

## **Supplementary Material**

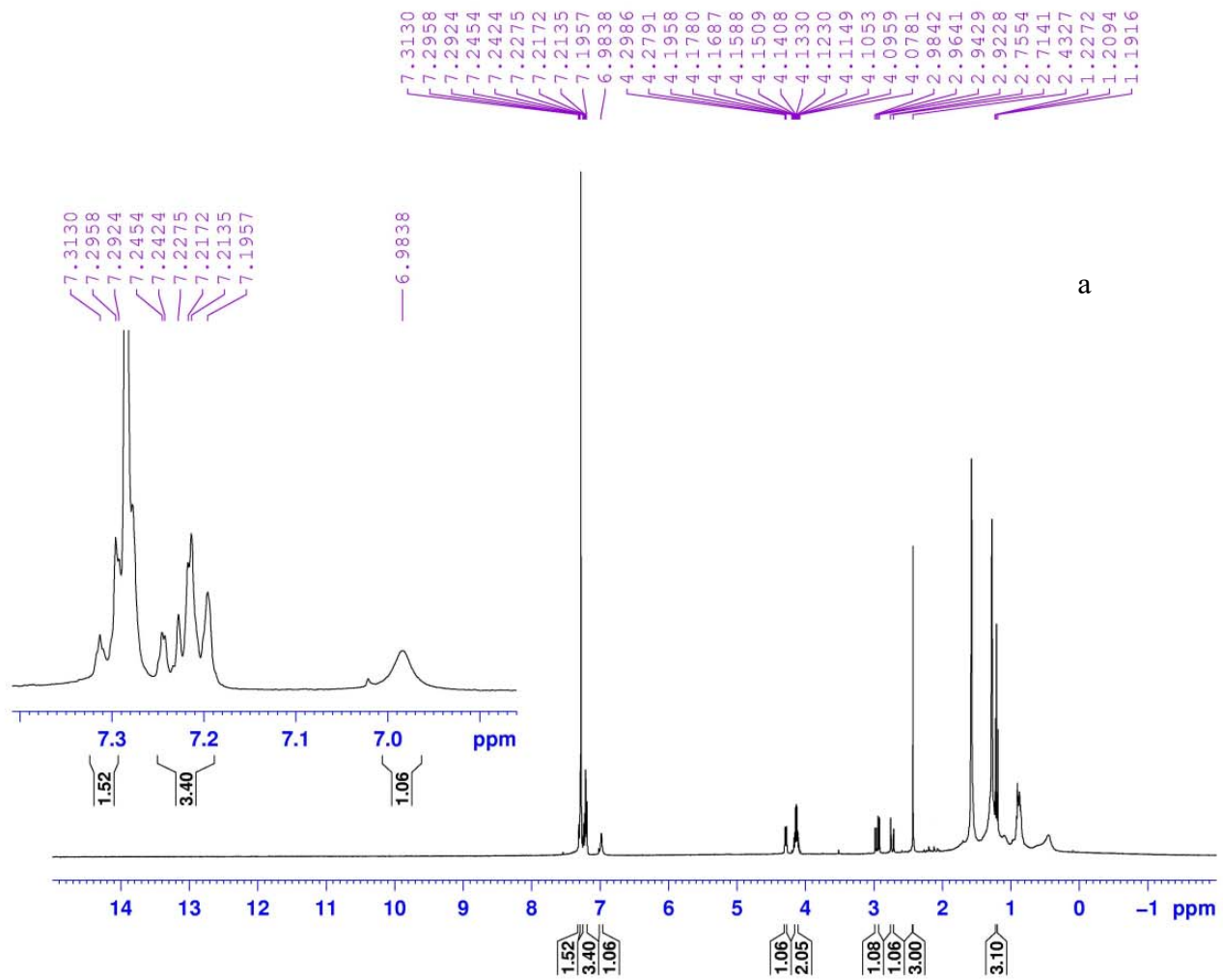
### **NMR and DFT Studies of 2-Oxo-1,2,3,4-tetrahydropyridines:**

### **Solvent and Temperature Effects**

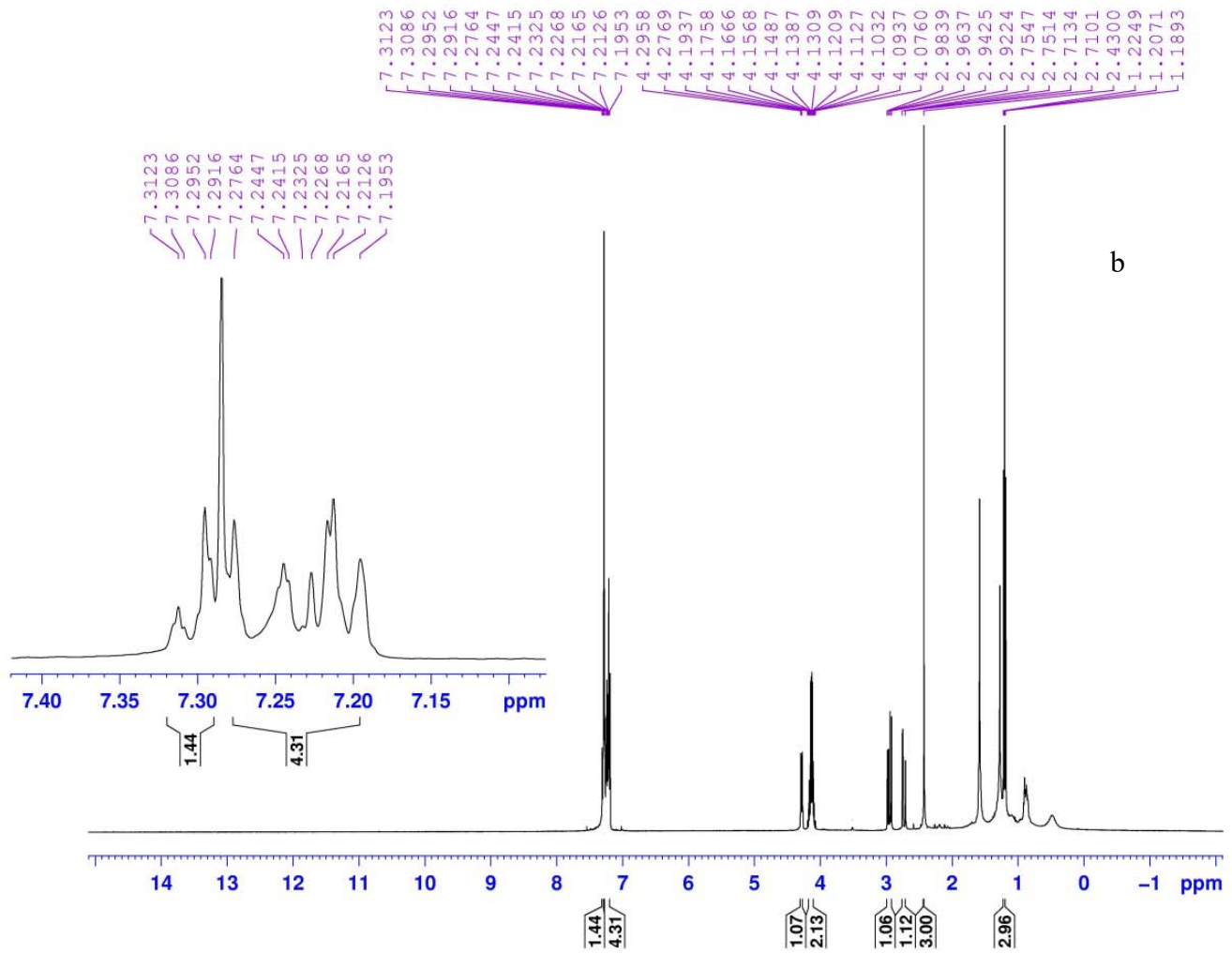
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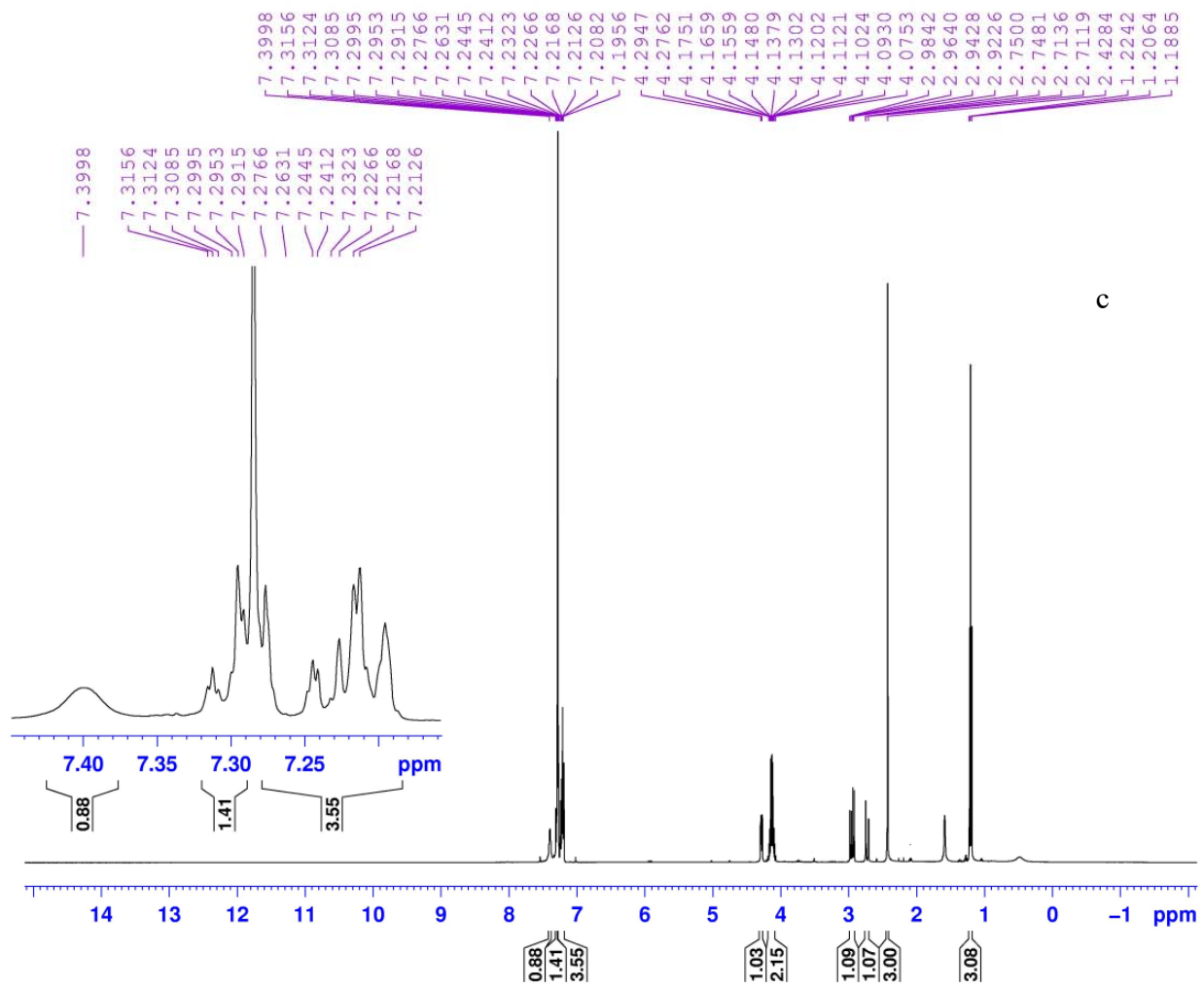
\*Email: [memarian@sci.ui.ac.ir](mailto:memarian@sci.ui.ac.ir), [sabzyan@sci.ui.ac.ir](mailto:sabzyan@sci.ui.ac.ir)

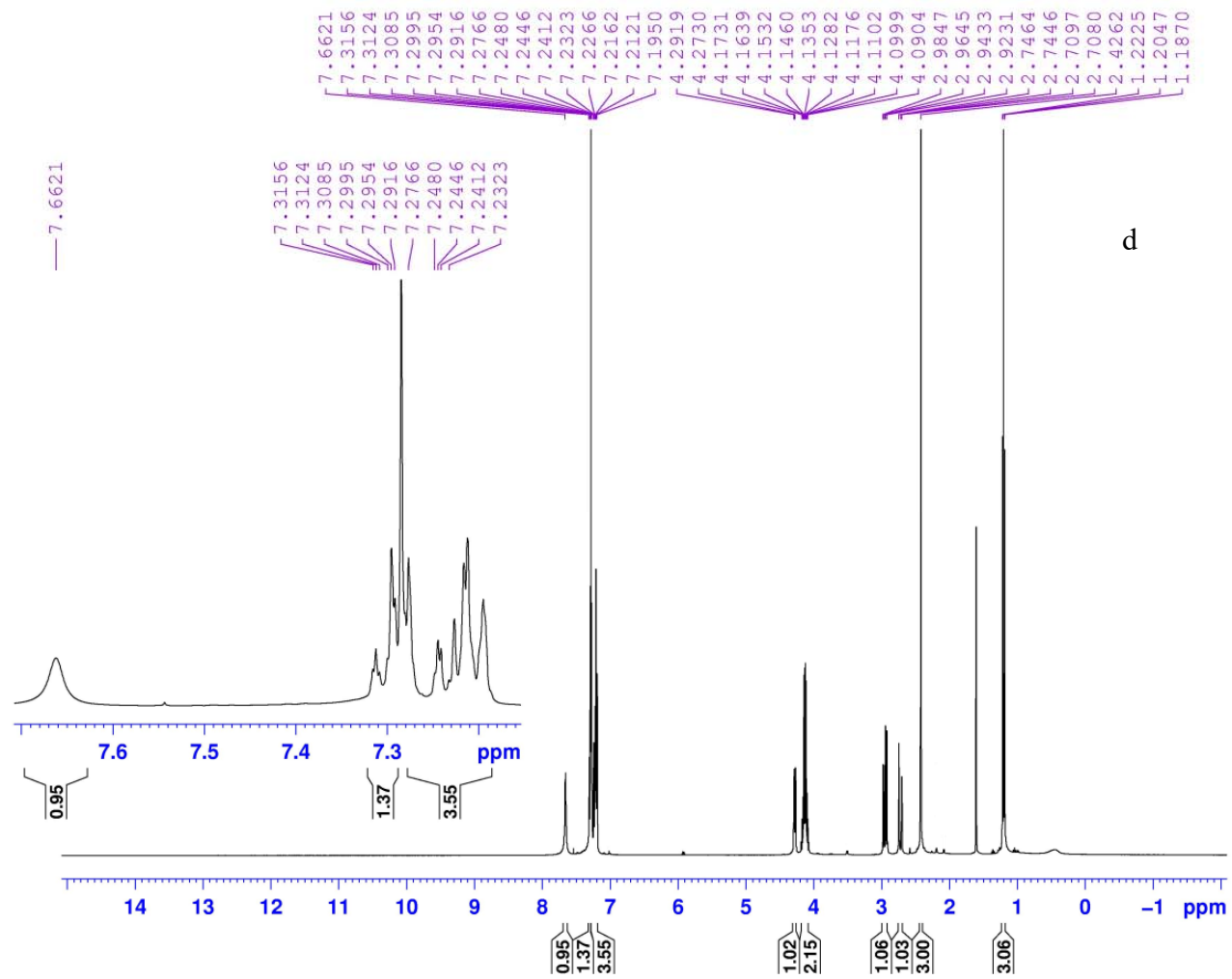


a



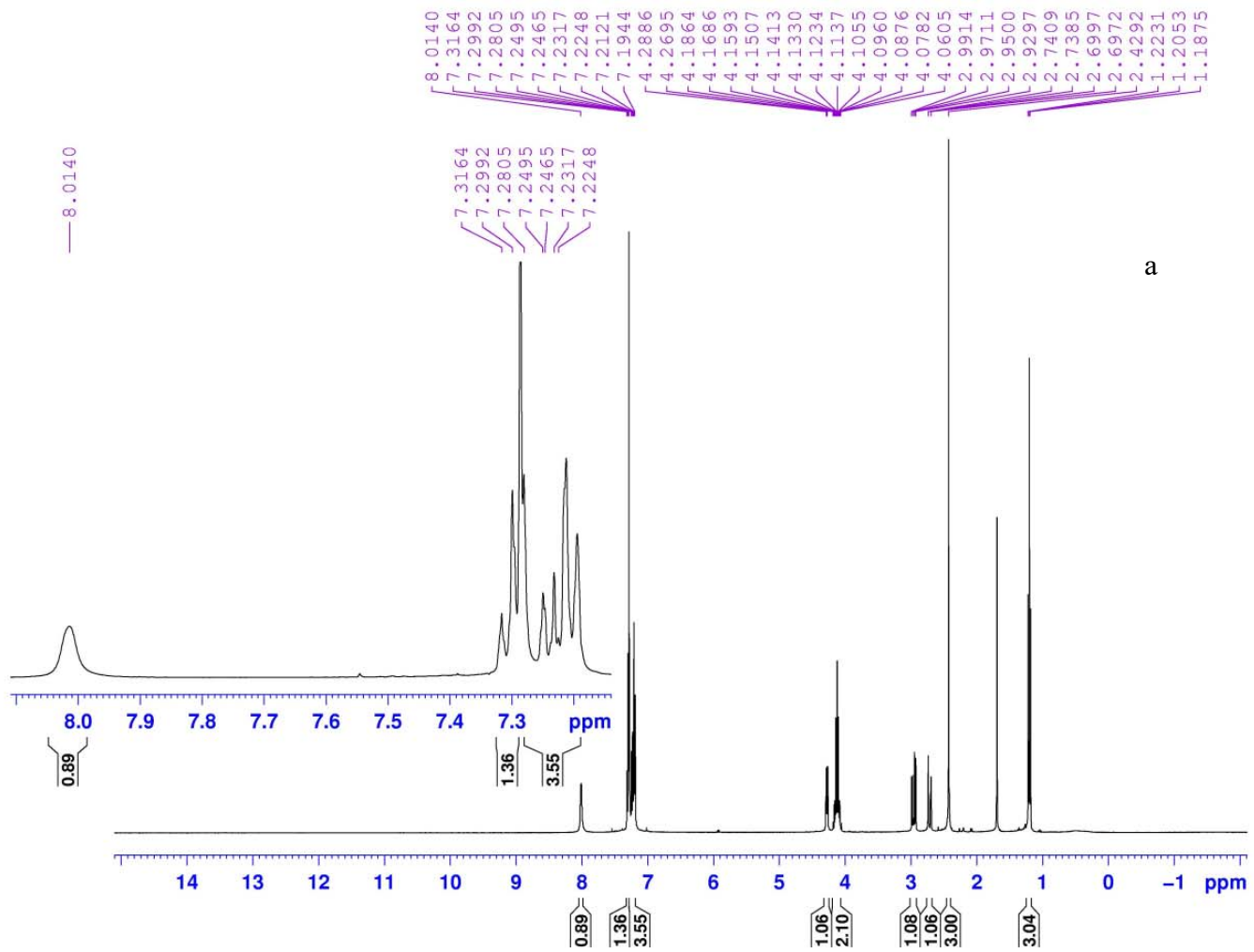
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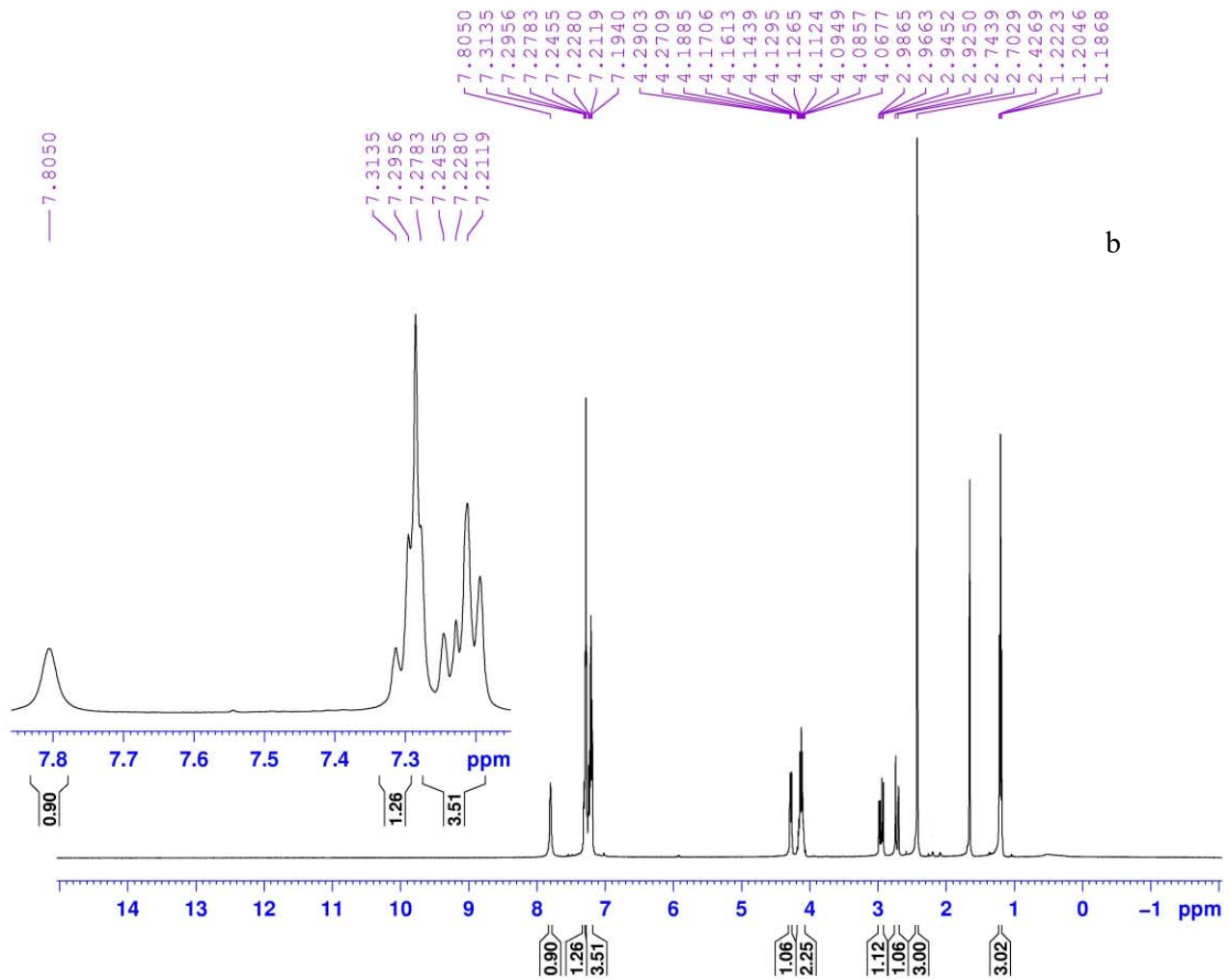


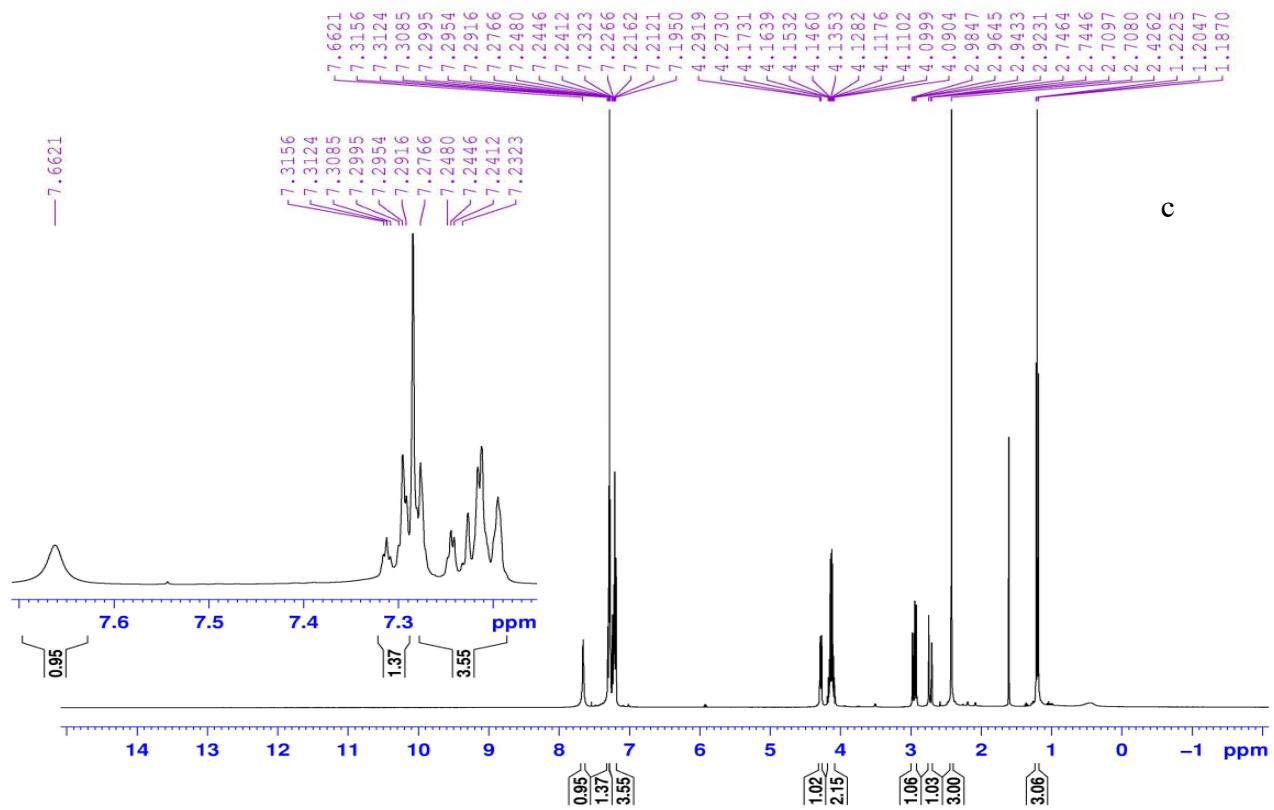


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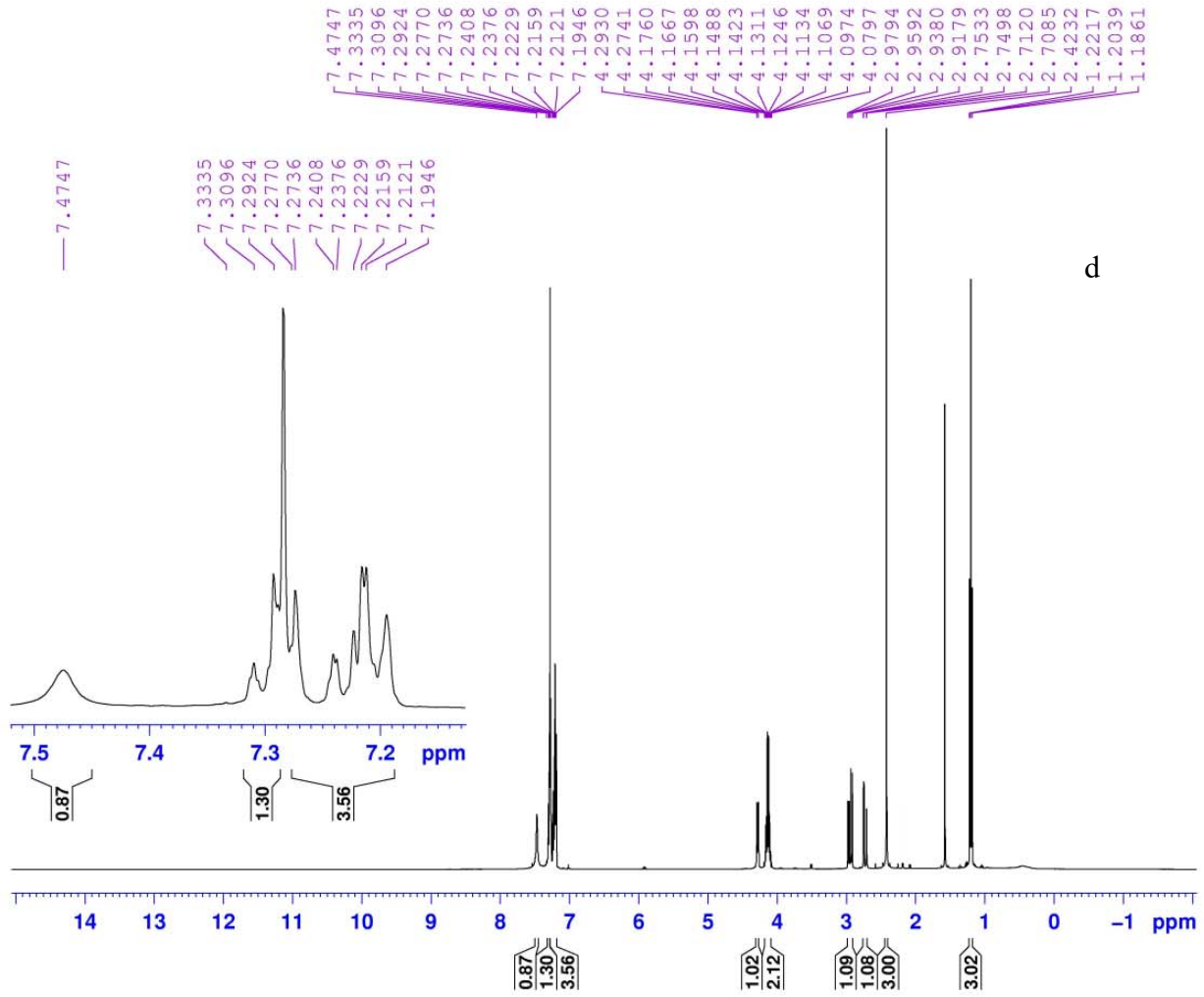
**Figure S1.**  $^1\text{H}$  NMR spectra of **1a** dissolved in  $\text{CDCl}_3$  at concentration of 0.002 M (a), 0.01 M (b), 0.02 M (c) and 0.03 M (d).



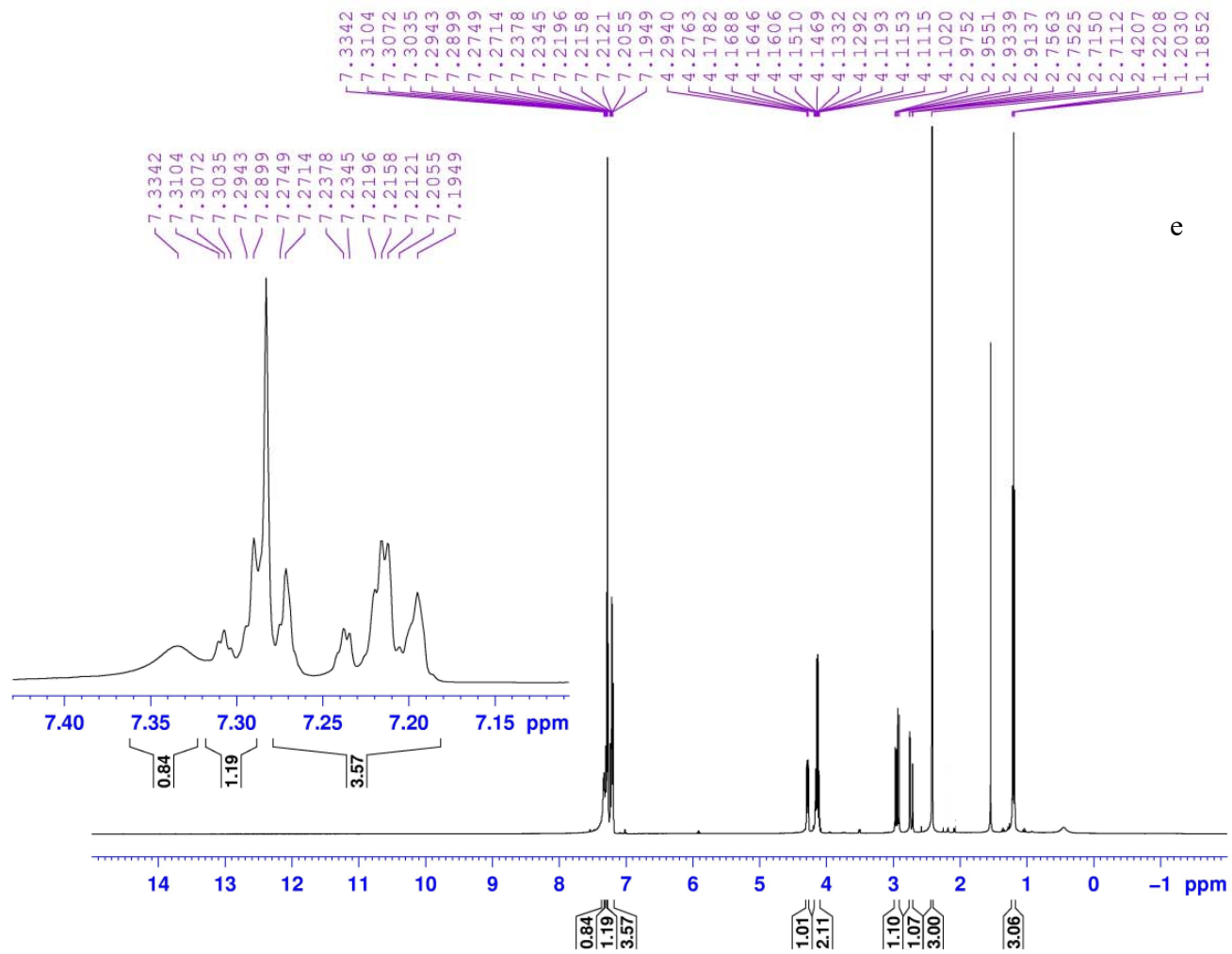




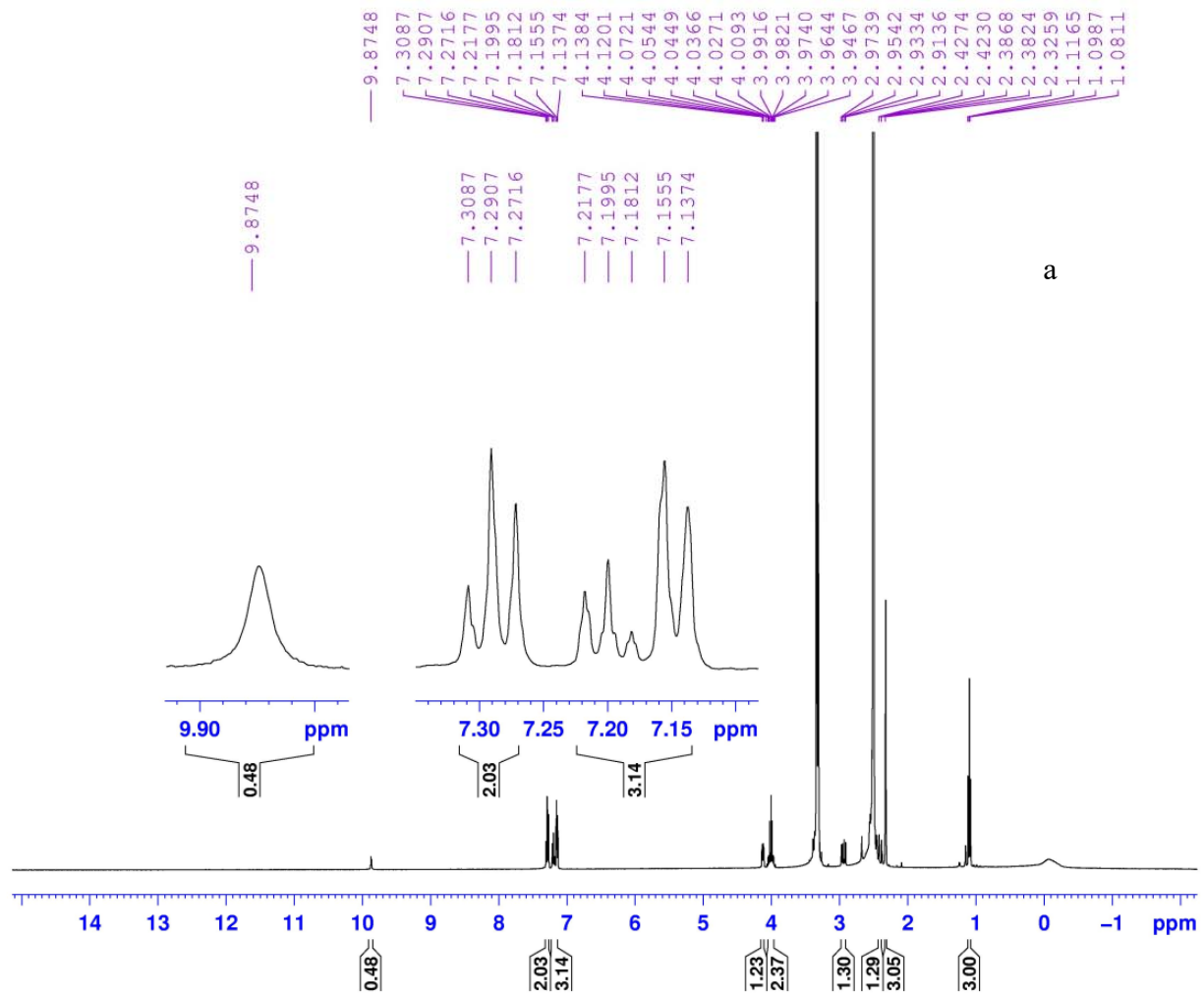


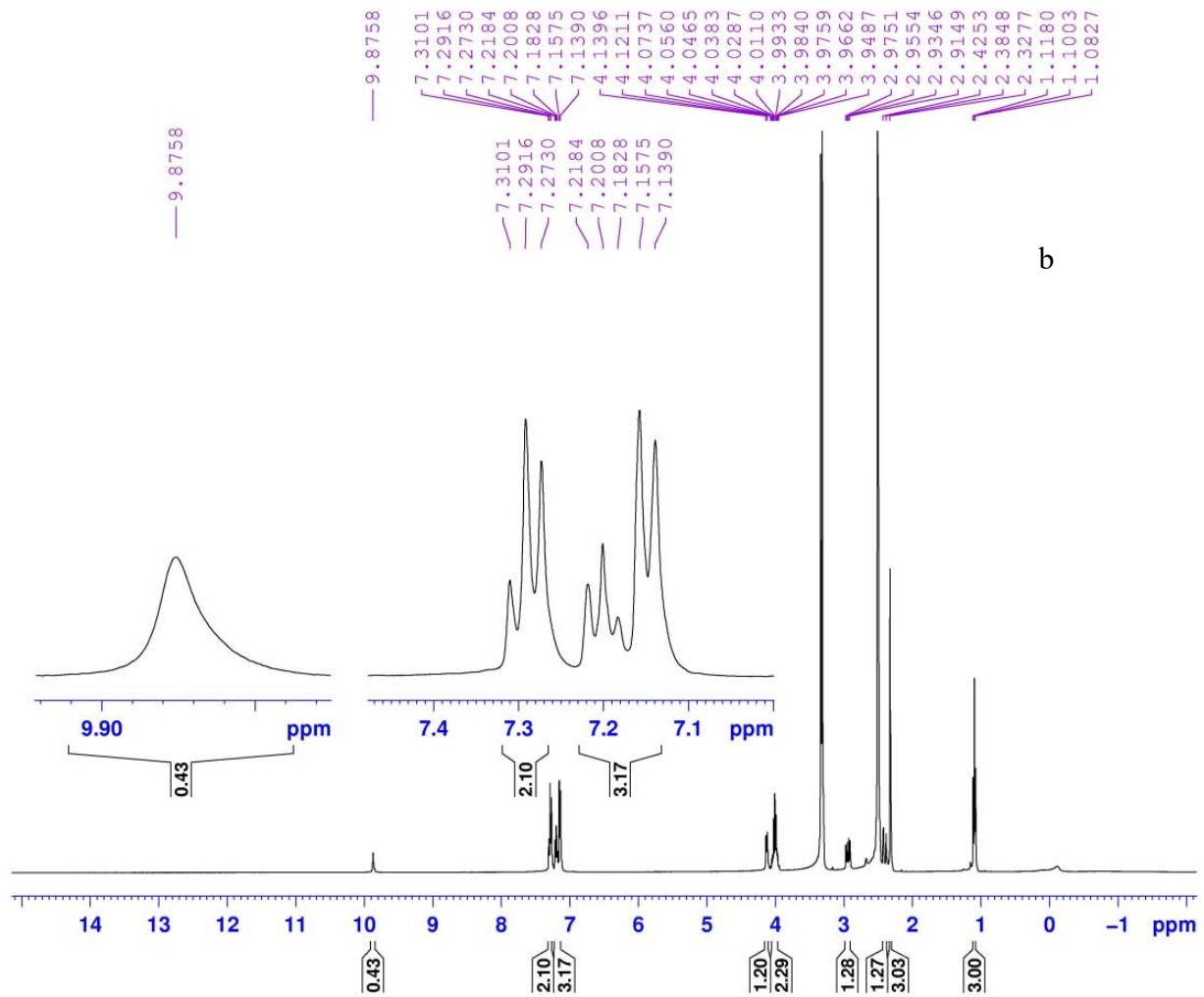


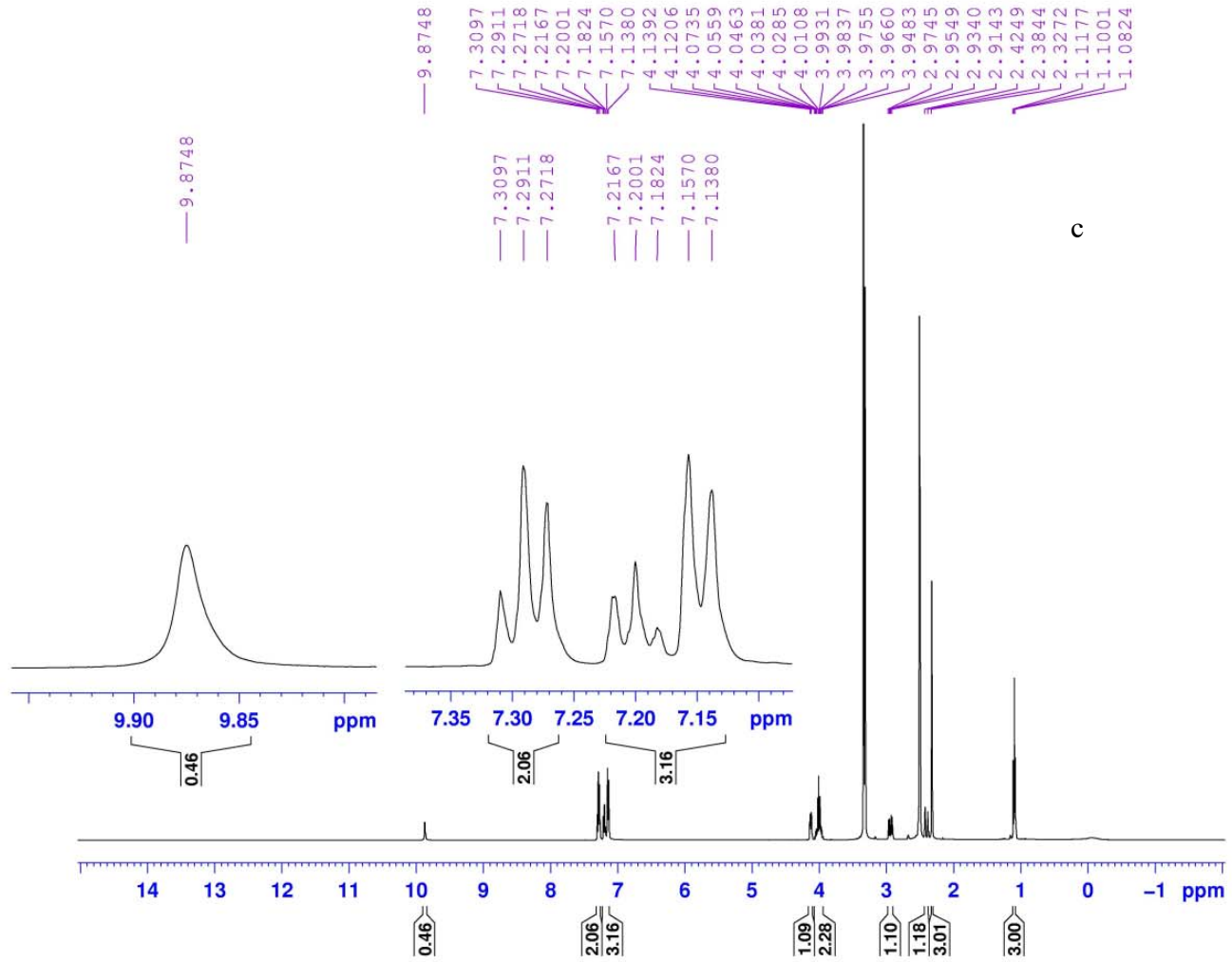
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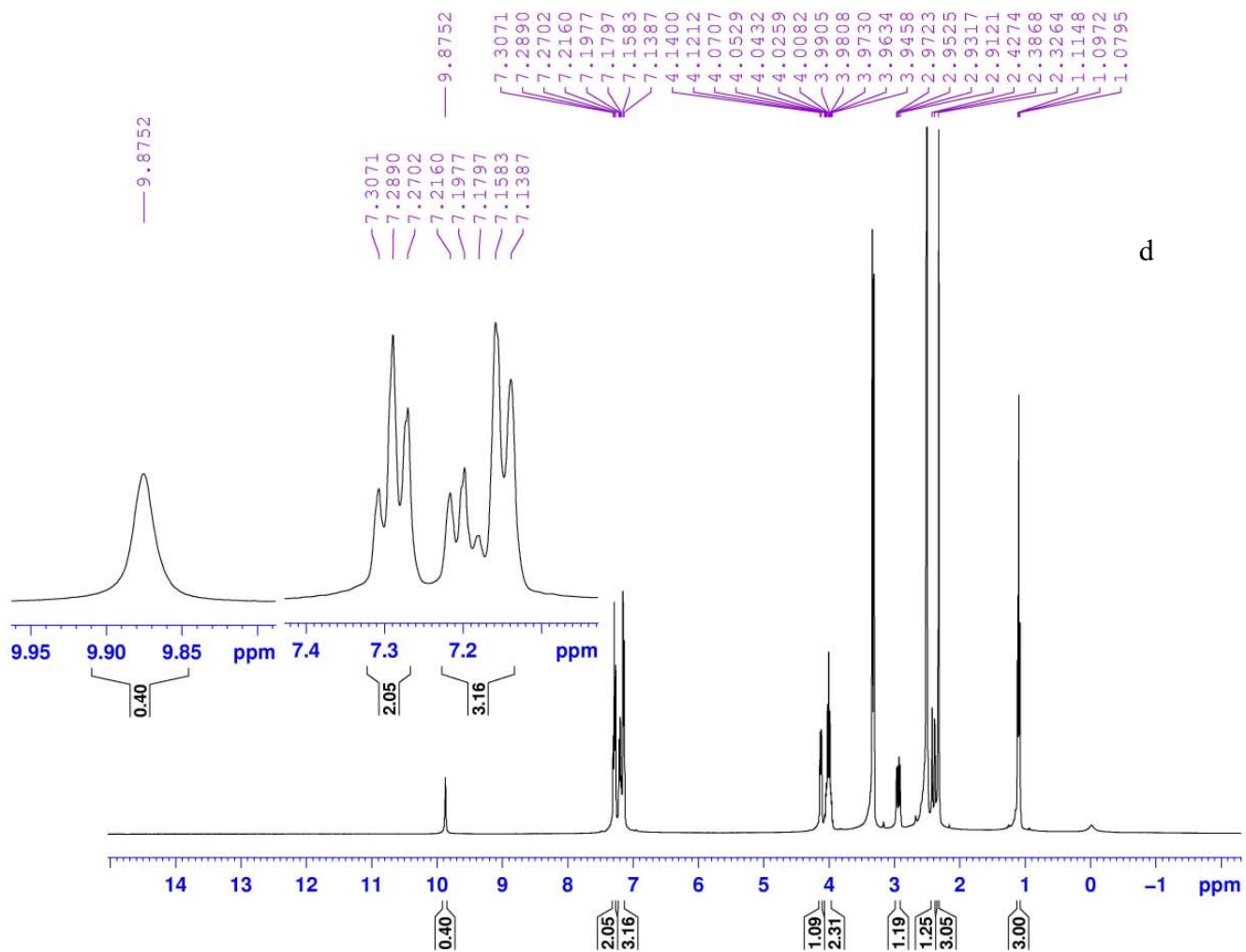


**Figure S2.**  $^1\text{H}$  NMR spectra of 0.03 M solutions of **1a** in  $\text{CDCl}_3$  at 278 K (a), 288 K (b), 298 K (c), 308 K (d) and 318 K (e).



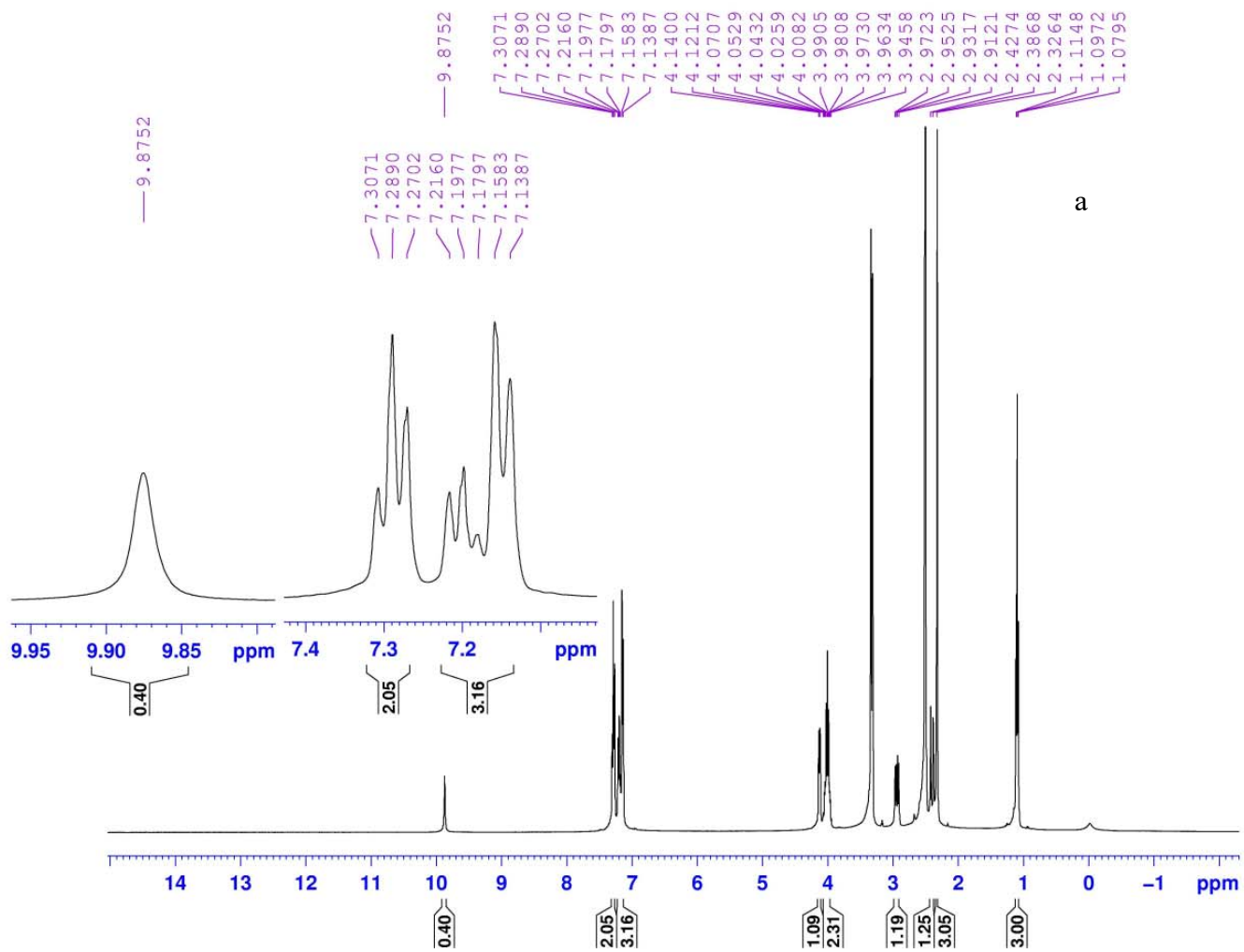




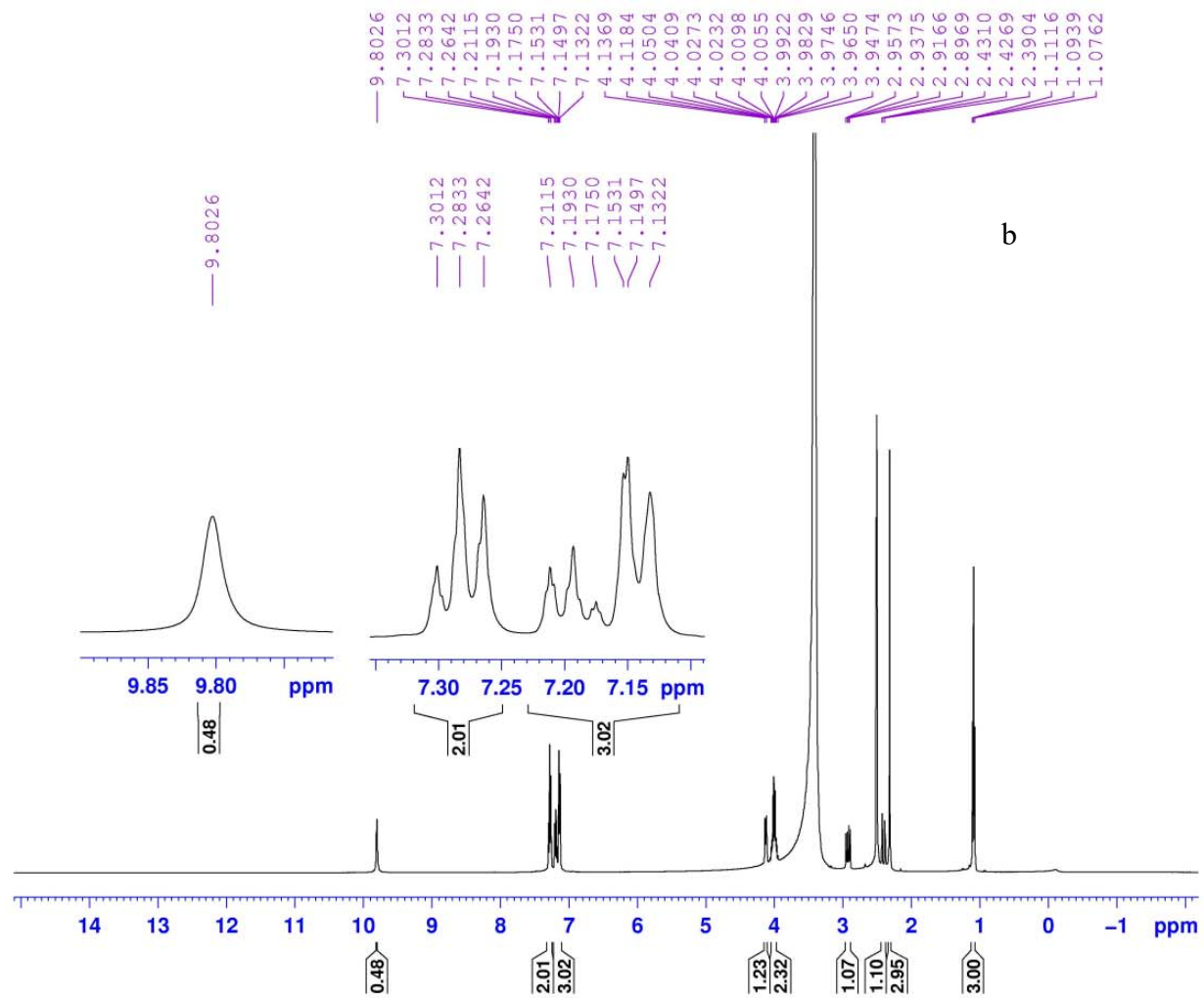


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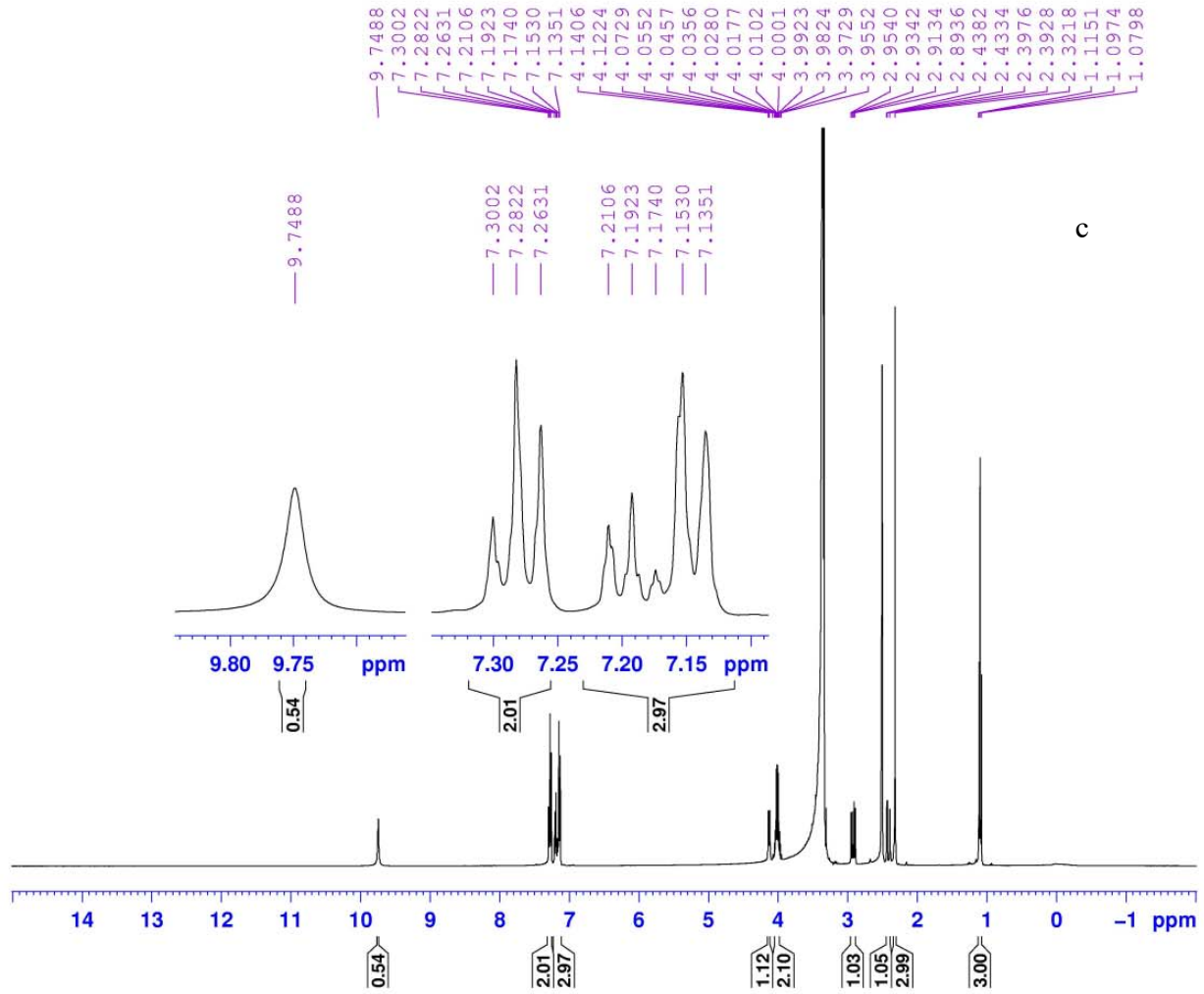
**Figure S3.**  $^1\text{H}$  NMR spectra of **1a** dissolved in DMSO- $d_6$  at concentration of 0.002 M (a), 0.01 M (b), 0.02 M (c) and 0.03 M (d).

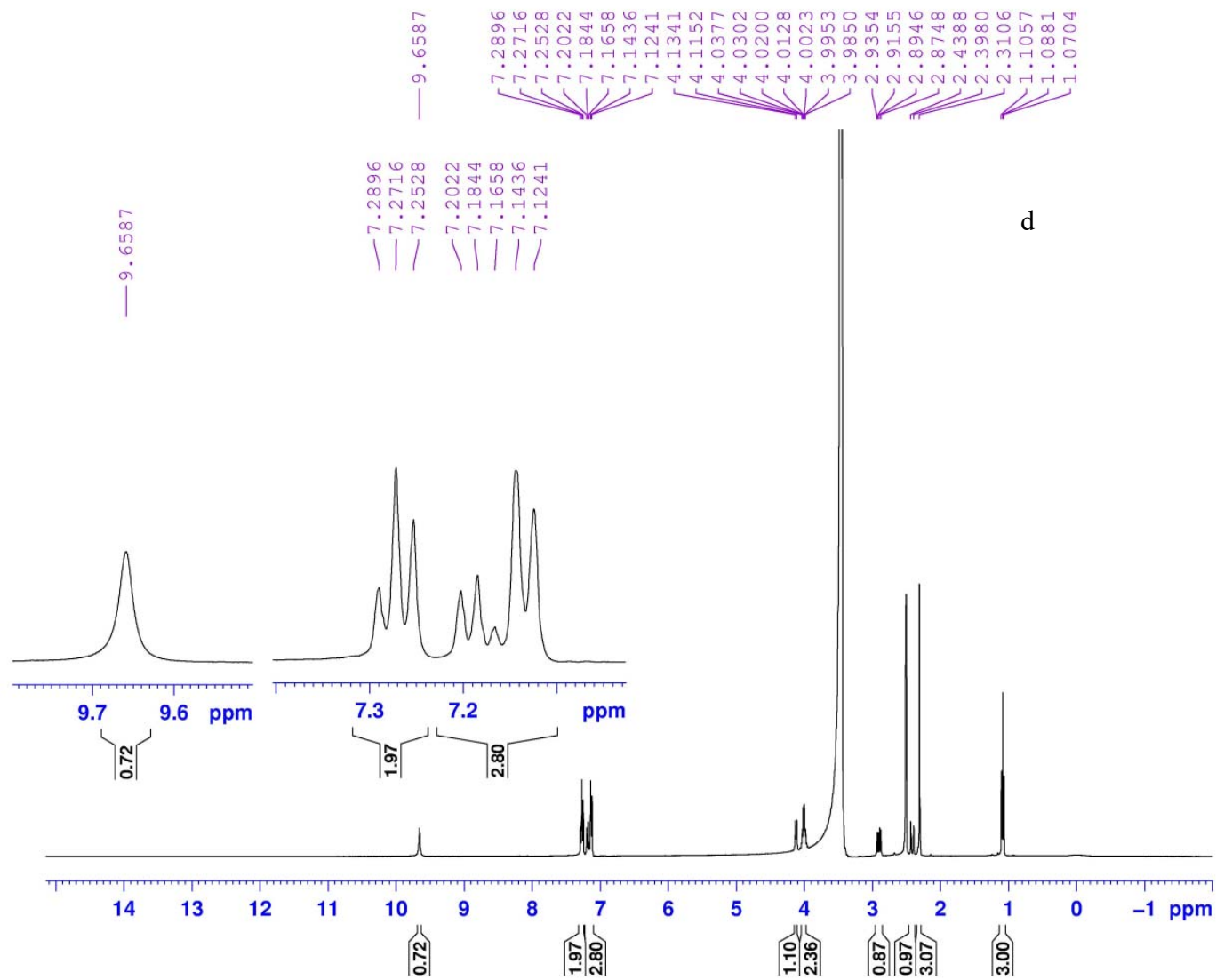


a

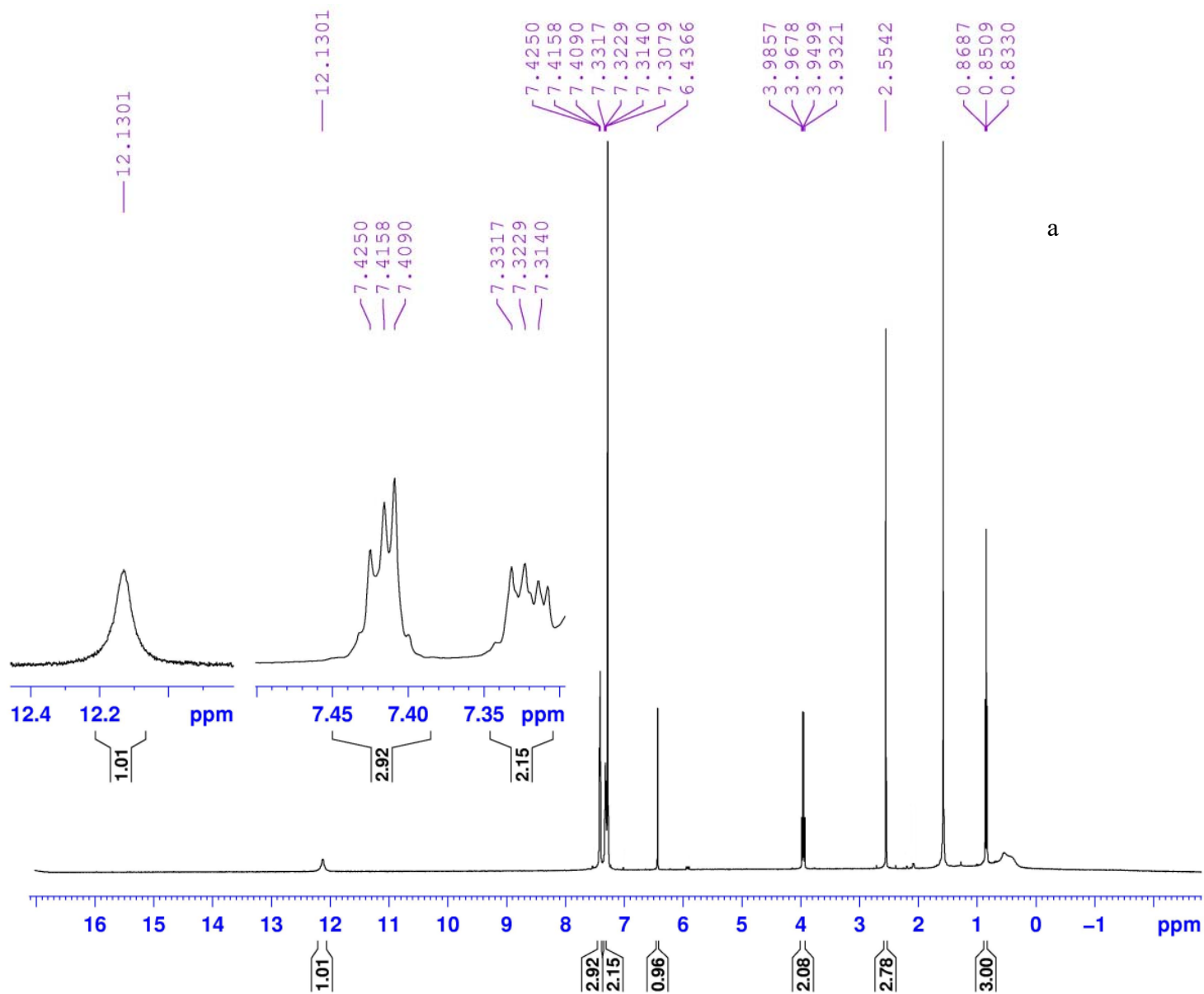


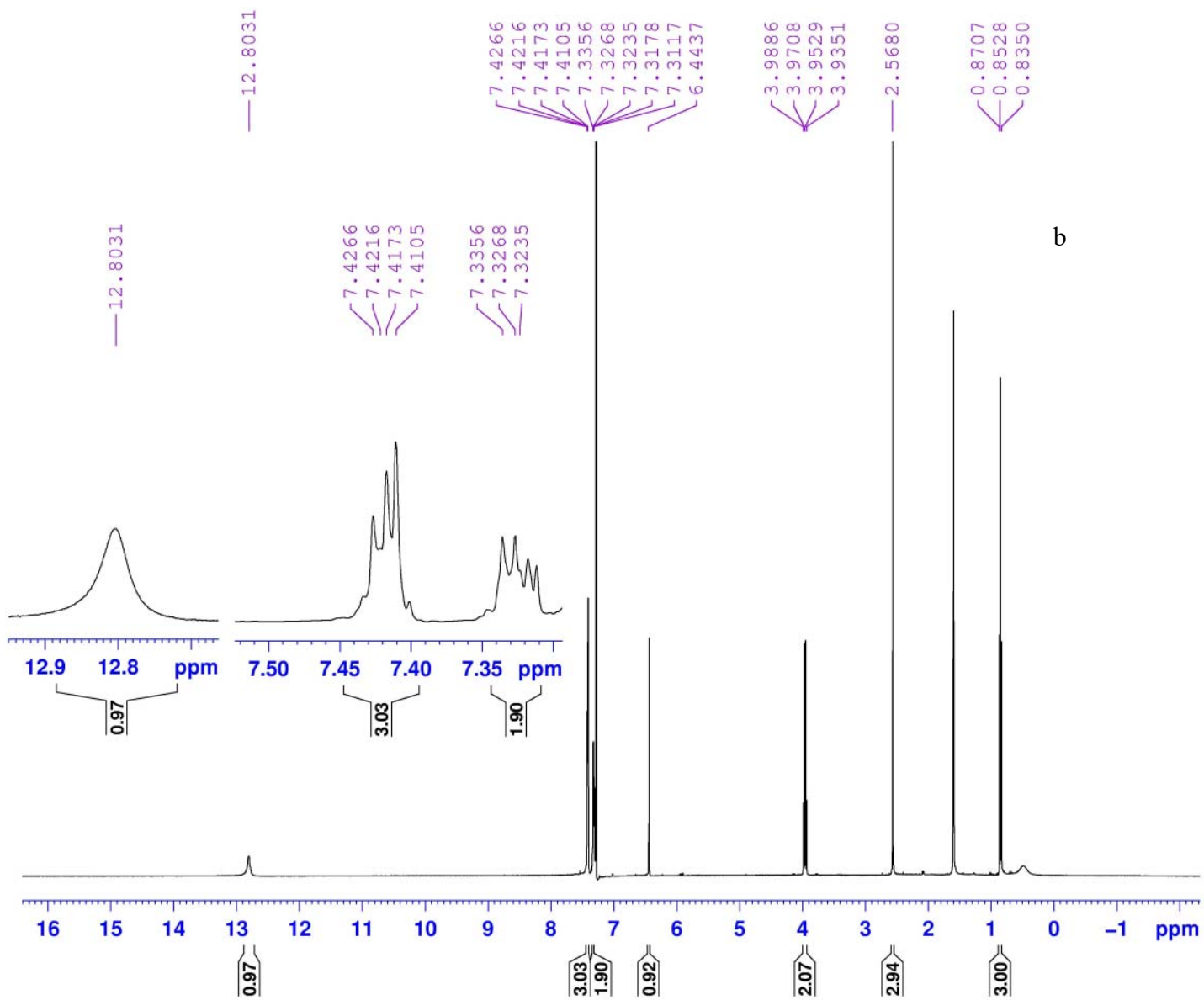




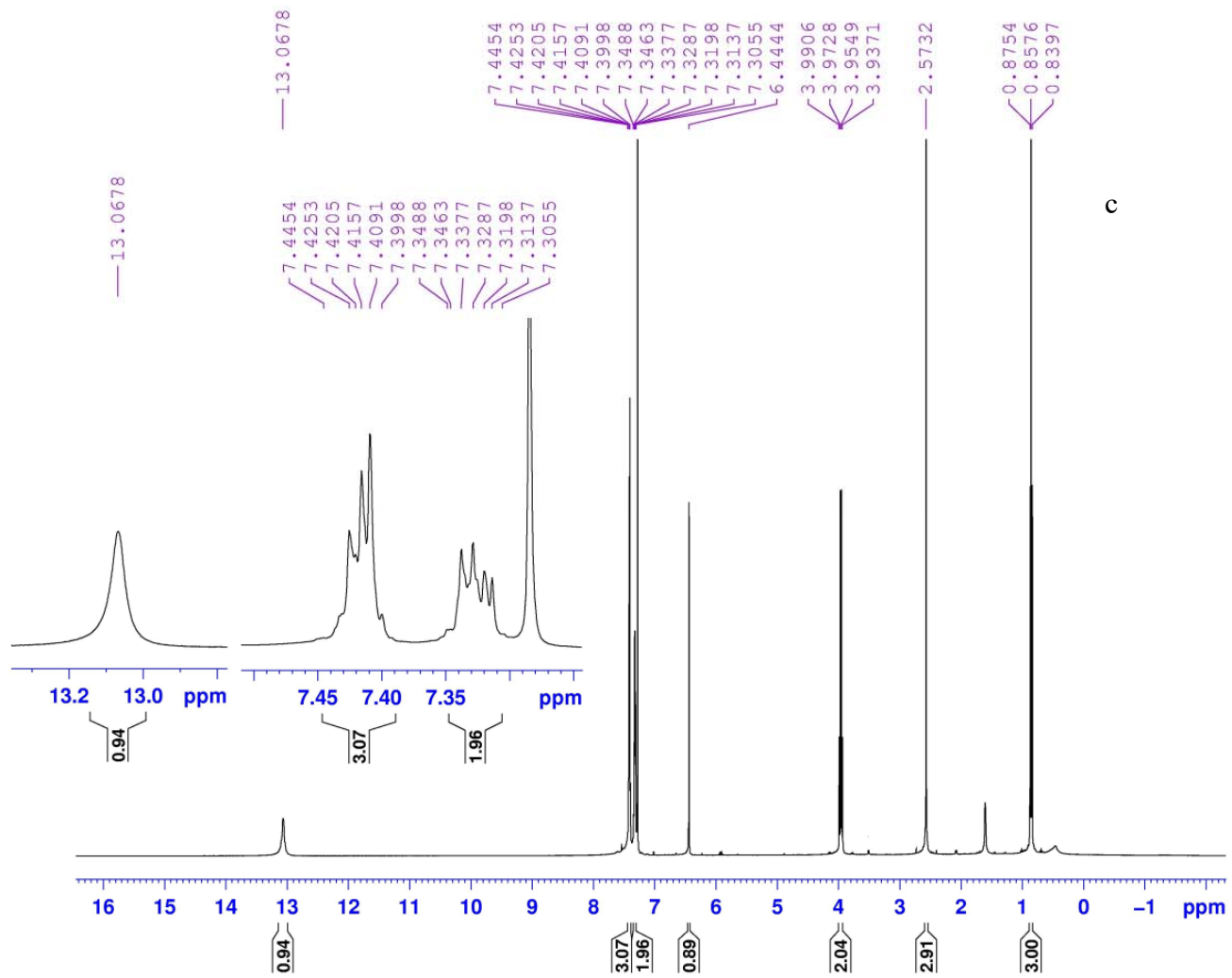


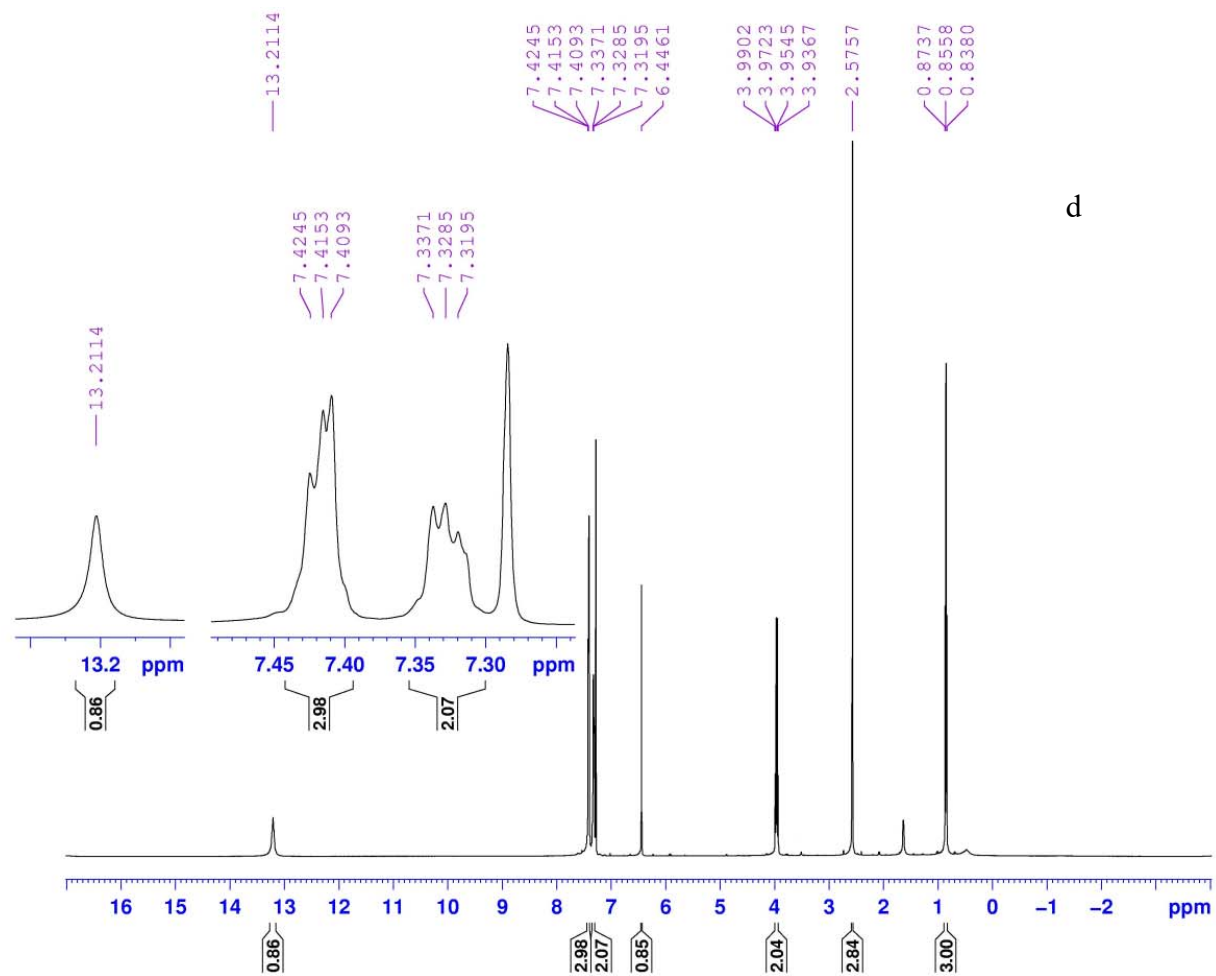
**Figure S4.**  $^1\text{H}$  NMR spectra of 0.03 M solutions of **1a** in DMSO- $d_6$  at 298 K (a), 308 K (b), 318 K (c) and 328 K (d).





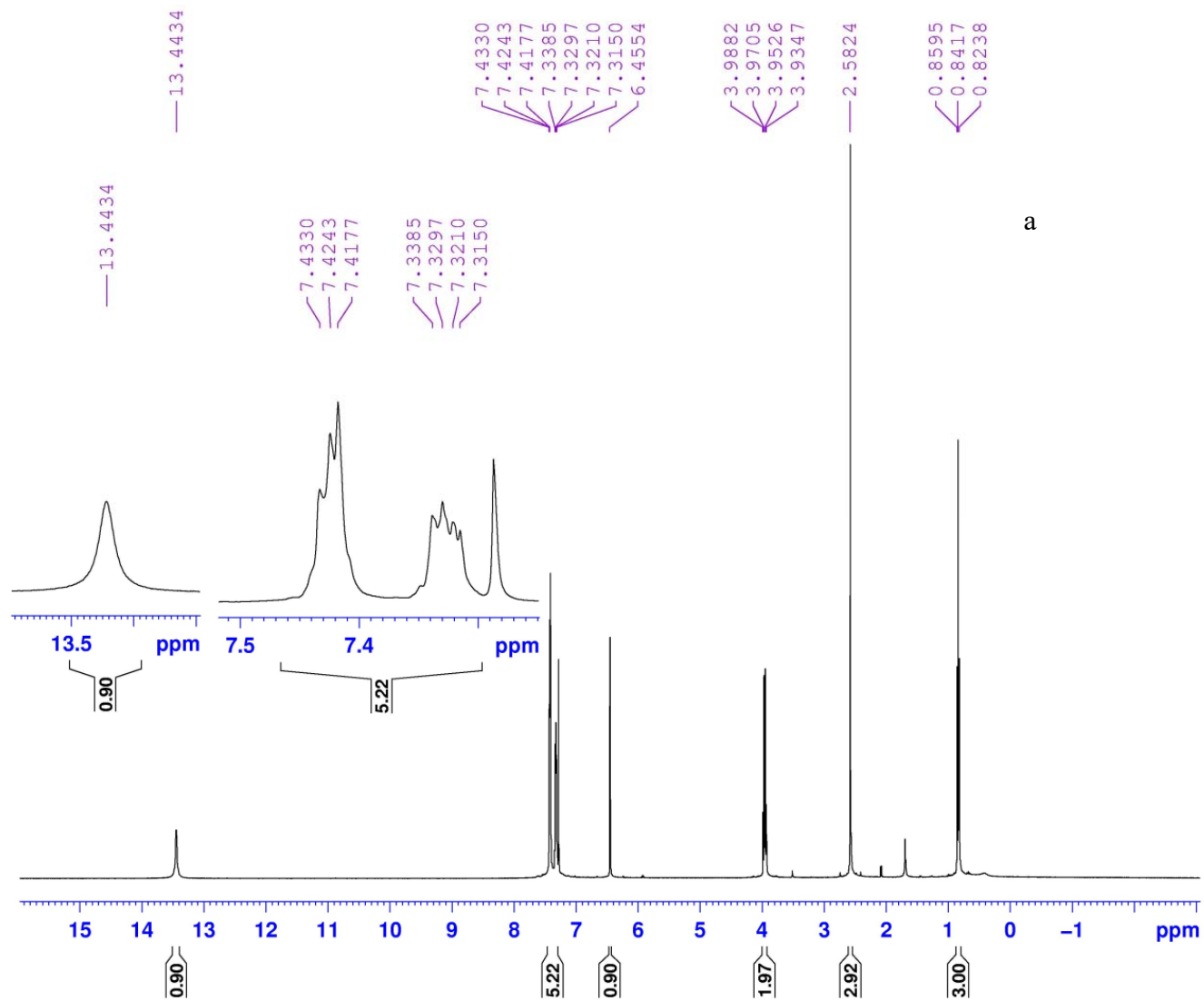
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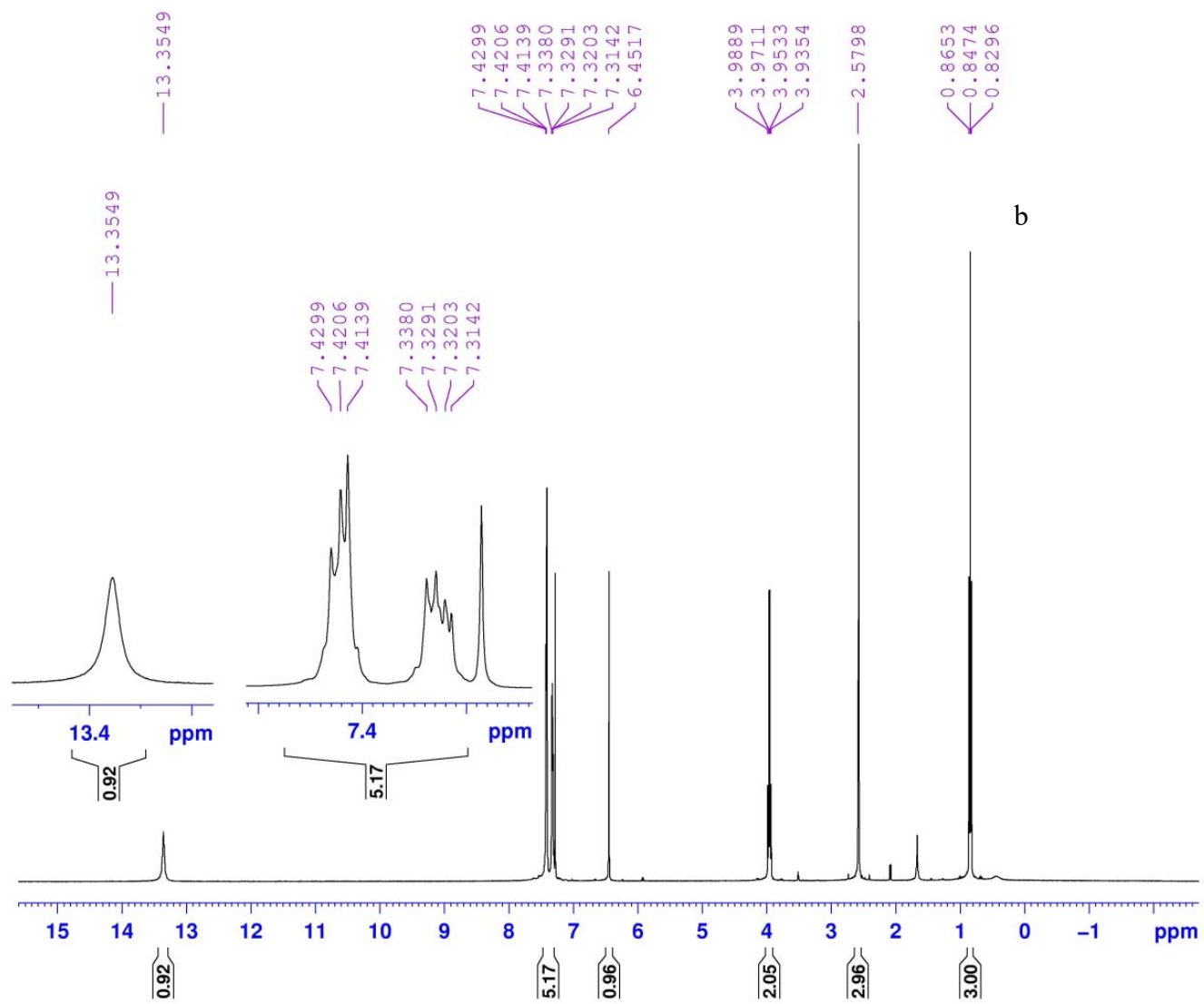




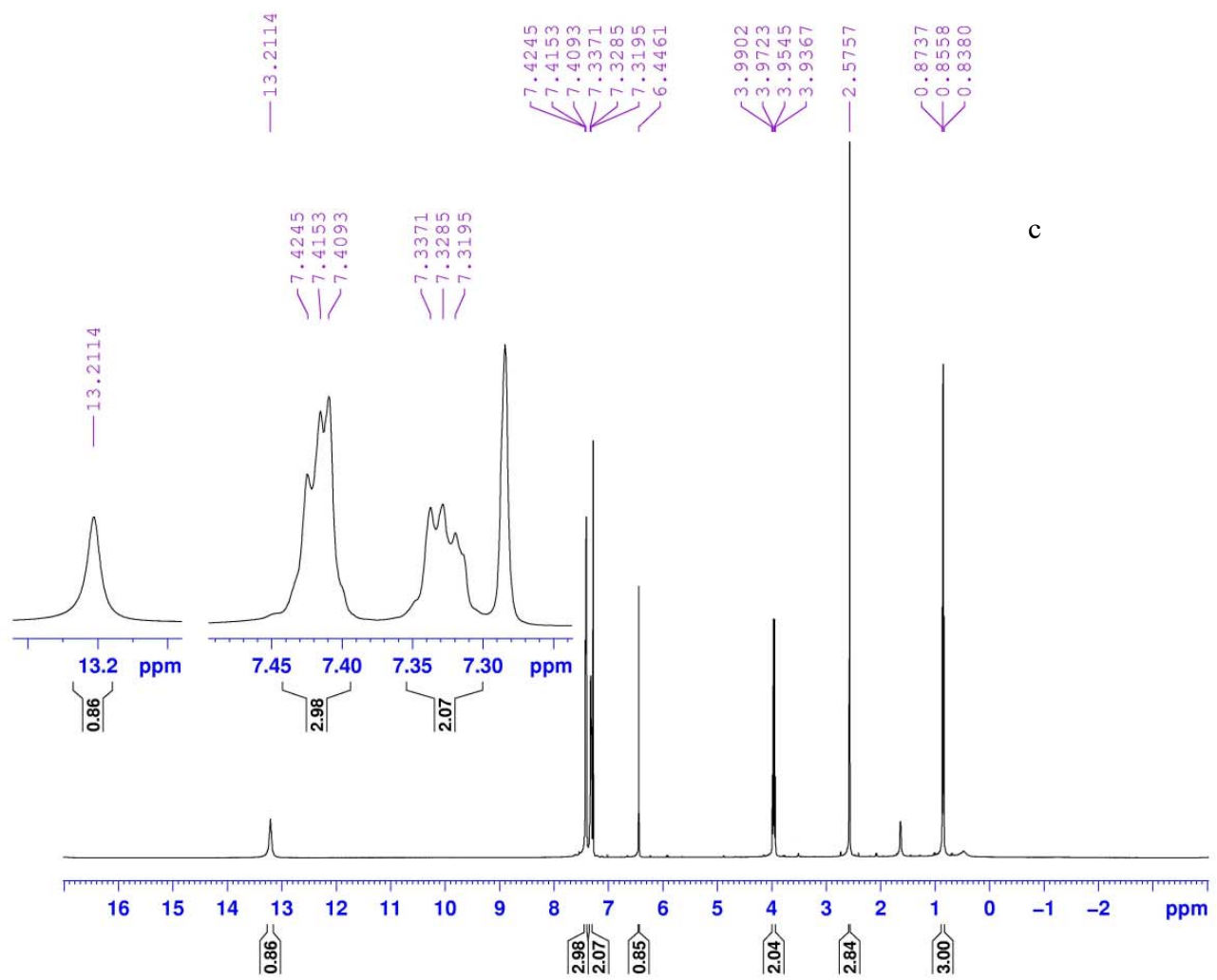
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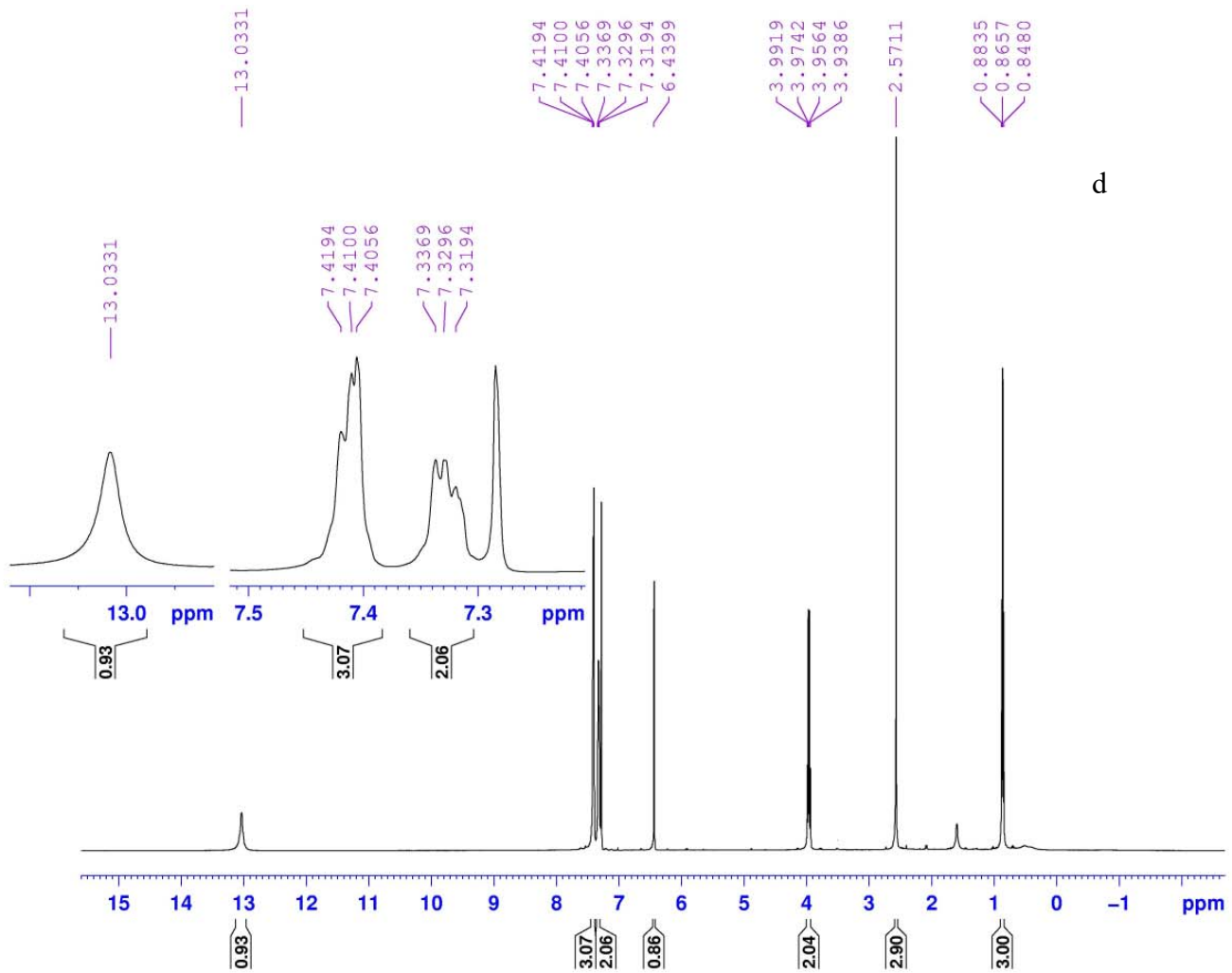
**Figure S5.**  $^1\text{H}$  NMR spectra of **2a** dissolved in  $\text{CDCl}_3$  at concentration of 0.002 M (a), 0.01 M (b), 0.02 M (c) and 0.03 M (d).



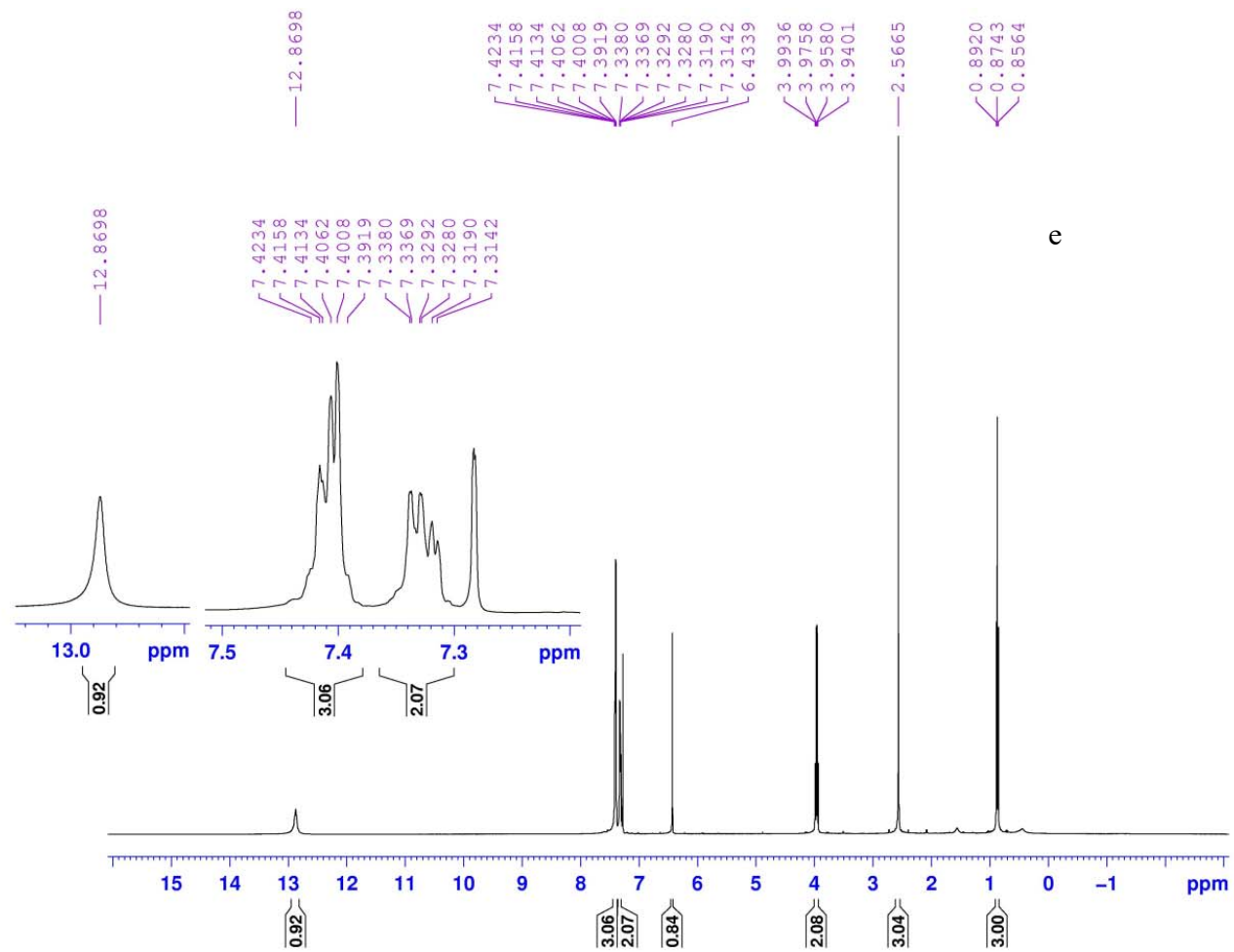




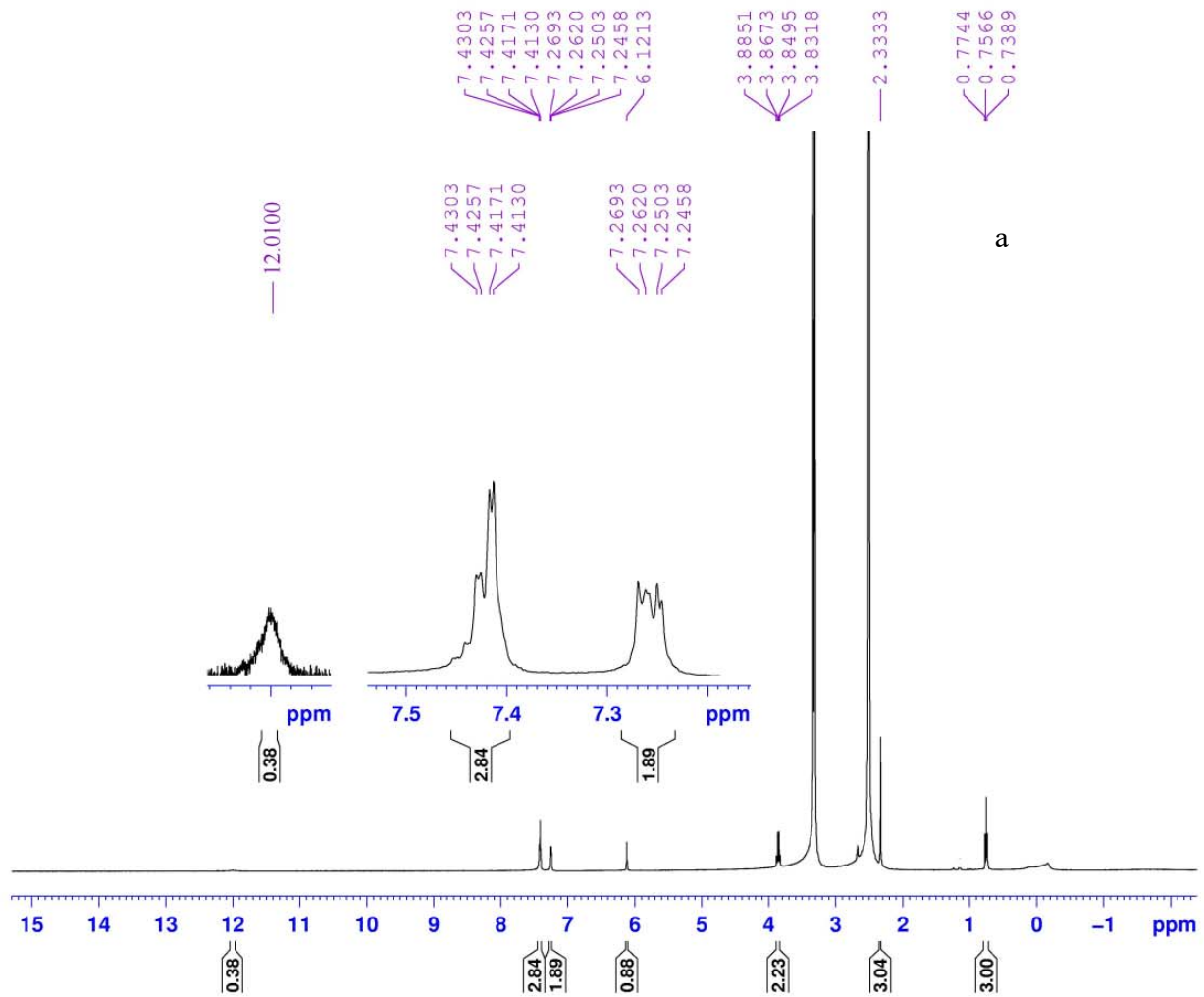


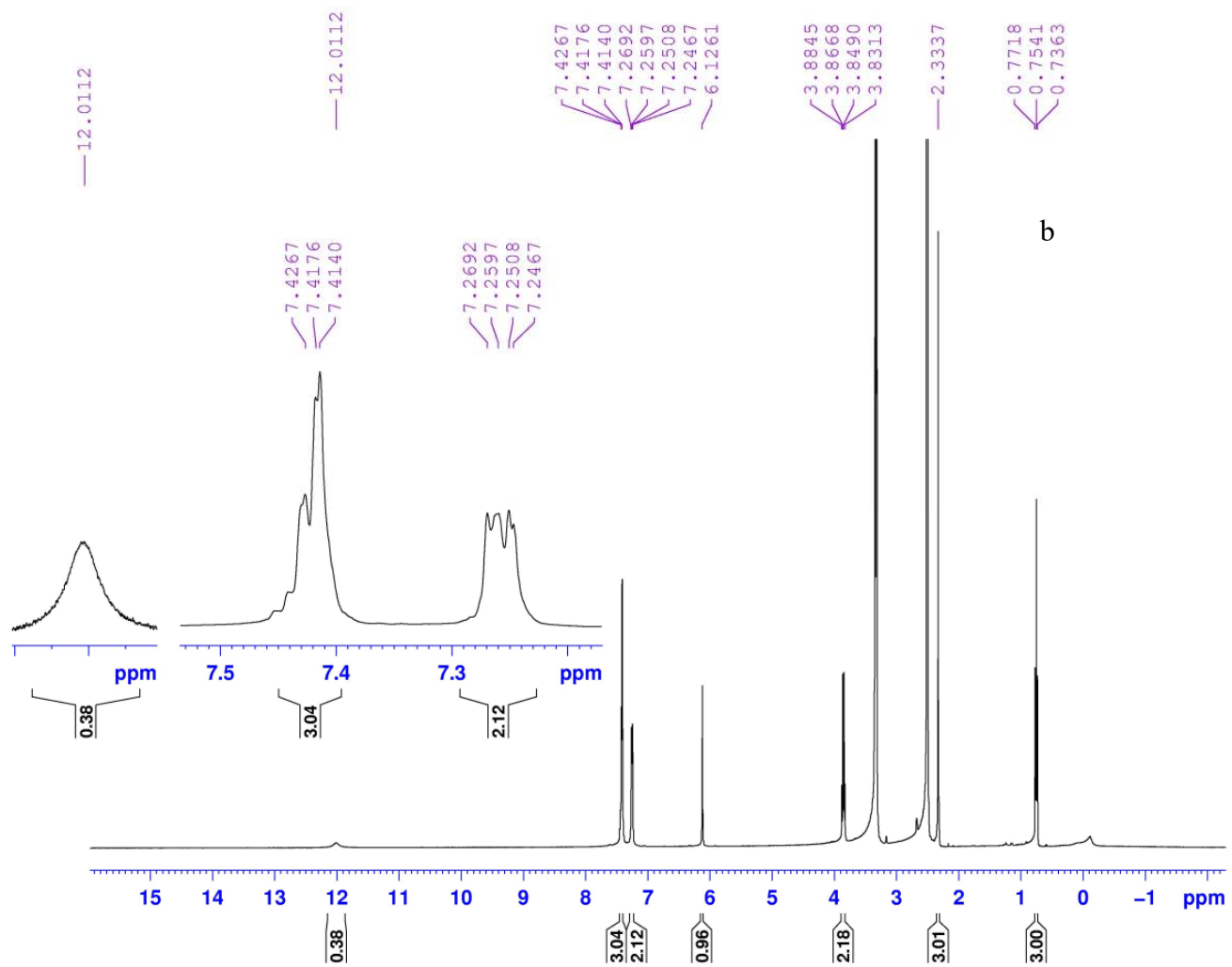


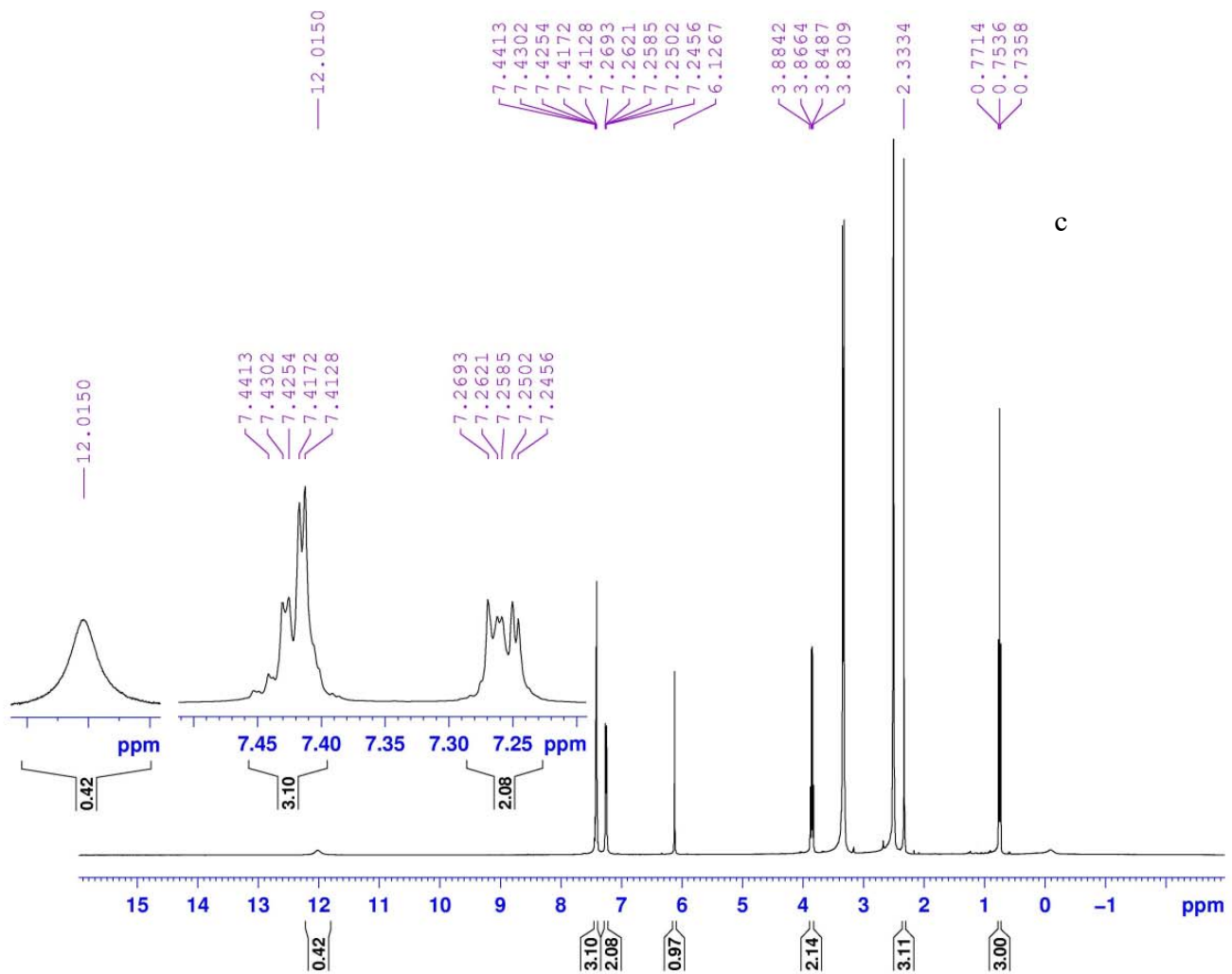
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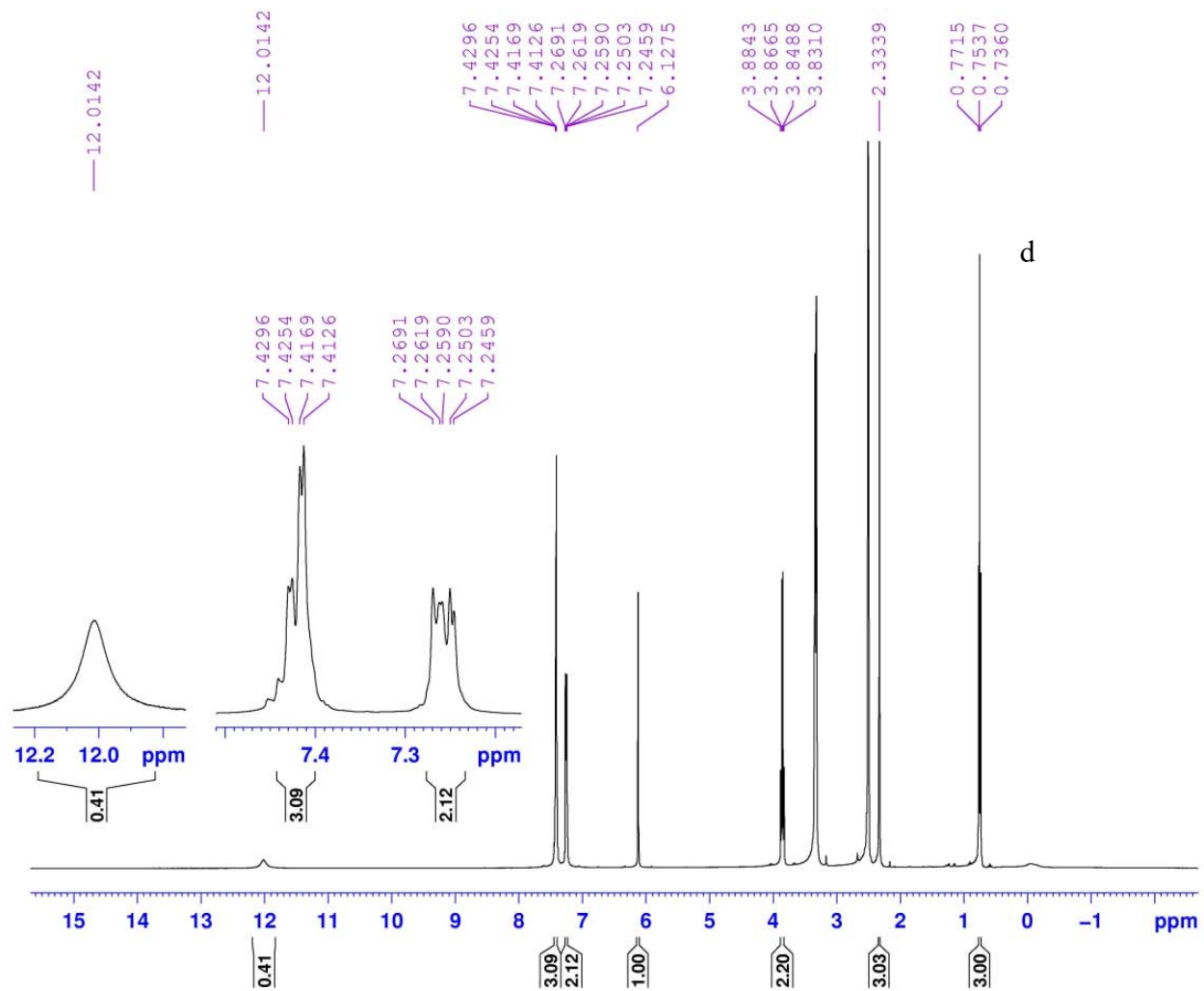
**Figure S6.**  $^1\text{H}$  NMR spectra of 0.03 M solutions of **2a** in  $\text{CDCl}_3$  at 278 K (a), 288 K (b), 298 K (c), 308 K (d) and 318 K (e).



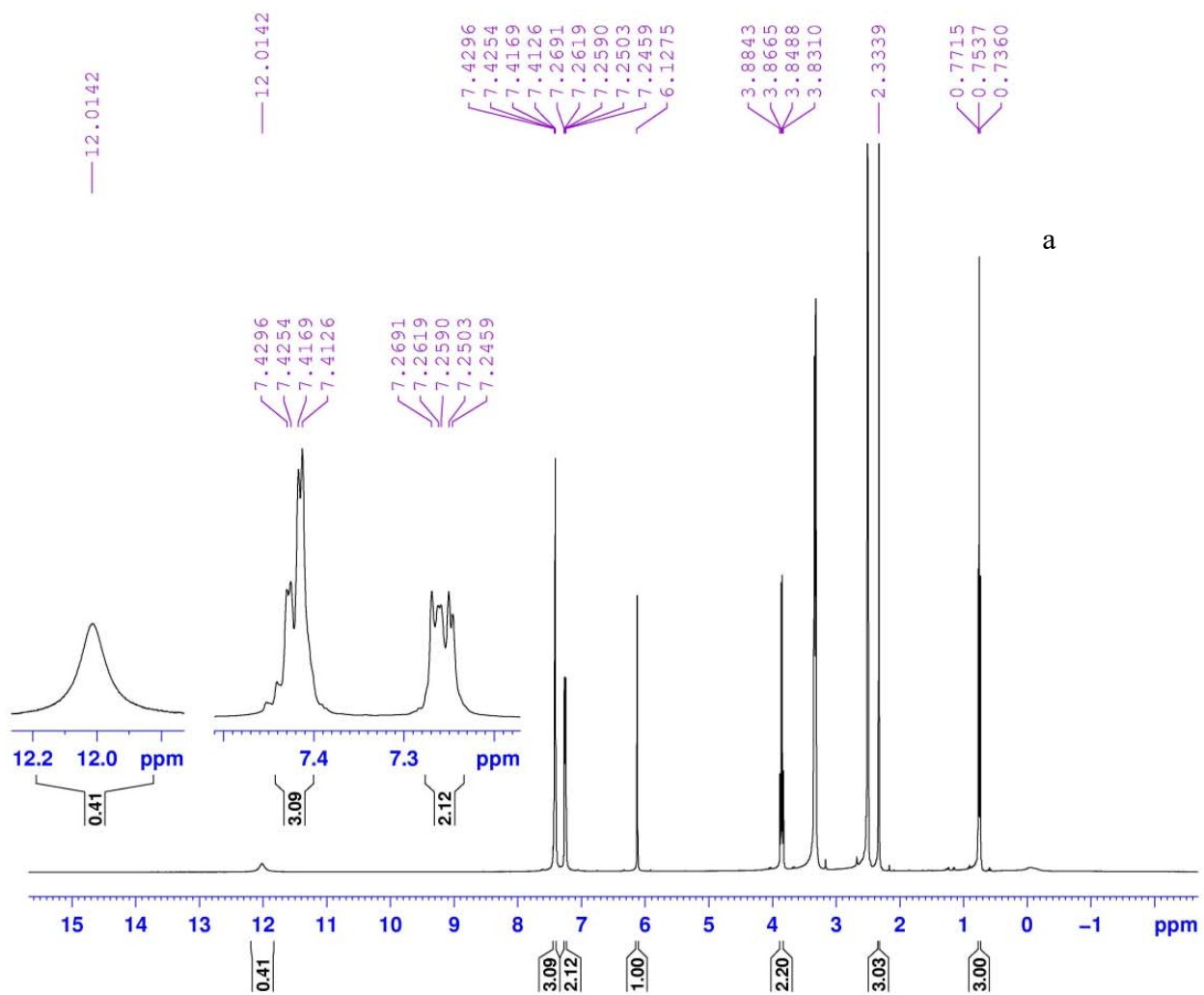




c

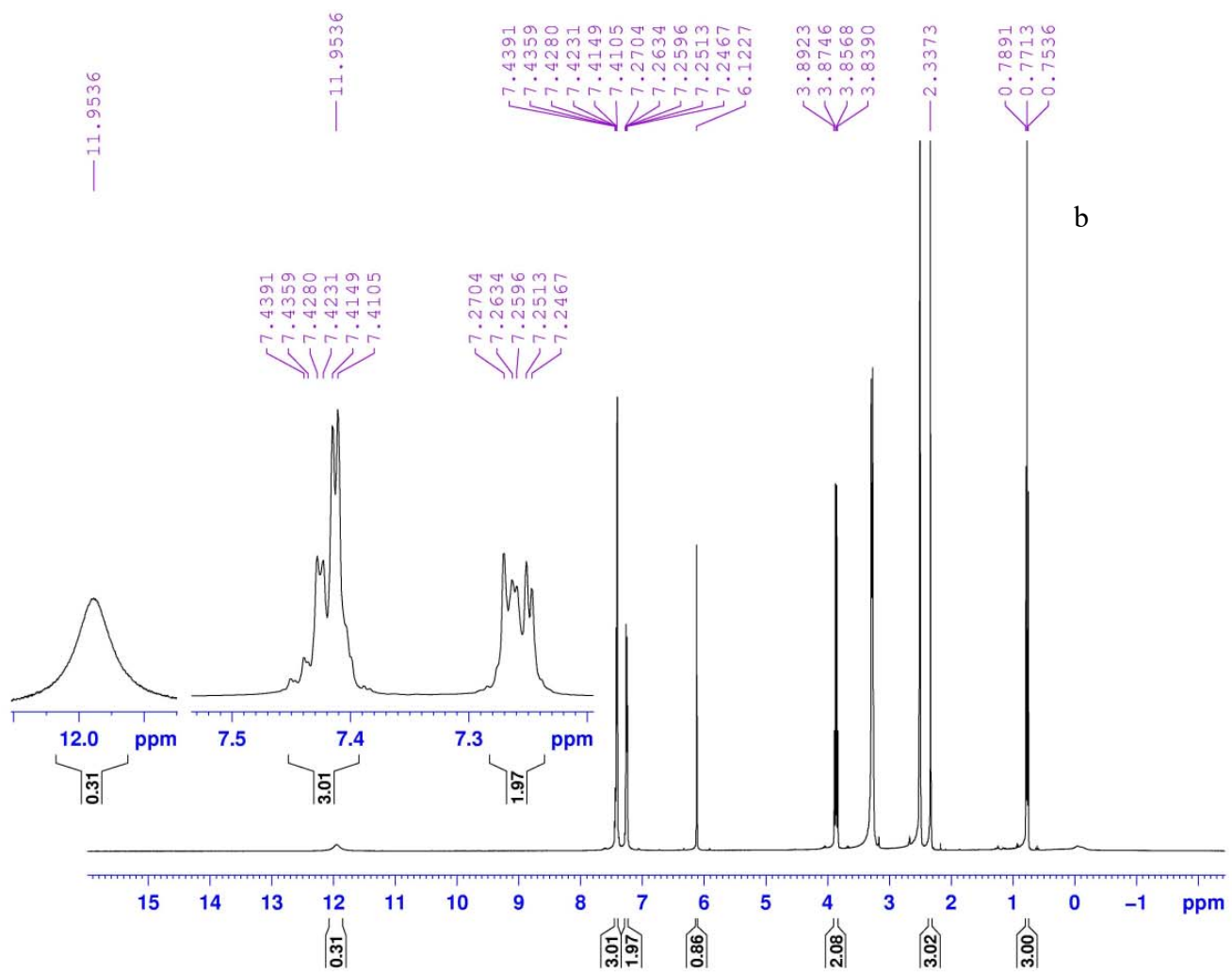


**Figure S7.**  $^1\text{H}$  NMR spectra of **2a** dissolved in DMSO- $d_6$  at concentration of 0.002 M (a), 0.01 M (b), 0.02 M (c) and 0.03 M (d).

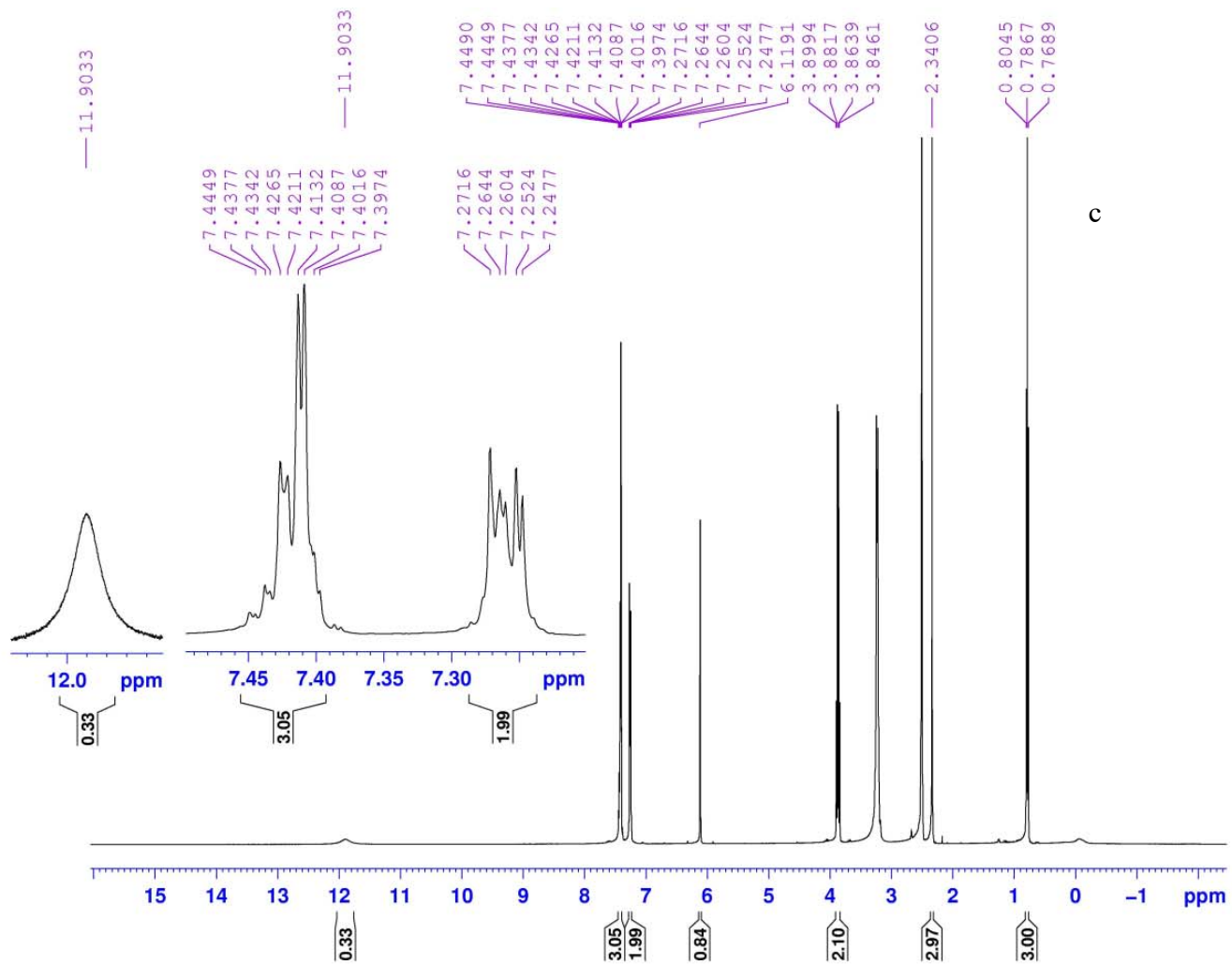


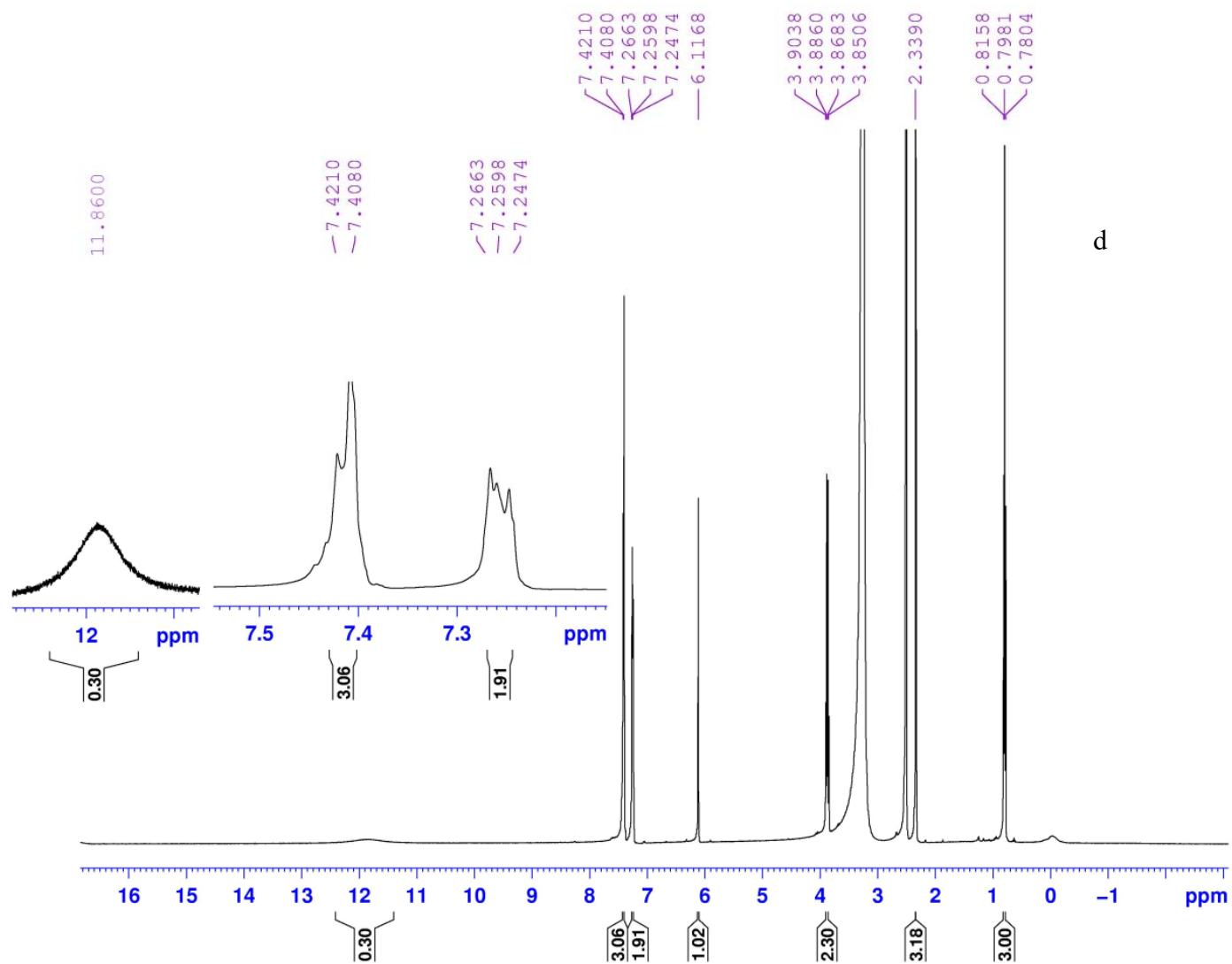
a





b





d

**Figure S8.**  $^1\text{H}$  NMR spectra of 0.03 M solutions of **2a** in DMSO- $d_6$  at 298 K (a), 308 K (b), 318 K (c) and 328 K (d).