

## Supporting Information

# Development of an Efficient and Sustainable Synthesis of 2-(3-Methyl-1*H*-1,2,4-triazol-1-yl) Acetic Acid under Continuous-Flow Conditions

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## *Analytical methods*

### **Gas chromatography–mass spectrometry**

ISQ LT

Injection volume: 0.30  $\mu$ L  
Column: Zebron ZB-5, 15mx0.25mm, 0.25 $\mu$ m  
Column flow: 1.20 mL/min  
Gas: Helium  
Method: 60 to 300 °C in 11.10 min  
50 to 650 amu\_EI+

The purity is given in area percent (% a/a).

### **Liquid chromatography–mass spectrometry**

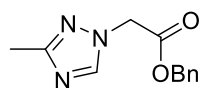
Waters iClass, Thermo MSQ Plus and DAD

Injection volume: 0.15  $\mu$ L  
Column: Zorbax RRHD SB-AQ, 1.8  $\mu$ m, 2.1 $\times$ 50 mm  
Column flow: 0.8 mL/min  
Eluent: Water, 0.04% TFA (Eluent A)  
Acetonitrile (Eluent B)  
Gradient: 0.00 min 5% B  
1.20 min 95% B  
1.90 min 95% B  
2.1 min 5% B  
Temperature: 40°C

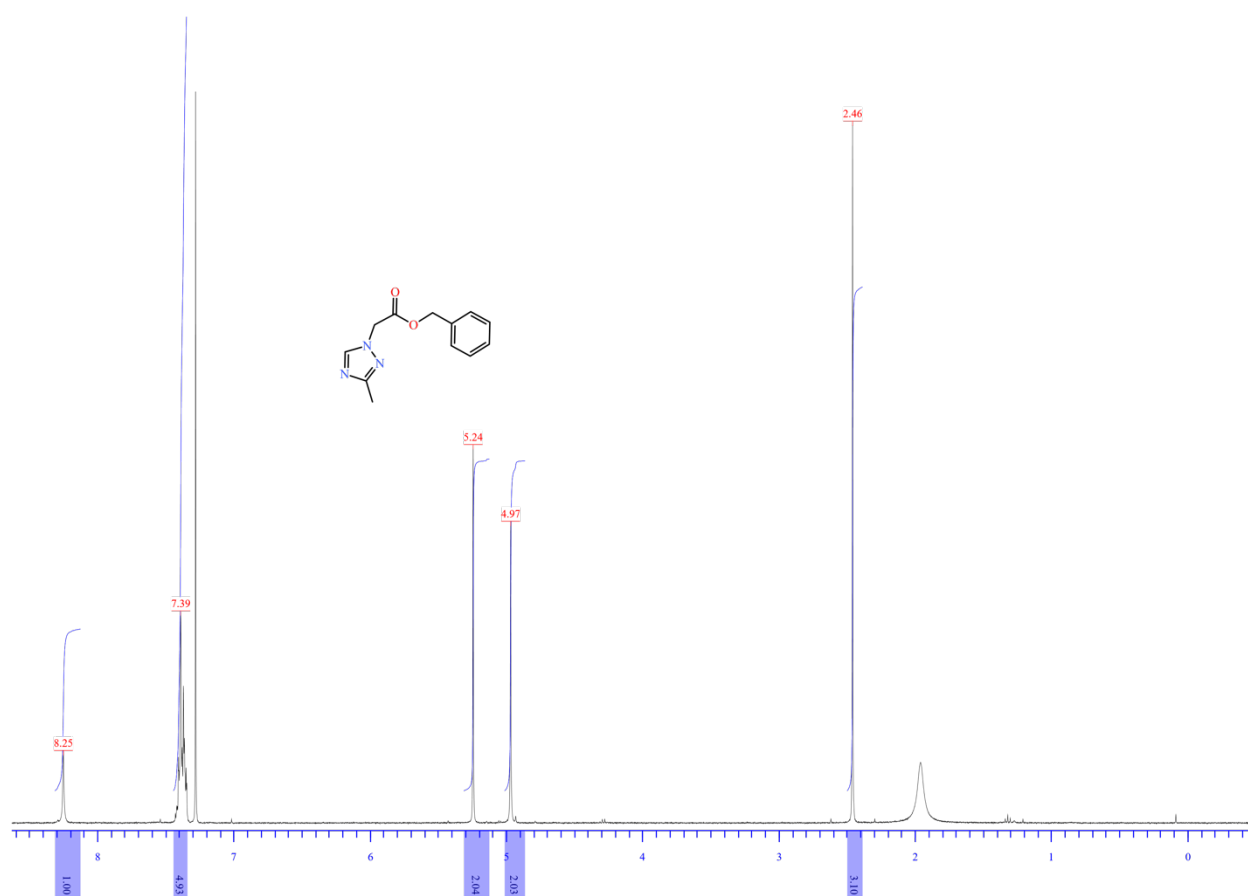
The purity is given in area percent (% a/a).

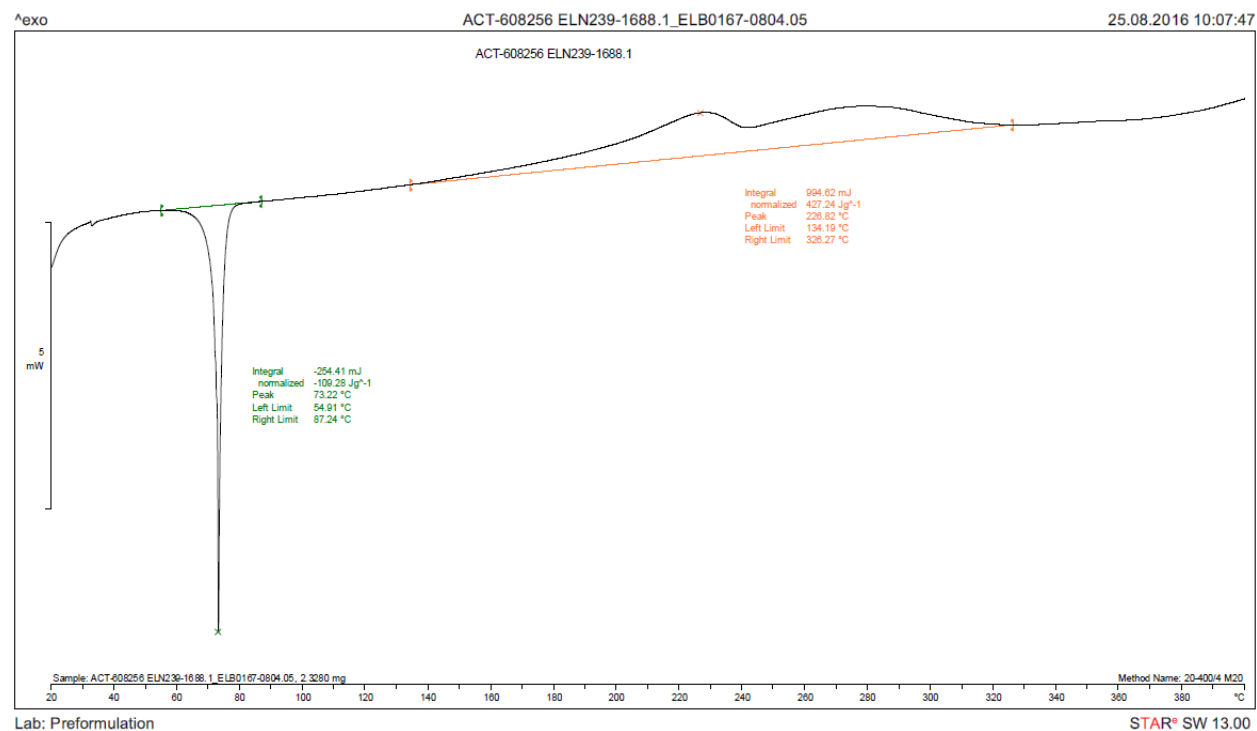
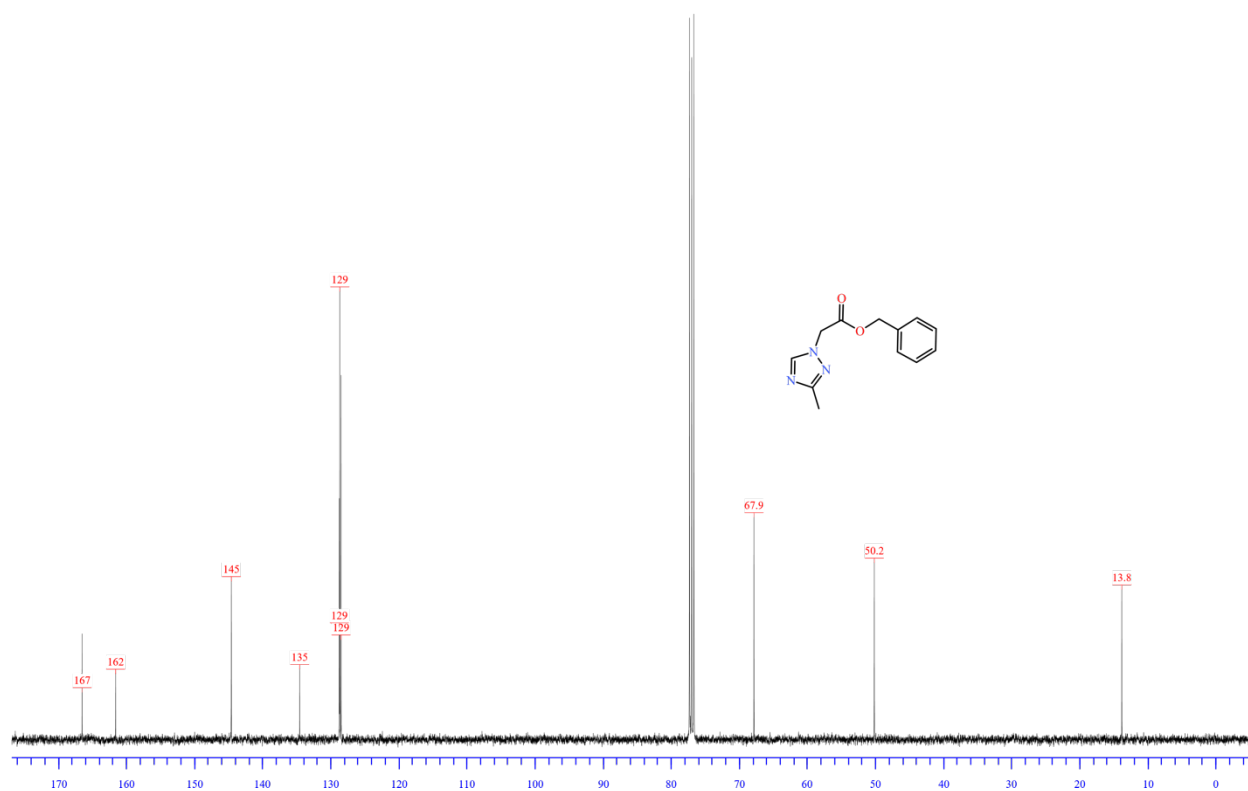
## Products characterization

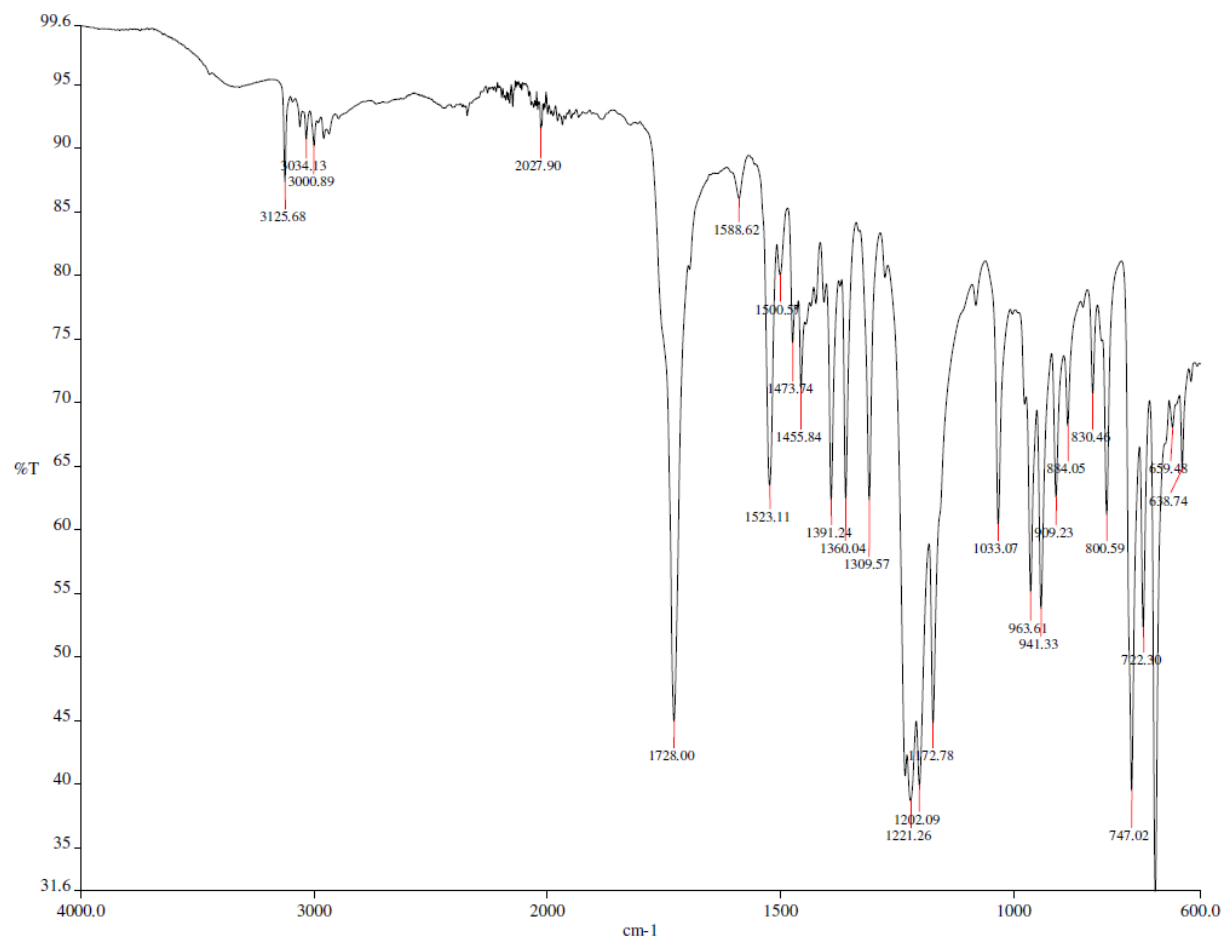
### benzyl 2-(3-methyl-1*H*-1,2,4-triazol-1-yl)acetate



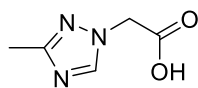
**11a**



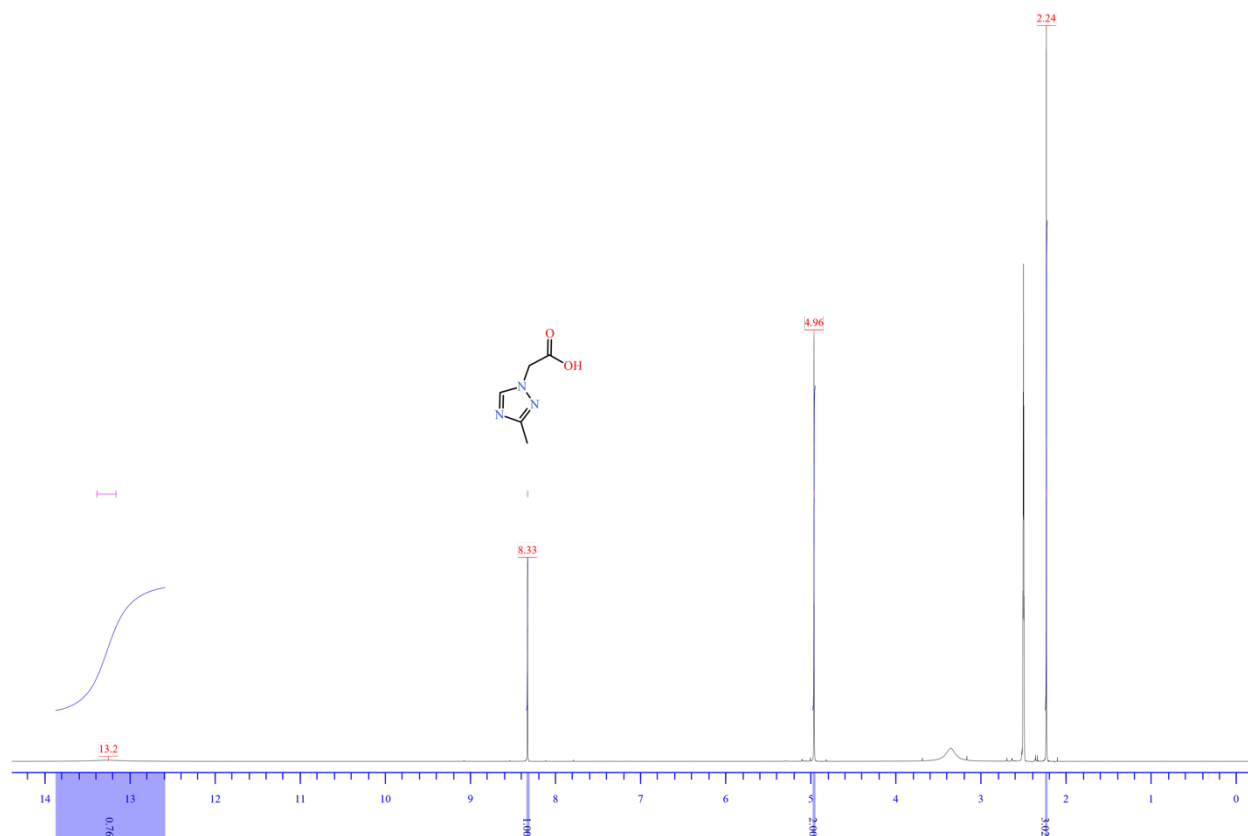


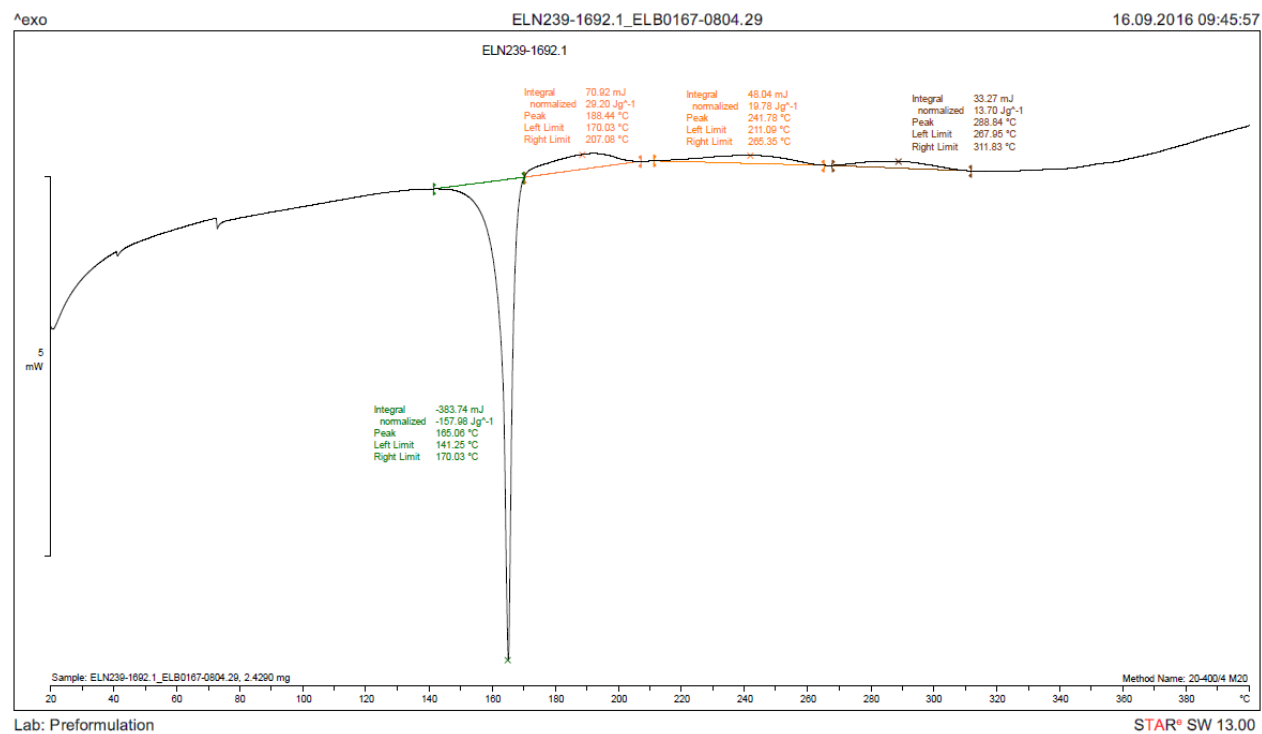
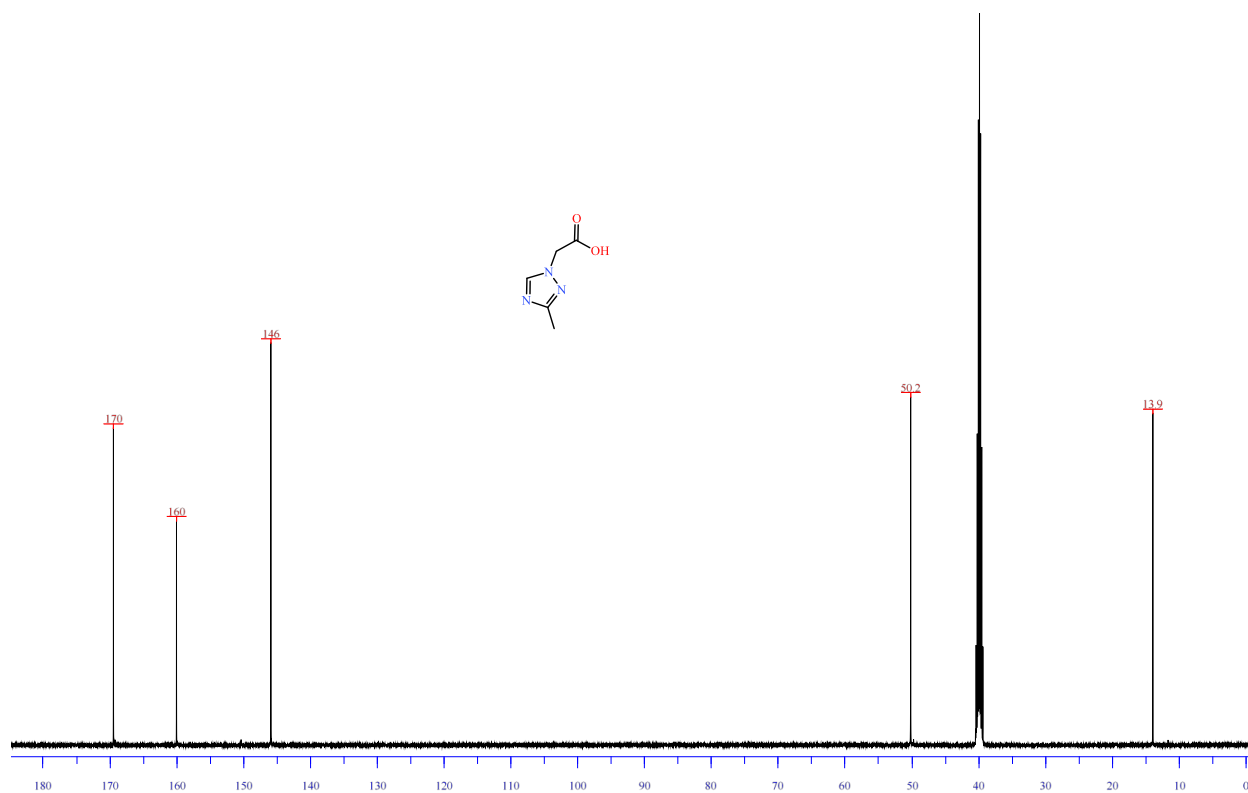


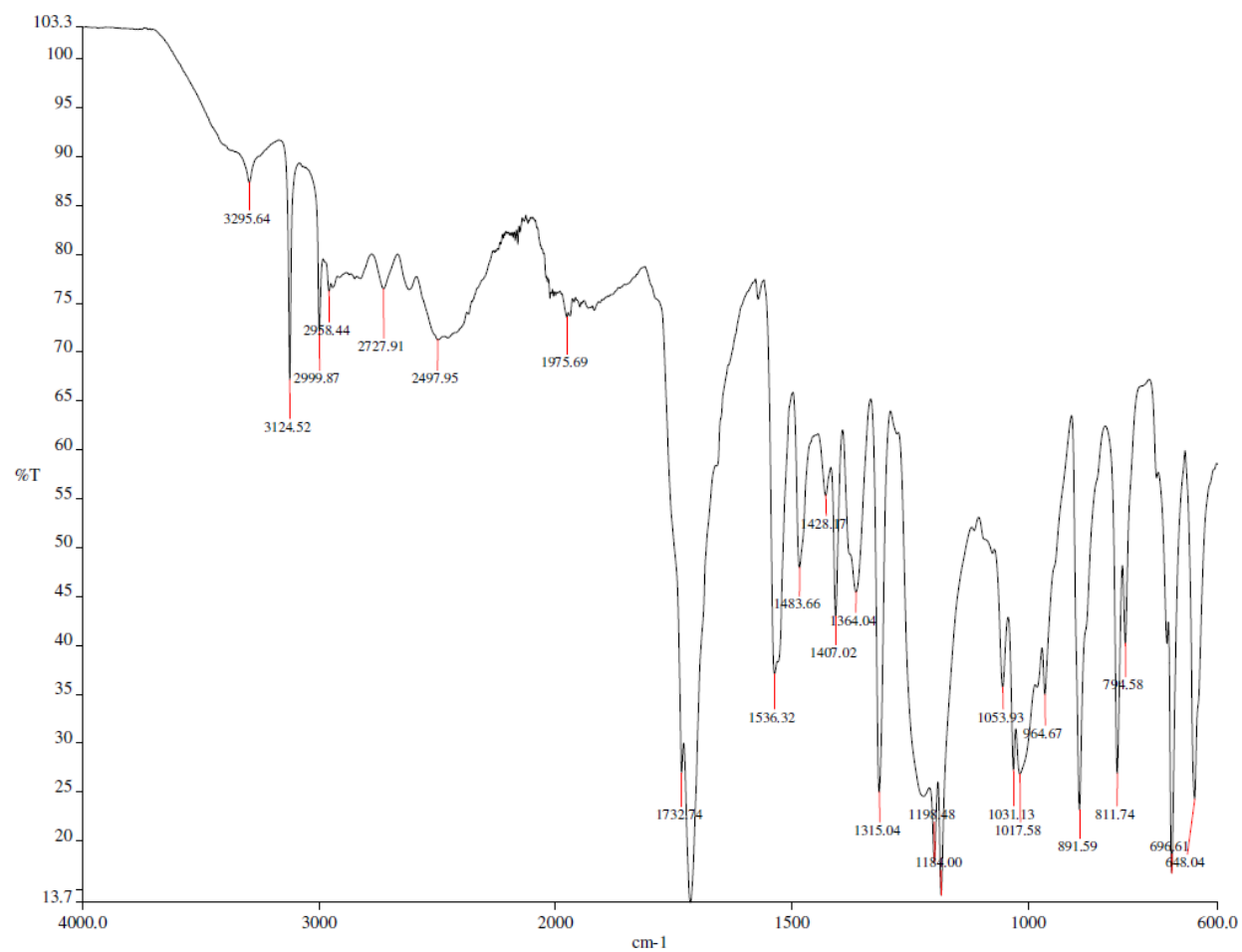
# 2-(3-methyl-1*H*-1,2,4-triazol-1-yl)acetic acid



1

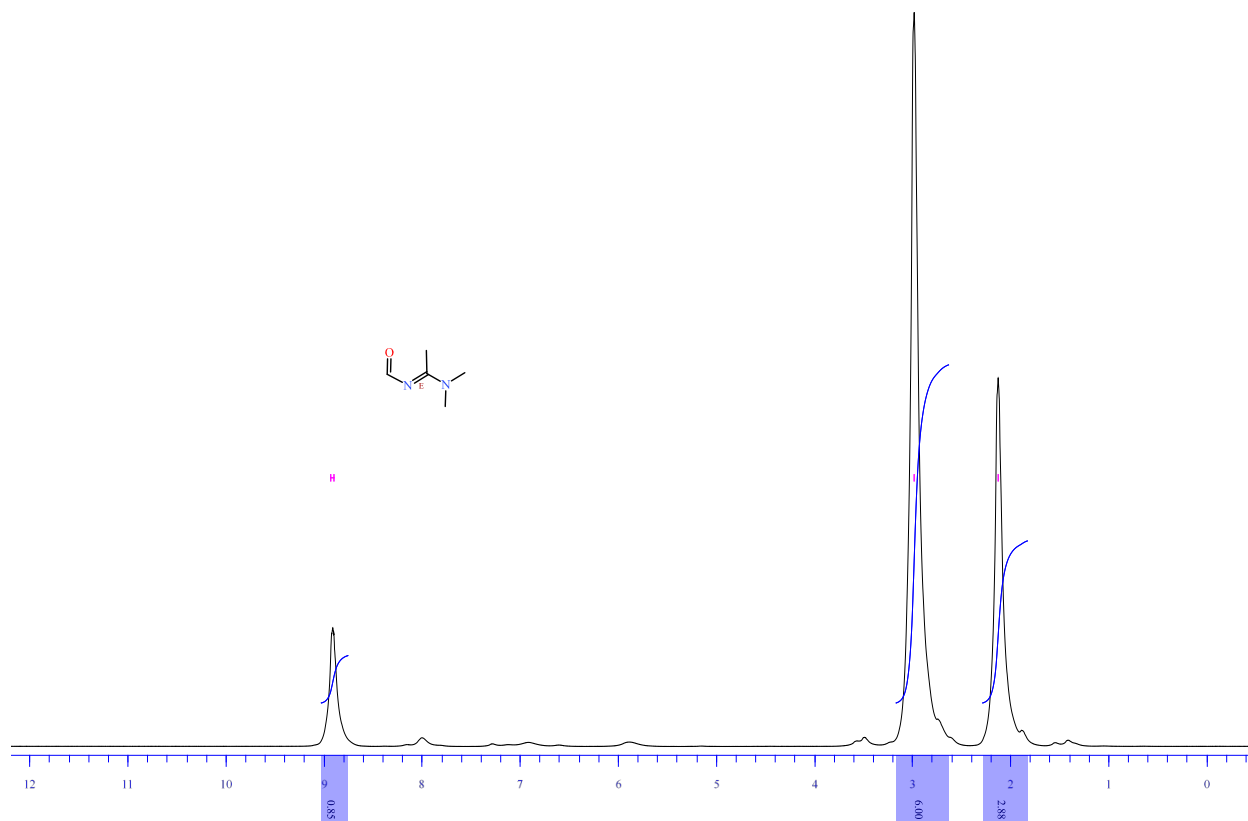
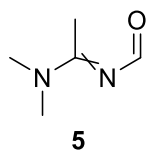


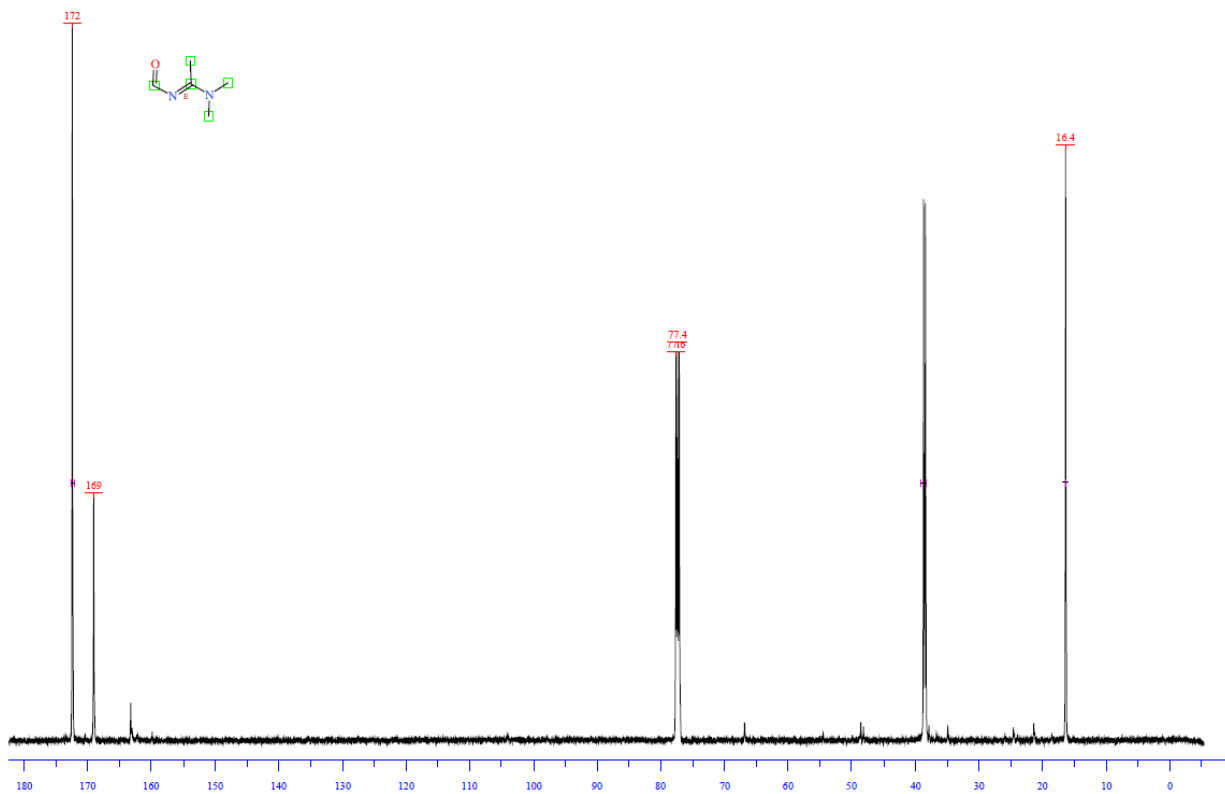




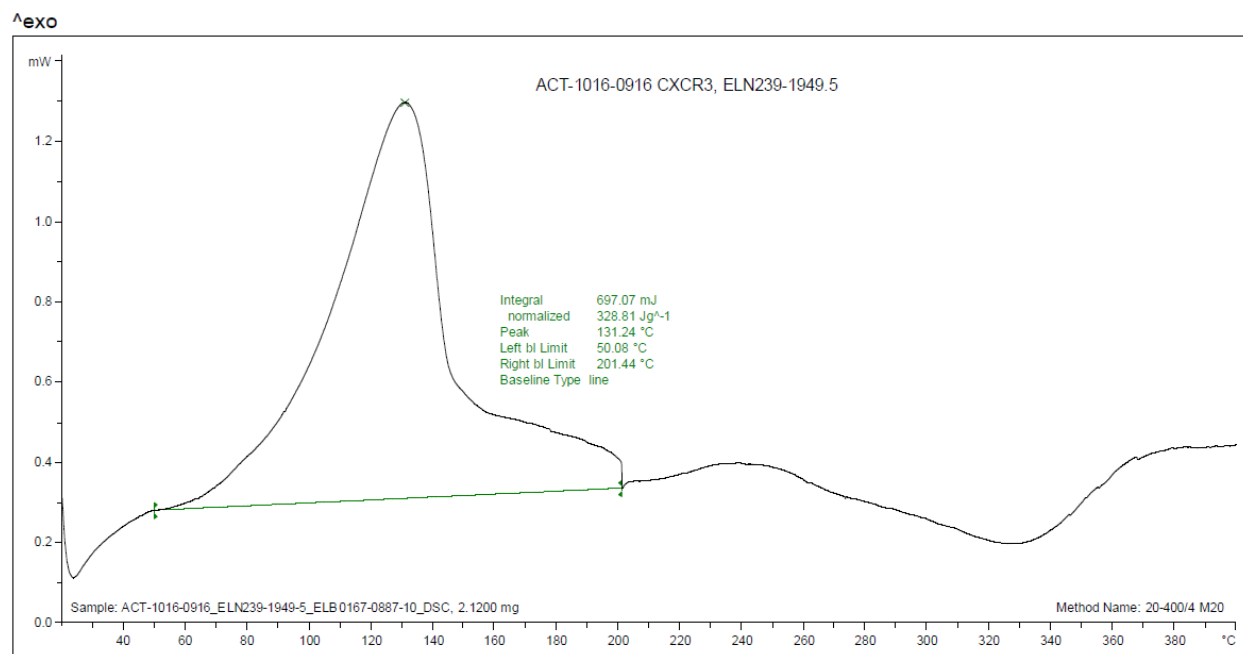


***N'*-formyl-*N,N*-dimethylacetimidamide**





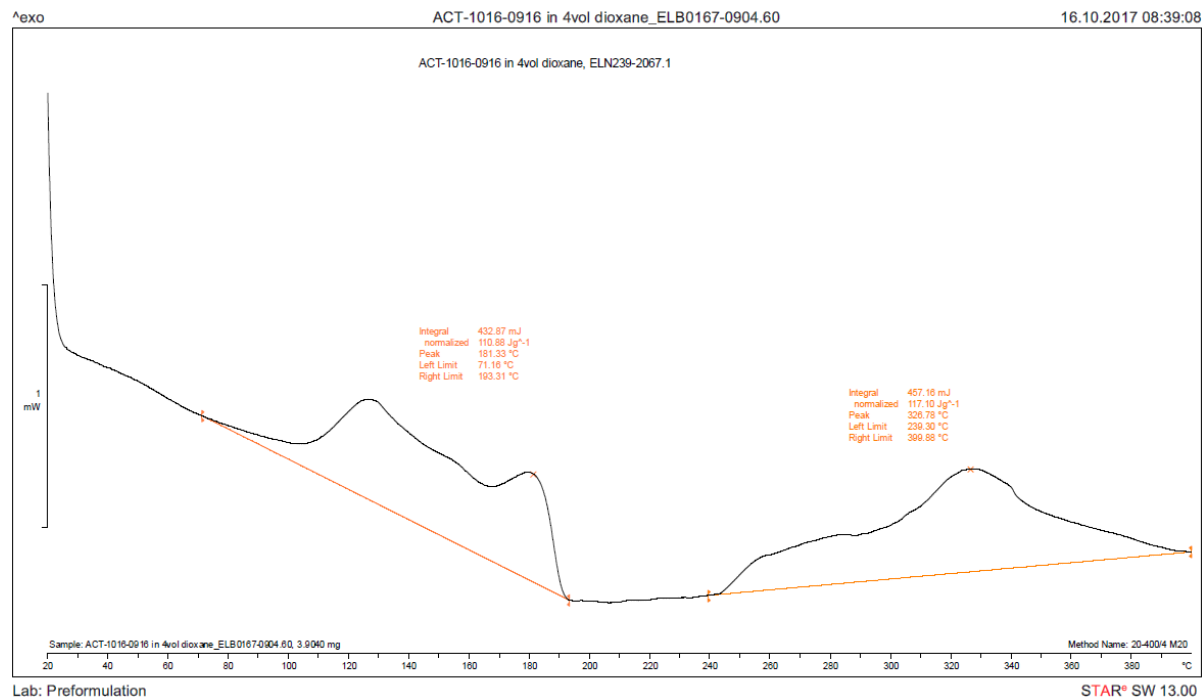
pure:



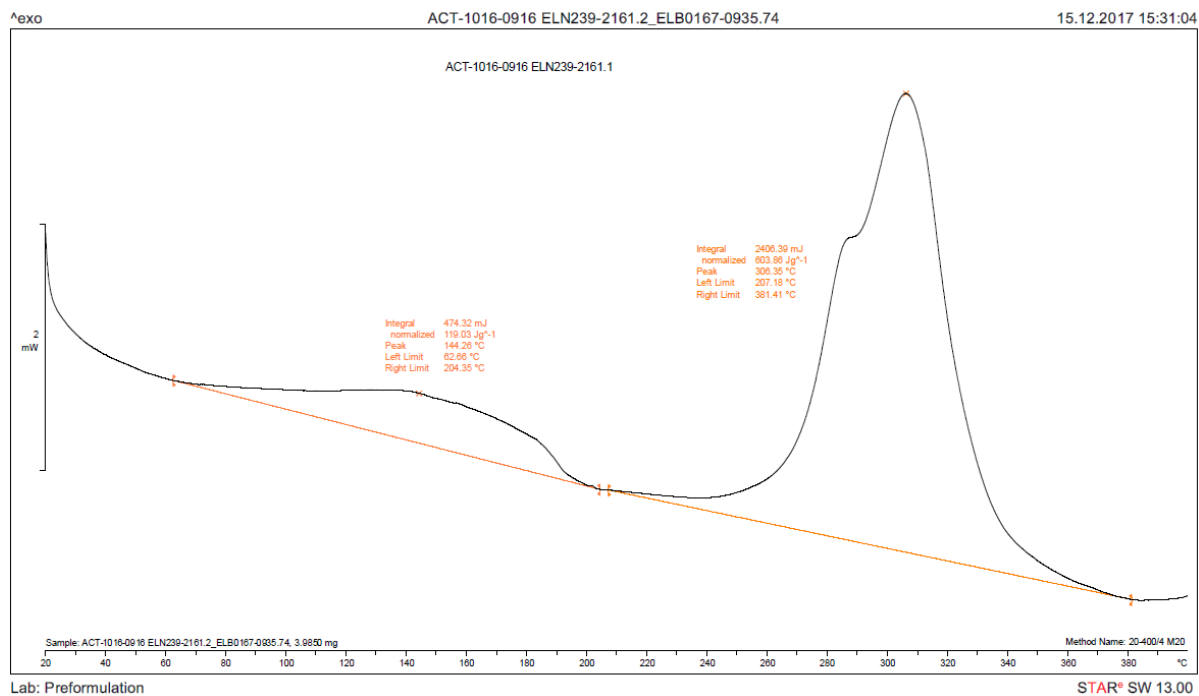
ACTELION: Preformulation

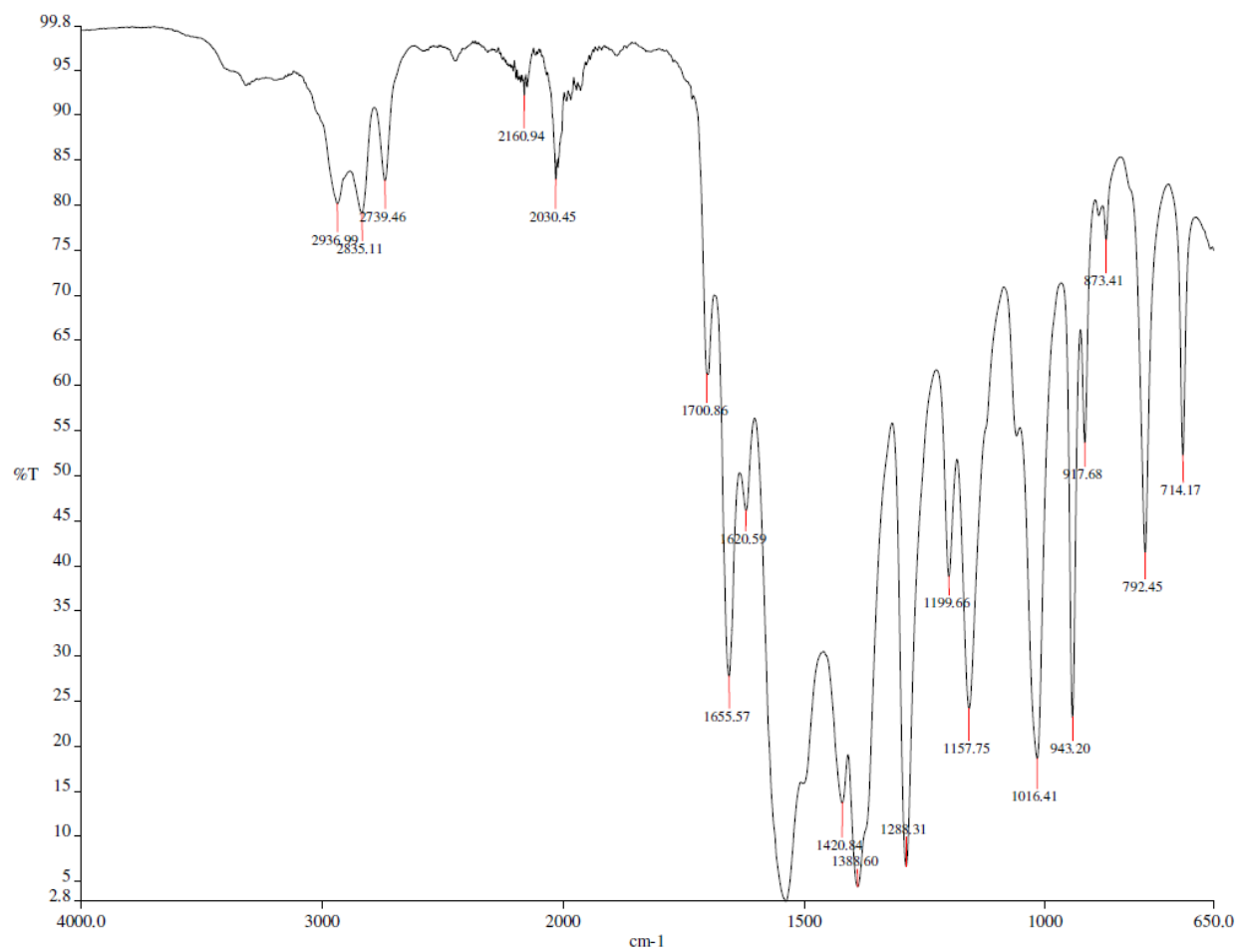
STAR® SW 13.00

in dioxane:

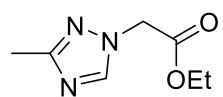


in DMSO:

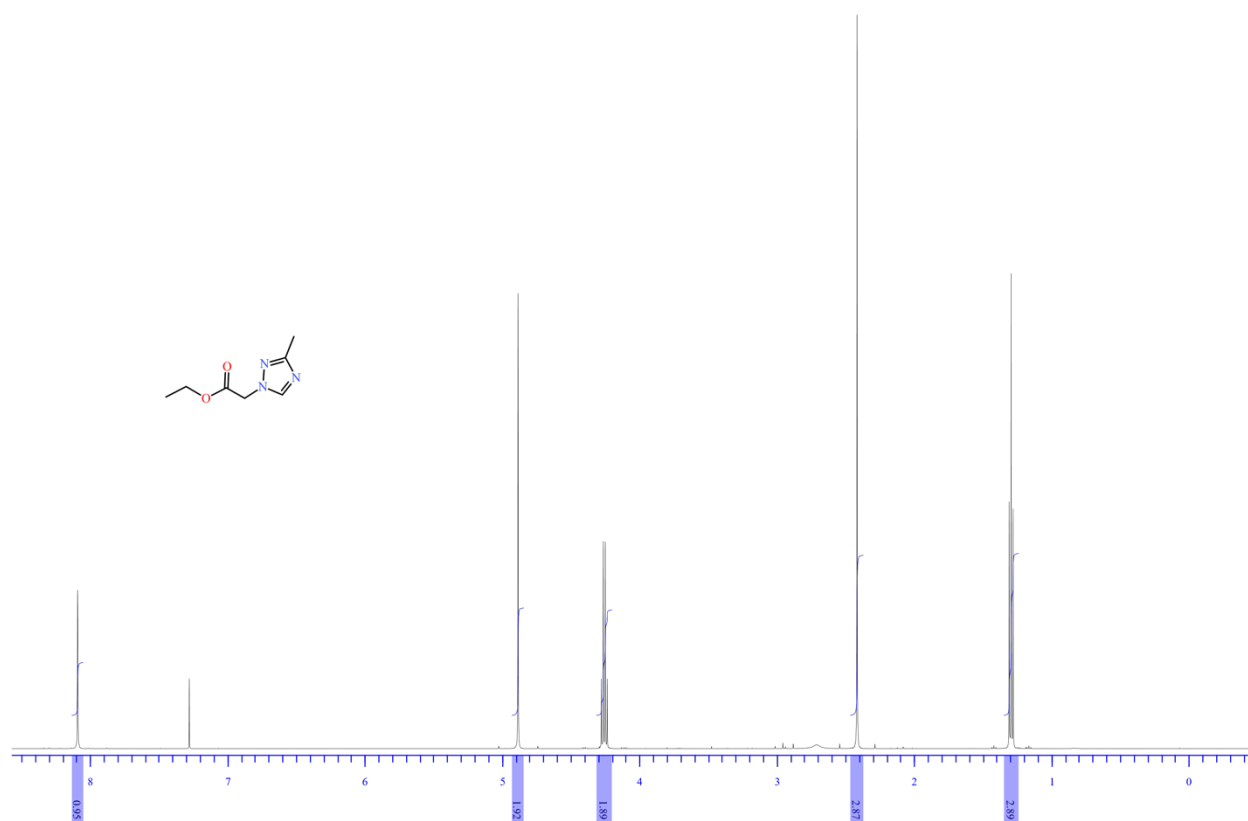


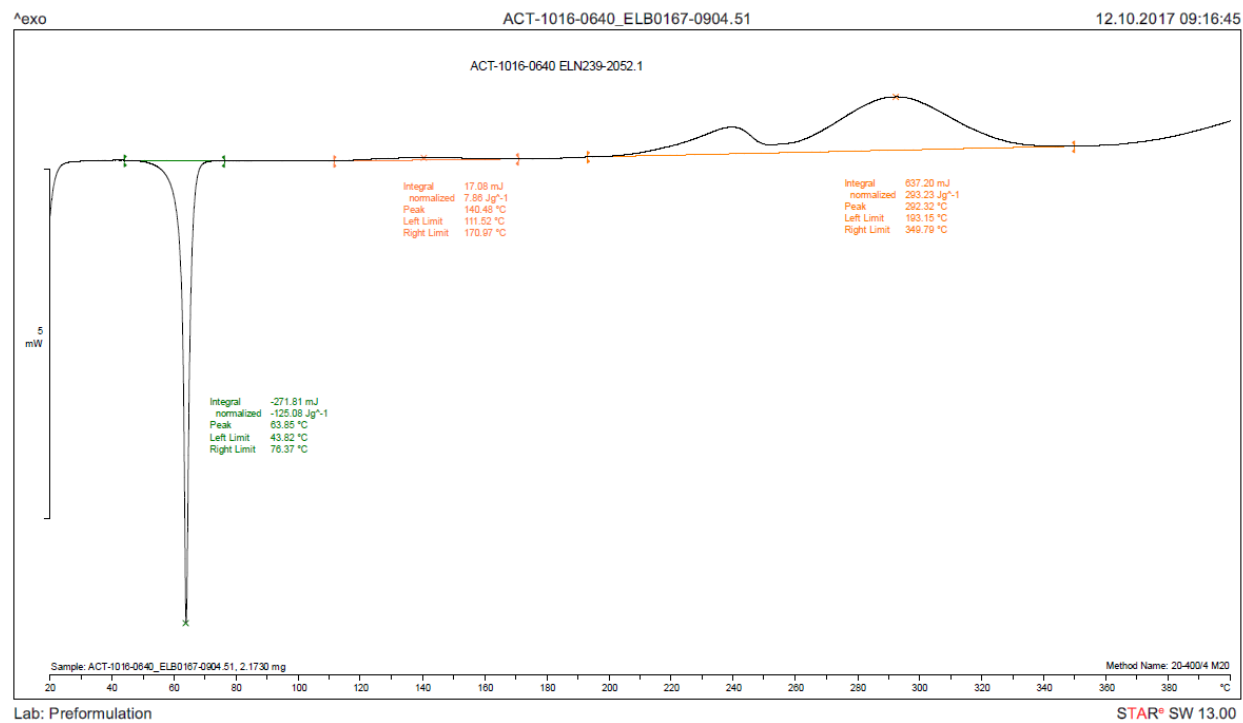
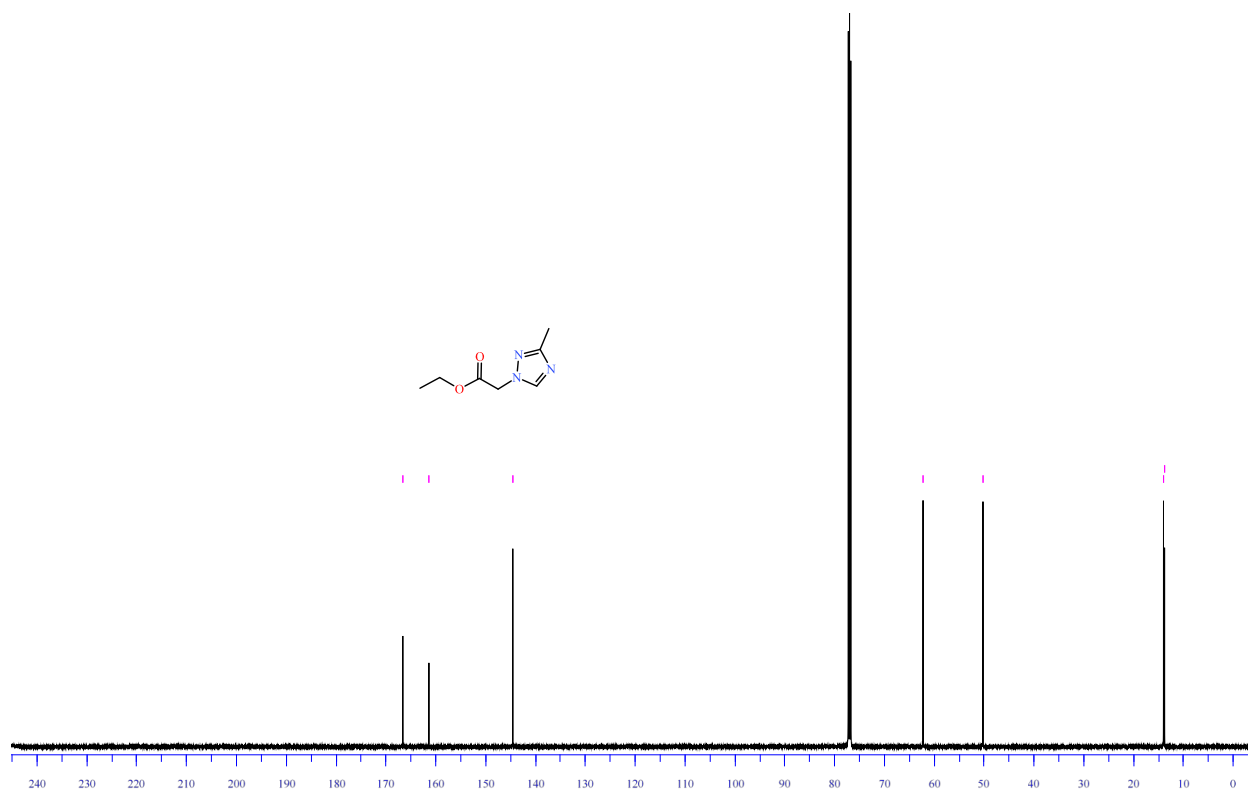


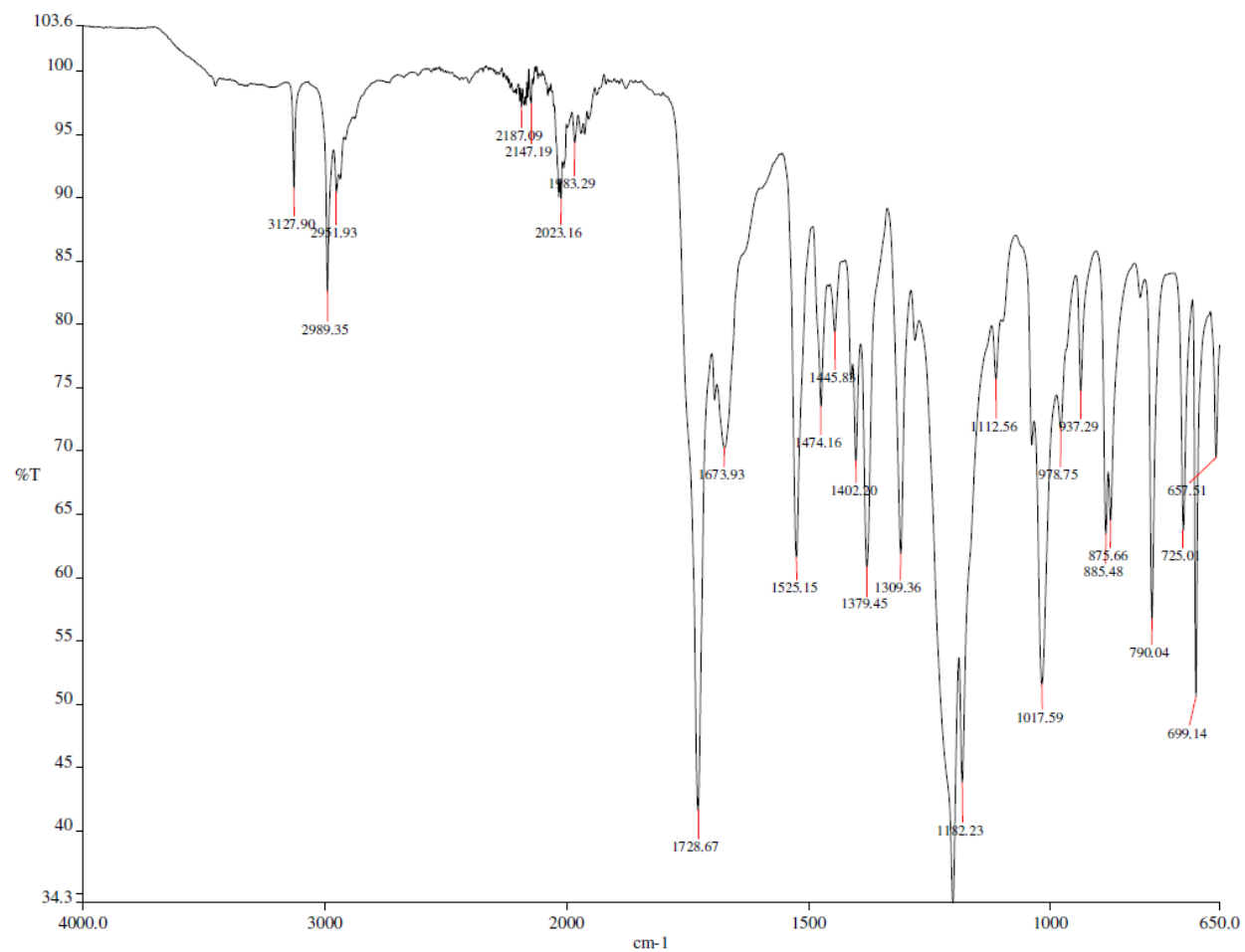
ethyl 2-(3-methyl-1*H*-1,2,4-triazol-1-yl)acetate



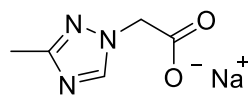
**11b**







**2-(3-methyl-1*H*-1,2,4-triazol-1-yl) acetate sodium(I) salt**



**12**

