

Supporting Information

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## SUPPORTING INFORMATION

### **Halolactonization of *N*-acyl-*N*-(2-cyclohex-1-en-1-yl)-6-methylphenylglycines: towards production of 4,1-benzoxazoheterocycles**

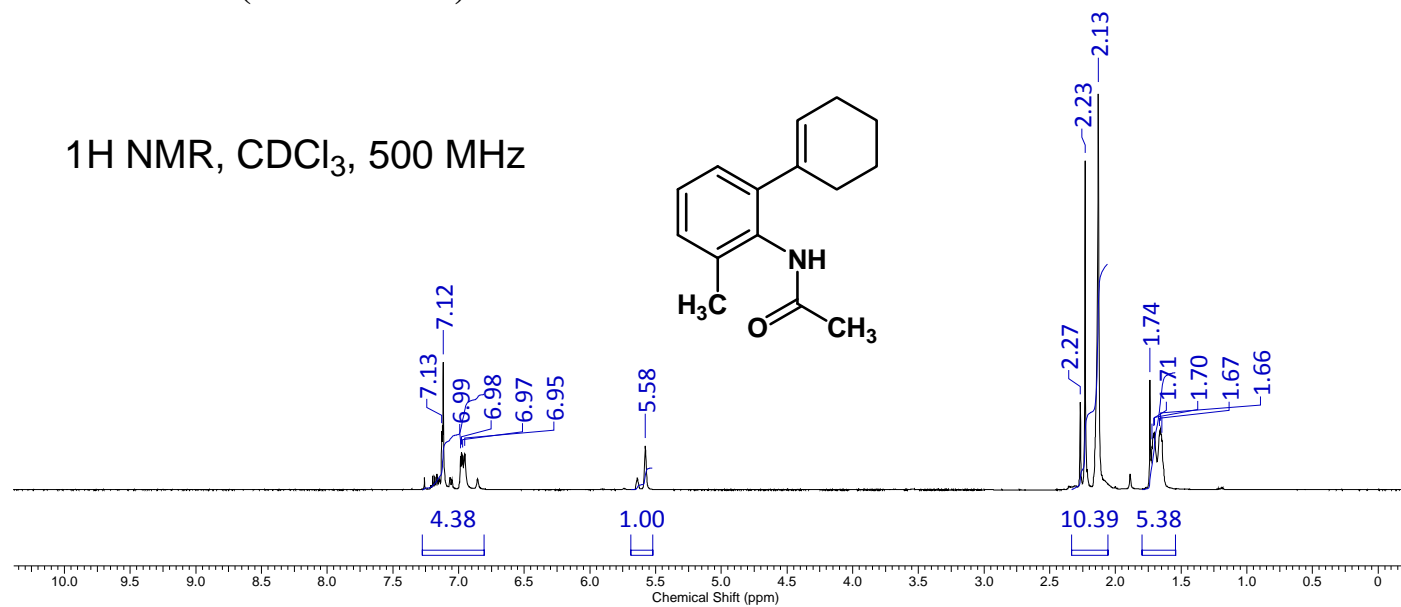
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[gataullin@anrb.ru](mailto:gataullin@anrb.ru)

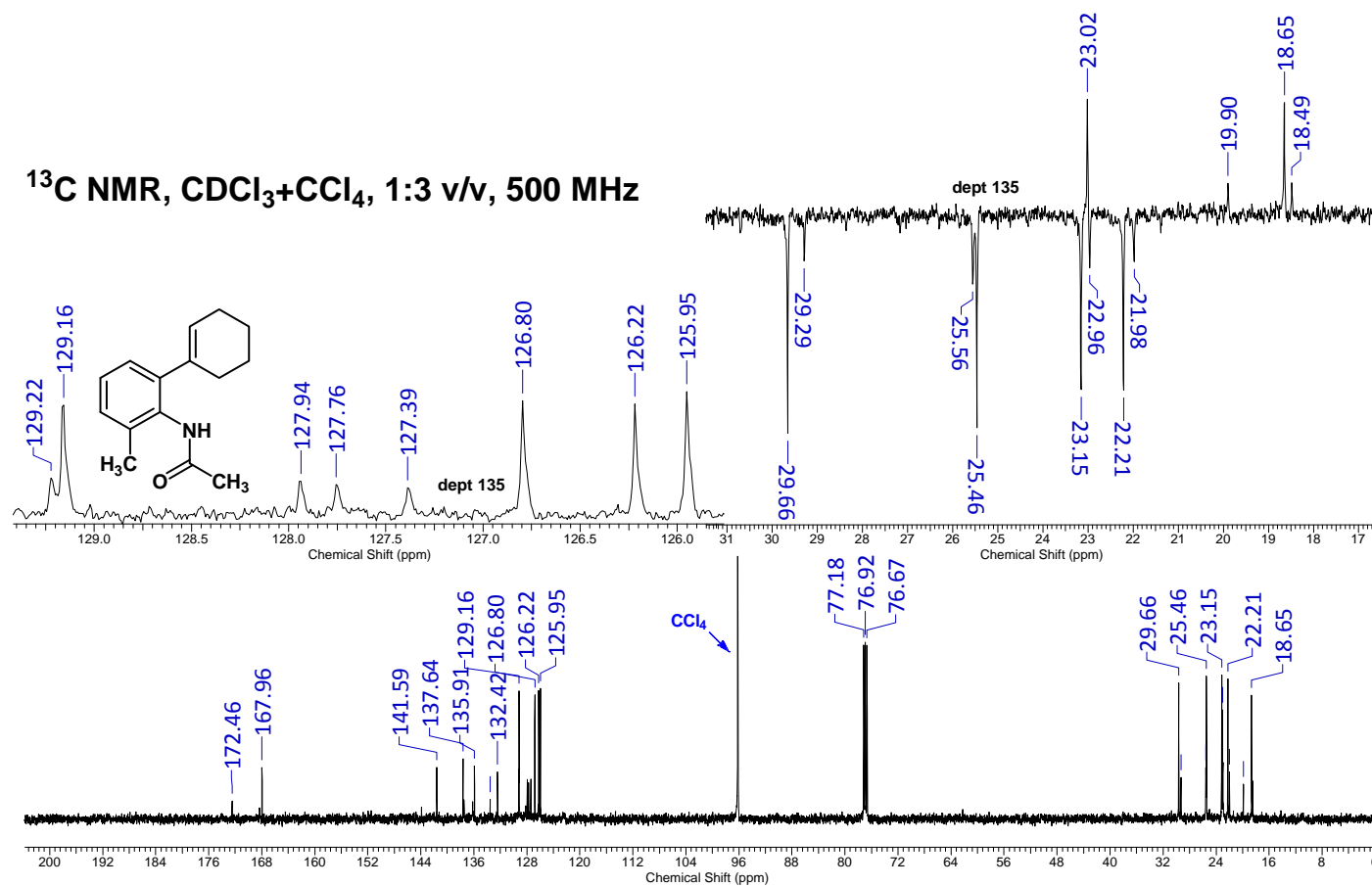
# S 2

## Acetamide 2a (rotamers 1:3)

<sup>1</sup>H NMR, CDCl<sub>3</sub>, 500 MHz

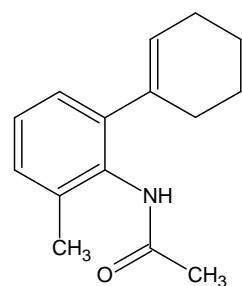


<sup>13</sup>C NMR, CDCl<sub>3</sub>+CCl<sub>4</sub>, 1:3 v/v, 500 MHz



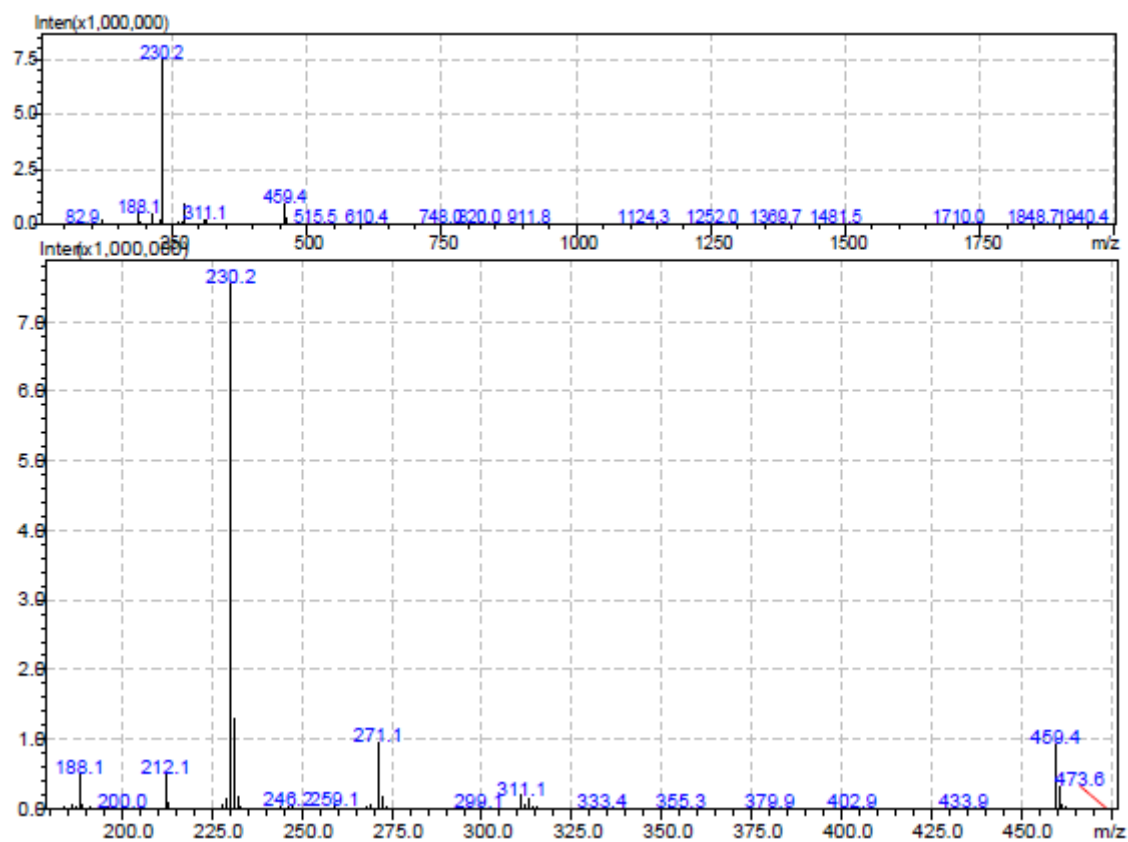
S 3

Acetamide 2a



$C_{15}H_{19}NO$ ,  $M_r = 229.31$

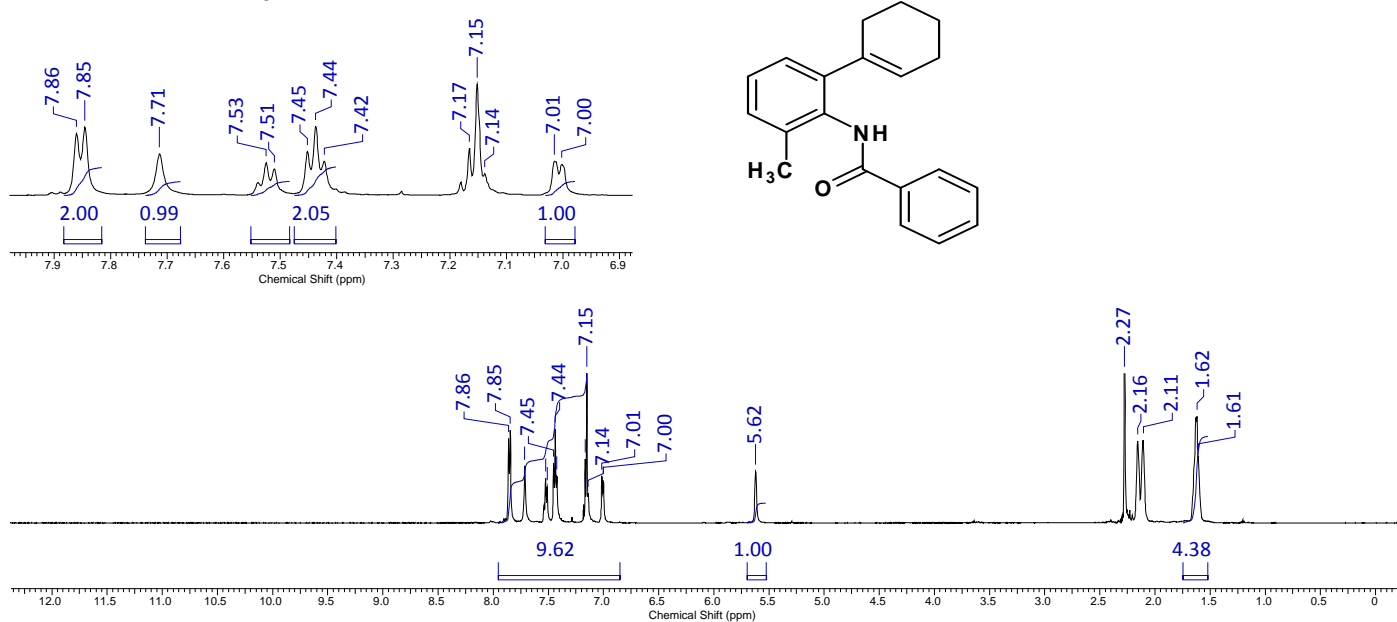
MS (APCI, MeCN/HOH 100/0, 0.1 ml/min). Scan(C+) Ret. Time : 26.900 min



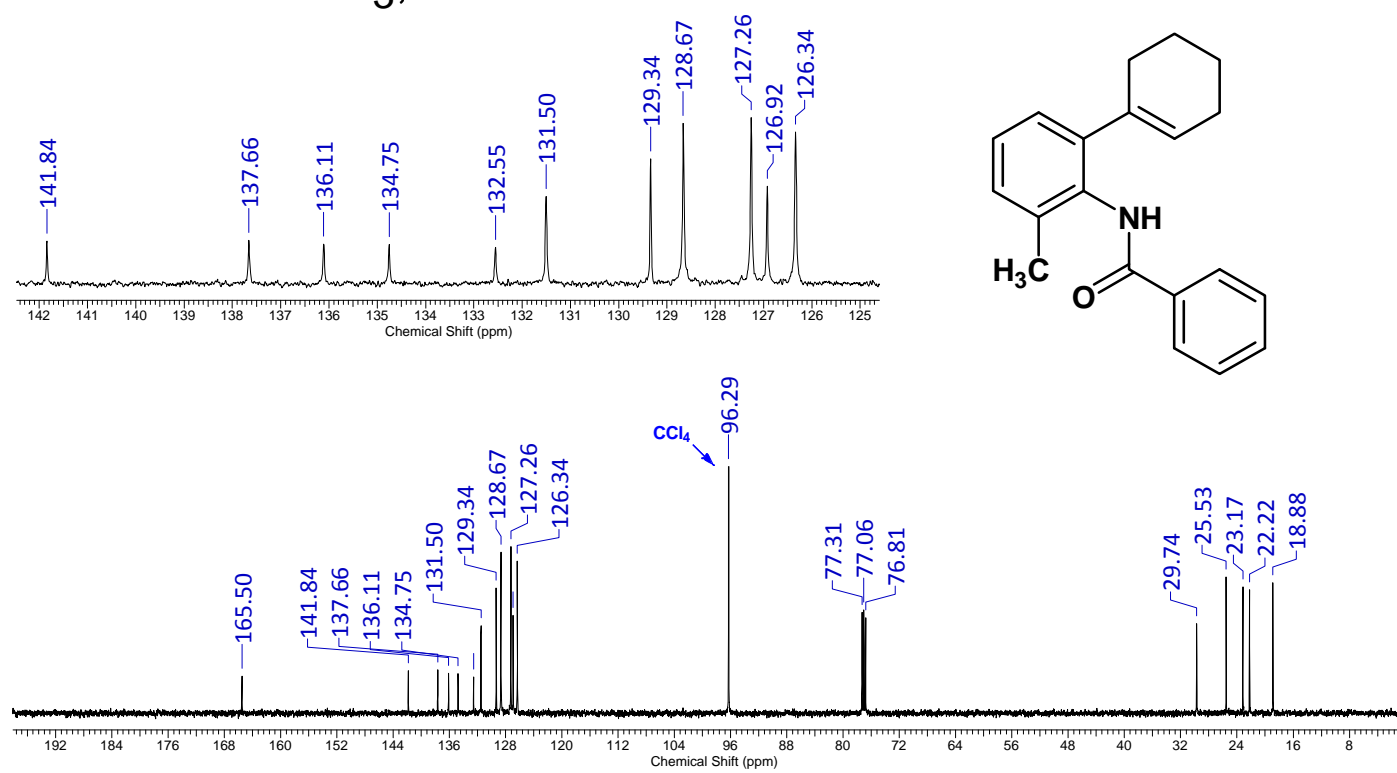
# S 4

## Benzamide 2b

$^1\text{H}$  NMR  $\text{CDCl}_3$ , 500 MHz

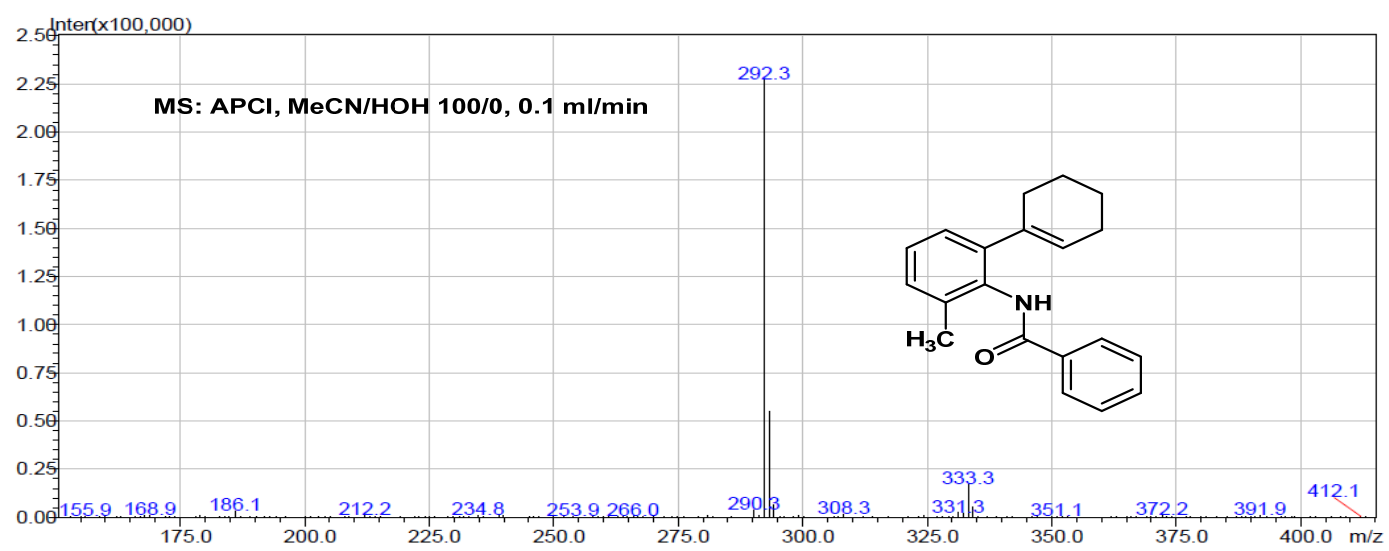


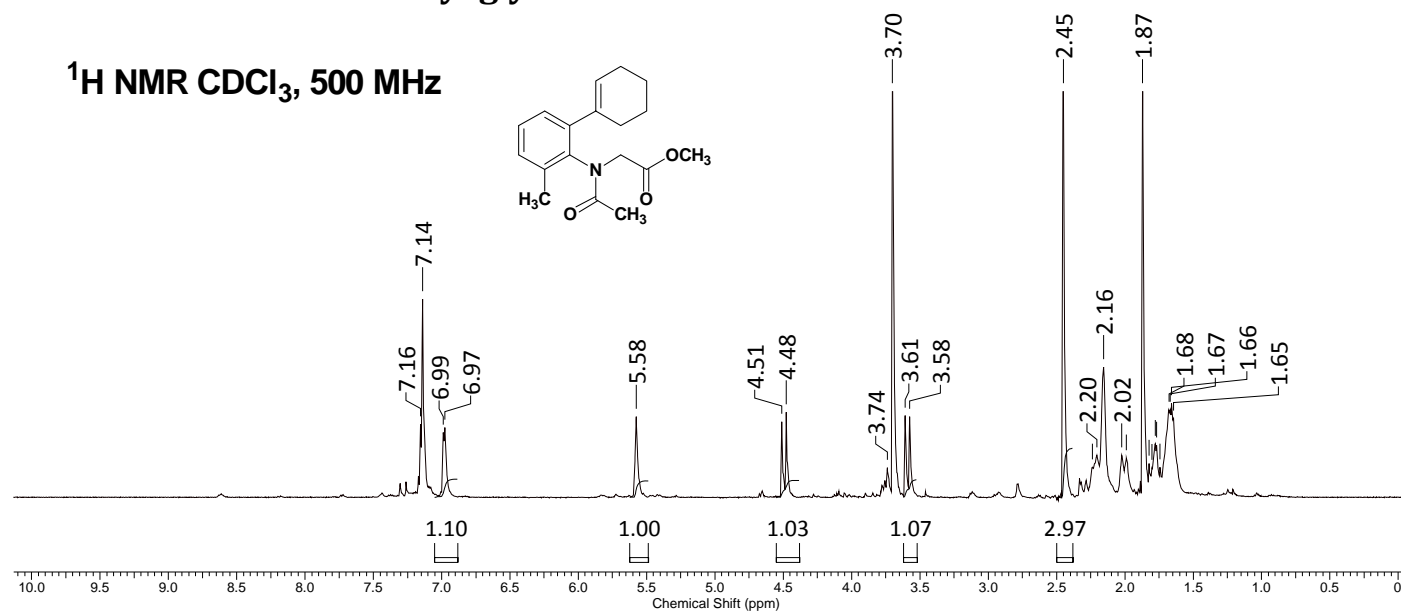
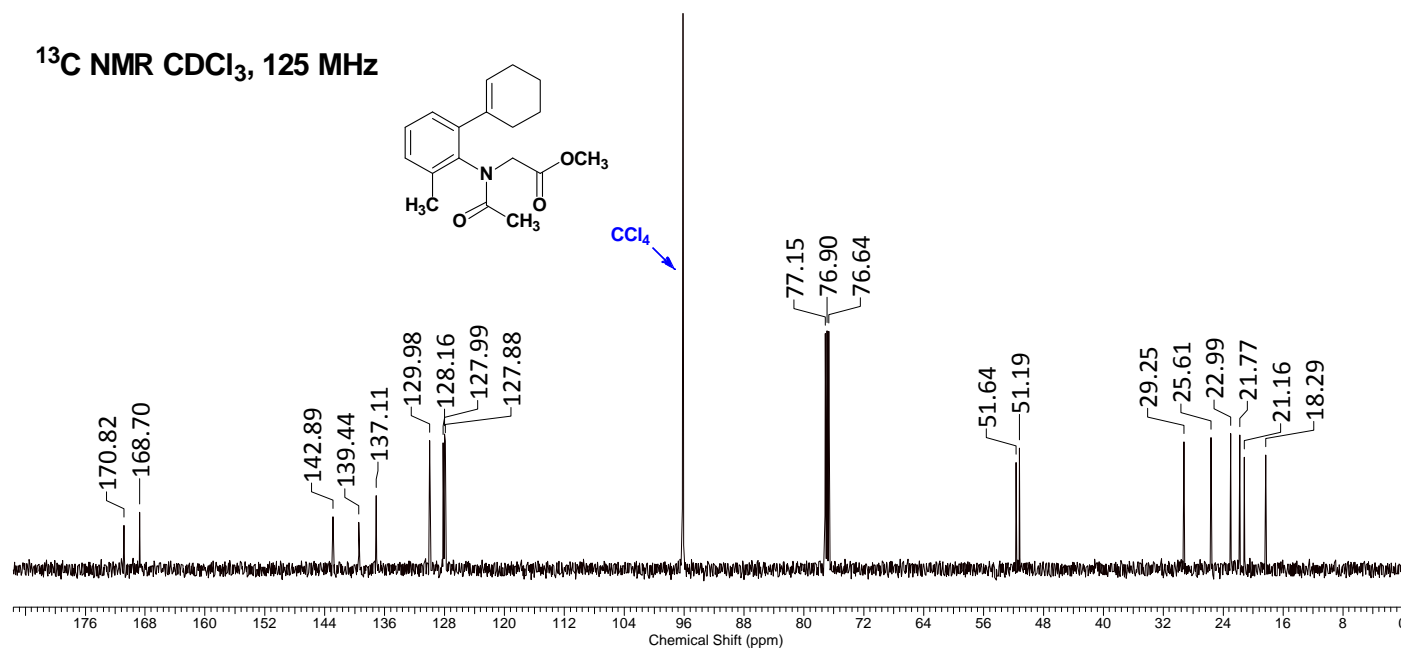
$^{13}\text{C}$  NMR  $\text{CDCl}_3$ , 125 MHz



S 5

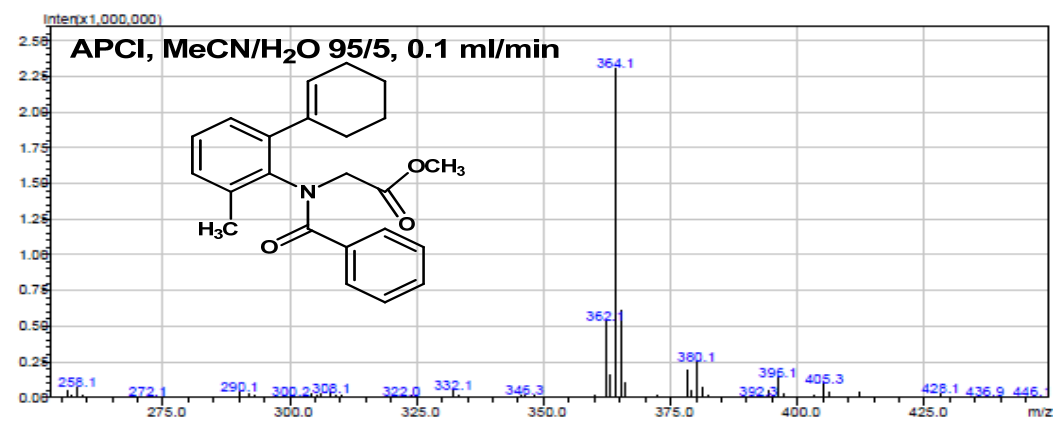
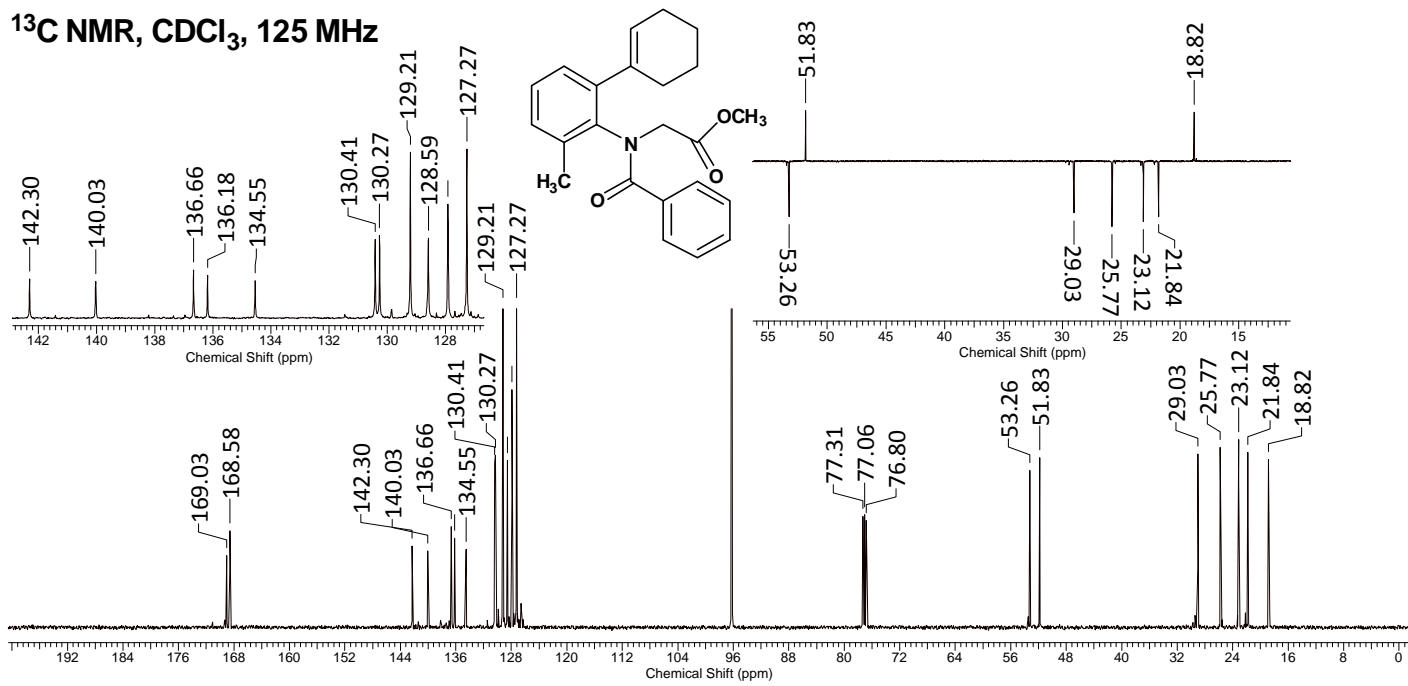
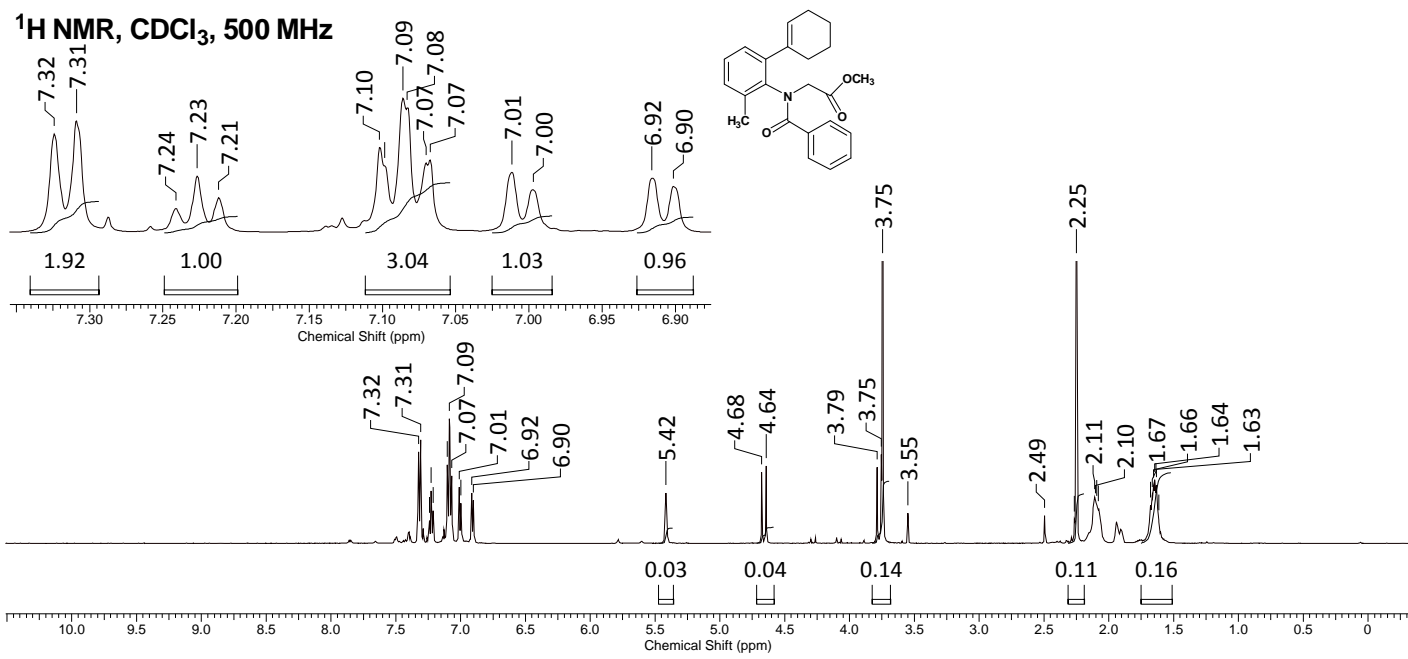
Benzamide 2b



**S 6****Methyl glycinate 3a****<sup>1</sup>H NMR CDCl<sub>3</sub>, 500 MHz****<sup>13</sup>C NMR CDCl<sub>3</sub>, 125 MHz**

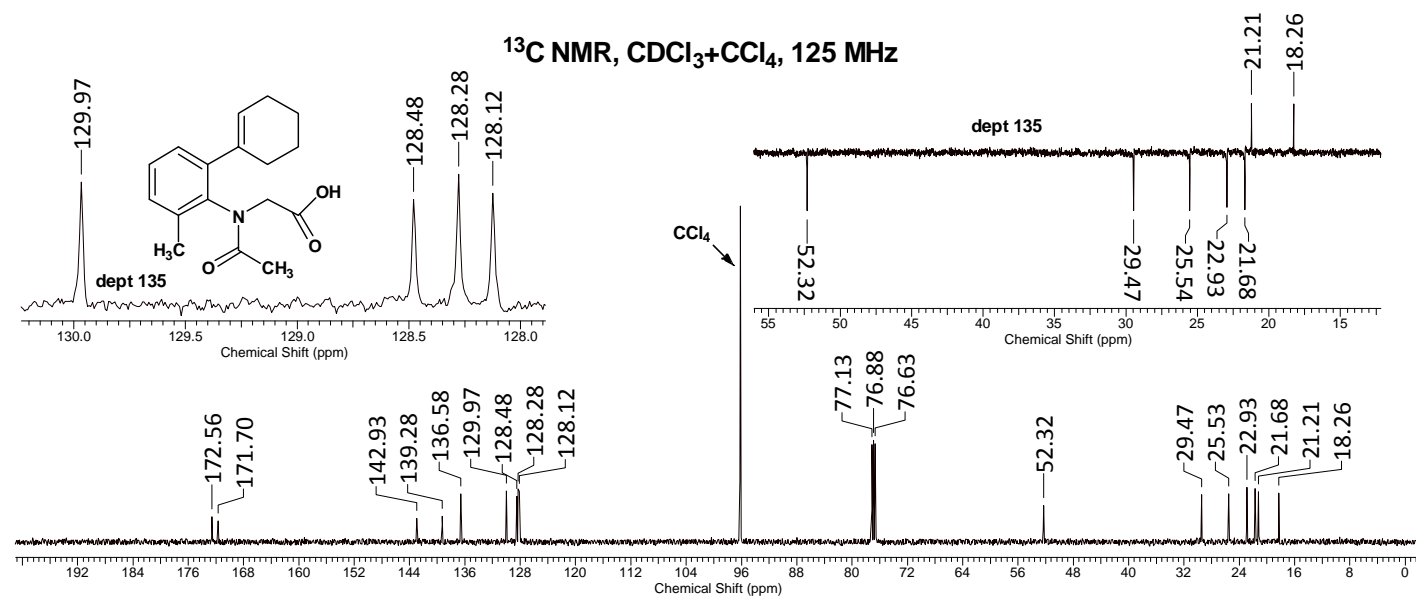
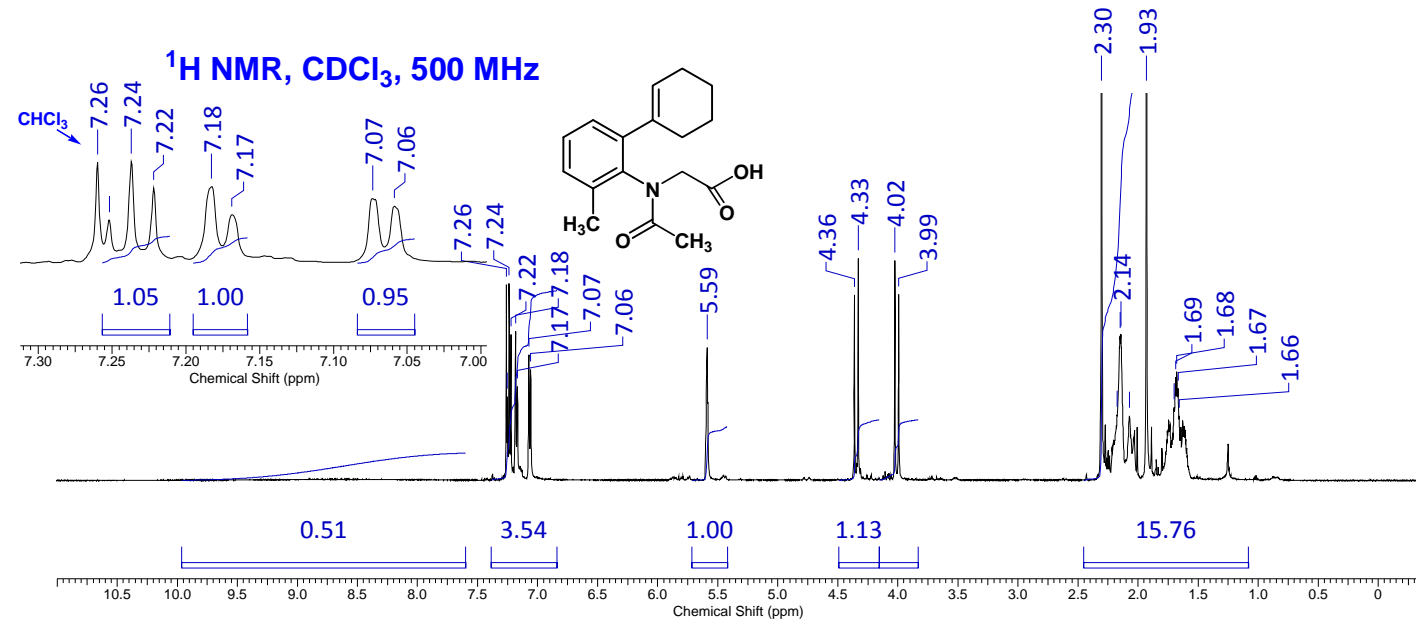
S 7

## Methyl glycinate 3b



S 8

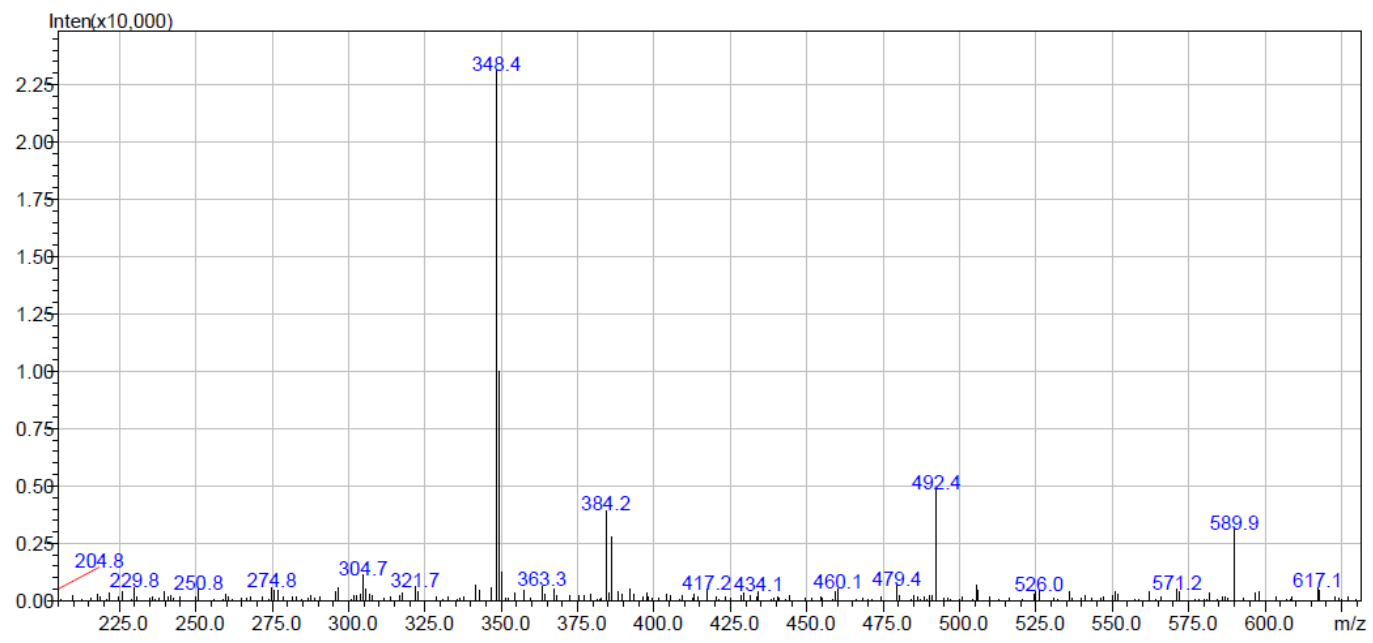
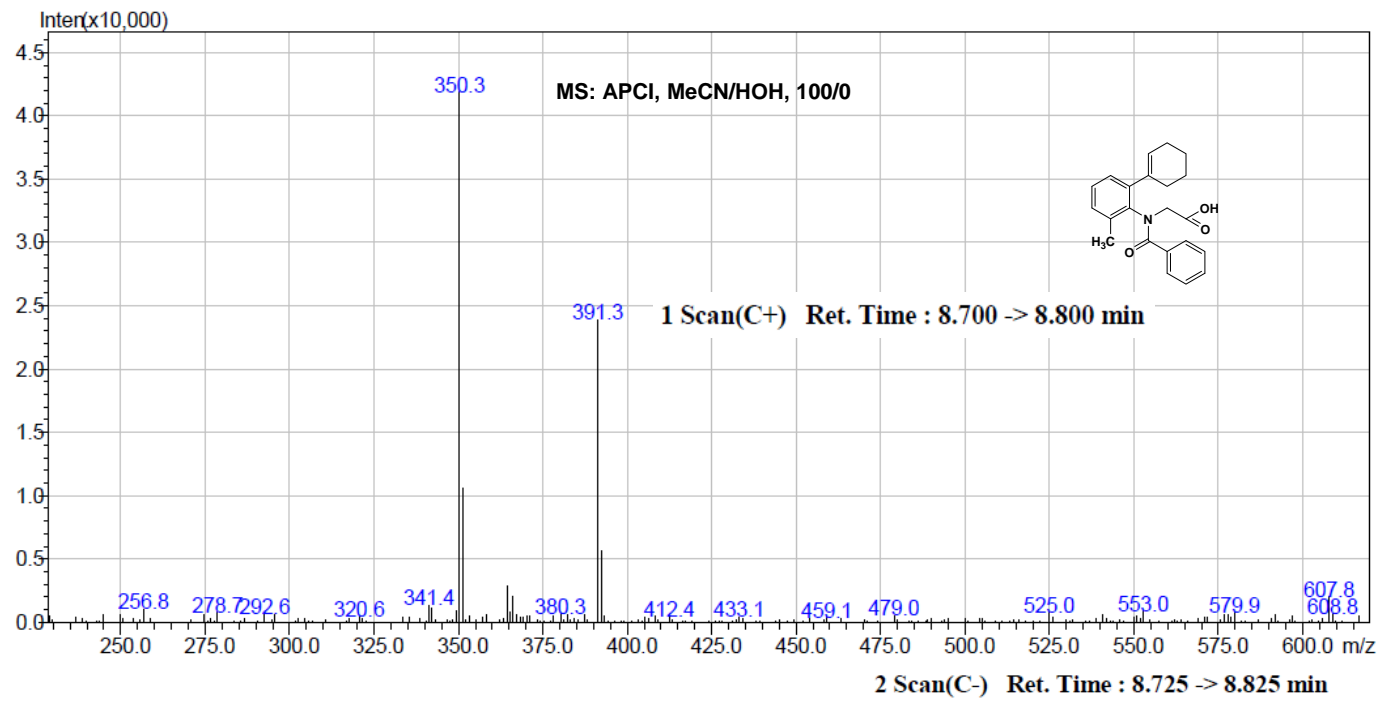
## N-Acetyl glycine 4a

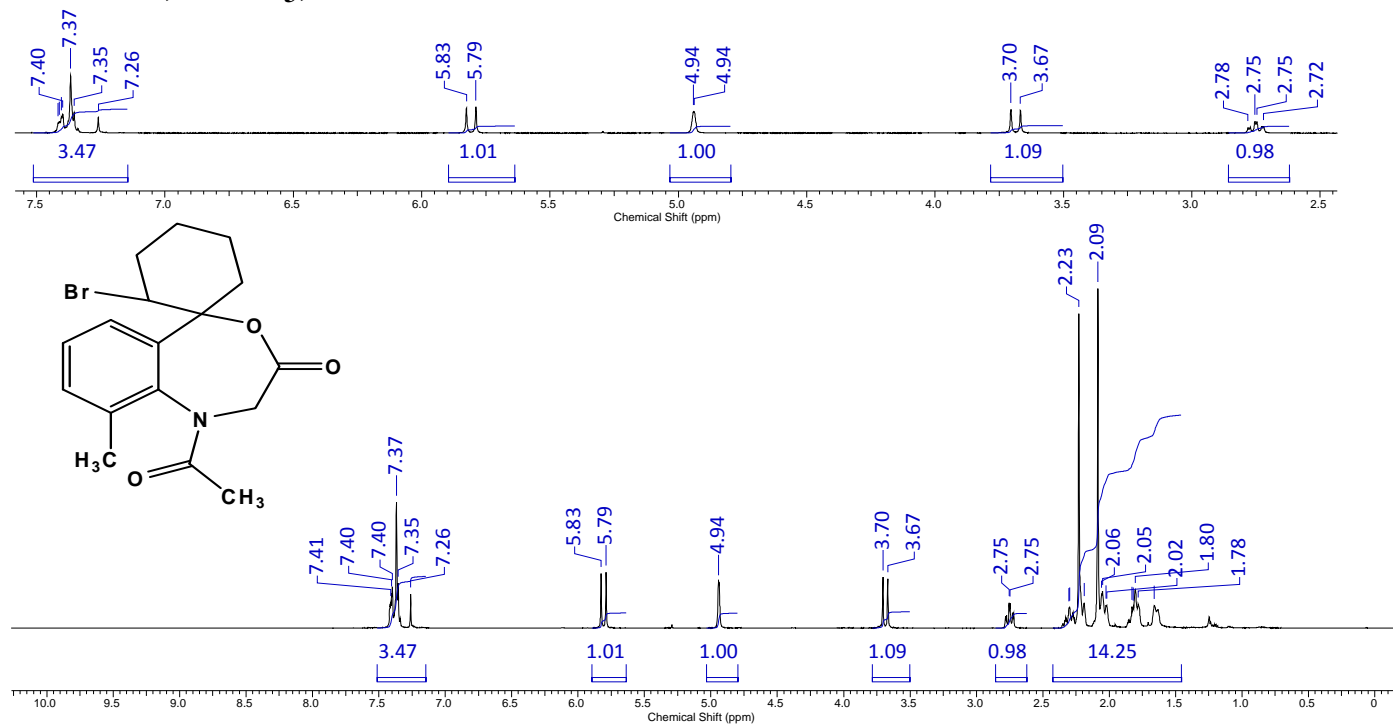
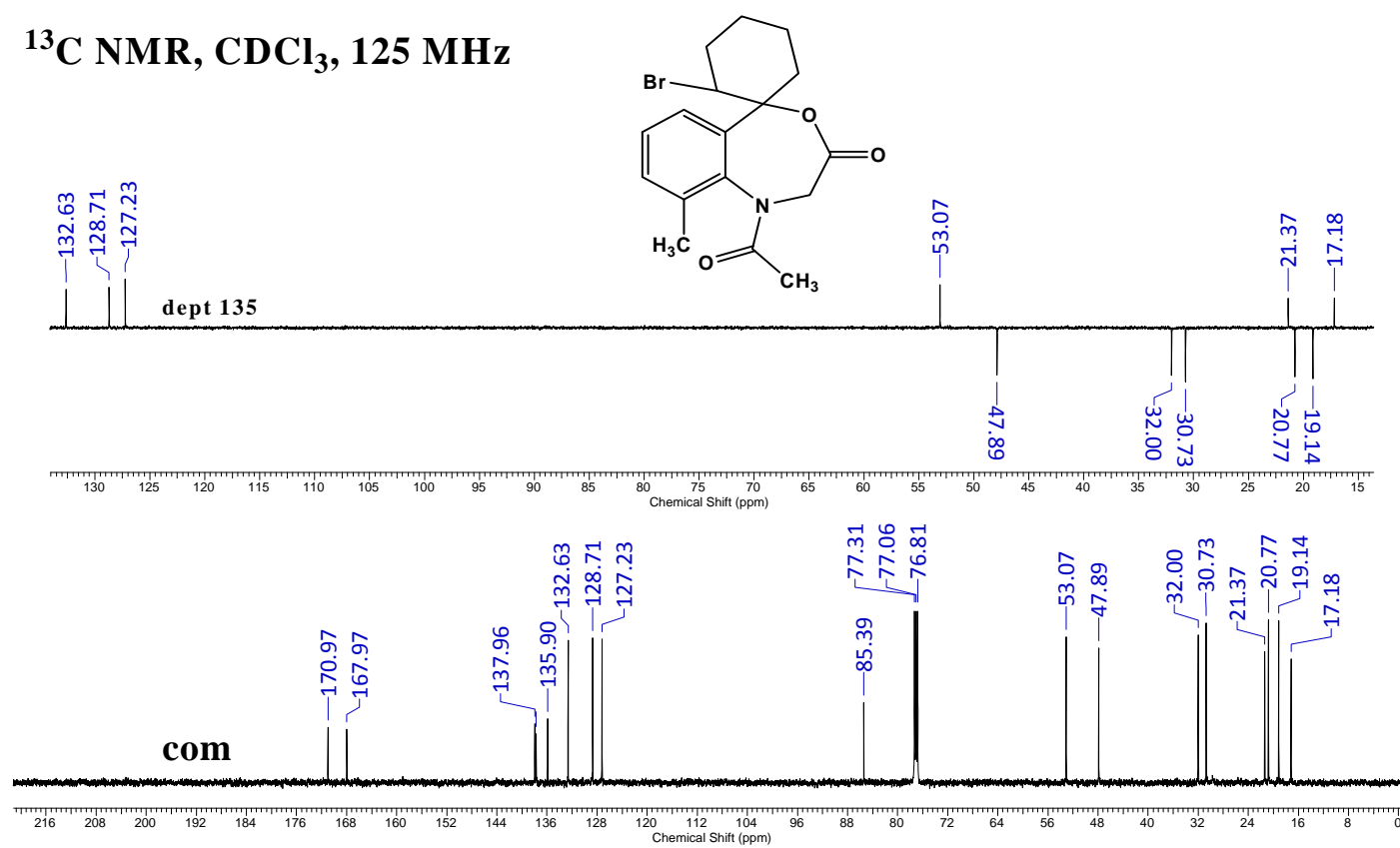




S 10

N-Benzoyl glycine 4b

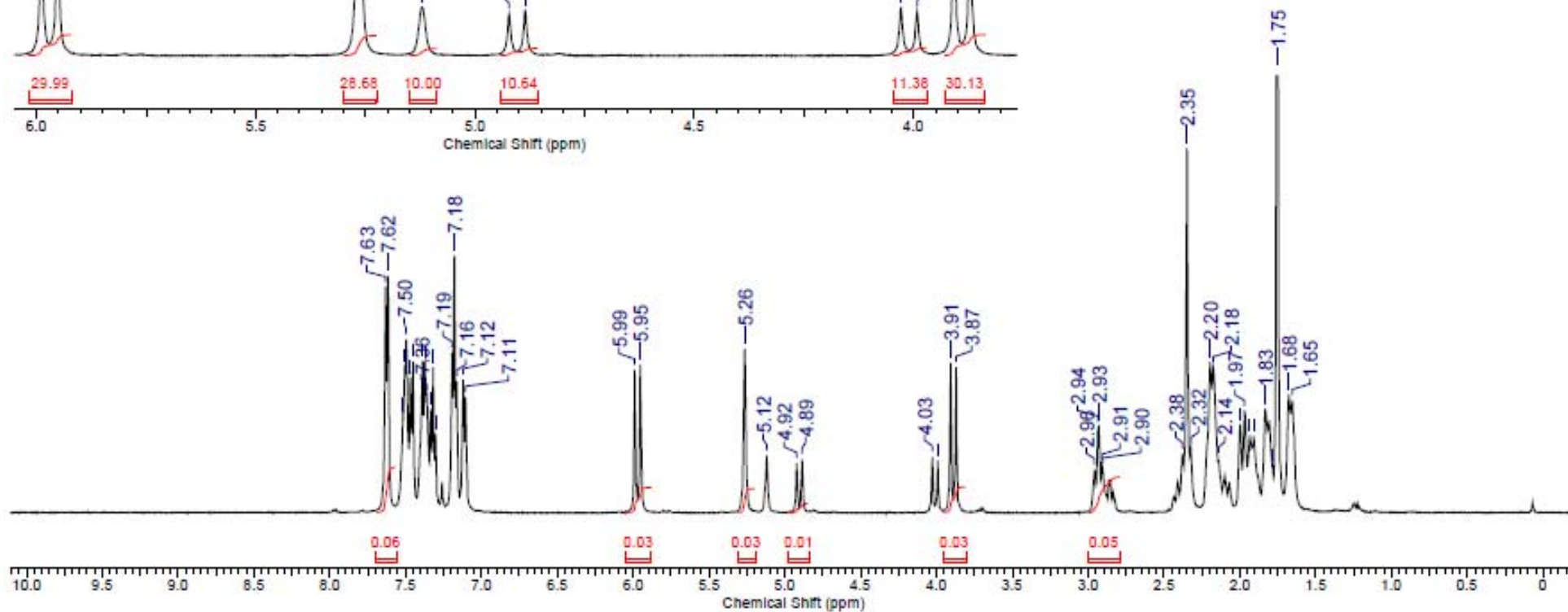
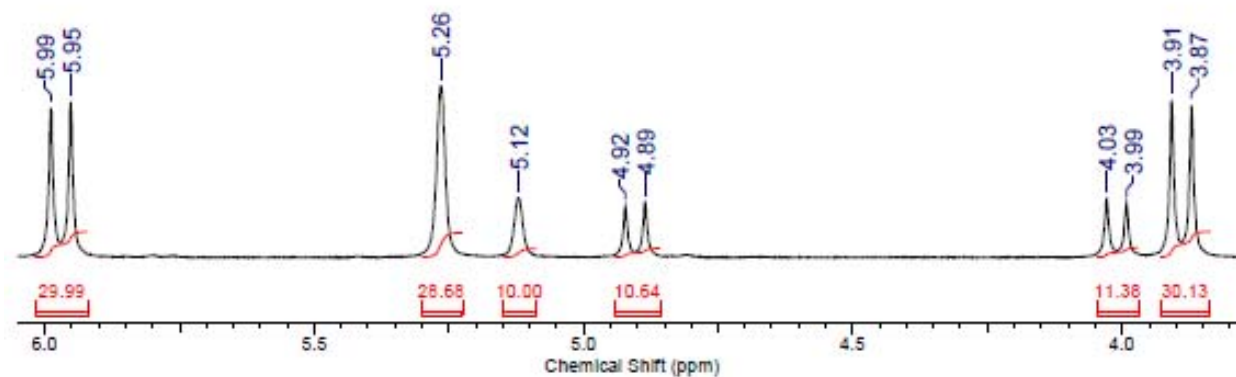
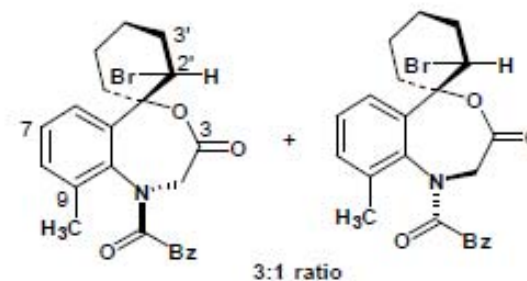


**S 11****Benzoxazepinone 5a****<sup>1</sup>H NMR, CDCl<sub>3</sub>, 500 MHz****<sup>13</sup>C NMR, CDCl<sub>3</sub>, 125 MHz**

S 12

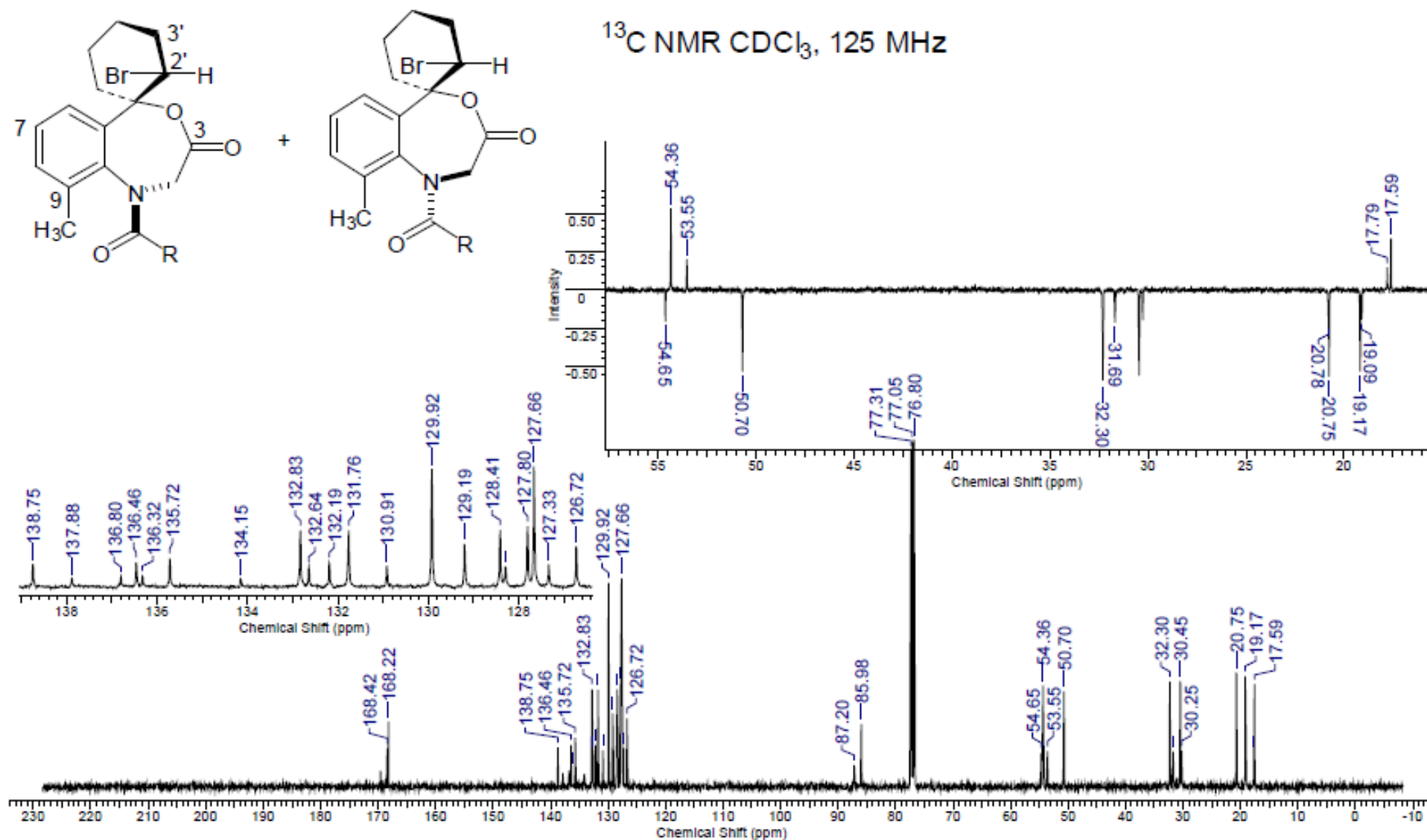
# Benzoxazepinone 5b

$^1\text{H}$  NMR  $\text{CDCl}_3$ , 500 MHz



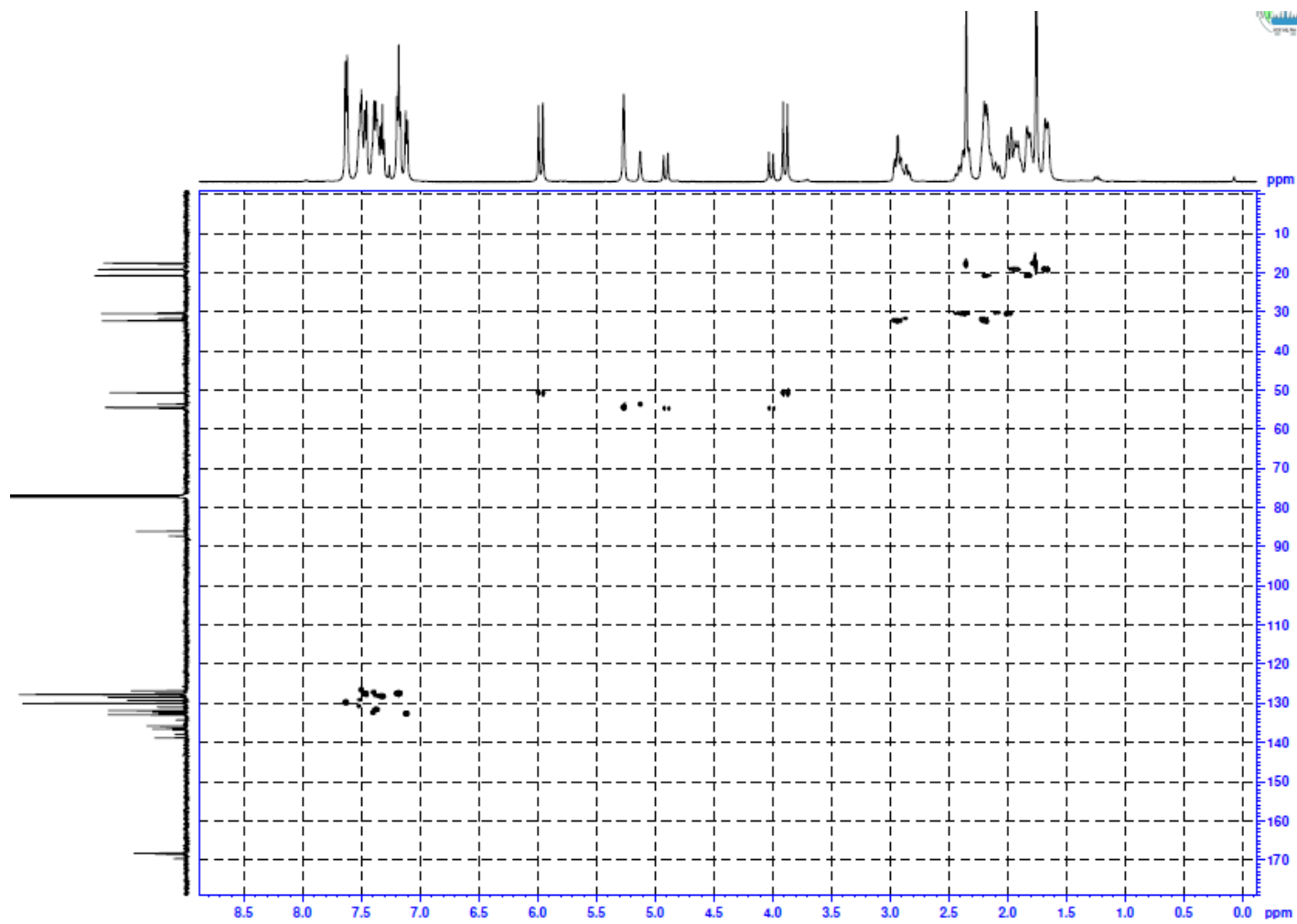
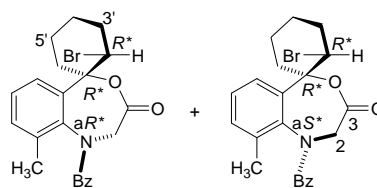
S 13

## Benzoxazepinone 5b



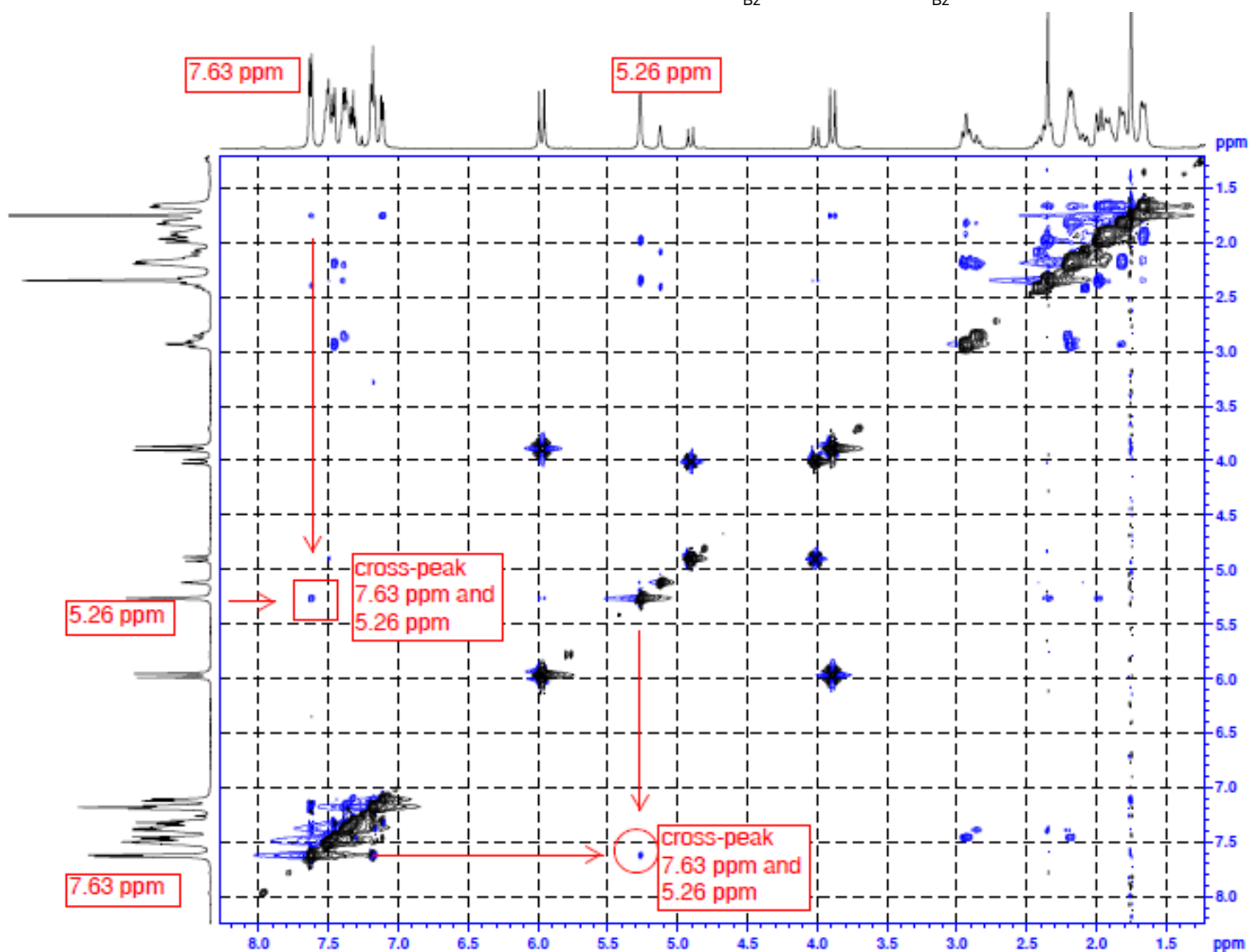
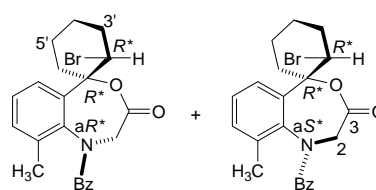
S 14

# HSQC of Benzoxazepinone 5b



S 15

# NOESY of Benzoxazepinone 5b



# S 16

# NMR of Benzoxazocinone 6

