

## Supplementary Material

### **Design, synthesis and biological evaluation of nitrate derivatives of sauropunol A and B as potent vasodilatory agents**

Lu Lu <sup>1</sup>, Xuemin Rao <sup>1</sup>, Rigang Cong <sup>2</sup>, Chenxi Zhang <sup>1</sup>, Zhimei Wang <sup>1</sup>, Jinyi Xu <sup>1</sup>, Genzoh Tanabe <sup>3</sup>, Osamu Muraoka <sup>3</sup>, Xiaoming Wu <sup>1\*</sup> and Weijia Xie <sup>1\*</sup>

<sup>1</sup> State Key Laboratory of Natural Medicines and Department of Medicinal Chemistry, China Pharmaceutical University, 24 Tong Jia Xiang, Nanjing 210009, PR China;

<sup>2</sup> National-certified Enterprise Technology Center; Disha Pharmaceutical Group Co., Ltd;

<sup>3</sup> Faculty of Pharmacy, Kinki University, 3-4-1 Kowakae, Higashi-Osaka, Osaka 577-8502, Japan;

\*Corresponding authors:

\*E-Mail: xmwu@cpu.edu.cn (Xiaoming Wu),

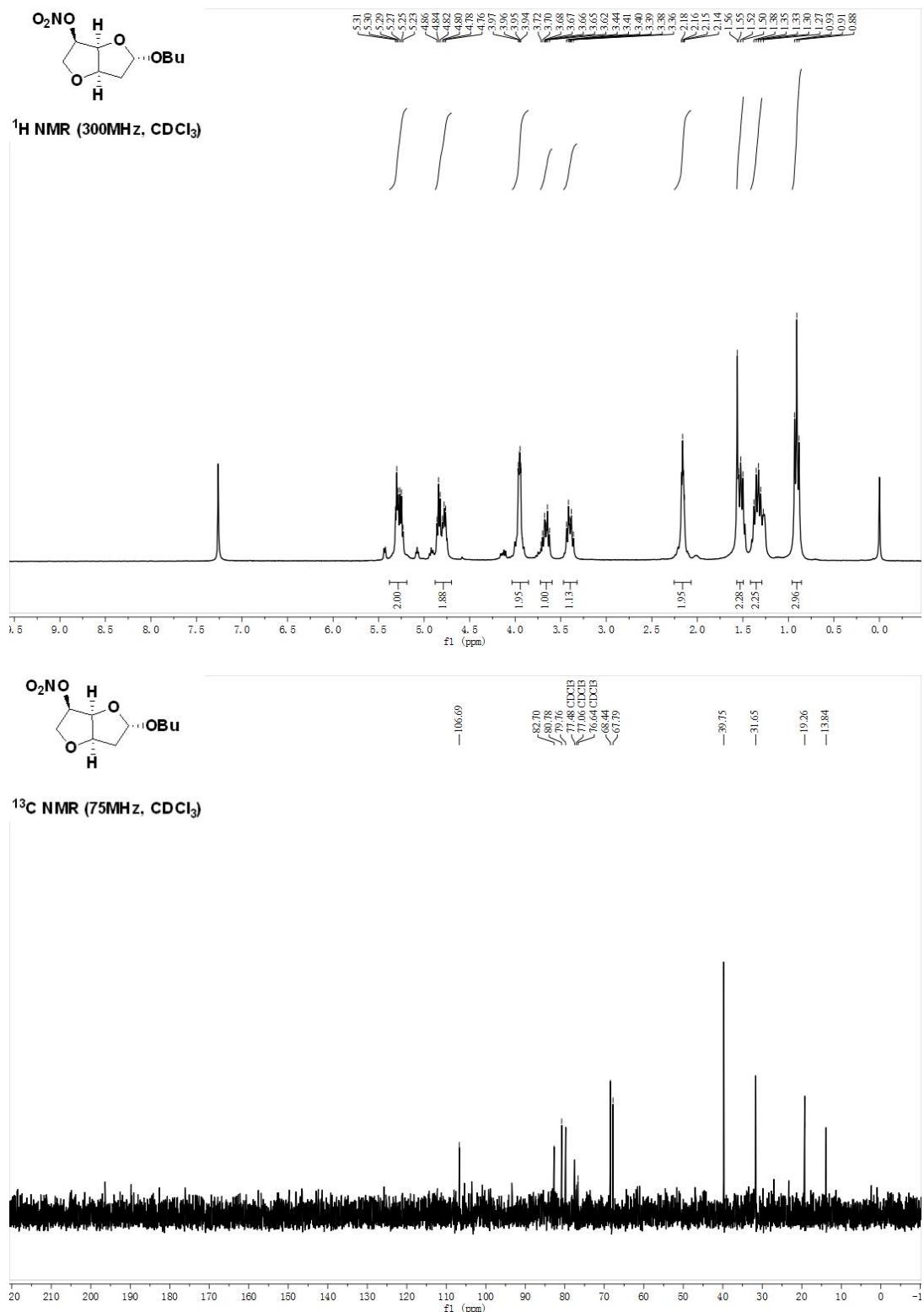
\*E-mail: weijiaxie@cpu.edu.cn (Weijia Xie); Tel.: +86-25-8327-1414 (Weijia Xie).

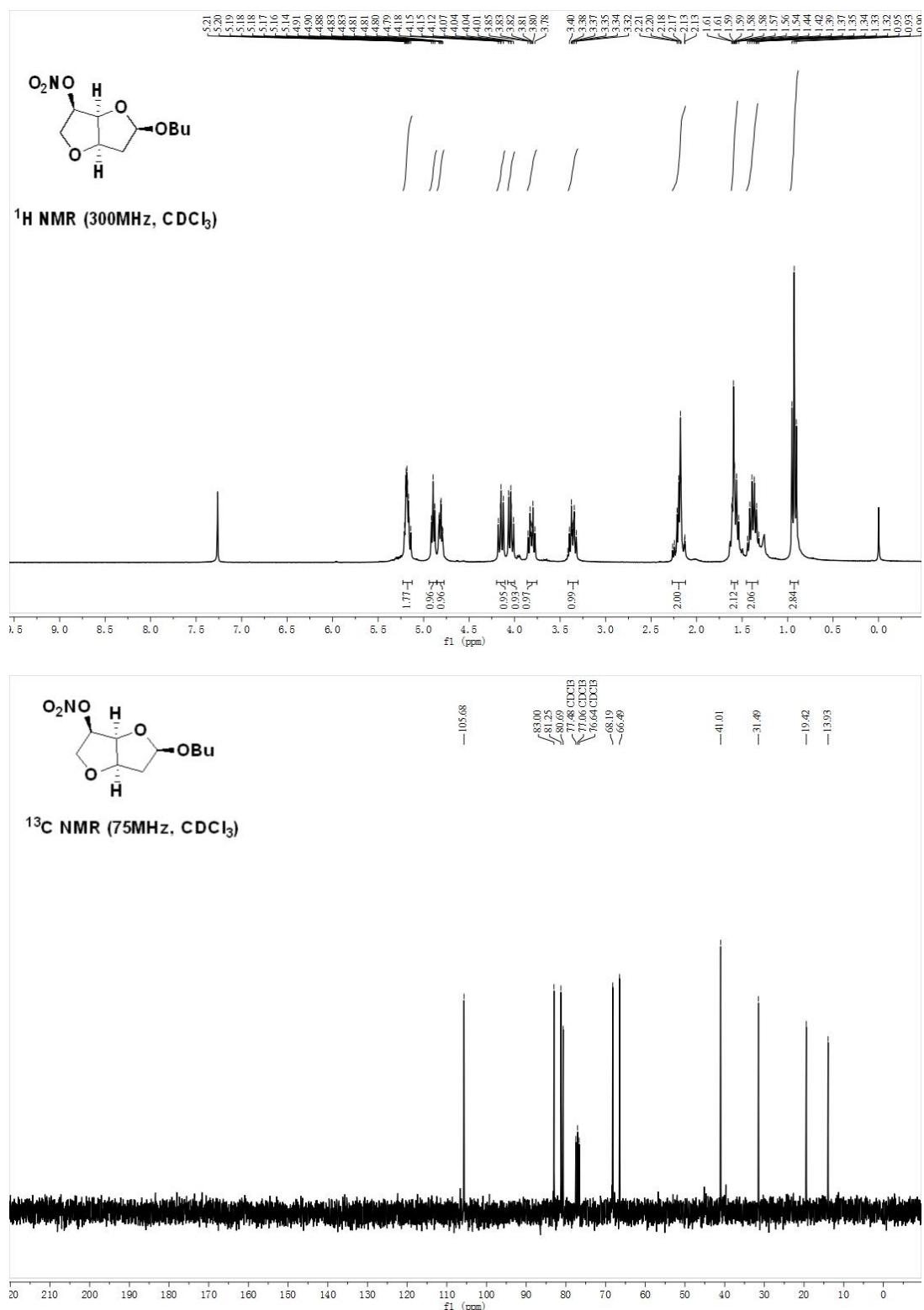
---

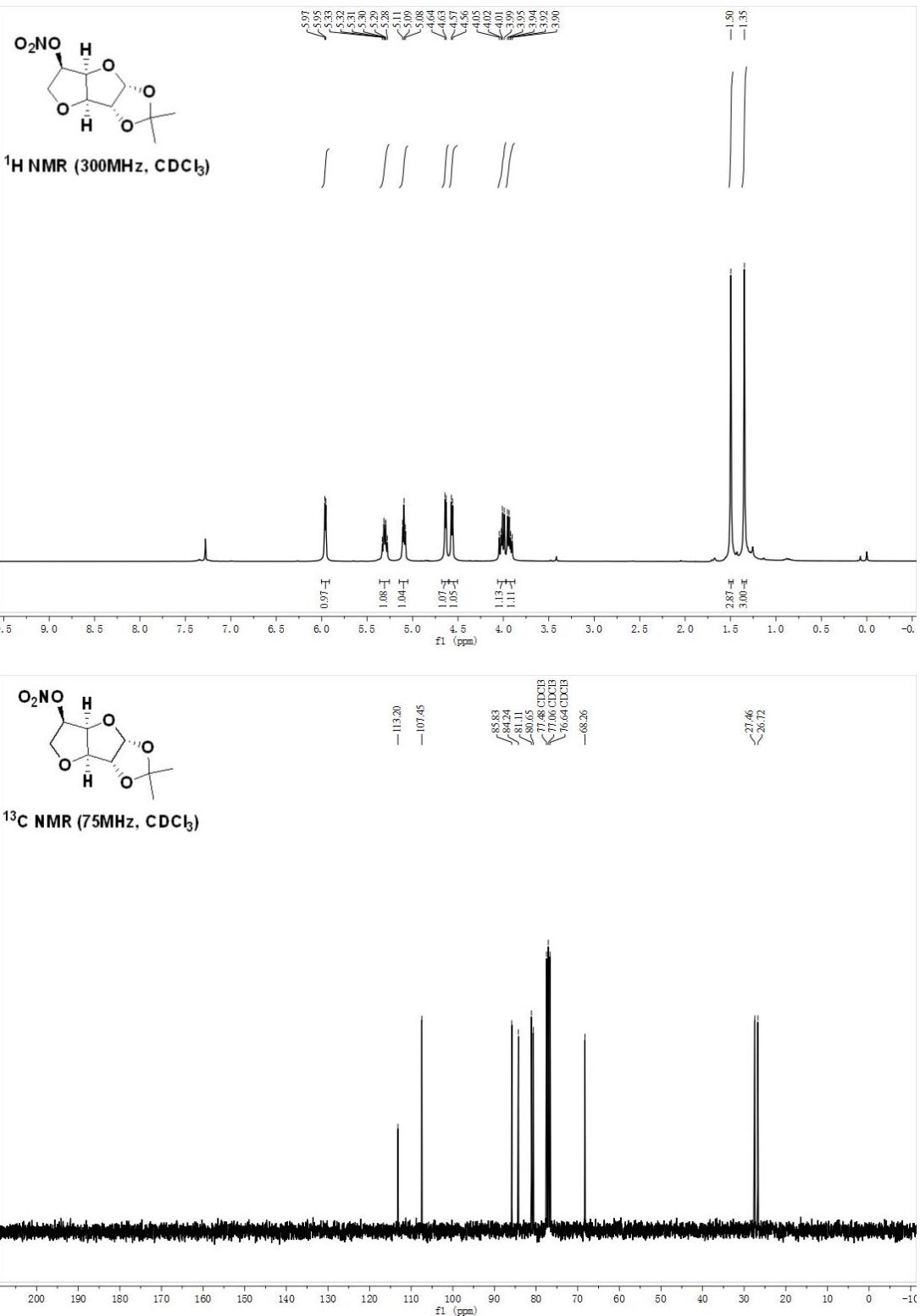
## **Contents**

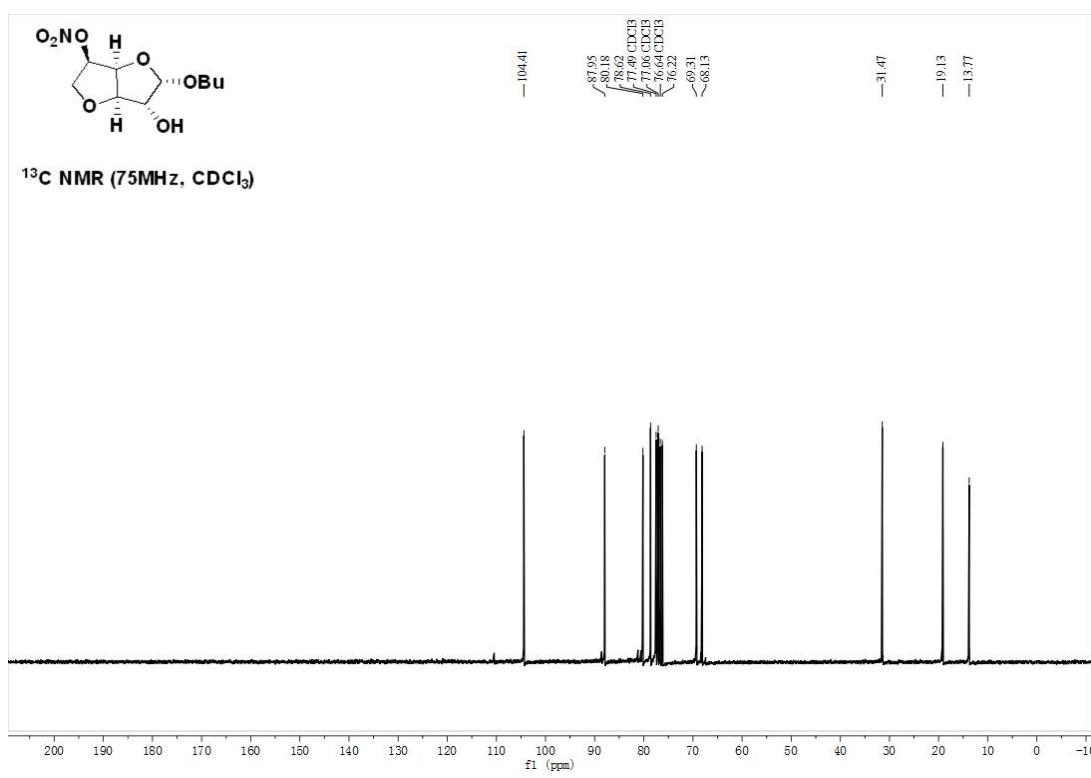
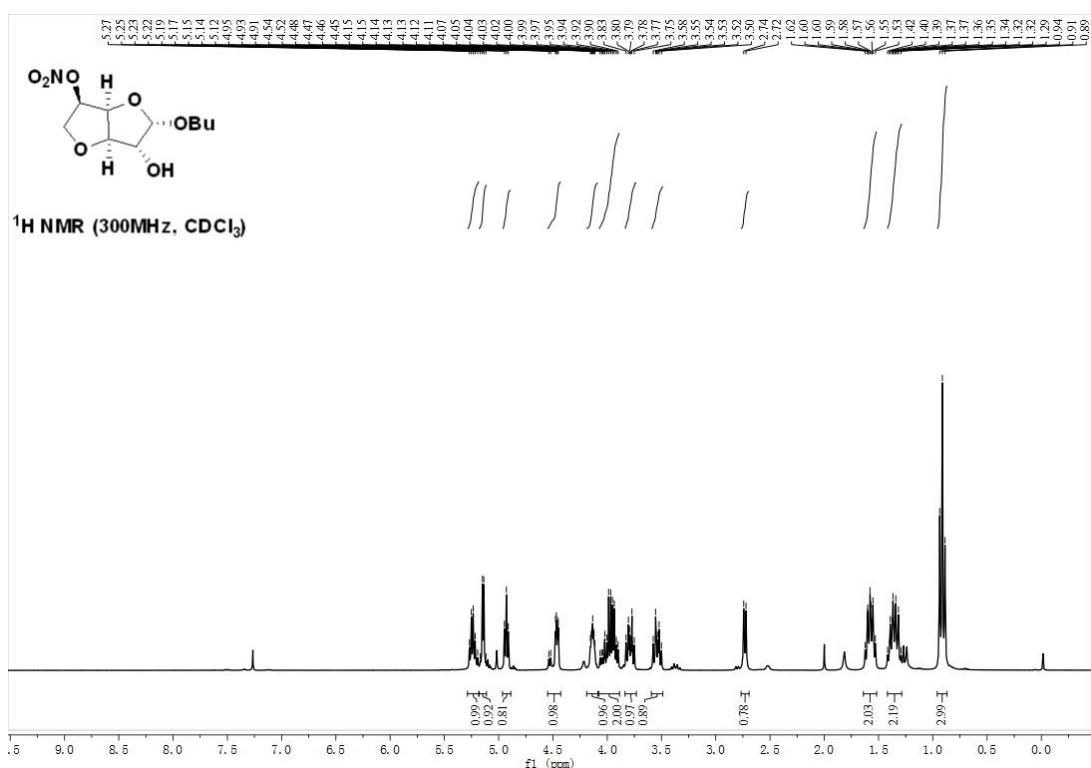
1. Copies of <sup>1</sup> H NMR and <sup>13</sup> C NMR.....	2
2. Copies of IR.....	21
3. The inhibitory effect of nitrates derivatives on the contraction induced by phenylephrine in mesenteric artery rings.....	31
4. The inhibitory effect of nitrates derivatives on the contraction induced by KCl in mesenteric artery rings.....	31

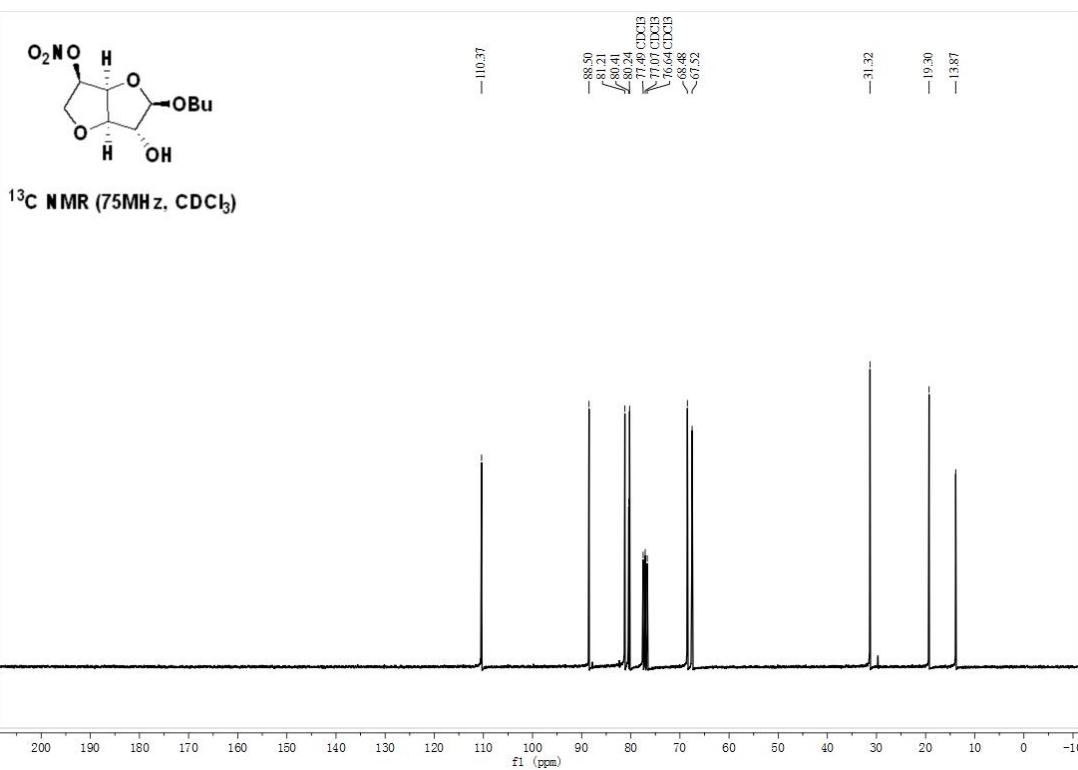
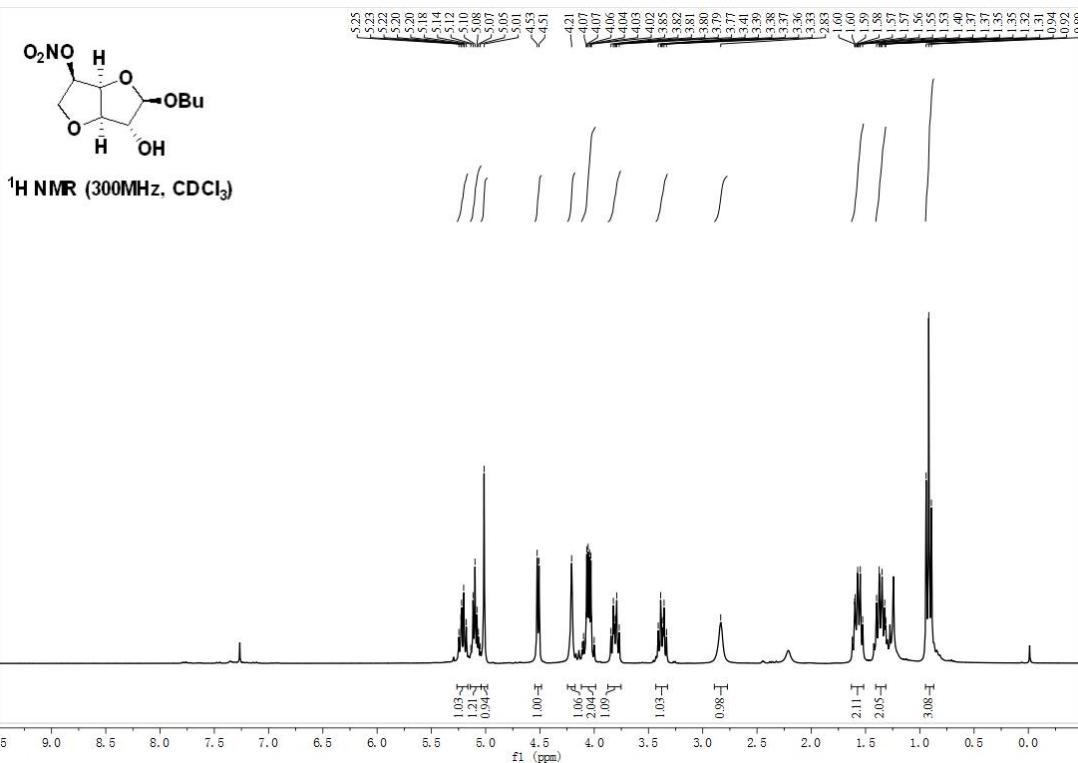
1. Copies of  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR

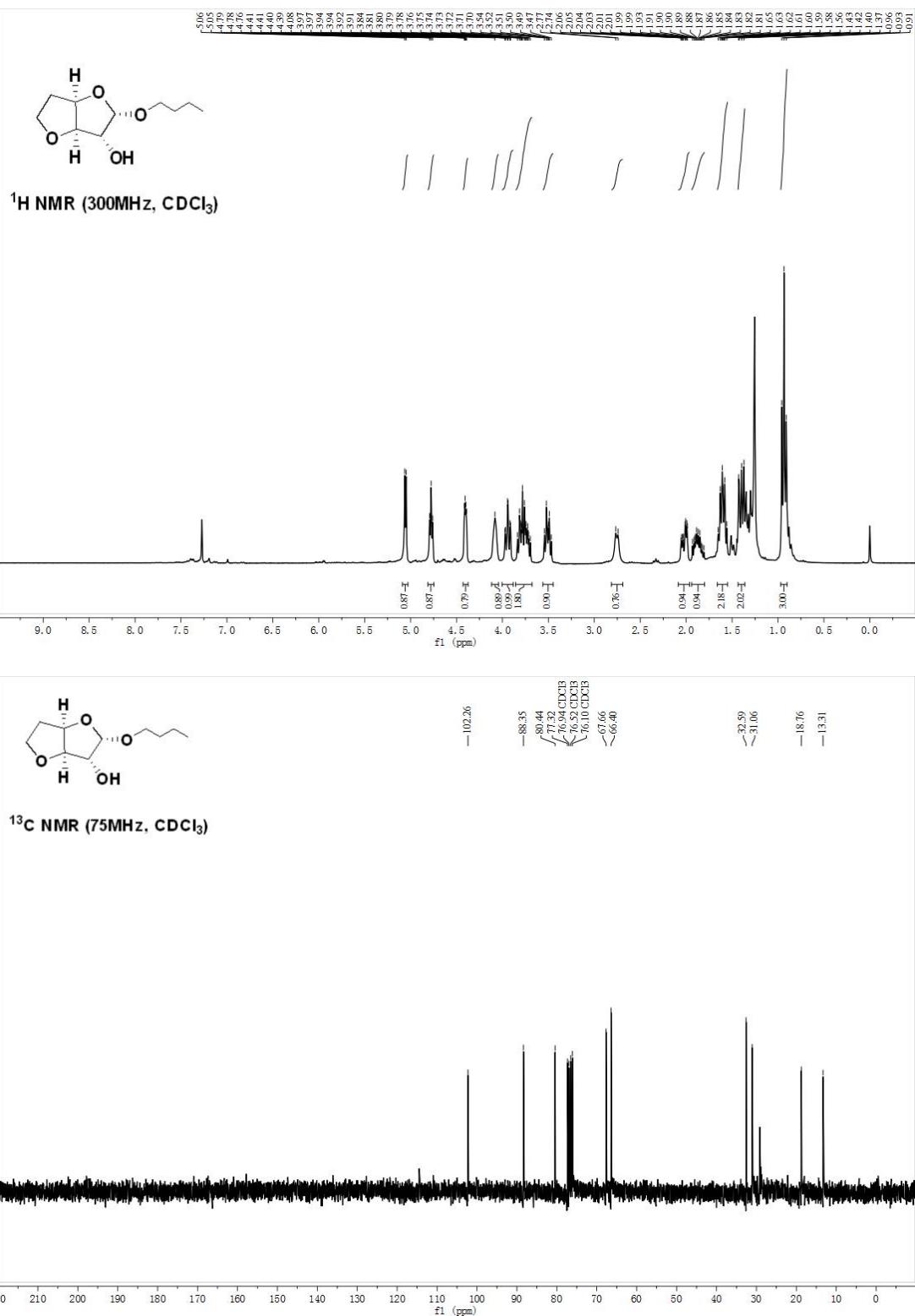


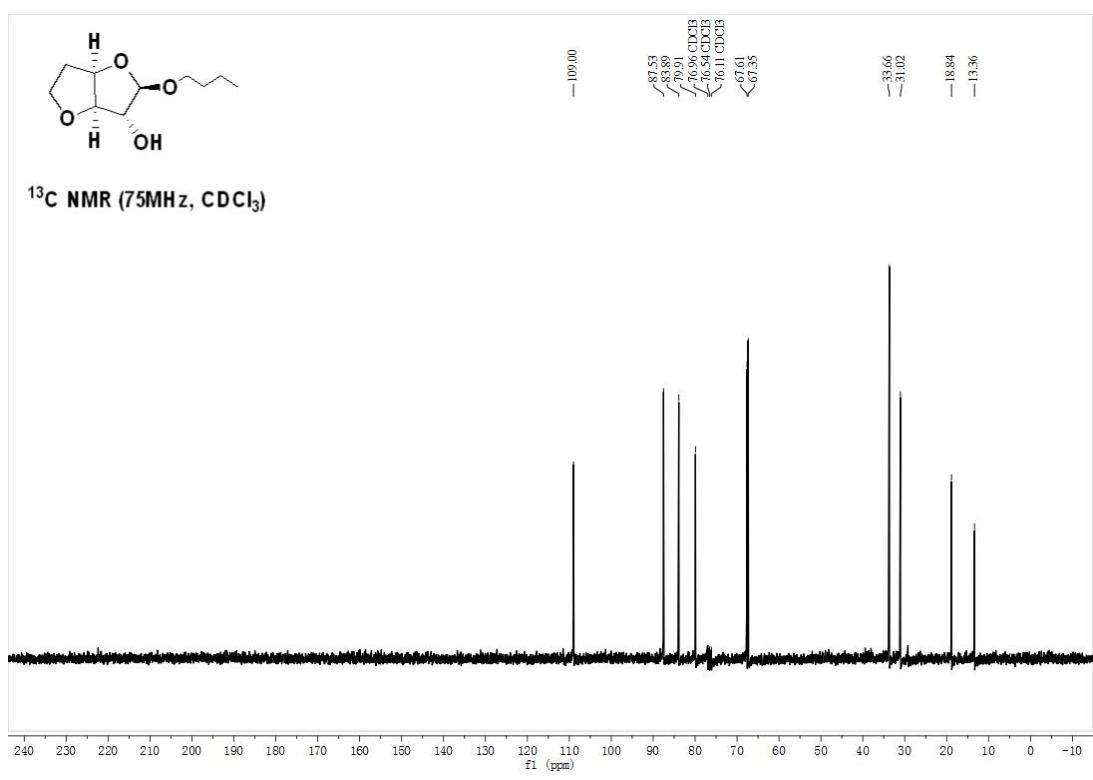
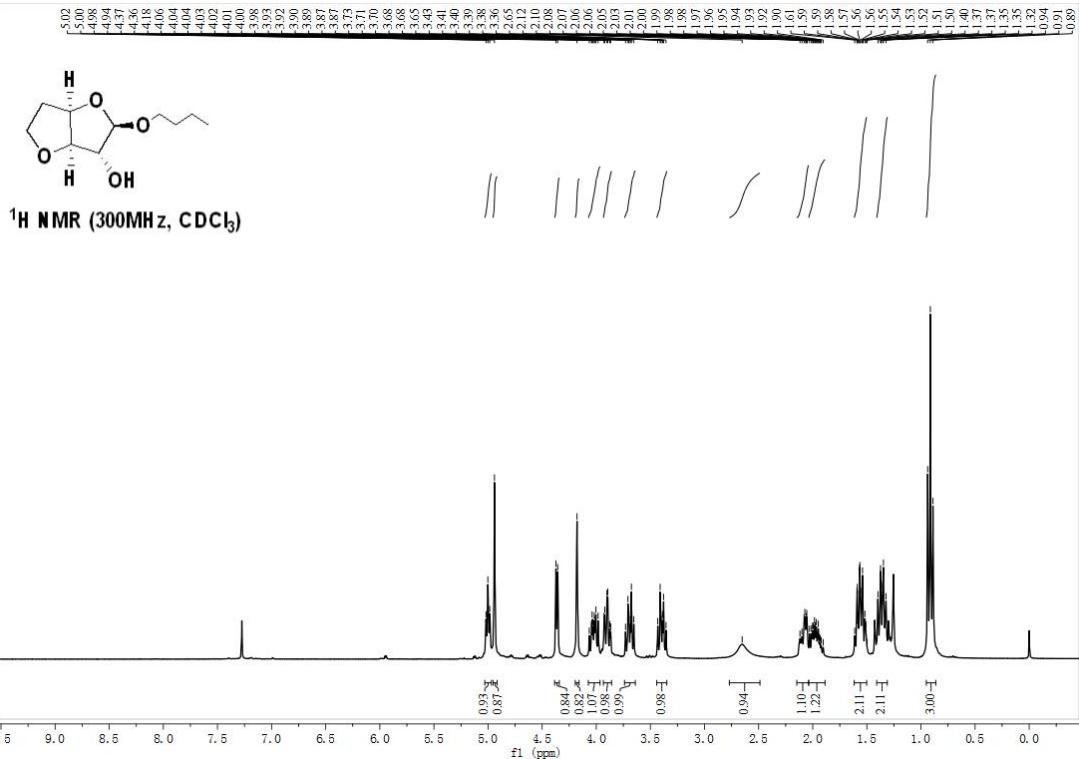




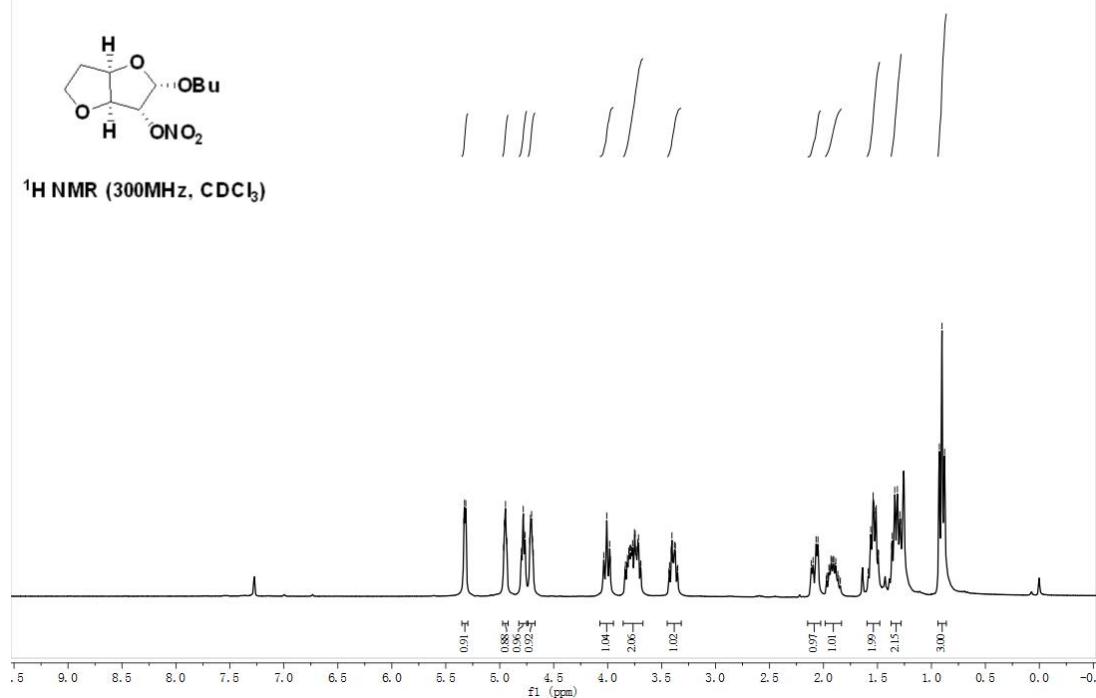




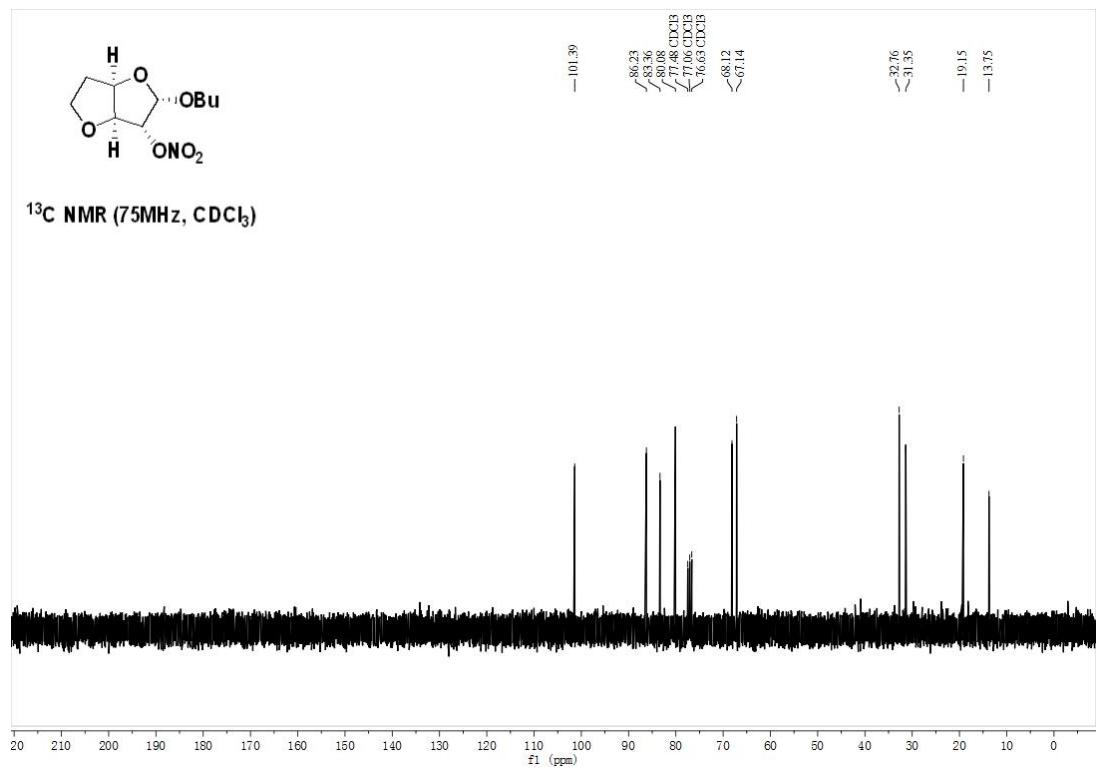


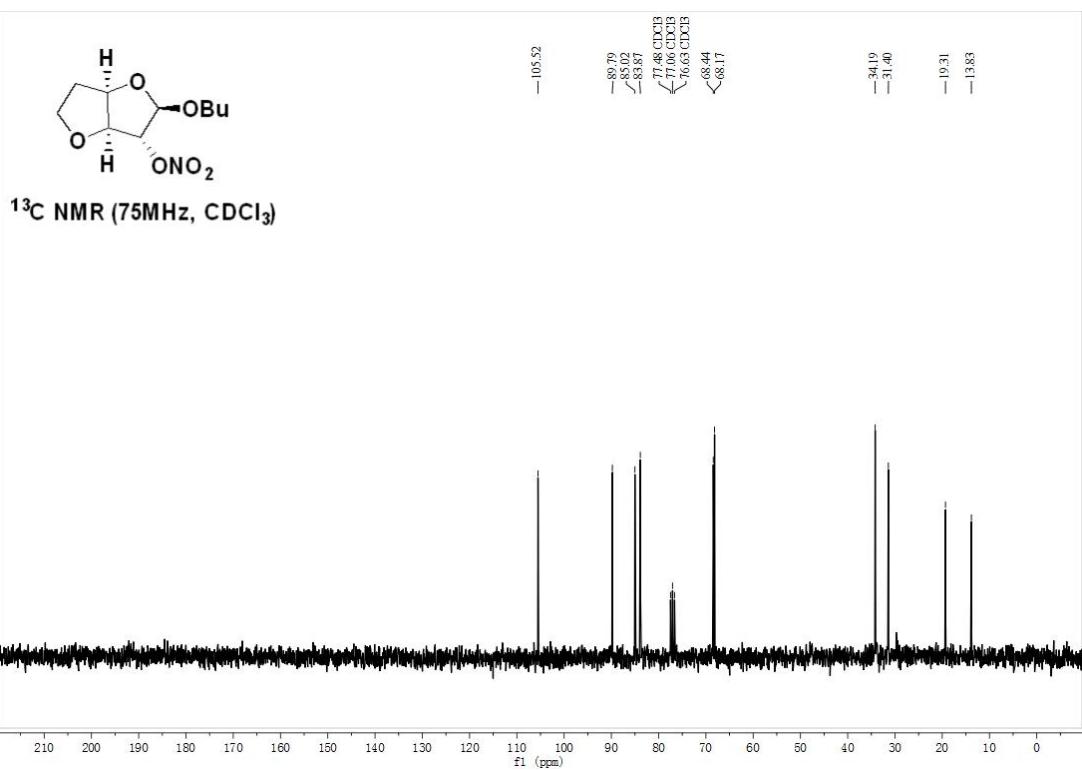
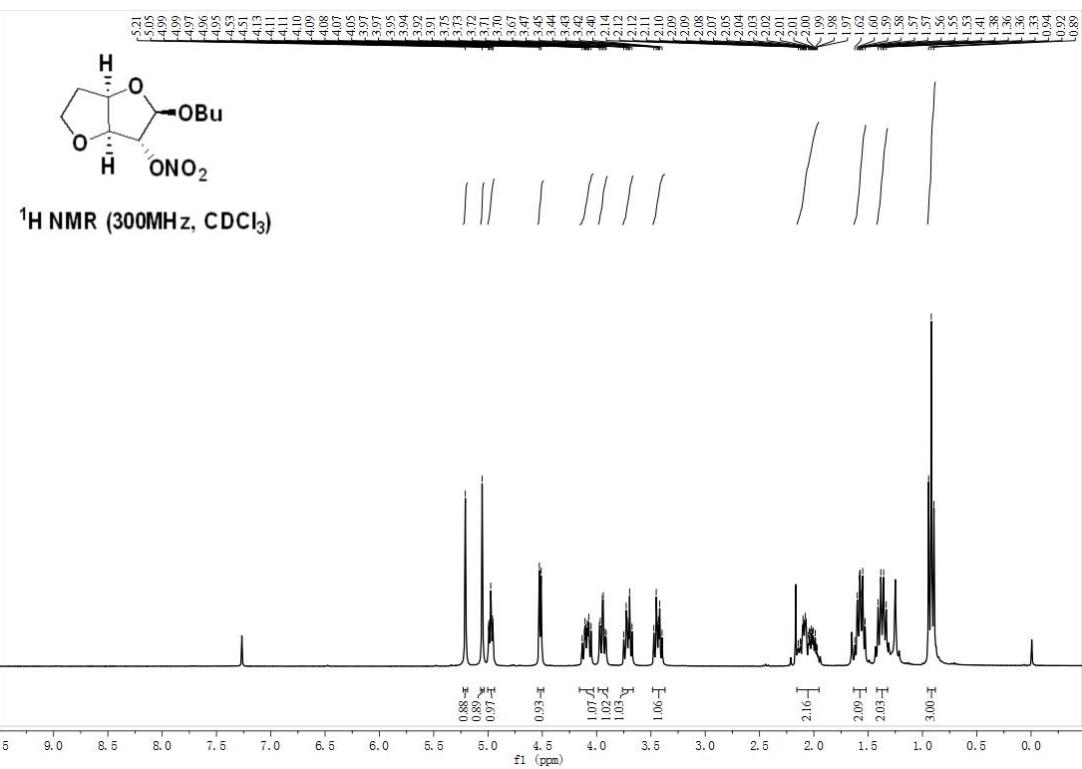


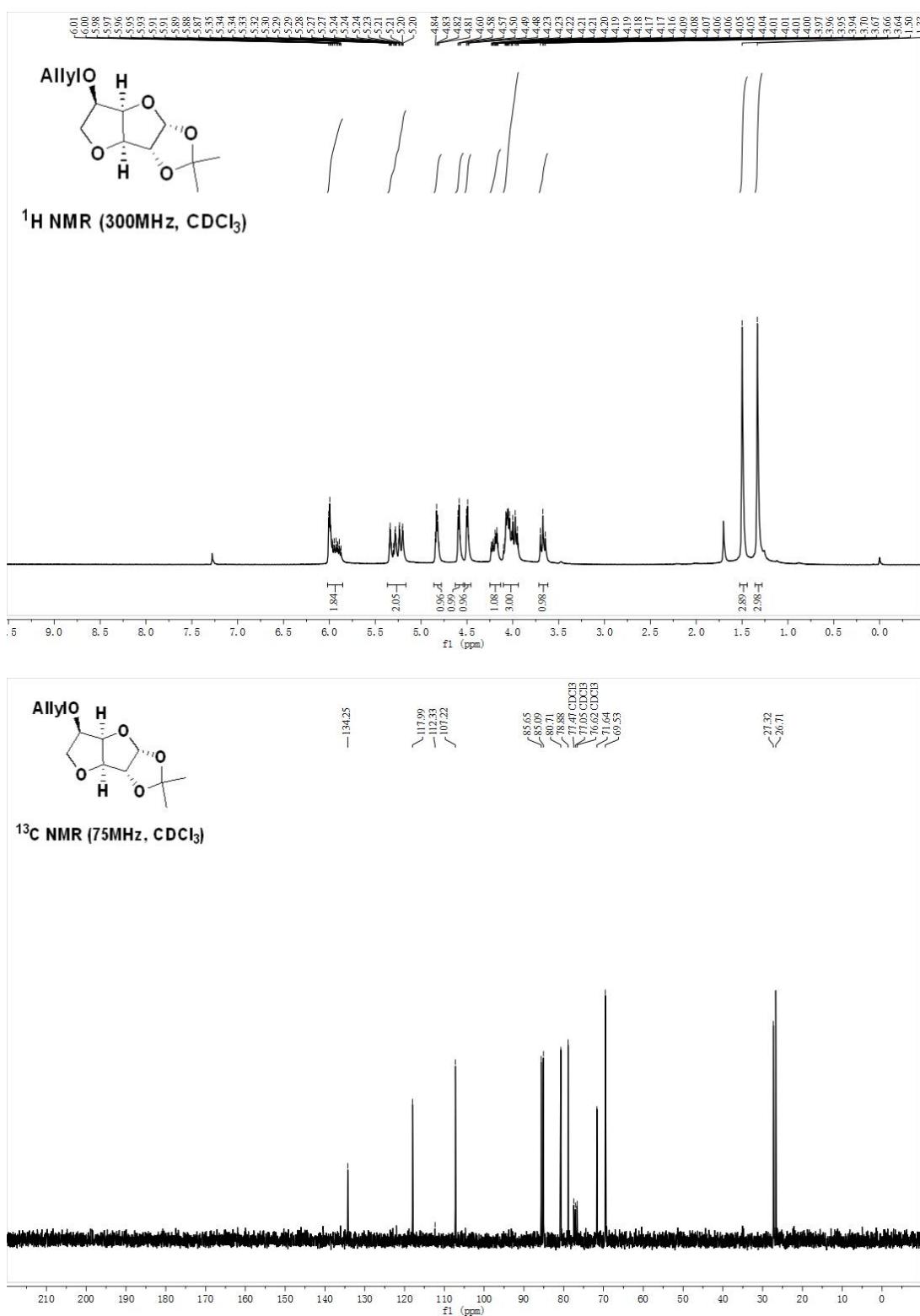
<sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>)

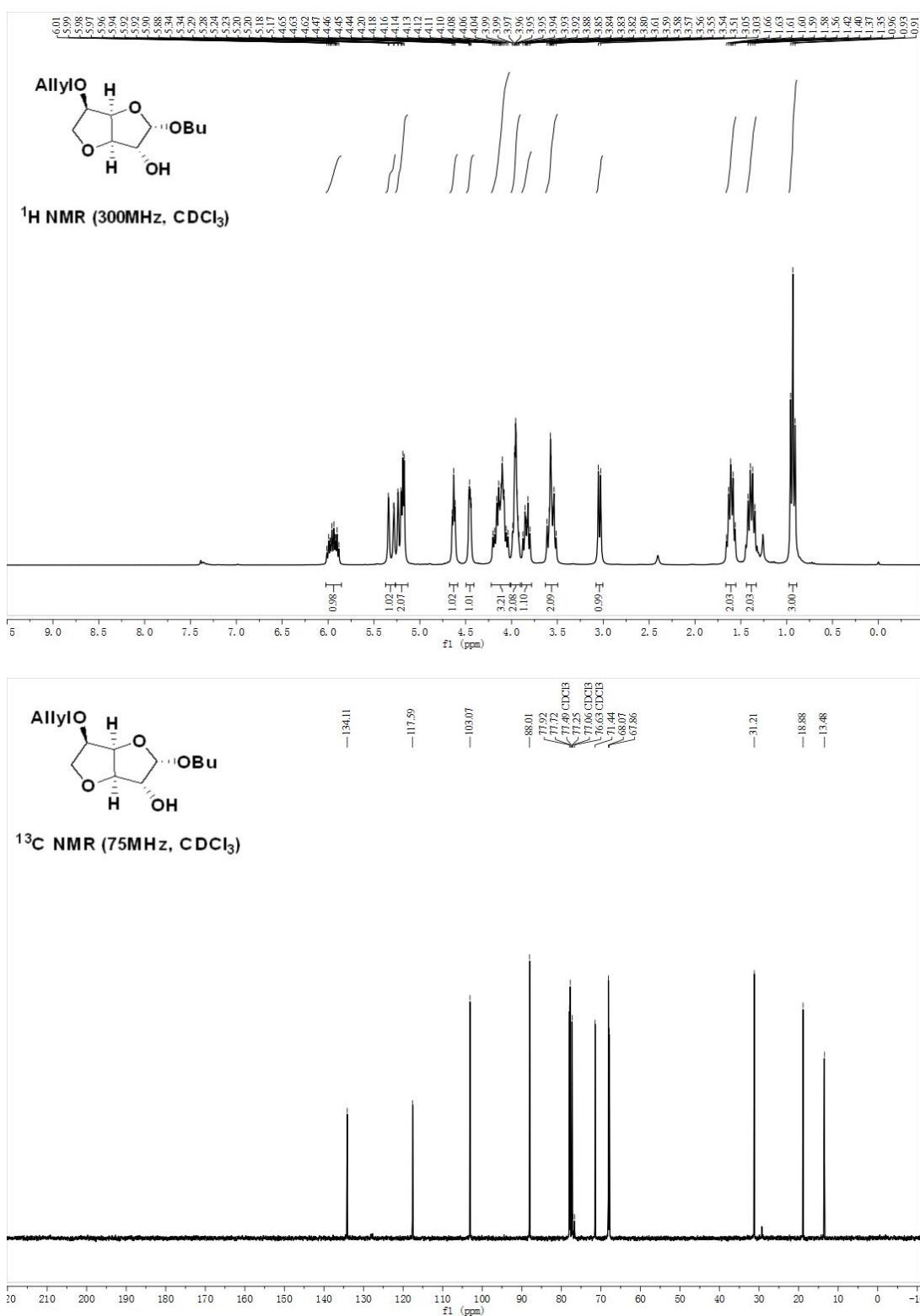


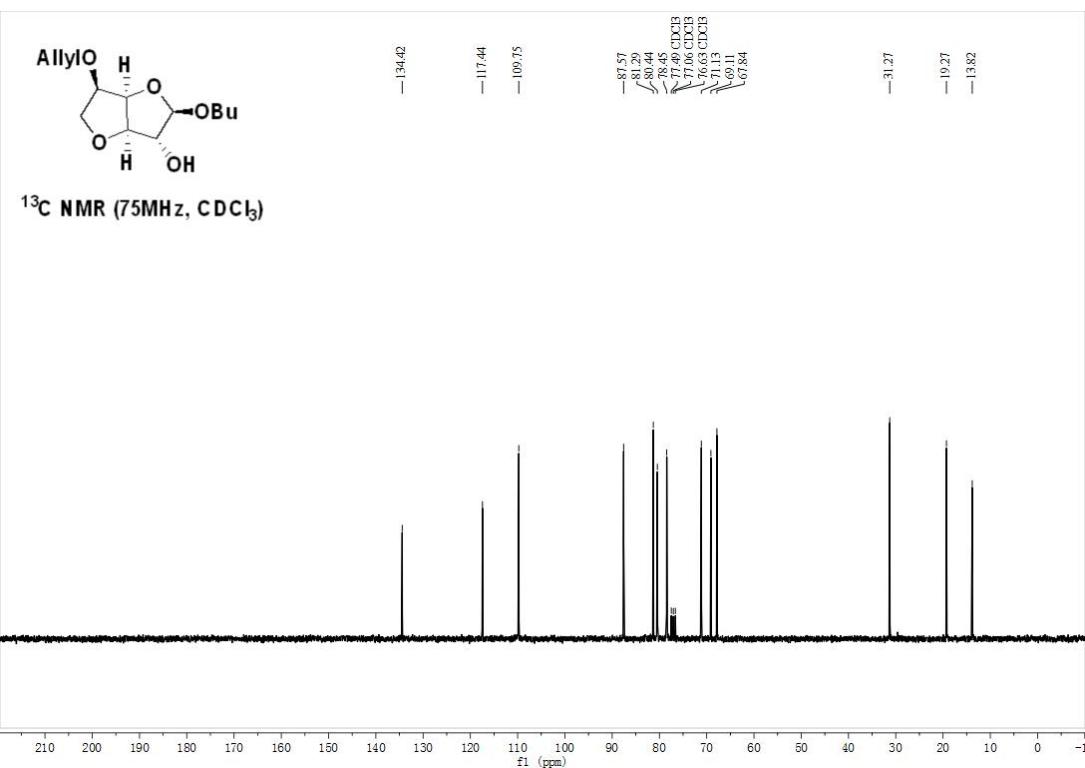
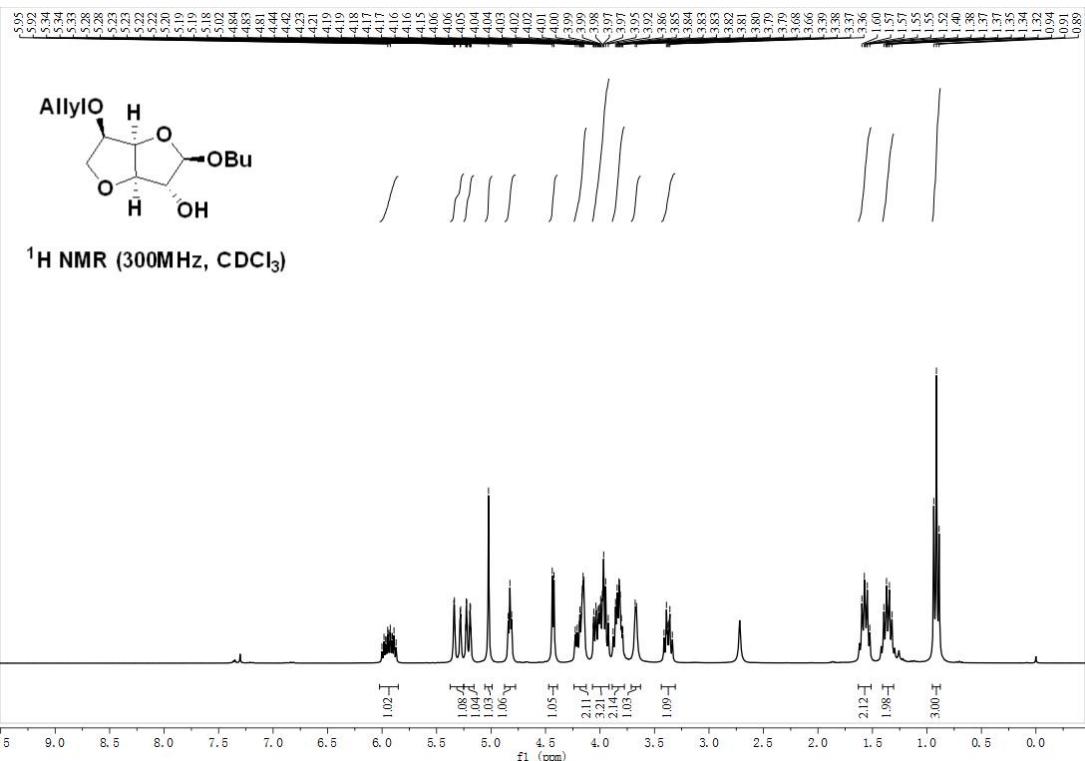
<sup>13</sup>C NMR (75MHz, CDCl<sub>3</sub>)

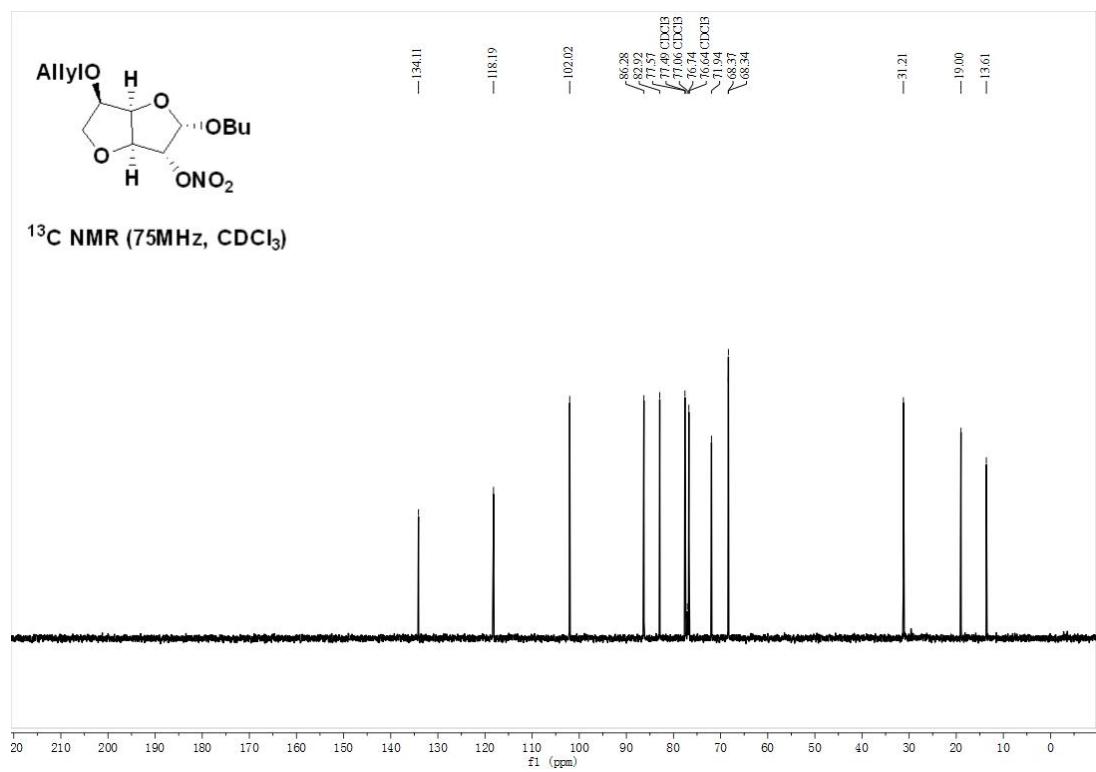
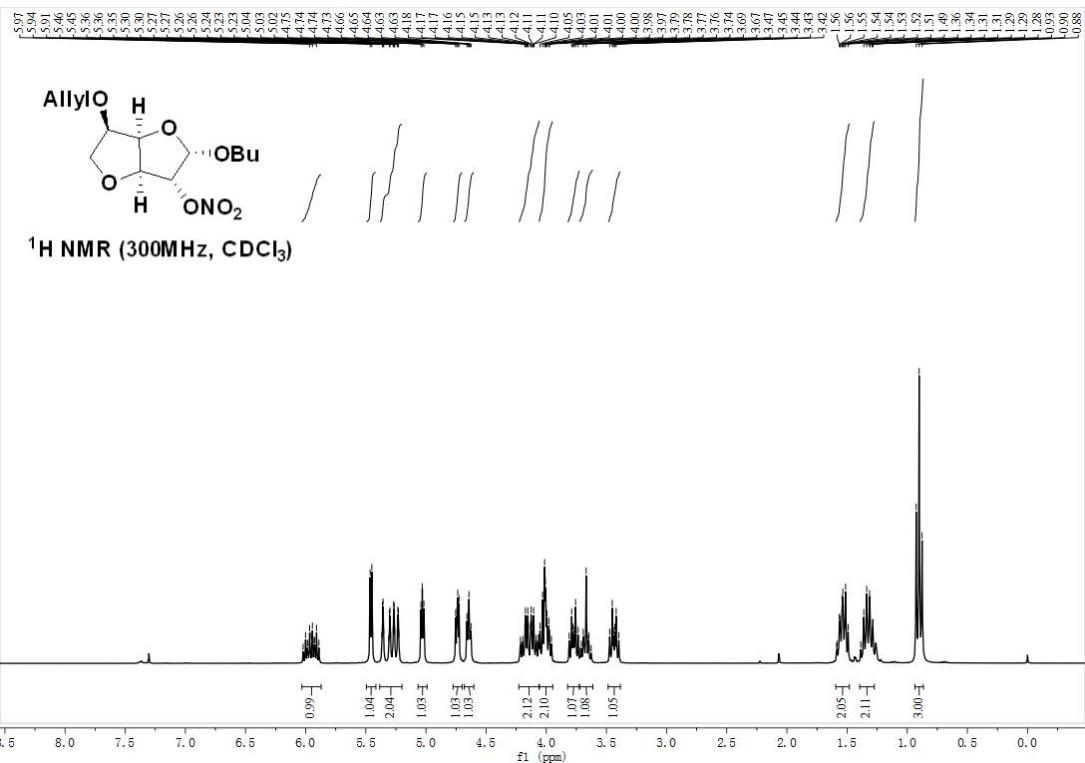


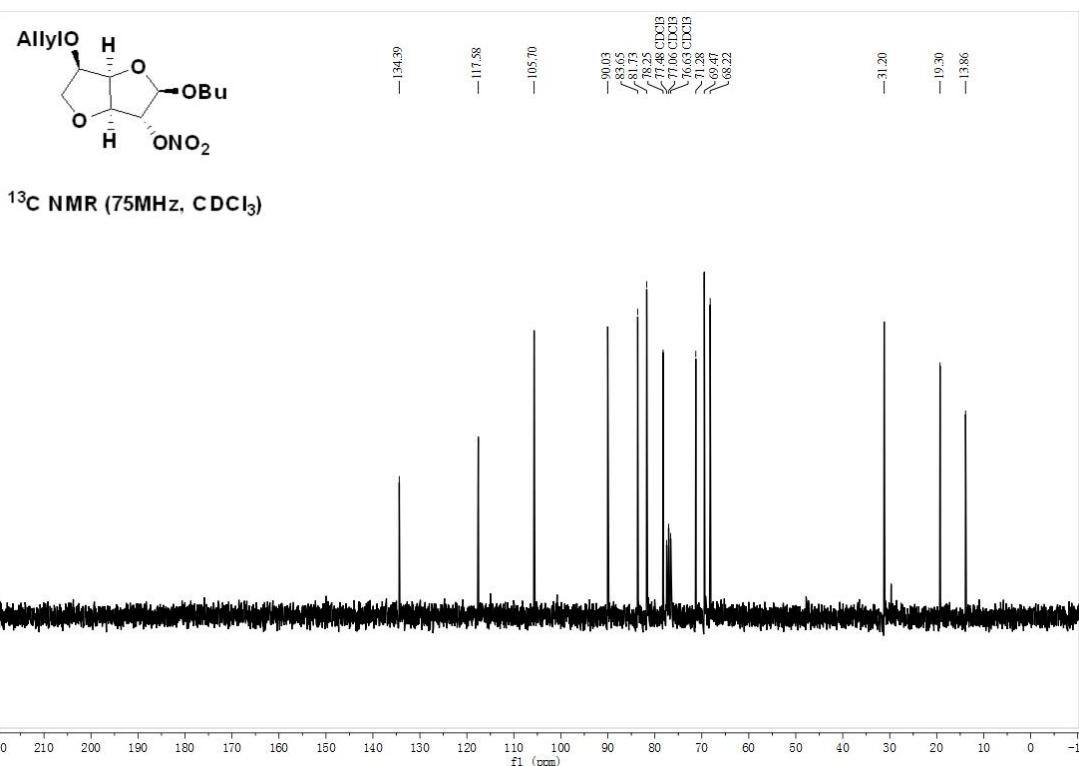
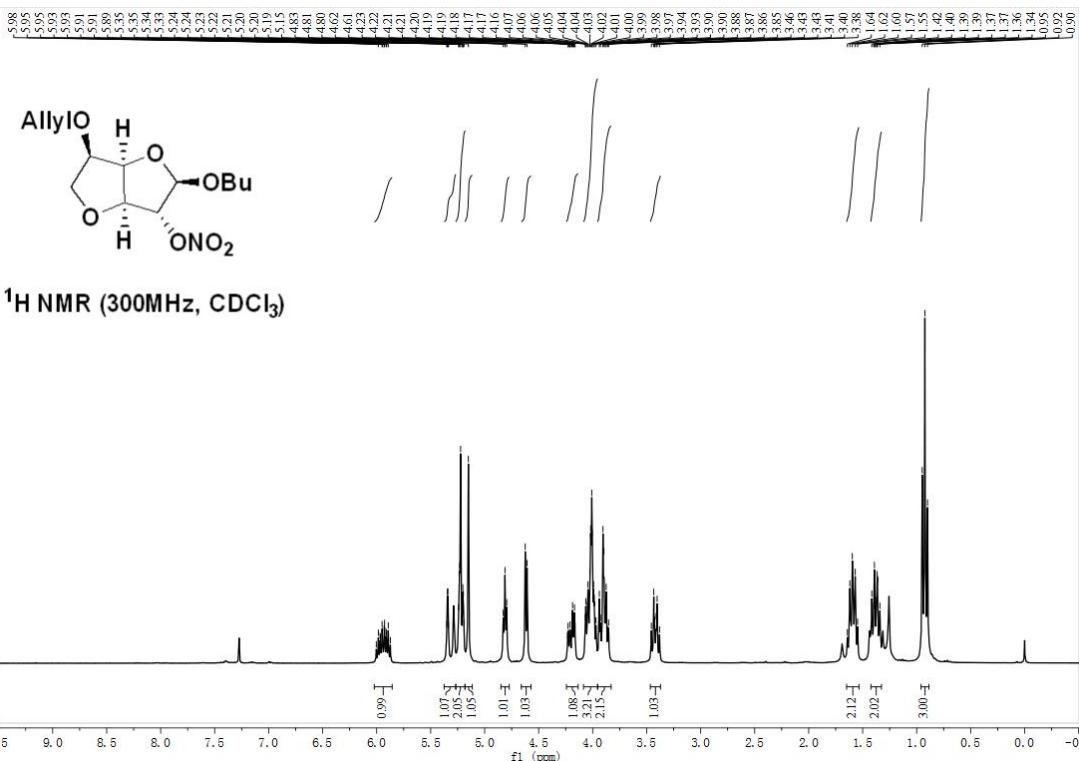


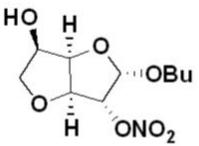




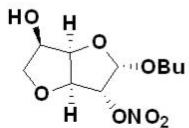
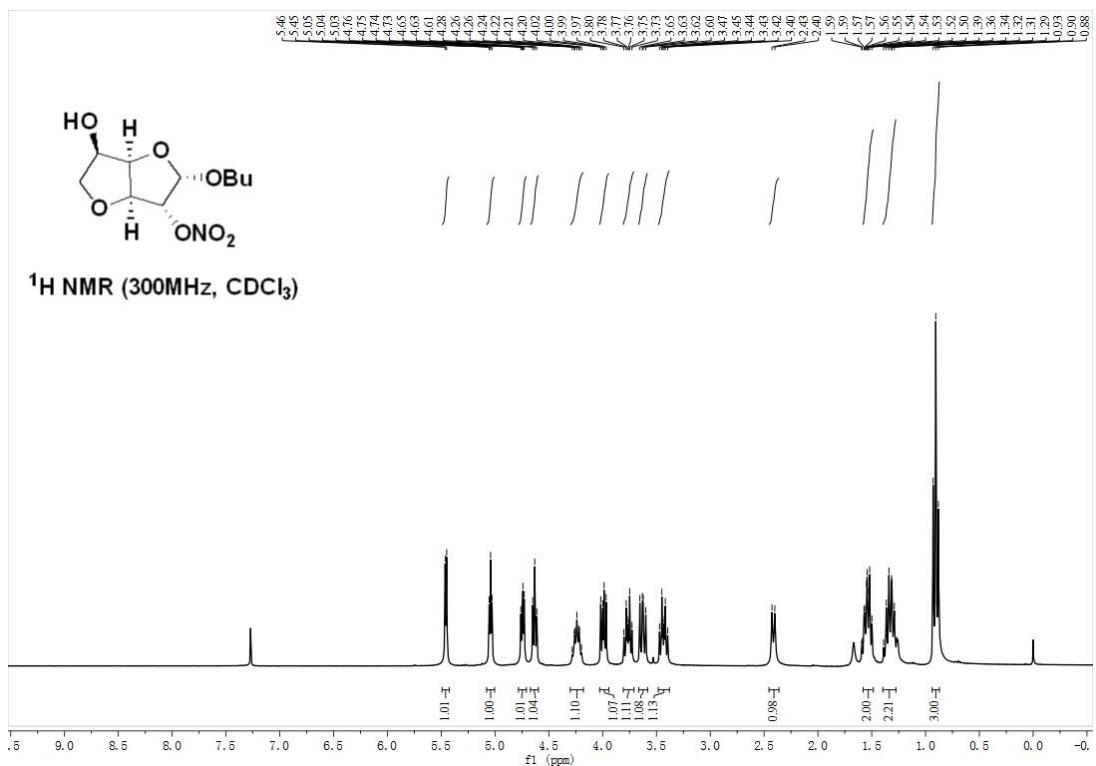




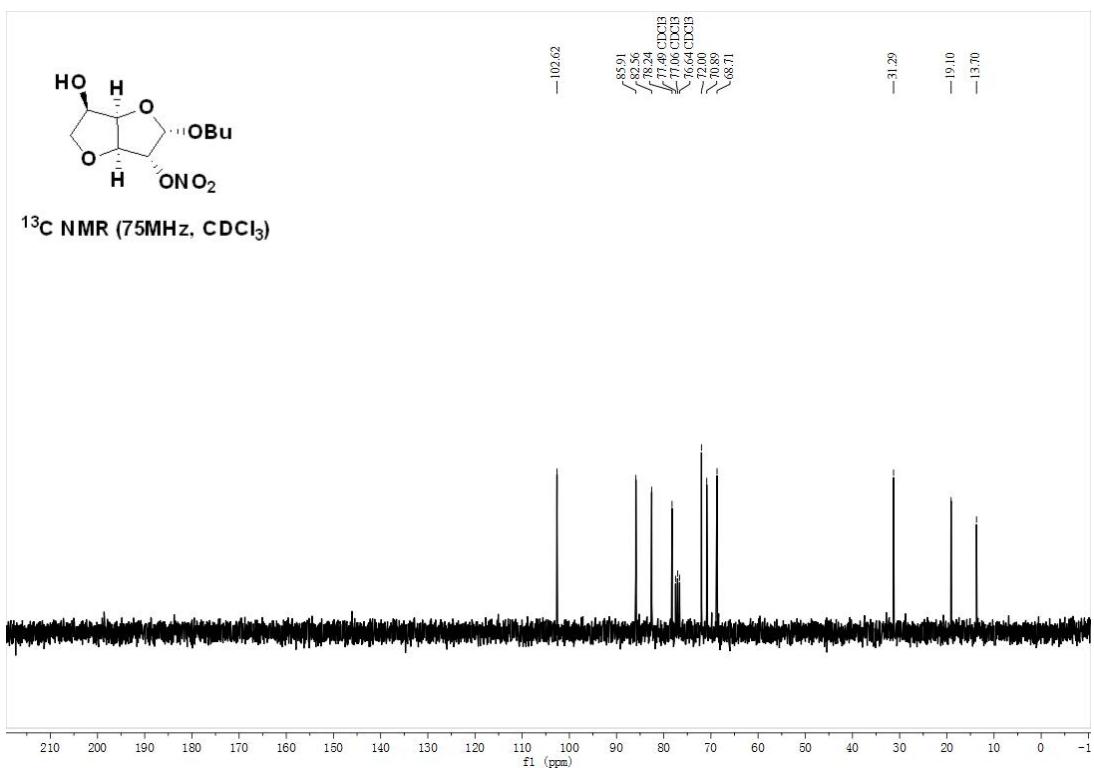


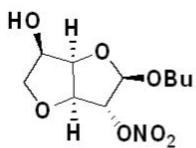


<sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>)

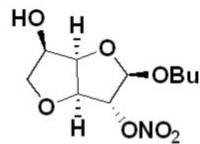
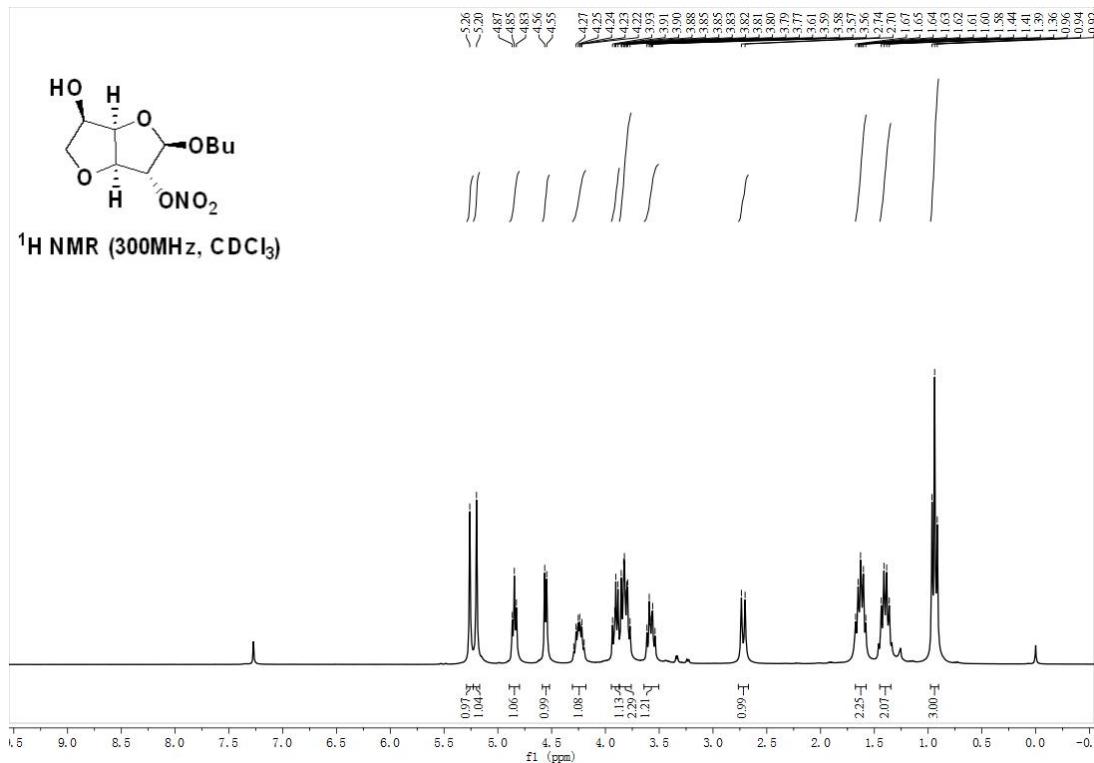


**<sup>13</sup>C NMR (75MHz, CDCl<sub>3</sub>)**

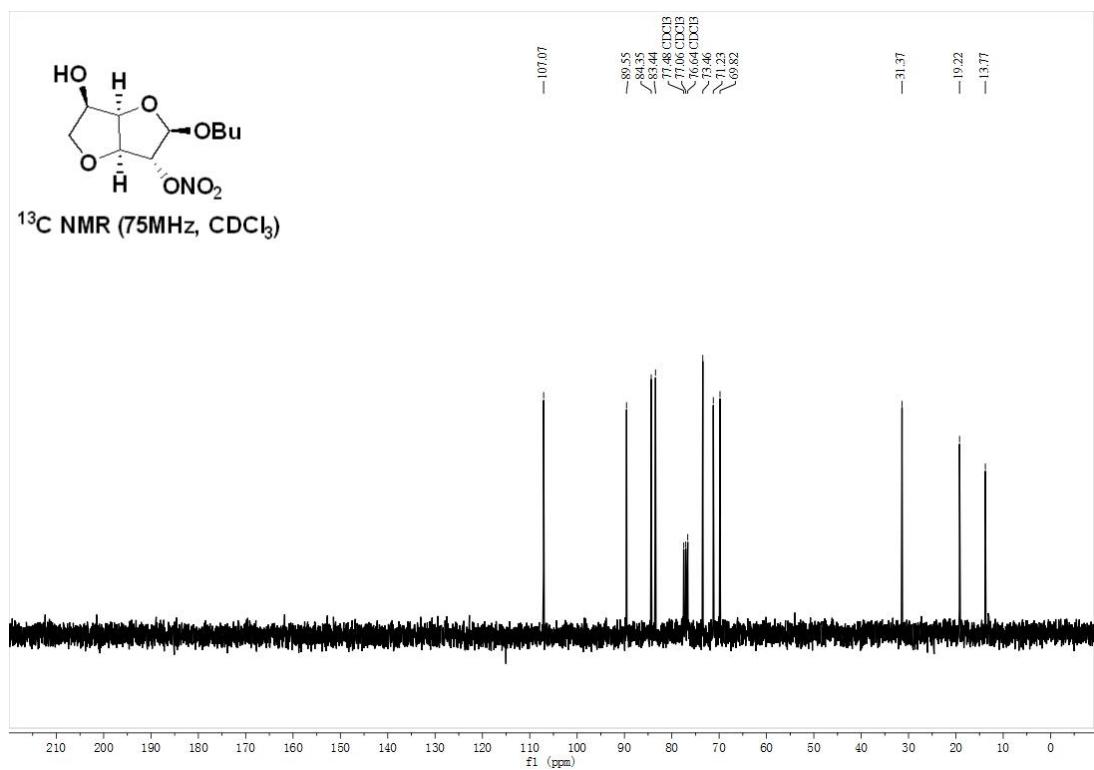


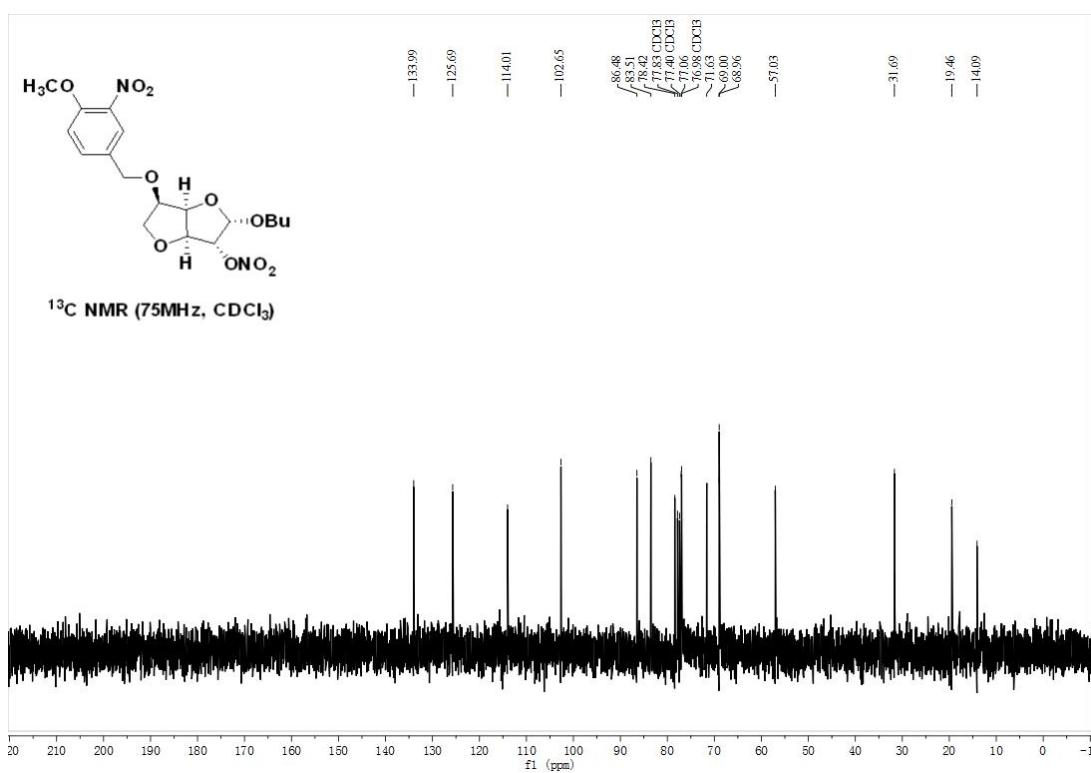
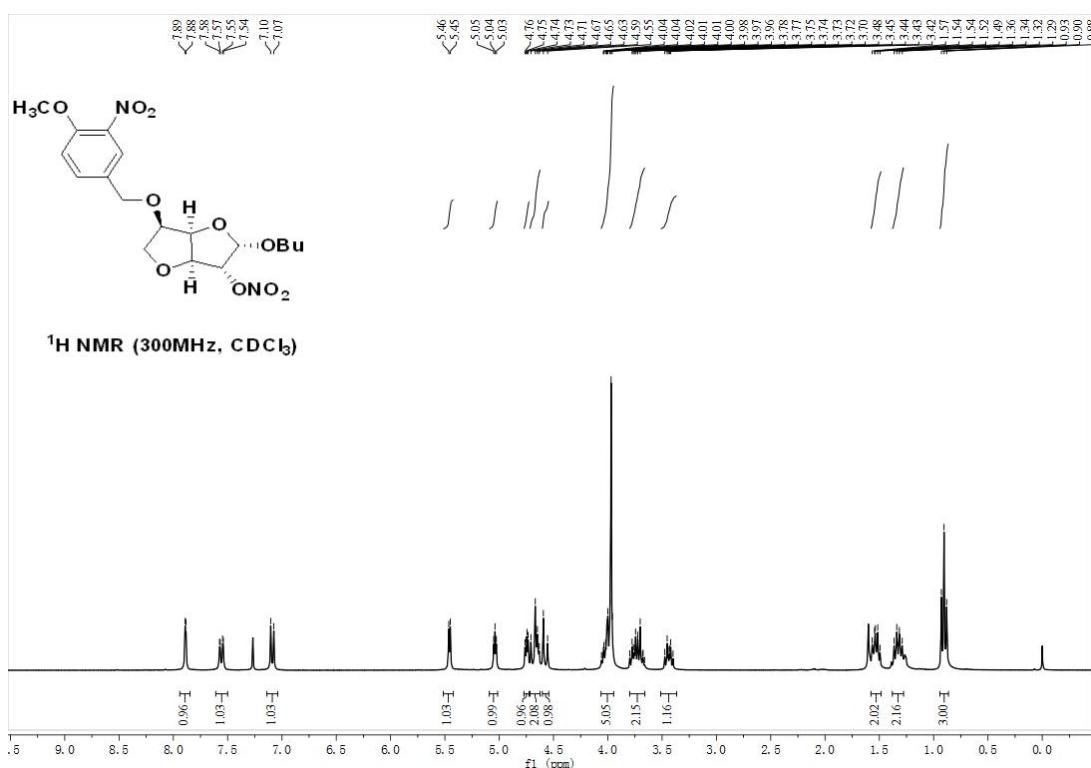


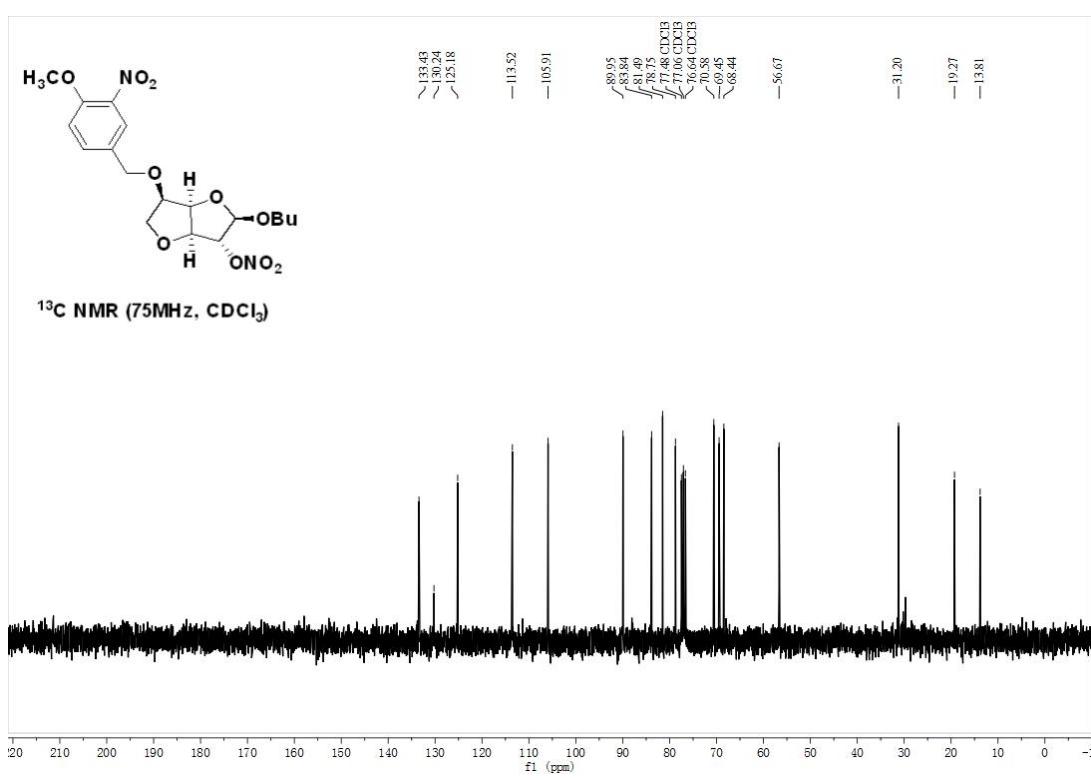
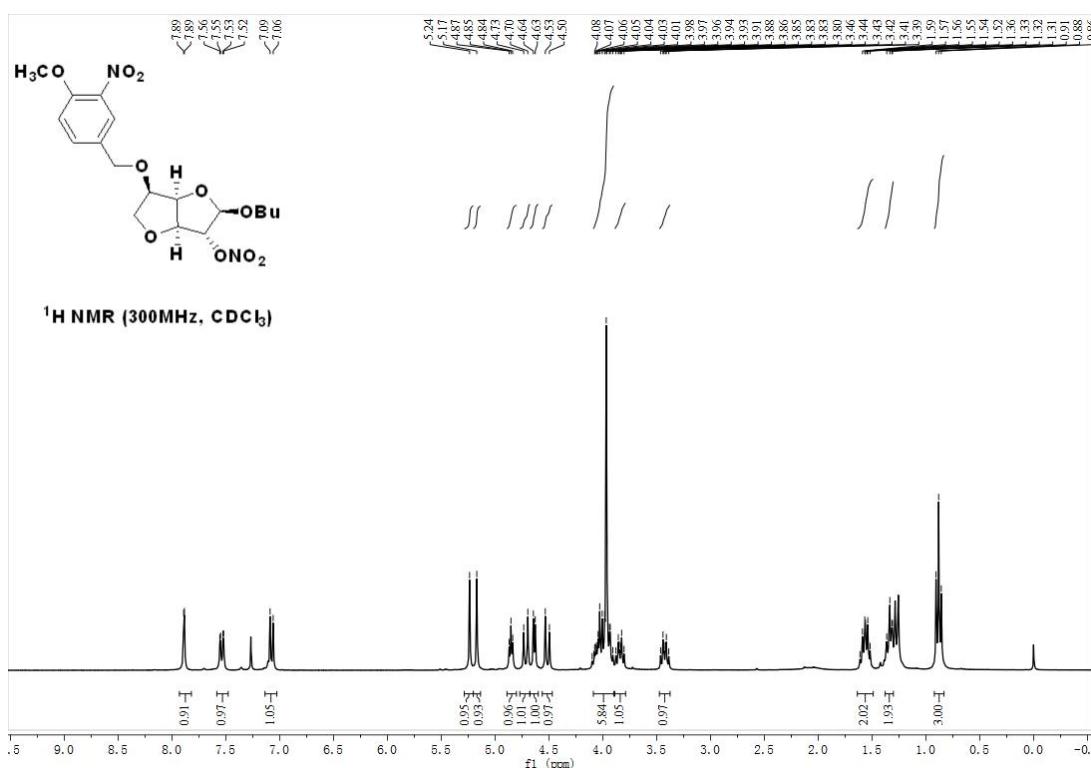
<sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>)

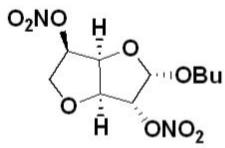


<sup>13</sup>C NMR (75MHz, CDCl<sub>3</sub>)

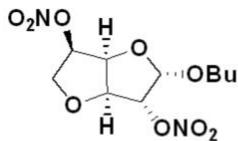
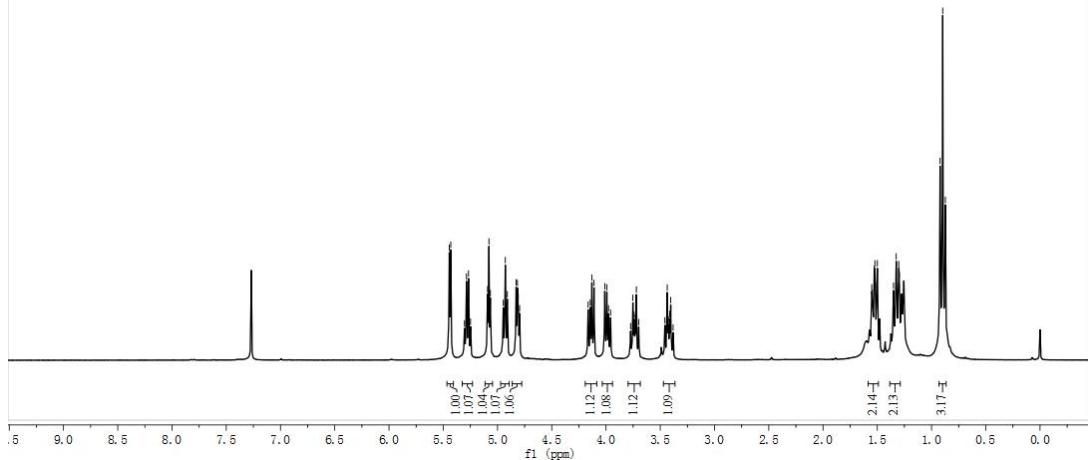




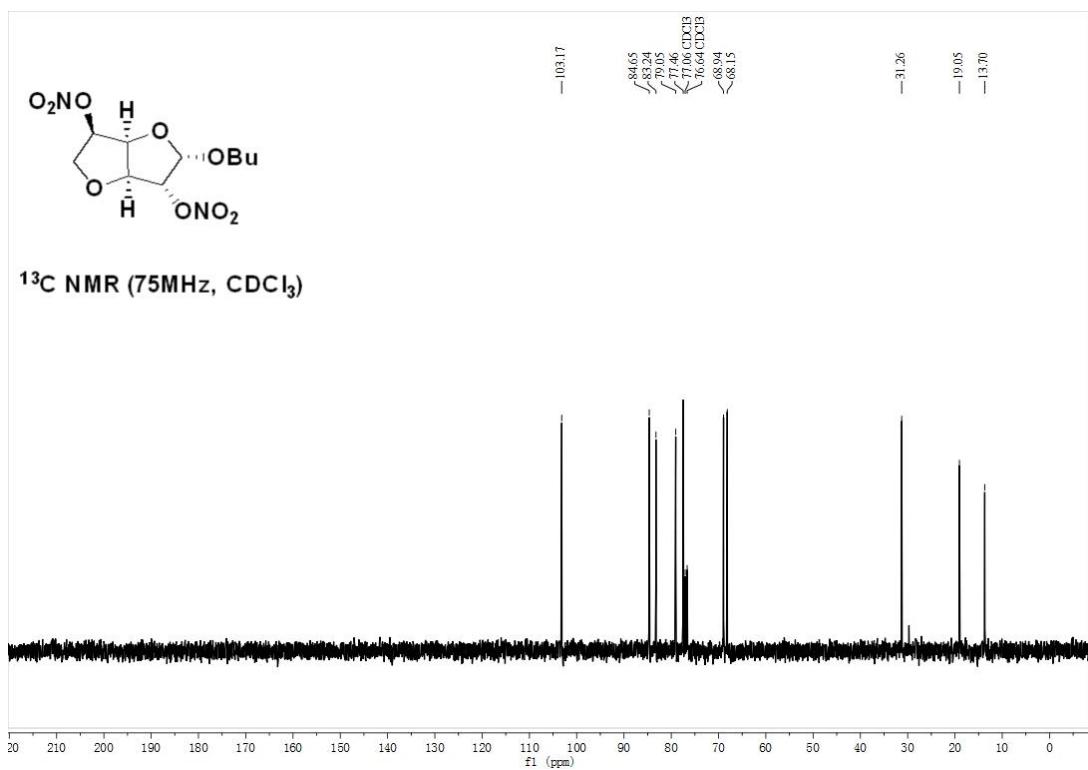


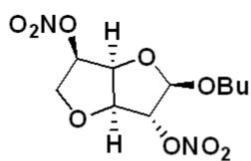


<sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>)

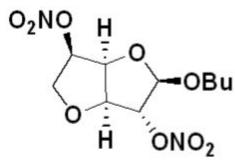
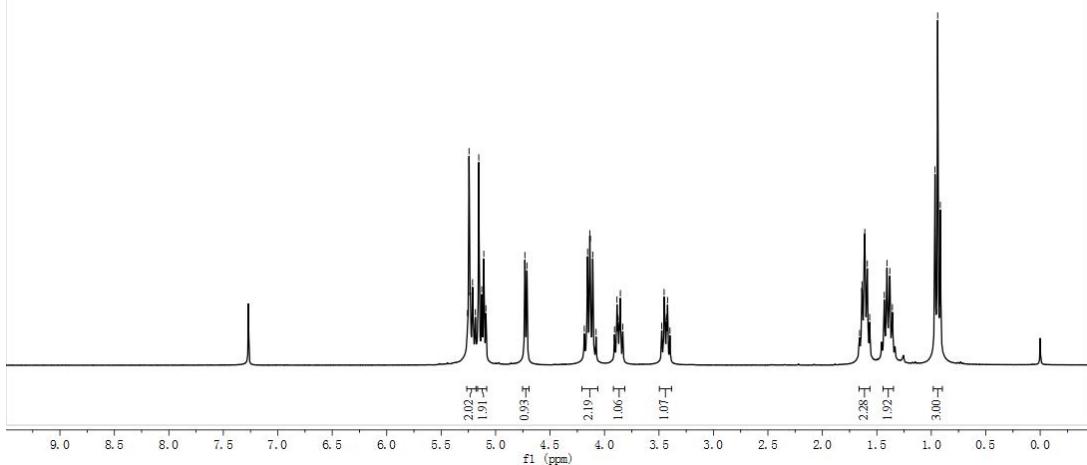


<sup>13</sup>C NMR (75MHz, CDCl<sub>3</sub>)

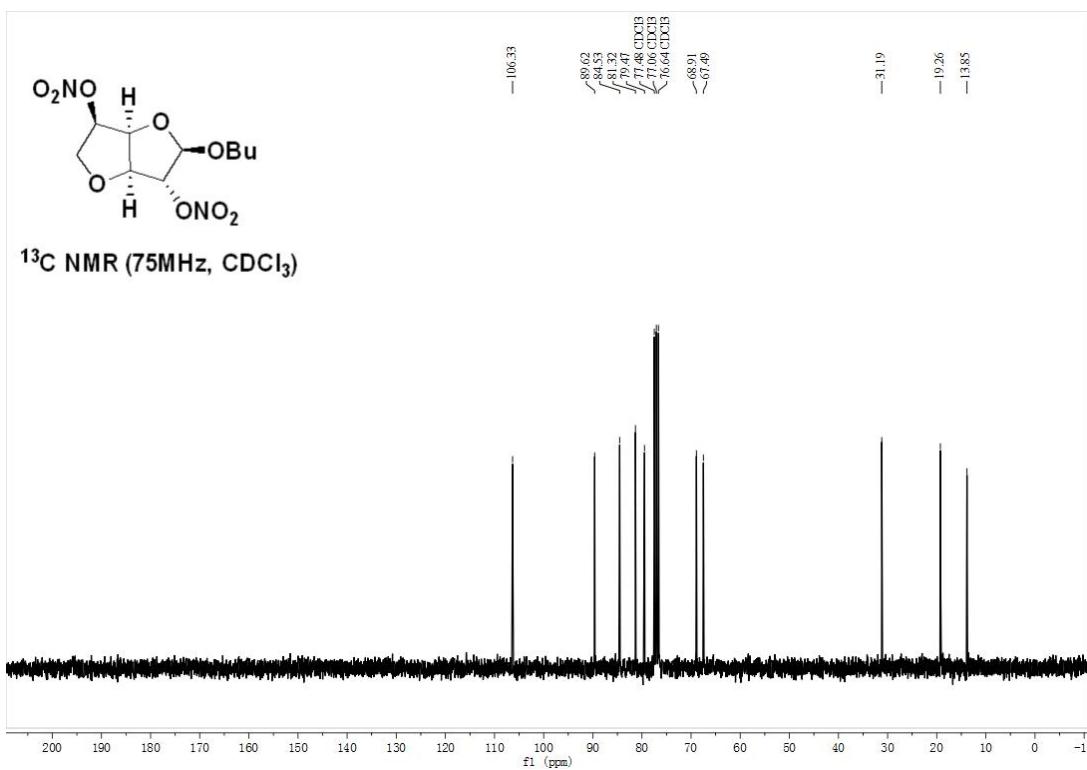




<sup>1</sup>H NMR (300MHz, CDCl<sub>3</sub>)

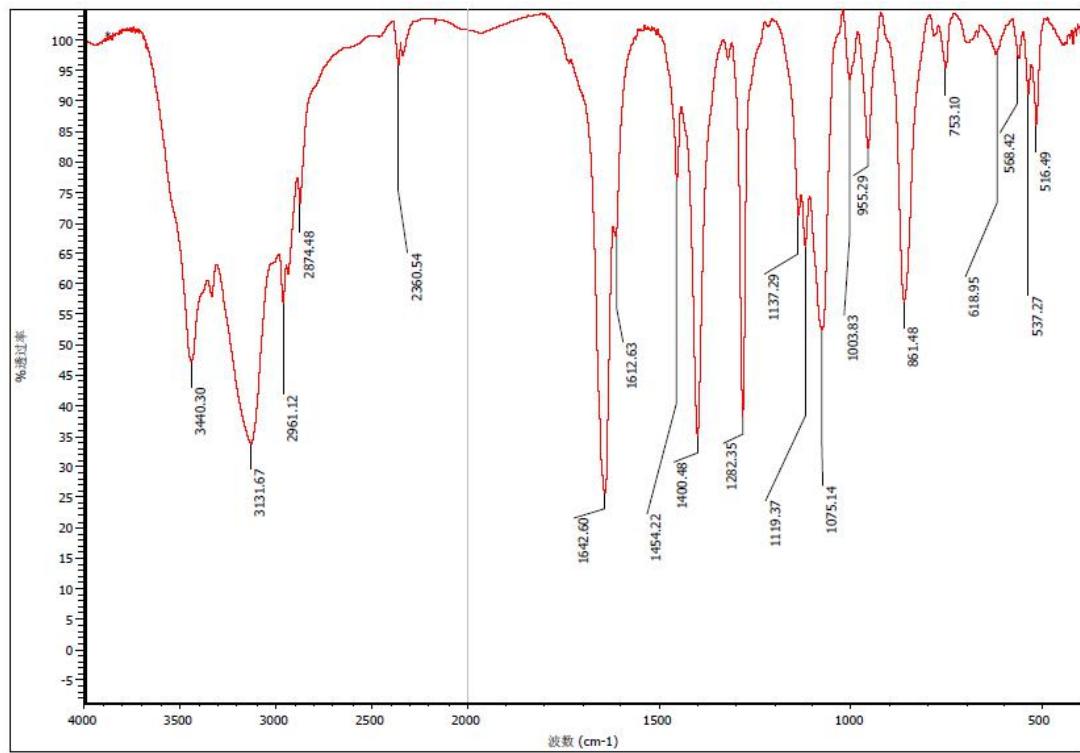


<sup>13</sup>C NMR (75MHz, CDCl<sub>3</sub>)

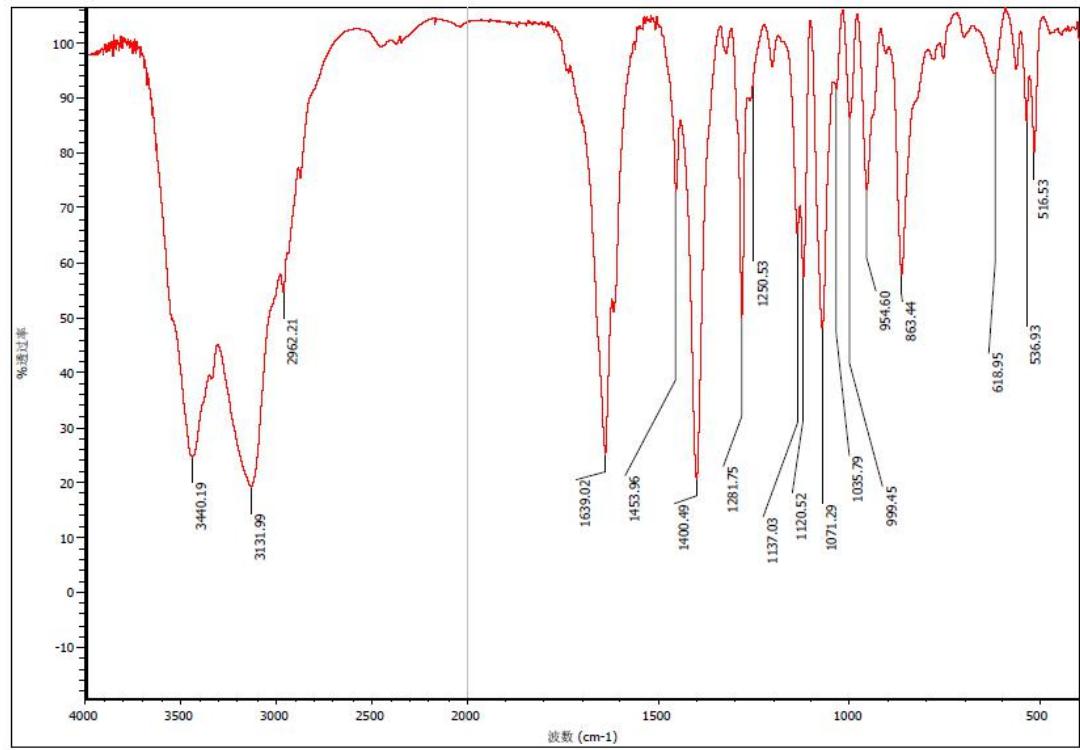


## 2. Copies of IR

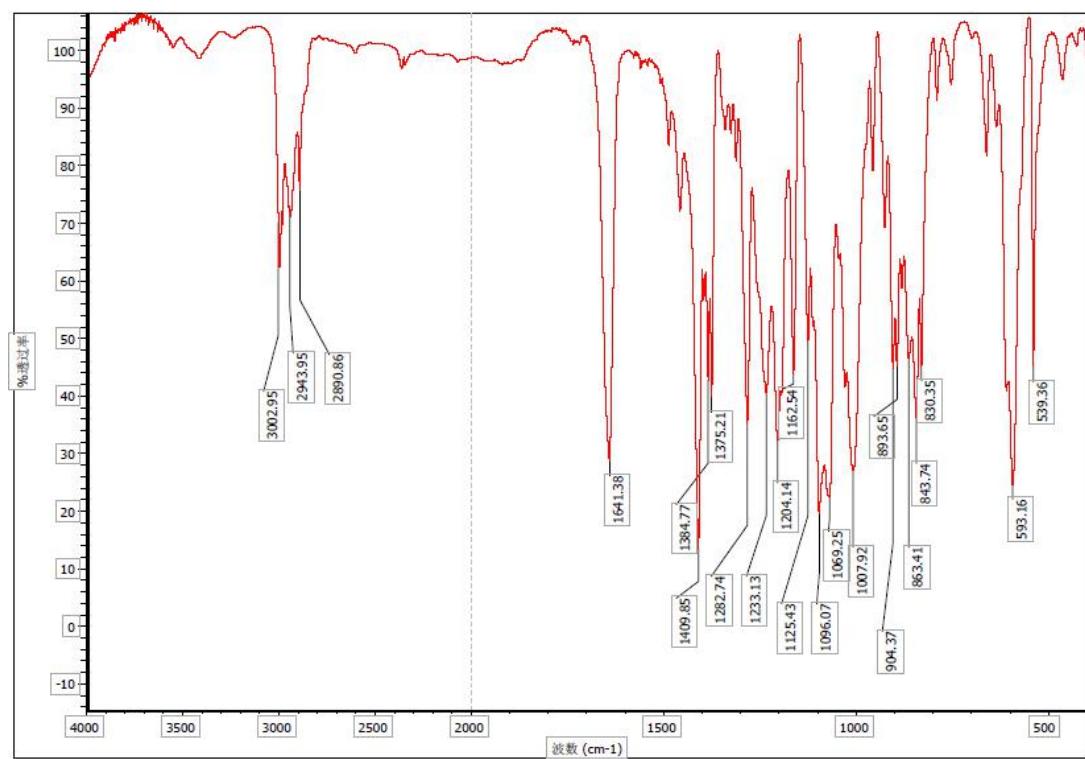
### Copies of IR of 5MNS-1



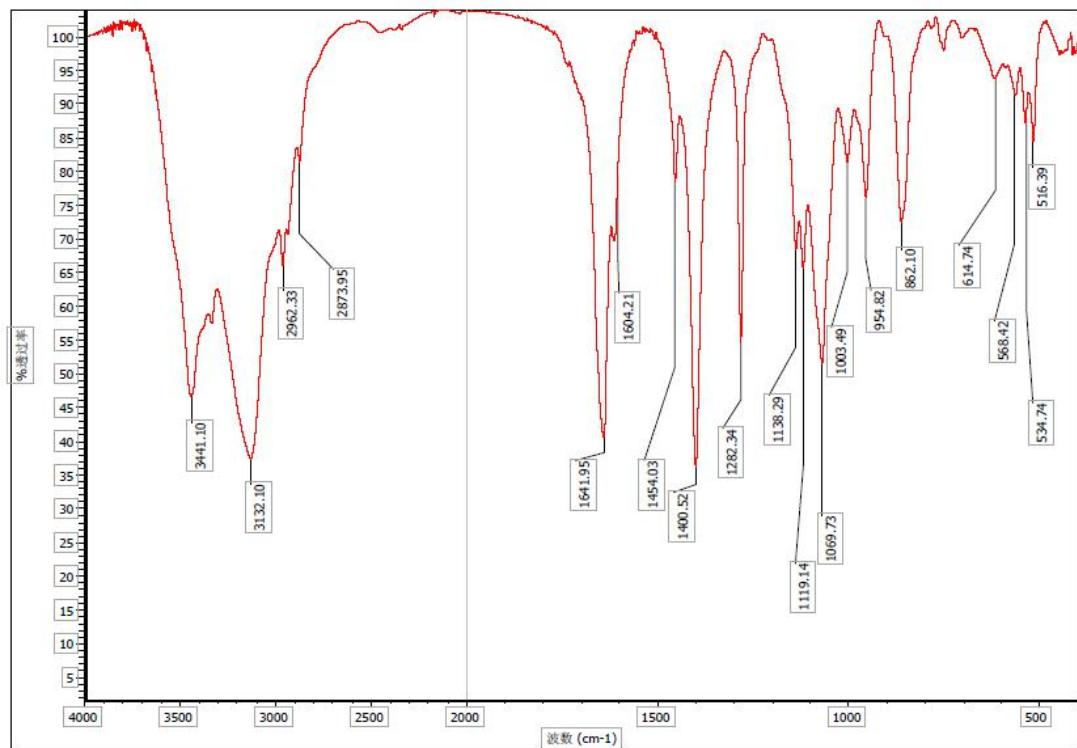
### Copies of IR of 5MNS-2



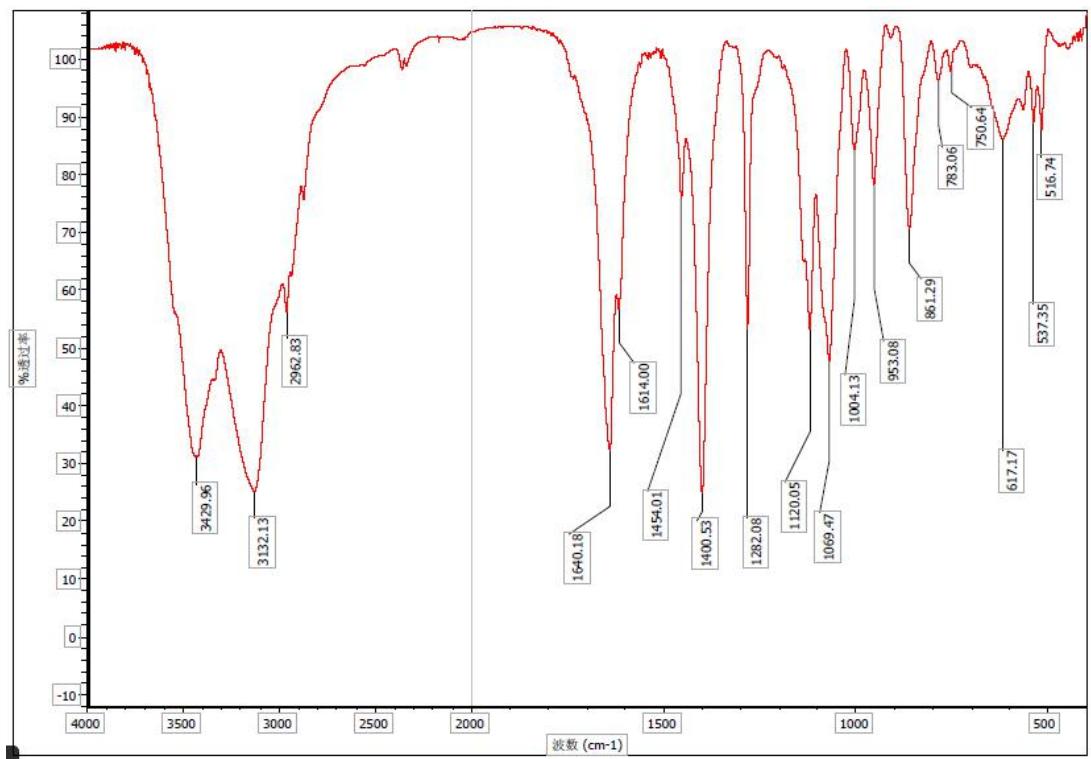
Copies of IR of 5MNS-3



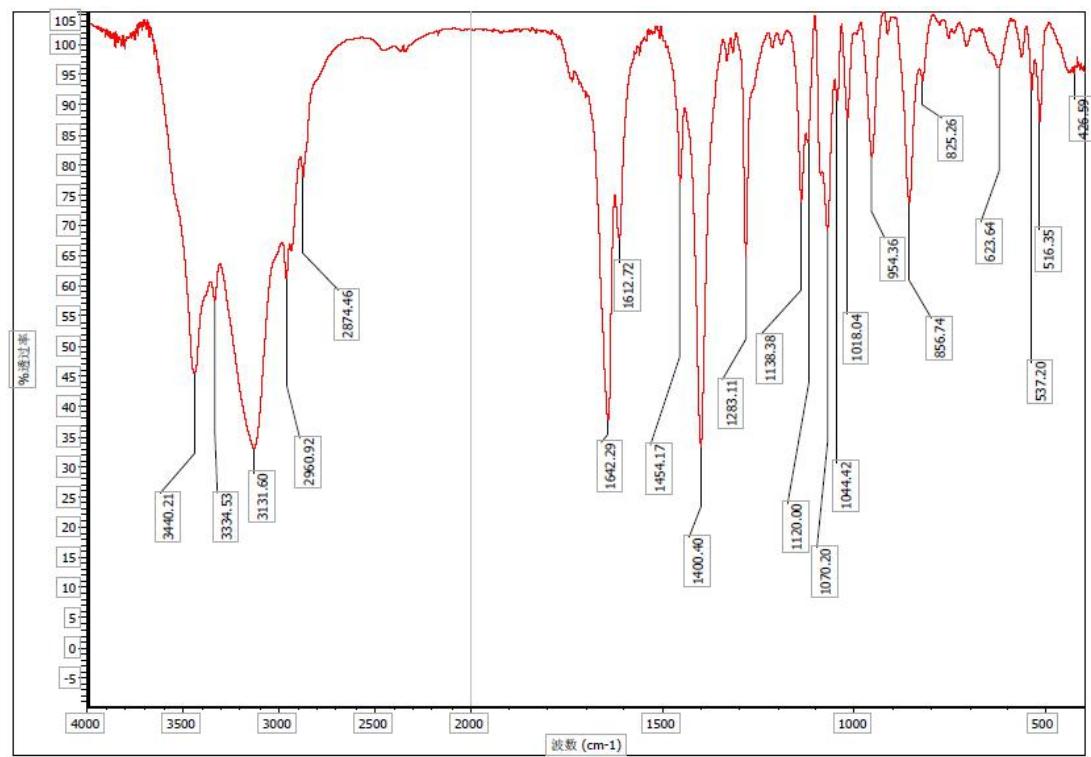
Copies of IR of 5MNS-4



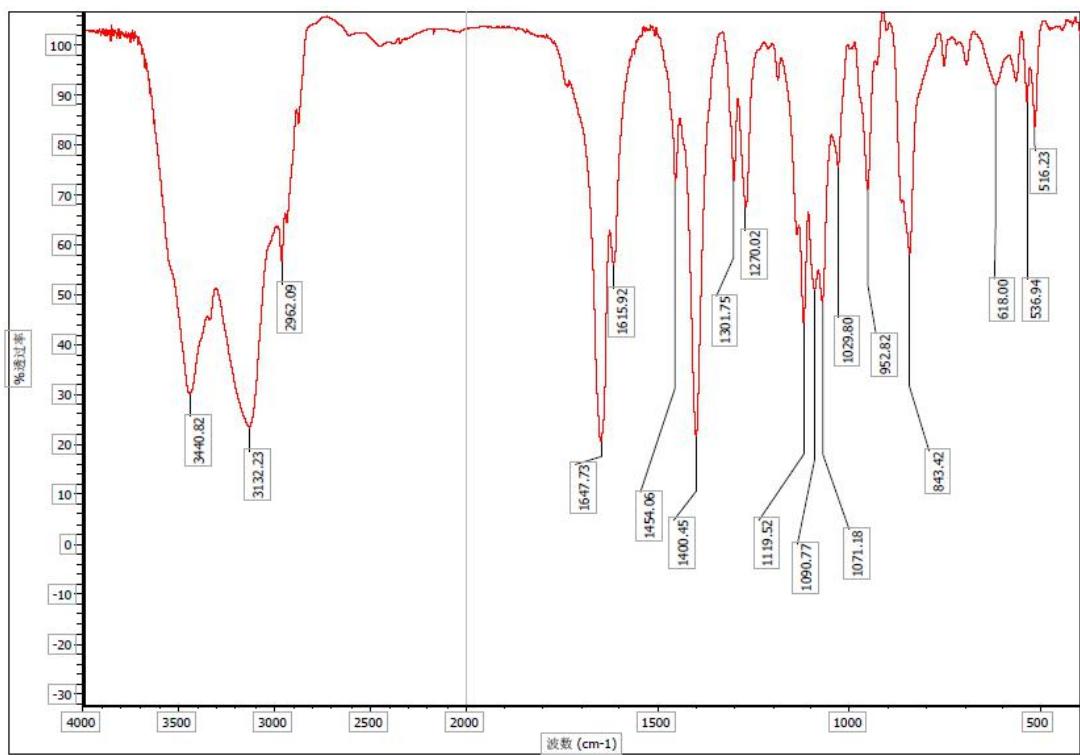
Copies of IR of 5MNS-5



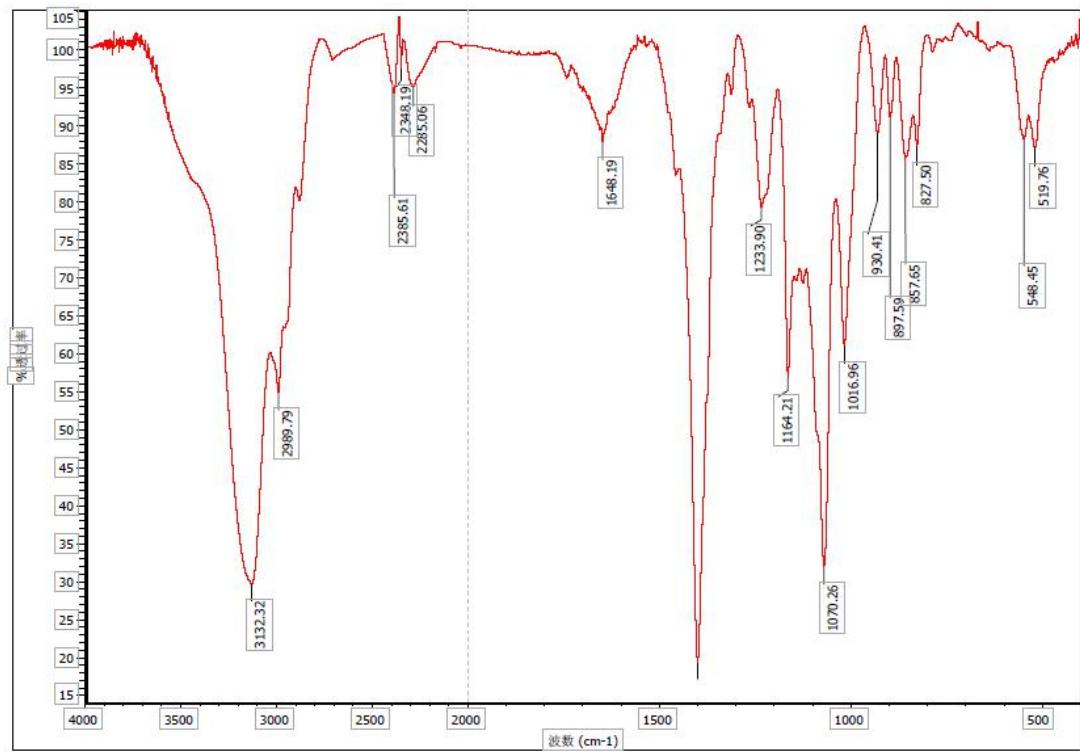
Copies of IR of 2MNS-1



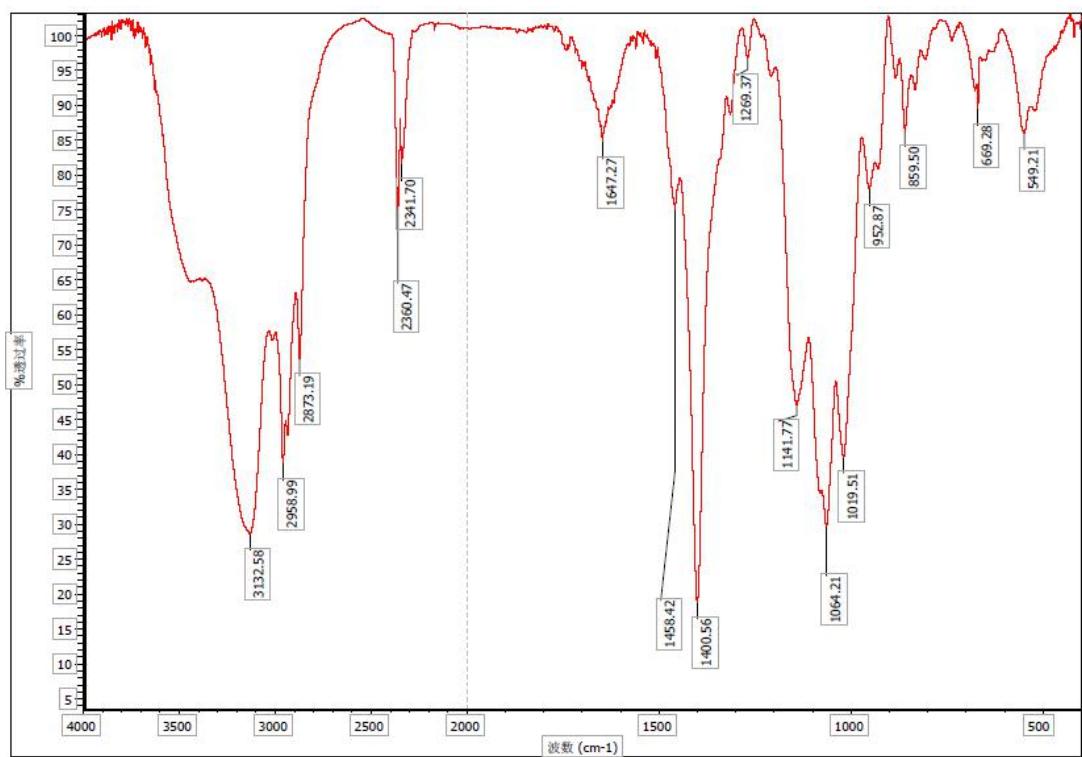
Copies of IR of 2MNS-2



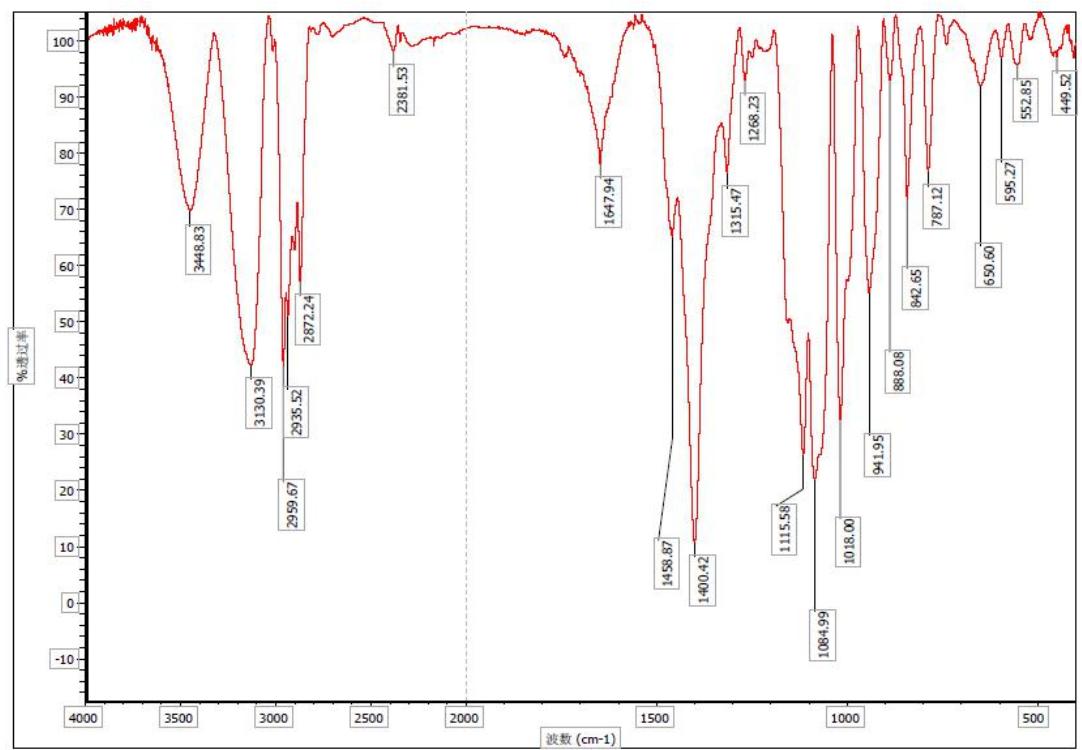
Copies of IR of 8



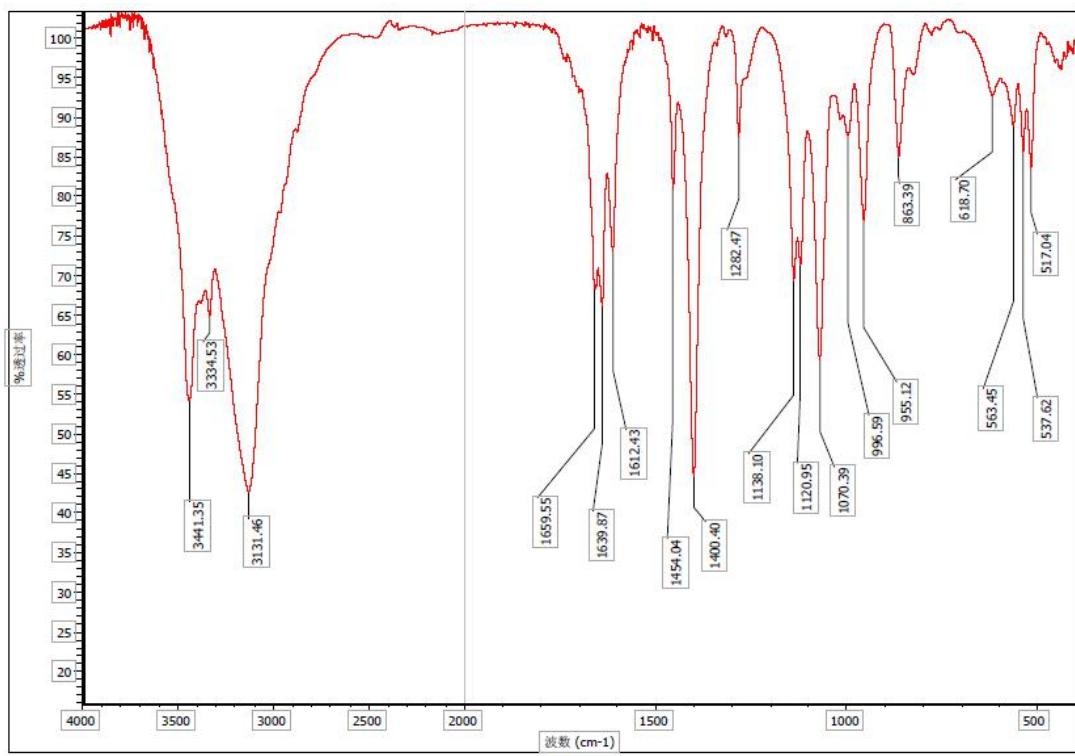
Copies of IR of **9a**



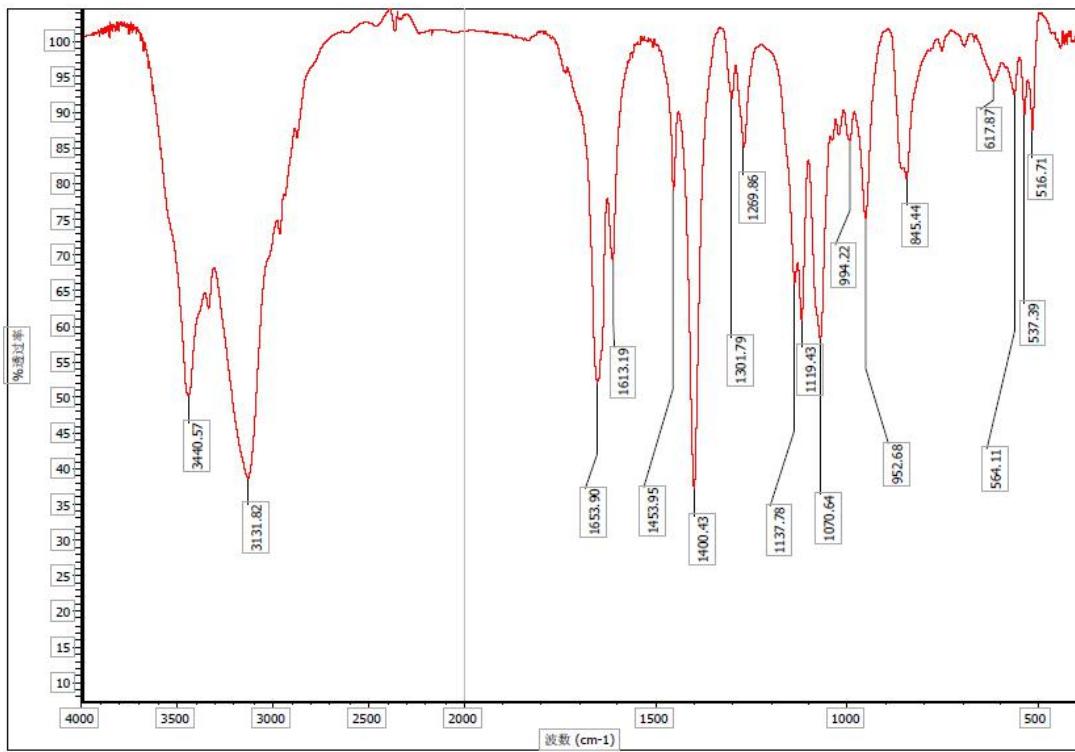
Copies of IR of **9b**



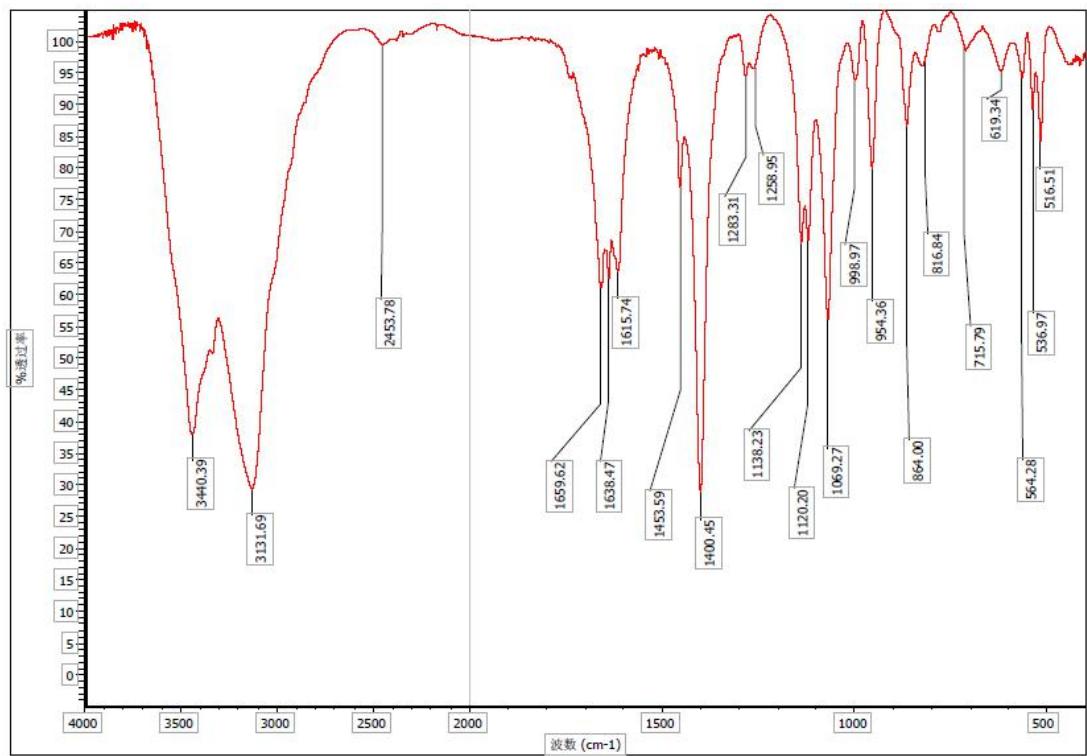
Copies of IR of 2MNS-3



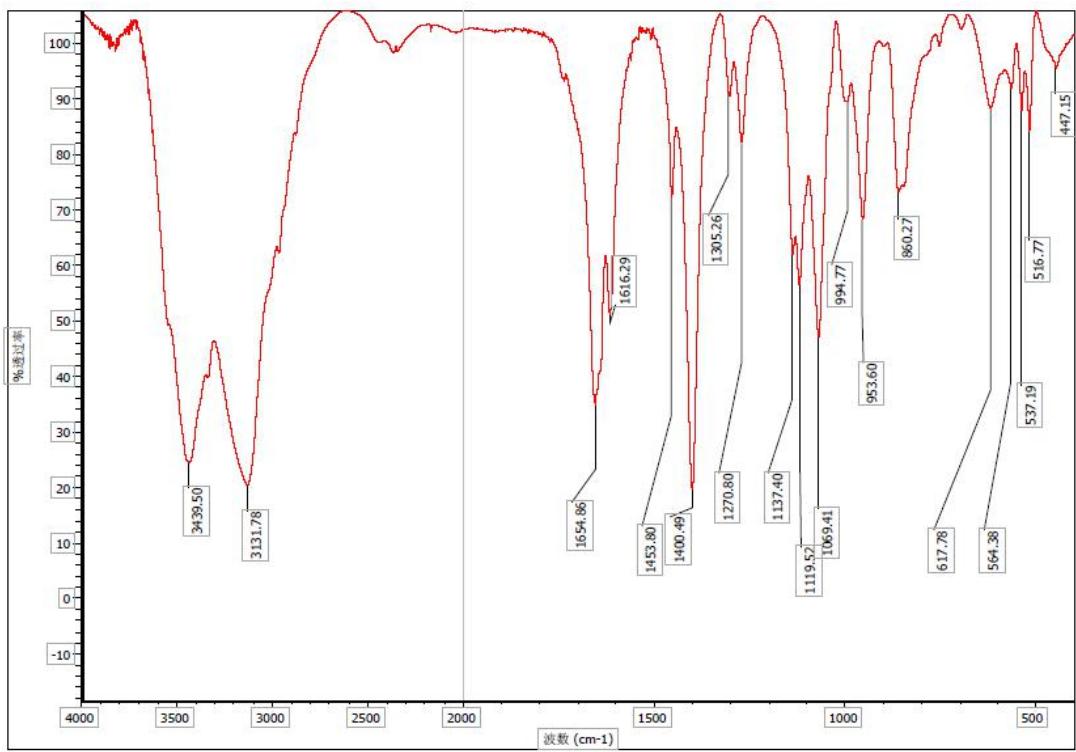
Copies of IR of 2MNS-4



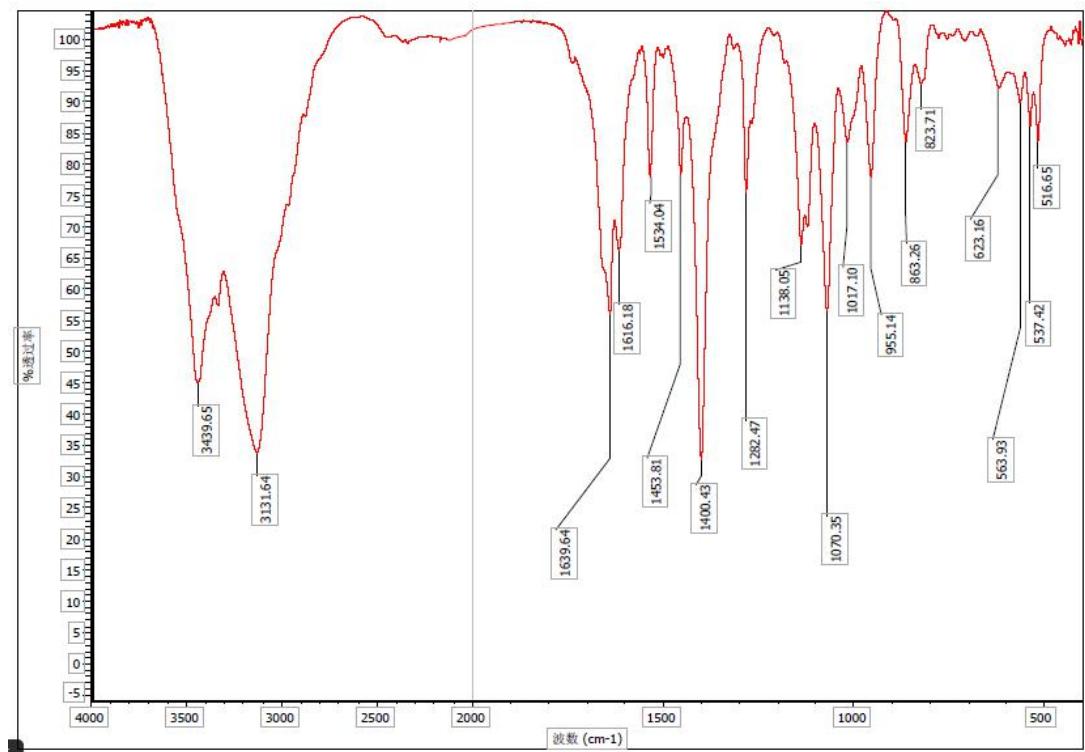
Copies of IR of 2MNS-5



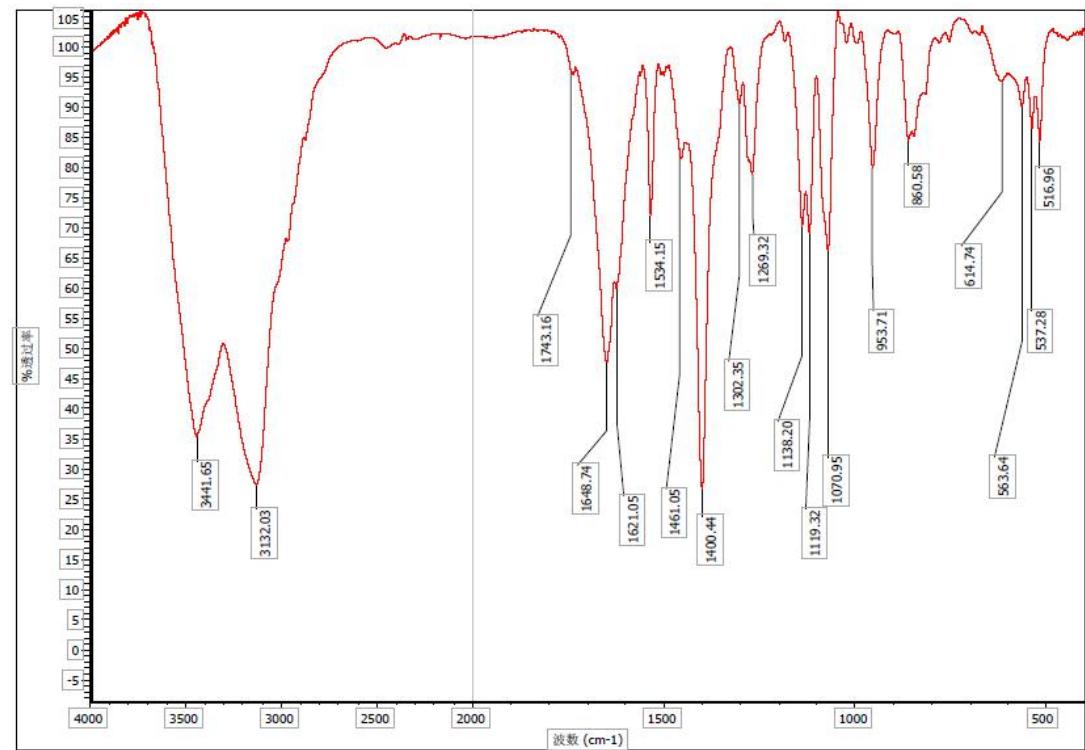
Copies of IR of 2MNS-6



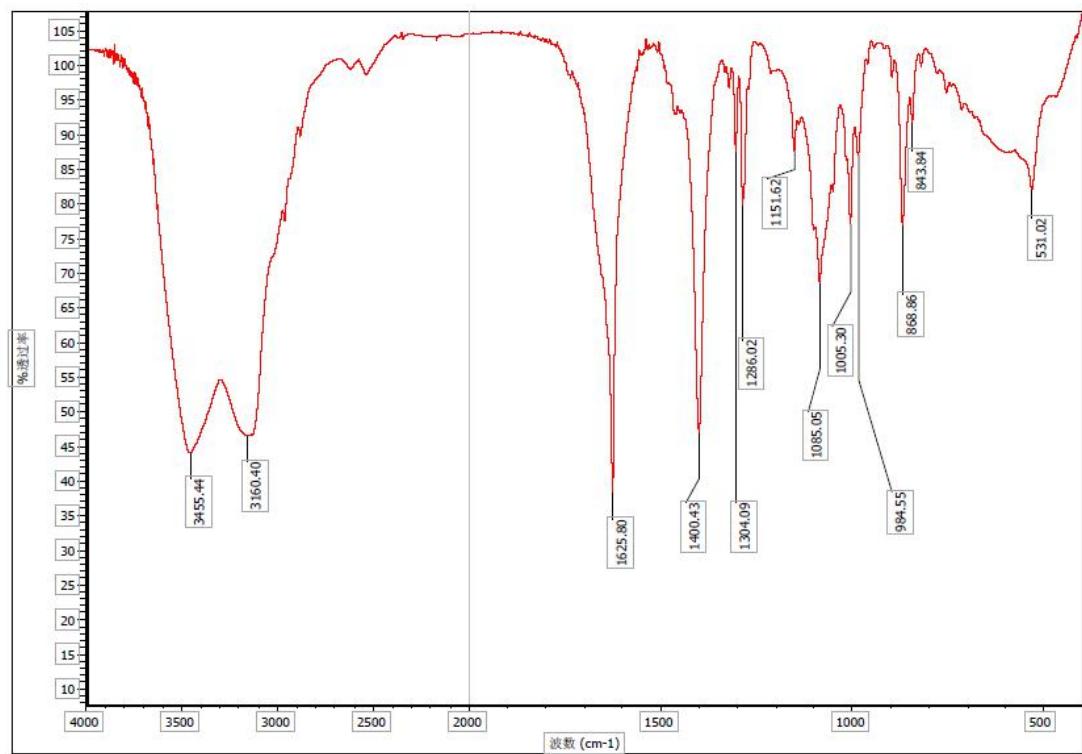
Copies of IR of 2MNS-7



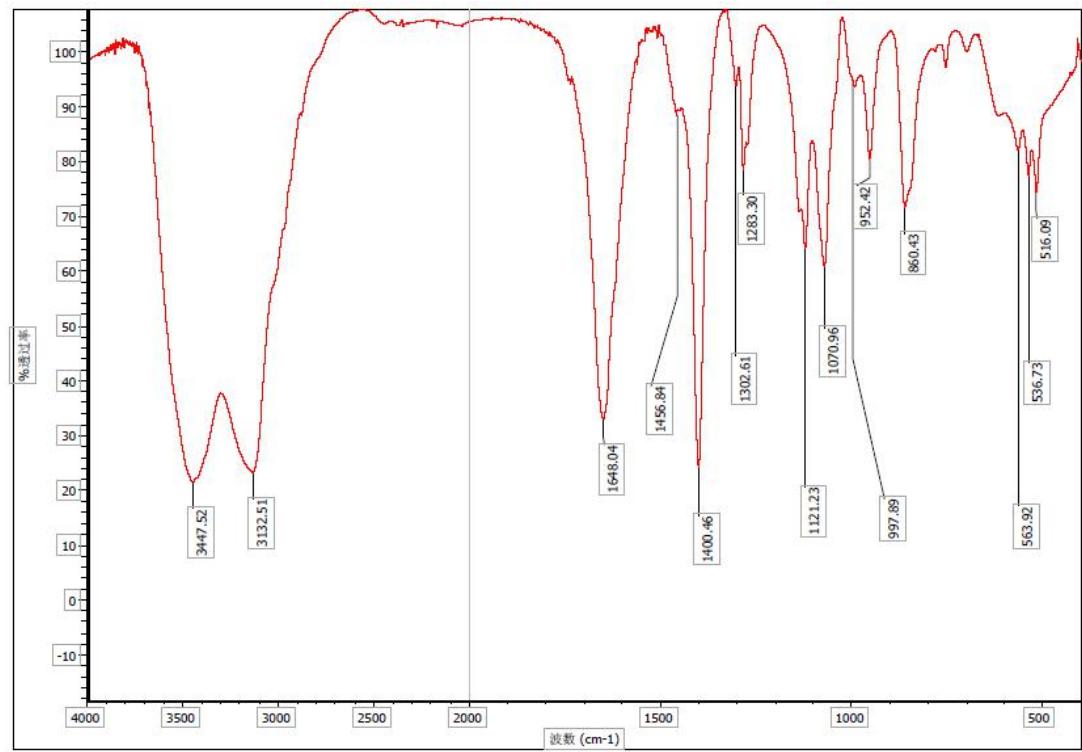
Copies of IR of 2MNS-8



Copies of IR of DNS-1



Copies of IR of DNS-2



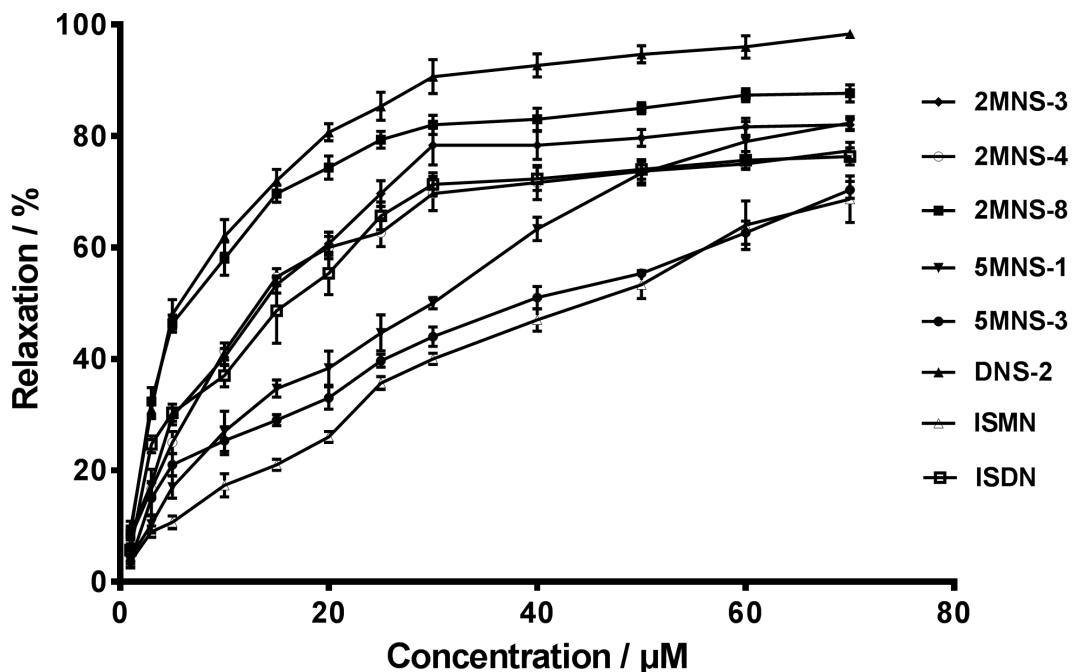


Figure.1S. The inhibitory effect of nitrates derivatives on the contraction induced by phenylephrine in mesenteric artery rings.

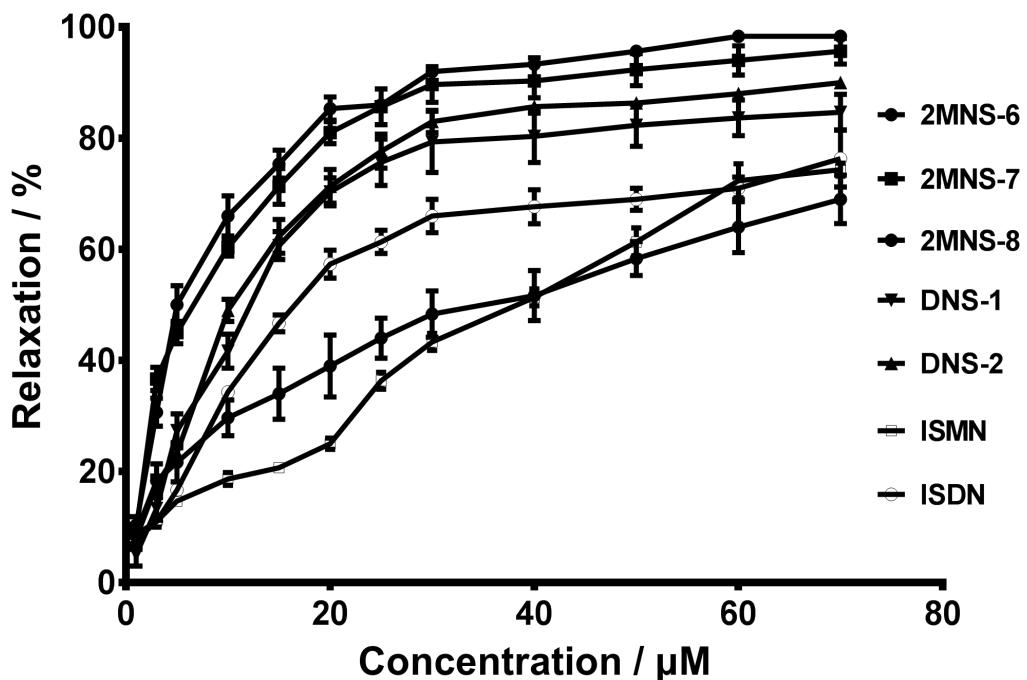


Figure.2S. The inhibitory effect of nitrates derivatives on the contraction induced by KCl in mesenteric artery rings.