

Supplementary Information

Design, synthesis of novel pyrazolopyridine derivatives and CREBBP bromodomain inhibitors docking and molecular dynamics

M Saamanthi^{*a}, S Aruna^a, R Girija^a & D Vinod^b

^a PG & Research Department of Chemistry, Queen Mary's College, Chennai 600 004, India

^b Vellore Institute of Technology, Vellore 632 014, India

E-mail: samanthishanmugam92@gmail.com

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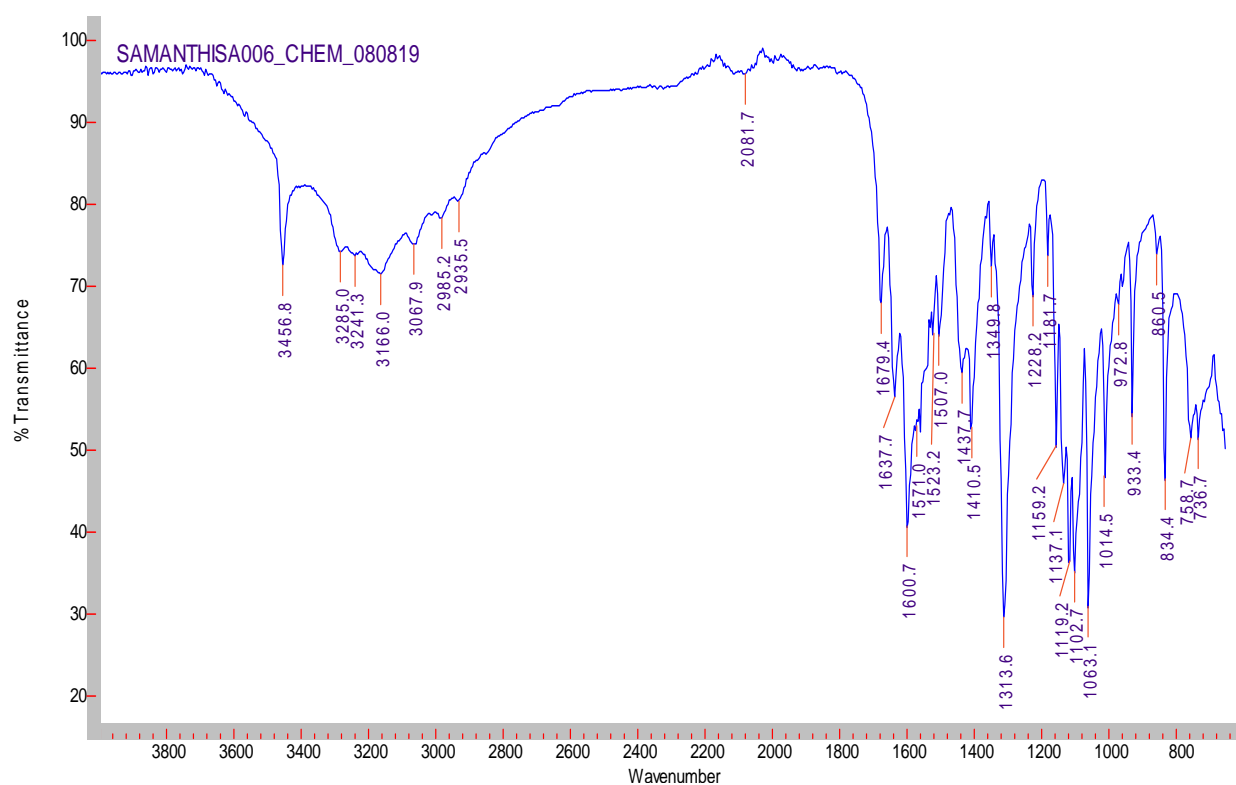


Figure. 1 IR Spectrum of the compound 4a

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SA006

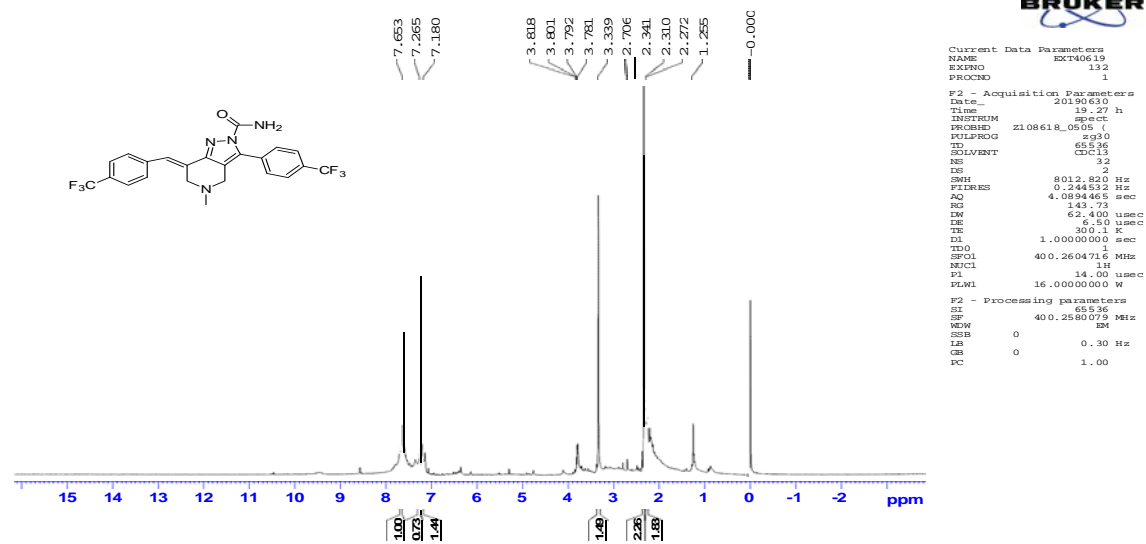


Figure .2 ¹H NMR Spectrum of the compound 4a

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SA006

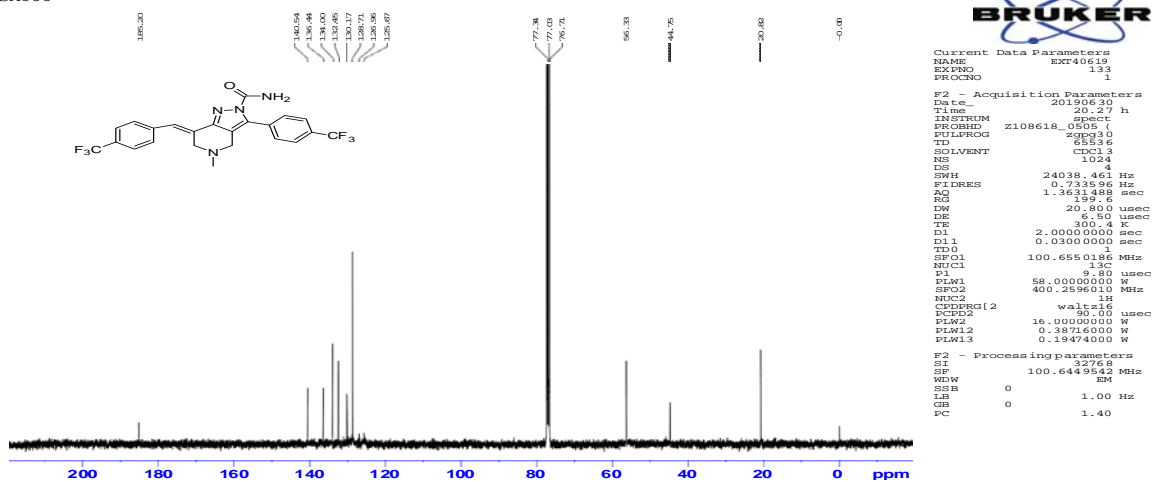


Figure. 3 ¹³C NMR Spectrum of the compound 4a

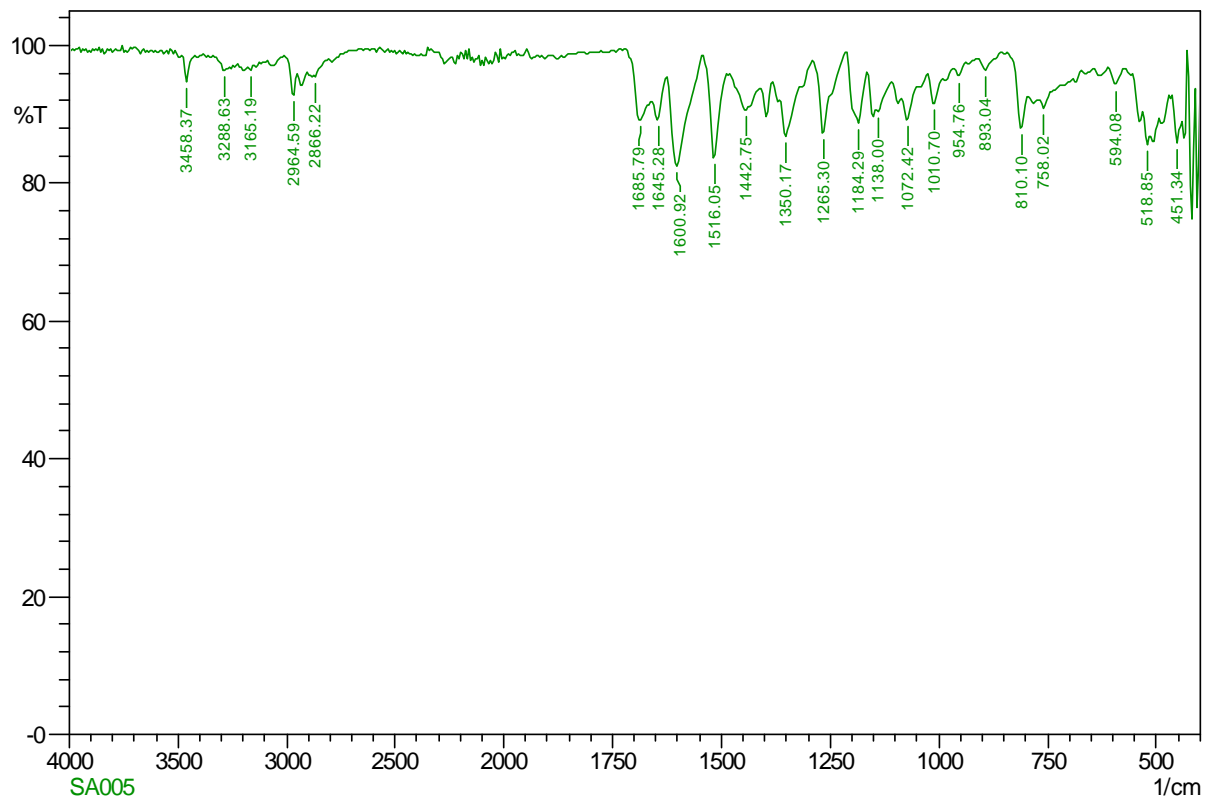


Figure . 4 IR Spectrum of the compound 4c

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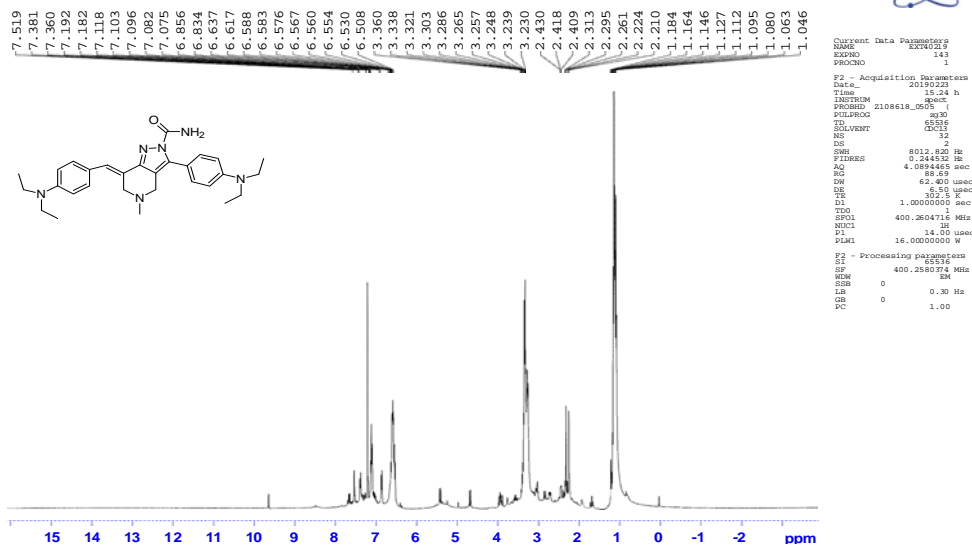


Figure .5 ^1H NMR Spectrum of the compound 4c

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SA005

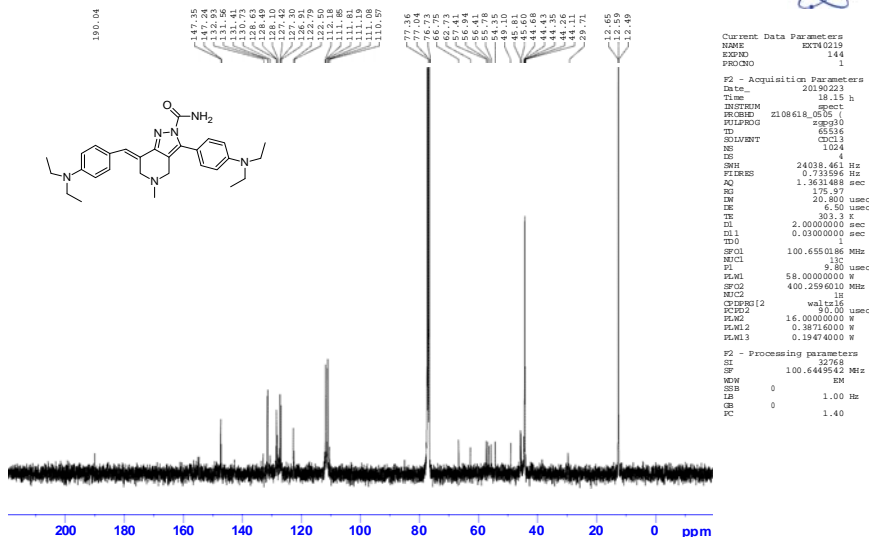


Figure .6 ^{13}C NMR Spectrum of the compound 4c

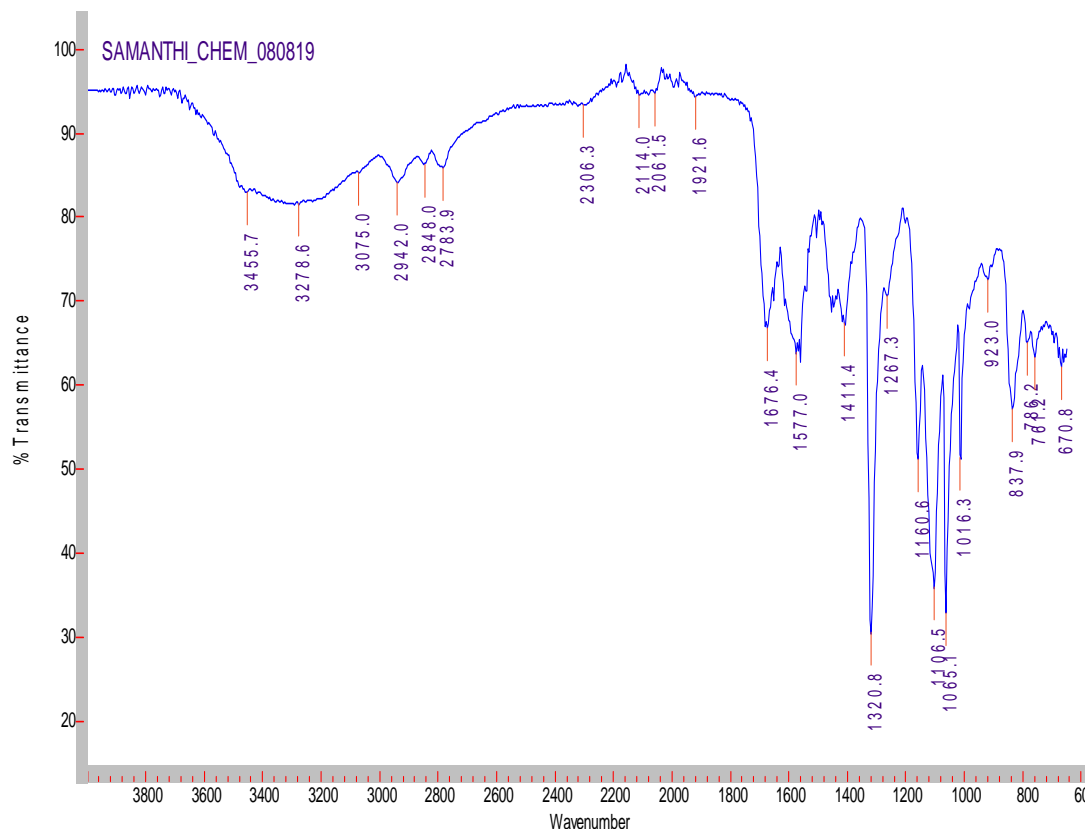
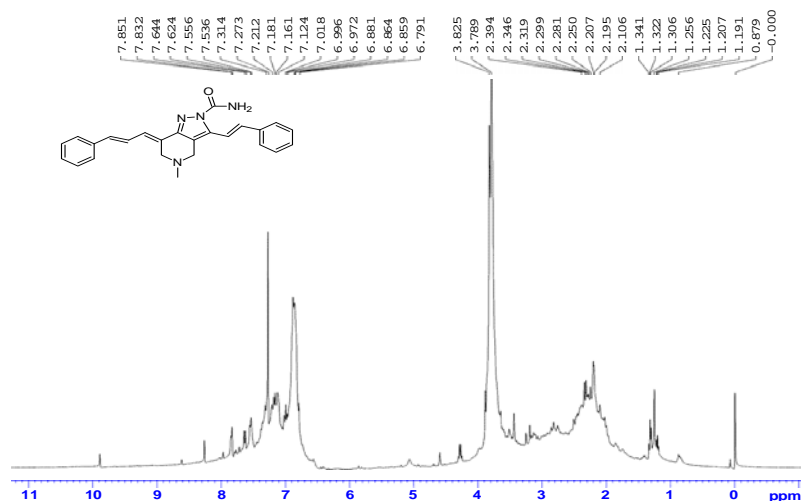


Figure. 7 IR Spectrum of the compound 4d

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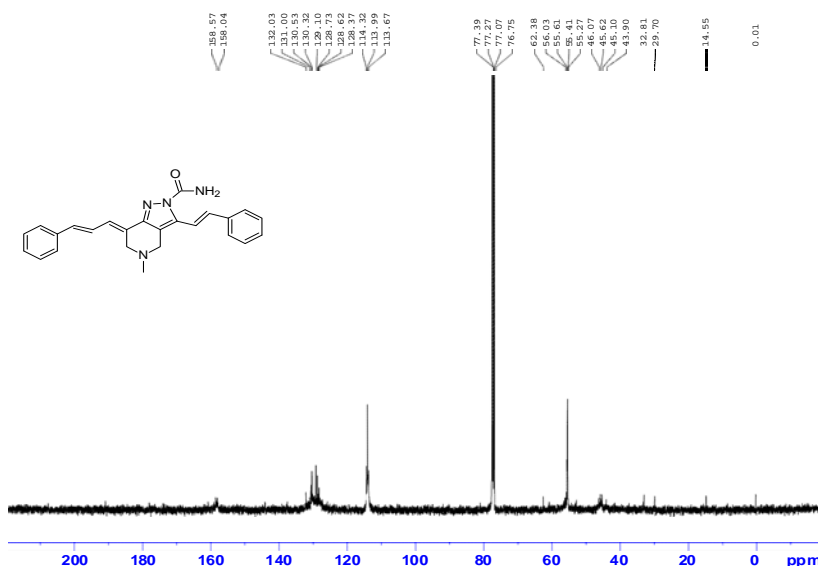


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Figure .8 ^1H NMR Spectrum of the compound 4d

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SA007



Current Data Parameters
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EXPNO 109
PROCNO 1

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NS 1024
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Figure .9 ^{13}C NMR Spectrum of the compound 4d

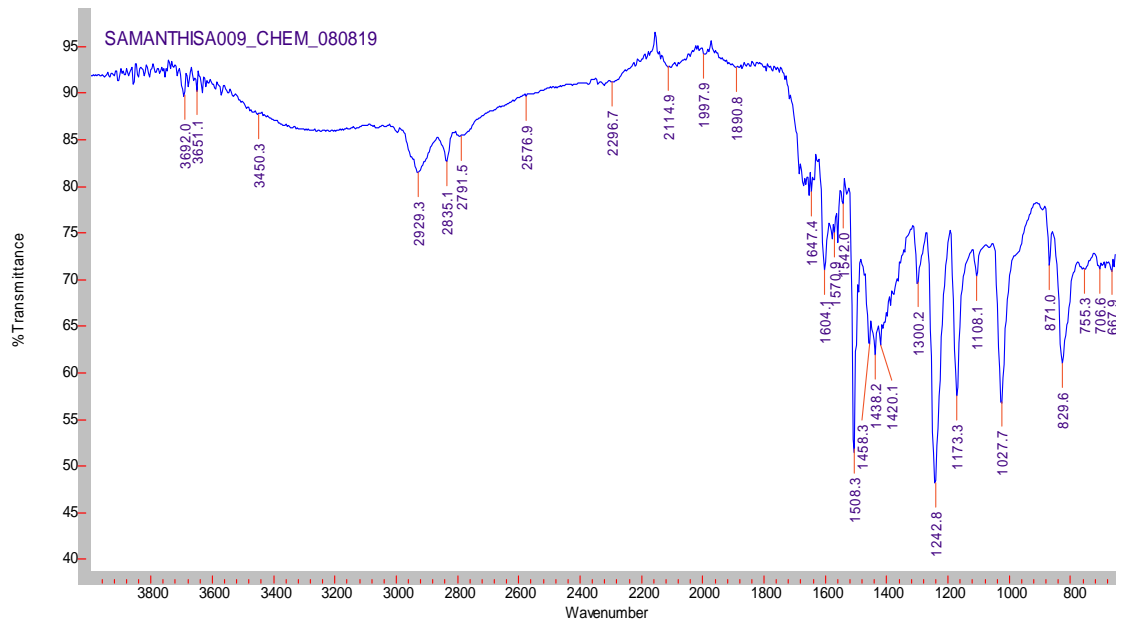


Figure . 10 IR Spectrum of the compound 4f

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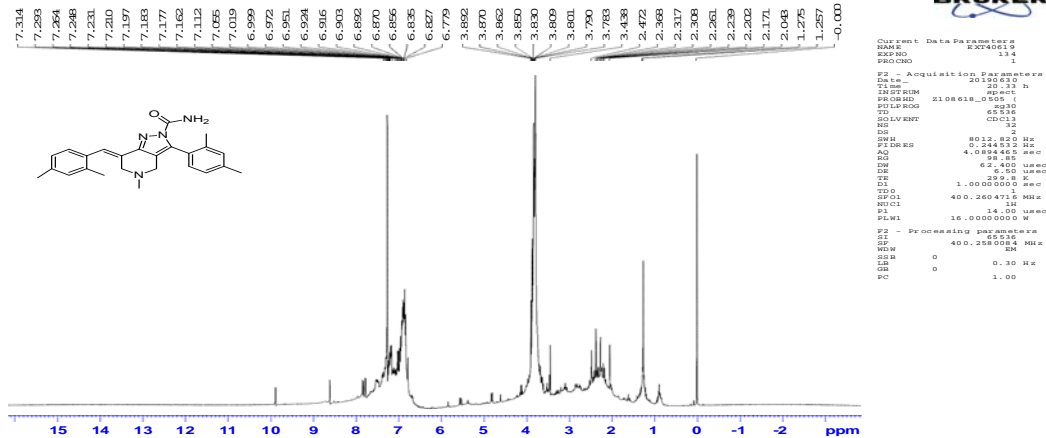


Figure .11 ¹H NMR Spectrum of the compound 4f

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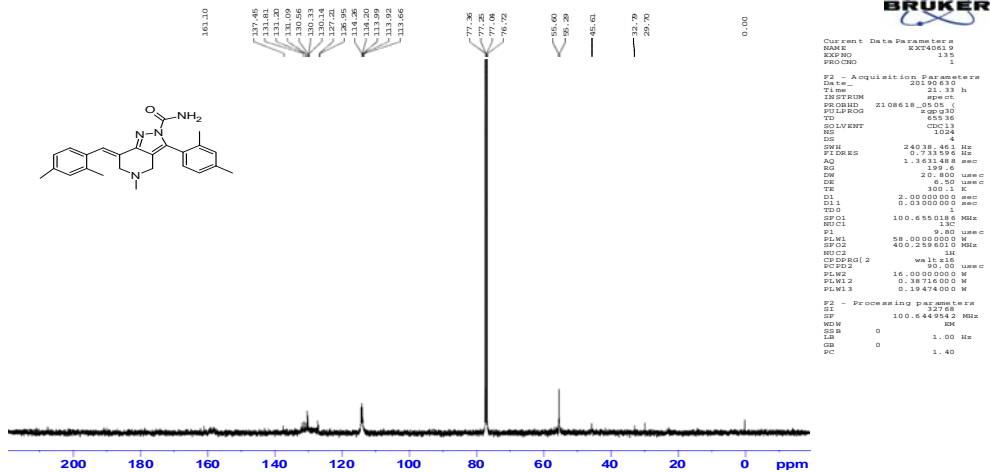


Figure . 12 ¹³C NMR Spectrum of the compound 4f

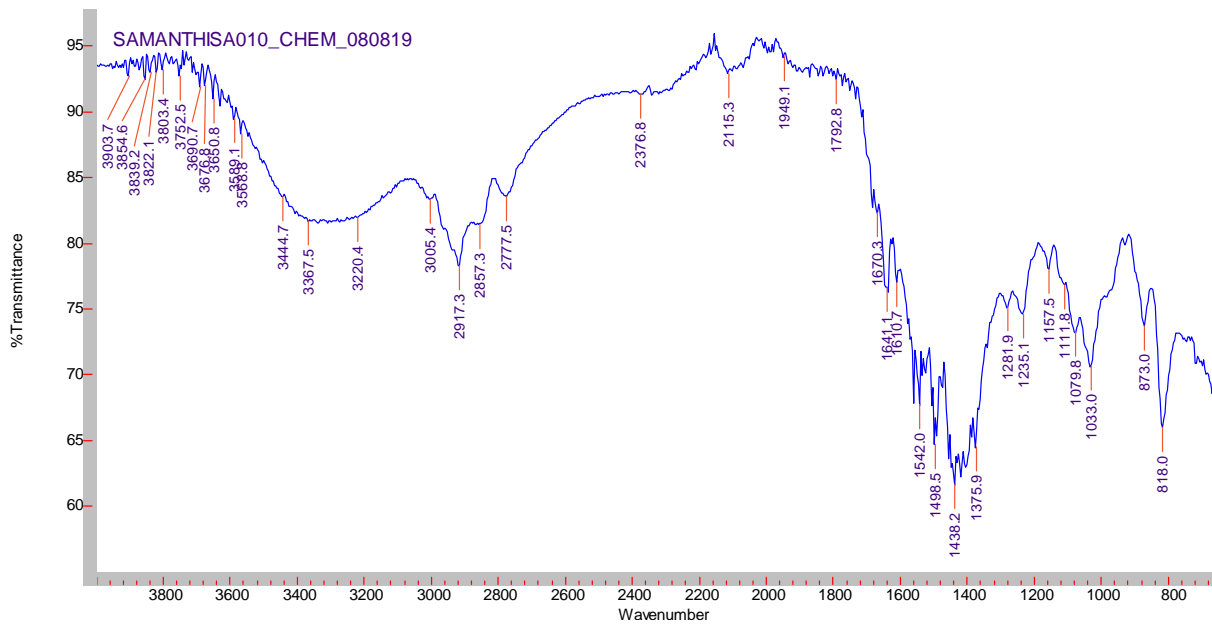


Figure . 13 IR Spectrum of the compound 4g

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SA010

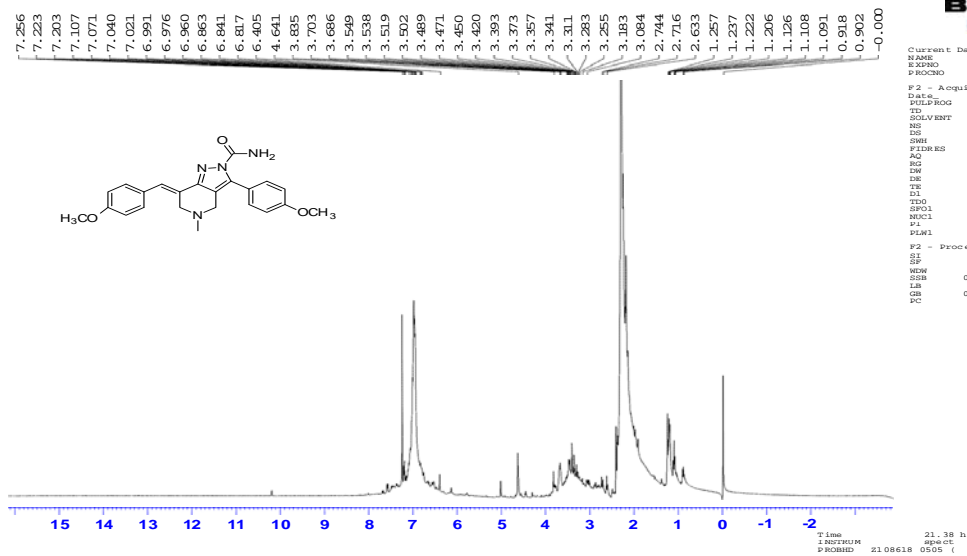


Figure .14 ¹H NMR Spectrum of the compound 4g

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SA010

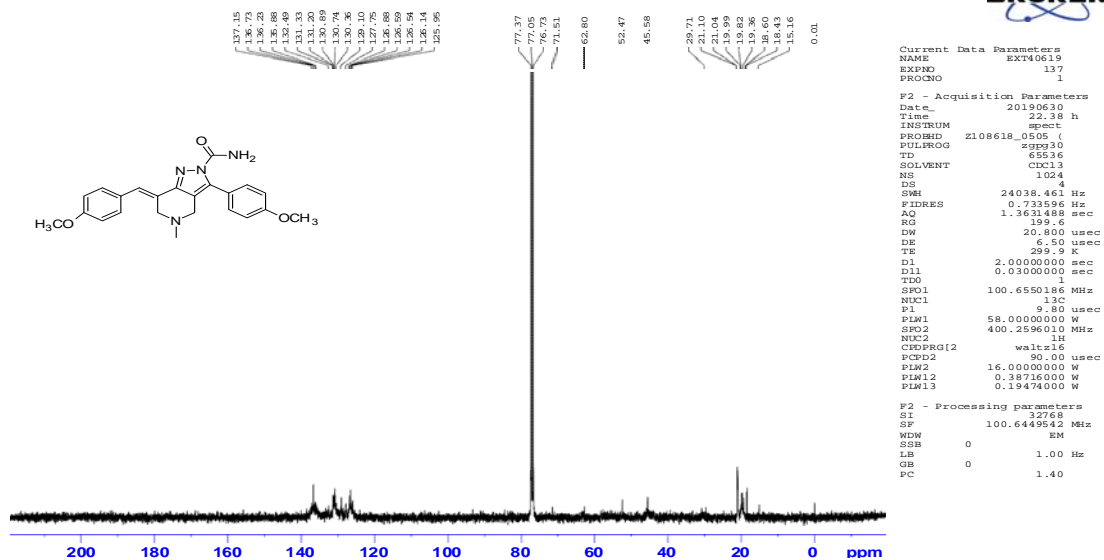


Figure .15 ¹³C NMR Spectrum of the compound 4g

SA006

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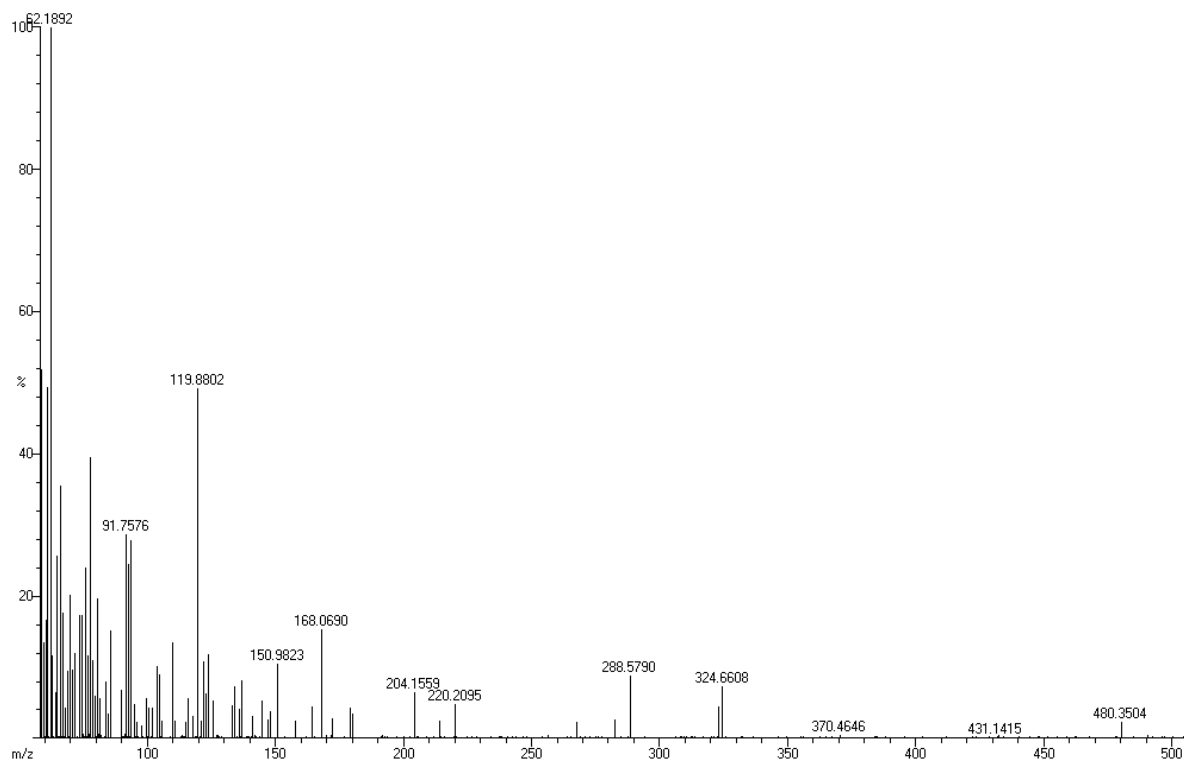
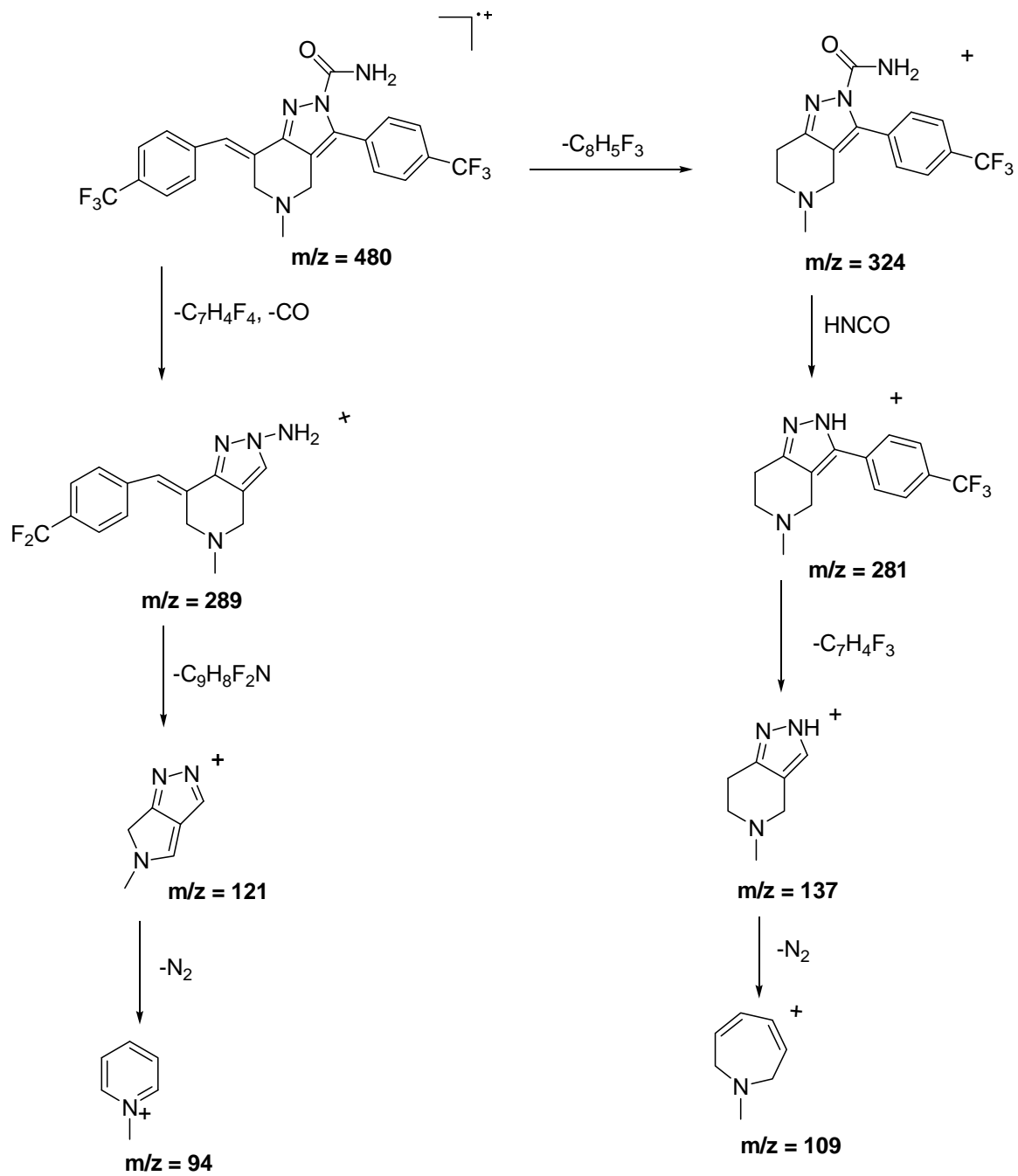


Figure . 16 Mass Spectrum of the compound 4a

The mass spectral fragmentation pattern of the pyrazolo pyridine **4a**



SA005

Scan: 14 TIC=21897120 Base=100%FS #ions=1460 RT=.33

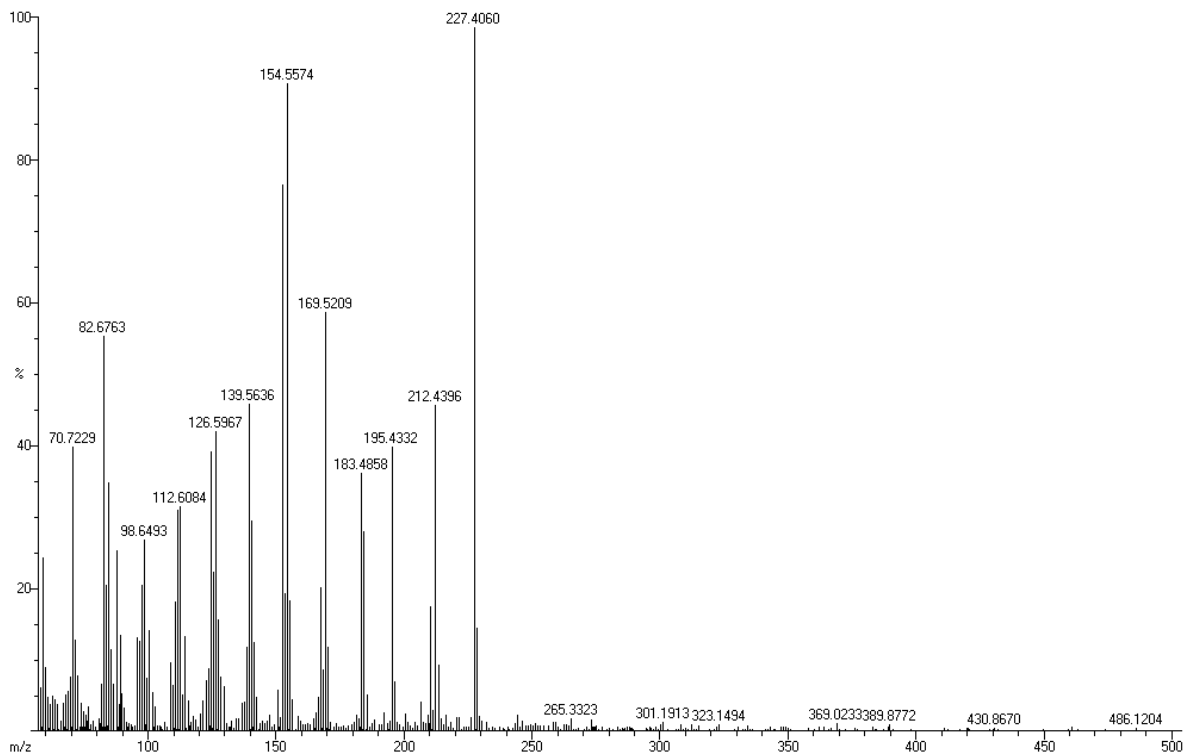


Figure . 17 Mass Spectrum of the compound 4c

SA007

Scan: 55 TIC=14391440 Base=51.5%FS #Ions=1421 RT=1.37

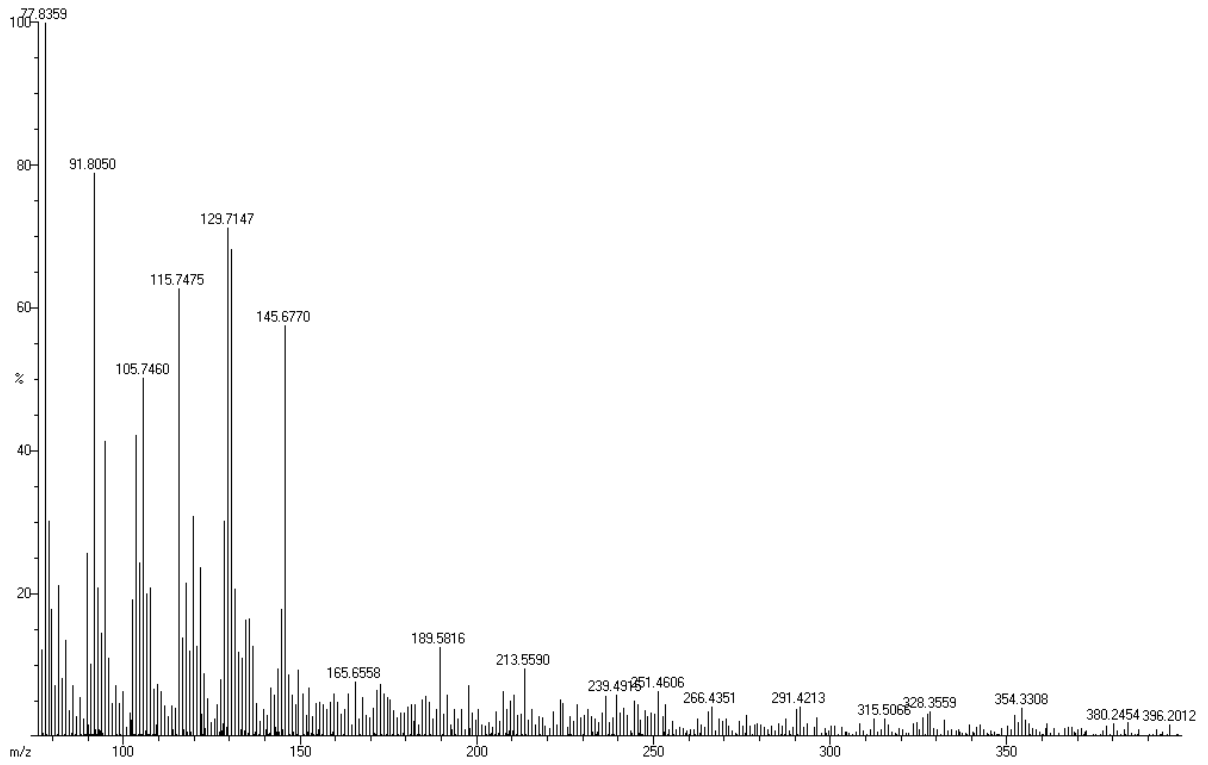


Figure .18 Mass Spectrum of the compound 4d

SA009

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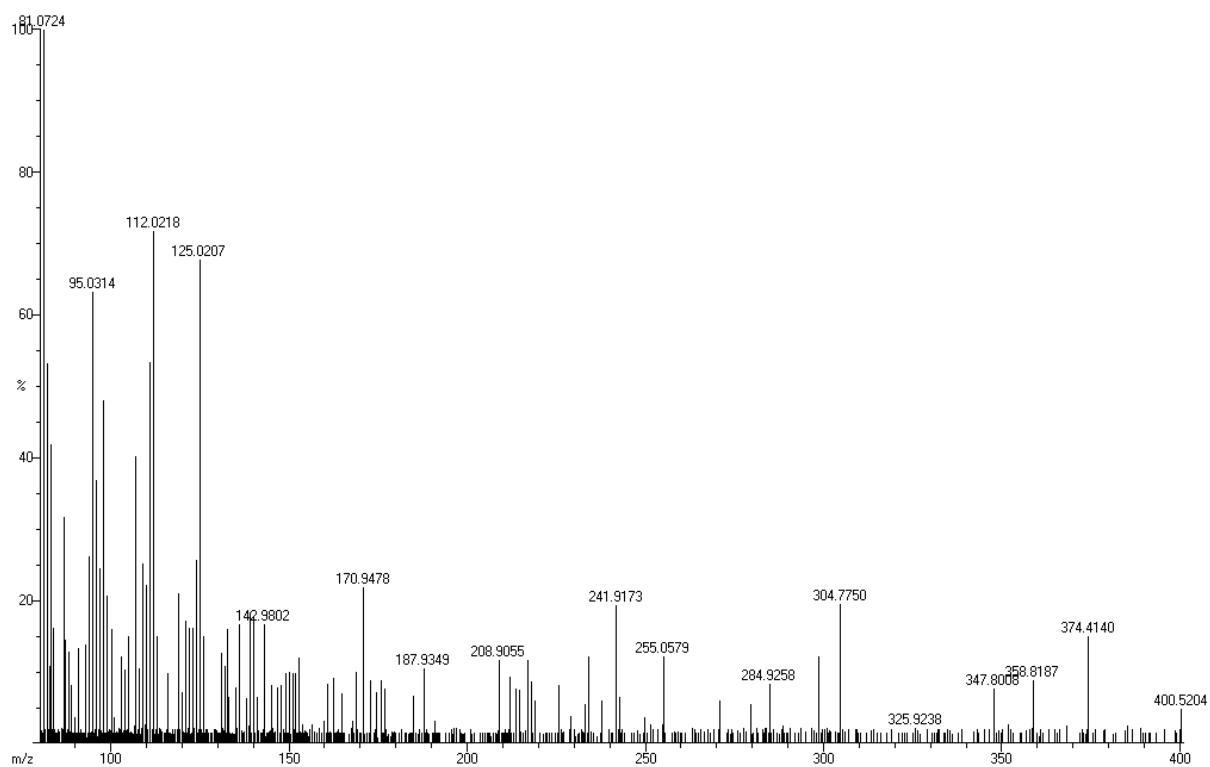
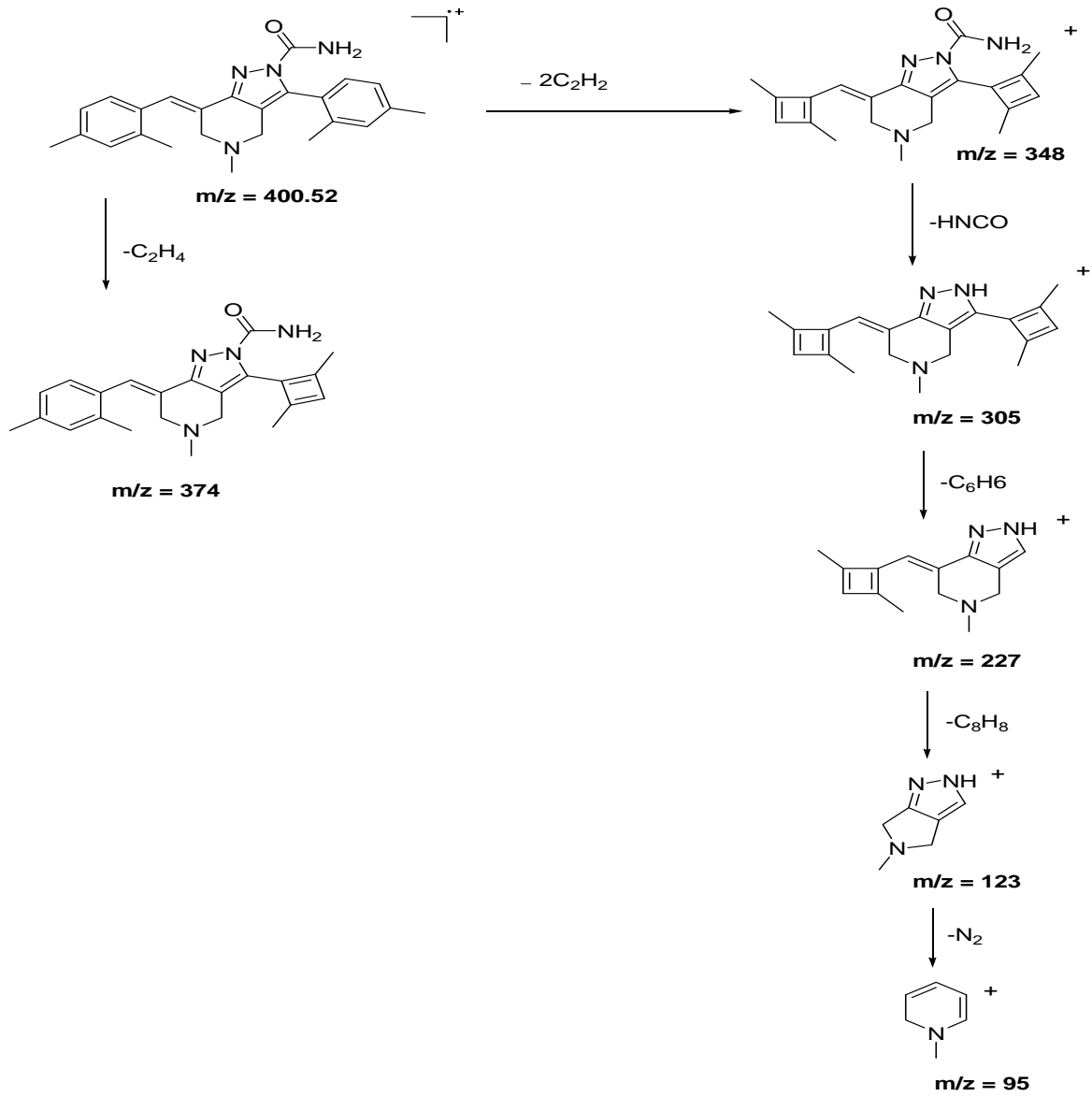


Figure . 19 Mass Spectrum of the compound 4f

The mass spectral fragmentation pattern of the pyrazolo pyridine **4f**



SA010

Scan: 52 TIC=1558560 Base=4.7%FS #ions=890 RT=52

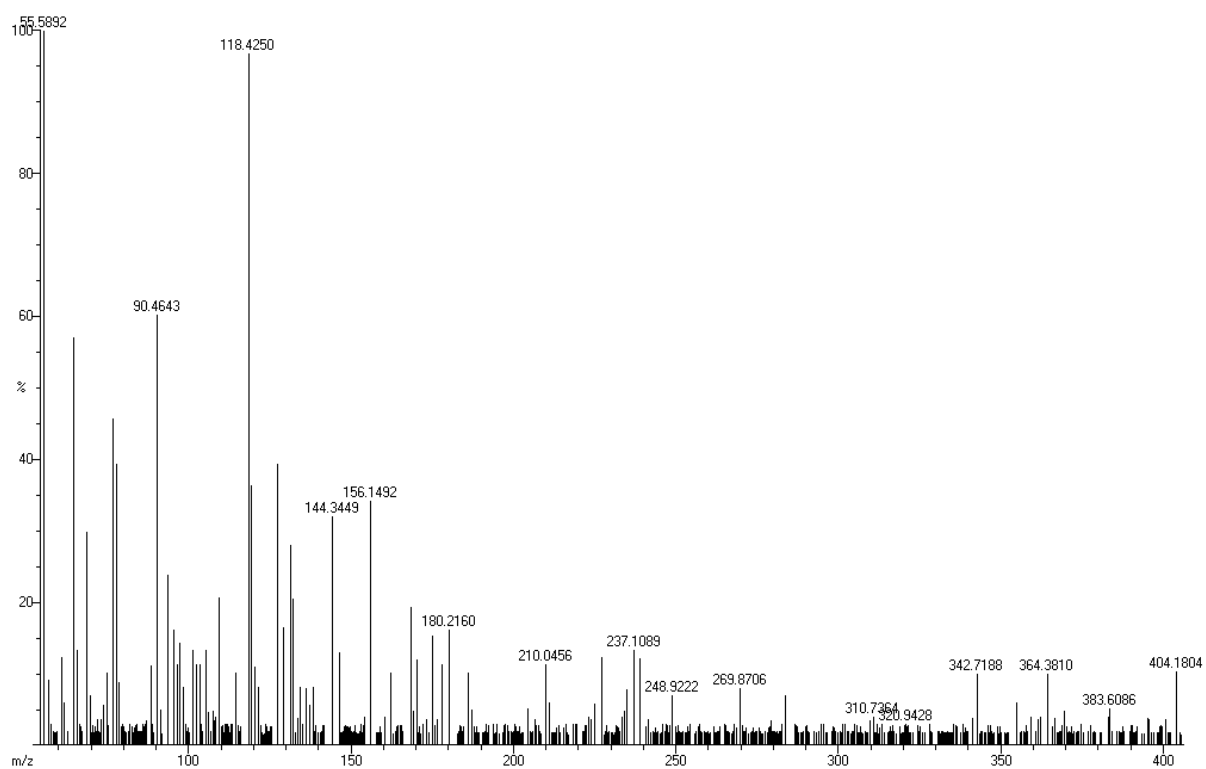
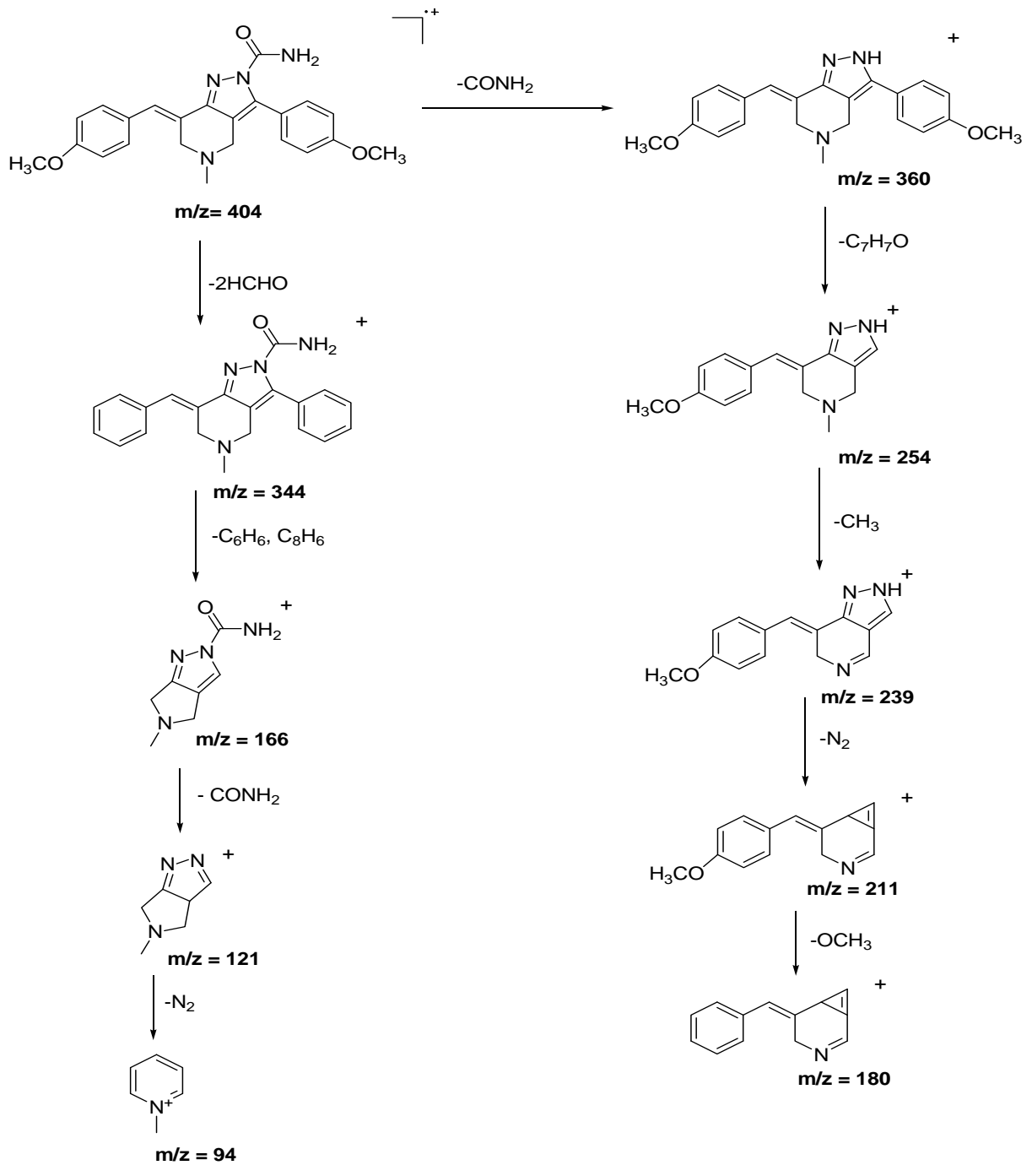
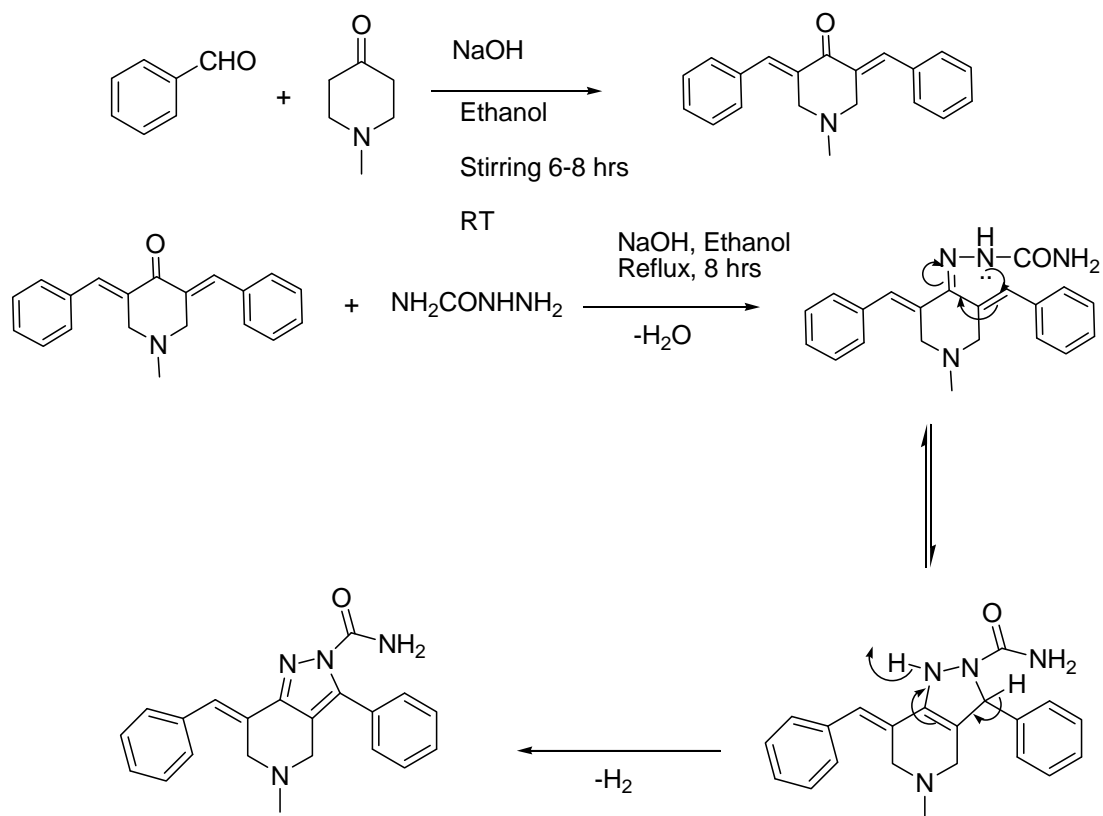


Figure. 20 Mass Spectrum of the compound 4g

The mass spectral fragmentation pattern of the pyrazolo pyridine **4j**

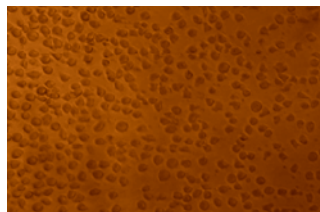


Reaction Mechanism

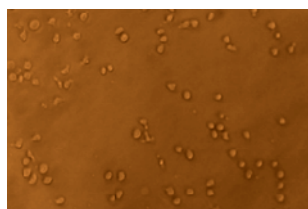


Anticancer effect of 4a on U937 cell line

Control



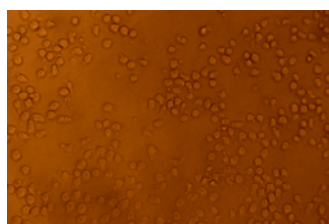
1000µg/ml



62.5µg/ml

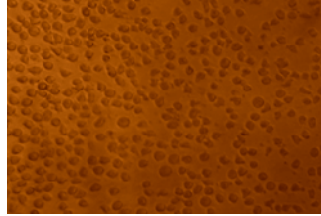


7.8µg/ml

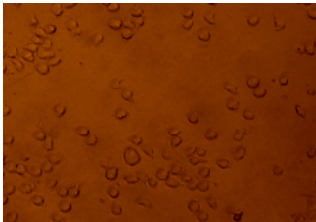


Anticancer effect of 4b on U937 cell line

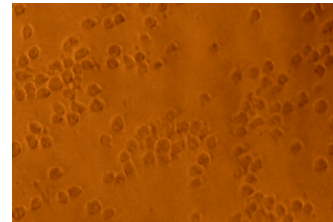
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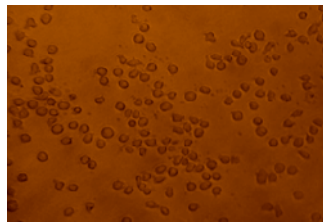
1000 μ g/ml



31.2 μ g/ml

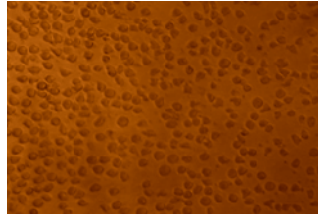


7.8 μ g/ml

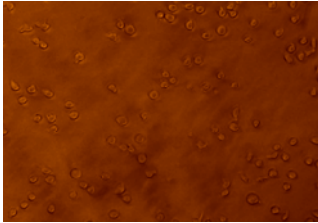


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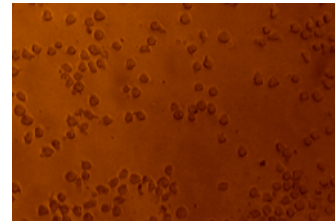
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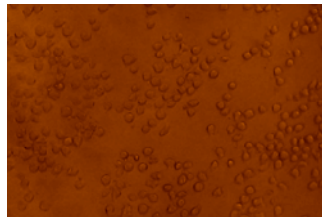
1000 μ g/ml



31.2 μ g/ml

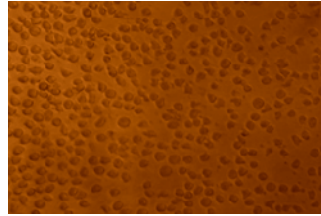


7.8 μ g/ml

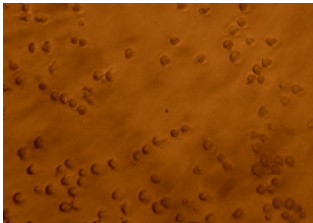


Anticancer effect of 5b on U937 cell line

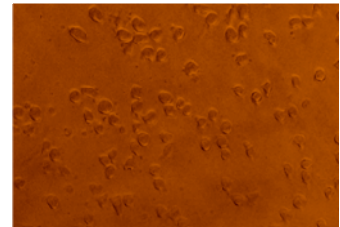
Control



1000µg/ml



62.5µg/ml



7.8µg/ml

