

Novel Pyrazoline linked acyl thiourea pharmacophores: Design synthesis, antimicrobial, urease, amylase and α -glucosidase inhibition, SAR and molecular docking study.

Aamer Saeed^a Atteeque Ahmed^a Main Bilal Haider^a, Hammad Ismail^b Khizar Hayat^c, Ghulam Shabir^a, Hesham R El-Seedi^{de}

^a Department of Chemistry, Quaid I Azam University, Islamabad, 45320, Pakistan.

^b Department of Biochemistry and Biotechnology, University of Gujrat, Gujrat, 50700, Pakistan

^c Department of Botany, University of Gujrat, Gujrat, 50700, Pakistan

^d International Research Centre for Food Nutrition and Safety, Jiangsu University, Zhenjiang 212013, China.

^e Department of Chemistry, Faculty of Science, Islamic University of Madinah, Madinah, 42351, Saudi Arabia

Correspondence

Prof. Dr. Aamer Saeed

Email: asaheed@qau.edu.pk; ORCID: <http://orcid.org/0000-0002-7112-9296>

Contact number: +92-51-9064-2128, Fax: +92-51-9064-2241

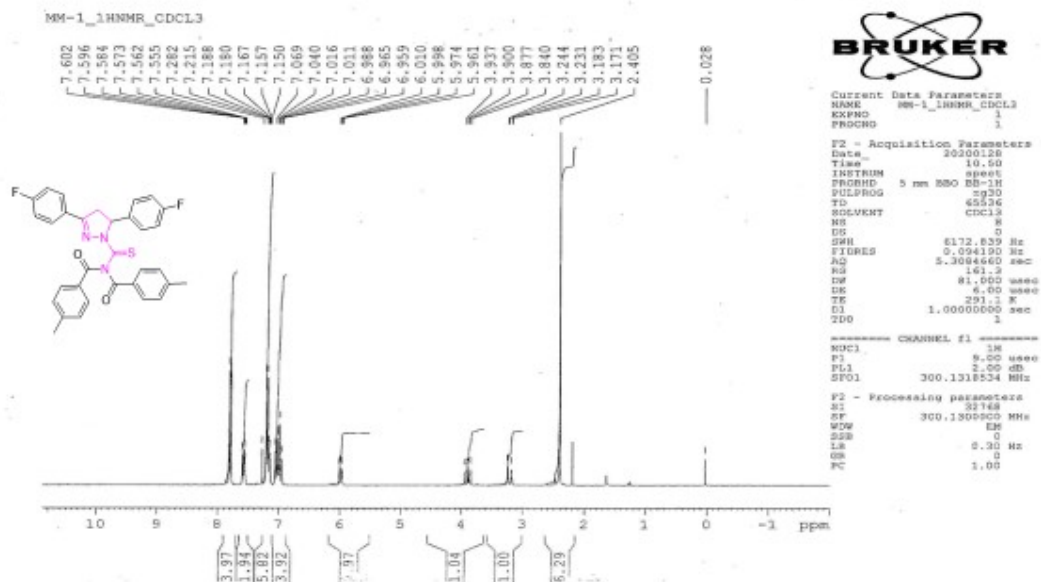
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Figure 1. $^1\text{H-NMR}$ Spectrum of **5a**

***N*-(3,5-bis(4-fluorophenyl)-4,5-dihydro-1*H*-pyrazole-1-carbonothioyl)-4-methyl-*N*-(4-methylbenzoyl)benzamide (**5a**):**



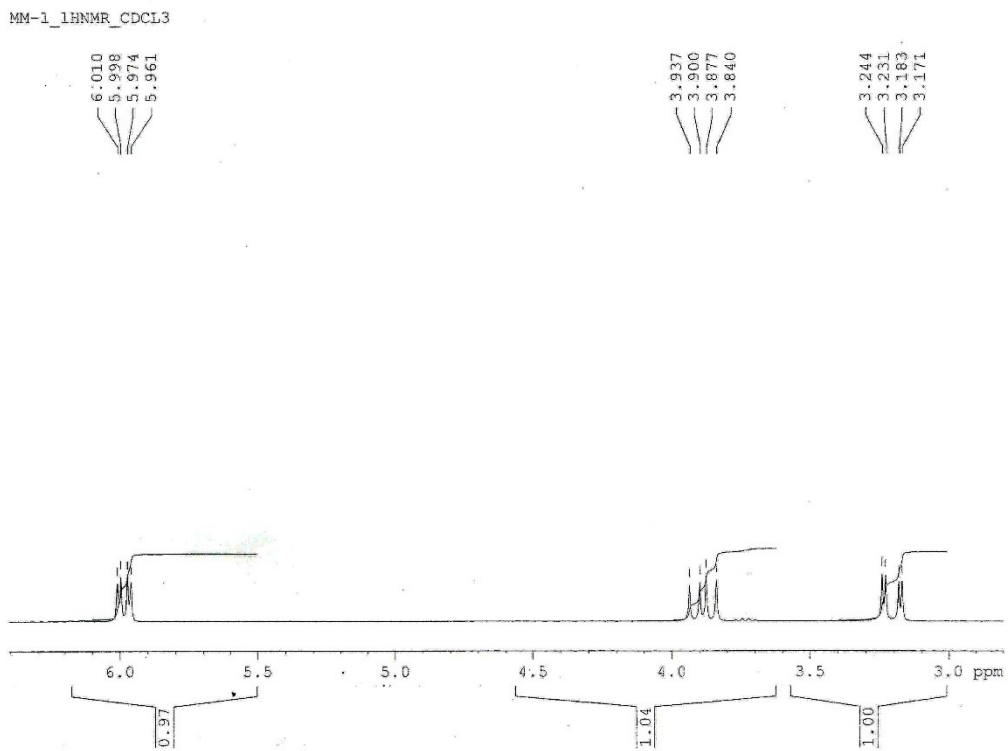
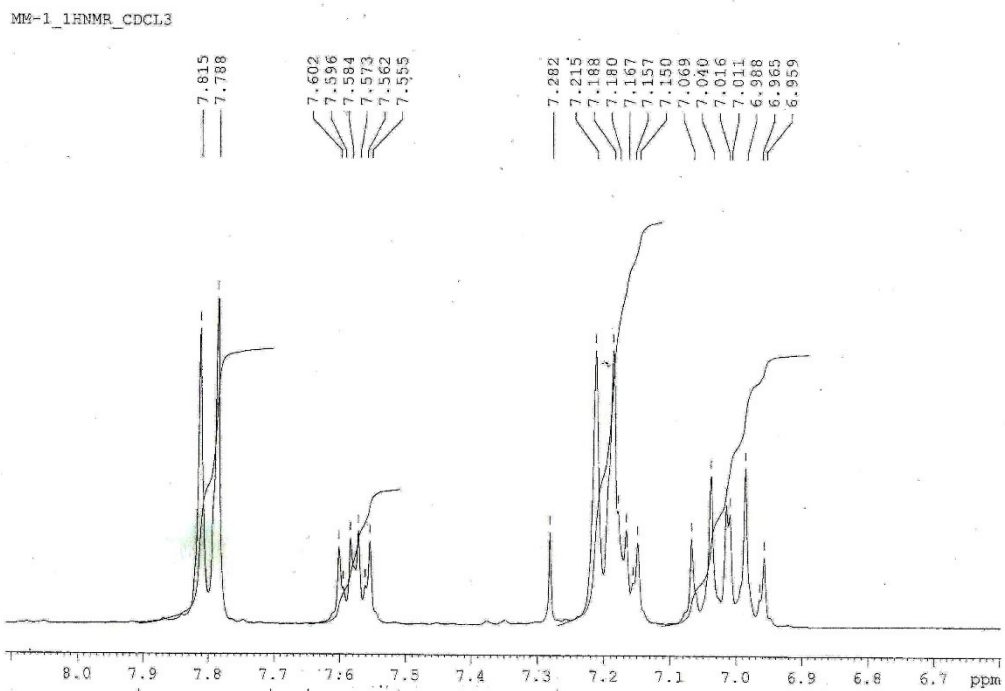


Figure 2. ^{13}C -NMR Spectrum of 5a

***N*-(3,5-bis(4-fluorophenyl)-4,5-dihydro-1*H*-pyrazole-1-carbonothioyl)-4-methyl-*N*-(4-methylbenzoyl)benzamide (5a):**

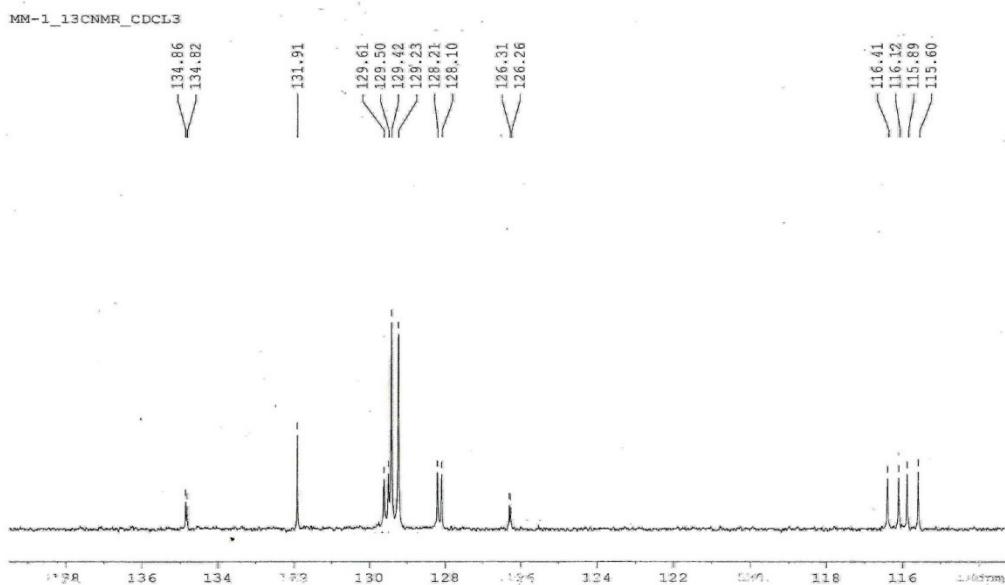
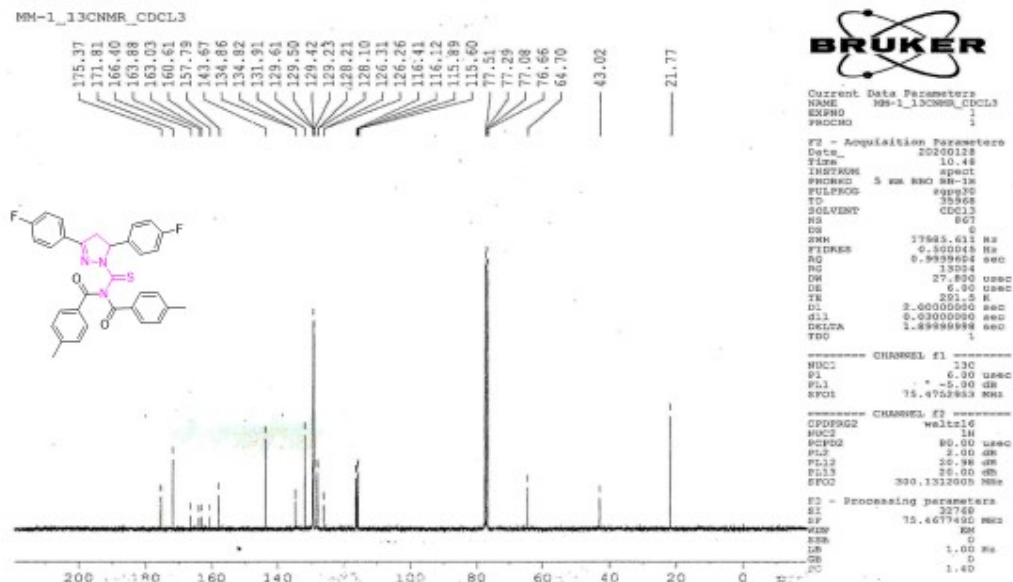


Figure 3. FT-IR Spectrum *N*-(3,5-bis(4-fluorophenyl)-4,5-dihydro-1*H*-pyrazole-1-carbonothioyl)-4-methyl-*N*-(4-methylbenzoyl)benzamide (5a):

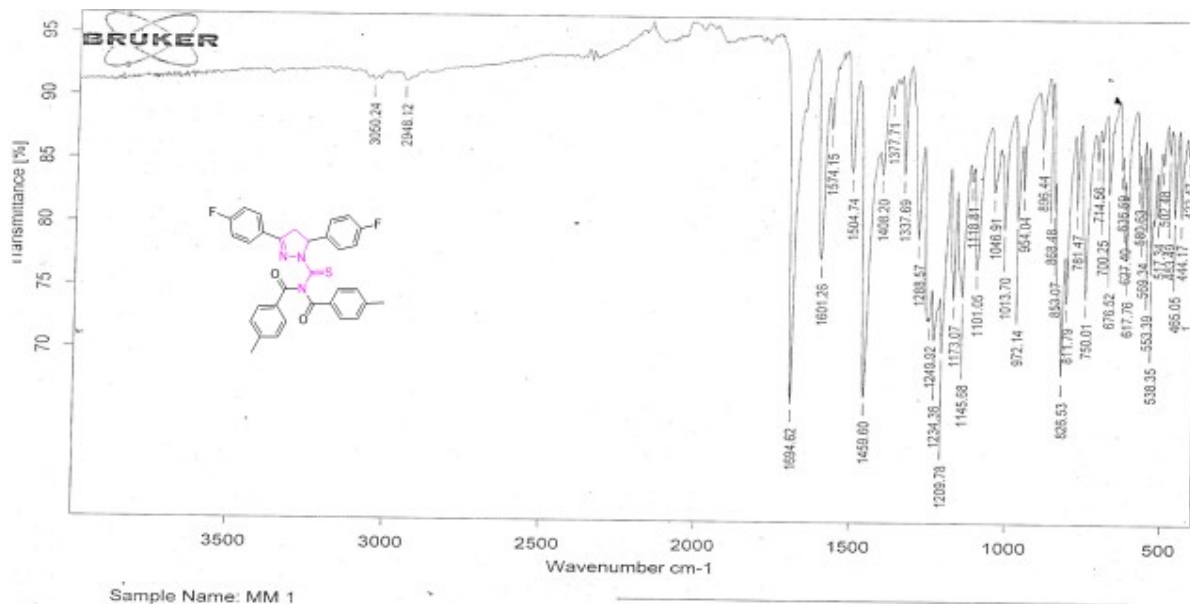
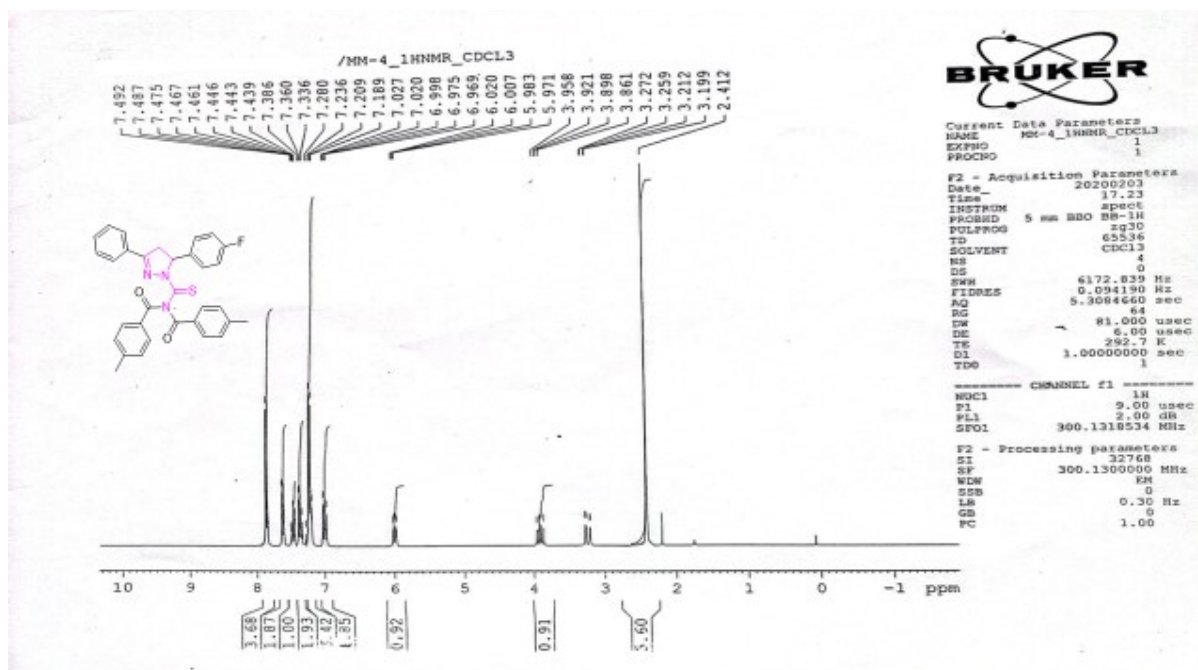


Figure 4. ¹H-NMR Spectrum of 5d

N-(5-(4-fluorophenyl)-3-phenyl-4,5-dihydro-1*H*-pyrazole-1-carbonothioyl)-4-methyl-*N*-(4-methylbenzoyl)benzamide (5d):



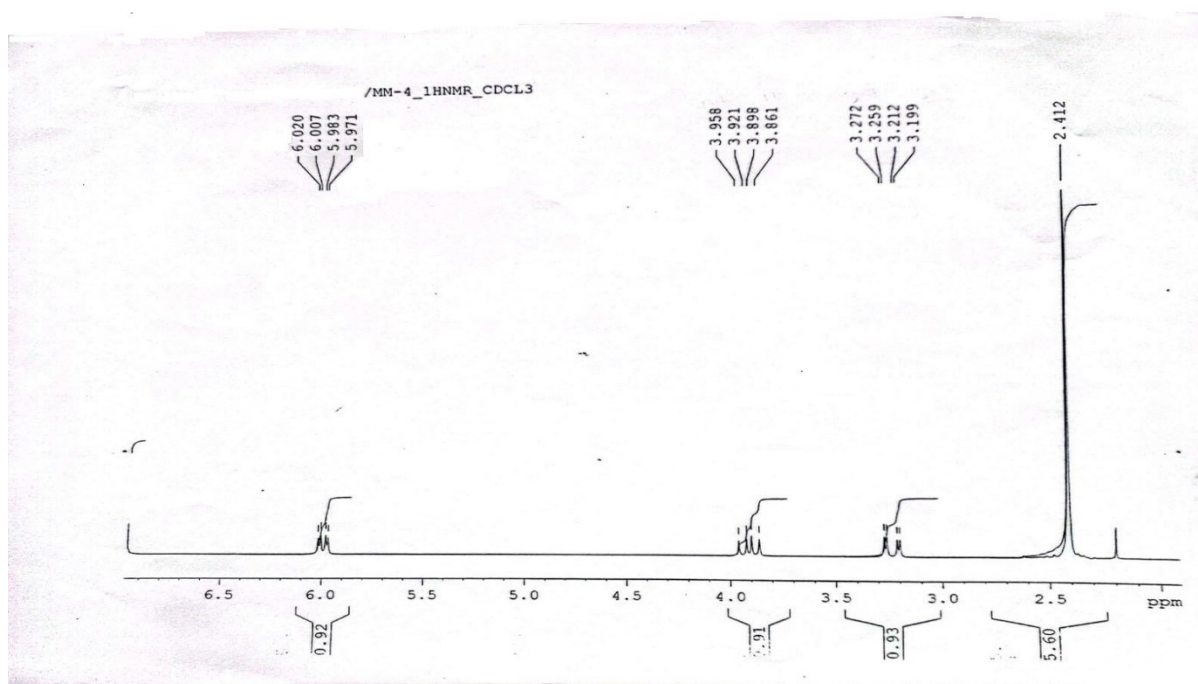
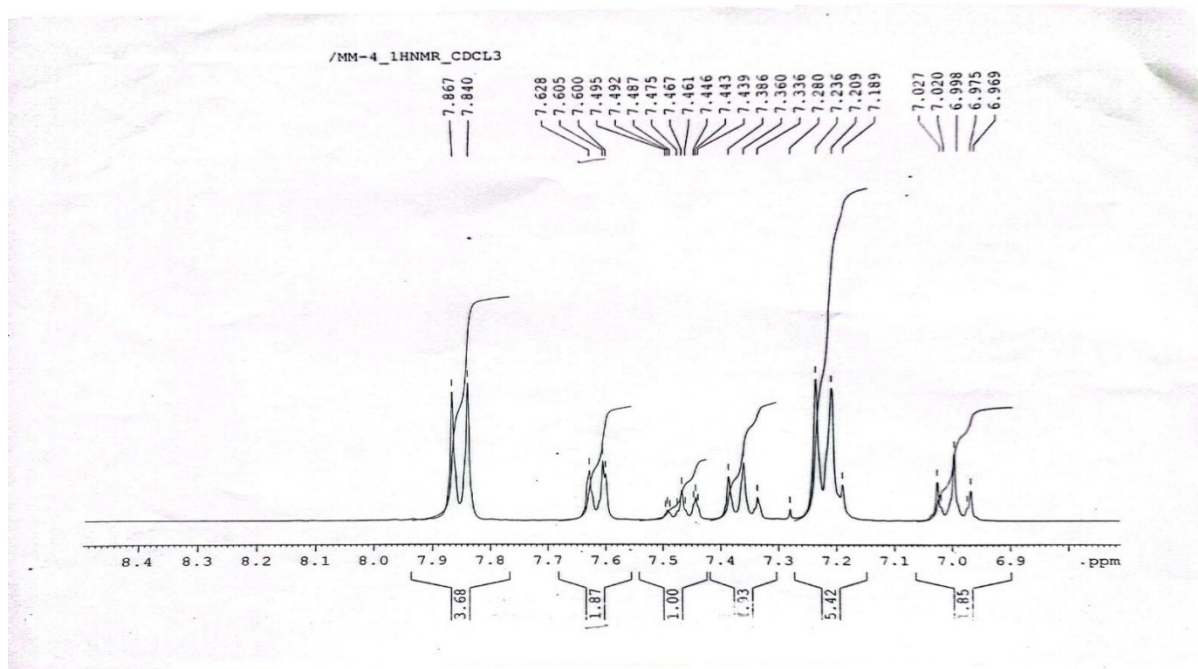


Figure 5. ^{13}C -NMR Spectrum of **5d**

***N*-(5-(4-fluorophenyl)-3-phenyl-4,5-dihydro-1*H*-pyrazole-1-carbonothioyl)-4-methyl-*N*-(4-methylbenzoyl)benzamide (**5d**):**

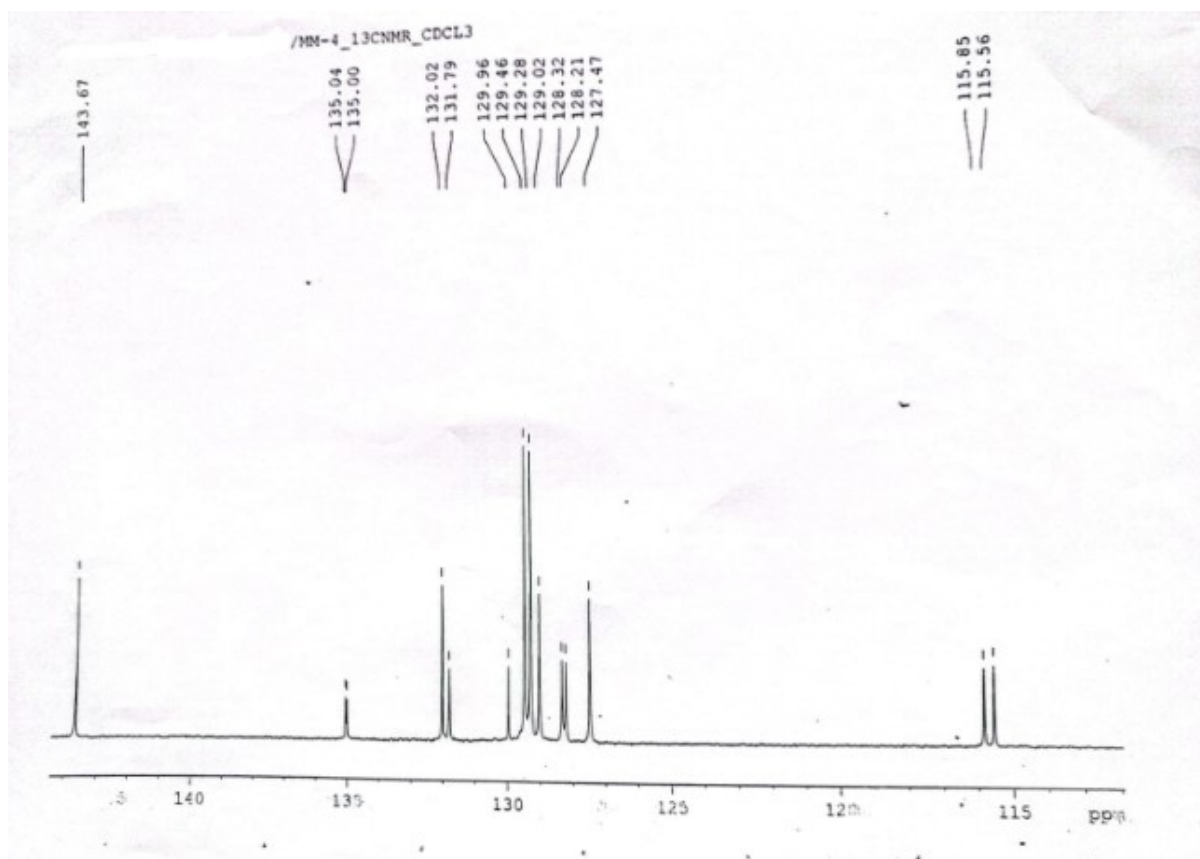
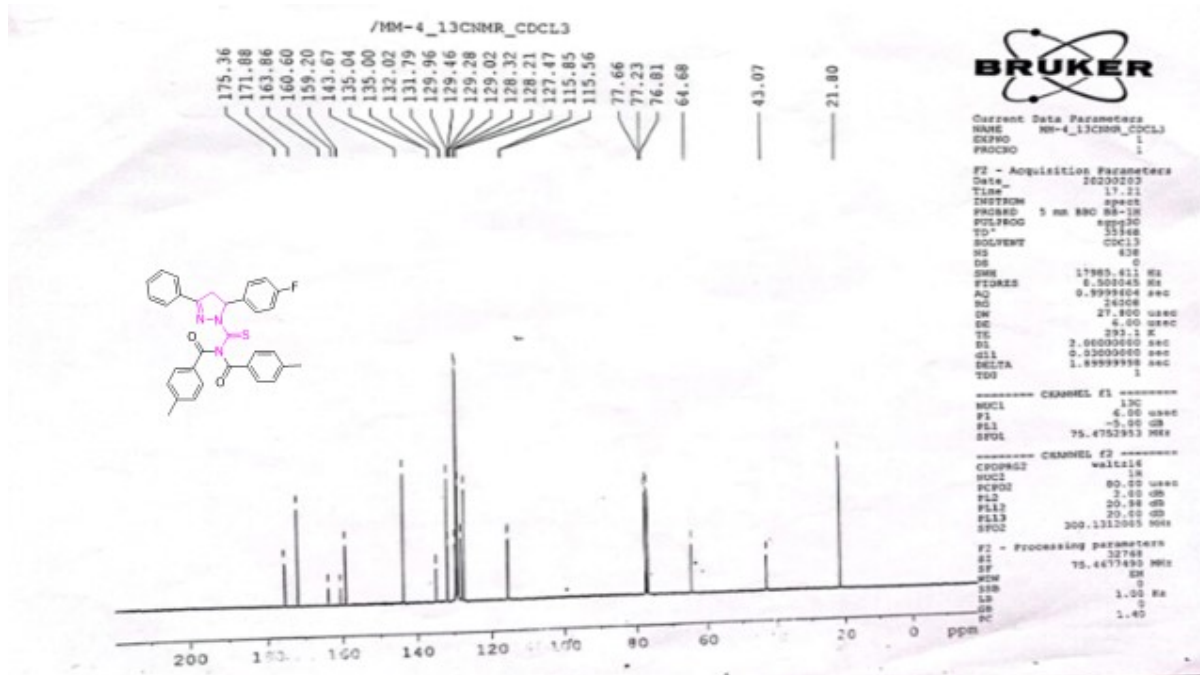


Figure 6. FT-IR Spectrum of **5d**

N-(5-(4-fluorophenyl)-3-phenyl-4,5-dihydro-1*H*-pyrazole-1-carbonothioyl)-4-methyl-*N*-(4-methylbenzoyl)benzamide (**5d**):

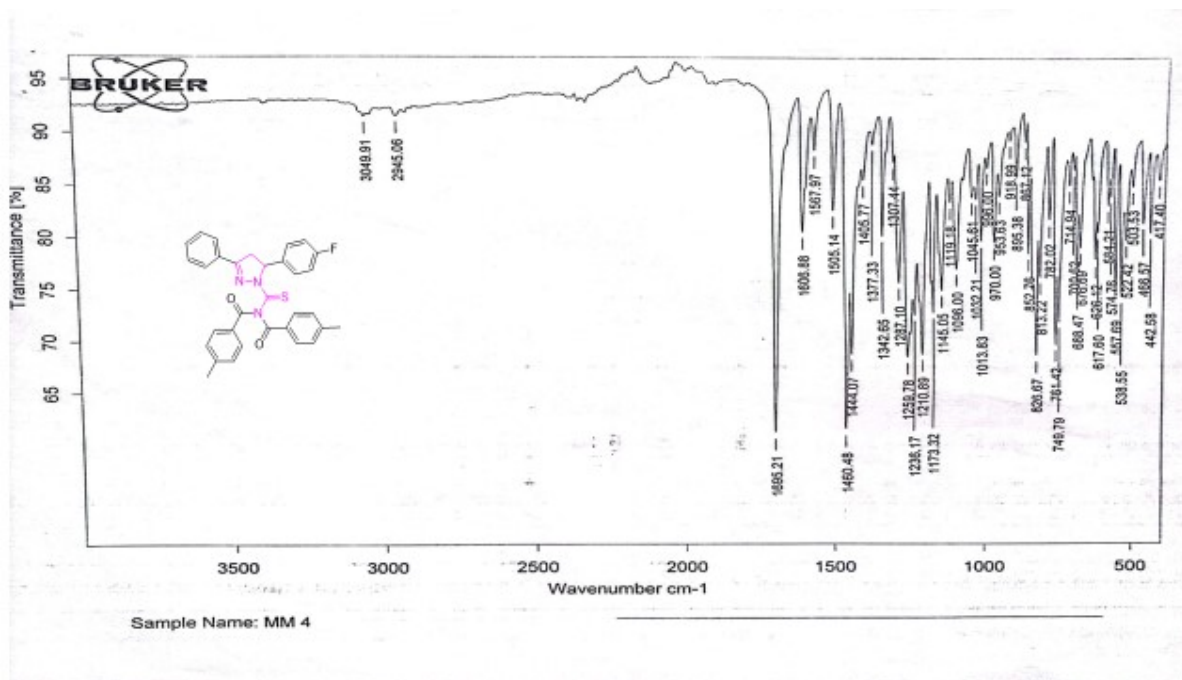
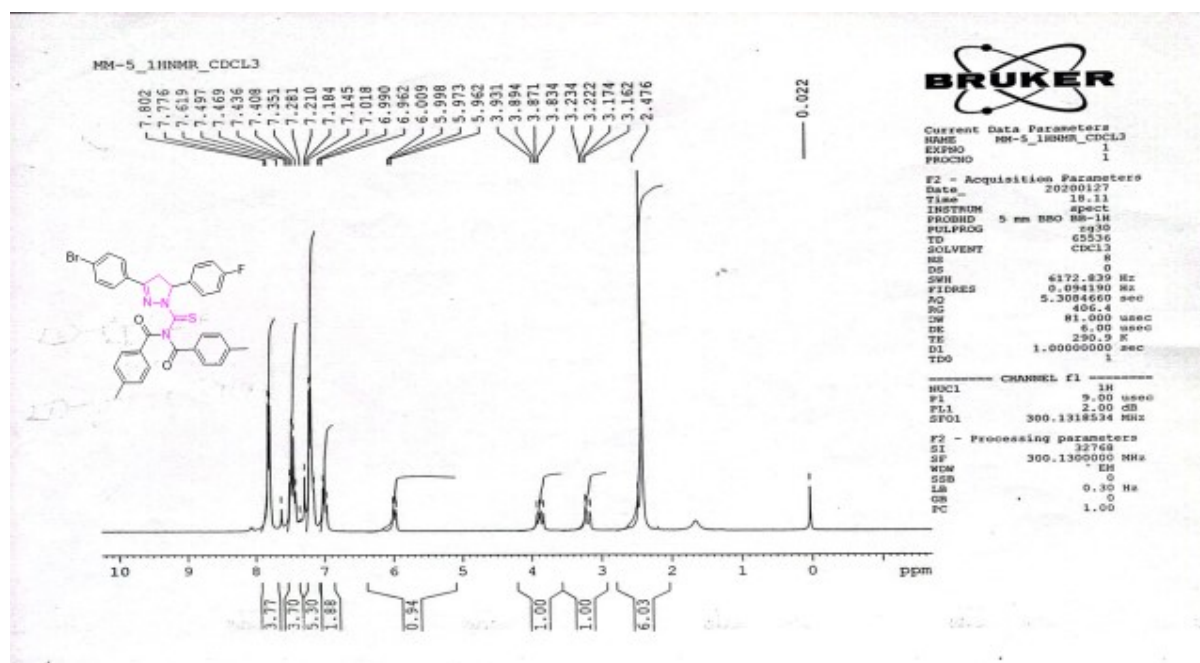


Figure 7. ¹H-NMR Spectrum of 5e

N-(3-(4-bromophenyl)-5-(4-fluorophenyl)-4,5-dihydro-1*H*-pyrazole-1-carbonothioyl)-4-methyl-*N*-(4-methylbenzoyl)benzamide (5e):



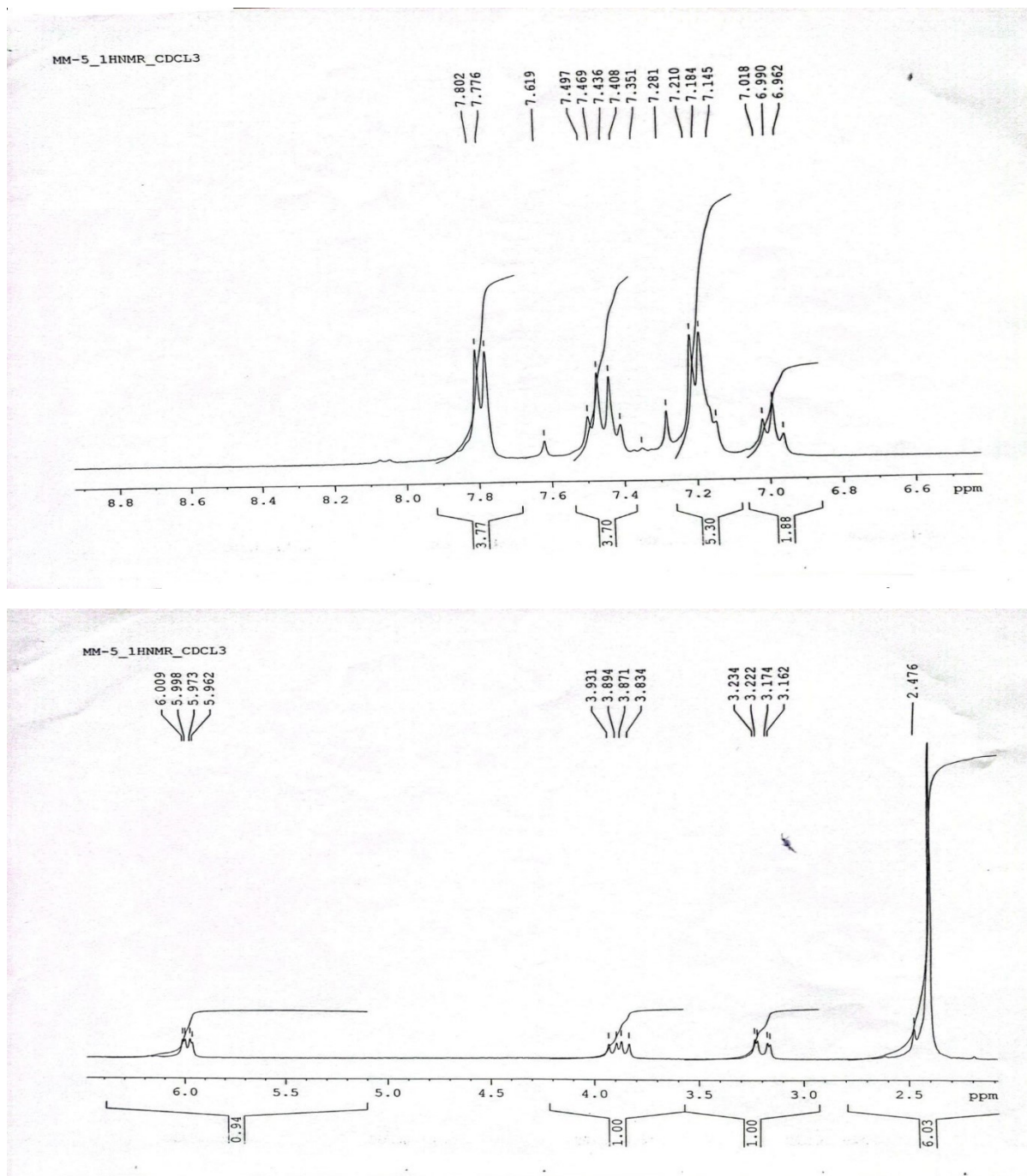


Figure 8. ^1H -NMR Spectrum of **5e**

N-(3-(4-bromophenyl)-5-(4-fluorophenyl)-4,5-dihydro-1*H*-pyrazole-1-carbonothioyl)-4-methyl-*N*-(4-methylbenzoyl)benzamide (**5e**):

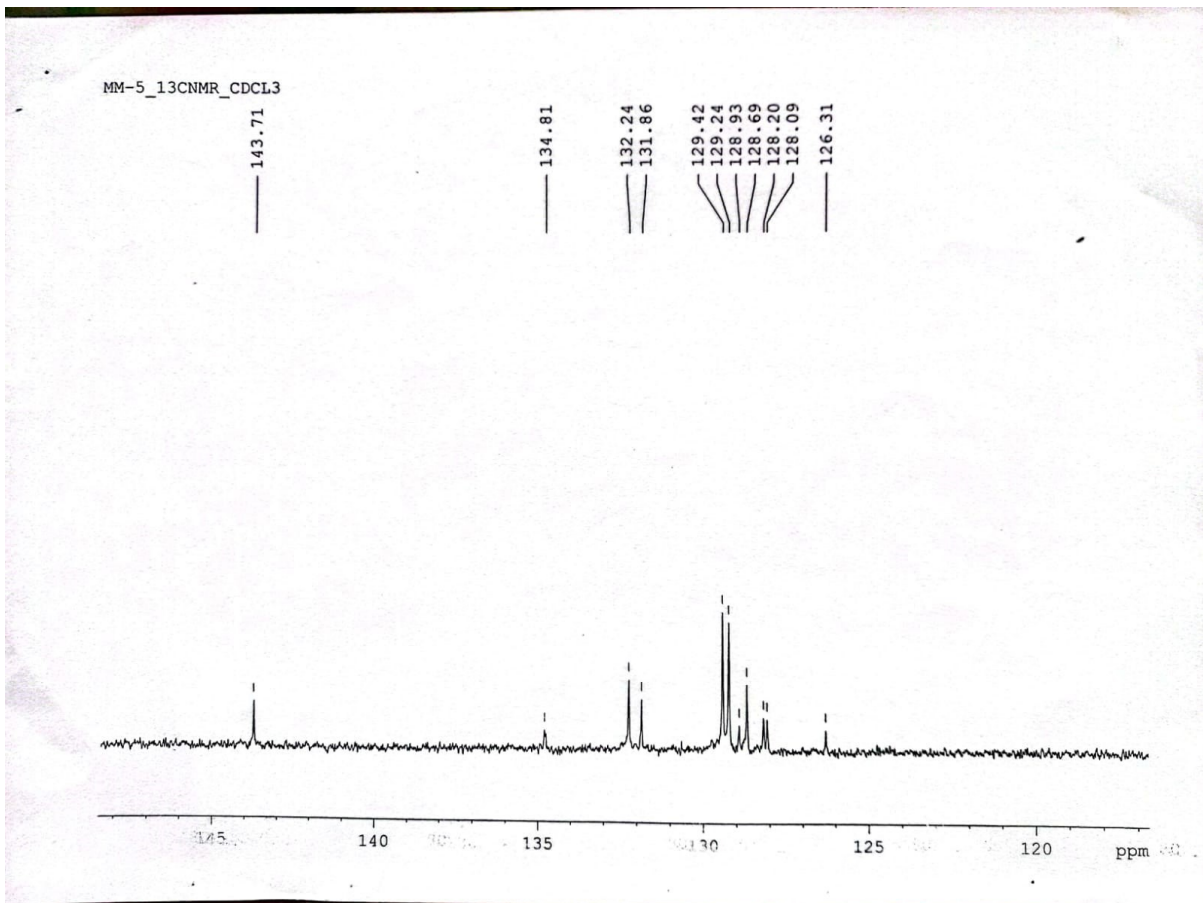
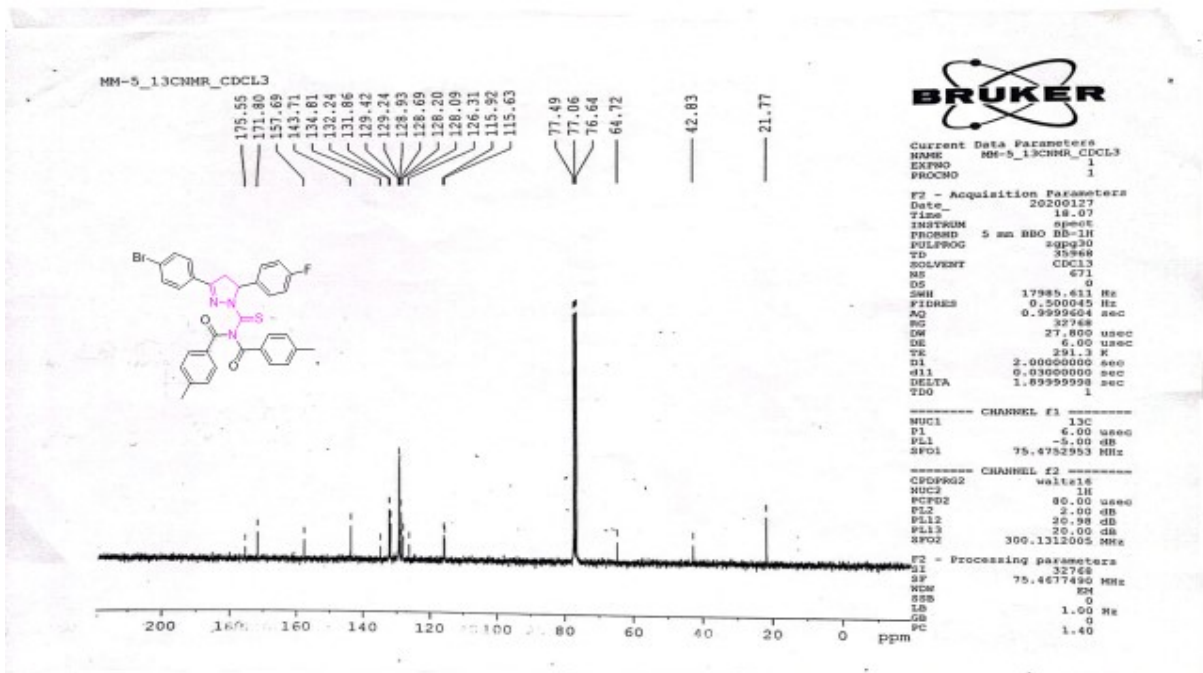


Figure 9. FT-IR Spectrum of 5e

***N*-3-(4-bromophenyl)-5-(4-fluorophenyl)-4,5-dihydro-1*H*-pyrazole-1-carbonothioyl)-4-methyl-*N*-(4-methylbenzoyl)benzamide (5e):**

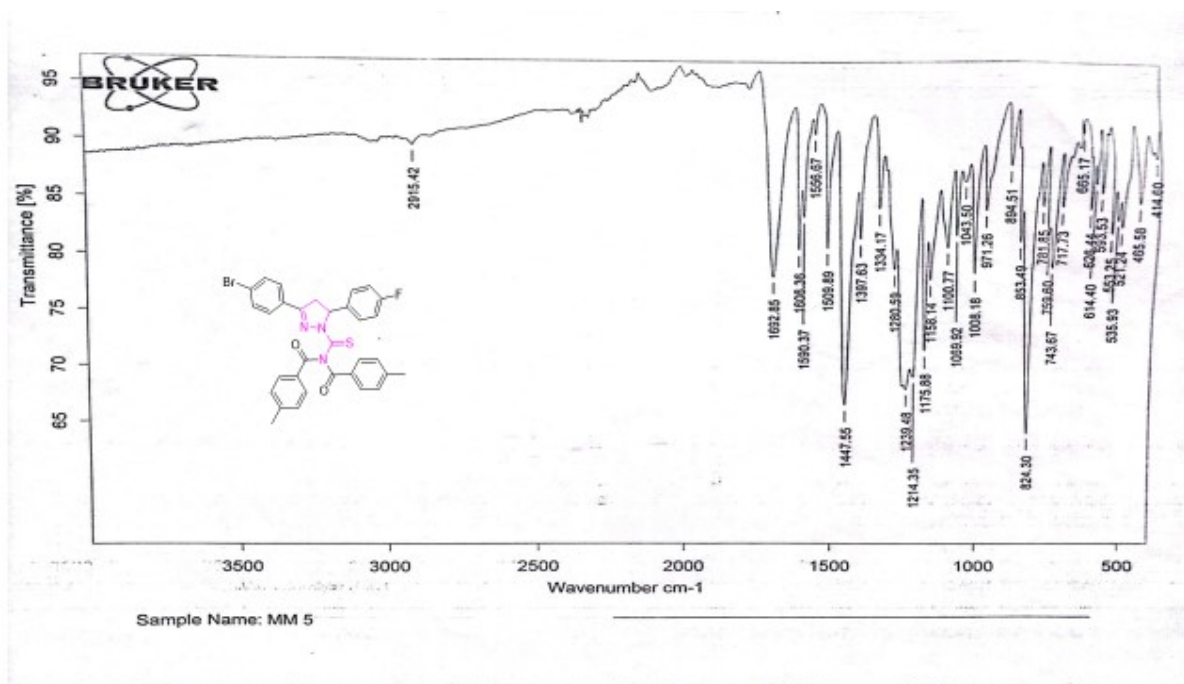
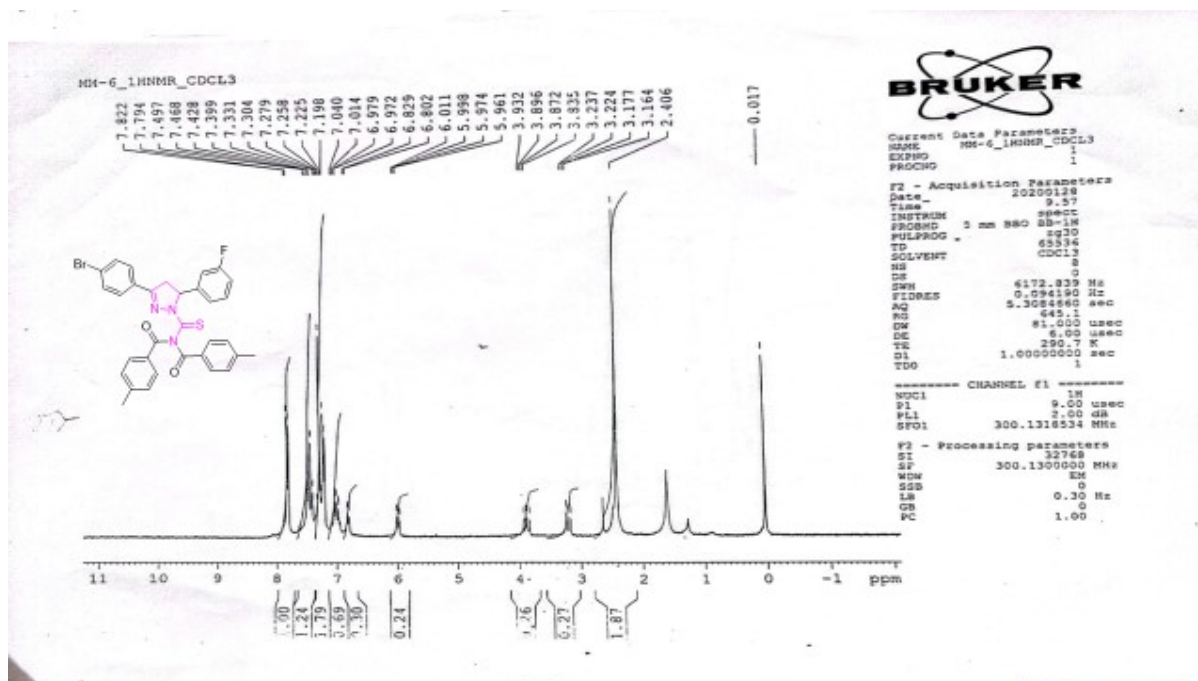


Figure 10. ¹H-NMR Spectrum of 5f

***N*-3-(4-bromophenyl)-5-(3-fluorophenyl)-4,5-dihydro-1*H*-pyrazole-1-carbonothioyl)-4-methyl-*N*-(4-methylbenzoyl)benzamide (5f):**



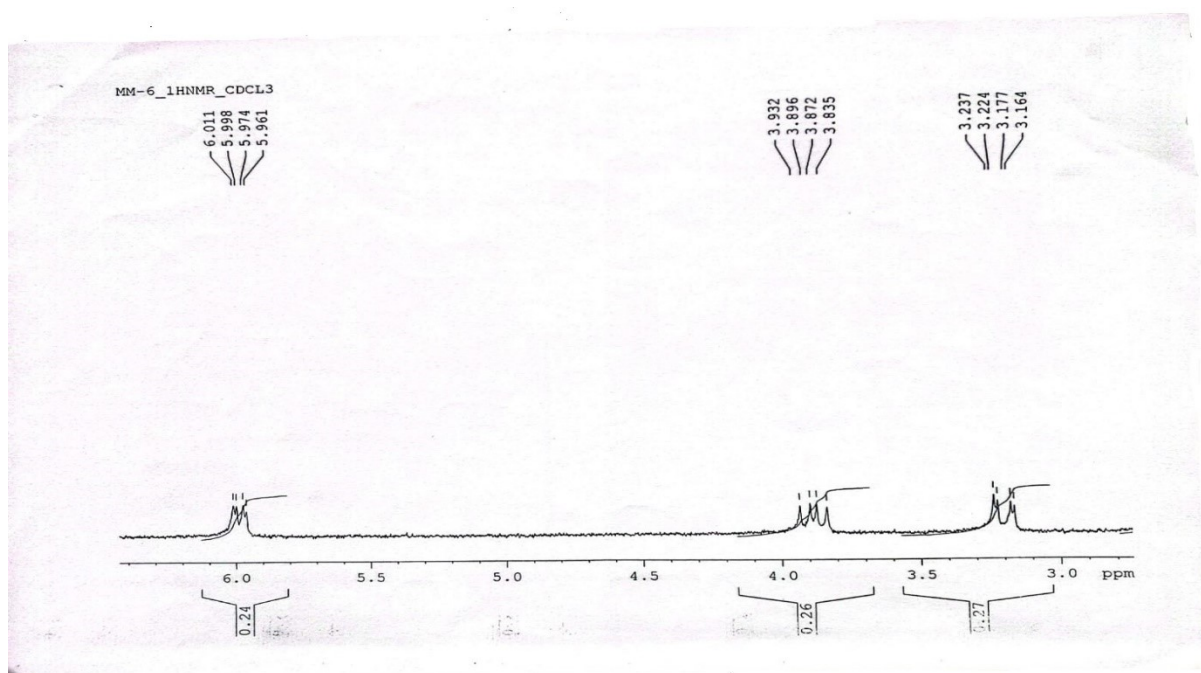
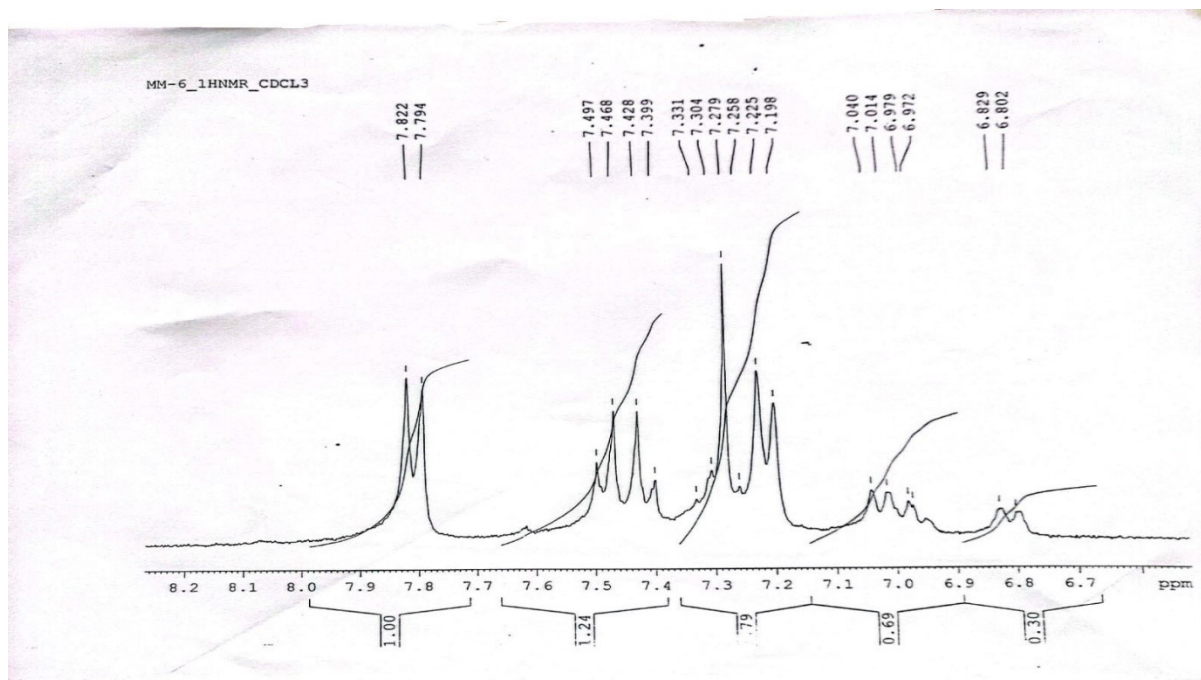
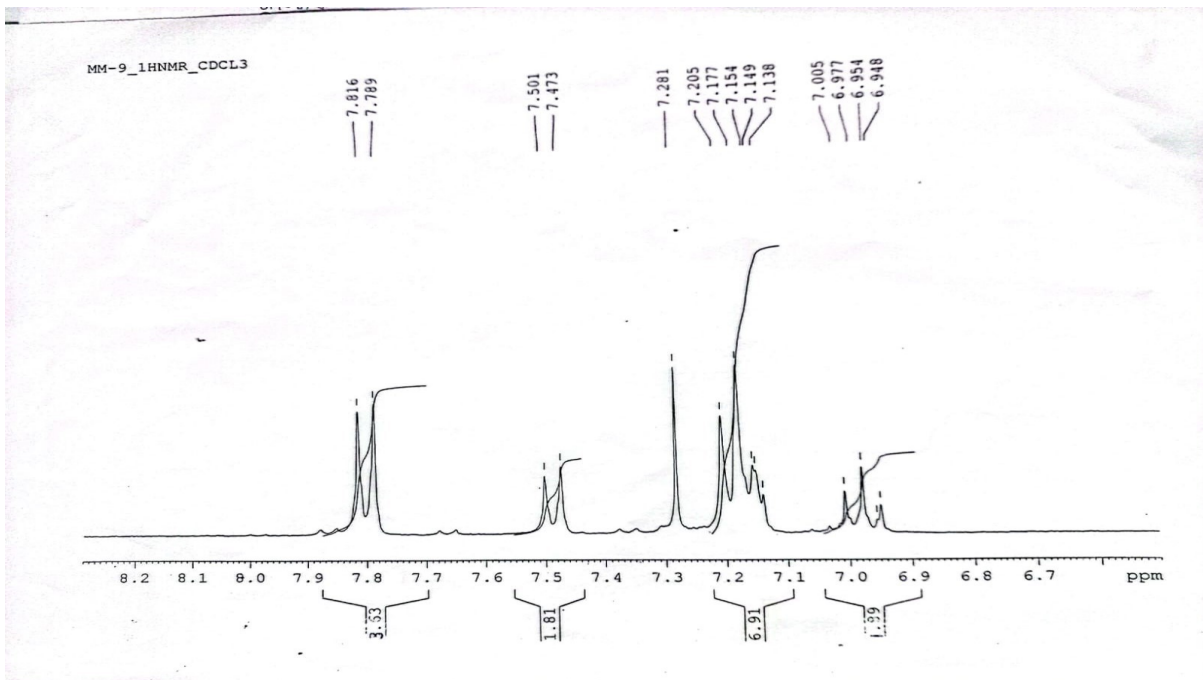
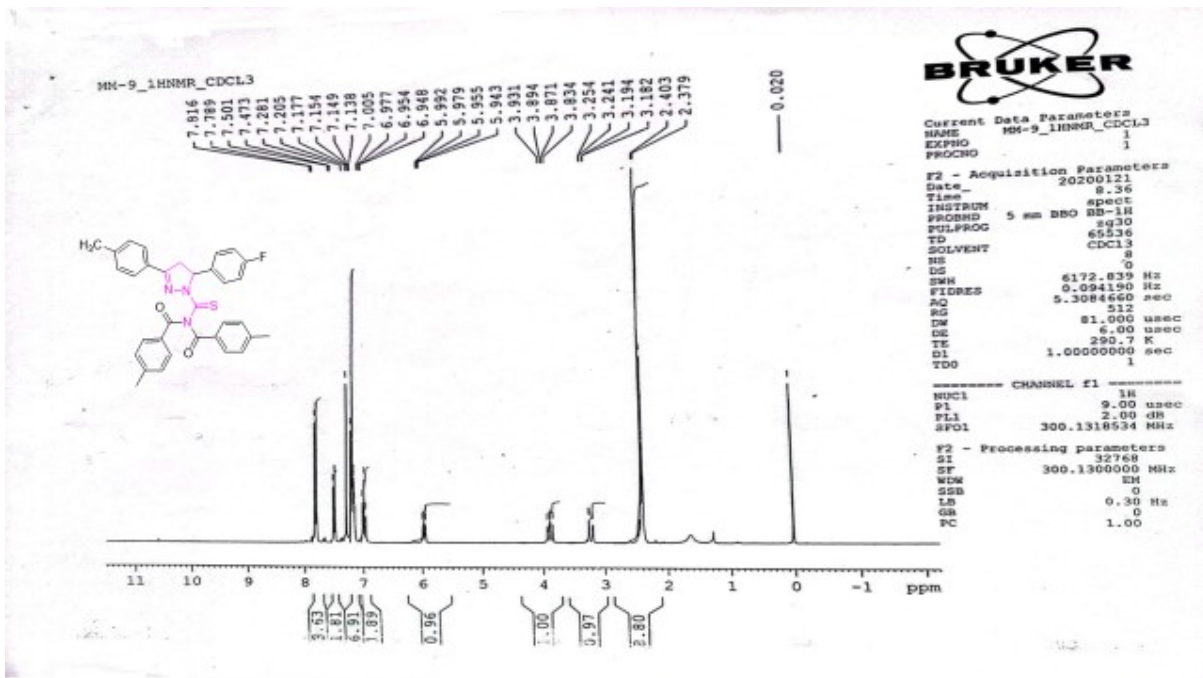


Figure 11. $^1\text{H-NMR}$ Spectrum of **5i**

N-(5-(4-fluorophenyl)-3-(*p*-tolyl)-4,5-dihydro-1*H*-pyrazole-1-carbonothioyl)-4-methyl-*N*-(4-methylbenzoyl)benzamide (**5i**):



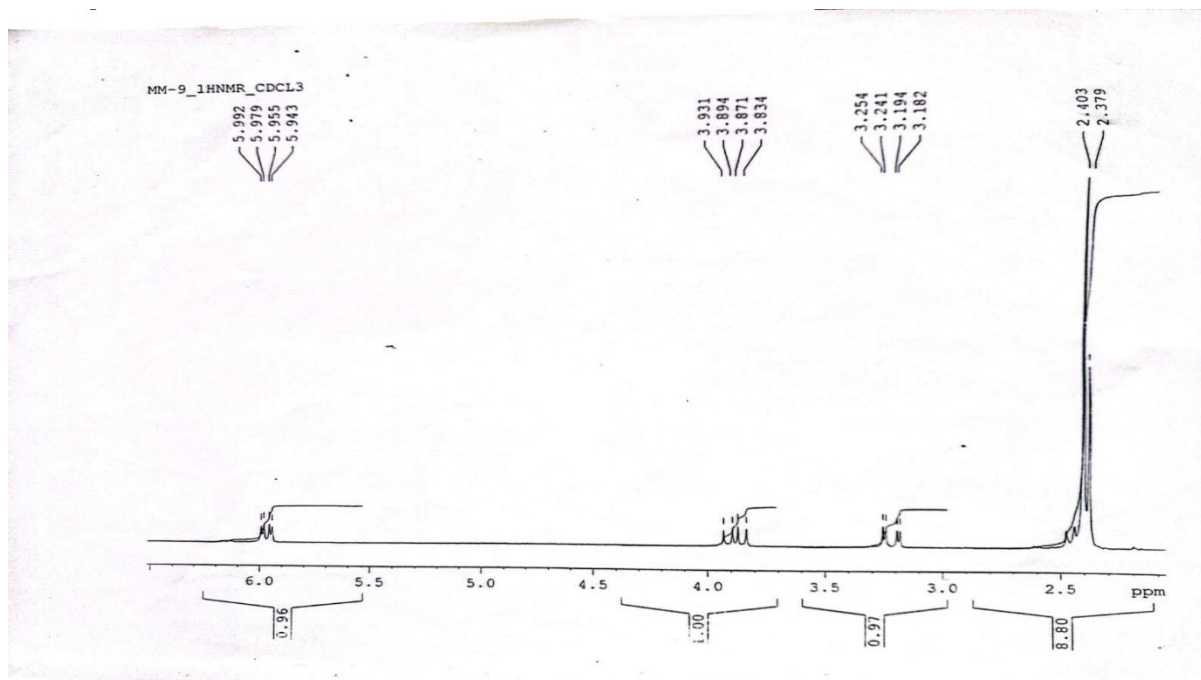
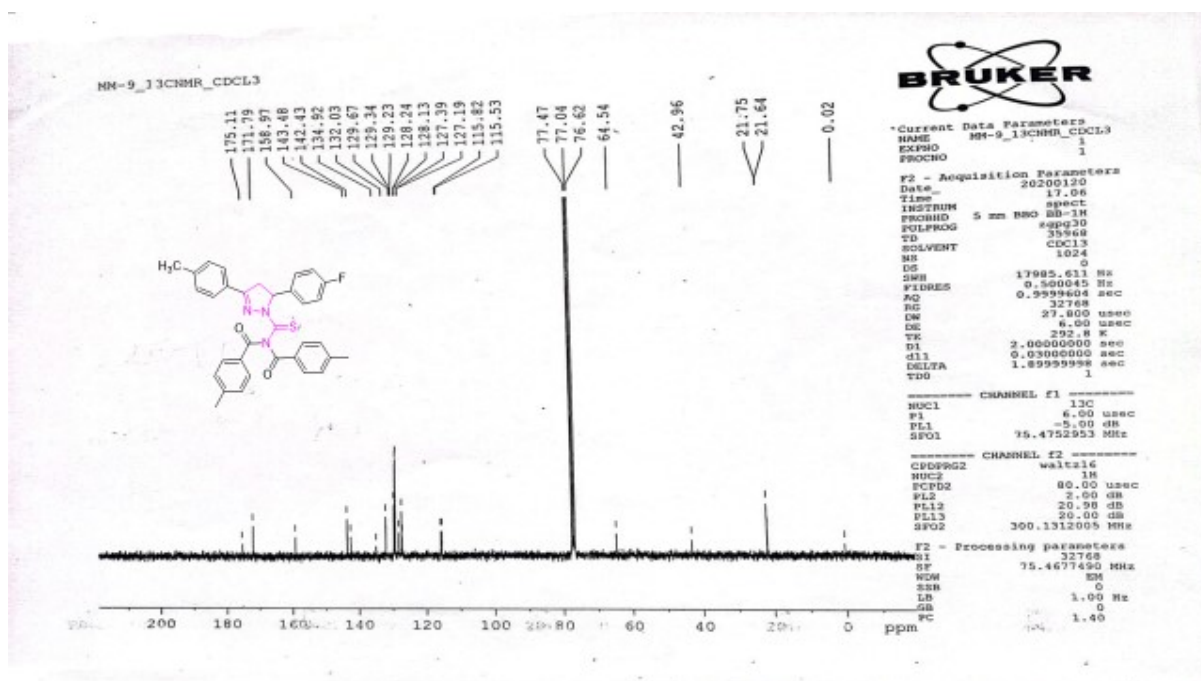


Figure 12. ^1H -NMR Spectrum of **5i**

N-(5-(4-fluorophenyl)-3-(*p*-tolyl)-4,5-dihydro-1*H*-pyrazole-1-carbonothioyl)-4-methyl-*N*-(4-methylbenzoyl)benzamide (**5i**):



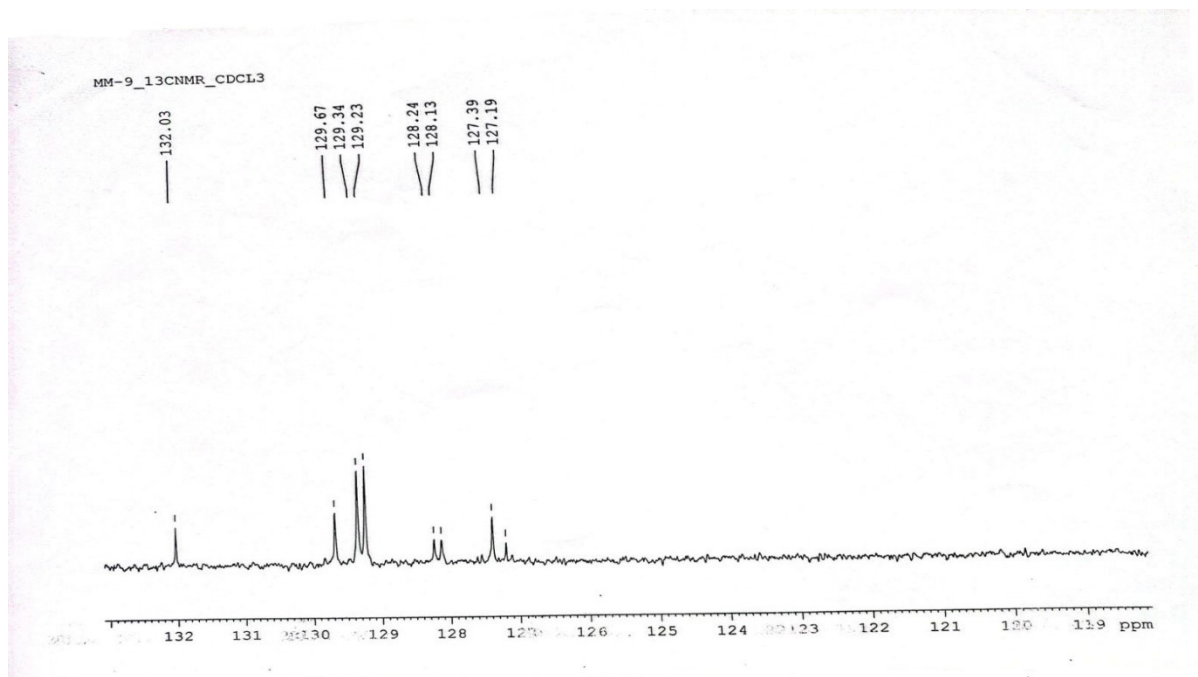


Figure 13. FT-IR Spectrum of **5j**

N-(5-(4-chlorophenyl)-3-(*p*-tolyl)-4,5-dihydro-1*H*-pyrazole-1-carbonothioyl)-4-methyl-*N*-(4-methylbenzoyl)benzamide (**5j**):

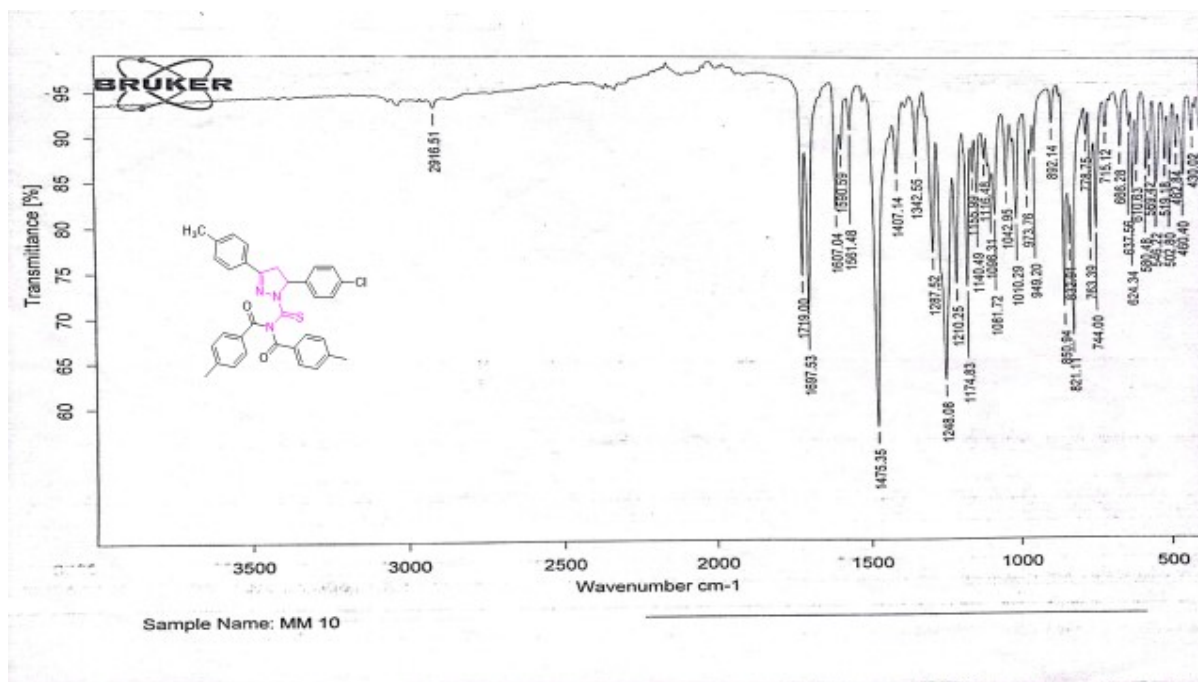
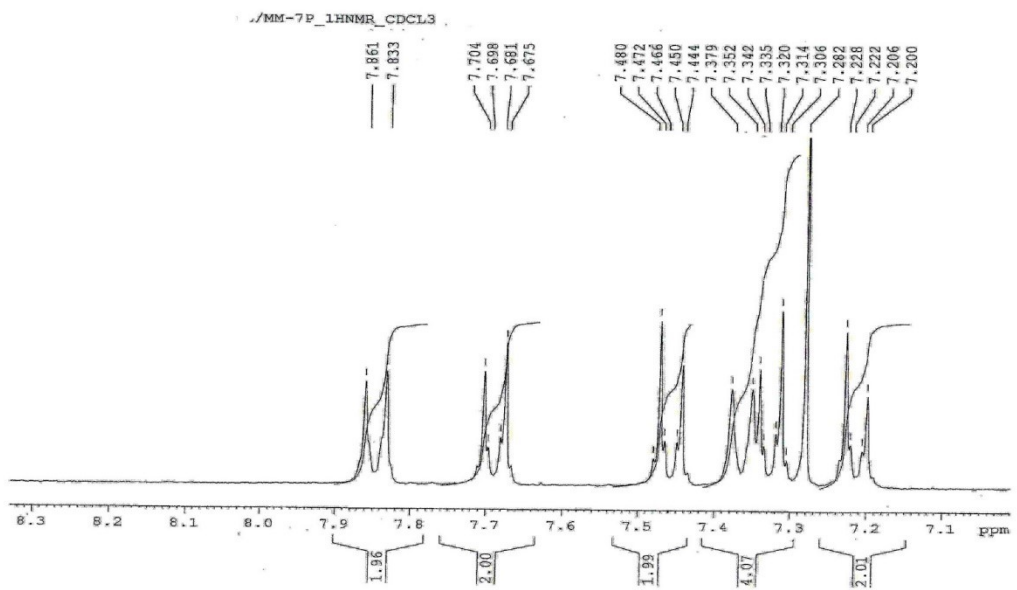
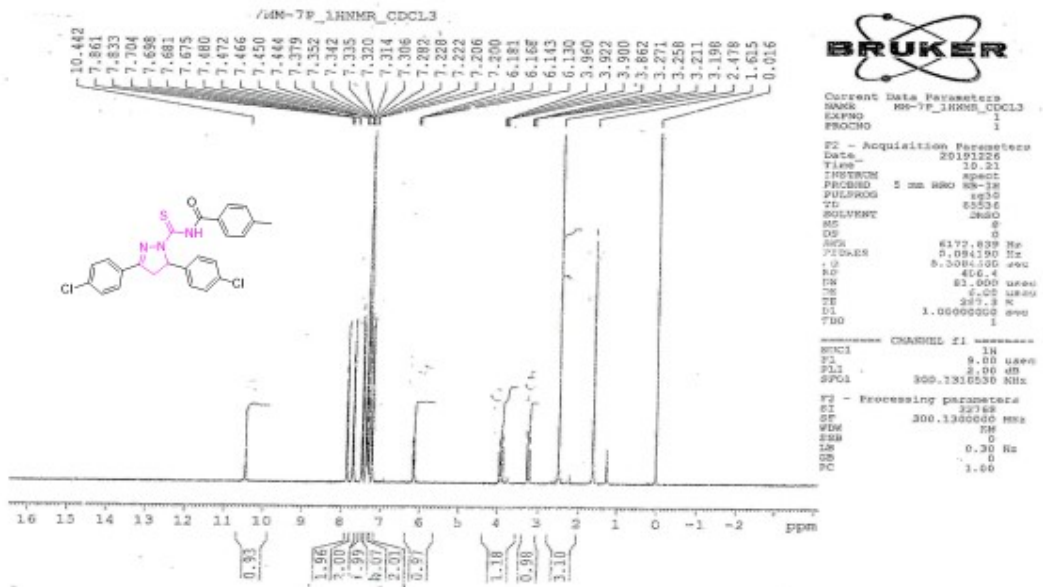


Figure 14. ¹H-NMR Spectrum of **5k**

N-(3,5-bis(4-chlorophenyl)-4,5-dihydro-1*H*-pyrazole-1-carbonothioyl)-4-methylbenzamide (**5k**):



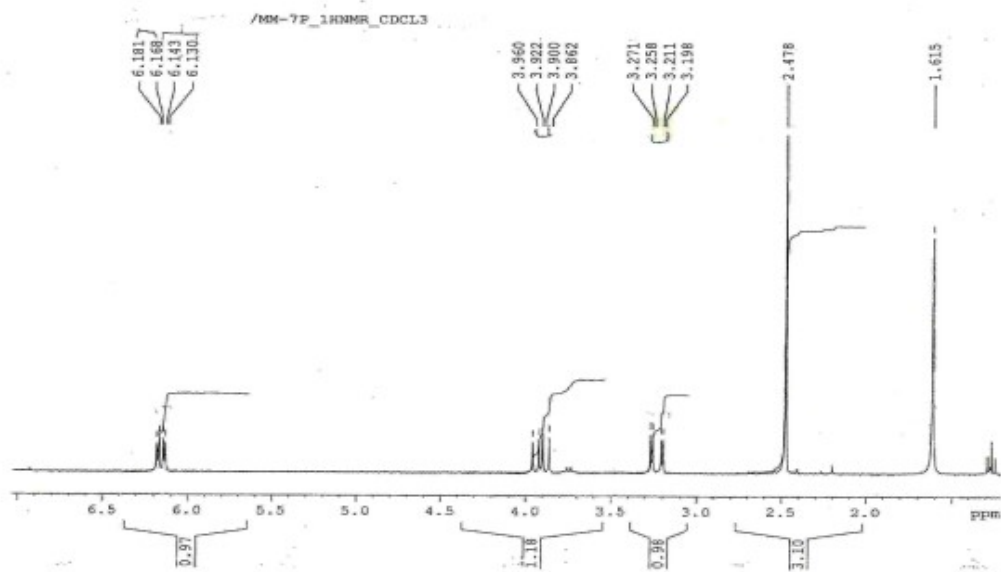
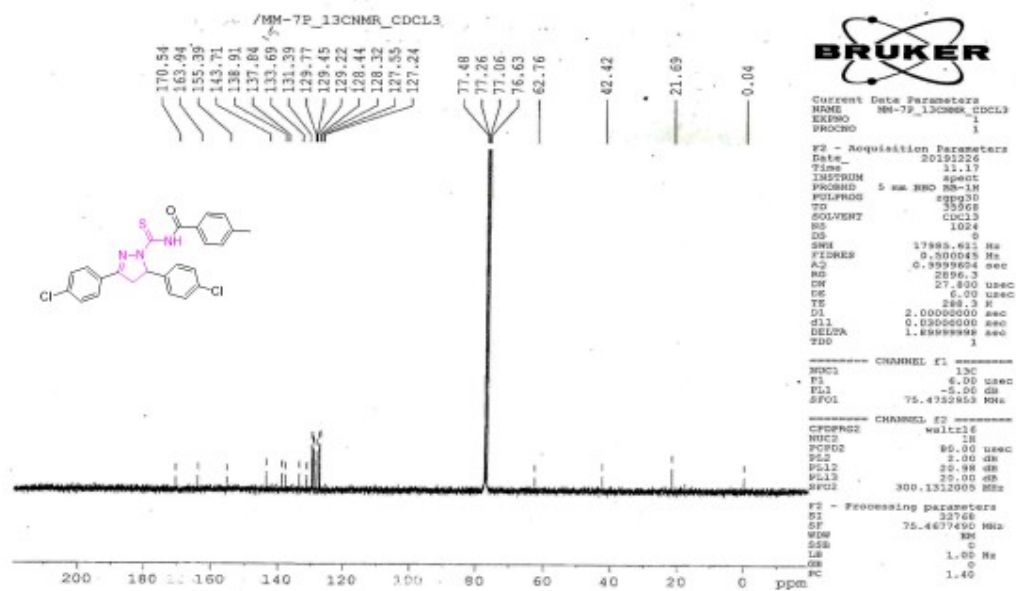


Figure 15. ¹³C-NMR Spectrum of **5k**

N-(3,5-bis(4-chlorophenyl)-4,5-dihydro-1*H*-pyrazole-1-carbonothioyl)-4-methylbenzamide (**5k**):



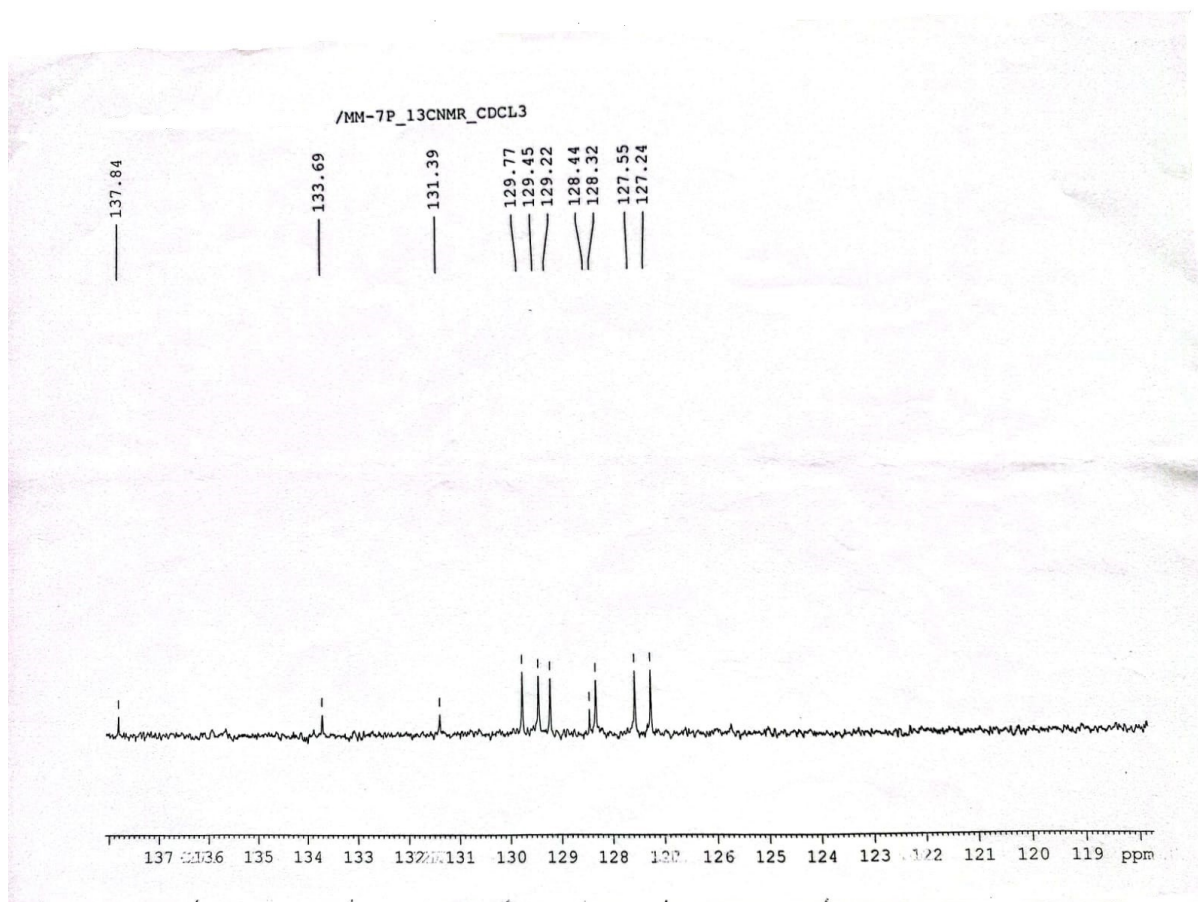
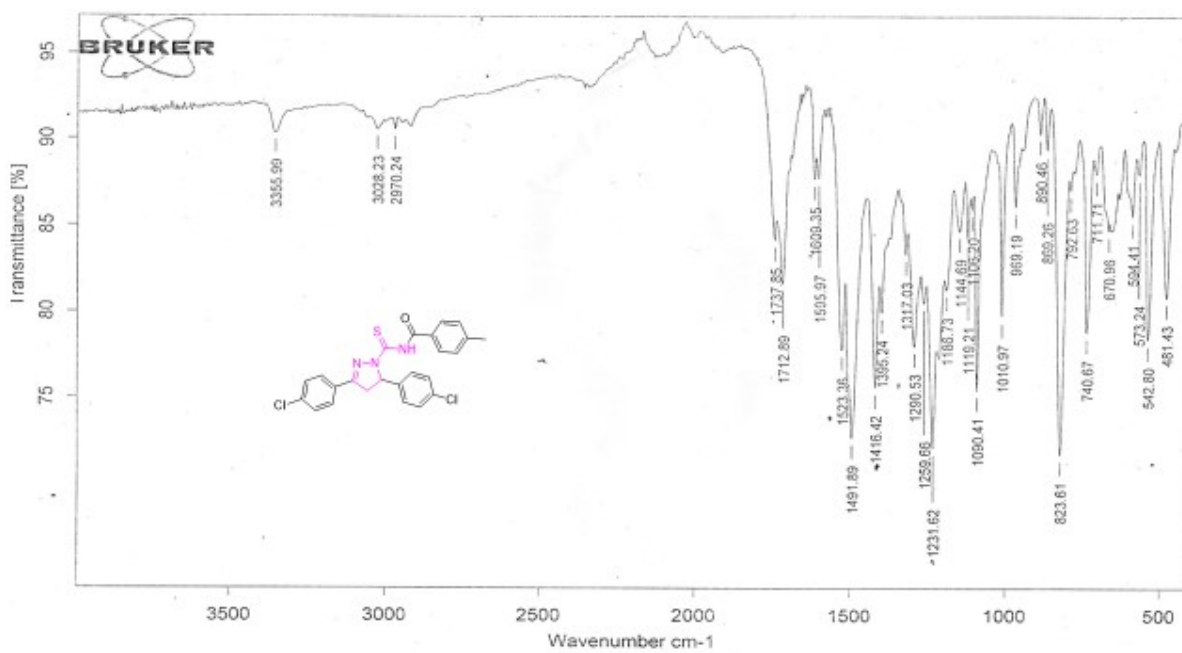


Figure 16. FT-IR Spectrum of 5k

***N*-(3,5-bis(4-chlorophenyl)-4,5-dihydro-1*H*-pyrazole-1-carbonothioyl)-4-methylbenzamide (5k):**



Sample Name: MM 7

Figure 17. FT-IR Spectrum of 5m

N-(5-(4-fluorophenyl)-3-phenyl-4,5-dihydro-1*H*-pyrazole-1-carbonothioyl)-4-methylbenzamide (5m):

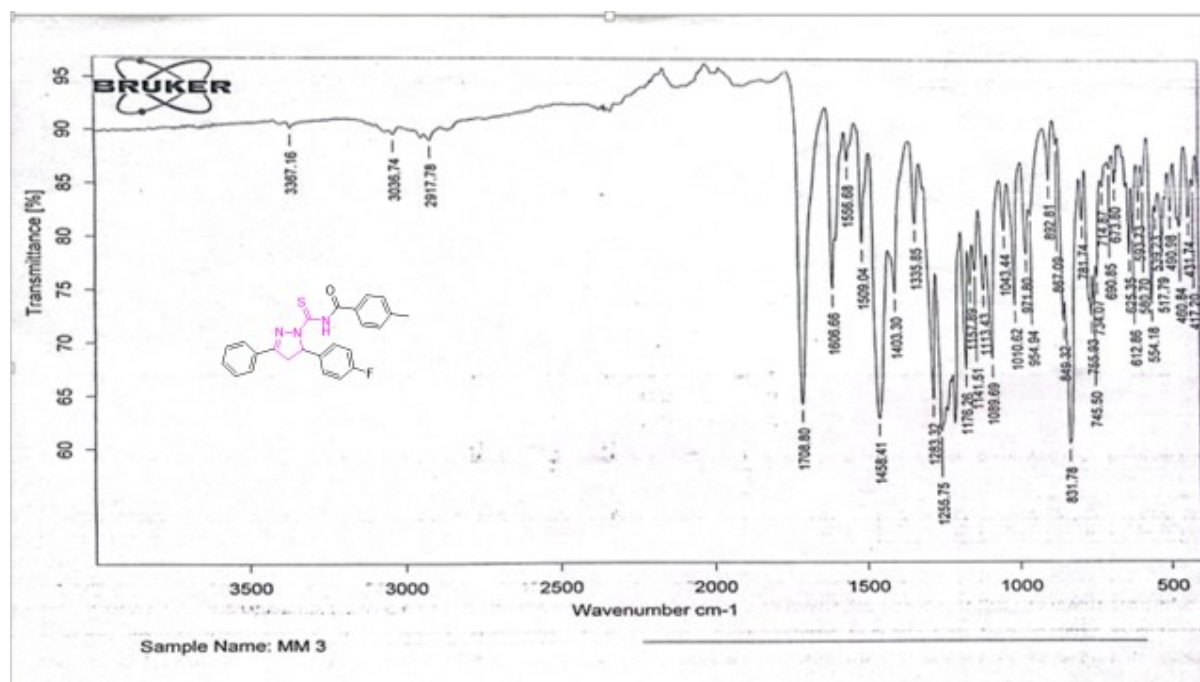
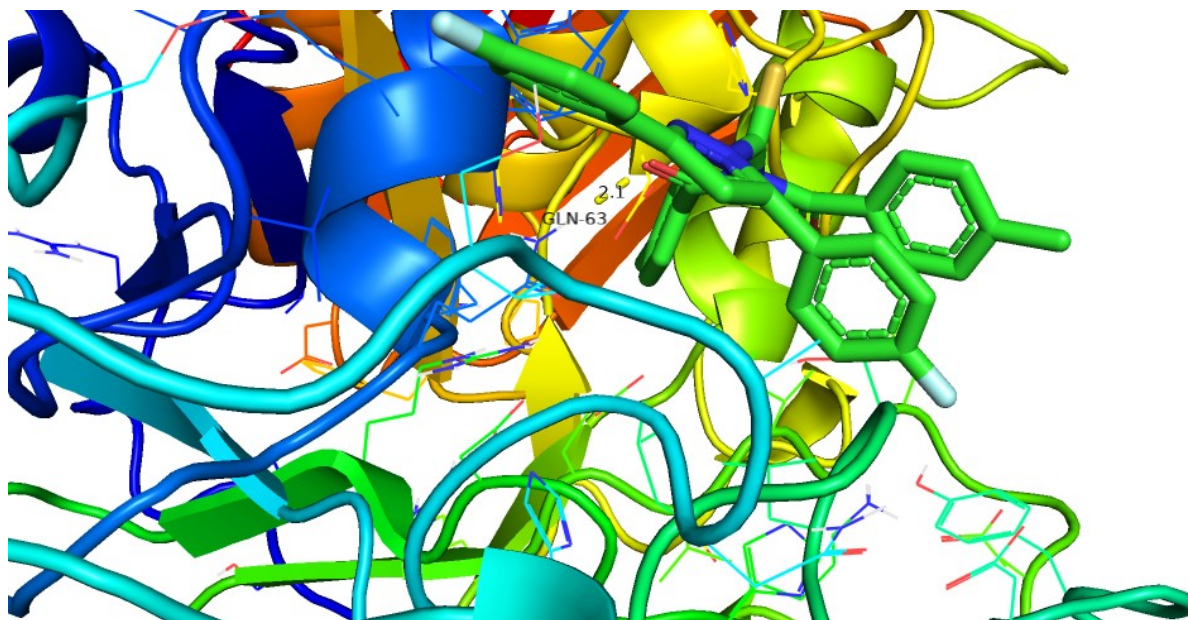
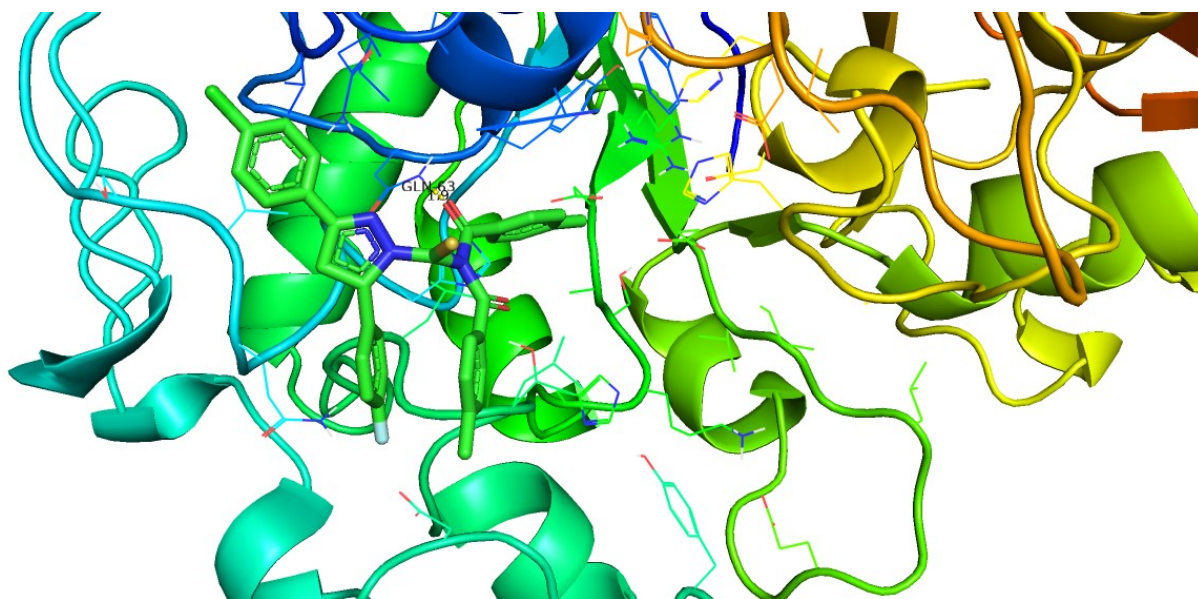


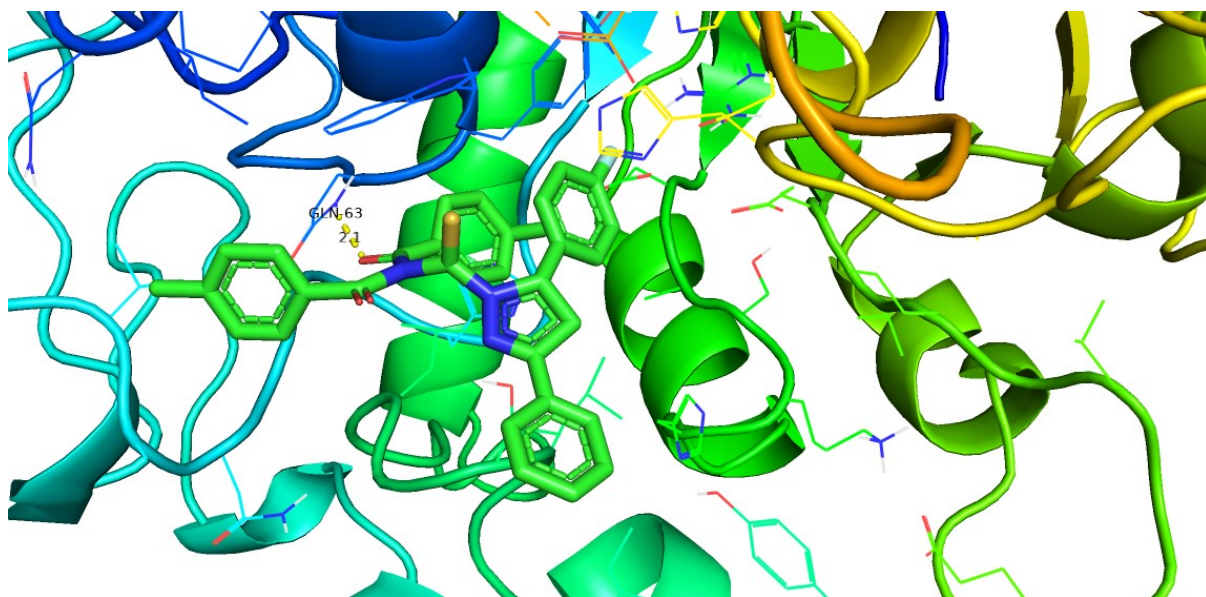
Figure 18. Amylase interaction images of compounds 5a, 5c, 5d, 5e, 5g, 5h, 5i, 5j.



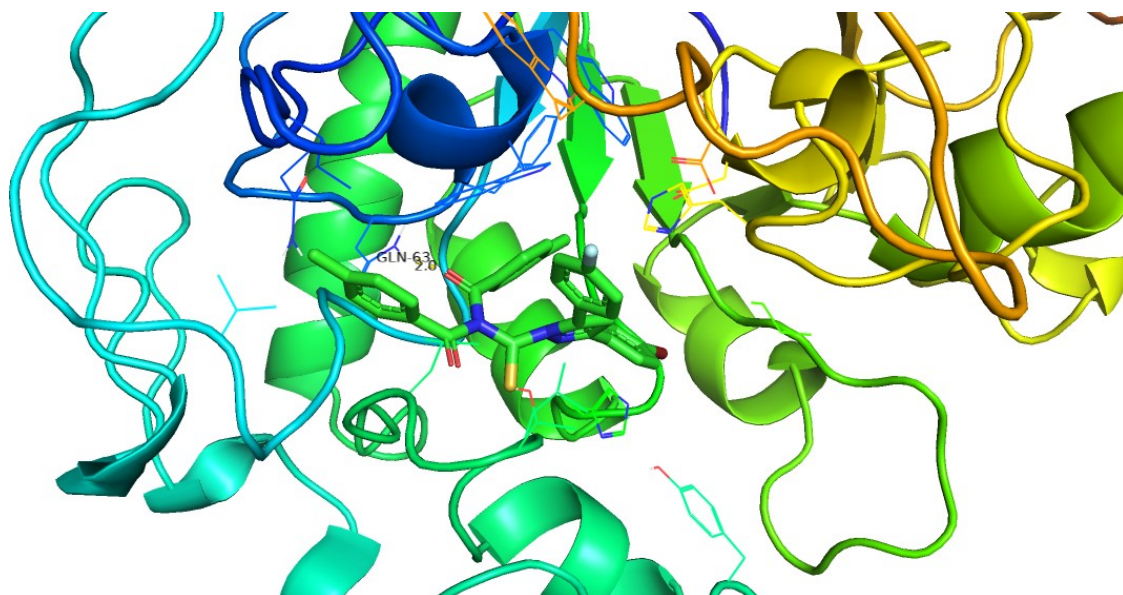
5a



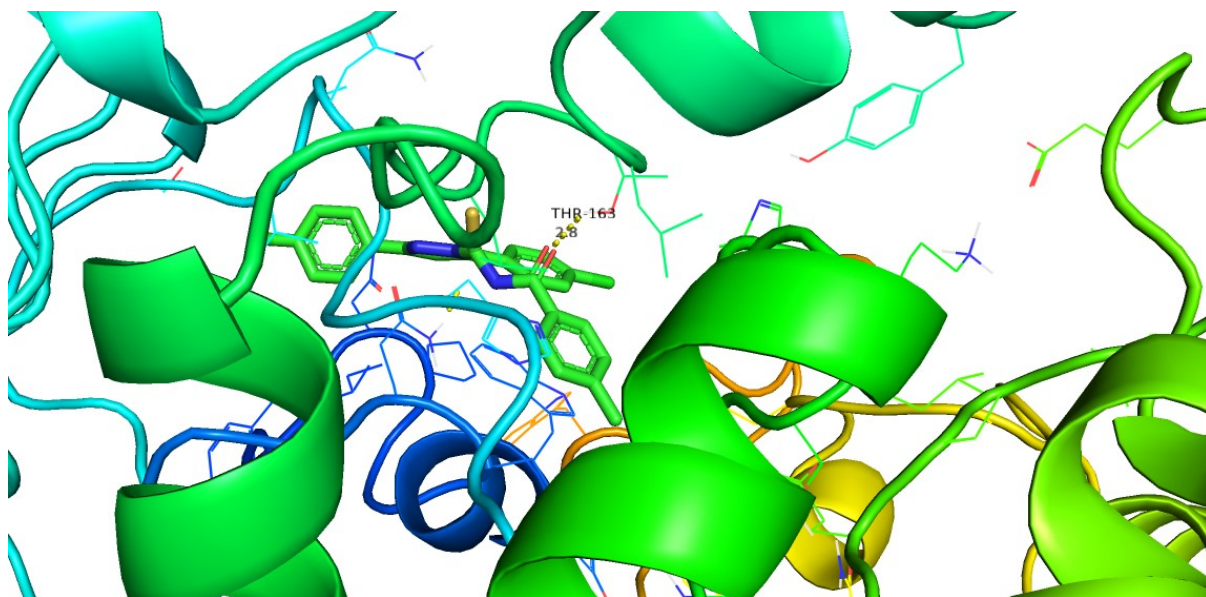
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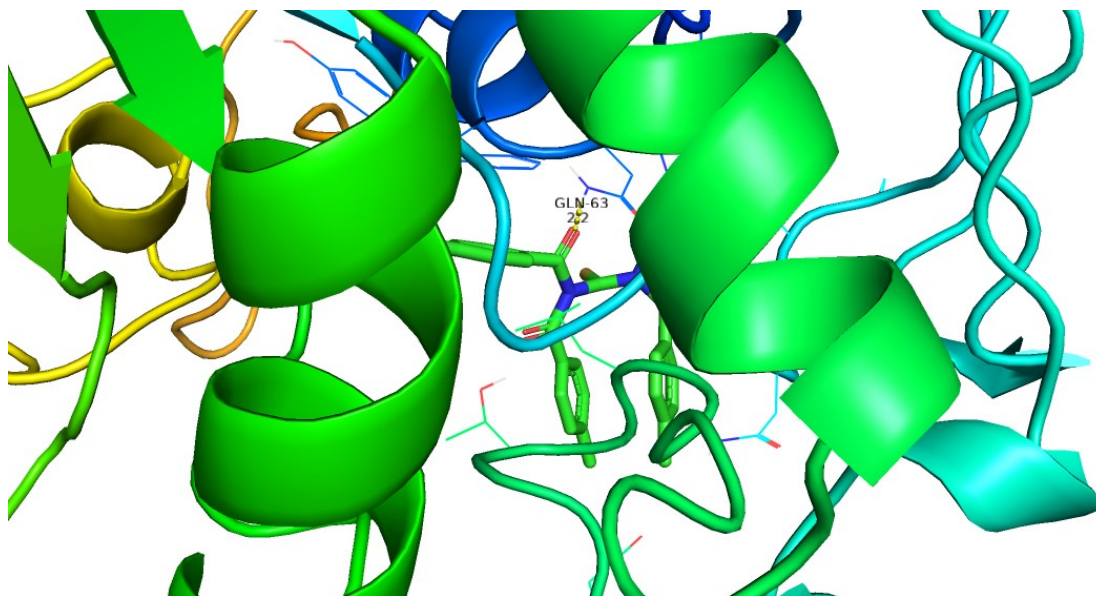
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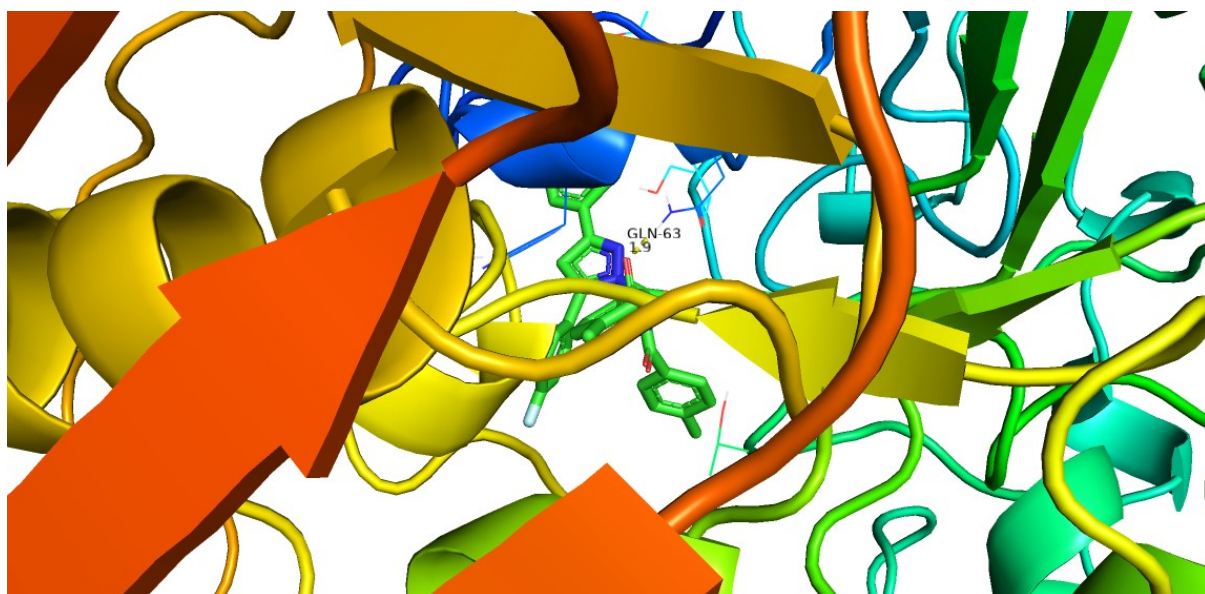
5e



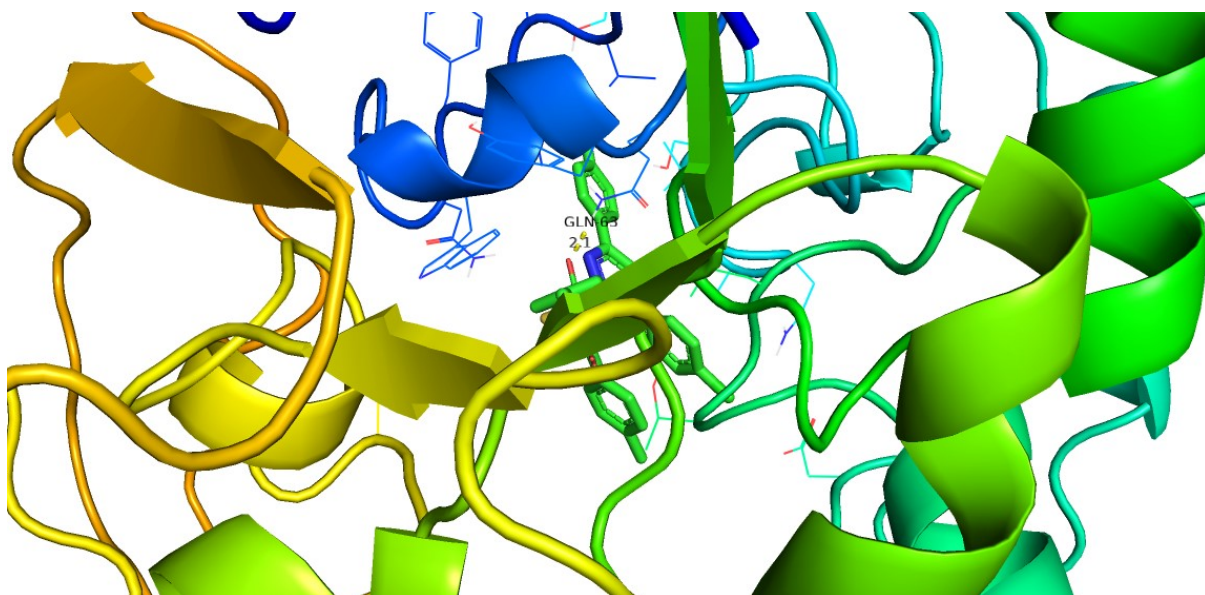
5g



5h

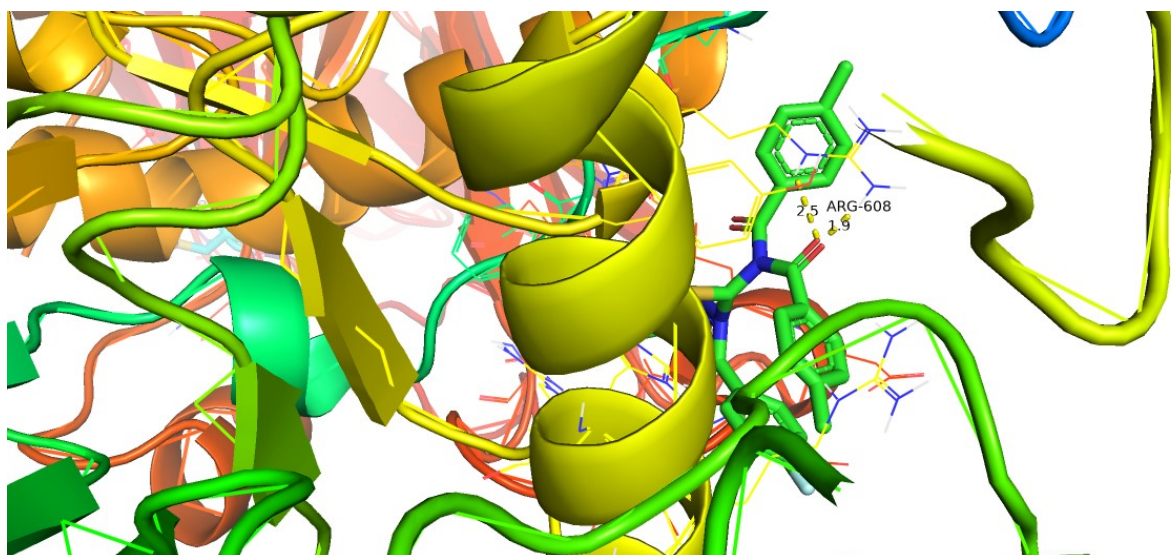


5i

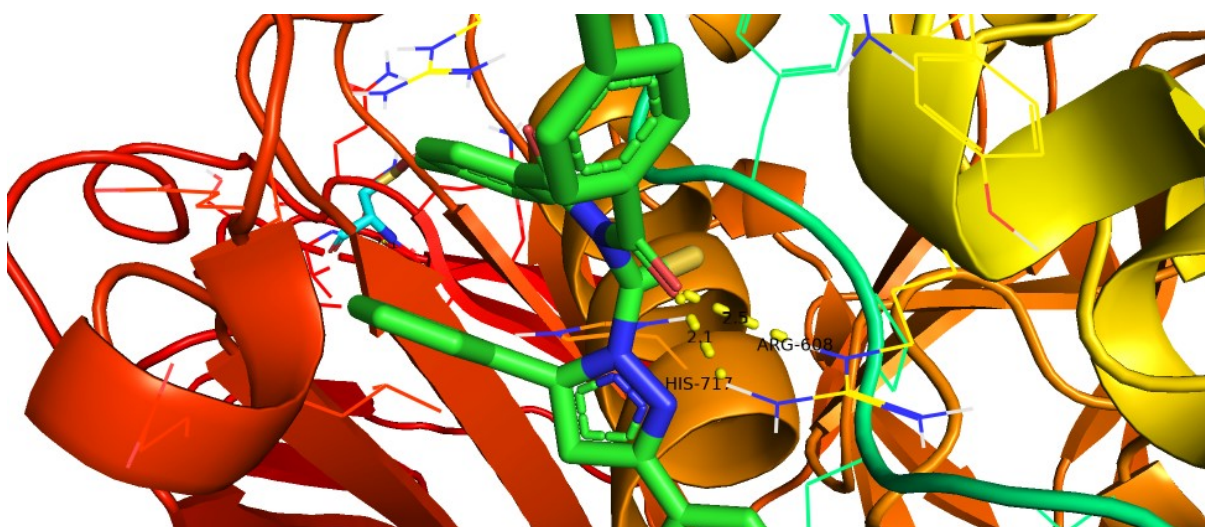


5j

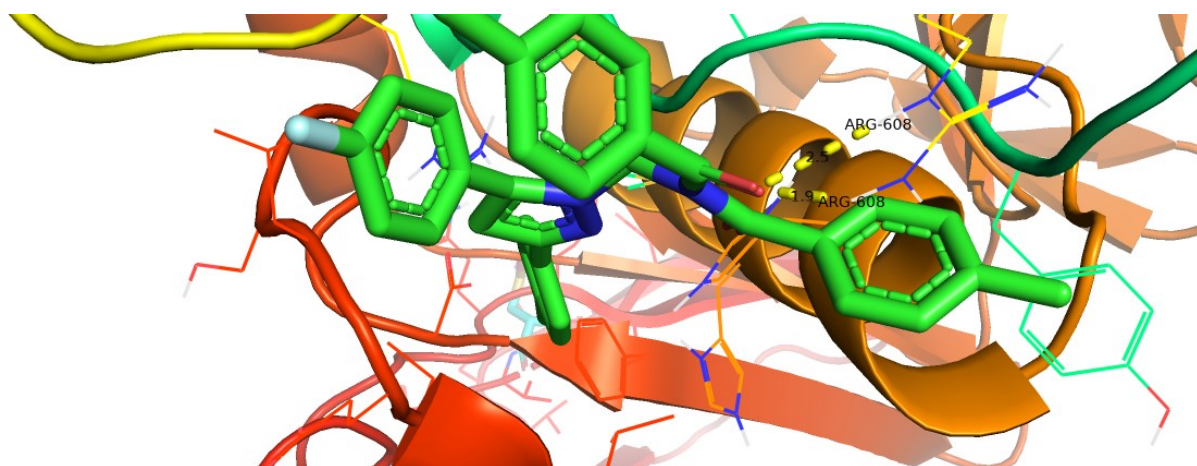
Figure 19. A-Glucosidase interaction images of compounds 5a, 5b 5c, 5d, 5e, 5f, 5g, 5h, 5i, 5j.



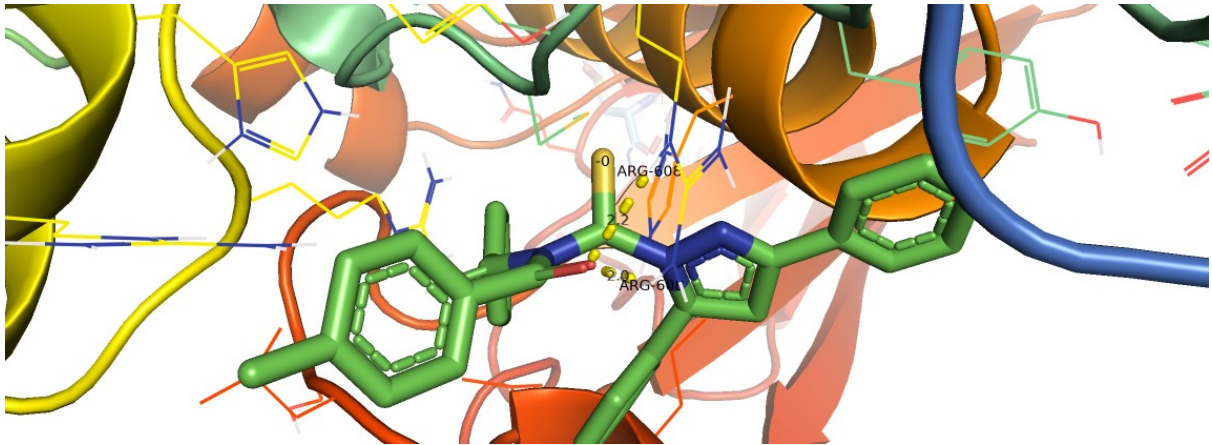
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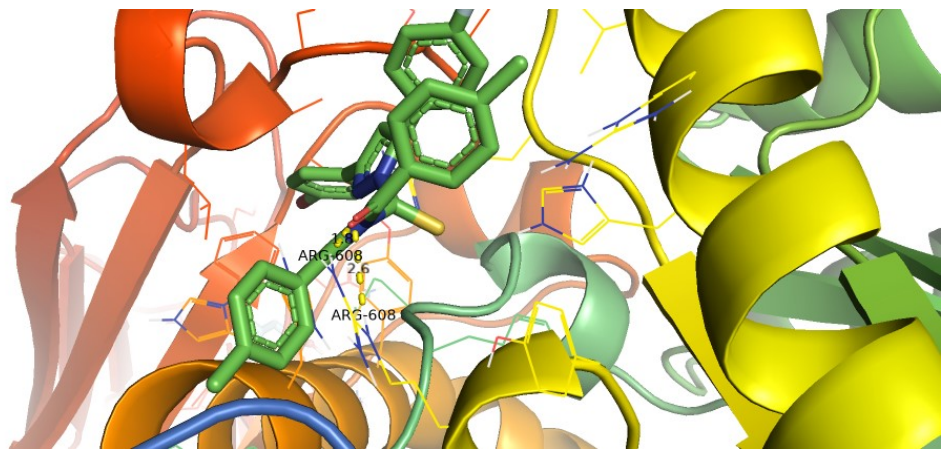
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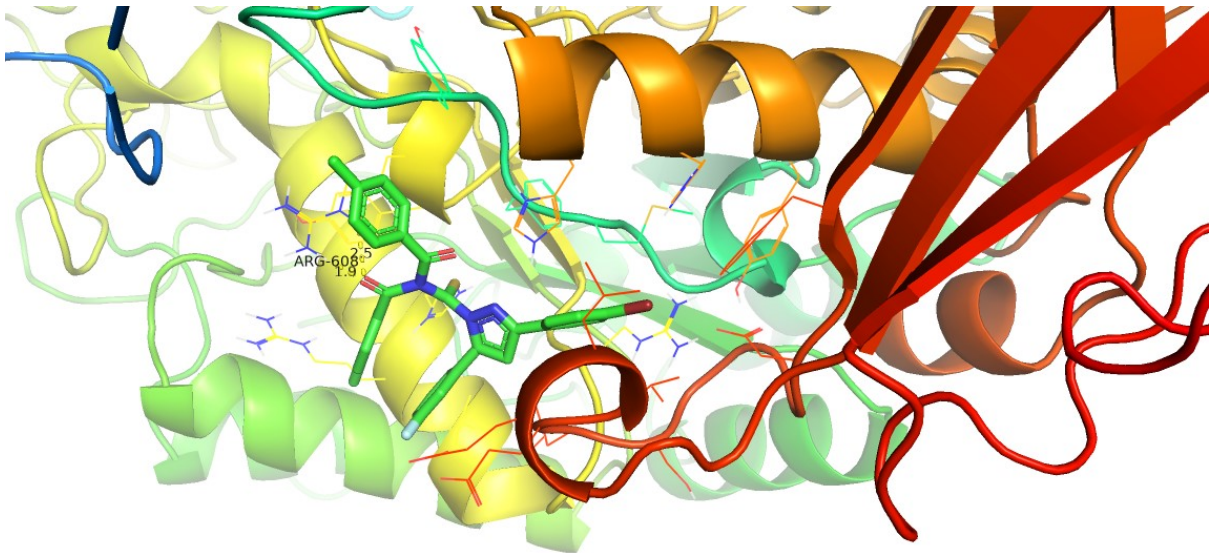
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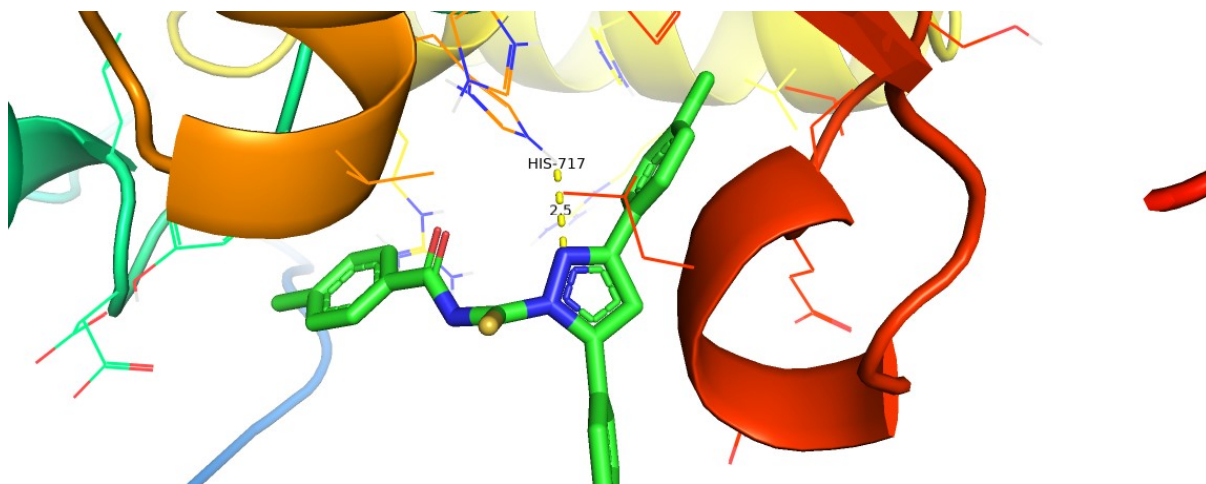
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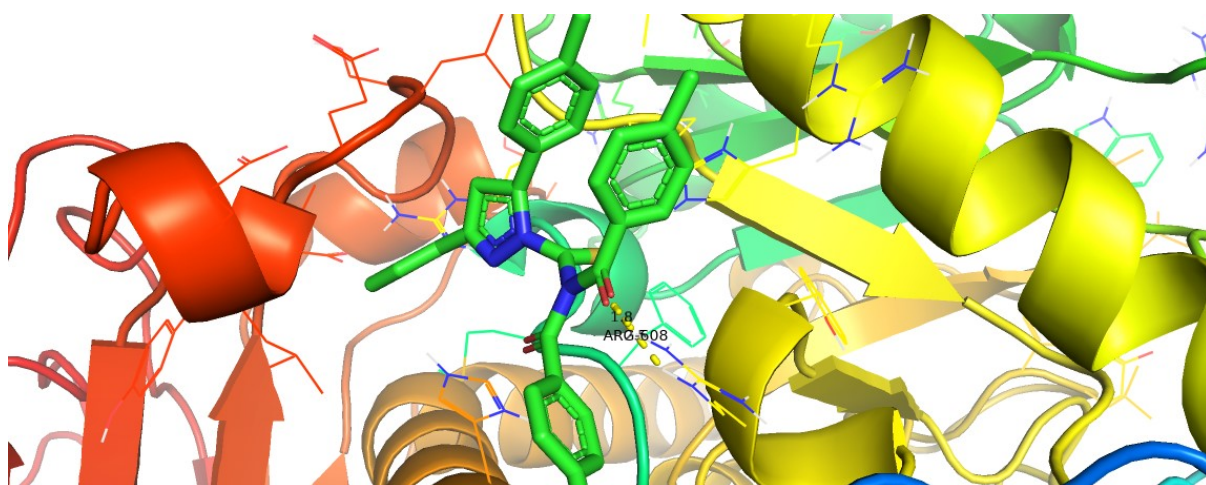
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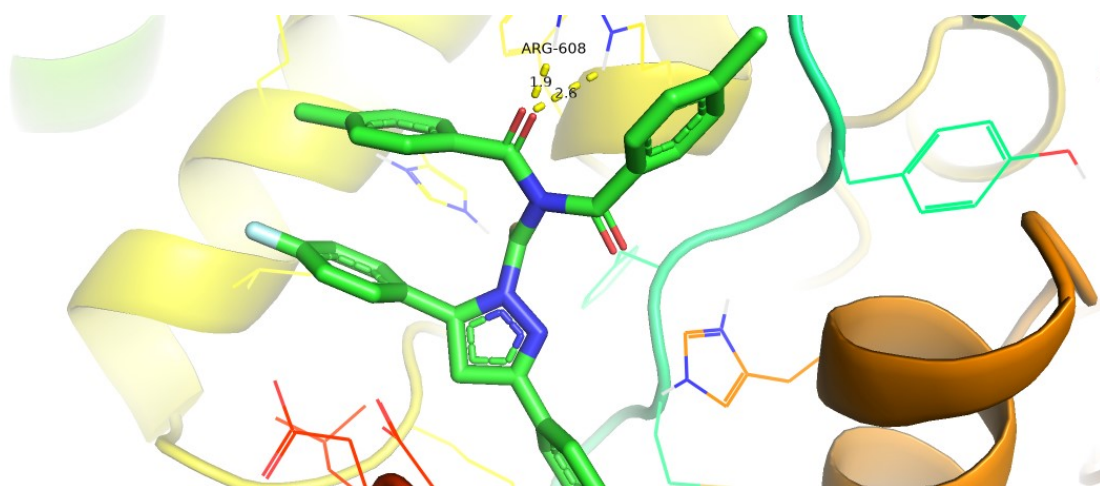
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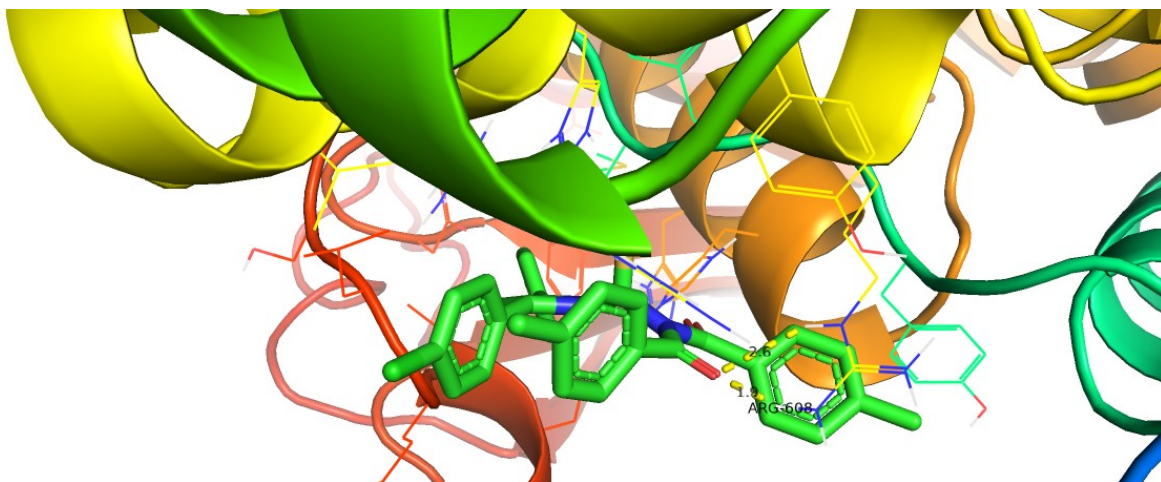
5g



5h

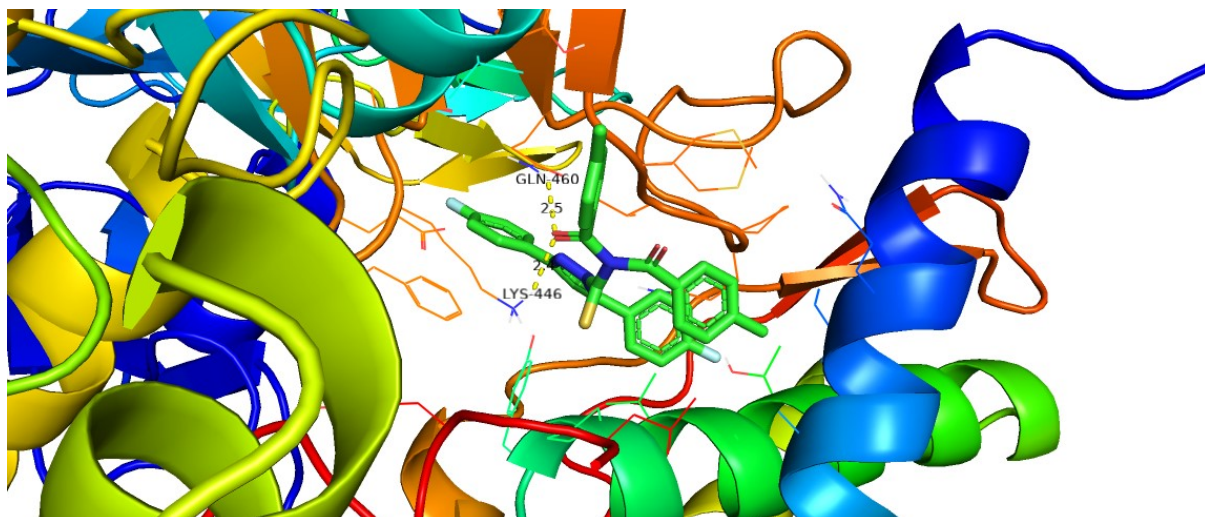


5i

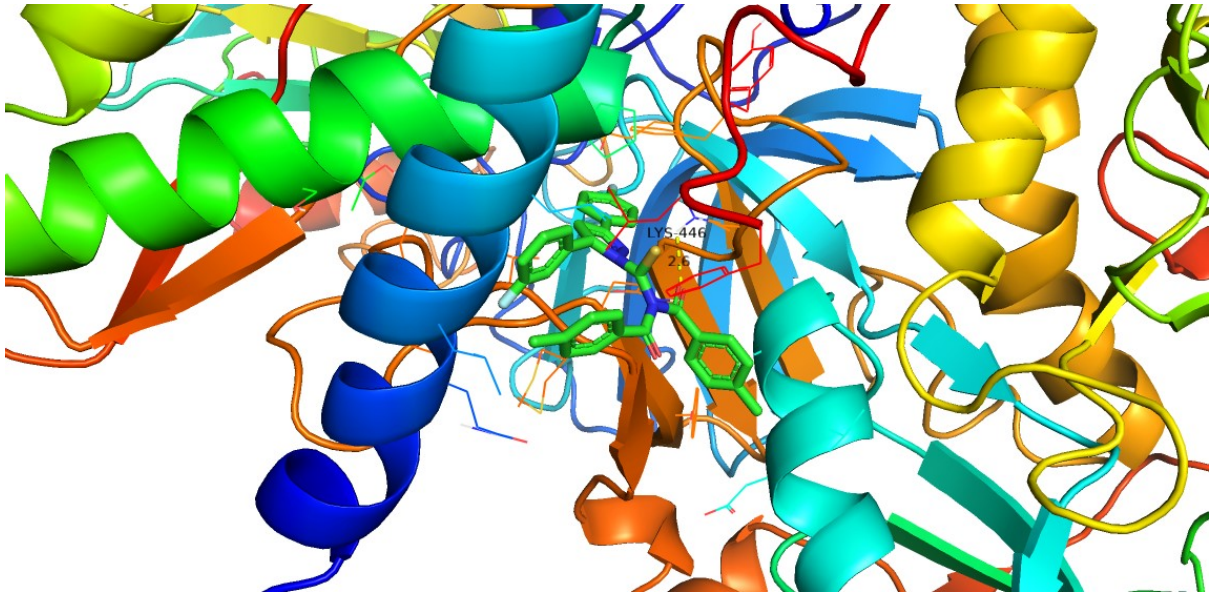


5j

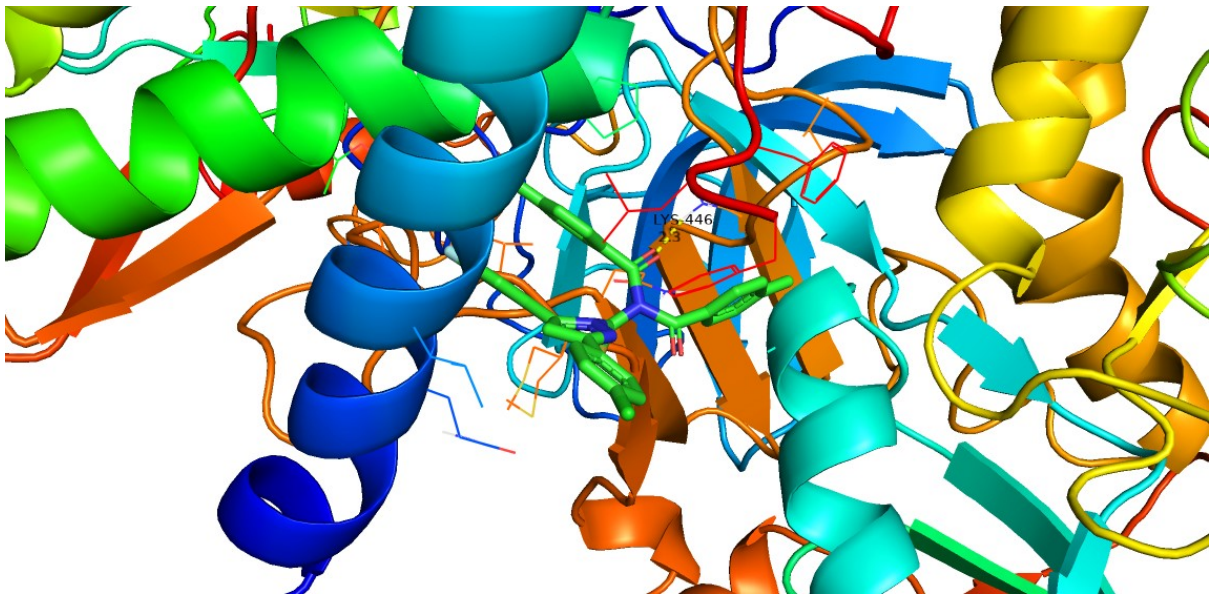
Figure 20. Urease interaction images of compounds 5a, 5b 5c, 5d, 5e, 5f, 5g, 5h, 5i, 5j.



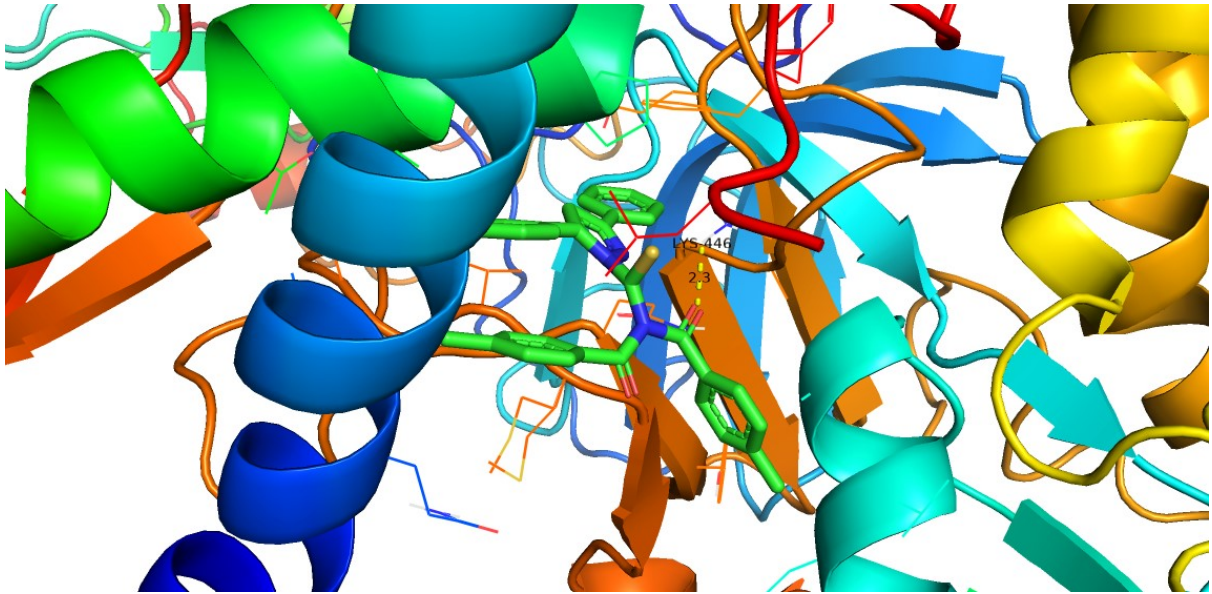
5a



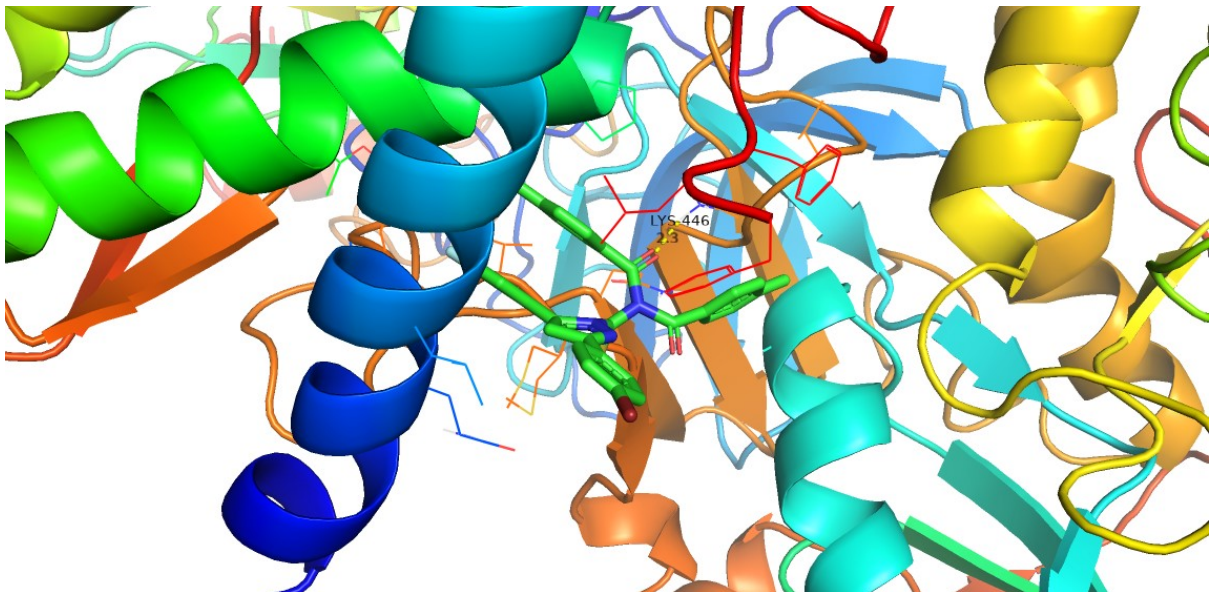
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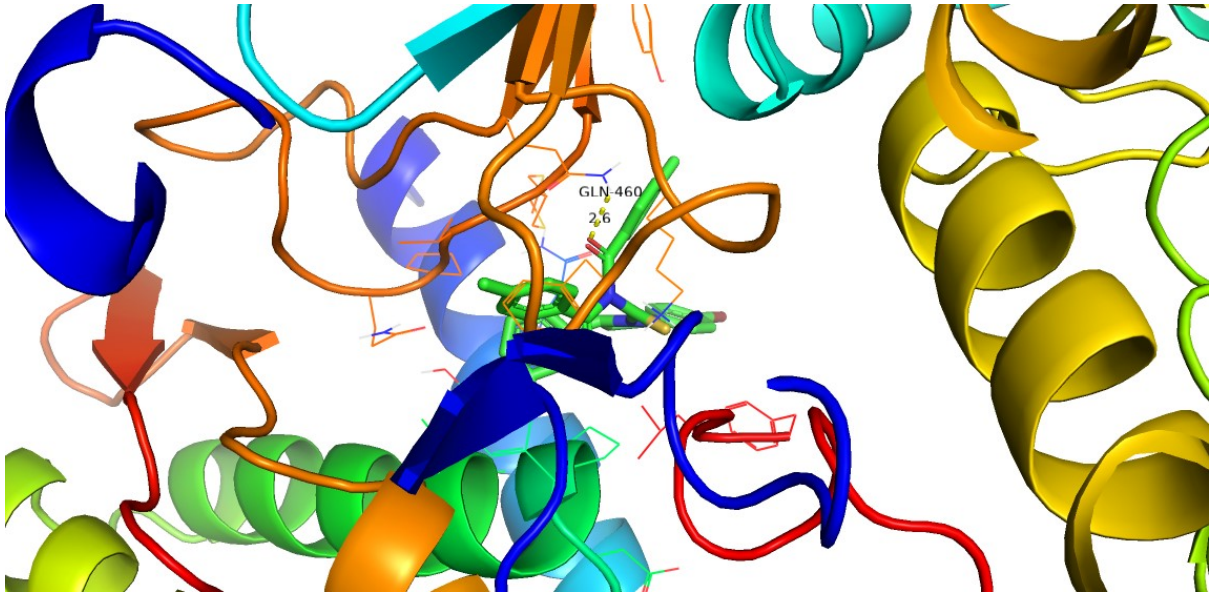
5c



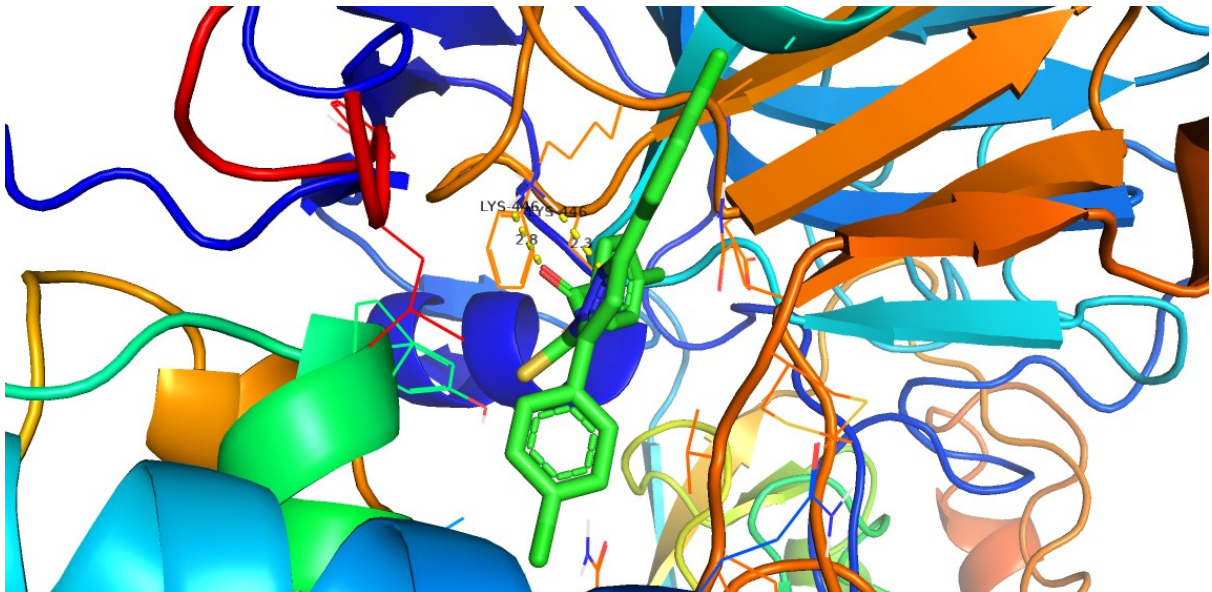
5d



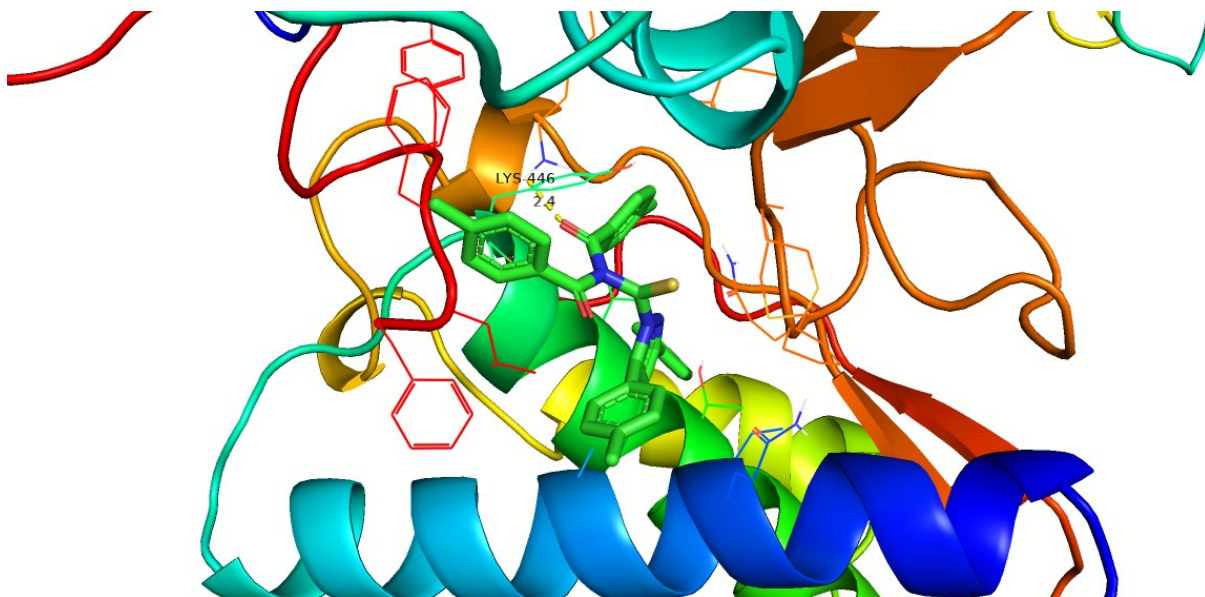
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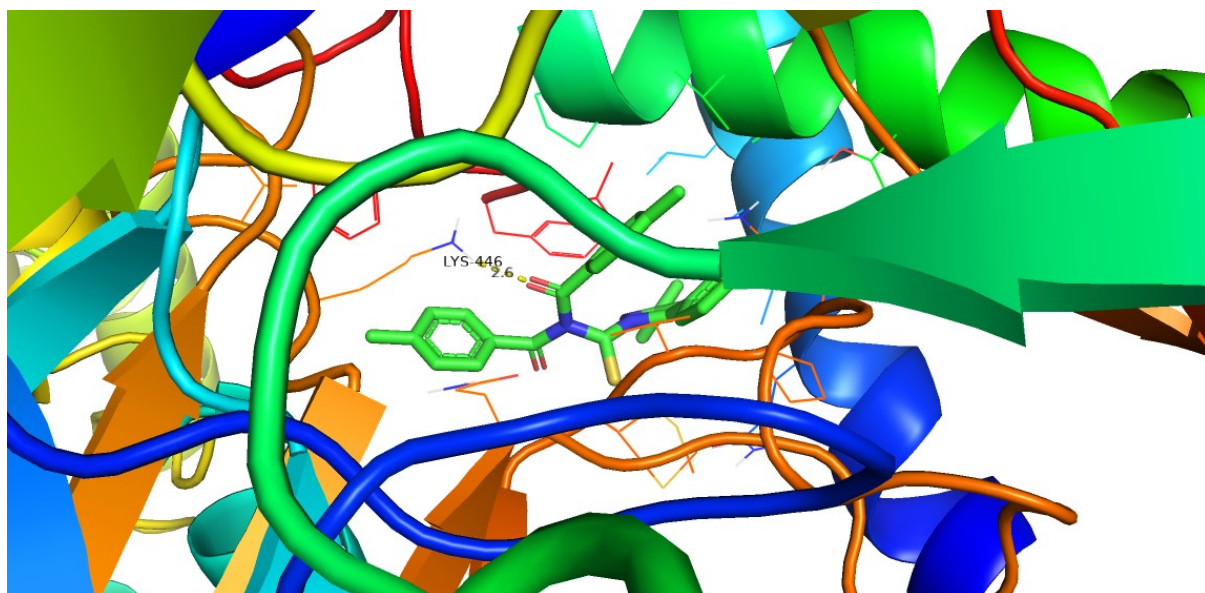
5f



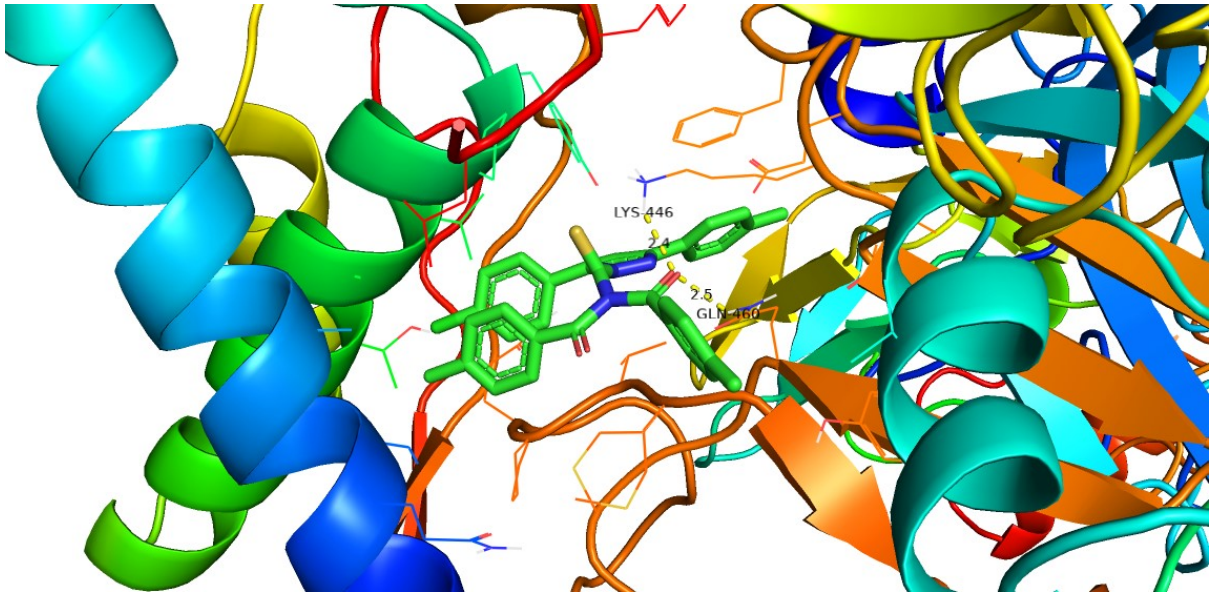
5g



5h



5i



5j