Supplementary Information

Novel Pyrimidine Linked Acyl Thiourea Derivatives as Potent α-Amylase and Proteinase K Inhibitors: Design, Synthesis, Molecular Docking and ADME Studies

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List of Figures

25. Figure 25. FT-IR Spectrum of compound **(6i)**

26. Figure 26. FT-IR Spectrum of compound **(6j)**

27. Figure 27. 3D docking pose and 2D binding interactions of compounds **(6a-j)** in the binding pocket of α-amylase

28. Fig 28. 3D docking pose and 2D binding interactions of compounds **(6a-j)** in the binding pocket of proteinase K

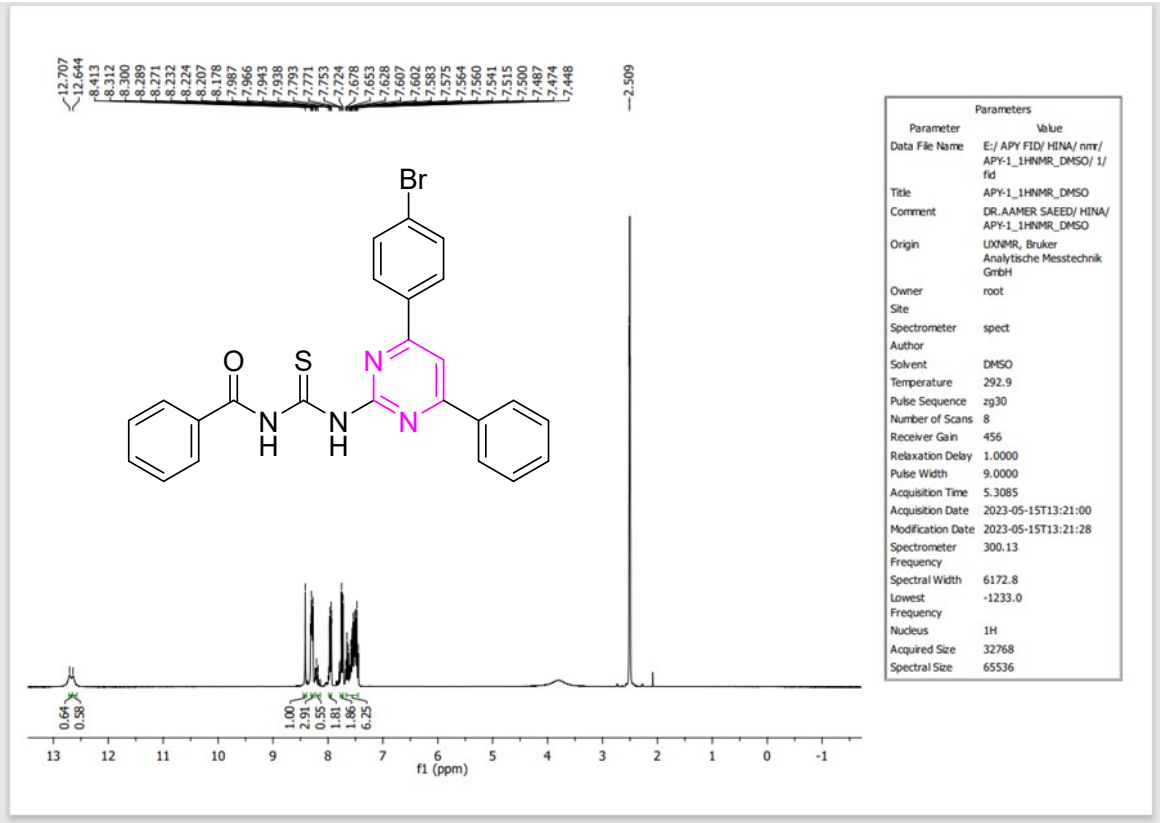
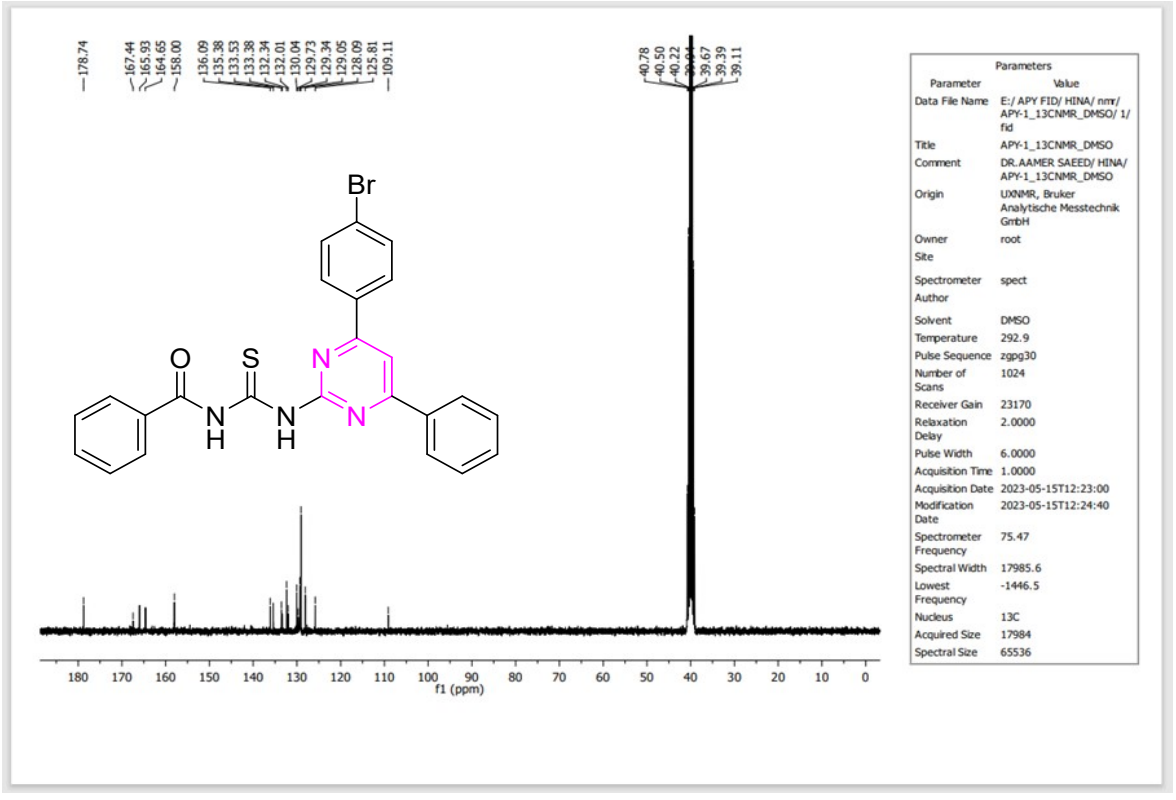


Figure 1. [1]H-NMR Spectrum of compound **(6a)**



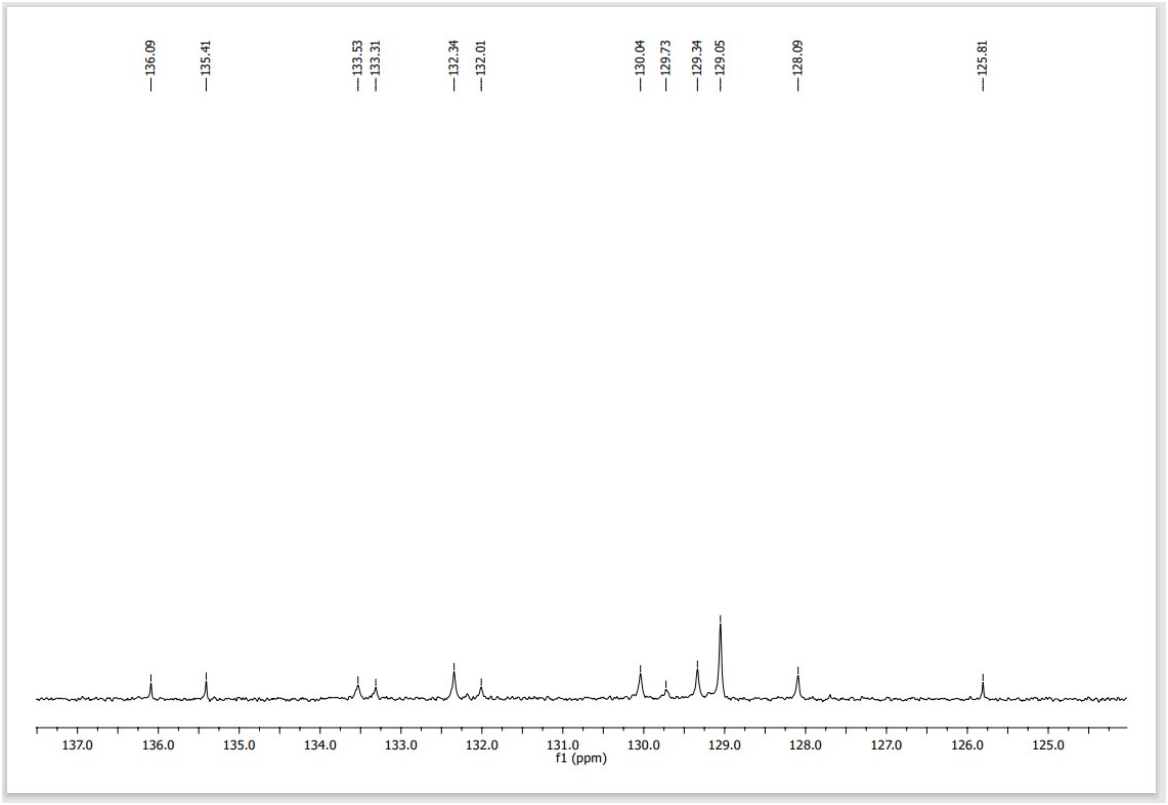


Figure 2.^{13}C-NMR Spectrum of compound **(6a)**

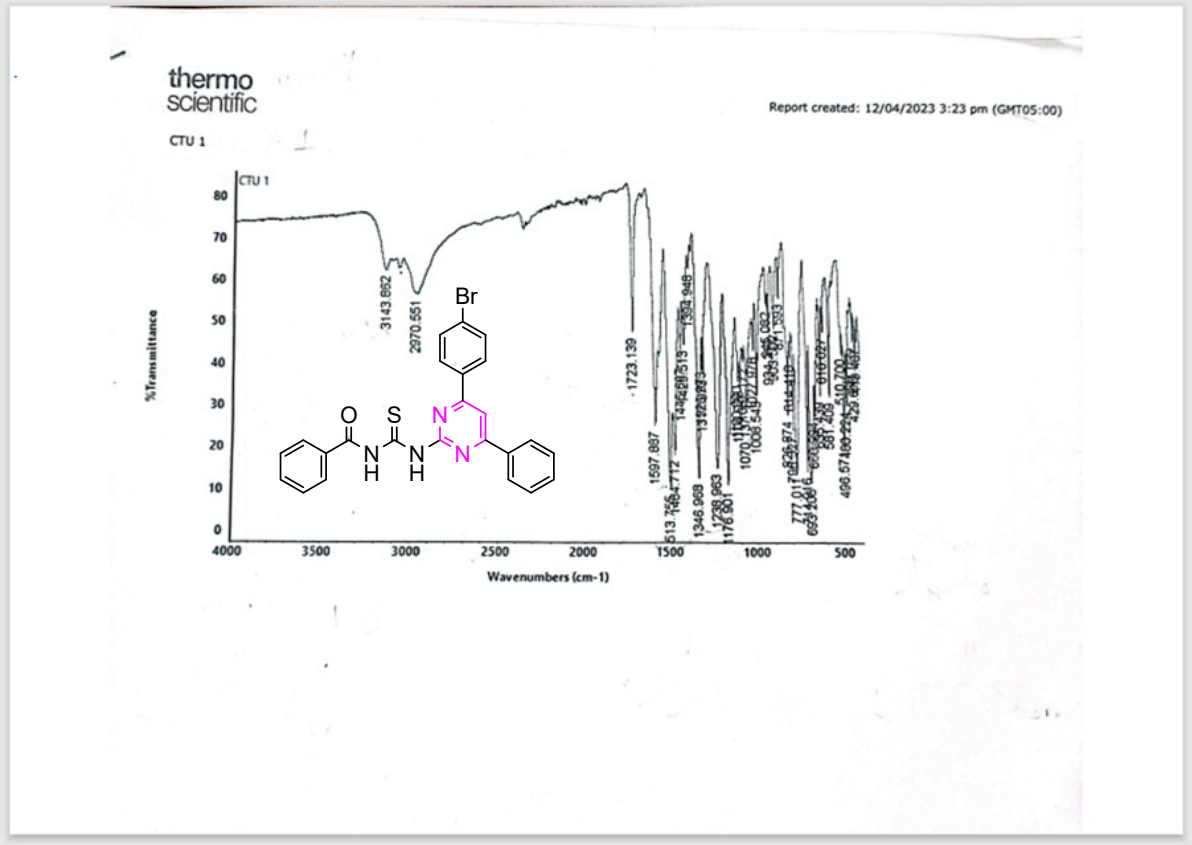
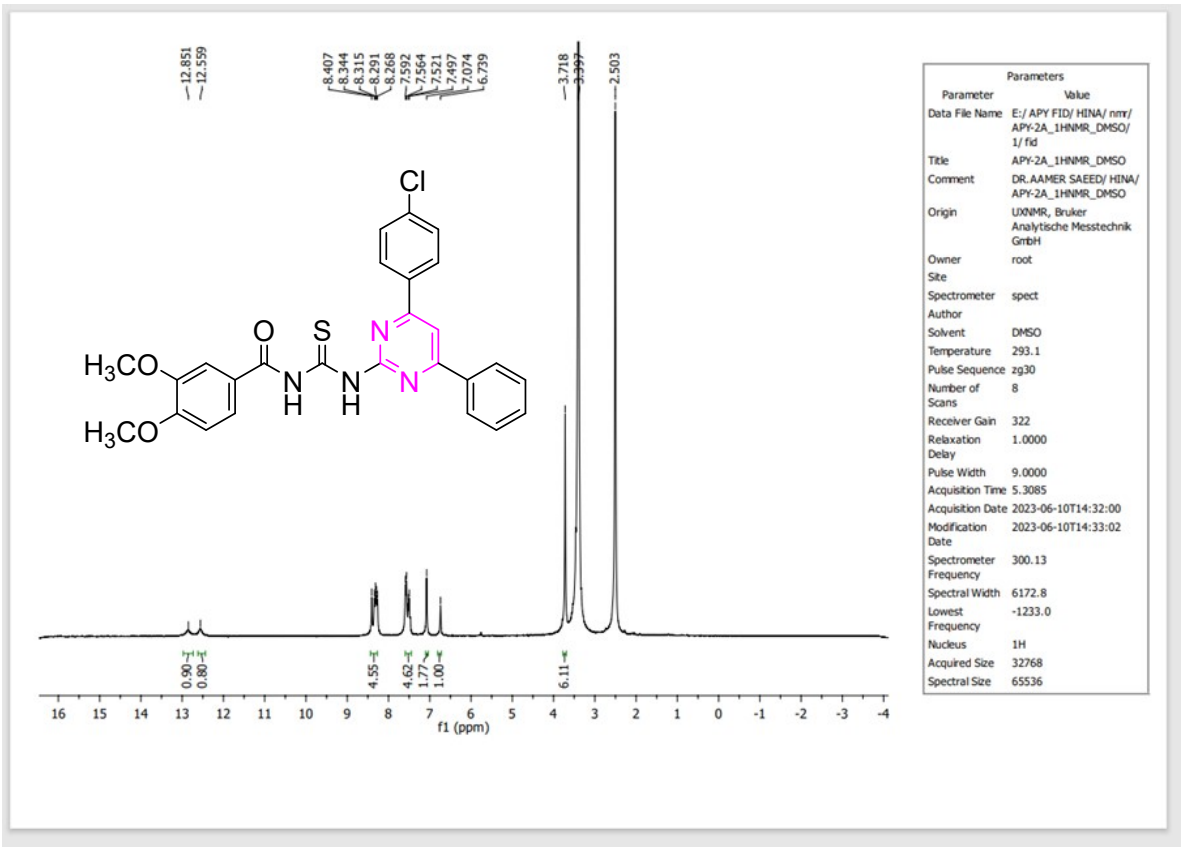


Figure 3. FT-IR Spectrum of compound **(6a)**



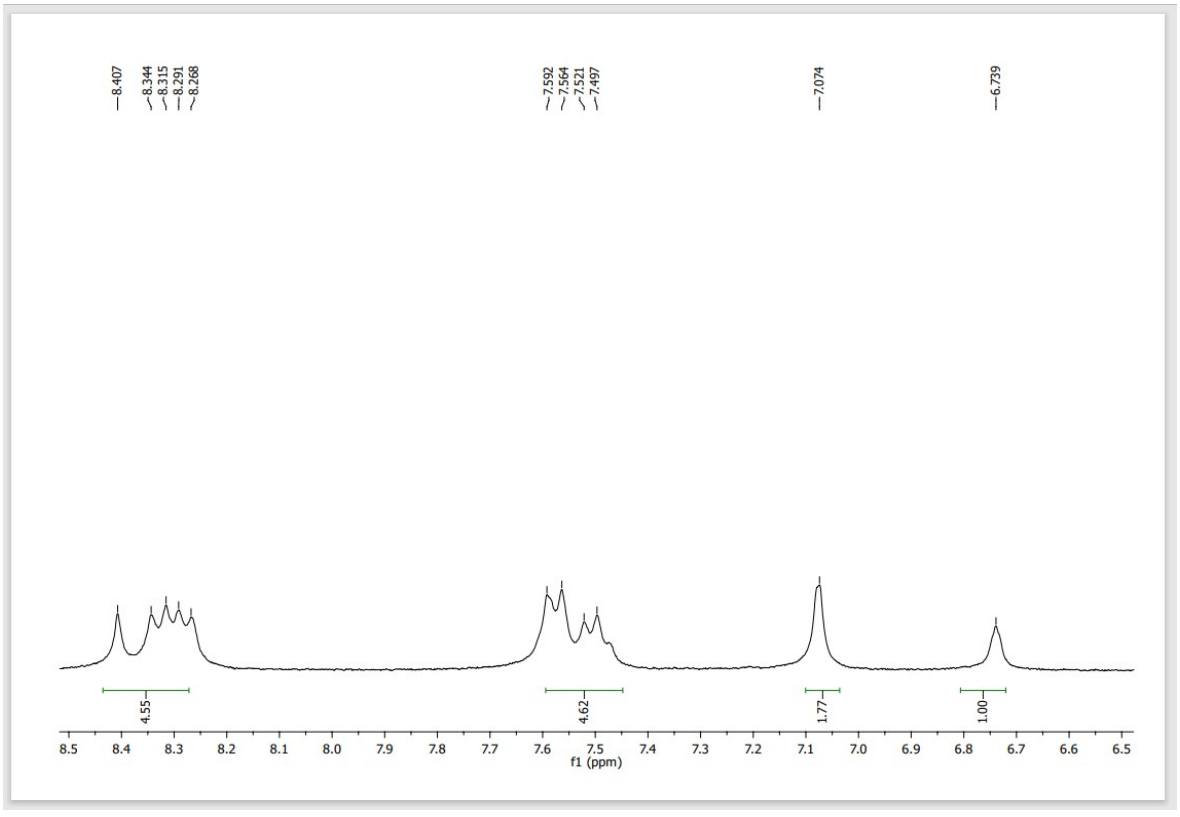


Figure 4. [1]H-NMR Spectrum of compound **(6b)**

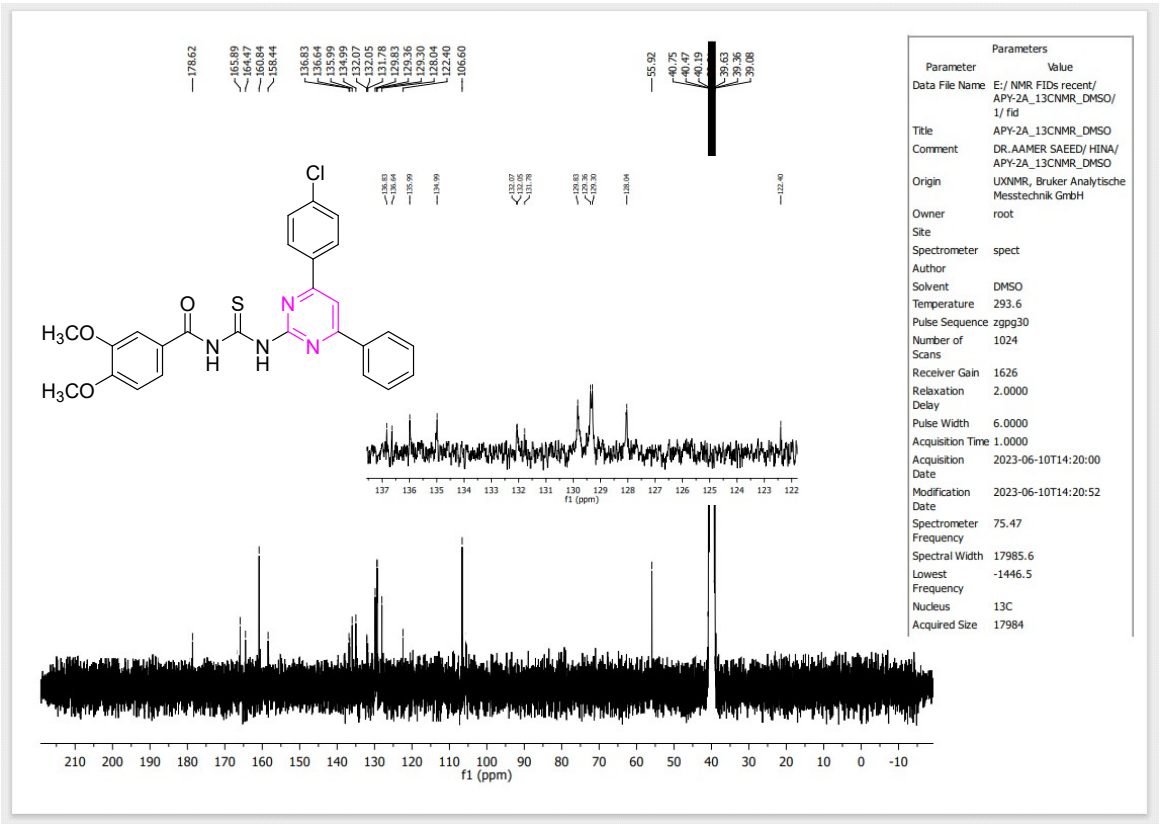


Figure 5.^{13}C-NMR Spectrum of compound **(6b)**

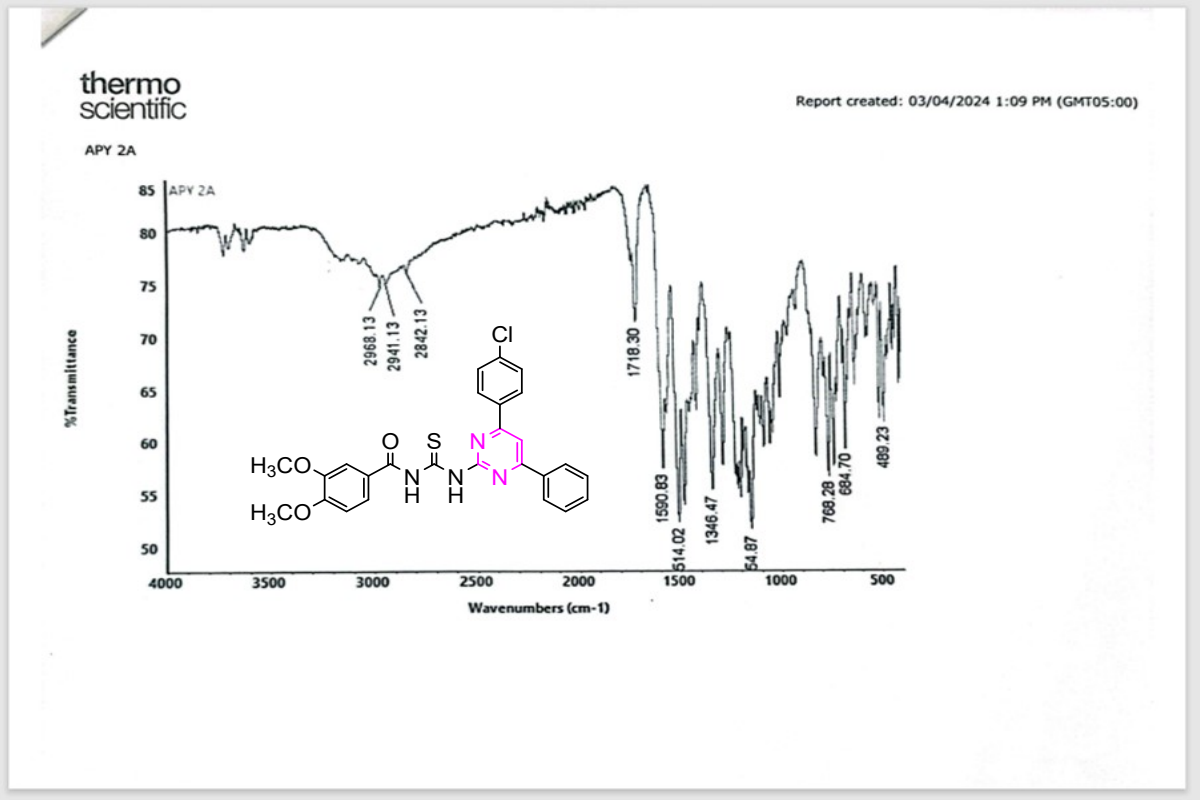
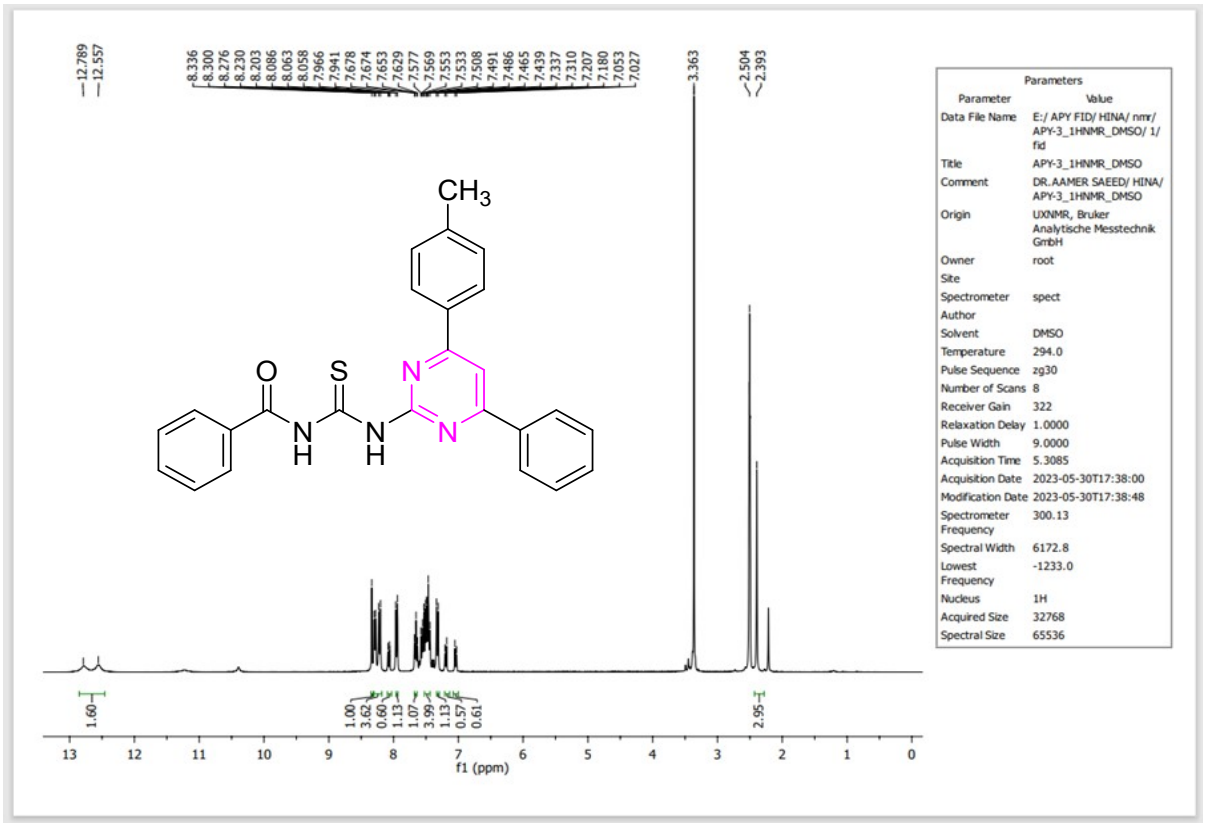


Figure 6. FT-IR Spectrum of compound **(6b)**



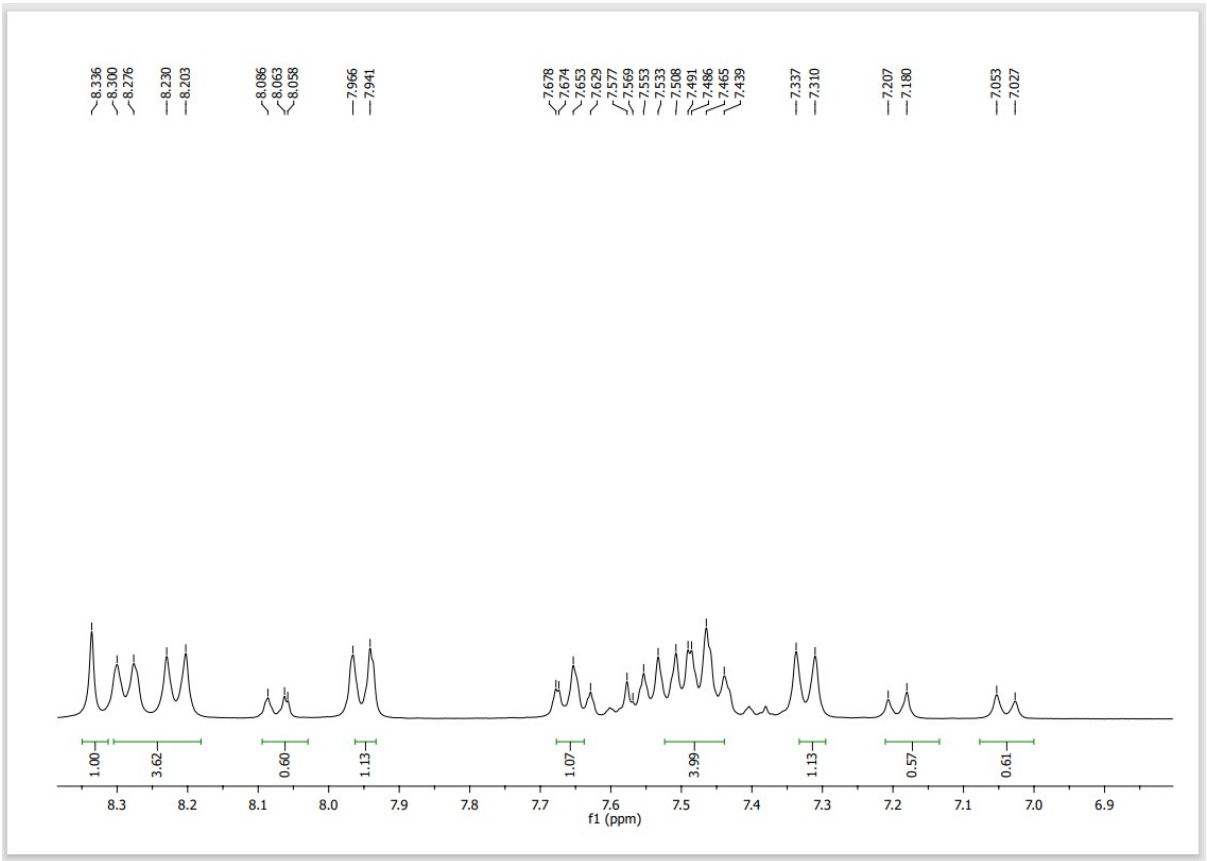
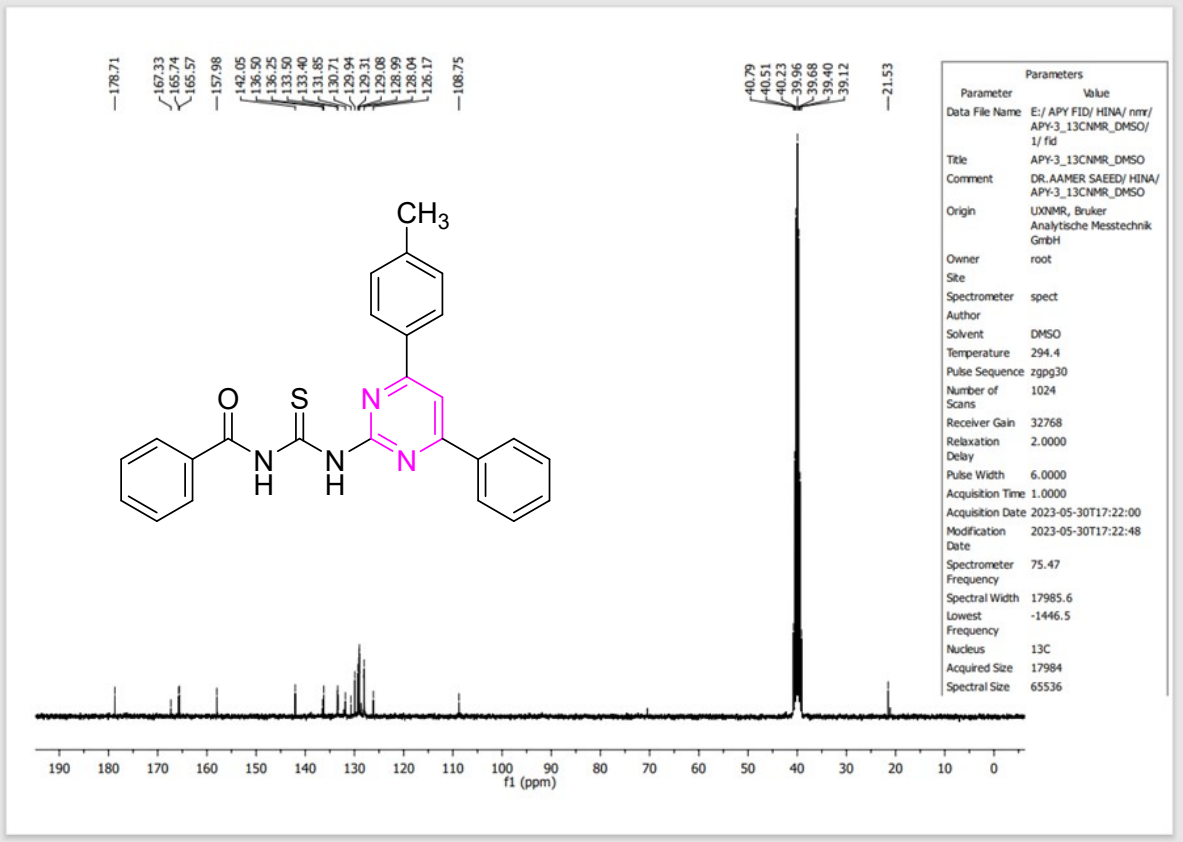


Figure 7. ^{1}H-NMR Spectrum of compound **(6c)**



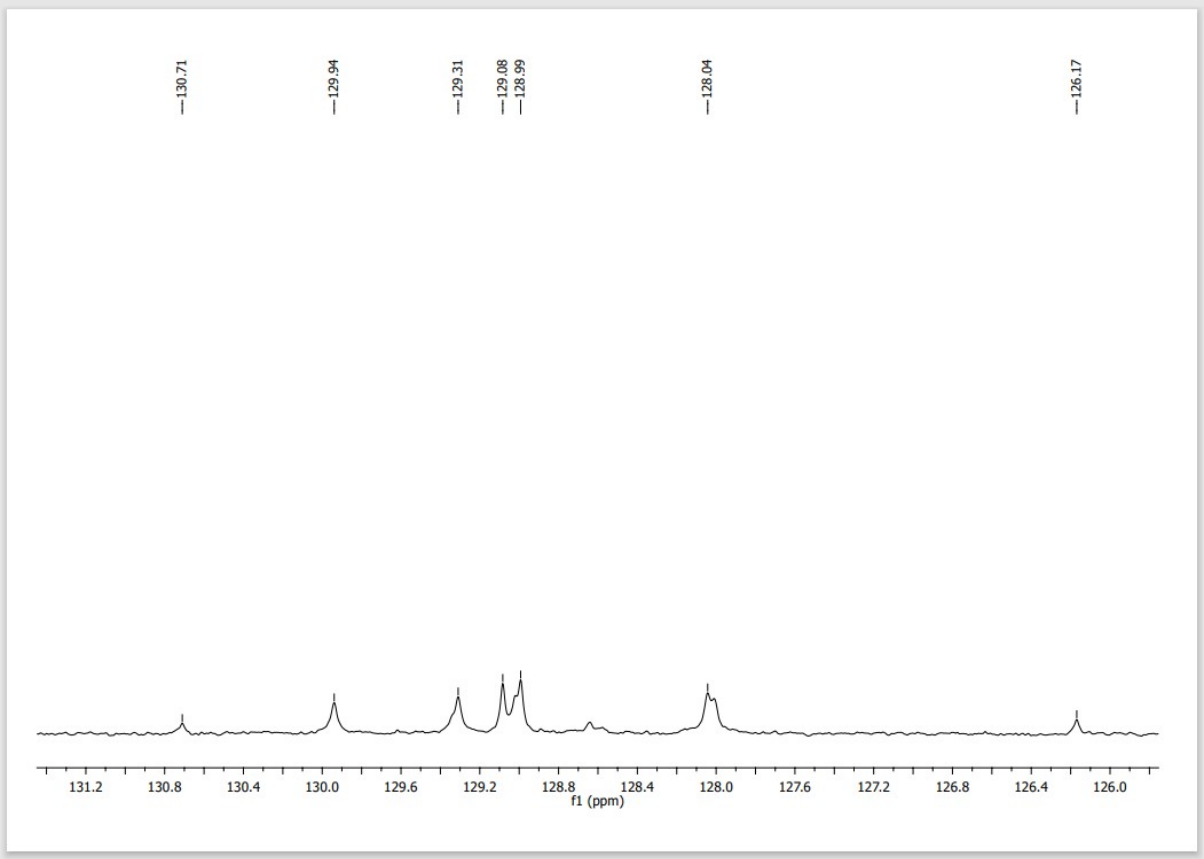


Figure 8. ^{13}C-NMR Spectrum of compound **(6c)**

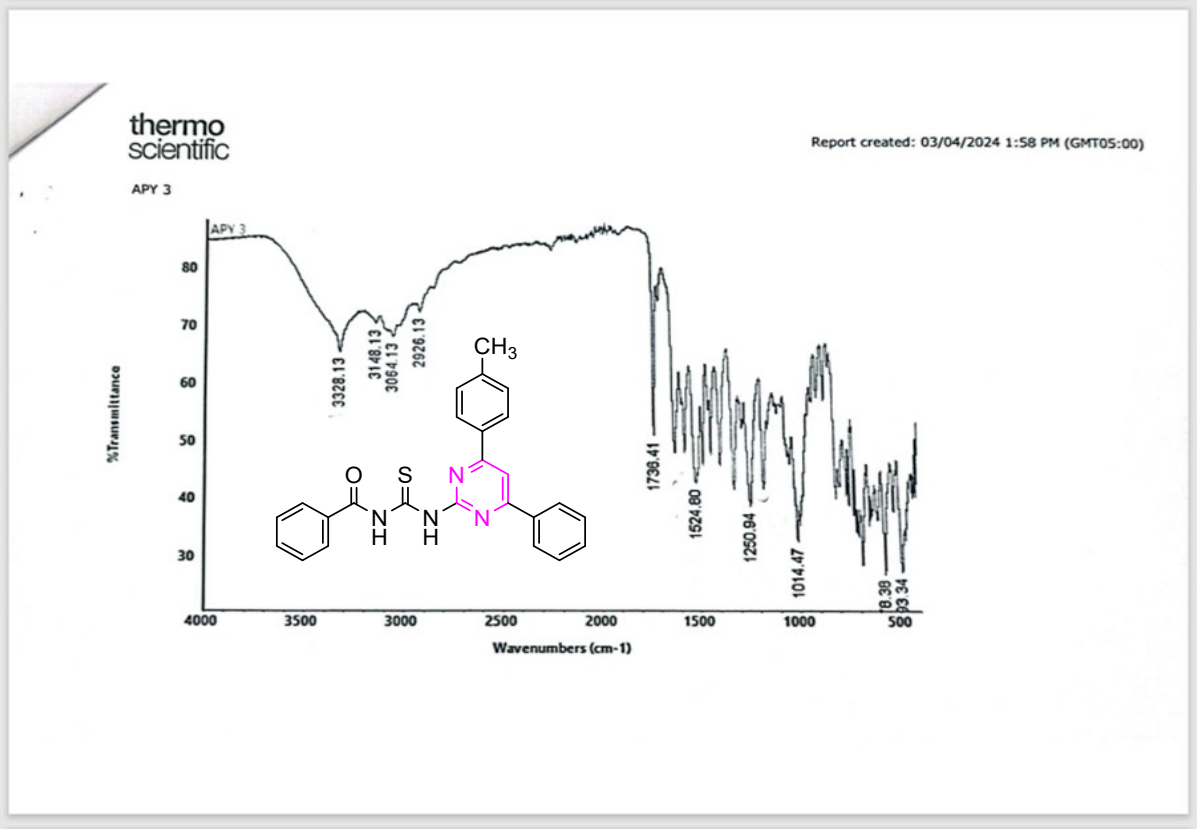


Figure 9. FT-IR Spectrum of compound **(6c)**

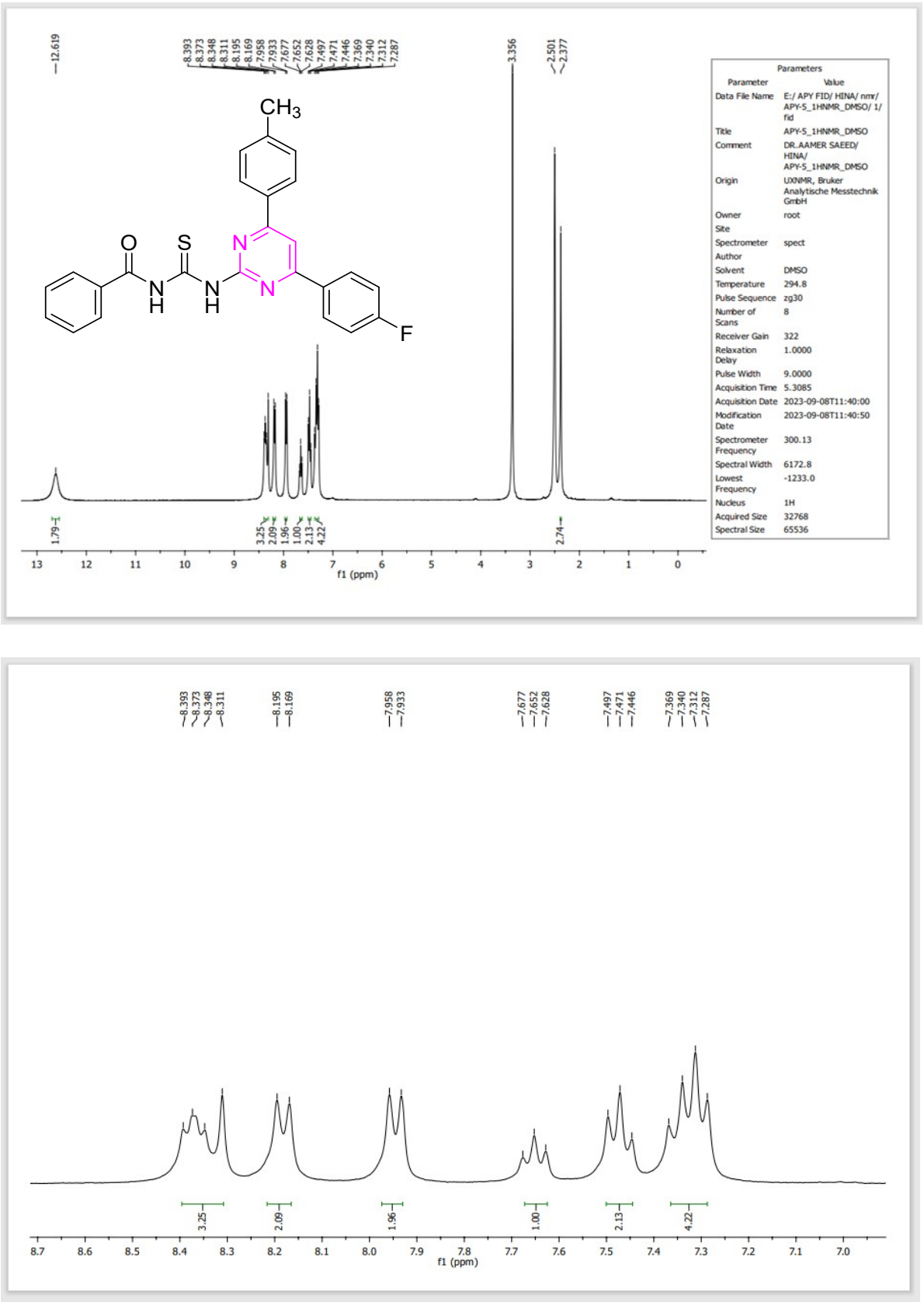


Figure 10. ^{1}H-NMR Spectrum of compound **(6d)**

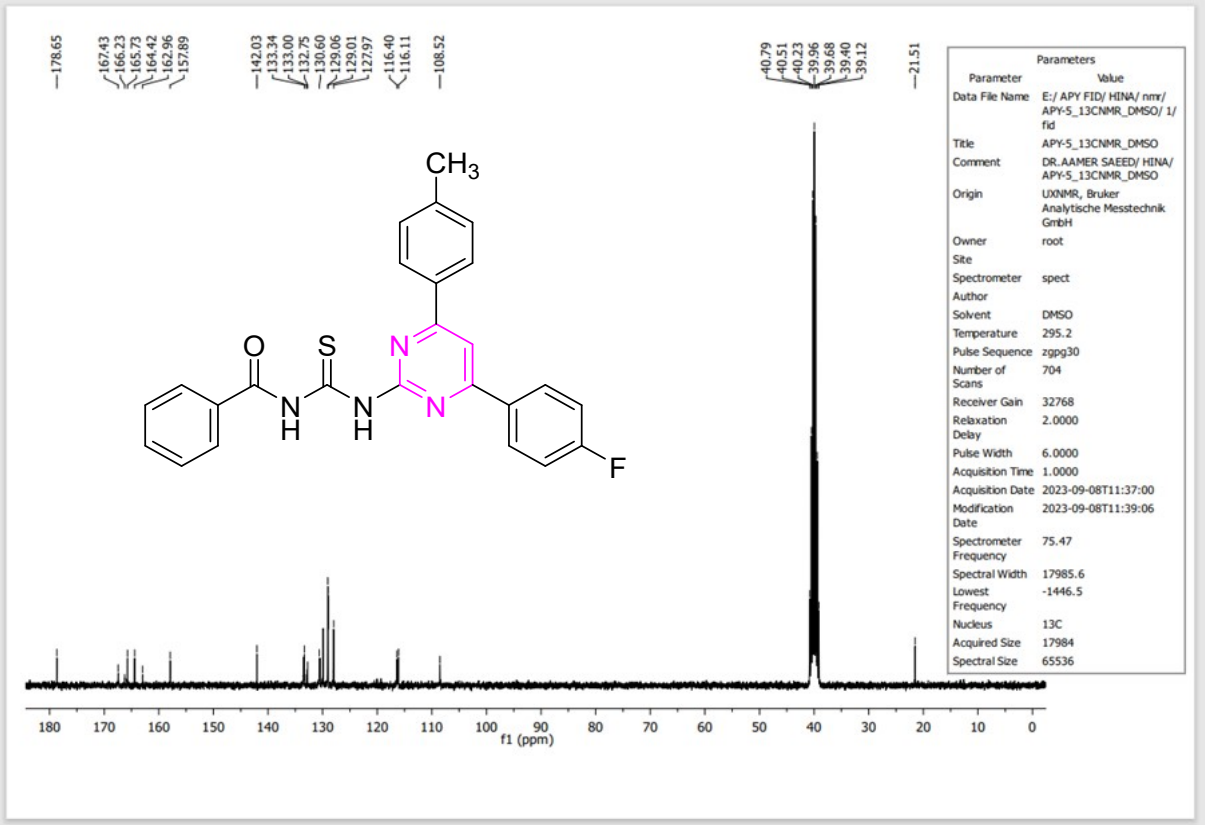


Figure 11.[13]C-NMR Spectrum of compound **(6d)**

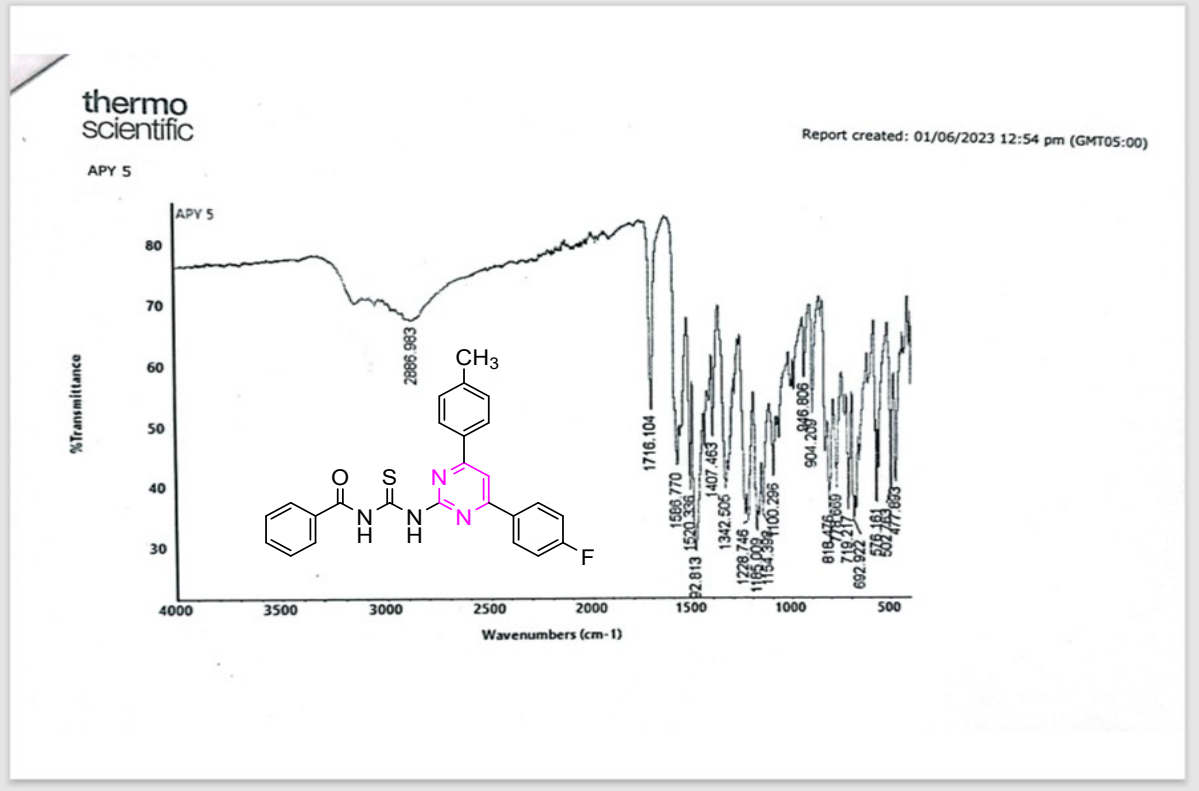


Figure 12. FT-IR Spectrum of compound **(6d)**

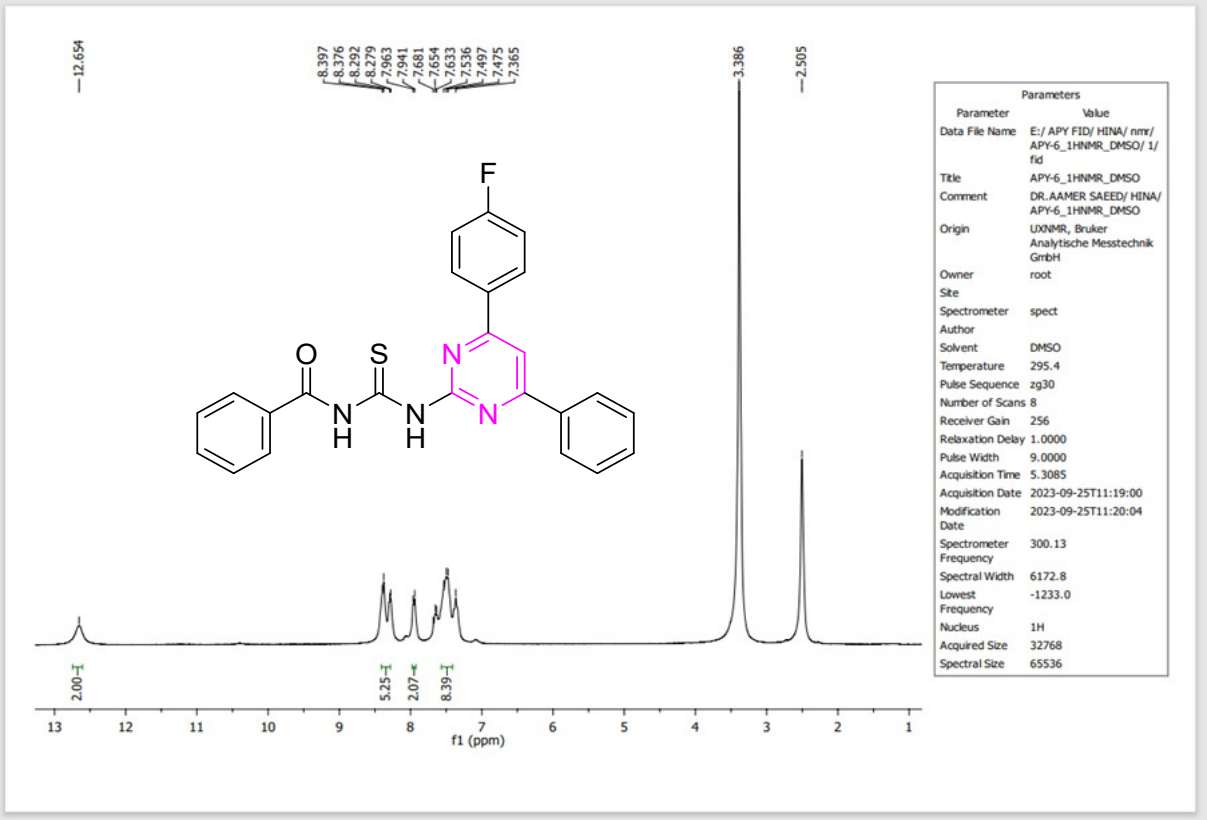
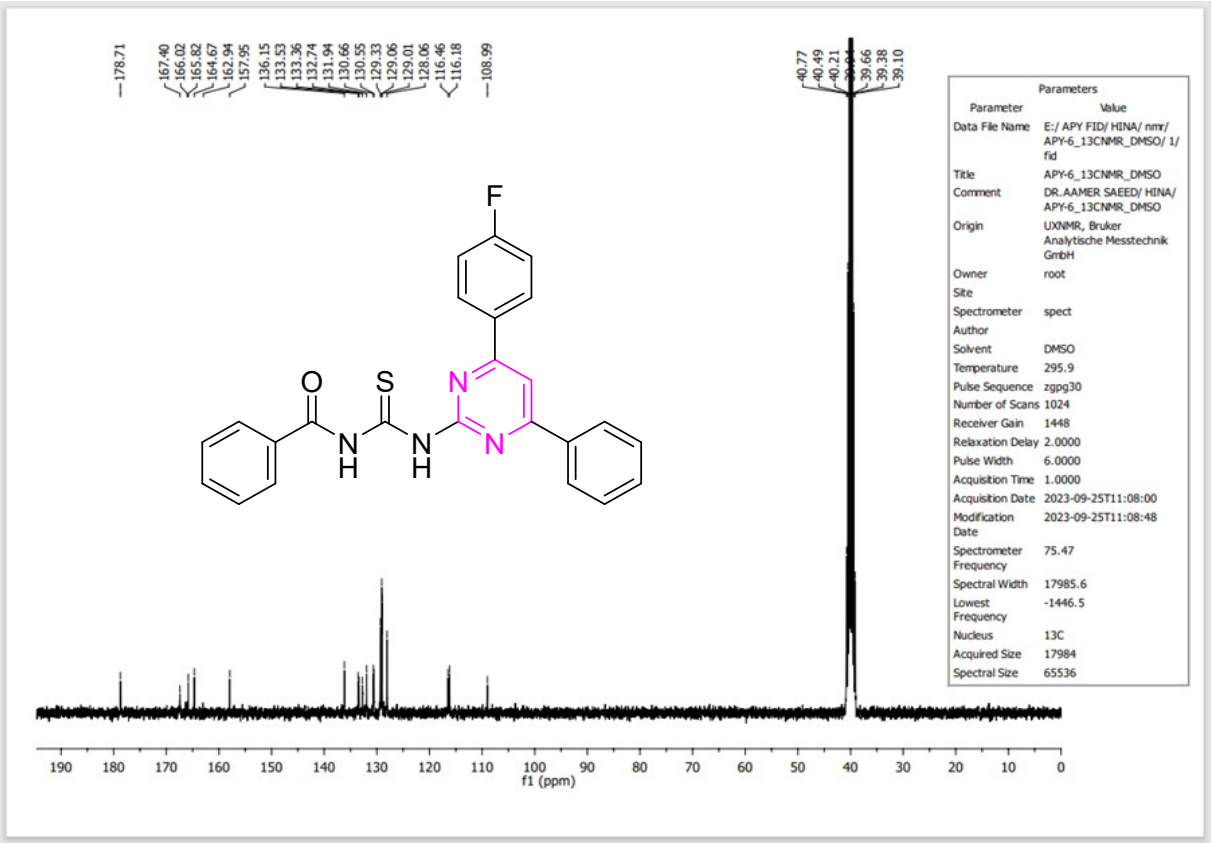


Figure 13. ^{1}H-NMR Spectrum of compound **(6e)**



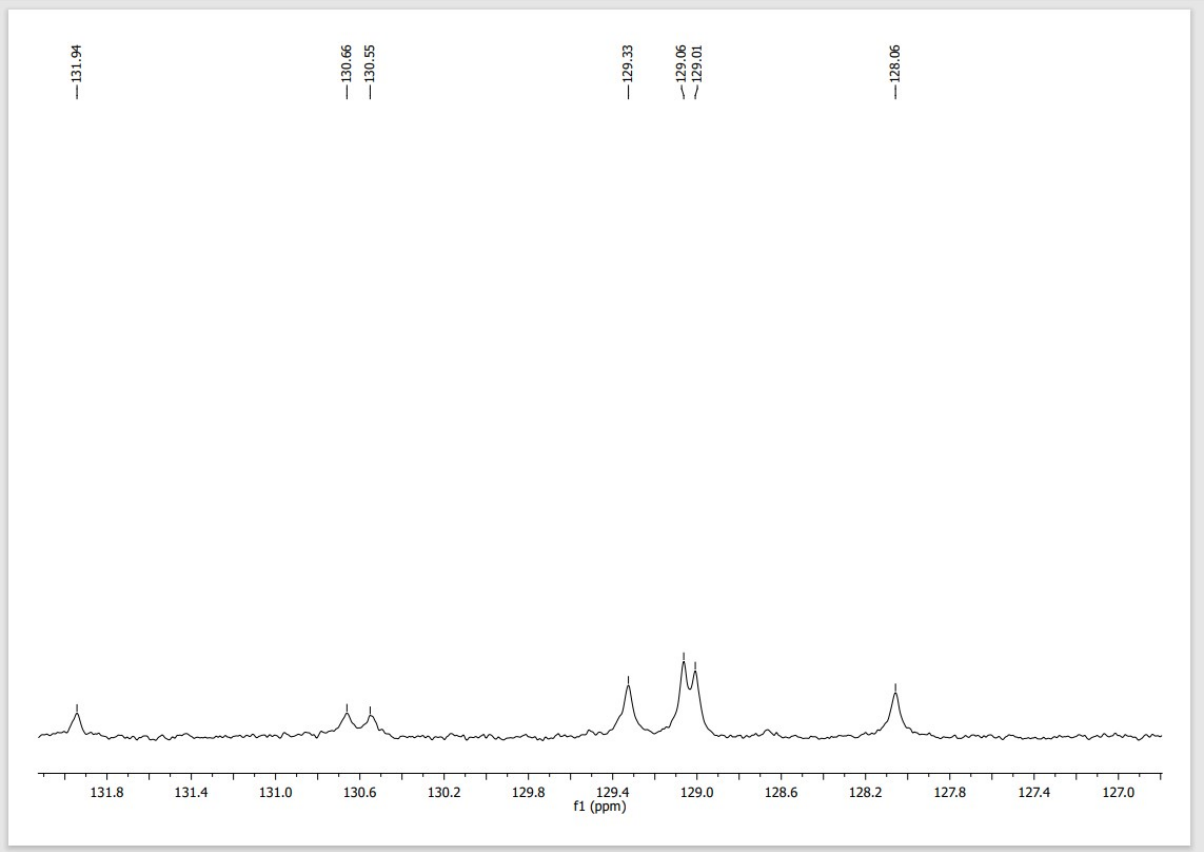


Figure 14. ^{13}C-NMR Spectrum of compound **(6e)**

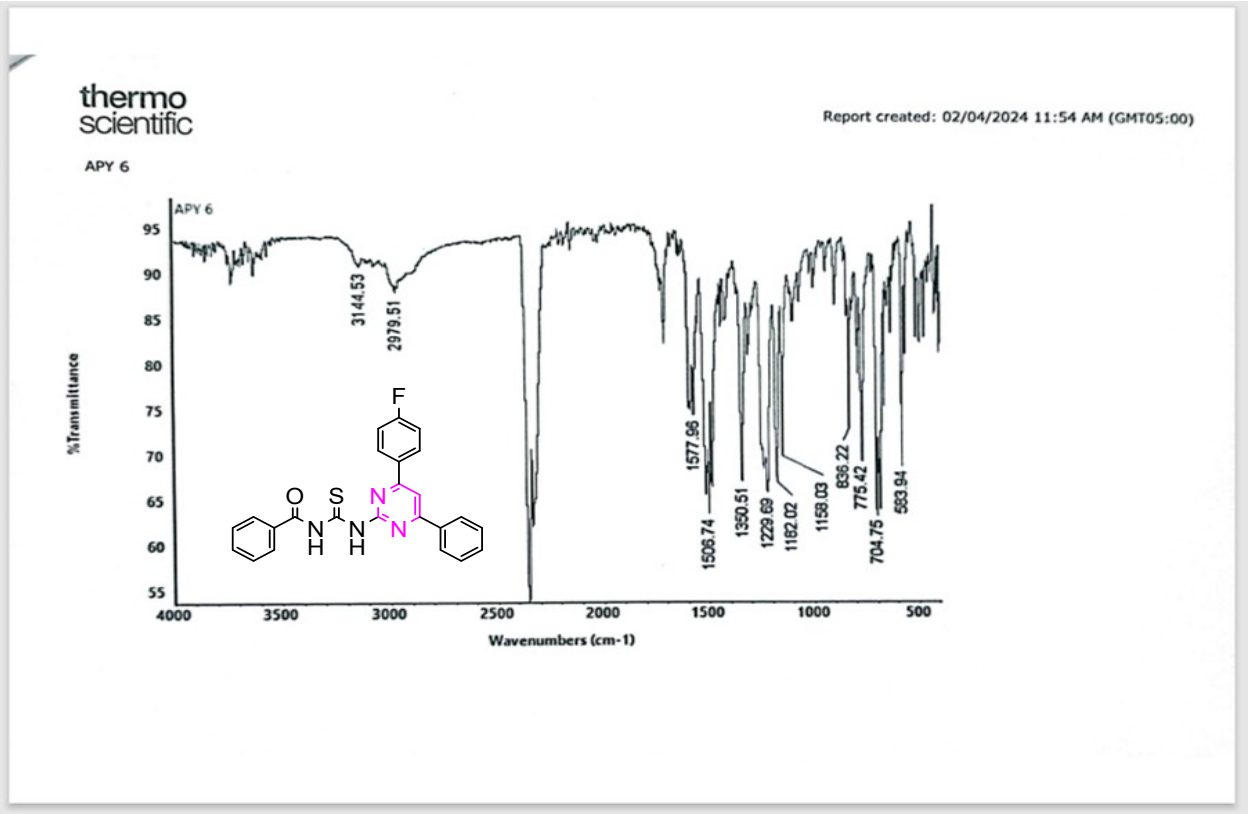
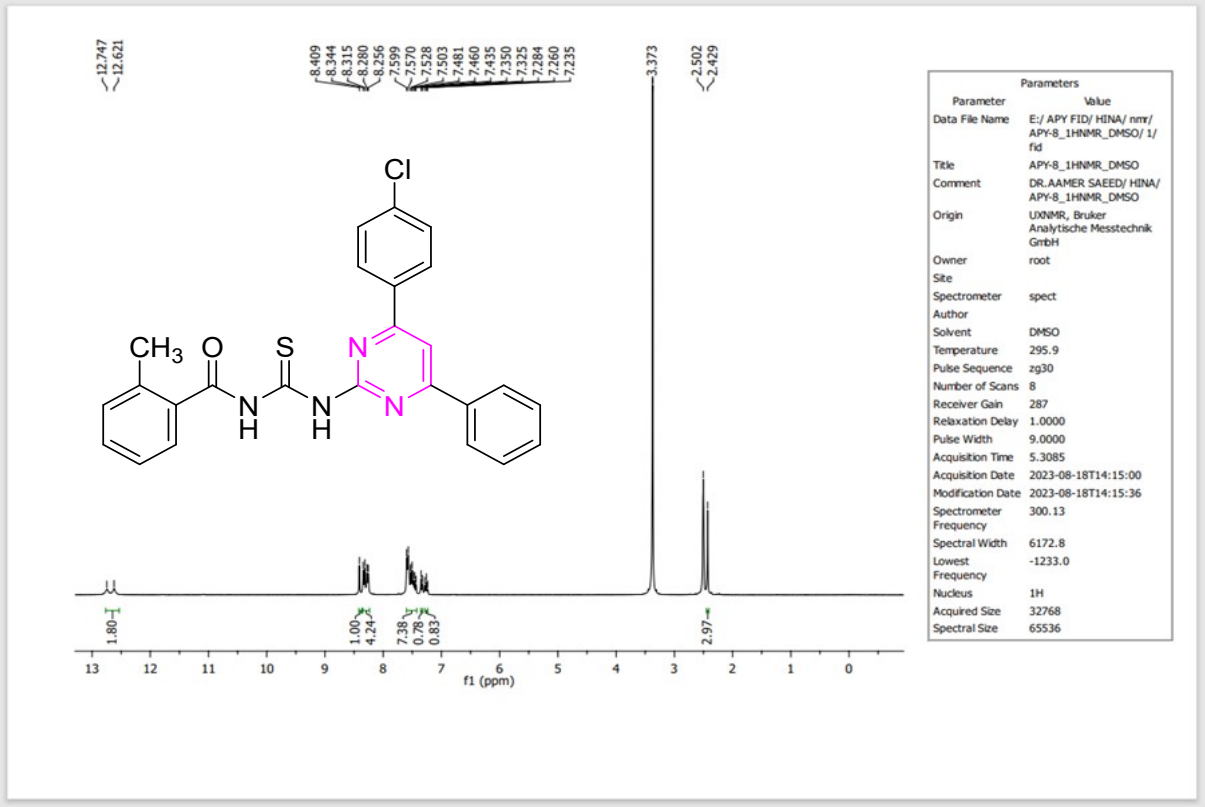


Figure 15. FT-IR Spectrum of compound **(6e)**



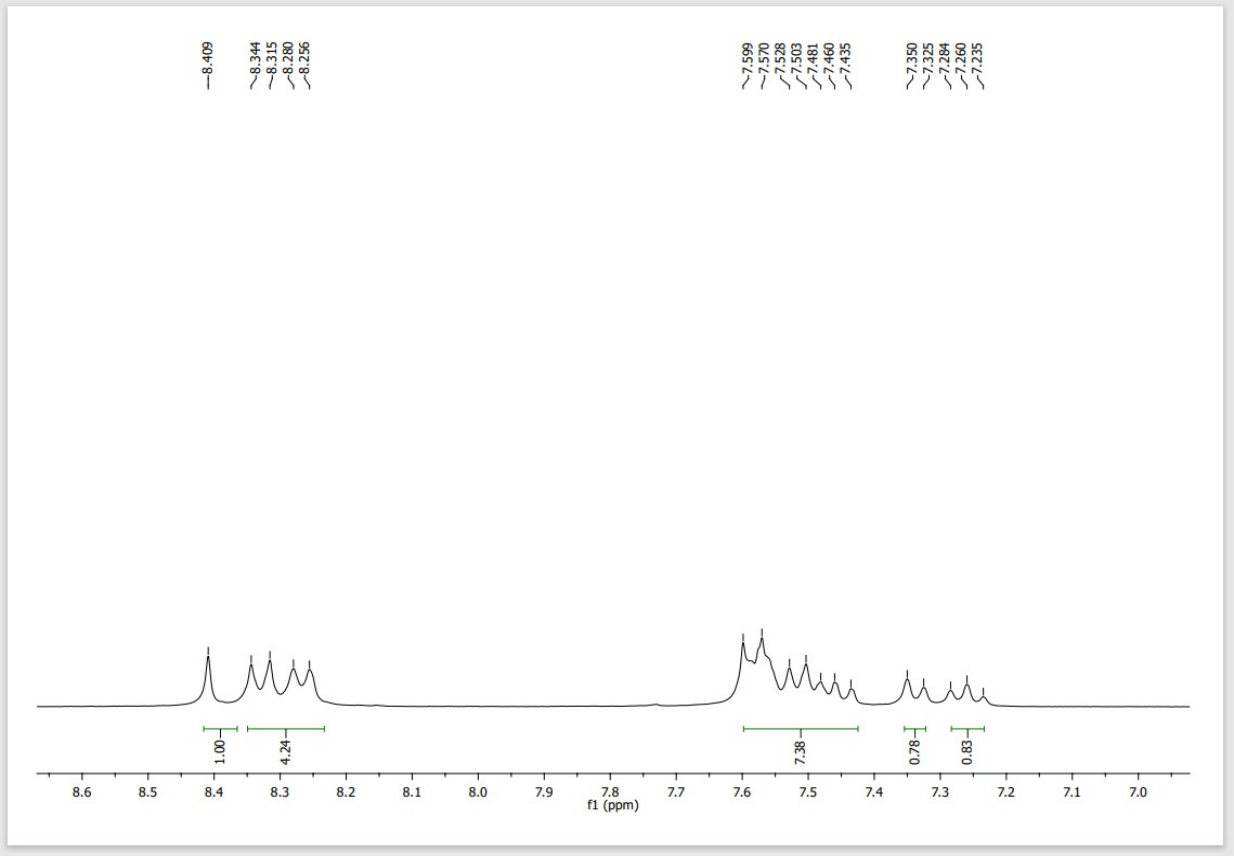
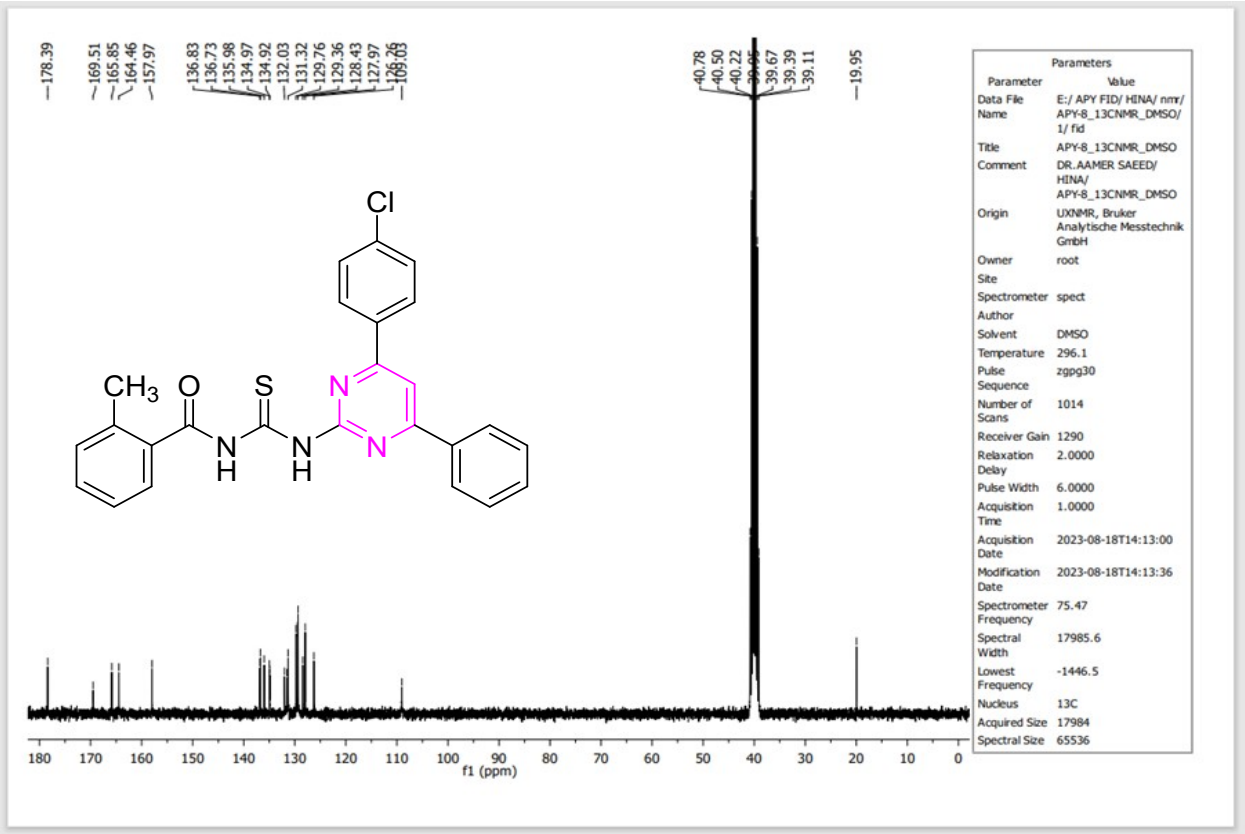


Figure 16. ^{1}H-NMR Spectrum of compound **(6f)**



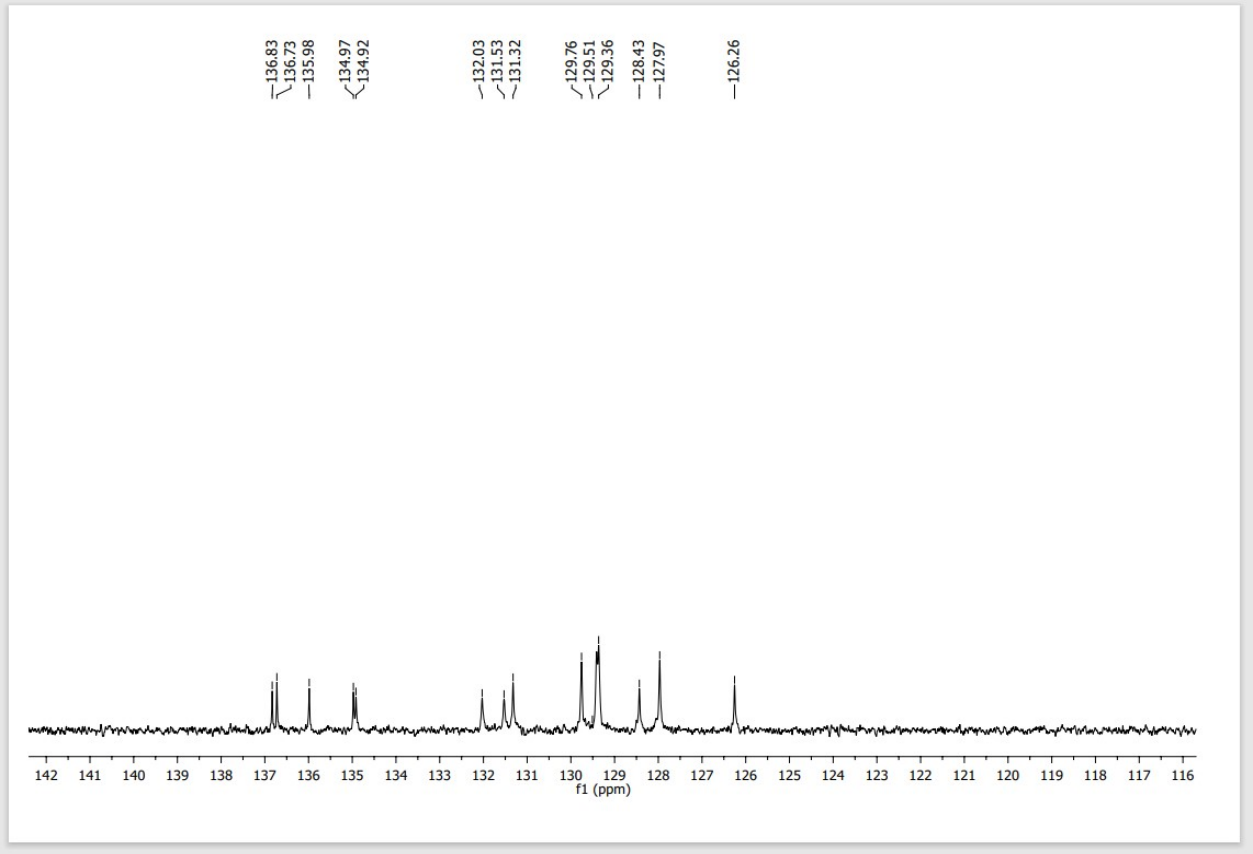


Figure 17.[13]C-NMR Spectrum of compound **(6f)**

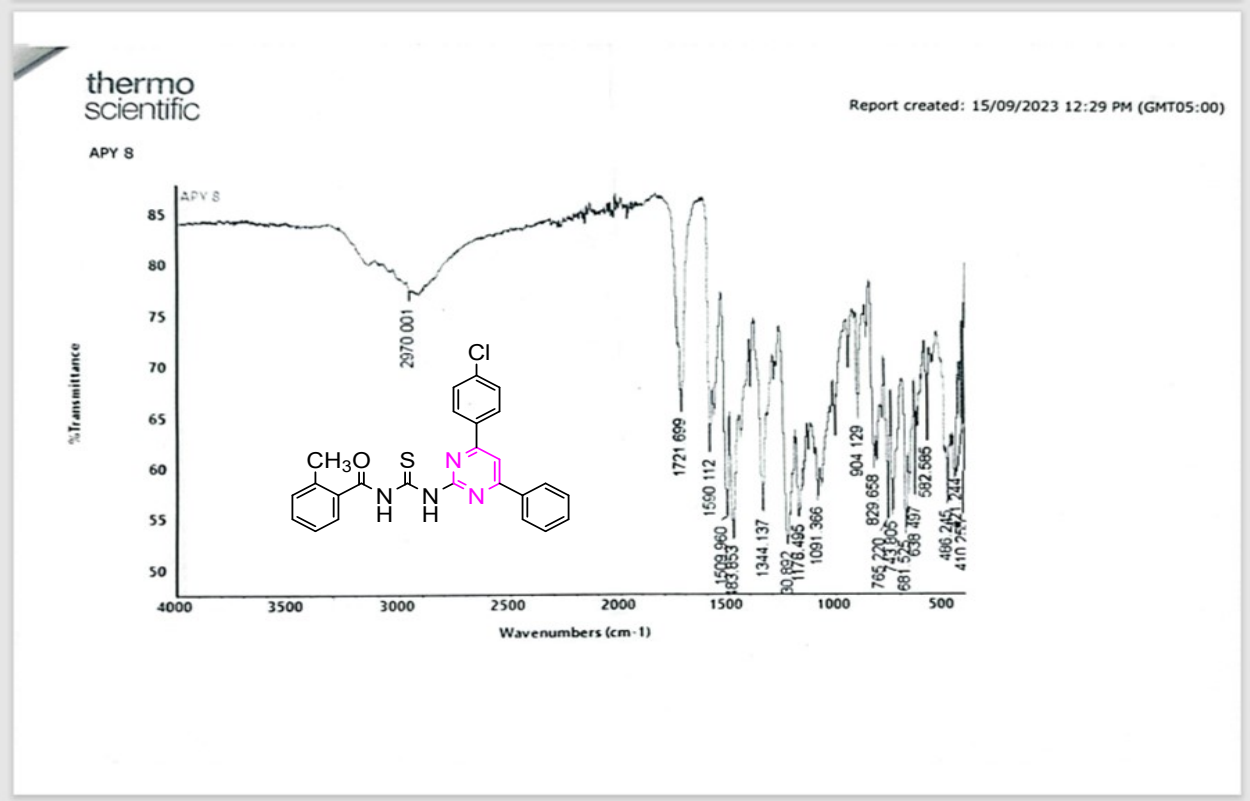
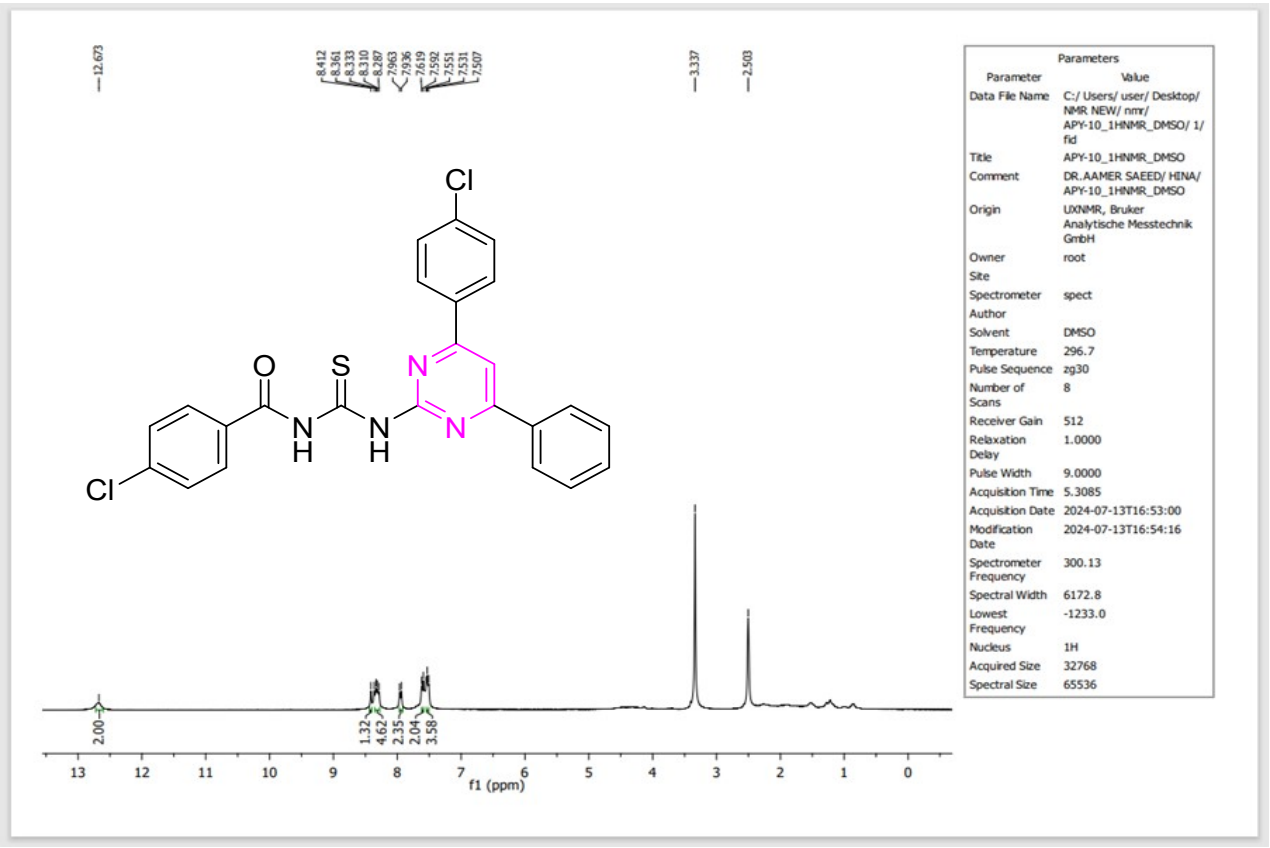


Figure 18. FT-IR Spectrum of compound **(6f)**



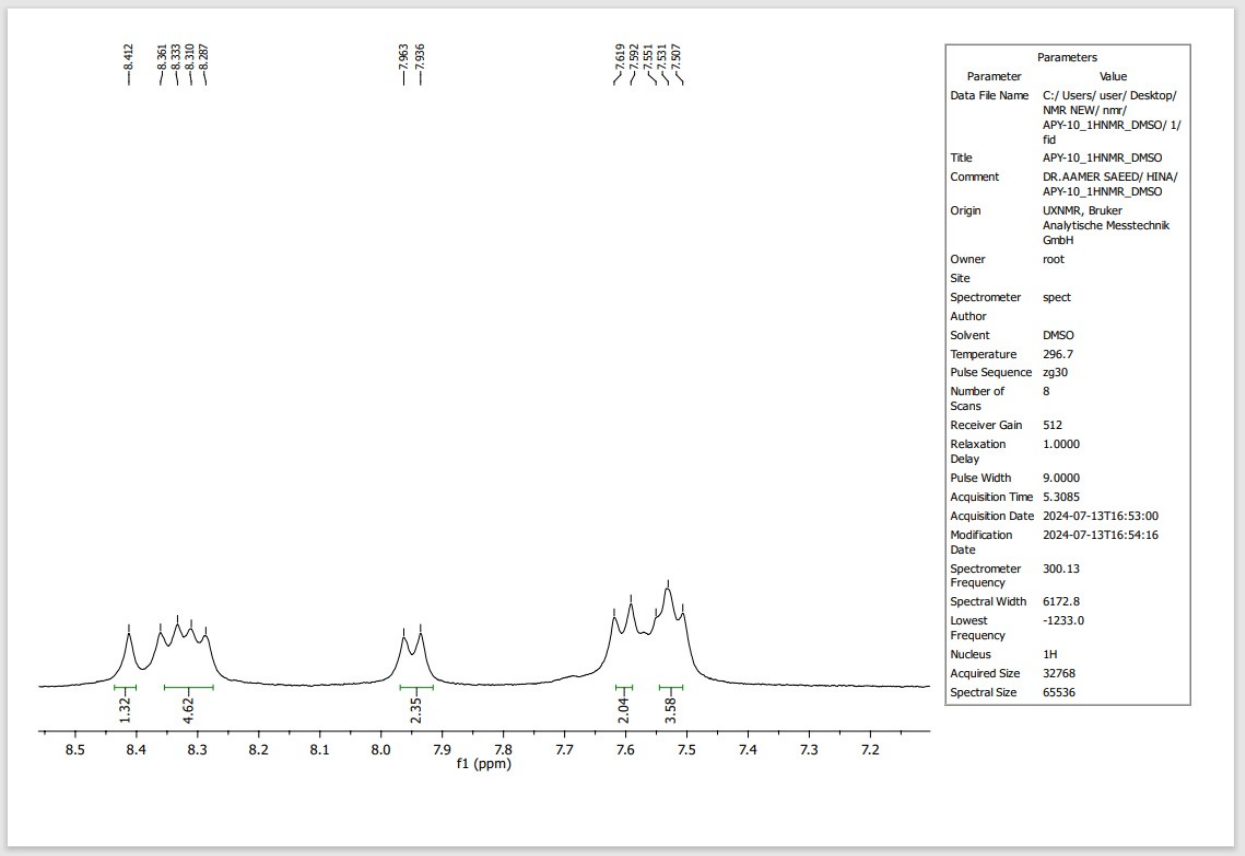


Figure 19. ^{1}H-NMR Spectrum of compound (**6g)**

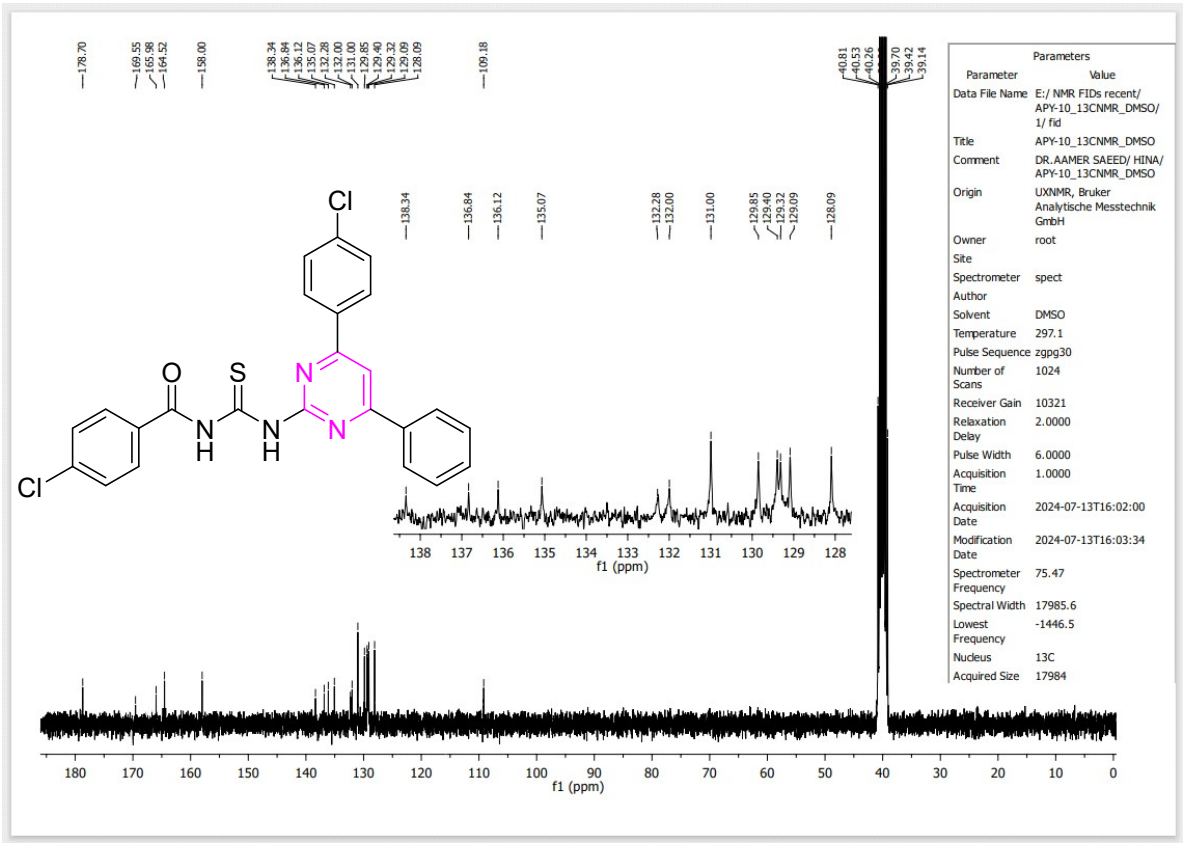


Figure 20.[13]C-NMR Spectrum of compound **(6g)**

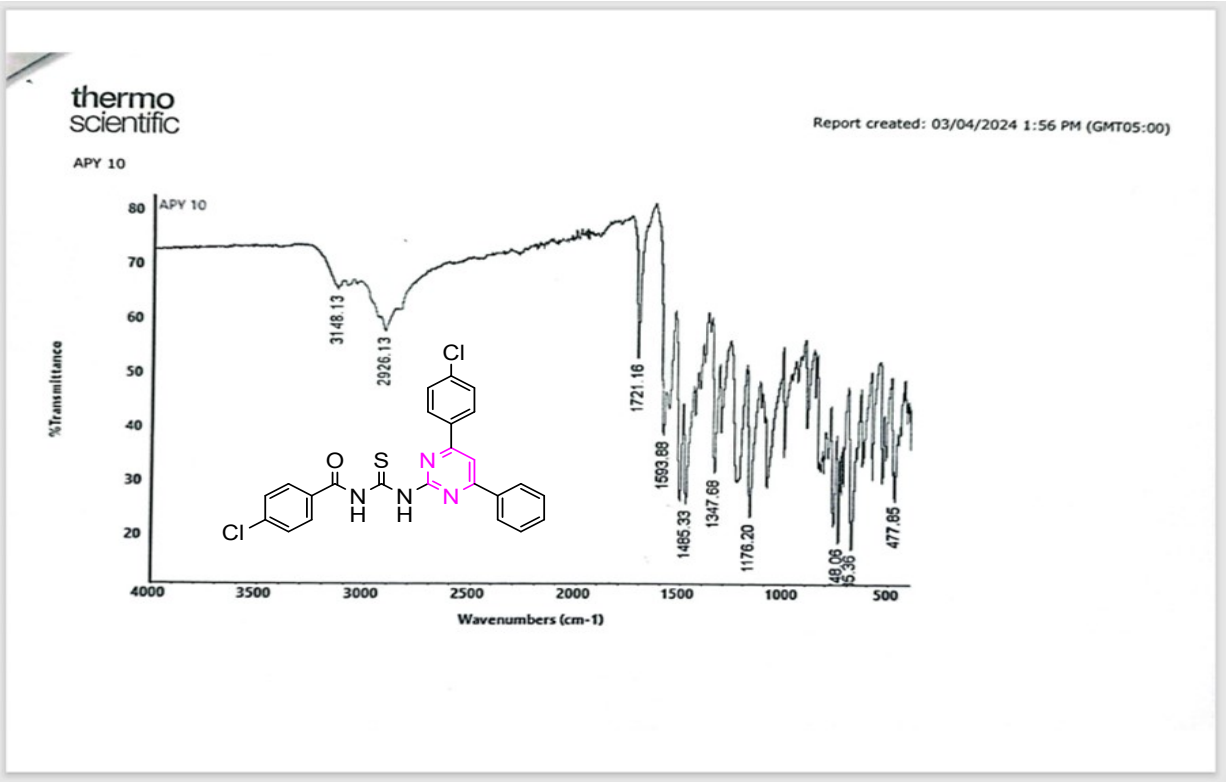
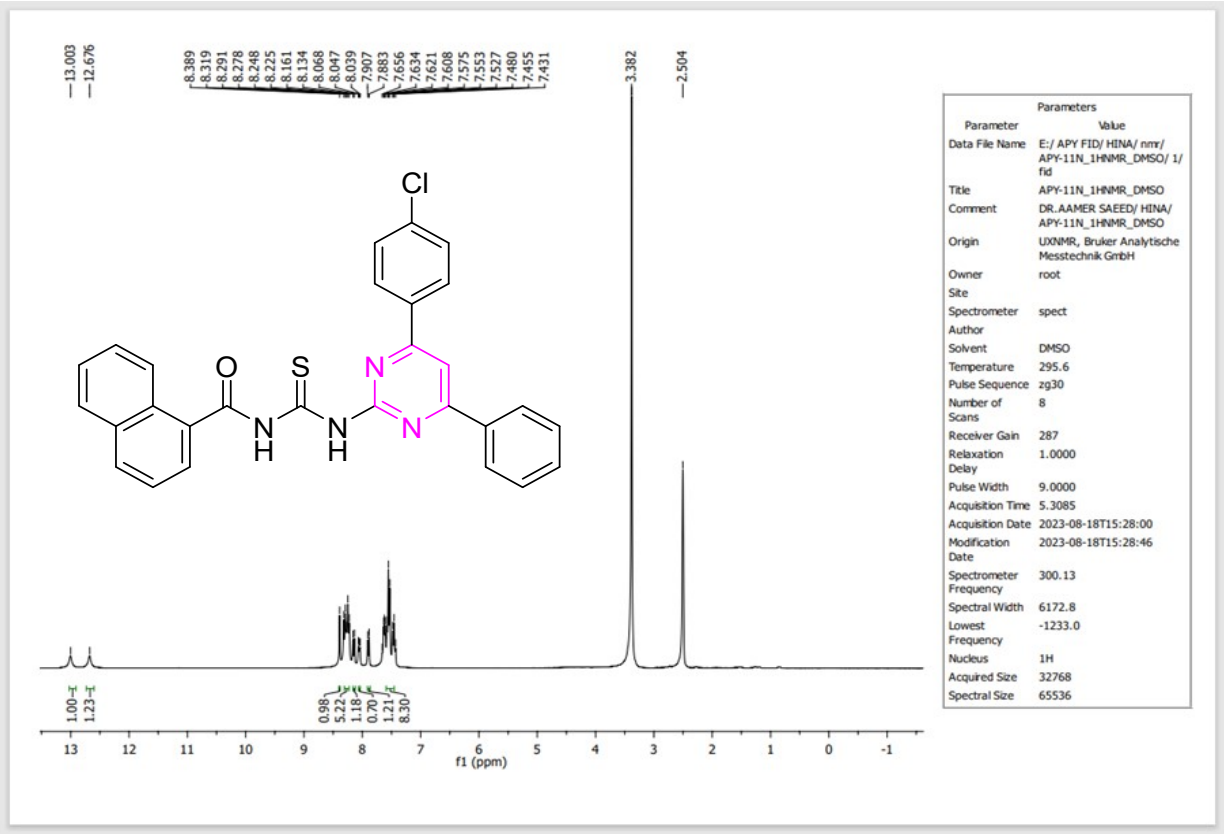


Figure 21. FT-IR Spectrum of compound **(6g)**



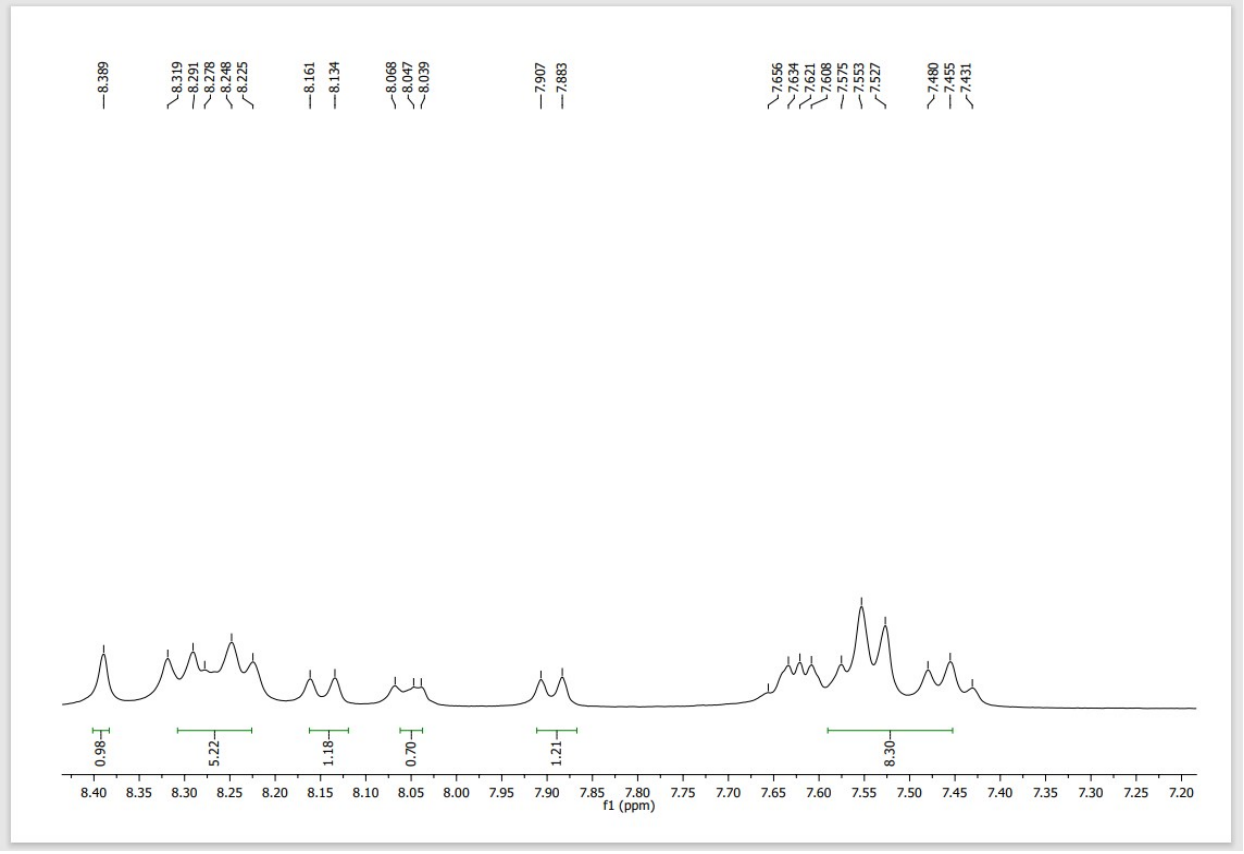
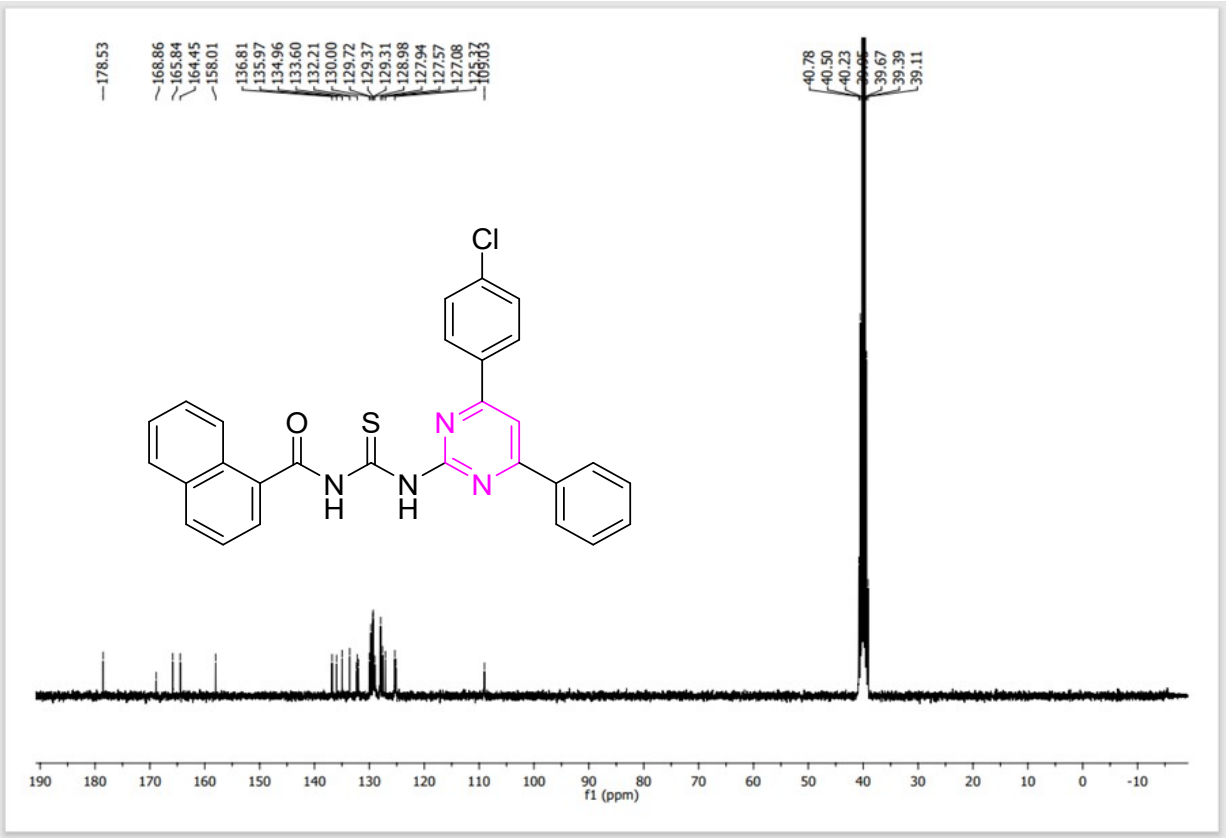


Figure 22. [1]H-NMR Spectrum of compound **(6h)**



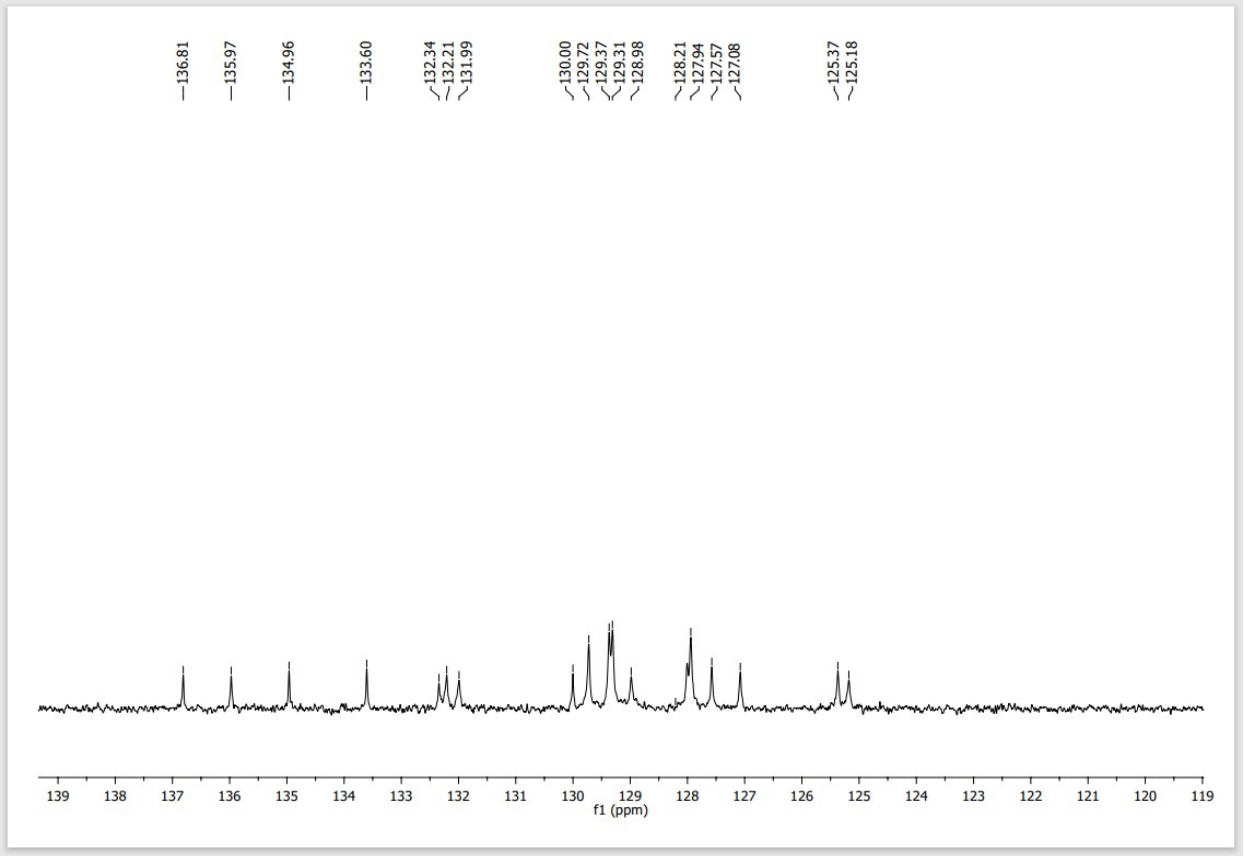


Figure 23. ^{13}C-NMR Spectrum of compound **(6h)**

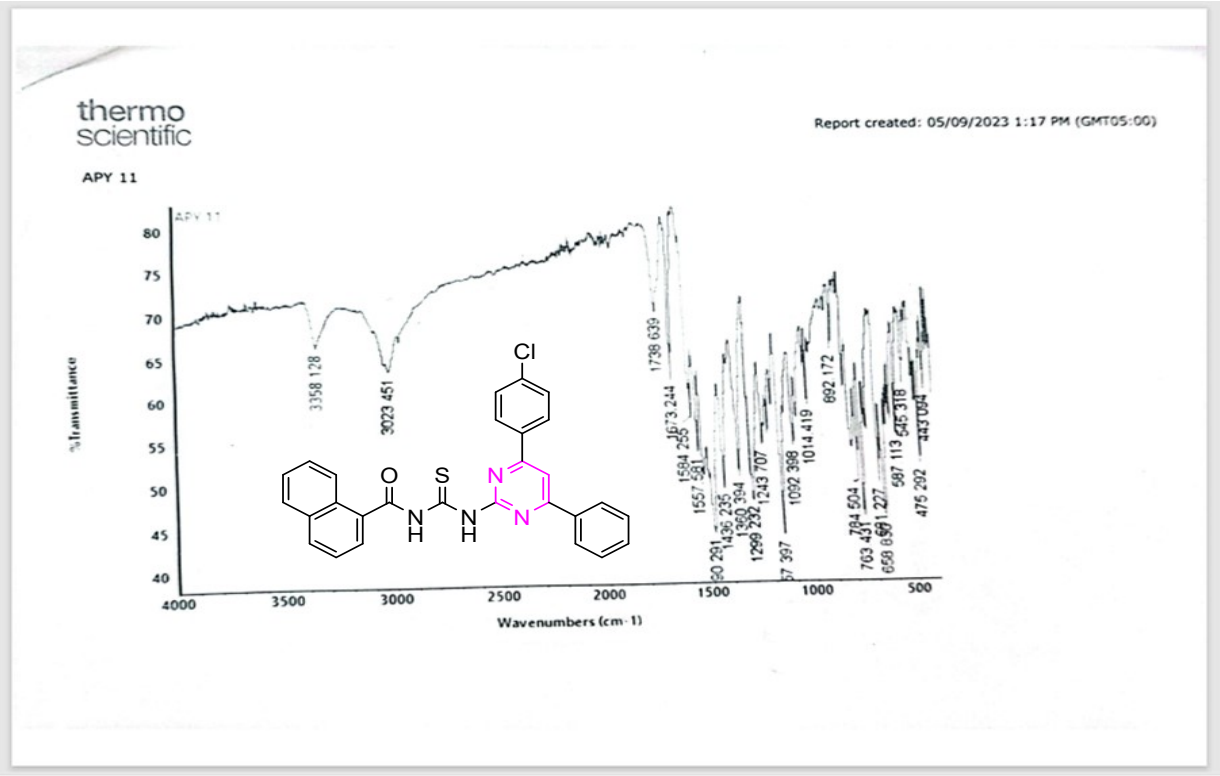


Figure 24. FT-IR Spectrum of compound **(6h)**

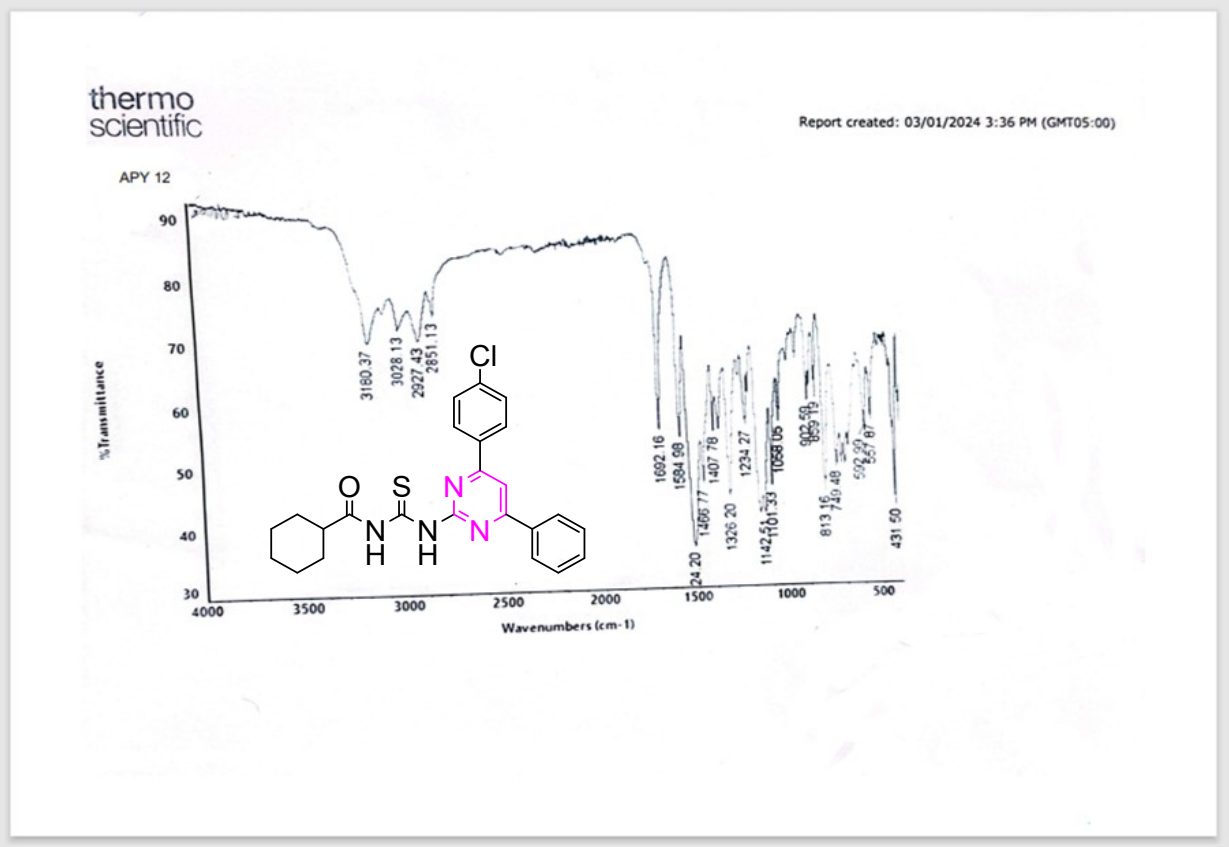


Figure 25. FT-IR Spectrum of compound **(6i)**

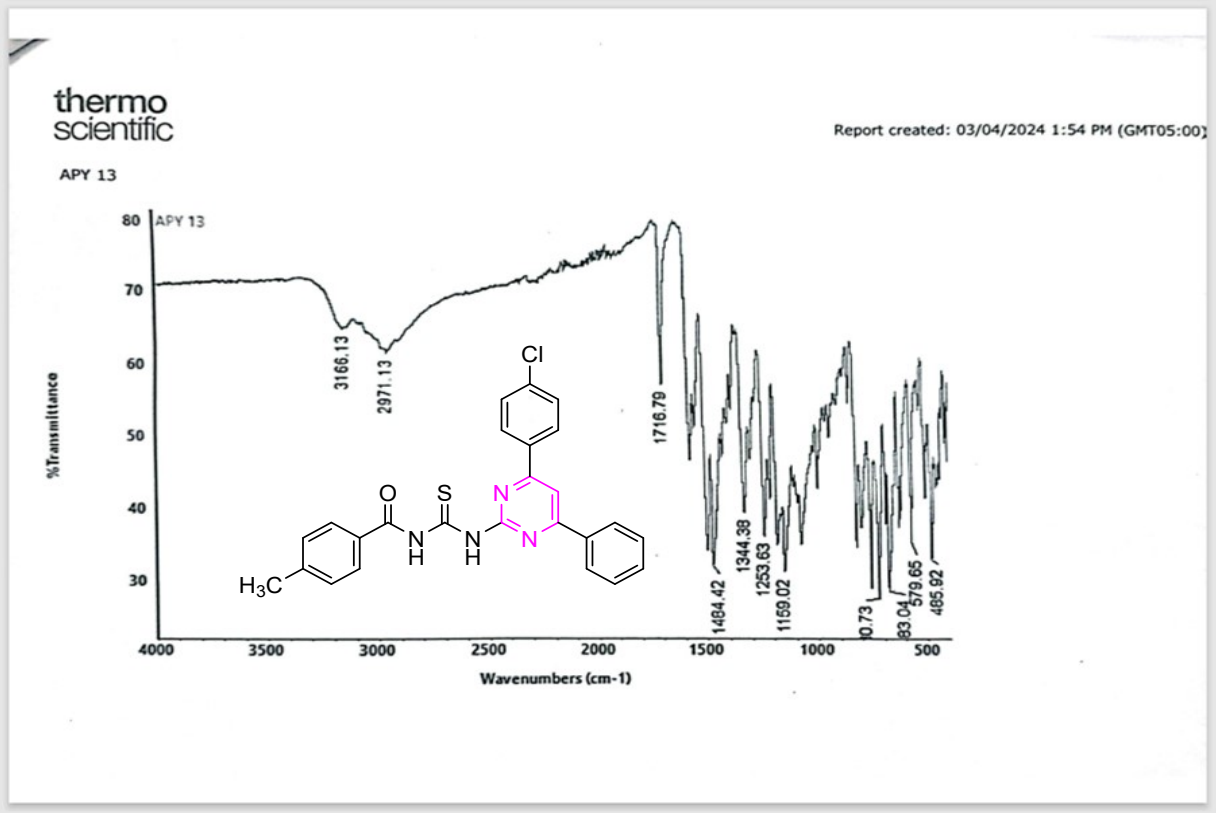


Figure 26. FT-IR Spectrum of compound **(6j)**

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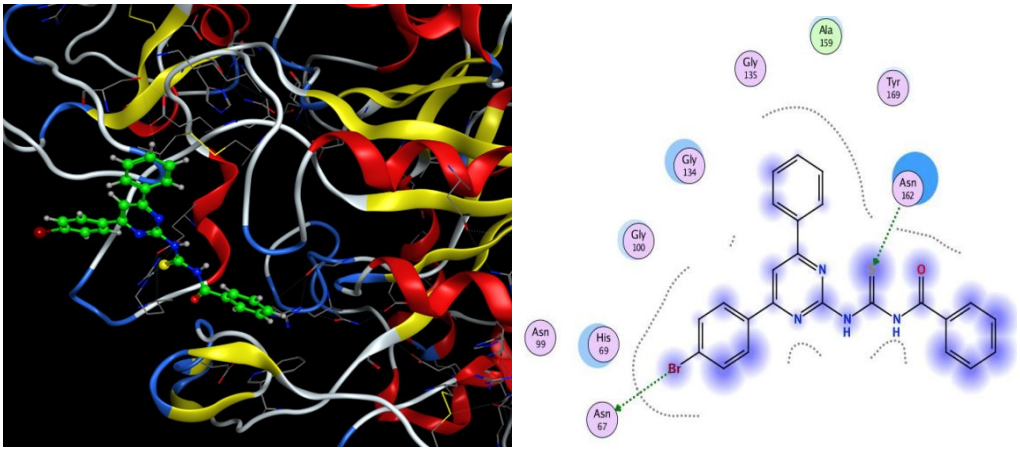
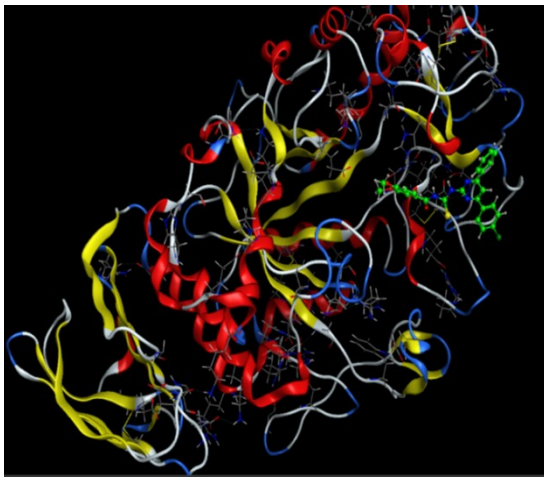
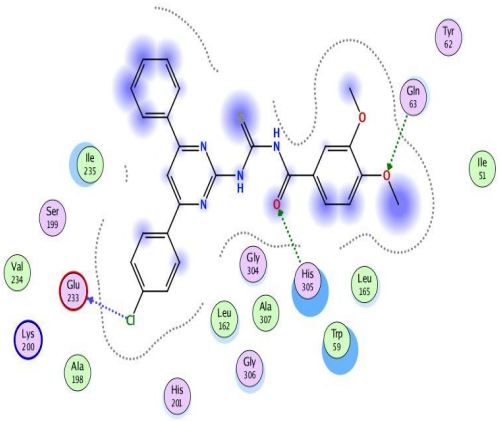


6b

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Gln 63
Ile 51
Ile 235
Ser 199
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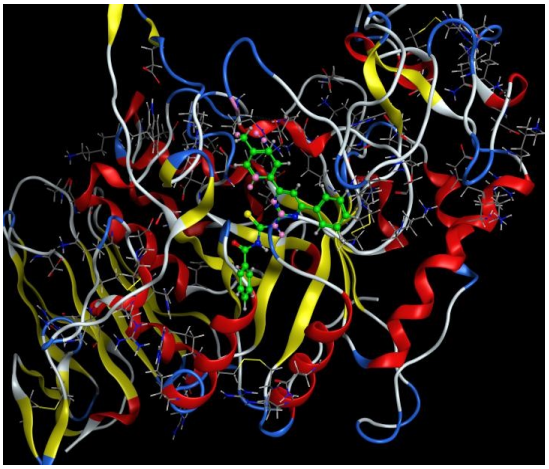
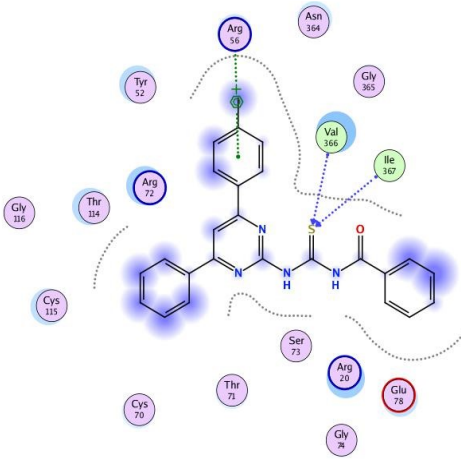
His 201

6c

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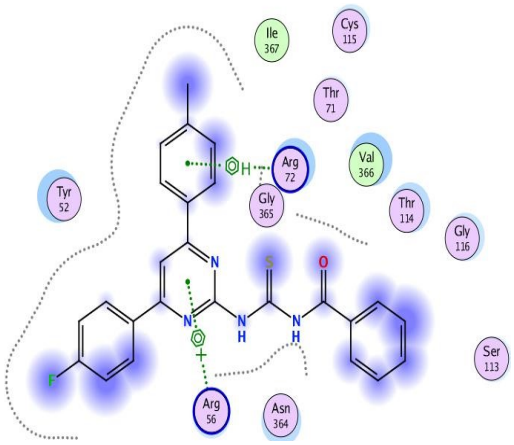
Gly 74

6d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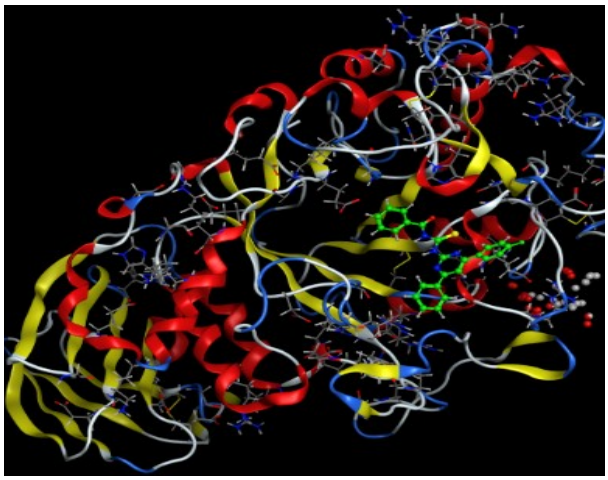
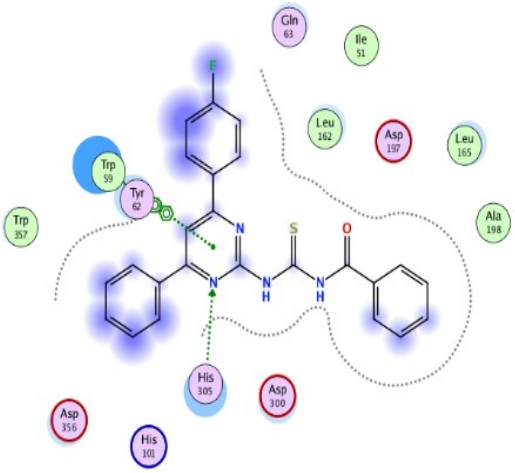
6e

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Asp 197
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Trp 59
Tyr 62
Trp 357
Ala 198
His 305
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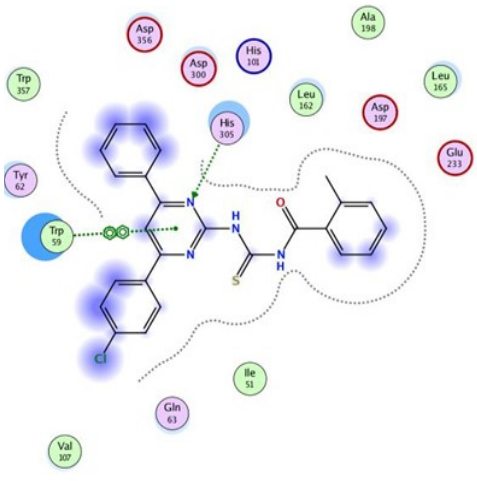
His 101

6f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Asp 300
His 101
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His 305
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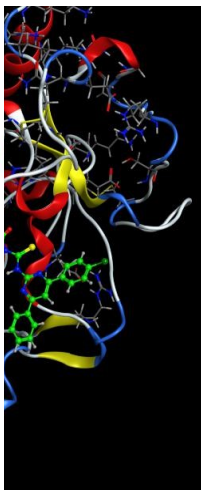
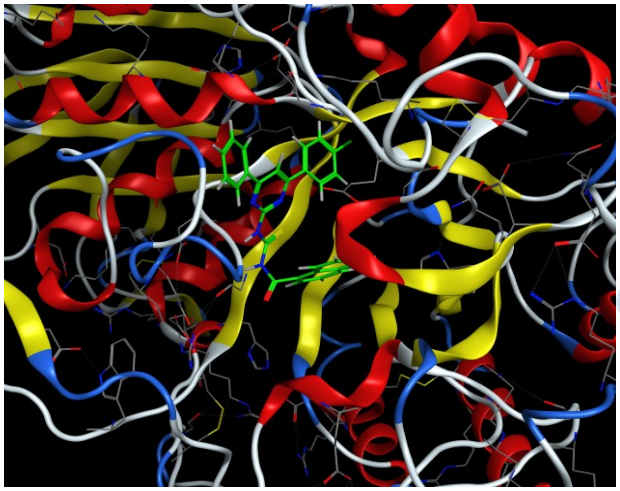
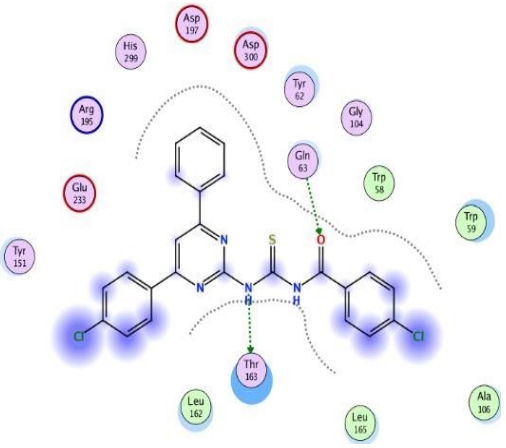


6g

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Leu 165
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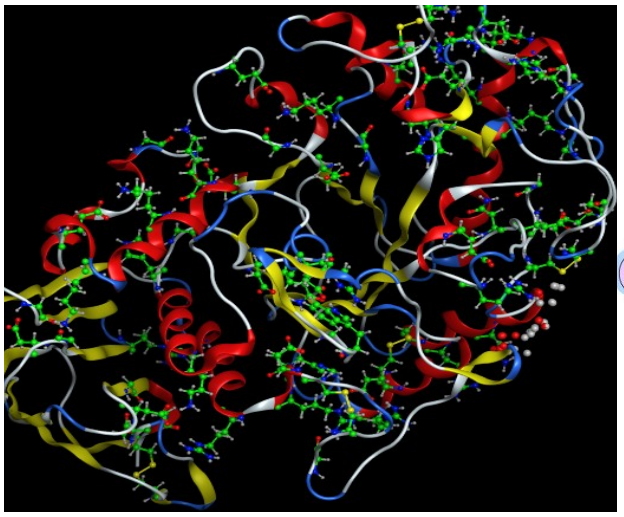
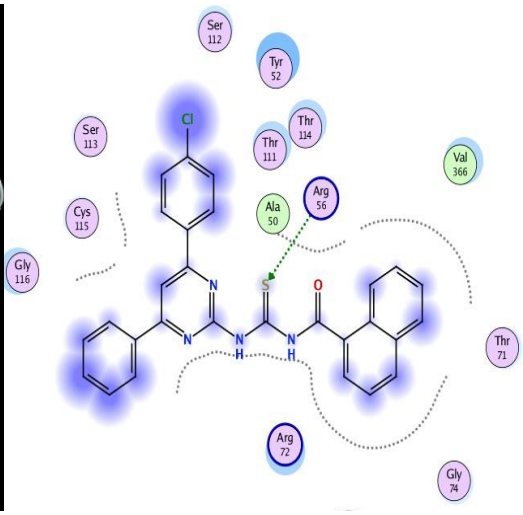
6h

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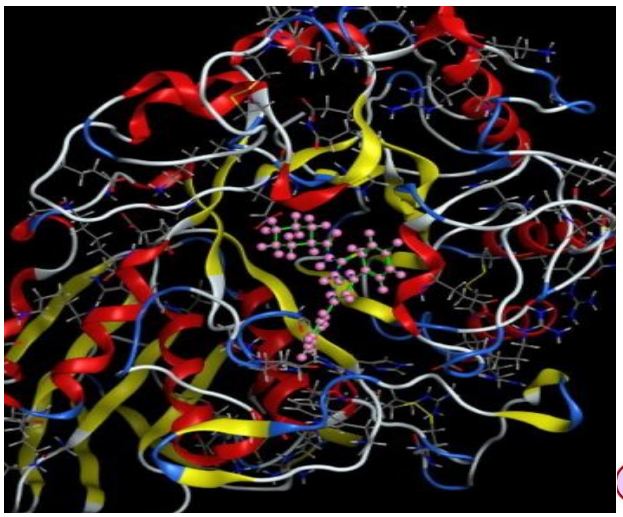
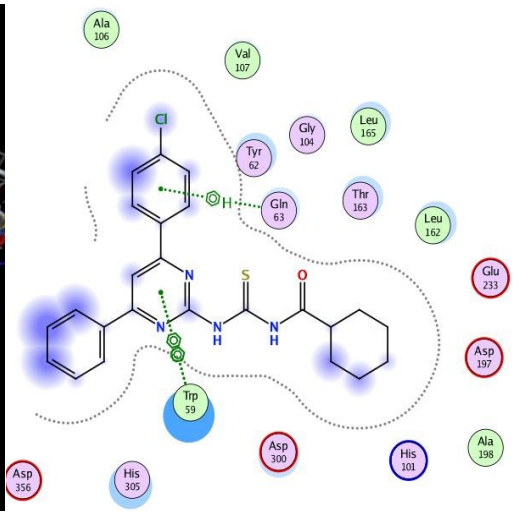
6i

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Gly 104
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Trp 59
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His 101
Ala 198
Asp 356
His 305

6j

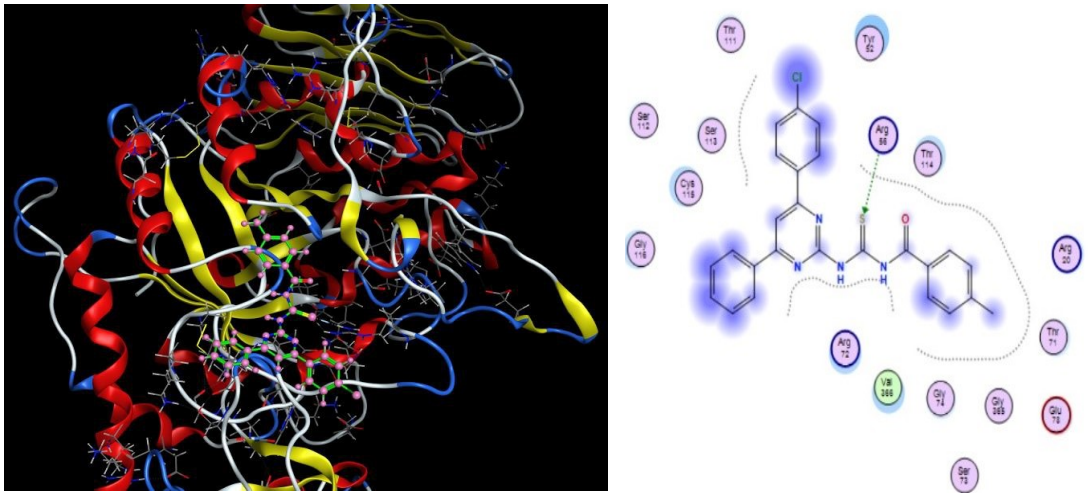
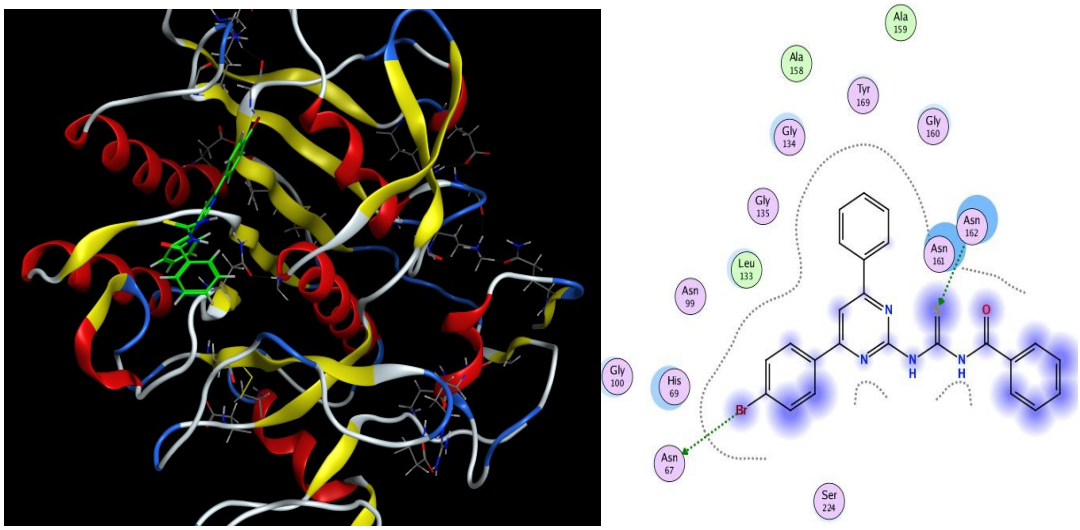
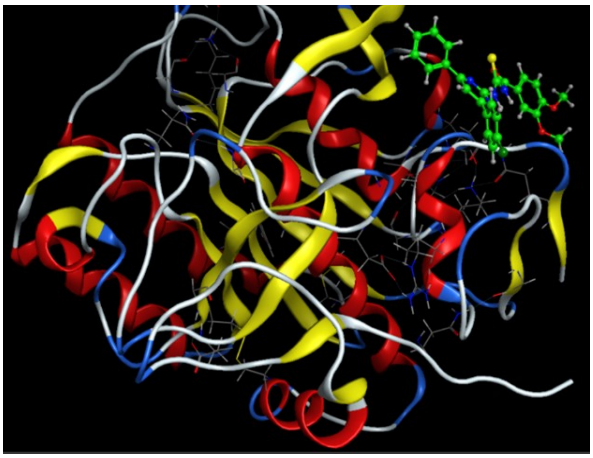


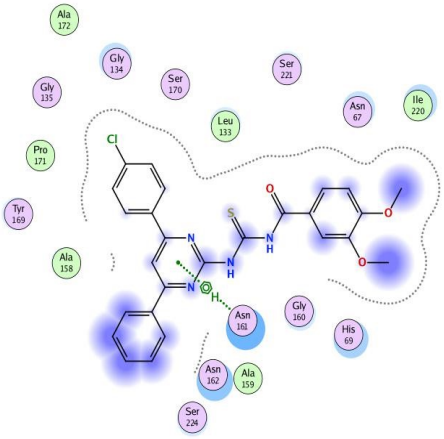
Fig 27. 3D docking pose and 2D binding interaction of the synthesized compounds (**6a-j**) in the binding pocket of *α*-amylase

6a

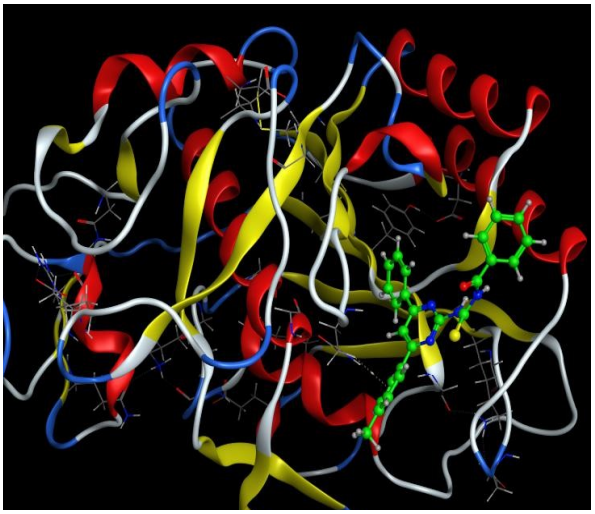


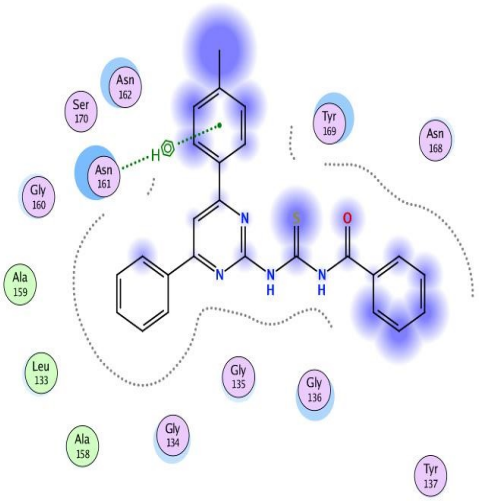
6b



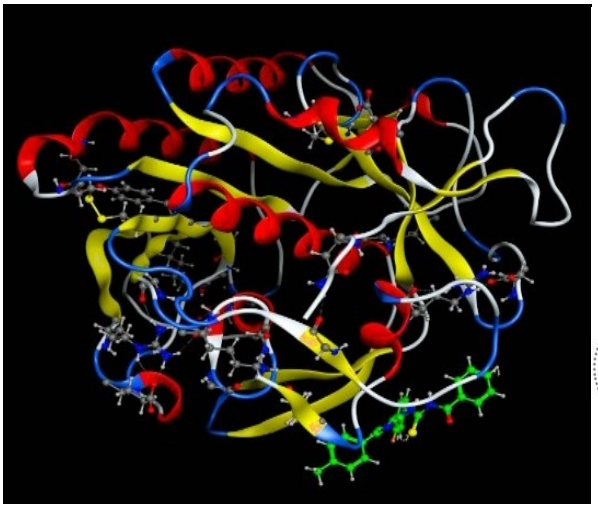

Ala 172
Gly 134
Ser 170
Ser 221
Gly 135
Asn 67
Ile 220
Leu 133
Pro 171
Cl
Tyr 169
Ala 158
Gly 160
Asn 161
His 69
Asn 162
Ala 159
Ser 224

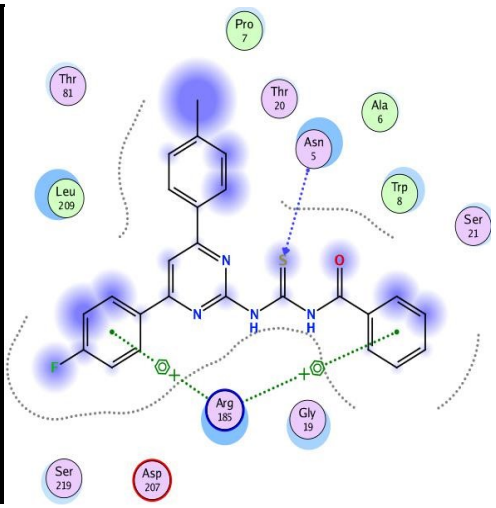
6c



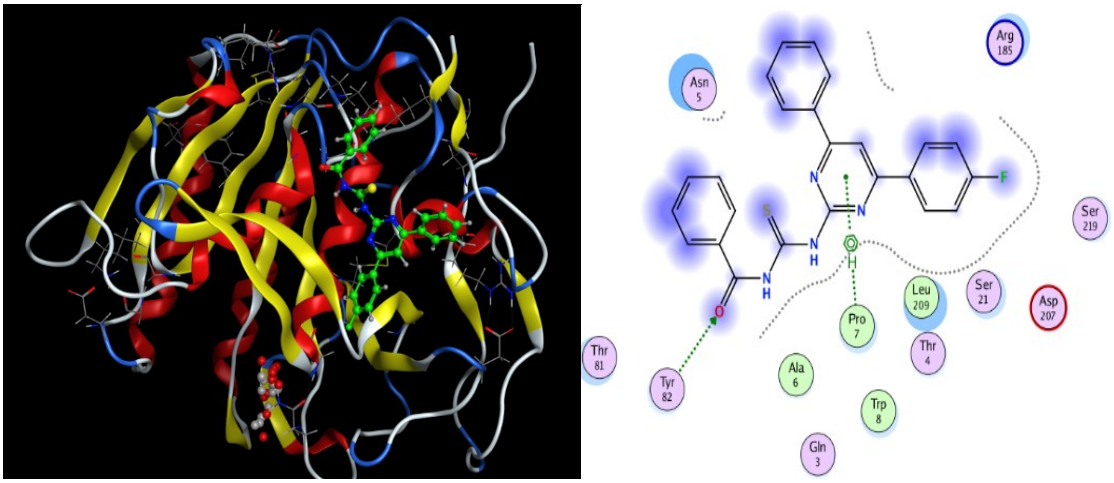

Asn 162
Ser 170
Tyr 169
Asn 168
Asn 161
Gly 160
Ala 159
Leu 133
Gly 135
Gly 136
Gly 134
Ala 158
Tyr 137

6d

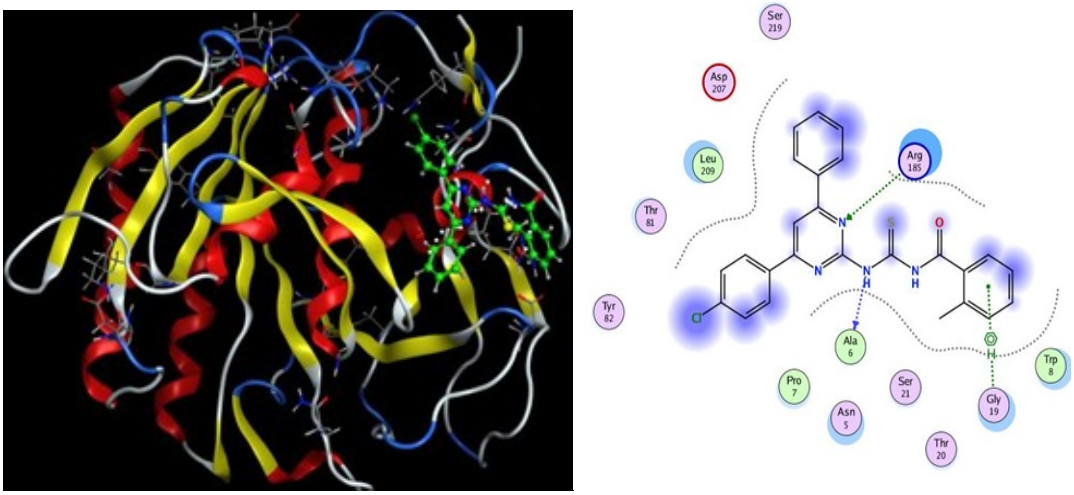



Pro 7
Thr 81
Thr 20
Ala 6
Asn 5
Leu 209
Trp 8
Ser 21
F
Arg 185
Gly 19
Ser 219
Asp 207

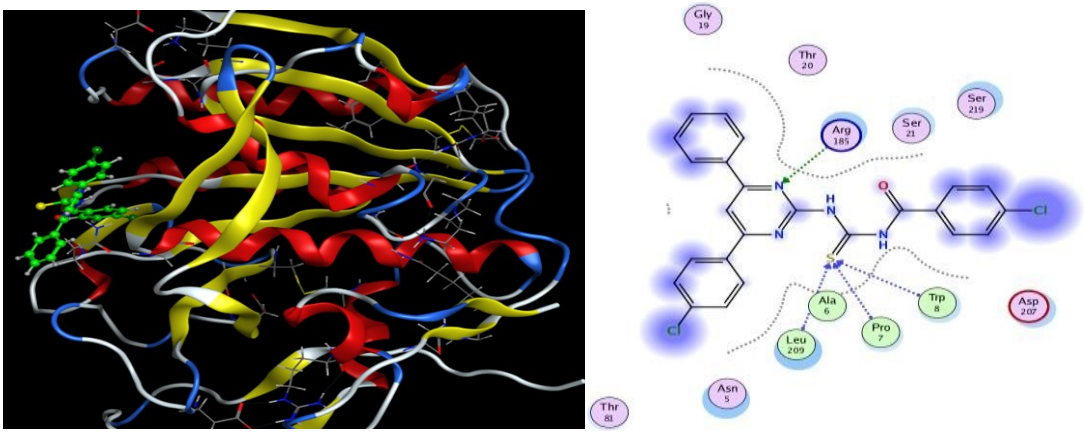
6e


Arg 185
Asn 5
Ser 219
Leu 209
Ser 21
Asp 207
Pro 7
Thr 4
Thr 81
Ala 6
Tyr 82
Trp 8
Gln 3

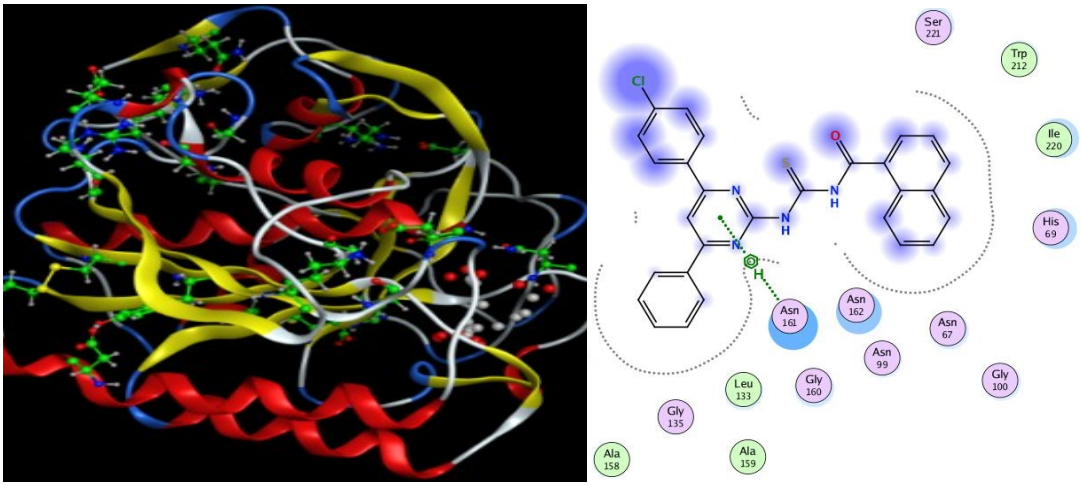
6f


Ser 219
Asp 207
Leu 209
Arg 185
Thr 81
Tyr 82
Ala 6
Trp 8
Pro 7
Ser 21
Gly 19
Asn 5
Thr 20

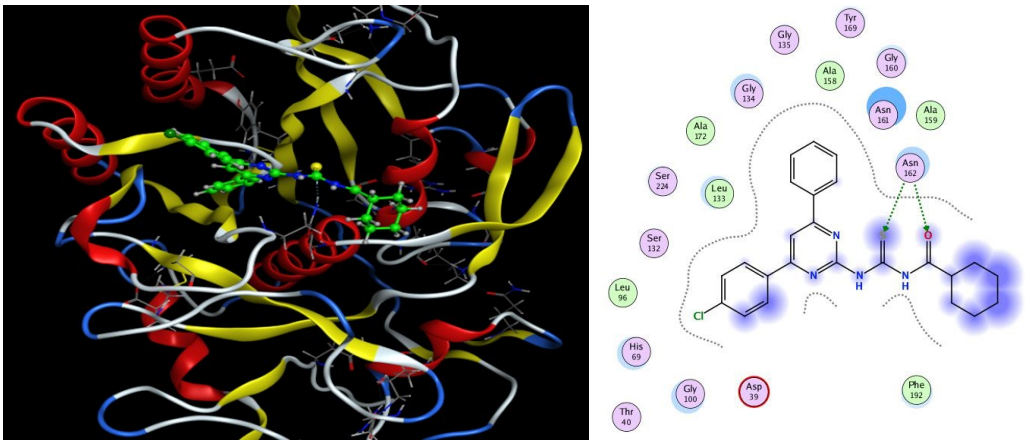
6g


Gly 19
Thr 20
Ser 219
Arg 185
Ser 21
Ala 6
Trp 8
Asp 207
Pro 7
Leu 209
Asn 5
Thr 81

6h



6i



6j

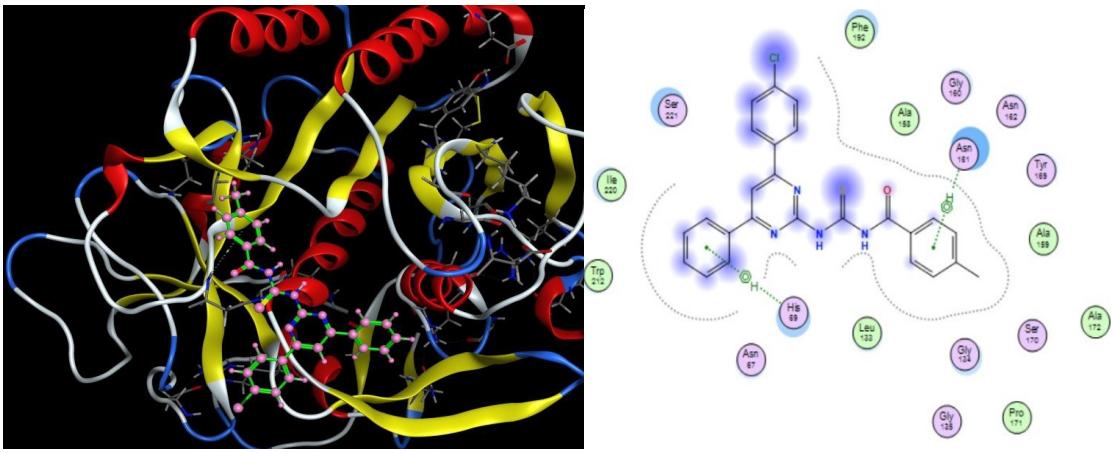


Fig 28. 3D docking pose and 2D binding interaction of the synthesized compounds (**6a-j**) in the binding pocket of Proteinase K