

Design, Eco-friendly synthesis, molecular modeling, and anticancer evaluation of thiazol-5(4*H*)-ones as potential tubulin polymerization inhibitors targeting colchicine binding site

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Pharmaceutical Medicinal Chemistry & Drug Design Department, Faculty of Pharmacy (Boys), Al-Azhar University, Cairo, 11884, Egypt

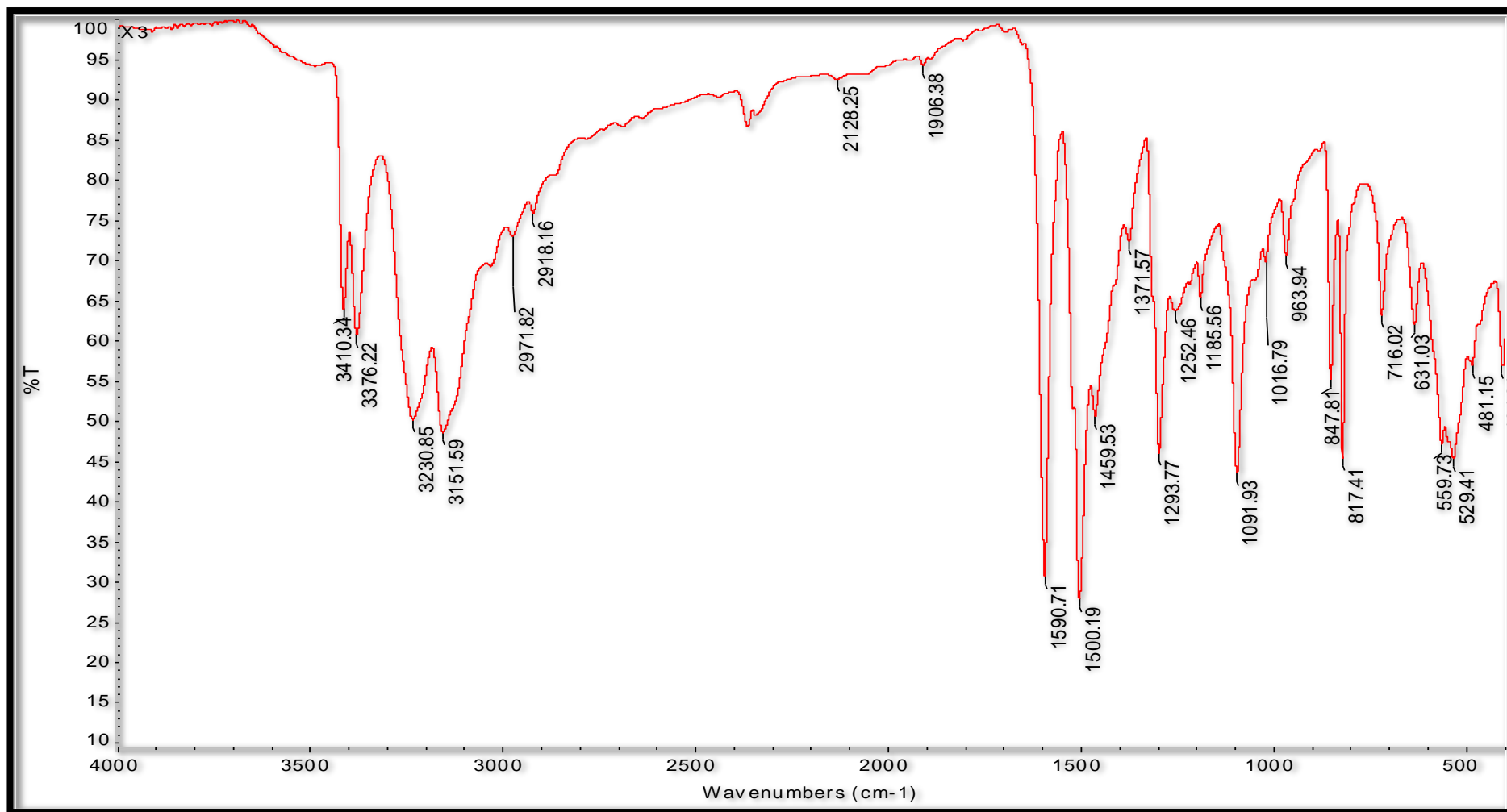
Email: Ibrahimeissa@azhar.edu.eg

Abeer M. El-Naggar

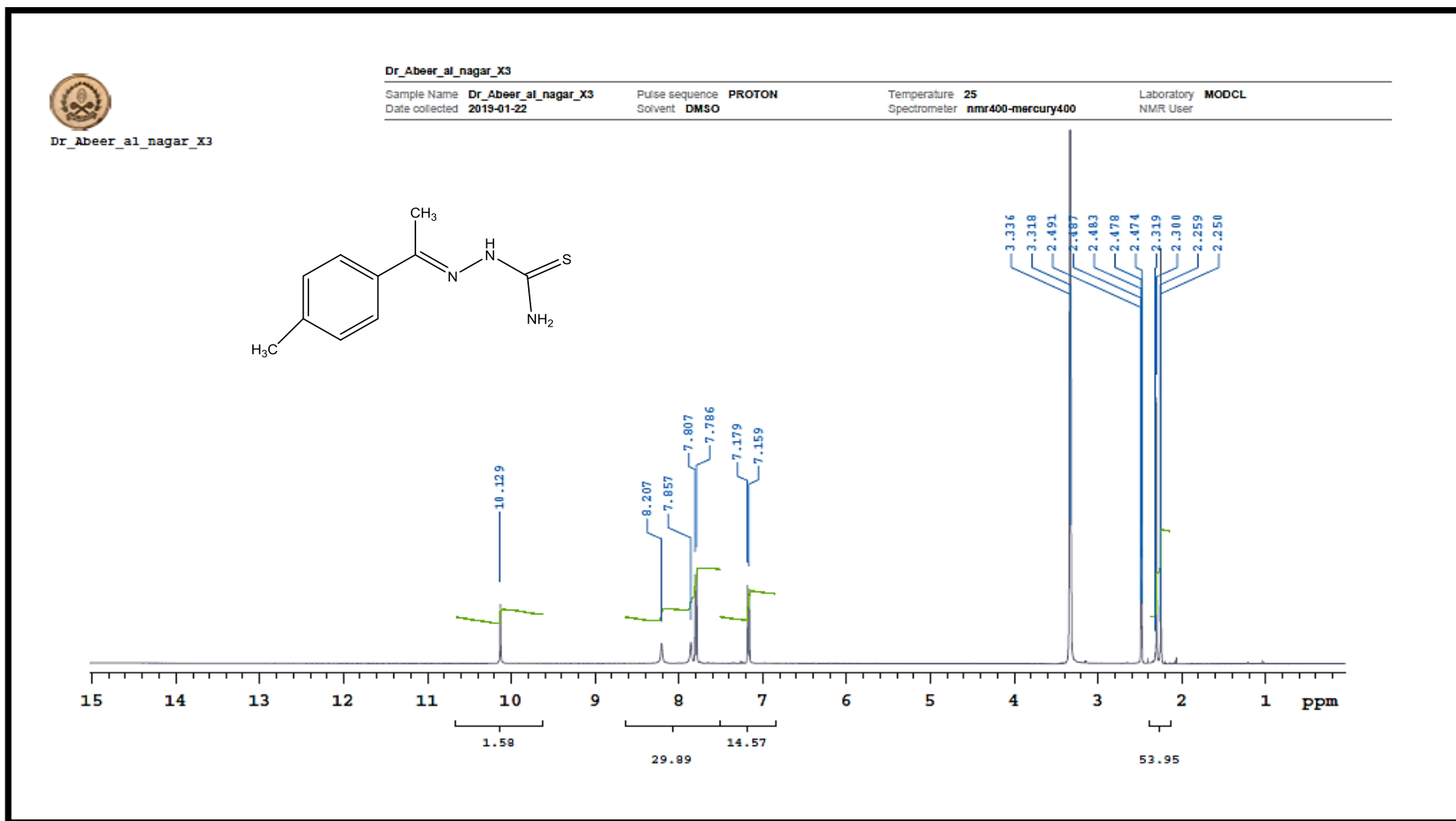
Chemistry Department, Faculty of science, Ain shams University, Abbassia, Cairo-11566, Egypt.

E-mail: elsayedam@sci.asu.edu.eg

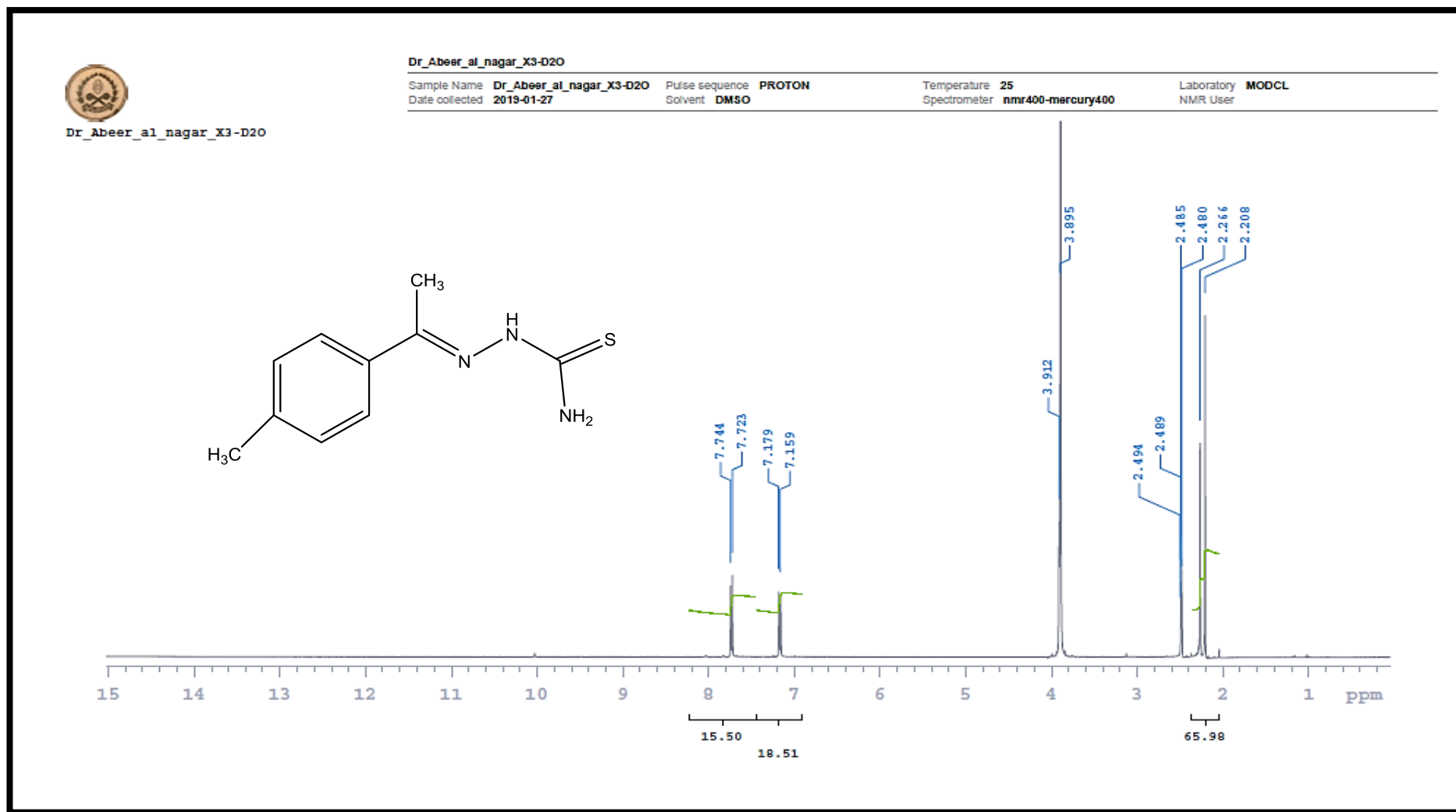
IR of compound (3a)



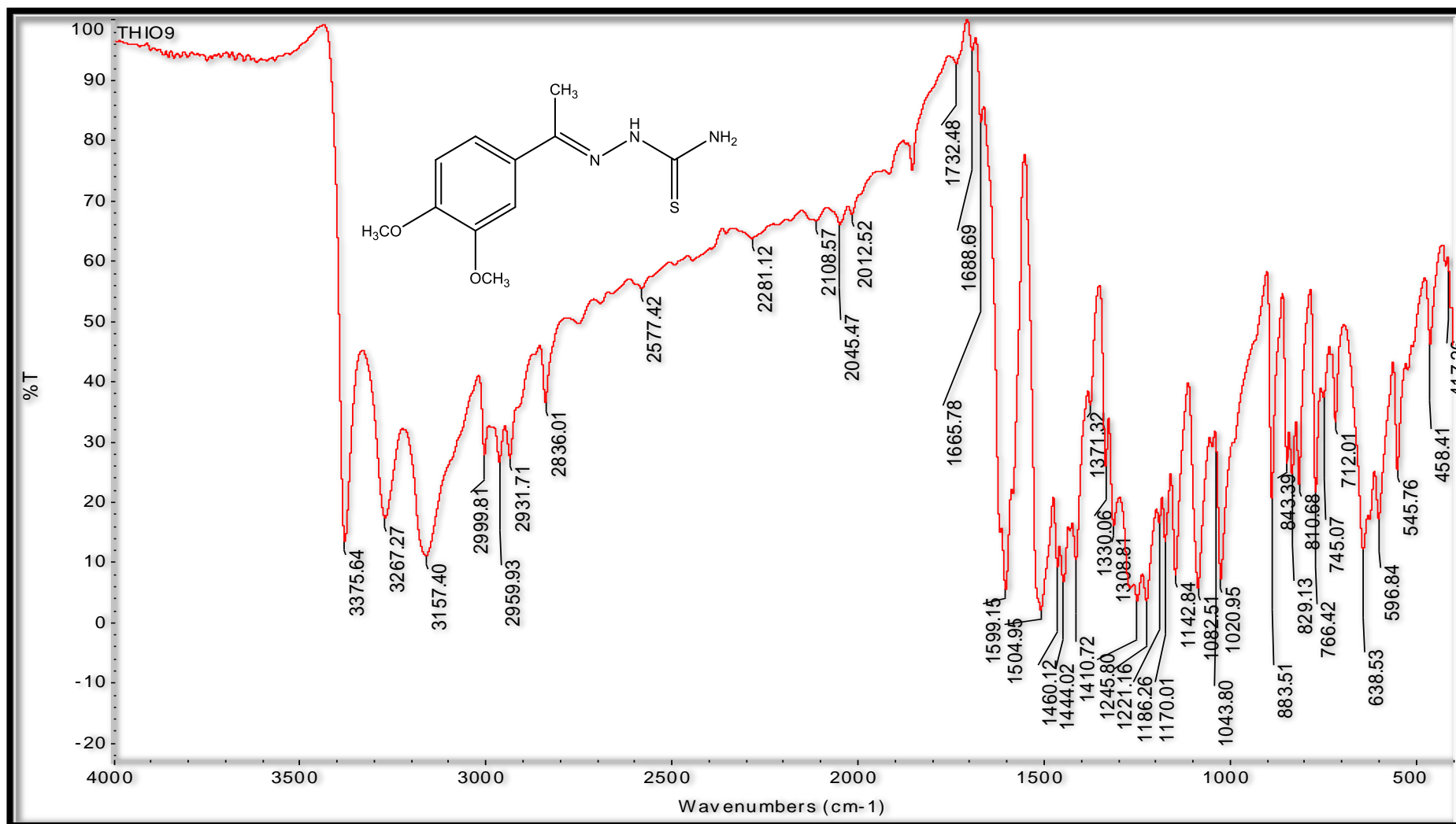
¹H NMR of compound (3a)



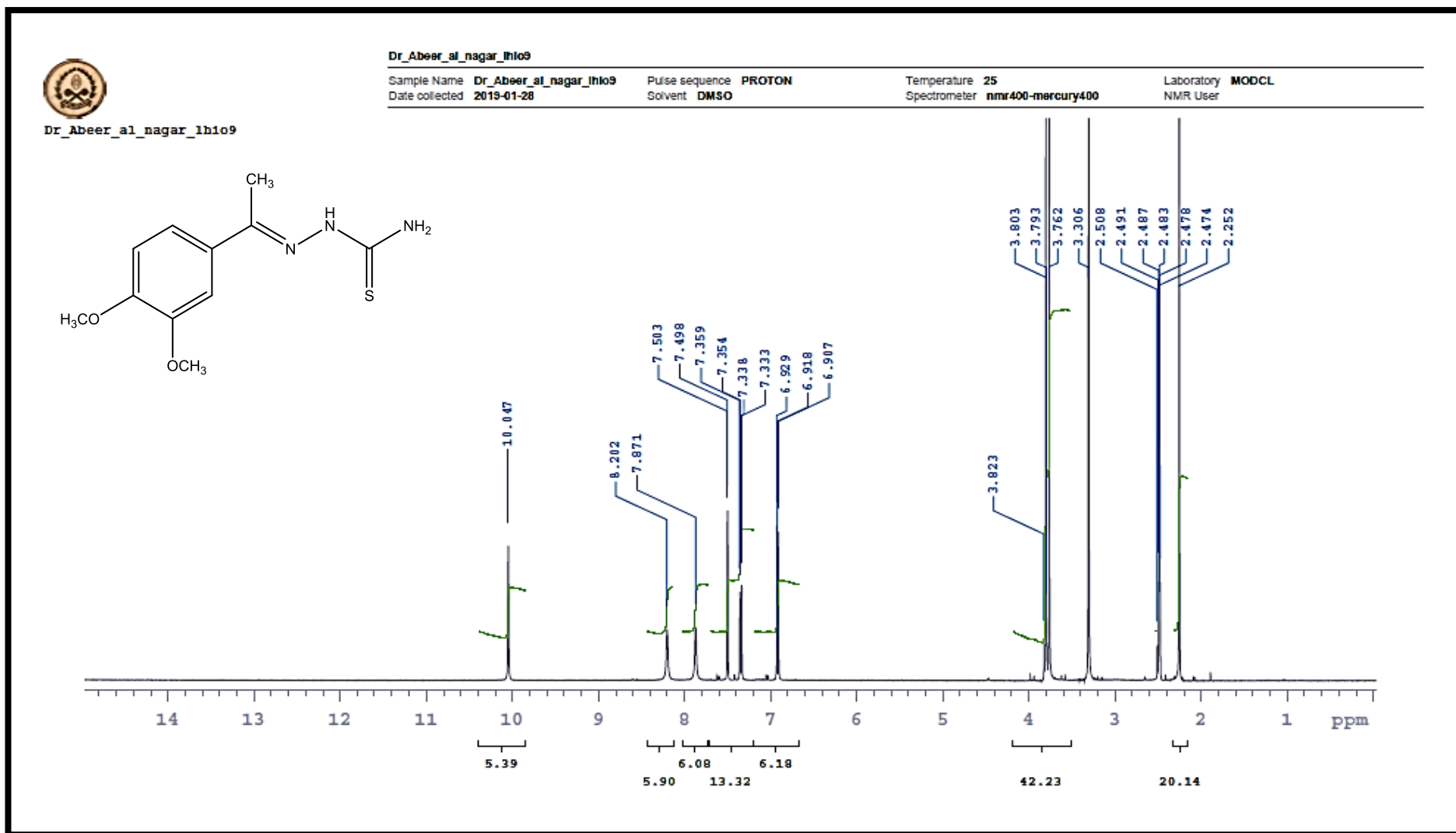
D₂O ¹H NMR of compound (3a)



IR of compound (3b)



¹H NMR of compound (3b)



¹³C NMR of compound (3b)



Dr_Abeer_al_nagar_1h1o9

Dr_Abeer_al_nagar_1h1o9

Sample Name Dr_Abeer_al_nagar_1h1o9

Pulse sequence CARBON

Temperature 25

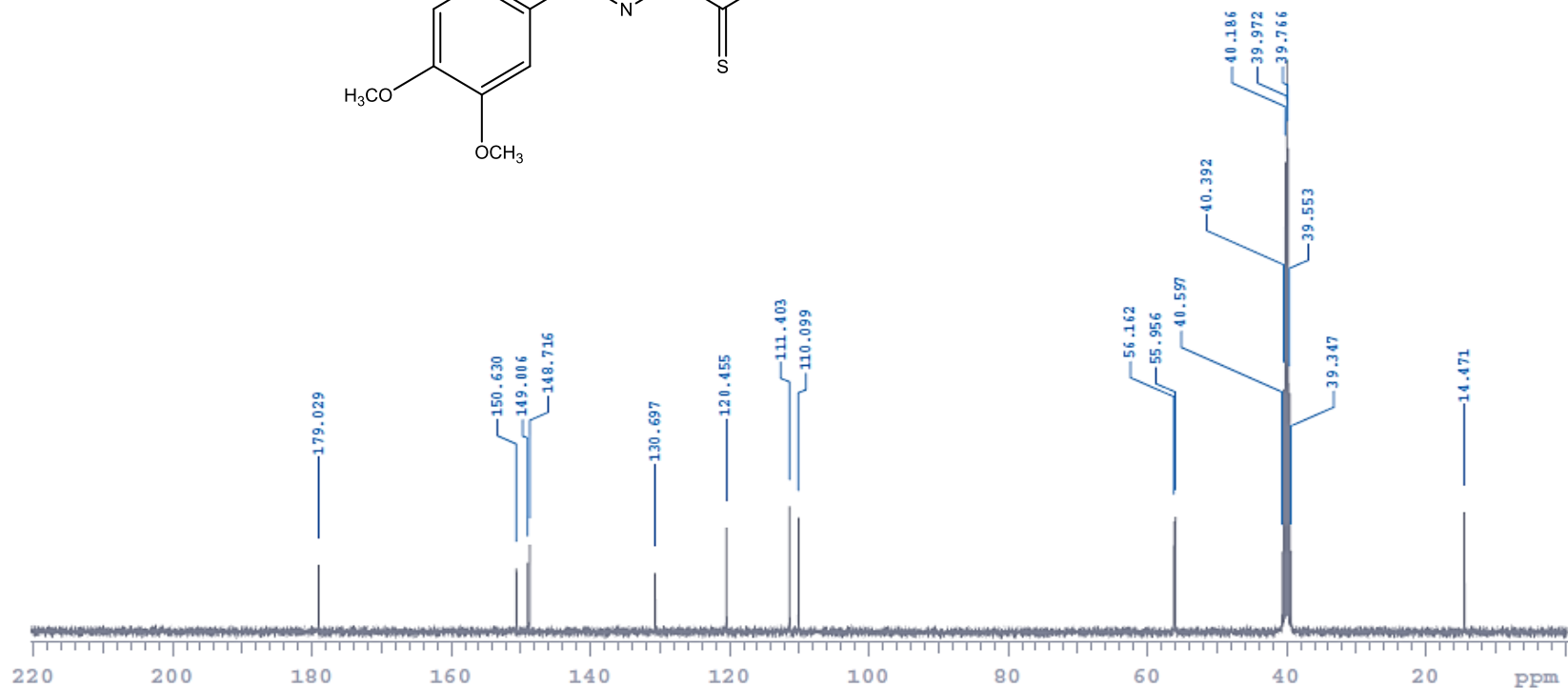
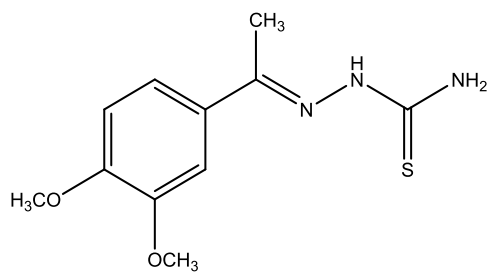
Laboratory MODCL

Date collected 2019-01-28

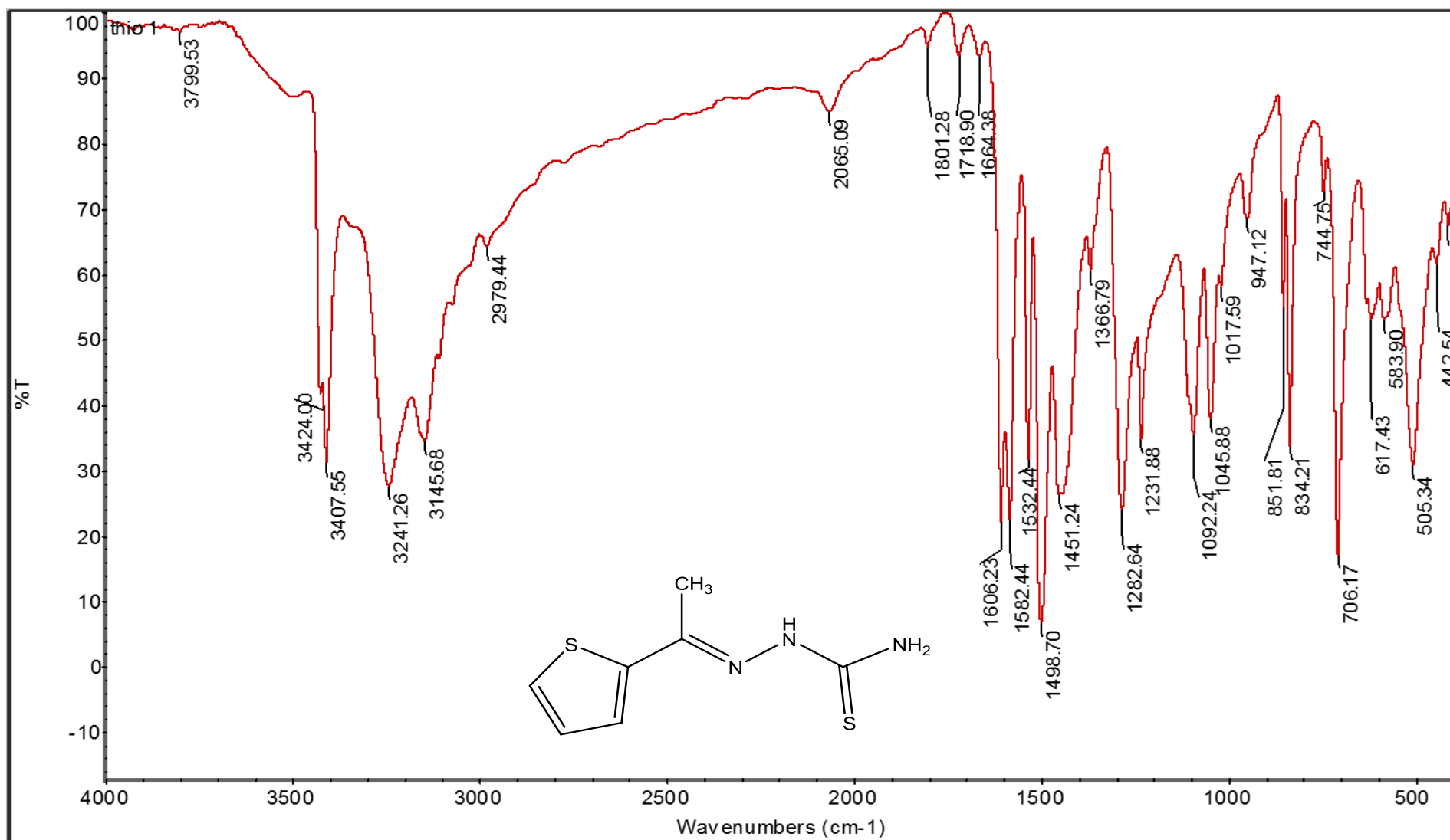
Solvent DMSO

Spectrometer nmr400-mercury400

NMR User



IR of compound (7a)



¹H NMR of compound (7a)



Dr_AbeerElnagar-thio1

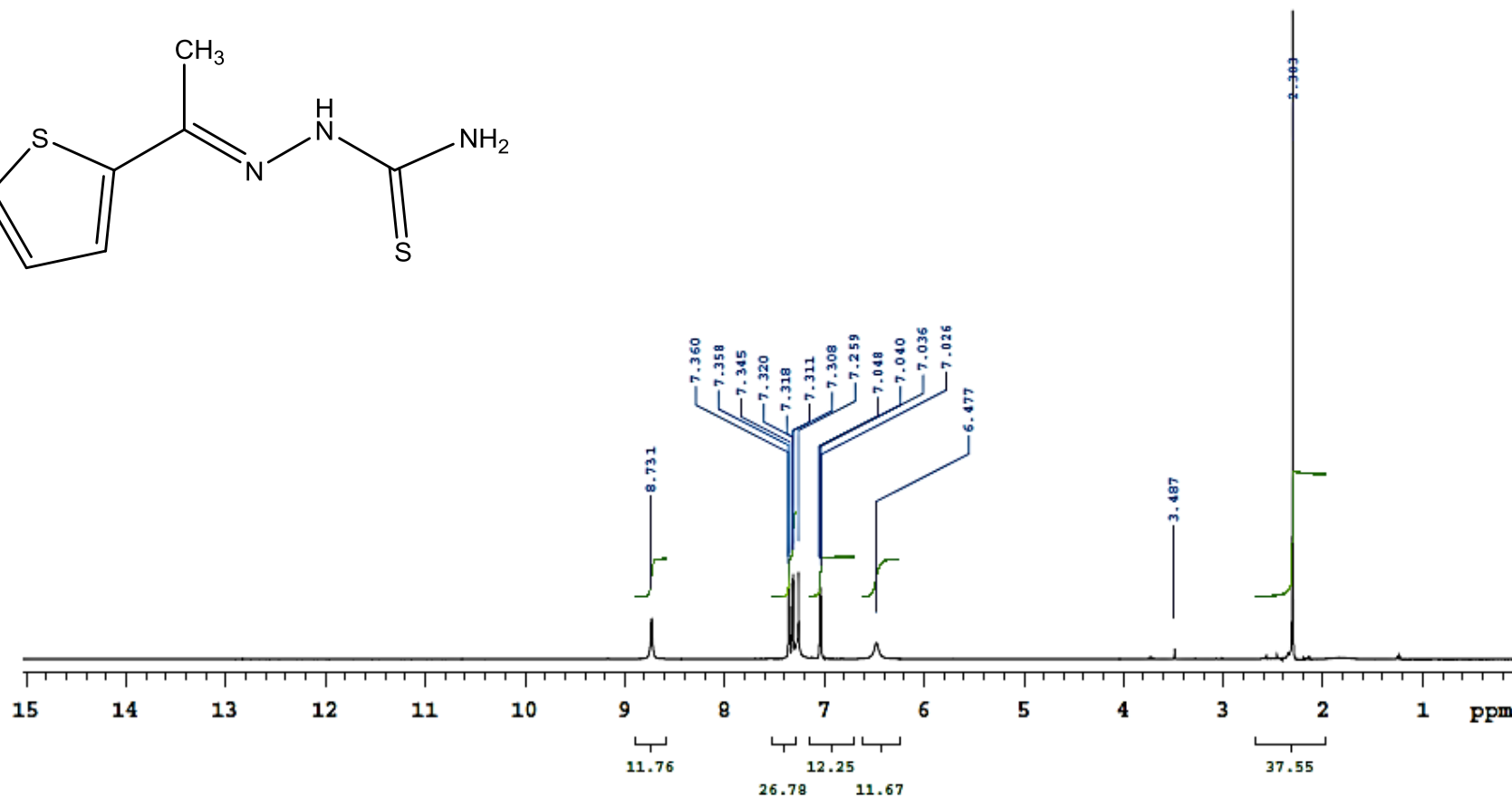
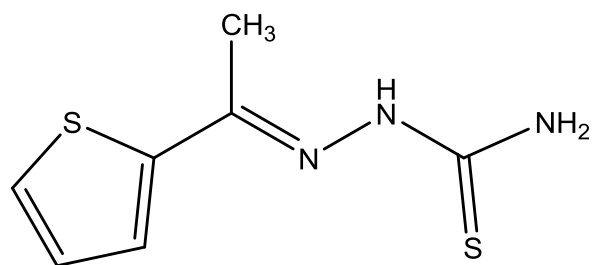
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Sample Name Dr_AbeerElnagar-thio1
Date collected 2017-11-12

Pulse sequence PROTON
Solvent cdcl3

Temperature 25
Spectrometer nmr400-mercury400

Study owner vnmr1
Operator vnmr1



D₂O H NMR of compound (7a)



Dr_AbeerElmagar-th1o1-D2O

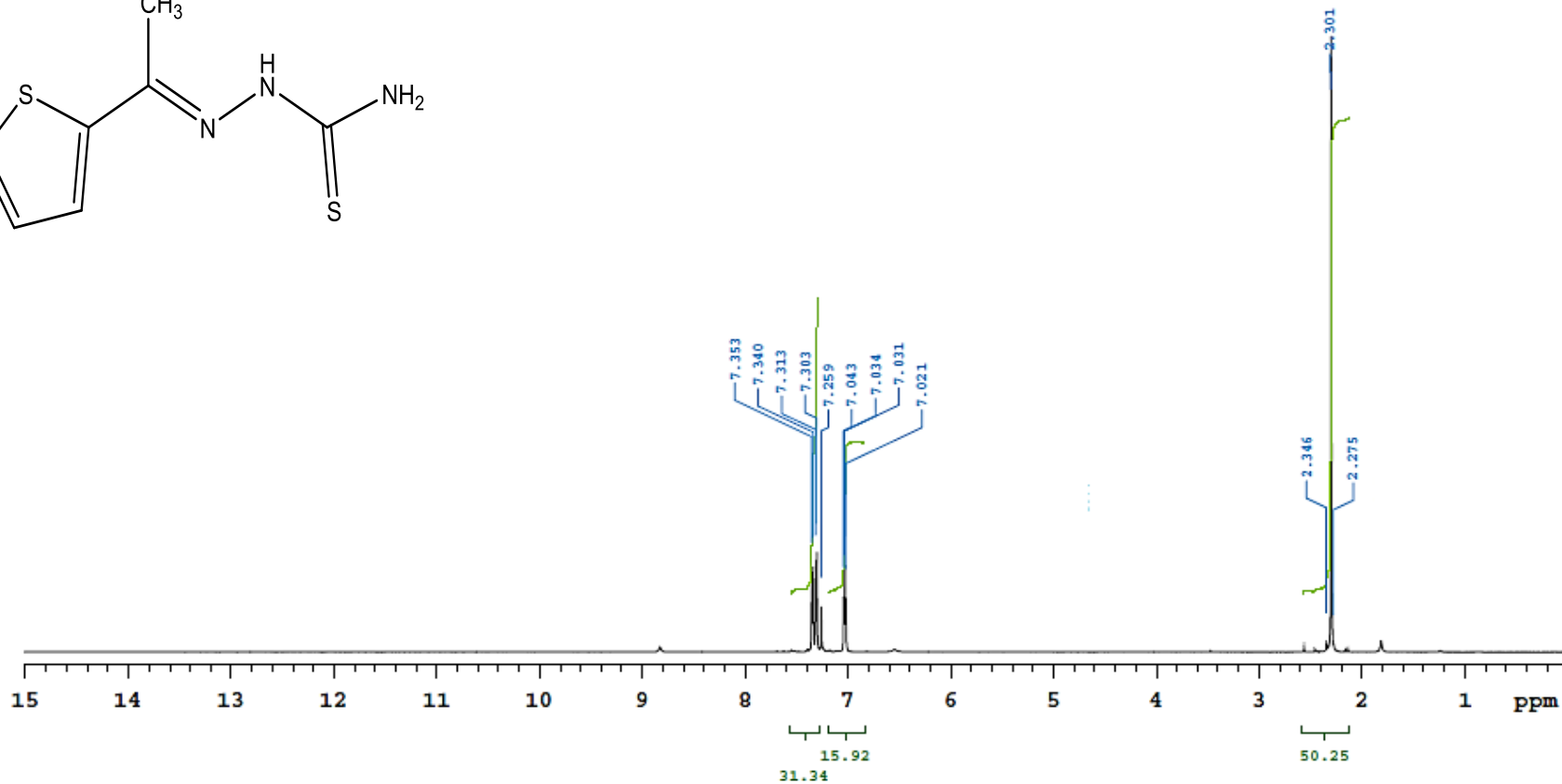
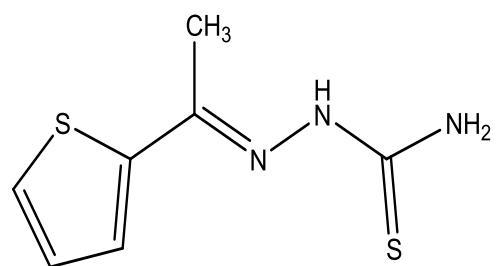
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Date collected 2017-11-13

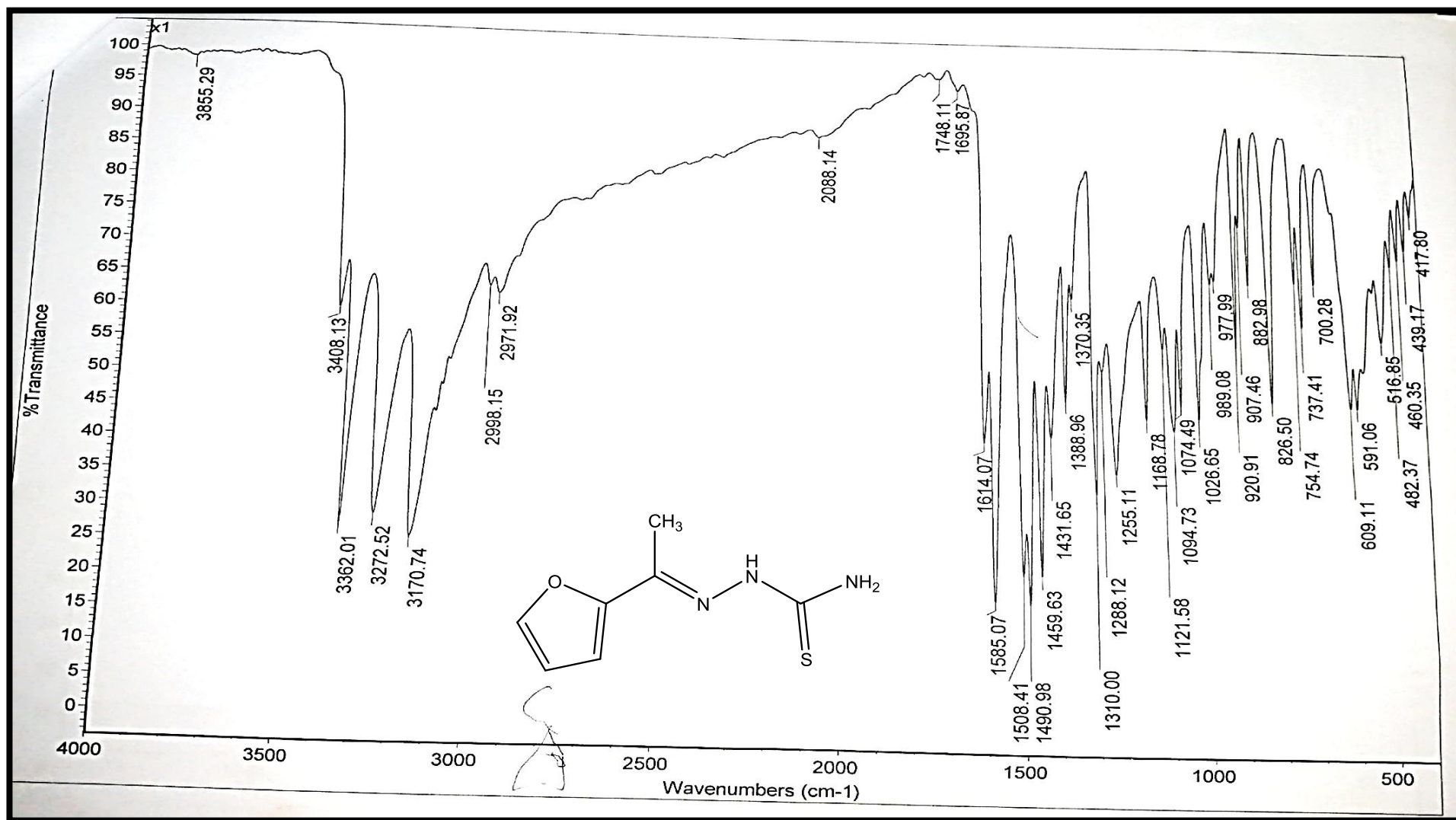
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Solvent cdcl3

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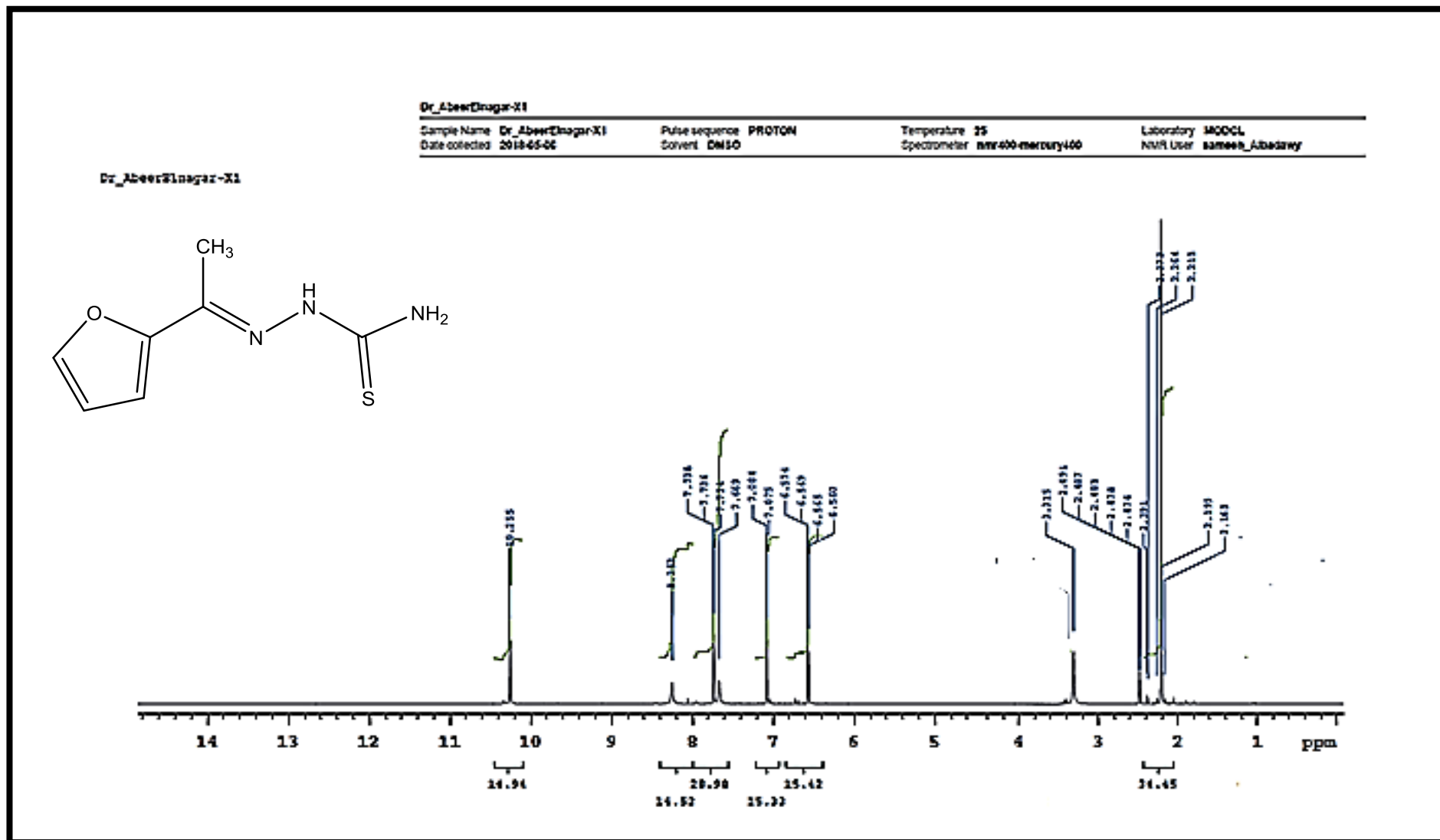
Study owner vnmr1
Operator vnmr1



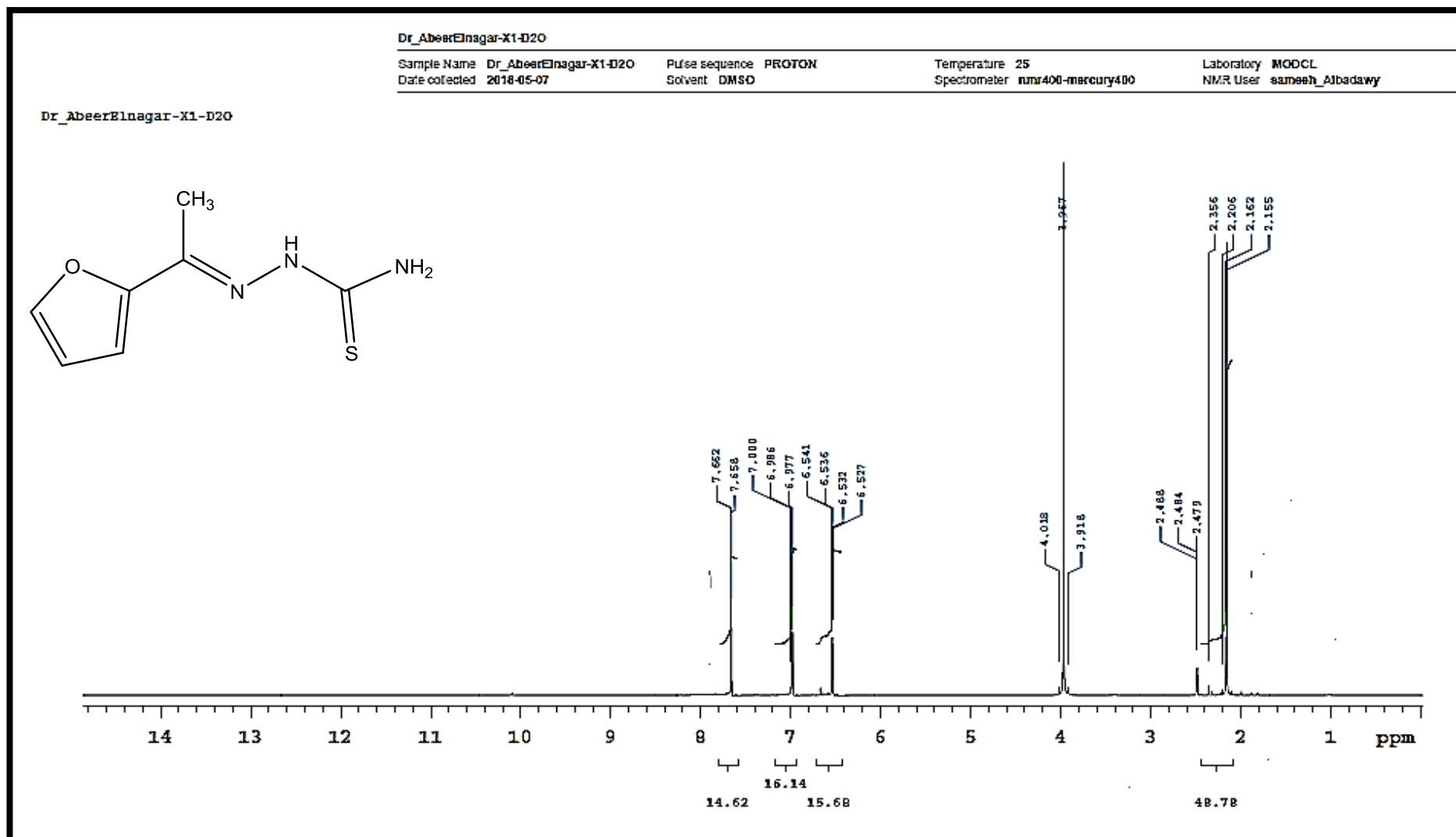
IR of compound (7b)



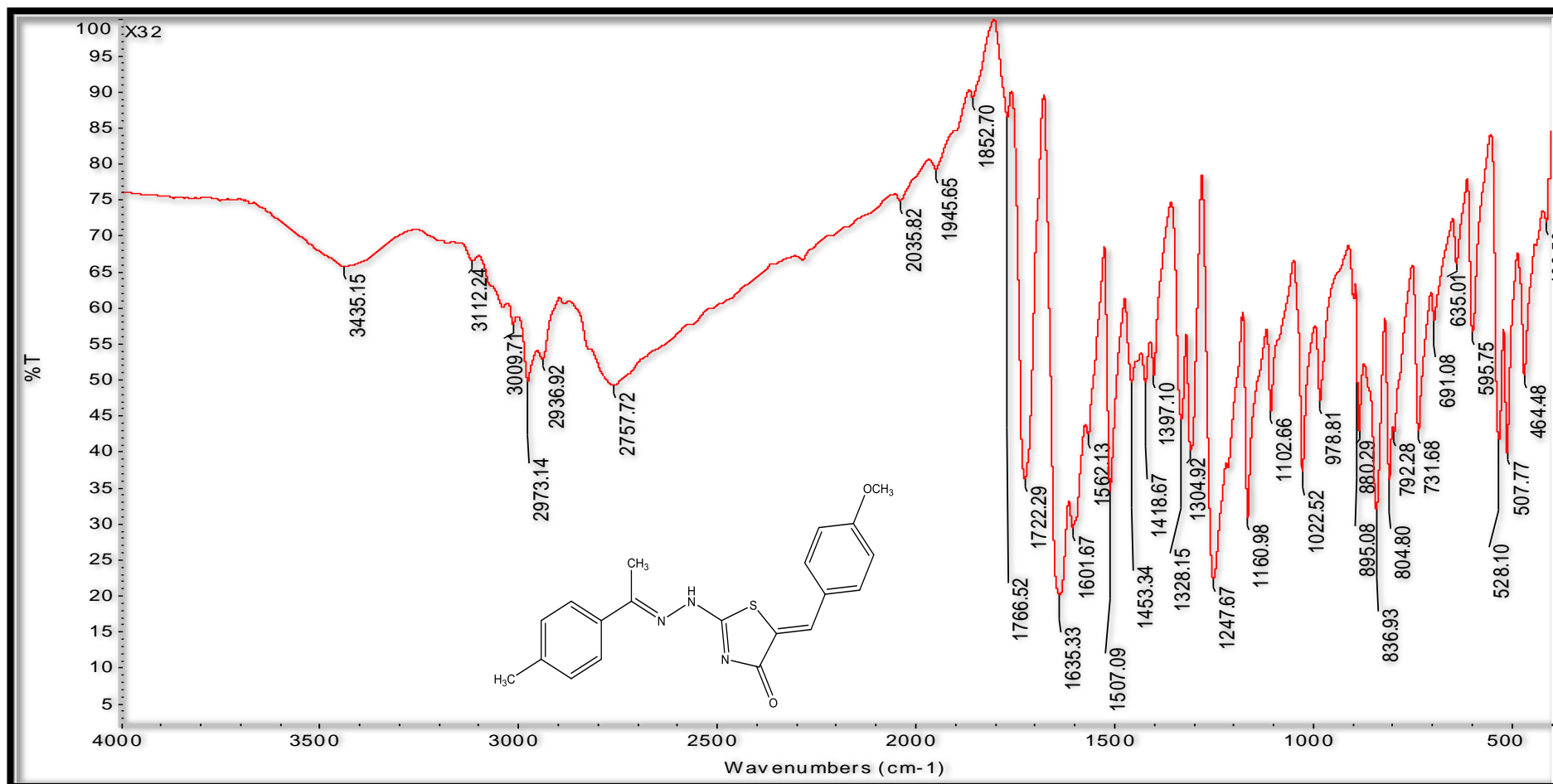
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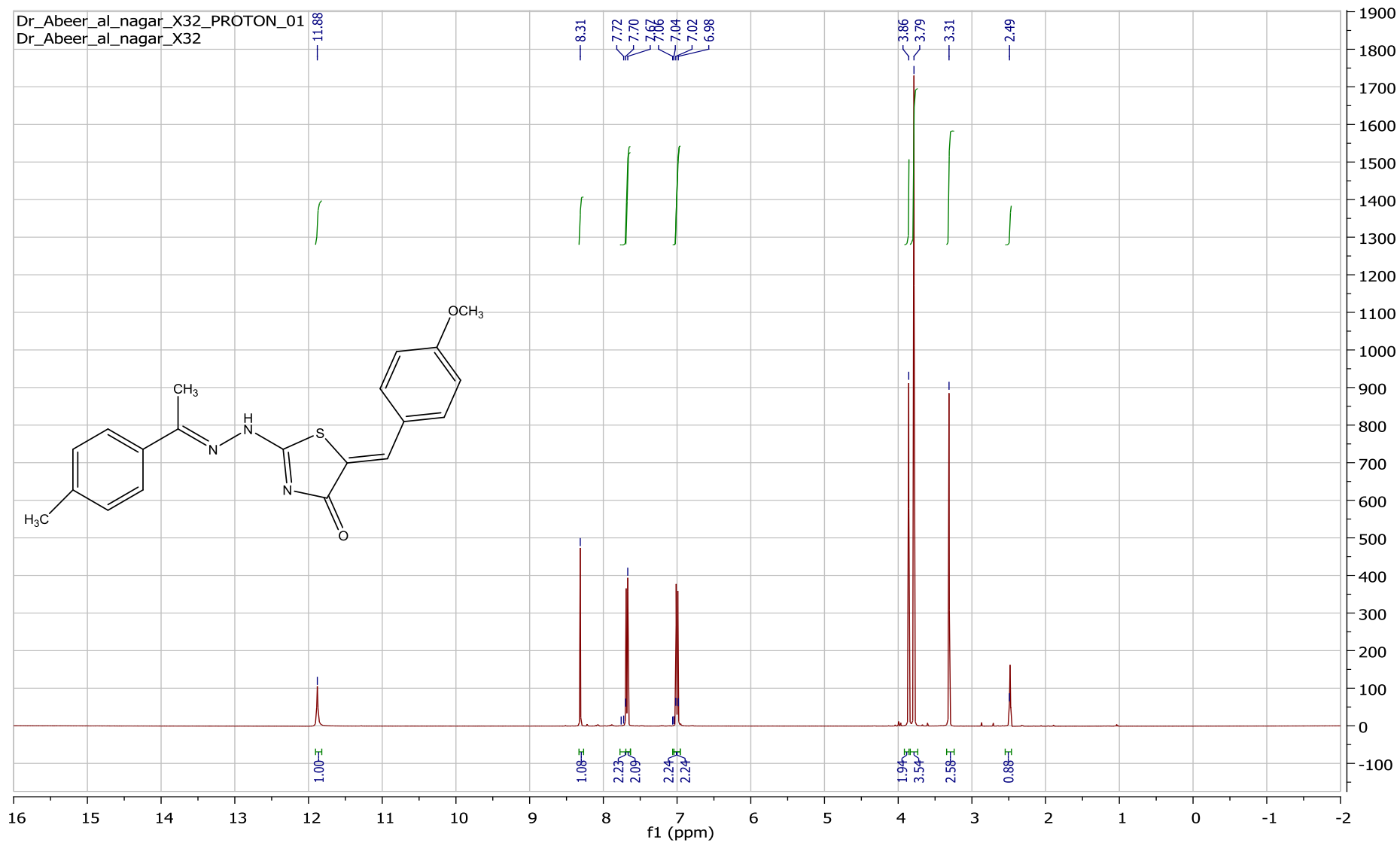
D₂O ¹H NMR of compound (7b)



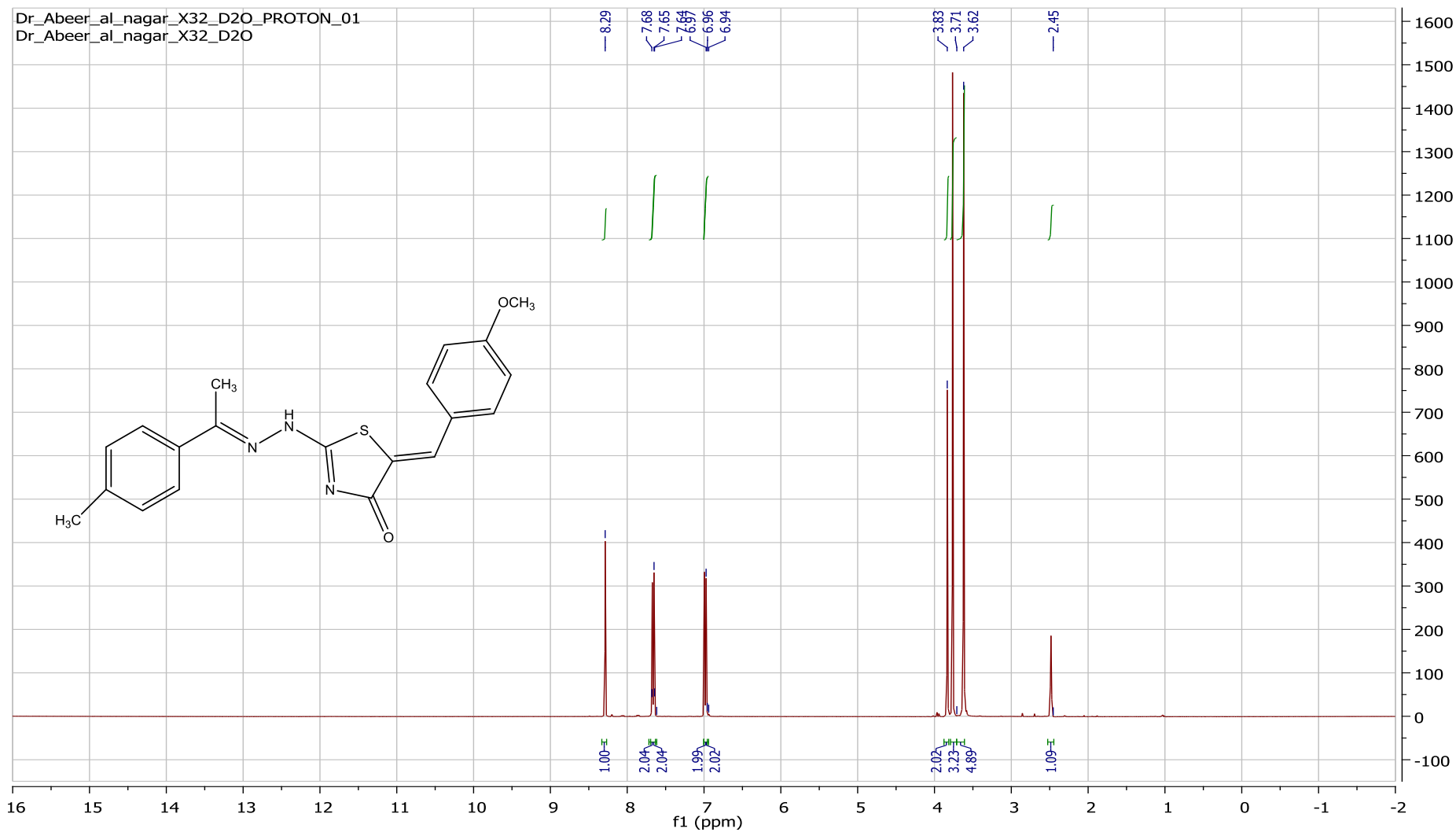
IR of compound (4a).



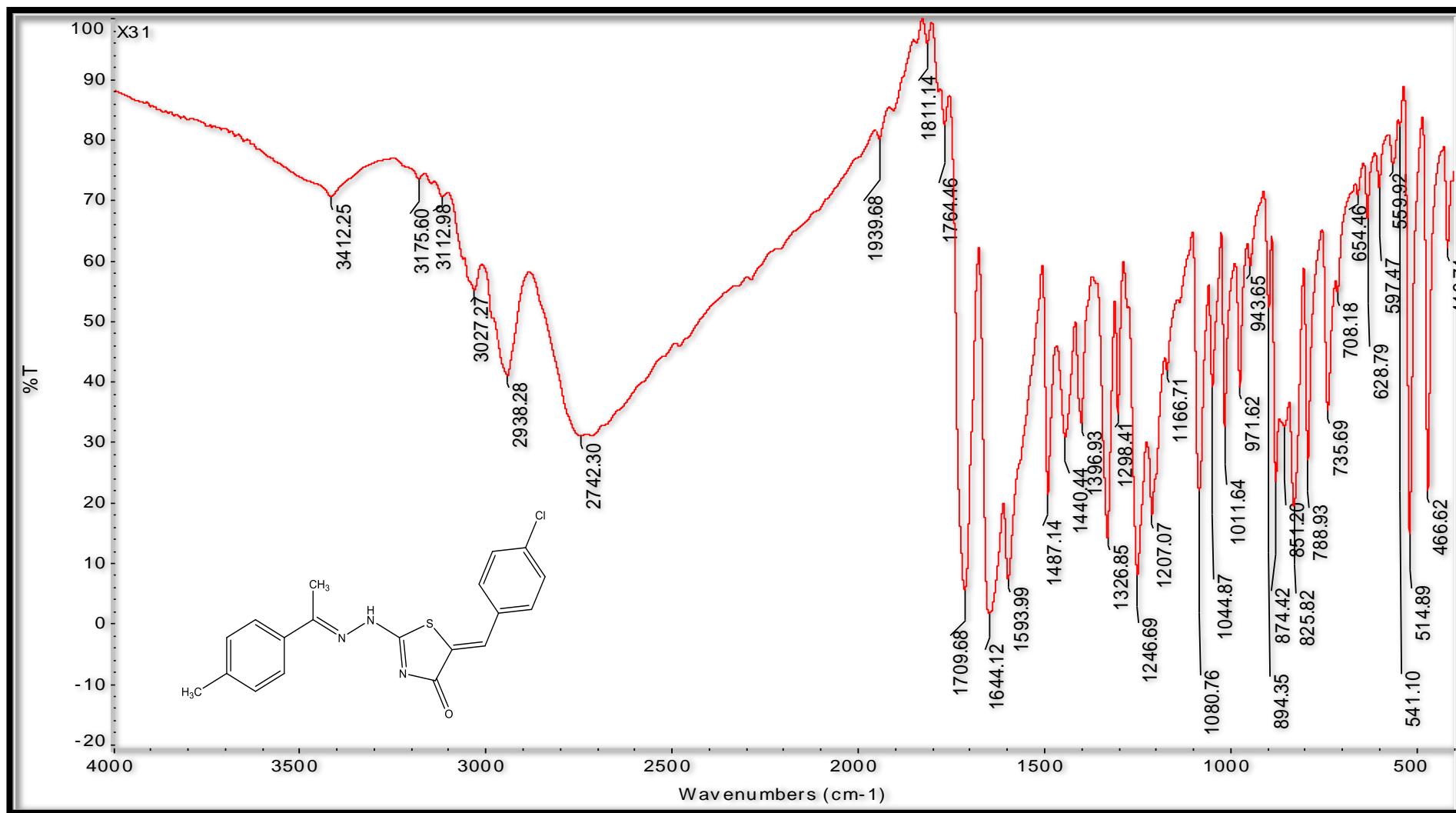
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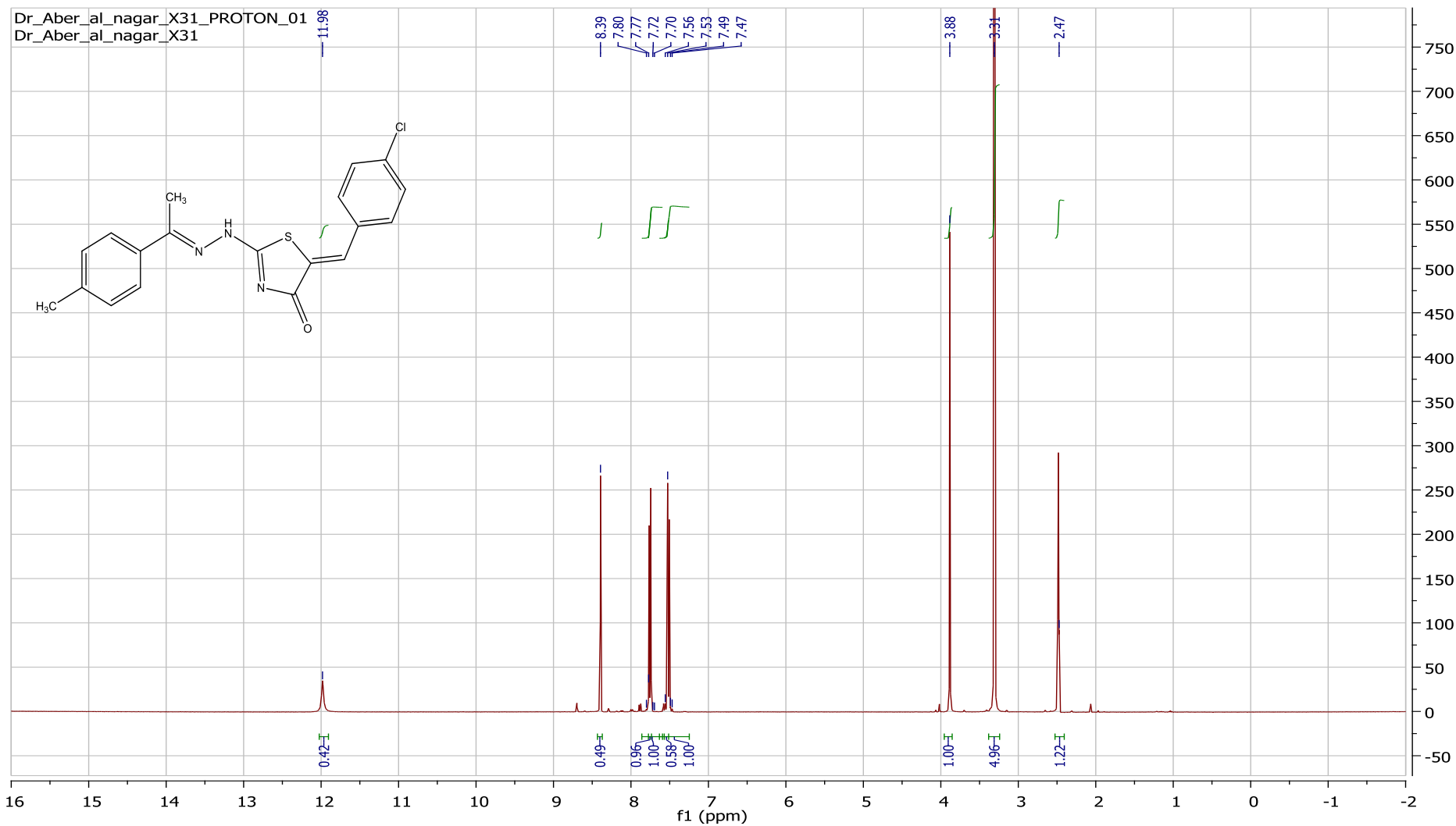
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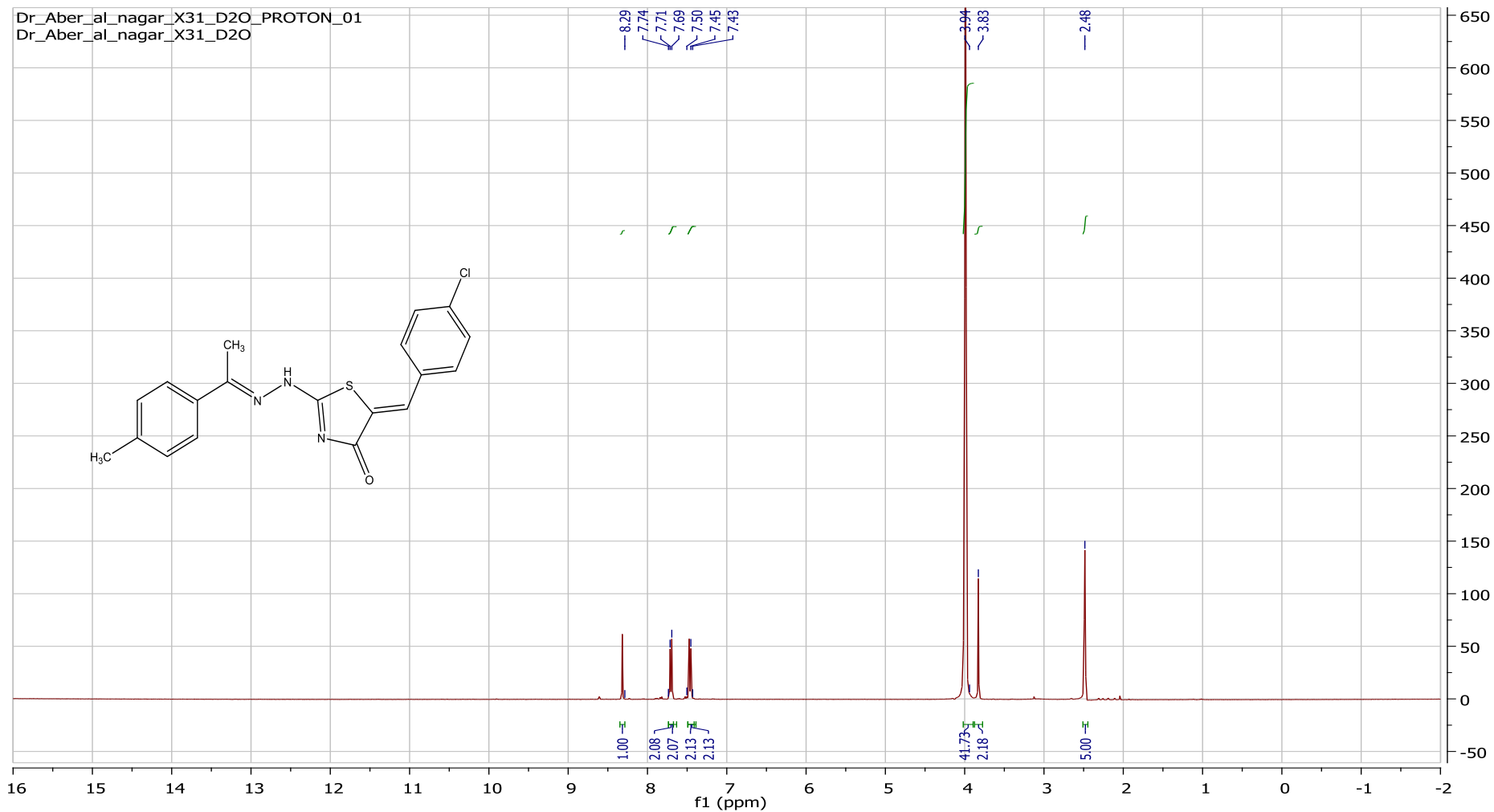
IR of compound (4b)



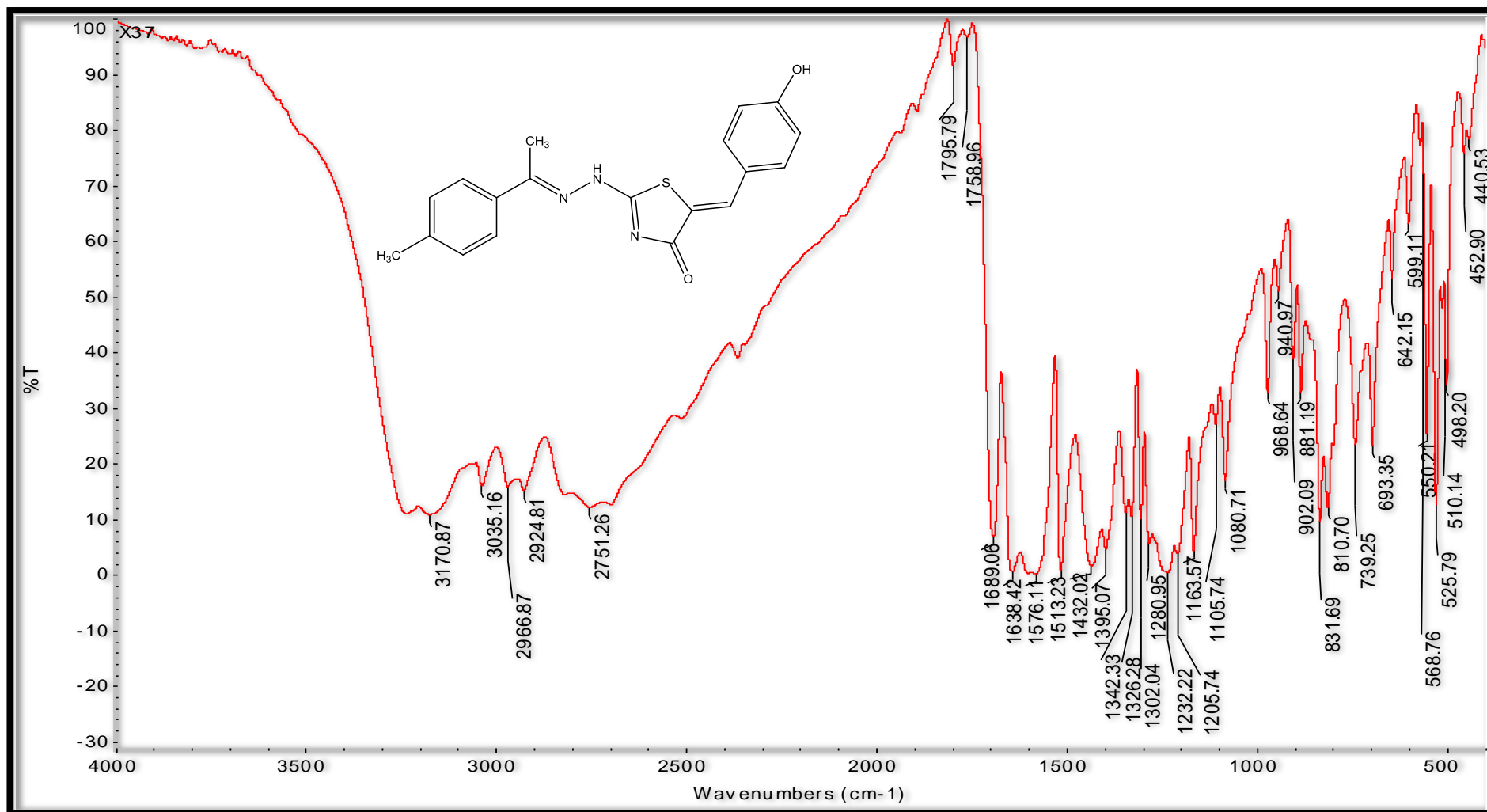
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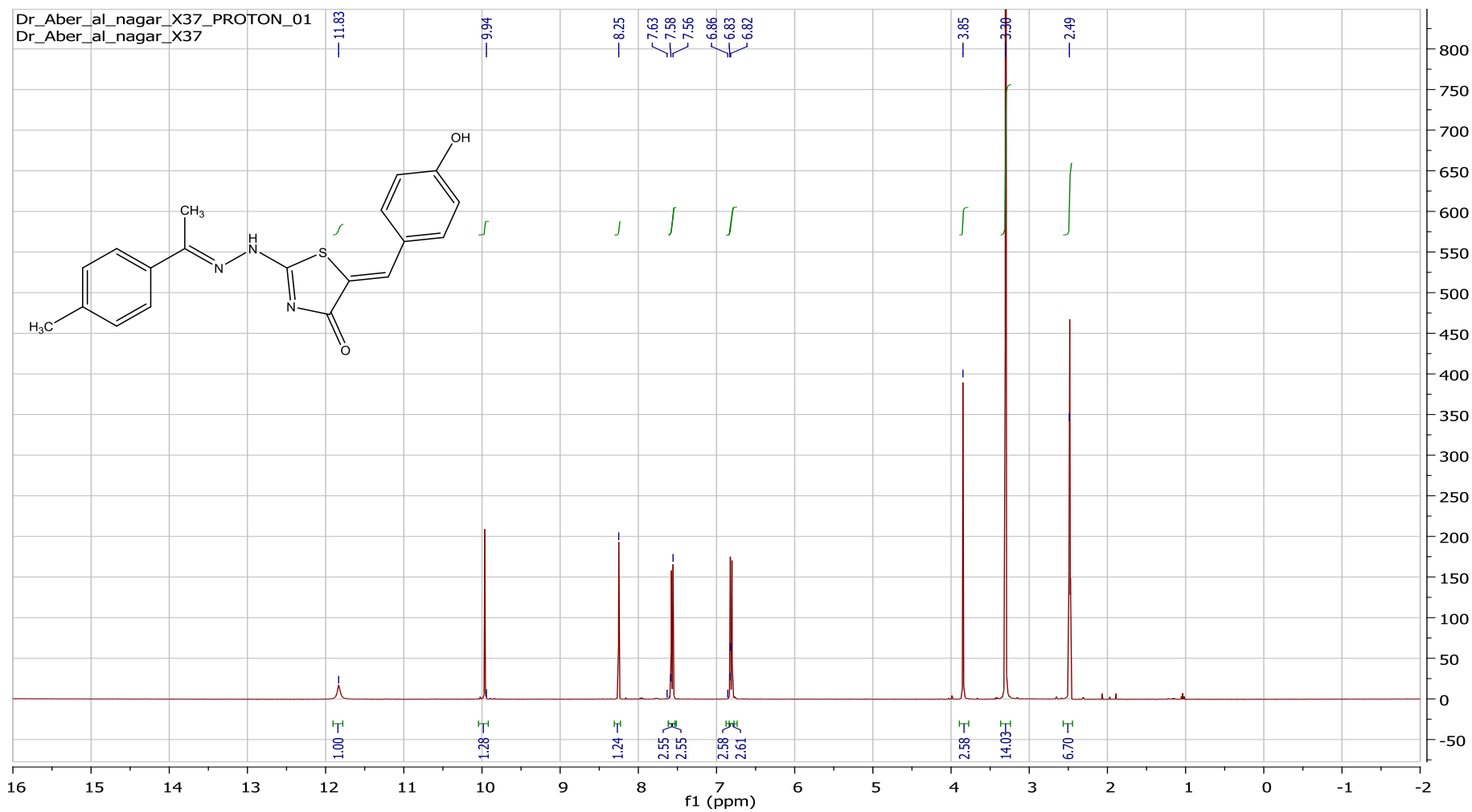
D₂O ¹H NMR of compound (4b)



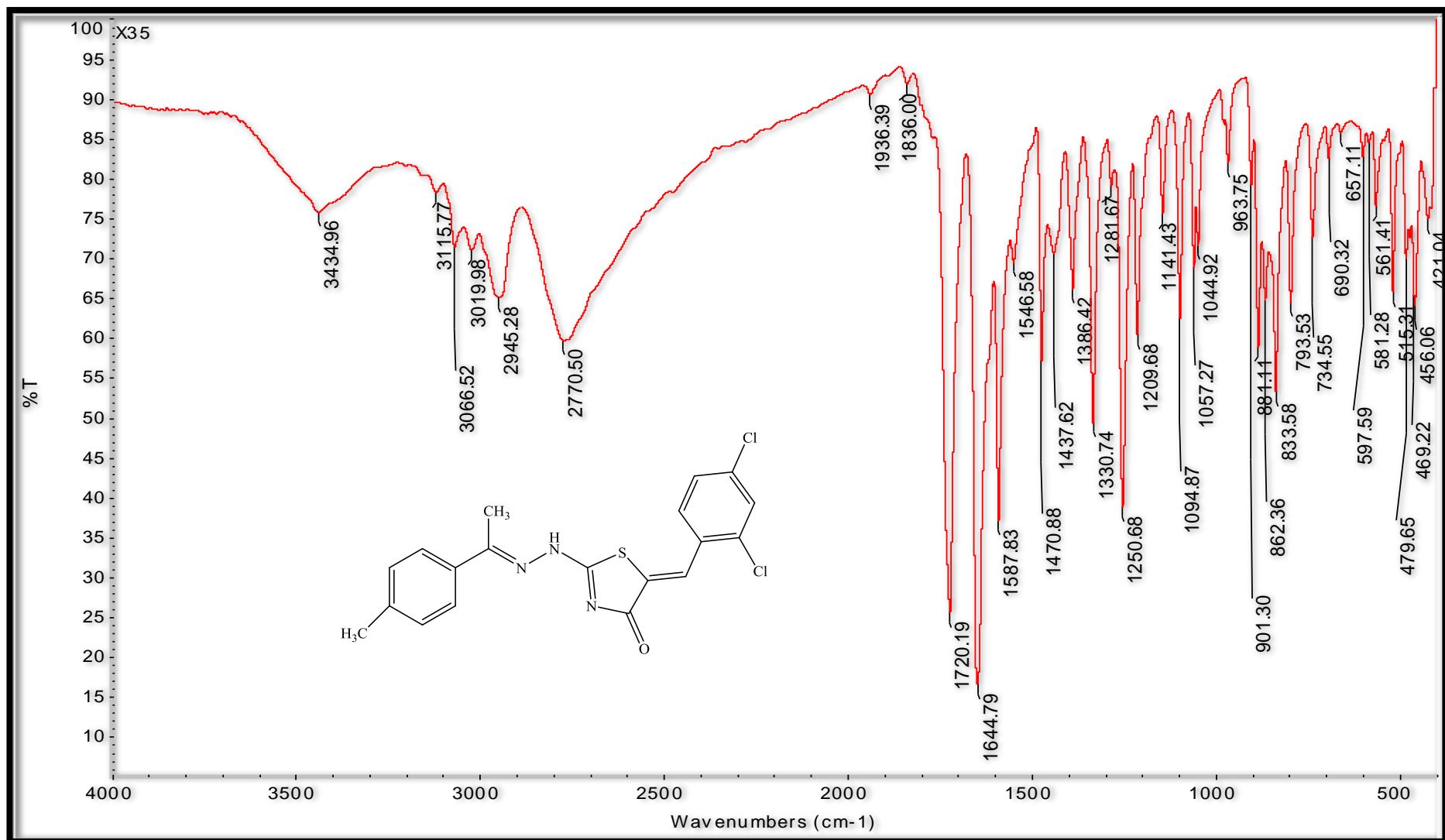
IR of compound (4c)



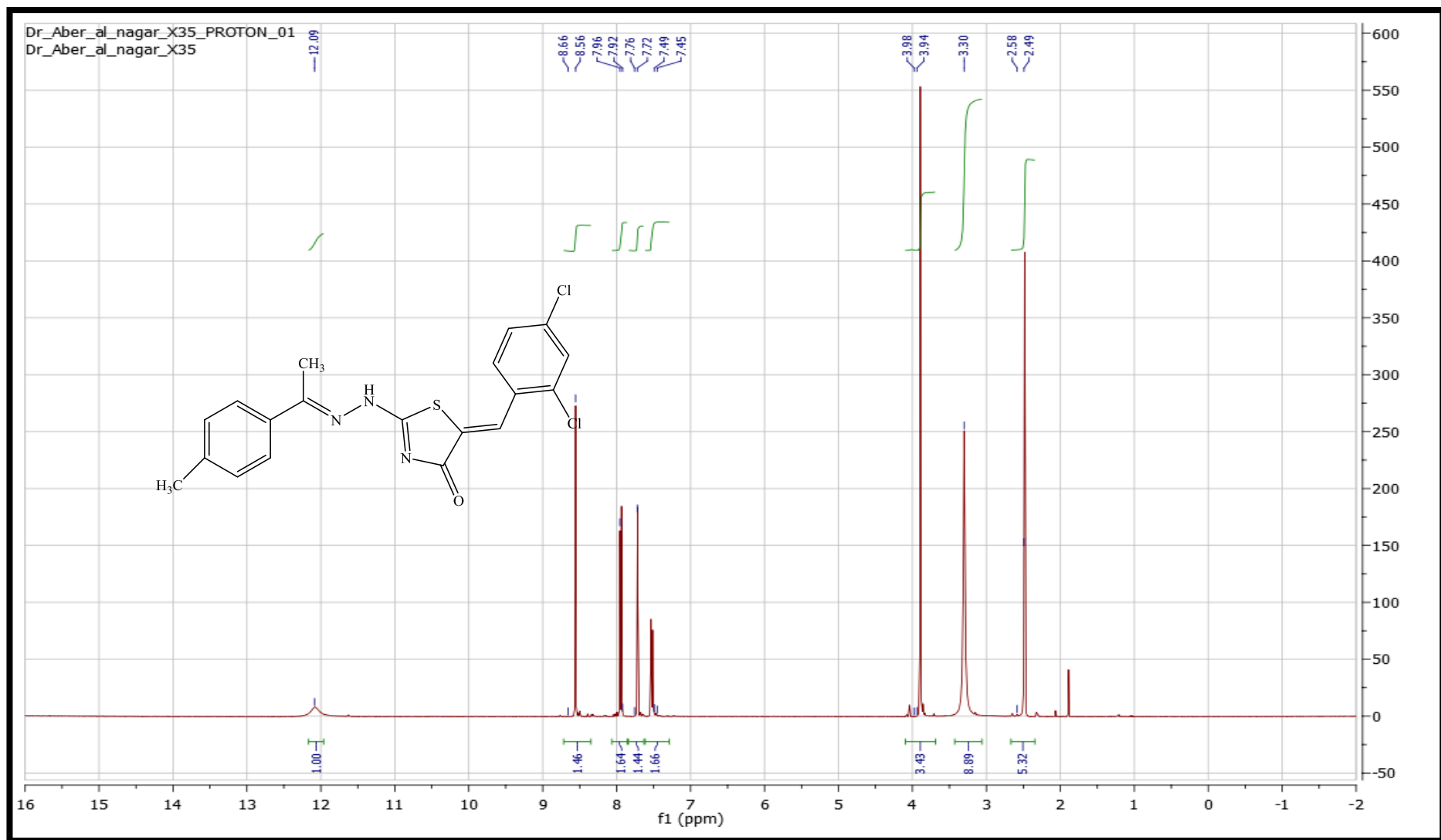
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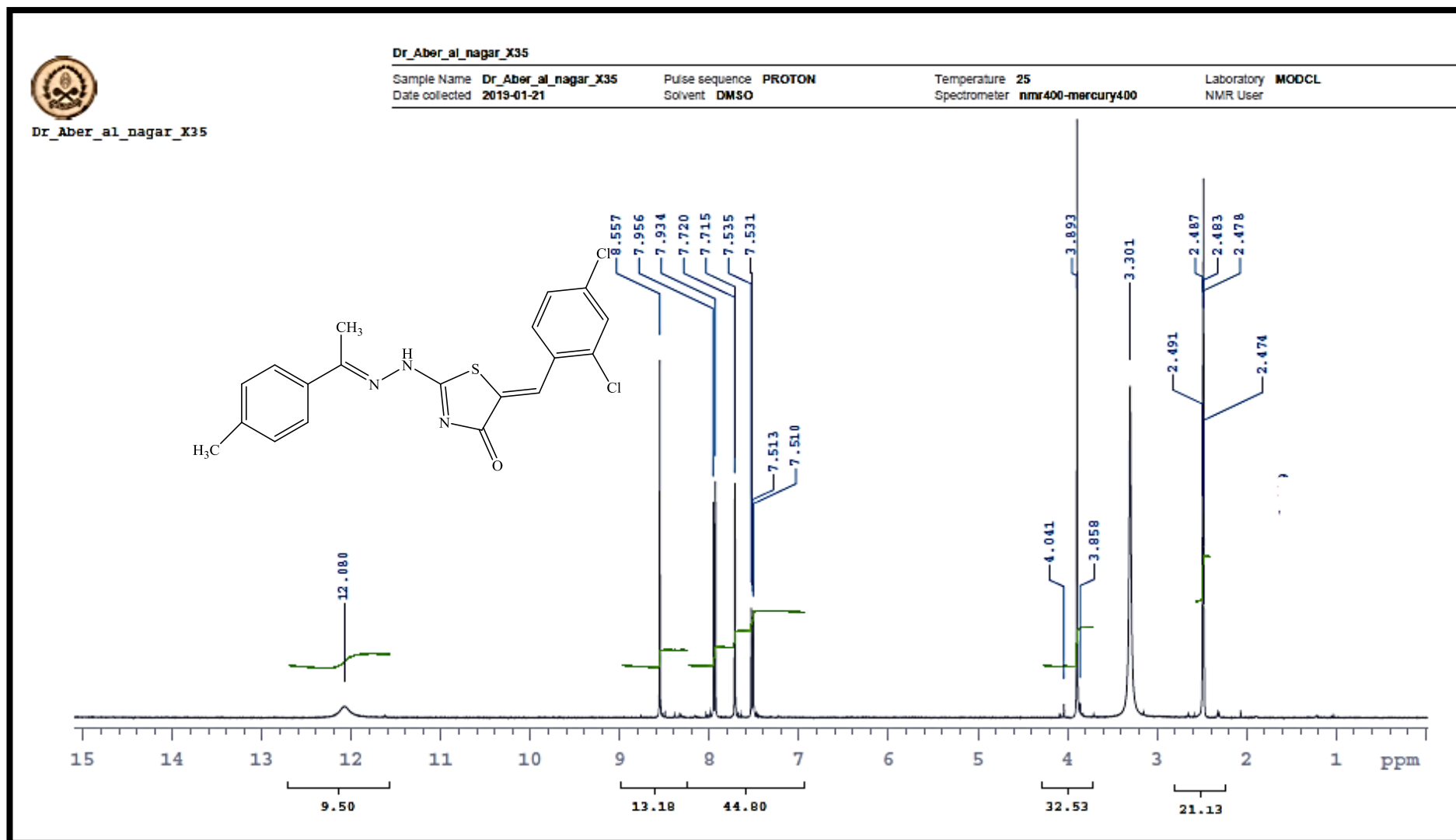
IR of compound (4d)



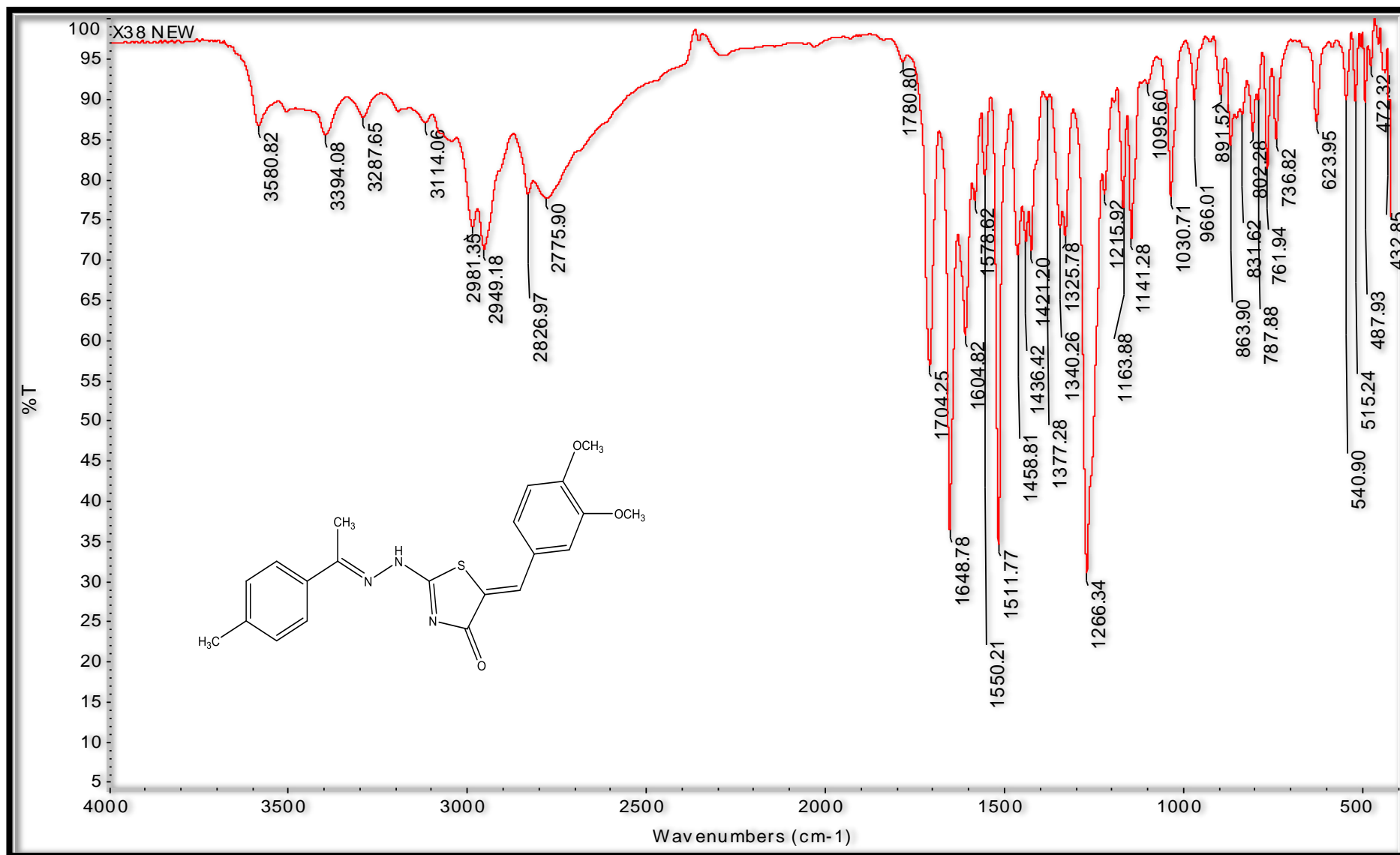
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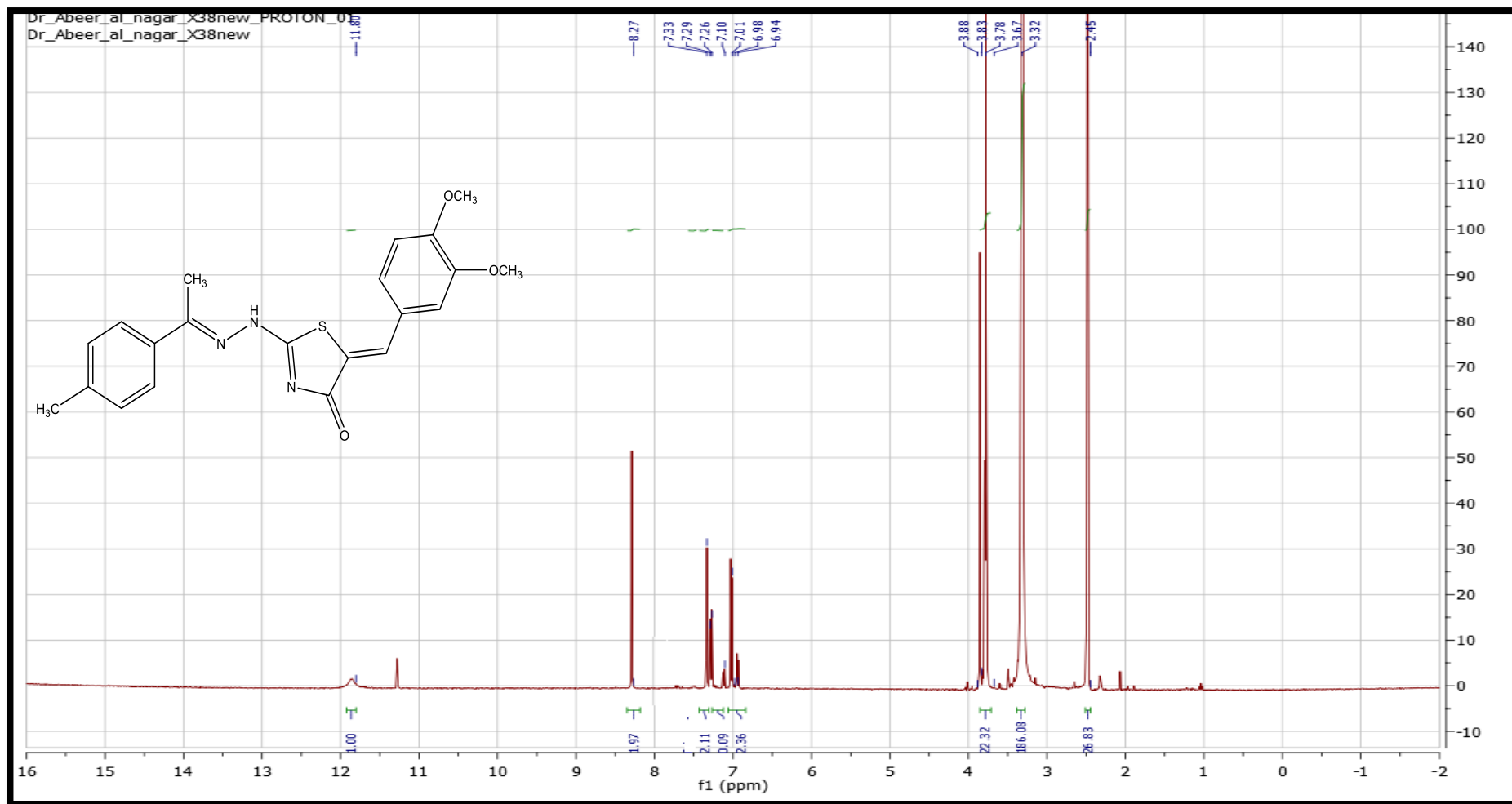
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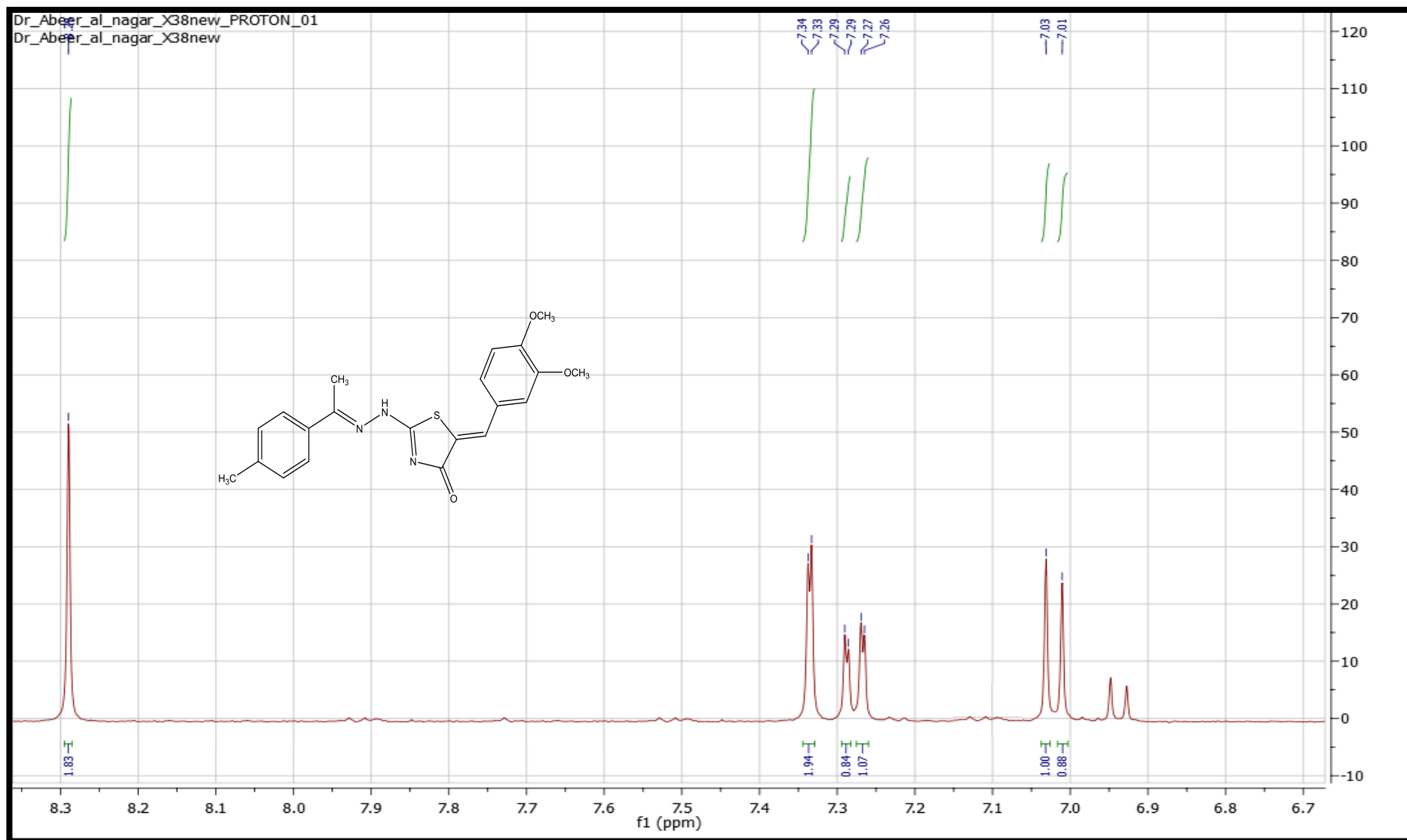
IR of compound (4e)



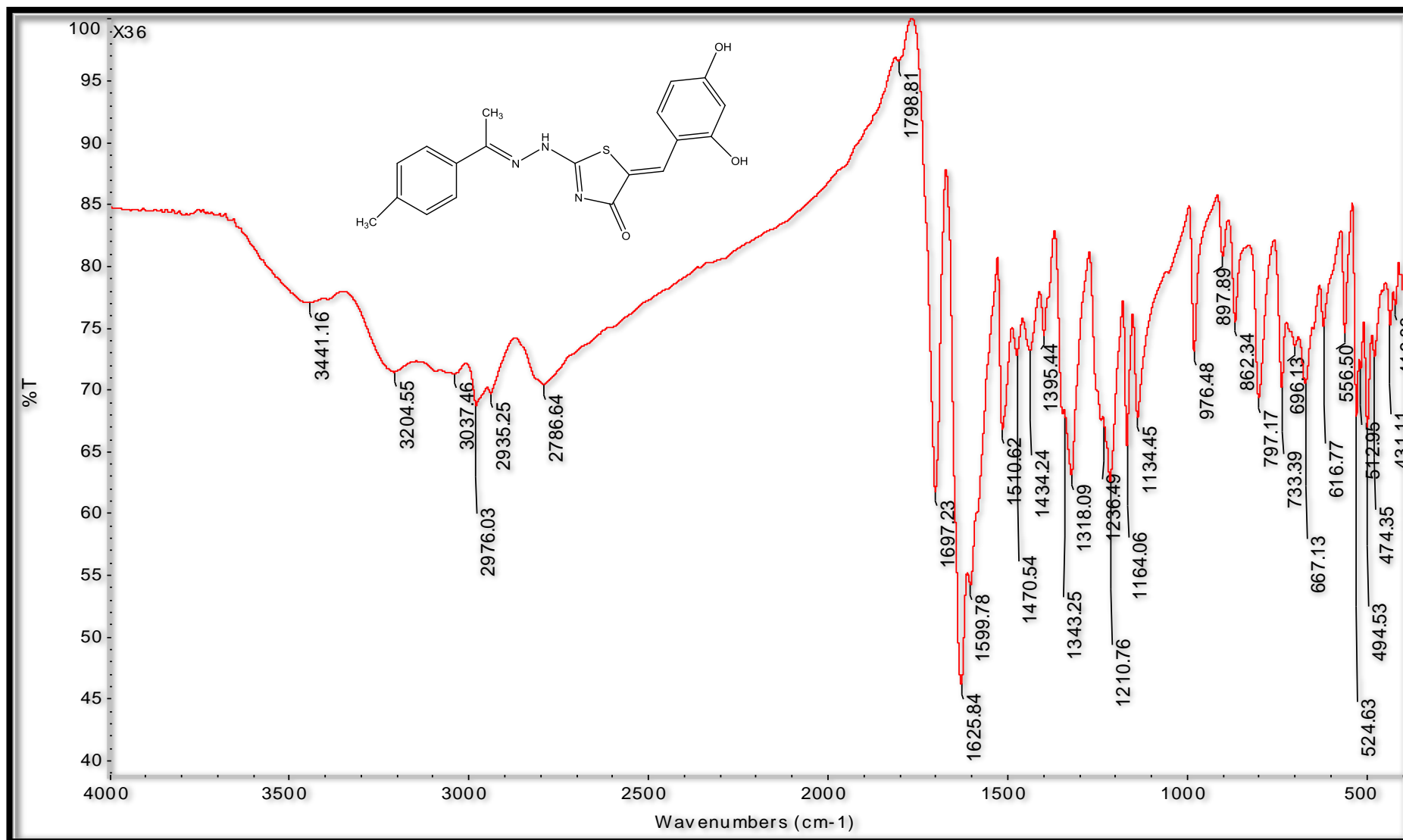
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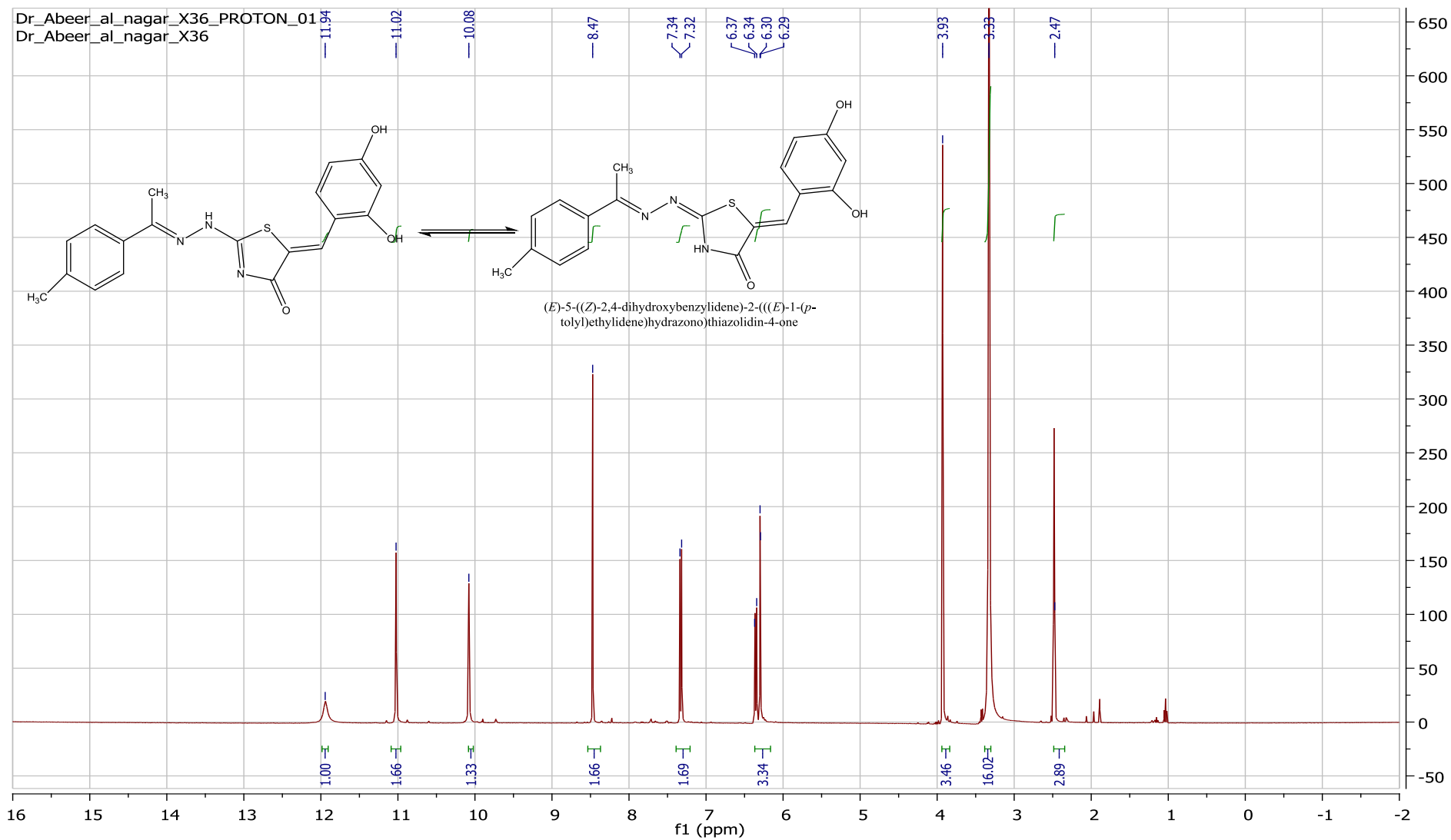
¹H NMR of compound (4e)



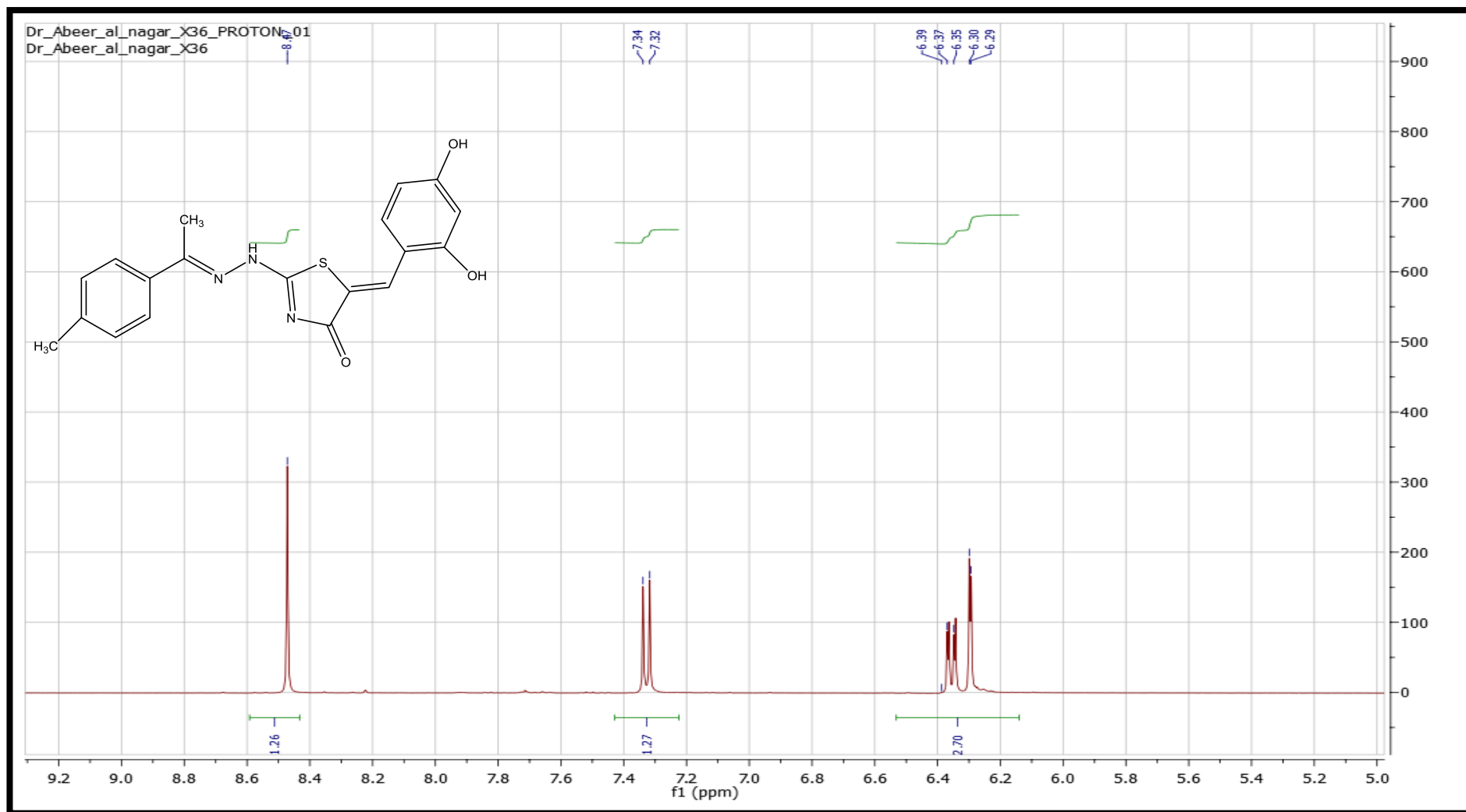
IR of compound (4f)



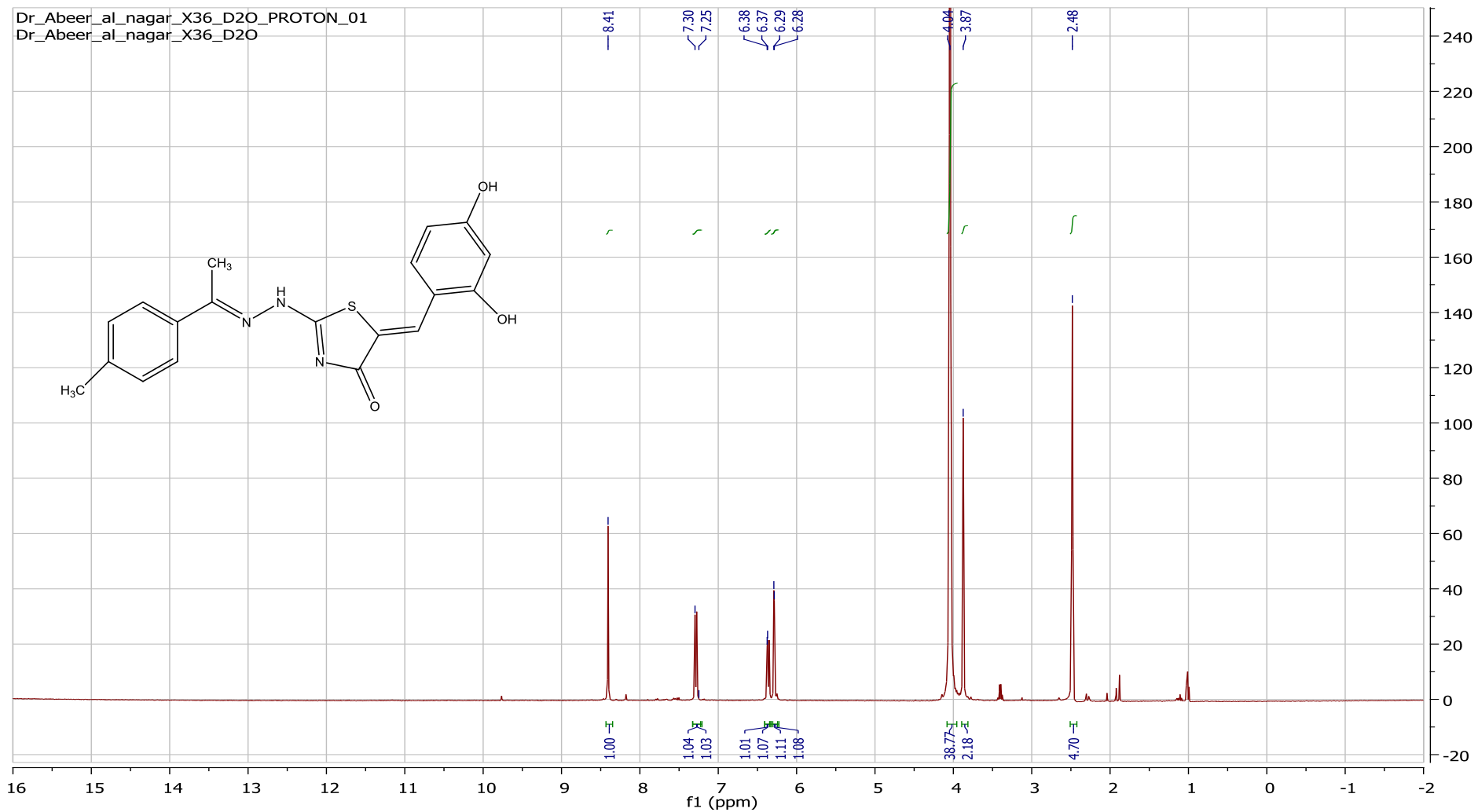
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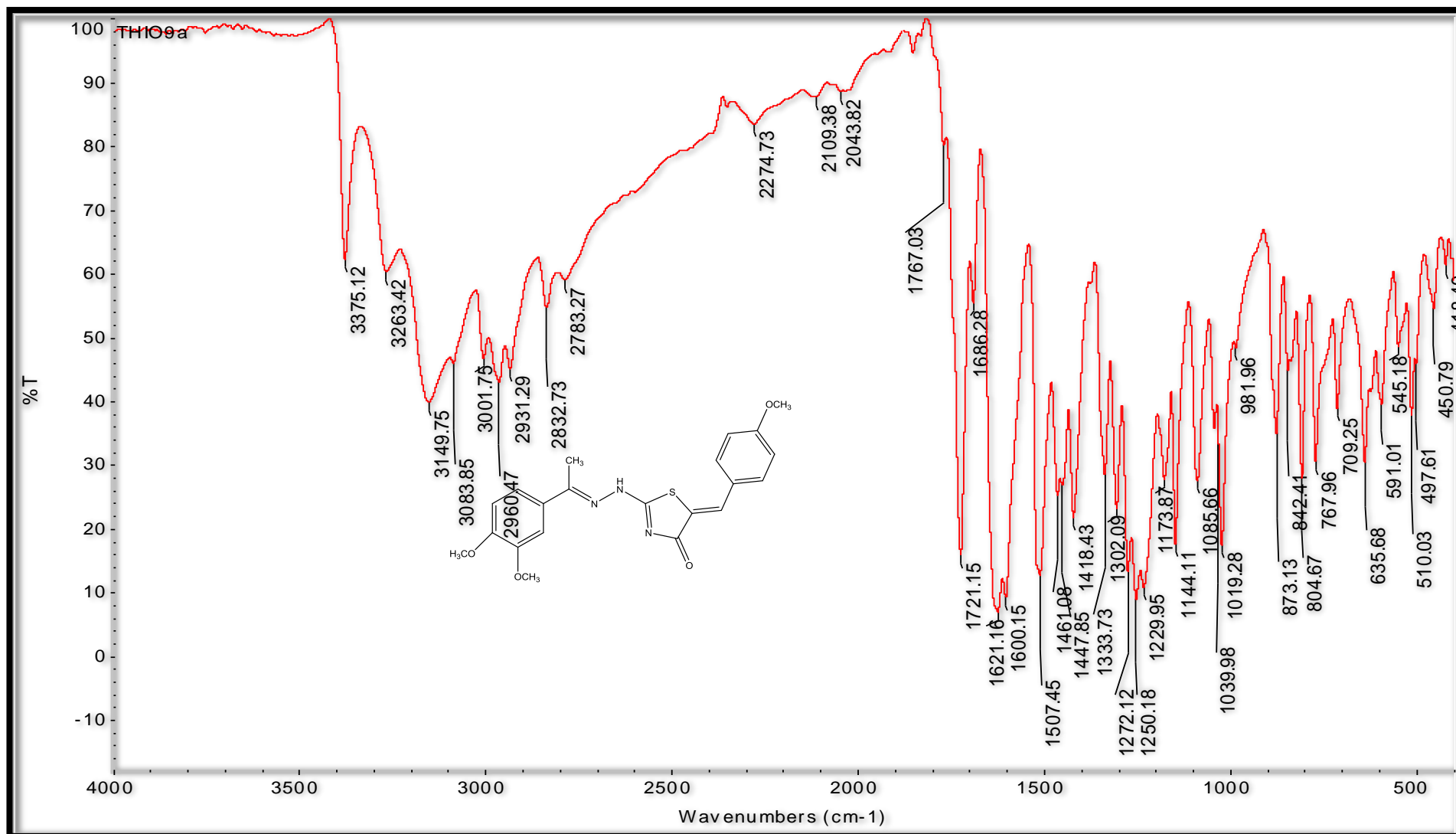
¹H NMR of compound (4f)



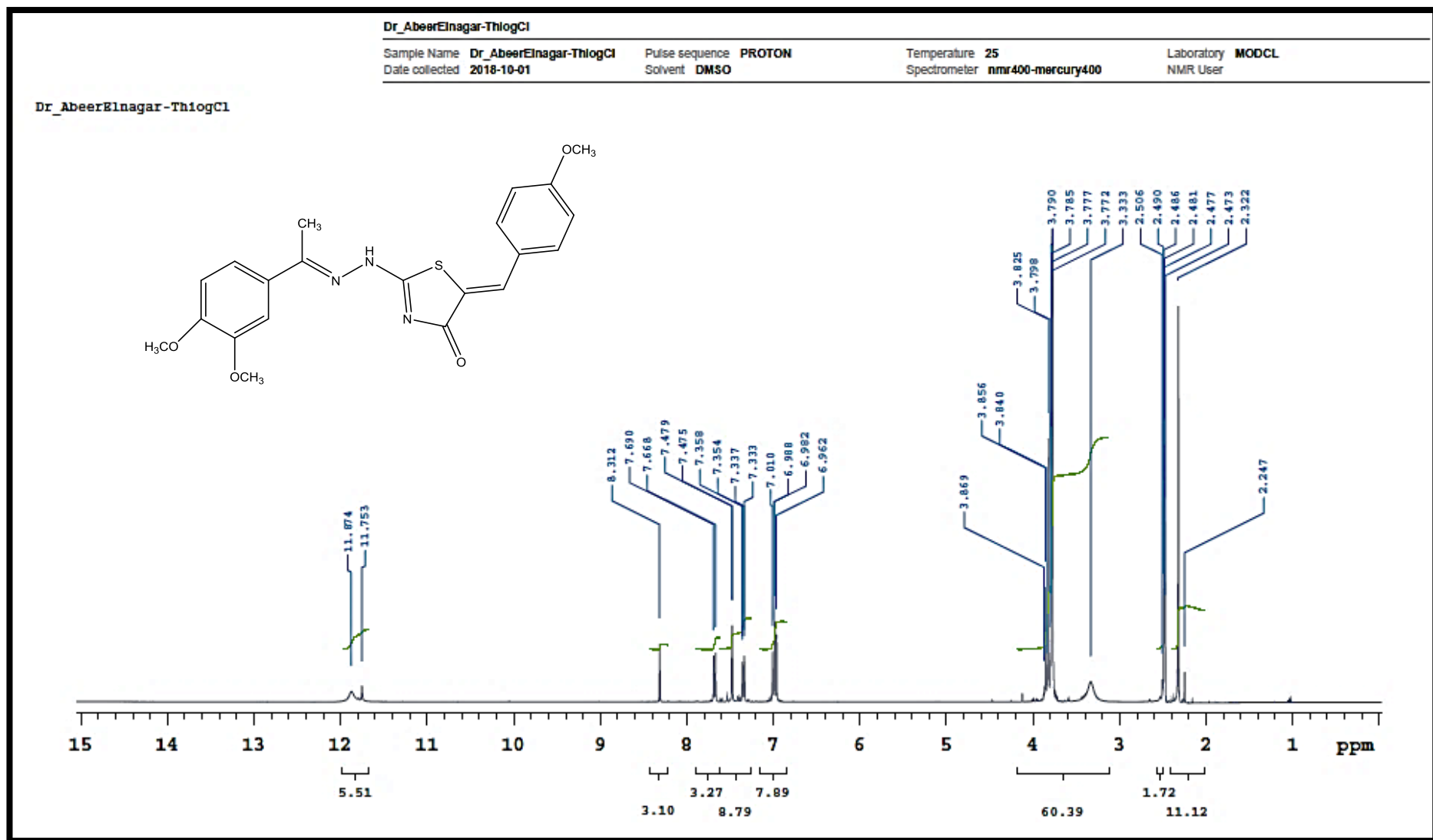
D₂O ¹H NMR of compound (4f)



IR of compound (4g).



¹H NMR of compound (4g).



D₂O ¹H NMR of compound (4g)

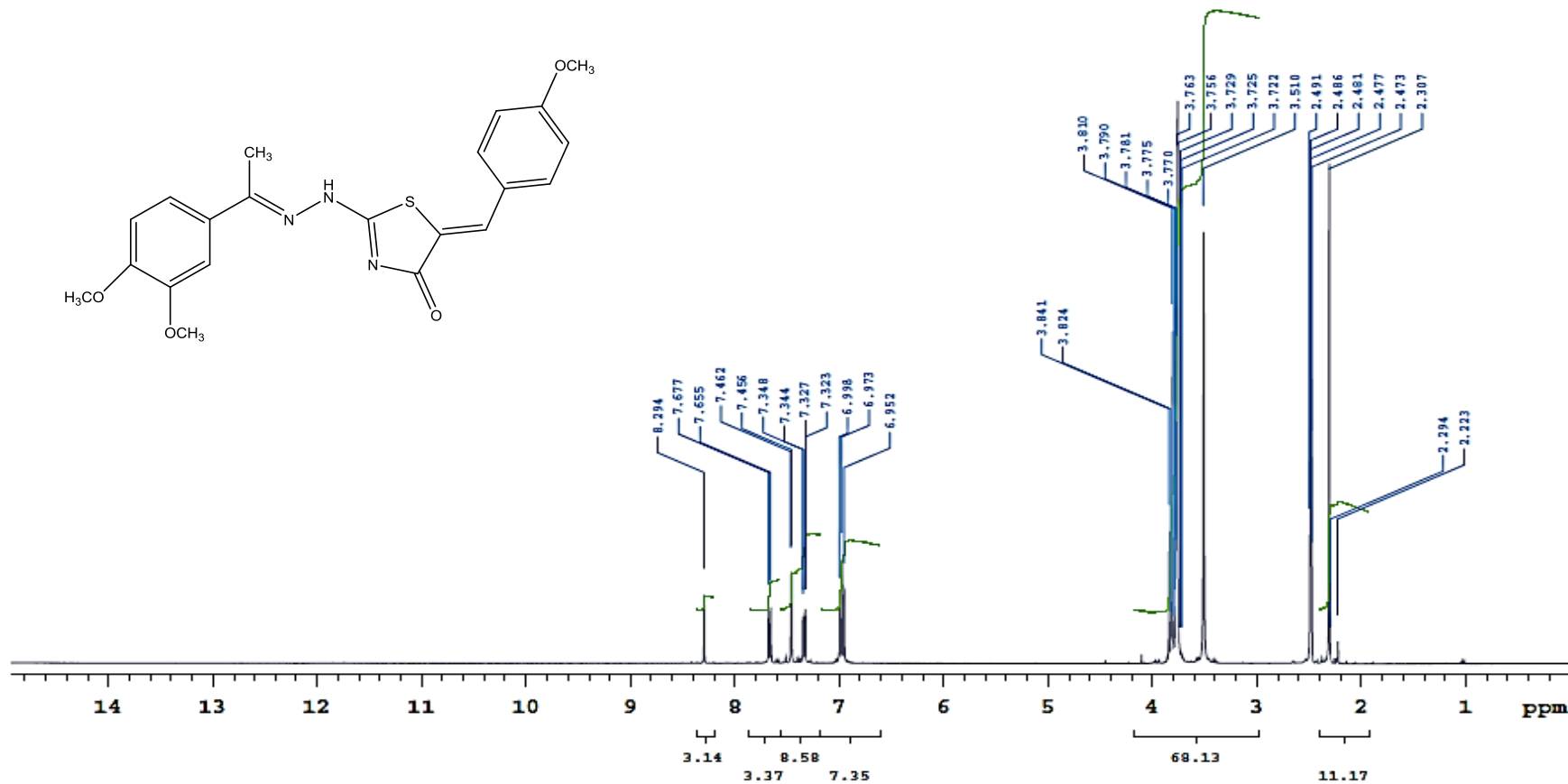
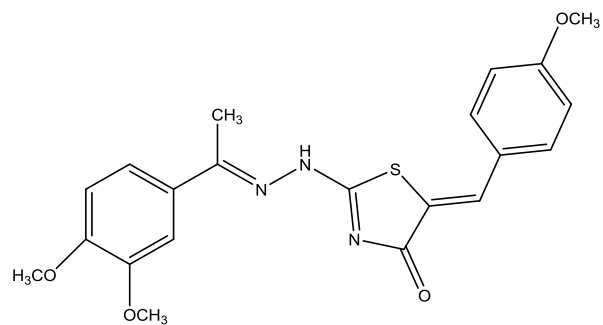
Dr_AbeerElmagar-ThiogCl-D2O

Sample Name **Dr_AbeerElmagar-ThiogCl-D2O** Pulse sequence **PROTON**
Date collected **2018-10-02** Solvent **DMSO**

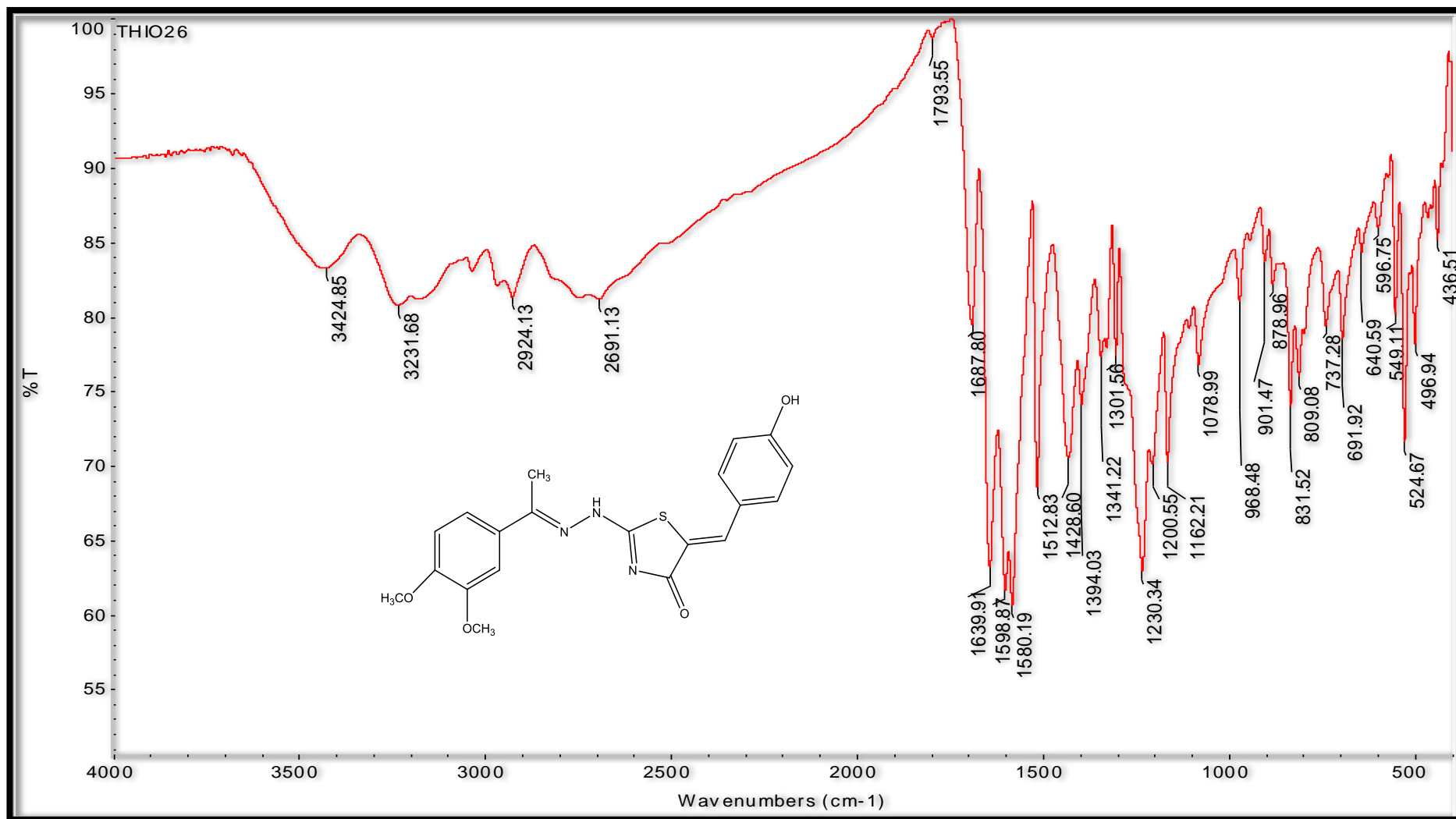
Temperature **25**
Spectrometer **nmr400-mercury400**

Laboratory **MODCL**
NMR User **sameeh_Albadawy**

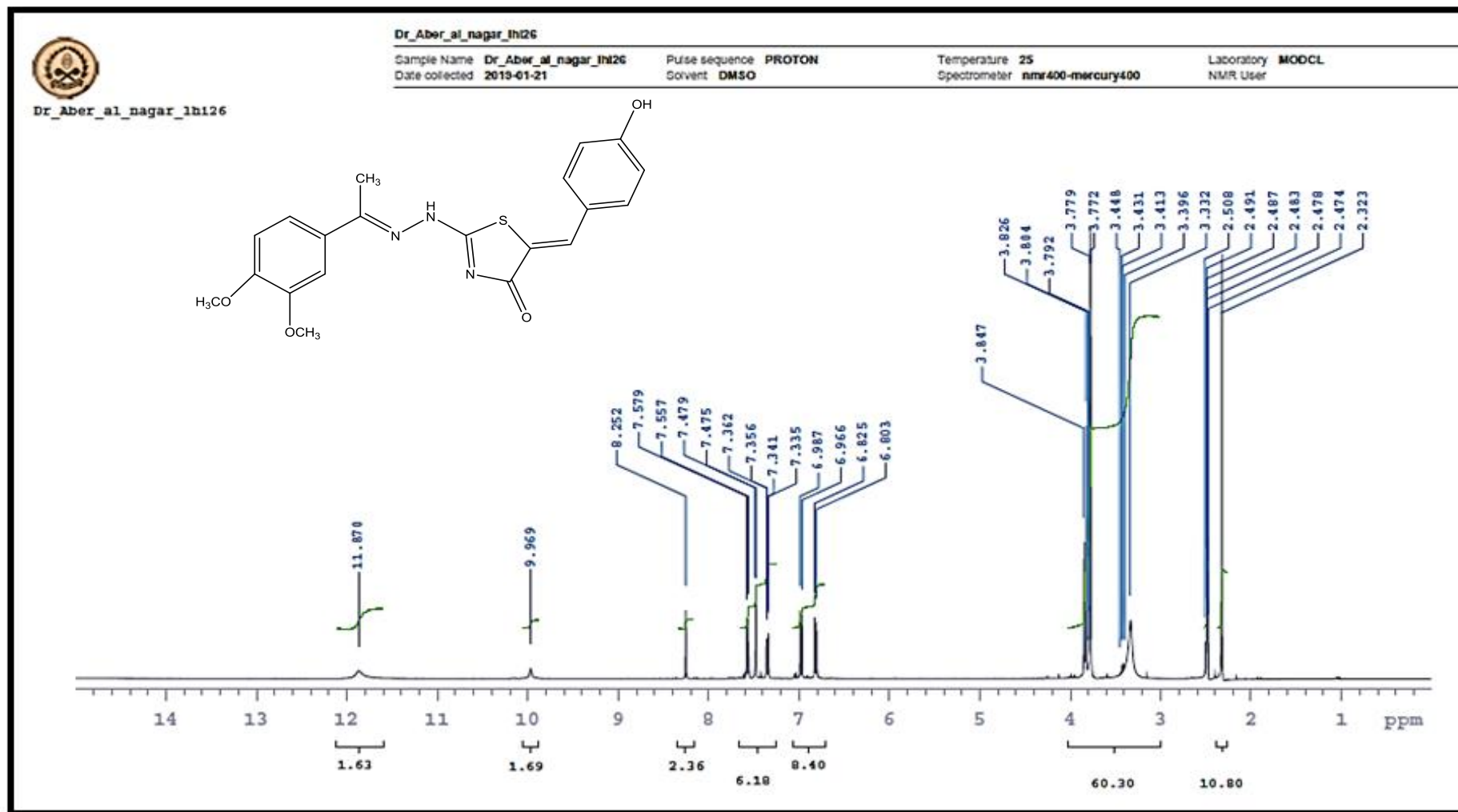
Dr_AbeerElmagar-ThiogCl-D2O



IR of compound (4h).

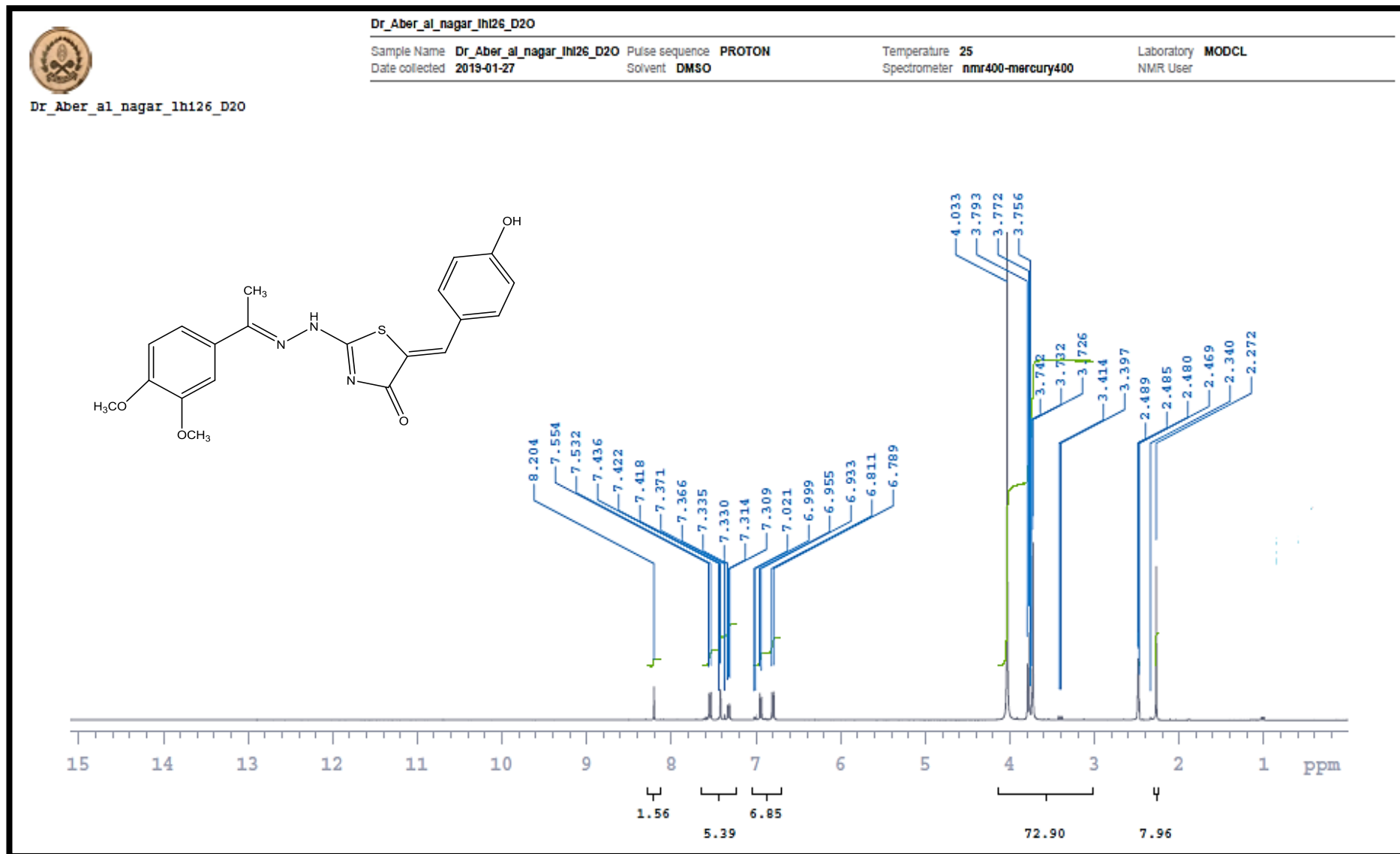


¹H NMR of compound (4h)

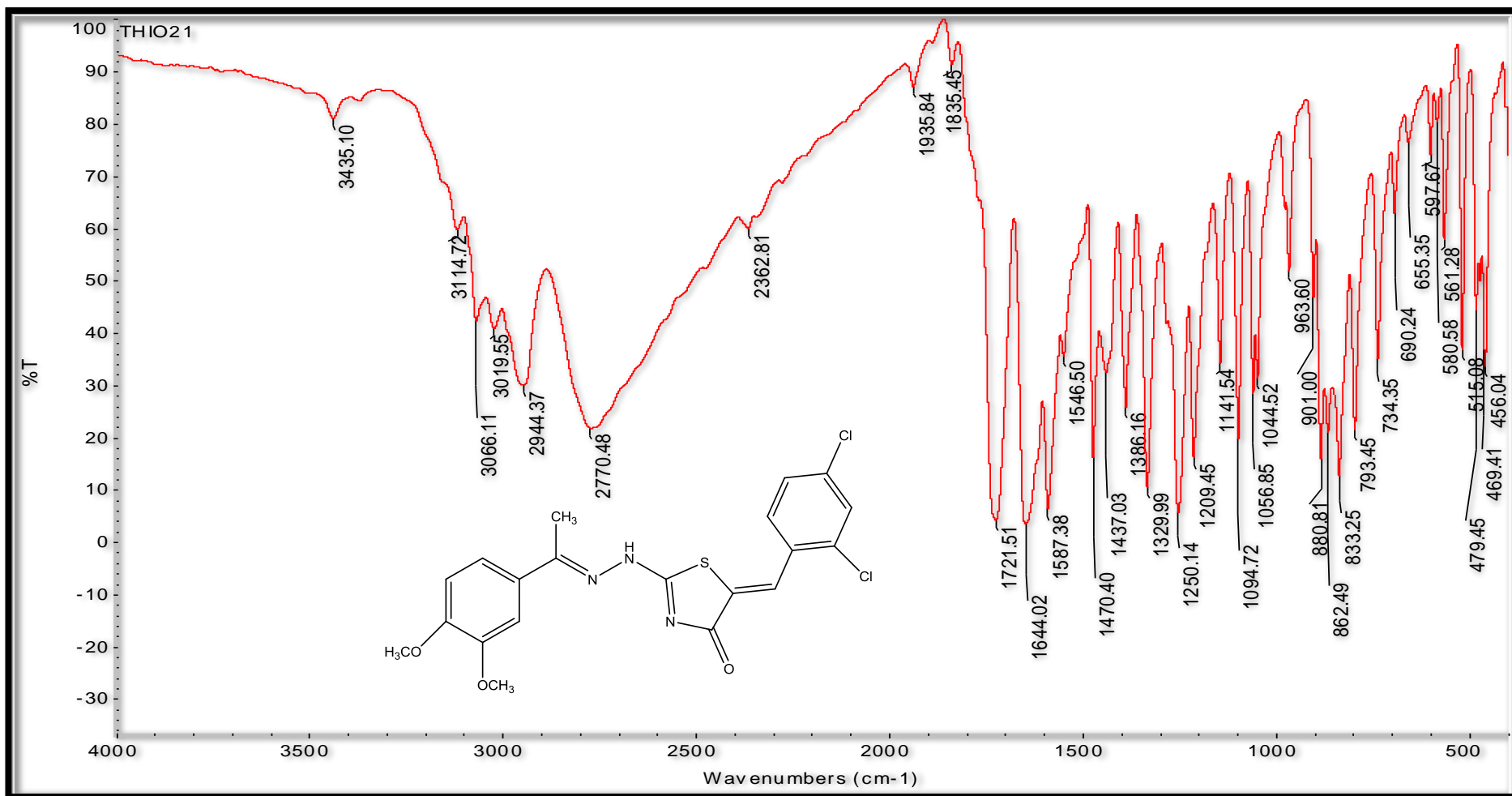


OH

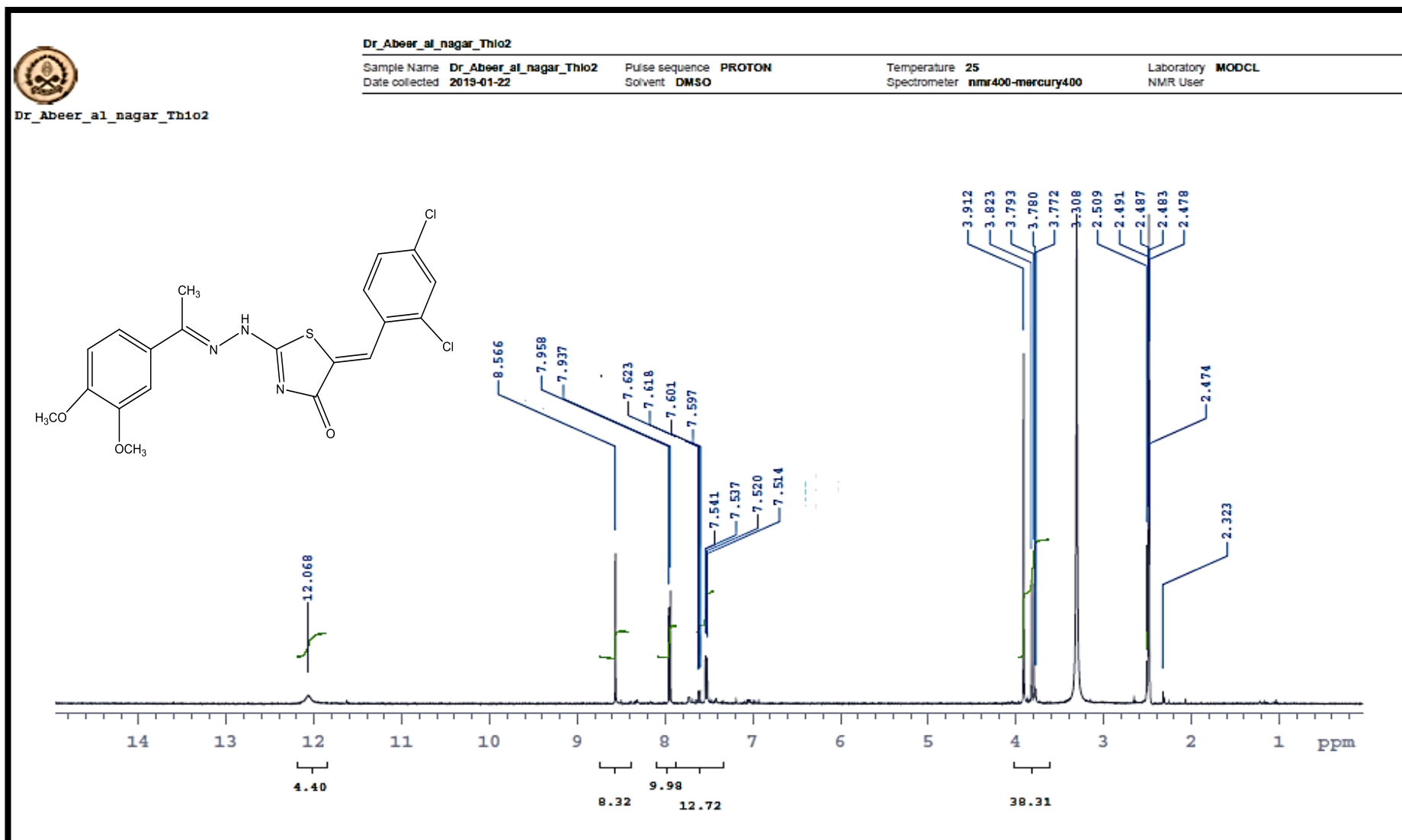
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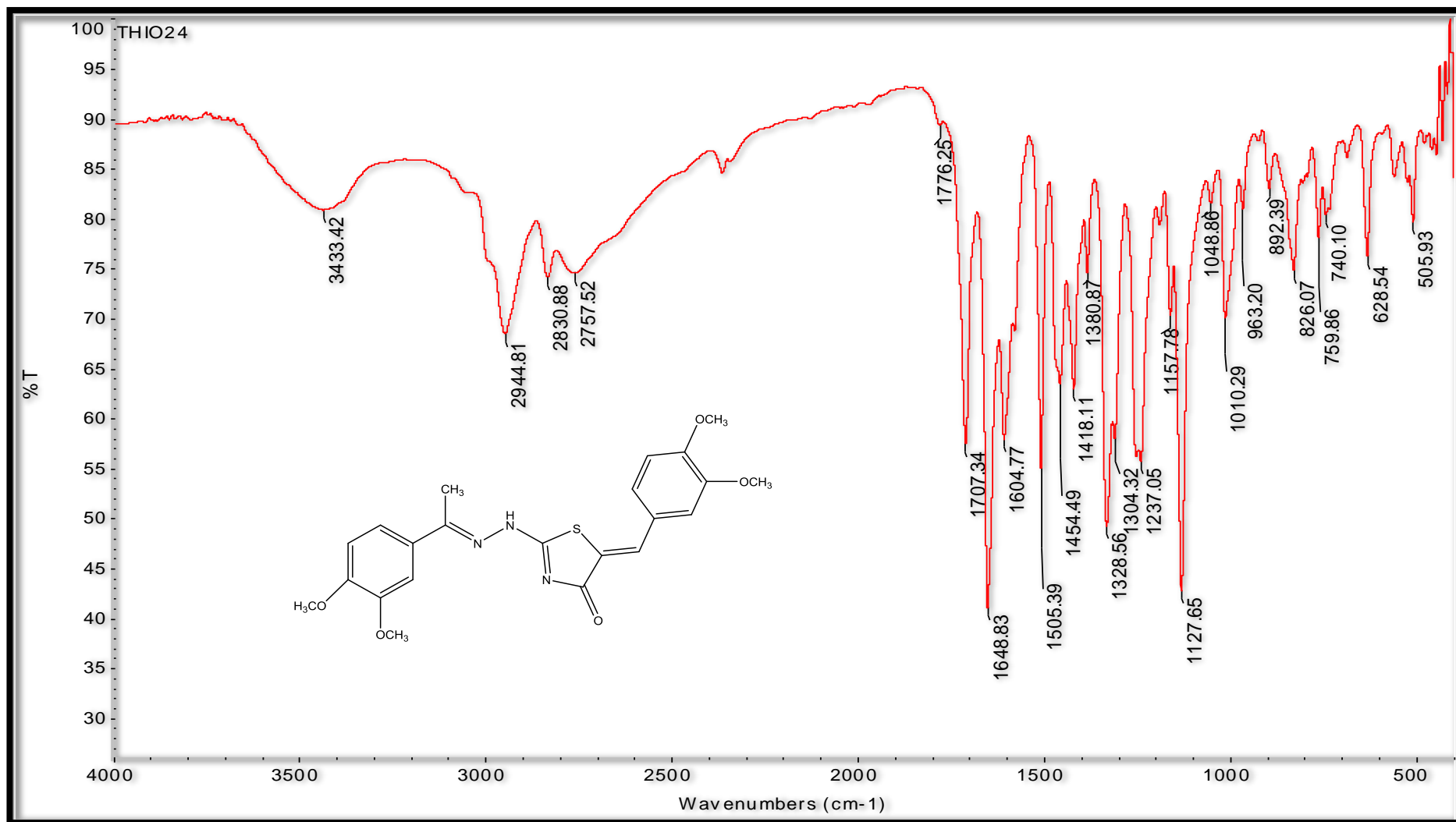
IR of compound (4i)



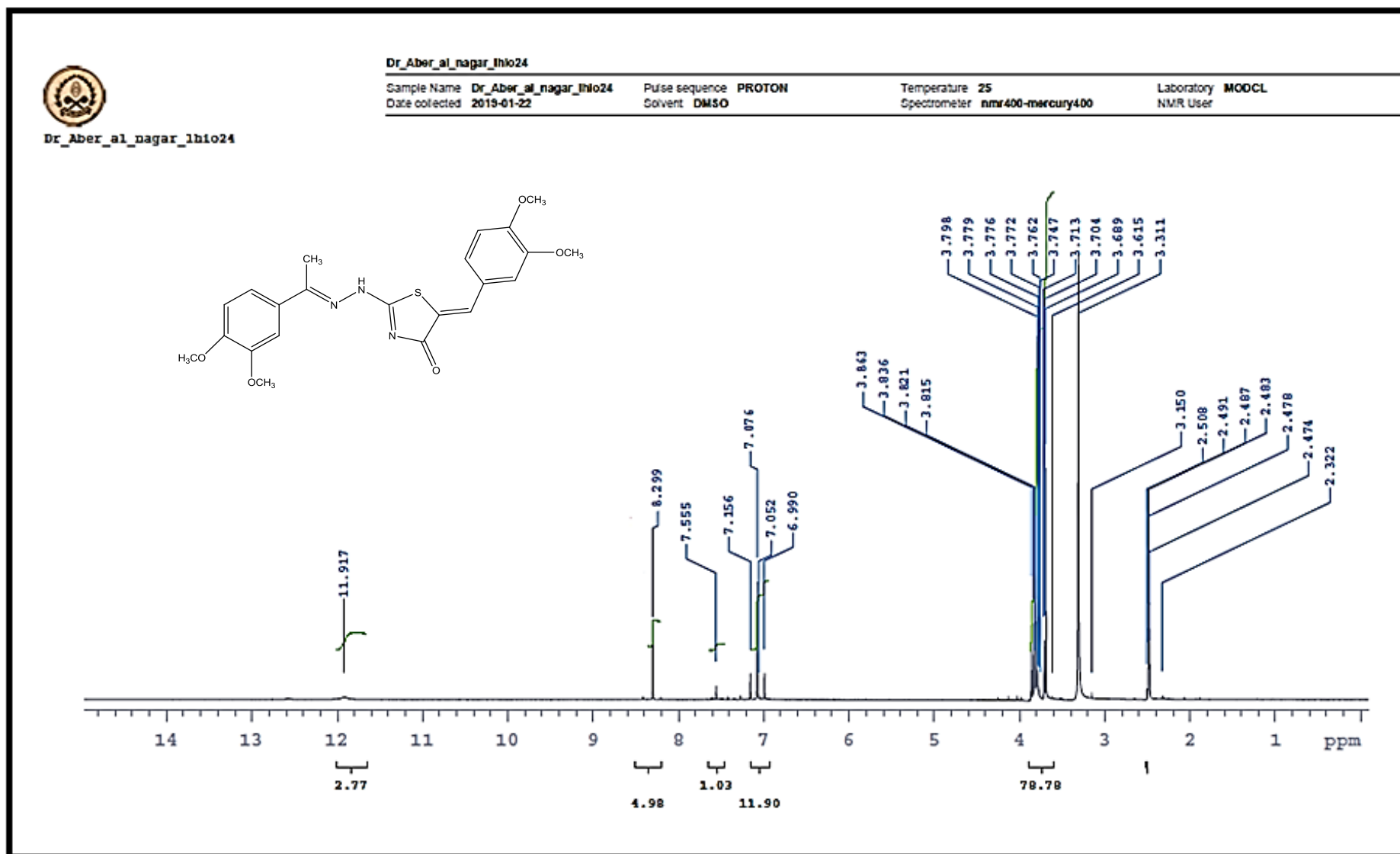
¹H NMR of compound (4i)



IR of compound (4j)



¹H NMR of compound (4j)



D₂O ¹H NMR of compound(4j)



Dr_Aber_al_nagar_1h1o24_D2O

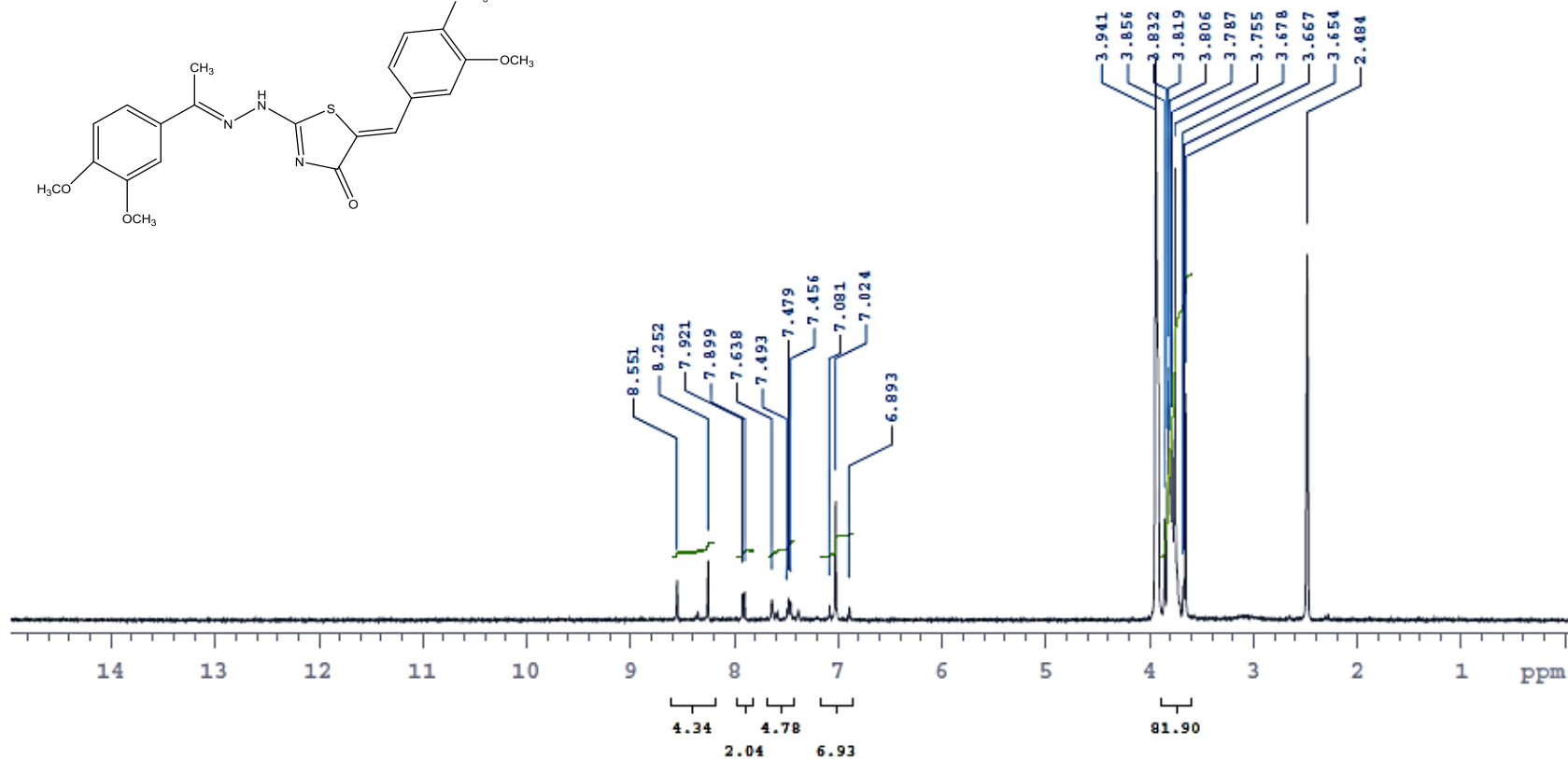
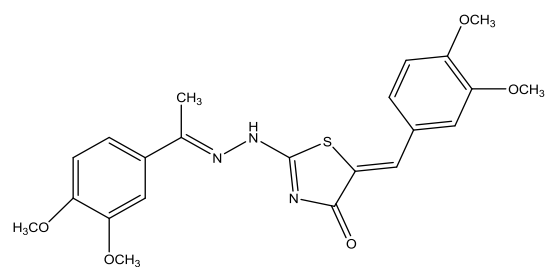
Dr_Aber_al_nagar_1h1o24_D2O

Sample Name Dr_Aber_al_nagar_1h1o24_D2O
Date collected 2019-01-27

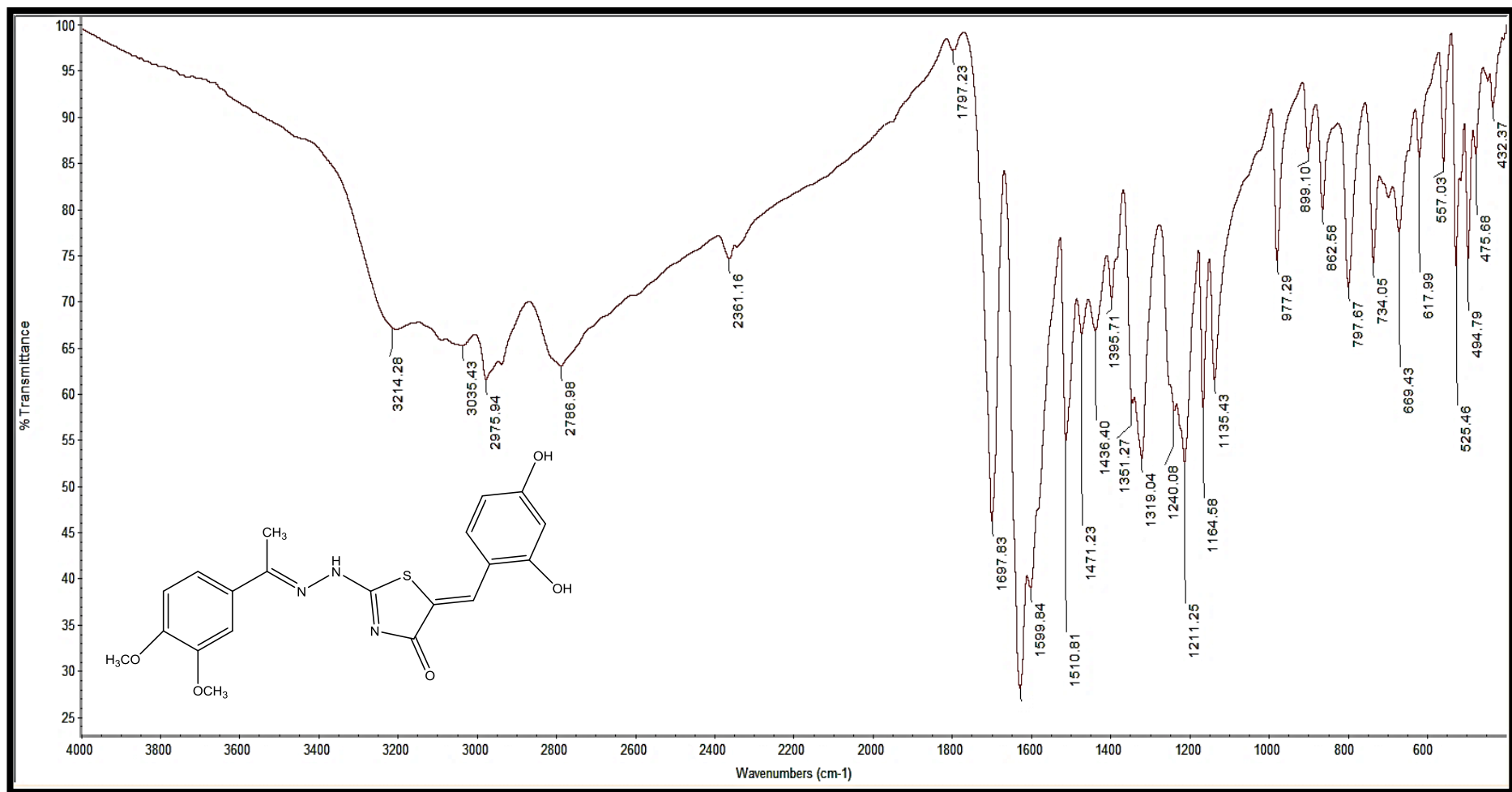
Pulse sequence PROTON
Solvent DMSO

Temperature 25
Spectrometer nmr400-mercury400

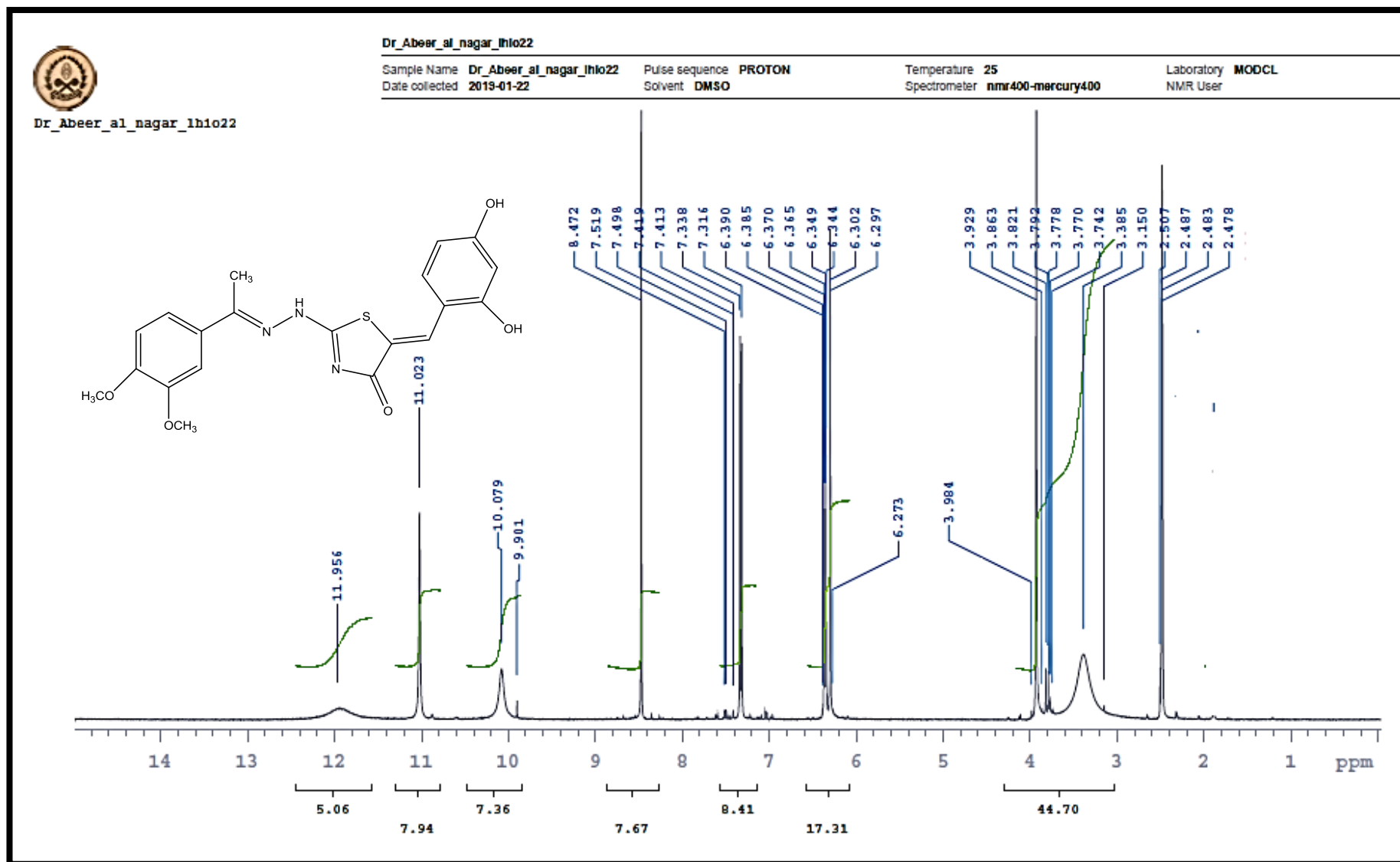
Laboratory MODCL
NMR User Cap-Ahmed Salah Elkholy



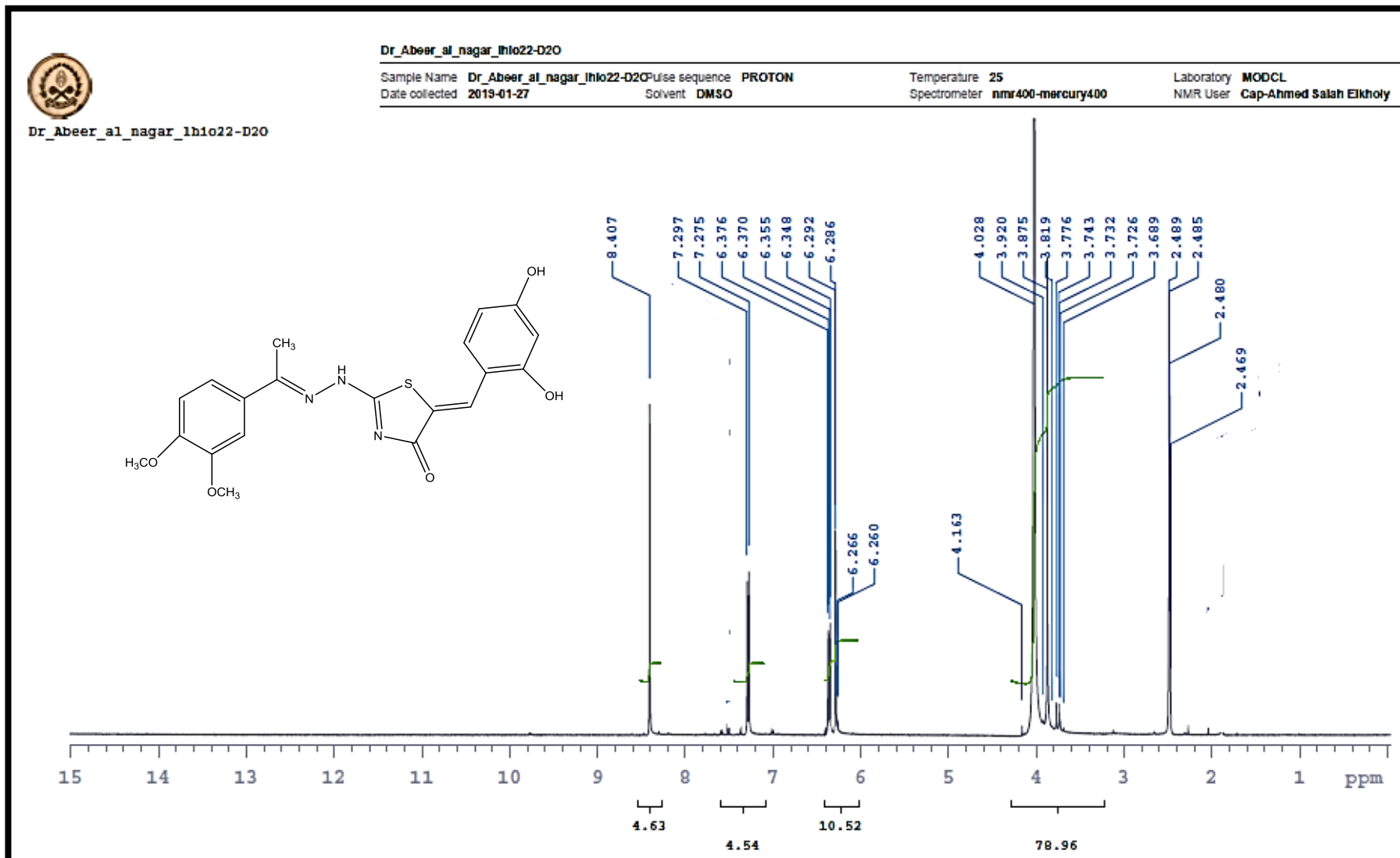
IR of compound (4k)



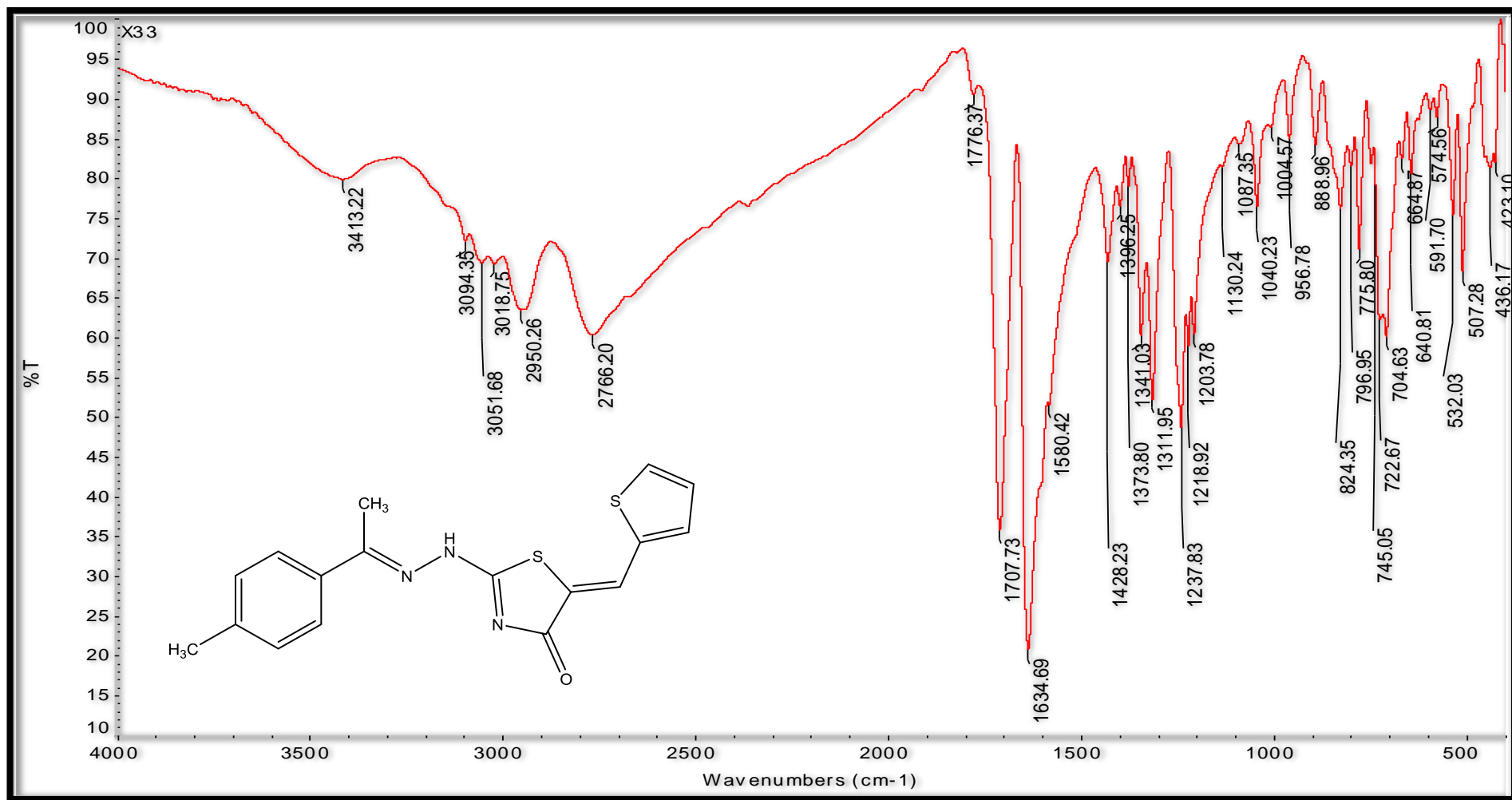
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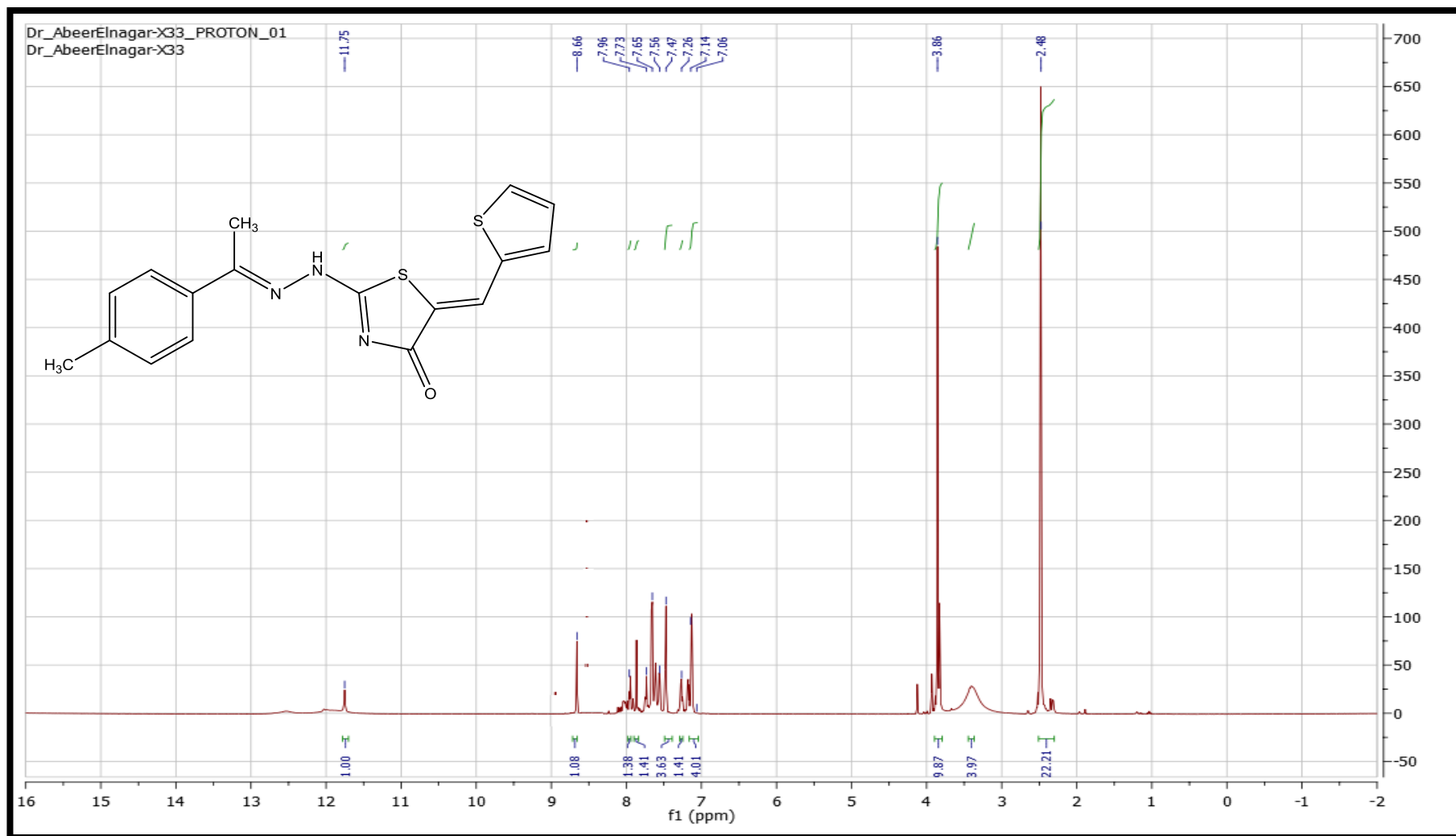
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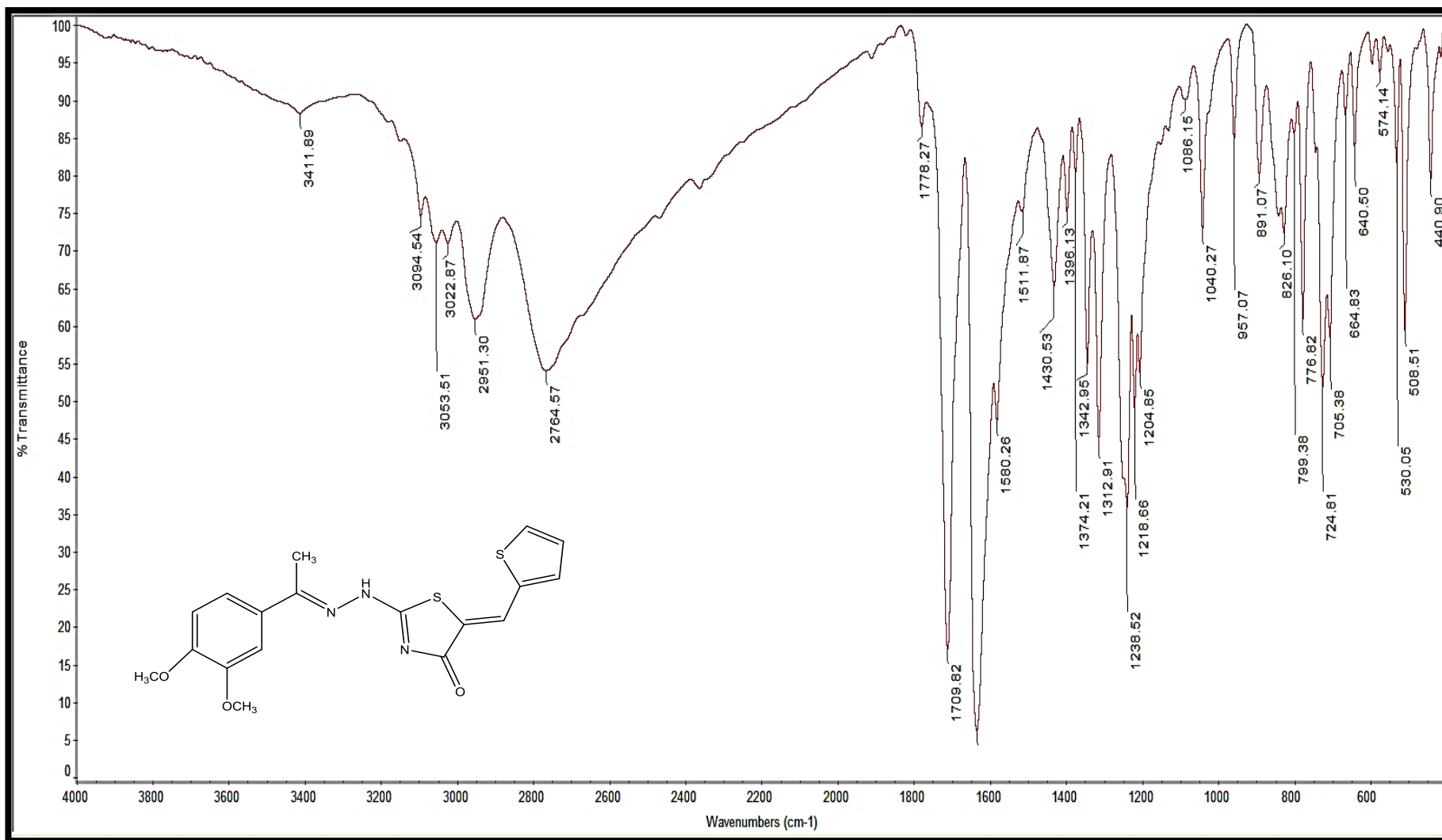
IR of compound (5a).



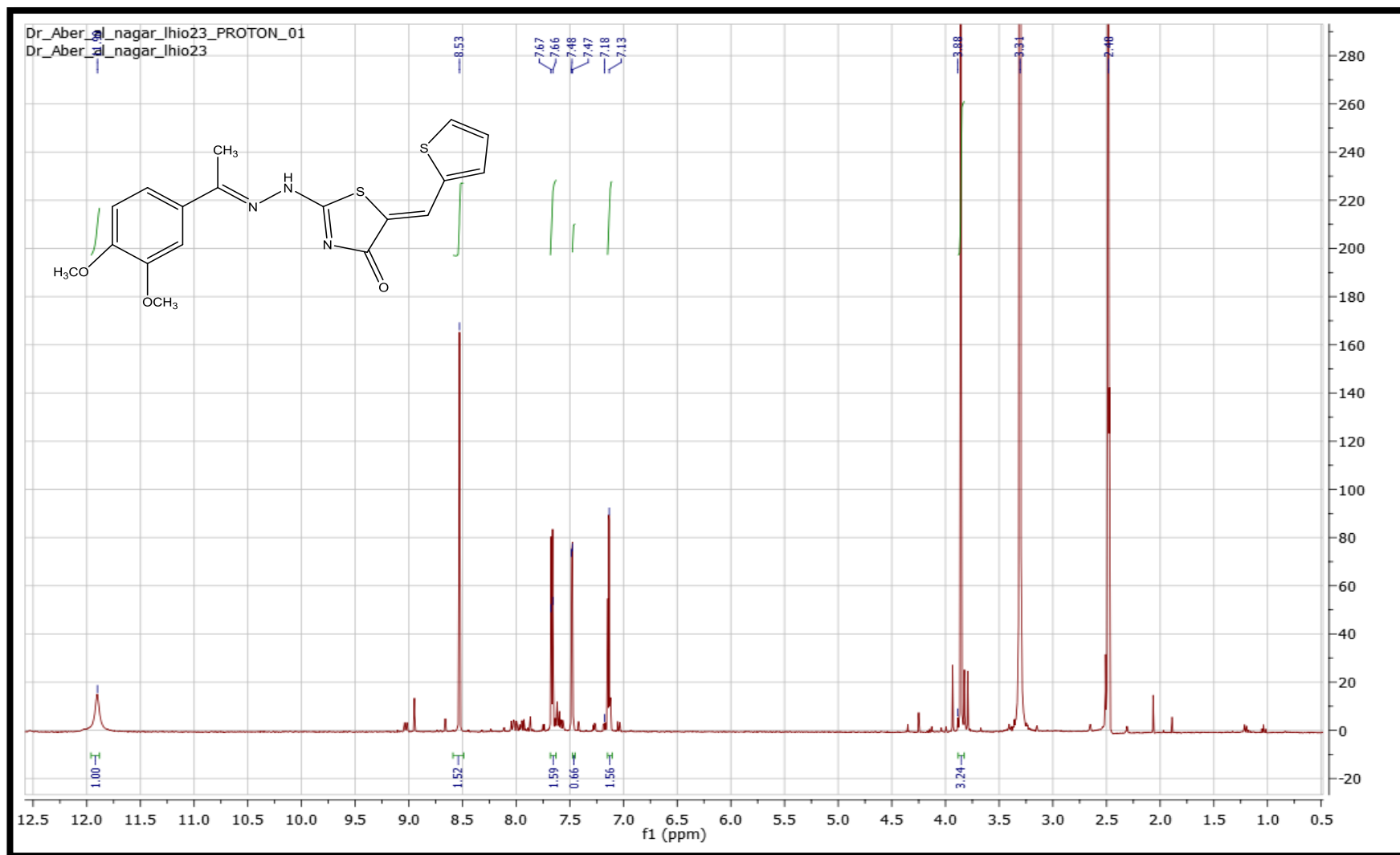
¹H NMR of compound (5a)



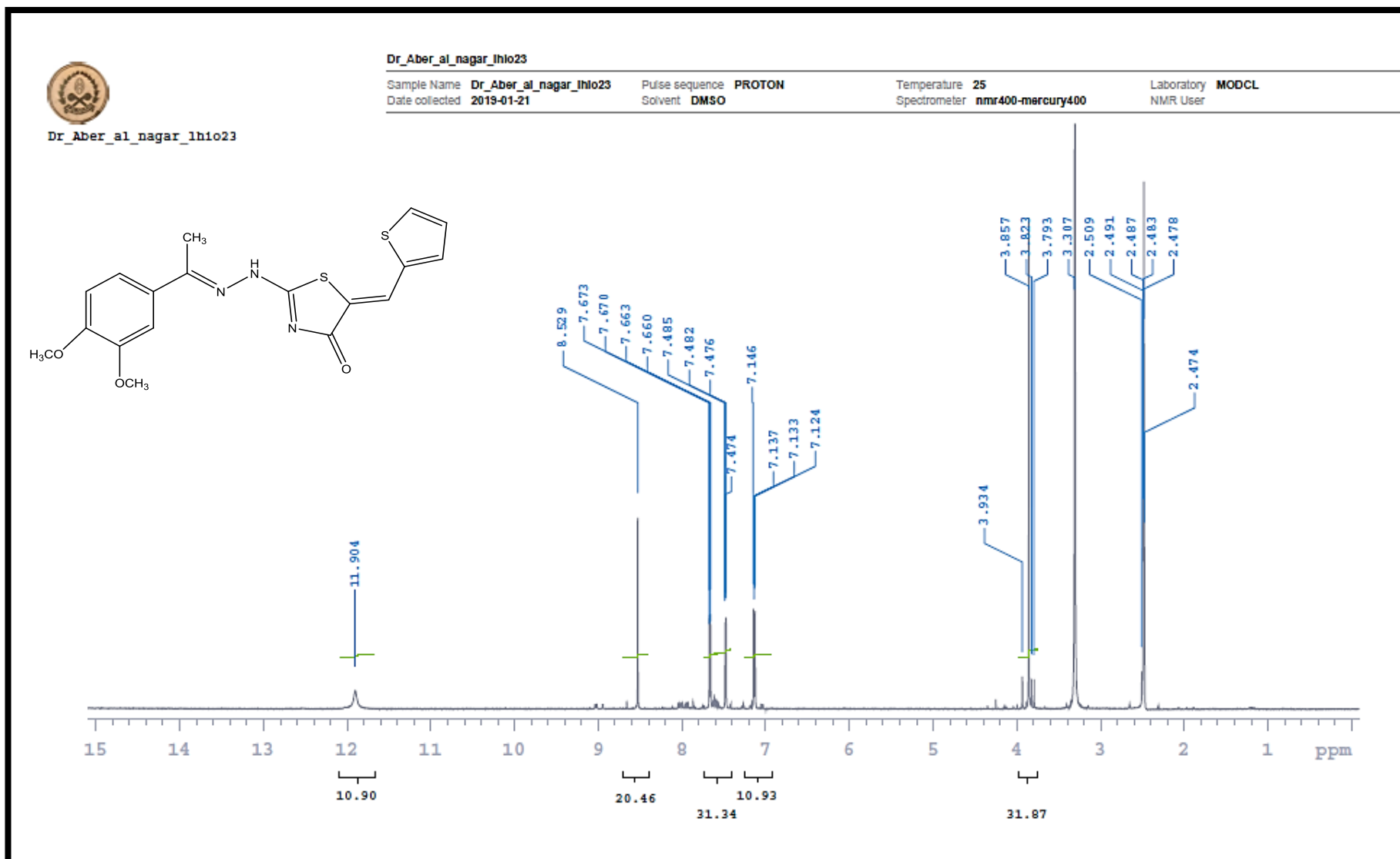
IR of compound (5b)



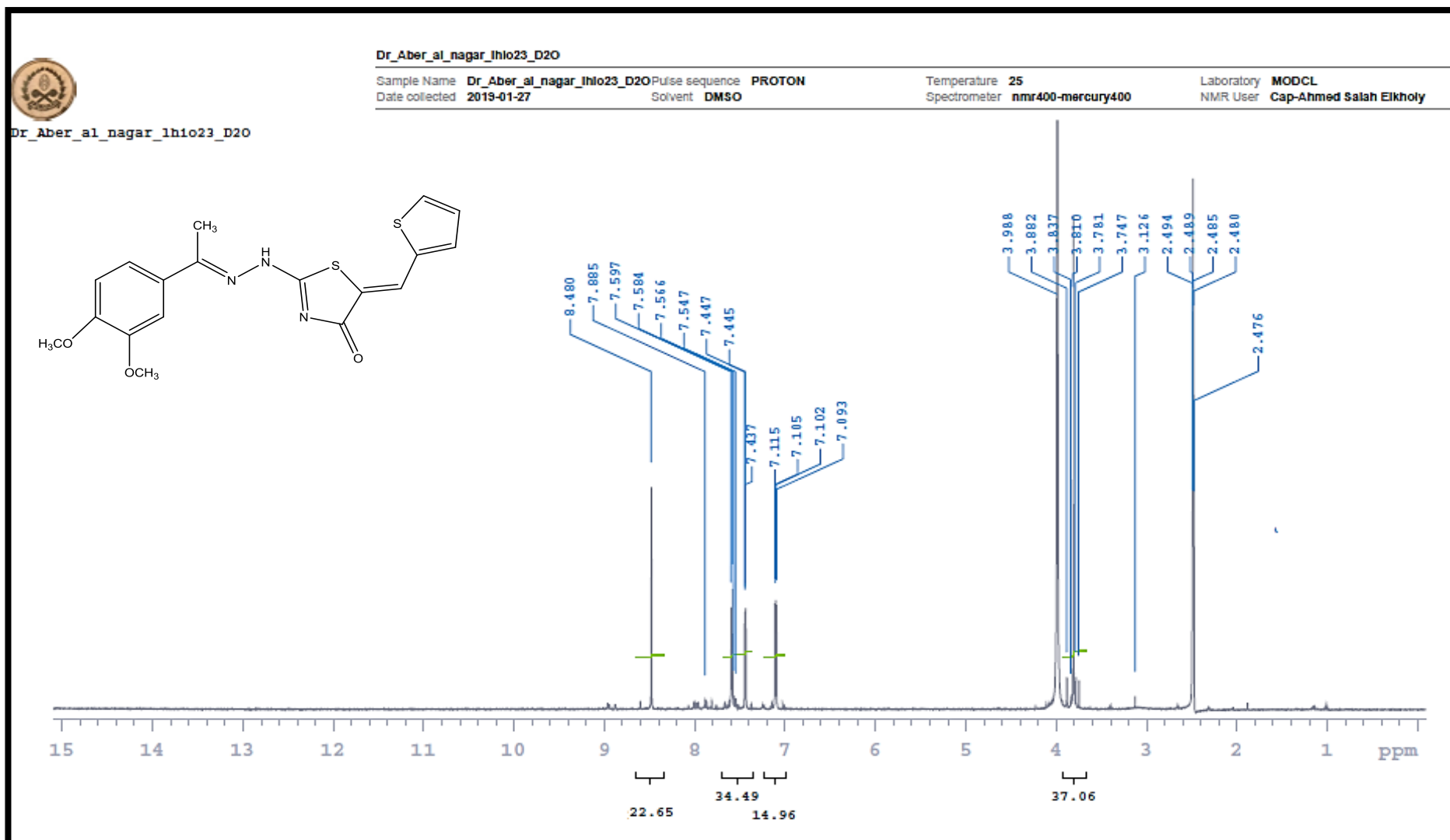
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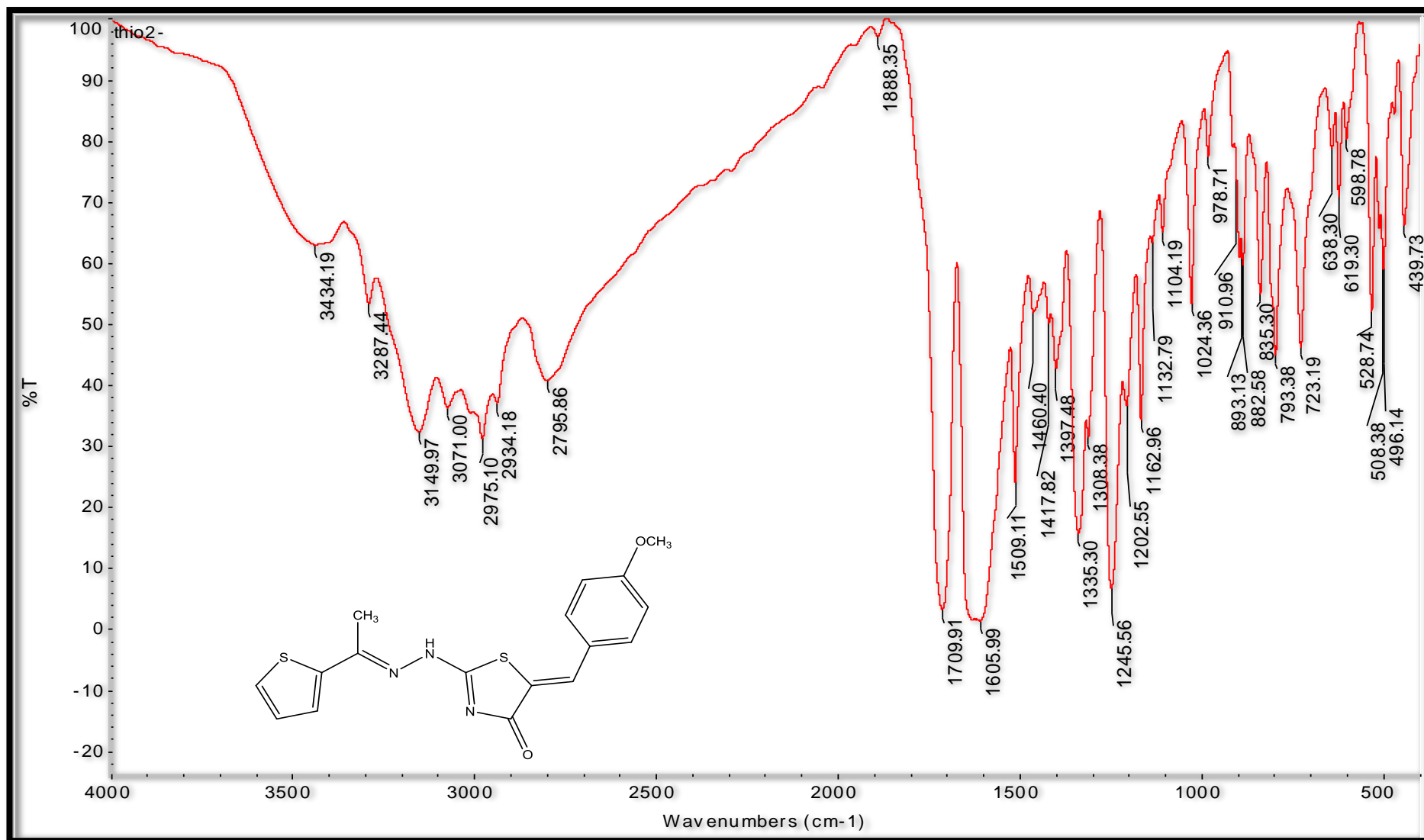
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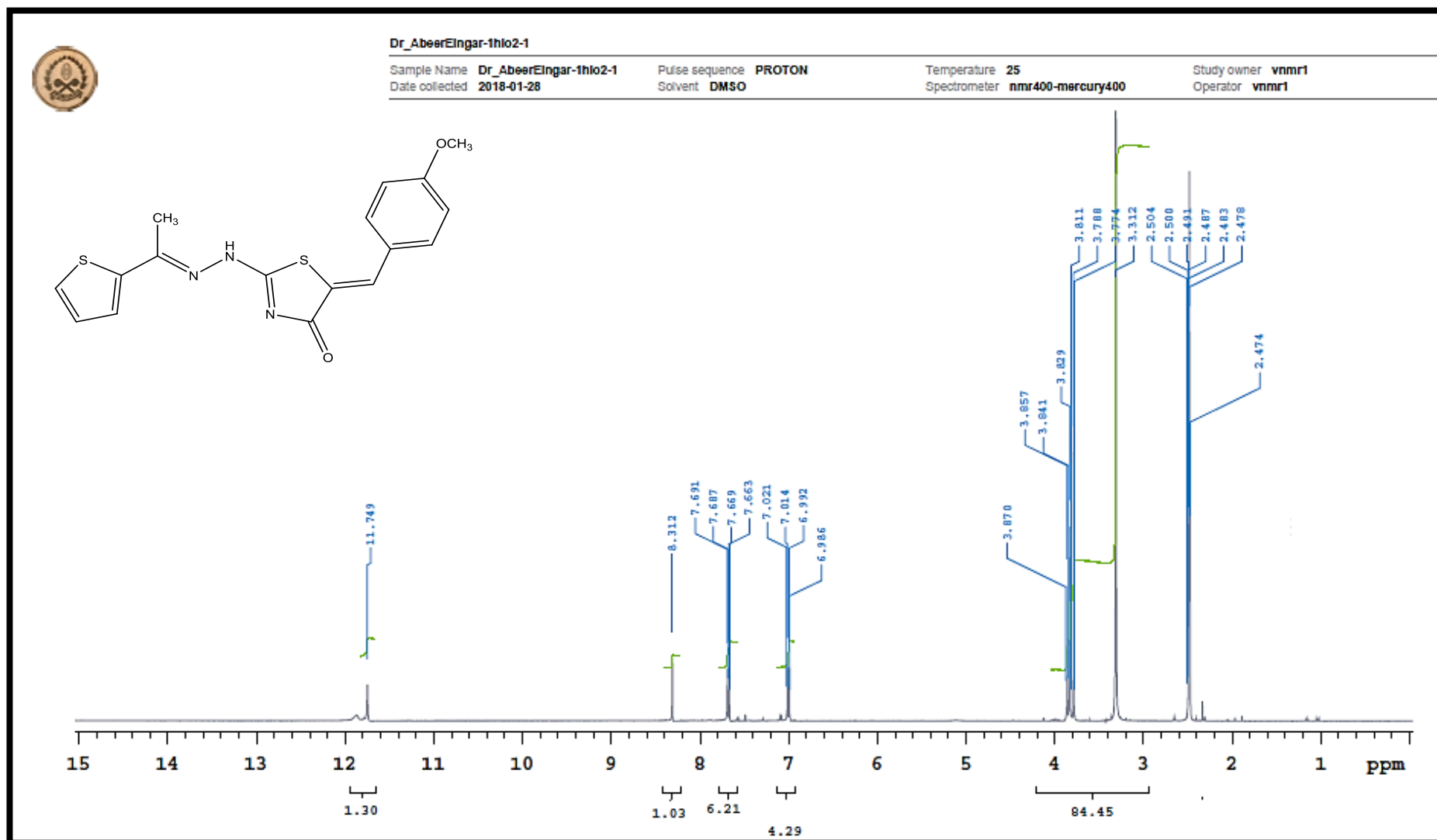
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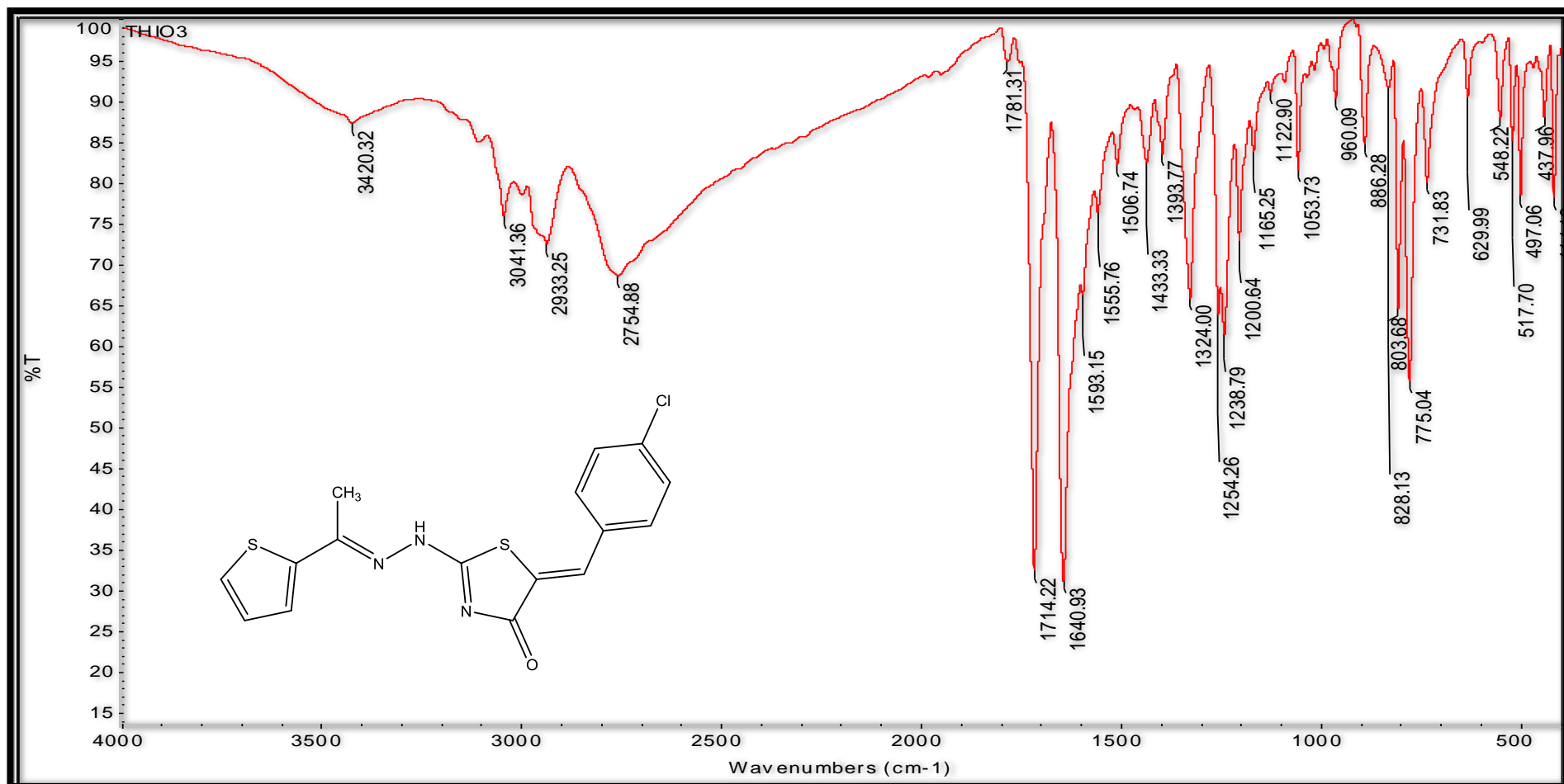
IR of compound (8a)



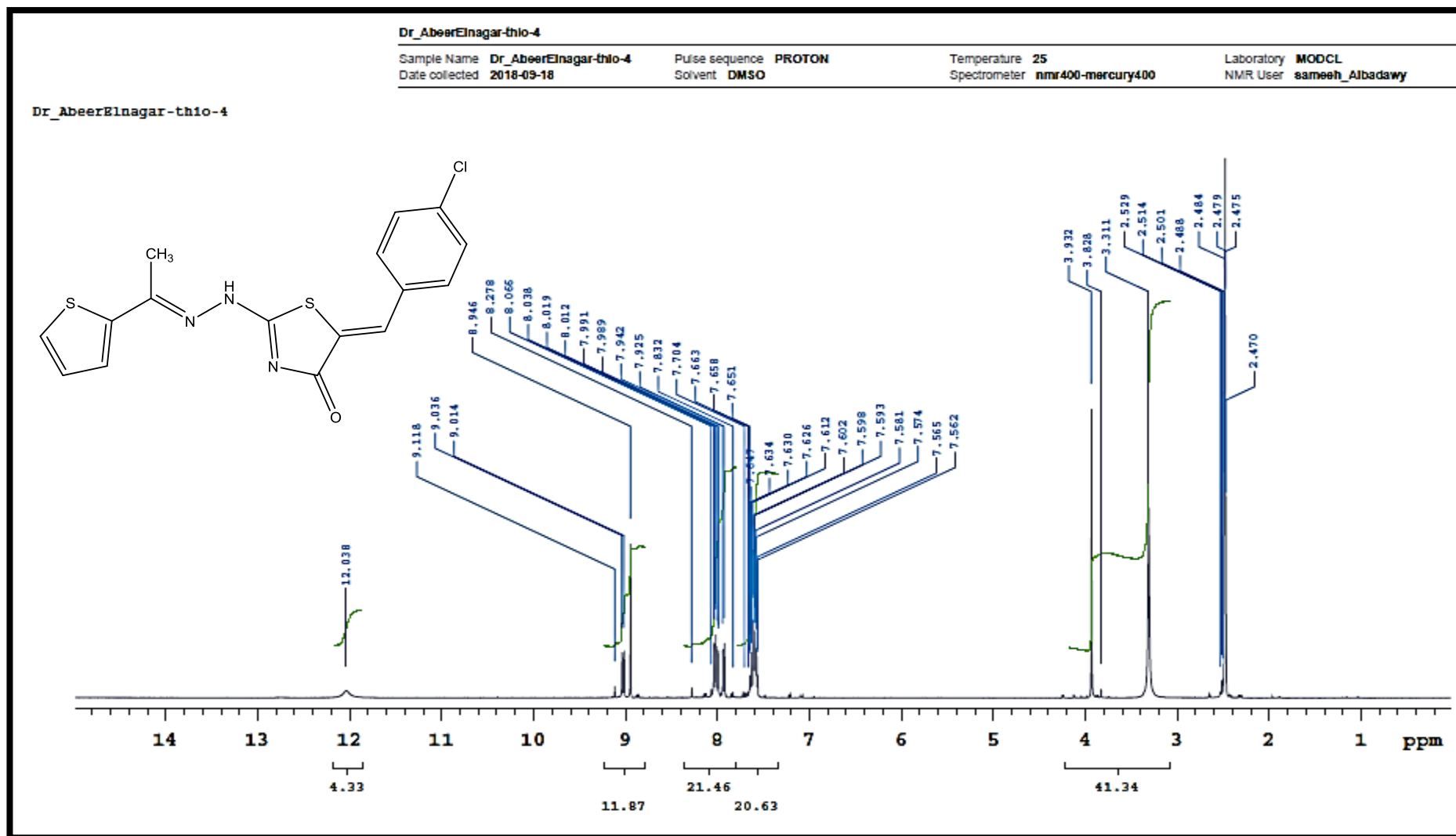
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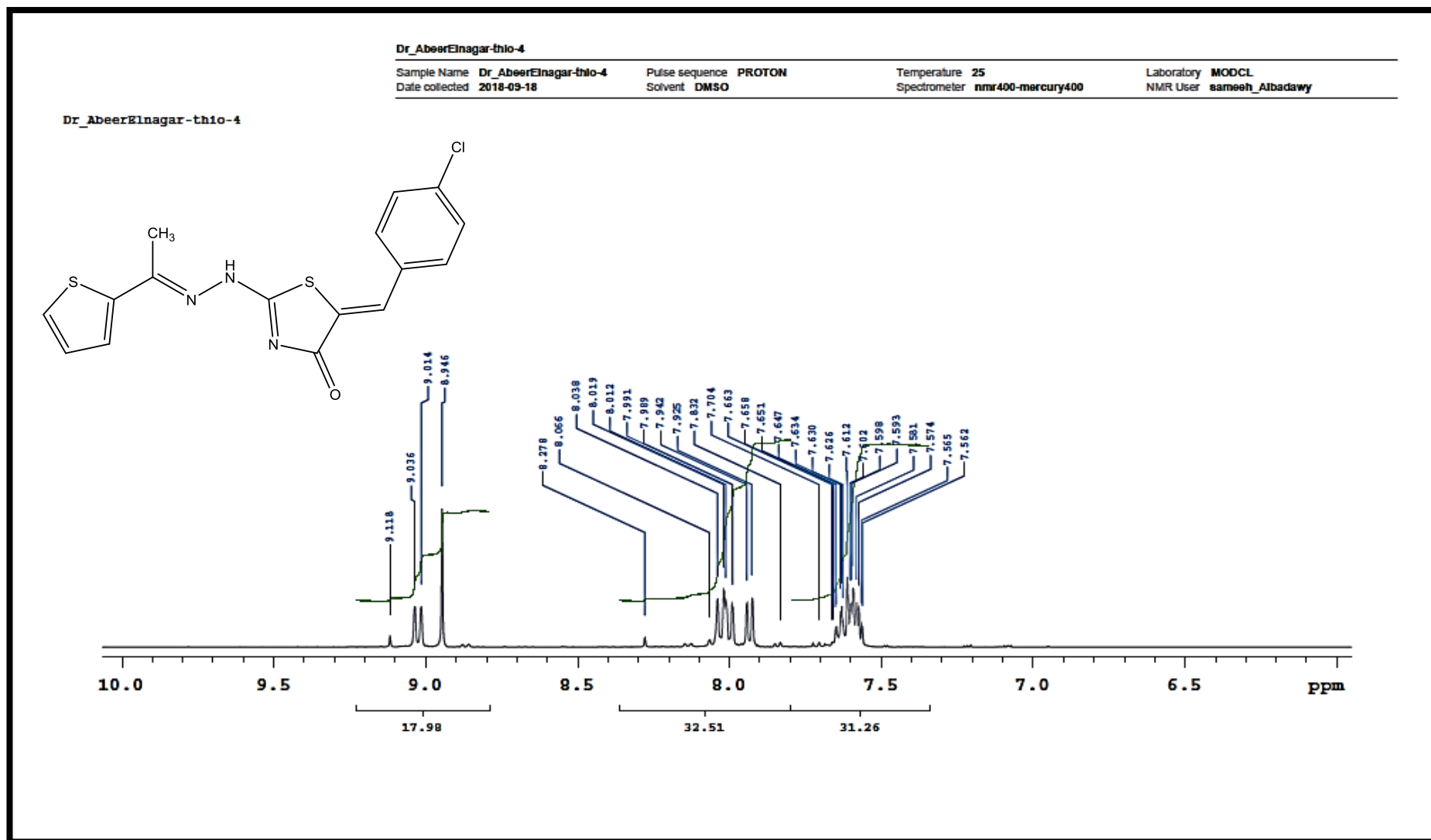
IR of compound (8b)



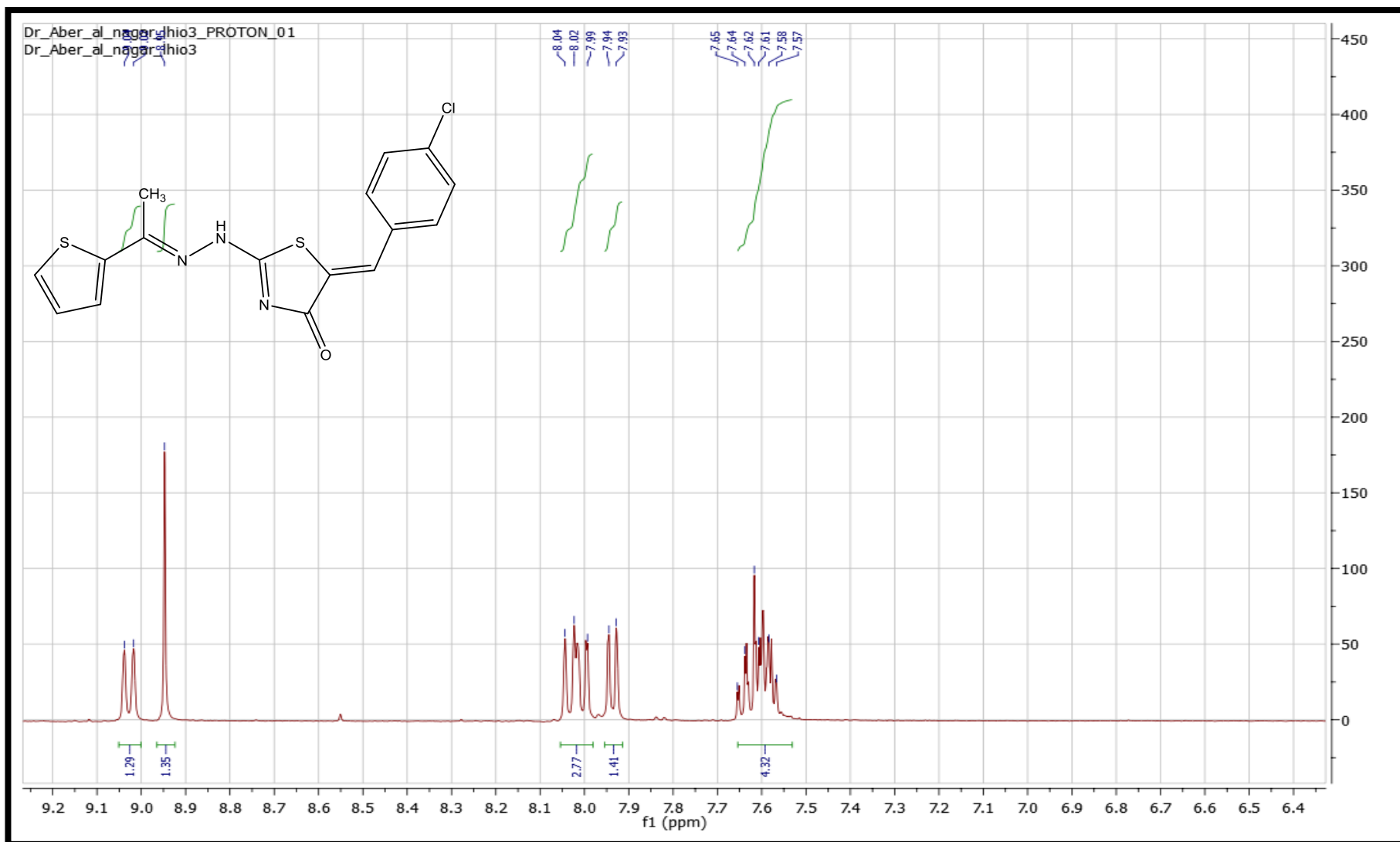
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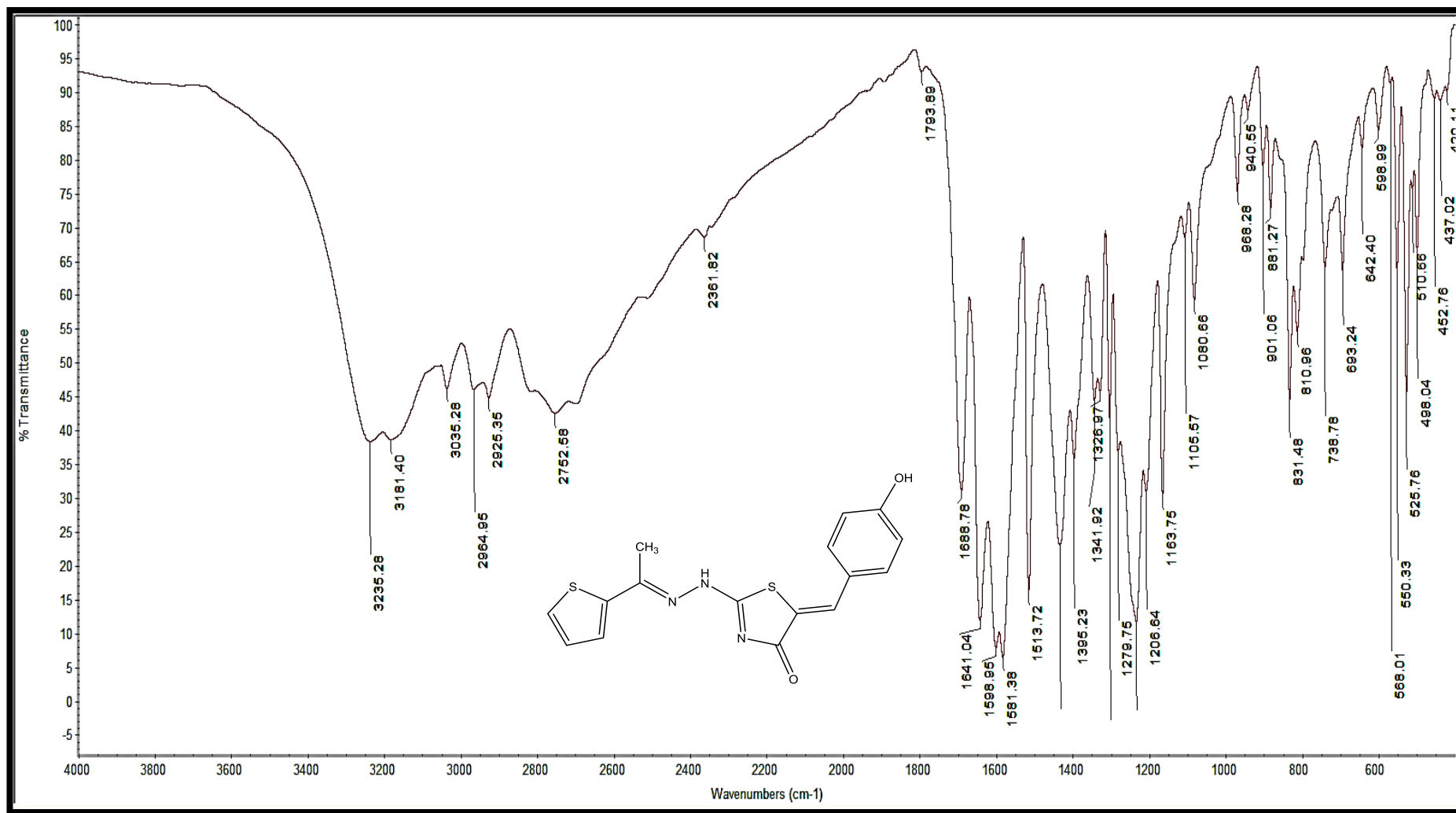
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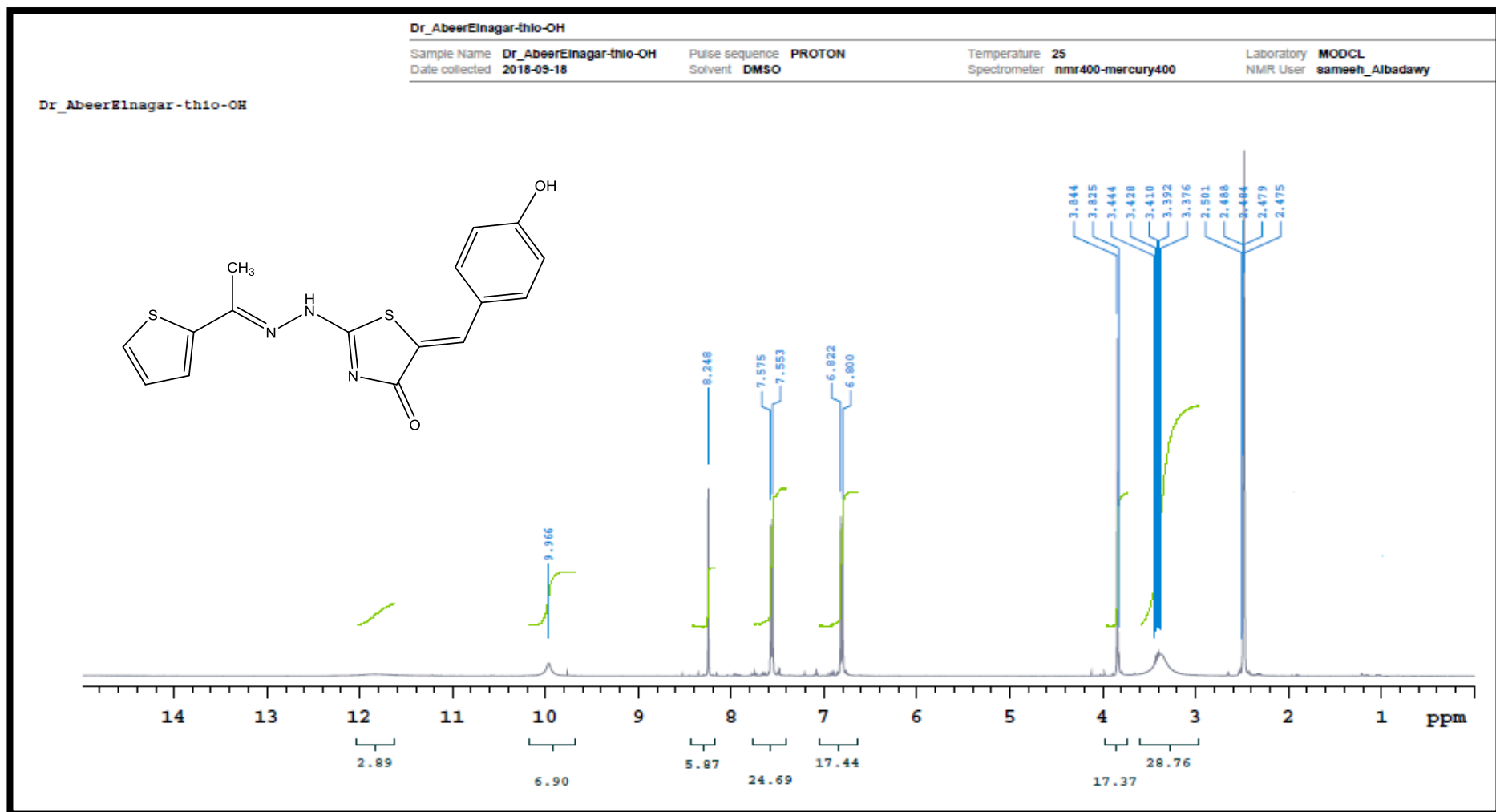
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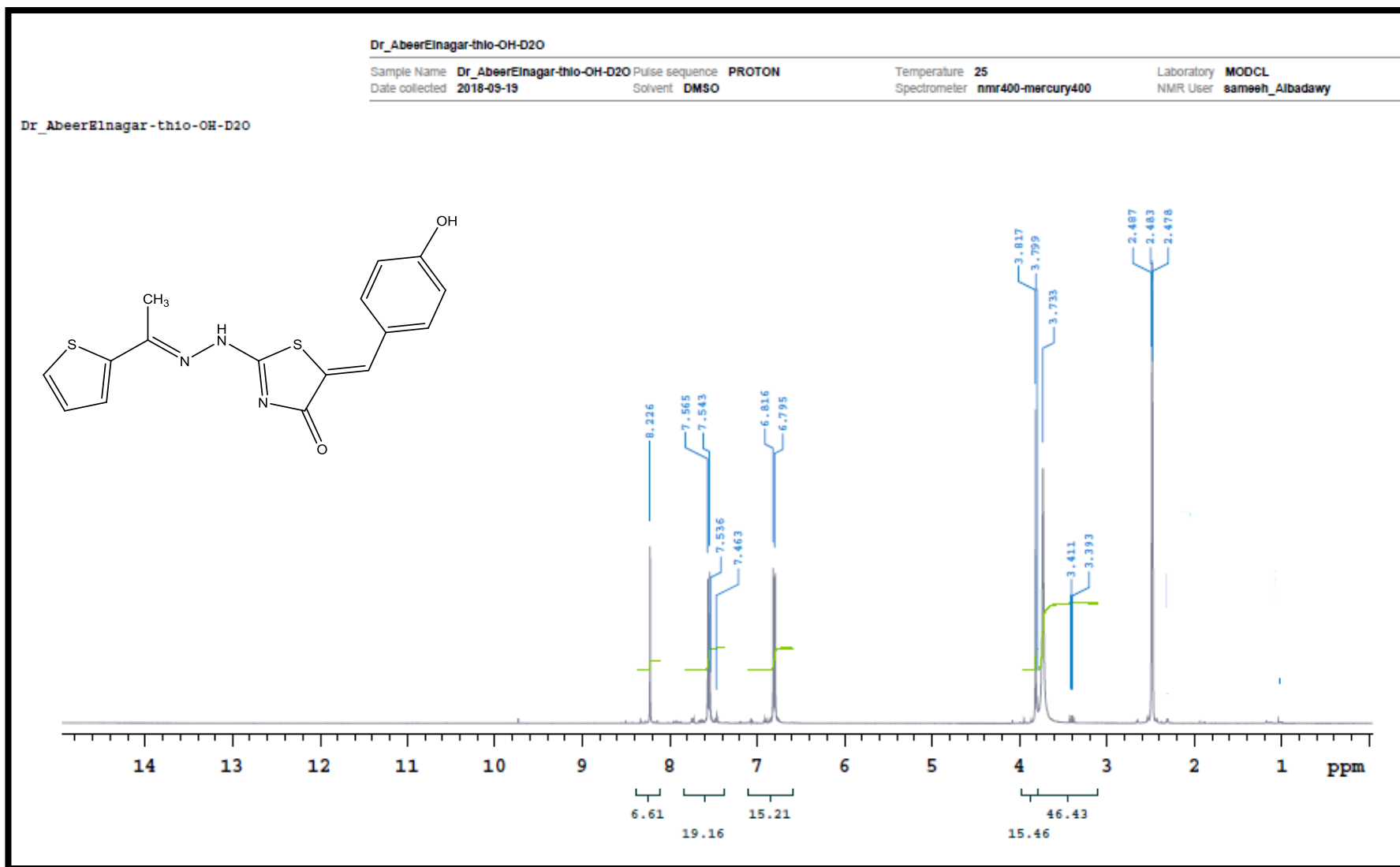
IR of compound (8c)



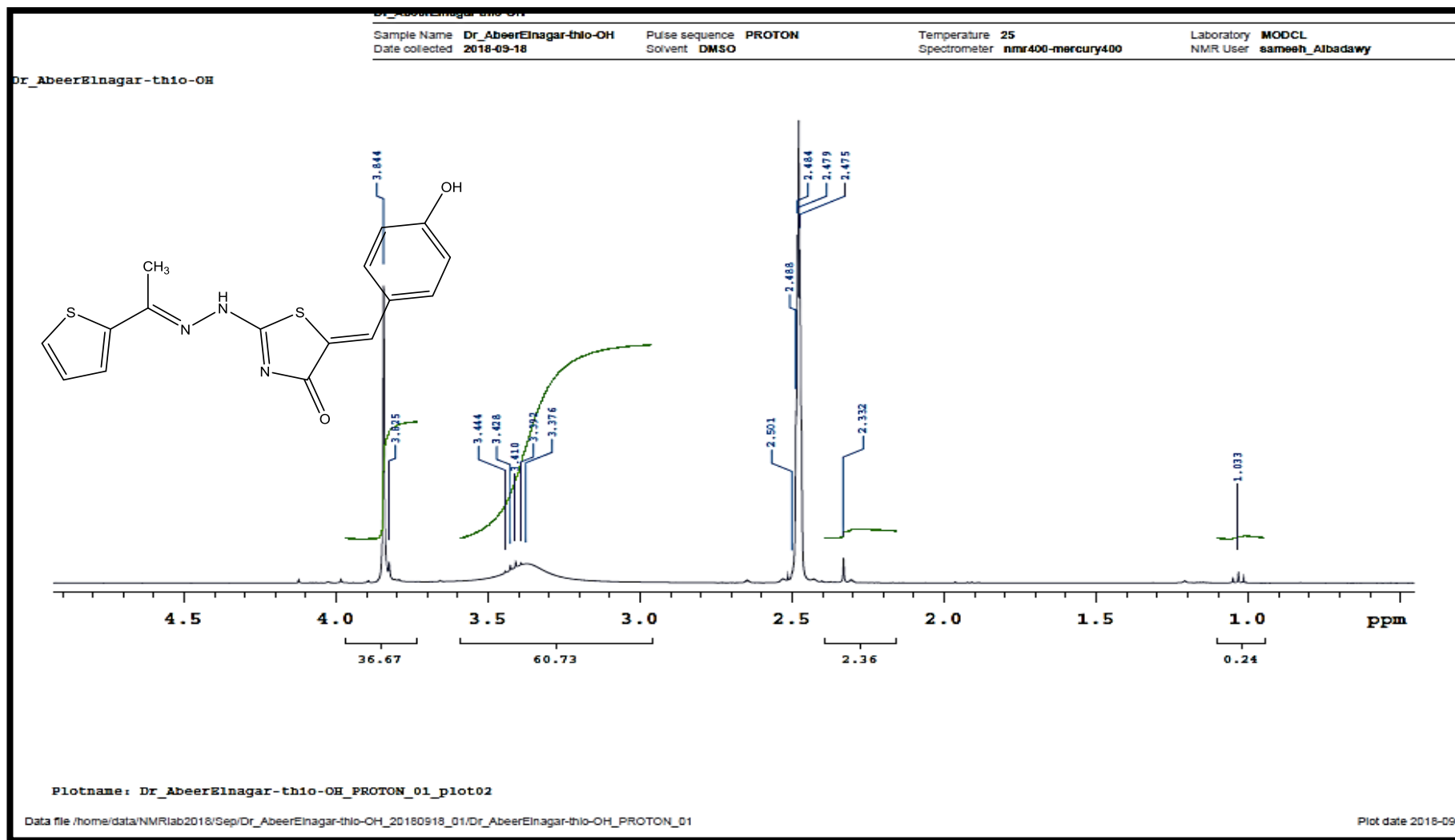
¹H NMR of compound (8c)



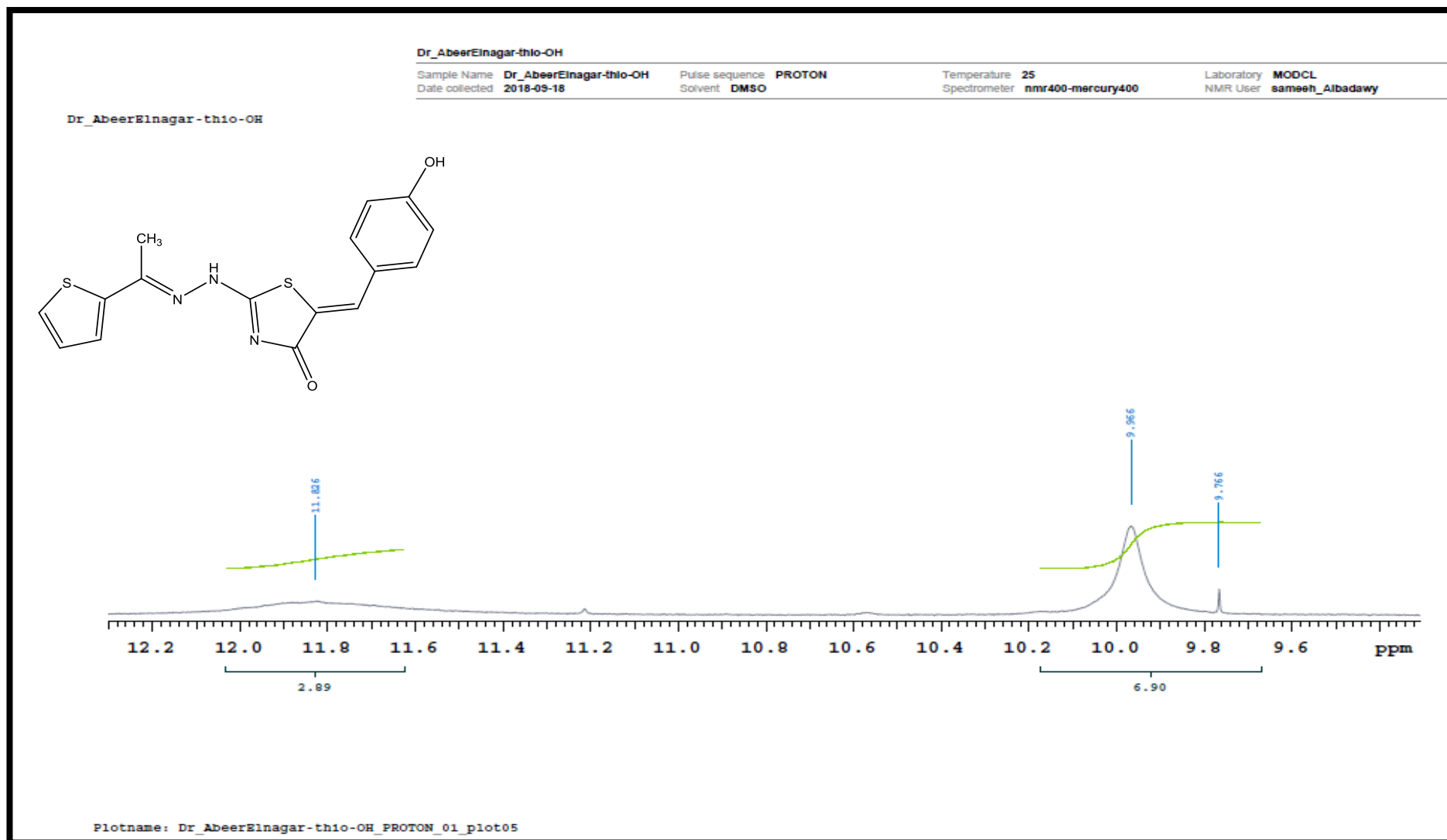
D₂O ¹H NMR of compound (8c)



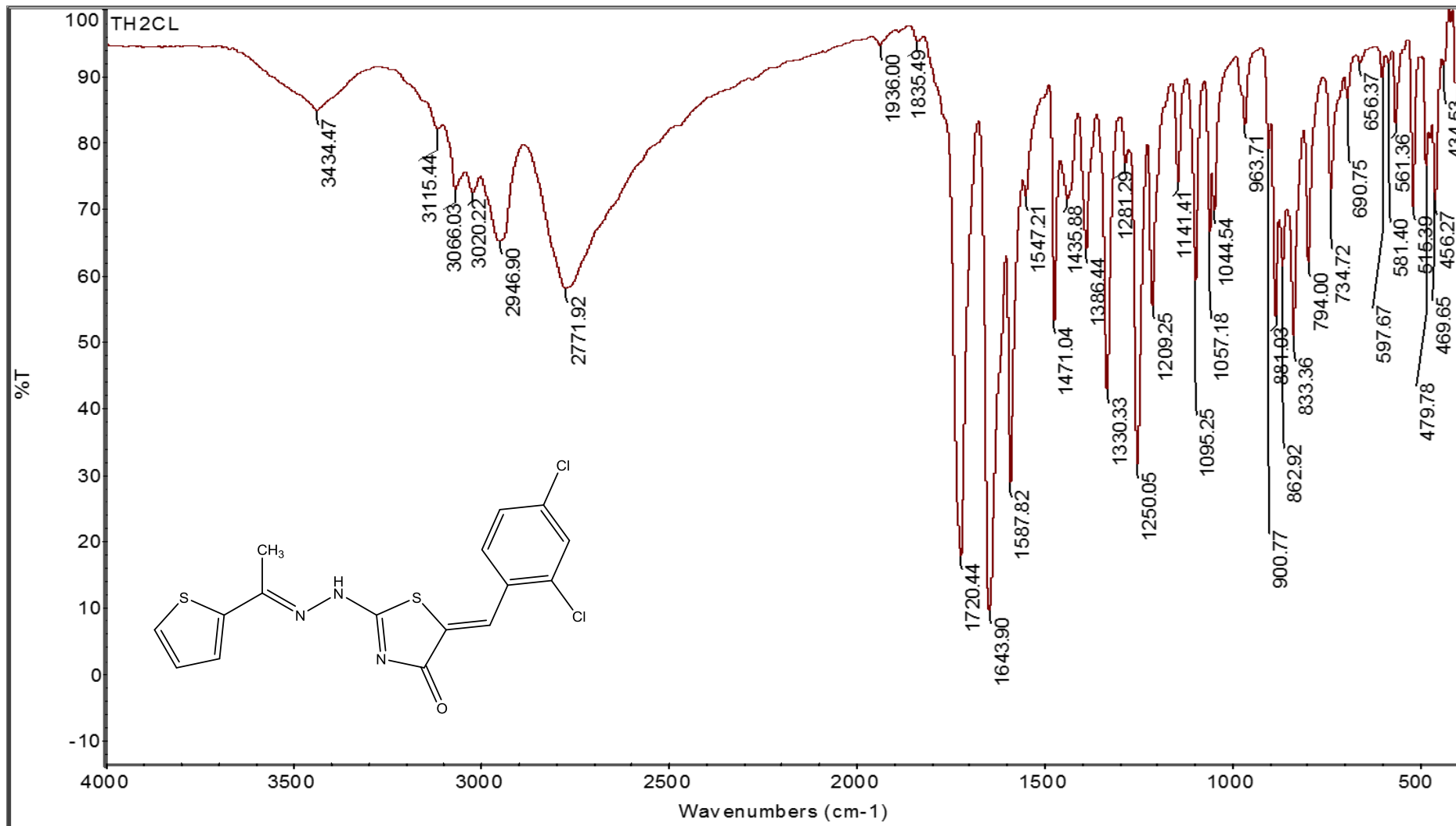
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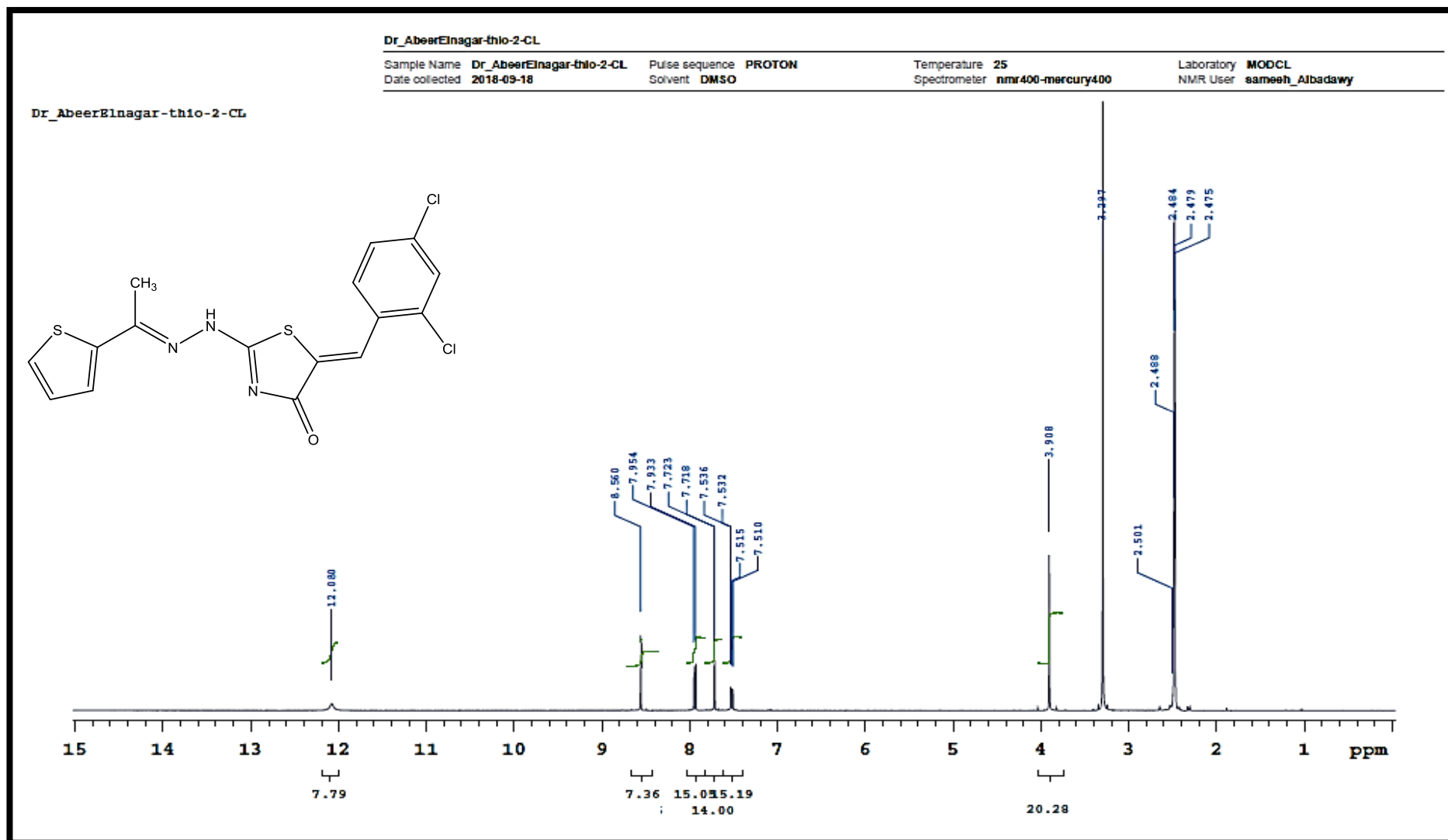
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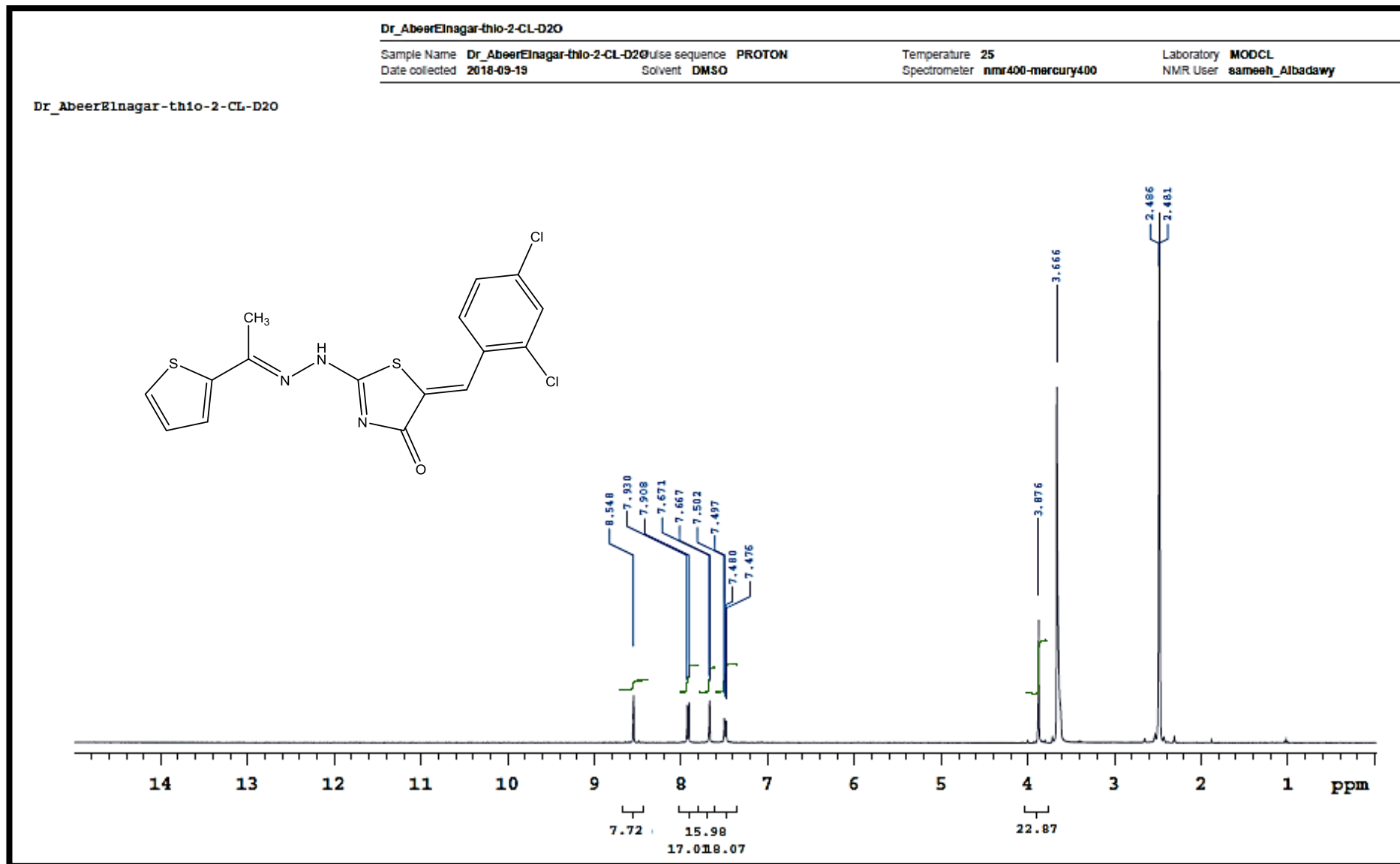
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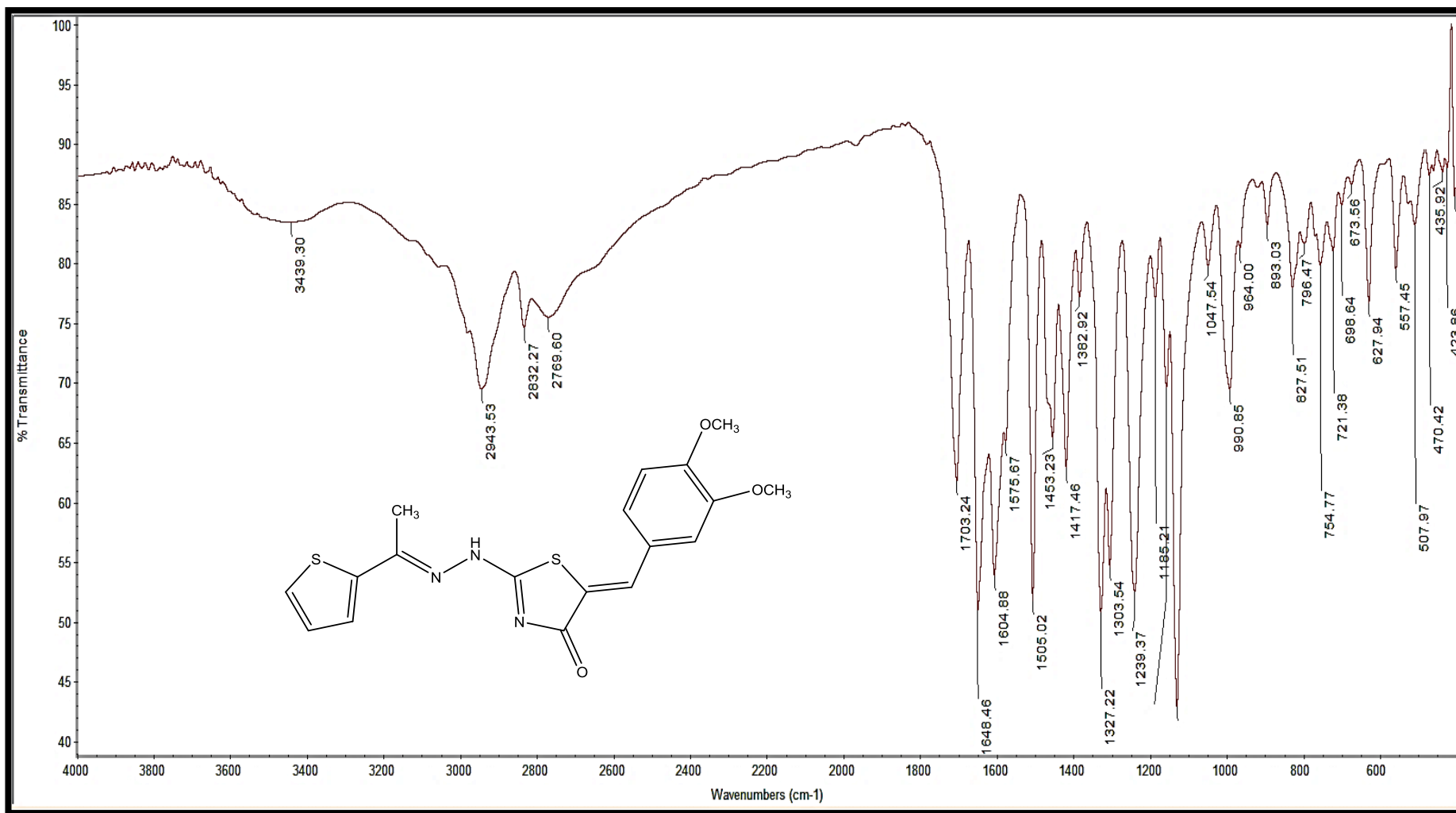
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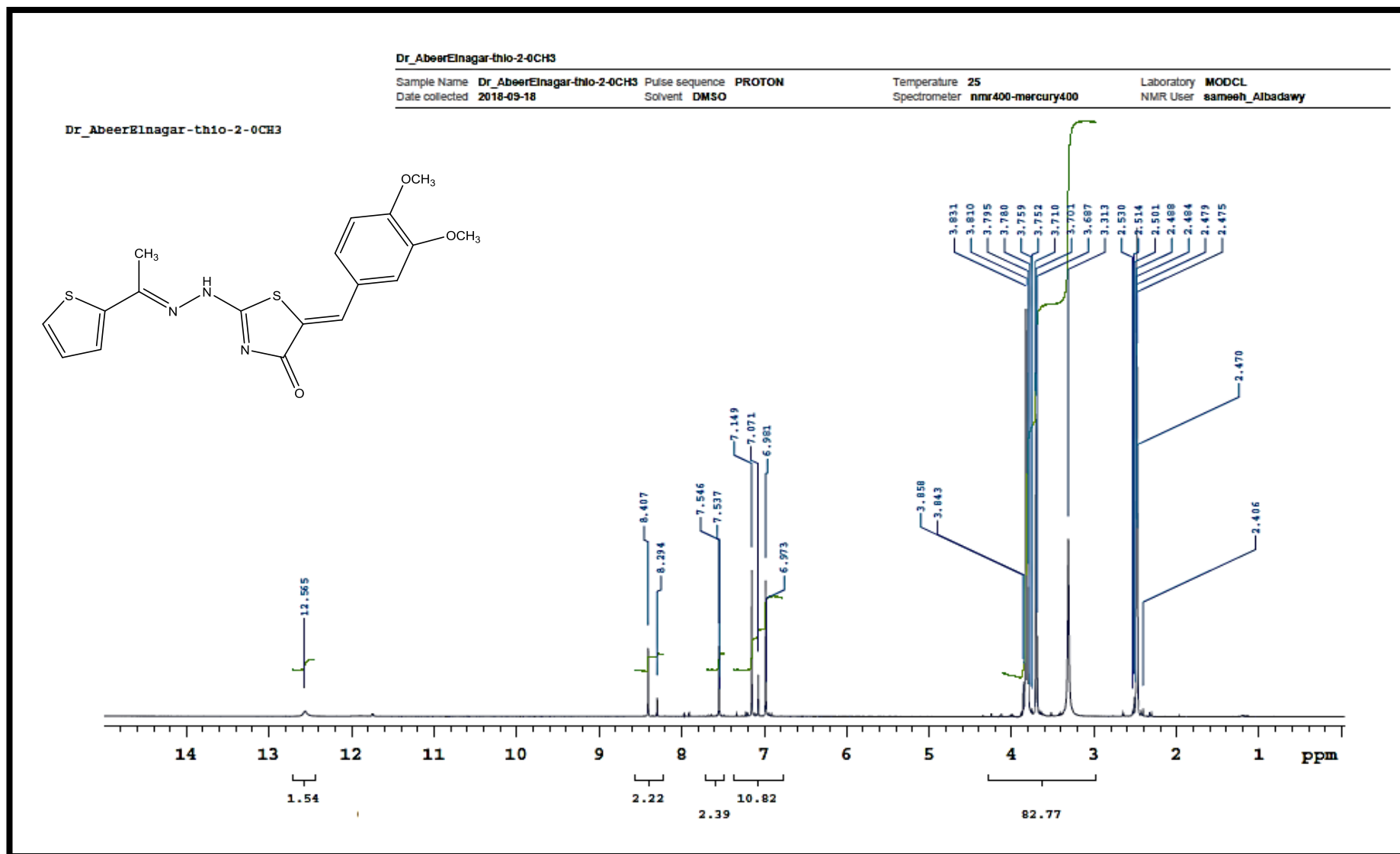
D₂O ¹H NMR of compound (8d)



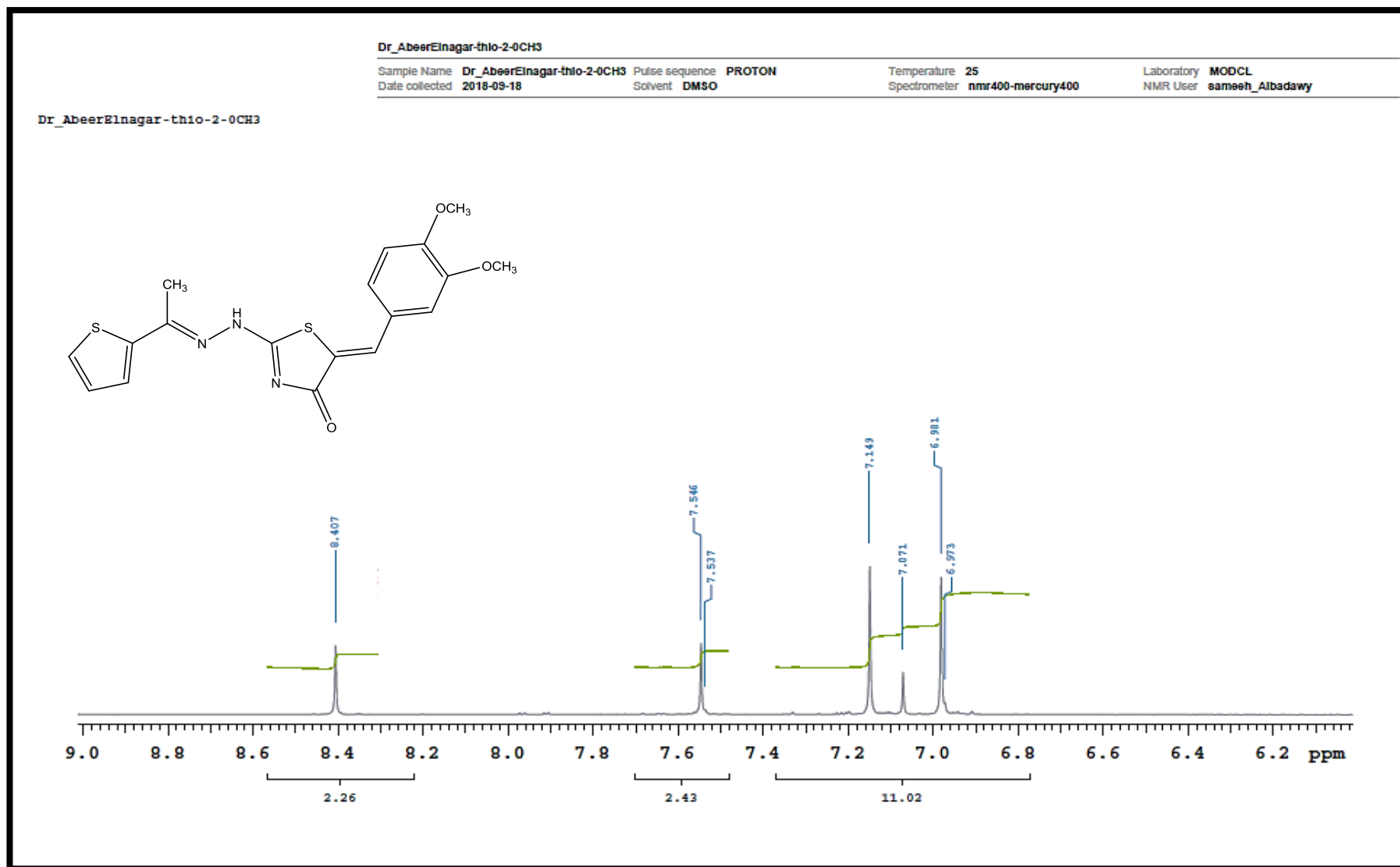
IR of compound (8e)



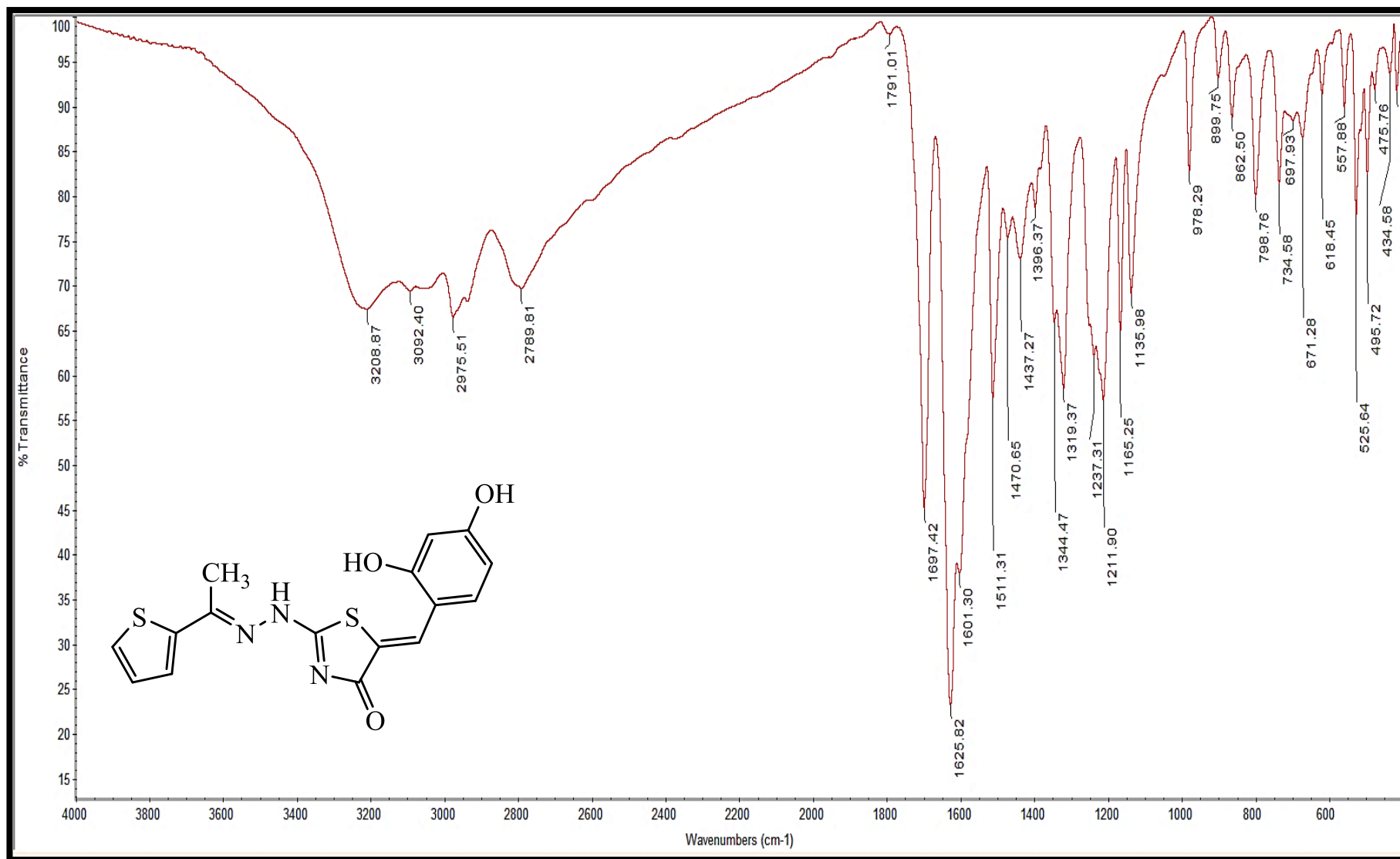
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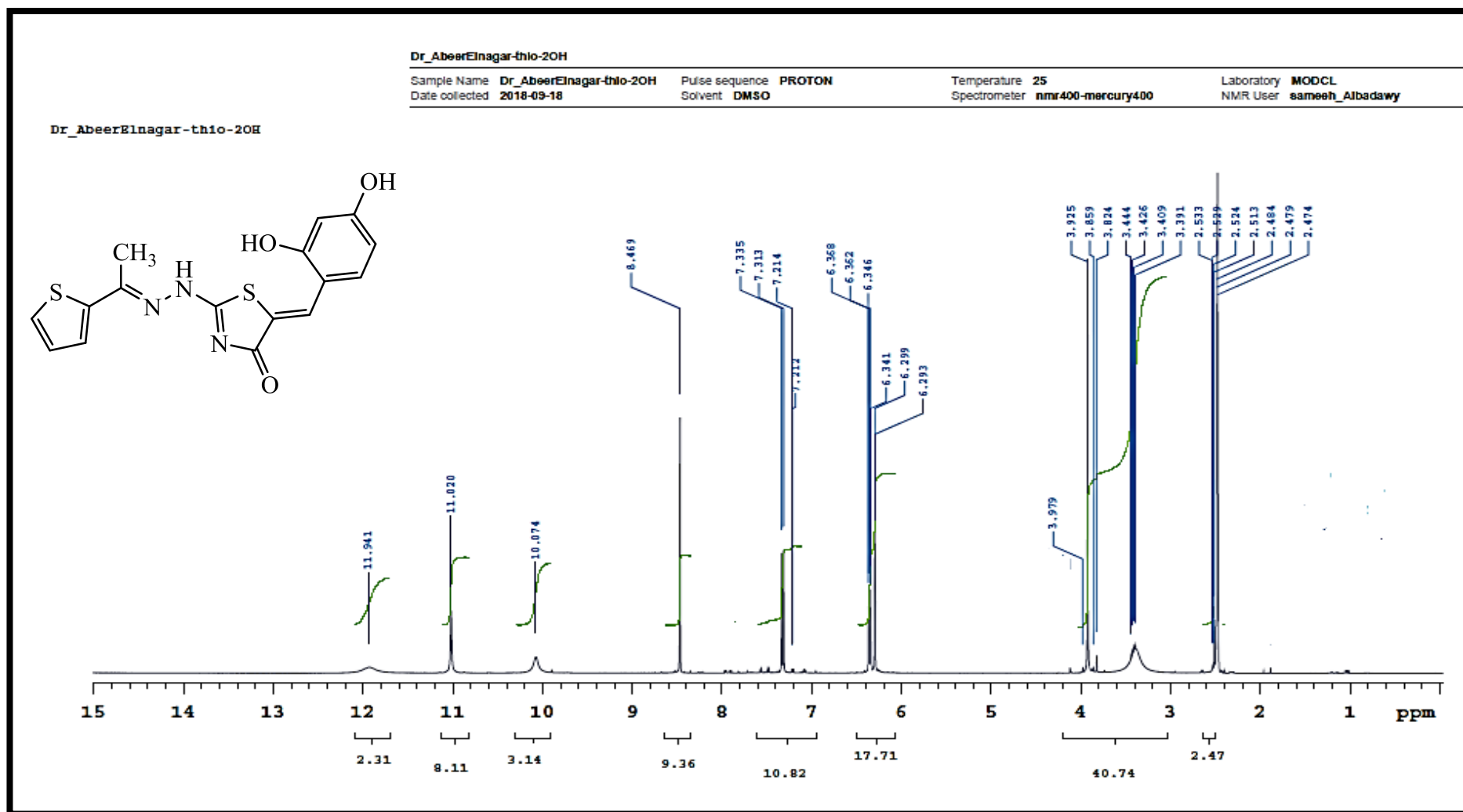
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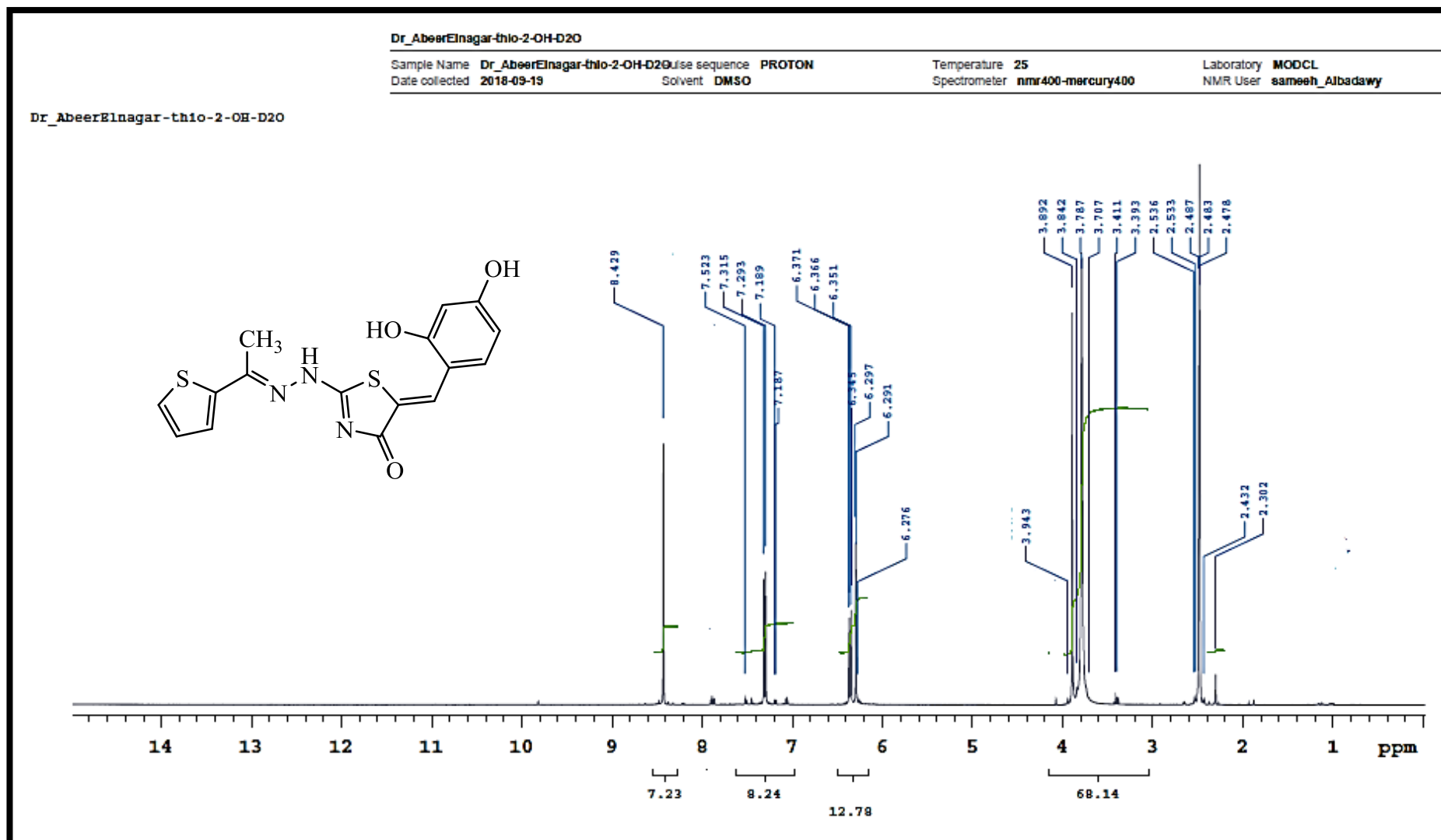
IR of compound (8f)



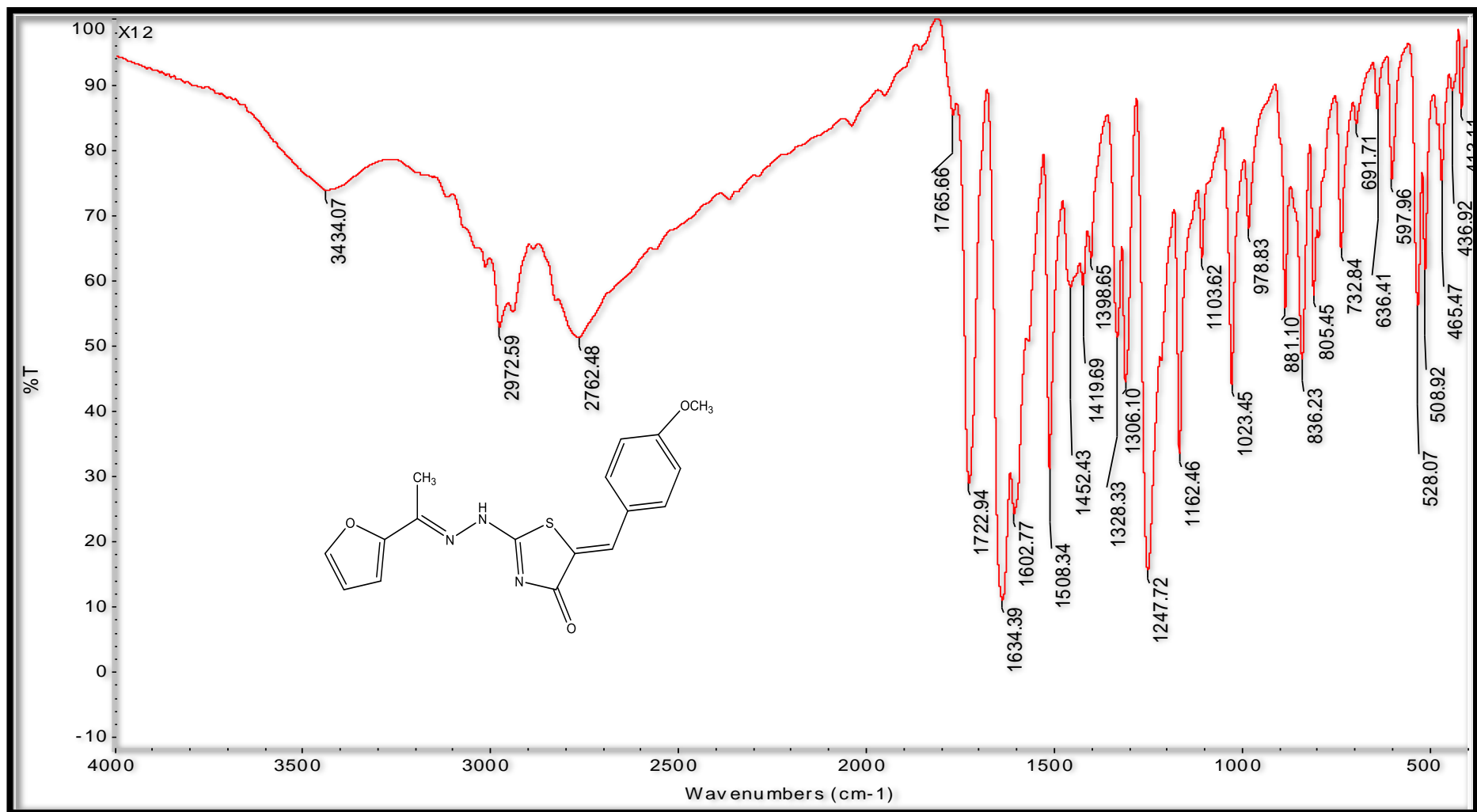
¹H NMR of compound (8f)



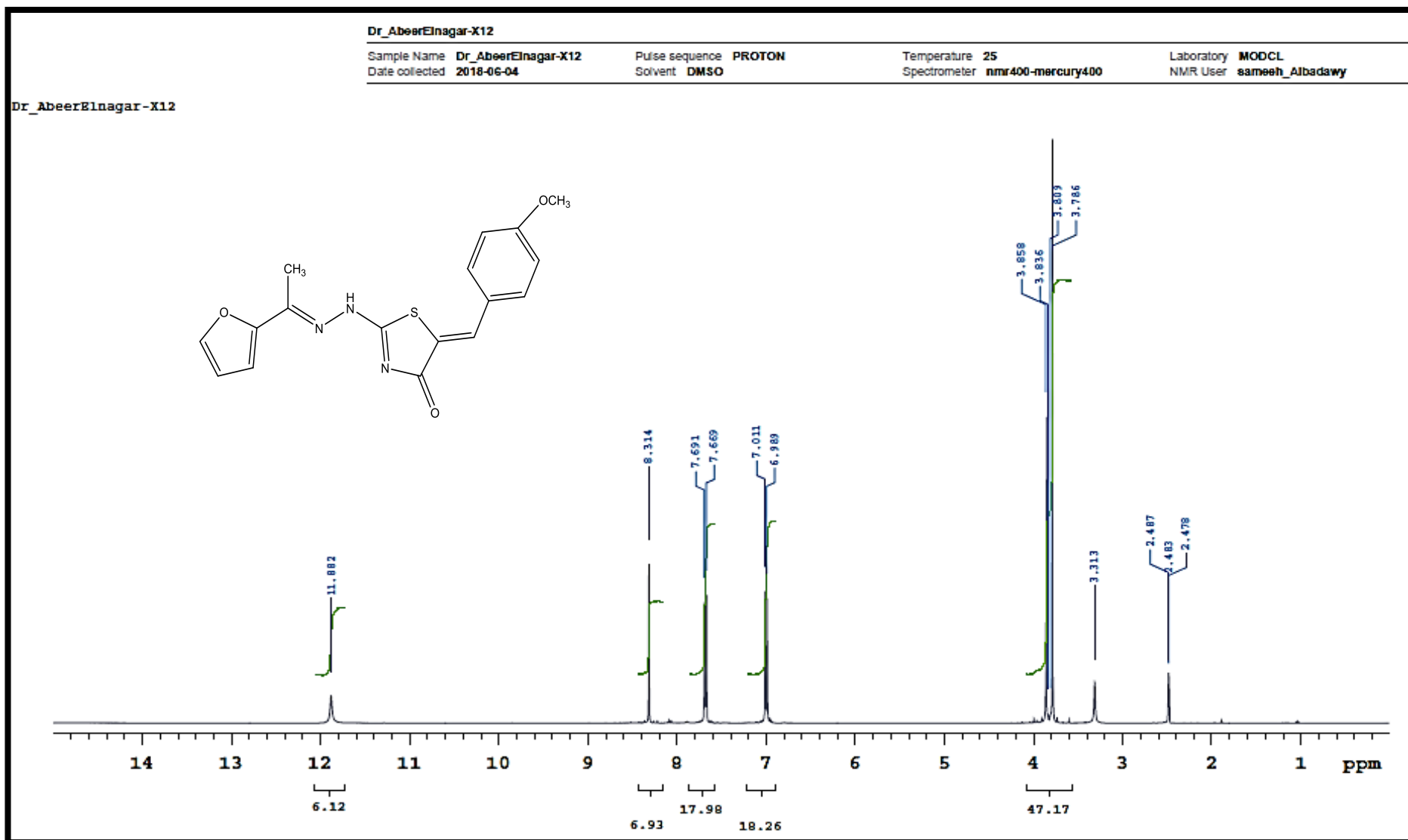
D₂O ¹H NMR of compound (8f)



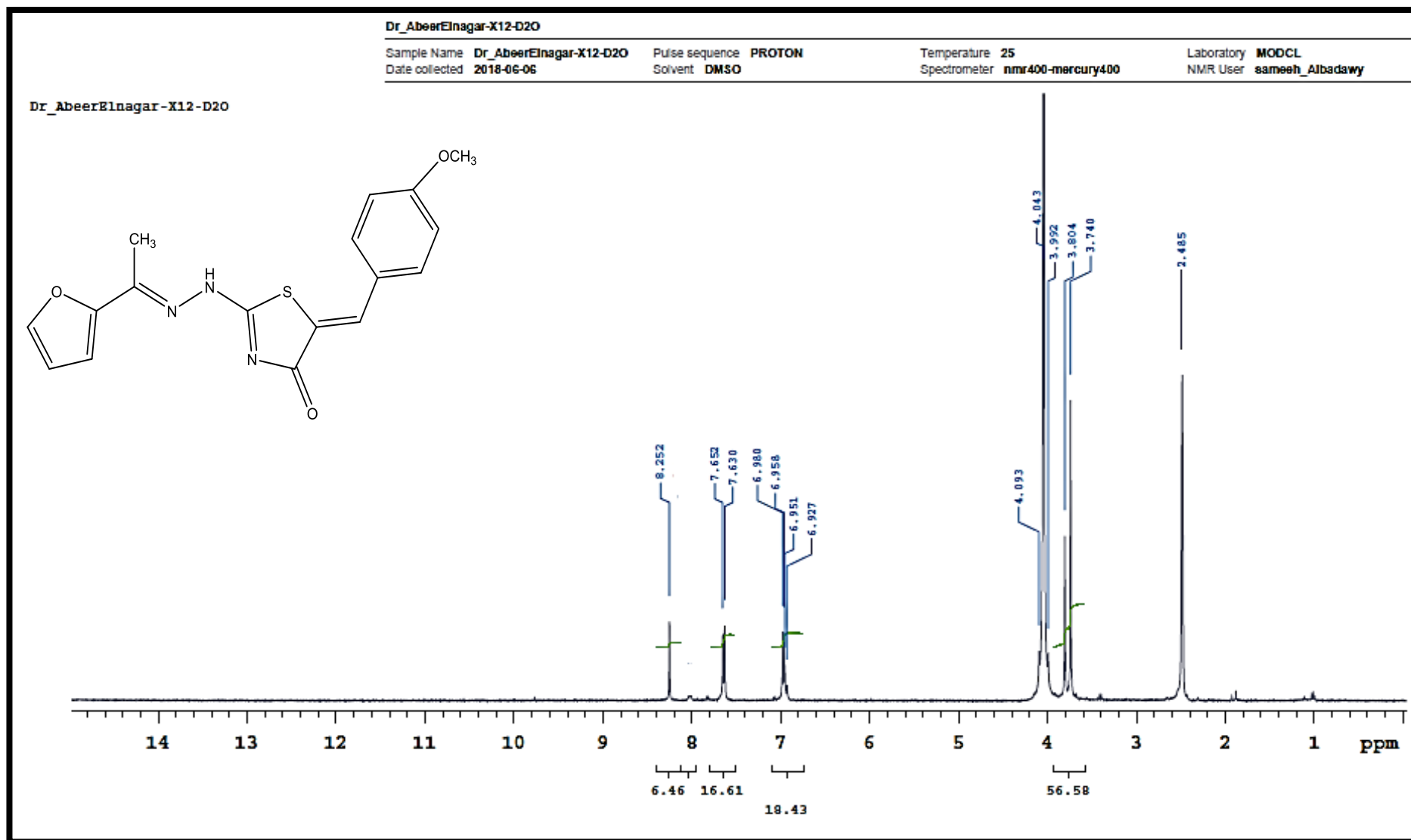
IR of compound (8g)



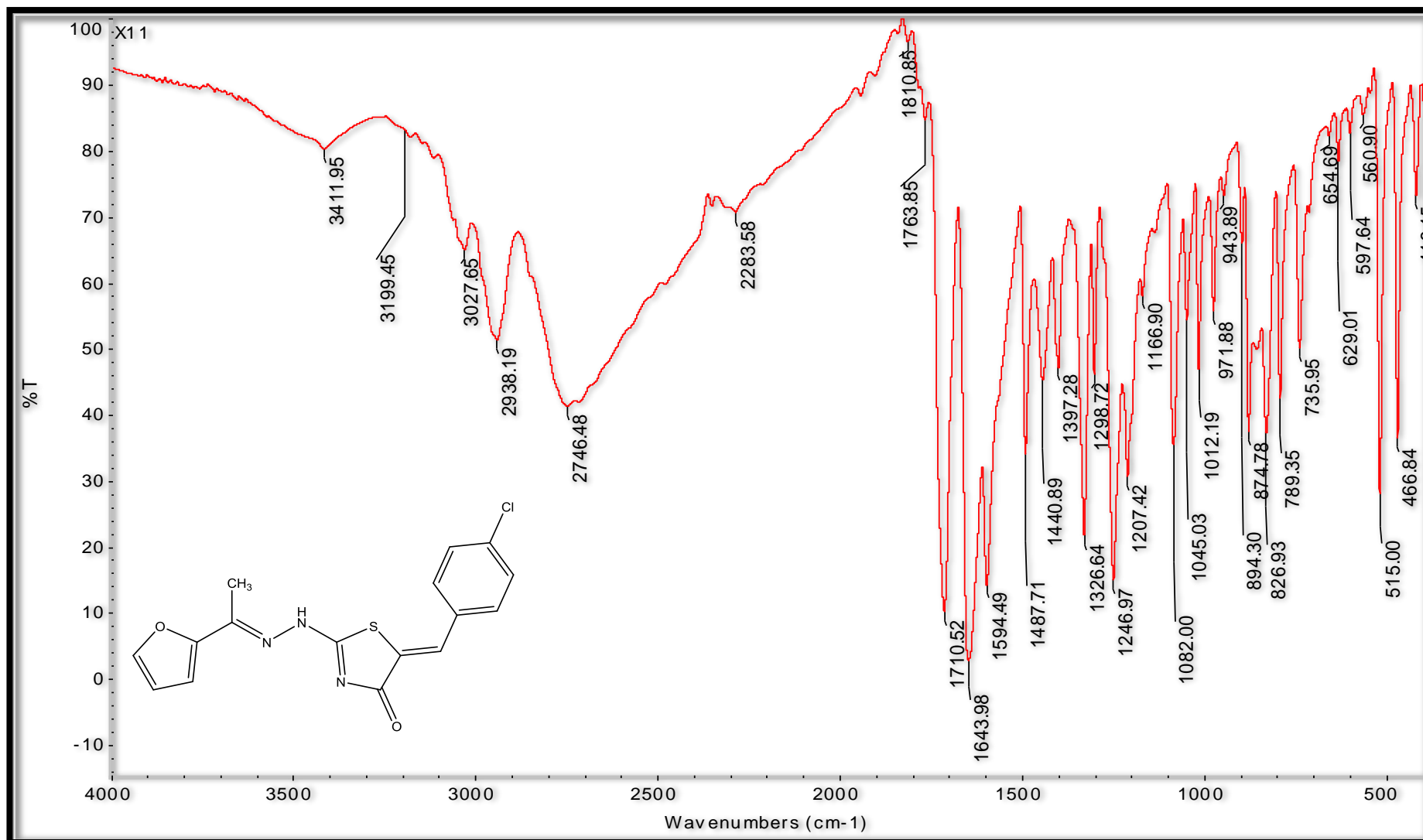
¹H NMR of compound (8g)



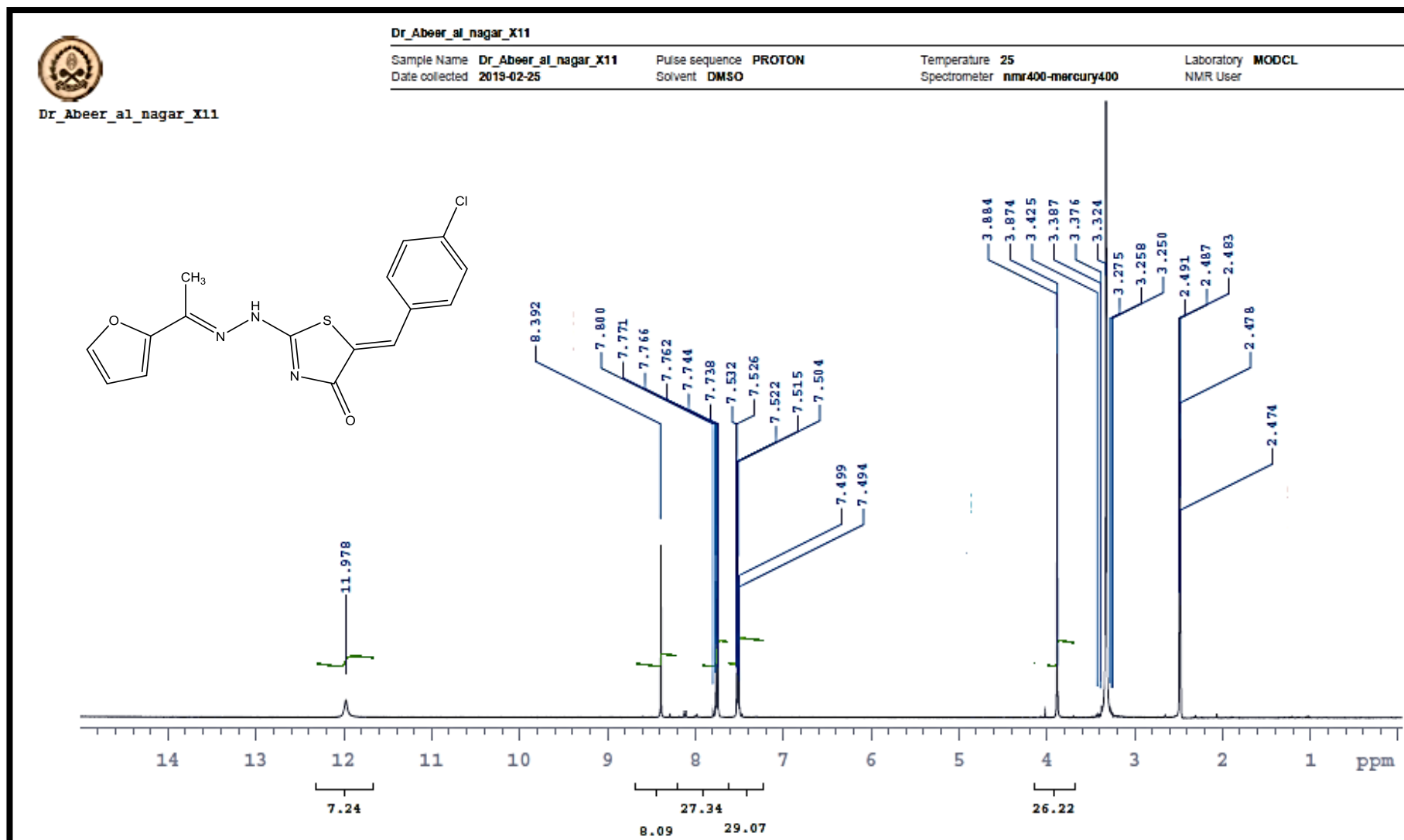
D₂O ¹H NMR of compound (8g)



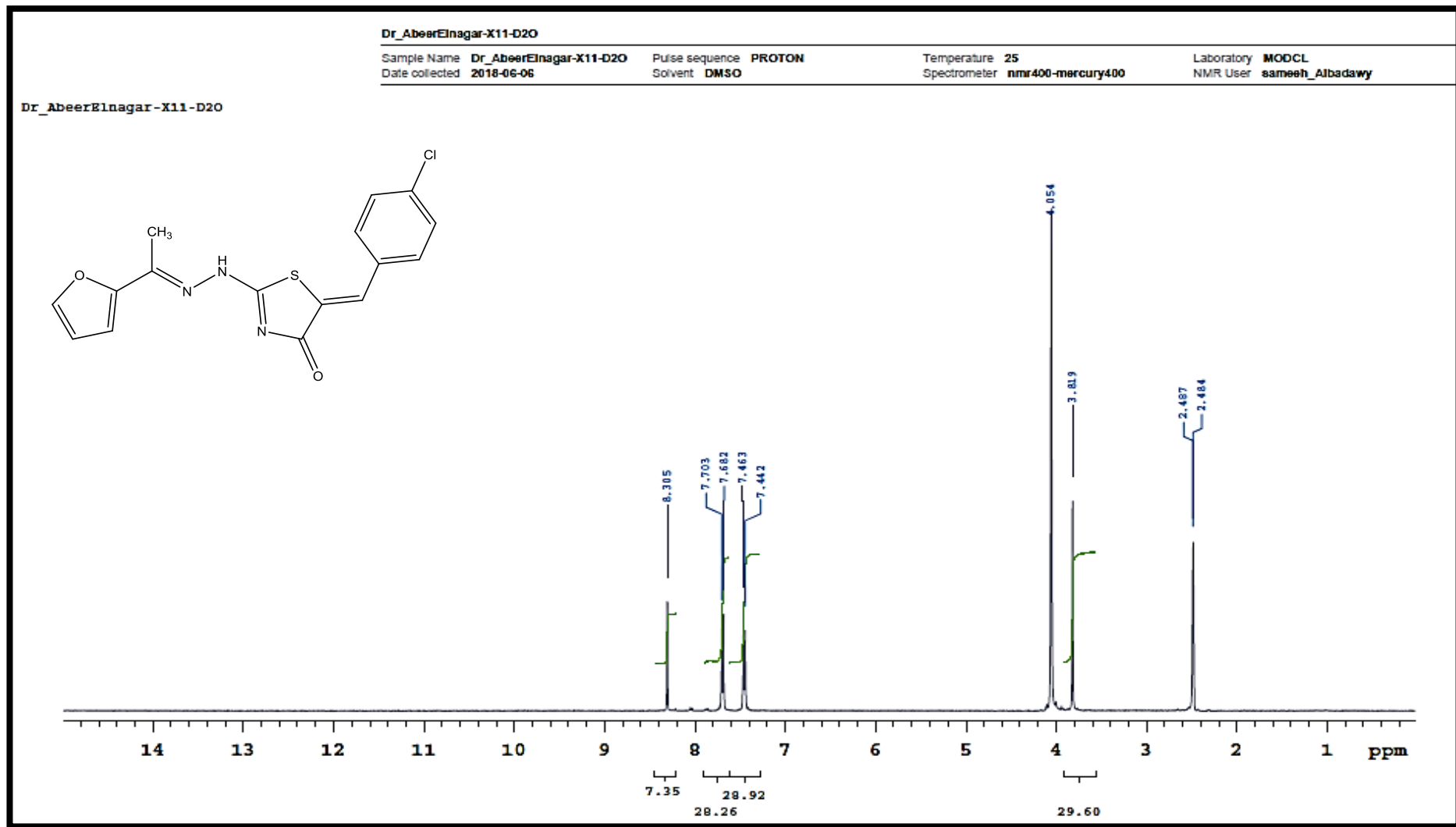
IR of compound (8h)



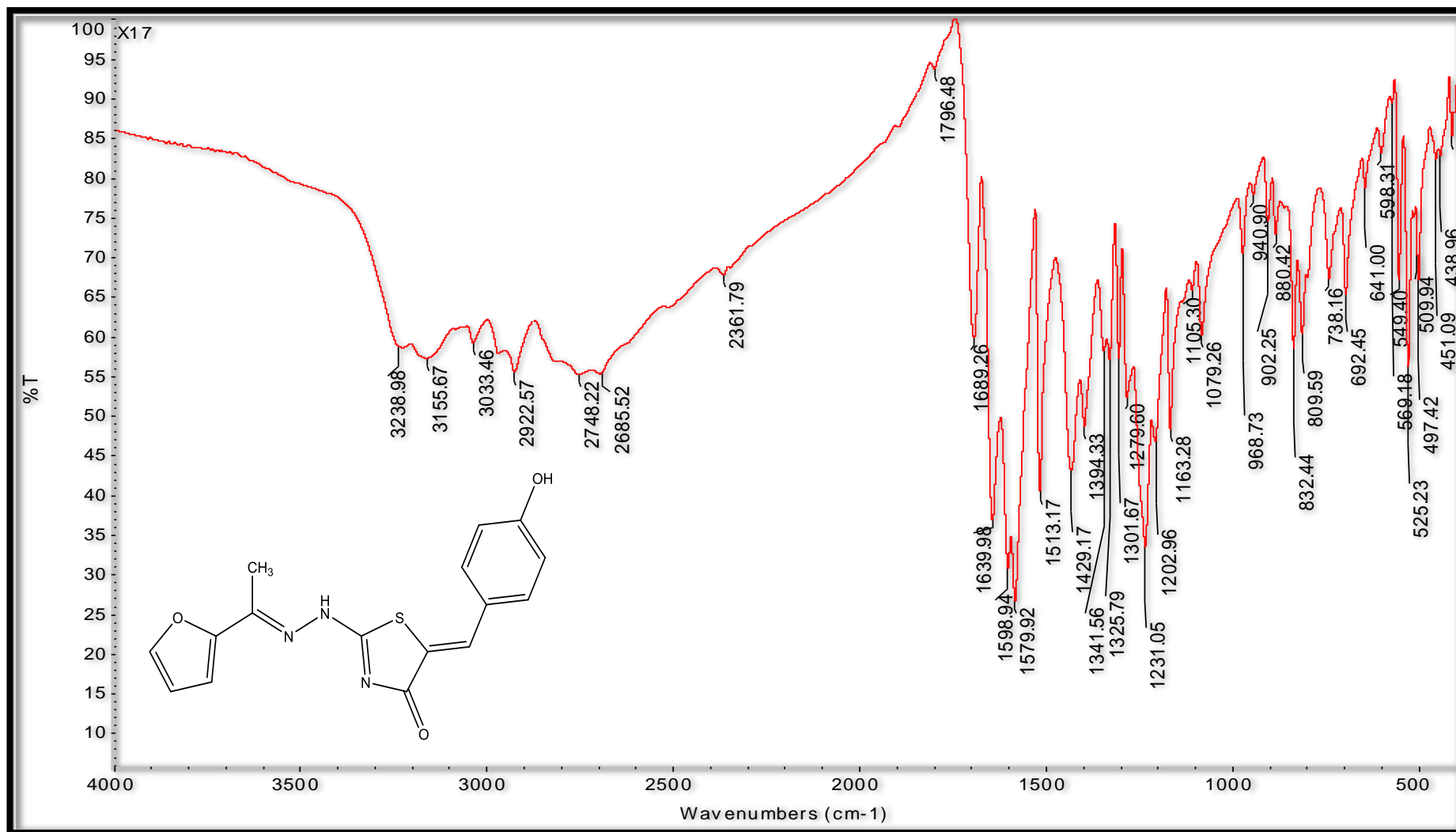
¹H NMR of compound (8h)



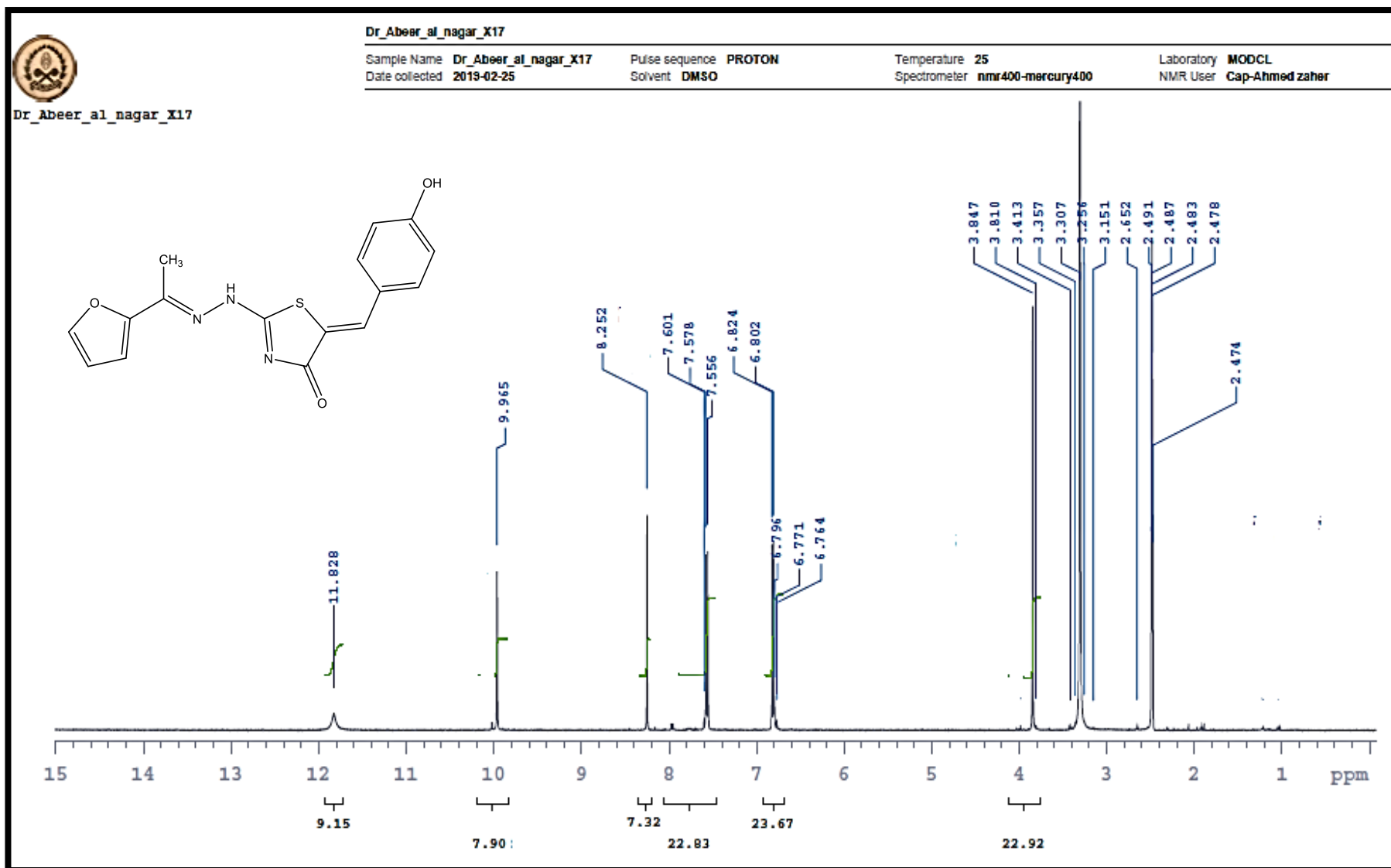
D₂O ¹H NMR of compound (8h)



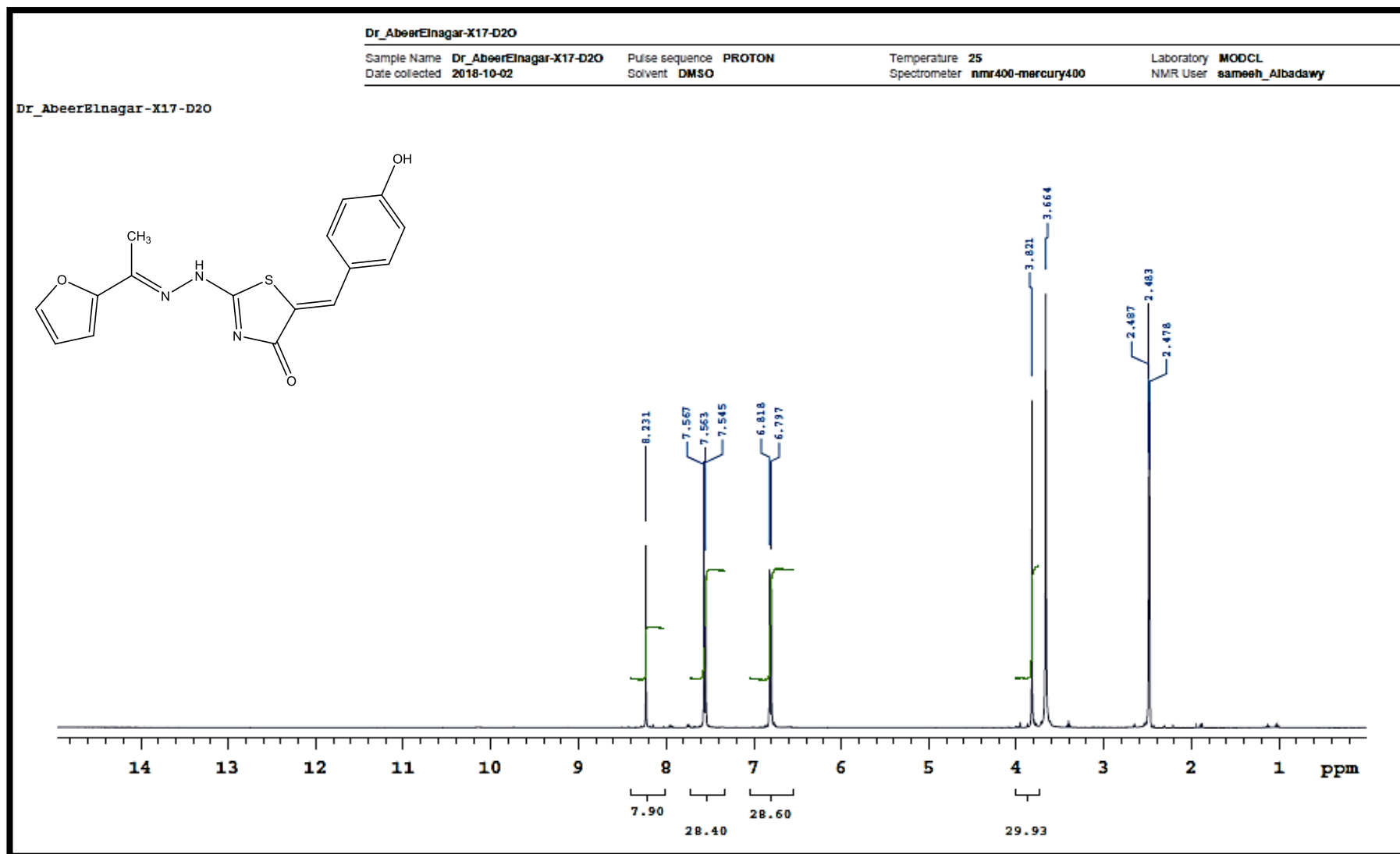
IR of compound (8i)



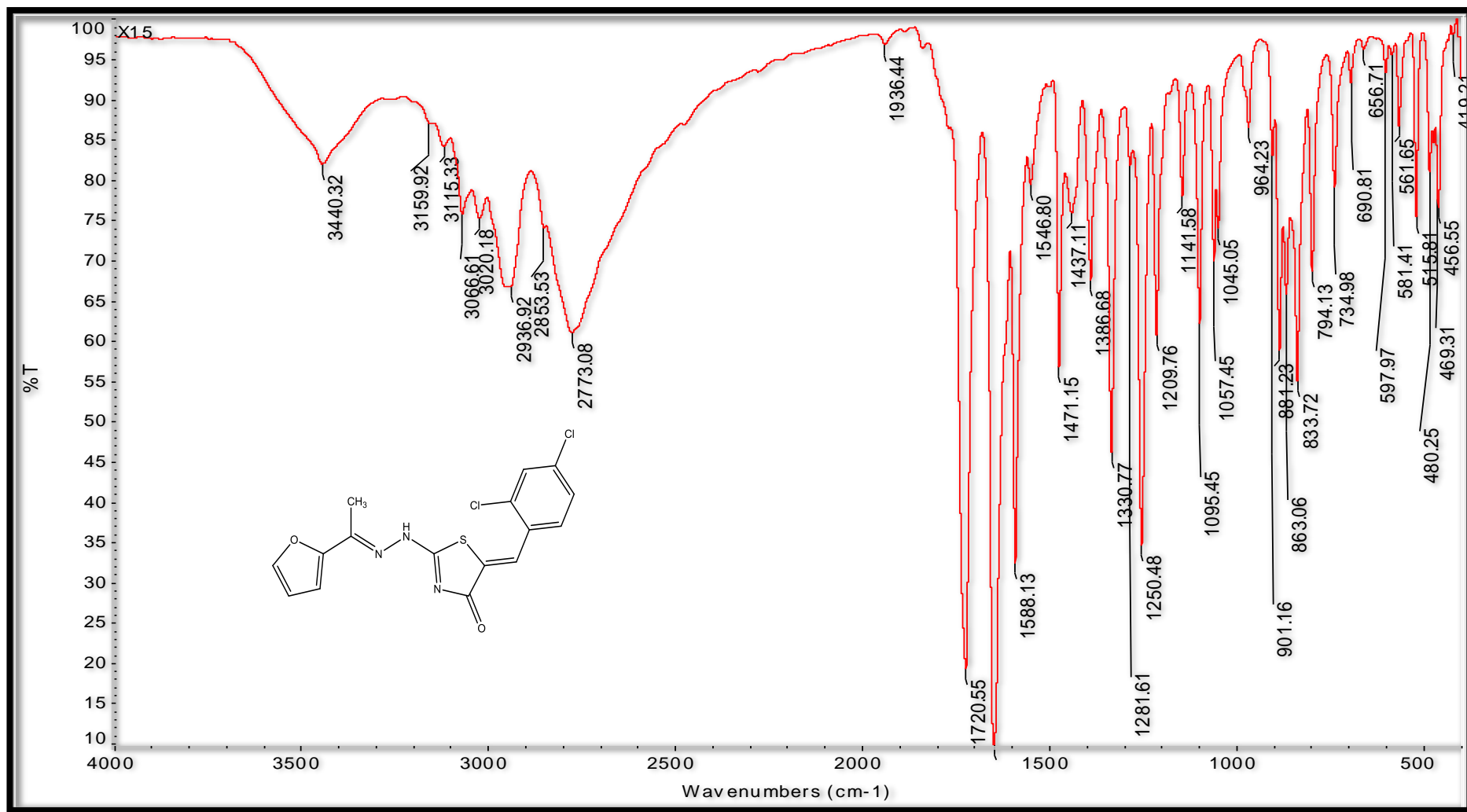
¹H NMR of compound (8i)



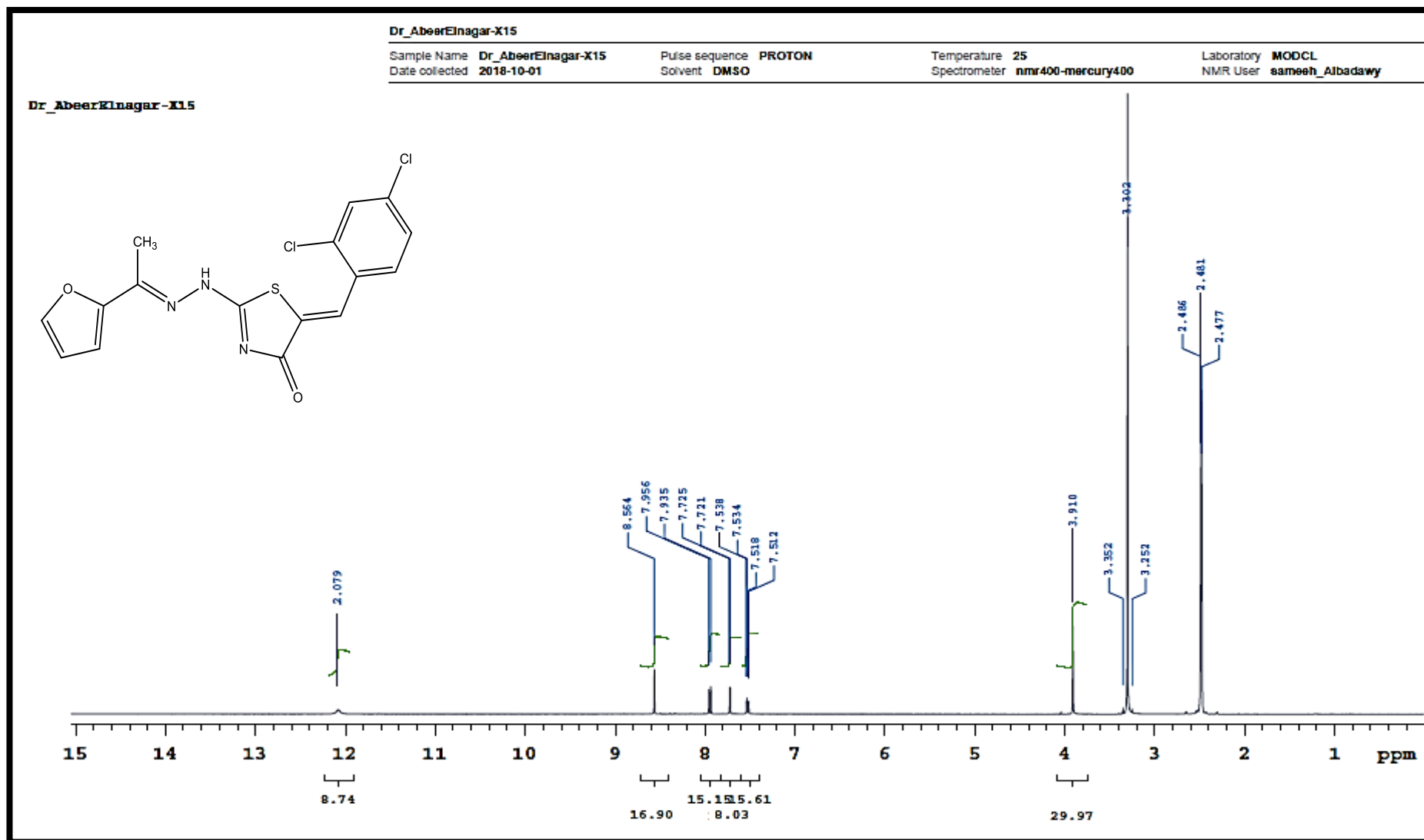
¹H NMR of compound (8i)



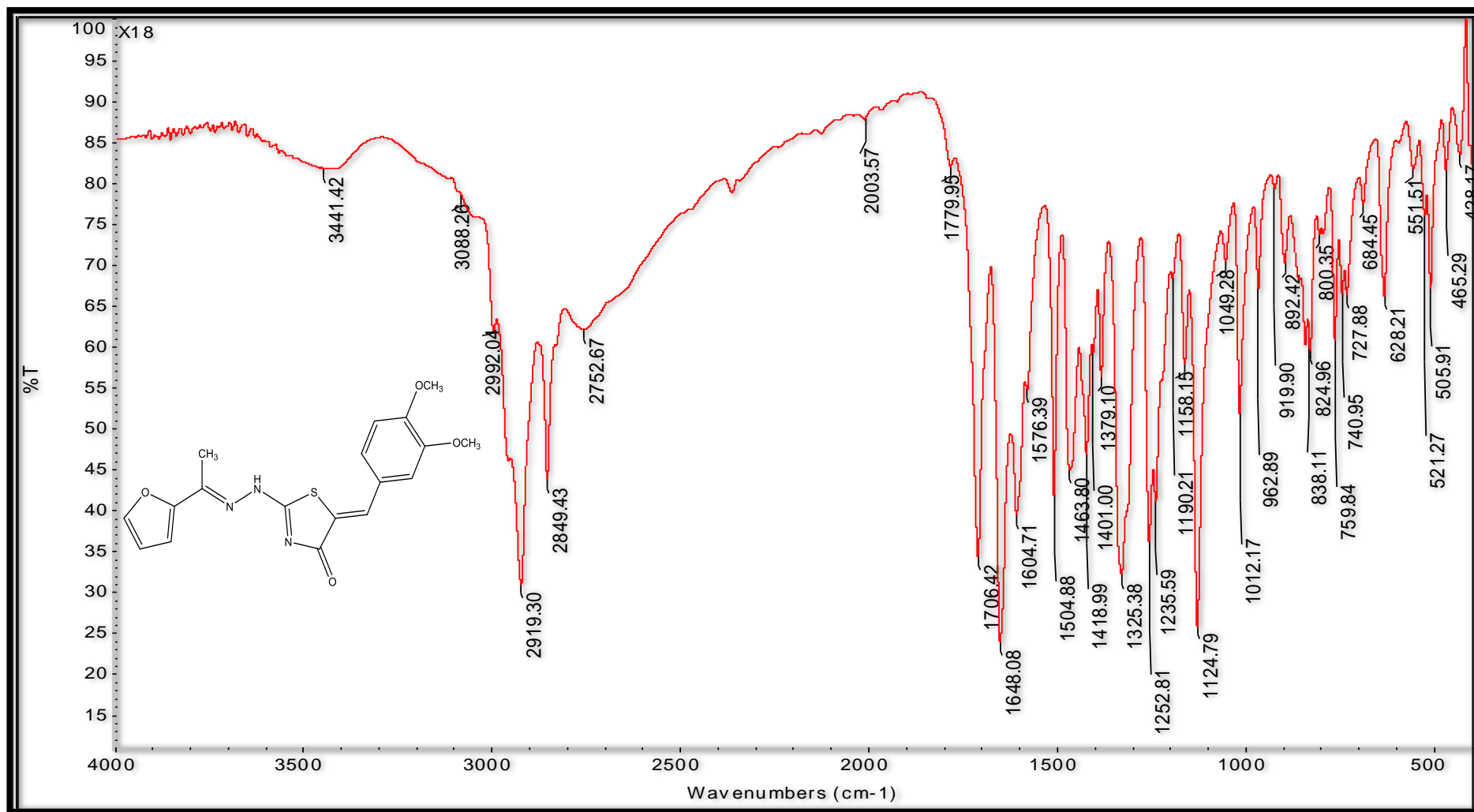
IR of compound (8j)



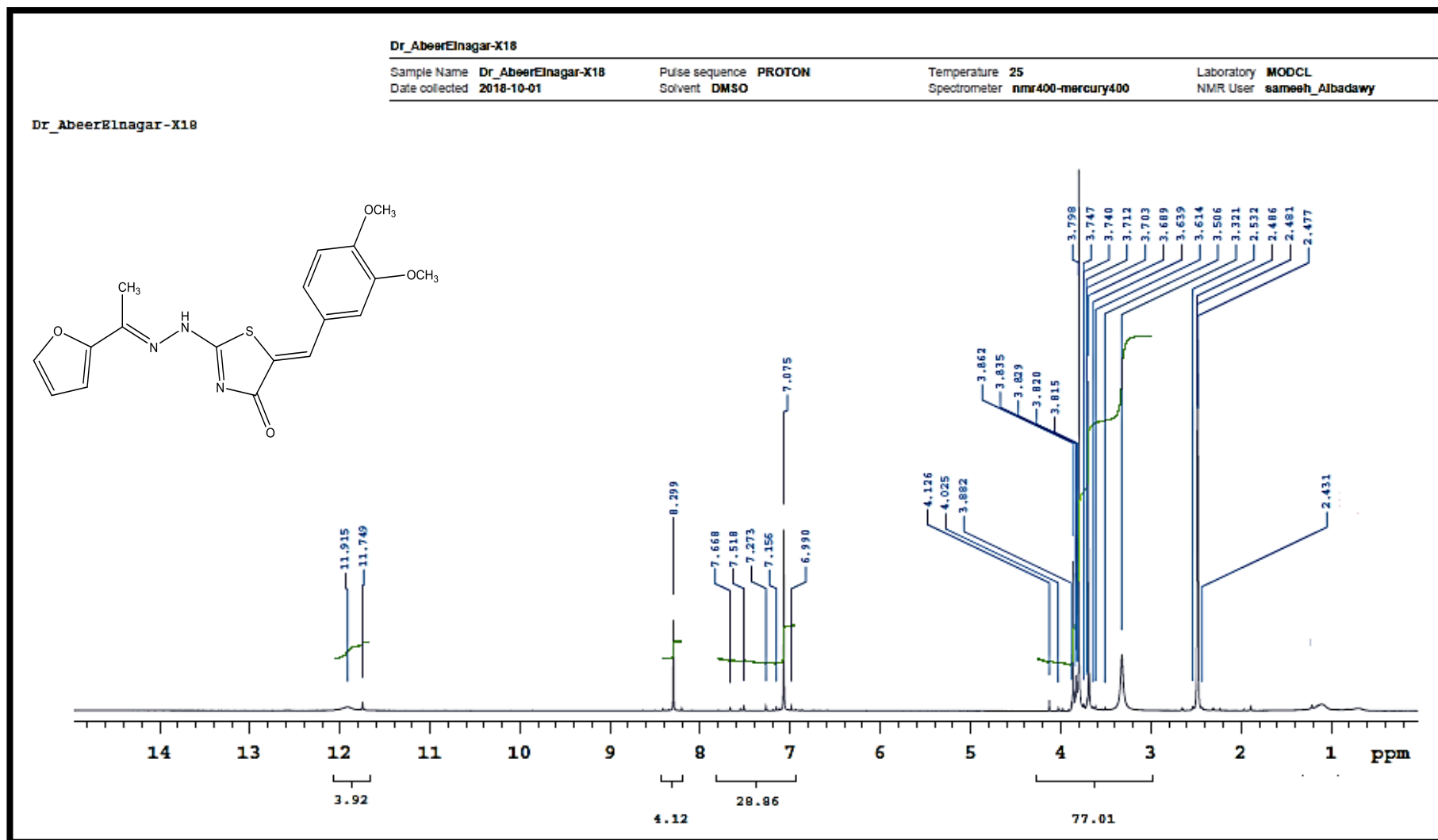
¹H NMR of compound (8j)



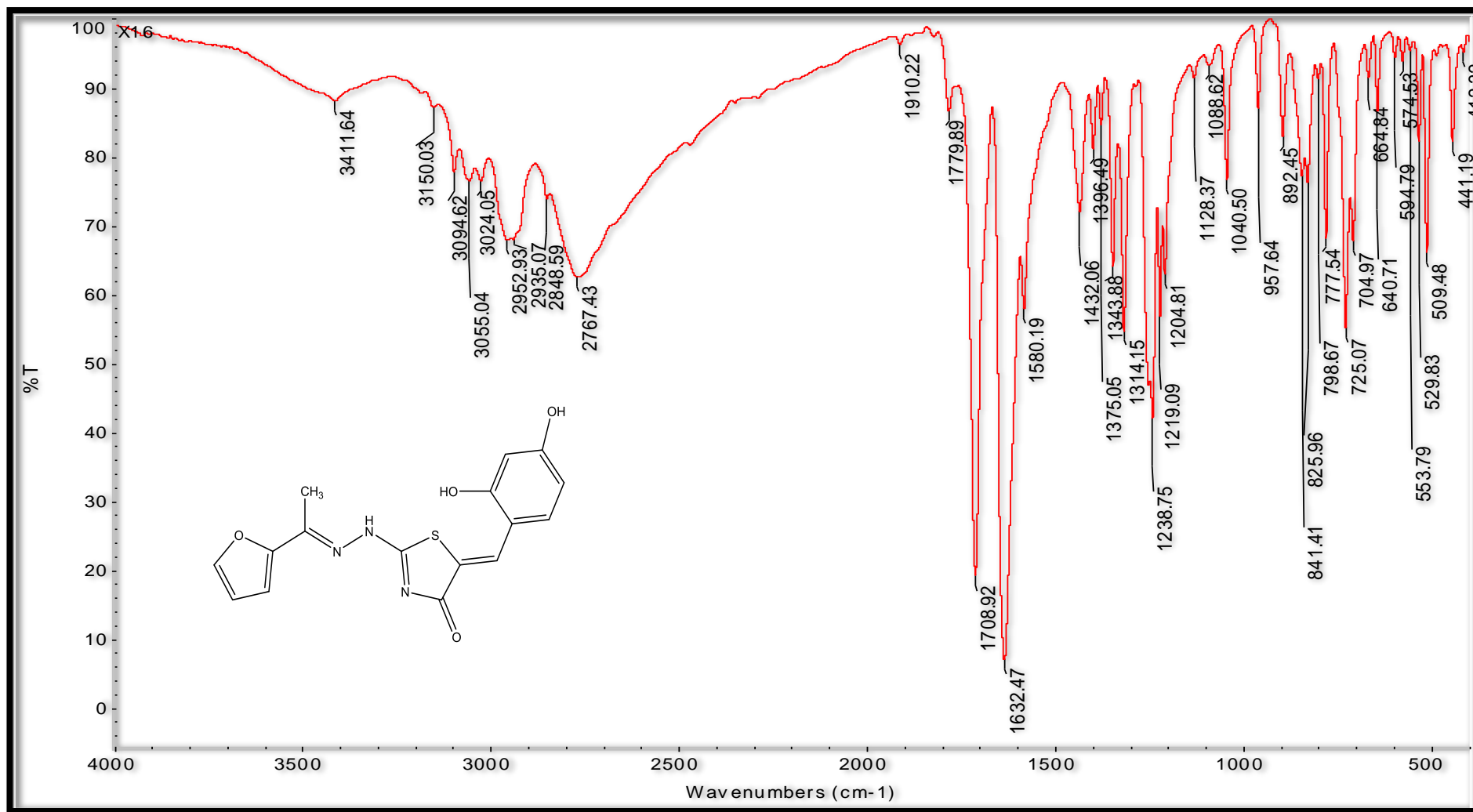
IR of compound (8k)



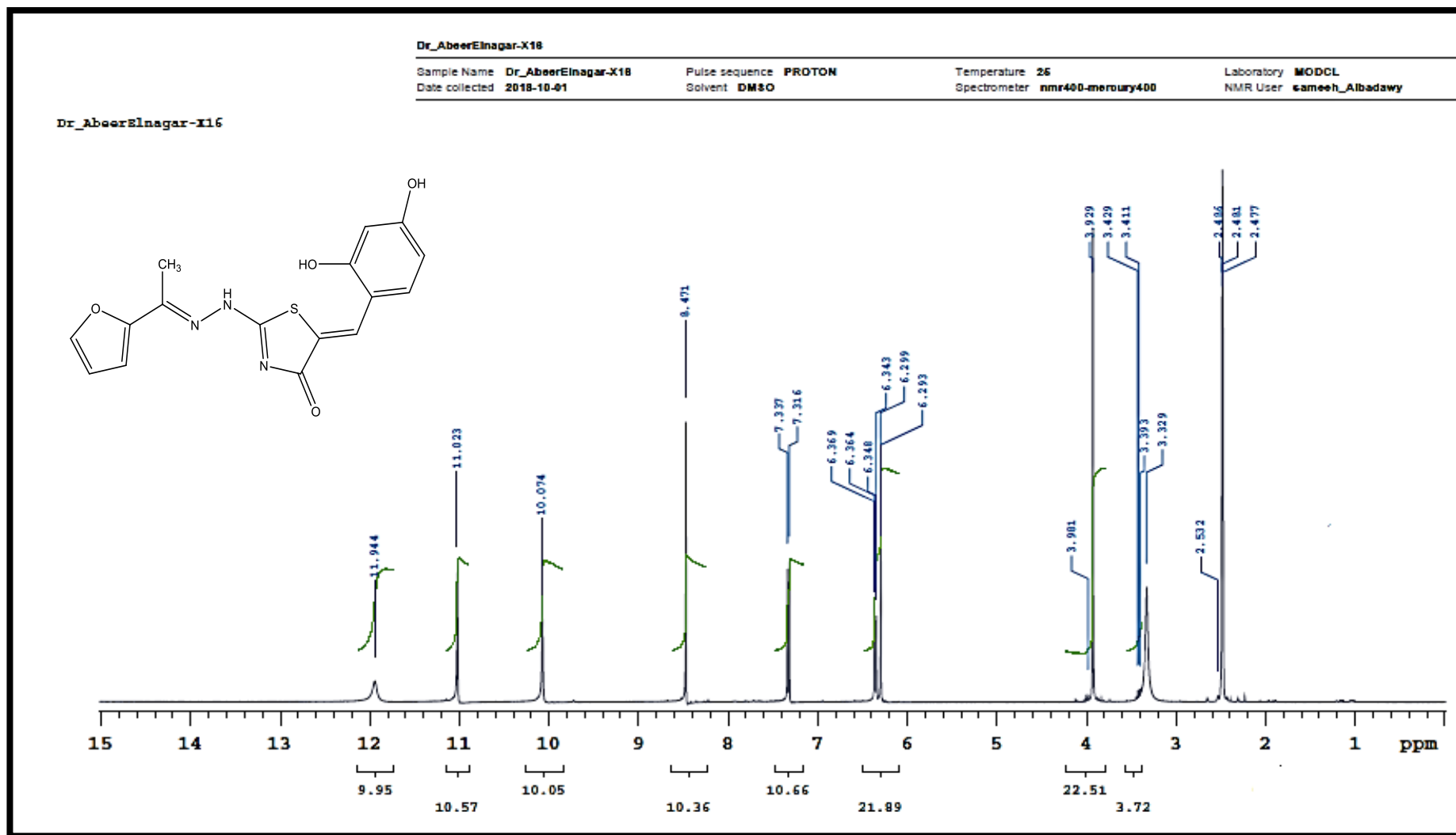
¹H NMR of compound (8k)



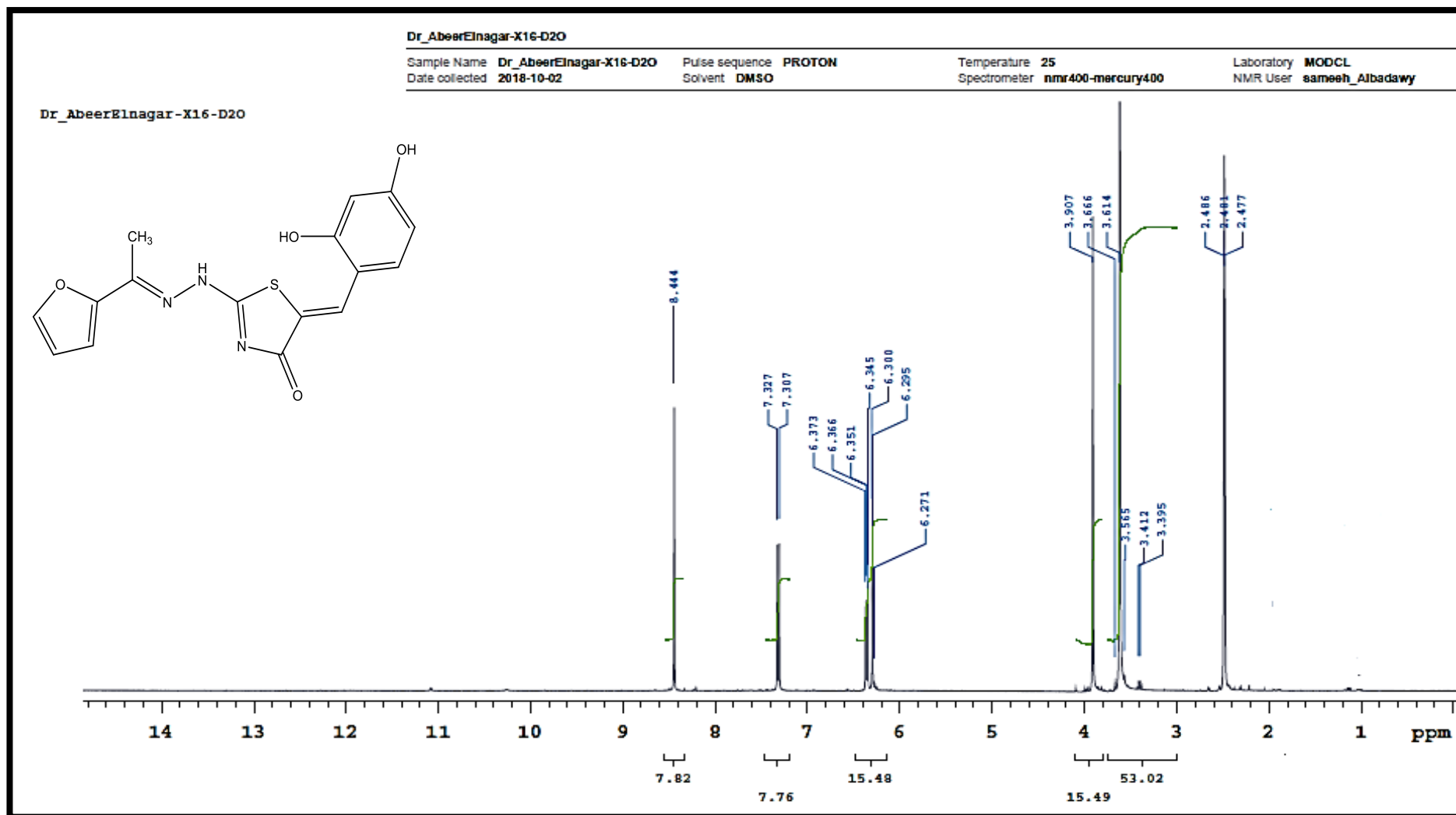
IR of compound (8l)



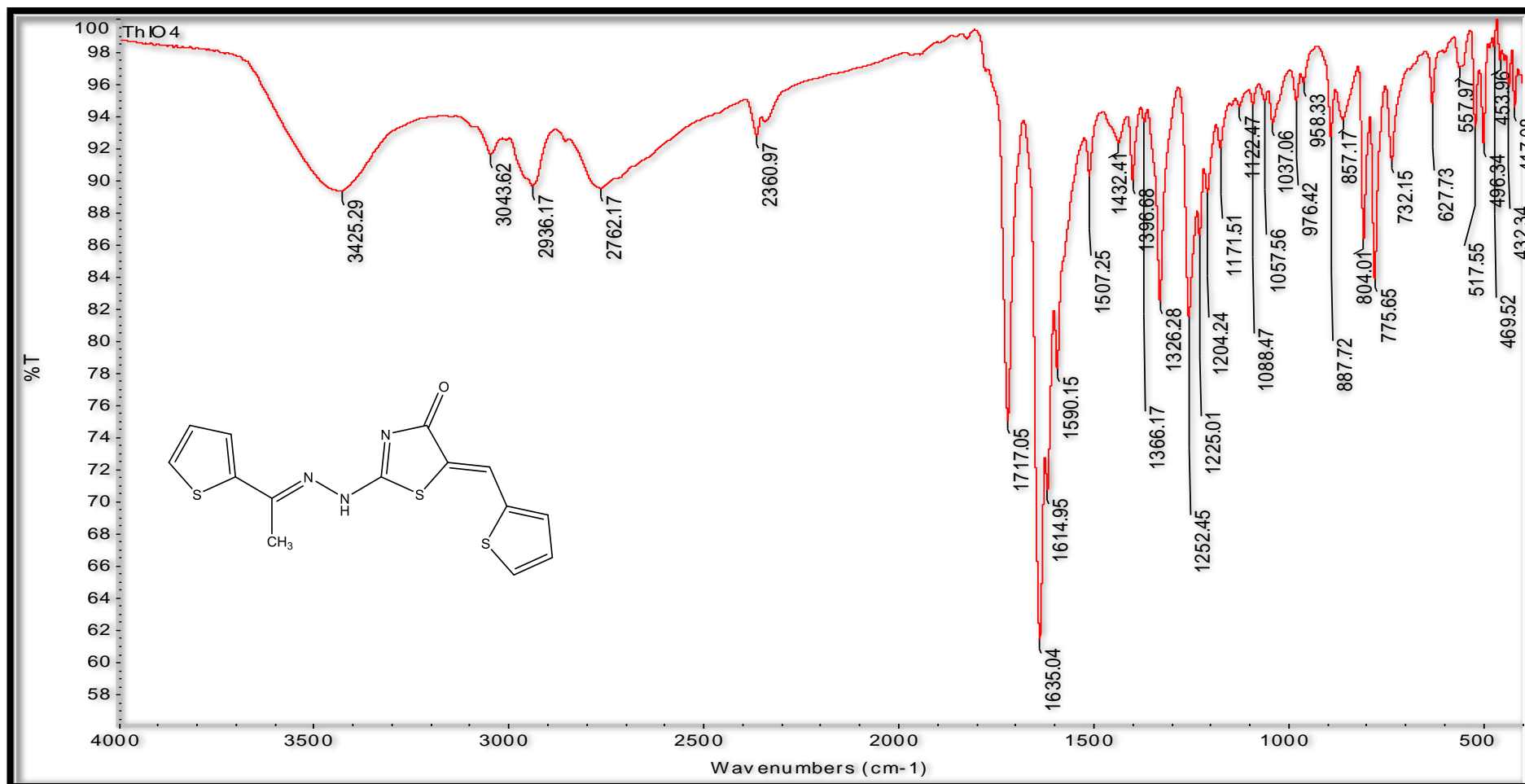
¹H NMR of compound (8I)



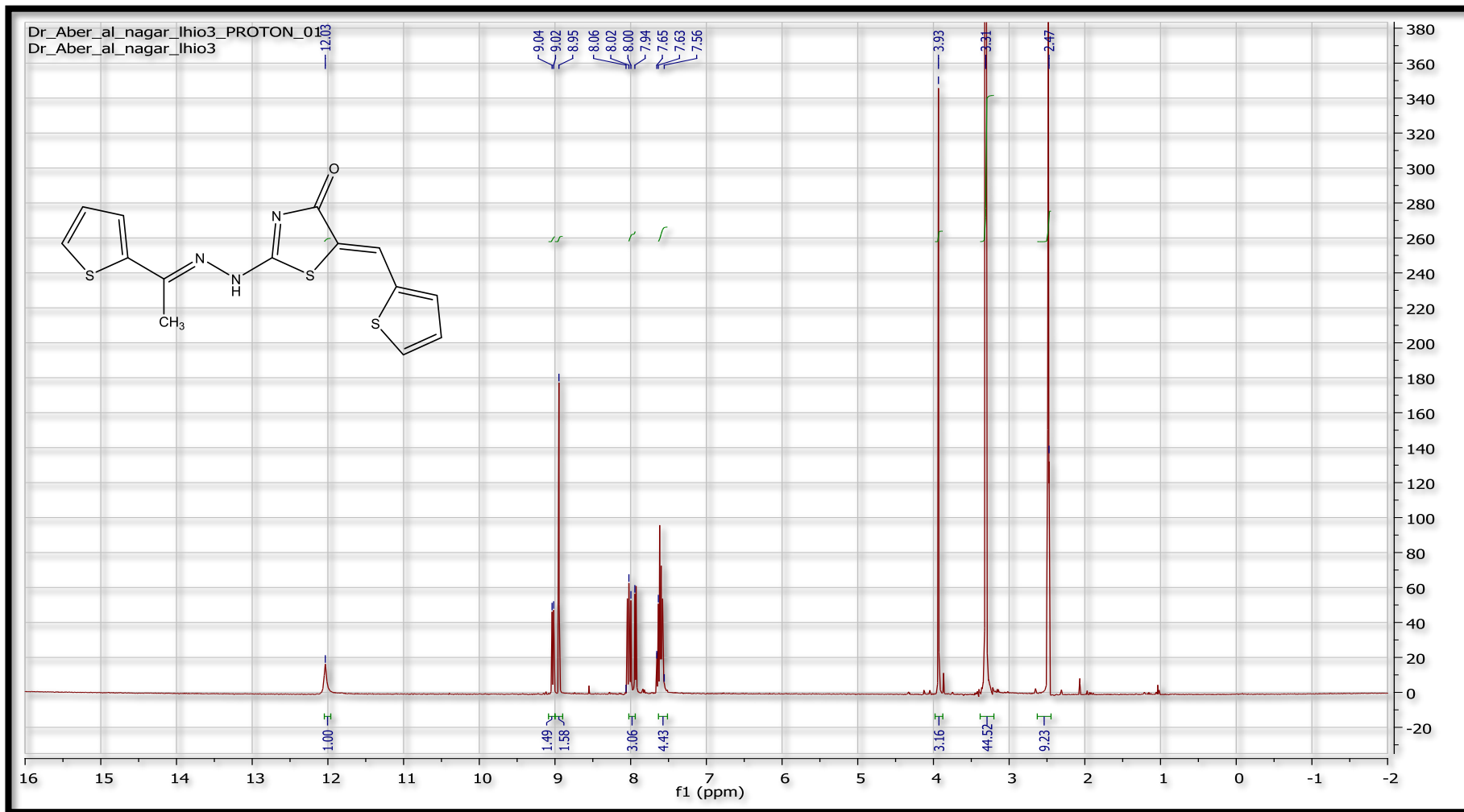
D₂O ¹H NMR of compound (8l)



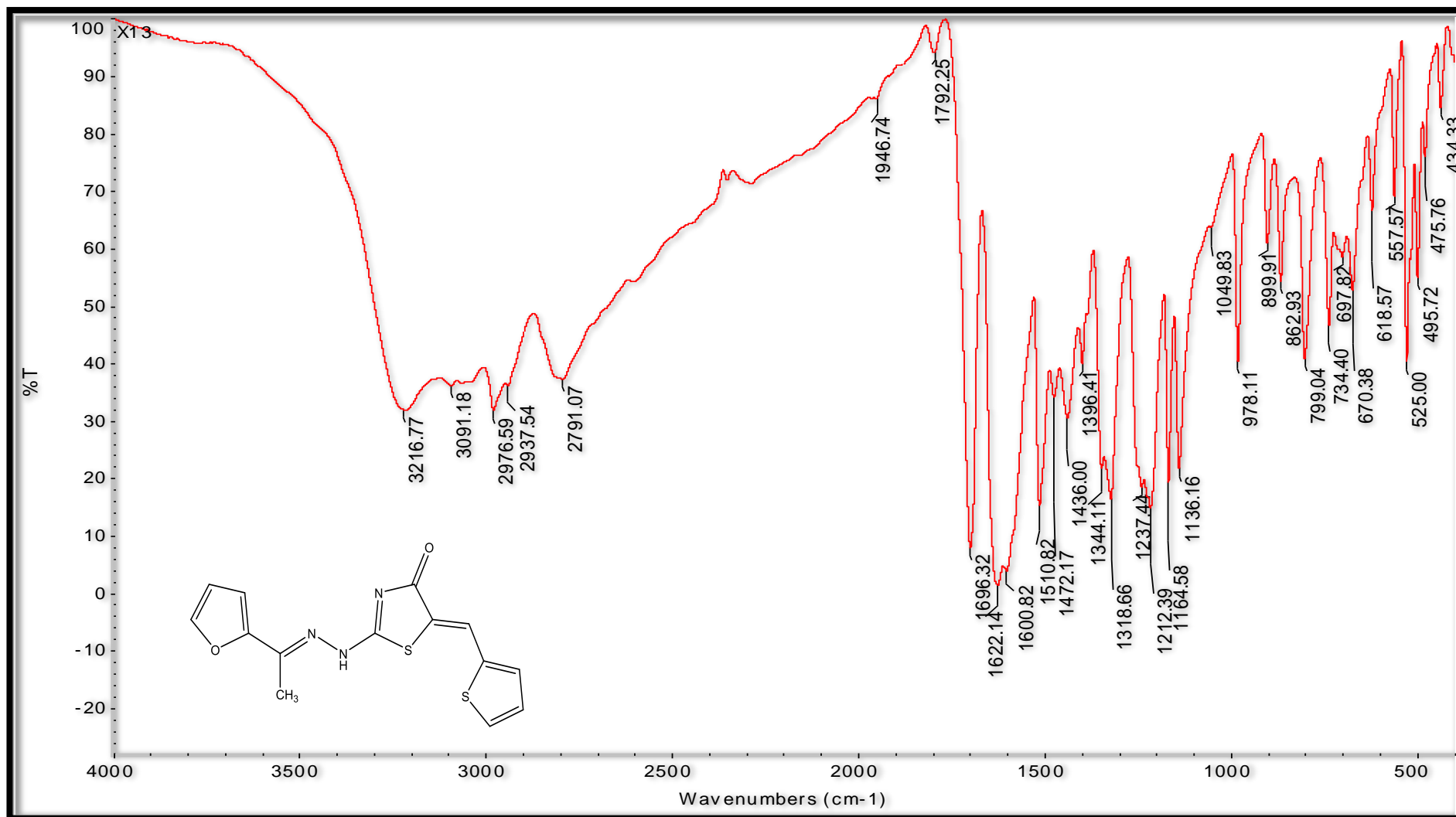
IR of compound (9a)



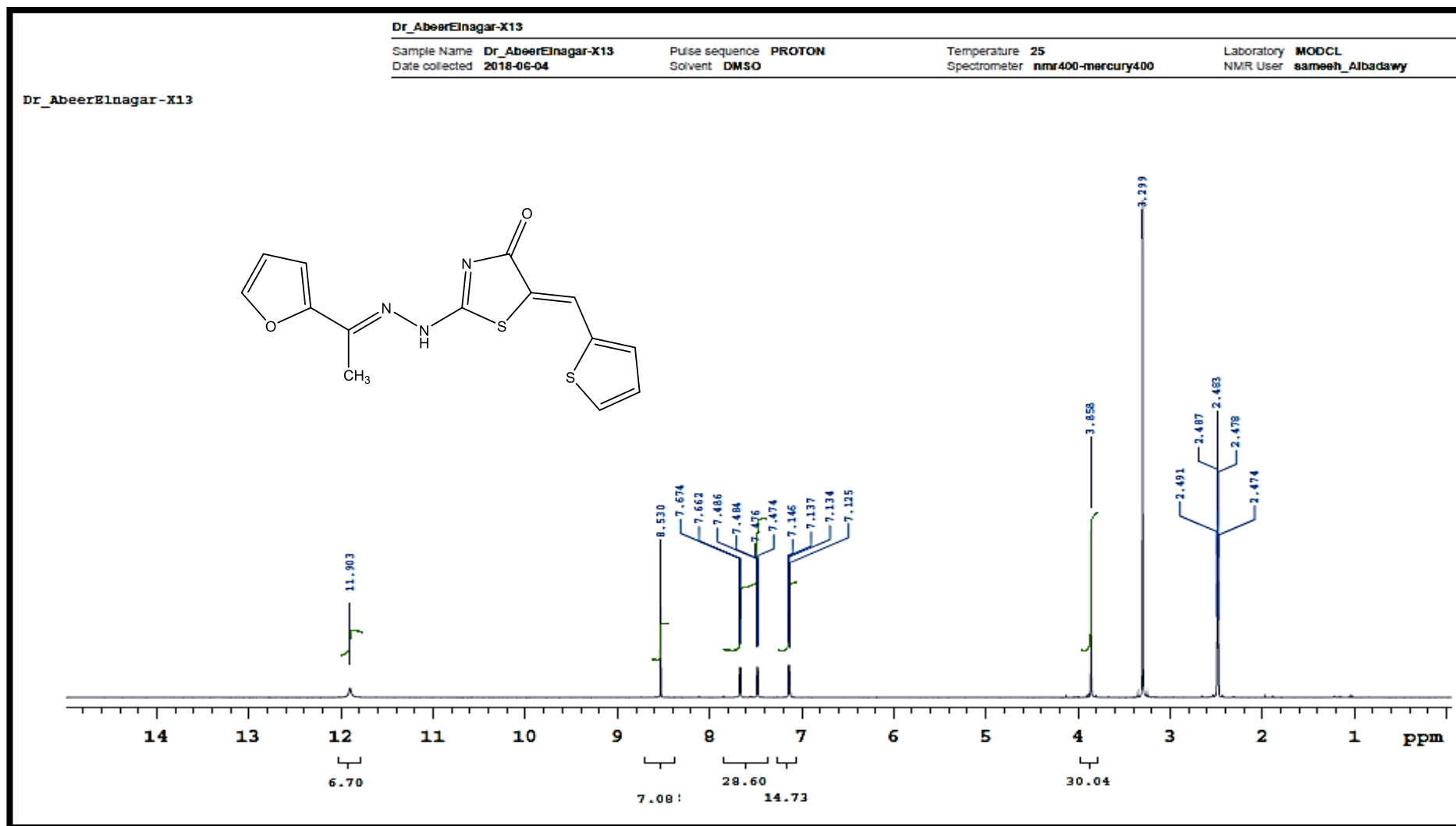
¹H NMR of compound (9a)



IR of compound (9b)



¹H NMR of compound (9b)



¹H NMR of compound (9b)

