

Supporting Information of

Dynamic ¹H-NMR Spectroscopic Study of the Ring Inversion in *N*-Sulfonyl Morpholines–Studies on N-S Interactions

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1. Experimental

1.1 General

Melting points were uncorrected. Variable temperature $^1\text{H-NMR}$ spectra were calibrated with a standard methanol sample.¹ The temperature was measured at the probe (± 0.1 °C).

Samples were allowed to equilibrate for 10 min at each temperature before recording the spectrum.

1.2 Chemicals

All starting materials and solvents were purified with appropriate purification techniques before use, when necessary.² *N*-(aryl-alkylsulfonyl) morpholines **1a-d** are known compounds and identified by comparison of some their spectral data (IR, ¹H and ¹³C NMR) and physical properties with those of authentic samples and were prepared from morpholine and sulfonylchlorides according to literature.³⁻¹⁴

1.3 General Procedure for preparation of *N*-(aryl-alkylsulfonyl) morpholines **1a-d**³

To a solution of morpholine (1 mmol) in pyridine (3 ml), aryl or alkyl sulfonyl chloride (2 mmol) was added and the mixture was stirred for appropriate time. Completion of the reaction was indicated by TLC. After completion, water was added and the solid product was filtered. The desired pure products were recrystallised in ethanol; **1a**, mp = 93-95 °C, lit.¹¹ mp = 95 °C; **1b**, mp = 142-144 °C, lit.¹² mp = 143-145 °C; **1c**, mp = 117-119 °C, lit.¹³ mp = 117-118 °C; **1d**, mp = 151-153 °C; **1e**, mp = 170-172 °C, lit.¹⁴ mp = 172-174 °C. Unfortunately, any melting point was not found for **1d** in literature in spite of the fact that there were many papers for the synthesis of this compound; so, the melting point obtained by us, is still included.

2. Dynamic behavior of *N*-(aryl-alkylsulfonyl) morpholines **1a-1e** in variable temperatures

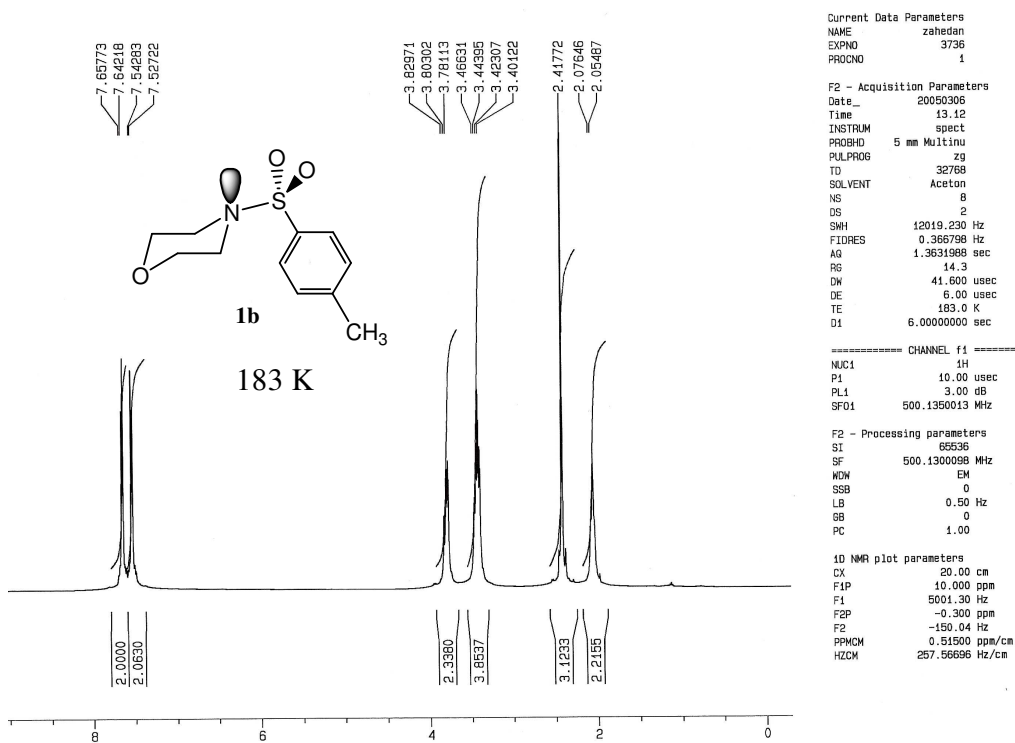
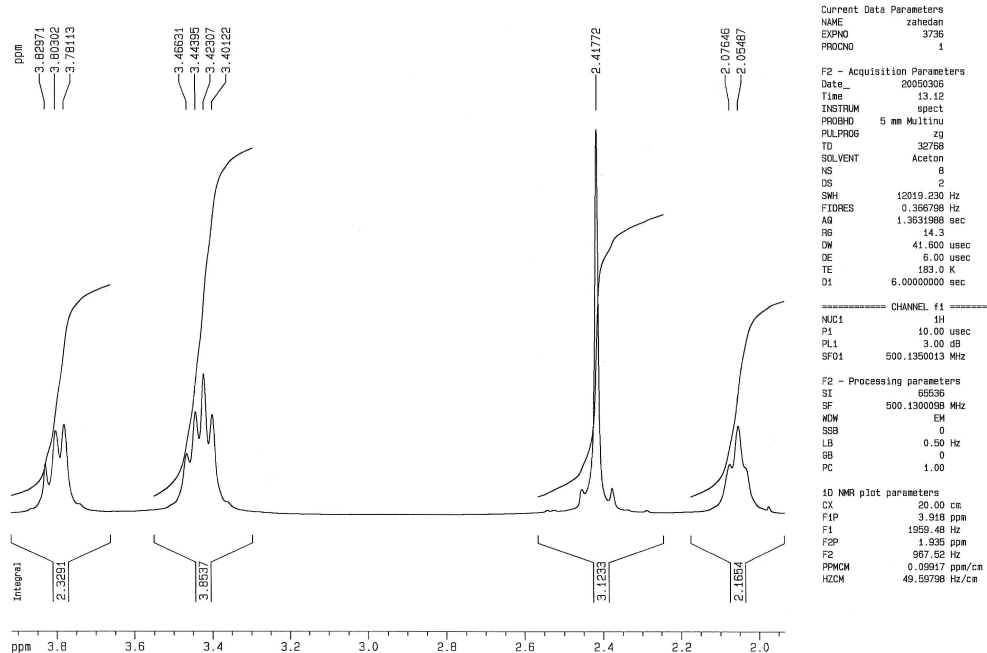


Figure S1. $^1\text{H-NMR}$ (500 MHz) spectrum of 4-methylbenzenesulfonyl morpholine **1b** in CD_3COCD_3 (at 183 K).



Continued Figure S1.

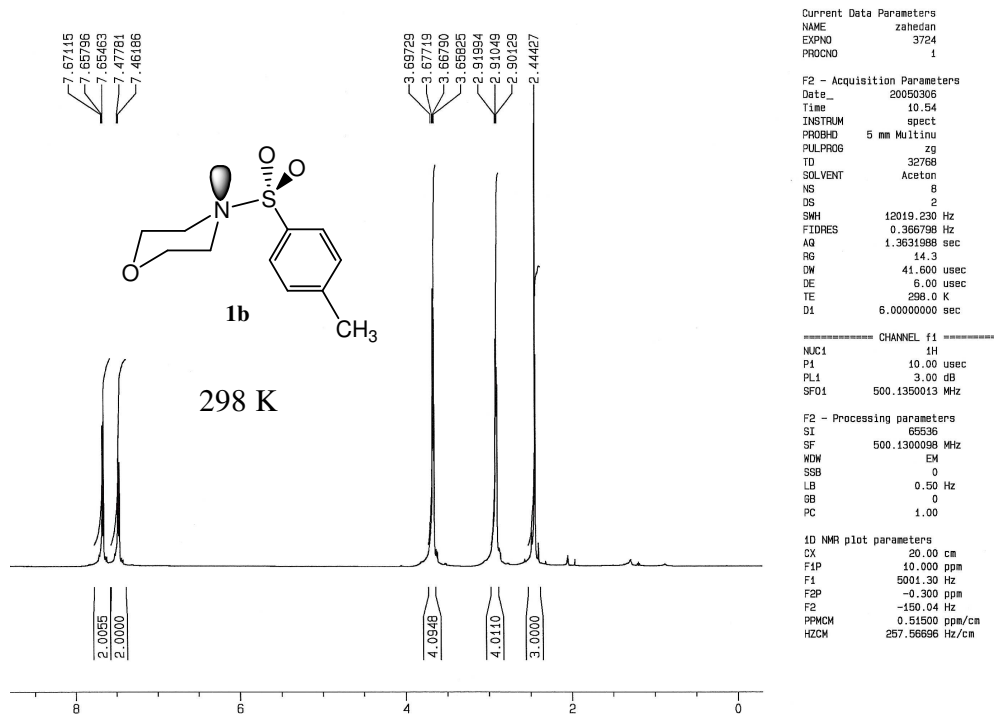
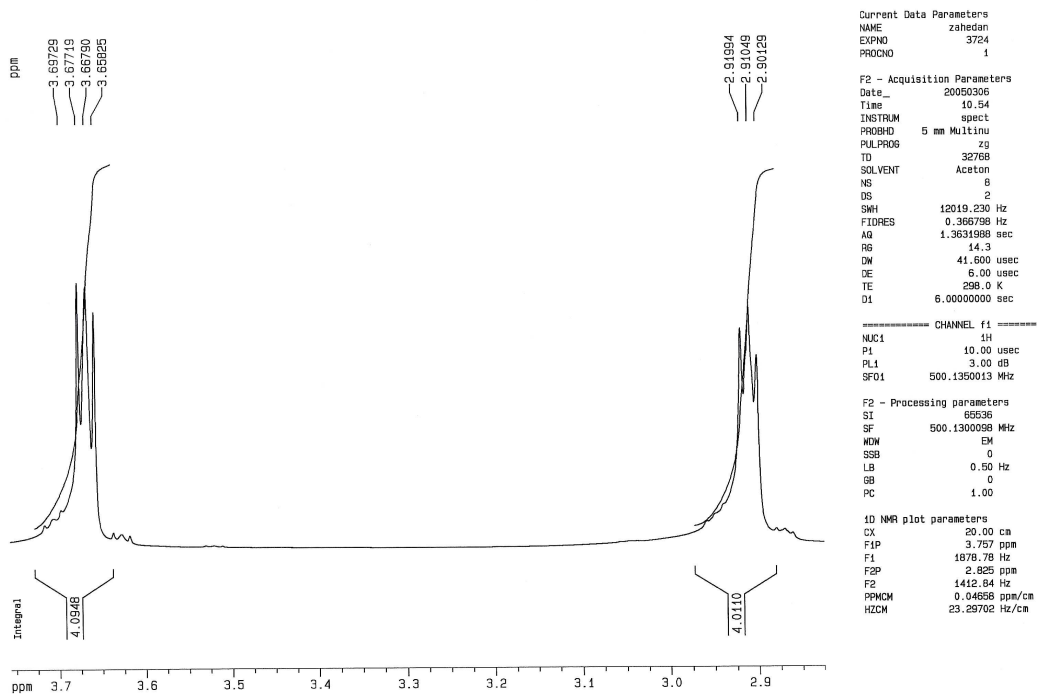
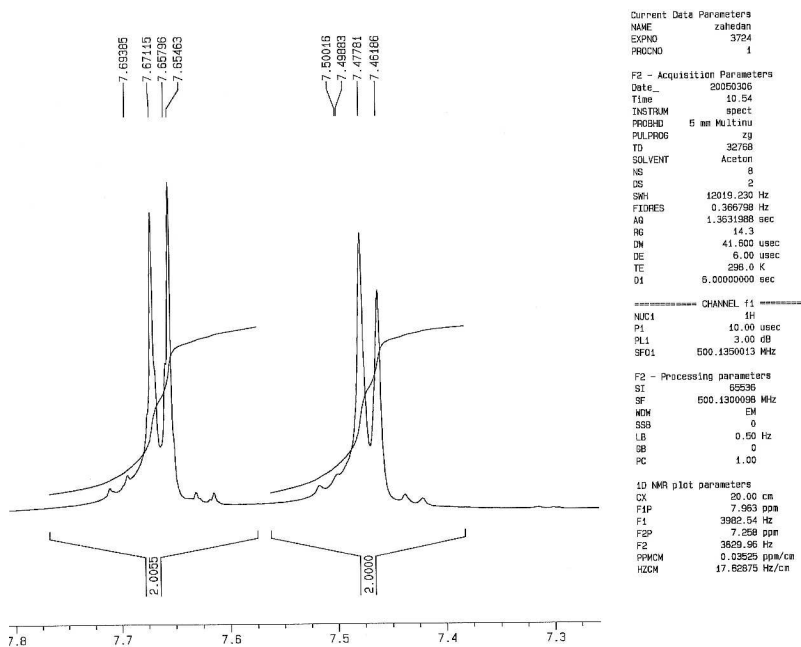


Figure S2. ¹H-NMR (500 MHz) spectrum of 4-methylbenzenesulfonyl morpholine **1b** in CD₃COCD₃ (at 298 K).



Continued Figure S2.



Continued Figure S2.

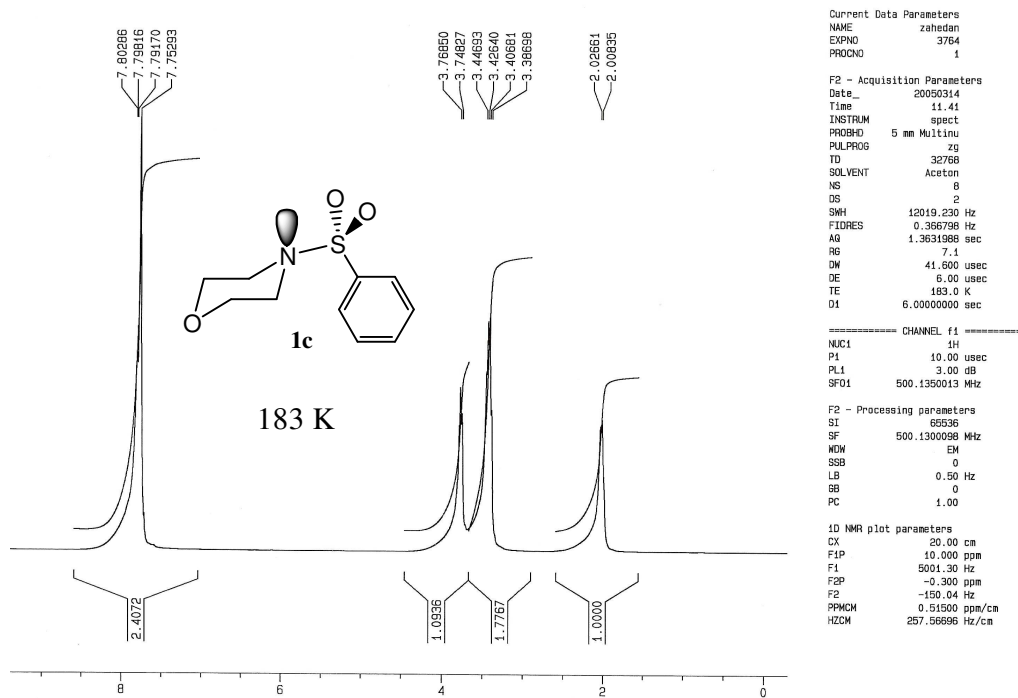
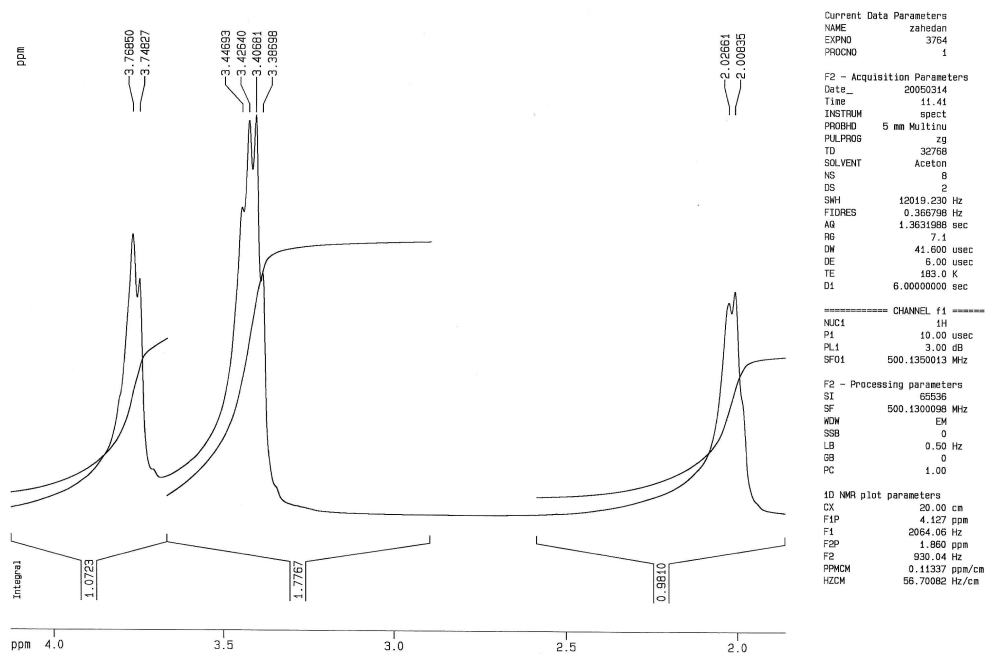


Figure S3. $^1\text{H-NMR}$ (500 MHz) spectrum of benzenesulfonyl morpholine **1c** in CD_3COCD_3 (at 183 K).



Continued Figure S3.

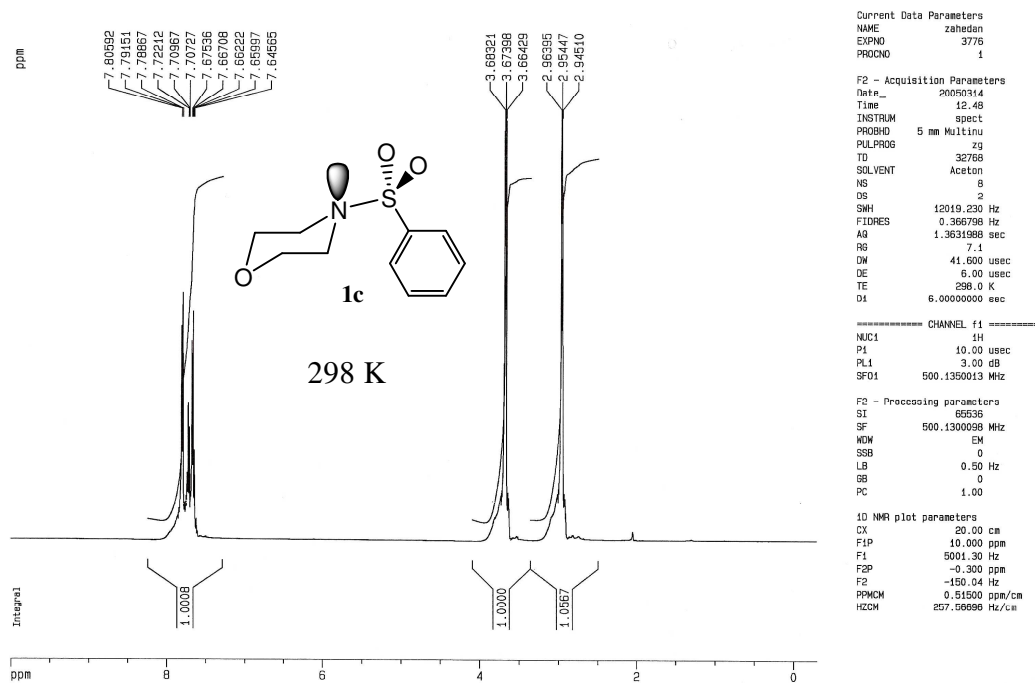
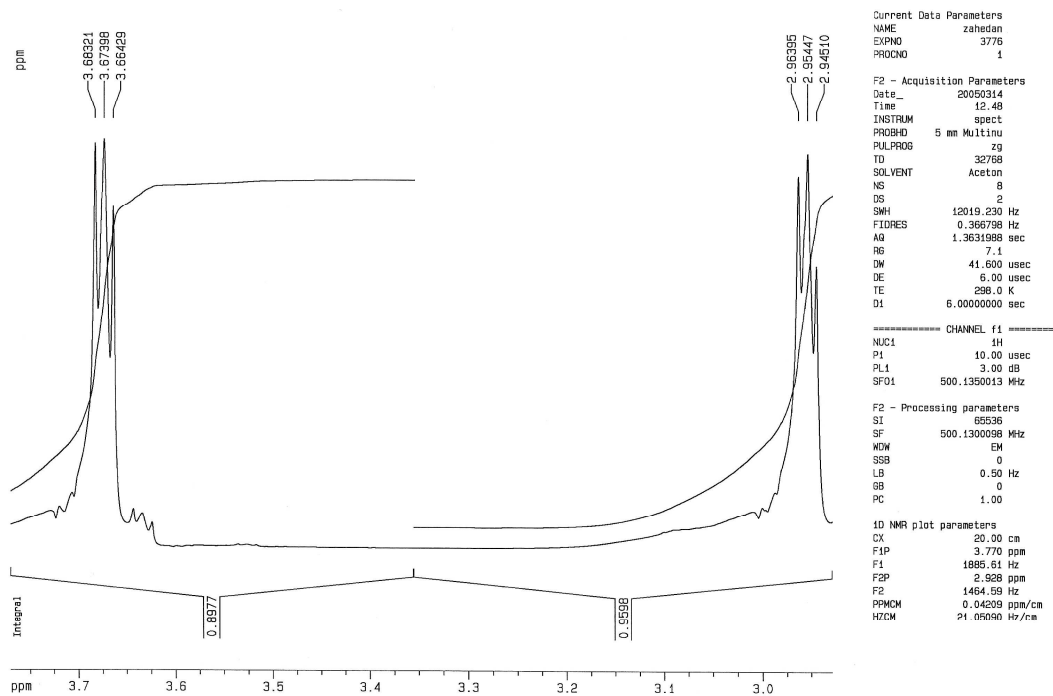
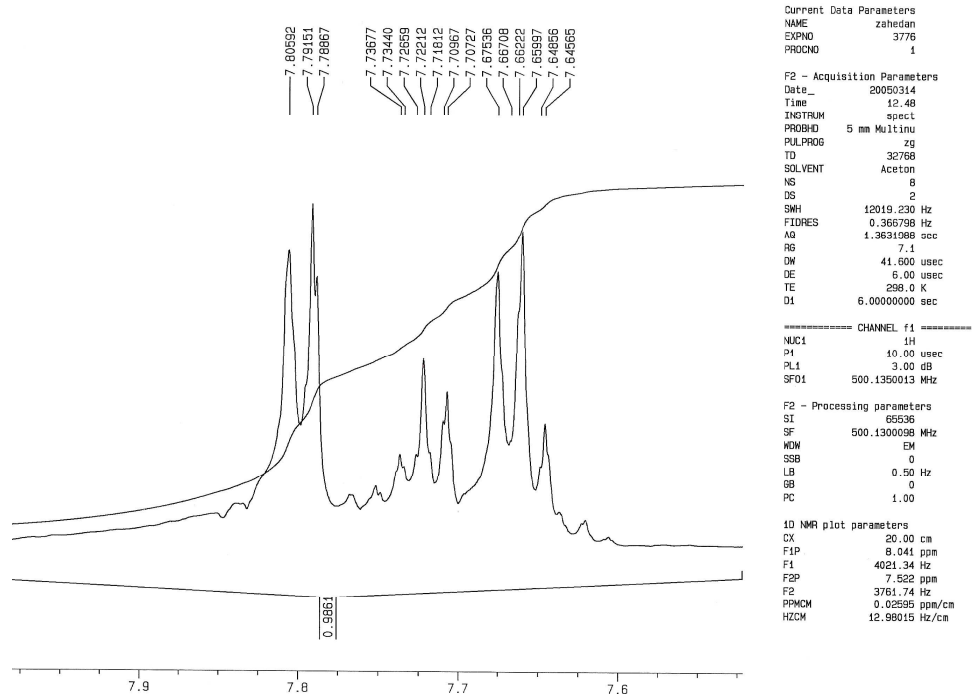


Figure S4. $^1\text{H-NMR}$ (500 MHz) spectrum of benzenesulfonyl morpholine **1c** in CD_3COCD_3 (at 298 K).



Continued Figure S4.



Continued Figure S4.

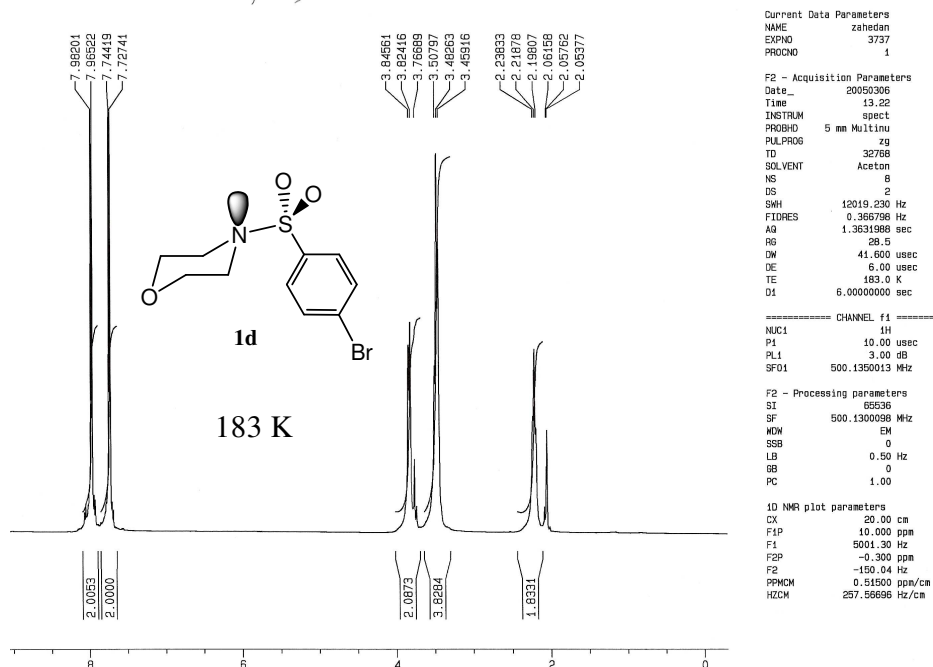
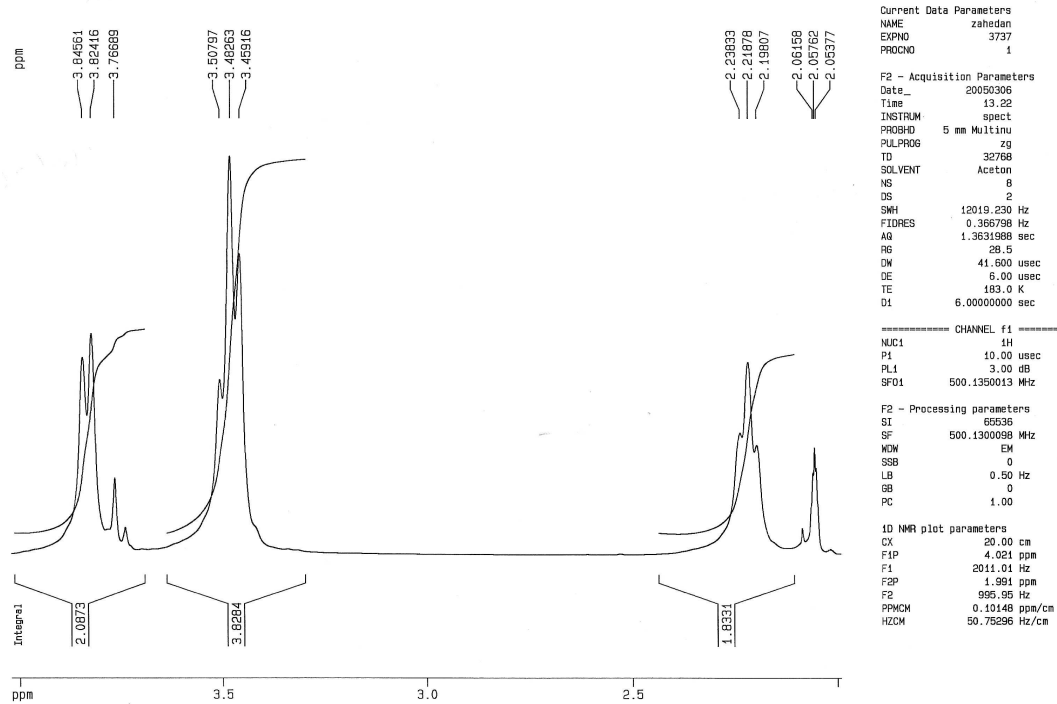
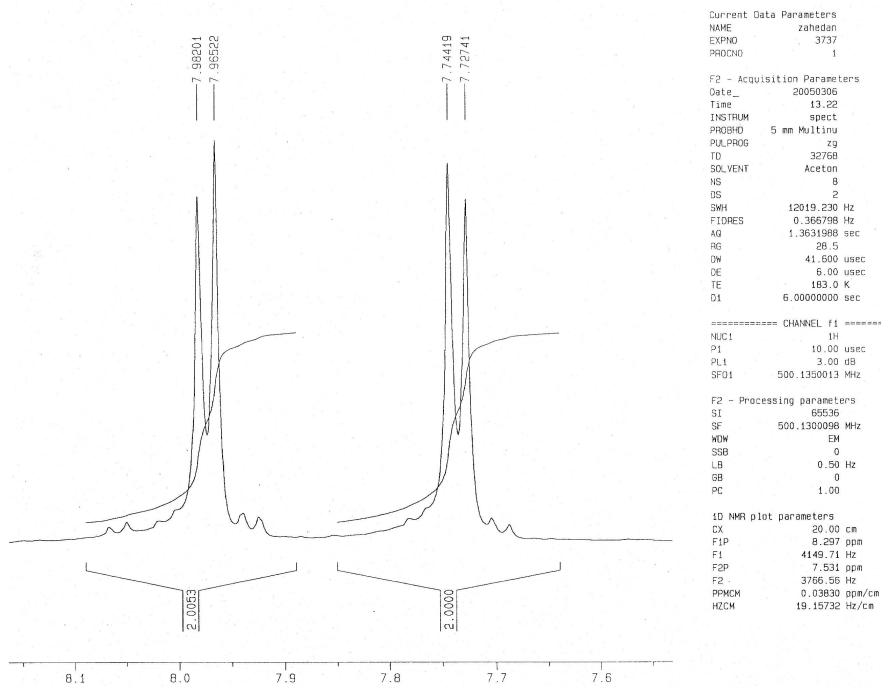


Figure S5. ¹H-NMR (500 MHz) spectrum of 4-bromobenzenesulfonyl morpholine **1d** in CD₃COCD₃ (at 183 K).



Continued Figure S5.



Continued Figure S5.

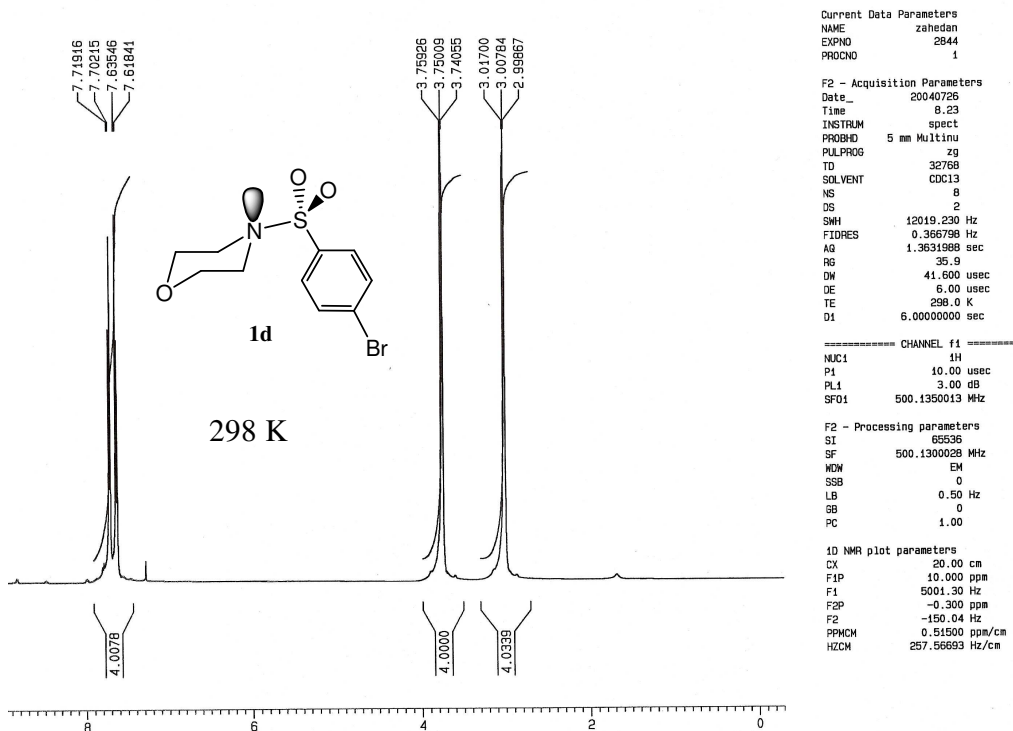
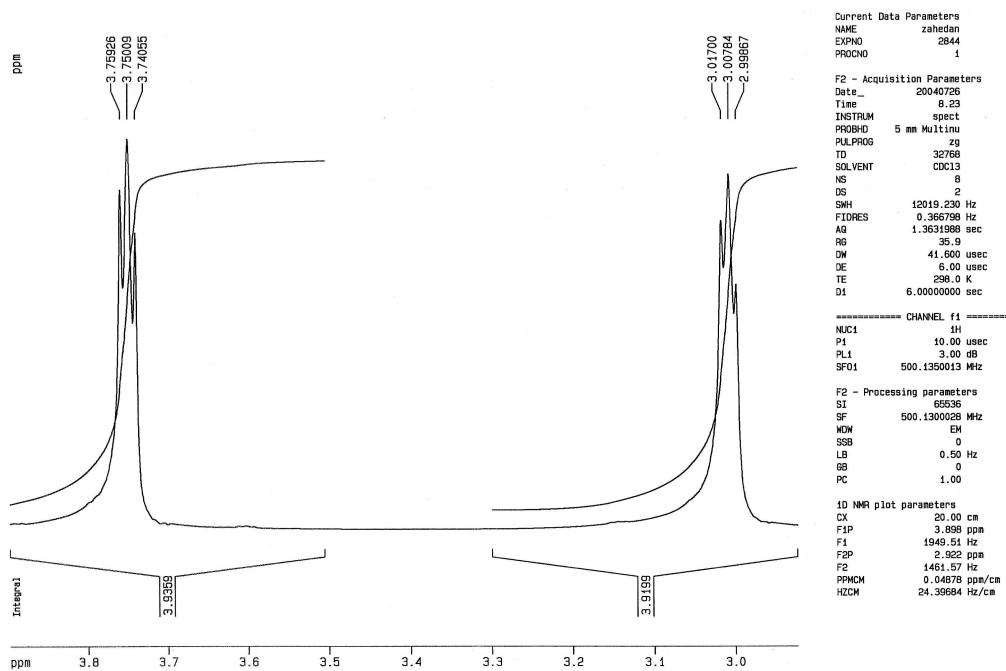
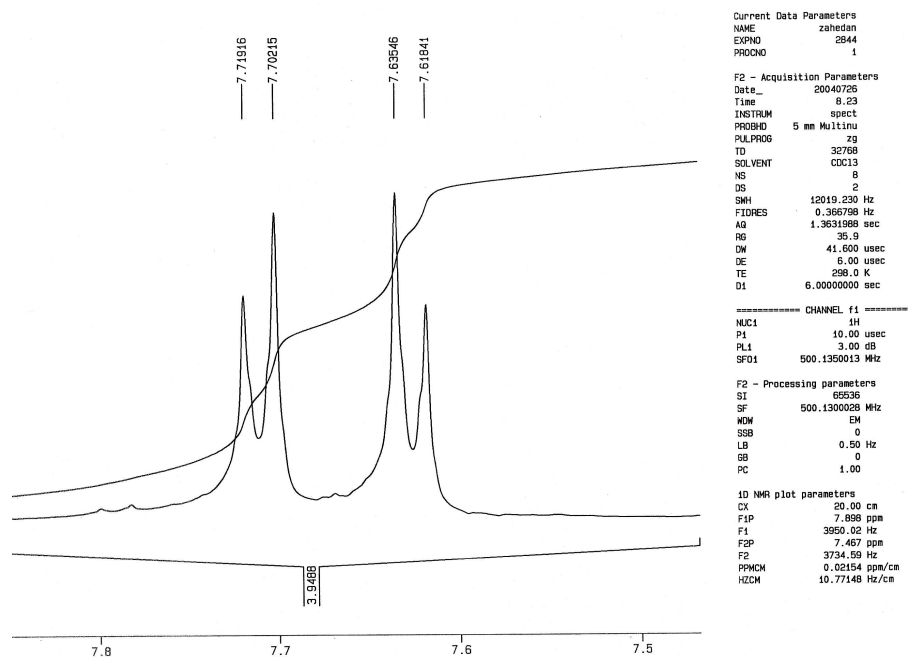


Figure S6. ¹H-NMR (500 MHz) spectrum of 4-bromobenzenesulfonyl morpholine **1d** in CD₃COCD₃ (at 298 K).



Continued Figure S6.



Continued Figure S6.

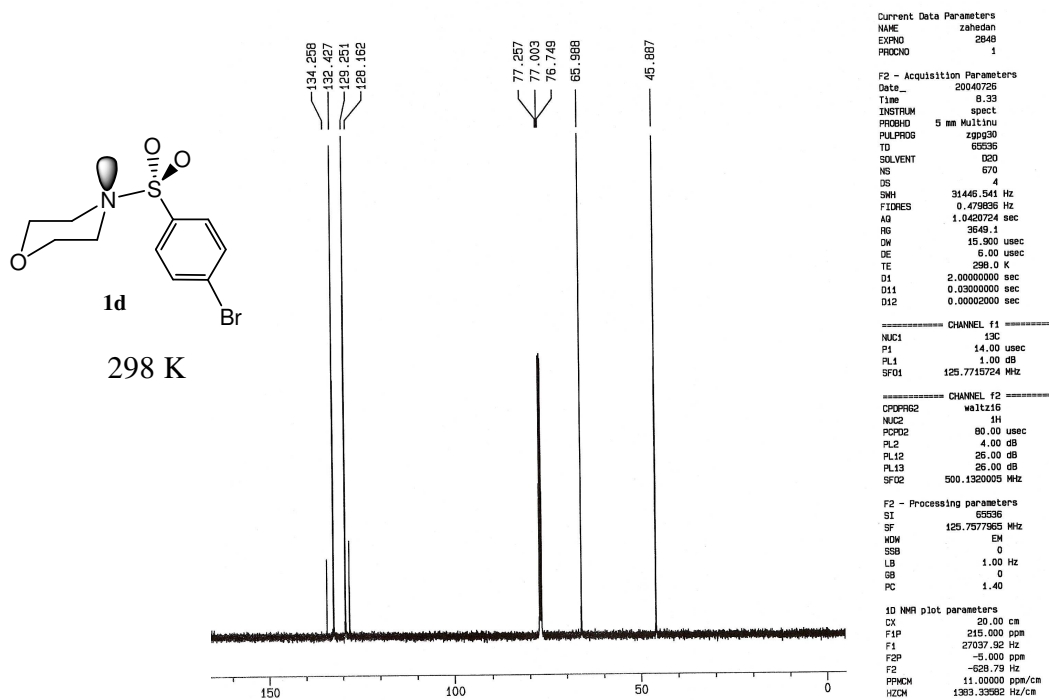


Figure S7. ^{13}C -NMR (125 MHz) spectrum of 4-bromobenzenesulfonyl morpholine **1d** in CD_3COCD_3 (at 298 K).

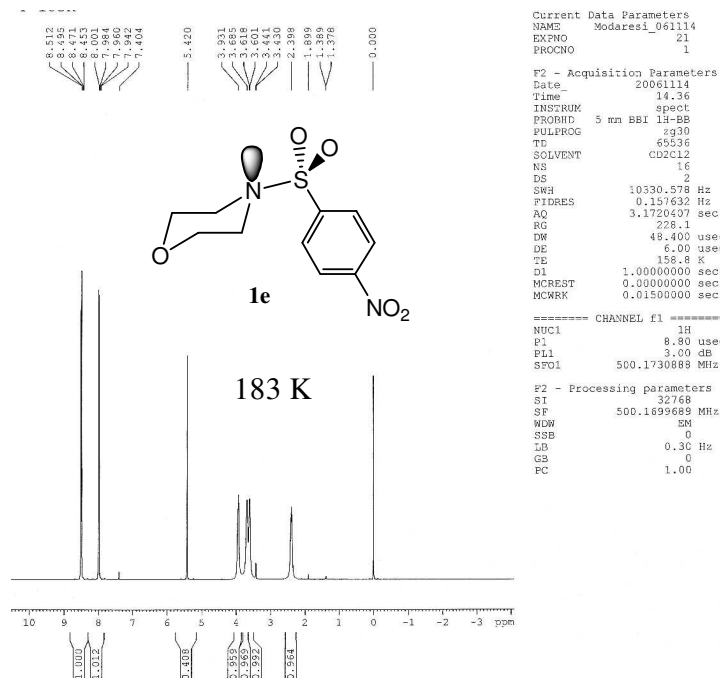
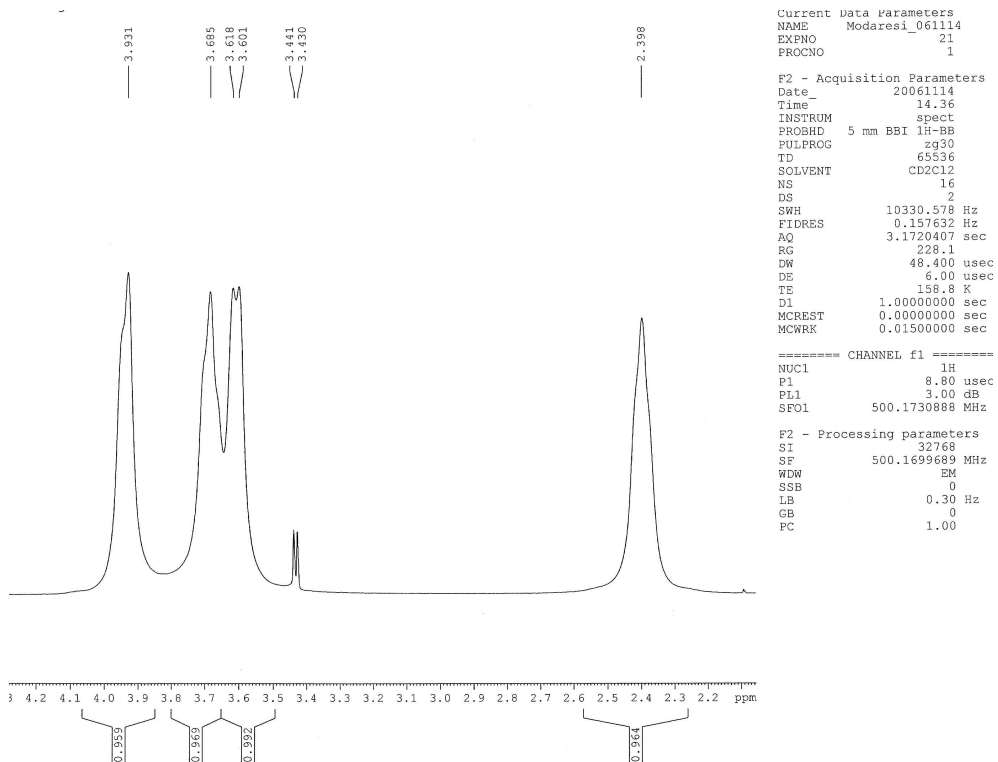
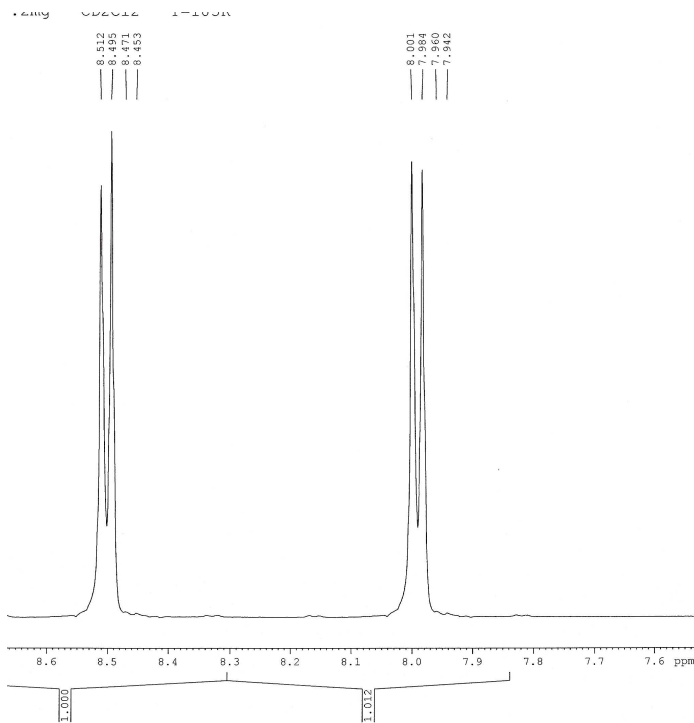


Figure S8. $^1\text{H-NMR}$ (500 MHz) spectrum of 4-nitrobenzenesulfonyl morpholine **1e** in CD_2Cl_2 (at 183 K).



Continued Figure S8.



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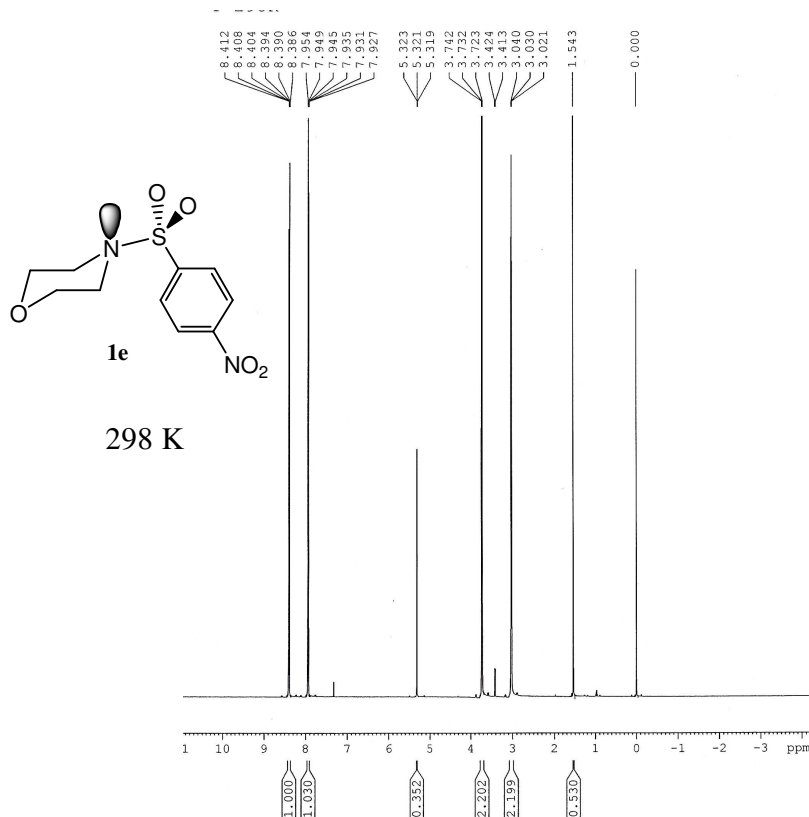
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Continued Figure S8.



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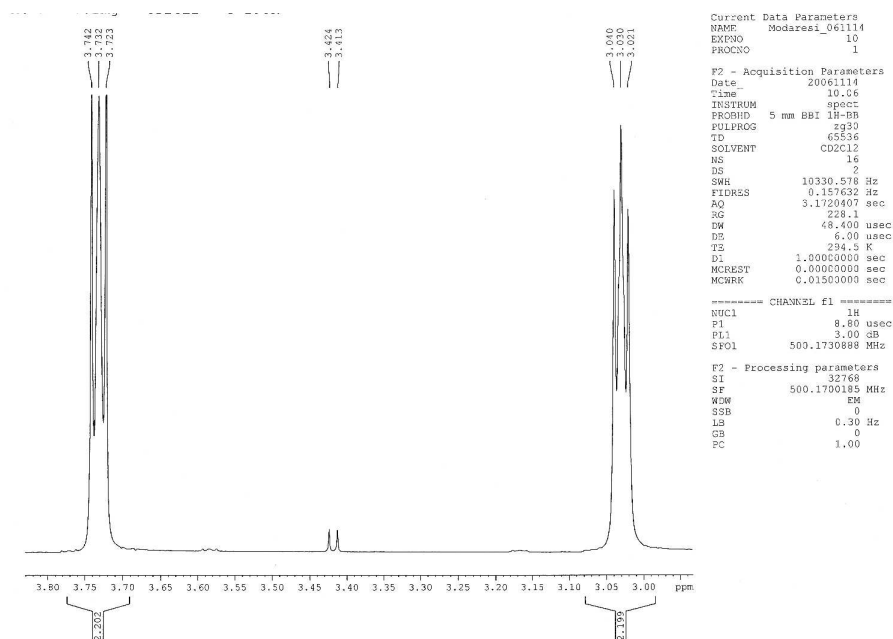
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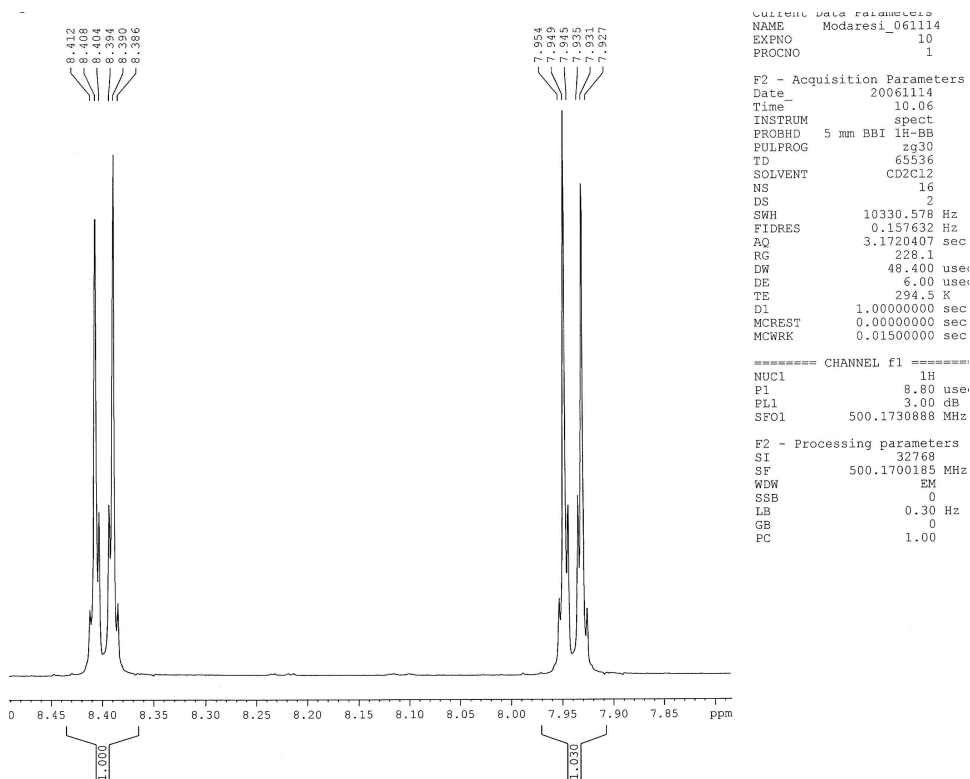
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Figure S9. $^1\text{H-NMR}$ (500 MHz) spectrum of 4-nitrobenzenesulfonyl morpholine **1e** in CD_2Cl_2 (at 298 K).



Continued Figure S9.



Continued Figure S9.

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