

Supporting Information

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A catalyst-free and eco-friendly approach to synthesis of 1,8-naphthyridines *via* natural deep eutectic solvents

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General Procedure for Synthesis of 2-amino-4-phenyl-1,8-naphthyridine-3-carbonitrile (**1-27**)

A mixture of 2-aminopyridine (5 mmol), malononitrile (5 mmol), and the corresponding aromatic aldehyde (5 mmol) was added to a lactic acid-based DES prepared from Lactic acid, Maltose, and Amla Juice (Indian gooseberry Juice) in a 3:1:3 molar ratio. The reaction mixture was stirred at room temperature for the appropriate time, as listed in Table 3. The progress of the reaction was monitored by thin-layer chromatography (TLC) using petroleum ether and ethyl acetate (9:1, v/v) as the eluent. Upon completion, the reaction mixture was poured into water to precipitate the product. The solid was collected by filtration, washed thoroughly with water, and dried. The crude product was then recrystallized from a mixture of ethanol (4 mL) and water (0.5 mL) to afford the pure 2-amino-4-phenyl-1,8-naphthyridine-3-carbonitrile.

Solvent Characterization

Density measured by using Pyknometer and Refractive Index measured by using Refractometer

Table S1 : Density measured by using pyknometer and refractive index measured by using refractometer

Sr. No.	Deep Eutectic Solvents	Test Parameter		
		Refractive Index at 27°C	Density at 27°C g/cc	P ^H
1.	Lactic Acid-Maltose-Amla Juice	1.309	1.1820	1.37
2.	Lactic Acid -Maltose- Water	1.401	1.1887	2.48
3.	Lactic Acid-Proline-SnCl ₂	1.447	1.3412	2.56
4.	Lactic Acid- Maltose - Aloe vera Juice	1.310	1.1693	1.39
5.	Lactic Acid - Proline - Aloe Vera Juice	1.309	1.1717	2.60

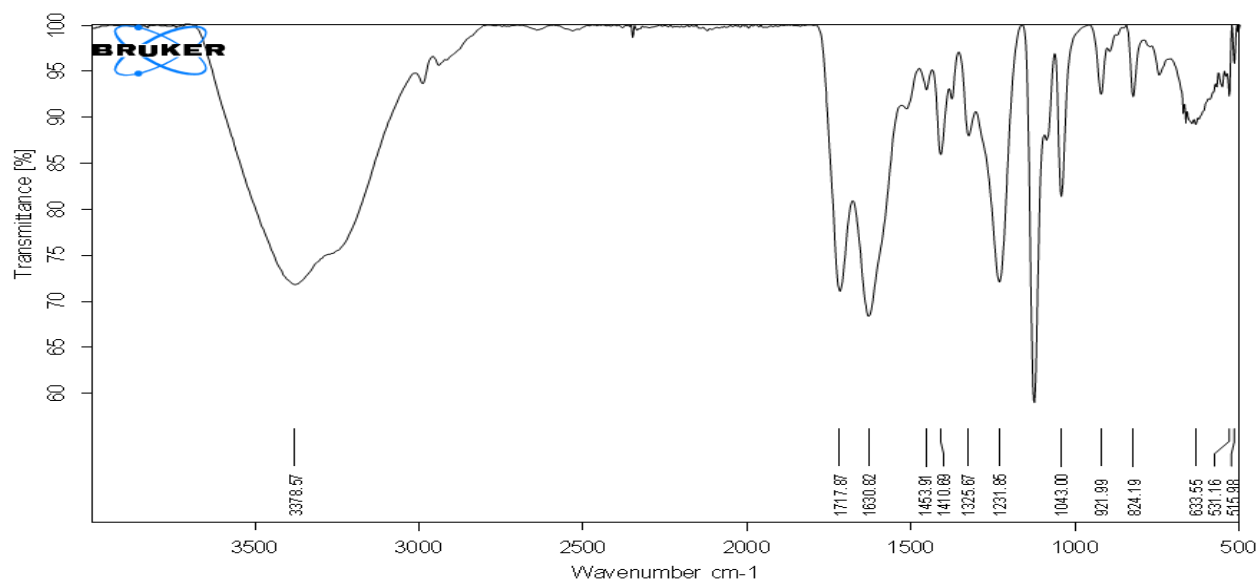


Figure S1: IR Spectra of L1 Lactic Acid-Maltose- Amla Juice

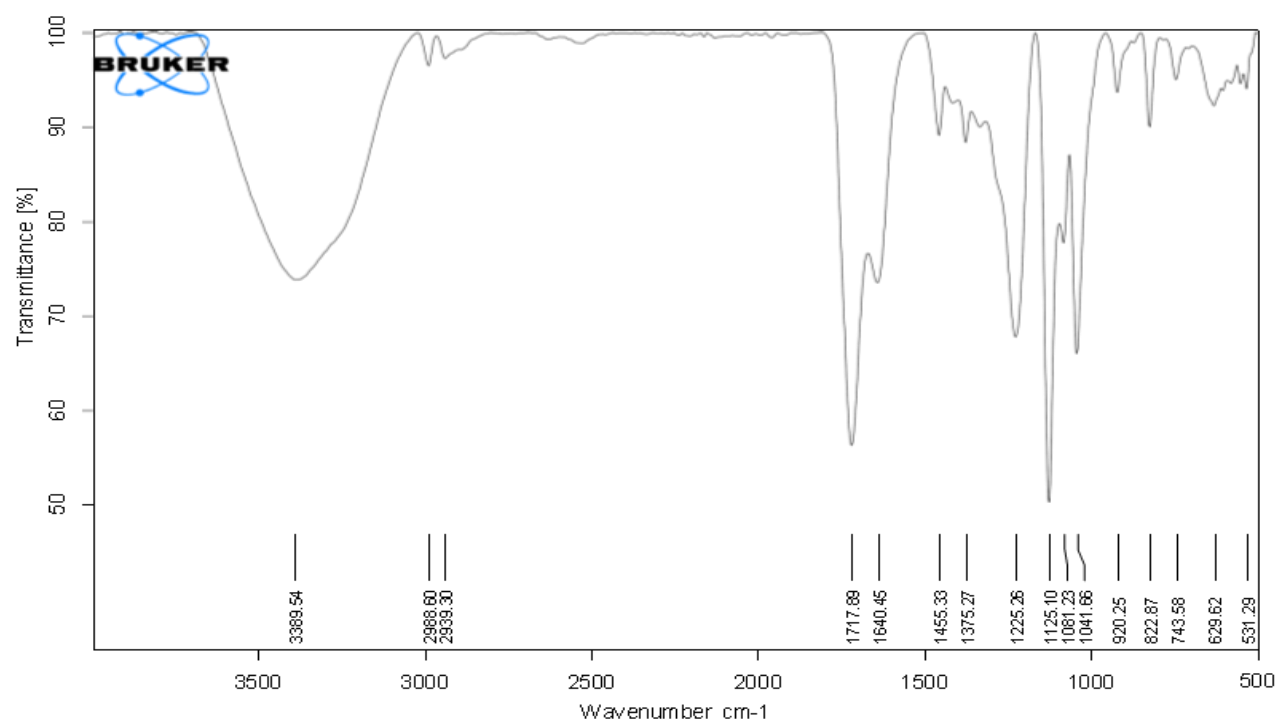


Figure S2: IR Spectra of L2 Lactic Acid-Maltose- Water

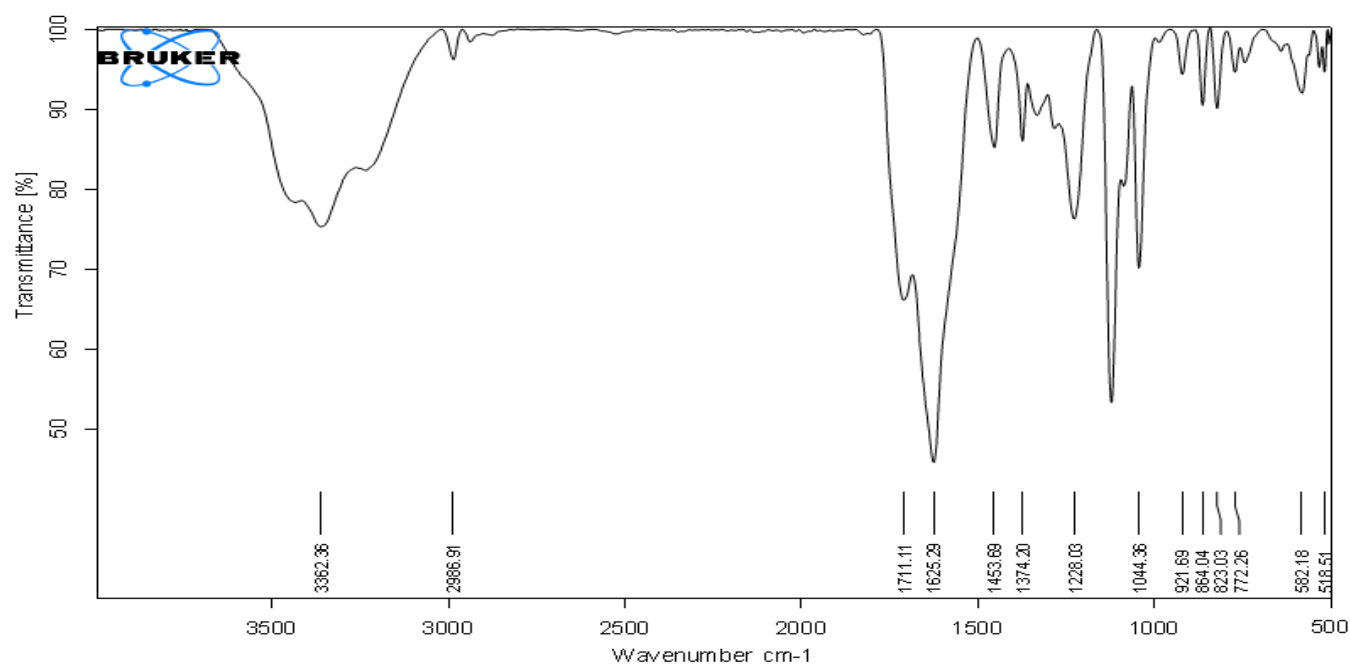


Figure S3: IR Spectra of L3 Lactic Acid-Proline-SnCl₂

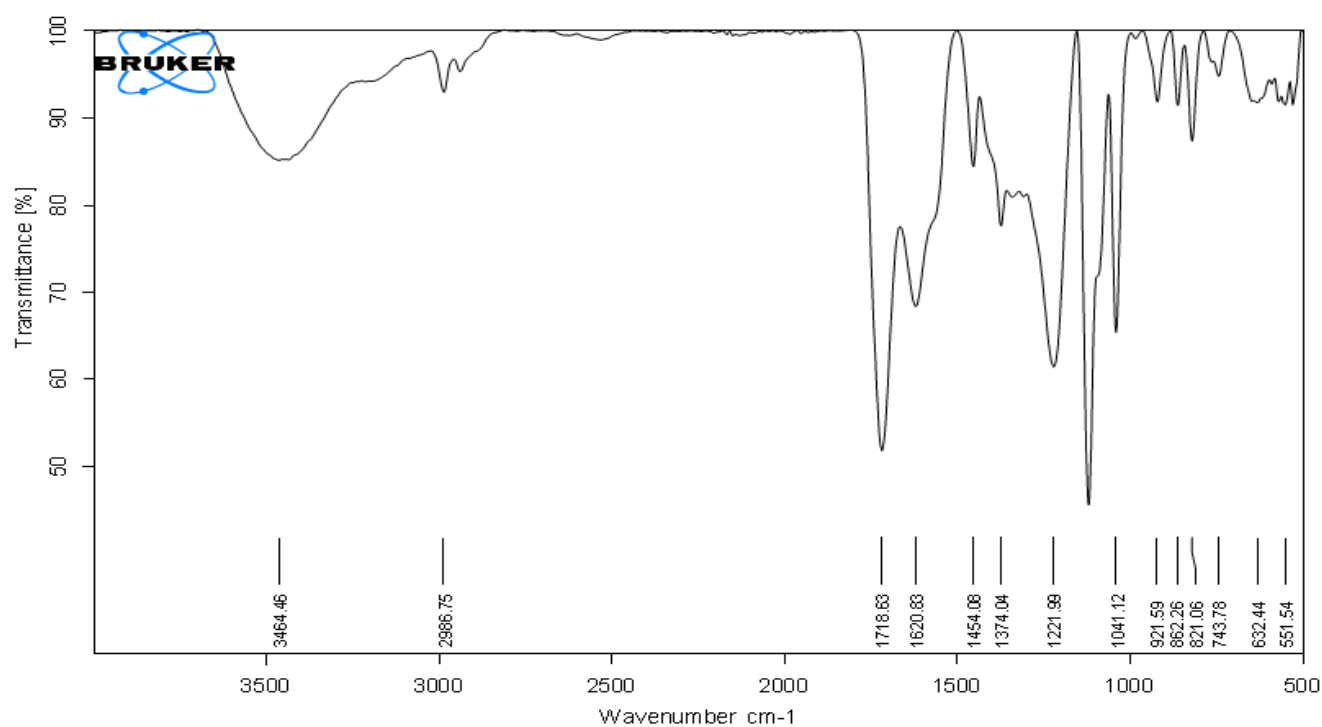


Figure S4: IR Spectra of L4 Lactic Acid-Maltose- Aloe Vera Juice

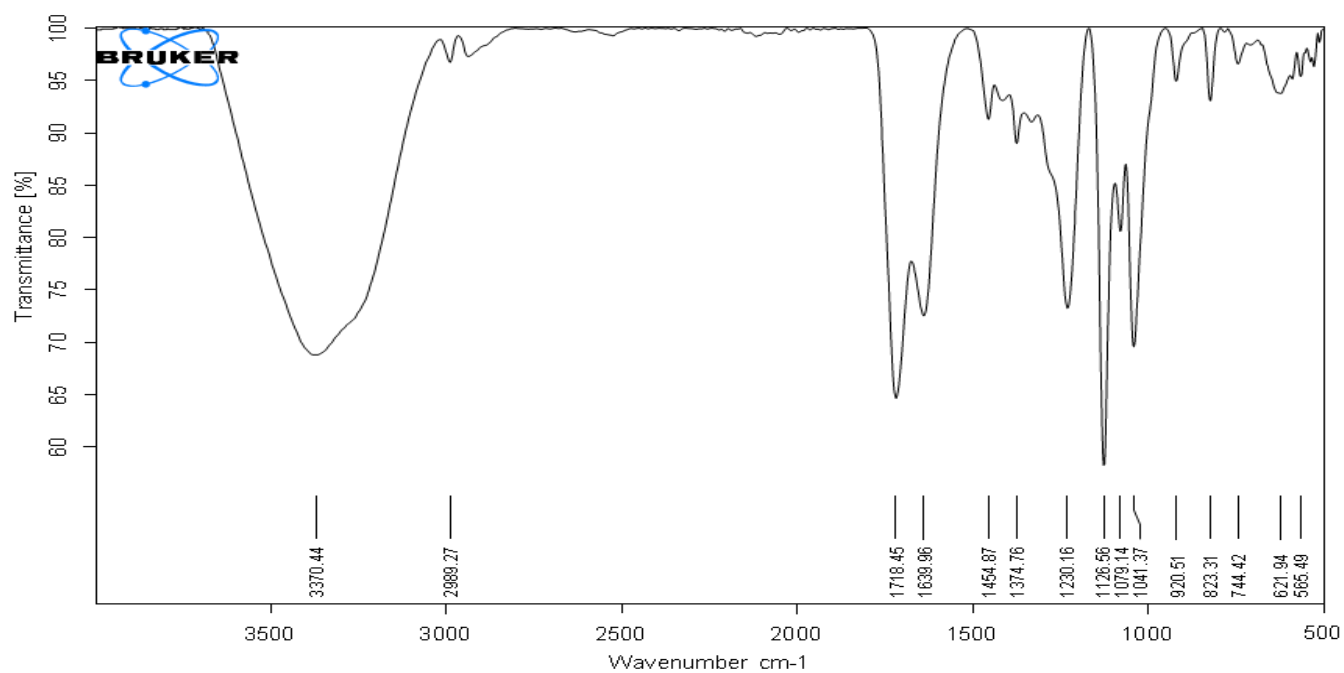


Figure S5: IR Spectra of L5 Lactic Acid-Proline-Aloe Vera Juice

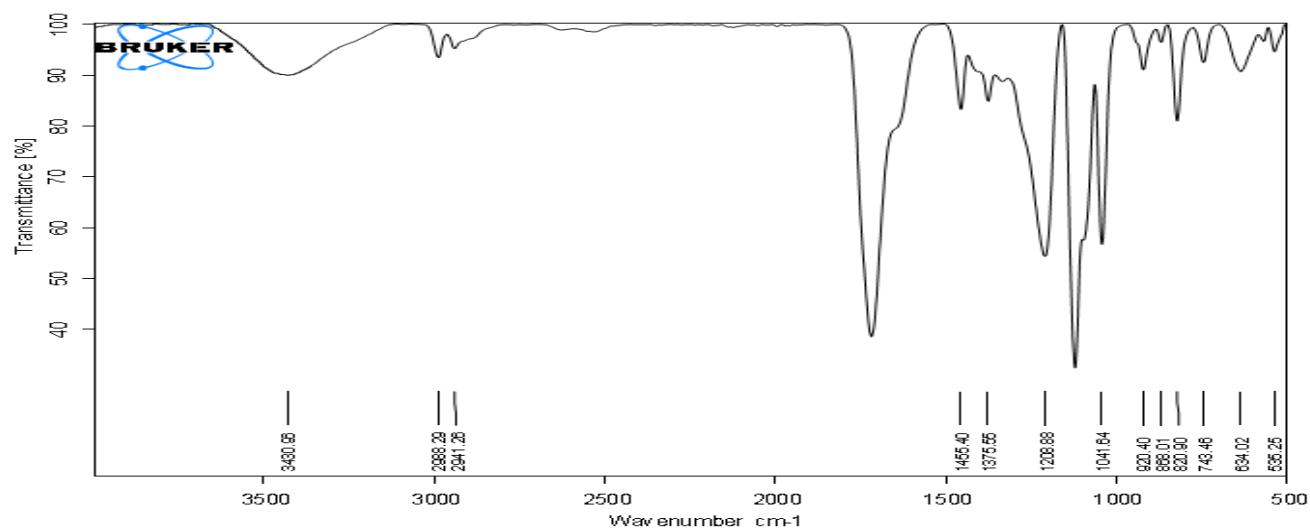


Figure S6: IR Spectra of Pure Lactic Acid

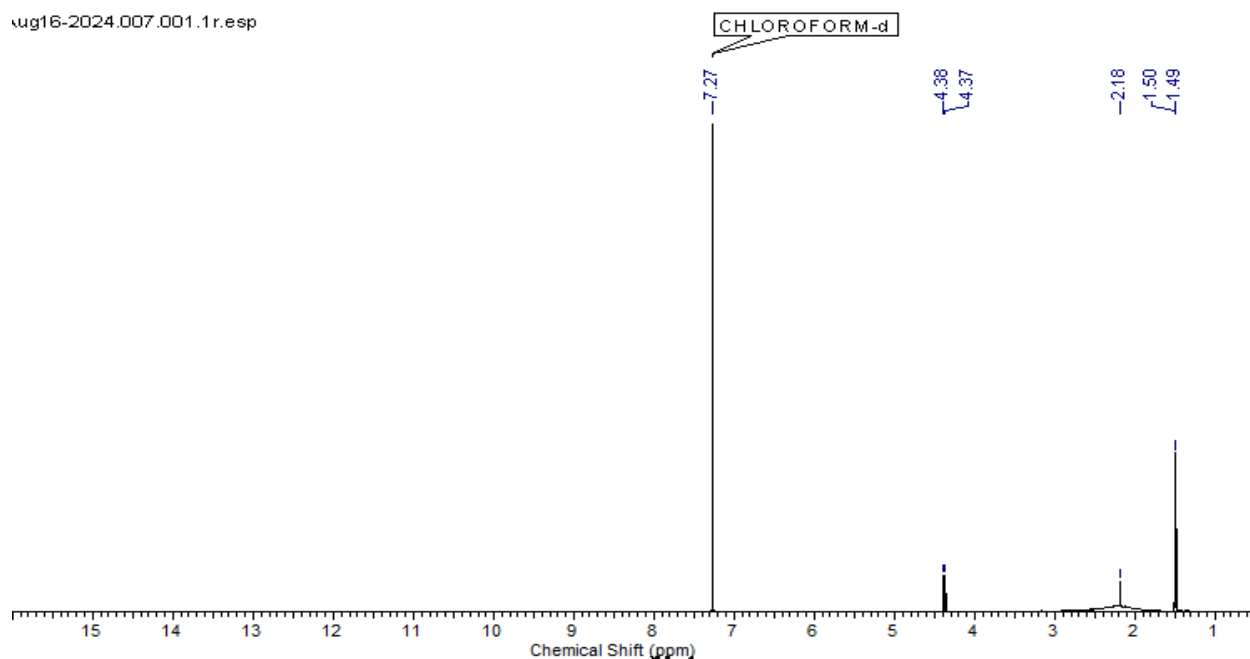


Figure S7: ^1H -NMR (500 MHz, CDCl_3) Spectrum of L1 Lactic Acid-Maltose- Amla Juice

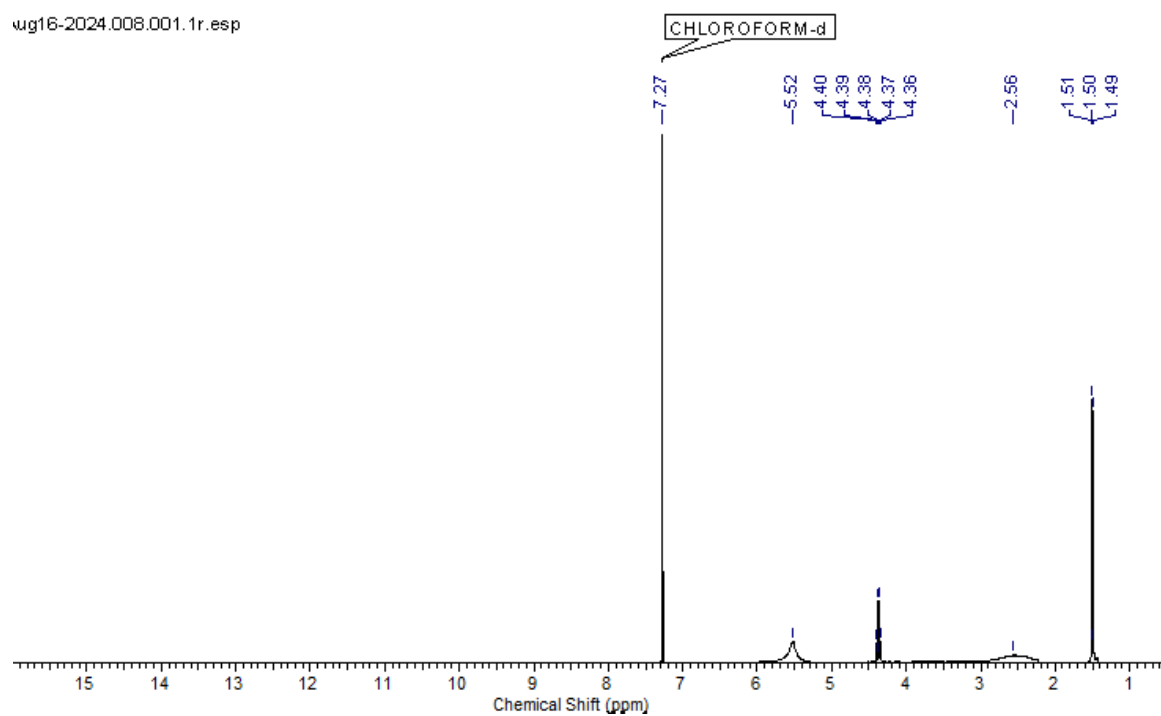


Figure S8: ^1H -NMR (500 MHz, CDCl_3) Spectrum of L2 Lactic Acid-Maltose- Water

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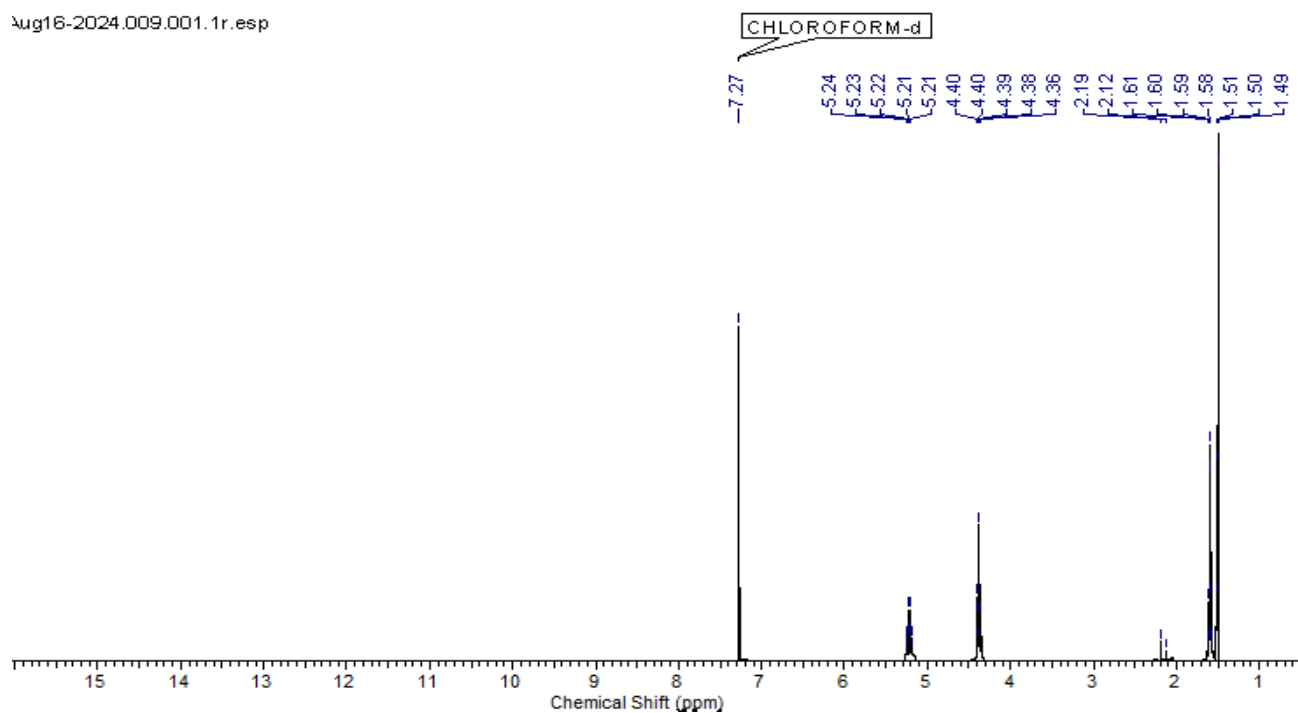


Figure S9: ^1H -NMR (500 MHz, CDCl_3) Spectrum of L3 Lactic Acid-Proline- SnCl_2

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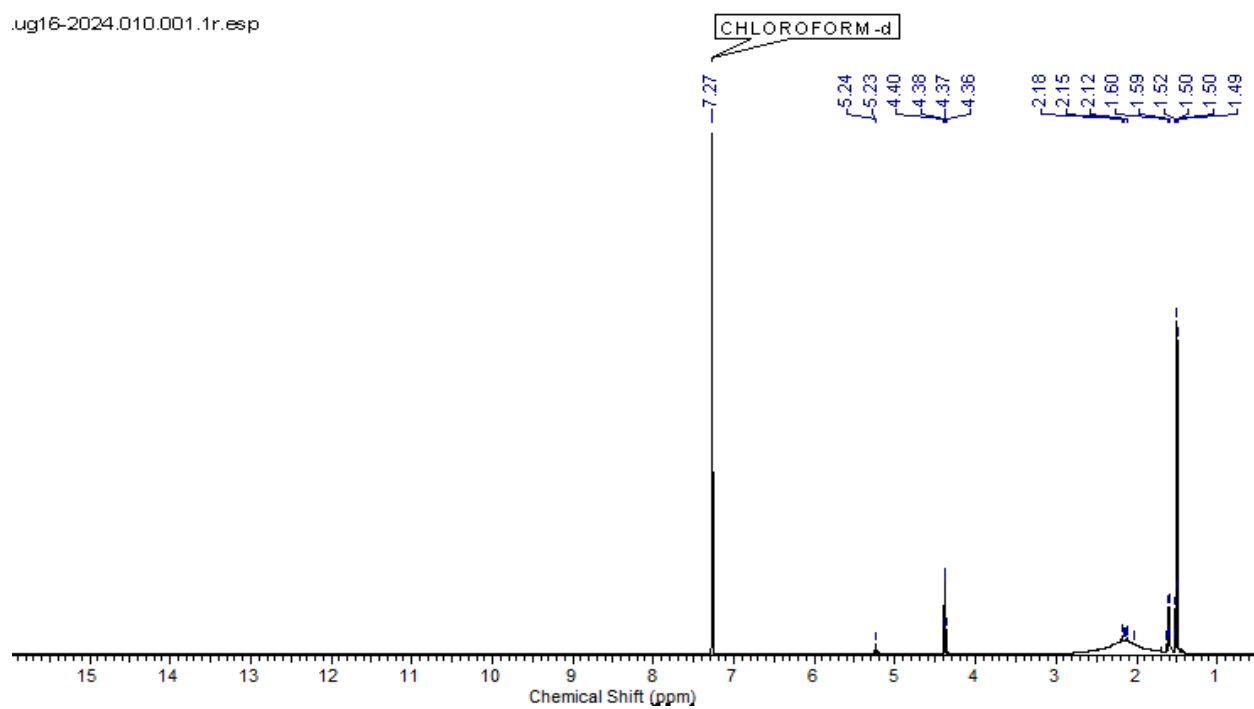


Figure S10: ^1H -NMR (500 MHz, CDCl_3) Spectrum of L4 Lactic Acid-Maltose- Aloe Vera Juice

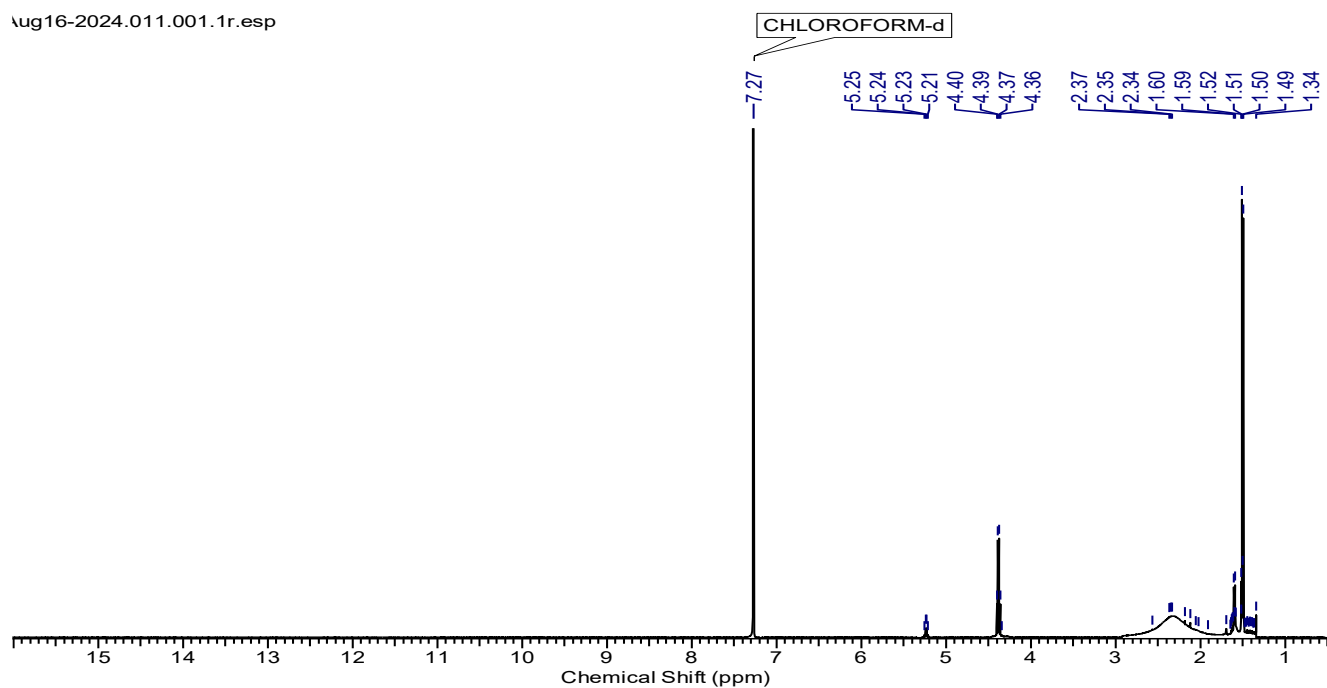


Figure S11: ^1H -NMR (500 MHz, CDCl_3) Spectrum of L5 Lactic Acid-Proline-Aloe Vera Juice

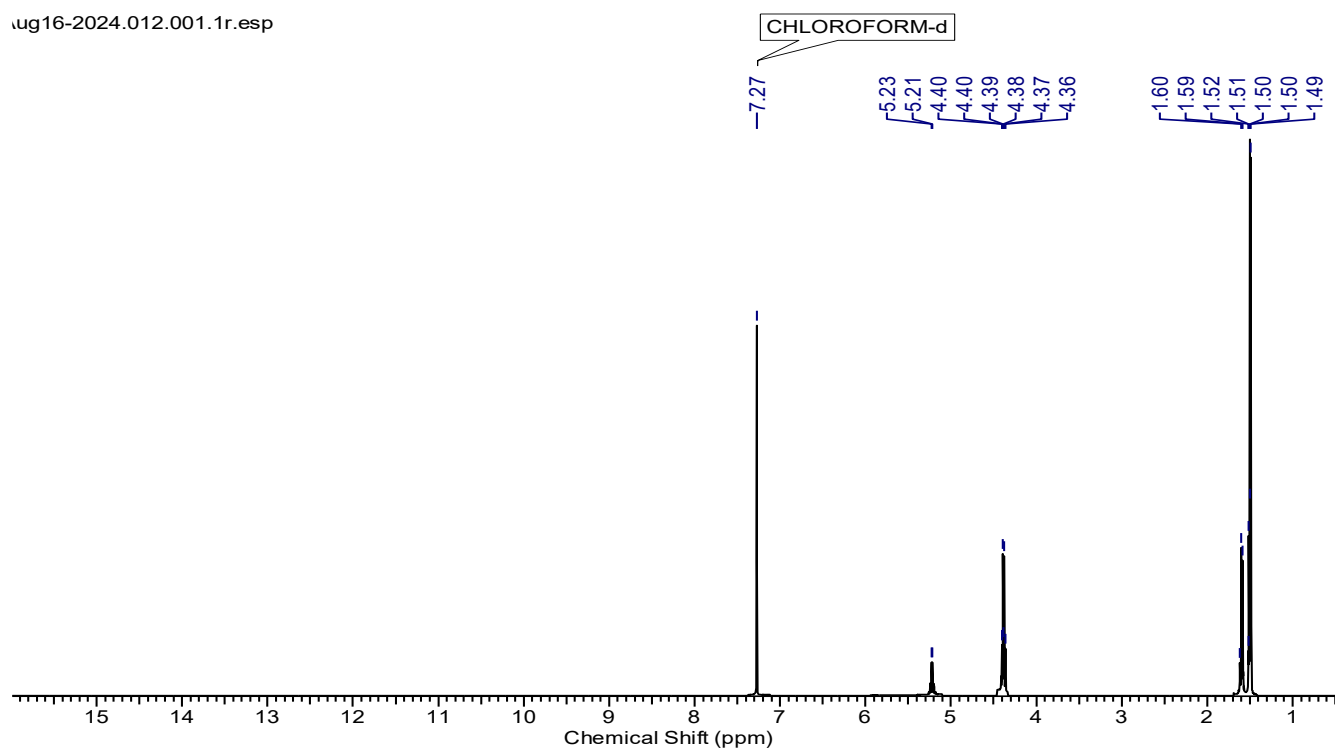


Figure S12: ^1H -NMR (500 MHz, CDCl_3) Spectrum of Pure Lactic Acid

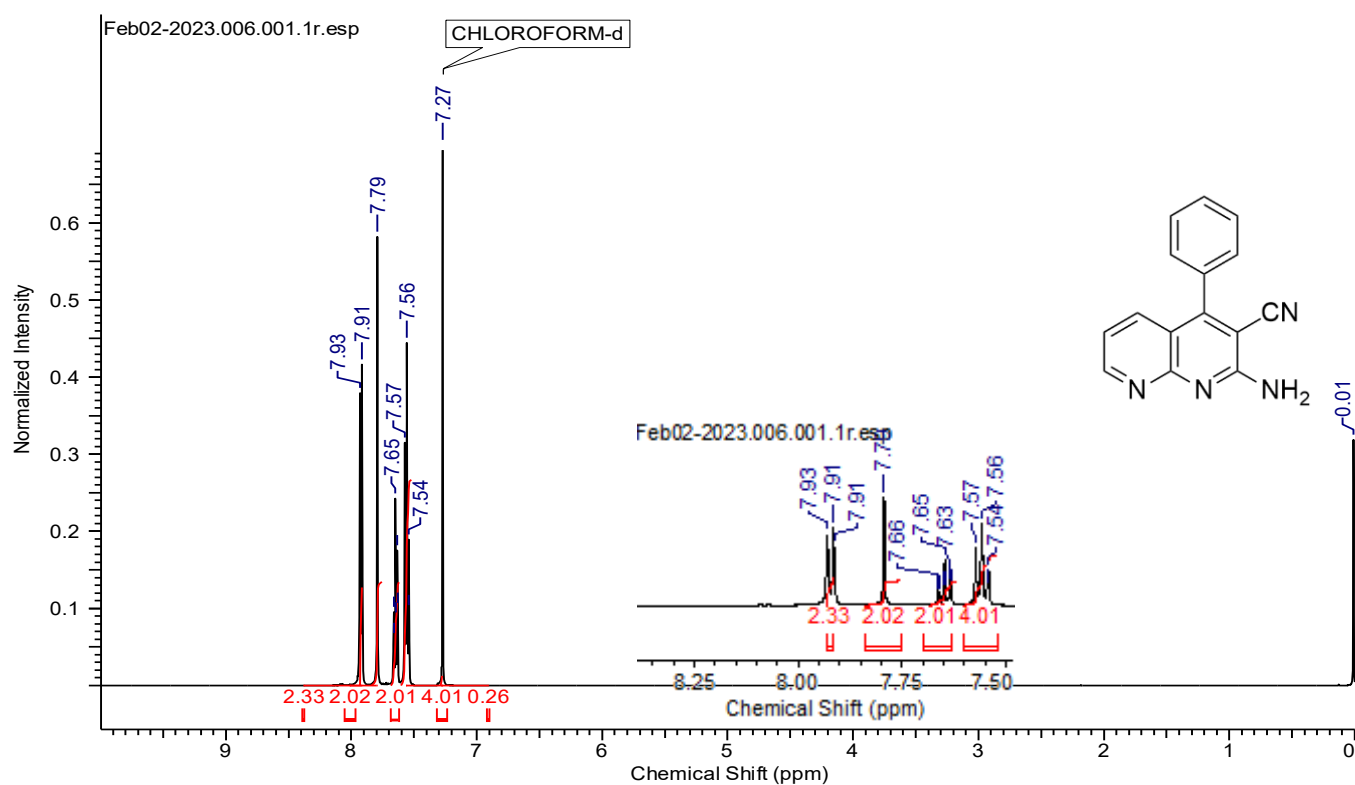


Figure S13: ^1H -NMR (500 MHz, CDCl_3) Spectrum of 2-Amino-4-phenyl-1,8-naphthyridine-3-carbonitrile (**4a**)

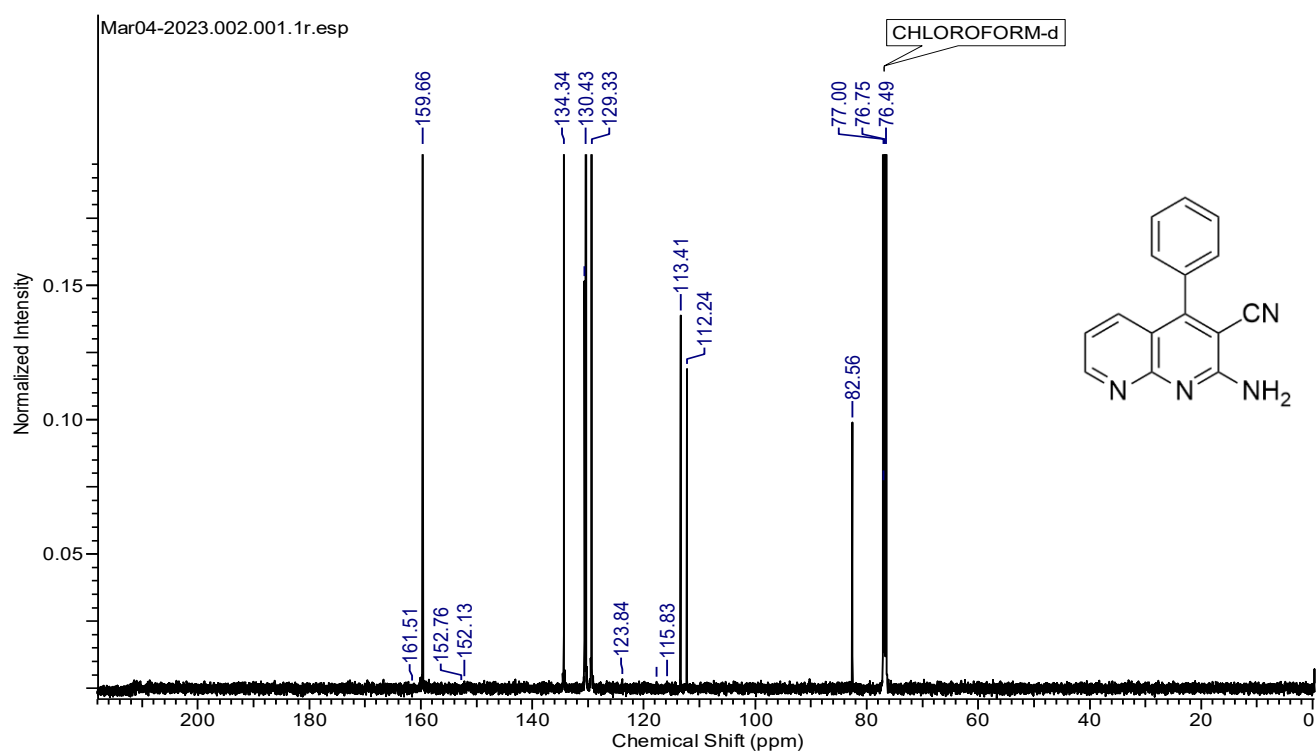
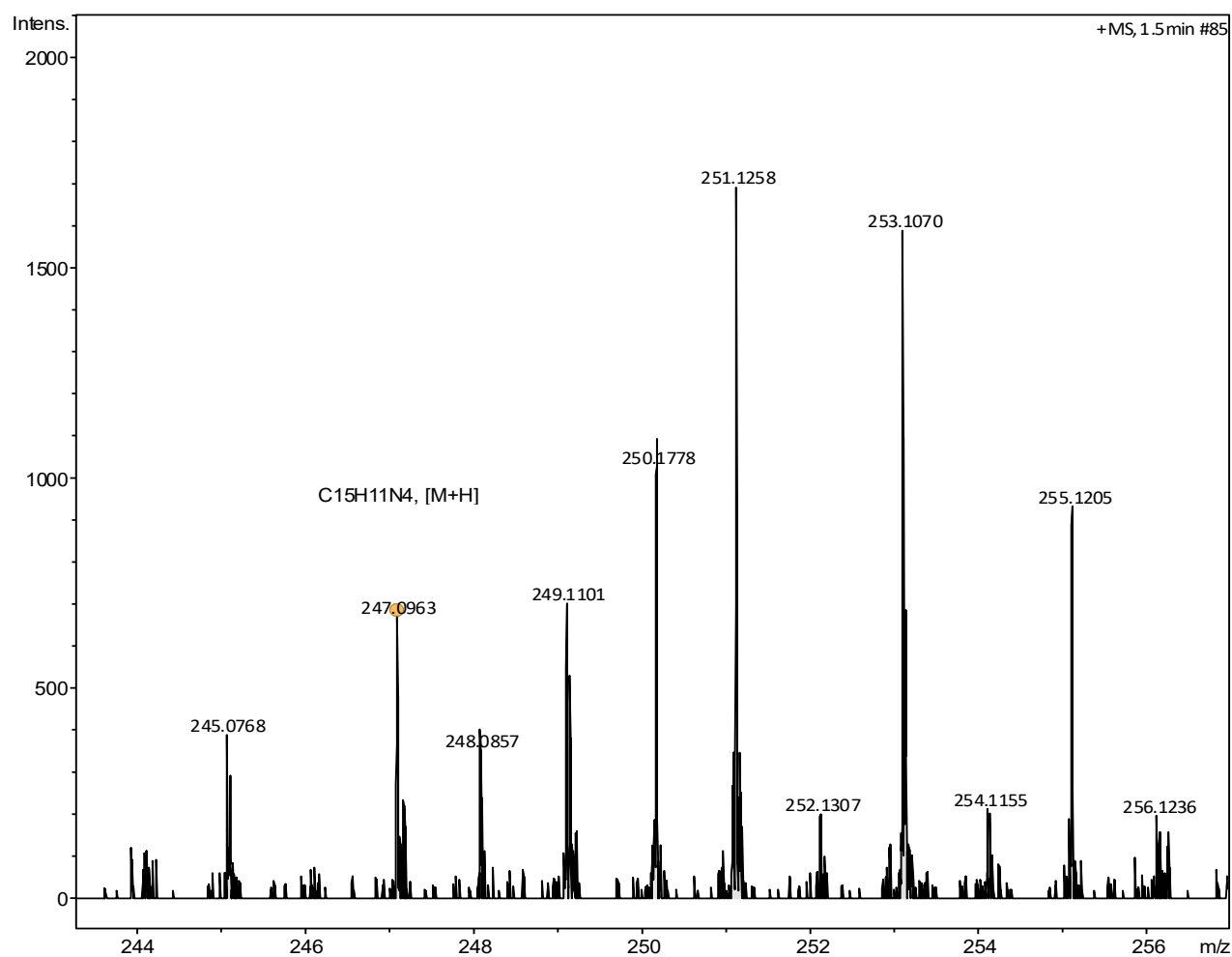


Figure S14: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 2-Amino-4-phenyl-1,8-naphthyridine-3-carbonitrile (**4a**)

Savitribai Phule Pune University - Central Instrumentation Facility

Analysis Info		Acquisition Date 10/16/2023 5:28:31 PM	
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Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



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	2	C ₁₁ H ₁₁ N ₄ O ₃	0.00	247.082567	-13.8	-55.8	607.3	8.5	even		ok	M+H

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Figure S15: HR-ESI-MS Spectrum of 2-Amino-4-phenyl-1,8-naphthyridine-3-carbonitrile (**4a**)

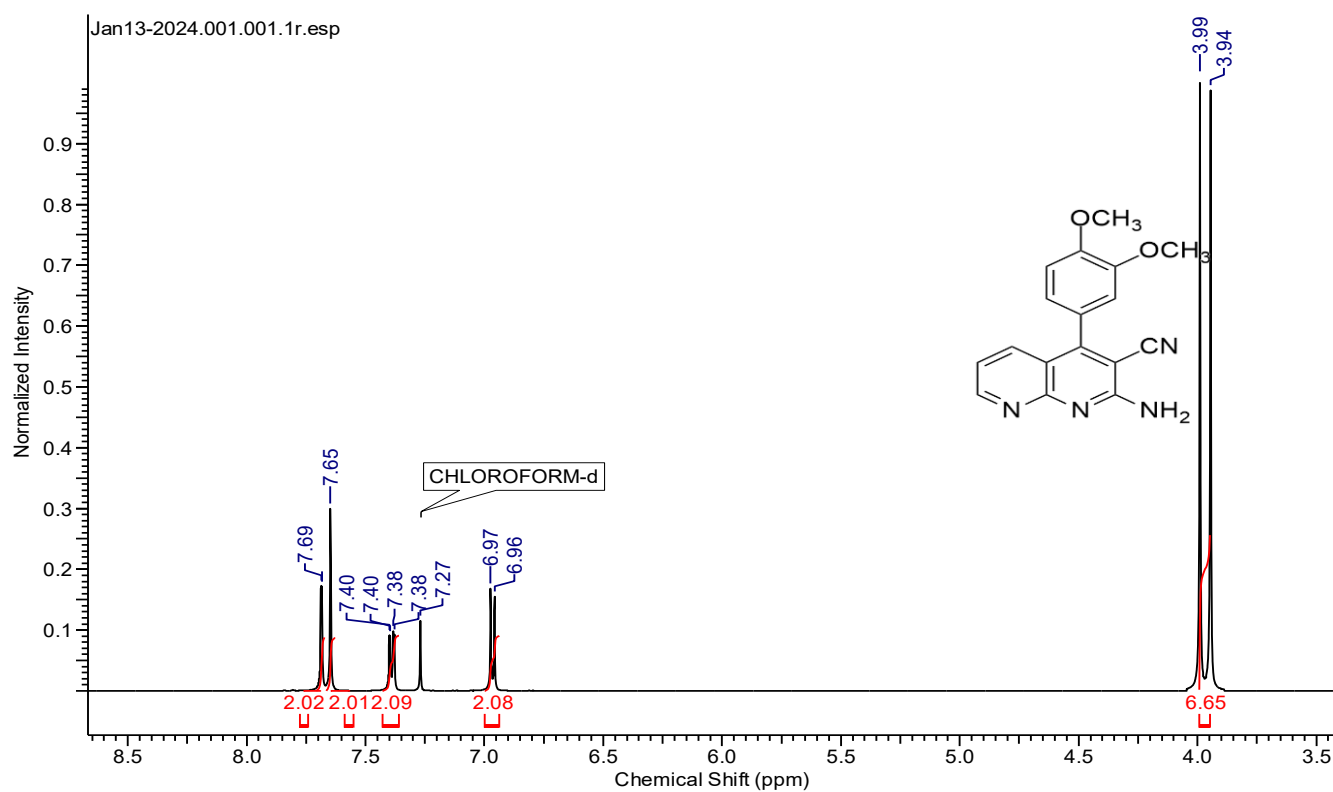


Figure S16: ^1H -NMR (500 MHz, CDCl_3) Spectrum of 2-Amino-4-(3,4-dimethoxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4b**)

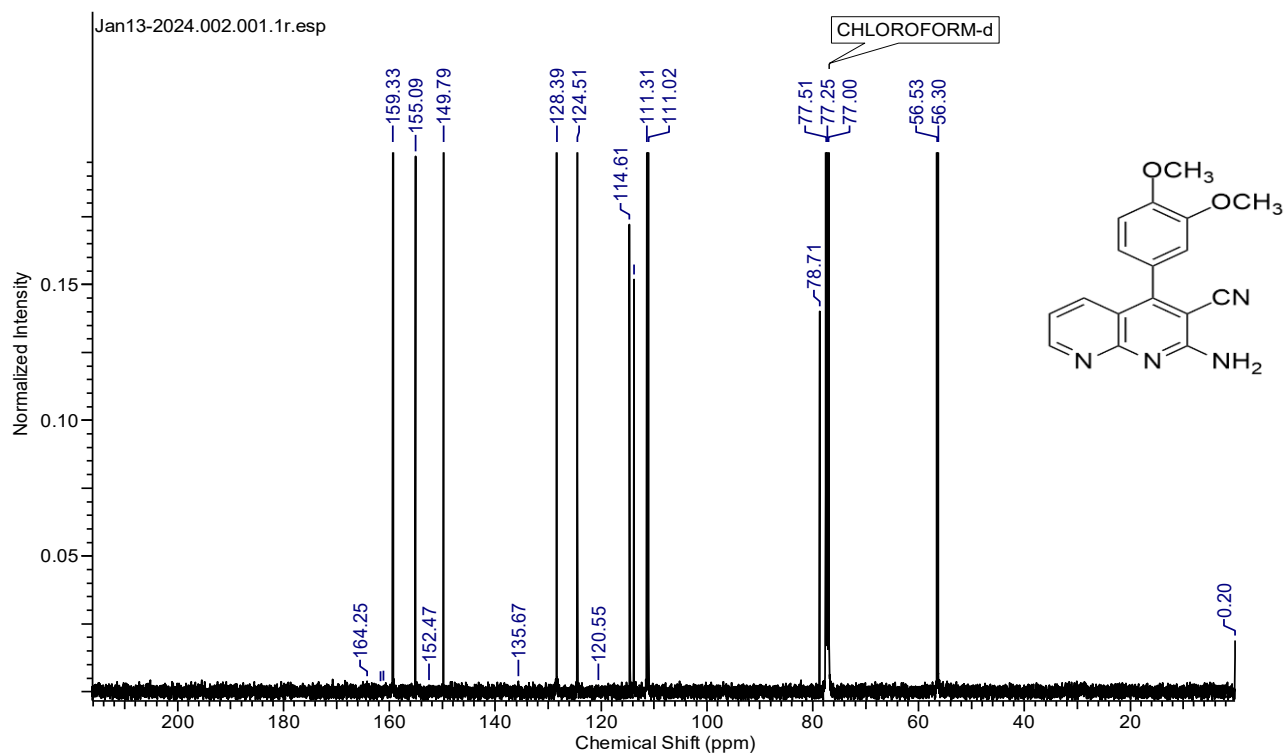


Figure S17: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 2-Amino-4-(3,4-dimethoxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4b**)

Analysis Info

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Sample Name D1

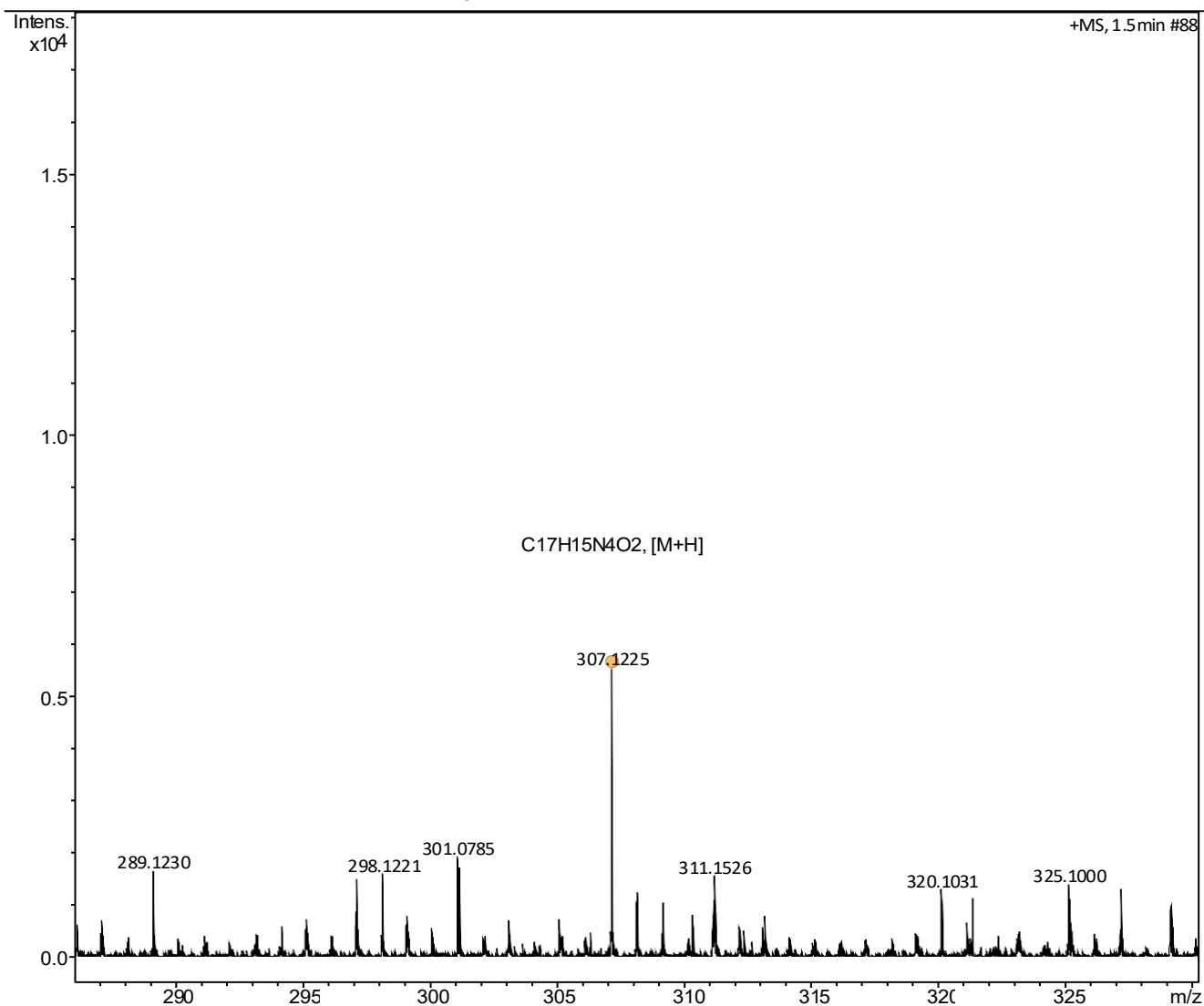
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Operator Nitin S. Kadam CIF

Instrument impactHD 1819696.00184

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Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule	Adduct
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406.335028	1	C ₁₅ H ₄ O ₂ N ₁	100.00	406.336096	1.1	2.6	30.5	1.5	even		ok	M+H
418.181797	1	C ₁₄ H ₂ O ₂ N ₁	71.16	418.180658	-1.1	-2.7	18.0	11.5	even		ok	M+H

Figure S18: HR-ESI-MS Spectrum of 2-Amino-4-(3,4-dimethoxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4b**)

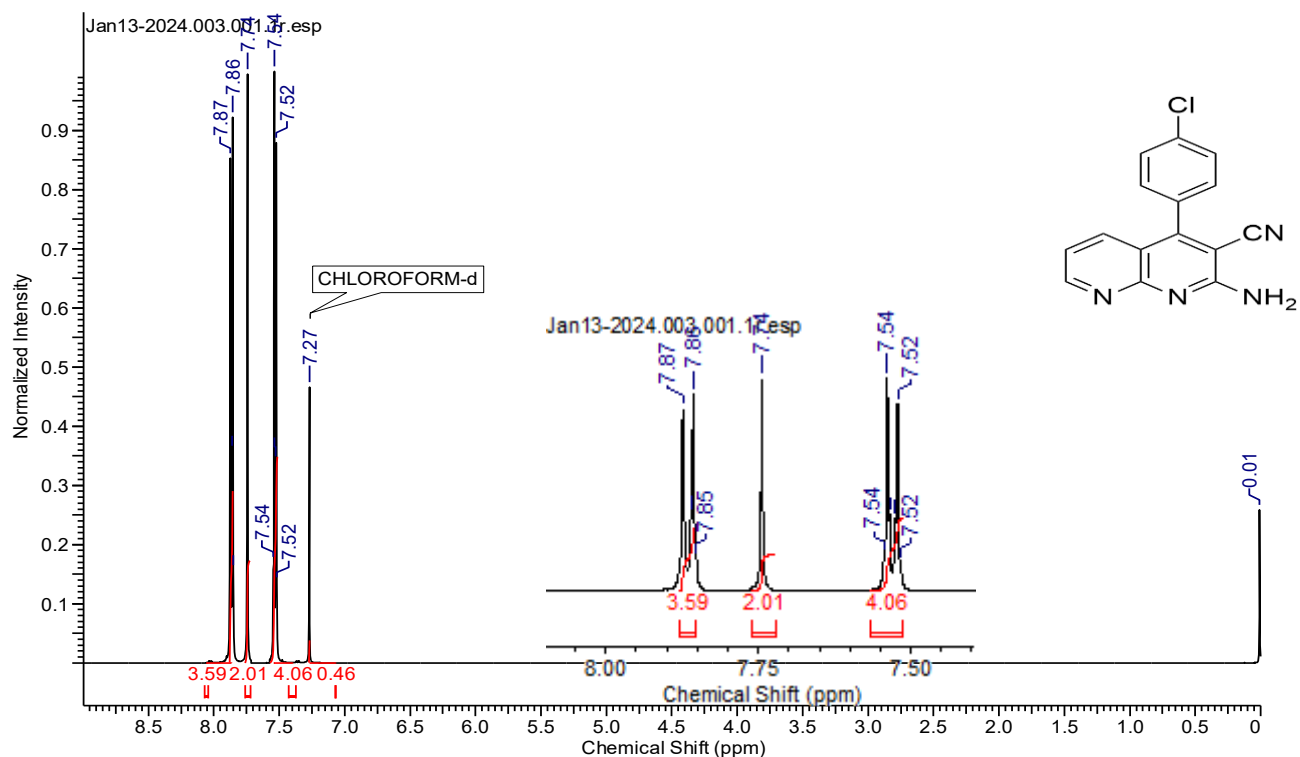


Figure S19: ^1H -NMR (500 MHz, CDCl_3) Spectrum of 2-Amino-4-(4-chlorophenyl)-1,8-naphthyridine-3-carbonitrile (**4c**)

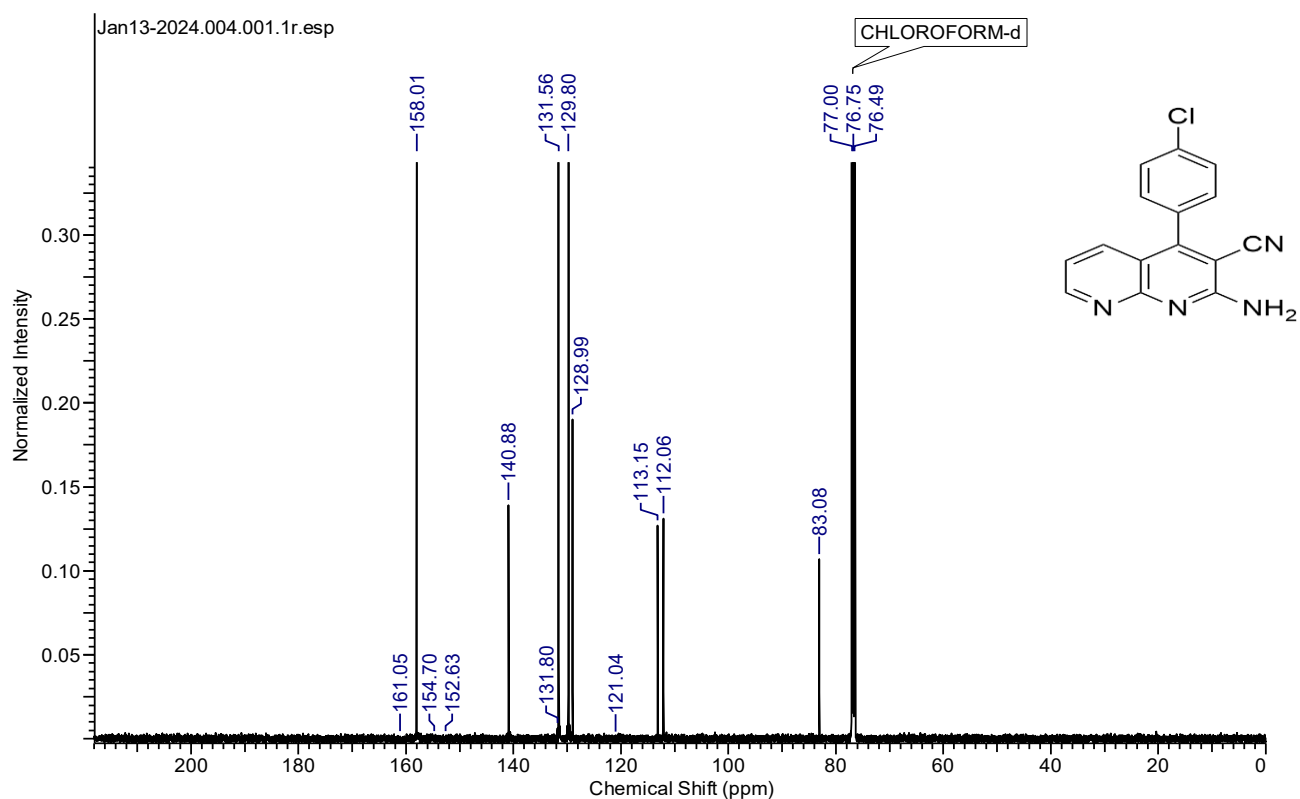


Figure S20: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 2-Amino-4-(4-chlorophenyl)-1,8-naphthyridine-3-carbonitrile (**4c**)

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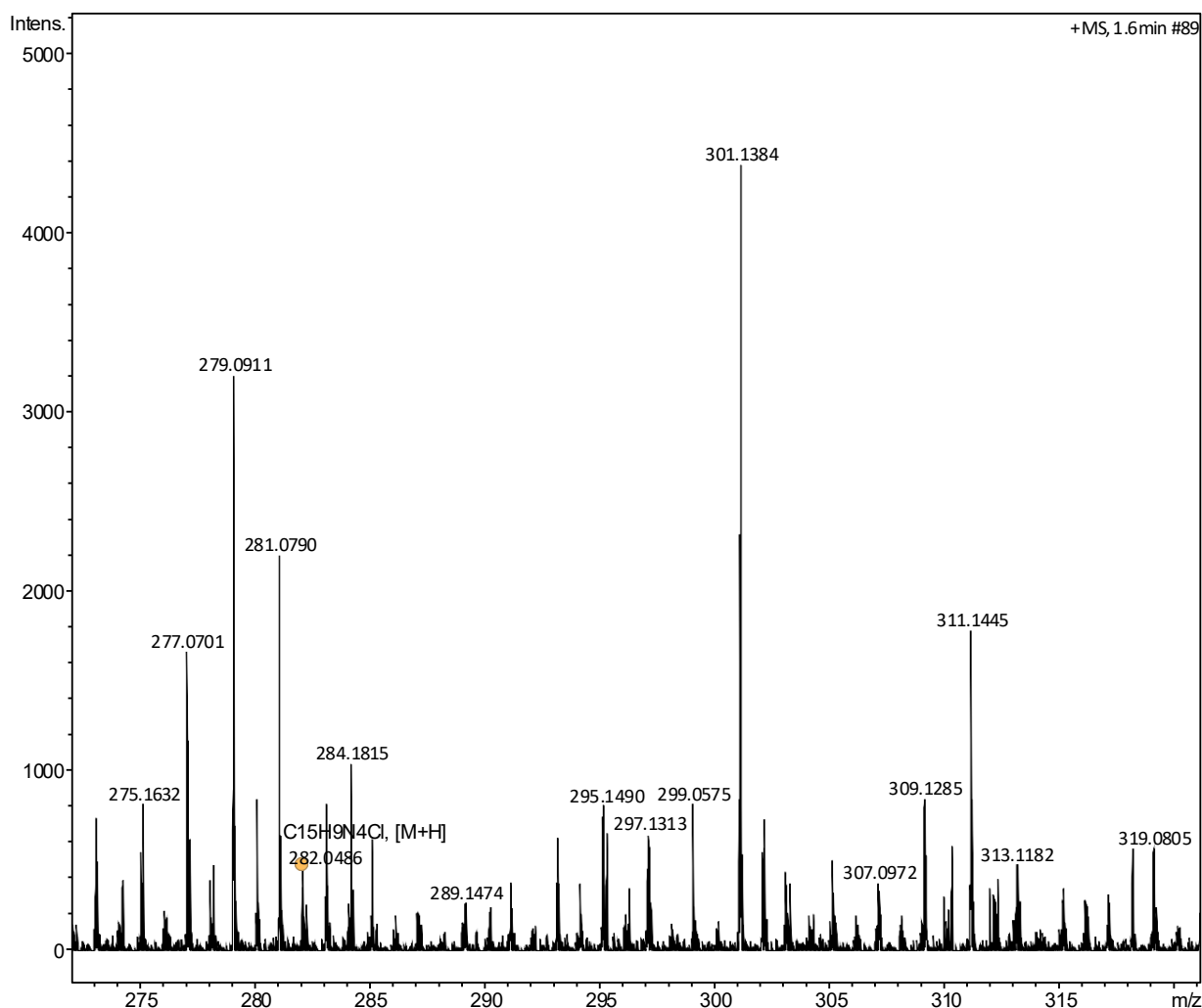
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Operator Nitin S. Kadam CIF

Instrument impactHD 1819696.00184

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Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



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Figure S21: HR-ESI-MS Spectrum of 2-Amino-4-(4-Chlorophenyl)-1,8-naphthyridine-3-carbonitrile (**4c**)

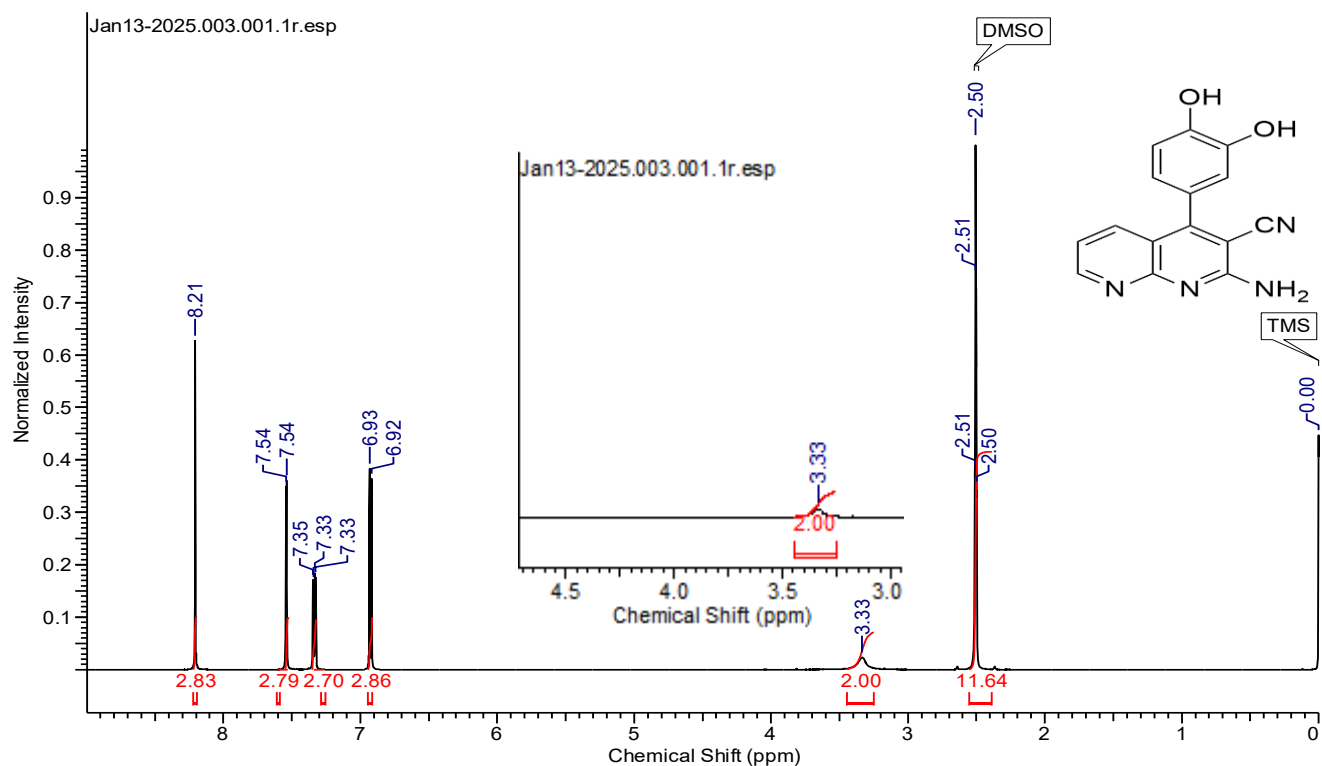


Figure S22: ^1H -NMR (500 MHz, CDCl_3) Spectrum of 2-Amino-4-(3,4-dihydroxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4d**)

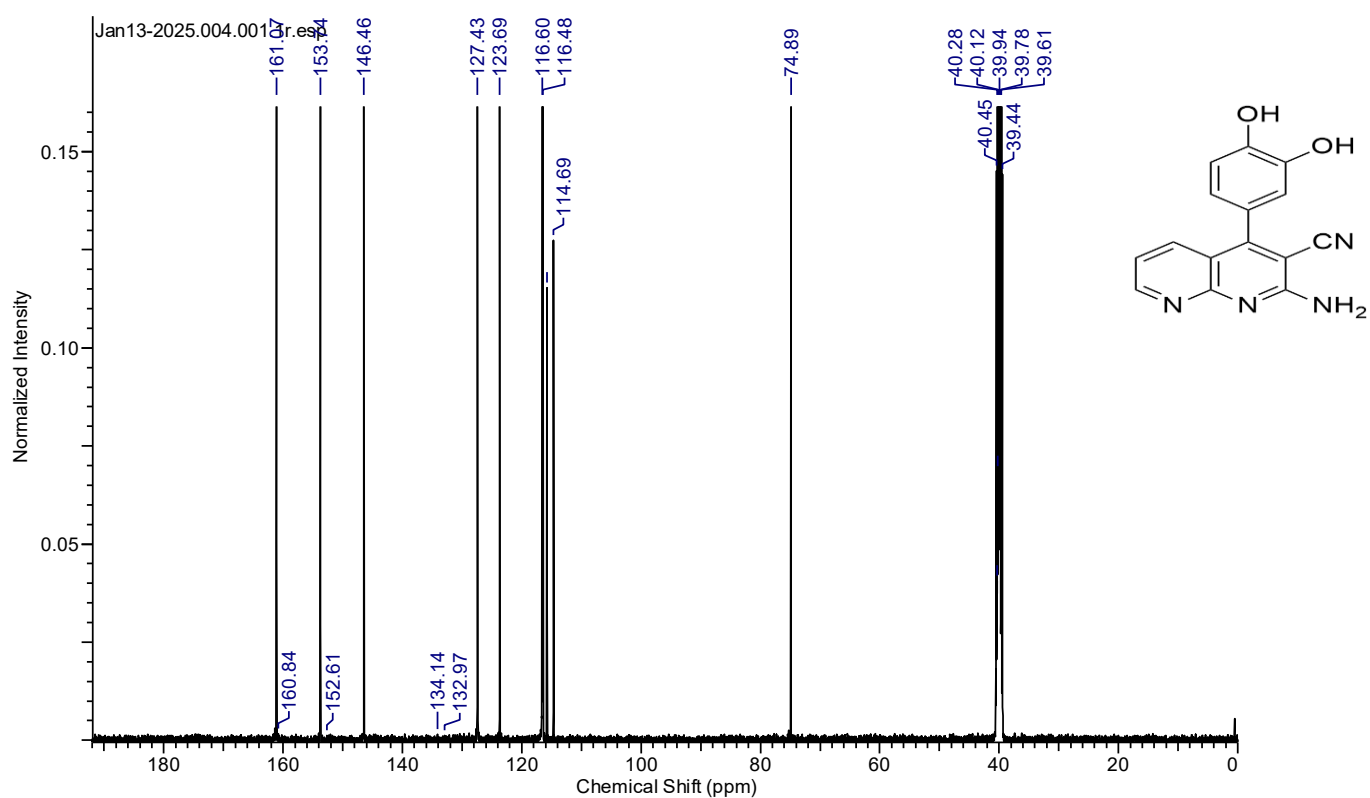
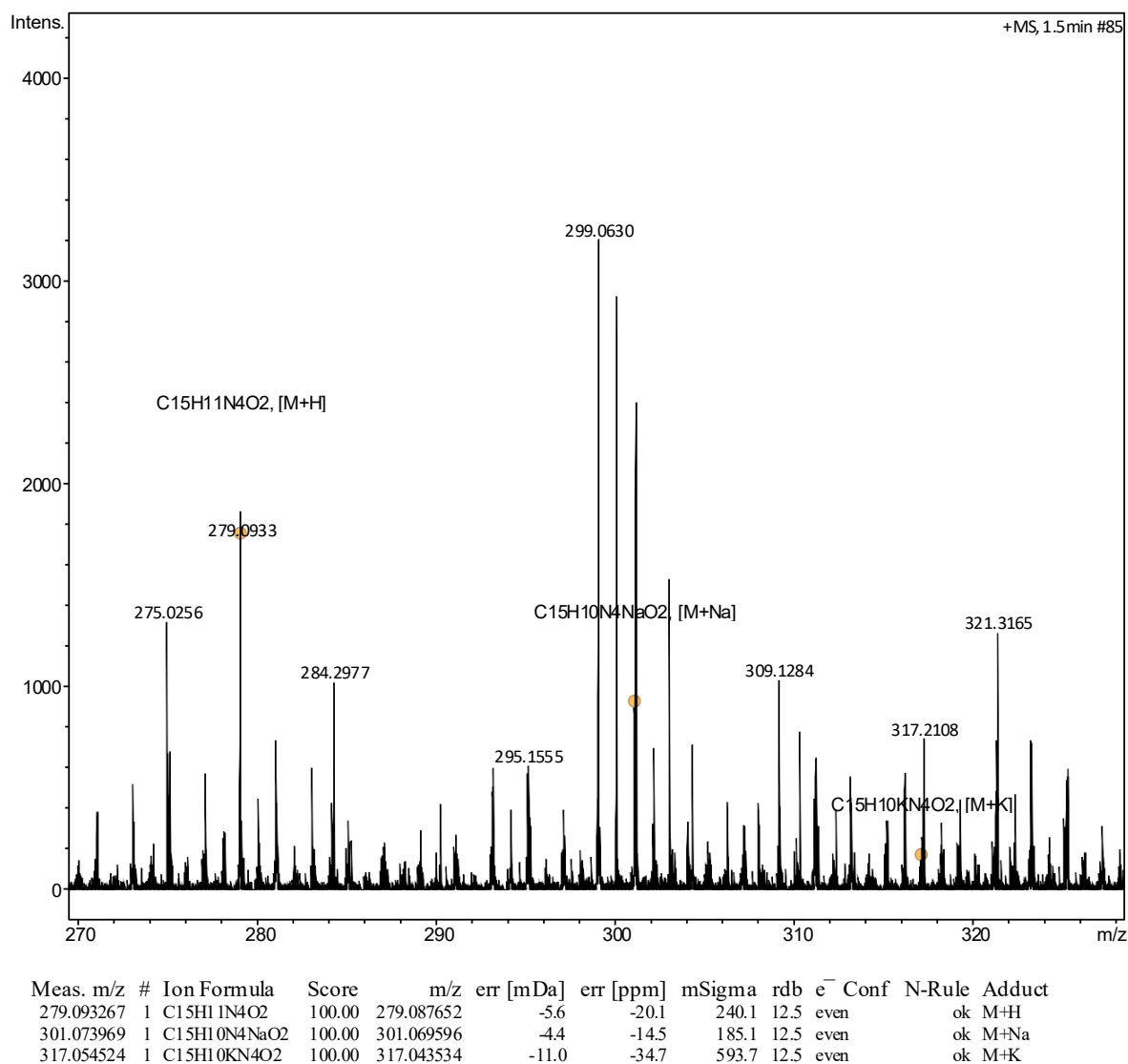


Figure S23: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 2-Amino-4-(3,4-dihydroxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4d**)

Analysis Info Acquisition Date 1/12/2024 3:15:19 PM
 Analysis Name D:\Data\2024\JAN\SPPU COLLEGE\H. R. M. Rajgurunagar\RUPALI VADAK\D3_RE3_01_6771.d Method
 dlc_ms20-1200mz_10min_0.120ml flow_90b_dec 23.m Operator Nitin S. Kadam CIF
 Sample Name D3 Instrument impact HD 1819696.00184

Acquisition Parameter
 Source Type ESI Ion Polarity Positive Set Nebulizer 0.8 Bar
 Focus Active Set Capillary 4500 V Set Dry Heater 200 °C
 ScanBegin 20 m/z Set End Plate Offset -500 V Set Dry Gas 7.0 l/min
 Scan End 1200 m/z Set Charging Voltage 2000 V Set Divert Valve Source
 Set Corona 0 nA Set APCI Heater 0 °C



D3_RE3_01_6771.d

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Figure S24: HR-ESI-MS Spectrum of 2-Amino-4-(3,4-dihydroxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4d**)

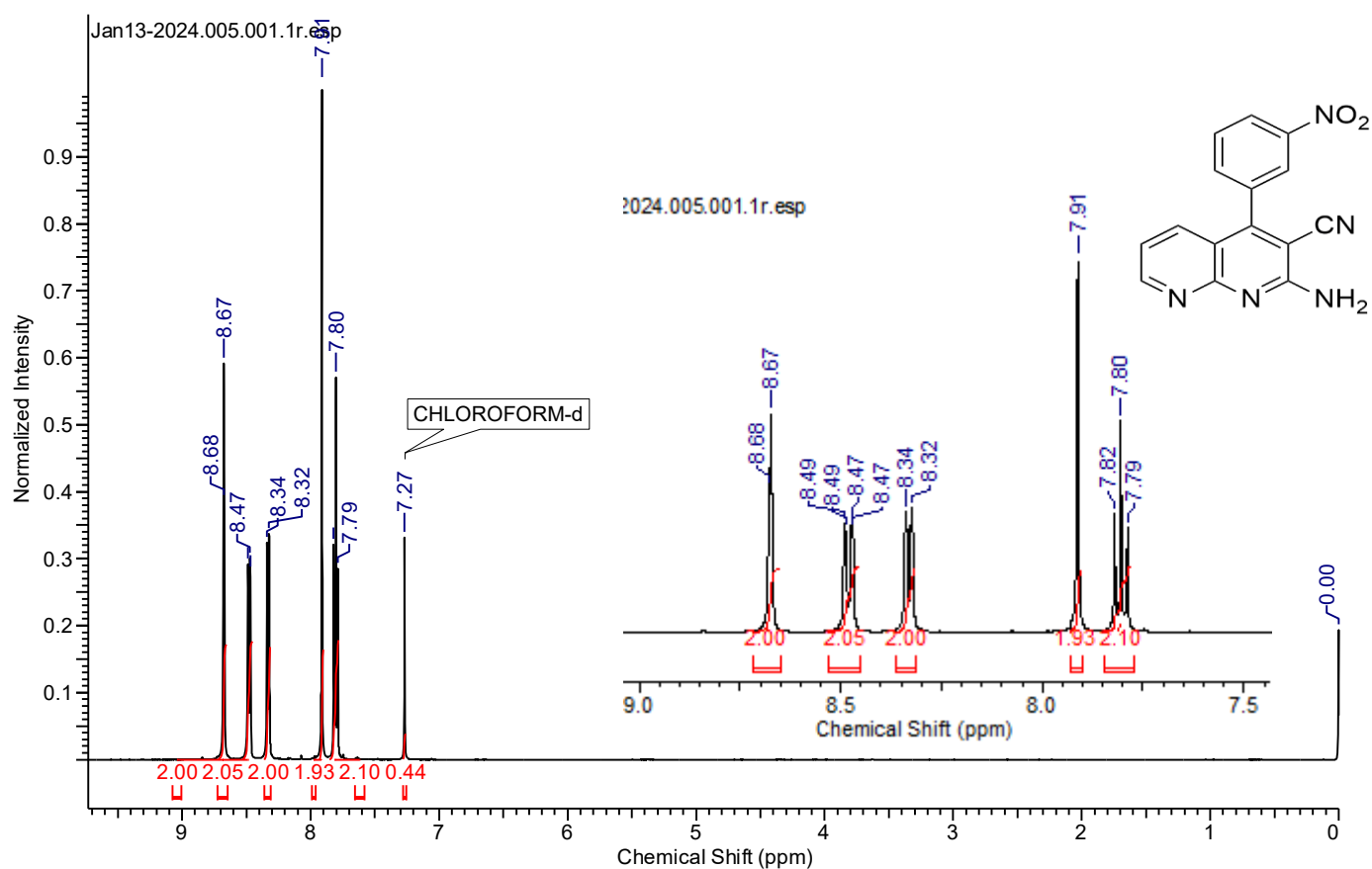


Figure S25: ^1H -NMR (500 MHz, CDCl_3) Spectrum of 2-Amino-4-(3-nitrophenyl)-1,8-naphthyridine-3-carbonitrile (**4e**)

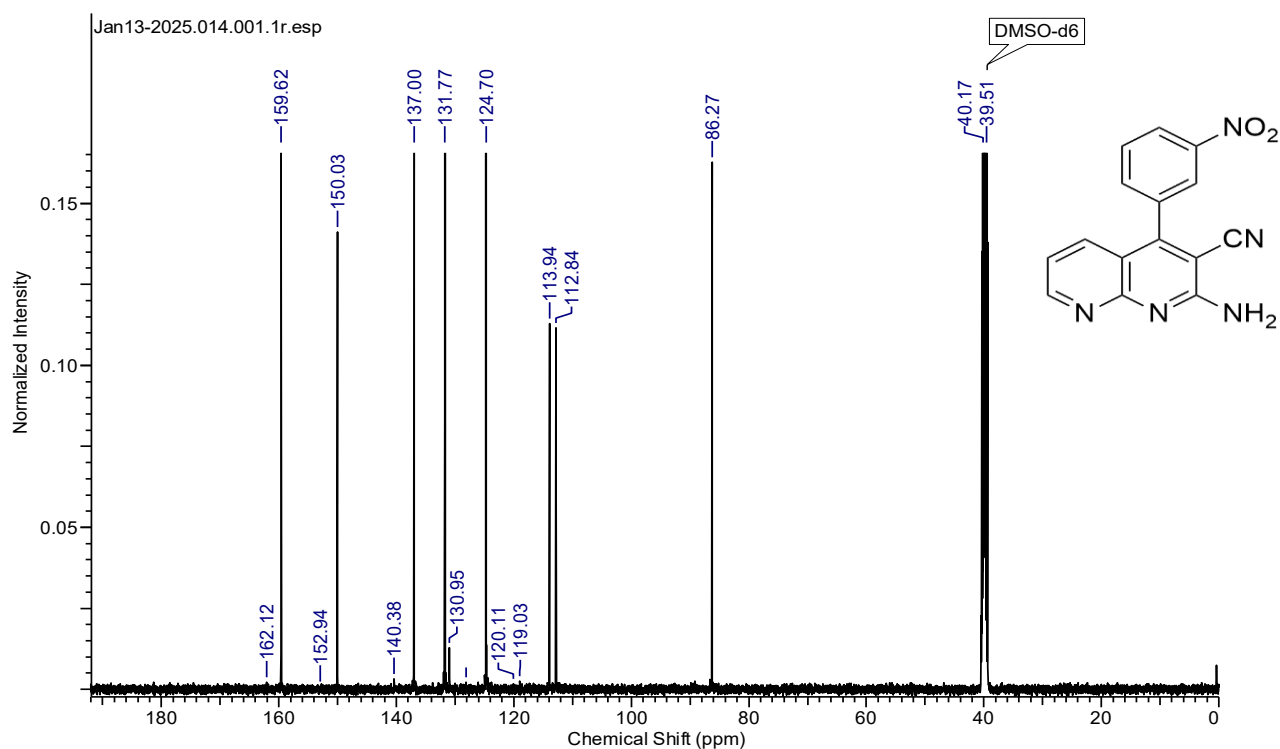


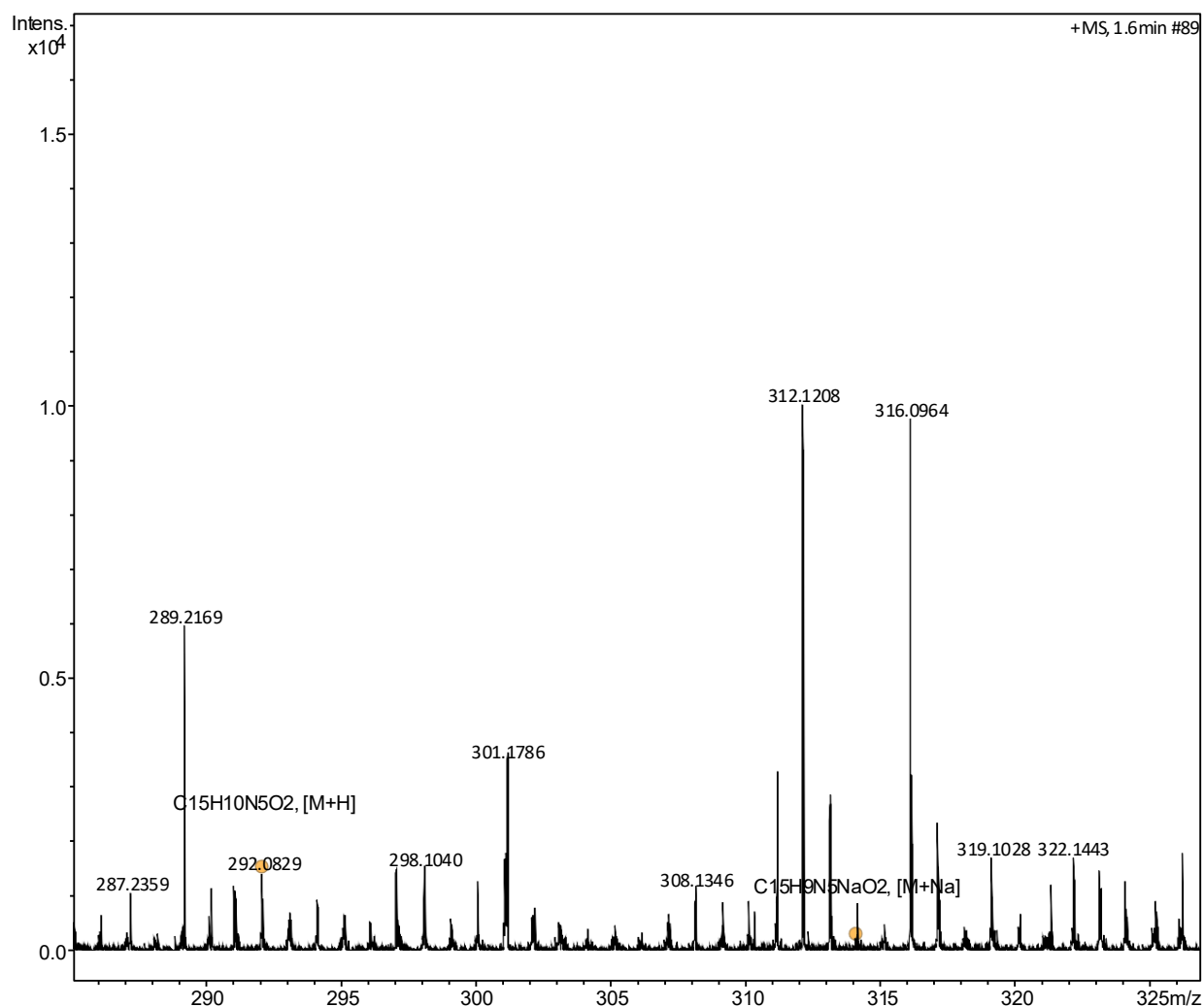
Figure S26: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 2-Amino-4-(3-nitrophenyl)-1,8-naphthyridine-3-carbonitrile (**4e**)

Analysis Info

Acquisition Date 1/12/2024 4:34:21 PM
 Analysis Name D:\Data\2024\JAN\SPPU COLLEGE\H. R. M. Rajgurunagar\RUPALI VADAK\D4_RA6_01_6777.d
 Method dlc_ms20-1200mz_10min_0.120ml flow_90b_dec23.m Operator Nitin S. Kadam CIF
 Sample Name D4 Instrument impactHD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule	Adduct
292.082899	1	C ₁₅ H ₁₀ N ₅ O ₂	100.00	292.082901	0.0	0.0	133.9	13.5	even		ok	M+H
314.067045	1	C ₁₅ H ₉ N ₅ NaO ₂	100.00	314.064845	-2.2	-7.0	495.9	13.5	even		ok	M+Na

D4_RA6_01_6777.d

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Figure S27: HR-ESI-MS Spectrum of 2-Amino-4-(3-nitrophenyl)-1,8-naphthyridine-3-carbonitrile (4e)

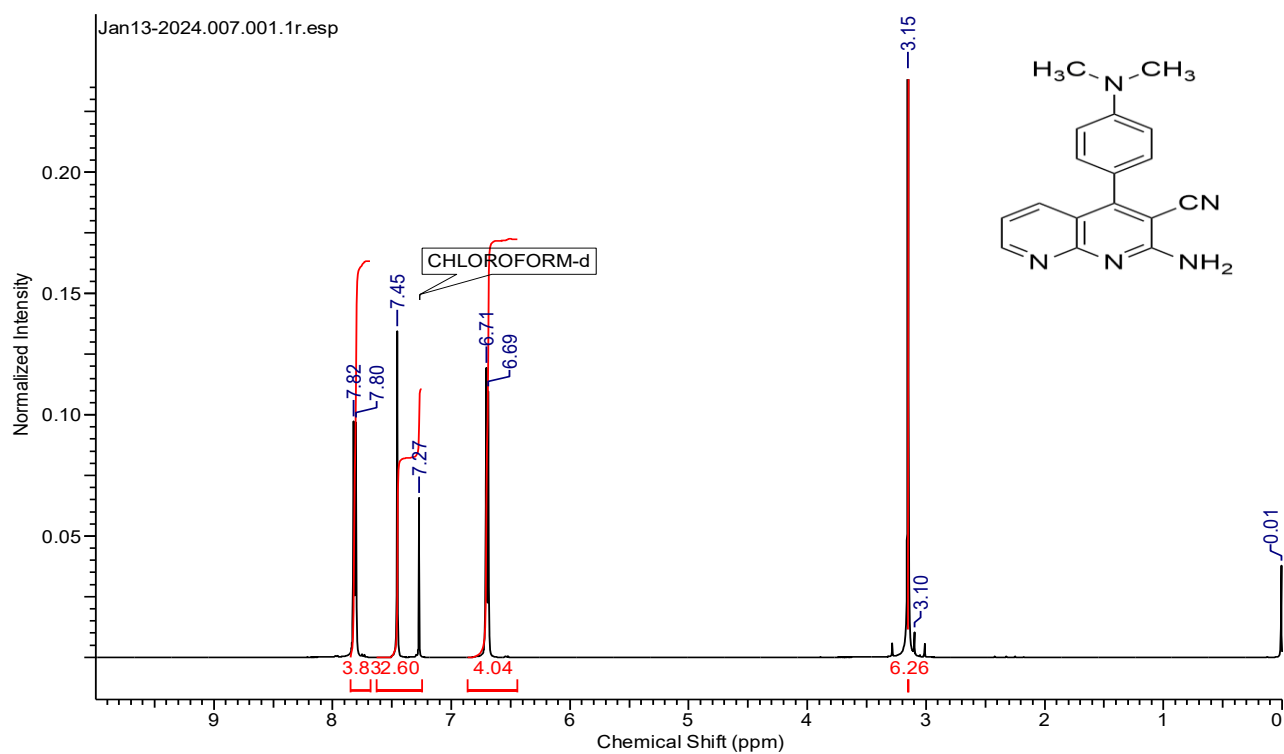


Figure S28: ^1H -NMR (500 MHz, CDCl_3) Spectrum of 2-amino-4-(4-dimethylaminophenyl)-1,8-naphthyridine-3-carbonitrile (**4f**)

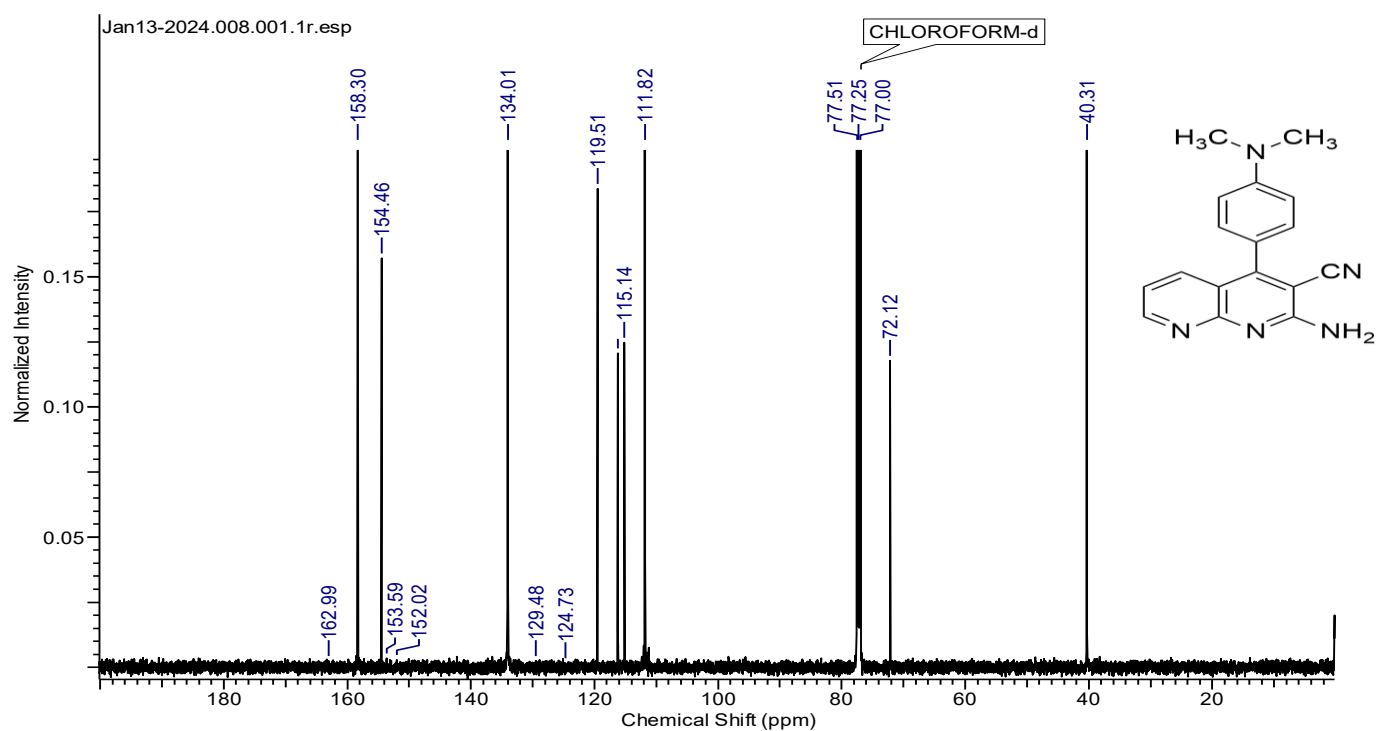
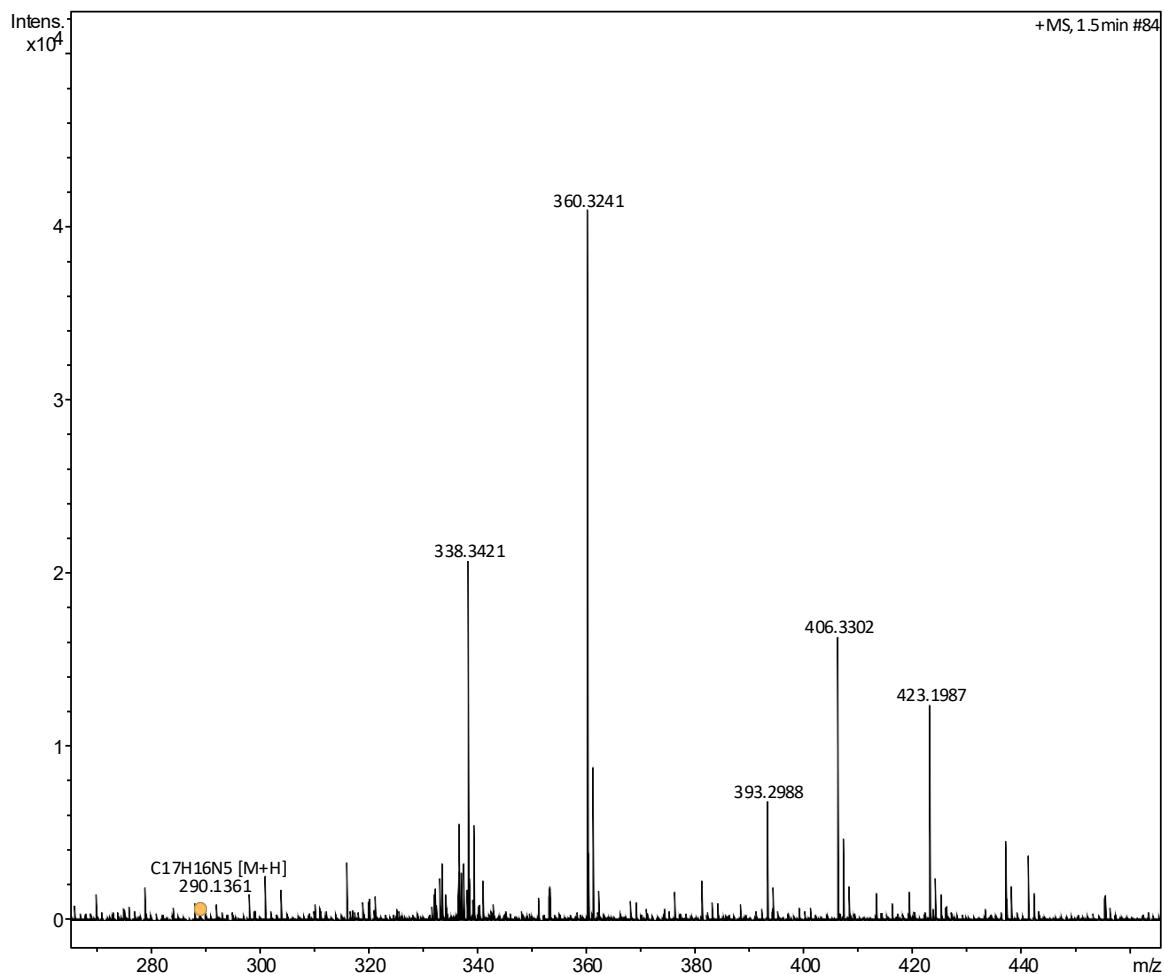


Figure S29: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 2-amino-4-(4-dimethylaminophenyl)-1,8-naphthyridine-3-carbonitrile (**4f**)

Analysis Info	Acquisition Date	1/10/2024 9:29:33 PM
Analysis Name	D:\Data\2024\JAN\SPPU COLLEGE\H. R. M. Rajgurunagar\RUPALI VADAKID5_RE5_01_6750.d	
Method	dlc_ms20-1200mz_10min_0.120ml flow_90b_dec 23.m	Operator Nitin S. Kadam CIF
Sample Name	D5	Instrument impactHD 1819696.00184

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
ScanBegin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



D5_RE5_01_6750.d

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Figure S30: HR-ESI-MS Spectrum of 2-amino-4-(4-dimethylaminophenyl)-1,8-naphthyridine-3-carbonitrile (**4f**)

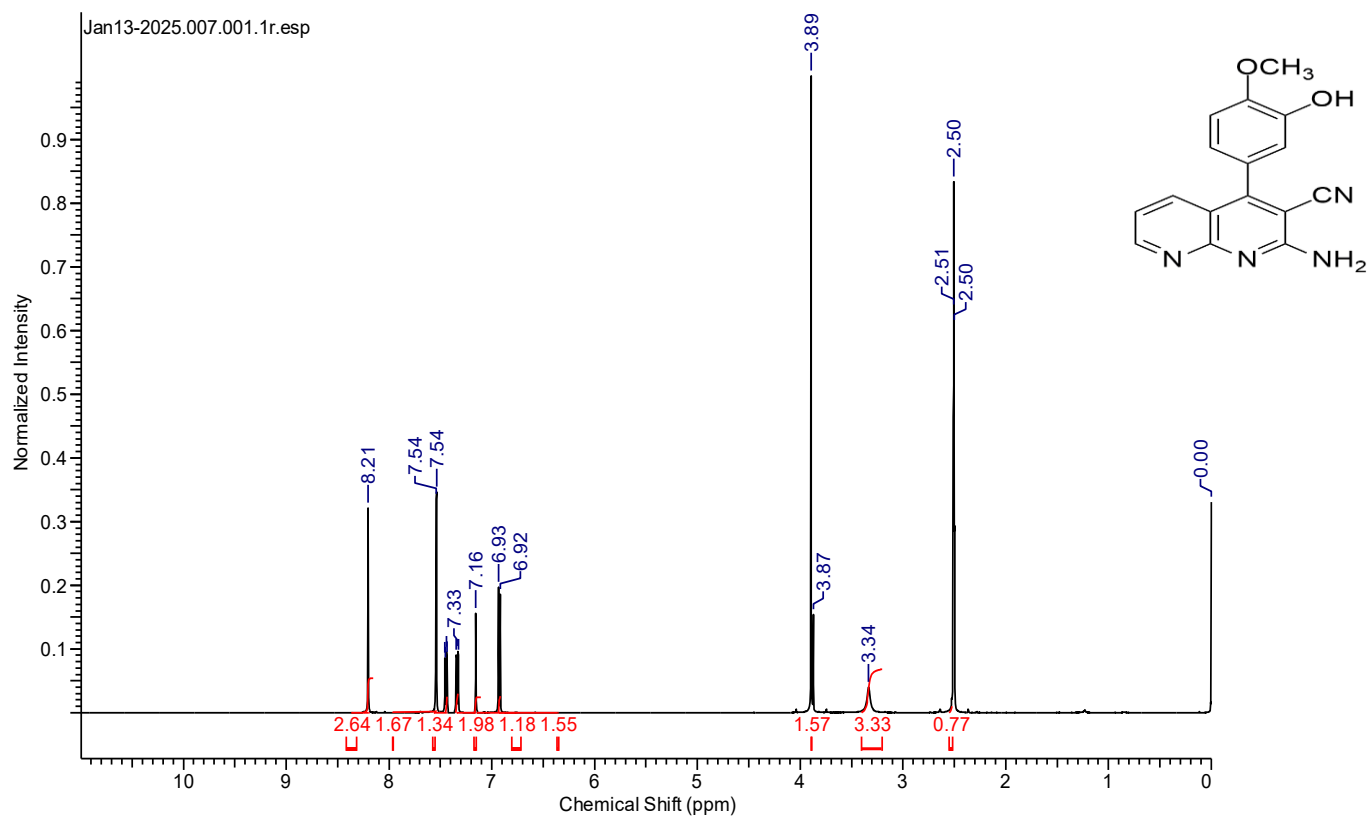


Figure S31: ^1H -NMR (500 MHz, CDCl_3) Spectrum of 2-amino-4-(3-hydroxy-4-methoxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4g**)

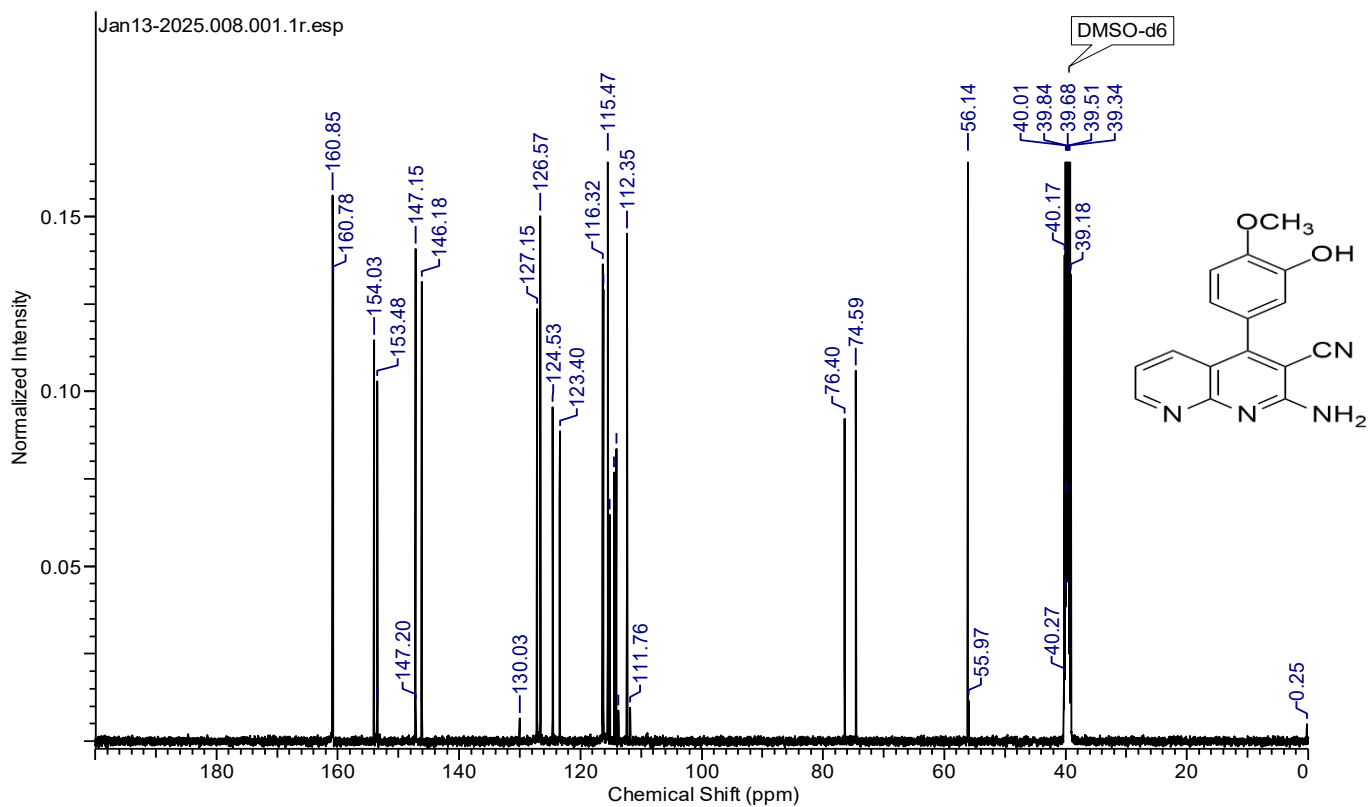


Figure S32: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 2-amino-4-(3-hydroxy-4-methoxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4g**)

Analysis Info

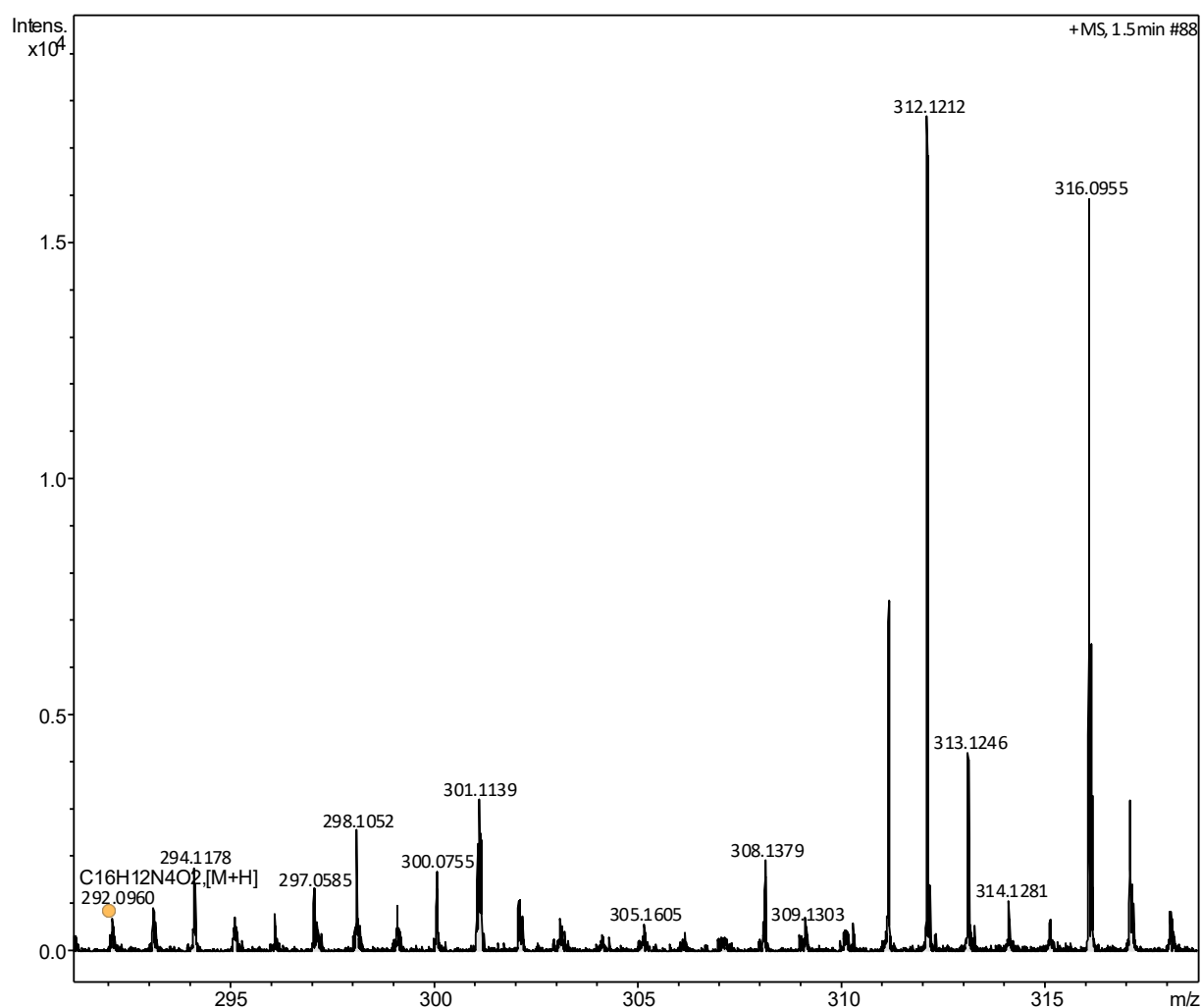
Analysis Name D:\Data\2024\JAN\SPPU COLLEGE\H. R. M. Rajgurunagar\RUPALI VADAK\D6_RA7_01_6778.d
 Method dlc_ms20-1200mz_10min_0.120ml flow_90b_dec 23.m
 Sample Name D6

Acquisition Date 1/12/2024 4:45:04 PM

Operator Nitin S. Kadam CIF
 Instrument impactHD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ⁻	Conf	N-Rule	Adduct
293.119655	1	C ₁₆ H ₁₃ N ₄ O ₂	100.00	293.103302	-16.4	-55.8	580.8	12.5	even		ok	M+H

D6_RA7_01_6778.d

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Figure S33: HR-ESI-MS Spectrum of 2-amino-4-(3-hydroxy-4-methoxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4g**)

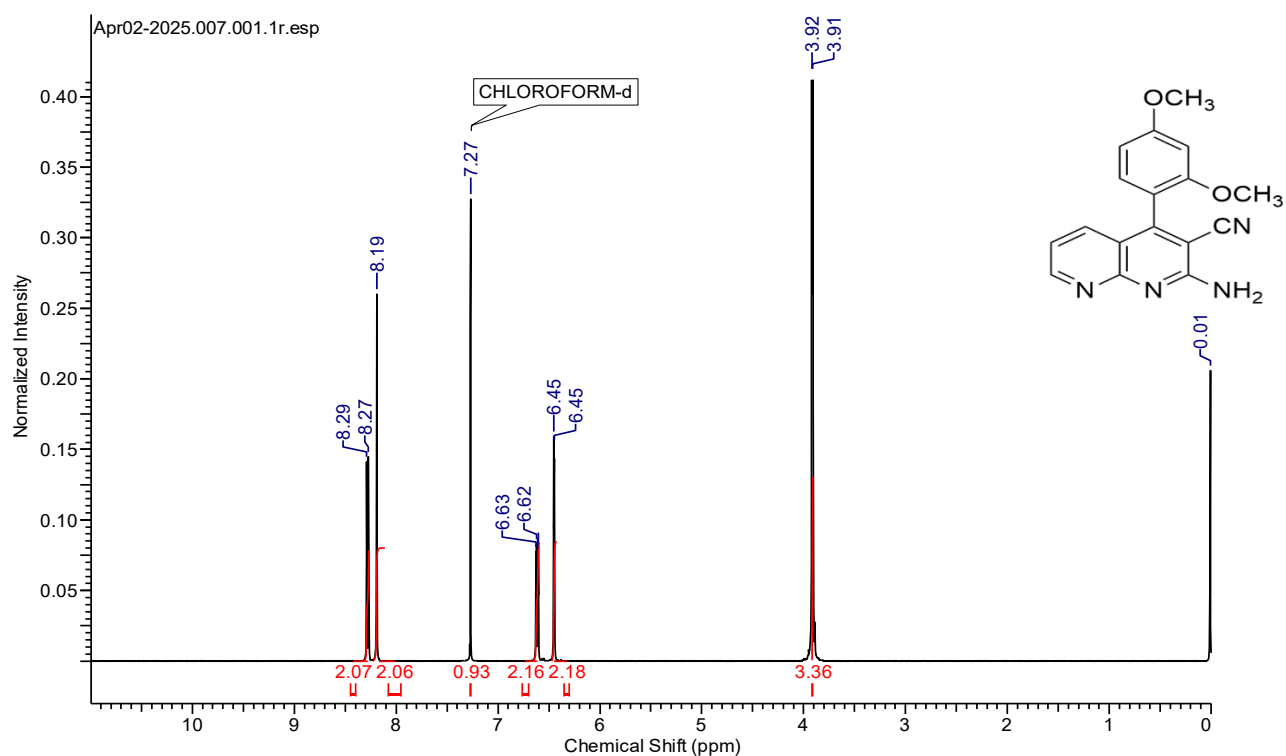


Figure S34: ^1H -NMR (500 MHz, CDCl_3) Spectrum of 2-amino-4-(2,4-dimethoxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4h**)

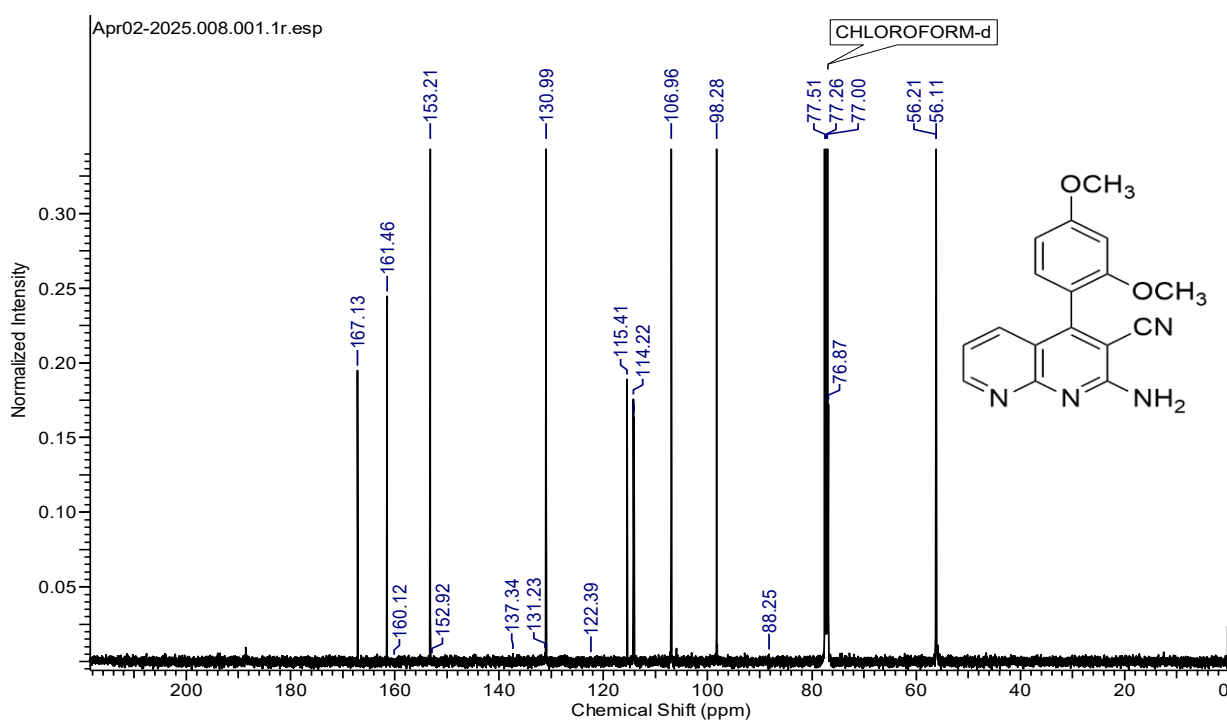


Figure S35: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 2-amino-4-(2,4-dimethoxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4h**)

Analysis Info

Analysis Name D:\Data\2025\APRIL\SPPU COLLEGE\HRM COLLEGE\HUNDARE PAYAL\D23_RE3_01_9260.d

Method dlc_50-1200mz_pos_mode_7min_0.2ml.m

Sample Name D7

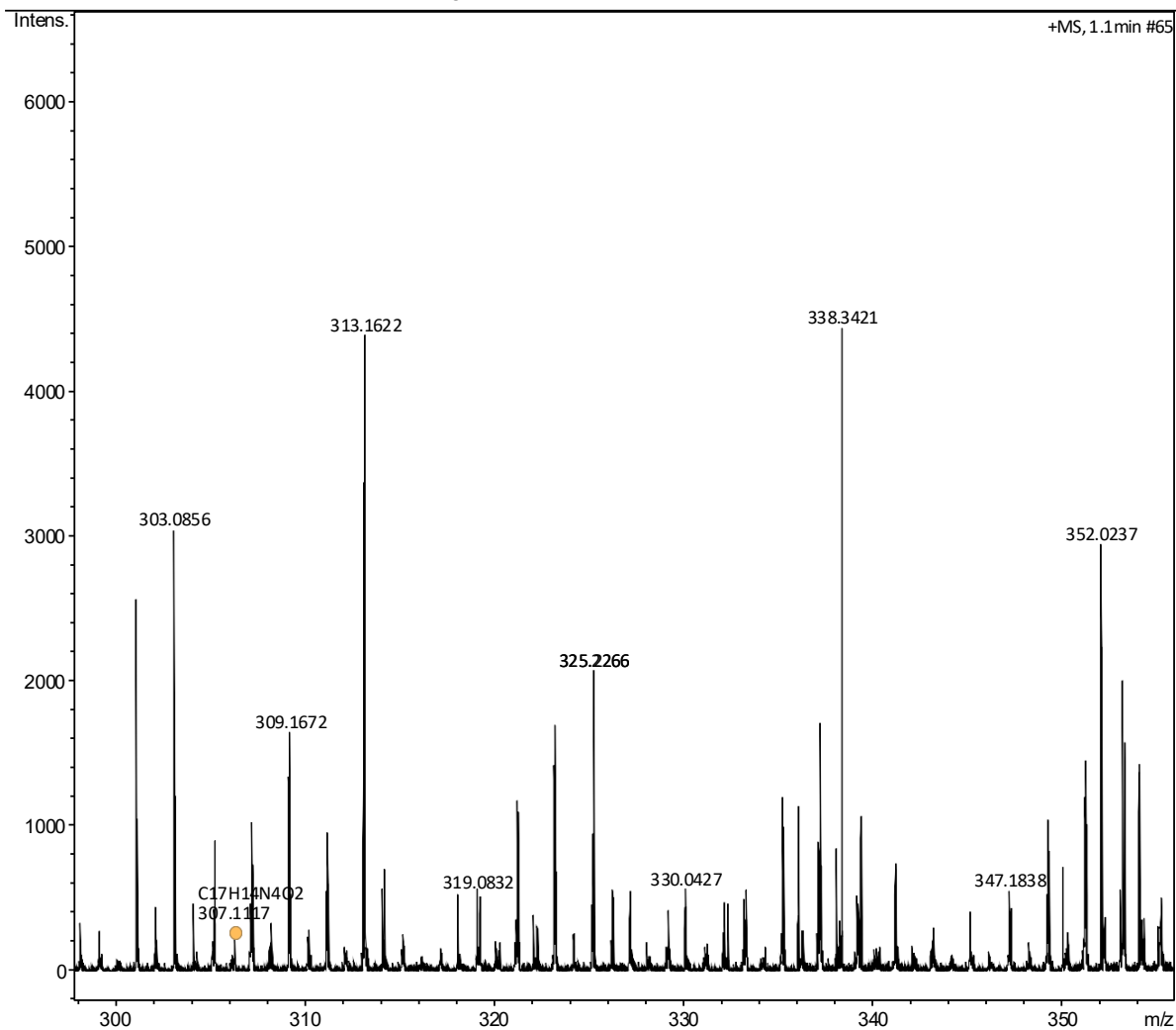
Acquisition Date 4/3/2025 7:05:52 PM

Analyst: Nitin S. Kadam CIF

Instrument impactHD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.7 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
ScanBegin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



D23_RE3_01_9260.d

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Figure S36: HR-ESI-MS Spectrum of 2-amino-4-(2,4-dimethoxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4h**)

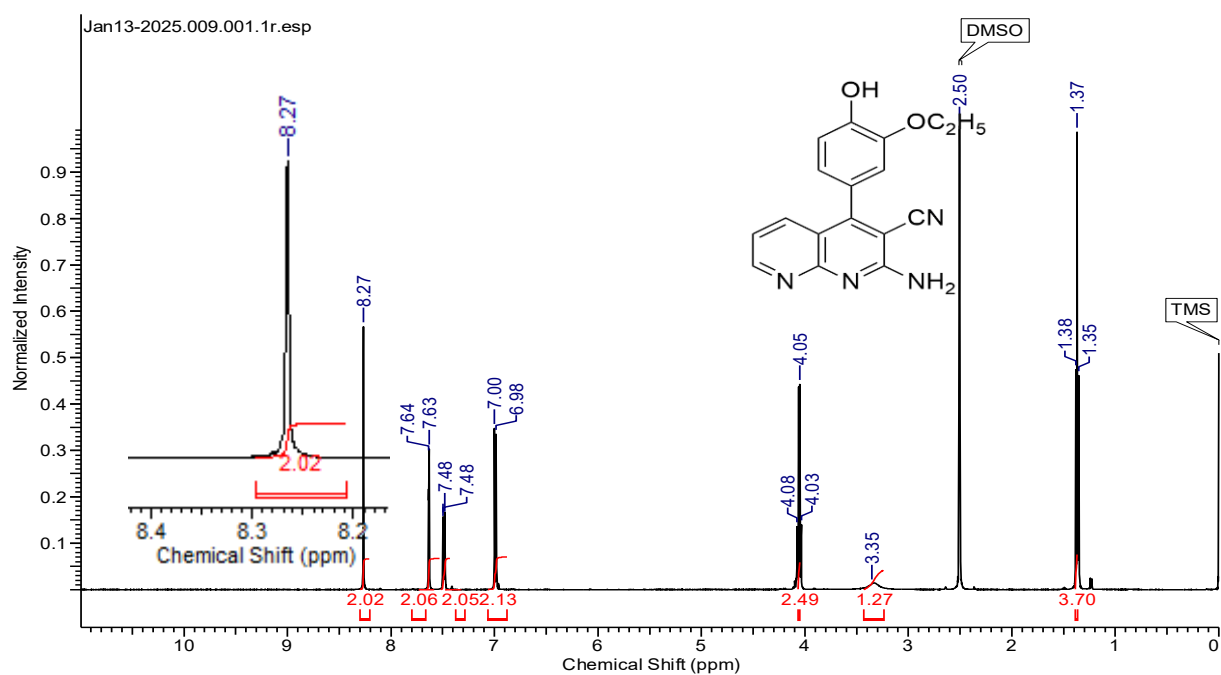


Figure S37: ^1H -NMR (500 MHz, CDCl_3) Spectrum of 2-amino-4-(3-ethoxy-4-hydroxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4i**)

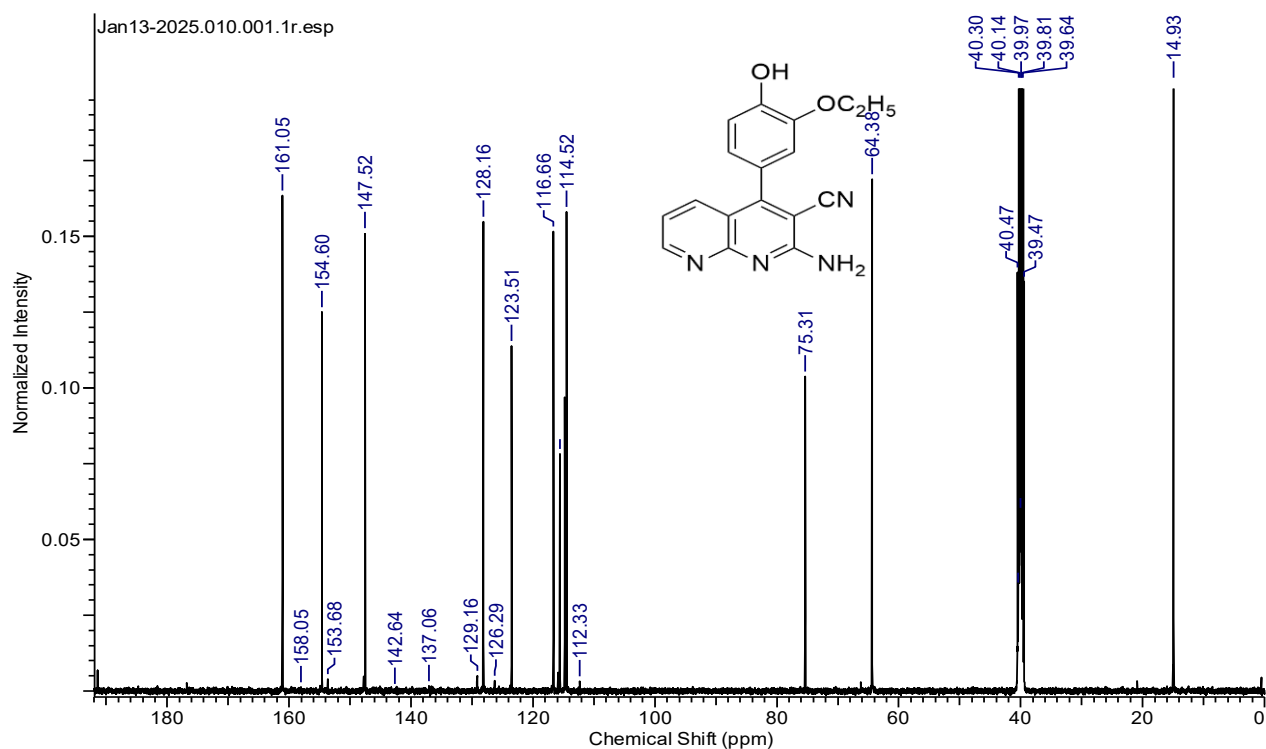


Figure S38: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 2-amino-4-(3-ethoxy-4-hydroxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4i**)

Analysis Info

Analysis Name D:\Data\2024\JAN\SPPU COLLEGE\H. R. M. Rajgurunagar\RUPALI VADAK\D8_RA8_01_6779.d
Method dlc_ms20-1200mz_10min_0.120ml flow_90b_dec23.m
Sample Name D8

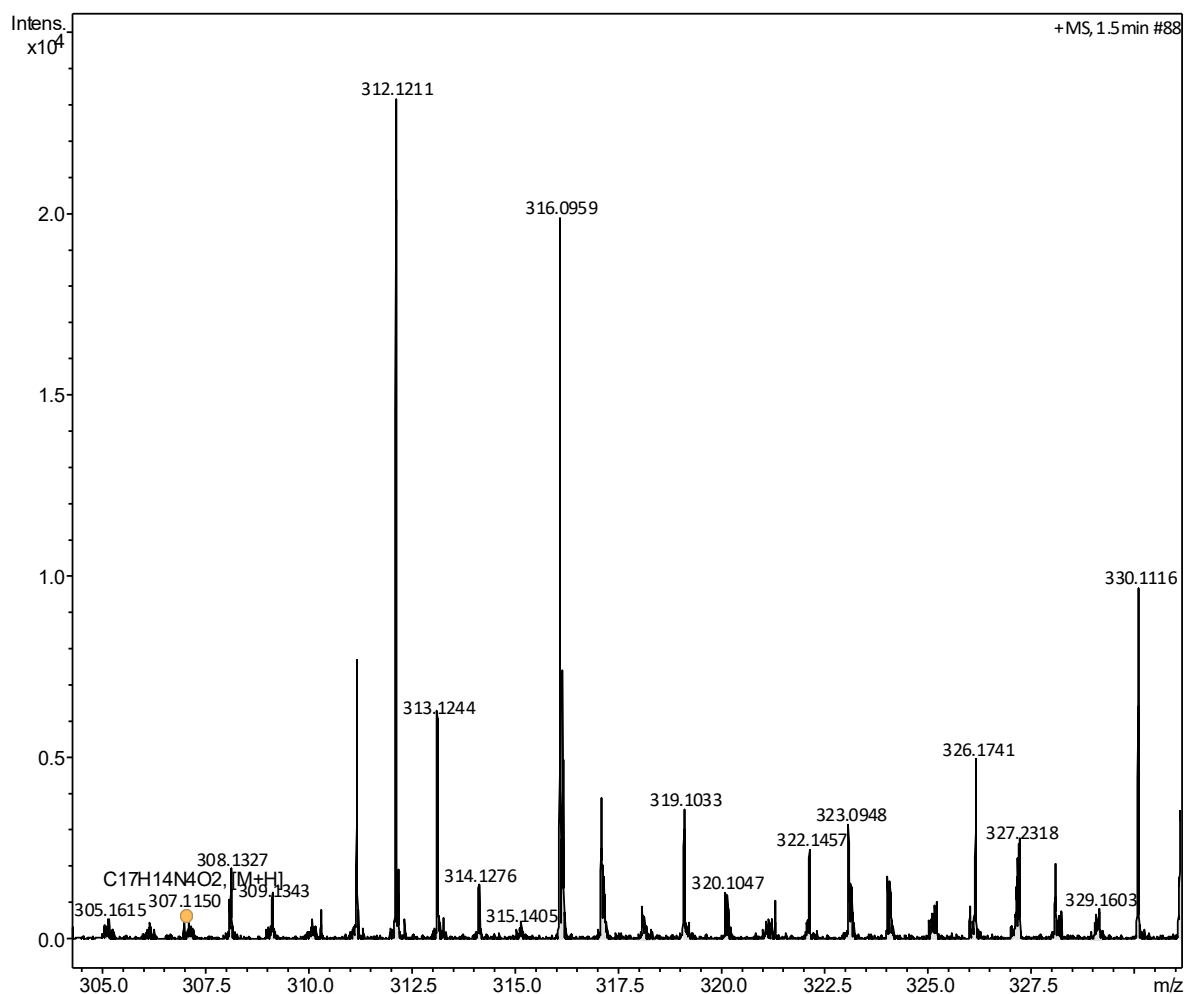
Acquisition Date 1/12/2024 4:55:45 PM

Operator Nitin S. Kadam CIF

Instrument impactHD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
ScanBegin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



D8_RA8_01_6779.d

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Figure S39: HR-ESI-MS Spectrum of 2-amino-4-(3-ethoxy-4-hydroxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4i**)

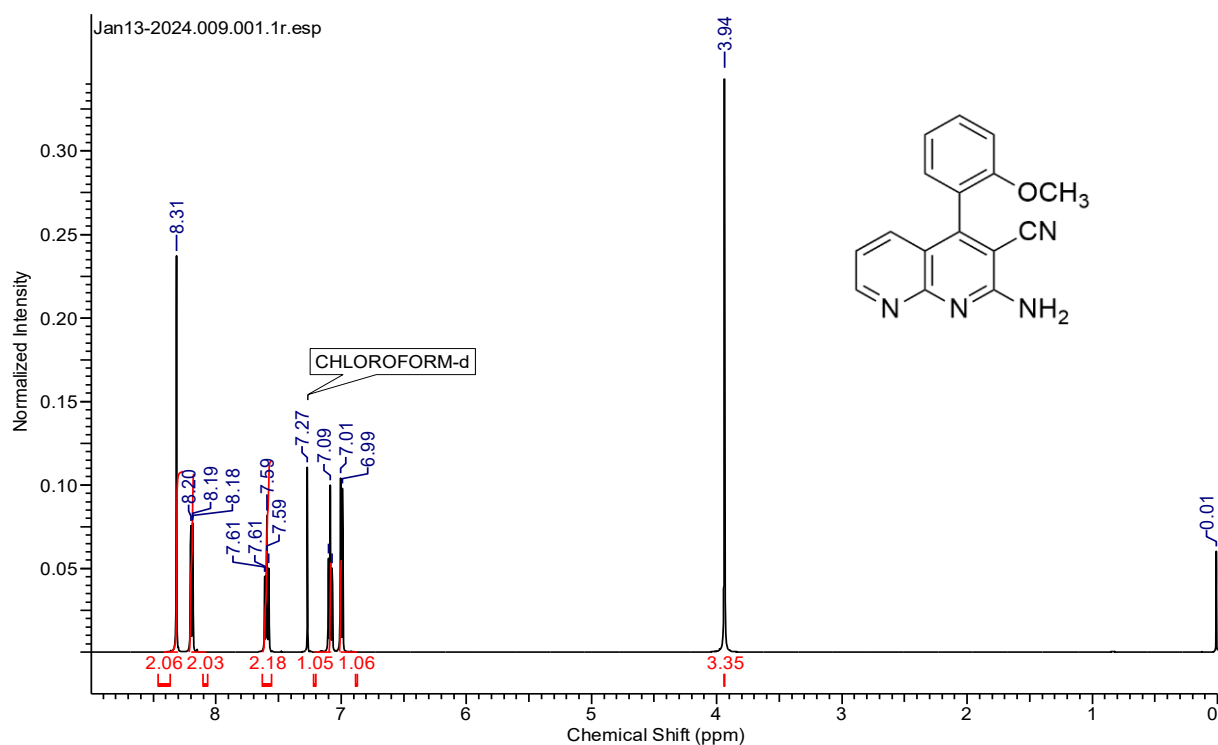


Figure S40: ^1H -NMR (500 MHz, CDCl_3) Spectrum of 2-Amino-4-(2-methoxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4j**)

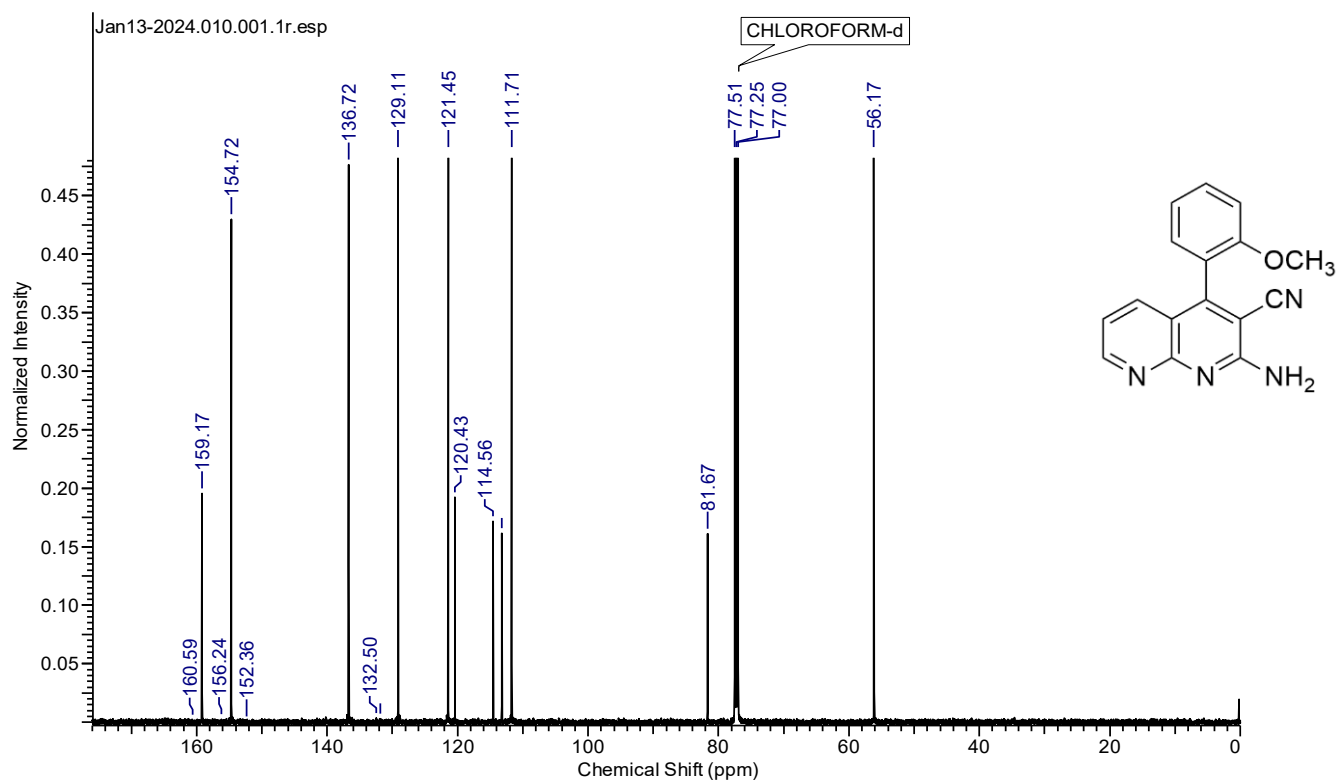


Figure S41: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 2-Amino-4-(2-methoxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4j**)

Analysis Info

Analysis Name D:\Data\2024\JAN\SPPU COLLEGE\H. R. M. Rajgurunagar\RUPALI VADAK\D10_RB1_01_6780.d
Method dlc_ms20-1200mz_10min_0.120ml flow_90b_dec 23.m
Sample Name D10

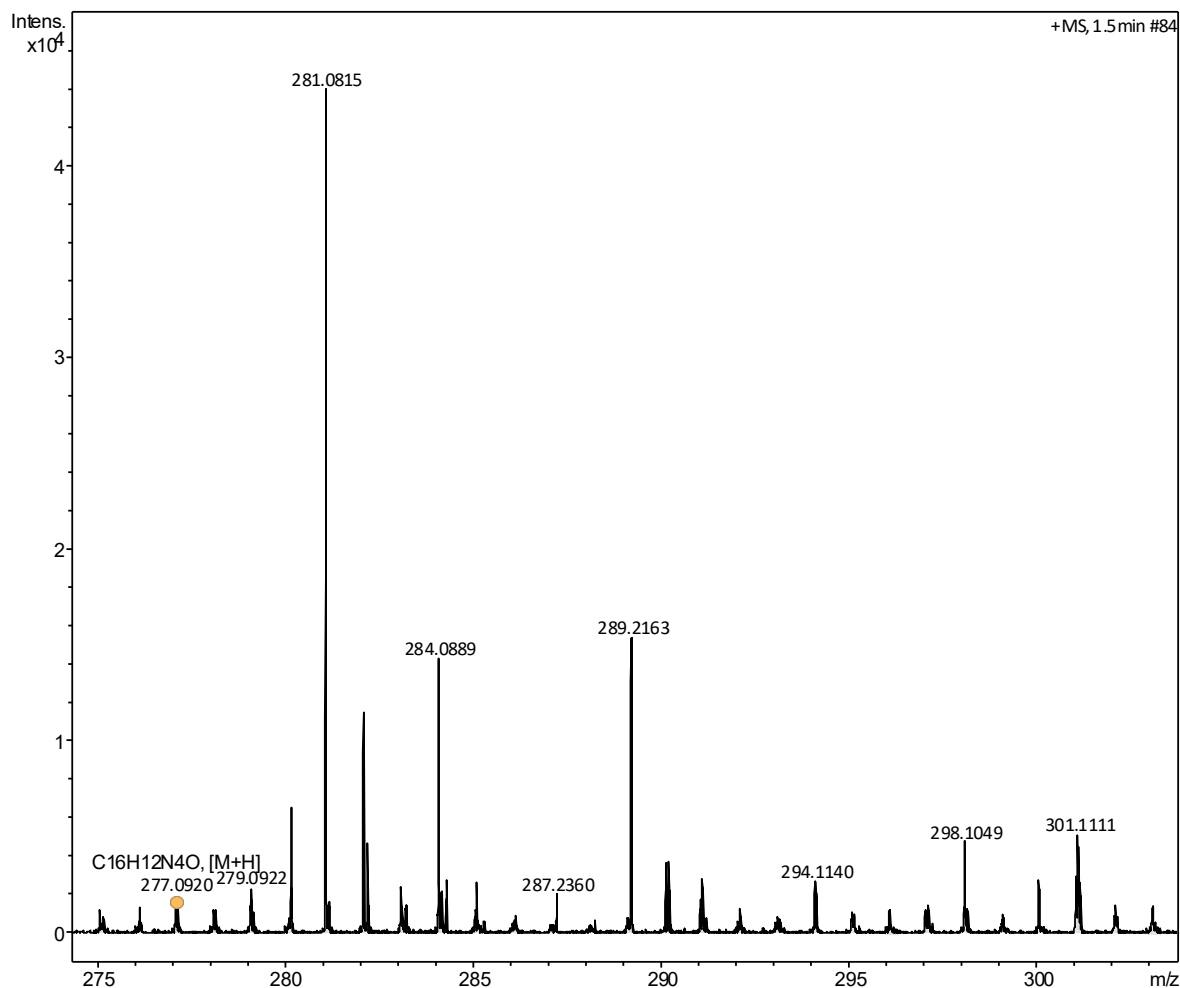
Acquisition Date 1/12/2024 5:06:26 PM

Operator Nitin S. Kadam CIF

Instrument impactHD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
ScanBegin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



D10_RB1_01_6780.d

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Figure S42: HR-ESI-MS Spectrum of 2-Amino-4-(2-methoxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4j**)

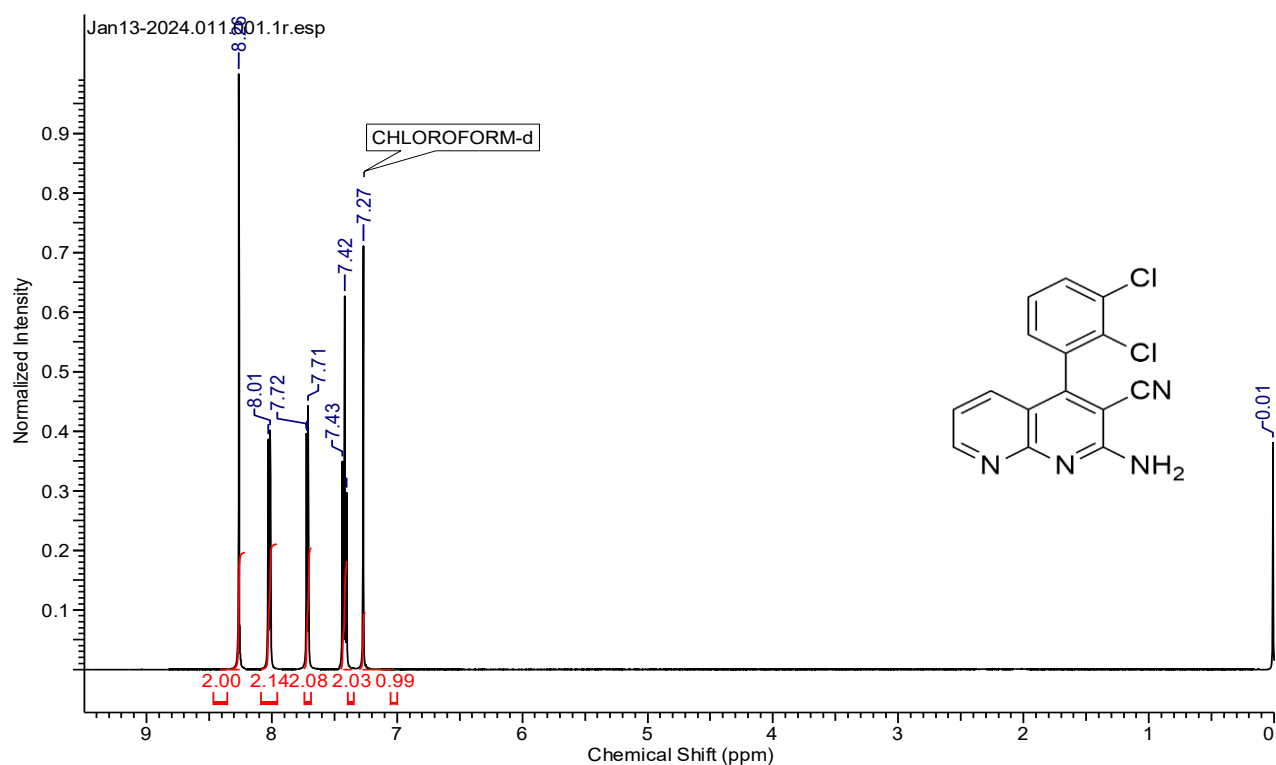


Figure S43: ^1H -NMR (500 MHz, CDCl_3) Spectrum of 2-Amino-4-(2,3-dichlorophenyl)-1,8-naphthyridine-3-carbonitrile (**4k**)

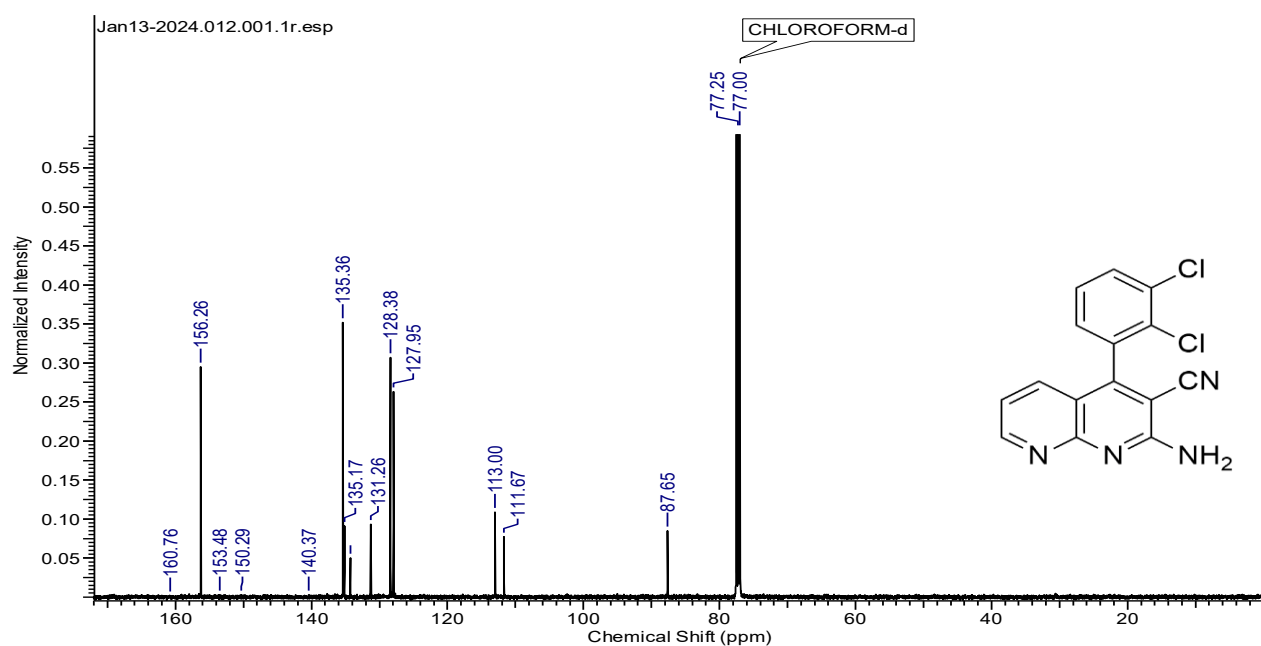
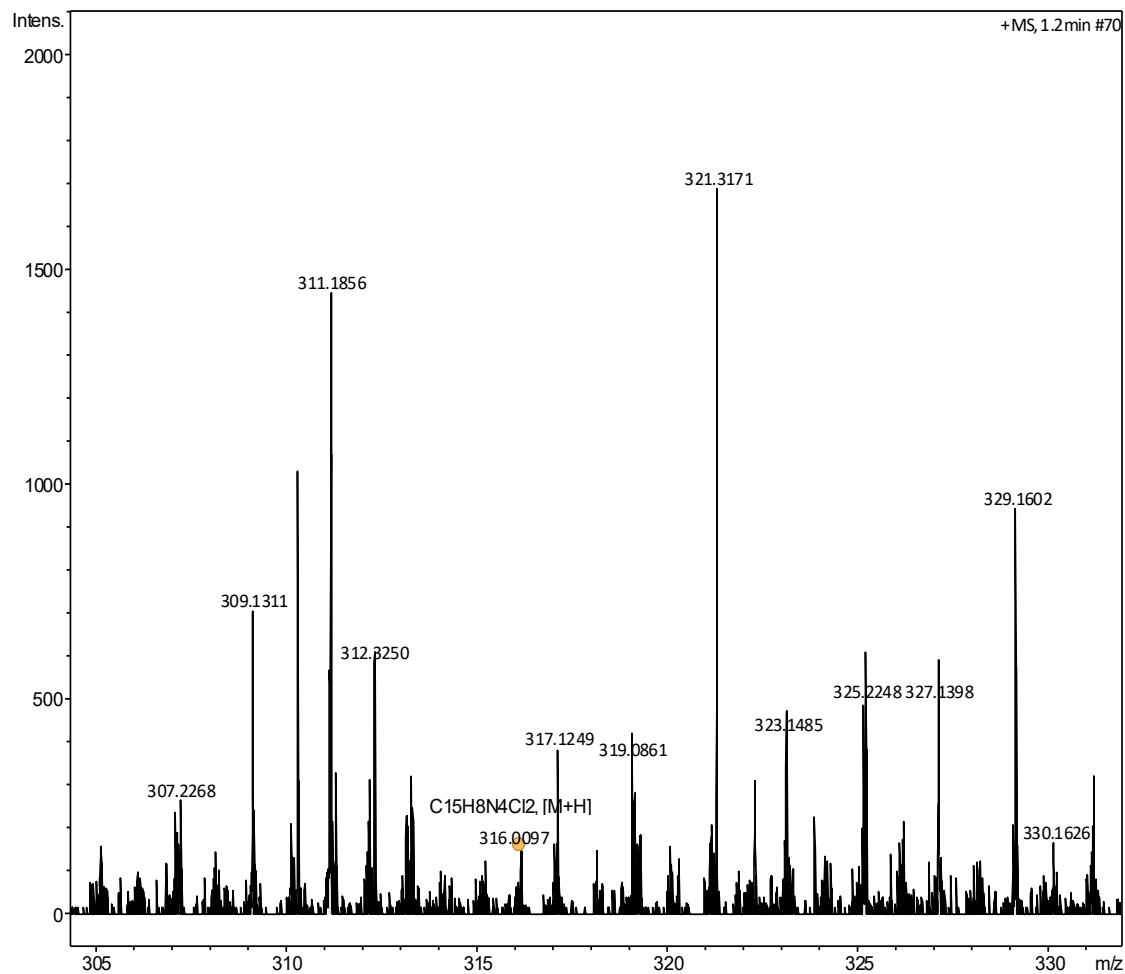


Figure S44: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 2-Amino-4-(2,3-dichlorophenyl)-1,8-naphthyridine-3-carbonitrile (**4k**)

Analysis Info	Acquisition Date	1/12/2024 5:17:09 PM
Analysis Name	D:\Data\2024\JAN\SPPU COLLEGE\H. R. M. Rajgurunagar\RUPALI VADAK\11_RB2_01_6781.d	
Method	dlc_ms20-1200mz_10min_0.120ml flow_90b_dec23.m	Operator Nitin S. Kadam CIF
Sample Name	D11	Instrument impactHD 1819696.00184

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
ScanBegin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



D11_RB2_01_6781.d

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Figure S45: HR-ESI-MS Spectrum of 2-Amino-4-(2,3-dichlorophenyl)-1,8-naphthyridine-3-carbonitrile (**4k**)

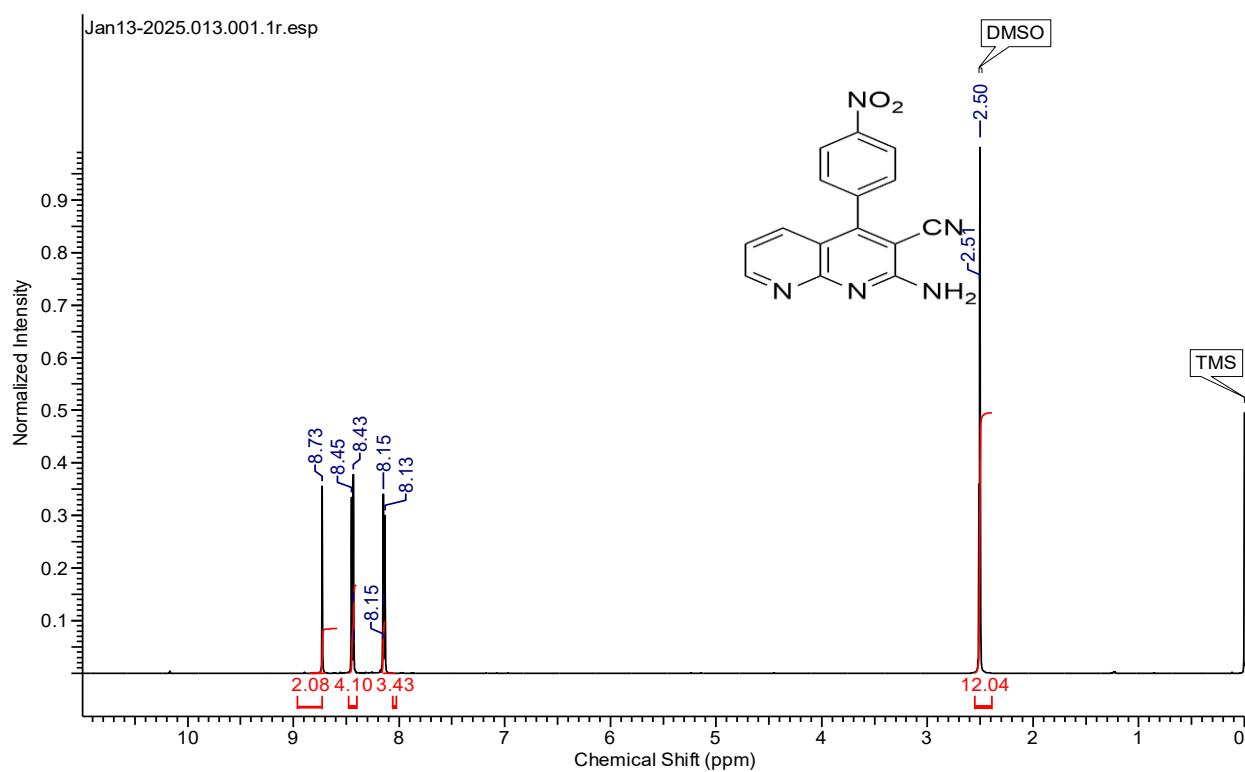


Figure S46: ^1H -NMR (500 MHz, CDCl_3) Spectrum of 2-Amino-4-(4-nitrophenyl)-1,8-naphthyridine-3-carbonitrile (**4I**)

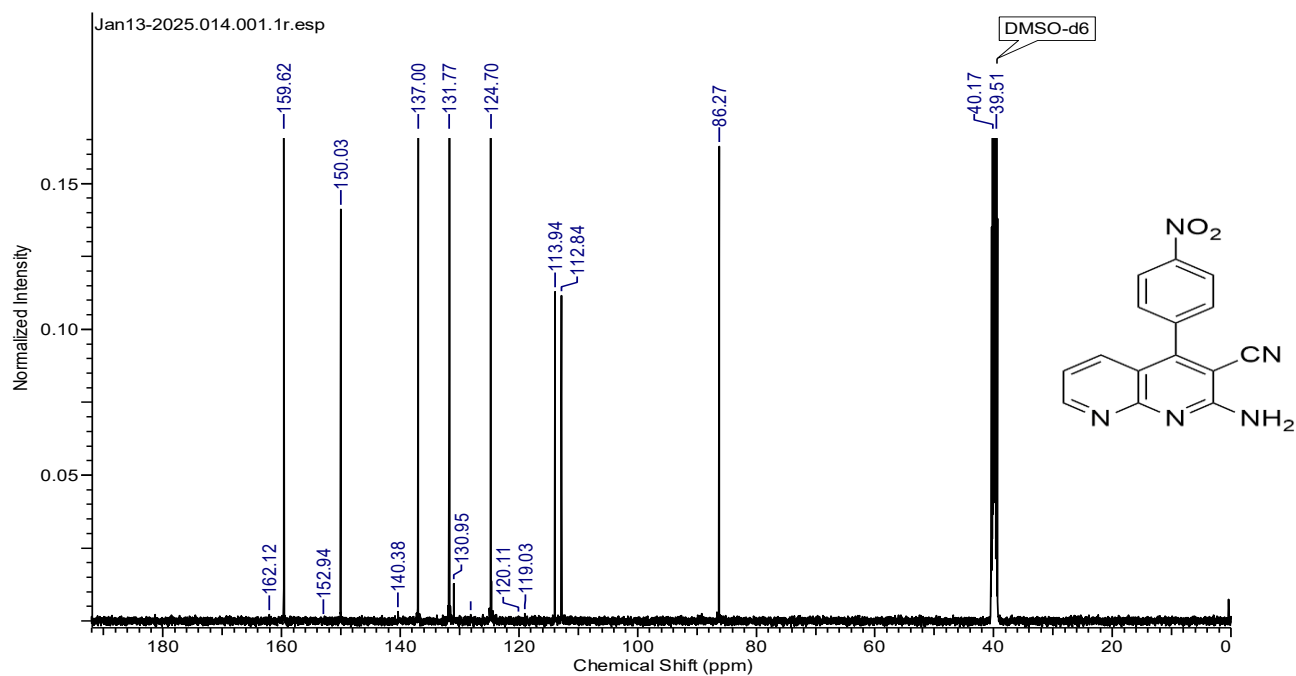


Figure S47: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 2-Amino-4-(4-nitrophenyl)-1,8-naphthyridine-3-carbonitrile (**4I**)

Analysis Info

Analysis Name D:\Data\2024\JAN\SPPU COLLEGE\H. R. M. Rajgurunagar\RUPALI VADAK\12_BA2_01_6755.d
 Method dlc_ms20-1200mz_10min_0.120ml flow_90b_dec 23.m
 Sample Name D12

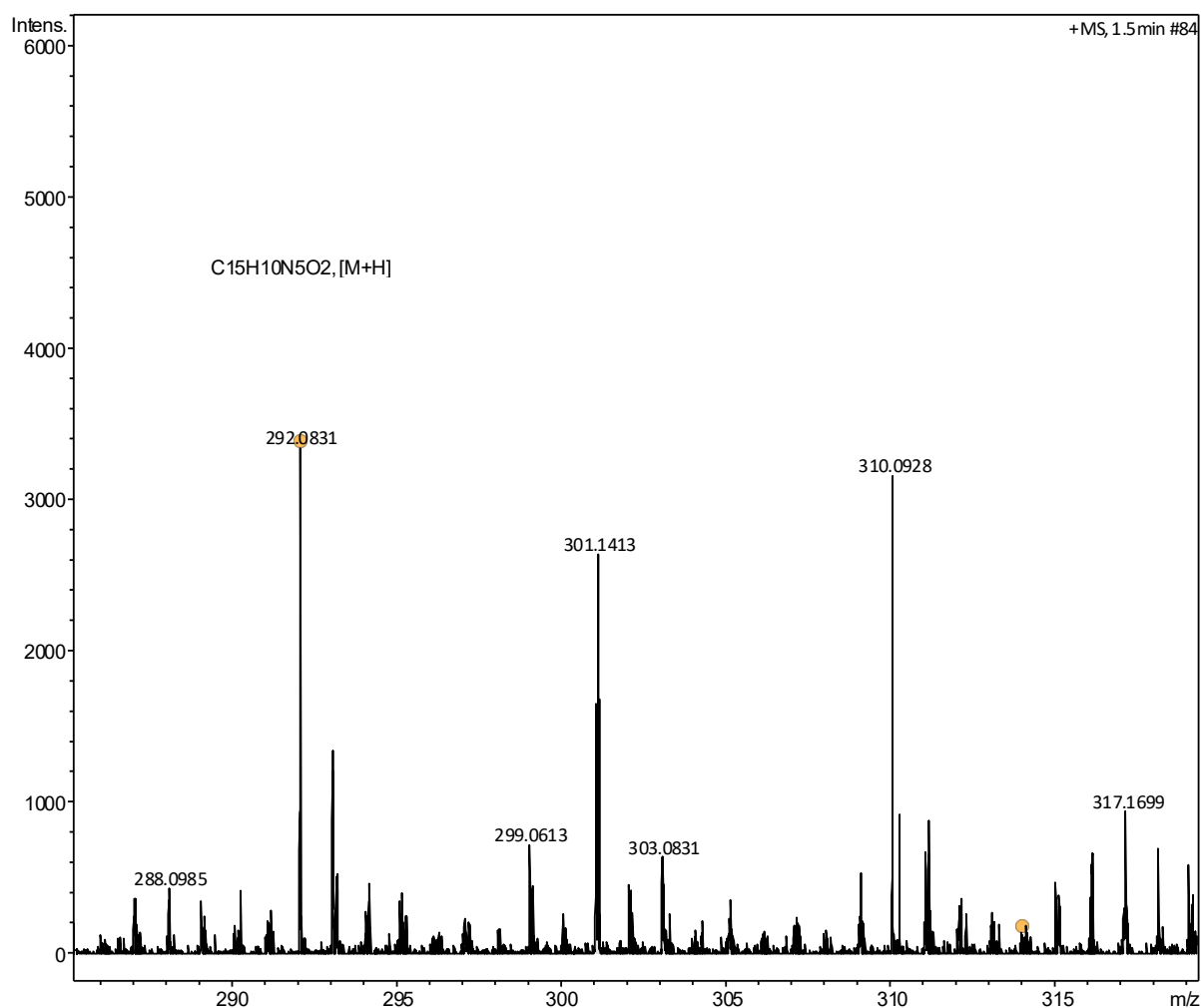
Acquisition Date 1/10/2024 10:22:57 PM

Operator Nitin S. Kadam CIF

Instrument impact HD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule	Adduct
292.083064	1	C ₁₅ H ₁₀ N ₅ O ₂	100.00	292.082901	-0.2	-0.6	130.3	13.5	even		ok	M+H
314.043788	1	C ₁₅ H ₉ N ₅ NaO ₂	100.00	314.064845	21.1	67.0	634.5	13.5	even		ok	M+Na

D12_BA2_01_6755.d

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Figure S48: HR-ESI-MS Spectrum of 2-Amino-4-(4-nitrophenyl)-1,8-naphthyridine-3-carbonitrile (4I)

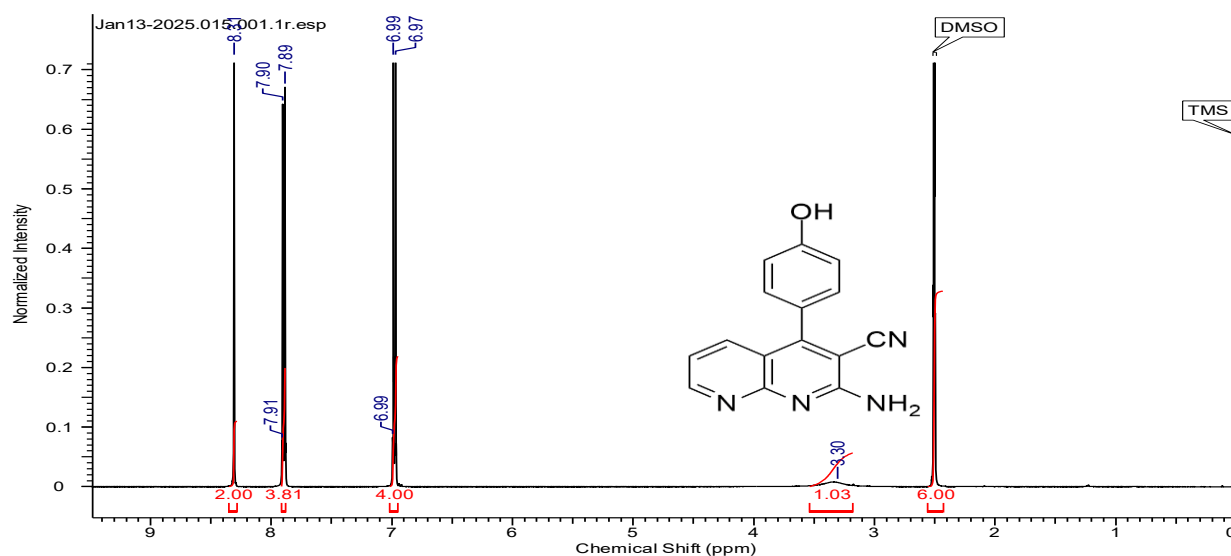


Figure S49: ^1H -NMR (500 MHz, CDCl_3) Spectrum of 2-Amino-4-(4-hydroxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4m**)

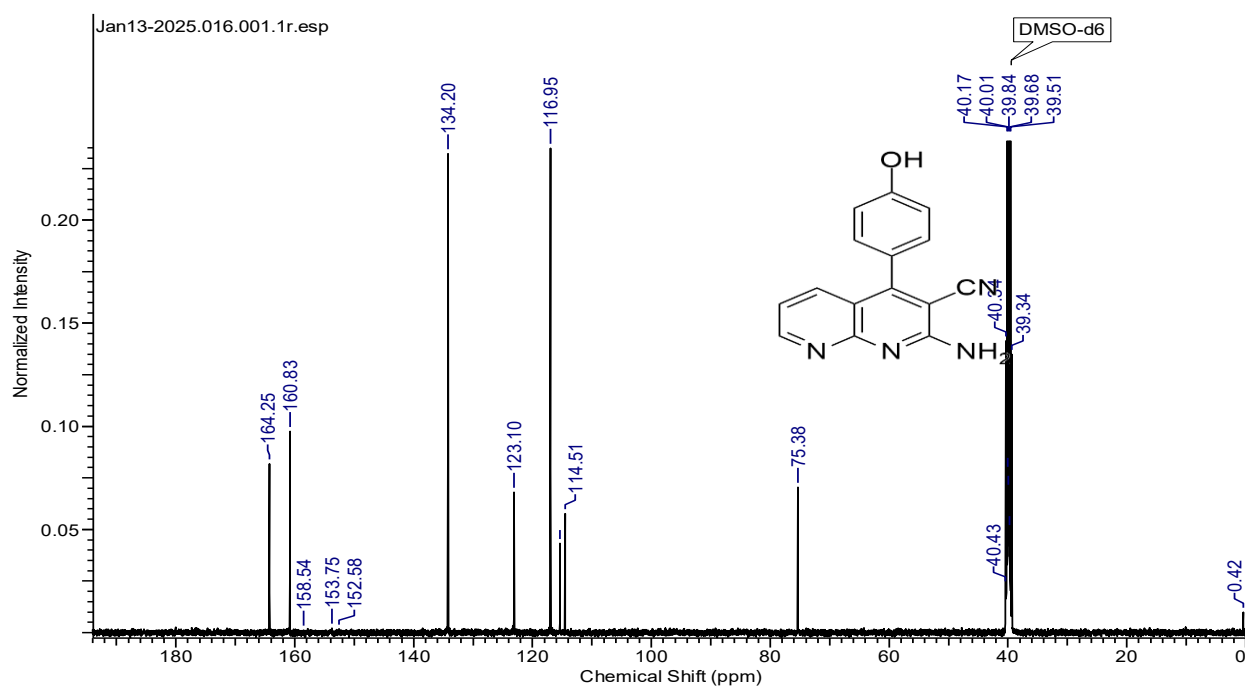


Figure S50: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 2-Amino-4-(4-hydroxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4m**)

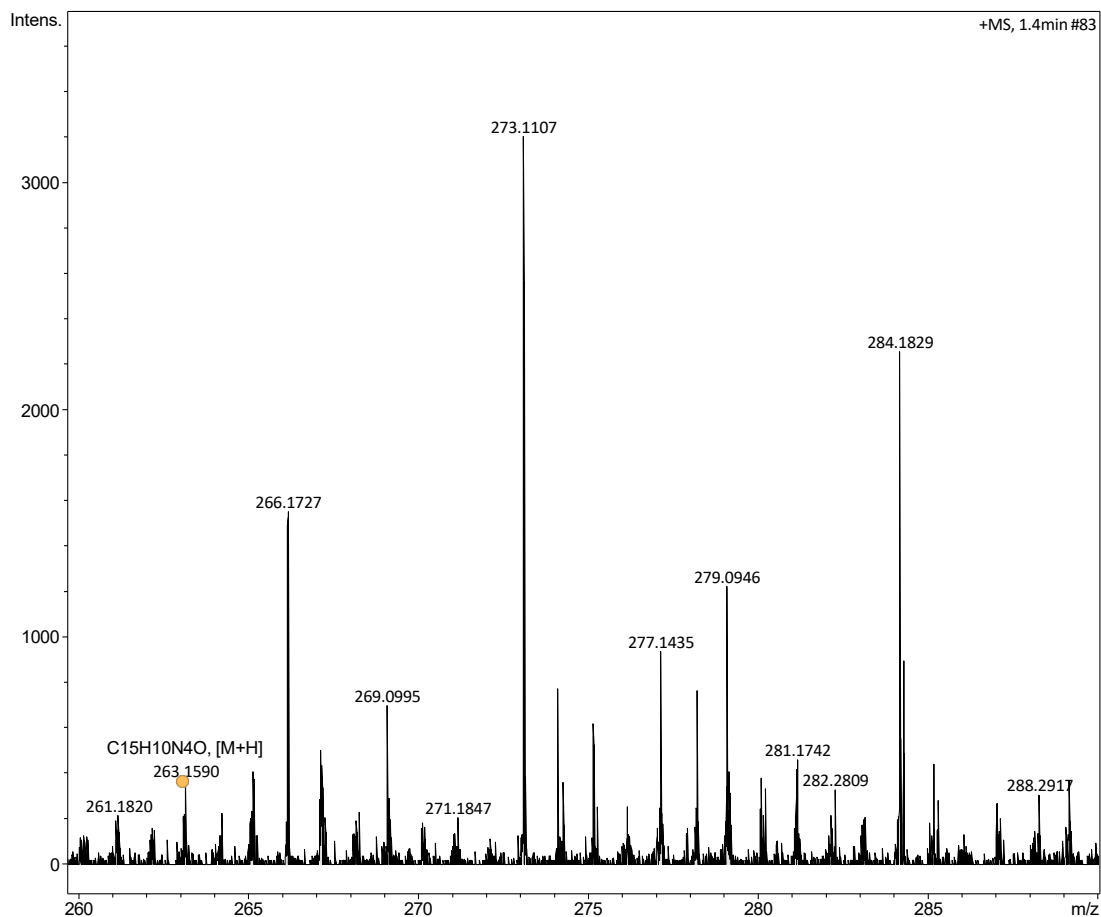
Savitribai Phule Pune University - Central Instrumentation Facility

Analysis Info

Analysis Name	D:\Data\2024\JAN\SPPU COLLEGE\H. R. M. Rajgurunagar\RUPALI VADAK\ID13_BA3_01_6756.d	Acquisition Date	1/10/2024 10:33:38 PM
Method	dlc_ms20-1200mz_10min_0.120ml flow_90b_dec 23.m	Operator	Nitin S. Kadam CIF
Sample Name	D13	Instrument	impact HD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



D13_BA3_01_6756.d

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Figure S51: HR-ESI-MS Spectrum of 2-Amino-4-(4-hydroxyphenyl)-1,8-naphthyridine-3-carbonitrile (4m)

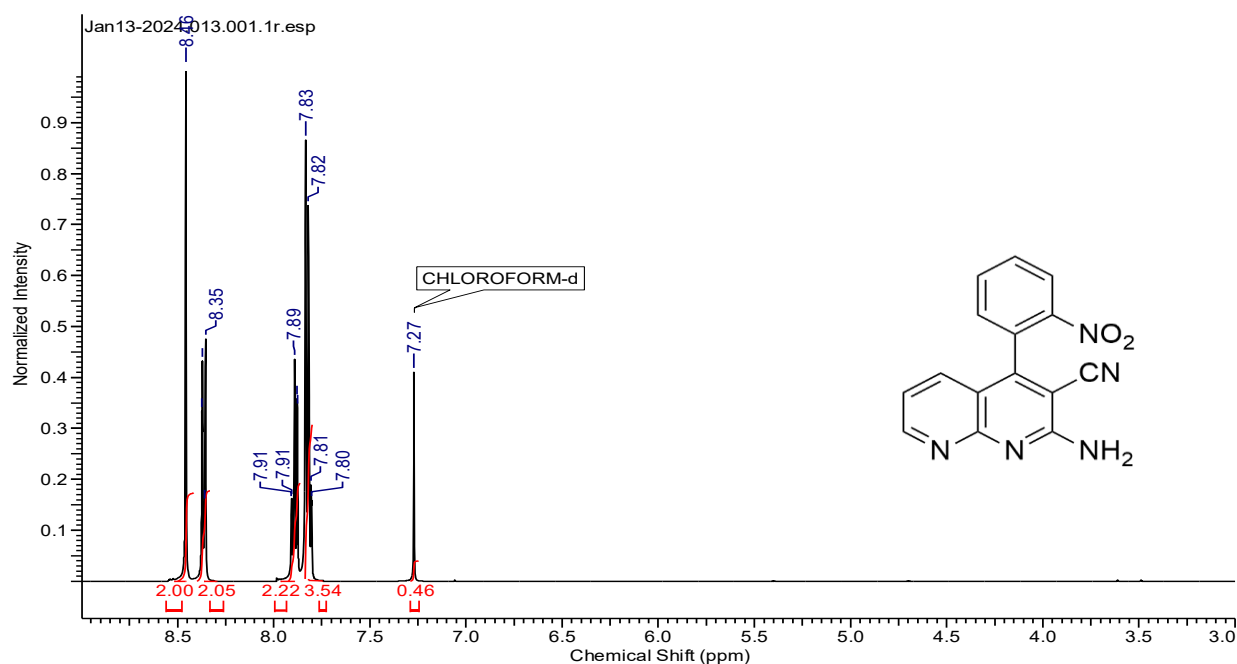


Figure S52: ^1H -NMR (500 MHz, CDCl_3) Spectrum of 2-amino-4-(2-nitrophenyl)-1,8-naphthyridine-3-carbonitrile (**4n**)

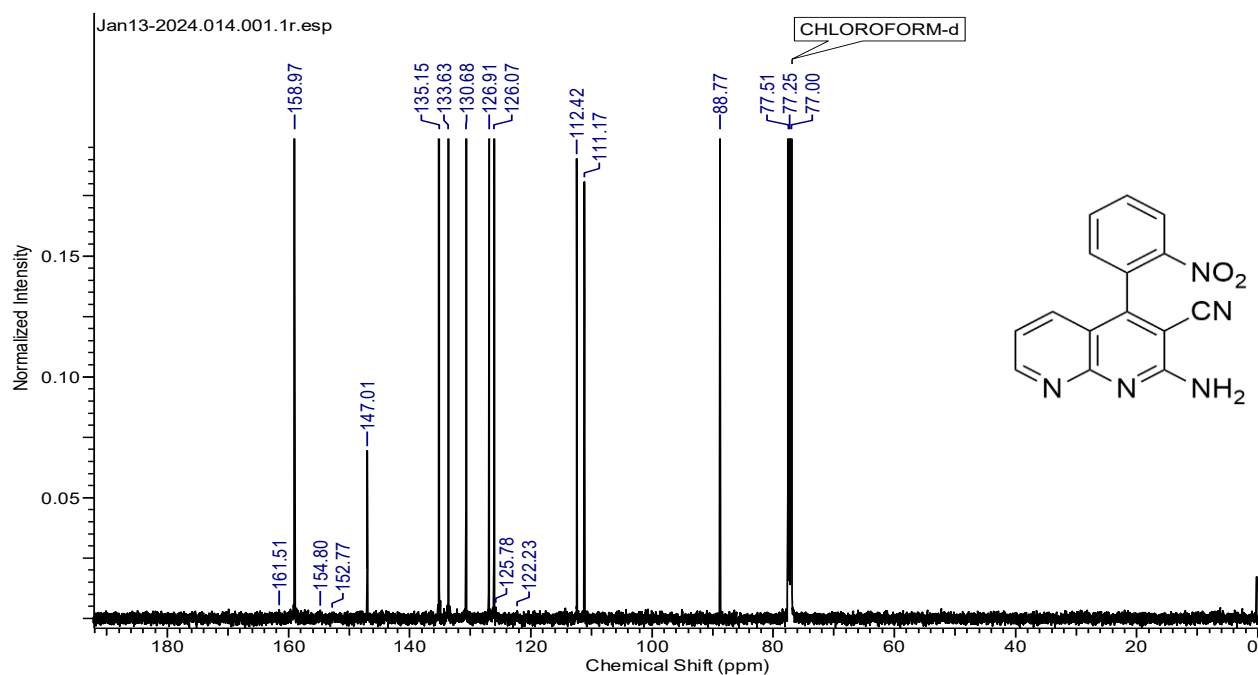
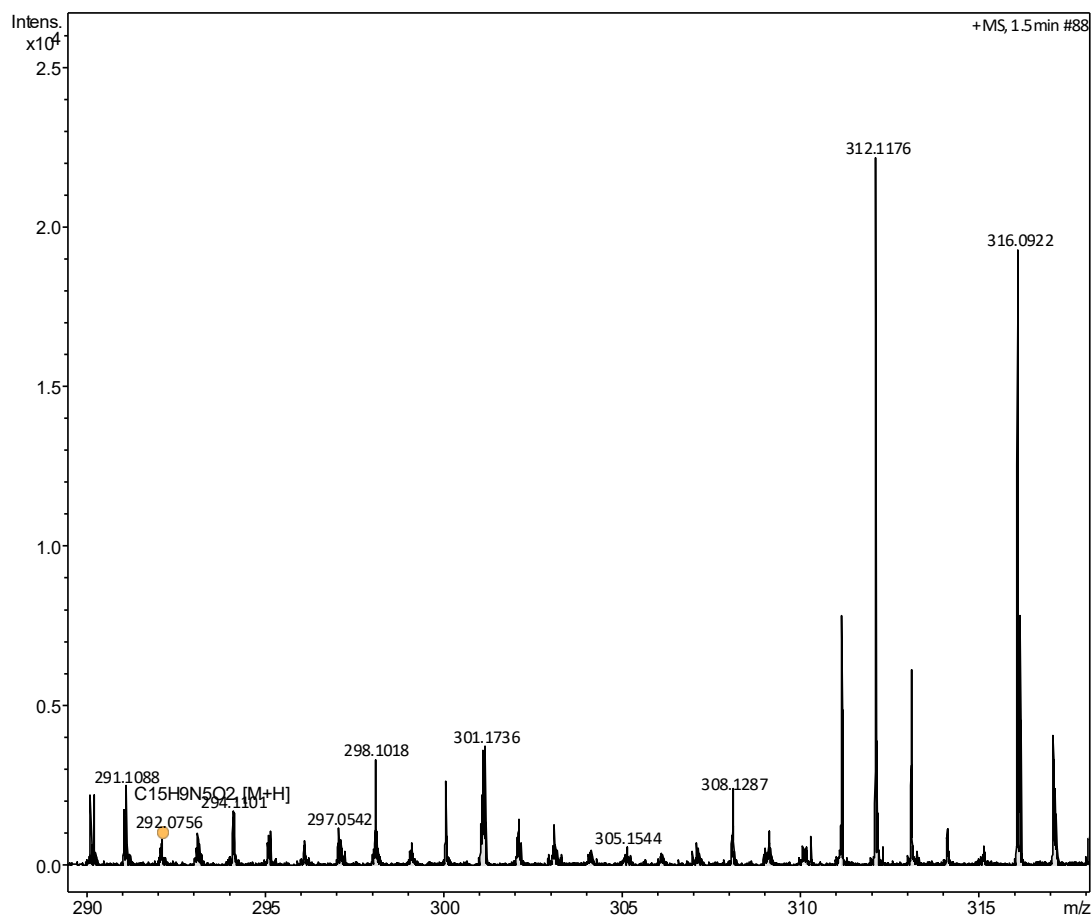


Figure S53: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 2-amino-4-(2-nitrophenyl)-1,8-naphthyridine-3-carbonitrile (**4n**)

Analysis Info		Acquisition Date	1/12/2024 5:27:50 PM	
Analysis Name	D:\Data\2024\JAN\SPPU COLLEGE\H. R. M. Rajgurunagar\RUPALI VADAK\14_RB3_01_6782.d			
Method	dlc_ms20-1200mz_10min_0.120ml flow_90b_dec23.m		Operator	Nitin S. Kadam CIF
Sample Name	D14	Instrument	impactHD	1819696.00184

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
ScanBegin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



D14_RB3_01_6782.d

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Figure S54: HR-ESI-MS Spectrum of 2-amino-4-(2-nitrophenyl)-1,8-naphthyridine-3-carbonitrile (4n)

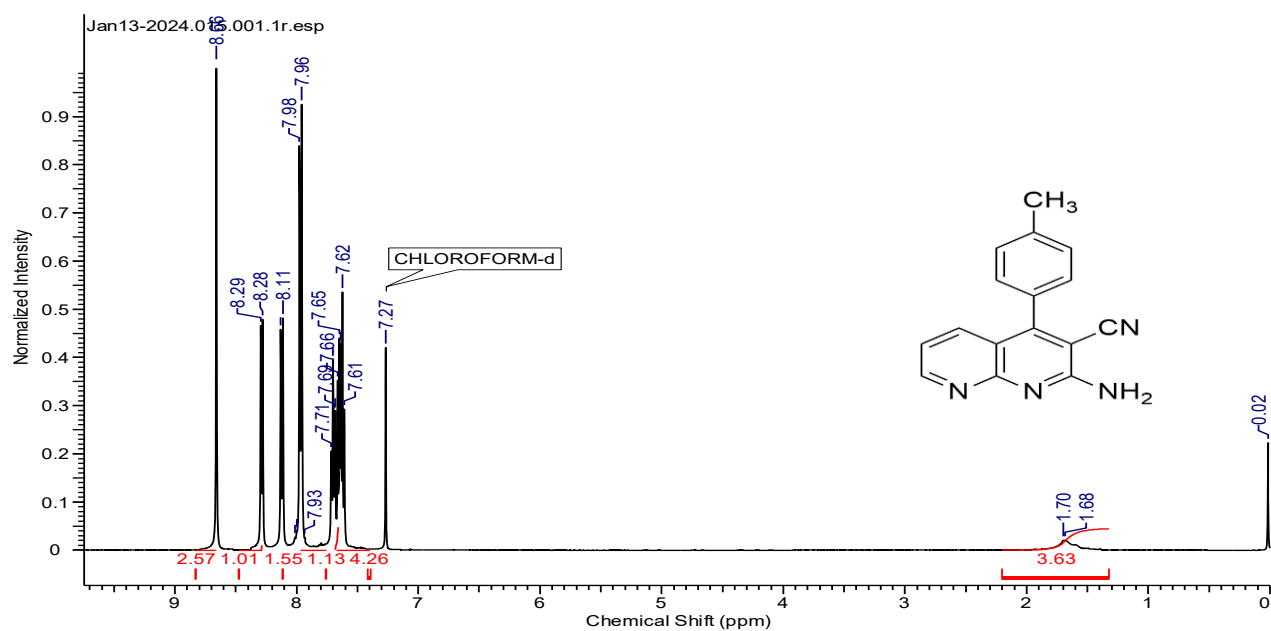


Figure S55: ¹H-NMR (500 MHz, CDCl₃) Spectrum of 2-amino-4-(4-methylphenyl)-1,8-naphthyridine-3-carbonitrile (40)

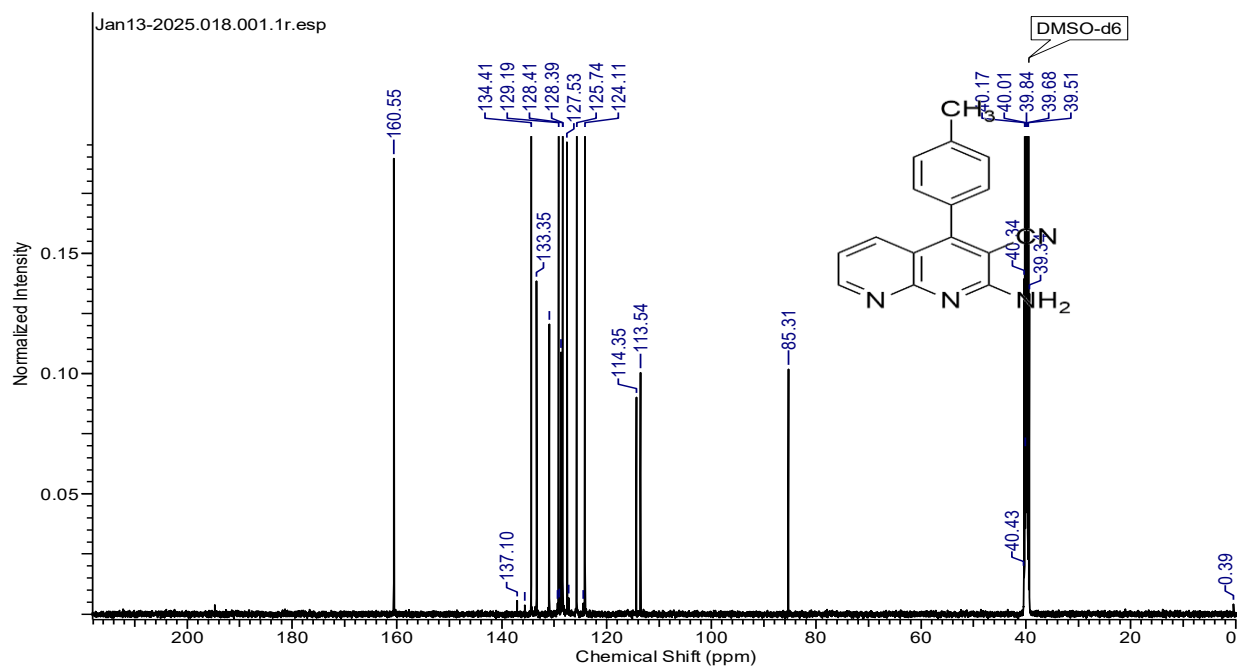
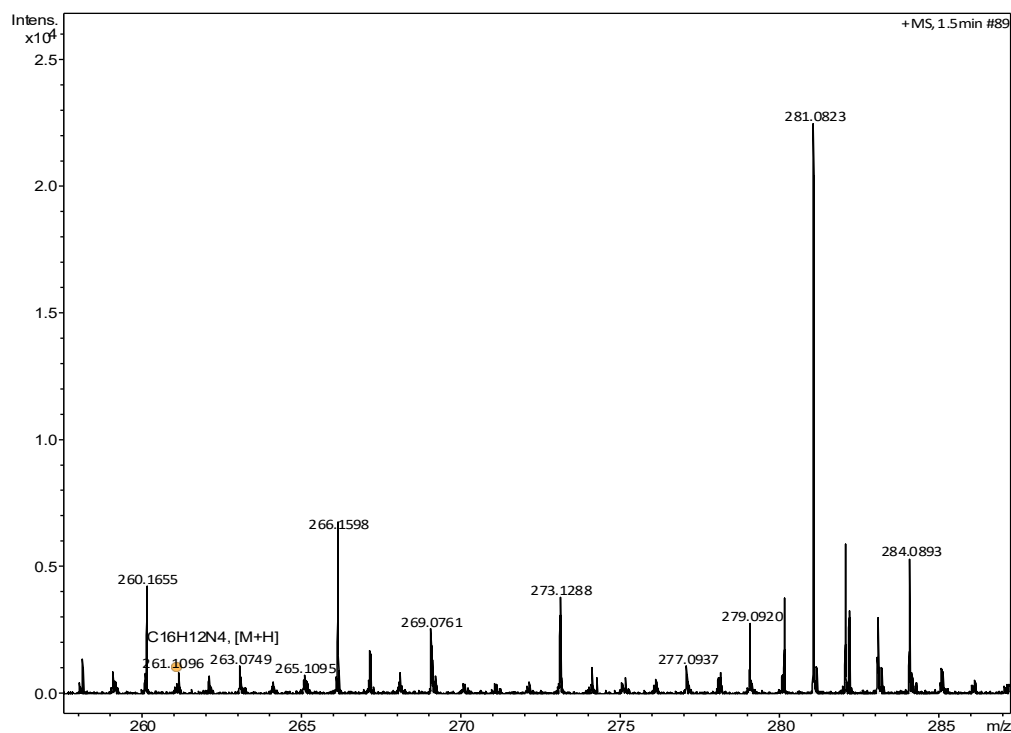


Figure S56: ¹³C-NMR (125 MHz, CDCl₃) Spectrum of 2-amino-4-(4-methylphenyl)-1,8-naphthyridine-3-carbonitrile (40)

Analysis Info		Acquisition Date	1/12/2024 5:38:30 PM
Analysis Name	D:\Data\2024\JAN\SPPU COLLEGE\H. R. M. Rajgurunagar\RUPALI VADAK\15_RB4_01_6783.d	Operator	Nitin S. Kadam CIF
Method	dlc_ms20-1200mz_10min_0.120ml flow_90b_dec 23.m	Instrument	impactHD
Sample Name	D15		1819696.00184

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
ScanBegin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



D15_RB4_01_6783.d

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Figure S57: HR-ESI-MS Spectrum of 2-amino-4-(4-methylphenyl)-1,8-naphthyridine-3-carbonitrile (4o)

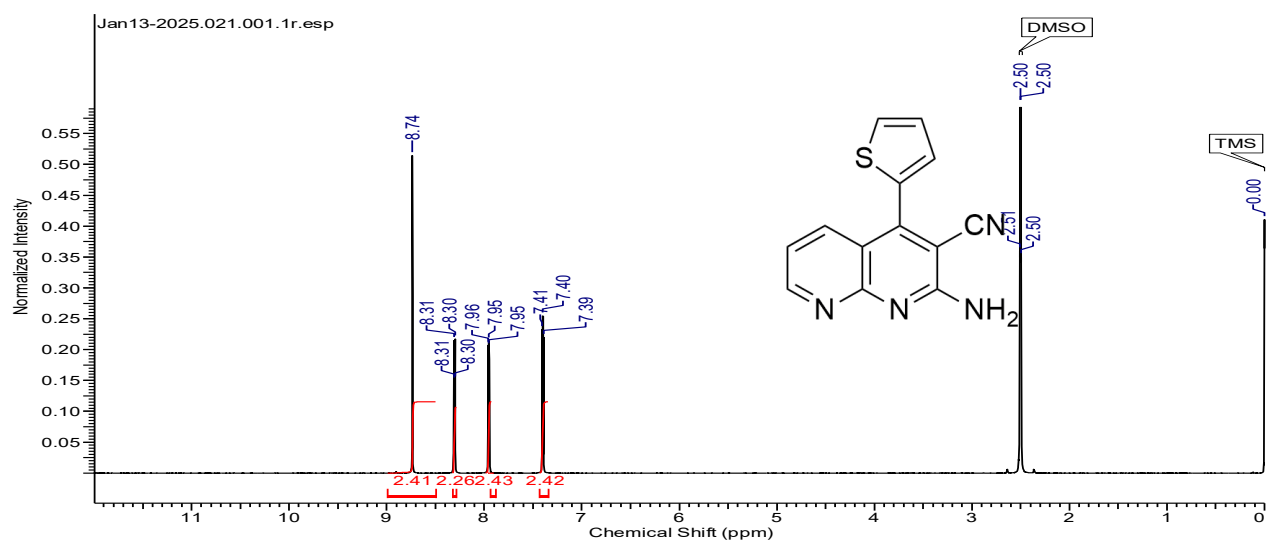


Figure S58: ^1H -NMR (500 MHz, CDCl_3) Spectrum of 2-Amino-4-(2-thiophenophenyl)-1,8-naphthyridine-3-carbonitrile (**4p**)

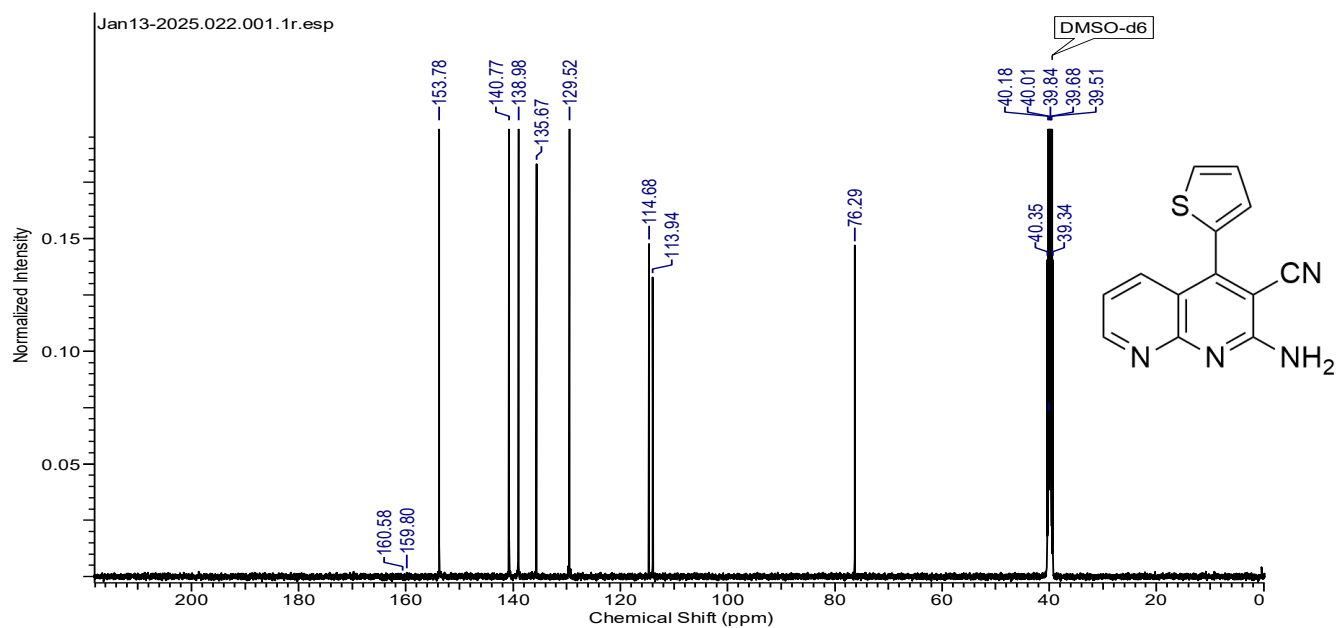
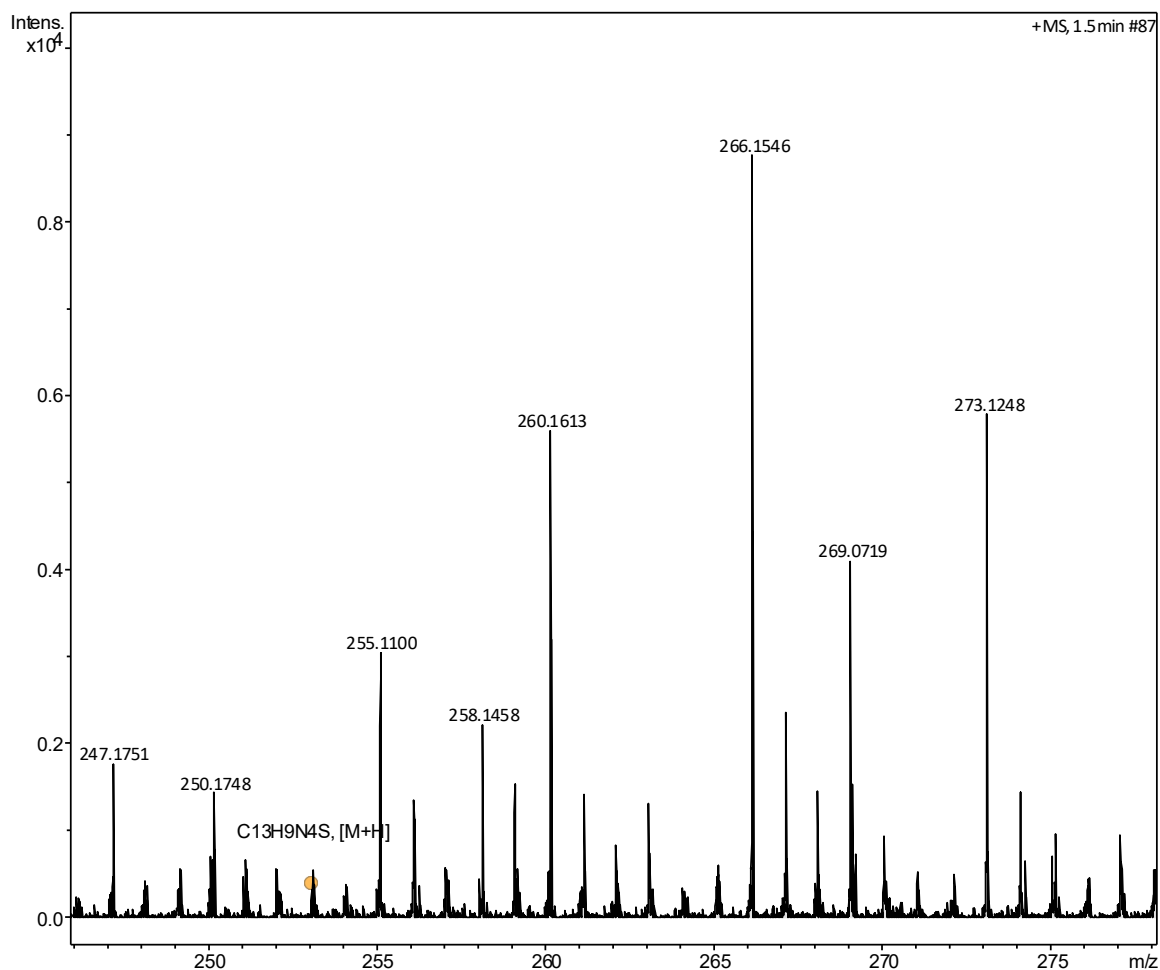


Figure S59: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 2-Amino-4-(2-thiophenophenyl)-1,8-naphthyridine-3-carbonitrile (**4p**)

Analysis Info	Acquisition Date	1/12/2024 5:59:51 PM
Analysis Name	D:\Data\2024\JAN\SPPU COLLEGE\H. R. M. Rajgurunagar\RUPALI VADAK\19_RB6_01_6785.d	
Method	dlc_ms20-1200mz_10min_0.120ml flow_90b_dec 23.m	Operator Nitin S. Kadam CIF
Sample Name	D19	Instrument impactHD 1819696.00184

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	20 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ⁻	Conf	N-Rule	Adduct
253.062978	1	C13H9N4S	100.00	253.054244	-8.7	-34.5	669.8	11.5	even		ok	M+H

D19_RB6_01_6785.d

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Figure S60: HR-ESI-MS Spectrum 2-Amino-4-(2-thiophenophenyl)-1,8-naphthyridine-3-carbonitrile (4p)

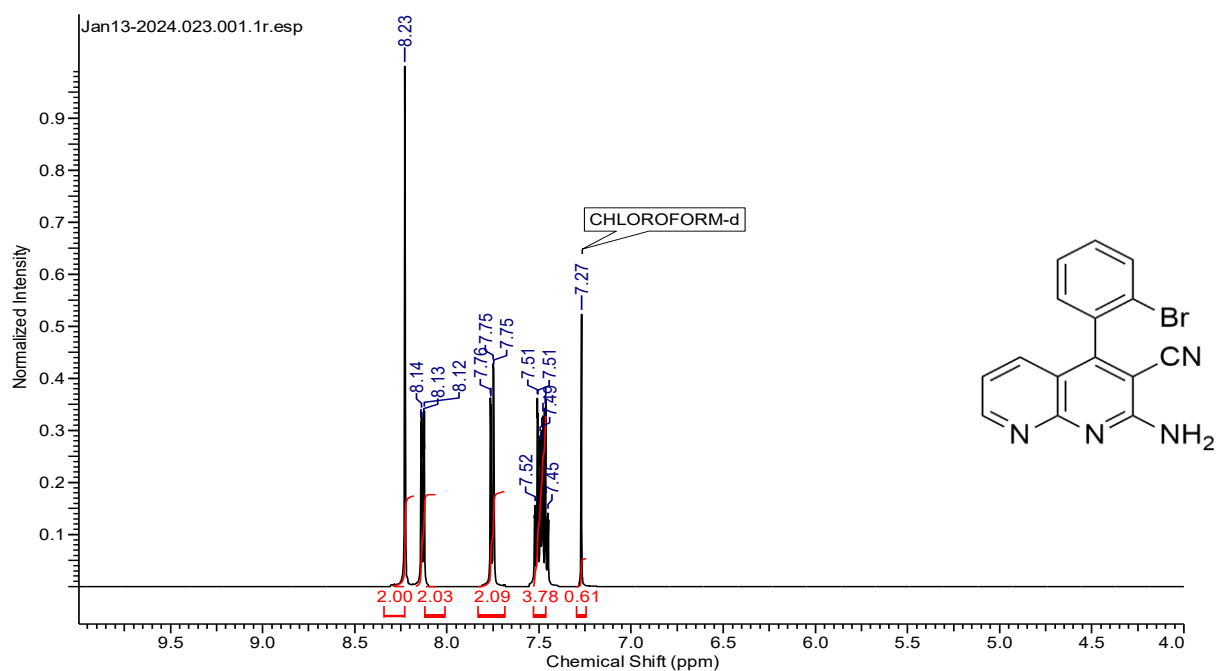


Figure S61: ^1H -NMR (500 MHz, CDCl_3) Spectrum of 2-Amino-4-(2-bromophenyl)-1,8-naphthyridine-3-carbonitrile (**4q**)

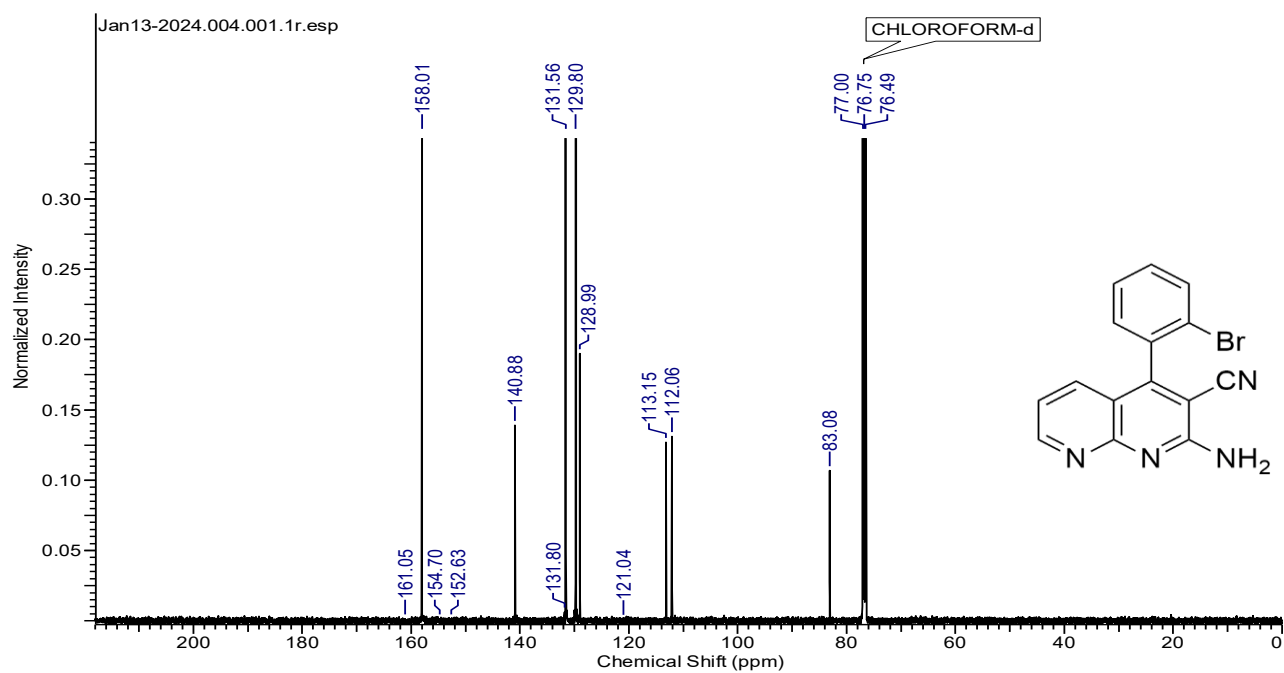
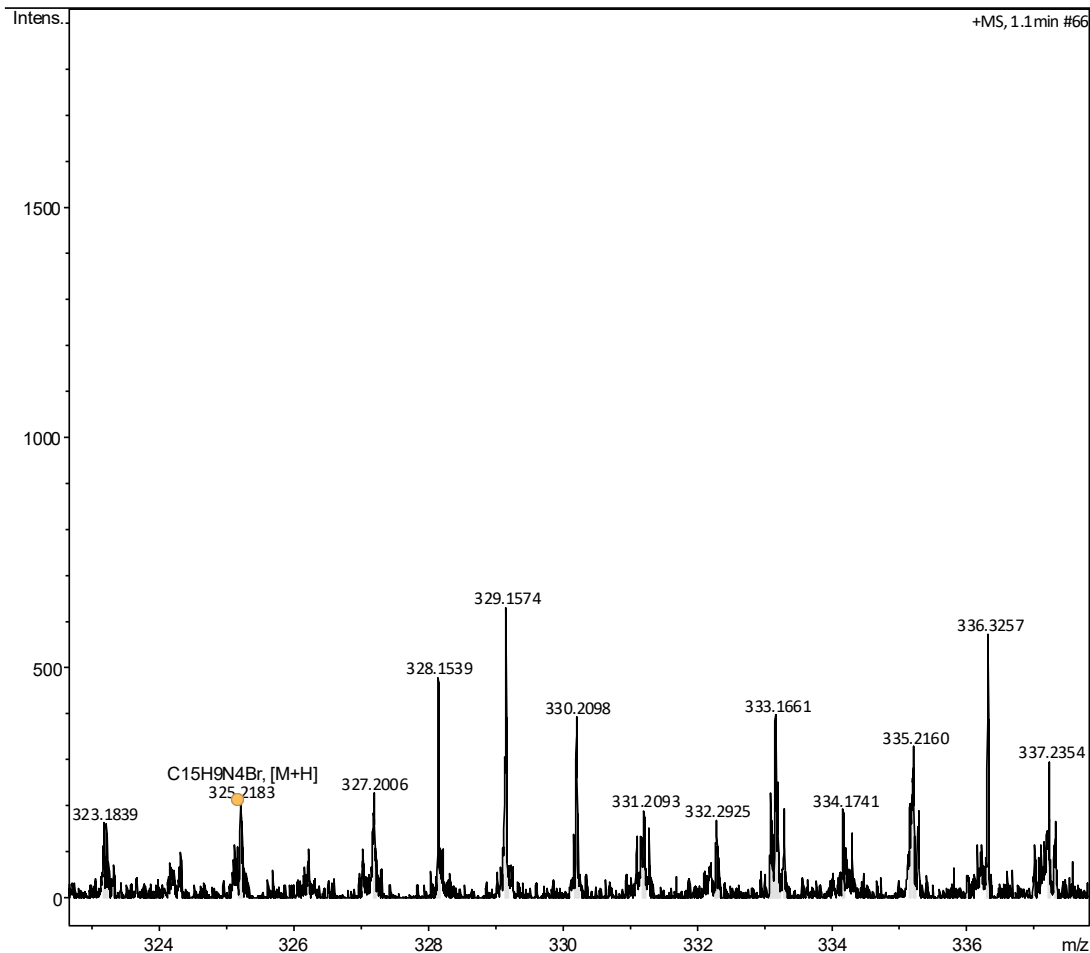


Figure S62: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 2-Amino-4-(2-bromophenyl)-1,8-naphthyridine-3-carbonitrile (**4q**)

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Analysis Info		Acquisition Date	1/24/2025 2:01:42 PM
Analysis Name	D:\Data\2025\JAN\SPPU COLLEGE\HRM COLLEGE\DR. PRAMOD KULKARNI\VADAK RUPALI\D22_RB7_01_8727.d		
Method	dlc_50-1200mz_pos_mode_7min_0.2ml.m	Analyst:	Nitin S. Kadam CIF
Sample Name	D22	Instrument	impactHD 1819696.00184

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.7 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
ScanBegin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



D22_RB7_01_8727.d

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Figure S63: HR-ESI-MS Spectrum of 2-Amino-4-(2-bromophenyl)-1,8-naphthyridine-3-carbonitrile (4q)

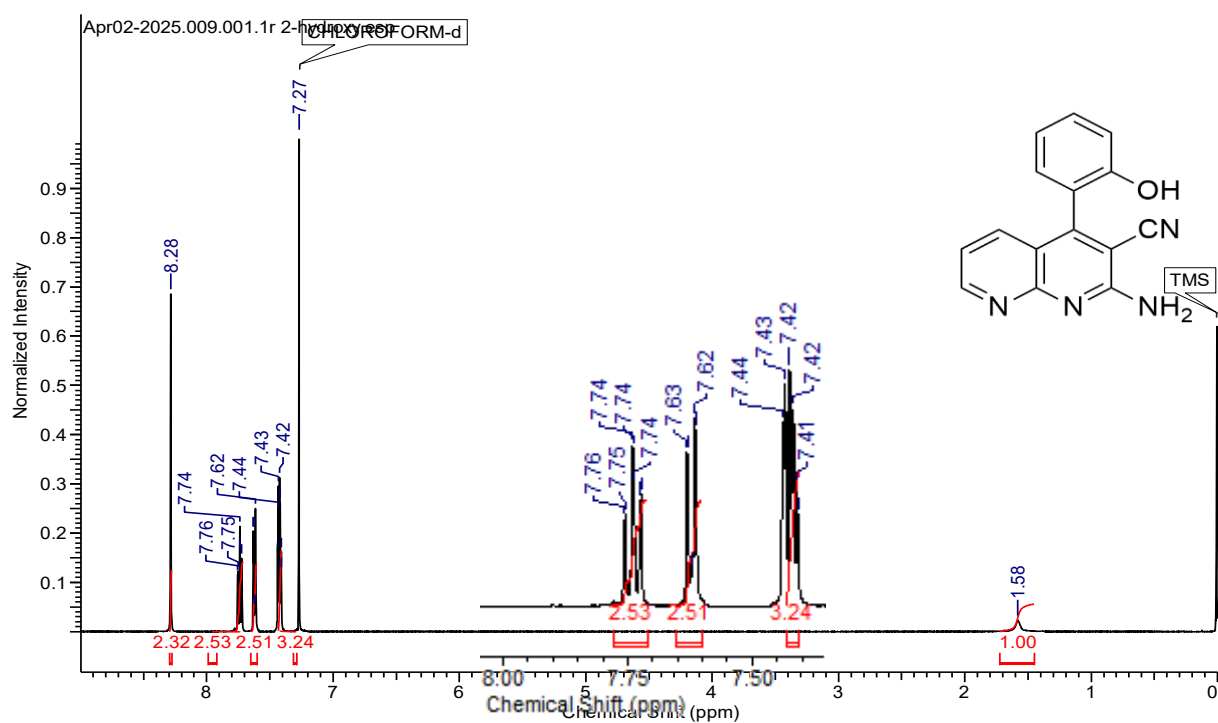


Figure S64: ^1H -NMR (500 MHz, CDCl_3) Spectrum of 2-amino-4-(2-hydroxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4r**)

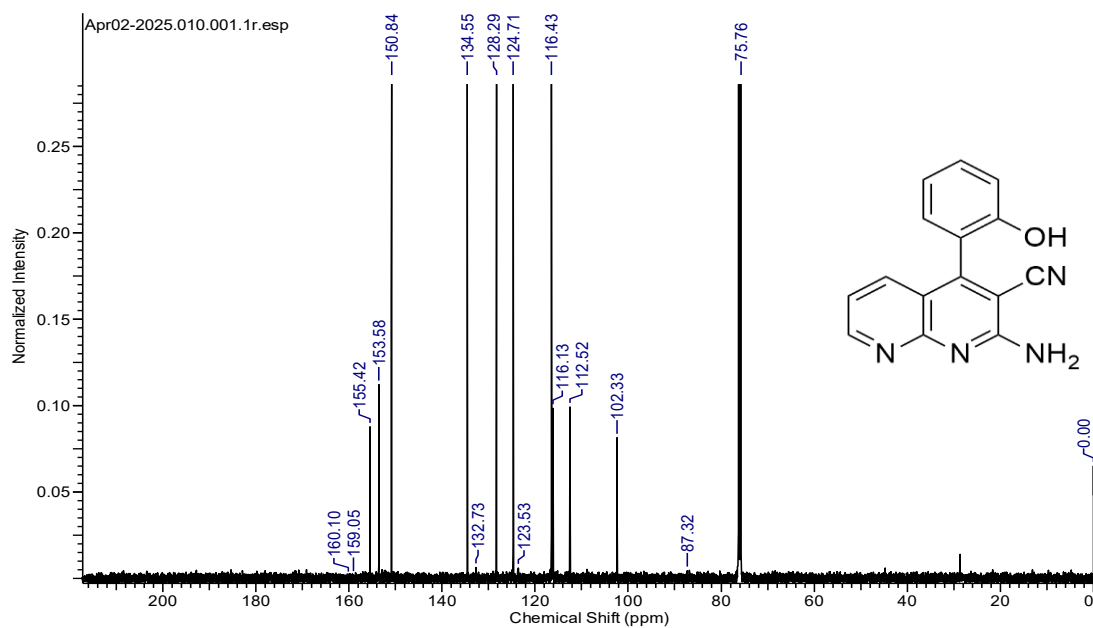
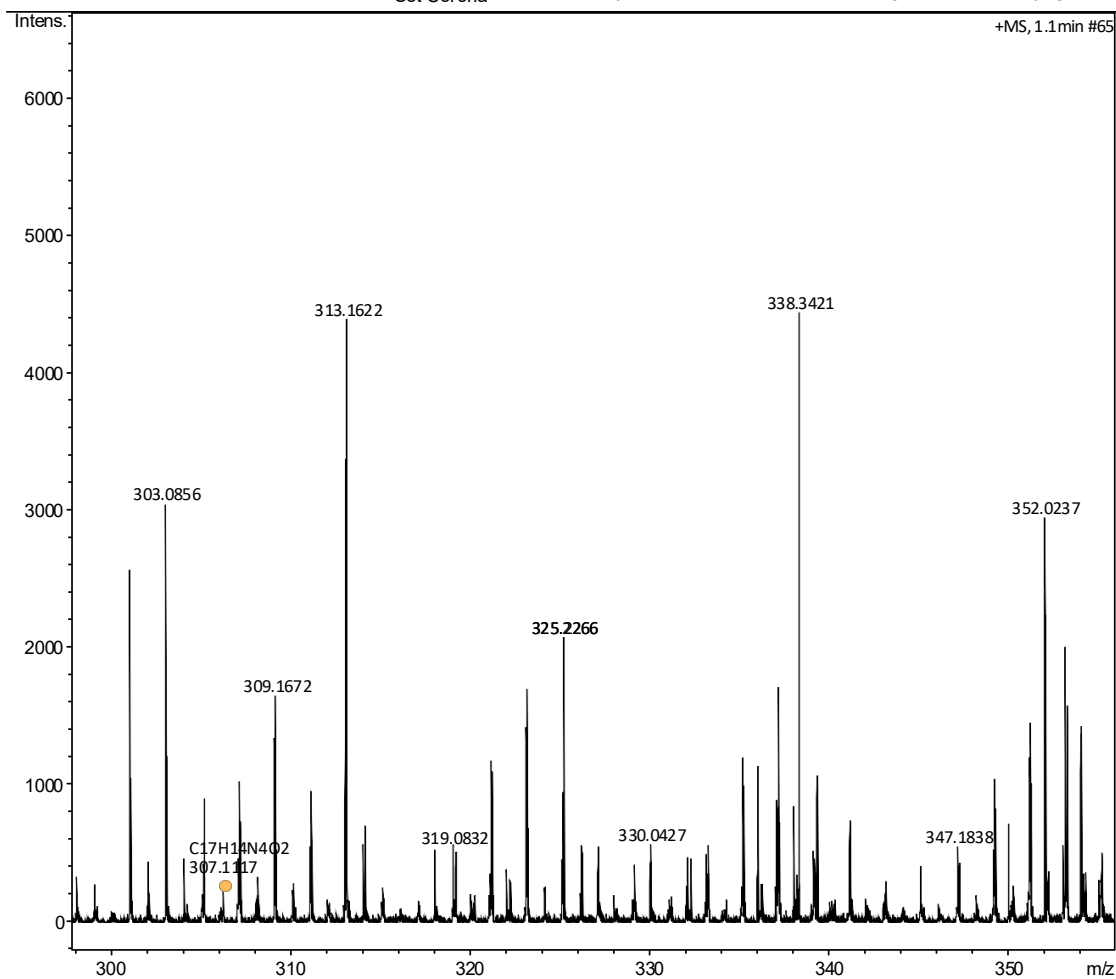


Figure S65: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 2-amino-4-(2-hydroxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4r**)

Analysis Info	Acquisition Date	4/3/2025 7:05:52 PM
Analysis Name	D:\Data\2025\APRIL\SPPU COLLEGE\HRM COLLEGE\HUNDARE PAYAL\D23_RE3_01_9260.d	
Method	dlc_50-1200mz_pos_mode_7min_0.2ml.m	Analyst: Nitin S. Kadam CIF
Sample Name	D23	Instrument impact HD 1819696.00184

Acquisition Parameter	Ion Polarity	Positive	Set Nebulizer	0.7 Bar
Source Type	Set Capillary	4000 V	Set Dry Heater	200 °C
Focus	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan Begin	Set Charging Voltage	2000 V	Set Divert Valve	Source
Scan End	Set Corona	0 nA	Set APCI Heater	0 °C



D23_RE3_01_9260.d

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Figure S66: HR-ESI-MS Spectrum of 2-amino-4-(2-hydroxyphenyl)-1,8-naphthyridine-3-carbonitrile (4r)

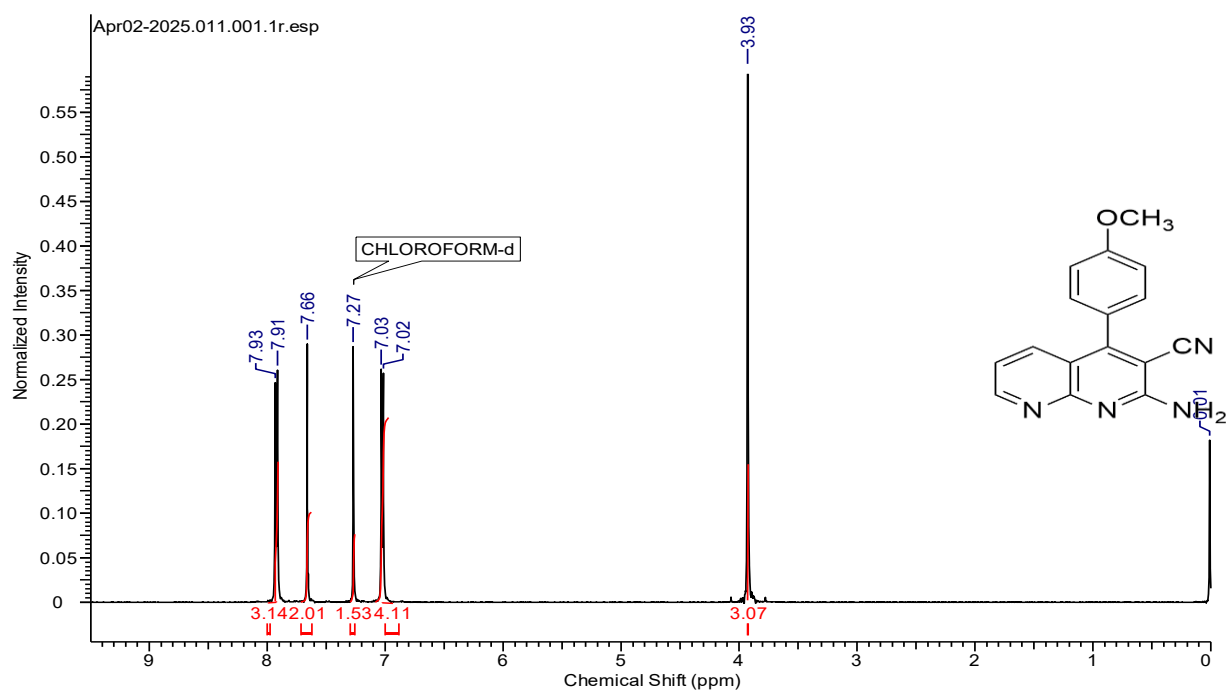


Figure S67: ^1H -NMR (500 MHz, CDCl_3) Spectrum of 2-amino-4-(4-methoxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4s**)

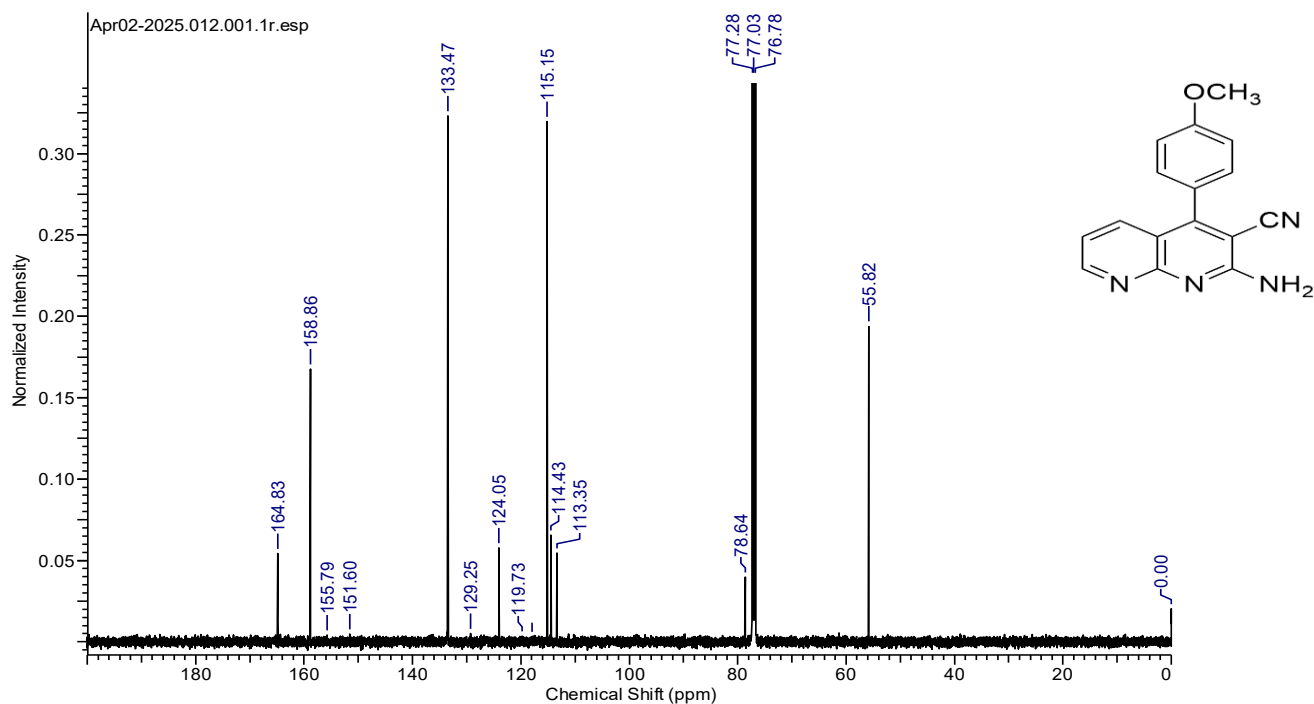
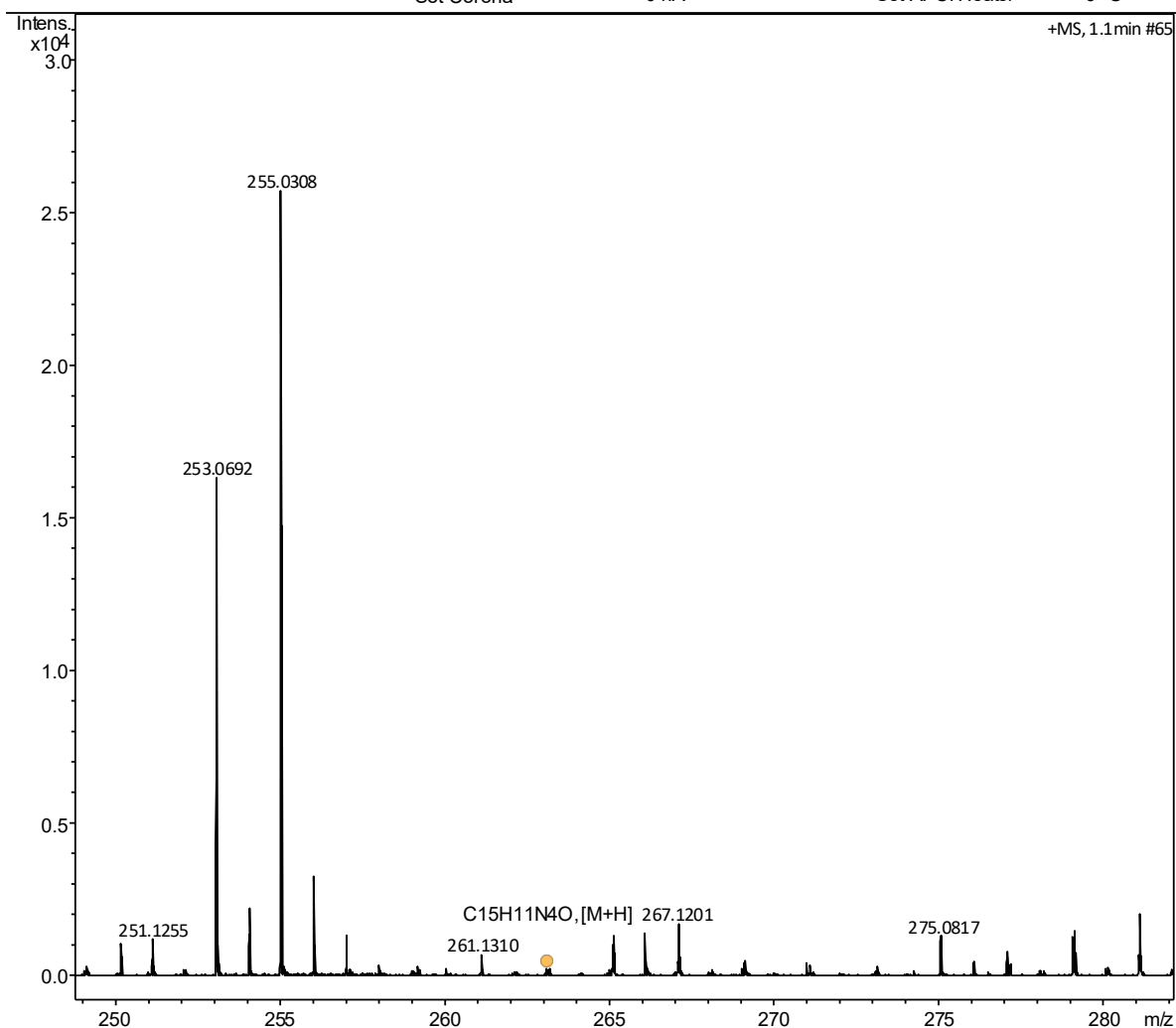


Figure S68: ^{13}C -NMR (125 MHz, CDCl_3) Spectrum of 2-amino-4-(4-methoxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4s**)

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Analysis Info		Acquisition Date	4/3/2025 6:58:18 PM
Analysis Name	D:\Data\2025\APRIL\SPPU COLLEGE\HRM COLLEGE\HUNDARE PAYAL\D24_RE2_01_9259.d		
Method	dlc_50-1200mz_pos_mode_7min_0.2ml.m	Analyst:	Nitin S. Kadam CIF
Sample Name	D24	Instrument	impactHD 1819696.00184

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.7 Bar
Focus	Active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z #	Ion Formula	Score	m/z err [mDa]	err [ppm]	mSigma	rdB	e ⁻	Conf	N-Rule	Adduct
263.091420 1	C ₁₅ H ₁₁ N ₄ O	100.00	263.092737	1.3	5.0	724.3	12.5	even	ok	M+H

Figure S69: HR-ESI-MS Spectrum of 2-amino-4-(4-methoxyphenyl)-1,8-naphthyridine-3-carbonitrile (**4s**)