

# Crystal Structure, Hirshfeld Surface Analysis, In-Silico and Antimycotic Investigations of Methyl 6-methyl-4-(4-nitrophenyl)-2-oxo-1,2-dihydropyrimidine-5-carboxylate

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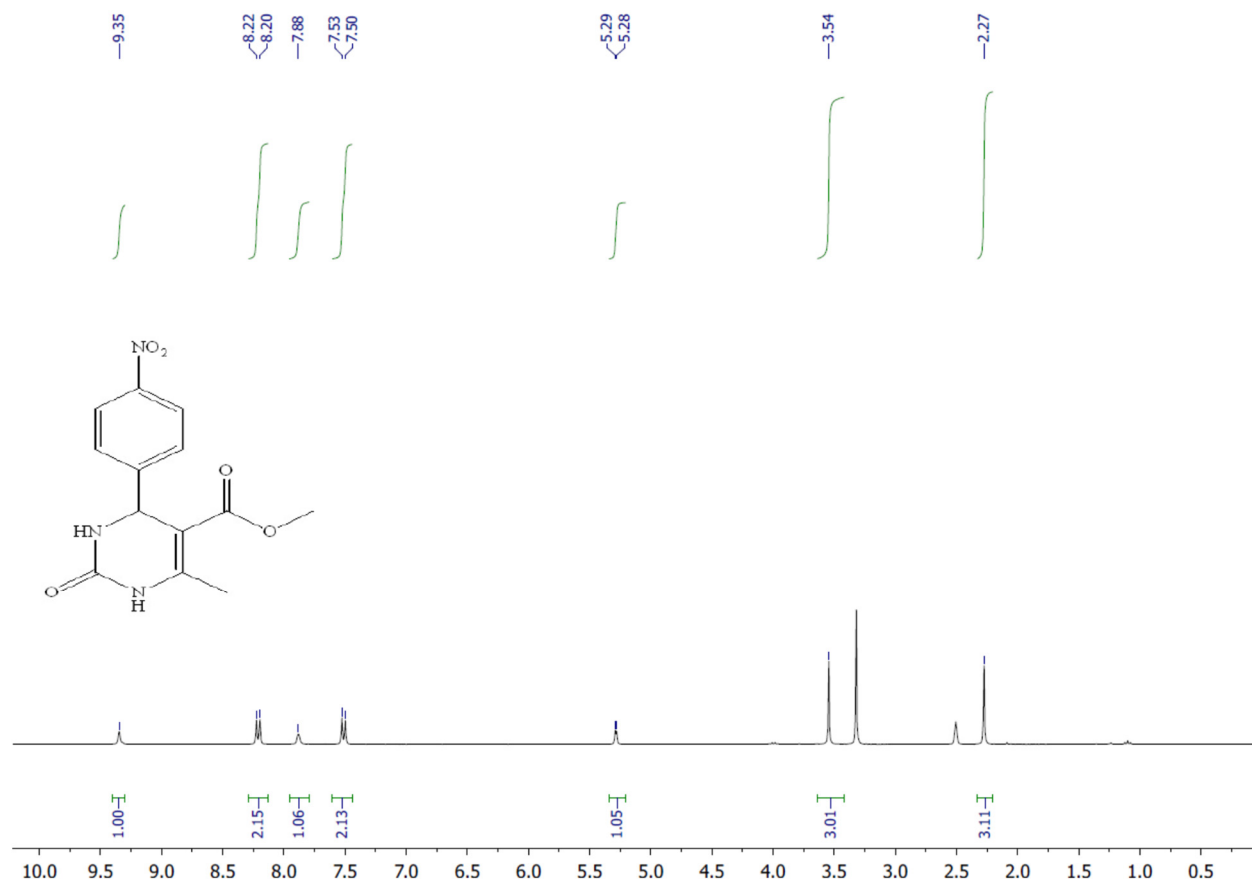
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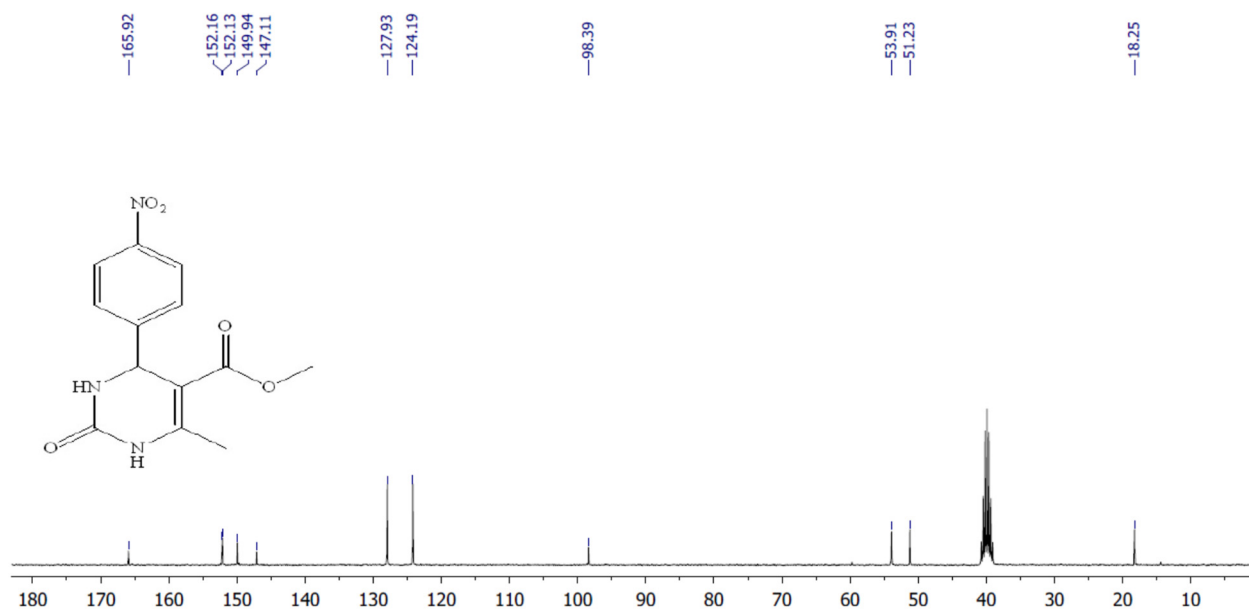
## Supplementary Materials

### Table of contents

|   |    |
|---|----|
| 1. NMR spectra.....                     | S2 |
| 2. X-ray data.....                      | S4 |
| 3. Hirshfeld surface analysis data..... | S5 |



**Figure S1.** <sup>1</sup>H NMR spectrum of the synthesized dihydropyrimidine **1**.



**Figure S2.** <sup>13</sup>C NMR spectrum of the synthesized dihydropyrimidine **1**.

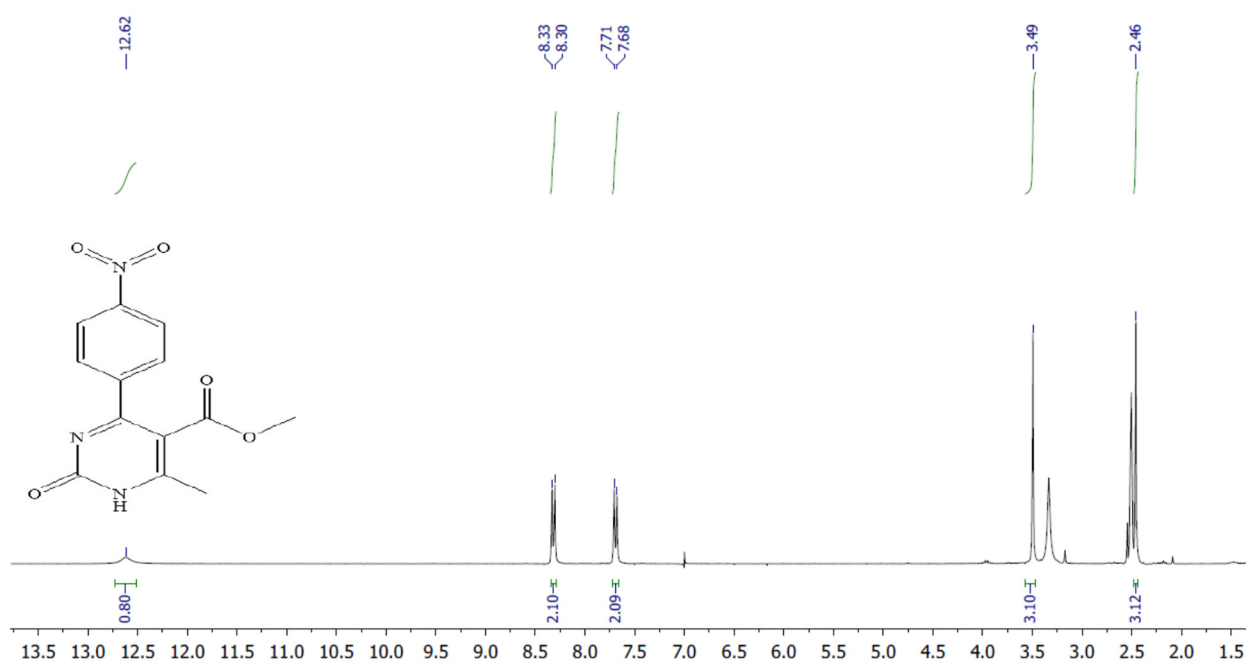


Figure S3.  $^1\text{H}$  NMR spectrum of the synthesized dihydropyrimidine 2.

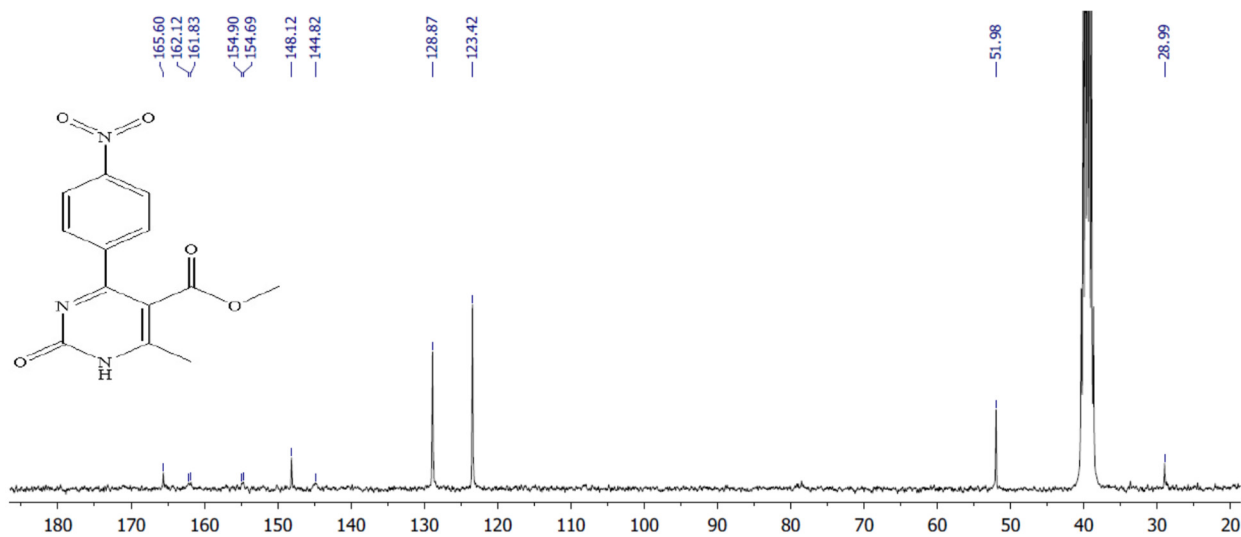


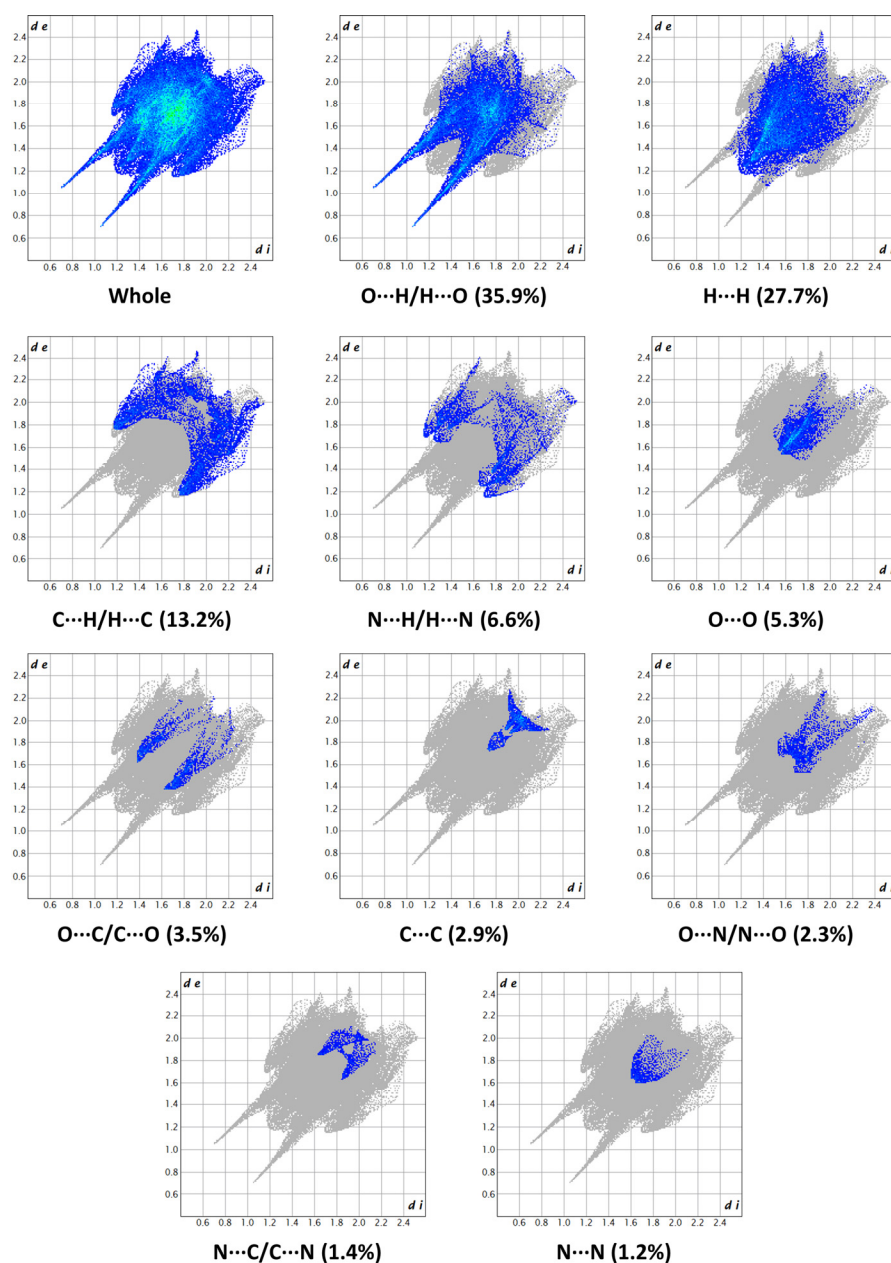
Figure S4.  $^{13}\text{C}$  NMR spectrum of the synthesized dihydropyrimidine 2.

**Table S1.** Bond lengths [Å] and angles [°] for the crystal structure of **2**.

| Atoms        | Distance (Å) | Atoms               | Angle (°)  |
|--------------|--------------|---------------------|------------|
| O(1)-N(1)    | 1.221(3)     | C(11)-O(5)-C(12)    | 116.28(15) |
| O(2)-N(1)    | 1.216(3)     | O(2)-N(1)-O(1)      | 124.1(2)   |
| O(3)-C(10)   | 1.233(2)     | O(2)-N(1)-C(1)      | 118.1(2)   |
| O(4)-C(11)   | 1.204(2)     | O(1)-N(1)-C(1)      | 117.8(2)   |
| O(5)-C(11)   | 1.333(2)     | C(7)-N(2)-C(10)     | 118.84(16) |
| O(5)-C(12)   | 1.446(2)     | C(9)-N(3)-C(10)     | 124.73(16) |
| N(1)-C(1)    | 1.472(3)     | C(9)-N(3)-H(3)      | 117.6      |
| N(2)-C(7)    | 1.328(2)     | C(10)-N(3)-H(3)     | 117.6      |
| N(2)-C(10)   | 1.359(2)     | C(2)-C(1)-C(6)      | 122.05(19) |
| N(3)-C(9)    | 1.344(2)     | C(2)-C(1)-N(1)      | 119.0(2)   |
| N(3)-C(10)   | 1.379(2)     | C(6)-C(1)-N(1)      | 118.9(2)   |
| N(3)-H(3)    | 0.8600       | C(1)-C(2)-C(3)      | 118.8(2)   |
| C(1)-C(2)    | 1.372(3)     | C(1)-C(2)-H(2)      | 120.6      |
| C(1)-C(6)    | 1.374(3)     | C(3)-C(2)-H(2)      | 120.6      |
| C(2)-C(3)    | 1.372(3)     | C(2)-C(3)-C(4)      | 120.4(2)   |
| C(2)-H(2)    | 0.9300       | C(2)-C(3)-H(3A)     | 119.8      |
| C(3)-C(4)    | 1.390(3)     | C(4)-C(3)-H(3A)     | 119.8      |
| C(3)-H(3A)   | 0.9300       | C(5)-C(4)-C(3)      | 119.27(19) |
| C(4)-C(5)    | 1.383(3)     | C(5)-C(4)-C(7)      | 120.08(17) |
| C(4)-C(7)    | 1.487(3)     | C(3)-C(4)-C(7)      | 120.64(17) |
| C(5)-C(6)    | 1.373(3)     | C(6)-C(5)-C(4)      | 120.6(2)   |
| C(5)-H(5)    | 0.9300       | C(6)-C(5)-H(5)      | 119.7      |
| C(6)-H(6)    | 0.9300       | C(4)-C(5)-H(5)      | 119.7      |
| C(7)-C(8)    | 1.424(3)     | C(5)-C(6)-C(1)      | 118.7(2)   |
| C(8)-C(9)    | 1.379(3)     | C(5)-C(6)-H(6)      | 120.7      |
| C(8)-C(11)   | 1.483(2)     | C(1)-C(6)-H(6)      | 120.7      |
| C(9)-C(13)   | 1.492(3)     | N(2)-C(7)-C(8)      | 123.41(17) |
| C(12)-H(12A) | 0.9600       | N(2)-C(7)-C(4)      | 115.10(17) |
| C(12)-H(12B) | 0.9600       | C(8)-C(7)-C(4)      | 121.49(16) |
| C(12)-H(12C) | 0.9600       | C(9)-C(8)-C(7)      | 117.24(16) |
| C(13)-H(13A) | 0.9600       | C(9)-C(8)-C(11)     | 120.98(17) |
| C(13)-H(13B) | 0.9600       | C(7)-C(8)-C(11)     | 121.01(16) |
| C(13)-H(13C) | 0.9600       | N(3)-C(9)-C(8)      | 117.46(17) |
|              |              | N(3)-C(9)-C(13)     | 115.29(16) |
|              |              | C(8)-C(9)-C(13)     | 127.08(16) |
|              |              | O(3)-C(10)-N(2)     | 122.88(18) |
|              |              | O(3)-C(10)-N(3)     | 118.92(17) |
|              |              | N(2)-C(10)-N(3)     | 118.20(16) |
|              |              | O(4)-C(11)-O(5)     | 123.47(17) |
|              |              | O(4)-C(11)-C(8)     | 124.32(17) |
|              |              | O(5)-C(11)-C(8)     | 112.20(15) |
|              |              | O(5)-C(12)-H(12A)   | 109.5      |
|              |              | O(5)-C(12)-H(12B)   | 109.5      |
|              |              | H(12A)-C(12)-H(12B) | 109.5      |
|              |              | O(5)-C(12)-H(12C)   | 109.5      |
|              |              | H(12A)-C(12)-H(12C) | 109.5      |
|              |              | H(12B)-C(12)-H(12C) | 109.5      |
|              |              | C(9)-C(13)-H(13A)   | 109.5      |
|              |              | C(9)-C(13)-H(13B)   | 109.5      |
|              |              | H(13A)-C(13)-H(13B) | 109.5      |

|                     |       |
|---------------------|-------|
| C(9)-C(13)-H(13C)   | 109.5 |
| H(13A)-C(13)-H(13C) | 109.5 |
| H(13B)-C(13)-H(13C) | 109.5 |

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**Figure S5.** 2D HS Fingerprint plots of 2, providing a visual summary of the frequency of each combination of  $d_e$  and  $d_i$  across the HS. Points with a contribution to the surface are colored blue for a small contribution to green for a great contribution.