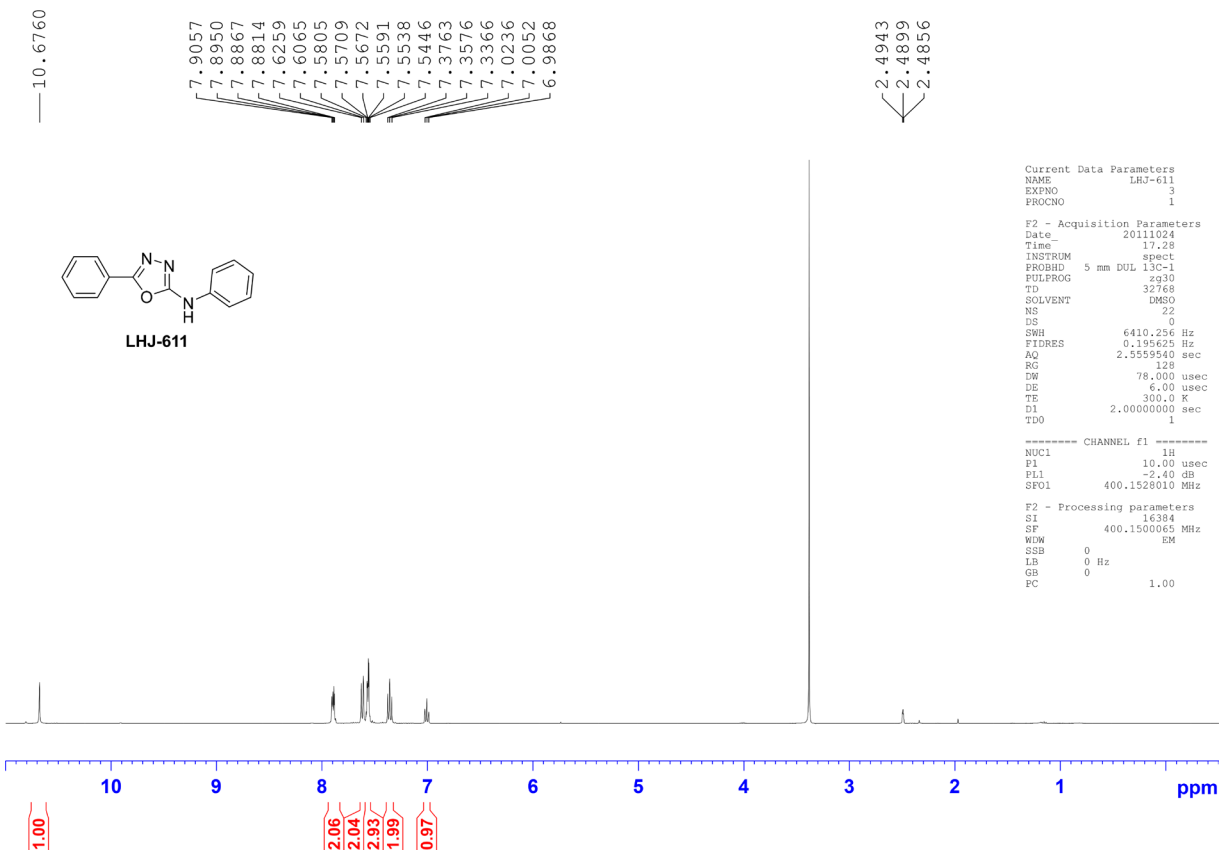
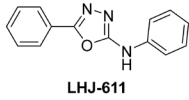


# Characterization of a novel androgen receptor (AR) coregulator RIPK1 and related chemicals that suppress AR-mediated prostate cancer growth via peptide and chemical screening

## Supplementary Materials



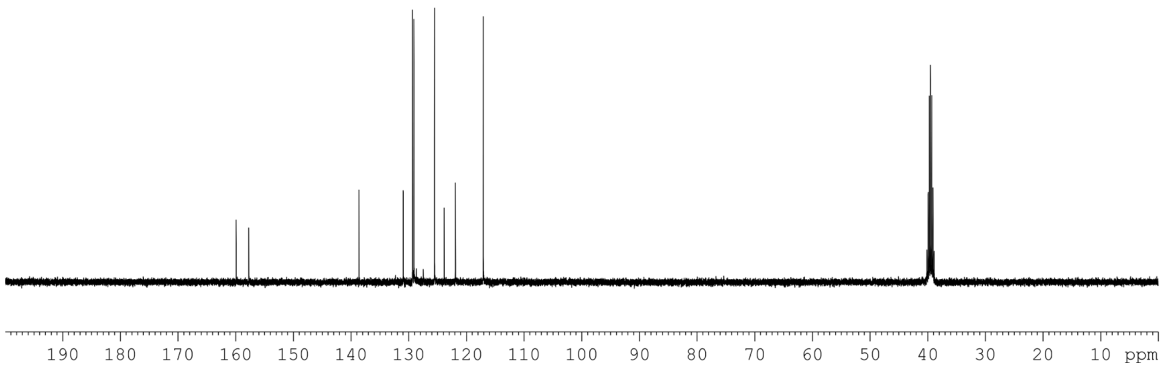


159.9184  
157.7449

138.6302  
130.9529  
129.3293  
129.0934  
125.5364  
123.8488  
121.8997  
117.0776

40.1258  
39.9159  
39.7087  
39.4992  
39.2905  
39.0819  
38.8754

Current Data Parameters  
NAME LHJ-611-13C.fid  
EXPNO 1  
PROCNO 1  
F2 - Processing parameters  
SI 65536  
SF 100.5219769 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



LHJ-611 (HR-ESI MS)  
Elemental Composition Report

Single Mass Analysis

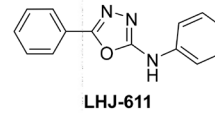
Tolerance = 100.0 PPM / DBE: min = -100.0, max = 1000.0  
Element prediction: Off  
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions  
15 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)  
Elements Used:  
C: 0-1000 H: 0-4000 N: 3-3 O: 1-1  
LHJ-611

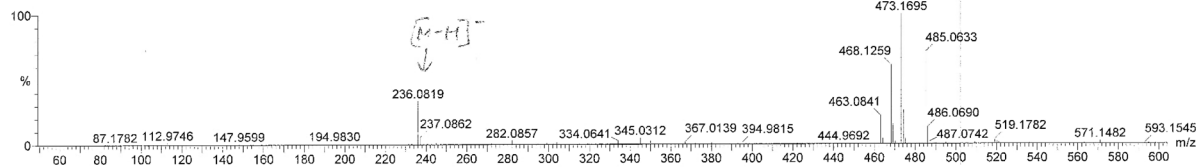
KE267

1031\_LHJ-611 34 (3.365) Cm (34:35:2)

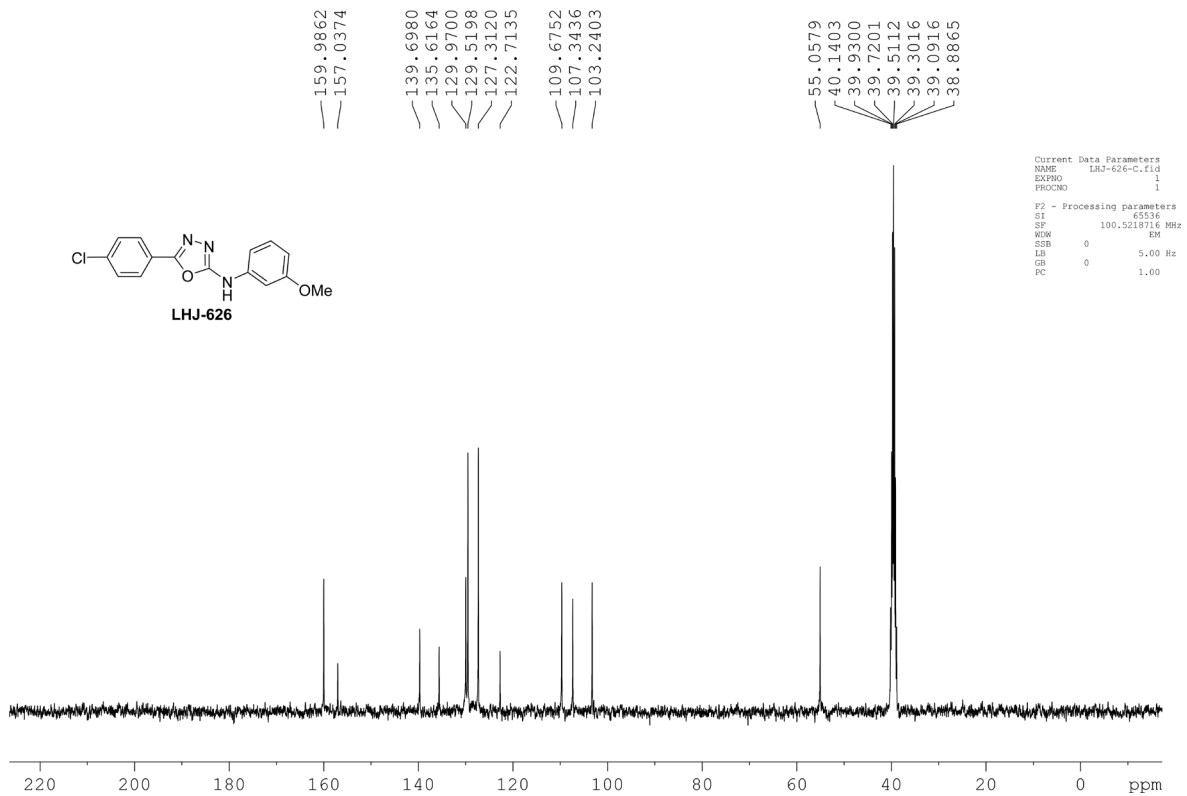
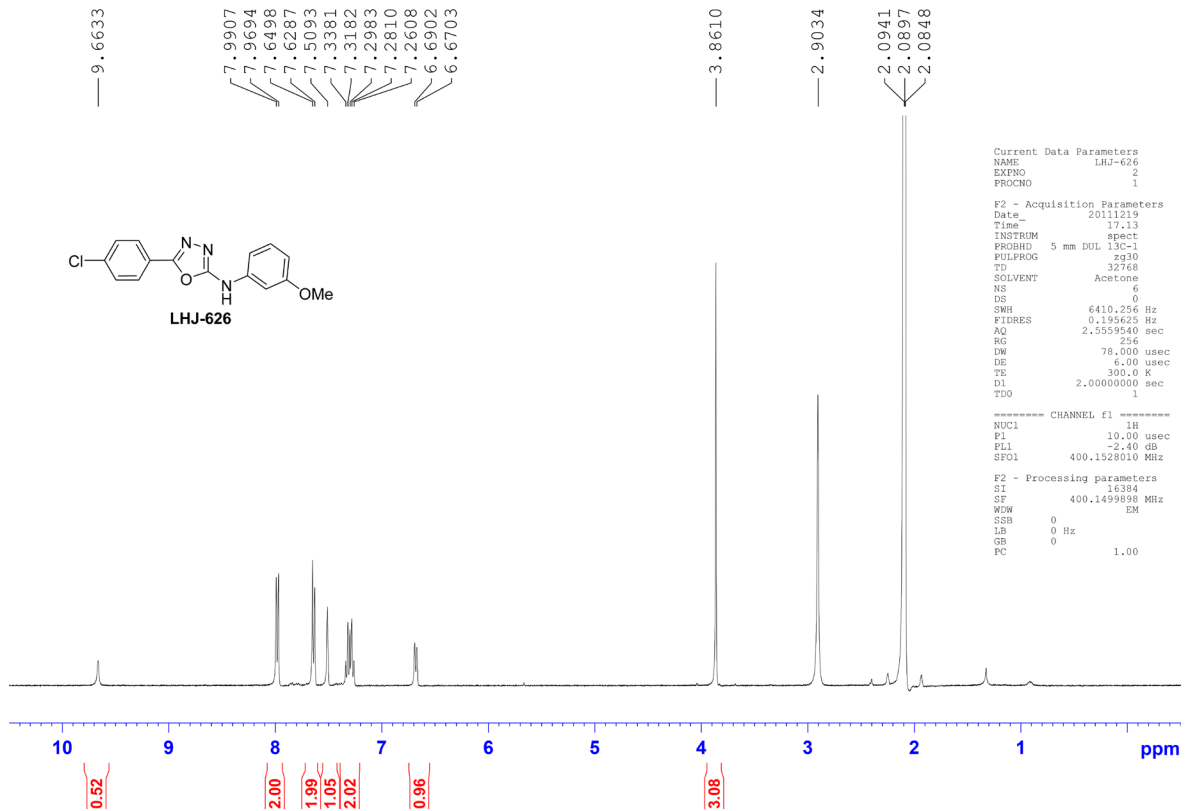
Page 1



31-Oct-2011  
13:46:34  
2: TOP MS ES-  
1.66e+004



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
236.0819	236.0824	-0.5	-2.1	11.5	34.9	0.0	C14 H10 N3 O



LHJ-626 (cur-E51mg)

### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -100.0, max = 1000.0  
Element prediction: Off  
Number of isotope peaks used for i-FIT = 2

#### Monoisotopic Mass, Even Electron Ions

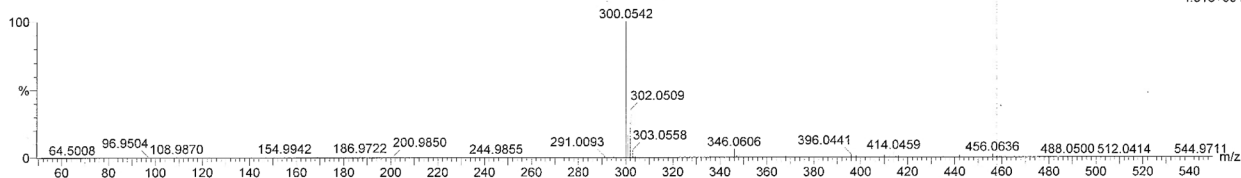
17 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

#### Elements Used:

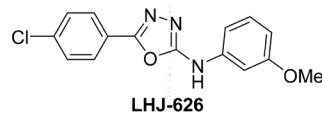
C: 0-4000 H: 0-4000 N: 3-3 O: 2-2 Cl: 1-1

LHJ-626

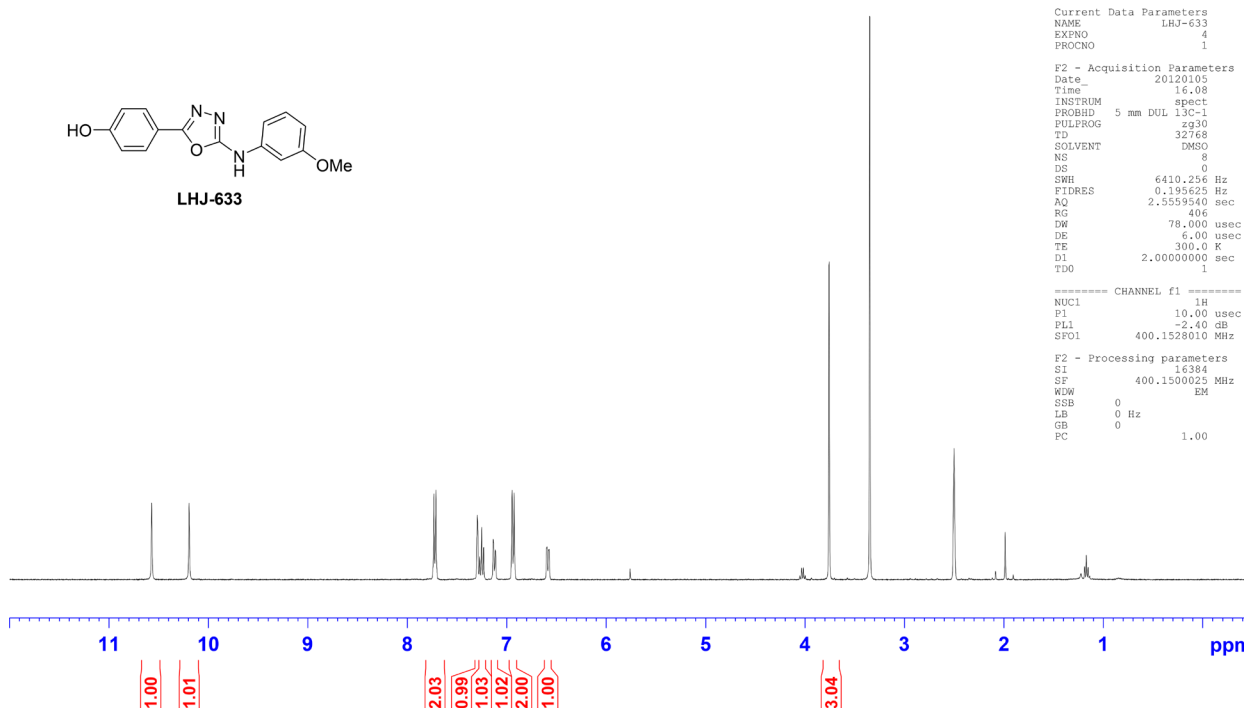
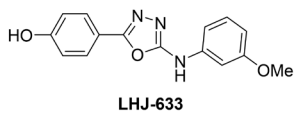
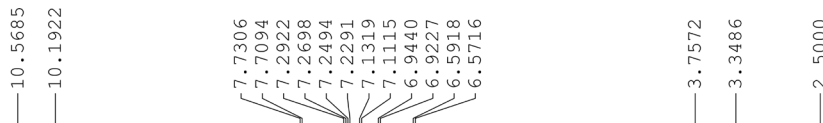
0113\_LHJ-626 22 (2.189)



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
300.0542	300.0540	0.2	0.7	11.5	102.0	0.0	C15 H11 N3 O2 Cl



13-Jan-2012  
12:45:16  
2: TOF MS ES-  
4.31e+004

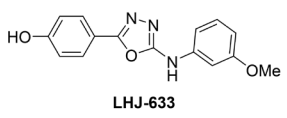
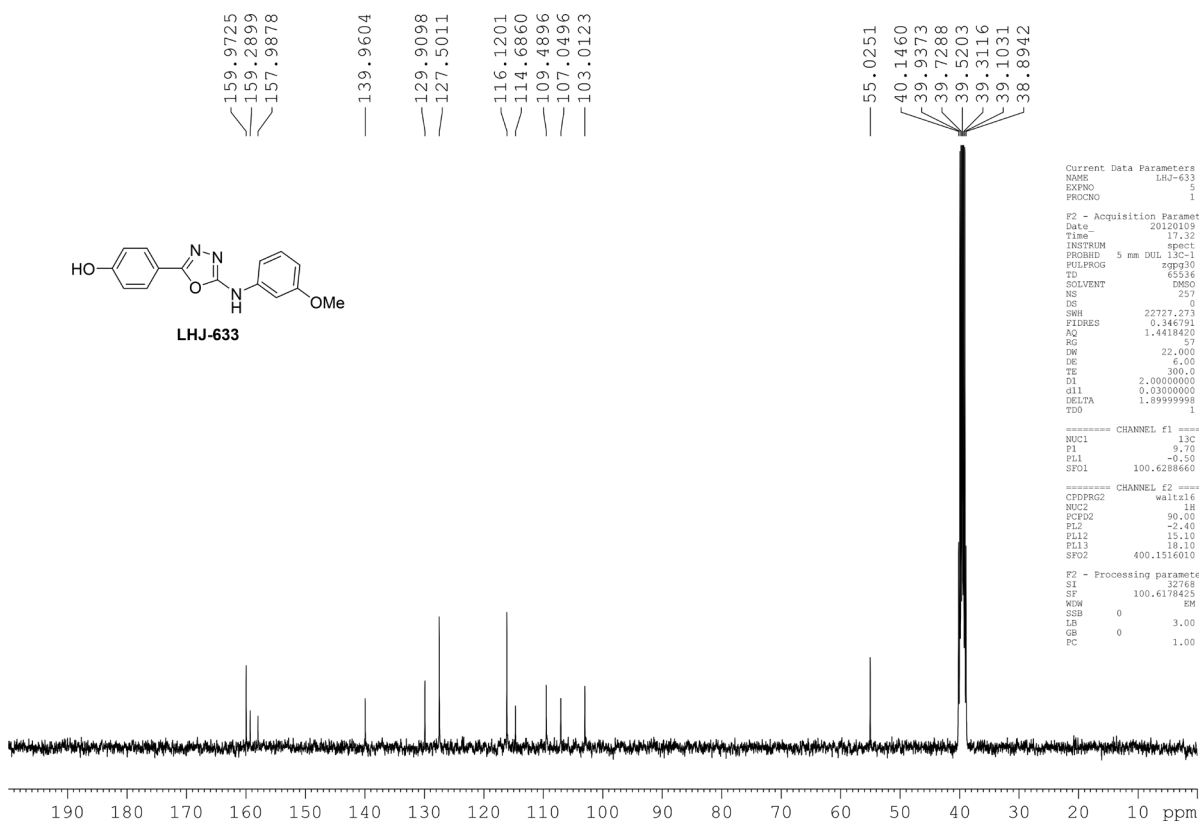


Current Data Parameters  
NAME LHJ-633  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120105  
Time 16.08  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT DMSO  
NS 8  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 406  
DW 78.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -2.40 dB  
SFO1 400.1528010 MHz

F2 - Processing parameters  
SI 16384  
SF 400.1500025 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



```

Current Data Parameters
NAME      LHJ-633
EXPNO     5
PROCNO    1

F2 - Acquisition Parameters
Date_     20120109
Time      17.32
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         227
DS         0
SWH        22727.273 Hz
FIDRES     0.346791 Hz
AQ         1.4418420 sec
RG         57
DW         22.000 use
DE         6.00 use
TE         300.0 K
D1         2.0000000 sec
d11        0.0300000 sec
DELTA     1.8999999 sec
TDO        1

===== CHANNEL f1 =====
NUC1       13C
P1         9.70 use
PL1        -0.50 dB
SFO1      100.6288600 MHz

===== CHANNEL f2 =====
CFDPRG2   waitz16
NUC2       1H
PCPD2     90.00 use
PL2        -2.40 dB
PL12       15.10 dB
PL13       18.10 dB
SFO2      400.1516010 MHz

F2 - Processing parameters
SI         32768
SF         100.6178425 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.00
  
```

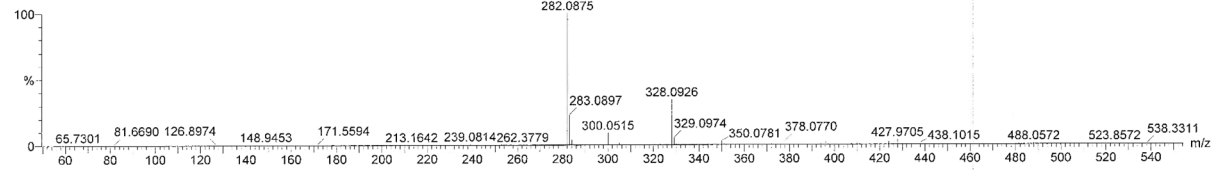
LHJ-633 (HR-ESI MS)

### Elemental Composition Report

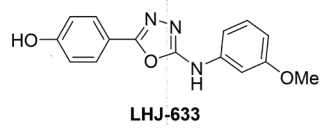
**Single Mass Analysis**  
 Tolerance = 100.0 PPM / DBE: min = -100.0, max = 1000.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions  
 35 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)  
 Elements Used:  
 C: 0-4000 H: 0-4000 N: 3-3 O: 2-3  
 LHJ-633

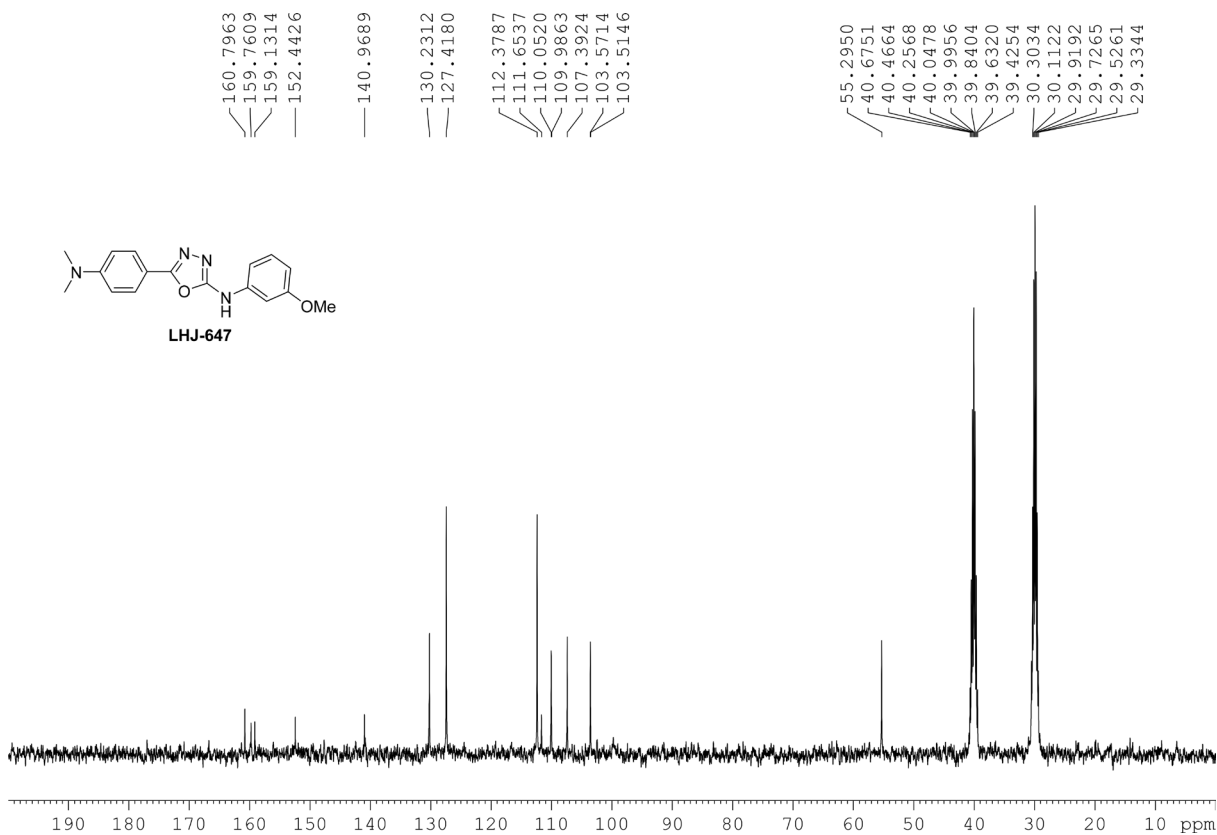
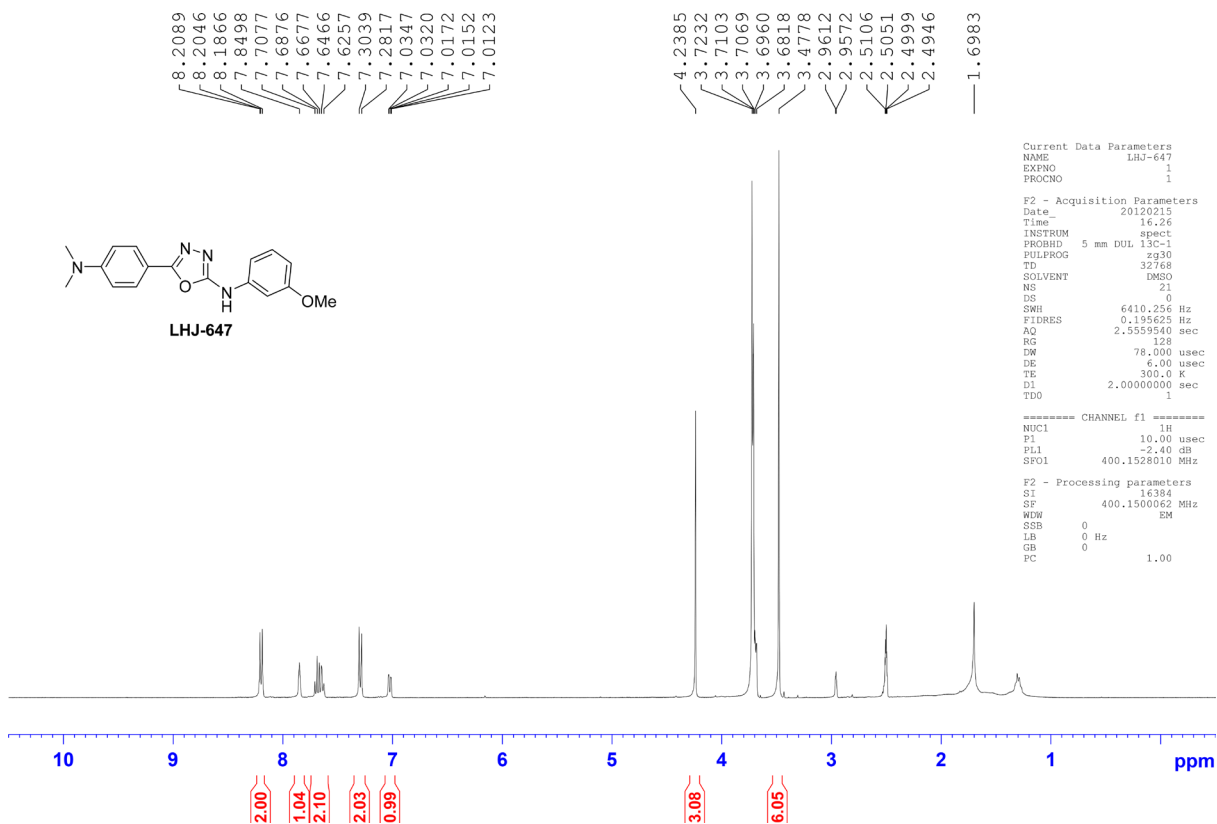
0113\_LHJ-633 21 (2.110) Cm (21-101x5.000)



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
282.0875	282.0879	-0.4	-1.4	11.5	90.1	0.0	C15 H12 N3 O3



Page 1  
 13-Jan-2012  
 12:56:28  
 2: TOF MS ES-  
 1.01e+004



LHJ-647 (HR-ESI-MS)

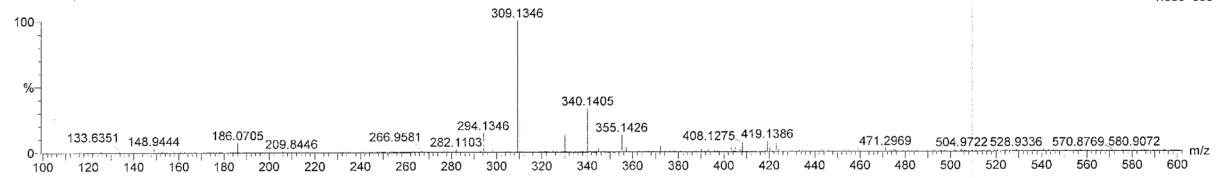
Elemental Composition Report

Single Mass Analysis

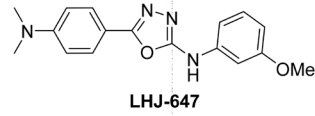
Tolerance = 20.0 PPM / DBE: min = -100.0, max = 1000.0  
Element prediction: Off  
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions  
18 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)  
Elements Used:  
C: 0-4000 H: 0-4000 N: 4-4 O: 2-2  
LHJ-647

0221\_LHJ-647 29 (2.896) Cm (29-101x10.000)



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
309.1346	309.1352	-0.6	-1.9	11.5	37.6	0.0	C17 H17 N4 O2

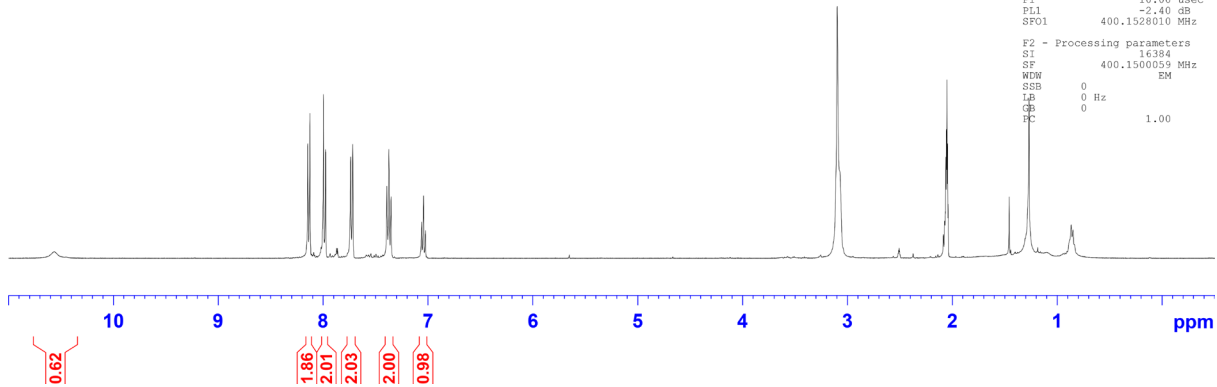
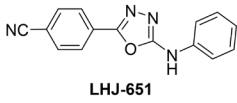


21-Feb-2012  
16:14:35  
2: TOF MS ES-  
1.08e+003

10.5662

8.1447  
8.1233  
7.9954  
7.9749  
7.9737  
7.7353  
7.7158  
7.3898  
7.3709  
7.3501  
7.0590  
7.0406  
7.0220

2.0609  
2.0553  
2.0501  
2.0444  
2.0393

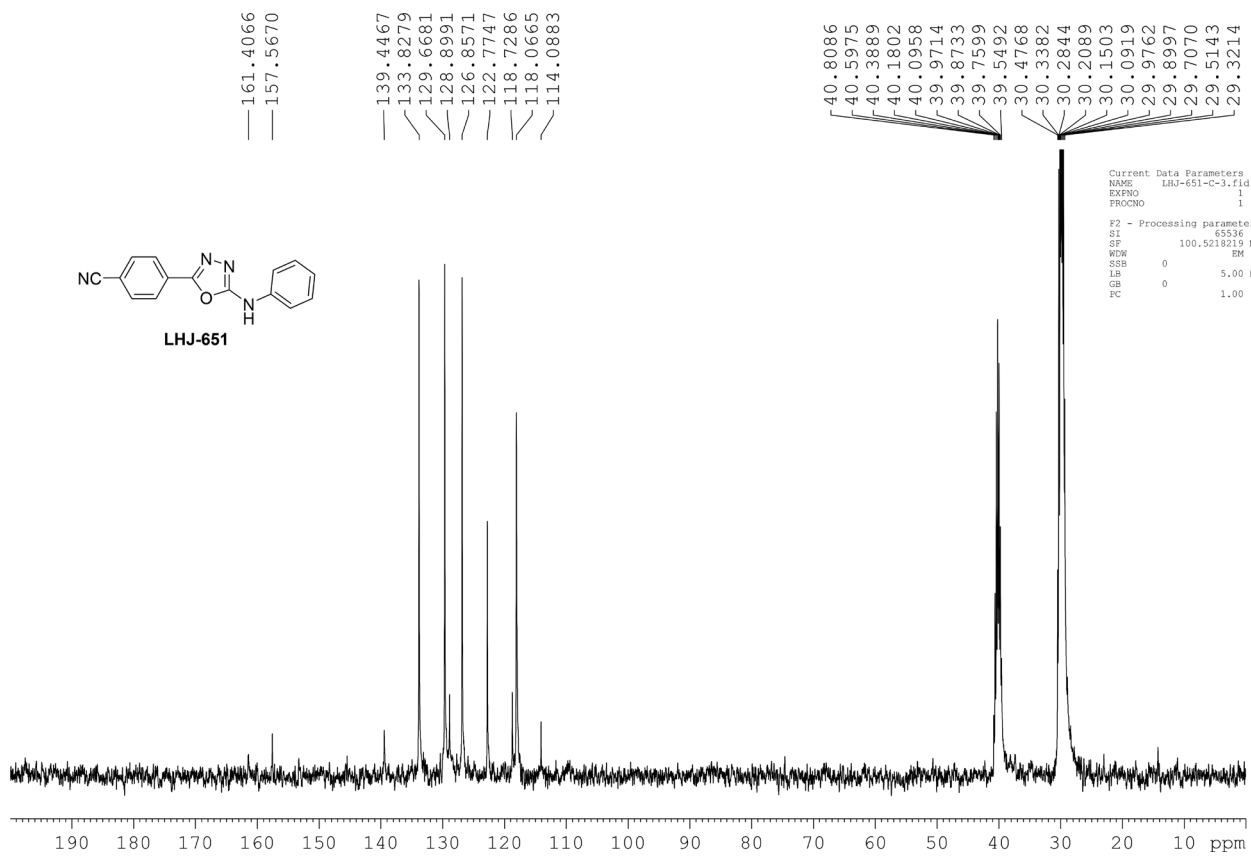


Current Data Parameters  
NAME LHJ-651  
EXFNO 5  
PROCNO 1

F2 - Acquisition Parameters  
Date 20120223  
Time 15.29  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT Acetone  
NS 19  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 287  
DW 78.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
TDO 1

----- CHANNEL f1 -----  
NUC1 1H  
P1 10.00 usec  
PL1 -2.40 dB  
SFO1 400.1528010 MHz

F2 - Processing parameters  
SI 16384  
SF 400.1500059 MHz  
WDW EM  
SSB 0  
LA 0 Hz  
GB 0  
PC 1.00



LHJ-651 (HR ESI neg)

Elemental Composition Report

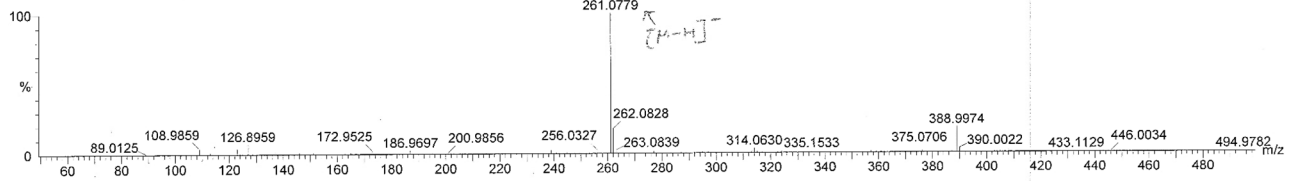
Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -100.0, max = 1000.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions  
 16 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)  
 Elements Used:

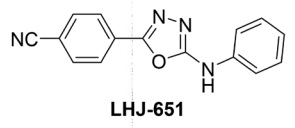
C: 0-4000 H: 0-4000 N: 4-4 O: 1-1  
 LHJ-651

0328\_LHJ-651 10 (1.013)

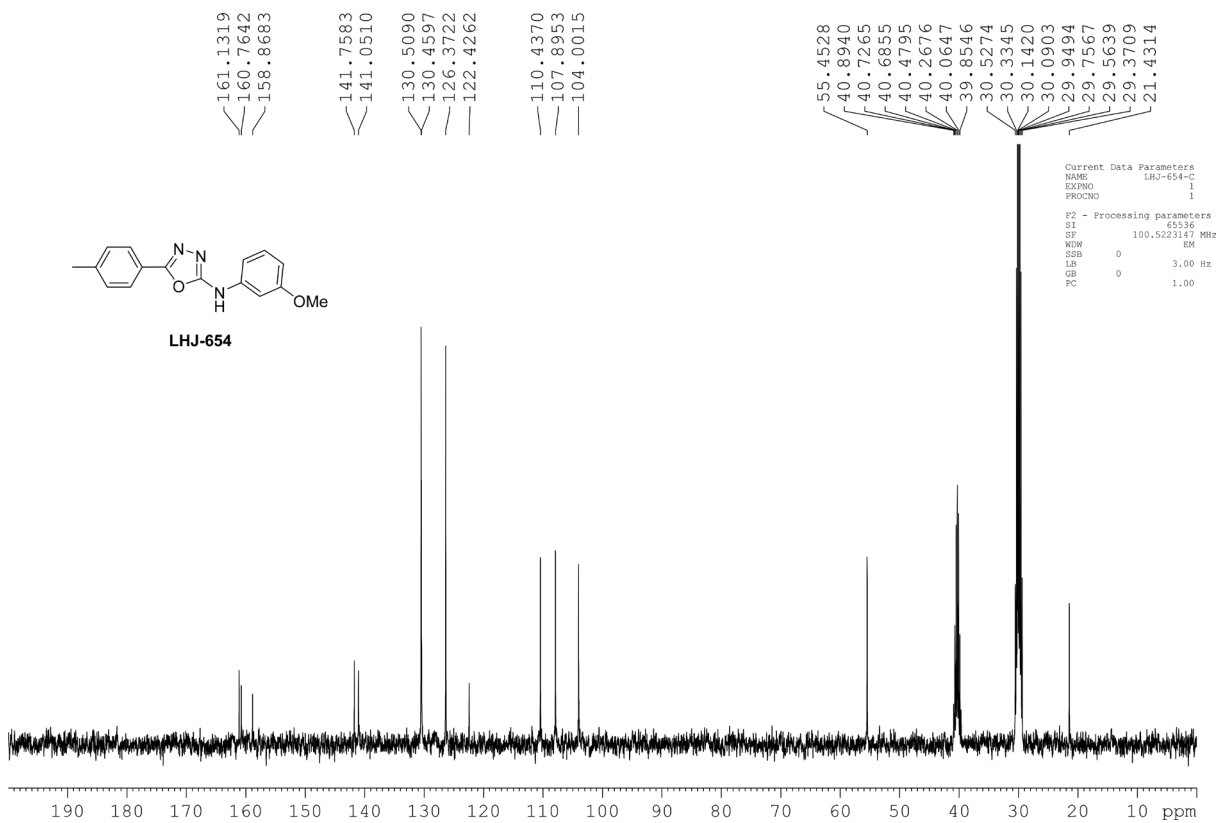
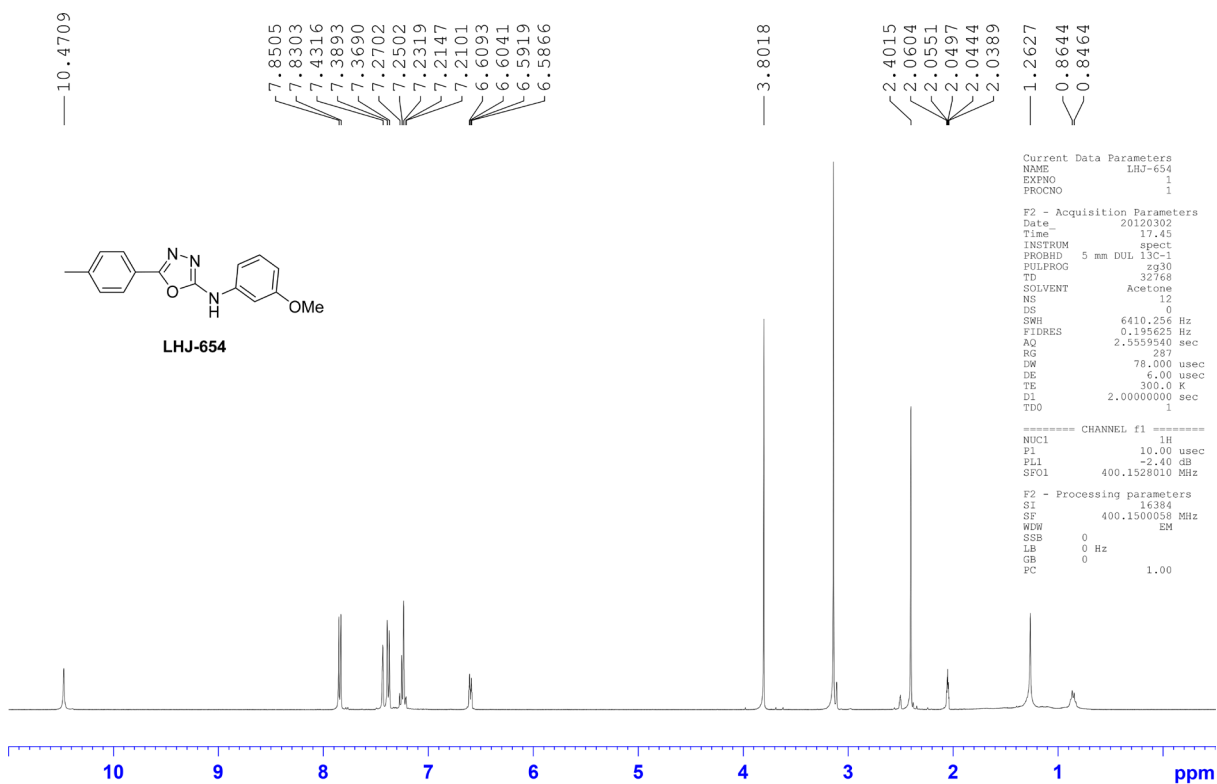


Minimum: -100.0  
 Maximum: 5.0 50.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
261.0779	261.0776	0.3	1.1	13.5	81.4	0.0	C15 H9 N4 O







LHJ-654 (HR-ESI neg)

### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -100.0, max = 1000.0  
Element prediction: Off  
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

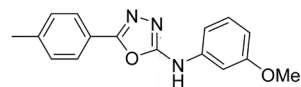
18 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-4000 H: 0-4000 N: 3-3 O: 2-2

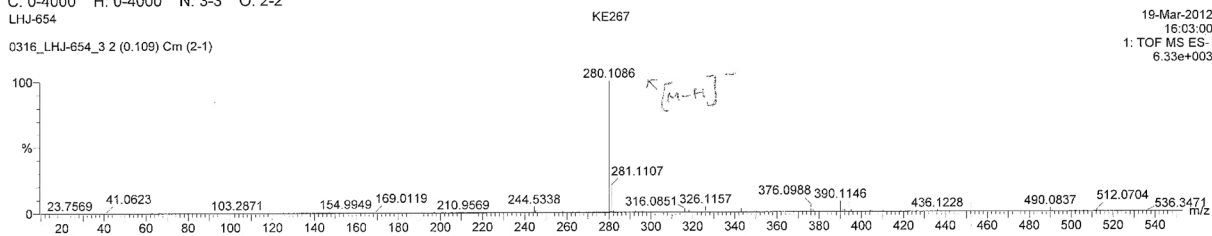
LHJ-654

0316\_LHJ-654\_3\_2 (0.109) Cm (2-1)

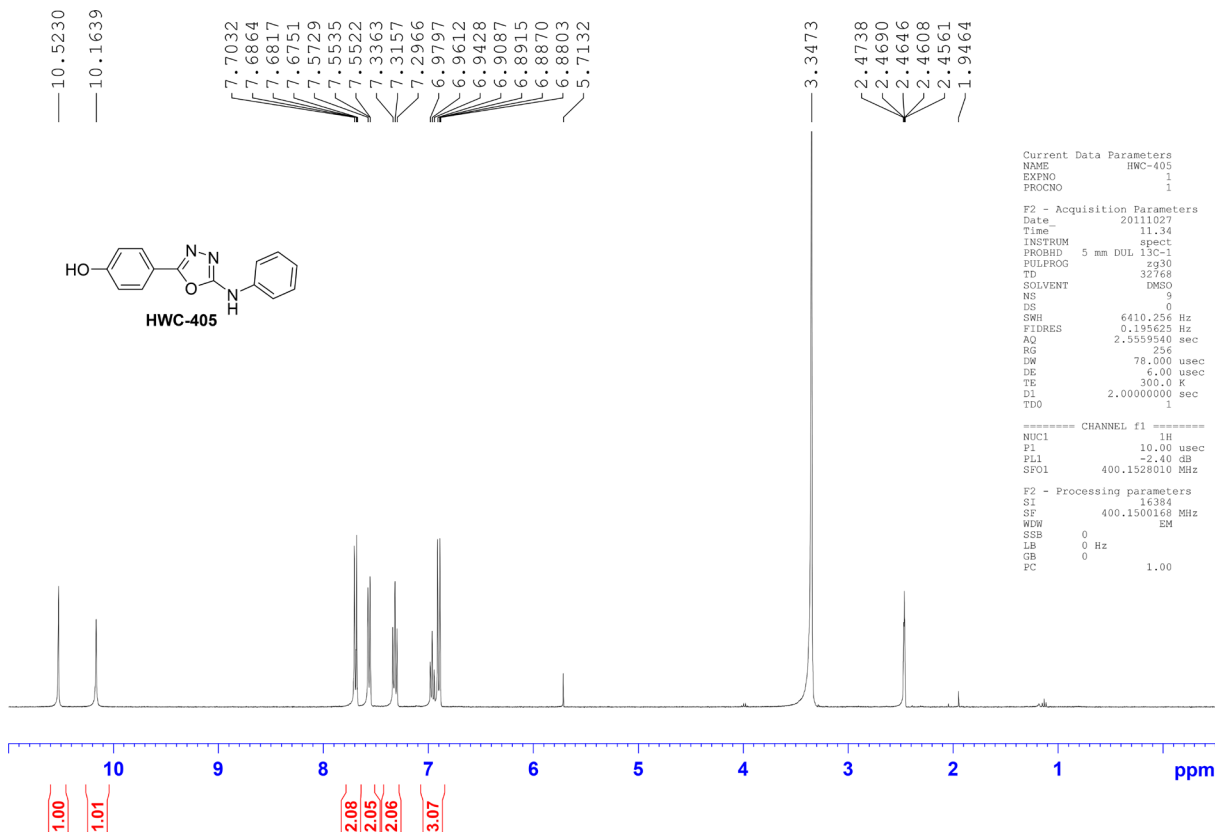


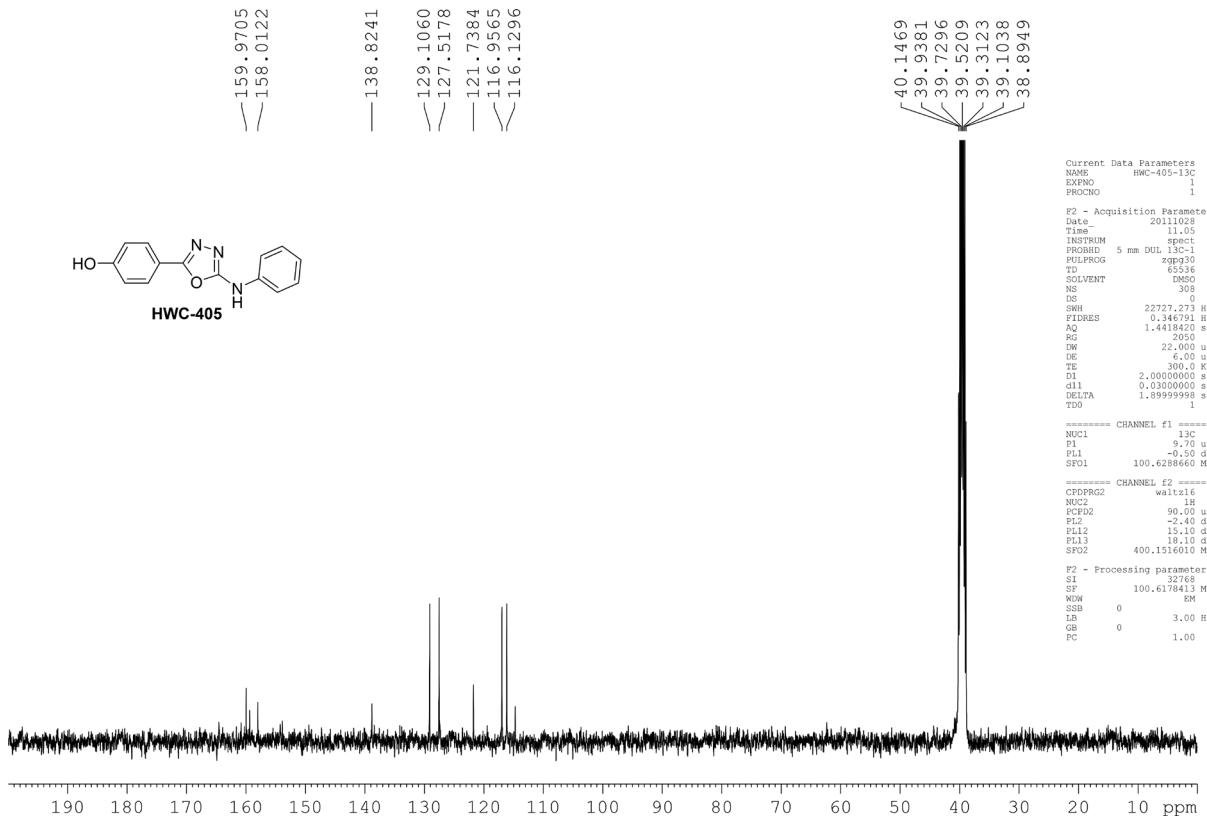
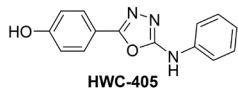
LHJ-654

19-Mar-2012  
16:03:00  
1: TOF MS ES-  
6.33e+003



Minimum:	Maximum:	Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
-100.0	1000.0	280.1086	280.1086	0.0	0.0	11.5	125.3	0.0	C16 H14 N3 O2





```

Current Data Parameters
NAME      HWC-405-13C
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    2011028
Time     11:05
INSTRUM  spect
PROBHD   5 mm DUL 13C-1
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        308
DS        0
SWH       22727.273 Hz
FIDRES   0.346791 Hz
AQ        1.4418420 sec
RG        2050
DW        22.000 use
DE        6.000 use
TE        300.0 K
D1        2.00000000 sec
d11       0.03000000 sec
DELTA    1.89999999 sec
TD0       1

===== CHANNEL f1 =====
NUC1      13C
P1        9.70 use
PL1       -0.50 dB
SFO1      100.6288660 MHz

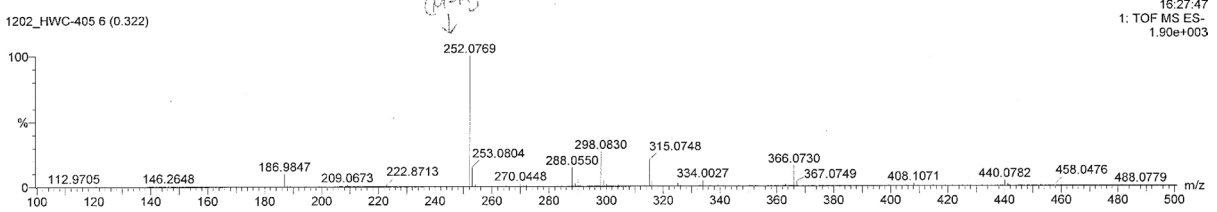
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2    90.00 use
PL2      -2.40 dB
PL12     15.10 dB
PL13     18.10 dB
SFO2     400.1516010 MHz

F2 - Processing parameters
SI        32768
SF        100.6178413 MHz
WDW       EM
SSB       0
LB        3.00 Hz
GB        0
PC        1.00
  
```

HWC-405 (HR-ESI-MS)  
**Elemental Composition Report**

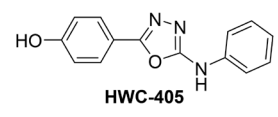
**Single Mass Analysis**  
 Tolerance = 100.0 PPM / DBE: min = -100.0, max = 1000.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 2

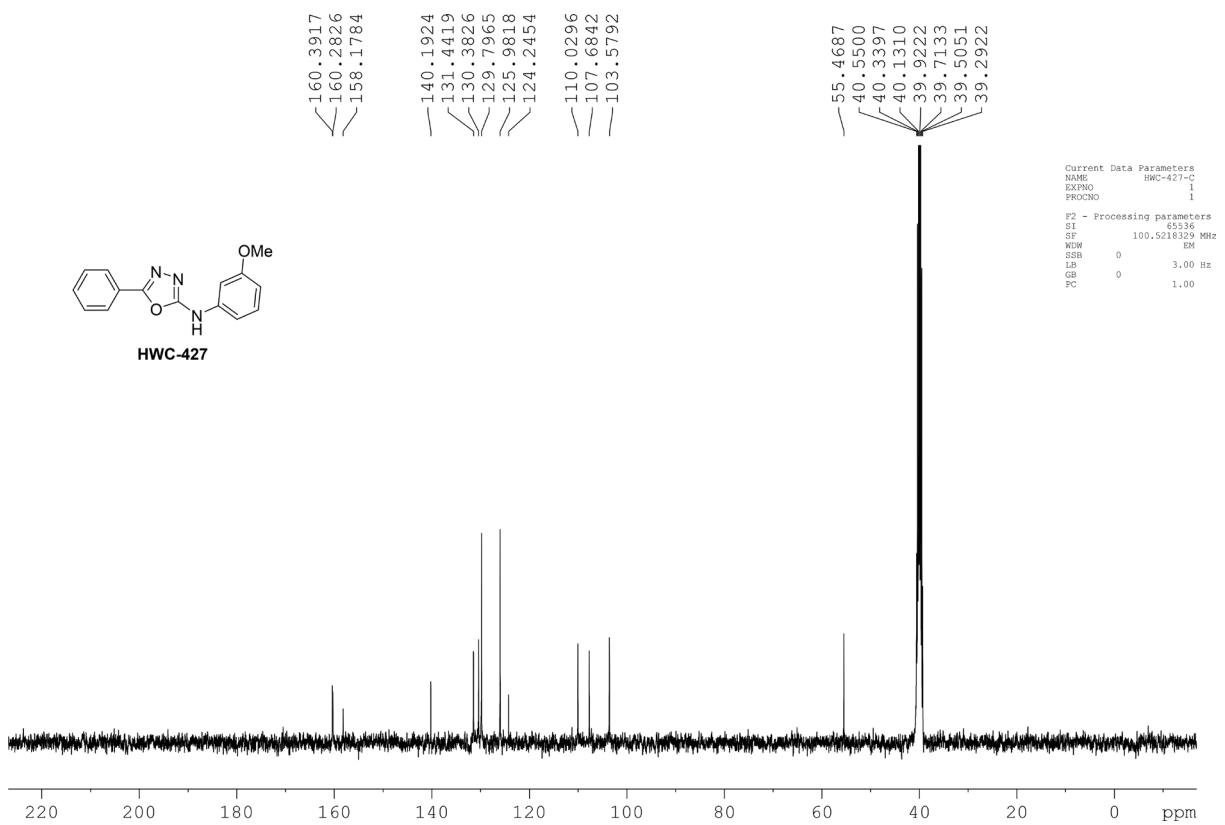
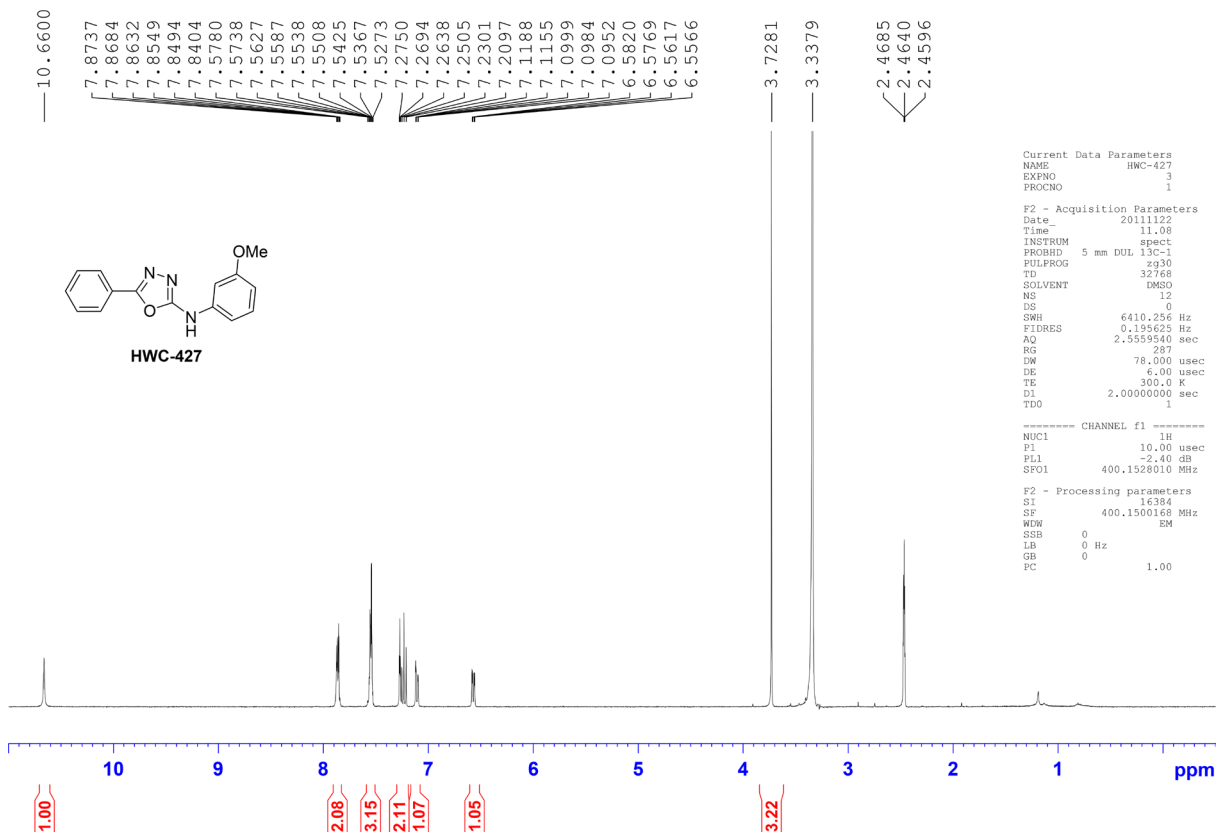
Monoisotopic Mass, Even Electron Ions  
 15 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)  
 Elements Used:  
 C: 0-1000 H: 0-4000 N: 3-3 O: 2-2  
 HWC-405



1202\_HWC-405 6 (0.322)

Minimum:	5.0	100.0	-100.0						
Maximum:			1000.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula		
252.0769	252.0773	-0.4	-1.6	11.5	62.1	0.0	C14 H10 N3 O2		





HWC-427 (HR-ESI-MS)

### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -100.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

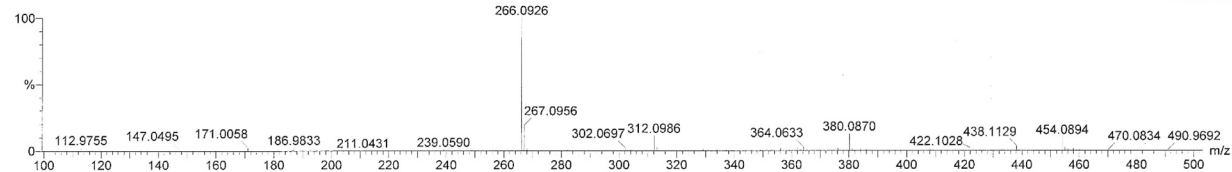
17 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-1000 H: 0-4000 N: 3-3 O: 2-2

HWC-427

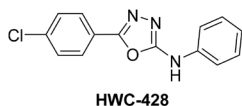
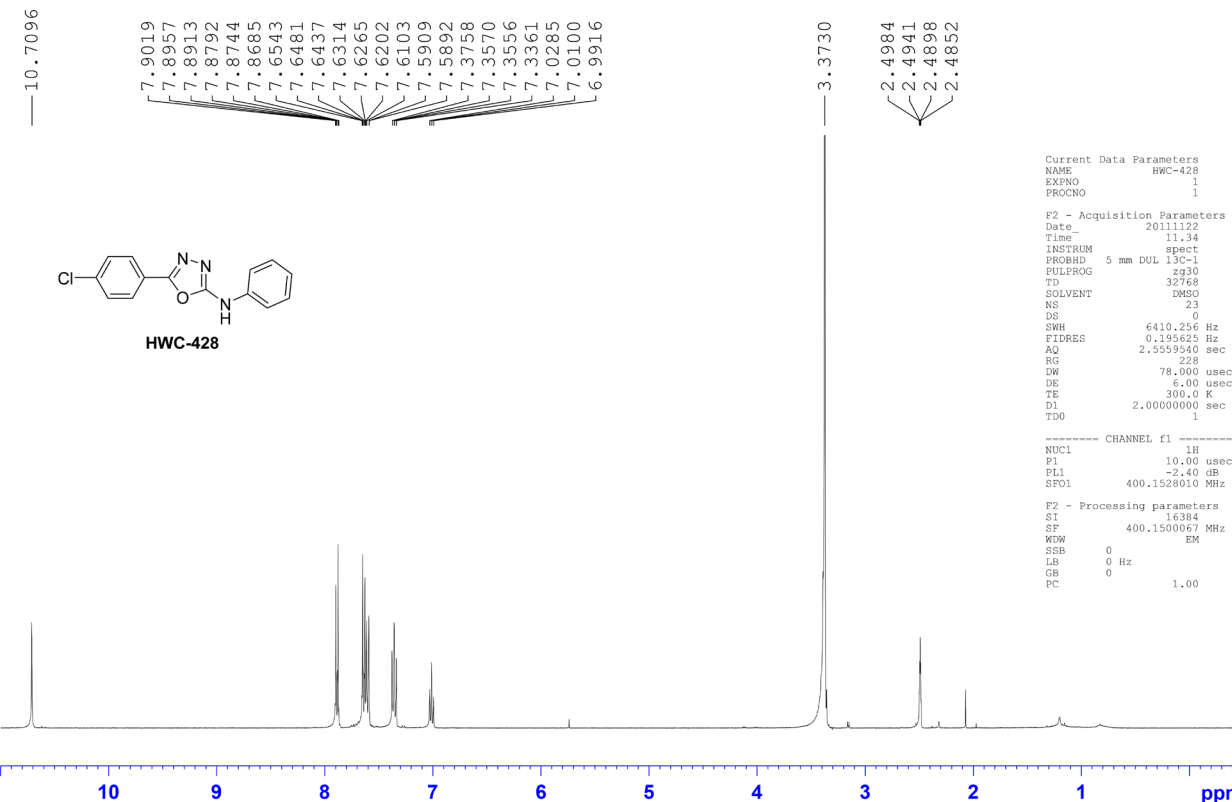
1202\_HWC-427 19 (1.037) Cm (19-1)



Minimum:  
Maximum:

5.0 100.0 -100.0  
1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
266.0926	266.0930	-0.4	-1.5	11.5	183.2	0.0	C15 H12 N3 O2

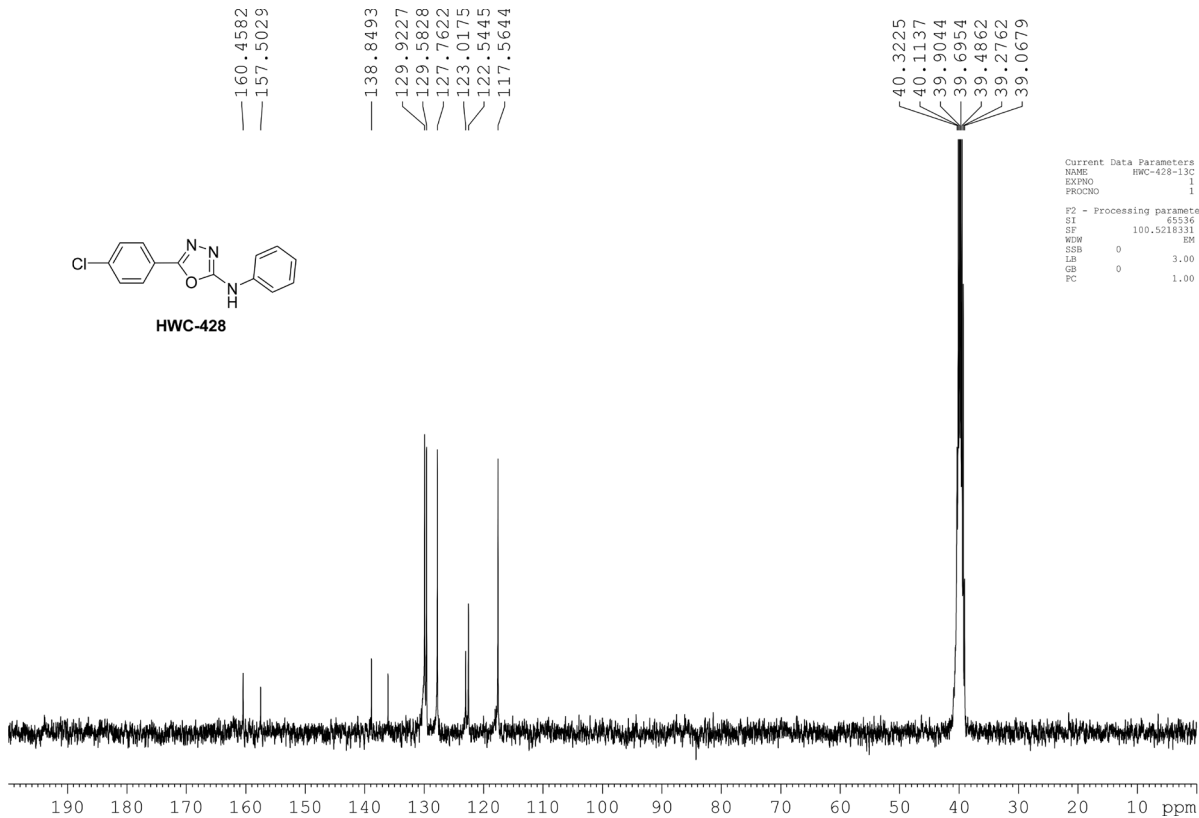
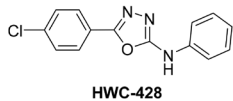


Current Data Parameters  
NAME HWC-428  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 2011122  
Time 11.34  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
FULPROG zg30  
TD 32768  
SOLVENT DMSO  
NS 23  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.19525 Hz  
AQ 2.5559540 sec  
RG 228  
DW 78.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.0000000 sec  
TD0 1

CHANNEL f1  
NUC1 1H  
P1 10.00 usec  
PL1 -2.40 dB  
SFO1 400.1528010 MHz

F2 - Processing parameters  
SI 16384  
SF 400.1500067 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

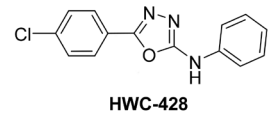


Current Data Parameters  
 NAME HWC-428-13C  
 EXPNO 1  
 PROCNO 1  
 F2 - Processing parameters  
 SI 5536  
 SF 100.5218131 MHz  
 KW EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00

HWC-428 (4K-ESS mag)

**Elemental Composition Report**

**Single Mass Analysis**  
 Tolerance = 100.0 PPM / DBE: min = -100.0, max = 1000.0  
 Element prediction: Off  
 Number of isotope peaks used for i-FIT = 2

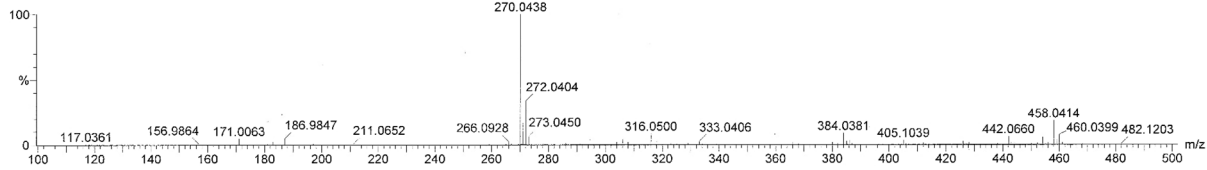


Monoisotopic Mass, Even Electron Ions  
 15 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)  
 Elements Used:  
 C: 0-1000 H: 0-4000 N: 3-3 O: 1-1 Cl: 1-1  
 HWC-428

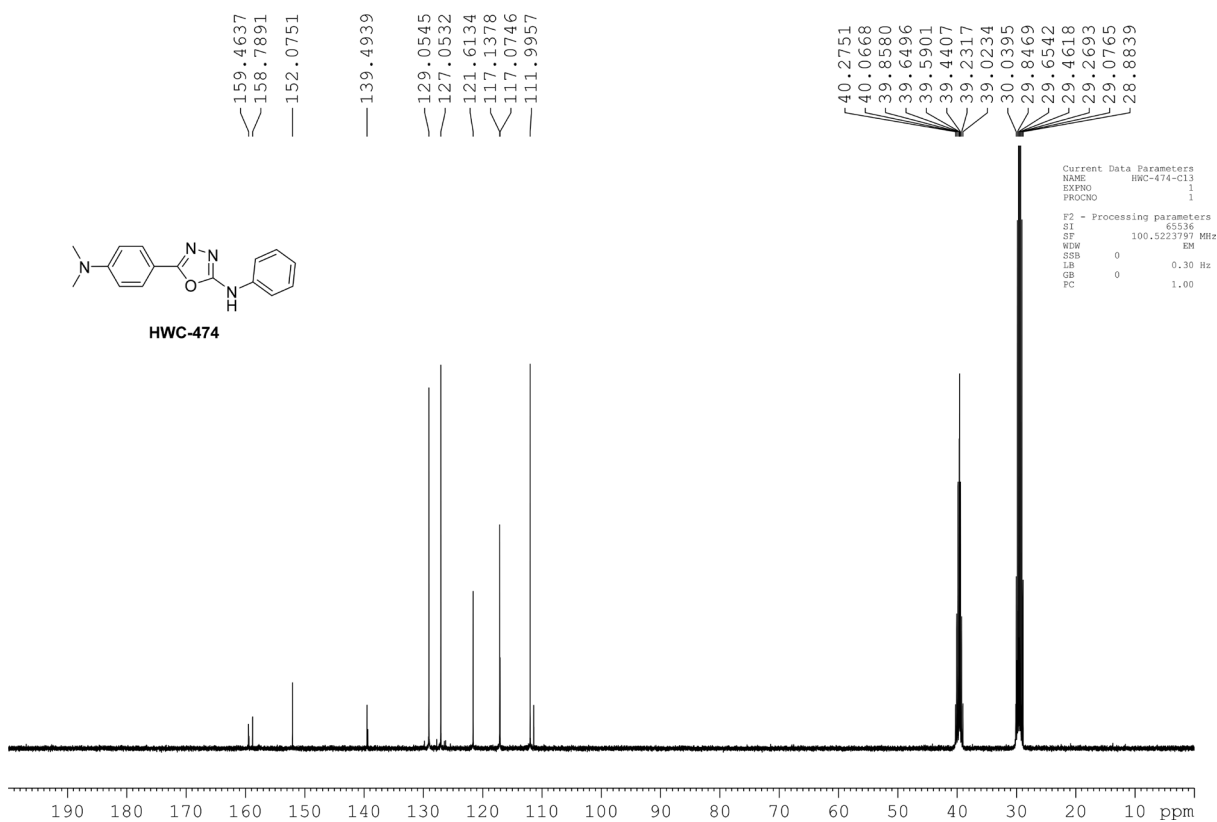
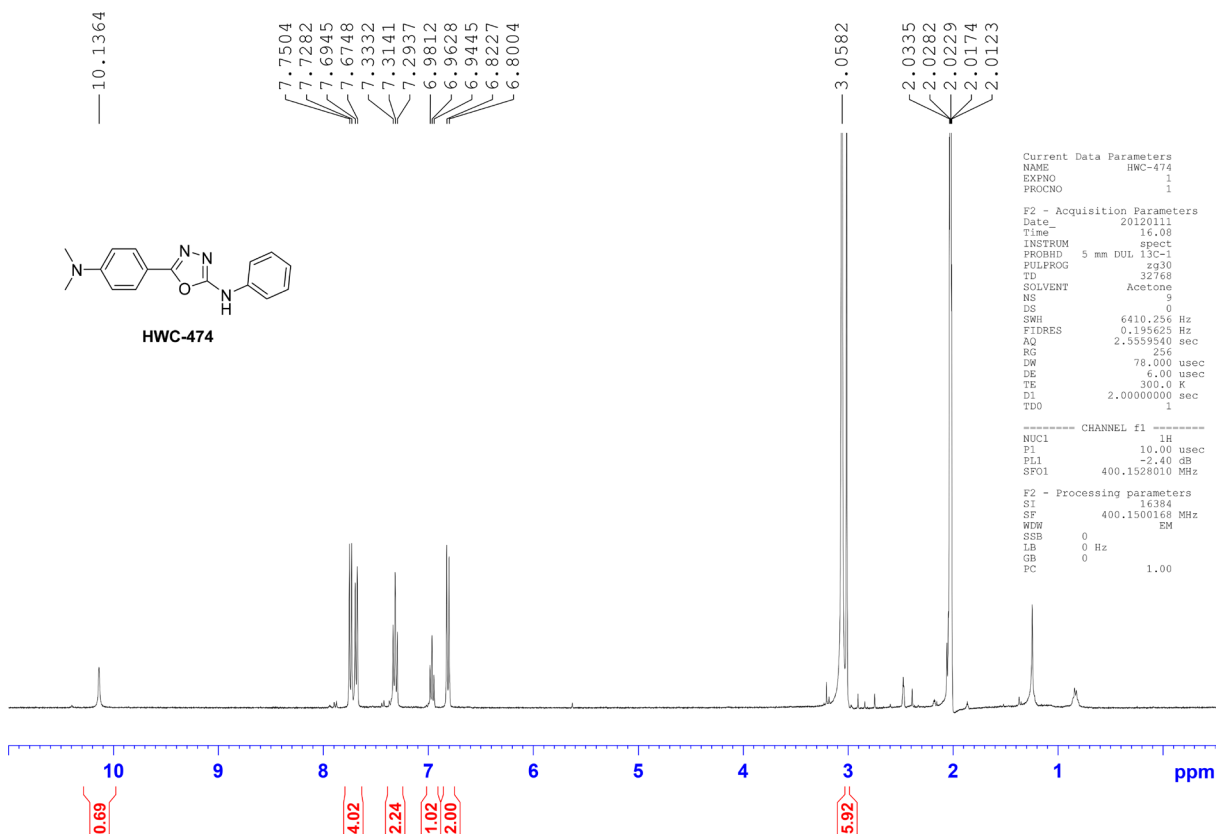
1202\_HWC-428 4 (0.216) Cm (4-1)

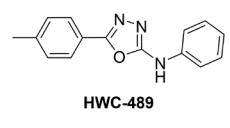
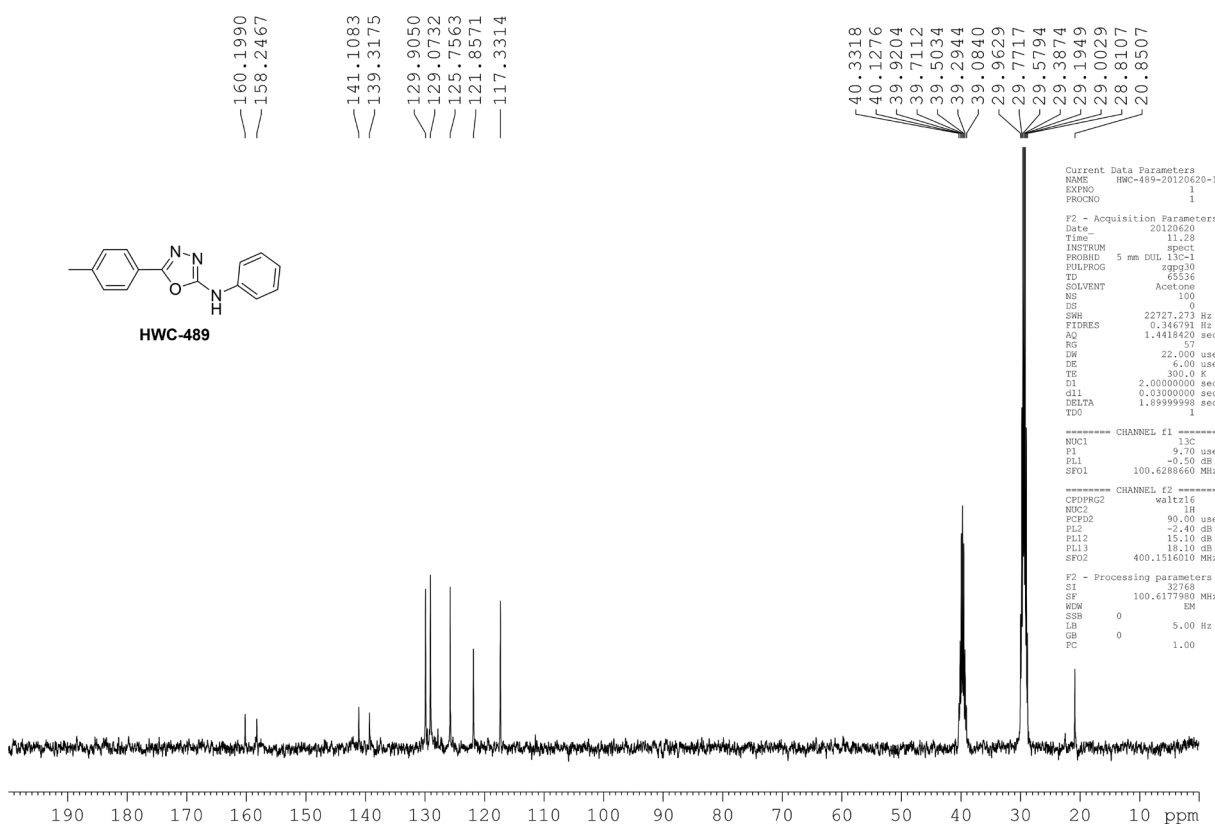
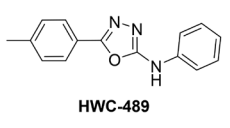
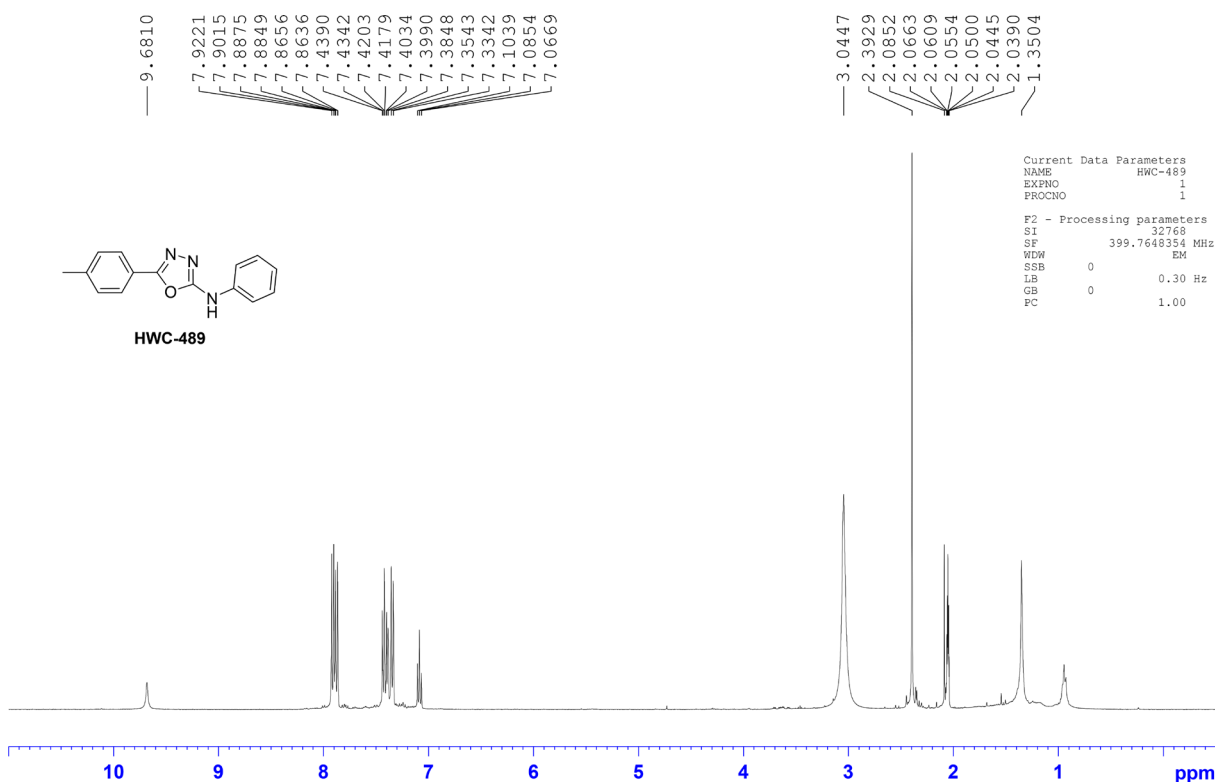
$[M+H]^+$  KE267

05-Dec-2011  
 17:01:31  
 1: TOF MS ES-  
 1.97e+004



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
270.0438	270.0434	0.4	1.5	11.5	217.7	0.0	C14 H9 N3 O Cl







HWC-489 CHR-ESI neg?

### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -100.0, max = 1000.0  
Element prediction: Off  
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

17 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

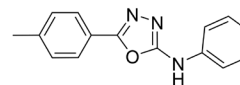
Elements Used:

C: 0-4000 H: 0-4000 N: 3-3 O: 1-1

HWC-489

KE267

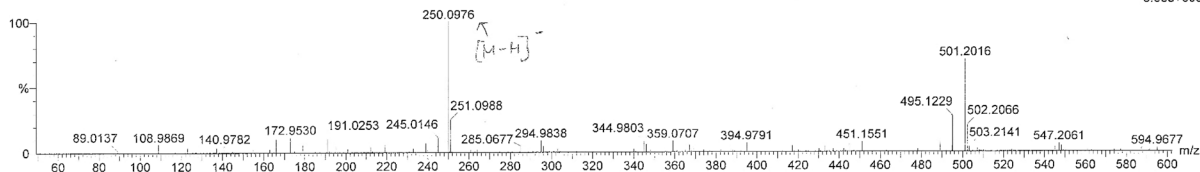
Page 1



HWC-489

0307\_HWC-489 10 (1.013) Cm (10-2)

07-Mar-2012  
12:33:52  
2: TOF MS ES-  
3.58e+003



Minimum: -100.0  
Maximum: 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
250.0976	250.0980	-0.4	-1.6	11.5	57.3	0.0	C15 H12 N3 O

Supplementary Figure 1: Synthesis pathways of oxadiazole derivatives.