Supplementary Information

Synthesis and antimicrobial screening of novel oxadiazole doped pyrazoline derivatives

Ajay Rathod*[a], Chirag Patel*[a], Akhil Hadiya[b] & Falguni Bhabhor[c]

[a] Department of Chemistry, KSKV Kachchh University, Bhuj 370 015, Gujarat, India

[b] Department of Chemistry, Saurashtra University, Rajkot 360 005, Gujarat, India

[c] Bhavan's Sheth R A College of Science,Gujarat University, Ahmedabad 380 001, Gujarat, India

E-mail: ajayrathod.chem@gmail.com, patel87chirag@gmail.com

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SUPPORTING DATA

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General procedure:

Synthesis of 5-(4-chloro phenyl)-1,3,4-oxadiazol-2-thiol

4-chloro benzoic acid (0.1mol) in 100 ml CH_3OH with catalytic amount of H_2SO_4 was refluxed for 7 hours. Reaction was monitored through TLC. (Hexane: ethyl acetate; 60:40) Reaction mixture was poured in cold water and methyl 4-chlorobenzoatewas collected. Further methyl 4-chlorobenzoate (0.08 mol) was refluxed for 8 hours with (0.08 mol) hydrazine hydrated. After completion of reaction, reaction mixture was poured in cold water to get 4-chlorobenzohydrazide.

of 5-(4-chloro phenyl)-1,3,4-oxadiazol-2-thiol was synthesized by mixing (0.06 mol) of 4-chlorobenzohydrazide in (0.09 mol) KOH and 100 ml methanol in RBF. Then (0.09 mol) CS_2 was added portion wise and reaction mixture was being refluxed with stirring for 11 hours. Reaction progress was monitored through TLC. (Hexane: ethyl acetate; 80:20). Reaction mixture was poured in cold water and acidified with dil. HCl to get oxadiazole. Solid was filtered, dried and re crystallized with ethanol

Synthesis of chloro acetyl pyrazoline :

Various chalcone (0.03 mol) and hydrazine hydrate (0.03 mol) were dissolved in ethanol in RBF. It was refluxed for 12 hours. Reaction progress was monitored through TLC (Hexane: ethyl acetate; 80:20). After the completion of reaction solids wered obtained through distillation and dissolved in a DCM. Chloro acetyl chloride (0.03 mol) was added to reaction mass and stirred for 7 to 8 hours. Solid were obtained through vacuum distillation and re crystallized by ethanol.

General Procedure for Synthesis of 2-(5-(4-chloro phenyl)-1,3,4-oxadiazol-2-thiol)-1-(5-(phenyl)-3-phenyl-1*H*-pyrazol-1-yl)ethanone derivatives :

5-(4-chloro phenyl)-1,3,4-oxadiazol-2-thiol(2.12 gm, 0.01 mol), 2-chloro-1-(4,5-dihydro-5-(3-aryl)-3-arylpyrazol-1-yl)ethanone (0.01mol) and (1.24gm, 0.01mol) of anhydrous K_2CO_3 were dissolved in 100 ml of dimethyl formamide in a FBF. The reaction mass was agitated at 30-32 °C for 8–9 hours**.** TLC (hexane: ethyl acetate; 70:30) was used to monitor the reaction. The mixture was added to cooled water once the reaction was completed. Solids were filtered off as well as recrystallized with ethyl alcohol.

Spectral Data :

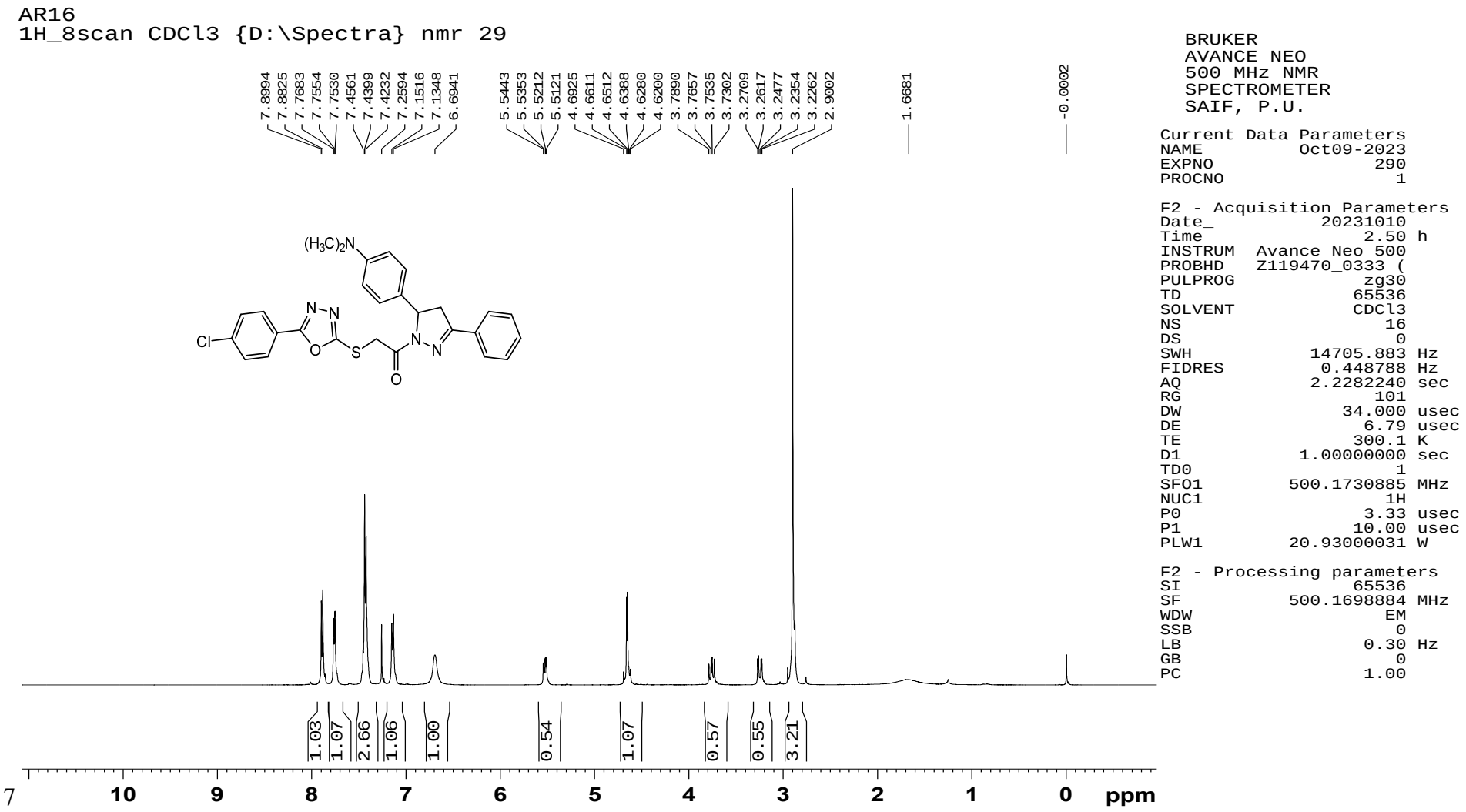


Figure S1: ^{1}H NMR spectra of compound 6d

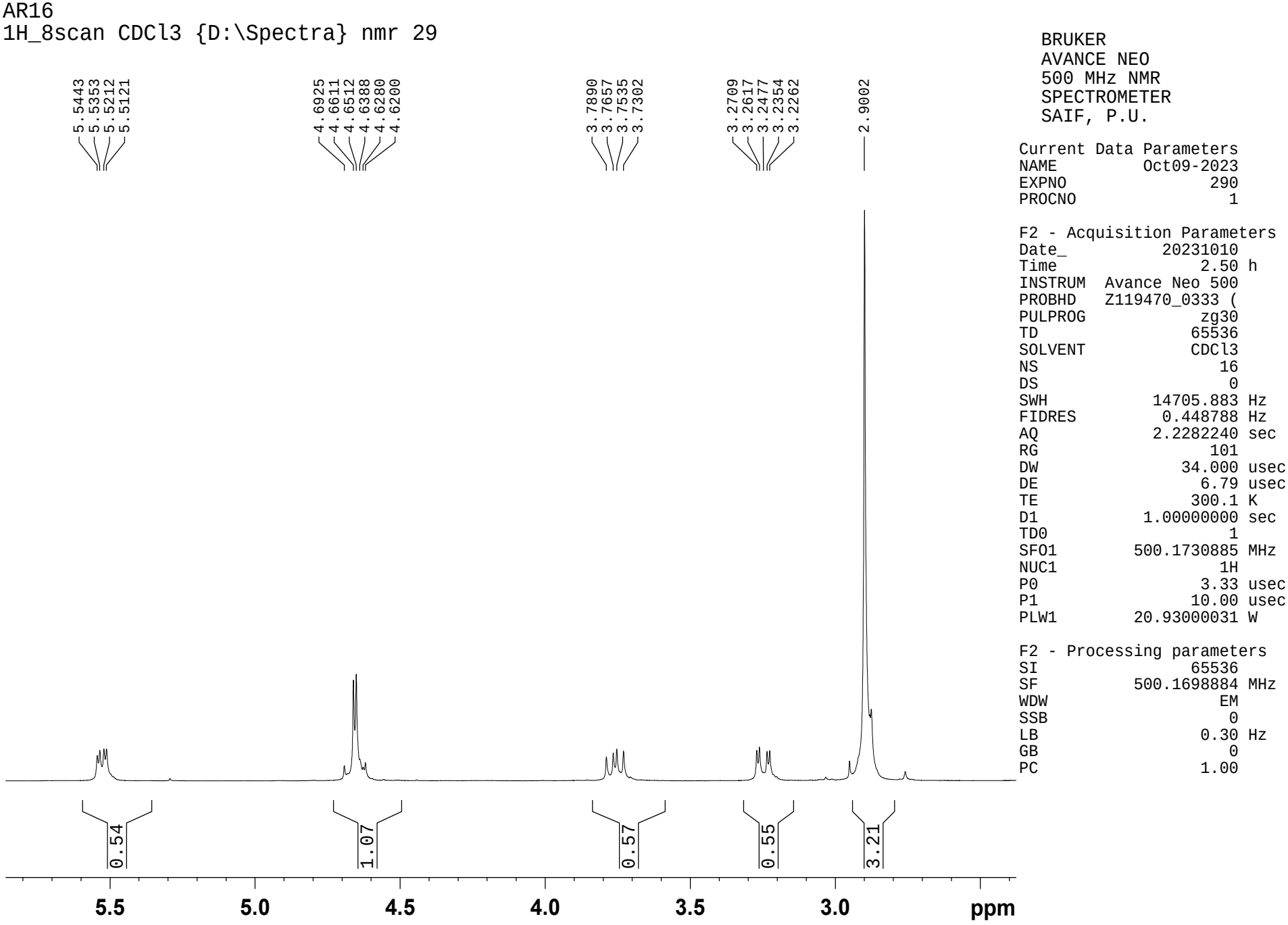


Figure S2: Expanded ^{1}H NMR spectra of compound 6d

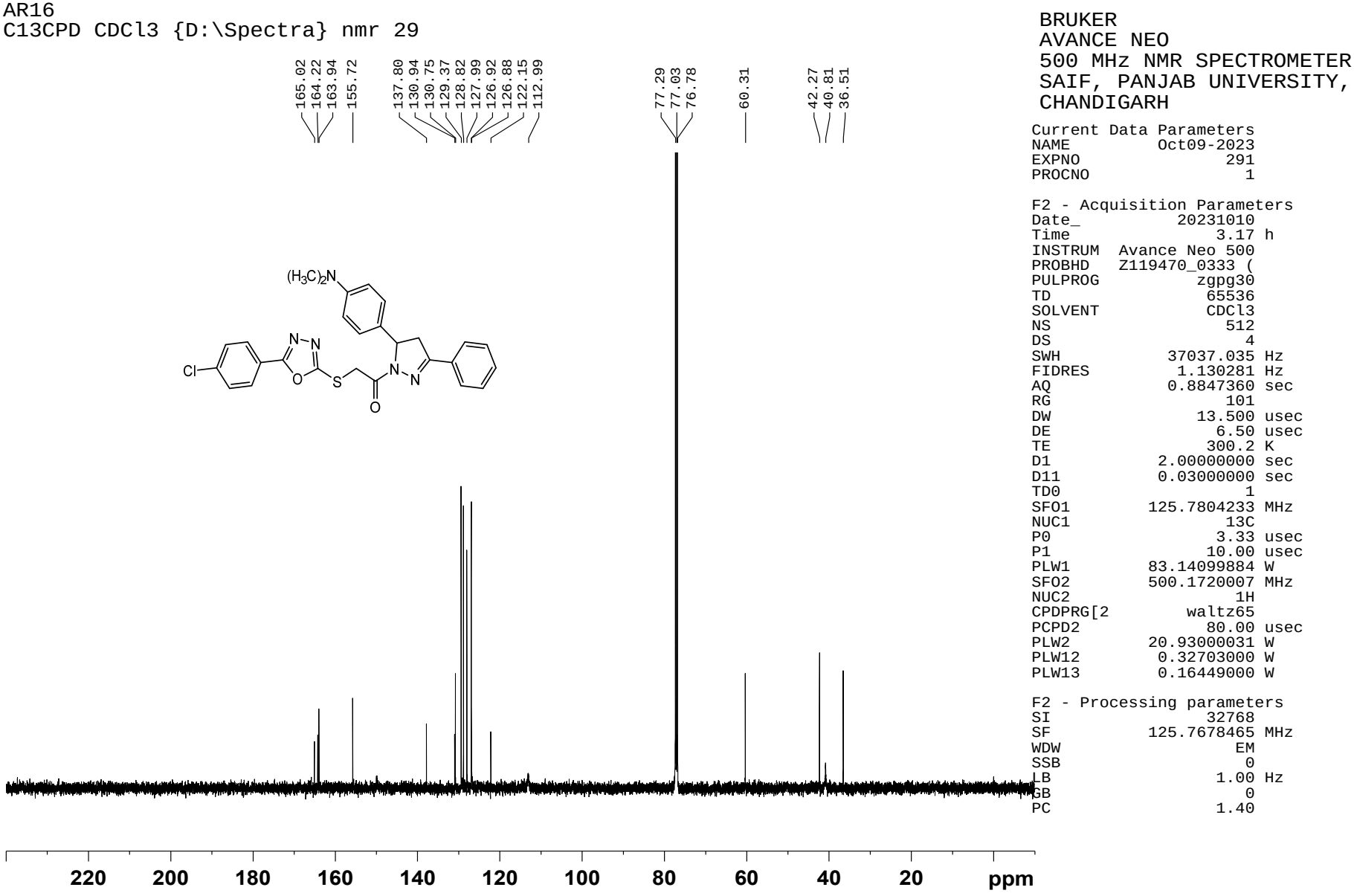
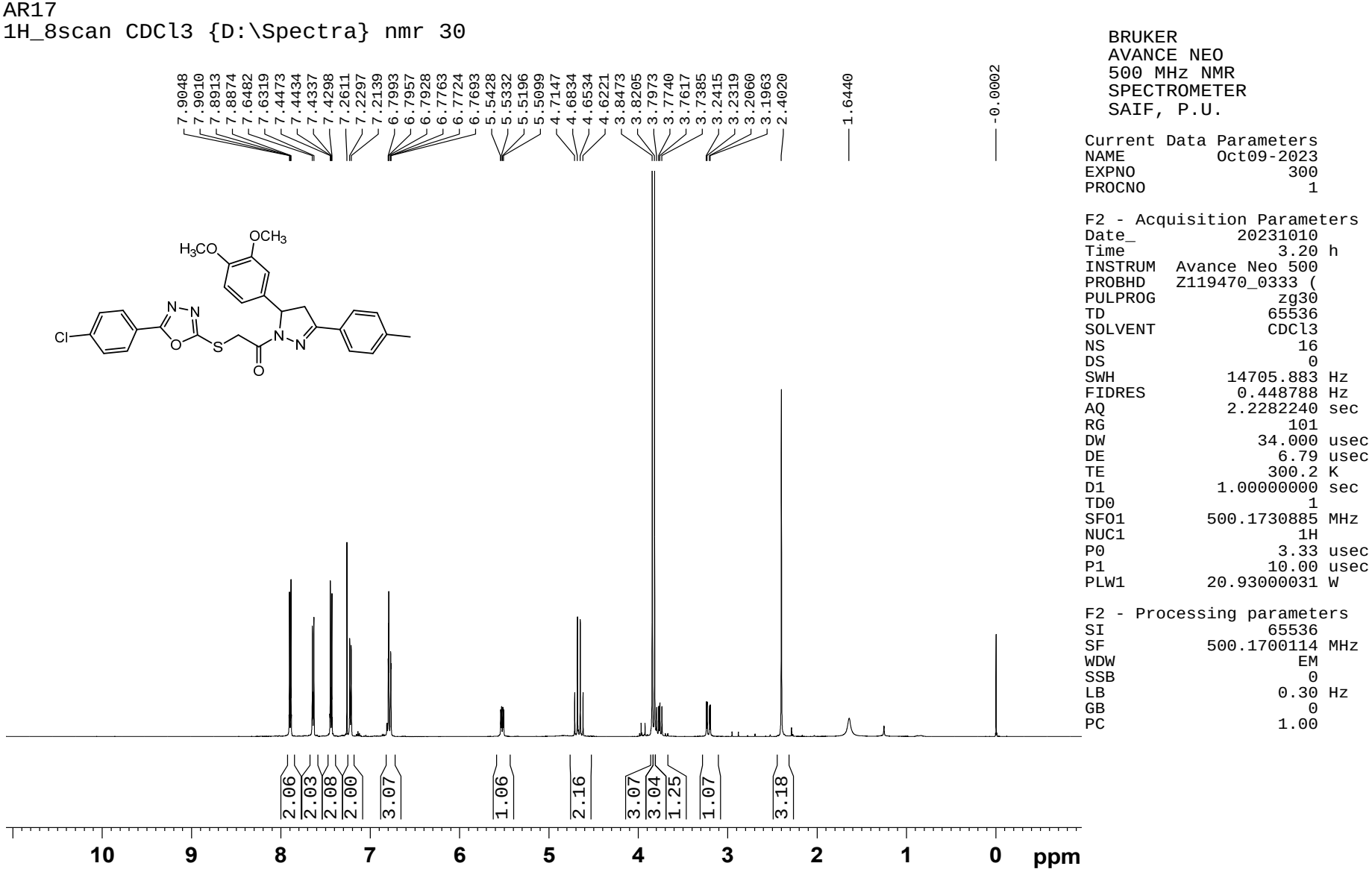


Figure S3: ^{13}C NMR spectra of compound 6d



BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

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EXPNO	300
PROCNO	1

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NS	16
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SWH	14705.883 Hz
FIDRES	0.448788 Hz
AQ	2.2282240 sec
RG	101
DW	34.000 usec
DE	6.79 usec
TE	300.2 K
D1	1.00000000 sec
TD0	1
SFO1	500.1730885 MHz
NUC1	1H
P0	3.33 usec
P1	10.00 usec
PLW1	20.93000031 W

F2 - Processing parameters	
SI	65536
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PC	1.00

Figure S4: ^{1}H NMR spectra of compound 6h

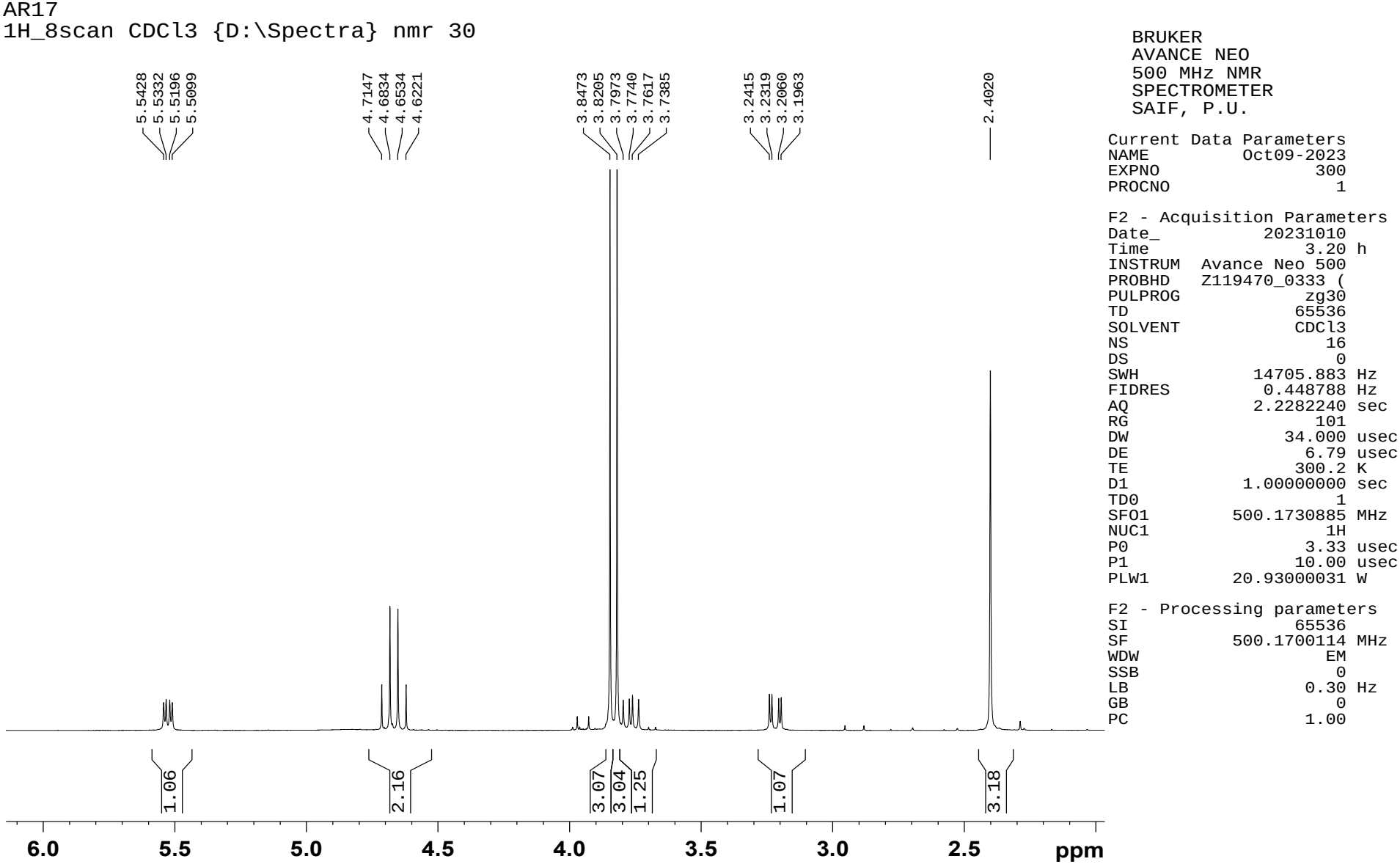
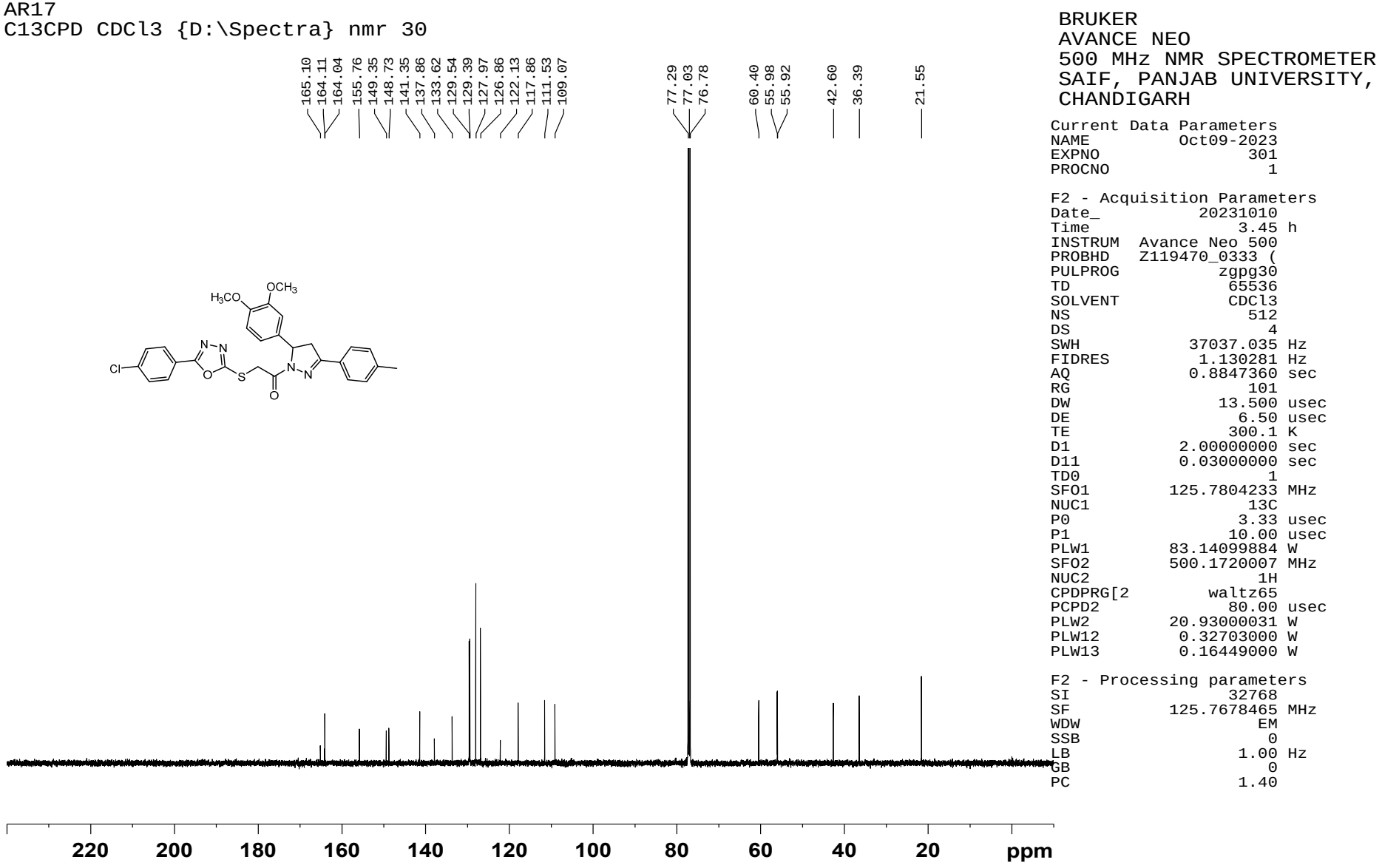


Figure S5: Expanded ^{1}H NMR spectra of compound 6h




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BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

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PROCNO                 1

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FIDRES          1.130281 Hz
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RG                   101
DW                13.500 usec
DE                 6.50 usec
TE                300.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         125.7804233 MHz
NUC1                 13C
P0                3.33 usec
P1               10.00 usec
PLW1         83.14099884 W
SFO2         500.1720007 MHz
NUC2                 1H
CPDPRG[2         waltz65
PCPD2              80.00 usec
PLW2         20.93000031 W
PLW12         0.32703000 W
PLW13         0.16449000 W

F2 - Processing parameters
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SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Figure S6: ^{13}C NMR spectra of compound 6h

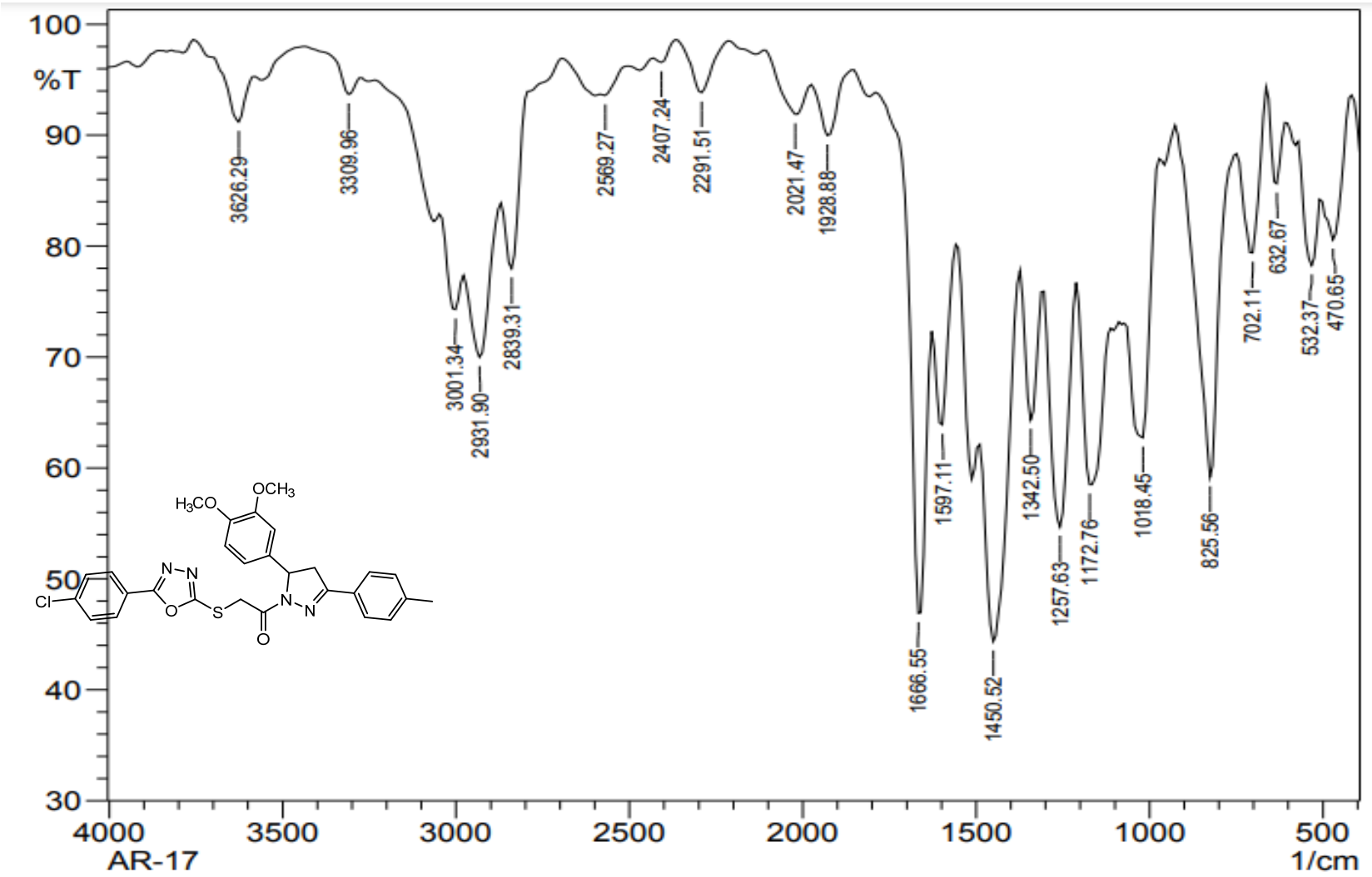


Figure S7: FT-IR spectra of compound 6h

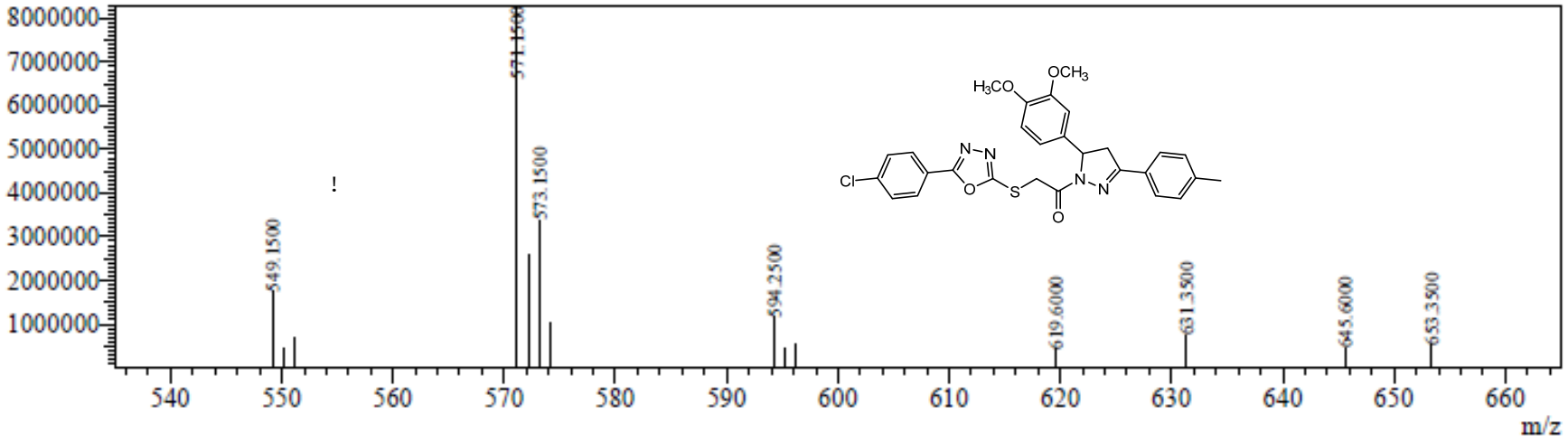


Figure S8: LCMS spectra of compound 6h

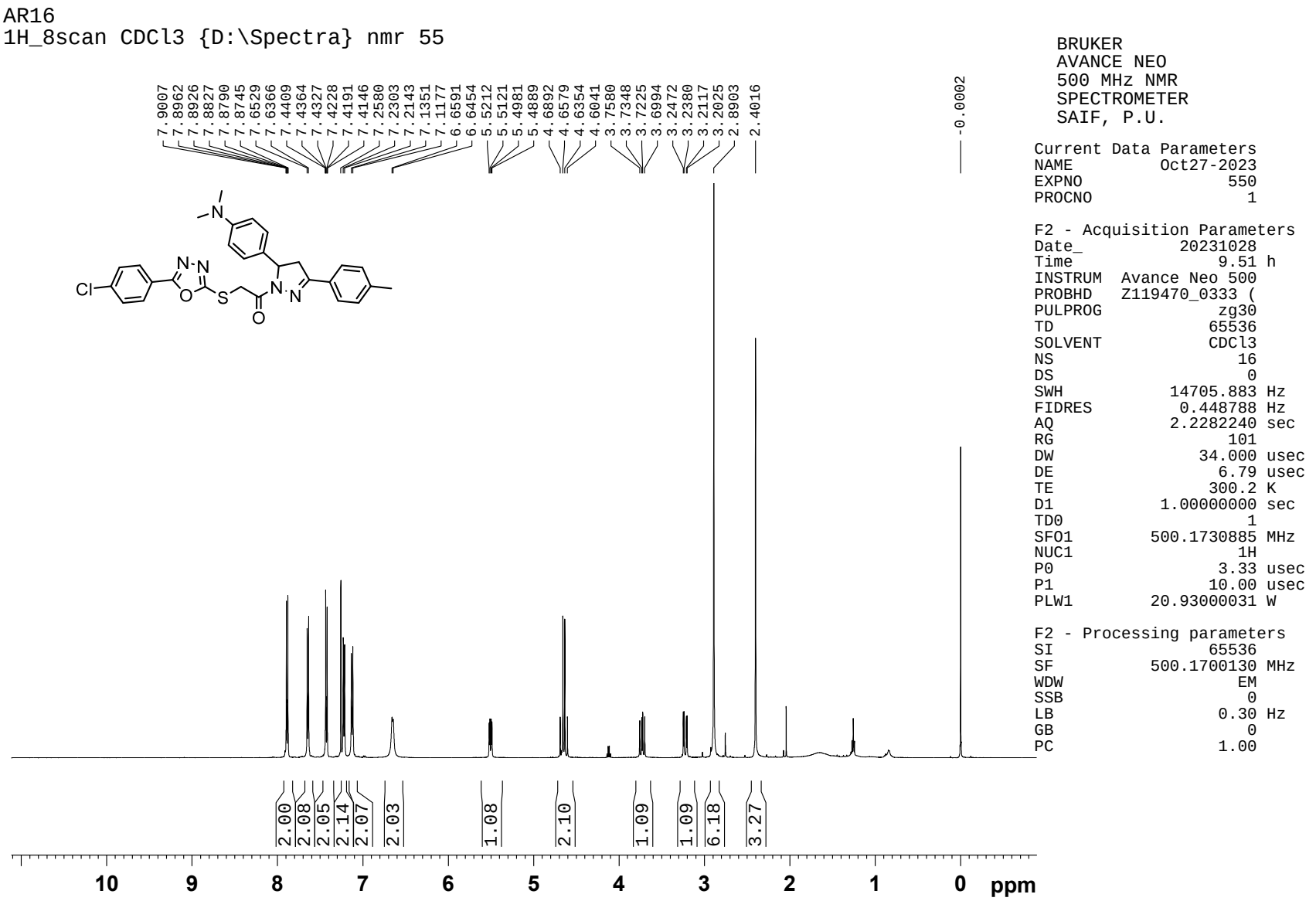


Figure S9: ^{1}H NMR spectra of compound 6i

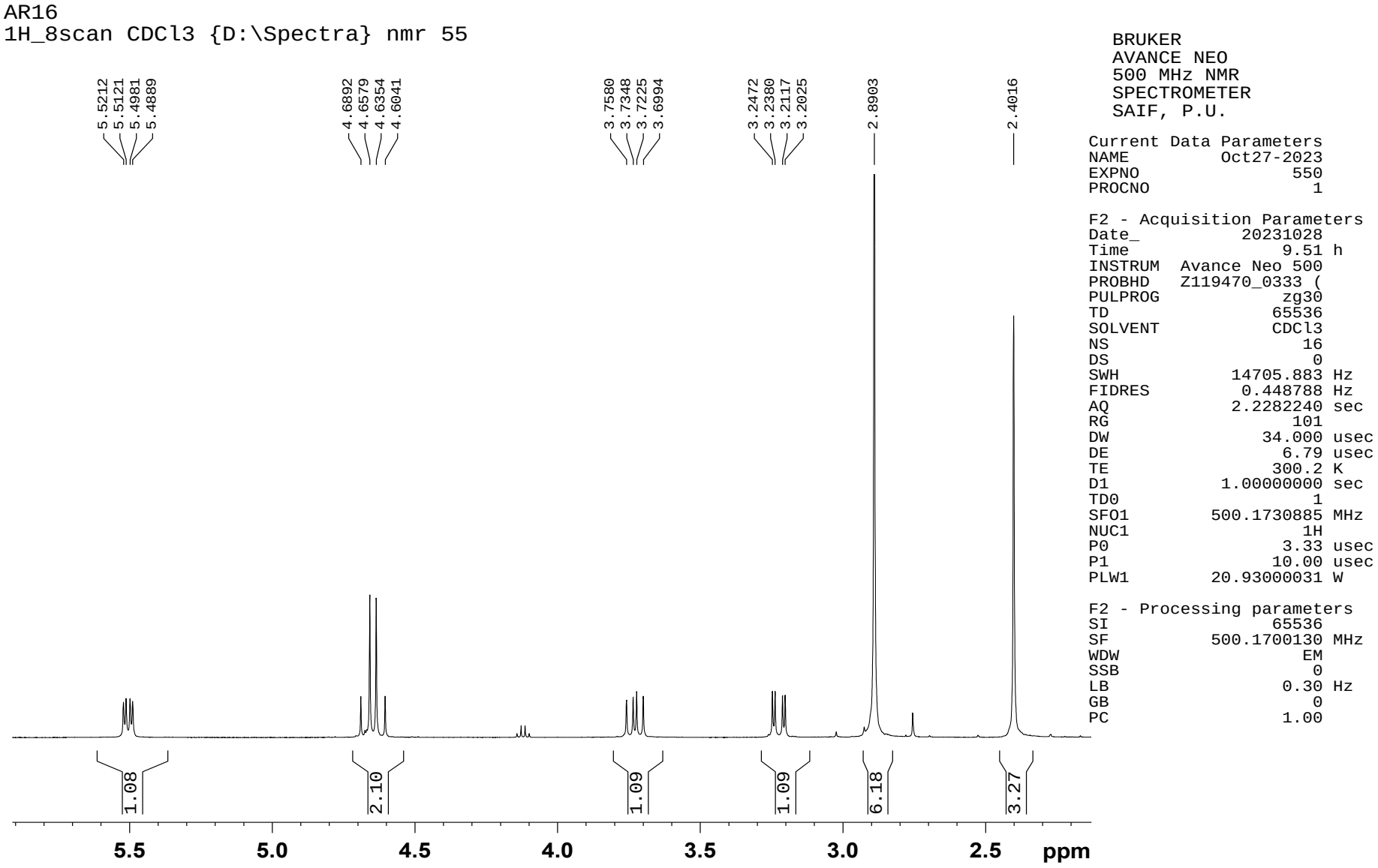


Figure S10: Expanded ^{1}H NMR spectra of compound 6i

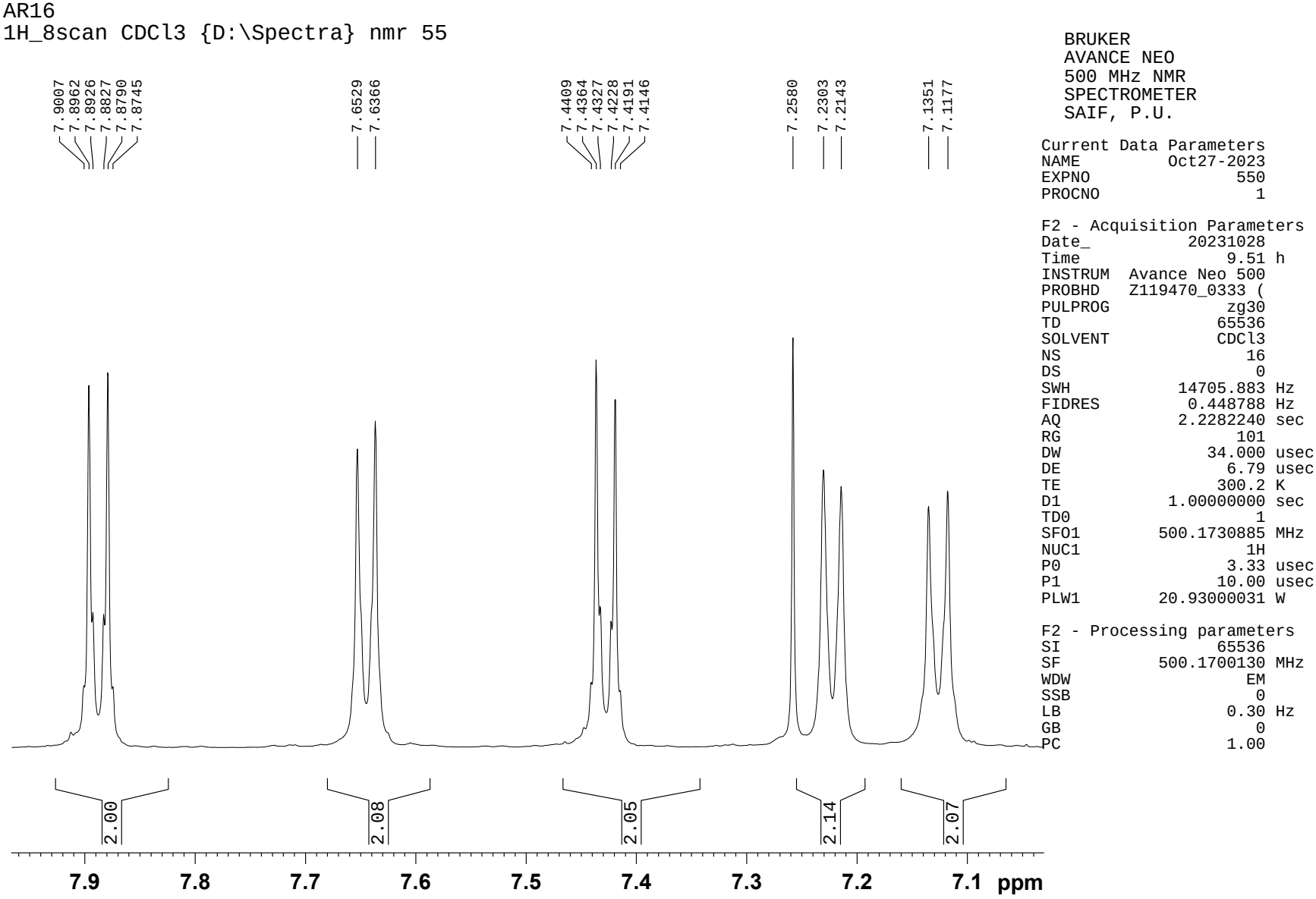


Figure S10: Expanded ^{1}H NMR spectra of compound 6i

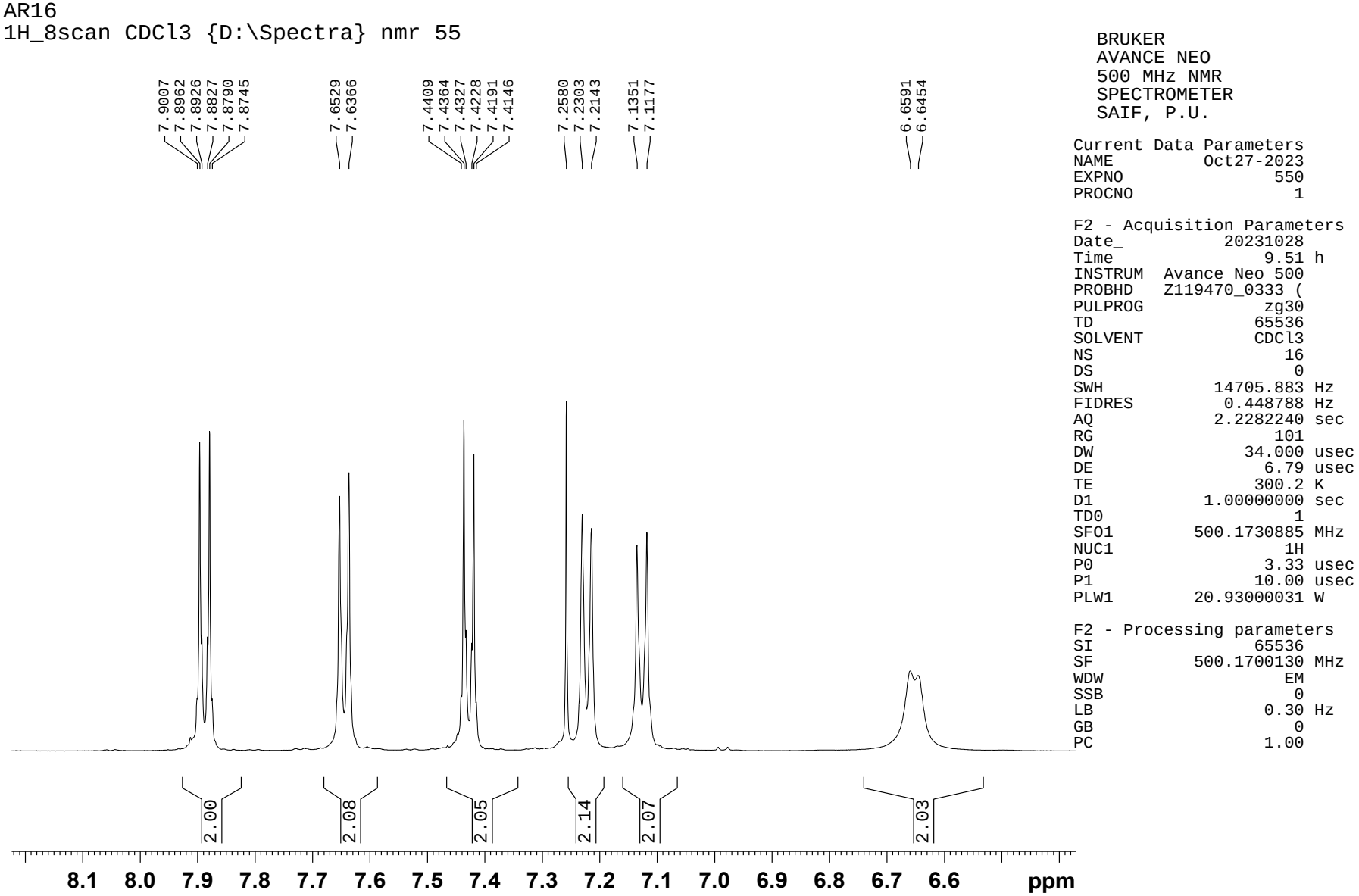


Figure S10: Expanded ^{1}H NMR spectra of compound 6i

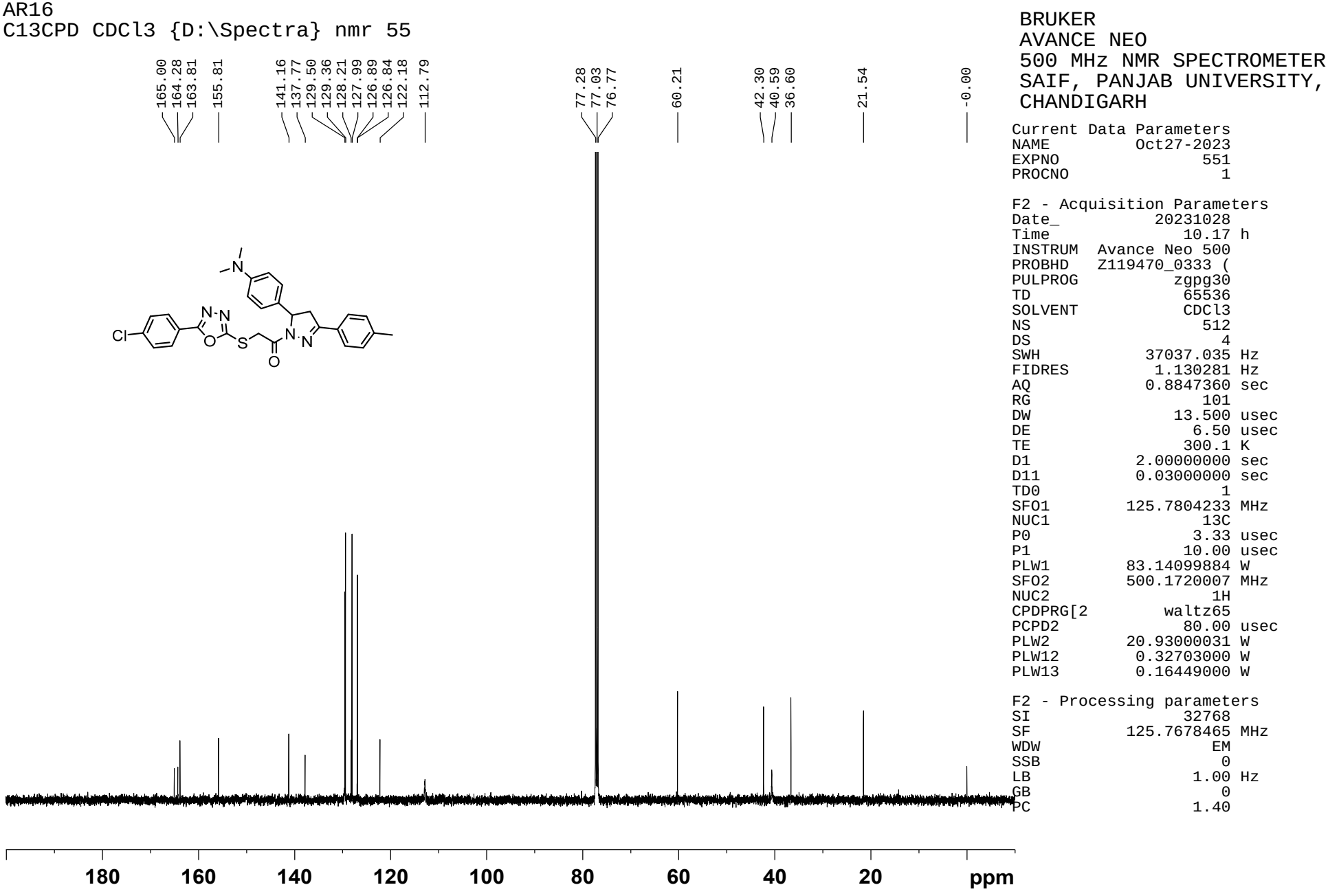


Figure S11: ^{13}C NMR spectra of compound 6i

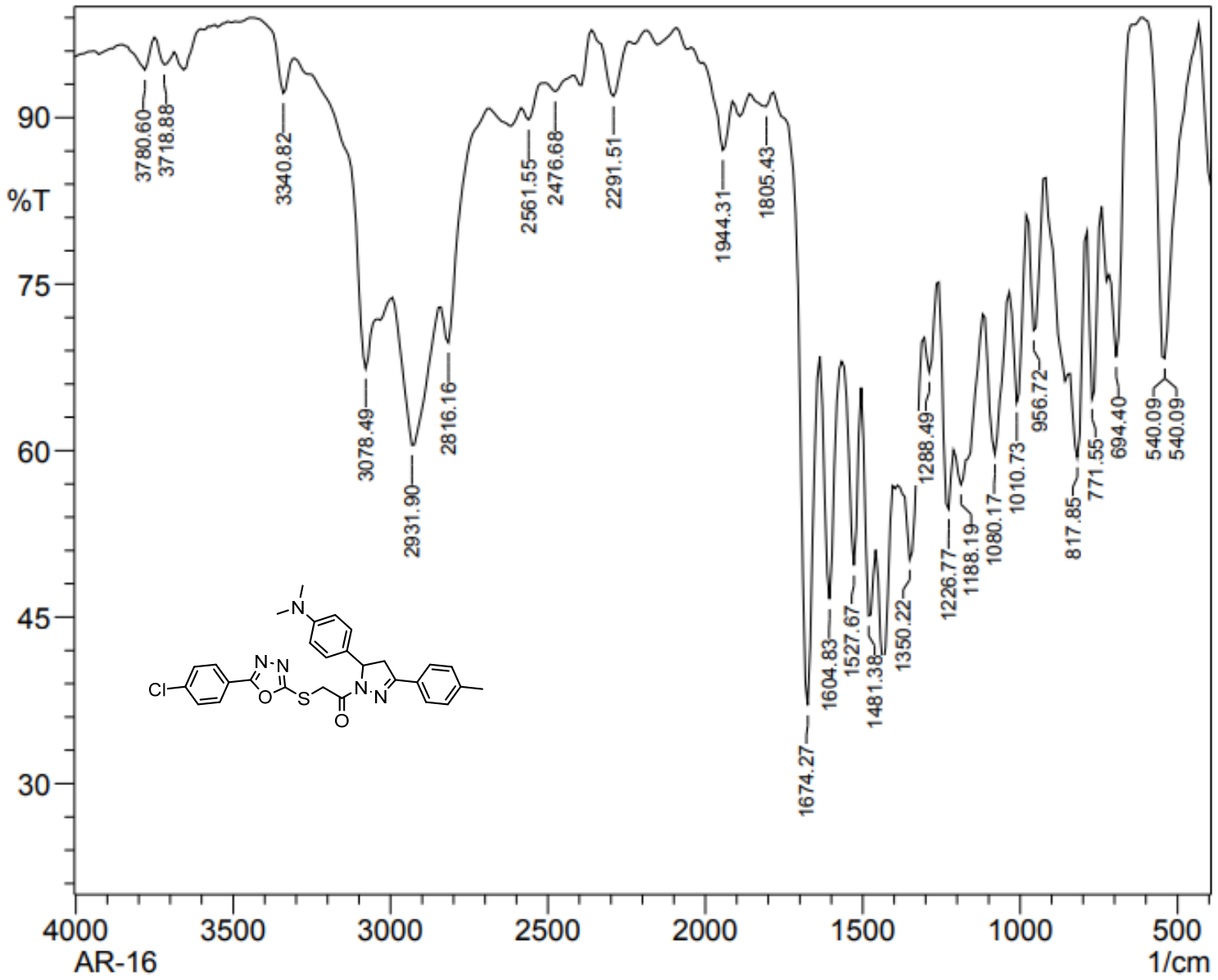


Figure S12: FT-IR spectra of compound 6i

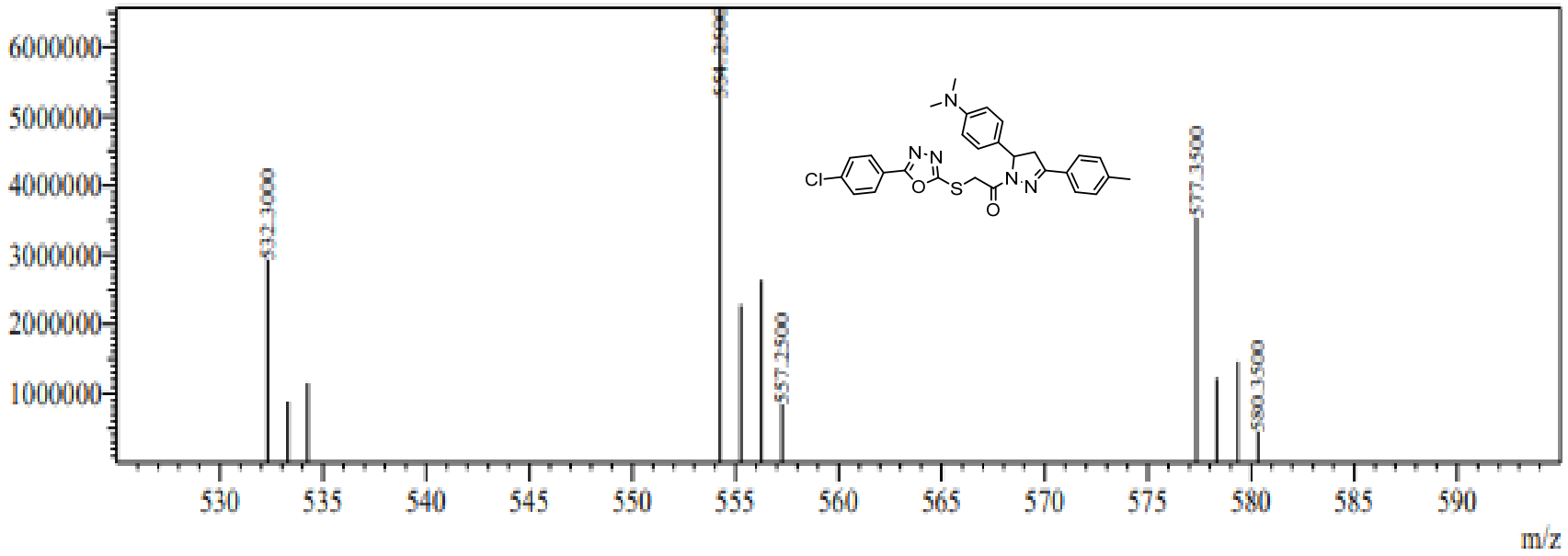


Figure S13: LCMS spectra of compound 6i

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