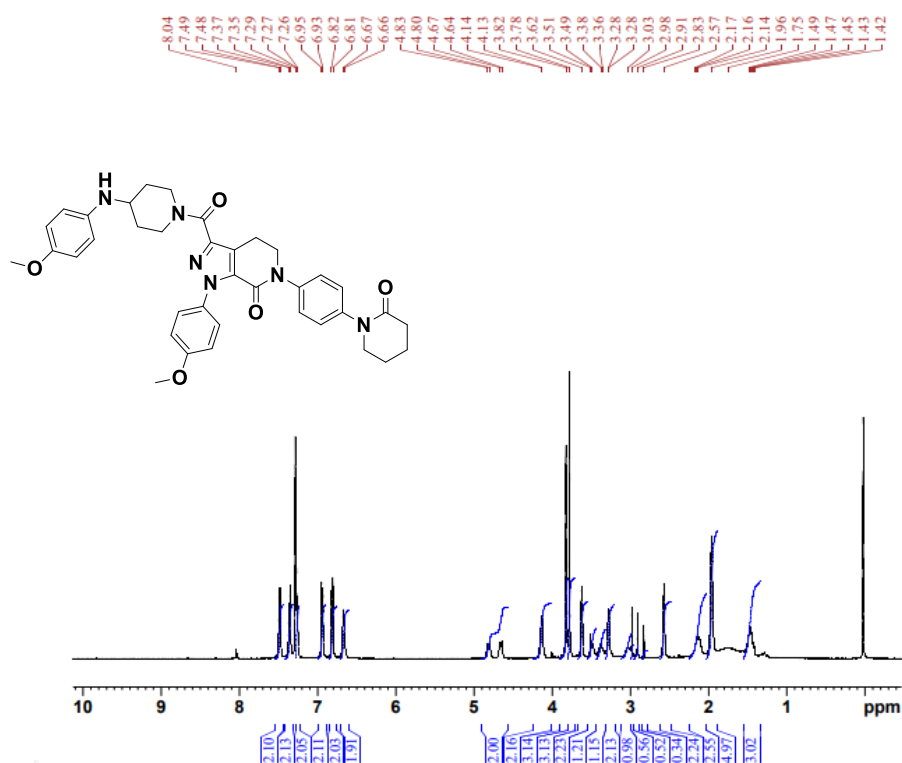


kishor.jadhavi
Current Data Parameters
NAME 10.12.2022
EXPNO 42
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221210
Time_ 22.45 h
INSTRUM Avance Neo 500MHz
PROBHD z167419_0052 (z
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1500
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DW 16.600 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.05000000 sec
TD0 1
SFO1 125.6848627 MHz
NUC1 13C
P0 3.00 usec
P1 9.00 usec
PLM1 102.40000153 W
SFO2 499.7919992 MHz
NUC2 1H
CPDPRG2 waltz165
PCPD2 80.00 usec
PLM2 25.08499908 W
PLM12 0.21249931 W
PLM13 0.12154060 W

F2 - Processing parameters
SI 32768
SF 125.6722955 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Fraction 10
SPL ID: S22-0296838



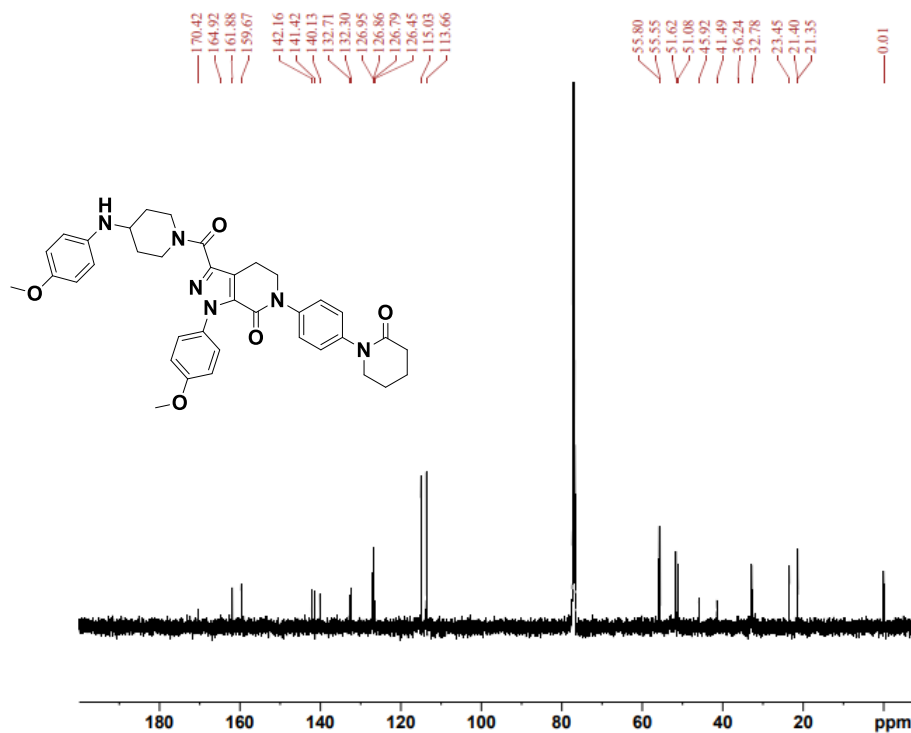
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kishor.jadhavi
Current Data Parameters
NAME      10.12.2022
EXPNO    51
PROCNO   1

F2 - Acquisition Parameters
Date_    20221210
Time     22:50 h
INSTRUM  Avance Neo 500MHz
PROBHD   2167419_0052 (
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       10000.000 Hz
FIDRES    0.305176 Hz
AQ        3.2767999 sec
RG         101
DN         50.000 usec
DE         11.14 usec
TE         295.9 K
D1         1.00000000 sec
TDO        1
SFO1      499.7930862 MHz
NUC1       1H
PC         2.67 usec
P1         8.00 usec
PLW1      25.08499908 W

F2 - Processing parameters
SI         65536
SF         499.7900000 MHz
WDW        EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00
    
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Fraction 10
SPL ID: S22-0296838



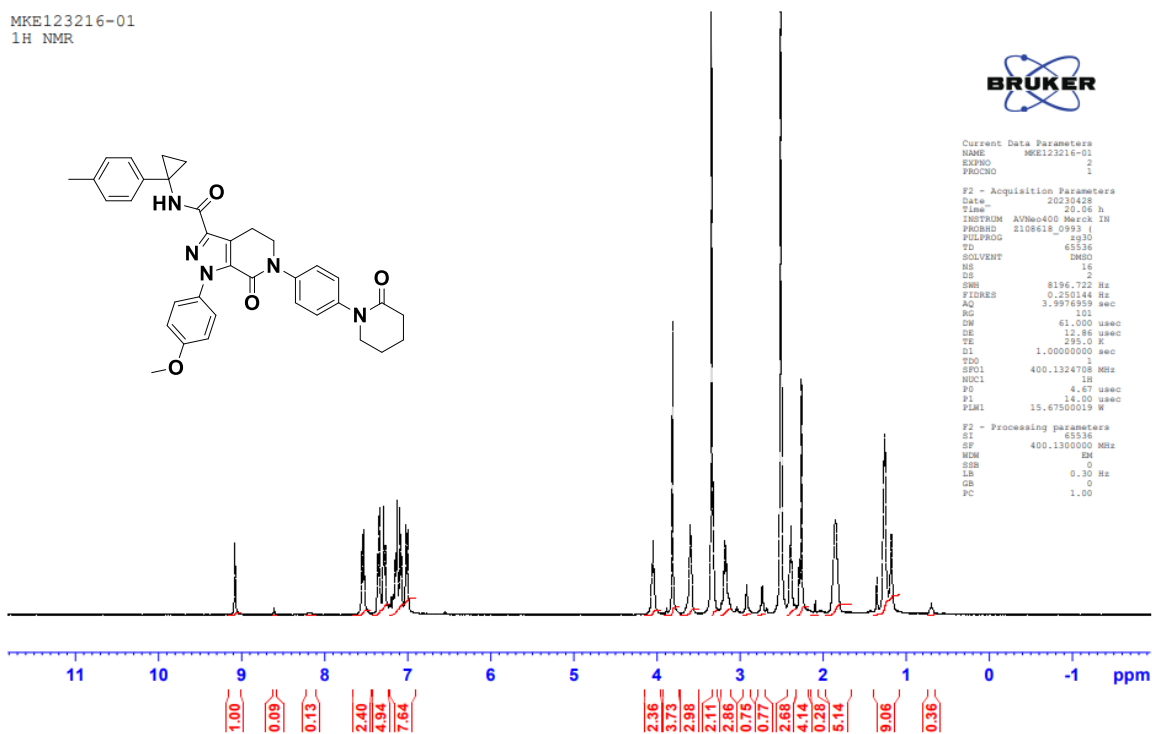
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kishor.jadhavi
Current Data Parameters
NAME      10.12.2022
EXPNO    52
PROCNO   1

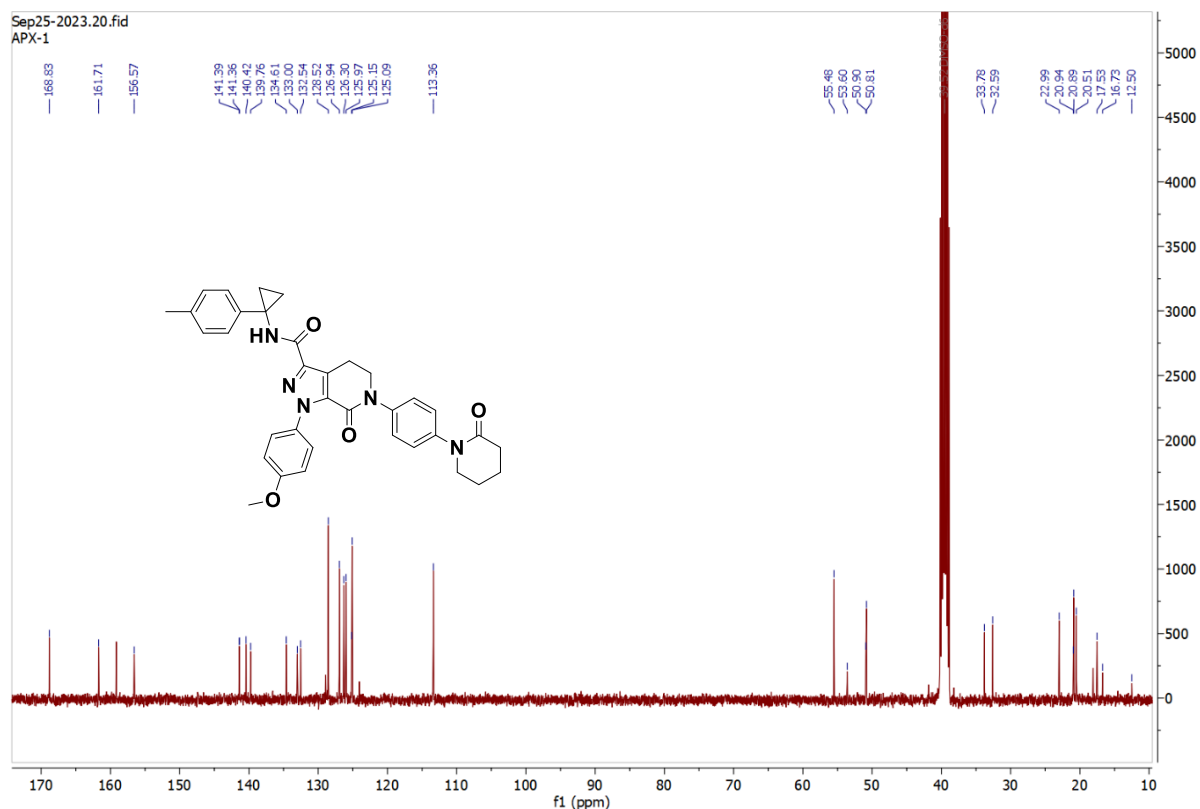
F2 - Acquisition Parameters
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Time     0:10 h
INSTRUM  Avance Neo 500MHz
PROBHD   2167419_0052 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        1500
DS        4
SWH       30120.482 Hz
FIDRES    0.919204 Hz
AQ        1.0878977 sec
RG         101
DN         16.600 usec
DE         6.50 usec
TE         297.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1
SFO1      125.6848627 MHz
NUC1       13C
PC         3.00 usec
P1         9.00 usec
PLW1      102.40000153 W
SFO2      499.7919992 MHz
NUC2       1H
CPDPRG2  waltz65
PCPD2     80.00 usec
PLW2      25.08499908 W
PLW12     0.24249931 W
PLW13     0.12154060 W

F2 - Processing parameters
SI         32768
SF         125.6722955 MHz
WDW        EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
    
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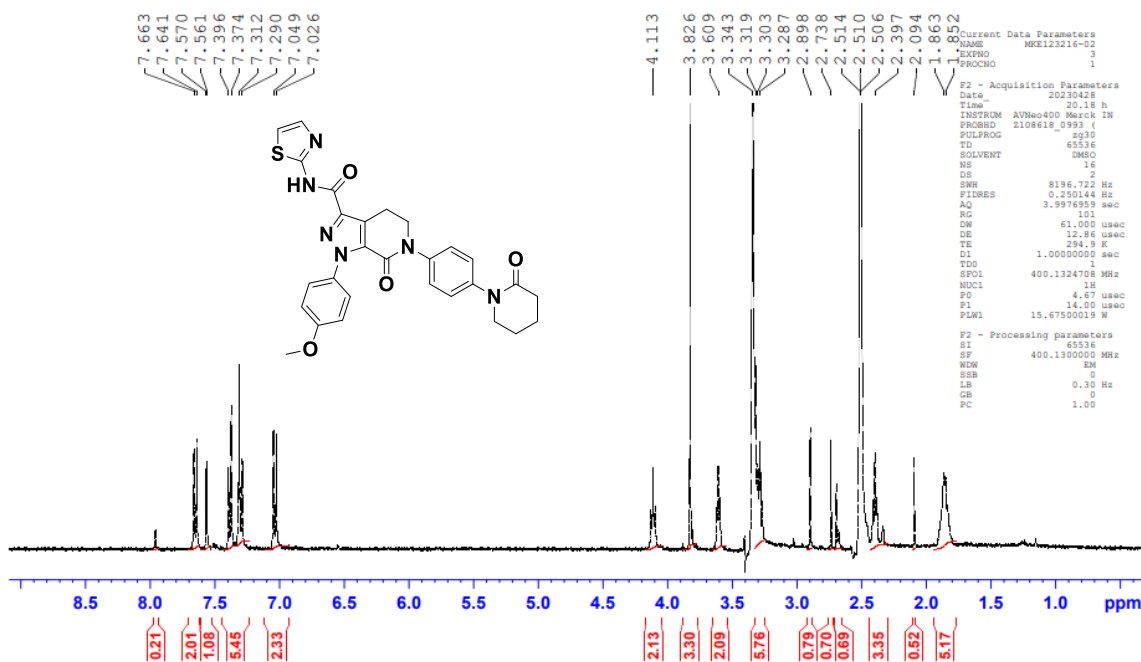
MKE123216-01
1H NMR



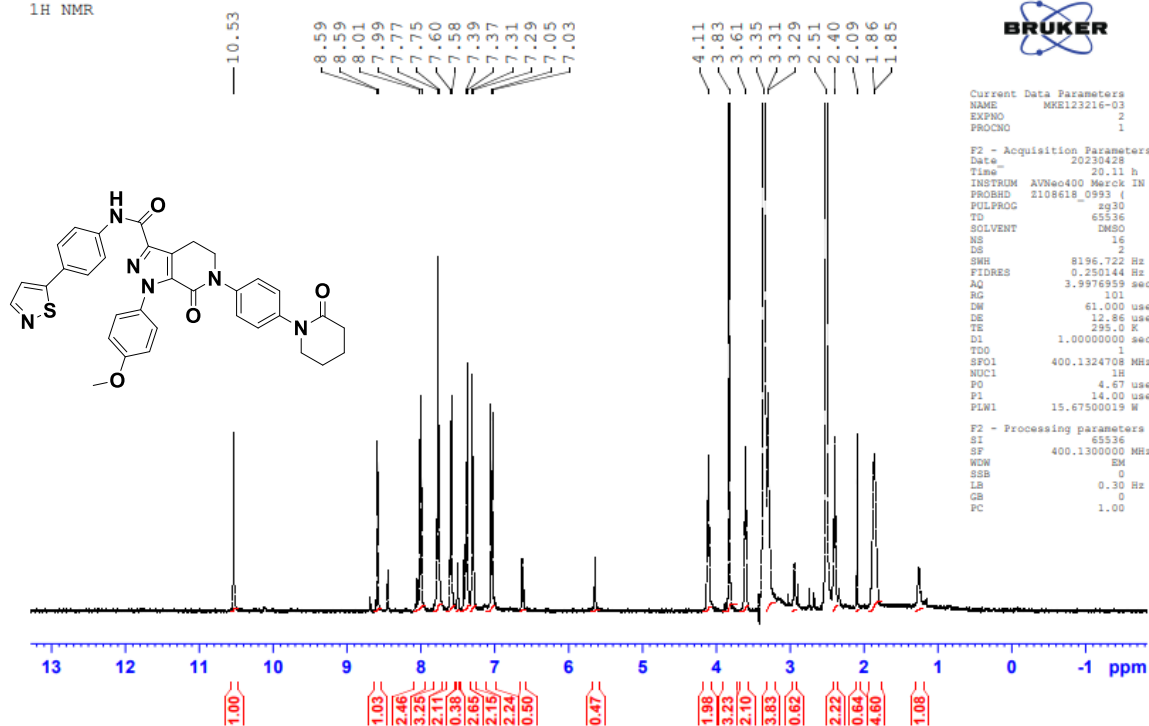
Sep25-2023.20.fid
APX-1



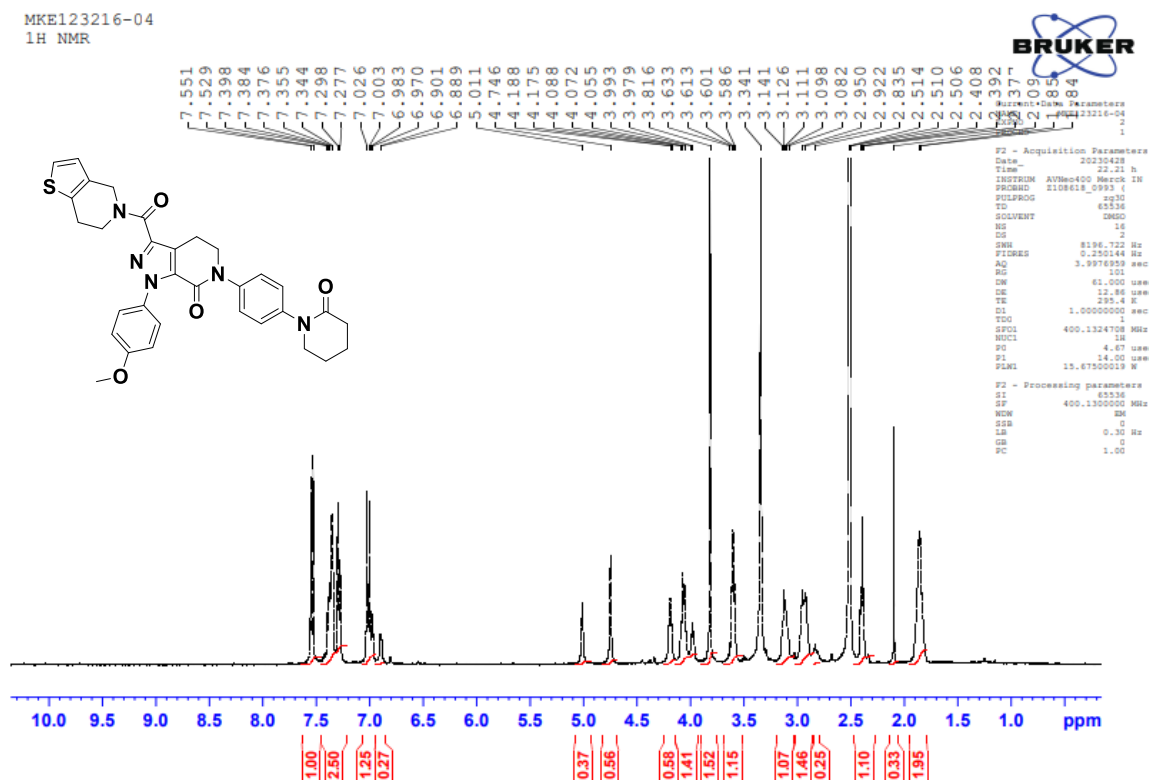
MKE123216-02
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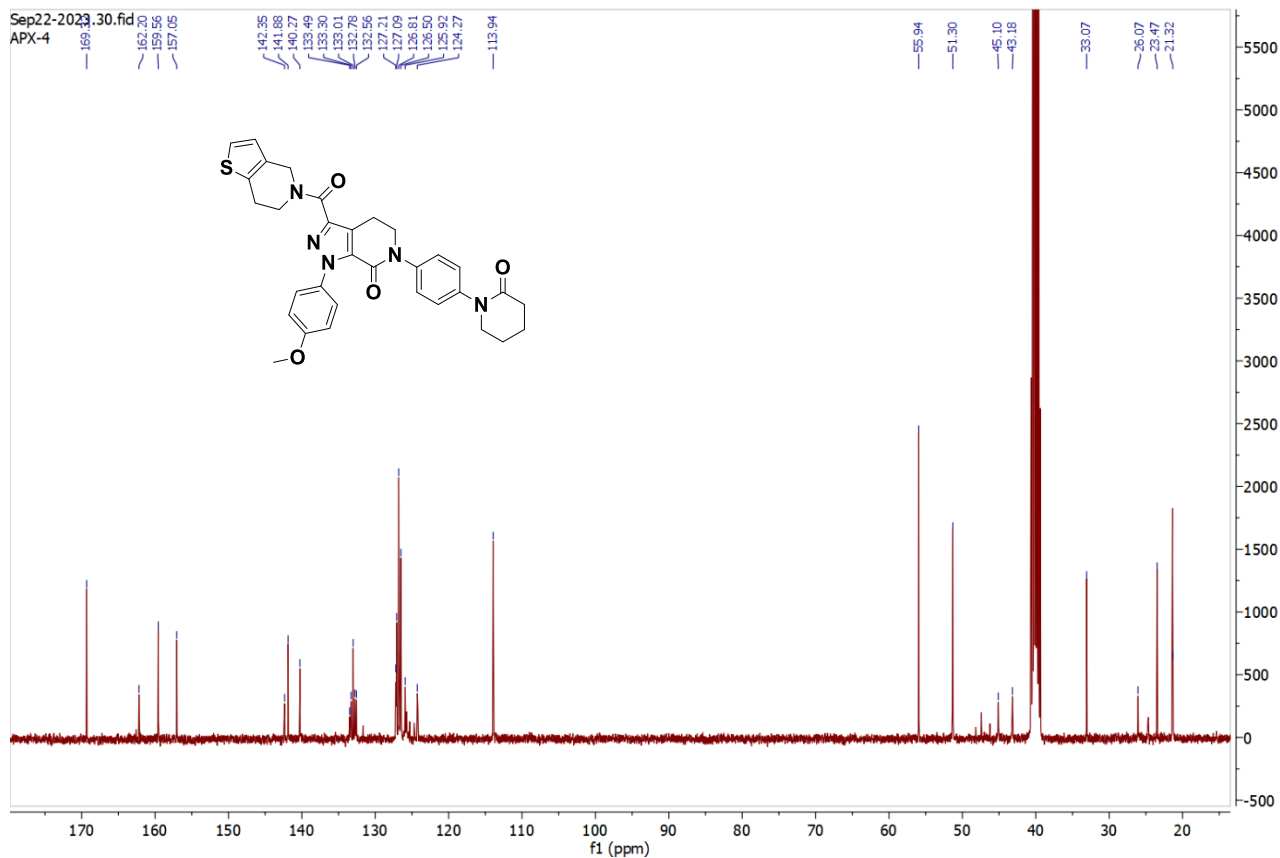
MKE123216-03
1H NMR



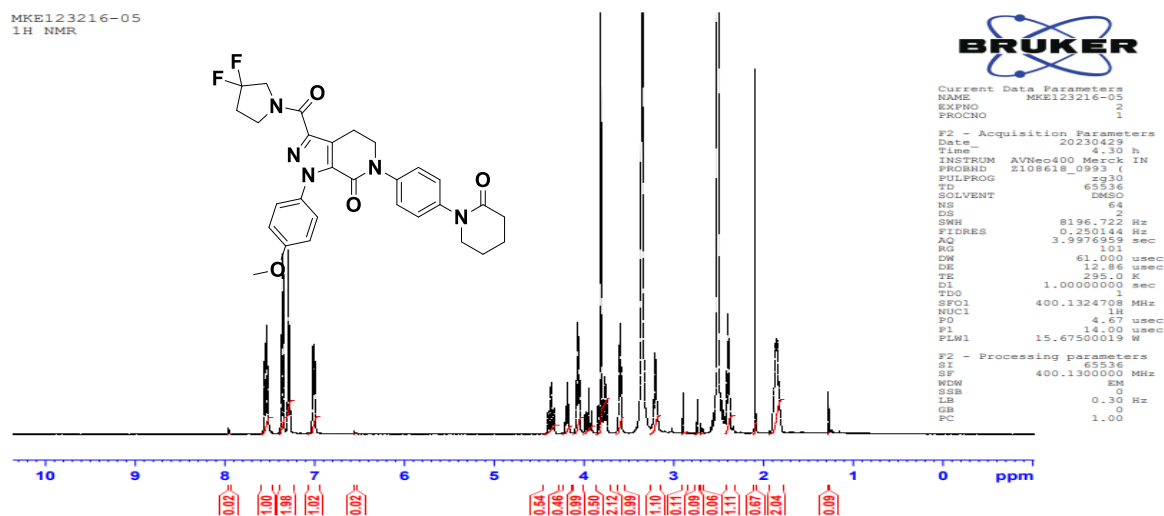
MKE123216-04
1H NMR



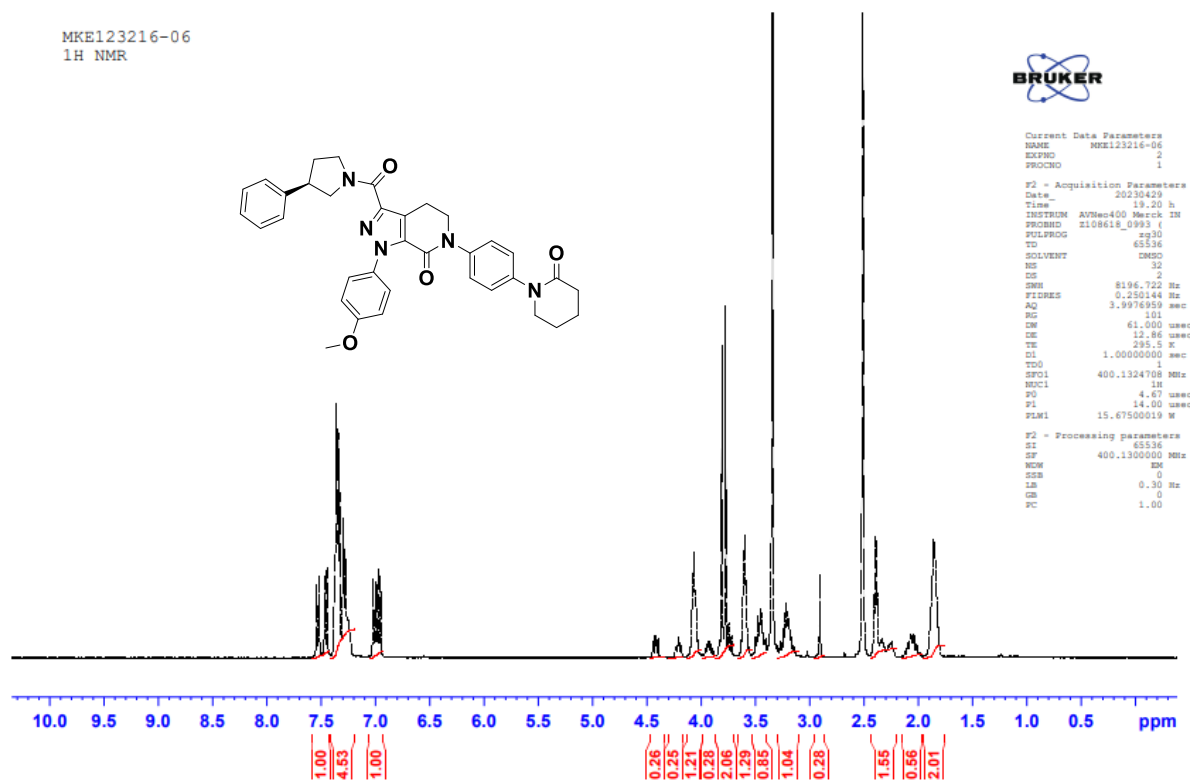
¹³C NMR (101 MHz, DMSO-*d*₆) δ 169.32, 162.20, 159.56, 157.05, 141.88, 140.27, 133.01, 132.56, 127.21, 127.09, 126.81, 126.50, 125.92, 124.27, 113.94, 55.94, 51.30, 45.10, 43.18, 33.07, 26.07, 23.47, 21.32.

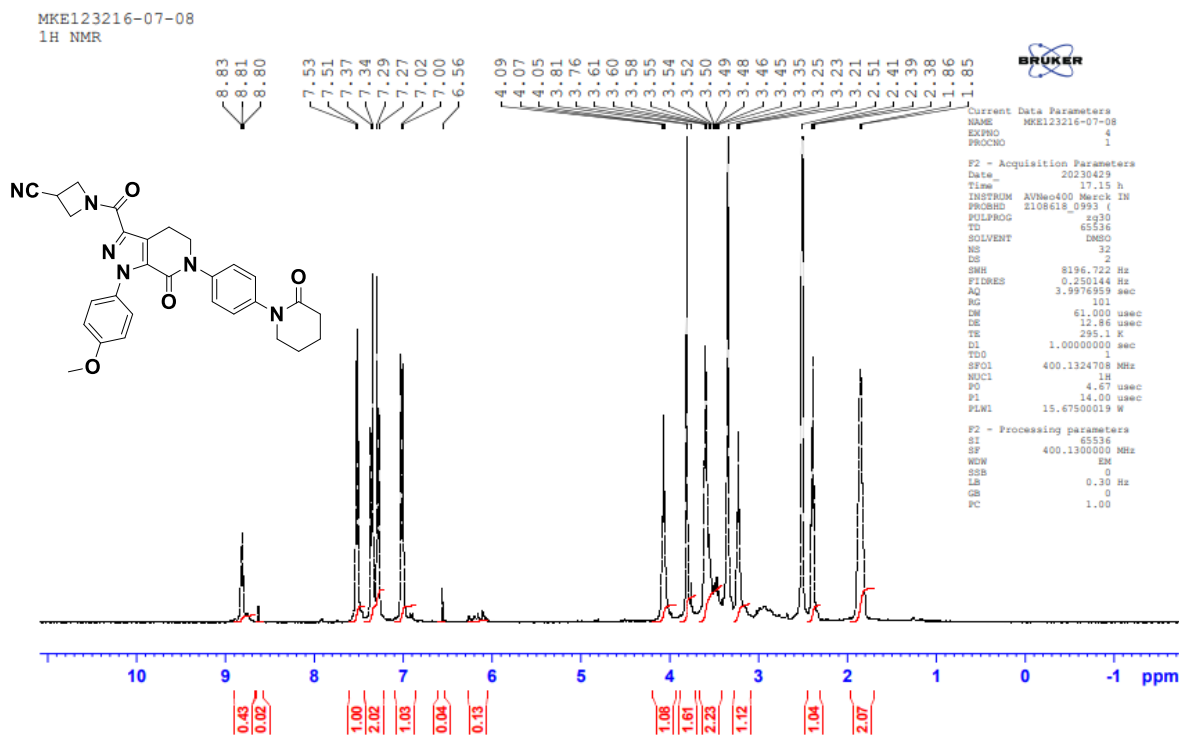
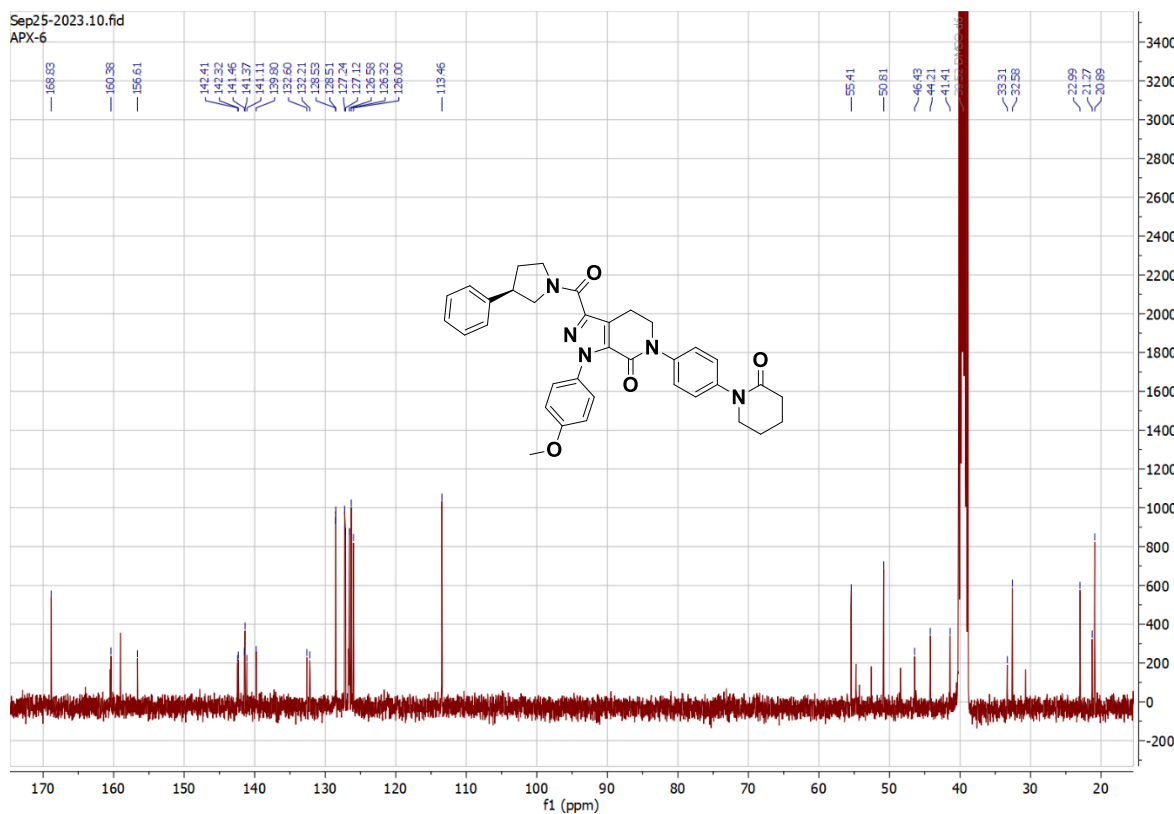


MKE123216-05
1H NMR

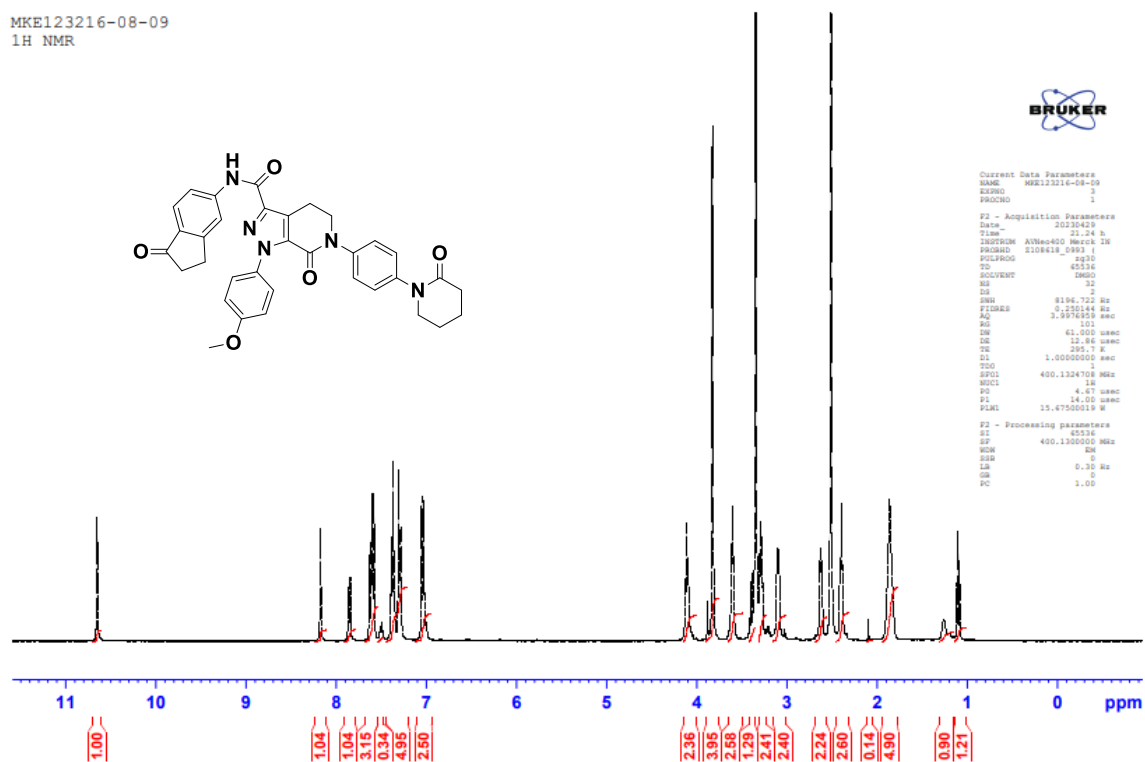


MKE123216-06
1H NMR

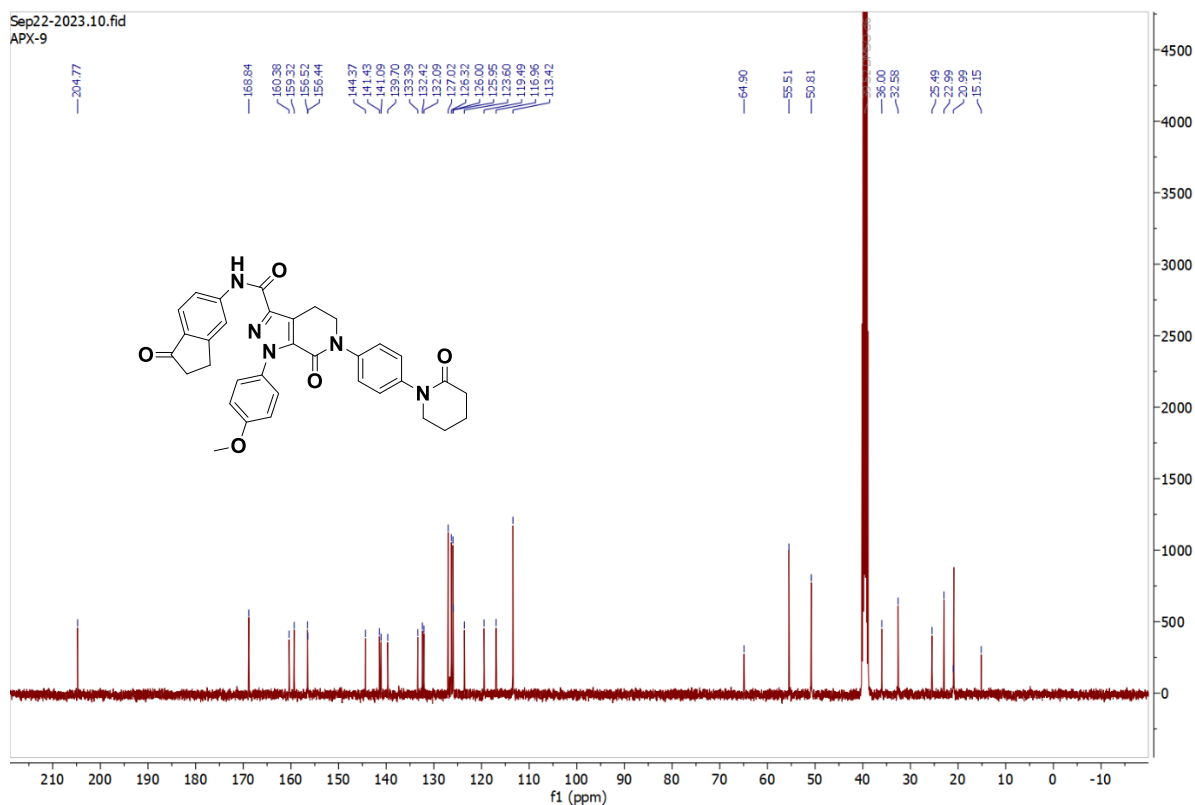




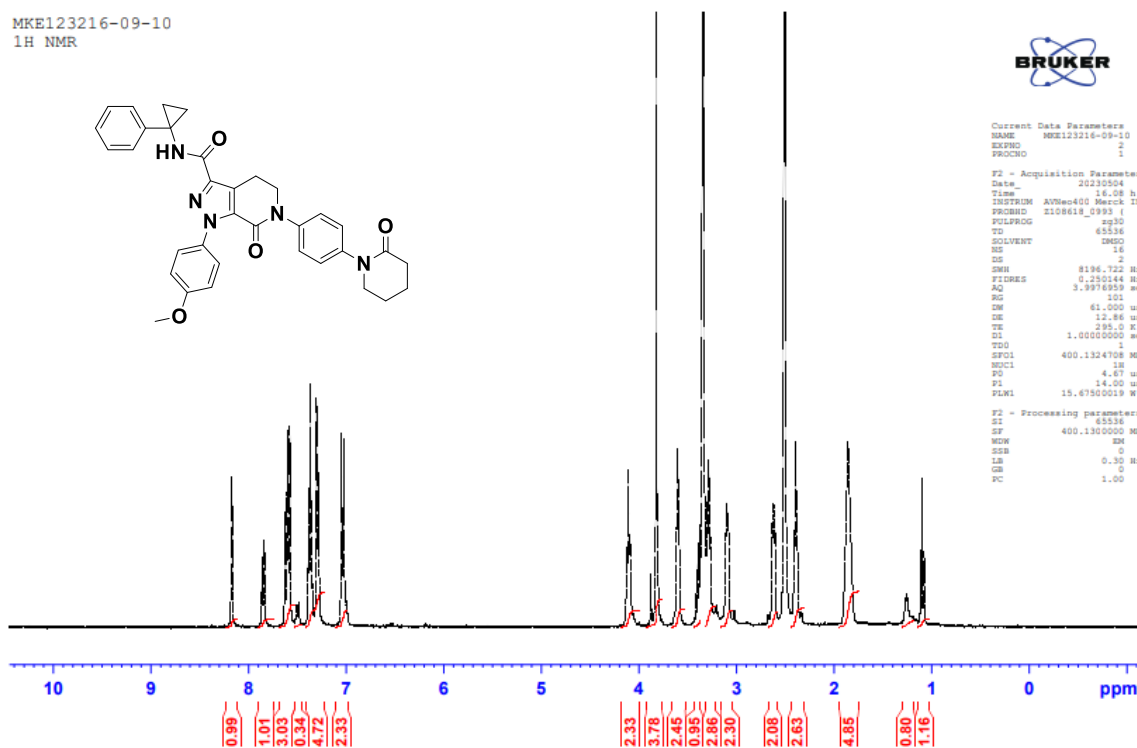
MKE123216-08-09
1H NMR



Sep22-2023.10.fid
APX-9



MKE123216-09-10
1H NMR



Sep25-2023.30.fid
APX-10

