

## SUPPORTING INFORMATION

### Fluconazole Cocrystals with Dicarboxylic Acids

**Authors:** Jože Kastelic, Žiga Hodnik, Primož Šket, Janez Plavec, Nina Lah, Ivan Leban, Matjaž Pajk,

Odon Planinšek, Danijel Kikelj

#### Figure

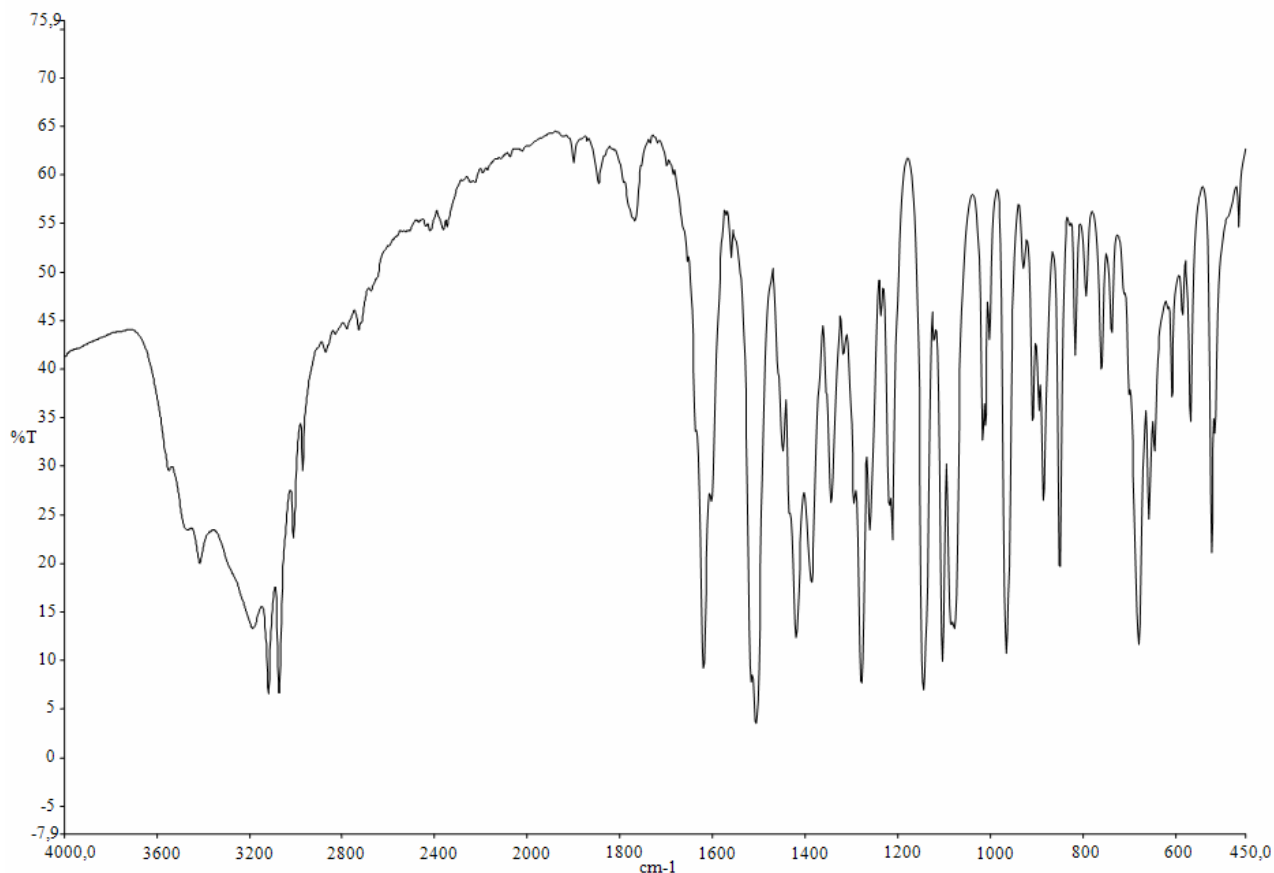
**Figure S1 - S4.** IR spectra of fluconazole, cocrystal formers and cocrystals

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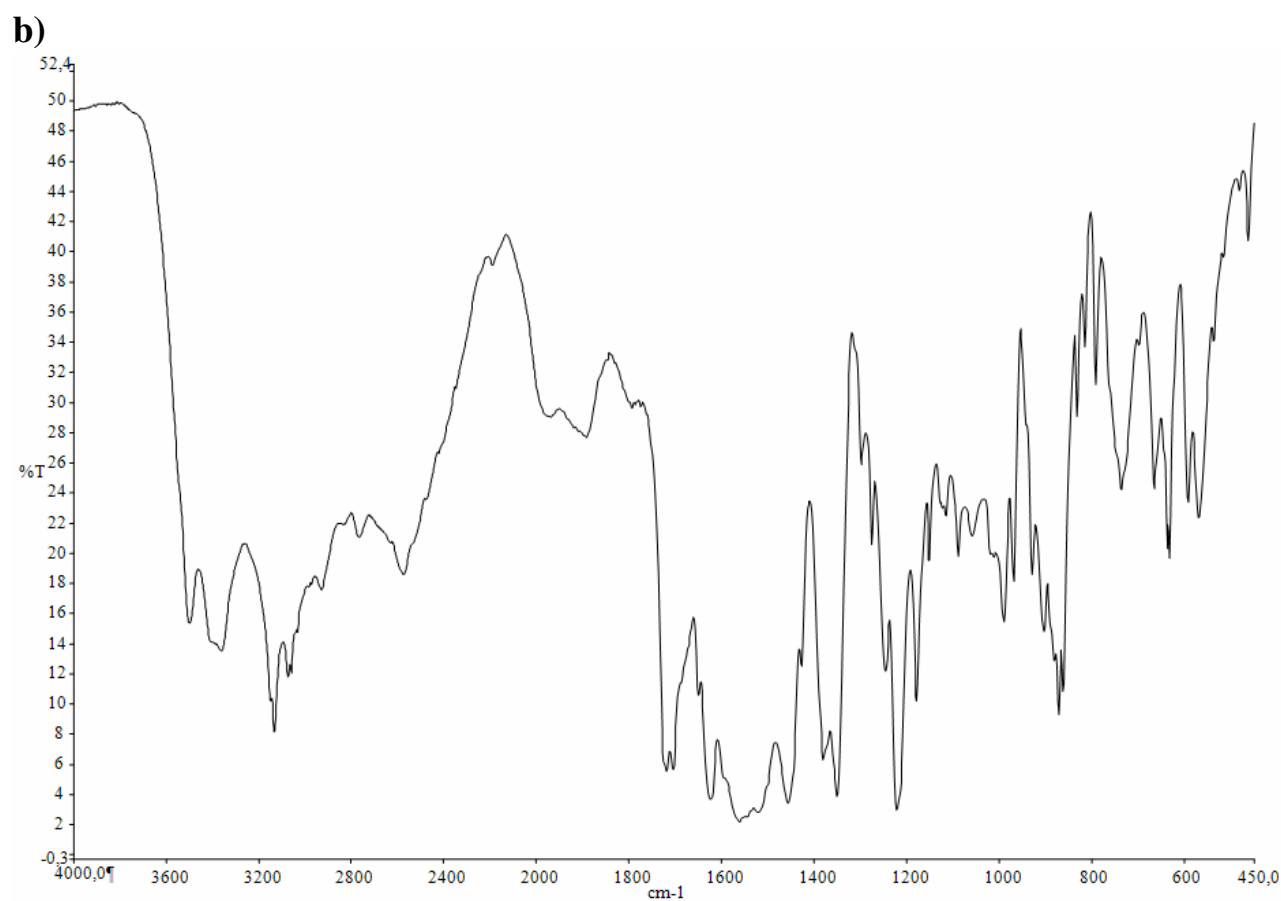
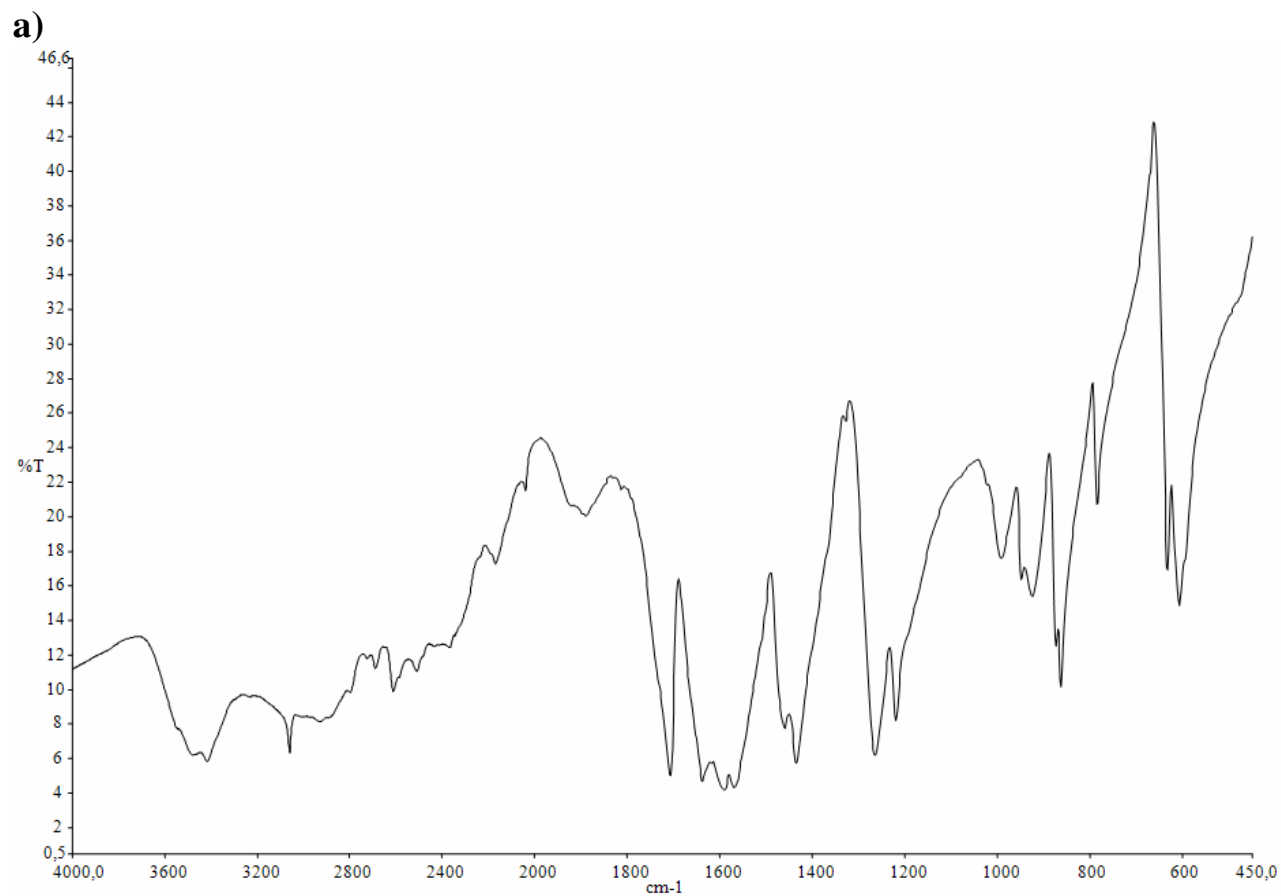
1 - 4

**Figure S5 – S8.** Solution  $^1\text{H}$  NMR spectra of fluconazole, cocrystal formers and cocrystals

5 - 8

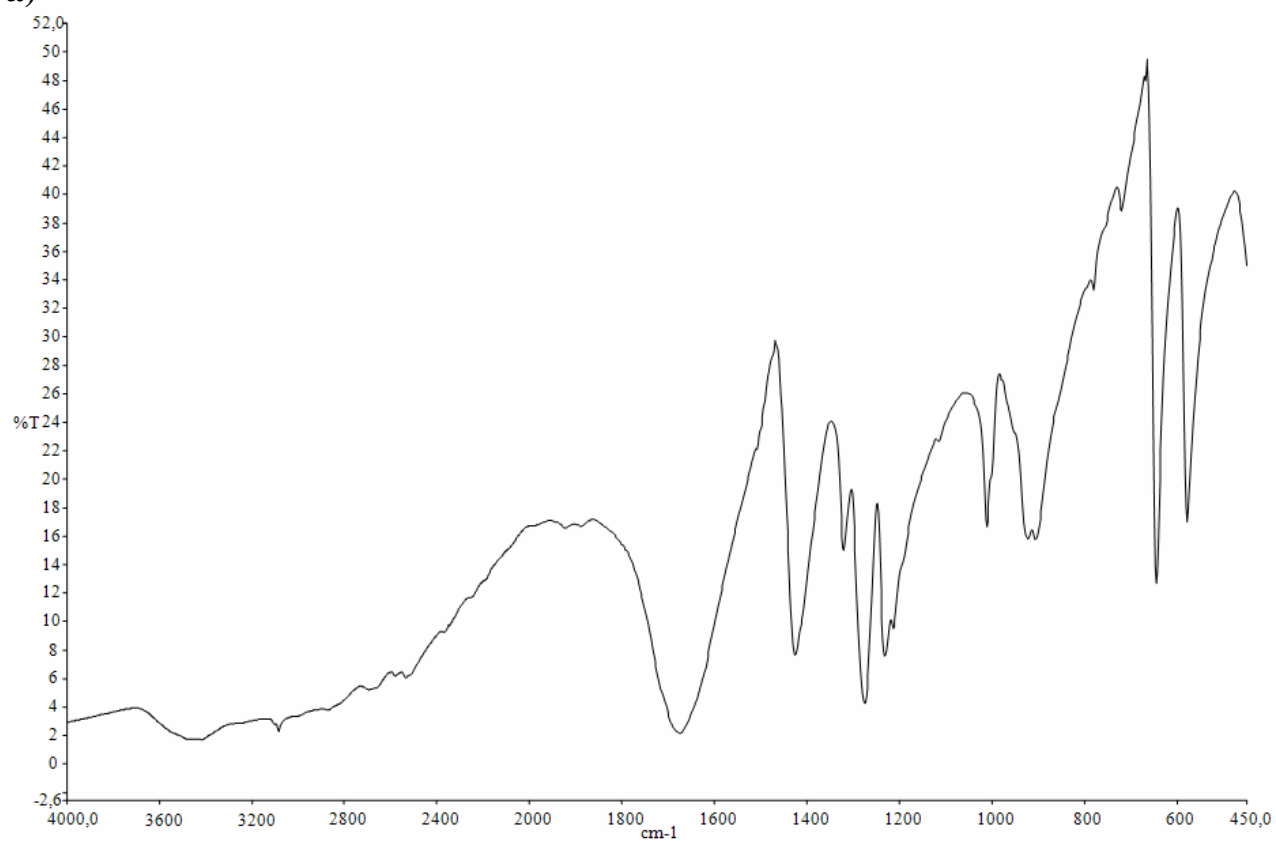


**Figure S1.** IR spectra of fluconazole form III.

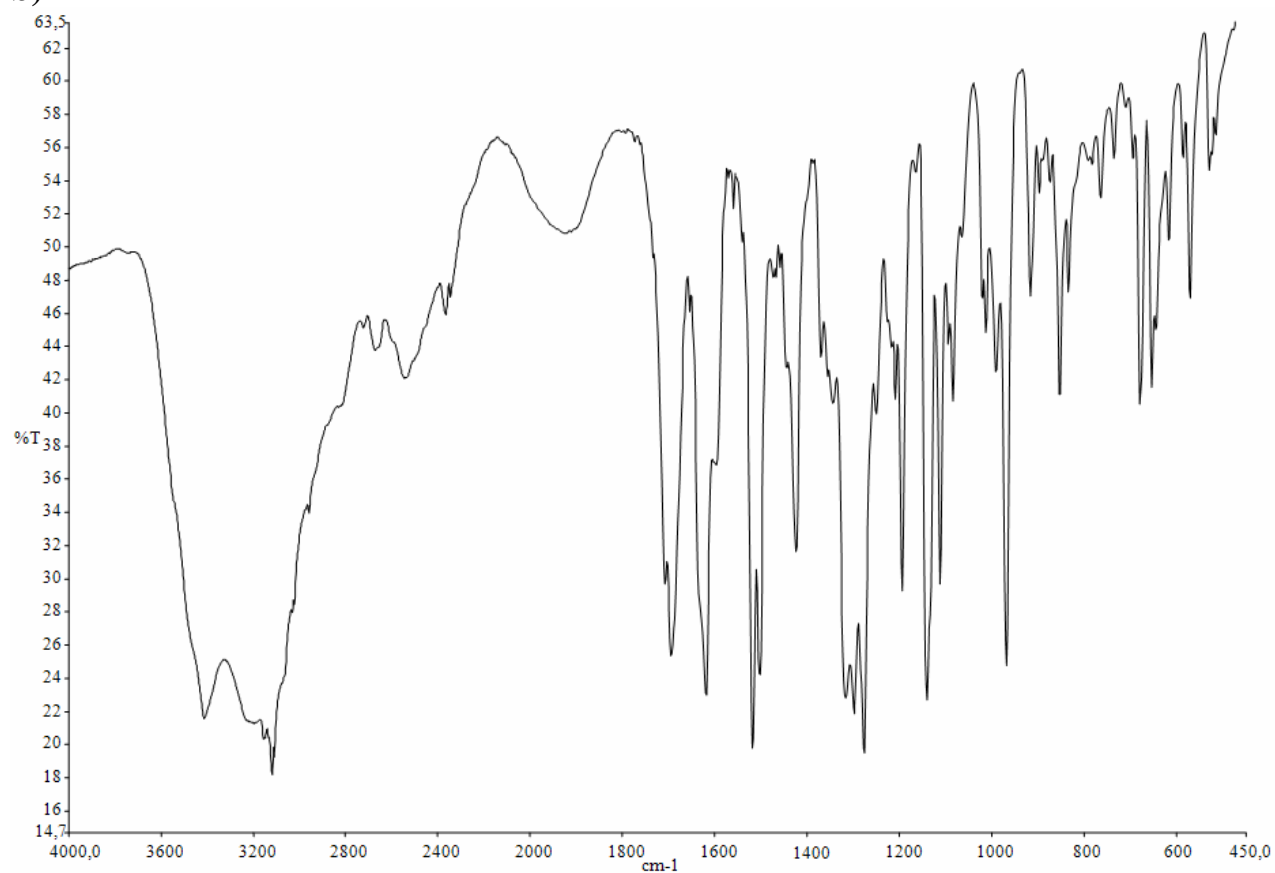


**Figure S2.** IR spectra of a) maleic acid and b) cocrystal 1.

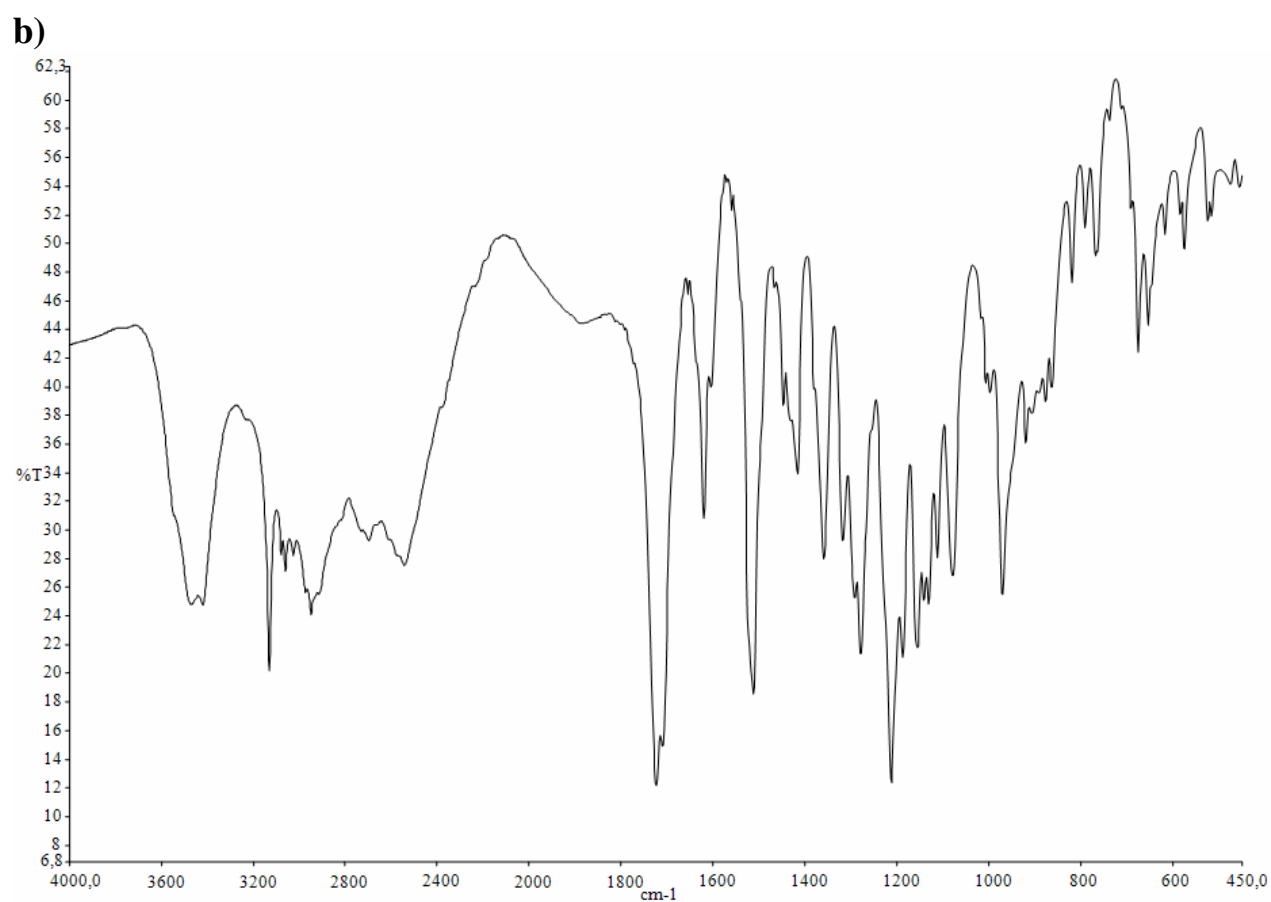
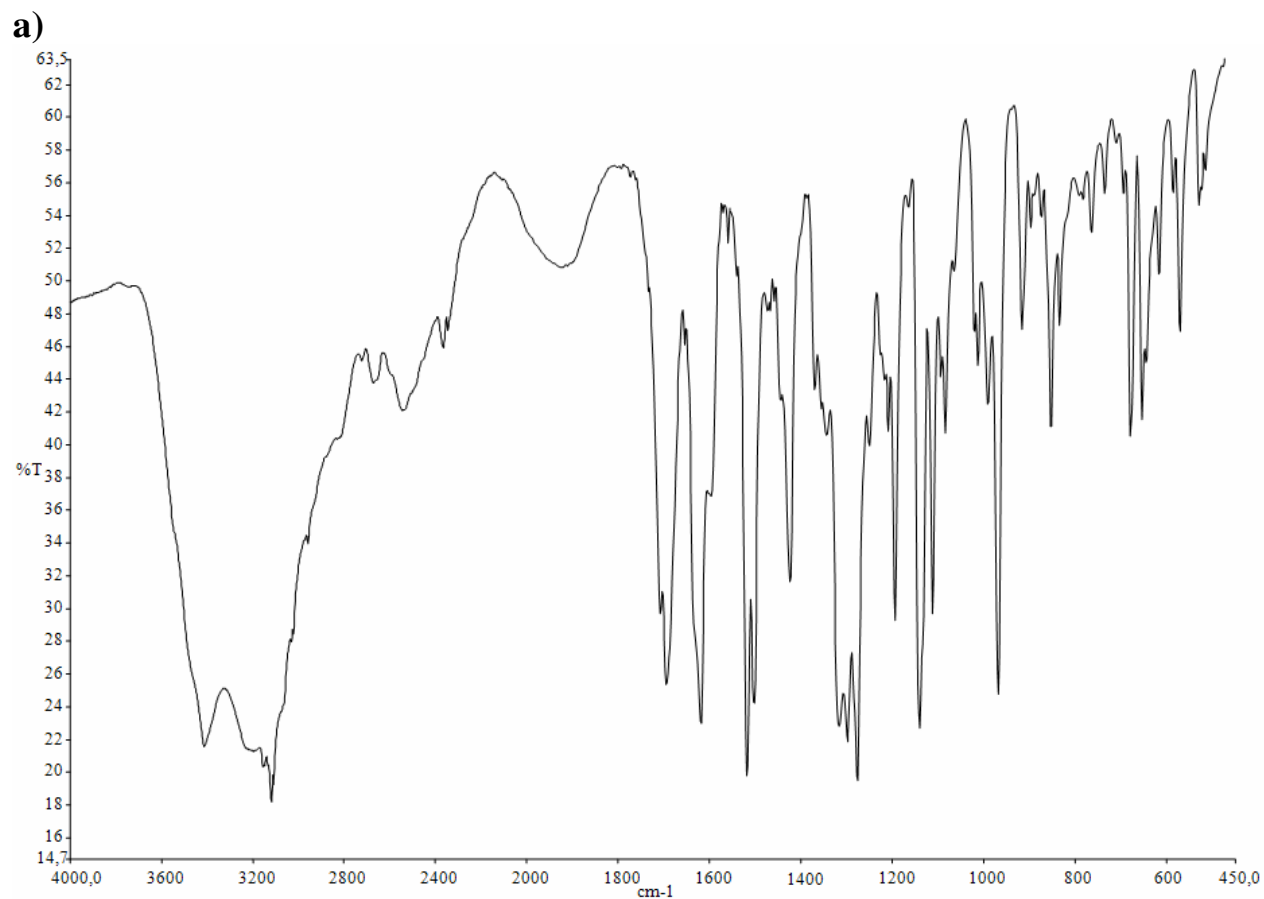
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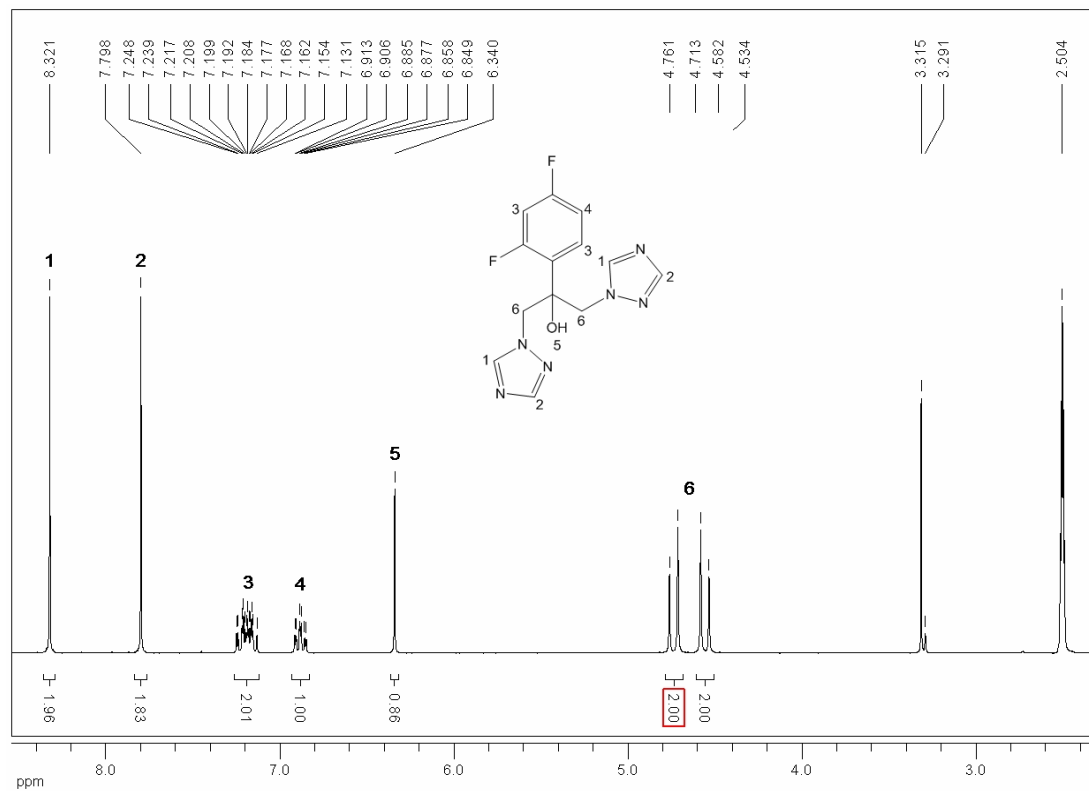
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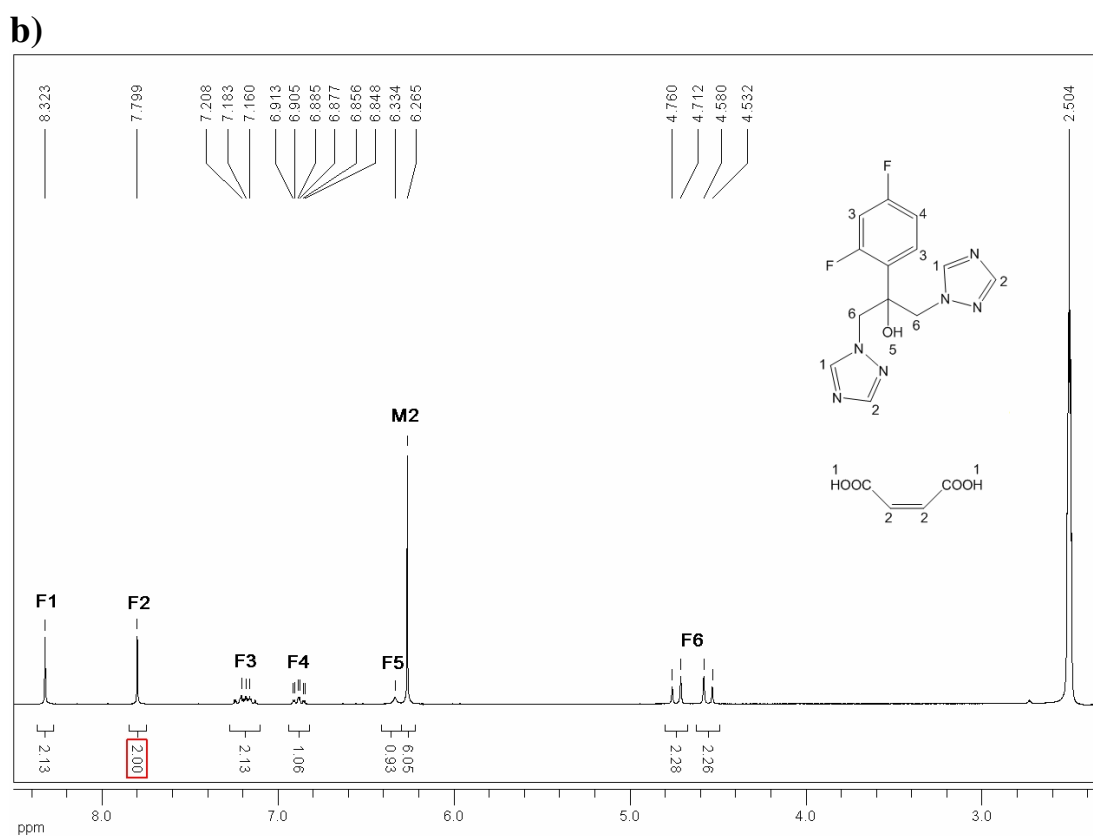
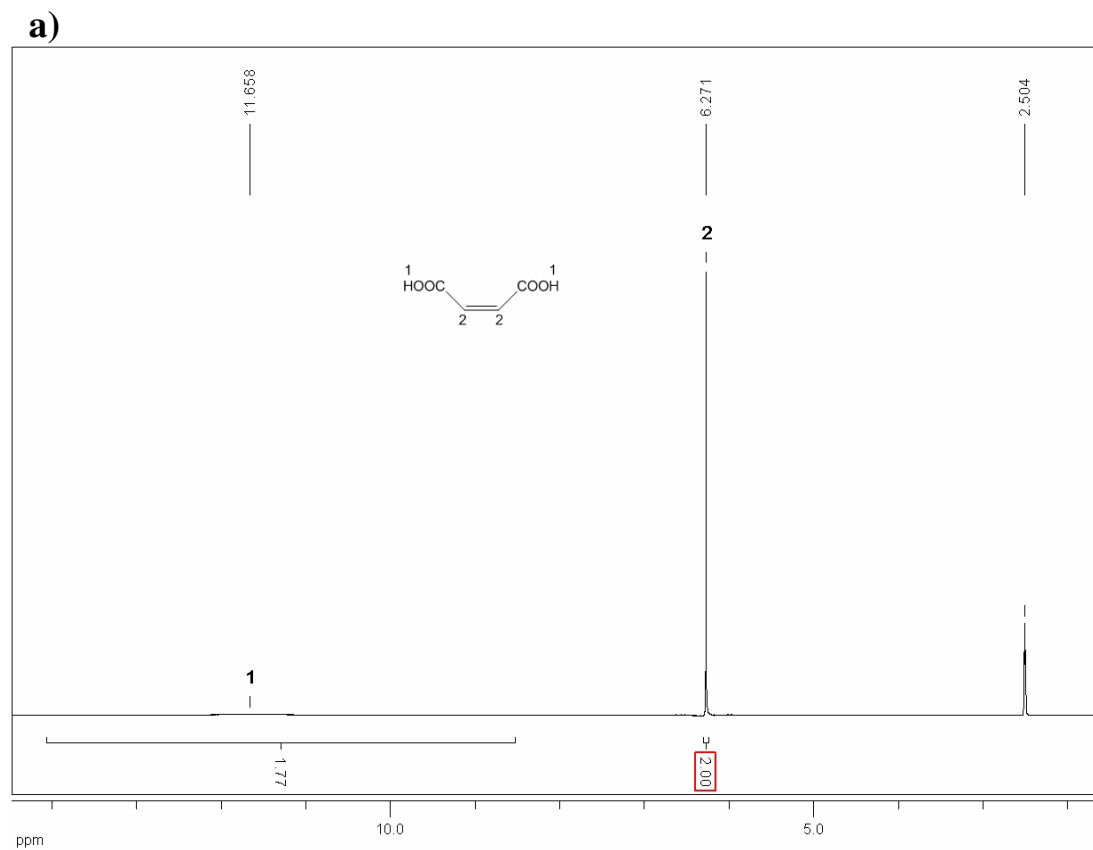
**Figure S3.** IR spectra of a) fumaric acid and b) cocrystal 2.



**Figure S4.** IR spectra of a) glutaric acid and b) cocrystal **3**.

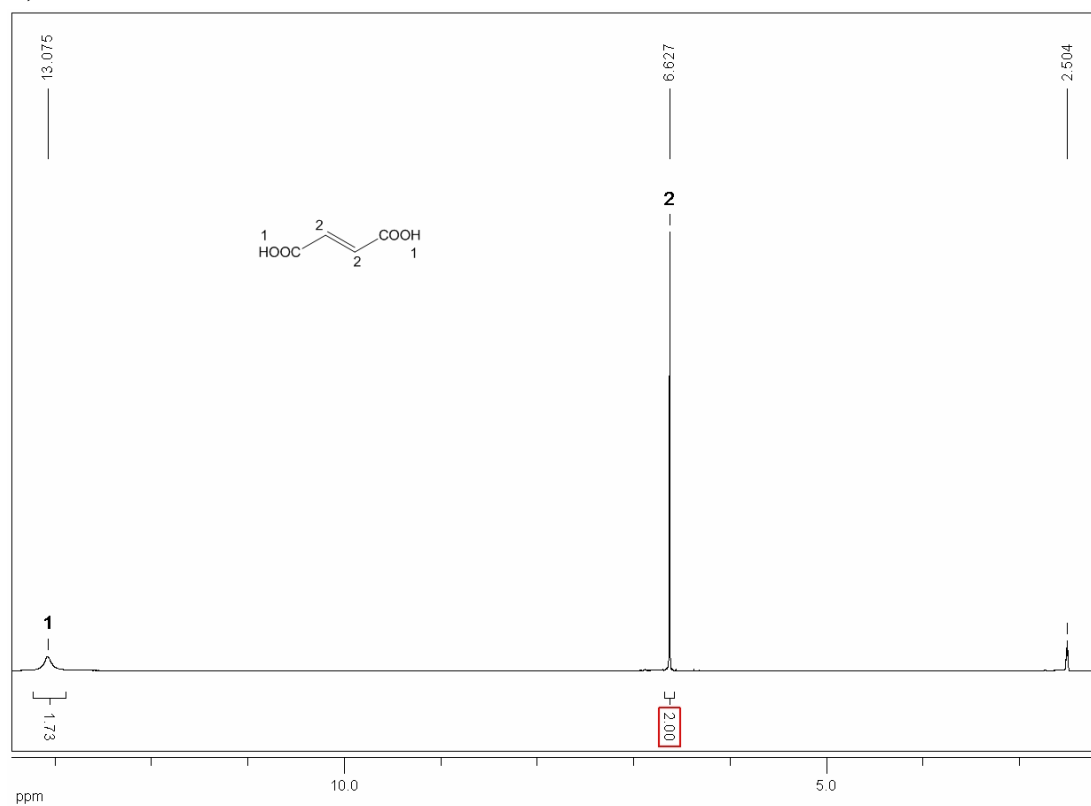


**Figure S5.** Solution <sup>1</sup>H NMR spectra of fluconazole.

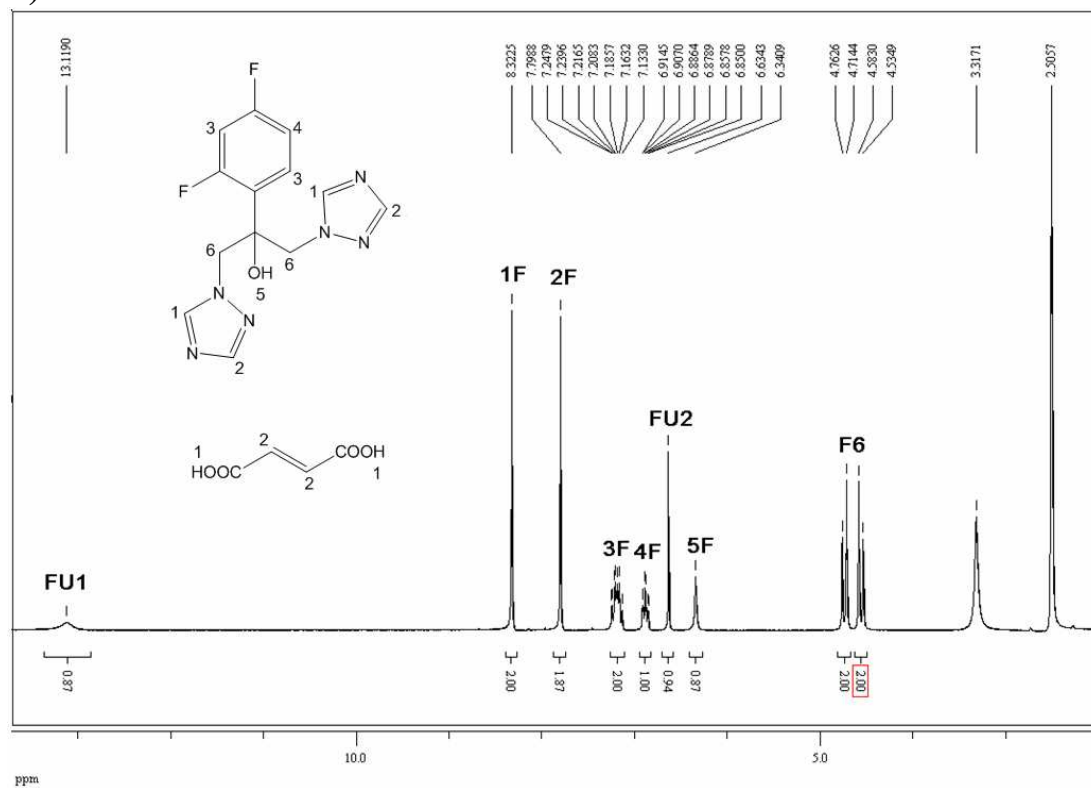


**Figure S6.** Solution  $^1\text{H}$  NMR spectra of a) maleic acid and b) cocrystal of fluconazole with maleic acid (1). Signals of protons are correspondingly assigned (F – fluconazole, M – maleic acid).

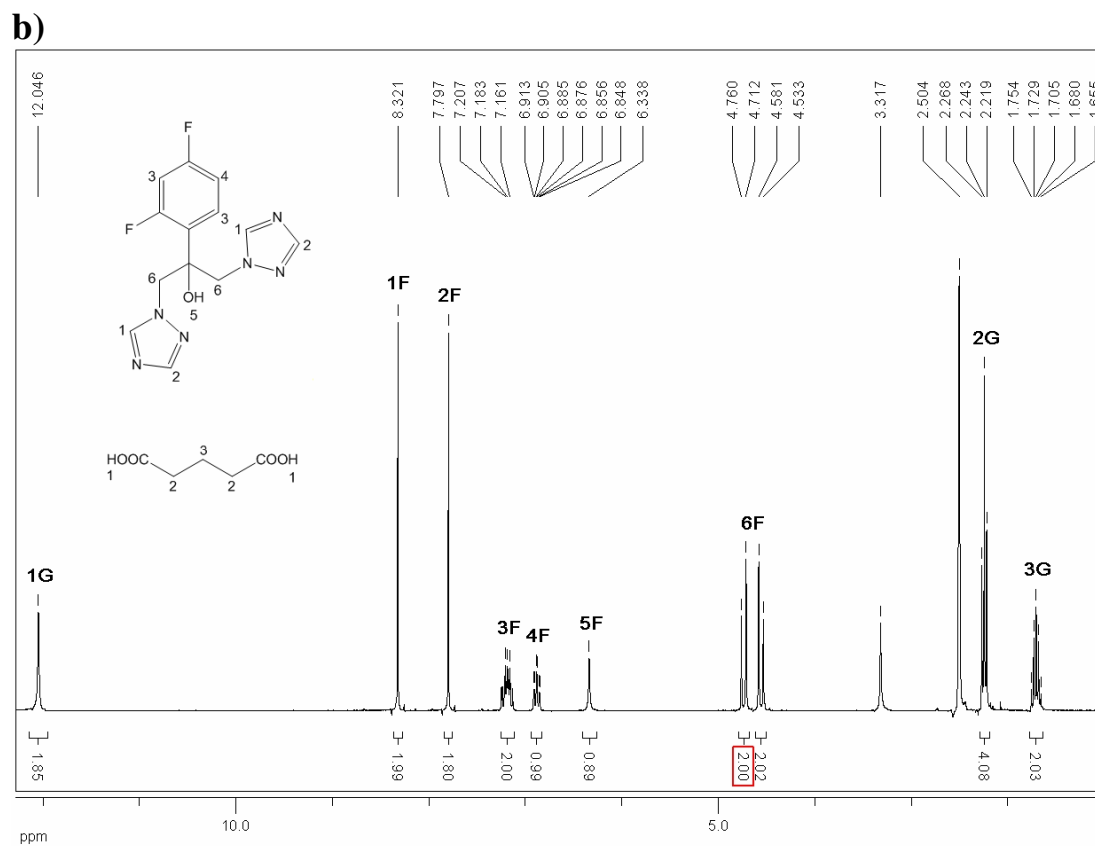
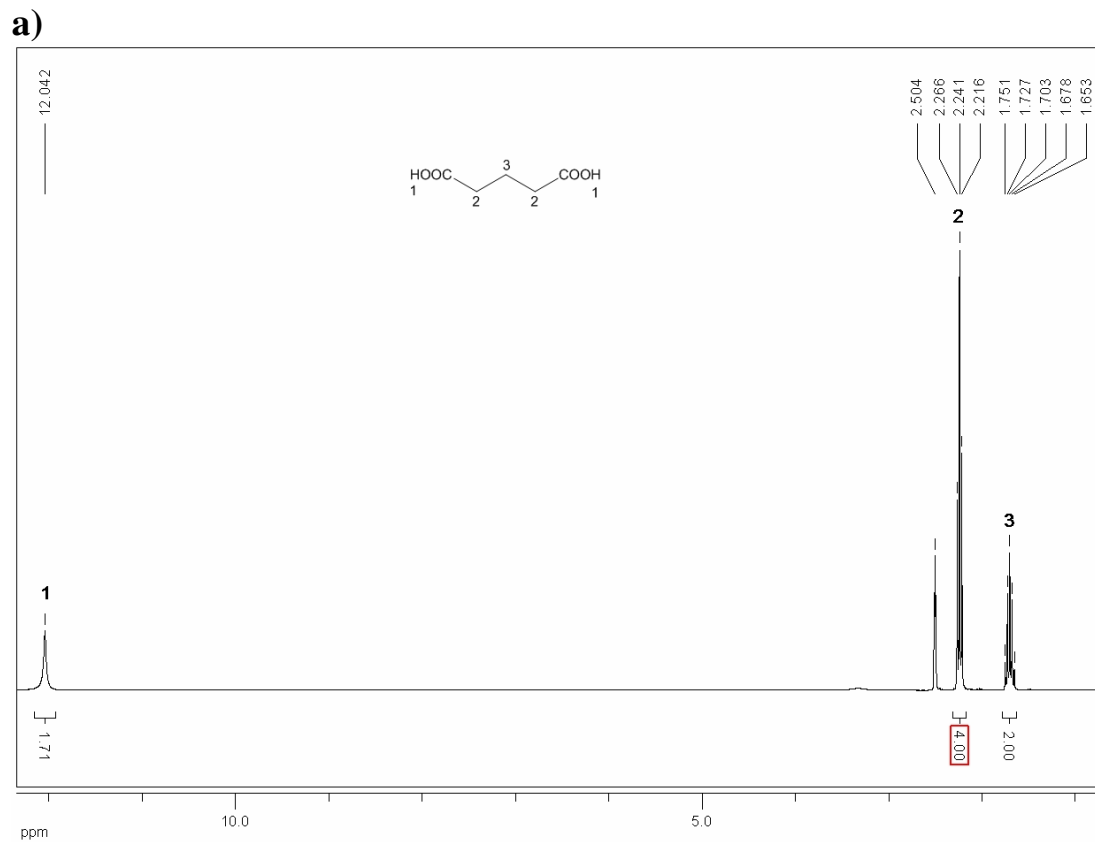
a)



b)



**Figure S7.** Solution  $^1\text{H}$  NMR spectra of a) fumaric acid and b) cocrystal with fumaric acid (**2**). Signals of protons are correspondingly assigned (F – fluconazole, Fu – fumaric acid).



**Figure S8.** Solution  $^1\text{H}$  NMR spectra of a) glutaric acid and b) cocrystal with glutaric acid (3). Signals of protons are correspondingly assigned (F – fluconazole, G – glutaric acid).



The stoichiometric ratios were established by comparison of fluconazole F6 and maleic acid M2 signal intensities for cocrystal **1**, fluconazole F6 and fumaric acid FU2 signal intensities for cocrystal **2** and fluconazole F6 and glutaric acid G3 signal intensities for cocrystal **3**.