Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting information

The design, synthesis, and biological evaluation of novel YC-1 derivatives as potent anti-Hepatic Fibrosis agents

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† These authors contributed equally to this work.

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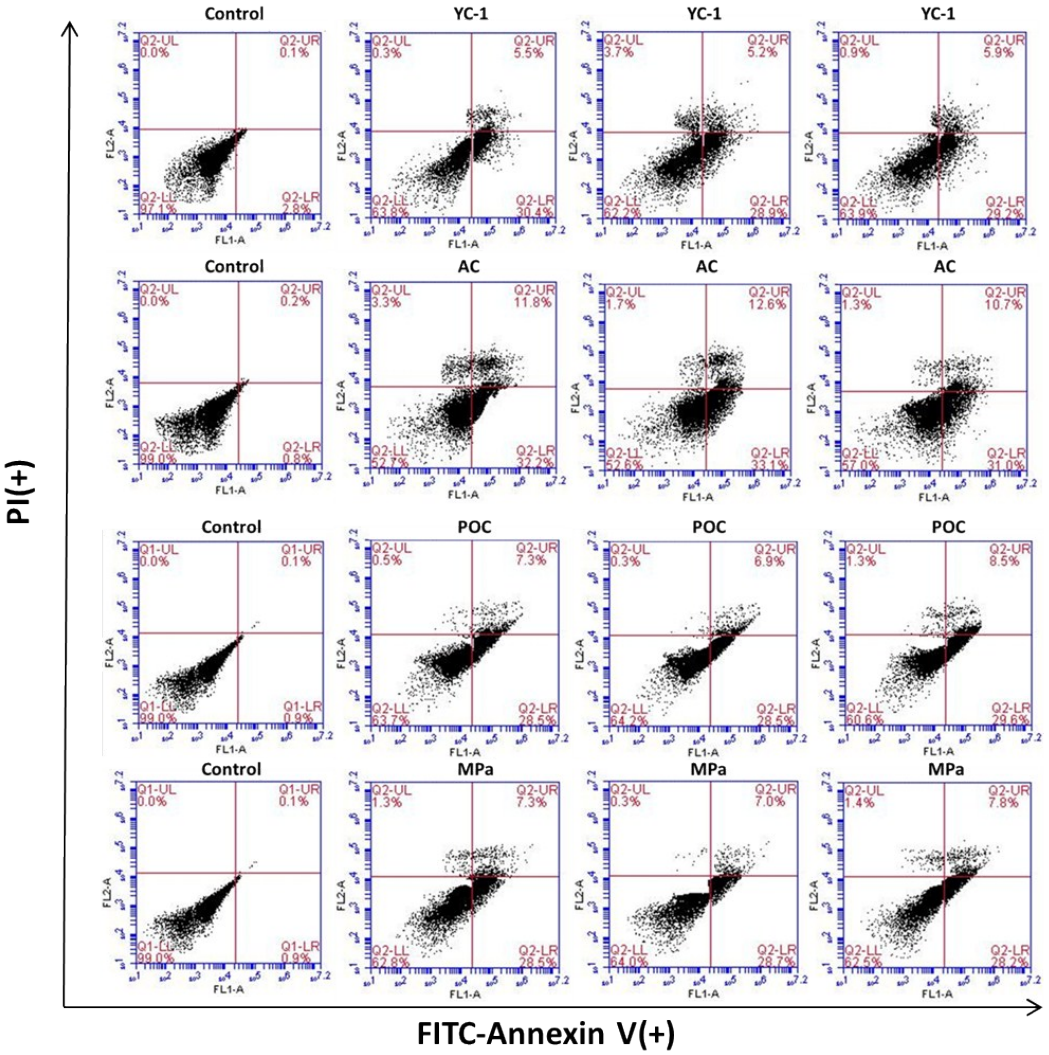
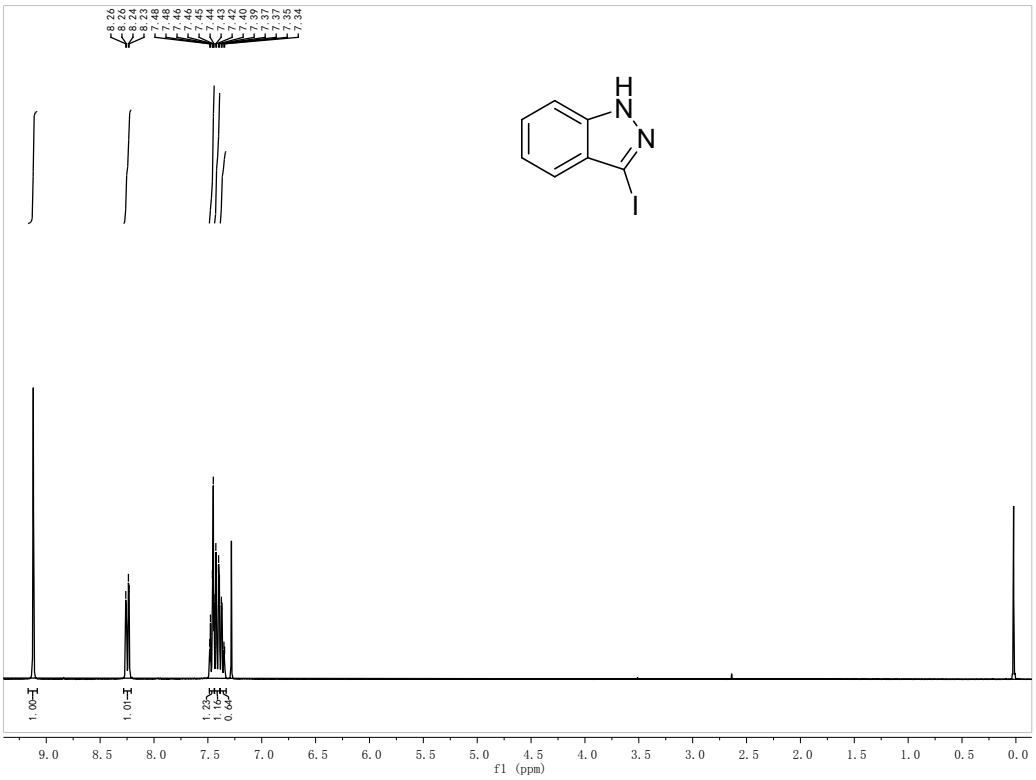


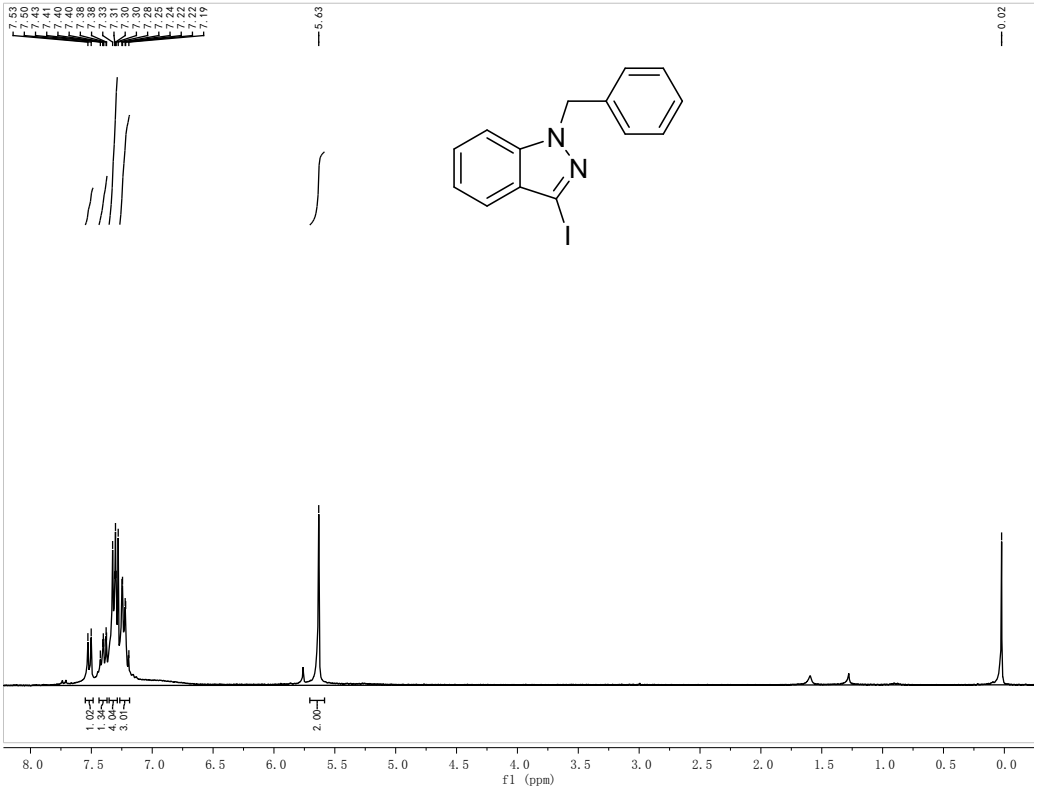
Figure S1. The effects of **YC-1**, **AC**, **POC** and **MPa** on LX-2 apoptosis. Activated LX-2 (2×10^5 cells/well in 6-well plate) were incubated with 25 uM **YC-1**, **AC** and **MPa** for 24h. Cells were then harvested and incubated with FITC conjugated annexin-V and PI. FITC-positive/PI-negative cell were measured by flow cytometry (n = 3/group).

Tof-MS and NMR Spectra

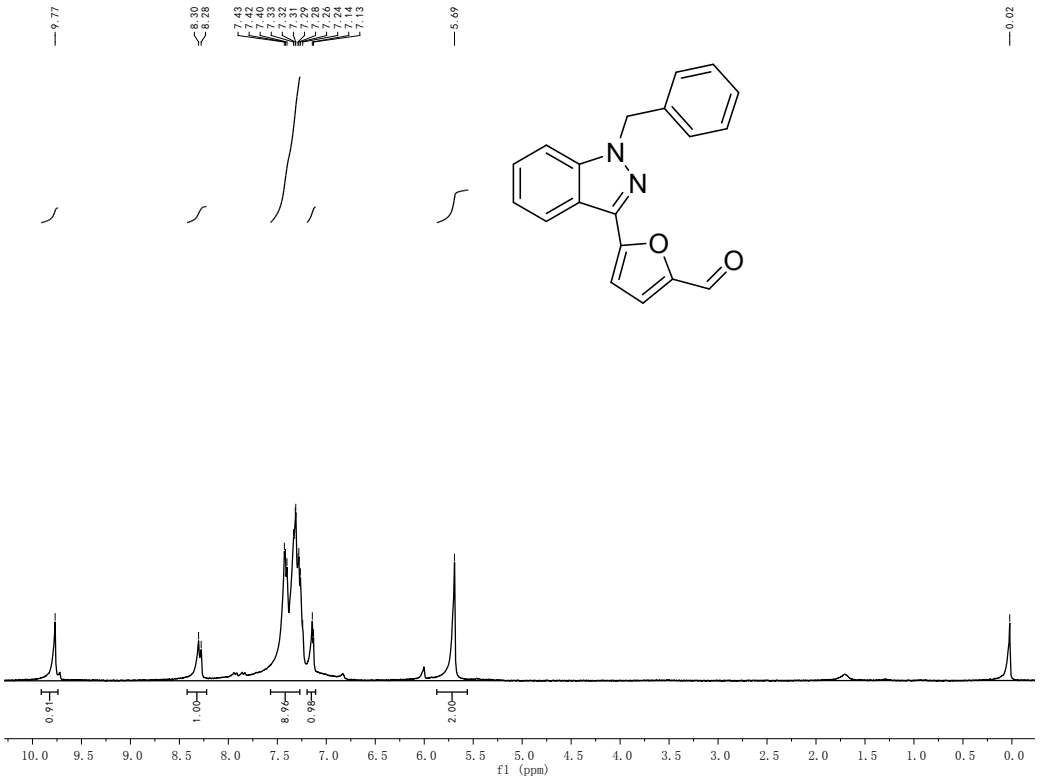
3-iodoindazole (1):



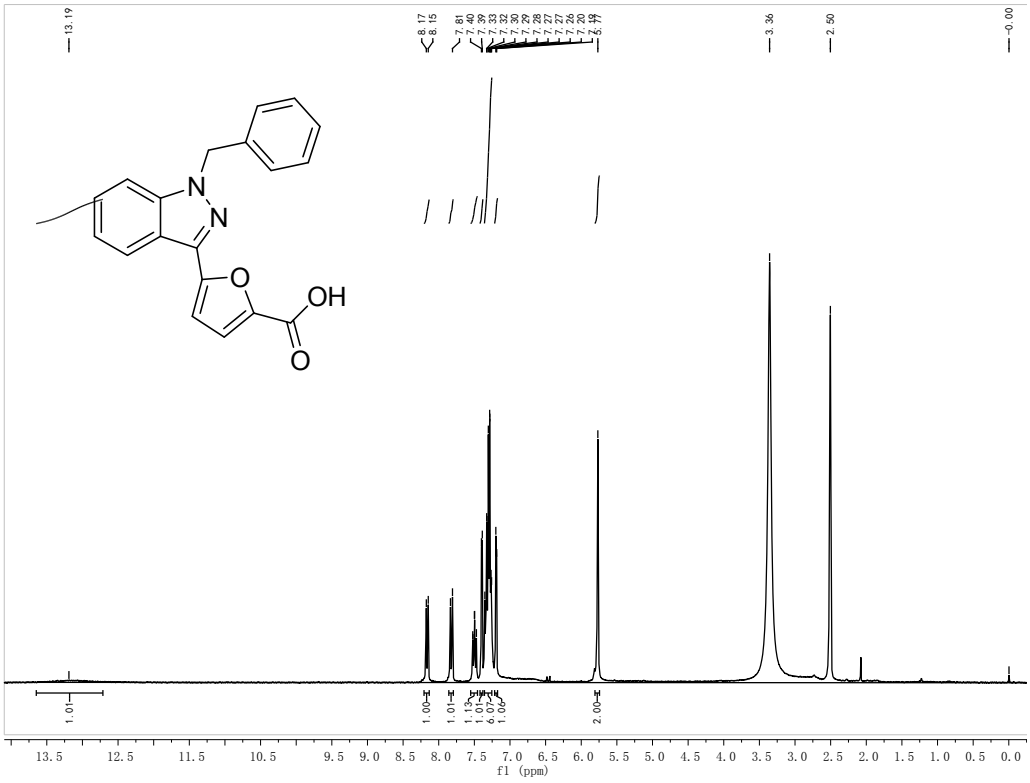
1-Benzyl-3-iodoindazole (2):

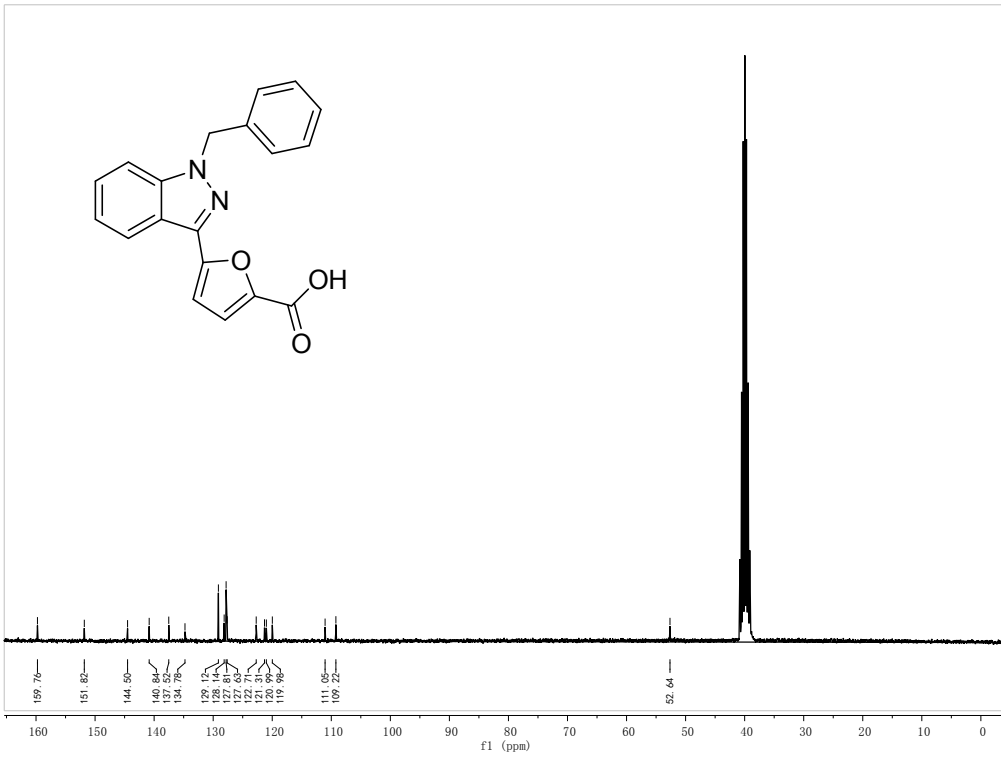


5-(1′-benzyl-1H-indazol-3′-yl) furan-2-carbaldehyde (3):

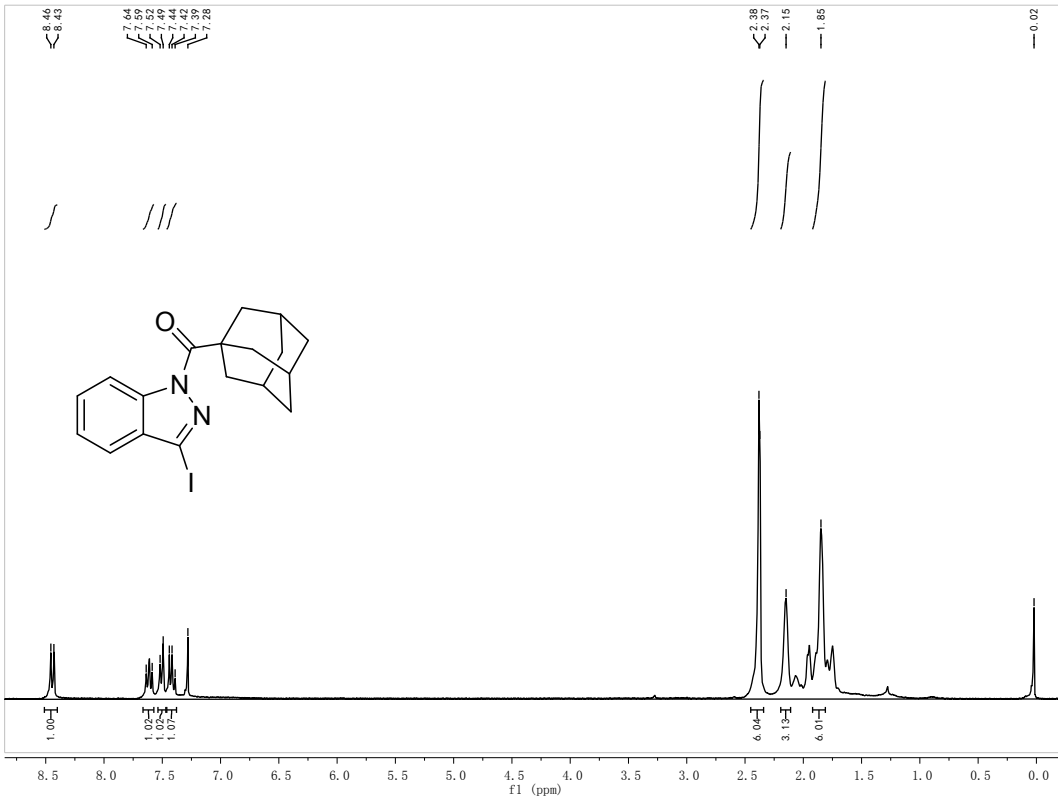


5-(1′-benzyl-1H-indazol-3′-yl)furan-2-carboxylic acid (4):

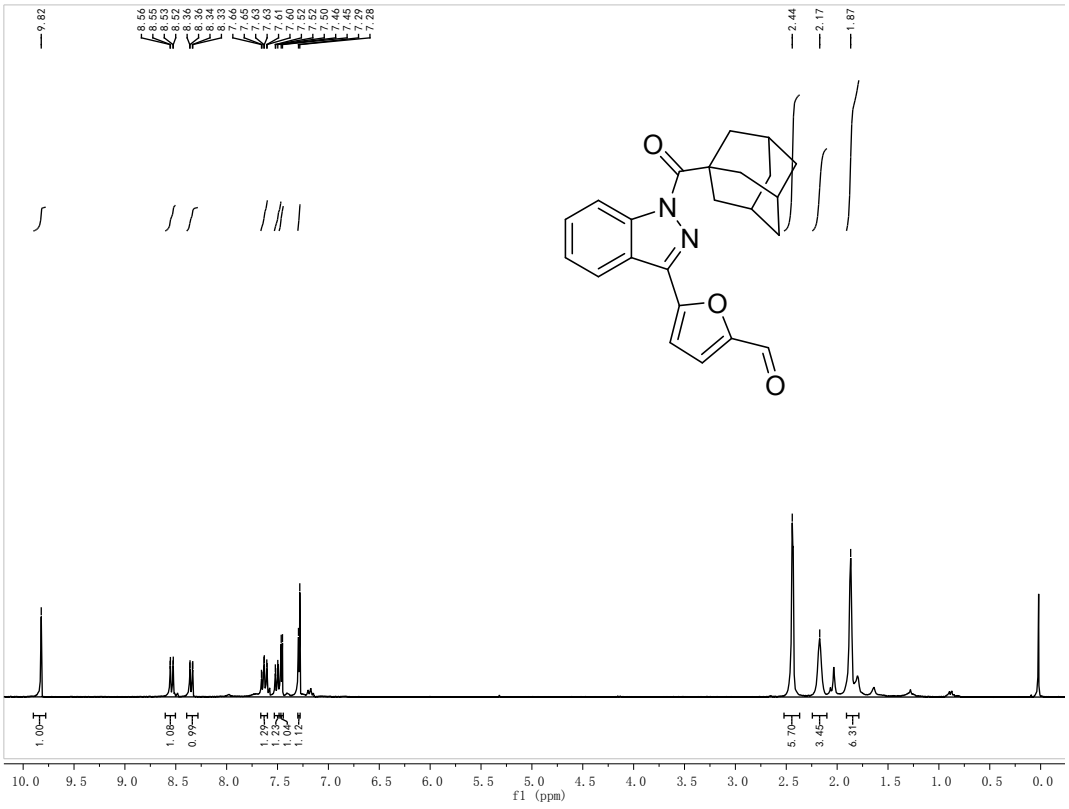




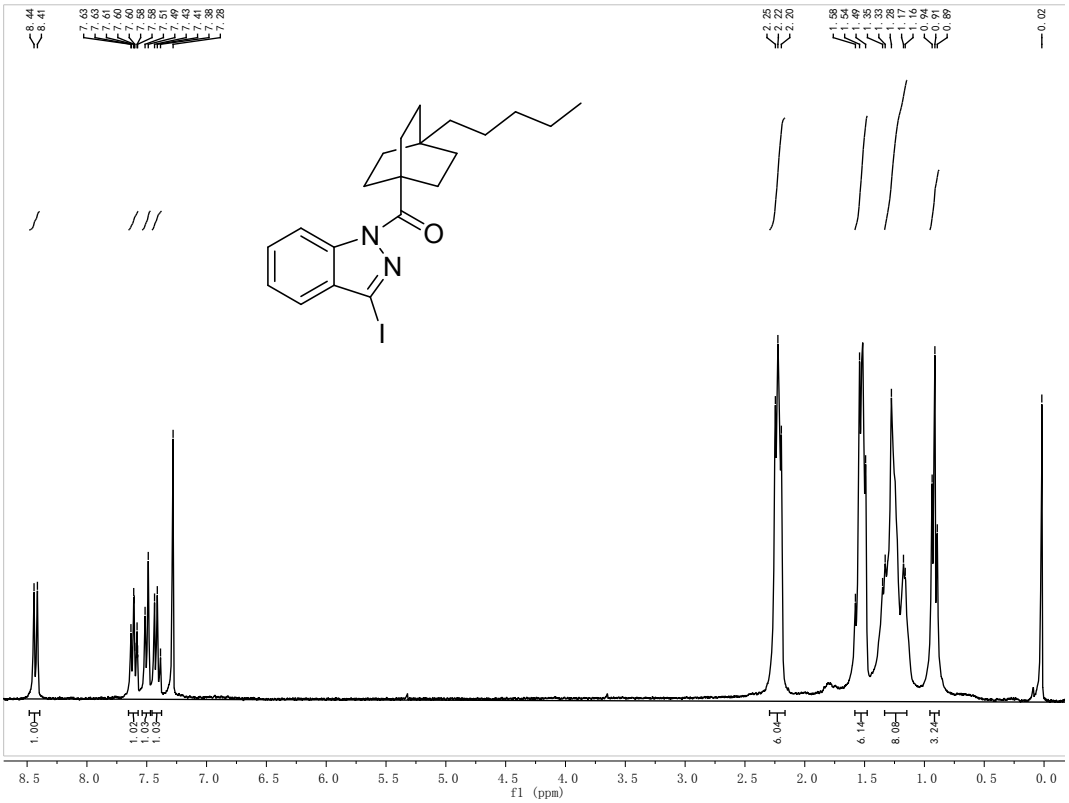
1- Adamantaneformoxyl-3-iodoindazole (5):



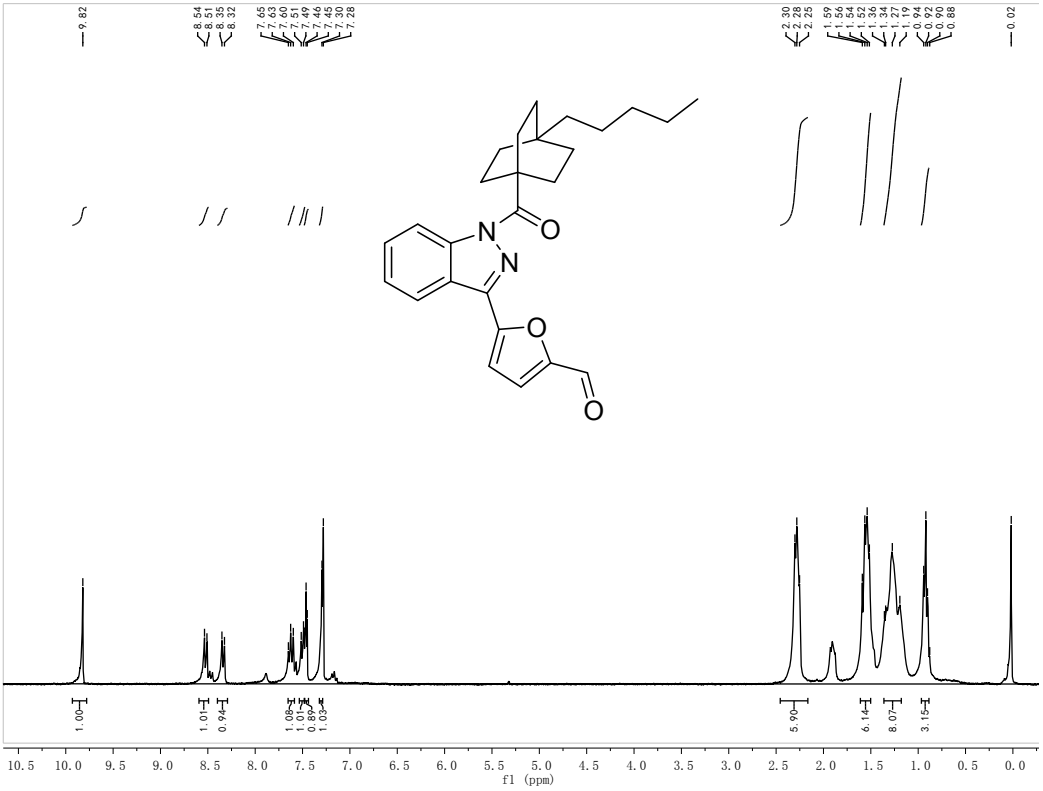
5-(1′-adamantaneformoxyl -1H-indazol-3′-yl)furan-2-carbaldehyde (6):



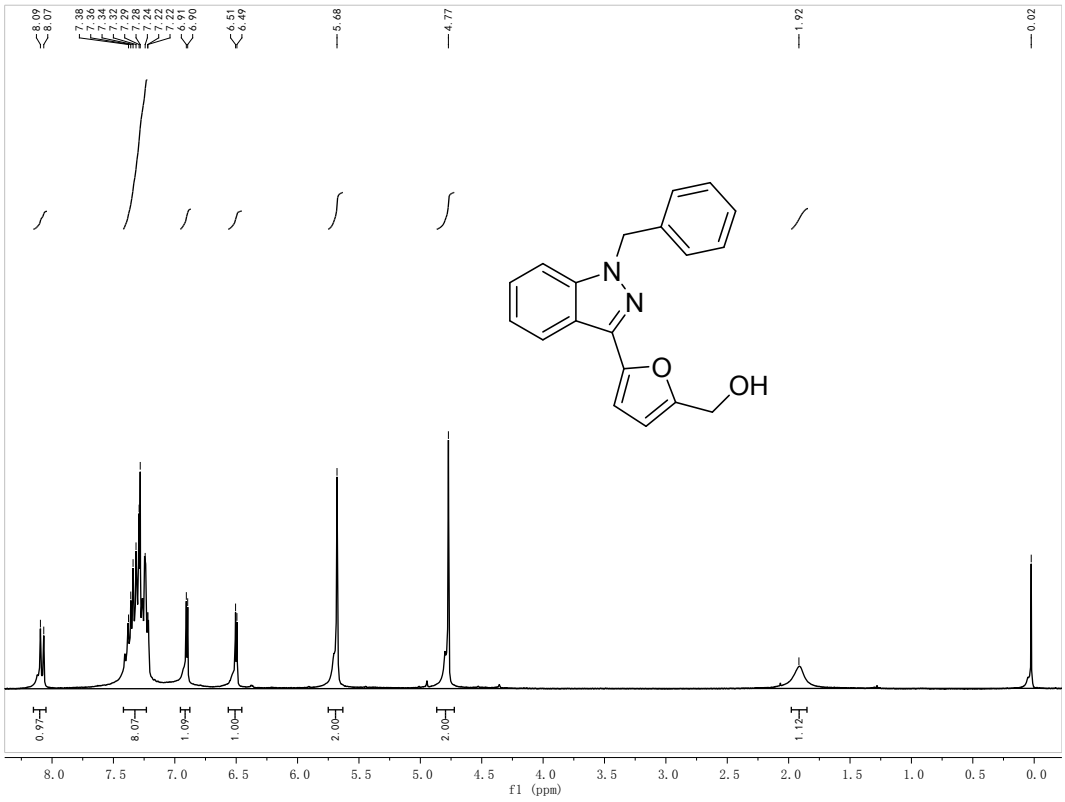
1-(4'-pentylbicyclo[2.2.2]octan-1'-formoxyl)- 3-iodoindazole (7):



5-(4'-pentylbicyclo[2.2.2]octan-1'-formoxyl-1H-indazol-3-yl)furan-2-carbaldehyde (8):



1-benzyl-3-(5'-hydroxymethyl-2'-furyl)indazole (YC-1):



1-adamantaneformoxyl-3-(5'-hydroxymethyl-2'-furyl)indazole (AC):

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Method	Sample 5 min.m		
Sample Name	Bb153	Instrument / Ser#	micrOTOF 10328
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active			Set Dry Heater	180 °C
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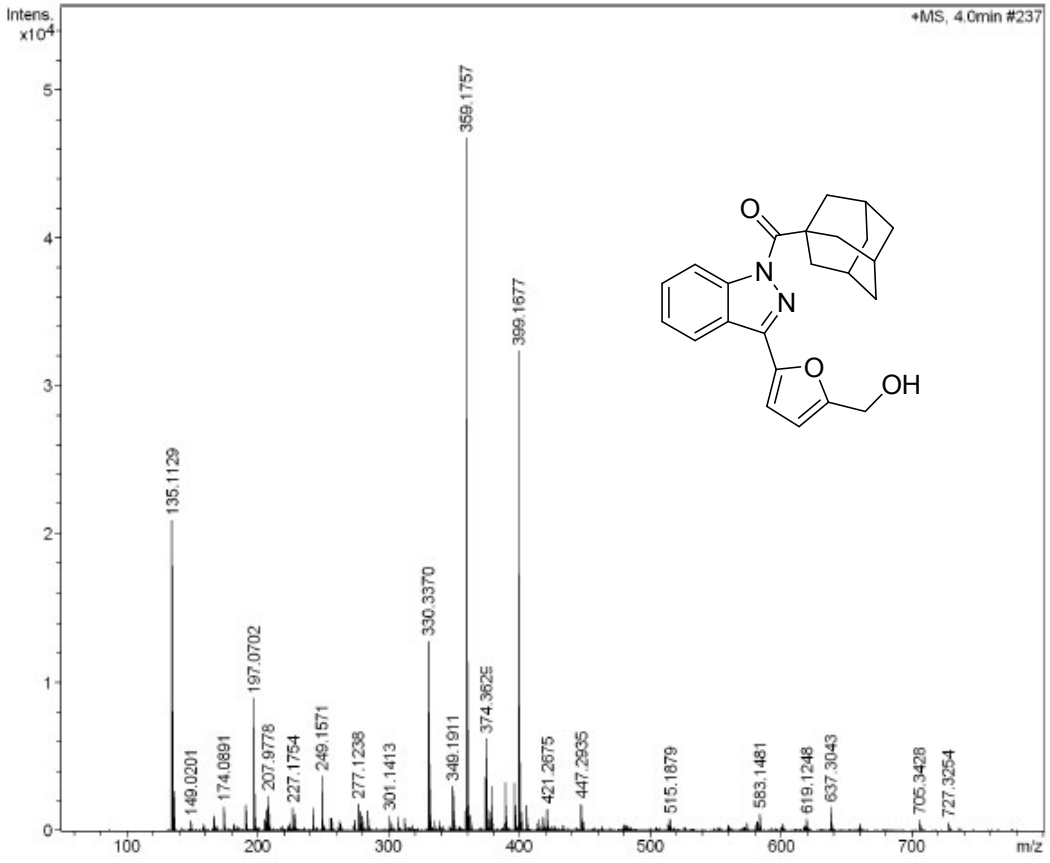
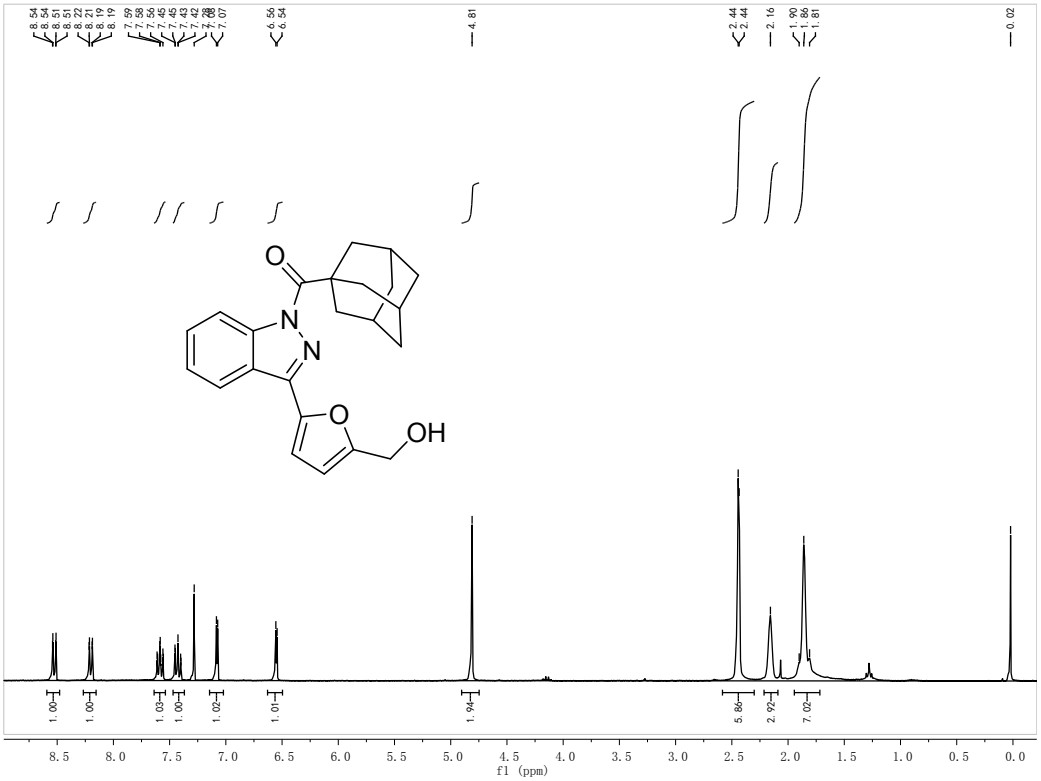
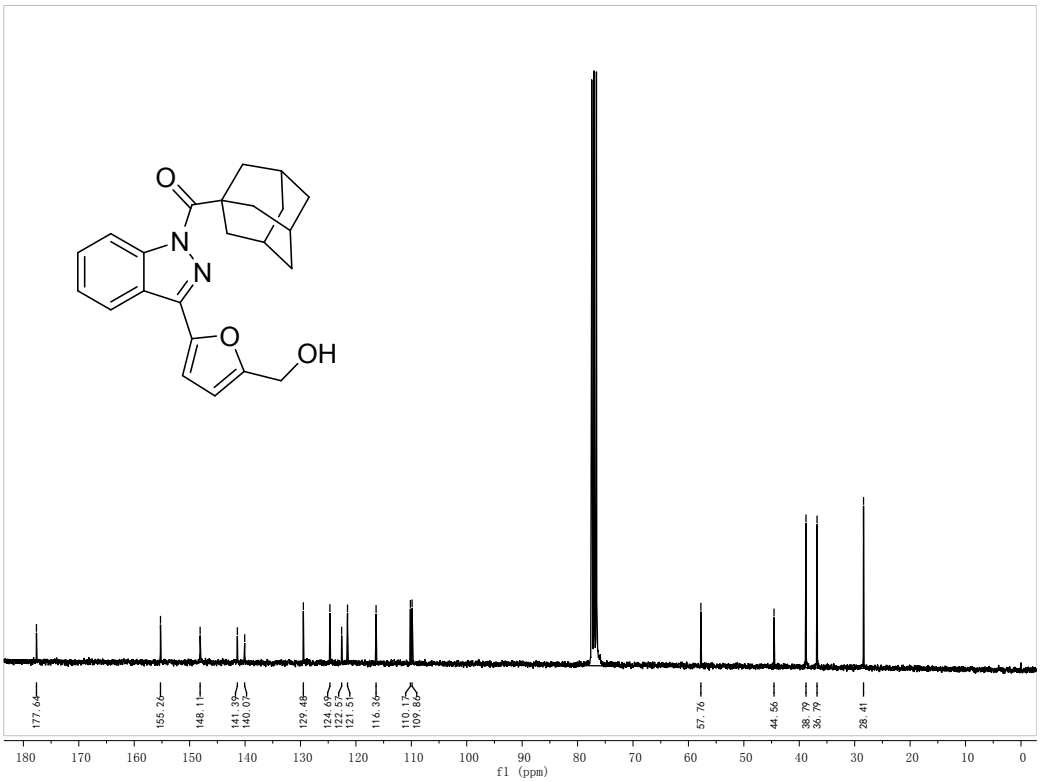
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
399.1677	1	C 23 H 24 N 2 Na O 3	100.00	399.1679	0.5	0.3	3.2	12.5	even	ok





1-(4'-pentylbicyclo[2.2.2]octan-1'-formoxyl)-3-(5'-hydroxymethyl-2'-furyl)indazole (POC):

Analysis Info

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Method	Sample 5 min.m		
Sample Name	Bb154	Instrument / Ser#	micrOTOF 10328
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active			Set Dry Heater	180 °C
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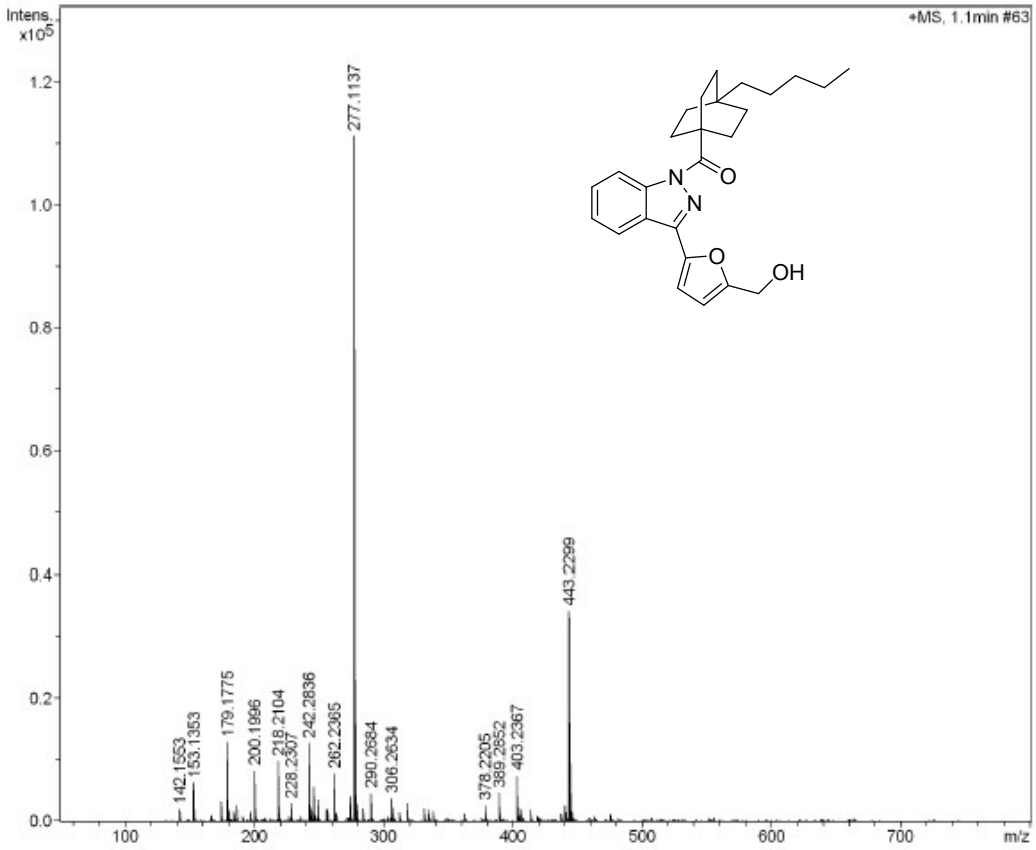
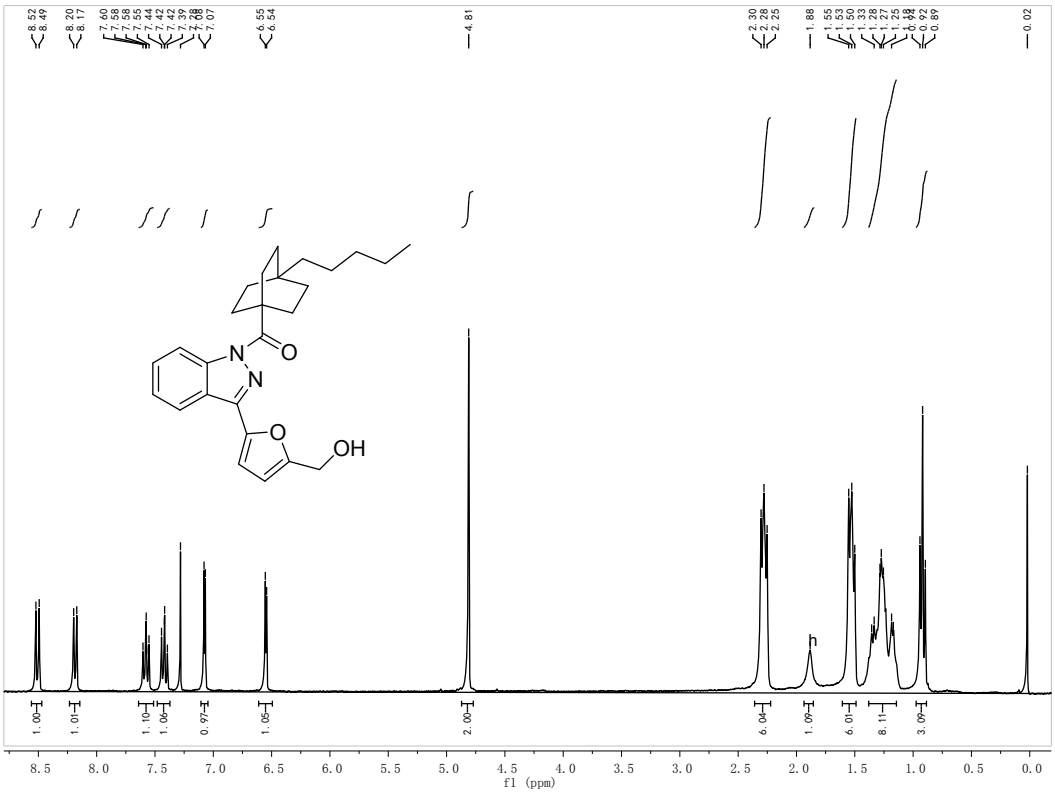
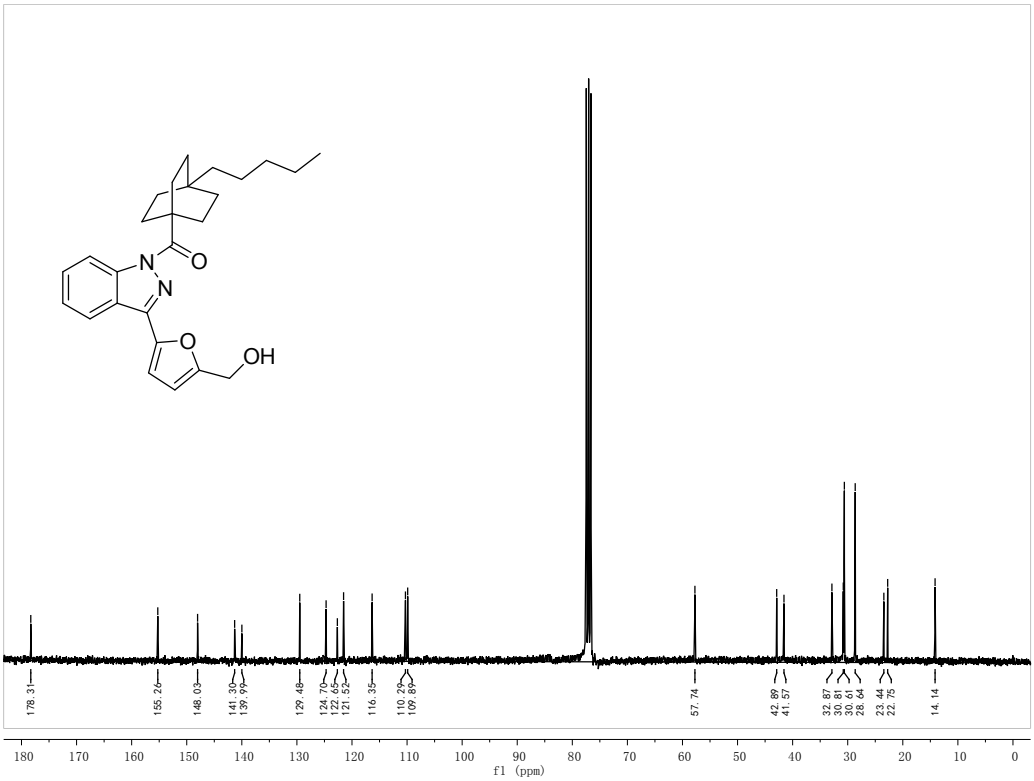
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
443.2299	1	C 26 H 32 N 2 Na O 3	100.00	443.2305	1.4	1.6	2.3	11.5	even	ok





5-(1-benzyl-1H-indazol-3-yl)-N-(prop-2-yn-1-yl)furan-2-carboxamide (MPa):

Analysis Info

Analysis Name	D:\Data\user\B2015\Bb155_38_01_9295.d	Acquisition Date	5/21/2015 12:37:51 PM
Method	Sample 5 min.m		
Sample Name	Bb155	Instrument / Ser#	micrOTOF 10328
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
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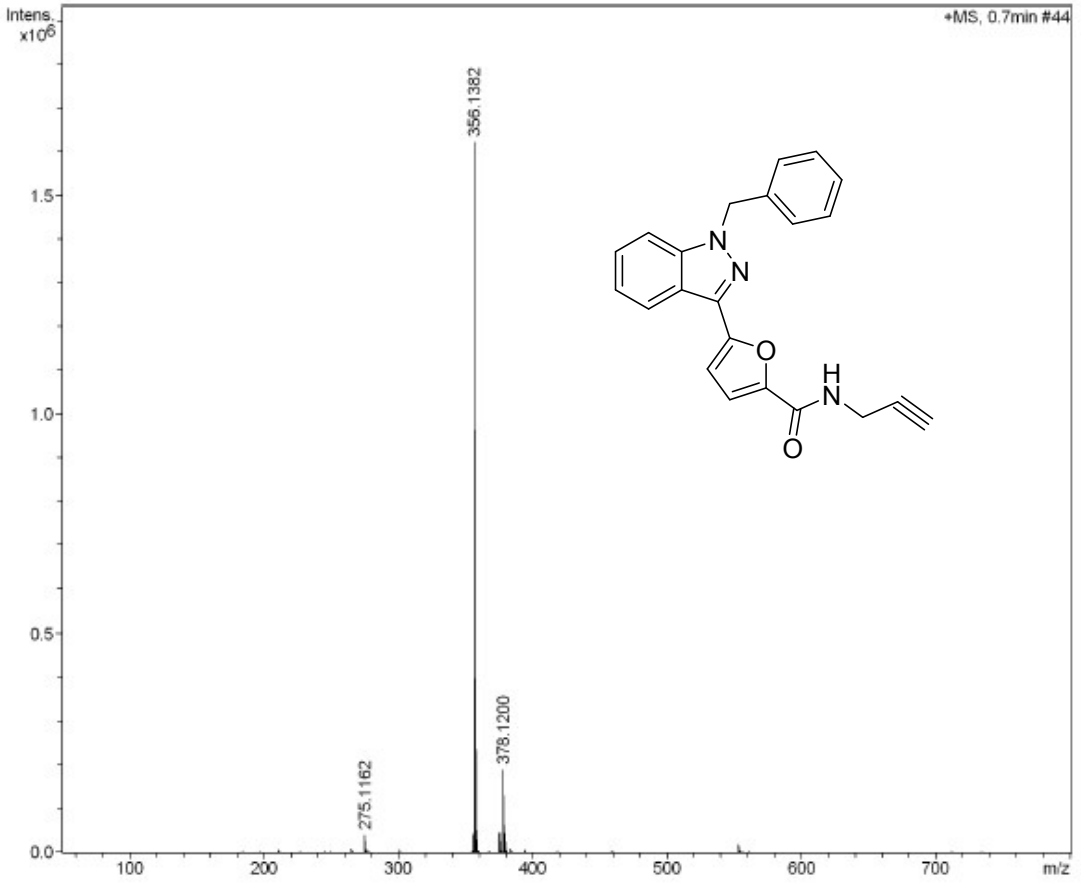
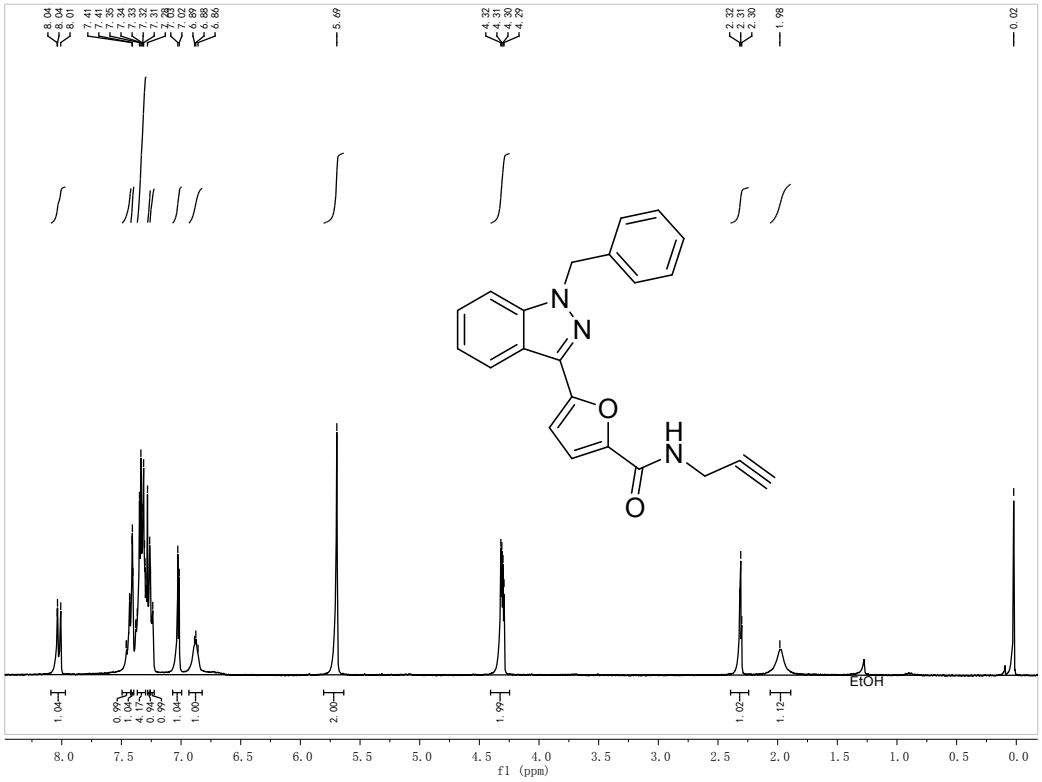
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
356.1382	1	C 22 H 18 N 3 O 2	100.00	356.1394	3.2	3.5	2.0	15.5	even	ok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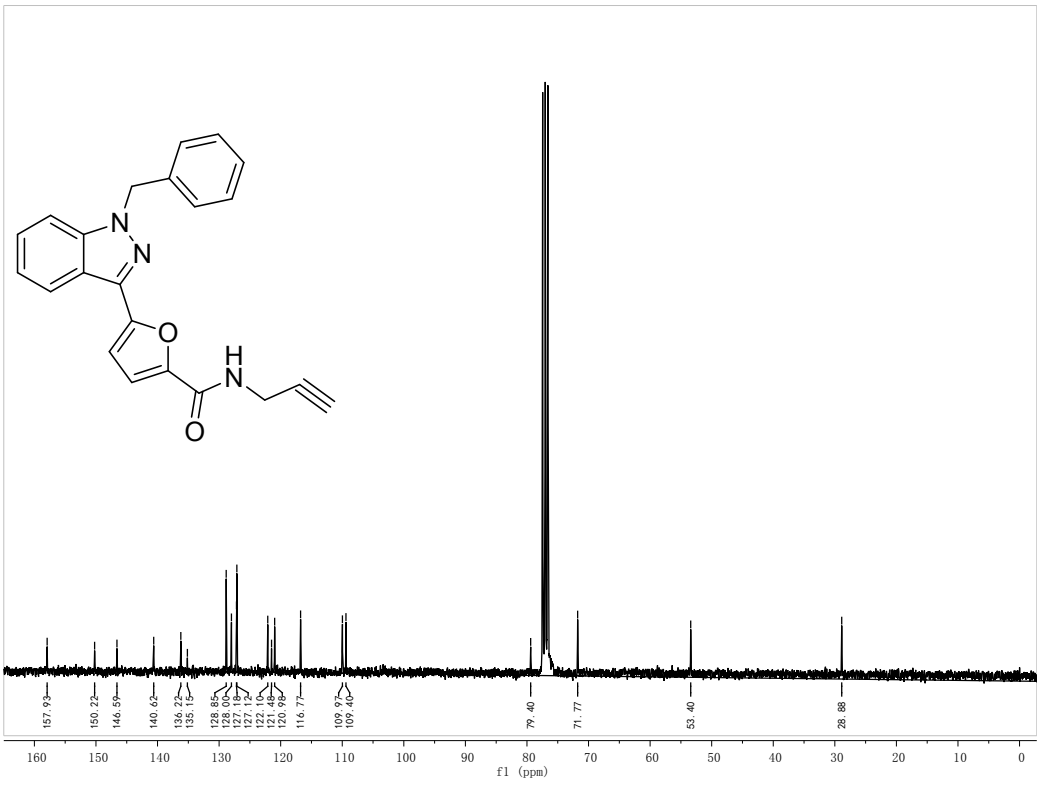
7.41
7.41
7.35
7.34
7.33
7.32
7.31
7.03
7.02
6.89
6.88
6.86
5.69
4.32
4.31
4.30
4.29
2.32
2.31
2.30
1.98
0.02
N
N
O
H
N
O
EtOH
1.04
0.99
1.04
4.17
0.94
0.99
1.04
1.00
2.00
1.99
1.02
1.12
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


N
N
O
H
N
O
157.93
150.22
146.59
140.62
136.22
135.15
128.85
128.05
127.18
127.12
122.10
121.46
120.99
116.77
109.97
109.40
79.40
71.77
53.40
28.88
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)