

## Supplementary Materials

### Evidence of Isomerization in the Michael-Type Thiol-Maleimide Addition: Click Reaction Between L-Cysteine and 6-Maleimidehexanoic acid.

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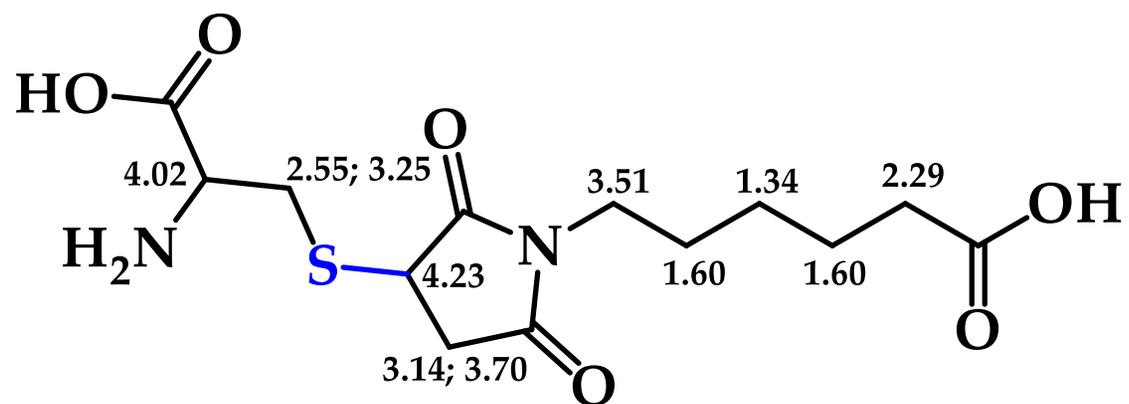
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**Figure S9.** MS/MS for TIC of 4.6 min corresponding to compound **2**.

**Figure S10.** <sup>1</sup>H-NMR spectrum (400MHz, MeOD, 303 K) of mix products.



COMPOUND 1: Cys-S-Mhx

P-2 (RMN-210166) BBO  
P-2 (RMN-210166) BBO  
Neo Avance 1H-MeOD  
24 de Marzo de 2021

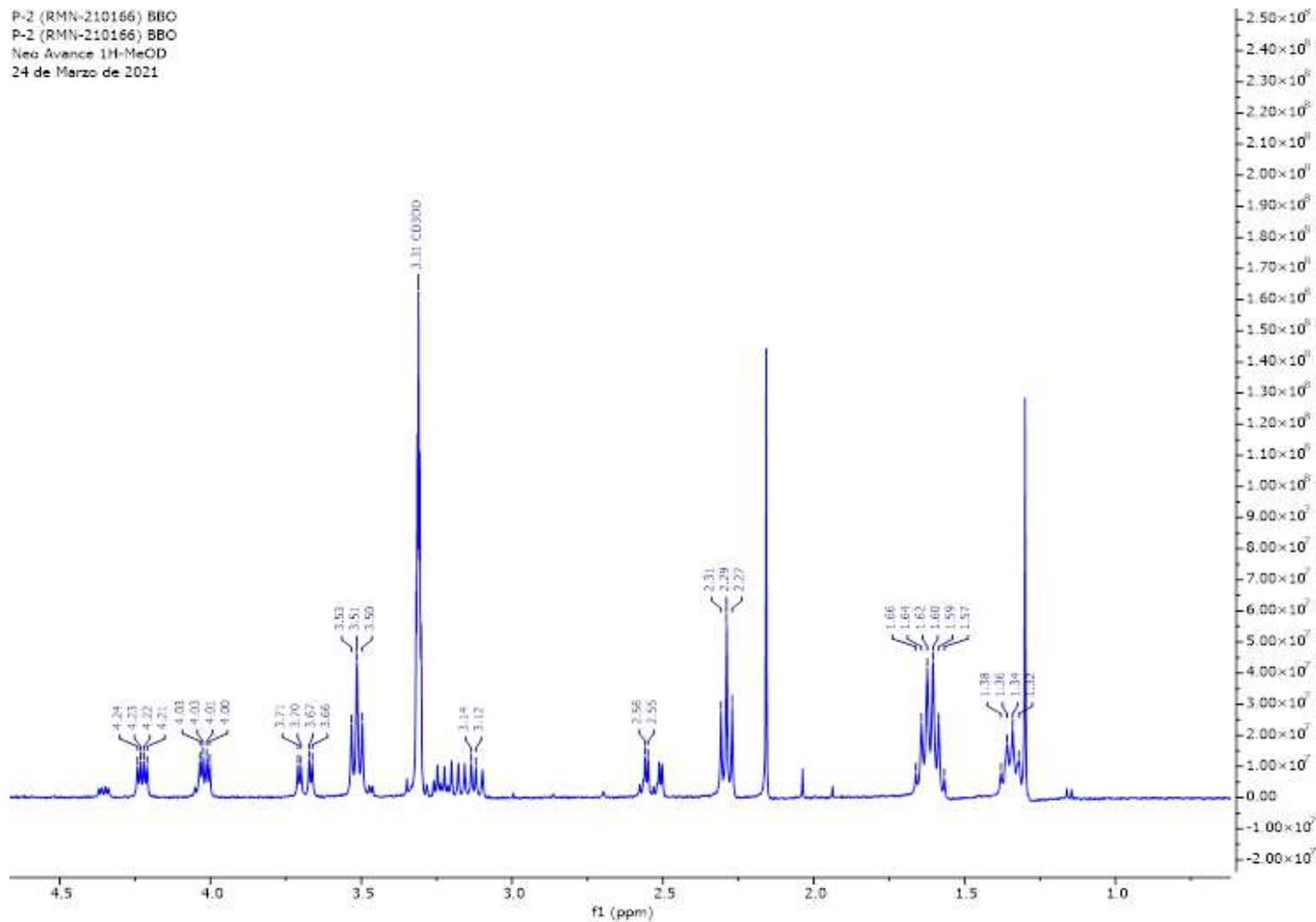


Figure S1. <sup>1</sup>H-NMR spectrum (400MHz, MeOD, 303 K) of compound 1.



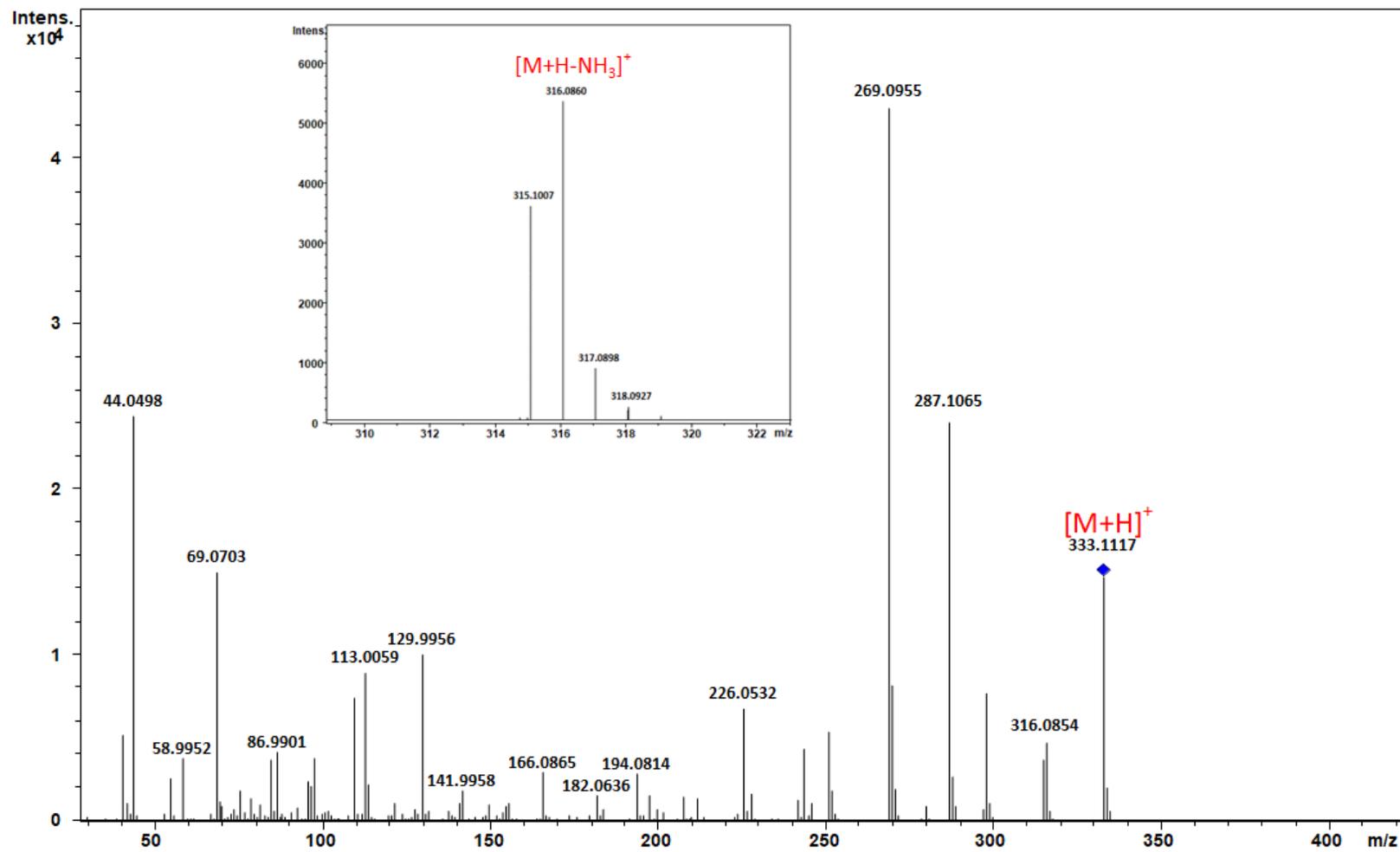
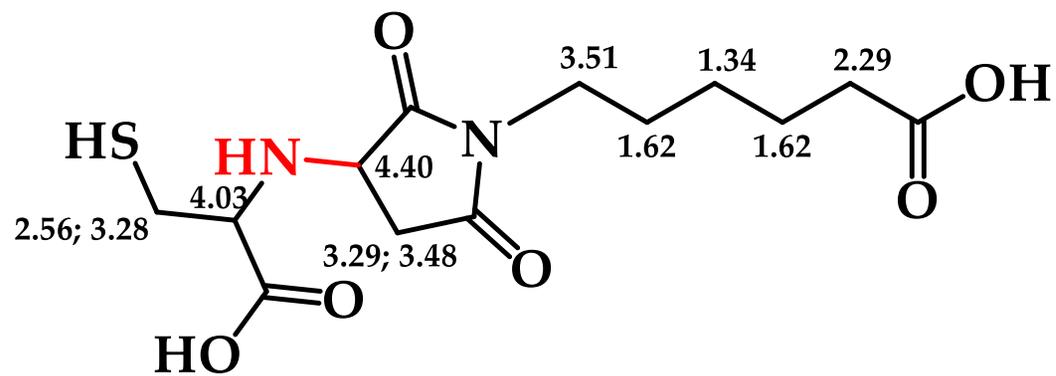
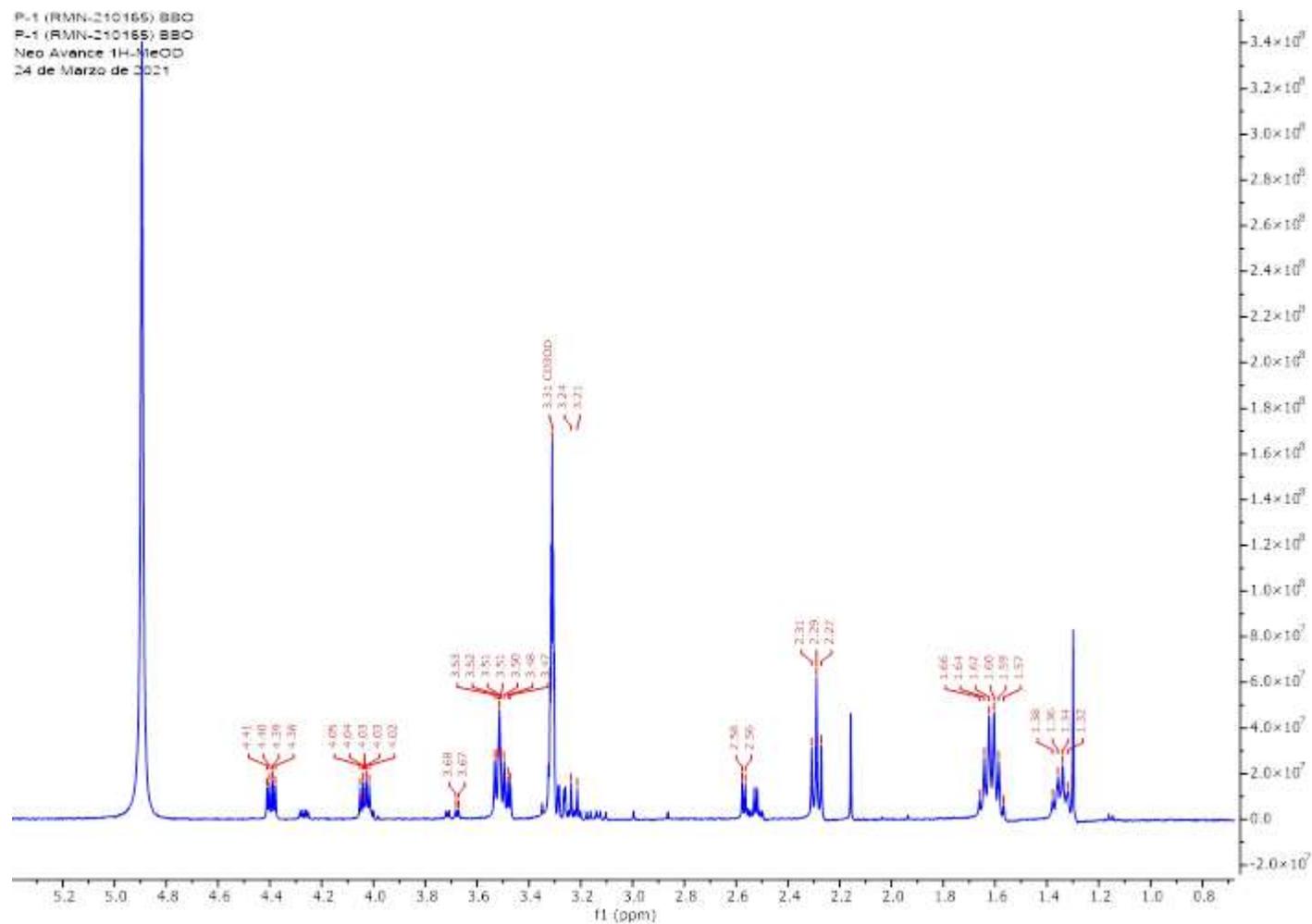


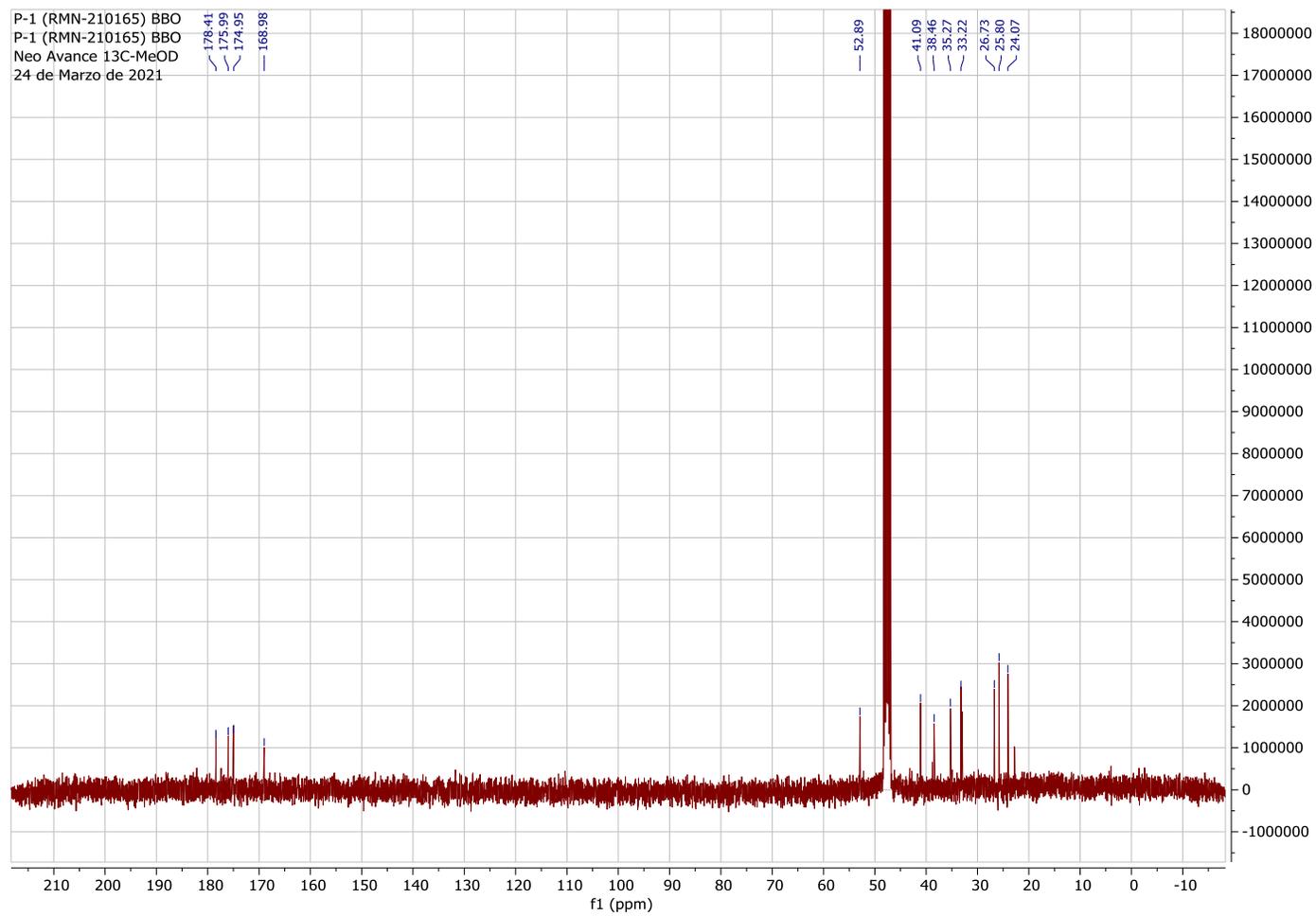
Figure S3. MS/MS for TIC of 4.7 min corresponding to compound 1.



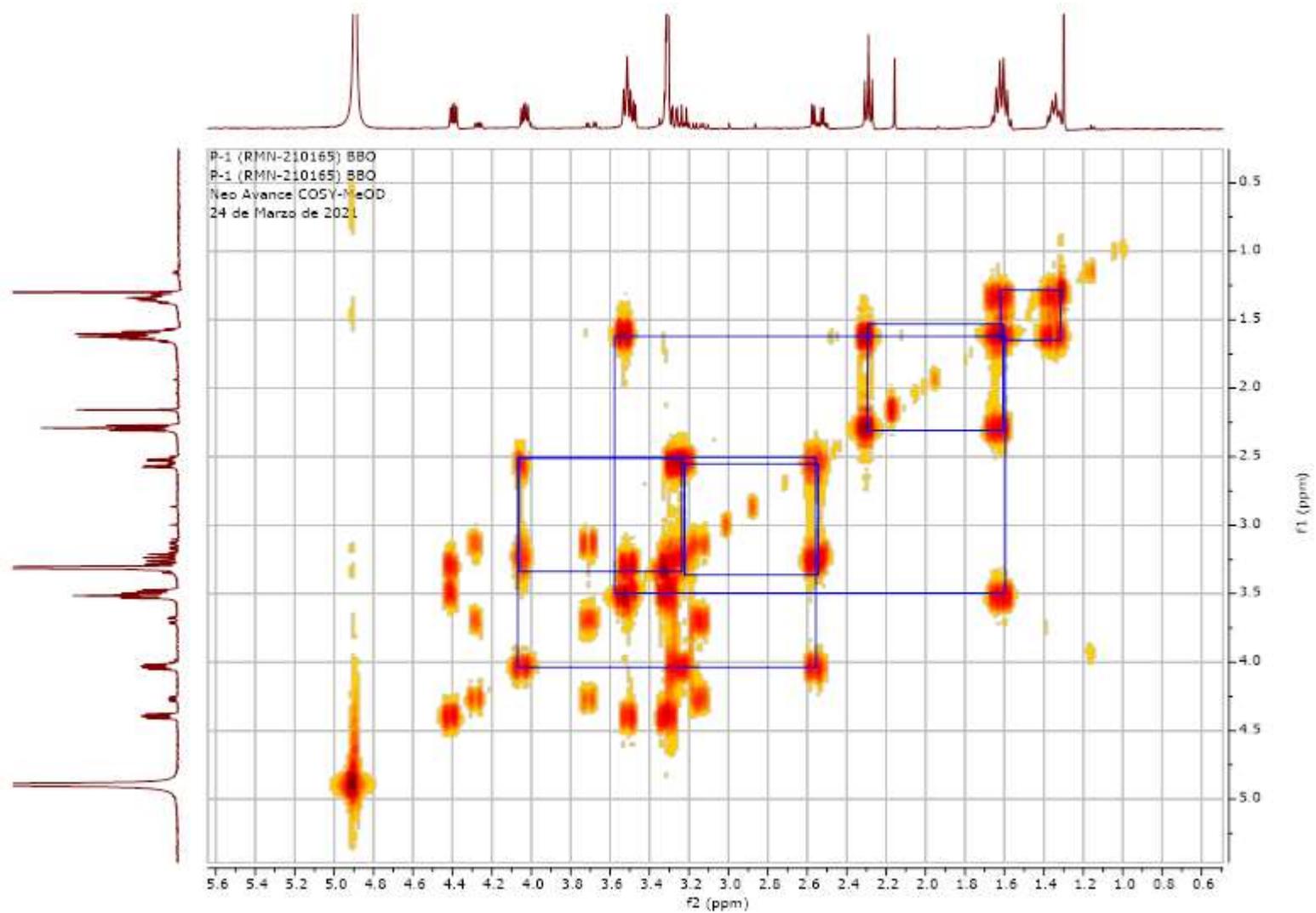
COMPOUND 2: Cys-N-Mhx



**Figure S4.**  $^1\text{H}$ -NMR spectrum (400MHz, MeOD, 303 K) of compound 2.



**Figure S5.**  $^{13}\text{C}$ -NMR spectrum (400MHz, MeOD, 303 K) of compound **2**.



**Figure S6.**  $^1\text{H-NMR}$  COSY spectrum (400MHz, MeOD, 303 K) of compound 2.

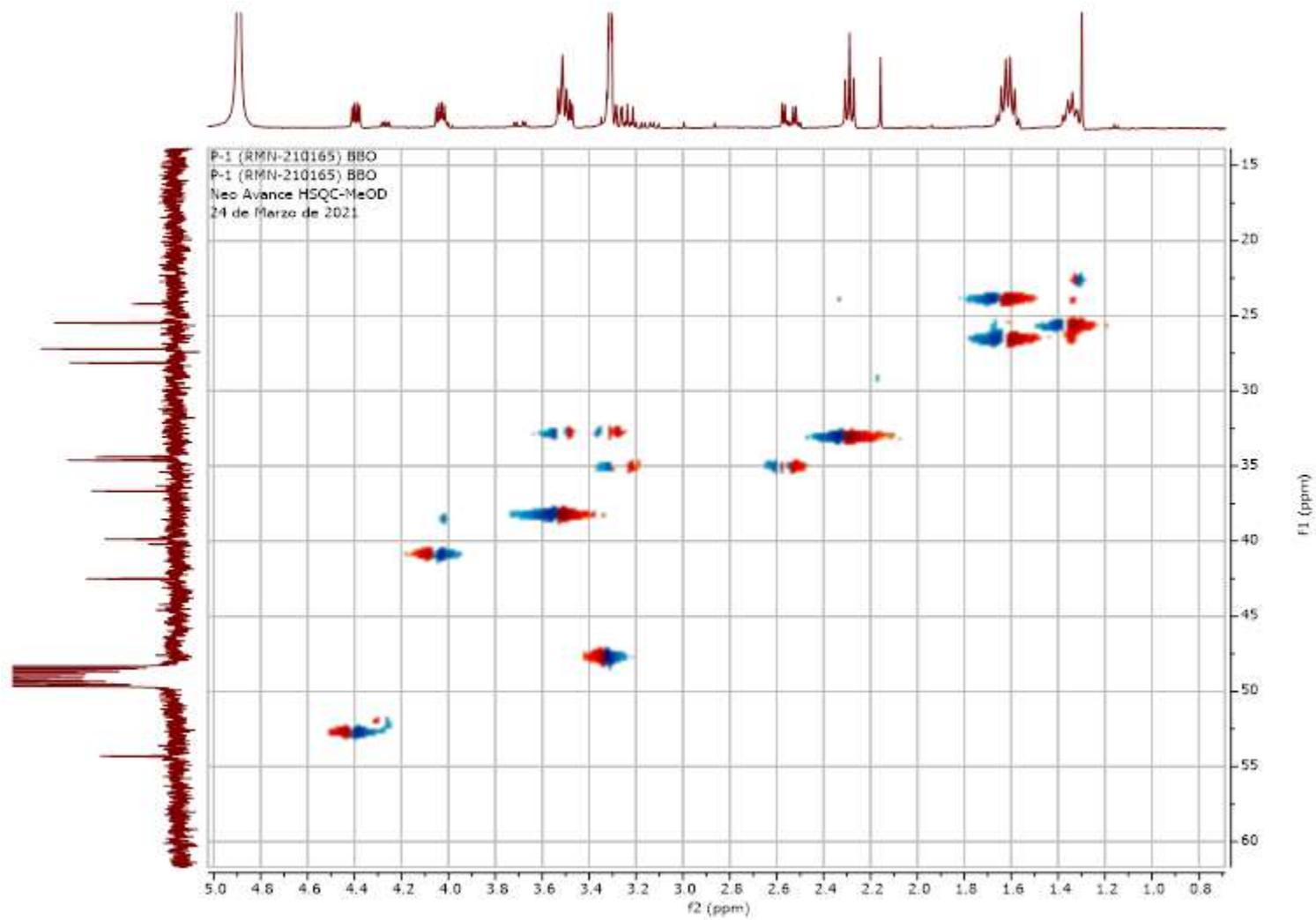


Figure S7.  $^1\text{H}$ -NMR HSQC spectrum (400MHz, MeOD, 303 K) of compound 2.

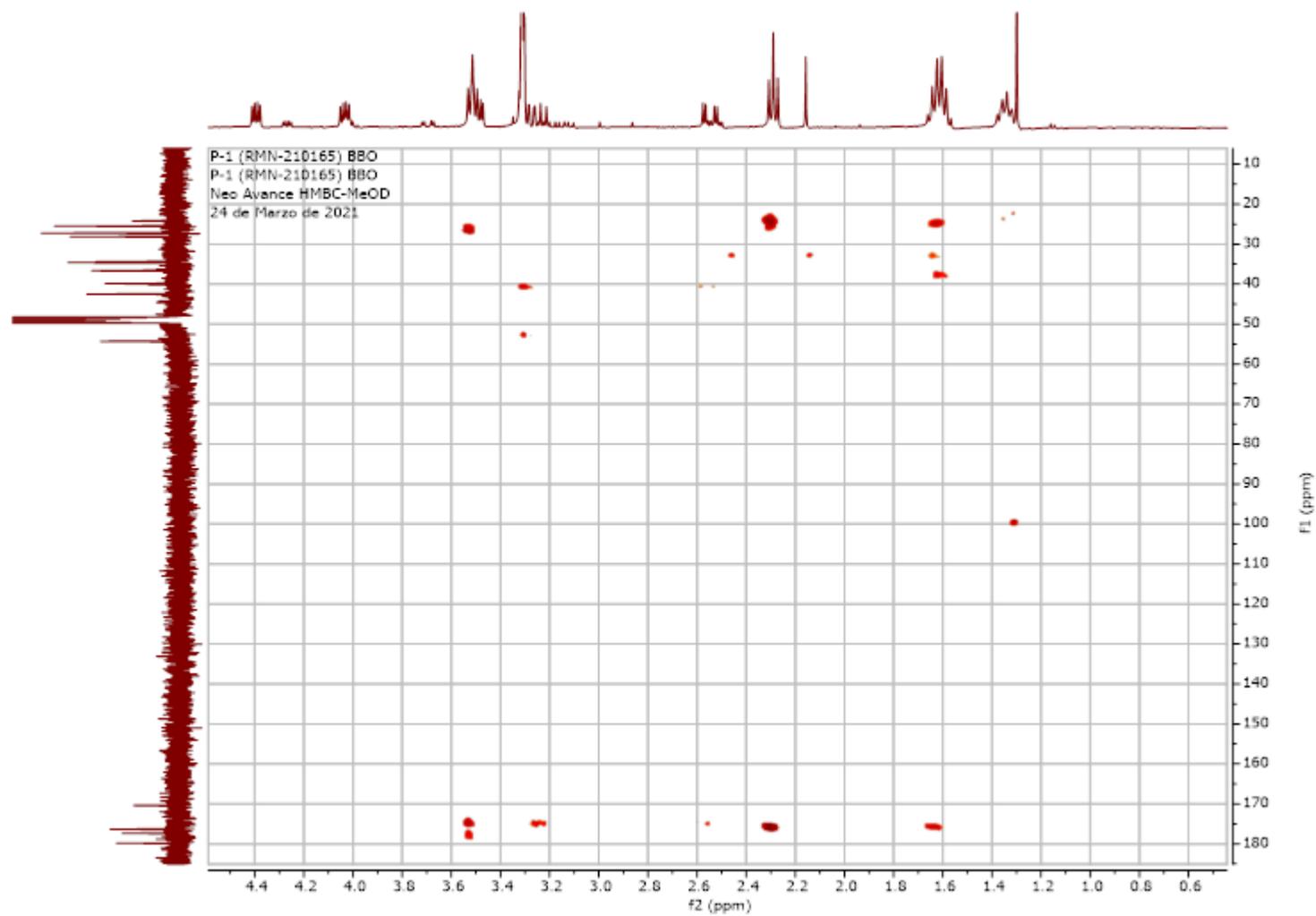


Figure S8.  $^1\text{H}$ -NMR HMBC spectrum (400MHz, MeOD, 303 K) of compound 2.

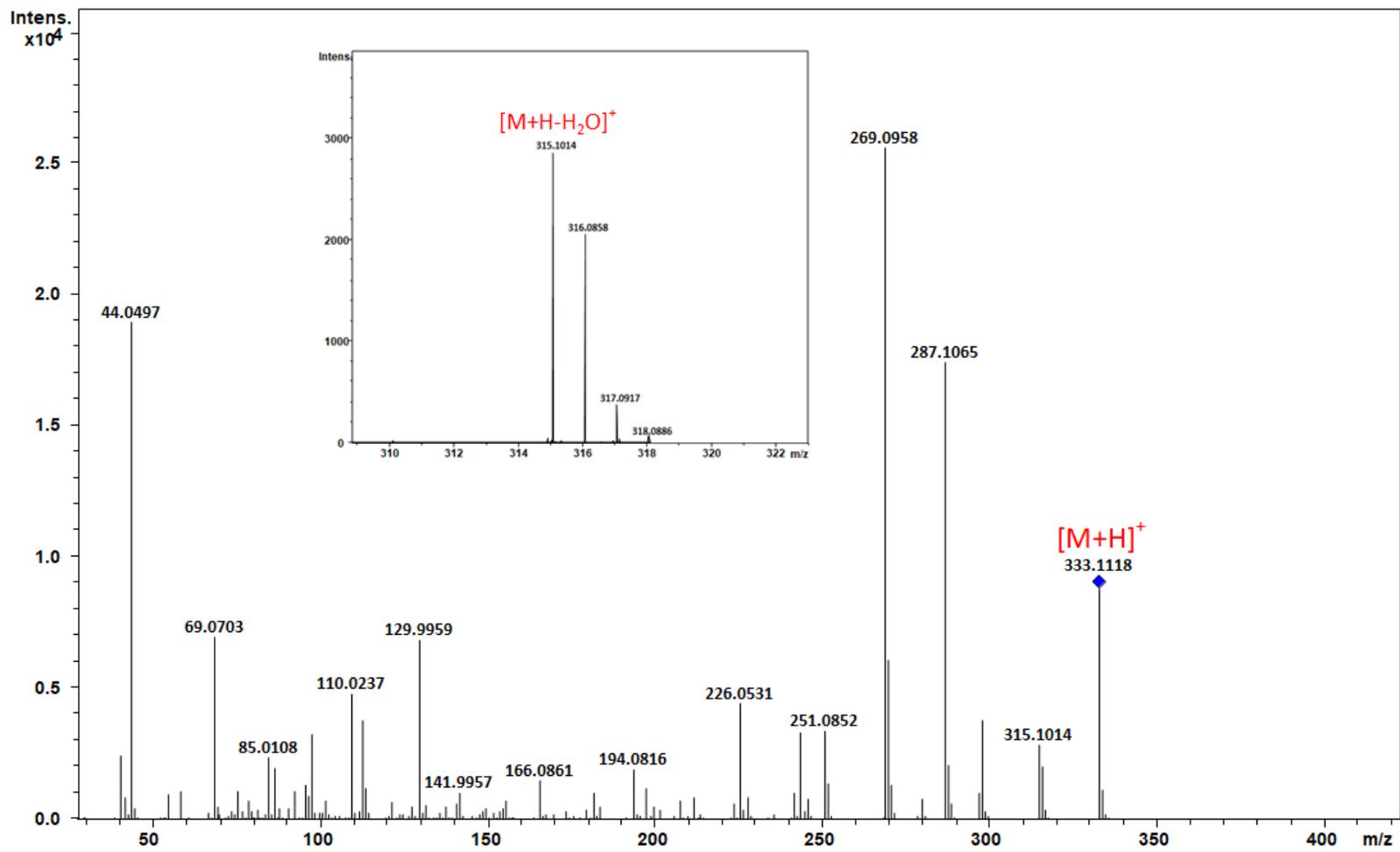


Figure S9. MS/MS for TIC of 4.6 min corresponding to compound 2.

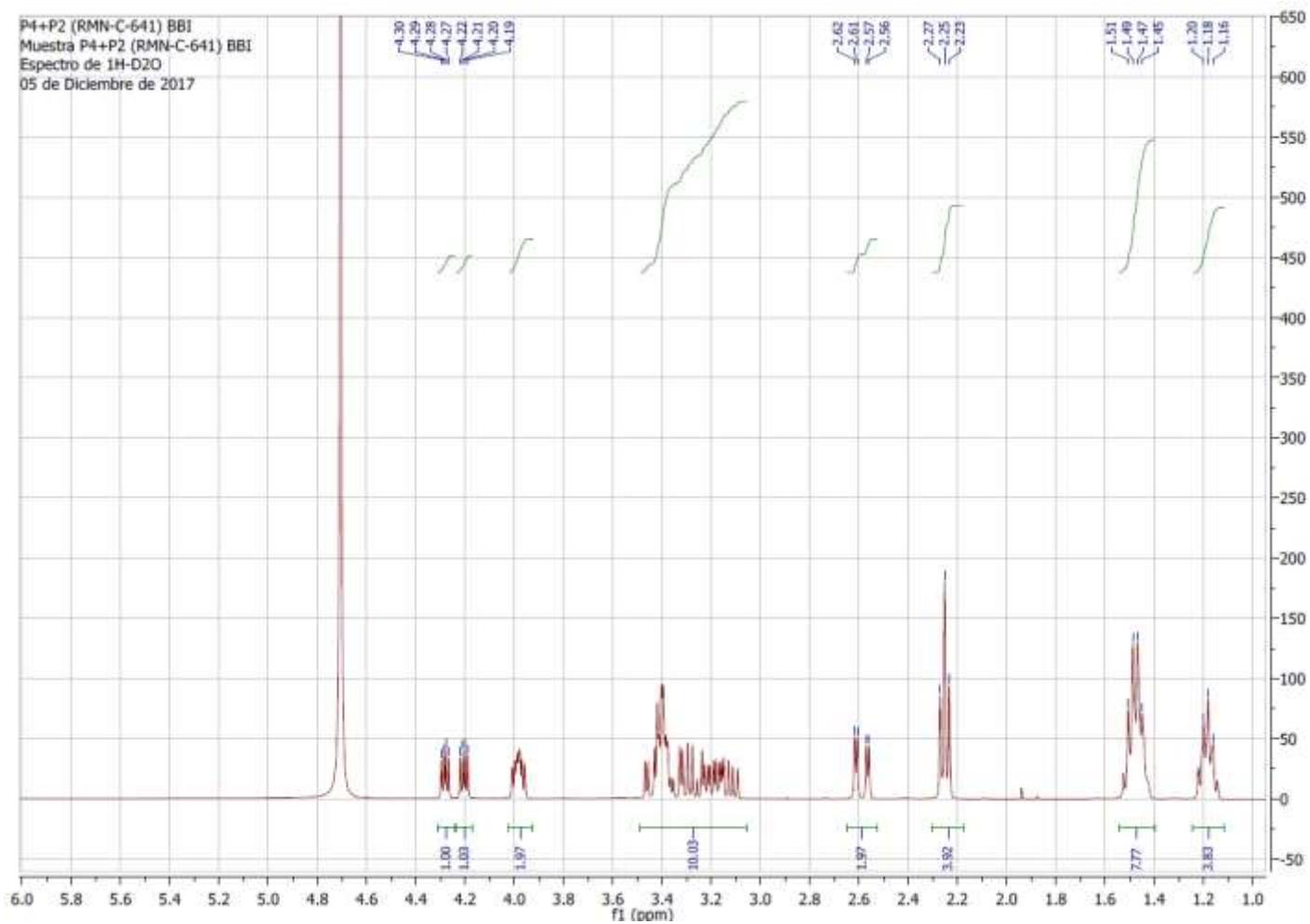


Figure S10. <sup>1</sup>H-NMR spectrum (400MHz, MeOD, 303 K) of mix products.