

Supplementary material

Design, synthesis and bioevaluation of 1*H*-indole-4-carboxamide derivatives as potent Poly (ADP-ribose) polymerase-1 inhibitors

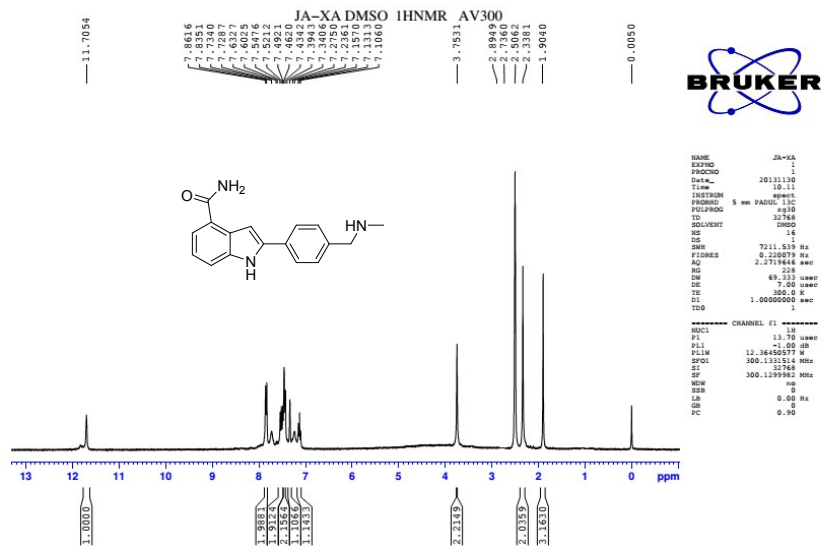
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^a*Jiangsu Key Laboratory of Drug Design and Optimization, China Pharmaceutical University, Nanjing 21009, China*

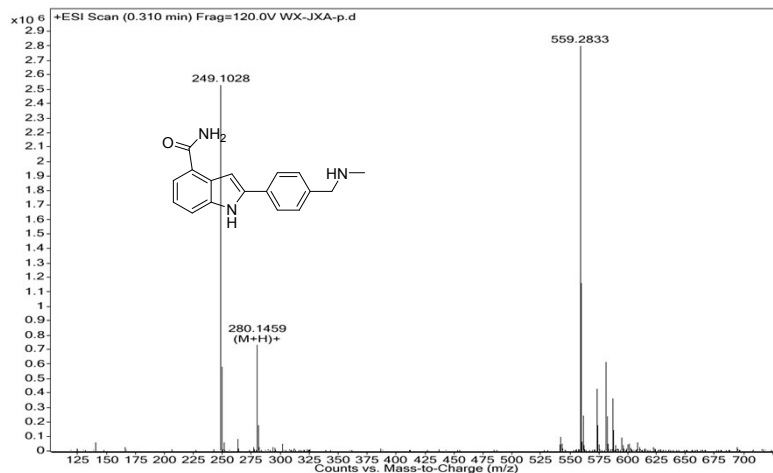
Contents

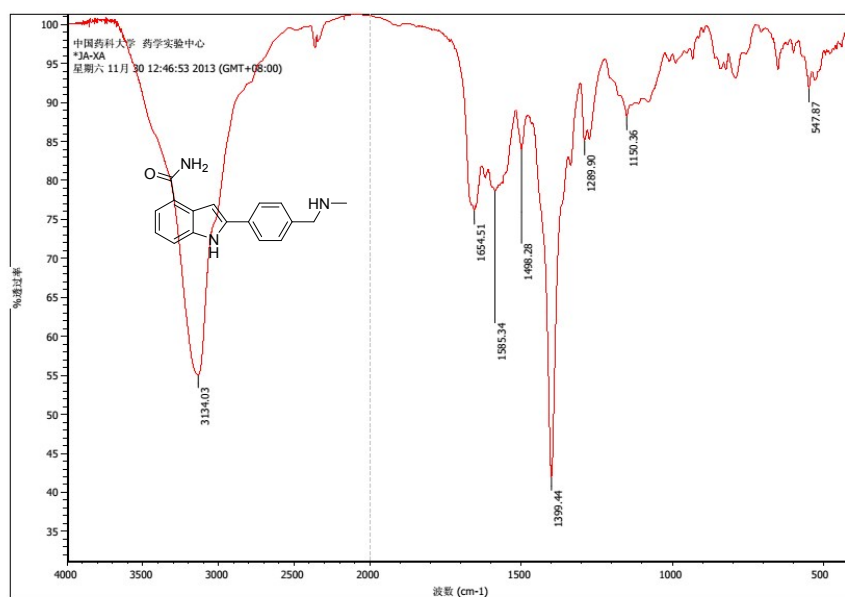
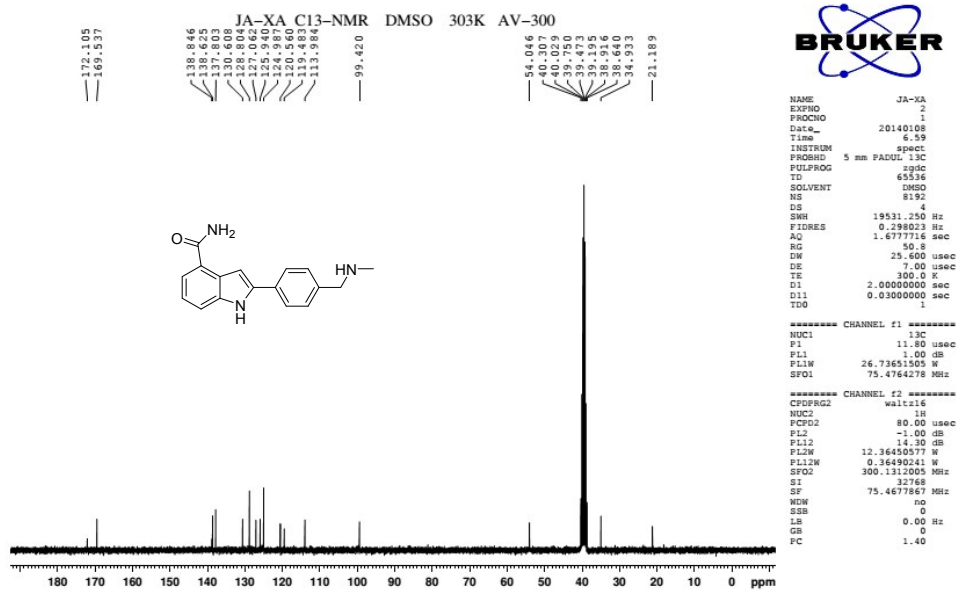
Compound characterization

Compound LX1

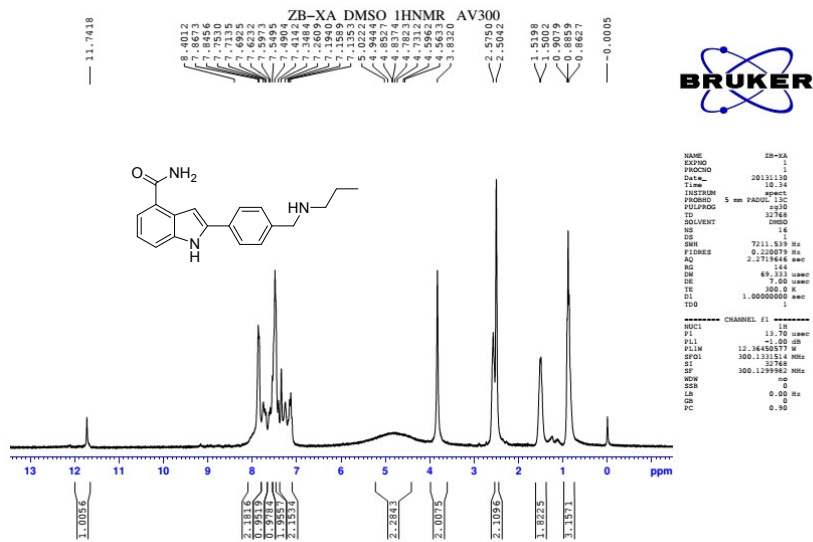


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Data Filename	WX-JXA-p.d	ACQ Method		Comment		Acquired Time	12/13/2013 10:04:09 PM

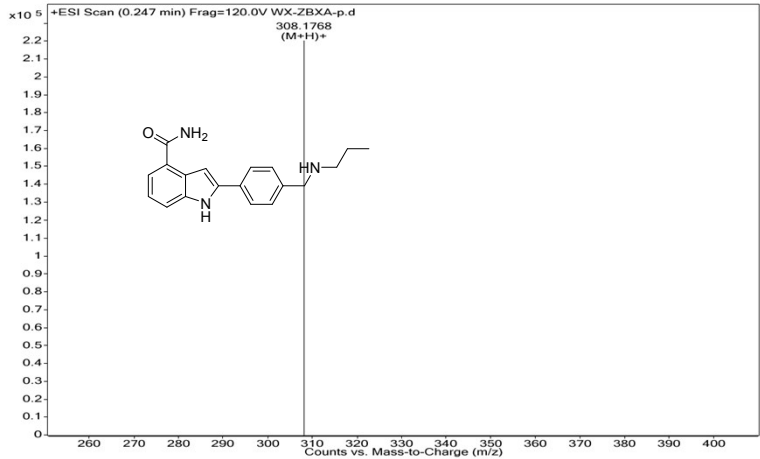


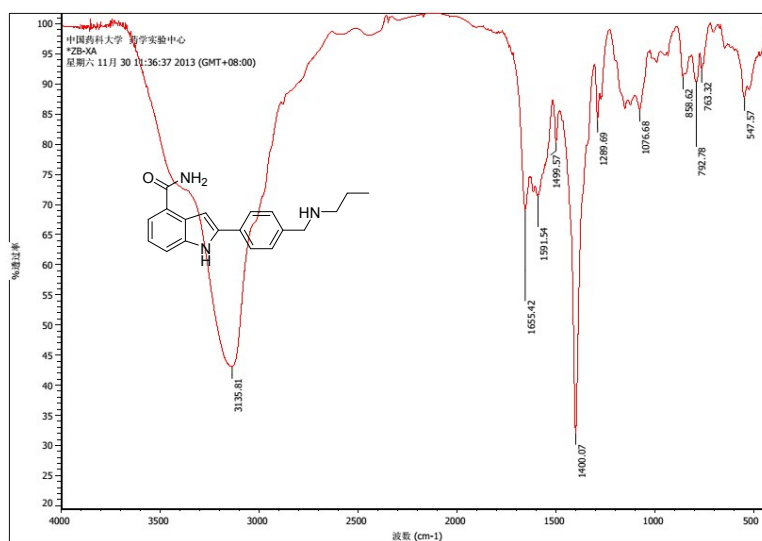
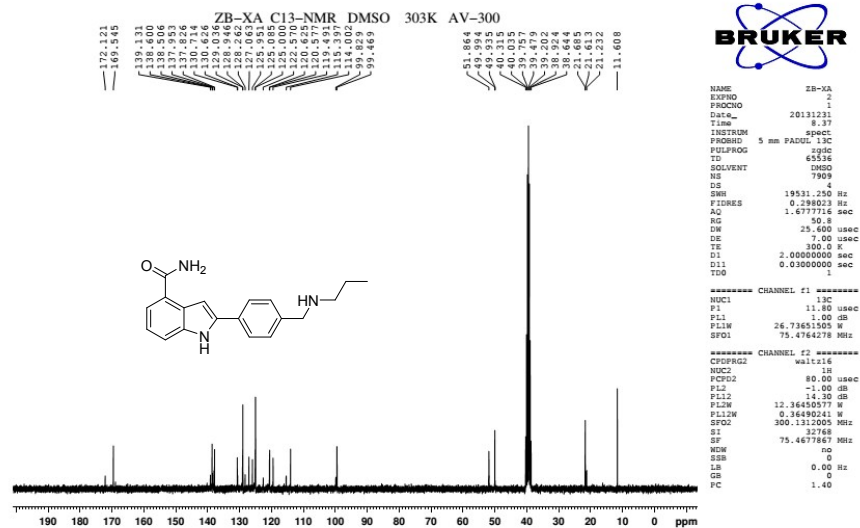


Compound LX2

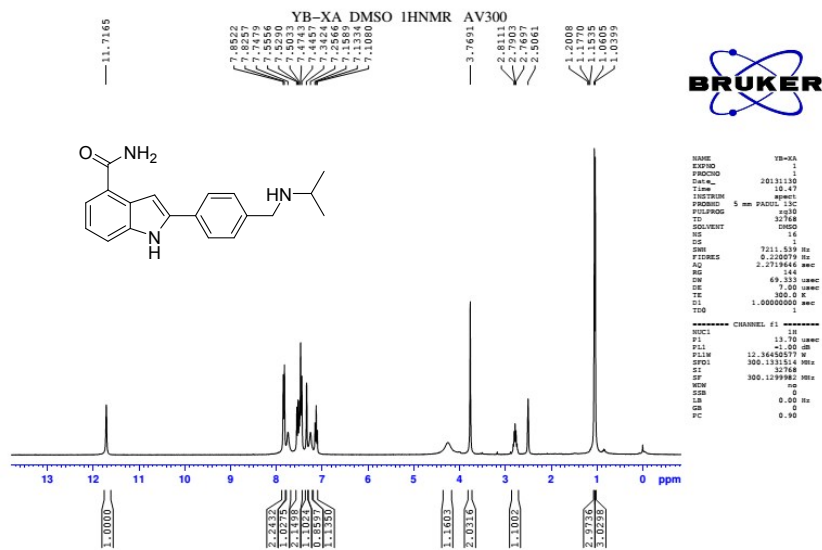


Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	WX-ZBXA-p.d	Acq Method	Unavailable	Comment	Sample Information is unavailable	Acquired Time	Unavailable

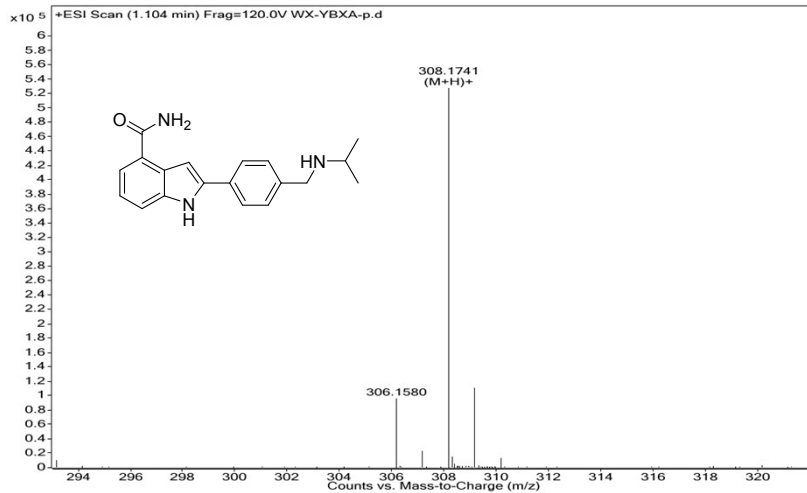


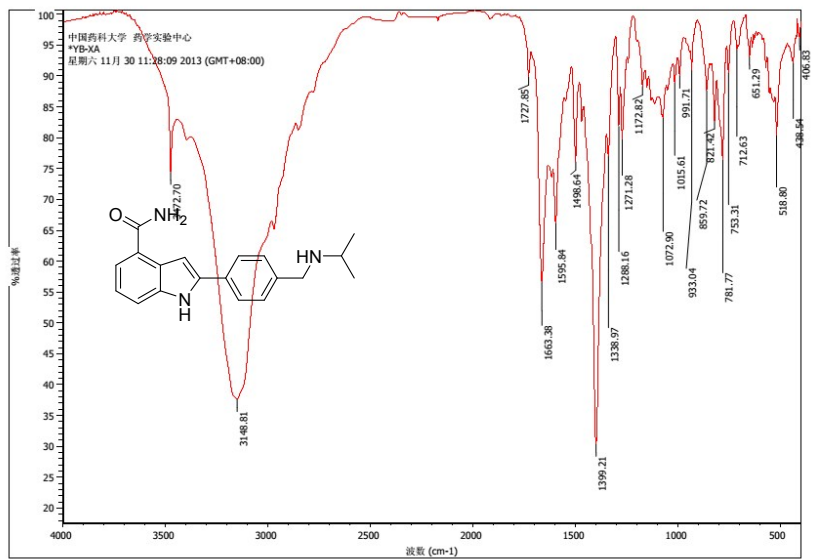
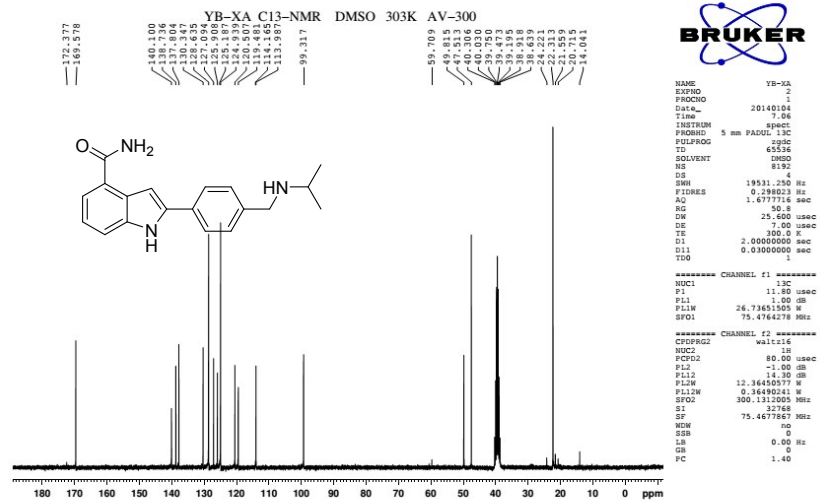


Compound LX3

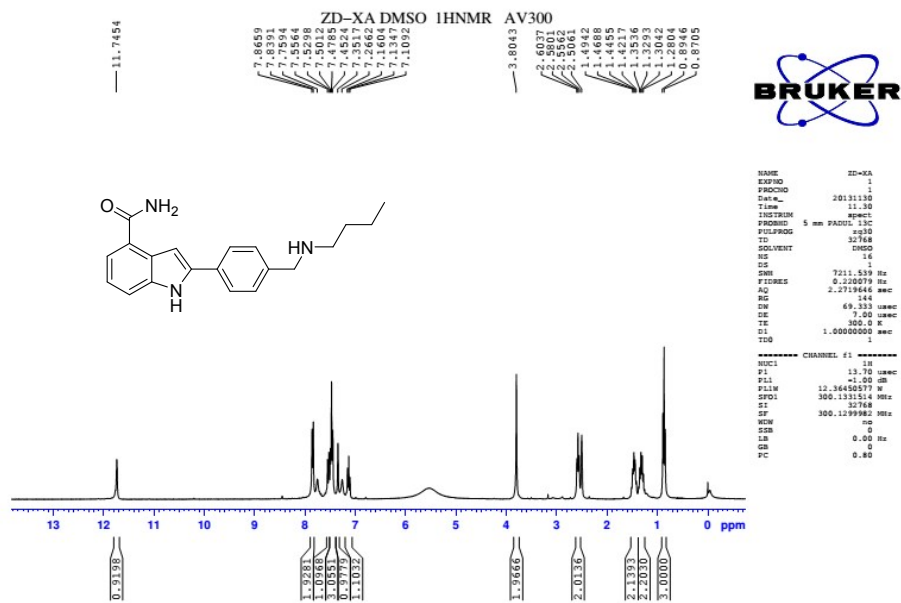


Sample Name	5	Position	P2-B7	Instrument Name	Instrument 1	User Name	
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Data Filename	WX-YBXA-p.d	ACQ Method		Comment		Acquired Time	1/3/2014 11:35:00 PM

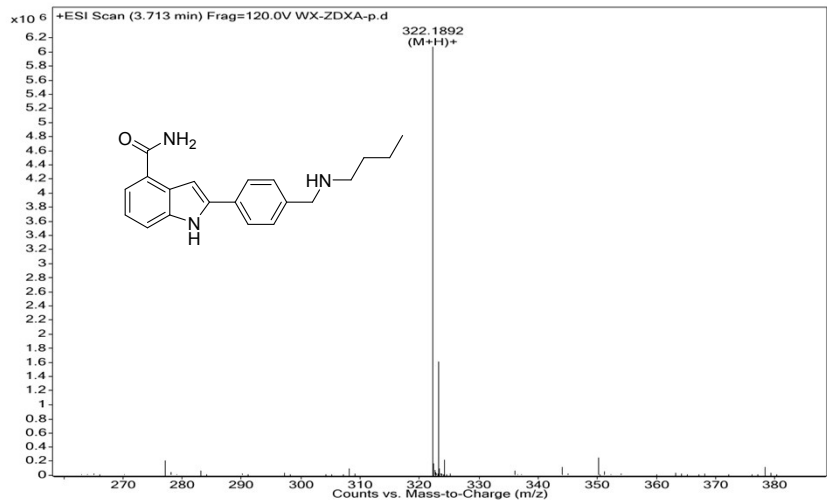


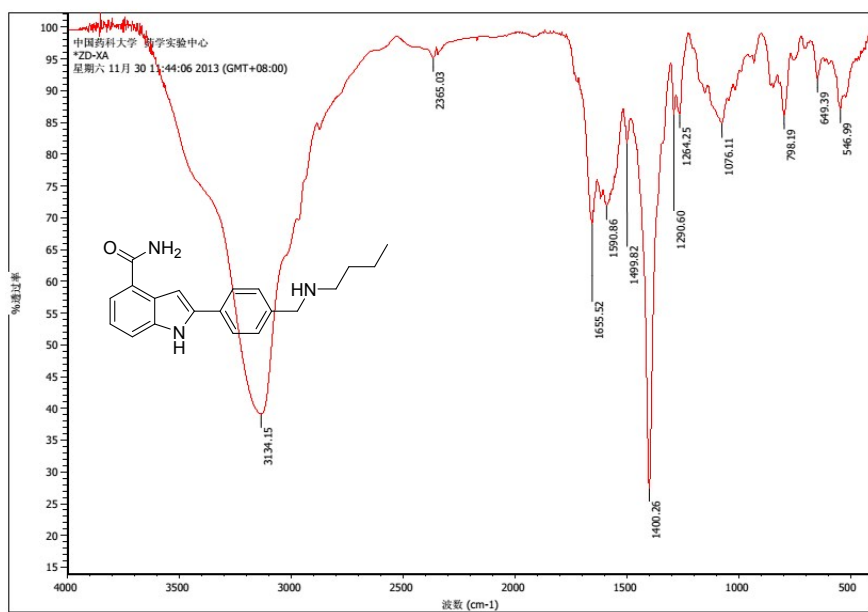
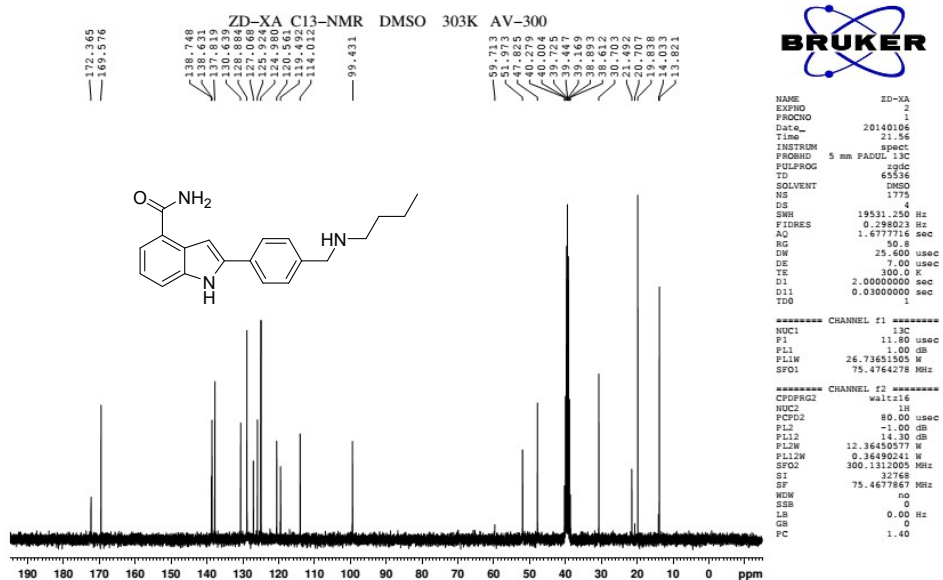


Compound LX4

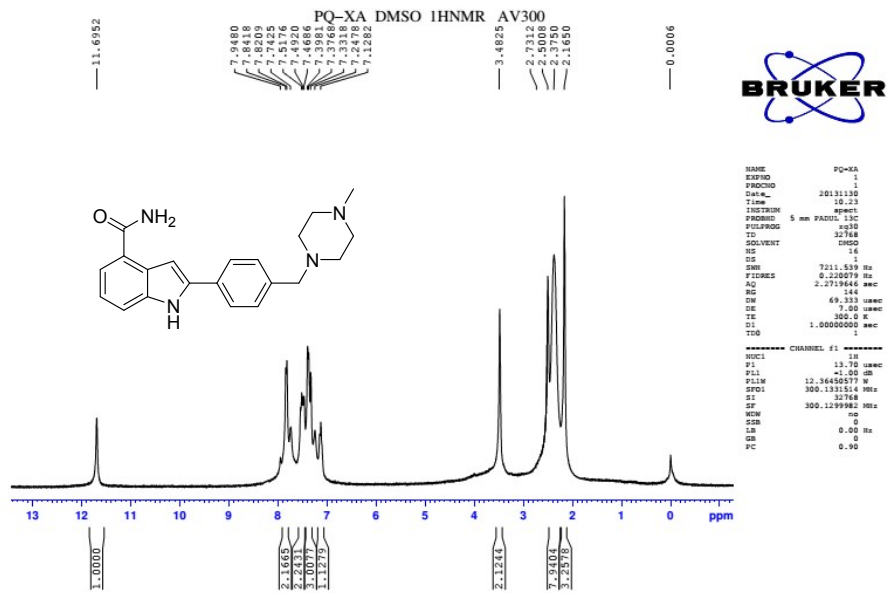


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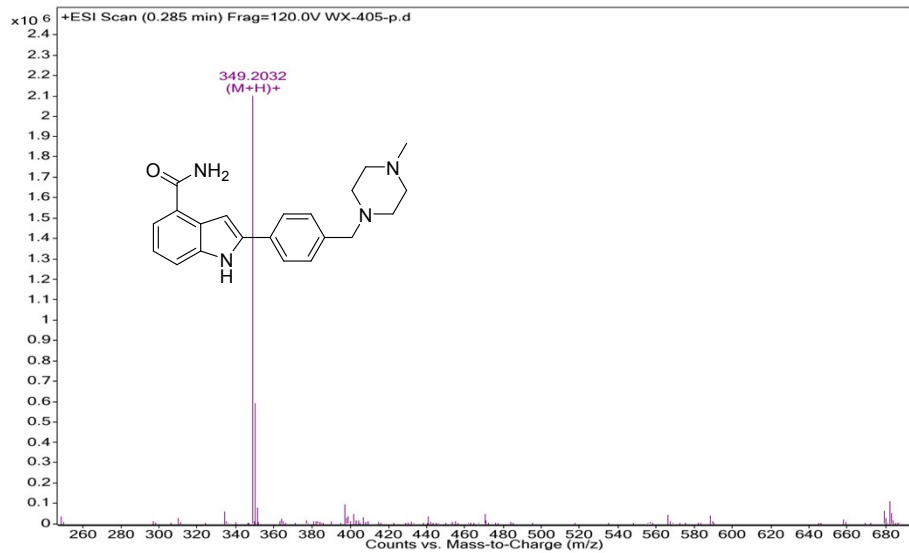


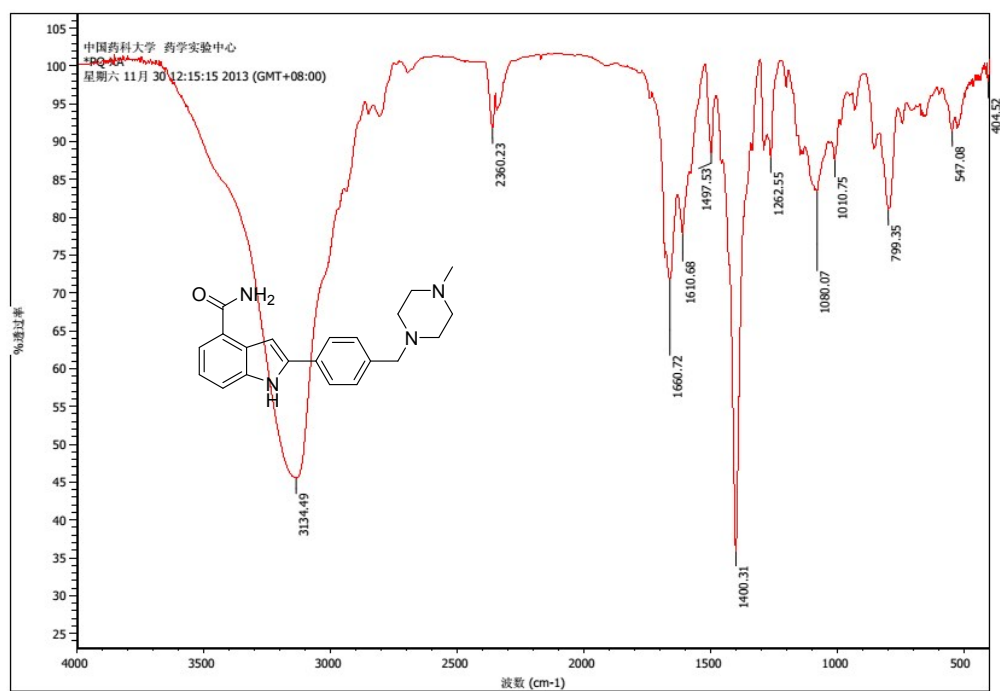
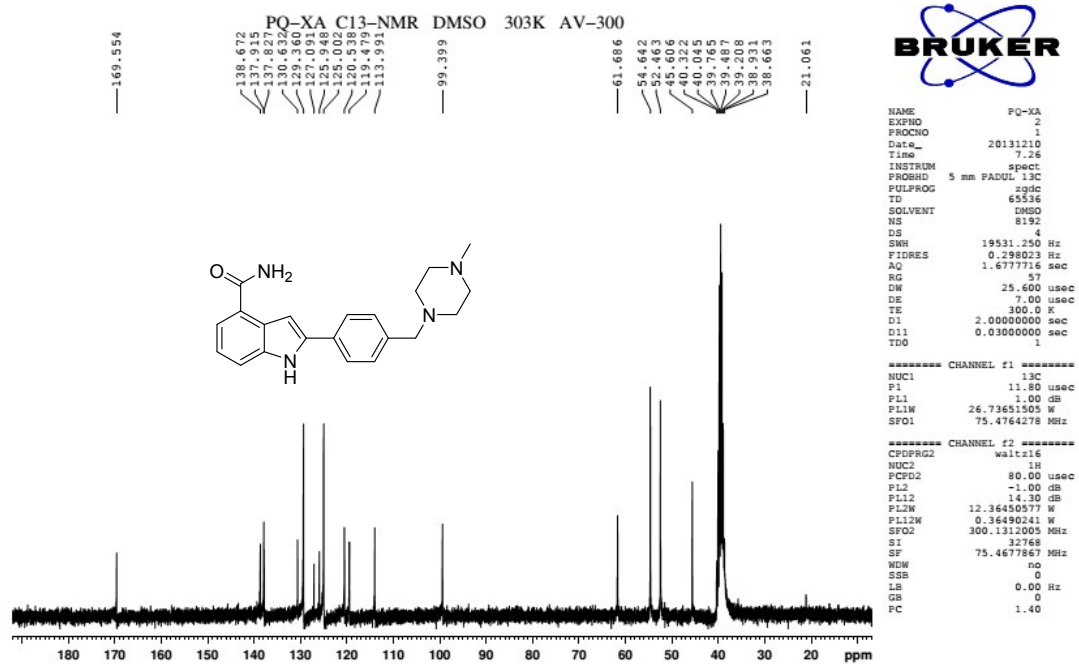


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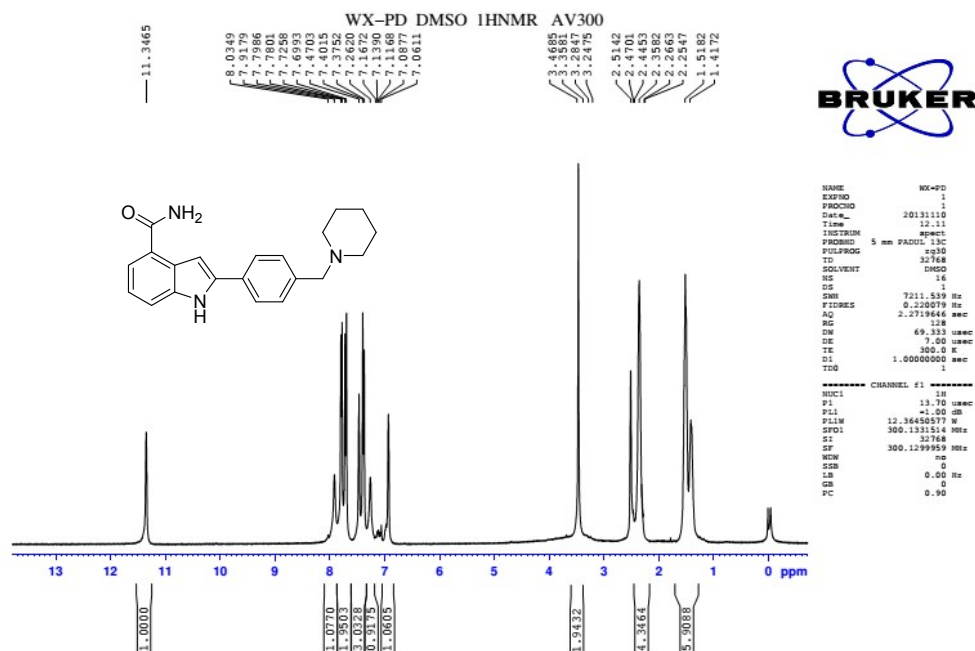


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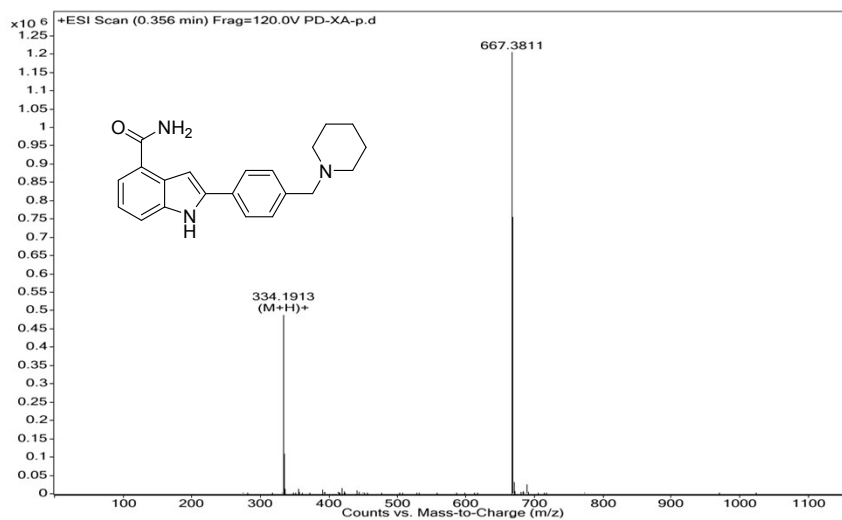


Compound LX6

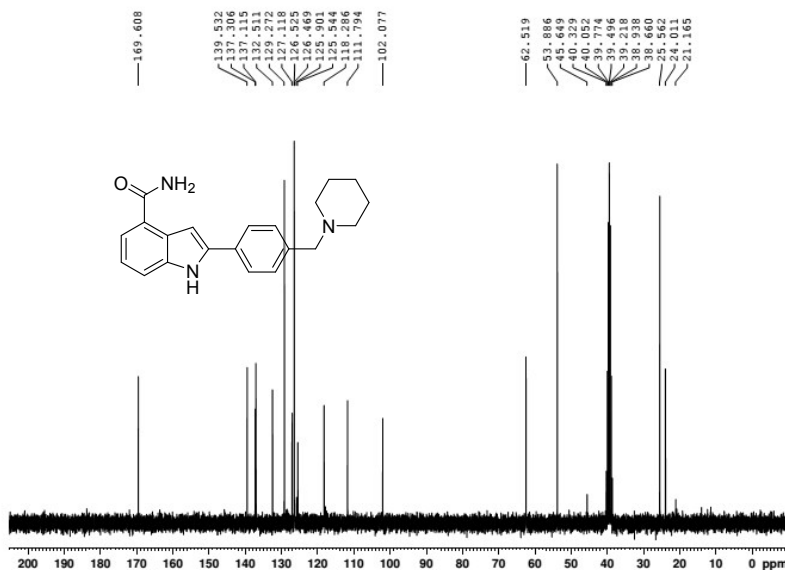


Sample Name	Position	Instrument Name	User Name
PD-XA-p.d	P1-E3	Instrument 1	IRM Calibration Status
		Sample	Acquired Time

Success 4/22/2014 11:16:44 AM



WX-PD C13-NMR DMSO 303K AV-300

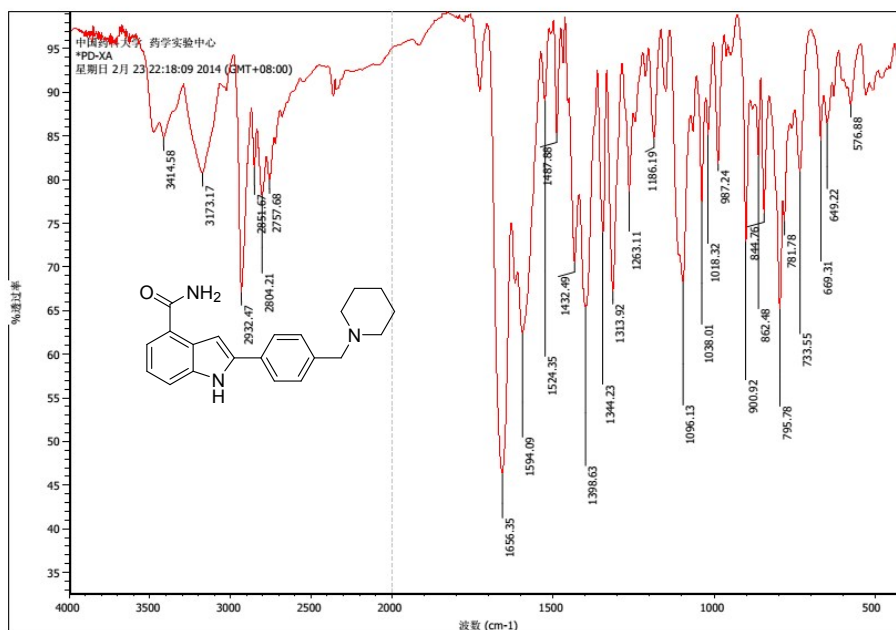


```

NAME          WX-PD
EXPNO         2
PROCNO        1
Date_         20131110
Time          18.10
INSTRUM       spect
PROBHD        5 mm PADUL 13C
PULPROG       zgpg
TD             65536
SOLVENT       DMSO
NS            864
DS            4
SWH           19531.250 Hz
FIDRES        0.298023 Hz
AQ            1.6777716 sec
RG            50.8
DW            25.600 usec
DE            7.00 usec
TE            300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

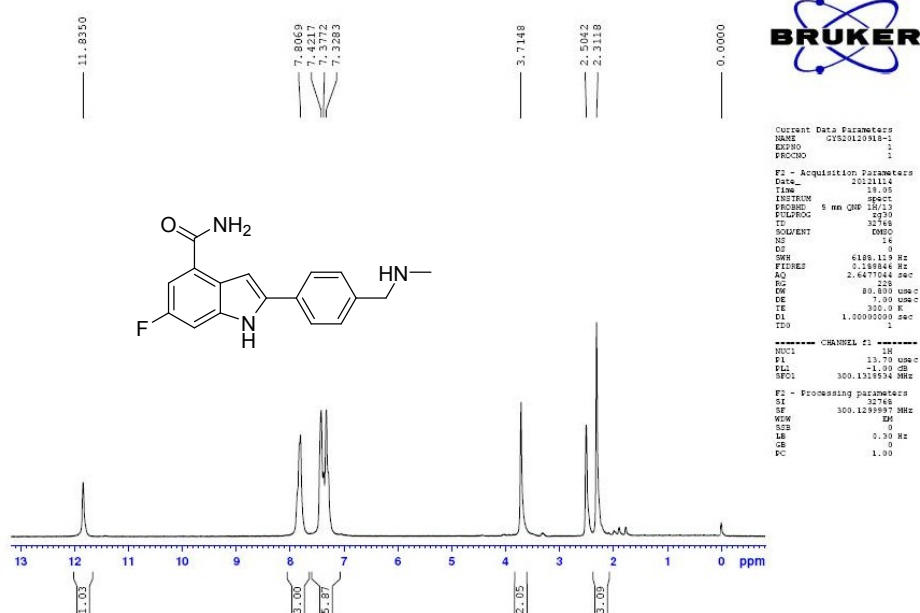
===== CHANNEL f1 =====
NUC1           13C
P1            11.80 usec
PL1           -1.00 dB
PL1W          26.73651505 W
SFO1          75.4764278 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2         80.00 usec
PL2           -1.00 dB
PL12          14.30 dB
PL1W          12.36450577 W
PL12W         0.36490241 W
SFO2          300.1312005 MHz
SI            32768
SF           75.4677867 MHz
WDW           no
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
  
```

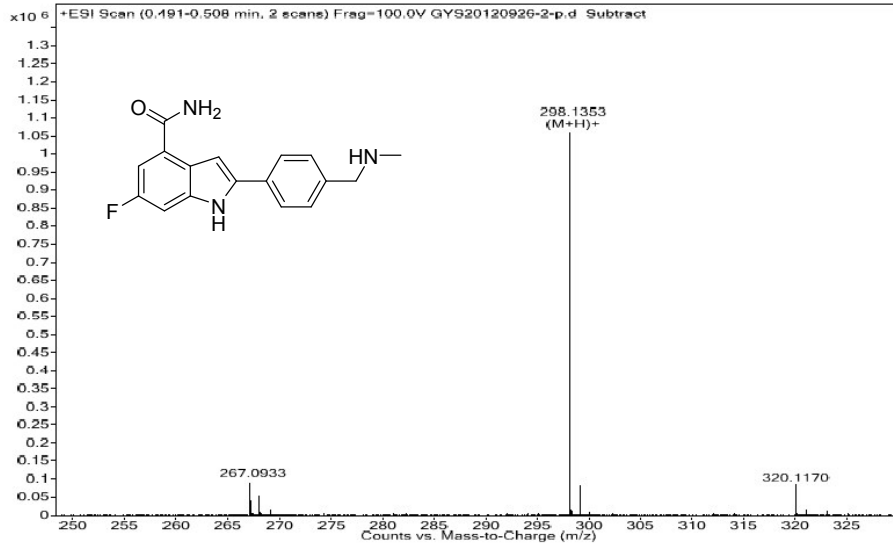


Compound LX7

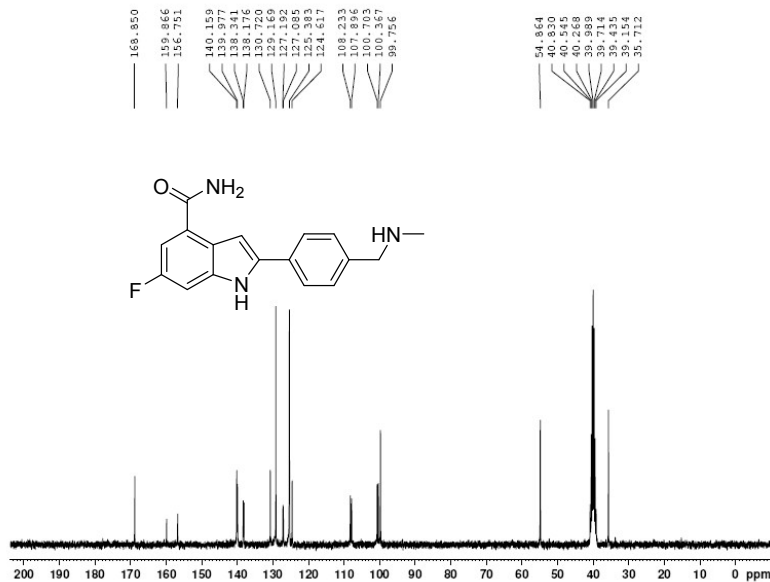
GYS20120918-1 DMSO 303K AV-300



Sample Name	0.3	Position	P2-B9	Instrument Name	Instrument 1	User Name	
Inj Vol		Inj Position		Sample Type	Sample	IRM Calibration Status	Success
Data Filename	GYS20120926-2-p.d	ACQ Method		Comment		Acquired Time	9/26/2012 7:57:48 PM



GYS20120918-1 C13-NMR DMSO 303K AV-300



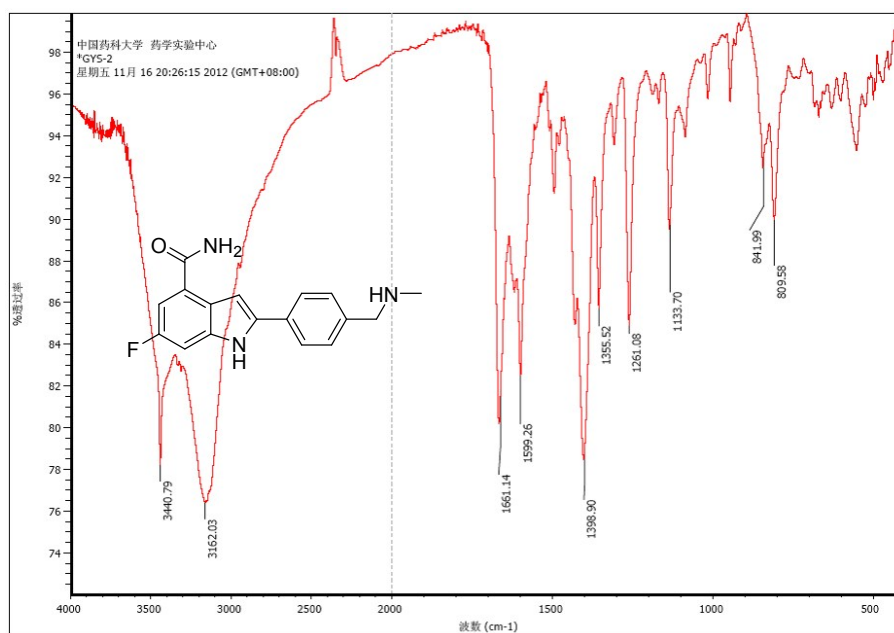
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NAME GYS20120918-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121116
Time 7.57
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 659
DS 4
SWH 16666.666 Hz
FIDRES 0.284113 Hz
AQ 1.9661300 sec
RG 362
DW 30.000 usec
DE 7.00 usec
TE 301.0 K
D1 2.0000000 sec
S11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 11.80 usec
PL1 1.00 dB
SFO1 75.4752203 MHz

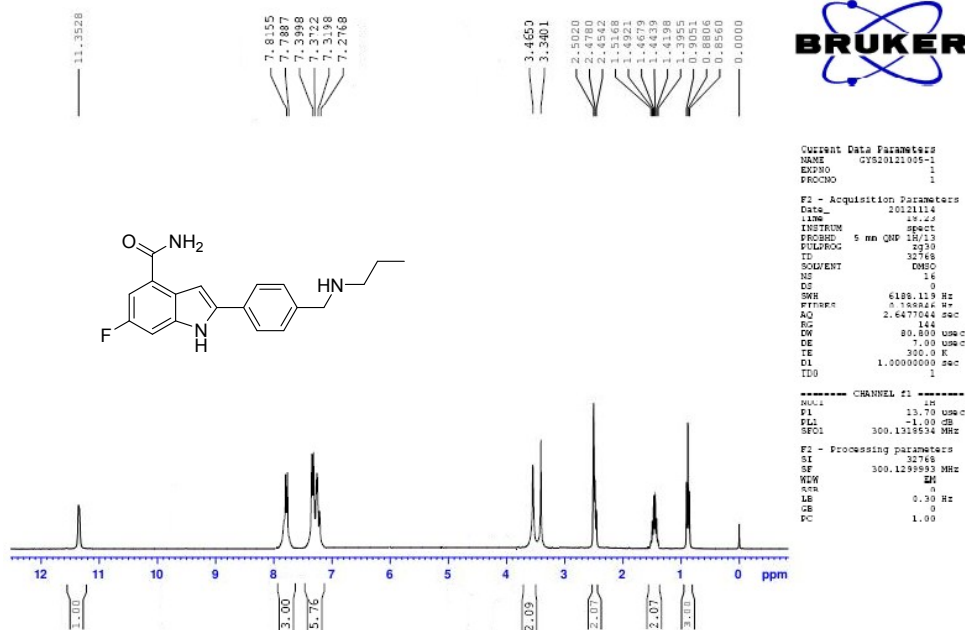
===== CHANNEL f2 =====
CDEPR2 wait+16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.30 dB
SFO2 300.131305 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

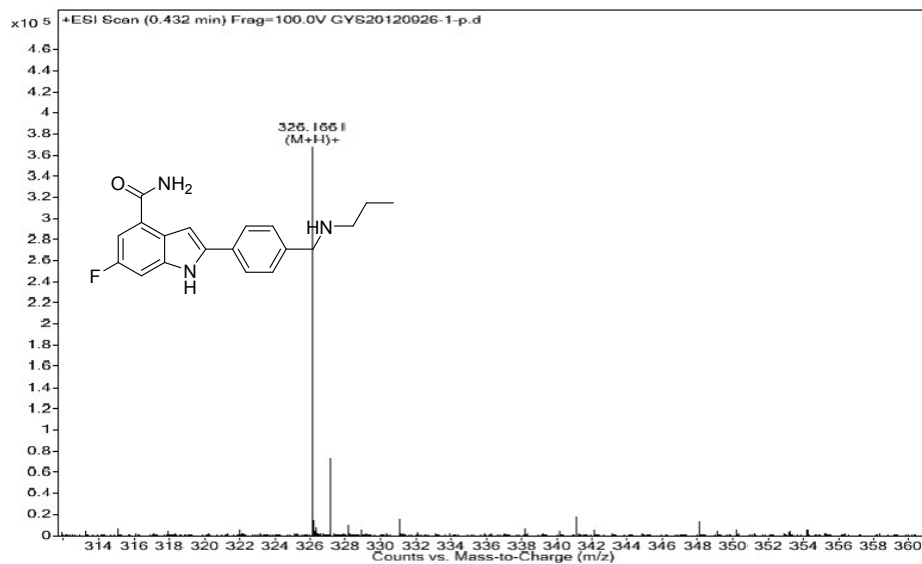


Compound LX8

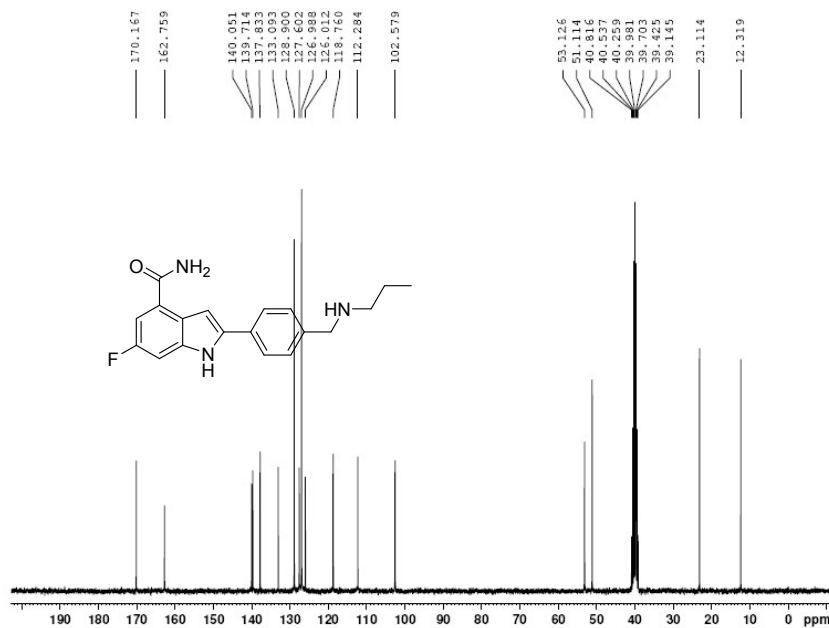
GYS20121005-1 DMSO 303K AV-300



Sample Name	Position	Instrument Name	Instrument 1	User Name
Inj Vol: 0.3	P2-B8	SampleType	Sample	IRM Calibration Status
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GYS20121005-1 C13-NMR DMSO 303K AV-300



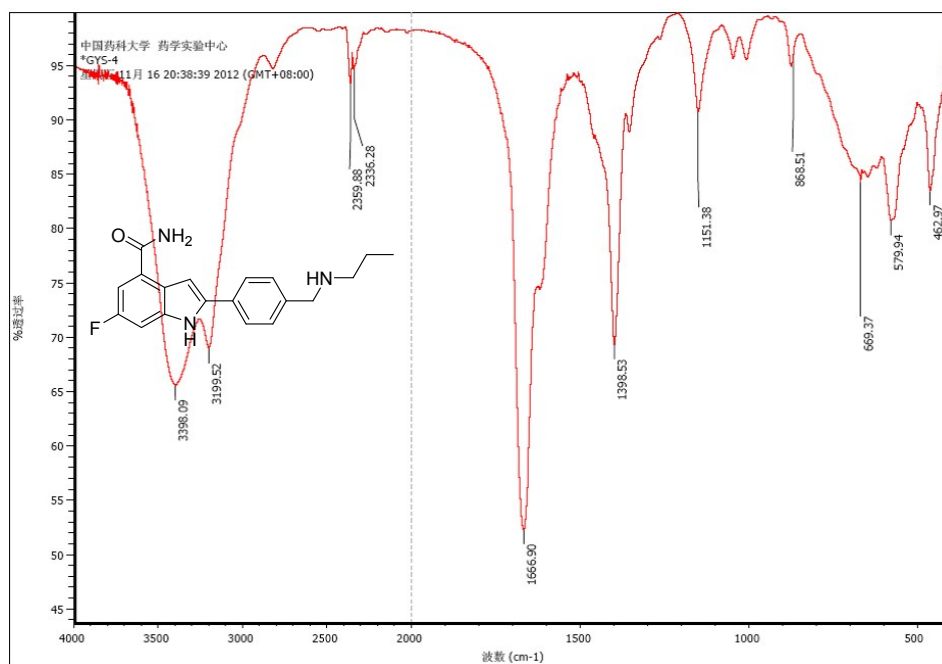
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NAME GYS20121005-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121118
Time 22.49
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 8192
DS 4
SWH 16666.666 Hz
FIDRES 0.254313 Hz
AQ 1.9661300 sec
RG 203
DM 30.900 usec
DE 1.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 11.80 usec
PL1 1.00 dB
SFO1 75.4752203 MHz

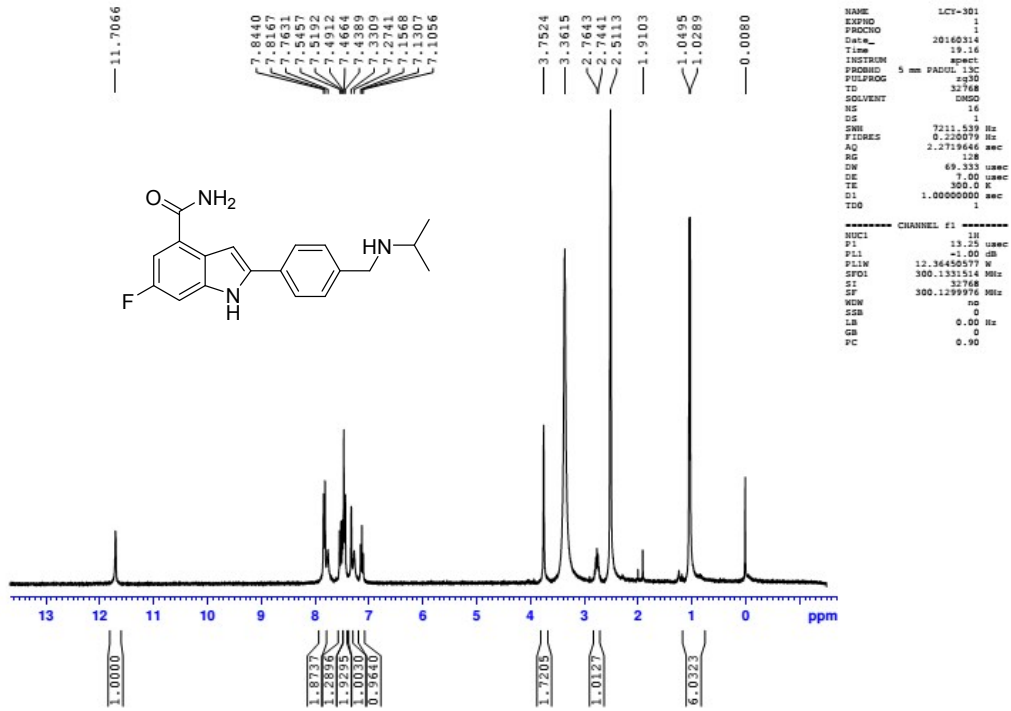
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 14.30 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

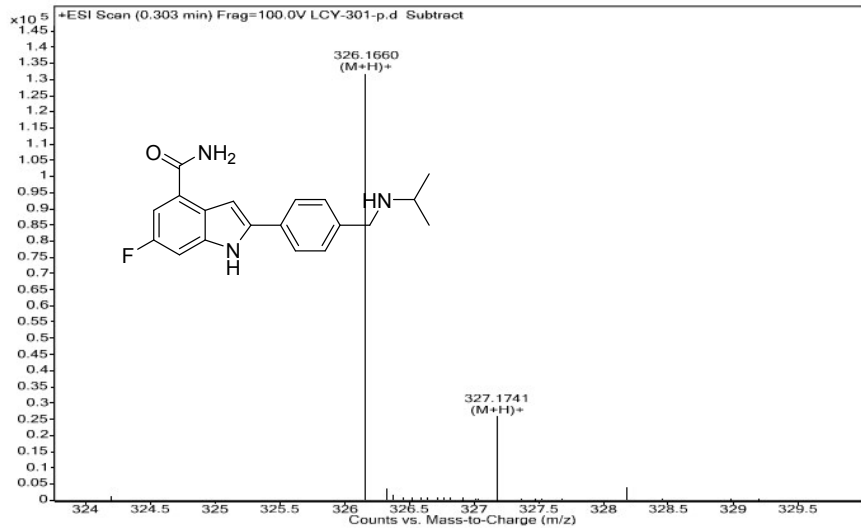


Compound LX9

LCY-301 DMSO 1HNMR AV300

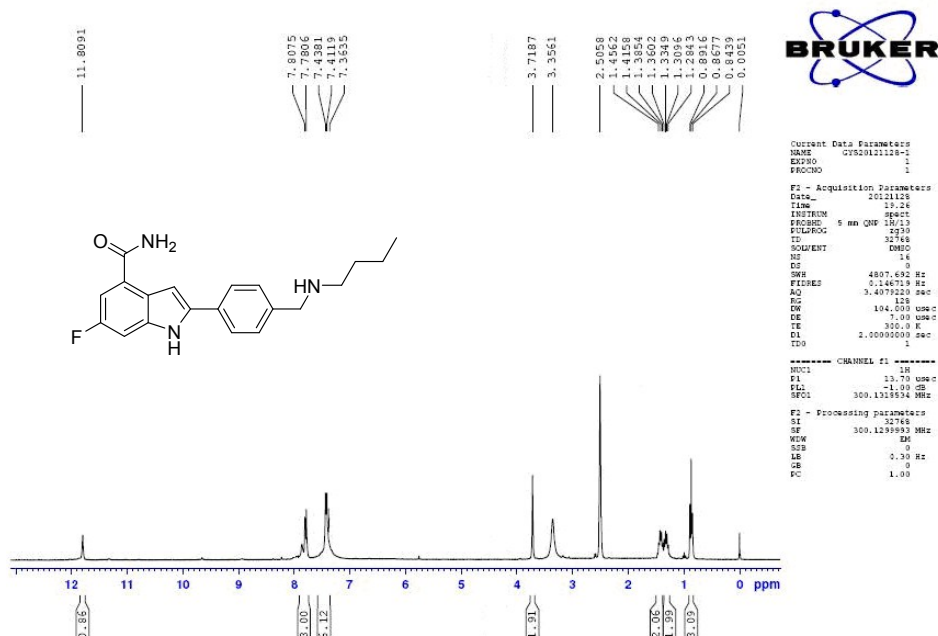


Sample Name	Position	Instrument Name	User Name
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Inj Vol	20	Sample	Success
Data Filename	LCY-301-p.d	Comment	Acquired Time

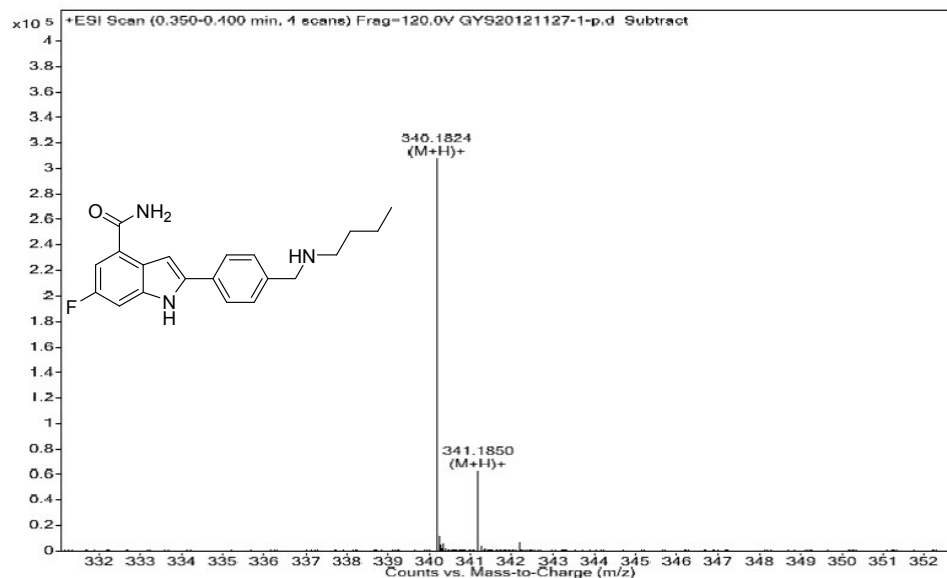


Compound LX10

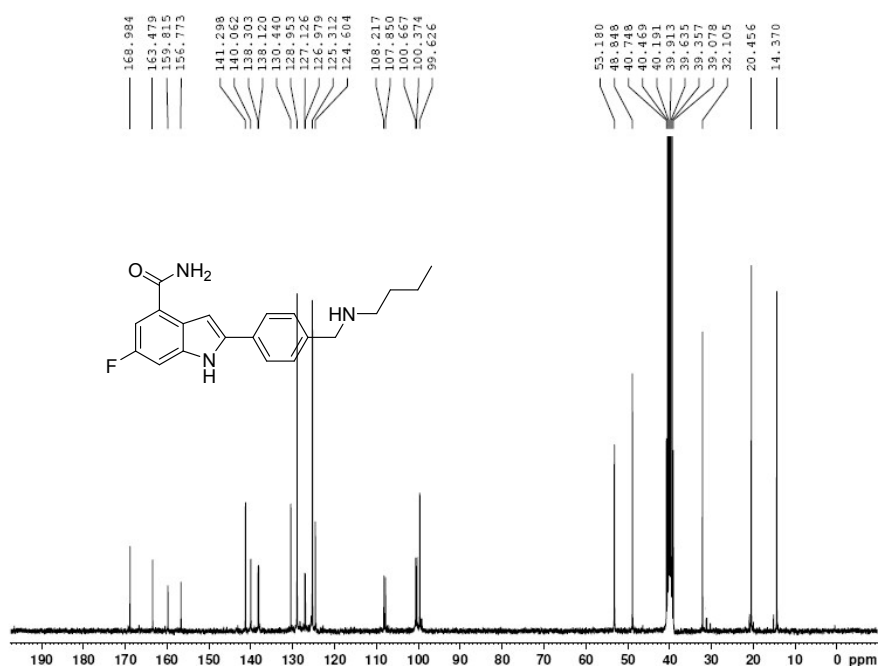
GYS20121128-1 H1-NMR DMSO 303K AV-300



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Inj Vol: 0.3	InjPosition		SampleType	Sample	IRM Calibration Status
Data Filename: GYS20121127-1-p.d	ACQ Method		Comment		Success
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GY20121128-1 C13-NMR DMSO 303K AV-300



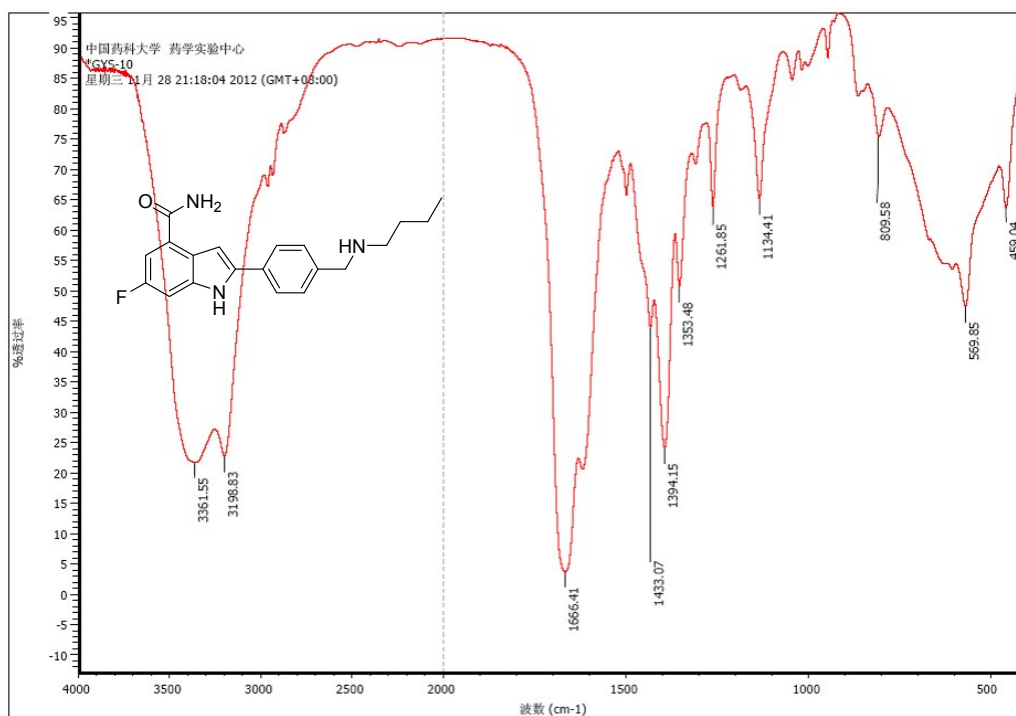
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EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121129
Time 7.20
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 8192
DS 4
SWH 16666.666 Hz
FIDRES 0.254313 Hz
AQ 1.9661300 sec
RG 228
DW 30.000 usec
DE 7.00 usec
TE 300.2 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 11.80 usec
PL1 1.00 dB
SFO1 75.4752203 MHz

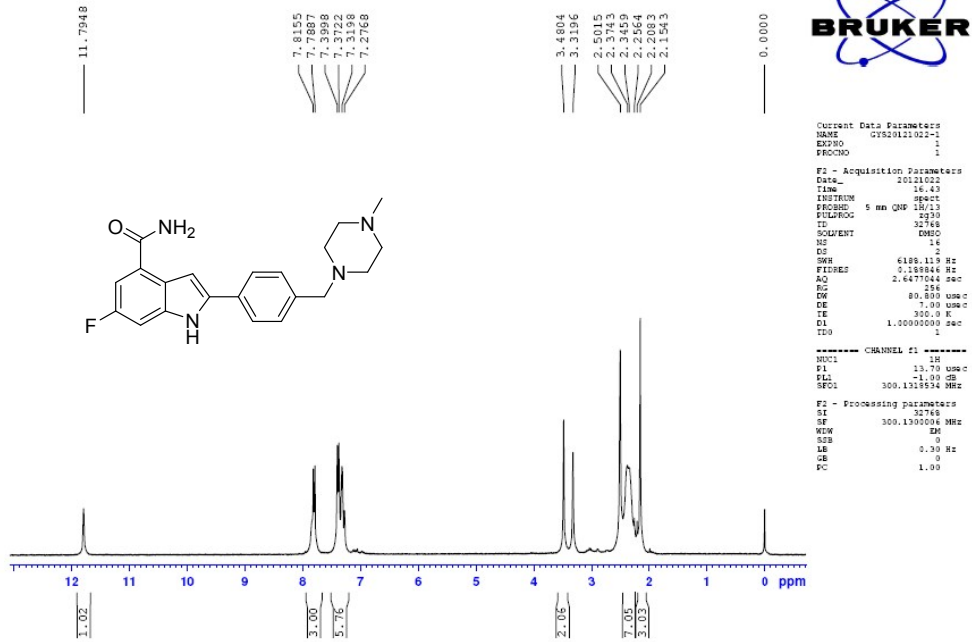
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 1.00 dB
PL12 14.30 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
S1 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

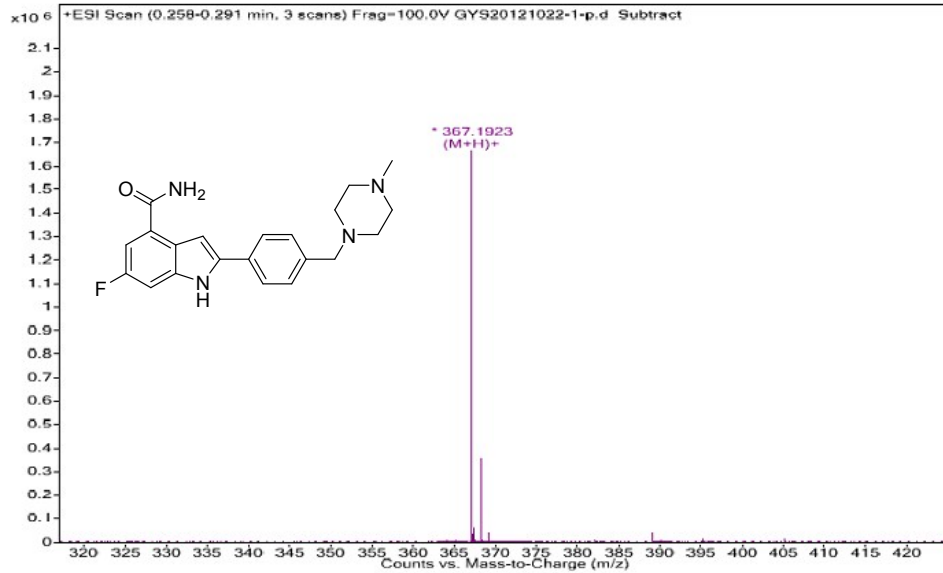


Compound LX11

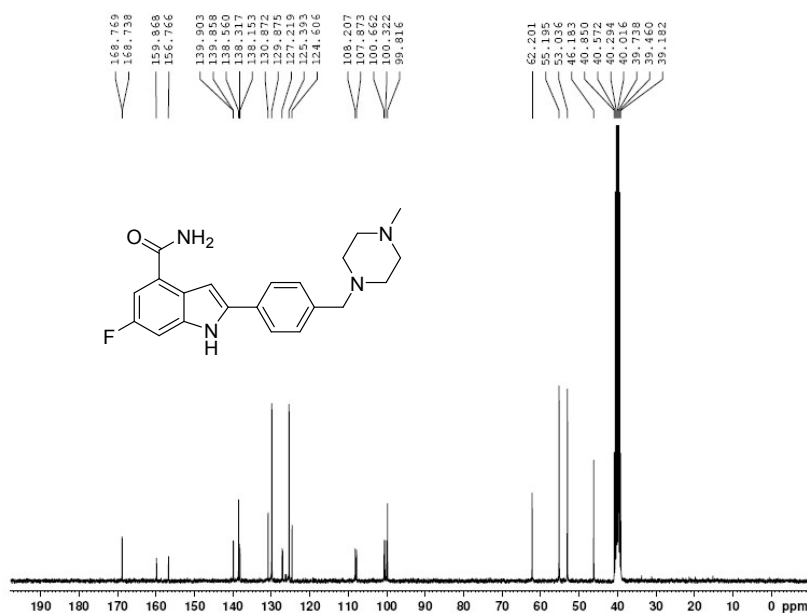
GYS20121022-1 HNMR DMSO 303K AV-300



Sample Name	Position	P1-F3	Instrument Name	Instrument 1	User Name	
Inj Vol	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ACQ Method		Comment		Acquired Time	10/23/2012 3:15:10 PM



GY520121022-1 C13-NMR DMSO 303K AV-300



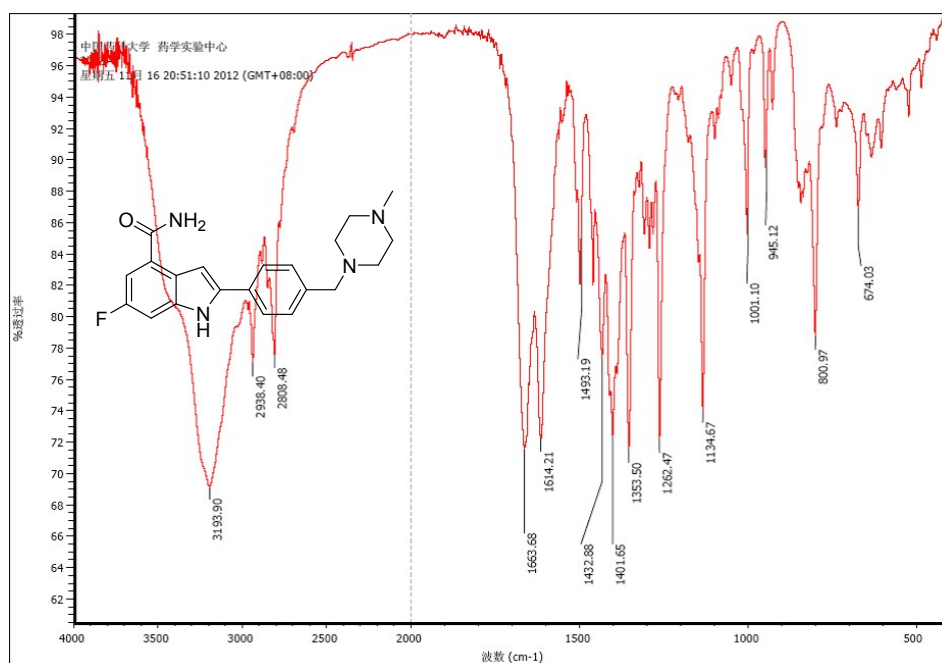
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EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121025
Time 7.32
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 8192
DS 2
SWH 16666.666 Hz
FIDRES 0.254313 Hz
AQ 1.9661300 sec
RG 322
DW 30.000 usec
DE 7.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
TDO 1

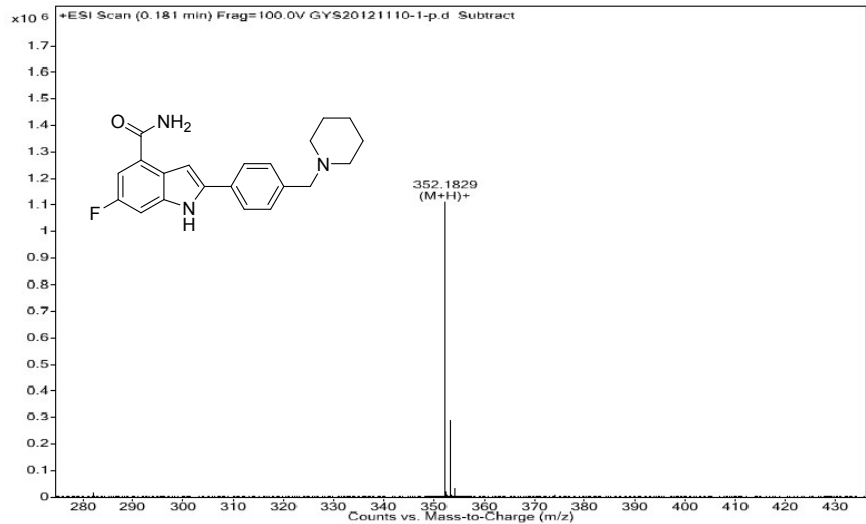
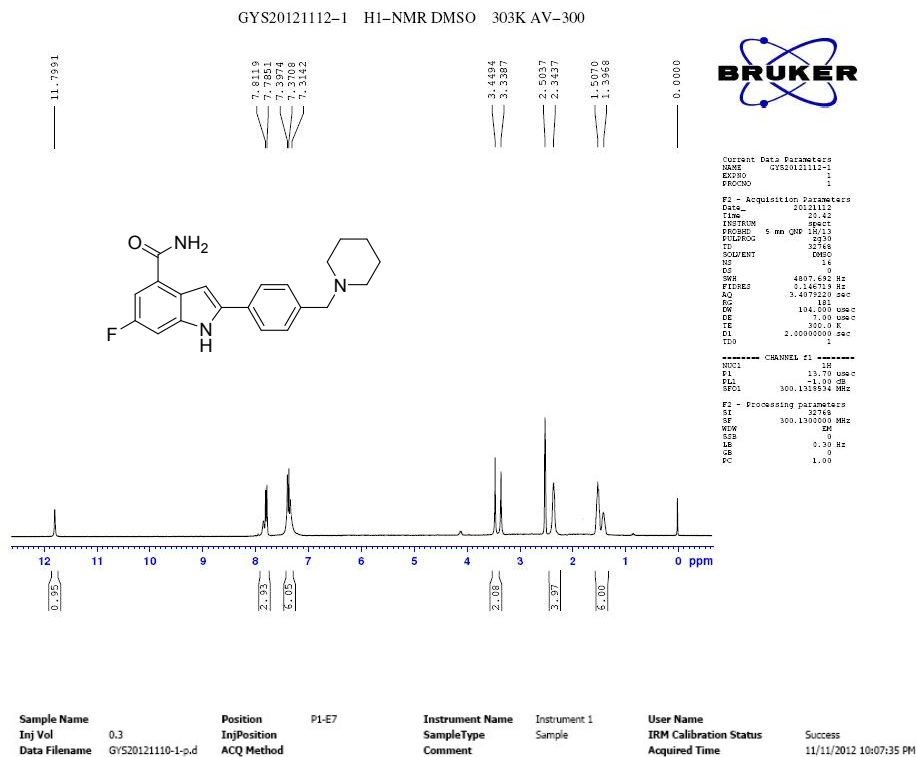
===== CHANNEL f1 =====
NUC1 13C
P1 11.80 usec
PL1 1.00 dB
SFO1 75.4752203 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.30 dB
SFO2 300.1312005 MHz

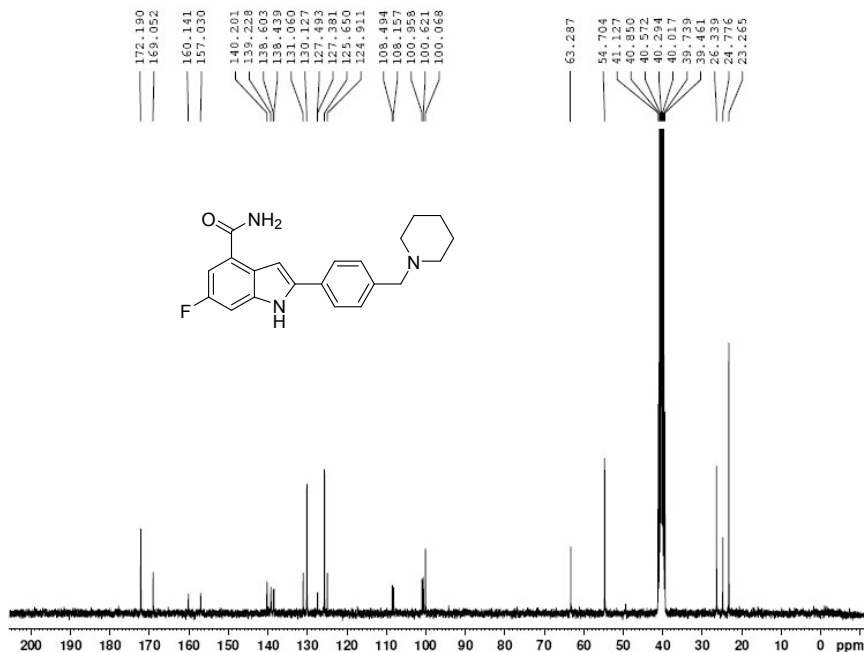
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Compound LX12



GY520121112-1-C C13-NMR DMSO 303K AV-300



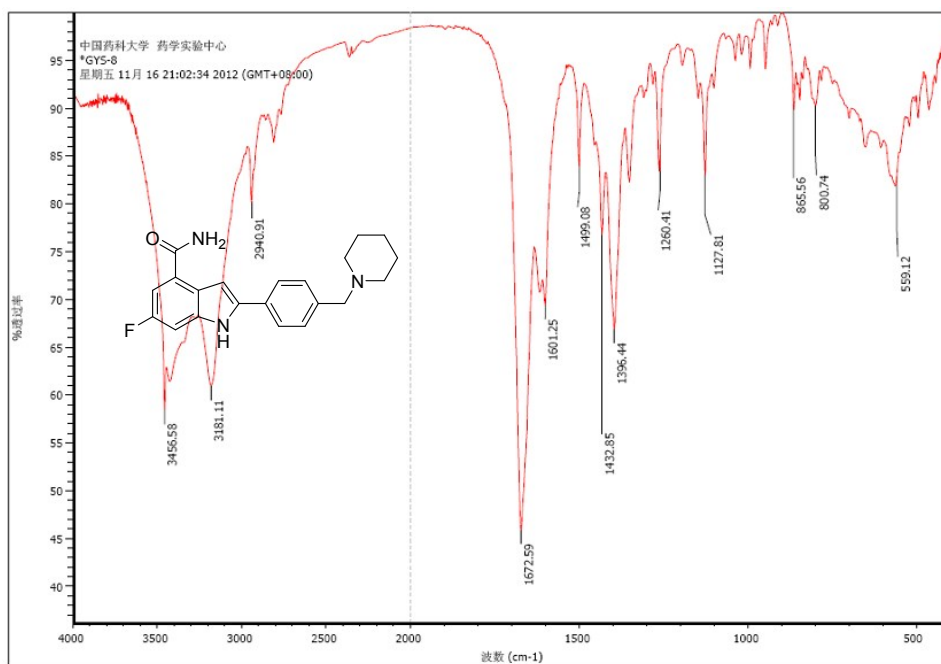
Current Data Parameters
NAME GY520121112-1-C
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121115
Time 7.49
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 8192
DS 4
SWH 16666.666 Hz
FIDRES 0.254313 Hz
AQ 1.9661300 sec
RG 203
SW 30.900 usec
DE 1.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
TD0 1

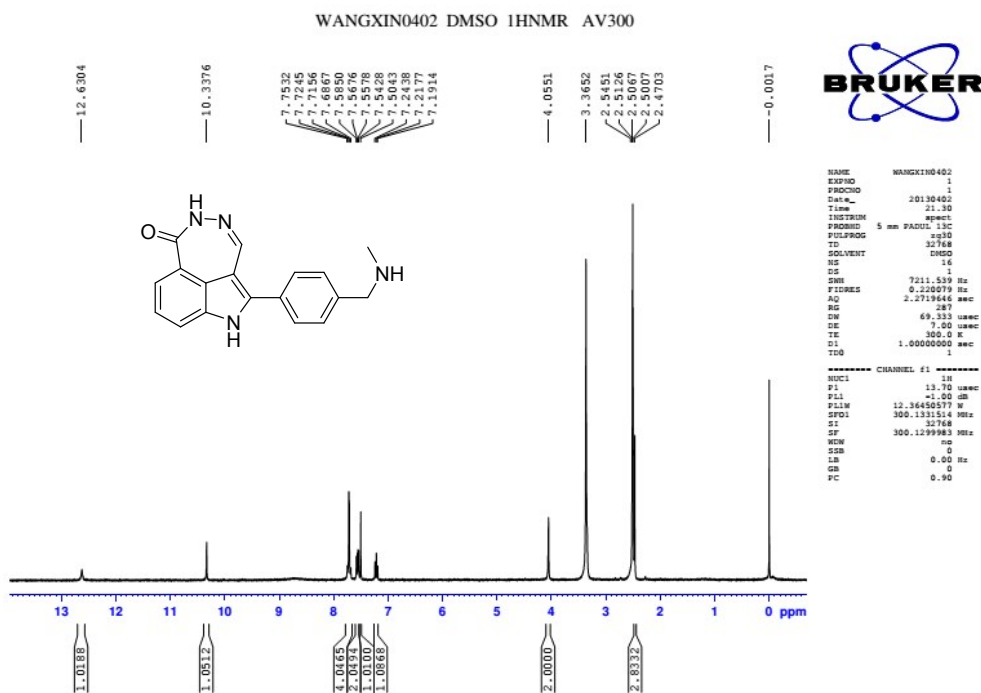
===== CHANNEL f1 =====
NUC1 13C
P1 11.80 usec
PL1 1.00 dB
SFO1 75.4752203 MHz

===== CHANNEL f2 =====
CDEPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 14.30 dB
SFO2 300.1312005 MHz

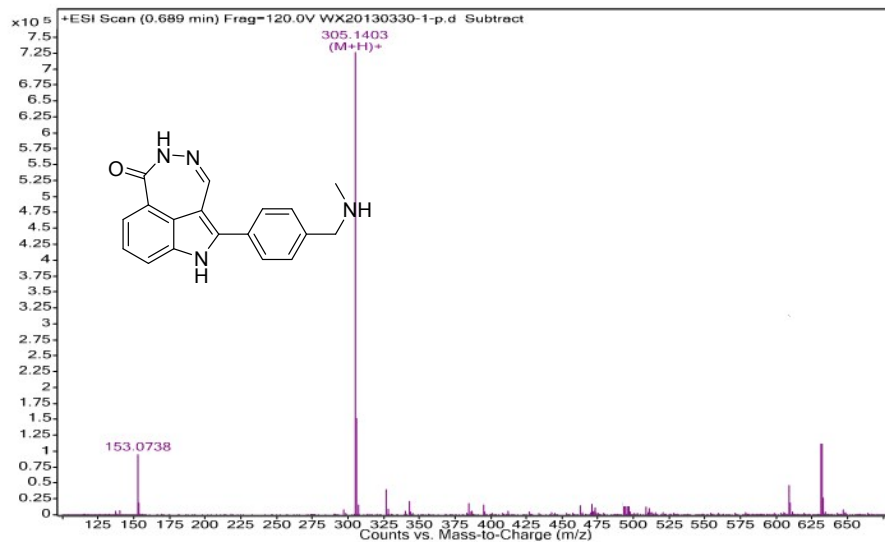
F2 - Processing parameters
SI 32768
SF 75.4677261 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



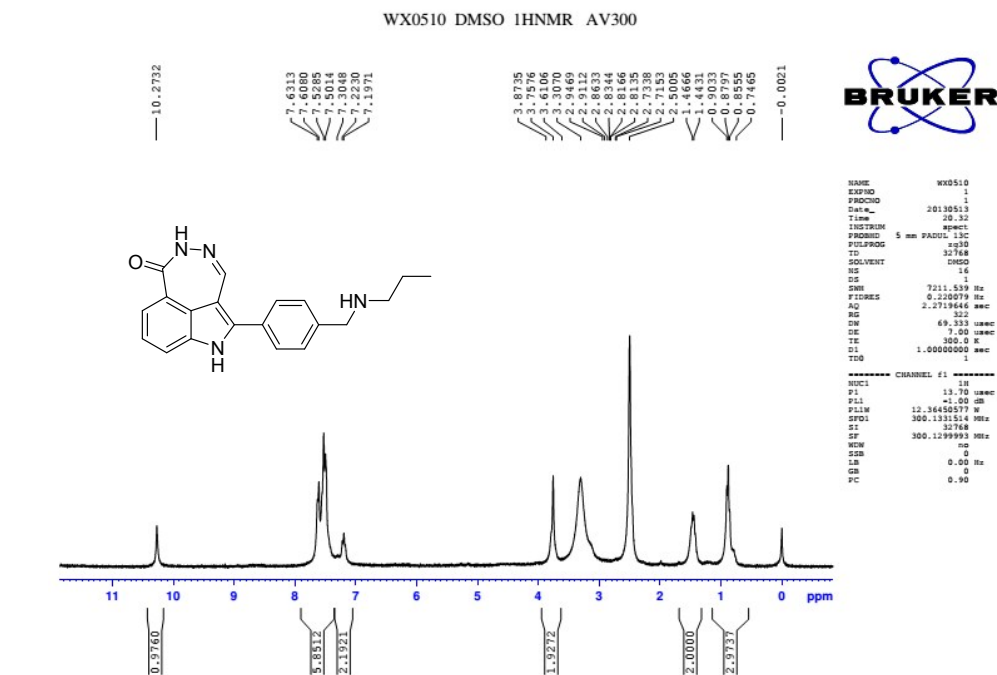
Compound LX13



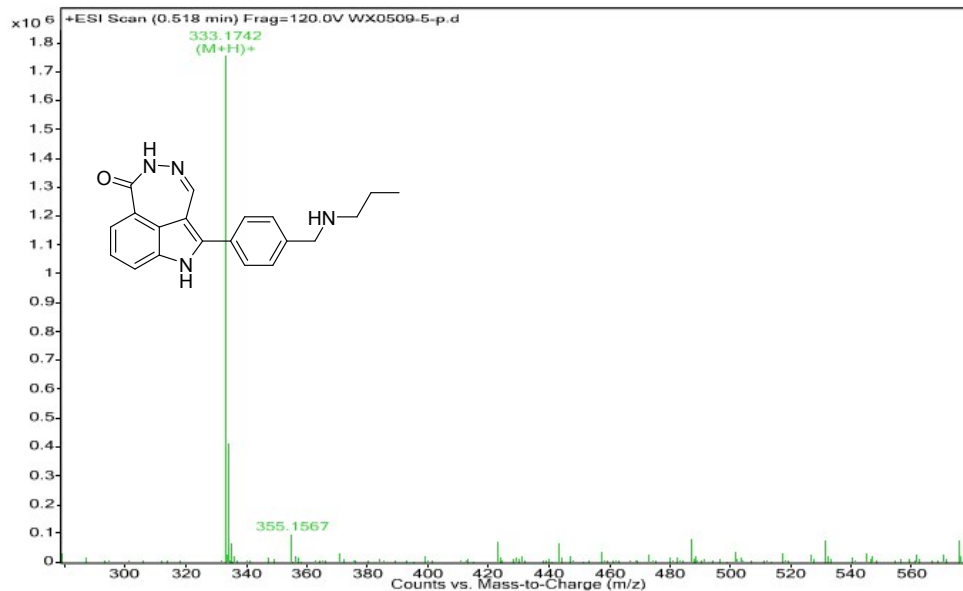
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Inj Vol	0.6		SampleType	Sample	IRM Calibration Status
Data Filename	WX20130330-1-p.d	ACQ Method	Comment		Acquired Time



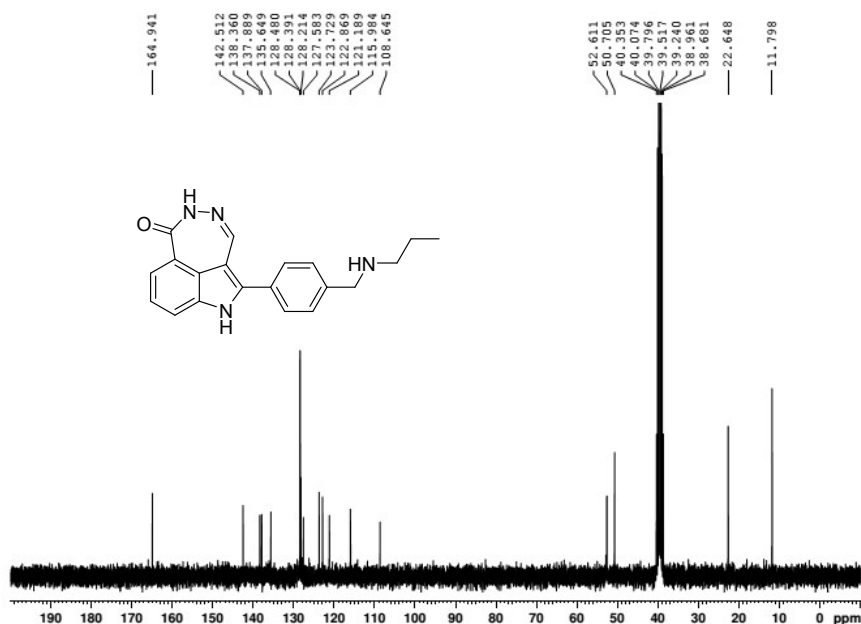
Compound LX14



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Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
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WX0510 C13-NMR DMSO 303K AV-300

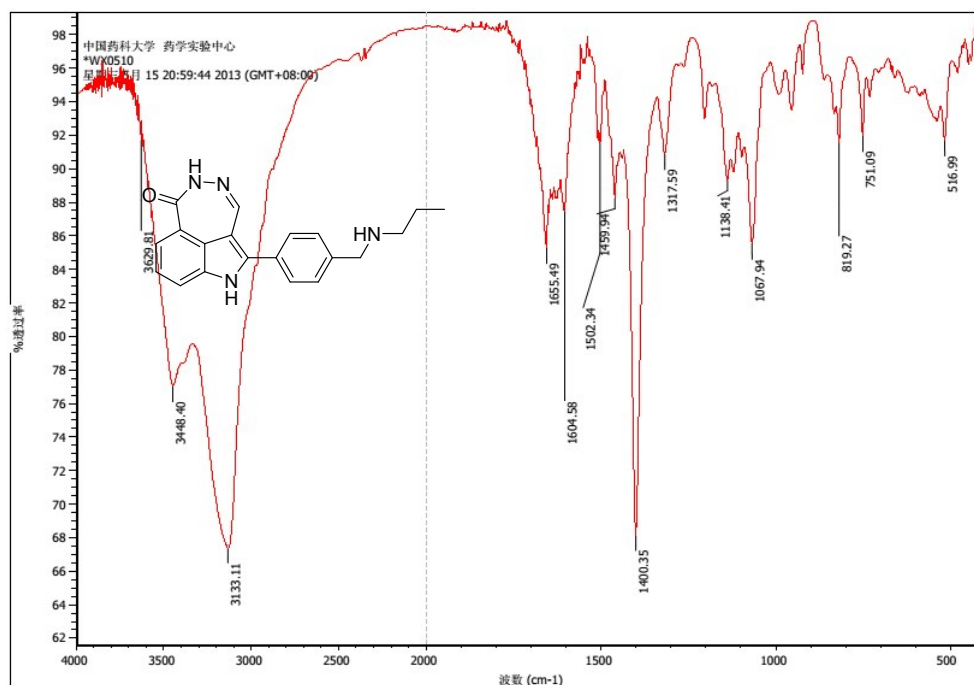


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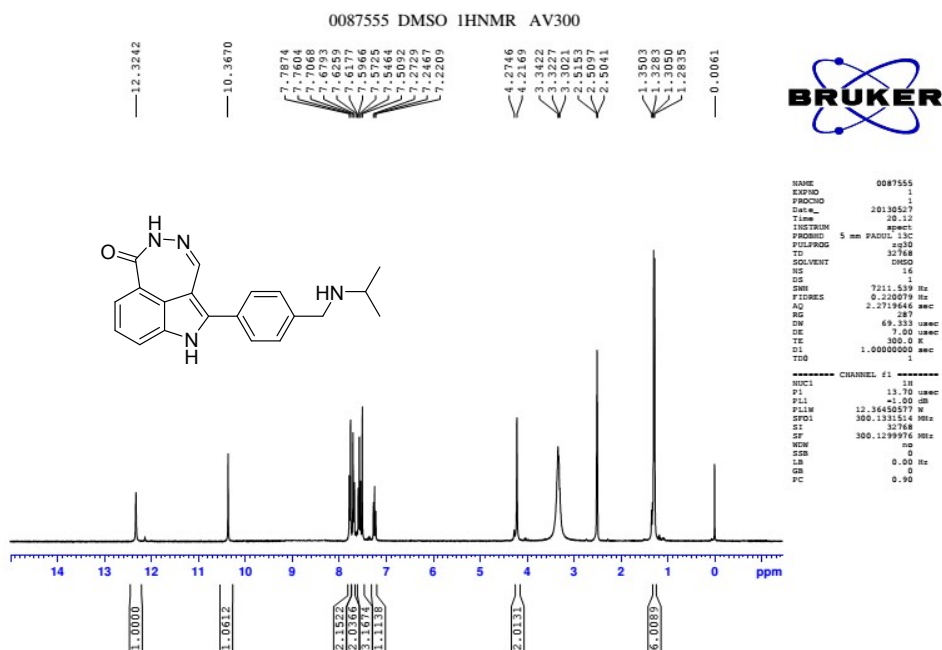
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EXPNO         2
PROCNO        1
Date_         20130515
Time         20.30
INSTRUM       spect
PROBHD        5 mm PABUL 13C
PULPROG       zgpg
TD            65536
SOLVENT       DMSO
NS            2355
DS            4
SWH           19531.250 Hz
FIDRES        0.298023 Hz
AQ            1.6777716 sec
RG            57
DW            25.600 usec
DE            7.00 usec
TE            300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            11.80 usec
PL1           1.00 dB
PL1W          26.73651505 W
SFO1          75.4764278 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -1.00 dB
PL12          14.30 dB
PL1W          12.36450577 W
PL12W         0.36490241 W
SFO2          300.1312005 MHz
SI            32768
SF            75.4677867 MHz
WDW           no
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
    
```



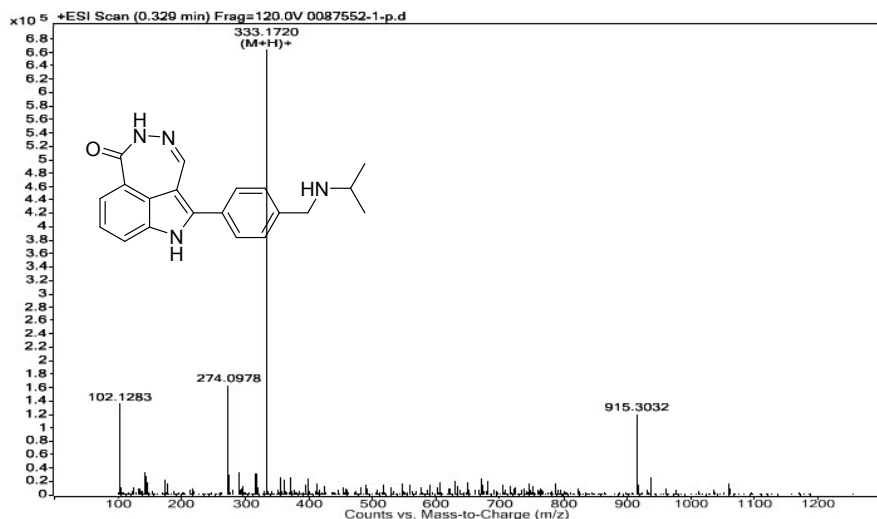
Compound LX15



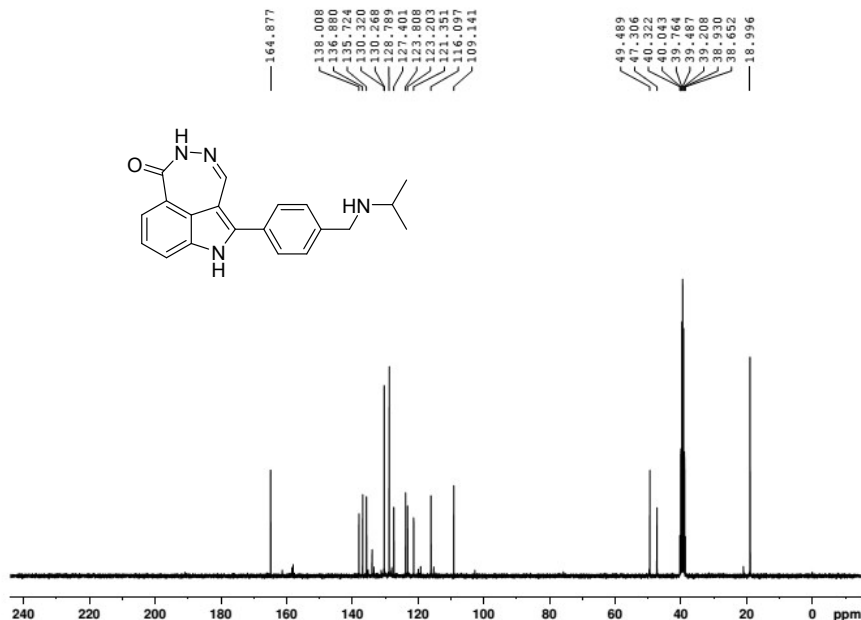
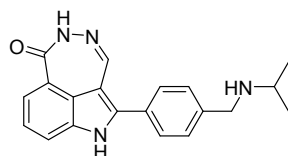
Sample Name	Position	Instrument Name	User Name
0087552-1-p.d	P2-C4	Instrument 1	

Inj Vol	InjPosition	SampleType	IRM Calibration Status
0.5		Sample	Success

Data Filename	ACQ Method	Comment	Acquired Time
0087552-1-p.d			5/21/2013 6:44:59 PM



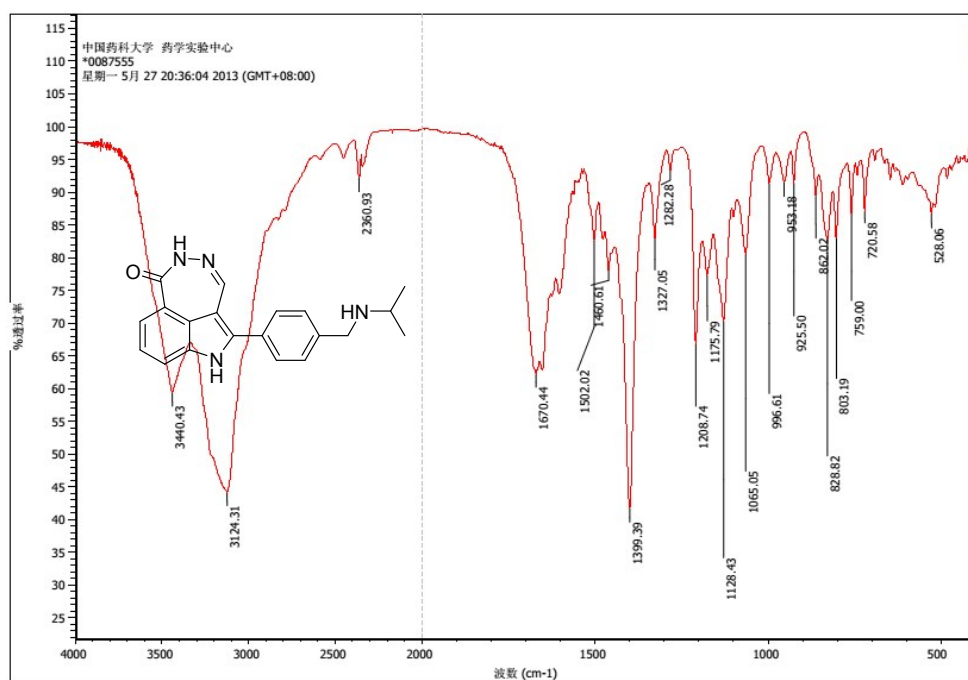
0087555 C13-NMR DMSO 303K AV-300



NAME 0087555
EXPNO 2
PROCNO 1
Date_ 20130530
Time 5.26
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 8192
DS 4
SWH 19531.250 Hz
FIDRES 0.298023 Hz
AQ 1.6777716 sec
RG 90.5
DW 25.600 usec
DE 7.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

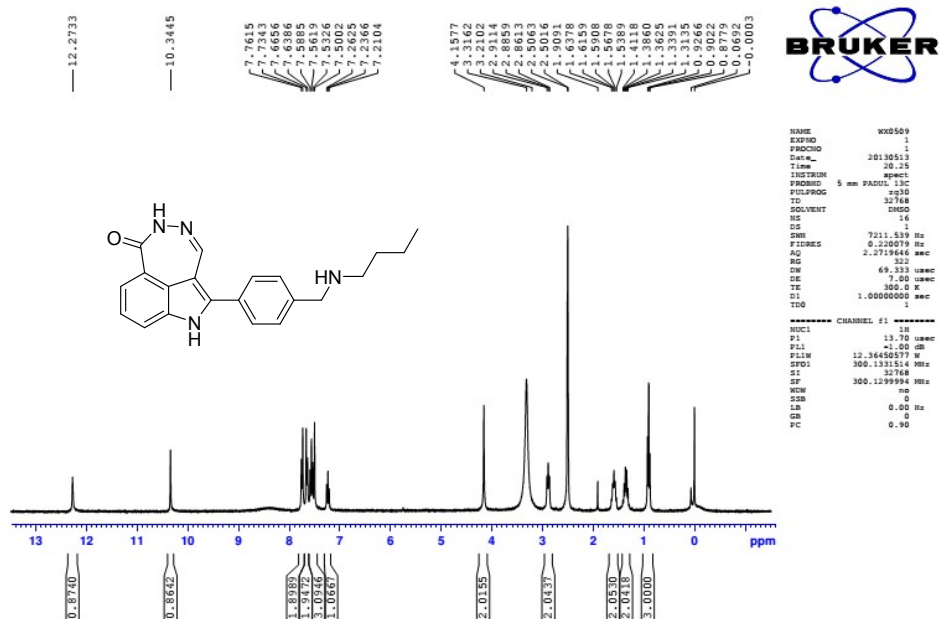
===== CHANNEL f1 =====
NUC1 13C
P1 11.80 usec
PL1 1.00 dB
PL1W 26.73651505 W
SFO1 75.4764278 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.30 dB
PL1W 12.36450577 W
PL12W 0.36490241 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677867 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

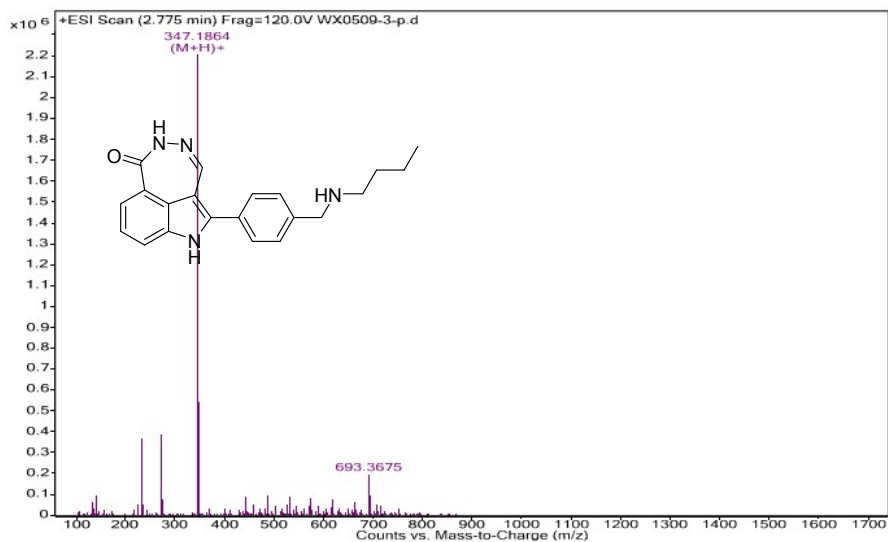


Compound LX16

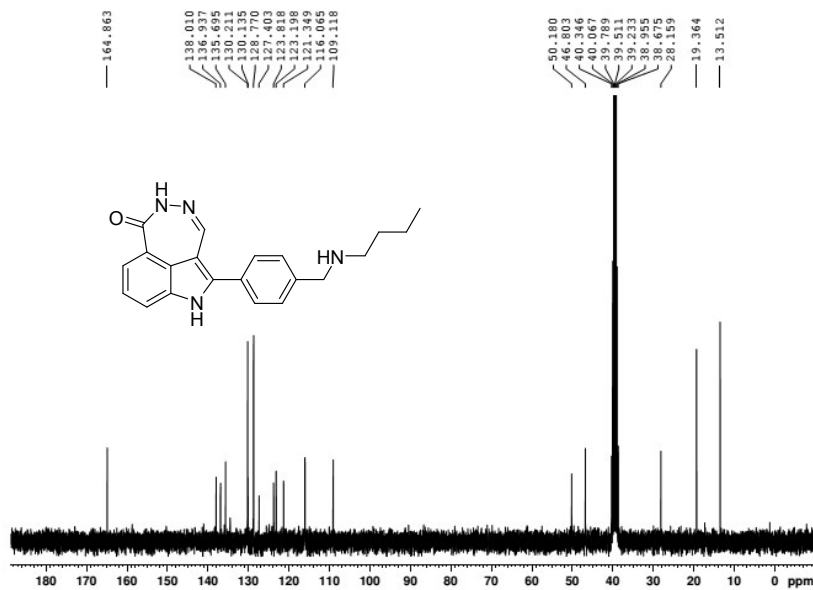
WX0509 DMSO 1HNMR AV300



Sample Name: 0.3
Inj Vol: 0.3
Data Filename: WX0509-3-p.d
Position: P2-C4
InjPosition: P2-C4
ACQ Method: P2-C4
Instrument Name: Instrument 1
SampleType: Sample
User Name: User Name
IRM Calibration Status: Success
Acquired Time: 5/9/2013 3:33:28 PM



WX0509 C13-NMR DMSO 303K AV-300

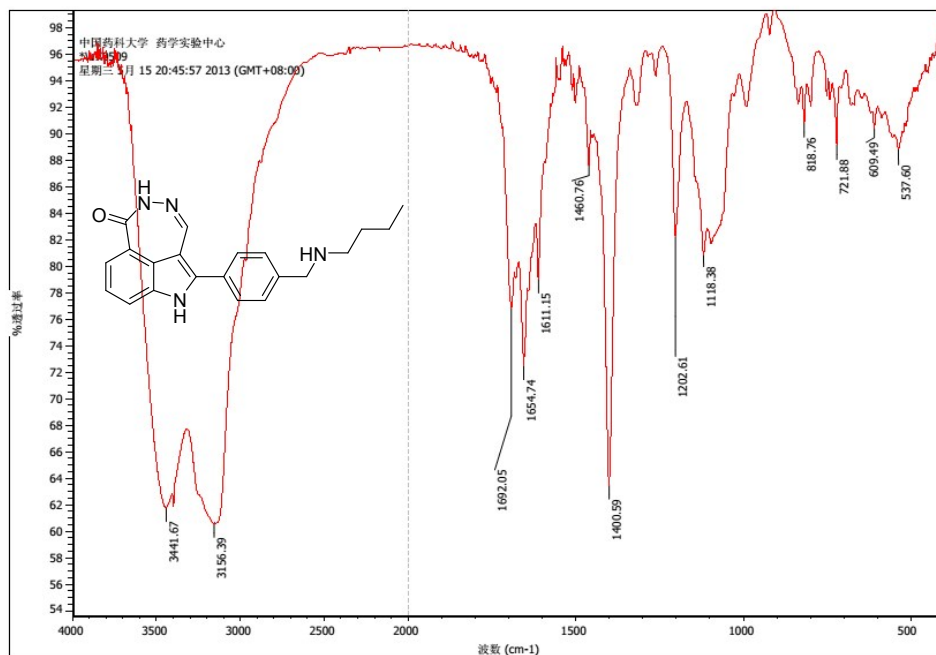


```

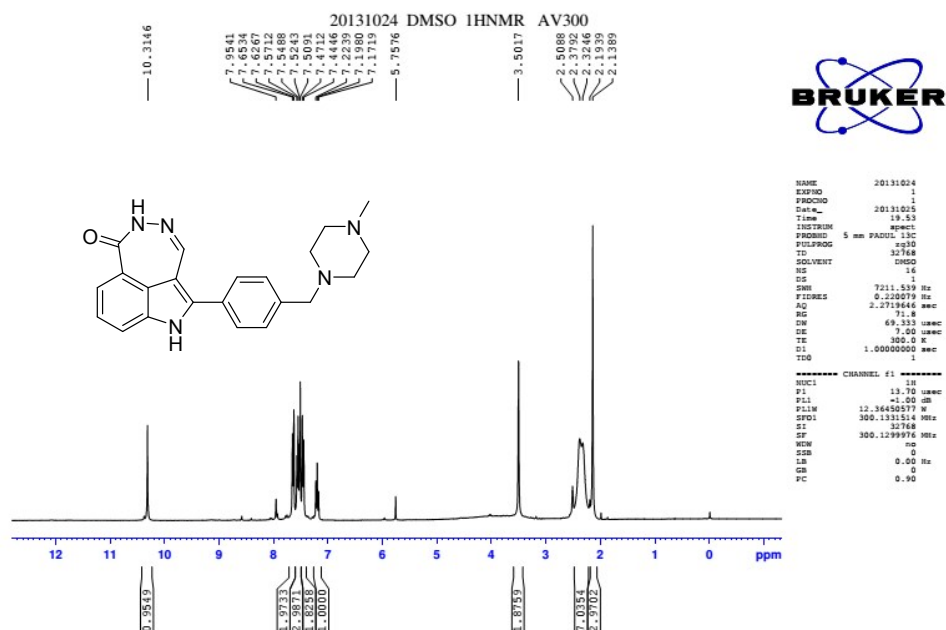
NAME          WX0509
EXPNO         2
PROCNO        1
Date_         20130513
Time          21.10
INSTRUM       spect
PROBHD        5 mm PABDZ-13C
PULPROG       zgpg30
TD            65536
SOLVENT       DMSO
NS            1441
DS            4
SWH           19531.250 Hz
FIDRES        0.298023 Hz
AQ            1.6777716 sec
RG            57
DW            25.600 usec
DE            7.00 usec
TE            300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1          13C
P1            11.80 usec
PL1           1.00 dB
PL1W          26.73651505 W
SFO1          75.4764278 MHz

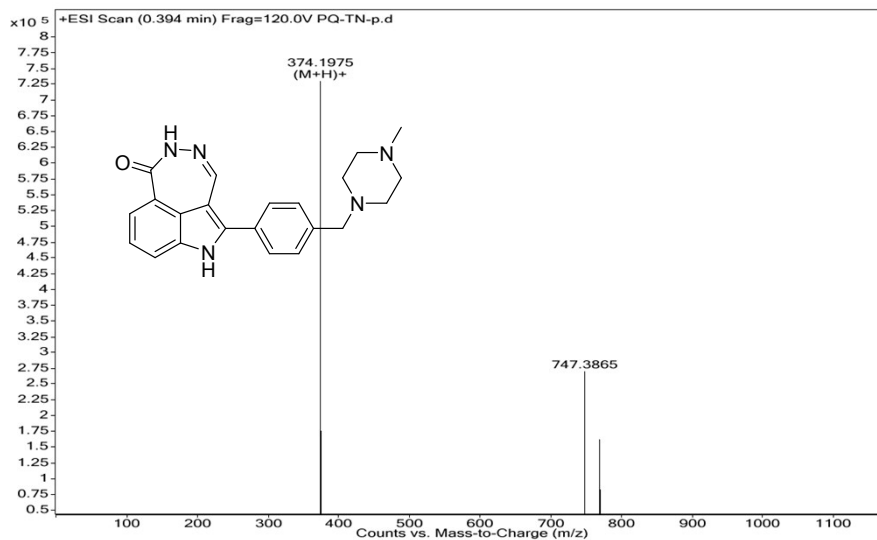
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           1.00 dB
PL12          14.30 dB
PL2W          12.36450577 W
PL12W         0.36490241 W
SFO2          300.1312005 MHz
SI            32768
SF            75.4677867 MHz
WDW           no
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
    
```



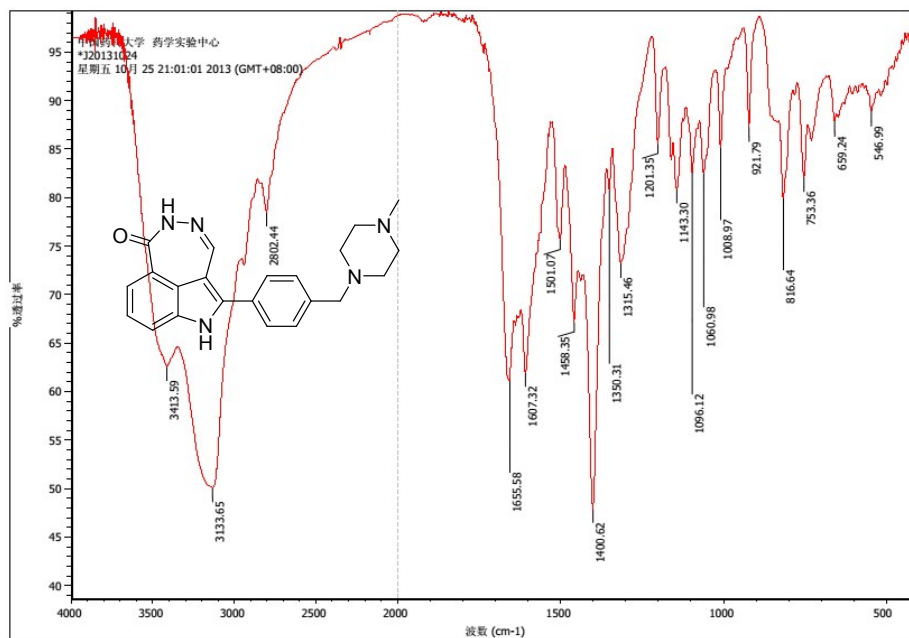
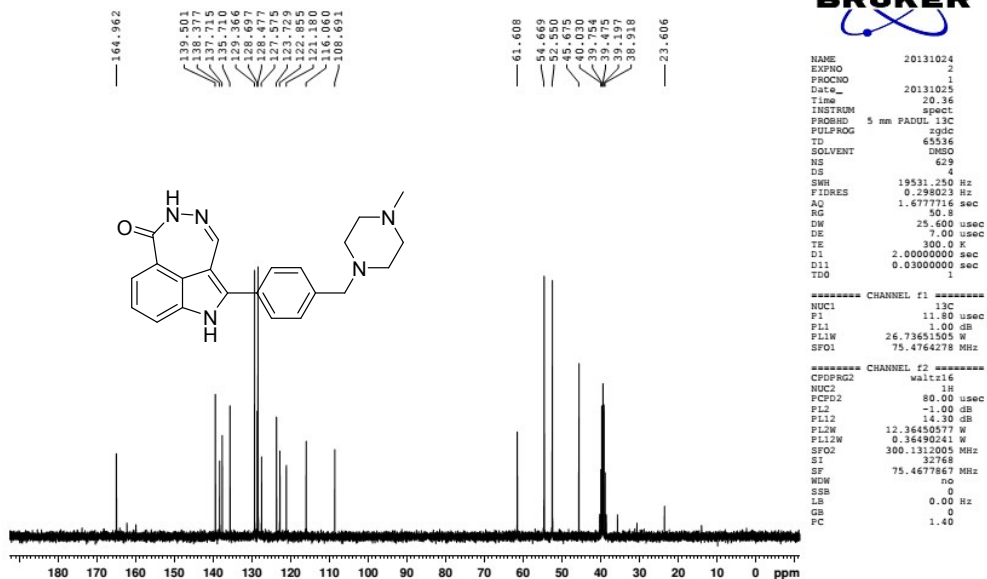
Compound LX17



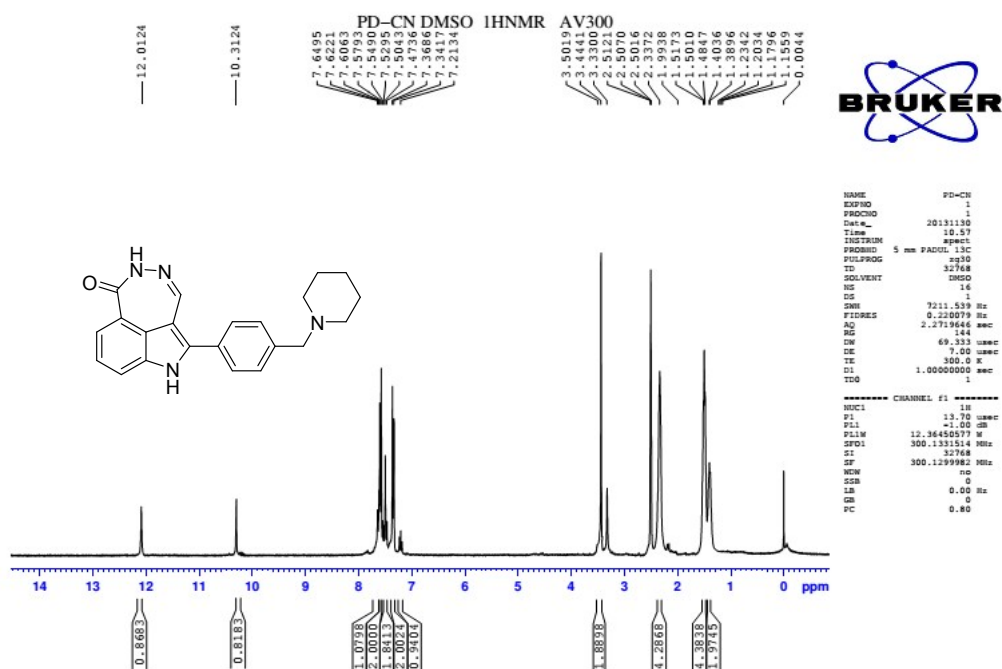
Sample Name	0.5	Position	P1-E6	Instrument Name	Instrument 1	User Name	
Inj Vol		InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	PQ-TN-p.d	ACQ Method		Comment		Acquired Time	4/22/2014 12:42:22 PM



20131024 C13-NMR DMSO 303K AV-300

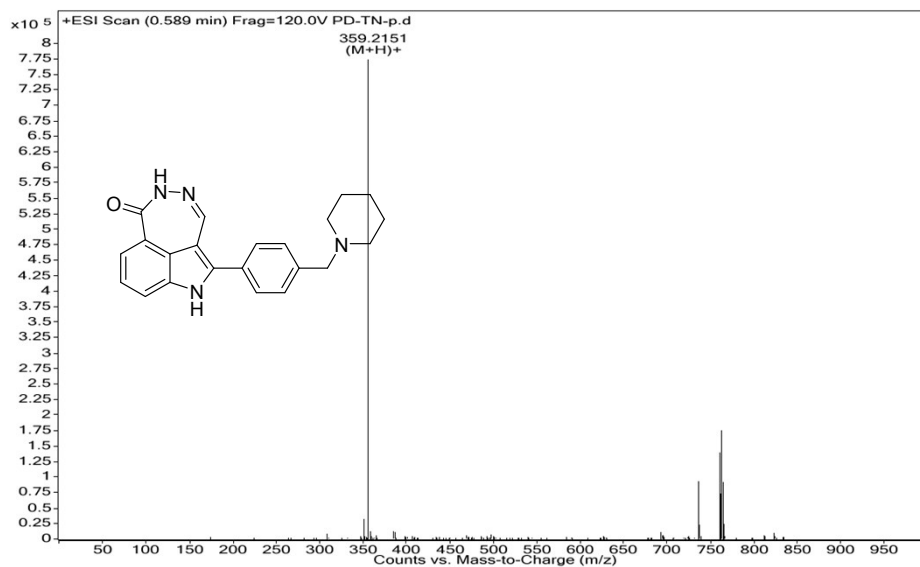


Compound LX18

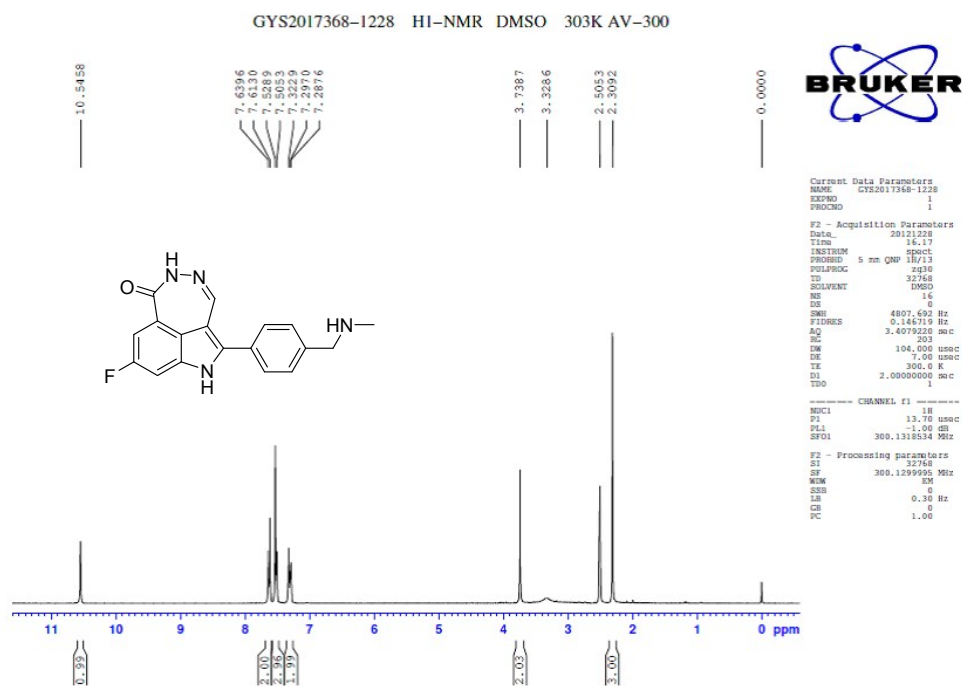


Sample Name	Position	P1-E4	Instrument Name	Instrument 1	User Name
Inj Vol	0.5	InjPosition	SampleType	Sample	IRM Calibration Status
Data Filename	PD-TN-p.d	ACQ Method	Comment		Acquired Time

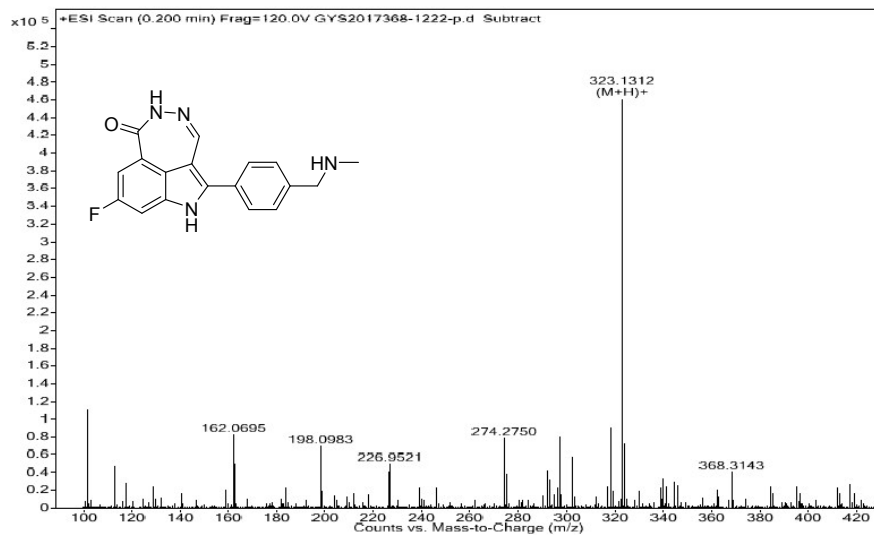
Success 4/22/2014 12:21:58 PM



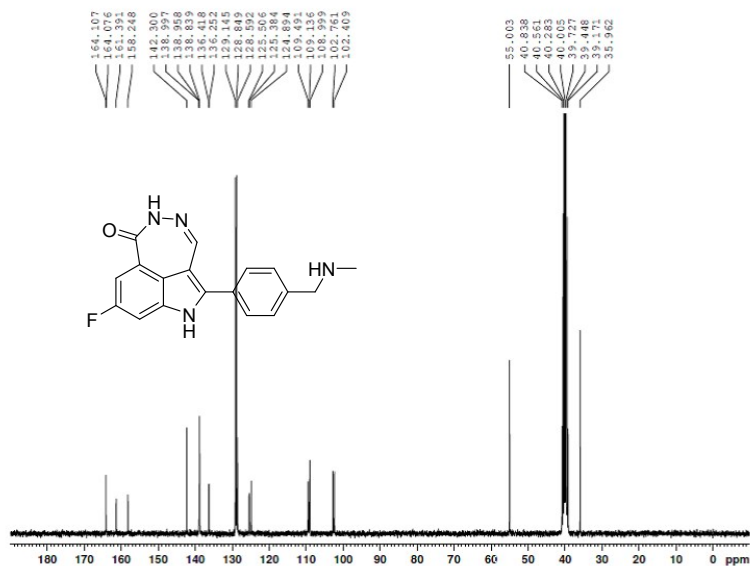
Compound LX19



Sample Name	Position	Instrument Name	User Name
GYS2017368-1222-p.d	P1-C1	Instrument 1	IRM Calibration Status
Inj Vol: 0.3	InjPosition	Sample	Acquired Time
Data Filename	ACQ Method	Comment	Success 12/24/2012 8:21:09 PM



GYS2017368-1228 C13-NMR DMSO 303K AV-300



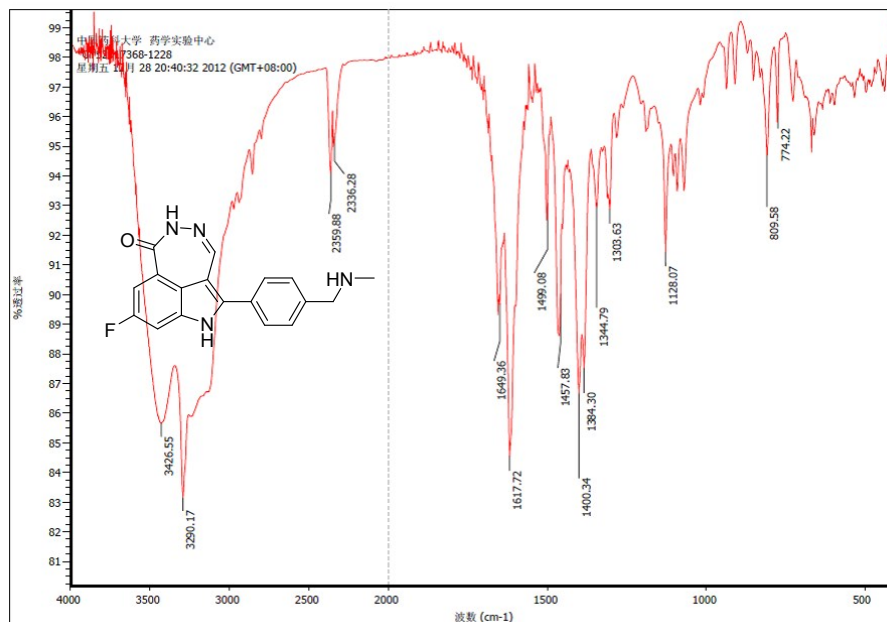
Current Data Parameters
 NAME: GYS2017368-1228
 EXPNO: 2
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20121228
 Time: 16.38
 INSTRUM: spect
 PULPROG: zgpg
 TD: 65536
 SOLVENT: DMSO
 NS: 2656
 DS: 4
 SWH: 16666.666 Hz
 FIDRES: 0.254313 Hz
 AQ: 1.9661305 sec
 RG: 228
 DW: 30.000 usec
 DE: 7.00 usec
 TE: 300.0 K
 D1: 2.00000000 sec
 d11: 0.03000000 sec
 TDO: 1

==== CHANNEL f1 =====
 NUC1: 13C
 P1: 11.80 usec
 PL1: 1.00 dB
 SFO1: 75.4752203 MHz

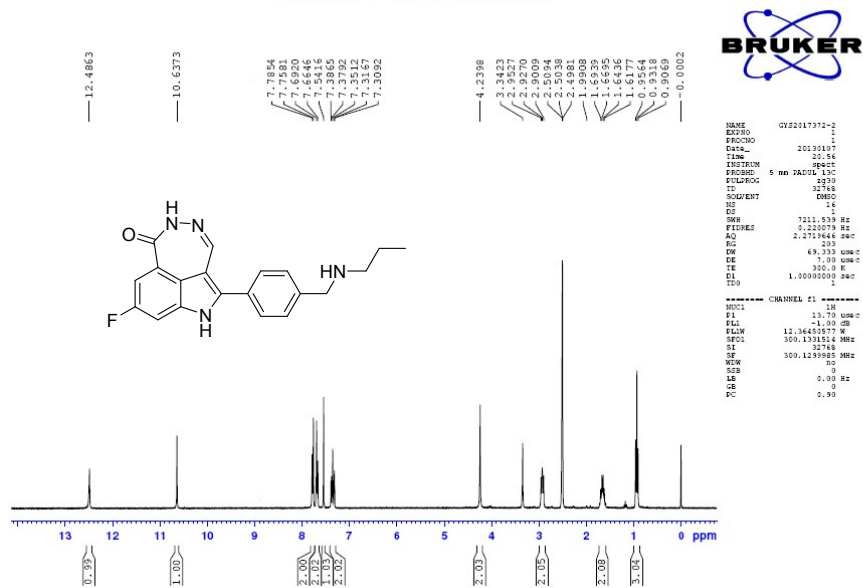
==== CHANNEL f2 =====
 CPDPRG2: waltz16
 NUC2: 1H
 PCPD2: 80.00 usec
 PL2: -1.00 dB
 PL12: 14.30 dB
 SFO2: 300.1312005 MHz

F2 - Processing parameters
 SI: 32768
 SF: 75.4677490 MHz
 MEW: RM
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

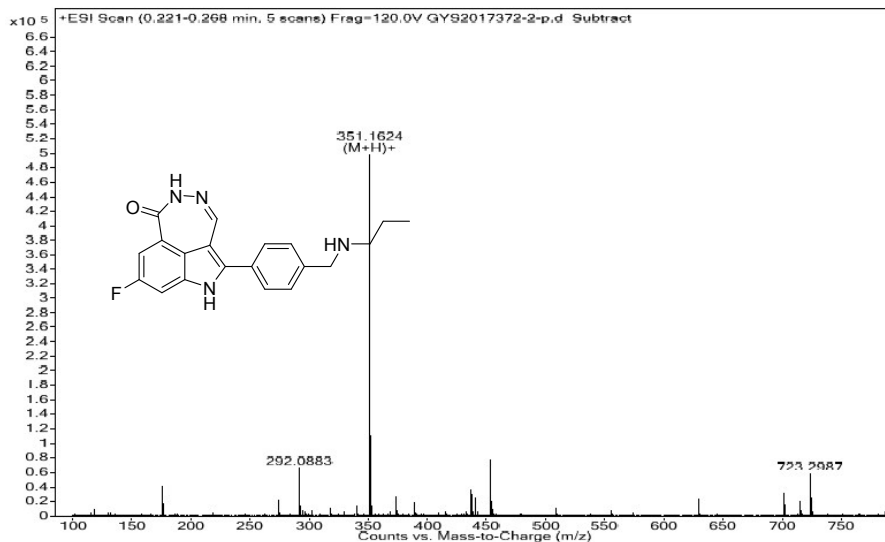


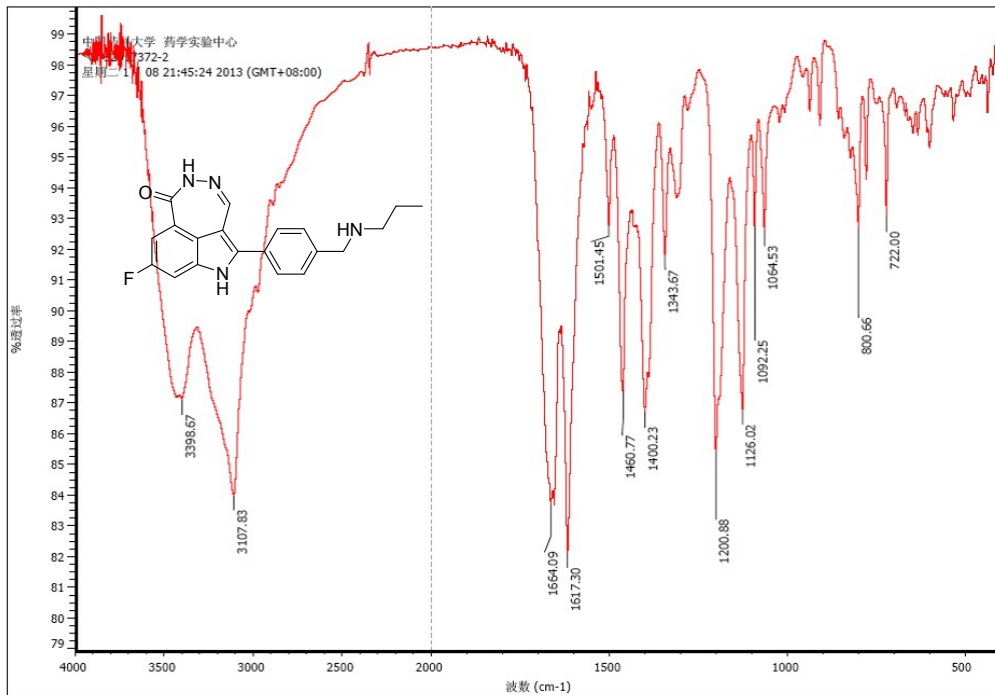
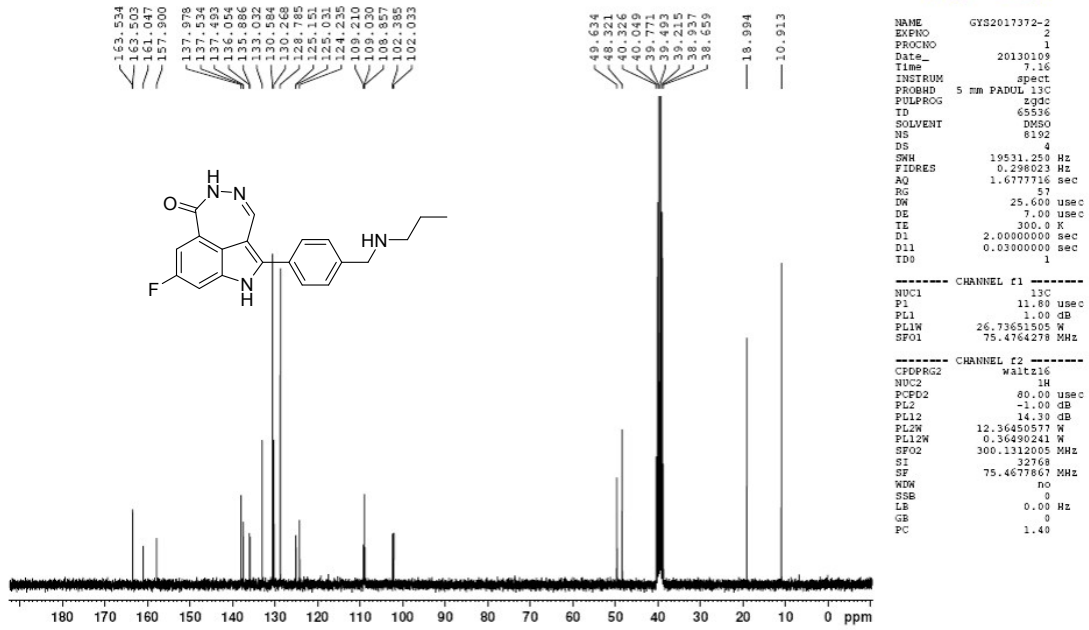
Compound LX20

GYS2017372-2 DMSO 1HNMR AV300



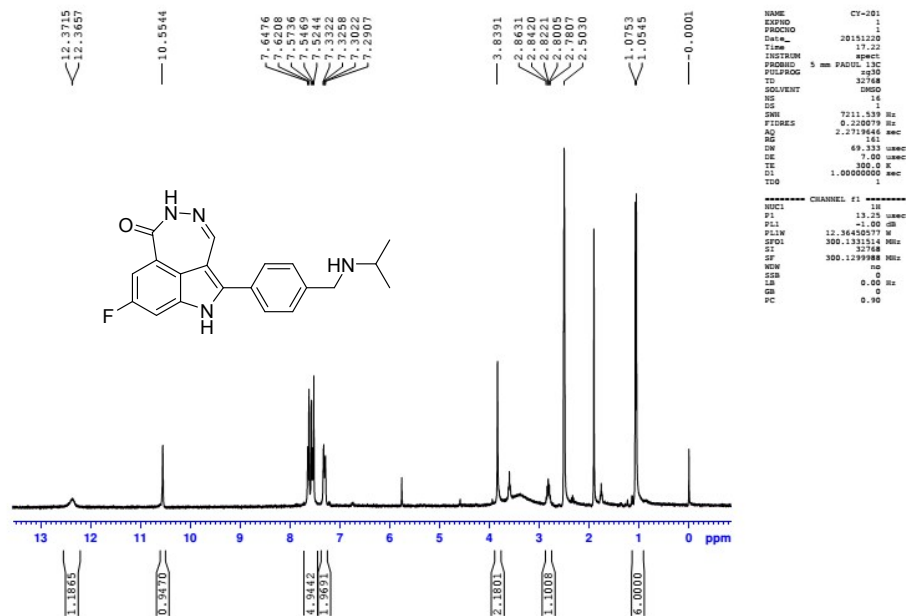
Sample Name	Position	P2-01	Instrument Name	Instrument 1	User Name
Inj Vol	0.3	InjPosition	SampleType	Sample	IRM Calibration Status
Data Filename	GYS2017372-2.p.d	ACQ Method	Comment		Acquired Time



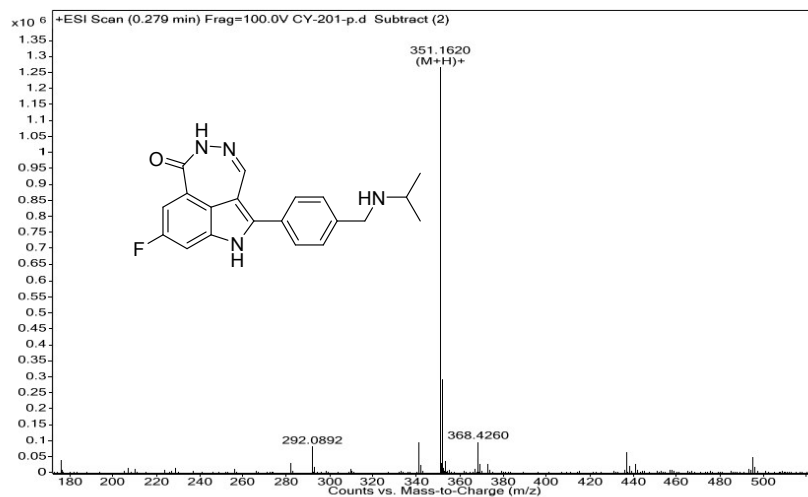


Compound LX21

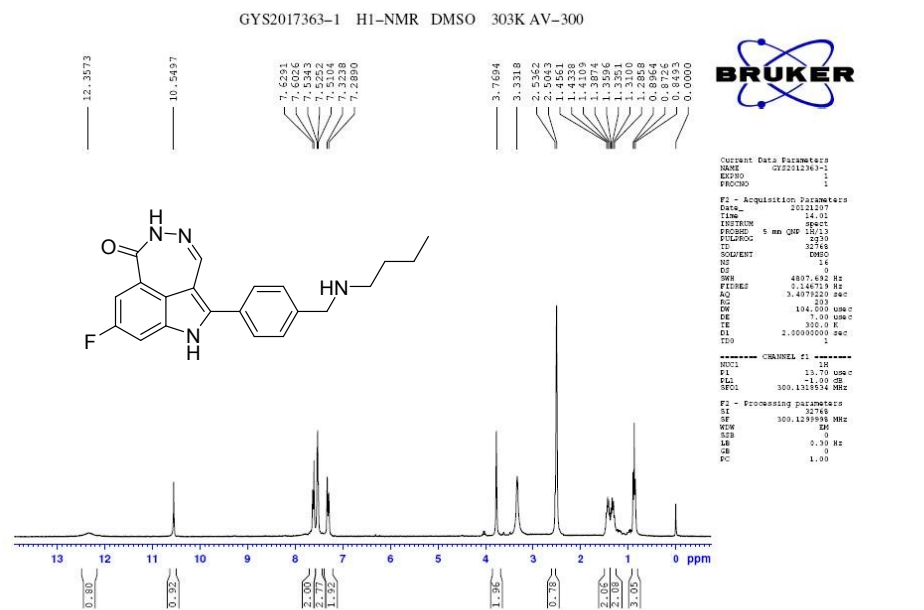
CY-201 DMSO 1HNMR AV300



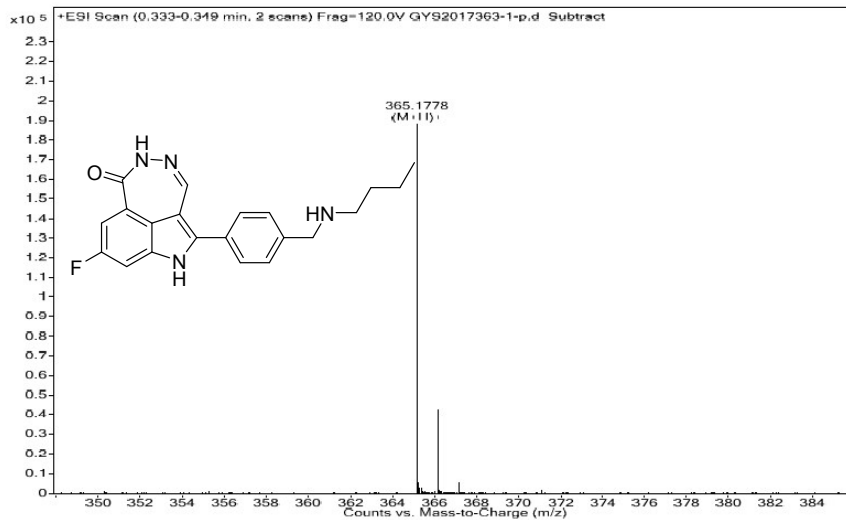
Sample Name	0.1	Position	P1-F5	Instrument Name	Instrument 1	User Name	
Inj Vol		InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	CY-201-p.d	ACQ Method		Comment		Acquired Time	12/16/2015 6:47:48 PM



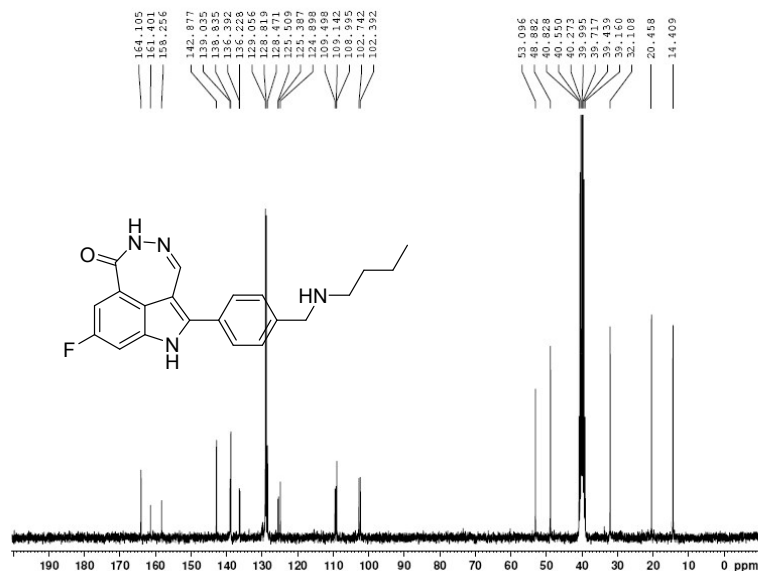
Compound LX22



Sample Name	Position	P1-A7	Instrument Name	Instrument 1	User Name	
Inj Vol	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ACQ Method		Comment		Acquired Time	12/6/2012 8:06:39 PM



GYS2017363-1 C13-NMR DMSO 303K AV-300



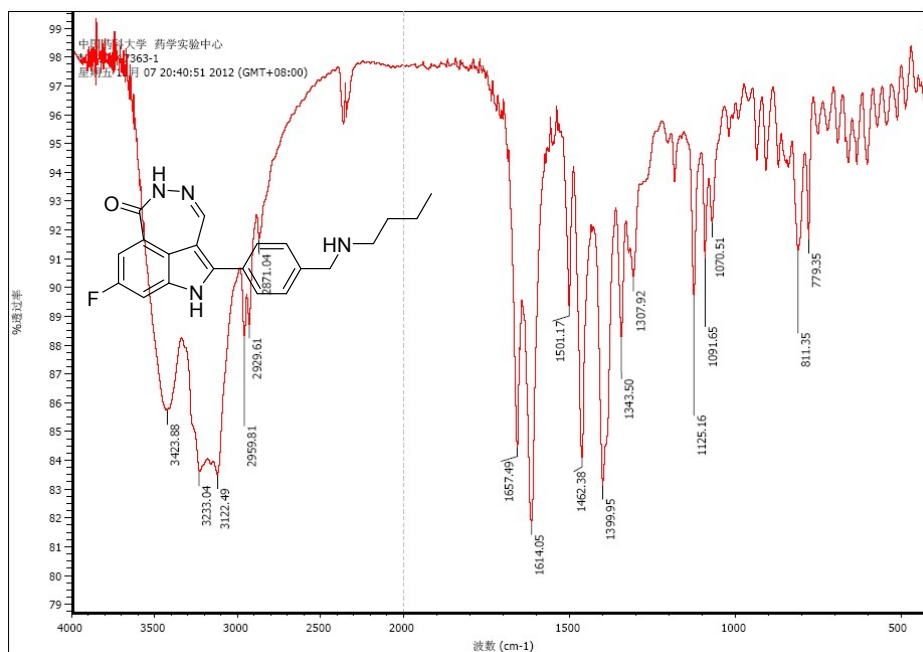
Current Data Parameters
NAME GYS2017363-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121207
Time 15.00
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 2061
DS 4
SWH 16666.666 Hz
FIDRES 0.244113 Hz
AQ 1.9661300 sec
RG 203
SW 30.100 usec
DE 7.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
TD 1

===== CHANNEL f1 =====
NUC1 13C
P1 11.80 usec
PL1 1.00 dB
SFO1 75.4752203 MHz

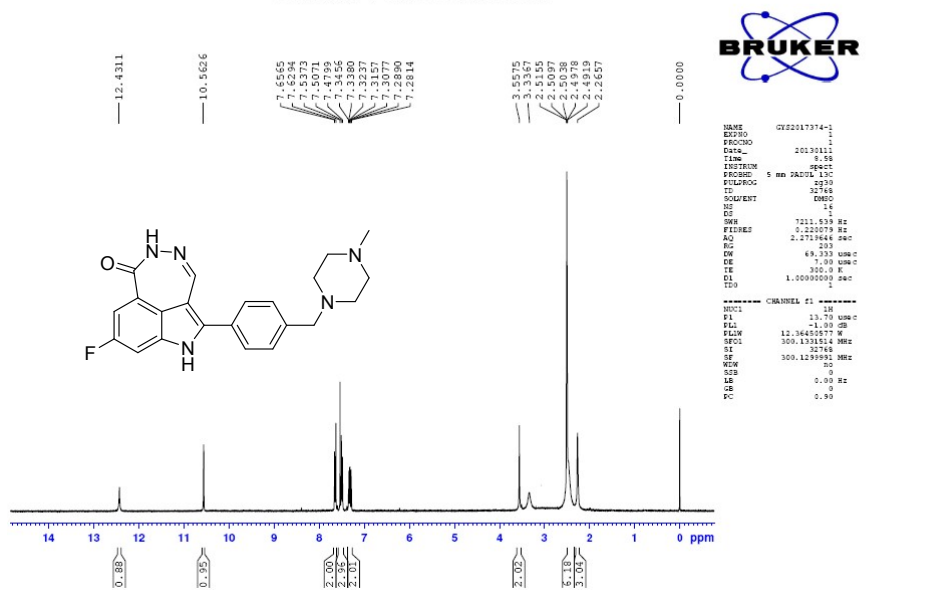
===== CHANNEL f2 =====
PCPRG2 waltz16
NUC2 1H
P2 80.00 usec
PL2 -1.00 dB
PL12 14.30 dB
SFO2 300.1312103 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

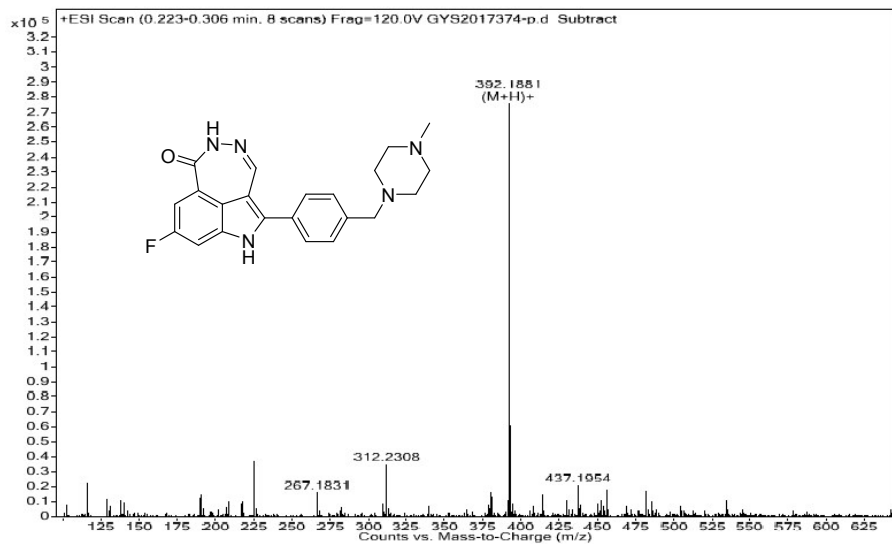


Compound LX23

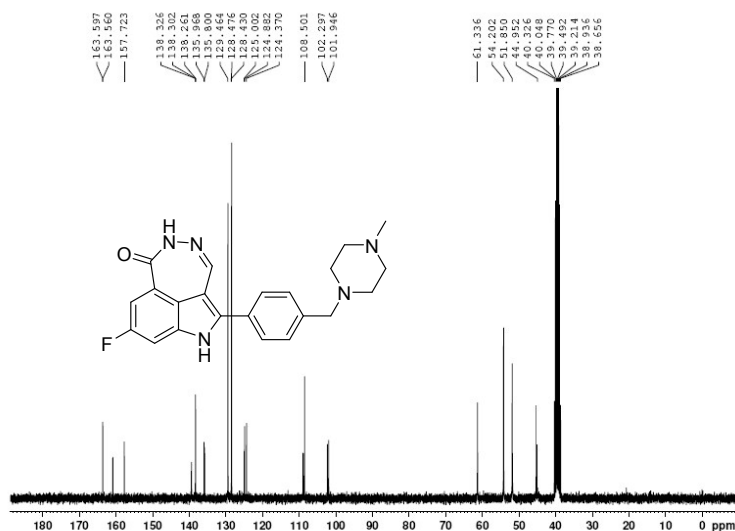
GYS2017374-1 DMSO 1HNMR AV300



Sample Name	Position	P1-A8	Instrument Name	Instrument 1	User Name	
Inj Vol	1	InjPosition	SampleType	Sample	IRM Calibration Status	Success
Data Filename	GY52017374-p.d	ACQ Method	Comment		Acquired Time	1/10/2013 7:27:14 PM



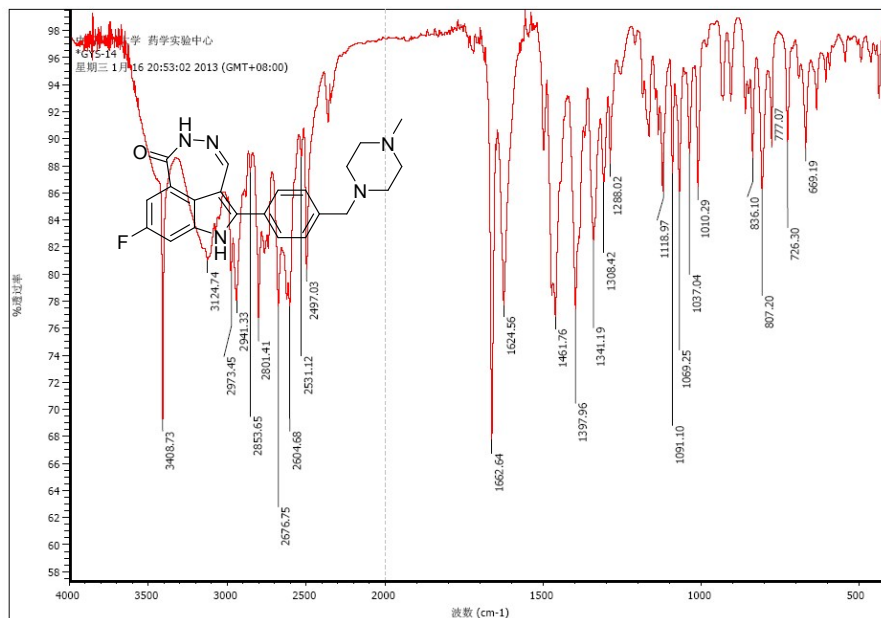
GYS2017374-1 C13-NMR DMSO 303K AV-300



NAME GYS2017374-1
 EXPNO 2
 PROCNO 1
 Date_ 20130113
 Time 16:19
 INSTRUM spect
 PROBRD 5 mm PADUL 13C
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 6262
 DS 4
 SWH 19531.250 Hz
 FIDRES 0.258023 Hz
 AQ 1.677718 sec
 RG 57
 DW 25.600 usec
 DE 7.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D3 1

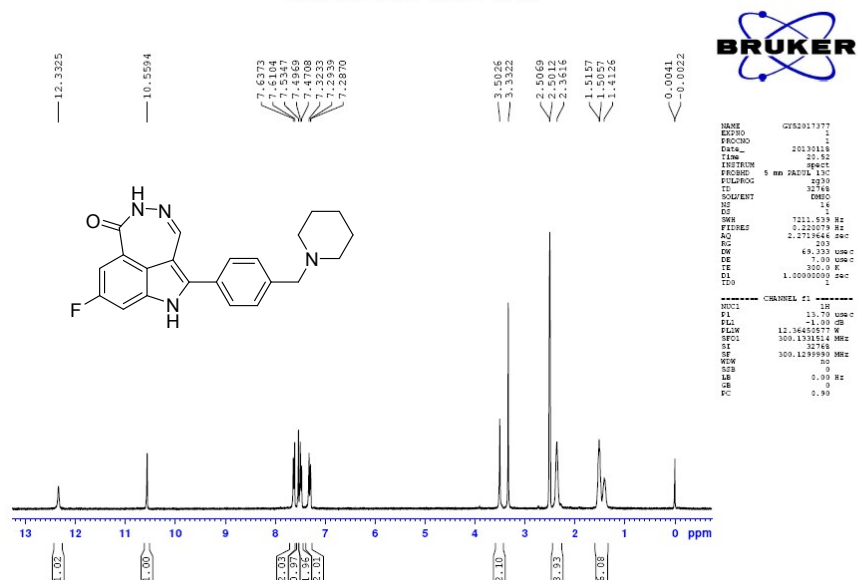
----- CHANNEL f1 -----
 NUC1 13C
 P1 11.00 usec
 PL1 0.00 dB
 PL1W 26.73651905 W
 SF01 75.4764278 MHz

----- CHANNEL f2 -----
 CPGPRG2 waltz16
 MUC2 1H
 P2 80.00 usec
 PL2 -1.00 dB
 PL12 14.30 dB
 PL1W 12.36450577 W
 PL12W 0.36450241 W
 SF02 300.1312005 MHz
 S1 32768
 SF 75.4677867 MHz
 NSW NO
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

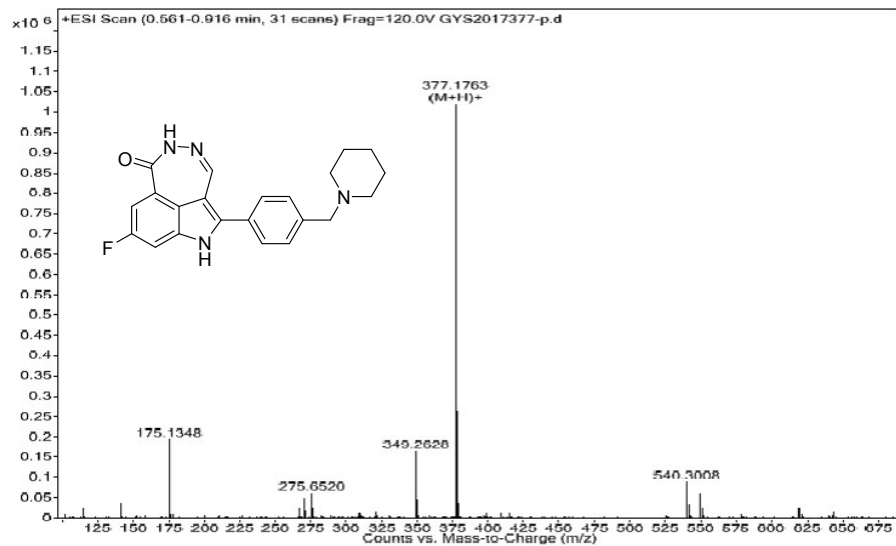


Compound LX24

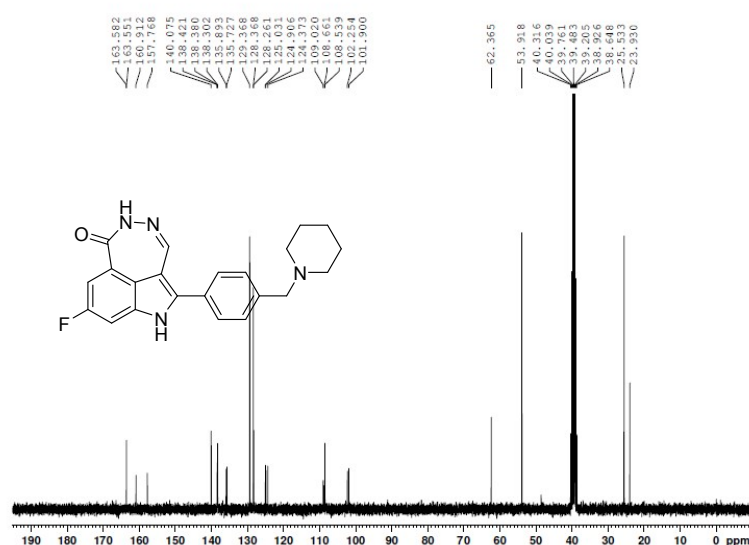
GYS2017377 DMSO 1HNMR AV300



Sample Name	Position	Instrument Name	User Name
1	P1-D4	Instrument 1	
Inj Vol	InjPosition	SampleType	IRM Calibration Status
1		Sample	Success
Data Filename	ACQ Method	Comment	Acquired Time
GYS2017377-p.d			1/19/2013 10:02:23 AM



GYS2017377 C13-NMR DMSO 303K AV-300



```

NAME      GYS2017377
EXPNO     2
PROCNO    1
Date_     20130119
Time      14.09
INSTRUM    spect
PROBHD     5 mm PADUL 13C
PULPROG    zgpg
TD          65536
SOLVENT    DMSO
NS          2816
DS          4
SWH         19531.250 Hz
FIDRES      0.298023 Hz
AQ          1.6777716 sec
RG          57
RG         25.600 usec
DE          7.00 usec
TE          300.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0         1

===== CHANNEL f1 =====
NUC1        13C
P1          11.80 usec
PL1         -1.00 dB
PL1W        26.73651505 W
SFO1        75.4764278 MHz

===== CHANNEL f2 =====
CPDPRG2     waltz16
NUC2         1H
PCPD2        80.00 usec
PL2          -1.00 dB
PL2W         14.30 dB
PL1W2        12.36450577 W
PL1W2W        0.36498241 W
SFO2         300.1312005 MHz
SI           32768
SF           75.4677867 MHz
KW           0
SSB          0
LB           0.00 Hz
GB           0
PC           1.40
    
```

