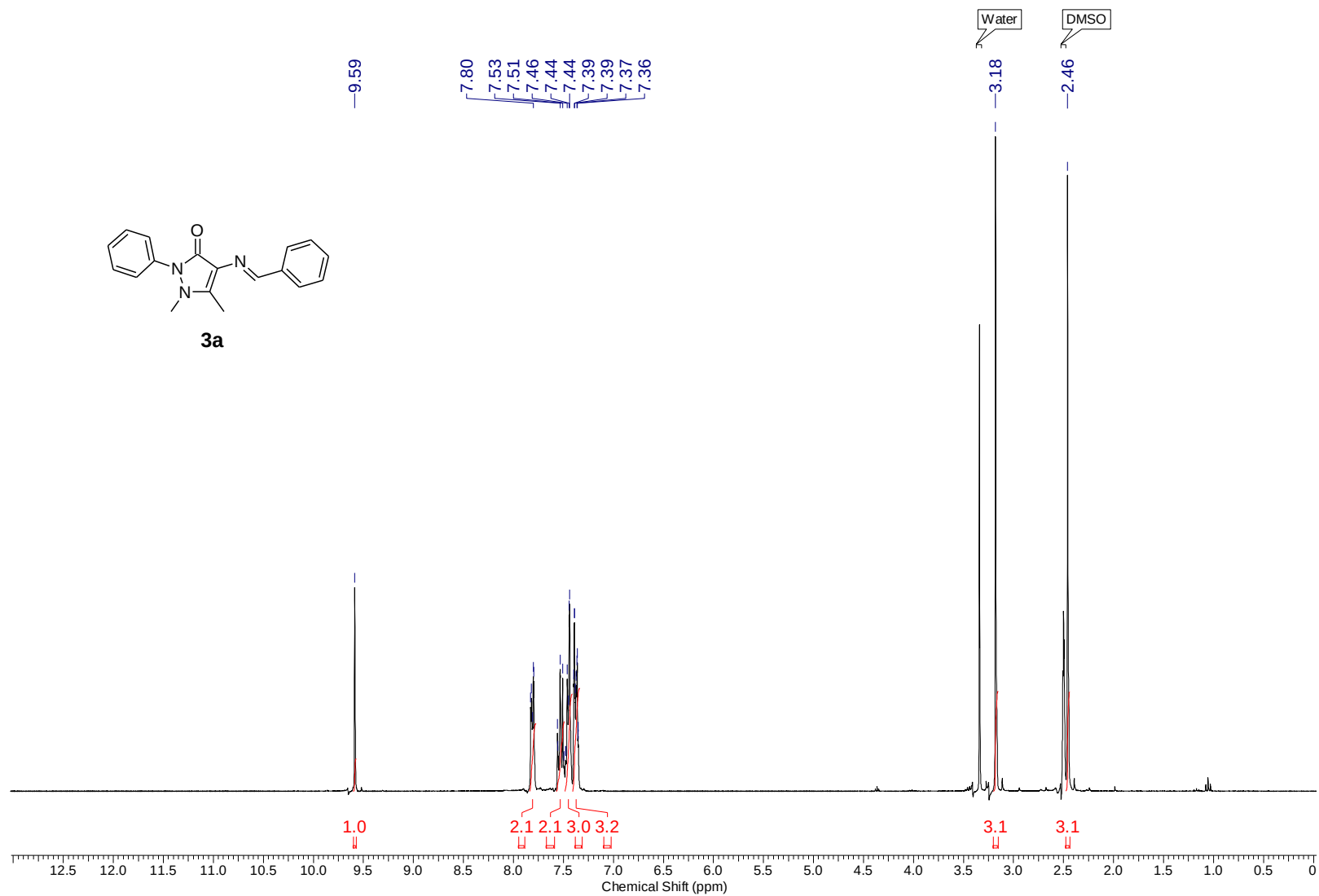




**Figure S1.**  $^1\text{H}$  NMR spectrum of compound **3a**.

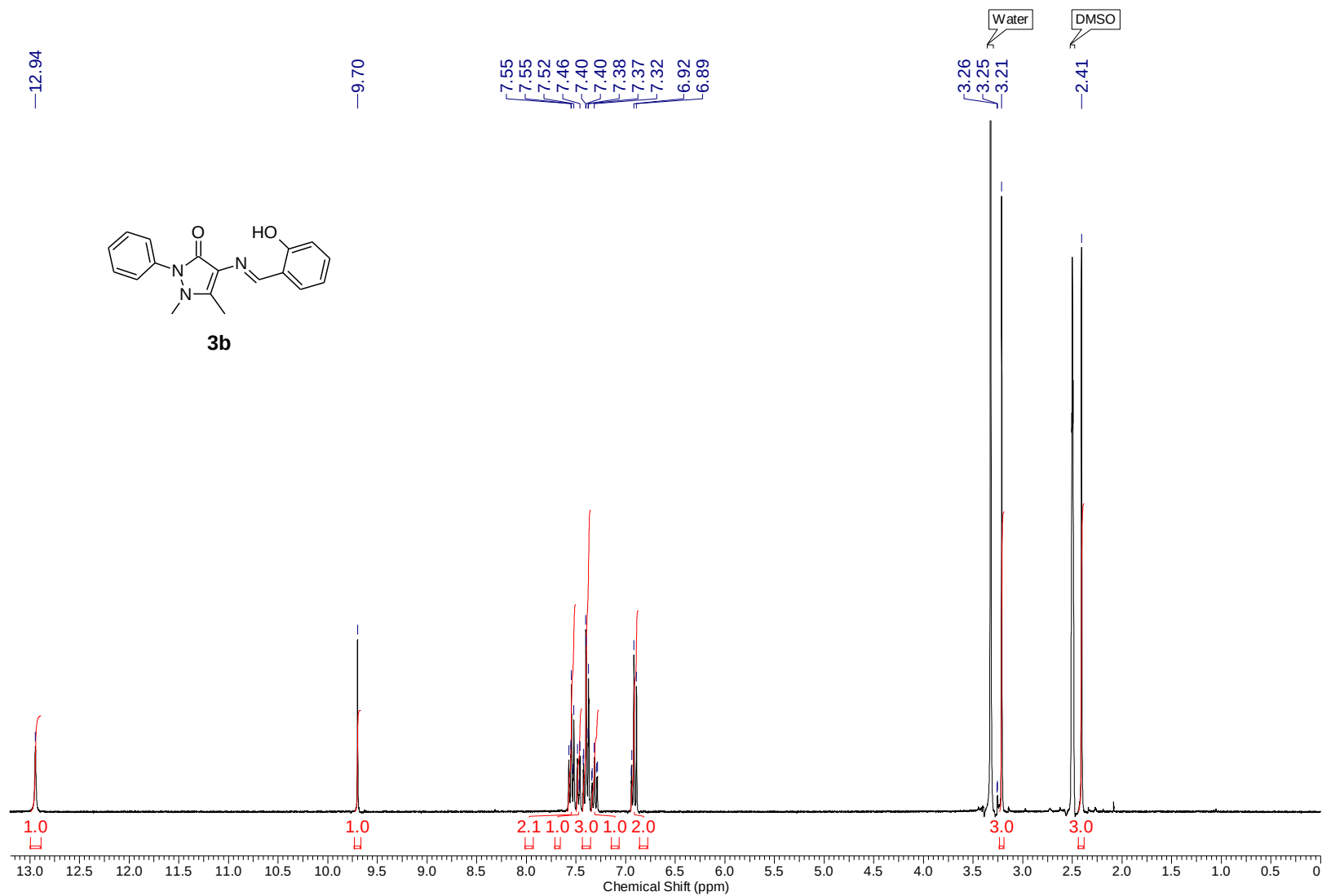


Figure S2. <sup>1</sup>H NMR spectrum of compound **3b**.

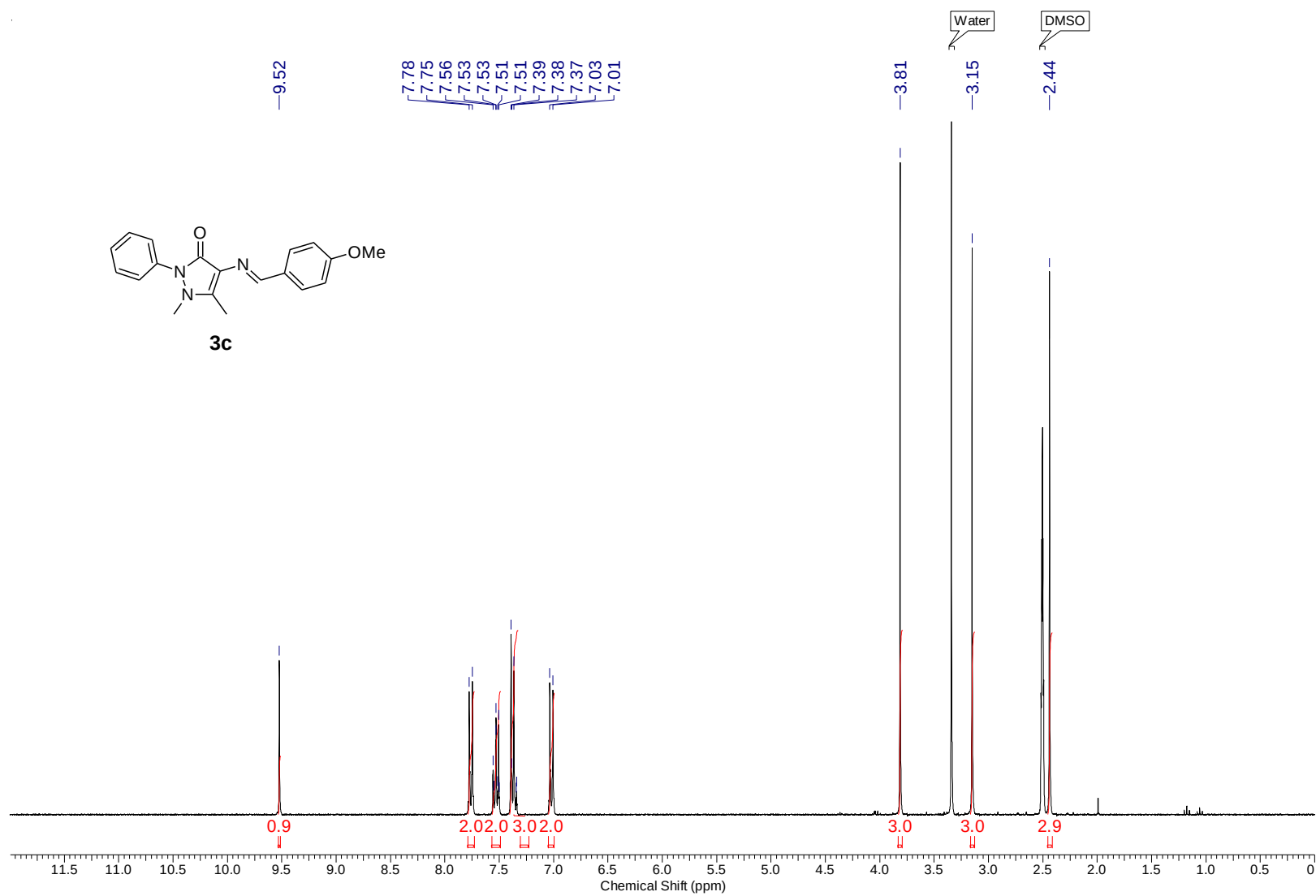
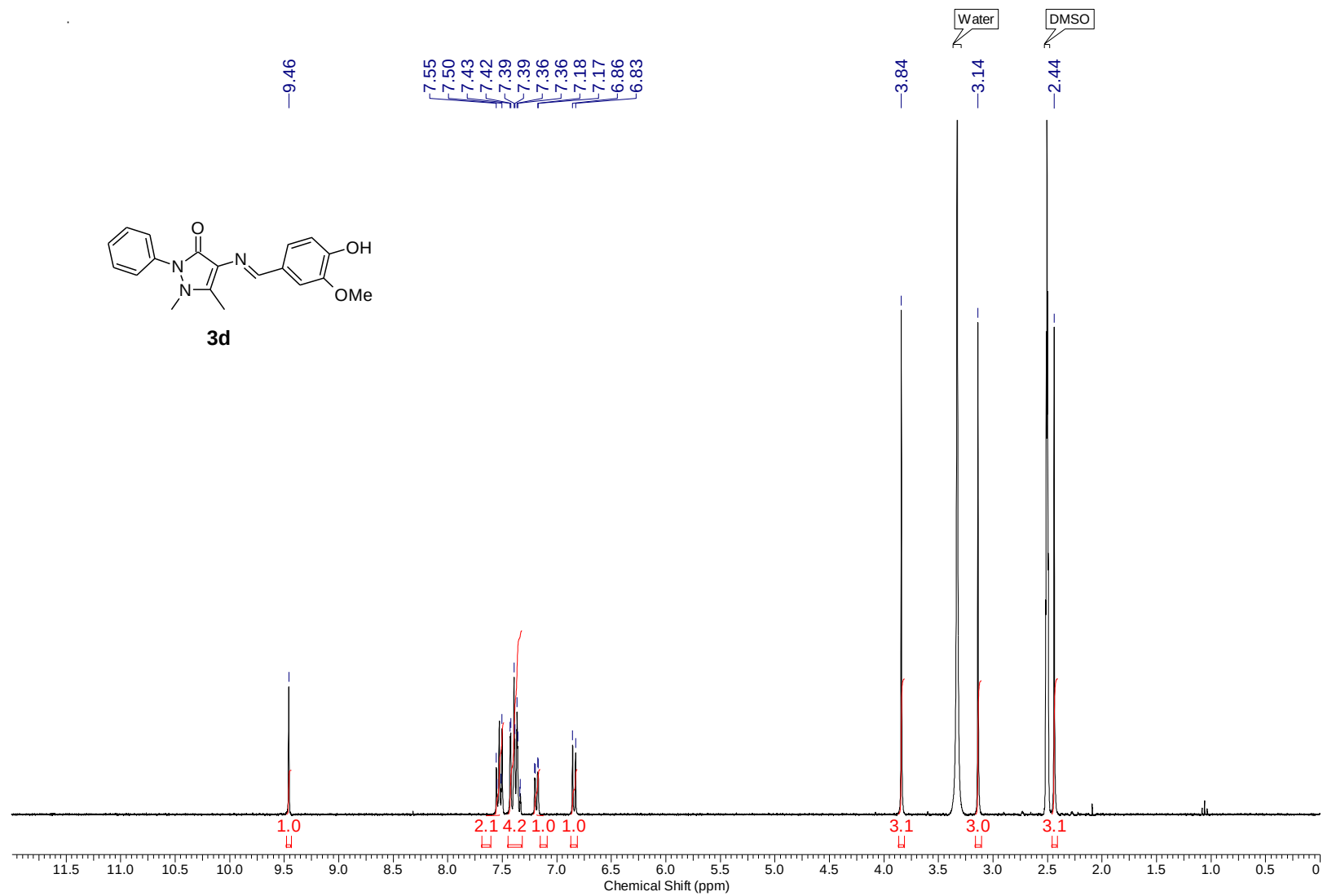
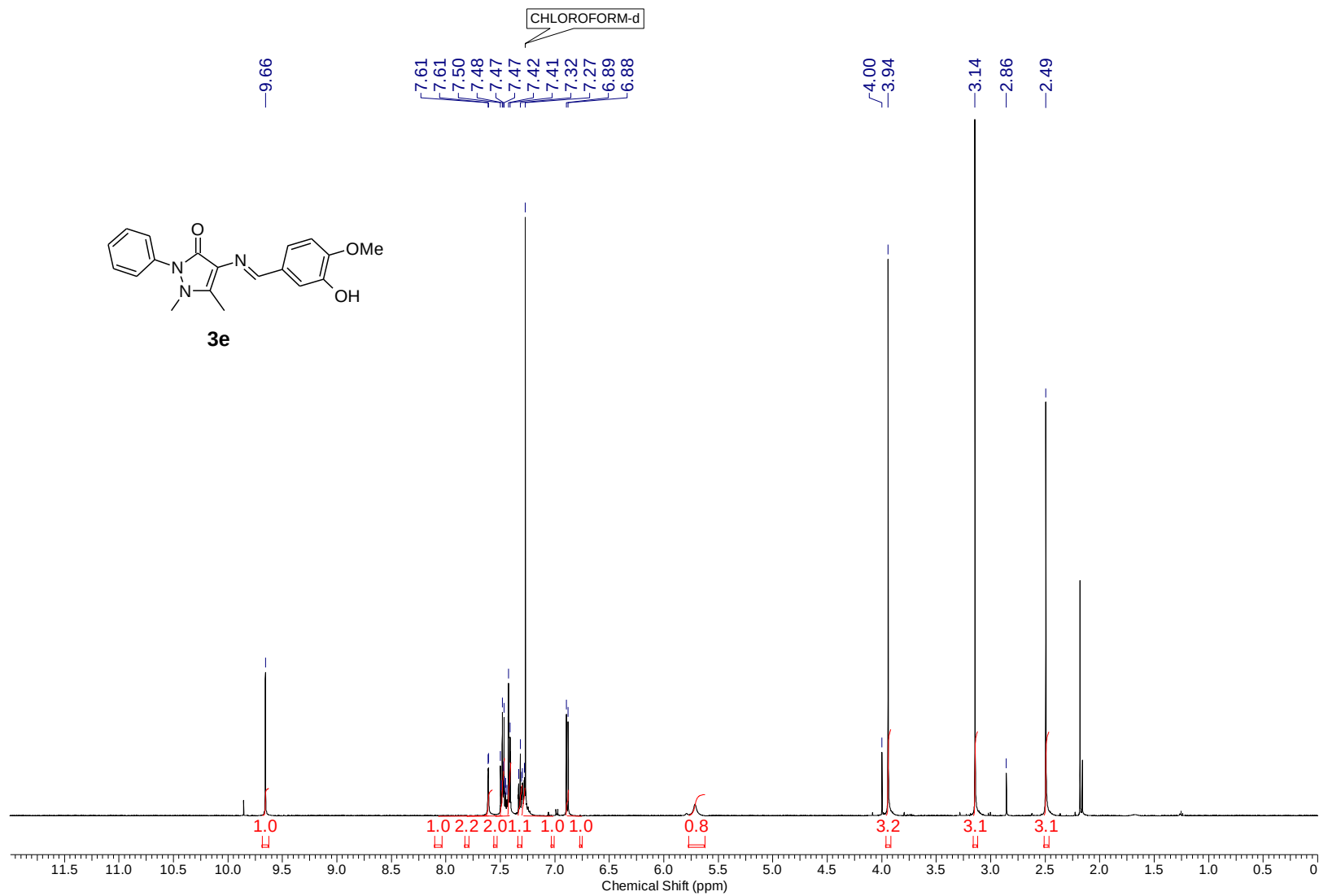


Figure S3. <sup>1</sup>H NMR spectrum of compound **3c**.



**Figure S4.** <sup>1</sup>H NMR spectrum of compound **3d**.



**Figure S5.**  $^1\text{H}$  NMR spectrum of compound **3e**.

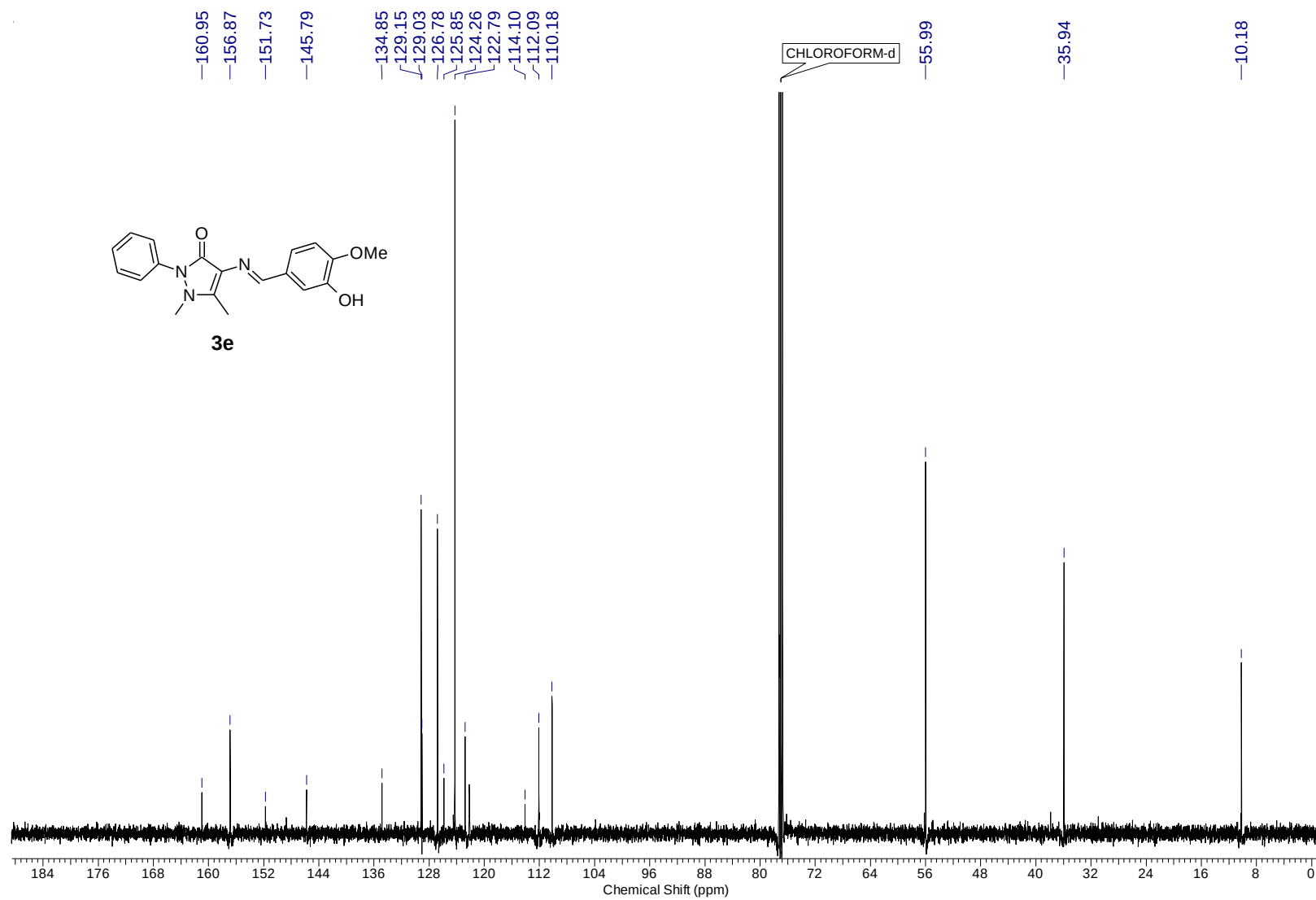


Figure S6.  $^{13}\text{C}$  NMR spectrum of compound **3e**.

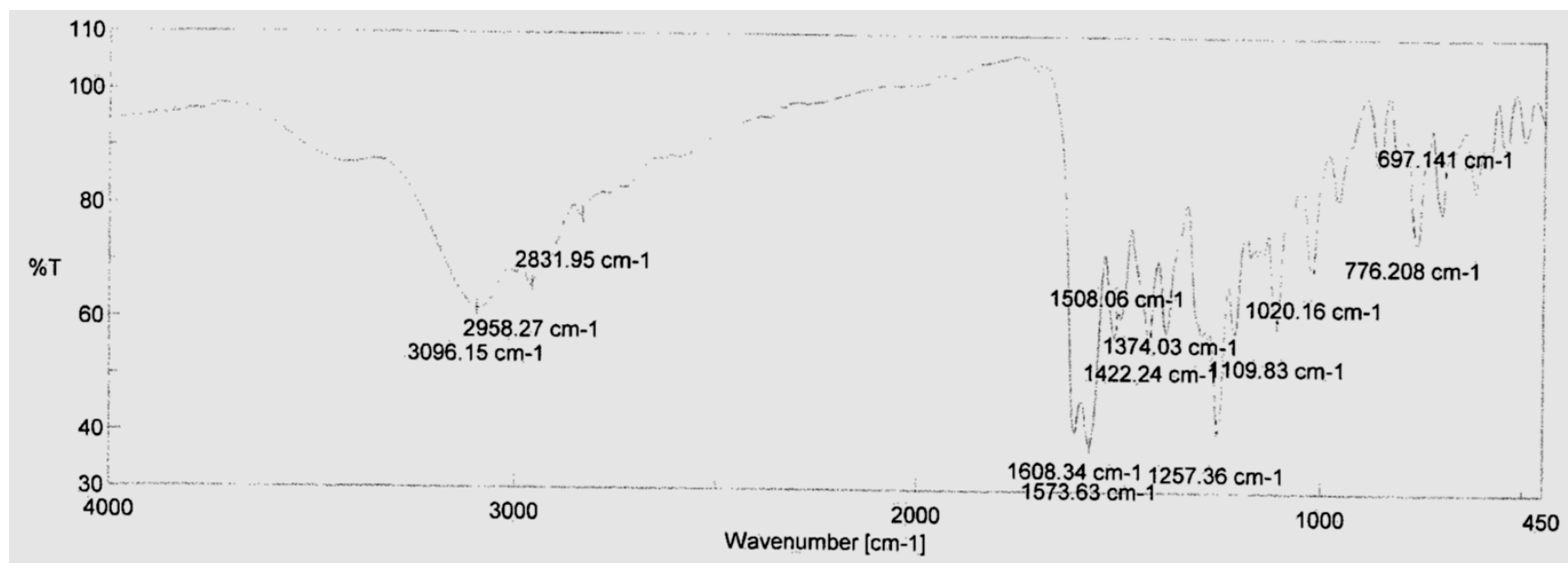


Figure S7. IR spectrum of compound 3e.

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -2.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

60 formula(e) evaluated with 3 results within limits (up to 19 closest results for each mass)

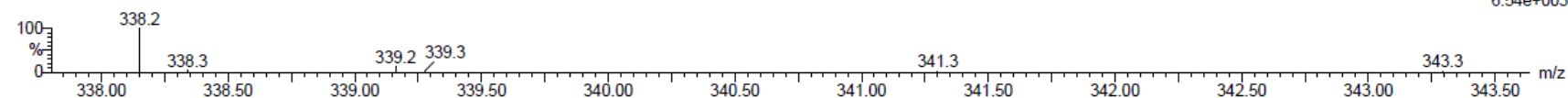
Elements Used:

C: 0-100 H: 0-200 N: 3-3 O: 0-30

24-Jun-2016

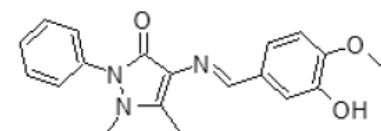
jhm-24jun16-77 284 (5.252) Cn (Cen,7, 50.00, Ar); Sm (SG, 3x5.00); Sb (12,5.00)

TOF MS ES+  
6.54e+003



Minimum: -2.0  
Maximum: 10.0 10.0 1000.0

| Mass     | Calc. Mass | mDa  | PPM   | DBE  | i-FIT | Formula       |
|----------|------------|------|-------|------|-------|---------------|
| 338.1506 | 338.1505   | 0.1  | 0.3   | 11.5 | n/a   | C19 H20 N3 O3 |
|          | 338.1563   | -5.7 | -16.9 | 2.5  | n/a   | C12 H24 N3 O8 |
|          | 338.1411   | 9.5  | 28.1  | -1.5 | n/a   | C8 H24 N3 O11 |



[M+H]<sup>+</sup> = 338.149918 Da

Figure S8. HRMS of compound 3e.



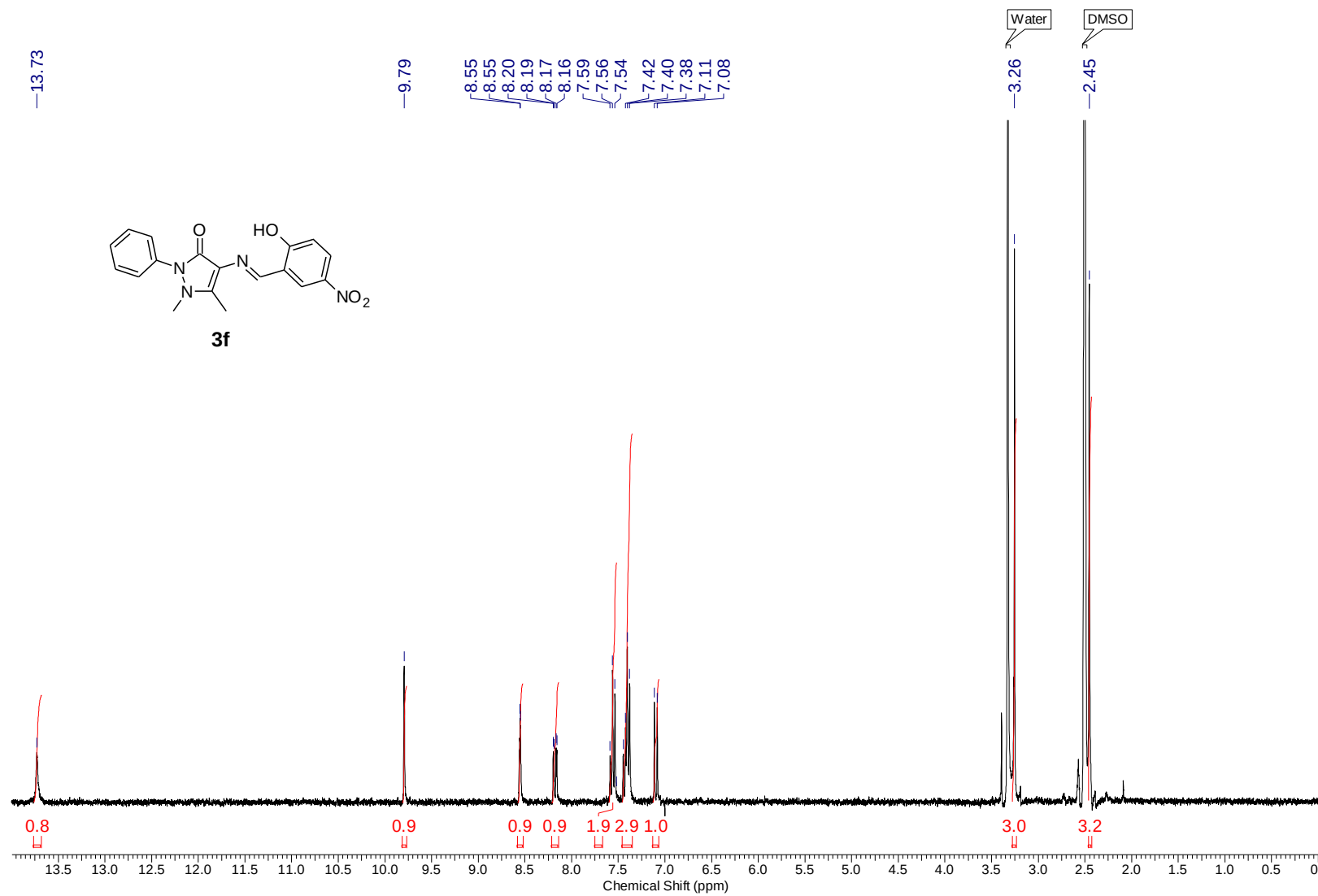


Figure S9.  $^1\text{H}$  NMR spectrum of compound **3f**.

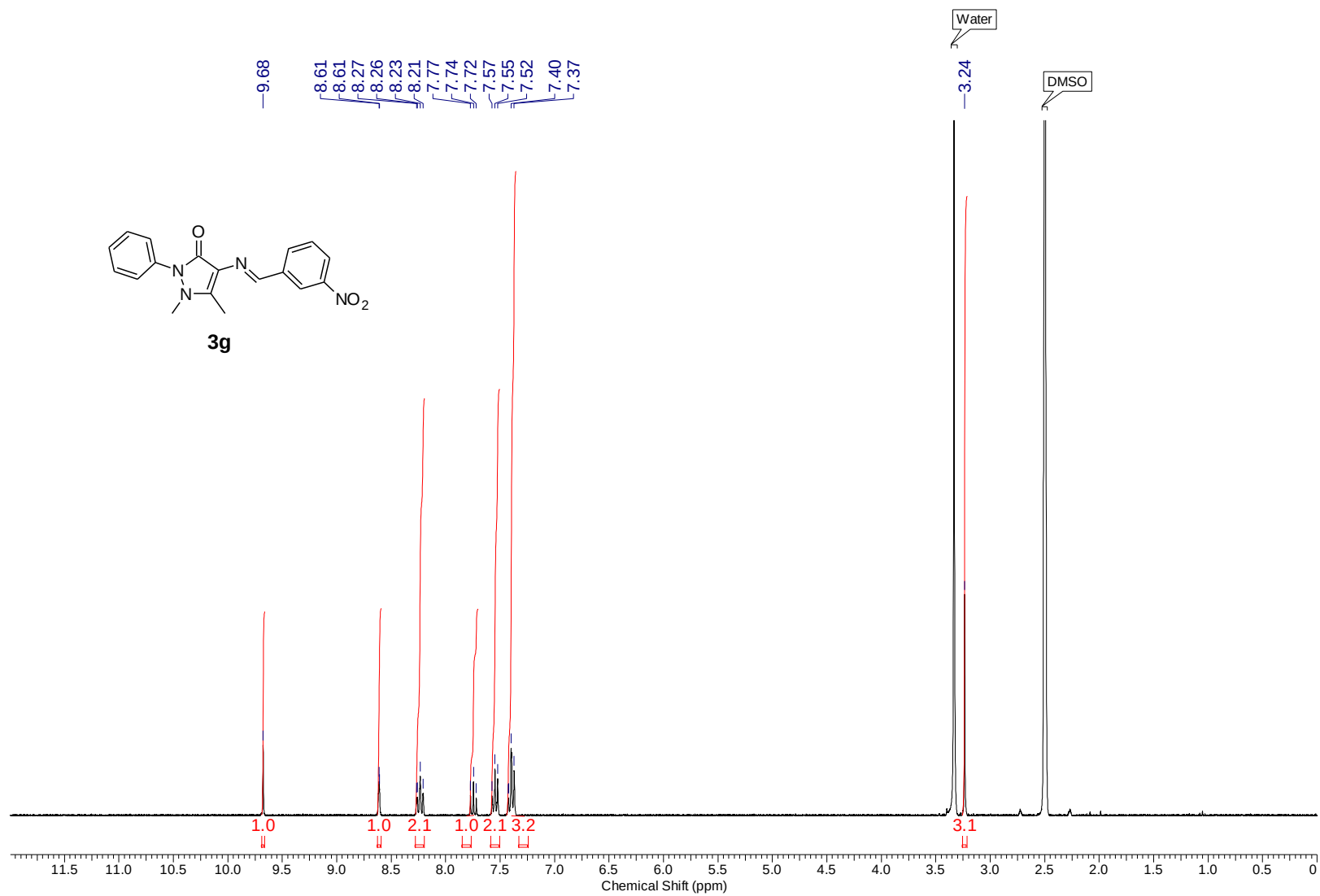


Figure S10. <sup>1</sup>H NMR spectrum of compound **3g**.

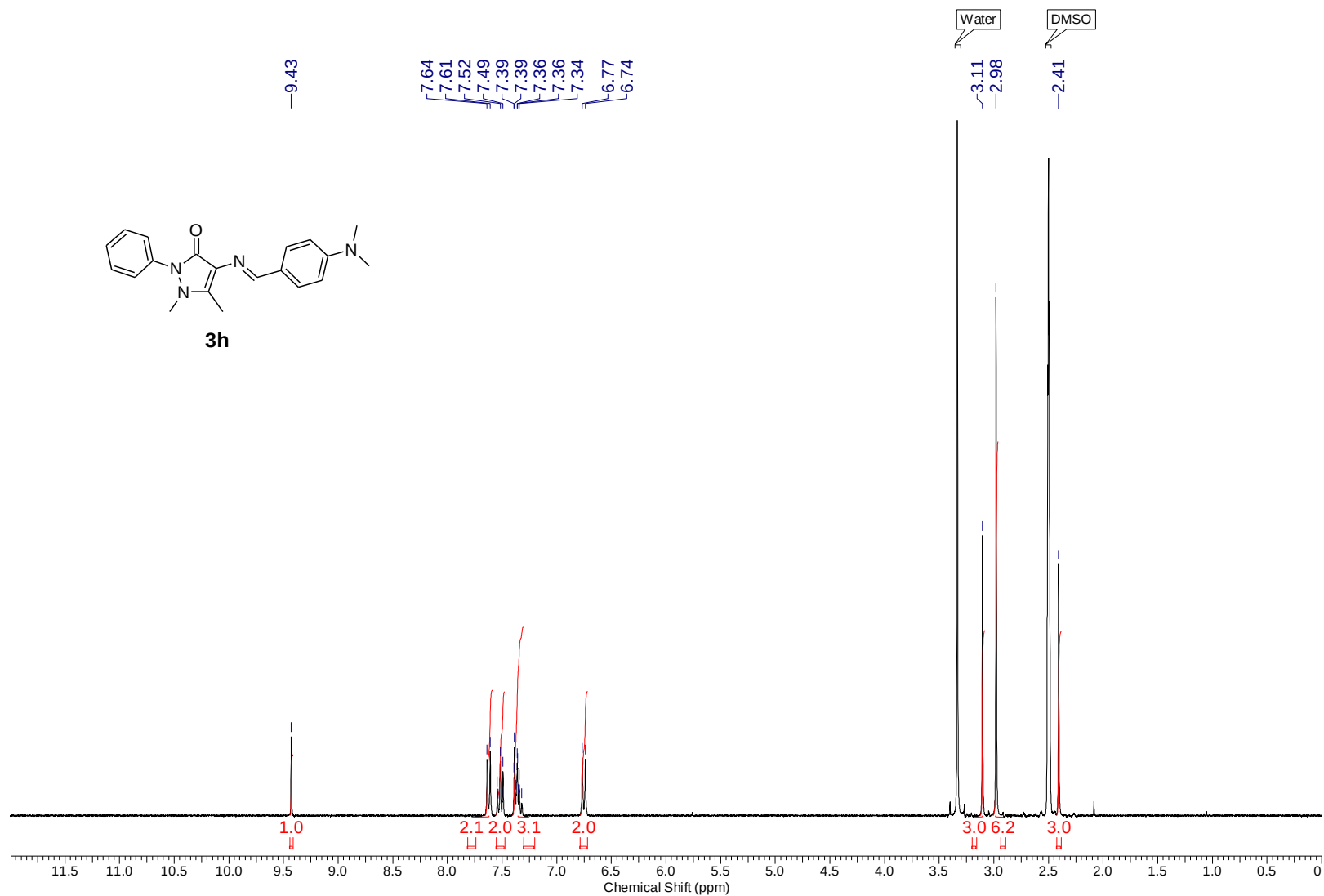
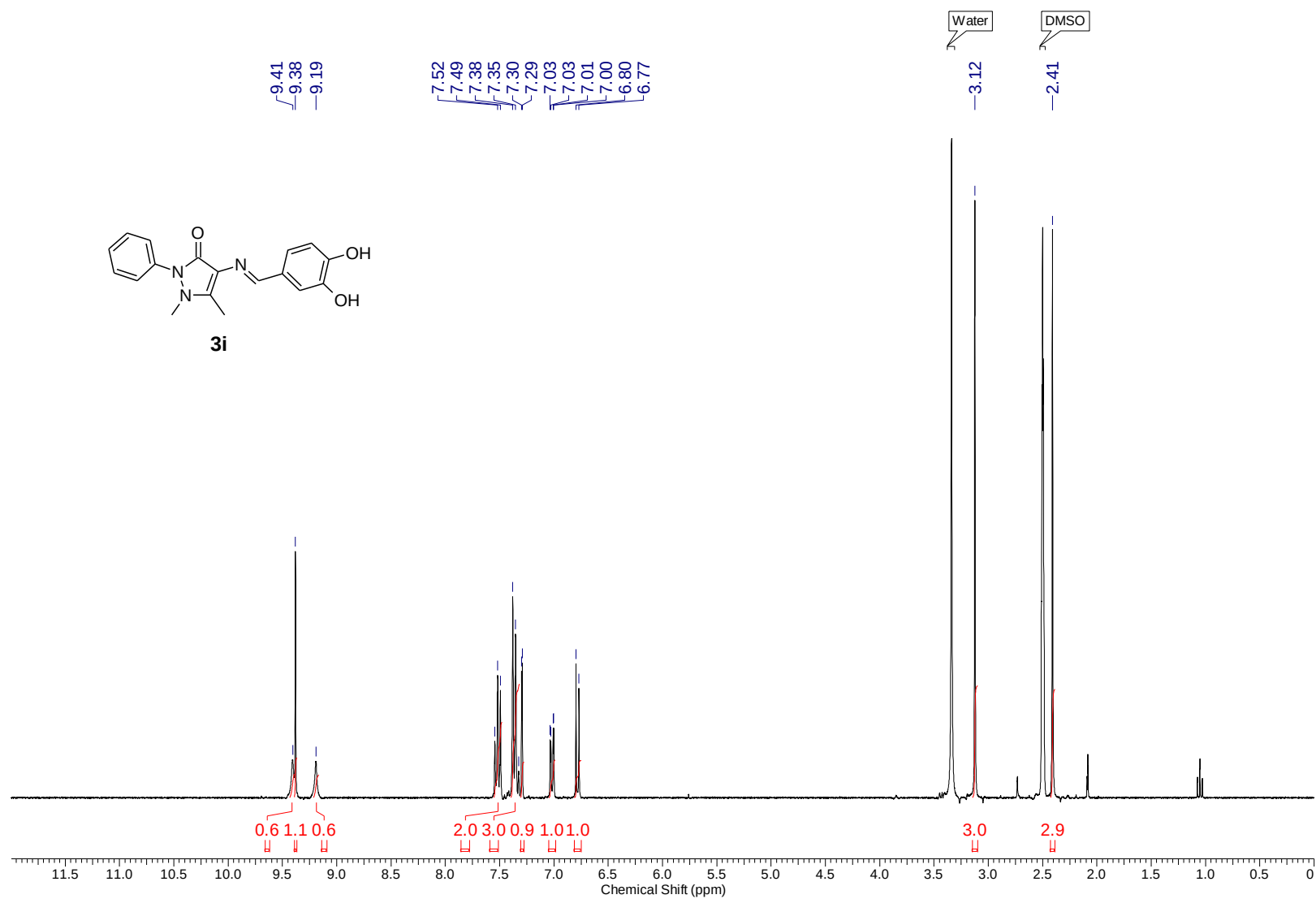


Figure S11.  $^1\text{H}$  NMR spectrum of compound **3h**.



**Figure S12.** <sup>1</sup>H NMR spectrum of compound **3i**.

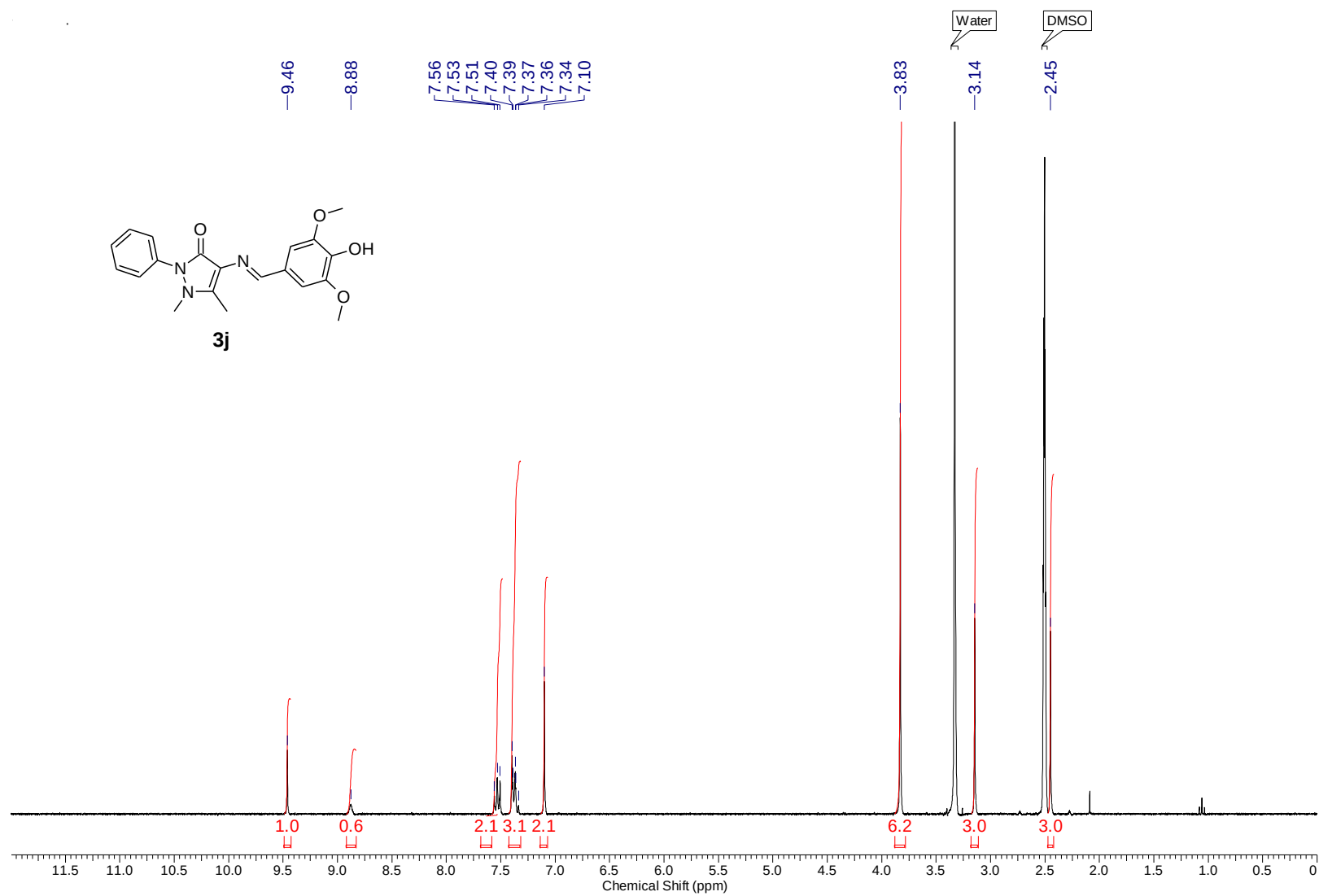


Figure S13. <sup>1</sup>H NMR spectrum of compound **3j**.

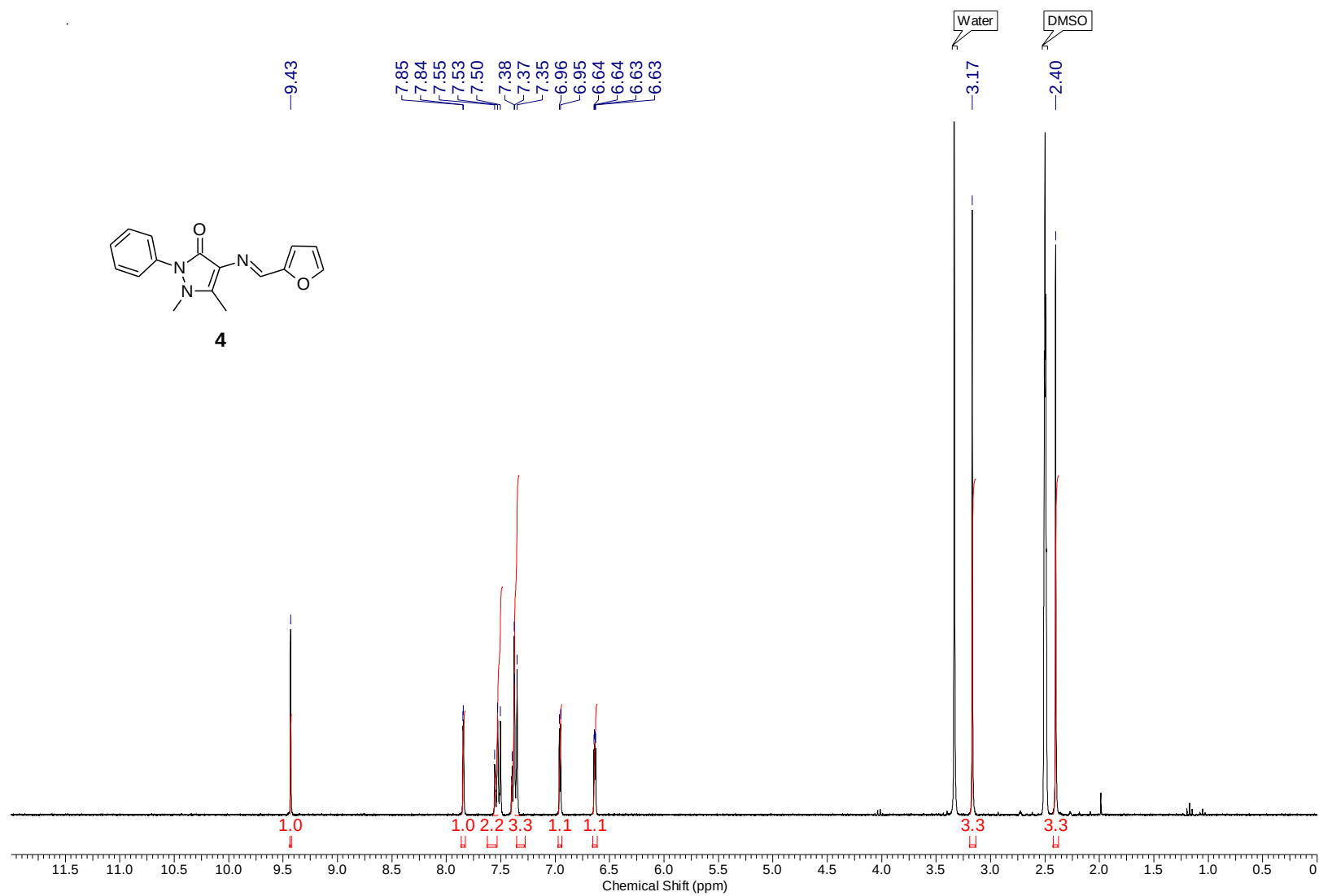


Figure S14.  $^1\text{H}$  NMR spectrum of compound 4.

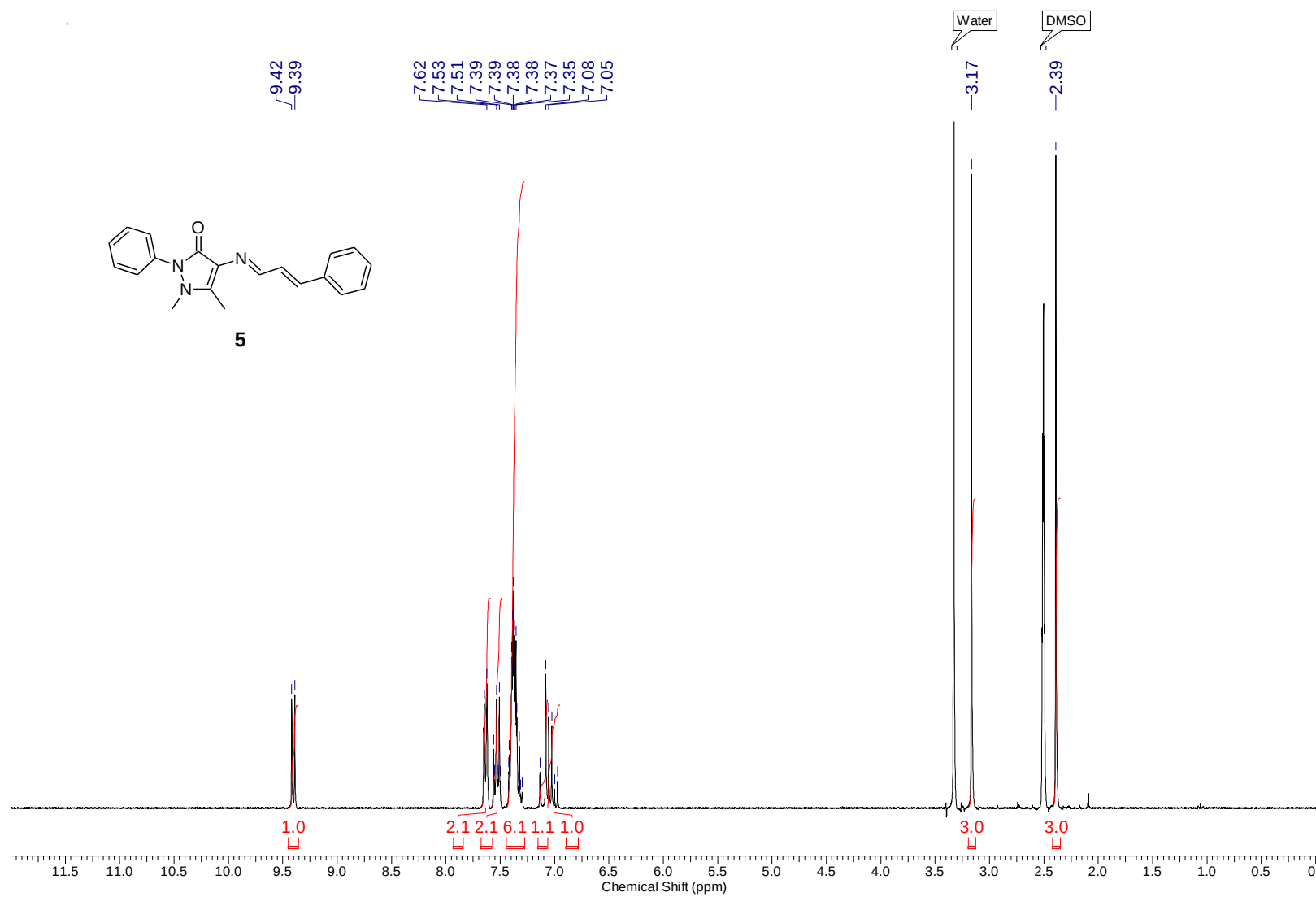
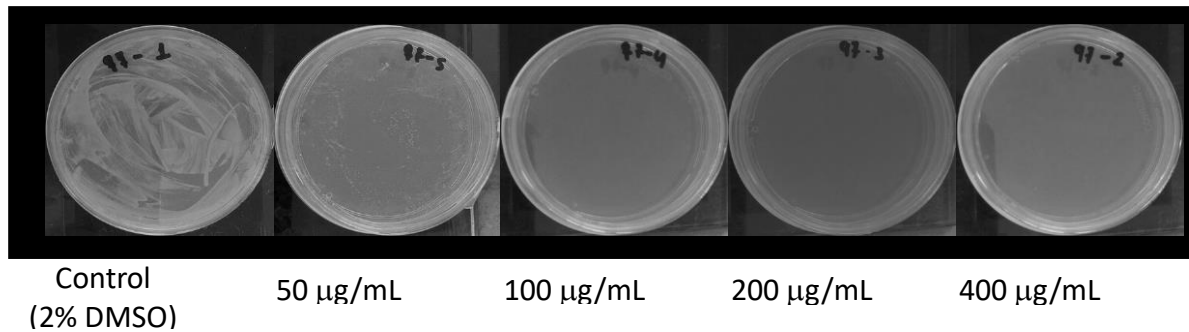


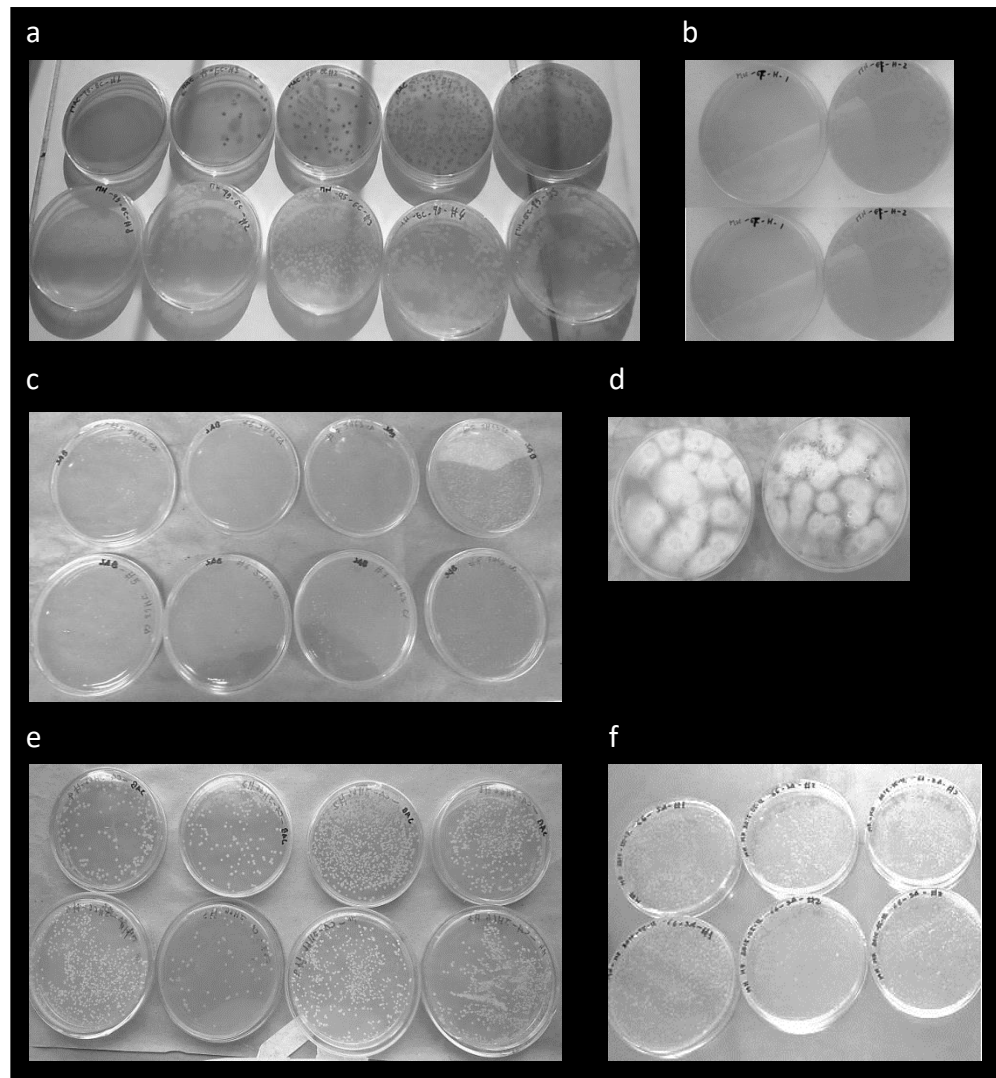
Figure S15. <sup>1</sup>H NMR spectrum of compound 5.

## Supplementary figure S16. Evaluation of –cide/-static effect

### A. Fungicide effect. *S. cerevisiae* (W303) exposed to Schiff base 5



B. Bacteriostatic and fungistatic effect. a. *Escherichia coli* exposed to Schiff base **3d**; b. *Enterococcus faecalis* exposed to Schiff base **3a**; c. *Candida albicans* exposed to Schiff base **3b**; d. *Candida albicans* exposed to Schiff base **3f**; e. *Aspergillus niger* exposed to Schiff base **3f**; f. *Staphylococcus aureus* exposed to Schiff base **3f**.





**Supplemental Table S1. Theoretical prediction of ADME properties<sup>a</sup> of some drug used in chemotherapy.**

| Compound         | MW      | HBA | HBD | nrotb | PSA    | M    | T    | RE   | I    | cLogP | cLogS | DL     | DS   | IARC <sup>b</sup> |
|------------------|---------|-----|-----|-------|--------|------|------|------|------|-------|-------|--------|------|-------------------|
| Cyclophosphamide | 261.09  | 4   | 1   | 4     | 51.38  | high | high | high | none | 0.73  | -1.90 | -10.32 | 0.10 | 1                 |
| Methotrexate     | 454.45  | 13  | 5   | 9     | 210.54 | none | high | none | none | -1.23 | -3.77 | -7.59  | 0.22 | 3                 |
| Fluorouracil     | 130.08  | 4   | 2   | 0     | 58.20  | high | high | high | high | -0.84 | -1.77 | -4.50  | 0.06 | 3                 |
| Doxorubicin      | 543.52  | 12  | 6   | 5     | 206.07 | none | none | none | high | 0.17  | -4.51 | 6.65   | 0.33 | NR                |
| Procarbazine     | 221.3   | 4   | 3   | 5     | 53.16  | high | high | high | none | 0.24  | -2.41 | 3.86   | 0.20 | 2A                |
| Prednisolone     | 360.45  | 5   | 3   | 2     | 94.83  | none | none | none | none | 1.14  | -2.96 | 4.10   | 0.85 | NR                |
| Bleomycin        | 1415.57 | 38  | 20  | 36    | 683.55 | none | none | none | none | -9.96 | -2.70 | 5.30   | 0.48 | 2B                |
| Etoposide        | 588.56  | 13  | 3   | 5     | 160.83 | none | none | none | none | 0.67  | -3.95 | -1.98  | 0.30 | 1                 |
| Cisplatin        | 300.05  | 2   | 2   | 0     | 55.28  | none | none | none | none | 0.00  | -1.93 | -3.18  | 0.49 | 2A                |
| Epirubicin       | 543.52  | 12  | 6   | 5     | 206.07 | none | none | none | high | 0.17  | -4.51 | 6.65   | 0.33 | NR                |
| Capecitabine     | 359.35  | 9   | 3   | 6     | 120.69 | high | none | low  | low  | 0.47  | -3.37 | -21.33 | 0.16 | NR                |
| Folinic acid     | 473.44  | 14  | 7   | 9     | 215.55 | none | none | none | none | -2.21 | -4.08 | -6.77  | 0.34 | NR                |
| Temozolomide     | 194.15  | 8   | 1   | 1     | 105.94 | high | high | high | none | -0.50 | -1.90 | -1.80  | 0.12 | NR                |
| Anastrozole      | 293.37  | 5   | 0   | 4     | 78.29  | none | high | low  | none | 2.61  | -4.17 | -4.16  | 0.19 | NR                |

<sup>a</sup> MW: molecular weight; HBA: number of hydrogen bond acceptor; HBD: number of hydrogen bond donor; nrotb: number of rotatable bonds; PSA: polar surface area; M: mutagenicity; T: tumorigenicity; RE: reproductive effect; I: irritant effect; cLogP: logarithm of compound partition coefficient between n-octanol and water; cLogS: logarithm of compound aqueous solubility; DL: drug-likeness; DS: drug score. VR: voriconazole; CP: ciprofloxacin.

<sup>b</sup> Group of classification of IARC; NR = no reported.