

Supplementary Material

In search of cocrystals and tricrystals of natural products.

A sustainable approach

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Table of Contents

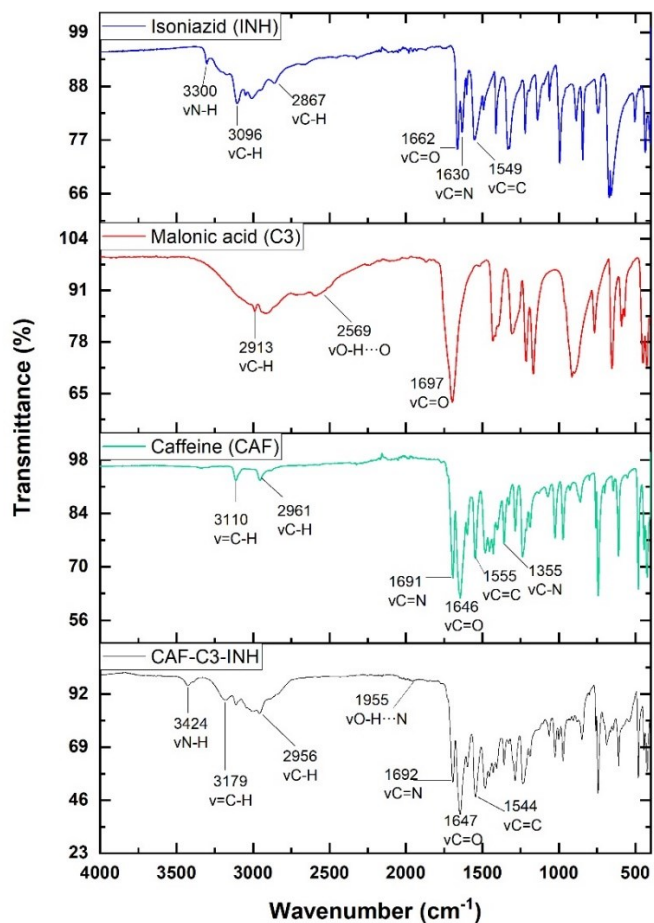
1. IR spectra of isoniazid, malonic acid, caffeine and the product CAF-C3-INH	S3
2. Thermal analysis, DSC of CAF-C3-INH	S3
3. Comparison of Powder Diffraction Patterns of reagents and synthesized compounds in the CAF-C3-INH system.	S4
4. Comparison of ¹³ C CPMAS NMR spectra of reagents and synthesized compounds in the CAF-C3-INH system.	S4
5. IR spectra of isoniazid, succinic acid, caffeine and the product CAF-C4-INH	S5
6. Thermal analysis, DSC of CAF-C4-INH	S5
7. Comparison of Powder Diffraction Patterns of reagents and synthesized compounds in the CAF-C4-INH system.	S6
8. Comparison of ¹³ C CPMAS NMR spectra of reagents and synthesized compounds in the CAF-C4-INH system.	S6
9. IR spectra of isoniazid, glutaric acid, caffeine and the product CAF-C5-INH	S7
10. Thermal analysis of CAF-C5-INH . The DSC curve in grey and the TGA curve in black.....	S7
11. Comparison of Powder Diffraction Patterns of reagents and synthesized compounds in the CAF-C5-INH system.	S8
12. Comparison of ¹³ C CPMAS NMR spectra of reagents and synthesized compounds in the CAF-C5-INH system.	S8
13. IR spectra of isoniazid, adipic acid, caffeine and the product CAF-C6-INH	S9
14. Thermal analysis of CAF-C6-INH . The DSC curve in red and the TGA curve in black.....	S9
15. Comparison of Powder Diffraction Patterns of reagents and synthesized compounds in the CAF-C6-INH system.	S10
16. Comparison of ¹³ C CPMAS NMR spectra of reagents and synthesized compounds in the CAF-C6-INH system.....	S10
17. IR spectra of isoniazid, pimelic acid, caffeine, and the product CAF-C7-INH	S11
18. Thermal analysis of CAF-C7-INH . The DSC curve in brown and the TGA curve in black.	S11
19. Comparison of Powder Diffraction Patterns of reagents and synthesized compounds in the CAF-C7-INH system.	S12
20. Comparison of ¹³ C CPMAS NMR spectra of reagents and synthesized compounds in the CAF-C7-INH system.....	S12
21. IR spectra of isoniazid, suberic acid, caffeine and the product CAF-C8-INH	S13

22. Thermal analysis of CAF-C8-INH . The DSC curve in blue and the TGA curve in black.....	S13
23. Comparison of Powder Diffraction Patterns of reagents and synthesized compounds in the CAF-C8-INH system.....	S14
24. Comparison of ¹³ C CPMAS NMR spectra of reagents and synthesized compounds in the CAF-C8-INH system.....	S14
25. IR spectra of isoniazid, azelaic acid, caffeine and the product CAF-C9-INH	S15
26. Thermal analysis, DSC of CAF-C9-INH	S15
27. Comparison of Powder Diffraction Patterns of reagents and synthesized compounds in the CAF-C9-INH system.....	S16
28. Comparison of ¹³ C CPMAS NMR spectra of reagents and synthesized compounds in the CAF-C9-INH system.....	S16
29. IR spectra of isoniazid, sebacic acid, caffeine and the product CAF-C10-INH	S17
30. Thermal analysis, DSC of CAF-C10-INH	S17
31. Comparison of Powder Diffraction Patterns of reagents and synthesized compounds in the CAF-C10-INH system.....	S18
32. Comparison of ¹³ C CPMAS NMR spectra of reagents and synthesized compounds in the CAF-C10-INH system.....	S18

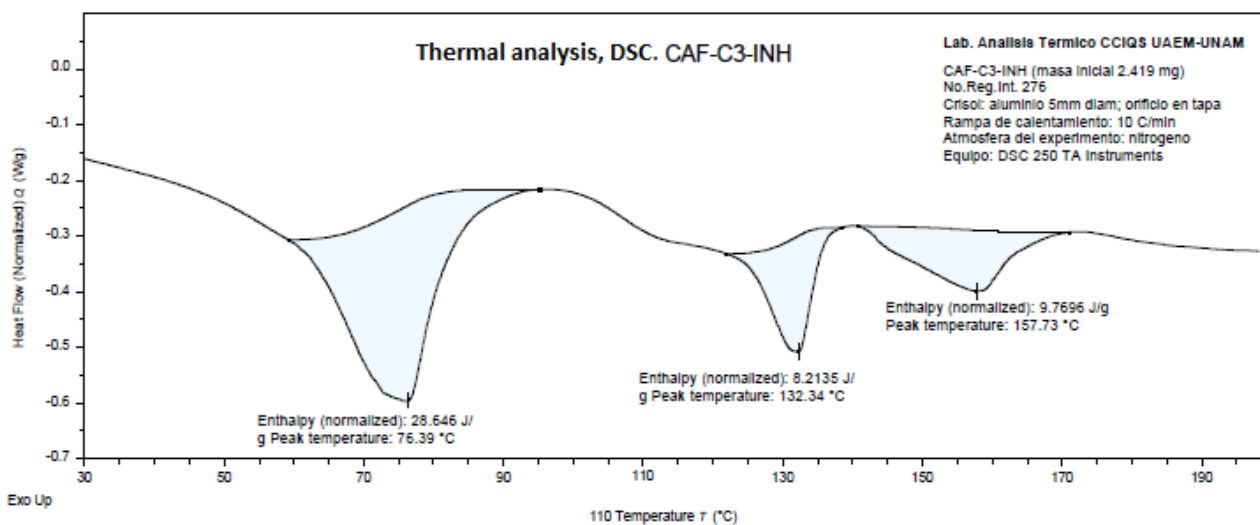
This supplementary material contains the FT-IR spectra, thermal analysis (DSC/TGA), powder X-ray diffraction patterns, and solid-state ¹³C CP/MAS NMR spectra used for the characterization of the CAF–Cn–INH ternary systems.

COMPOUND 1. CAF-C3-INH (CAFFEINE + MALONIC ACID + ISONIAZID)

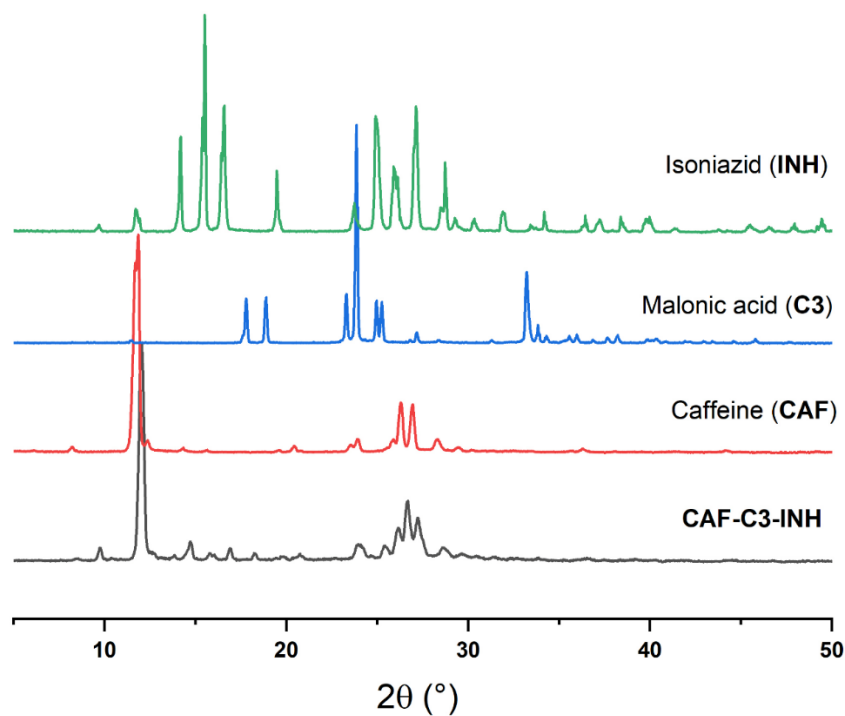
1. IR spectra of isoniazid, malonic acid, caffeine, and the product CAF-C3-INH.



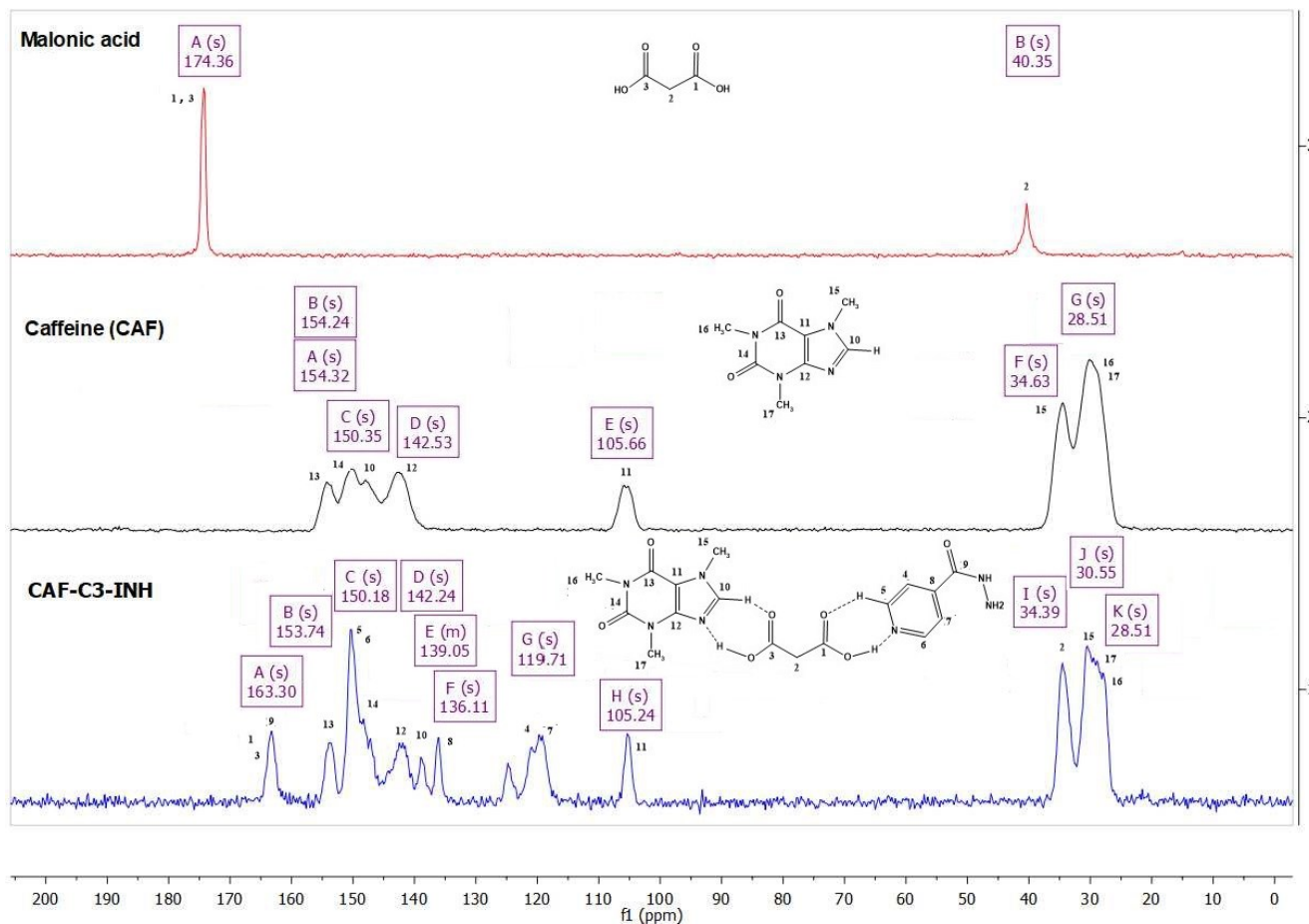
2. Thermal analysis, DSC of **CAF-C3-INH**.



3. Comparison of Powder Diffraction Patterns of reagents and synthesized compounds in the **CAF-C3-INH** system.

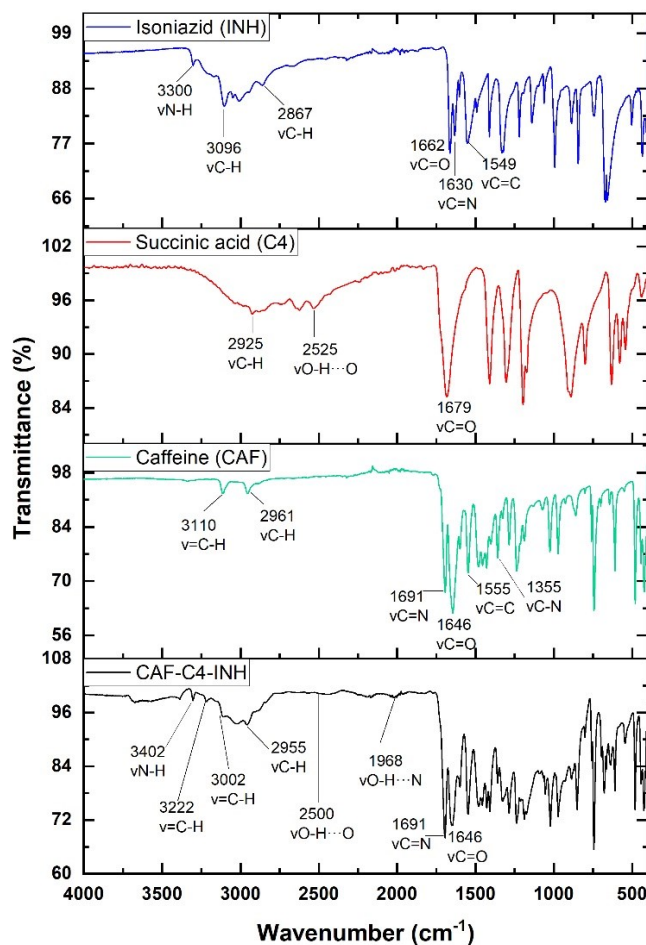


4. Comparison of ^{13}C CPMAS NMR spectra of reagents and synthesized compounds in the **CAF-C3-INH** system.



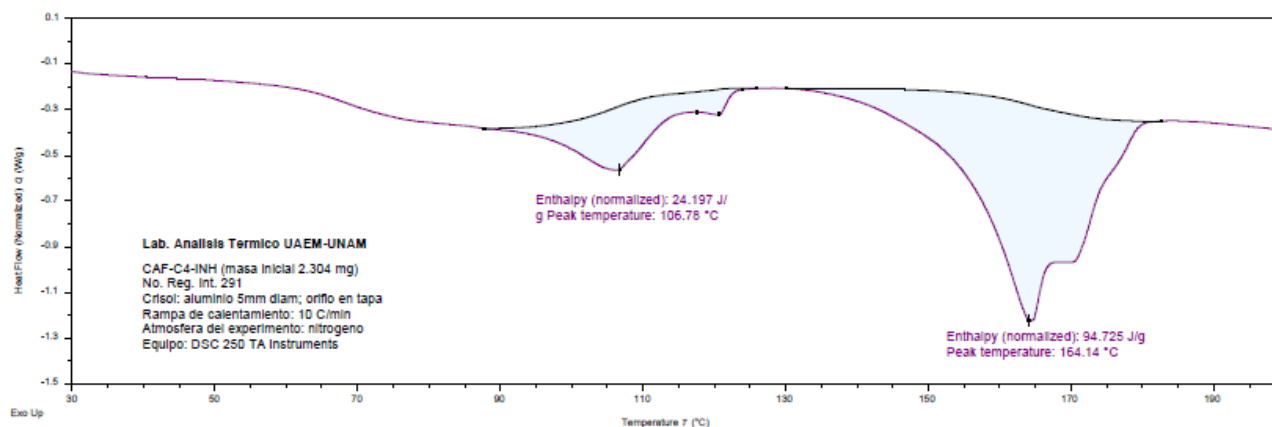
COMPOUND 2. **CAF-C4-INH** (CAFFEINE + SUCCINIC ACID + ISONIAZID)

5. IR spectra of isoniazid, succinic acid, caffeine, and the product **CAF-C4-INH**.



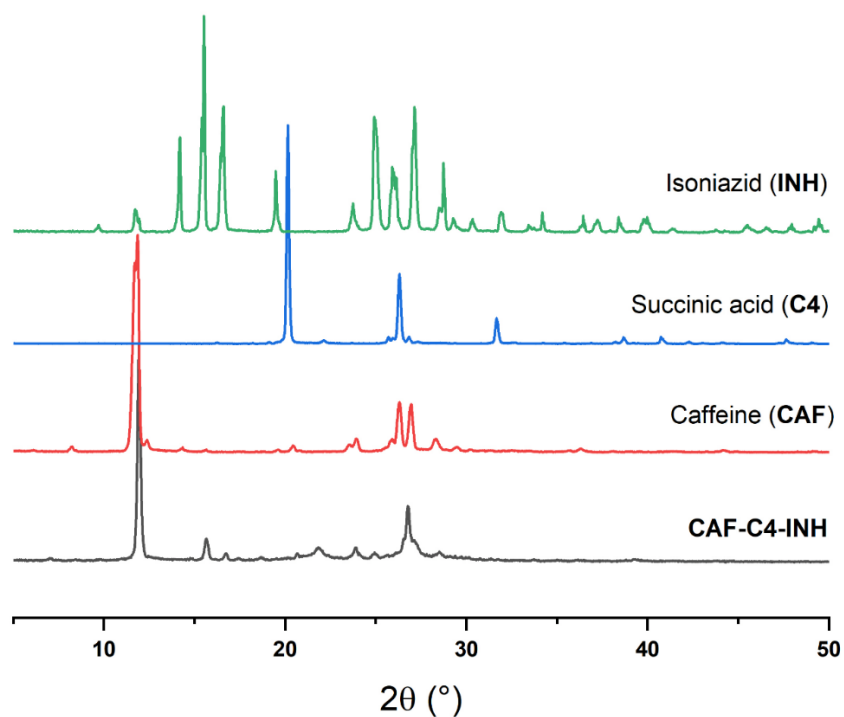
6. Thermal analysis, DSC of **CAF-C4-INH**.

Thermal analysis, DSC. CAF-C4-INH

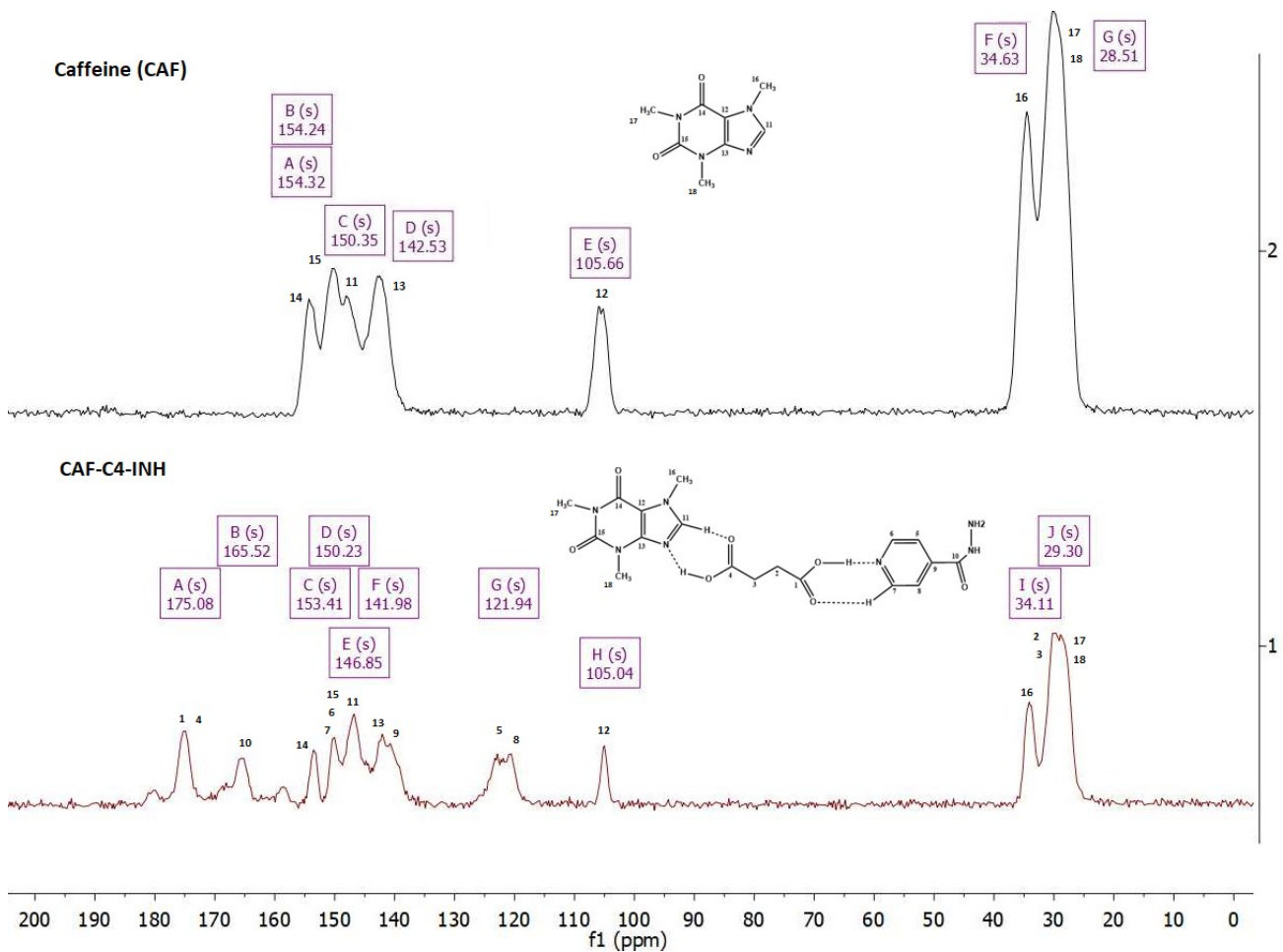


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7. Comparison of Powder Diffraction Patterns of reagents and synthesized compounds in the **CAF-C4-INH** system.

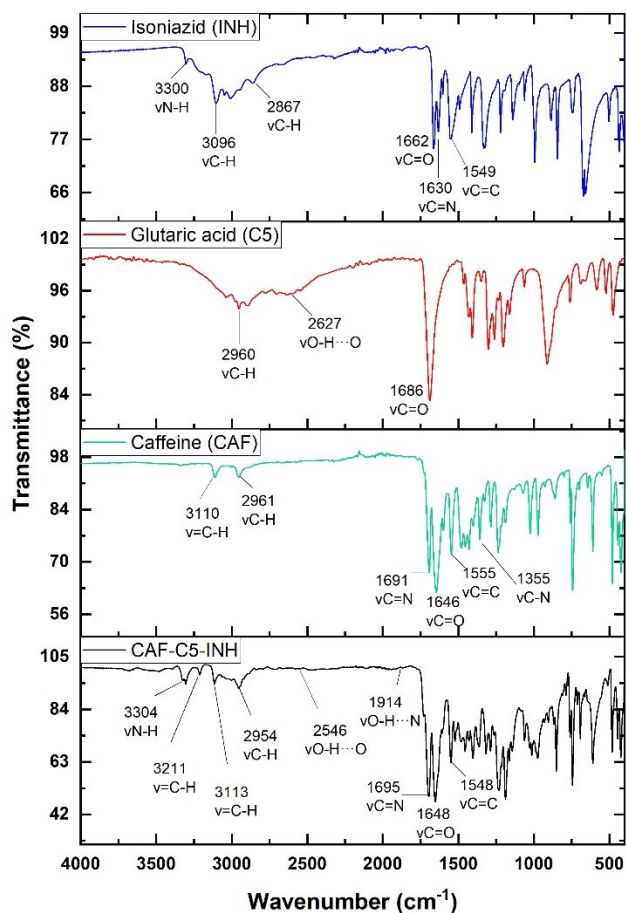


8. Comparison of ^{13}C CPMAS NMR spectra of reagents and synthesized compounds in the **CAF-C4-INH** system.

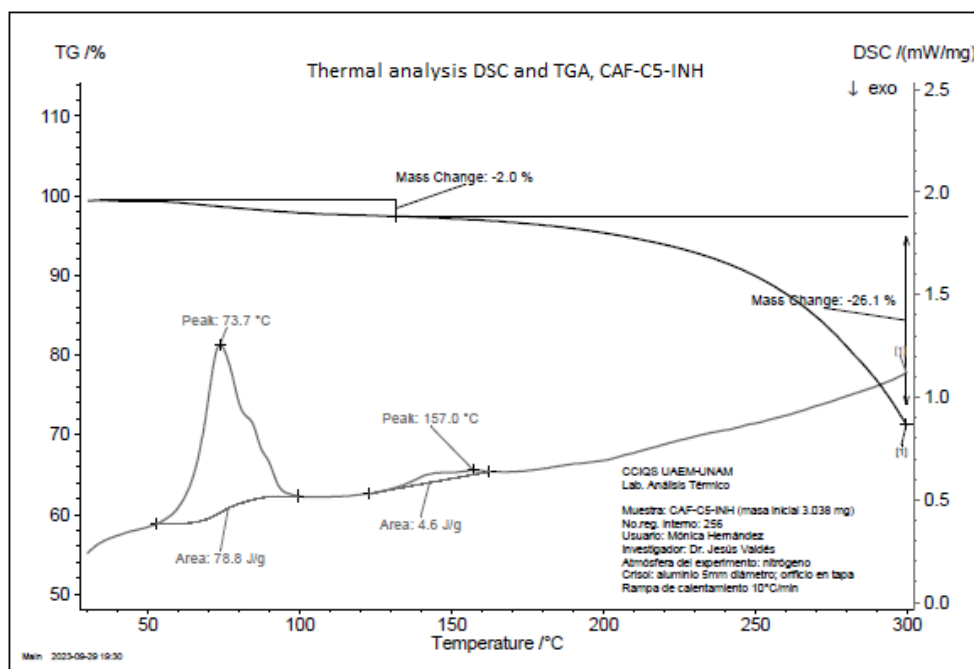


COMPOUND 3. CAF-C5-INH (CAFFEINE + GLUTARIC ACID + ISONIAZID)

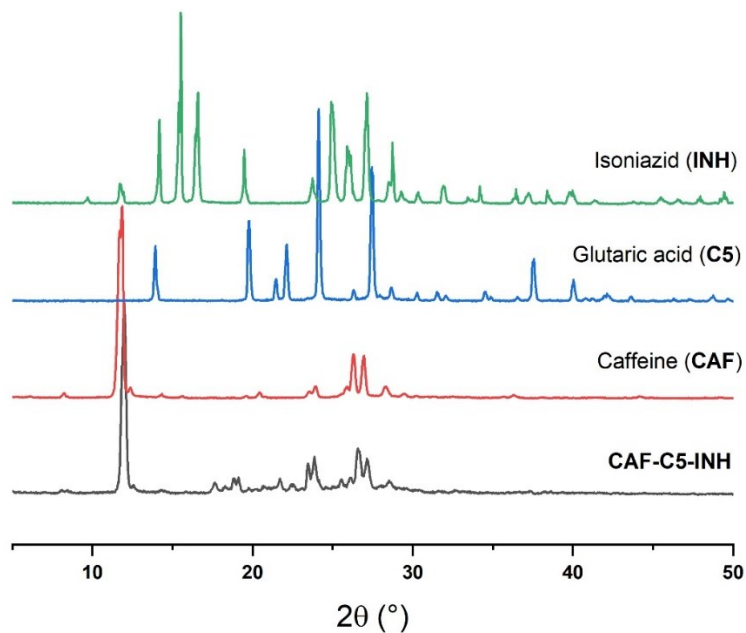
9. IR spectra of isoniazid, glutaric acid, caffeine and the product **CAF-C5-INH**.



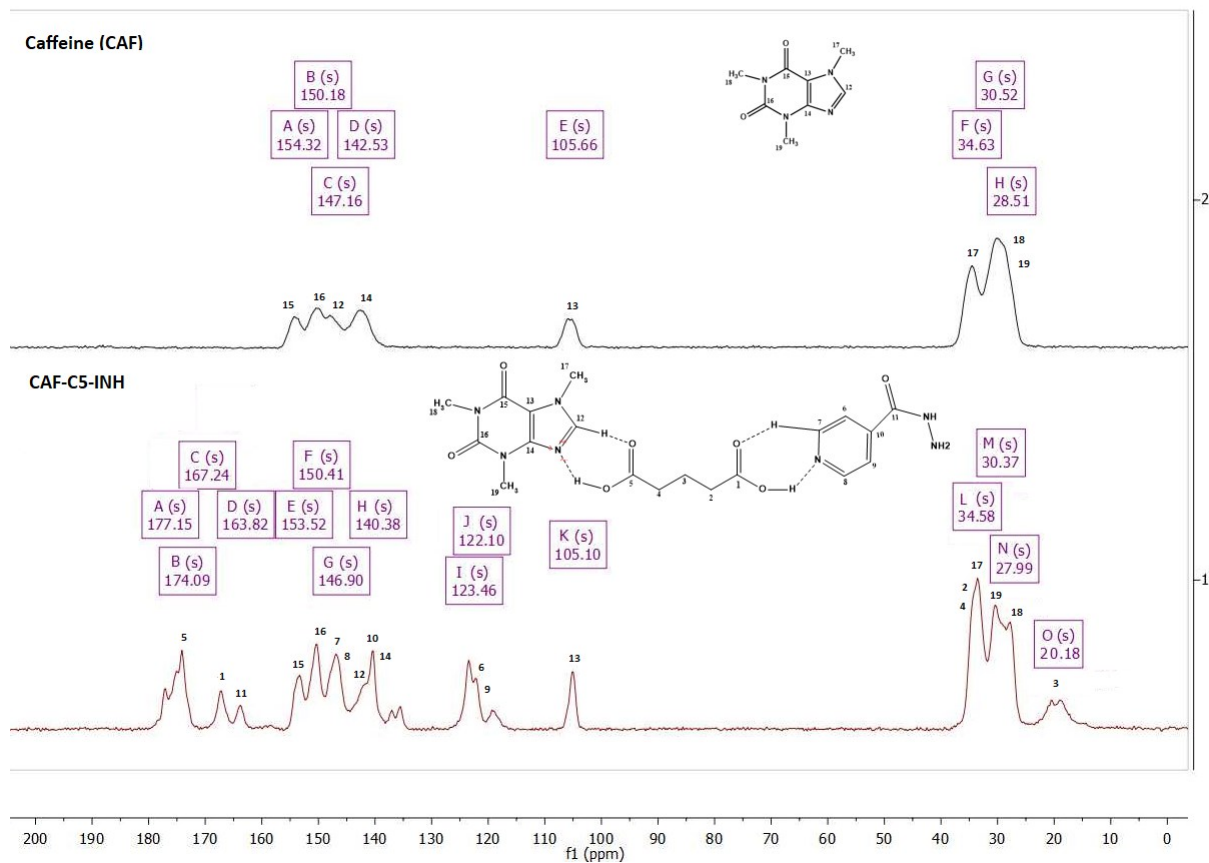
10. Thermal analysis of **CAF-C5-INH**. The DSC curve in grey and the TGA curve in black.



11. Comparison of Powder Diffraction Patterns of reagents and synthesized compounds in the **CAF-C5-INH** system.

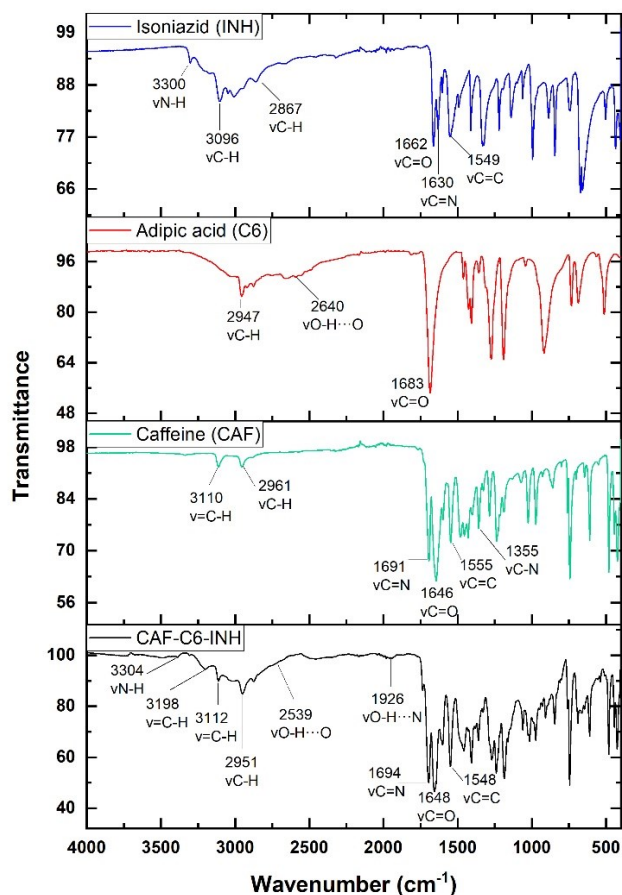


12. Comparison of ¹³C CPMAS NMR spectra of reagents and synthesized compounds in the **CAF-C5-INH** system.

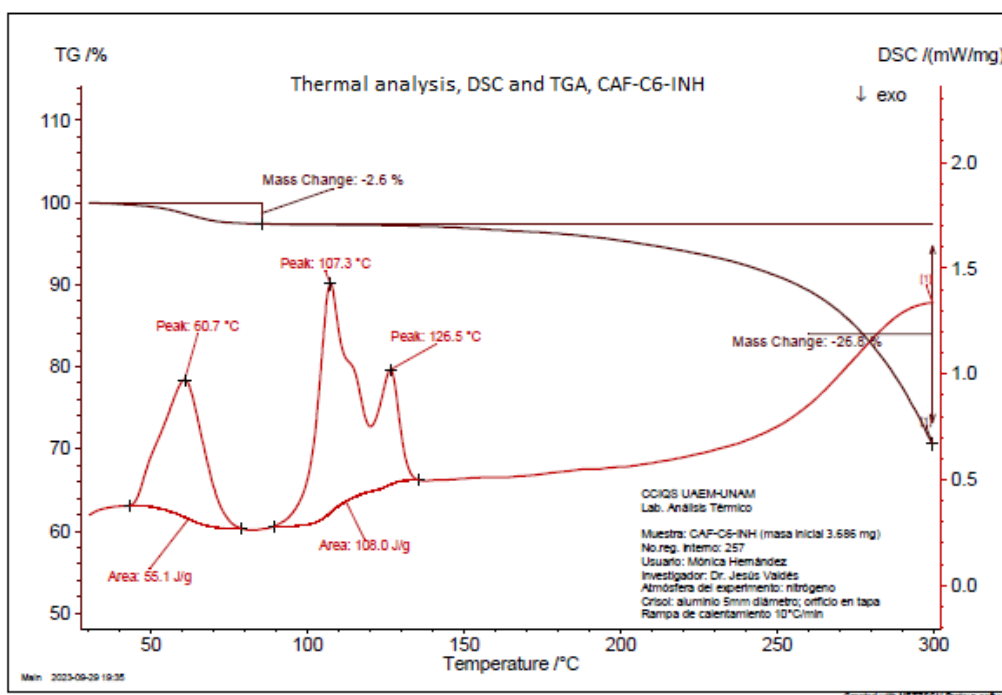


COMPOUND 4. CAF-C6-INH (CAFFEINE + ADIPIC ACID + ISONIAZID)

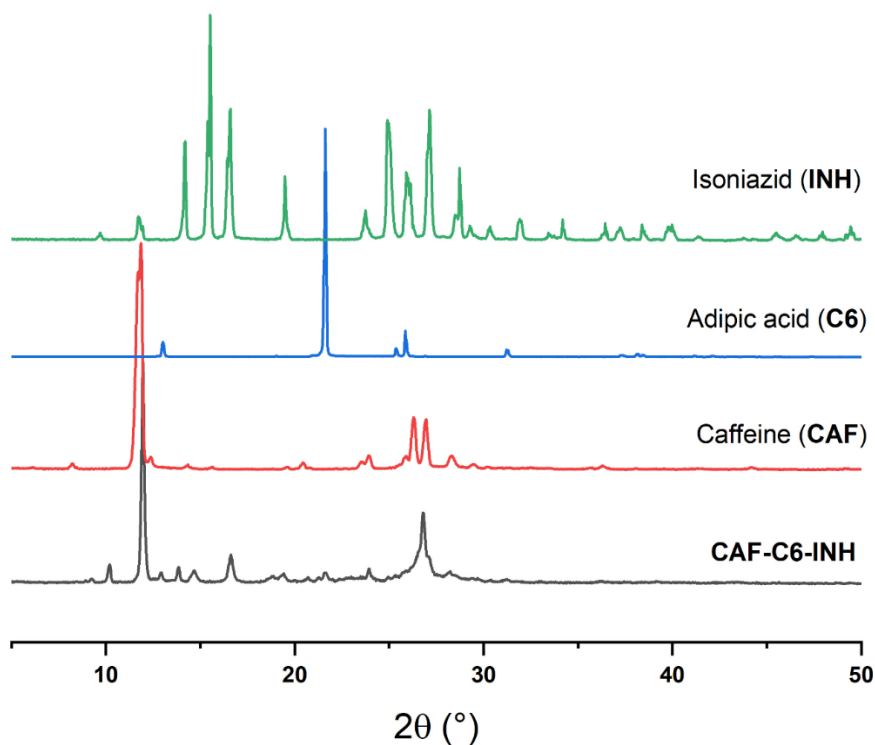
13. IR spectra of isoniazid, adipic acid, caffeine and the product **CAF-C6-INH**.



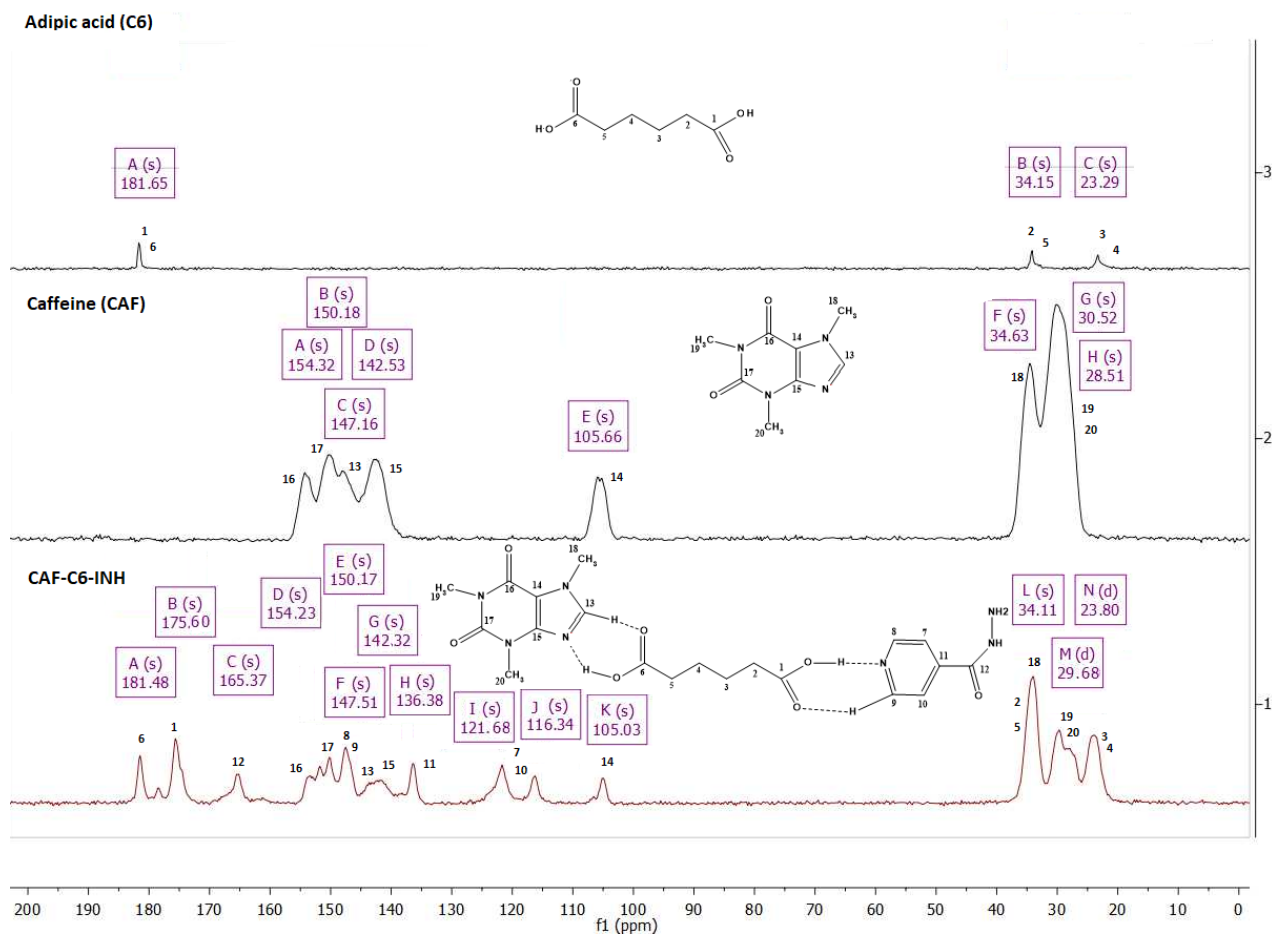
14. Thermal analysis of **CAF-C6-INH**. The DSC curve in red and the TGA curve in black.



15. Comparison of Powder Diffraction Patterns of reagents and synthesized compounds in the **CAF-C6-INH** system.

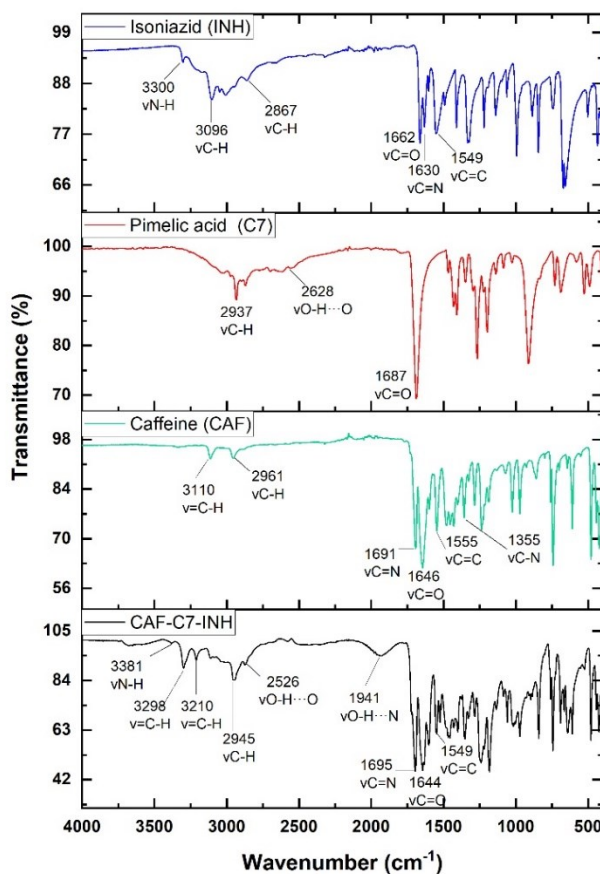


16. Comparison of ^{13}C CPMAS NMR spectra of reagents and synthesized compounds in the **CAF-C6-INH** system

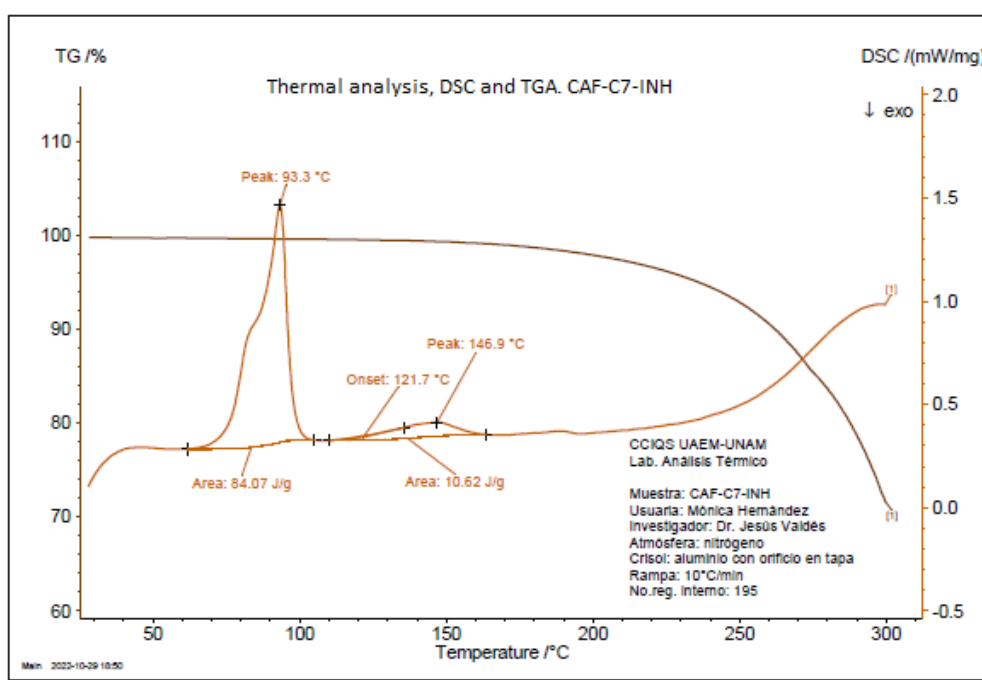


COMPOUND 5. CAF-C7-INH (CAFFEINE + PIMELIC ACID + ISONIAZID)

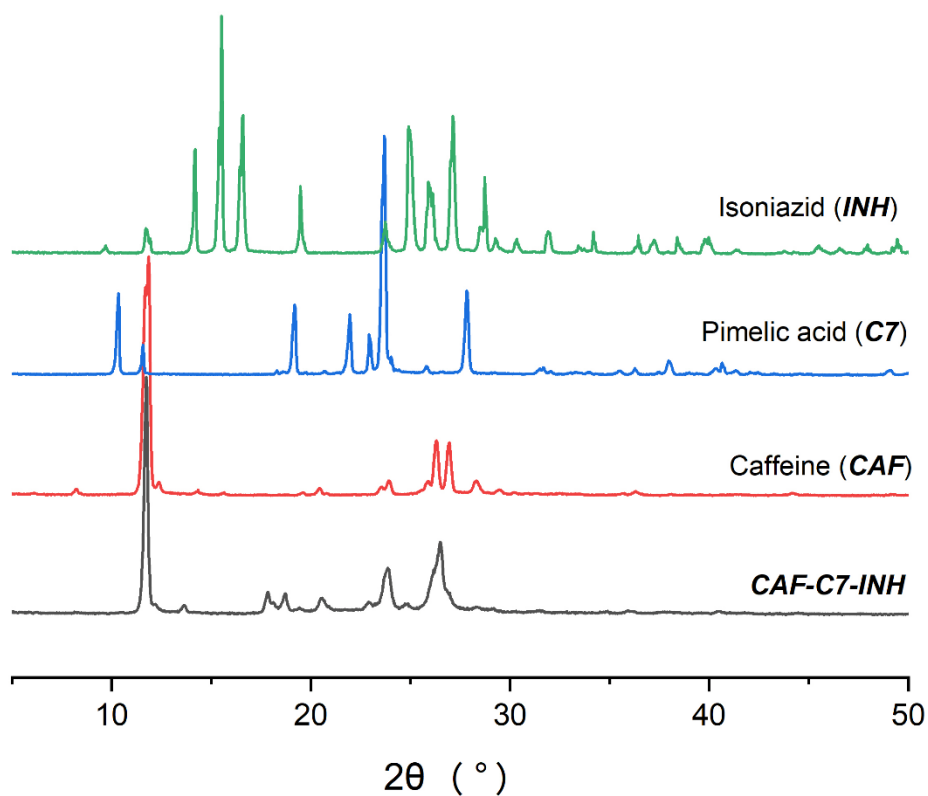
17. IR spectra of isoniazid, pimelic acid, caffeine and the product **CAF-C7-INH**.



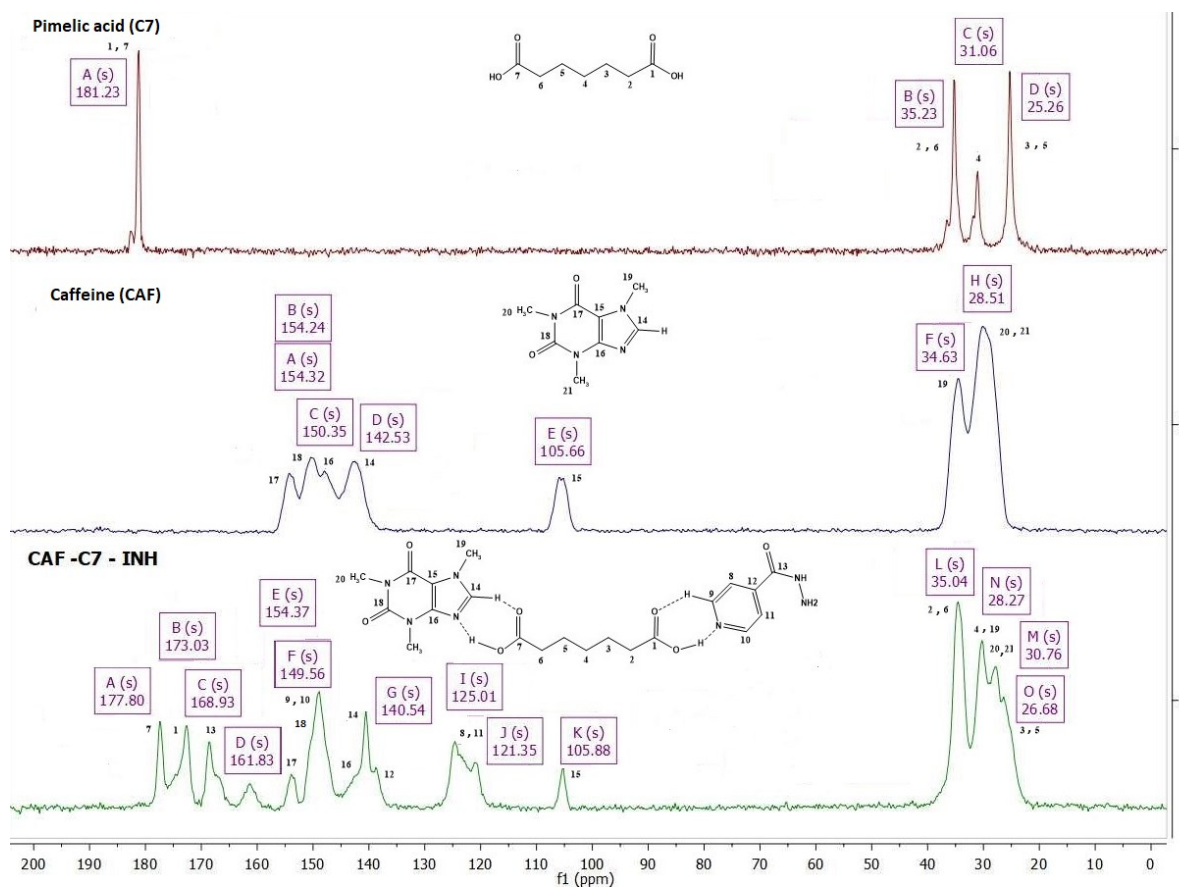
18. Thermal analysis of **CAF-C7-INH**. The DSC curve in brown and the TGA curve in black.



19. Comparison of Powder Diffraction Patterns of reagents and synthesized compounds in the **CAF-C7-INH** system.

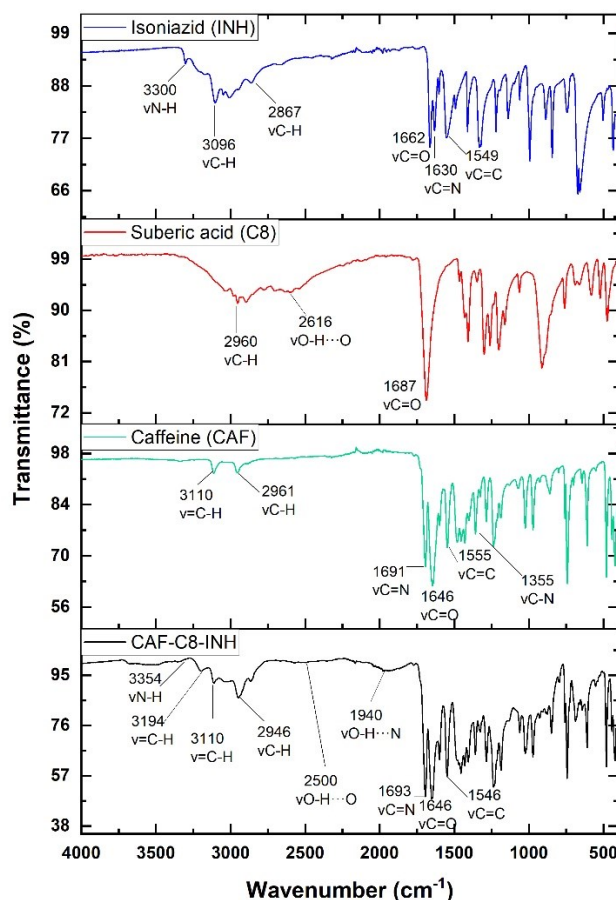


20. Comparison of ^{13}C CP/MAS NMR spectra of reagents and synthesized compounds in the **CAF-C7-INH** system

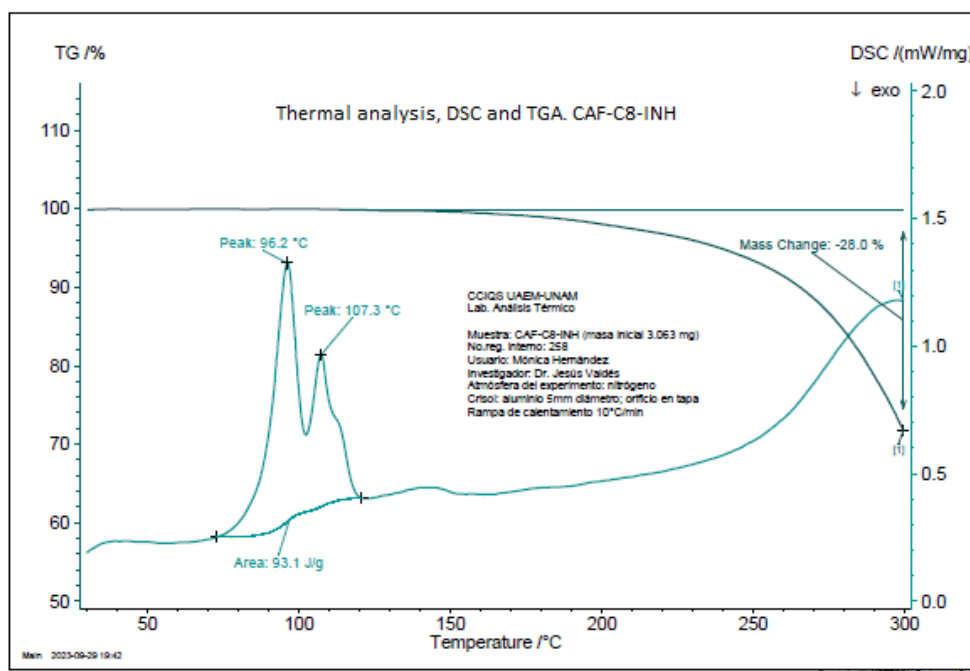


COMPOUND 6. CAF-C8-INH (CAFFEINE + SUBERIC ACID + ISONIAZID)

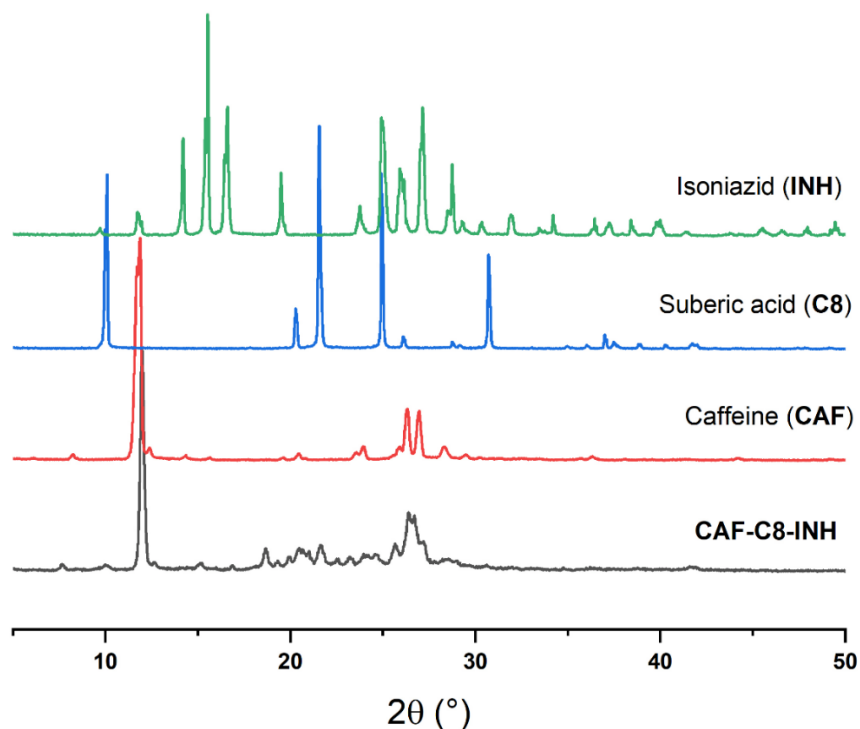
21. IR spectra of isoniazid, suberic acid, caffeine, and the product **CAF-C8-INH**.



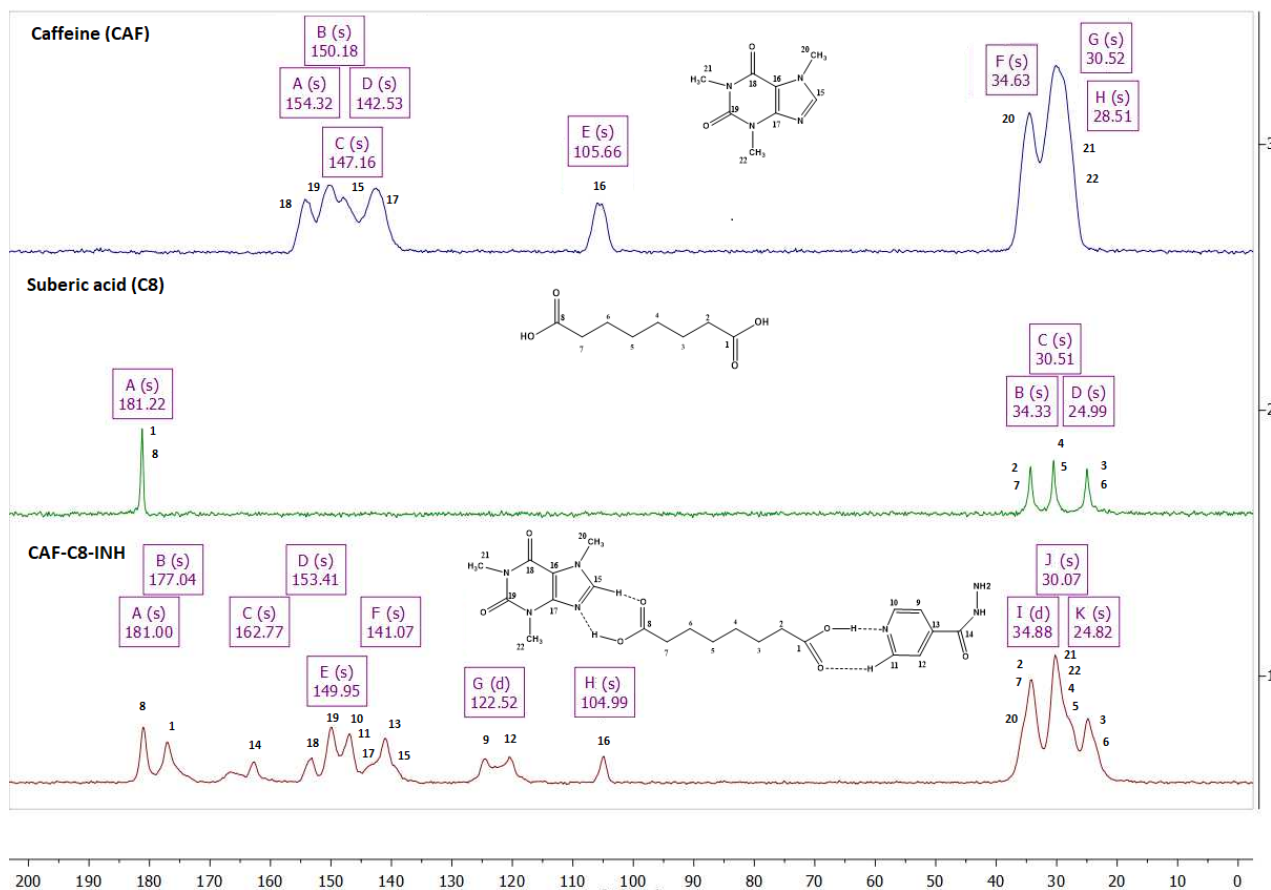
22. Thermal analysis of **CAF-C8-INH**. The DSC curve is in blue, and the TGA curve is in black.



23. Comparison of Powder Diffraction Patterns of reagents and synthesized compounds in the **CAF-C8-INH** system.

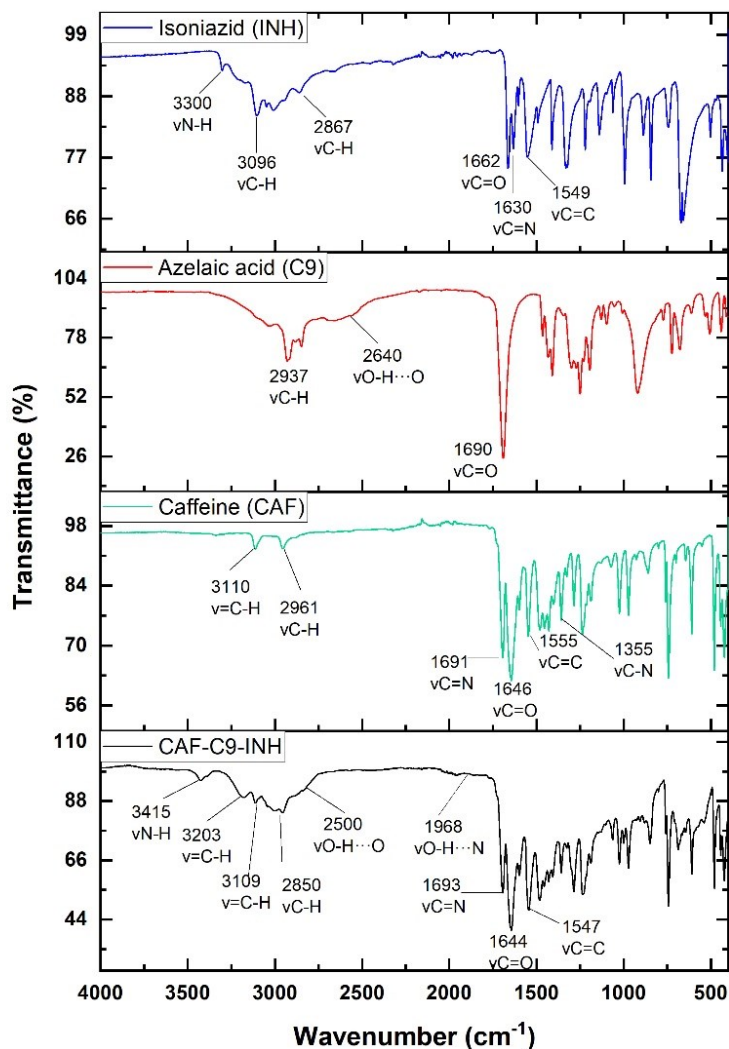


24. Comparison of ^{13}C CP/MAS NMR spectra of reagents and synthesized compounds in the **CAF-C8-INH** system

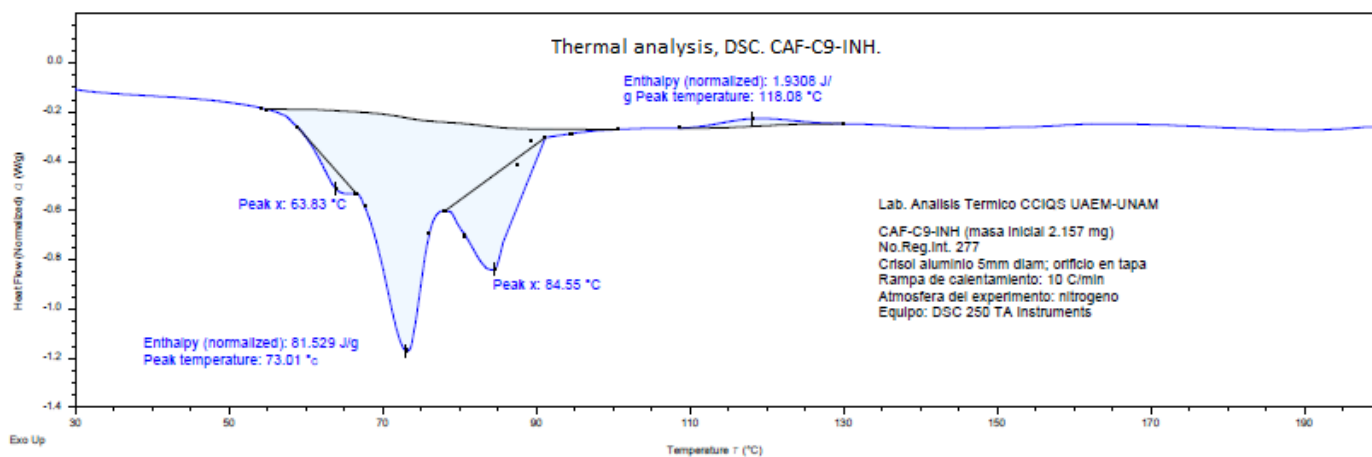


COMPOUND 7. CAF-C9-INH (CAFFEINE + AZELAIC ACID + ISONIAZID)

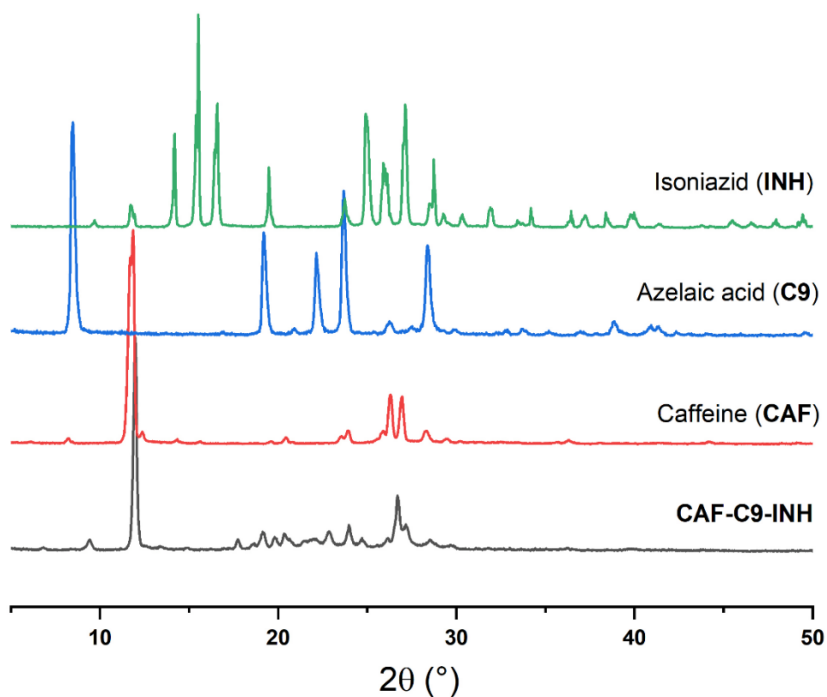
25. IR spectra of isoniazid, azelaic acid, caffeine and the product **CAF-C9-INH**.



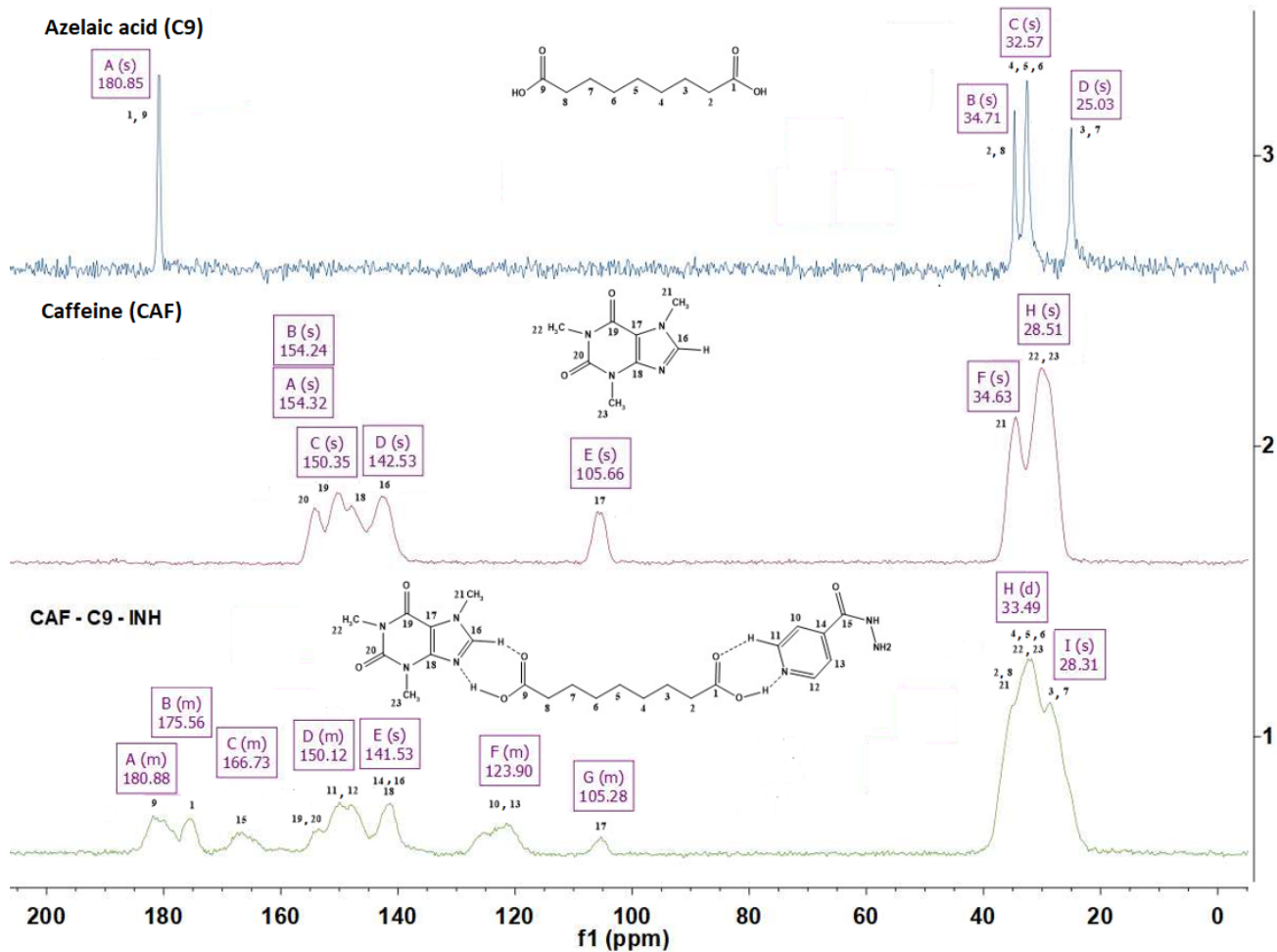
26. Thermal analysis, DSC of **CAF-C9-INH**.



27. Comparison of Powder Diffraction Patterns of reagents and synthesized compounds in the **CAF-C9-INH** system.

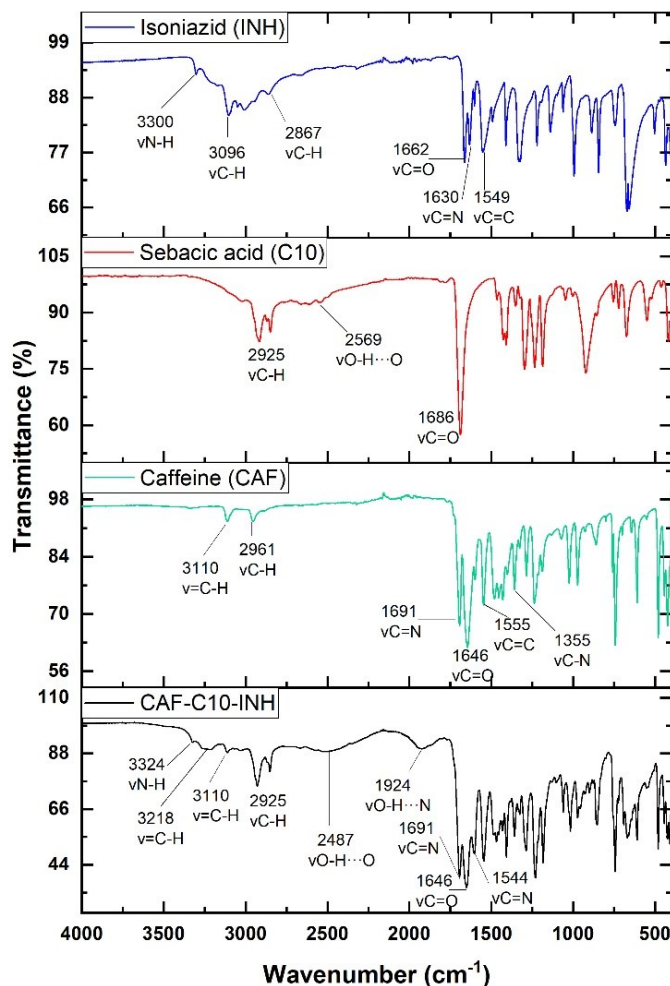


28. Comparison of ^{13}C CPMAS NMR spectra of reagents and synthesized compounds in the **CAF-C9-INH** system.

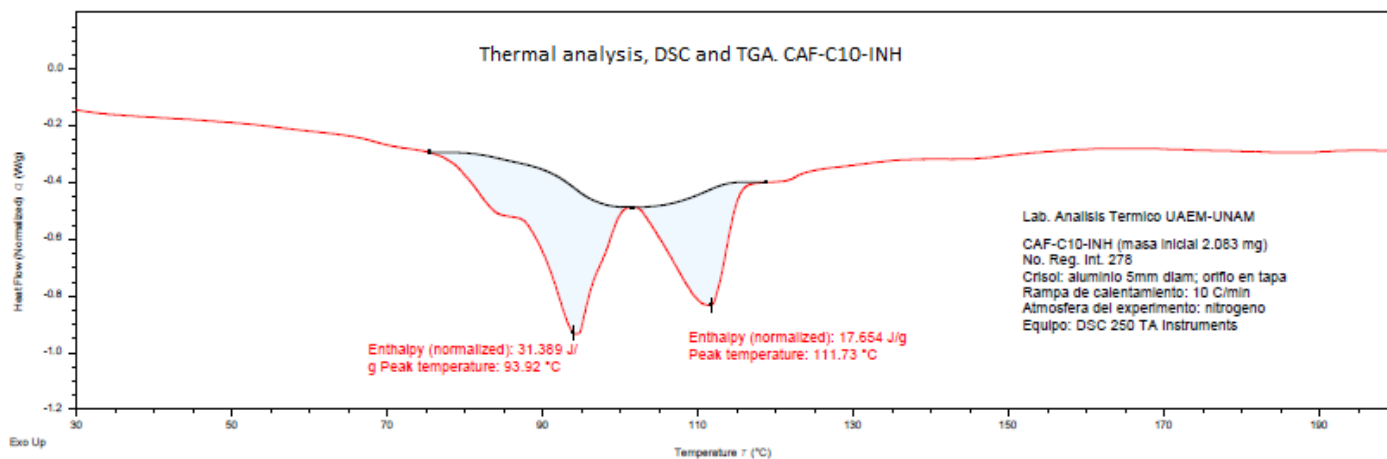


COMPOUND 8. CAF-C10-INH (CAFFEINE + SEBACIC ACID + ISONIAZID)

29. IR spectra of isoniazid, sebacic acid, caffeine, and the product **CAF-C10-INH**.

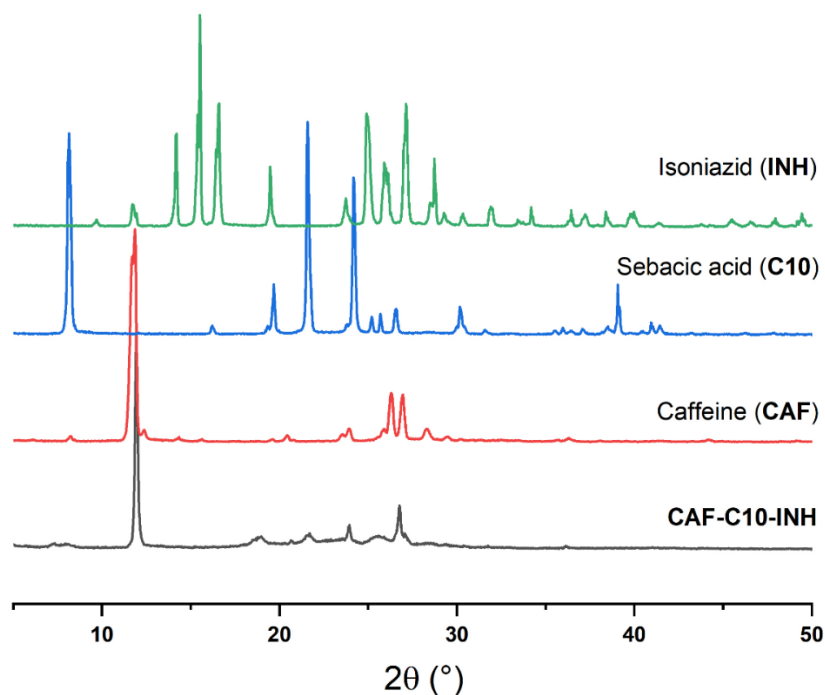


30. Thermal analysis, DSC of **CAF-C10-INH**.



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31. Comparison of Powder Diffraction Patterns of reagents and synthesized compounds in the **CAF-C10-INH** system.



32. Comparison of ^{13}C CPMAS NMR spectra of reagents and synthesized compounds in the **CAF-C10-INH** system.

