

Efficient Synthesis and Bioactivity of Novel Triazole Derivatives

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Supporting Information

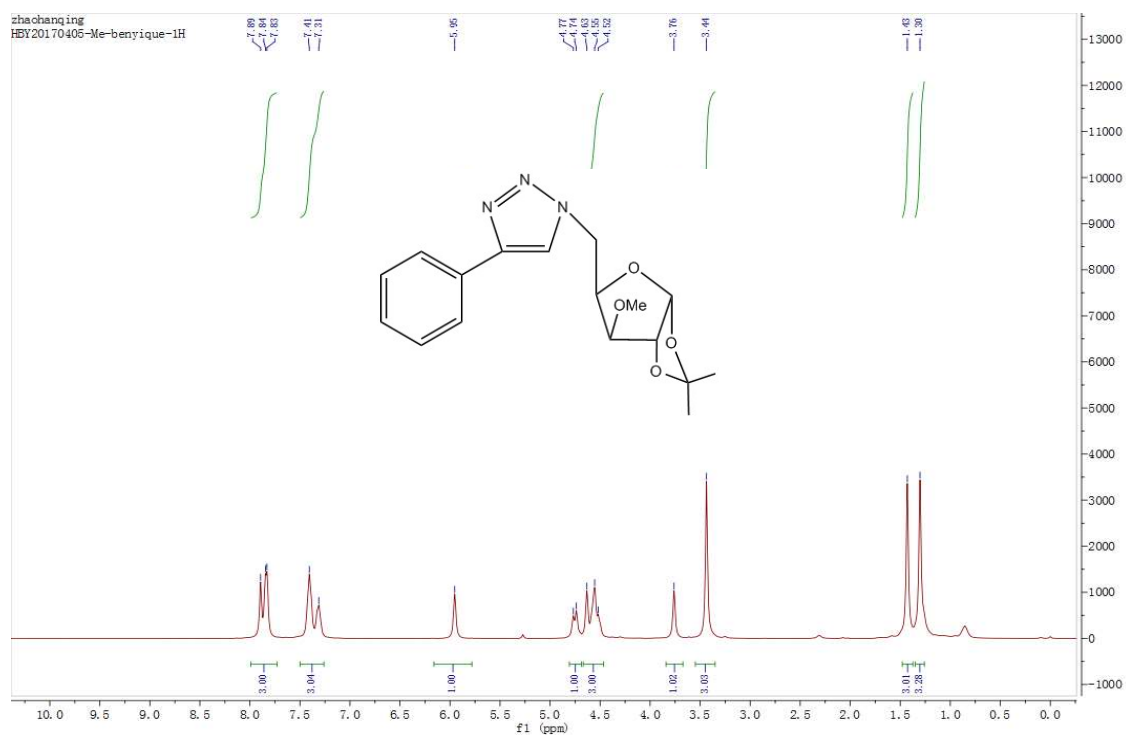
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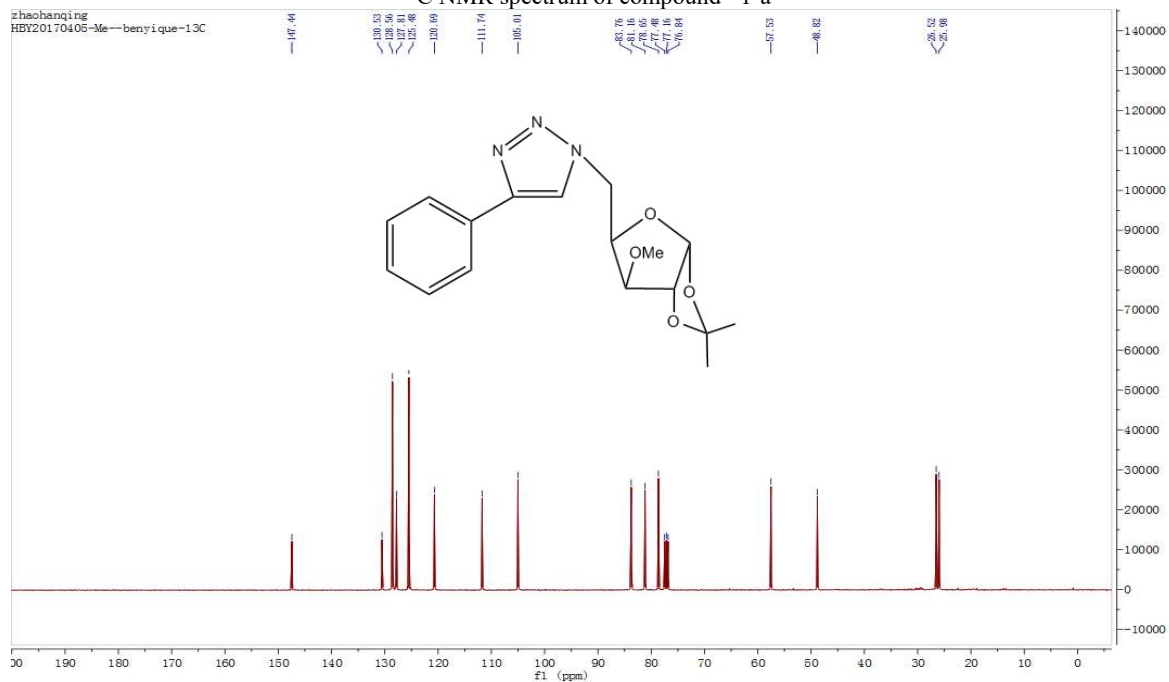
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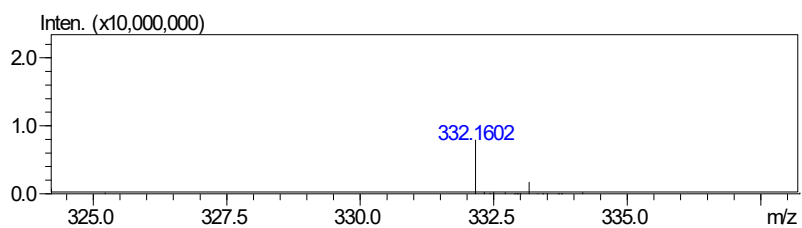
¹H NMR spectrum of compound 1-a



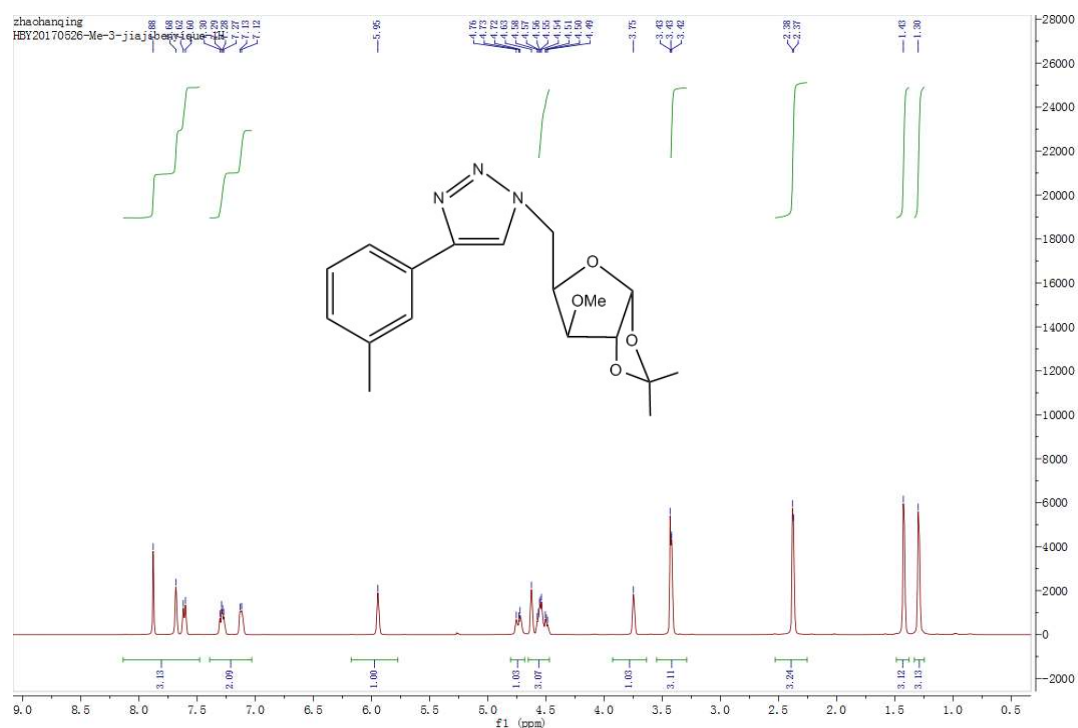
¹³C NMR spectrum of compound 1-a



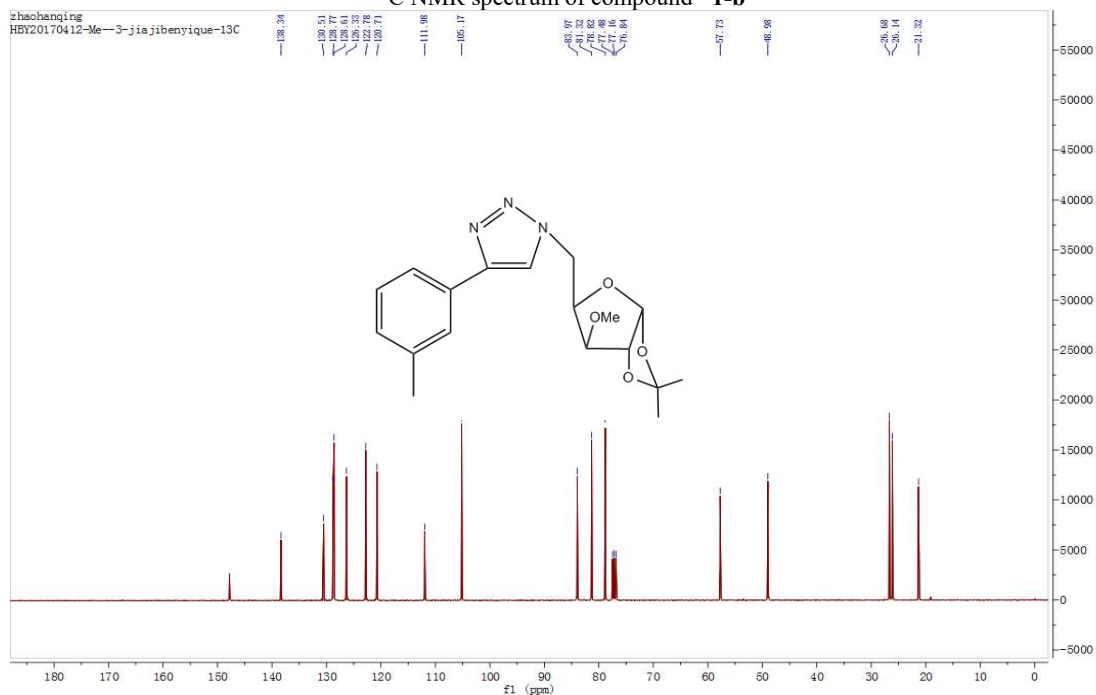
HRMS spectrum of compound 1-a



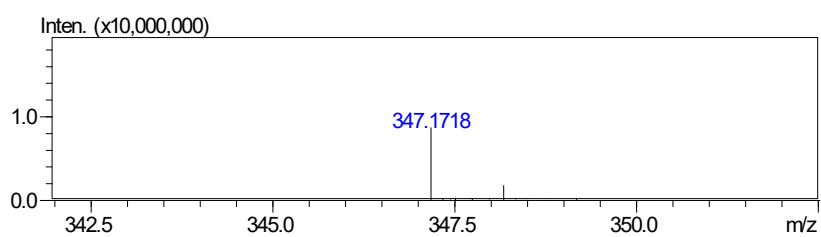
¹H NMR spectrum of compound **1-b**



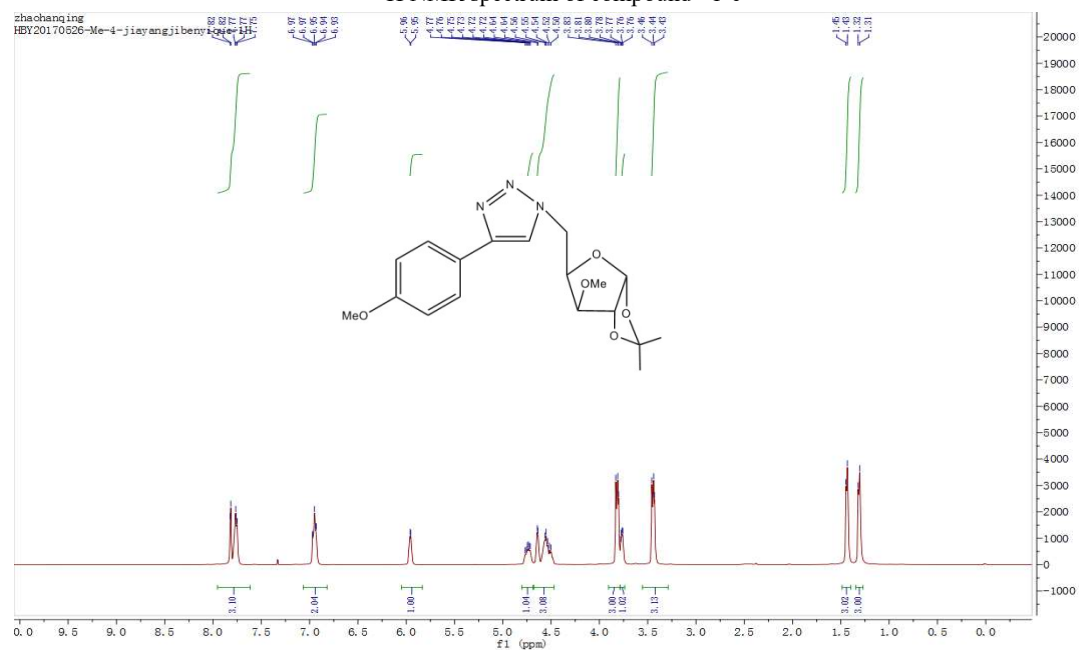
¹³C NMR spectrum of compound **1-b**



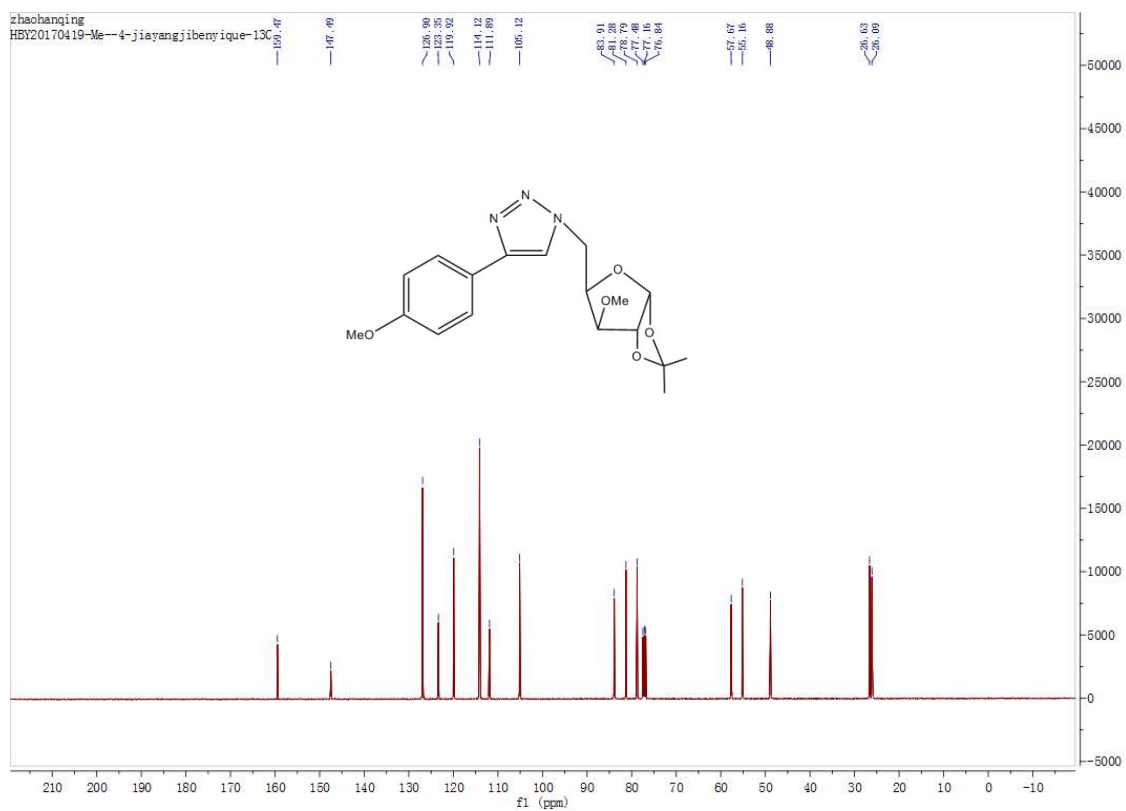
HRMS spectrum of compound **1-b**



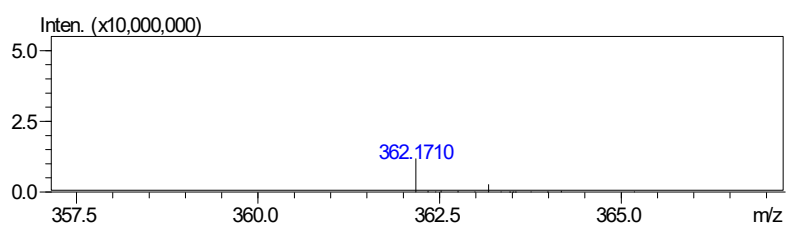
¹H NMR spectrum of compound 1-c



¹³C NMR spectrum of compound 1-c



HRMS spectrum of compound 1-c



Chemical structure of the compound is shown above the spectrum. The spectrum displays peaks corresponding to the structure, with chemical shifts (ppm) and integrations (area) indicated below the baseline.

Peak Data:

Chemical Shift (ppm)	Integration (Area)
~7.7	3.08
~7.1	2.02
~5.9	1.00
4.4 - 4.8	1.00, 3.02
~3.9	1.02
~3.5	3.04
~1.3	3.09, 3.10

¹³C NMR spectrum of compound 1-a

Chemical structure of compound 1-a is shown above the spectrum.

The spectrum displays peaks corresponding to the following chemical shifts (ppm):

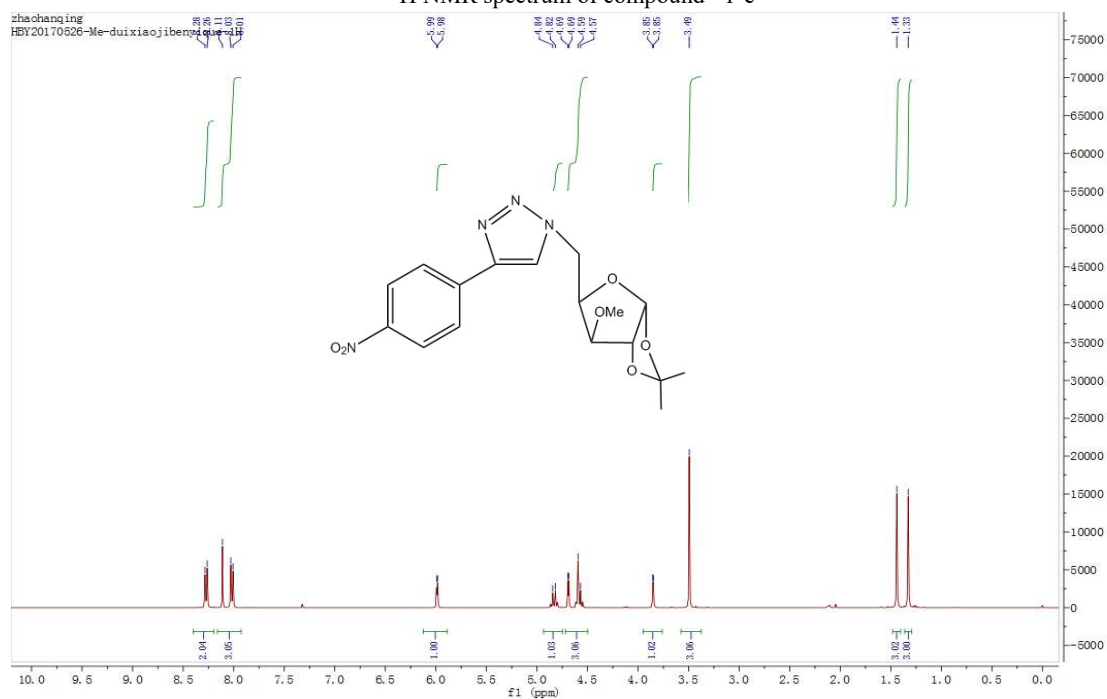
- 163.77
- 161.31
- 148.82
- 127.46
- 127.37
- 127.09
- 126.94
- 120.57
- 119.57
- 115.55
- 112.00
- 105.19
- 84.83
- 81.33
- 78.62
- 77.36
- 77.10
- 76.84
- 57.73
- 49.12
- 28.67
- 28.12

The x-axis represents the chemical shift in ppm, ranging from -10 to 210. The y-axis represents intensity.

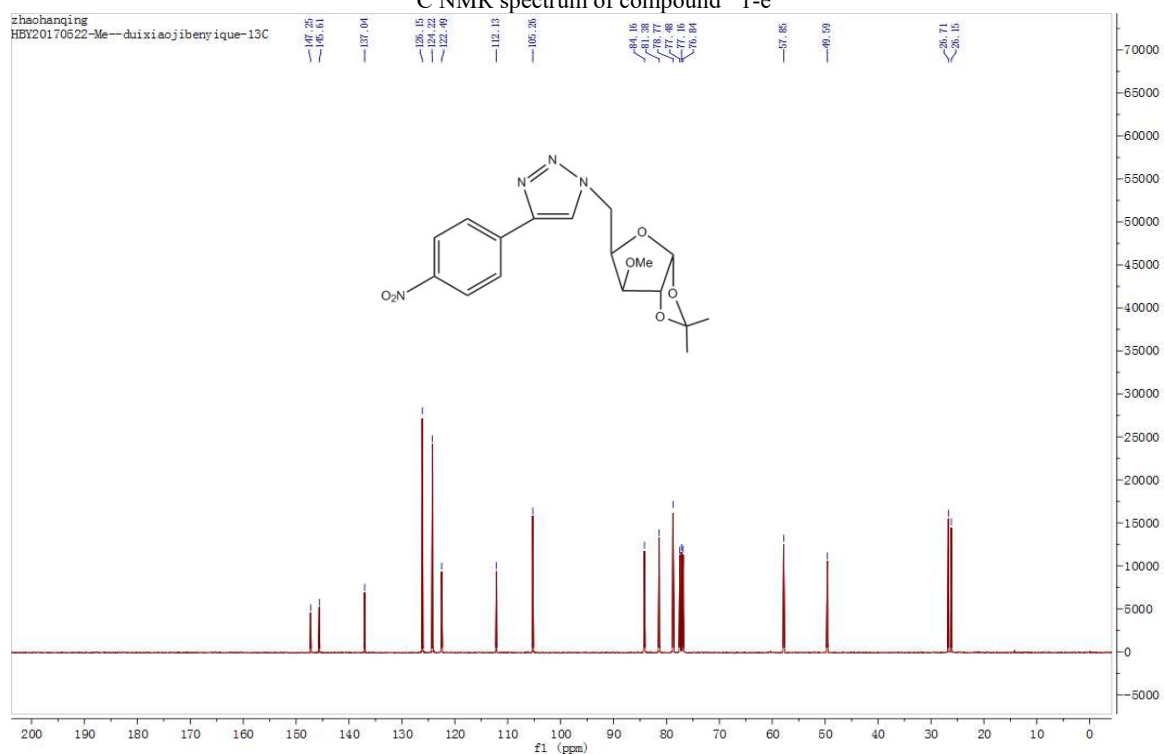
Mass spectrum of compound 10. The x-axis represents the mass-to-charge ratio (m/z) from 345.0 to 355.0. The y-axis represents intensity (Inten. (x10,000,000)) from 0.0 to 2.0. The base peak is at m/z 350.1515.

m/z	Intensity (x10,000,000)
350.1515	1.0
351.1515	0.2

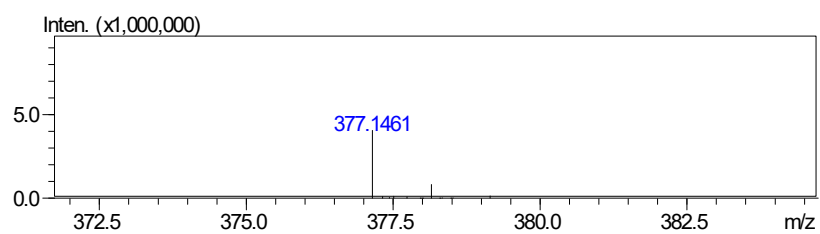
¹H NMR spectrum of compound 1-e



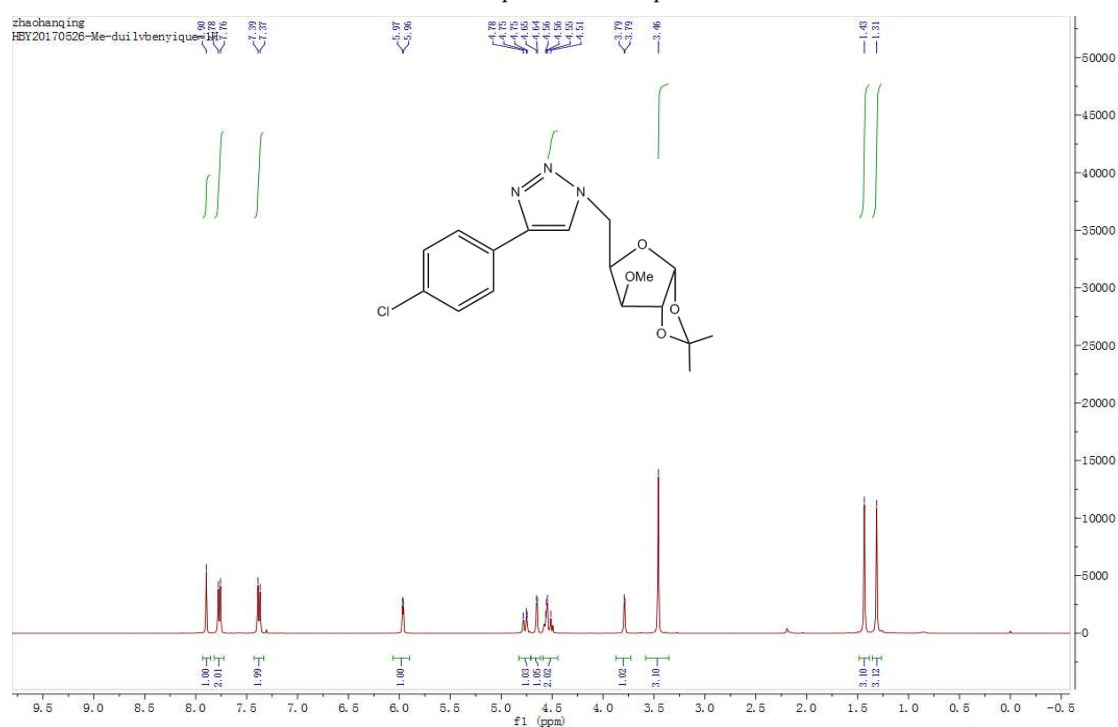
¹³C NMR spectrum of compound 1-e



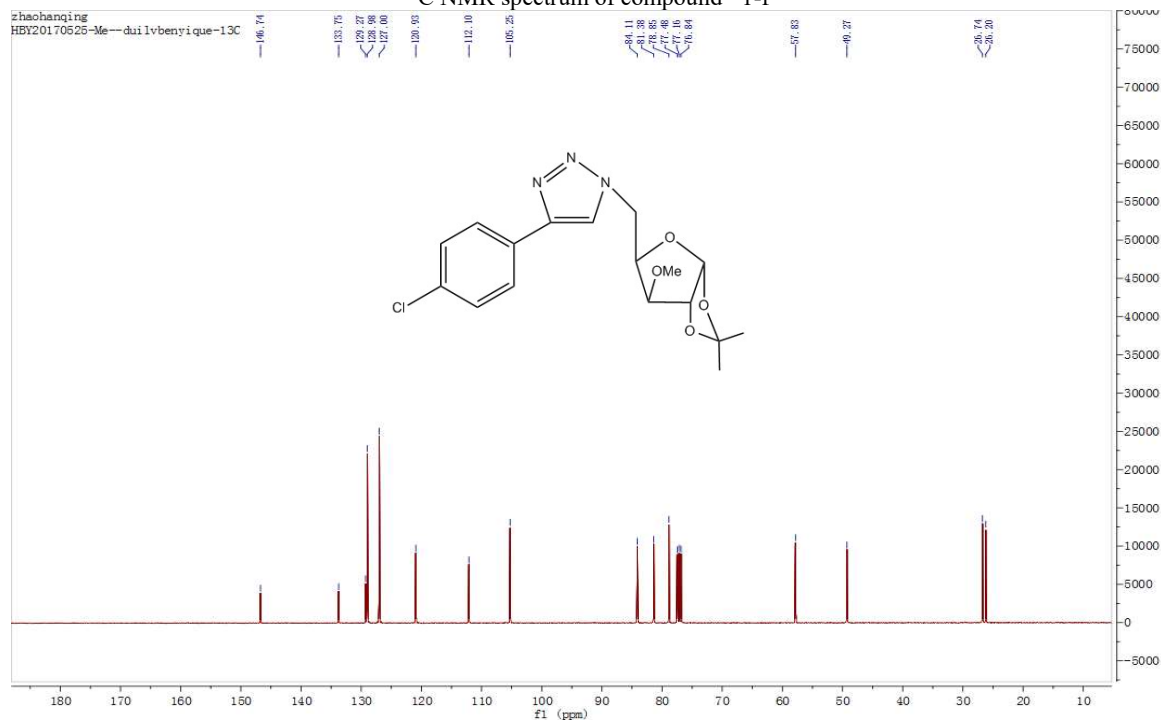
HRMS spectrum of compound 1-e



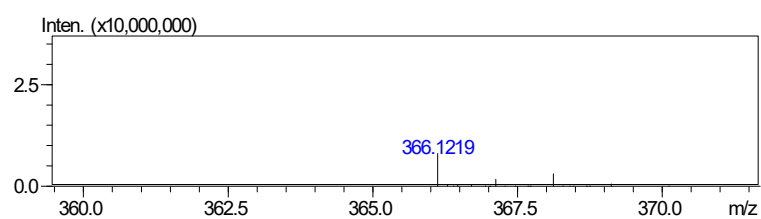
¹H NMR spectrum of compound 1-f



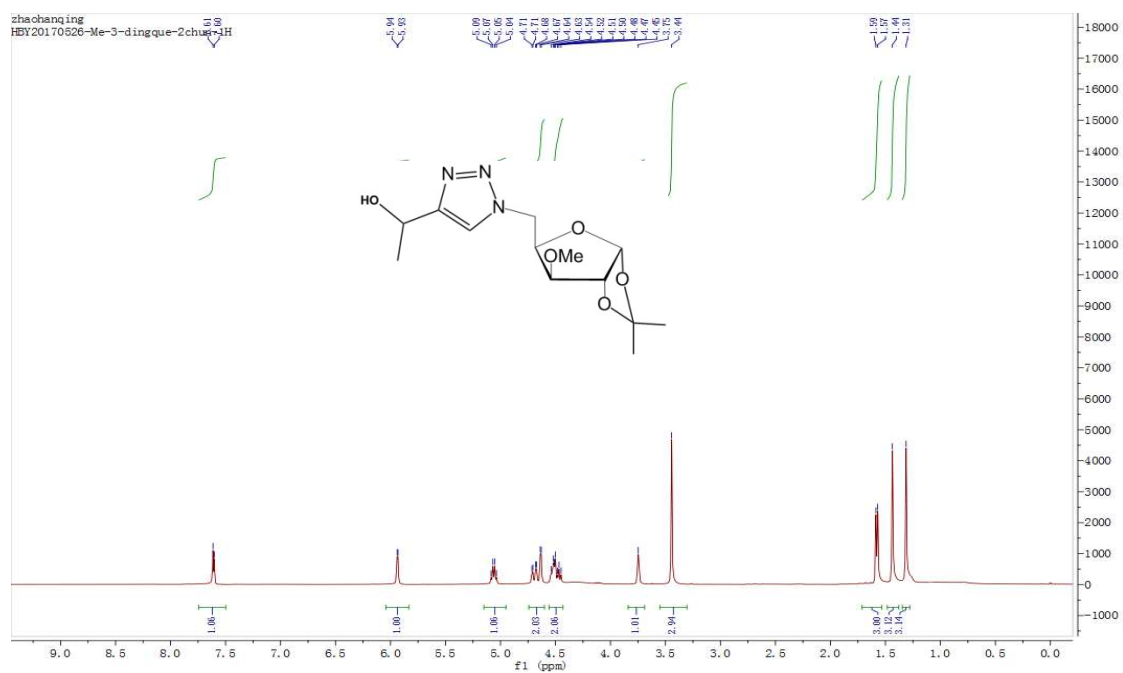
¹³C NMR spectrum of compound 1-f



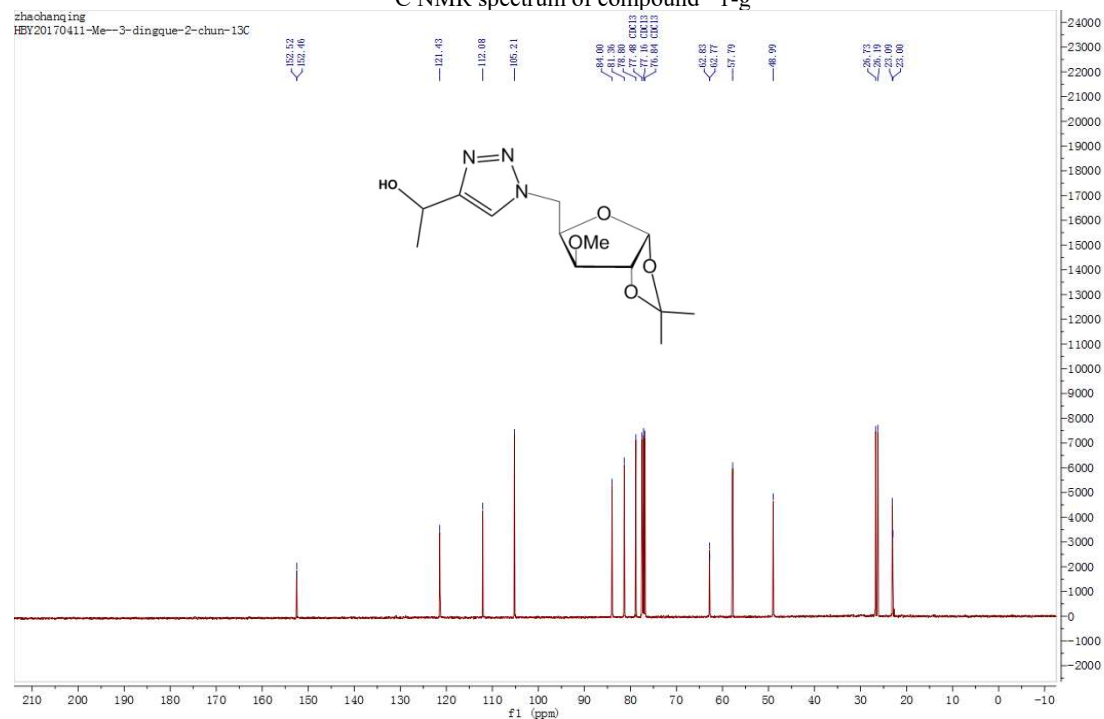
HRMS spectrum of compound 1-f



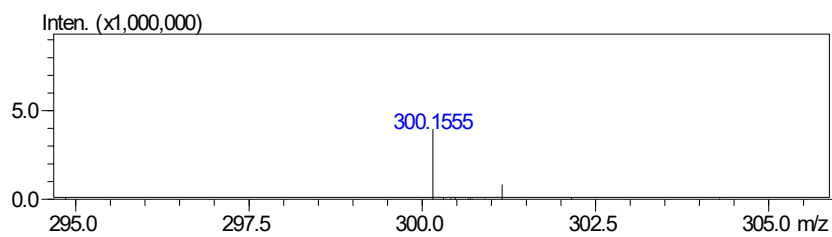
¹H NMR spectrum of compound 1-g



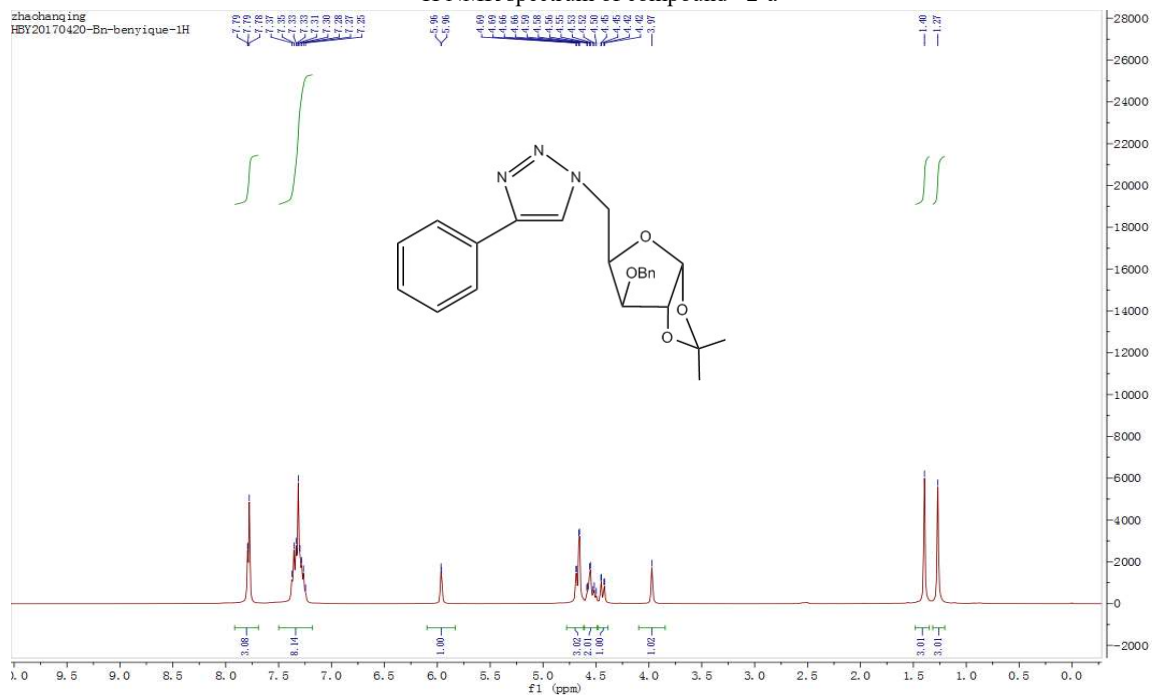
¹³C NMR spectrum of compound 1-g



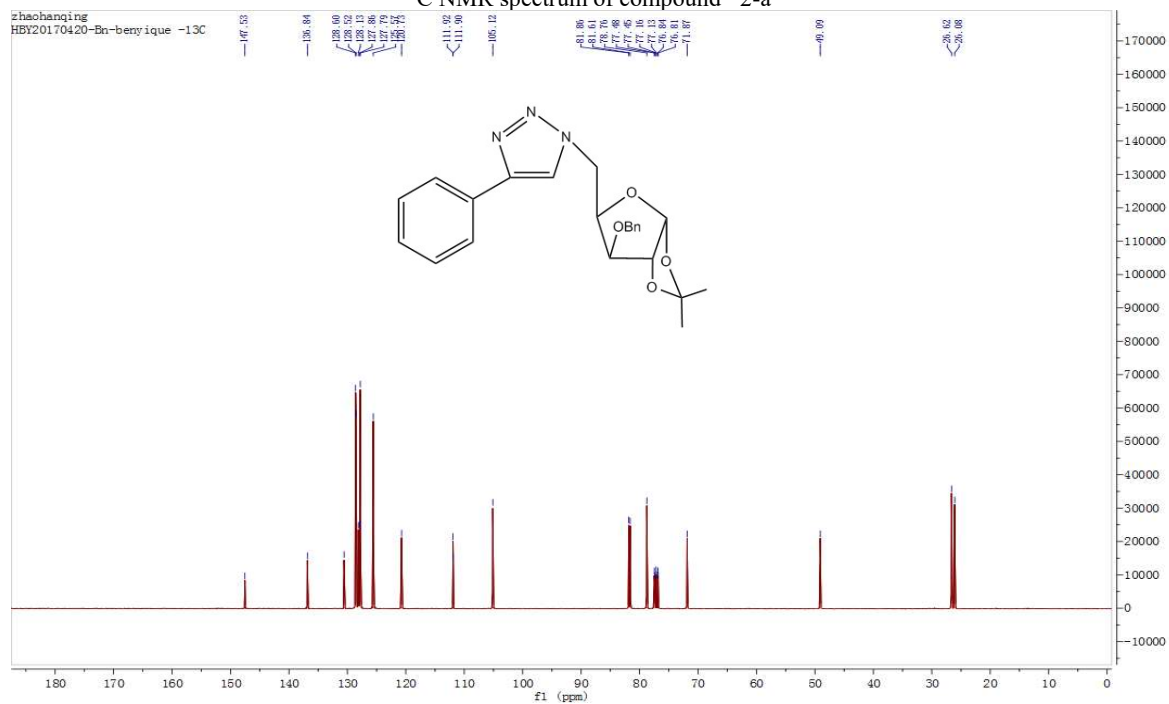
HRMS spectrum of compound 1-g



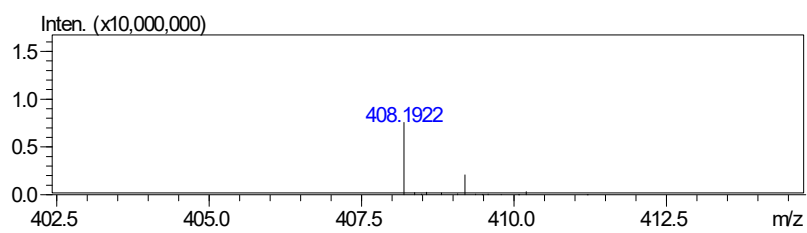
¹H NMR spectrum of compound 2-a



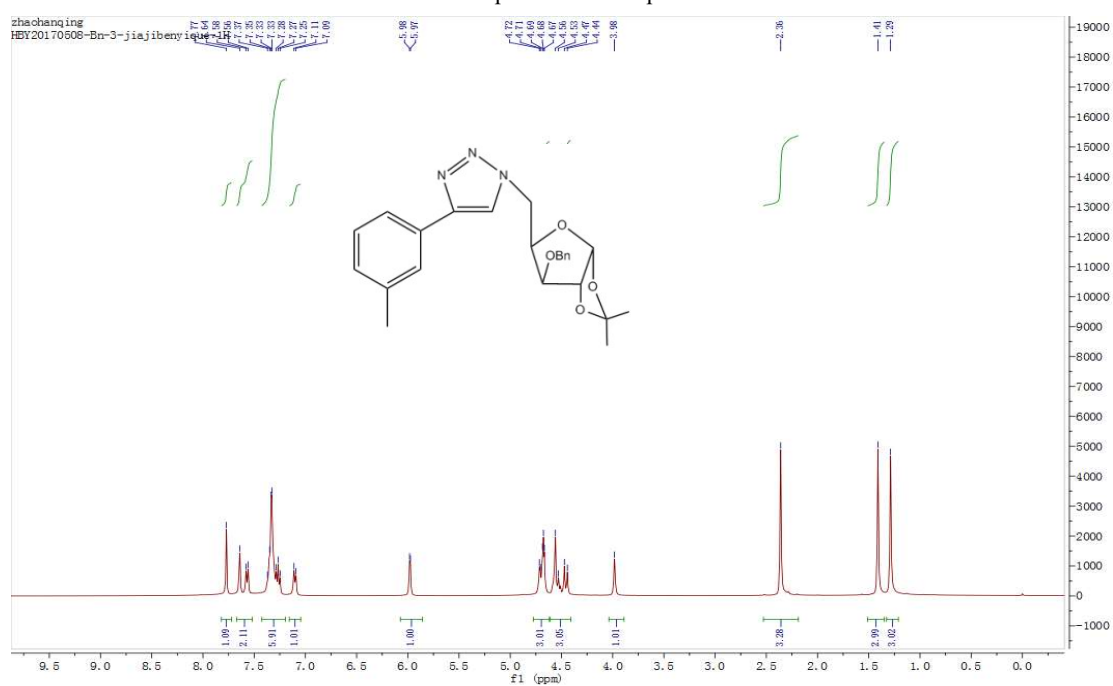
¹³C NMR spectrum of compound 2-a



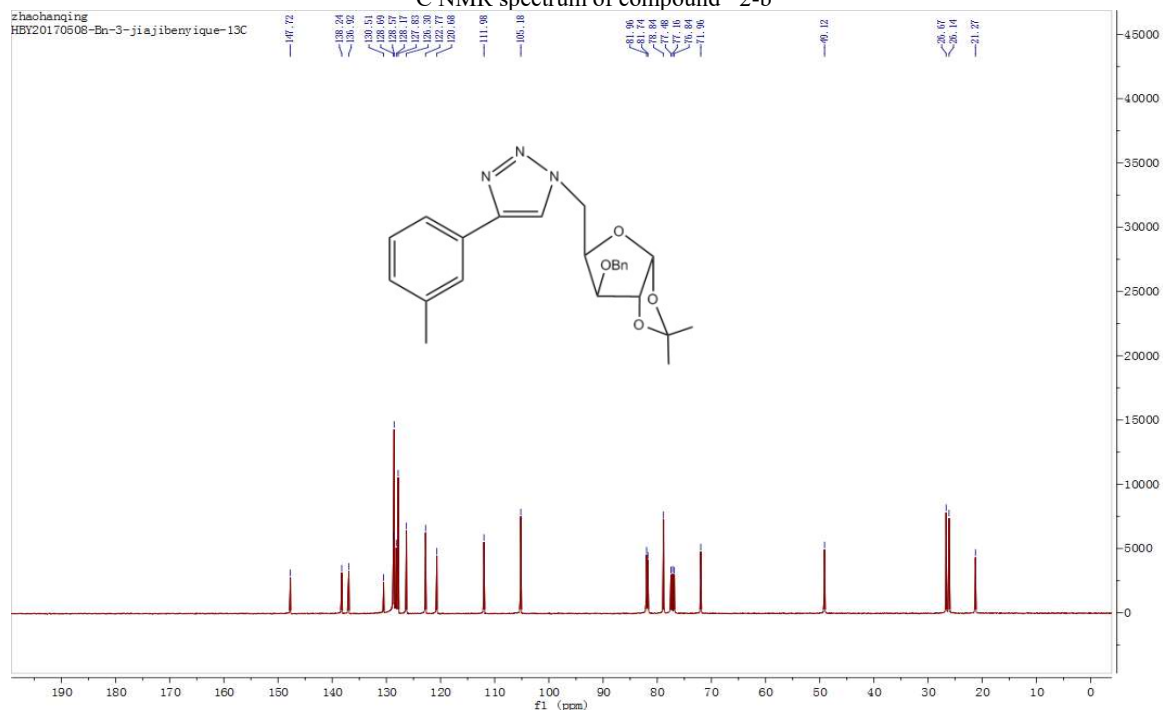
HRMS spectrum of compound 2-a



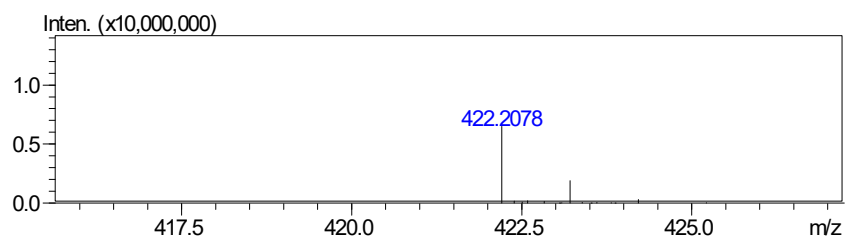
¹H NMR spectrum of compound 2-b

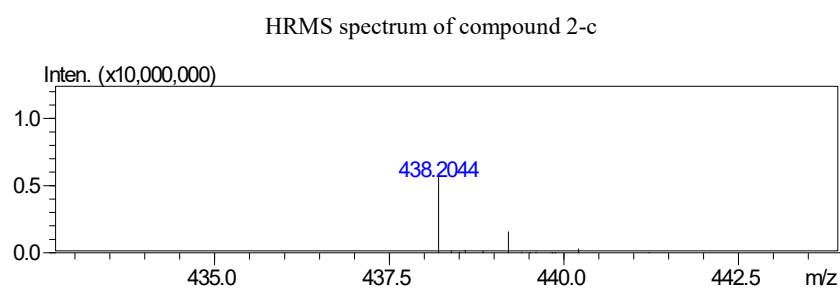
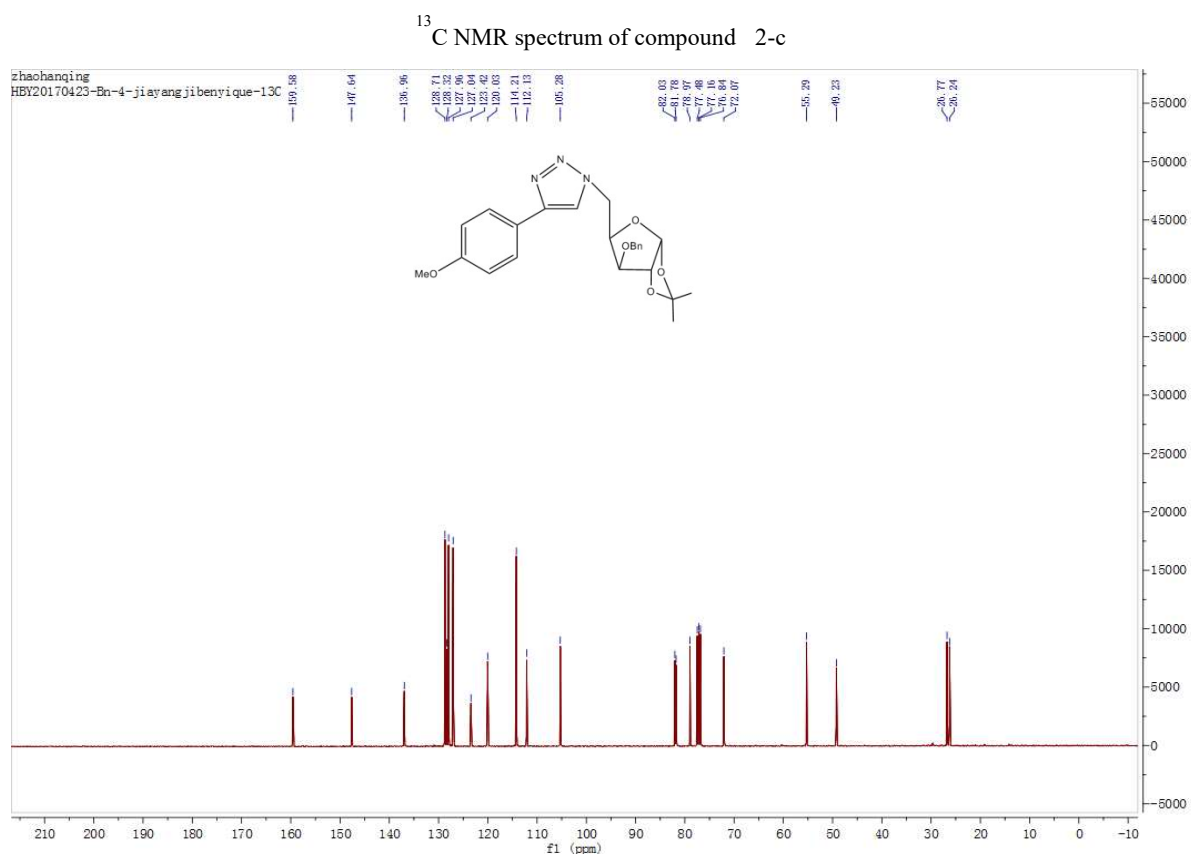
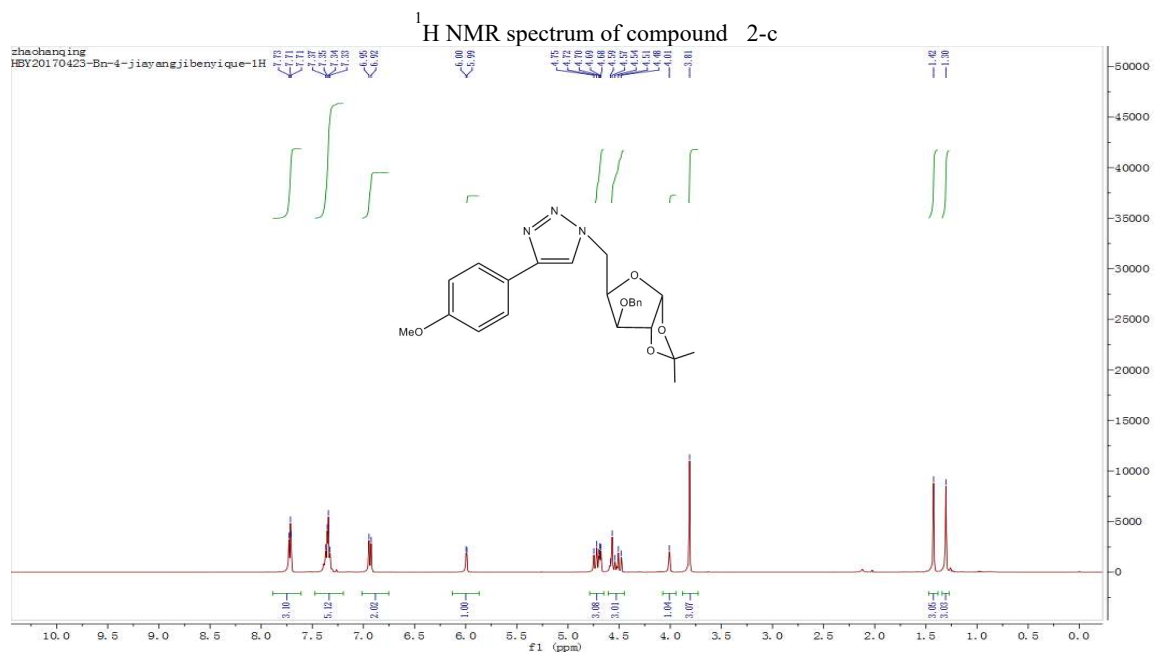


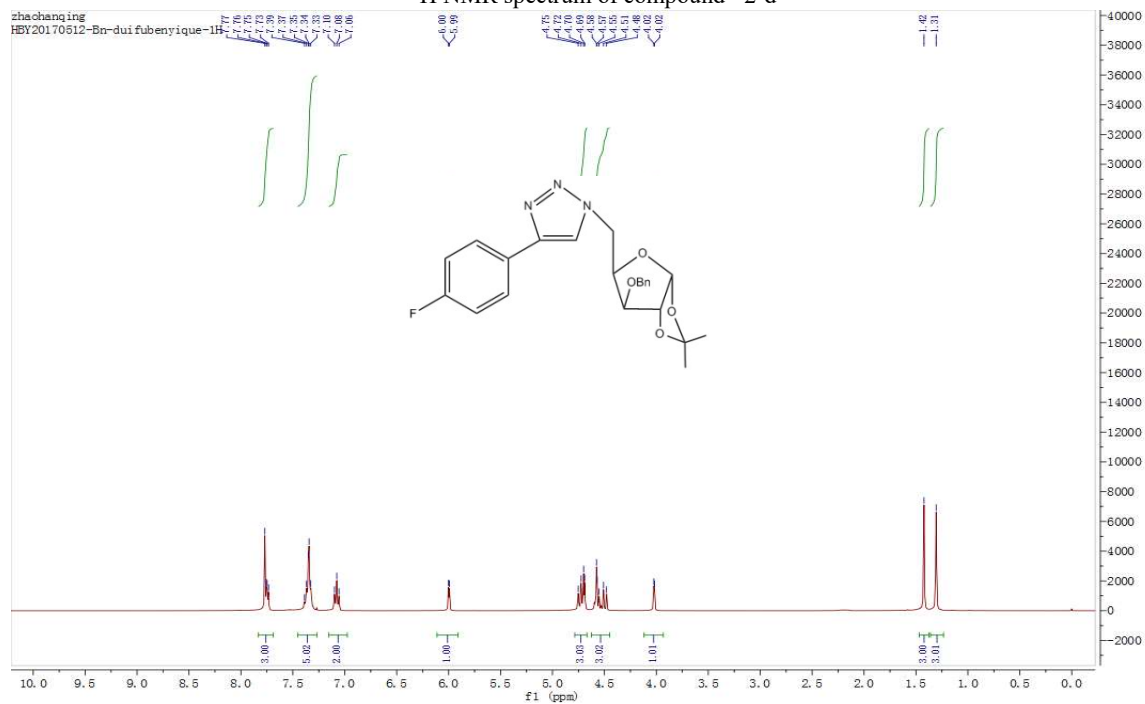
¹³C NMR spectrum of compound 2-b



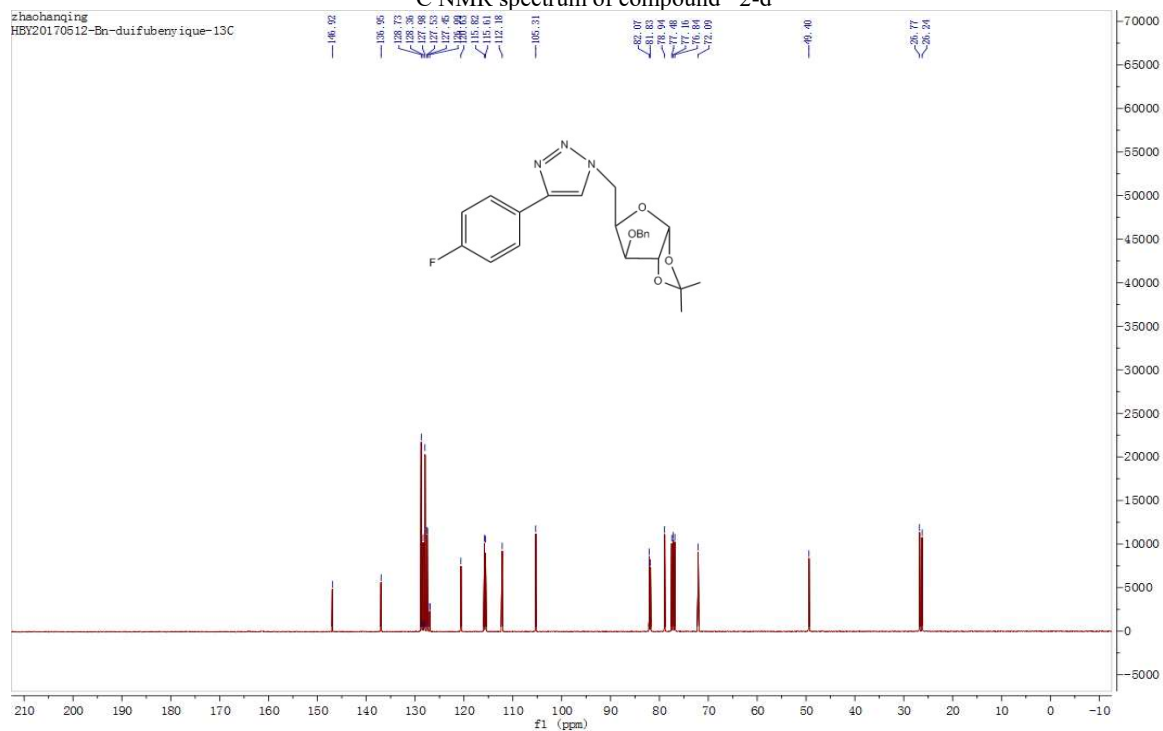
HRMS spectrum of compound 2-b



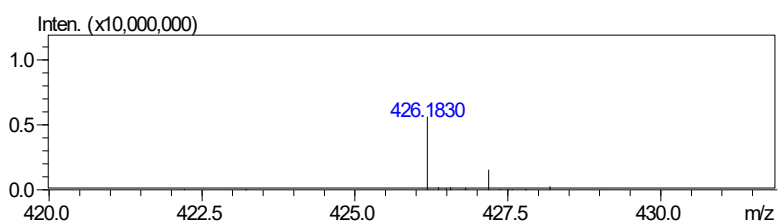


¹H NMR spectrum of compound 2-d

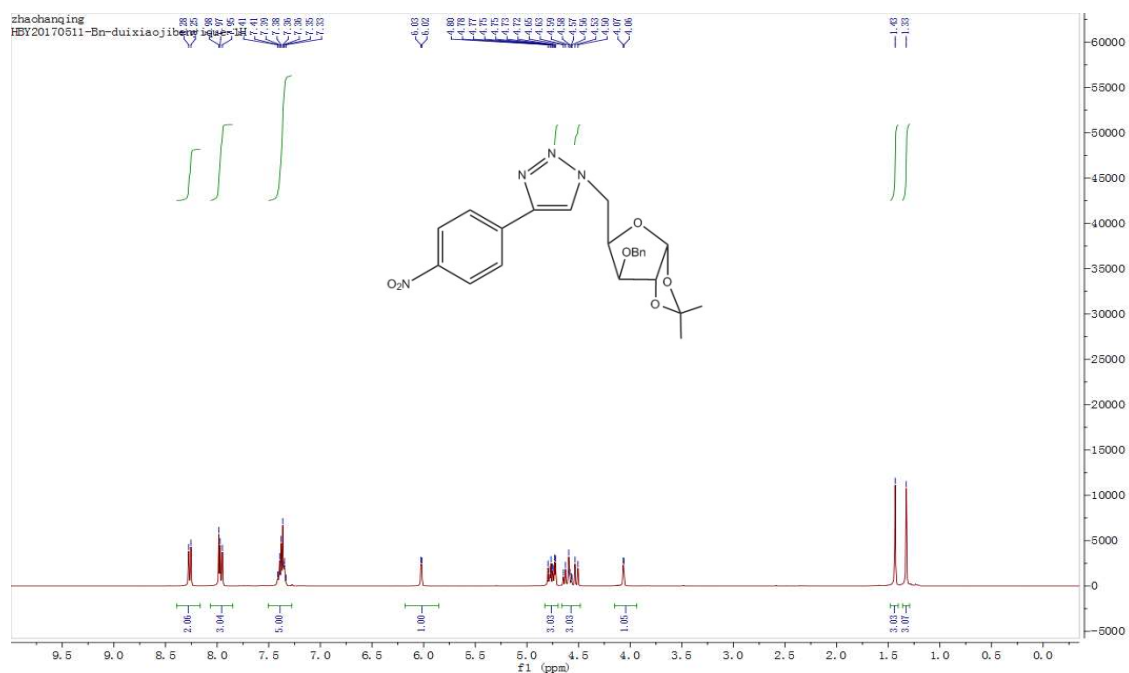
¹³C NMR spectrum of compound 2-d



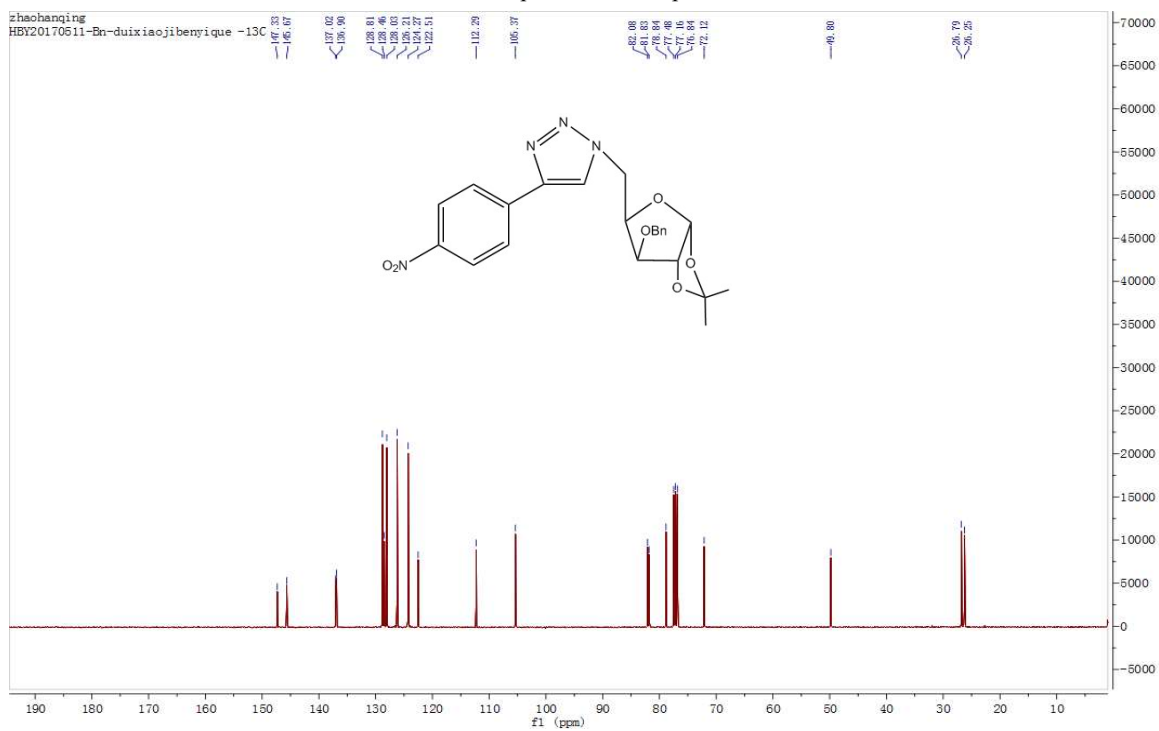
HRMS spectrum of compound 2-d



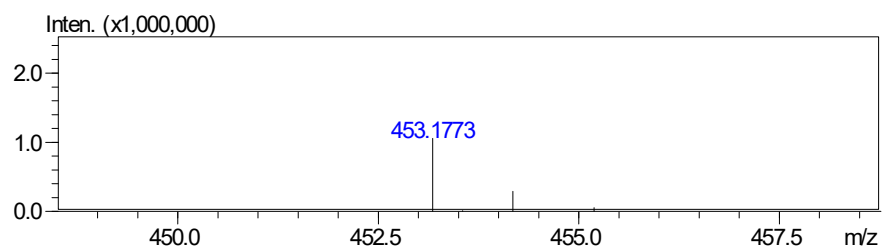
¹H NMR spectrum of compound 2-e



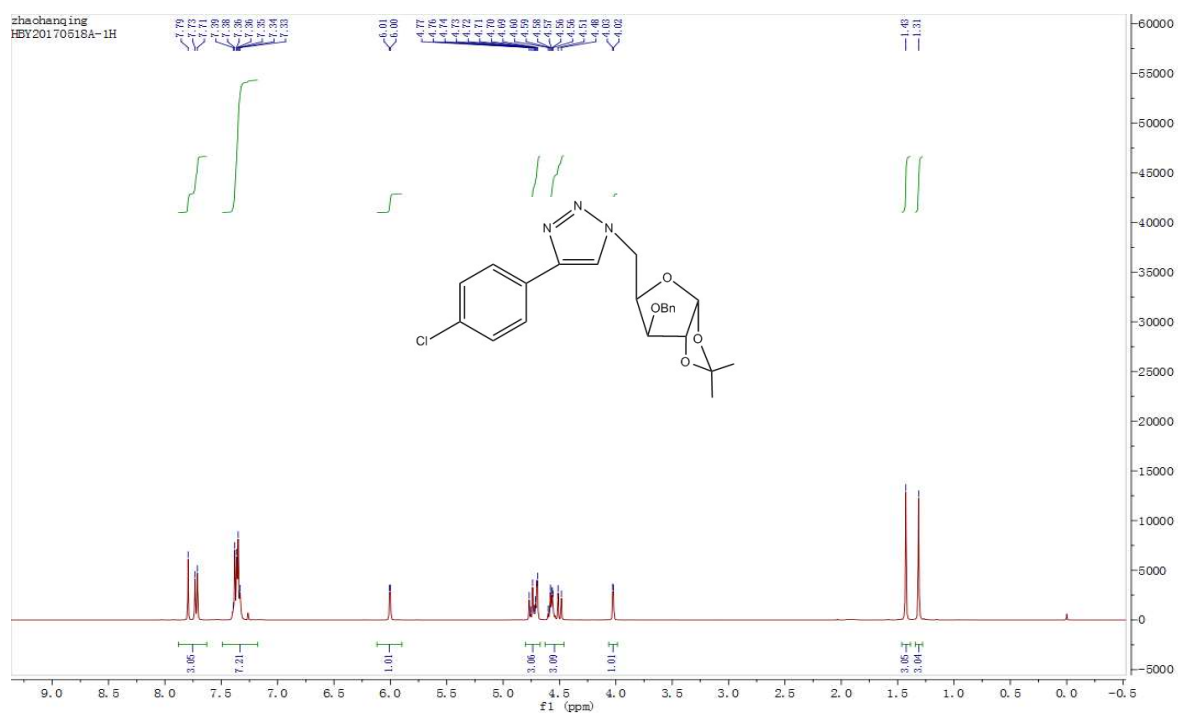
¹³C NMR spectrum of compound 2-e



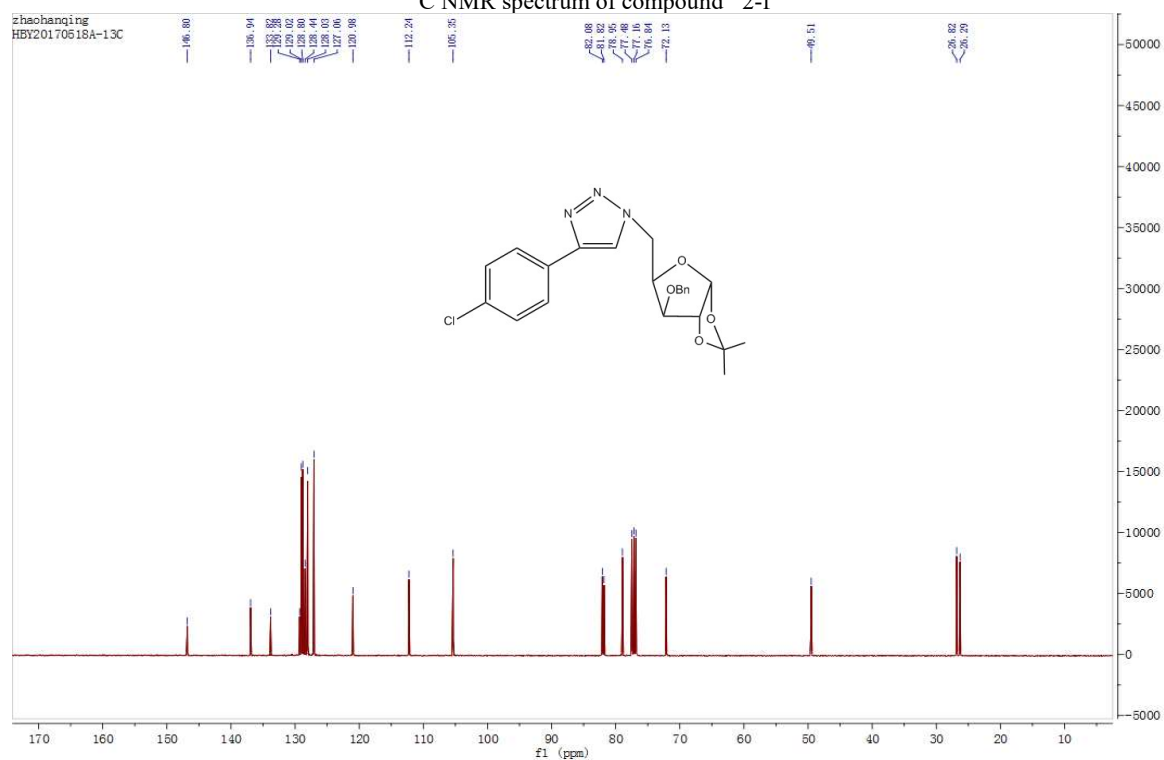
HRMS spectrum of compound 2-e



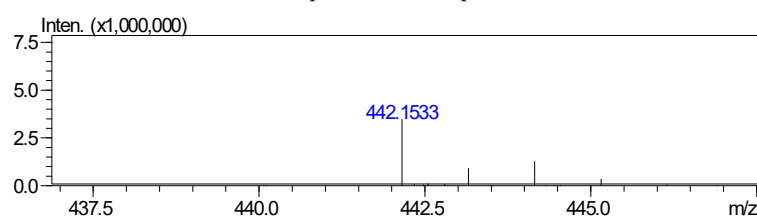
¹H NMR spectrum of compound 2-f



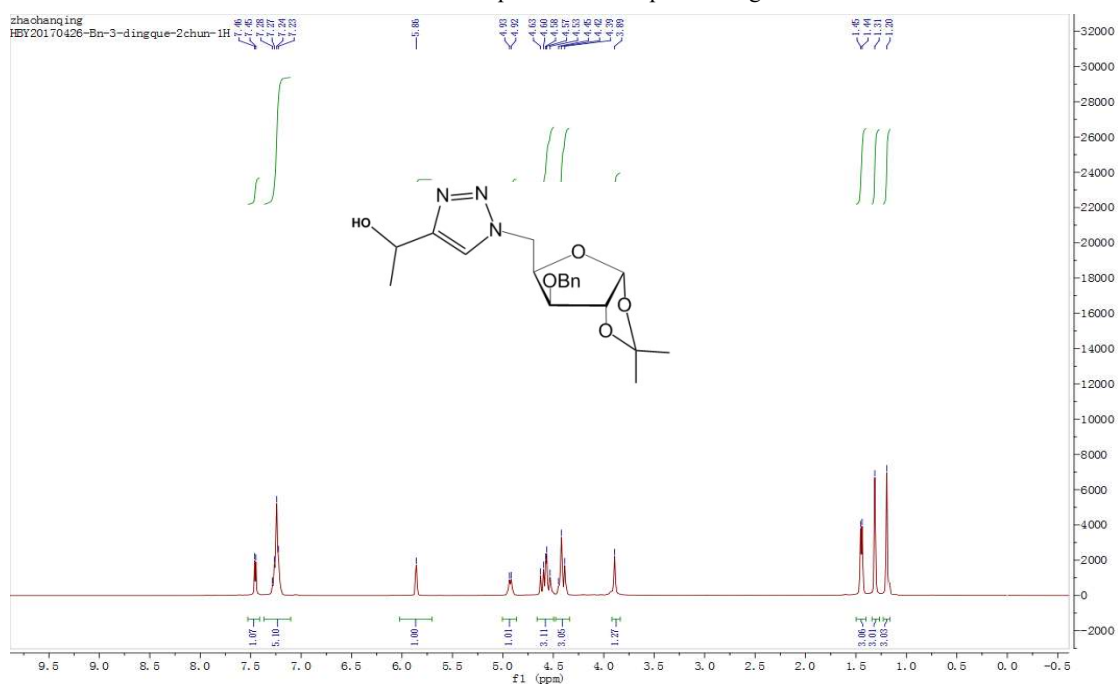
¹³C NMR spectrum of compound 2-f



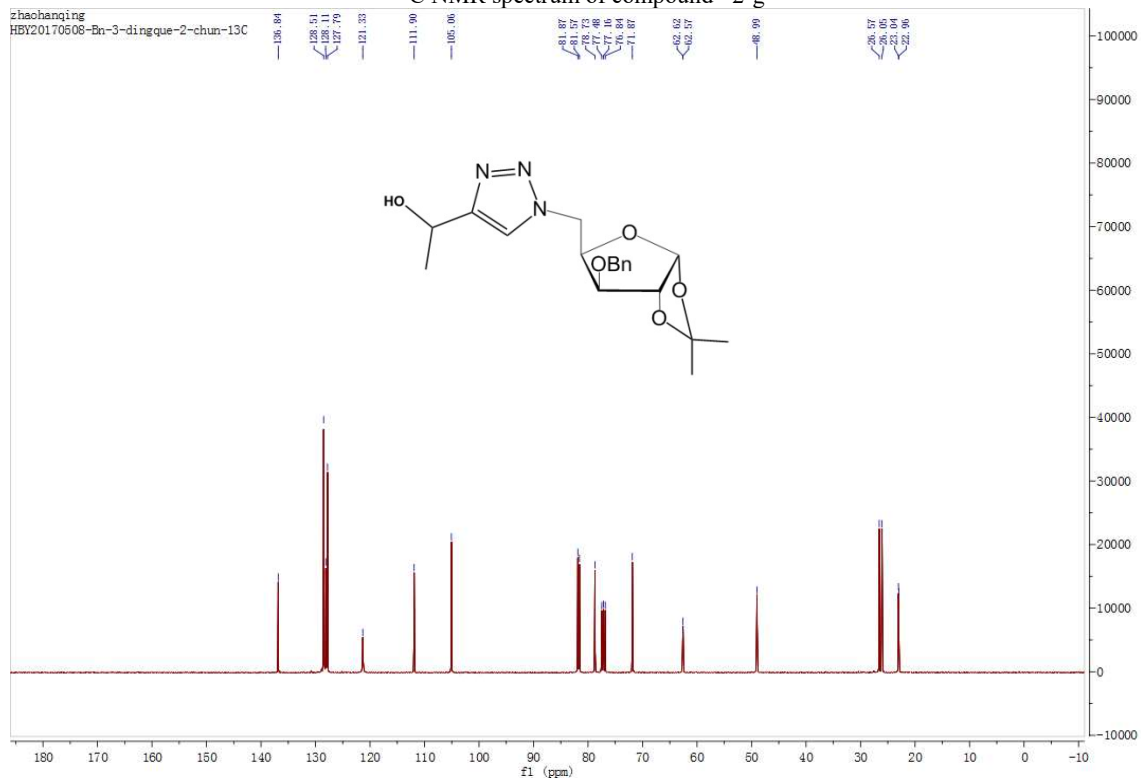
HRMS spectrum of compound 2-f



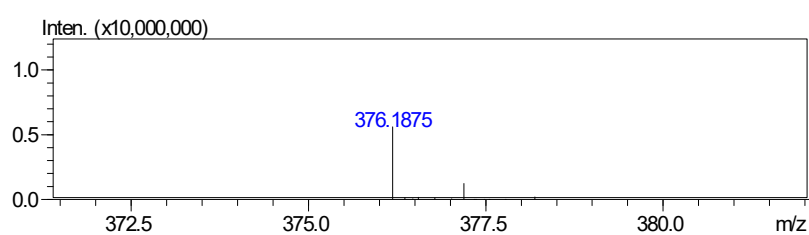
¹H NMR spectrum of compound 2-g

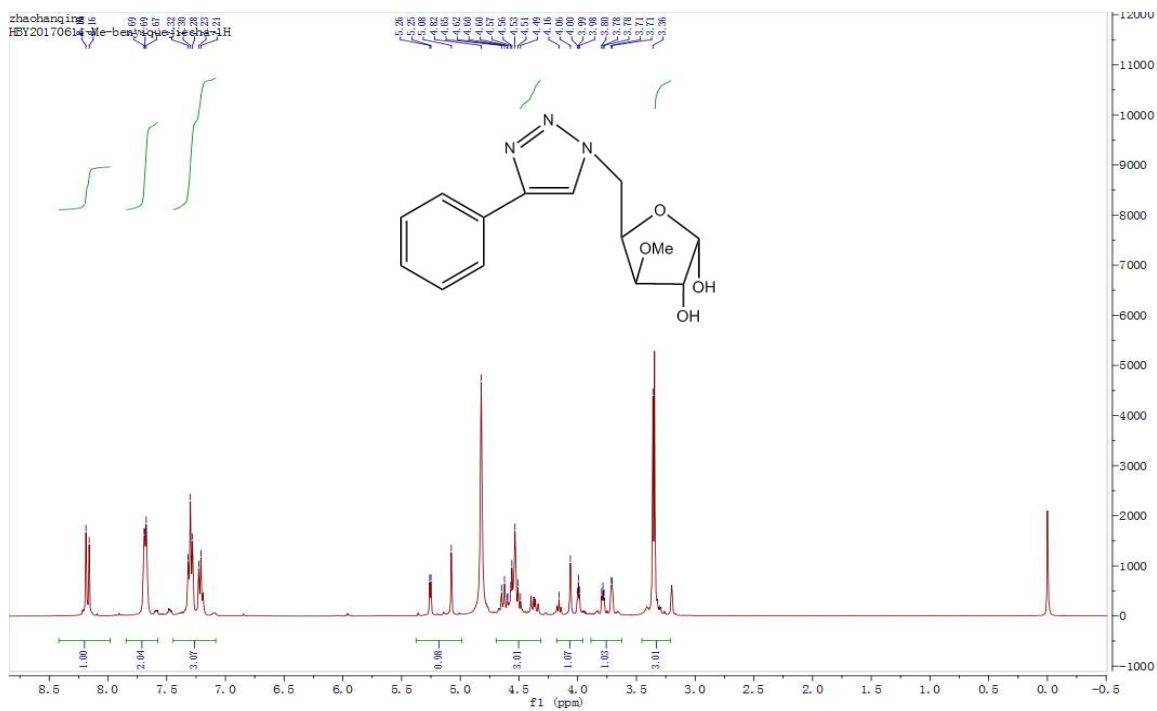


¹³C NMR spectrum of compound 2-g

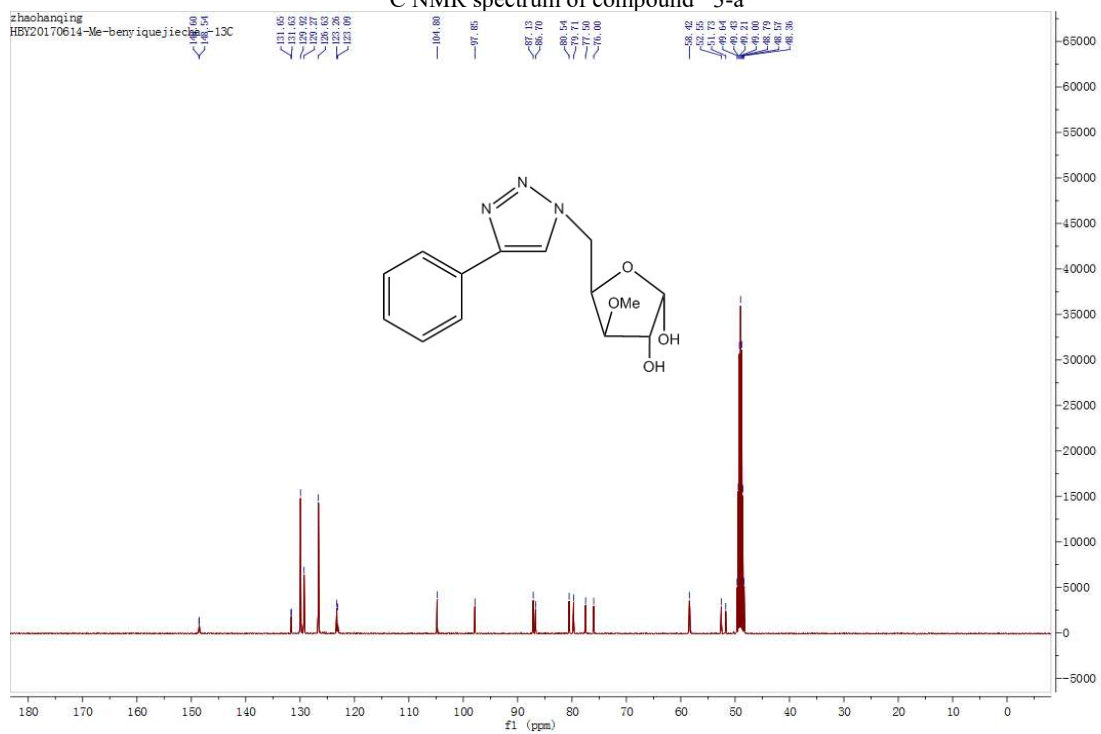


HRMS spectrum of compound 2-g

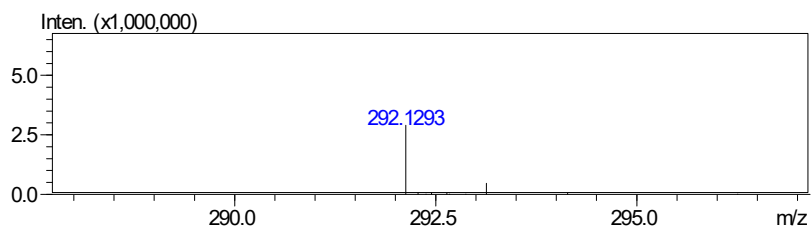


¹H NMR spectrum of compound 3-a

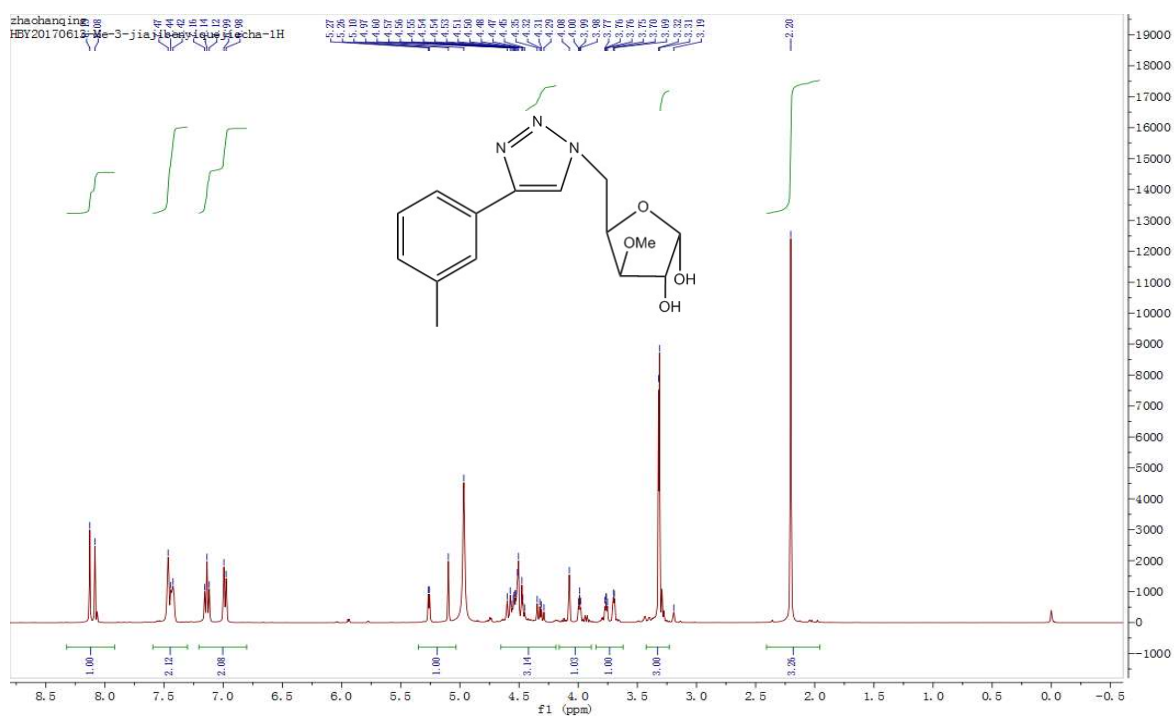
¹³C NMR spectrum of compound 3-a



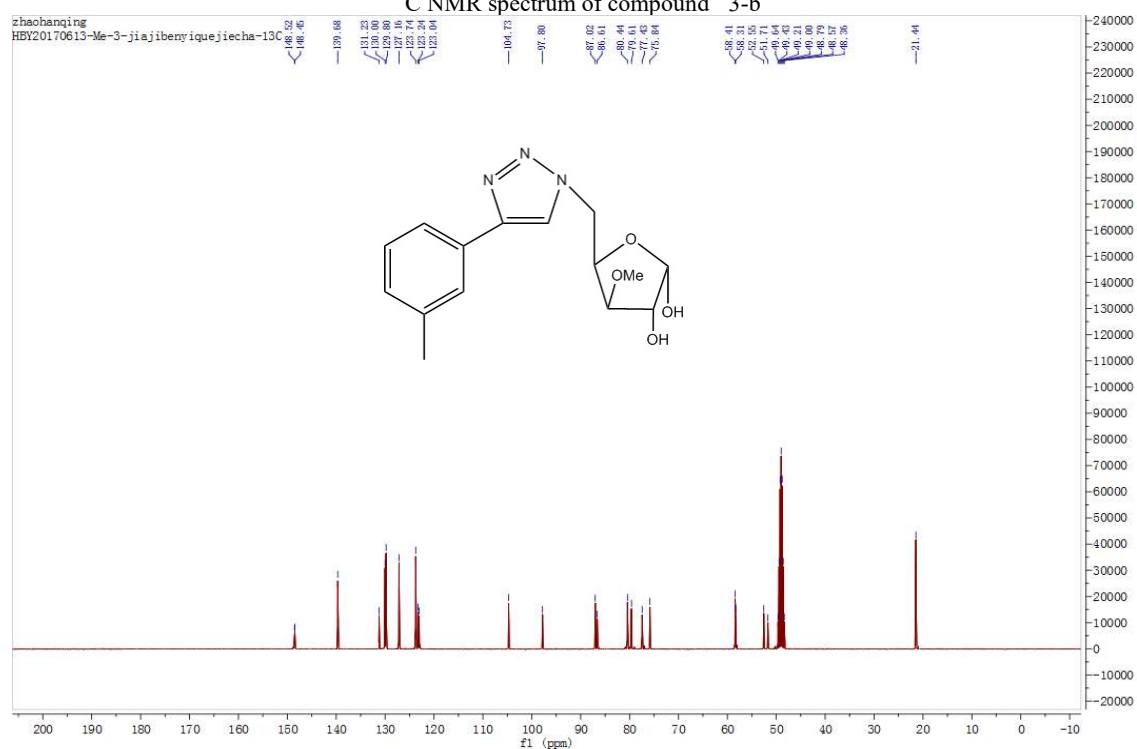
HRMS spectrum of compound 3-a



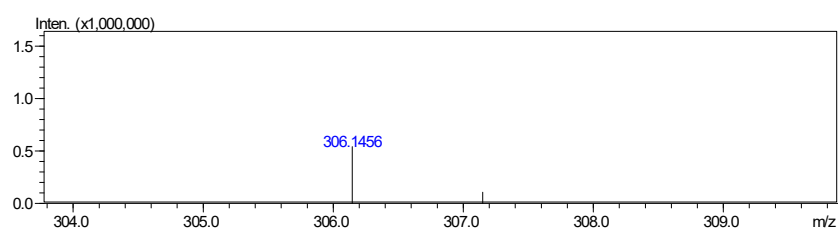
¹H NMR spectrum of compound 3-b

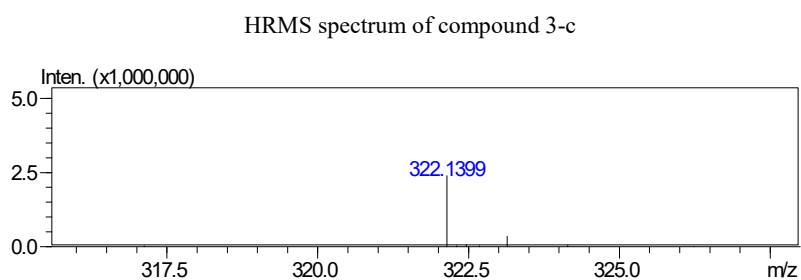
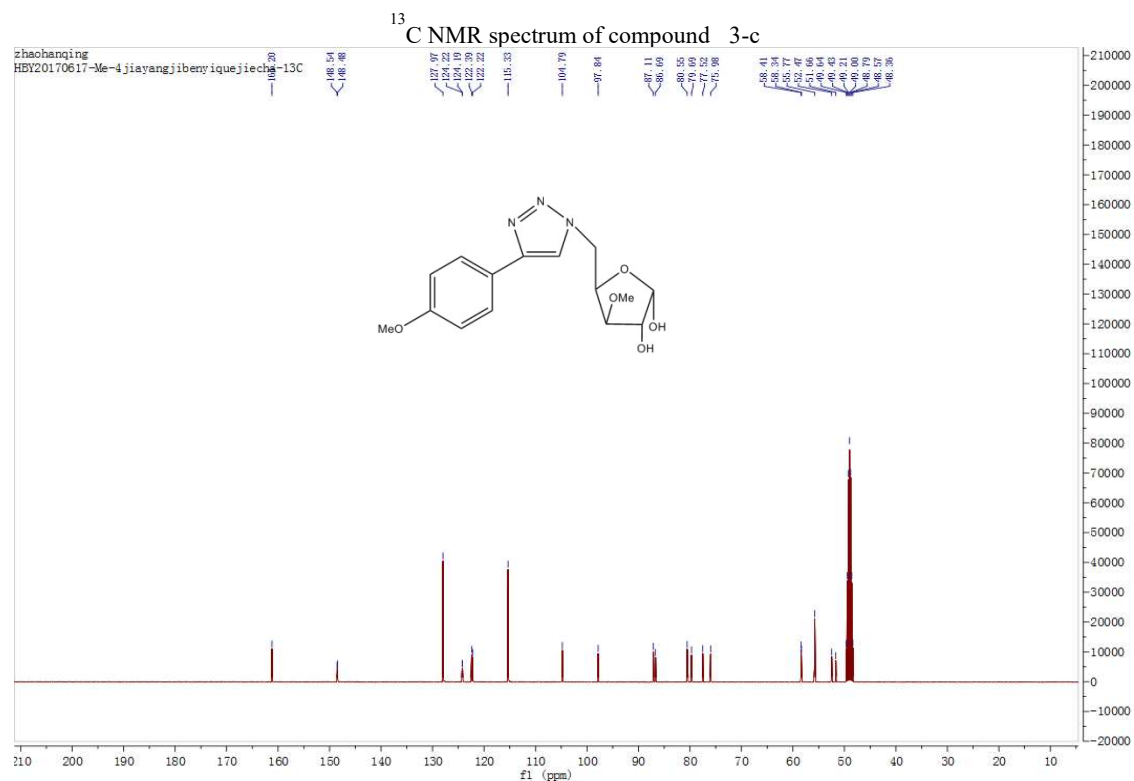
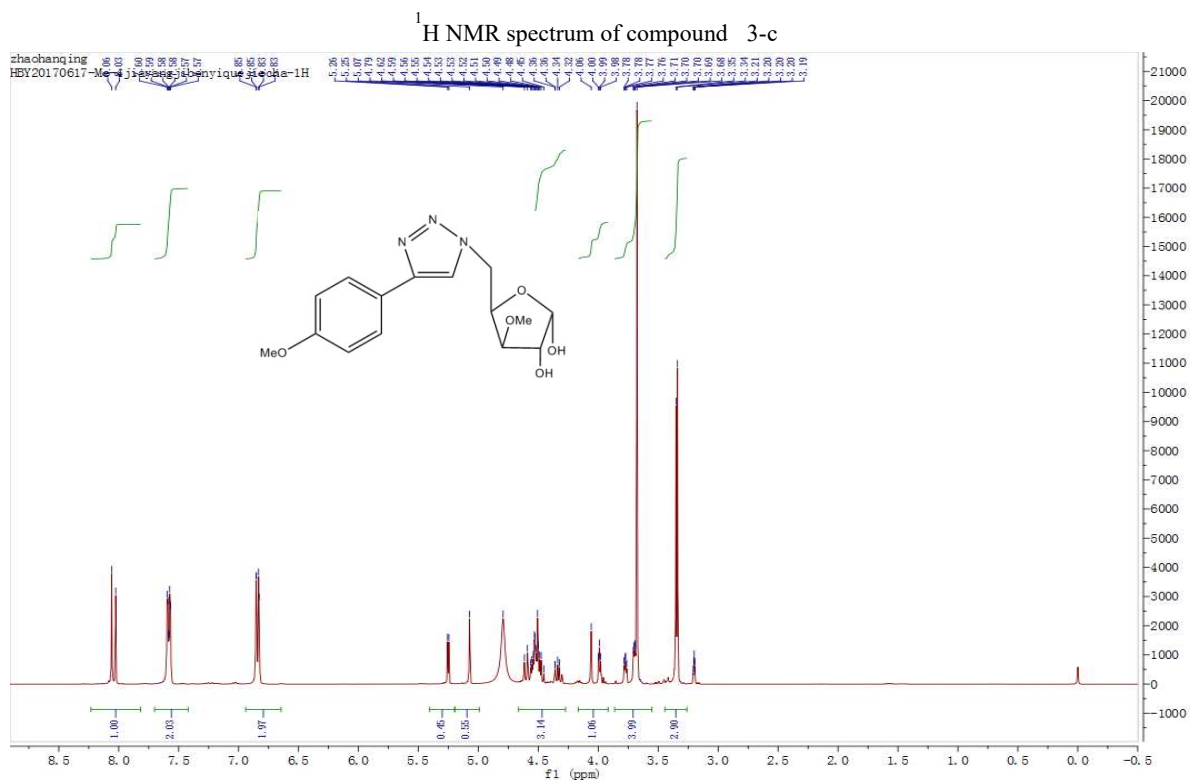


¹³C NMR spectrum of compound 3-b



HRMS spectrum of compound 3-b





Chemical structure of the compound is shown above the spectrum. The structure is 4-(4-fluorophenyl)-1H-1,2,4-triazole-3-ylmethyl 2,3-dihydro-4H-pyran-4-ylmethanol derivative. The spectrum shows peaks corresponding to the structure, with integration values provided below the baseline.

Integration values (from left to right): 1.00, 2.00, 1.98, 1.00, 3.00, 1.02, 1.01, 3.00.

Chemical structure: CO[C@H]1O[C@H](Cn2cnc(C3=CC=C(C=C3)F)c2)[C@H](O)[C@H]1O

Chemical structure of compound 5a is shown above the spectrum. The structure is 4-fluorophenyl-1-(4-methoxyphenyl)-1H-1,2,3-triazole. The spectrum displays peaks corresponding to the structure, with the following chemical shifts (ppm) labeled above the peaks:

163.49, 163.47, 148.48, 148.33, 127.28, 127.21, 126.85, 126.81, 126.78, 126.71, 121.63, 118.48, 115.29, 108.49, 96.55, 85.80, 85.39, 79.20, 78.39, 78.20, 74.66, 57.11, 57.03, 51.21, 50.95, 49.91, 48.12, 47.91, 47.48, 47.27, 47.06.

The spectrum shows a series of peaks in the aromatic region (120-160 ppm) and a cluster of peaks in the aliphatic region (47-57 ppm). The peak at 163.49 ppm is the most intense in the aromatic region. The peak at 47.06 ppm is the most intense in the aliphatic region.

Mass spectrum of compound 10. The x-axis represents the mass-to-charge ratio (m/z) from 305.0 to 315.0. The y-axis represents intensity (Inten. (x1,000,000)) from 0.0 to 2.5. A single prominent peak is observed at m/z 310.1204, which is the base peak.

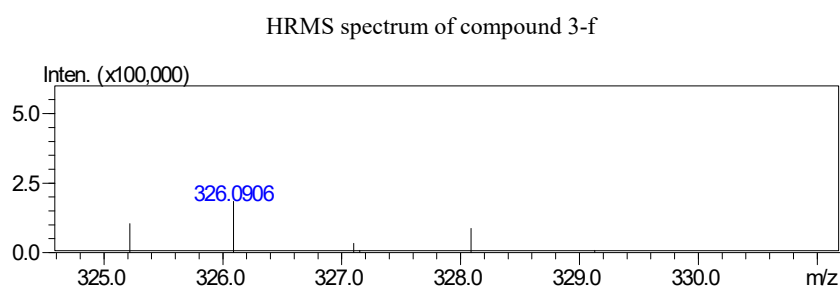
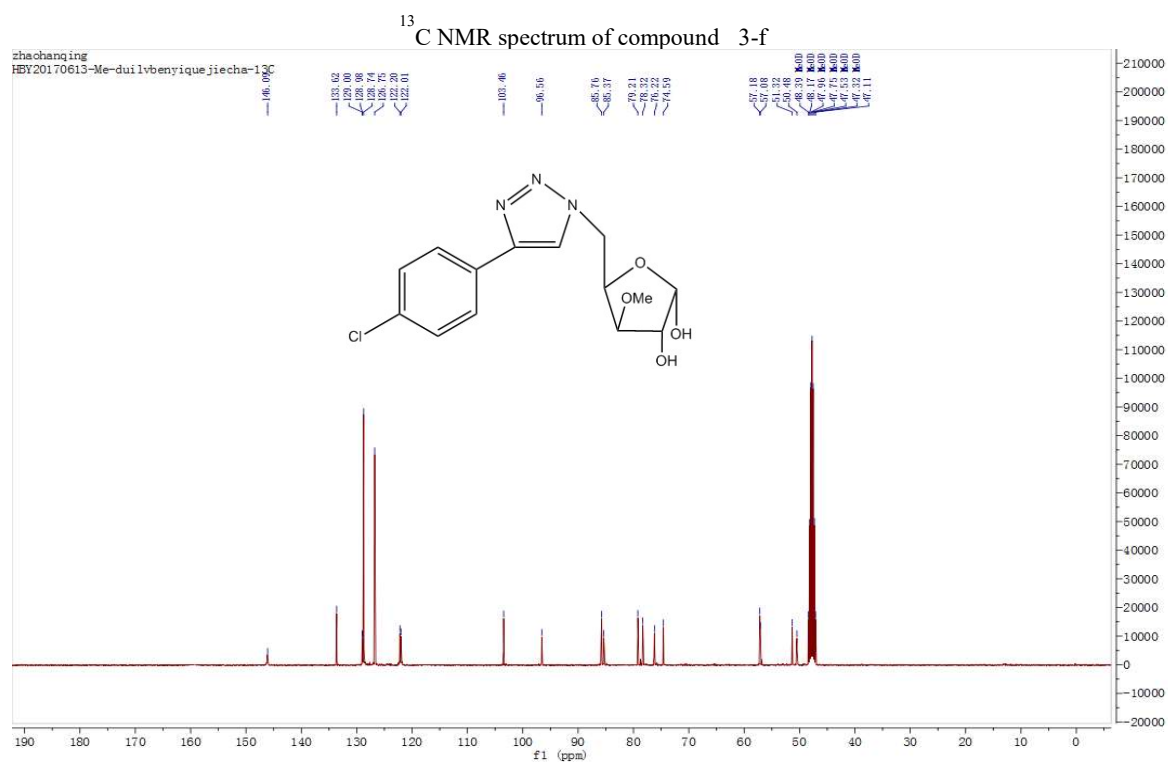
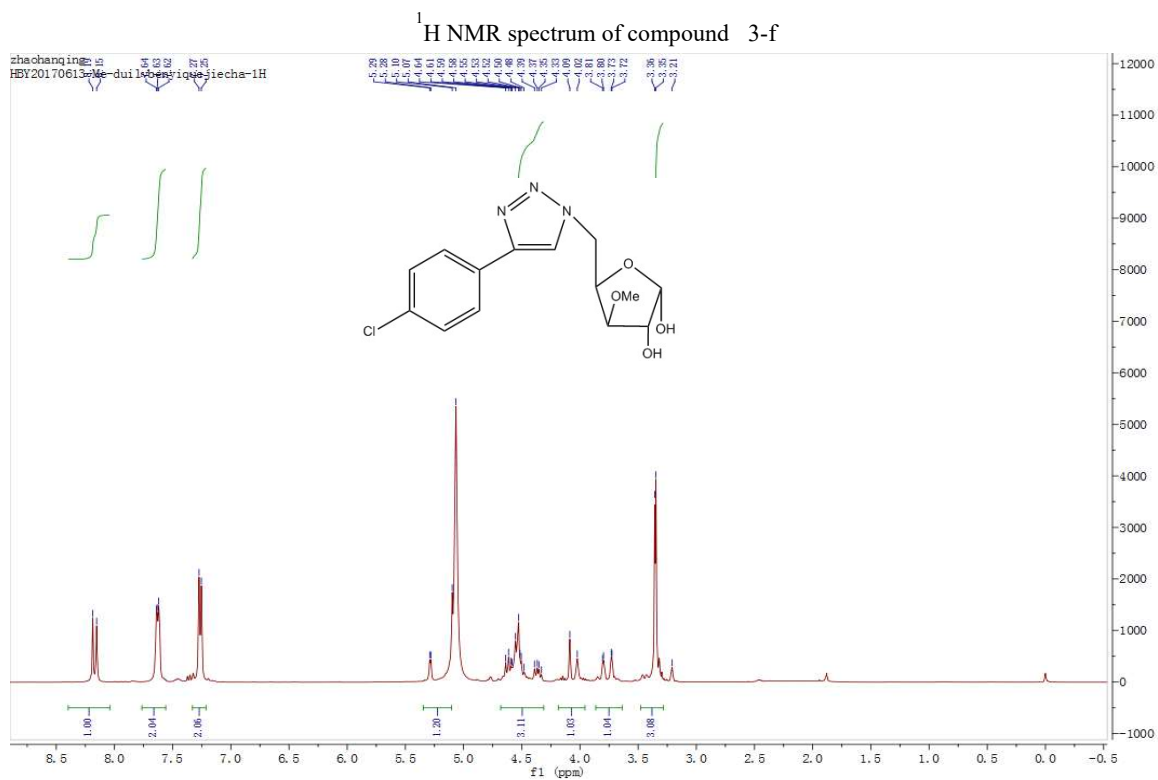
m/z	Intensity (x1,000,000)
310.1204	2.5

Desktop
(DMSO)-HBY-20180126-Merck-sojibenyiquejiecha-1H

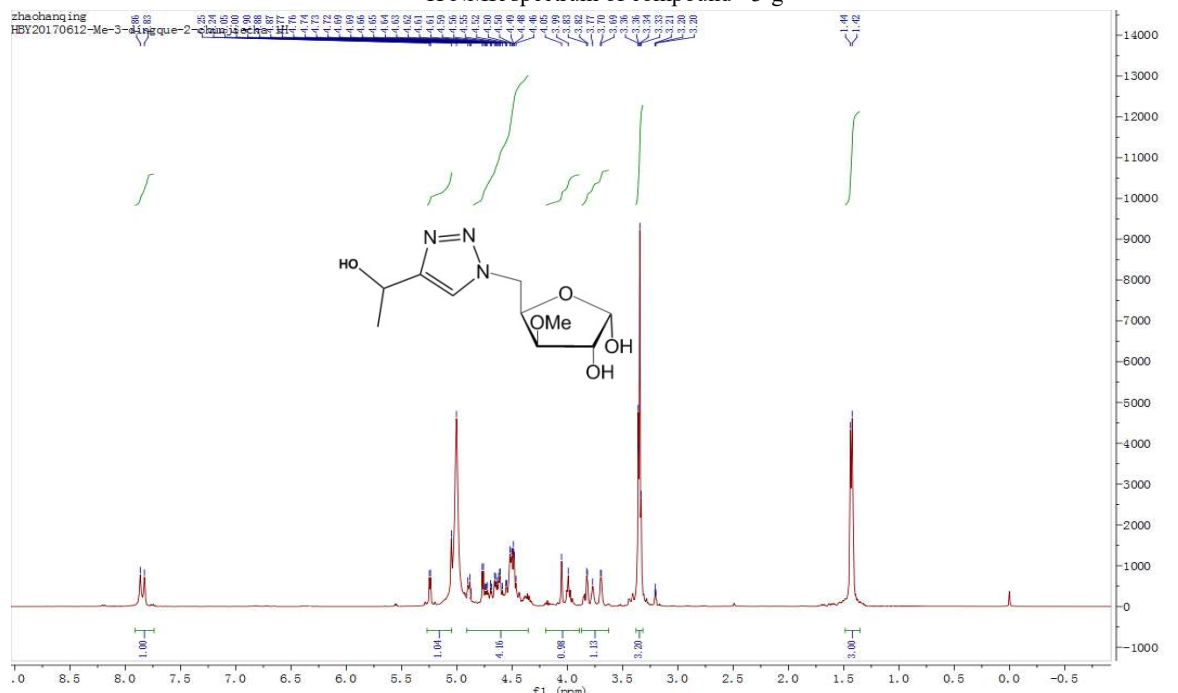
Chemical structure of compound 5c is shown above the spectrum. The structure is 4-(4-nitrophenyl)-1-(4-methoxy-2,3-dihydro-4H-pyran-2-yl)-1H-1,2,4-triazole.

Integration values are provided below the baseline: 1.06, 2.15, 2.09, 1.00, 3.00, 1.23, 1.09, 3.63, and 1.00.

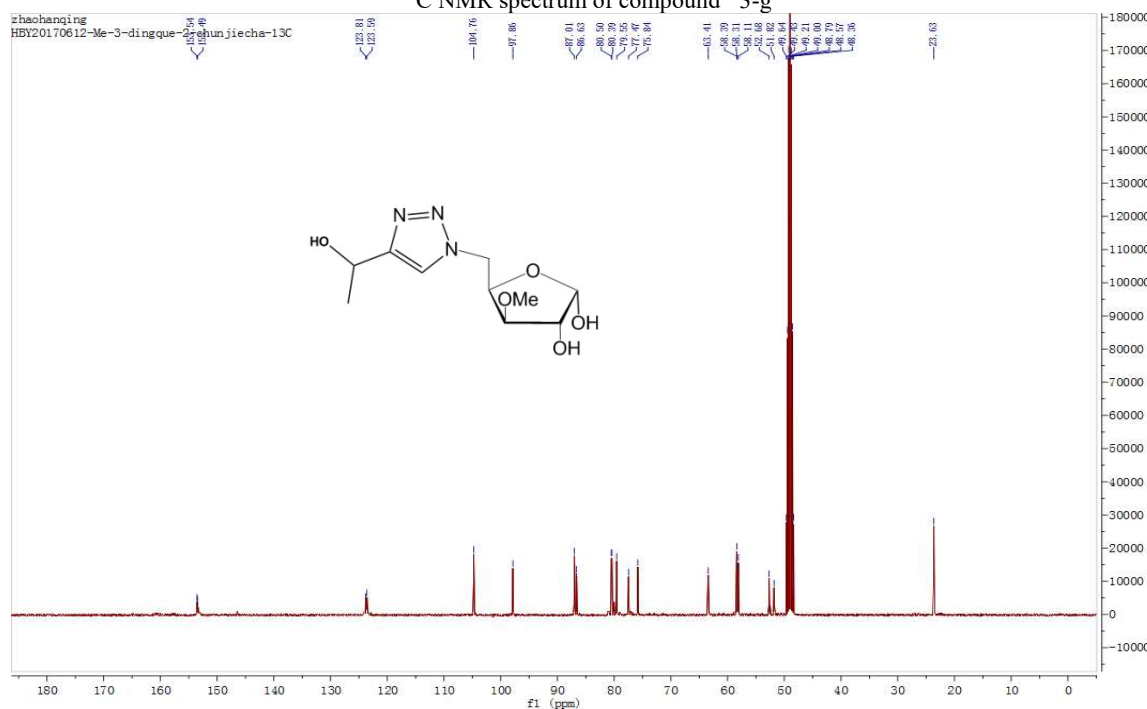
Zhaohanqing
HBV20170612-Me-3-duixiaoji benyiguan
Chemical structure: COC1OC(CO)CN1Cc2ncnc2-c3ccc([N+](=O)[O-])cc3
NMR spectrum (ppm): 125.98, 125.86, 124.53, 103.29, 96.29, 85.89, 85.87, 78.89, 78.11, 76.39, 74.31, 57.50, 57.44, 51.06, 50.39, 39.54, 39.48, 39.46, 39.10.



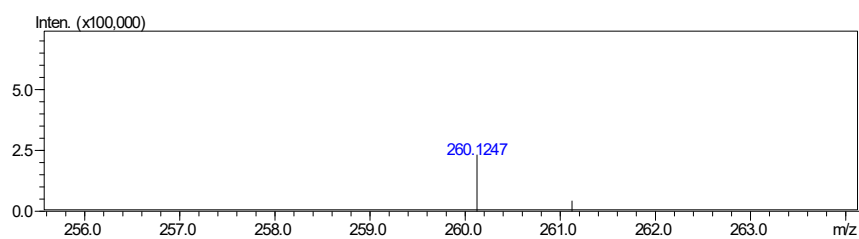
¹H NMR spectrum of compound 3-g



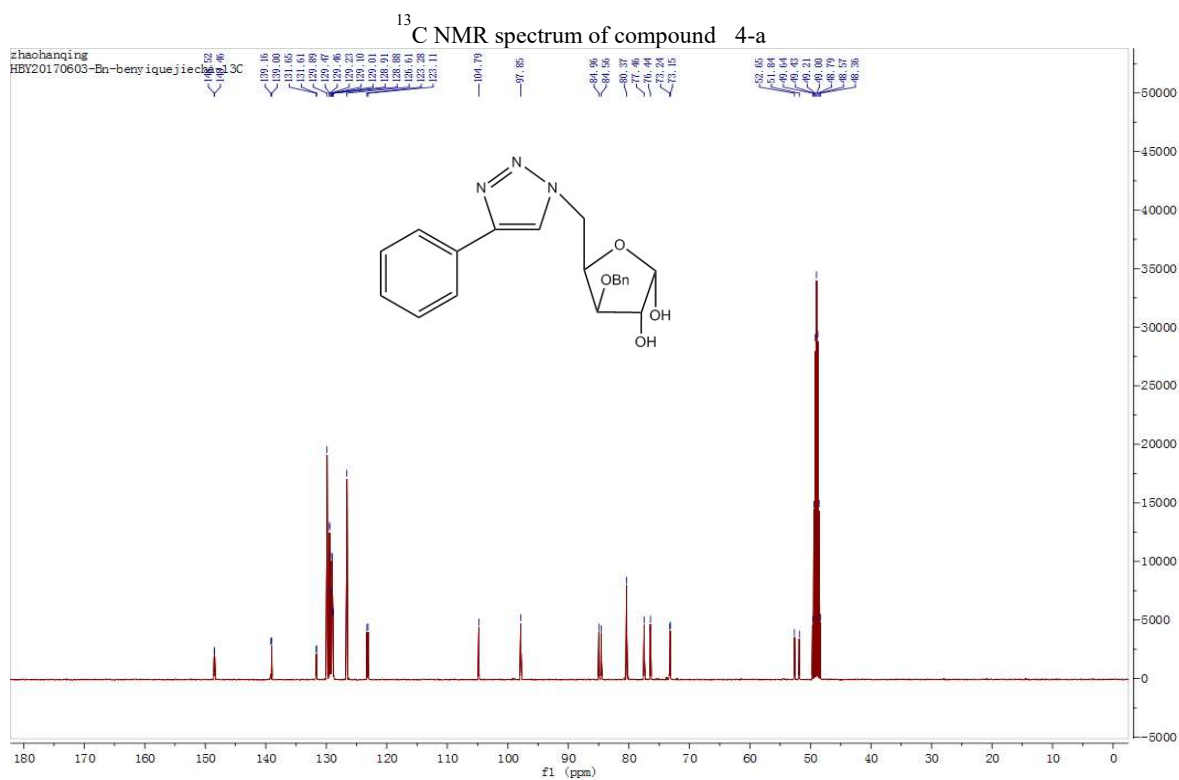
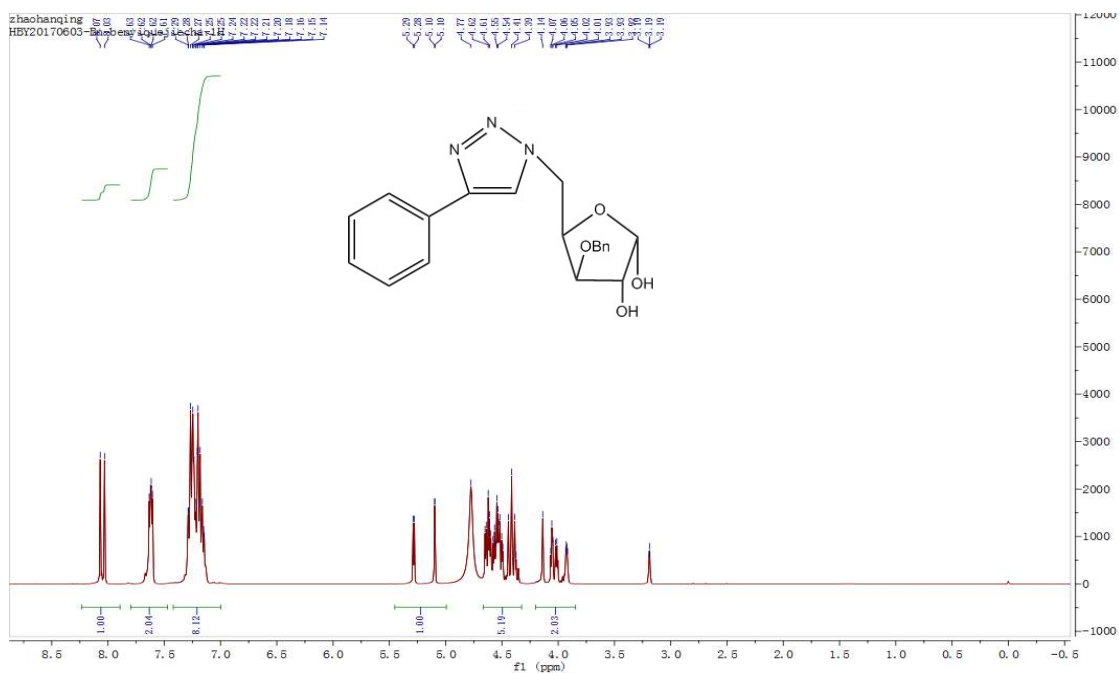
¹³C NMR spectrum of compound 3-g



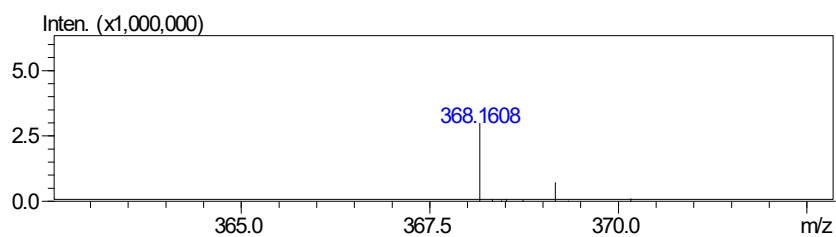
HRMS spectrum of compound 3-g



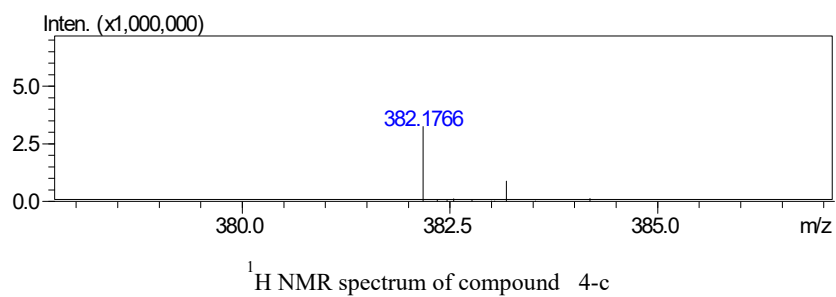
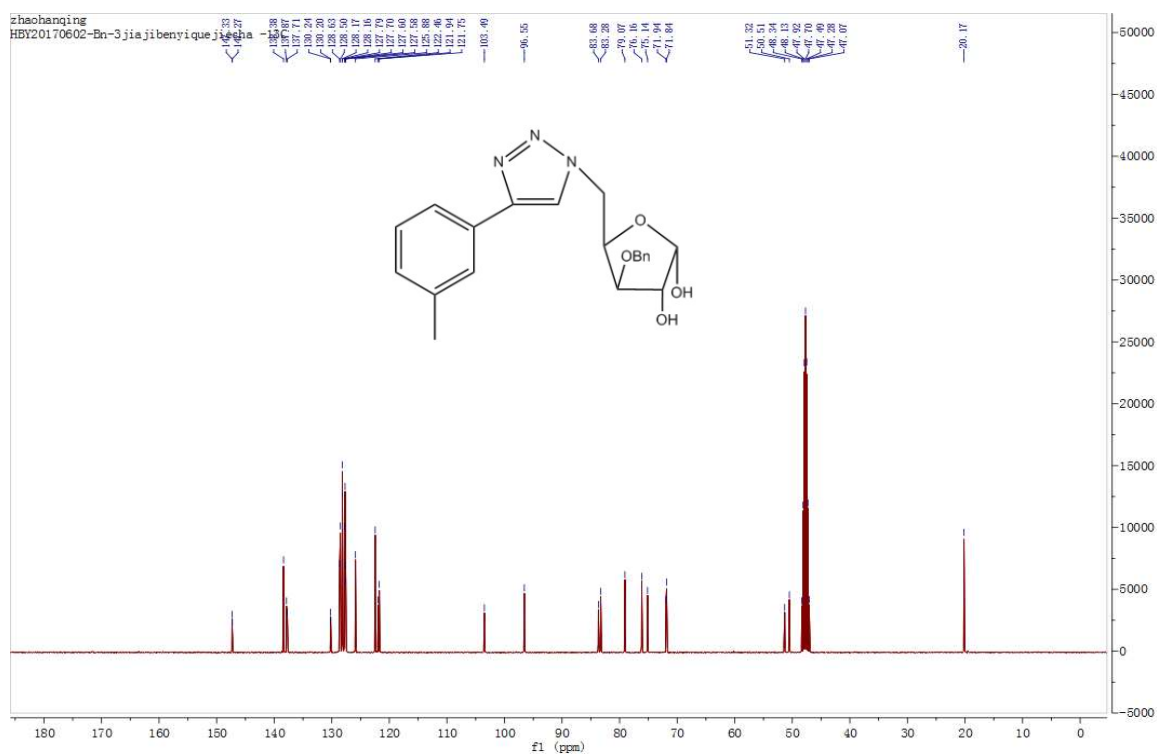
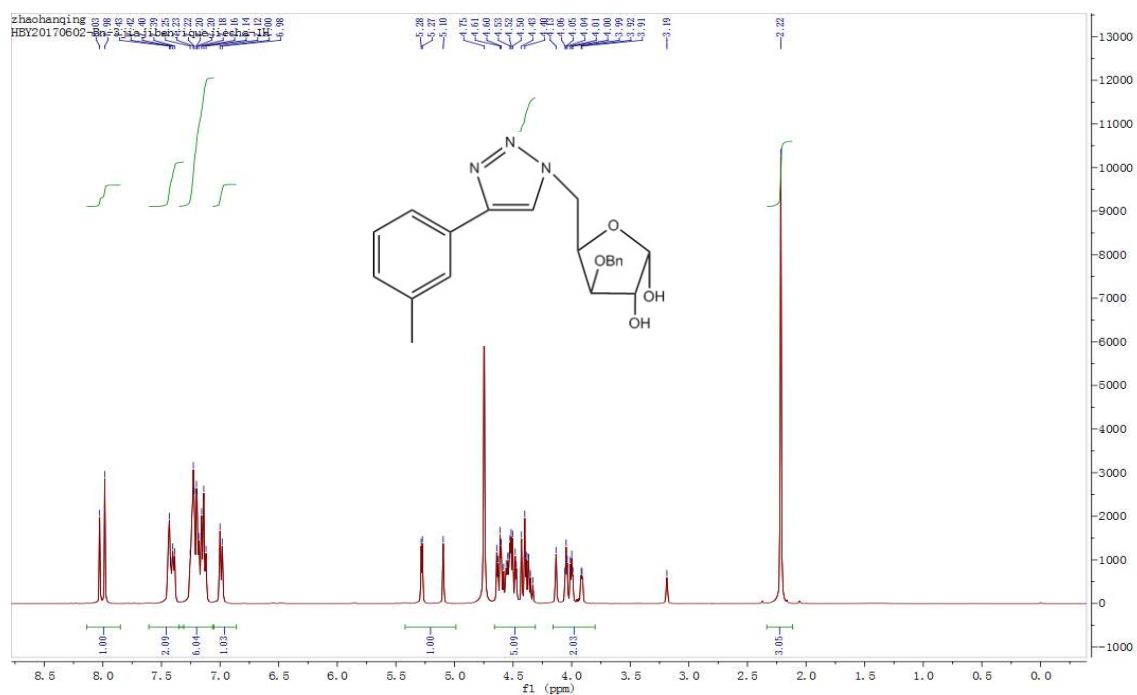
¹H NMR spectrum of compound 4-a

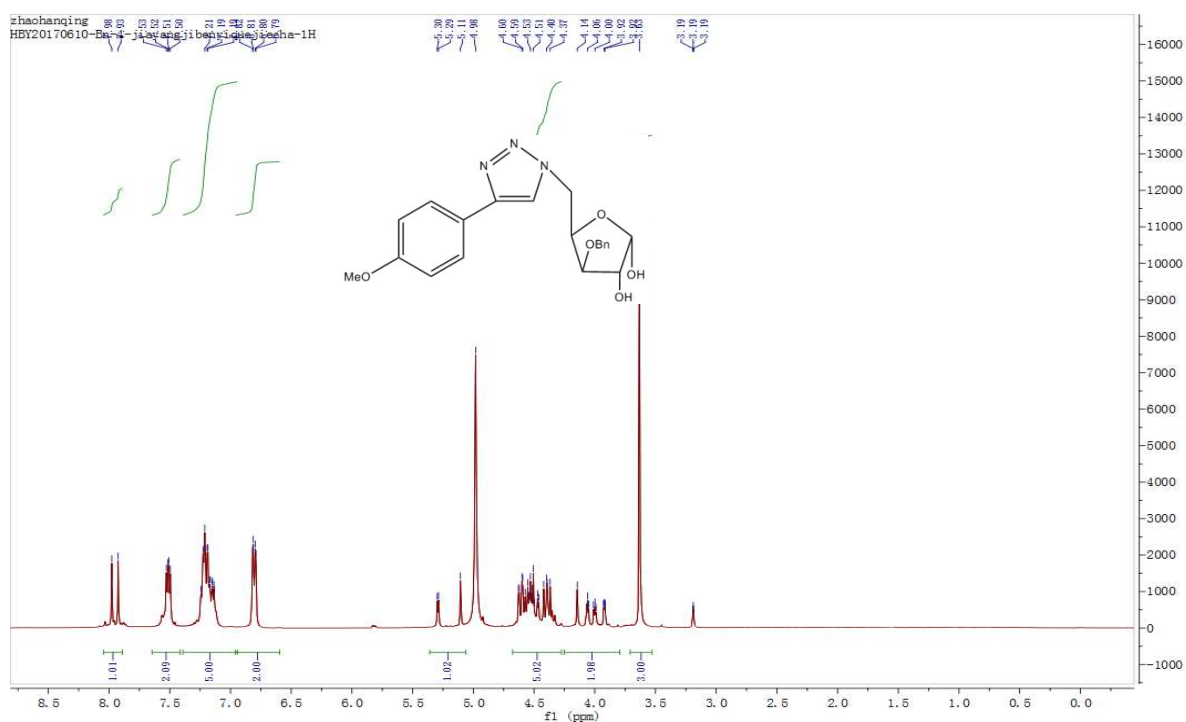


HRMS spectrum of compound 4-a

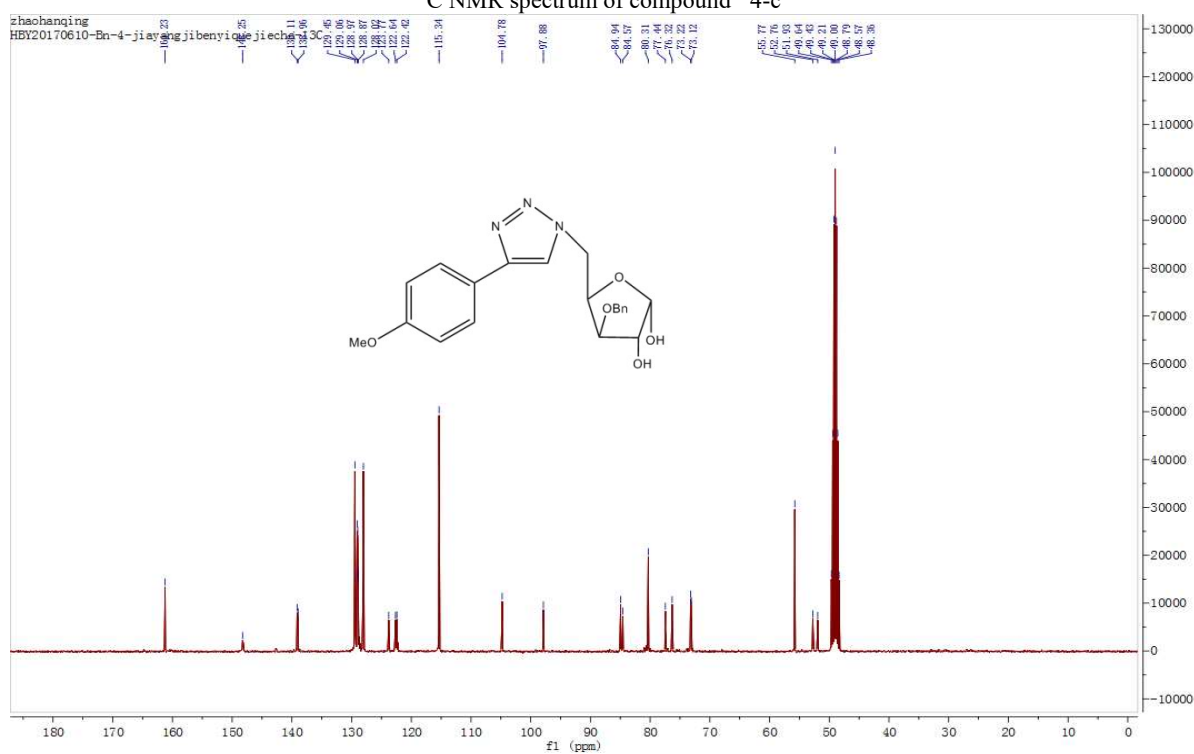


^1H NMR spectrum of compound 4-b

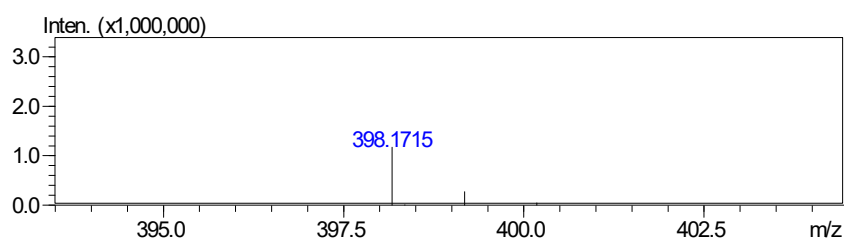




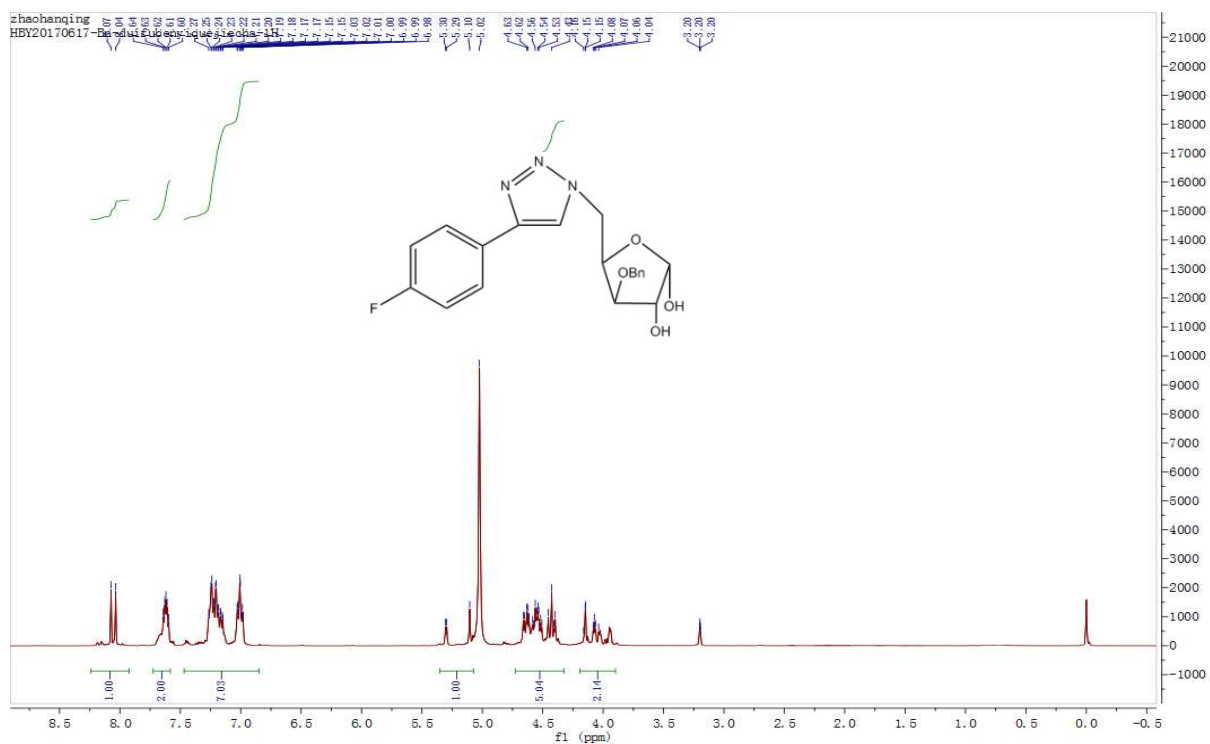
¹³C NMR spectrum of compound 4-c



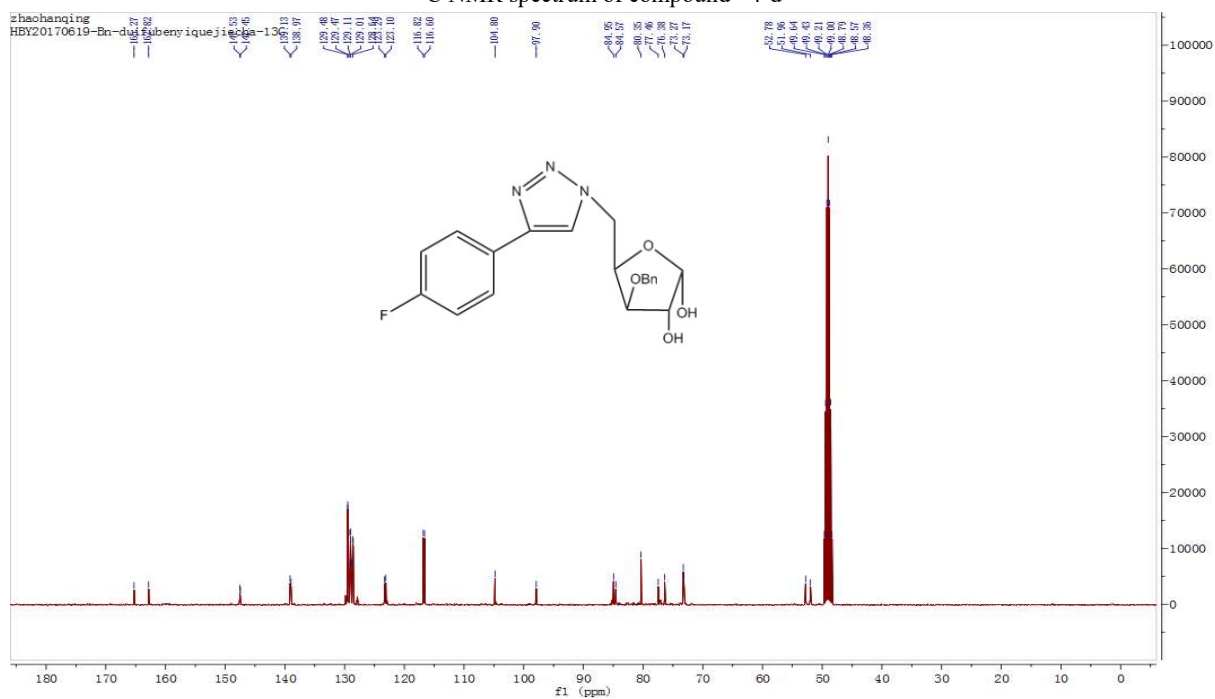
HRMS spectrum of compound 4-c



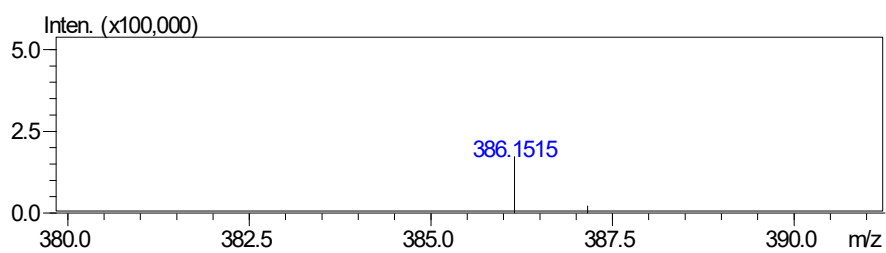
¹H NMR spectrum of compound 4-d



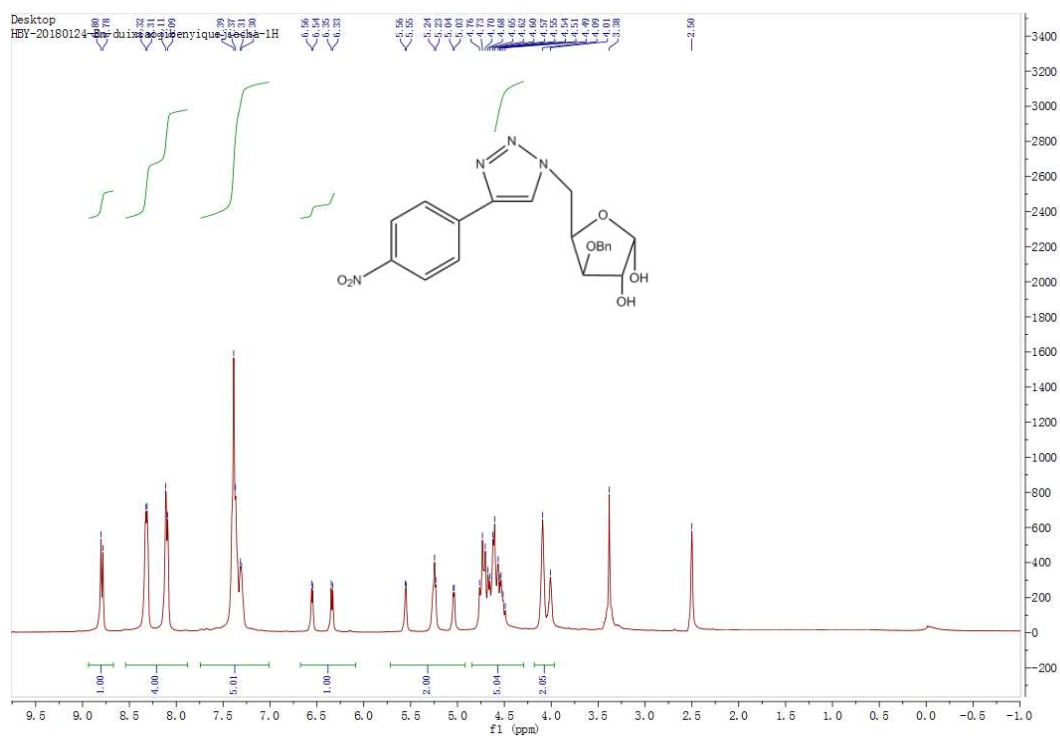
¹³C NMR spectrum of compound 4-d



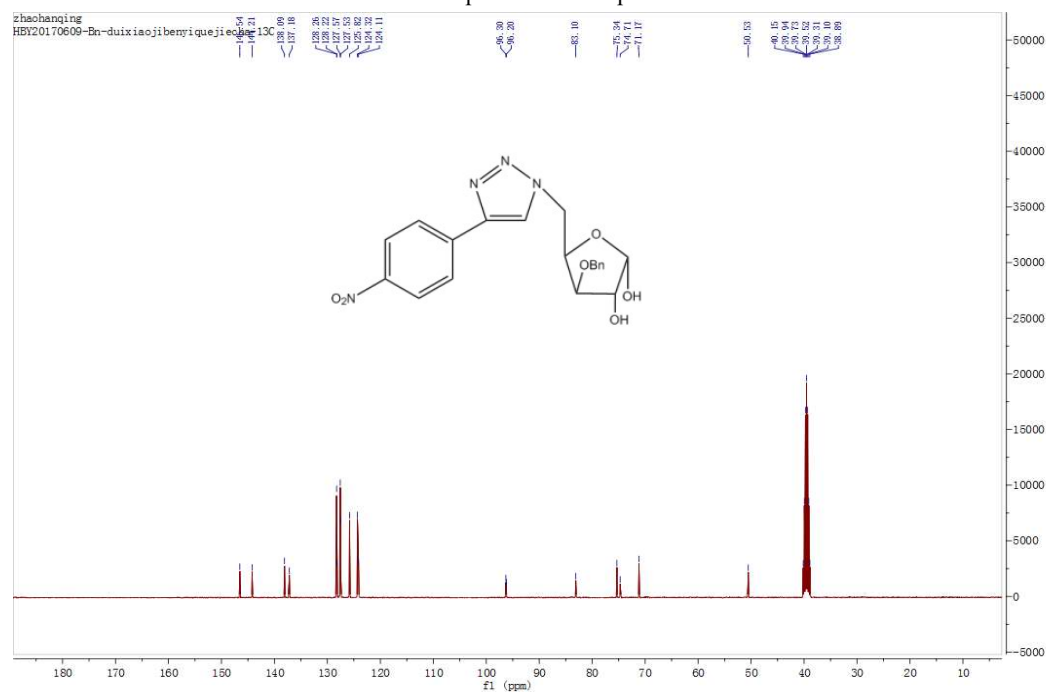
HRMS spectrum of compound 4-d



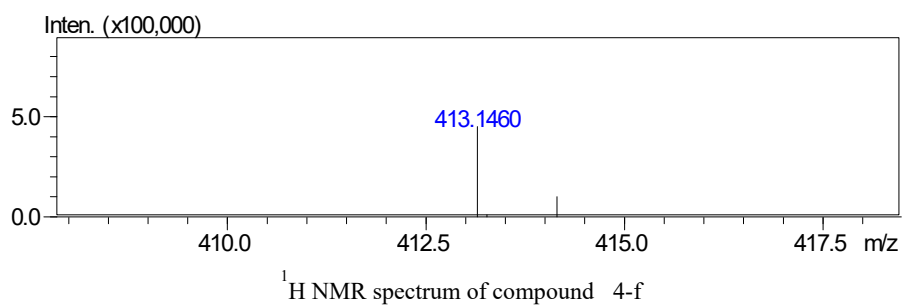
¹H NMR spectrum of compound 4-e



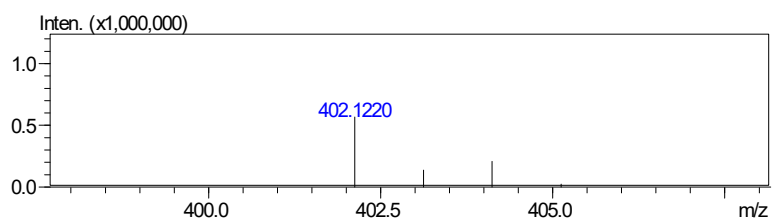
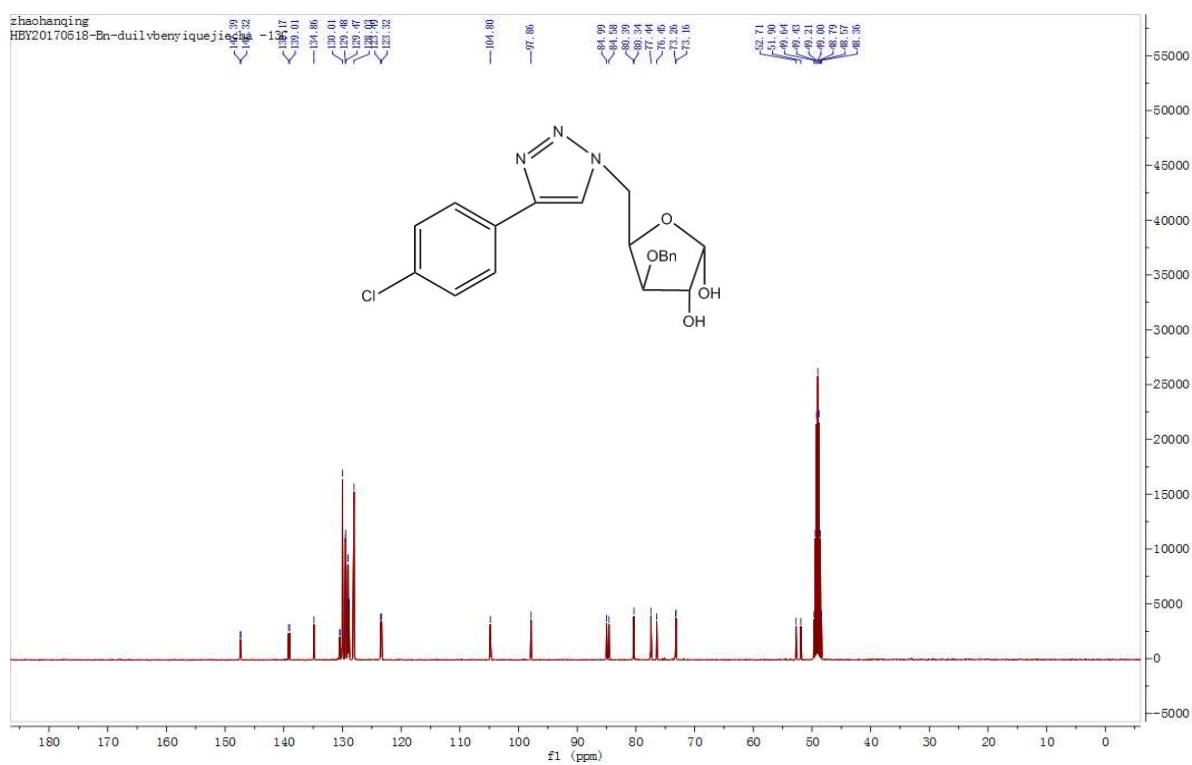
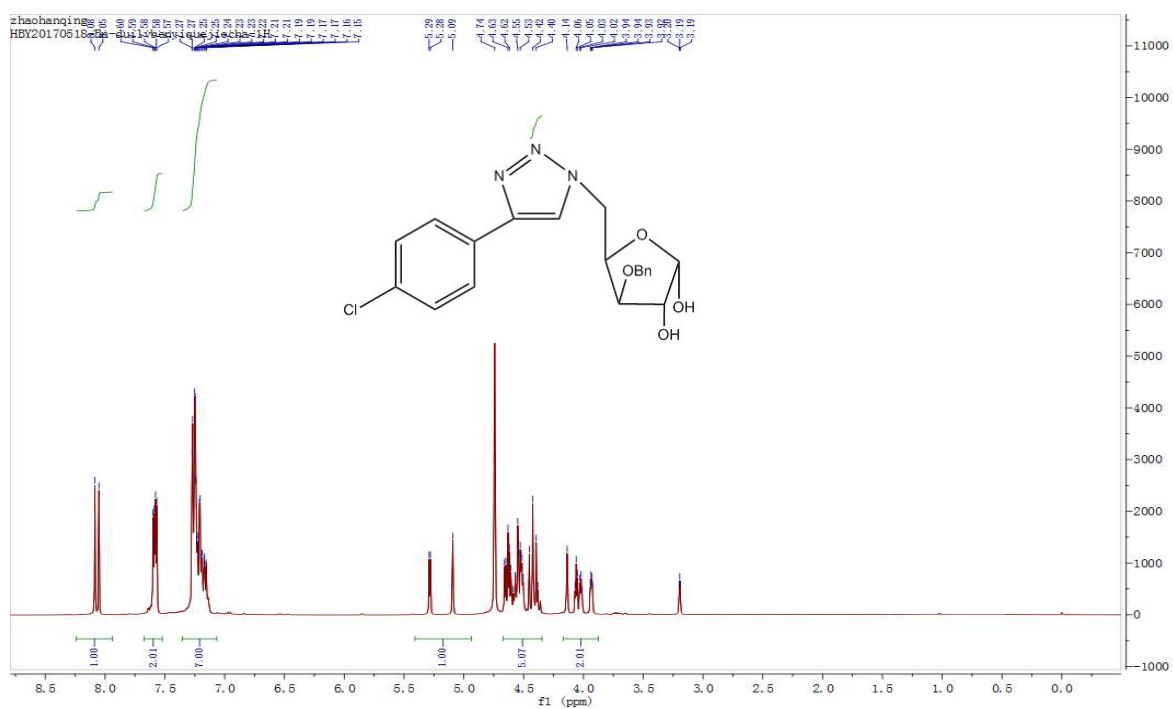
^{13}C NMR spectrum of compound 4-e



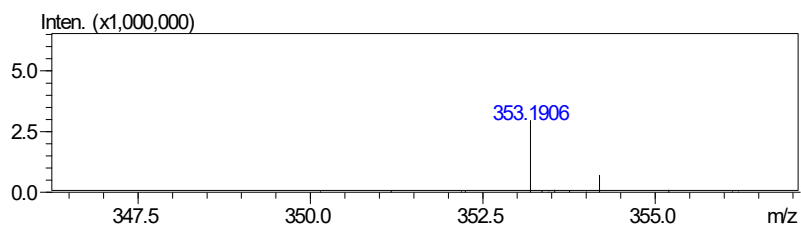
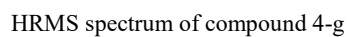
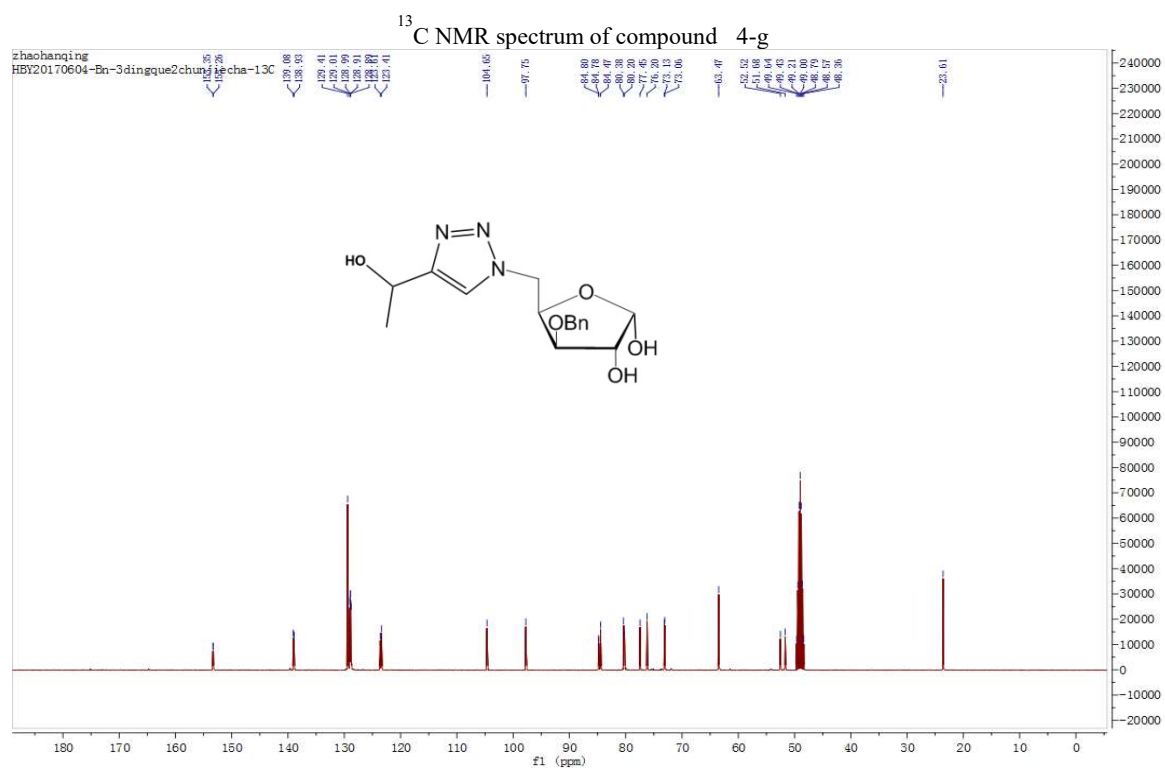
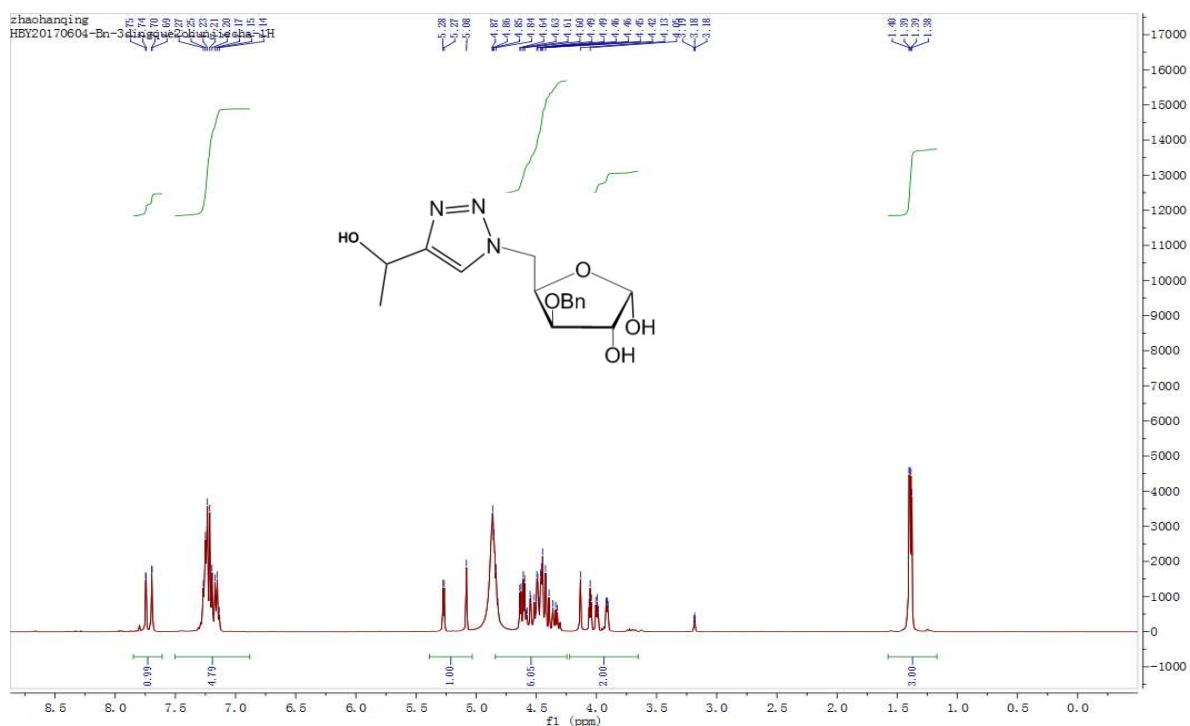
HRMS spectrum of compound 4-e

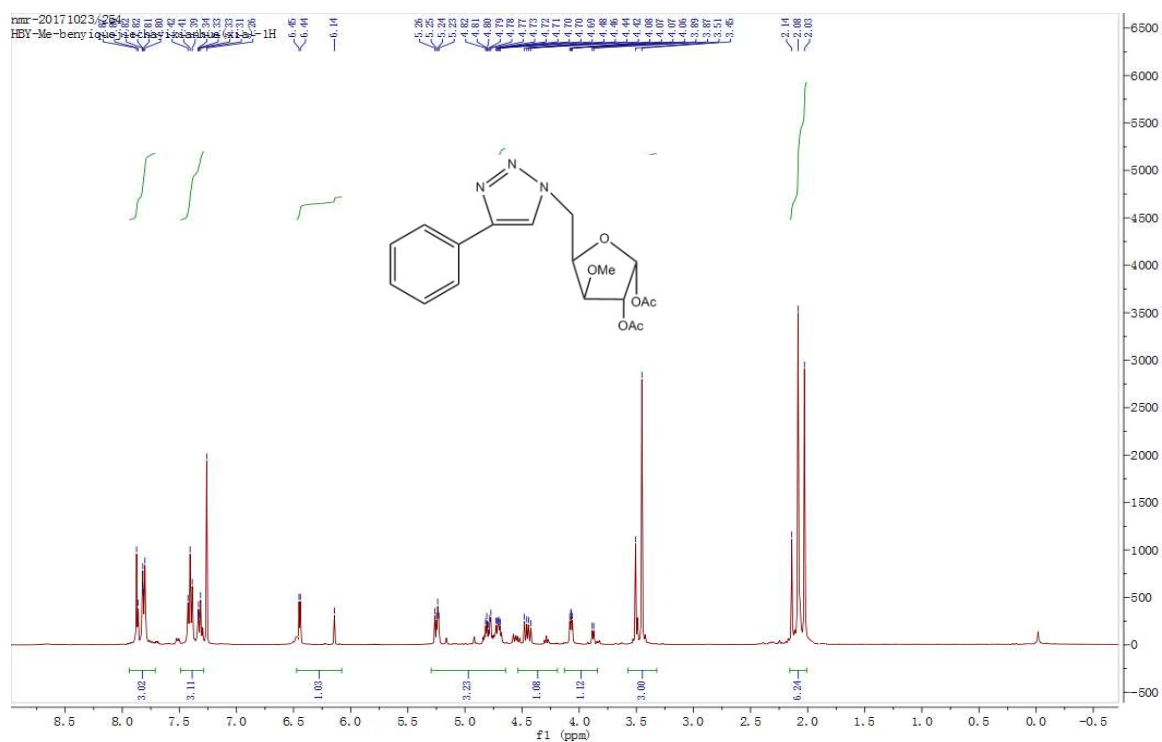


^1H NMR spectrum of compound 4-f

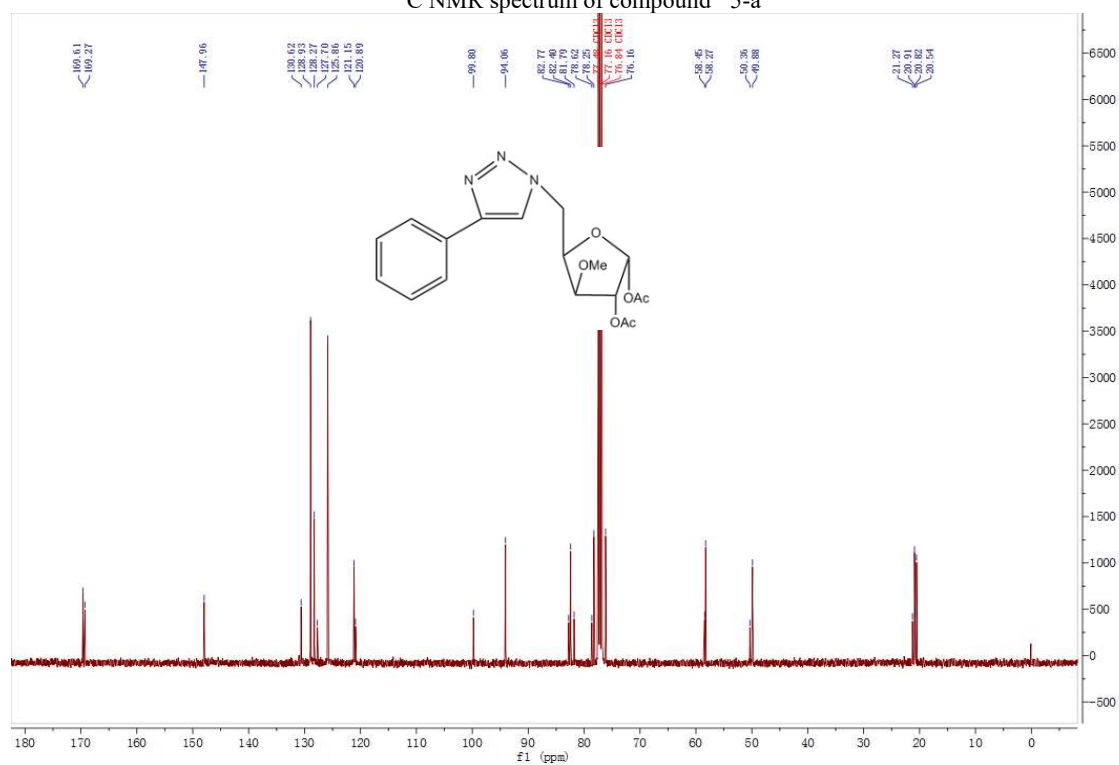


^1H NMR spectrum of compound 4-g

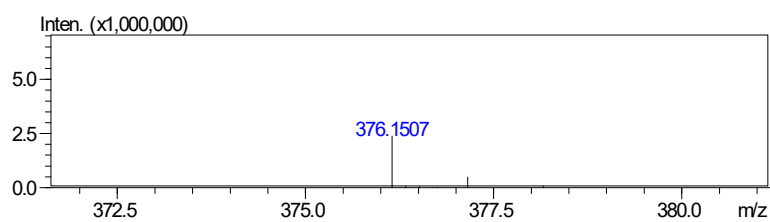


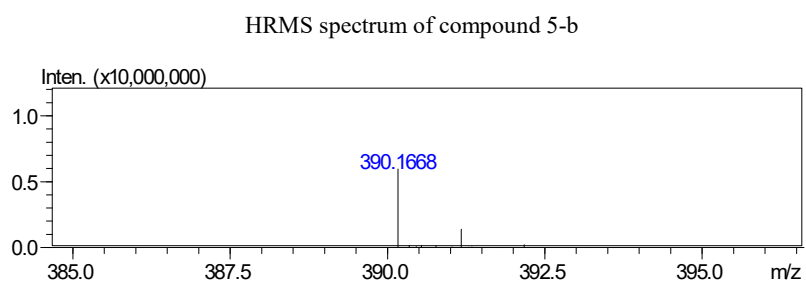
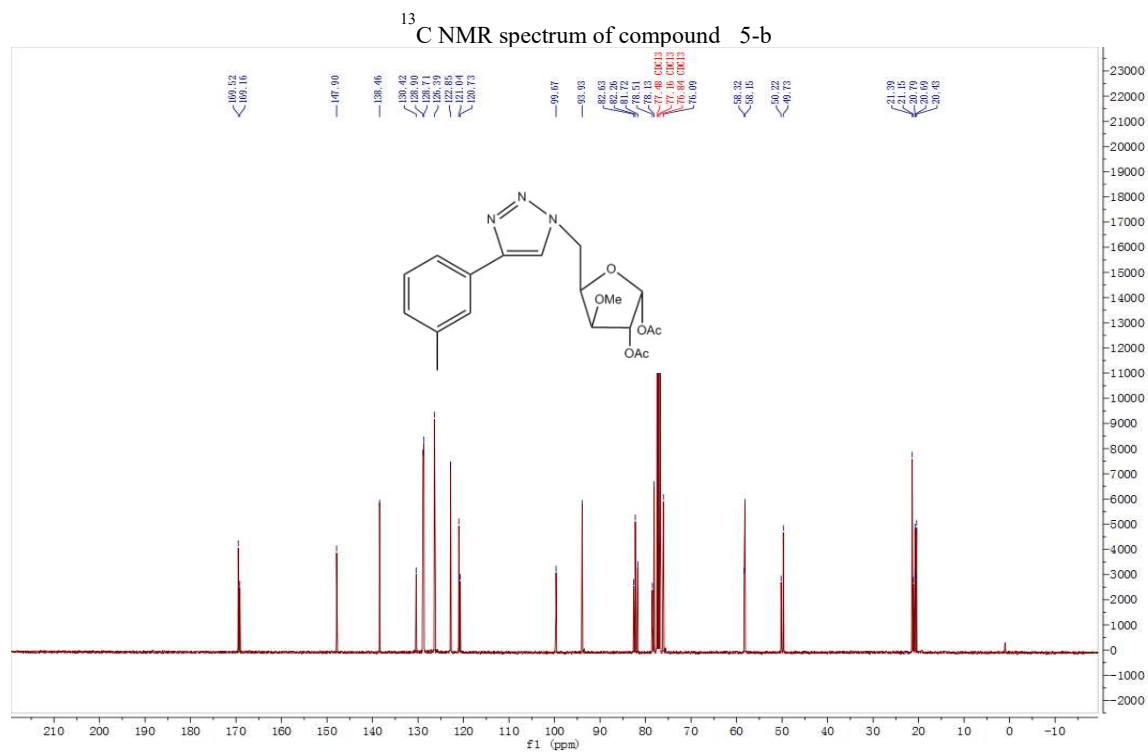
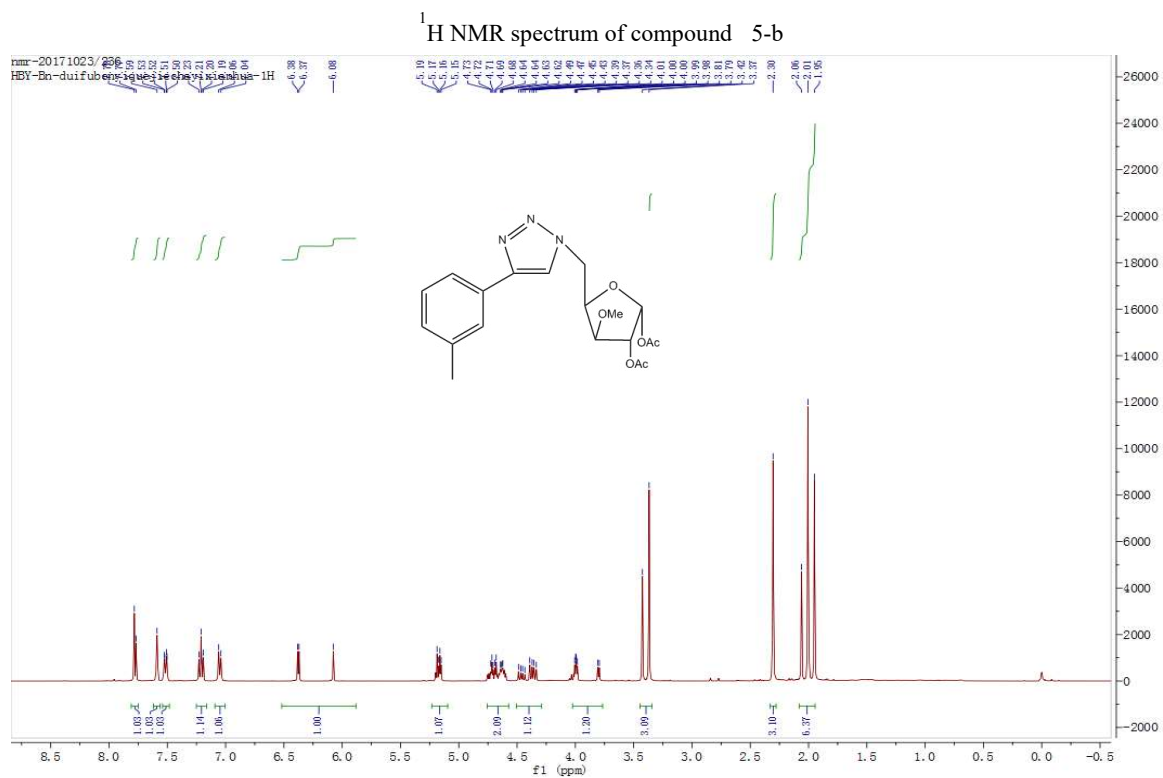


¹³C NMR spectrum of compound 5-a

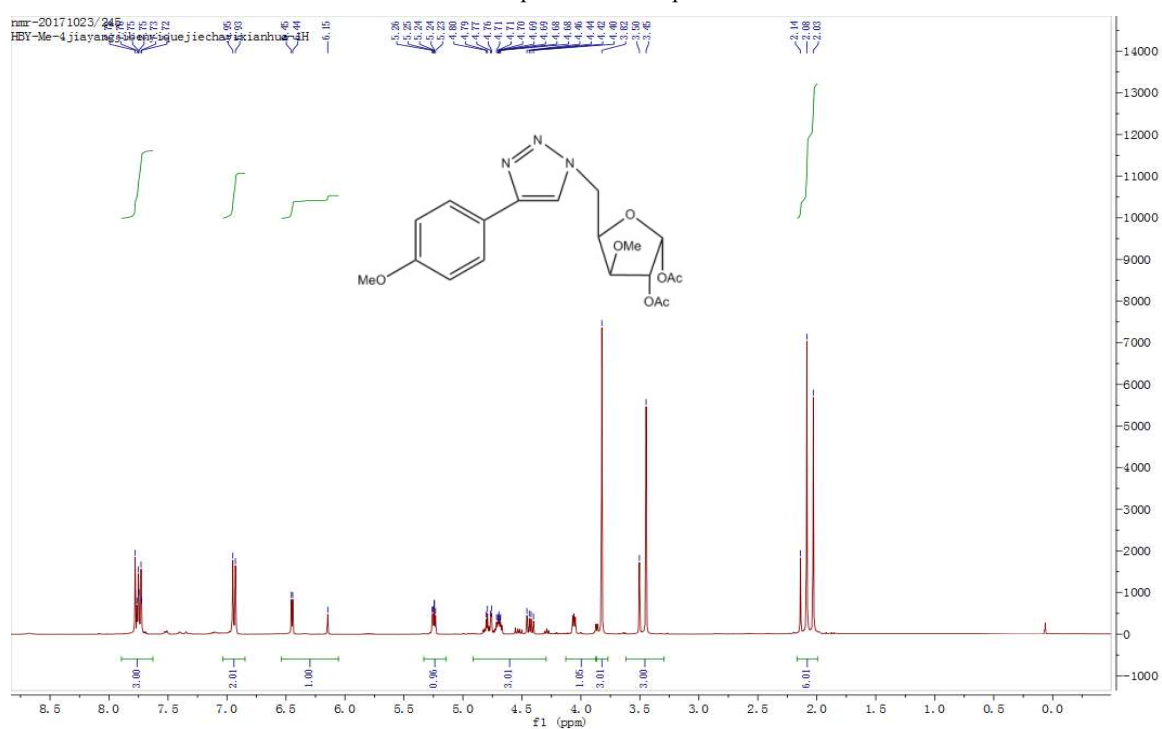


HRMS spectrum of compound 5-a

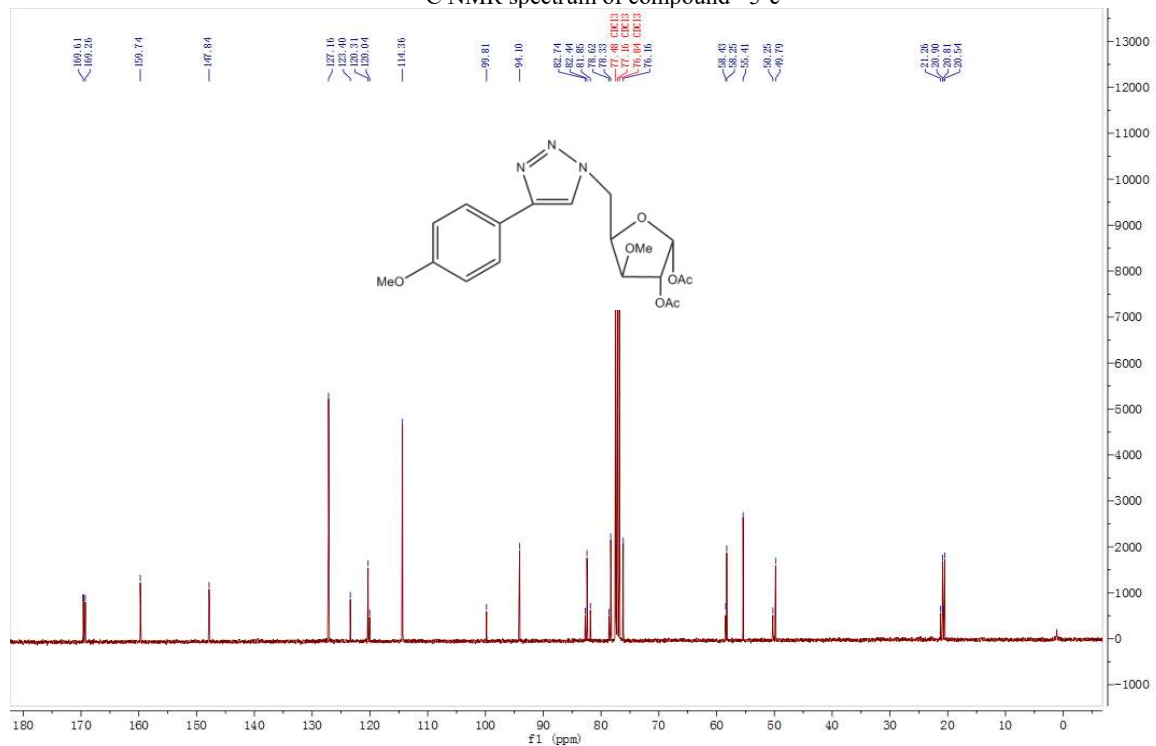




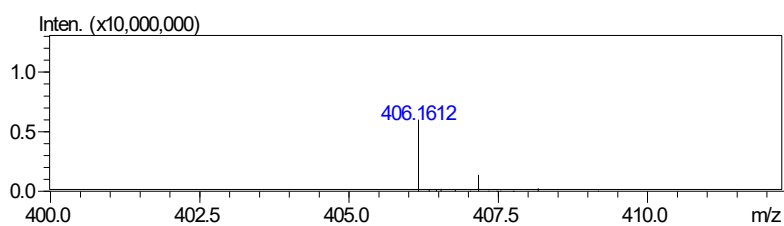
¹H NMR spectrum of compound 5-c



¹³C NMR spectrum of compound 5-c



HRMS spectrum of compound 5-c



nmr-20171023/228
HYB20170930-Me-ds-Subenrique-jac-hayixianhu-1H

Chemical structure of compound 10b: CCOC1C(OC(=O)C)OC(CN2C=NC(c3ccc(F)cc3)=C2)O1

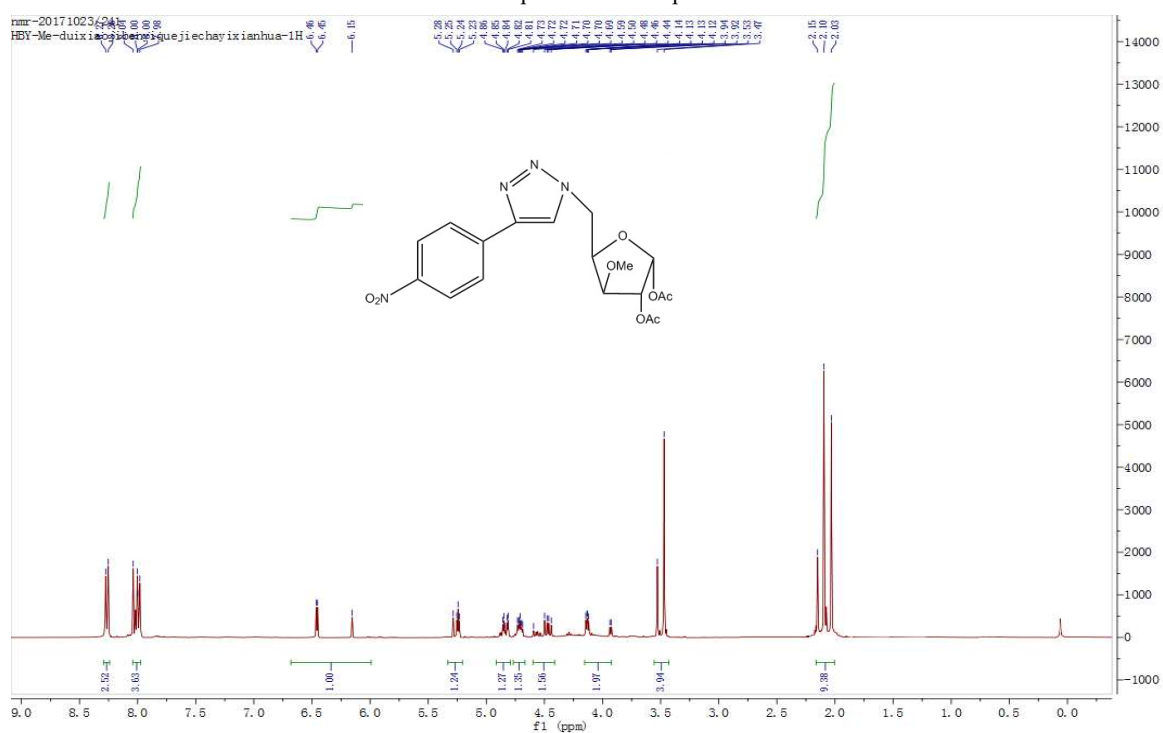
Integration values (from left to right): 3.06, 2.12, 1.00, 1.00, 2.09, 1.03, 1.21, 3.01, 6.05.

Chemical structure of compound 5-d is shown above the spectrum. The structure is a 4-fluorophenyl-1H-imidazole-2-ylmethyl 2,3-diacetate-4-methoxy-β-D-ribofuranoside. The spectrum displays peaks corresponding to the structure, with chemical shifts (ppm) labeled above the peaks: 174.03, 169.98, 162.18, 132.41, 130.83, 128.53, 115.84, 115.62, 99.66, 98.03, 82.05, 82.03, 82.01, 81.99, 81.97, 81.95, 81.93, 81.91, 81.89, 81.87, 81.85, 81.83, 81.81, 81.79, 81.77, 81.75, 81.73, 81.71, 81.69, 81.67, 81.65, 81.63, 81.61, 81.59, 81.57, 81.55, 81.53, 81.51, 81.49, 81.47, 81.45, 81.43, 81.41, 81.39, 81.37, 81.35, 81.33, 81.31, 81.29, 81.27, 81.25, 81.23, 81.21, 81.19, 81.17, 81.15, 81.13, 81.11, 81.09, 81.07, 81.05, 81.03, 81.01, 80.99, 80.97, 80.95, 80.93, 80.91, 80.89, 80.87, 80.85, 80.83, 80.81, 80.79, 80.77, 80.75, 80.73, 80.71, 80.69, 80.67, 80.65, 80.63, 80.61, 80.59, 80.57, 80.55, 80.53, 80.51, 80.49, 80.47, 80.45, 80.43, 80.41, 80.39, 80.37, 80.35, 80.33, 80.31, 80.29, 80.27, 80.25, 80.23, 80.21, 80.19, 80.17, 80.15, 80.13, 80.11, 80.09, 80.07, 80.05, 80.03, 80.01, 79.99, 79.97, 79.95, 79.93, 79.91, 79.89, 79.87, 79.85, 79.83, 79.81, 79.79, 79.77, 79.75, 79.73, 79.71, 79.69, 79.67, 79.65, 79.63, 79.61, 79.59, 79.57, 79.55, 79.53, 79.51, 79.49, 79.47, 79.45, 79.43, 79.41, 79.39, 79.37, 79.35, 79.33, 79.31, 79.29, 79.27, 79.25, 79.23, 79.21, 79.19, 79.17, 79.15, 79.13, 79.11, 79.09, 79.07, 79.05, 79.03, 79.01, 78.99, 78.97, 78.95, 78.93, 78.91, 78.89, 78.87, 78.85, 78.83, 78.81, 78.79, 78.77, 78.75, 78.73, 78.71, 78.69, 78.67, 78.65, 78.63, 78.61, 78.59, 78.57, 78.55, 78.53, 78.51, 78.49, 78.47, 78.45, 78.43, 78.41, 78.39, 78.37, 78.35, 78.33, 78.31, 78.29, 78.27, 78.25, 78.23, 78.21, 78.19, 78.17, 78.15, 78.13, 78.11, 78.09, 78.07, 78.05, 78.03, 78.01, 77.99, 77.97, 77.95, 77.93, 77.91, 77.89, 77.87, 77.85, 77.83, 77.81, 77.79, 77.77, 77.75, 77.73, 77.71, 77.69, 77.67, 77.65, 77.63, 77.61, 77.59, 77.57, 77.55, 77.53, 77.51, 77.49, 77.47, 77.45, 77.43, 77.41, 77.39, 77.37, 77.35, 77.33, 77.31, 77.29, 77.27, 77.25, 77.23, 77.21, 77.19, 77.17, 77.15, 77.13, 77.11, 77.09, 77.07, 77.05, 77.03, 77.01, 76.99, 76.97, 76.95, 76.93, 76.91, 76.89, 76.87, 76.85, 76.83, 76.81, 76.79, 76.77, 76.75, 76.73, 76.71, 76.69, 76.67, 76.65, 76.63, 76.61, 76.59, 76.57, 76.55, 76.53, 76.51, 76.49, 76.47, 76.45, 76.43, 76.41, 76.39, 76.37, 76.35, 76.33, 76.31, 76.29, 76.27, 76.25, 76.23, 76.21, 76.19, 76.17, 76.15, 76.13, 76.11, 76.09, 76.07, 76.05, 76.03, 76.01, 75.99, 75.97, 75.95, 75.93, 75.91, 75.89, 75.87, 75.85, 75.83, 75.81, 75.79, 75.77, 75.75, 75.73, 75.71, 75.69, 75.67, 75.65, 75.63, 75.61, 75.59, 75.57, 75.55, 75.53, 75.51, 75.49, 75.47, 75.45, 75.43, 75.41, 75.39, 75.37, 75.35, 75.33, 75.31, 75.29, 75.27, 75.25, 75.23, 75.21, 75.19, 75.17, 75.15, 75.13, 75.11, 75.09, 75.07, 75.05, 75.03, 75.01, 74.99, 74.97, 74.95, 74.93, 74.91, 74.89, 74.87, 74.85, 74.83, 74.81, 74.79, 74.77, 74.75, 74.73, 74.71, 74.69, 74.67, 74.65, 74.63, 74.61, 74.59, 74.57, 74.55, 74.53, 74.51, 74.49, 74.47, 74.45, 74.43, 74.41, 74.39, 74.37, 74.35, 74.33, 74.31, 74.29, 74.27, 74.25, 74.23, 74.21, 74.19, 74.17, 74.15, 74.13, 74.11, 74.09, 74.07, 74.05, 74.03, 74.01, 73.99, 73.97, 73.95, 73.93, 73.91, 73.89, 73.87, 73.85, 73.83, 73.81, 73.79, 73.77, 73.75, 73.73, 73.71, 73.69, 73.67, 73.65, 73.63, 73.61, 73.59, 73.57, 73.55, 73.53, 73.51, 73.49, 73.47, 73.45, 73.43, 73.41, 73.39, 73.37, 73.35, 73.33, 73.31, 73.29, 73.27, 73.25, 73.23, 73.21, 73.19, 73.17, 73.15, 73.13, 73.11, 73.09, 73.07, 73.05, 73.03, 73.01, 72.99, 72.97, 72.95, 72.93, 72.91, 72.89, 72.87, 72.85, 72.83, 72.81, 72.79, 72.77, 72.75, 72.73, 72.71, 72.69, 72.67, 72.65, 72.63, 72.61, 72.59, 72.57, 72.55, 72.53, 72.51, 72.49, 72.47, 72.45, 72.43, 72.41, 72.39, 72.37, 72.35, 72.33, 72.31, 72.29, 72.27, 72.25, 72.23, 72.21, 72.19, 72.17, 72.15, 72.13, 72.11, 72.09, 72.07, 72.05, 72.03, 72.01, 71.99, 71.97, 71.95, 71.93, 71.91, 71.89, 71.87, 71.85, 71.83, 71.81, 71.79, 71.77, 71.75, 71.73, 71.71, 71.69, 71.67, 71.65, 71.63, 71.61, 71.59, 71.57, 71.55, 71.53, 71.51, 71.49, 71.47, 71.45, 71.43, 71.41, 71.39, 71.37, 71.35, 71.33, 71.31, 71.29, 71.27, 71.25, 71.23, 71.21, 71.19, 71.17, 71.15, 71.13, 71.11, 71.09, 71.07, 71.05, 71.03, 71.01, 70.99, 70.97, 70.95, 70.93, 70.91, 70.89, 70.87, 70.85, 70.83

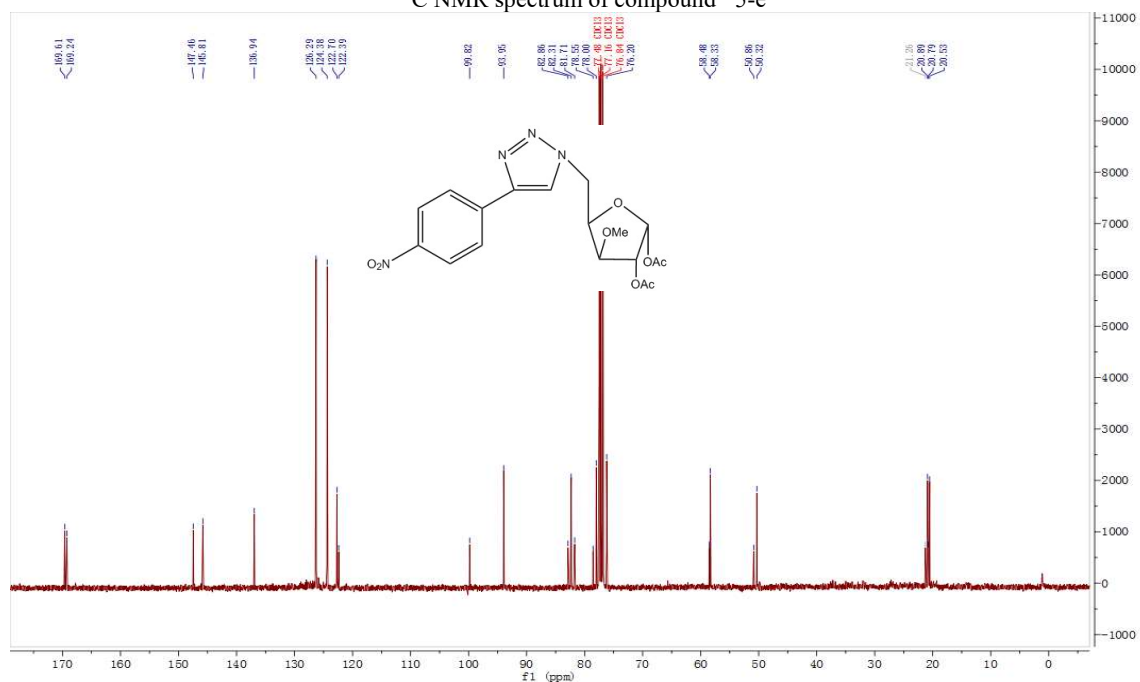
Mass spectrum of compound 10. The x-axis represents the mass-to-charge ratio (m/z) from 390.0 to 400.0. The y-axis represents intensity (Inten. (x1,000,000)) from 0.0 to 7.5. The base peak is at m/z 394.1414.

m/z	Intensity (x1,000,000)
394.1414	~3.0
395.0	~0.5

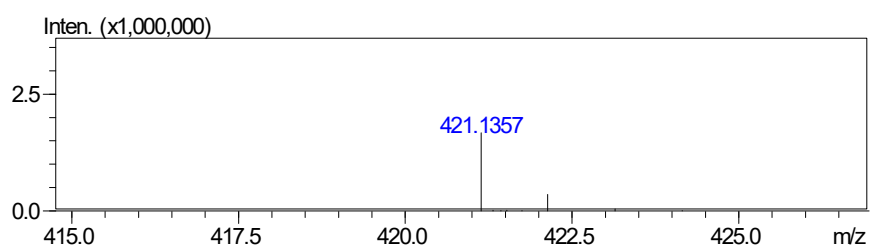
¹H NMR spectrum of compound 5-e



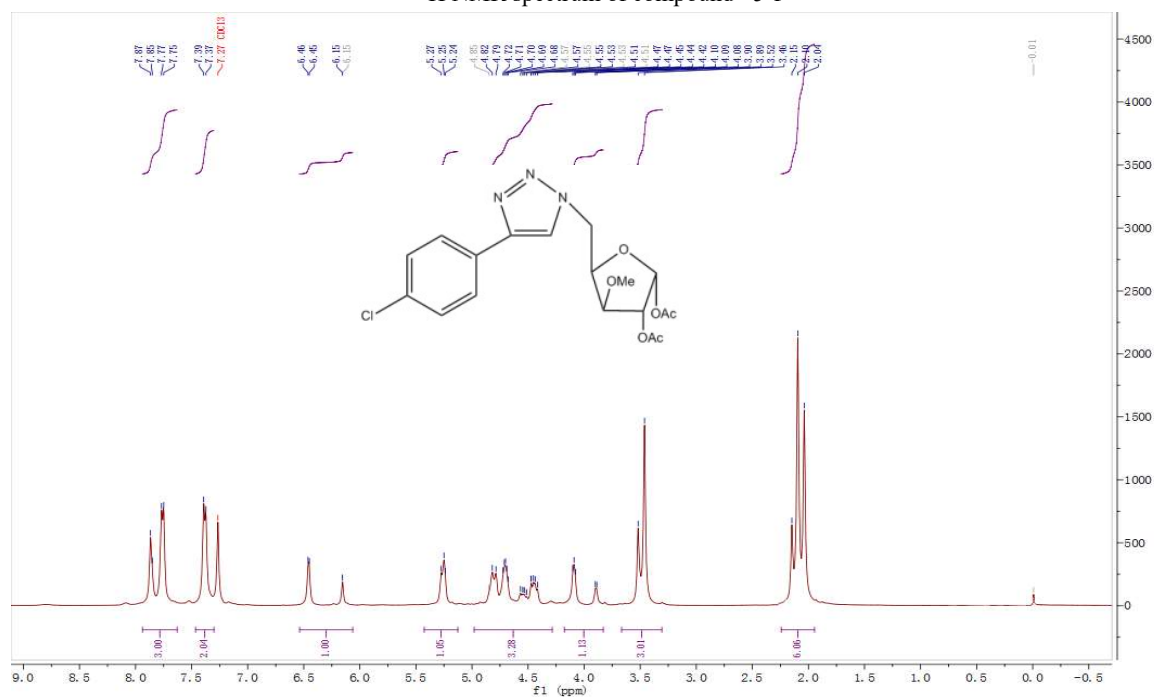
¹³C NMR spectrum of compound 5-e



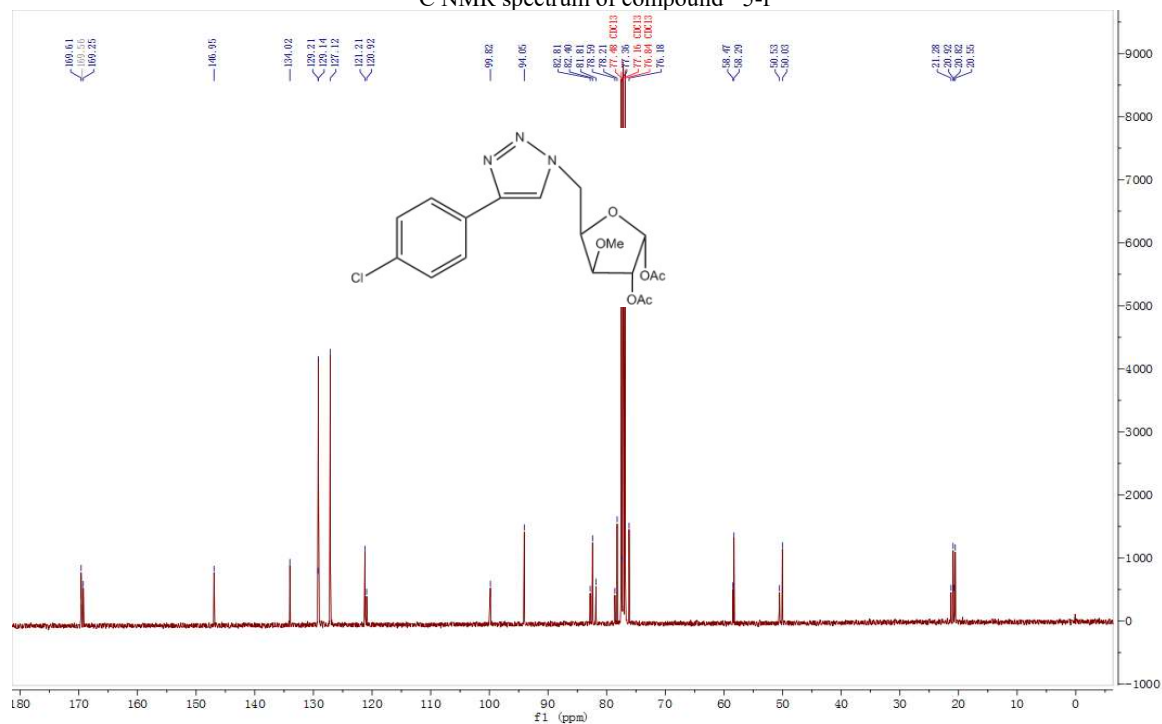
HRMS spectrum of compound 5-e



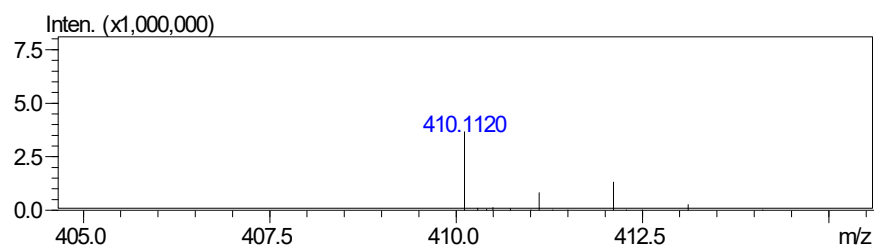
¹H NMR spectrum of compound 5-f

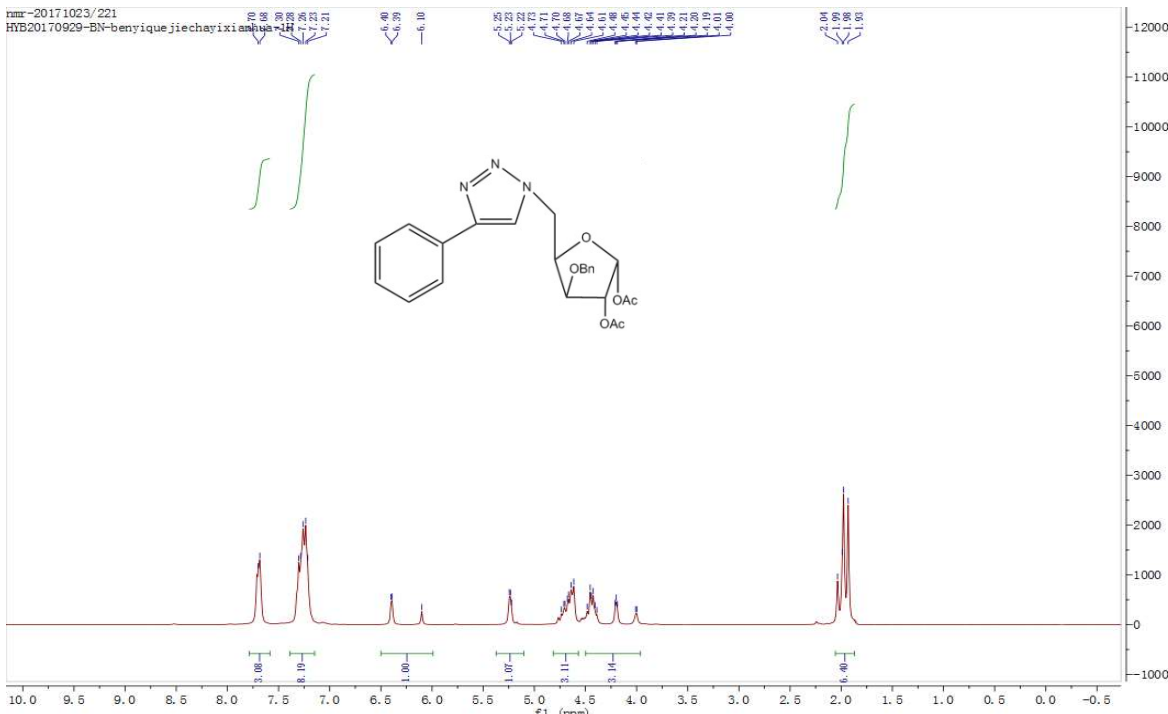


¹³C NMR spectrum of compound 5-f

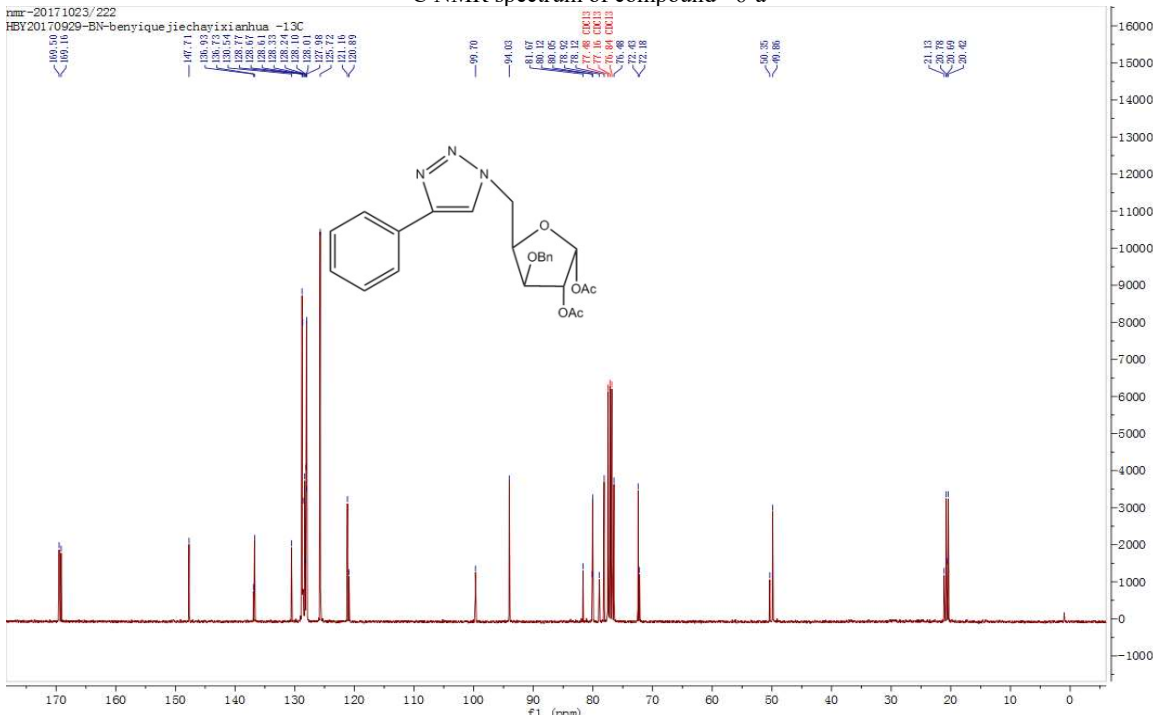


HRMS spectrum of compound 5-f

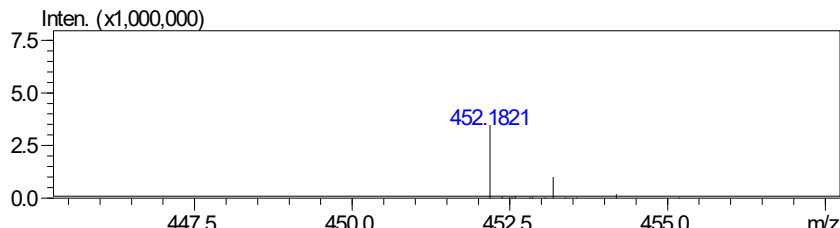


¹H NMR spectrum of compound 6-a

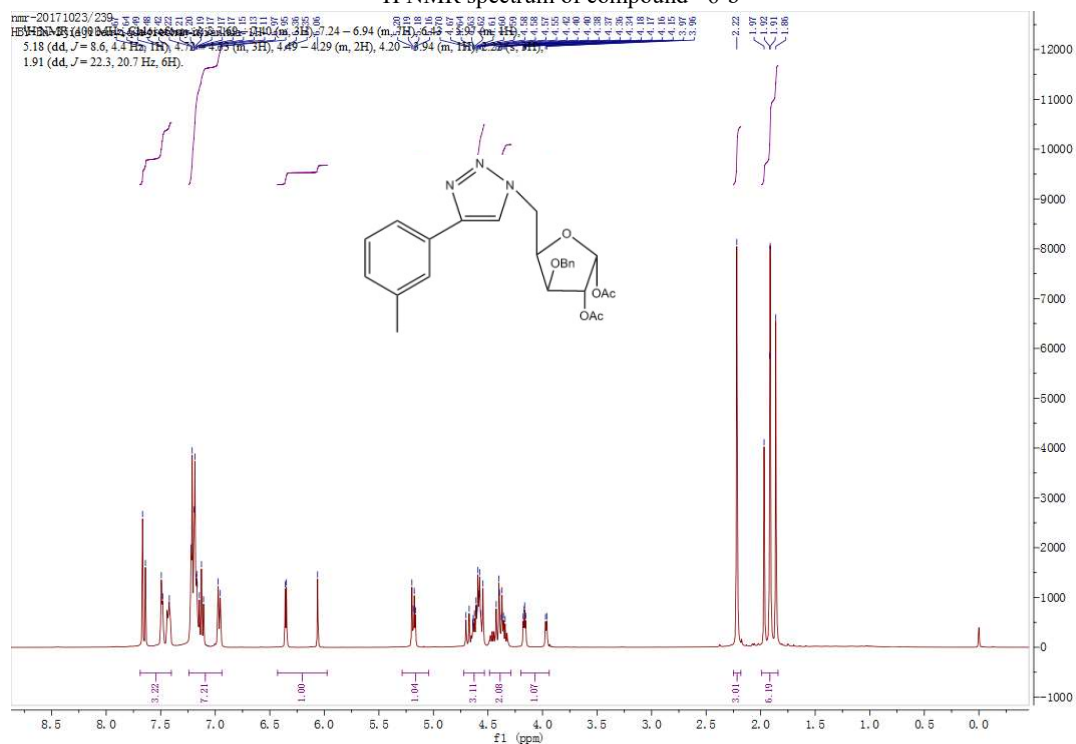
¹³C NMR spectrum of compound 6-a



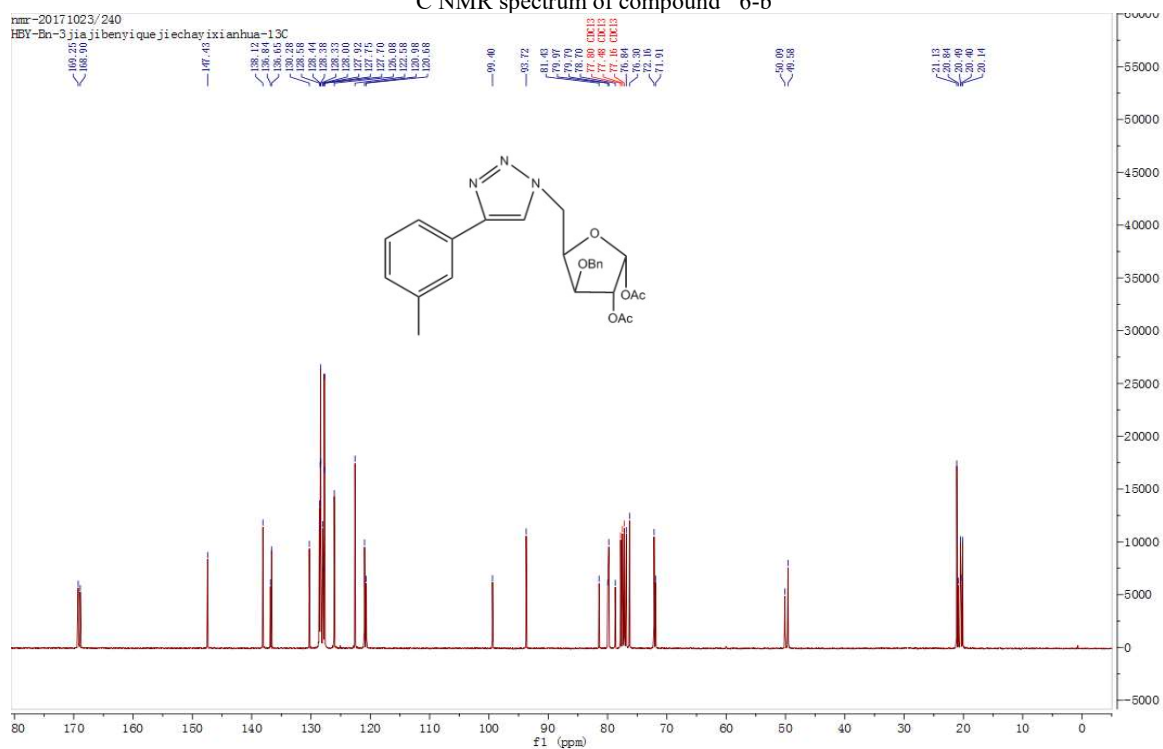
HRMS spectrum of compound 6-a



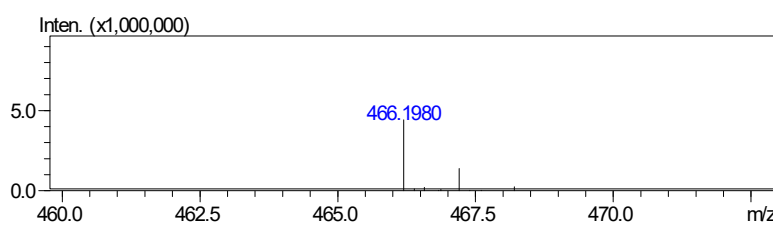
¹H NMR spectrum of compound 6-b

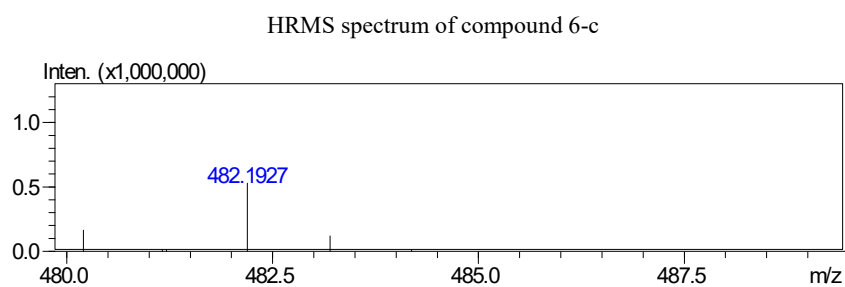
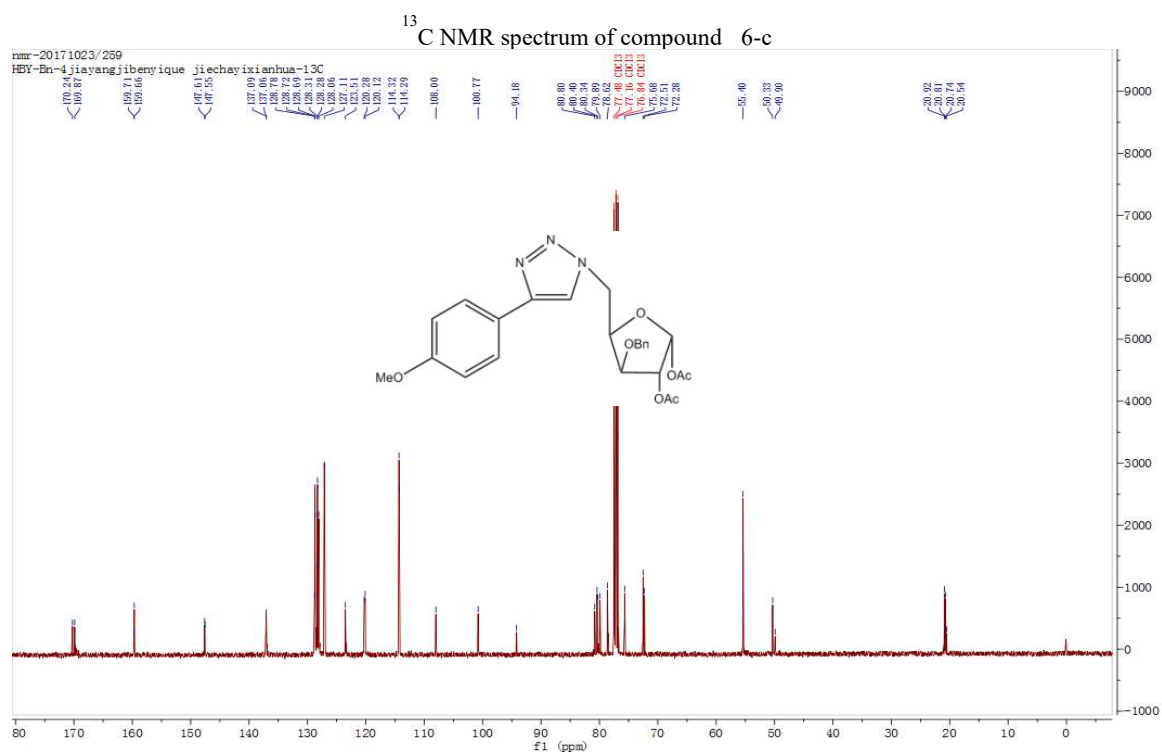
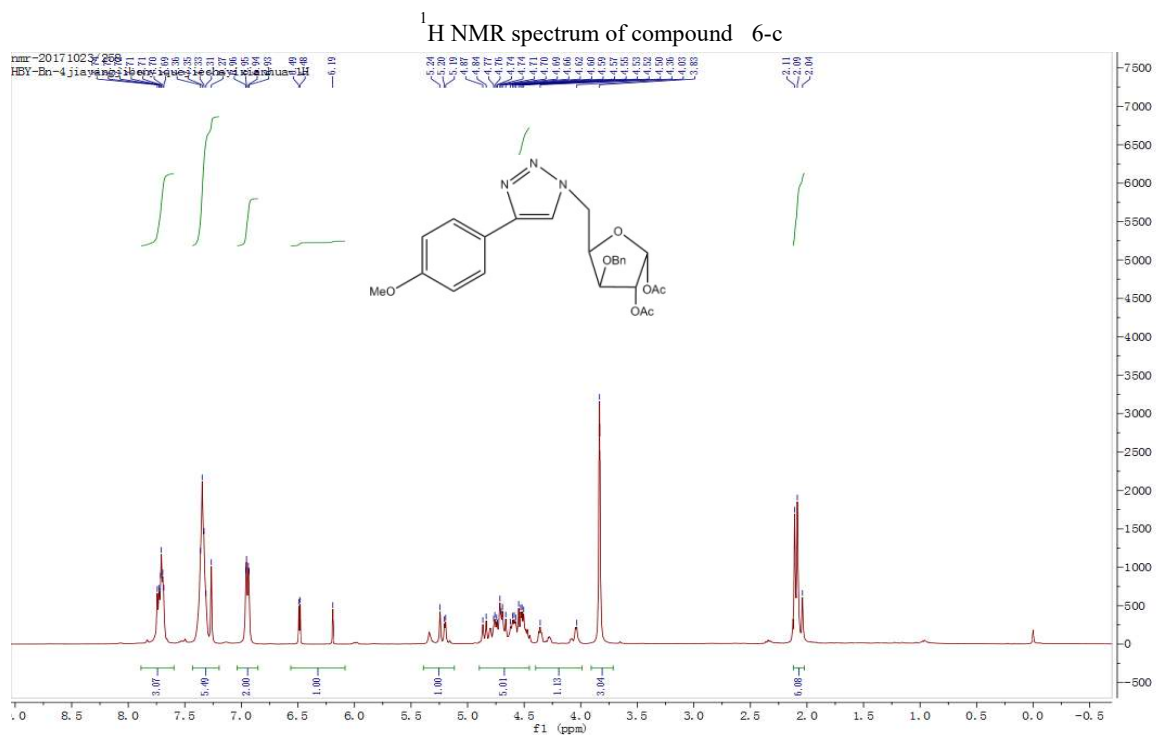


¹³C NMR spectrum of compound 6-b

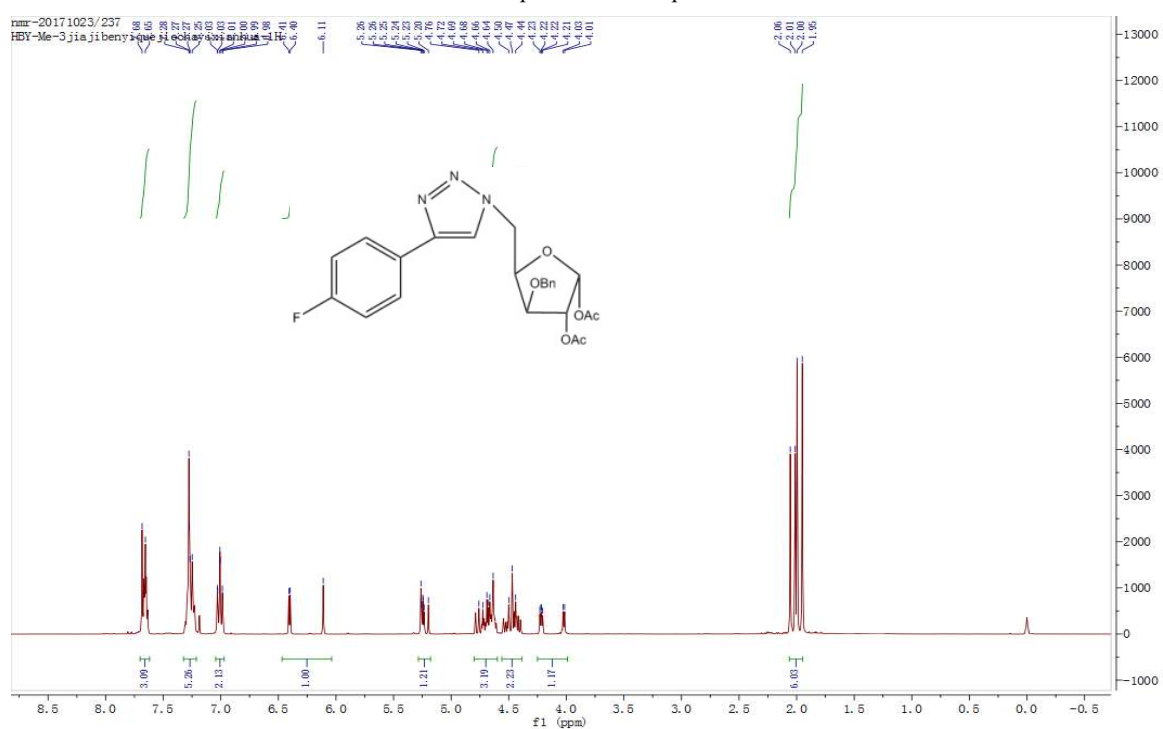


HRMS spectrum of compound 6-b

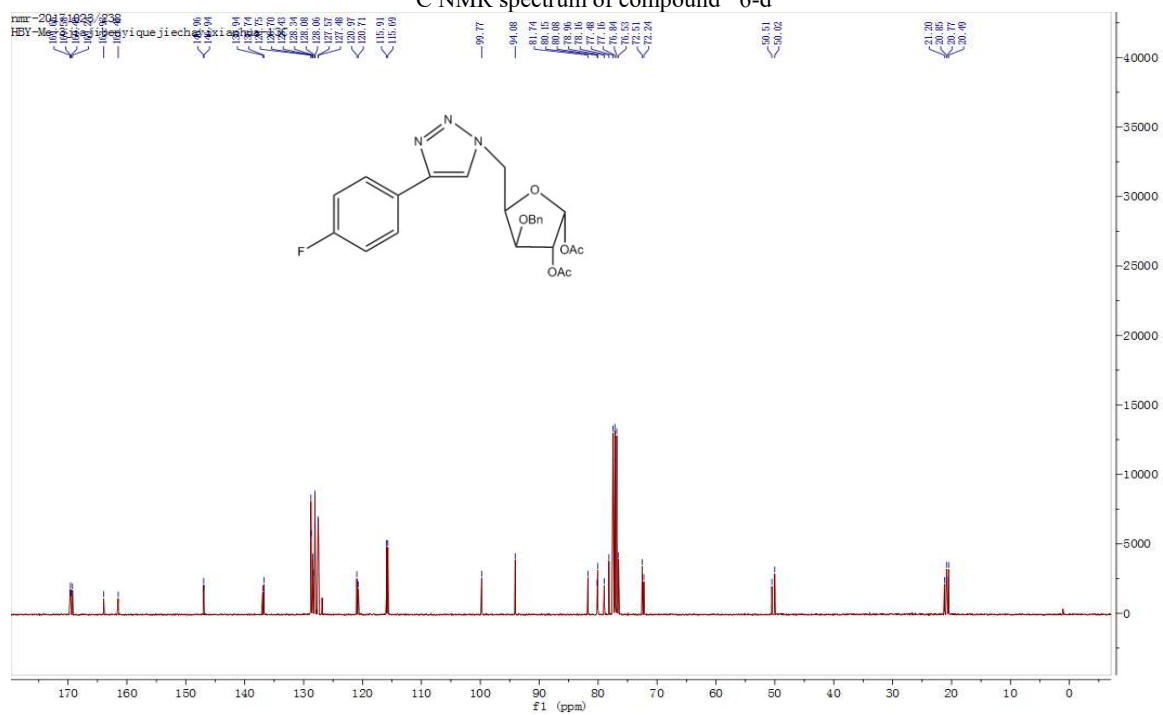




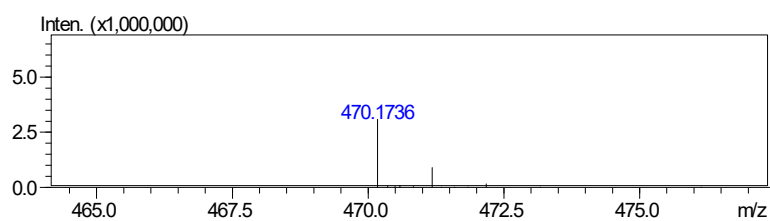
¹H NMR spectrum of compound 6-d



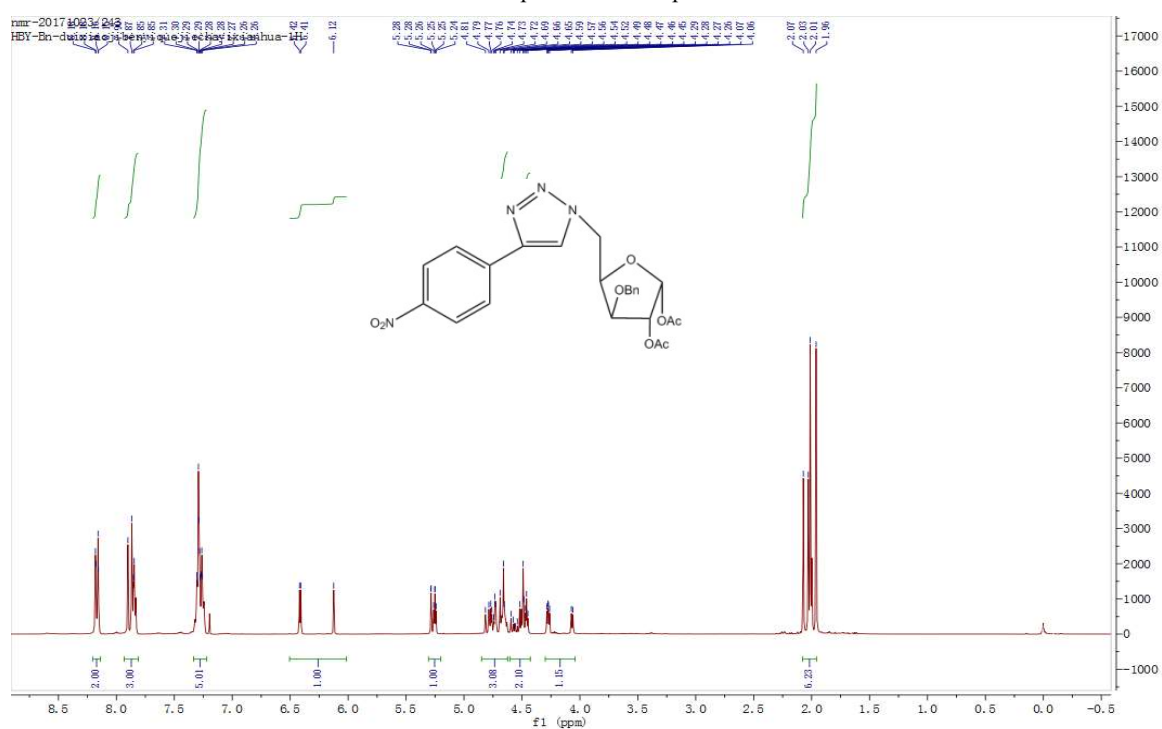
¹³C NMR spectrum of compound 6-d



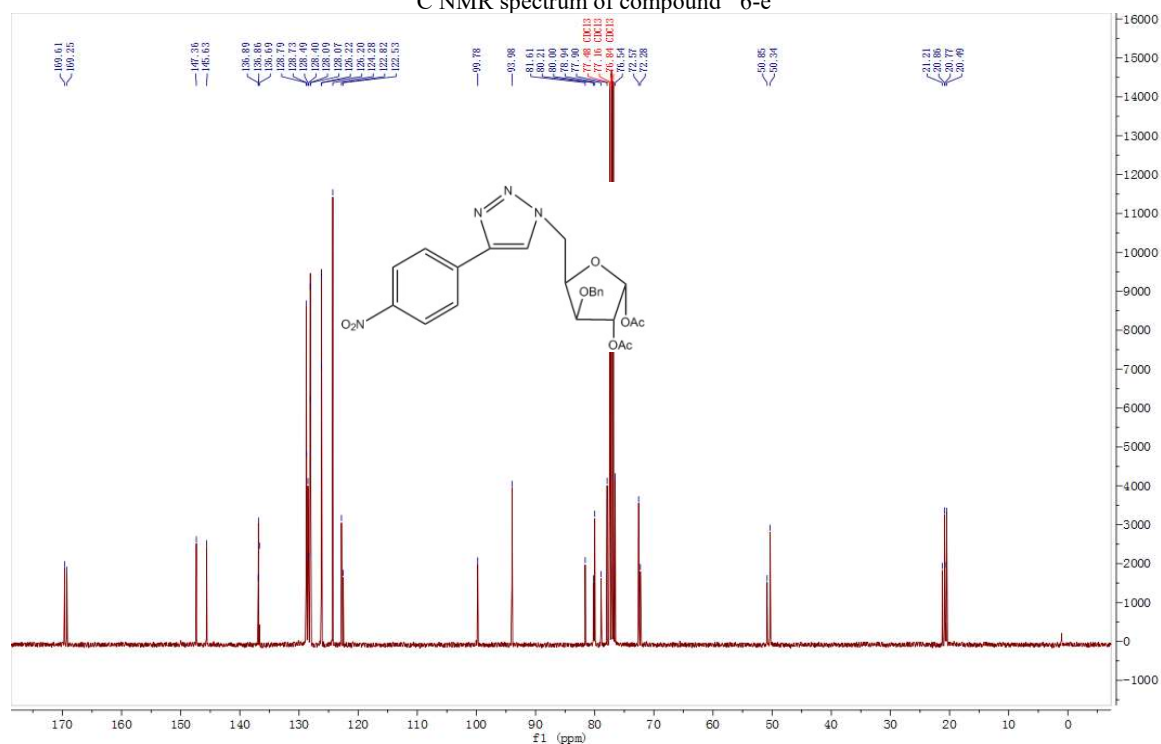
HRMS spectrum of compound 6-d



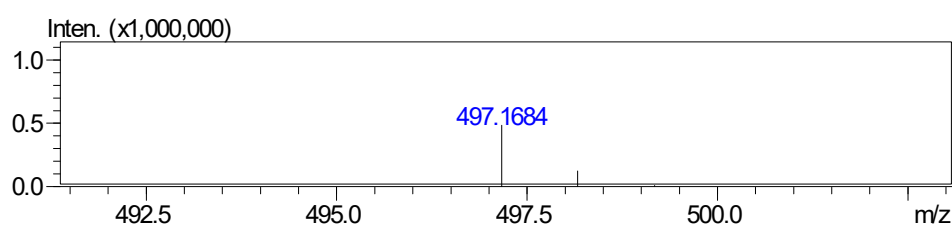
¹H NMR spectrum of compound 6-e



¹³C NMR spectrum of compound 6-e



HRMS spectrum of compound 6-e



nmr-20171023_233
HB20170930-D4-D41-Ven-Hu-jiechayixia-H

Chemical structure of compound 10b: CC(=O)OC[C@H]1O[C@H](Cn2cc(Cc3ccc(Cl)cc3)nn2)[C@@H](OC(=O)C)[C@H](O)[C@H]1O

¹H NMR spectrum (CDCl₃) of compound 10b. The spectrum shows peaks at 7.53 (d, 3.27), 7.47 (d, 7.17), 6.53 (d, 1.00), 6.47 (d, 1.09), 5.33 (m, 3.15), 5.29 (m, 2.02), 5.25 (m, 1.16), 2.07 (s, 6.07), and 2.01 (s, 3.01). The chemical structure of 10b is shown above the spectrum.

C NMR spectrum of compound 6-1

Chemical structure of compound 6-1: CC(=O)OC1C(OC(=O)C)OC(C1)C2=CN=C(C=C2)c3ccc(Cl)cc3

Peak list (ppm):

- 169.49, 169.14
- 149.52, 146.57
- 136.91, 136.71, 136.11, 135.15, 130.15, 129.97, 129.44, 128.37, 128.28, 128.02, 127.92, 126.90, 126.98, 123.75, 120.97
- 99.71, 94.00, 81.05, 80.15, 80.03, 78.92, 78.94, 77.16, 76.84, 76.83, 72.47, 72.20
- 59.46, 49.99
- 21.14, 20.70, 20.43

Mass spectrum of compound 10. The x-axis represents the mass-to-charge ratio (m/z) from 482.5 to 490.0. The y-axis represents the relative intensity in units of $1,000,000$ from 0.0 to 2.5. The base peak is at m/z 486.1437.

m/z	Relative Intensity ($\times 1,000,000$)
486.1437	~2.3
487.1	~0.1
488.1	~0.1
489.1	~0.05