

Supplementary Material

Copper-catalyzed, oxidative sp^2 C-H cyanation: facile synthesis of aromatic carbonitriles

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Luoyang 471022, China

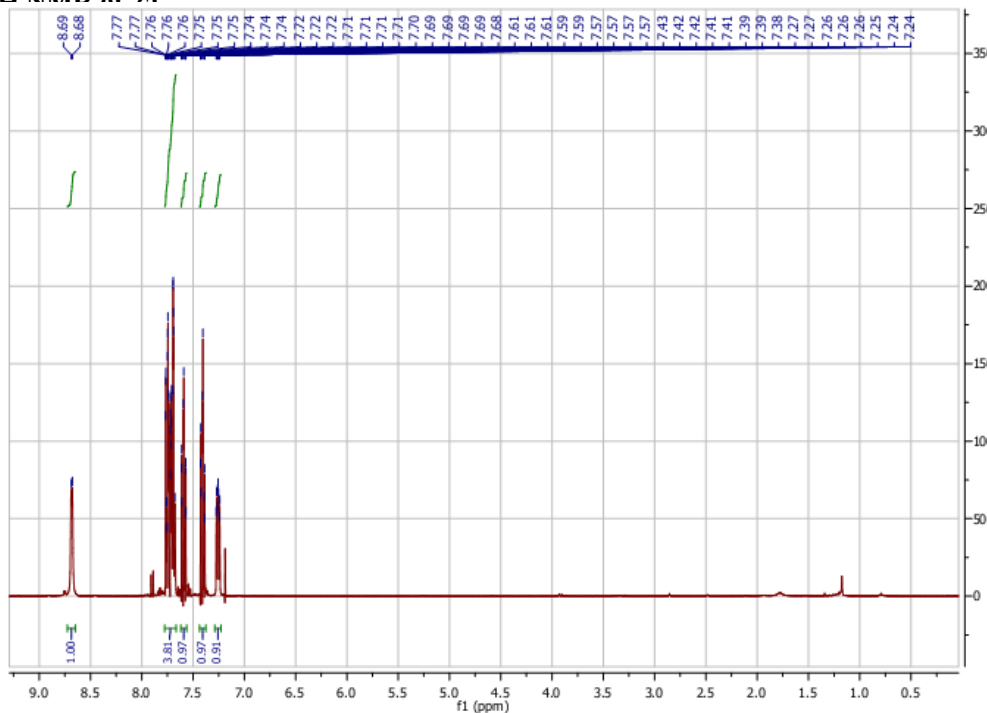
^b Hutchison MediPharma Limited, Shanghai 201203. China

^c Department of Chemical and Biological Engineering, Zhejiang University,
Hangzhou 310027, China

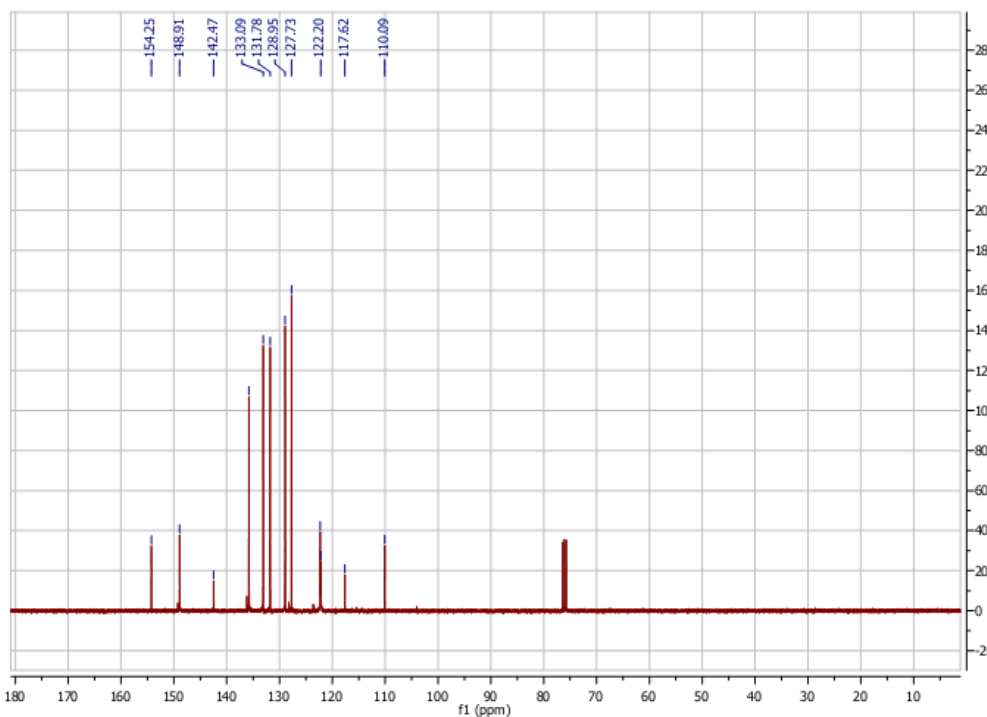
Email: liuque.zju@hotmail.com

Spectral data (^1H , ^{13}C , LC MS) of compounds 2a-1'v

pages 1-80

¹H NMR of 2a

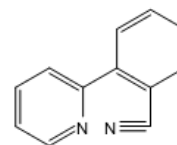
¹H NMR (400 MHz, cdcl₃) δ 8.68 (d, *J* = 4.3, 1H), 7.68 – 7.77 (m, 4H), 7.57 – 7.61 (m, 1H), 7.38 – 7.43 (m, 1H), 7.24 – 7.27 (m, 1H).

¹³C NMR of 2a

Hutchison Medi Pharma

Acquisition Parameters
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 Owner: jrhong
 DATE: 2013-04-11T00:44:05
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 PULPROG: s2pul
 TE: 34 C
 NS: 8
 SFO1: 399.59 MHz
 SWH: 6410.3 Hz
 NUC: 1H
 TD: 13132

F2 - Processing Parameters
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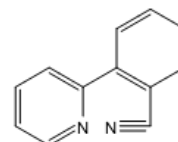


C₁₂H₈N₂
 Exact Mass: 180.07
 Mol. Wt.: 180.21

Hutchison Medi Pharma

Acquisition Parameters
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 Origin: vnmrs
 Owner: jrhong
 DATE: 2013-04-11T02:07:35
 Solvent: cdcl3
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 SWH: 24509.8 Hz
 NUC: 13C
 TD: 31875

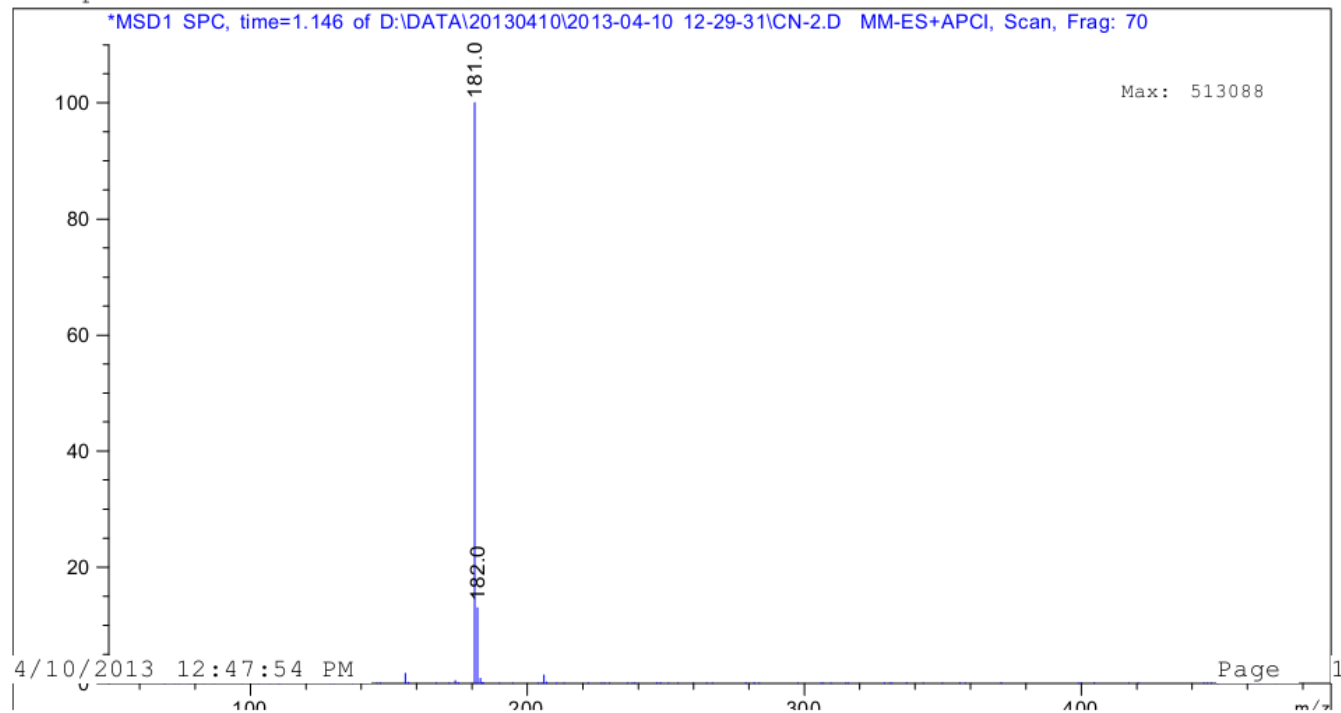
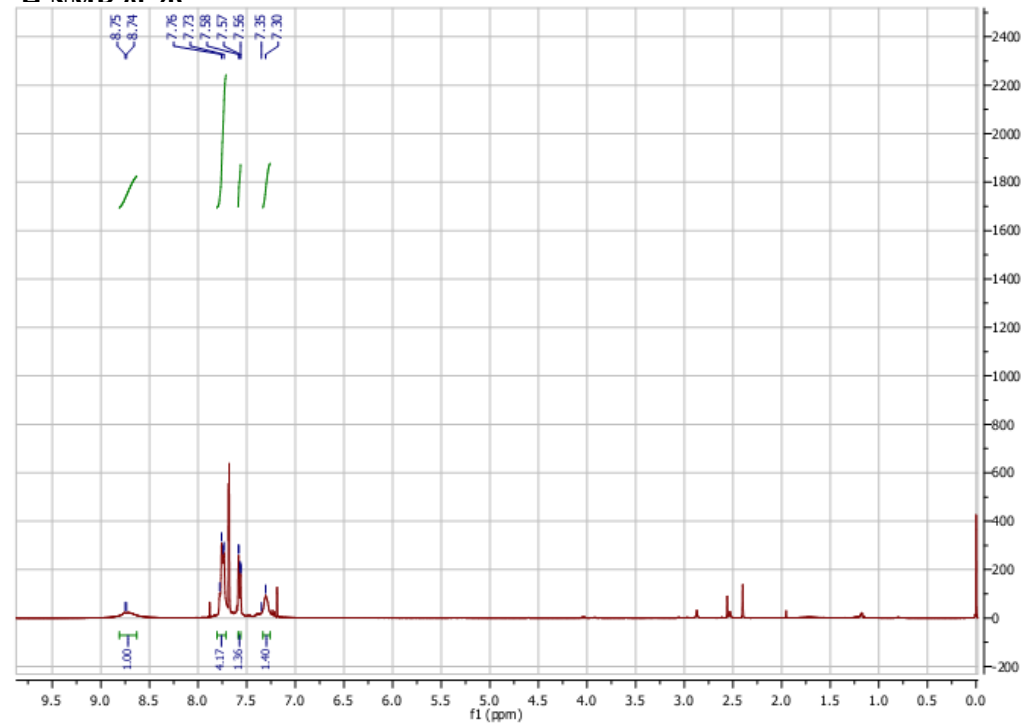
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C₁₂H₈N₂
 Exact Mass: 180.07
 Mol. Wt.: 180.21

LC-MS of 2a

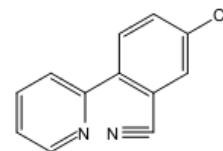
MS Spectrum

¹H NMR of 2a¹H NMR (400 MHz, cdcl₃) δ 8.74 (d, *J* = 4.3, 1H), 7.73 - 7.78 (m, 4H), 7.56 - 7.58 (m, 1H), 7.30 - 7.35 (m, 1H).

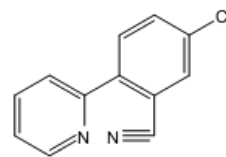
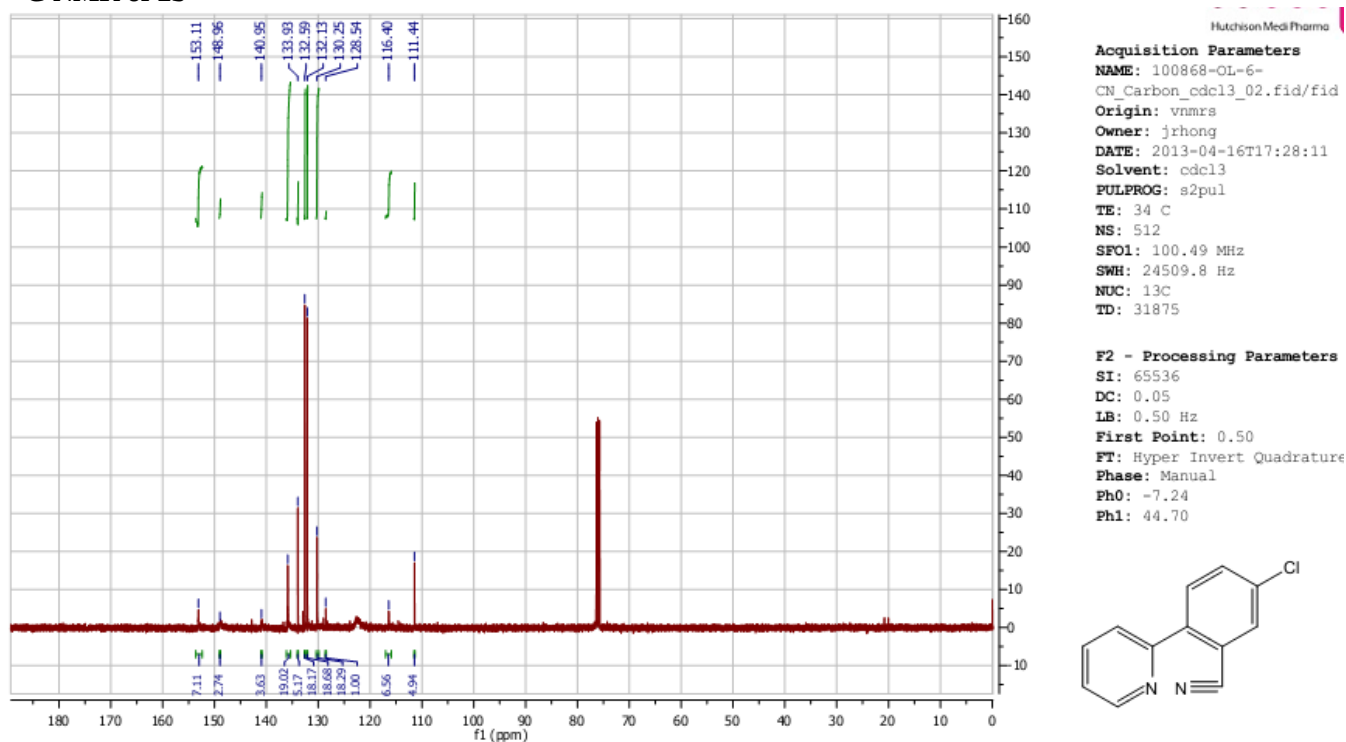
Hutchison MediPharma

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Origin: vnmrs
Owner: jrhong
DATE: 2013-04-16T11:28:06
Solvent: cdcl3
PULPROG: s2pul
TE: 34 C
NS: 32
SF01: 399.59 MHz
SWH: 6410.3 Hz
NUC: 1H
TD: 13132

F2 - Processing Parameters
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FT: Hyper Invert Quadrature
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Ph0: -156.03
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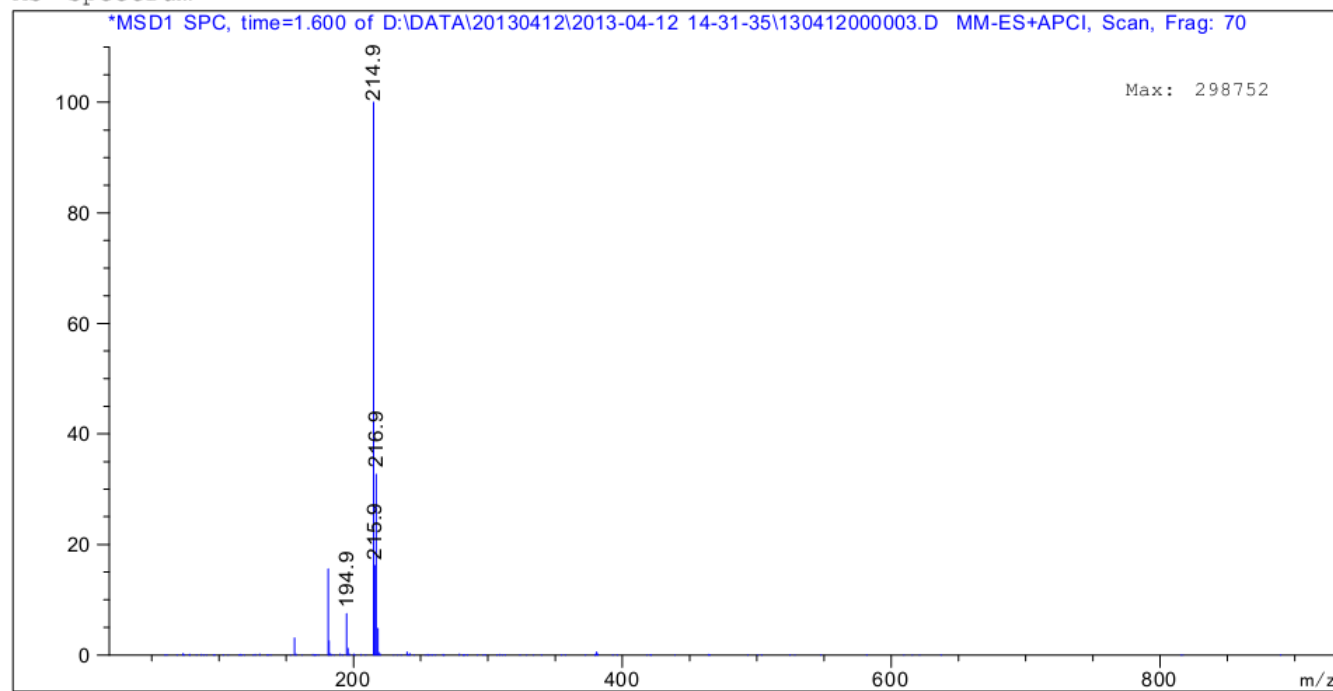
C12H7ClN2
Exact Mass: 214.03
Mol. Wt.: 214.65

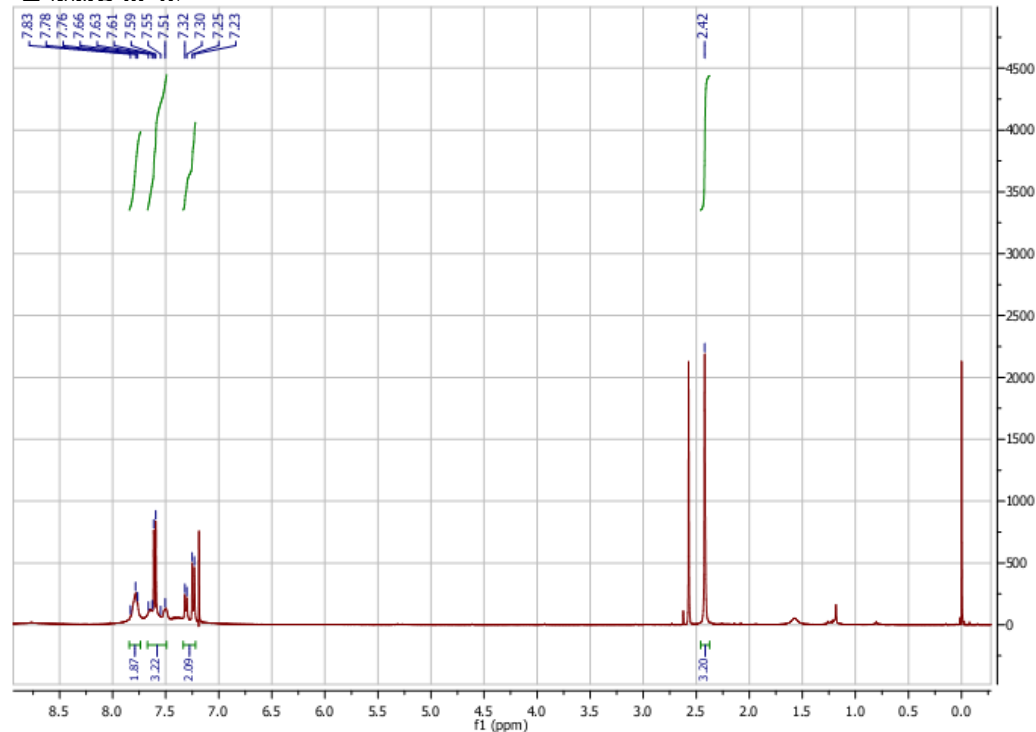
¹³C NMR of 2b

C12H7ClN2
Exact Mass: 214.03
Mol. Wt.: 214.65

LC-MS of 2b

MS Spectrum



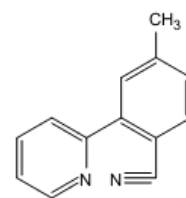
¹H NMR of 2c

¹H NMR (400 MHz, cdcl₃) δ 7.76 – 7.83 (m, 2H), 7.51 – 7.66 (m, 3H), 7.23 – 7.32 (m, 2H), 2.42 (s, 3H).

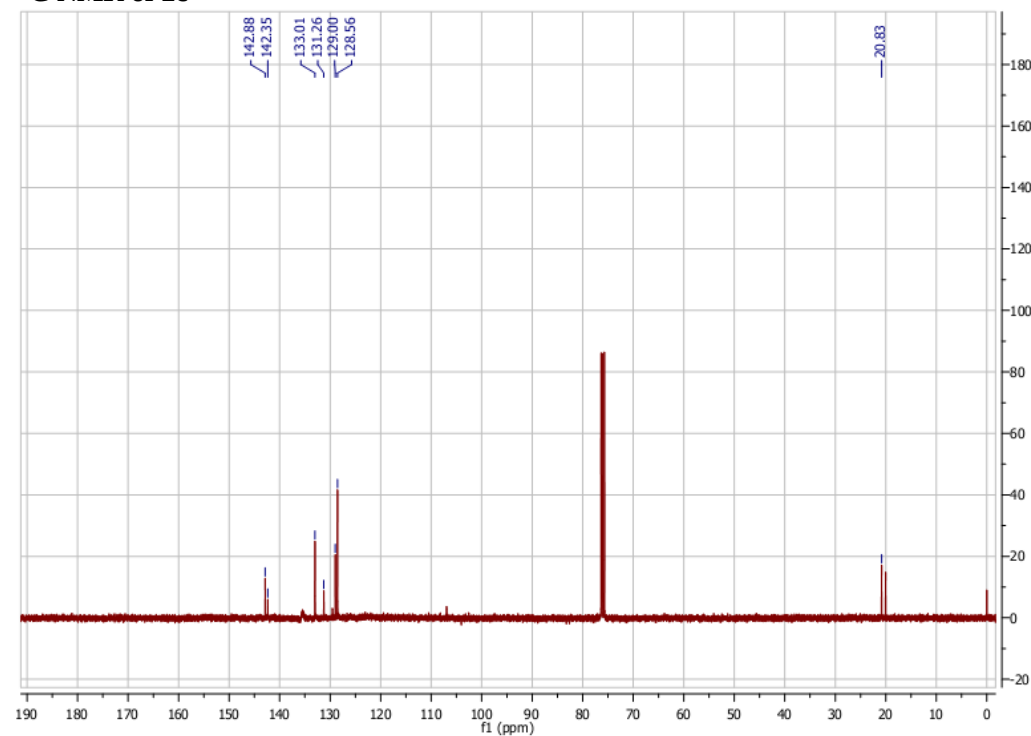
Hutchison Medi Pharma

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 PULPROG: s2pul
 TE: 34 C
 NS: 32
 SFOL: 399.59 MHz
 SWH: 6410.3 Hz
 NUC: 1H
 TD: 13132

F2 - Processing Parameters
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 Phase: Manual
 Ph0: -159.27
 Ph1: 9.76



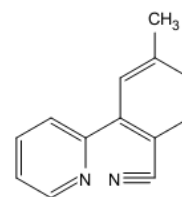
C13H10N2
 Exact Mass: 194.08
 Mol. Wt.: 194.23

¹³C NMR of 2c

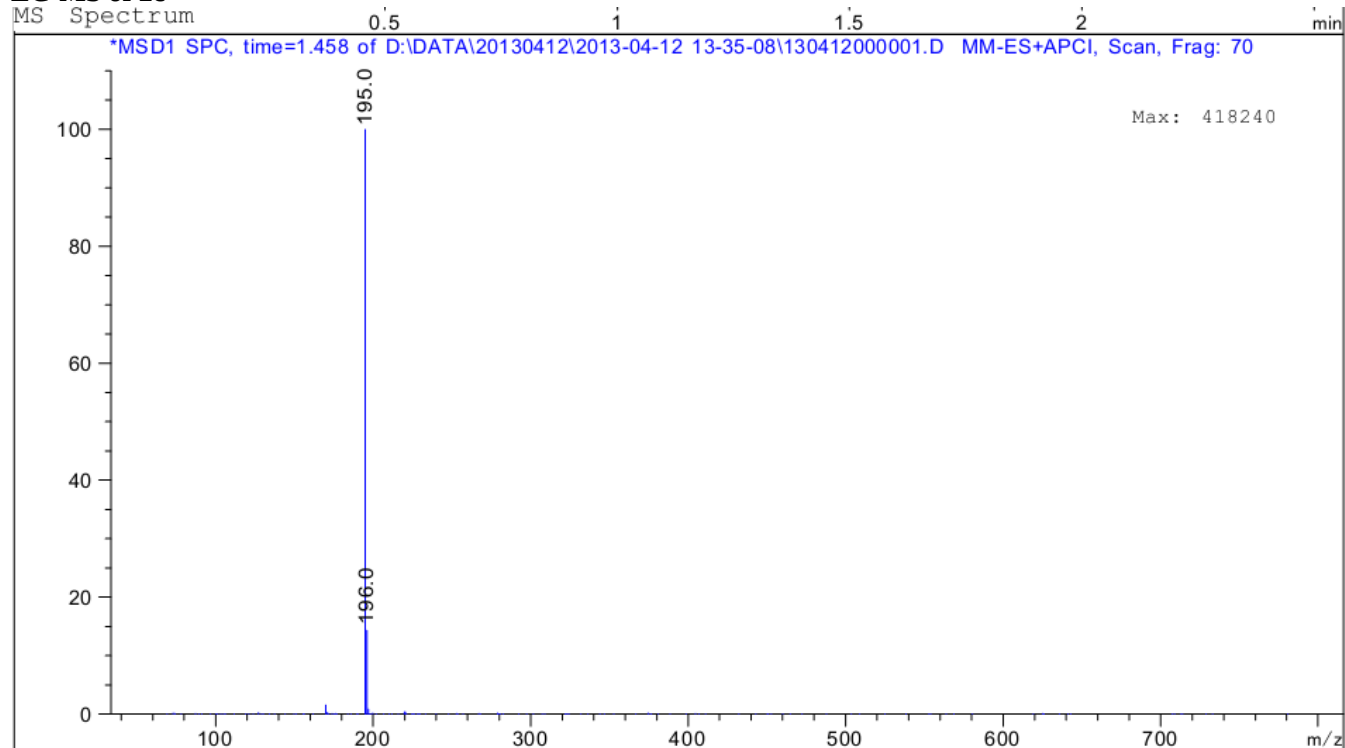
Hutchison Medi Pharma

Acquisition Parameters
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 Origin: vnmrs
 Owner: jrhong
 DATE: 2013-04-16T12:50:45
 Solvent: cdcl3
 PULPROG: s2pul
 TE: 34 C
 NS: 768
 SFOL: 100.49 MHz
 SWH: 24509.8 Hz
 NUC: 13C
 TD: 31875

F2 - Processing Parameters
 SI: 65536
 DC: 0.05
 LB: 0.50 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: -5.08
 Ph1: 48.61



MS Spectrum



¹H NMR spectrum of compound 10a in CDCl₃. The spectrum shows several peaks in the aromatic region (7.0-8.8 ppm) and a small peak in the aliphatic region (1.0 ppm). Integration values are provided below the peaks.

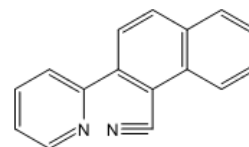
Chemical Shift (ppm)	Integration
8.77	1.00
8.32	0.91
8.32	1.05
8.07	1.03
7.68	0.95
7.57	0.94
7.34	0.95
7.33	
7.31	
1.0	

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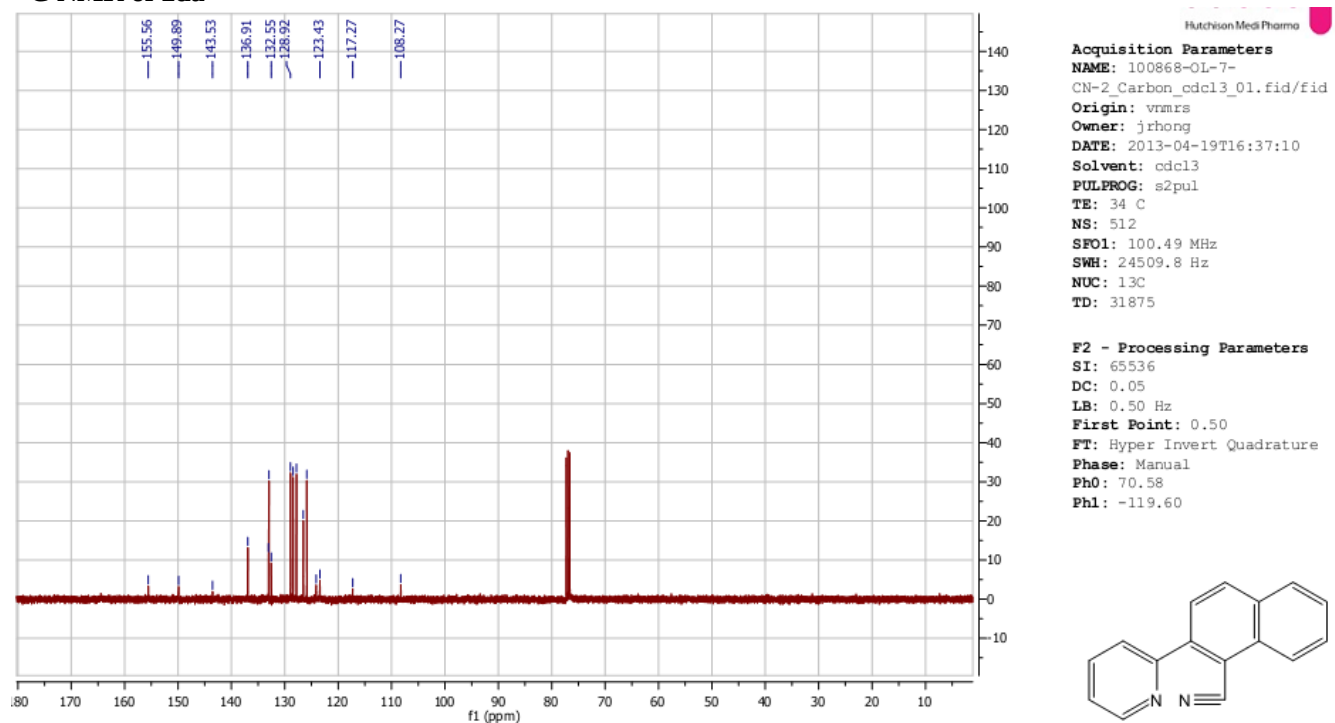
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Origin: vnmrs
Owner: jrhong
DATE: 2013-04-19T01:06:37
Solvent: cdc13
PULPROG: s2pul
TE: 34 C
NS: 8
SF01: 399.59 MHz
SWH: 6410.3 Hz
NUC: 1H
TD: 13132

F2 - Processing Parameters
SI: 32768
DC: 0.05
LB: 0.00 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: -149.03
Ph1: 0.00

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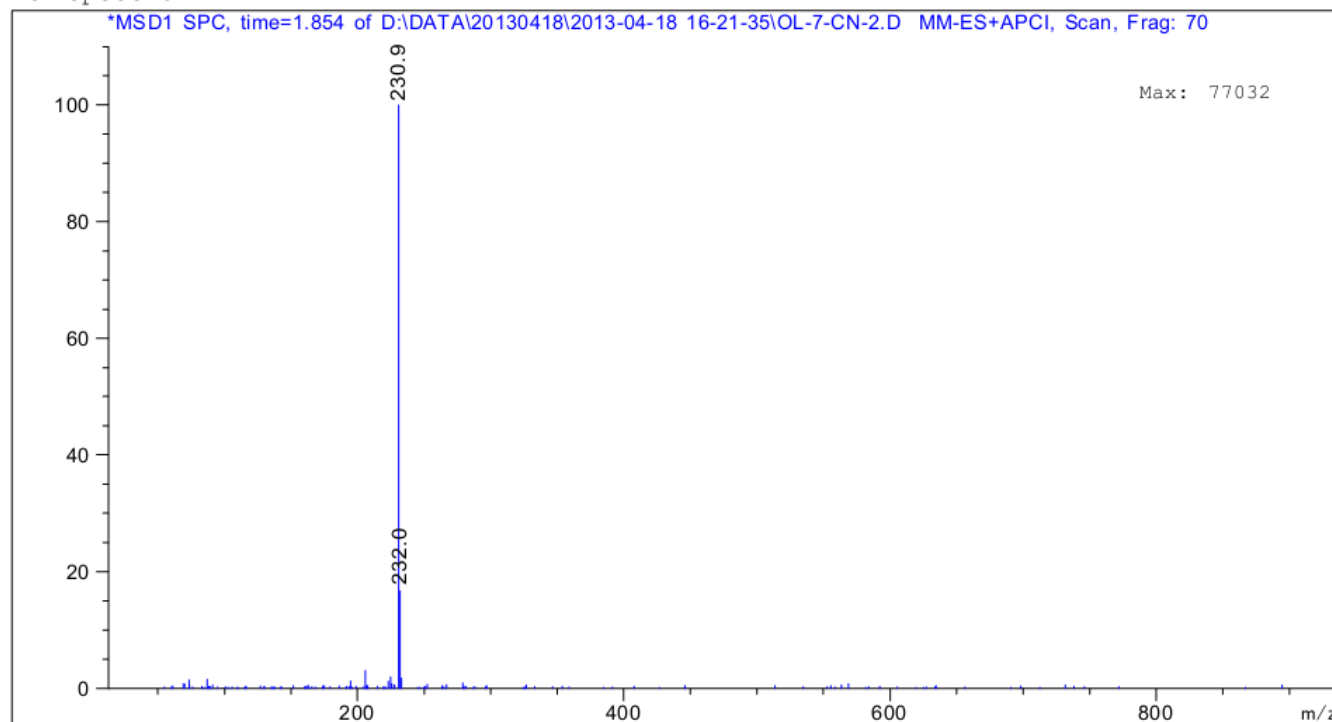


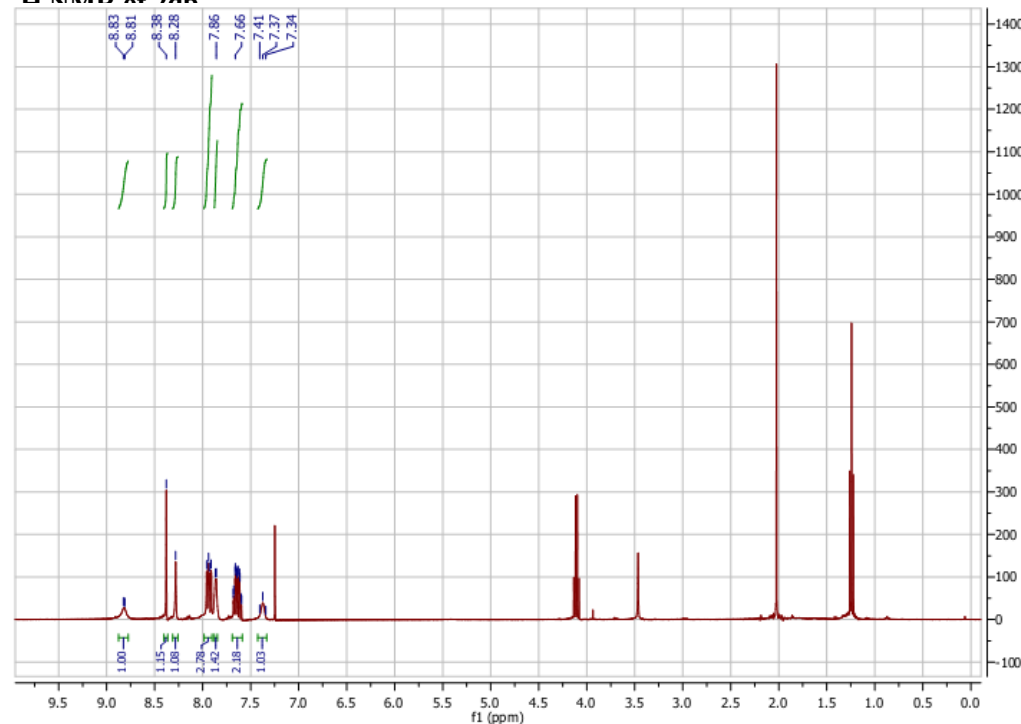
C₁₆H₁₀N₂
Exact Mass: 230.08
Mol. Wt.: 230.26

¹³C NMR of 2da

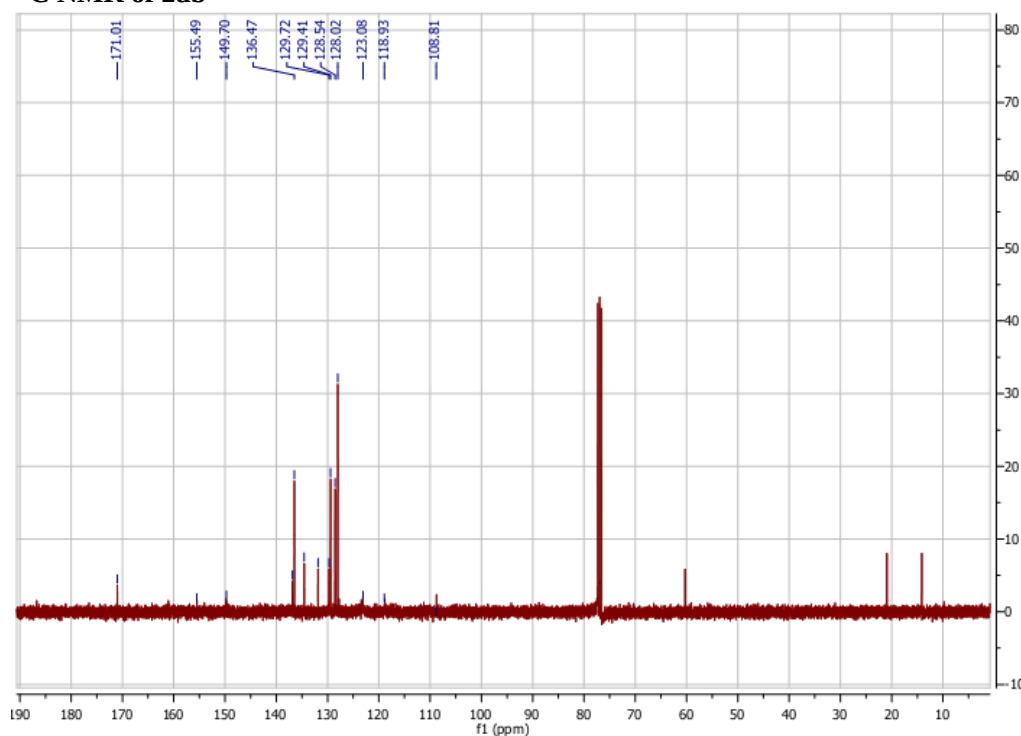
LC-MS of 2da

MS Spectrum



¹H NMR of 2ab

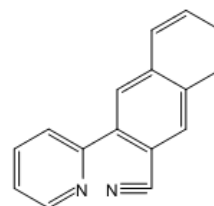
¹H NMR (400 MHz, cdcl₃) δ 8.82 (d, *J* = 4.8 Hz, 1H), 8.38 (s, 1H), 8.28 (s, 1H), 7.91 - 7.96 (m, 3H), 7.86 - 7.87 (m, 2H), 7.59 - 7.66 (m, 2H), 7.34 - 7.41 (m, 1H).

¹³C NMR of 2db

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Acquisition Parameters
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 Origin: vmrs
 Owner: jrhong
 DATE: 2013-04-19T01:02:47
 Solvent: cdcl3
 PULPROG: s2pul
 TE: 34 C
 NS: 8
 SFO1: 399.59 MHz
 SWH: 6410.3 Hz
 NUC: 1H
 TD: 13132

F2 - Processing Parameters
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 LB: 0.00 Hz
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 FT: Hyper Invert Quadrature
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 Ph1: -23.51

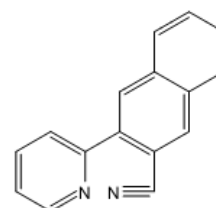


C16H10N2
 Exact Mass: 230.08
 Mol. Wt.: 230.26

Hutchison Medi Pharma

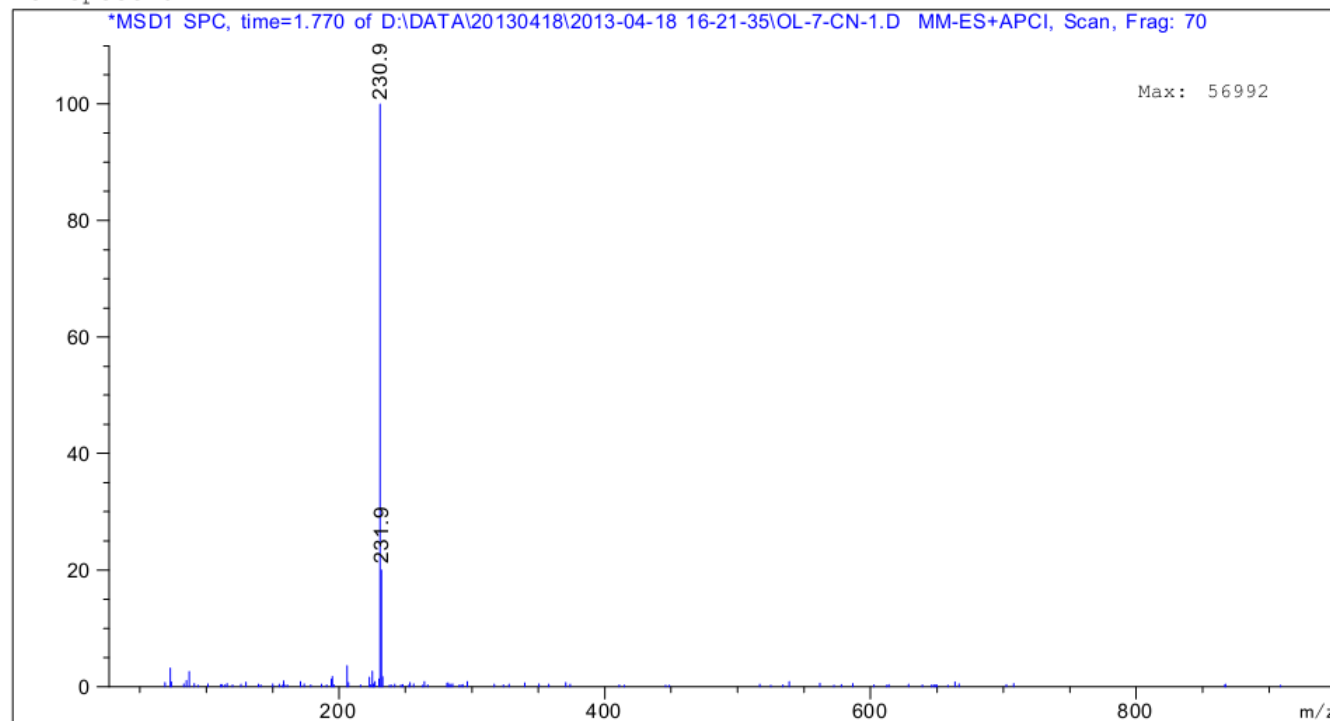
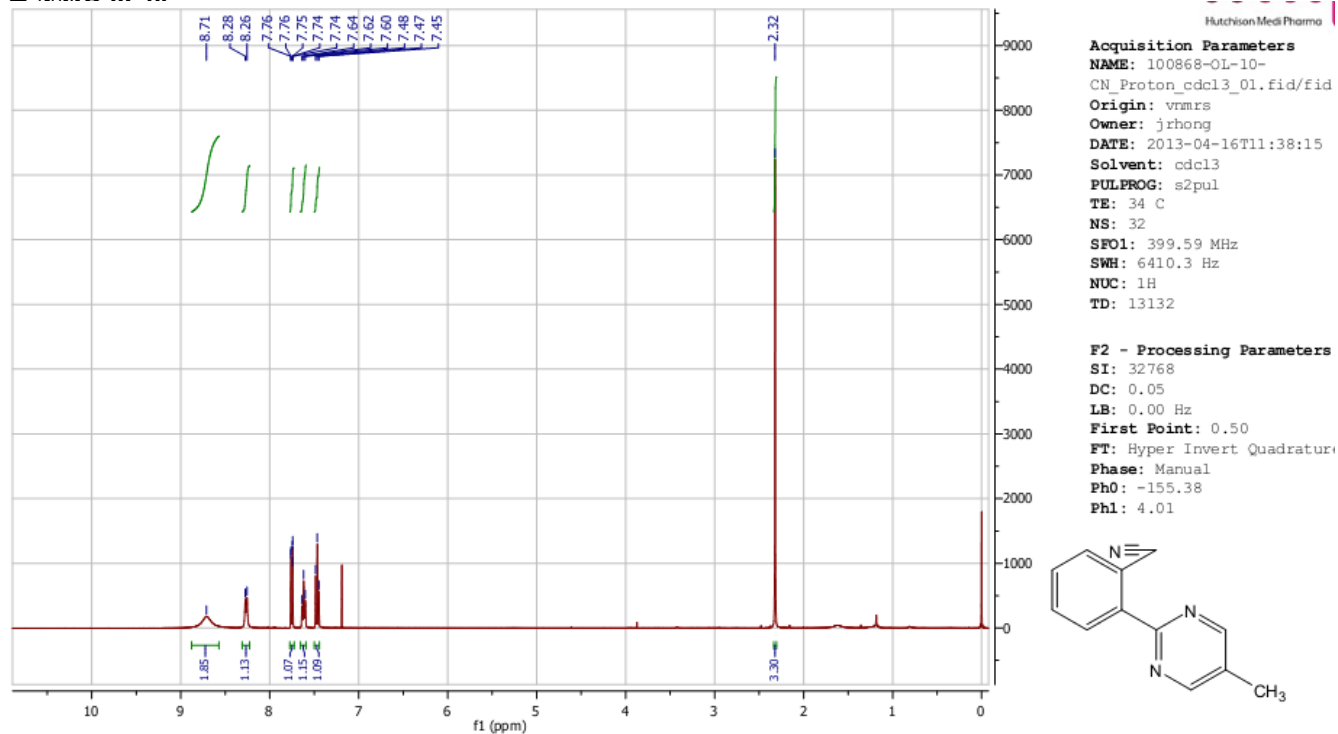
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 Owner: jrhong
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 Solvent: cdcl3
 PULPROG: s2pul
 TE: 34 C
 NS: 512
 SFO1: 100.49 MHz
 SWH: 24509.8 Hz
 NUC: 13C
 TD: 31875

F2 - Processing Parameters
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 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: -8.27
 Ph1: 31.85



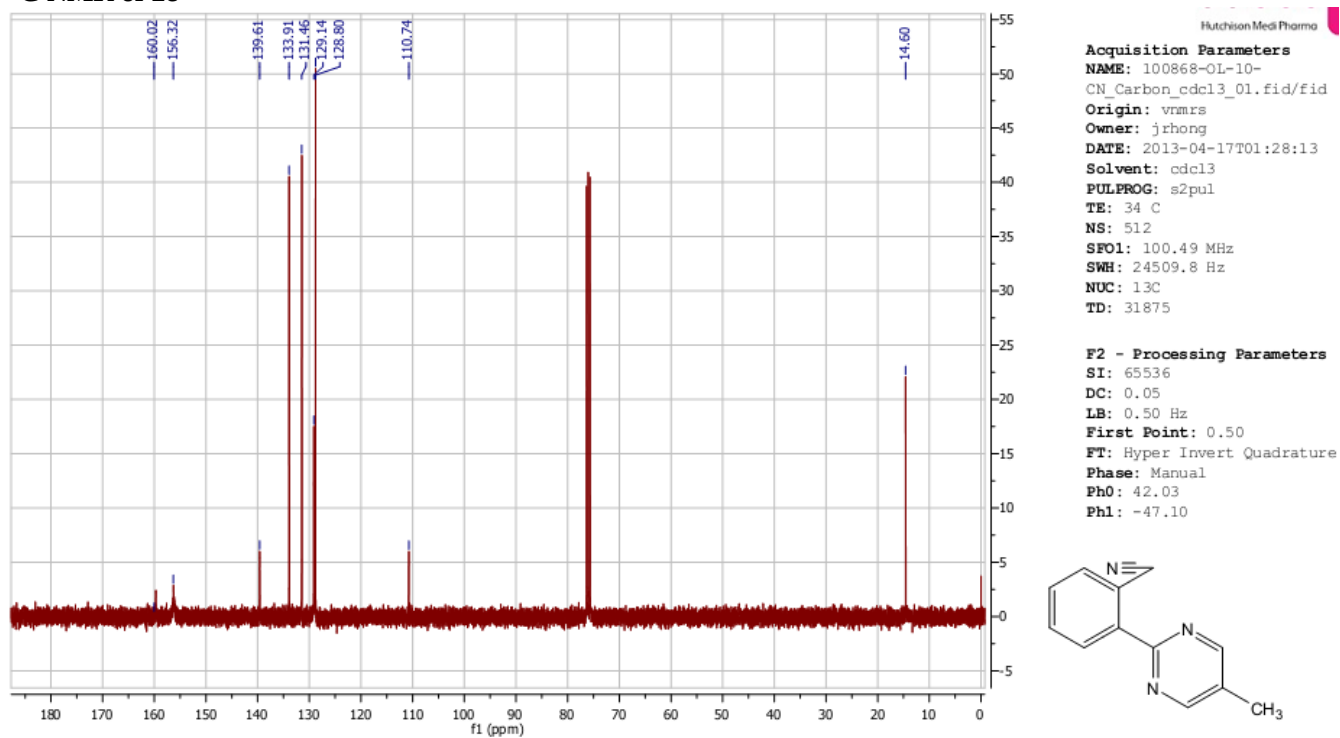
LC-MS of 2db

MS Spectrum

¹H NMR of 2db

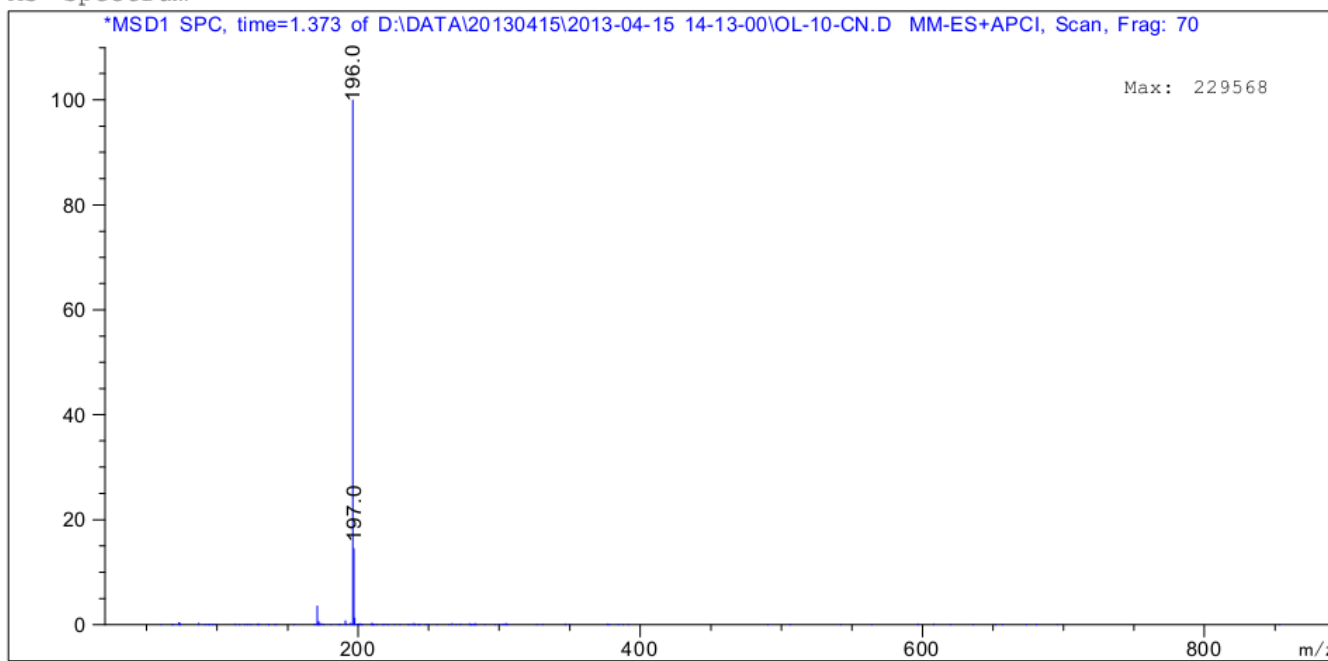
¹H NMR (400 MHz, cdcl₃) δ 8.71 (s, 2H), 8.27 (d, *J* = 7.8, 1H), 7.74–7.76 (m, 1H), 7.60–7.62 (m, 1H), 7.45–7.48 (m, 1H), 2.32 (s, 3H).

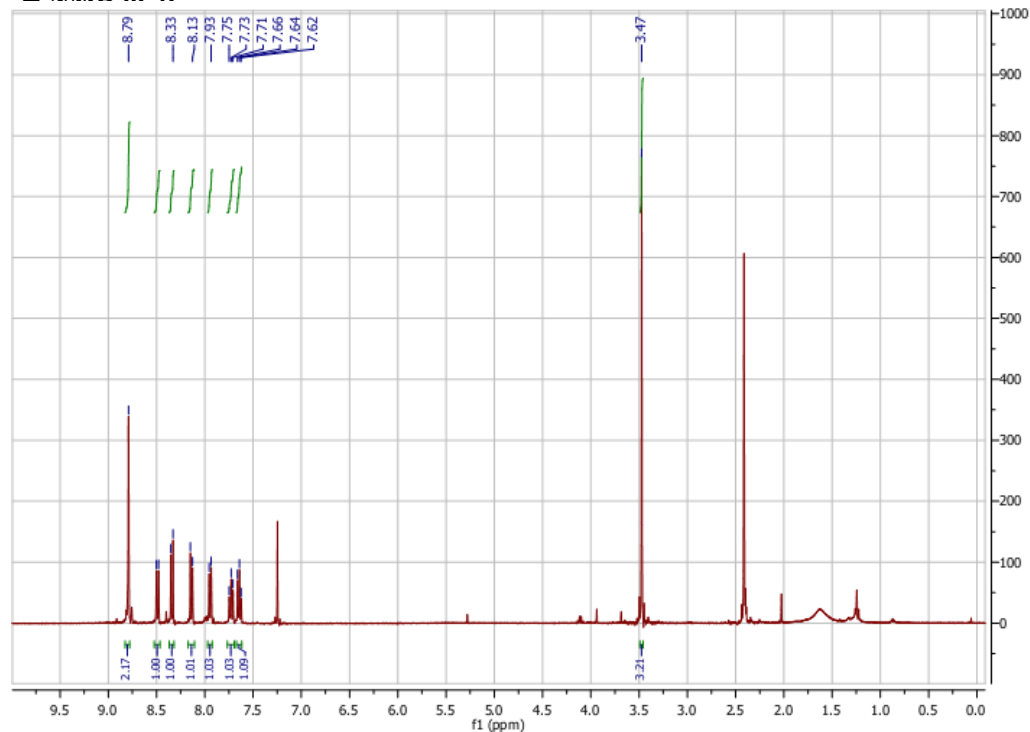
C₁₂H₉N₃
Exact Mass: 195.08
Mol. Wt.: 195.22

¹³C NMR of 2e

LC-MS of 2e

MS Spectrum



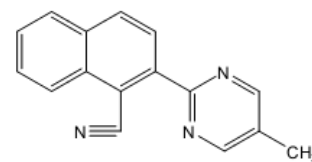
¹H NMR of 2f

¹H NMR (400 MHz, cdcl₃) δ 8.79 (s, 2H), 8.49 (d, *J* = 8.5 Hz, 1H), 8.34 (d, *J* = 8.7 Hz, 1H), 8.14 (d, *J* = 8.8 Hz, 1H), 7.94 (d, *J* = 8.2 Hz, 1H), 7.73 (t, *J* = 7.5 Hz, 1H), 7.64 (t, *J* = 7.5 Hz, 1H), 3.47 (s, 3H).

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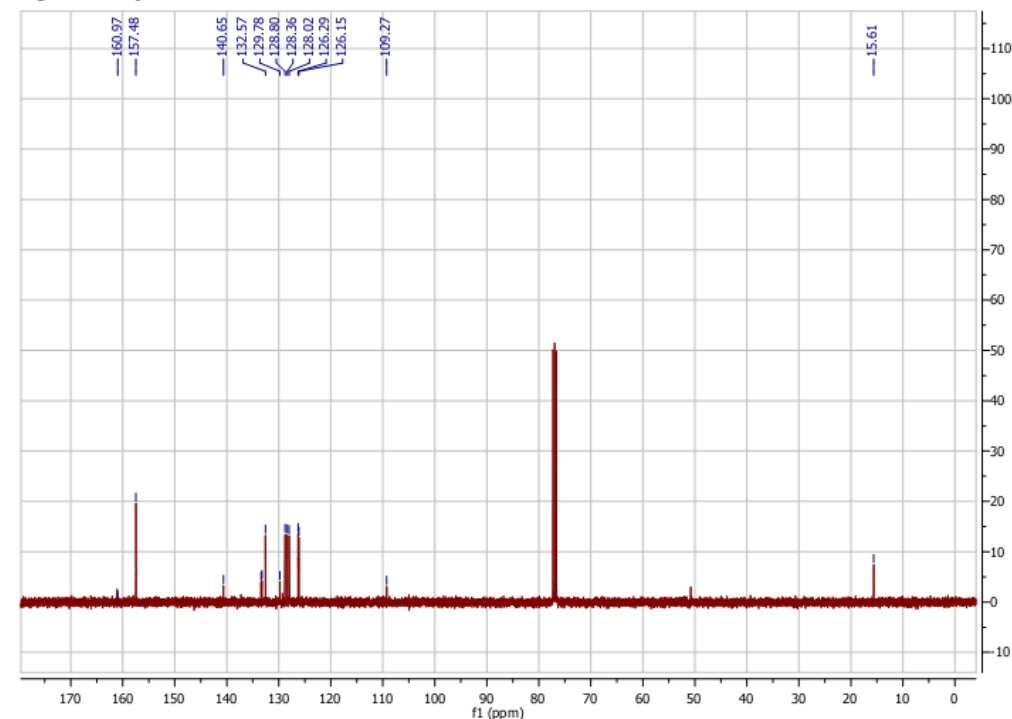
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 DATE: 2013-04-19T01:10:27
 Solvent: cdcl3
 PULPROG: s2pul
 TE: 34 C
 NS: 8
 SFO1: 399.59 MHz
 SWH: 6410.3 Hz
 NUC: 1H
 TD: 13132

F2 - Processing Parameters
 SI: 32768
 DC: 0.05
 LB: 0.00 Hz
 First Point: 0.50
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 Phase: Manual
 Ph0: -142.11
 Ph1: -14.21

C₁₆H₁₁N₃

Exact Mass: 245.1

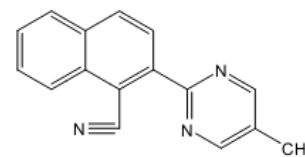
Mol. Wt.: 245.28

¹³C NMR of 2f

Hutchison Medi Pharma

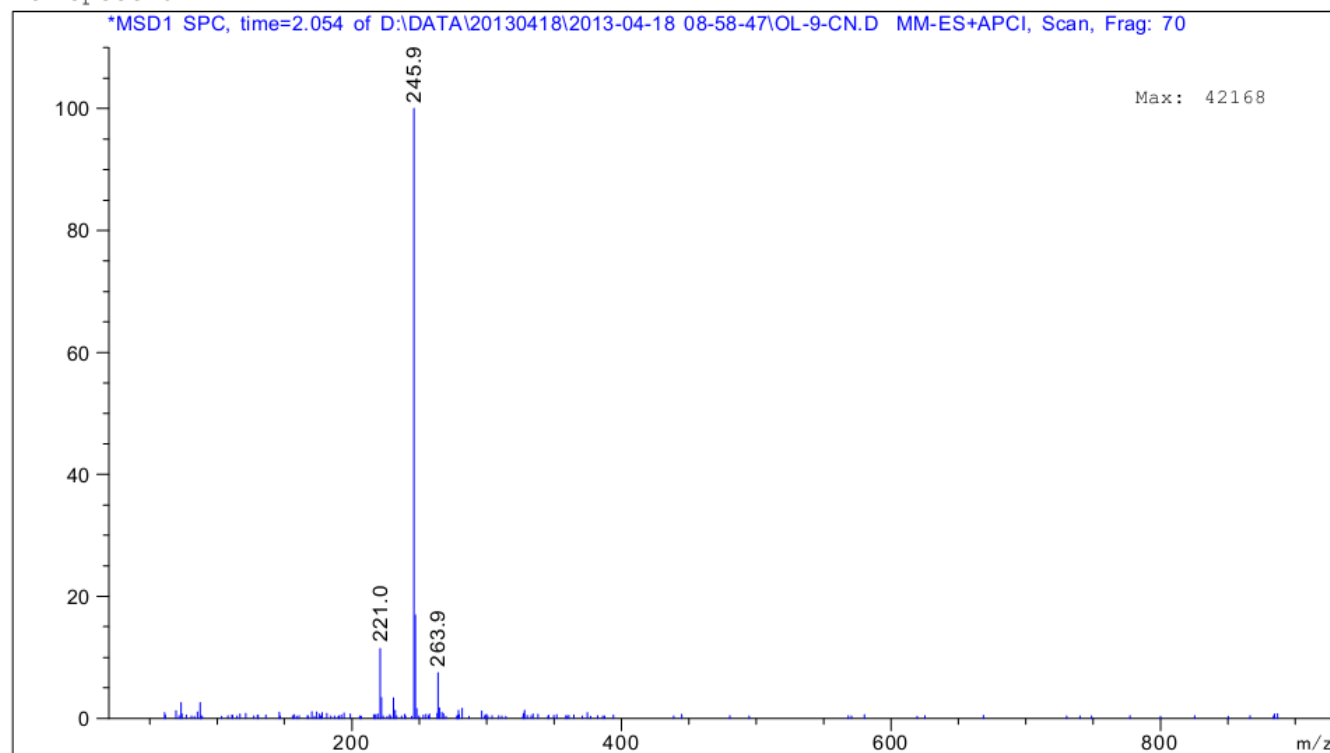
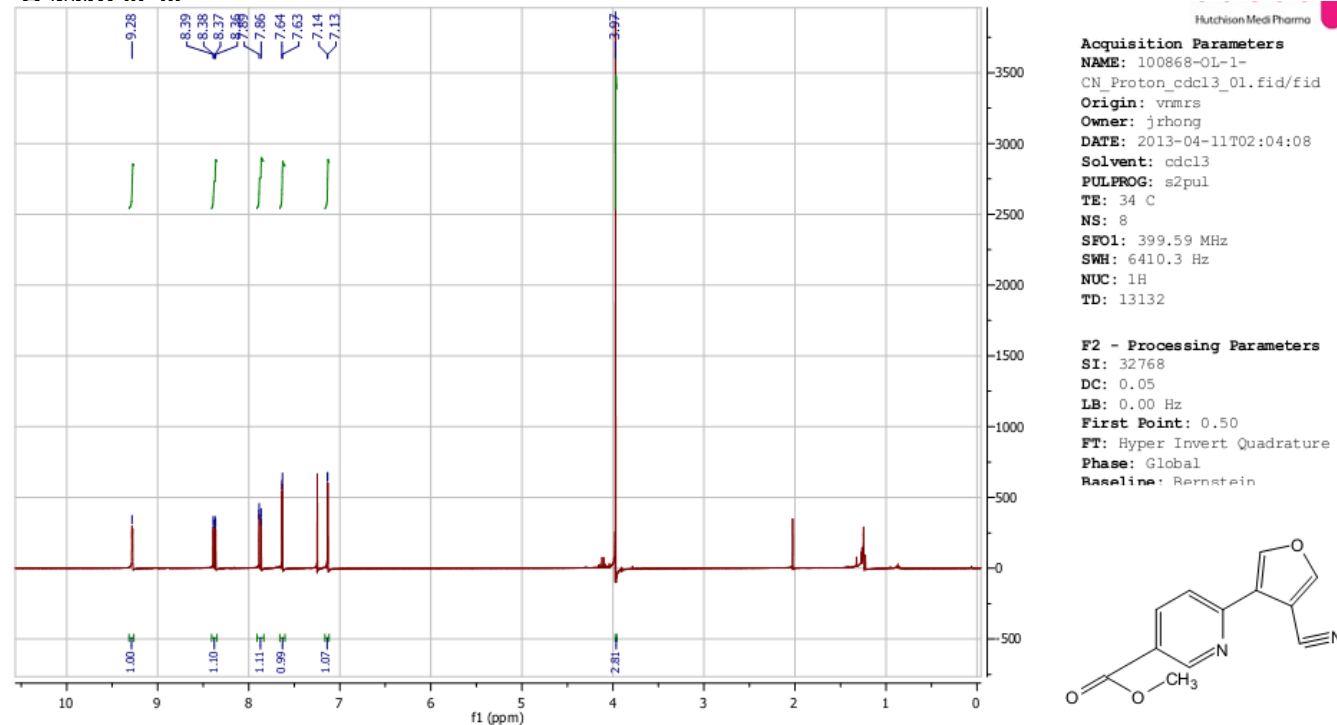
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 DATE: 2013-04-19T02:16:06
 Solvent: cdcl3
 PULPROG: s2pul
 TE: 34 C
 NS: 512
 SFO1: 100.49 MHz
 SWH: 24509.8 Hz
 NUC: 13C
 TD: 31875

F2 - Processing Parameters
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 Ph1: -15.08



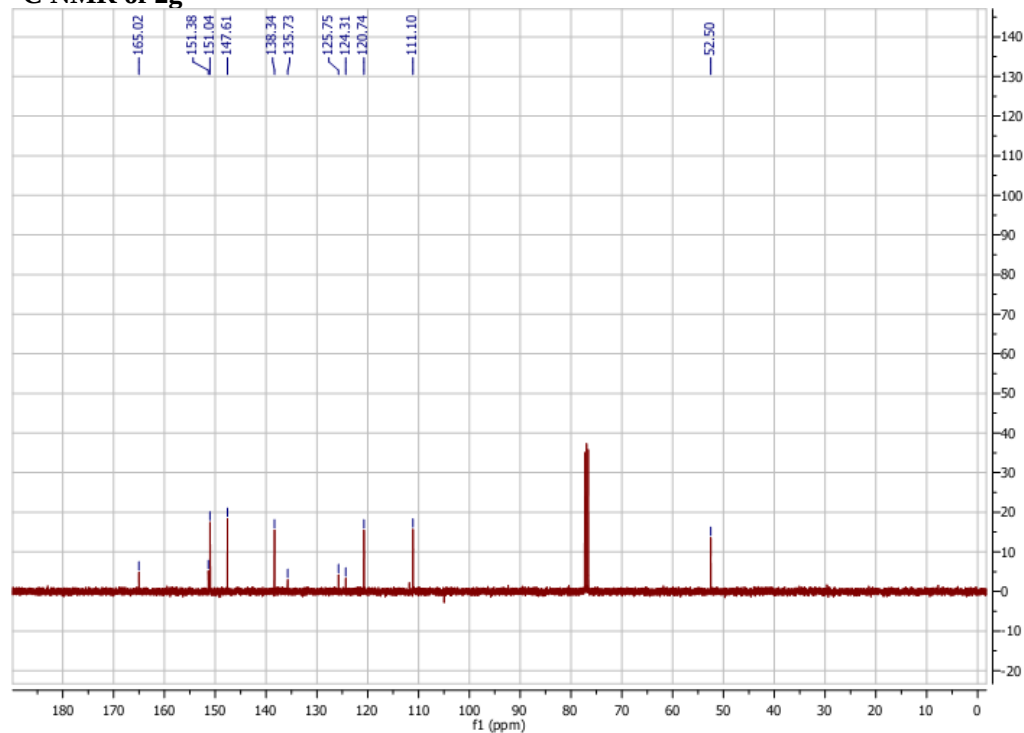
LC-MS of 2f

MS Spectrum

¹H NMR of 2f

¹H NMR (400 MHz, cdcl₃) δ 9.28 (s, 1H), 8.36 - 8.38 (m, 1H), 7.86 - 7.89 (m, 1H), 7.63 (d, *J* = 4.0 Hz, 1H), 7.13 (d, *J* = 4.0 Hz, 1H), 3.97 (s, 3H).

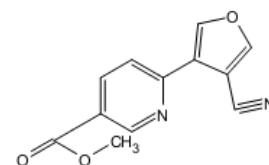
C12H8N2O3
Exact Mass: 228.05
Mol. Wt.: 228.2

¹³C NMR of 2g

Hutchison MediPharm

Acquisition Parameters
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Owner: jrhong
DATE: 2013-04-11T16:07:55
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NUC: 13C
TD: 31875

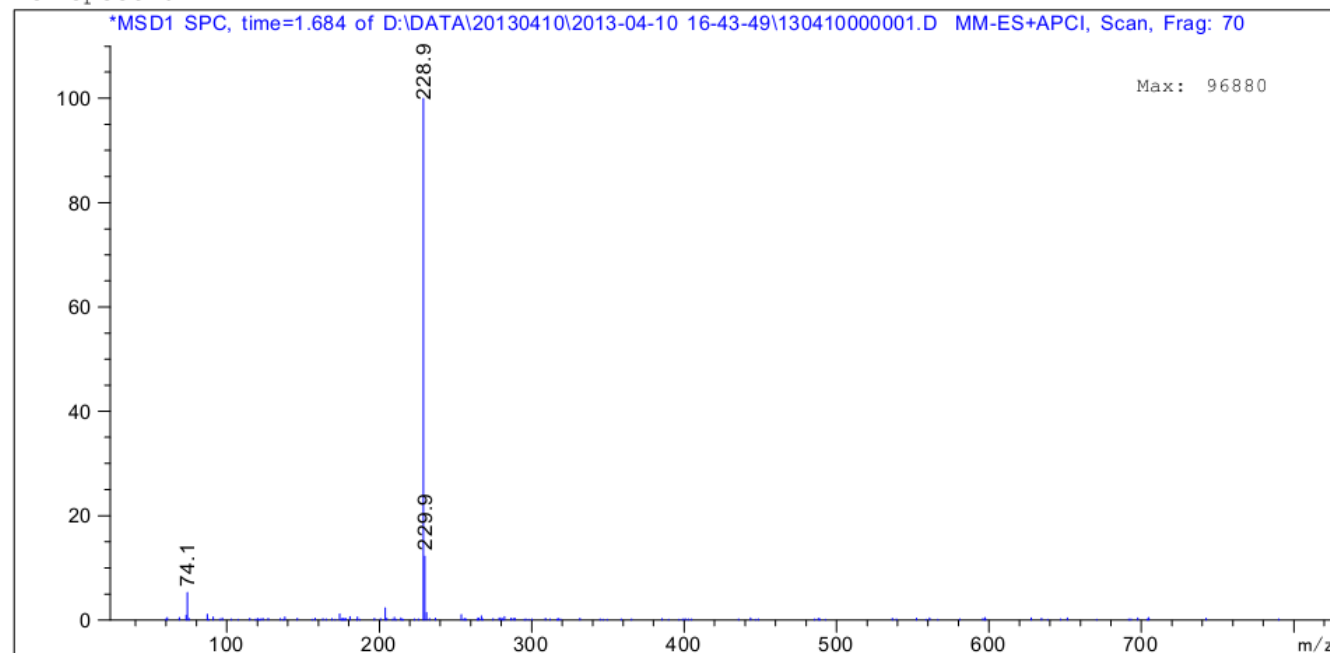
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Ph1: 0.00

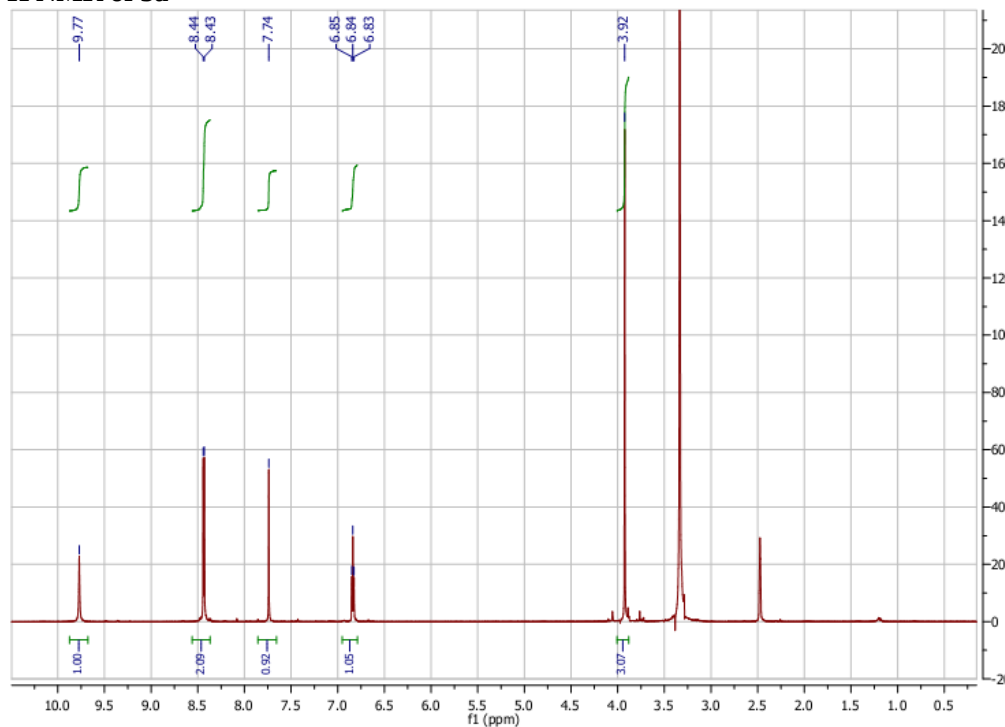


C12H8N2O3
Exact Mass: 228.05
Mol. Wt.: 228.2

LC-MS of 2g

MS Spectrum

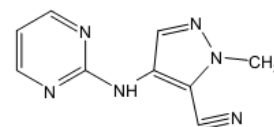


¹H NMR of 3a

¹H NMR (400 MHz, dmsO) δ 9.77 (s, 1H), 8.44 (d, J = 4.8, 2H), 7.74 (s, 1H), 6.84 (t, J = 4.8, 1H), 3.92 (s, 3H).

Hutchison Medi Pharma
Acquisition Parameters
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Origin: vmrs
Owner: jrhong
DATE: 2012-12-05T01:20:48
Solvent: dmsO
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SWH: 6410.3 Hz
NUC: 1H
TD: 13132

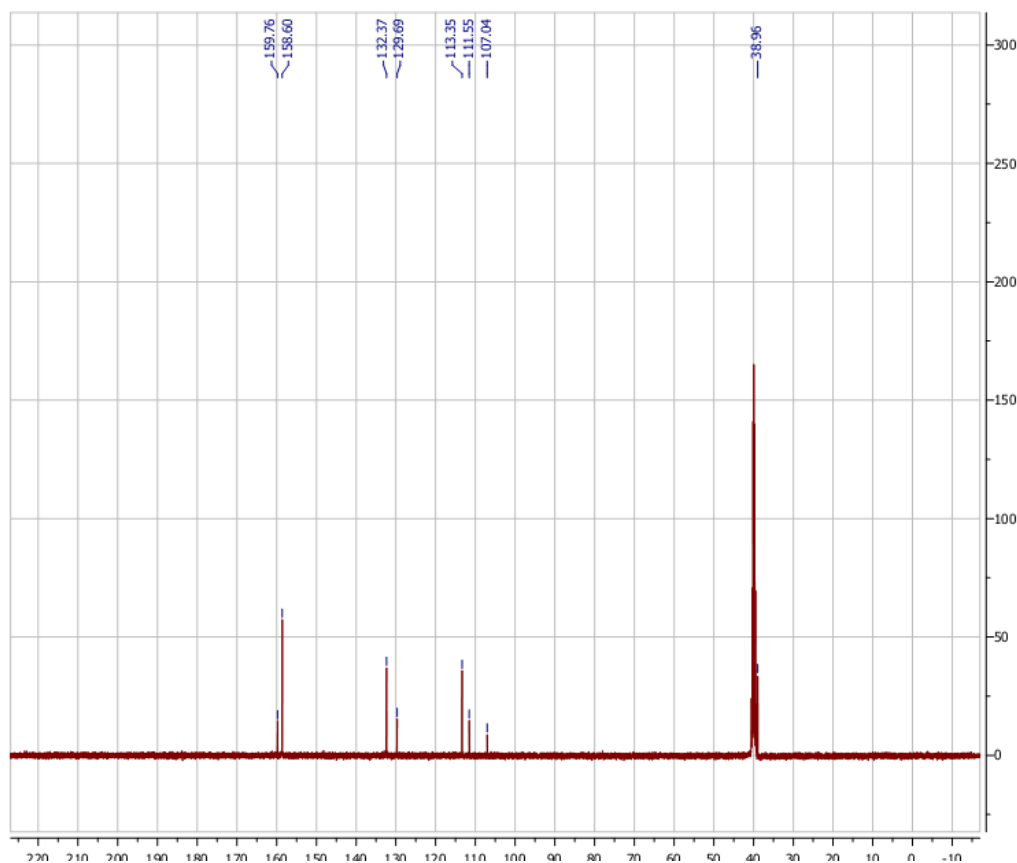
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Ph1: -4.93



C₉H₈N₆

Exact Mass: 200.08

Mol. Wt.: 200.2

¹³C NMR of 3a

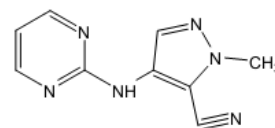
Hutchison Medi Pharma

Acquisition Parameters

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DATE: 2012-12-05T01:32:57
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SWH: 24509.8 Hz
NUC: 13C
TD: 31875

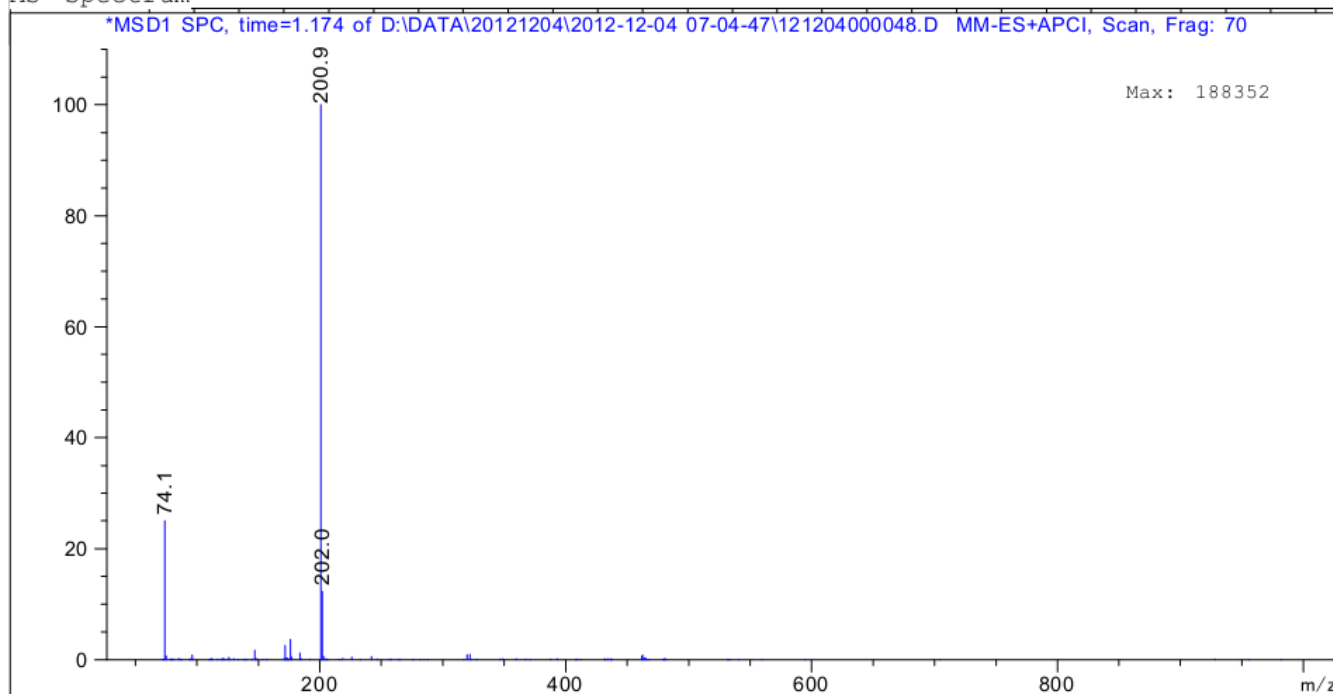
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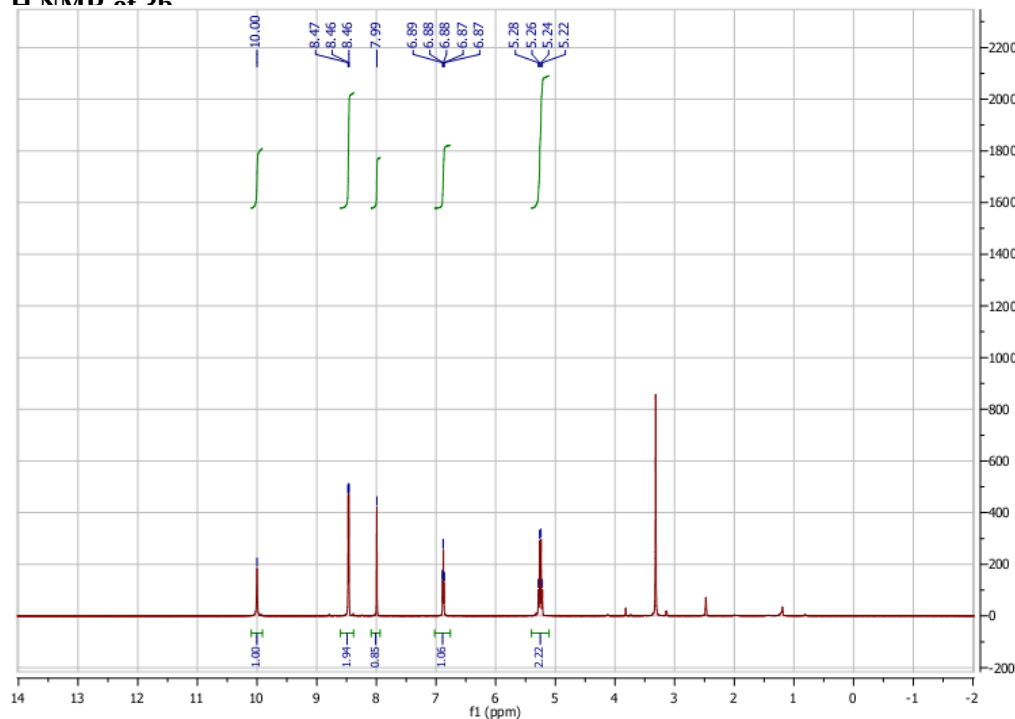
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C₉H₈N₆

Exact Mass: 200.08

Mol. Wt.: 200.2

LC-MS of 3a
MS Spectrum

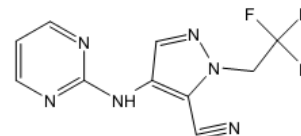
¹H NMR of 2b

¹H NMR (400 MHz, dmsol) δ 10.00 (s, 1H), 8.47 (dd, *J* = 4.8, 1.0, 2H), 7.99 (s, 1H), 6.87 - 6.89 (m, 1H), 5.22 - 5.28 (m, 2H).

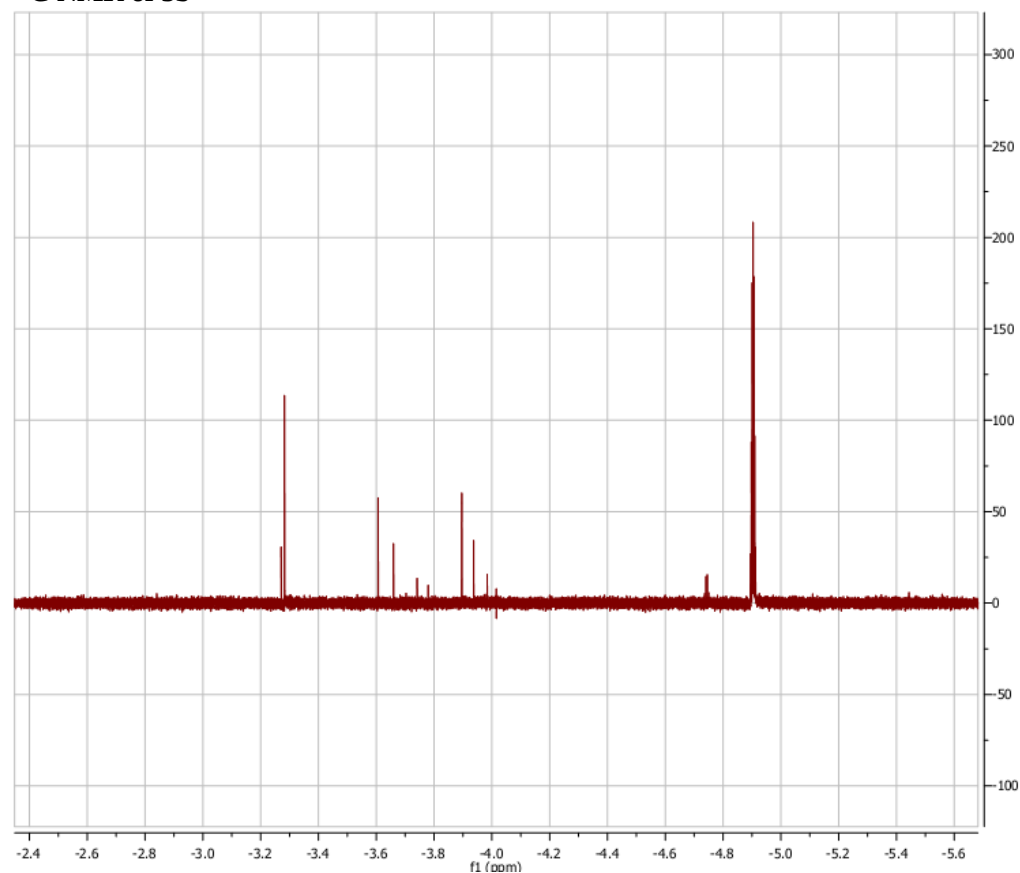
Hutchison Medi Pharma

Acquisition Parameters
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Owner: jrhong
DATE: 2013-01-15T01:05:47
Solvent: dmsol
PULPROG: s2pul
TE: 30 C
NS: 8
SFOL: 399.6 Mhz
SWH: 6410.3 Hz
NUC: 1H
TD: 13132

F2 - Processing Parameters
SI: 32768
DC: 0.05
LB: 0.00 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: -52.07
Ph1: -5.11



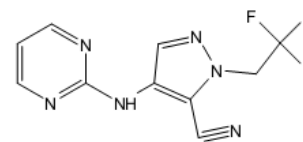
C10H7F3N6
Exact Mass: 268.07
Mol. Wt.: 268.2

¹³C NMR of 3b

Hutchison Medi Pharma

Acquisition Parameters
NAME: 100868-
ff-18_Carbon_dms0_03.fid/fid
Origin: Varian-NMR:vnms
Owner: jrhong
DATE: 2012-12-22T04:22:17
Solvent:
PULPROG:
TE: 0 C
NS: 0
SF01: 300 MHz
SWH: 1000 Hz
NUC:
TD: 0

F2 - Processing Parameters
SI: 65536
DC: 0.05
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: 188.24
Ph1: 18.63
Baseline: Bernstein



C10H7F3N6
Exact Mass: 268.07
Mol. Wt.: 268.2

Noesy analysis of 3b

100868-ff-18

exp8 Noesy

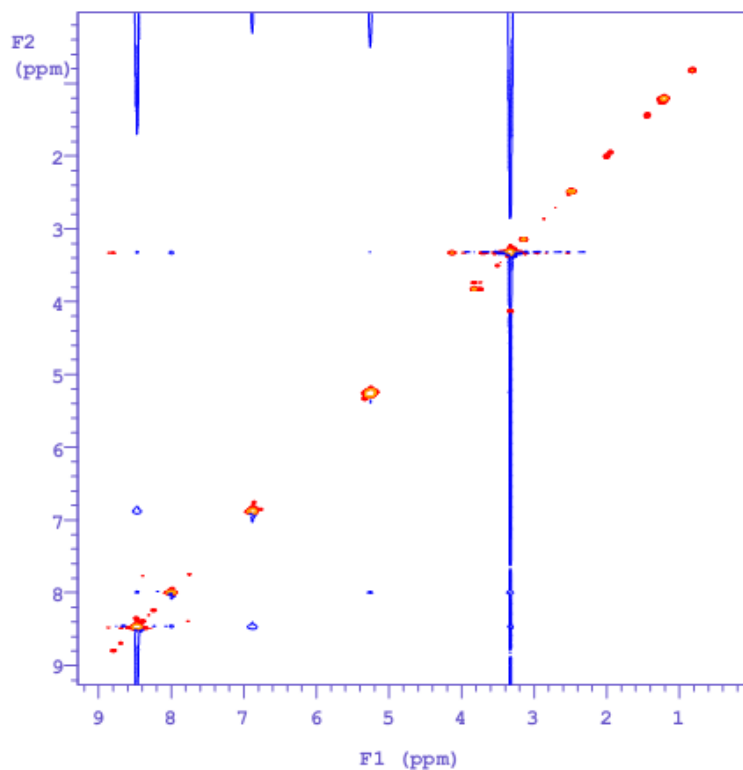
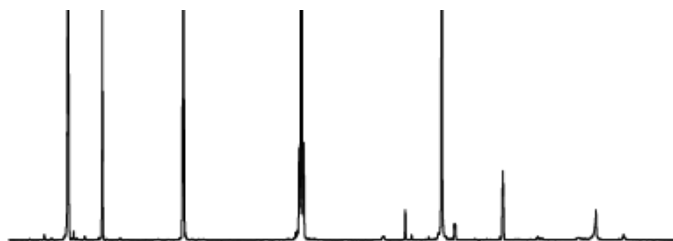
SAMPLE		2D DISPLAY		ACQUISITION ARRAYS	
date	Jan 14 2013	sp1	11.5	array	phase
solvent	dmsc	vp1	3697.0	arraydim	400
file	/home/jrhong/~	sc2	0		
vnarray	/data/10086~	vc2	155	i	phase
8-ff-18_Noesy_dmsc~	rf11	-7.2		1	1
_02_fid	rfp1	0		2	2

ACQUISITION		DEC. & VT	
afrq	399.601	dfreq	100.489
tn	81	dn	C13
at	0.229	dpwr	31
rp	2048	dof	0
sw	4464.3	dm	n
fb	4000	dms	c
bs	32	dmf	29412
as	16	dseq	
tpwr	59	dres	9.0
pw	12.3	homo	n
compfl	1.0680	temp	30.0
dl	1.000	PROCESSING	
nix	1.000	gf	0.106
tof	241.3	gfs	not used
nt	16	wtfile	
ct	16	proc	ft
gain	34	fn	2048
aspul	y	math	f
gt1	0.0025	asf1	not used
gr1vl1	1604	asorder	3
hugt	0.0020	santaps	3
huglvi	1203	2D PROCESSING	
satmode	sum	gf1	0.029
satpwr	-13	gfal	not used
satdly	0	wtfile1	
scuba	n	procl	lp
rqflg	y	fn1	2048
alt_grd	n		

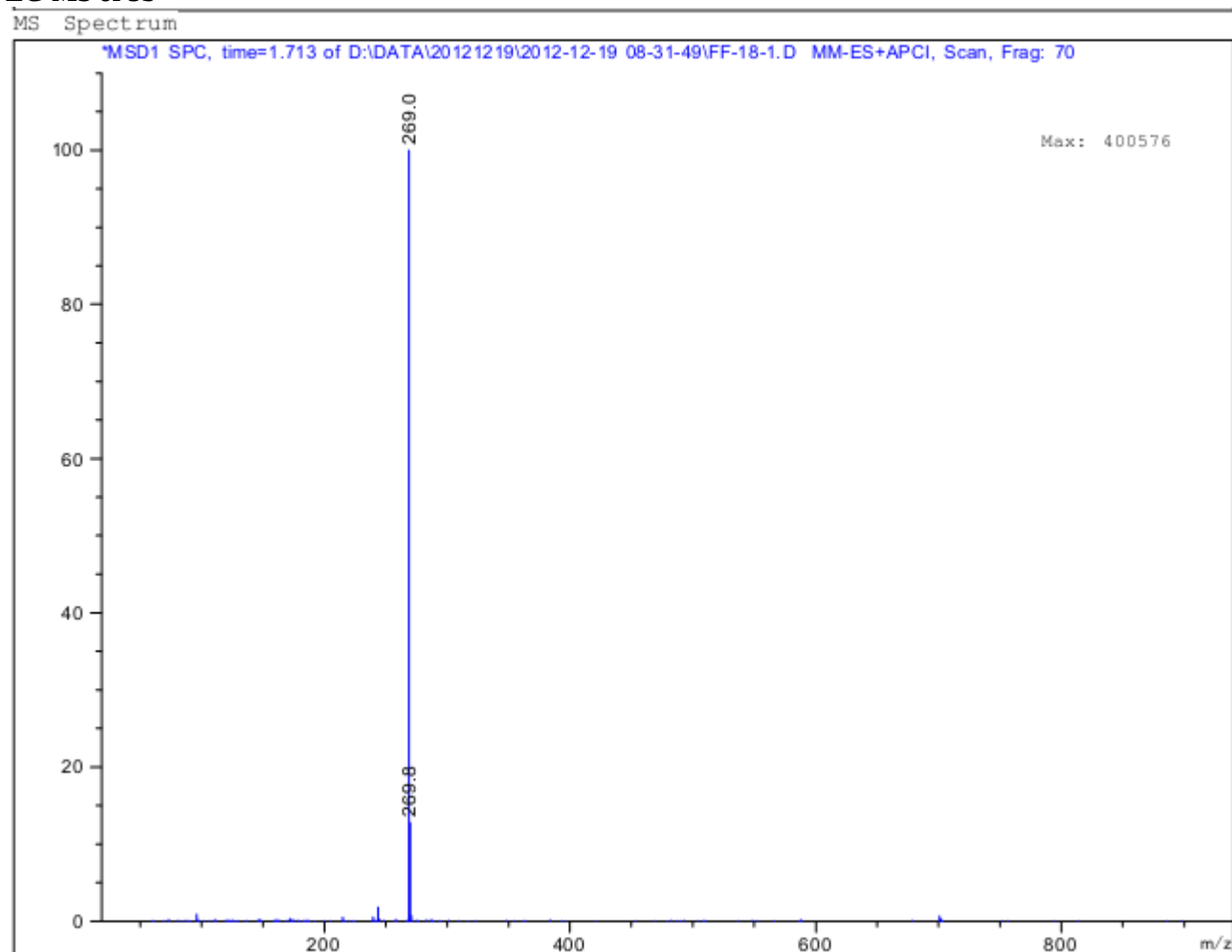
FLAGS	
il	n
in	n
dp	y
hs	nn
aspul	y

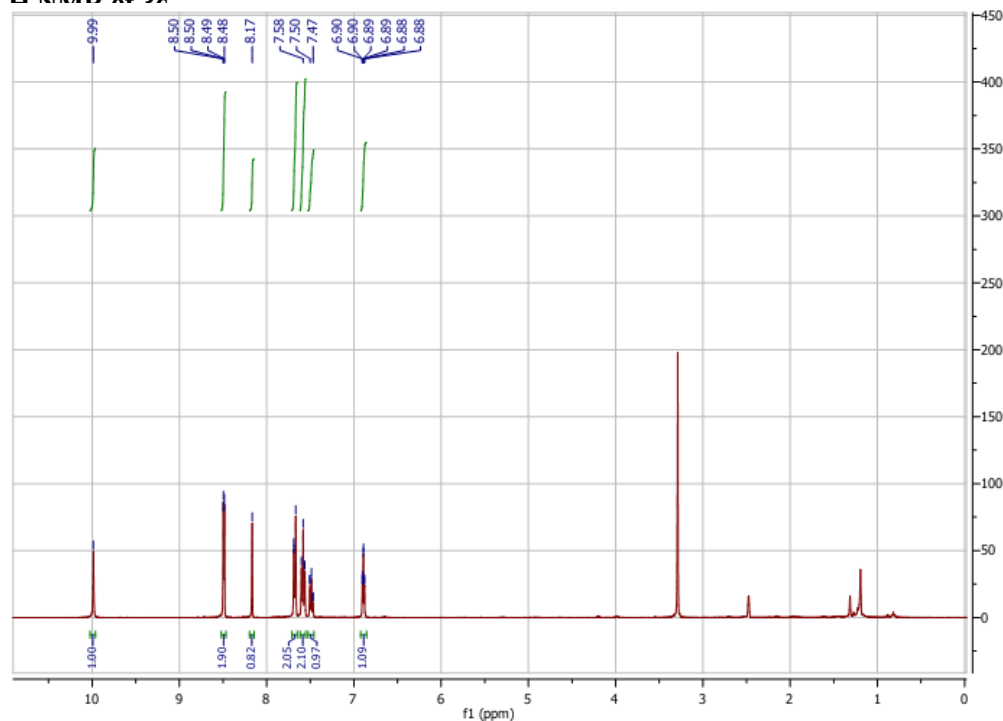
2D ACQUISITION	
sw1	4464.3
ni	200
phase	arrayed

DISPLAY	
sp	11.5
vp	3688.3
vs	5750
sc	0
vc	250
hnm	25.64
is	744.69
rf1	-7.2
rfp	0
th	2
ins	100.000
ai	cdc ph



LC-MS of 3b

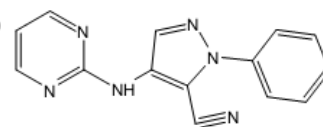


¹H NMR of 2a

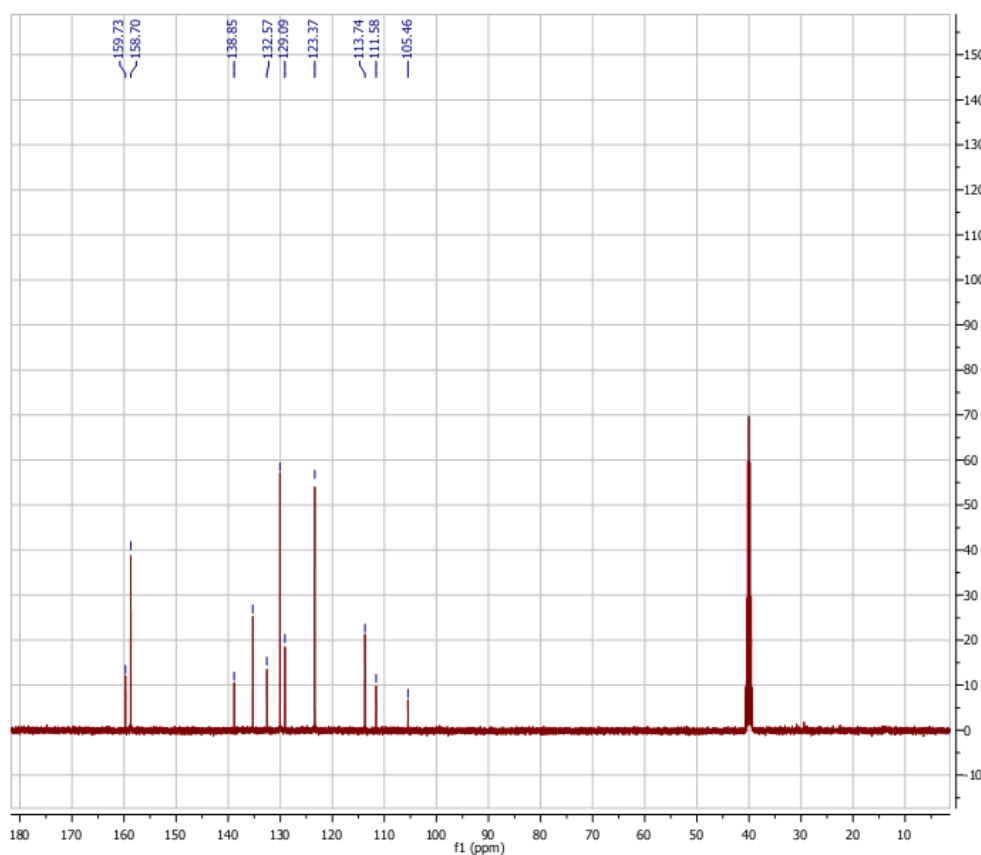
¹H NMR (400 MHz, dmsO) δ 9.99 (s, 1H), 8.48 - 8.50 (m, 2H), 8.17 (s, 1H), 7.67 - 7.69 (m, 2H), 7.56 - 7.60 (m, 2H), 7.47 - 7.51 (m, 1H), 6.88 - 6.90 (m, 1H).

Acquisition Parameters
 NAME: 100868-
 ff-39_Proton_dmsO_02.fid/fid
 Origin: vnmrs
 Owner: jrhong
 DATE: 2013-01-18T01:24:14
 Solvent: dmsO
 PULPROG: s2pul
 TE: 30 C
 NS: 8
 SF01: 399.6 MHz
 SWH: 6410.3 Hz
 NUC: 1H
 TD: 13132

F2 - Processing Parameters
 SI: 32768
 DC: 0.05
 LB: 0.00 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: -52.55
 Ph1: -4.87

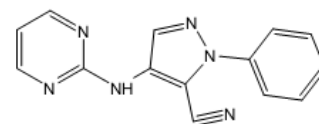


C₁₄H₁₀N₆
 Exact Mass: 262.1
 Mol. Wt.: 262.27

¹³C NMR of 3c

Acquisition Parameters
 NAME: 100868-
 ff-39_Carbon_dmsO_01.fid/fid
 Origin: vnmrs
 Owner: jrhong
 DATE: 2013-01-18T20:08:25
 Solvent: dmsO
 PULPROG: s2pul
 TE: 30 C
 NS: 824
 SF01: 100.49 MHz
 SWH: 24509.8 Hz
 NUC: 13C
 TD: 31875

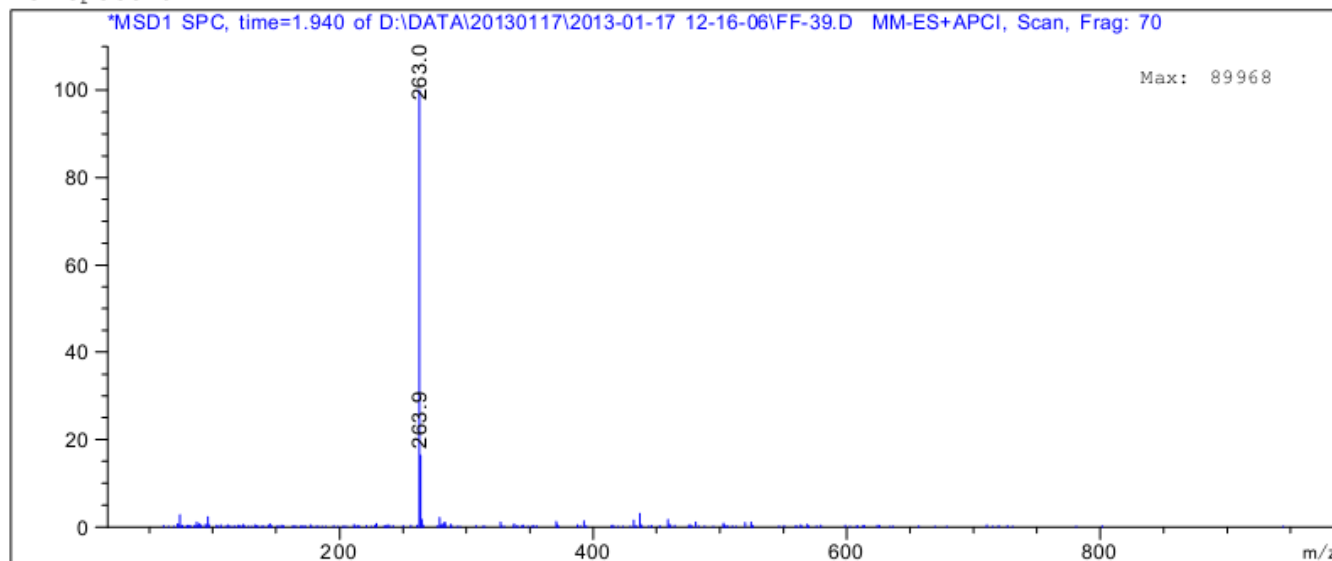
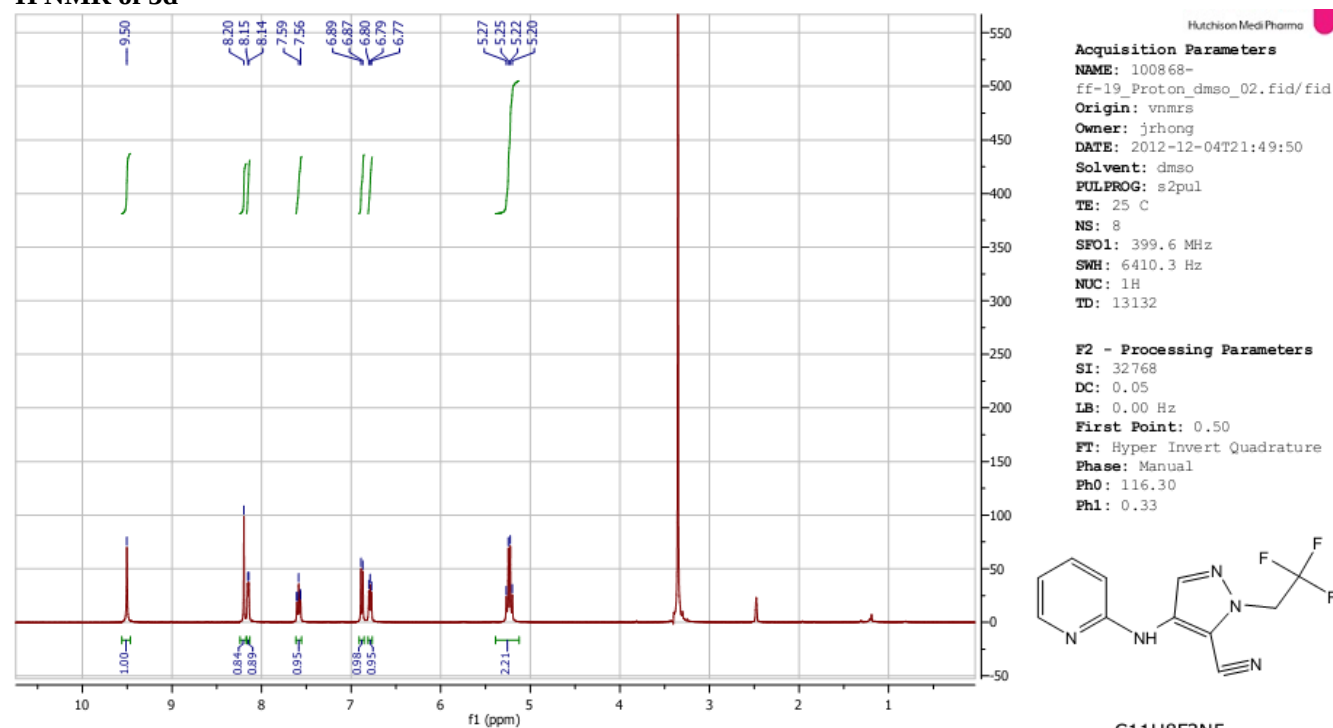
F2 - Processing Parameters
 SI: 65536
 DC: 0.05
 LB: 0.50 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: 155.72
 Ph1: -18.64



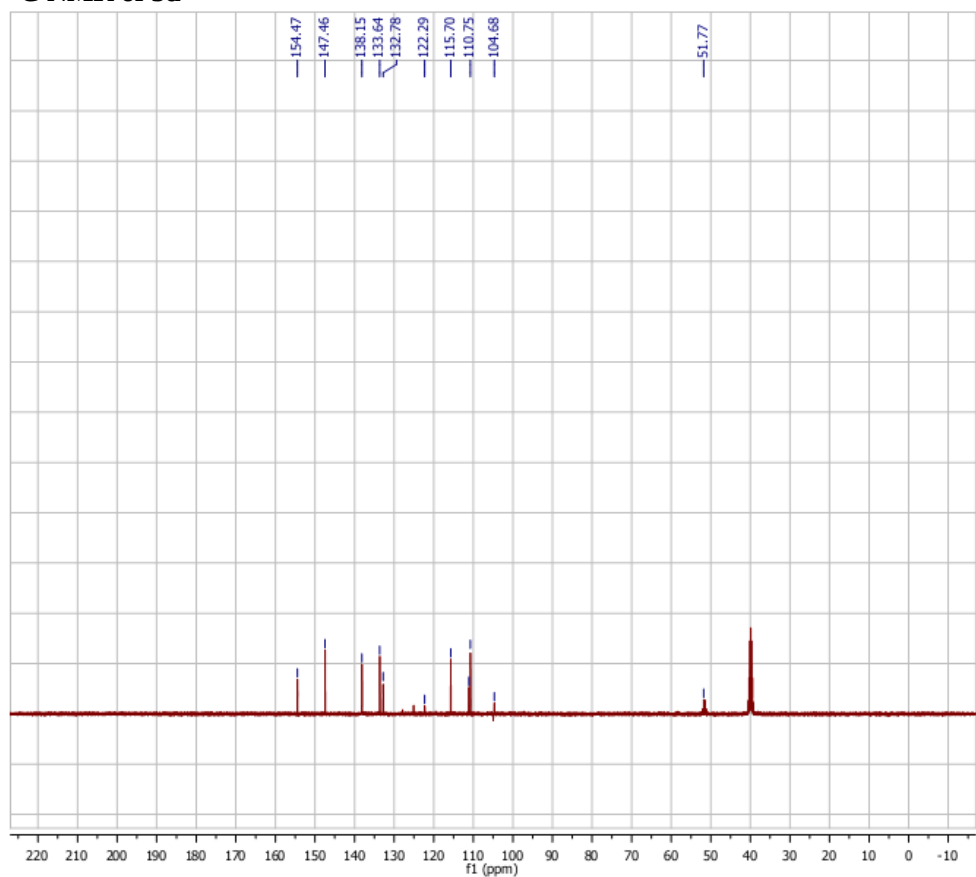
C₁₄H₁₀N₆
 Exact Mass: 262.1
 Mol. Wt.: 262.27

LC-MS of 3c

MS Spectrum

¹H NMR of 3d

¹H NMR (400 MHz, dms0) δ 9.50 (s, 1H), 8.20 (s, 1H), 8.15 (d, *J* = 4.1, 1H), 7.55 – 7.62 (m, 1H), 6.88 (d, *J* = 8.3, 1H), 6.76 – 6.81 (m, 1H), 5.20–5.27 (m, 2H).

¹³C NMR of 3d

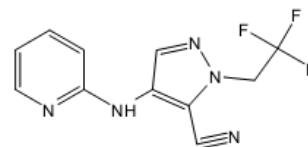
Hutchison Medi Pharma

Acquisition Parameters

NAME: 100868-
ff-19_Carbon_dmsd_02.fid/fid
Origin: vnmrs
Owner: jrhong
DATE: 2012-12-05T16:51:51
Solvent: dmsd
PULPROG: s2pul
TE: 25 C
NS: 256
SF01: 100.49 MHz
SWH: 24509.8 Hz
NUC: 13C
TD: 31875

F2 - Processing Parameters

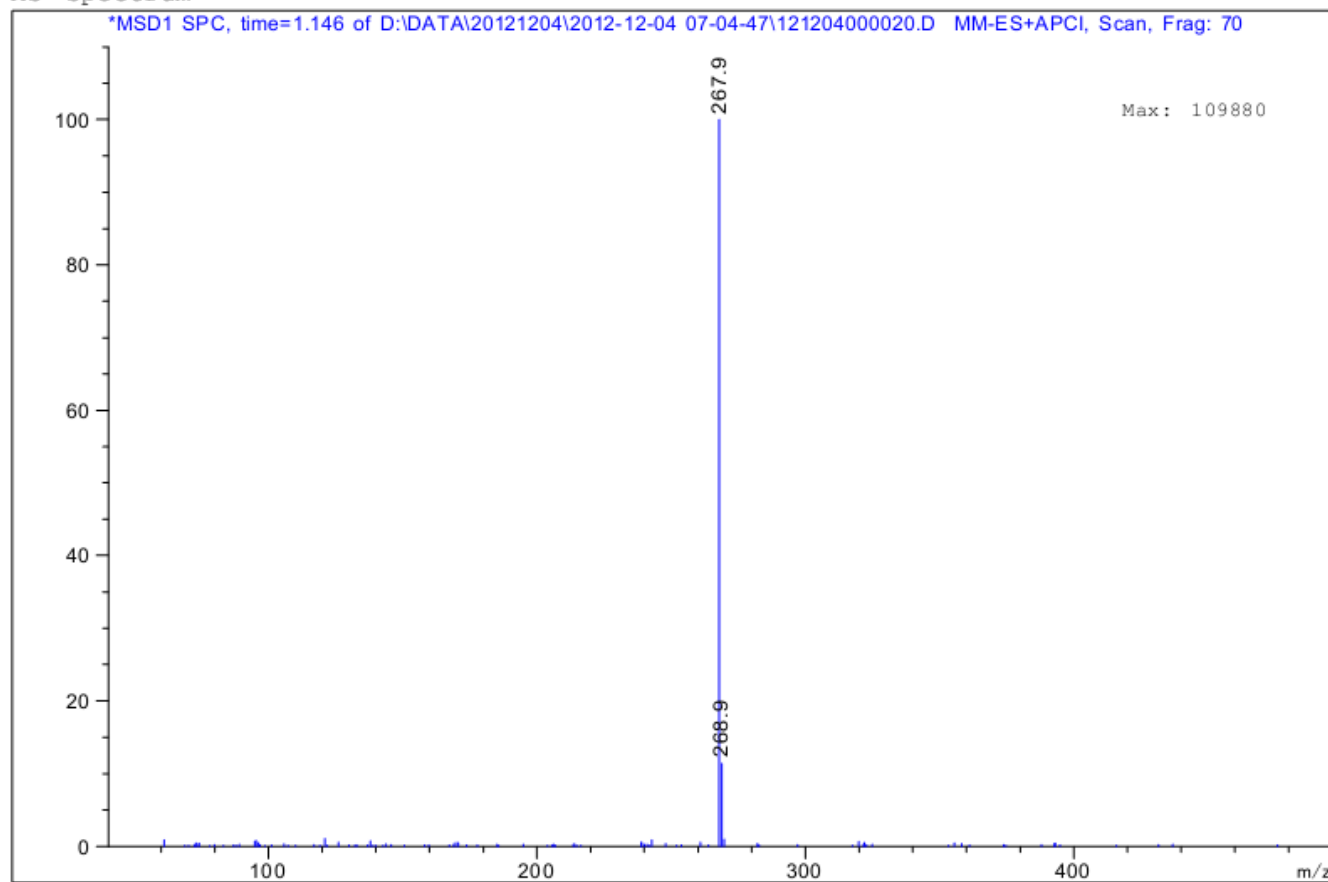
SI: 65536
DC: 0.05
LB: 0.50 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: -153.24
Ph1: -15.43

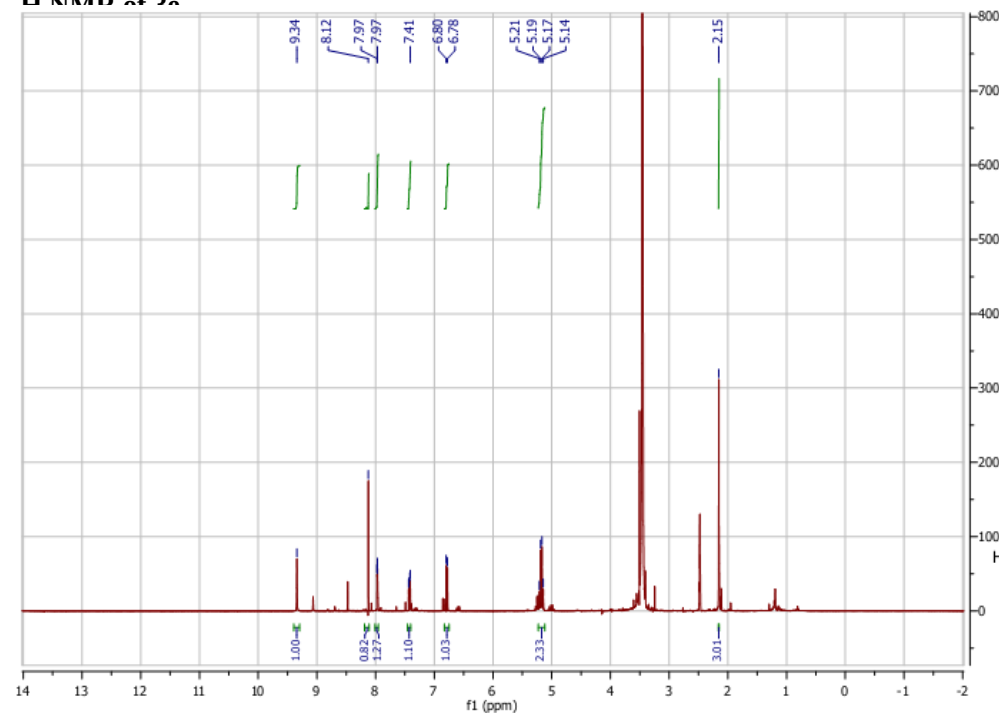


C₁₁H₈F₃N₅
Exact Mass: 267.07
Mol. Wt.: 267.21

LC-MS of 3d

MS Spectrum



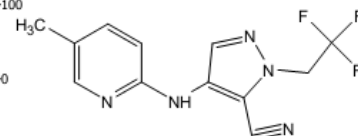
¹H NMR of 2a

¹H NMR (400 MHz, dmsO) δ 9.34 (s, 1H), 8.12 (s, 1H), 7.97–8.12 (m, 1H), 7.42 (dd, J = 8.5, 2.4, 1H), 6.79 (d, J = 8.4, 1H), 5.14–5.21 (m, 2H), 2.15 (s, 3H).

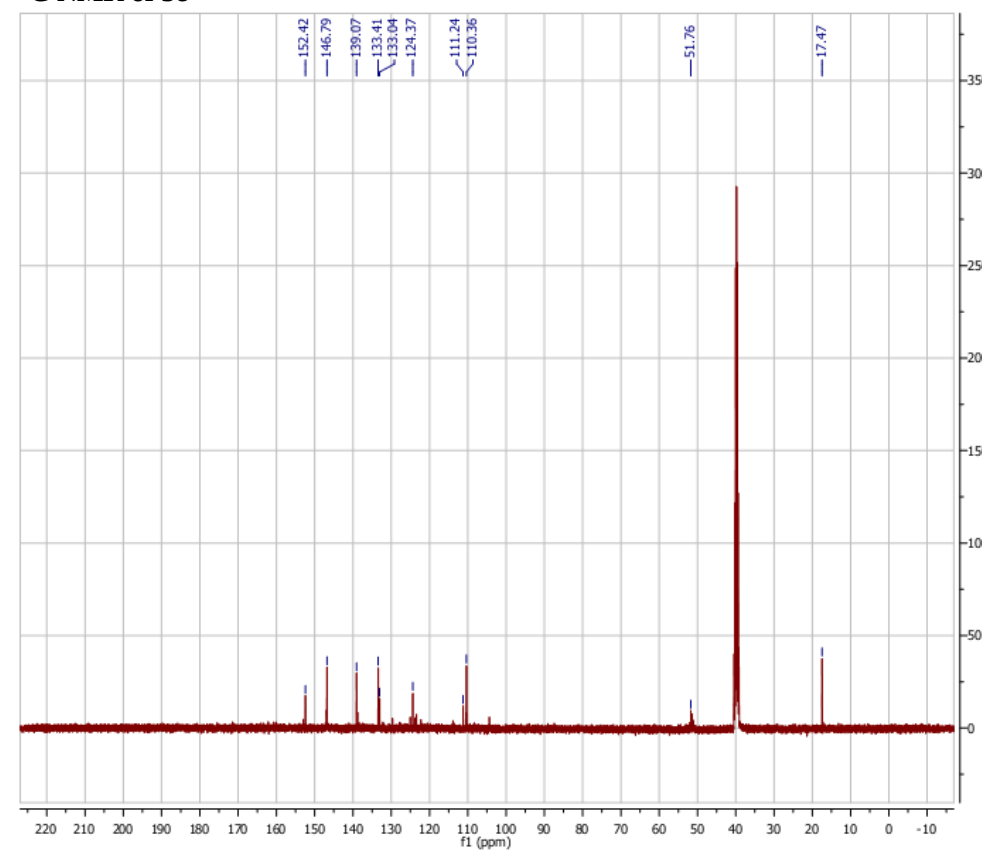
Hutchison Medi Pharma

Acquisition Parameters
 NAME: 100868-
 ff-31_Proton_dmsO_01.fid/fid
 Origin: vnmrs
 Owner: jrhong
 DATE: 2012-12-14T18:30:49
 Solvent: dmsO
 PULPROG: s2pul
 TE: 30 C
 NS: 32
 SFO1: 399.6 MHz
 SWH: 6410.3 Hz
 NUC: 1H
 TD: 13132

F2 - Processing Parameters
 SI: 32768
 DC: 0.05
 LB: 0.00 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: 113.70
 Ph1: 2.52



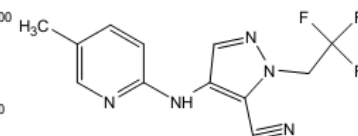
C12H10F3N5
 Exact Mass: 281.09
 Mol. Wt.: 281.24

¹³C NMR of 3e

Hutchison Medi Pharma

Acquisition Parameters
 NAME: 100868-
 ff-31_Carbon_dmsO_01.fid/fid
 Origin: vnmrs
 Owner: jrhong
 DATE: 2012-12-20T04:09:41
 Solvent: dmsO
 PULPROG: s2pul
 TE: 30 C
 NS: 2400
 SFO1: 100.49 MHz
 SWH: 24509.8 Hz
 NUC: 13C
 TD: 31875

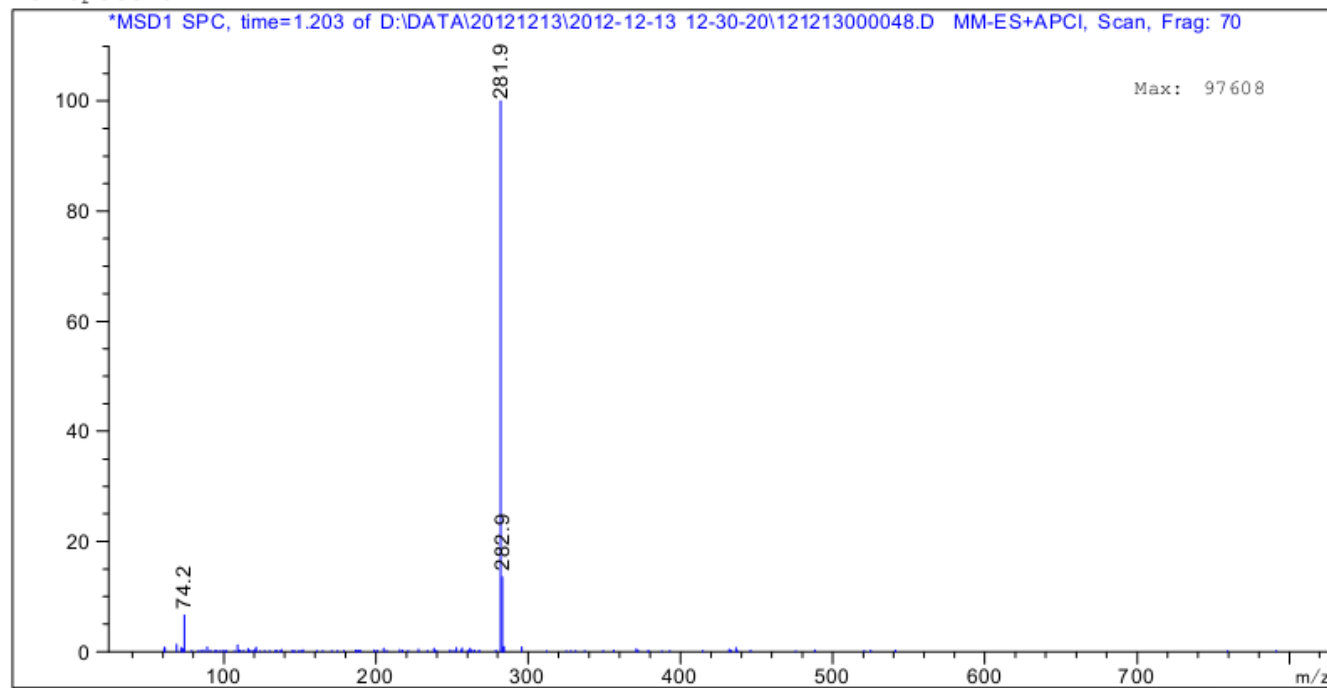
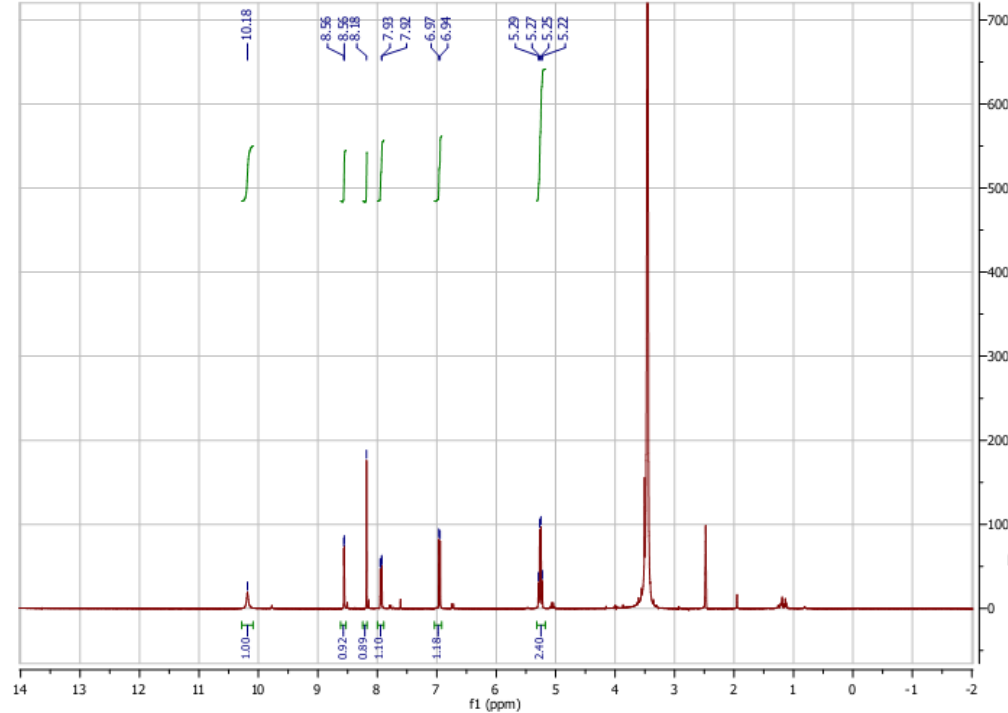
F2 - Processing Parameters
 SI: 65536
 DC: 0.05
 LB: 0.50 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: 165.67
 Ph1: 1.51



C12H10F3N5
 Exact Mass: 281.09
 Mol. Wt.: 281.24

LC-MS of 3e

MS Spectrum

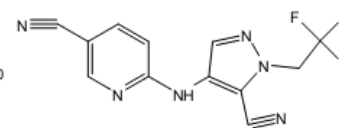
¹H NMR of 3e

Acquisition Parameters

NAME: 100868-
ff-32_Proton_dms0_01.fid/fid
Origin: vnmsr
Owner: jrhong
DATE: 2012-12-14T18:35:21
Solvent: dms0
PULPROG: s2pul
TE: 30 C
NS: 32
SFO1: 399.6 MHz
SWH: 6410.3 Hz
NUC: 1H
TD: 13132

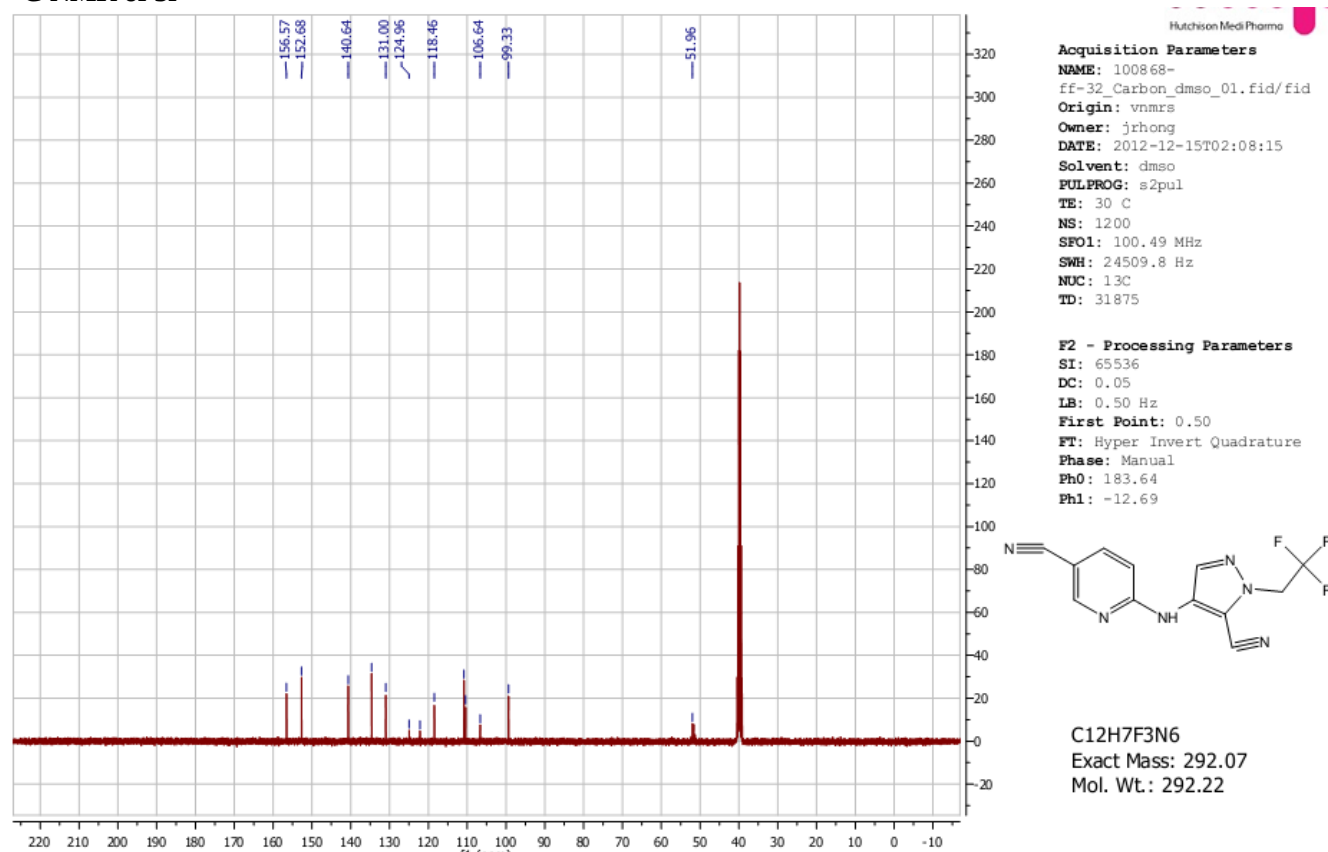
F2 - Processing Parameters

SI: 32768
DC: 0.05
LB: 0.00 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: 111.38
Ph1: 8.96



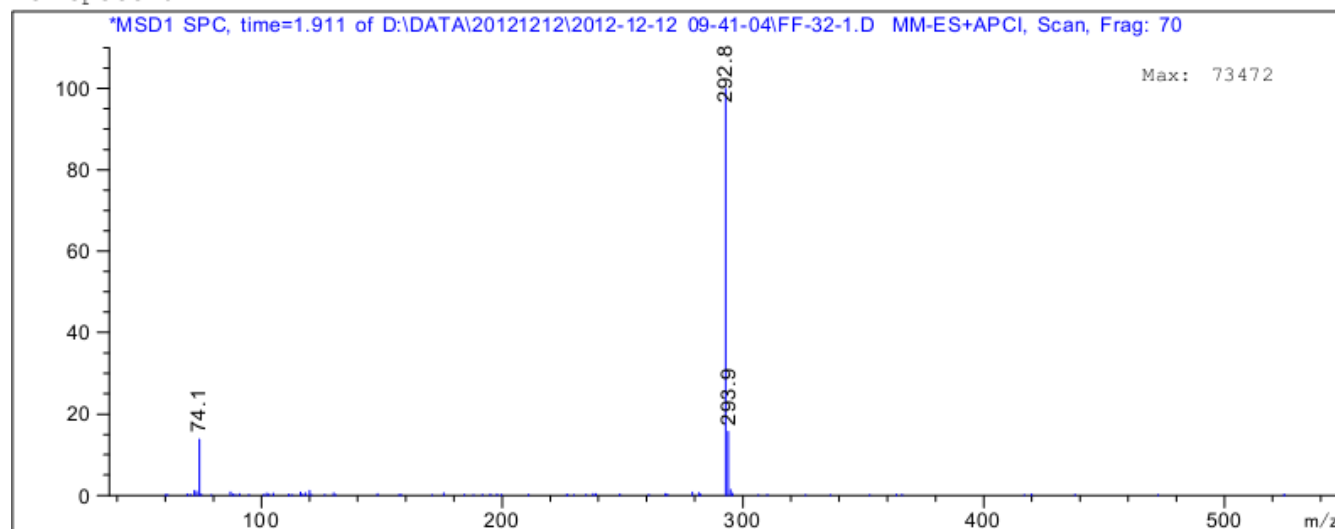
C₁₂H₇F₃N₆
Exact Mass: 292.07
Mol. Wt.: 292.22

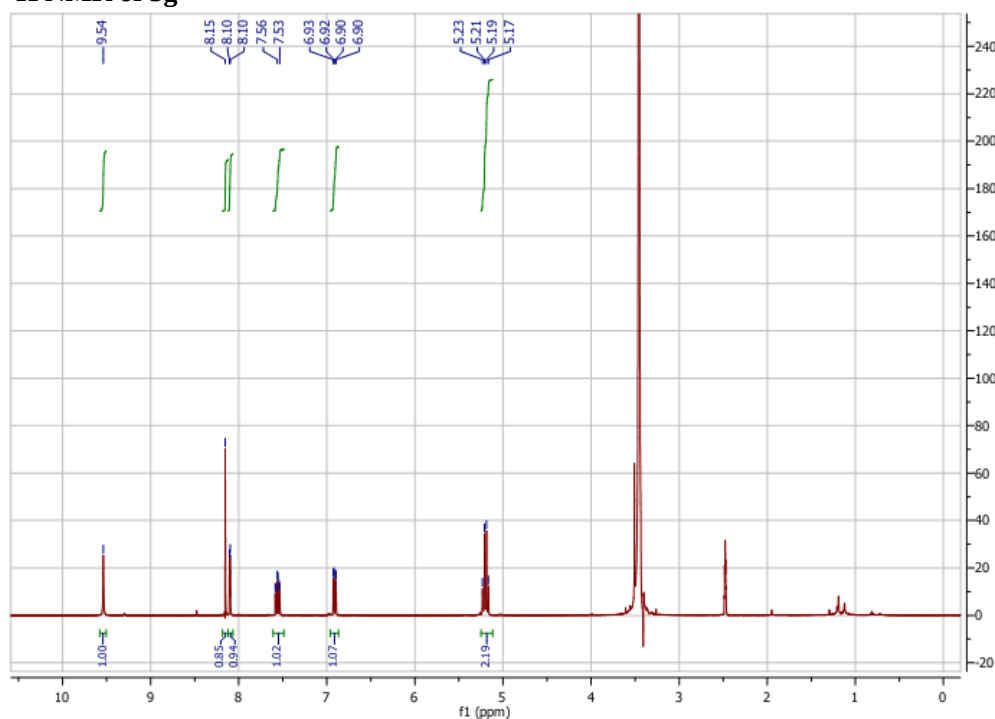
¹H NMR (400 MHz, dms0) δ 10.18 (s, 1H), 8.56 (d, $J = 2.2$, 1H), 8.18 (s, 1H), 7.94 (dd, $J = 8.8, 2.3$, 1H), 6.96 (d, $J = 8.8$, 1H), 5.22 - 5.29 (m, 2H).

¹³C NMR of 3f

LC-MS of 3f

MS Spectrum



¹H NMR of 3g

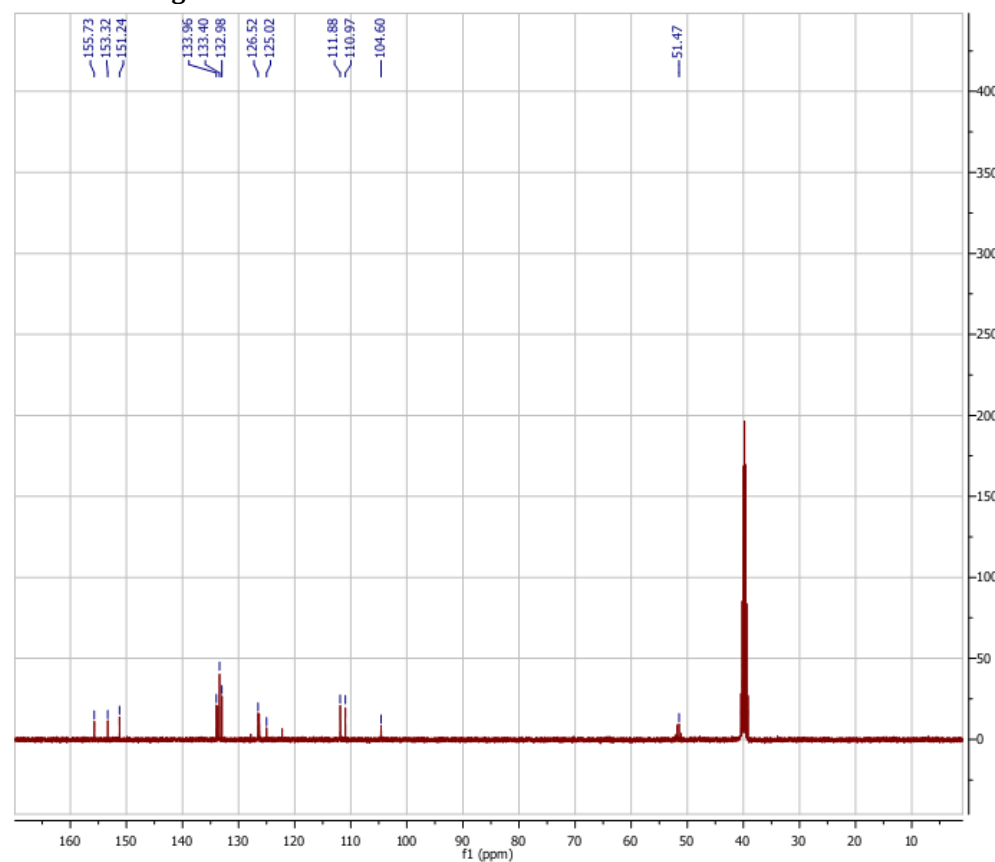
Hutchison Medi Pharma

Acquisition Parameters
NAME: 100868-ff-33_Proton_dms0_01.fid/fid
Origin: vnmrs
Owner: jrhong
DATE: 2012-12-14T18:54:17
Solvent: dms0
PULPROG: s2pul
TE: 30 C
NS: 8
SF01: 399.6 MHz
SWH: 6410.3 Hz
NUC: 1H
TD: 13132

F2 - Processing Parameters
SI: 32768
DC: 0.05
LB: 0.00 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: 117.39
Ph1: 0.89

C₁₁H₇F₄N₅
Exact Mass: 285.06
Mol. Wt.: 285.2

¹H NMR (400 MHz, dms0) δ 9.54 (s, 1H), 8.15 (s, 1H), 8.10 (d, J = 3.0, 1H), 7.53 - 7.56 (m, 1H), 6.91 (dd, J = 9.1, 3.7, 1H), 5.17 - 5.23 (m, 2H).

¹³C NMR of 3g

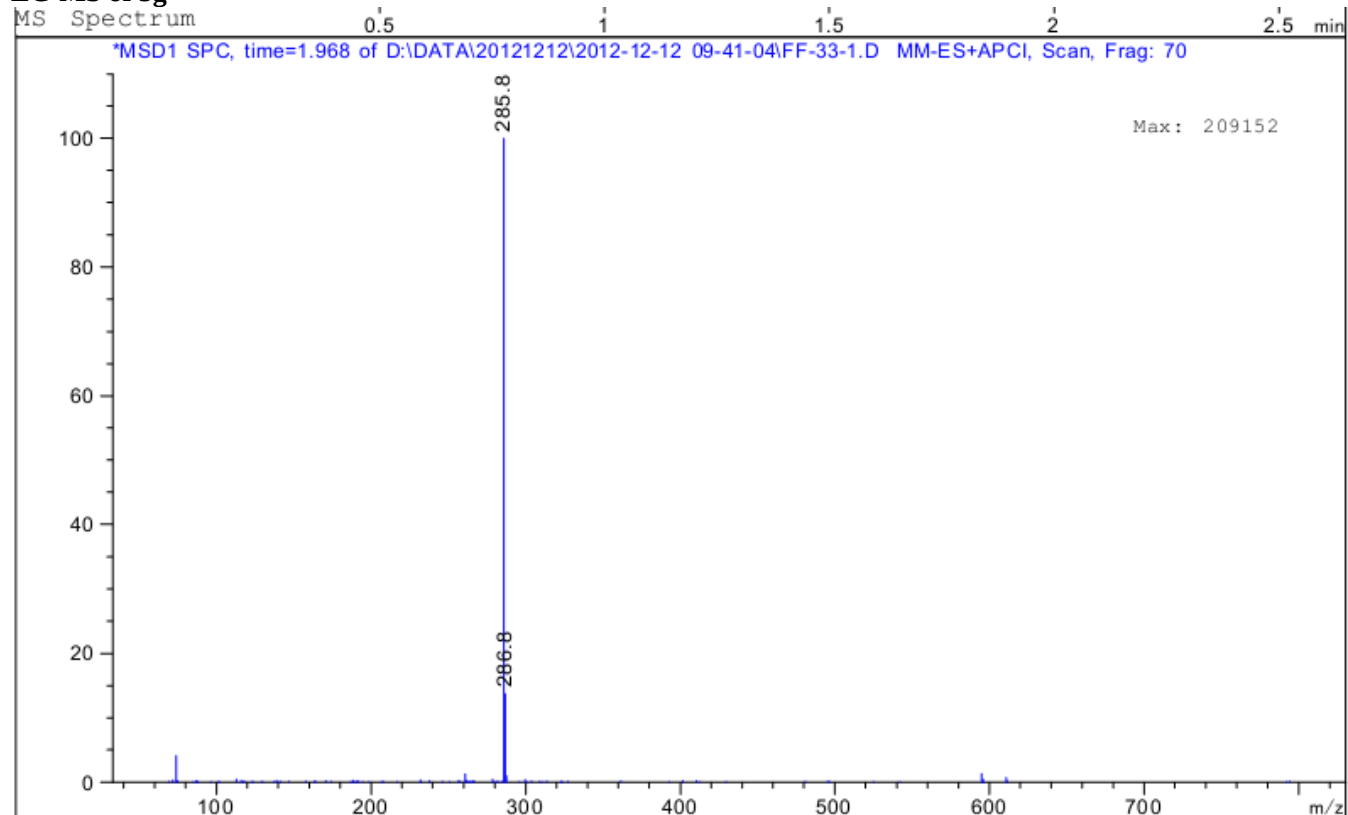
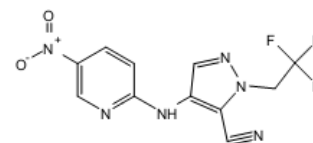
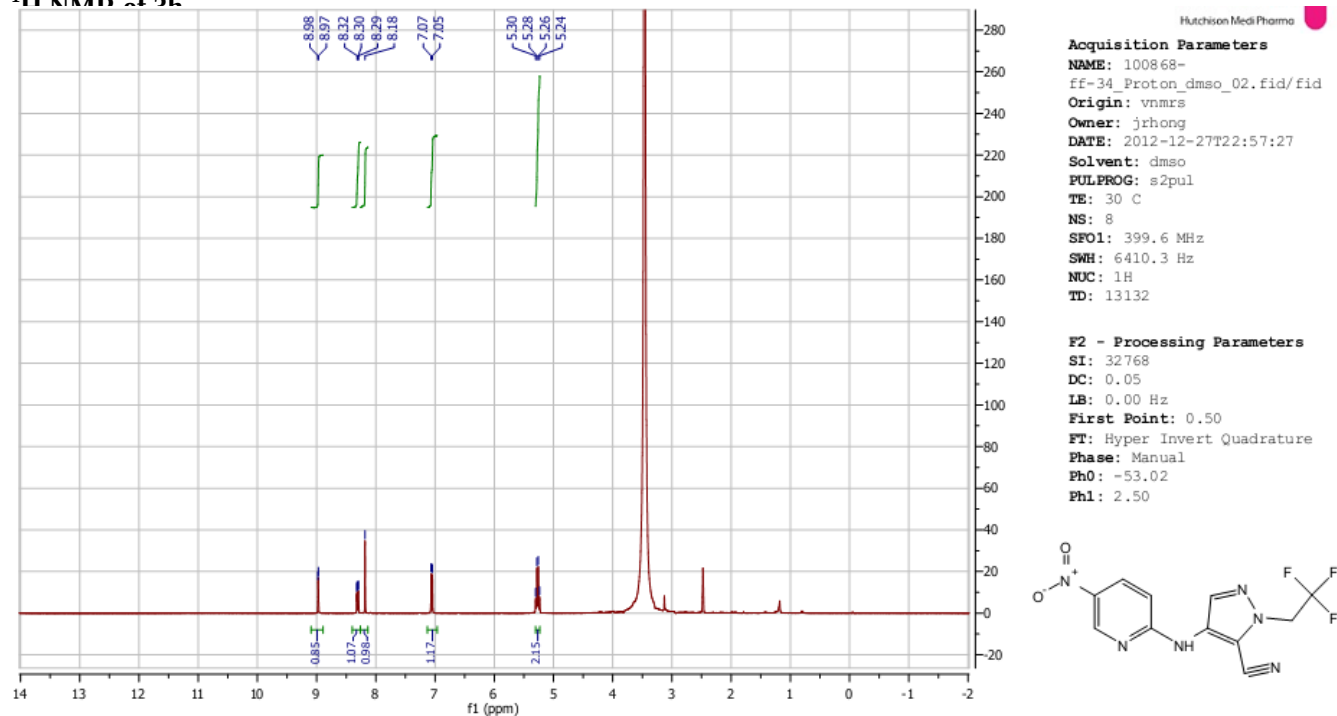
Hutchison Medi Pharma

Acquisition Parameters
NAME: 100868-ff-33_Carbon_dms0_01.fid/fid
Origin: vnmrs
Owner: jrhong
DATE: 2012-12-15T02:57:00
Solvent: dms0
PULPROG: s2pul
TE: 30 C
NS: 1200
SF01: 100.49 MHz
SWH: 24509.8 Hz
NUC: 13C
TD: 31875

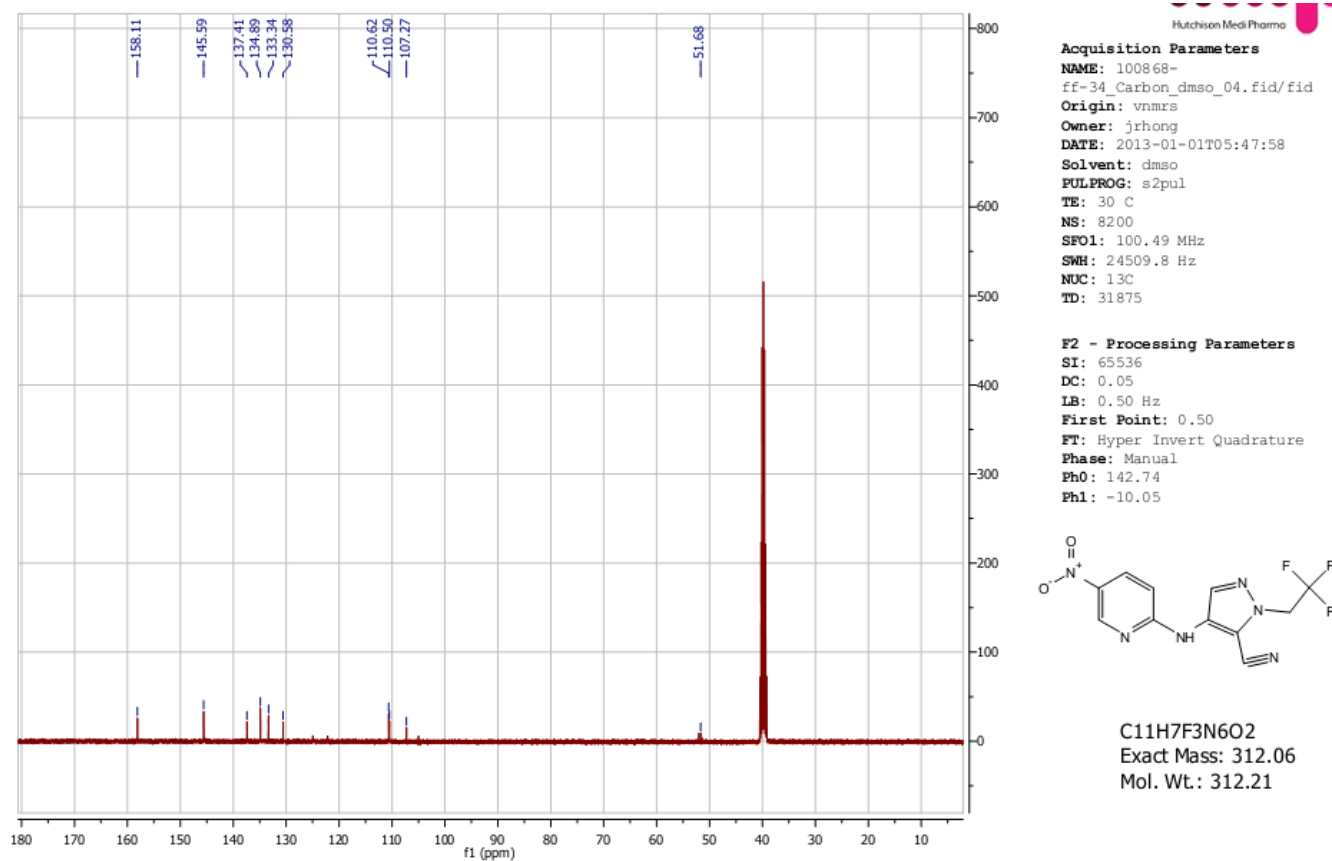
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.50 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: 207.79
Ph1: -27.90

C₁₁H₇F₄N₅
Exact Mass: 285.06
Mol. Wt.: 285.2

LC-MS of 3g

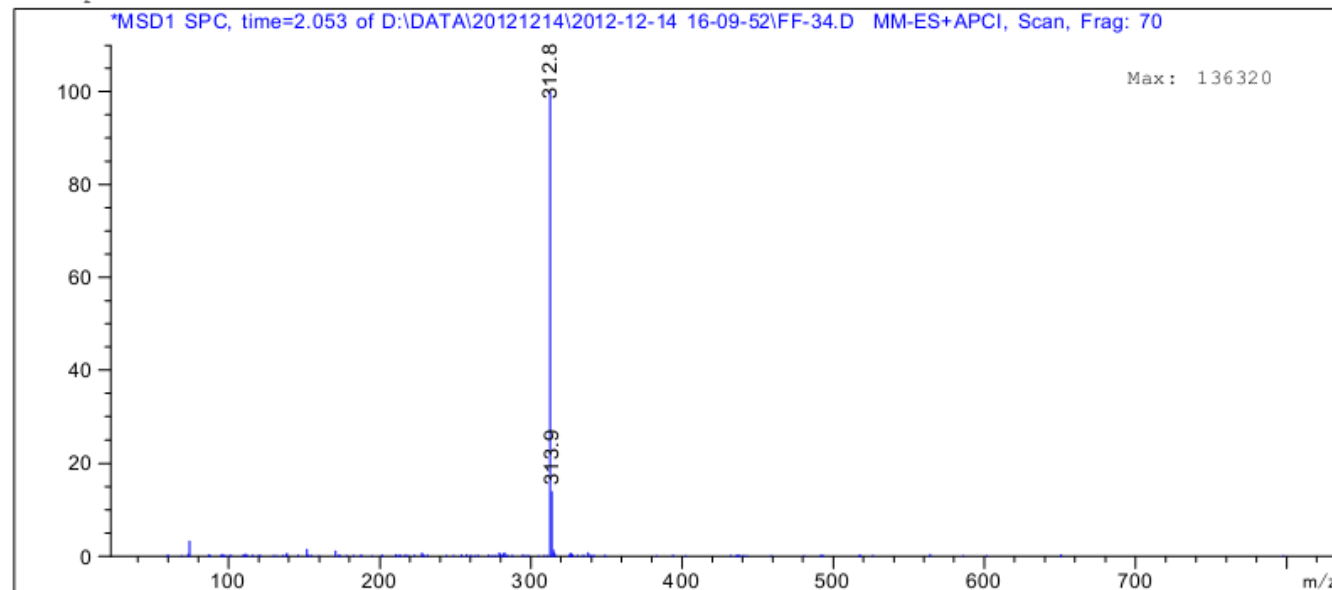
¹H NMR of 3g

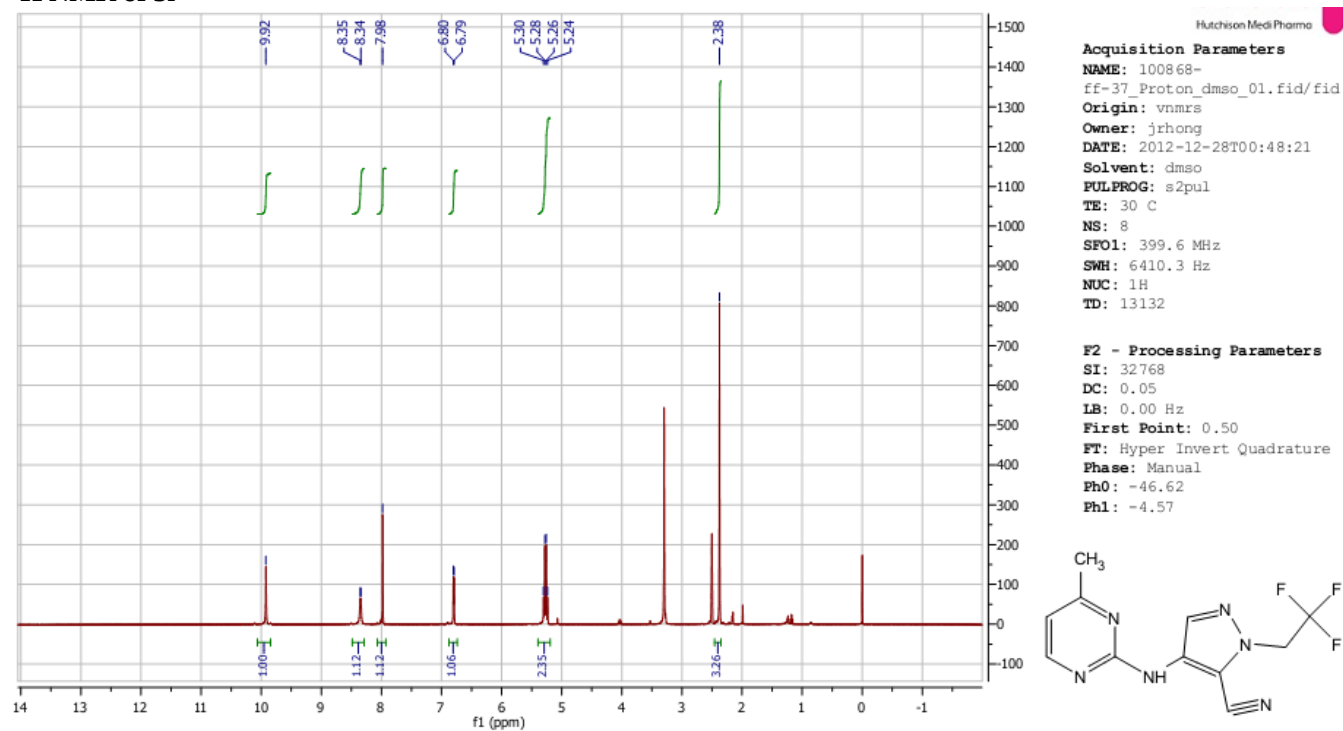
C11H7F3N6O2
Exact Mass: 312.06
Mol. Wt.: 312.21

¹³C NMR of 3h

LC-MS of 3h

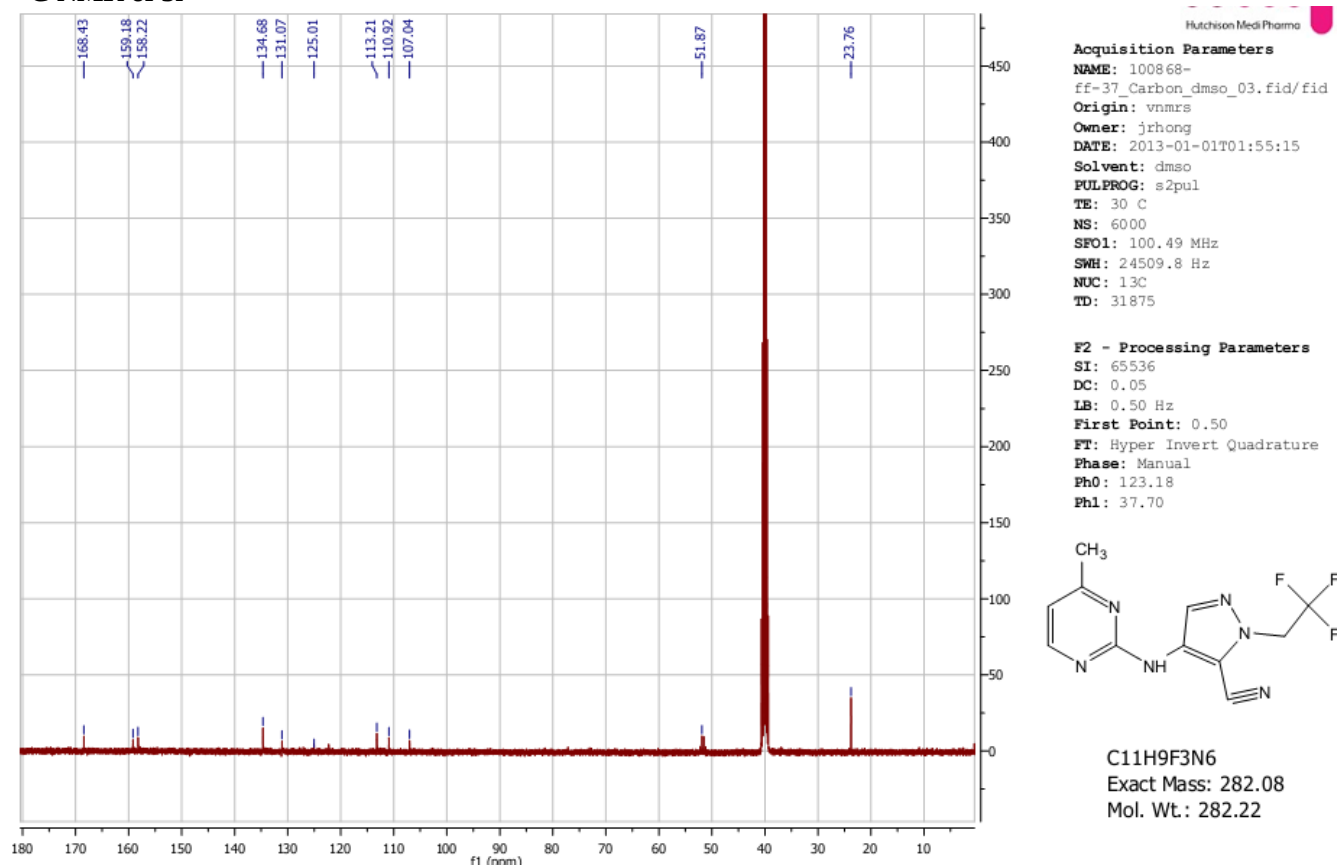
MS Spectrum



¹H NMR of 3i

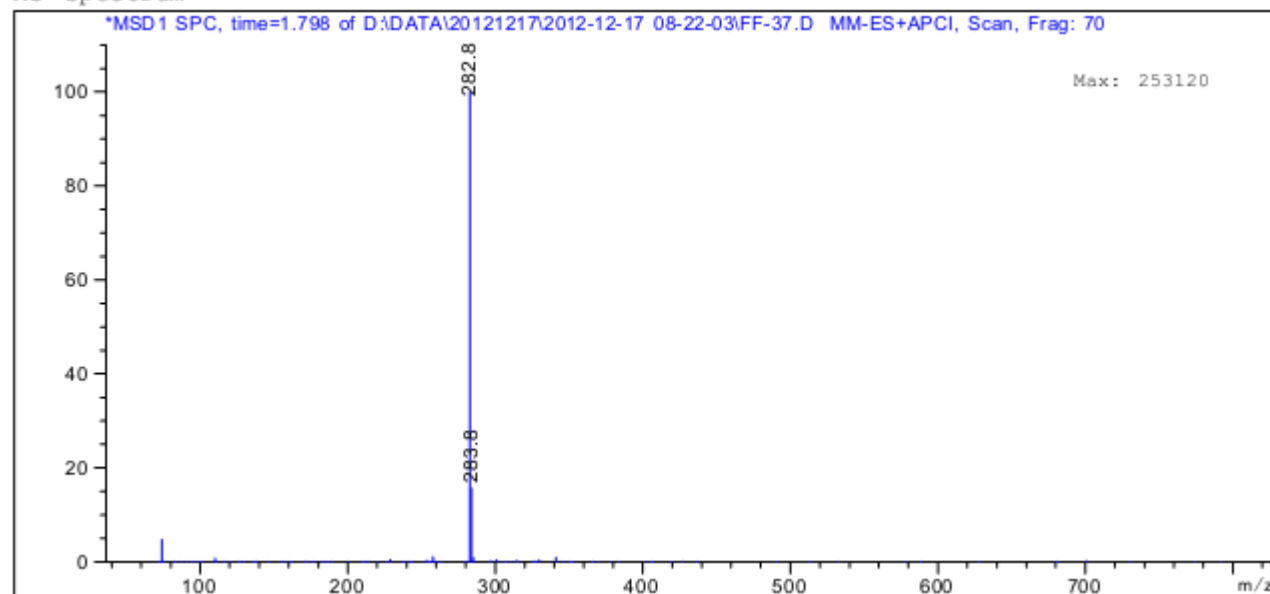
¹H NMR (400 MHz, dms0) δ 9.92 (s, 1H), 8.35 (d, J = 4.1, 1H), 7.98 (s, 1H), 6.80 (d, J = 4.9, 1H), 5.24 - 5.30 (m, 2H), 2.38 (s, 3H).

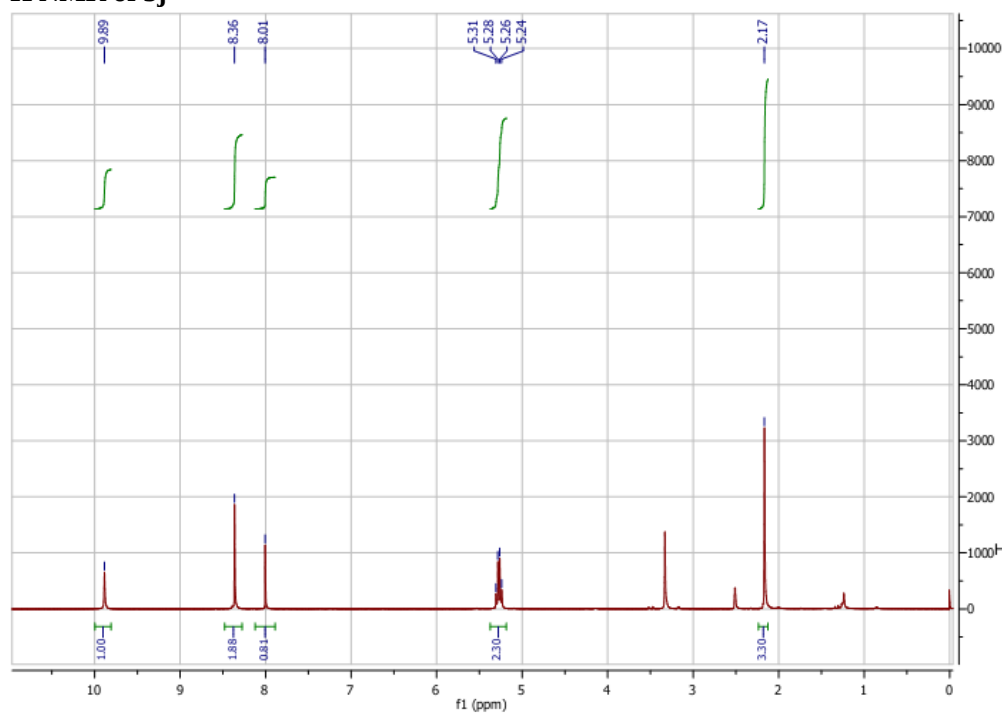
C11H9F3N6
Exact Mass: 282.08
Mol. Wt.: 282.22

¹³C NMR of 3i

LC-MS of 3i

MS Spectrum



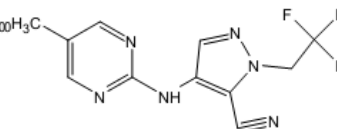
¹H NMR of 3j

¹H NMR (400 MHz, dms) δ 9.89 (s, 1H), 8.36 (s, 2H), 8.01 (s, 1H), 5.24 - 5.31 (m, 2H), 2.17 (s, 3H).

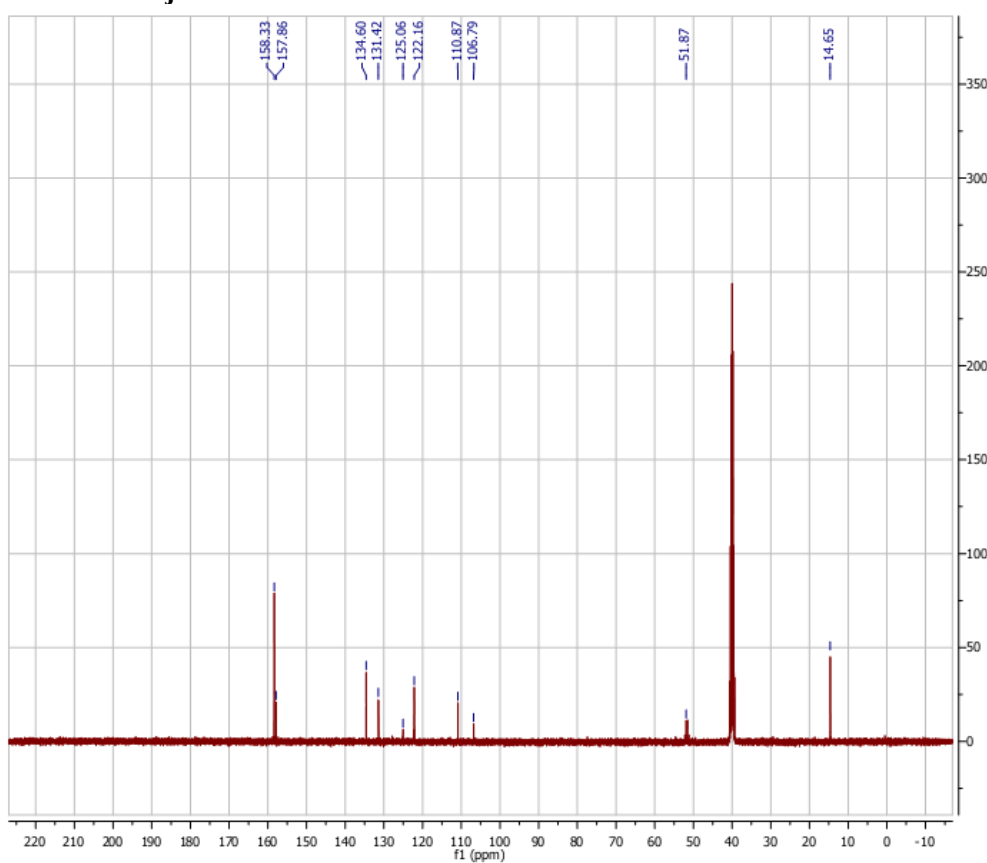
Hutchison MediPharma

Acquisition Parameters
 NAME: 100868-
 ff-36_Proton_dms0_04.fid/fid
 Origin: vnms
 Owner: jrhong
 DATE: 2012-12-20T22:43:36
 Solvent: dms0
 PULPROG: s2pul
 TE: 30 C
 NS: 32
 SFO1: 399.6 MHz
 SWH: 6410.3 Hz
 NUC: 1H
 TD: 13132

F2 - Processing Parameters
 SI: 32768
 DC: 0.05
 LB: 0.00 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: 126.64
 Ph1: -10.23



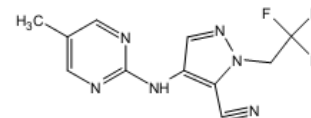
C11H9F3N6
 Exact Mass: 282.08
 Mol. Wt.: 282.22

¹³C NMR of 3j

Hutchison MediPharma

Acquisition Parameters
 NAME: 100868-
 ff-36_Carbon_dms0_02.fid/fid
 Origin: vnms
 Owner: jrhong
 DATE: 2012-12-22T02:47:40
 Solvent: dms0
 PULPROG: s2pul
 TE: 30 C
 NS: 2400
 SFO1: 100.49 MHz
 SWH: 24509.8 Hz
 NUC: 13C
 TD: 31875

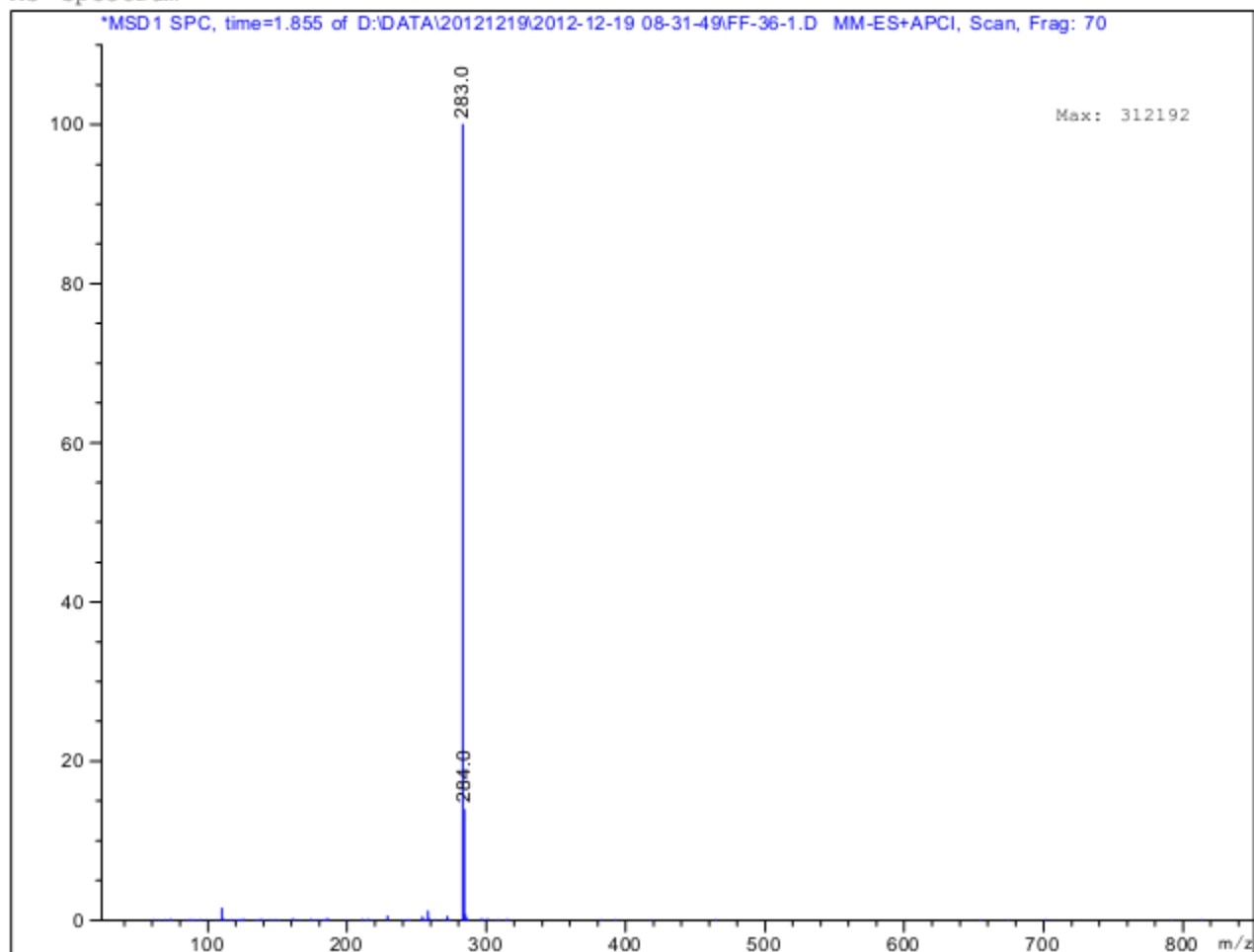
F2 - Processing Parameters
 SI: 65536
 DC: 0.05
 LB: 0.50 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: -138.64
 Ph1: -19.55

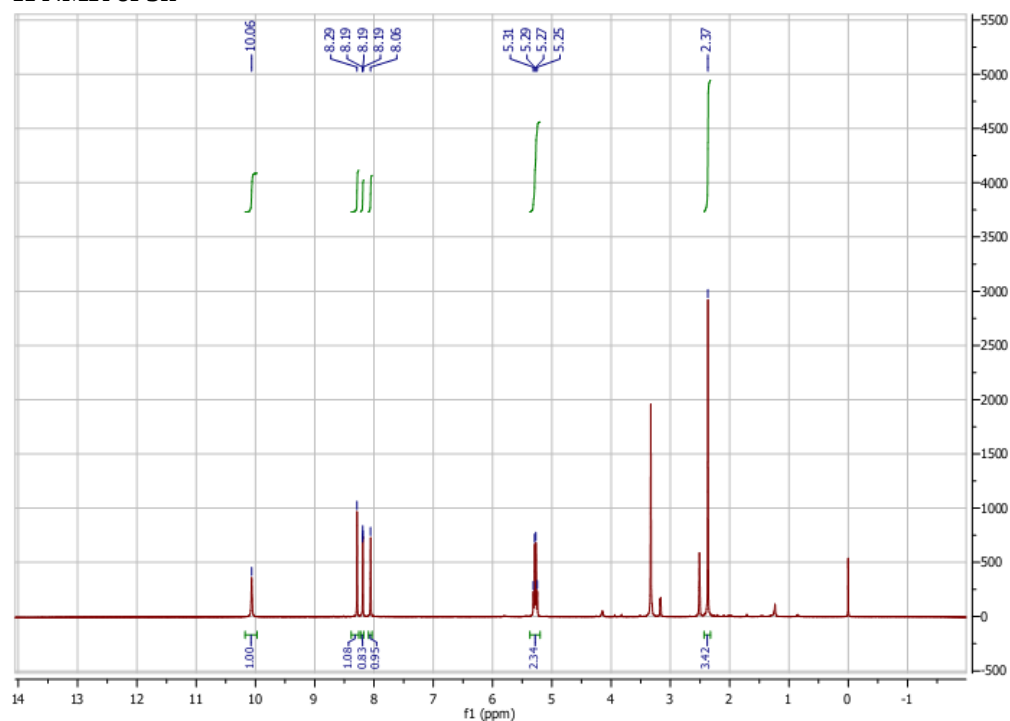


C11H9F3N6
 Exact Mass: 282.08
 Mol. Wt.: 282.22

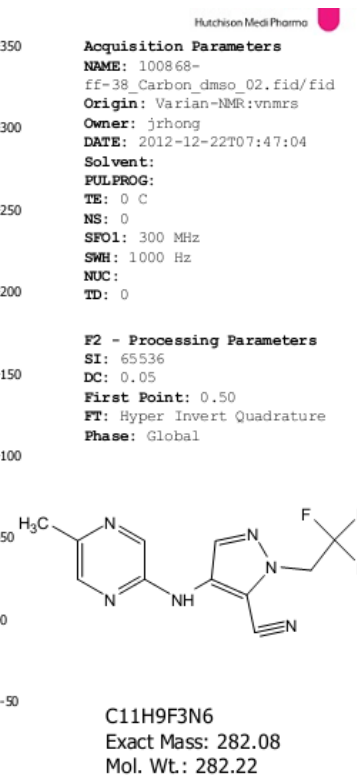
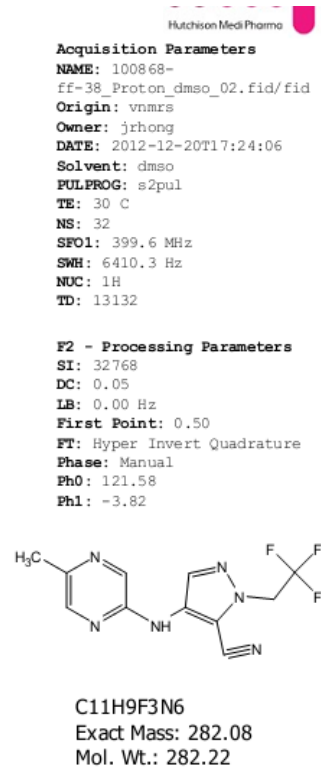
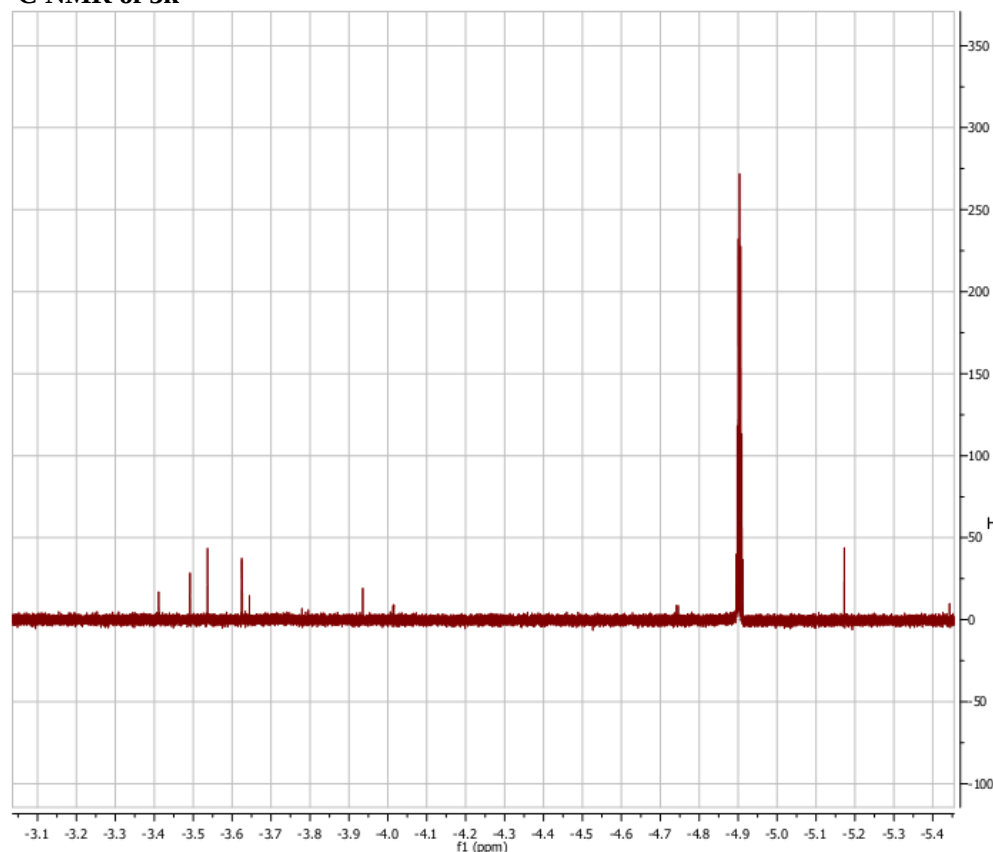
LC-MS of 3j

MS Spectrum



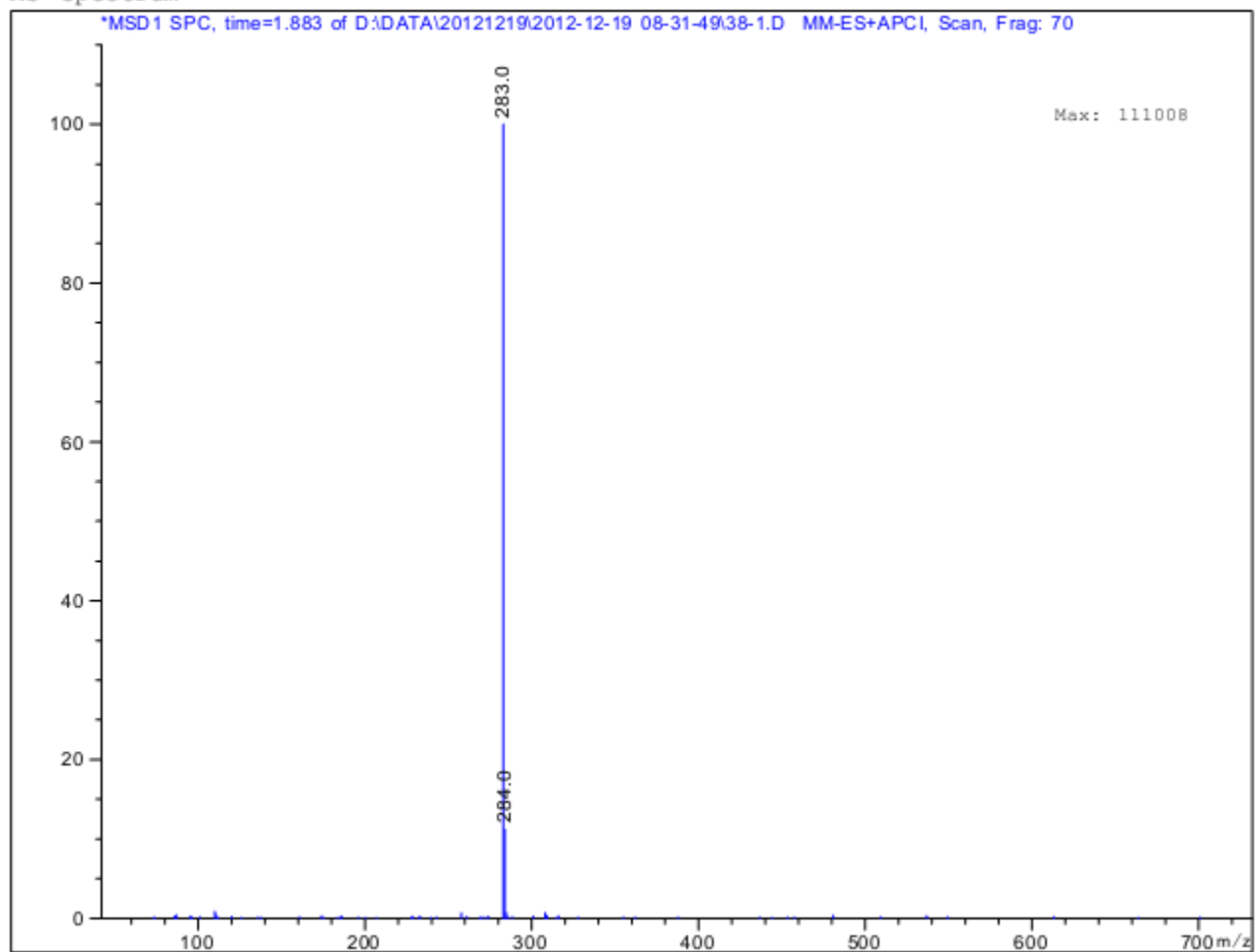
¹H NMR of 3k

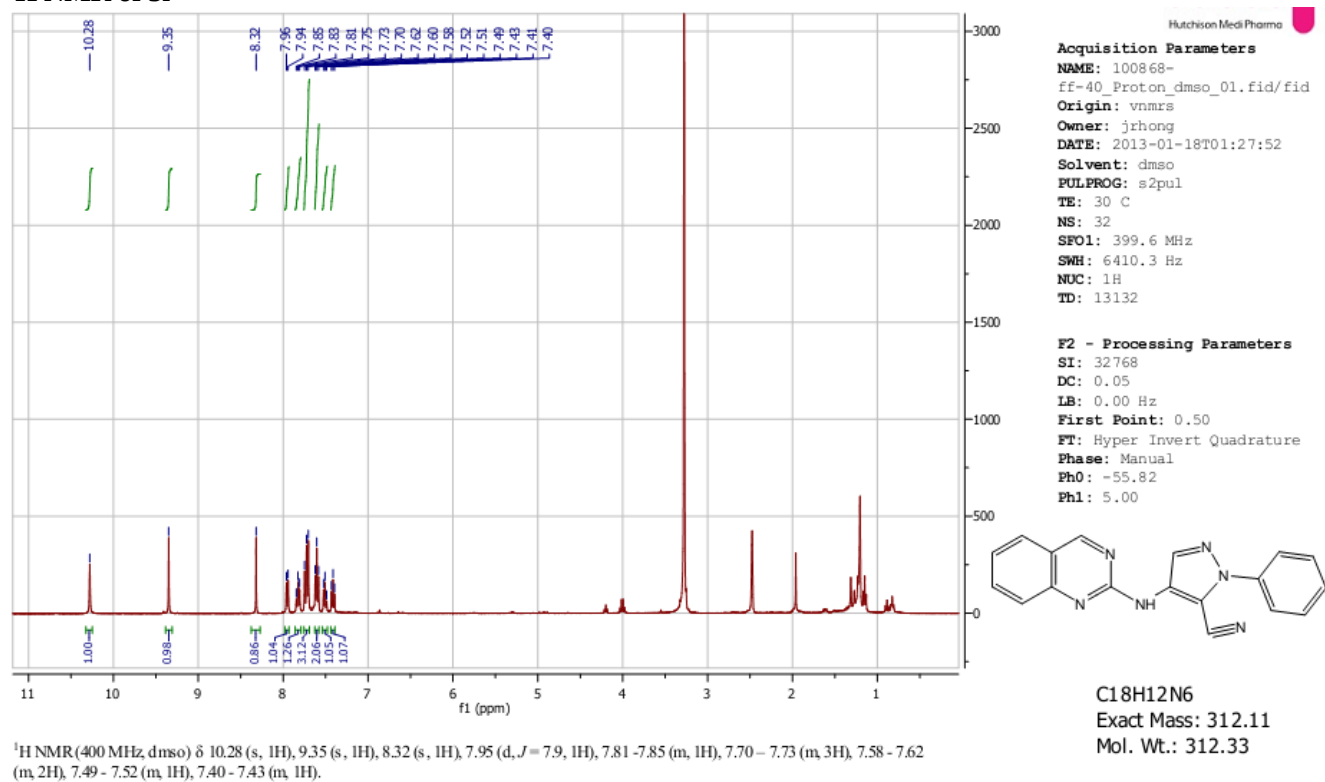
¹H NMR (400 MHz, dmsO) δ 10.06 (s, 1H), 8.29 (s, 1H), 8.17 – 8.19 (m, 1H), 8.06 (s, 1H), 5.25 – 5.31 (m, 2H), 2.37 (s, 3H).

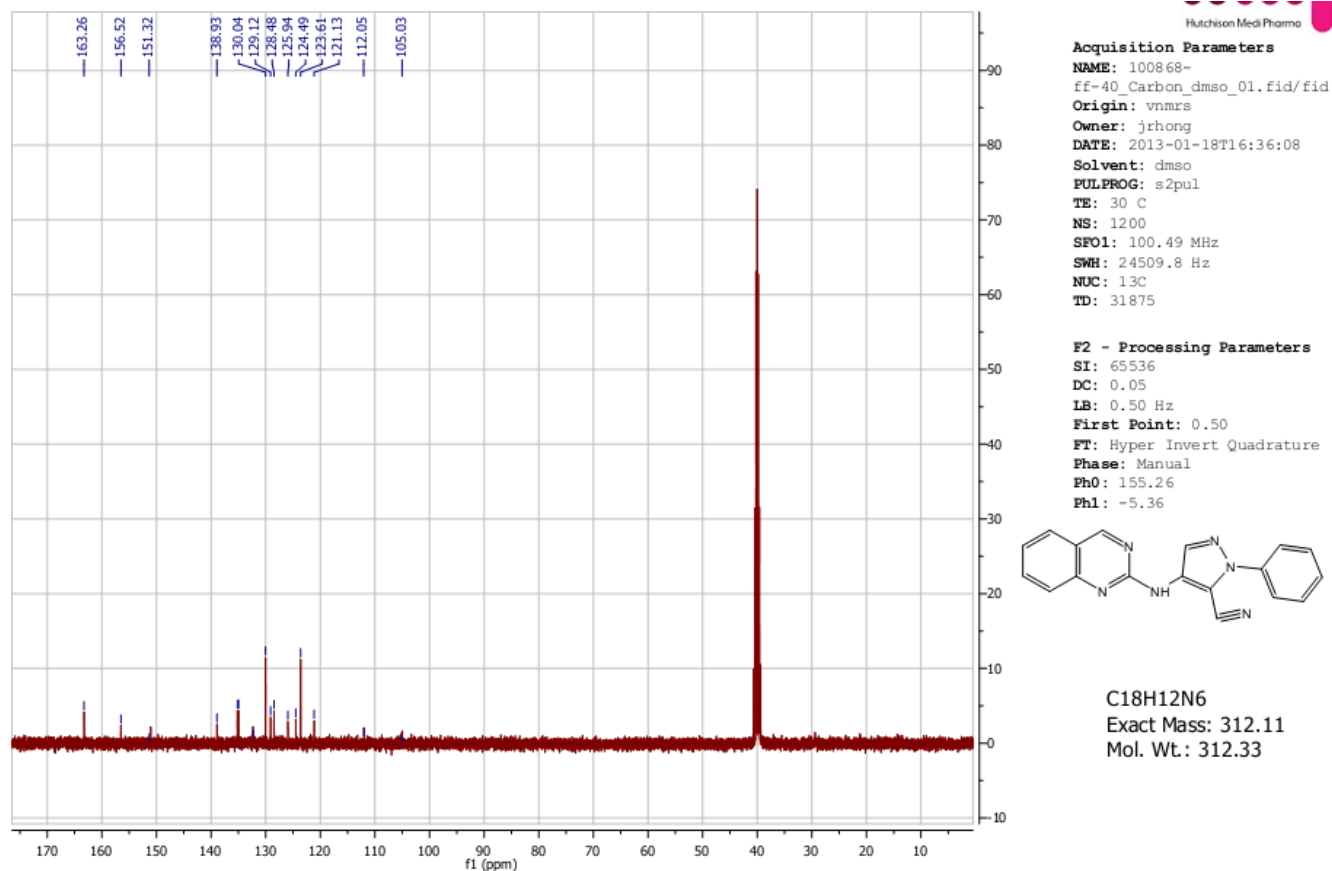
¹³C NMR of 3k

LC-MS of 3k

MS Spectrum

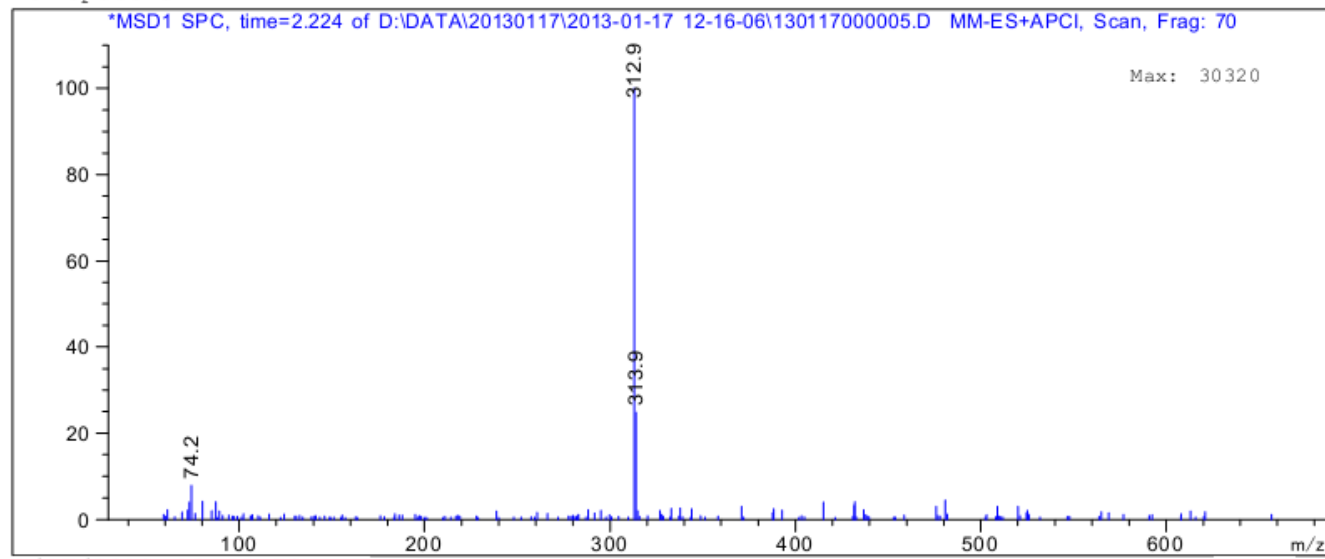


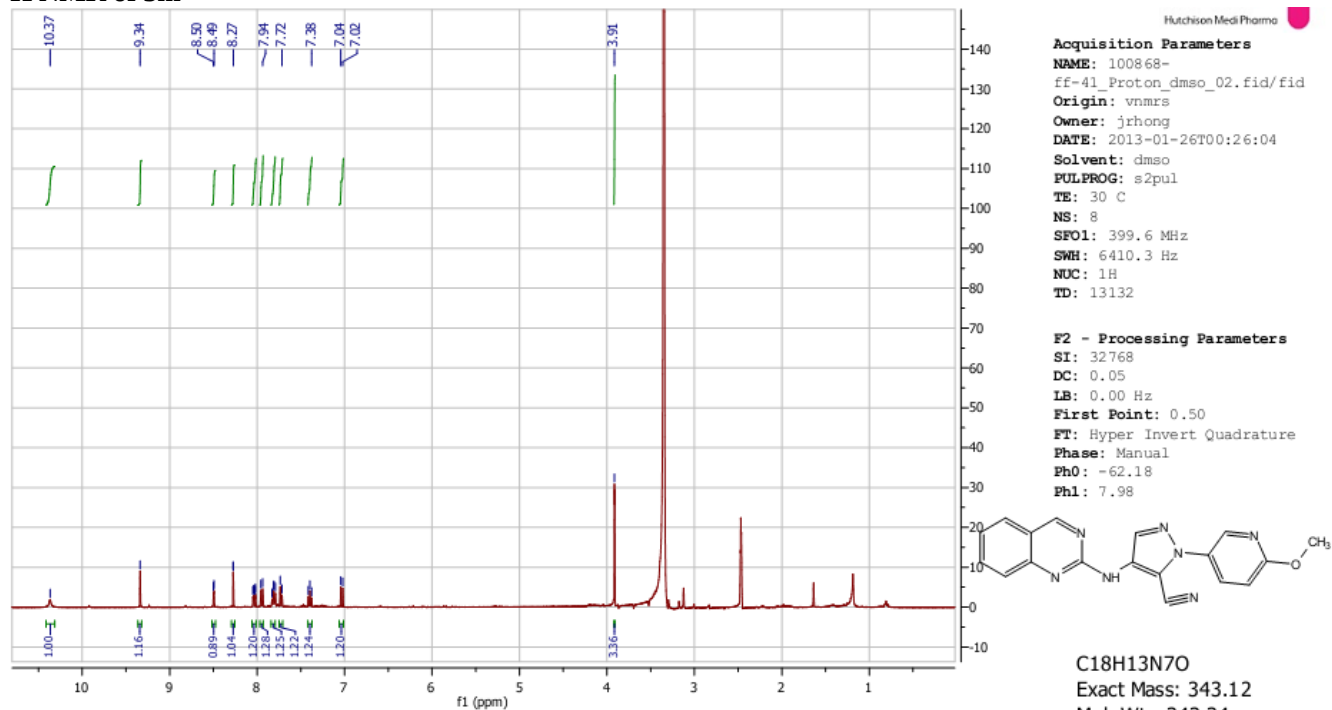
¹H NMR of 31

¹³C NMR of 3l

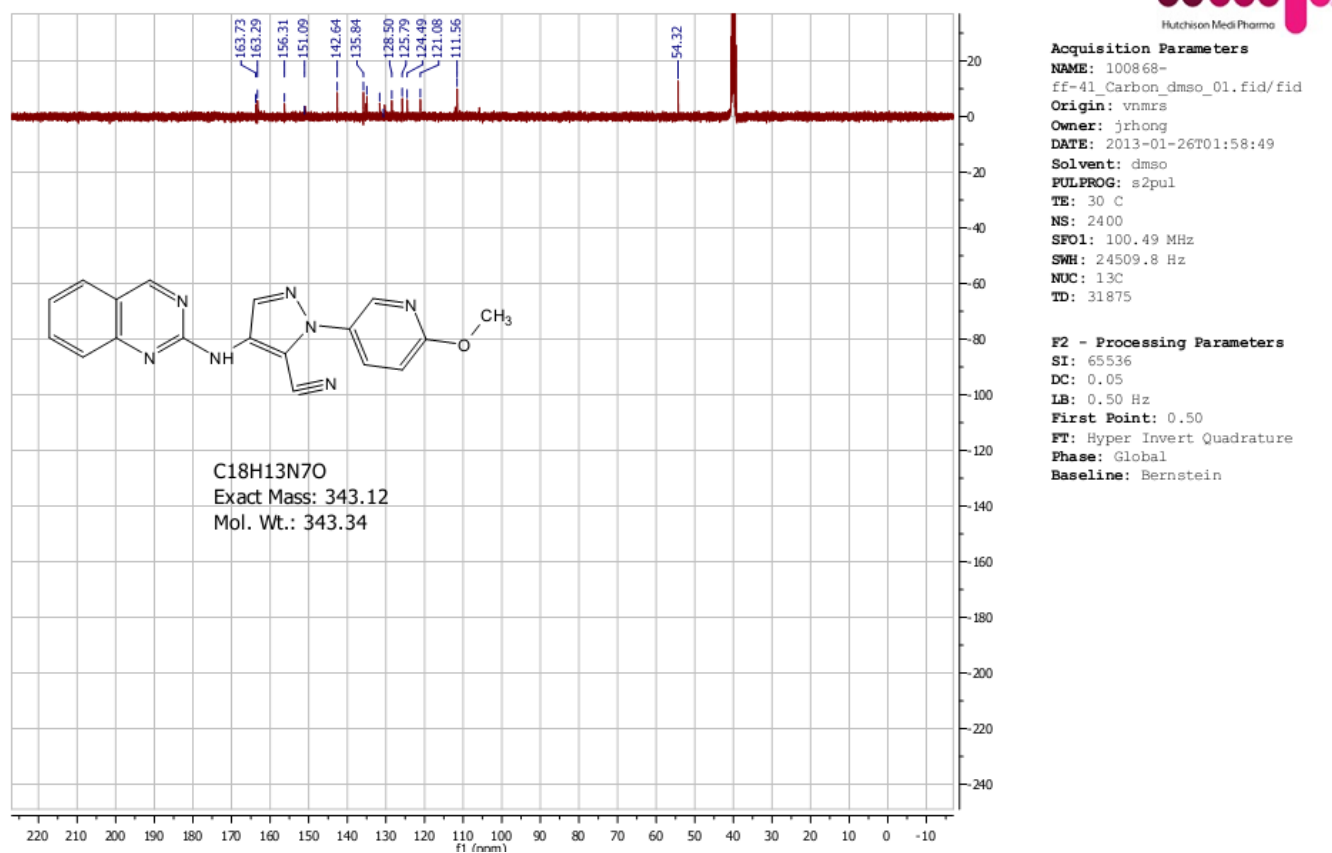
LC-MS of 3l

MS Spectrum



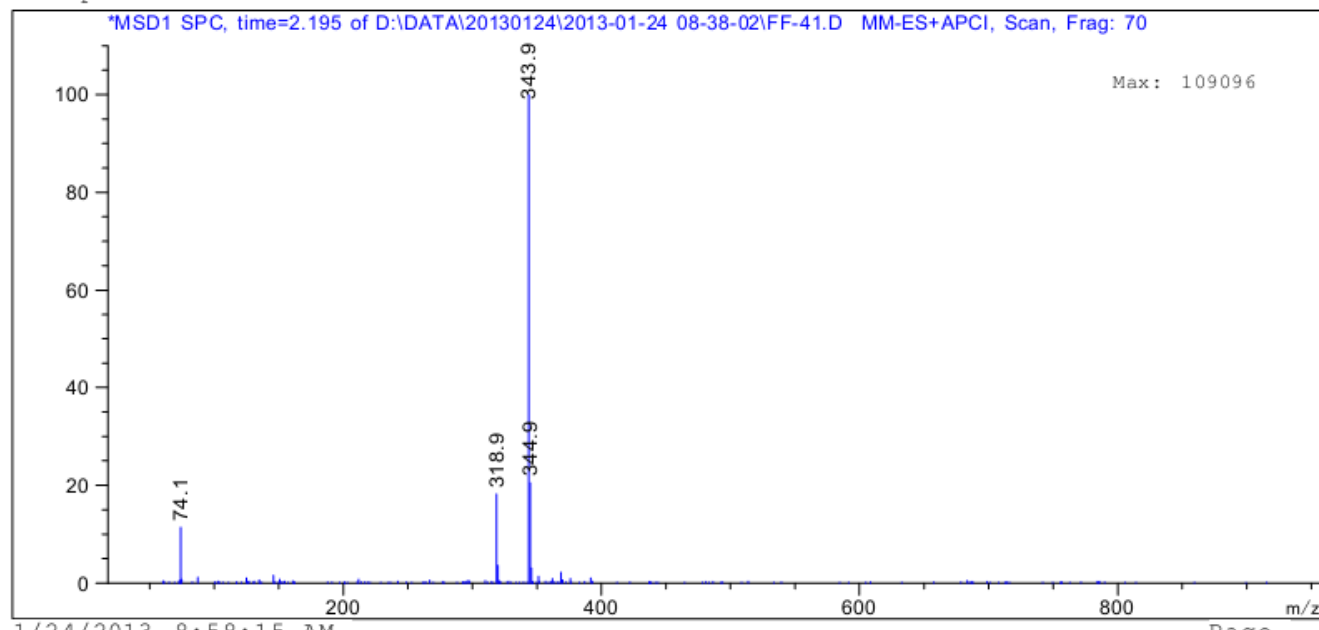
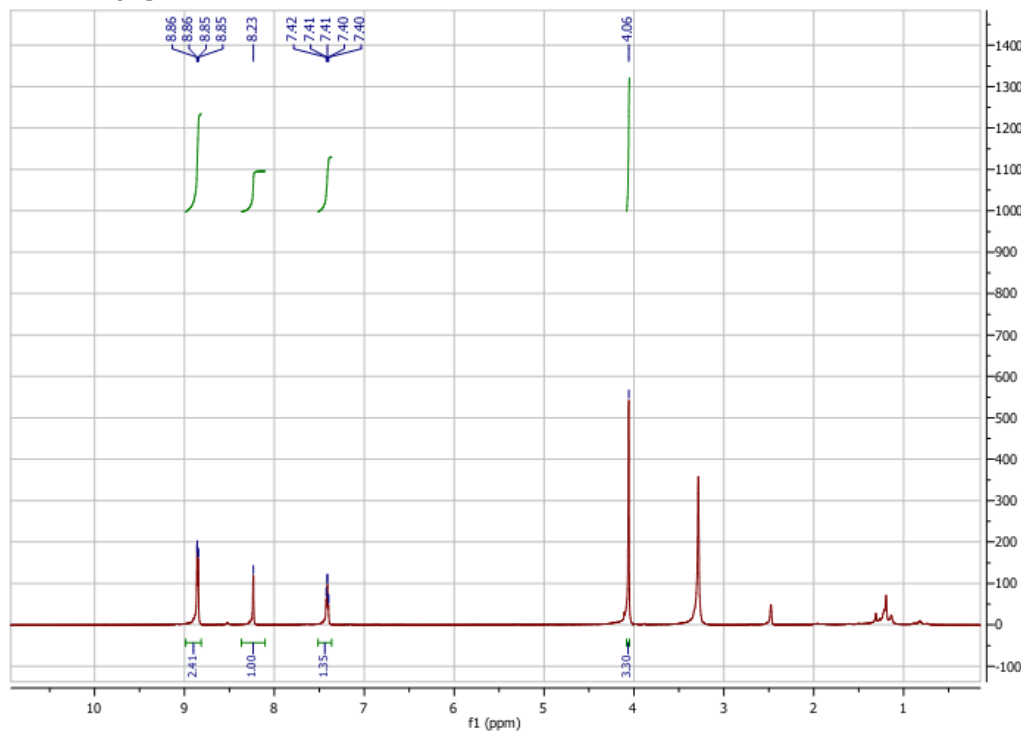
¹H NMR of 3m

¹H NMR (400 MHz, dms0) δ 10.37 (s, 1H), 9.34 (s, 1H), 8.50 (d, $J = 2.7$, 1H), 8.27 (d, $J = 1.5$, 1H), 8.02 – 8.03 (m, 1H), 7.94 – 7.96 (m, 1H), 7.79 – 7.84 (m, 1H), 7.72 – 7.74 (m, 1H), 7.40 (t, $J = 7.4$, 1H), 7.02 – 7.04 (m, 1H), 3.91 (s, 3H).

¹³C NMR of 3m

LC-MS of 3m

MS Spectrum

¹H NMR of 3n¹H NMR (400 MHz, dmsO) δ 8.85 - 8.86 (m, 2H), 8.23 (s, 1H), 7.40 - 7.42 (m, 1H), 4.06 (s, 3H).

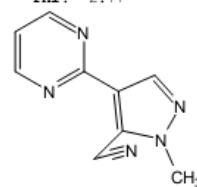
Hutchison MediPharma

Acquisition Parameters

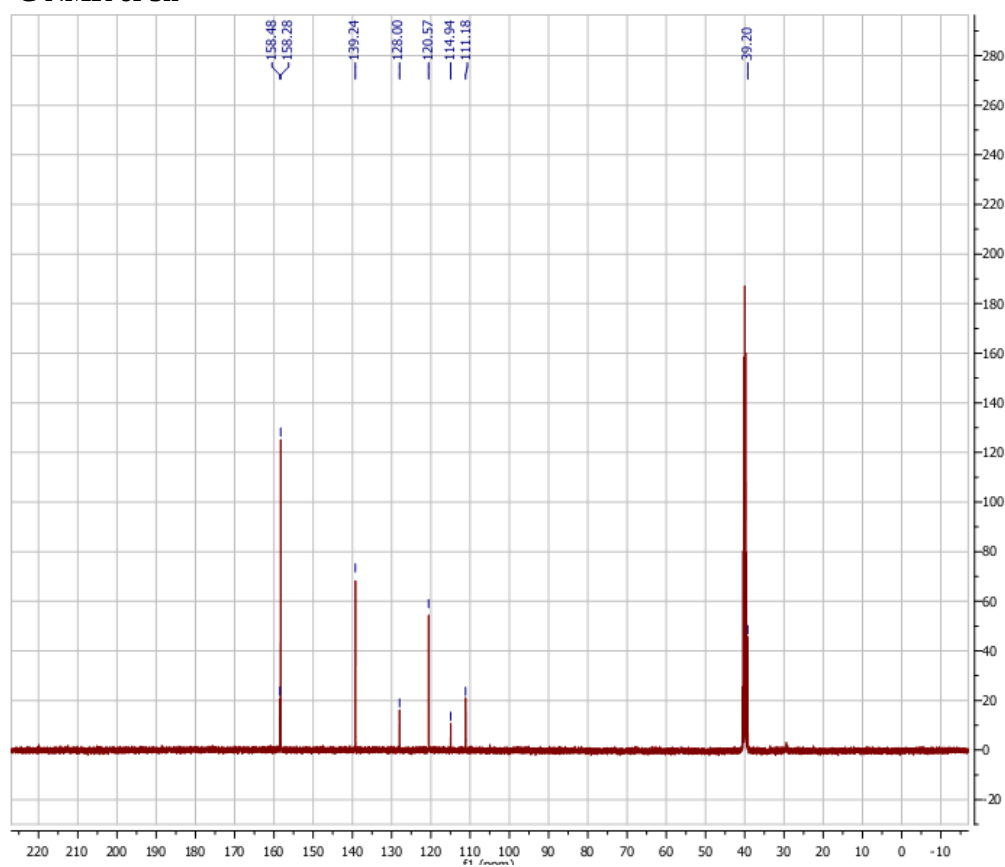
NAME: 100868-ff-09_Proton_dmsO_01.fid/fid
Origin: vnmrs
Owner: jrhong
DATE: 2012-12-27T22:54:08
Solvent: dmsO
PULPROG: s2pul
TE: 30 C
NS: 8
SFO1: 399.6 MHz
SWH: 6410.3 Hz
NUC: 1H
TD: 13132

F2 - Processing Parameters

SI: 32768
DC: 0.05
LB: 0.00 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: -46.56
Ph1: -2.77



C9H7N5
Exact Mass: 185.07
Mol. Wt.: 185.19

¹³C NMR of 3n

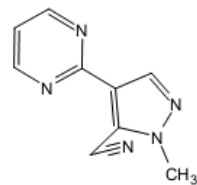
Hutchison Medi Pharma

Acquisition Parameters

NAME: 100868-
ff-09_Carbon_dms0_01.fid/fid
Origin: vnmrs
Owner: jrhong
DATE: 2012-12-28T02:58:48
Solvent: dms0
PULPROG: s2pul
TE: 30 C
NS: 2400
SF01: 100.49 MHz
SWH: 24509.8 Hz
NUC: 13C
TD: 31875

F2 - Processing Parameters

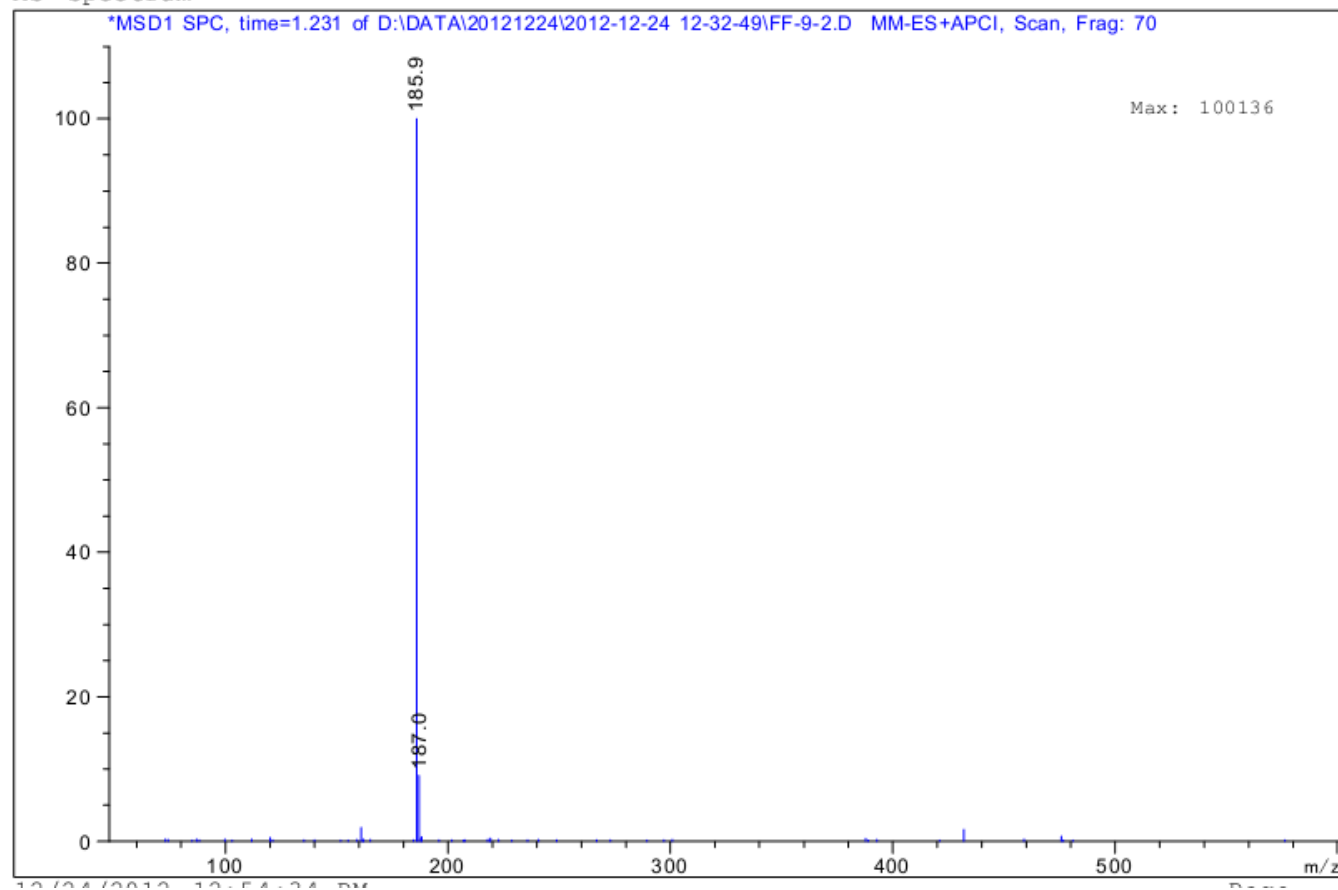
SI: 65536
DC: 0.05
LB: 0.50 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: 147.72
Ph1: -10.14

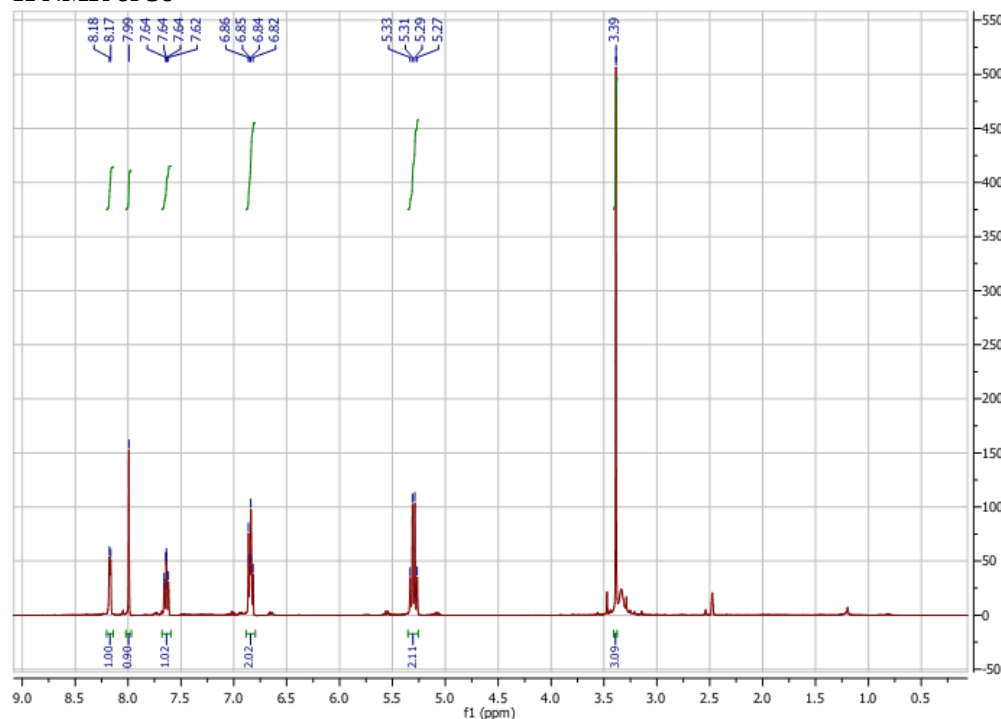


C₉H₇N₅
Exact Mass: 185.07
Mol. Wt.: 185.19

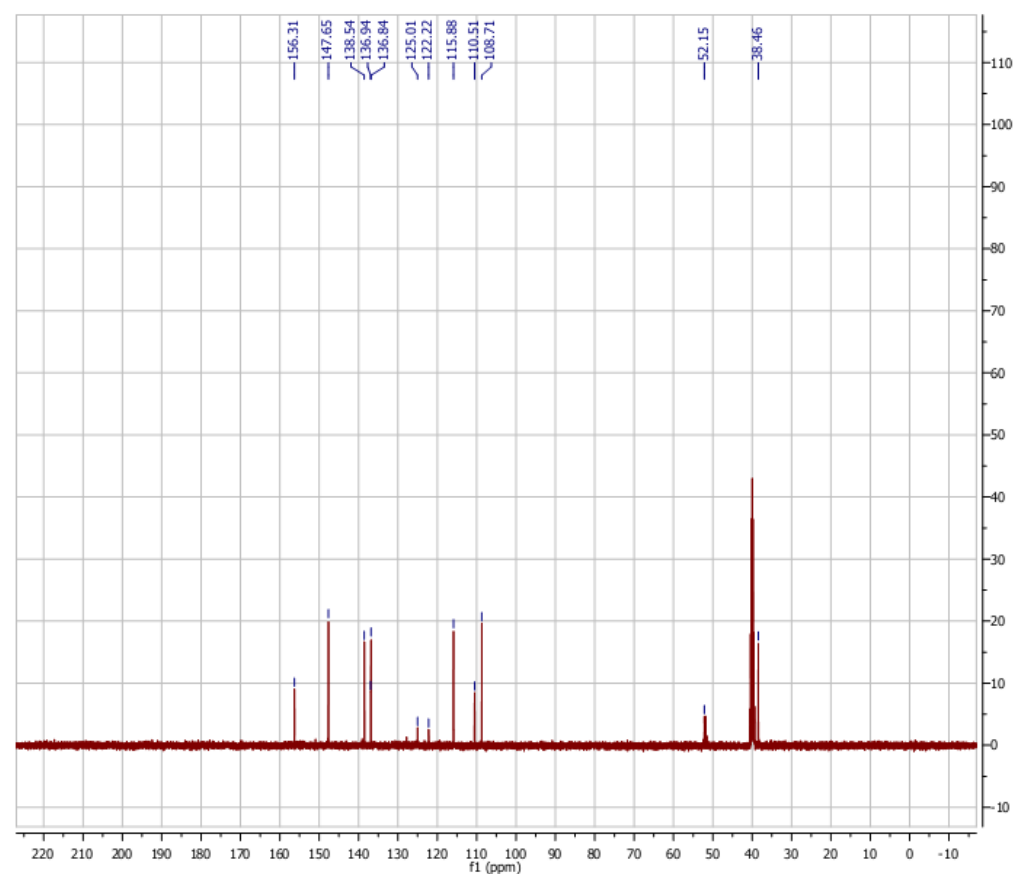
LC-MS of 3n

MS Spectrum

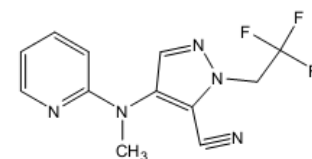


¹H NMR of 3o

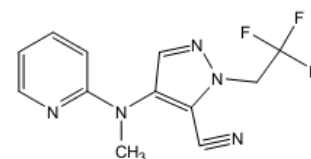
¹H NMR (400 MHz, dmsol) δ 8.17 (d, J = 4.8, 1H), 7.99 (s, 1H), 7.62 - 7.64 (m, 1H), 6.82 - 6.86 (m, 2H), 5.27 - 5.33 (, 2H), 3.39 (s, 3H).

¹³C NMR of 3o

C₁₂H₁₀F₃N₅
Exact Mass: 281.09
Mol. Wt.: 281.24



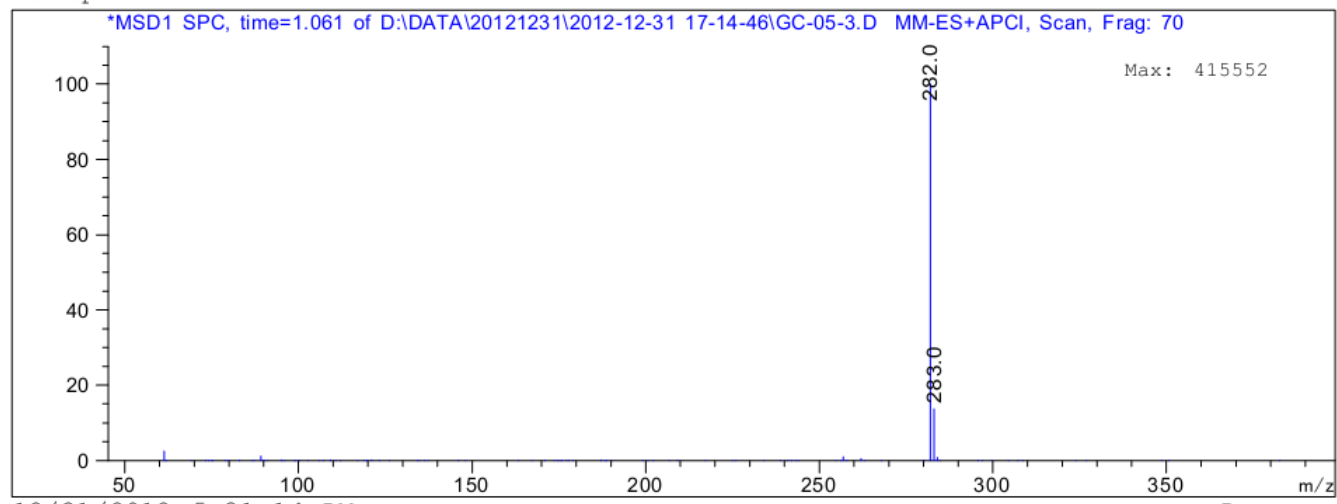
C₁₂H₁₀F₃N₅
Exact Mass: 281.09
Mol. Wt.: 281.24



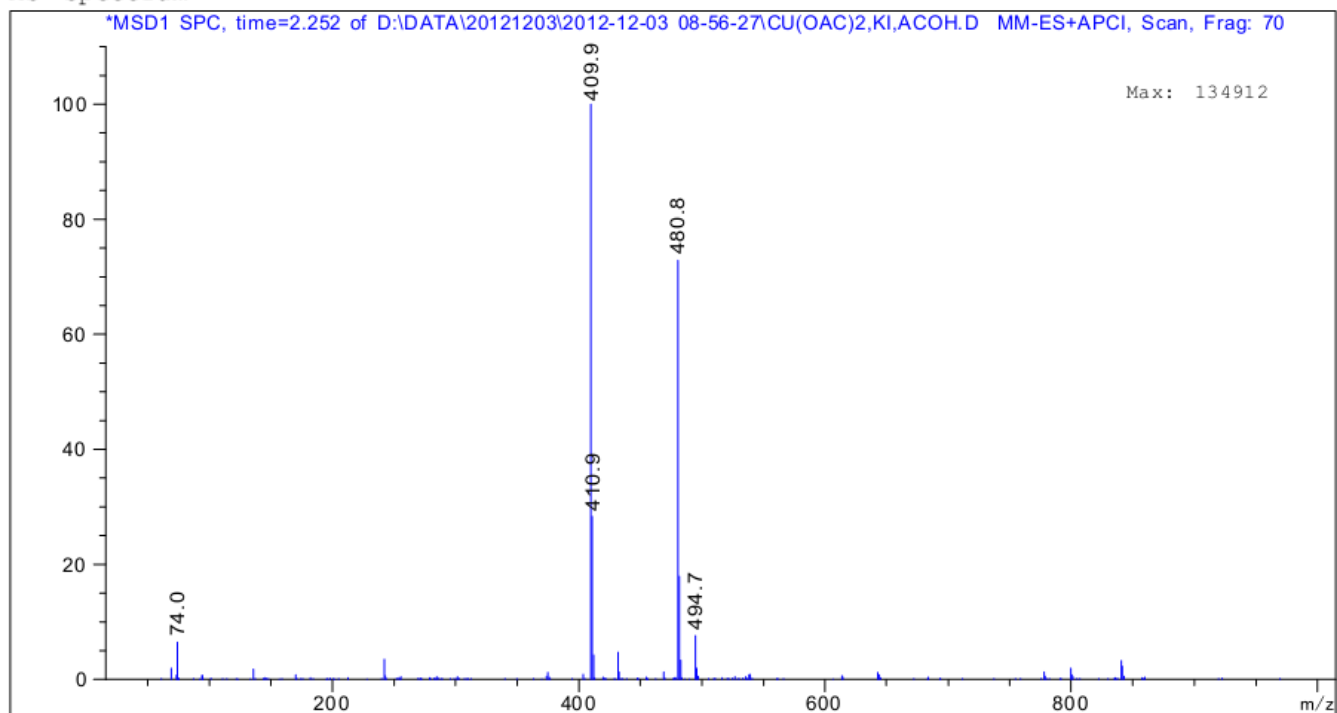
C₁₂H₁₀F₃N₅
Exact Mass: 281.09
Mol. Wt.: 281.24

LC-MS of 3o

MS Spectrum

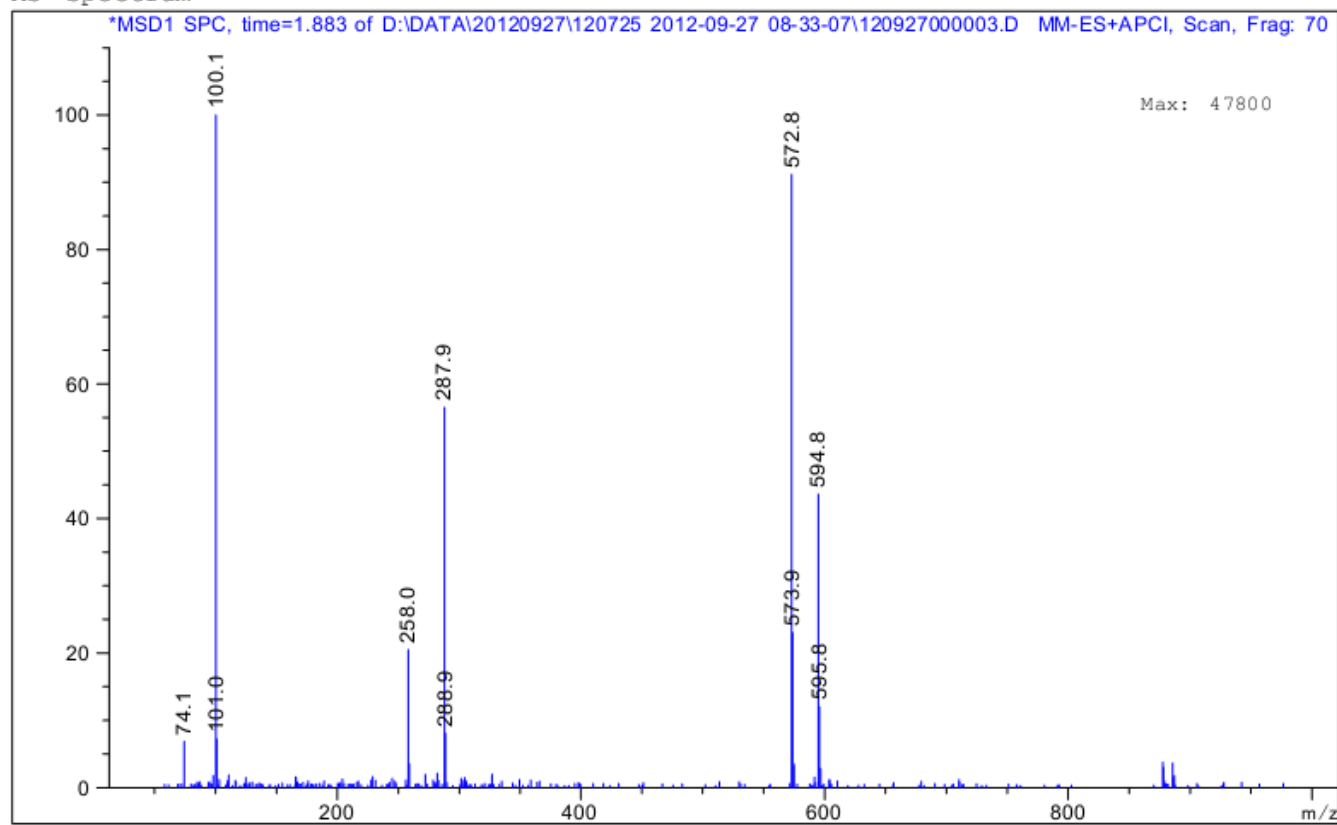
**LC-MS of 4p**

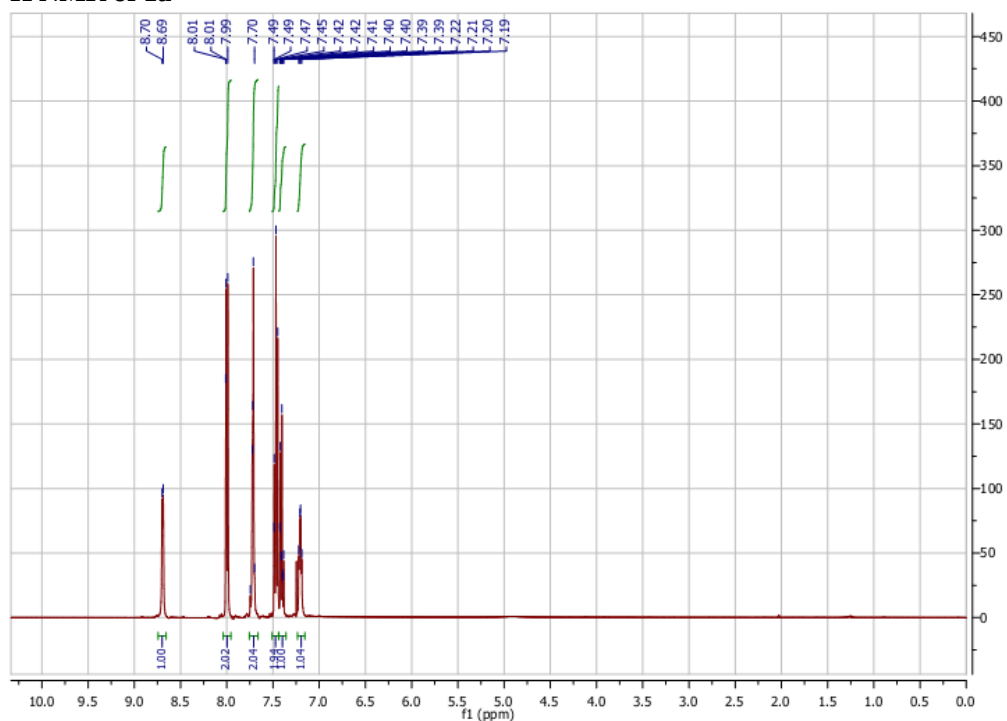
MS Spectrum



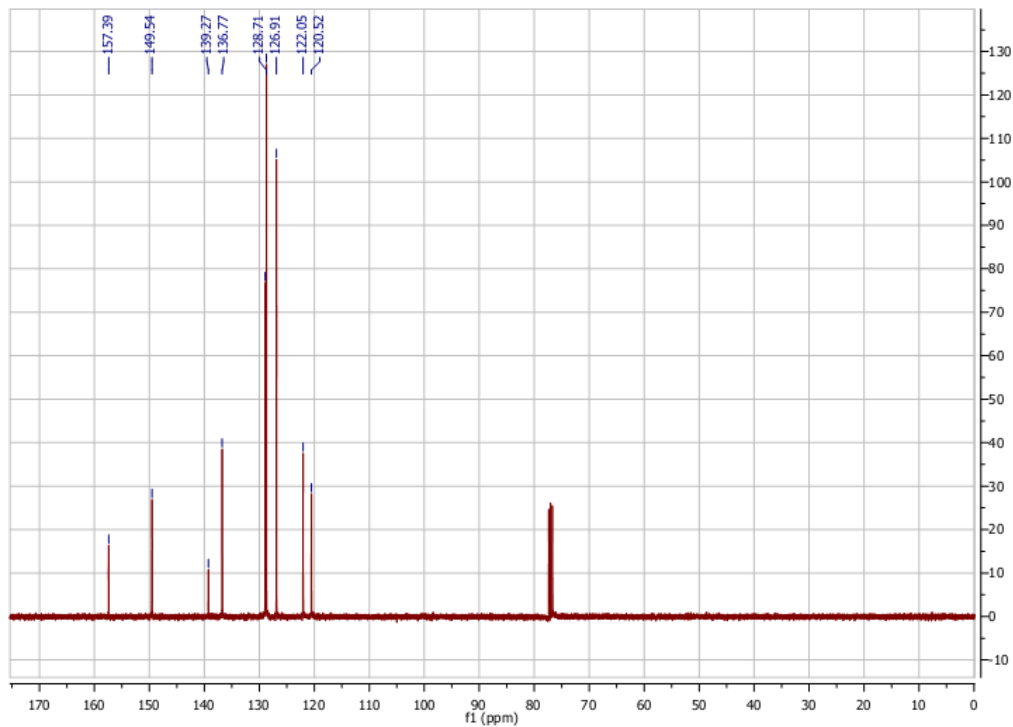
LC-MS of 5q

MS Spectrum



¹H NMR of 1a

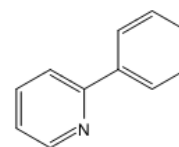
¹H NMR (400 MHz, cdcl₃) δ 8.69 - 8.70 (m, 1H), 7.99 - 8.01 (m, 2H), 7.70 - 7.74 (m, 2H), 7.45 - 7.49 (m, 2H), 7.39 - 7.42 (m, 1H), 7.19 - 7.22 (, 1H).

¹³C NMR of 1a

Hutchison MediPharma

Acquisition Parameters
 NAME: 100868-
 ol-3_Proton_cdcl3_01.fid/fid
 Origin: vmrms
 Owner: jrhong
 DATE: 2013-04-08T01:37:57
 Solvent: cdcl3
 PULPROG: s2pul
 TE: 34 C
 NS: 8
 SFO1: 399.59 MHz
 SWH: 6410.3 Hz
 NUC: 1H
 TD: 13132

F2 - Processing Parameters
 SI: 32768
 DC: 0.05
 LB: 0.00 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: -146.33
 Ph1: -30.96



C11H9N

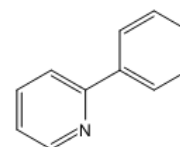
Exact Mass: 155.07

Mol. Wt.: 155.2

Hutchison MediPharma

Acquisition Parameters
 NAME: 100868-
 OL-3_Carbon_cdcl3_01.fid/fid
 Origin: vmrms
 Owner: jrhong
 DATE: 2013-04-08T22:23:14
 Solvent: cdcl3
 PULPROG: s2pul
 TE: 34 C
 NS: 256
 SFO1: 100.49 MHz
 SWH: 24509.8 Hz
 NUC: 13C
 TD: 31875

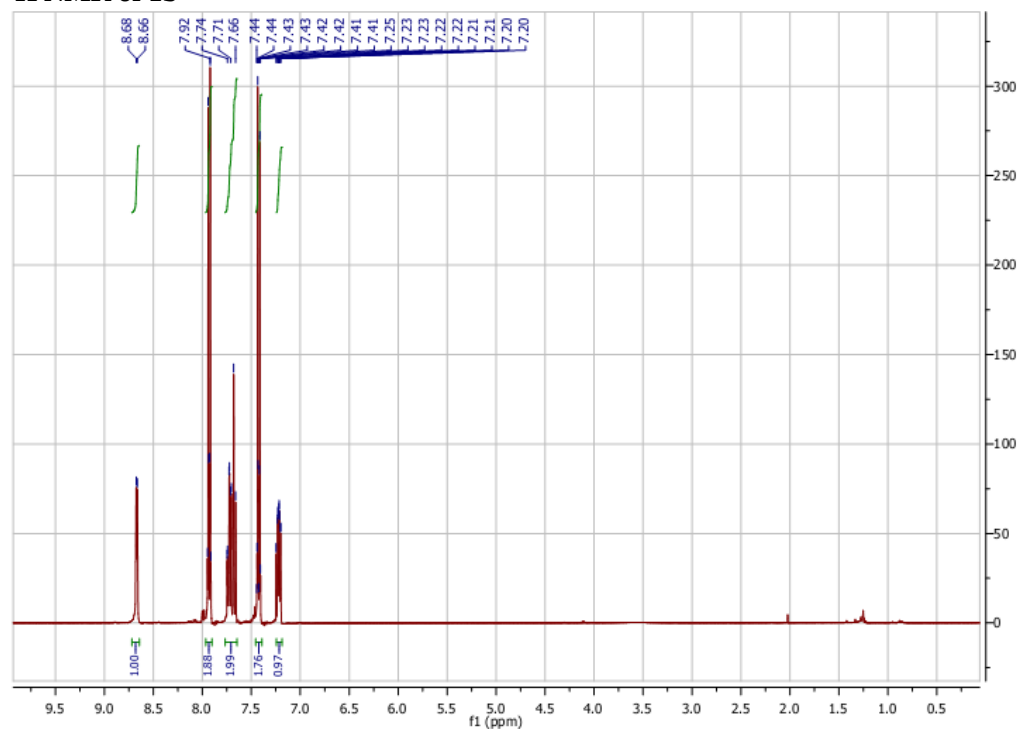
F2 - Processing Parameters
 SI: 65536
 DC: 0.05
 LB: 0.50 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: 49.56
 Ph1: -71.25



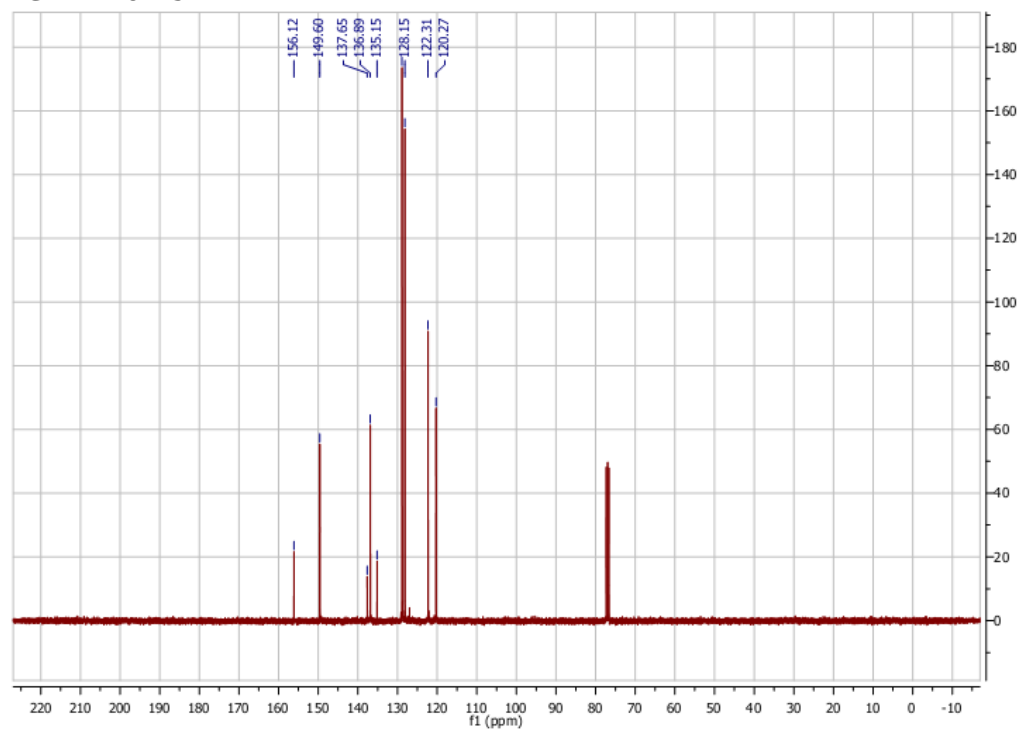
C11H9N

Exact Mass: 155.07

Mol. Wt.: 155.2

¹H NMR of 1b

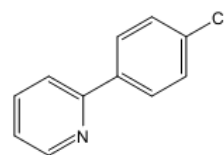
¹H NMR (400 MHz, CDCl_3) δ 8.66 – 8.68 (m, 1H), 7.91 – 7.95 (m, 2H), 7.66 – 7.75 (m, 2H), 7.41 – 7.43 (m, 2H), 7.20 – 7.23 (m, 1H).

¹³C NMR of 1b

Hutchison Medi Pharma

Acquisition Parameters
 NAME: 100868-
 OL-6_Proton_cdc13_01.fid/fid
 Origin: vmrs
 Owner: jrhong
 DATE: 2013-04-11T00:53:13
 Solvent: cdcl_3
 PULPROG: s2pul
 TE: 34 C
 NS: 8
 SF01: 399.59 MHz
 SWH: 6410.3 Hz
 NUC: ¹H
 TD: 13132

F2 - Processing Parameters
 SI: 32768
 DC: 0.05
 LB: 0.00 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: -155.72
 Ph1: 9.73

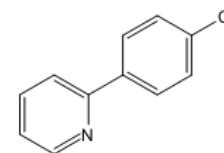


C₁₁H₈ClN
 Exact Mass: 189.03
 Mol. Wt.: 189.64

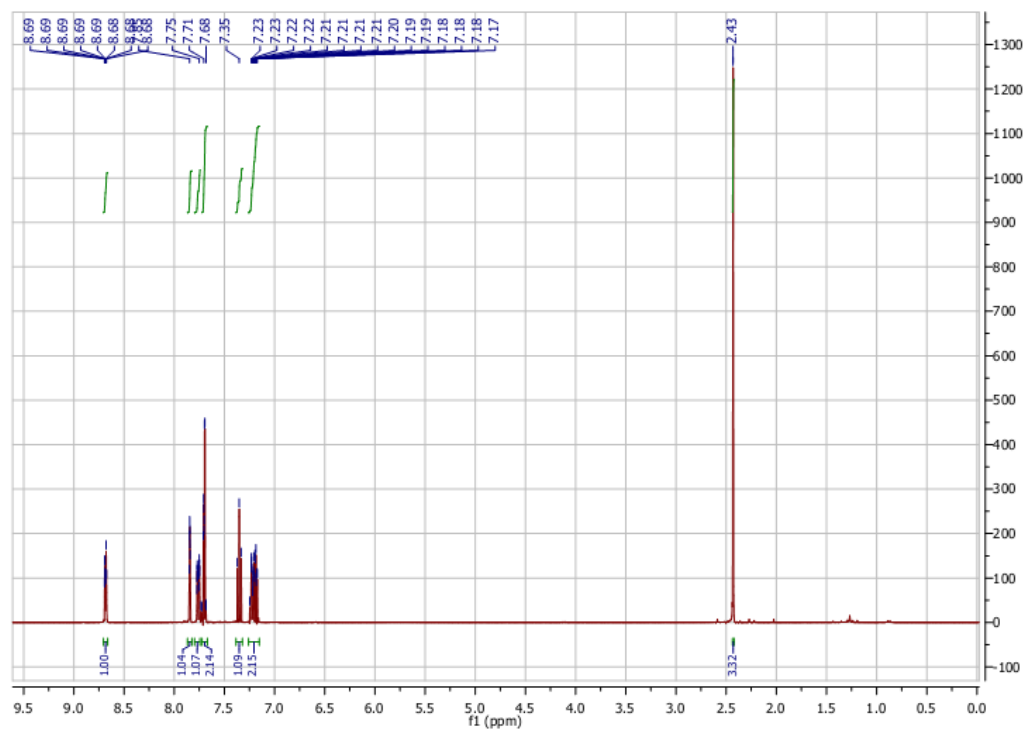
Hutchison Medi Pharma

Acquisition Parameters
 NAME: 100868-
 OL-6_Carbon_cdc13_01.fid/fid
 Origin: vmrs
 Owner: jrhong
 DATE: 2013-04-11T02:57:36
 Solvent: cdcl_3
 PULPROG: s2pul
 TE: 34 C
 NS: 512
 SF01: 100.49 MHz
 SWH: 24509.8 Hz
 NUC: ¹³C
 TD: 31875

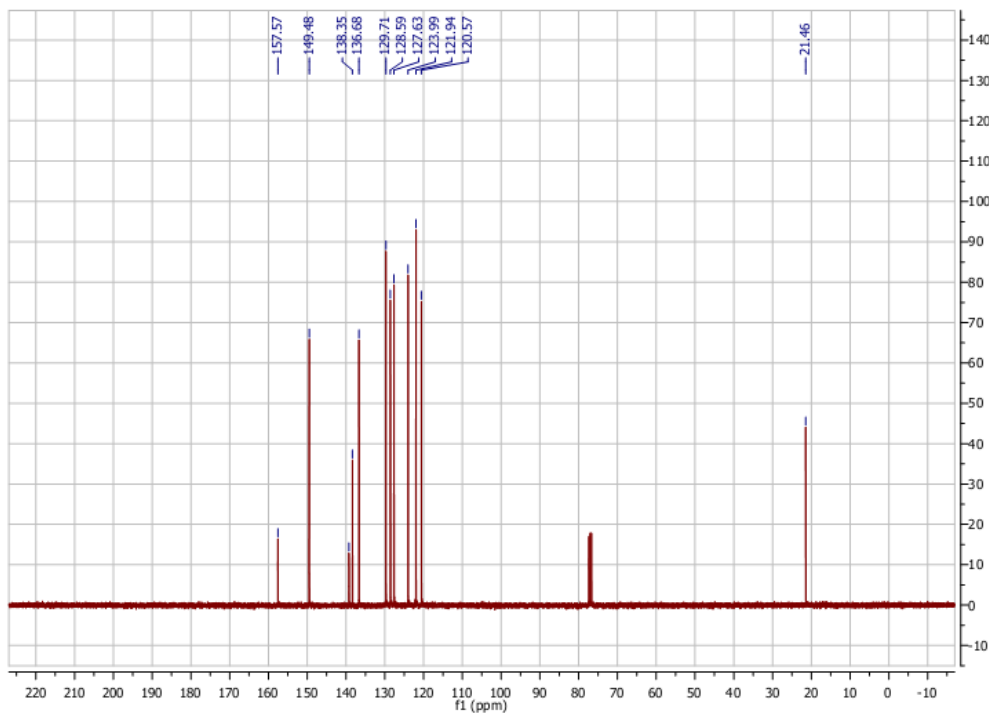
F2 - Processing Parameters
 SI: 65536
 DC: 0.05
 LB: 0.50 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: 15.66
 Ph1: 5.92



C₁₁H₈ClN
 Exact Mass: 189.03
 Mol. Wt.: 189.64

¹H NMR of 1c

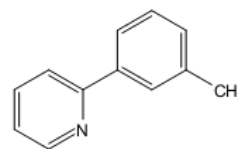
¹H NMR (400 MHz, CDCl_3) δ 8.68–8.69 (m, 1H), 7.84–7.85 (m, 1H), 7.75–7.77 (m, 1H), 7.68–7.71 (m, 2H), 7.33–7.37 (m, 1H), 7.17–7.25 (m, 2H), 2.43 (s, 3H).

¹³C NMR of 1c

Hutchison Medipharma

Acquisition Parameters
 NAME: 100868-
 OL-5_Proton_cdc13_01.fid/fid
 Origin: vnmrs
 Owner: jrhong
 DATE: 2013-04-11T01:54:35
 Solvent: cdc13
 FULPROG: s2pul
 TE: 34 C
 NS: 8
 SFO1: 399.59 MHz
 SWH: 6410.3 Hz
 NUC: 1H
 TD: 13132

F2 - Processing Parameters
 SI: 32768
 DC: 0.05
 LB: 0.00 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: -150.58
 Ph1: -1.72

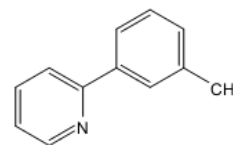


C12H11N
 Exact Mass: 169.09
 Mol. Wt.: 169.22

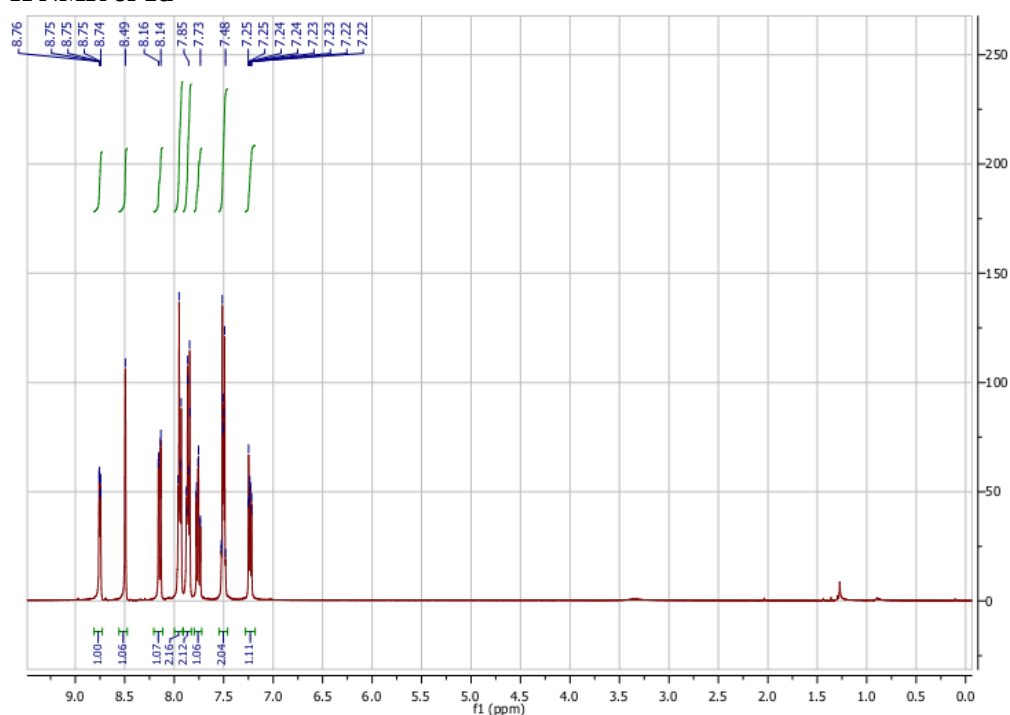
Hutchison Medipharma

Acquisition Parameters
 NAME: 100868-
 OL-5_Carbon_cdc13_01.fid/fid
 Origin: vnmrs
 Owner: jrhong
 DATE: 2013-04-11T02:42:54
 Solvent: cdc13
 FULPROG: s2pul
 TE: 34 C
 NS: 256
 SFO1: 100.49 MHz
 SWH: 24509.8 Hz
 NUC: 13C
 TD: 31875

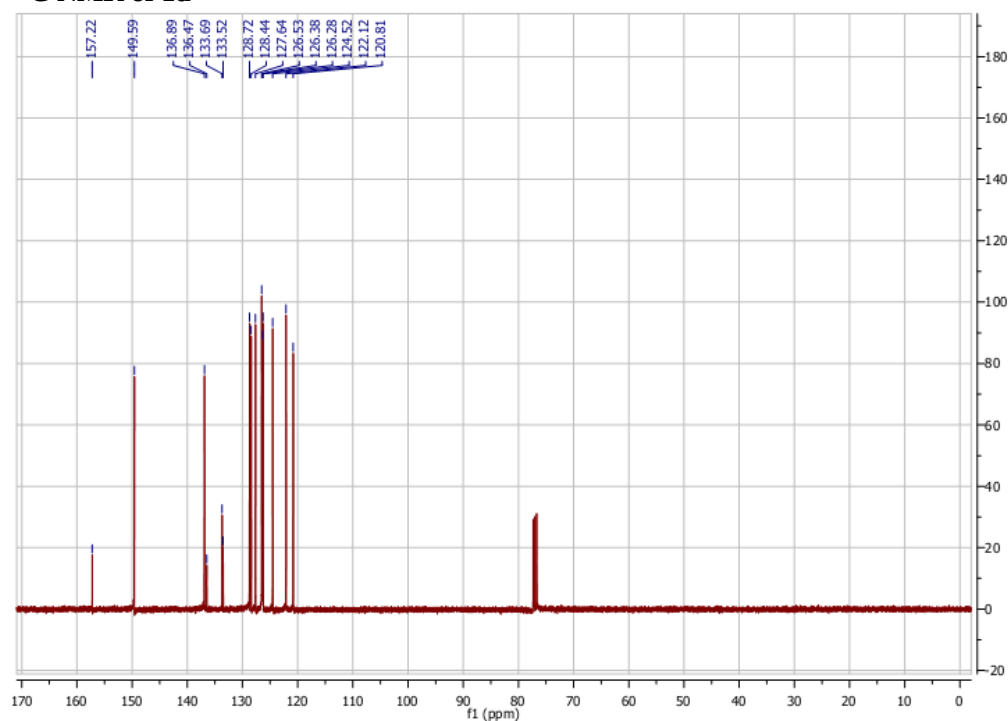
F2 - Processing Parameters
 SI: 65536
 DC: 0.05
 LB: 0.50 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: 26.08
 Ph1: -11.35



C12H11N
 Exact Mass: 169.09
 Mol. Wt.: 169.22

¹H NMR of 1d

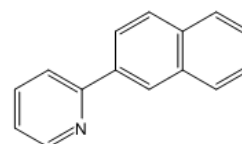
¹H NMR (400 MHz, CDCl_3) δ 8.74 – 8.76 (m, 1H), 8.49 (s, 1H), 8.14 – 8.16 (m, 1H), 7.93 – 7.93 (m, 2H), 7.84 – 7.86 (m, 2H), 7.73 – 7.78 (m, 1H), 7.48 – 7.52 (m, 2H), 7.22 – 7.25 (m, 1H).

¹³C NMR of 1d

Hutchison Medi Pharma

Acquisition Parameters
 NAME: 100868-
 OL-7_Proton_cdc13_01.fid/fid
 Origin: vmrs
 Owner: jrhong
 DATE: 2013-04-15T17:16:47
 Solvent: cdc13
 PULPROG: s2pul
 TE: 34 C
 NS: 8
 SFO1: 399.59 MHz
 SWH: 6410.3 Hz
 NUC: 1H
 TD: 13132

F2 - Processing Parameters
 SI: 32768
 DC: 0.05
 LB: 0.00 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Global

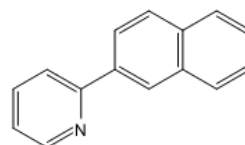


C15H11N
 Exact Mass: 205.09
 Mol. Wt.: 205.25

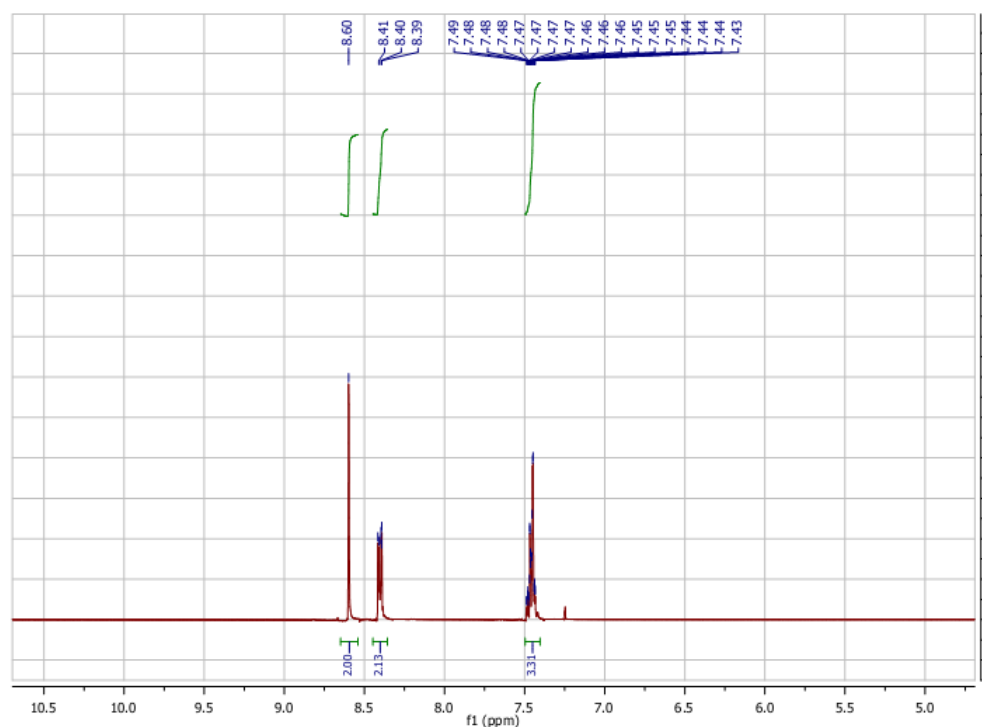
Hutchison Medi Pharma

Acquisition Parameters
 NAME: 100868-
 OL-7_Carbon_cdc13_01.fid/fid
 Origin: vmrs
 Owner: jrhong
 DATE: 2013-04-16T11:42:56
 Solvent: cdc13
 PULPROG: s2pul
 TE: 34 C
 NS: 512
 SFO1: 100.49 MHz
 SWH: 24509.8 Hz
 NUC: 13C
 TD: 31875

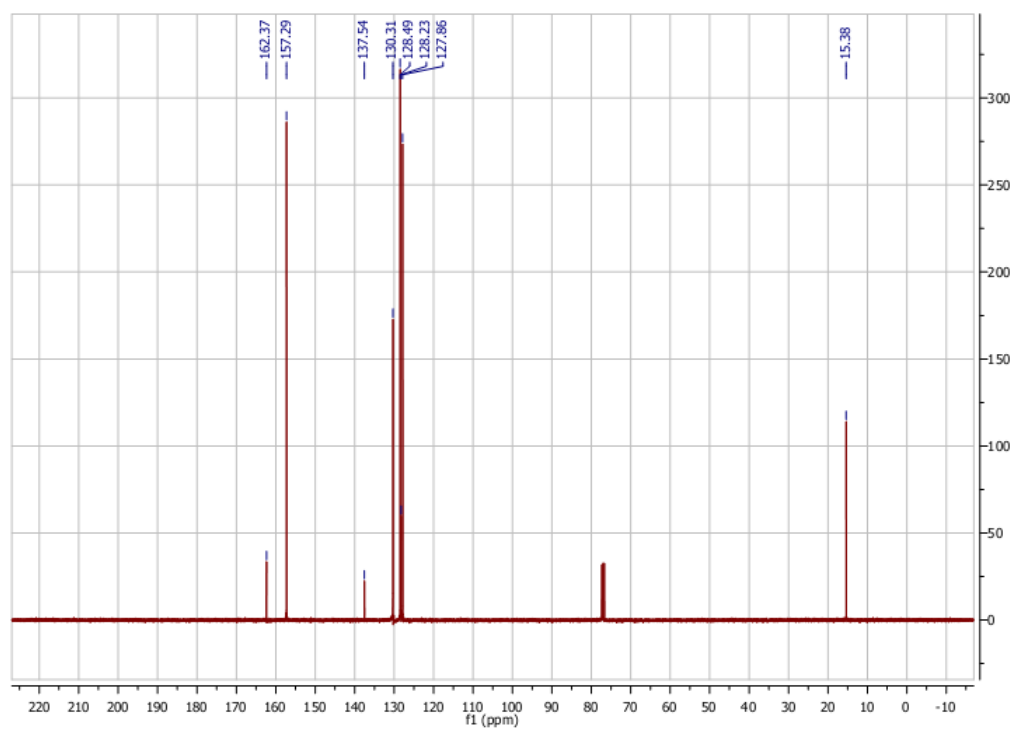
F2 - Processing Parameters
 SI: 65536
 DC: 0.05
 LB: 0.50 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: 82.95
 Ph1: -130.91



C15H11N
 Exact Mass: 205.09
 Mol. Wt.: 205.25

¹H NMR of 1e

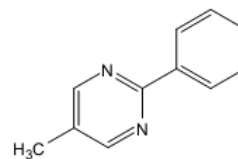
¹H NMR (400 MHz, CDCl_3) δ 8.60 (s, 2H), 8.39 – 8.41 (m, 2H), 7.43 – 7.49 (m, 3H), 2.29 (s, 3H).

¹³C NMR of 1e

Hutchison Medi Pharma

Acquisition Parameters
 NAME: 100868-
 OL-10_Proton_cdcl3_01.fid/fid
 Origin: vrmrs
 Owner: jrhong
 DATE: 2013-04-15T17:23:10
 Solvent: CDCl_3
 PULPROG: s2pul
 TE: 34 C
 NS: 8
 SFO1: 399.59 MHz
 SWH: 6410.3 Hz
 NUC: 1H
 TD: 13132

F2 - Processing Parameters
 SI: 32768
 DC: 0.05
 LB: 0.00 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: -163.93
 Ph1: 18.68

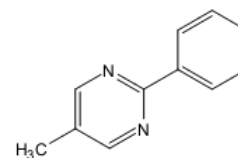


C11H10N2
 Exact Mass: 170.08
 Mol. Wt.: 170.21

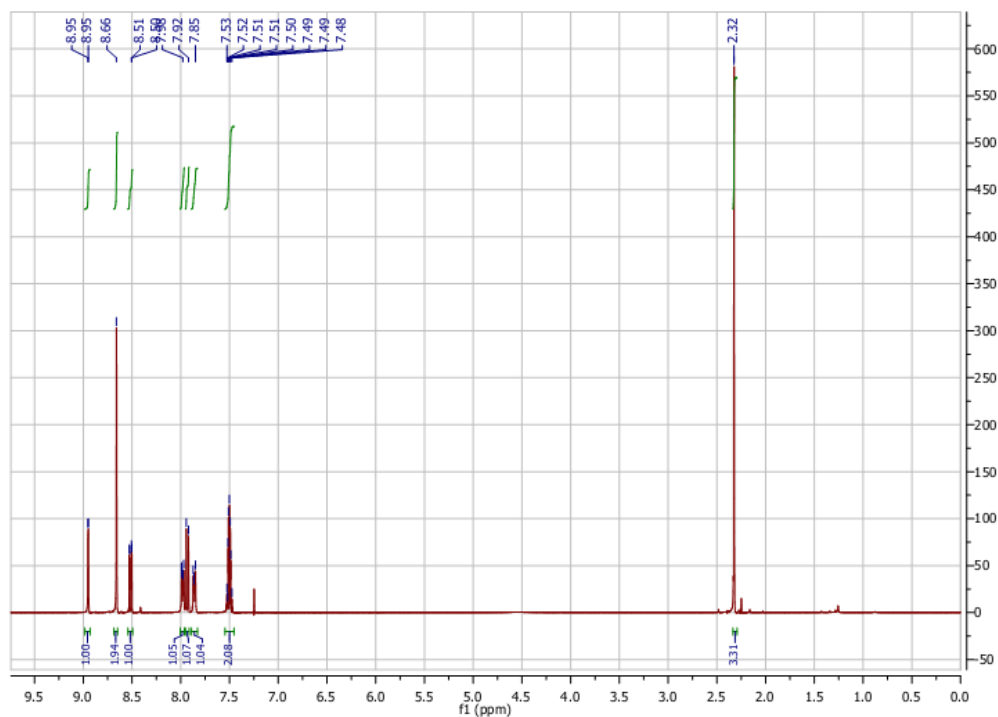
Hutchison Medi Pharma

Acquisition Parameters
 NAME: 100868-
 OL-10_Carbon_cdcl3_01.fid/fid
 Origin: vrmrs
 Owner: jrhong
 DATE: 2013-04-16T12:28:12
 Solvent: CDCl_3
 PULPROG: s2pul
 TE: 34 C
 NS: 512
 SFO1: 100.49 MHz
 SWH: 24509.8 Hz
 NUC: 13C
 TD: 31875

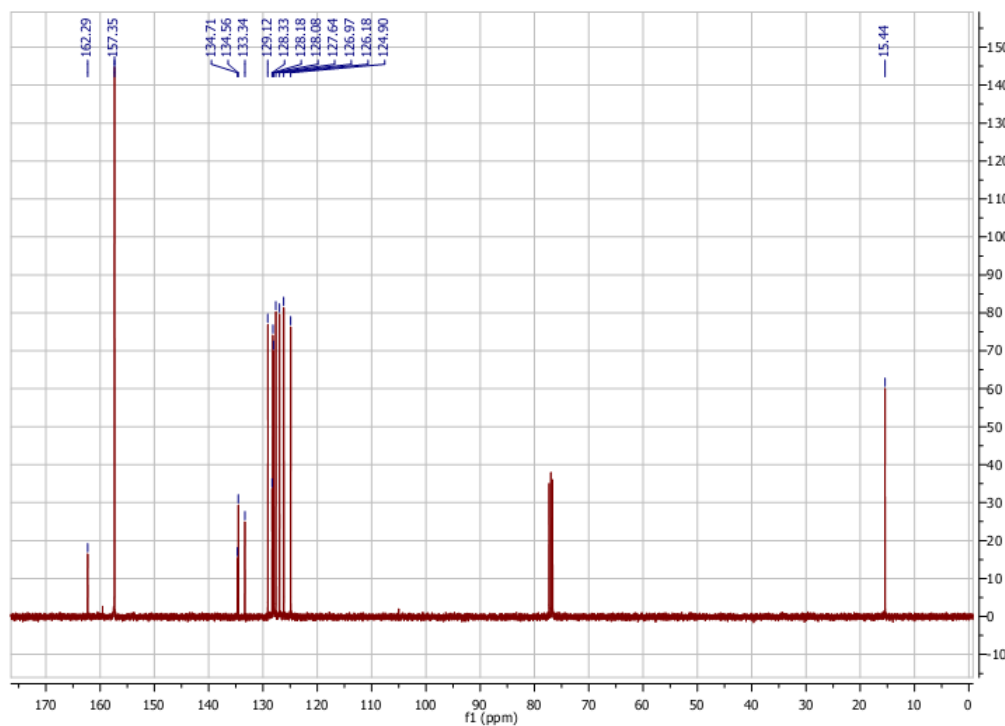
F2 - Processing Parameters
 SI: 65536
 DC: 0.05
 LB: 0.50 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: 37.26
 Ph1: -21.66



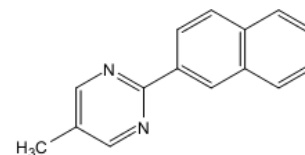
C11H10N2
 Exact Mass: 170.08
 Mol. Wt.: 170.21

¹H NMR of 1f

¹H NMR (400 MHz, CDCl_3) δ 8.95 (s, 1H), 8.66 (s, 2H), 8.50 - 8.53 (m, 1H), 7.97 - 7.99 (m, 1H), 7.92 - 7.94 (m, 1H), 7.85 - 7.87 (m, 1H), 7.48 - 7.53 (m, 2H), 2.32 (s, 3H).

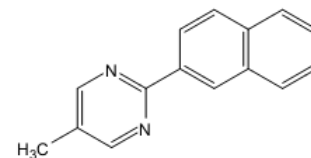
¹H NMR of 1f

C15H12N2
Exact Mass: 220.1
Mol. Wt.: 220.27

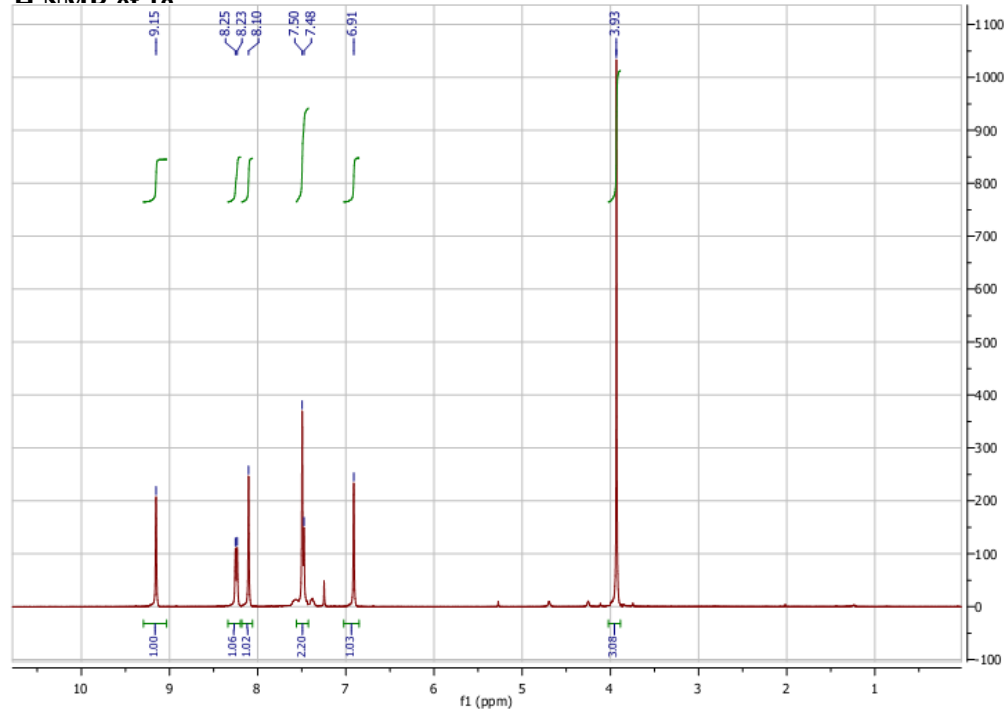


Acquisition Parameters
NAME: 100868-
OL-9_Carbon_cdcl3_01.fid/fid
Origin: vmrs
Owner: jrhong
DATE: 2013-04-16T12:05:37
Solvent: CDCl_3
PULPROG: s2pul1
TE: 34 C
NS: 512
SFO1: 100.49 MHz
SWH: 24509.8 Hz
NUC: 13C
TD: 31875

F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.50 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: 37.79
Ph1: -37.60



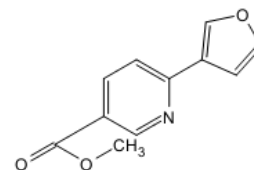
C15H12N2
Exact Mass: 220.1
Mol. Wt.: 220.27

¹H NMR of 1a

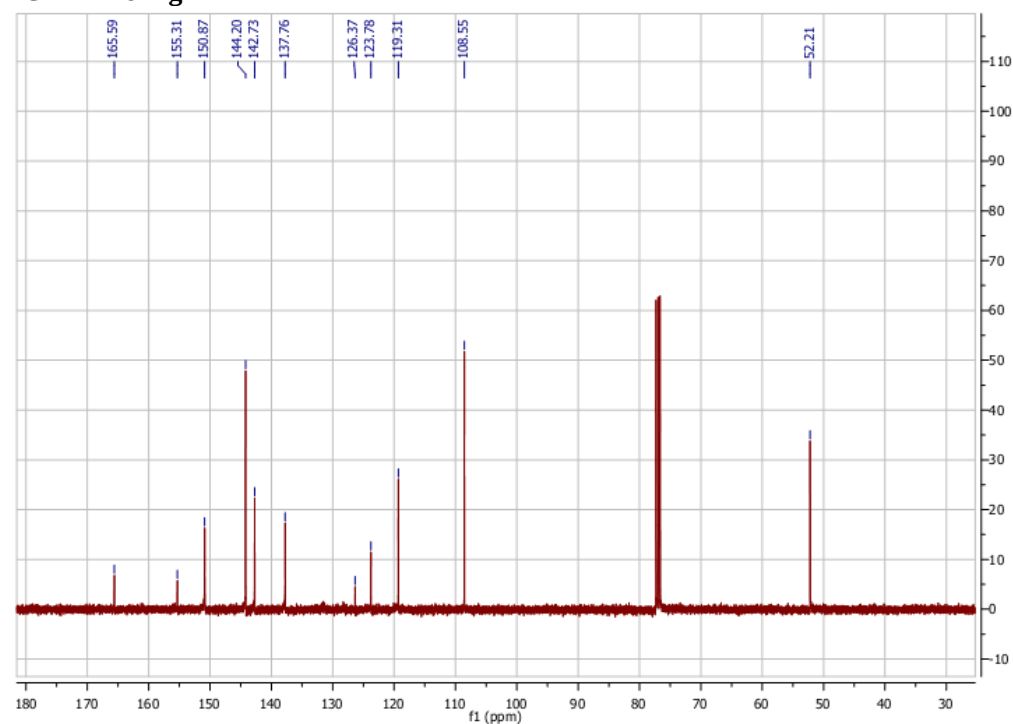
¹H NMR (400 MHz, cdcl₃) δ 9.15 (s, 1H), 8.24 (d, *J* = 8.1, 1H), 8.10 (s, 1H), 7.48-7.50 (m 2H), 6.91 (s, 1H), 3.93 (s, 3H).

Hutchison MediPharma
Acquisition Parameters
 NAME: 100868-
 ol-1_Proton_cdcl3_01.fid/fid
 Origin: vmrs
 Owner: jrhong
 DATE: 2013-04-08T01:25:39
 Solvent: cdcl3
 PULPROG: s2pul
 TE: 34 C
 NS: 8
 SF01: 399.59 MHz
 SWH: 6410.3 Hz
 NUC: 1H
 TD: 13132

F2 - Processing Parameters
 SI: 32768
 DC: 0.05
 LB: 0.00 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: -149.67
 Ph1: -9.91

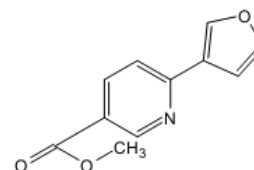


C11H9NO3
 Exact Mass: 203.06
 Mol. Wt.: 203.19

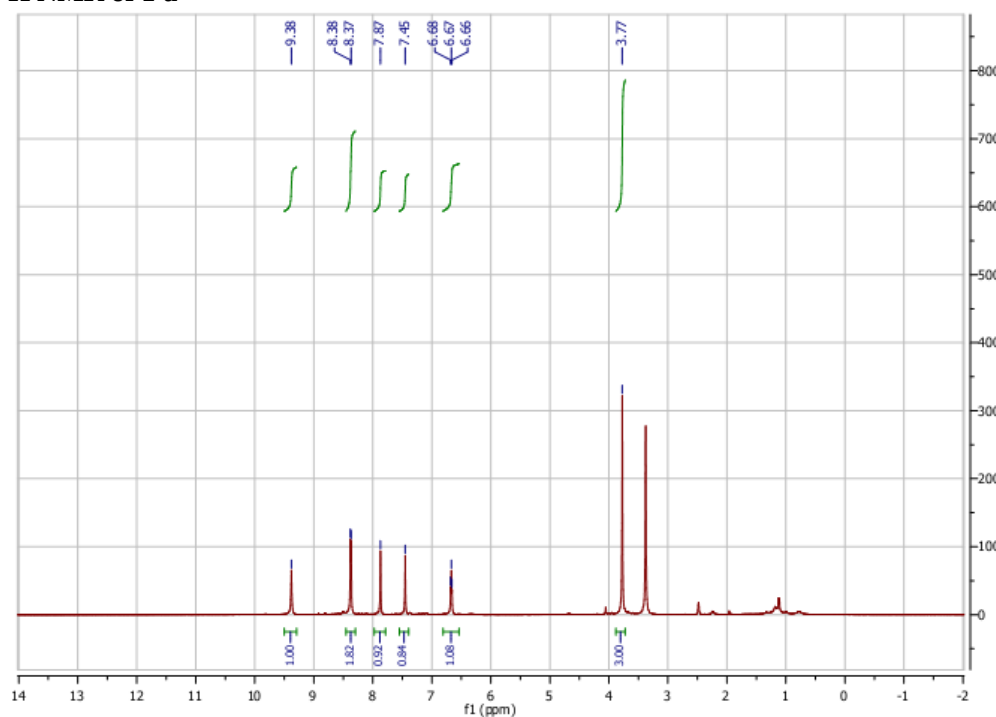
¹³C NMR of 1g

Hutchison MediPharma
Acquisition Parameters
 NAME: 100868-
 ol-1_Carbon_cdcl3_01.fid/fid
 Origin: vmrs
 Owner: jrhong
 DATE: 2013-04-08T01:49:33
 Solvent: cdcl3
 PULPROG: s2pul
 TE: 34 C
 NS: 512
 SF01: 100.49 MHz
 SWH: 24509.8 Hz
 NUC: 13C
 TD: 31875

F2 - Processing Parameters
 SI: 65536
 DC: 0.05
 LB: 0.50 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: 72.89
 Ph1: -97.36



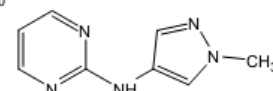
C11H9NO3
 Exact Mass: 203.06
 Mol. Wt.: 203.19

¹H NMR of 1'a

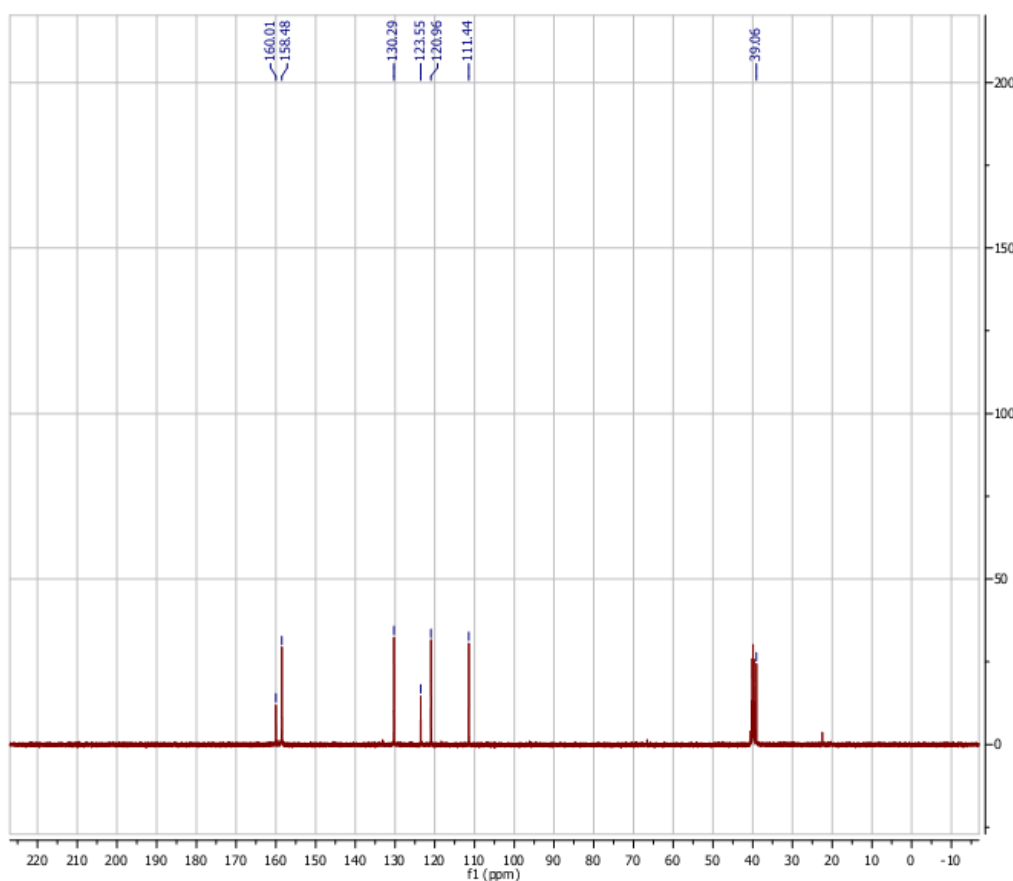
¹H NMR (400 MHz, dmsO) δ 9.38 (s, 1H), 8.37 (d, J = 4.6, 2H), 7.87 (s, 1H), 7.45 (s, 1H), 6.67 (t, J = 4.6, 1H), 3.77 (s, 3H).

Hutchison Medi Pharma
Acquisition Parameters
NAME: 100868-
ff-001-23_Proton_dmsO_01.fid/fid
Origin: vnmrs
Owner: jrhong
DATE: 2012-11-23T22:52:50
Solvent: dmsO
PULPROG: s2pul
TE: 25 C
NS: 8
SFO1: 399.61 MHz
SWH: 6410.3 Hz
NUC: 1H
TD: 13132

F2 - Processing Parameters
SI: 32768
DC: 0.05
LB: 0.00 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: 123.69
Ph1: -11.84

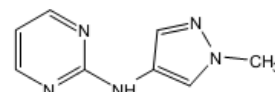


C8H9N5
Exact Mass: 175.09
Mol. Wt.: 175.19

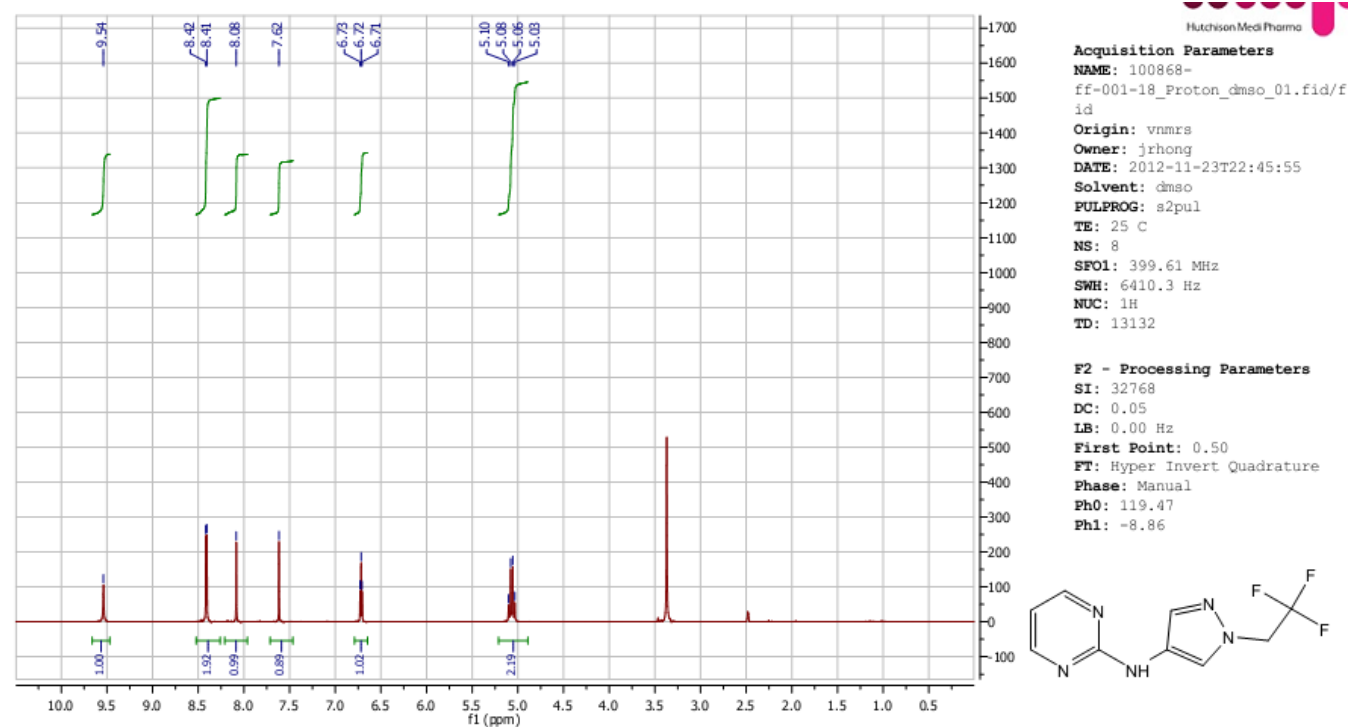
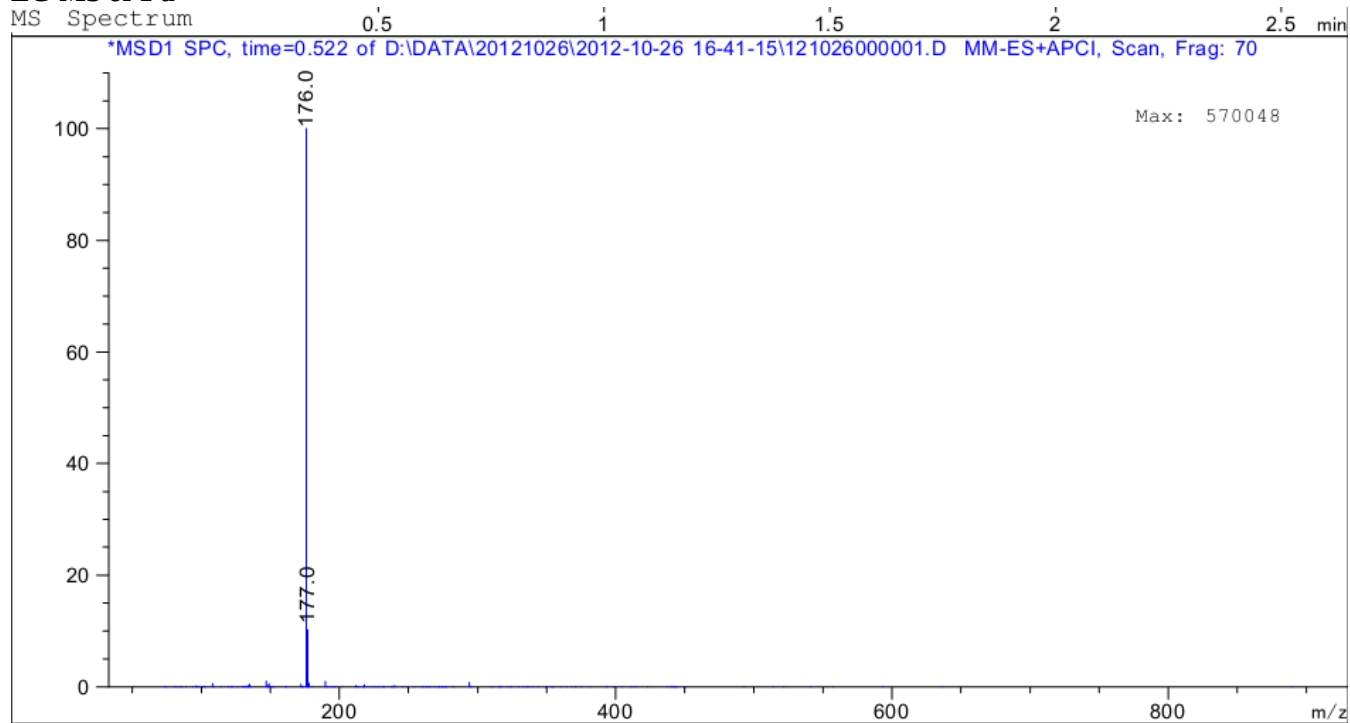
¹³C NMR of 1'a

Hutchison Medi Pharma
Acquisition Parameters
NAME: 100868-
ff-001-23_Carbon_dmsO_01.fid/fid
Origin: vnmrs
Owner: jrhong
DATE: 2012-11-26T22:11:15
Solvent: dmsO
PULPROG: s2pul
TE: 25 C
NS: 256
SFO1: 100.49 MHz
SWH: 24509.8 Hz
NUC: 13C
TD: 31875

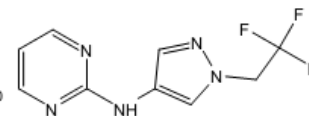
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.50 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: 204.30
Ph1: -25.66

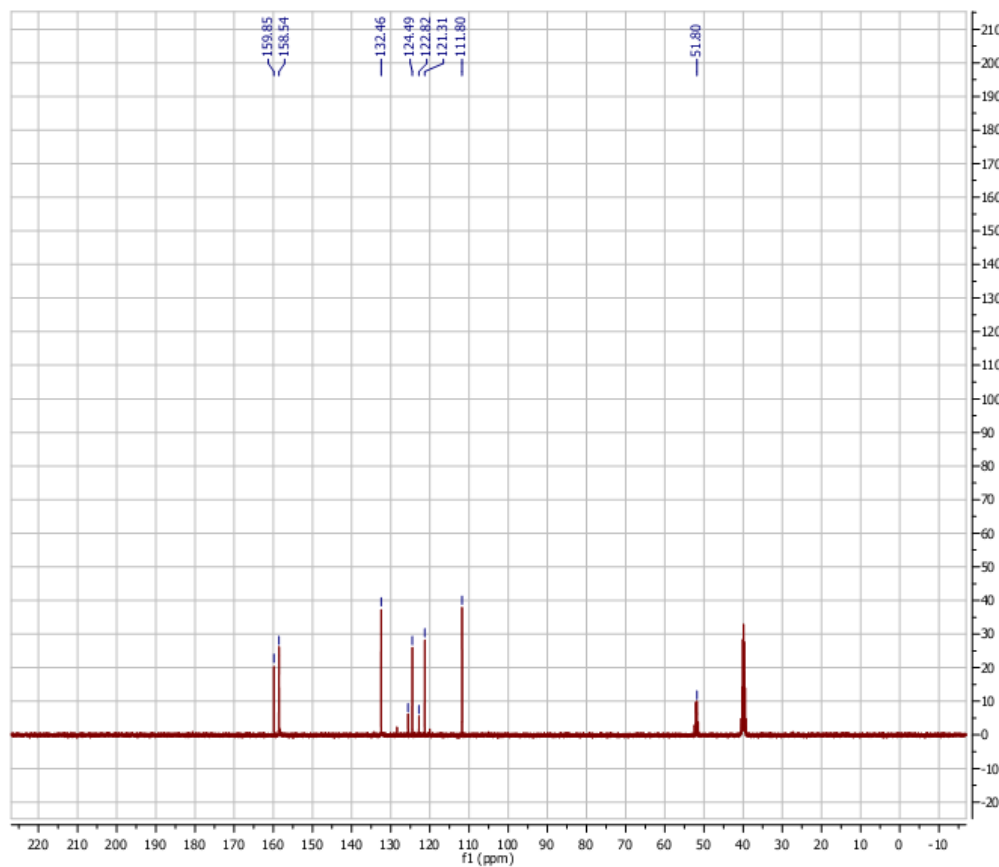


C8H9N5
Exact Mass: 175.09
Mol. Wt.: 175.19



C₉H₈F₃N₅
Exact Mass: 243.07
Mol. Wt.: 243.19



¹³C NMR of 1'b

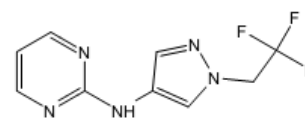
Hutchison MediPharma

Acquisition Parameters

NAME: 100868-
ff-001-18_Carbon_dms0_01.fid/f
id
Origin: vnmrs
Owner: jrhong
DATE: 2012-11-24T18:24:02
Solvent: dms0
PULPROG: s2pu1
TE: 25 C
NS: 256
SF01: 100.49 MHz
SWH: 24509.8 Hz
NUC: 13C
TD: 31875

F2 - Processing Parameters

SI: 65536
DC: 0.05
LB: 0.50 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: -159.06
Ph1: -7.63

C₉H₈F₃N₅

Exact Mass: 243.07

Mol. Wt.: 243.19

Noesy analysis of 1'b

100868-ff-001-18

exp8 Noesy

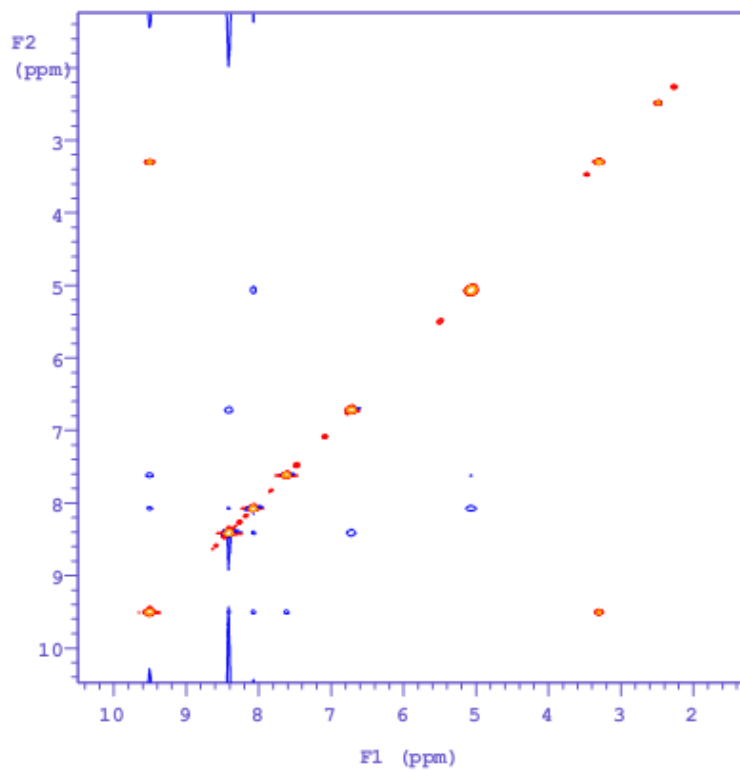
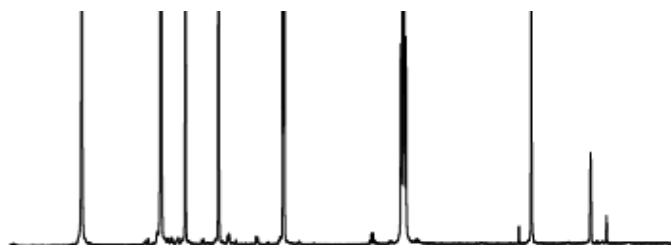
SAMPLE		2D DISPLAY		ACQUISITION ARRAYS	
date	Jan 14 2013	apl	499.6	array	phase
solvent	dmso	wpl	3691.2	arraydim	400
file	/home/jrhong/~	ac2	0		
vmrays/data/100868-	wo2	155		1	phase
8-ff-001-18 Noesy ~	rfl1	-492.3		1	1
dmso_01.fid	rflp1	0		2	2

ACQUISITION		DEC. & VT	
sfrq	399.601	dfrq	100.489
tn	E1	dn	C13
at	0.138	dpwr	31
np	1024	dof	0
sw	3720.2	dm	n
fb	4000	dsm	c
bs	32	dnt	29412
ss	16	dseq	
tpwr	59	dres	9.0
pw	12.3	homo	n
compW	1.0680	temp	30.0
dl	1.000	PROCESSING	
mix	1.000	gf	0.564
tof	354.4	qfs	not used
nt	16	wtfile	
ct	16	proc	ft
gain	32	fn	1024
aspl	y	math	f
gtl	0.0025	asfilter	not used
qslvll	1604	asorder	3
hagt	0.0020	asntaps	3
haglvi	1203	2D PROCESSING	
satnode	nmn	gfi	0.029
satpwr	-13	gfal	not used
satdly	0	wtfile1	
scuba	n	procl	lp
sqfig	y	fnl	1024
alt_grd	n		

FLAGS	
il	n
in	n
dp	y
hs	nn
aspl	y

2D ACQUISITION	
sw6	3720.2
ni	200
phase	arrayed

DISPLAY	
ap	499.6
vp	3683.9
vs	5750
sc	0
wc	250
hsmn	25.64
is	744.69
rfl	-492.3
rtp	0
th	2
lms	100.000
ai	cdc ph



100868-ff-001-18

exp8 Noesy

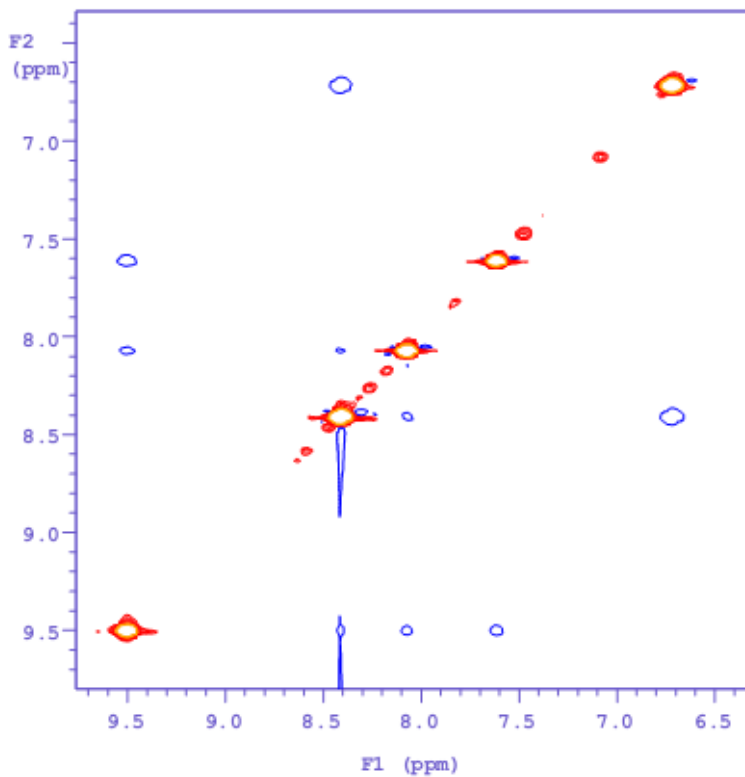
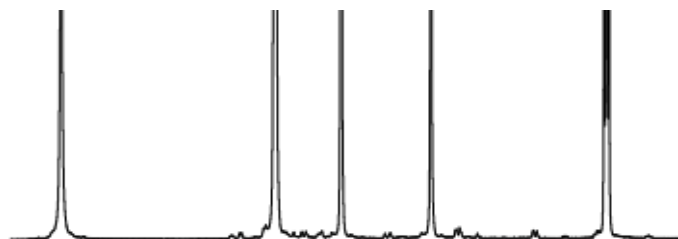
SAMPLE		2D DISPLAY		ACQUISITION ARRAYS	
date	Jan 14 2013	apl	2519.6	array	phase
solvent	dmsc	wpl	1380.6	arraydim	400
file	/home/jrhong/-	sc2	0		
vmrays/data/10086-	wc2		124	i	phase
8-ff-001-18 Noesy_-	rfil		-492.3	1	1
dmsc_01.fid	rfpl		0	2	2

ACQUISITION		DEC. & VT	
afreq	399.601	dfrq	100.489
tn	81	dn	C13
at	0.138	dpwr	31
np	1024	dof	0
sw	3720.2	dn	n
fb	4000	dms	c
bs	32	dmf	29412
ss	16	dseq	
tpwr	59	drax	9.0
pw	12.3	homo	n
comp	1.0680	temp	30.0
dl	1.000	PROCESSING	
mix	1.000	gf	0.064
tof	354.4	qfa	not used
nt	16	wtfile	
ct	16	proc	ft
gain	32	fn	1024
aspl	y	nath	f
gtl	0.0025	asfilter	not used
qtlvll	1604	asorder	3
hagt	0.0020	asntaps	3
haglvl	1203	2D PROCESSING	
satmode	nmn	gfl	0.029
satpwr	-13	gfal	not used
satdly	0	wtfile	
scuba	n	procl	lp
zqflg	y	fnl	1024
alt_grd	n		

FLAGS	
il	n
in	n
dp	y
bs	nm
aspl	y

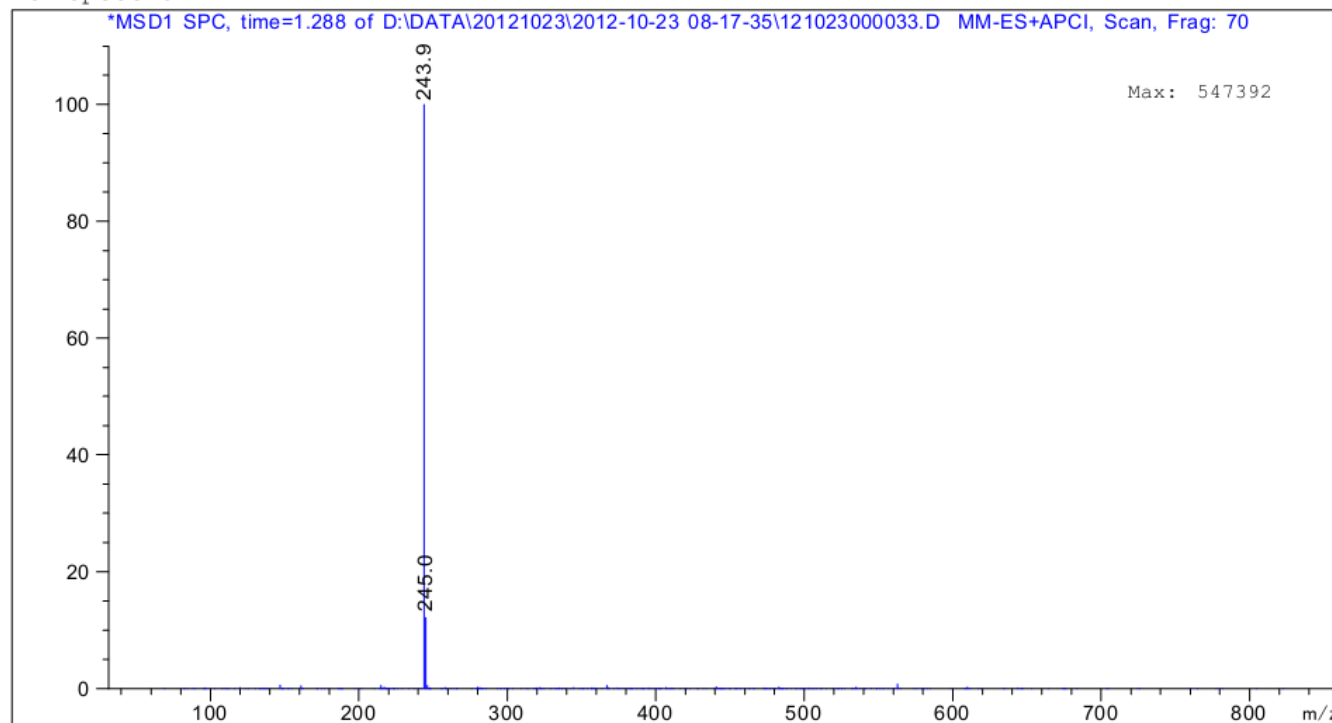
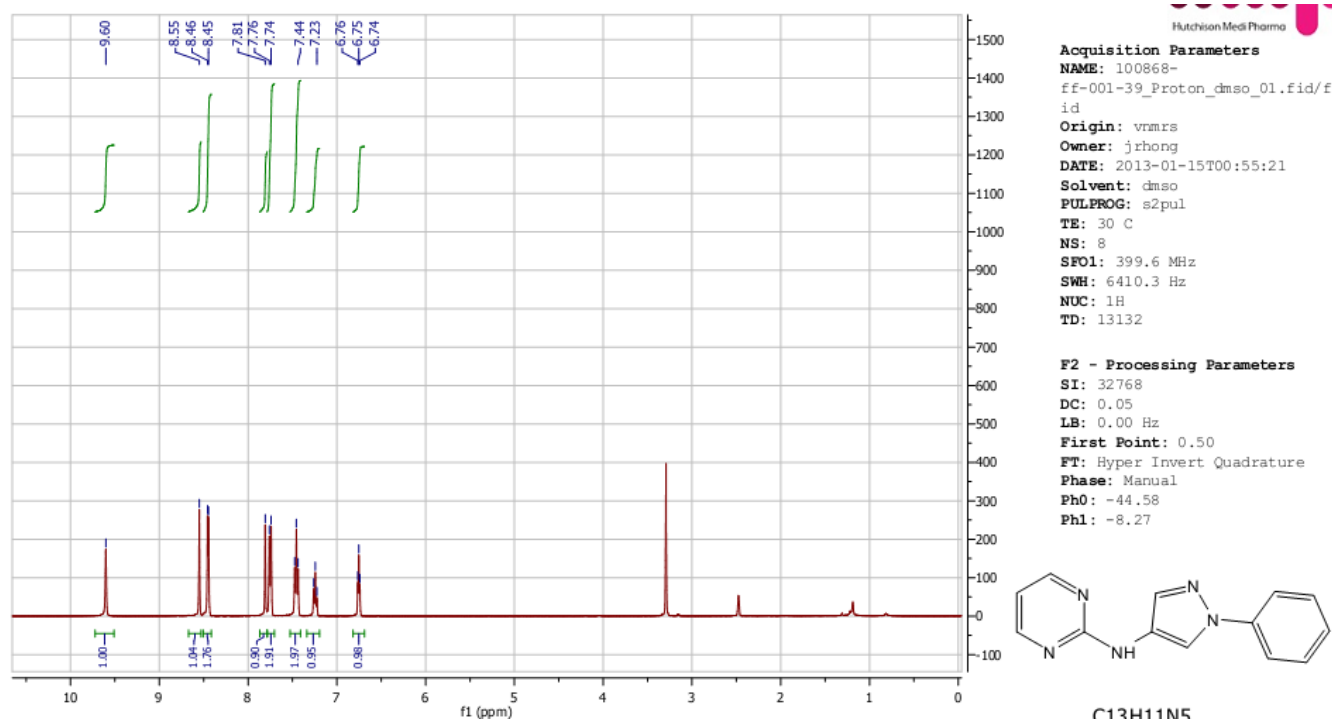
2D ACQUISITION	
swd	3720.2
ni	200
phase	arrayed

DISPLAY	
sp	2534.1
wp	1380.6
vs	5750
sc	6
wc	124
hmm	29.71
ls	744.69
rfl	-492.3
rfp	0
th	2
ins	100.000
al	cdc ph



LC-MS of 1'b

MS Spectrum

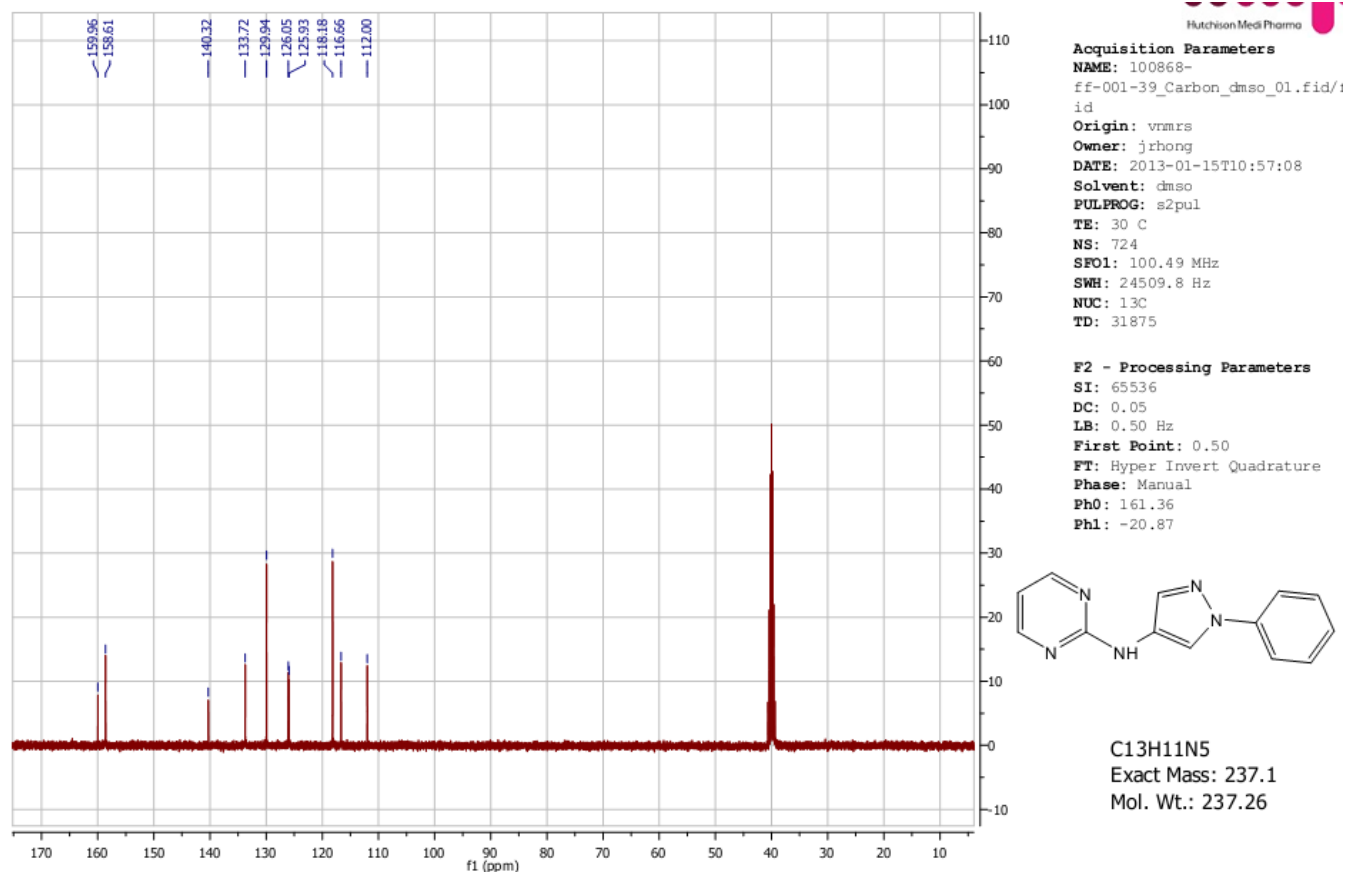
¹H NMR of 1'c

¹H NMR (400 MHz, dms0) δ 9.60 (s, 1H), 8.55 (s, 1H), 8.45 (d, J = 4.7, 2H), 7.81 (s, 1H), 7.75 (d, J = 7.9, 2H), 7.46 (t, J = 7.8, 2H), 7.24 (t, J = 7.3, 1H), 6.75 (t, J = 4.7, 1H).

C13H11N5

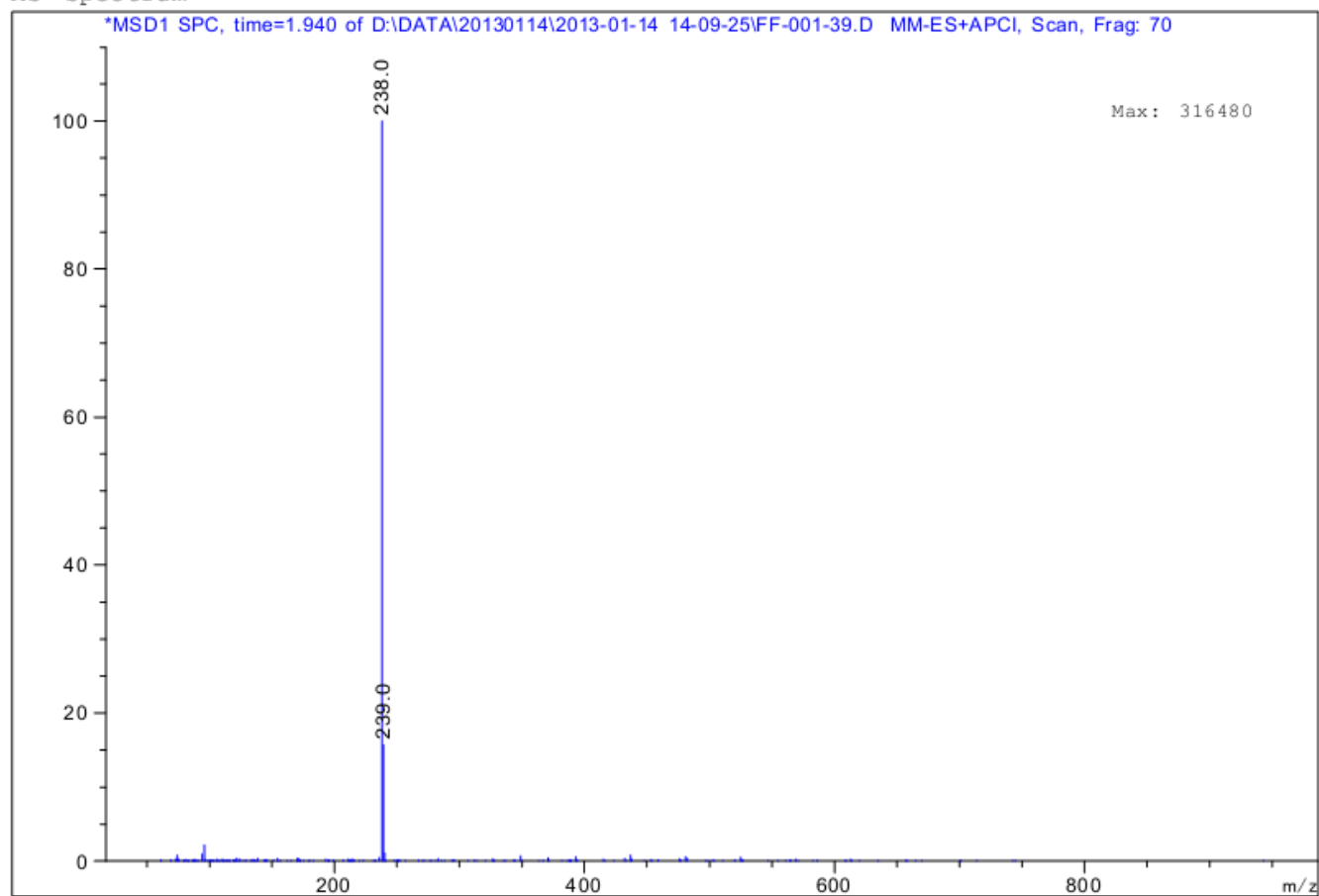
Exact Mass: 237.1

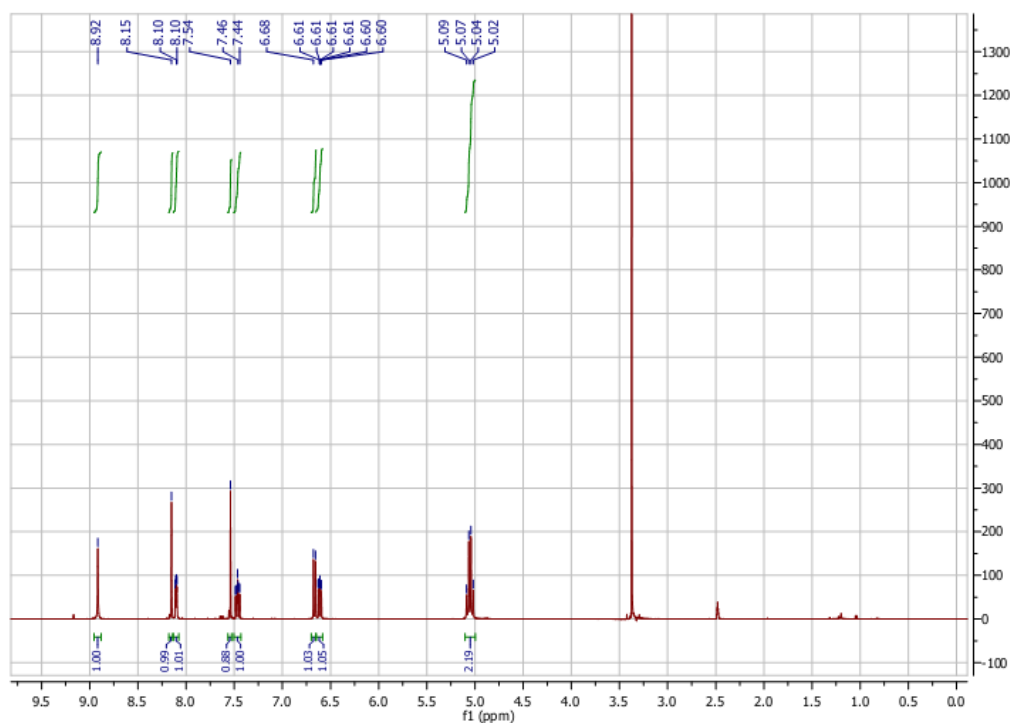
Mol. Wt.: 237.26

¹³C NMR of 1'c

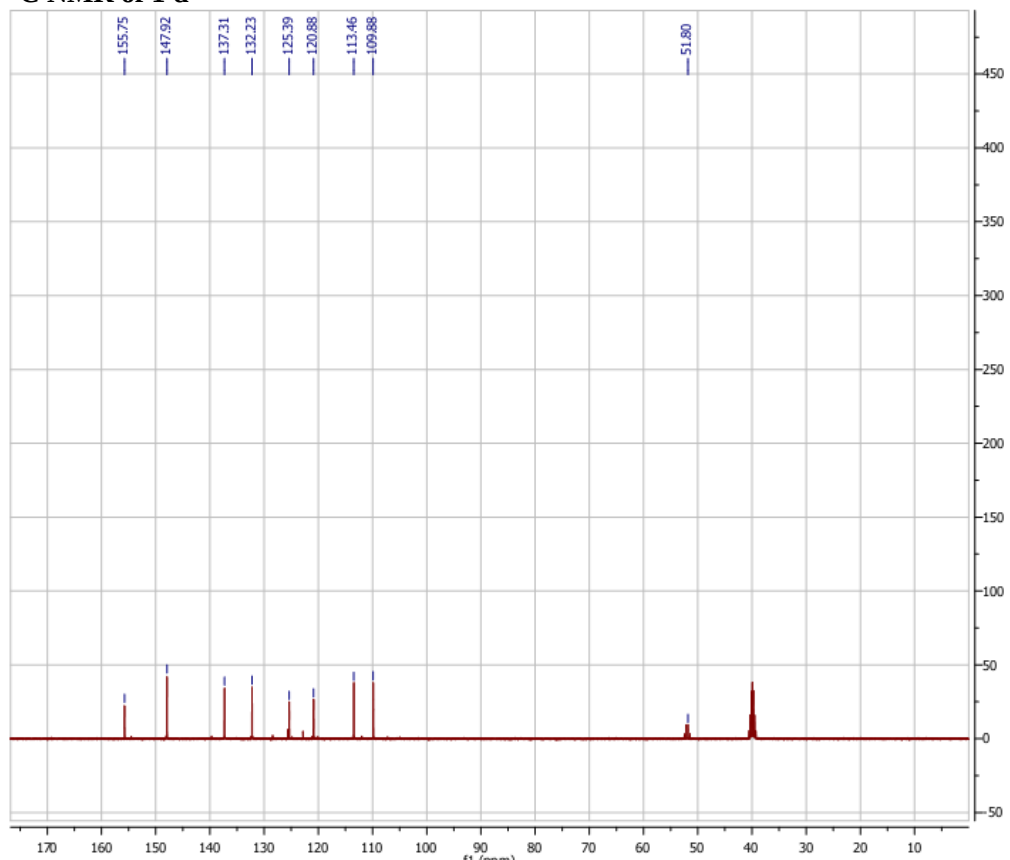
LC-MS of 1'**c**

MS Spectrum



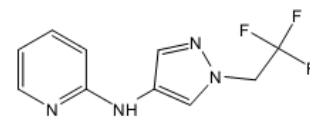
¹H NMR of 1'd

¹H NMR (400 MHz, DMSO) δ 8.92 (s, 1H), 8.15 (s, 1H), 8.10 - 8.11 (m, 1H), 7.54 (s, 1H), 7.44 - 7.49 (m, 1H), 6.66 - 6.68 (m, 1H), 6.60 - 6.63 (m, 1H), 5.02 - 5.09 (m, 2H).

¹³C NMR of 1'd

Acquisition Parameters
 NAME: 100868-ff-001-19_Proton_dms0_01.fid/fid
 Origin: vnmrs
 Owner: jrhong
 DATE: 2012-11-23T22:49:22
 Solvent: dms0
 PULPROG: s2pul
 TE: 25 C
 NS: 8
 SFO1: 399.61 MHz
 SWH: 6410.3 Hz
 NUC: 1H
 TD: 13132

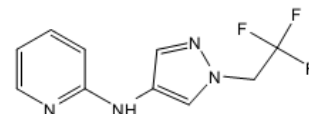
F2 - Processing Parameters
 SI: 32768
 DC: 0.05
 LB: 0.00 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: 120.56
 Ph1: -10.68



C₁₀H₉F₃N₄
 Exact Mass: 242.08
 Mol. Wt.: 242.2

Acquisition Parameters
 NAME: 100868-ff-001-19_Carbon_dms0_01.fid/fid
 Origin: vnmrs
 Owner: jrhong
 DATE: 2012-11-24T18:37:08
 Solvent: dms0
 PULPROG: s2pul
 TE: 25 C
 NS: 256
 SFO1: 100.49 MHz
 SWH: 24509.8 Hz
 NUC: 13C
 TD: 31875

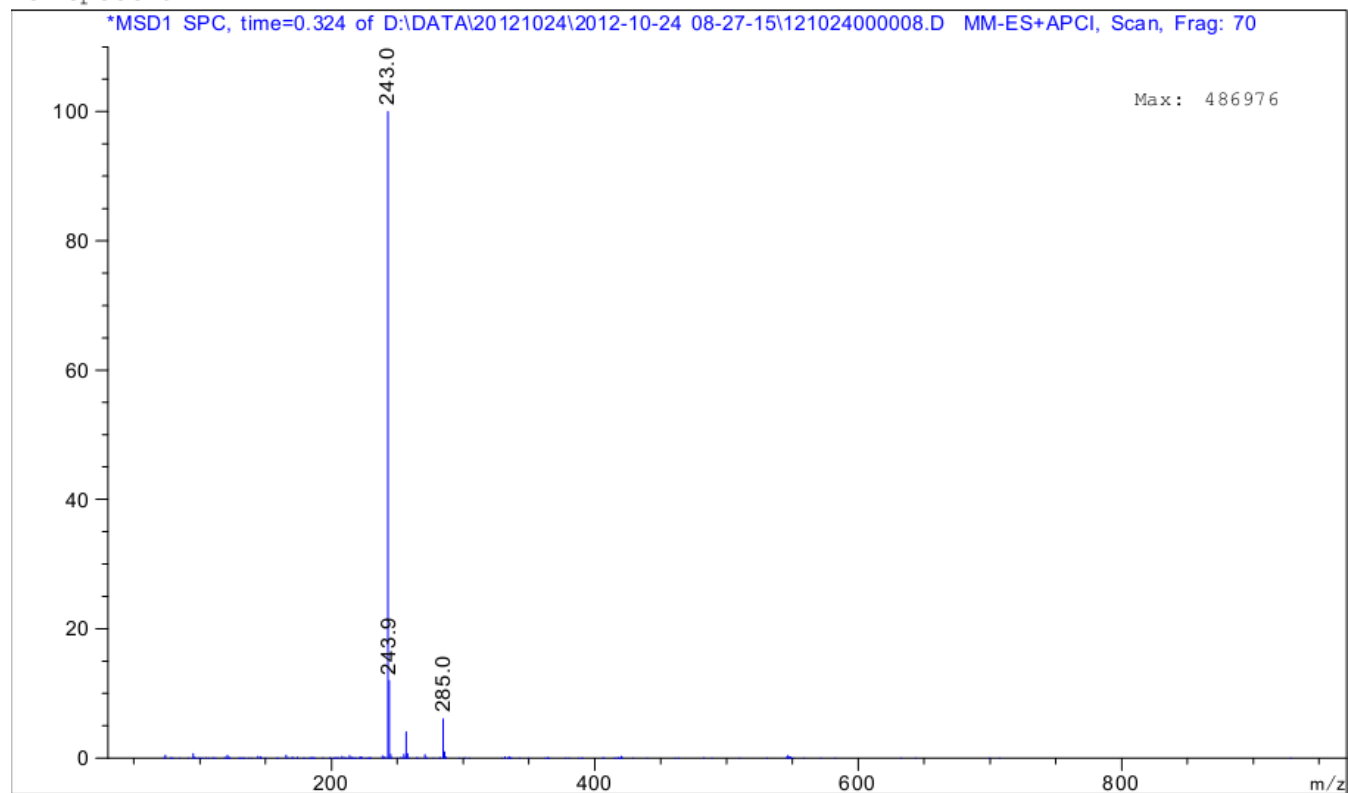
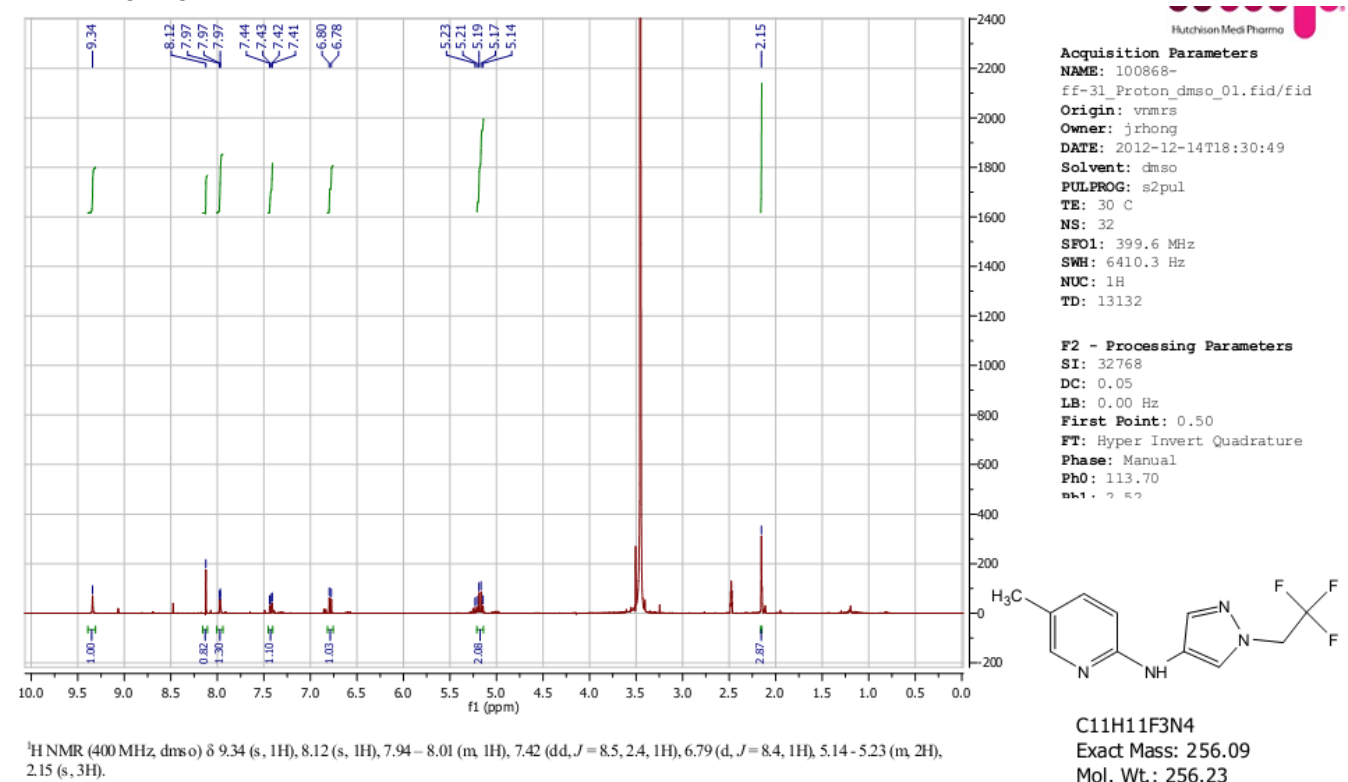
F2 - Processing Parameters
 SI: 65536
 DC: 0.05
 LB: 0.50 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: -161.48
 Ph1: -8.17

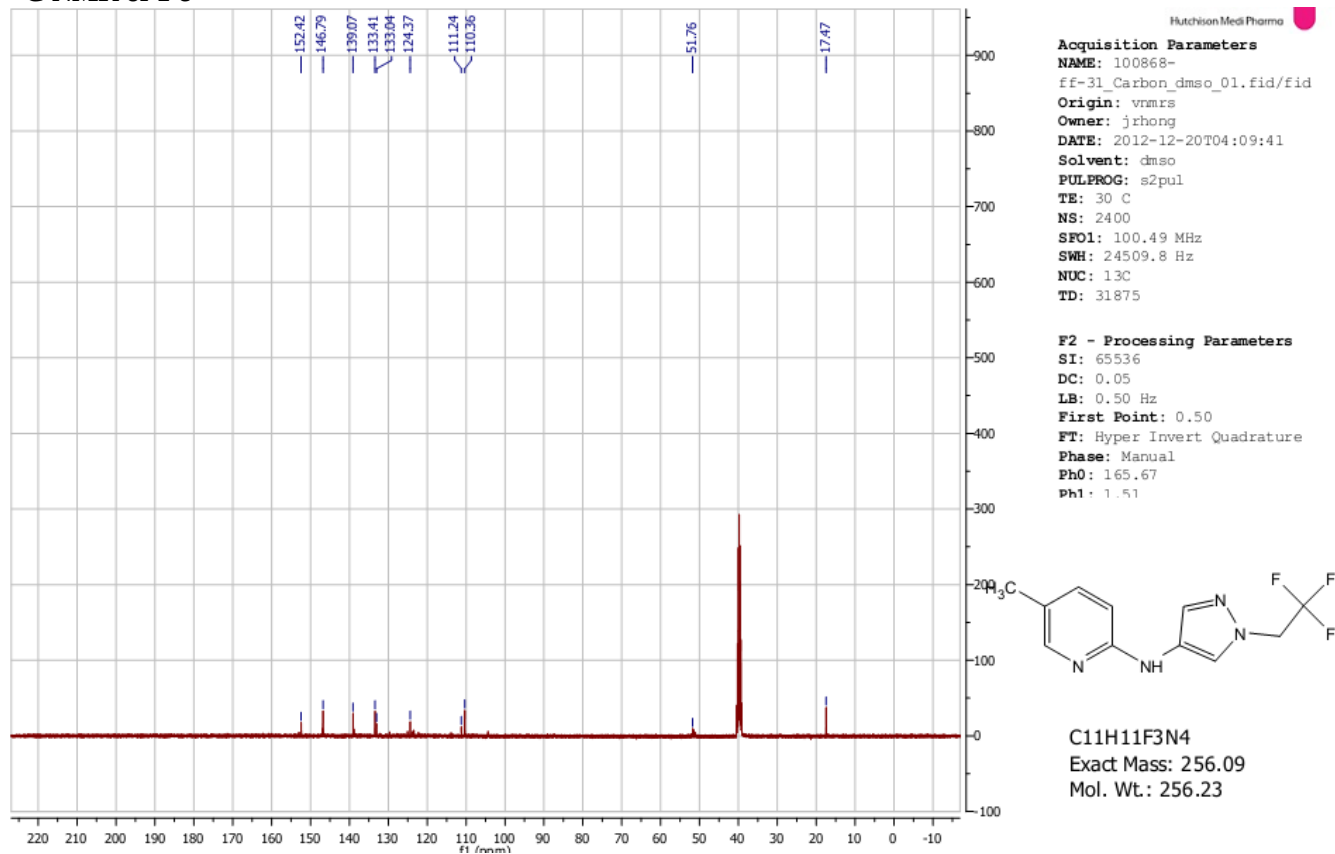


C₁₀H₉F₃N₄
 Exact Mass: 242.08
 Mol. Wt.: 242.2

LC-MS of 1'd

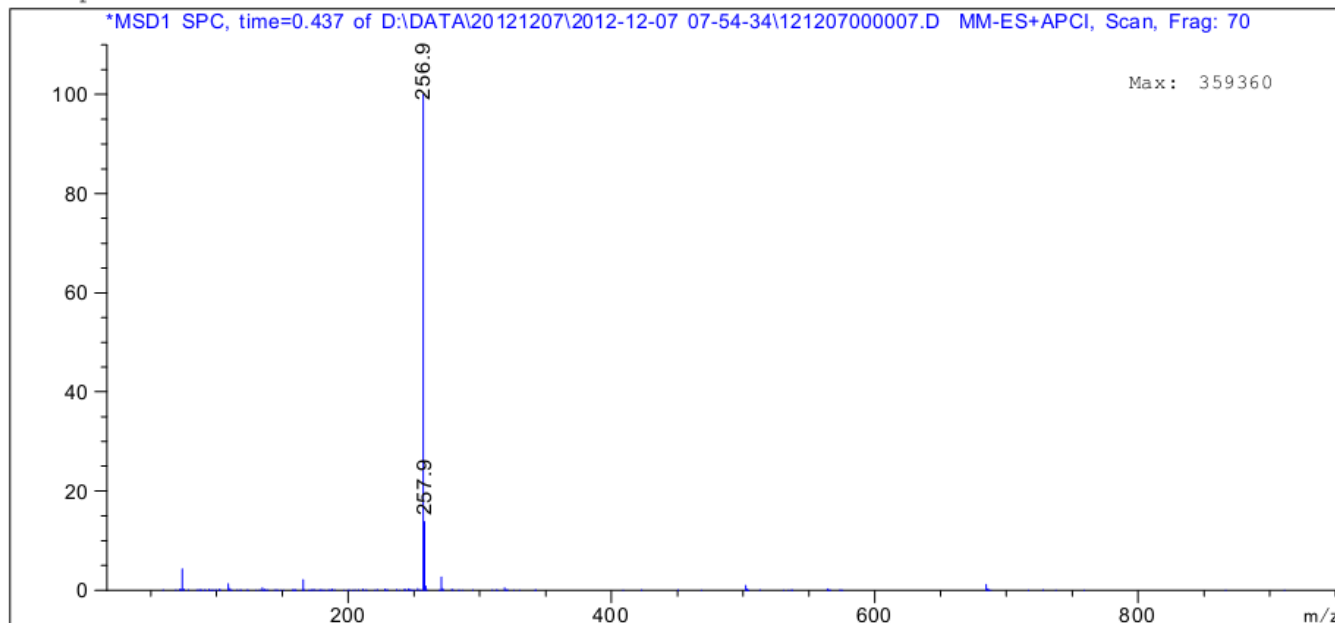
MS Spectrum

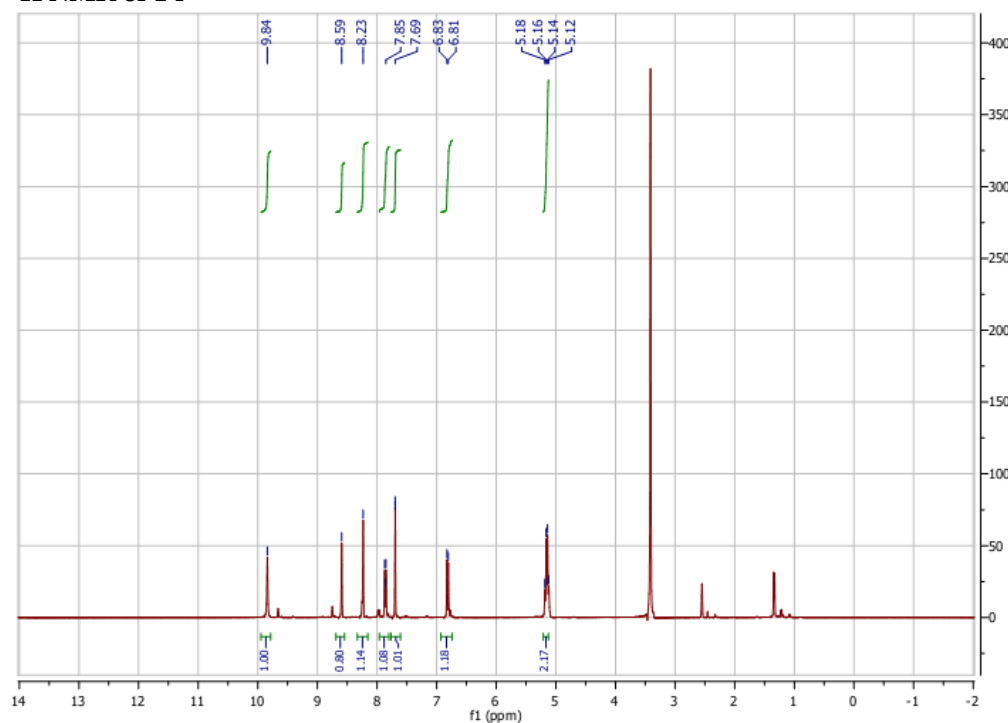
¹H NMR of 1'e

¹³C NMR of 1'e

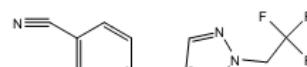
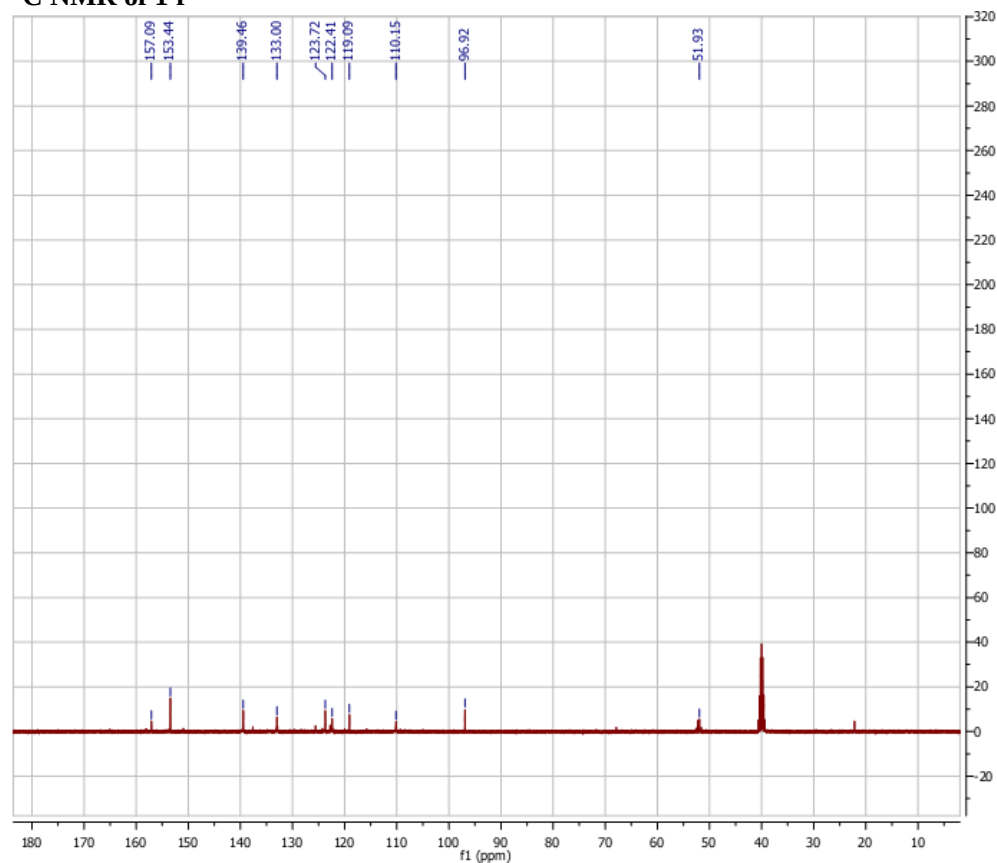
LC-MS of 1'e

MS Spectrum



¹H NMR of 1f

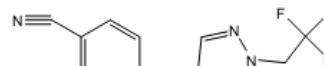
¹H NMR (400 MHz, dms-o) δ 9.84 (s, 1H), 8.59 (s, 1H), 8.23 (s, 1H), 7.80–7.96 (m, 1H), 7.70 (d, J = 0.7, 1H), 6.82 (d, J = 8.8, 1H), 5.12–5.21 (m, 2H).

¹³C NMR of 1f

C11H8F3N5
Exact Mass: 267.07
Mol. Wt.: 267.21

Acquisition Parameters
NAME: 100868-ff-001-32_Carbon_dms-o_01.fid/fid
Origin: vnmrs
Owner: jrhong
DATE: 2012-12-13T01:54:57
Solvent: dms-o
PULPROG: s2pul
TE: 30 C
NS: 256
SFO1: 100.49 MHz
SWH: 24509.8 Hz
NUC: 13C
TD: 31875

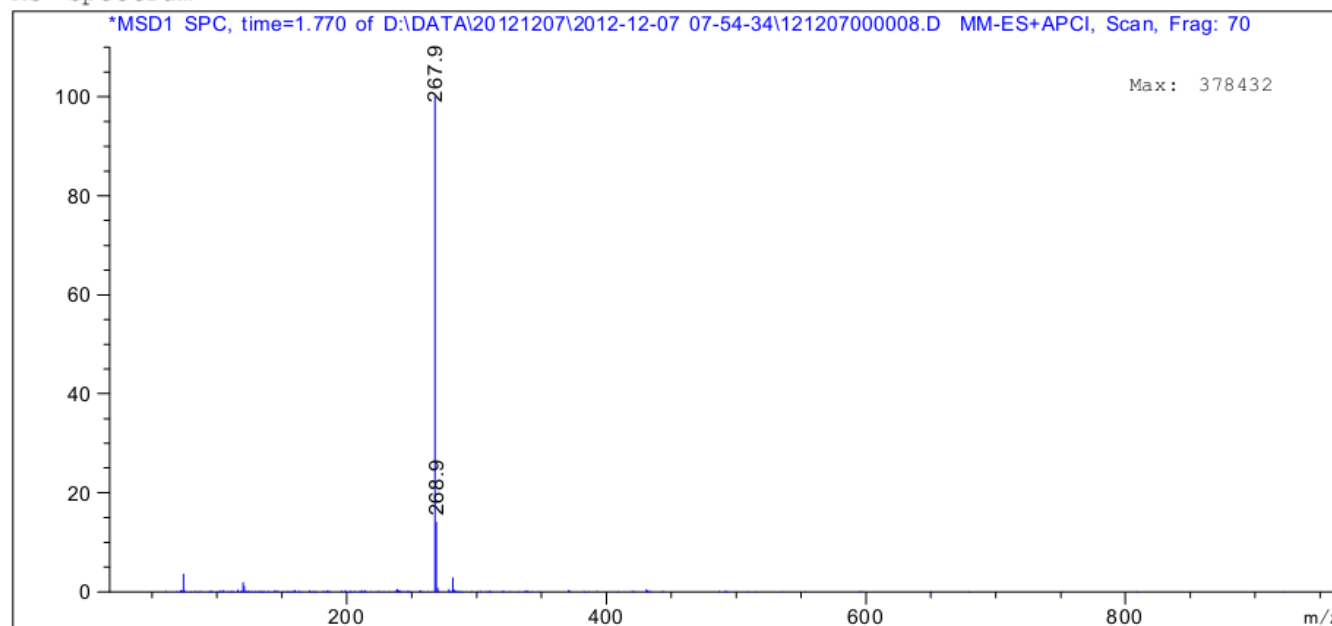
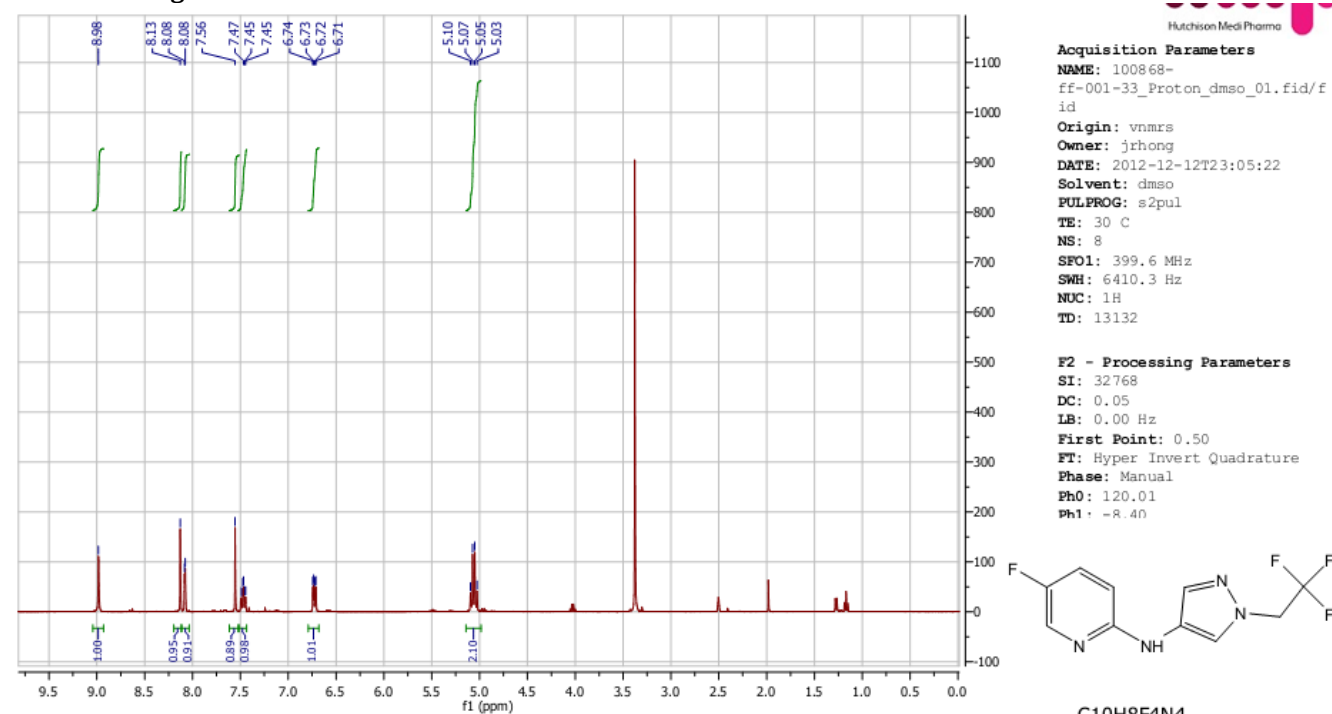
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.50 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: 220.50
Ph1: -48.19



C11H8F3N5
Exact Mass: 267.07
Mol. Wt.: 267.21

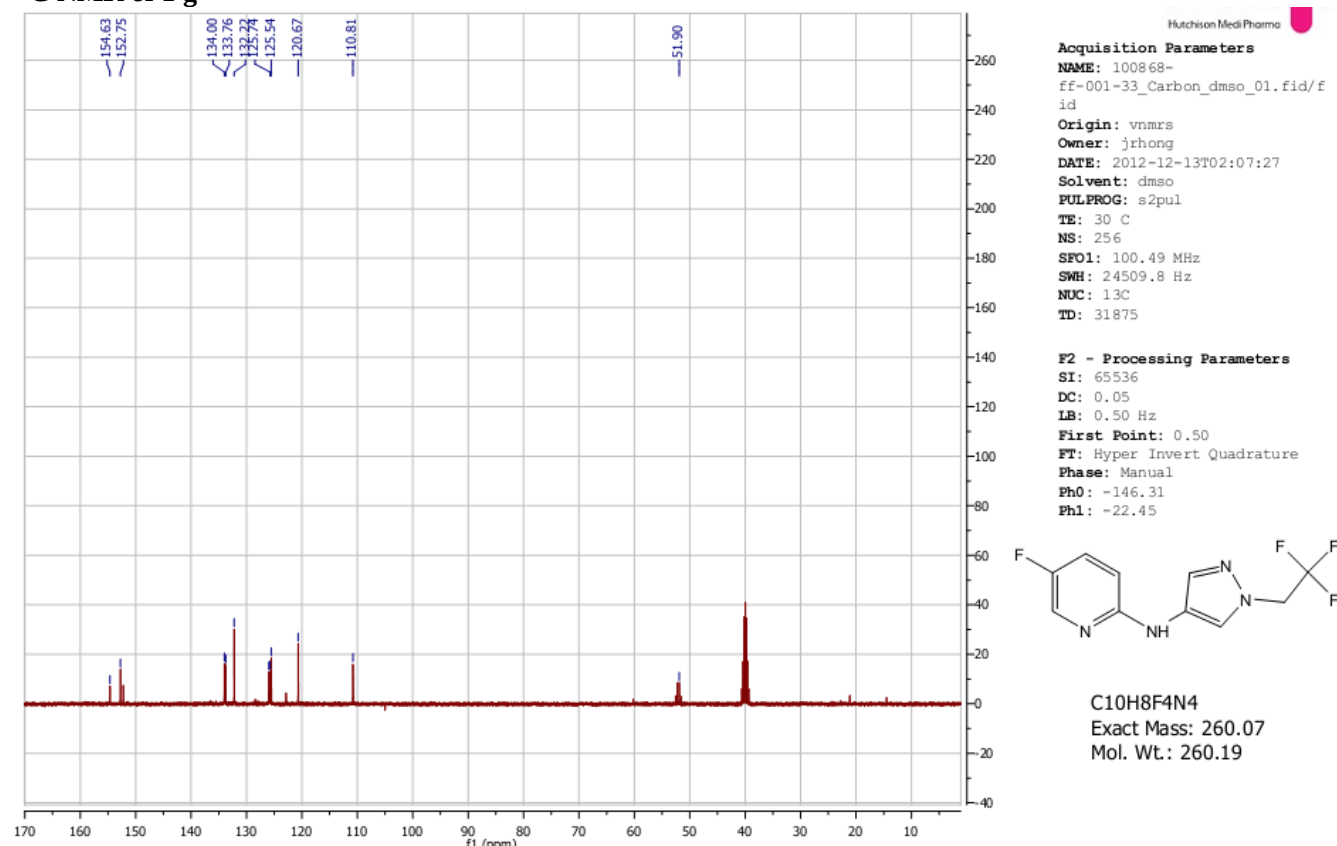
LC-MS of 1'f

MS Spectrum

¹H NMR of 1'g

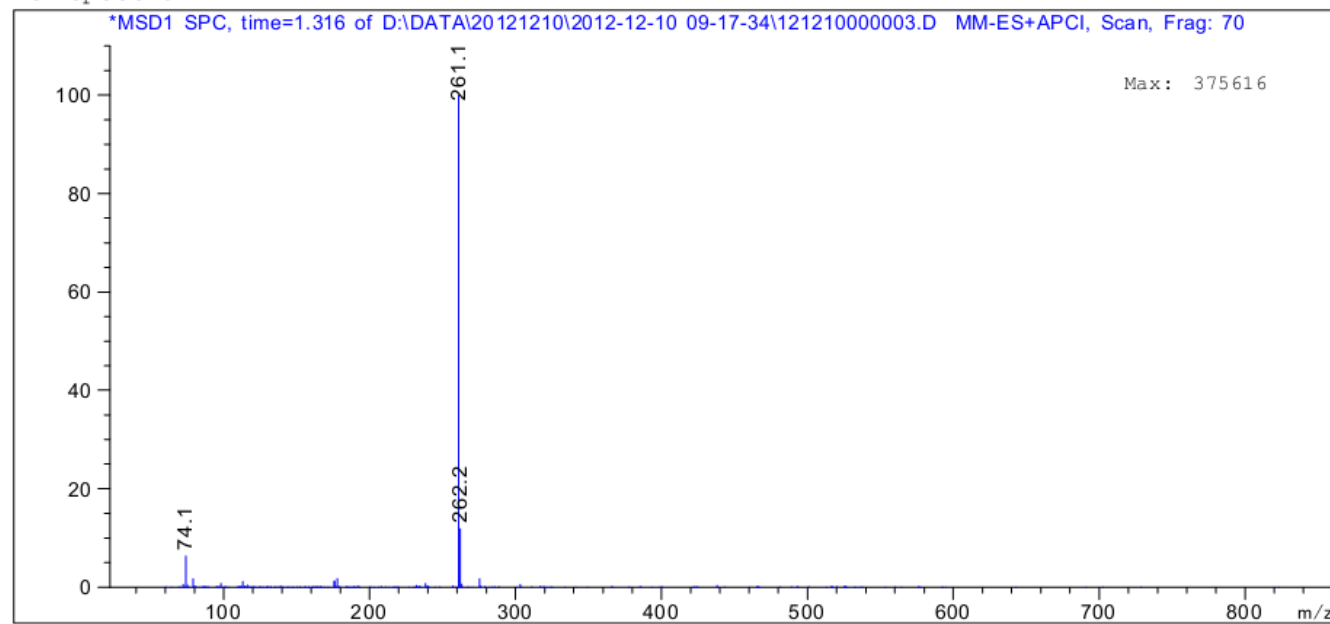
¹H NMR (400 MHz, dms0) δ 8.98 (s, 1H), 8.13 (s, 1H), 8.07 - 8.08 (m, 1H), 7.56 (s, 1H), 7.43 - 7.52 (m, 1H), 6.71 - 6.74 (m, 1H), 5.03 - 5.10 (m, 2H).

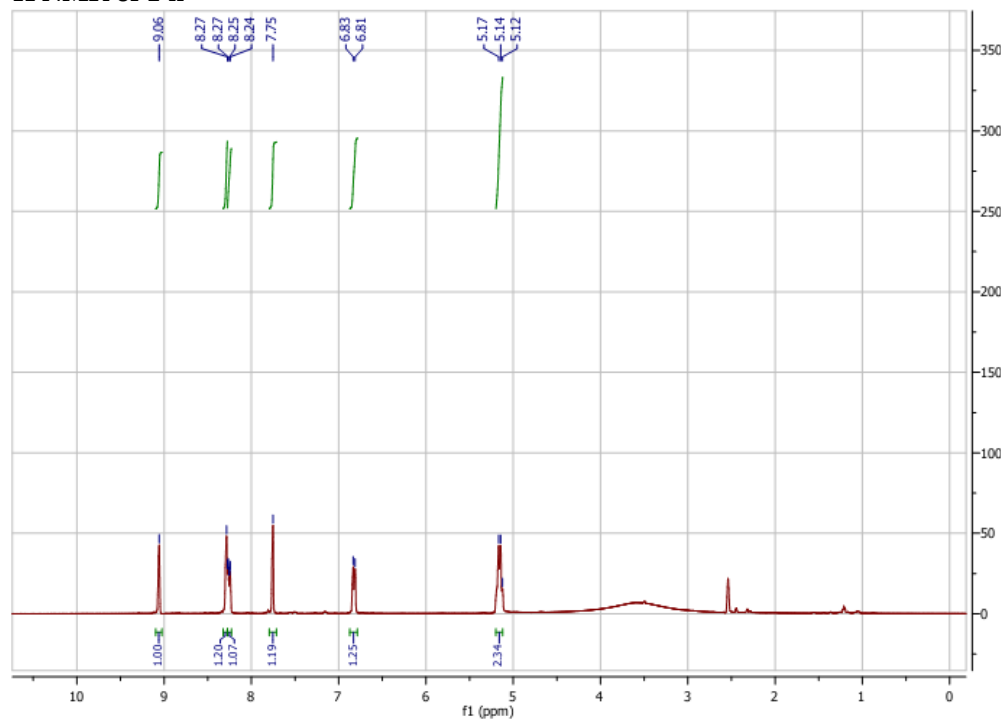
C10H8F4N4
Exact Mass: 260.07
Mol. Wt.: 260.19

¹³C NMR of 1'g

LC-MS of 1'g

MS Spectrum



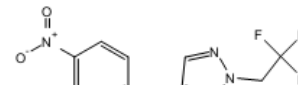
¹H NMR of 1'h

¹H NMR (400 MHz, dmsO) δ 9.06 (s, 1H), 8.29 (s, 1H), 8.27 – 8.23 (m, 1H), 7.75 (s, 1H), 6.81 – 6.83 (m, 1H), 5.12 – 5.20 (m, 2H).

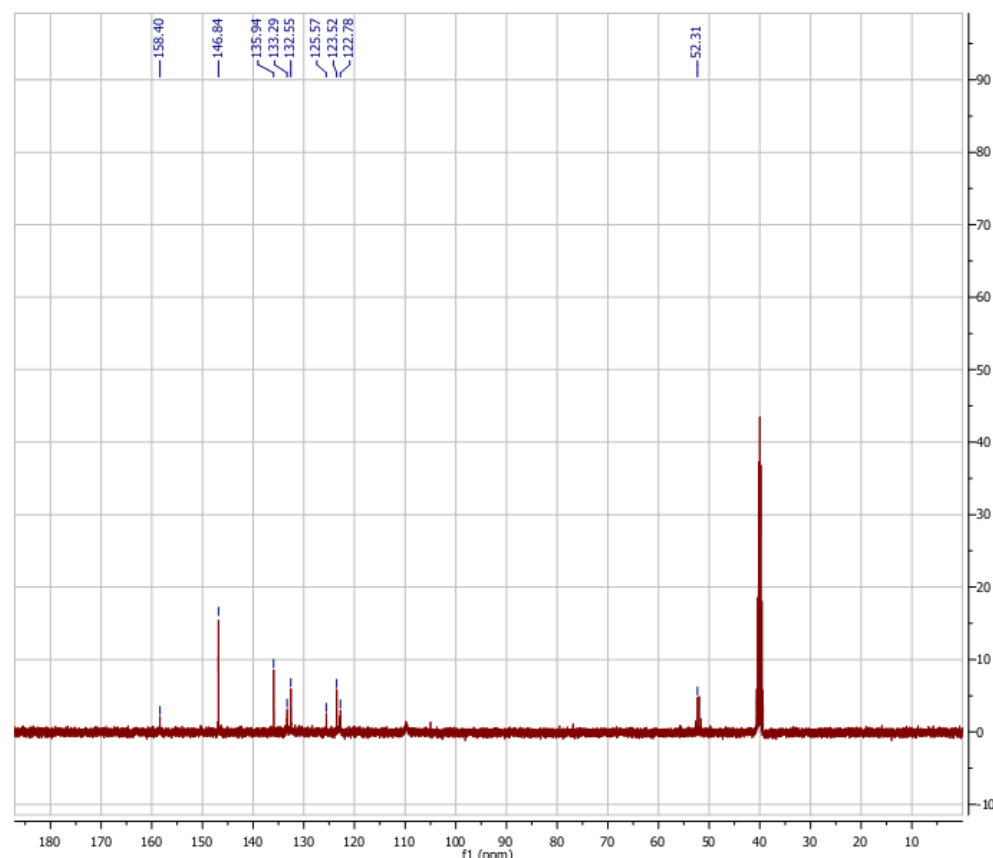
Hutchison Medi Pharma

Acquisition Parameters
 NAME: 100868-ff-001-34_Proton_dmsO_01.fid/fid
 Origin: vnmsr
 Owner: jrhong
 DATE: 2012-12-12T22:22:40
 Solvent: dmsO
 PULPROG: s2pul
 TE: 30 C
 NS: 8
 SFO1: 399.6 MHz
 SWH: 6410.3 Hz
 NUC: 1H
 TD: 13132

F2 - Processing Parameters
 SI: 32768
 DC: 0.05
 LB: 0.00 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: 123.22
 Ph1: -22.93



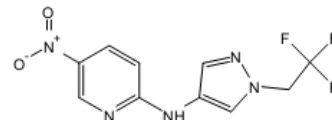
C10H8F3N5O2
 Exact Mass: 287.06
 Mol. Wt.: 287.2

¹³C NMR of 1'h

Hutchison Medi Pharma

Acquisition Parameters
 NAME: 100868-ff-001-34_Carbon_dmsO_01.fid/fid
 Origin: vnmsr
 Owner: jrhong
 DATE: 2012-12-13T17:17:00
 Solvent: dmsO
 PULPROG: s2pul
 TE: 30 C
 NS: 256
 SFO1: 100.49 MHz
 SWH: 24509.8 Hz
 NUC: 13C
 TD: 31875

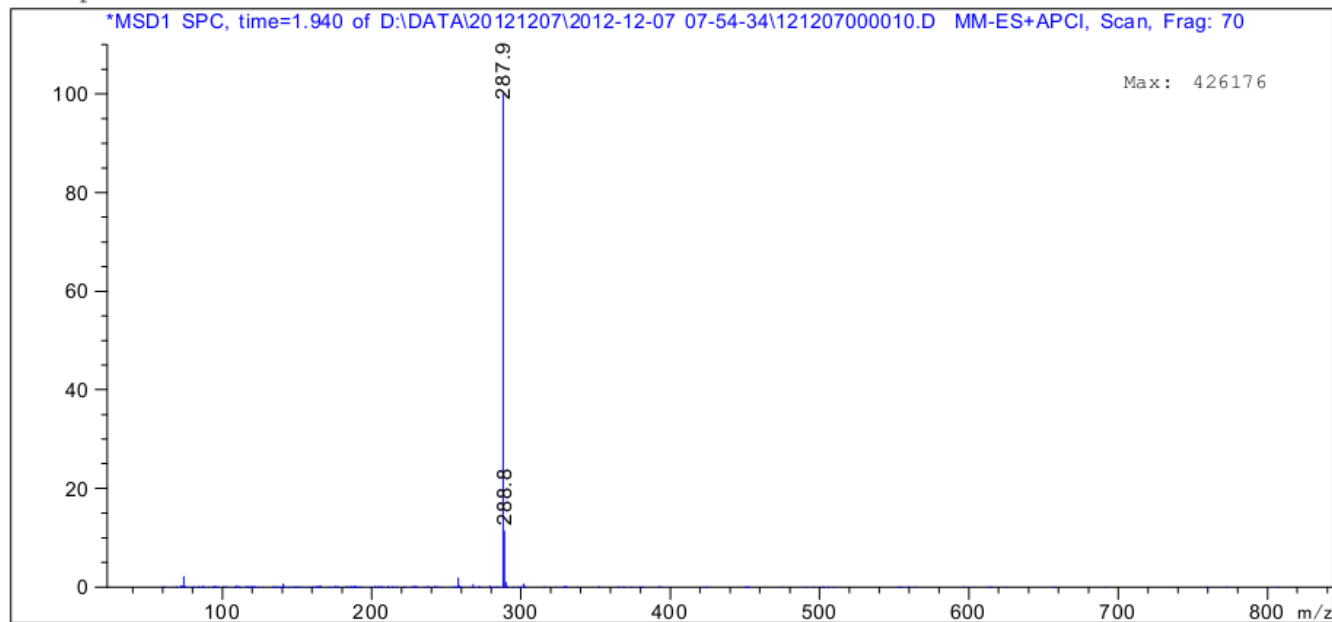
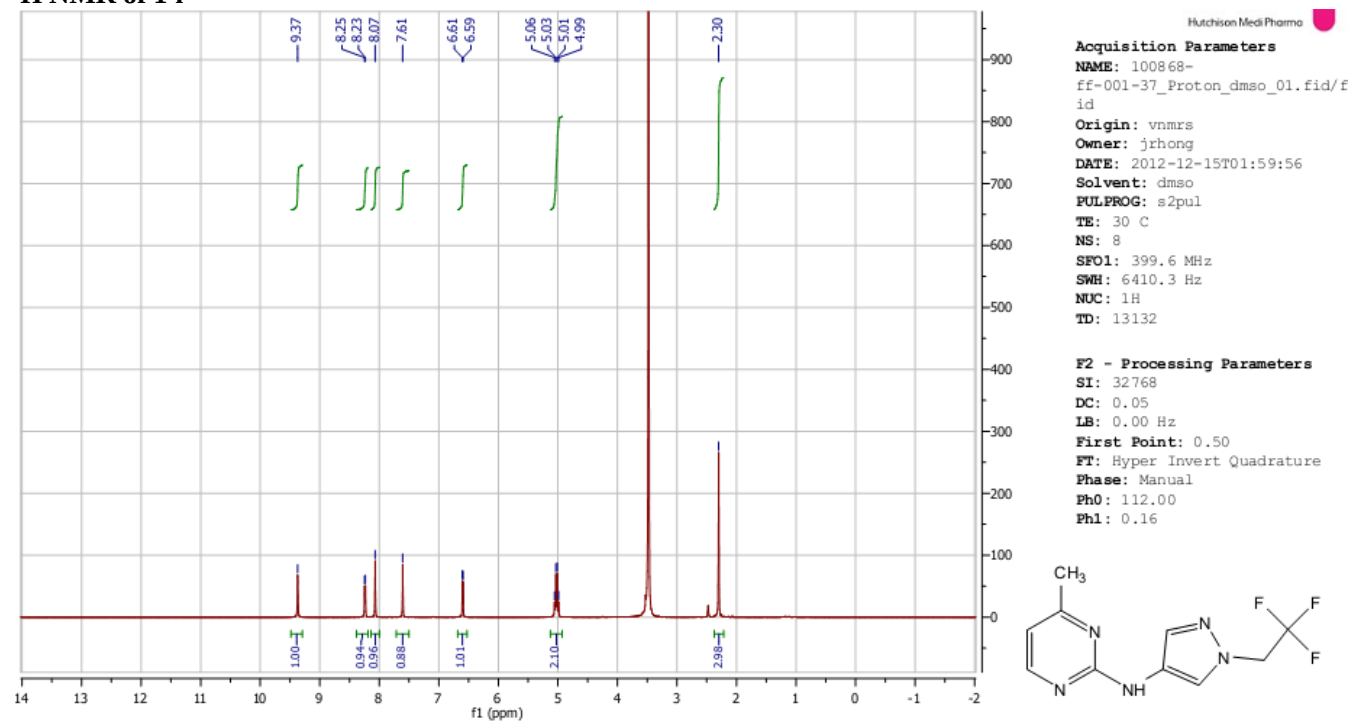
F2 - Processing Parameters
 SI: 65536
 DC: 0.05
 LB: 0.50 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: -151.47
 Ph1: -9.34



C10H8F3N5O2
 Exact Mass: 287.06
 Mol. Wt.: 287.2

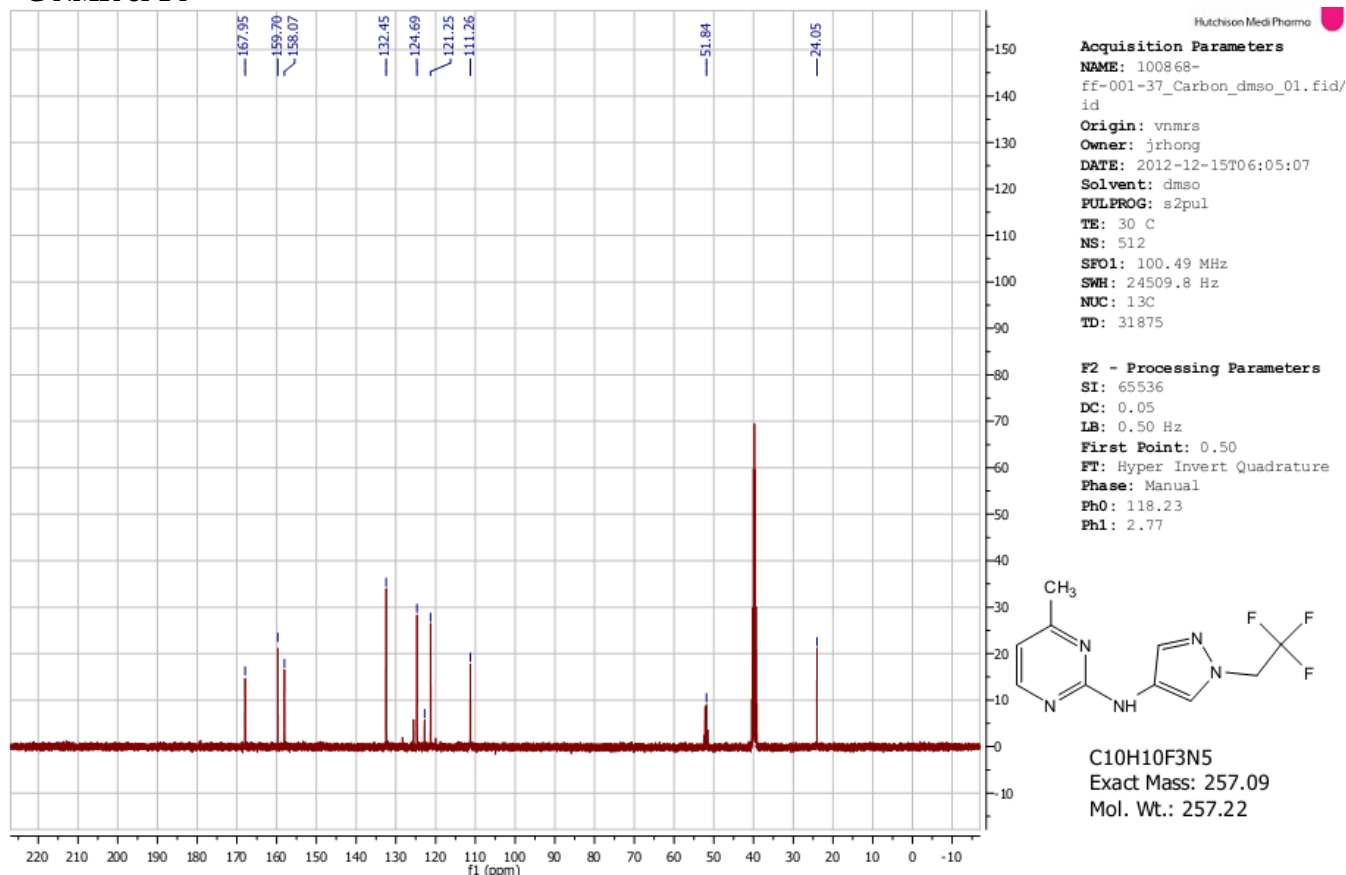
LC-MS of 1'h

MS Spectrum

¹H NMR of 1'i

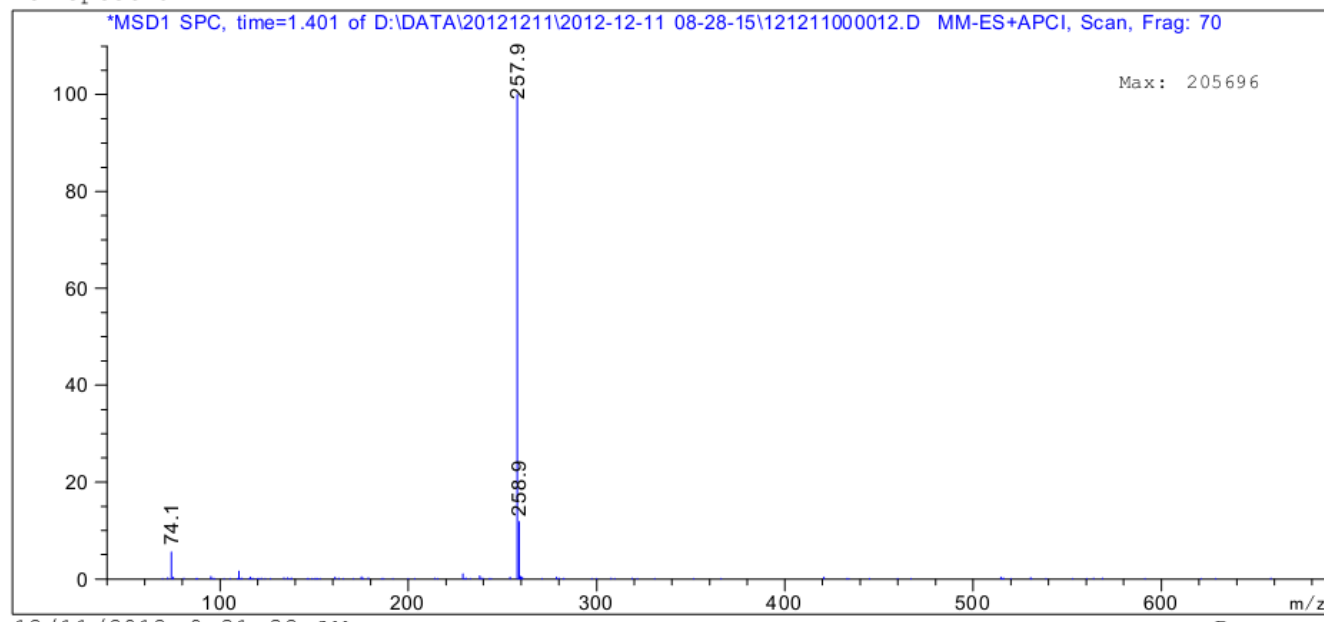
¹H NMR (400 MHz, dms0) δ 9.37 (s, 1H), 8.24 (d, $J=4.9$, 1H), 8.07 (s, 1H), 7.61 (s, 1H), 6.60 (d, $J=5.0$, 1H), 4.99 - 5.06 (m, 2H), 2.30 (s, 3H).

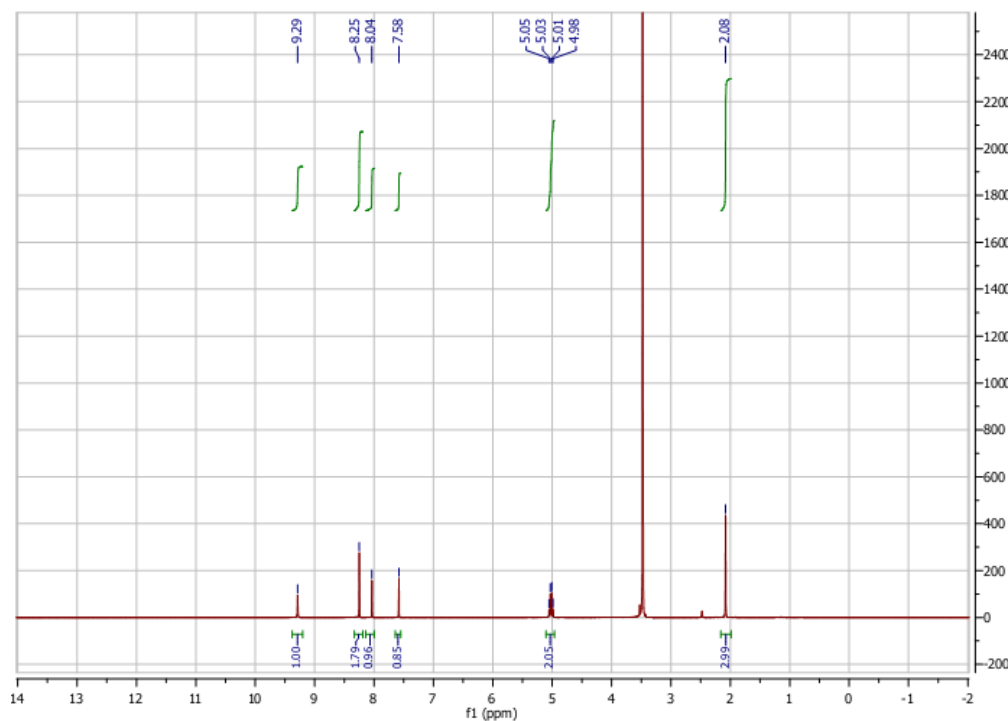
C₁₀H₁₀F₃N₅
Exact Mass: 257.09
Mol. Wt.: 257.22

¹³C NMR of 1'i

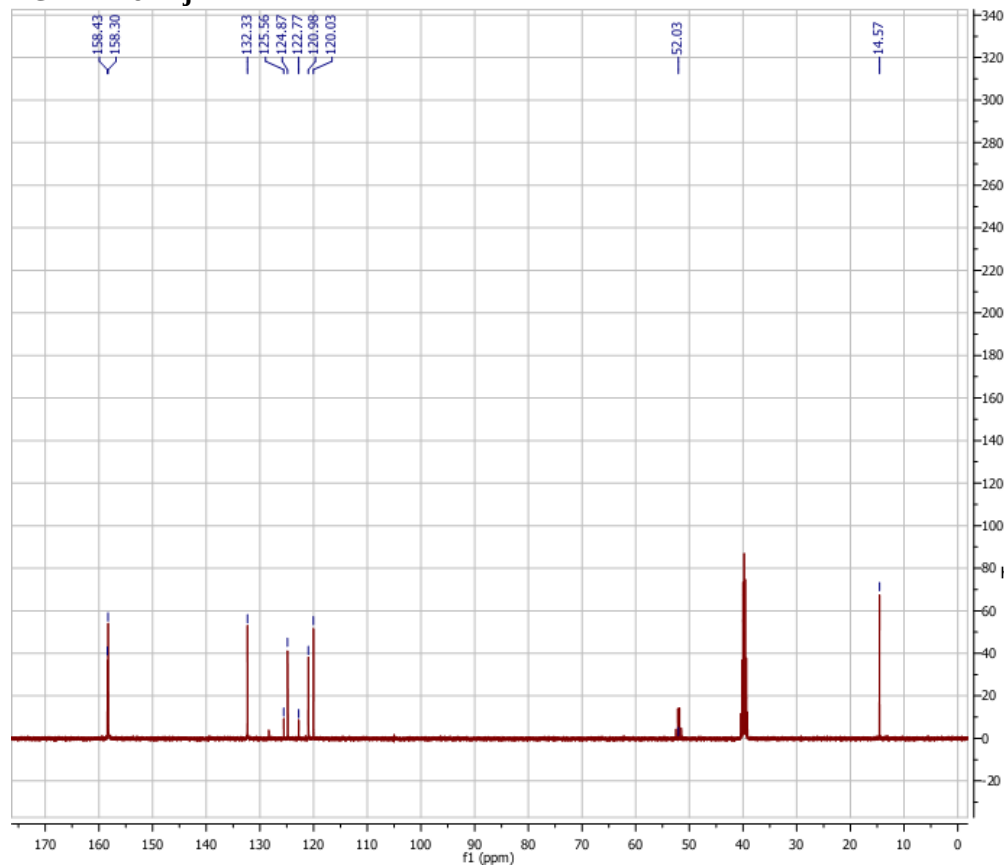
LC-MS of 1'i

MS Spectrum



¹H NMR of 1'j

¹H NMR (400 MHz, dmsO) δ 9.29 (s, 1H), 8.25 (s, 2H), 8.04 (s, 1H), 7.58 (s, 1H), 5.02 (q, J = 9.1, 2H), 2.08 (s, 3H).

¹³C NMR of 1'j

Hutchison Medi Pharma

Acquisition Parameters
 NAME: 100868-ff-001-36_Proton_dmsO_01.fid/fid
 Origin: vnmrs
 Owner: jrhong
 DATE: 2012-12-15T01:56:39
 Solvent: dmsO
 PULPROG: s2pul
 TE: 30 C
 NS: 8
 SFO1: 399.6 MHz
 SWH: 6410.3 Hz
 NUC: 1H
 TD: 13132

F2 - Processing Parameters
 SI: 32768
 DC: 0.05
 LB: 0.00 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: 122.03
 Ph1: -7.85

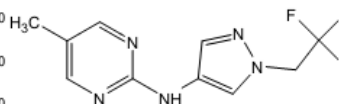


C10H10F3N5
 Exact Mass: 257.09
 Mol. Wt.: 257.22

Hutchison Medi Pharma

Acquisition Parameters
 NAME: 100868-ff-001-36_Carbon_dmsO_01.fid/fid
 Origin: vnmrs
 Owner: jrhong
 DATE: 2012-12-15T05:42:46
 Solvent: dmsO
 PULPROG: s2pul
 TE: 30 C
 NS: 512
 SFO1: 100.49 MHz
 SWH: 24509.8 Hz
 NUC: 13C
 TD: 31875

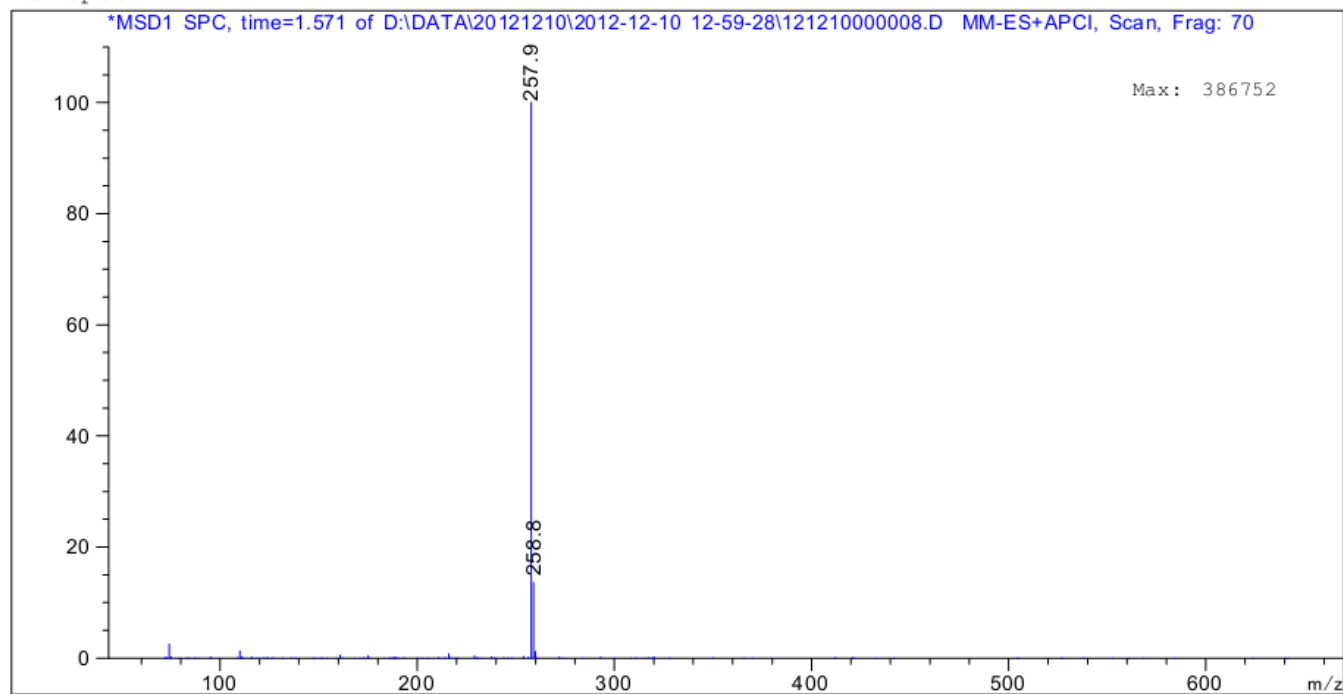
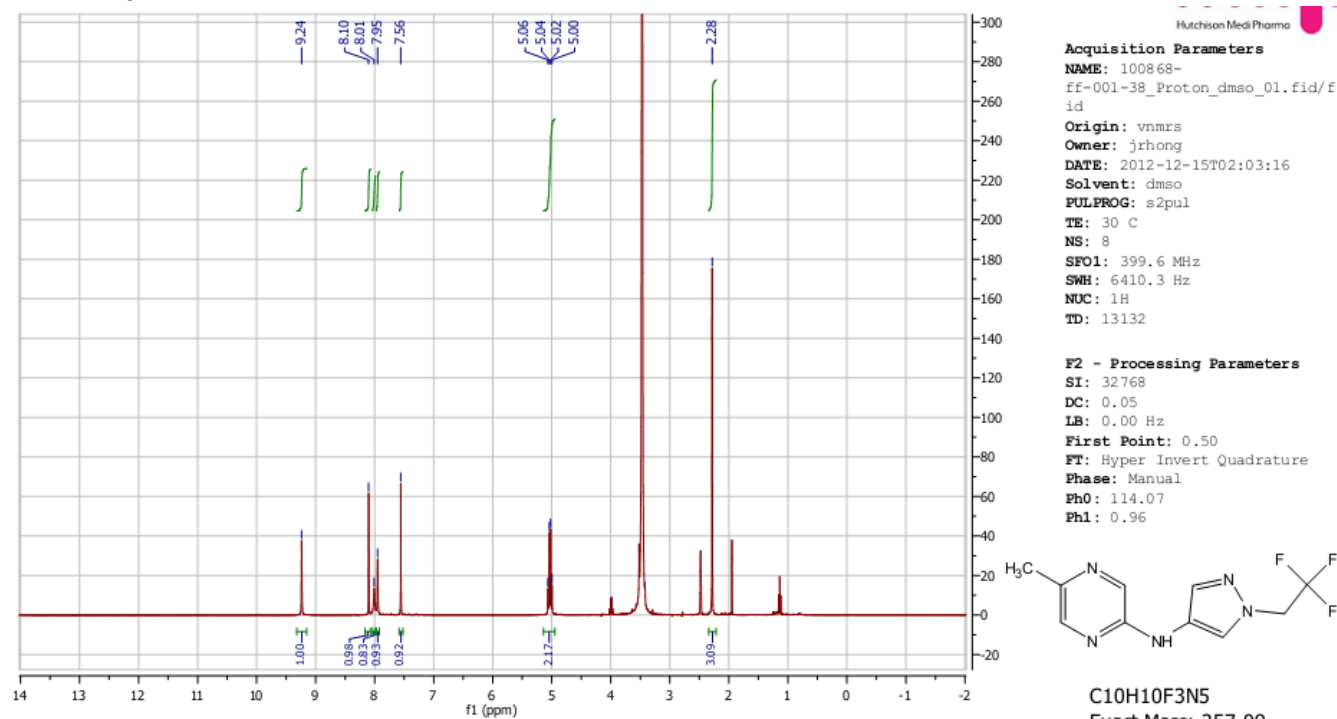
F2 - Processing Parameters
 SI: 65536
 DC: 0.05
 LB: 0.50 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: 187.80
 Ph1: -10.03

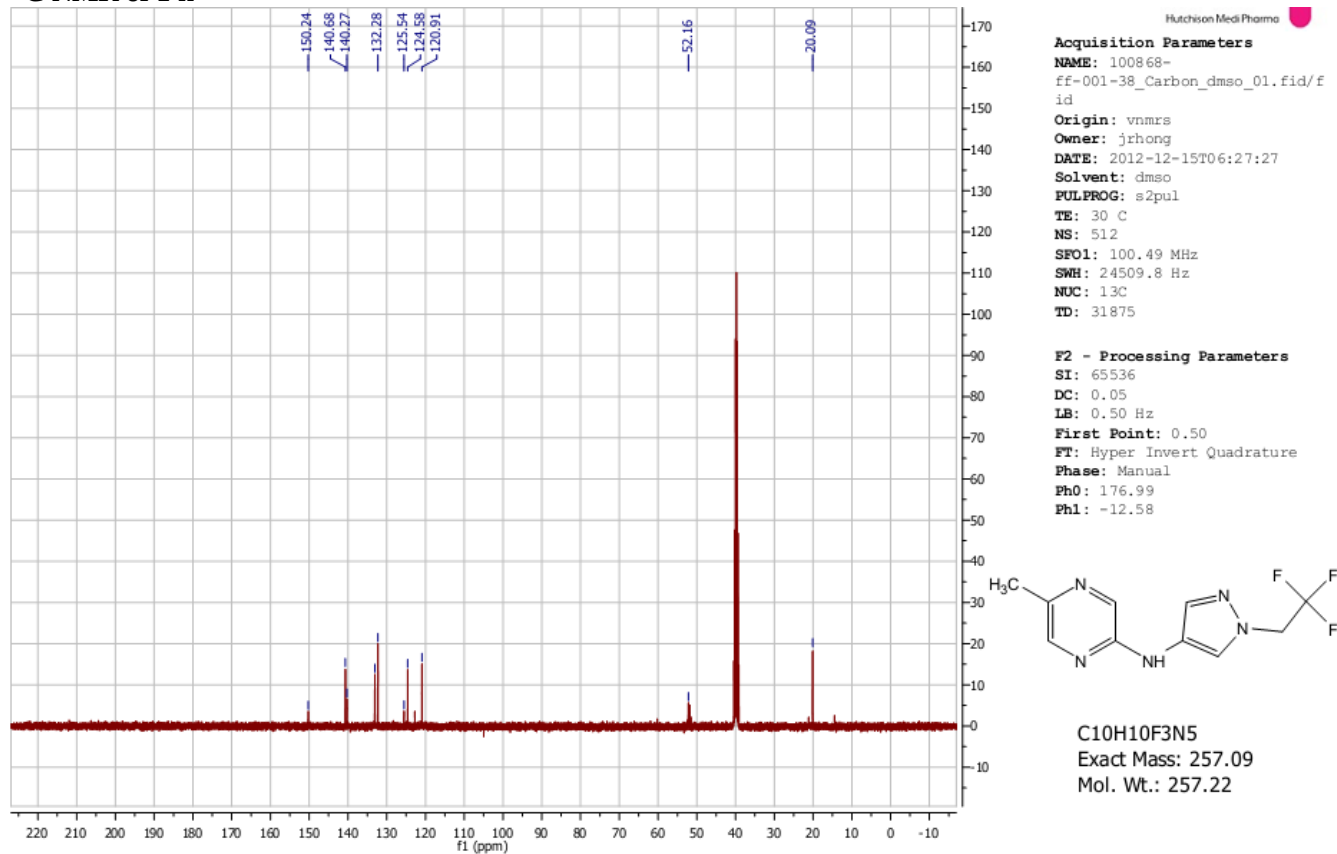
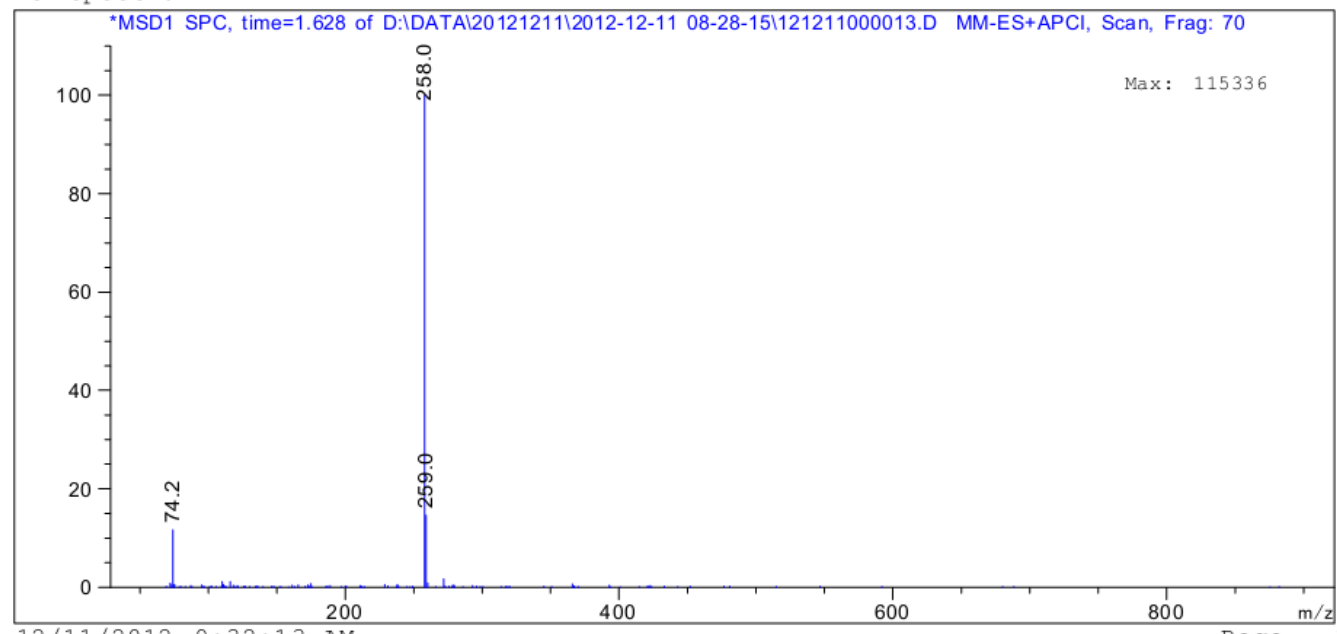


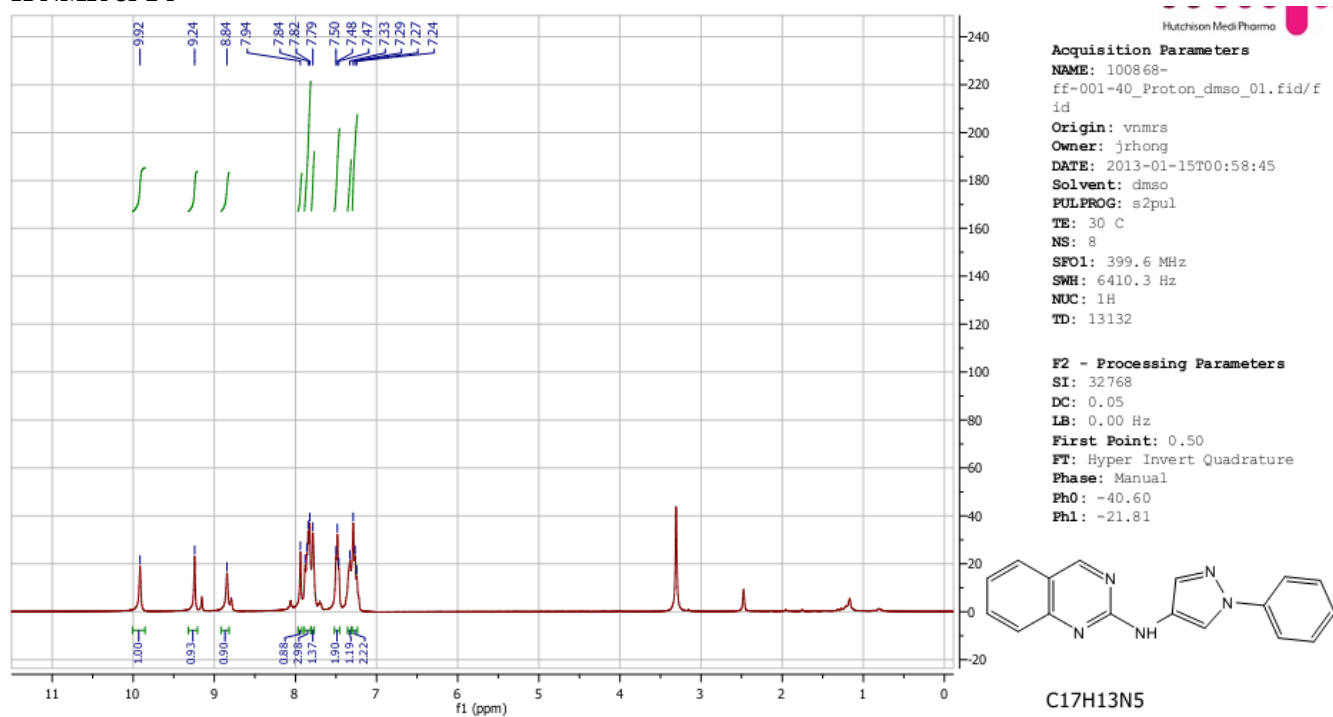
C10H10F3N5
 Exact Mass: 257.09
 Mol. Wt.: 257.22

LC-MS of 1'j

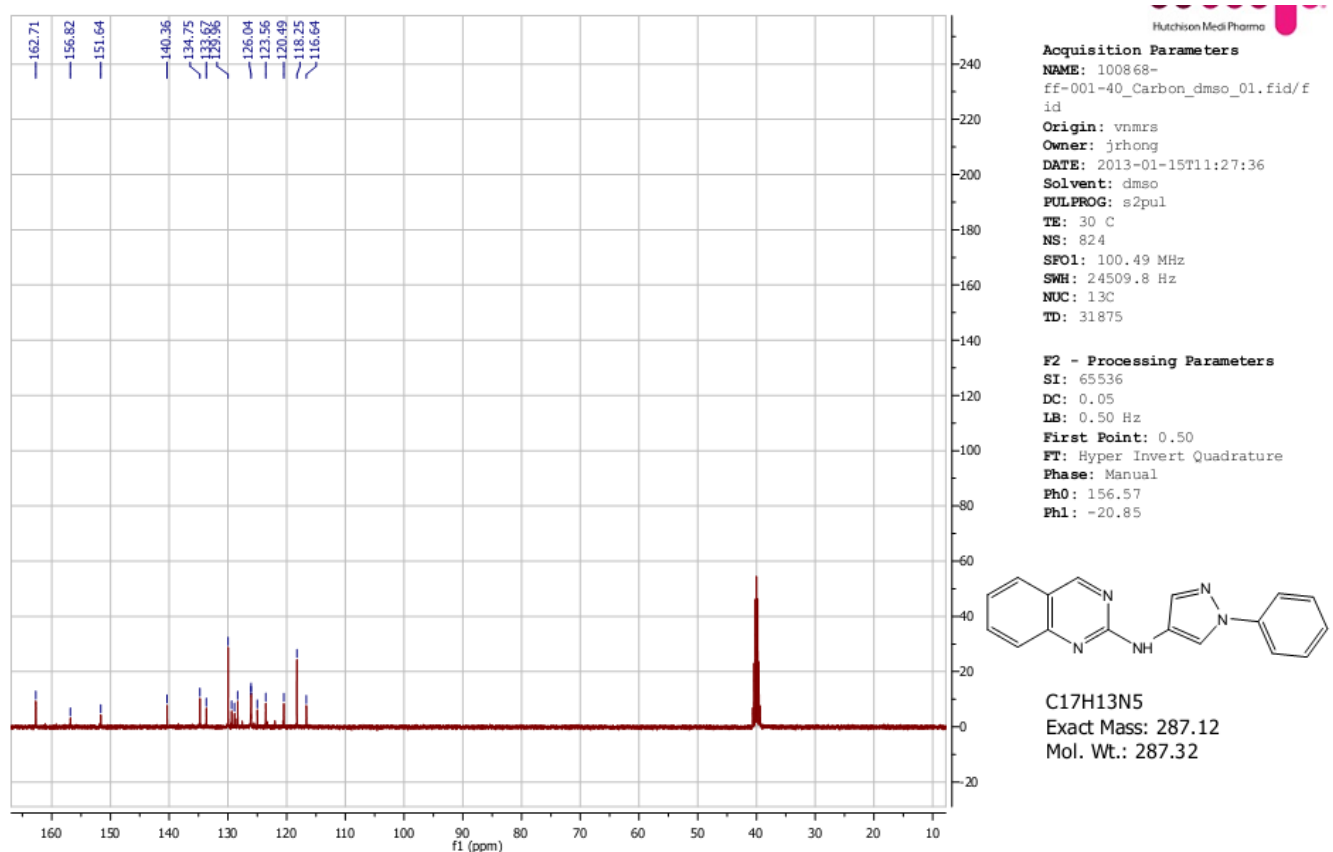
MS Spectrum

¹H NMR of 1'k¹H NMR (400 MHz, dms0) δ 9.24 (s, 1H), 8.10 (s, 1H), 8.01 (s, 1H), 7.95 (s, 1H), 7.56 (s, 1H), 5.00-5.06 (m, 2H), 2.28 (s, 3H).

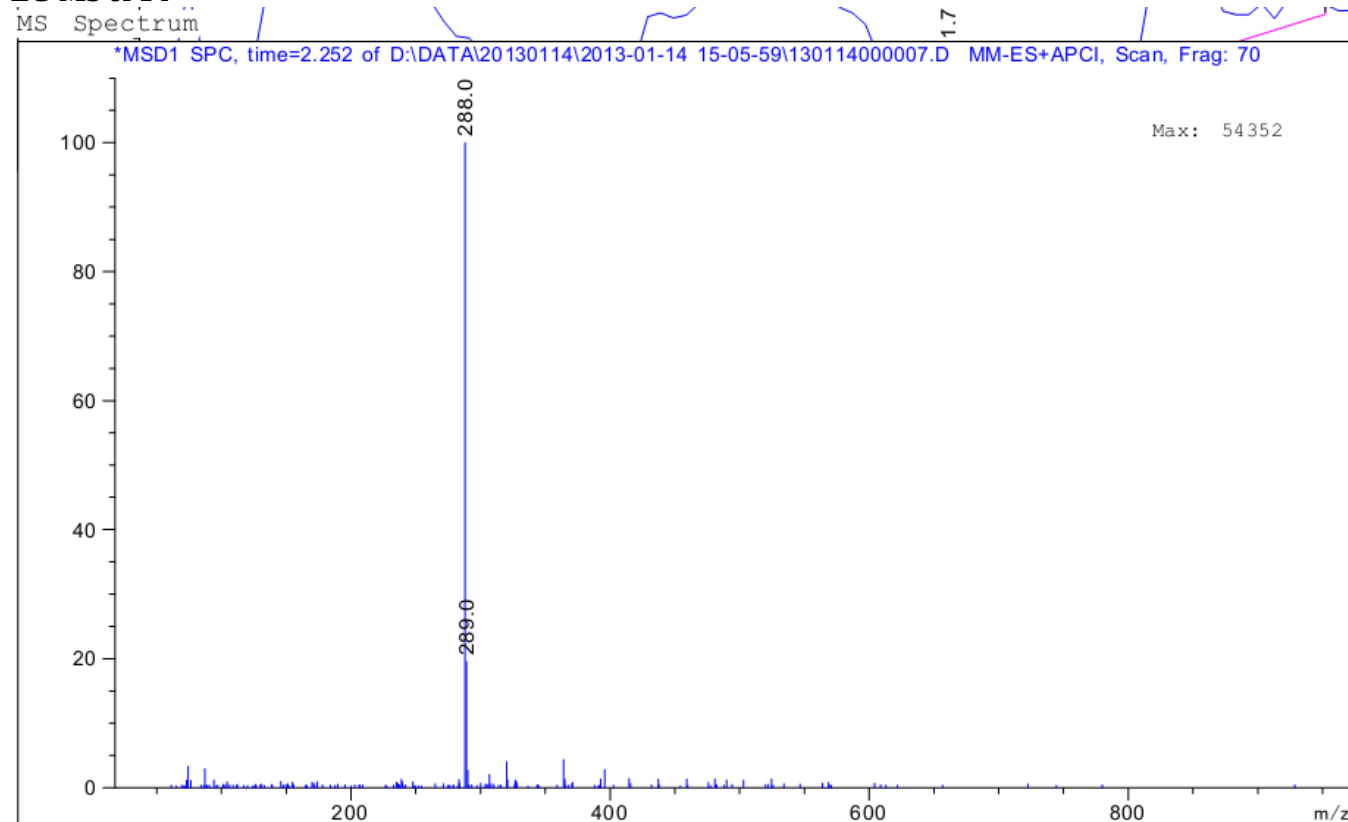
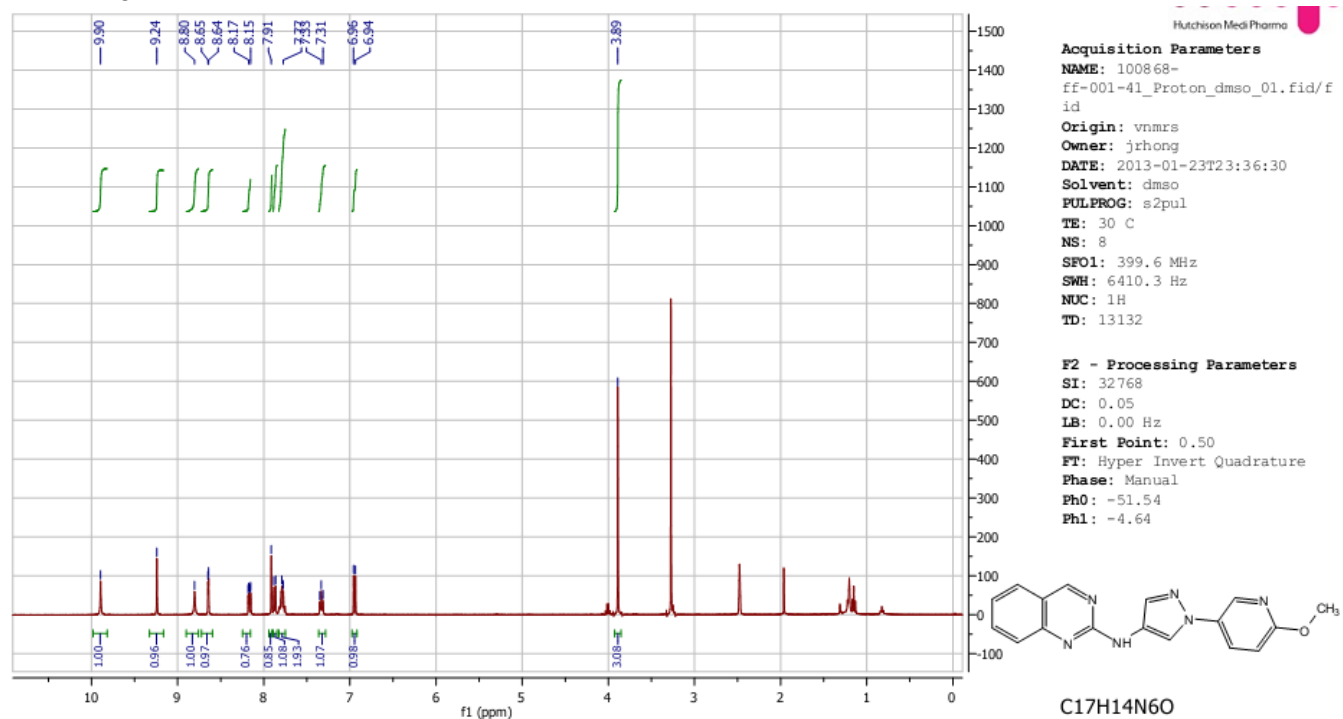
¹³C NMR of 1'kLC-MS of 1'k
MS Spectrum

¹H NMR of 1'

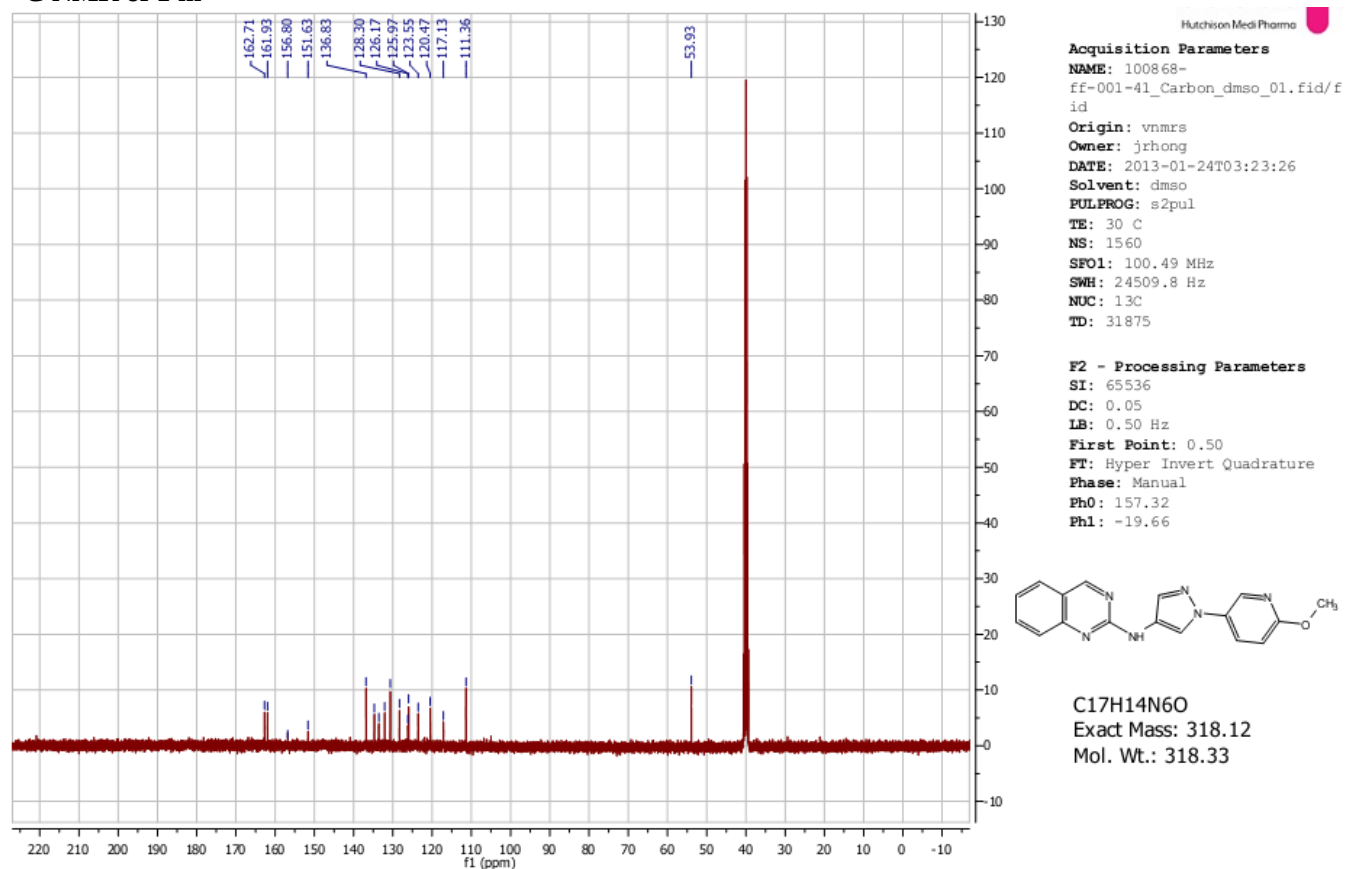
¹H NMR (400 MHz, dms0) δ 9.92 (s, 1H), 9.24 (s, 1H), 8.84 (s, 1H), 7.94 (s, 1H), 7.79 - 7.88 (m, 4H), 7.47 - 7.50 (m, 2H), 7.24 - 7.33 (m, 3H).

¹³C NMR of 1'

LC-MS of 1'

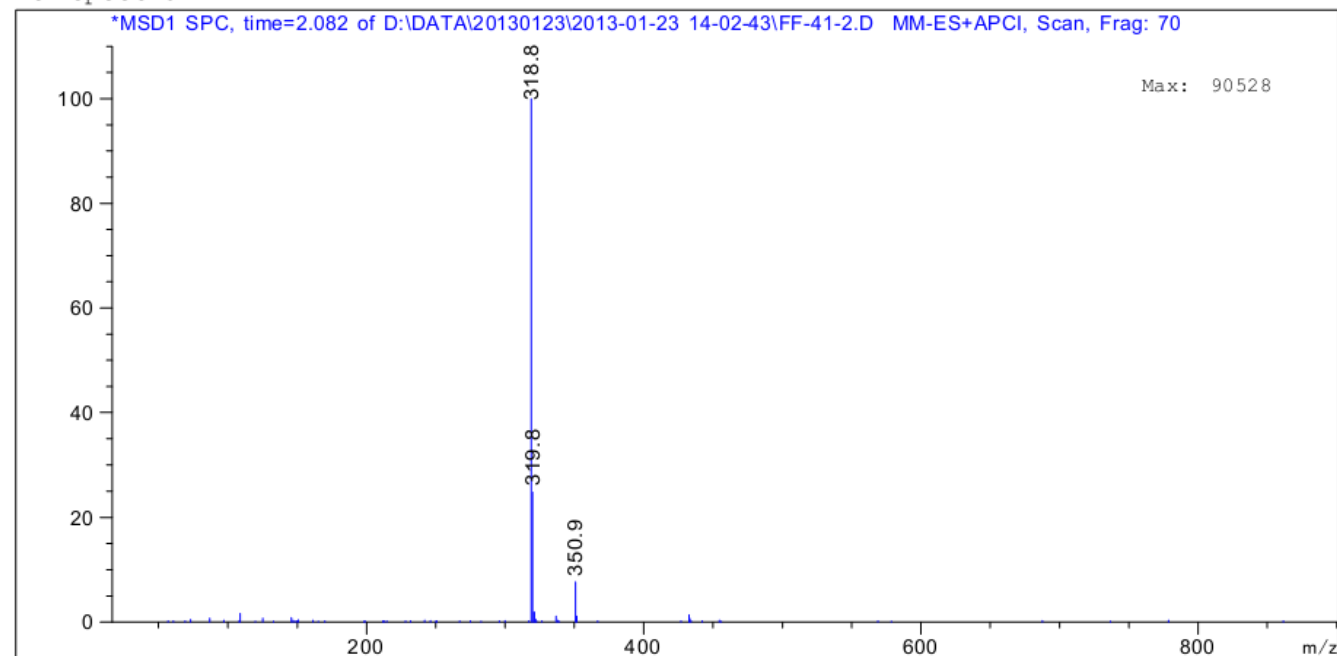
¹H NMR of 1'm

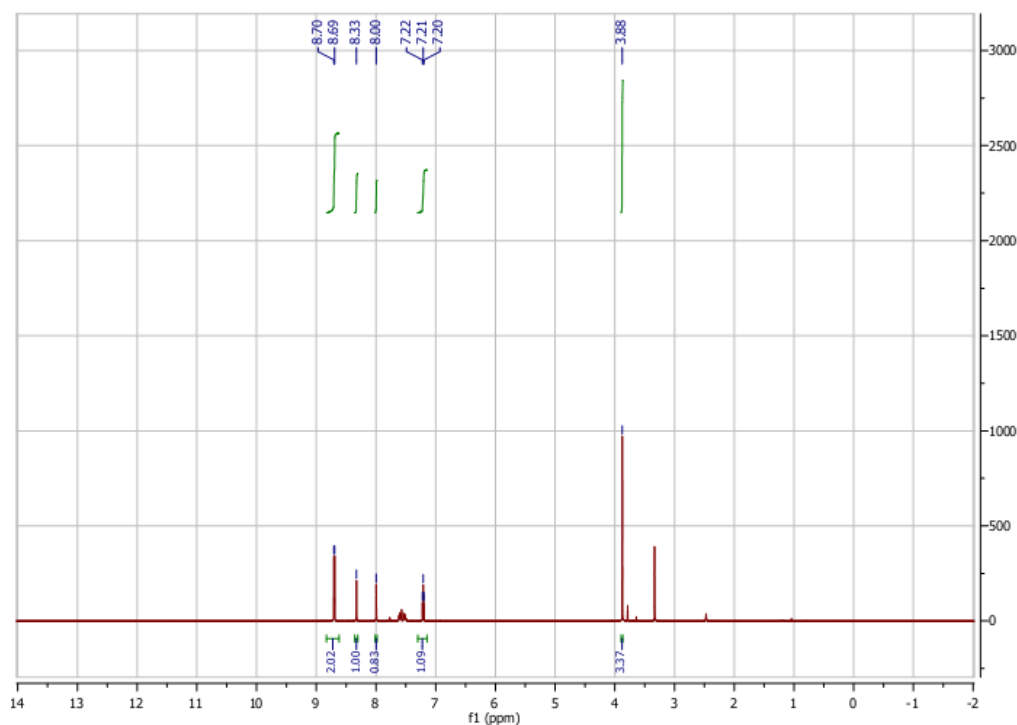
¹H NMR (400 MHz, dms0) δ 9.90 (s, 1H), 9.24 (s, 1H), 8.80 (s, 1H), 8.64 (d, J = 2.8, 1H), 8.15 – 8.25 (m, 1H), 7.91 (s, 1H), 7.87 (d, J = 8.0, 1H), 7.78 (d, J = 6.8, 2H), 7.33 (t, J = 7.6, 1H), 6.95 (d, J = 8.9, 1H), 3.89 (s, 3H).

¹³C NMR of 1'm

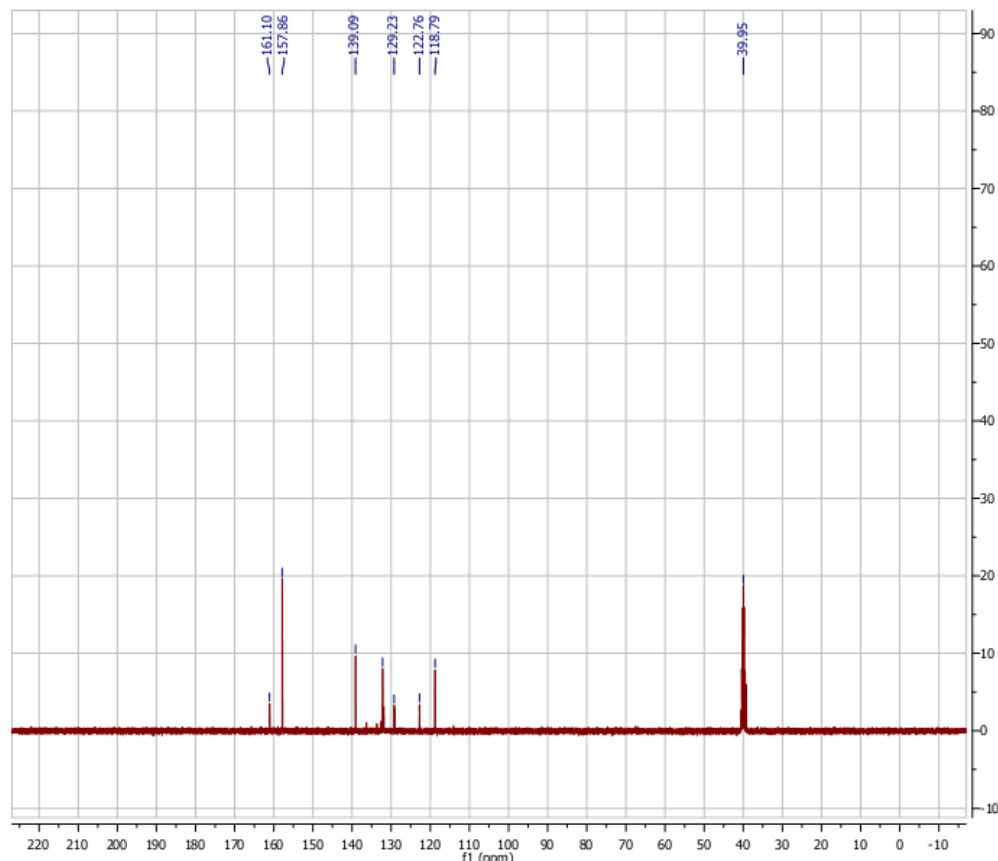
LC-MS of 1'm

MS Spectrum



¹H NMR of 1'n

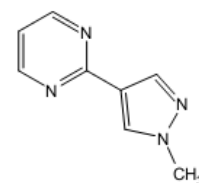
¹H NMR (400 MHz, DMSO) δ 8.70 (d, J = 4.9, 2H), 8.33 (s, 1H), 8.00 (s, 1H), 7.21 (t, J = 4.9, 1H), 3.88 (s, 3H).

¹³C NMR of 1'n

Hutchison Medi Pharma

Acquisition Parameters
 NAME: 100868-ff-001-9_Proton_dms0_01.fid/fid
 Origin: vnmrs
 Owner: jrhong
 DATE: 2012-09-28T22:59:22
 Solvent: dms0
 PULPROG: s2pul
 TE: 25 C
 NS: 8
 SFO1: 399.61 MHz
 SWH: 6410.3 Hz
 NUC: 1H
 TD: 13132

F2 - Processing Parameters
 SI: 32768
 DC: 0.05
 LB: 0.00 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: 127.81
 Ph1: -10.81

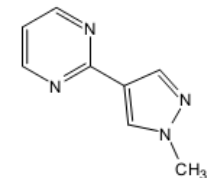


C8H8N4
 Exact Mass: 160.07
 Mol. Wt.: 160.18

Hutchison Medi Pharma

Acquisition Parameters
 NAME: 100868-ff-001-9_Carbon_dms0_01.fid/fid
 Origin: vnmrs
 Owner: jrhong
 DATE: 2012-09-29T18:24:36
 Solvent: dms0
 PULPROG: s2pul
 TE: 25 C
 NS: 256
 SFO1: 100.49 MHz
 SWH: 24509.8 Hz
 NUC: 13C
 TD: 31875

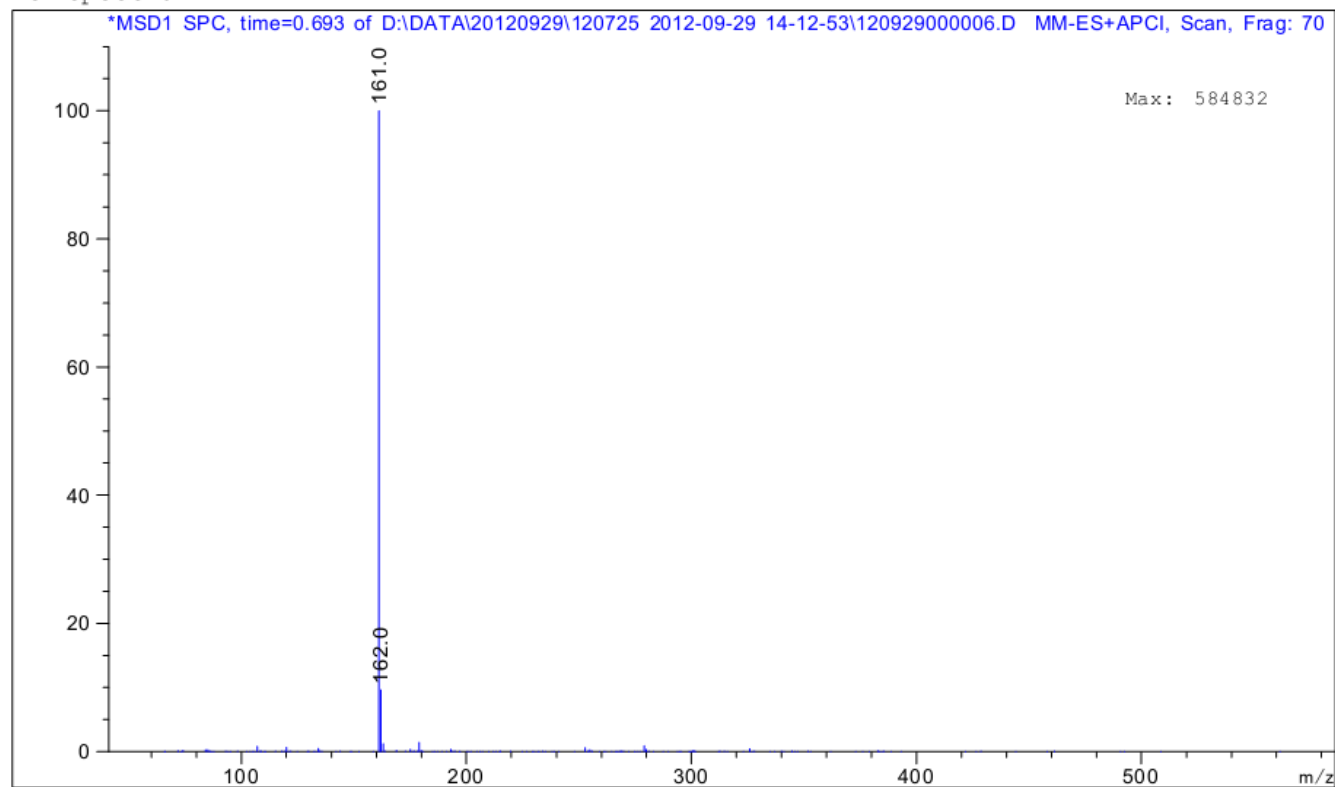
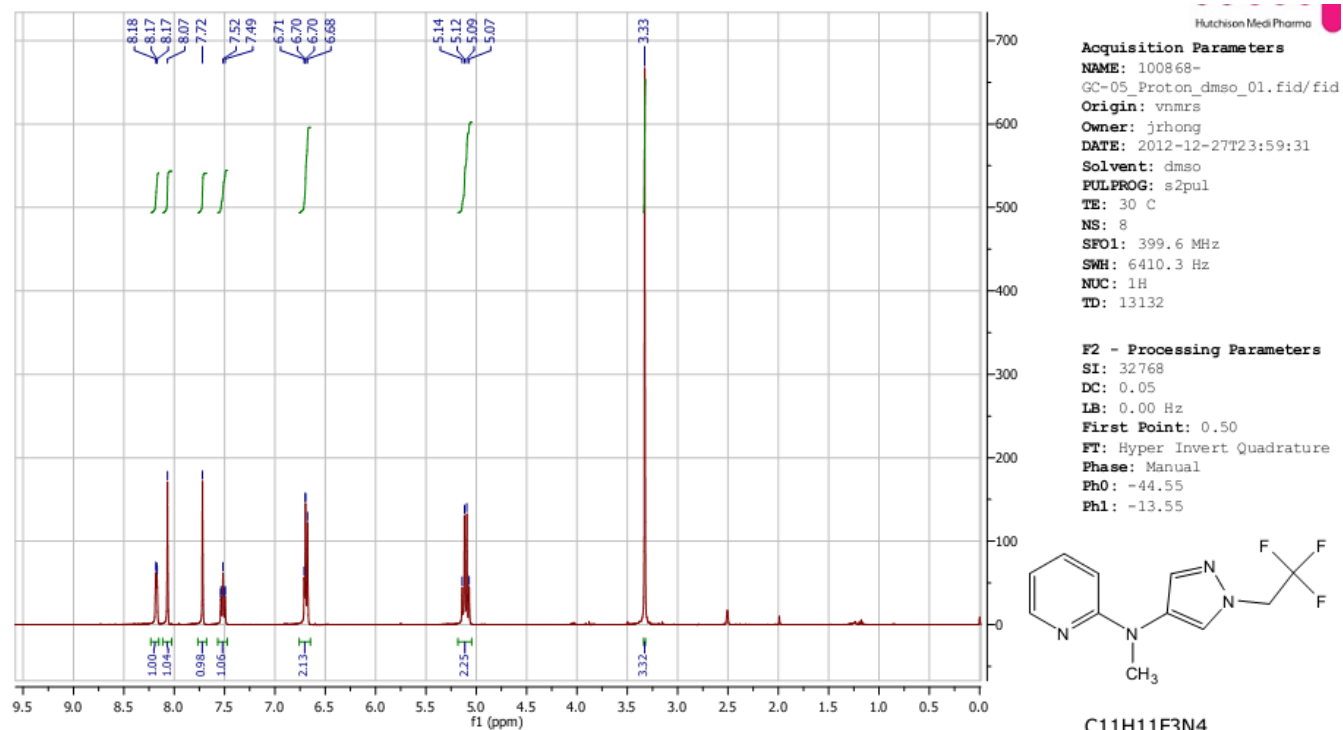
F2 - Processing Parameters
 SI: 65536
 DC: 0.05
 LB: 0.50 Hz
 First Point: 0.50
 FT: Hyper Invert Quadrature
 Phase: Manual
 Ph0: -26.78
 Ph1: -3.10



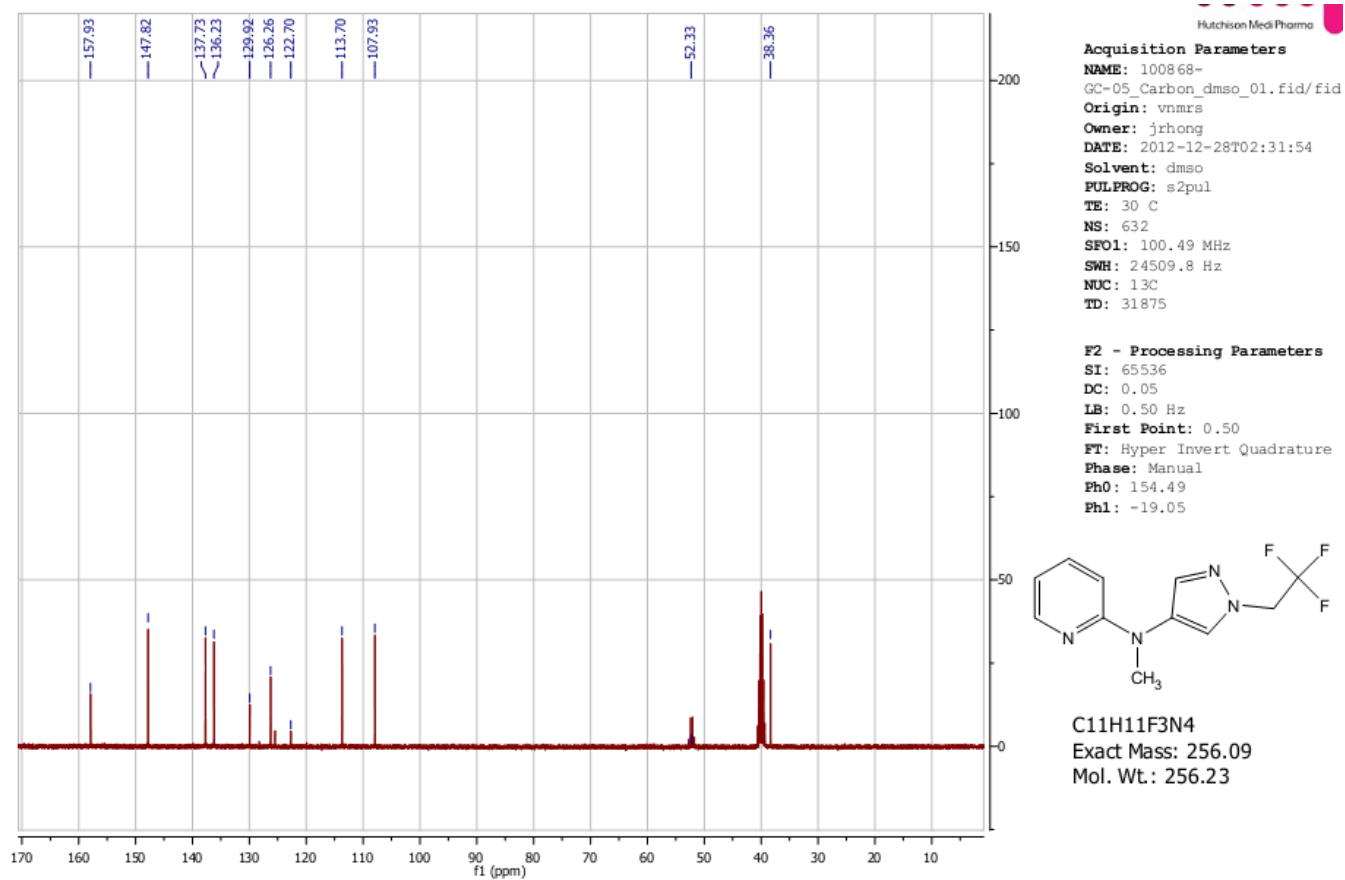
C8H8N4
 Exact Mass: 160.07
 Mol. Wt.: 160.18

LC-MS of 1'n

MS Spectrum

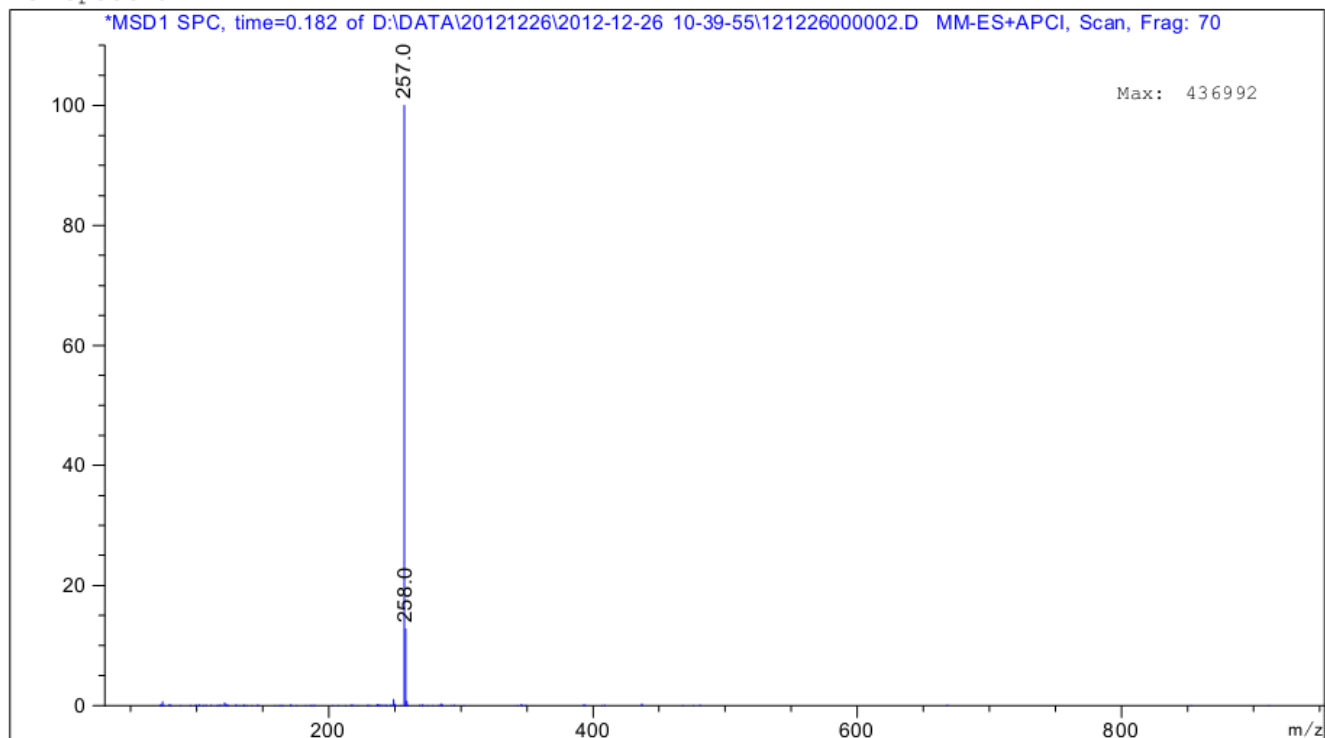
¹H NMR of 1'o

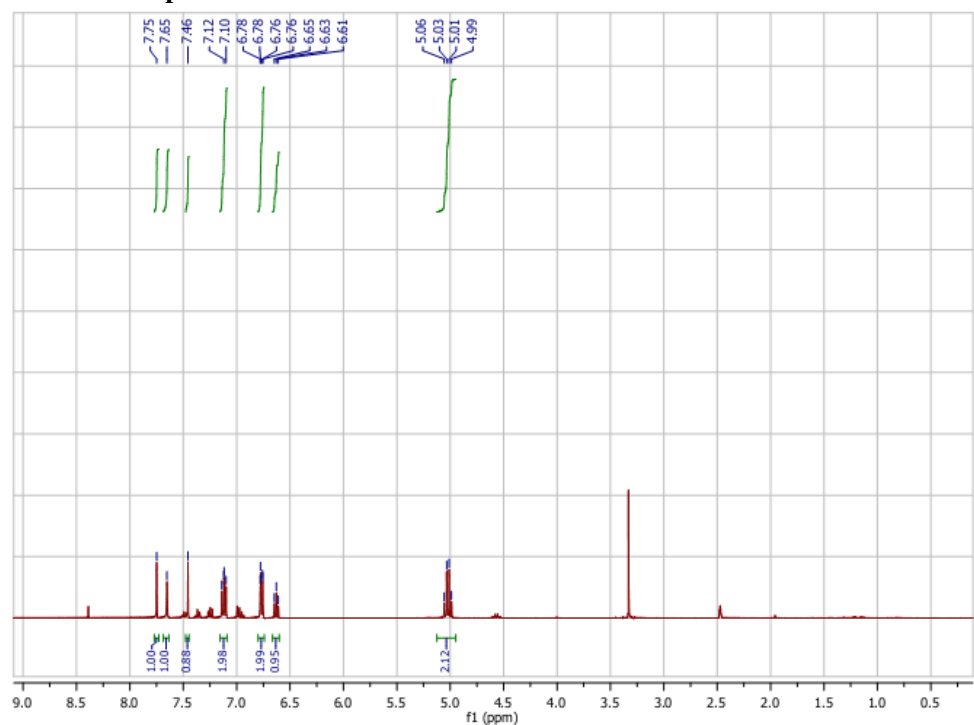
¹H NMR (400 MHz, dms0) δ 8.17 – 8.18 (m, 1H), 8.07 (s, 1H), 7.72 (s, 1H), 7.49 – 7.53 (m, 1H), 6.68 – 6.71 (m, 2H), 5.07 – 5.14 (m, 2H), 3.33 (s, 3H).

¹³C NMR of 1'o

LC-MS of 1'o

MS Spectrum



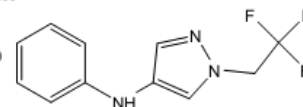
¹H NMR of 1'p

¹H NMR (400 MHz, dmsO) δ 7.75 (s, 1H), 7.65 (s, 1H), 7.46 (s, 1H), 7.10 - 7.14 (m, 2H), 6.76 - 6.78 (m, 2H), 6.63 (t, J = 7.3, 1H), 4.99 - 5.06 (q, J = 9.1, 2H).

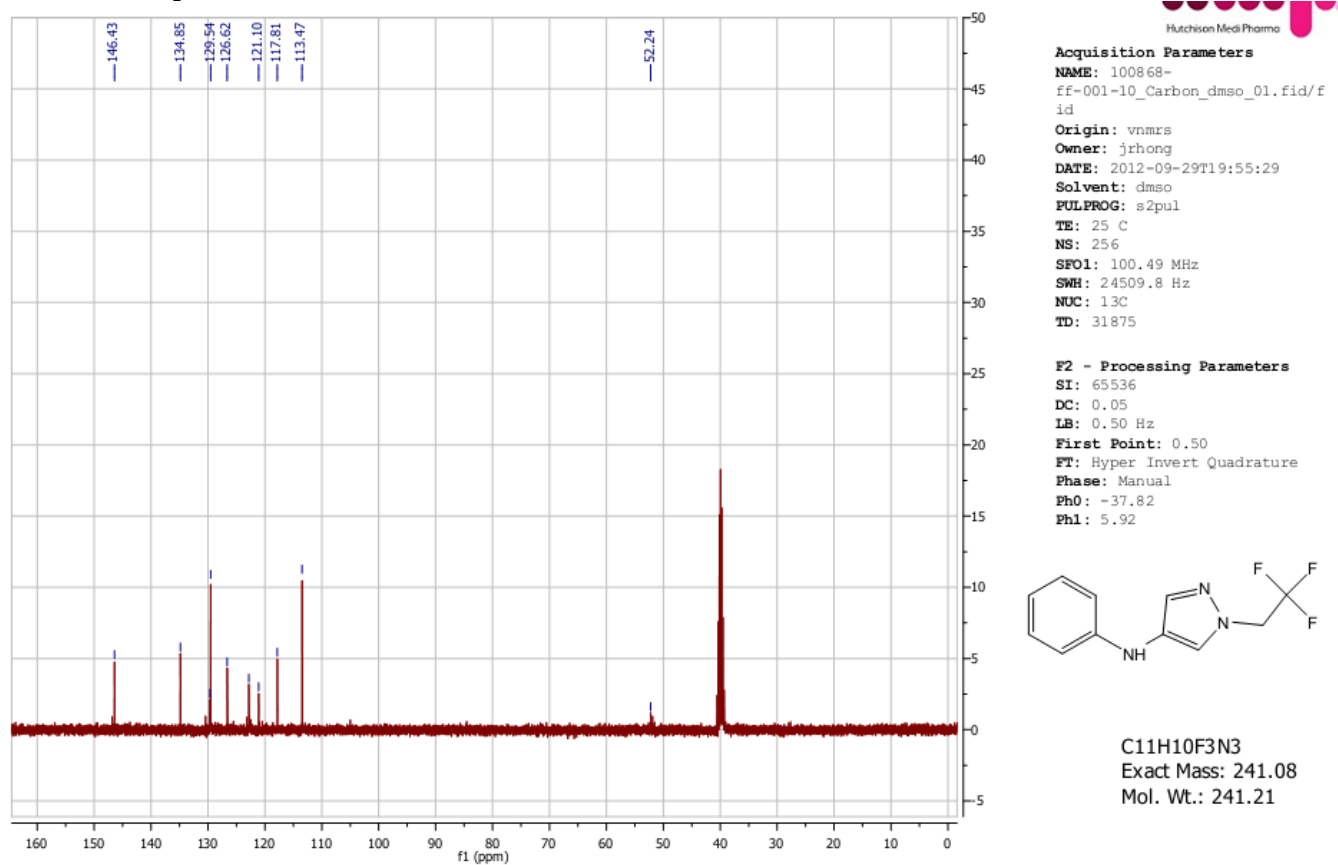
Hutchison Medi Pharma

Acquisition Parameters
NAME: 100868-
ff-001-10_Proton_dmsO_01.fid/
id
Origin: vnmsr
Owner: jrhong
DATE: 2012-09-29T16:57:45
Solvent: dmsO
PULPROG: s2pul
TE: 25 C
NS: 8
SFO1: 399.61 MHz
SWH: 6410.3 Hz
NUC: 1H
TD: 13132

F2 - Processing Parameters
SI: 32768
DC: 0.05
LB: 0.00 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: 147.31
Ph1: -33.27

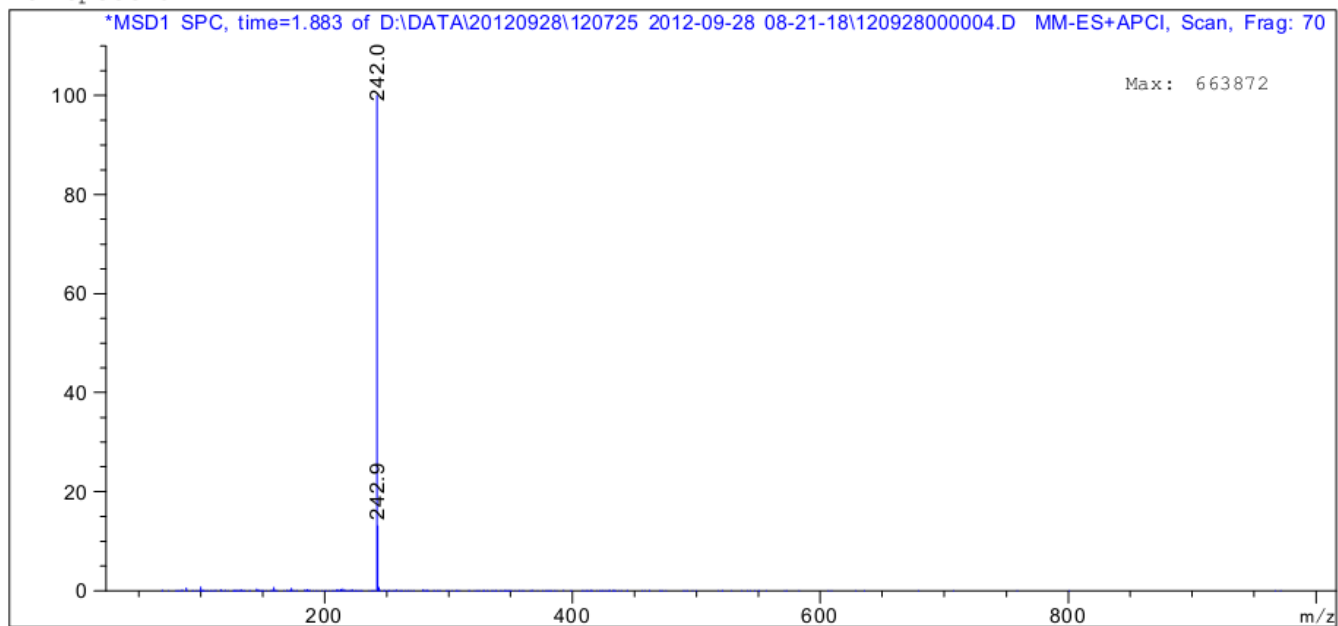


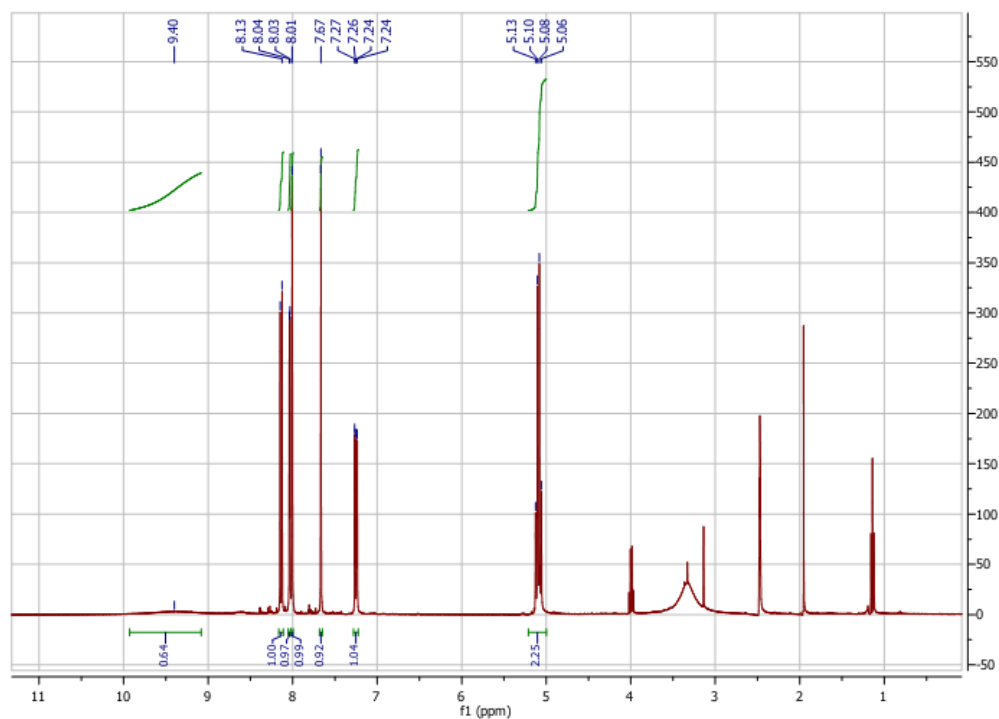
C₁₁H₁₀F₃N₃
Exact Mass: 241.08
Mol. Wt.: 241.21

¹³C NMR of 1'p

LC-MS of 1'p

MS Spectrum



¹H NMR of 1'q

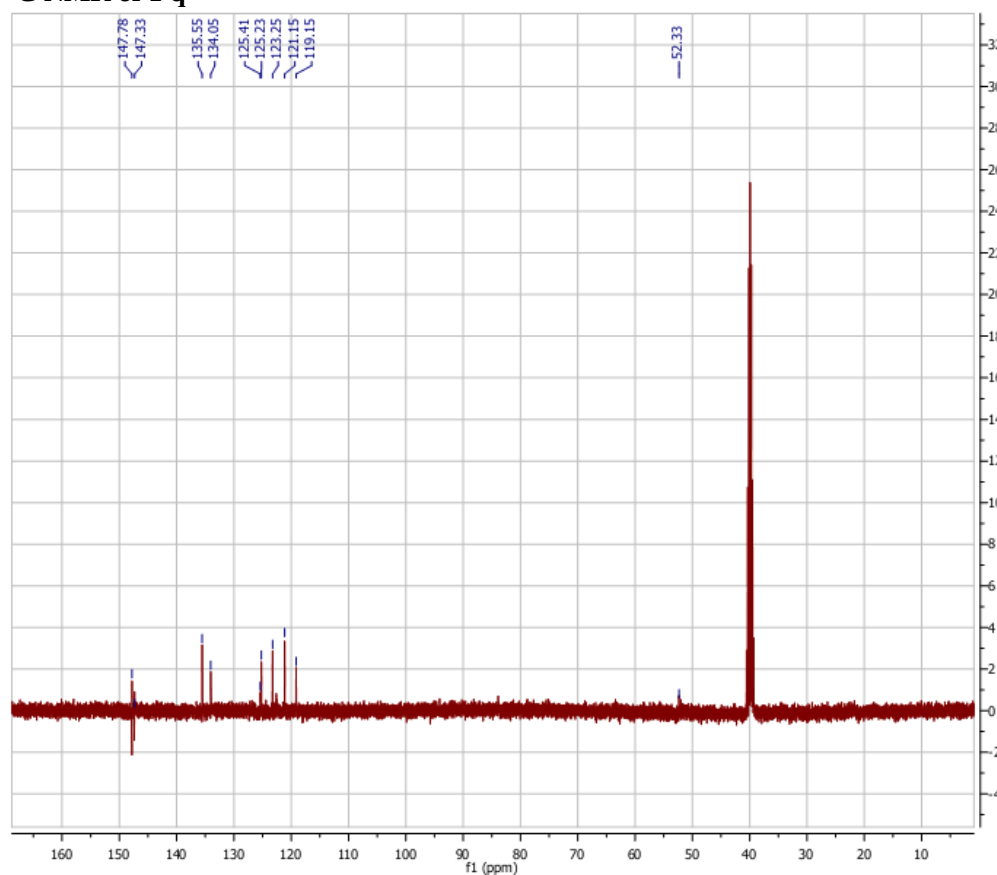
¹H NMR (400 MHz, dmsol-d₆) δ 9.40 (s, 1H), 8.14 (d, *J* = 9.1, 1H), 8.04 (d, *J* = 2.8, 1H), 8.01 (s, 1H), 7.67 (d, *J* = 0.5, 1H), 7.25 (dd, *J* = 9.1, 2.9, 1H), 5.09 (q, *J* = 9.1, 2H).

Hutchison Medi Pharma

Acquisition Parameters
NAME: 100868-
ff-001-11_Proton_dmsol_01.fid/f
id
Origin: vnmrs
Owner: jrhong
DATE: 2012-09-28T23:33:17
Solvent: dmsol
PULPROG: s2pul
TE: 25 C
NS: 8
SF01: 399.61 MHz
SWH: 6410.3 Hz
NUC: 1H
TD: 13132

F2 - Processing Parameters
SI: 32768
DC: 0.05
LB: 0.00 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: 133.39
Ph1: -24.81

C₁₀H₈F₃N₅O₂
Exact Mass: 287.06
Mol. Wt.: 287.2

¹³C NMR of 1'q

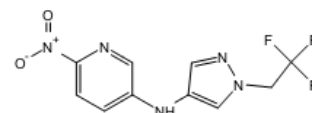
Hutchison Medi Pharma

Acquisition Parameters

NAME: 100868-
ff-001-11_Carbon_dms0_01.fid/
id
Origin: vnmsr
Owner: jrhong
DATE: 2012-09-29T22:51:34
Solvent: dms0
PULPROG: s2pul
TE: 25 C
NS: 256
SFO1: 100.49 MHz
SWH: 24509.8 Hz
NUC: 13C
TD: 31875

F2 - Processing Parameters

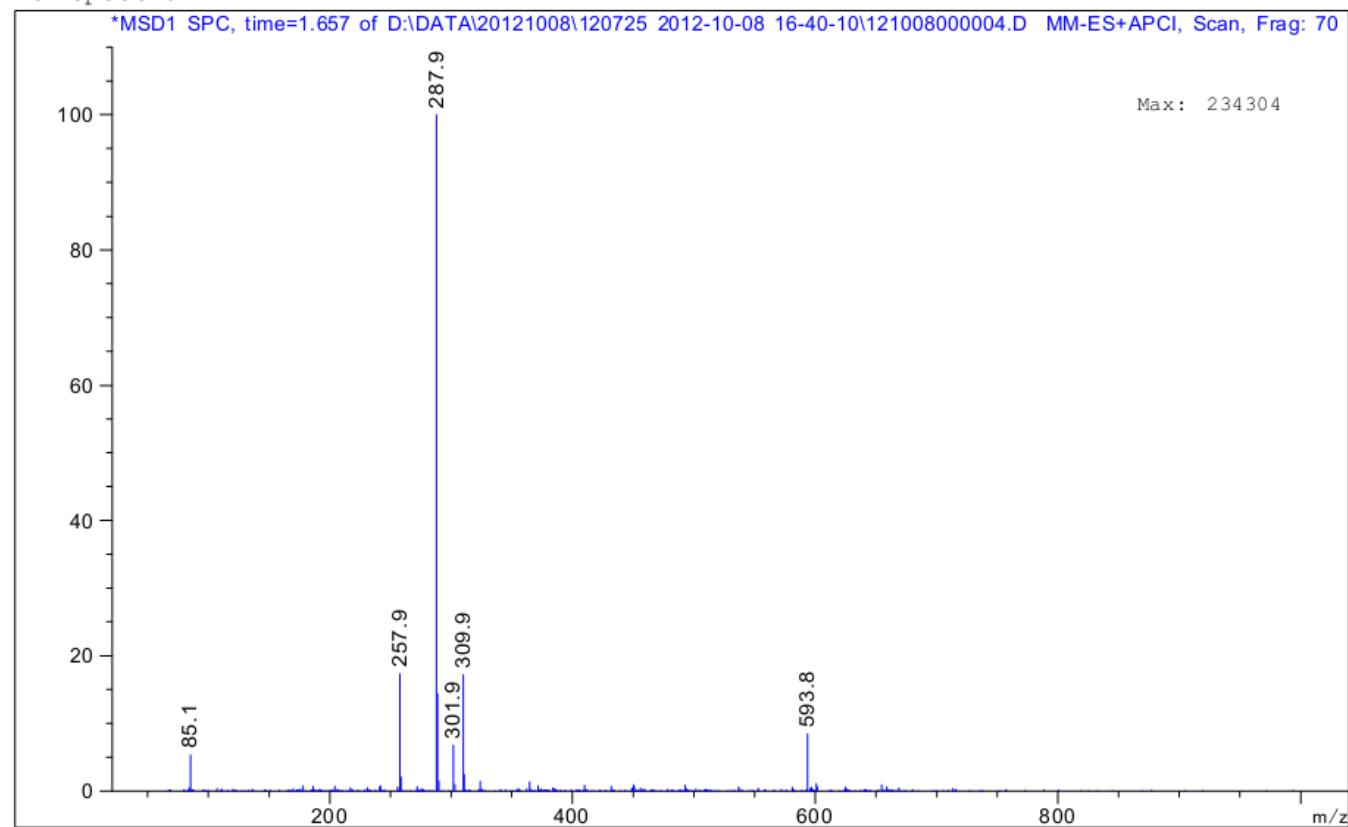
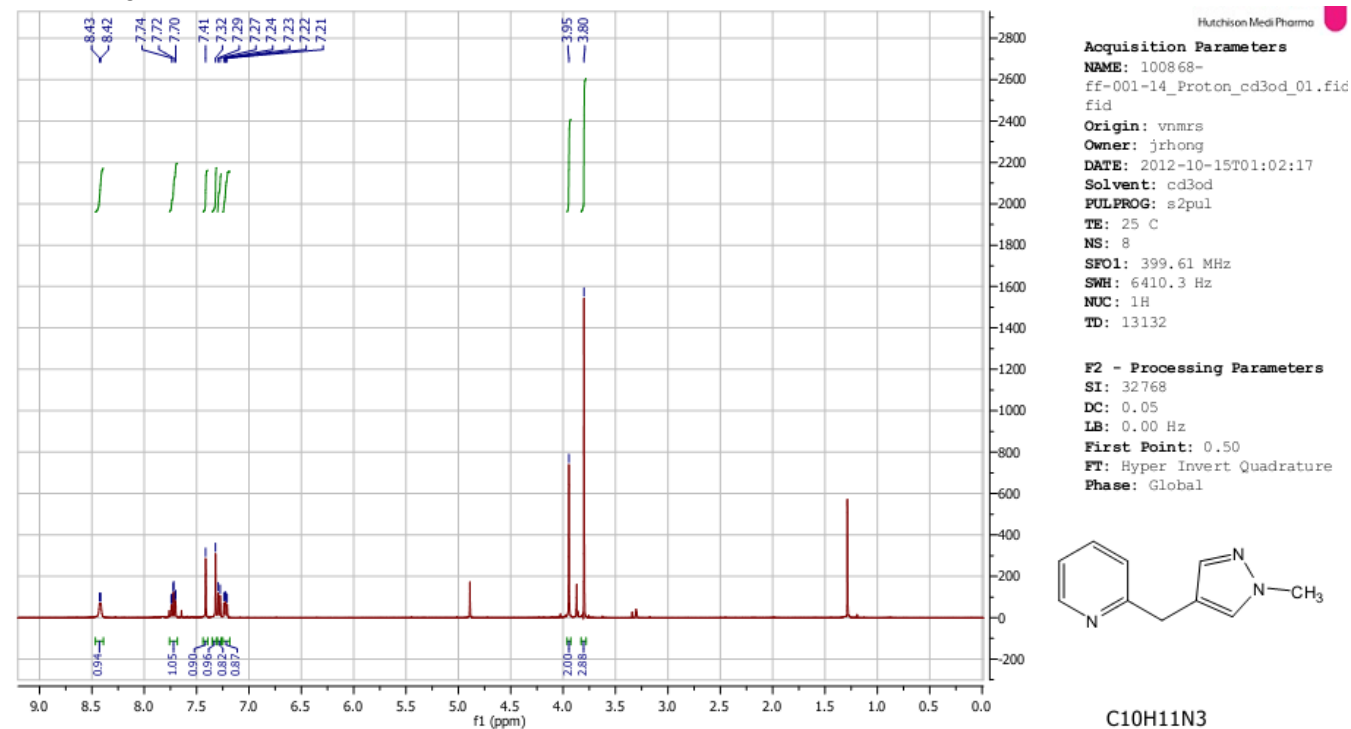
SI: 65536
DC: 0.05
LB: 0.50 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: -1191.67
Ph1: 1021.62



C10H8F3N5O2
Exact Mass: 287.06
Mol. Wt.: 287.2

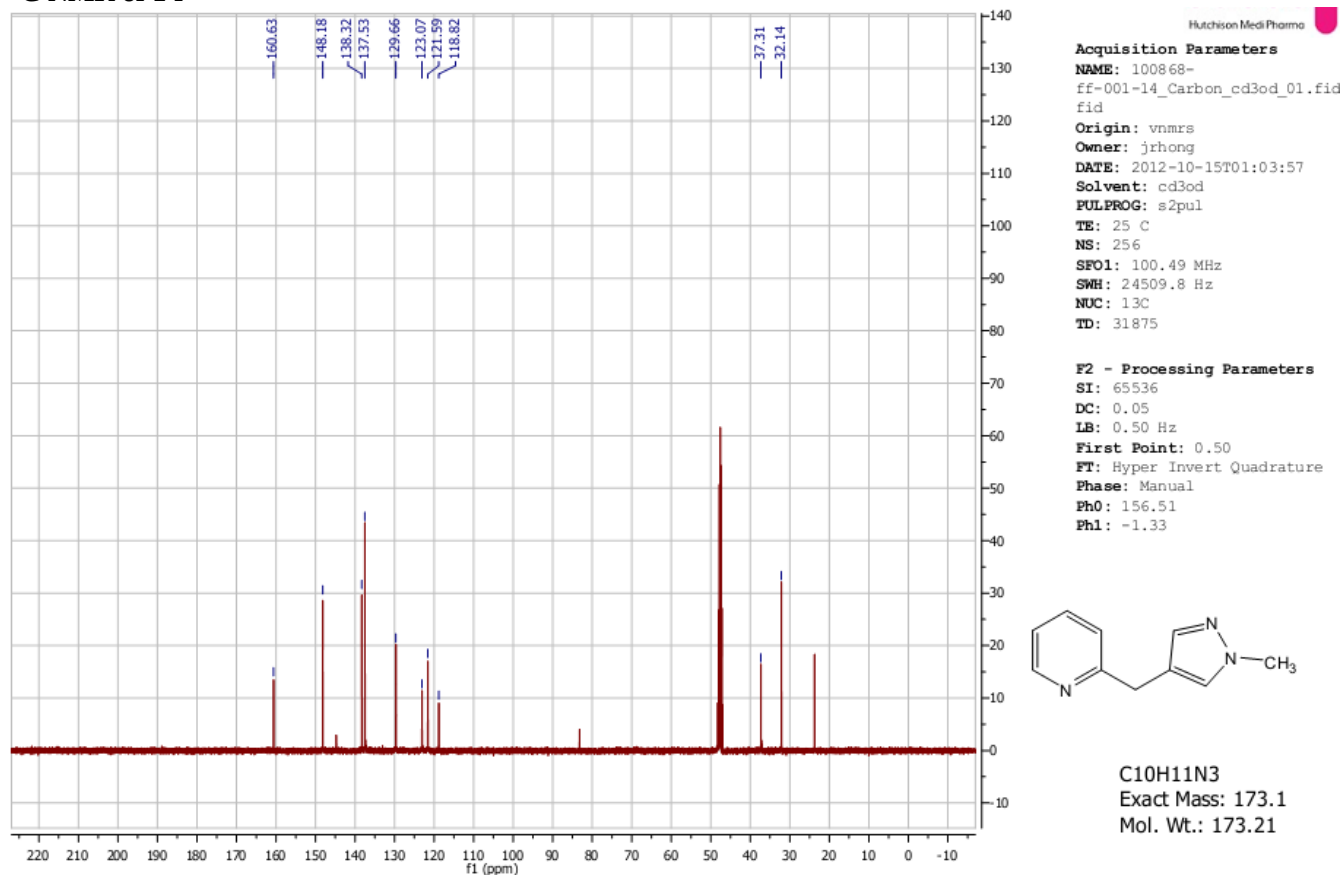
LC-MS of 1'q

MS Spectrum

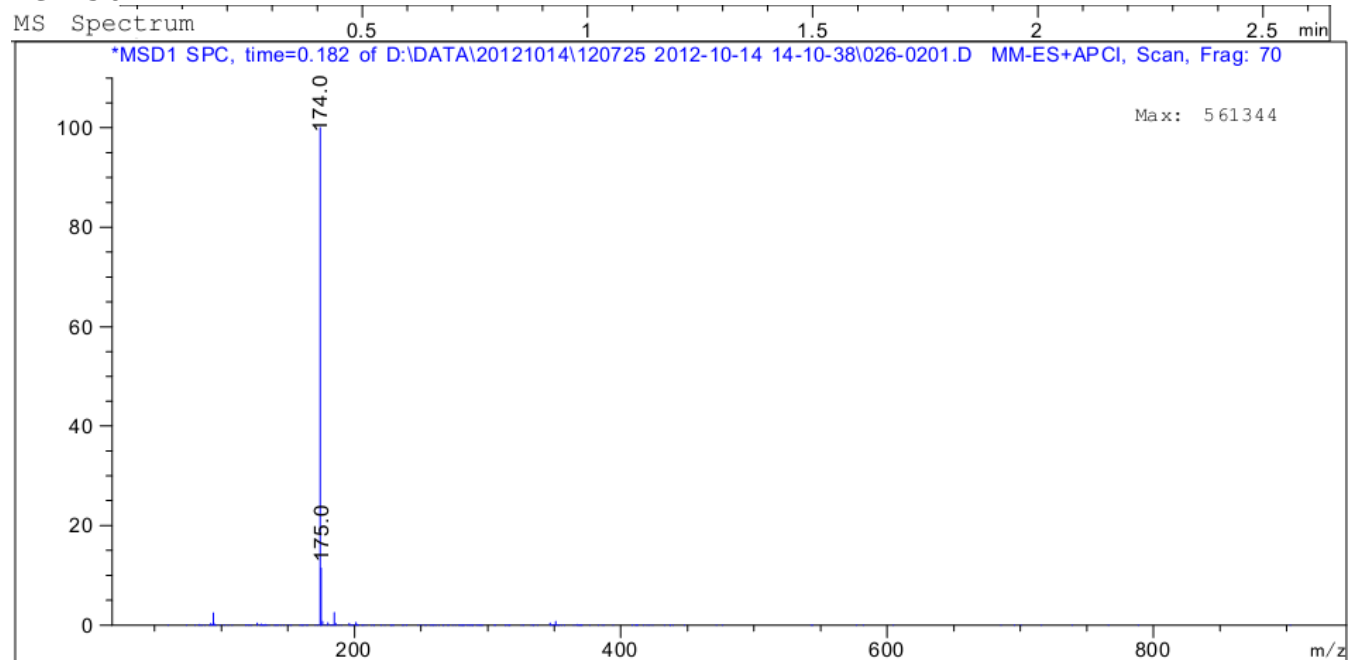
¹H NMR of 1'r

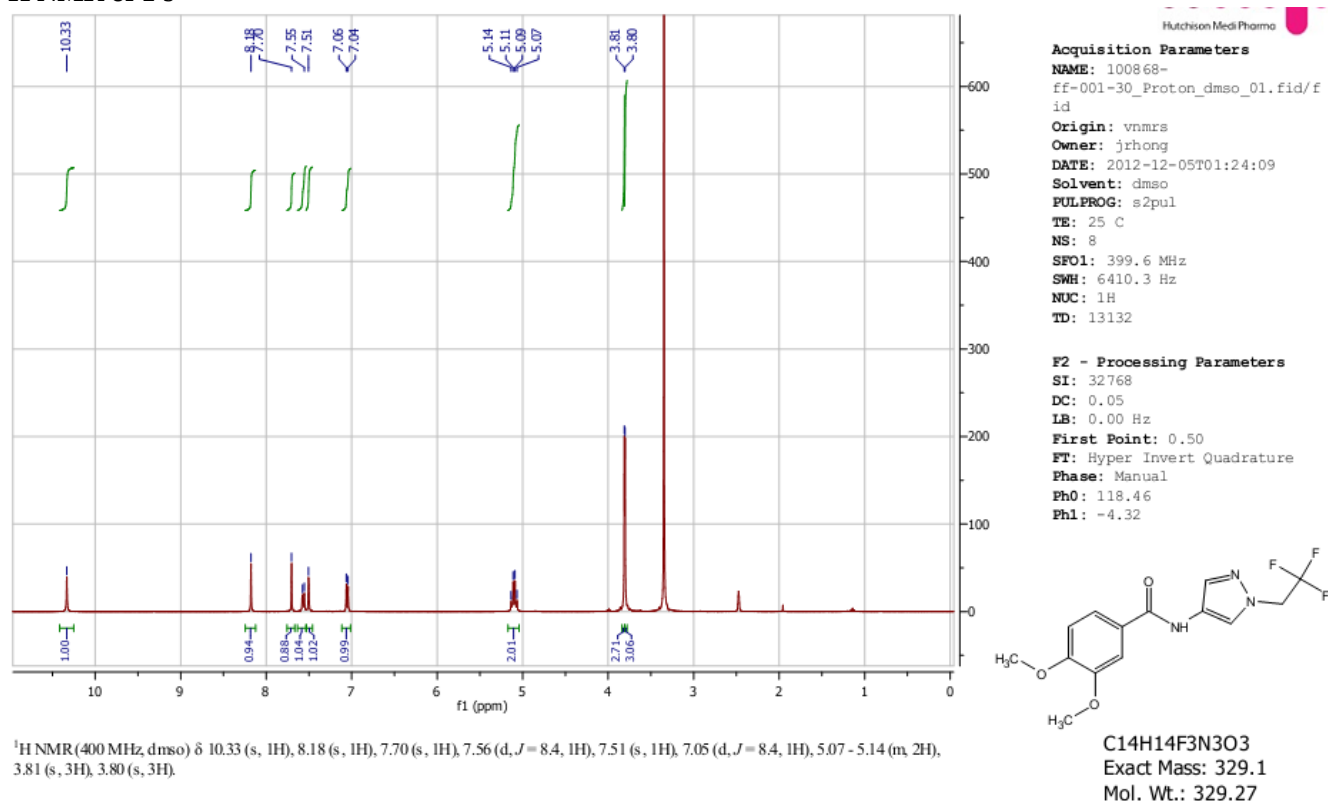
¹H NMR (400 MHz, cd₃od) δ 8.42 - 8.43 (m, 1H), 7.70 - 7.74 (m, 1H), 7.41 (s, 1H), 7.32 (s, 1H), 7.27 - 7.32 (m, 1H), 7.21 - 7.24 (m, 1H), 3.95 (s, 2H), 3.80 (s, 3H).

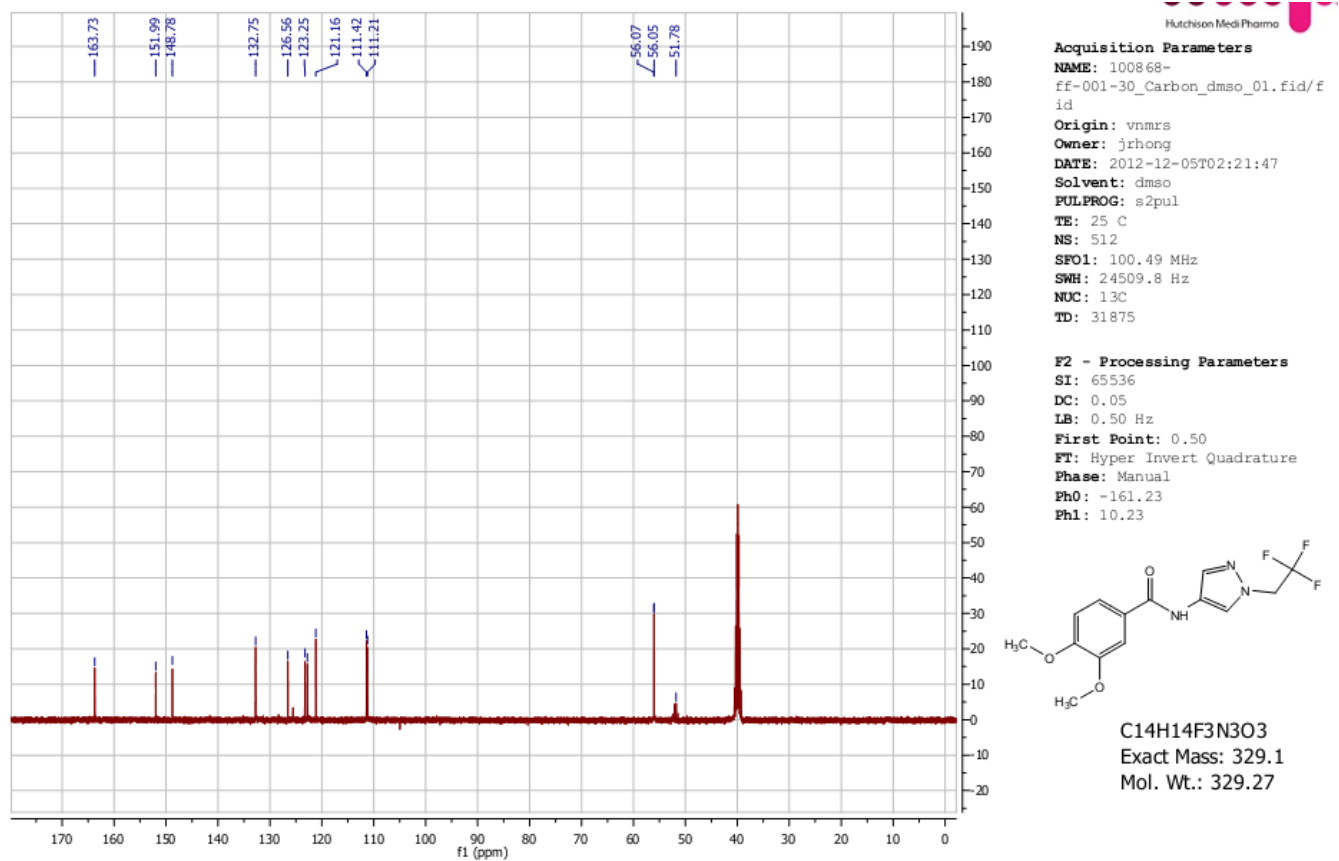
C10H11N3
Exact Mass: 173.1
Mol. Wt.: 173.21

¹³C NMR of 1'r

LC-MS of 1'r

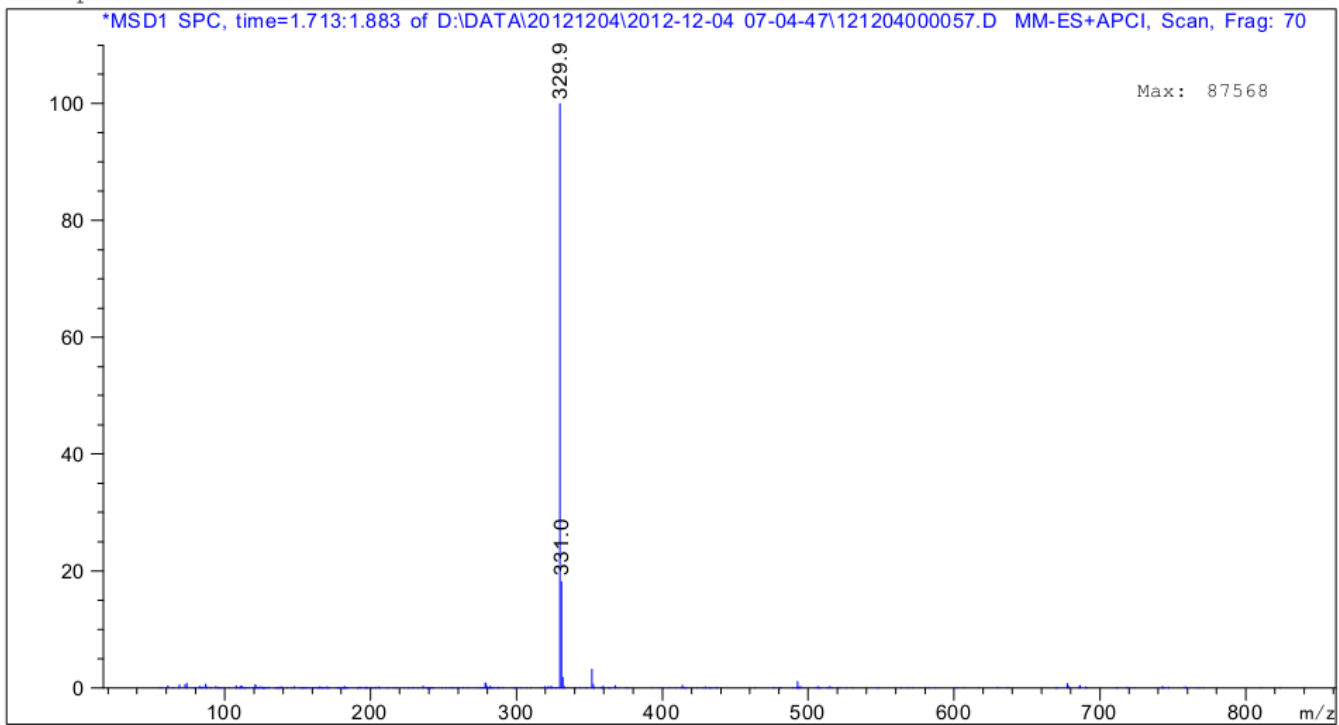


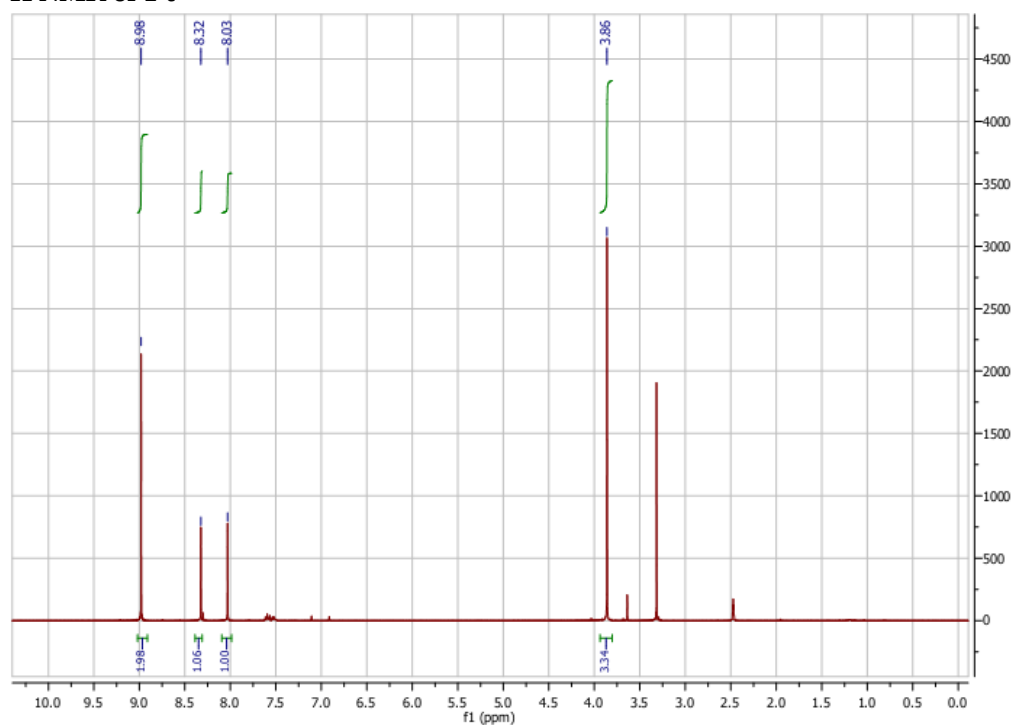
¹H NMR of 1's

¹³C NMR of 1's

LC-MS of 1's

MS Spectrum



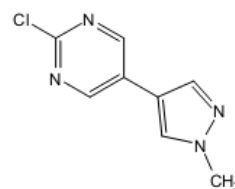
¹H NMR of 1't

¹H NMR (400 MHz, dms) δ 8.98 (s, 2H), 8.32 (s, 1H), 8.03 (s, 1H), 3.86 (s, 3H).

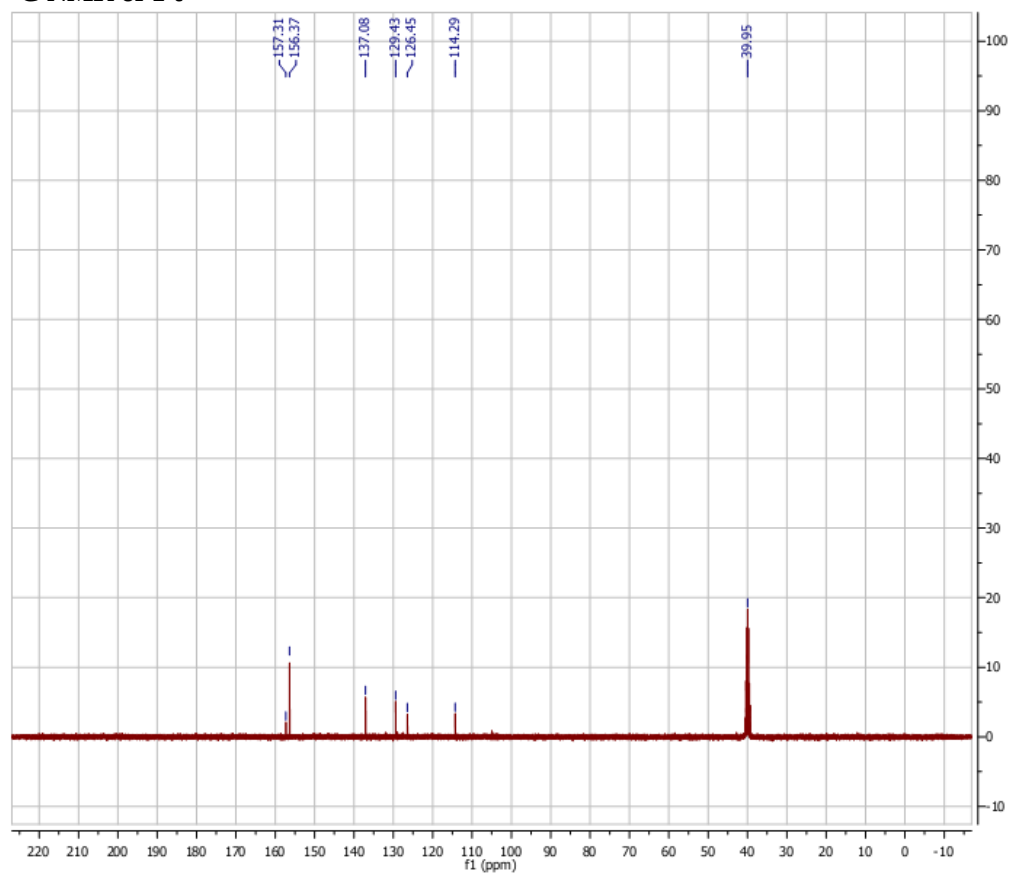
Hutchison MediPharma

Acquisition Parameters
NAME: 100868-
ff-001-7_Proton_dms0_01.fid/fi
d
Origin: vnmrs
Owner: jrhong
DATE: 2012-09-28T22:55:48
Solvent: dms0
PULPROG: s2pul
TE: 25 C
NS: 8
SF01: 399.61 MHz
SWH: 6410.3 Hz
NUC: 1H
TD: 13132

F2 - Processing Parameters
SI: 32768
DC: 0.05
LB: 0.00 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: 127.87
Ph1: -4.85



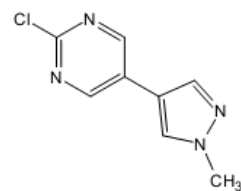
C8H7ClN4
Exact Mass: 194.04
Mol. Wt.: 194.62

¹³C NMR of 1't

Hutchison MediPharma

Acquisition Parameters
NAME: 100868-
ff-001-7_Carbon_dms0_01.fid/f:
d
Origin: vnms
Owner: jrhong
DATE: 2012-09-29T18:12:03
Solvent: dms0
PULPROG: s2pul
TE: 25 C
NS: 256
SFO1: 100.49 MHz
SWH: 24509.8 Hz
NUC: 13C
TD: 31875

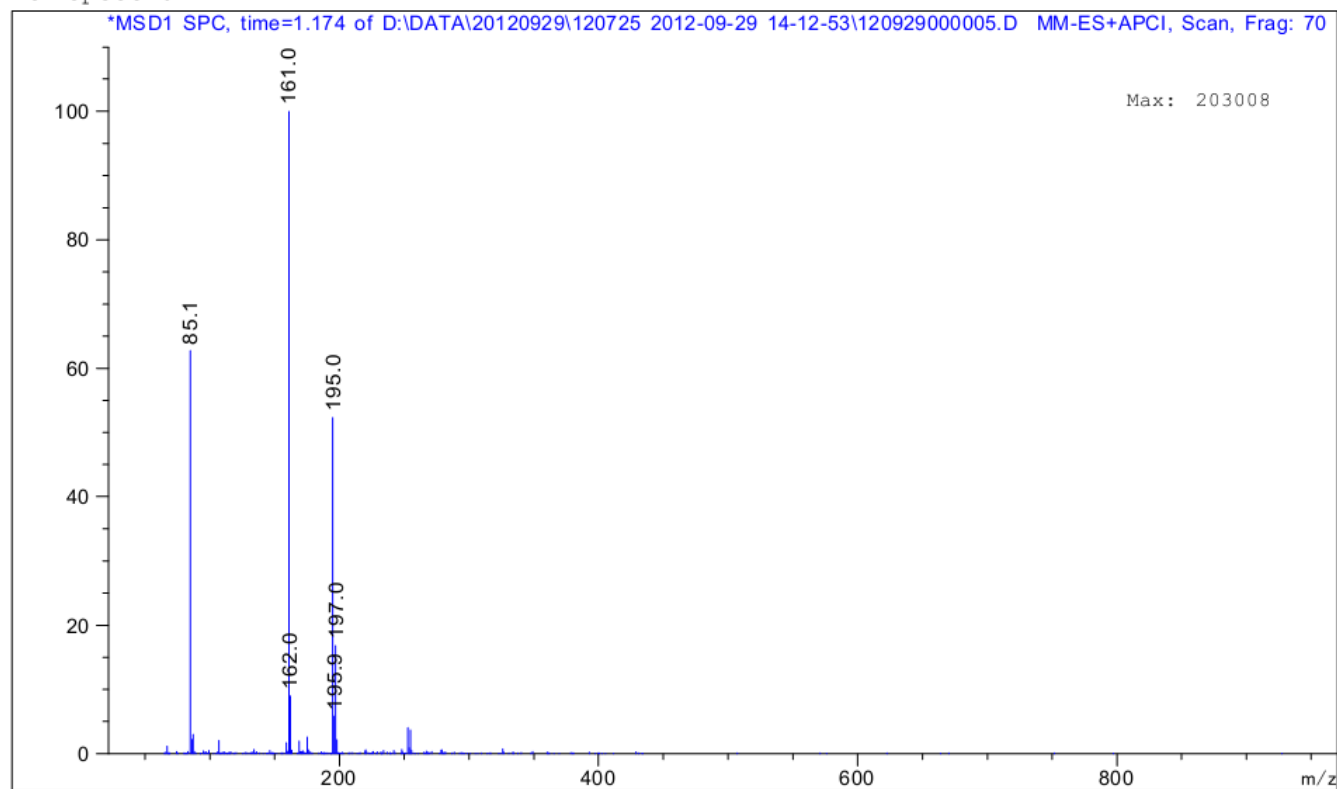
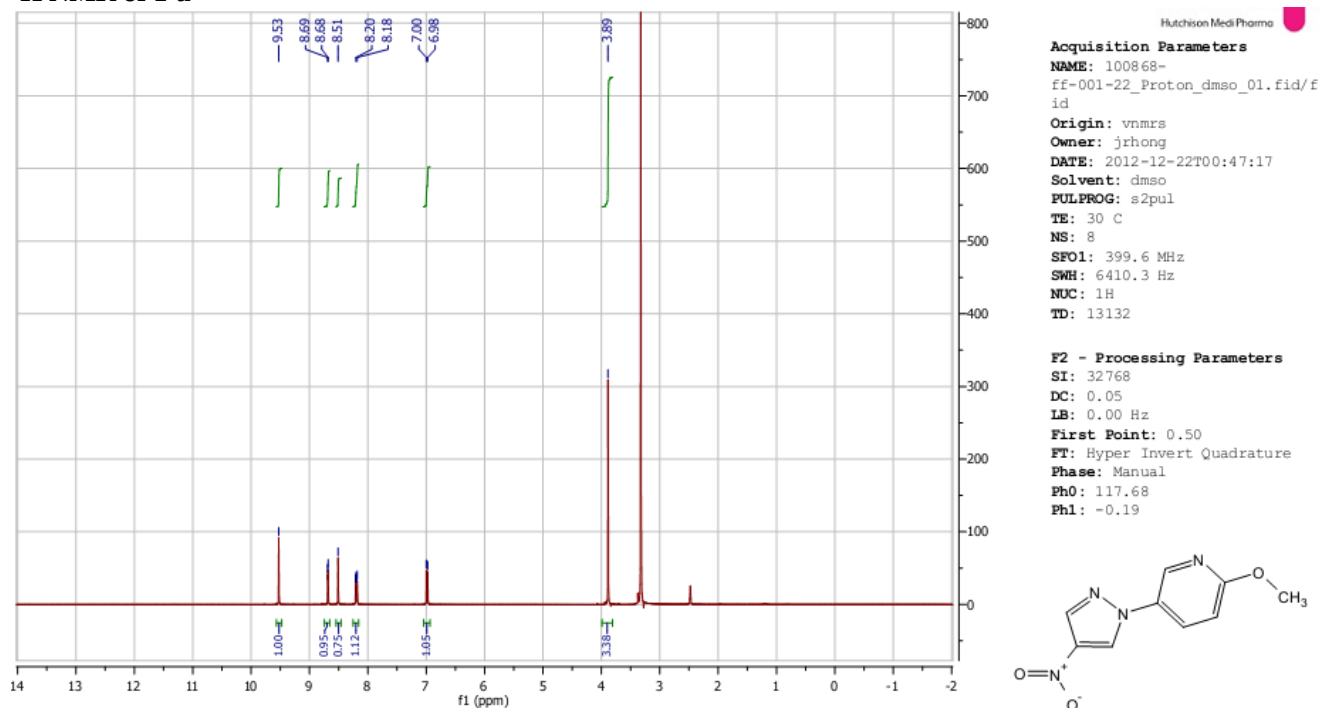
F2 - Processing Parameters
SI: 65536
DC: 0.05
LB: 0.50 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: -42.42
Ph1: 19.32



C₈H₇ClN₄
Exact Mass: 194.04
Mol. Wt.: 194.62

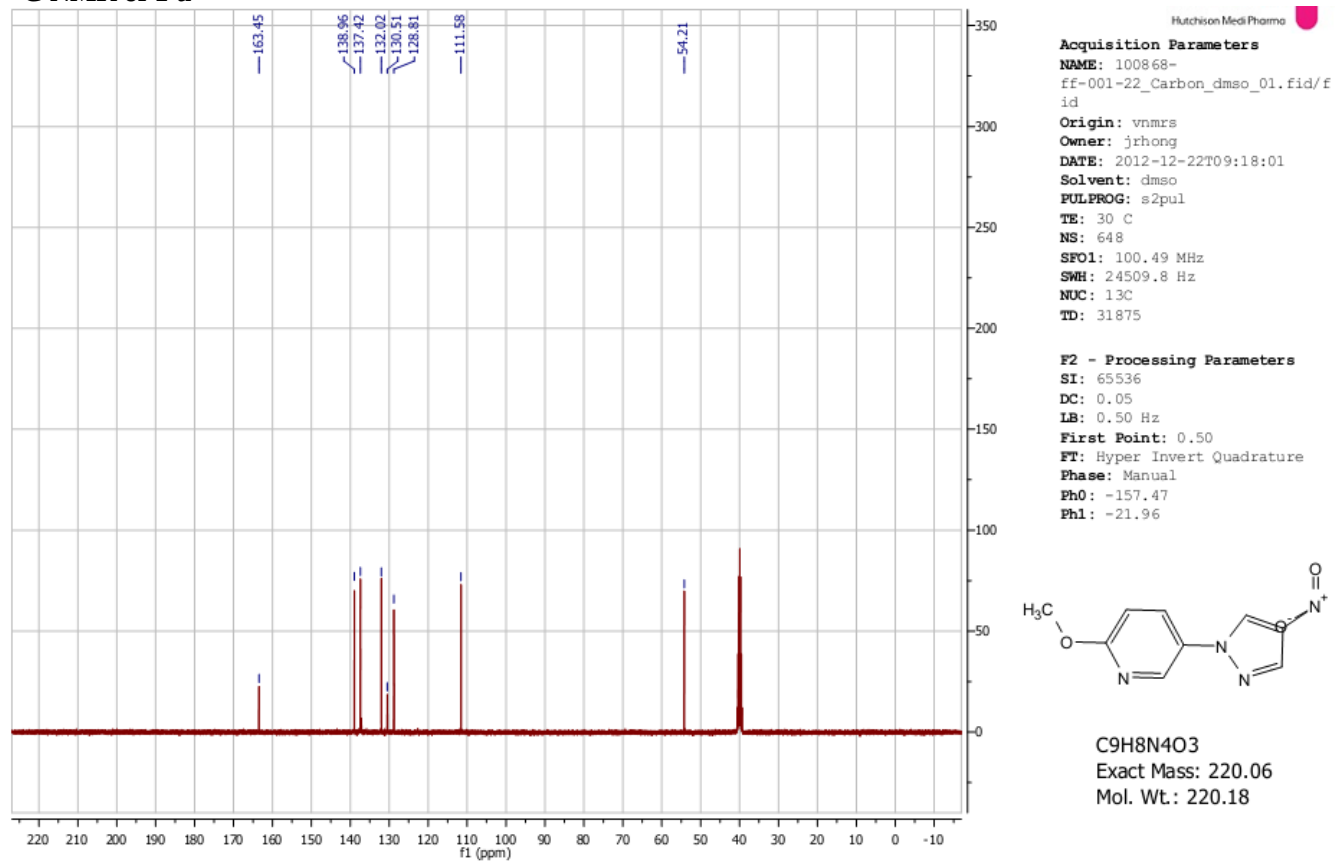
LC-MS of 1't

MS Spectrum

¹H NMR of 1'u

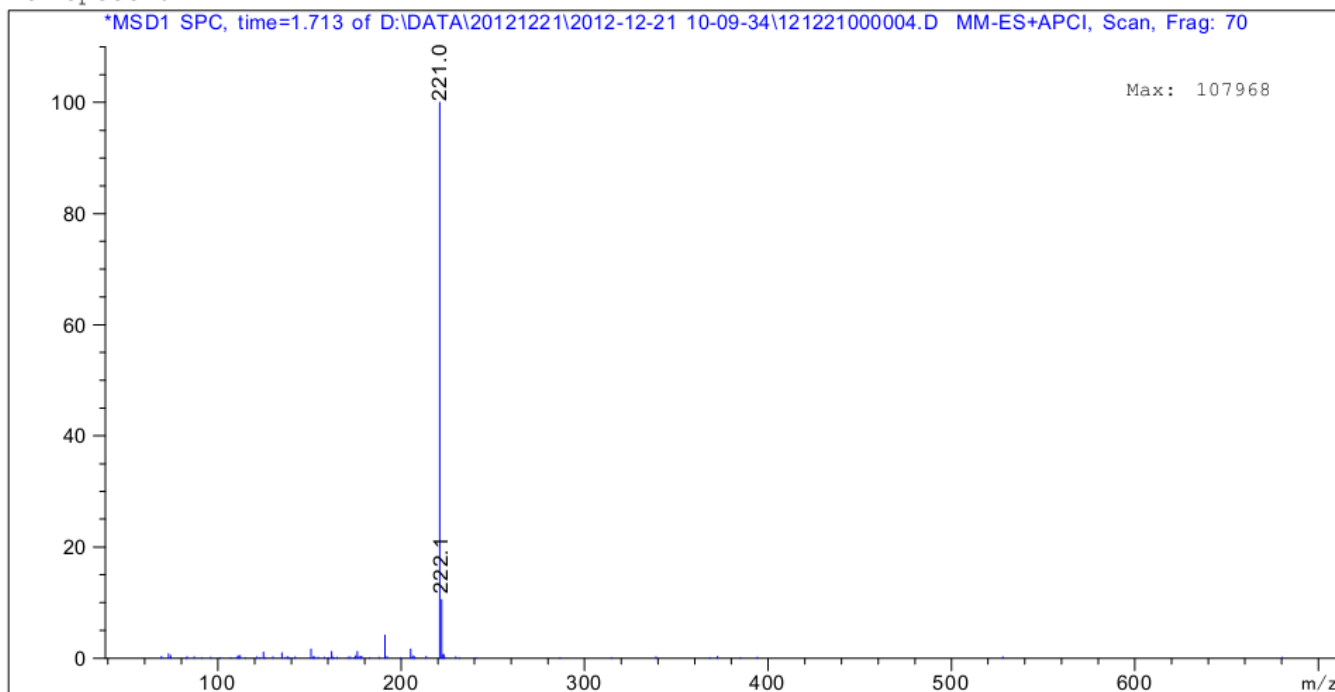
¹H NMR (400 MHz, dms0) δ 9.53 (s, 1H), 8.69 (d, *J* = 2.6, 1H), 8.51 (s, 1H), 8.20 (dd, *J* = 9.0, 2.8, 1H), 6.99 (d, *J* = 9.0, 1H), 3.89 (s, 3H).

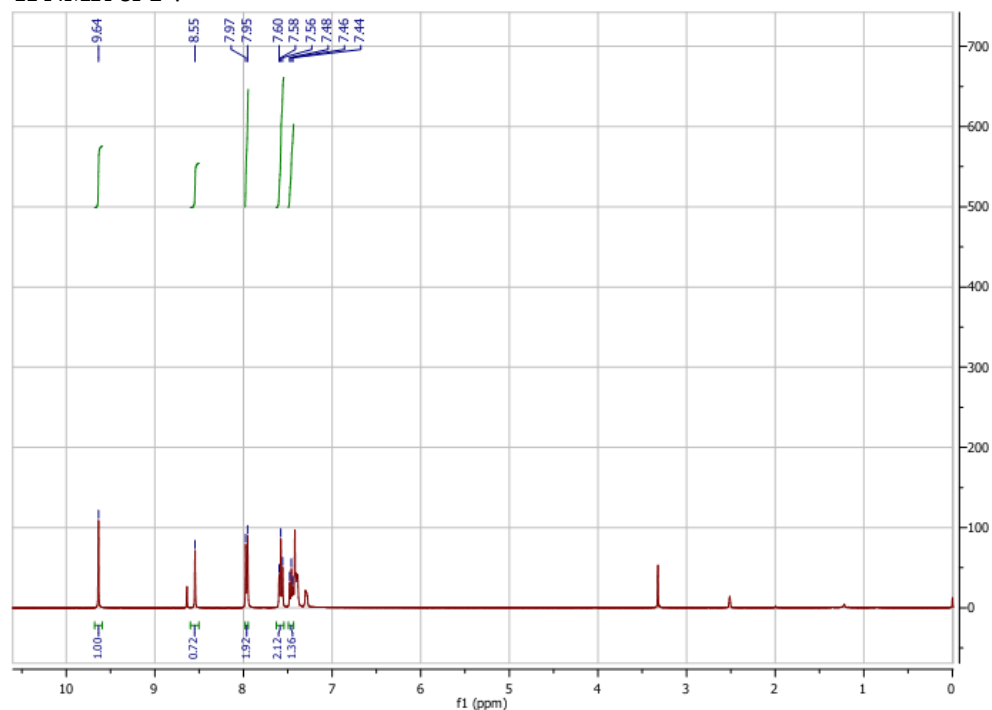
C9H8N4O3
Exact Mass: 220.06
Mol. Wt.: 220.18

¹³C NMR of 1'u

LC-MS of 1'u

MS Spectrum



¹H NMR of 1'v

¹H NMR (400 MHz, dmsO) δ 9.64 (s, 1H), 8.55 (s, 1H), 7.95 - 7.97 (m, 2H), 7.56 - 7.60 (m, 2H), 7.44 - 7.48 (m, 1H).

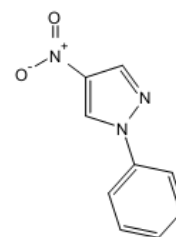
Hutchison Medi Pharma

Acquisition Parameters

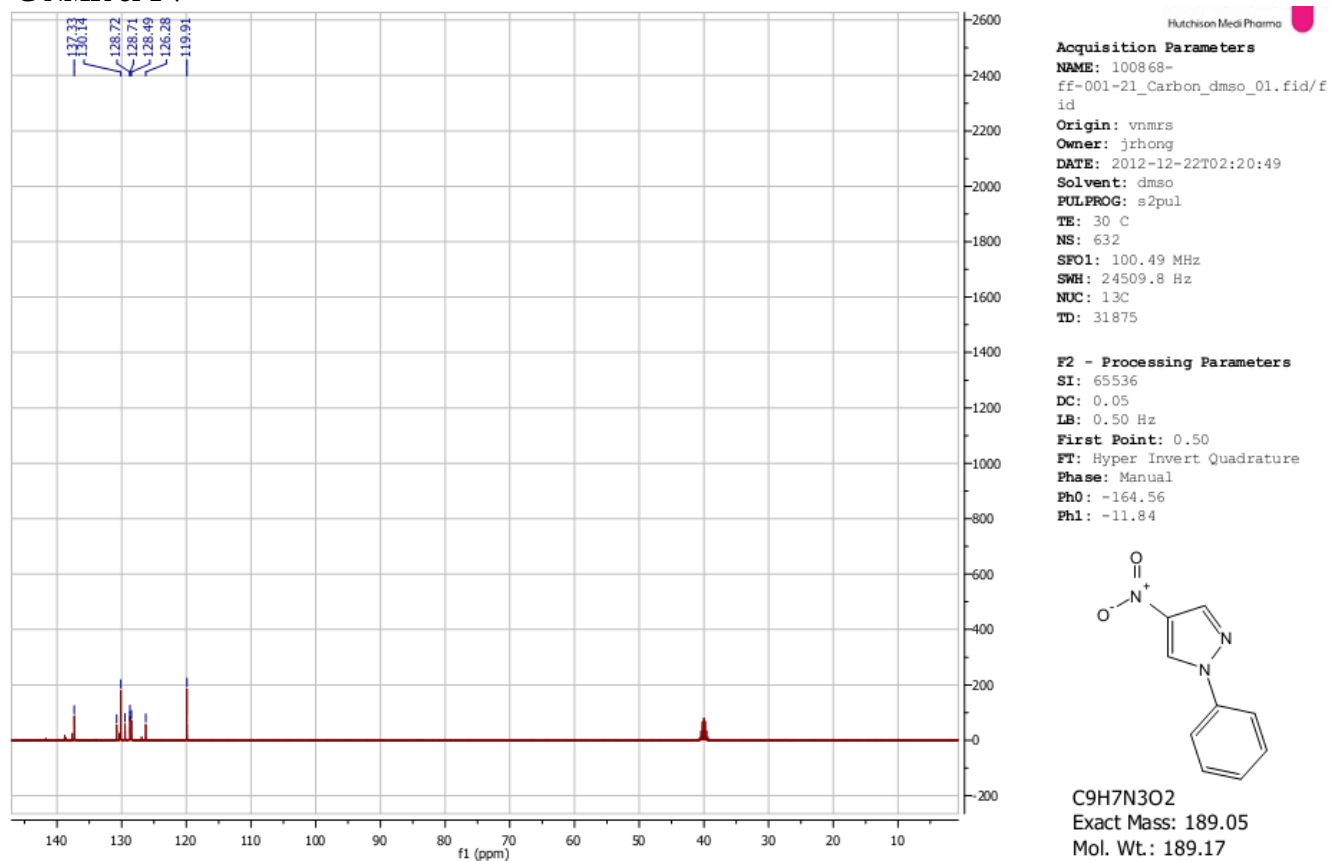
NAME: 100868-
ff-001-21_Proton_dmsO_01.fid/f
id
Origin: vnmrs
Owner: jrhong
DATE: 2012-12-21T20:45:00
Solvent: dmsO
PULPROG: s2pul
TE: 30 C
NS: 8
SF01: 399.6 MHz
SWH: 6410.3 Hz
NUC: 1H
TD: 13132

F2 - Processing Parameters

SI: 32768
DC: 0.05
LB: 0.00 Hz
First Point: 0.50
FT: Hyper Invert Quadrature
Phase: Manual
Ph0: 116.94
Ph1: 0.78



C₉H₇N₃O₂
Exact Mass: 189.05
Mol. Wt.: 189.17

¹³C NMR of 1'v

LC-MS of 1'v

MS Spectrum

