

Supporting Information

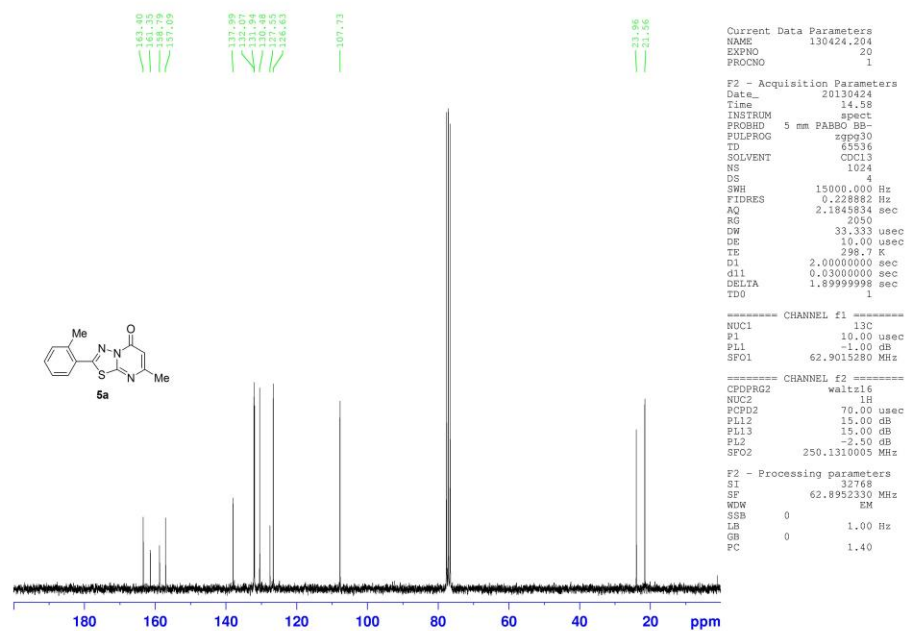
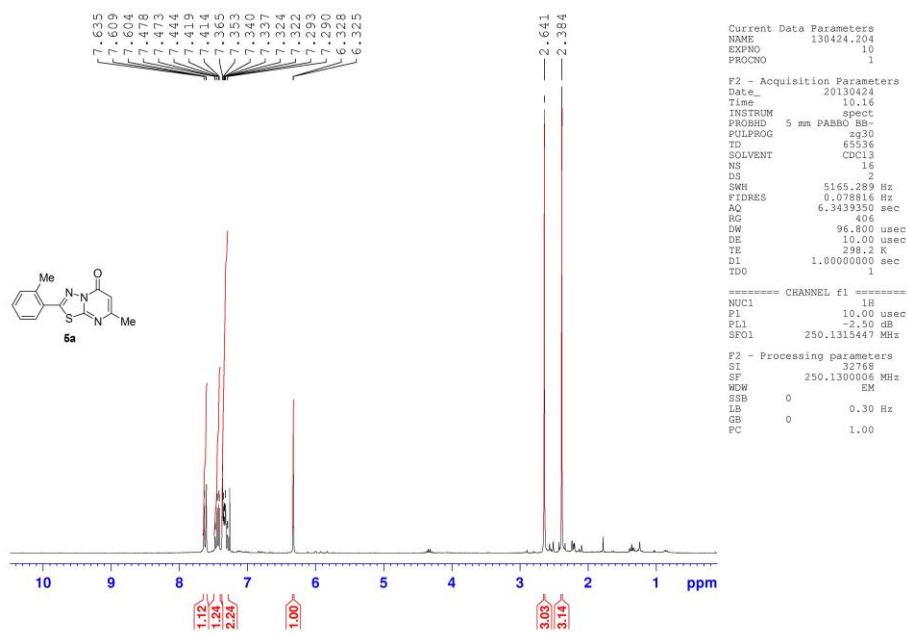
Synthesis of 2-Arylated Thiadiazolopyrimidones by Suzuki-Miyaura Cross-Coupling: A New Class of Nucleotide Pyrophosphatase (NPPs) Inhibitors

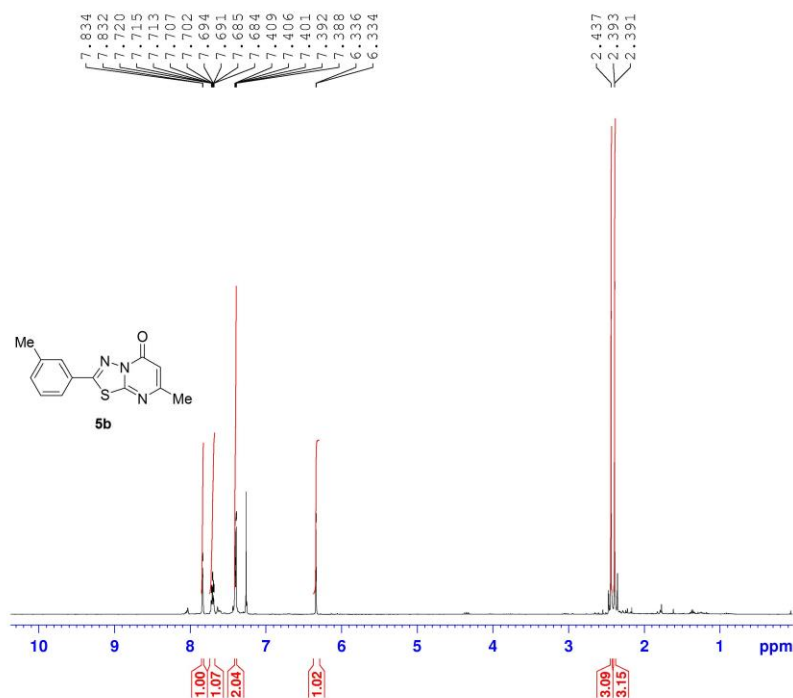
Behzad Jafari, Nazym Yelibayeva, Meirambek Ospanov, Syeda Abida Ejaz, Saira Afzal, Shafi Ullah Khan, Zharylkasyn A. Abilov, Mirgul Zh. Turmukhanova, Sergey N. Kalugin, Sayfidin Safarov, Joanna Lecka, Jean Sévigny, Qamar Rahman, Peter Ehlers, Jamshed Iqbal,* Peter Langer*

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NMR-Spectra



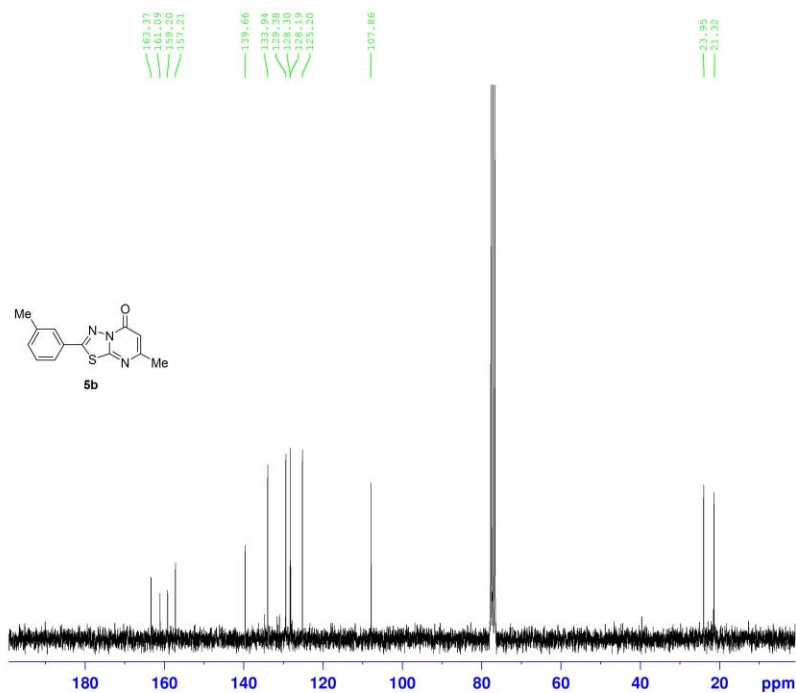


Current Data Parameters
NAME 130417.u310
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130417
Time 10.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 256
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



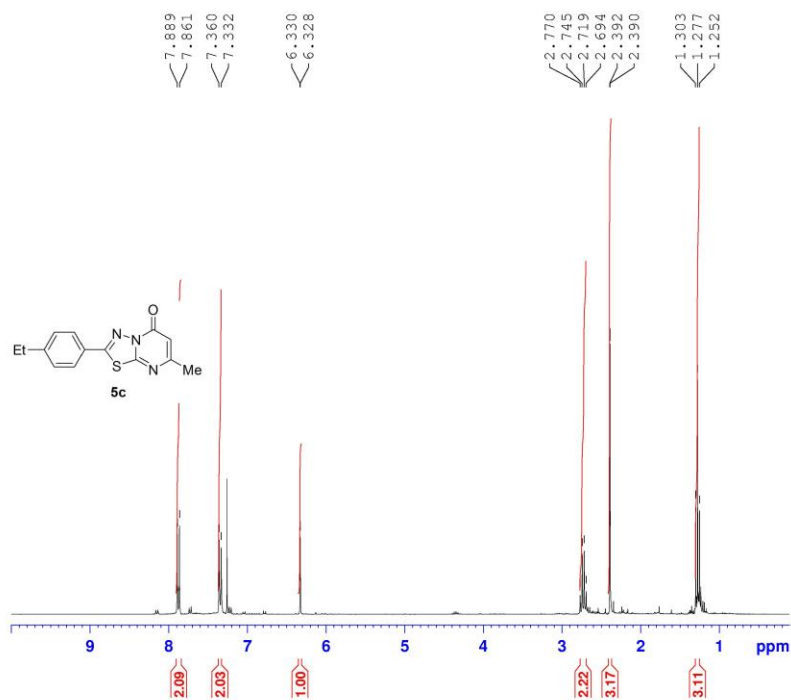
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NAME 130417.208
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130417
Time 15.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952300 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

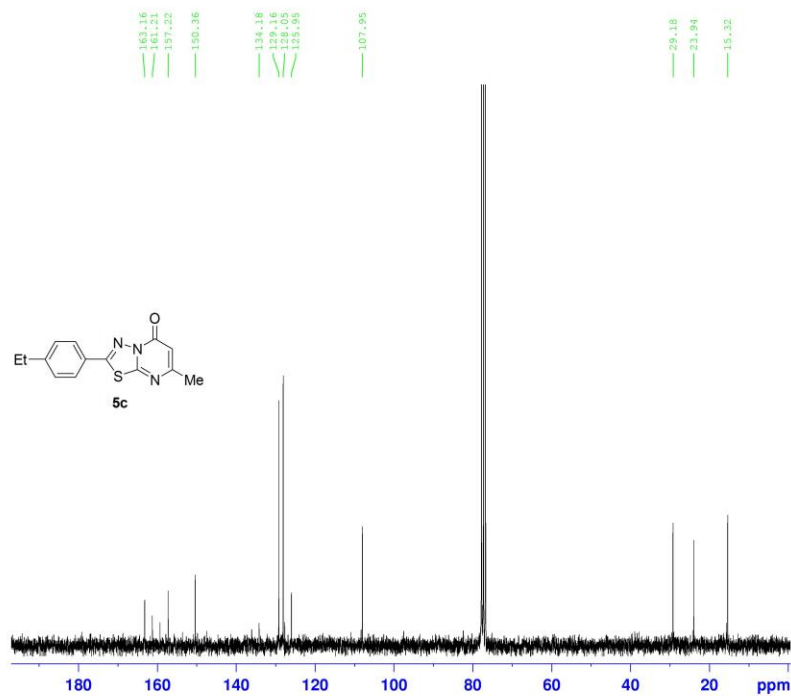


Current Data Parameters
NAME 130417.u312
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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Time 10.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 256
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



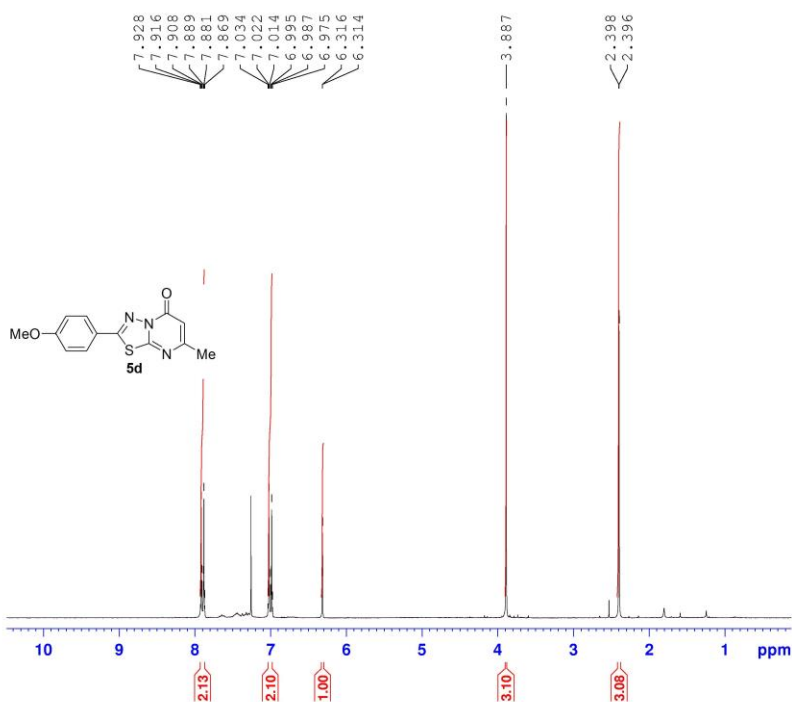
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NAME 130417.210
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130417
Time 19.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 299.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

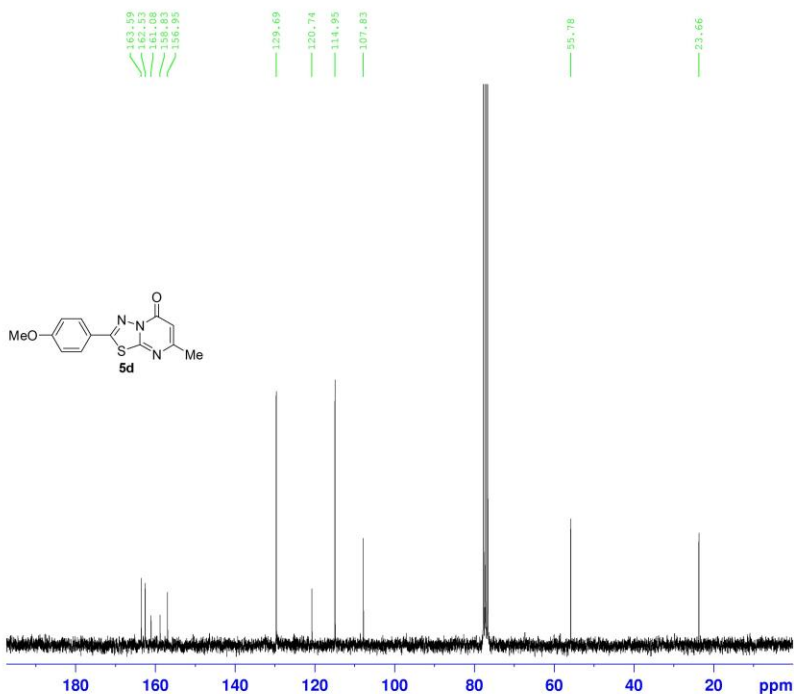
F2 - Processing parameters
SI 32768
SF 62.8952231 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
 NAME 130402.207
 EXPNO 10
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20130402
 Time 11.10
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 5165.289 Hz
 FIDRES 0.078816 Hz
 AQ 6.3439350 sec
 RG 645
 DW 96.800 usec
 DE 10.00 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 -2.50 dB
 SFO1 250.1315447 MHz

F2 - Processing parameters
 SI 32768
 SF 250.1300010 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 FC 1.00

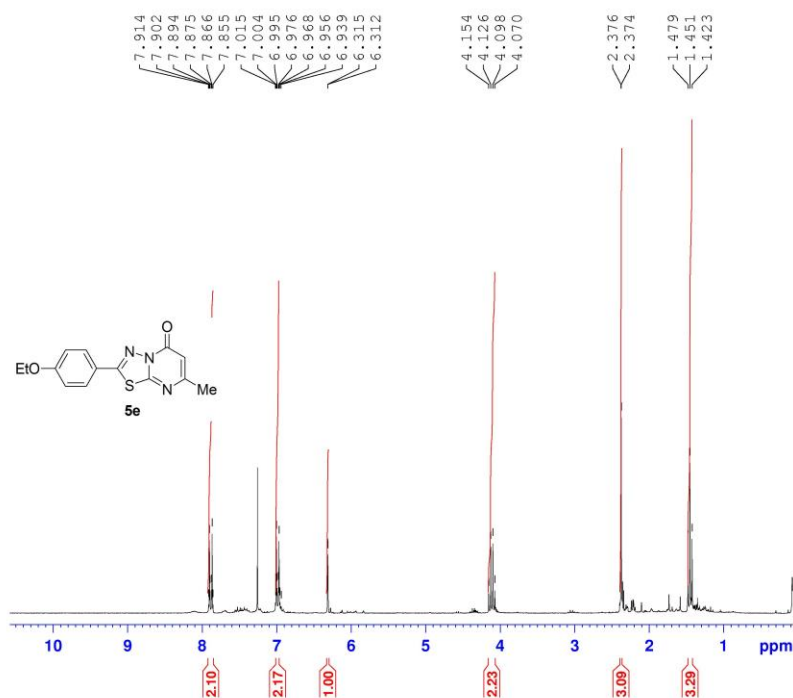


Current Data Parameters
 NAME 130403.216
 EXPNO 11
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20130404
 Time 6.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 15000.000 Hz
 FIDRES 0.228982 Hz
 AQ 2.1845834 sec
 RG 2050
 DW 33.333 usec
 DE 10.00 usec
 TE 297.8 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -1.00 dB
 SFO1 62.9015280 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 70.00 usec
 PL12 15.00 dB
 PL13 15.00 dB
 PL2 -2.50 dB
 SFO2 250.1310005 MHz

F2 - Processing parameters
 SI 32768
 SF 62.8952292 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 FC 1.40

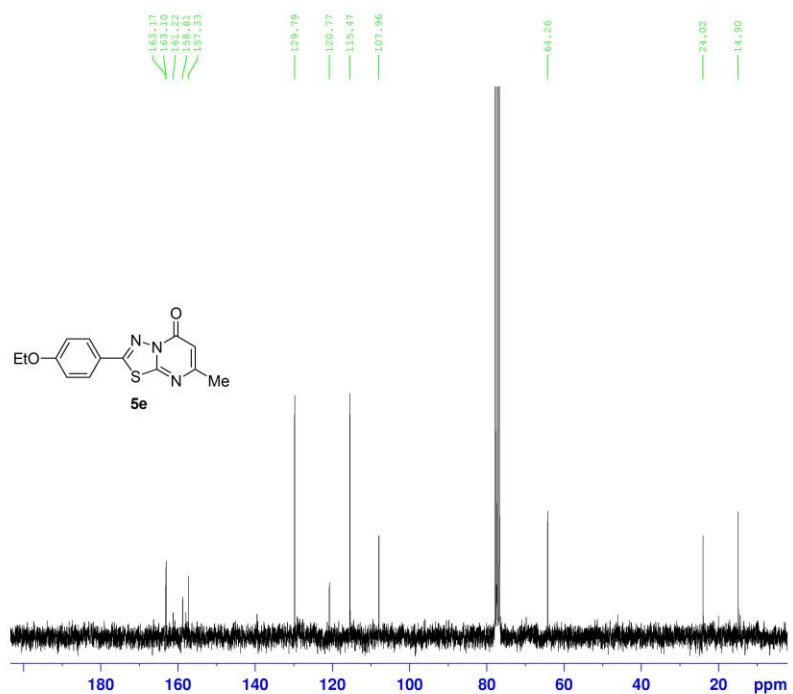


Current Data Parameters
 NAME 130410.205
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130410
 Time 9.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 5165.289 Hz
 FIDRES 0.078816 Hz
 AQ 6.3439350 sec
 RG 645
 DW 96.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 -2.50 dB
 SFO1 250.1315447 MHz

F2 - Processing parameters
 SI 32768
 SF 250.1300010 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



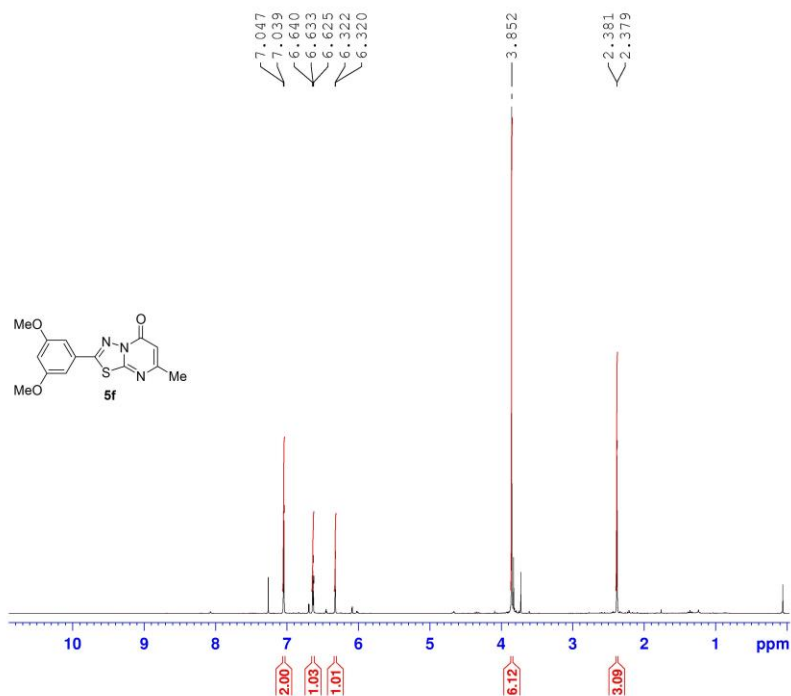
Current Data Parameters
 NAME 130410.205
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130411
 Time 2.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 15000.000 Hz
 FIDRES 0.228882 Hz
 AQ 2.1845834 sec
 RG 2050
 DW 33.333 usec
 DE 10.00 usec
 TE 298.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -1.00 dB
 SFO1 62.9015280 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 70.00 usec
 PL12 15.00 dB
 PL13 15.00 dB
 PL2 -2.50 dB
 SFO2 250.1310005 MHz

F2 - Processing parameters
 SI 32768
 SF 62.8952207 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

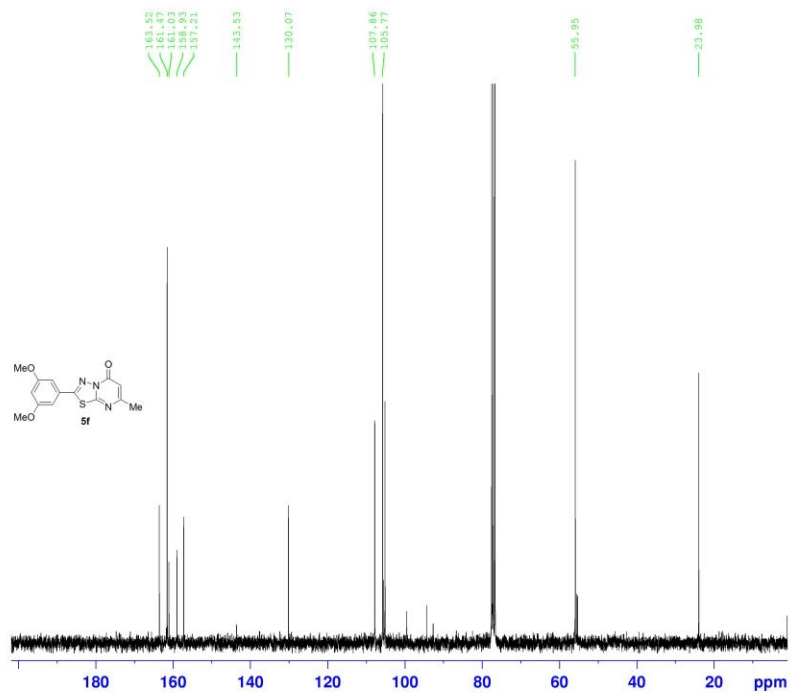


Current Data Parameters
NAME 130429.u301
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130429
Time 9.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 181
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



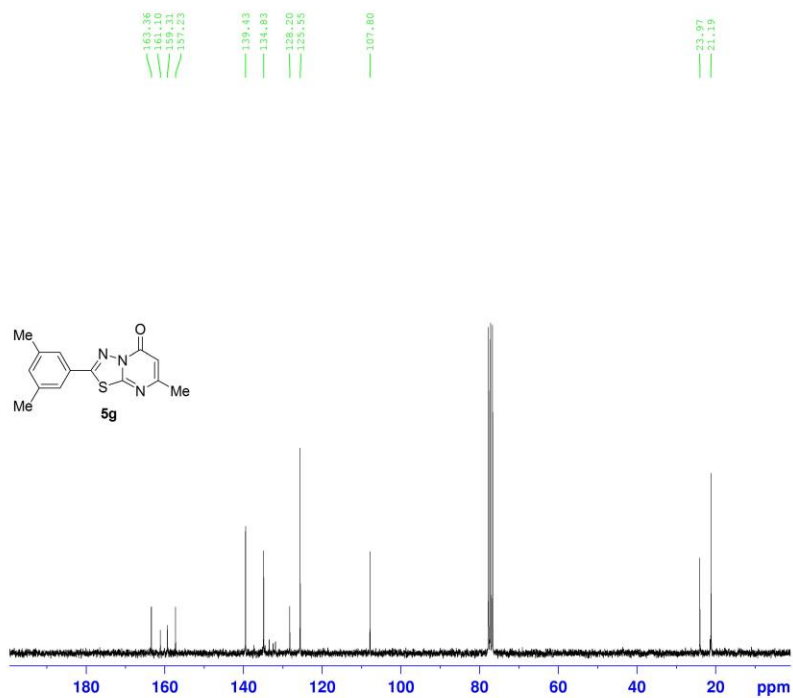
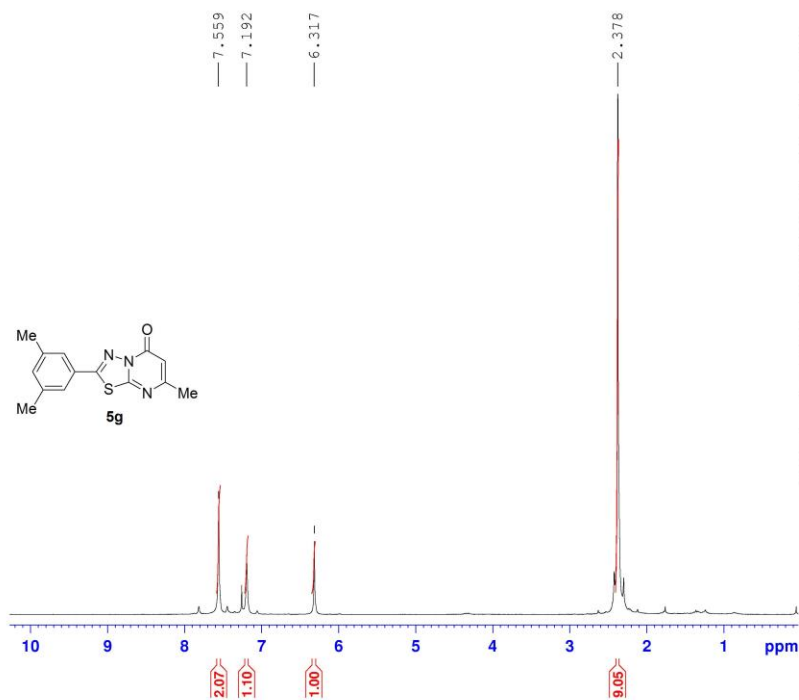
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EXPNO 12
PROCNO 1

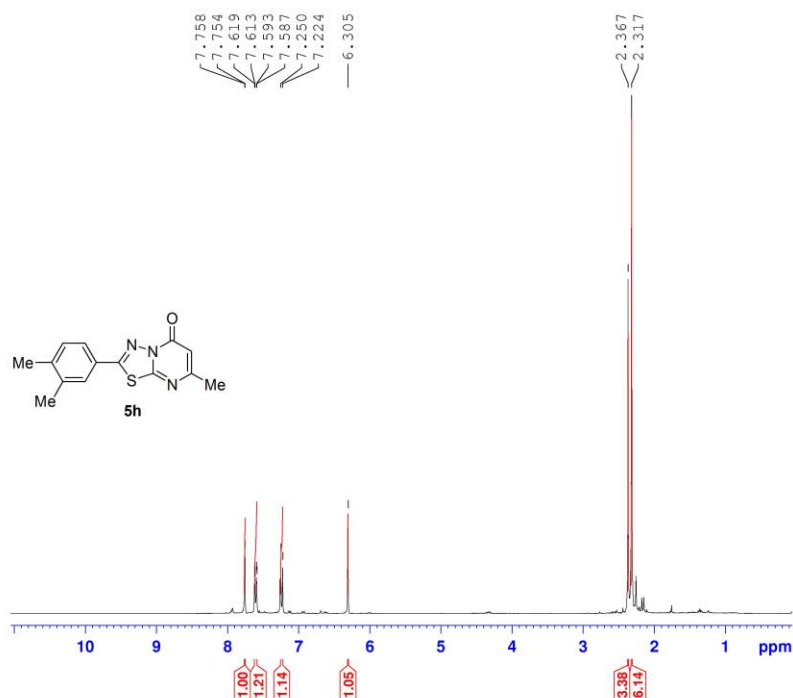
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Date_ 20130429
Time 13.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677411 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



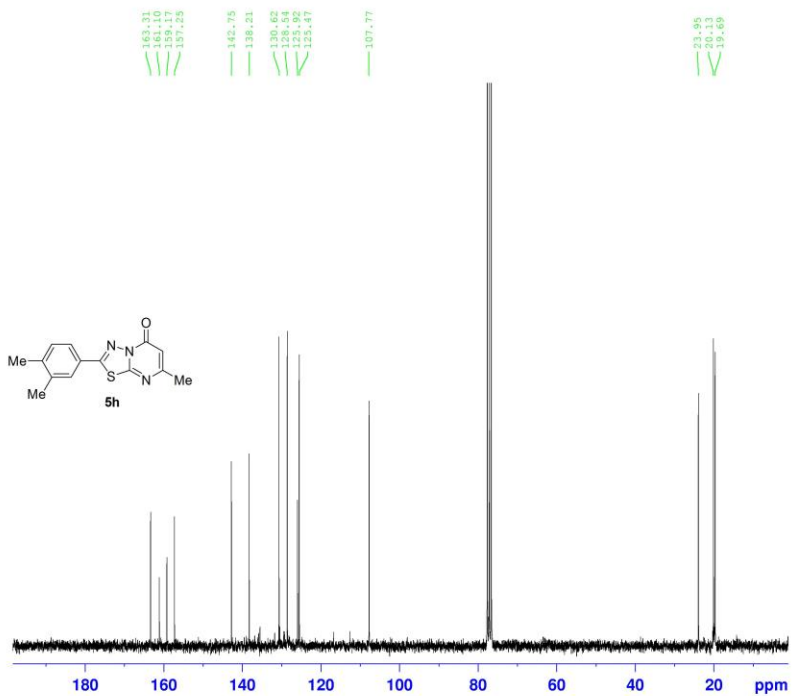


Current Data Parameters
NAME 130425.u304
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130425
Time 9.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 50.8
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0 dB
PLW 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



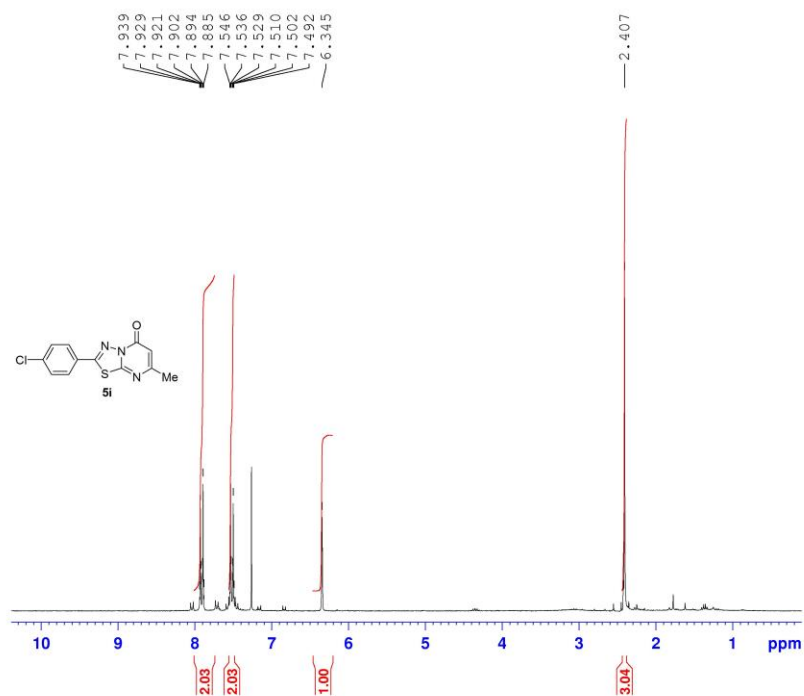
Current Data Parameters
NAME 130425.205
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130425
Time 18.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 299.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952303 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters

NAME	130410.203
EXPNO	10
PROCNO	1

F2 - Acquisition Parameters

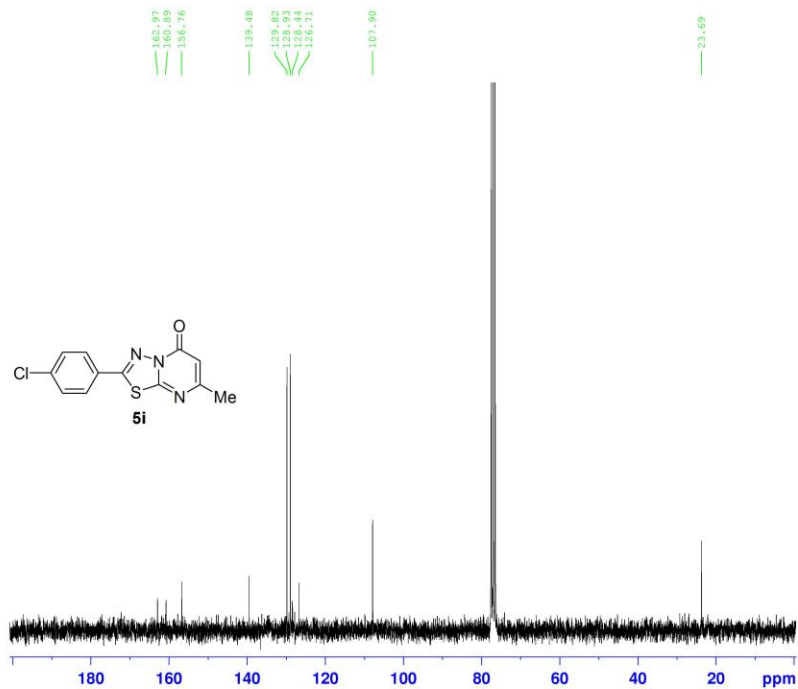
Date_	20130410
Time	9.29
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	5165.289 Hz
FTDRES	0.078816 Hz
AQ	6.3439350 sec
RG	645
DW	96.800 usec
DE	10.00 usec
TE	298.1 K
D1	1.00000000 sec
TD0	1

===== CHANNEL f1 =====

NUC1	1H
P1	10.00 usec
PL1	-2.50 dB
SFO1	250.1315447 MHz

F2 - Processing parameters

SI	32768
SF	250.1299994 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



Current Data Parameters

NAME	130410.203
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20130410
Time	13.21
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	15000.000 Hz
FTDRES	0.228882 Hz
AQ	2.1845834 sec
RG	2050
DW	33.333 usec
DE	10.00 usec
TE	298.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

===== CHANNEL f1 =====

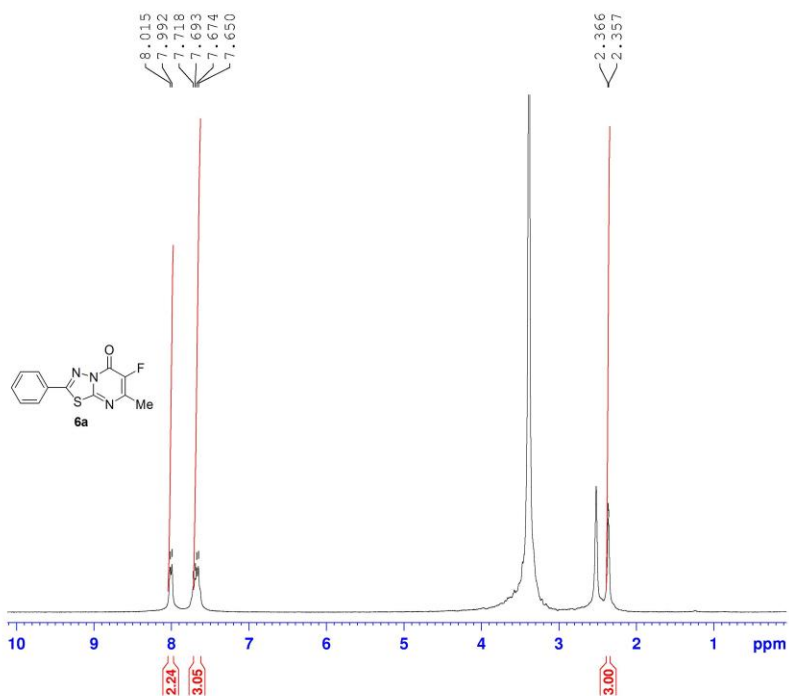
NUC1	13C
P1	10.00 usec
PL1	-1.00 dB
SFO1	62.9015280 MHz

===== CHANNEL f2 =====

CPDPRG2	waitz16
NUC2	1H
PCPD2	70.00 usec
PL12	15.00 dB
PL13	15.00 dB
PL2	-2.50 dB
SFO2	250.1310005 MHz

F2 - Processing parameters

SI	32768
SF	62.8952371 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



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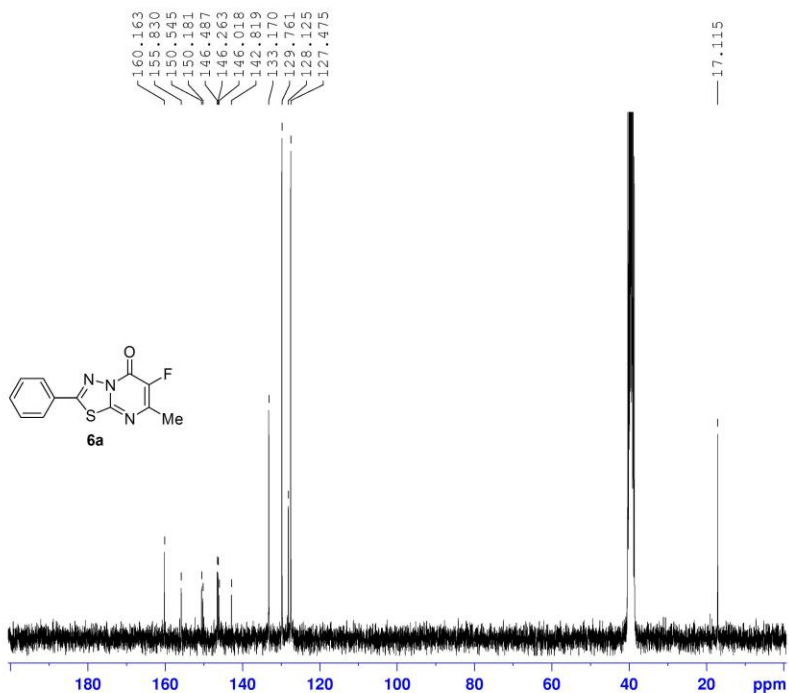
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EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20130906
Time      9.35
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD        65536
SOLVENT   DMSO
NS         16
DS         2
SWH        6188.119 Hz
FIDRES     0.094423 Hz
AQ         5.2953587 sec
RG         101
DW         80.800 usec
DE         10.00 usec
TE         298.2 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         10.00 usec
PL1        0 dB
PL1W       11.25325108 W
SFO1       300.1318534 MHz

F2 - Processing parameters
SI         32768
SF         300.1300398 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

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Current Data Parameters
NAME      130906.u313
EXPNO     12
PROCNO    1

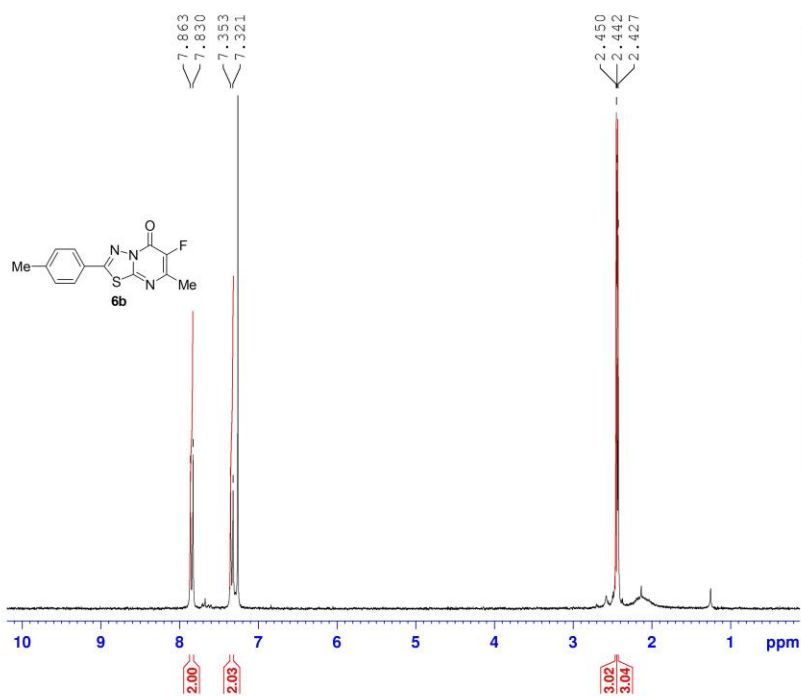
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Date_     20130906
Time      20.04
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS         2048
DS         4
SWH        18028.846 Hz
FIDRES     0.275098 Hz
AQ         1.8175818 sec
RG         2050
DW         27.733 usec
DE         10.00 usec
TE         298.7 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         10.00 usec
PL1        -0.50 dB
PL1W       33.25691986 W
SFO1       75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     72.00 usec
PL2        0 dB
PL12       17.00 dB
PL13       17.00 dB
PL2W       11.25325108 W
PL12W      0.22453187 W
PL13W      0.22453187 W
SFO2       300.1312005 MHz

F2 - Processing parameters
SI         32768
SF         75.4677891 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

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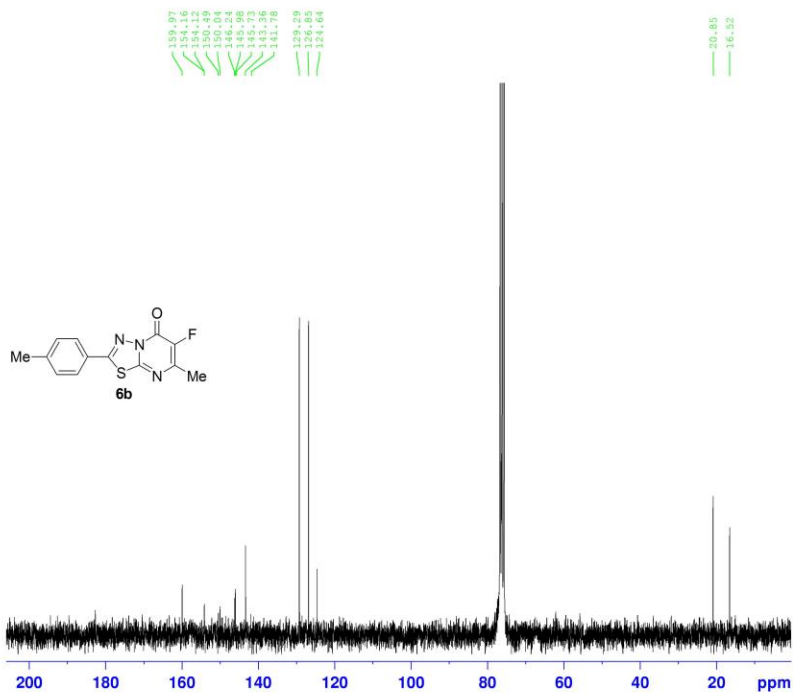


Current Data Parameters
NAME 160408.207
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160409
Time 4.45
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 5165.289 Hz
FIDRES 0.078816 Hz
AQ 6.3439350 sec
RG 1440
DW 96.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.40 usec
PL1 -3.00 dB
SFO1 250.1315447 MHz

F2 - Processing parameters
SI 32768
SF 250.1300005 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



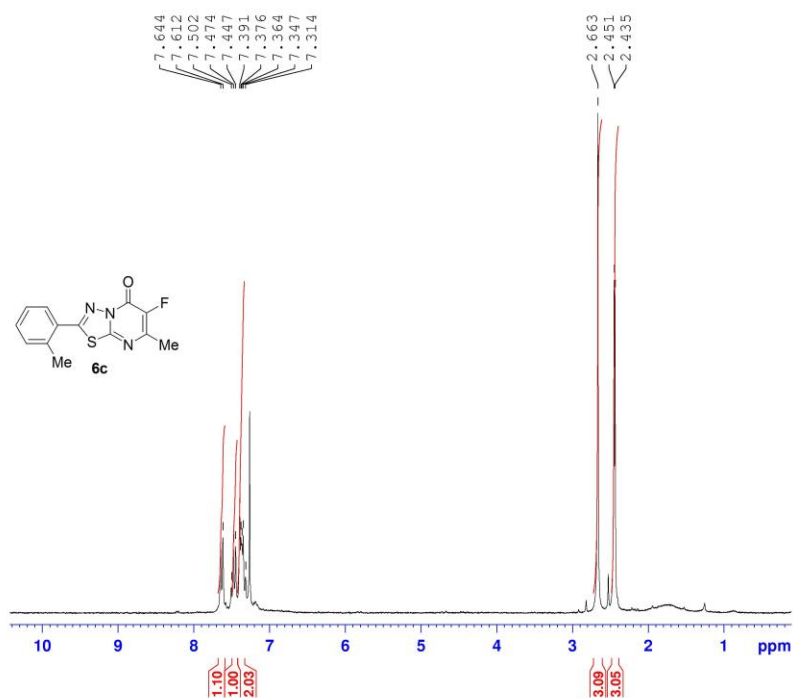
Current Data Parameters
NAME 160420.201
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160420
Time 16.08
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5000
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.20 usec
PL1 0 dB
SFO1 62.9015280 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
FCPD2 70.00 usec
PL12 14.00 dB
PL13 14.00 dB
PL2 -3.00 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952914 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

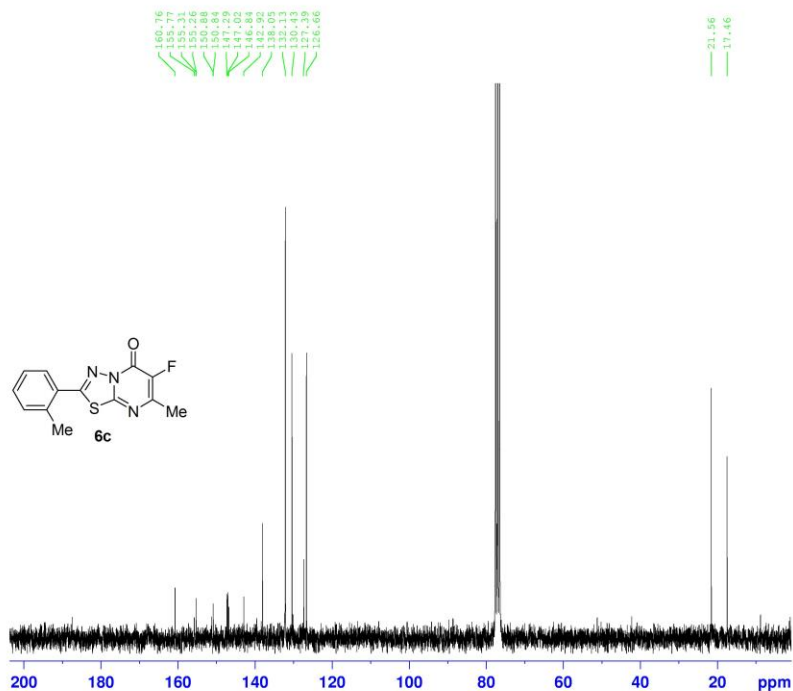


Current Data Parameters
 NAME 130920.201
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130920
 Time 8.33
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 5165.289 Hz
 FIDRES 0.078816 Hz
 AQ 6.3439350 sec
 RG 645
 DW 96.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 -2.50 dB
 SFO1 250.1315447 MHz

F2 - Processing parameters
 SI 32768
 SF 250.1300003 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



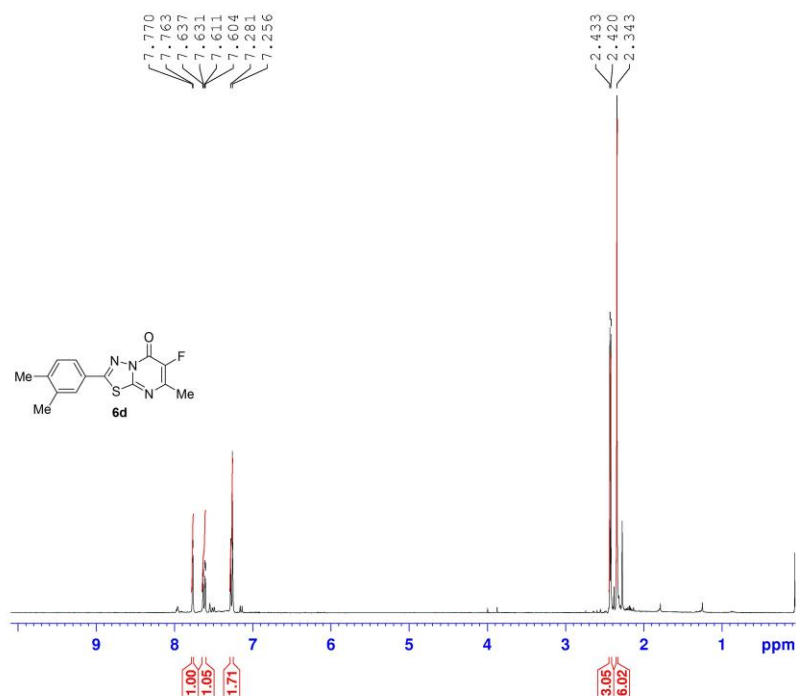
Current Data Parameters
 NAME 130920.207
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130921
 Time 2.34
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 5000
 DS 4
 SWH 15000.000 Hz
 FIDRES 0.228882 Hz
 AQ 2.1845834 sec
 RG 2050
 DW 33.333 usec
 DE 10.00 usec
 TE 298.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -1.00 dB
 SFO1 62.9015280 MHz

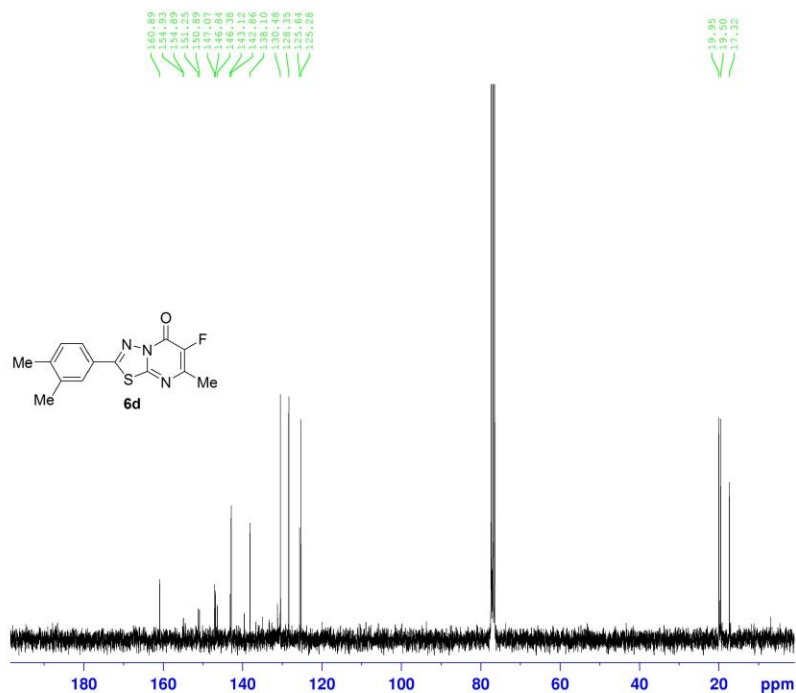
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 FCPD2 70.00 usec
 PL12 15.00 dB
 PL13 15.00 dB
 PL2 -2.50 dB
 SFO2 250.1310005 MHz

F2 - Processing parameters
 SI 32768
 SF 62.8952363 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



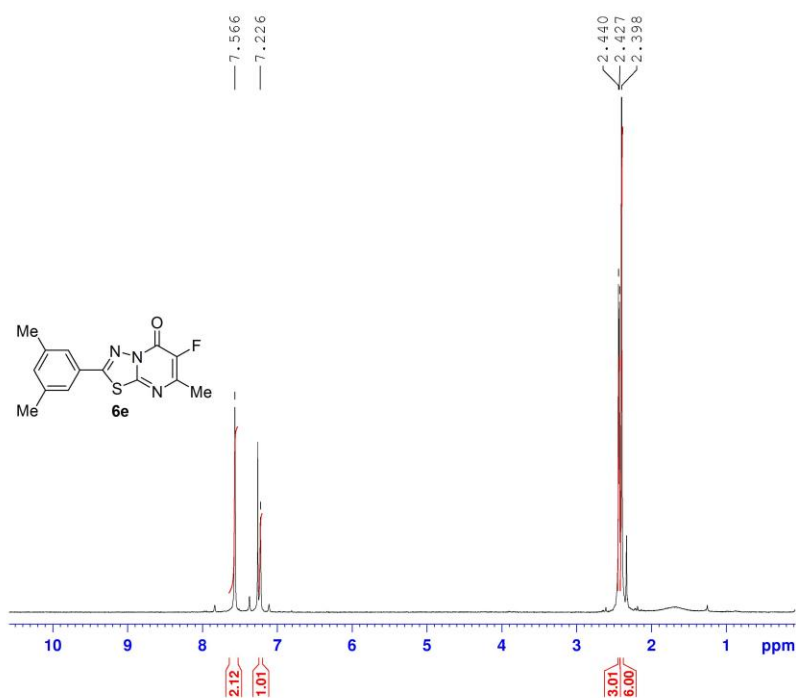
Current Data Parameters
 NAME 130924.u304
 EXPNO 10
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20130924
 Time 8.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 287
 DW 80.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PLL 0 dB
 PLLW 11.25325108 W
 SFO1 300.1318534 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1300105 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME 130924.u304
 EXPNO 13
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20130924
 Time 11.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175818 sec
 RG 2050
 DW 27.733 usec
 DE 10.00 usec
 TE 298.2 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PLL -0.50 dB
 PLLW 33.25691986 W
 SFO1 75.4752953 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 FCPD2 72.00 usec
 PL2 0 dB
 PL12 17.00 dB
 PL13 17.00 dB
 PL2W 11.25325108 W
 PLL2W 0.22453187 W
 PLL3W 0.22453187 W
 SFO2 300.1312005 MHz
 F2 - Processing parameters
 SI 32768
 SF 75.4677581 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



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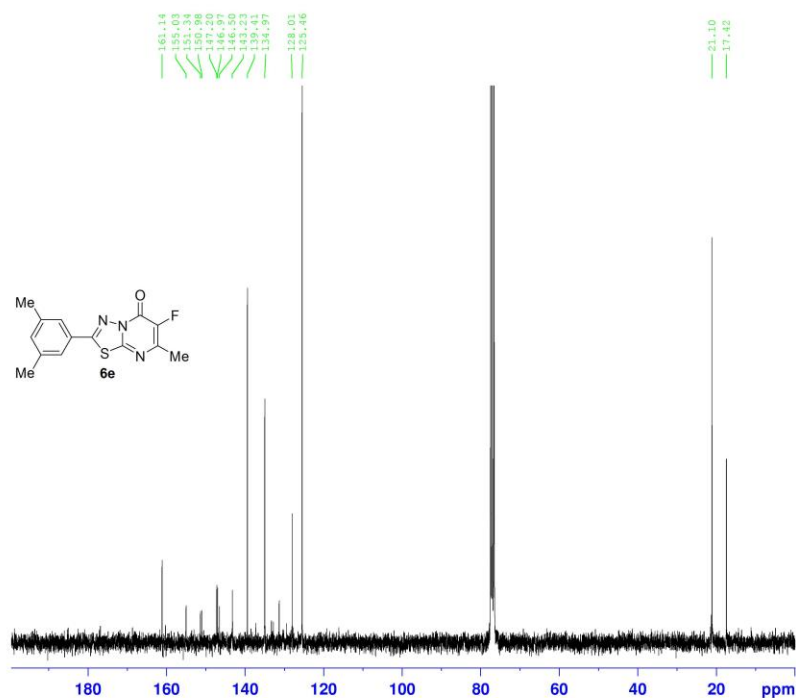
Current Data Parameters
NAME      130919.u303
EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20130919
Time      8.49
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        6188.119 Hz
FIDRES     0.094423 Hz
AQ         5.2953587 sec
RG         362
DW         80.800 usec
DE         10.00 usec
TE         298.2 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         10.00 usec
PL1        0 dB
PL1W       11.25325108 W
SFO1       300.1318534 MHz

F2 - Processing parameters
SI         32768
SF         300.1300118 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

```



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Current Data Parameters
NAME      130919.u303
EXPNO     12
PROCNO    1

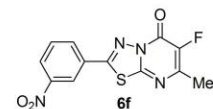
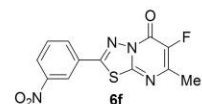
F2 - Acquisition Parameters
Date_     20130919
Time      23.54
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         5000
DS         4
SWH        18028.846 Hz
FIDRES     0.275098 Hz
AQ         1.8175818 sec
RG         2050
DW         27.733 usec
DE         10.00 usec
TE         298.2 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

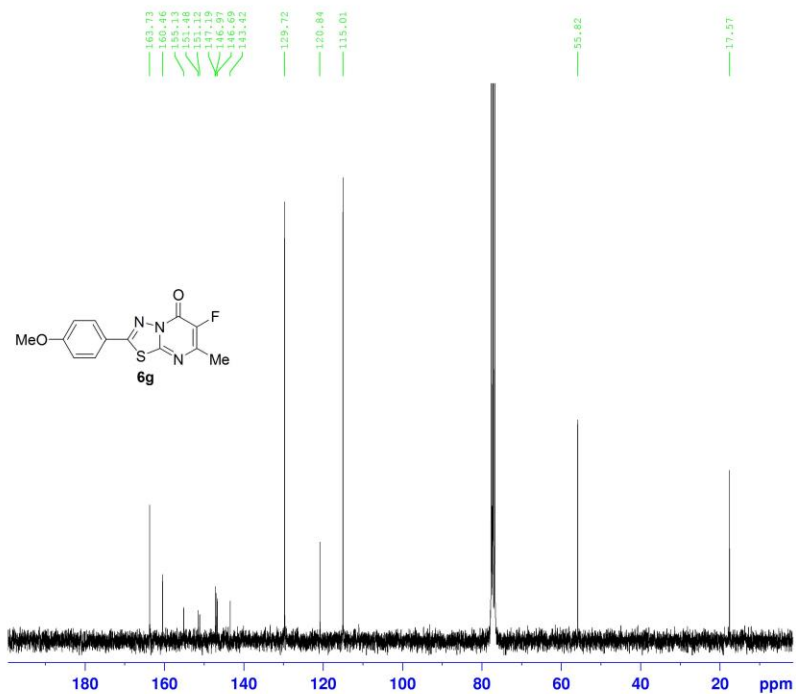
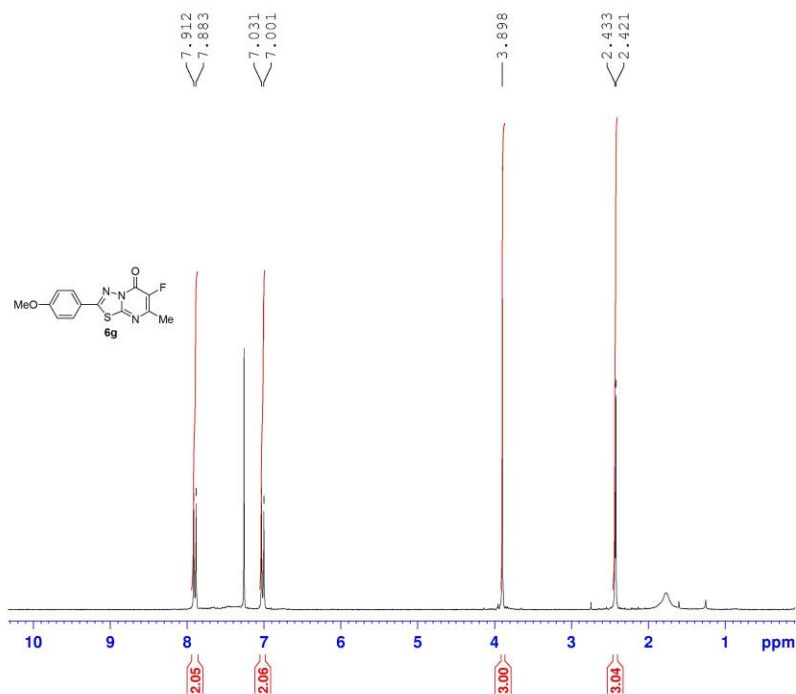
===== CHANNEL f1 =====
NUC1       13C
P1         10.00 usec
PL1        -0.50 dB
PL1W       33.25691986 W
SFO1       75.4752953 MHz

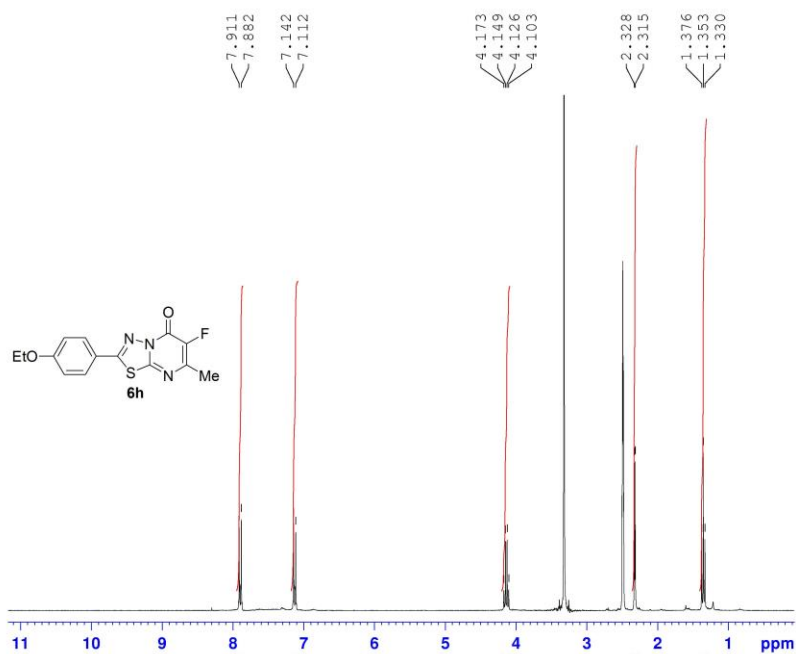
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     72.00 usec
PL2        0 dB
PL12       17.00 dB
PL13       17.00 dB
PL12W     11.25325108 W
PL12W     0.22453187 W
PL13W     0.22453187 W
SFO2       300.1312005 MHz

F2 - Processing parameters
SI         32768
SF         75.4677502 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

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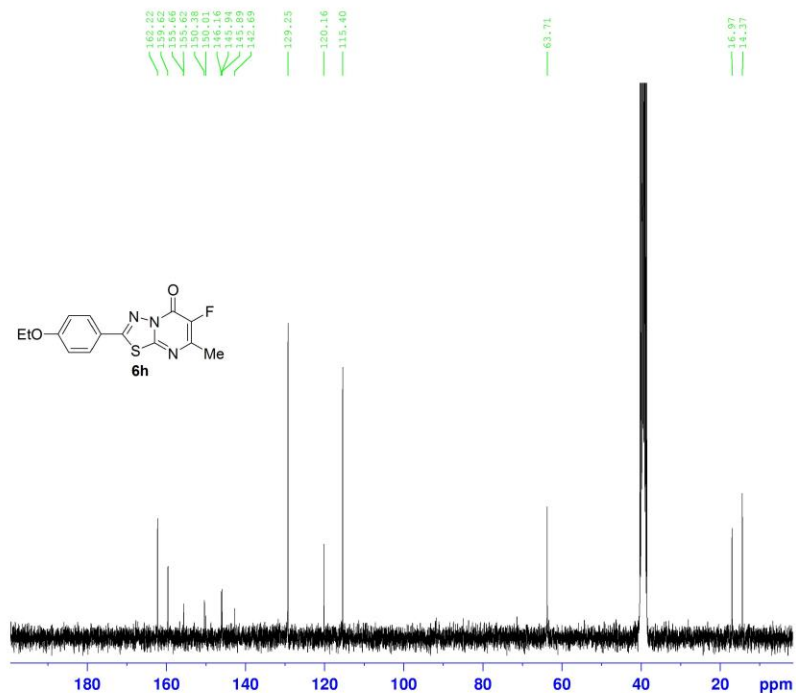


Current Data Parameters
 NAME 130913.u305
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130913
 Time 9.45
 INSTRUM spect
 PROBRD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 203
 DW 80.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0 dB
 PL1W 11.25325108 W
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300163 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



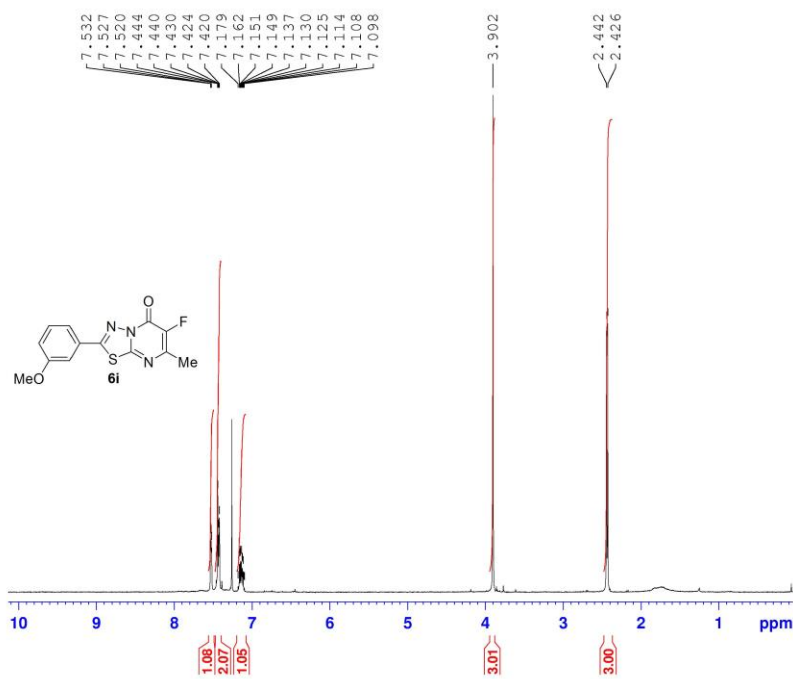
Current Data Parameters
 NAME 130913.u310
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130914
 Time 0.14
 INSTRUM spect
 PROBRD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 5000
 DS 4
 SWH 18028.846 Hz
 FIDRES 0.275098 Hz
 AQ 1.8175818 sec
 RG 2050
 DW 27.733 usec
 DE 10.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -0.50 dB
 PL1W 33.25691986 W
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 72.00 usec
 PL2 0 dB
 PL12 17.00 dB
 PL13 17.00 dB
 PL2W 11.25325108 W
 PL12W 0.22453187 W
 PL13W 0.22453187 W
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677933 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

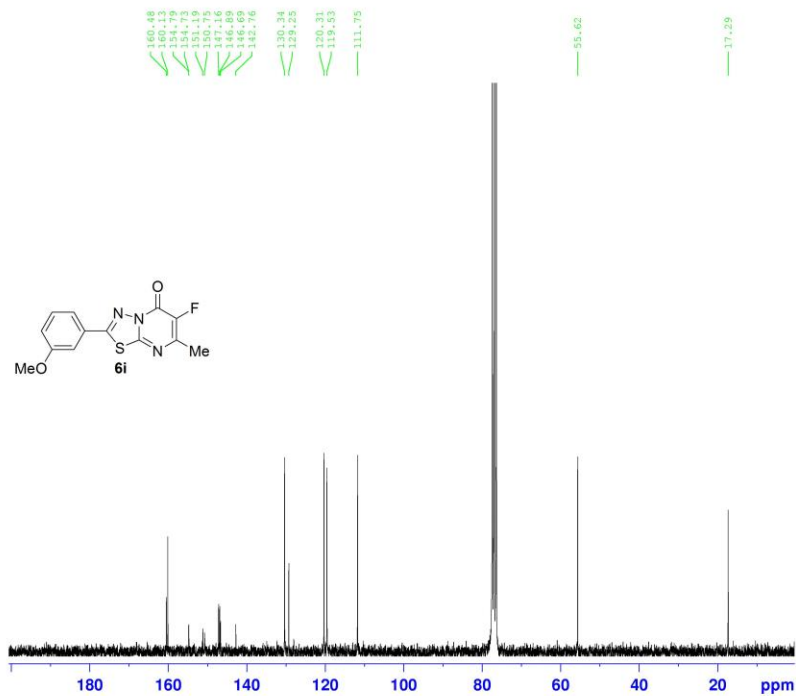


Current Data Parameters
NAME 130918.202
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130918
Time 9.27
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 5165.289 Hz
FIDRES 0.078816 Hz
AQ 6.3439350 sec
RG 1290
DW 96.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.40 usec
PL1 -3.00 dB
SFO1 250.1315447 MHz

F2 - Processing parameters
SI 32768
SF 250.1300007 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



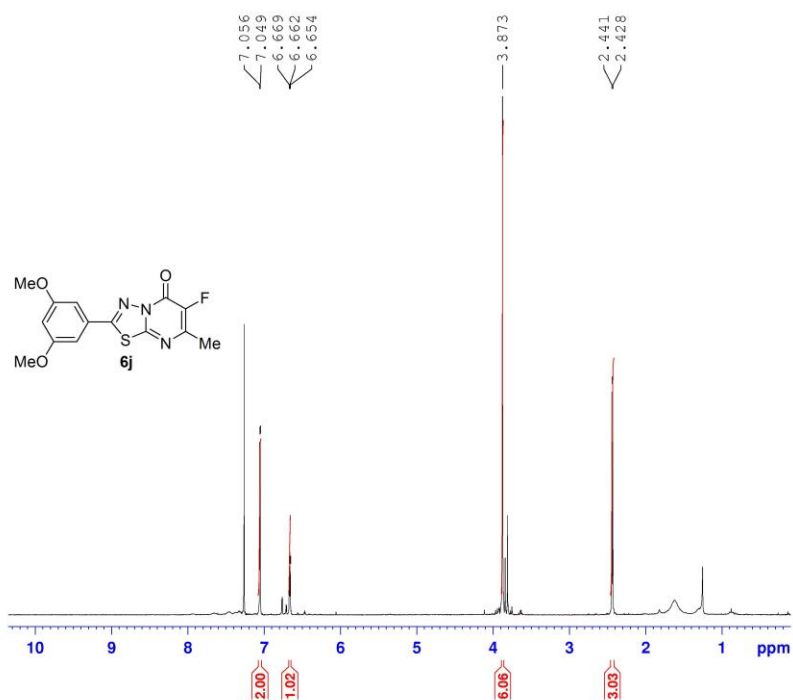
Current Data Parameters
NAME 160219.216
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160220
Time 12.45
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5000
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.20 usec
PL1 0 dB
SFO1 62.9015280 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 14.00 dB
PL13 14.00 dB
PL2 -3.00 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952478 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

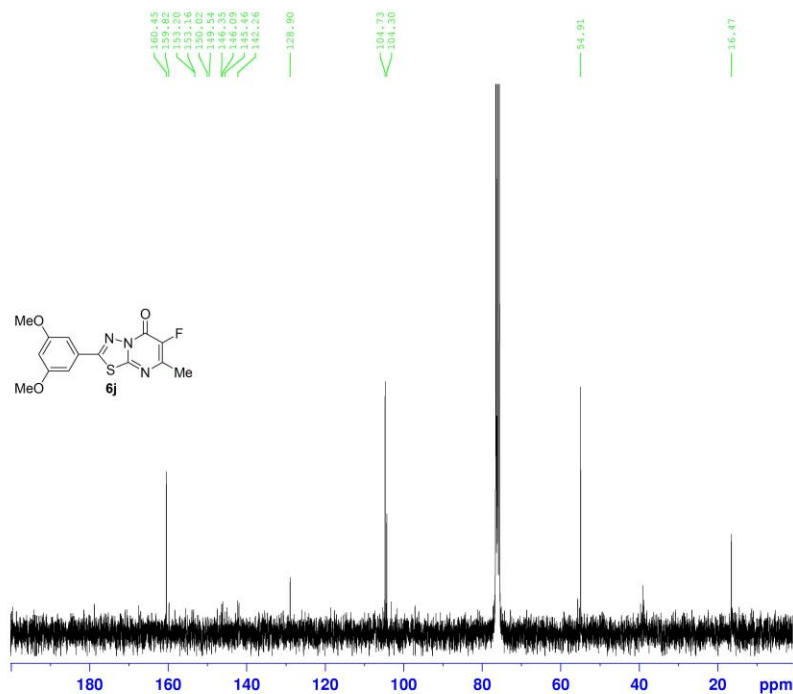


Current Data Parameters
NAME 131024.u314
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131024
Time 10.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 362
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300107 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



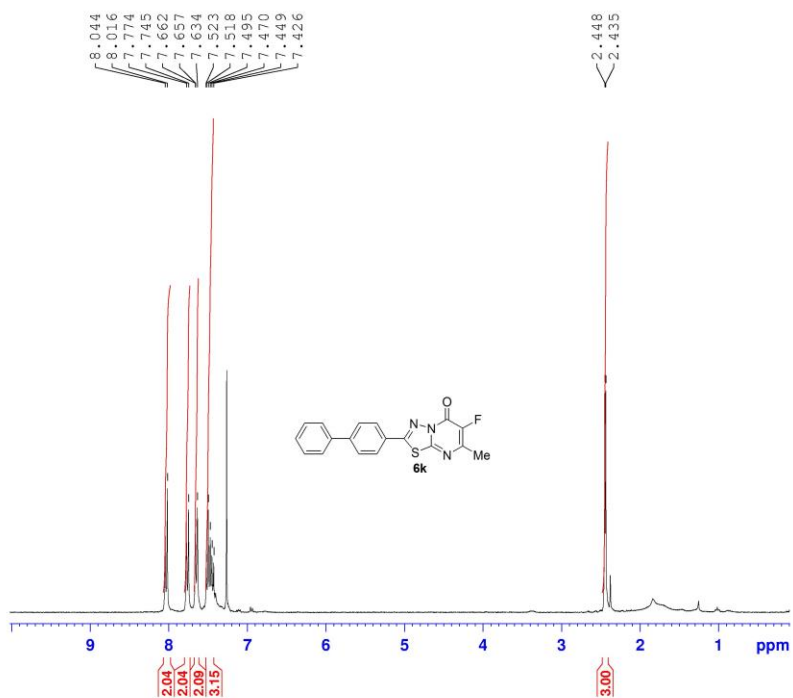
Current Data Parameters
NAME 160421.u331
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160422
Time 5.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5000
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4678216 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

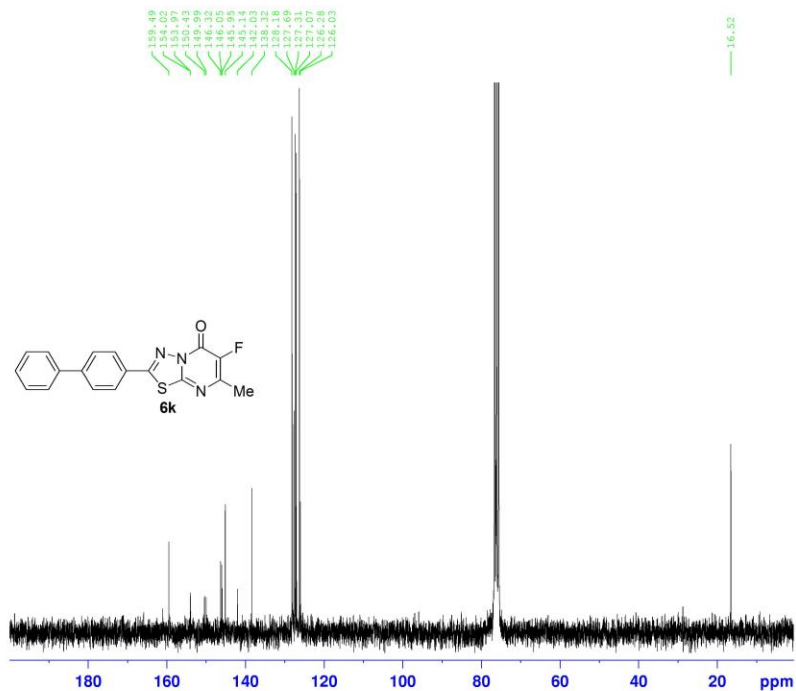


Current Data Parameters
 NAME 131022.u313
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131022
 Time 11.06
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 406
 DW 80.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0 dB
 PL1W 11.25325108 W
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300141 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



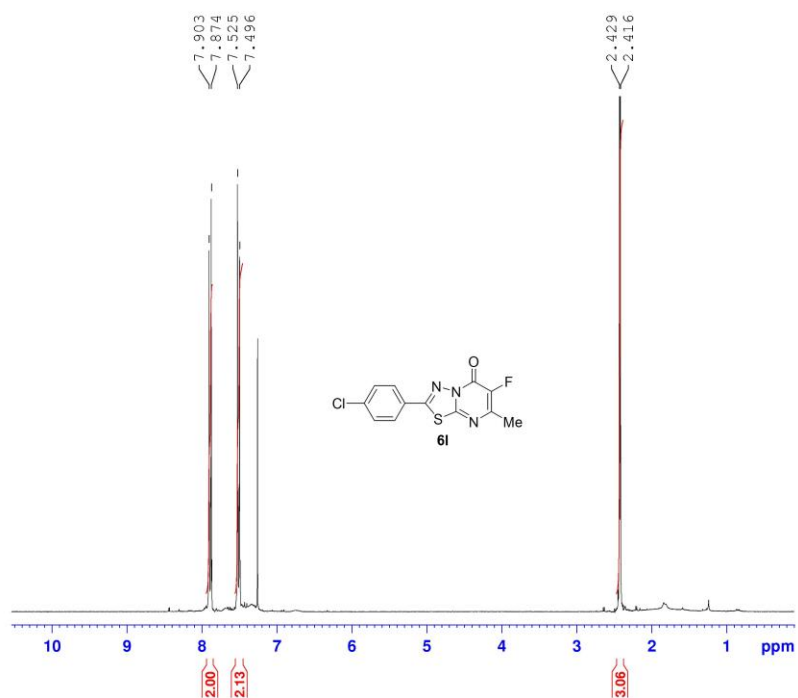
Current Data Parameters
 NAME 160414.208
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160415
 Time 4.52
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 5120
 DS 4
 SWH 15000.000 Hz
 FIDRES 0.228882 Hz
 AQ 2.1845834 sec
 RG 2050
 DW 33.333 usec
 DE 10.00 usec
 TE 298.1 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.20 usec
 PL1 0 dB
 SFO1 62.9015280 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 70.00 usec
 PL12 14.00 dB
 PL13 14.00 dB
 PL2 -3.00 dB
 SFO2 250.1310005 MHz

F2 - Processing parameters
 SI 32768
 SF 62.8952953 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

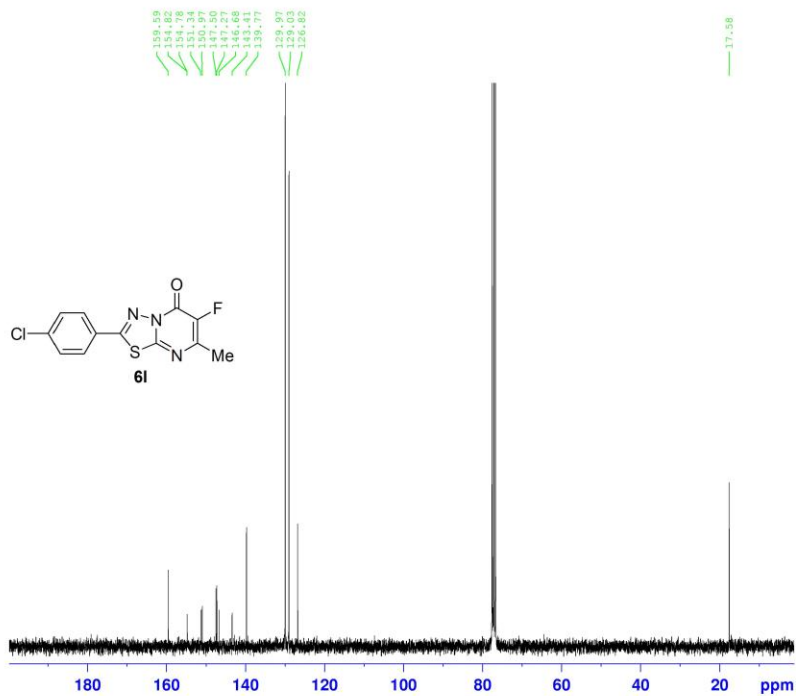


Current Data Parameters
NAME 130916.u304
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130916
Time 10.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 287
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



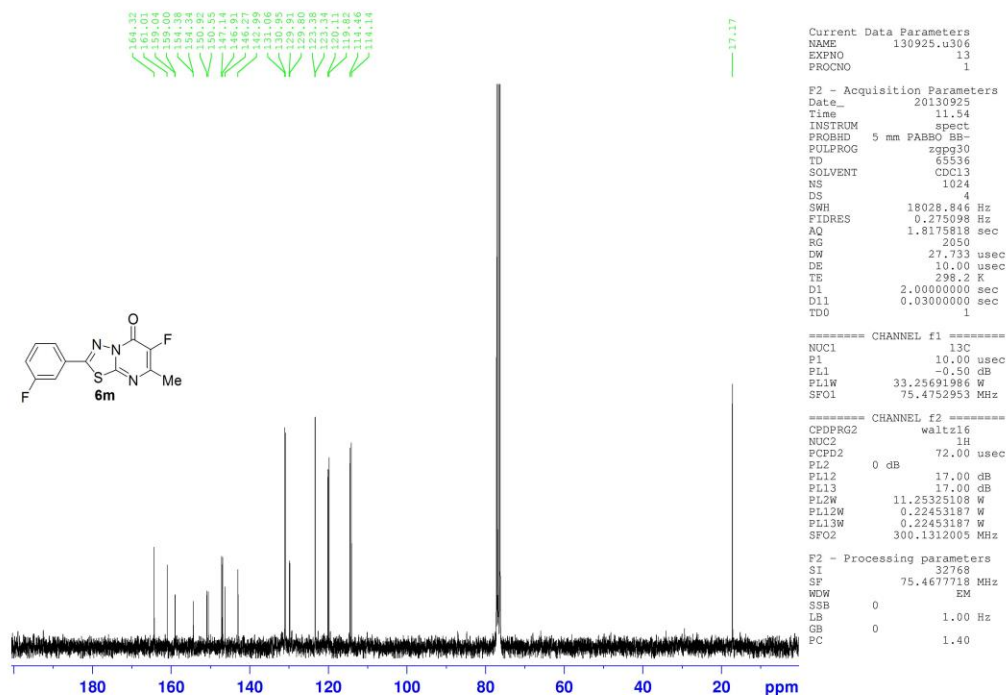
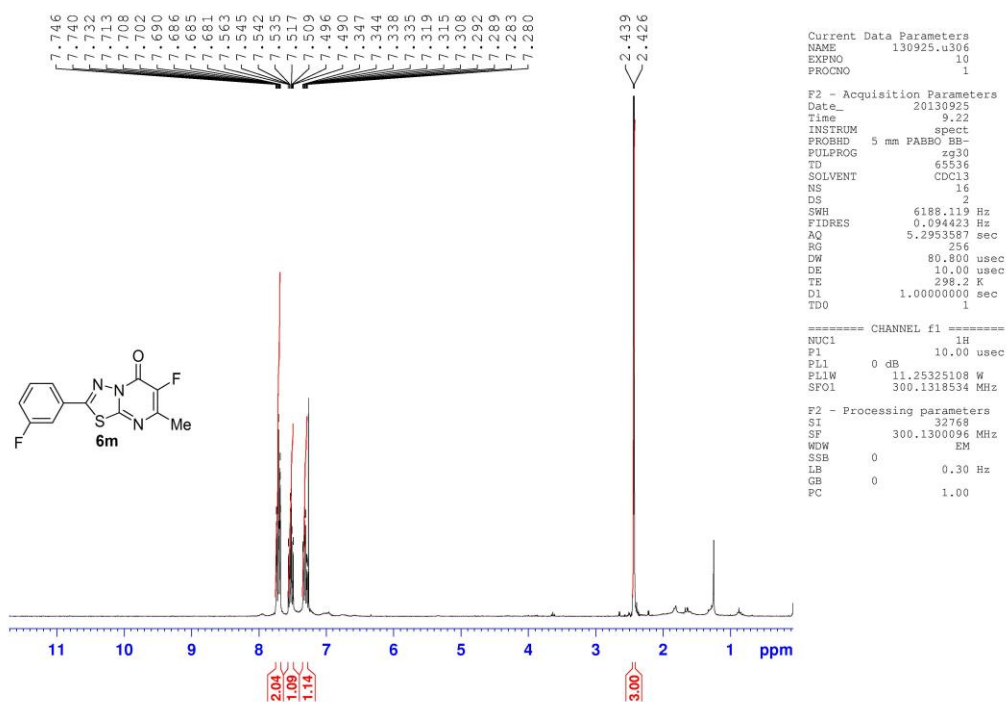
Current Data Parameters
NAME 130916.u304
EXPNO 13
PROCNO 1

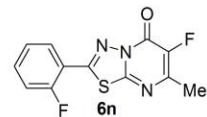
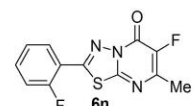
F2 - Acquisition Parameters
Date_ 20130916
Time 21.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 10.00 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

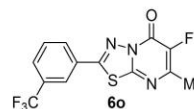
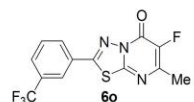
===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -0.50 dB
PL1W 33.25691986 W
SFO1 75.4752953 MHz

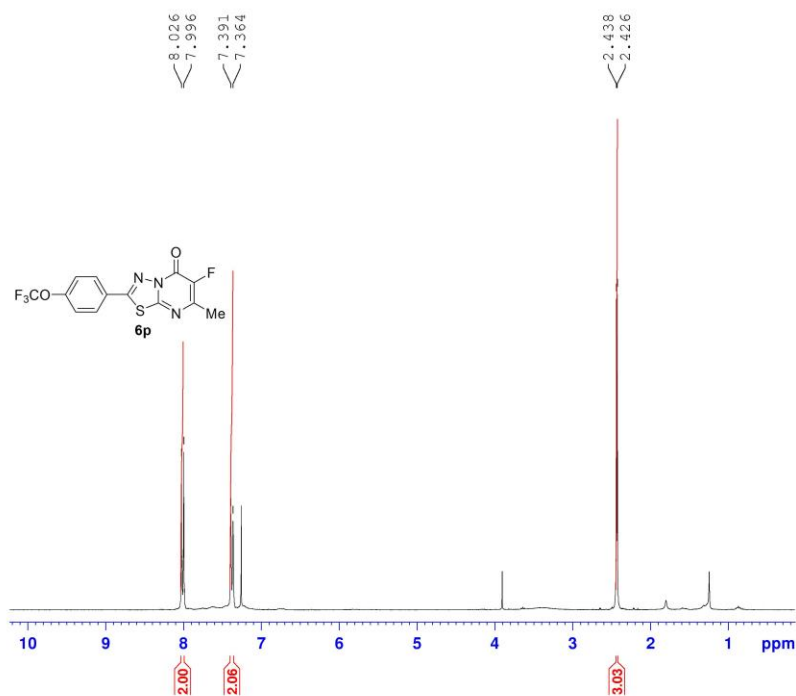
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 72.00 usec
PL2 0 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 11.25325108 W
PL12W 0.22453187 W
PL13W 0.22453187 W
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677403 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40







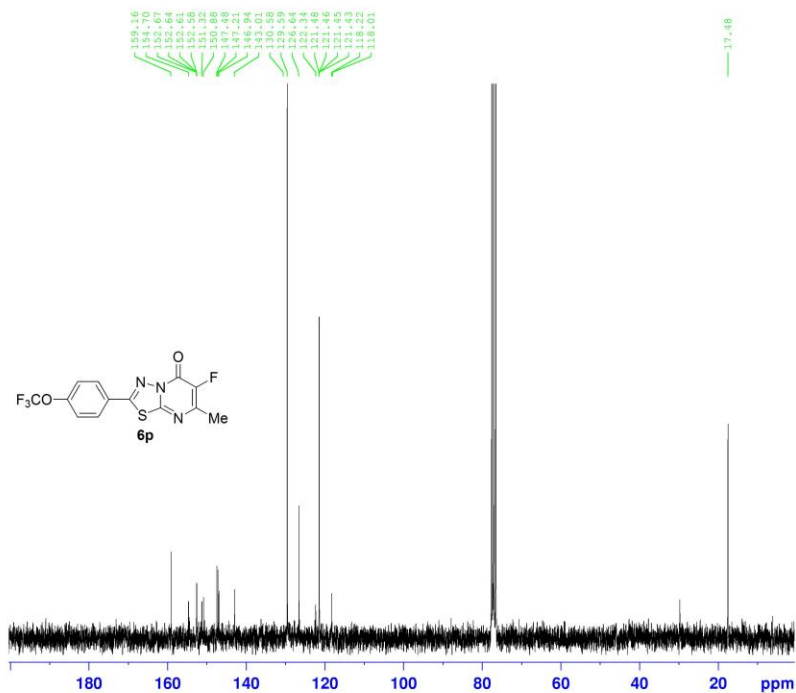


Current Data Parameters
 NAME 130927.u304
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130927
 Time 8.30
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 287
 DW 80.800 usec
 DE 10.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 0 dB
 PL1W 11.25325108 W
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1298248 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 FC 1.00



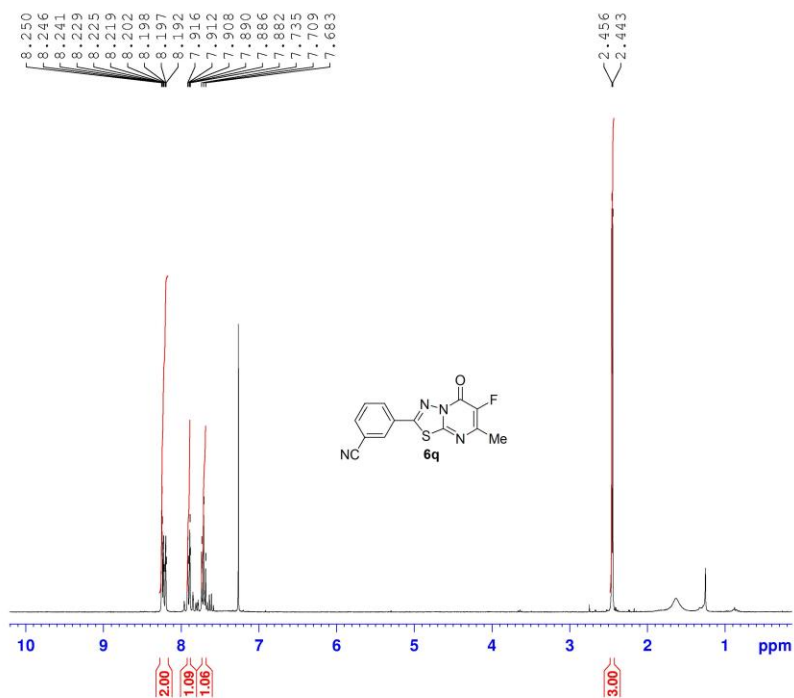
Current Data Parameters
 NAME 130927.201
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130927
 Time 9.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 15000.000 Hz
 FIDRES 0.228882 Hz
 AQ 2.1845834 sec
 RG 2050
 DW 33.333 usec
 DE 10.00 usec
 TE 298.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 -1.00 dB
 SFO1 62.9015280 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 70.00 usec
 PL12 15.00 dB
 PL13 15.00 dB
 PL2 -2.50 dB
 SFO2 250.1310005 MHz

F2 - Processing parameters
 SI 32768
 SF 62.8952351 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 FC 1.40

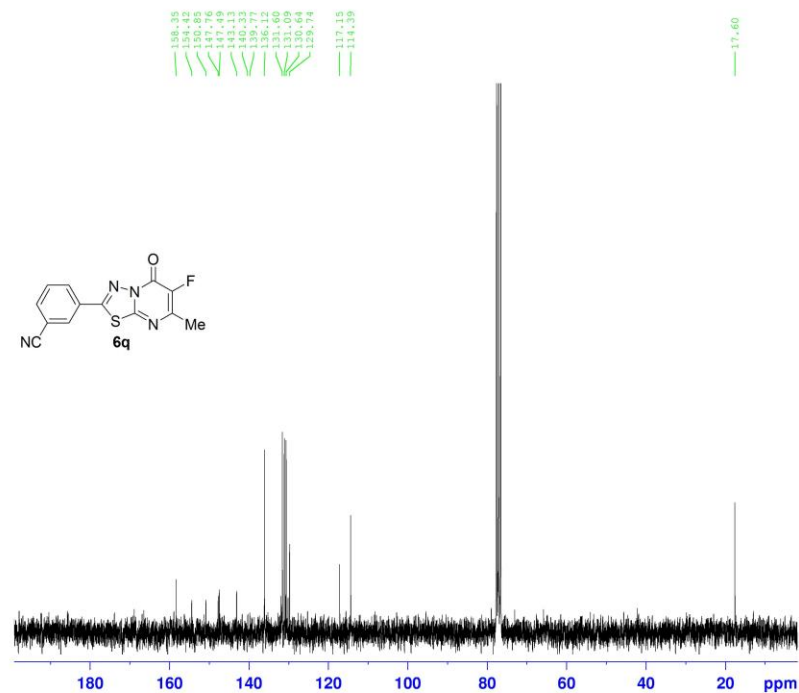


Current Data Parameters
NAME 131021.u305
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131021
Time 9.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 406
DW 80.800 usec
DE 10.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0 dB
PL1W 11.25325108 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 131024.203
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131024
Time 14.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 15000.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 2050
DW 33.333 usec
DE 10.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.00 dB
SFO1 62.9015280 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL12 15.00 dB
PL13 15.00 dB
PL2 -2.50 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952312 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Sequence alignment of human NPP-1

Mouse NPP-1....:1	5	10	15	20	25	30	35	40
Human NPP-1....:2								
Mouse NPP-1....:1	46	51	56	61	66	71	76	81
Human NPP-1....:2								
Mouse NPP-1....:1	87	92	97	102	107	112	117	122
Human NPP-1....:2								
Mouse NPP-1....:1	128	133	138	143	148	153	158	163
Human NPP-1....:2								
Mouse NPP-1....:1	169	174	179	184	189	194	199	204
Human NPP-1....:2								
Mouse NPP-1....:1	210	215	220	225	230	235	240	245
Human NPP-1....:2								
Mouse NPP-1....:1	251	256	261	266	271	276	281	286
Human NPP-1....:2								
Mouse NPP-1....:1	292	297	302	307	312	317	322	327
Human NPP-1....:2								
Mouse NPP-1....:1	333	338	343	348	353	358	363	368
Human NPP-1....:2								
Mouse NPP-1....:1	374	379	384	389	394	399	404	409
Human NPP-1....:2								
Mouse NPP-1....:1	415	420	425	430	435	440	445	450
Human NPP-1....:2								
Mouse NPP-1....:1	456	461	466	471	476	481	486	491
Human NPP-1....:2								

	497	502	507	512	517	522	527	532																																	
Mouse NPP-1....:1	P	I	Y	N	P	S	H	P	K	E	E	G	F	L	S	Q	C	P	I	K	S	T	S	N	D	L	G	C	T	C	D	P	W	I	V	P	I	K	D	F	E
Human NPP-1....:2	H	F	L	P	K	R	L	H	F	A	K	S	D	R	I	E	P	L	T	F	Y	L	D	P	Q	W	Q	L	A	L	N	P	S	E	R	K	Y	C	G	S	G
	538	543	548	553	558	563	568	573																																	
Mouse NPP-1....:1	K	Q	L	N	L	T	T	E	D	V	D	I	Y	H	M	T	V	P	Y	G	R	P	R	I	L	L	K	Q	H	H	V	C	L	L	Q	Q	Q	F	L		
Human NPP-1....:2	F	H	G	S	D	N	V	F	S	N	M	Q	A	L	F	V	G	Y	G	P	G	F	K	H	G	I	E	A	D	T	F	E	N	I	E	V	Y	N	L	M	C
	579	584	589	594	599	604	609	614																																	
Mouse NPP-1....:1	T	G	Y	S	L	D	L	L	M	P	L	W	A	S	Y	T	F	L	R	N	D	Q	F	S	R	D	D	F	S	N	C	L	Y	Q	D	L	R	I	P	L	S
Human NPP-1....:2	D	L	N	L	T	P	A	P	N	N	G	T	H	G	S	L	N	H	L	L	K	N	P	V	Y	T	P	K	H	P	K	E	V	H	P	L	V	Q	C	P	
	620	625	630	635	640	645	650	655																																	
Mouse NPP-1....:1	P	V	H	K	C	S	Y	Y	K	S	N	K	L	S	Y	G	F	L	T	P	P	R	L	N	R	V	S	N	H	I	Y	S	E	A	L	L	T	S	N	I	
Human NPP-1....:2	F	T	R	N	P	R	D	N	L	G	C	S	C	N	P	S	I	L	P	I	E	D	F	Q	T	Q	F	N	L	T	V	A	E	E	K	I	I	K	H	E	T
	661	666	671	676	681	686	691	696																																	
Mouse NPP-1....:1	V	P	M	Y	Q	S	F	Q	V	I	W	H	Y	L	H	D	T	L	L	Q	R	Y	A	H	E	R	N	G	I	N	V	V	S	G	P	V	F	D	F	D	Y
Human NPP-1....:2	L	P	Y	G	R	P	R	V	L	Q	K	E	N	T	I	C	L	L	S	Q	H	Q	F	M	S	G	Y	S	Q	D	I	L	M	P	L	W	T	S	Y	T	V
	702	707	712	717	722	727	732	737																																	
Mouse NPP-1....:1	D	G	R	Y	D	S	L	E	I	L	K	Q	N	S	R	V	I	R	S	Q	E	I	L	I	P	T	H	F	F	I	V	L	T	S	C	K	Q	L	S	E	T
Human NPP-1....:2	D	R	N	D	S	F	S	T	E	D	F	S	N	C	L	Y	Q	D	F	R	I	P	L	S	P	V	H	K	C	S	F	Y	K	N	N	T	K	V	S	Y	G
	743	748	753	758	763	768	773	778																																	
Mouse NPP-1....:1	P	L	E	C	S	A	L	E	S	S	A	Y	I	L	P	H	R	P	D	N	I	E	S	C	T	H	G	K	R	E	S	S	W	V	E	E	L	L	T	L	H
Human NPP-1....:2	F	L	S	P	P	Q	L	N	K	N	S	G	I	Y	S	E	A	L	L	T	T	N	I	V	P	M	Y	Q	S	F	Q	V	I	W	R	Y	F	H	D	T	
	784	789	794	799	804	809	814	819																																	
Mouse NPP-1....:1	R	A	R	V	T	D	V	E	L	I	T	G	L	S	F	Y	Q	D	R	Q	E	S	V	S	E	L	L	R	K	T	H	L	P	I	F	S					
Human NPP-1....:2	L	L	R	K	Y	A	E	E	R	N	G	V	N	V	S	G	P	V	F	D	F	D	Y	D	G	R	C	D	S	L	E	N	L	R	Q	R	R	V	I		
	825	830	835	840	845	850	855	860																																	
Mouse NPP-1....:1	R	N	Q	E	I	L	I	P	T	H	F	F	I	V	L	T	S	C	K	D	T	S	Q	T	P	L	H	C	E	N	L	D	T	L	A	F	I	L	P	H	R
Human NPP-1....:2	T	D	N	S	E	S	C	V	H	G	K	H	D	S	S	W	V	E	E	L	L	M	L	H	R	A	R	I	T	D	V	E	H	I	T	G	L	S	F	Y	Q
	866	871	876	881	886	891	896	901																																	
Mouse NPP-1....:1	T	D	N	S	E	S	C	V	H	G	K	H	D	S	S	W	V	E	E	L	L	M	L	H	R	A	R	I	T	D	V	E	H	I	T	G	L	S	F	Y	Q
Human NPP-1....:2	T	D	N	S	E	S	C	V	H	G	K	H	D	S	S	W	V	E	E	L	L	M	L	H	R	A	R	I	T	D	V	E	H	I	T	G	L	S	F	Y	Q
	907	912	917	922	927	932	937	942																																	
Mouse NPP-1....:1	Q	R	K	E	P	V	S	D	I	L	K	L	K	T	H	L	P	T	F	S	Q	E	D																		
Human NPP-1....:2	Q	R	K	E	P	V	S	D	I	L	K	L	K	T	H	L	P	T	F	S	Q	E	D																		

Figure SI-1. Sequence alignment of human NPP-1 (UniprotKB/Swiss-prot ID P22413) with mouse NPP-1 crystal structure (PDB ID 4B56). The color bars are secondary structure bars. Where, red bars indicate helices, yellow bars indicate β -sheets and blue bars indicate hydrogen bonded amino acids.

Sequence alignment of h-NPP-3

Mouse NPP-1....:1	5	10	15	20	25	30	35	40	
Human NPP-3....:2									
Mouse NPP-1....:1	46	51	56	61	66	71	76	81	
Human NPP-3....:2									
Mouse NPP-1....:1	87	92	97	102	107	112	117	122	
Human NPP-3....:2									
Mouse NPP-1....:1	128	133	138	143	148	153	158	163	
Human NPP-3....:2									
Mouse NPP-1....:1	169	174	179	184	189	194	199	204	
Human NPP-3....:2									
Mouse NPP-1....:1	210	215	220	225	230	235	240	245	
Human NPP-3....:2									
Mouse NPP-1....:1	251	256	261	266	271	276	281	286	
Human NPP-3....:2									
Mouse NPP-1....:1	292	297	302	307	312	317	322	327	
Human NPP-3....:2									
Mouse NPP-1....:1	333	338	343	348	353	358	363	368	
Human NPP-3....:2									
Mouse NPP-1....:1	374	379	384	389	394	399	404	409	
Human NPP-3....:2									
Mouse NPP-1....:1	415	420	425	430	435	440	445	450	
Human NPP-3....:2									
Mouse NPP-1....:1	456	461	466	471	476	481	486	491	
Human NPP-3....:2									

	497	502	507	512	517	522	527	532																																		
Mouse NPP-1....:1	P	I	Y	N	P	S	H	P	K	E	E	G	F	L	S	Q	C	P	I	K	S	T	S	N	D	L	G	C	T	C	D	P	W	I	V	P	I	K	D	F	E	
Human NPP-3....:2	E	A	I	F	L	A	H	G	P	S	F	K	E	K	T	E	V	E	P	F	E	N	I	E	V	Y	N	L	M	C	D	L	L	R	I	Q	P	A	P	N	N	
	538	543	548	553	558	563	568	573																																		
Mouse NPP-1....:1	K	Q	L	N	L	T	T	E	D	V	D	I	Y	H	M	T	V	P	Y	G	R	P	R	I	L	L	K	Q	H	H	V	C	L	L	Q	Q	Q	F	L			
Human NPP-3....:2	G	T	H	G	S	L	N	H	L	L	K	V	P	F	Y	E	P	S	H	A	E	E	V	S	K	F	S	V	C	G	F	A	N	P	L	P	T	E	S	L	D	
	579	584	589	594	599	604	609	614																																		
Mouse NPP-1....:1	T	G	Y	S	L	D	L	L	M	P	L	W	A	S	Y	T	F	L	R	N	D	Q	F	S	R	D	D	F	S	N	C	L	Y	Q	D	L	R	I	P	L	S	
Human NPP-3....:2	C	F	C	P	H	L	Q	N	S	T	Q	L	E	Q	V	N	Q	M	L	N	L	T	Q	E	E	I	T	A	T	V	K	V	N	L	P	F	G	R	P	R	V	
	620	625	630	635	640	645	650	655																																		
Mouse NPP-1....:1	P	V	H	K	C	S	Y	Y	K	S	N	S	K	L	S	Y	G	F	L	T	P	P	R	L	N	R	V	S	N	H	I	Y	S	E	A	L	L	T	S	N	I	
Human NPP-3....:2	L	Q	K	N	V	D	H	C	L	L	Y	H	R	E	Y	V	S	G	F	G	K	A	M	R	M	P	M	W	S	S	Y	T	V	P	Q	L	G	D	T	S	P	
	661	666	671	676	681	686	691	696																																		
Mouse NPP-1....:1	V	P	M	Y	Q	S	F	Q	V	I	W	H	Y	L	H	D	T	L	L	Q	R	Y	A	H	E	R	N	G	I	N	V	V	S	G	P	V	F	D	F	D	Y	
Human NPP-3....:2	L	P	P	T	V	P	D	C	L	R	A	D	V	R	V	P	P	S	E	S	Q	K	C	S	F	Y	L	A	D	K	N	I	T	H	G	F	L	P	P	A		
	702	707	712	717	722	727	732	737																																		
Mouse NPP-1....:1	D	G	R	Y	D	S	L	E	I	L	K	Q	N	S	R	V	I	R	S	Q	E	I	L	I	P	T	H	F	F	I	V	L	T	S	C	K	Q	L	S	E	T	
Human NPP-3....:2	S	N	R	T	S	D	S	Q	Y	D	A	L	I	T	S	N	L	V	P	M	Y	E	E	F	R	K	M	W	D	Y	F	H	S	V	L	L	I	K	H	A	T	
	743	748	753	758	763	768	773	778																																		
Mouse NPP-1....:1	P	L	E	C	S	A	L	E	S	S	A	Y	I	L	P	H	R	P	D	N	I	E	S	C	T	H	G	K	R	E	S	S	W	V	E	E	L	L	T	L	H	
Human NPP-3....:2	E	R	N	G	V	N	V	S	G	P	I	F	D	Y	N	Y	D	G	H	F	D	A	P	D	E	I	T	K	H	L	A	N	T	D	V	P	I	P	T	H		
	784	789	794	799	804	809	814	819																																		
Mouse NPP-1....:1	R	A	R	V	T	D	V	E	L	I	T	G	L	S	F	Y	Q	D	R	Q	E	S	V	S	E	L	L	R	L	K	T	H	L	P	I	F	S					
Human NPP-3....:2	Y	F	V	V	L	T	S	C	K	N	K	S	H	T	P	E	N	C	P	G	W	L	D	V	L	P	F	I	I	P	H	R	P	T	N	V	E	S	C	P	E	
	825	830	835	840	845	850	855	860																																		
Mouse NPP-1....:1	G	K	P	E	A	L	W	V	E	E	R	F	T	A	H	I	A	R	V	R	D	V	E	L	L	T	G	L	D	F	Y	Q	D	K	V	Q	P	V	S	E	I	
Human NPP-3....:2	L	Q	K	P	E	A	L	W	V	E	E	R	F	T	A	H	I	A	R	V	R	D	V	E	L	L	T	G	L	D	F	Y	Q	D	K	V	Q	P	V	S	E	I
	866	871	876	881	886	891	896	901																																		
Mouse NPP-1....:1	L	Q	L	K	T	Y	L	P	T	F	E	T	T	I																												
Human NPP-3....:2	L	Q	L	K	T	Y	L	P	T	F	E	T	T	I																												

Figure SI-2. Sequence alignment of h-NPP-3 (NCBI accession code O14638) with mouse NPP-1 crystal structure (PDB ID 4B56)

See description of Fig. **SI-1**

Ramachandran Plot generated for modelled h-NPP1

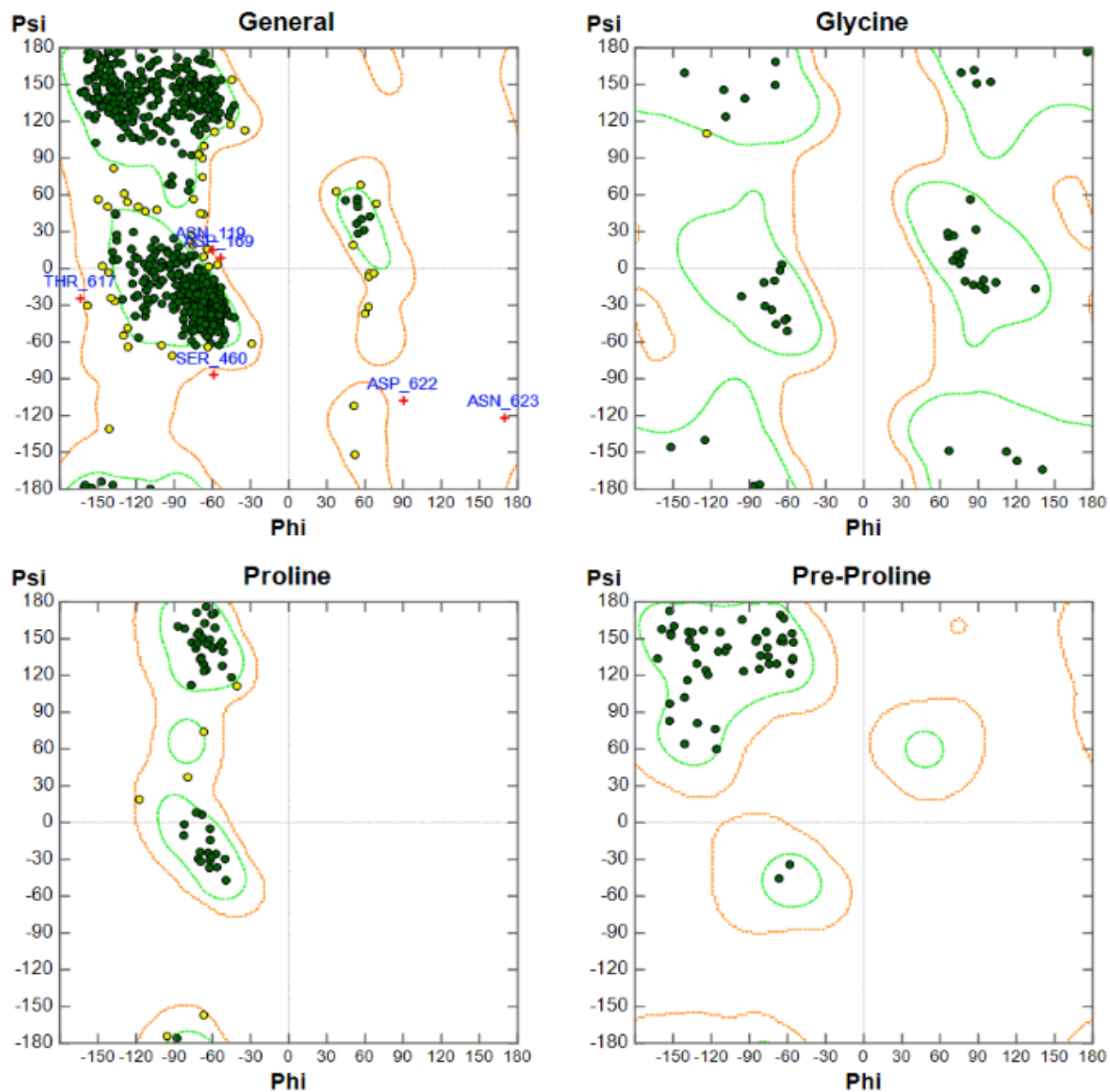


Figure SI-3. Ramachandran Plot generated for modelled h-NPP1 structure

Ramachandran Plot generated for modelled h-NPP3 structure

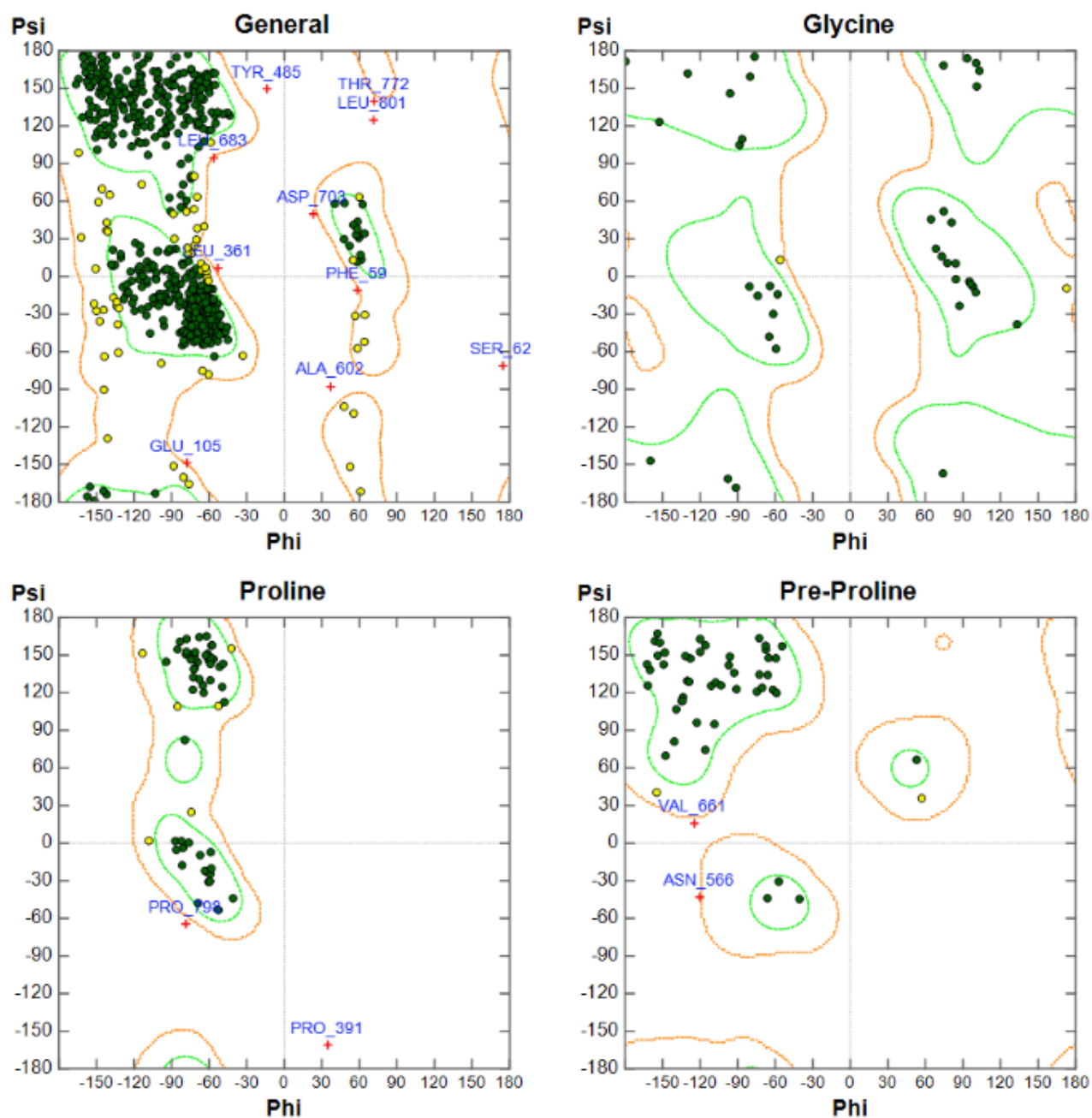


Figure SI-4. Ramachandran Plot generated for modelled h-NPP3 structure