

## Supplementary Data

Article

# Bio-Oriented synthesis and molecular docking studies of 1,2,4-Triazole based derivatives as potential Anticancer agents against HepG2 Cell Line

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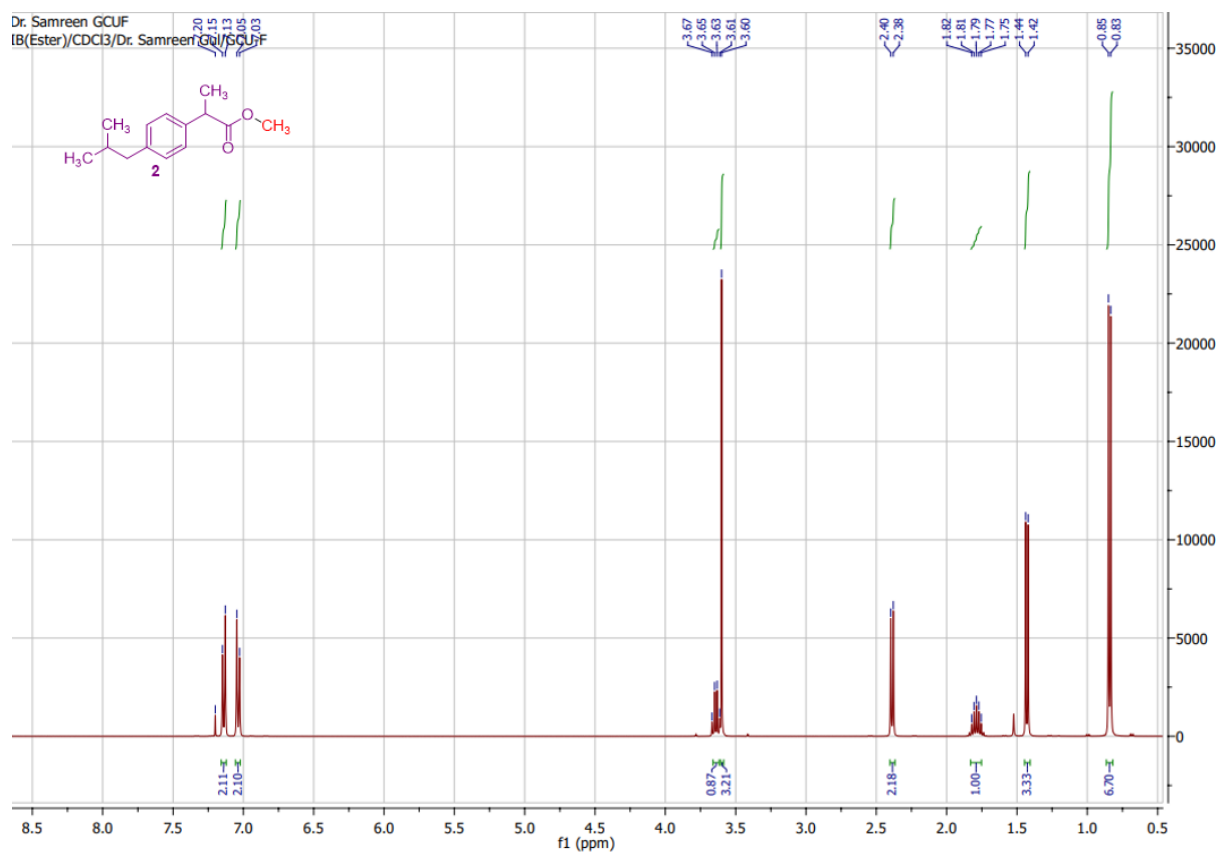
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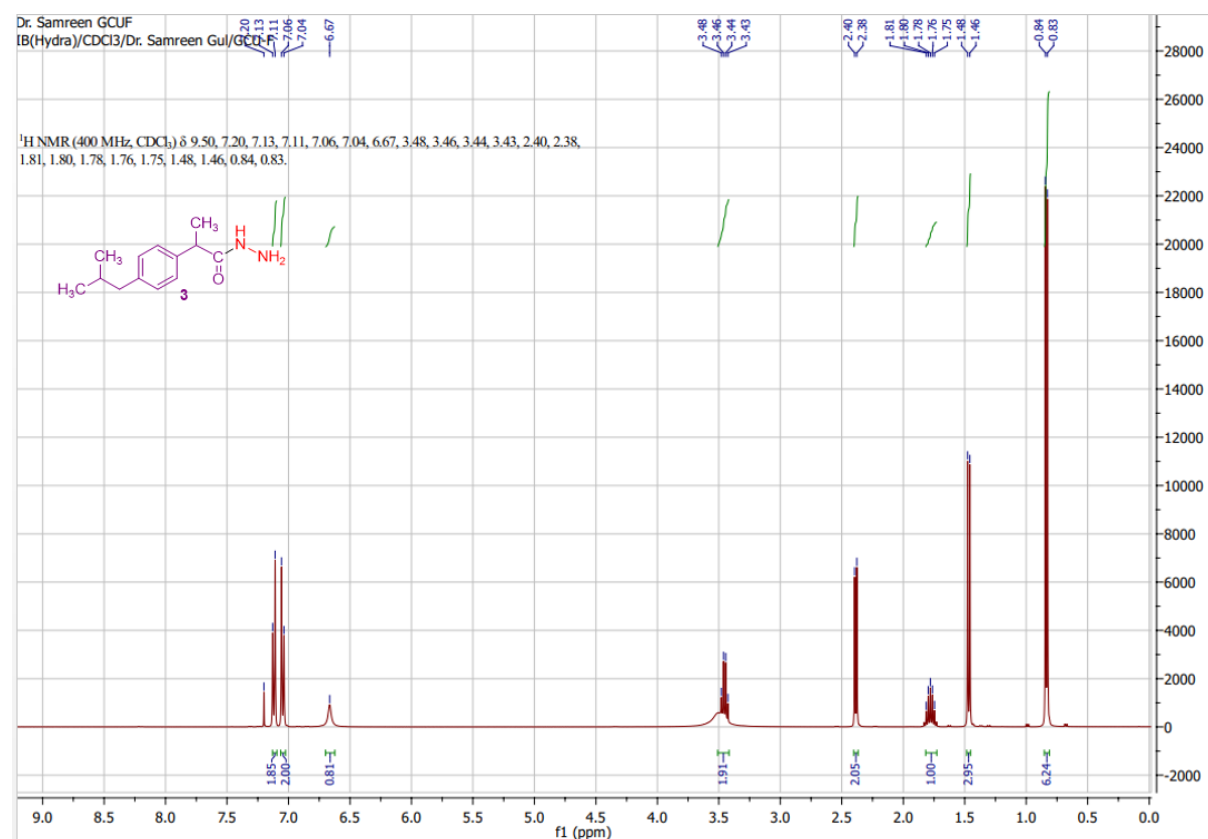
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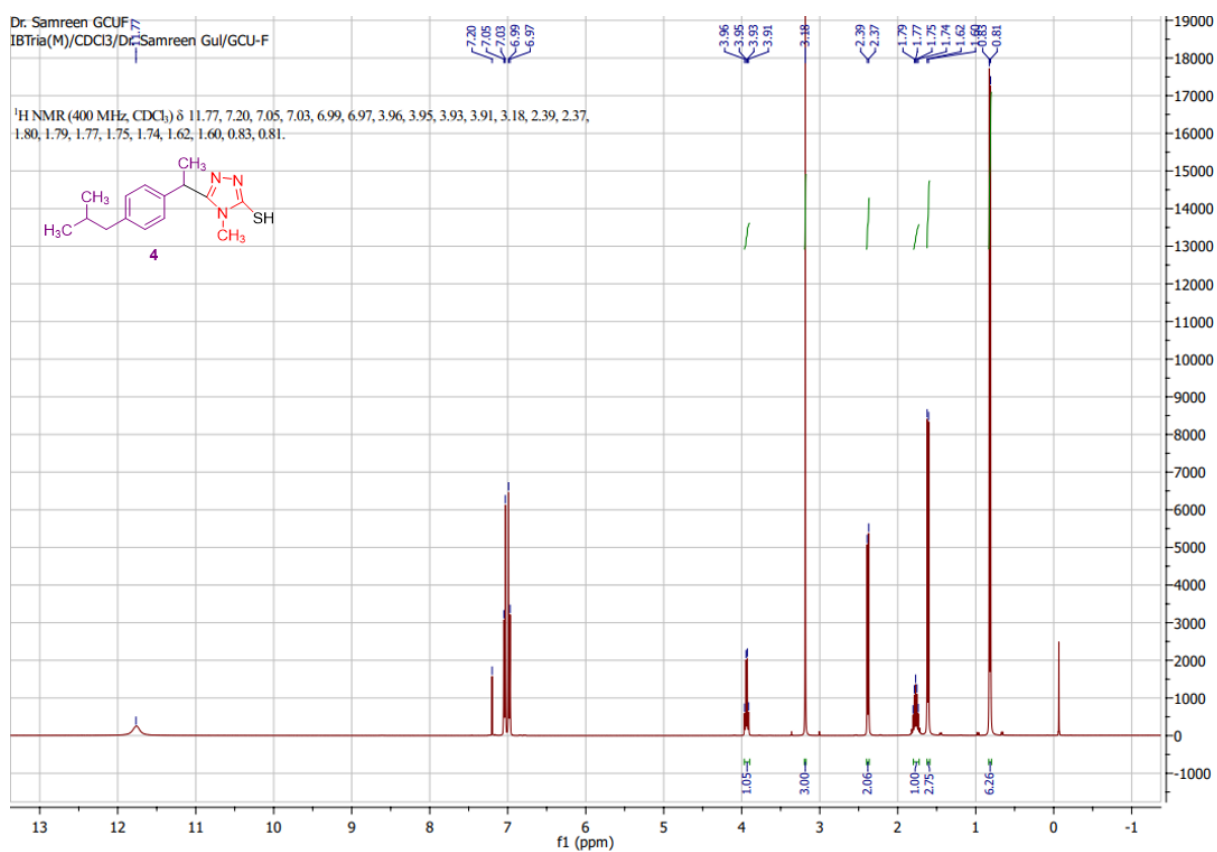
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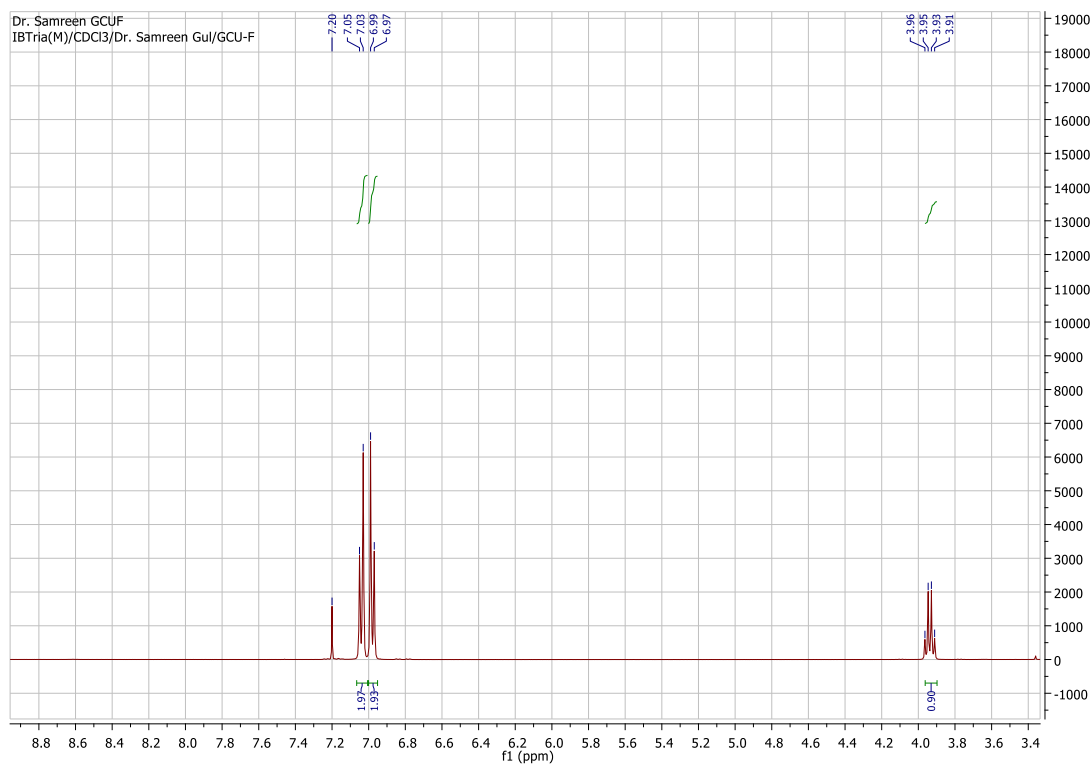
**Figure S1:** <sup>1</sup>H NMR spectrum of compound 2 (Full)



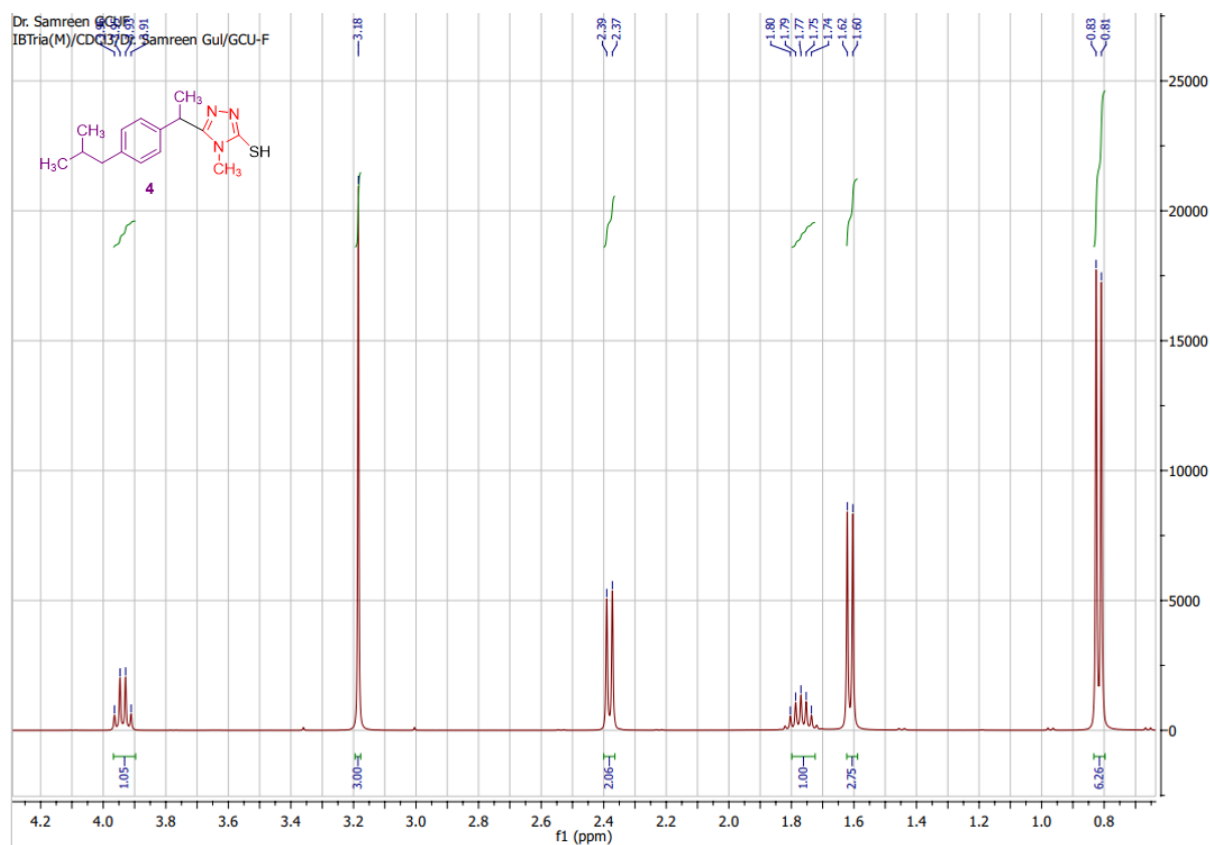
**Figure S2:** <sup>1</sup>H NMR spectrum of compound 3 (Full)



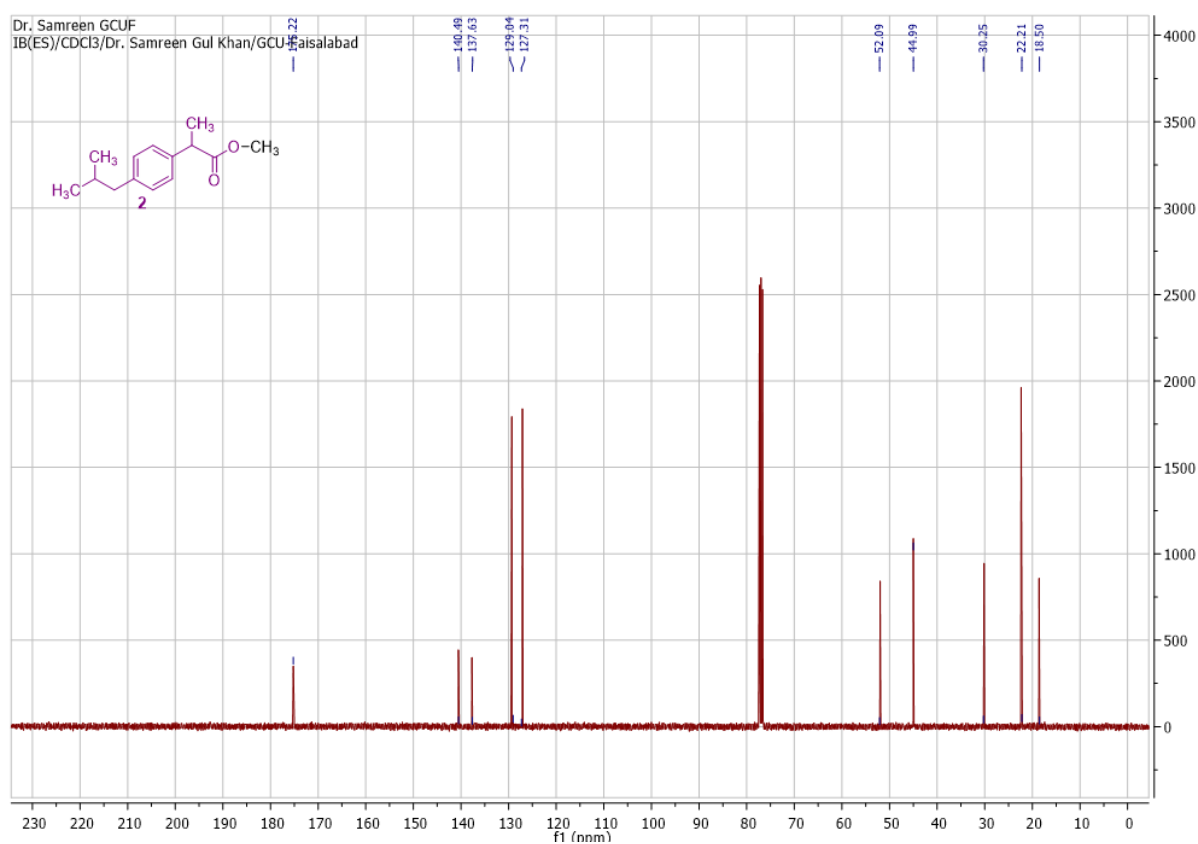
**Figure S3:** <sup>1</sup>H NMR spectrum of compound 4(Full)



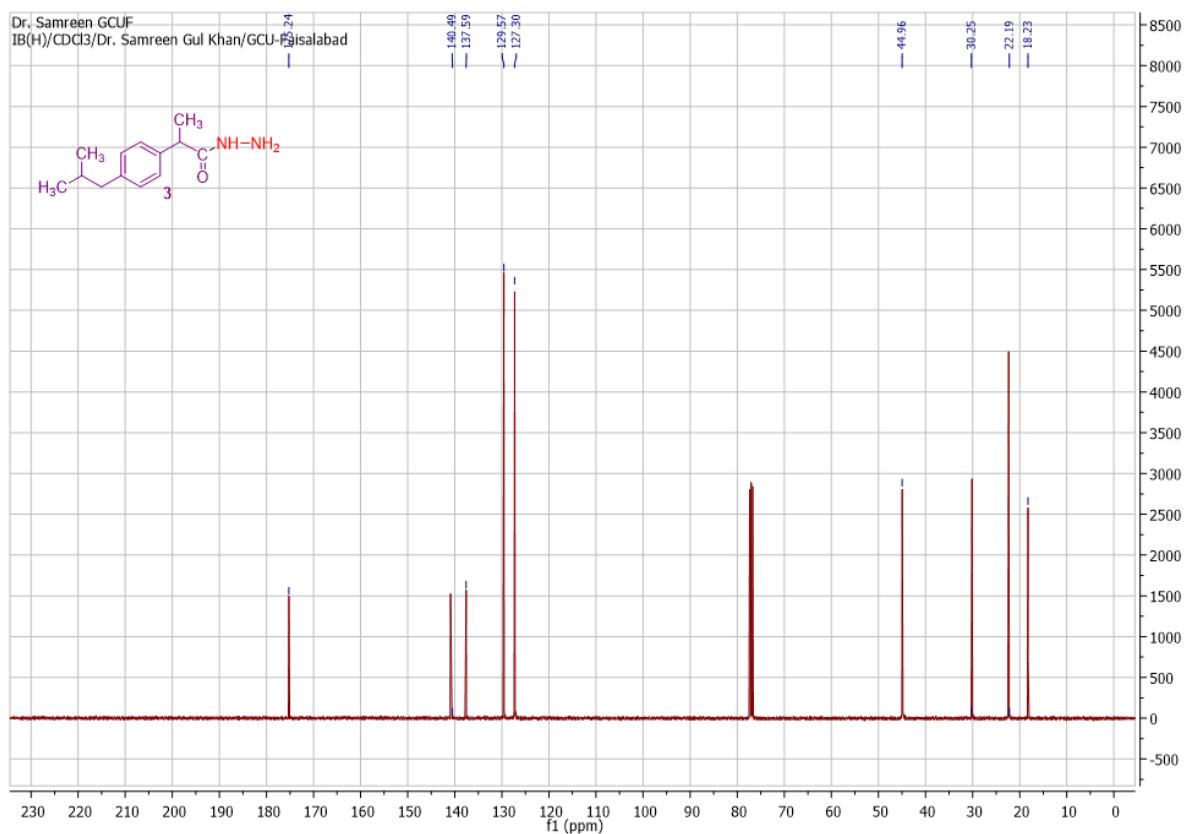
**Figure S4.** <sup>1</sup>H NMR spectrum of compound 4 (aromatic region)



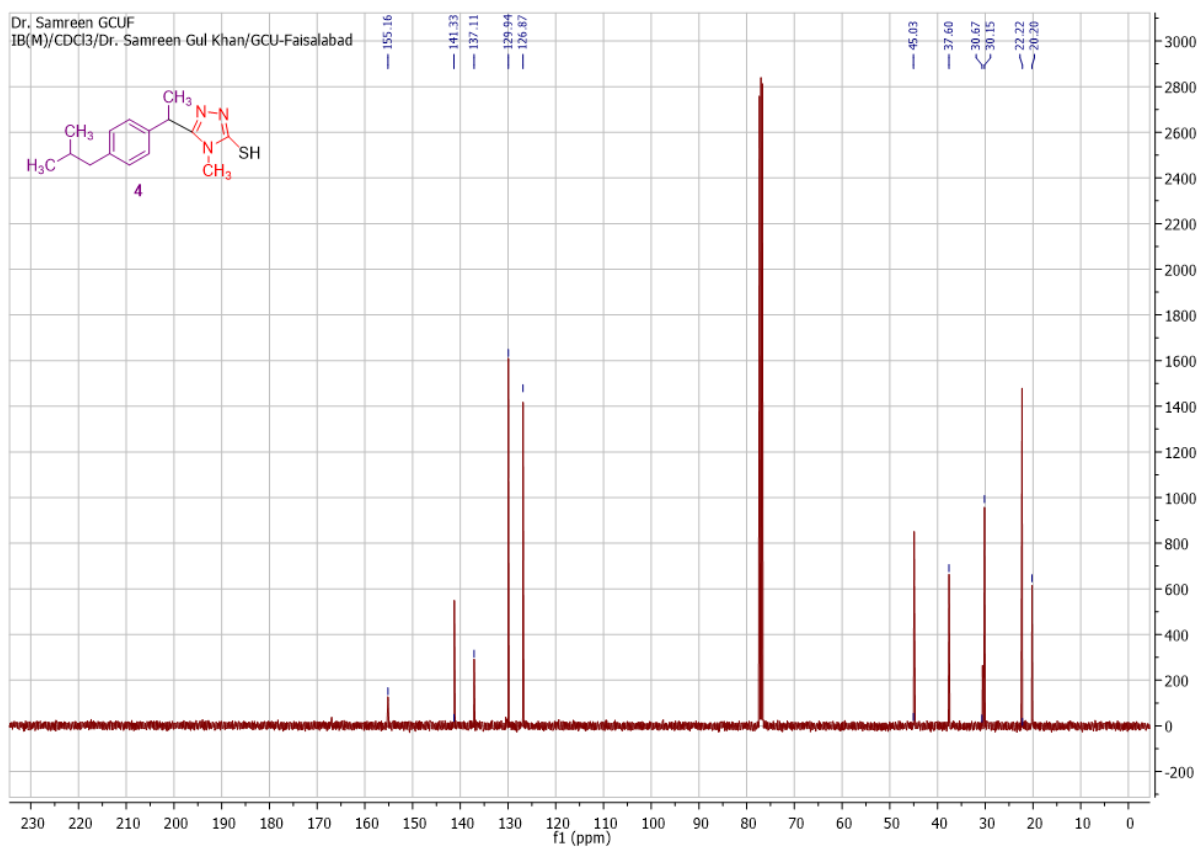
**Figure S5.** <sup>1</sup>H NMR spectrum of compound 4 (aliphatic region)



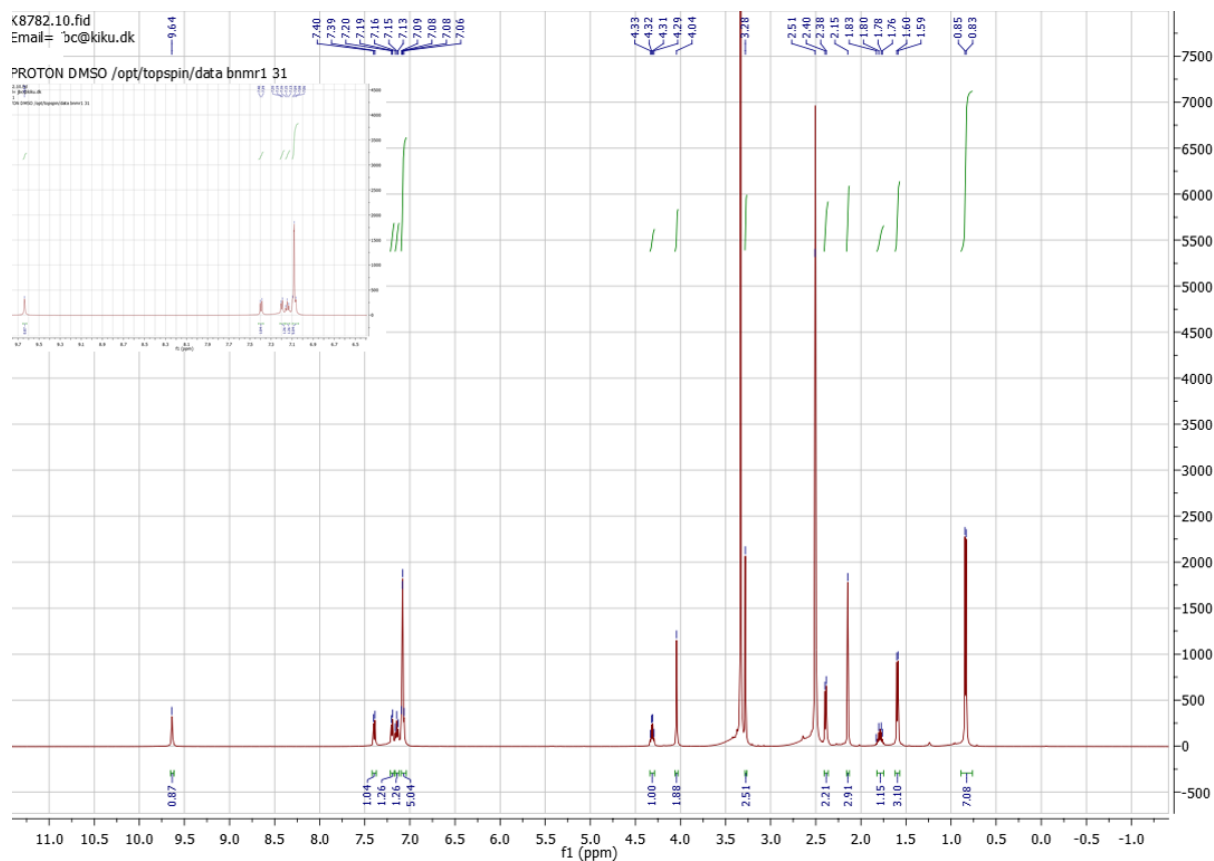
**Figure S6.** <sup>13</sup>C NMR spectrum of compound 2



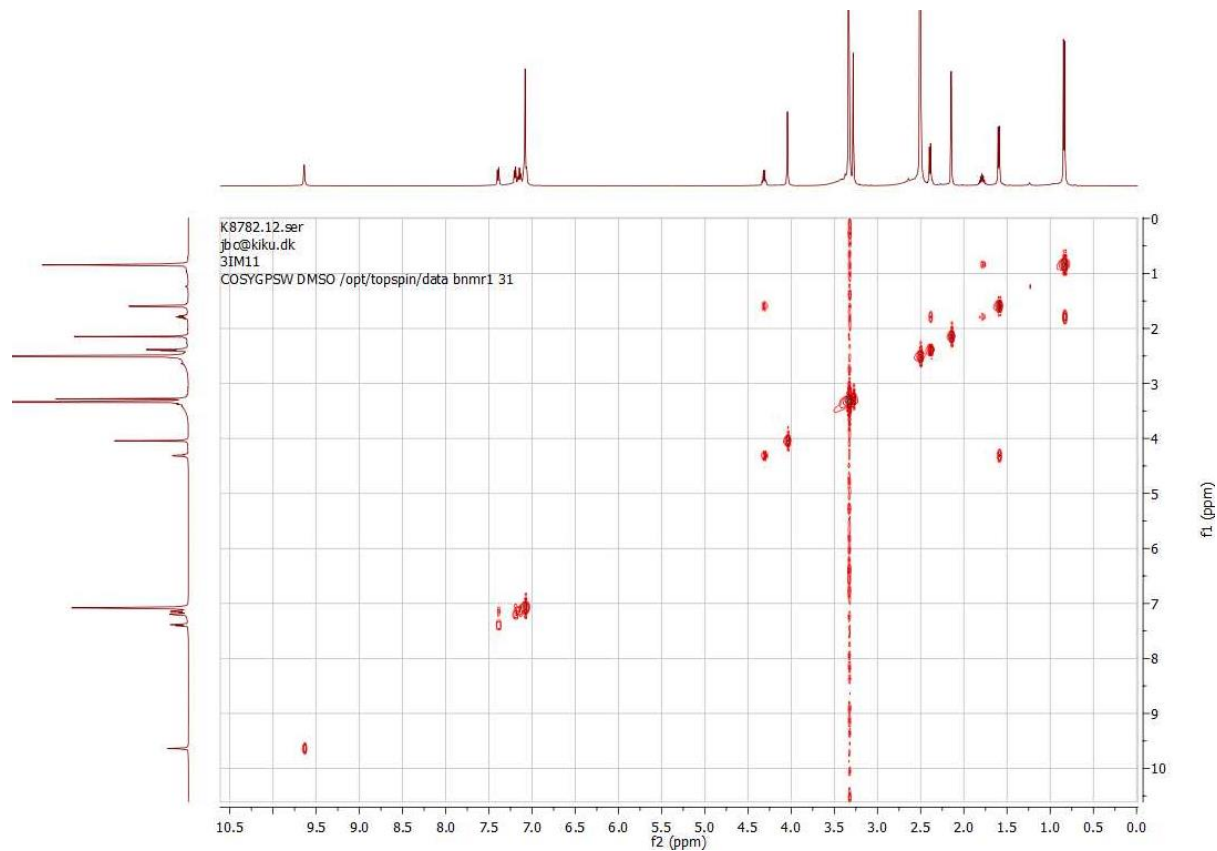
**Figure S7.** <sup>13</sup>C NMR spectrum of compound 3



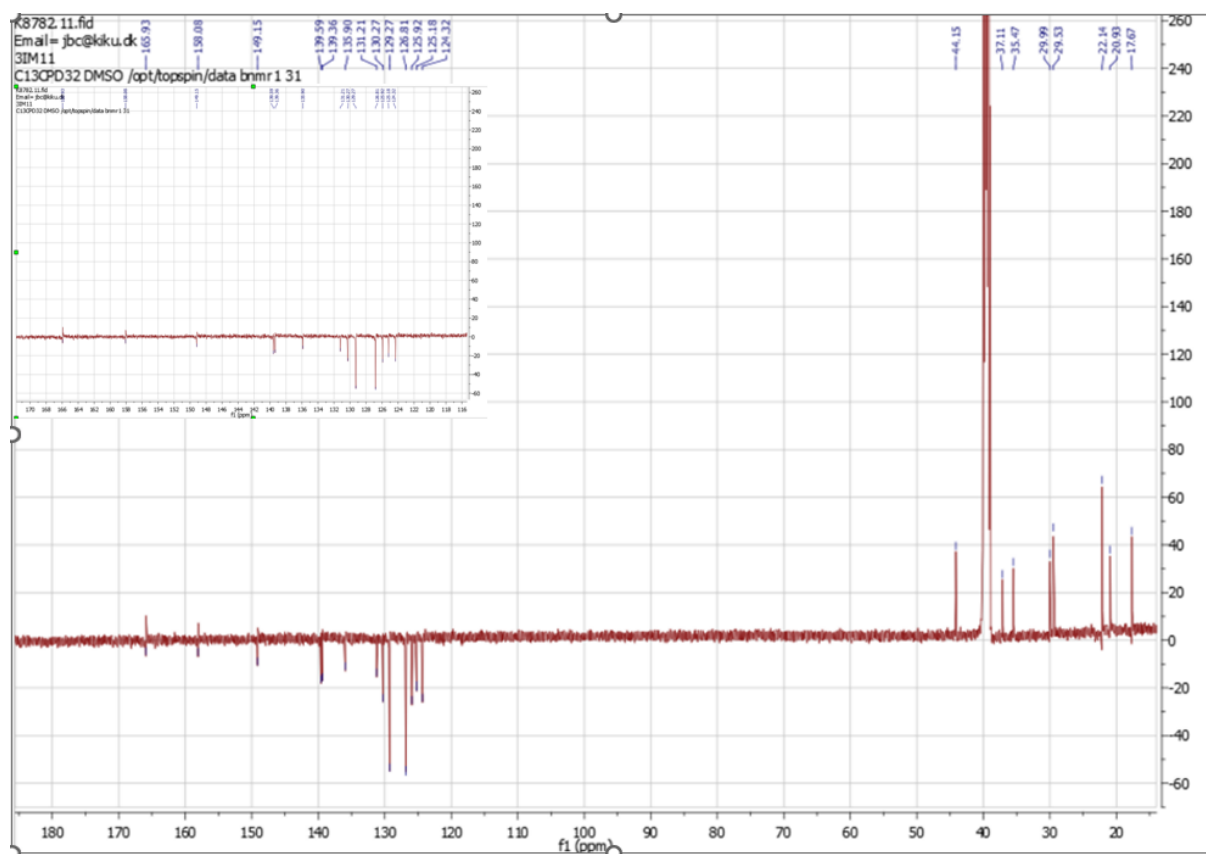
**Figure S8.** <sup>13</sup>C NMR spectrum of compound 4



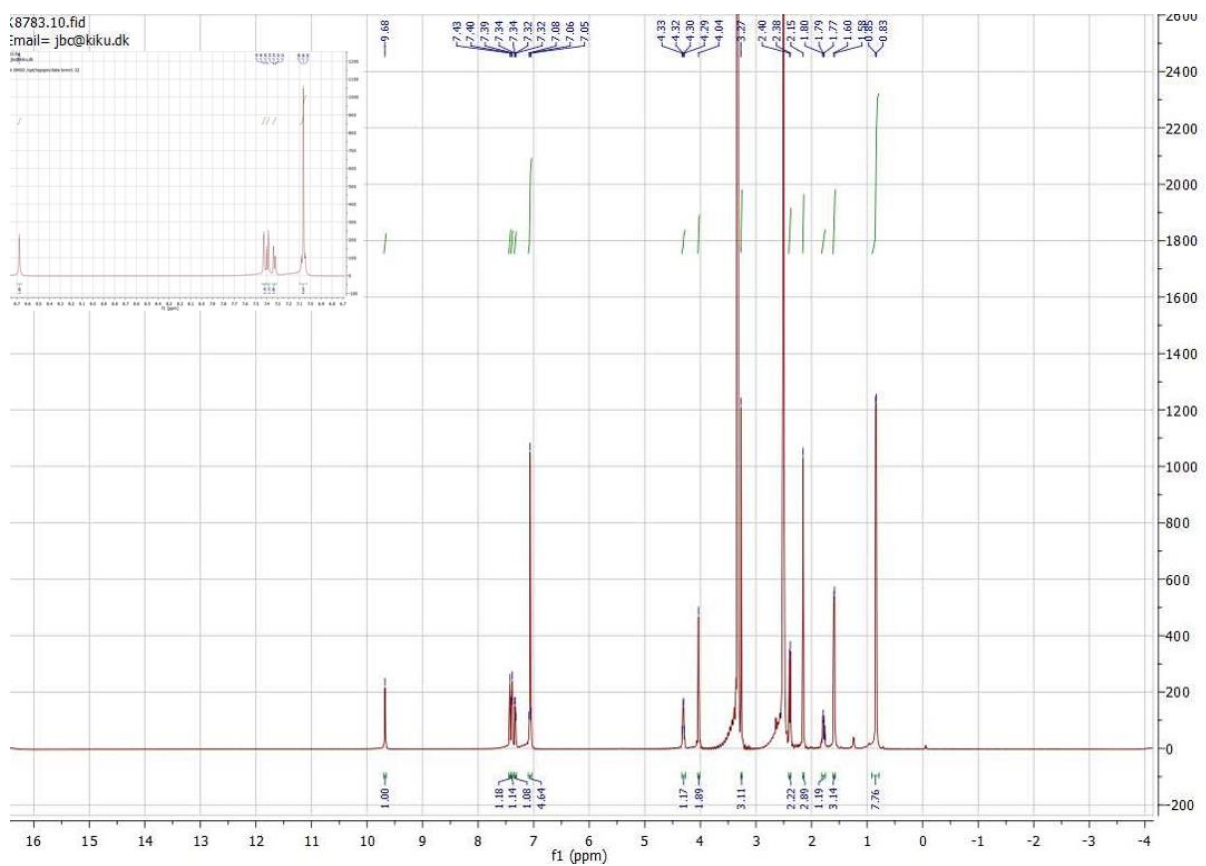
**Figure S9:**  $^1\text{H}$  NMR spectrum of compound **7a** (Full)



**Figure S10.** COSY- $^1\text{H}$  NMR spectrum of compound **7a**

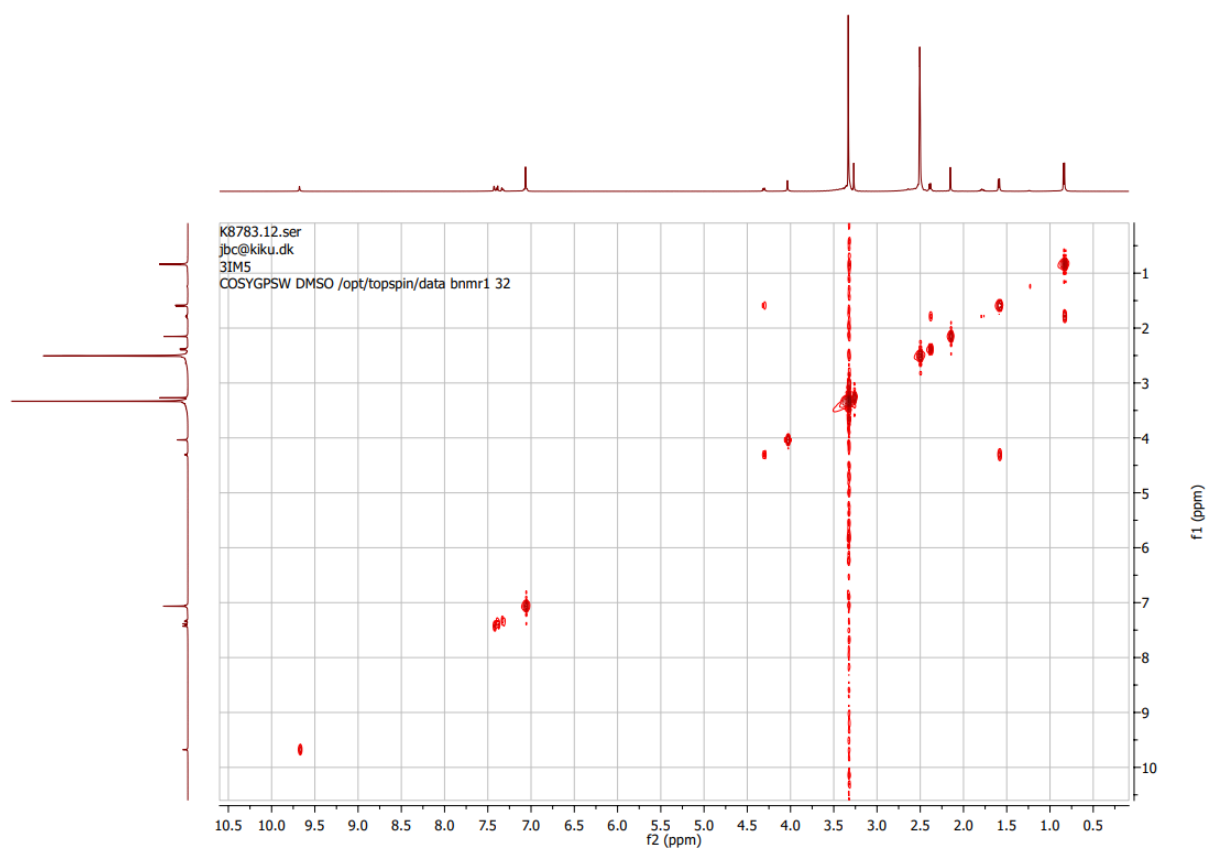


**Figure S11.**  $^{13}\text{C}$  NMR spectrum of compound **7a** (Full spectrum)

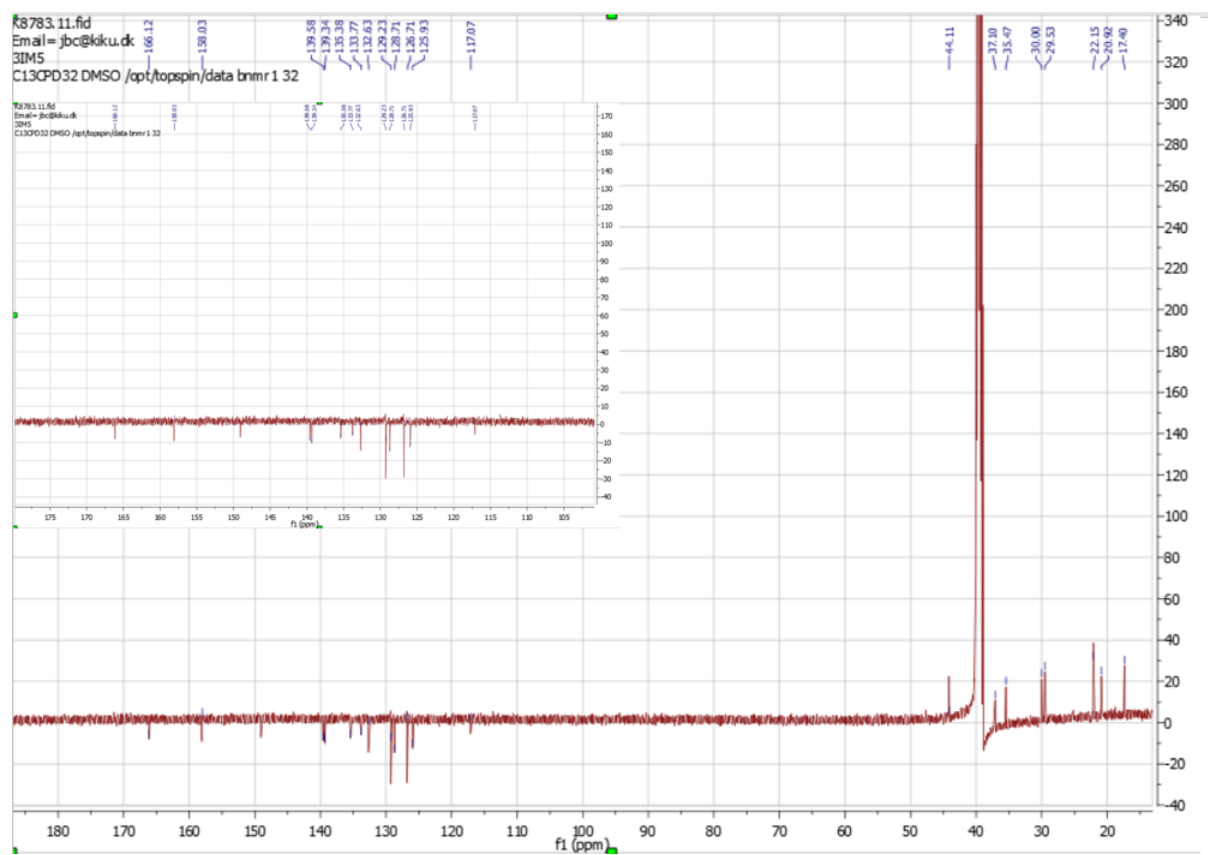


**Figure S12.**  $^1\text{H}$  NMR spectrum of compound **7b** (Full)

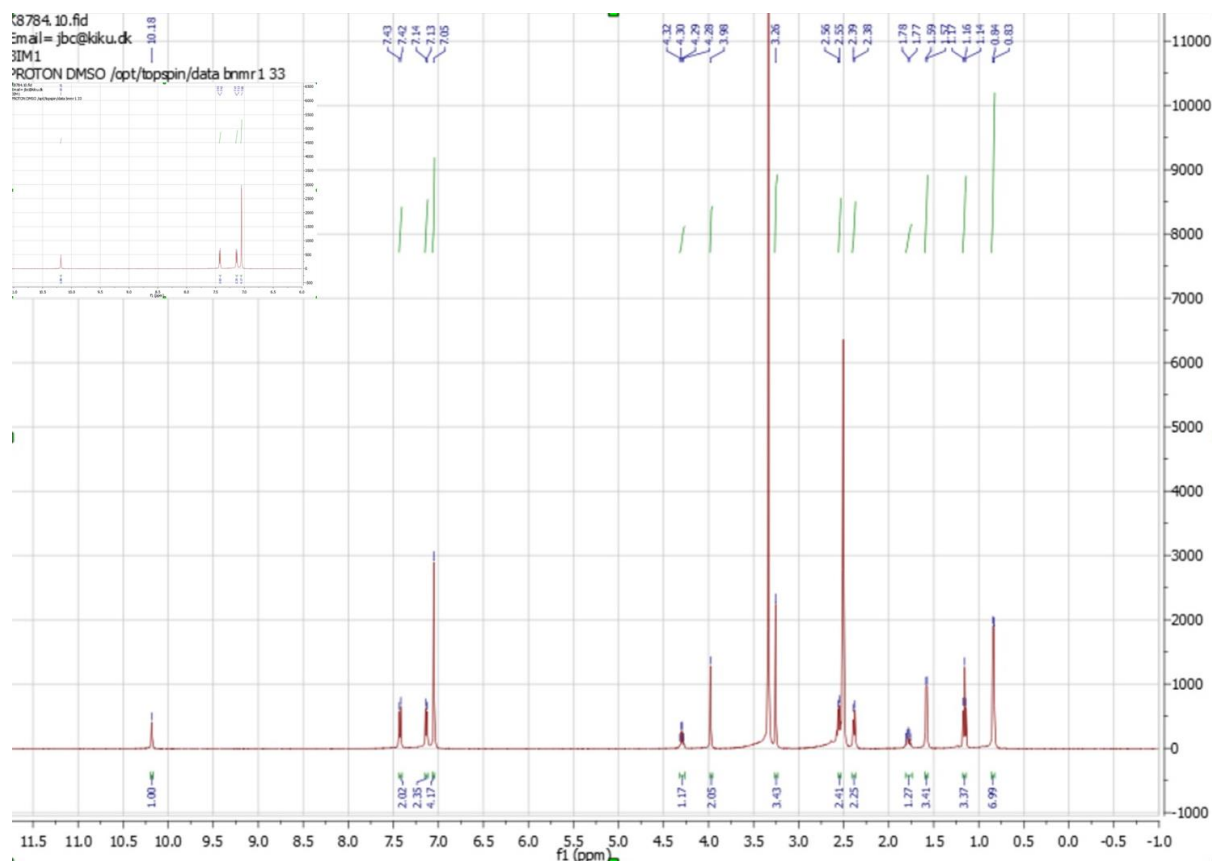




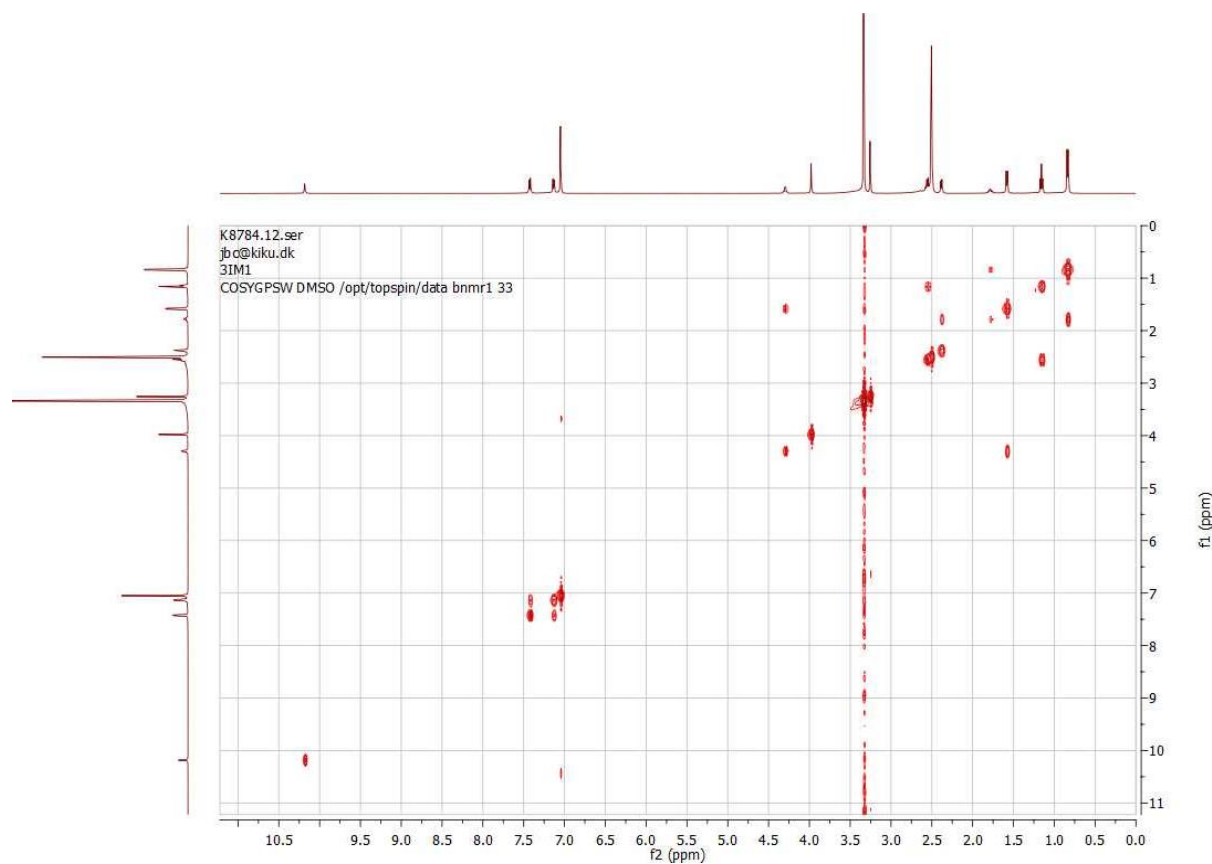
**Figure S13.** COSY- $^1\text{H}$  NMR spectrum of compound **7b**



**Figure S14.**  $^{13}\text{C}$  NMR spectrum of compound **7b** (Full spectrum)



**Figure S15.**  $^1\text{H}$  NMR spectrum of compound **7c** (Full spectrum)



**Figure S16.** COSY  $^1\text{H}$  NMR spectrum of compound **7c**

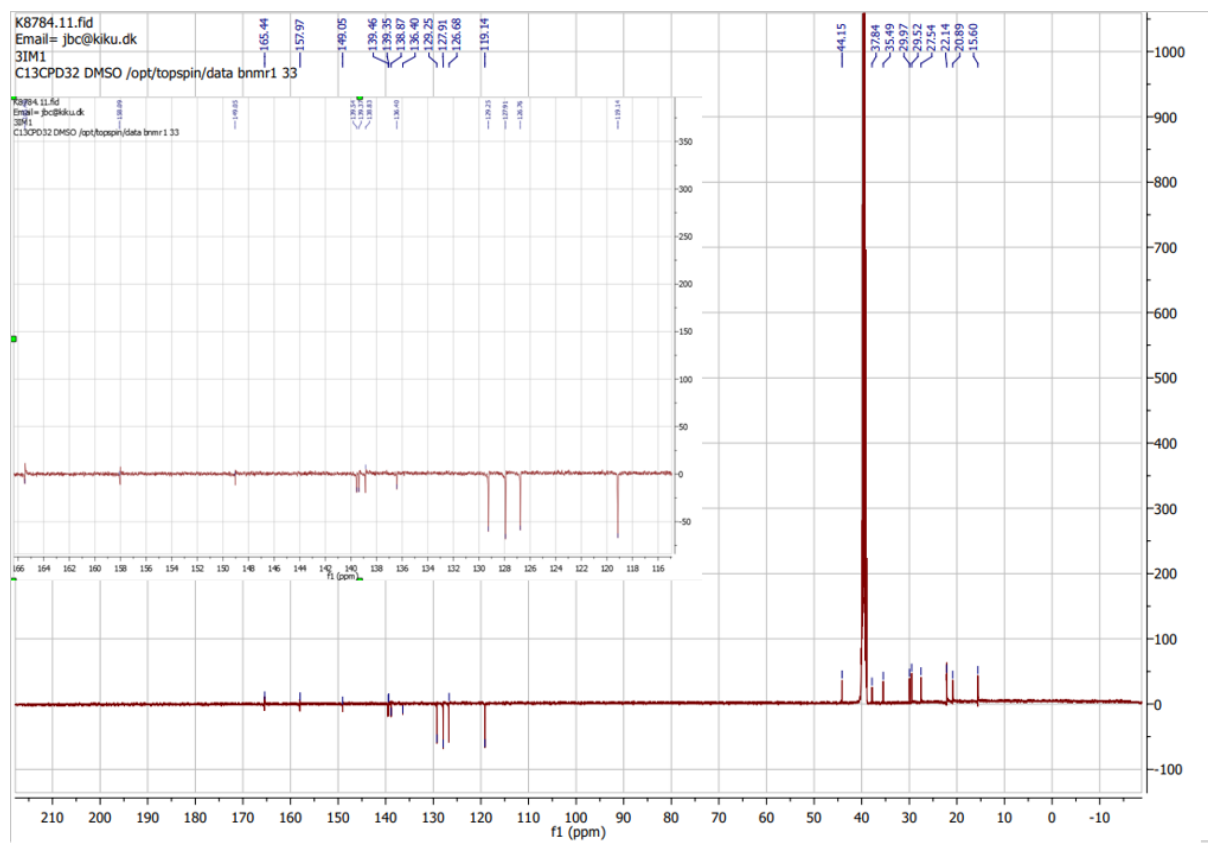


Figure S17.  $^{13}\text{C}$  NMR spectrum of compound **7c** (Full spectrum)

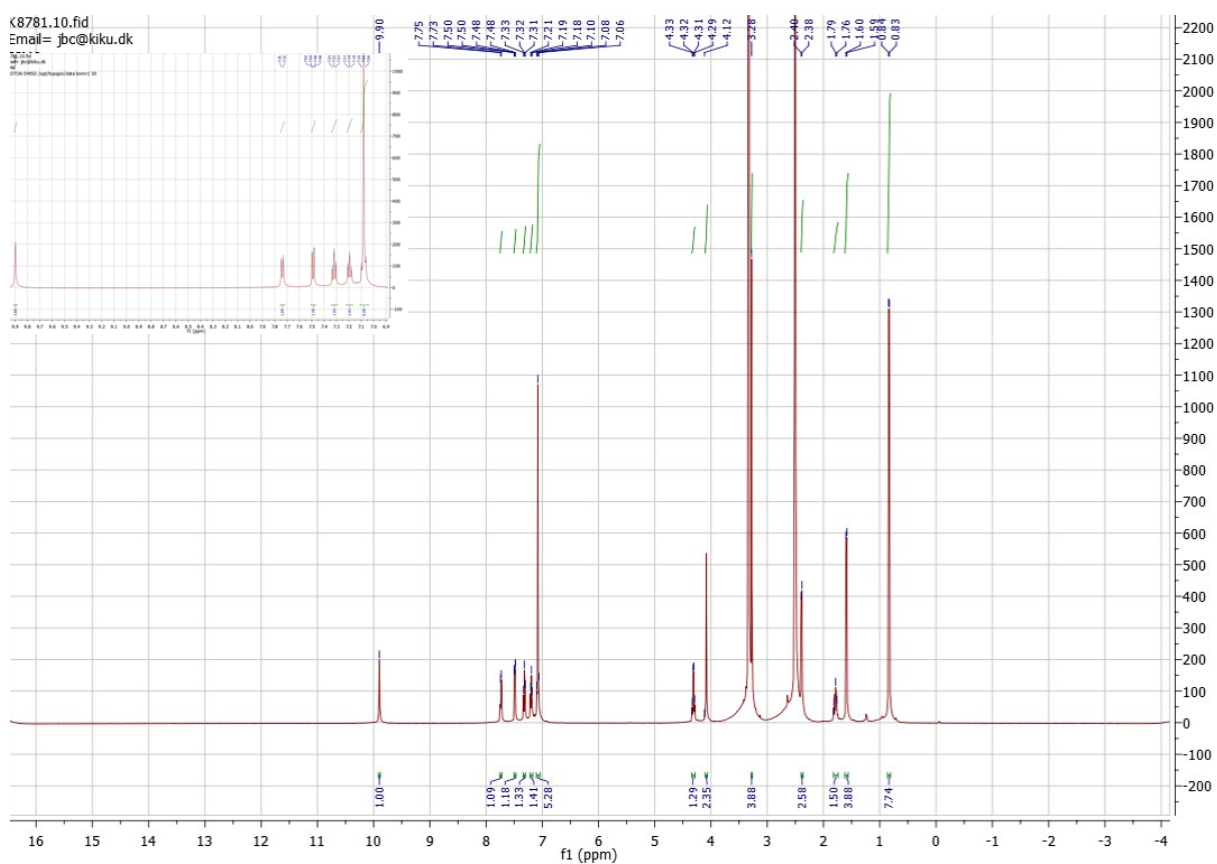
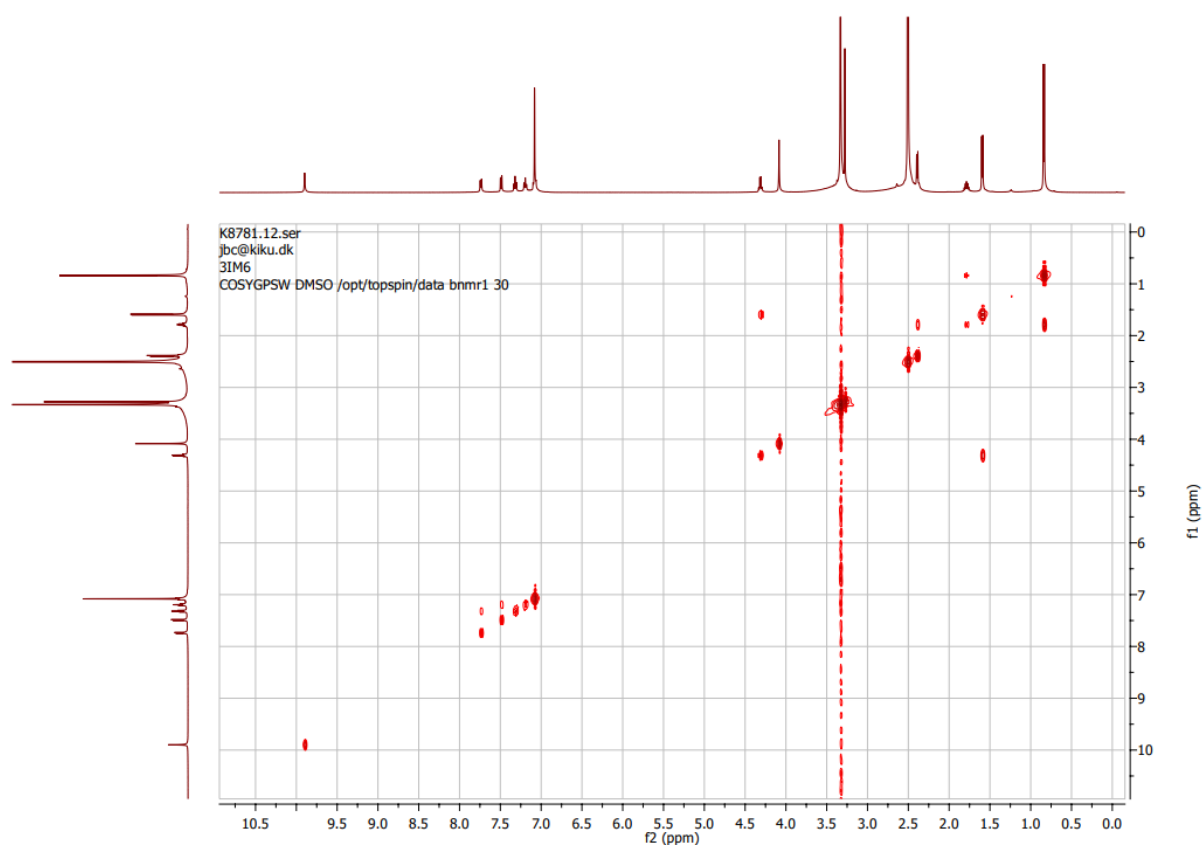
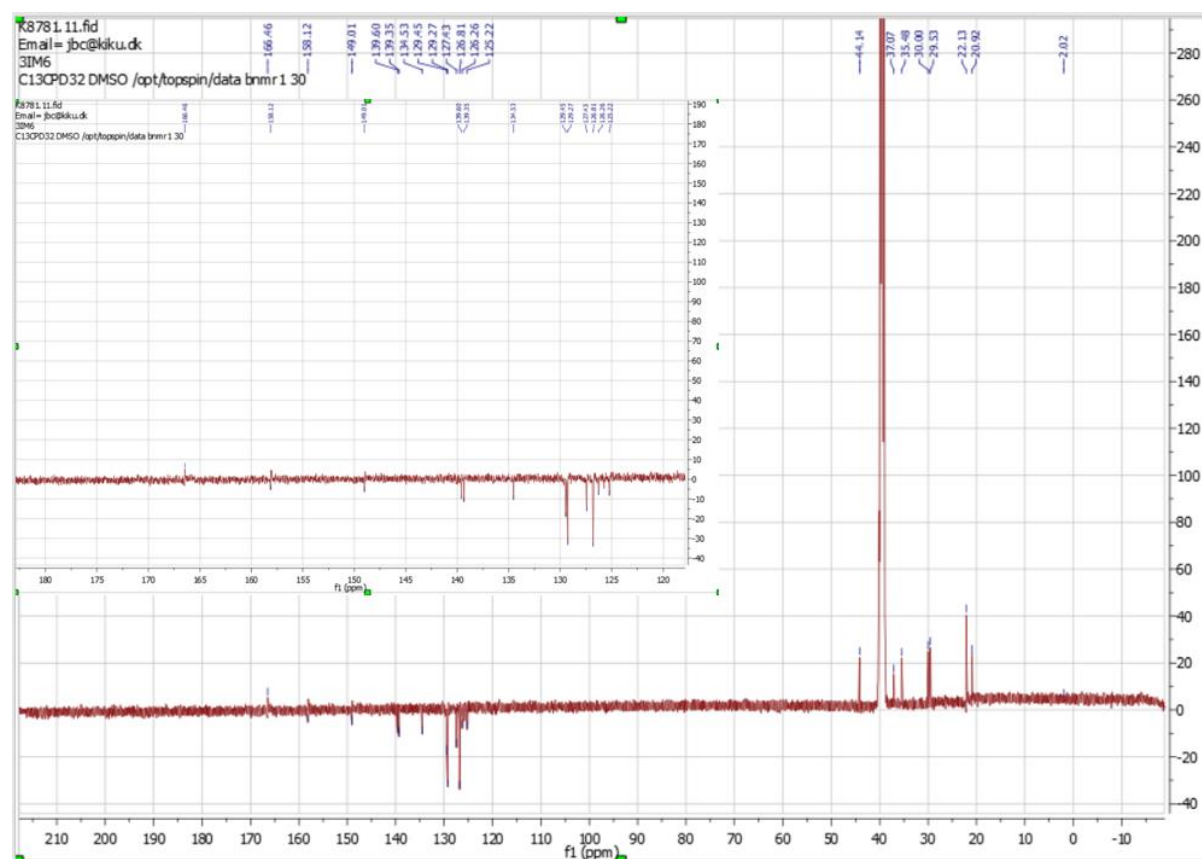


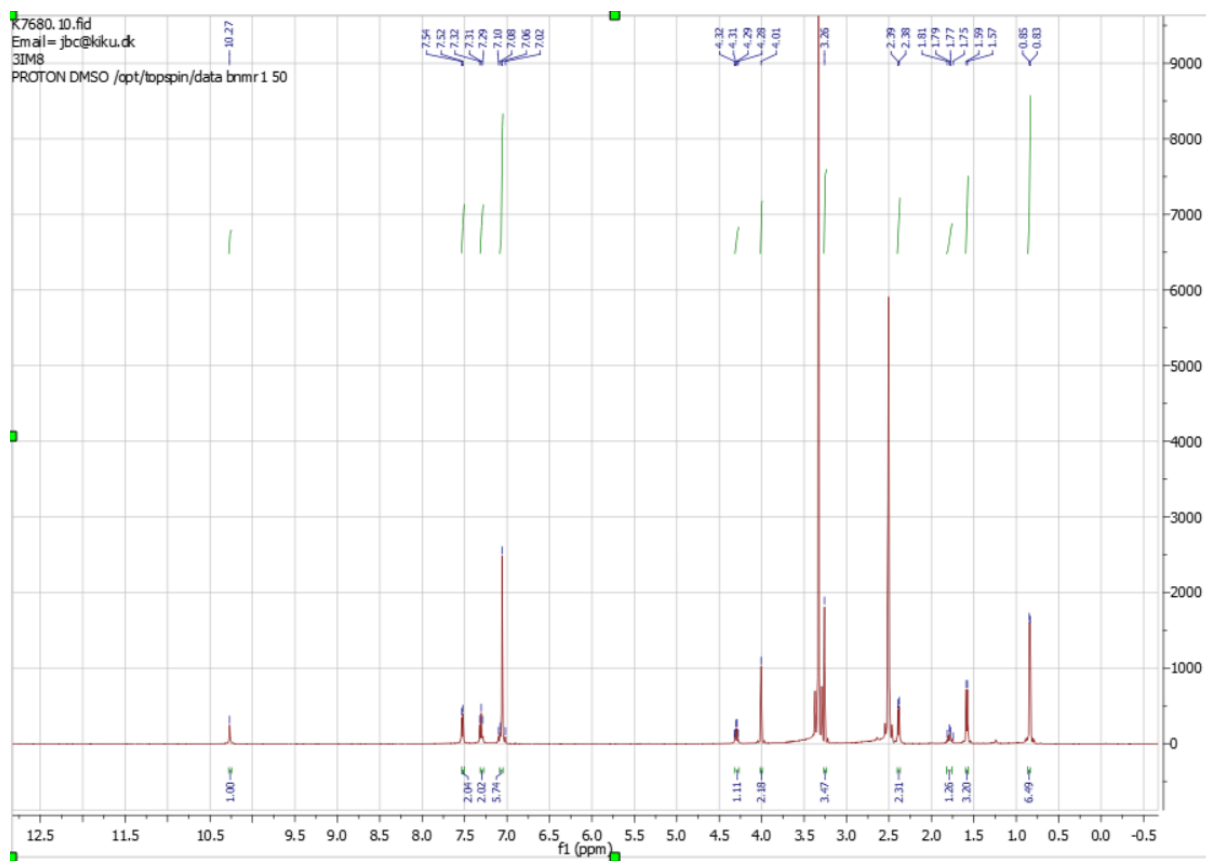
Figure S18:  $^1\text{H}$  NMR spectrum of compound **7d** (Full spectrum)



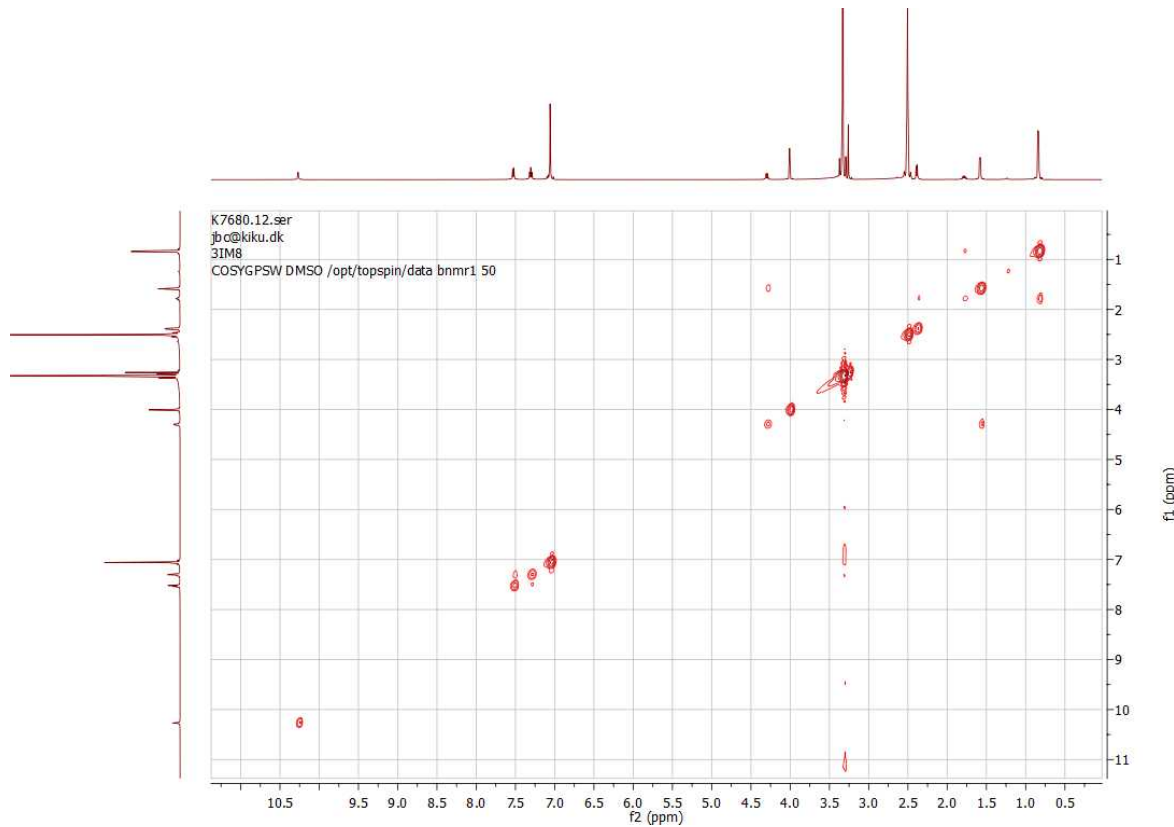
**Figure S19.** COSY- $^1\text{H}$  NMR spectrum of compound **7d**



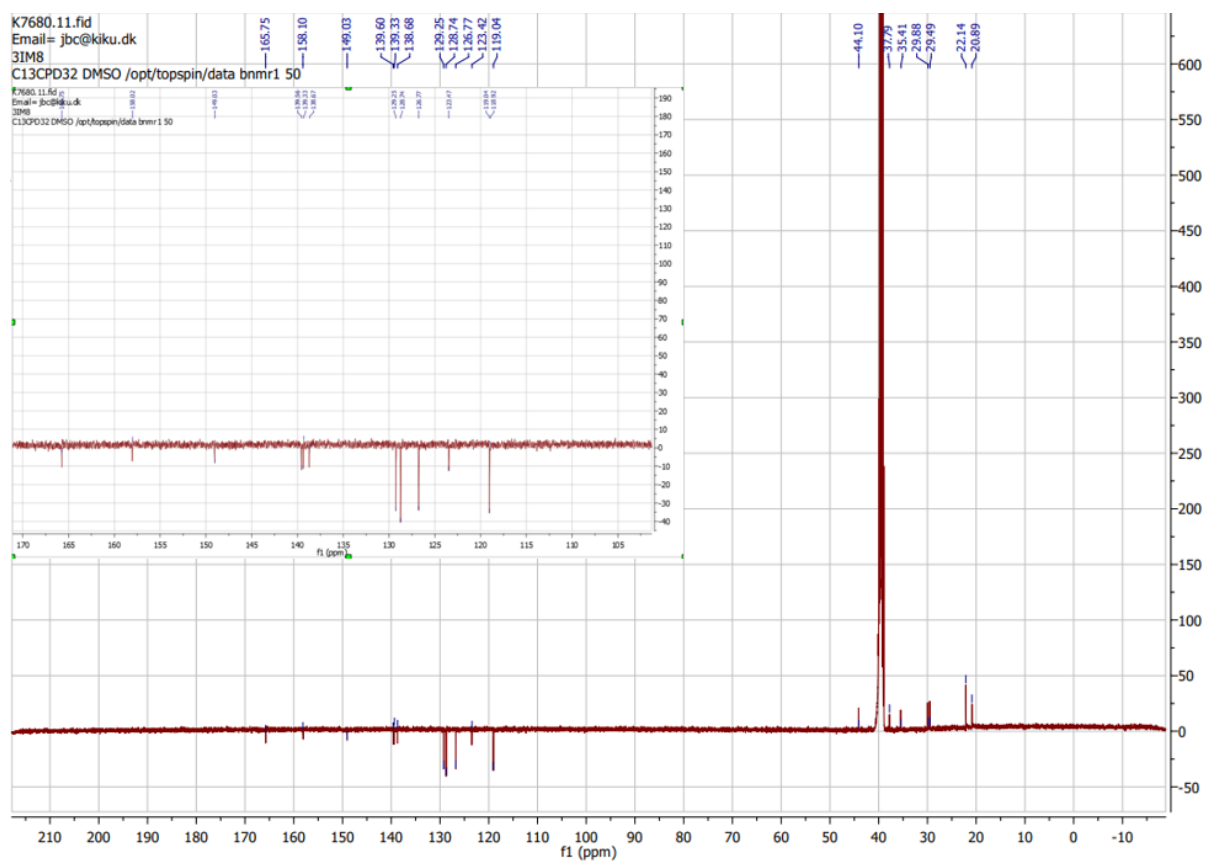
**Figure S20.**  $^{13}\text{C}$  NMR spectrum of compound **7d** (Full spectrum)



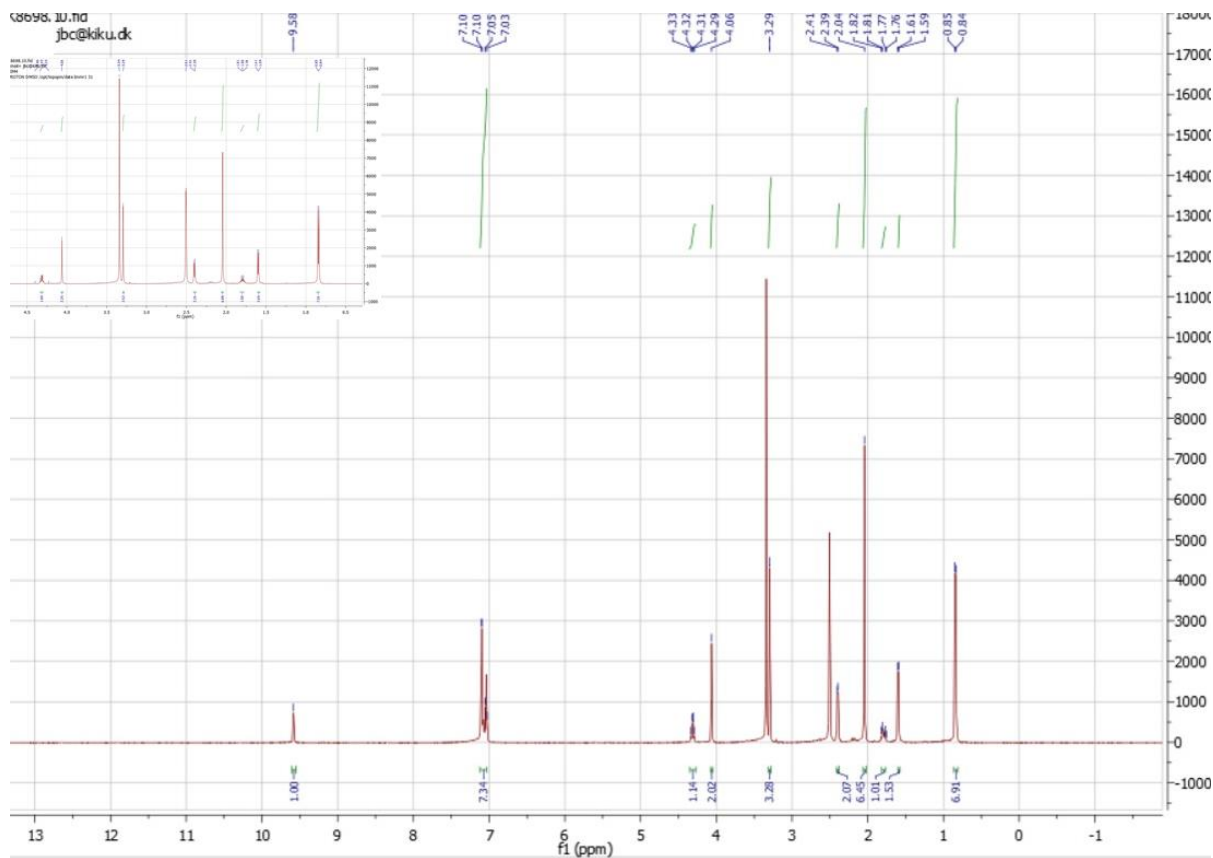
**Figure S21:**  $^1\text{H}$  NMR spectrum of compound **7e** (Full)



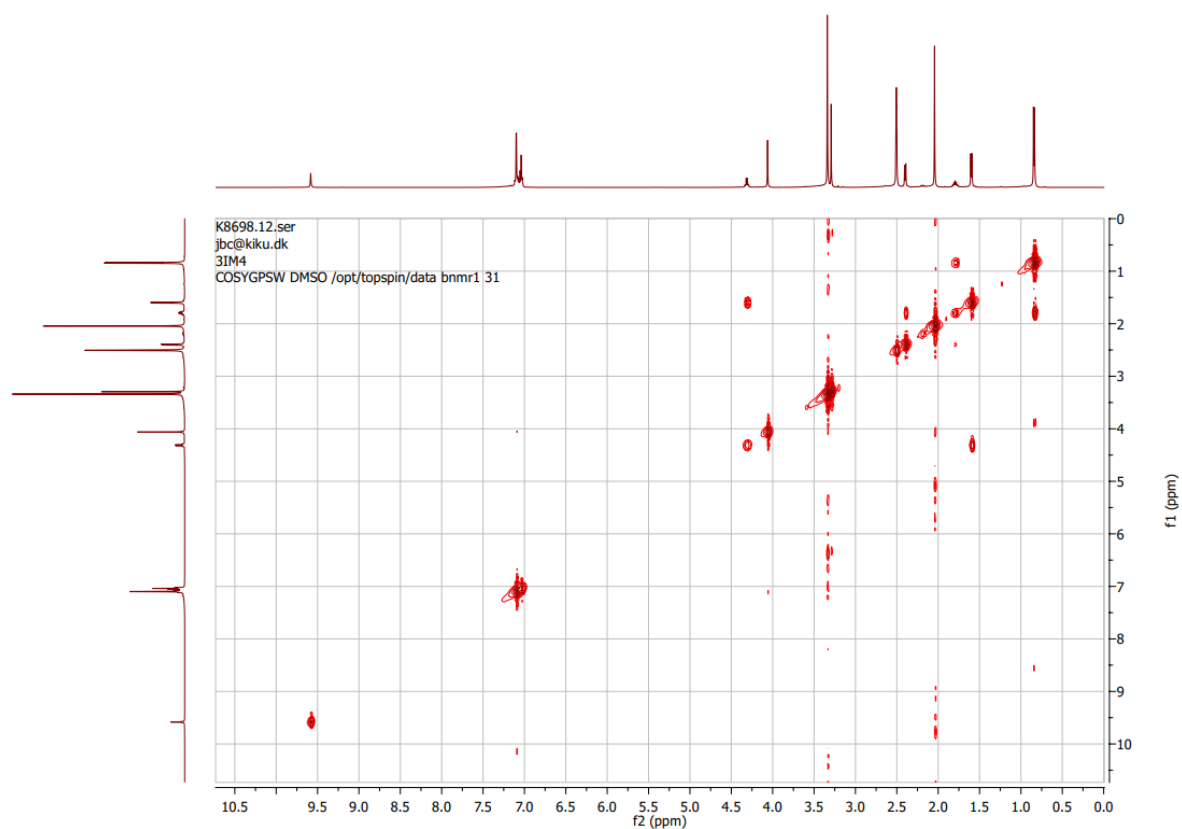
**Figure S22.** COSY- $^1\text{H}$  NMR spectrum of compound **7e**



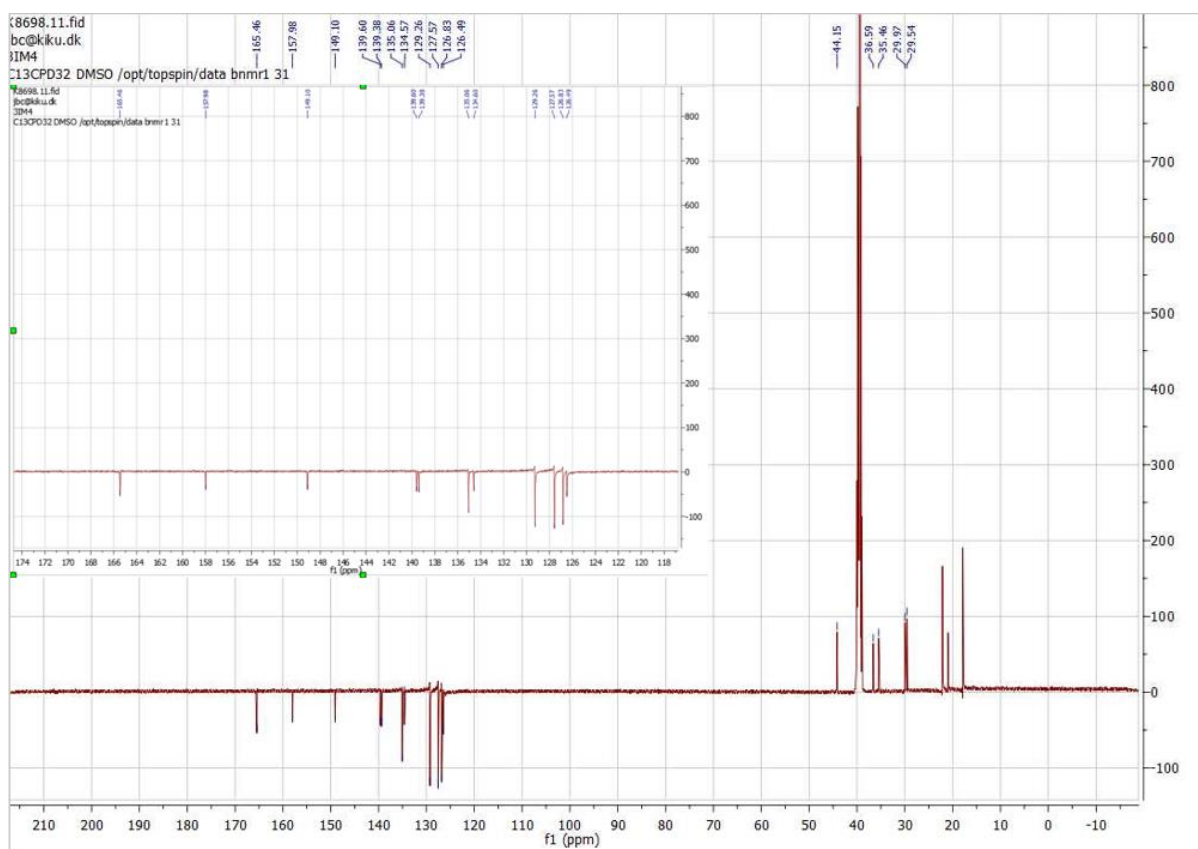
**Figure S23.**  $^{13}\text{C}$  NMR spectrum of compound **7e** (Full spectrum)



**Figure S24:**  $^1\text{H}$  NMR spectrum of compound **7f** (Full)



**Figure S25.** COSY-  $^1\text{H}$  NMR spectrum of compound **7f**



**Figure 26.**  $^{13}\text{C}$  NMR spectrum of compound **7f** (Full spectrum)

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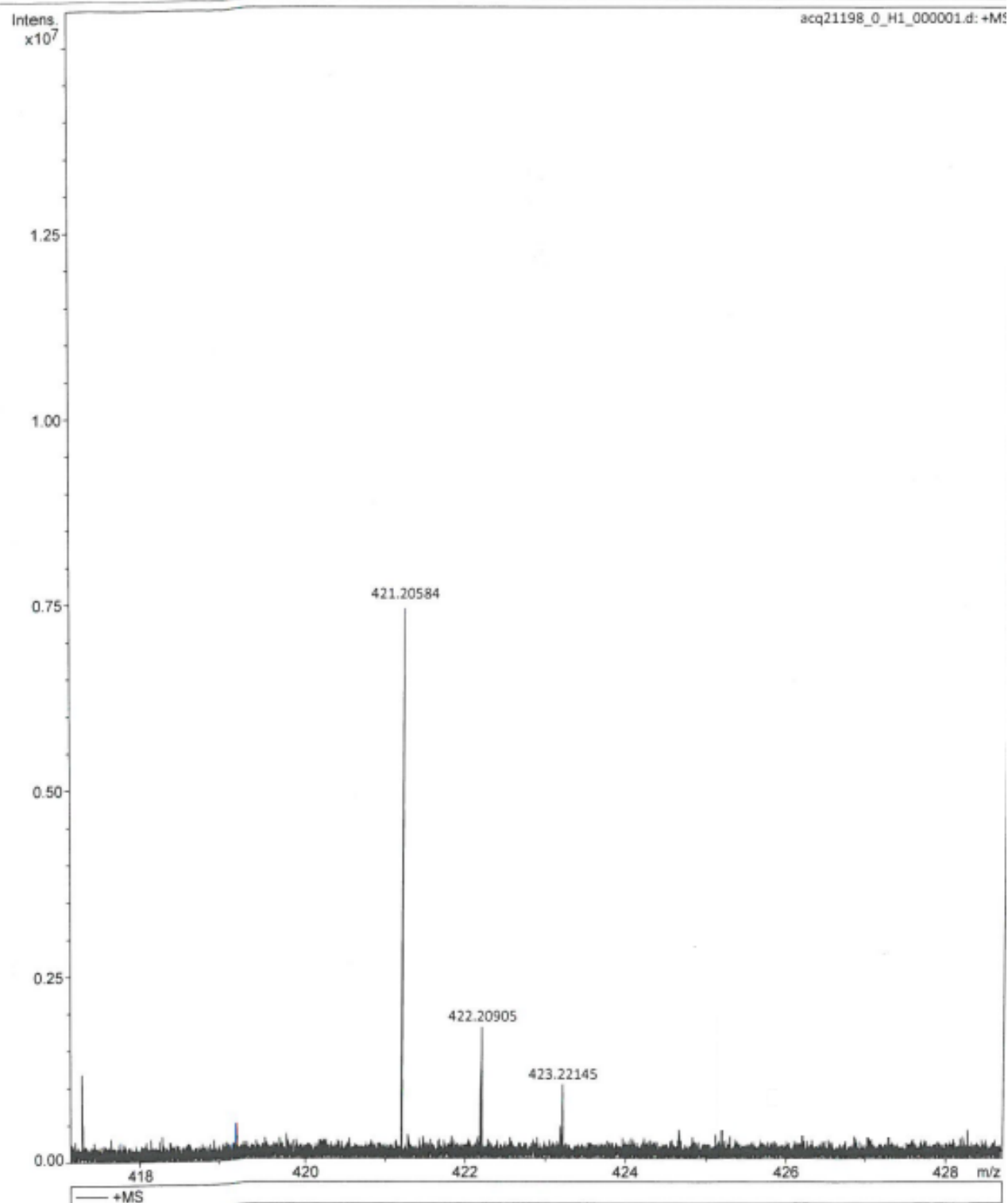


Figure S27. HRMS spectrum of compound **7a**



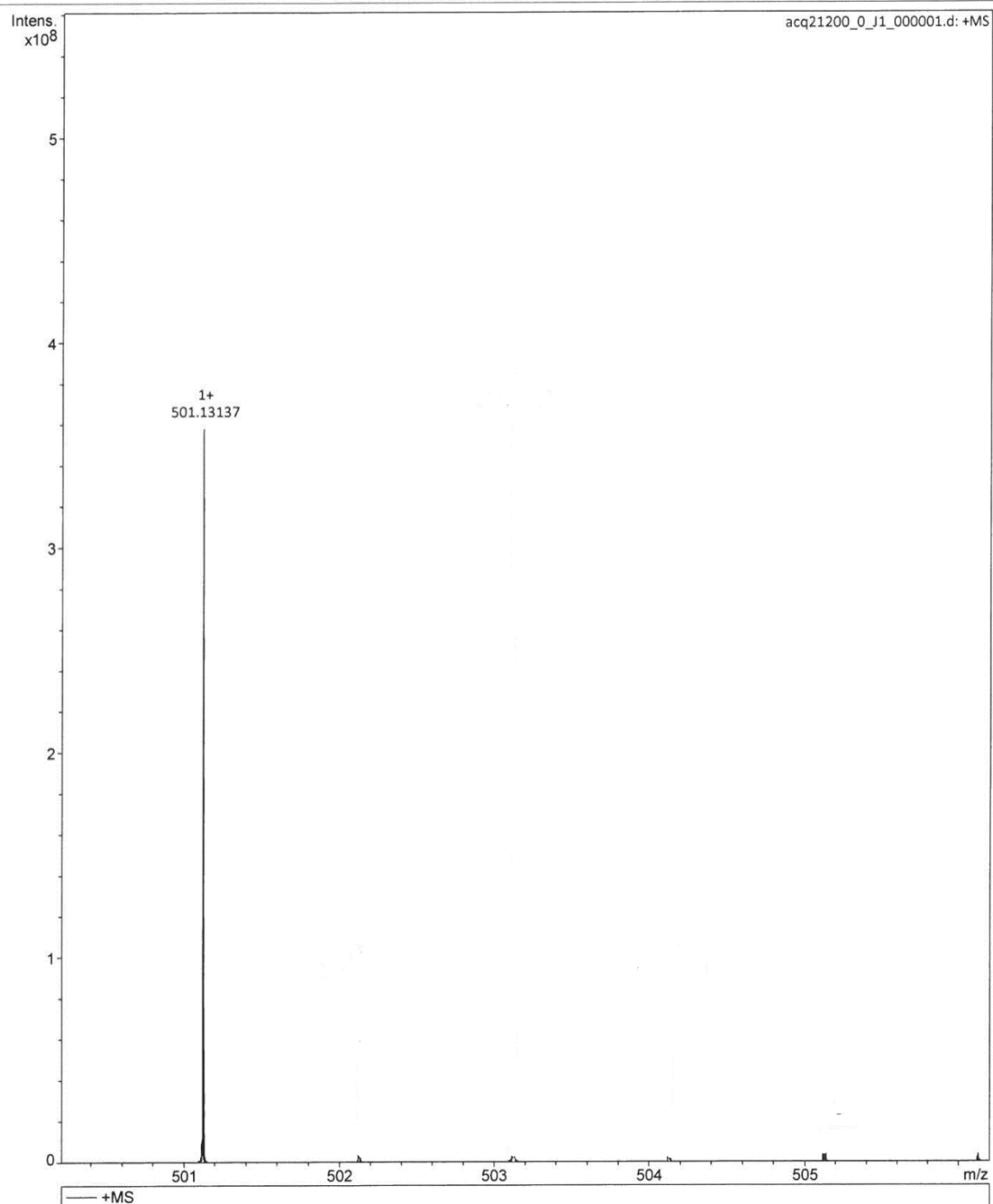
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**Figure S28.** HRMS spectrum of compound **7b**

## Generic Display Report

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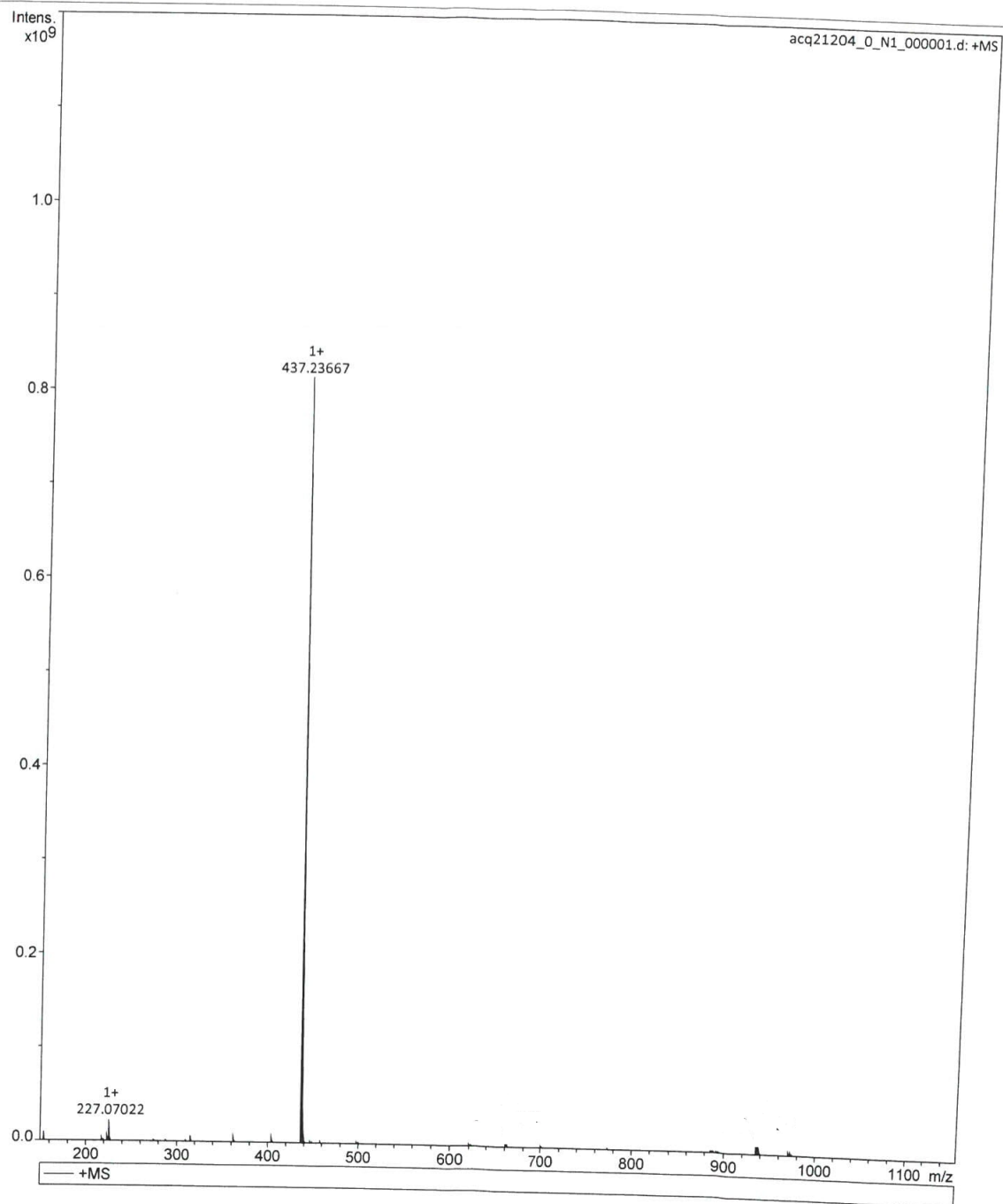


Figure S29. HRMS spectrum of compound 7c

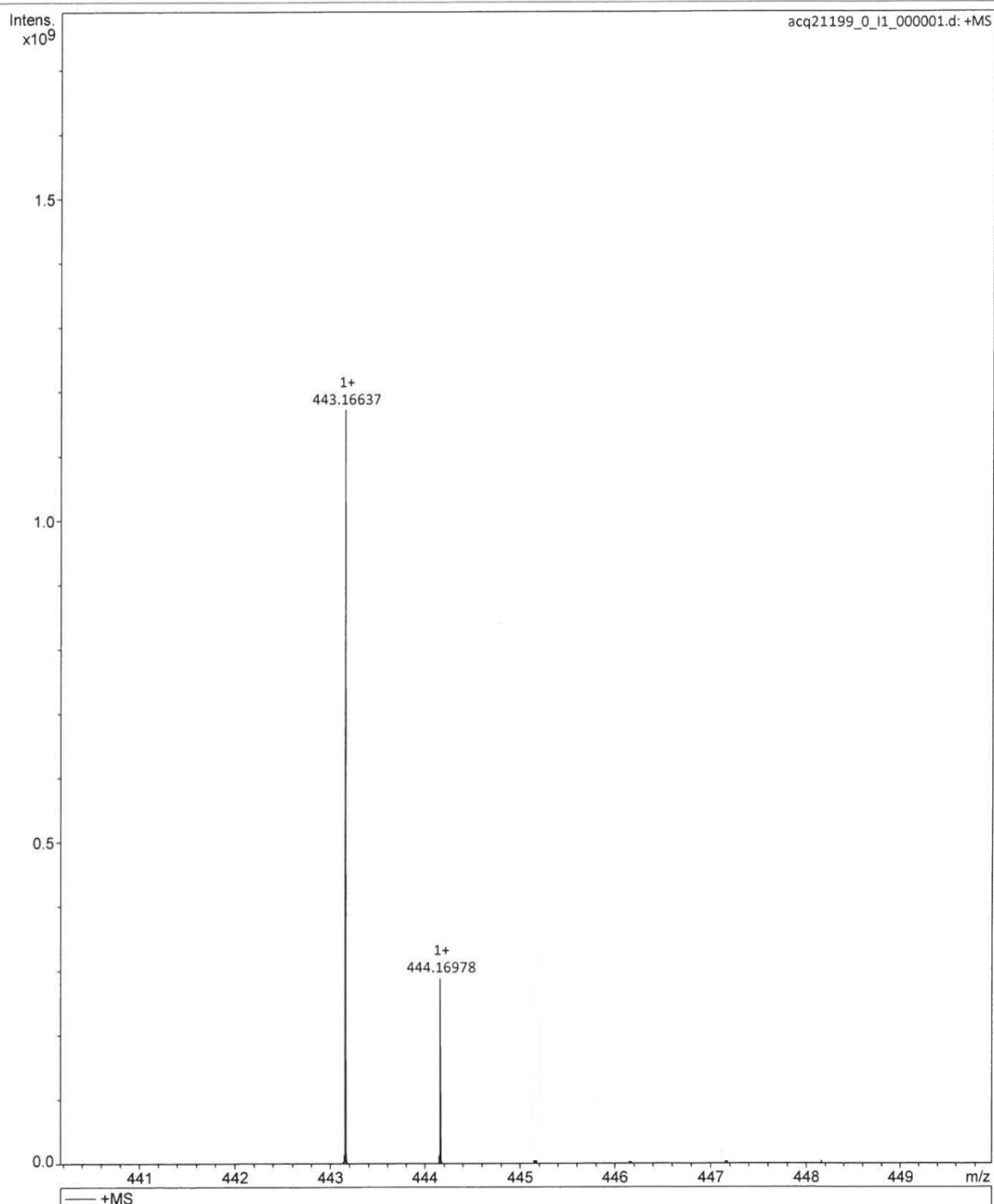
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**Figure S30.** HRMS spectrum of compound **7d**

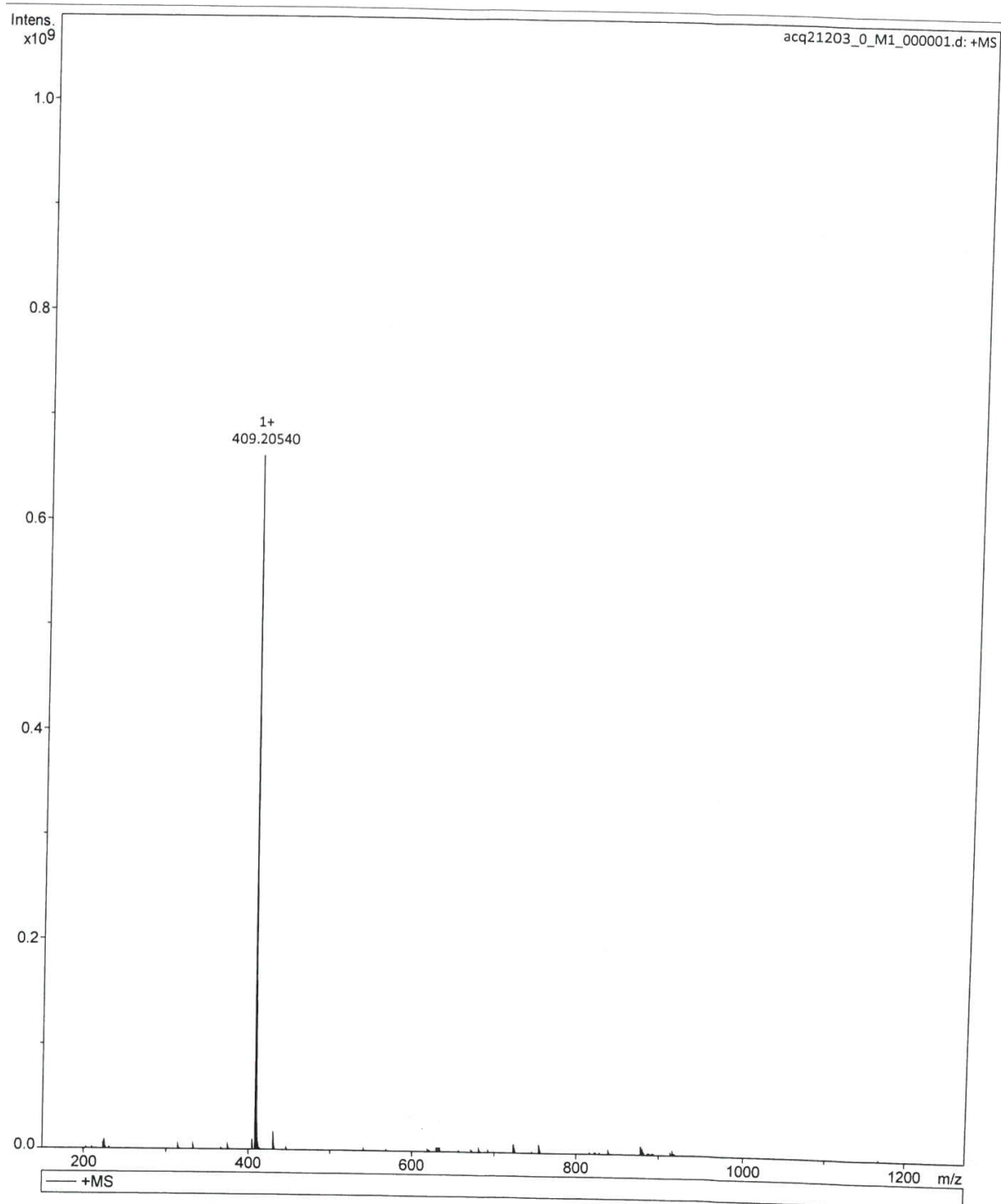
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Operator  
Instrument solarix XR



**Figure S31.** HRMS spectrum of compound **7e**

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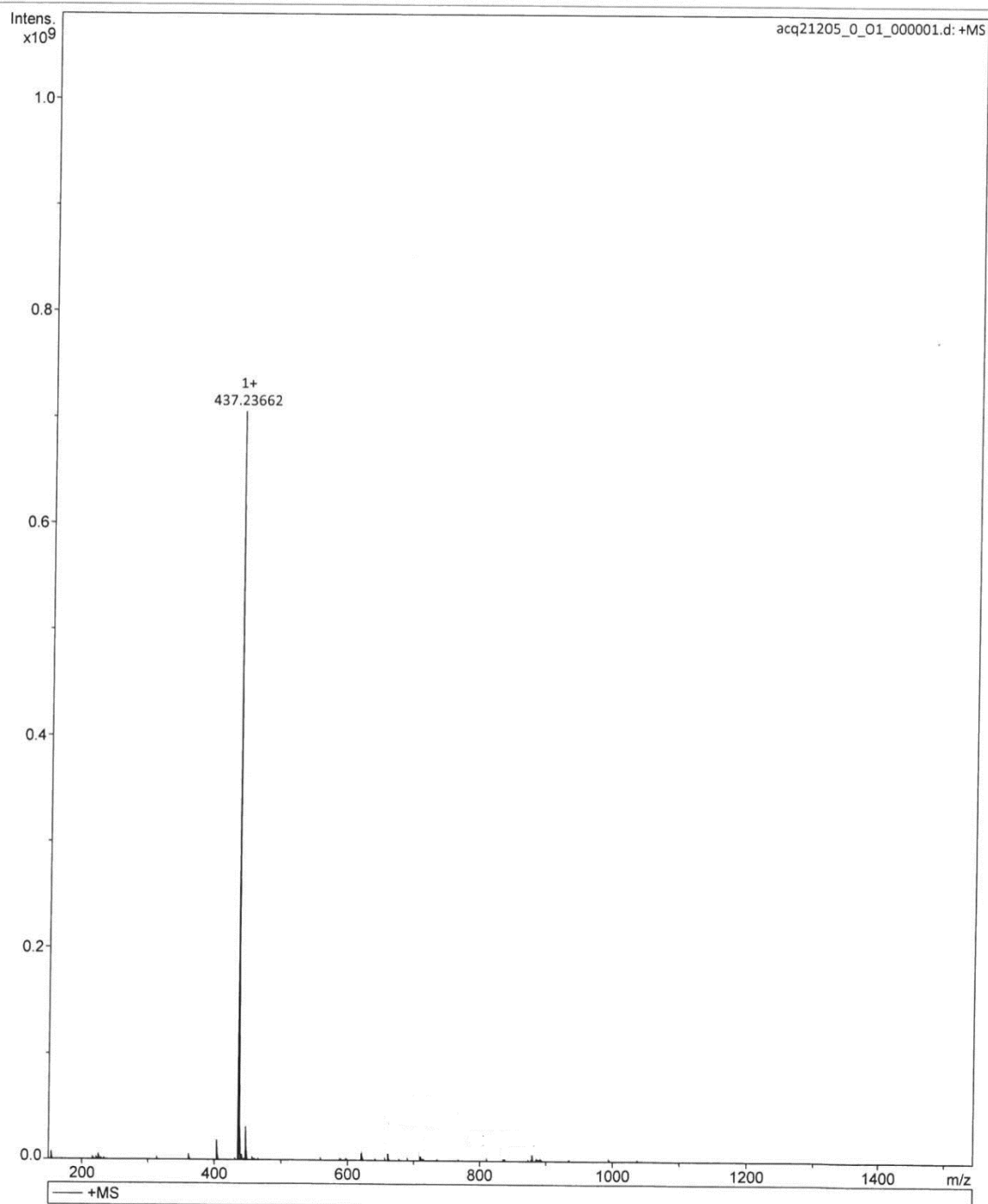
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**Figure S32.** HRMS spectrum of compound **7f**