Electronic Supplementary Information

An efficient and rapid intramolecular cyclization of quadruple Mannich reaction for the one-pot synthesis of pentaazaphenalenes and their antimicrobial activities

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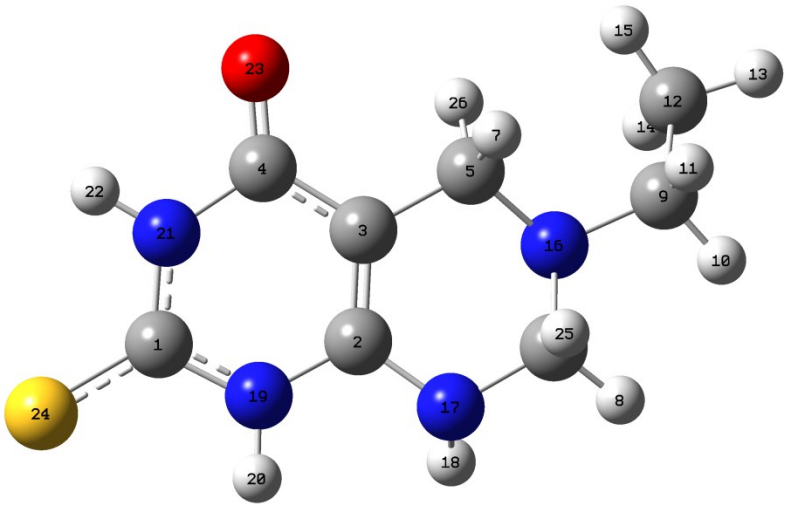
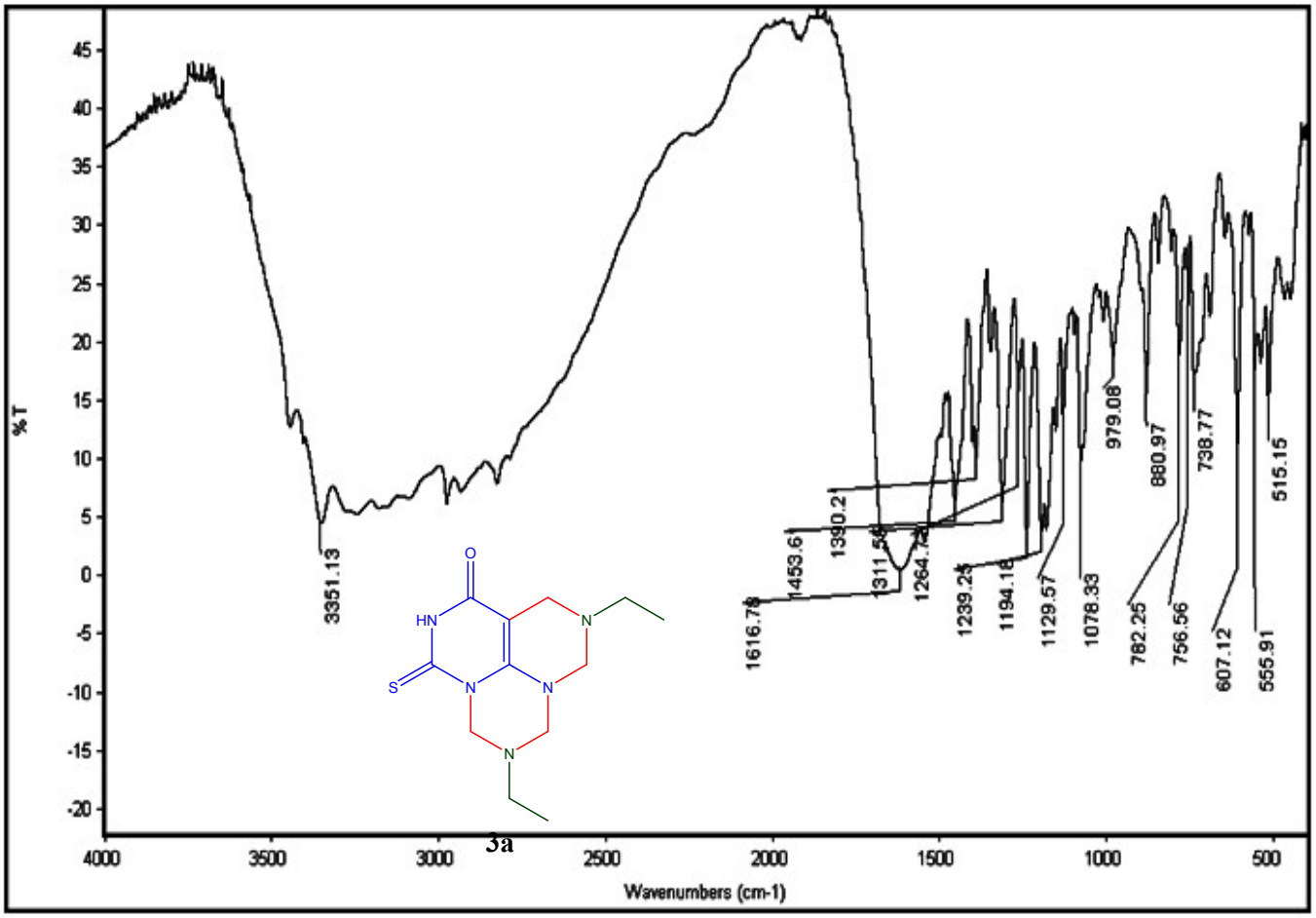


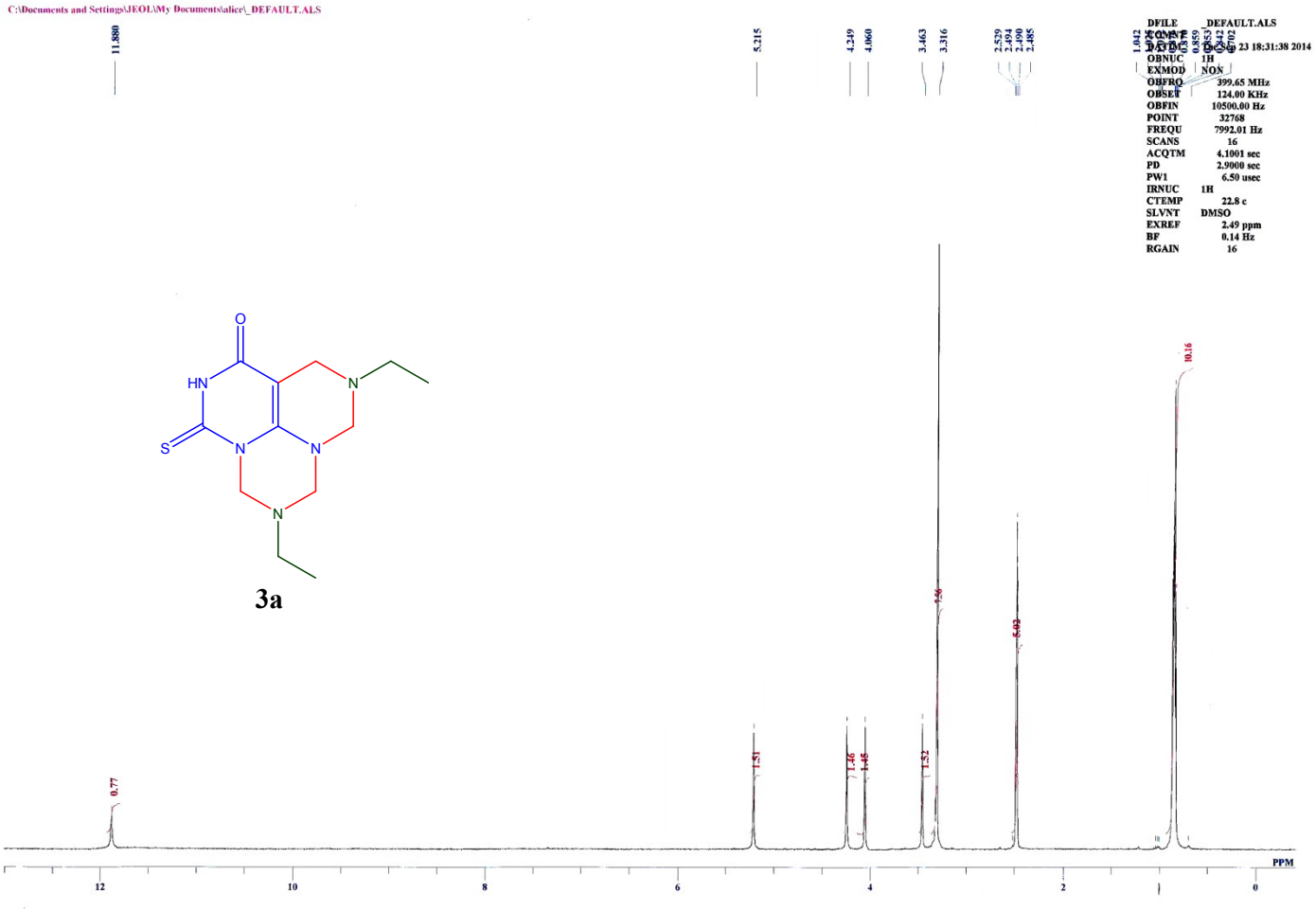
Figure S1. The geometry structure of intermediate tautomer **6a**. Atom color code: Carbon (gray), nitrogen (blue), oxygen (red), sulfur (yellow), bromine (orange) and hydrogen (white).

Table S1. Values of atomic charge of intermediate tautomer **6a**.

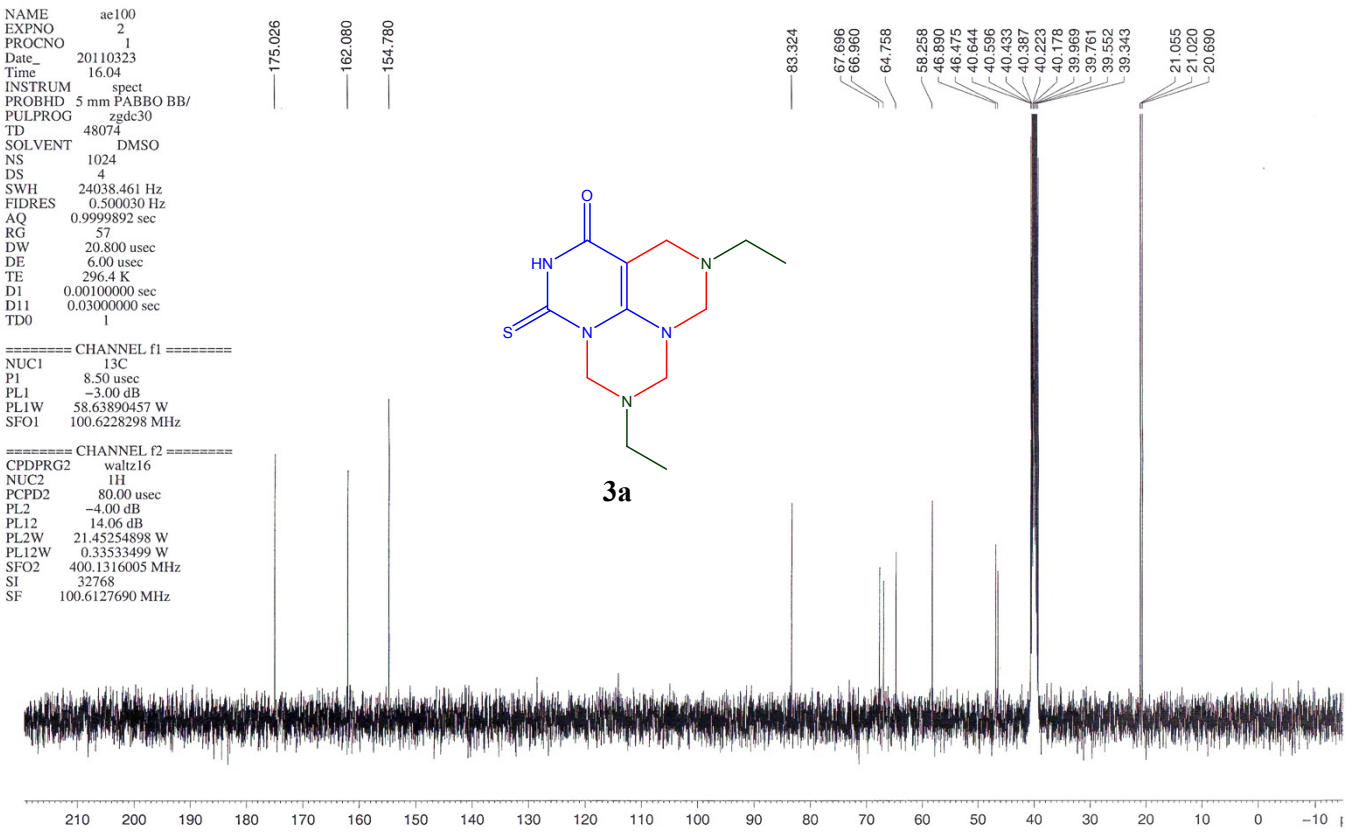
Atom	Number	Charge
C	1	0.24198
C	2	0.42319
C	3	- 0.23840
C	4	0.65682
C	5	- 0.26874
C	6	- 0.08130
H	7	0.22825
H	8	0.25065
C	9	- 0.27104
H	10	0.23901
H	11	0.21085
C	12	- 0.70967
H	13	0.24841
H	14	0.24718
H	15	0.24192
N	16	- 0.55760
N	17	- 0.67056
H	18	0.42809
N	19	- 0.61320
H	20	0.46452
N	21	- 0.64060
H	22	0.47049
O	23	- 0.61361
S	24	- 0.18107
H	25	0.21903
H	26	0.27539



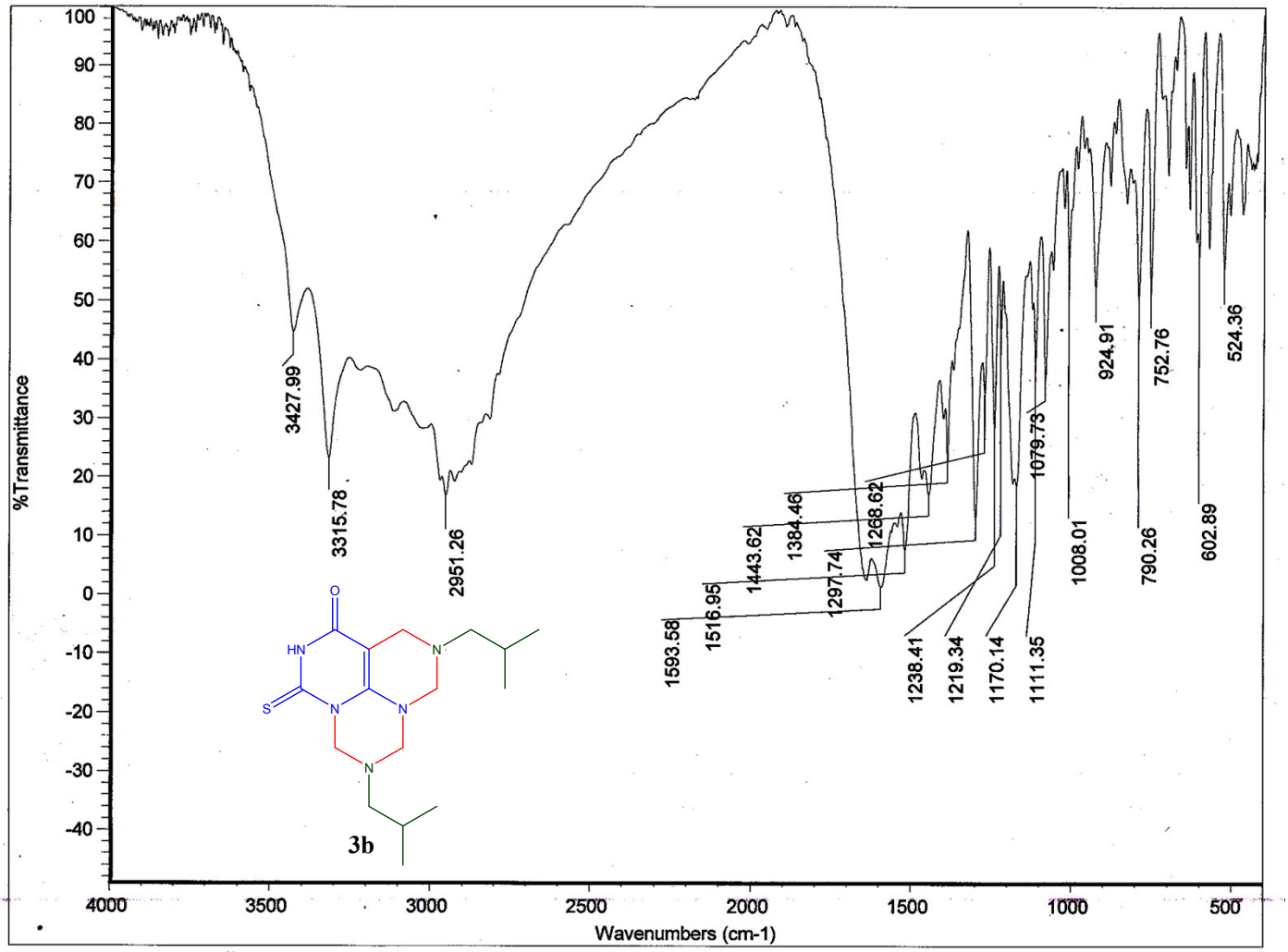
FTIR spectrum of compound **3a**.



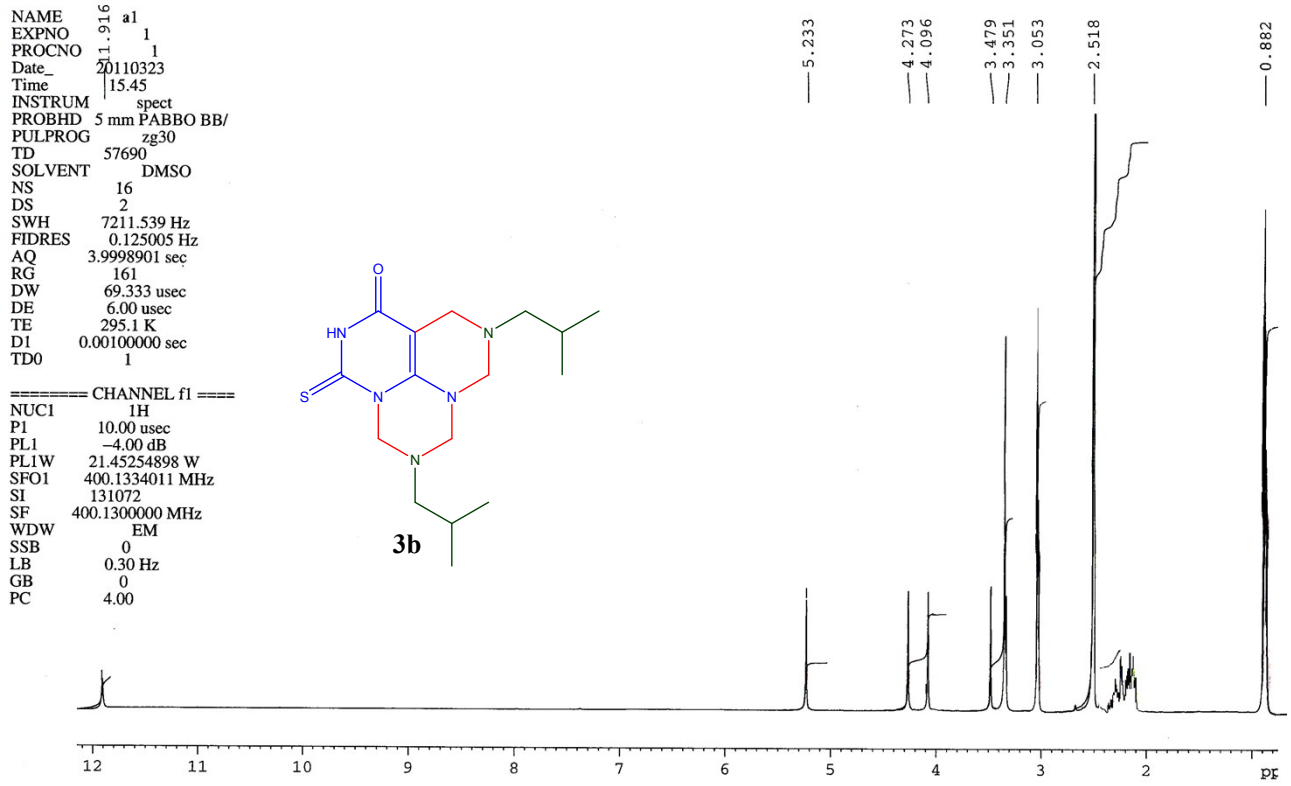
^{1}H-NMR spectrum of compound **3a** (400 MHz, DMSO-d_6).



^{13}C-NMR spectrum of compound **3a** (400 MHz, DMSO-d_6).

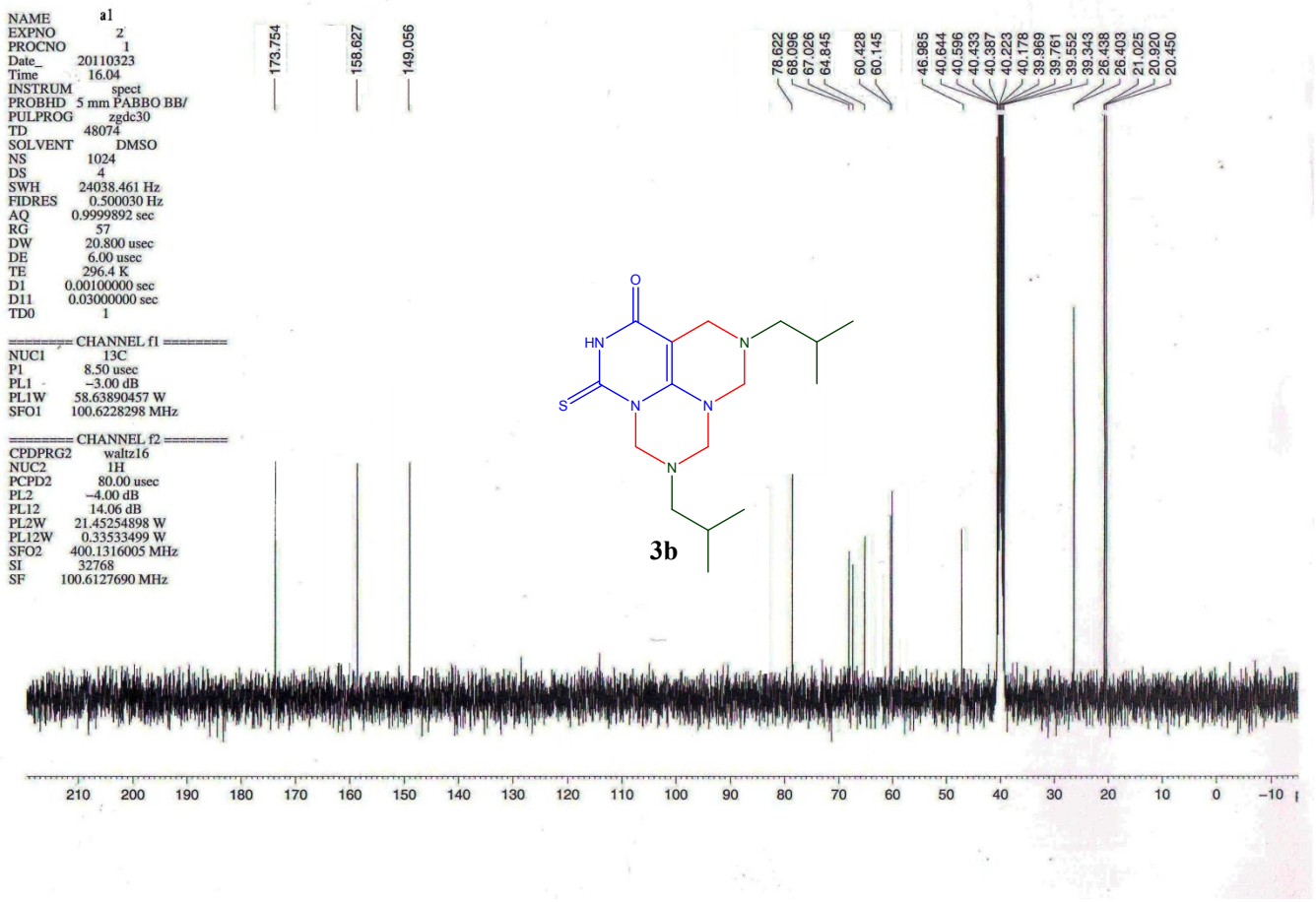


FTIR spectrum of compound **3b**

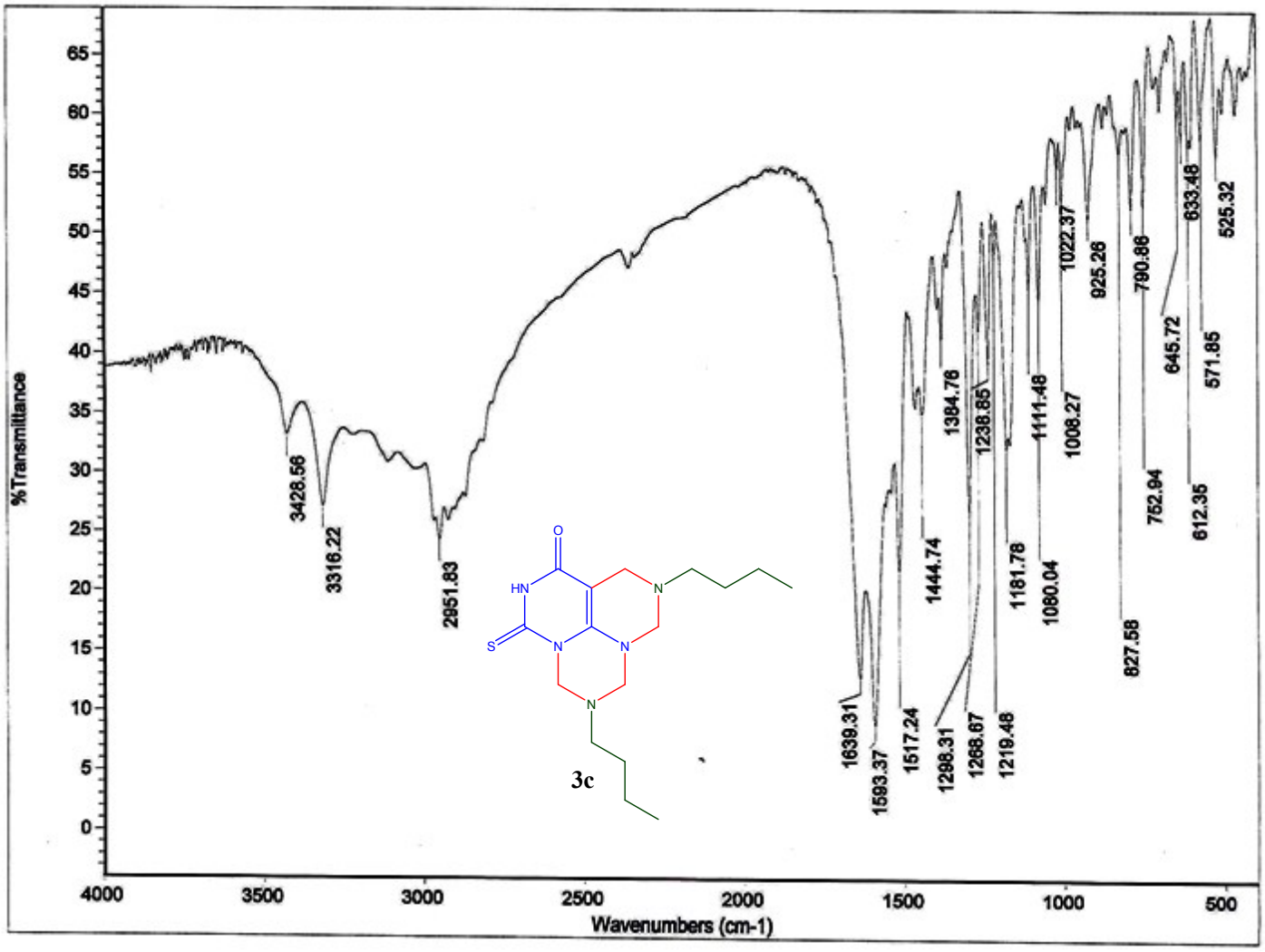


1

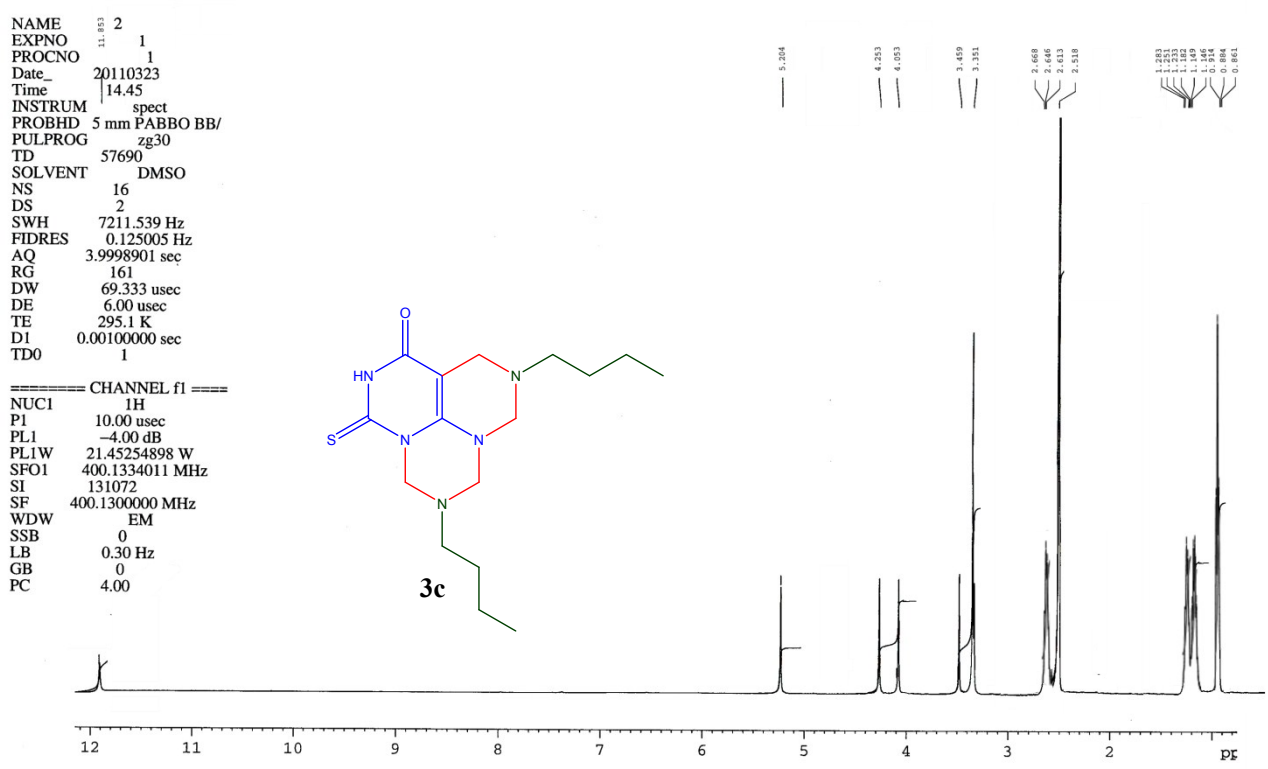
H-NMR spectrum of compound **3b** (400 MHz, DMSO-d_6).



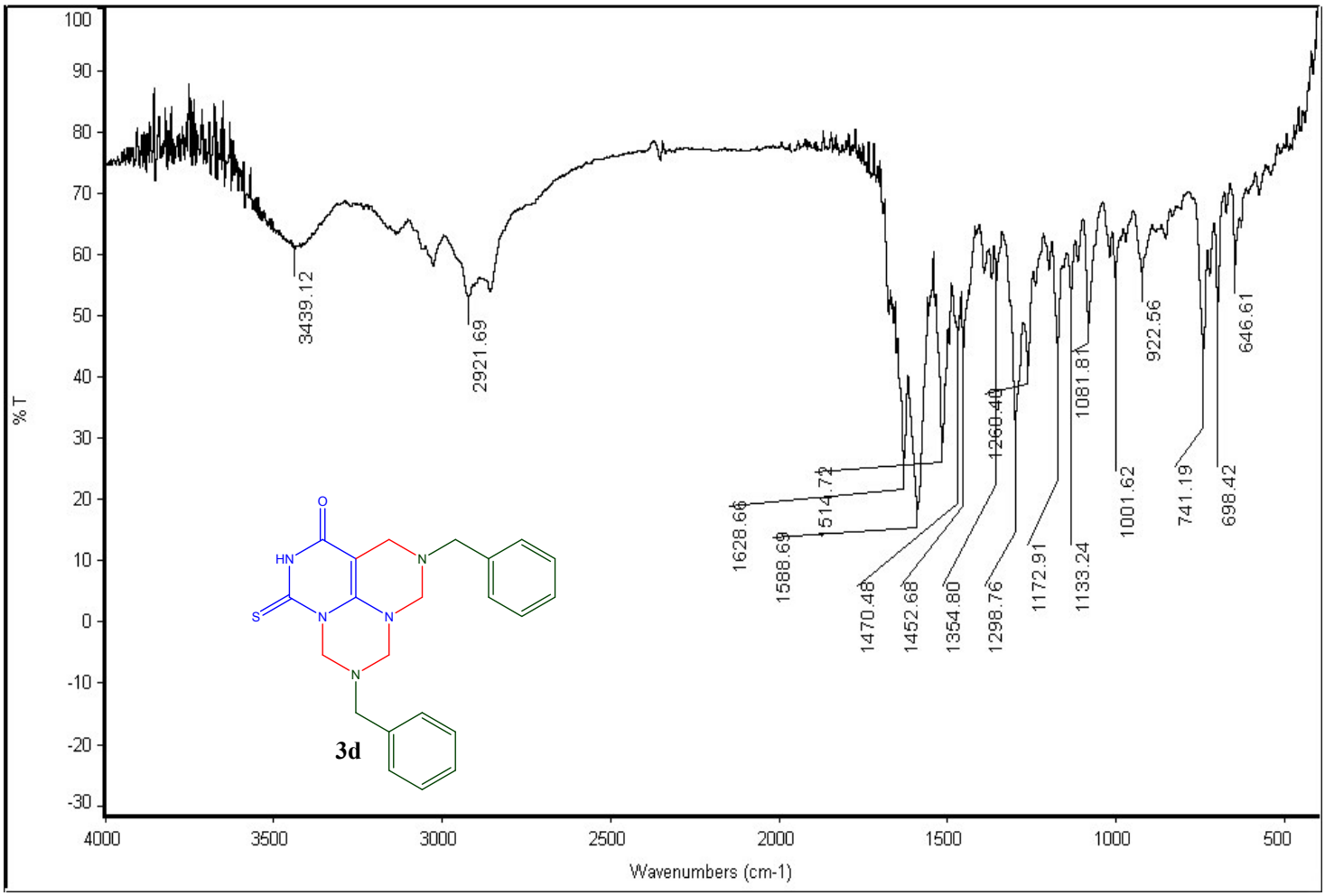
^{13}C-NMR spectrum of compound **3b** (400 MHz, DMSO-d_6).



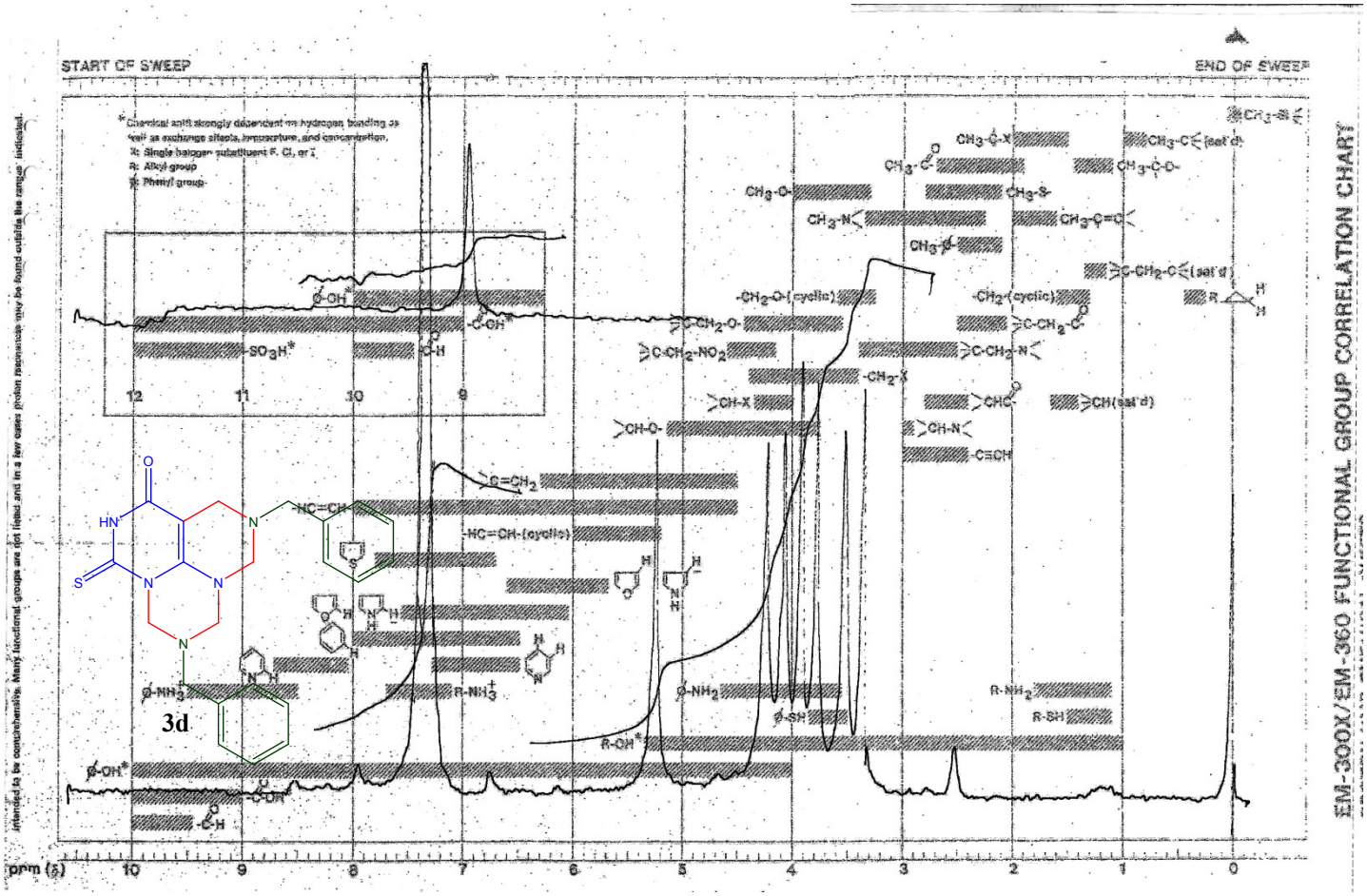
FTIR spectrum of compound **3c**



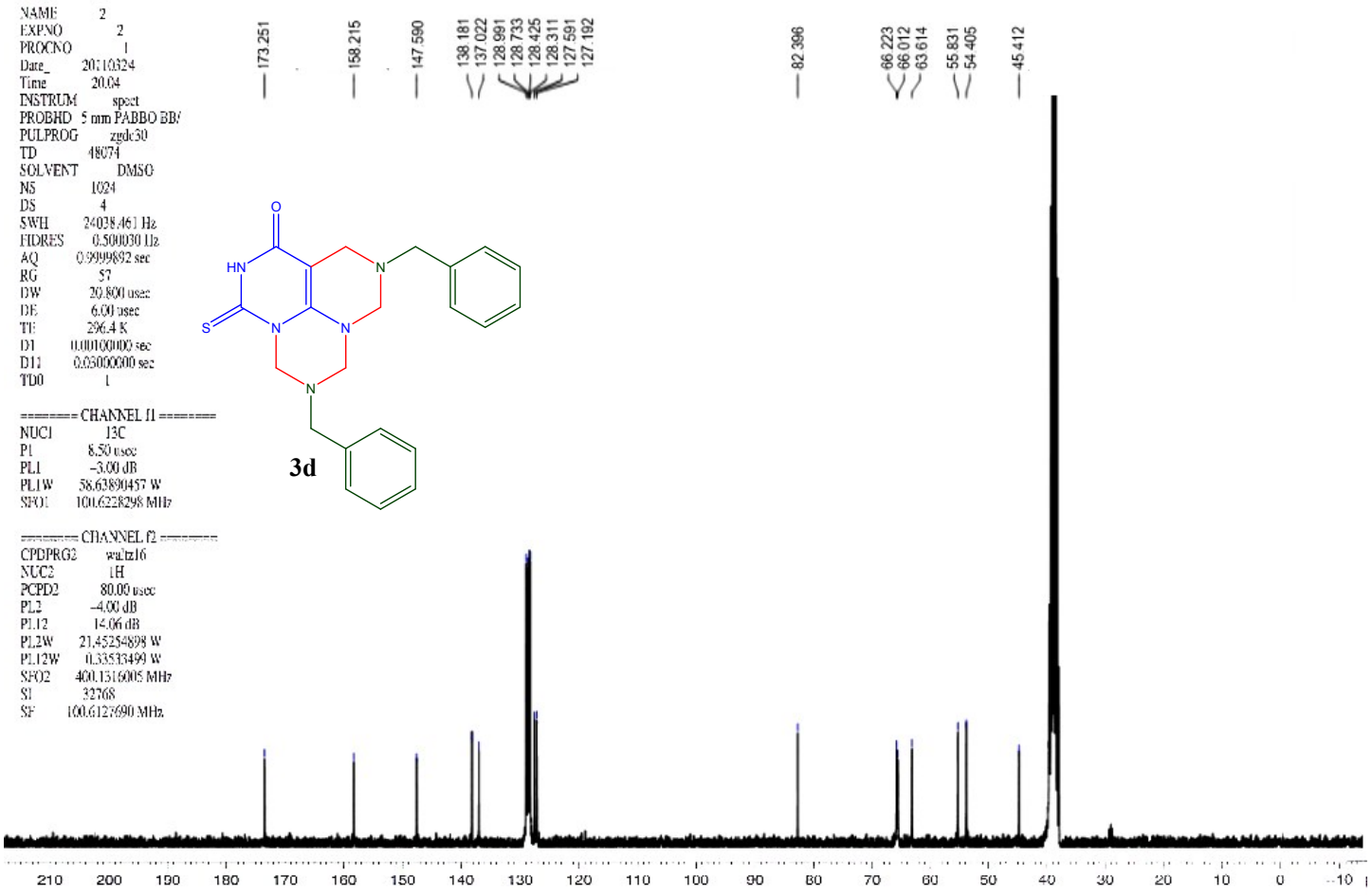
^{1}H-NMR spectrum of compound **3c** (400 MHz, DMSO-d_6).



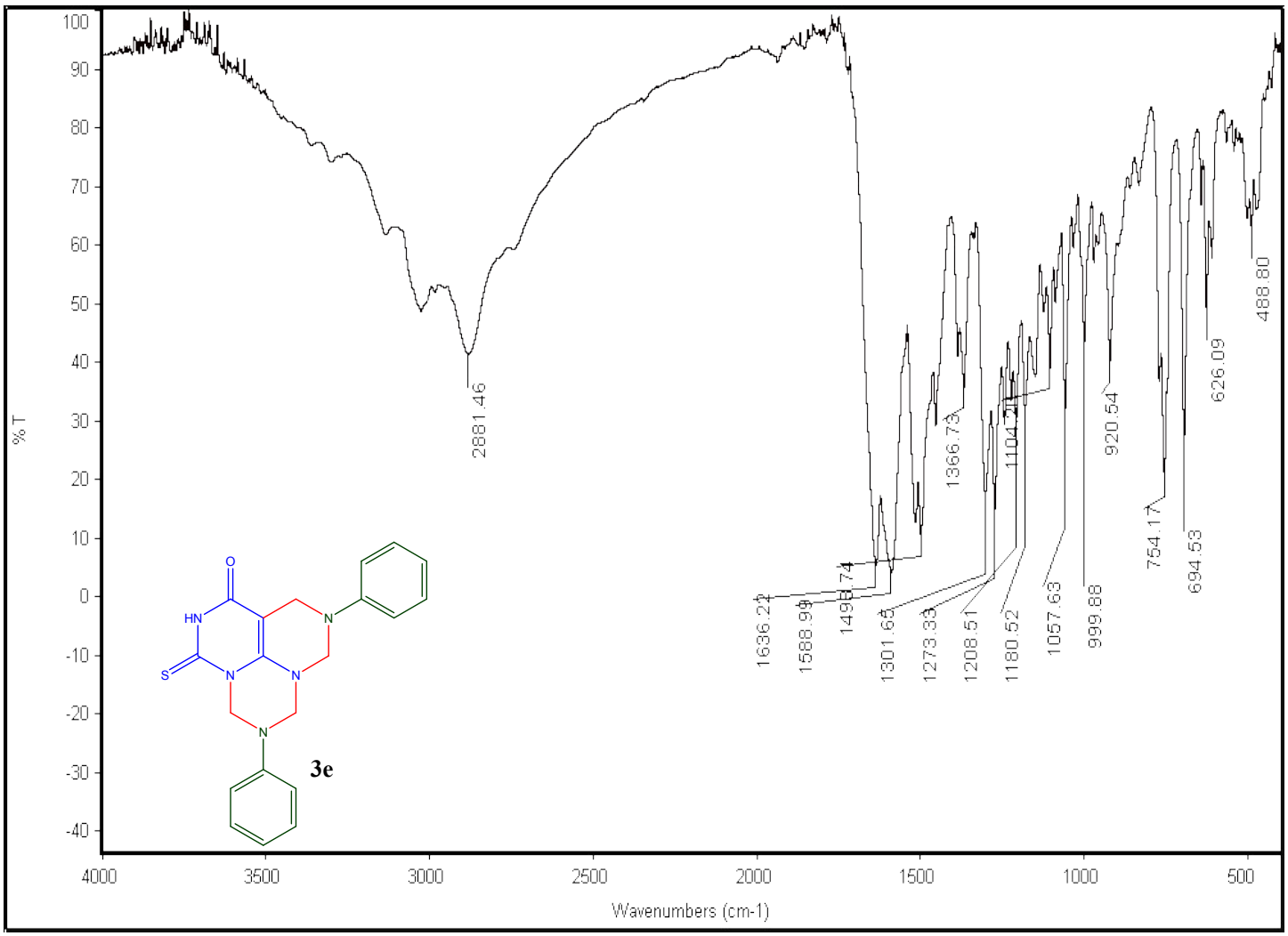
FTIR spectrum of compound **3d.**



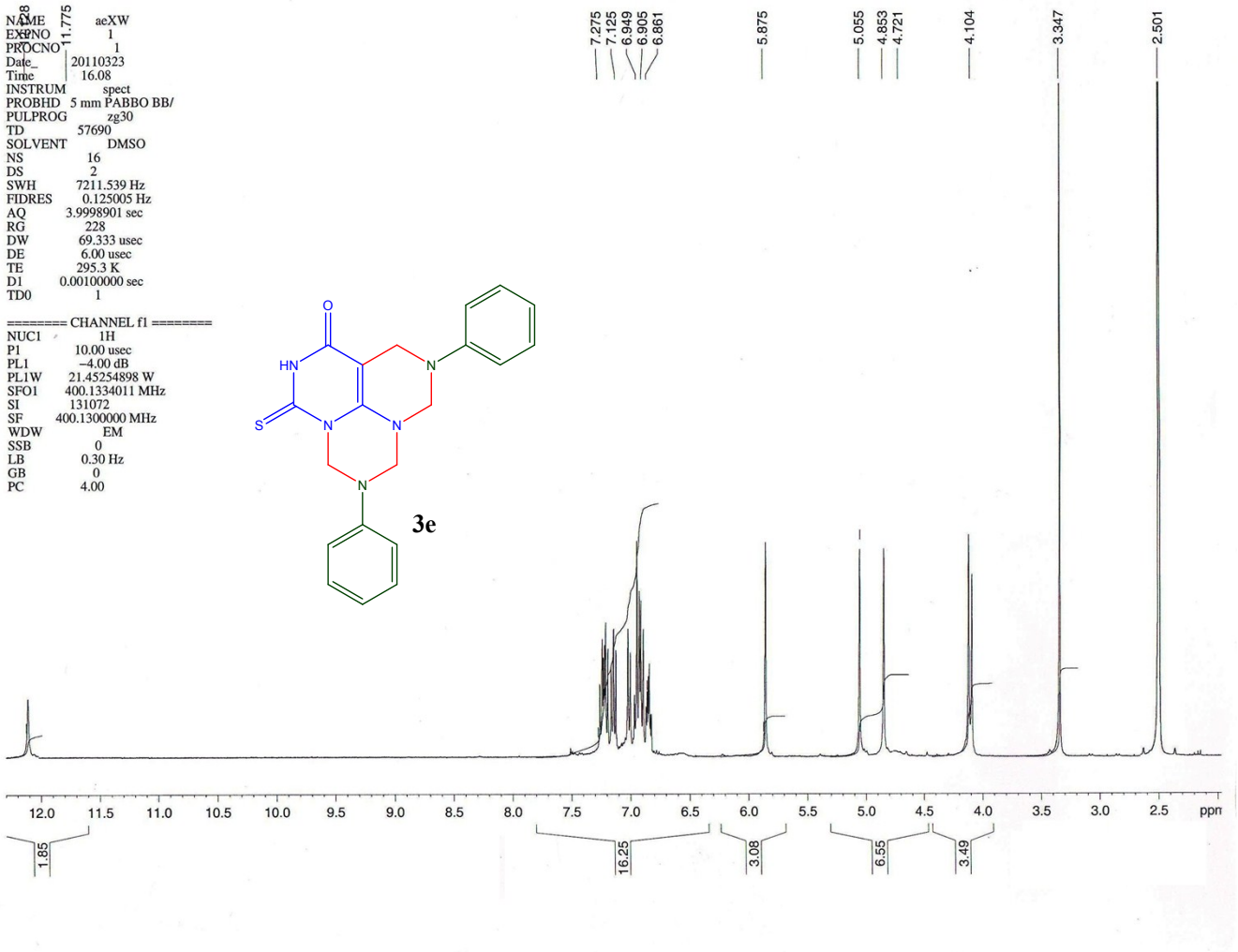
^{1}H-NMR spectrum of compound **3d** (90 MHz, DMSO-d_6).



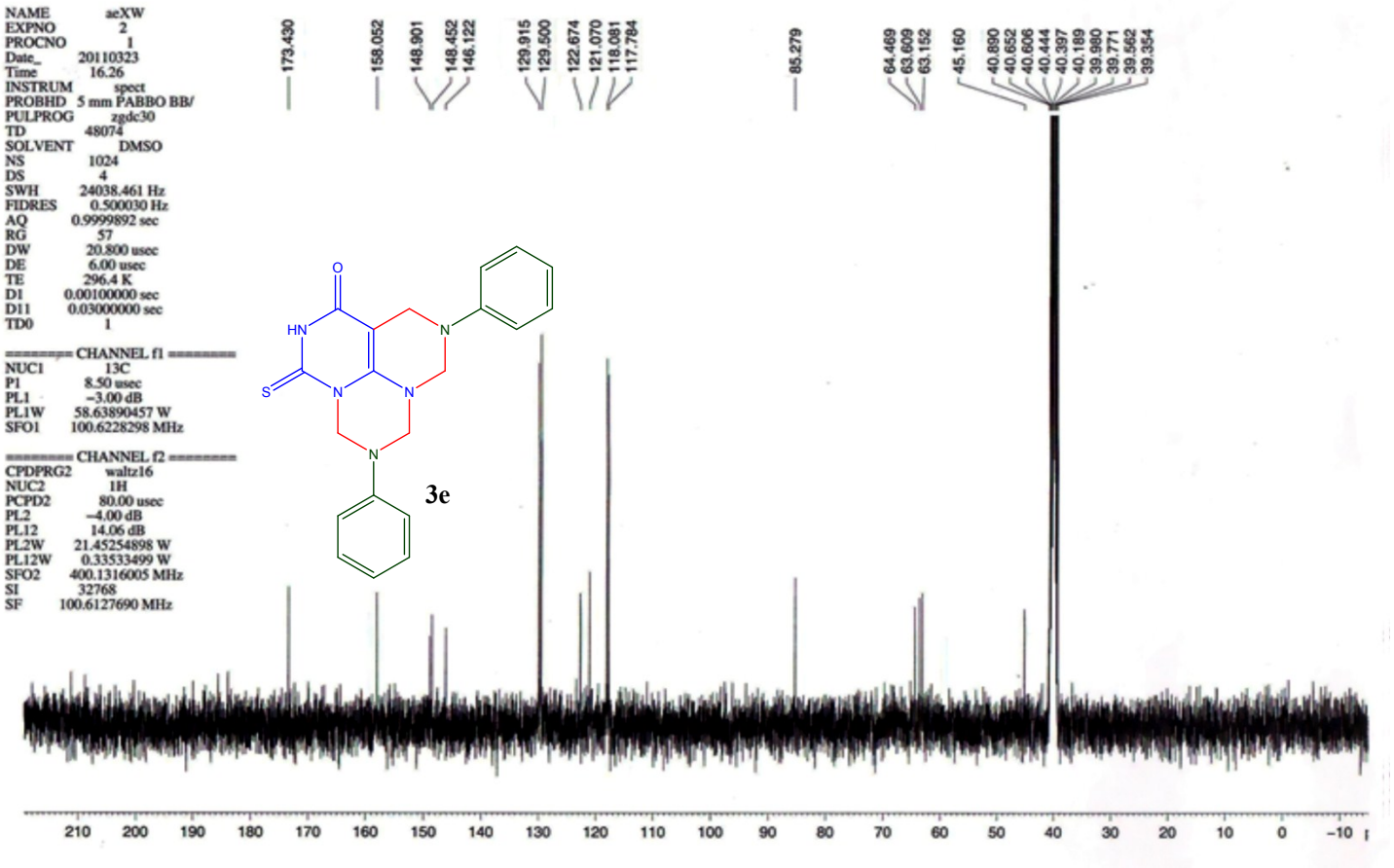
^{13}C-NMR spectrum of compound **3d** (400 MHz, DMSO-d_6).



FTIR spectrum of compound **3e**



^{1}H-NMR spectrum of compound **3e** (400 MHz, DMSO-d_6).



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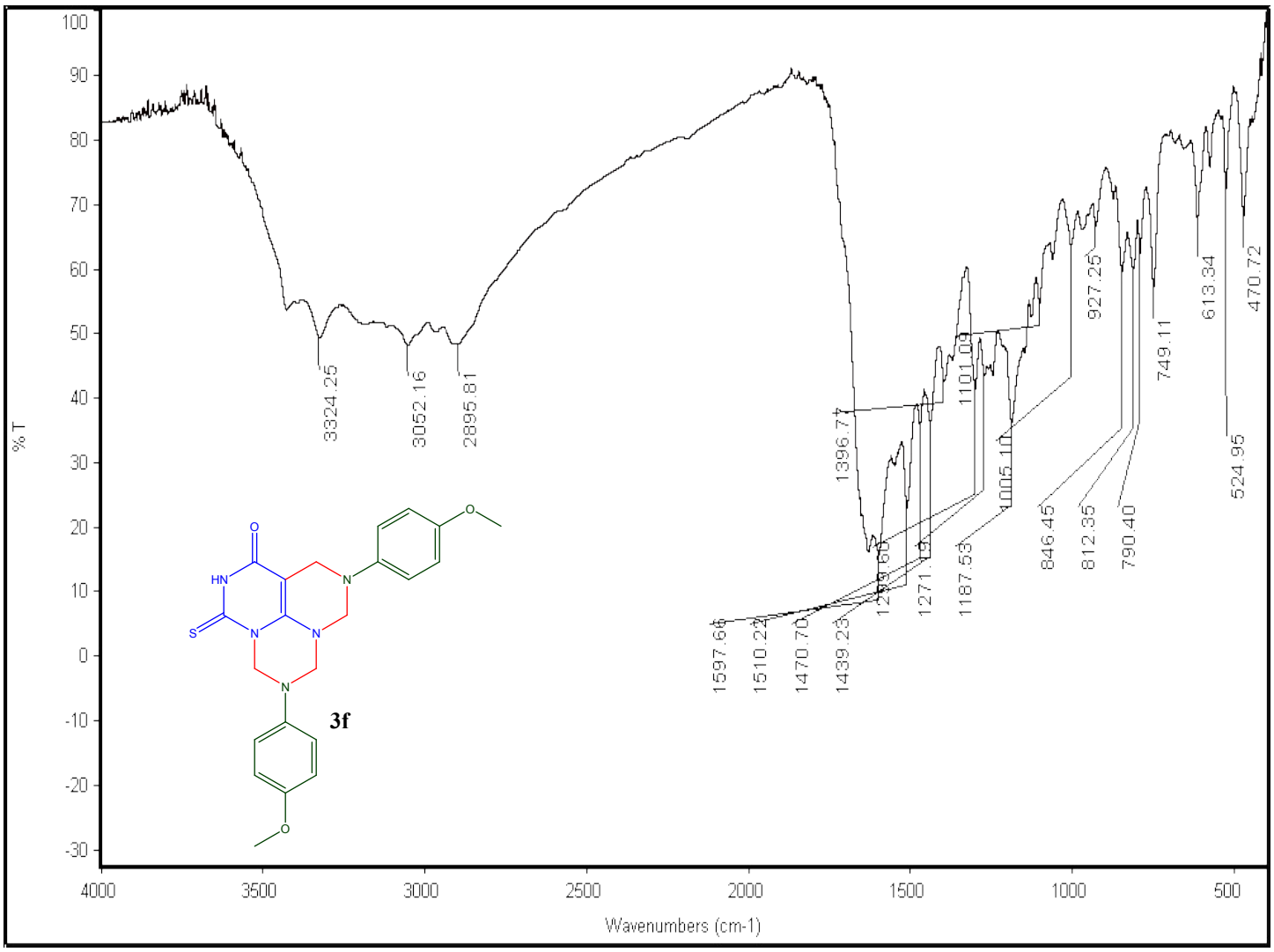

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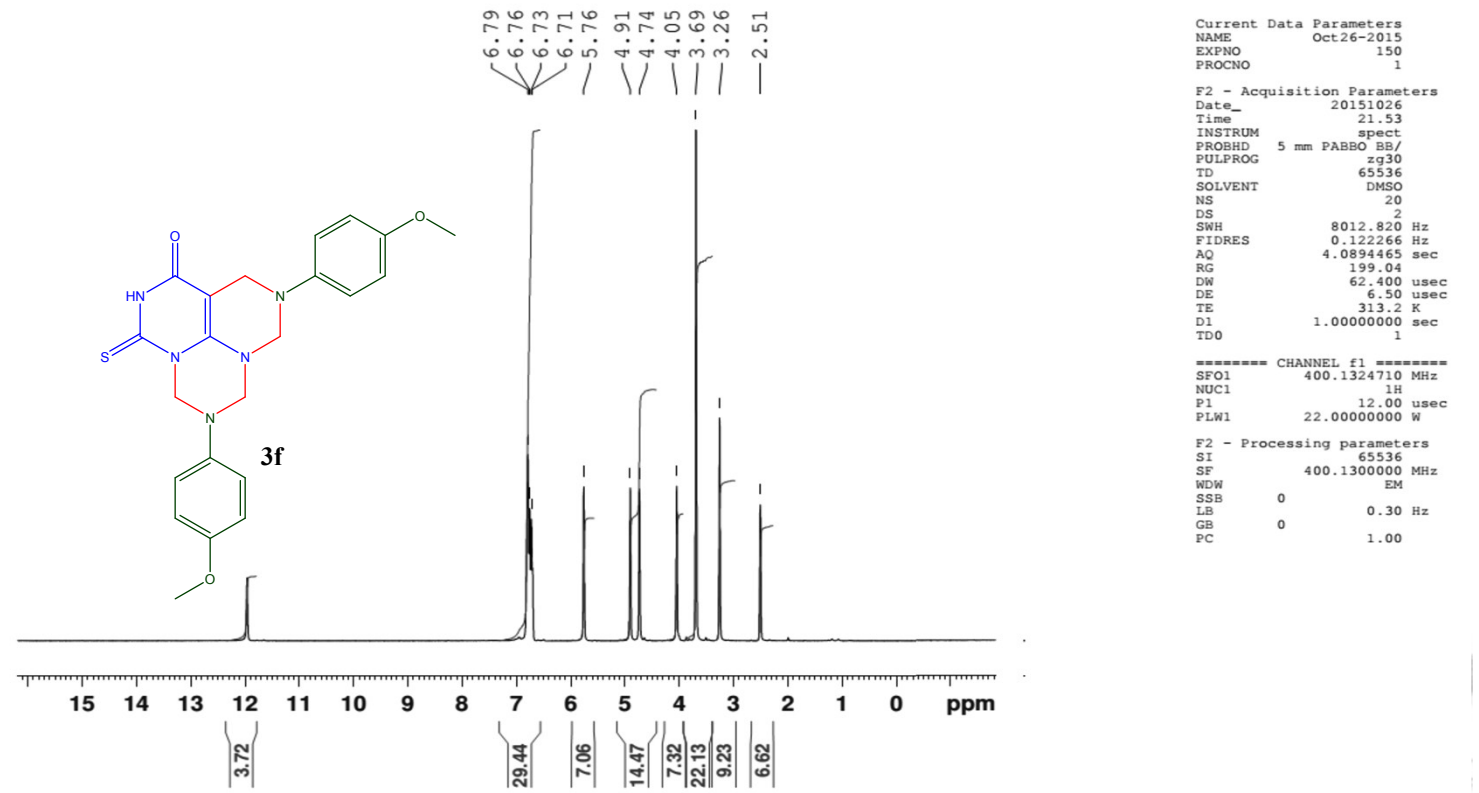


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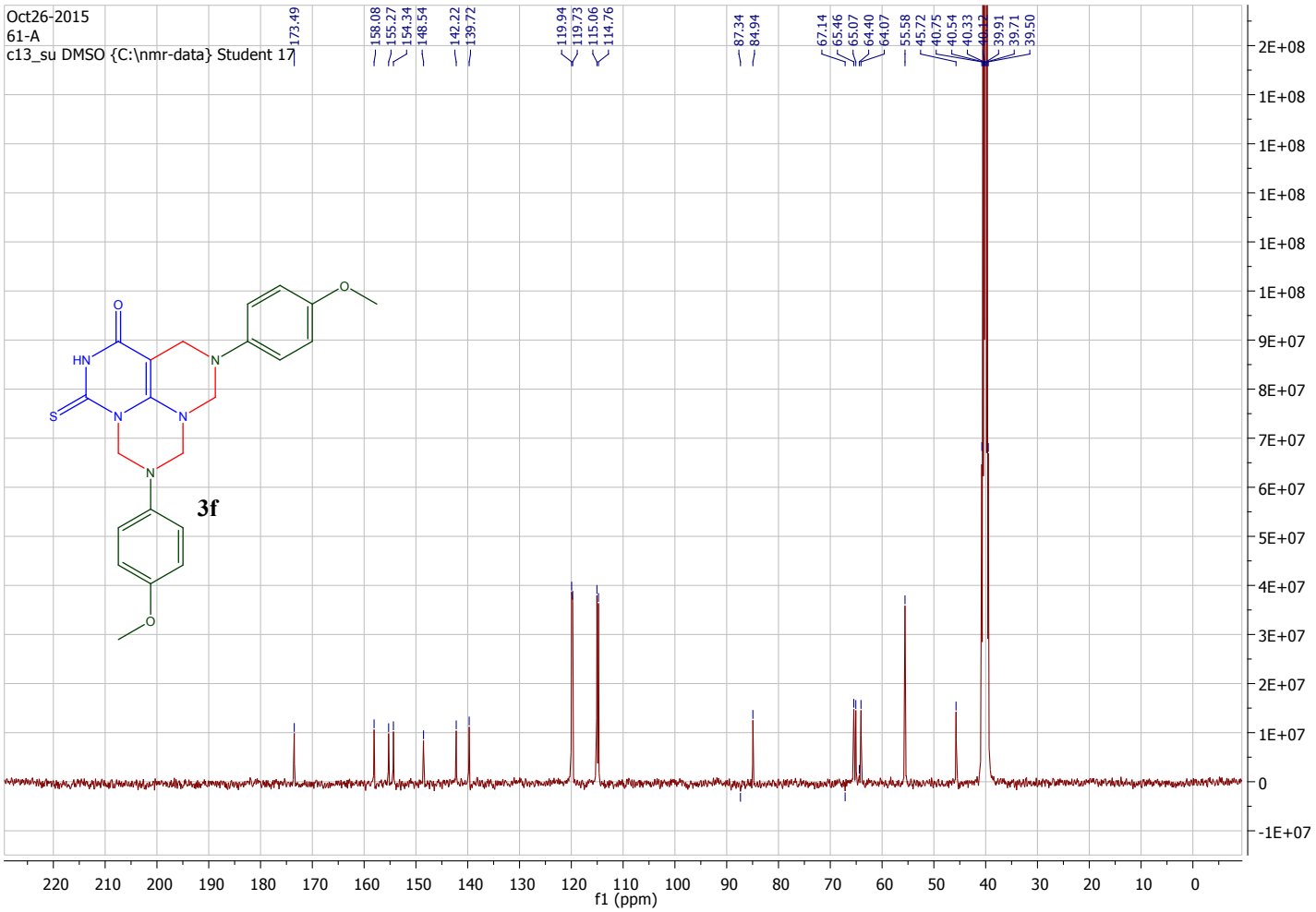

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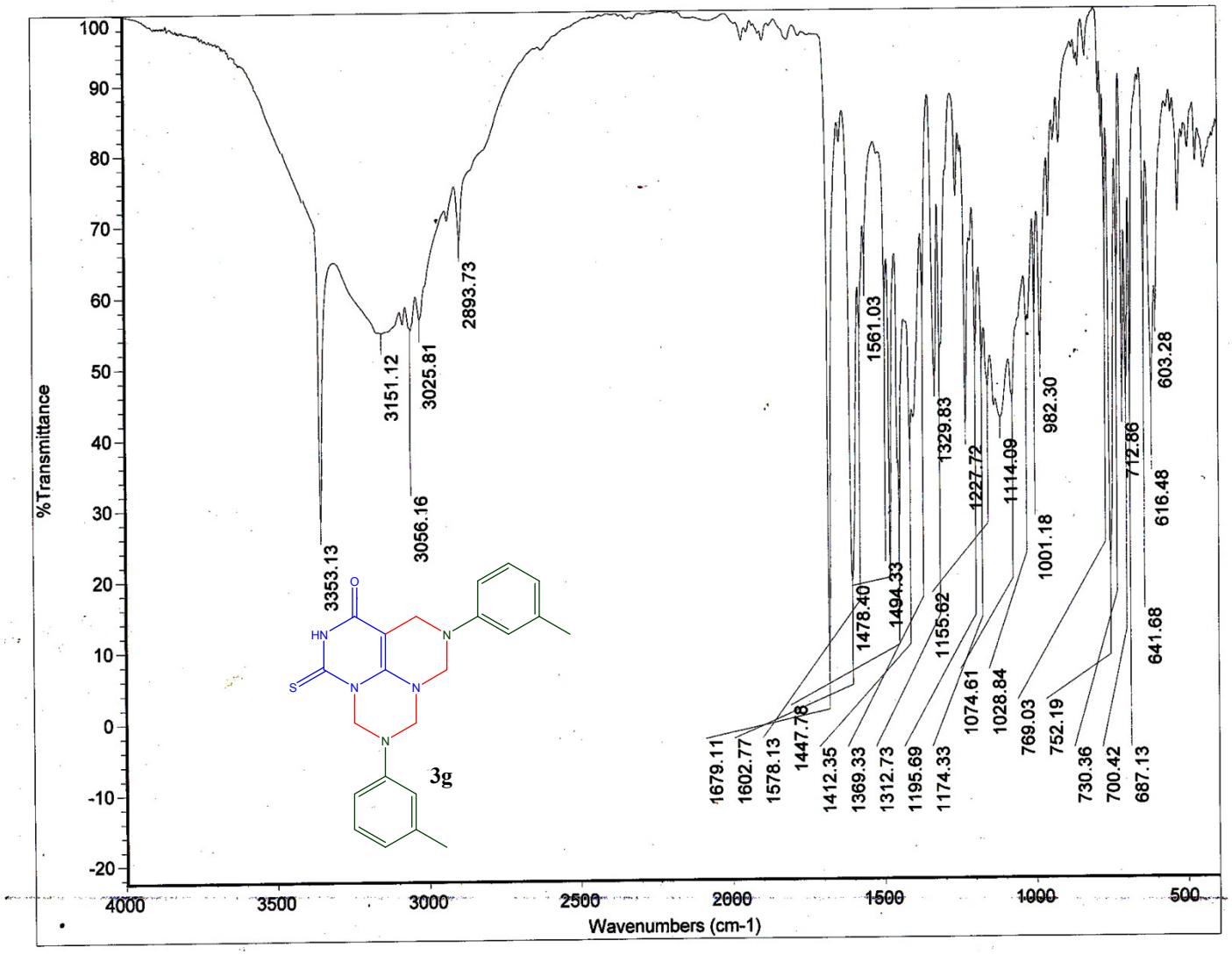

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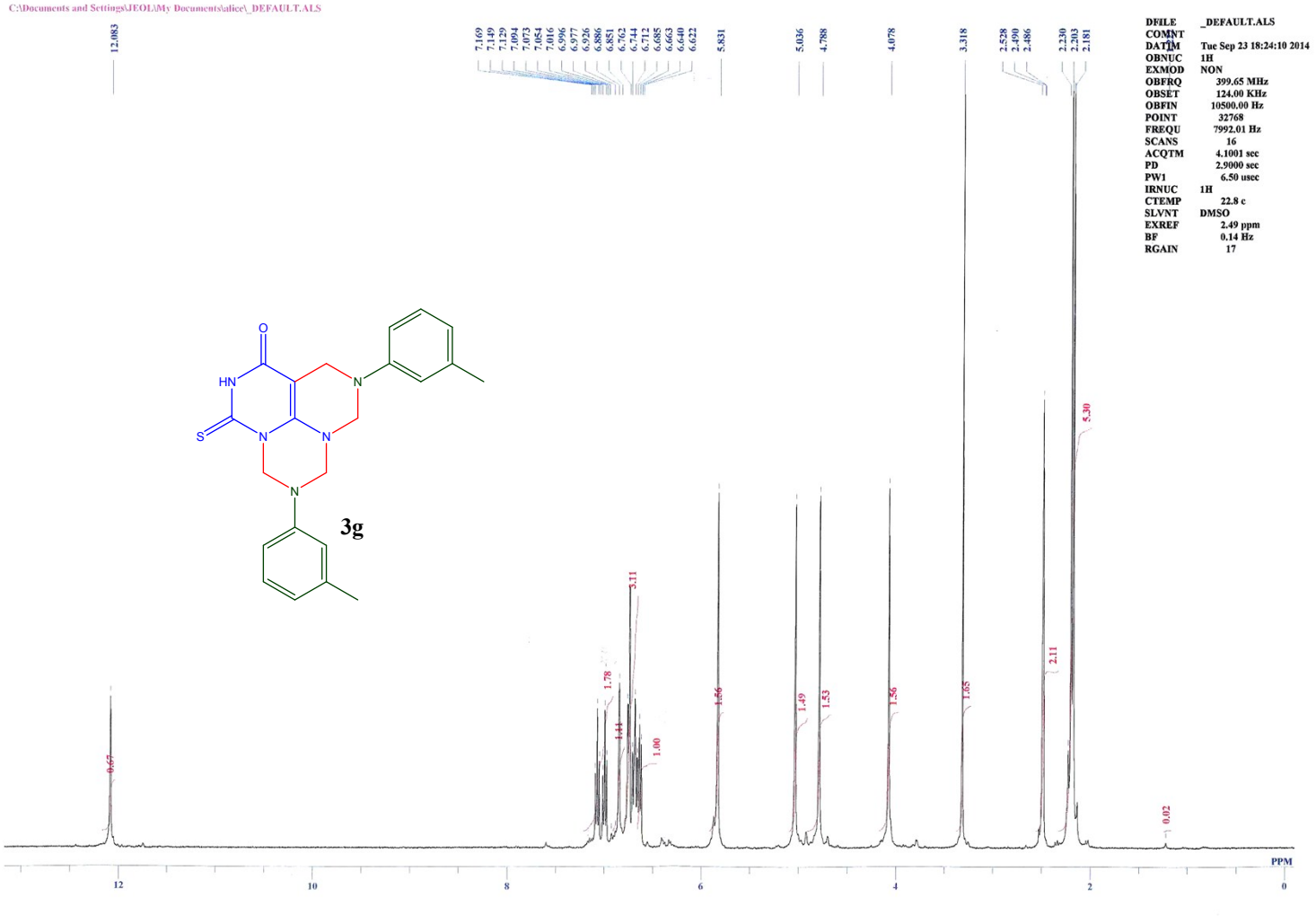
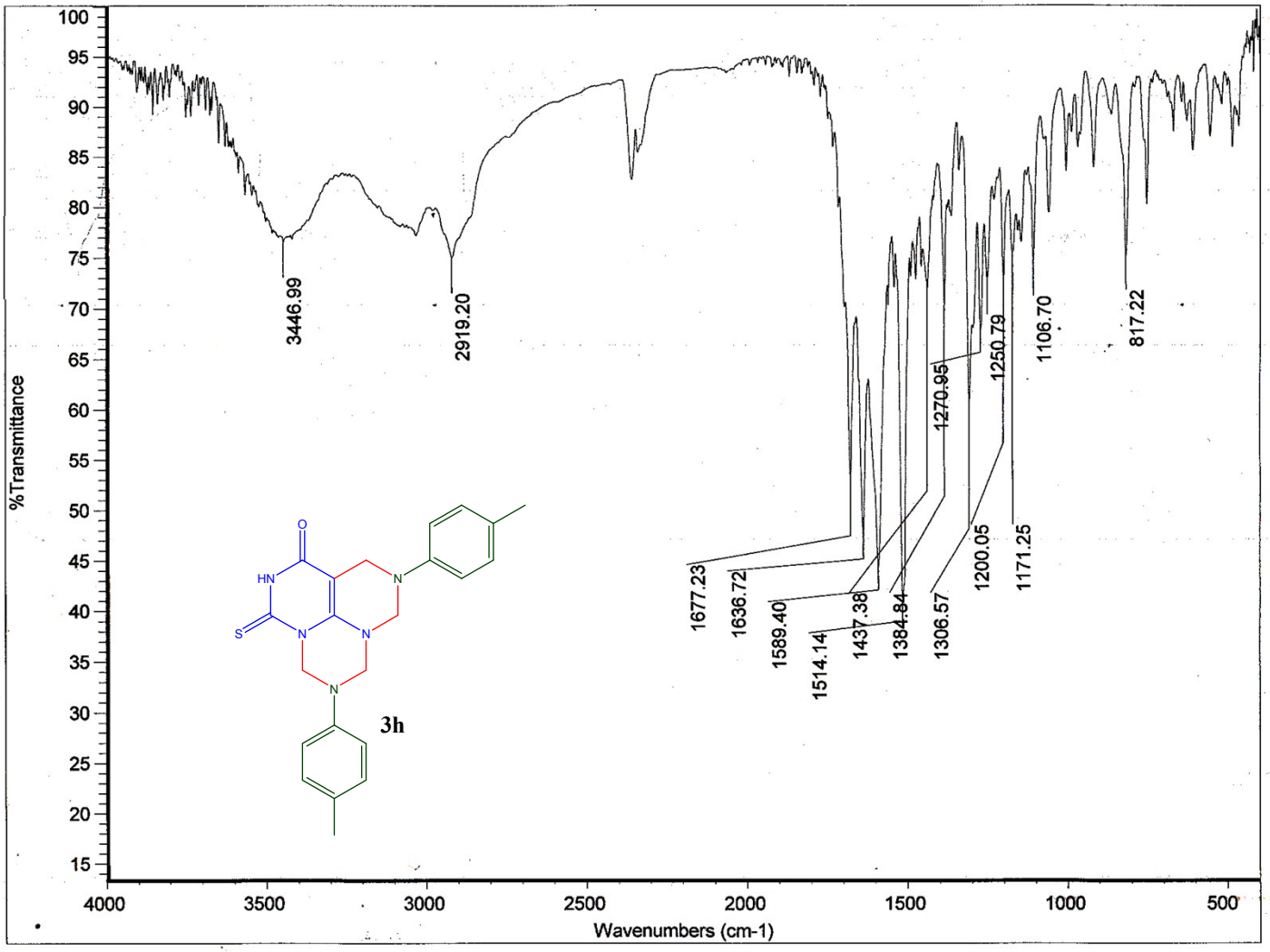


^{1}H-NMR spectrum of compound **3g** (400 MHz, DMSO-d_6).



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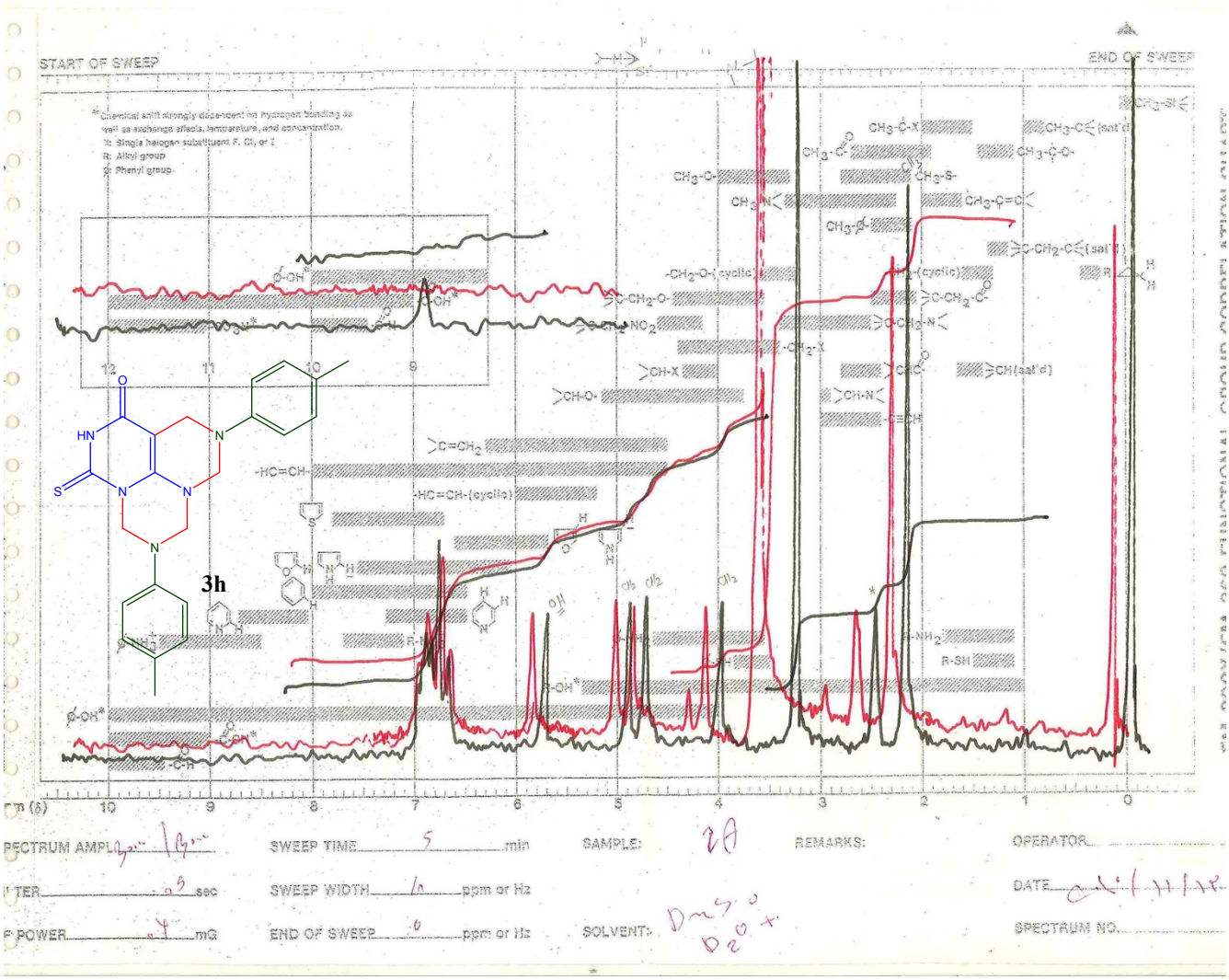
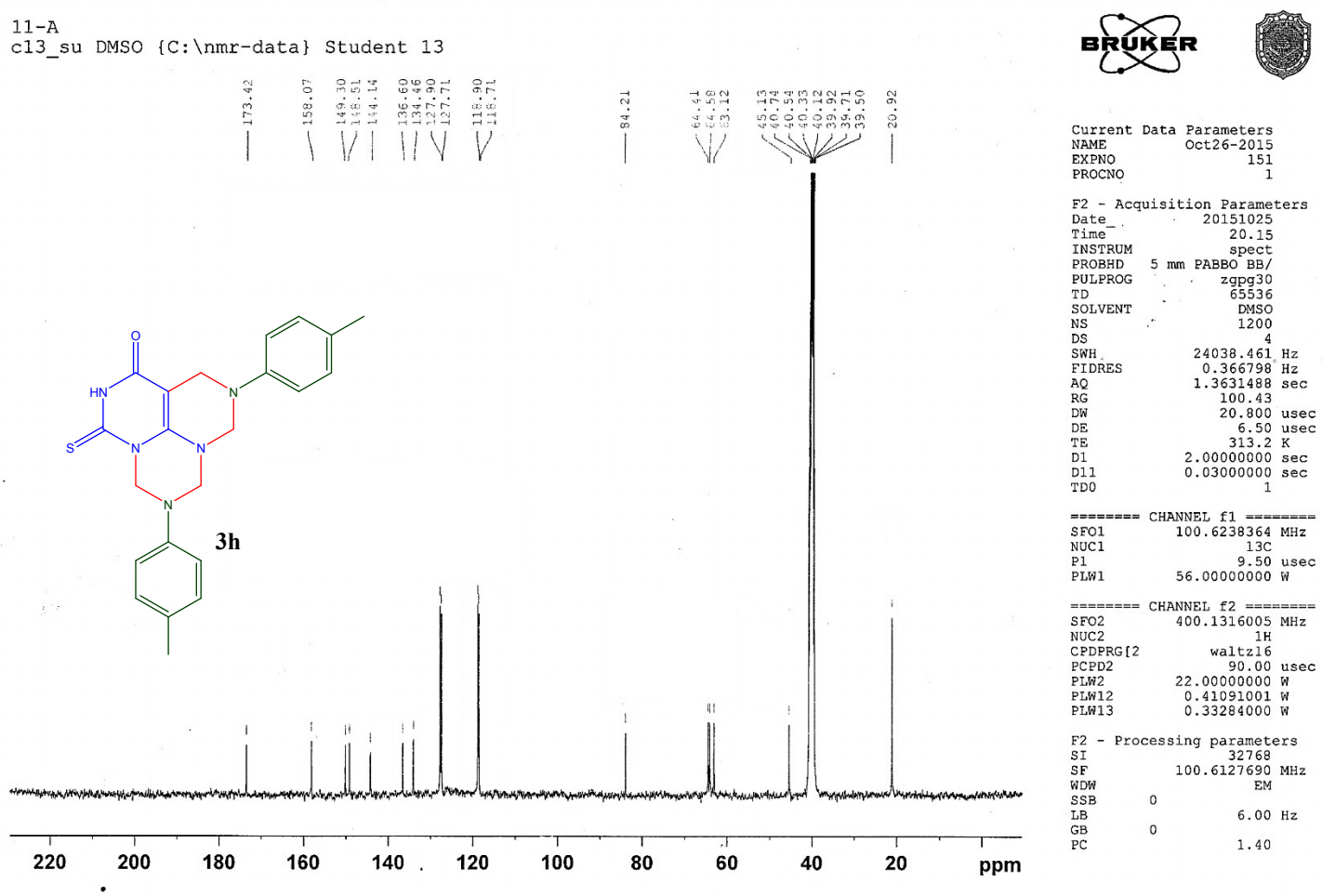
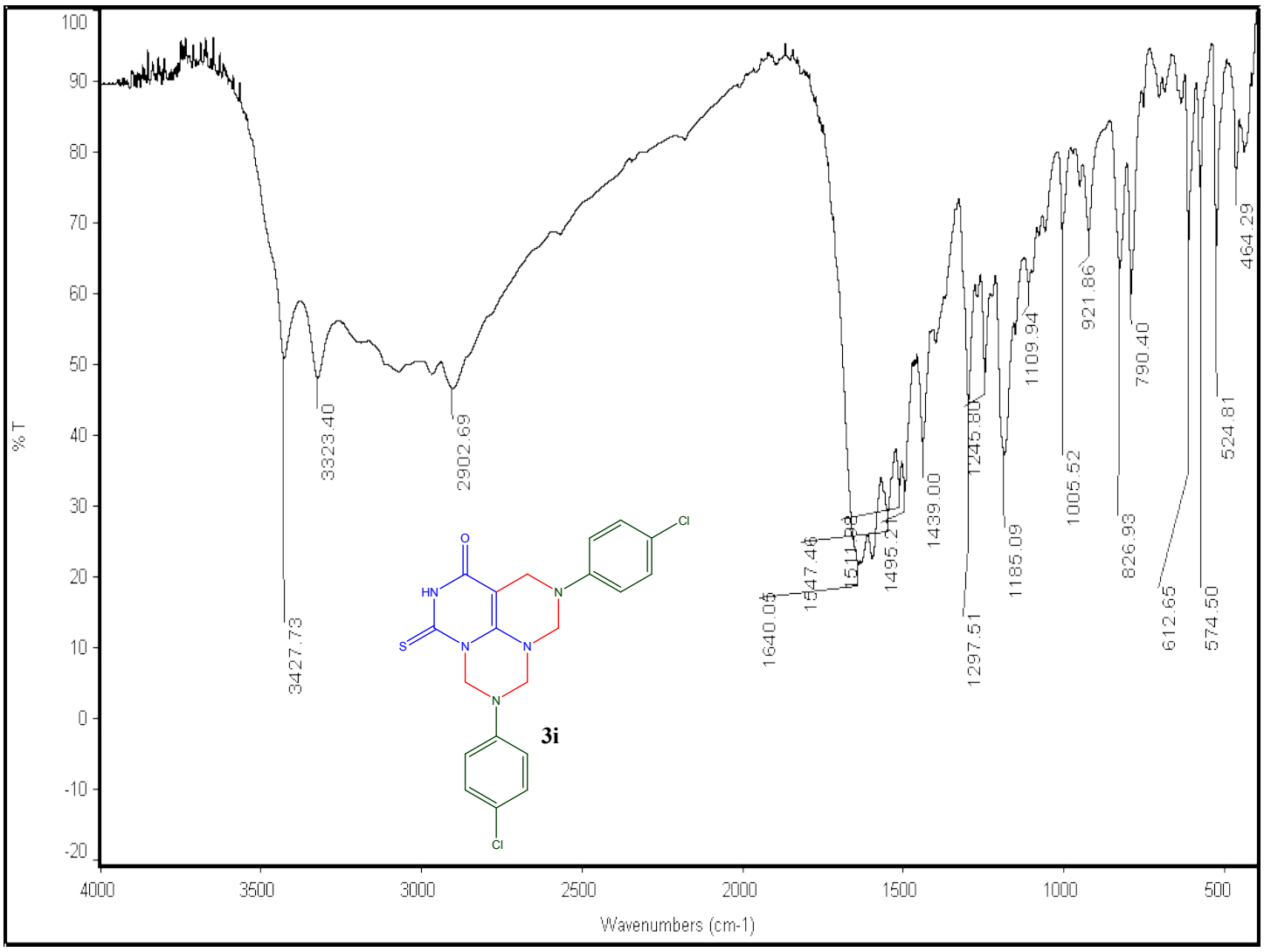


^{1}H-NMR spectrum of compound **3h** (90 MHz, DMSO-d_6).



^{13}C-NMR spectrum of compound **3h** (400 MHz, DMSO-d_6).



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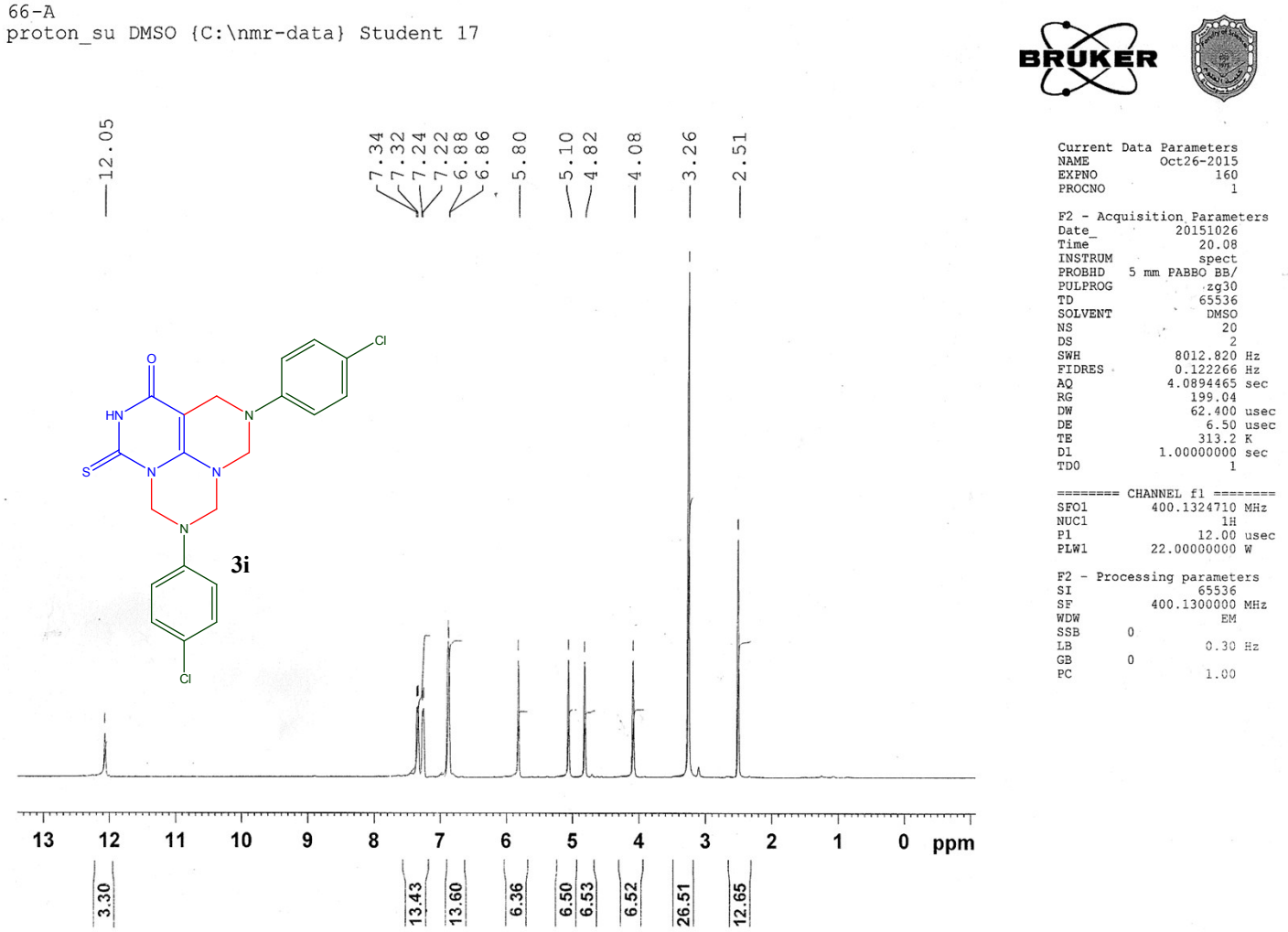
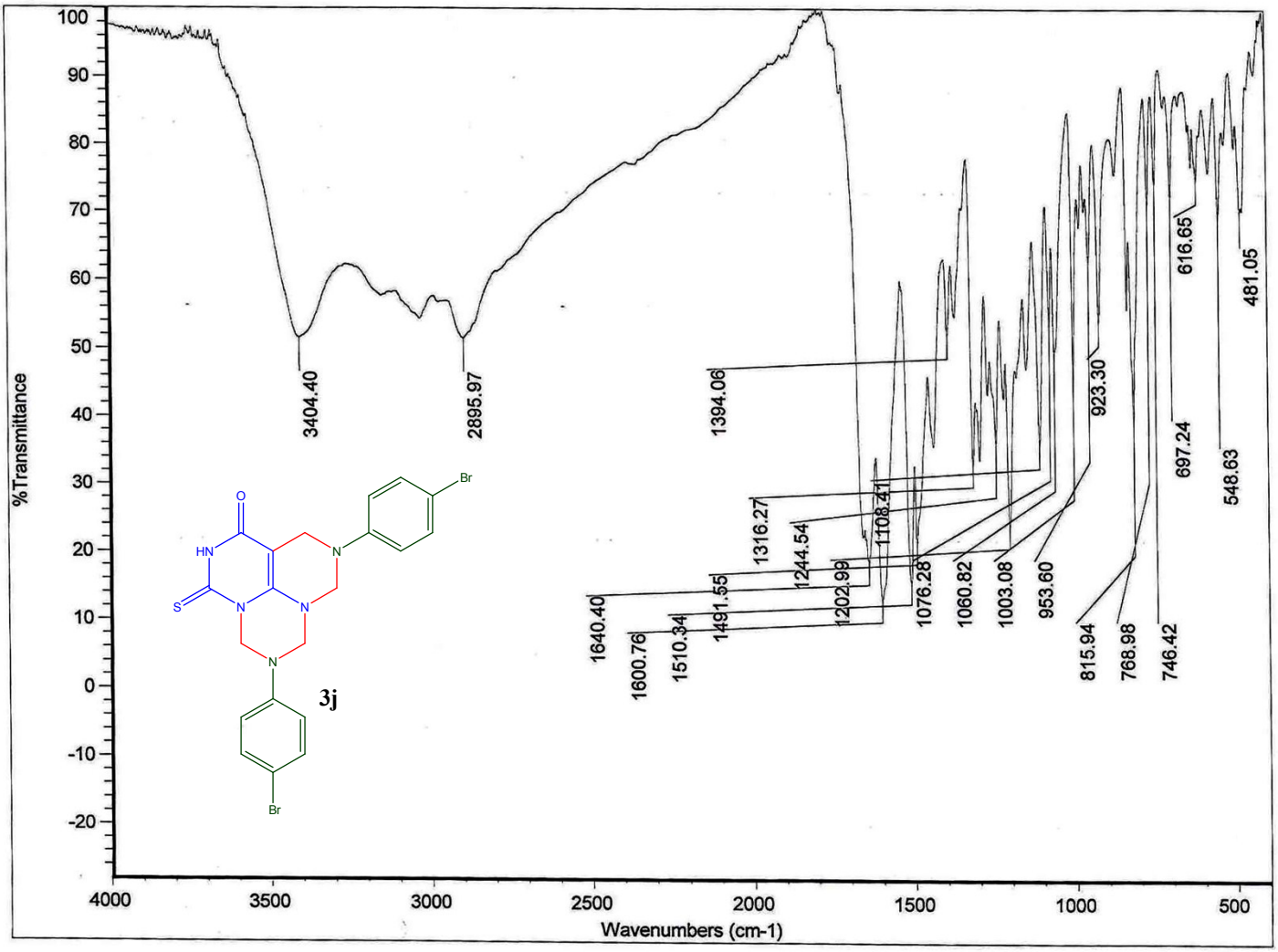
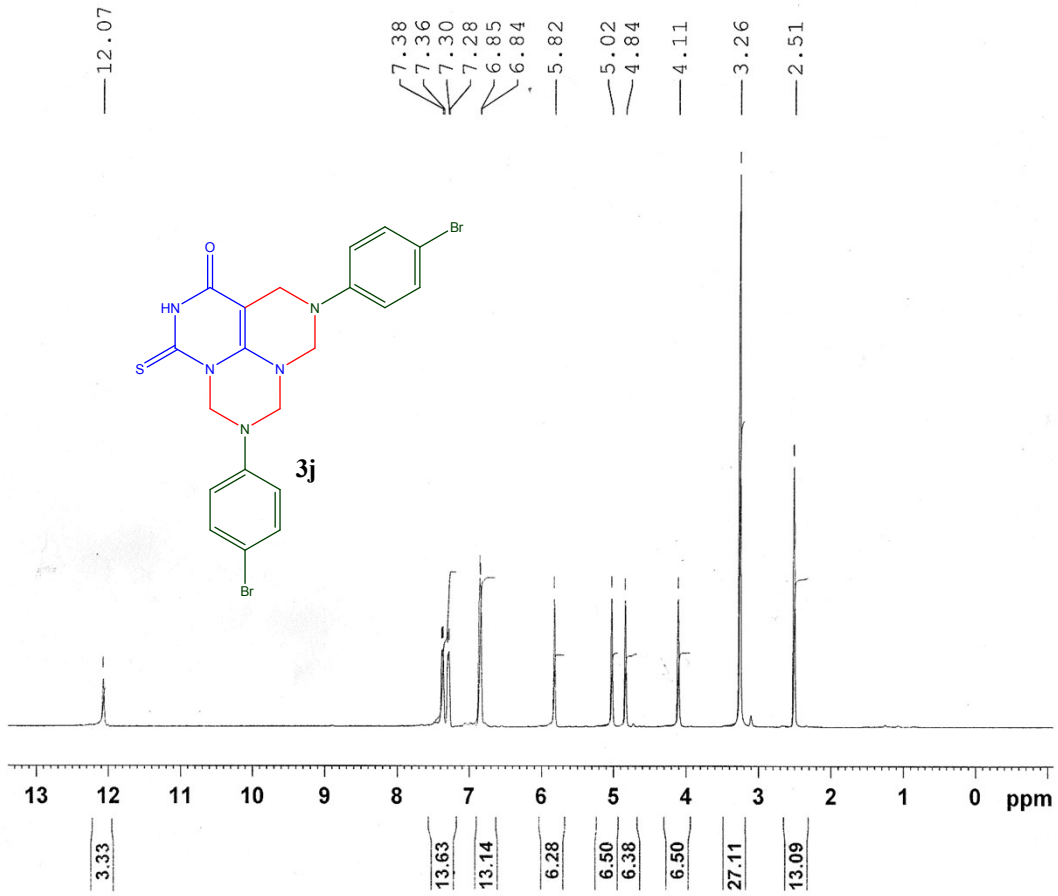


^{1}H-NMR spectrum of compound **3i** (400 MHz, DMSO-d_6).



FTIR spectrum of compound **3j**

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DS                     2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894465 sec
RG                 199.04
DW                 62.400 usec
DE                  6.50 usec
TE                313.2 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                 12.00 usec
PLW1          22.00000000 W

F2 - Processing parameters
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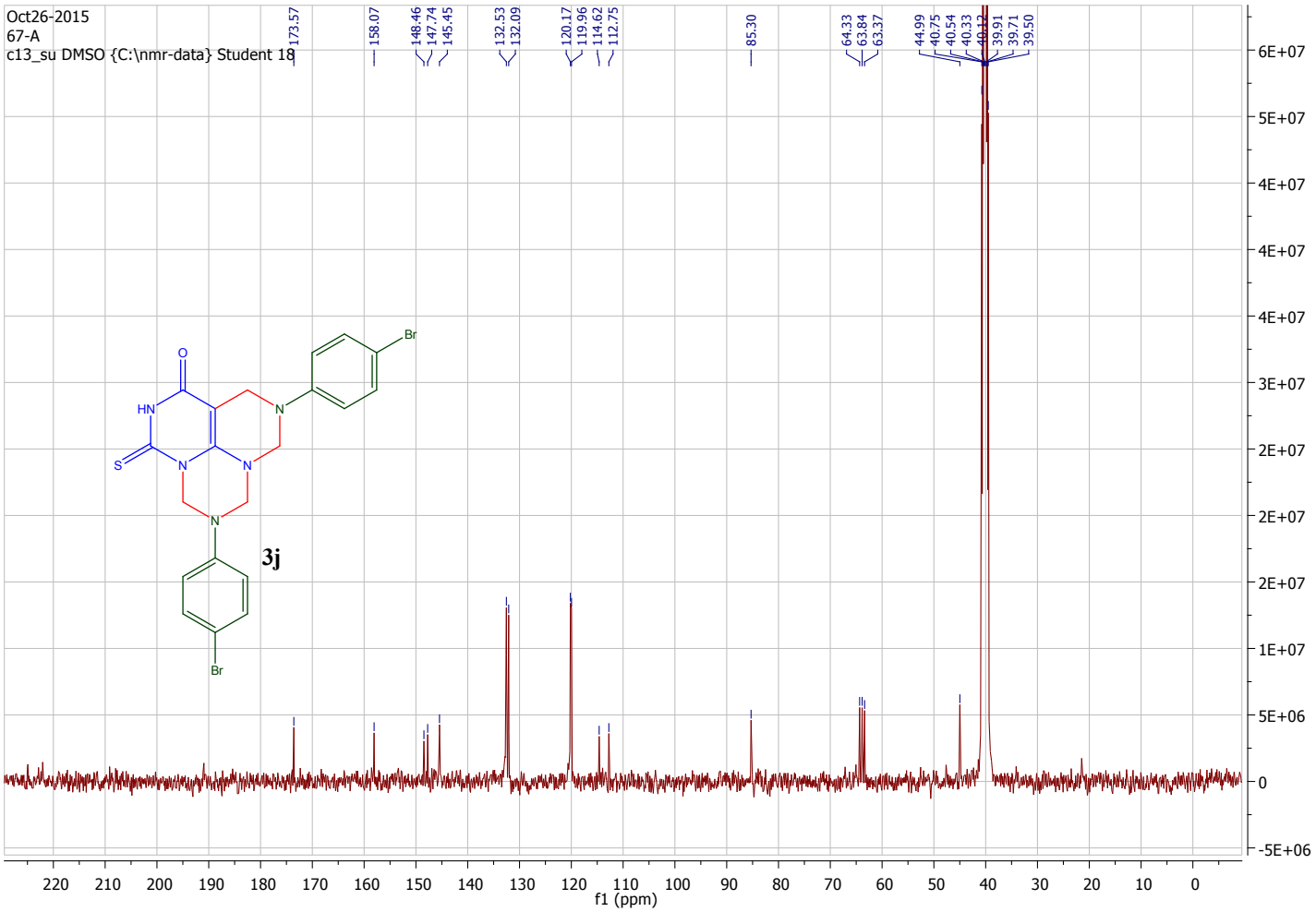
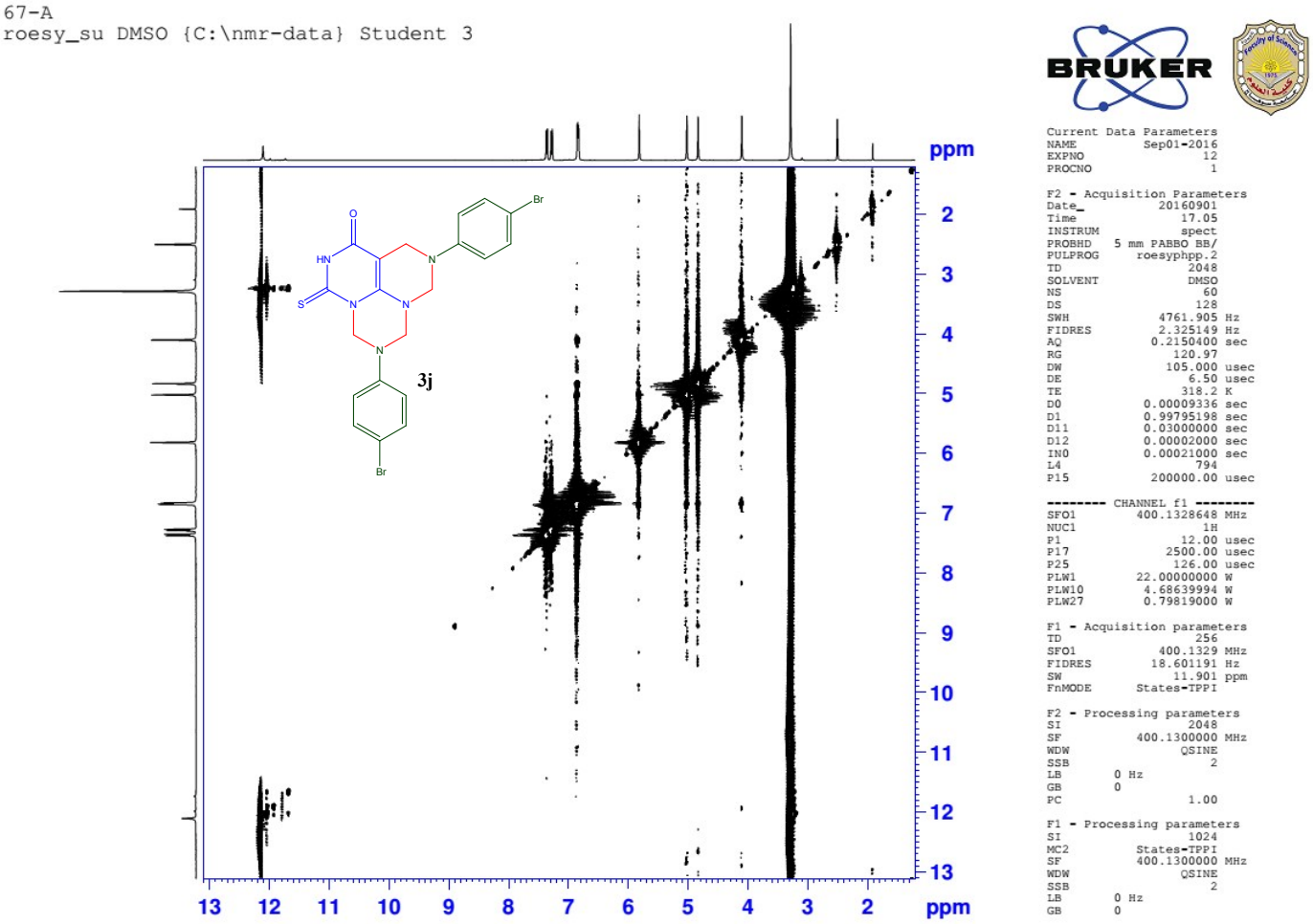
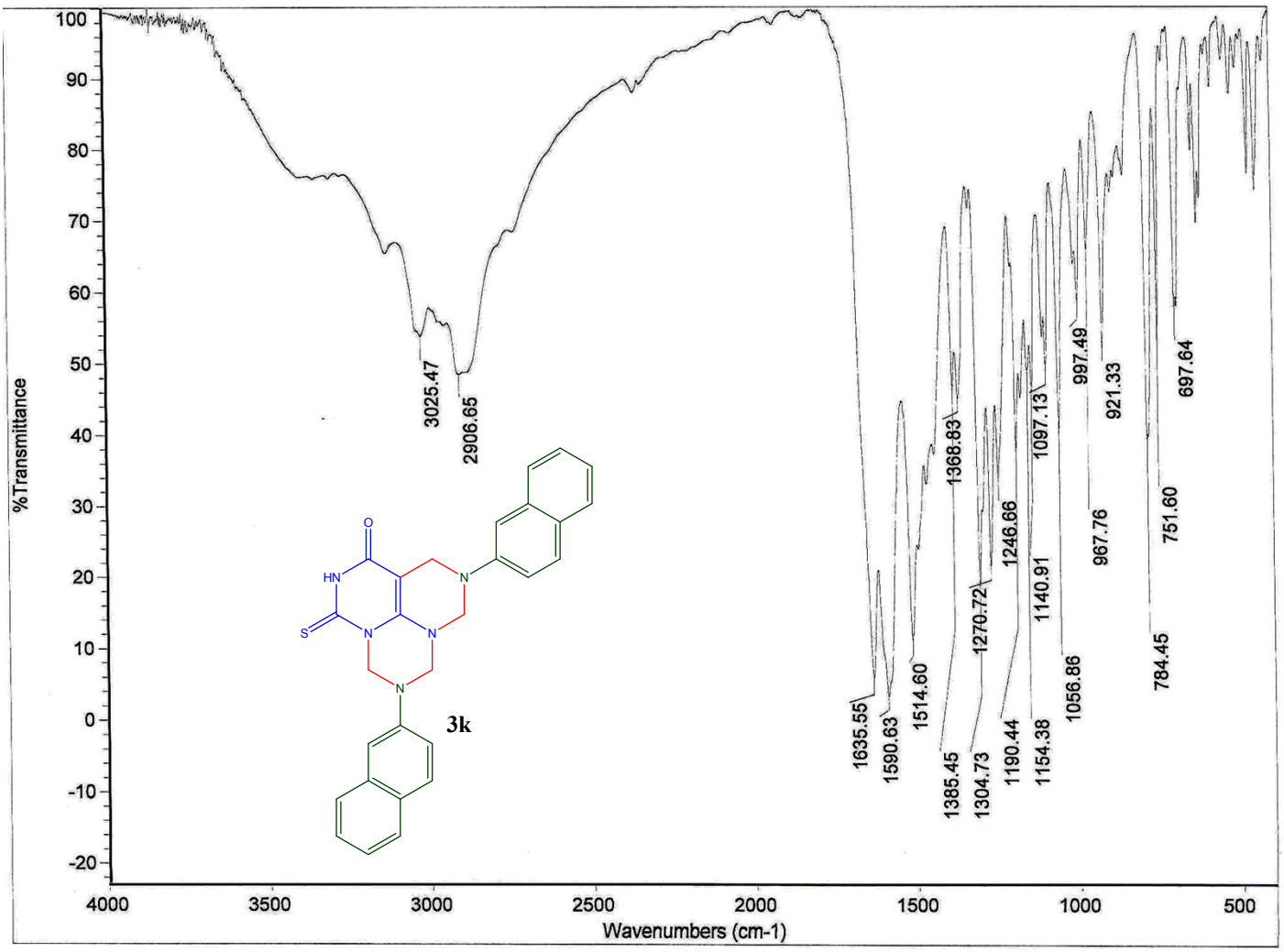
^{1}H-NMR spectrum of compound **3j** (400 MHz, DMSO-d_6).



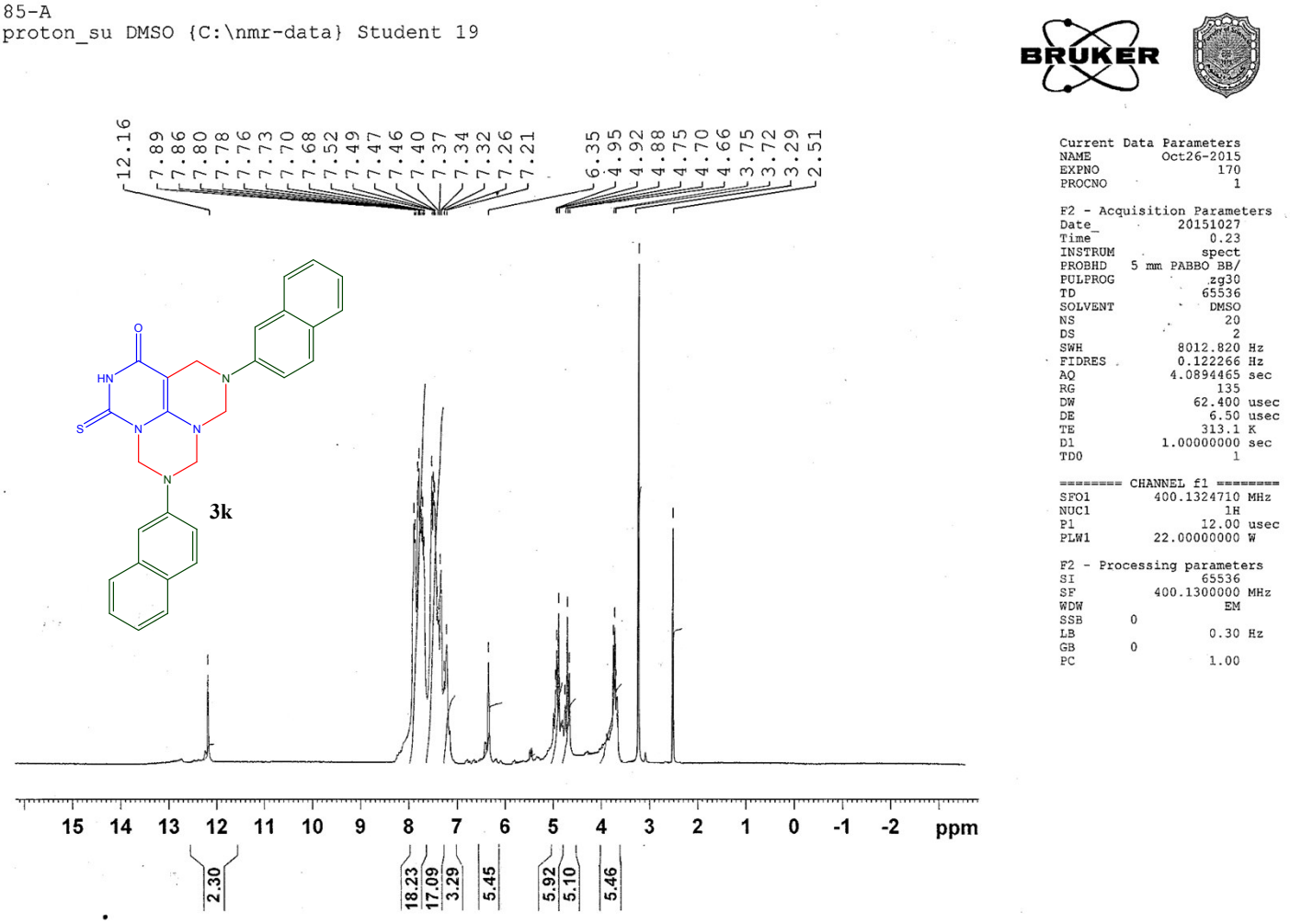
^{13}C-NMR spectrum of compound **3j** (400 MHz, DMSO-d_6).



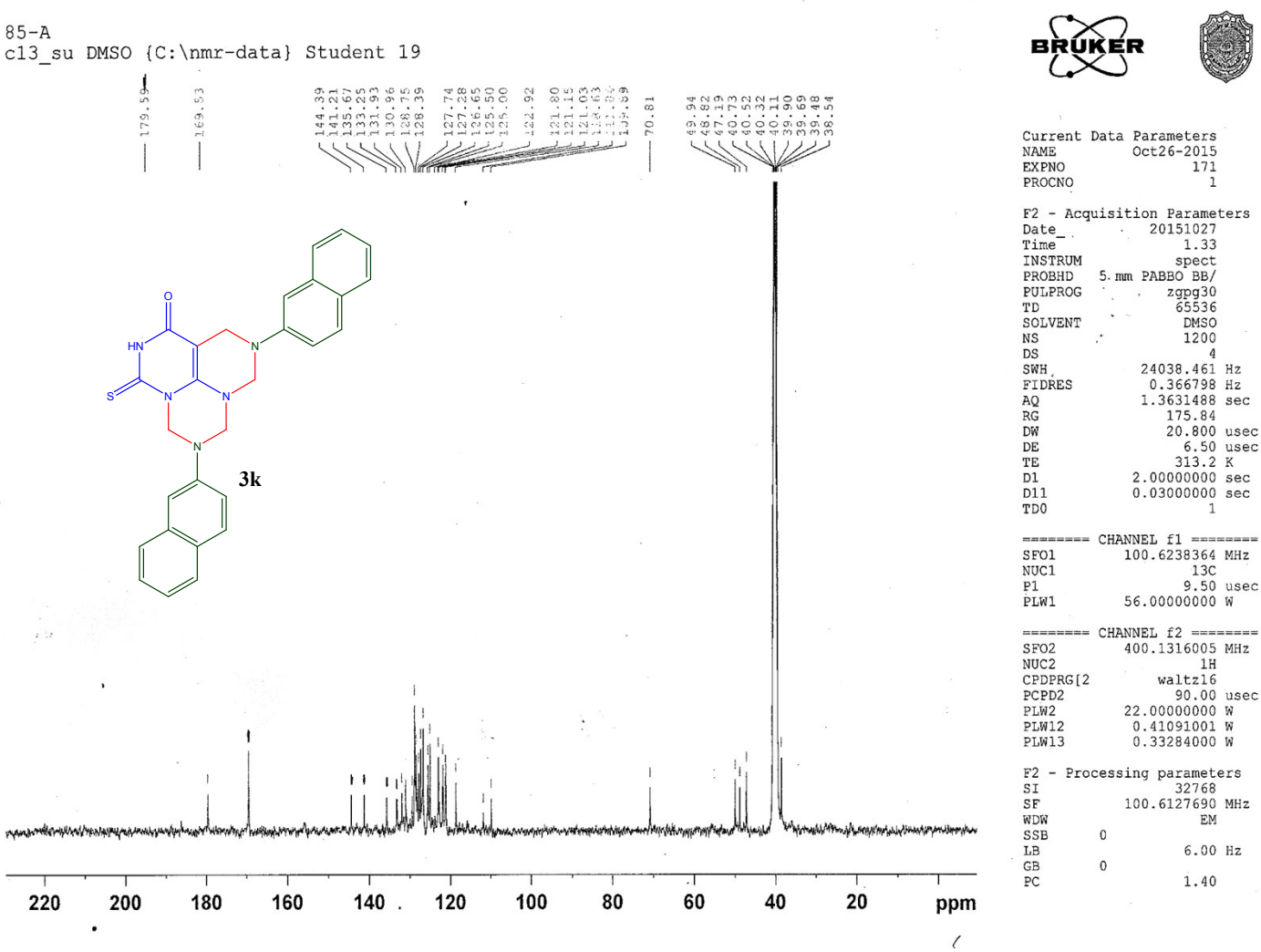
ROESY-NMR spectrum of compound **3j** (400 MHz, DMSO-d_6).



FTIR spectrum of compound **3k**



^{1}H-NMR spectrum of compound **3k** (400 MHz, DMSO-d_6).



^{13}C-NMR spectrum of compound **3k** (400 MHz, DMSO-d_6).