

supplementary materials

Targeting transcriptional CDKs 7, 8, and 9 with anilinopyrimidine derivatives as anticancer agents: Design, synthesis, and *in* *silico* studies

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¹Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, P.O.
Box 2457, Riyadh 11451, Saudi Arabia

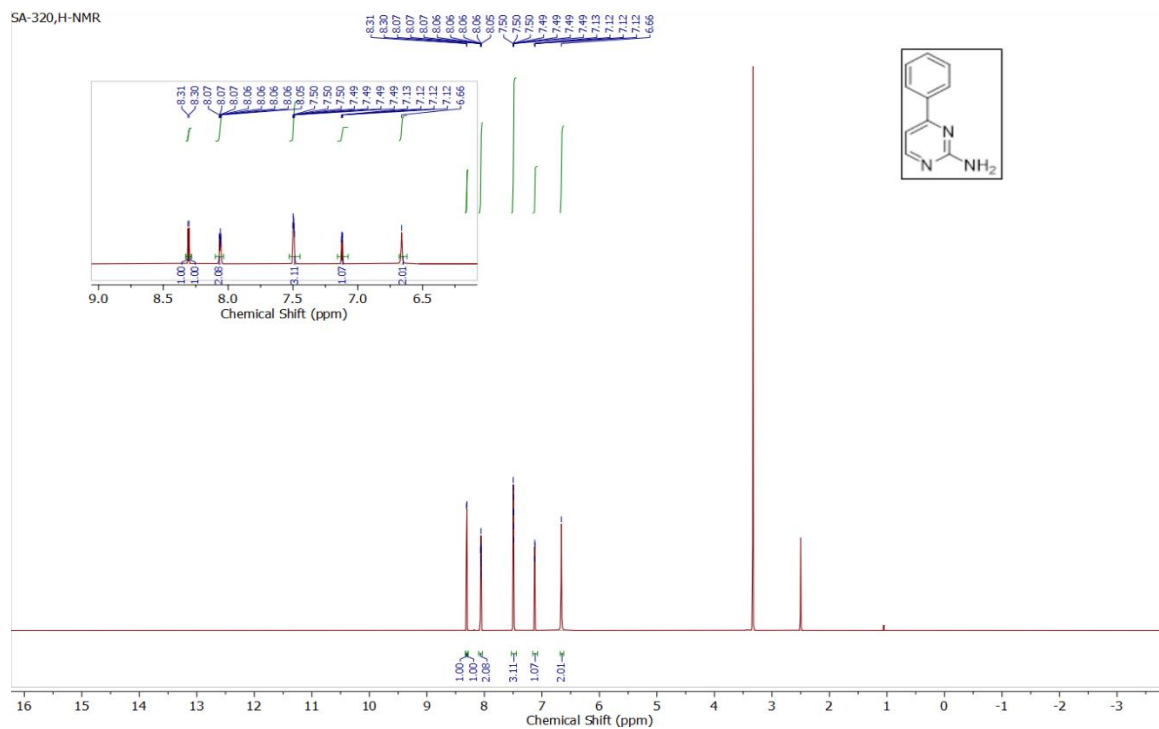
²Drug Exploration and Development (DEDC), Department of Pharmaceutical Chemistry,
College of Pharmacy, King Saud University, Riyadh 11451, Saudi Arabia

* Corresponding authors: Abdulrahman A. Almehizia, email: mehizia@ksu.edu.sa

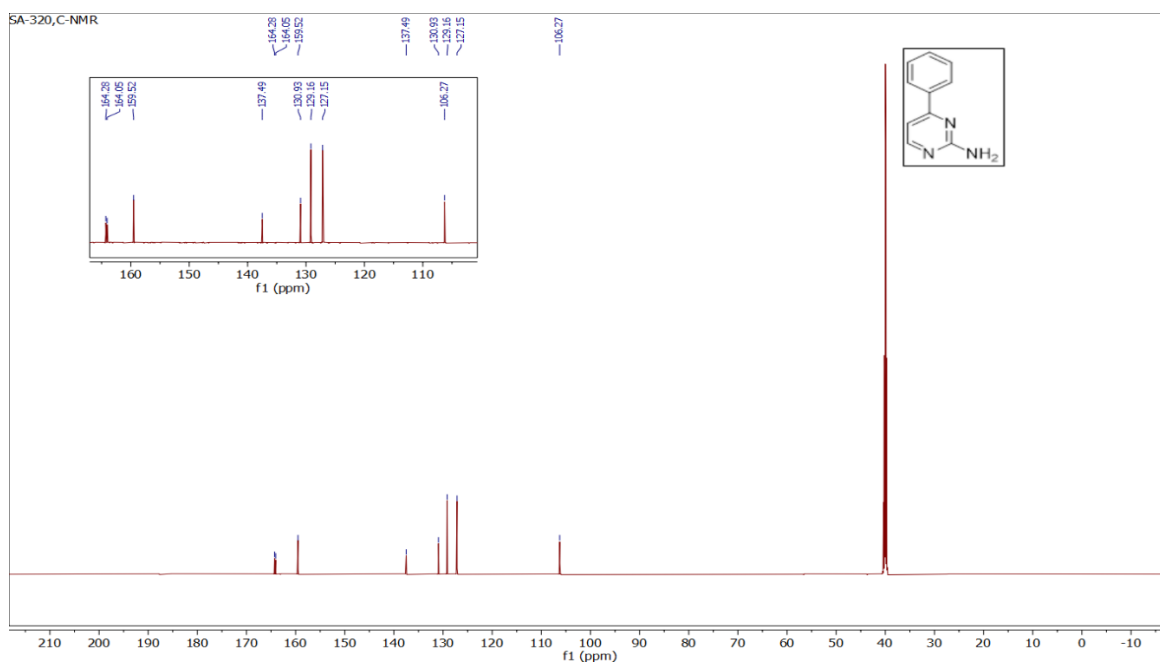
Hamad M. Alkahtani, email: ahamad@ksu.edu.sa

4.1.2.1. 4-phenylpyrimidin-2-amine (3a)

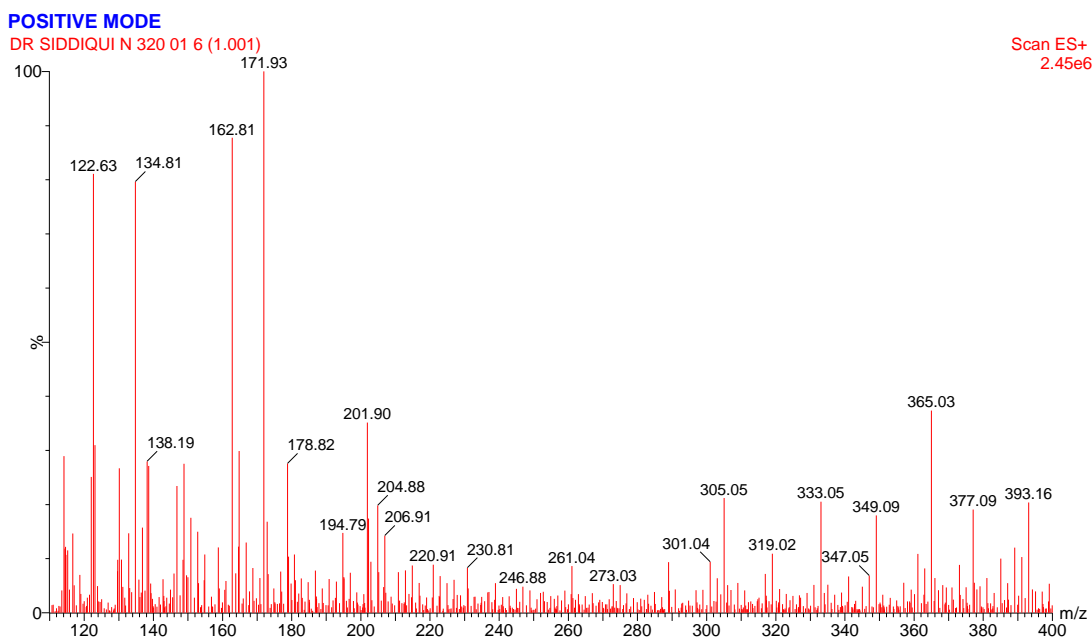
¹H-NMR spectra of compound (3a)



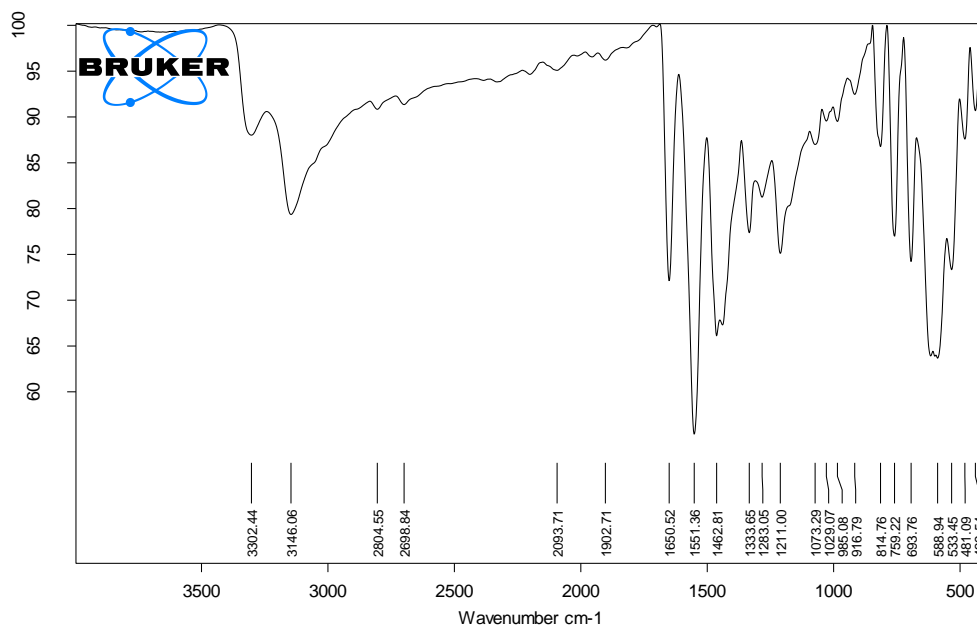
¹³C-NMR spectra of compound (3a)



Mass spectrum of compound (3a)



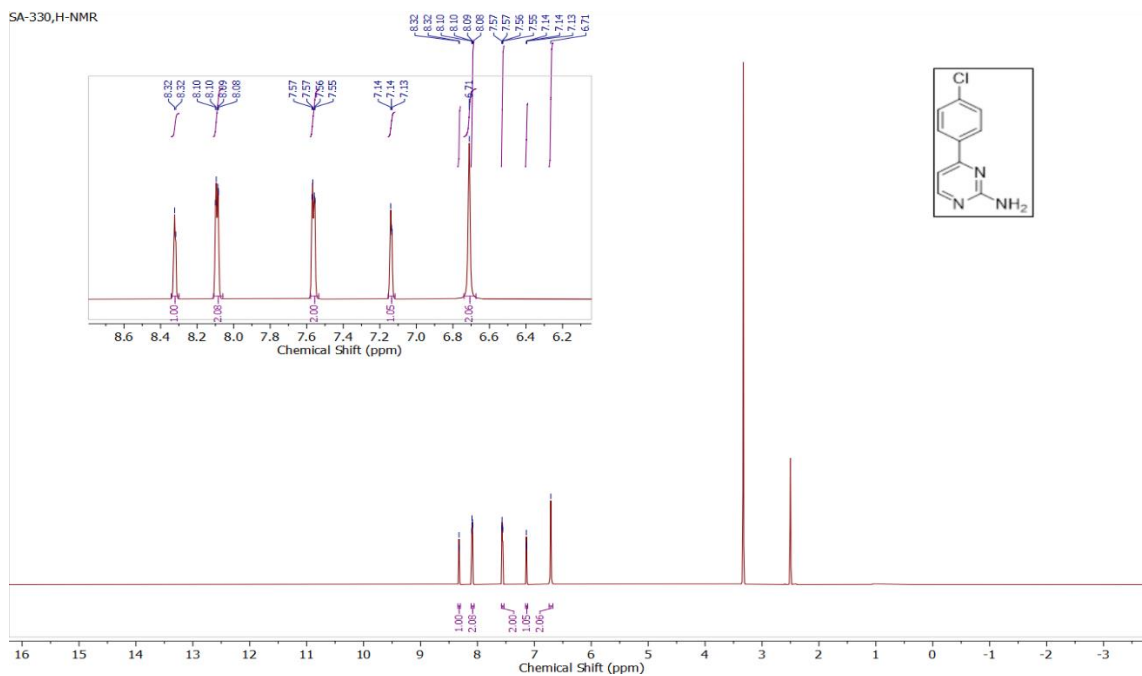
FTIR spectra of compound (3a)



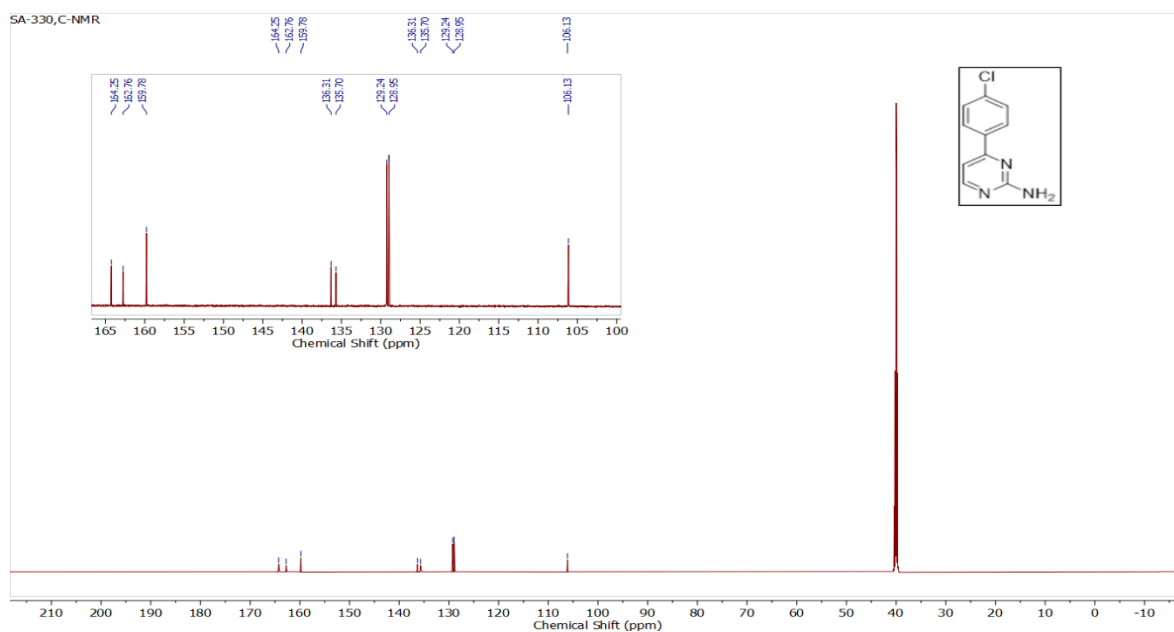
C:\Users\DELL\Documents\Bruker\OPUS_7.8.38\DATA\MEAS\AM-65 (320).0	AM-65 (320)	Instrument type and / or accessory	10/26/2022
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4.1.2.2. 4-(4-chlorophenyl)pyrimidin-2-amine (**3b**)

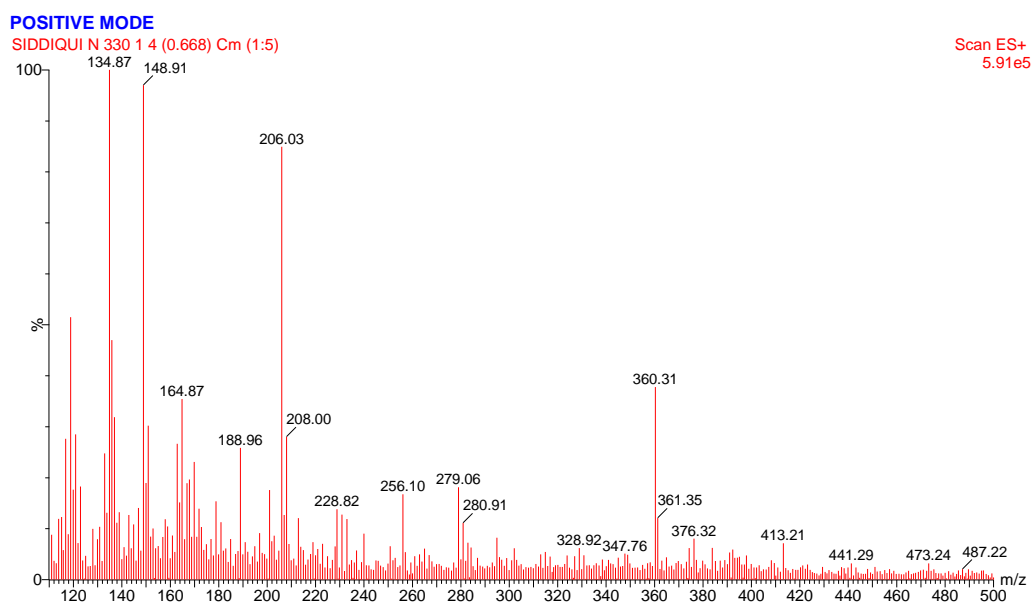
¹H-NMR spectra of compound (**3b**)



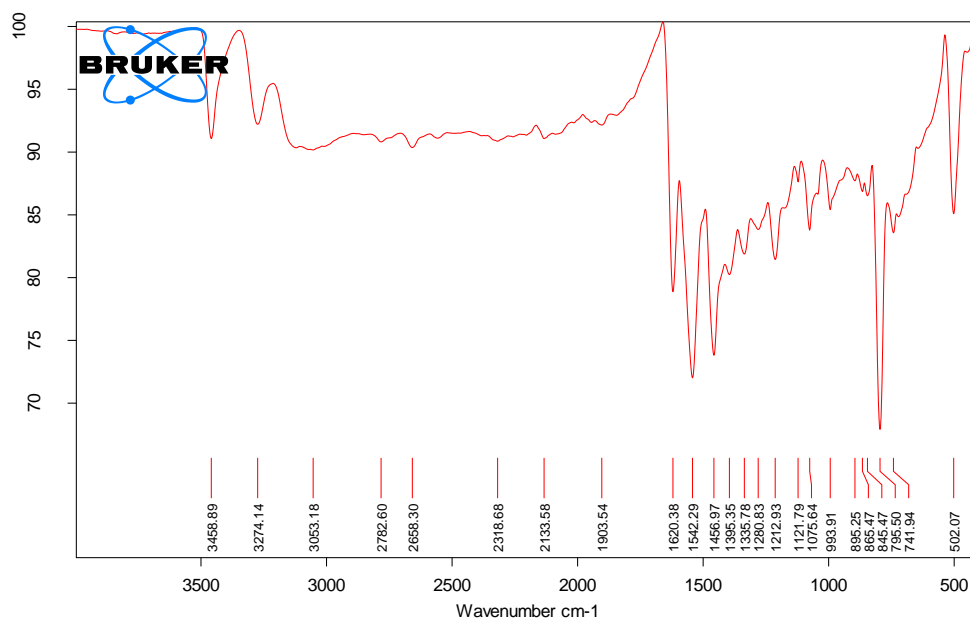
¹³C-NMR spectra of compound (**3b**)



Mass spectrum of compound (3b)



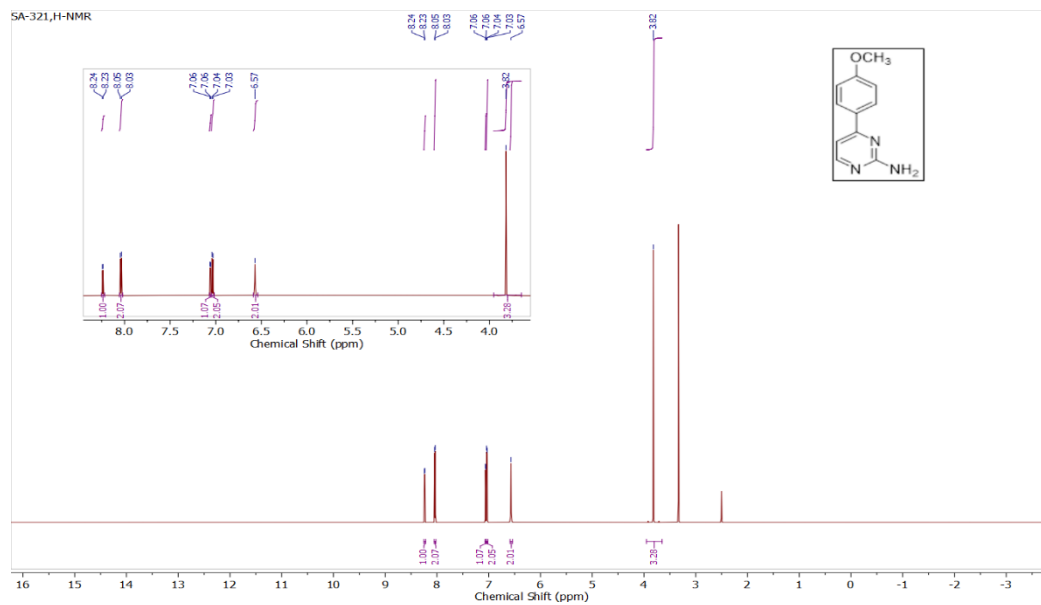
FTIR spectra of compound (3b)



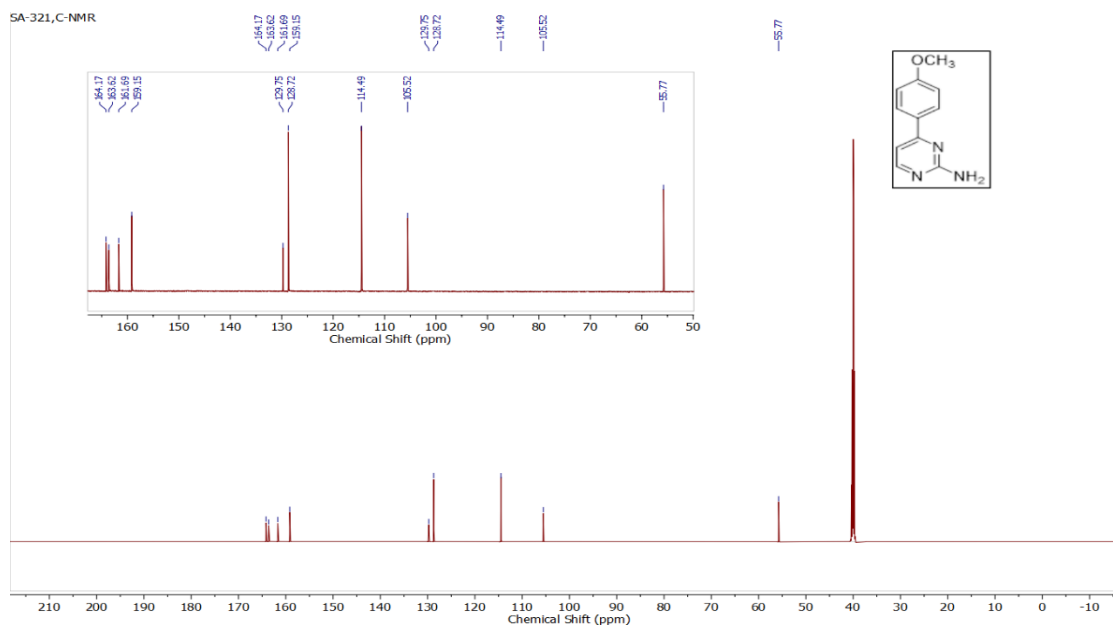
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4.1.2.3. 4-(4-methoxyphenyl)pyrimidin-2-amine (3c)

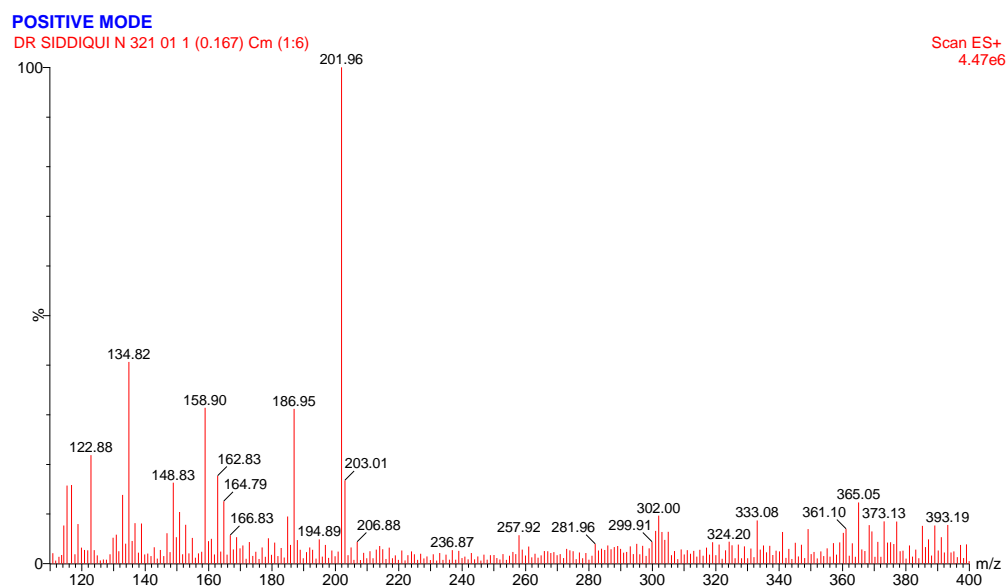
¹H-NMR spectra of compound (3c)



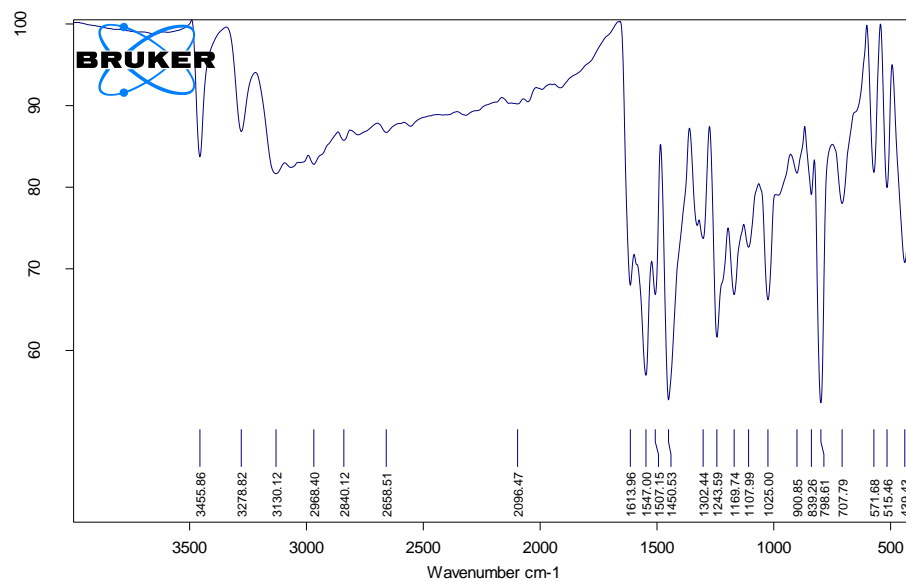
¹³C-NMR spectra of compound (3c)



Mass spectrum of compound (3c)



FTIR spectra of compound (3c)



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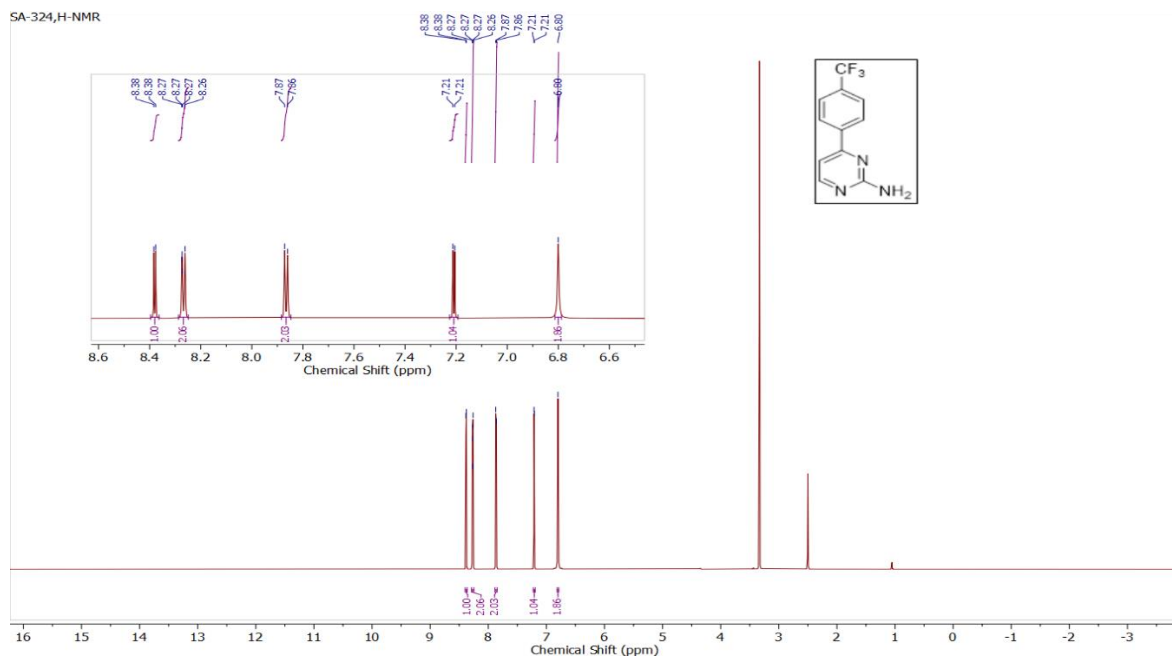
AM-65 (321)

Instrument type and / or accessory

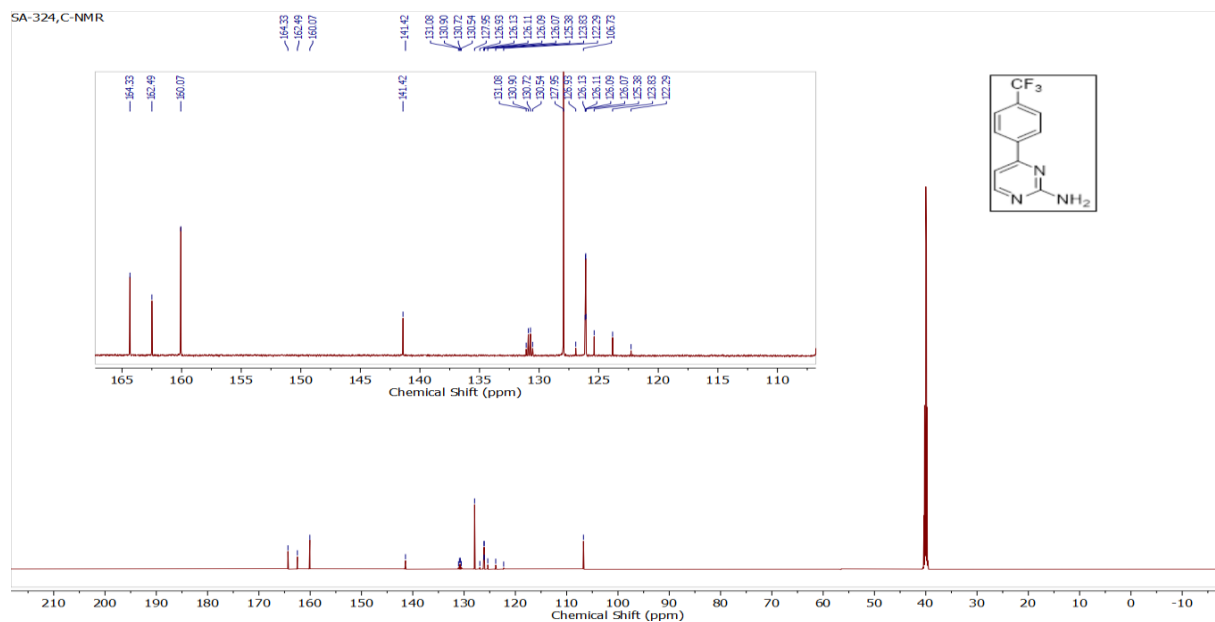
10/26/2022

4.1.2.4. 4-(4-(trifluoromethyl)phenyl)pyrimidin-2-amine (3d)

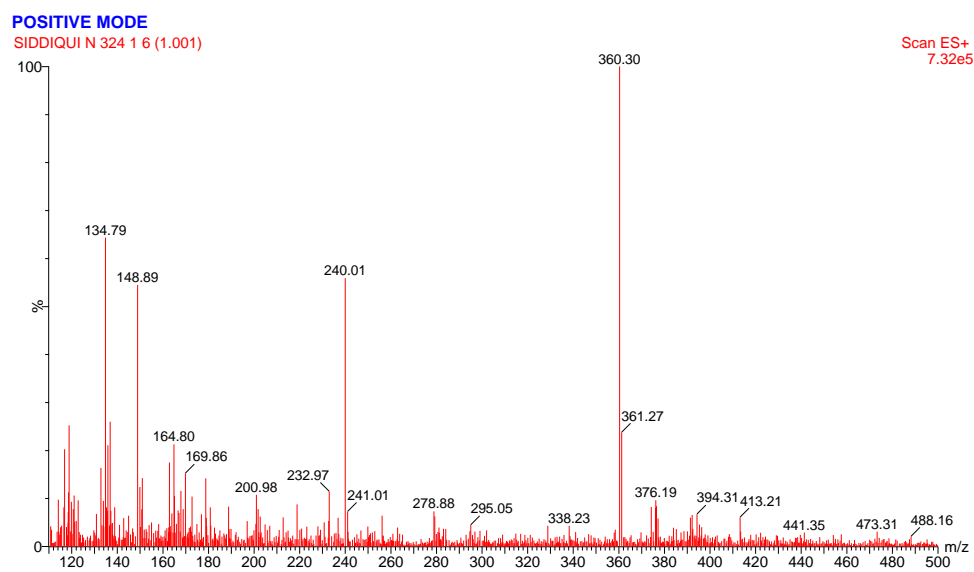
¹H-NMR spectra of compound (3d)



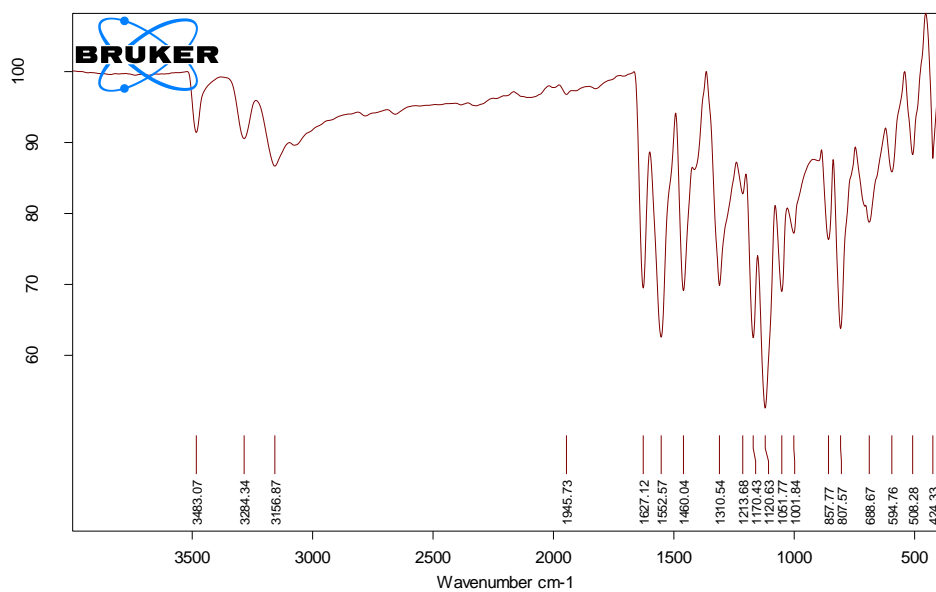
¹³C-NMR spectra of compound (3d)



Mass spectrum of compound (3d)

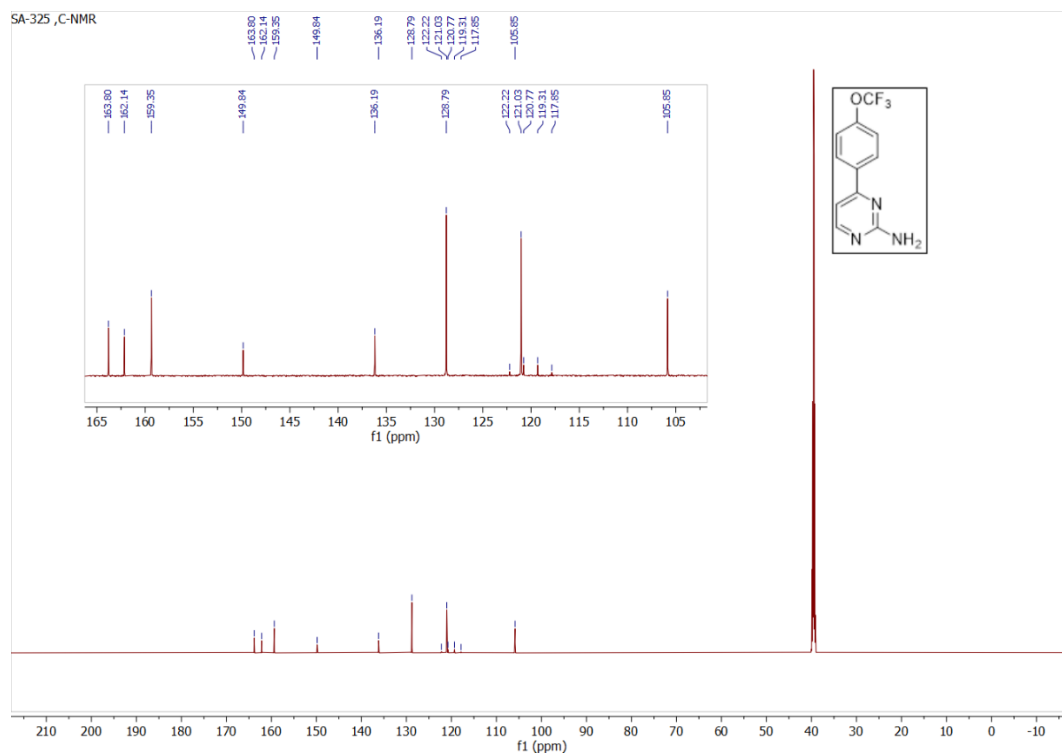
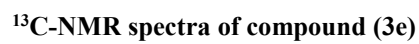


FTIR spectra of compound (3d)

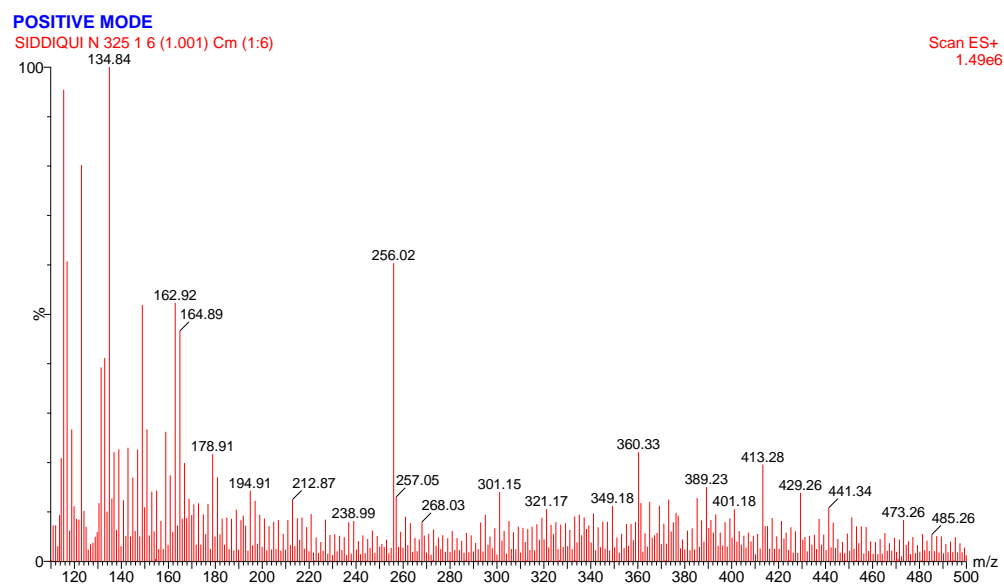


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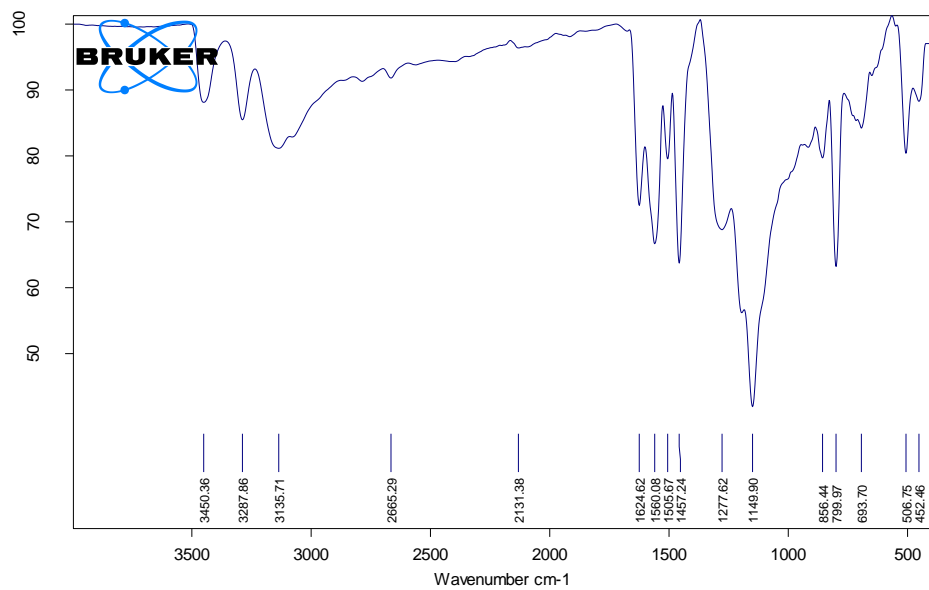
¹H-NMR spectra of compound (3e)



Mass spectrum of compound (3e)

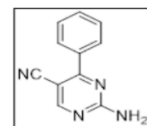


FTIR spectra of compound (3e)



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¹H-NMR spectra of compound (3f)



SA-273 C13-NMR

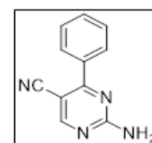
Chemical structure: Nc1nc(C#N)c(c1)-c2ccccc2

Chemical Shift (ppm):

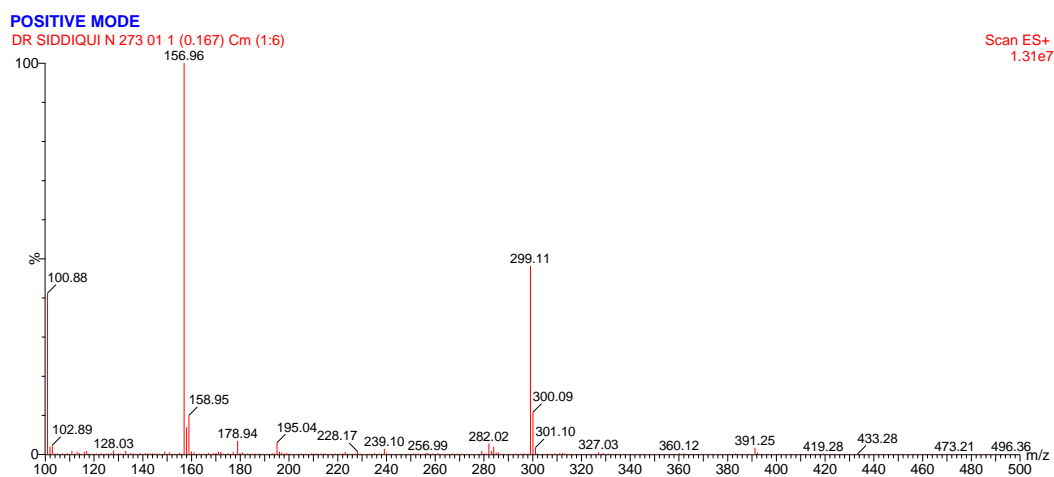
- 168.51
- 164.21
- 163.81
- 136.35
- 131.57
- 129.03
- 128.77
- 118.55
- 93.09

Chemical Shift (ppm):

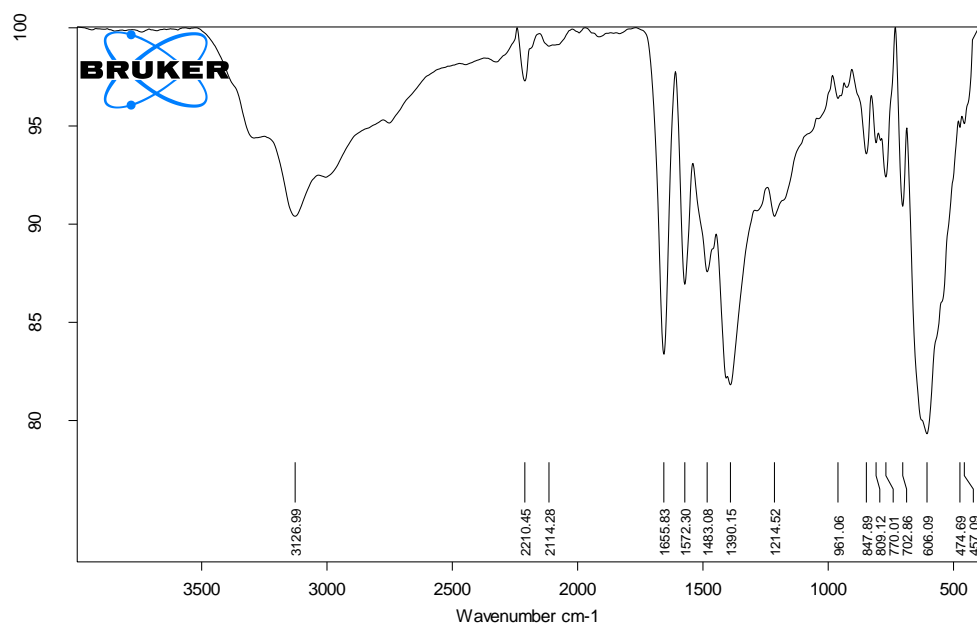
- 168.51
- 164.21
- 163.81
- 136.35
- 131.57
- 129.03
- 128.77
- 118.55
- 93.09



Mass spectrum of compound (3f)



FTIR spectra of compound (3f)



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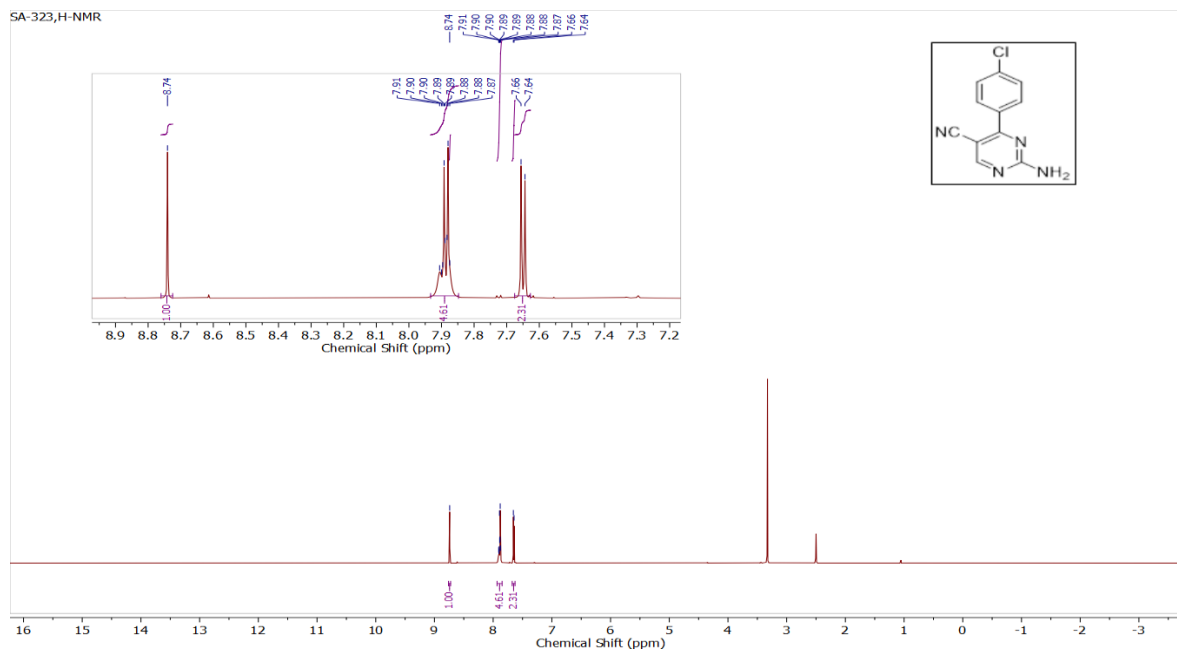
AM-65 (273)

Instrument type and / or accessory

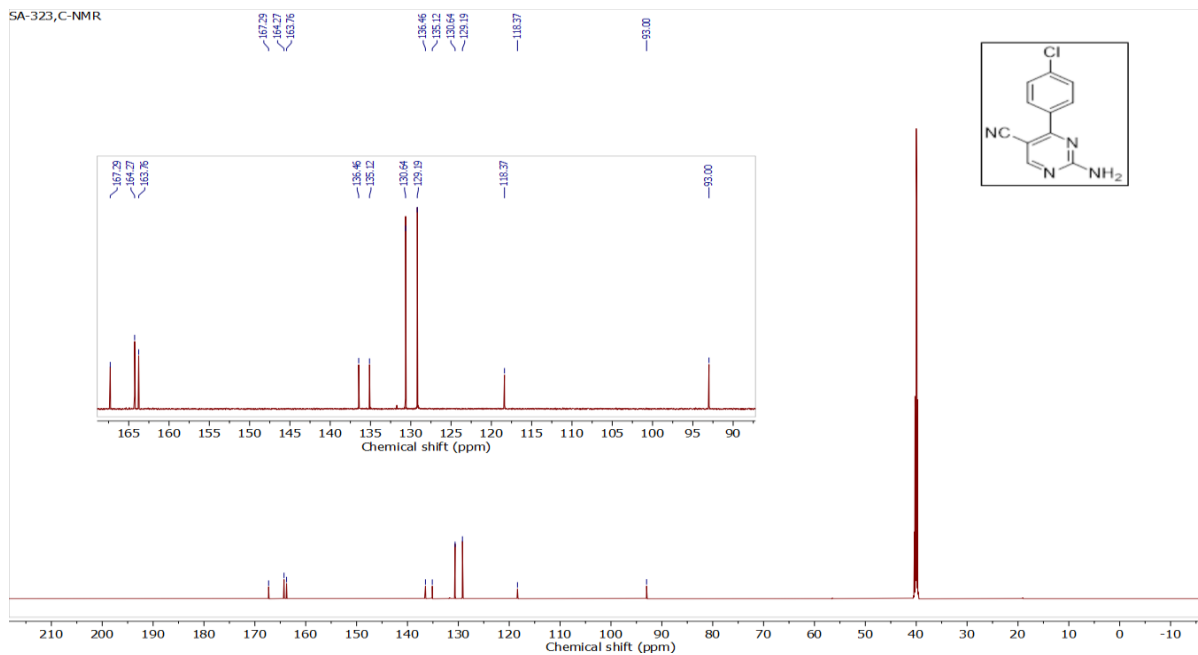
10/26/2022

4.1.2.7. 2-amino-4-(4-chlorophenyl)pyrimidine-5-carbonitrile (3g)

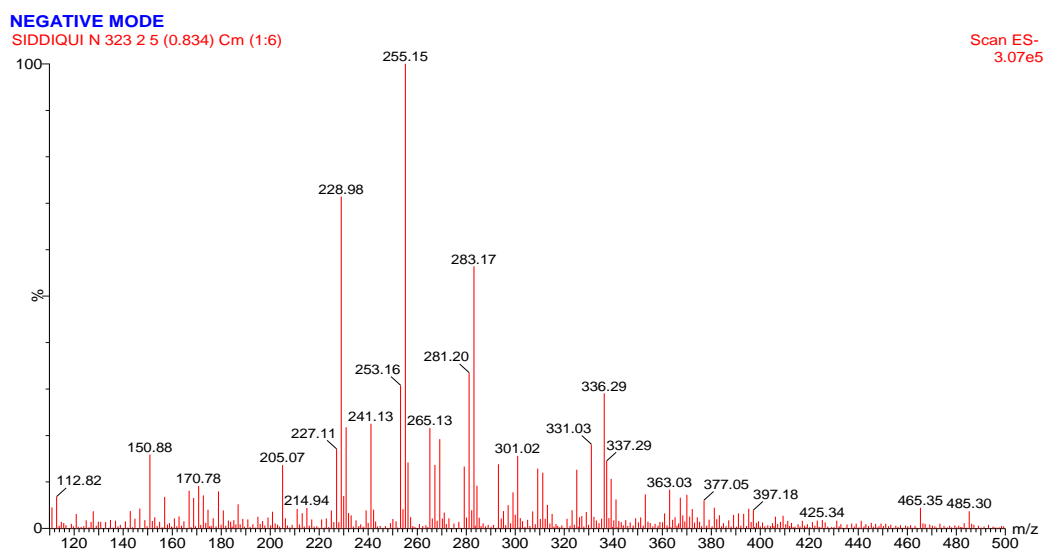
¹H-NMR spectra of compound (3g)



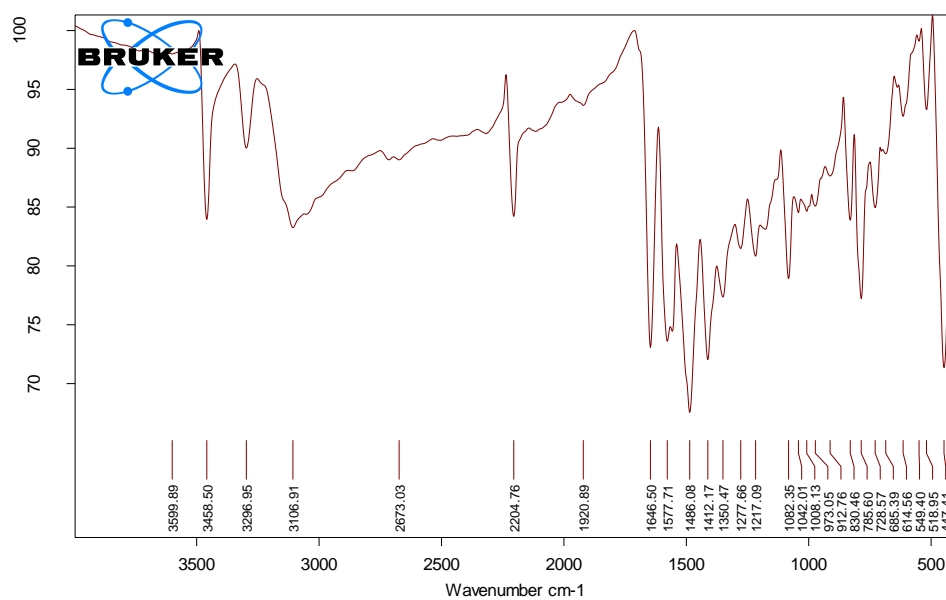
¹³C-NMR spectra of compound (3g)



Mass spectrum of compound (3g)



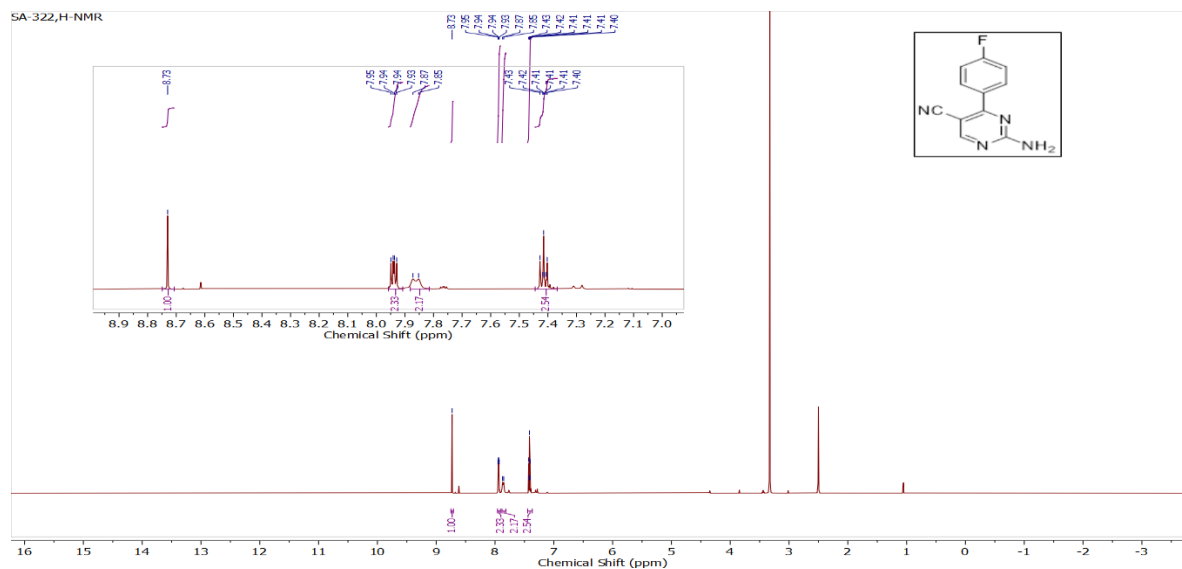
FTIR spectra of compound (3g)



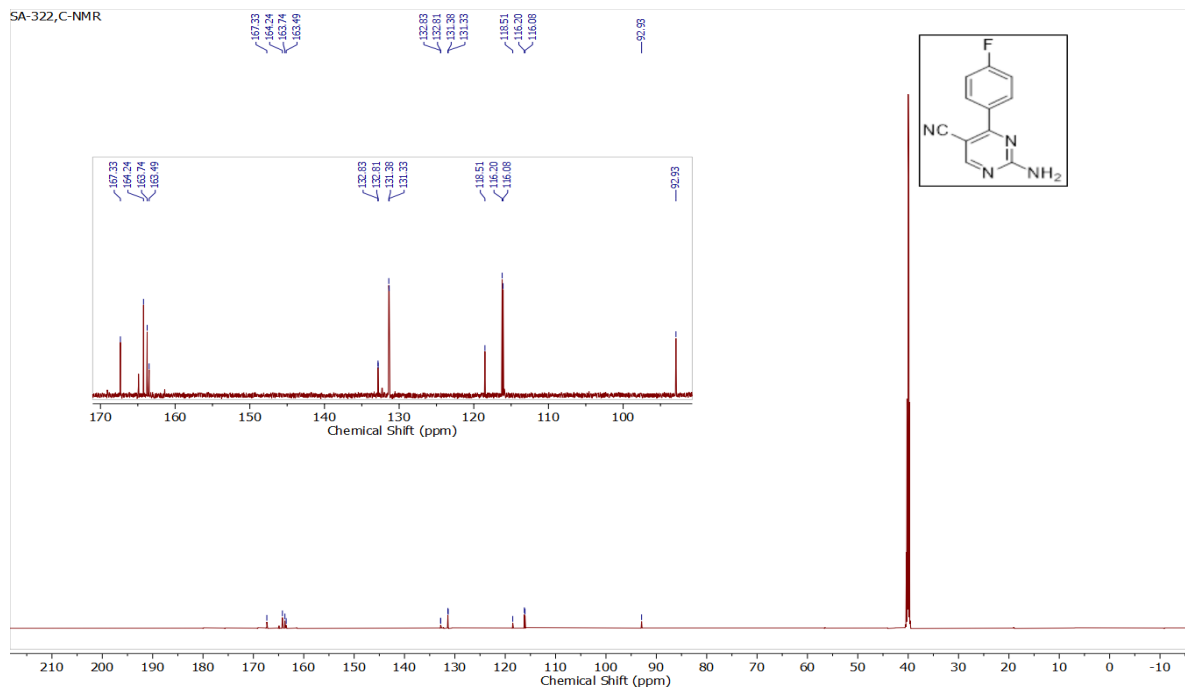
C:\Users\DELL\Documents\Bruker\OPUS_7.8.38\DATA\MEAS\AM-65 (323).0 AM-65 (323) Instrument type and / or accessory 10/26/2022

4.1.2.8. 2-amino-4-(4-fluorophenyl)pyrimidine-5-carbonitrile (3h)

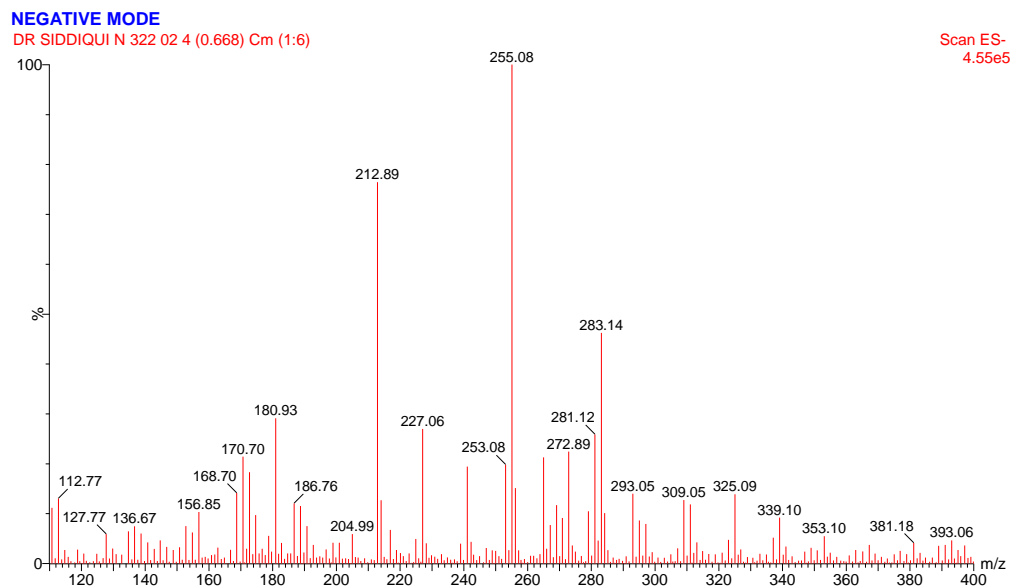
¹H-NMR spectra of compound (3h)



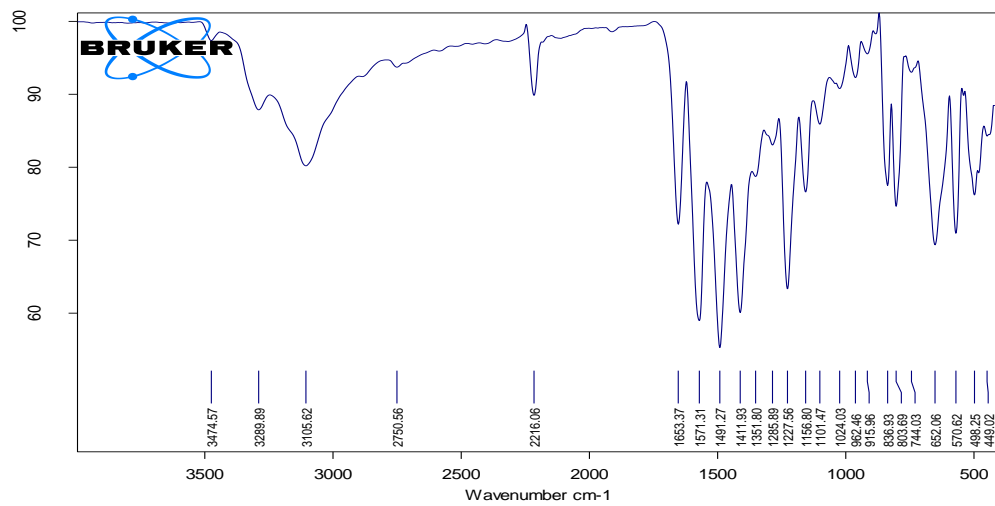
¹³C-NMR spectra of compound (3h)



Mass spectrum of compound (3h)



FTIR spectra of compound (3h)



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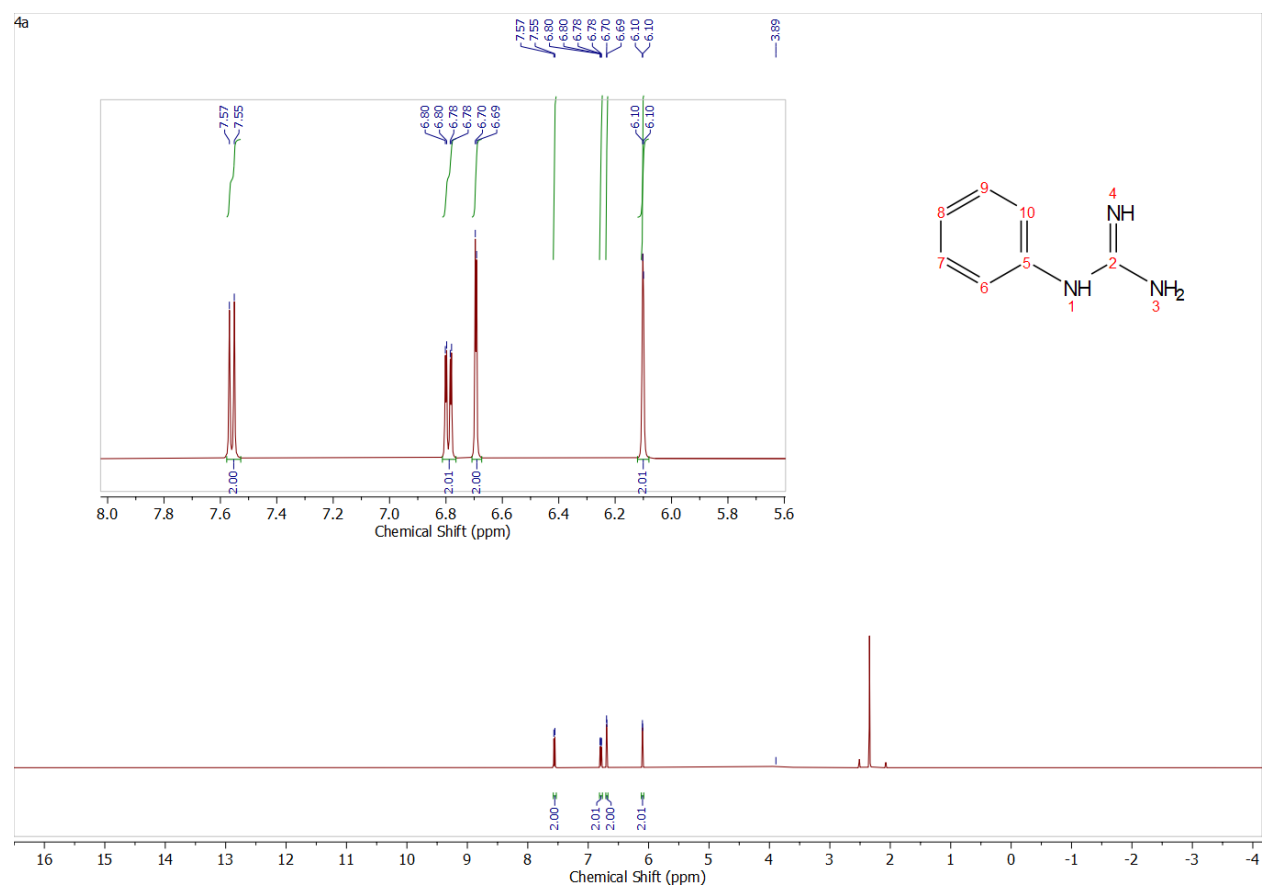
AM-65 (322)

Instrument type and / or accessory

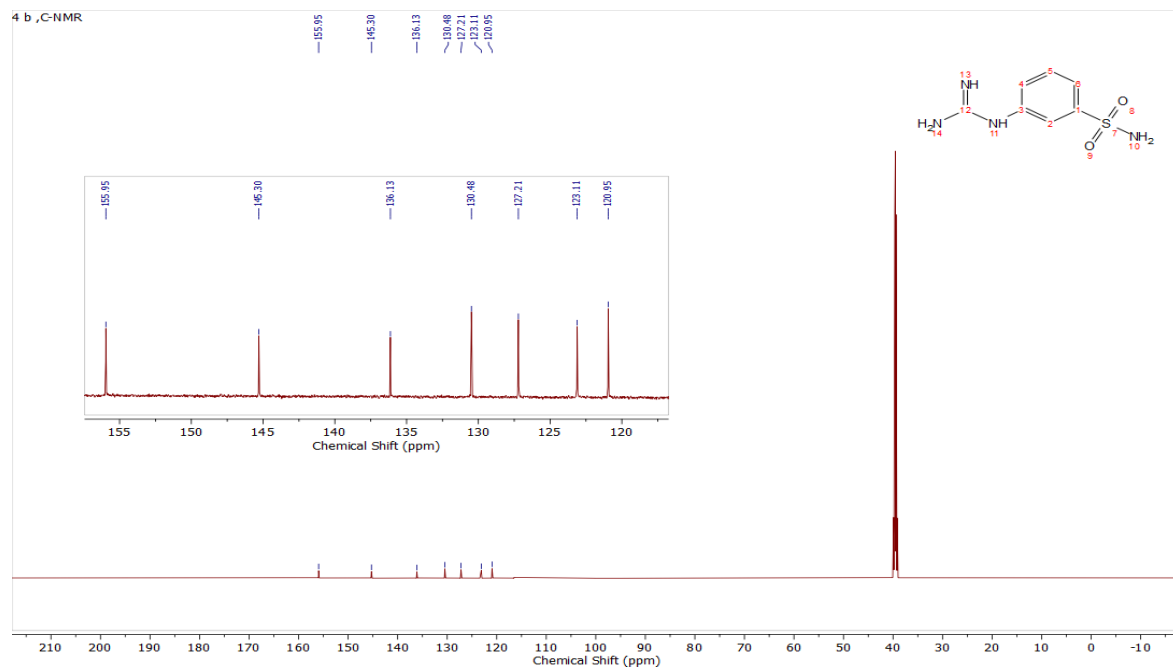
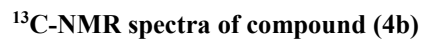
10/26/2022

4.1.3.1. 1-Phenylguanidine (4a)

¹H-NMR spectra of compound (4a)

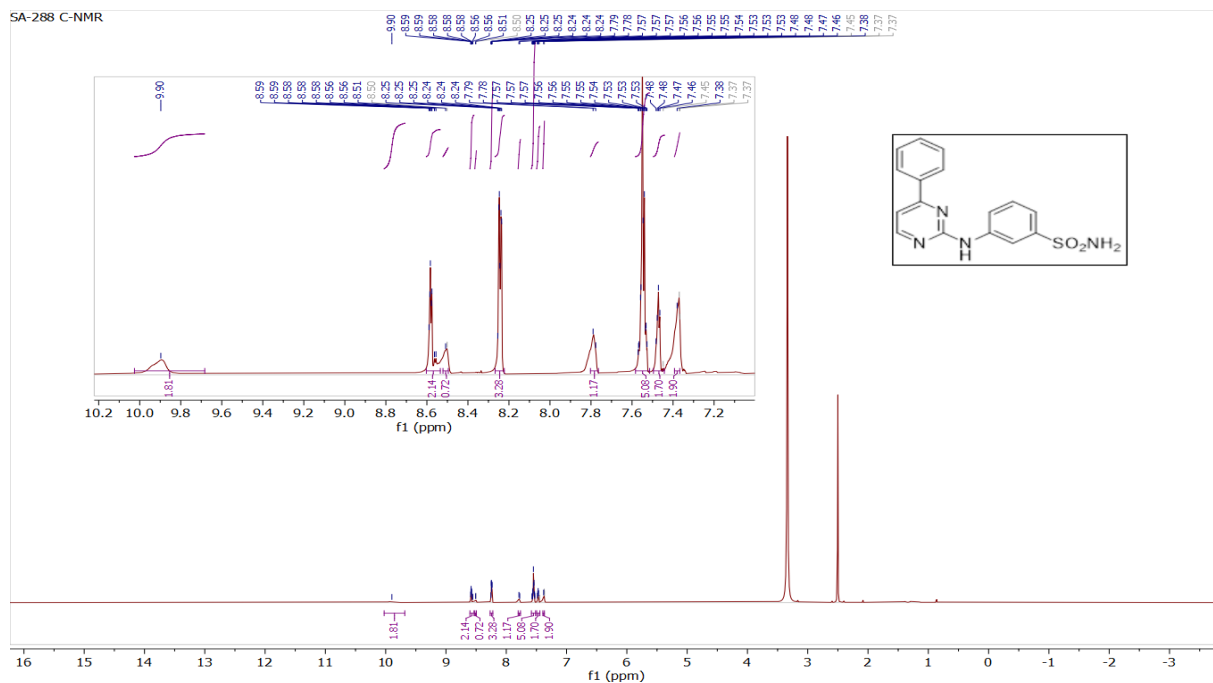


¹H-NMR spectra of compound (4b)

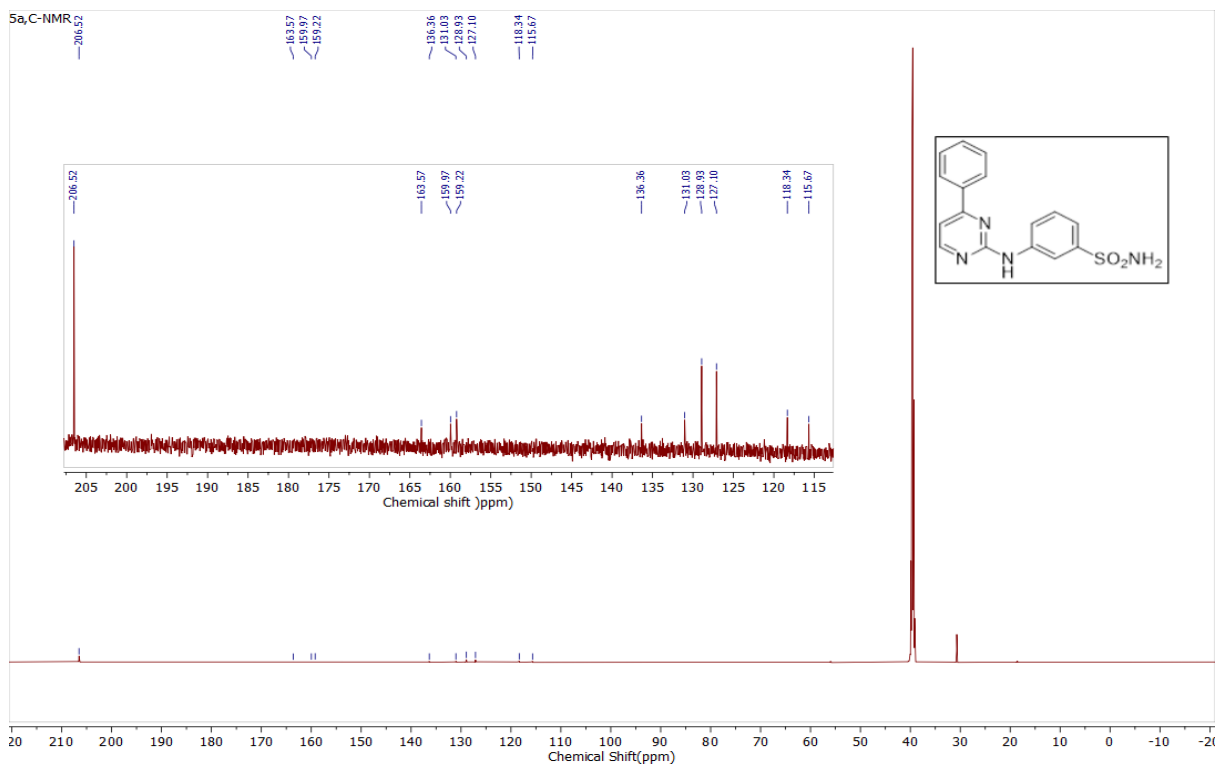


4.1.4.1. 3-((4-Phenylpyrimidin-2-yl)amino)benzenesulfonamide (5a)

¹H-NMR spectra of compound (5a)



¹³C-NMR spectra of compound (5a)

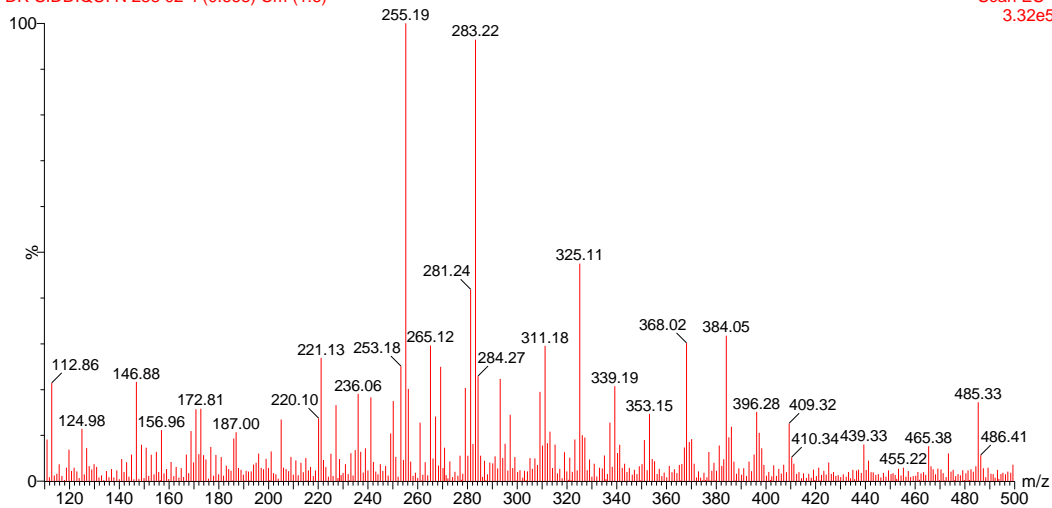


Mass spectrum of compound (5a)

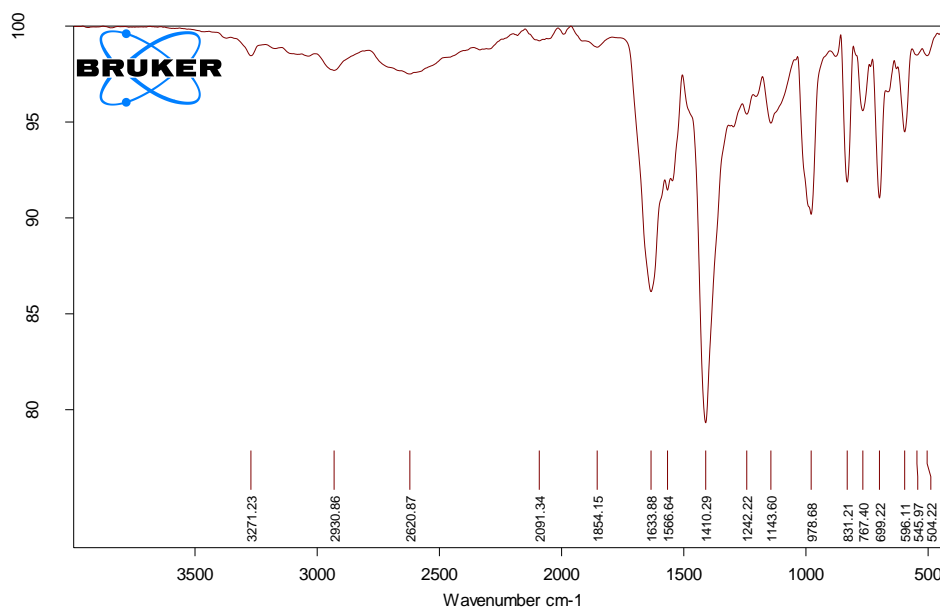
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DR SIDDIQUI N 288 02 4 (0.668) Cm (1:6)

Scan ES-
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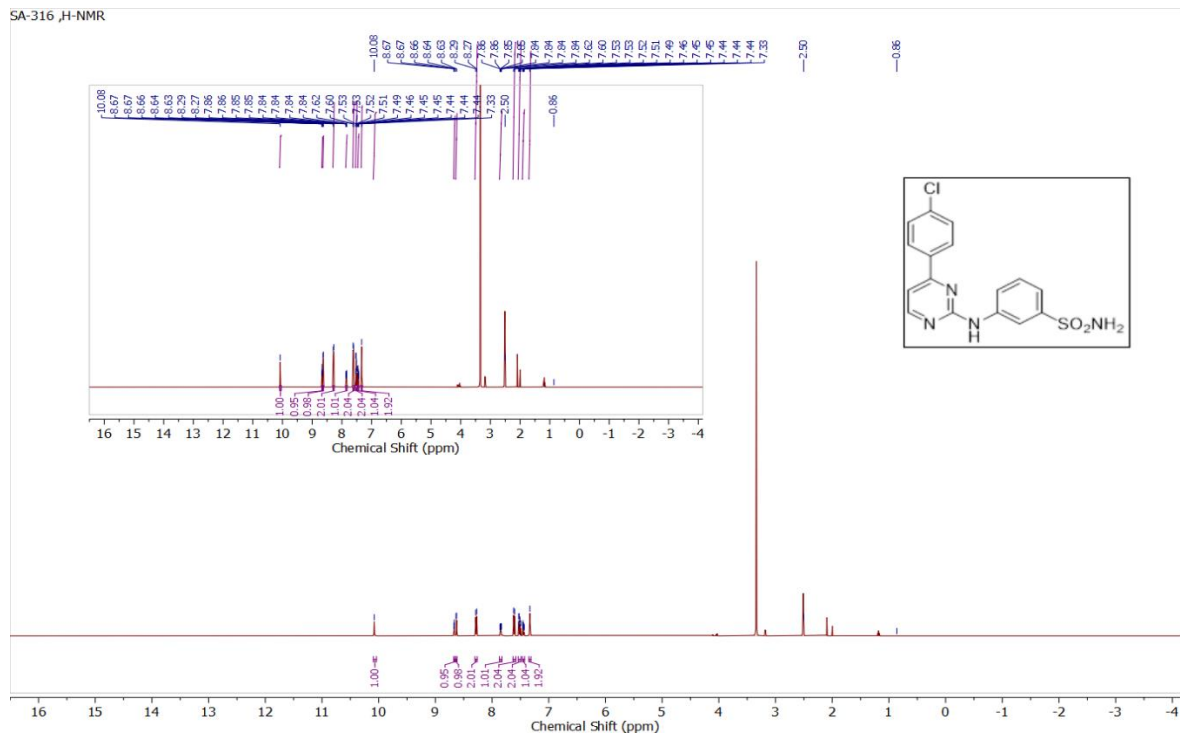
FTIR spectra of compound (5a)



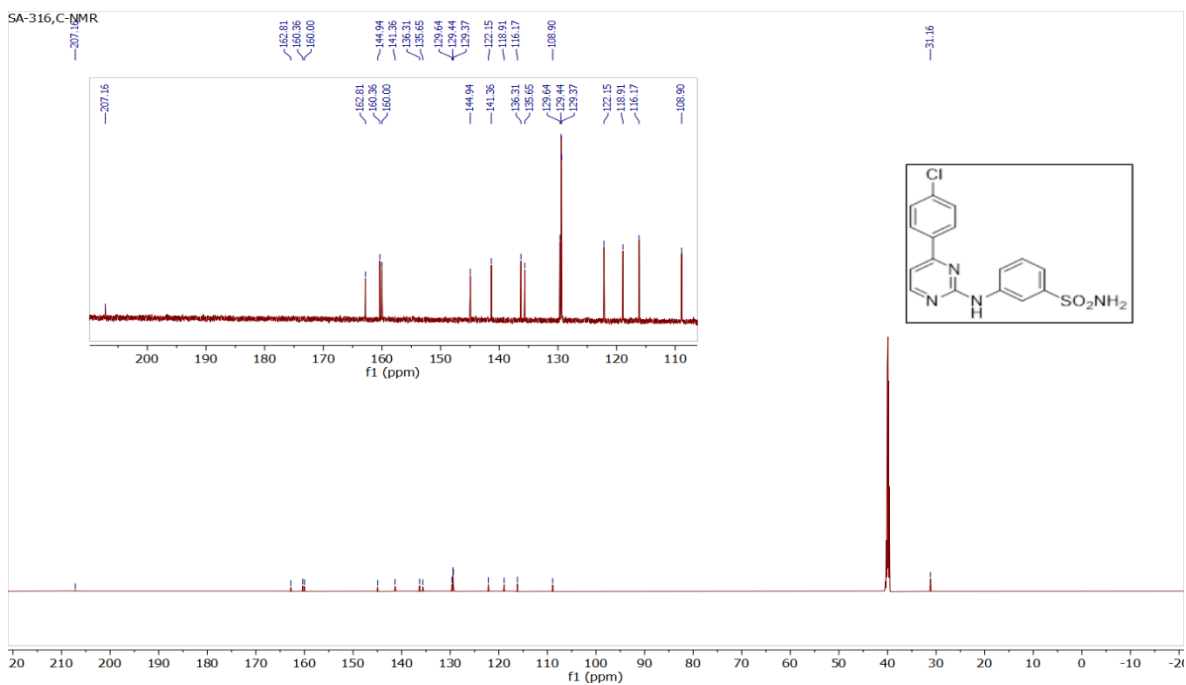
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4.1.4.2. 3-((4-(4-Chlorophenyl)pyrimidin-2-yl)amino)benzenesulfonamide (5b)

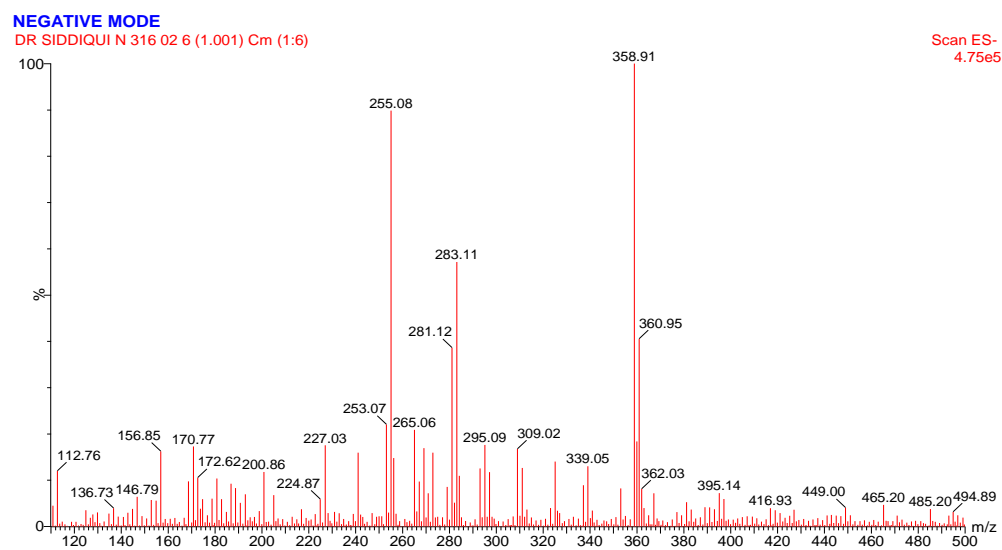
¹H-NMR spectra of compound (5b)



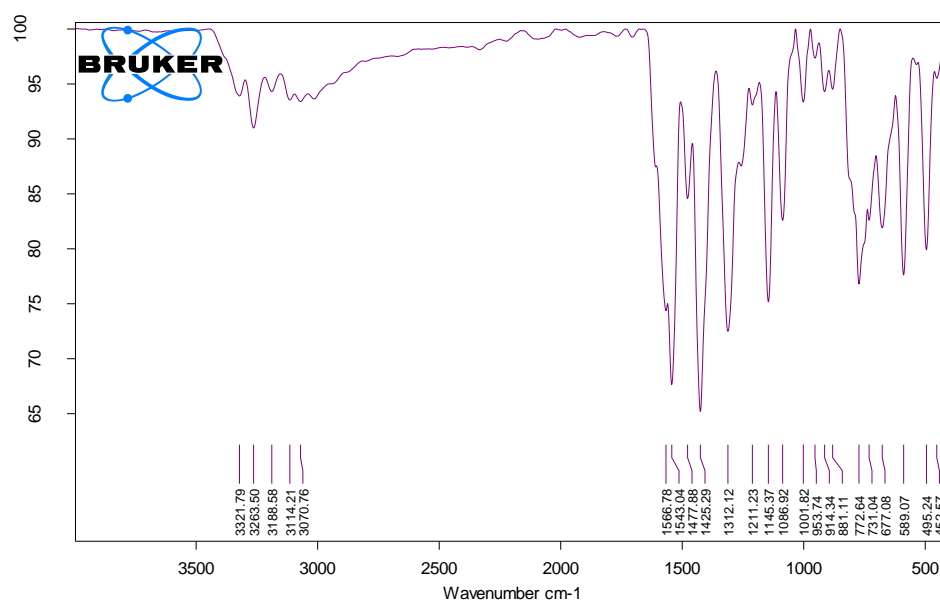
¹³C-NMR spectra of compound (5b)



Mass spectrum of compound (5b)



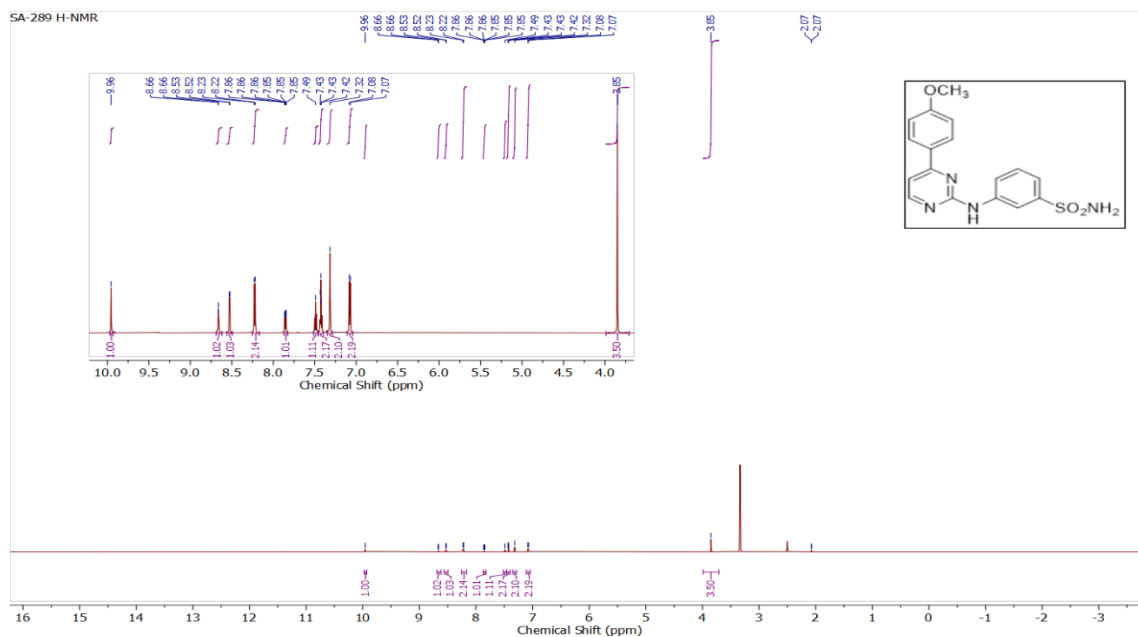
FTIR spectra of compound (5b)



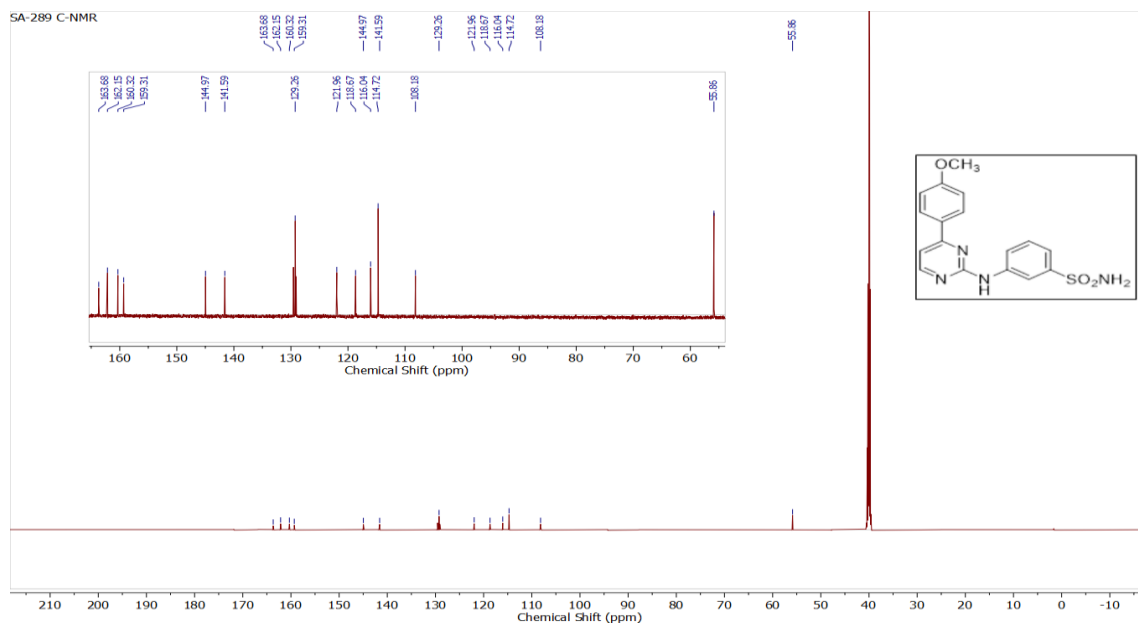
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4.1.4.3. 3-((4-(4-Methoxyphenyl)pyrimidin-2-yl)amino)benzenesulfonamide (5c)

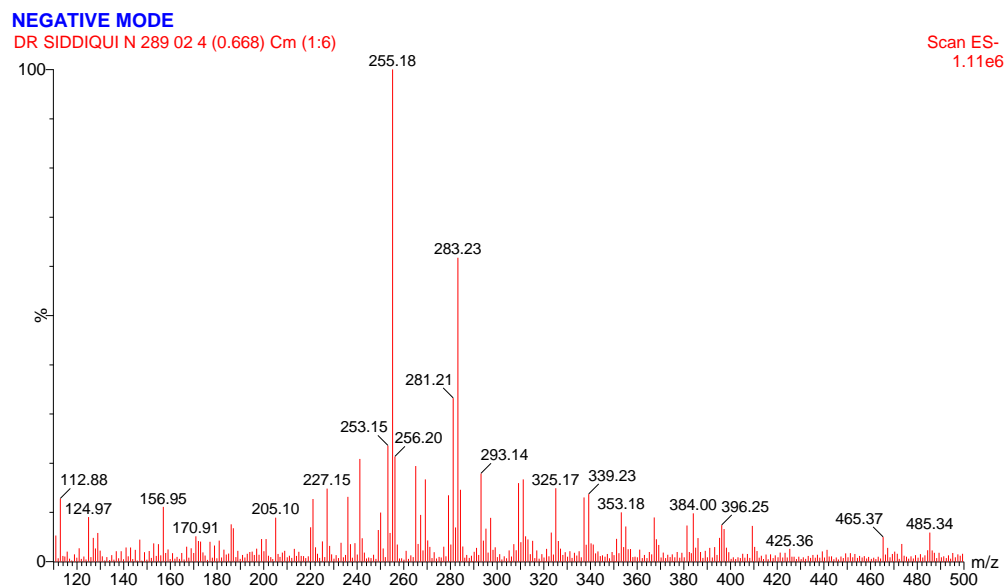
¹H-NMR spectra of compound (5c)



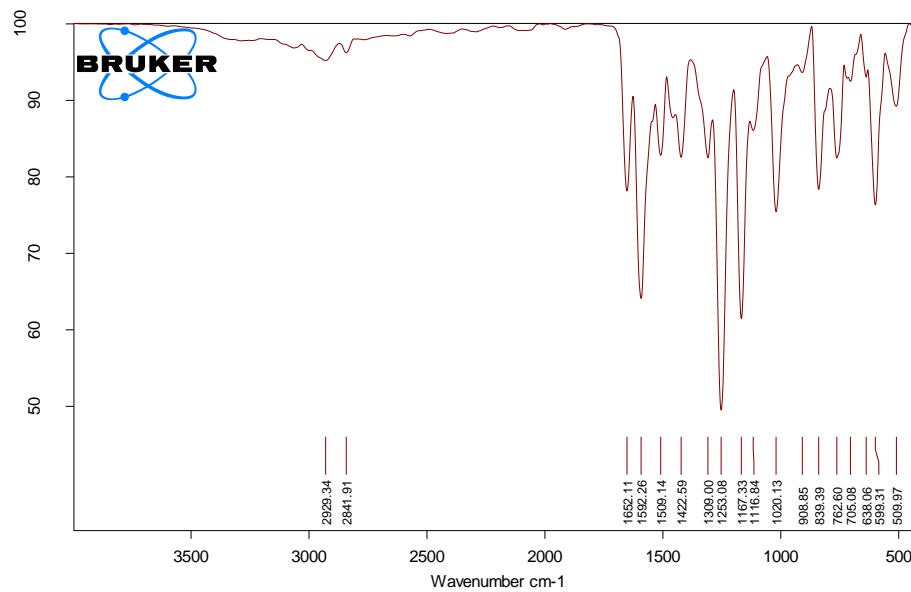
¹³C-NMR spectra of compound (5c)



Mass spectrum of compound (5c)



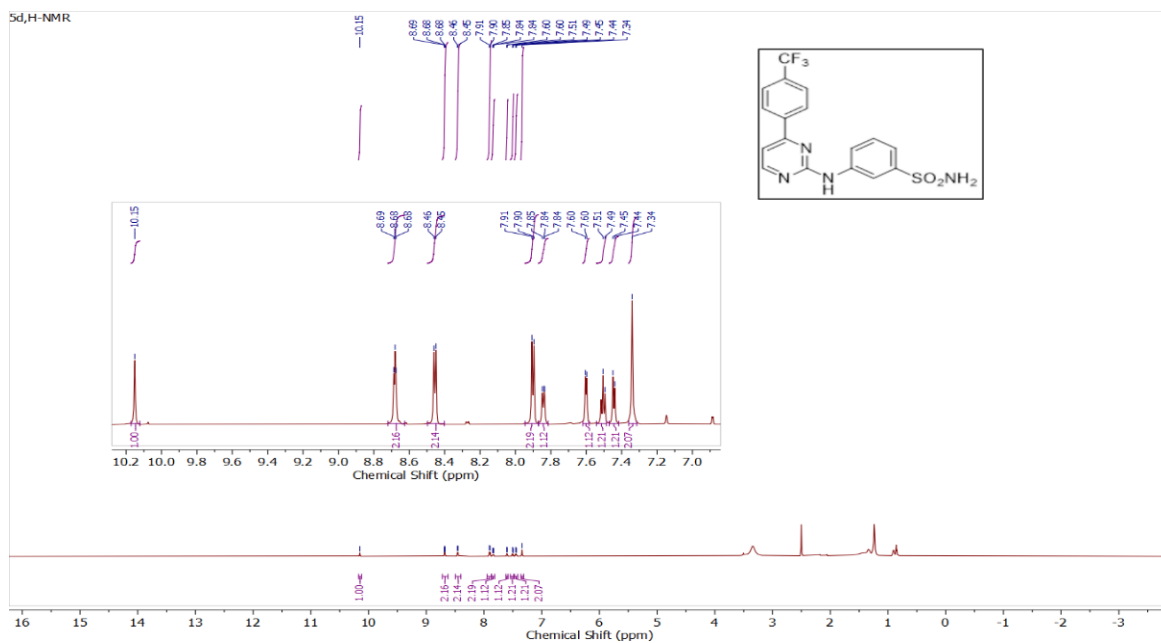
FTIR spectra of compound (5c)



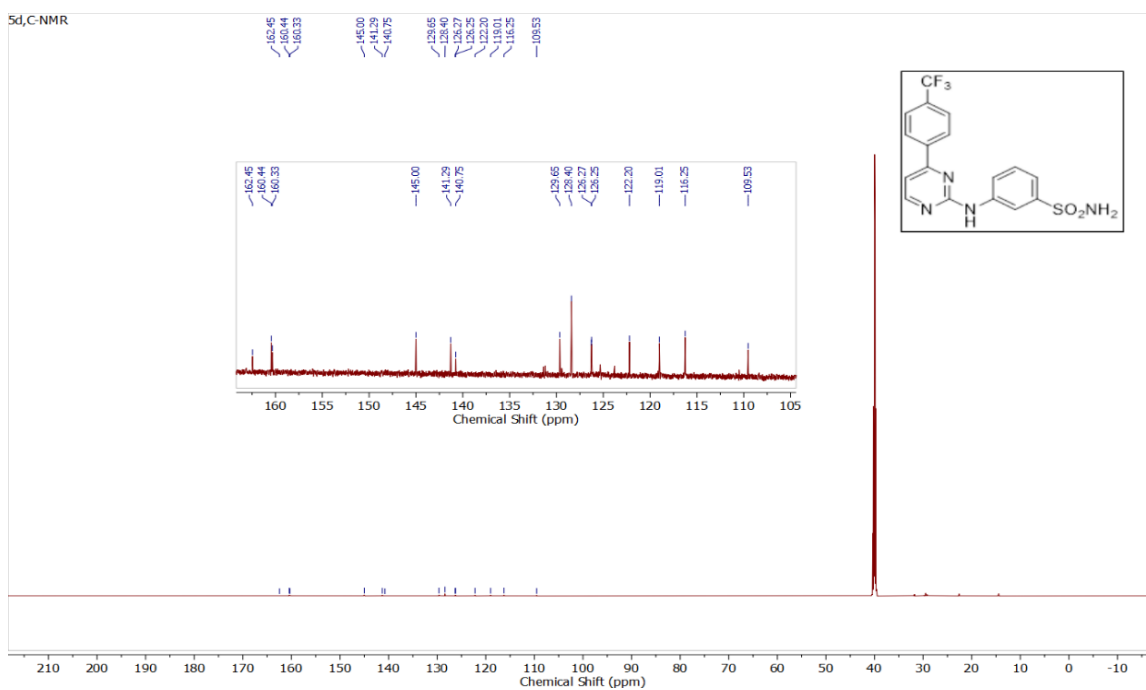
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4.1.4.4. 3-((4-(4-(Trifluoromethyl)phenyl)pyrimidin-2-yl)amino)benzenesulfonamide (5d)

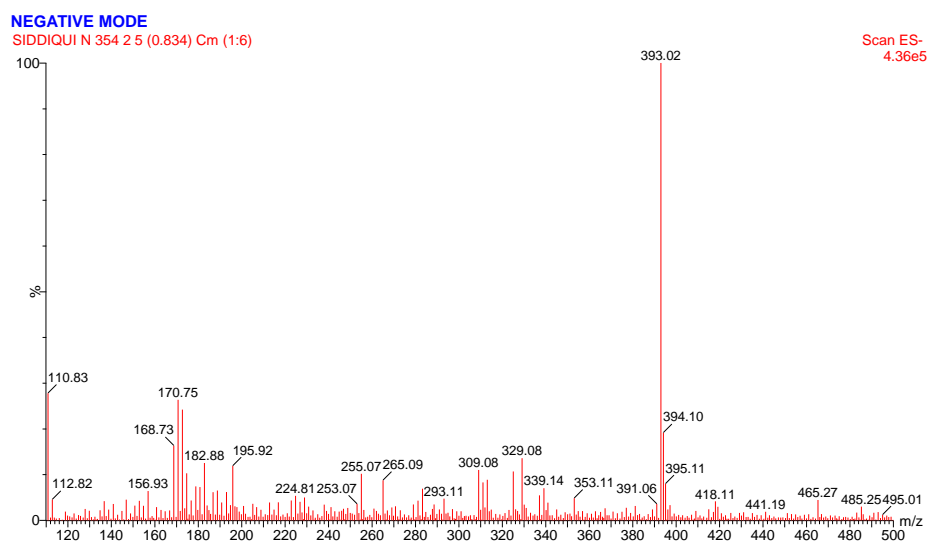
¹H-NMR spectra of compound (5d)



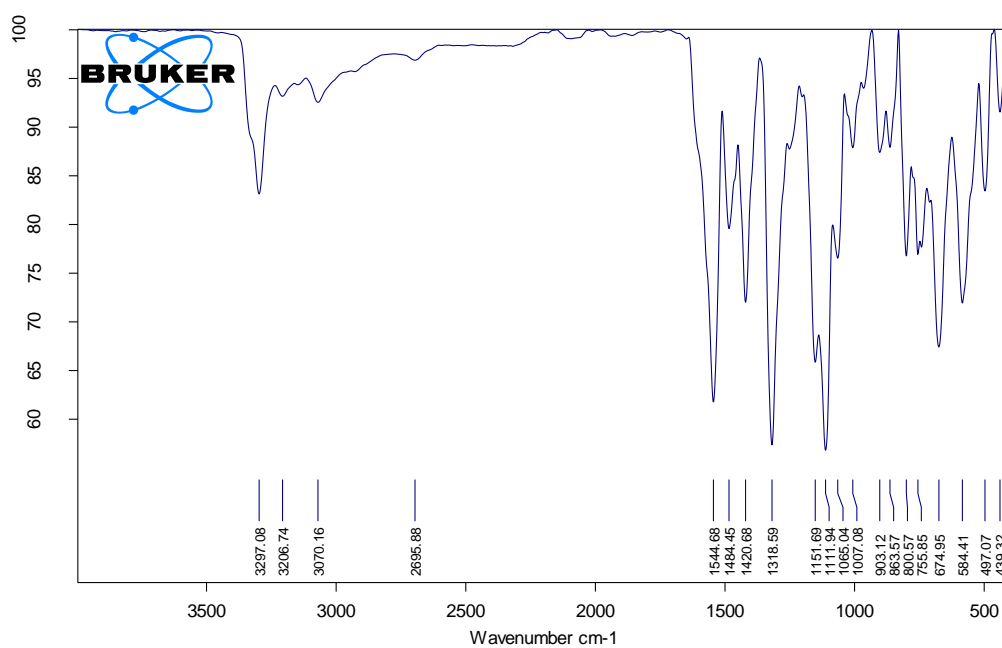
¹³C-NMR spectra of compound (5d)



Mass spectrum of compound (5d)



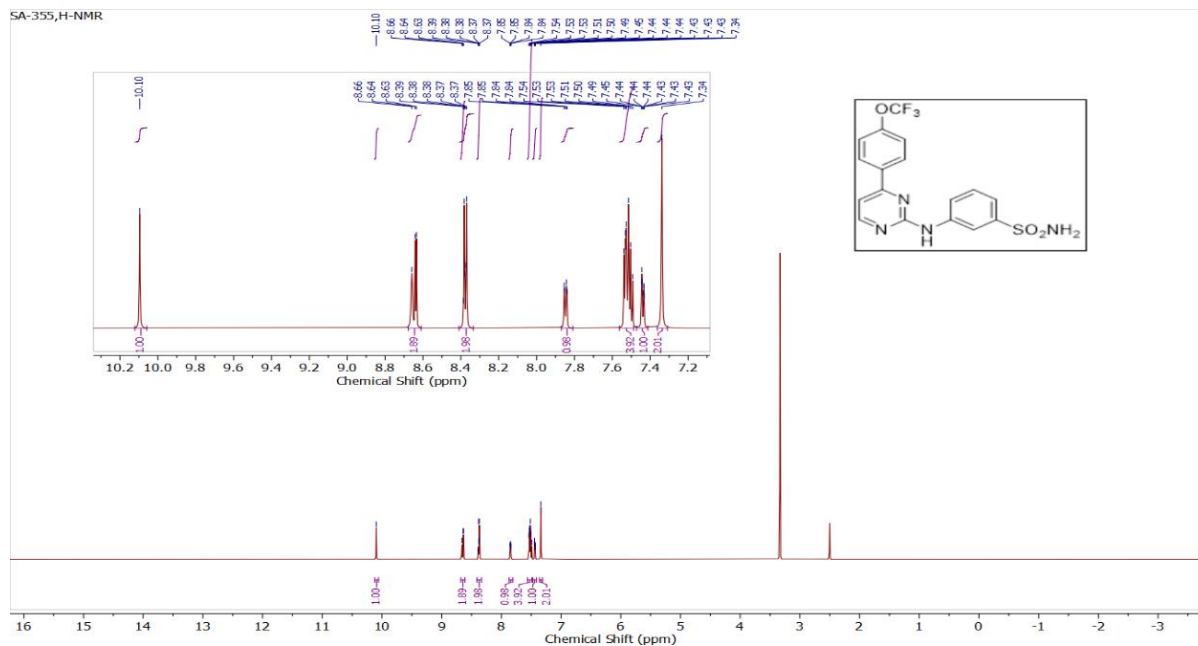
FTIR spectra of compound (5d)



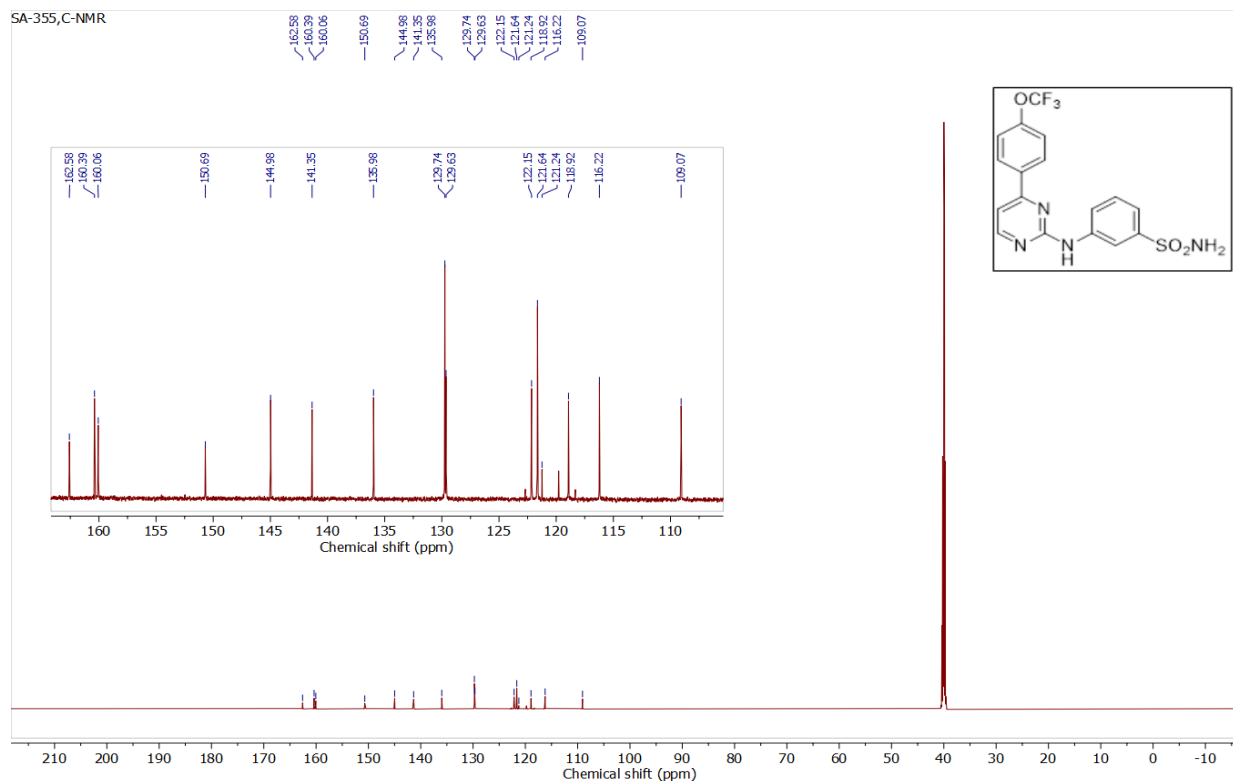
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4.1.4.5. 3-((4-(4-(Trifluoromethoxy)phenyl)pyrimidin-2-yl)amino)benzenesulfonamide (5e)

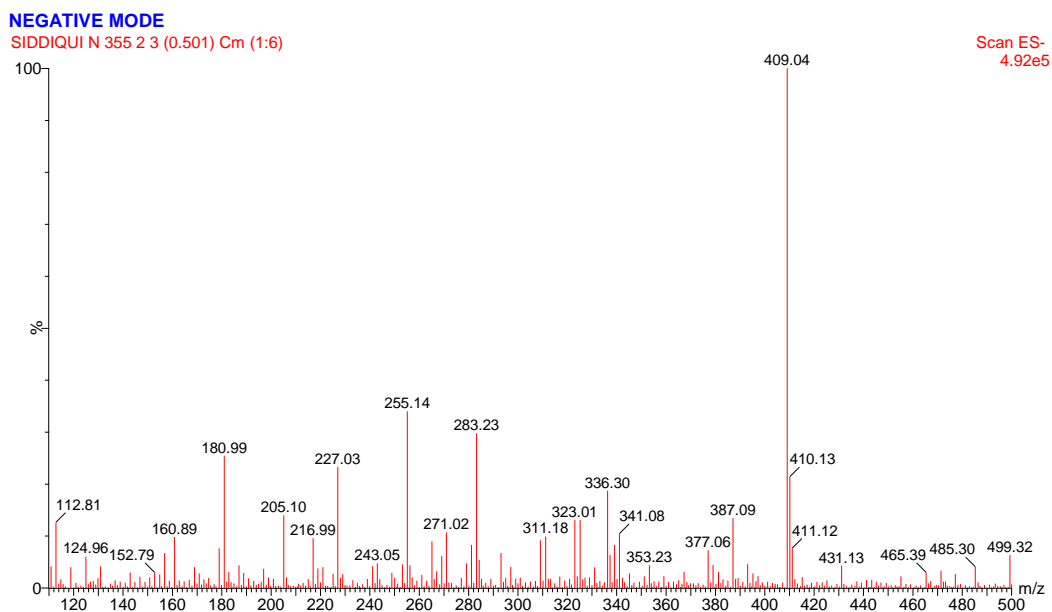
¹H-NMR spectra of compound (5e)



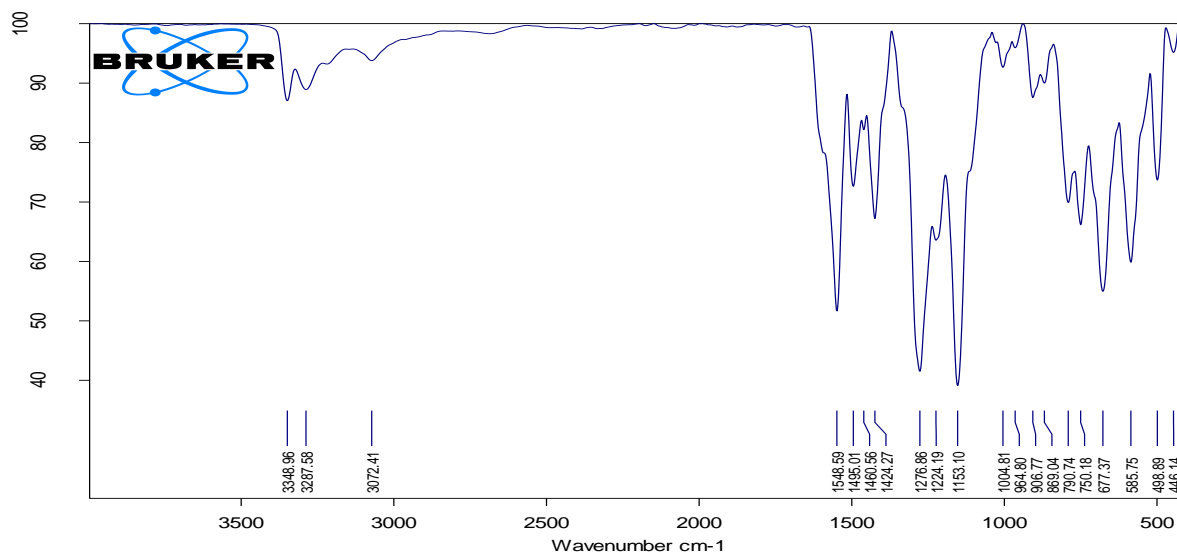
¹³C-NMR spectra of compound (5e)



Mass spectrum of compound (5e)



FTIR spectra of compound (5e)



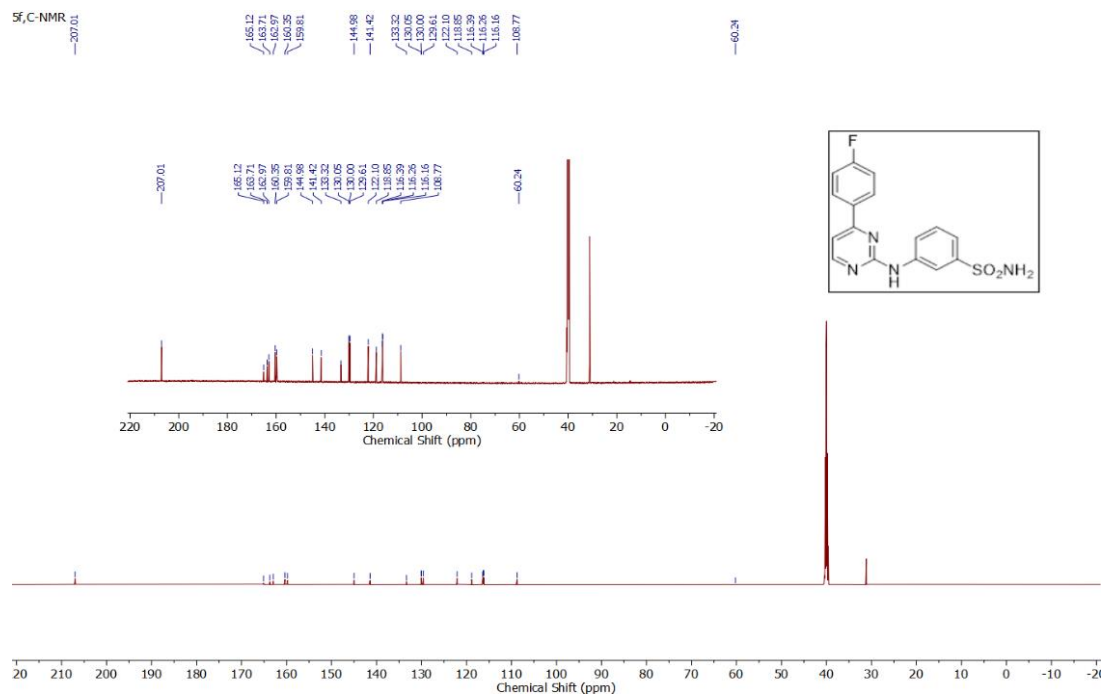
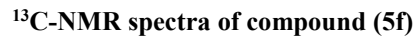
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AM-65 (355)

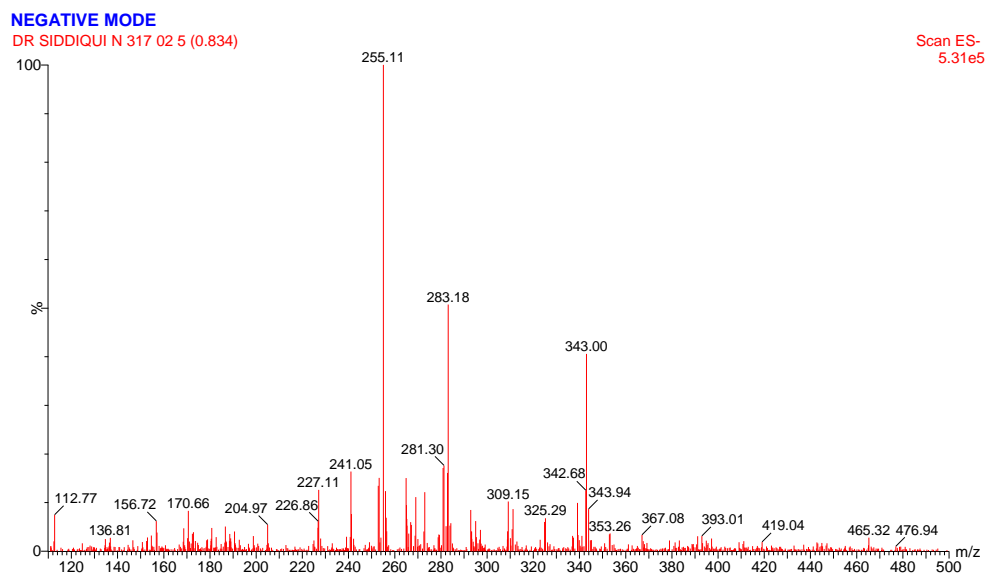
Instrument type and / or accessory

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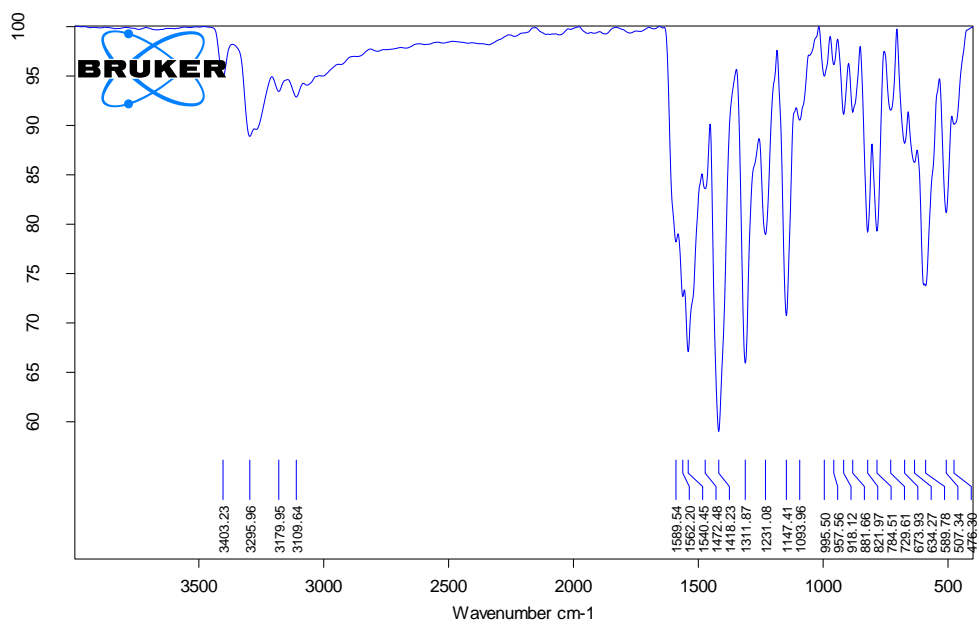
¹H-NMR spectra of compound (5f)



Mass spectrum of compound (5f)



FTIR spectra of compound (5f)



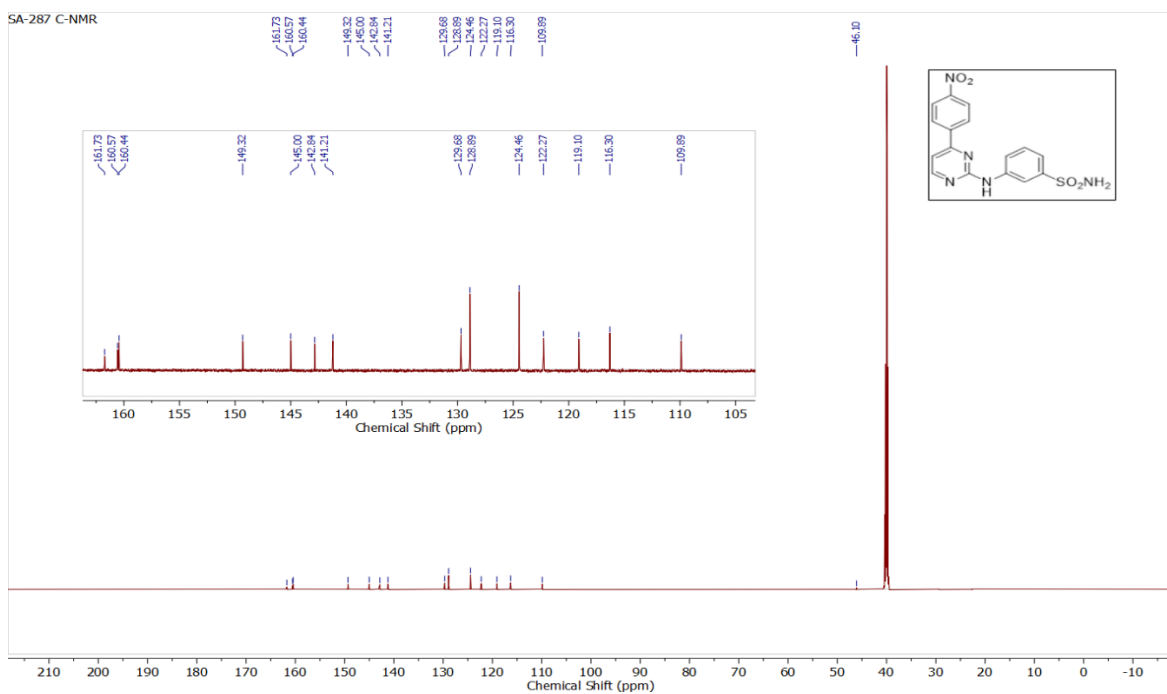
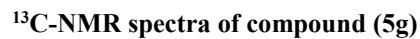
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AM-65 (317)

Instrument type and / or accessory

10/26/2022

¹H-NMR spectra of compound (5g)

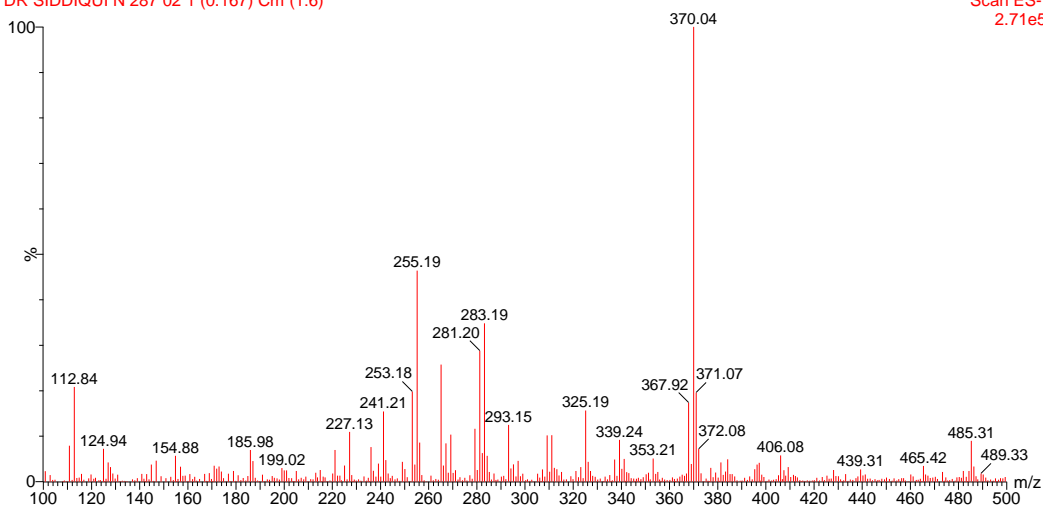


Mass spectrum of compound (5g)

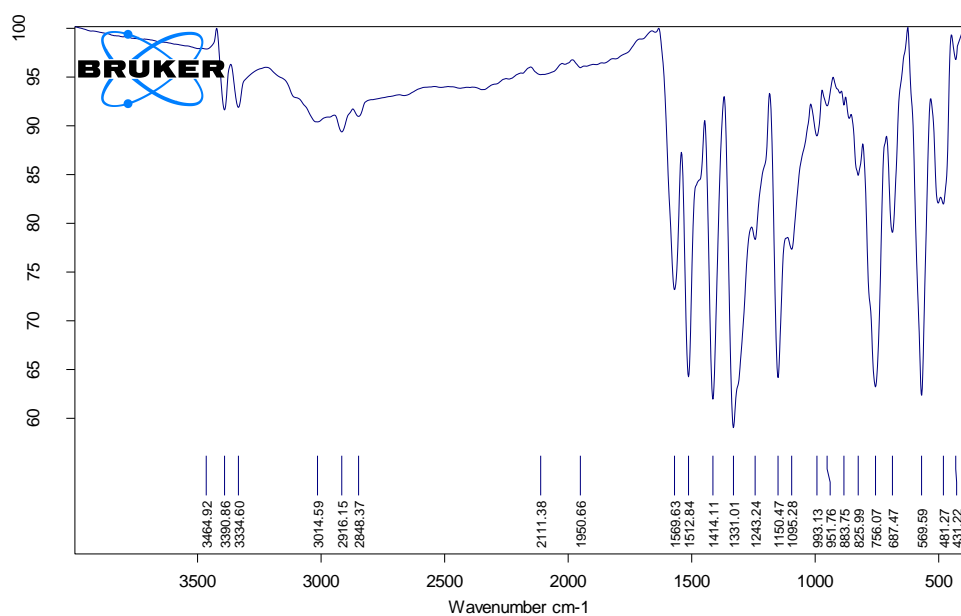
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Scan ES-
2.71e5



FTIR spectra of compound (5g)



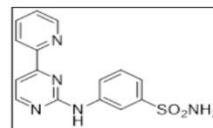
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AM-65 (287)

Instrument type and / or accessory

10/26/2022

¹H-NMR spectra of compound (5h)



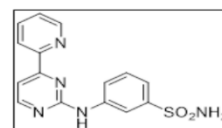
SA-312, C-NMR

Chemical structure of 2-(4-sulfamoylphenyl)-6-quinolinecarboxamide:

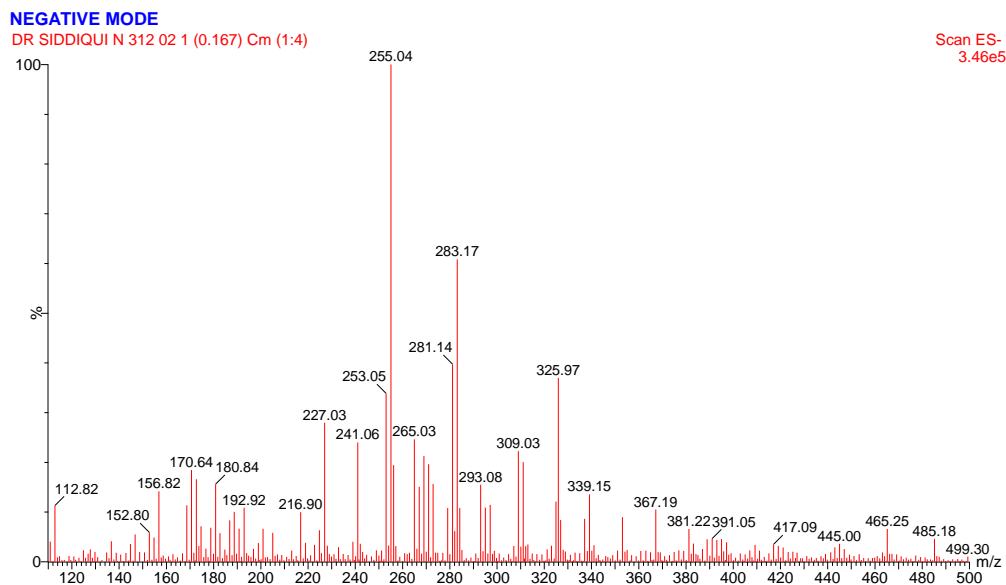
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Chemical Shift (ppm):

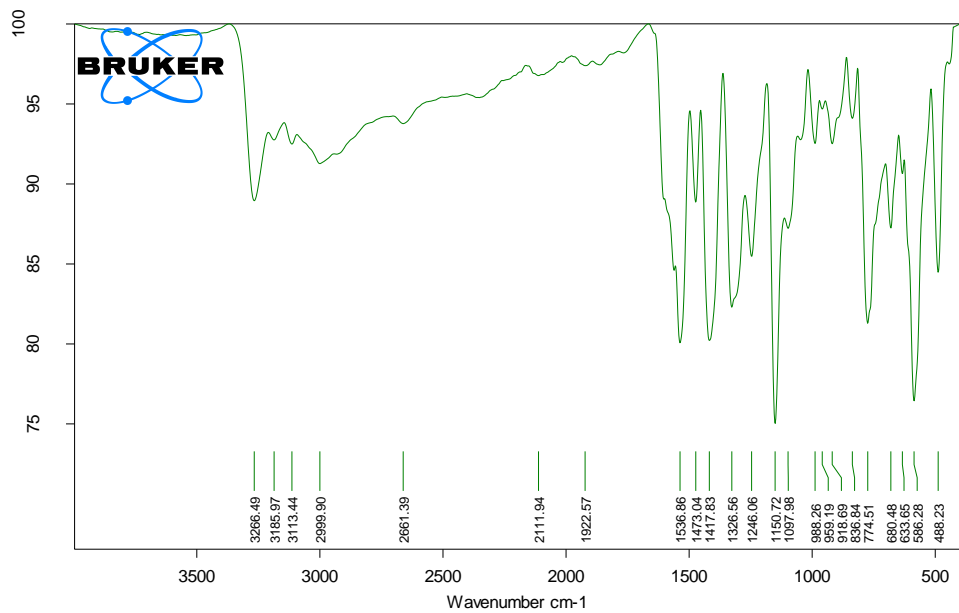
- 153.29
- 150.31
- 150.28
- 150.11
- 145.01
- 141.38
- 138.10
- 138.06
- 136.36
- 132.11
- 131.92
- 131.81
- 131.15
- 129.04
- 122.11
- 121.92
- 118.91
- 116.15
- 109.04



Mass spectrum of compound (5h)



FTIR spectra of compound (5h)



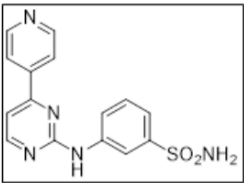
C:\Users\DELL\Documents\Bruker\OPUS_7.8.38\DATA\MEAS\AM-65 (312).0

AM-65 (312)

Instrument type and / or accessory

10/26/2022

¹H-NMR spectra of compound (5i)

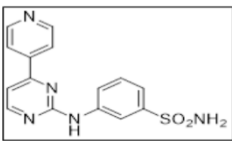


¹³C-NMR

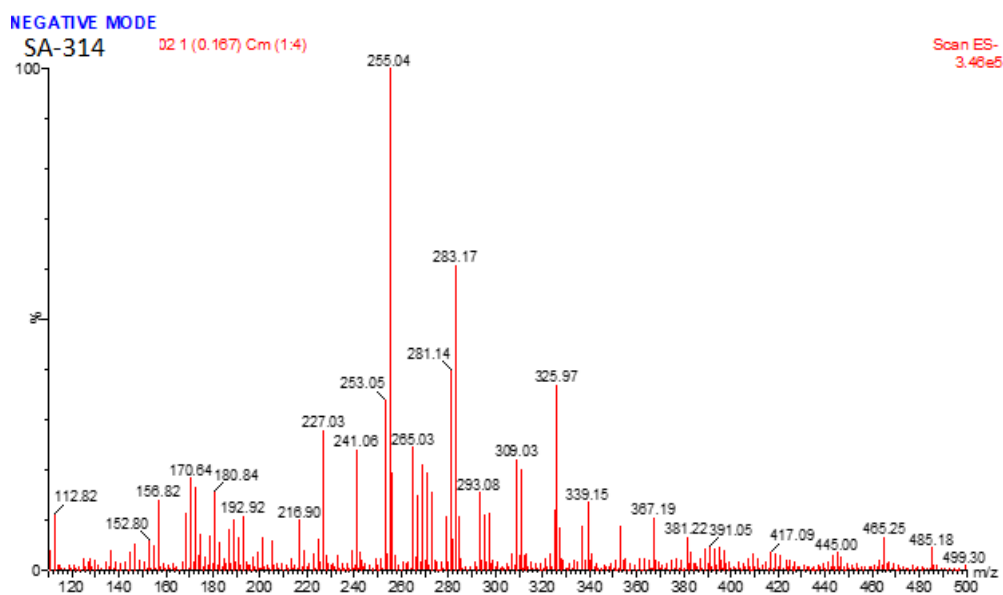
Chemical structure: Nc1ccc(NC2=NC3=CC=CC=C3N2)cc1

Chemical Shift (ppm):

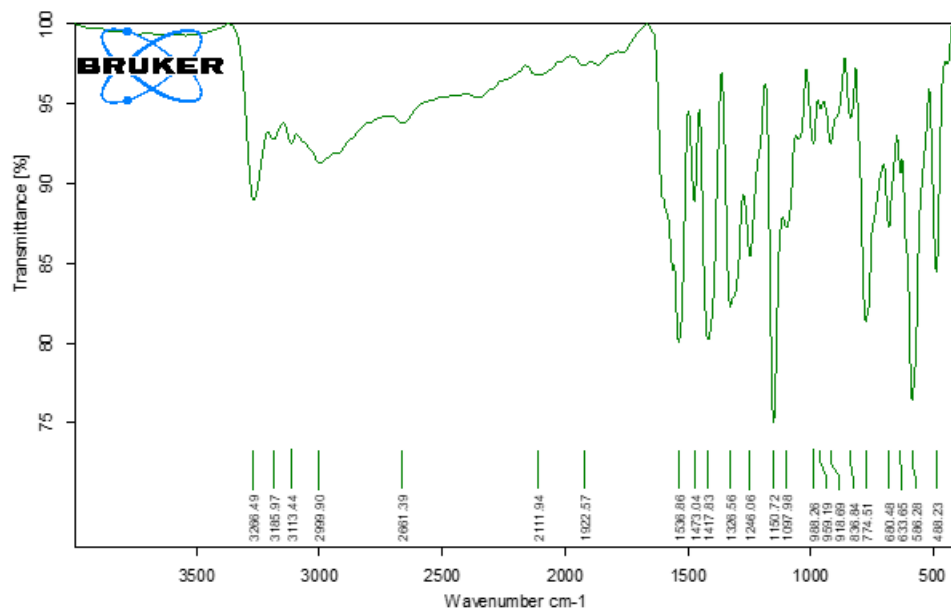
- 160.59
- 160.52
- 151.07
- 146.02
- 144.01
- 141.20
- 139.67
- 132.22
- 131.47
- 119.08
- 116.26
- 109.60



Mass spectrum of compound (5i)



FTIR spectra of compound (5i)



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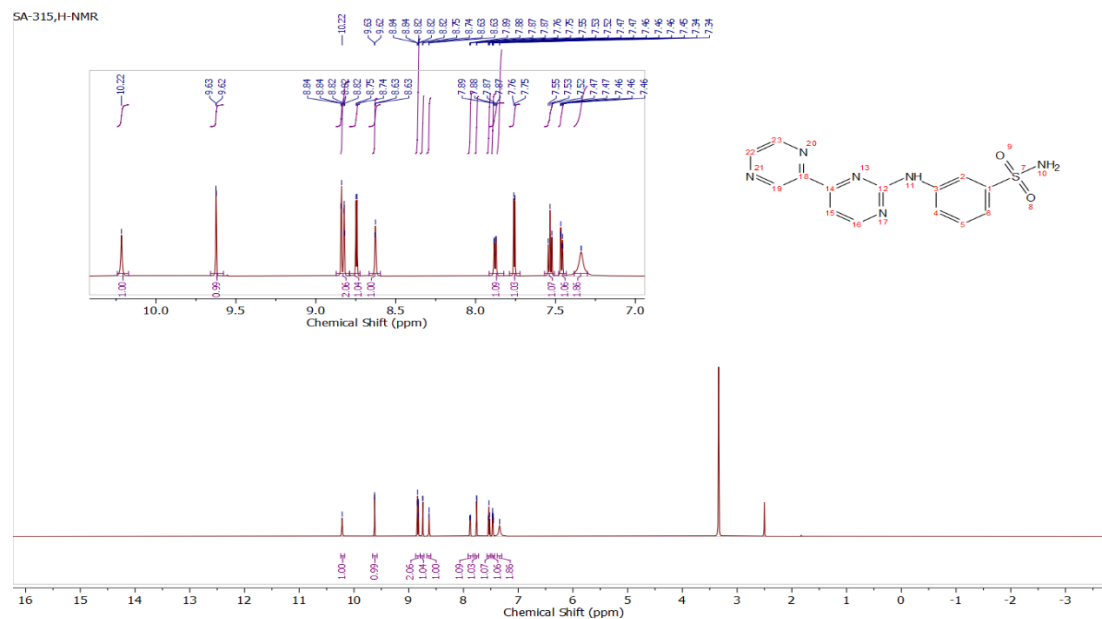
SA-314

Instrument type and / or accessory

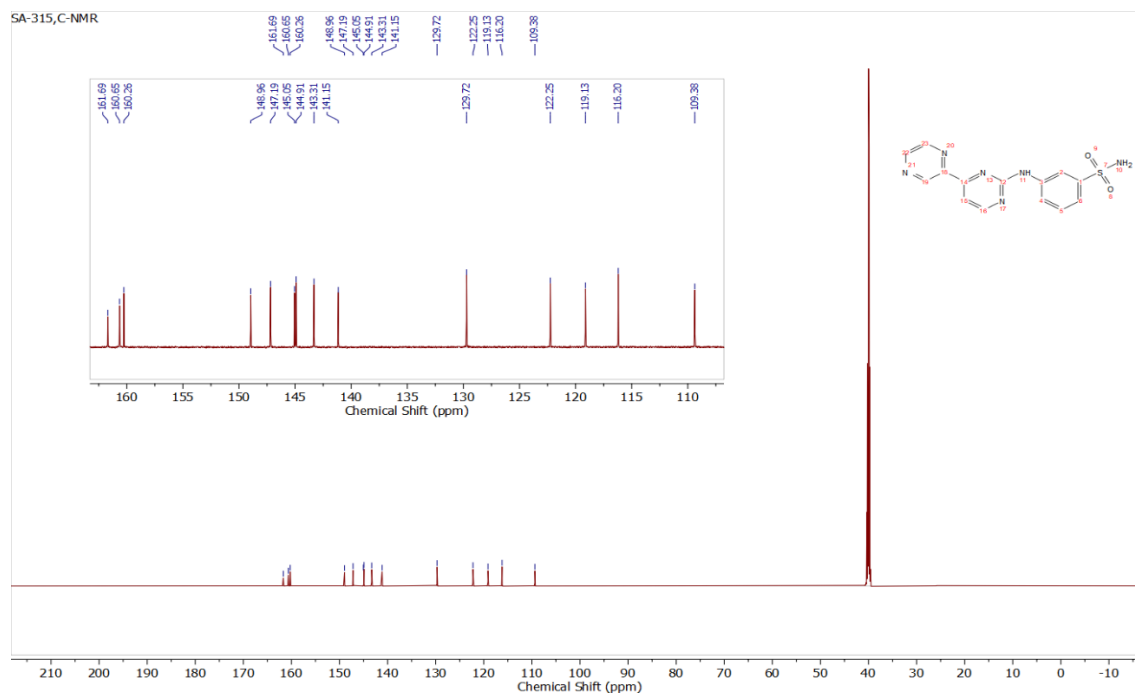
10/28/2022

4.1.4.10. 3-((4-(Pyrazin-2-yl)pyrimidin-2-yl)amino)benzenesulfonamide (5j)

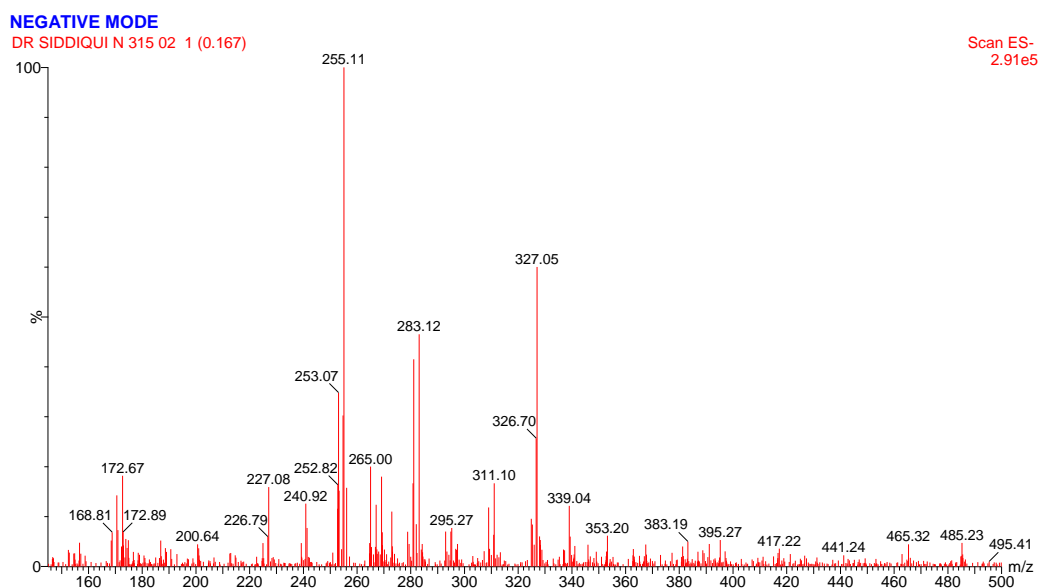
¹H-NMR spectra of compound (5j)



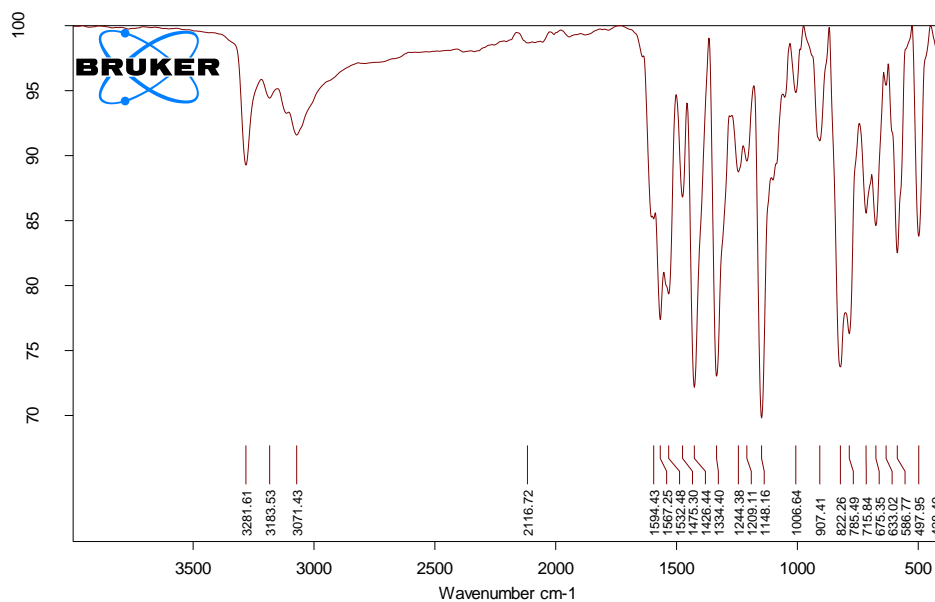
¹³C-NMR spectra of compound (5j)



Mass spectrum of compound (5j)



FTIR spectra of compound (5j)



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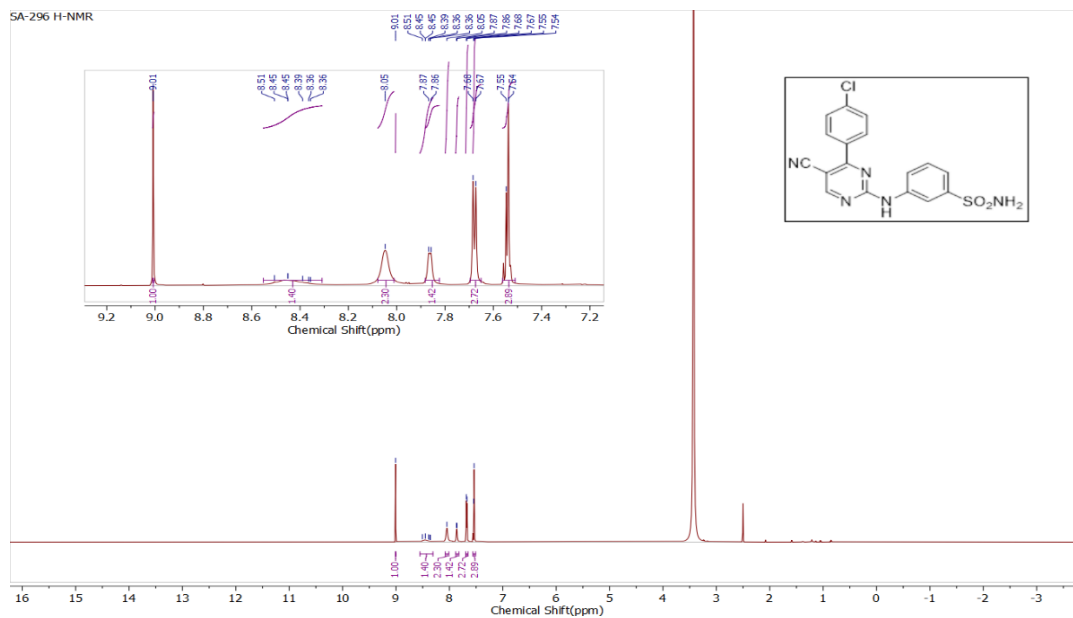
AM-65 (315)

Instrument type and / or accessory

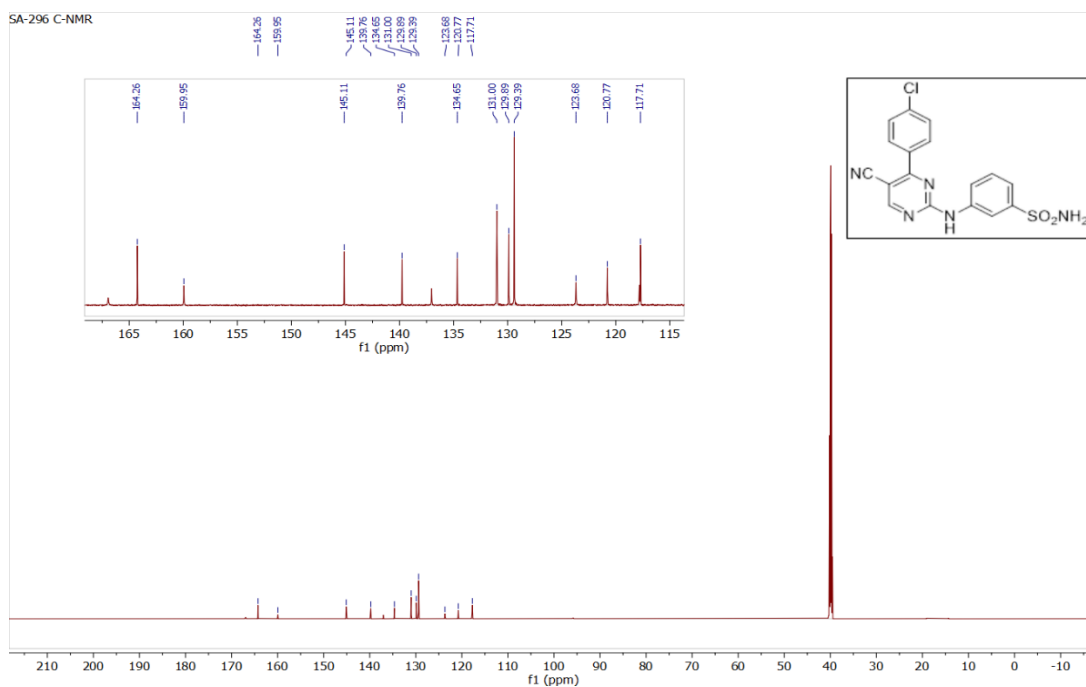
10/26/2022

4.1.4.11. 3-((4-(4-Chlorophenyl)-5-cyanopyrimidin-2-yl)amino)benzenesulfonamide (5k)

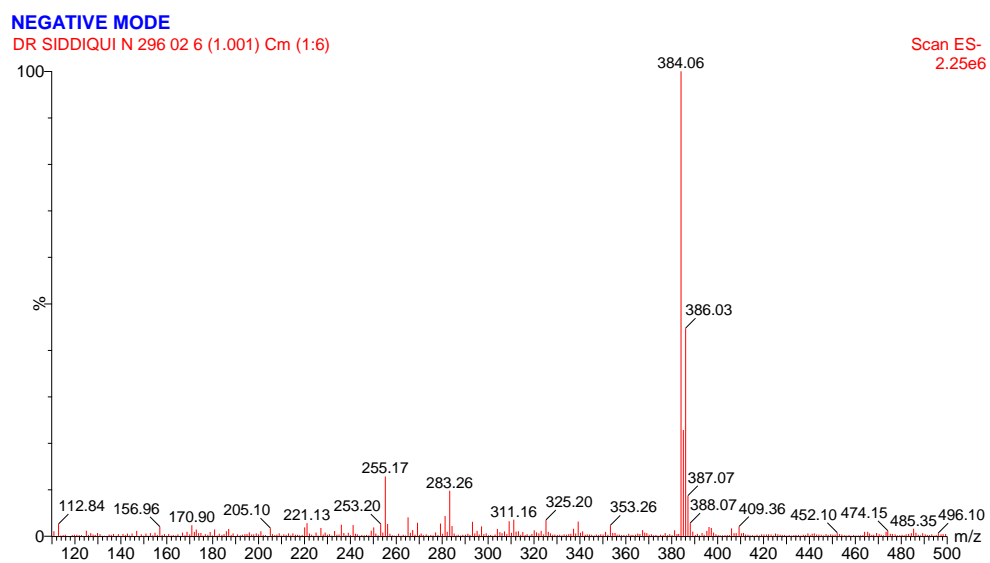
¹H-NMR spectra of compound (5k)



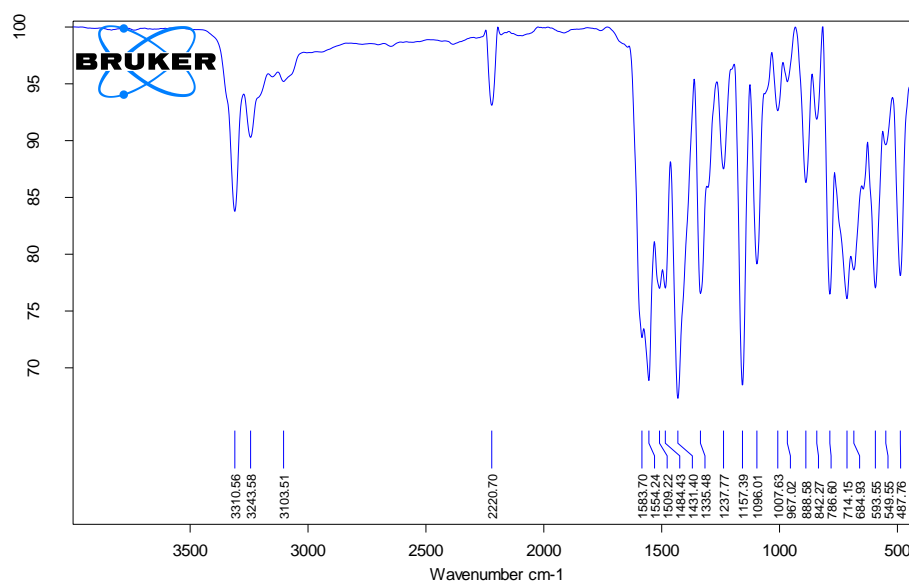
¹³C-NMR spectra of compound (5k)



Mass spectrum of compound (5k)

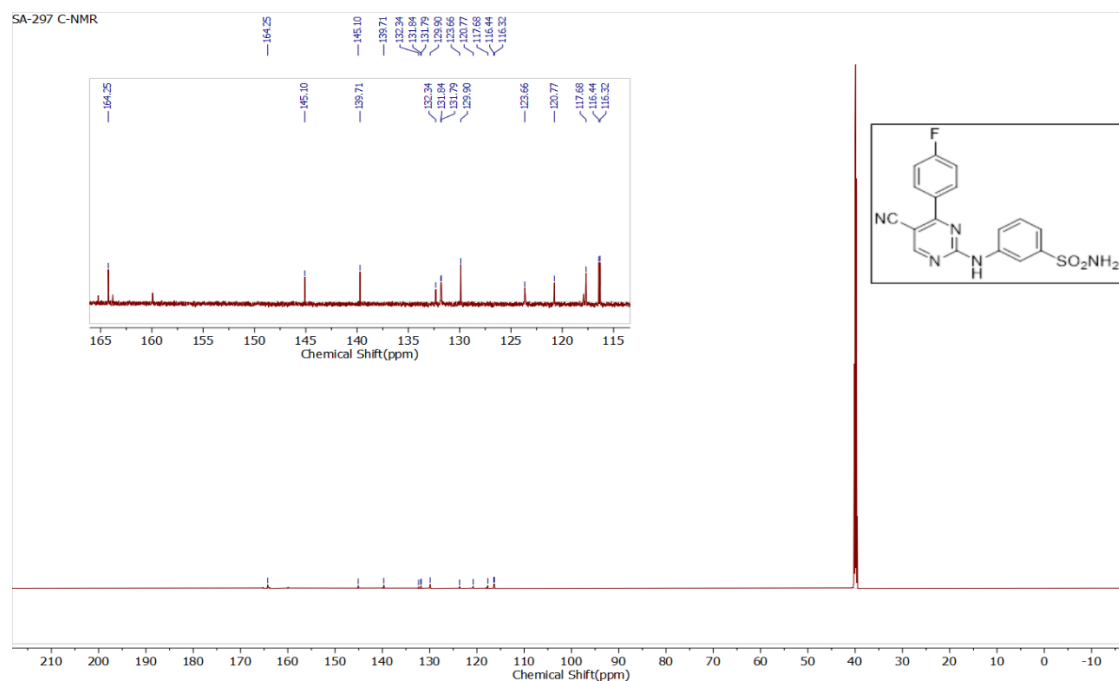
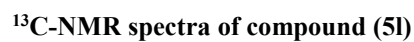


FTIR spectra of compound (5k)

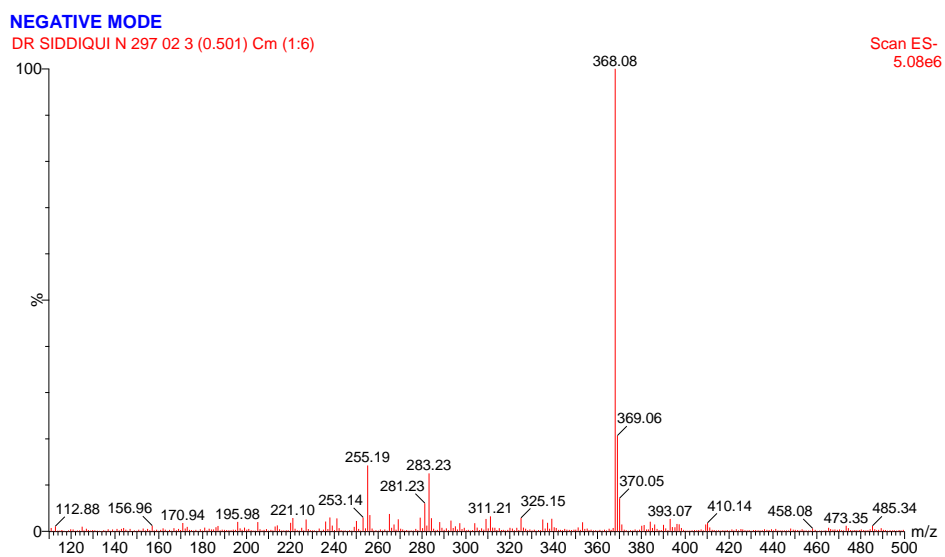


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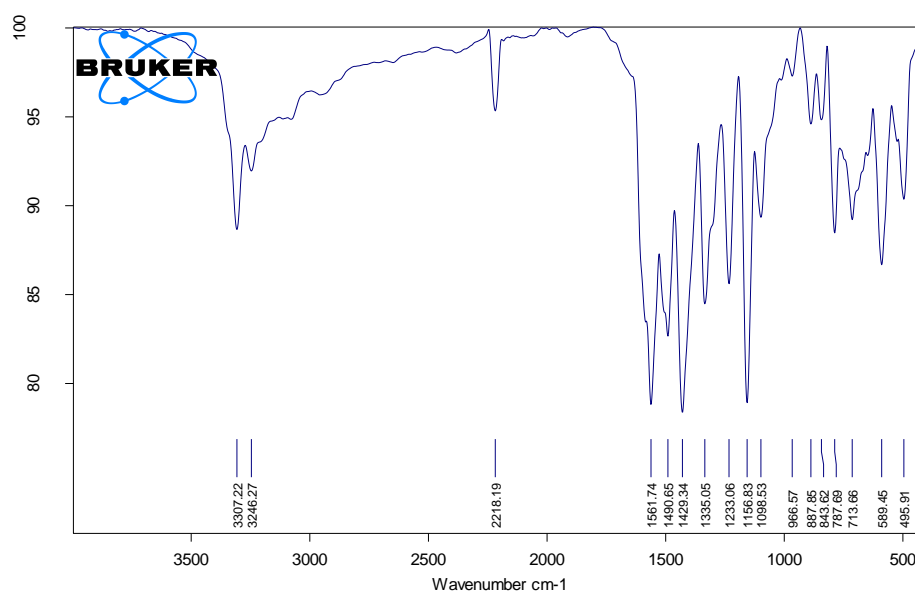
¹H-NMR spectra of compound (5l)



Mass spectrum of compound (5I)

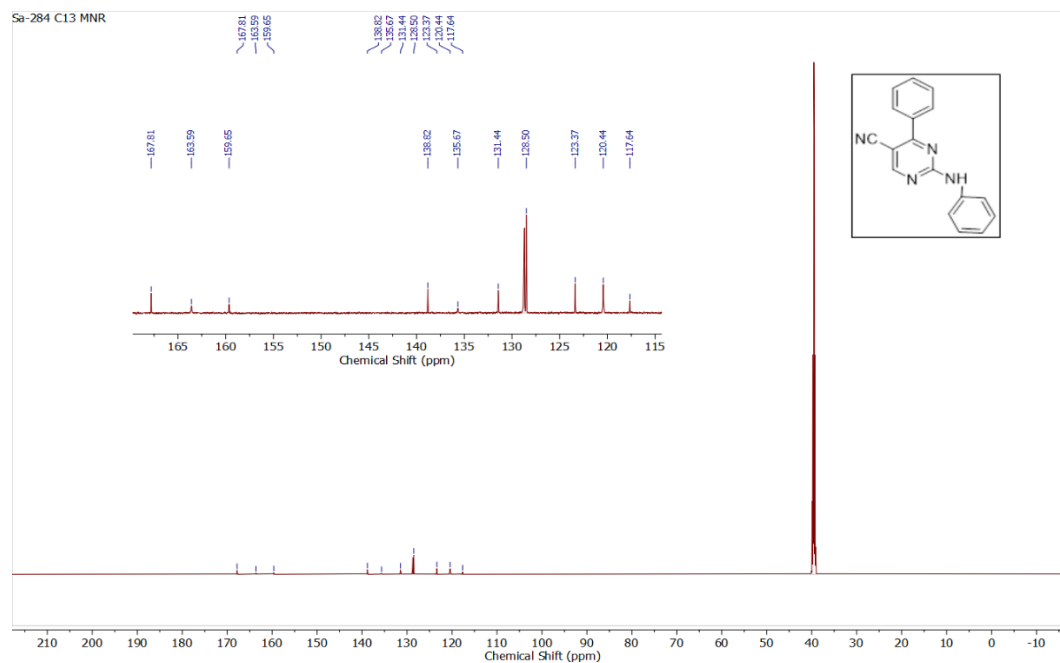
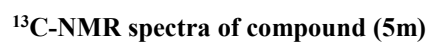


FTIR spectra of compound (5I)



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¹H-NMR spectra of compound (5m)

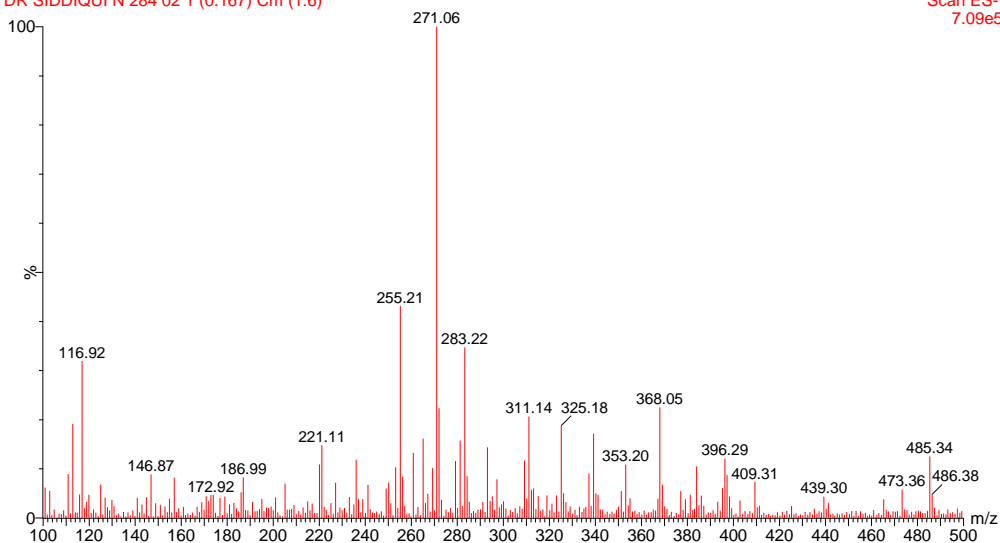


Mass spectrum of compound (5m)

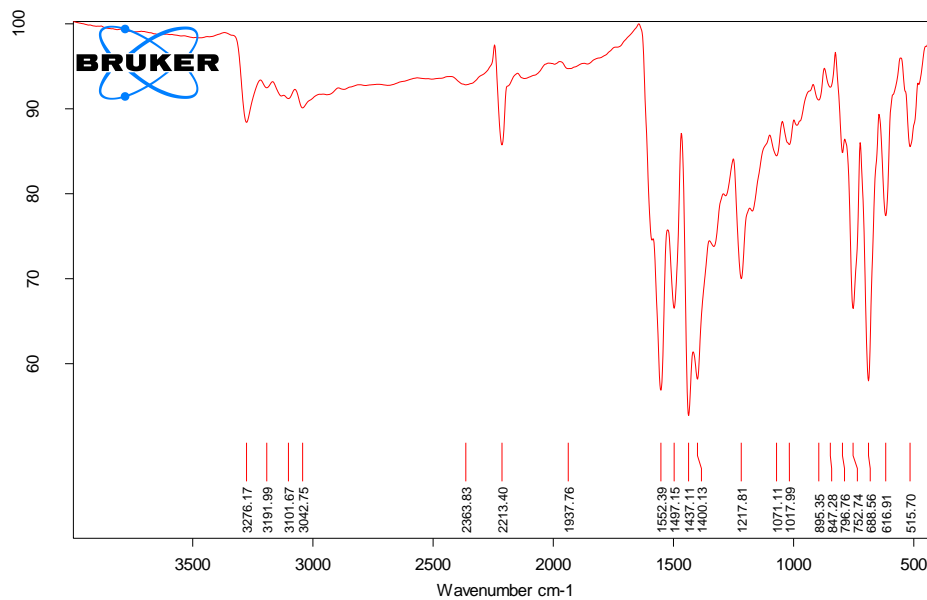
NEGATIVE MODE MODE

DR SIDDIQUI N 284 02 1 (0.167) Cm (1:6)

Scan ES-
7.09e5



FTIR spectra of compound (5m)



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AM-65 (284)

Instrument type and / or accessory

10/26/2022