

## Supplementary Materials

# Combination of Betulinic Acid Fragments and Carbonic Anhydrase Inhibitors – A New Drug Targeting Approach

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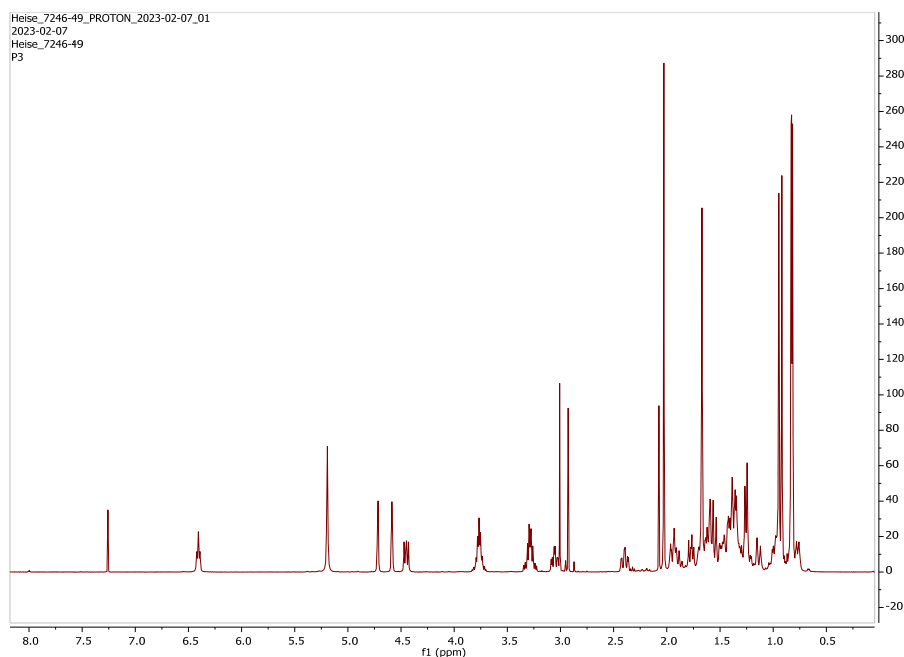
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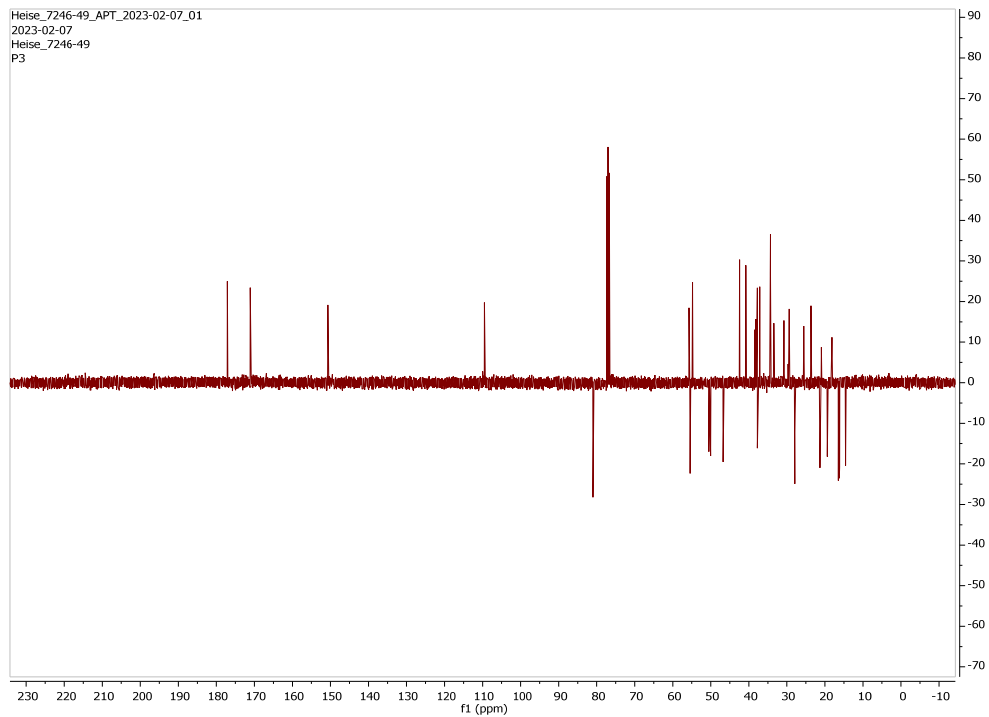
Figure S1: Representative <sup>1</sup>H- and <sup>13</sup>C- NMR spectra and ESI-MS spectra of the compounds synthesized in this work

### Compound 3

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz)

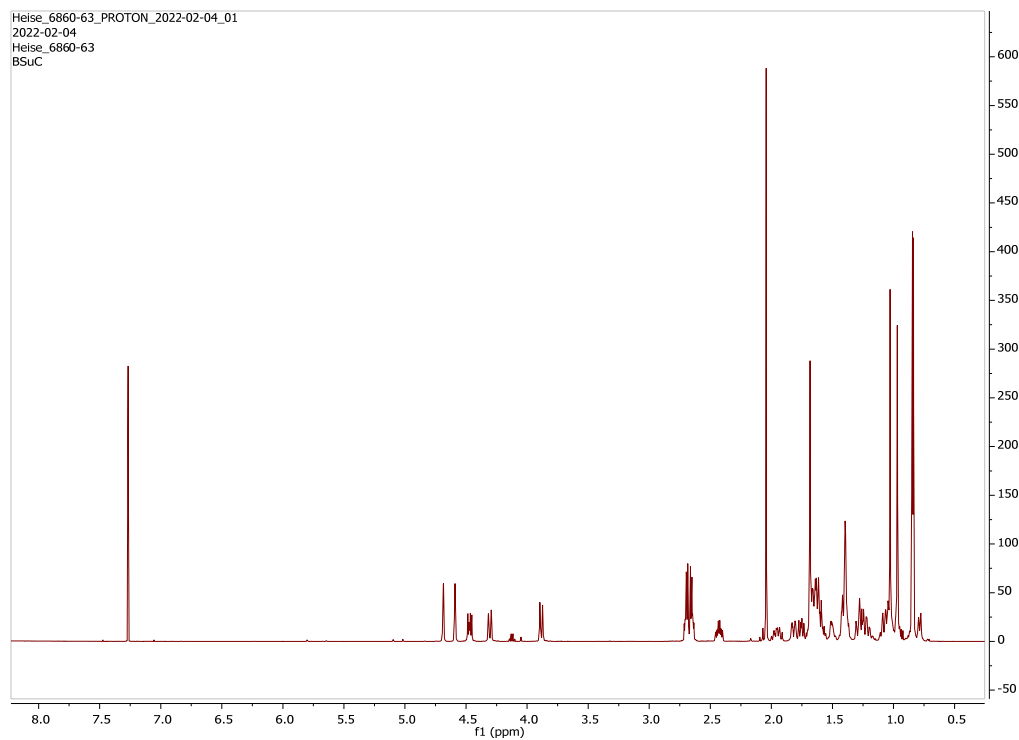


<sup>13</sup>C NMR (CDCl<sub>3</sub>, 101 MHz)

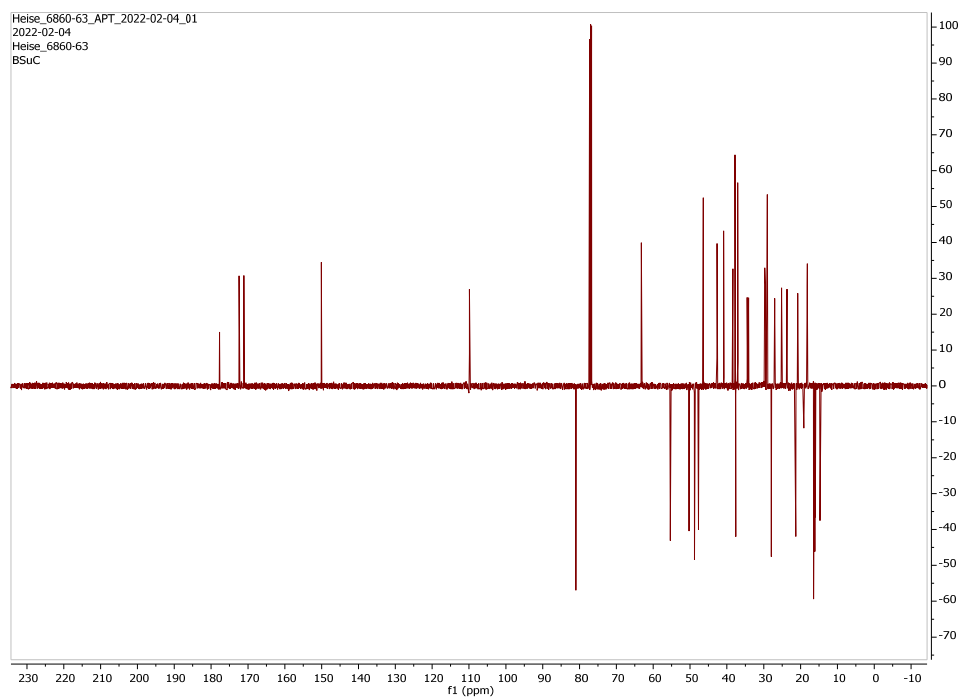


## Compound **4**

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



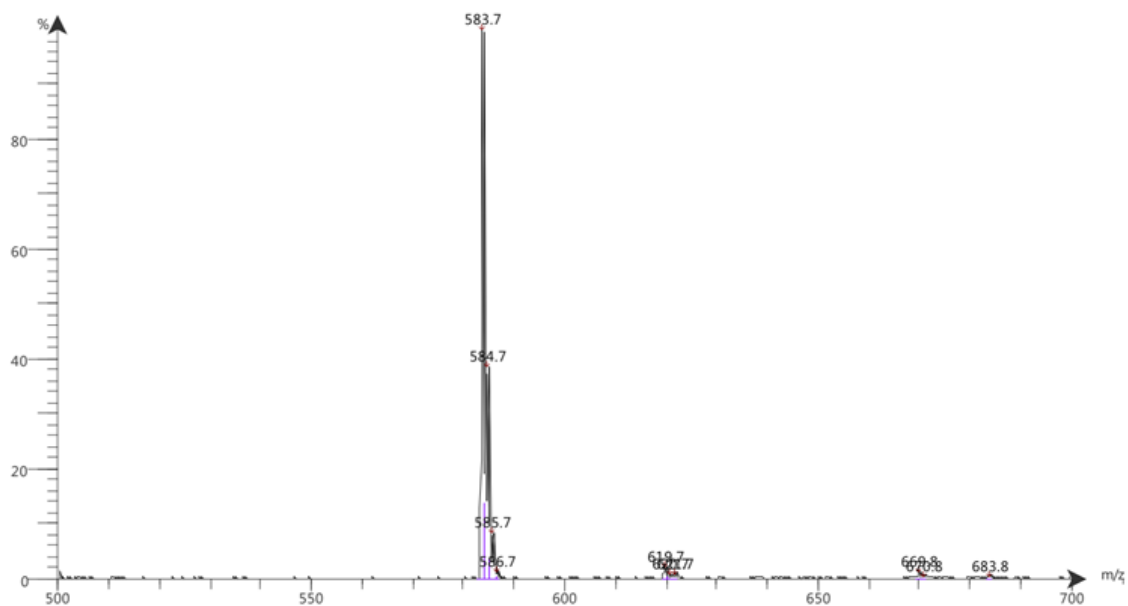
$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 126 MHz)



## ESI-MS

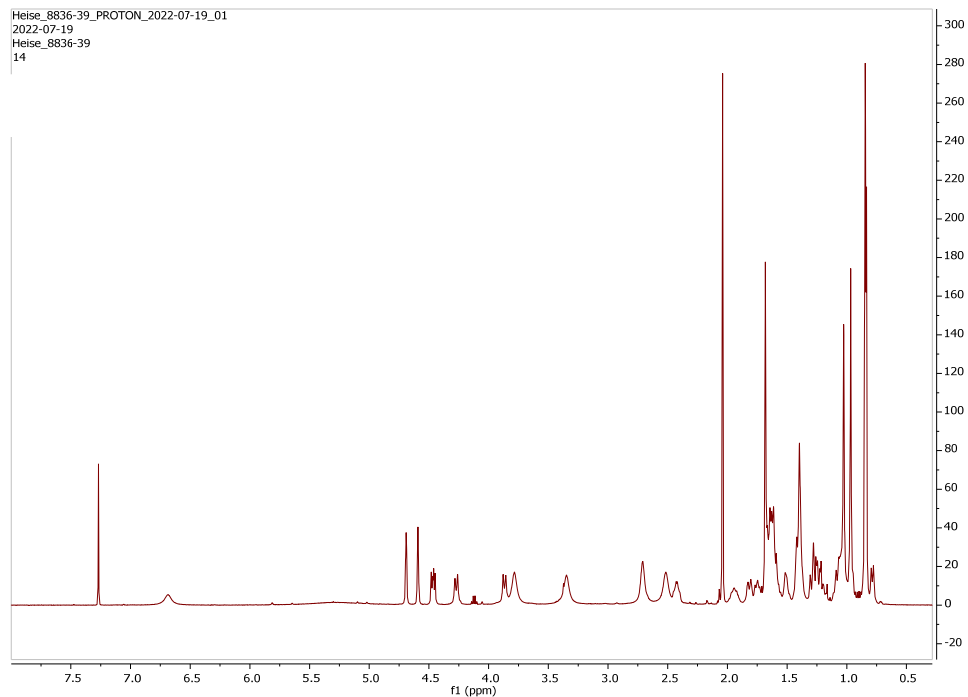
Spectrum RT 1:00 - 2:07 (138 scans) - Background Subtracted 0:02 - 0:48  
Heise-BSuc-2\_Scan1\_is1.datx 2022.02.08 13:05:36 ;  
ESI - Max: 3.5E7

Intensity

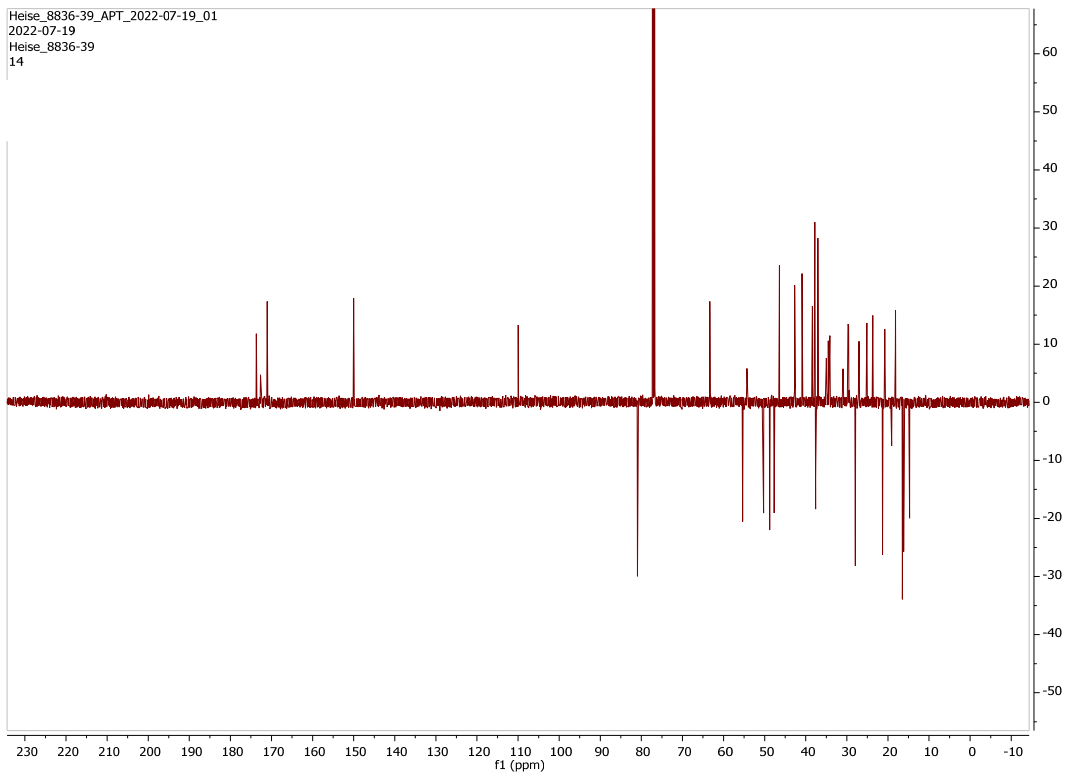


## Compound 5

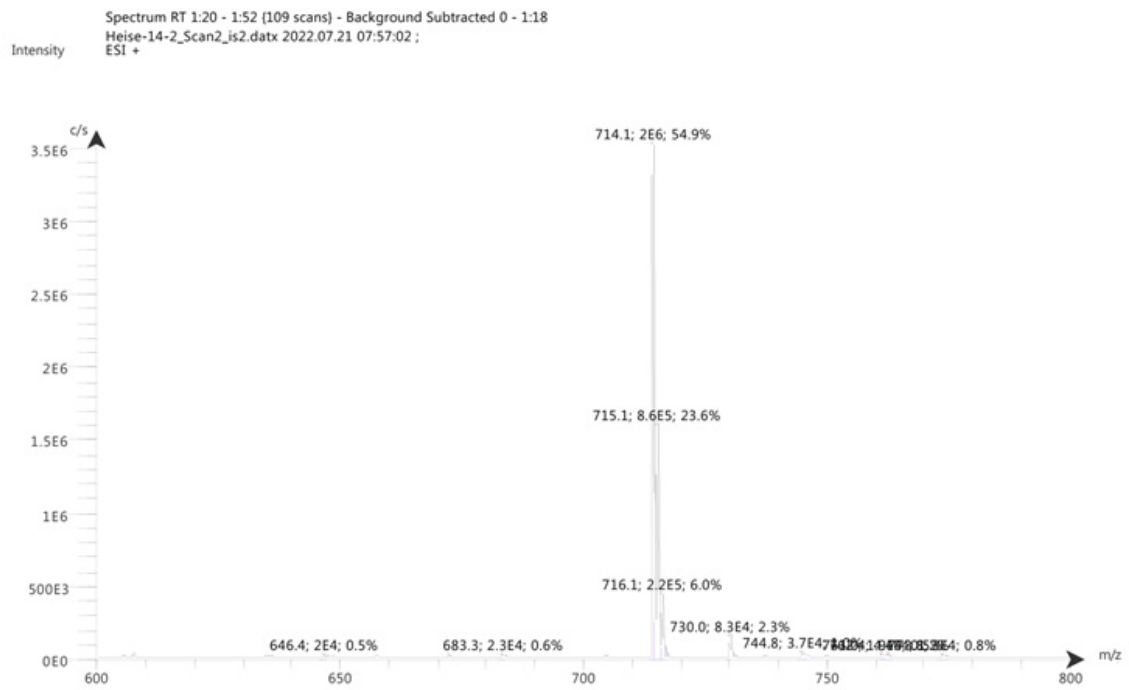
$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz)



$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 126 MHz)

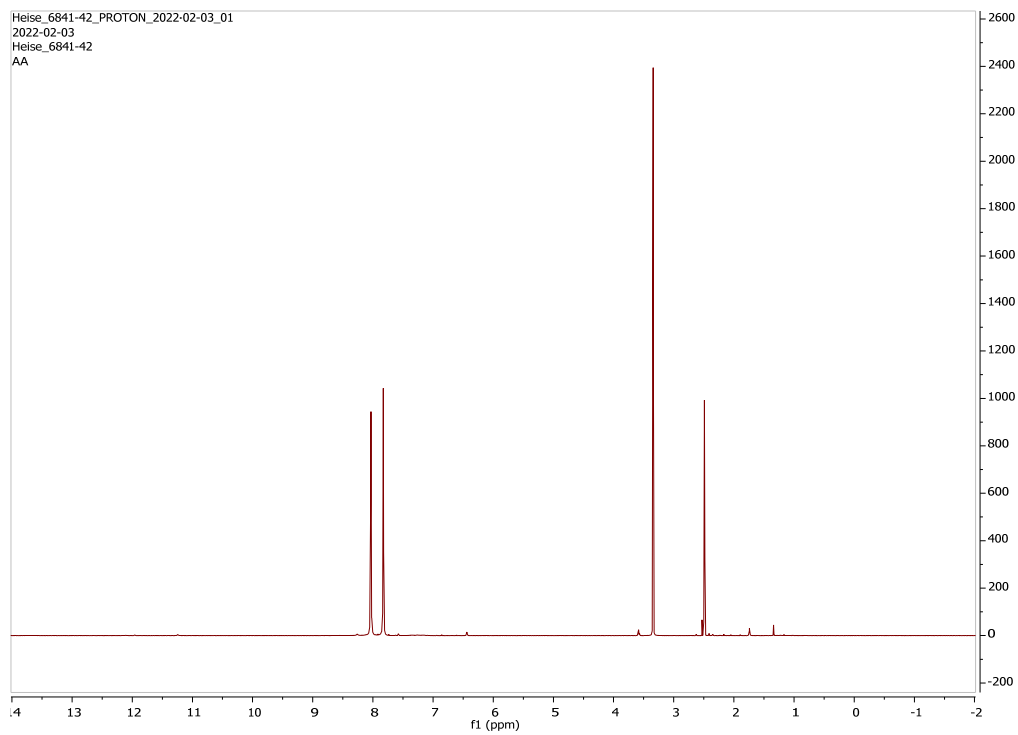


# ESI-MS

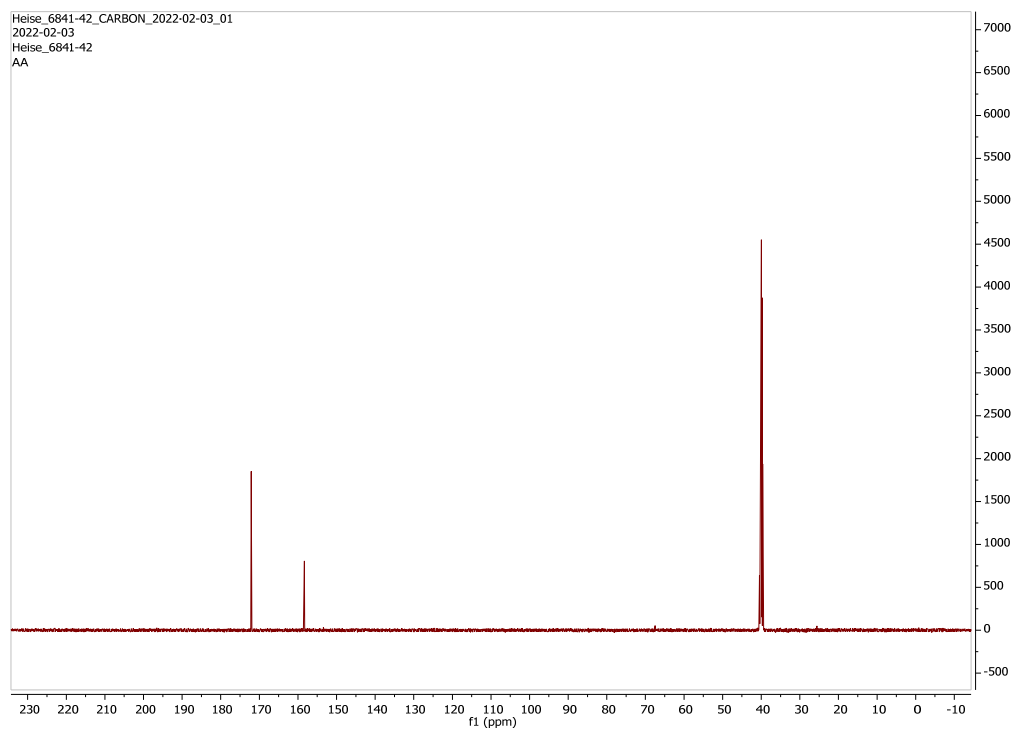


## Compound 6

$^1\text{H}$  NMR (DMSO- $d_6$ , 500 MHz)



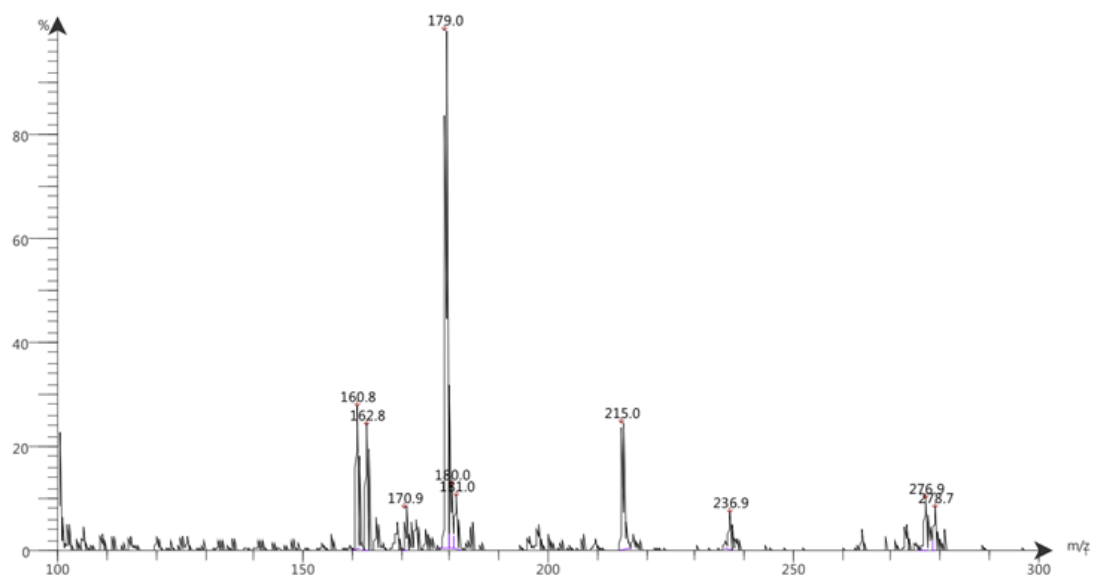
$^{13}\text{C}$  NMR (DMSO- $d_6$ , 126 MHz)



## ESI-MS

Spectrum RT 0:45 - 1:19 (70 scans) - Background Subtracted 0:06 - 0:34  
Heise-AA-2\_Scan1\_is1.datx 2022.02.08 12:36:23 ;  
ESI - Max: 5.1E6

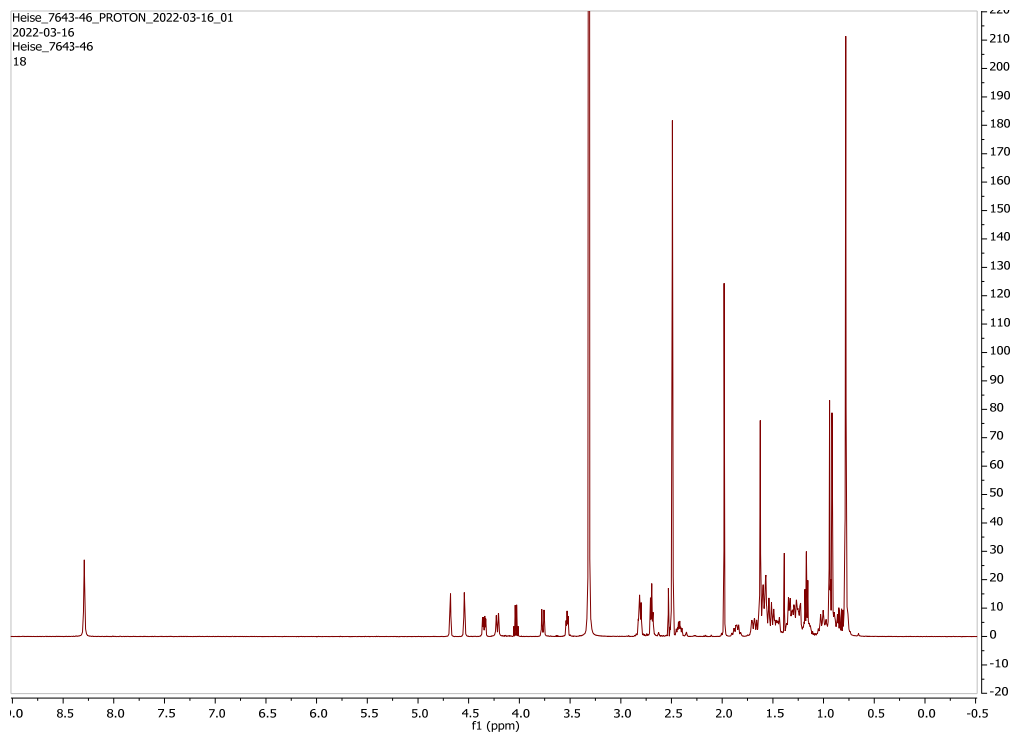
Intensity



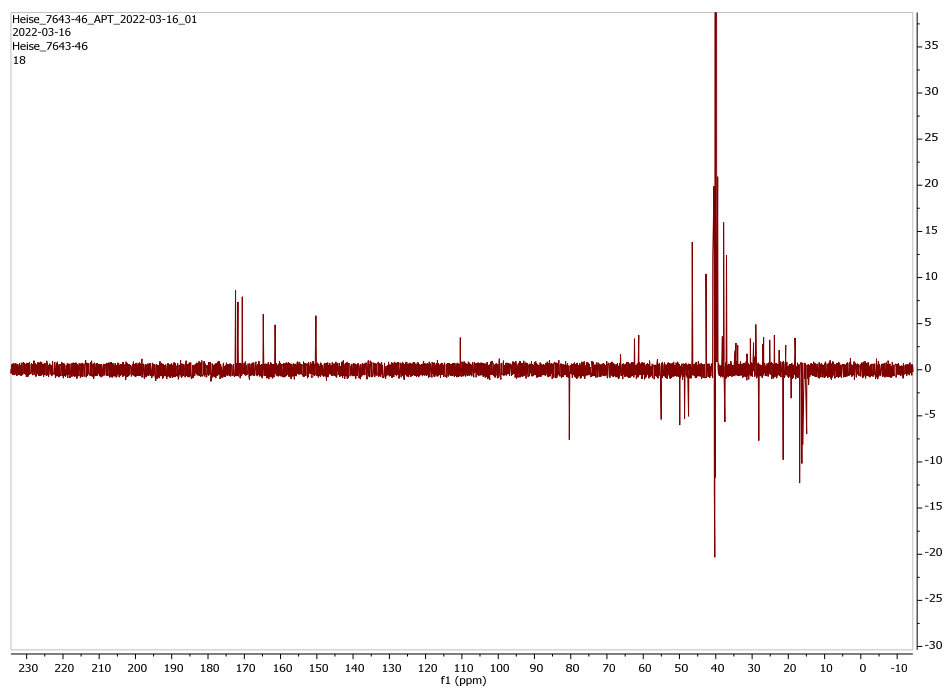


## Compound 9

$^1\text{H}$  NMR (DMSO- $d_6$ , 400 MHz)

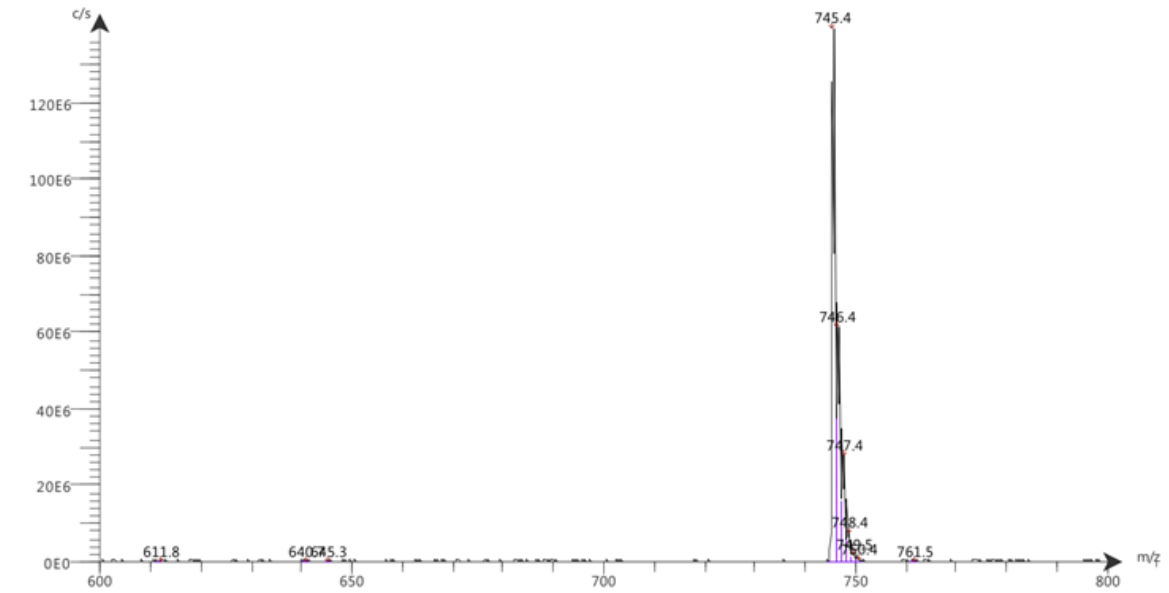


$^{13}\text{C}$  NMR (DMSO- $d_6$ , 101 MHz)



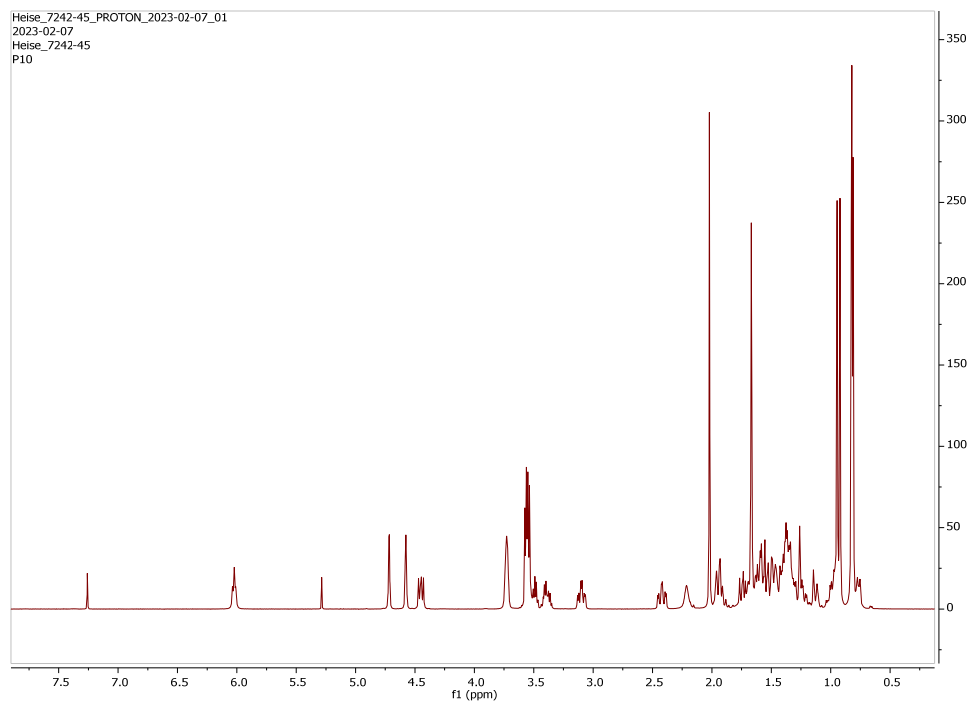
## ESI-MS

Spectrum RT 0:42 - 1:12 (61 scans) - Background Subtracted 0 - 0:37  
Heise\_BetAA-2\_Scan1\_is1.datx 2022.03.21 09:35:06 ;  
ESI -

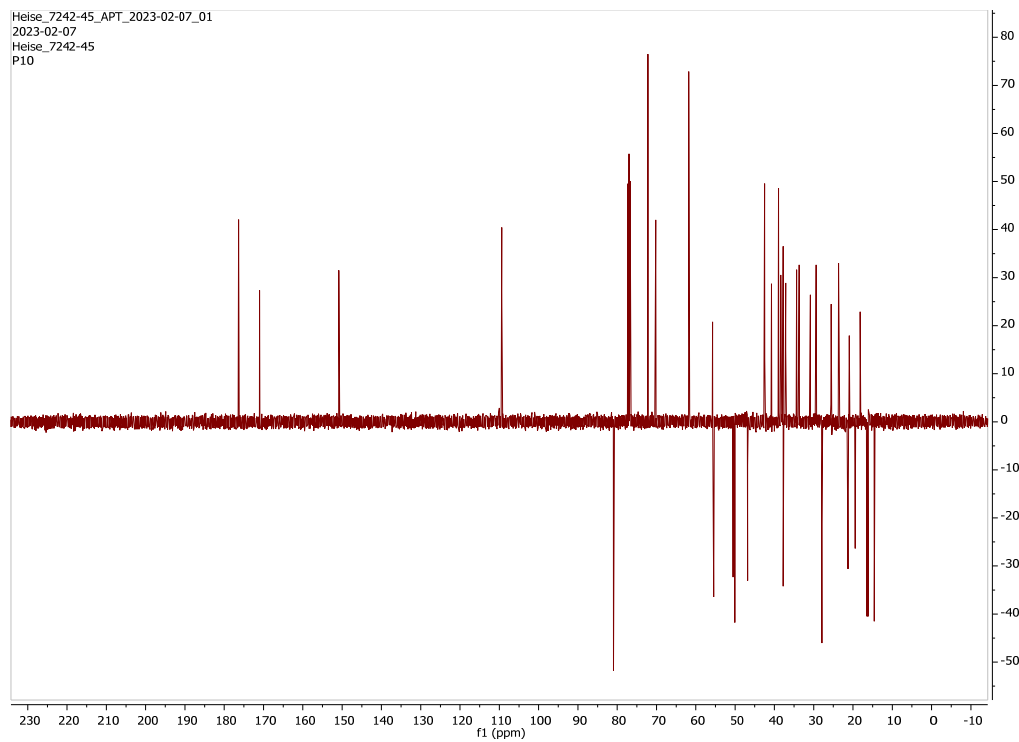


## Compound **10**

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)

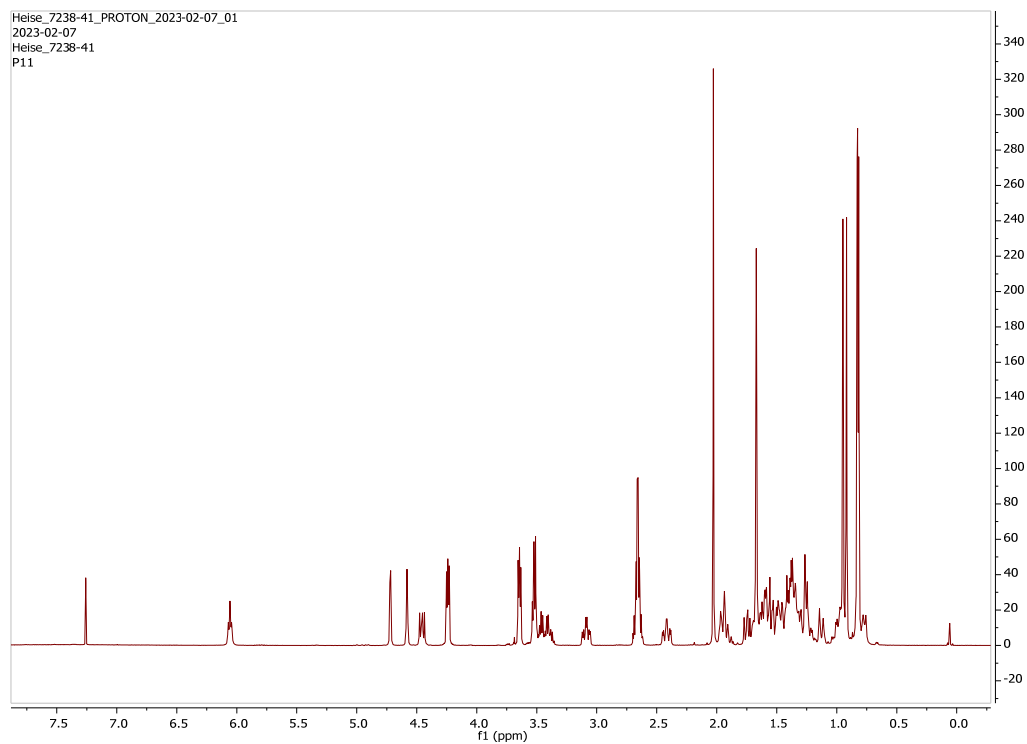


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 101 MHz)

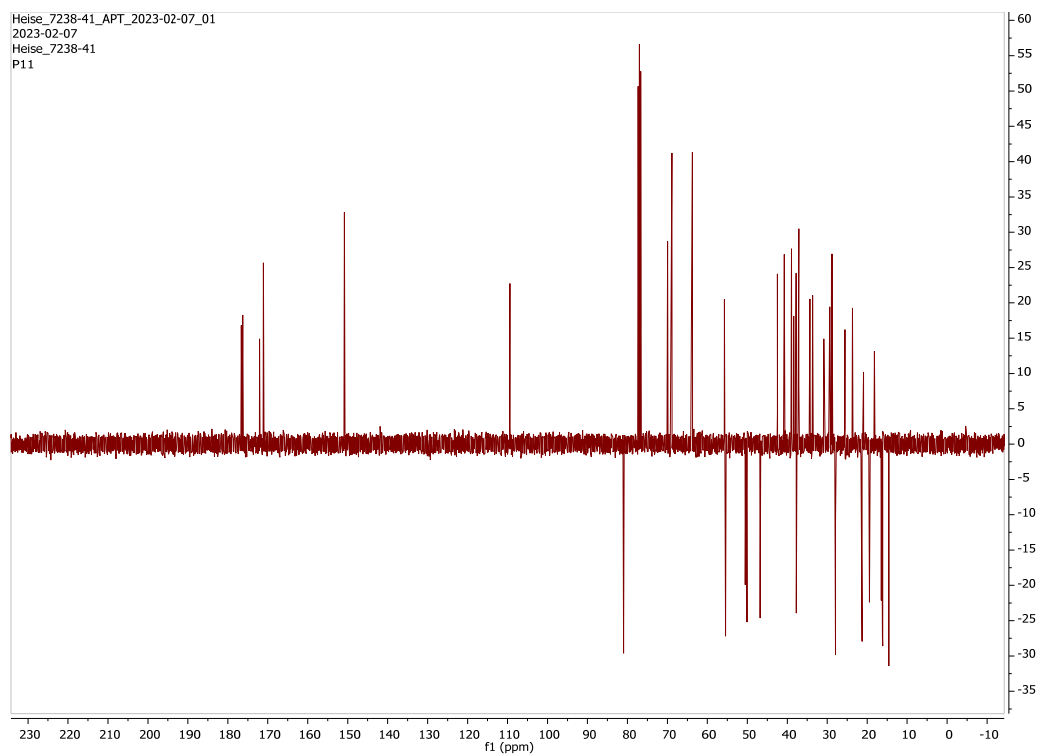


## Compound **11**

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz)

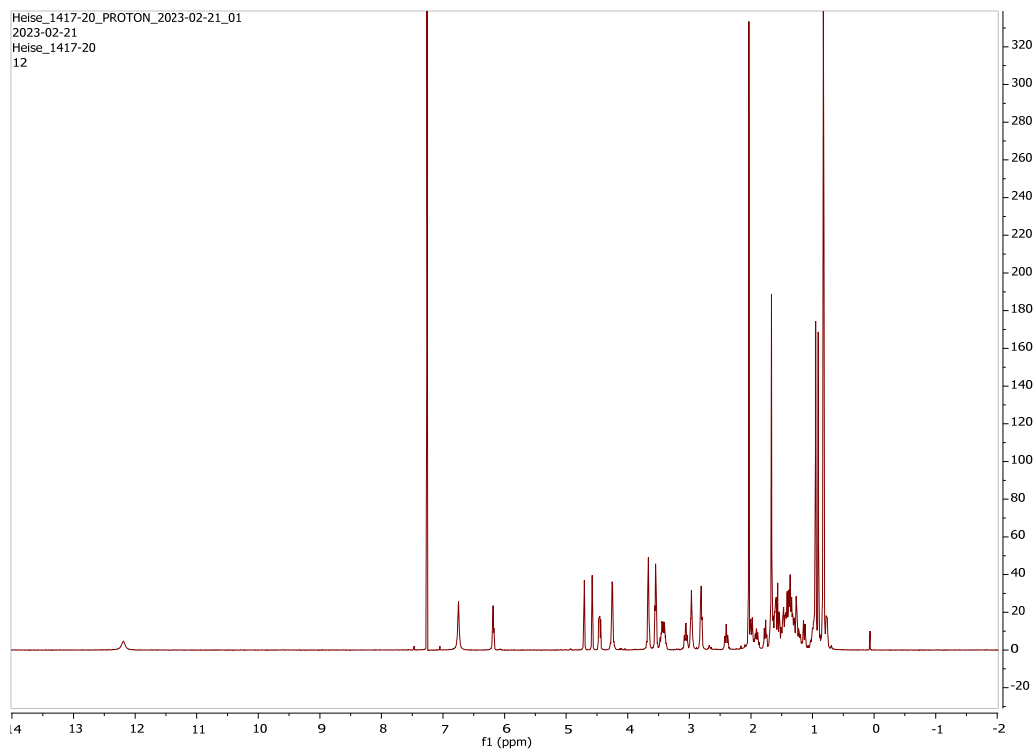


$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 101 MHz)

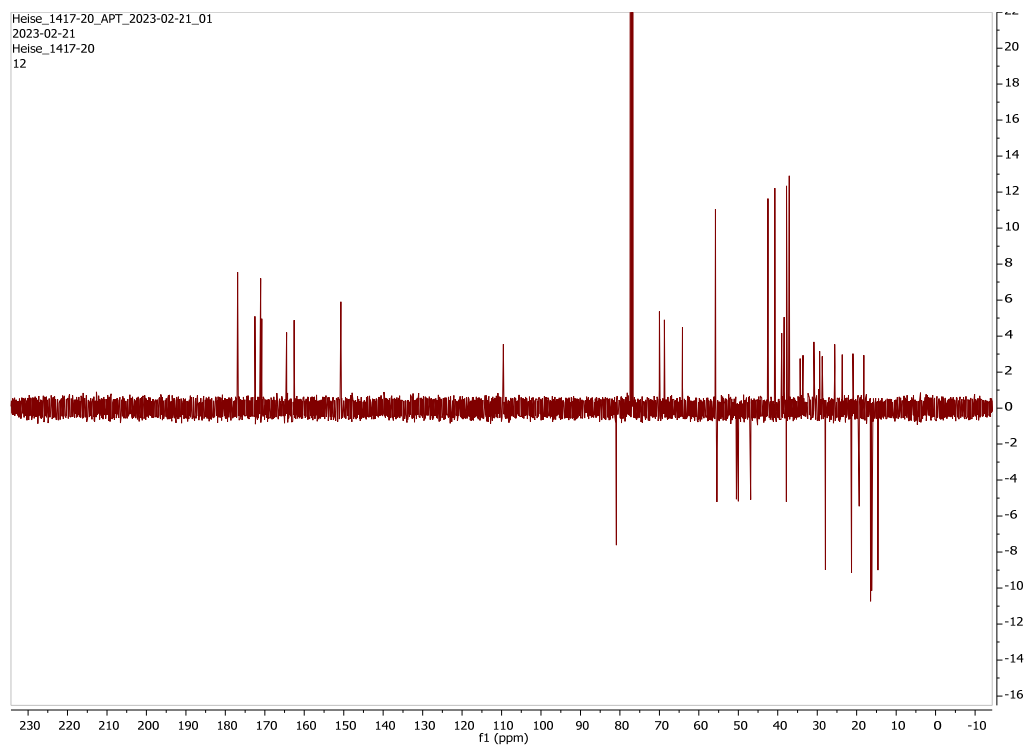


## Compound **12**

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



$^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 126 MHz)



## ESI-MS

Spectrum RT 0:60 - 1:37 (83 scans) - Background Subtracted 0 - 0:57  
Heise-12-2\_Scan2\_is2.datx 2023.02.27 09:05:41 ;  
ESI - Max: 1.3E8

