Supplementary Information

Synthesis of new imidazopyridine based 1,2,3-triazoles: Evaluation of antibacterial, antibiofilm and time kill studies

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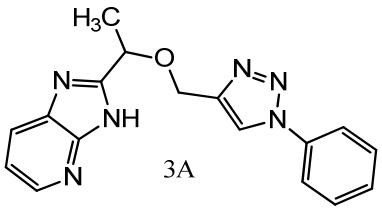
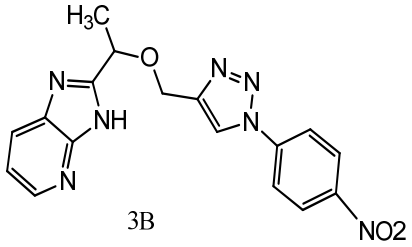


3A

2-(1-((1-phenyl-1H-1,2,3-triazol-4-yl)methoxy)ethyl)-3H-imidazo[4,5-b]pyridine (3a):

Yield : 62, (FT-IR)(KBr,cm^{-1}): 3325(-NH), 3144 (CH, triazole), 3038(CH, Ar),1595 (C=C) cm^{-1}; H^1NMR (400MHz, DMSO-d_6,δ ppm): 1.52 (d, *J*=6.45Hz ,3H,-CH_3), 3.98 (q,1H,-CH), 4.16 (s, 2H, -CH_2), 6.89-7.10 (m, 5H, Ar-H), 7.21-7.35 (m, 4H, Ar-H), 8.20 (s,1H,triazol), 9.45 (bs,1H,-NH).MS: *m/z* 320, $(M+H)^+$. Anal. Cal. for $C_{17}H_{16}N_6O$: C,63.74; H, 5.03; N, 26.23. Found: C, 63.59; H, 4.86; N, 25.91 %.

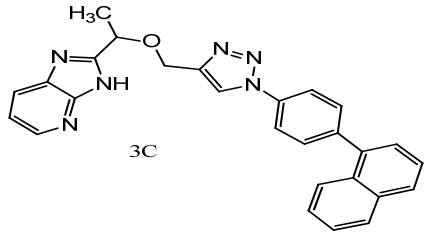
C17H16N6O



3B

2-(1-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl)methoxy)ethyl)-3H-imidazo[4,5-b]pyridine (3b):

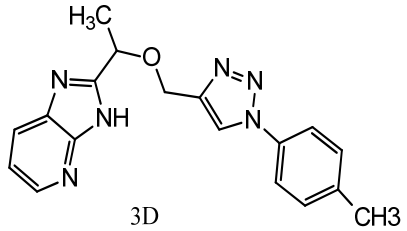
Yield : 65, FT-IR) (KBr,cm^{-1}):3367(-NH), 3132 (CH, triazole), 3069(CH, Ar), 1574(C=C) cm^{-1}; H^1NMR (400MHz, DMSO-d_6,δ ppm): 1.78 (d, *J*=4.21Hz, 3H,-CH_3), 3.98 (q,1H,-CH), 4.18 (s, 2H, -CH_2), 7.64-7.78 (m,4H, Ar-H), 7.92 (d, *J*=7.45Hz, 1H, Ar-H), 7.96 (d, *J*=7.55Hz, 1H, Ar-H), 8.04 (d, *J*=8.12Hz, 1H, Ar-H), 8.10 (d, *J*=8.23Hz, 1H, Ar-H), 8.56 (s,1H,triazol), 9.78 (bs,1H,-NH).MS: *m/z* 365, $(M+H)^+$. Anal. Cal. for $C_{17}H_{15}N_7O_3$: C, 55.89; H, 4.14; N, 26.84. Found: C, 55.44; H, 4.03;N, 26.05 %.



3C

2-(1((1-(napthalen-1-yl)-1H-1,2,3-triazol-4-yl)methoxy)ethyl)-3H-imidazo[4,5-b]pyridine (3c):

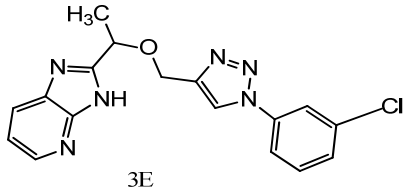
Yield :65 (FT-IR)(KBr,cm^{-1}): 3305(-NH), 3065 (CH, triazole), 3027(CH,Ar), 1556 (C=C) cm^{-1}; H^{I}NMR (400MHz, DMSO-$d_{6,}$δ ppm): 1.45 (d, *J*=4.05Hz, 3H,-CH_3), 3.67 (q,1H,-CH), 3.86 (s, 2H, -CH_2), 6.93-7.16 (m, 7H, Ar-H), 7.38-7.42 (m, 4H, Ar-H), 8.38 (s,1H,triazol), 11.05 (bs,1H,-NH).MS: *m*/*z* 370, $(M+H)^+$.Anal. Cal. for $C_{22}H_{19}N_5O$: C, 71.53; H, 5.18; N, 18.96. Found: C, 71.51; H, 5.17; N, 18.95 %.



3D

2-(1((1-(O-tolyl)-1H-1,2,3-triazol-4-yl)methoxy)ethyl)-3H-imidazo[4,5-b]pyridine (3d):

Yield : 66, (FT-IR)(KBr,cm^{-1}): 3355(-NH), 3074 (CH, triazole), 3056 (CH, Ar), 1563 (C=C) cm^{-1}; H^{I}NMR (400MHz, DMSO-$d_{6,}$δ ppm): 1.53 (d, *J*=4.53Hz, 3H,-CH_3), 2.36 (s, 3H,-CH_3), 3.80 (q,1H,-CH), 4.10 (s, 2H,-CH_2), 6.80-6.95 (m, 4H, Ar-H), 7.35-7.48 (m, 4H, Ar-H), 8.10 (s,1H,triazol), 11.10 (bs,1H,-NH).MS: *m*/*z* 334, $(M+H)^+$. Anal.Cal.for $C_{18}H_{18}N_6O$:C,64.66; H, 5.43; N,25.13.Found:C,64.43;H,5.23;N,24.90 %.

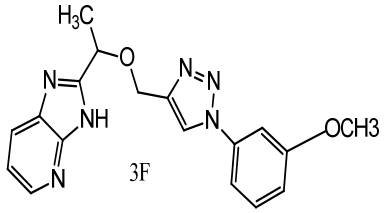


3E

2-(1-((1-(3-chlorophenyl)-1H-1,2,3-triazol-4-yl)methoxy)ethyl)-3H-imidazo[4,5-b] pyridine (3e):

Yield : 67 (FT-IR)(KBr,cm^{-1}): 3367 (-NH), 3112 (CH, triazole), 3086 (CH, Ar), 1595 (C=C) cm^{-1}; H^{I}NMR (400MHz, DMSO-$d_{6,}$δ ppm): 1.78 (d, *J*=6.45Hz, 3H,-CH_3), 3.90 (q,1H,-CH), 4.22 (s, 2H, -CH_2), 7.30-7.42 (m, 3H, Ar-H), 7.63-7.72 (d, 4H, Ar-H),7.76 (s,1H,Ar-H), 8.56 (s,1H,triazol), 11.46 (bs,1H,-NH).MS: *m*/*z* 354,$(M+H)^+$.

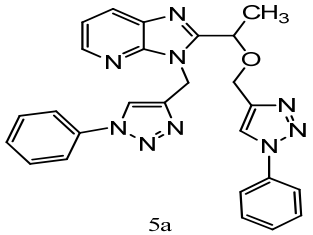
Anal. Cal. for $C_{17}H_{15}ClN_6O$: C, 57.55; H, 4.26; N, 23.69. Found: C, 57.25; H, 4.16; N, 23.34 %.



3F

2-(1-((1-(3-methoxyphenyl)-1H-1,2,3-triazol-4-yl)methoxy)ethyl)-3H-imidazo[4,5-b] pyridine (3f):

Yield : 68 (FT-IR)(KBr,cm^{-1}): 3326 (-NH), 3105 (CH, triazole), 3078 (CH,Ar), 1583 (C=C) cm^{-1}; H^INMR (400MHz, DMSO-d_6,δ ppm): 1.63 (d, *J*=5.67Hz, 3H,-CH_3),3.80 (s,3H,-OCH_3) 3.89 (q,1H,-CH), 4.10 (s, 2H, -CH_2), 7.32-7.43 (m, 3H, Ar-H), 7.46 (s, 1H, Ar-H), 7.52-7.63 (m, 4H, Ar-H), 8.46 (s,1H,triazol), 11.05 (bs,1H,-NH).MS: *m*/*z* 350,$(M+H)^+$. Anal. Cal. for $C_{18}H_{18}N_6O_2$: C, 61.70; H, 5.18; N, 23.99. Found: C, 61.32; H, 5.07; N, 22.62 %.

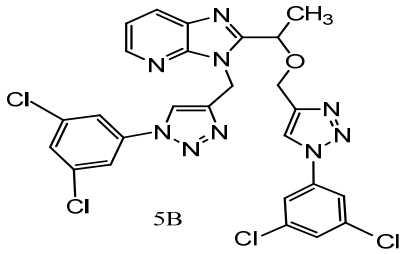


5a

2-(1-((1-phenyl-1H-1,2,3-triazol-4-yl)methoxy)ethyl)-3-((1-phenyl-1H-1,2,3-triazol-4-yl) methyl)-3H-imidazo[4,5-b]pyridine (5a):

Yield : 73.(FT-IR) (KBr,cm^{-1}): 3123 (CH, triazole), 3017 (CH, Ar), 2925(C-H) 1565 (C=N),1032(N-N)cm^{-1}; H^INMR (400MHz, DMSO-d_6,δ ppm): 1.56 (d, *J*= 3.65Hz, 3H,-CH_3), 4.32 (q,1H,-CH), 4.55 (s, 2H, -CH_2), 4.78 (s, 2H, -CH_2), 7.12-7.32 (m,5H,Ar-H), 7.38-7.53 (m,5H,Ar-H),7.56-7.68 (m,4H, Ar-H), 8.17 (s,1H,triazol), 8.21 (s,1H,triazol). MS: *m*/*z* 477, $(M+H)^+$. Anal. Cal. for $C_{26}H_{23}N_9O$: C, 65.40; H, 4.85; N,26.40. Found: C, 65.03; H, 4.68; N, 26.20 %.

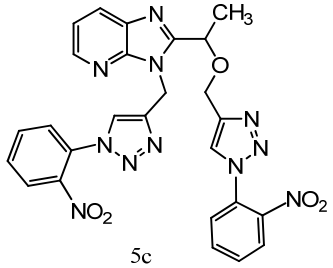
2-(1-((1-(3,5-dichlorophenyl)-1H-1,2,3,-triazol-4-yl)methoxy)ethyl)-3-((1-(3,5-dichloro phenyl) -1H-1,2,3-triazol-4-yl)methyl)- 3H-imidazo[4,5-b]pyridine (5b):



5B

Yield :71 (FT-IR) (KBr,cm^{-1}): 3169 (CH, triazole), 3063 (CH, Ar), 1597 (C=N),745(C-Cl) cm^{-1}; H^{I}NMR (400MHz, DMSO-$d_{6,}$δ ppm): 1.78 (d, *J*= 4.45Hz, 3H,-CH_3), 4.50 (q,1H,-CH), 4.62 (s, 2H, -CH_2), 4.89 (s, 2H, -CH_2), 7.30-7.43 (m,4H, Ar-H), 7.47 (s,1H, Ar-H), 7.56 (s,1H, Ar-H), 7.60 (s,1H, Ar-H), 7.65 (s, 1H, Ar-H), 7.72 (s,1H, Ar-H), 7.78 (s,1H, Ar-H), 8.38 (s,1H,triazol), 8.42 (s,1H,triazol). MS: *m*/*z* 613 $(M+H)^+$, 615(M+2), Anal. Cal. for $C_{26}H_{19}Cl_4N_9O$: C, 50.75; H, 3.11; N,20.49. Found: C, 50.68; H, 3.08; N, 19.93 %.

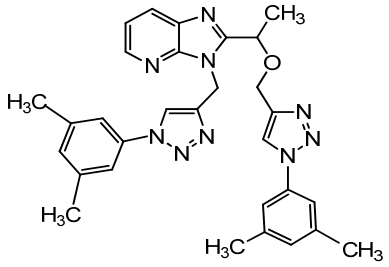
2-(1-((1-(2-nitrophenyl)-1H-1,2,3,-triazol-4-yl)methoxy)ethyl)-3-((1-(2-nitrophenyl)-1H-1,2,3-triazol-4-yl)methyl)- 3H-imidazo[4,5-b]pyridine (5c):



5c

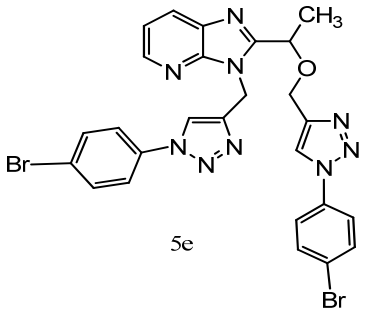
Yield :72 (FT-IR) (KBr,cm^{-1}): 3167 (CH, triazole), 3071 (CH, Ar),2853(C-H) 1598 (C=N) cm^{-1}; H^{I}NMR (400MHz, DMSO-$d_{6,}$δ ppm): 1.61 (d, *J*= 4.34Hz, 3H,-CH_3), 4.55 (q,1H,-CH),4.62(s,2H,-CH_2),4.65(s,2H,-CH_2),7.45-7.56(m,4H,Ar-H),7.63-7.74 (5H, Ar-H),7.76-7.86 (m,4H,Ar-H),8.35(s,1H,triazol), 8.39 (s,1H,triazol). MS:*m*/*z*567, $(M+H)^+$. Anal. Cal. for $C_{26}H_{21}N_{11}O_5$: C, 55.03; H, 3.73; N, 27.15. Found: C, 54.84; H, 3.55; N, 26.72%.

2-(1-((1-(3,5-dimethylphenyl)-1H-1,2,3,-triazol-4-yl) methoxy) ethyl)-3-((1-(3,5-dimethyl phenyl) -1H-1,2,3-triazol-4-yl)methyl)- 3H-imidazo[4,5-b]pyridine (5d):



Yield : 70, (FT-IR) (KBr,cm^{-1}): 3114 (CH, triazole), 3046 (CH, Ar), 1556 (C=C) cm^{-1}; H^{I}NMR (400MHz, DMSO-d_6,δ ppm): 1.52 (d, *J*= 3.52Hz, 3H,-CH_3), 2.32 (s, 3H,-CH_3), 2.34 (s, 3H,-CH_3), 2.41 (s, 3H,-CH_3), 2.44 (s, 3H,-CH_3), 4.48 (q,1H,-CH), 4.52 (s, 2H, -CH_2), 4.56 (s, 2H, -CH_2), 6.95 (s,1H, Ar-H), 7.15 (s,1H, Ar-H), 7.20 (s,1H, Ar-H), 7.25 (s,1H, Ar-H), 7.28 (s,1H, Ar-H), 7.35 (s,1H, Ar-H), 7.42-7.53 (m,4H, Ar-H), 8.22 (s,1H,triazol), 8.31 (s,1H,triazol). MS: *m*/*z* 533 $(M+H)^{+}$. Anal. Cal. for $C_{30}H_{31}N_9O$: C, 67.52; H, 5.86; N, 23.62. Found: C, 67.38; H, 5.55; N, 23.42 %.

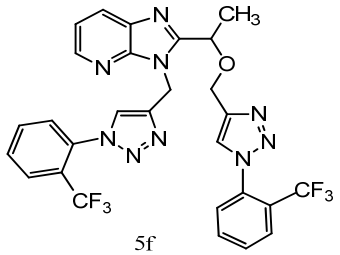
2-(1-((1-(4-bromophenyl)-1H-1,2,3,-triazol-4-yl)methoxy)ethyl)-3-((1-(4-bromophenyl)-1H-1,2,3-triazol-4-yl)methyl)- 3H-imidazo[4,5-b]pyridine (5e):



5e

Yield : 68, (FT-IR) (KBr,cm^{-1}): 3154 (CH, triazole), 3078 (CH, Ar), 1567 (C=C) cm^{-1}; H^{I}NMR (400MHz, DMSO-d_6,δ ppm): 1.82(d, *J*= 3.12Hz, 3H,-CH_3), 3.92 (q,1H,-CH), 4.18 (s, 2H, -CH_2), 4.84 (s, 2H, -CH_2), 7.61-7.72(m,4H, Ar-H),7.81(d, *J*=7.13Hz, 1H, Ar-H), 7.92 (d,*J*=7.26 Hz, 1H,Ar-H),8.02(d,*J*=7.31Hz, 1H, Ar-H), 8.12 (d, *J*=7.89Hz, 1H, Ar-H), 8.22 (d, *J*=6.14Hz, 1H, Ar-H),8.52 (s,1H,triazol), MS: *m*/*z* 633 (M+H),635(M++). Anal. Cal. for $C_{26}H_{21}Br_2N_9O$: C, 49.15; H, 3.33; N, 19.84. Found: C, 49.05; H, 3.21; N, 19.66 %.

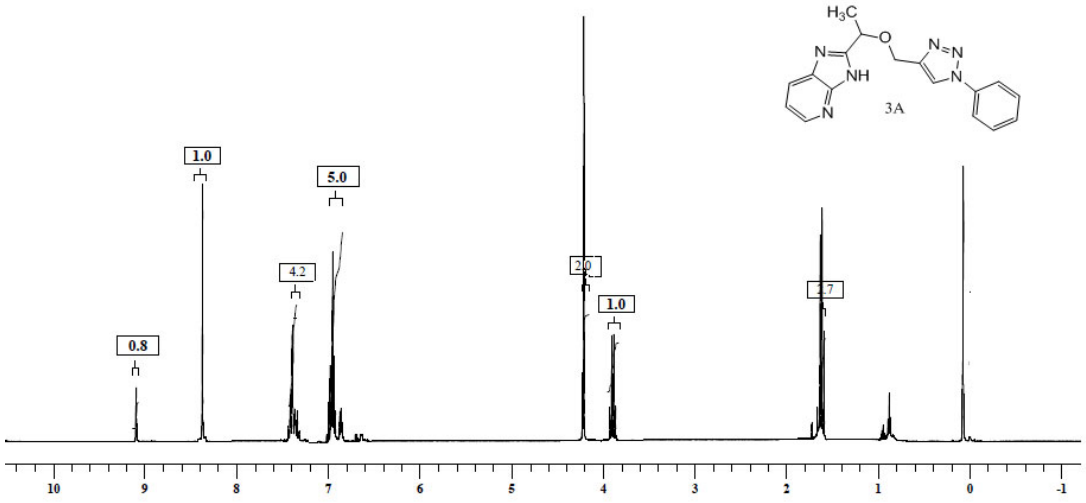
2-(1-((1-(2-(trifluoromethyl) phenyl)-1H-1,2,3,-triazol-4-yl) methoxy) ethyl)-3-((1-(2-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-4-yl)methyl)- 3H-imidazo[4,5-b]pyridine (5f):



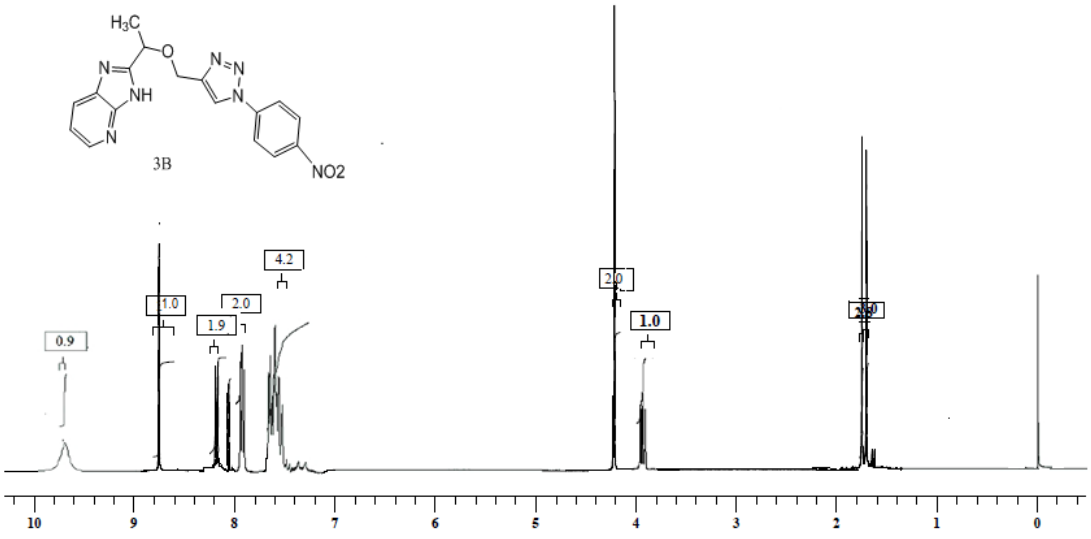
5f

Yield : 72, (FT-IR) (KBr,cm^{-1}): 3178 (CH, triazole), 3167 (CH, Ar), 1623 (C=C) cm^{-1}; H^{I}NMR (400MHz, DMSO-d_6,δ ppm): 1.82 (d, *J*= 4.02Hz, 3H,-CH_3), 4.62 (q,1H,-CH), 4.68 (s, 2H, -CH_2), 4.74 (s, 2H, -CH_2), 7.53-7.62 (m,4H, Ar-H), 7.78-7.94 (m, 8H, Ar-

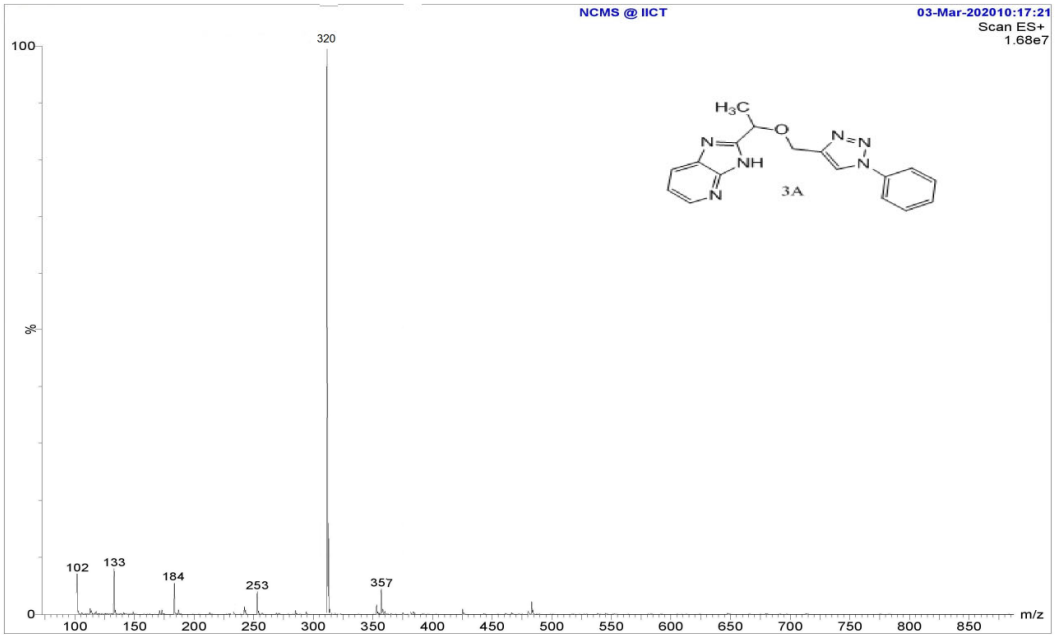
H), 8.67 (s,1H,triazol), 8.78 (s,1H,triazol). MS: *m/z* 613 $(M+H)^+$, Anal. Cal. for $C_{28}H_{21}F_6N_9O$: C, 54.82; H, 3.45; N, 20.25. Found: C, 54.55; H, 3.22; N, 19.98 %.



1HNMR Spectrum of compound 3a



1HNMR Spectrum of compound 3b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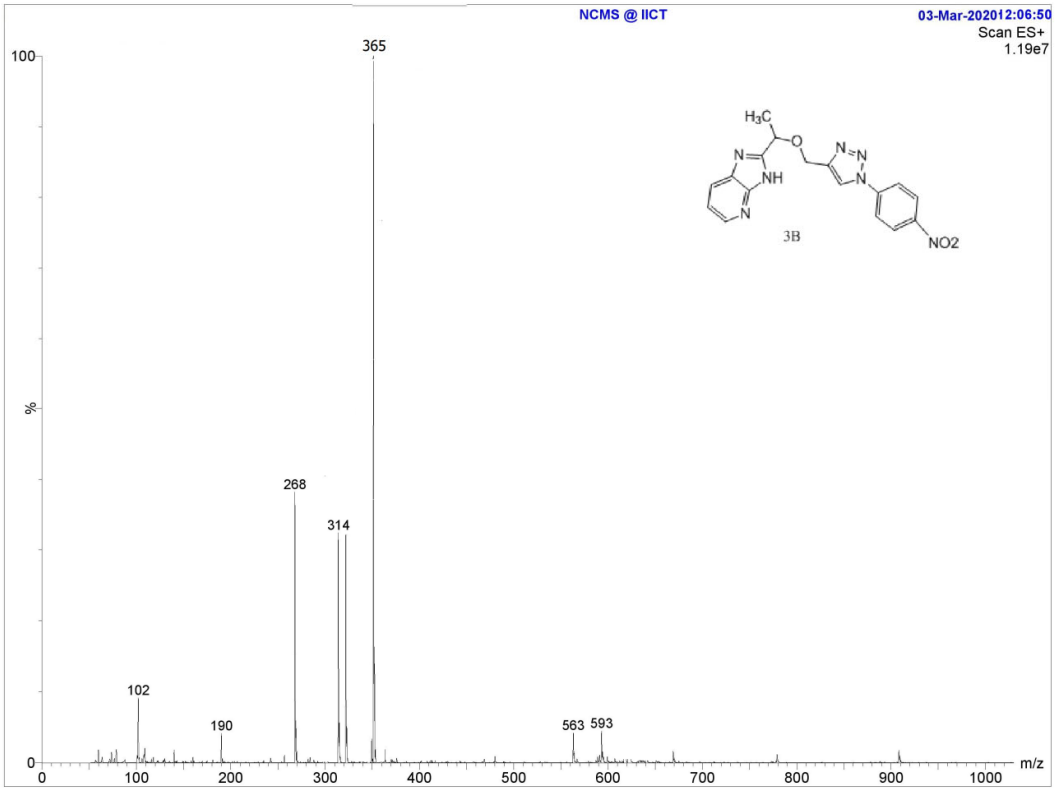
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m/z
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3B
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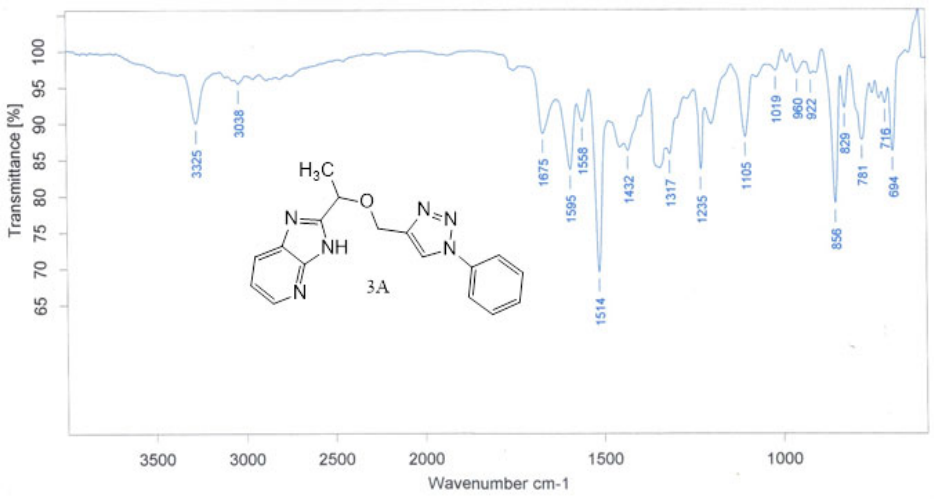
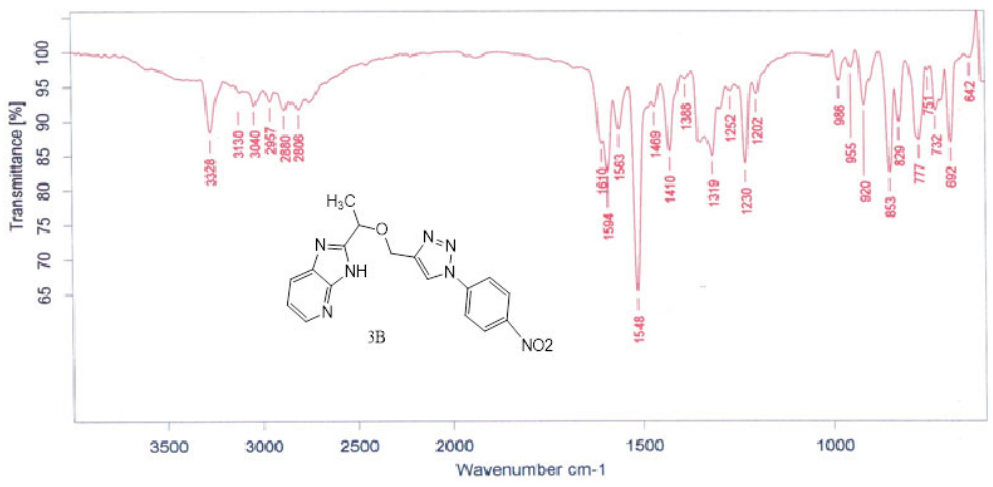
CENTRAL FACILITIES - OSMANIA UNIVERSITY

FTIR ANALYSIS REPORT



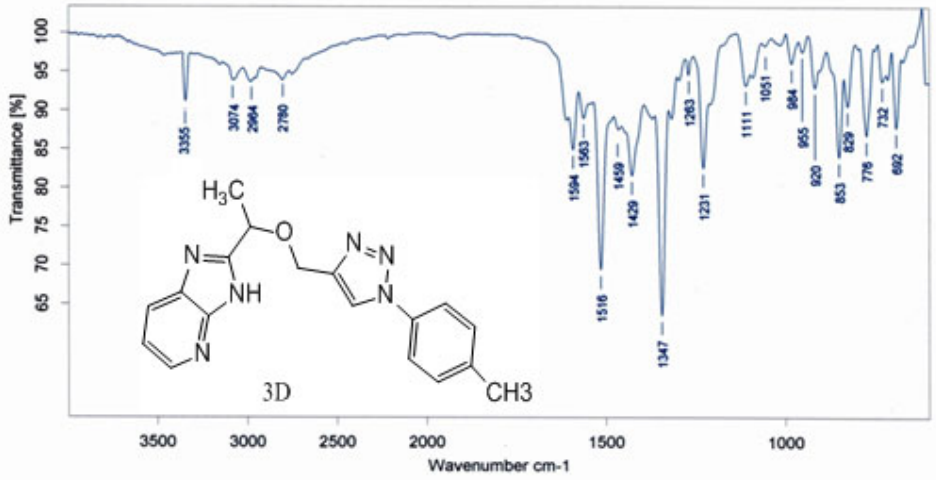
CENTRAL FACILITIES - OSMANIA UNIVERSITY

FTIR ANALYSIS REPORT



CENTRAL FACILITIES - OSMANIA UNIVERSITY

FTIR ANALYSIS REPORT



MASS REPORT

OSPC, Dr RATHOD

SHIMADZU LabSolutions

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Date Acquired	: 10/16/2020 3:17:42 PM
Batch File	: 16102020.lcb

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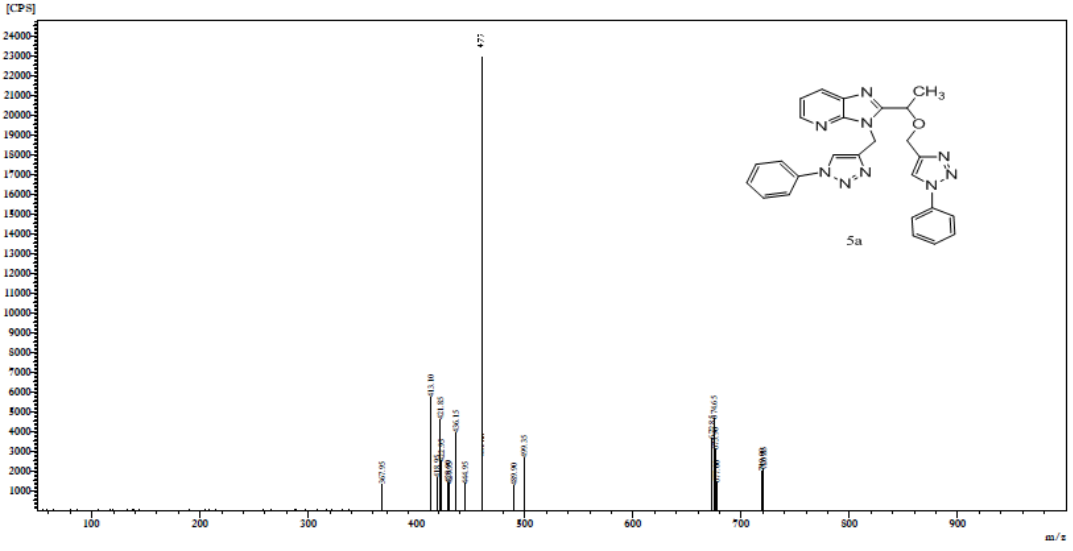

SHIMADZU
LabSolutions

MASS REPORT

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Date Acquired : 11/26/2020 1:29:08 PM
Batch File : 26112020.lcb

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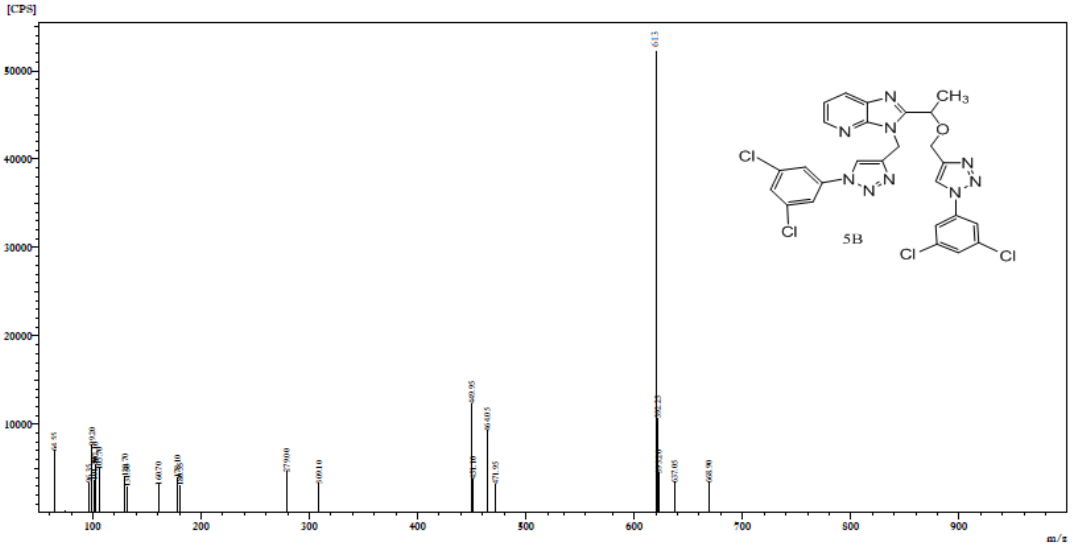

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OSPC, Dr RATHOD

SHIMADZU
LabSolutions

MASS REPORT

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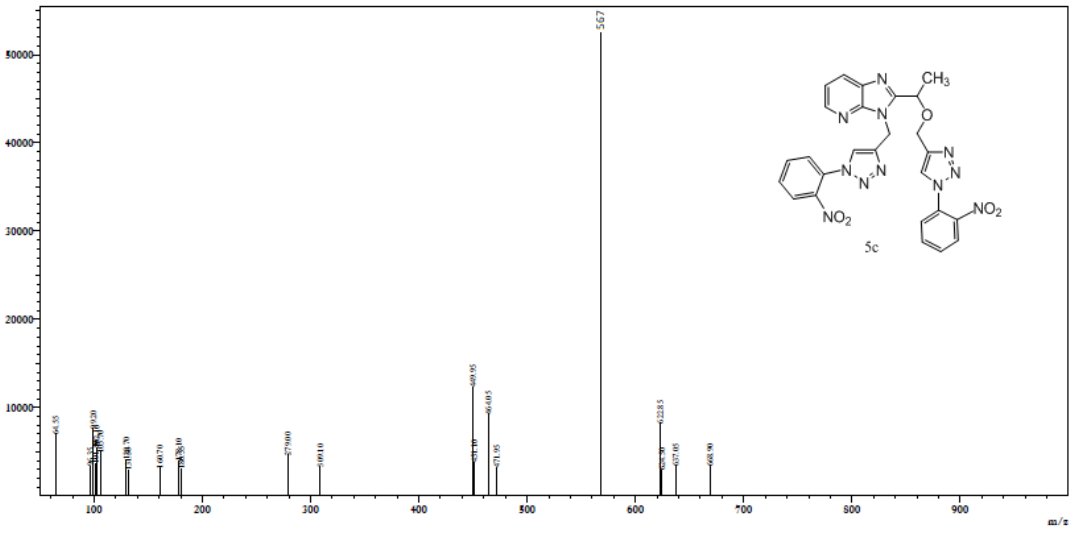

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SHIMADZU
LabSolutions

MASS REPORT

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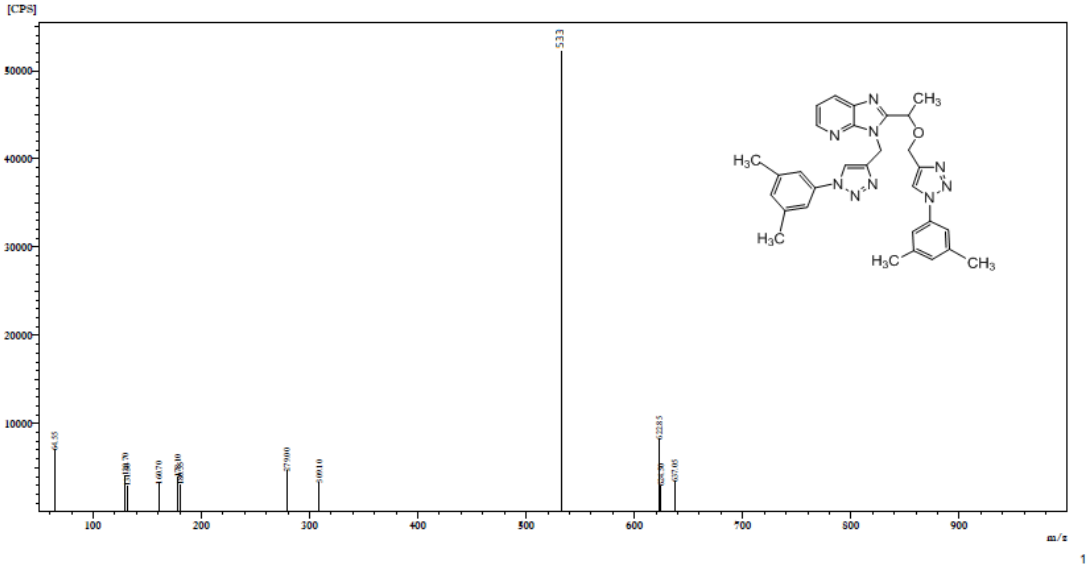
AveragedESI Positive+
Spectrum Mode:Averaged 0.378-0.966(163-415)



OSPC, Dr RATHOD

SHIMADZU
LabSolutions

MASS REPORT

Sample Name : DSB-12L-622
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Date Acquired : 11/26/2020 1:29:08 PM
Batch File : 26112020.lcb

MS Spectrum
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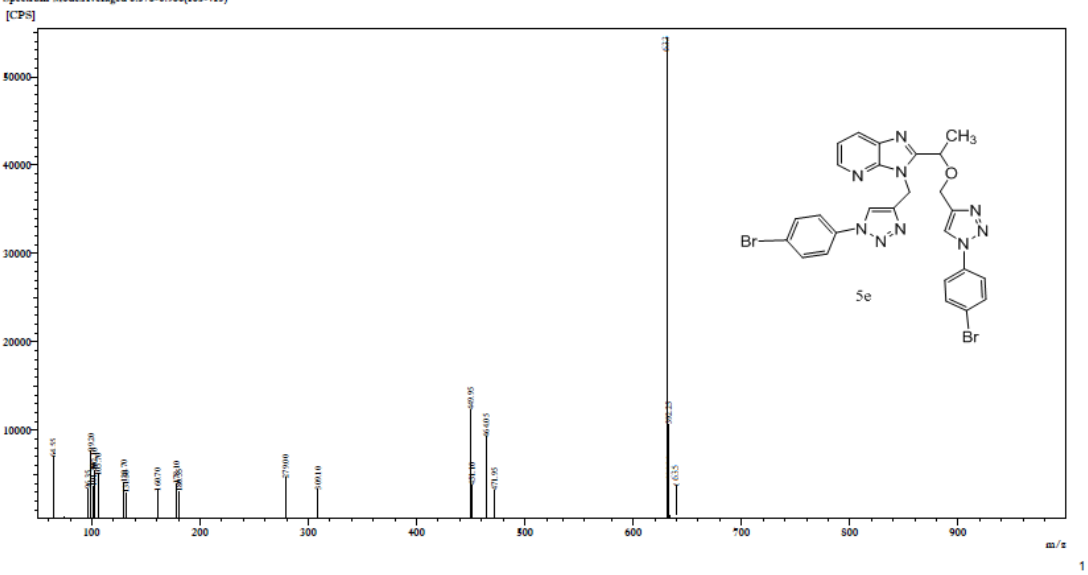
AveragedESI Positive+
Spectrum Mode:Averaged 0.378-0.966(163-415)



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SHIMADZU
LabSolutions

MASS REPORT

OSPC, Dr RATHOD

Sample Name : DSB-12L-622
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Date Acquired : 11/26/2020 3:17:42 PM
Batch File : 26112020.lcb

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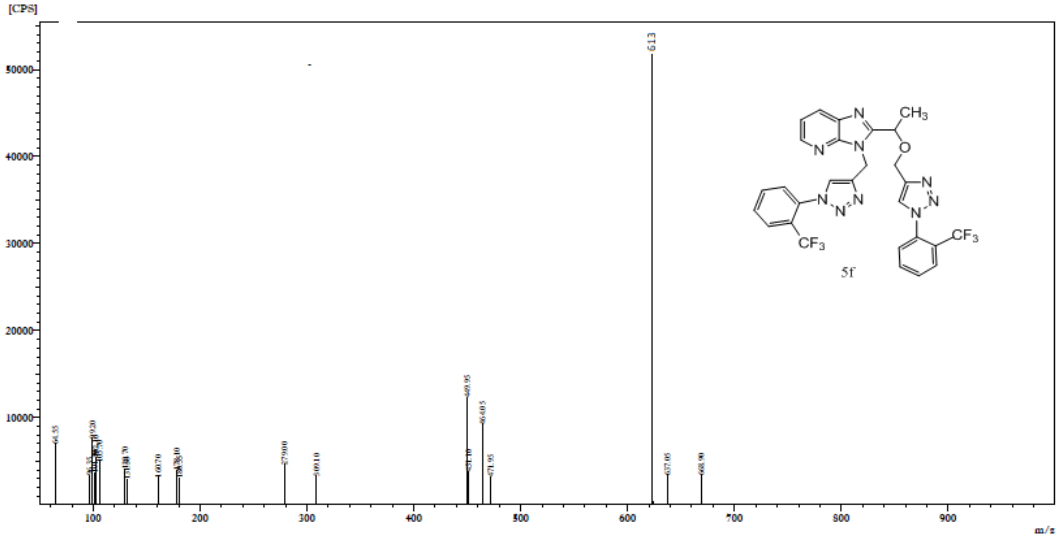
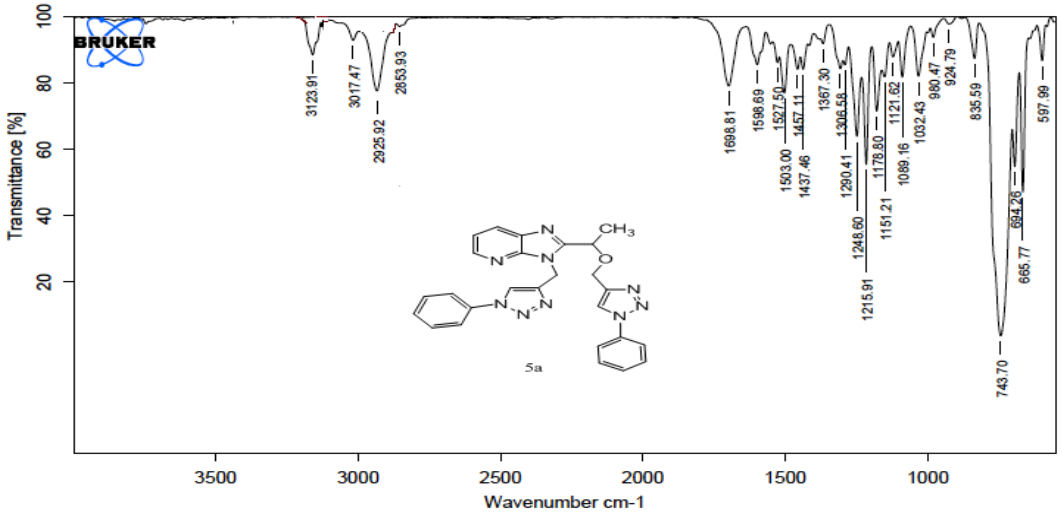
AveragedESI Positive+
Spectrum Mode:Averaged 0.378-0.966(163-415)



Indian Institute Of Chemical Technology, Hyderabad

Organic and BioMolecular Chemistry Division

FTIR Analysis Report



Sample Name:DSB-SP-OME-PURE
Sample Form:LIQUID
Collection Time:04/12/2020,6:00:13 PM
Instrument: Bruker Alpha Spectrometer.
Resolution: 4 cm-1

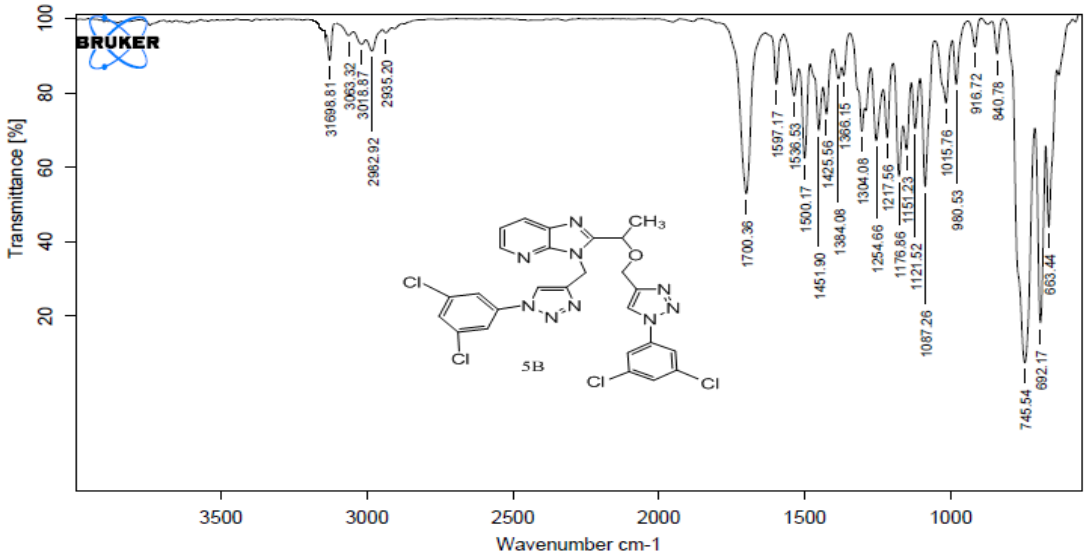
Detector:DLaTGS
Beam Splitter: ZnSe
Source:GloBar.

Analyst Name:

Indian Institute Of Chemical Technology, Hyderabad

Organic and BioMolecular Chemistry Division

FTIR Analysis Report



Sample Name:DSB-SP-H
Sample Form:LIQUID
Collection Time:04/12/2020,12:00:23 PM
Instrument: Bruker Alpha Spectrometer.
Resolution: 4 cm-1

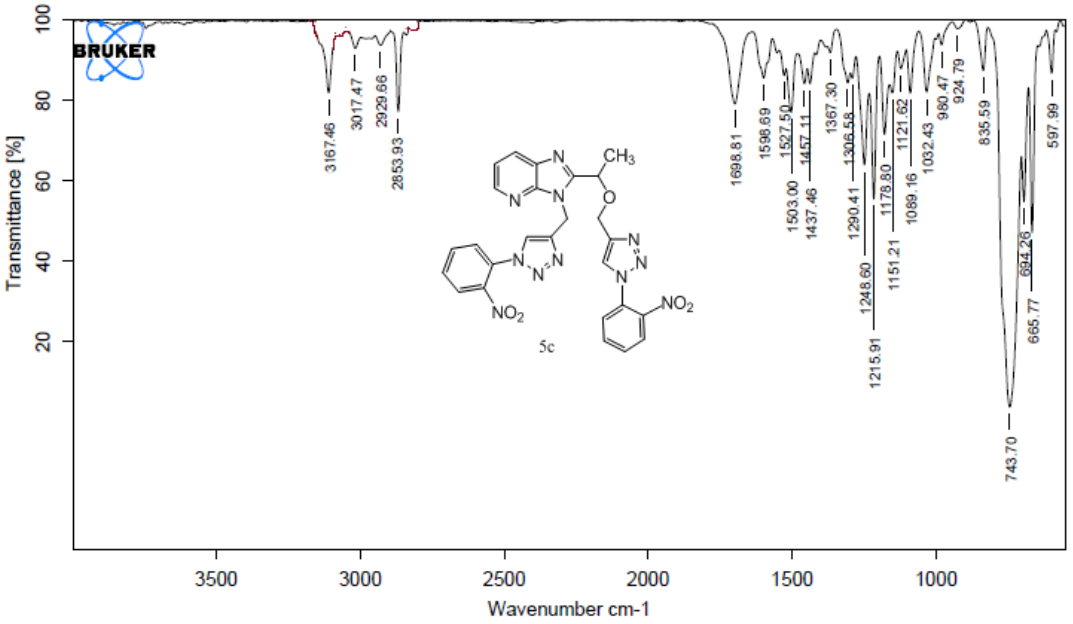
Detector:DLaTGS
Beam Splitter: ZnSe
Source:GloBar.

Analyst Name:

Indian Institute Of Chemical Technology, Hyderabad

Organic and BioMolecular Chemistry Division

FTIR Analysis Report



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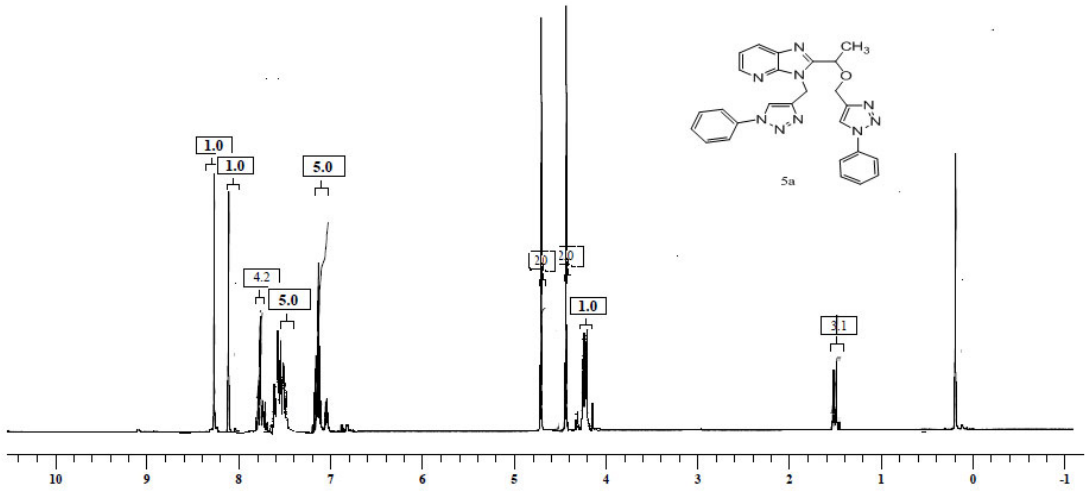
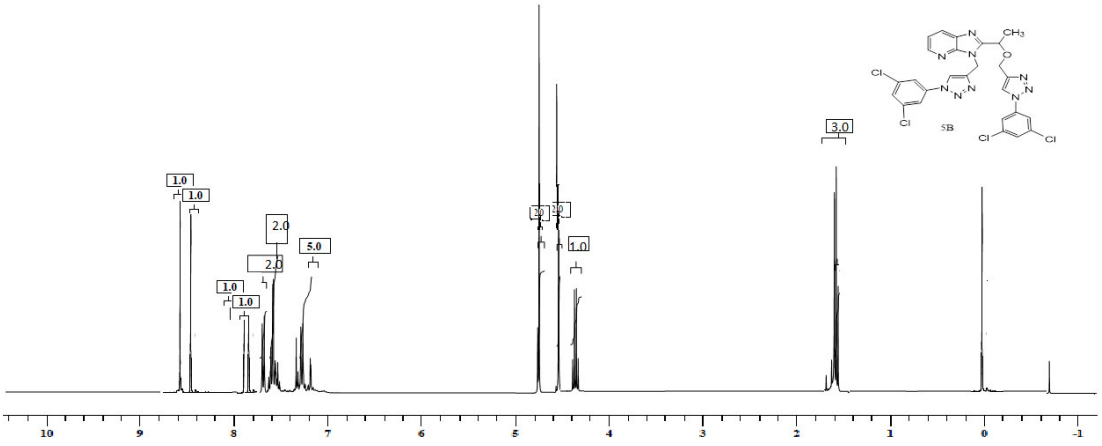
Sample Form:LIQUID
Collection Time:04/12/2020,12:00:23 PM
Instrument: Bruker Alpha Spectrometer.
Resolution: 4 cm-1

Detector:DLaTGS
Beam Splitter: ZnSe
Source:GloBar.

Analyst Name:

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1.0
1.0
2.0
2.0
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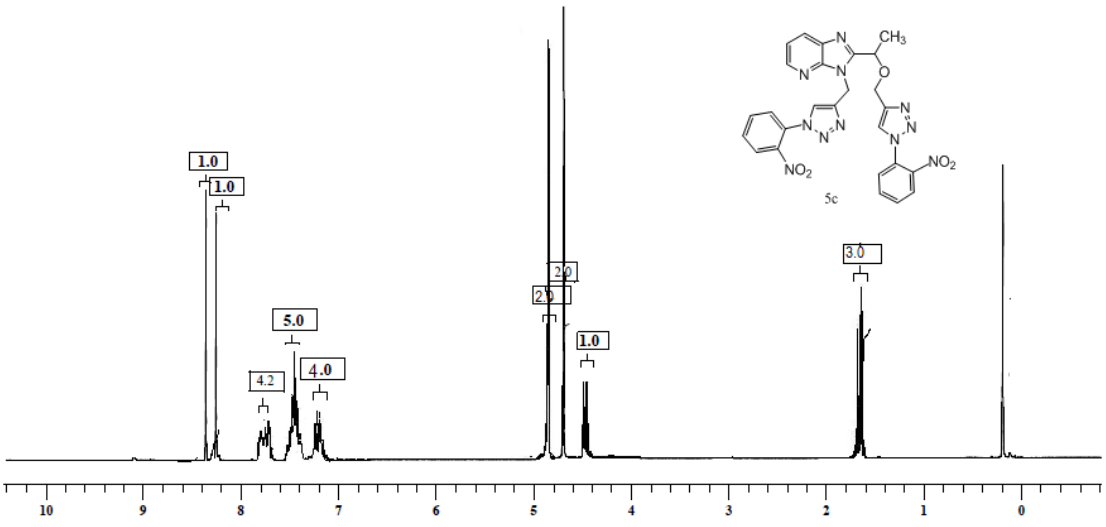
1.0
3.0
5B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5c