

Development of an efficient chemo-enzymatic process for the synthesis of Nilotinib

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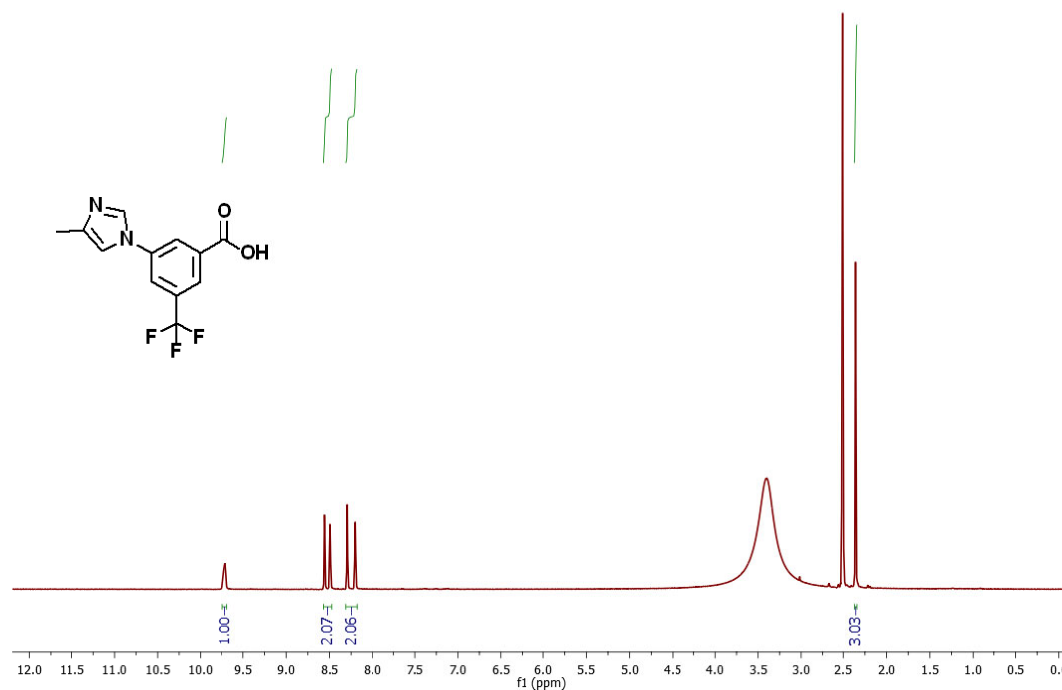
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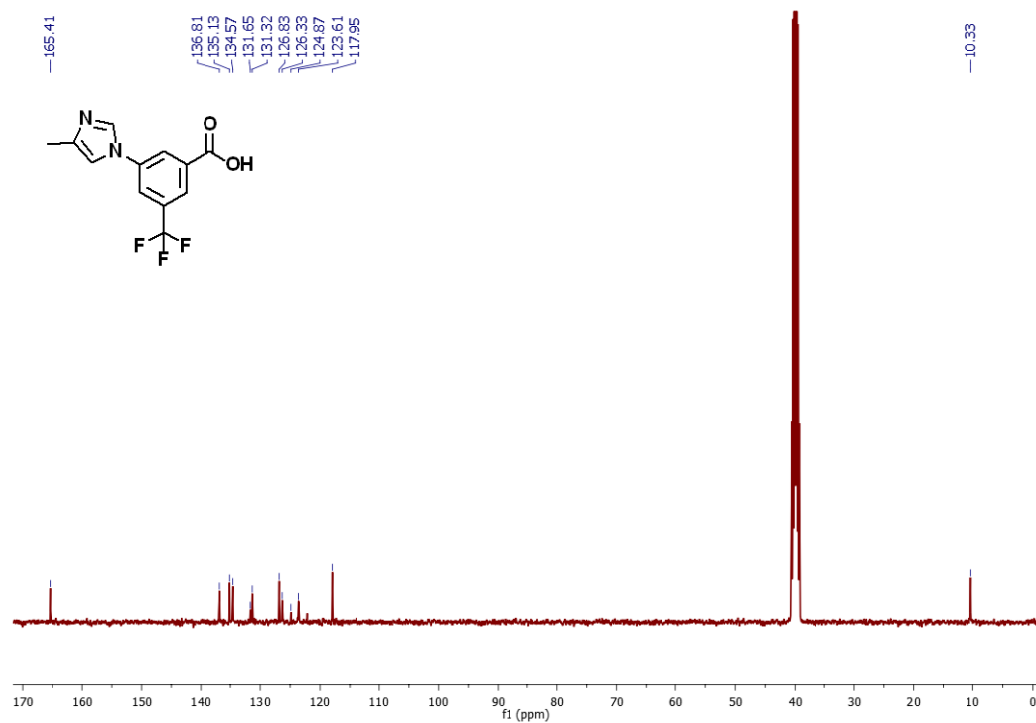
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Supplementary data

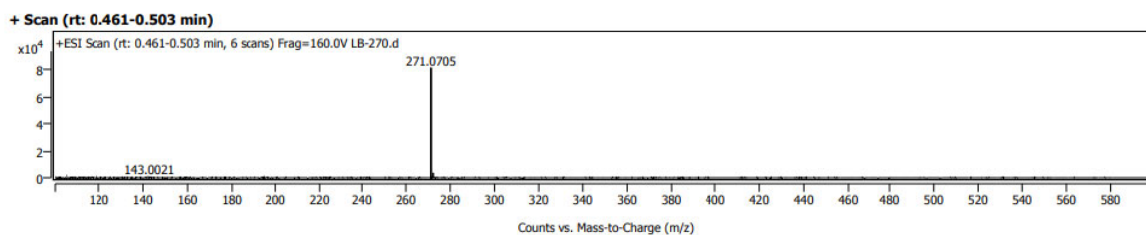
1. NMR Spectroscopy

1.1. ¹H NMR of 3-(4-methyl-1H-imidazol-1-yl)-5-(trifluoromethyl)benzoic acid



1.2. ^{13}C NMR of 3-(4-methyl-1H-imidazol-1-yl)-5-(trifluoromethyl)benzoic acid

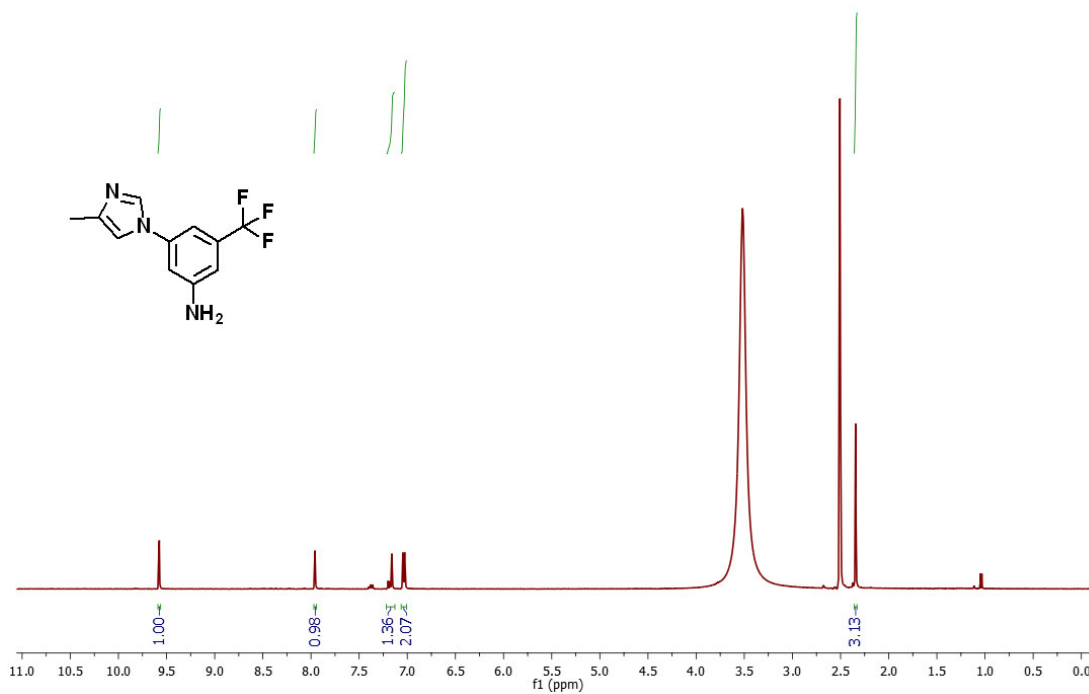
1.3. HRMS of 3-(4-methyl-1H-imidazol-1-yl)-5-(trifluoromethyl)benzoic acid.

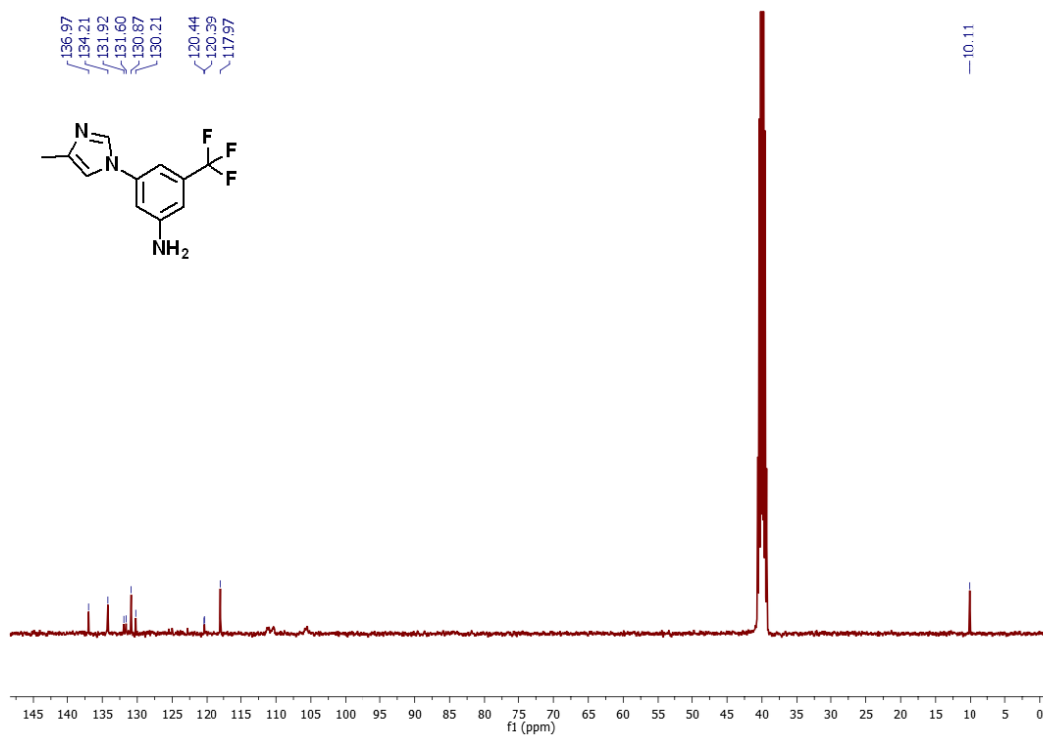


Spectrum Identification Table

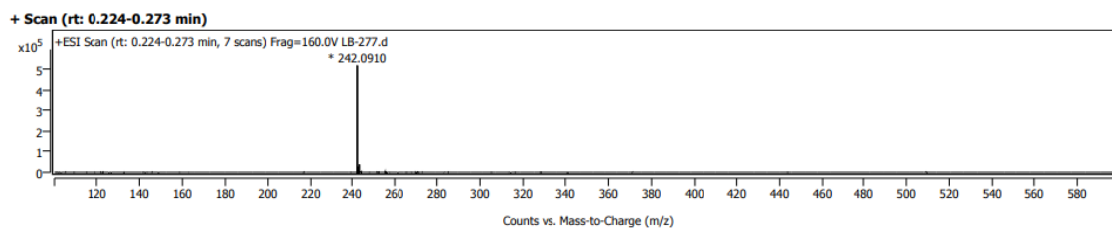
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No	MFG	C12 H10 F3 N2 O2	M+	271.0705	5.83	S8	271.0694			60.27	

MassHunter Qual 10.0
(End of Report)

1.4. ^1H NMR of 3-(4-methyl-1h-imidazol-1-yl)-5-(trifluoromethyl)aniline.**1.5. ^{13}C NMR of 3-(4-methyl-1h-imidazol-1-yl)-5-(trifluoromethyl)aniline**



1.6.HRMS of 3-(4-methyl-1h-imidazol-1-yl)-5-(trifluoromethyl)aniline

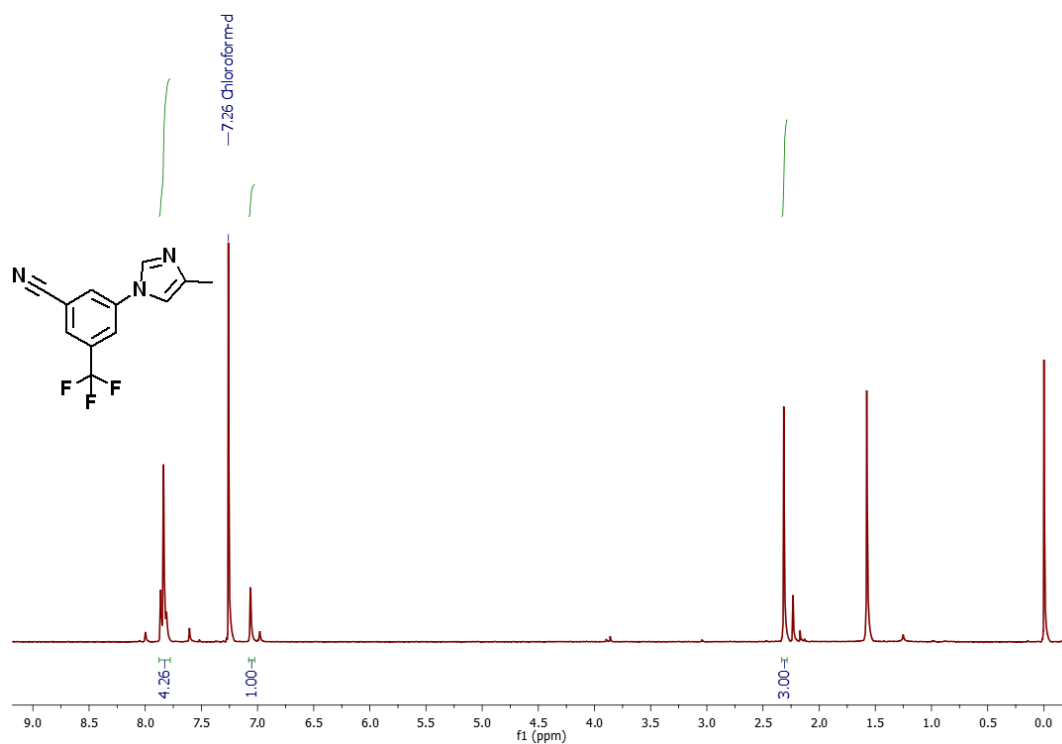


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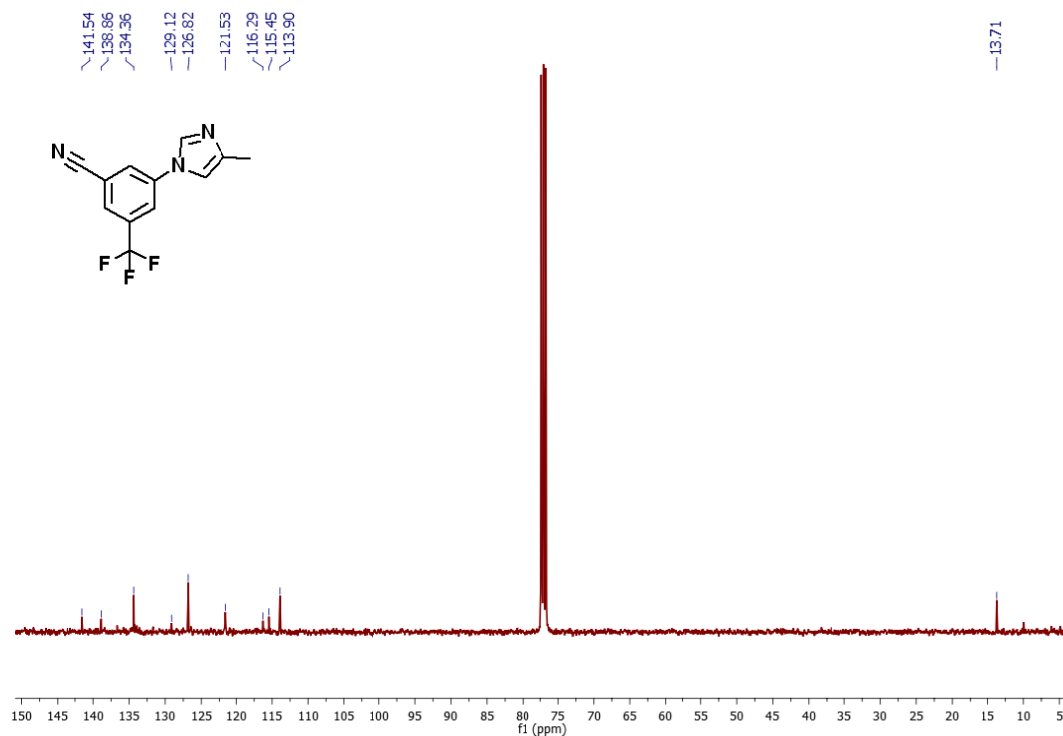
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No	MFG		C11 H11 F3 N3	M+	242.0910	4.31	58	242.0905			74.61	

MassHunter Qual 10.0
(End of Report)

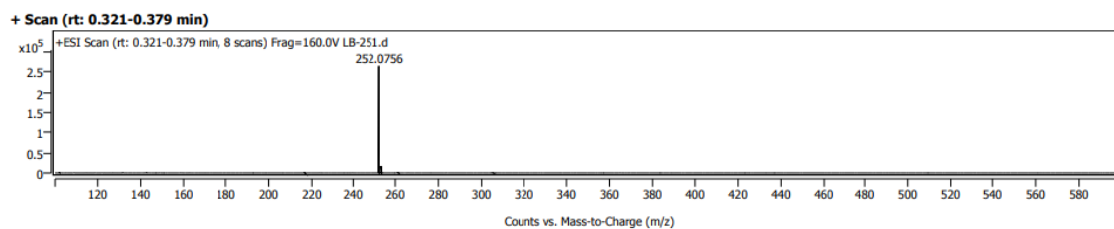
1.7.¹H NMR of 3-(4-methyl-1h-imidazol-1-yl)-5-(trifluoromethyl)benzonitrile



1.8. ^{13}C NMR of 3-(4-methyl-1H-imidazol-1-yl)-5-(trifluoromethyl)benzonitrile



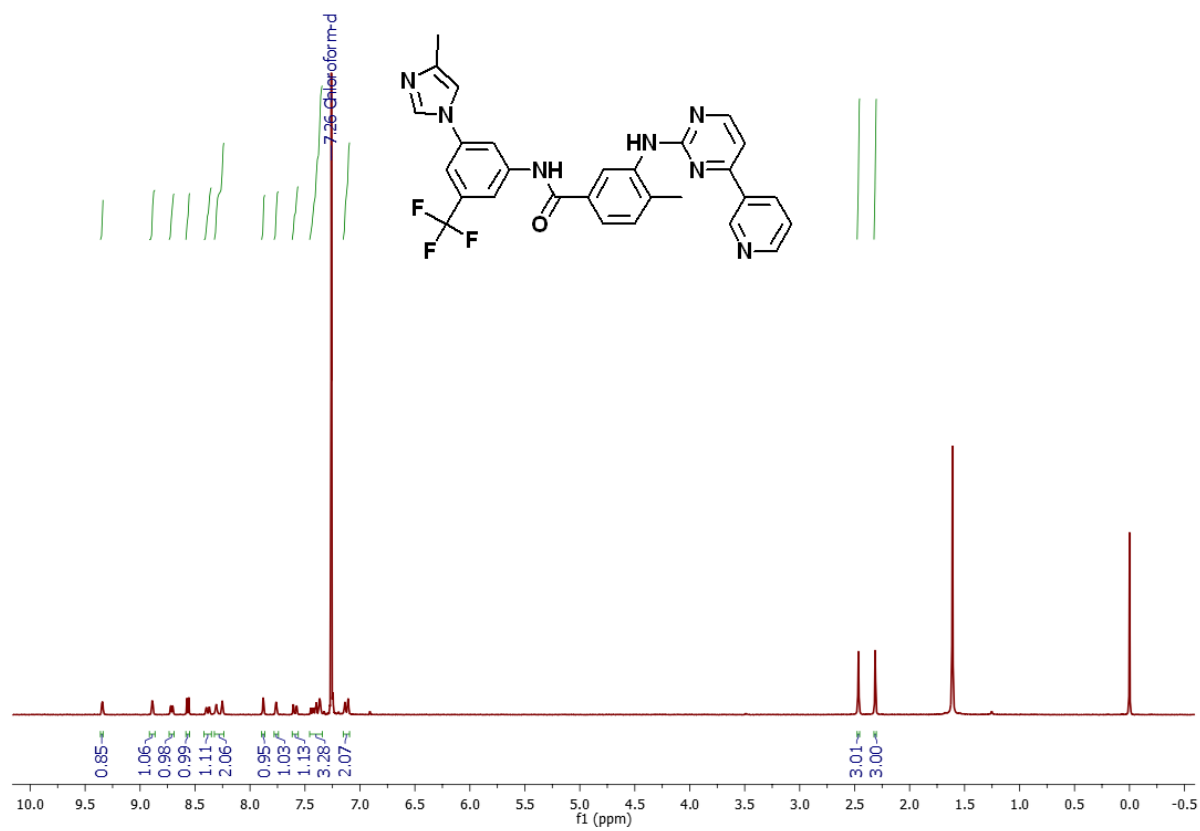
1.9. HRMS of 3-(4-methyl-1H-imidazol-1-yl)-5-(trifluoromethyl)benzonitrile

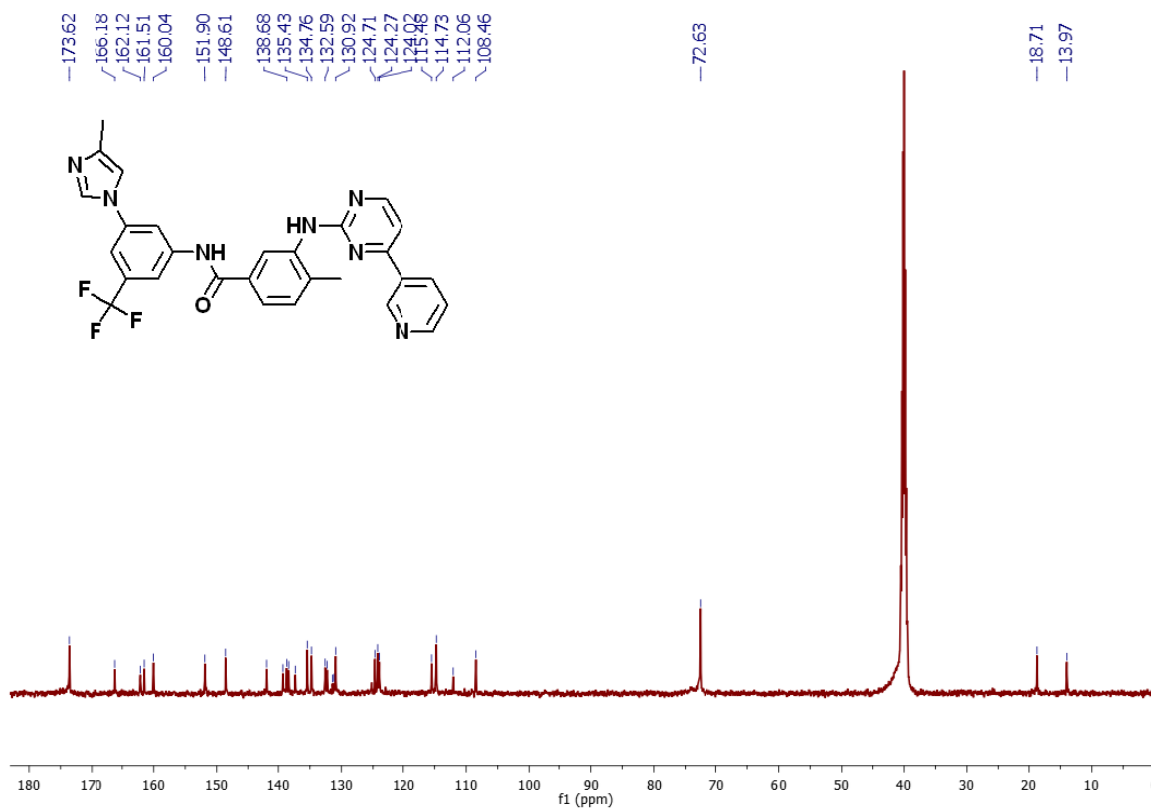


Spectrum Identification Table

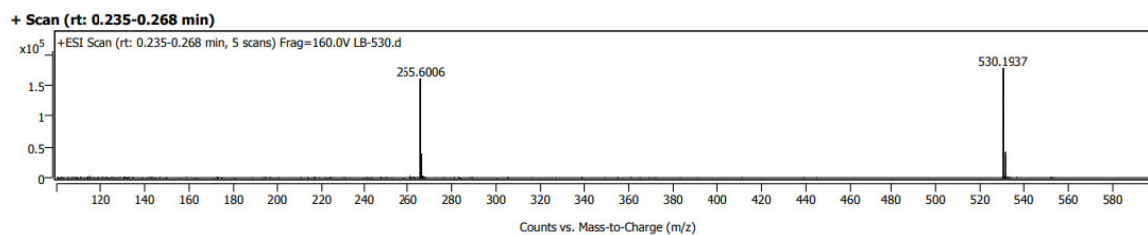
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No. MFG		C12 H9 F3 N3	M+	252.0756	5.18	58	252.0749			79.26	

MassHunter Qual 10.0
(End of Report)

1.10. ^1H NMR of Nilotinib

1.11. ^{13}C NMR of Nilotinib

1.12. HRMS of Nilotinib



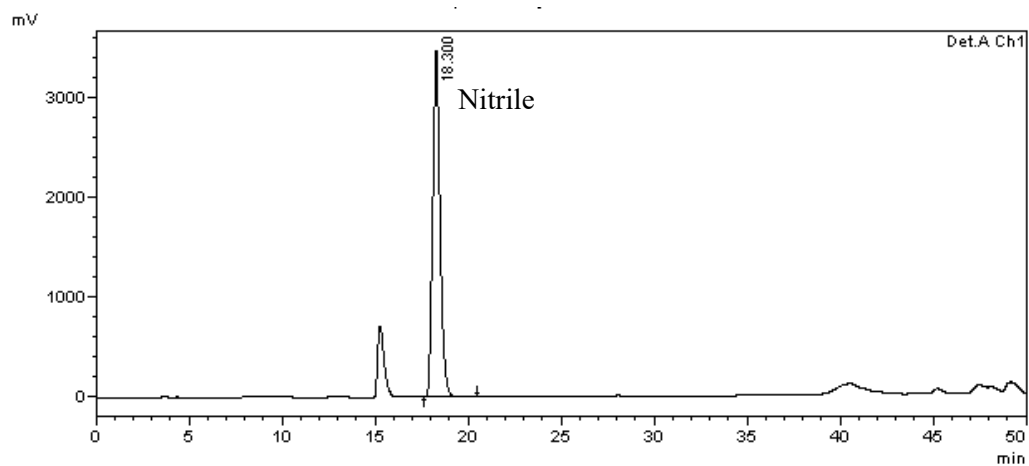
Spectrum Identification Table

Best ID Source	Name	Formula	Species	m/z	Diff (ppm)	Textbox2	Mass	Score (Lib)	Score (DB)	Score (MFG)	Lib/DB
No	MFG	C ₂₈ H ₂₃ F ₃ N ₇ O	M+	530.1937	5.06	S8	530.1916			74.22	

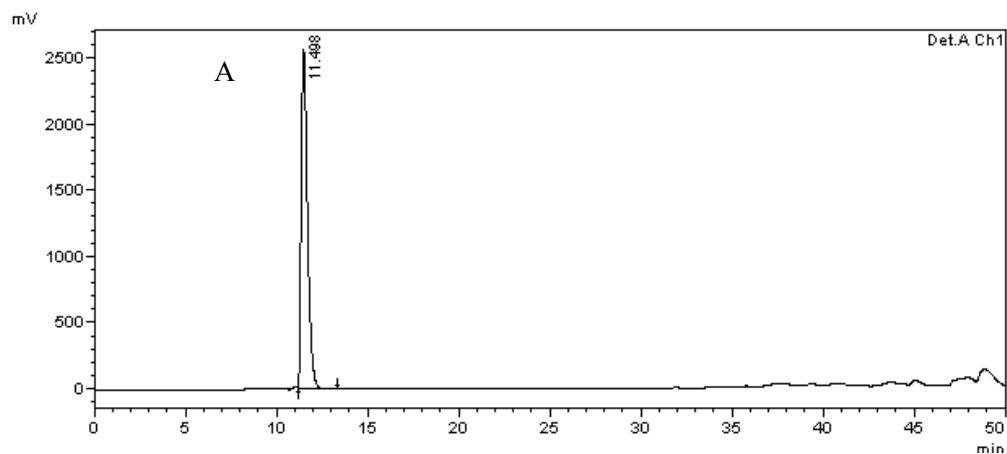
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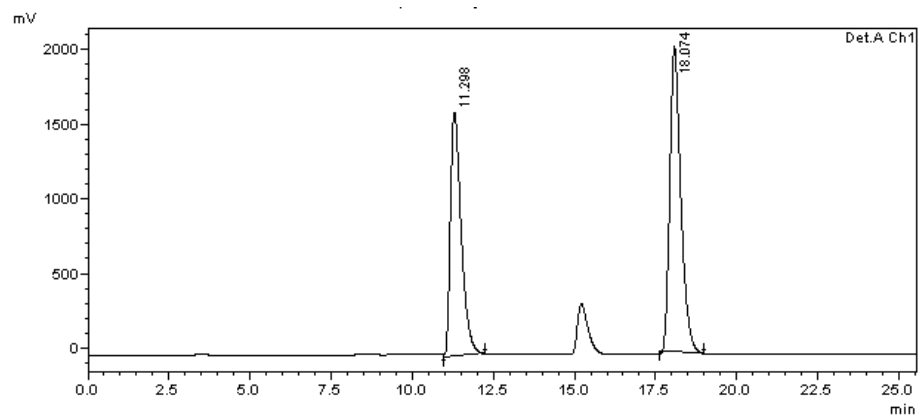
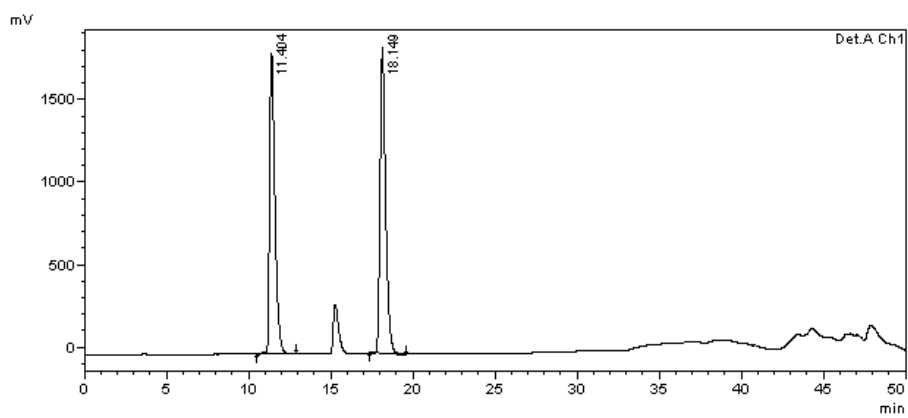
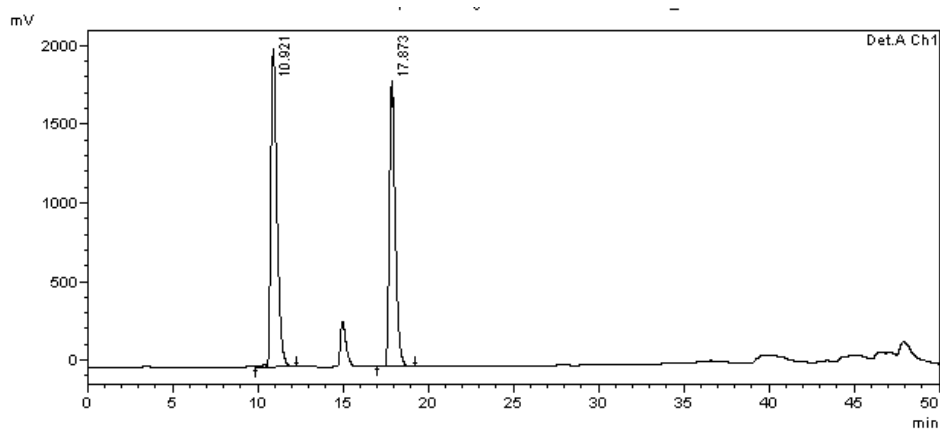
2. Nilotinib HPLC Data

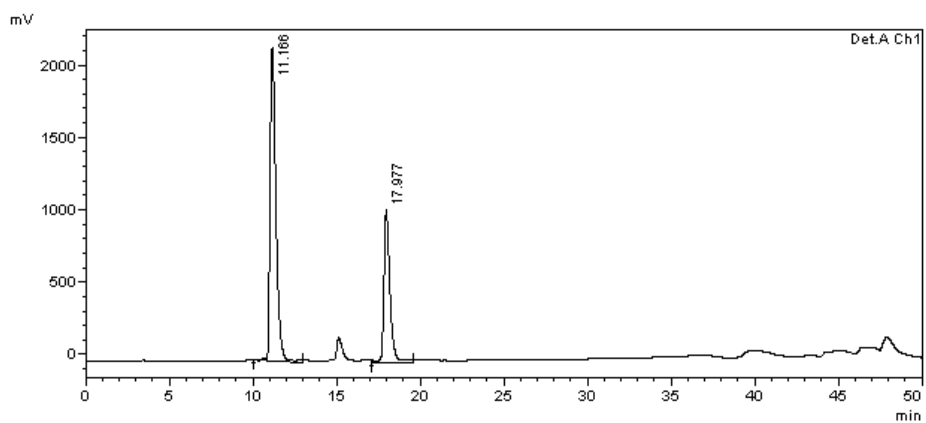
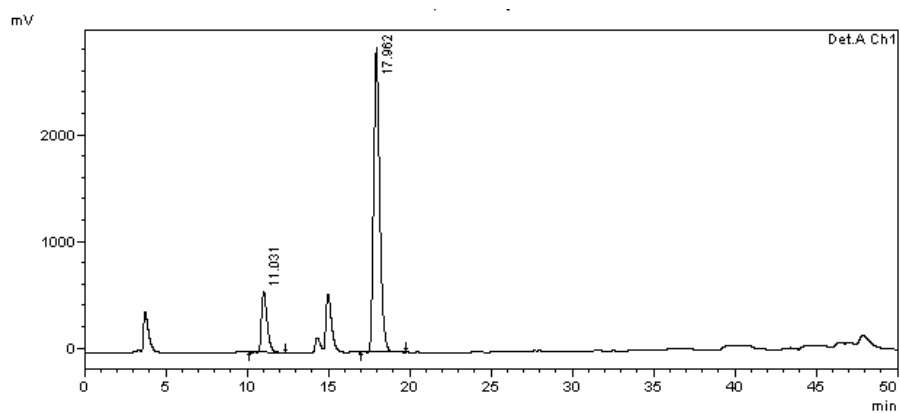
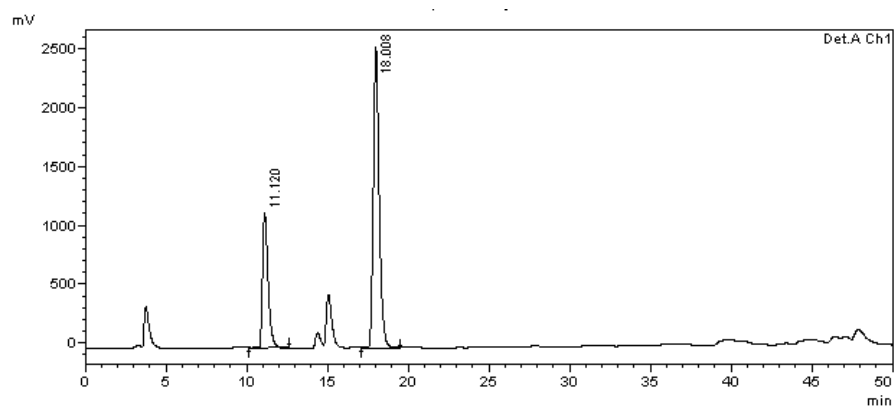
2.1.3-(4-methyl-1H-imidazol-1-yl)-5-(trifluoromethyl)benzonitrile.

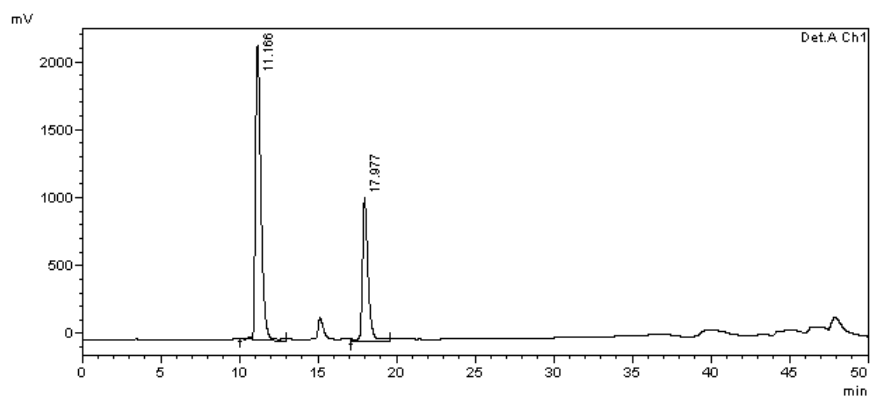


2.2.3-(3-methyl-1H-pyrrol-1-yl)-5-(trifluoromethyl)benzoic acid



2.3.NIT EW 104**2.4.NIT EW 103****2.5.NIT EW 102**

2.6. NIT EW 101**2.7. Reaction time – 6 Hrs****2.8. Reaction time – 12Hrs**

2.9. Reaction time – 24Hrs**2.10. Reaction time – 48Hrs**