

Supporting Information

Synthetic Access to Diverse Thiazetidines via One-Pot Microwave Assisted Telescopic Approach and its Interaction with Biomolecules

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Abha 61413, Saudi Arabia

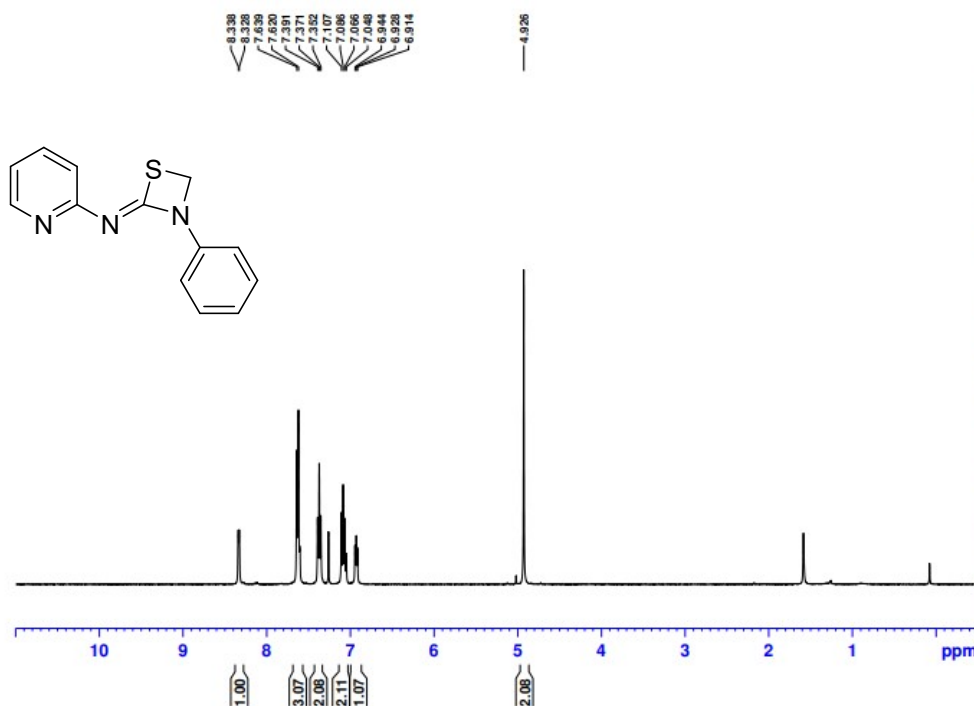
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mmbala@gmail.com

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Signature SIF VIT VELLORE
NR-118-TD-A

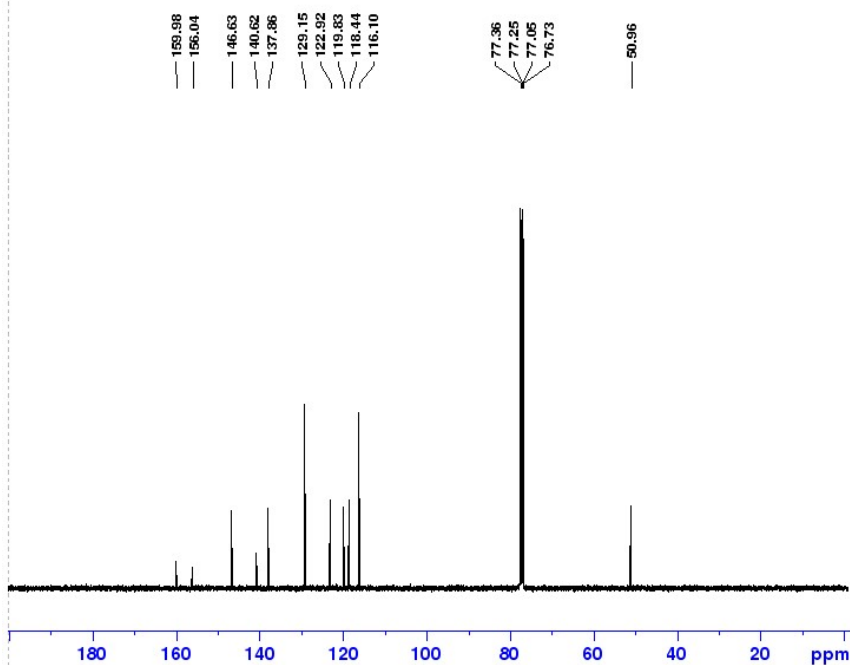


Current Data Parameters
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EXPNO 35
PROCNO 1

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TD 65536
SOLVENT CDCl3
NS 16
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FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 156.91
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DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MH
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Signature SIF VIT VELLORE
NR-118-TD-A



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EXPNO 36
PROCNO 1

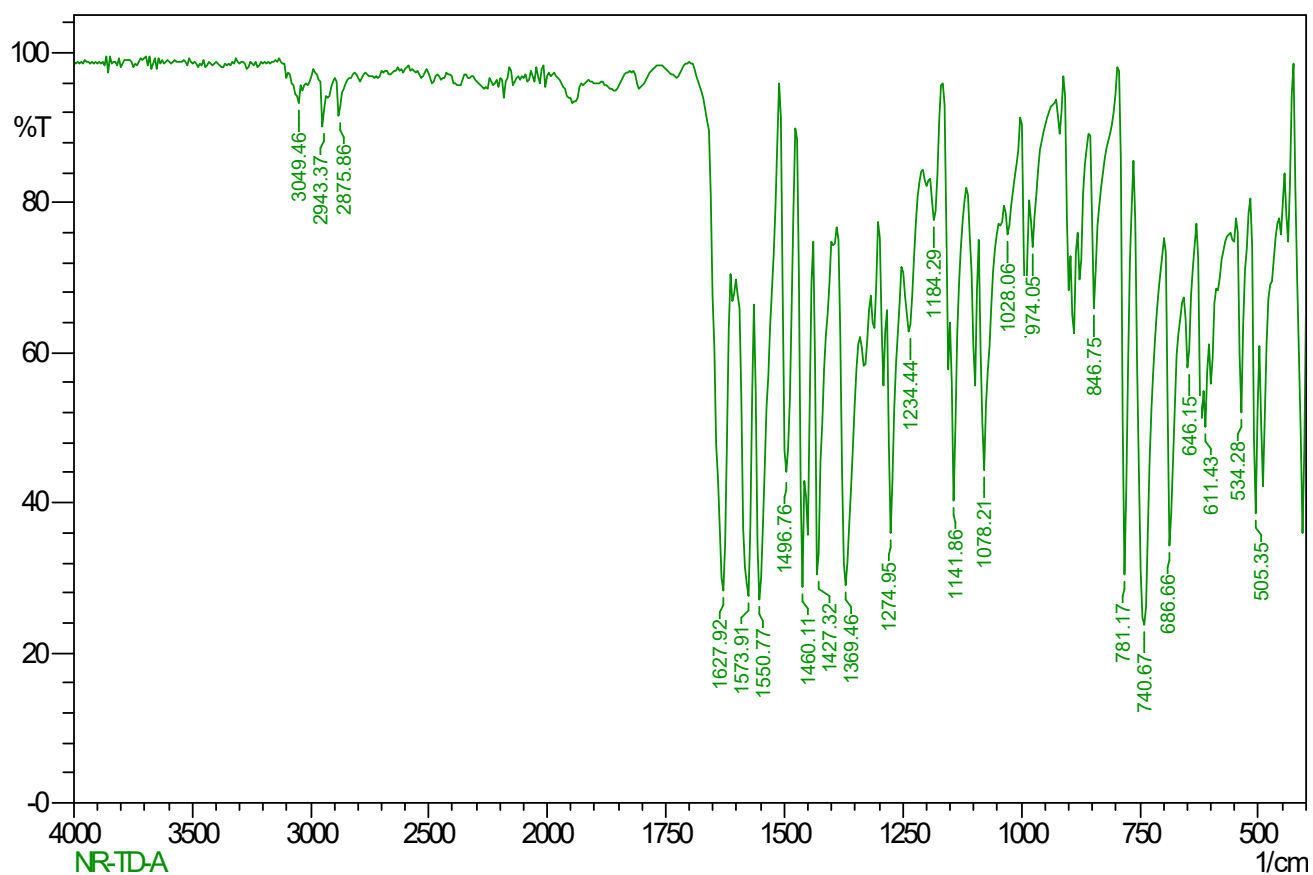
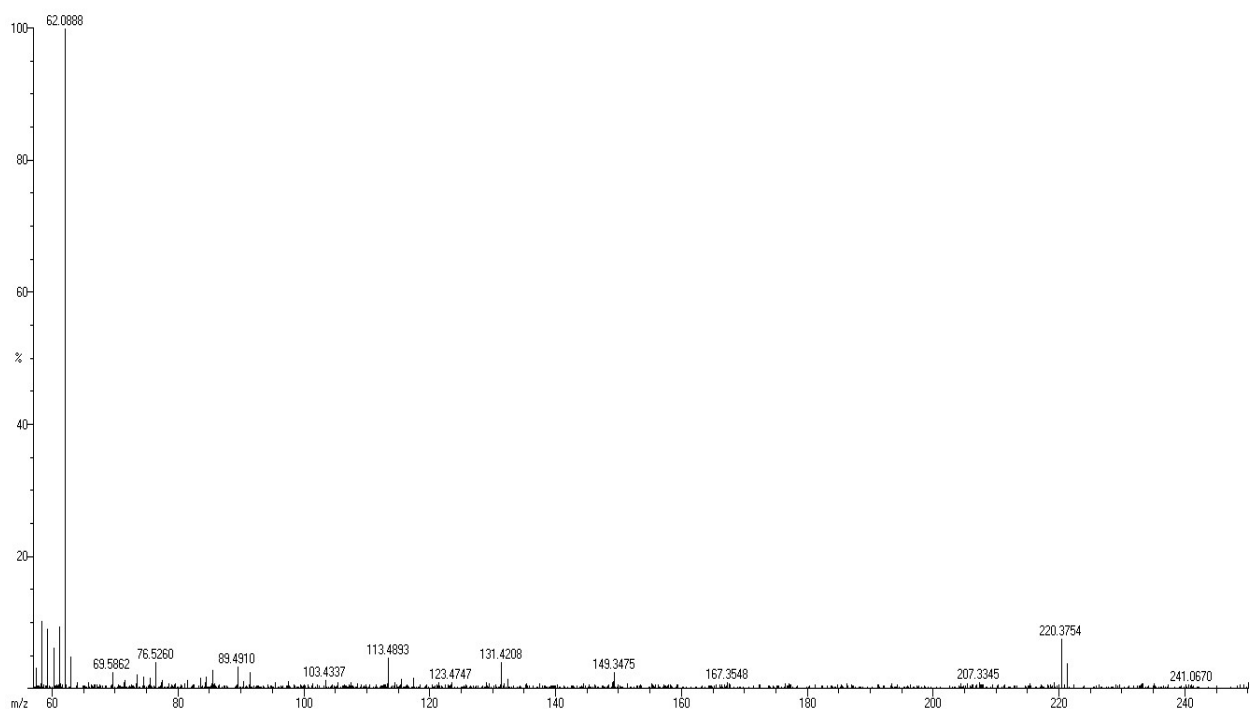
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NS 512
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SWH 24038.461 Hz
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AQ 1.3631488 sec
RG 88.69
DW 20.800 usec
DE 6.50 usec
TE 297.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
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¹H and ¹³C NMR spectra of compound 4a

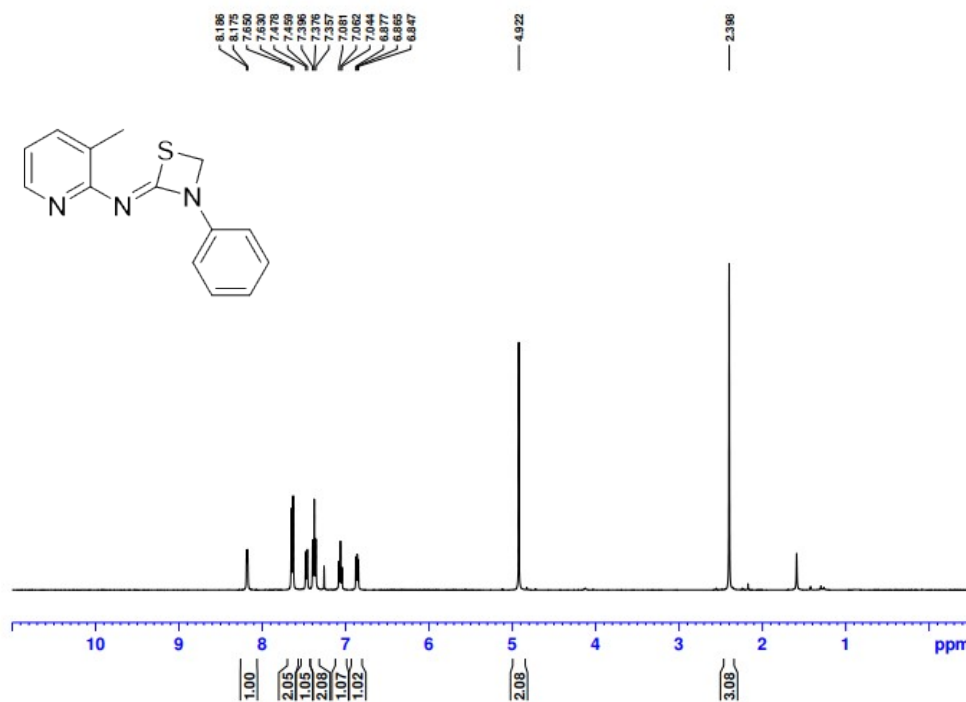
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HRMS and IR spectra compound 4a

Signature SIF VIT VELLORE
NR-TO0218-B

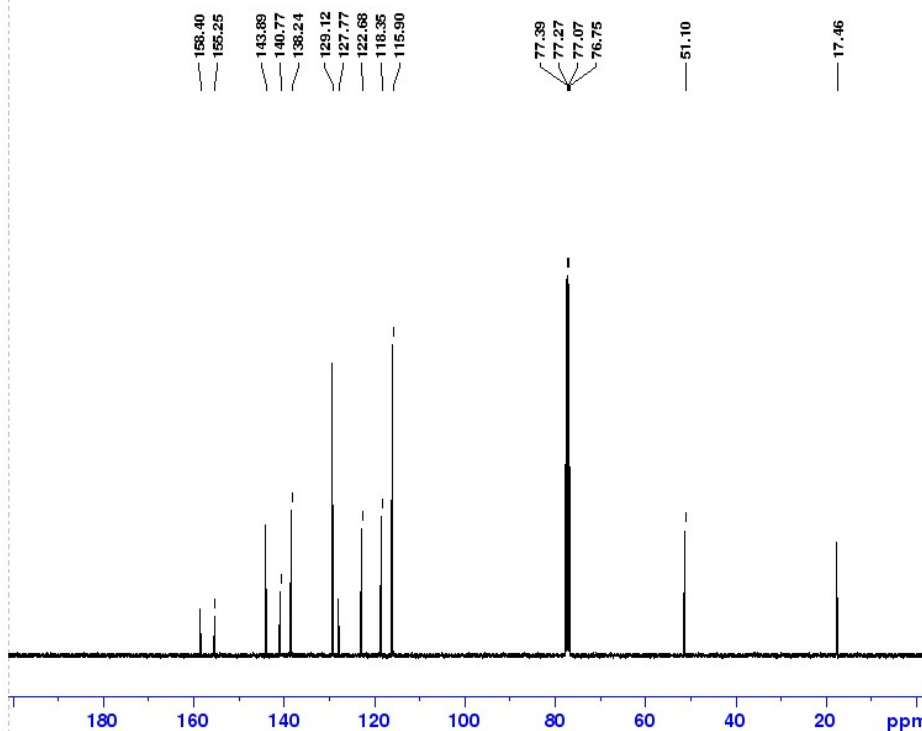


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EXPNO 19
PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 112.69
DW 62.400 usec
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TE 297.0 K
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SFO1 400.2604716 MH:
NUC1 1H
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PLW1 14.00000000 W

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Signature SIF VIT VELLORE
NR-TO0218-B



Current Data Parameters
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EXPNO 20
PROCNO 1

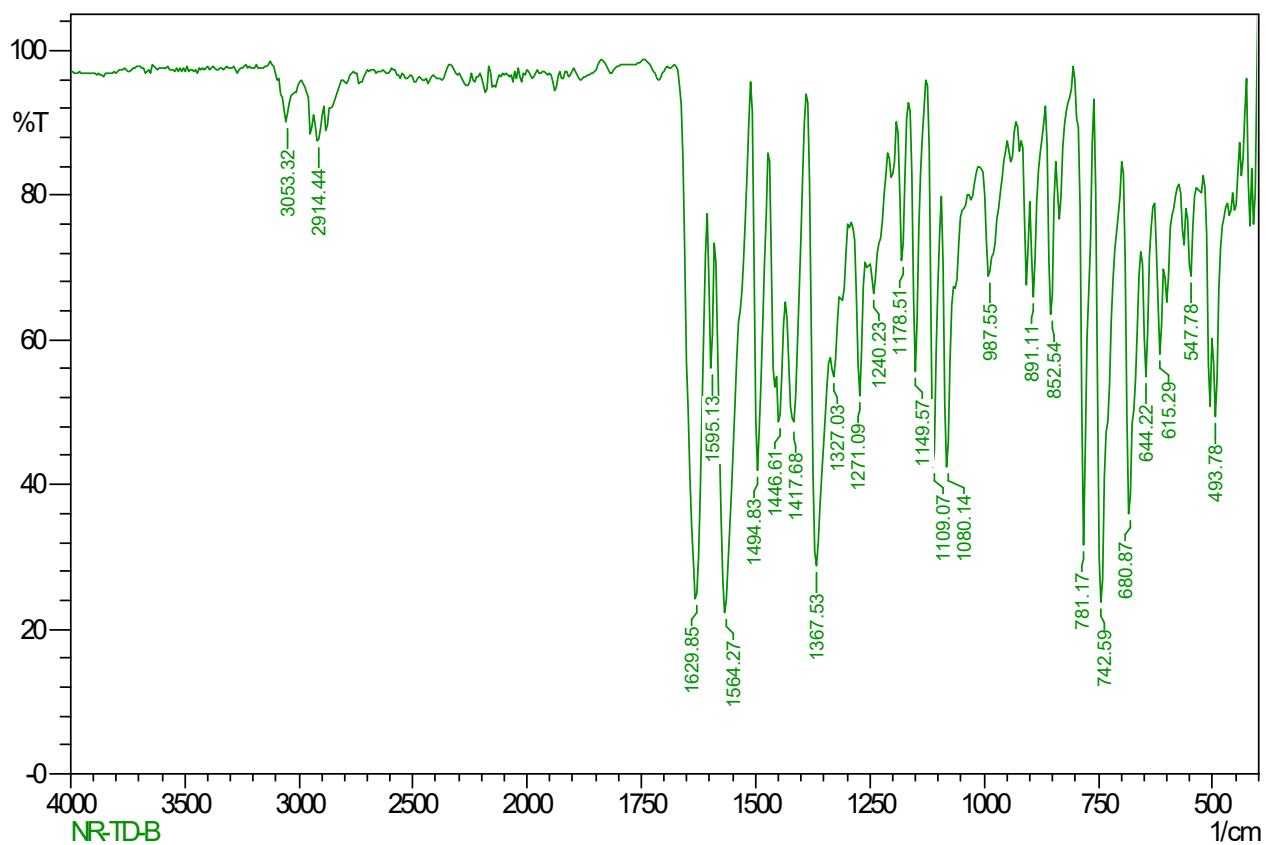
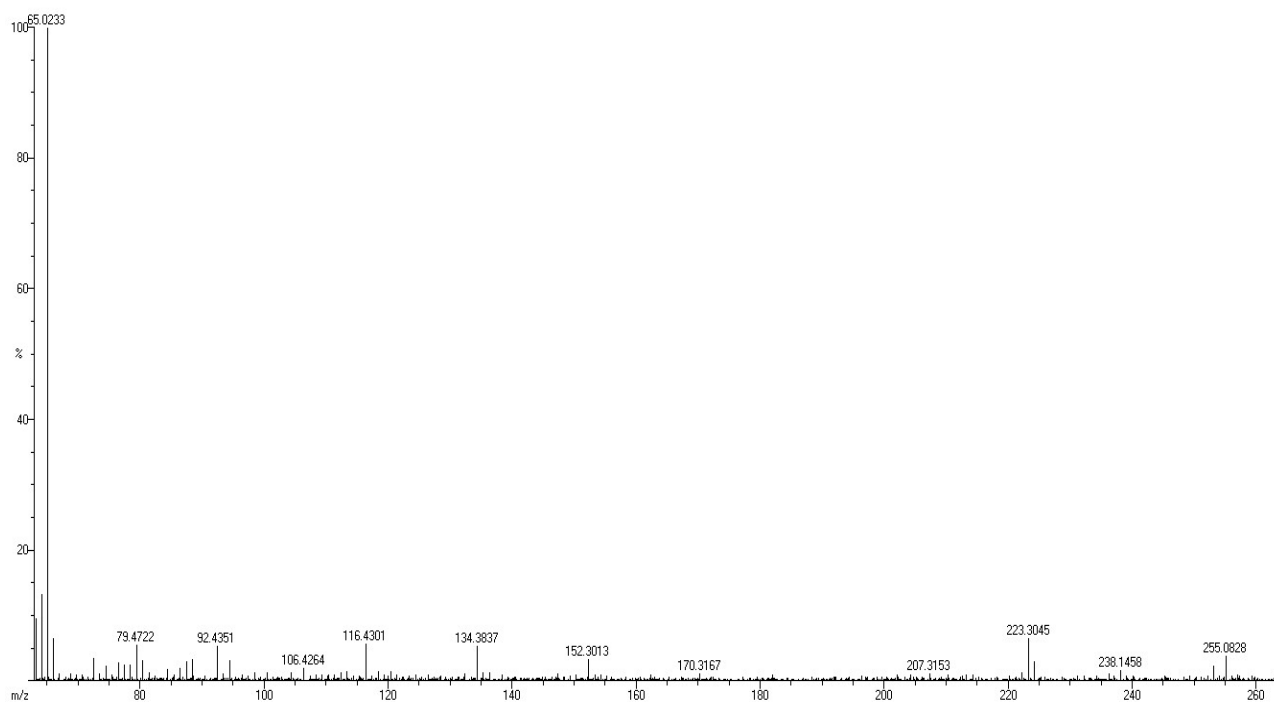
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SOLVENT CDCl3
NS 512
DS 4
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FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 77.73
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DE 6.50 usec
TE 297.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
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PLW13 0.17654000 W

F2 - Processing parameters
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¹H and ¹³C NMR spectra of compound 4b.

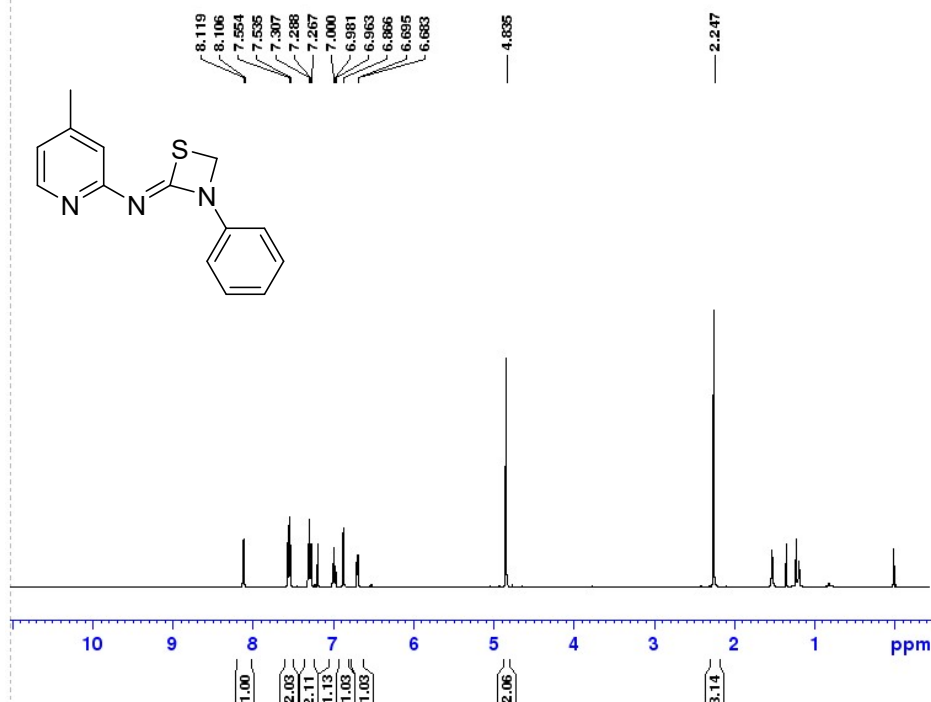
TD-8

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HRMS and IR spectra compound 4b

Signature SIF VIT VELLORE
NR-318-TD-D1

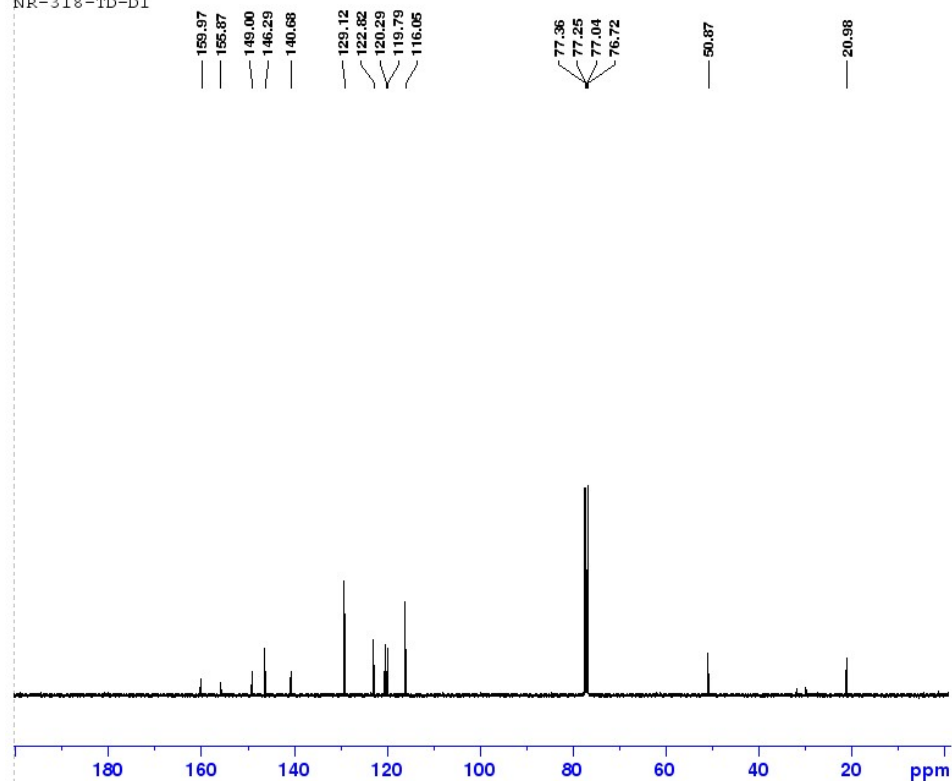


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EXPNO 20
PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 156.91
DW 62.400 usec
DE 6.50 usec
TE 298.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W

F2 - Processing parameters
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SF 400.2590401 MHz
WDW EM
SSB 0
LB 0.30 Hz
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Signature SIF VIT VELLORE
NR-318-TD-D1



Current Data parameters
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EXPNO 21
PROCNO 1

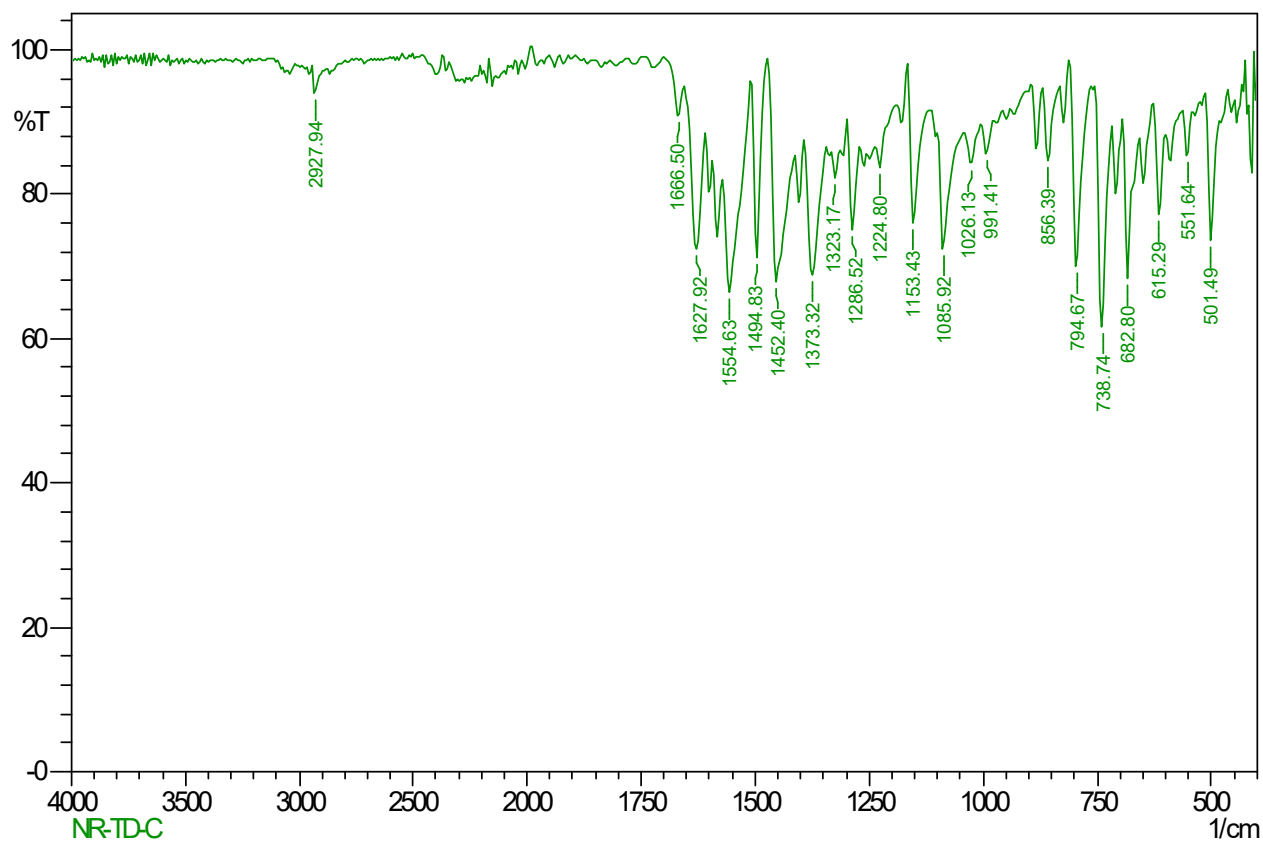
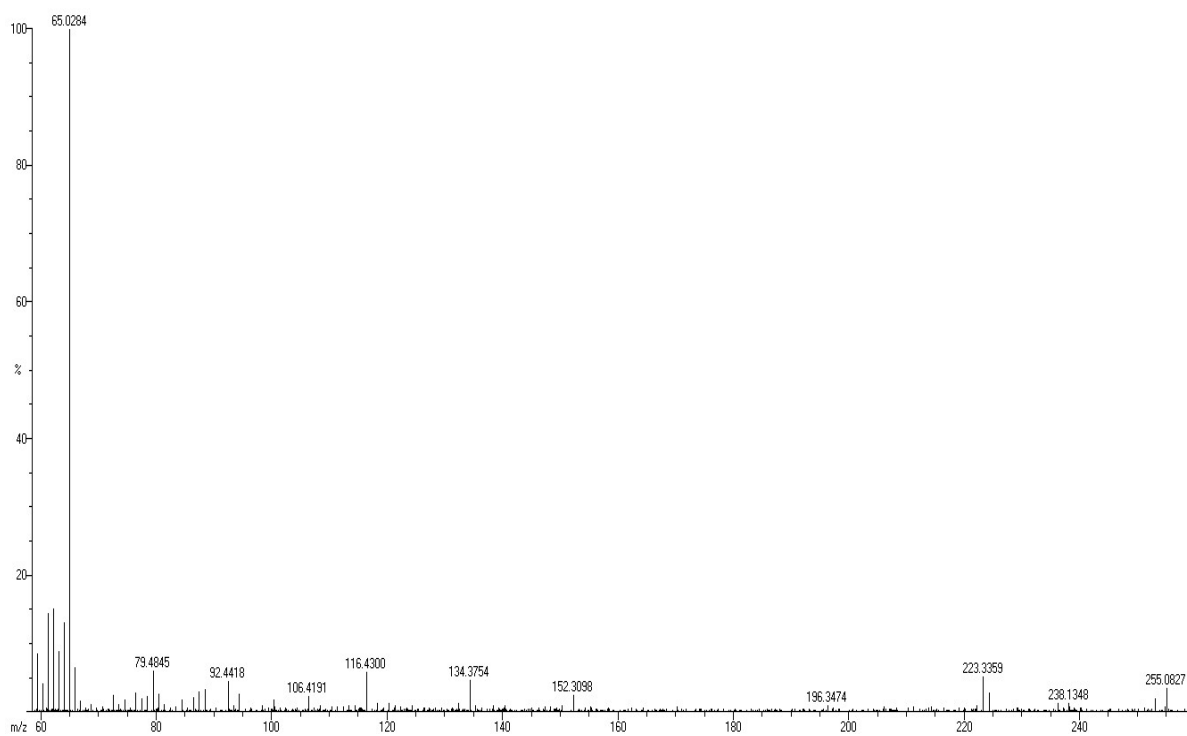
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TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 88.69
DW 20.800 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
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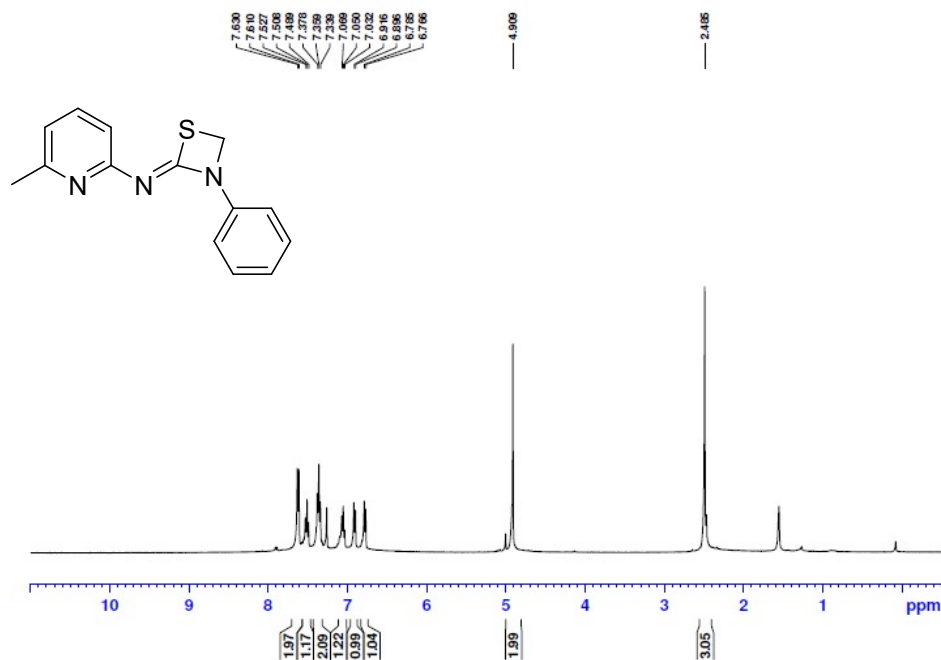
¹H and ¹³C NMR spectra of compound 4c.

TD-C

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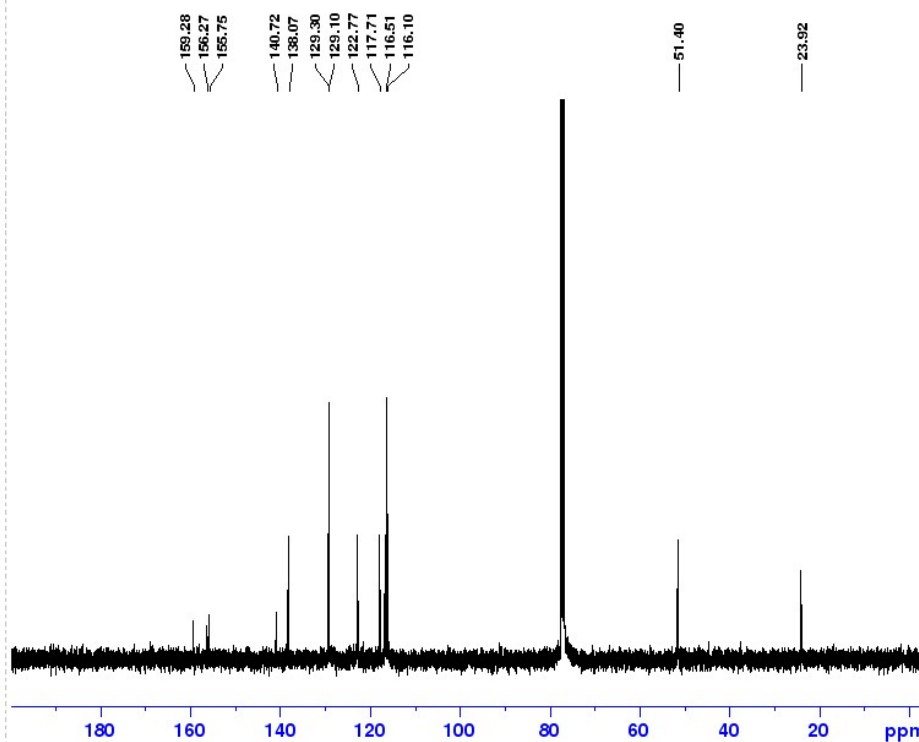
HRMS and IR spectra compound 4c.



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EXPNO 9
PROCNO 1

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Time 23.40 h
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PROBHD Z108618_0505 (Zg30)
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 175.97
DW 62.400 usec
DE 6.50 usec
TE 306.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MH
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W

F2 - Processing parameter
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NAME 6-Methyl amino pyridin
EXPNO 10
PROCNO 1

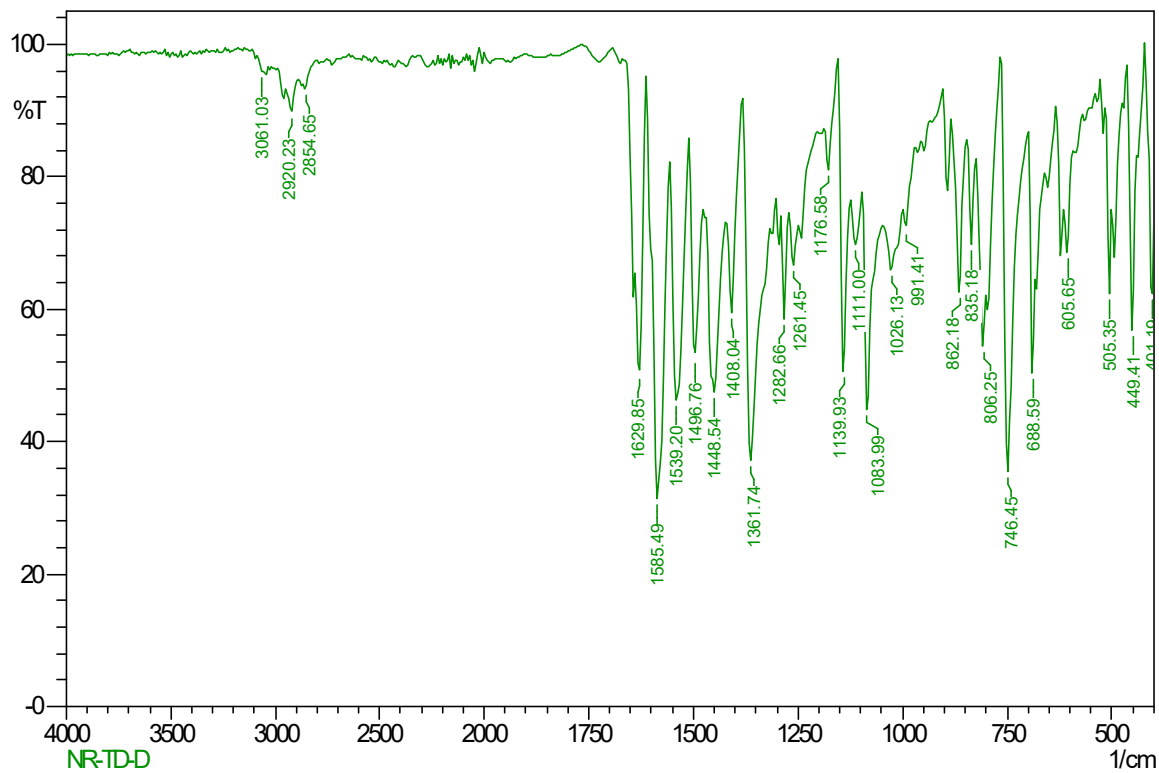
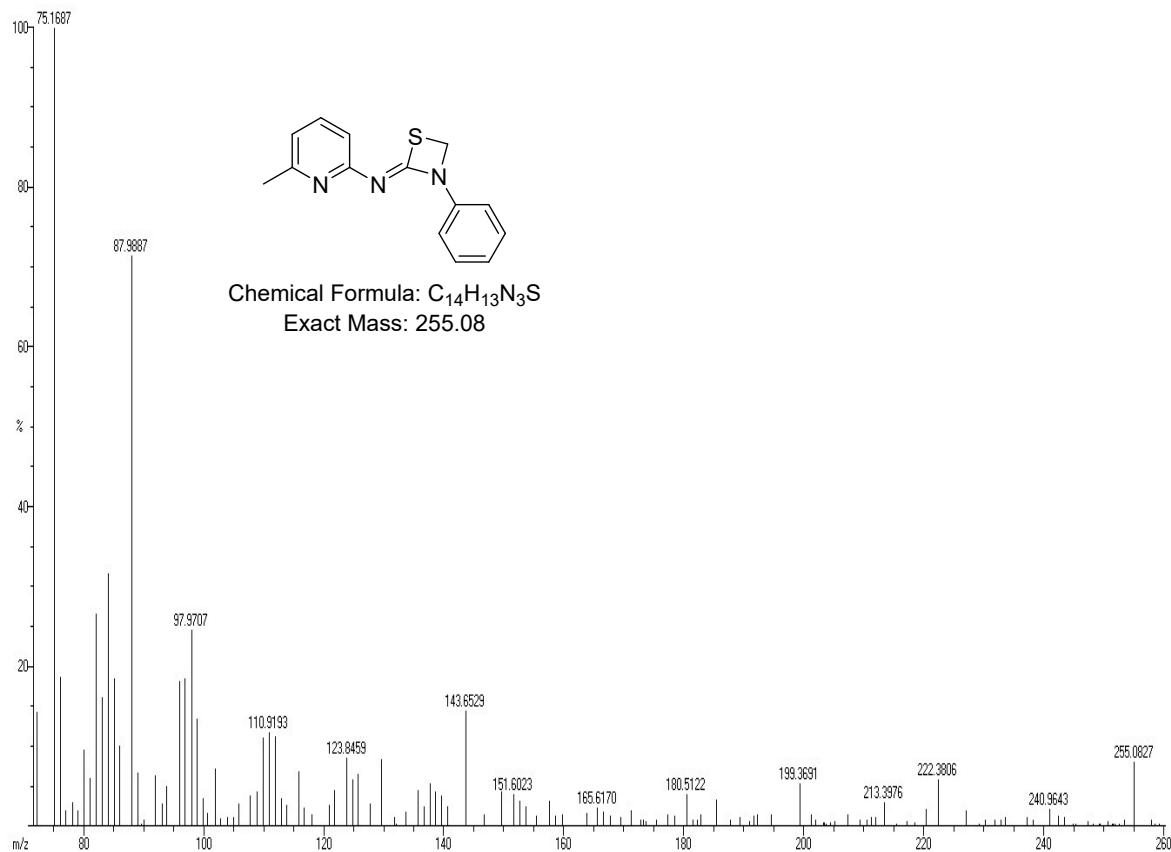
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PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 305.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.35097000 W
PLW13 0.17654000 W

F2 - Processing parameters
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PC 1.40

¹H and ¹³C NMR spectra of compound 4d.

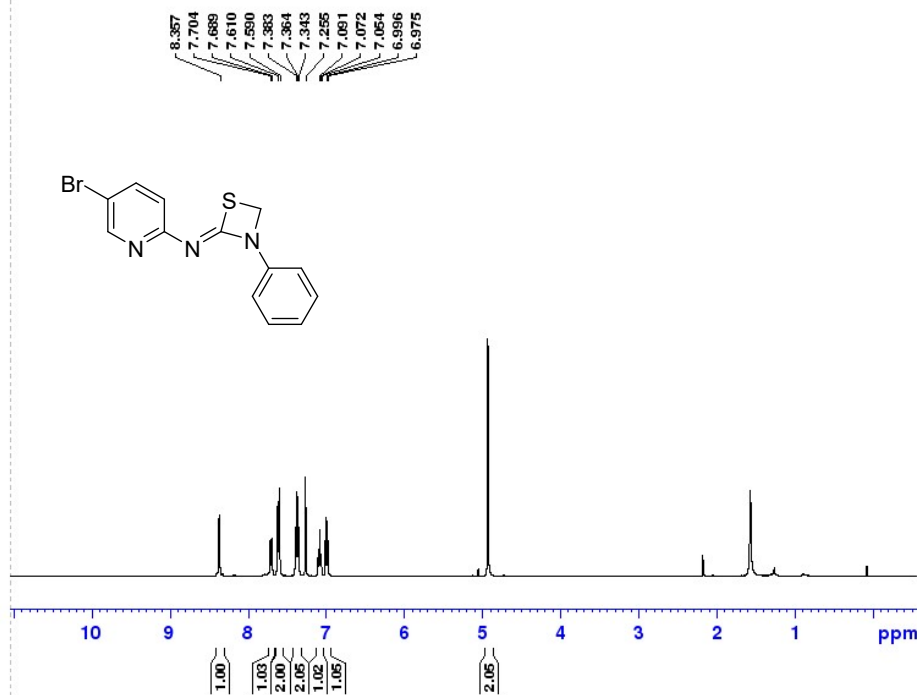
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HRMS and IR spectra compound 4d

Signature SIF VIT VELLORE
NR-318-TD-E

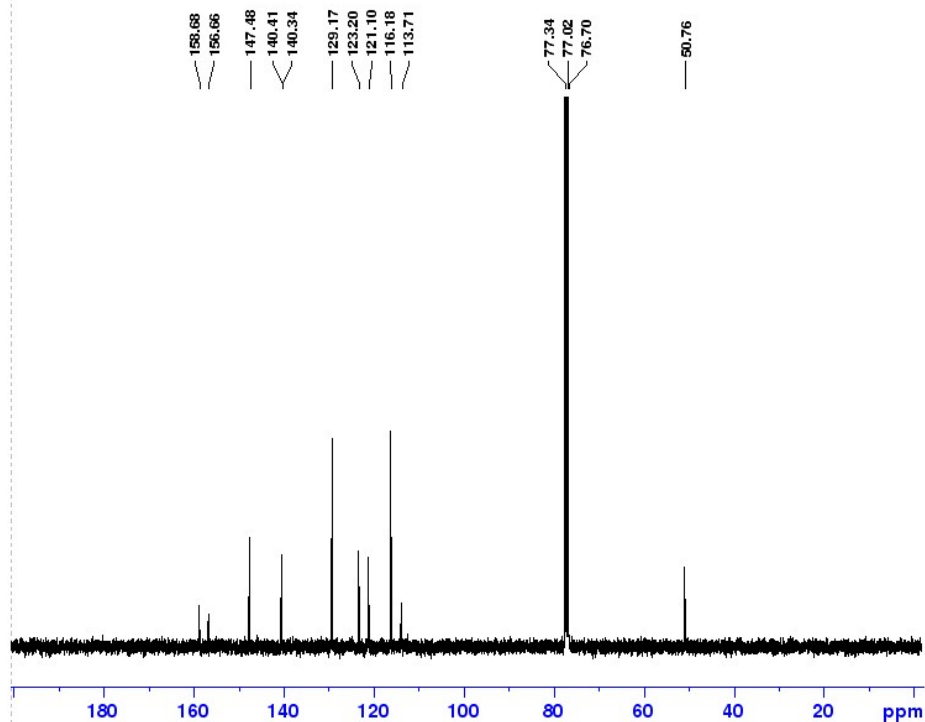


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NAME 5-Bromo-Amino Pyridi
EXPNO 24
PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 199.6
DW 62.400 usec
DE 6.50 usec
TE 300.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.25 usec
PLW1 14.0000000 W

F2 - Processing parameters
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LB 0.30 Hz
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PC 1.00

Signature SIF VIT VELLORE
NR-318-TD-E



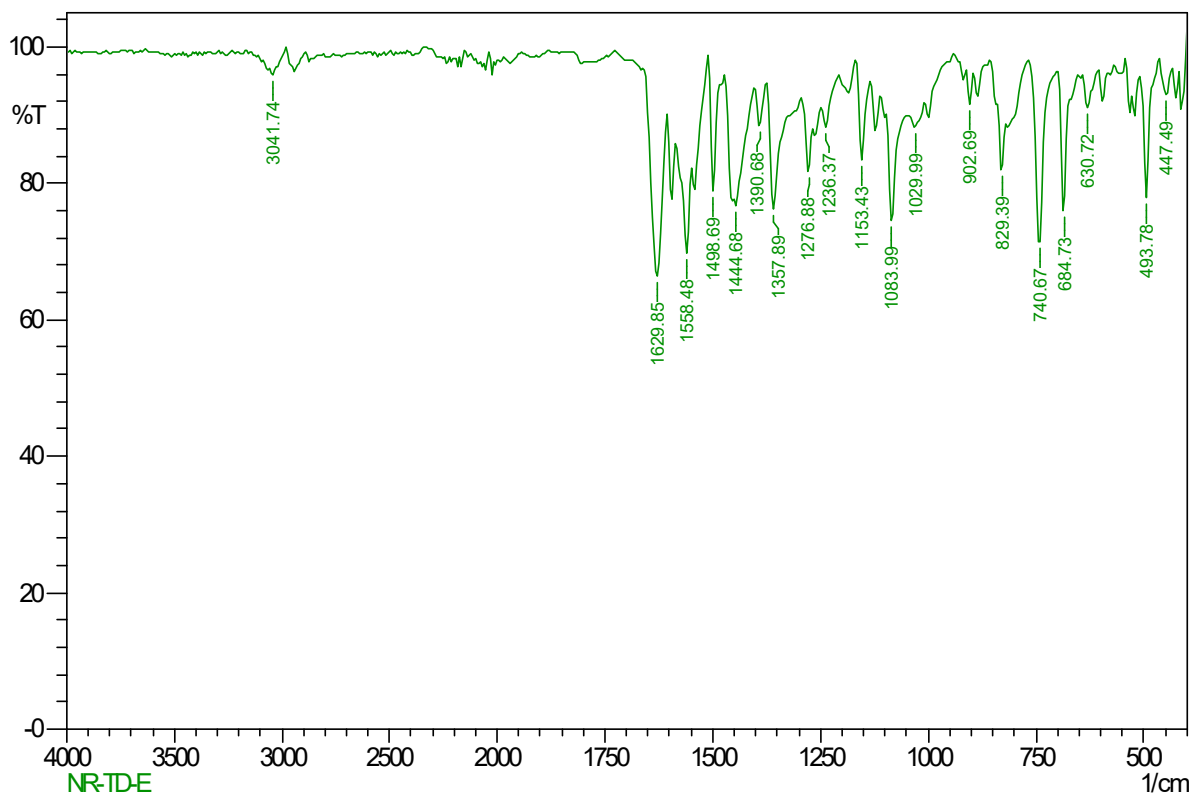
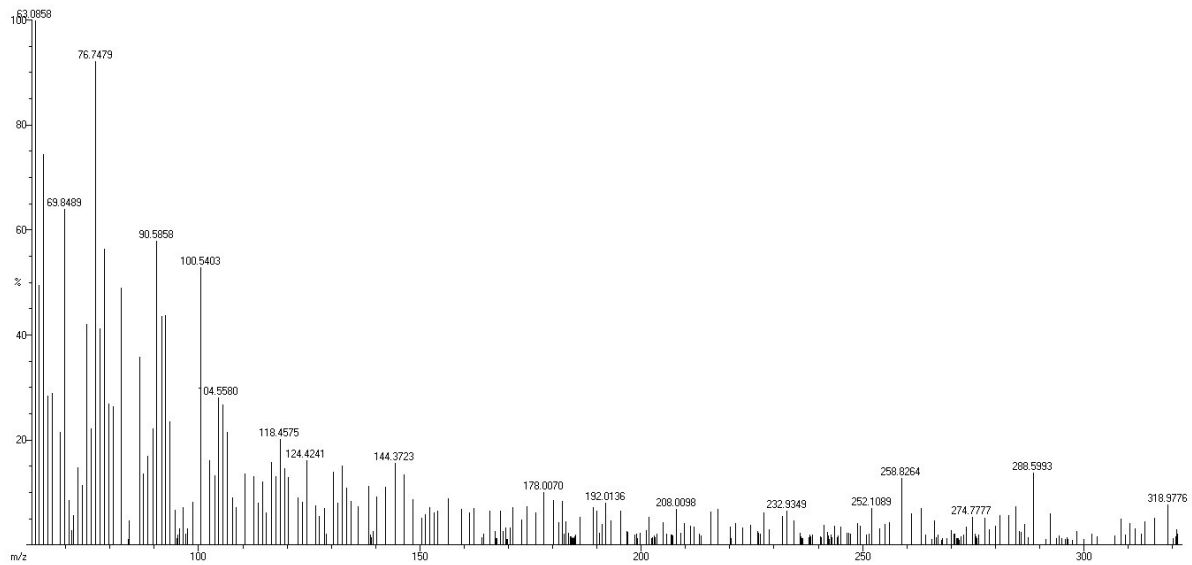
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NAME 5-Bromo-Amino Pyridi
EXPNO 25
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180315
Time 19.34 h
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PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 143.73
DW 20.800 usec
DE 6.50 usec
TE 301.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.0000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 14.0000000 W
PLW12 0.35097000 W
PLW13 0.17654000 W

F2 - Processing parameters
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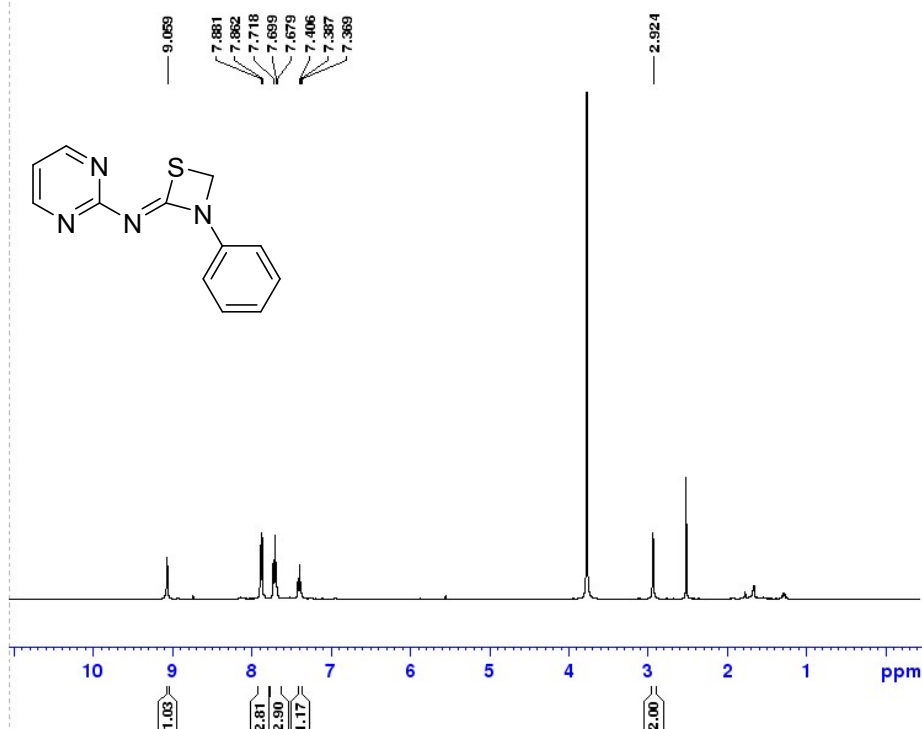
¹H and ¹³C NMR spectra of compound 4e

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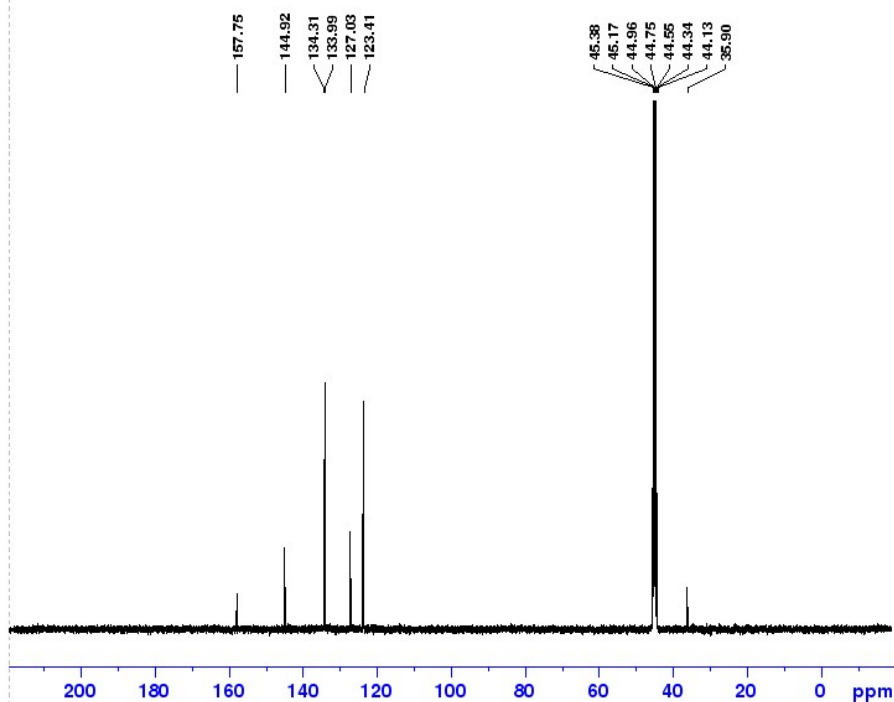


HRMS and IR spectra compound 4e

Signature SIF VIT VELLORE
NR-318-TO-F



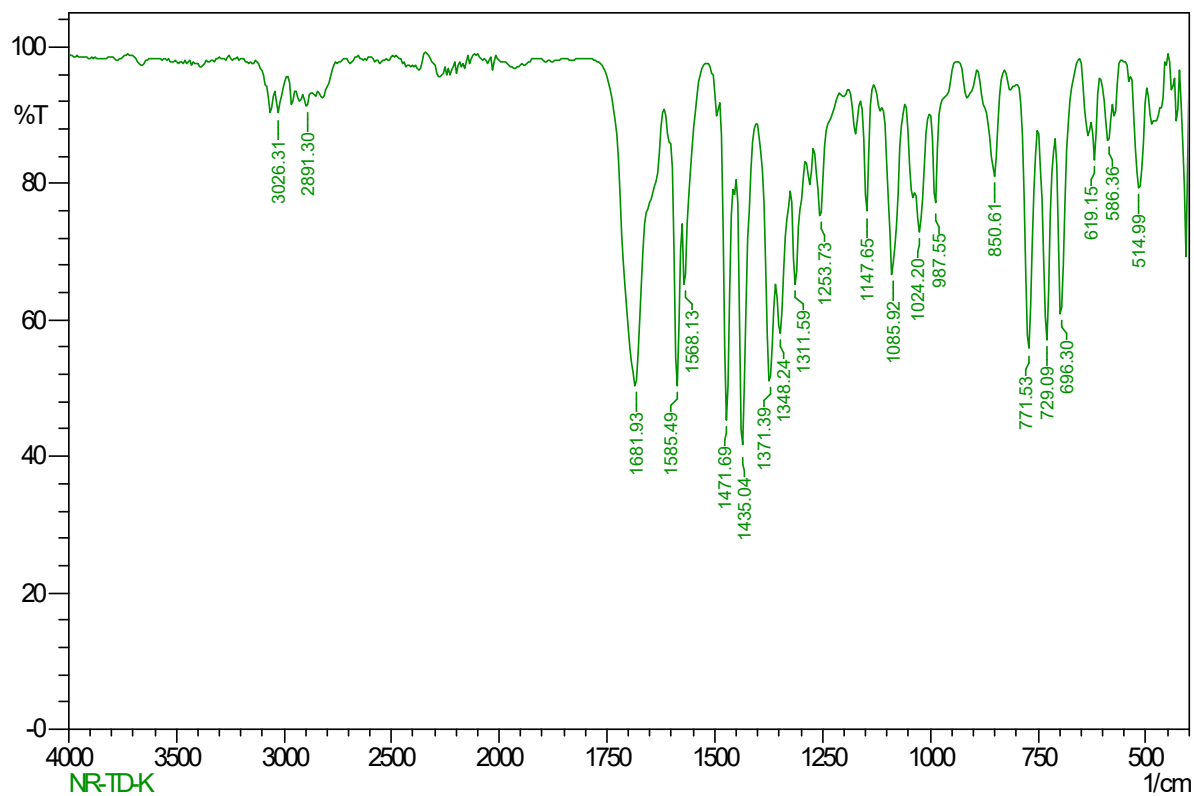
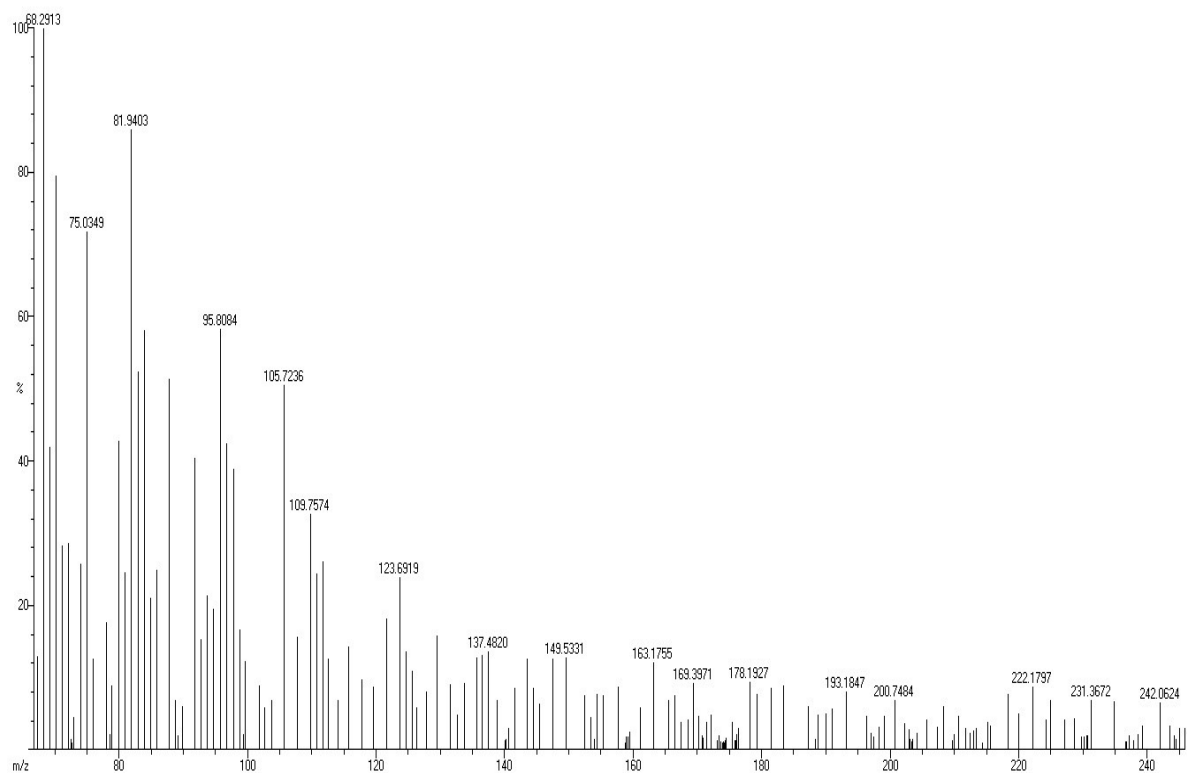
Signature SIF VIT VELLORE
NR-318-TO-F



¹H and ¹³C NMR spectra of compound 4f

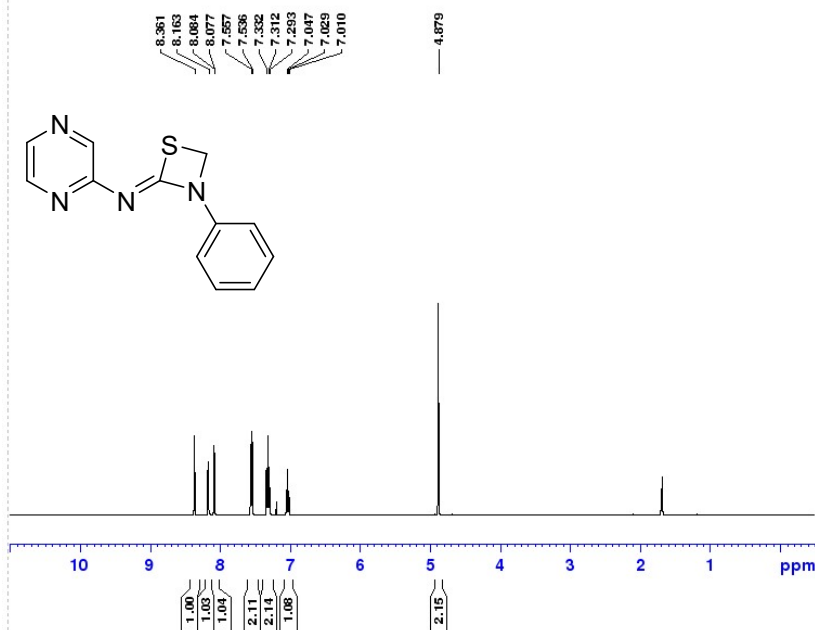
NR-TD.F

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HRMS and IR spectra compound 4f.

Signature SIF VIT VELLORE
NR-718-ID-T

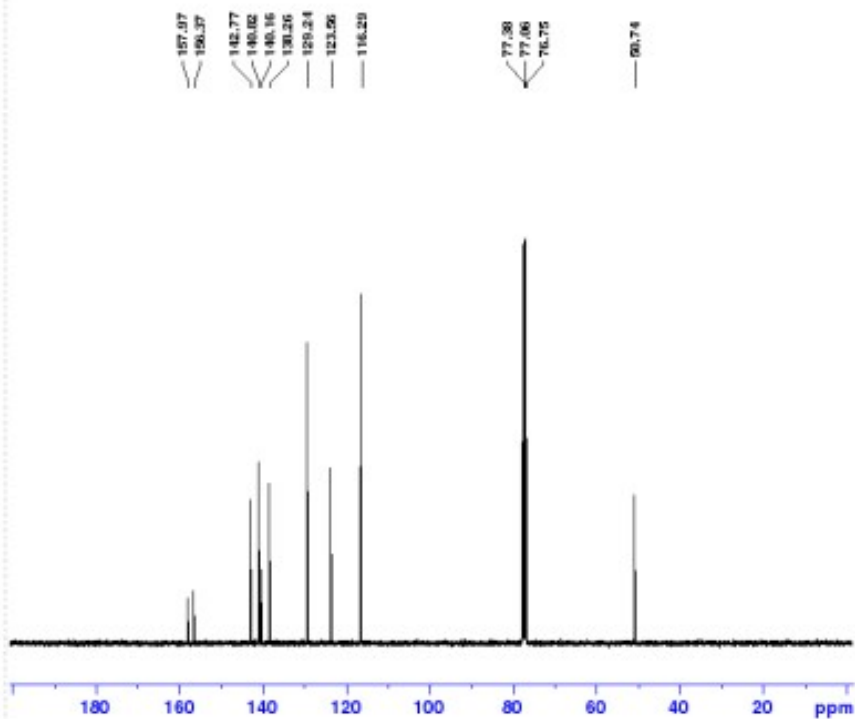


Current Data Parameters
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EXPNO 34
PROCNO 1

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SOLVENT CDCl3
NS 16
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FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 298.5 K
D1 1.0000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.27 usec
PLW1 15.0000000 W

F2 - Processing parameters
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PC 1.00

Signature SIF VIT VELLORE
NR-718-ID-T

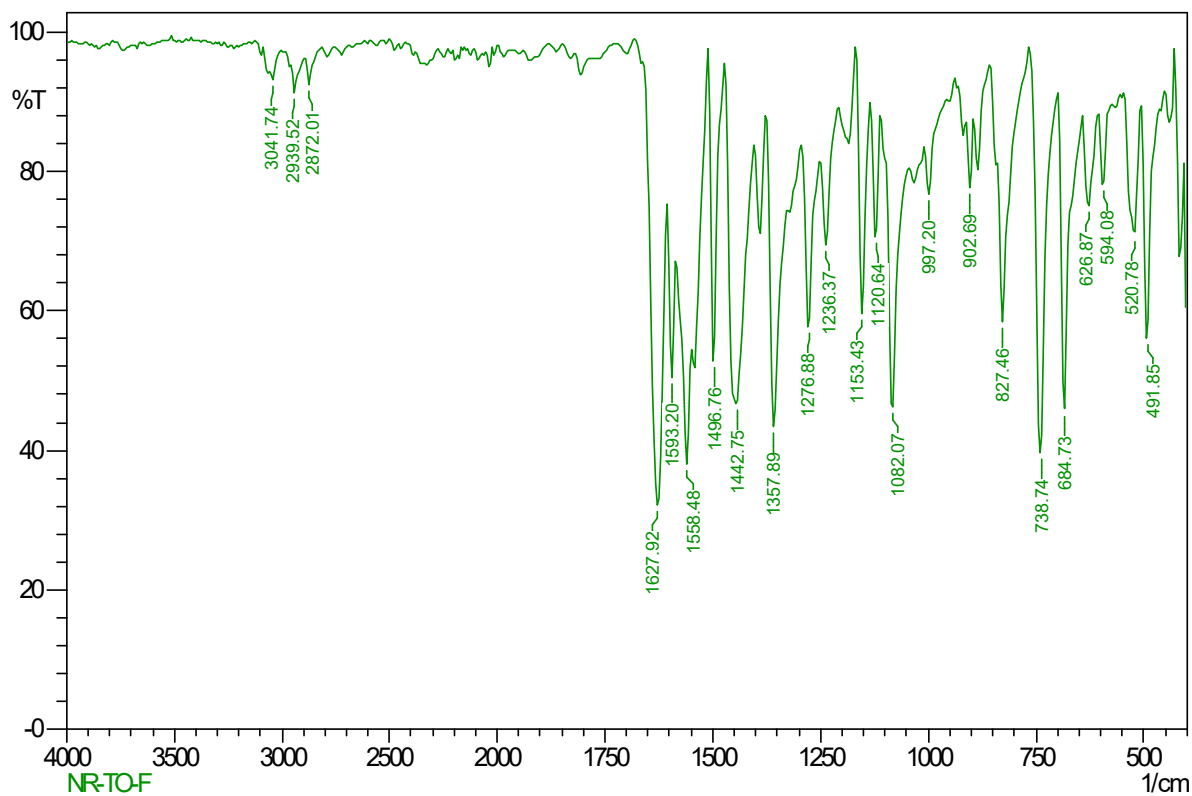
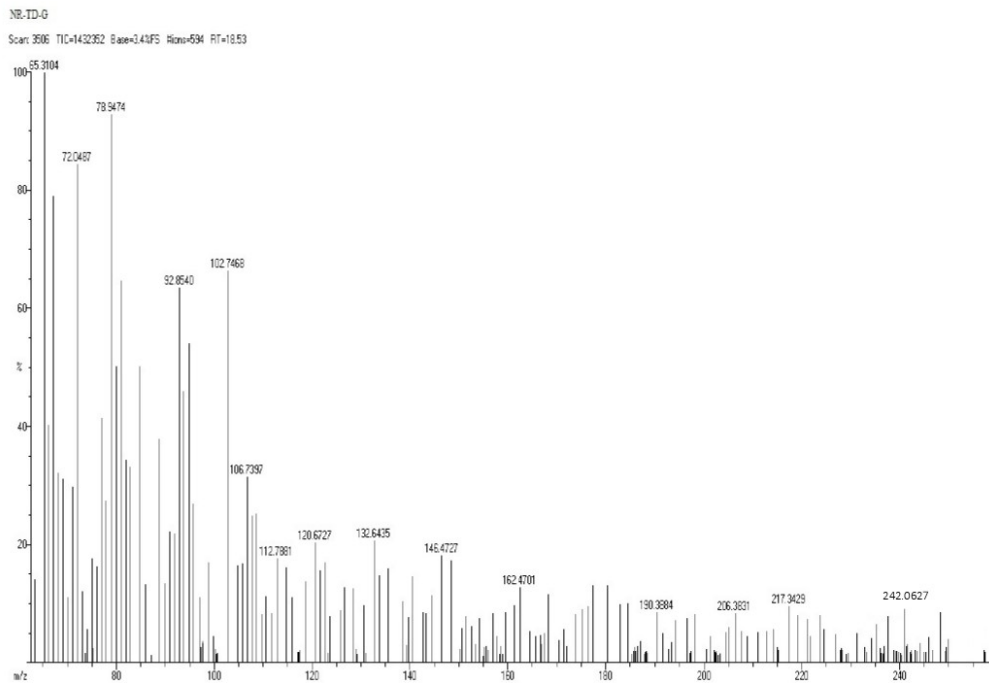


Current Data Parameters
NAME 2-Amino pyrazine with
EXPNO 35
PROCNO 1

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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631480 sec
RG 156.91
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6250186 MHz
NUC1 13C
P1 9.80 usec
PLW1 50.0000000 W
SFO2 400.2536010 MHz
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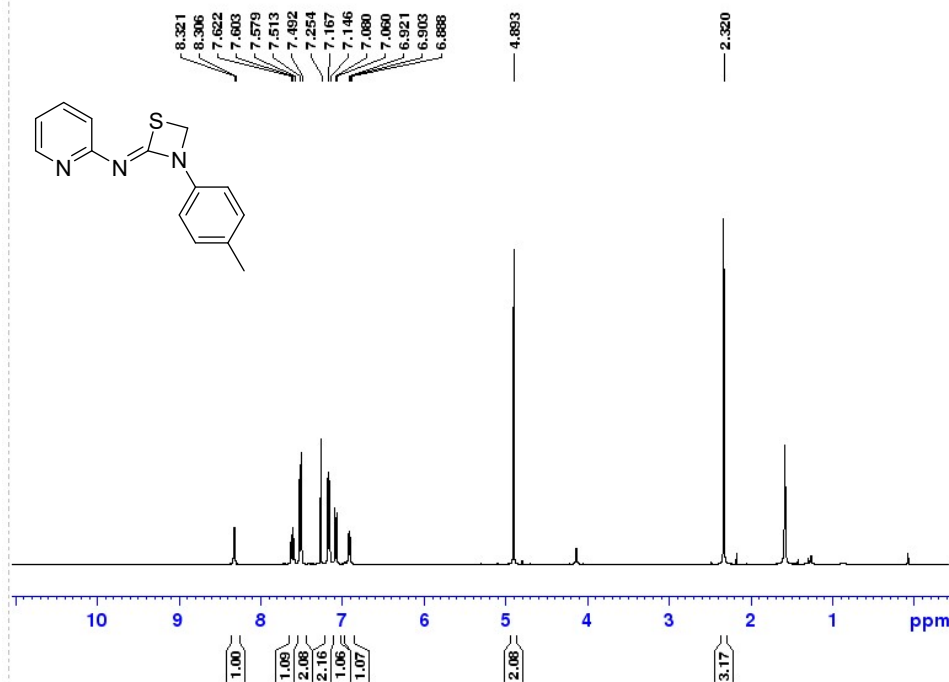
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¹H and ¹³C NMR spectra of compound 4g



HRMS and IR spectra compound 4g.

Signature SIF VIT VELLORE
NR-318-TD-H

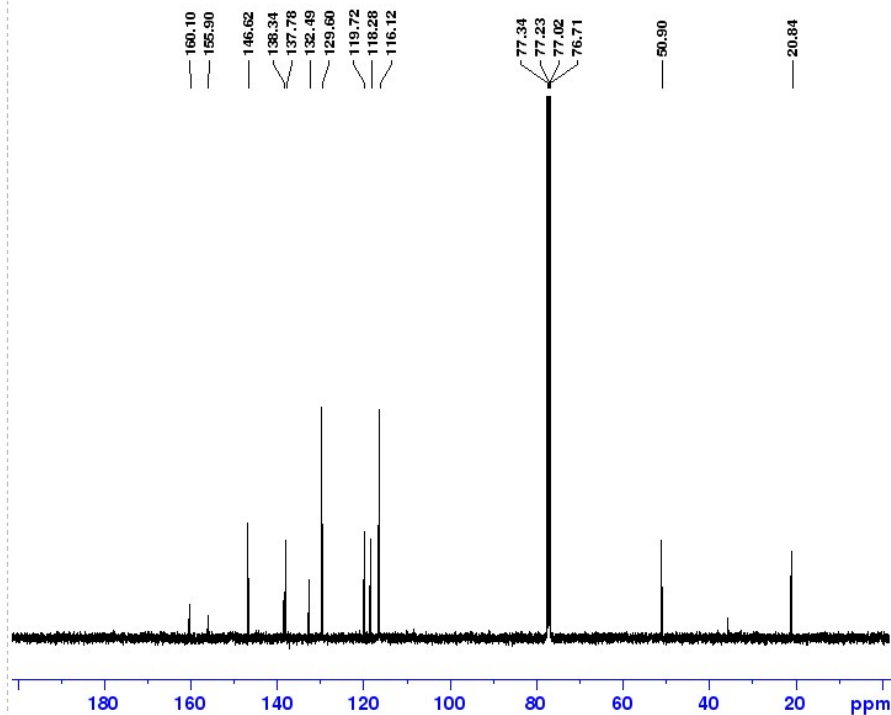


Current Data Parameters
NAME 2-Amino Pyridine
EXPNO 53
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180324
Time 7.59 h
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TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 175.97
DW 62.400 usec
DE 6.50 usec
TE 301.2 K
D1 1.0000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.27 usec
PLW1 15.0000000 W

F2 - Processing parameters
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SF 400.2580124 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Signature SIF VIT VELLORE
NR-318-TD-H



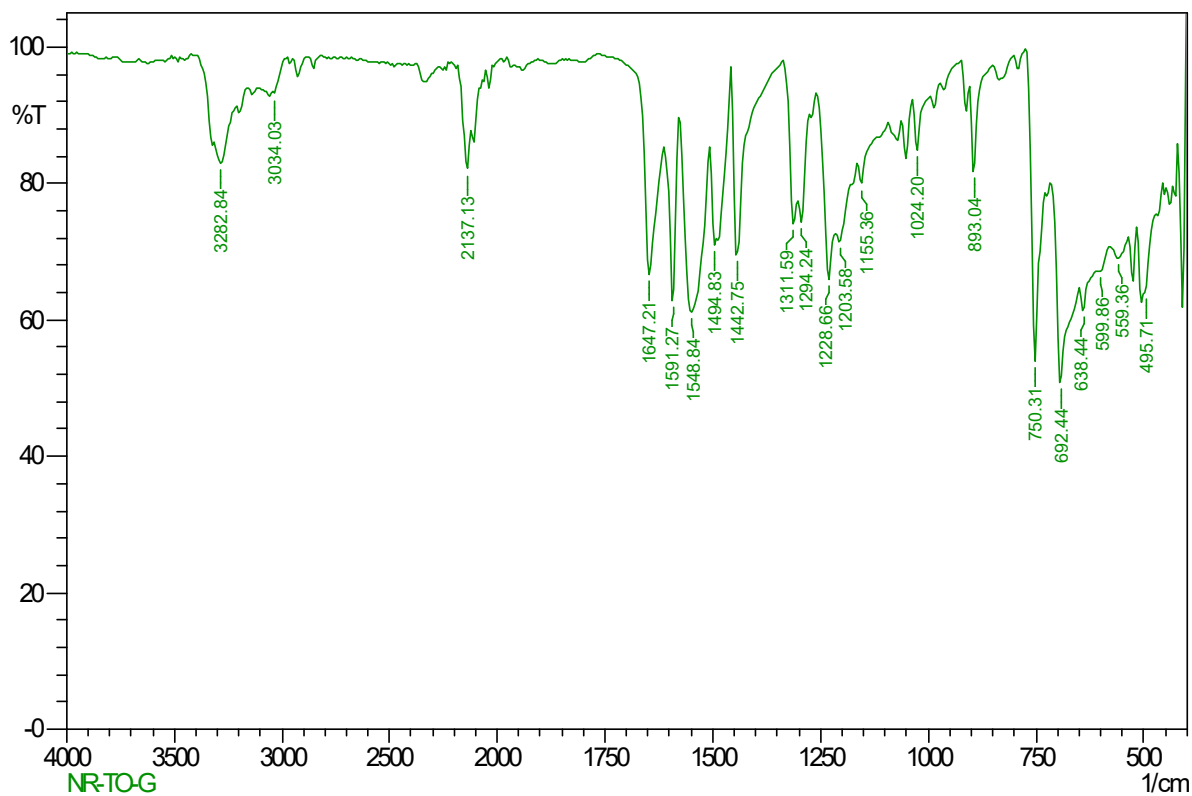
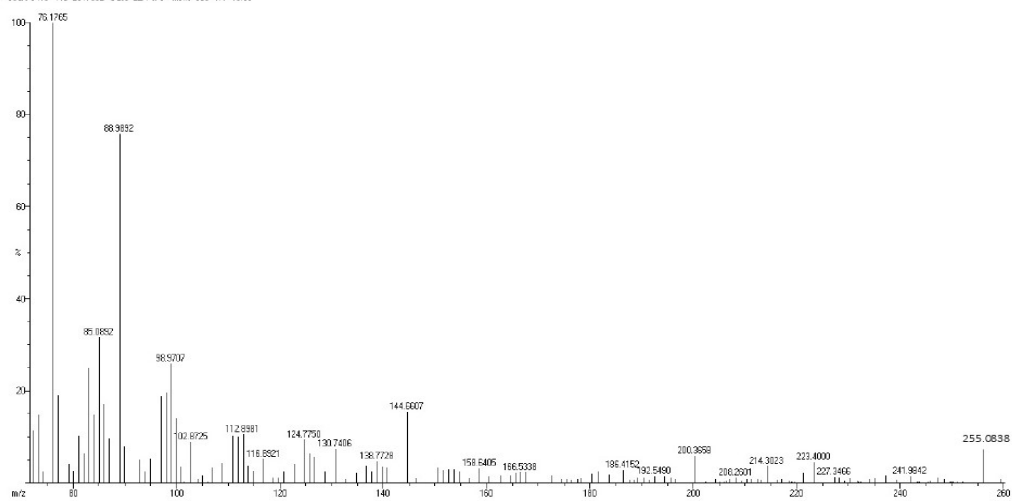
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EXPNO 54
PROCNO 1

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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 156.91
DW 20.800 usec
DE 6.50 usec
TE 302.3 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.0000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.0000000 W
PLW12 0.37709999 W
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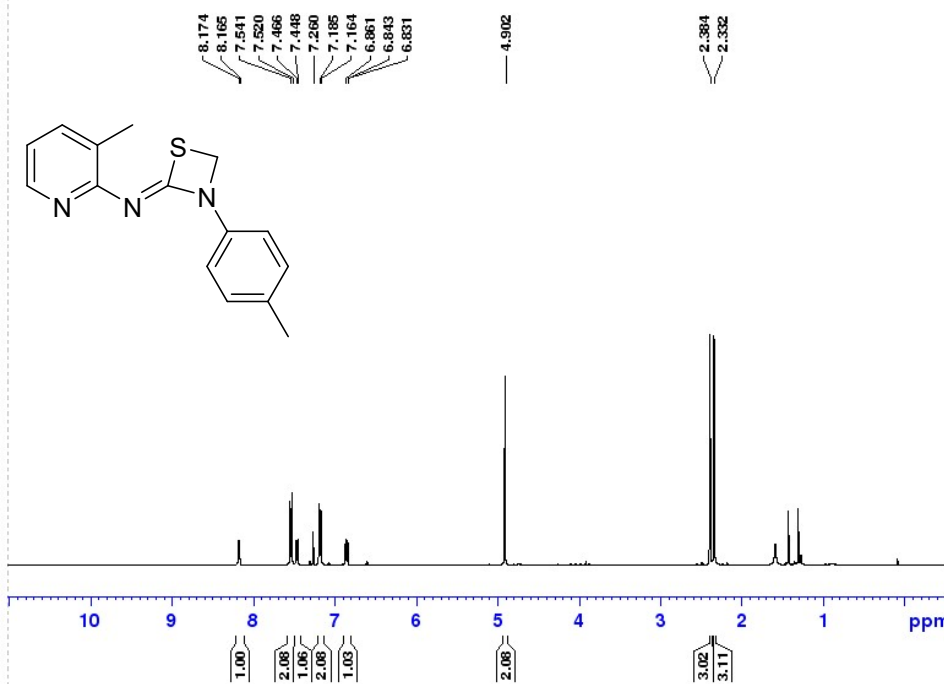
^1H and ^{13}C NMR spectra of compound 4h.

NR-TO-G
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HRMS and IR spectra compound 4h

Signature SIF VIT VELLORE
NR-318-TD-J

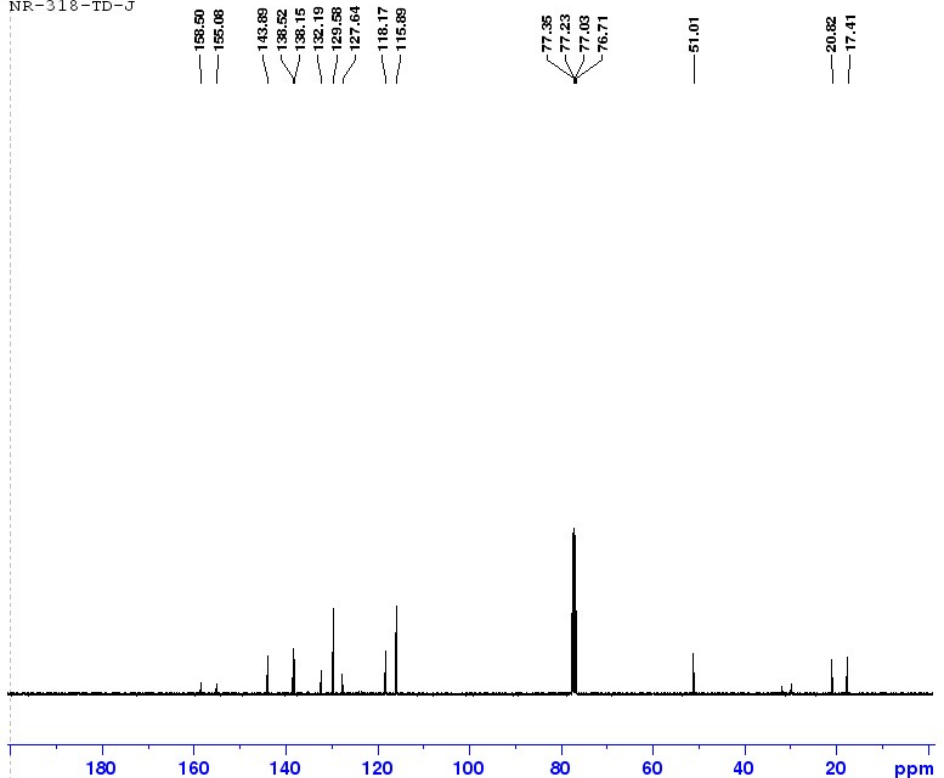


Current Data Parameters
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EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
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INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 143.73
DW 62.400 usec
DE 6.50 usec
TE 302.7 K
D1 1.0000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.27 usec
PLW1 15.0000000 W

F2 - Processing parameters
SI 65536
SF 400.2580099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Signature SIF VIT VELLORE
NR-318-TD-J



Current Data Parameters
NAME 3-Methyl Amino Pyridin
EXPNO 4
PROCNO 1

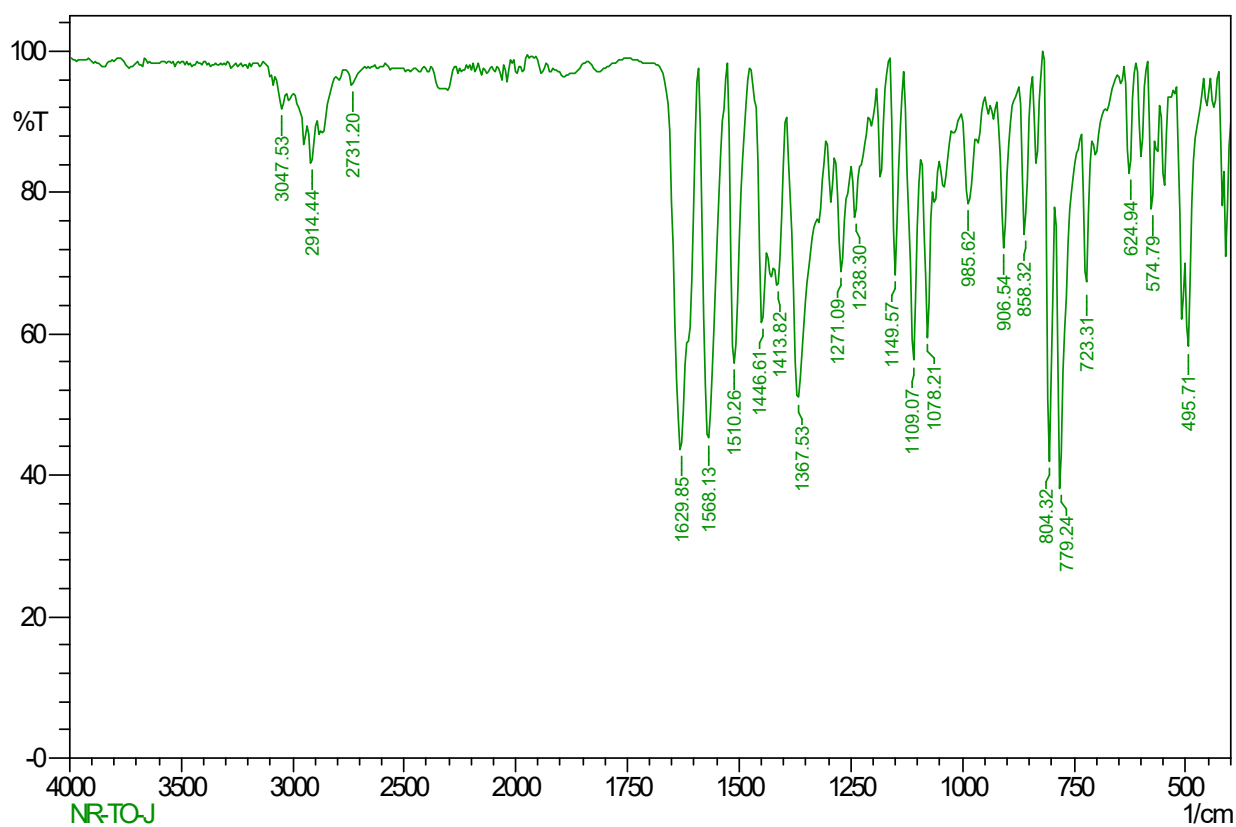
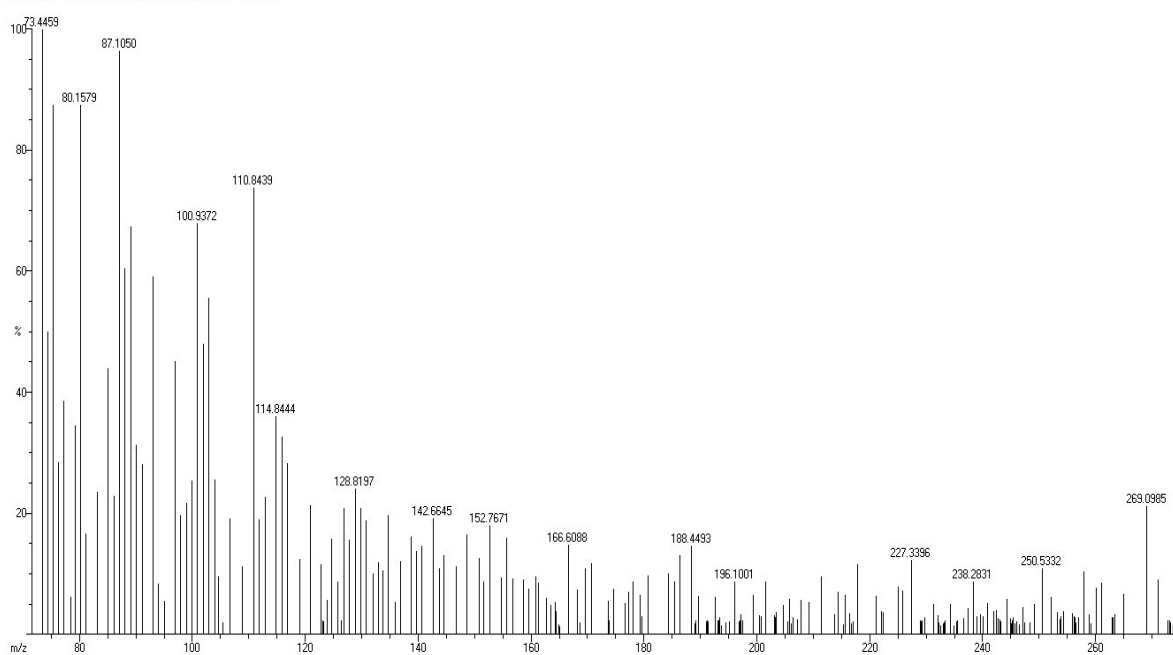
F2 - Acquisition Parameters
Date_ 20180410
Time 20.17 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 303.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6250186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.0000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 15.0000000 W
PLW12 0.37709999 W
PLW13 0.18968000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^1H and ^{13}C NMR spectra of compound 4i.

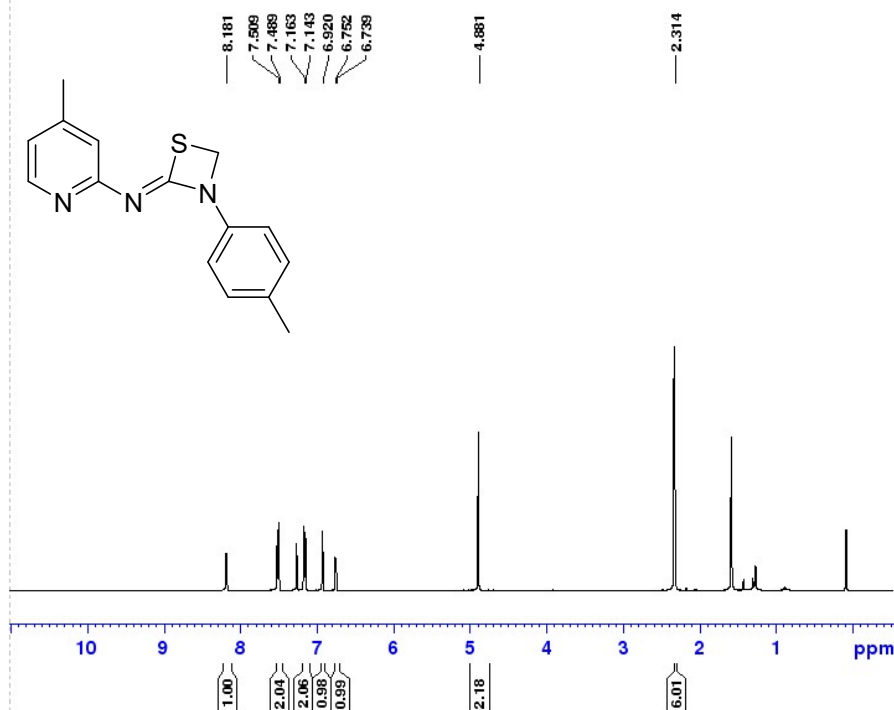
NR-TD-H

Scan: 3509 TIC=1434688 Base=3%FS #Ions=625 RT=18.54



HRMS and IR spectra compound 4i

Signature SIF VIT VELLORE
NR-318-TD-H

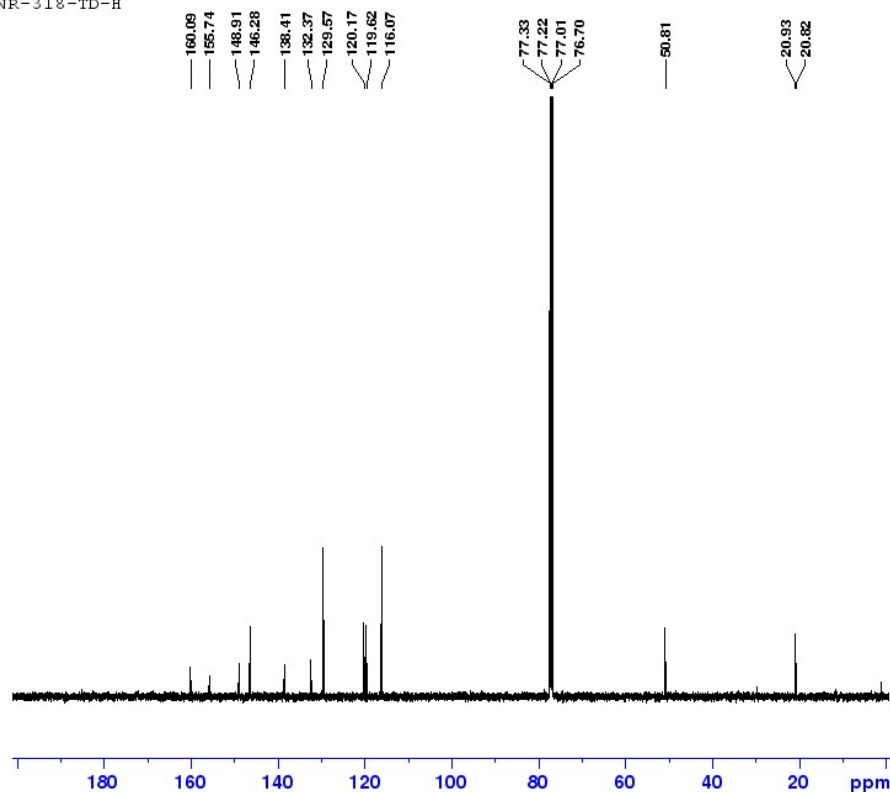


Current Data Parameters
NAME 4-Methyl Amino Pyridir
EXPNO 61
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180329
Time 23.24 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 175.97
DW 62.400 usec
DE 6.50 usec
TE 304.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.27 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2580106 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Signature SIF VIT VELLORE
NR-318-TD-H



NAME 4-Methyl Amino Pyridir
EXPNO 62
PROCNO 1

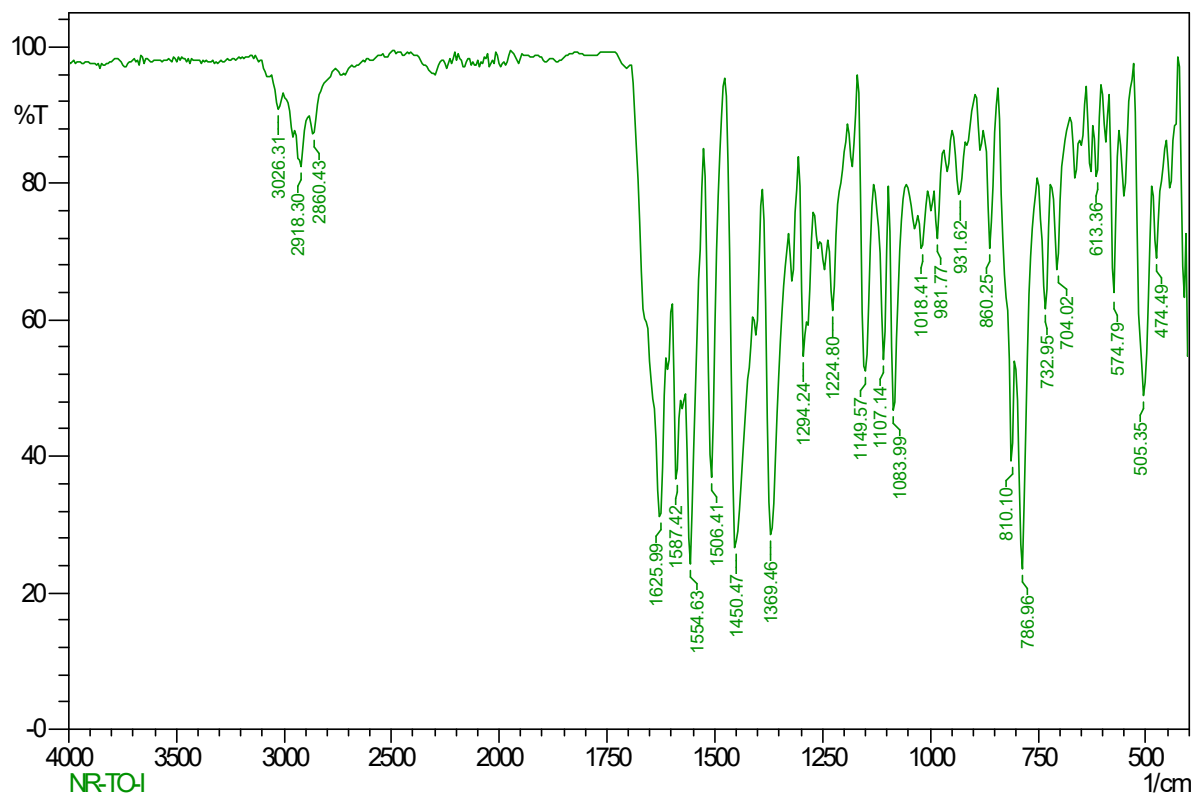
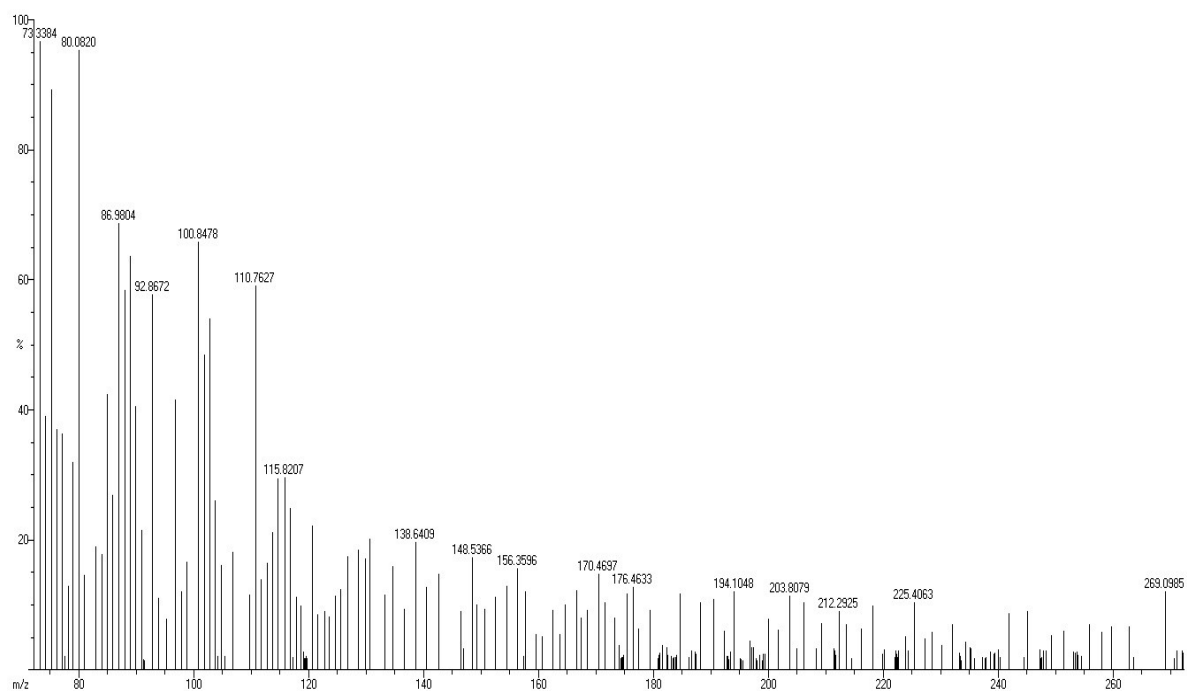
F2 - Acquisition Parameters
Date_ 20180329
Time 23.54 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 304.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.37709999 W
PLW13 0.18968000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H and ¹³C NMR spectra of compound 4j

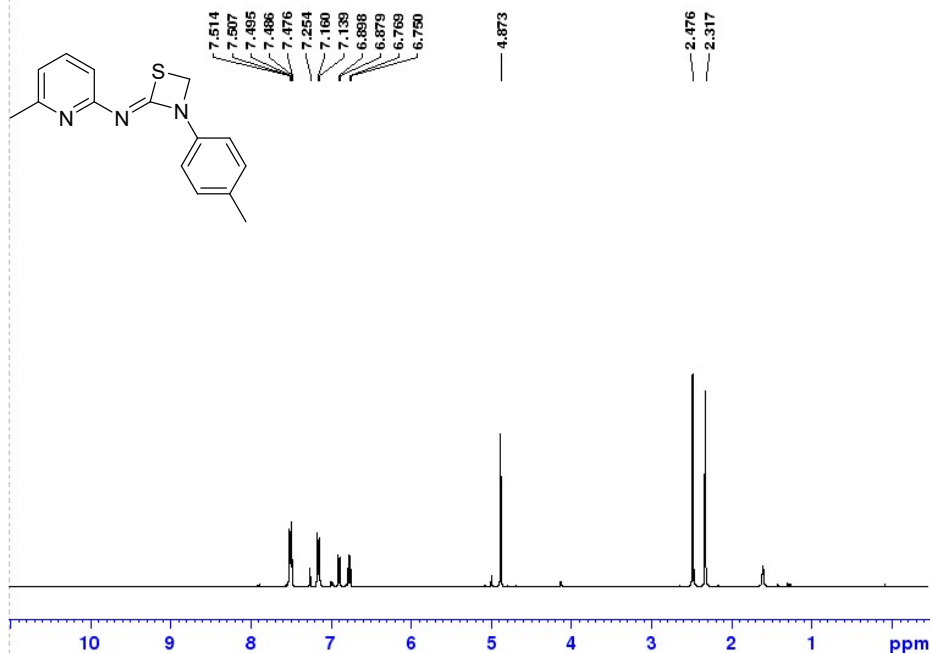
NR-TD-1

Scan: 3515 TIC=1409664 Base=3.12%FS #Ions=650 RT=18.57



HRMS and IR spectra compound 4j

Signature SIF VIT VELLORE
NR-318-TD-I

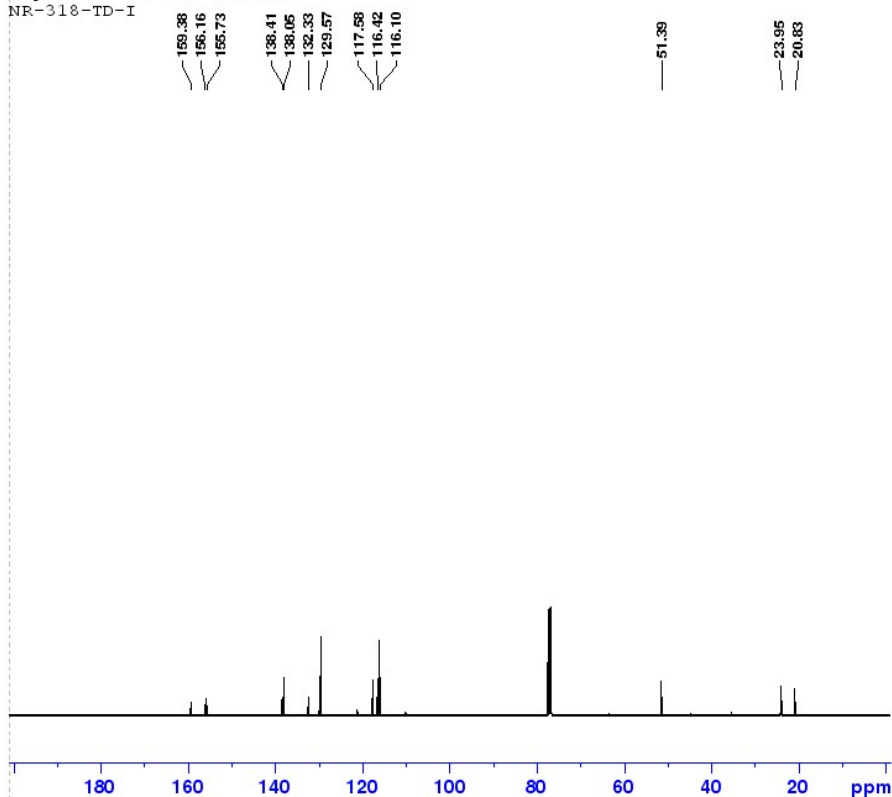


Current Data Parameters
NAME 6-Methyl Amino Pyridir
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180404
Time 20.06 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 112.69
DW 62.400 usec
DE 6.50 usec
TE 302.2 K
D1 1.0000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.27 usec
PLW1 15.0000000 W

F2 - Processing parameters
SI 65536
SF 400.2580122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Signature SIF VIT VELLORE
NR-318-TD-I



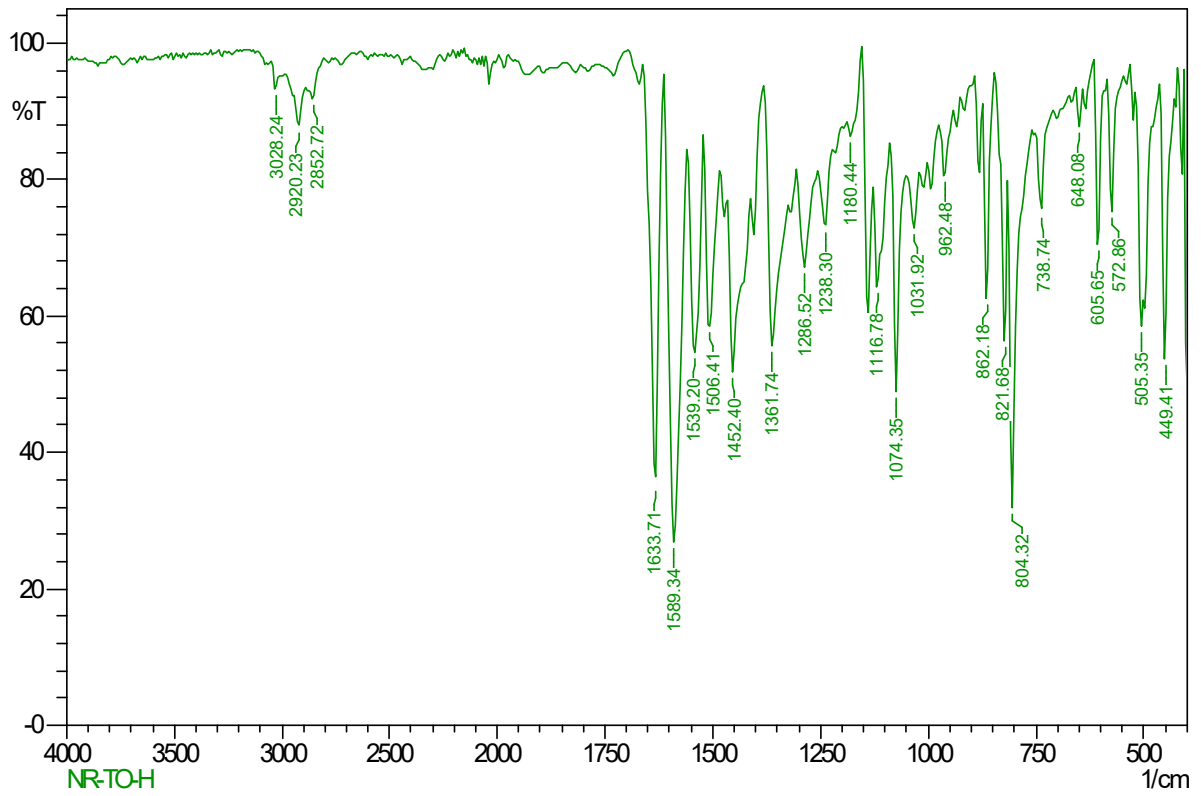
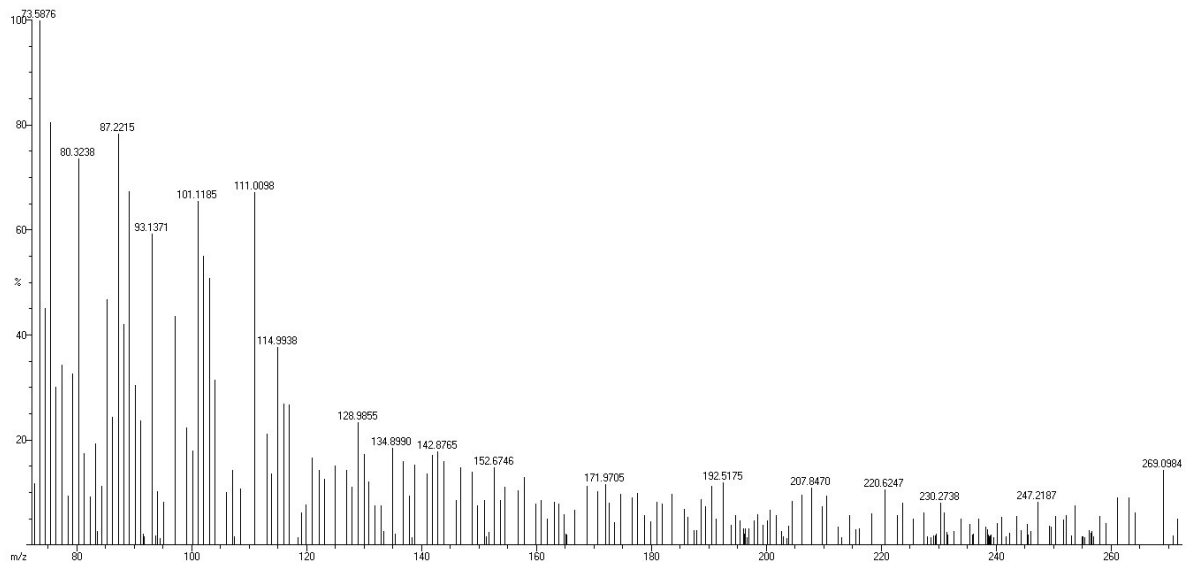
Current Data Parameters
NAME 6-Methyl Amino Pyridir
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180404
Time 20.36 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 303.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.0000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 15.0000000 W
PLW12 0.37709999 W
PLW13 0.18968000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H and ¹³C NMR spectra of compound 4k.

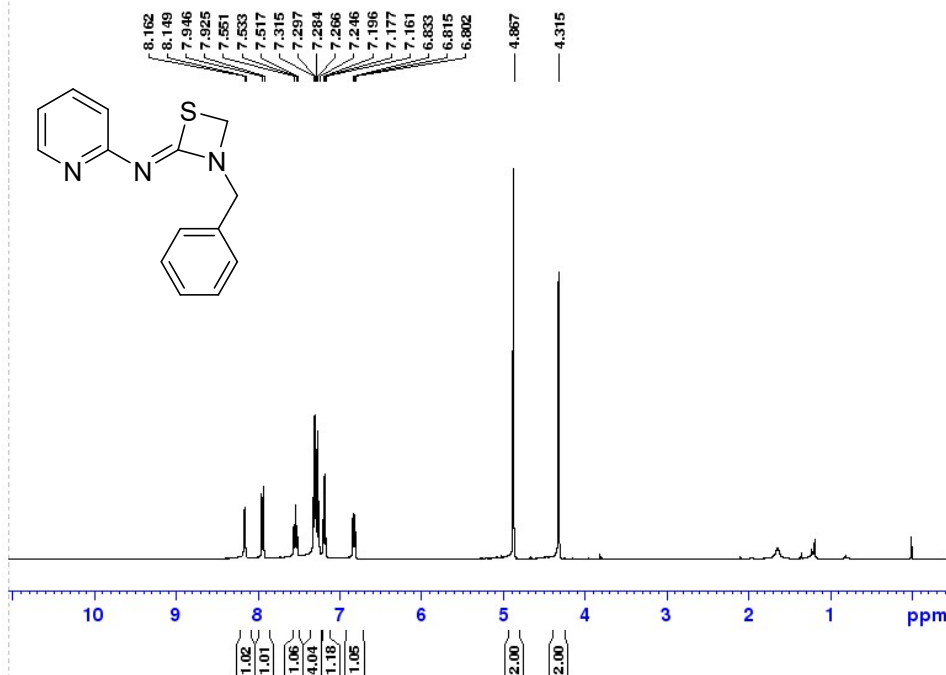
NR-TD-1
Scan: 3512 TIC=1427744 Base=3.2%FS #Ions=593 RT=18.56



NR-TO-H

HRMS and IR spectra compound 4k

Signature SIF VIT VELLORE
NR-318-TD-K

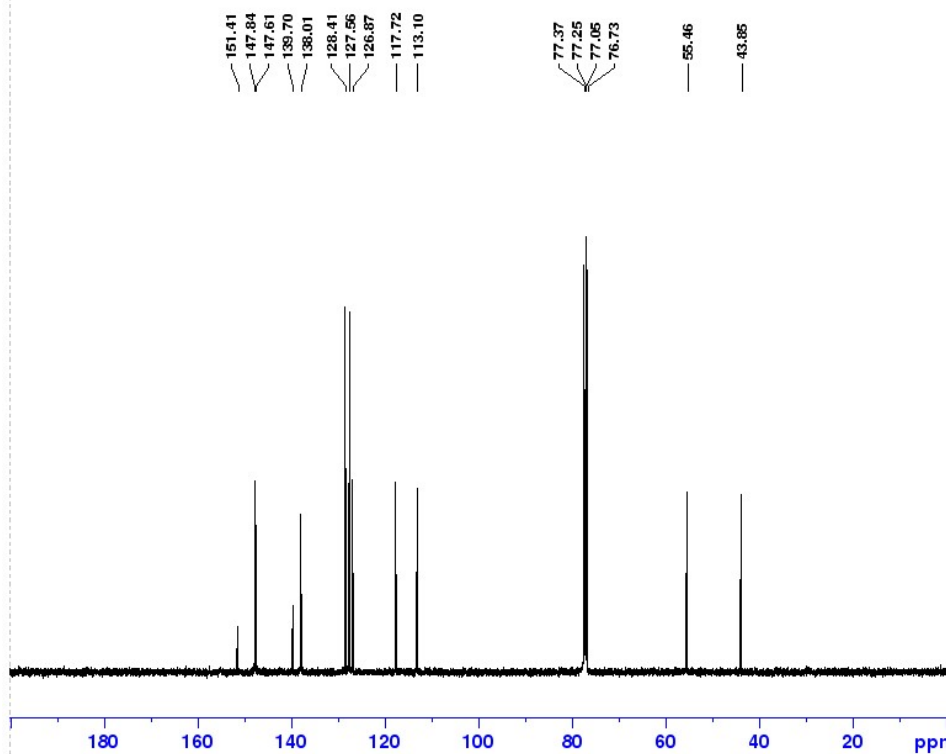


Current Data Parameters
NAME Aminopyridine
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180412
Time 3.26 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 112.69
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.27 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2580426 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Signature SIF VIT VELLORE
NR-318-TD-K



Current Data Parameters
NAME Aminopyridine
EXPNO 6
PROCNO 1

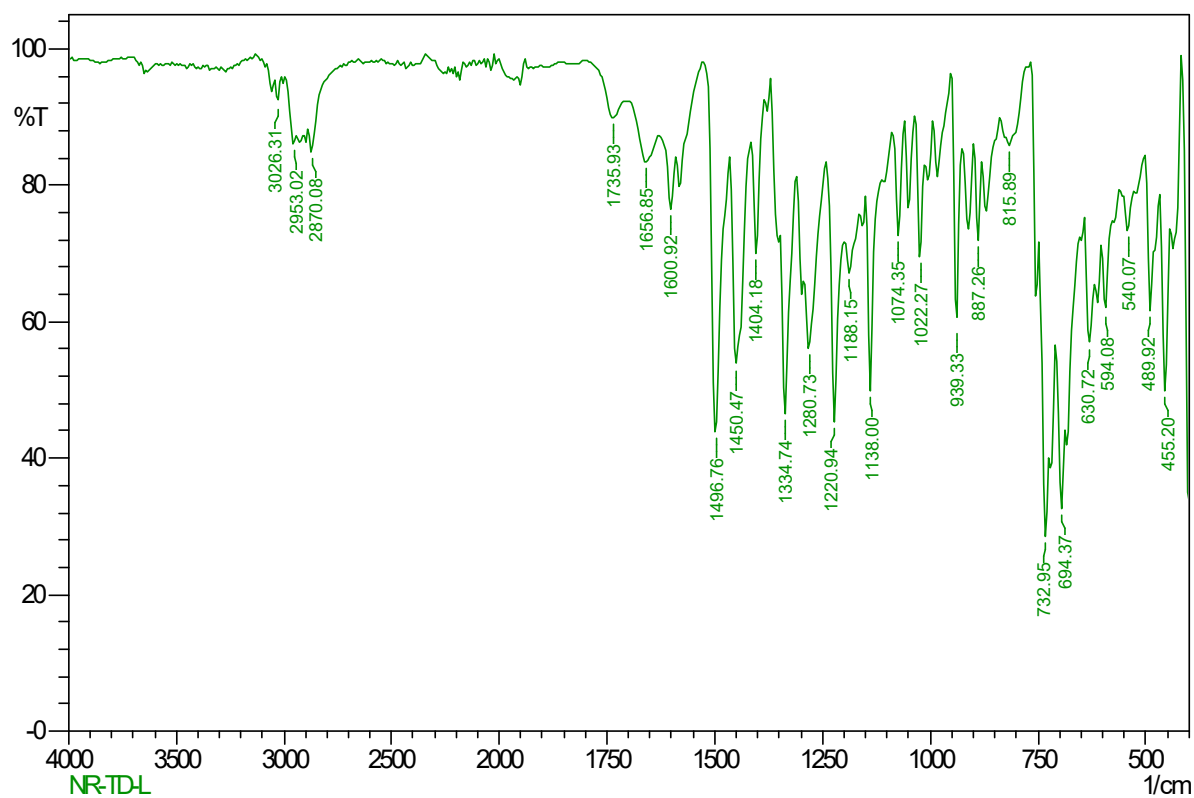
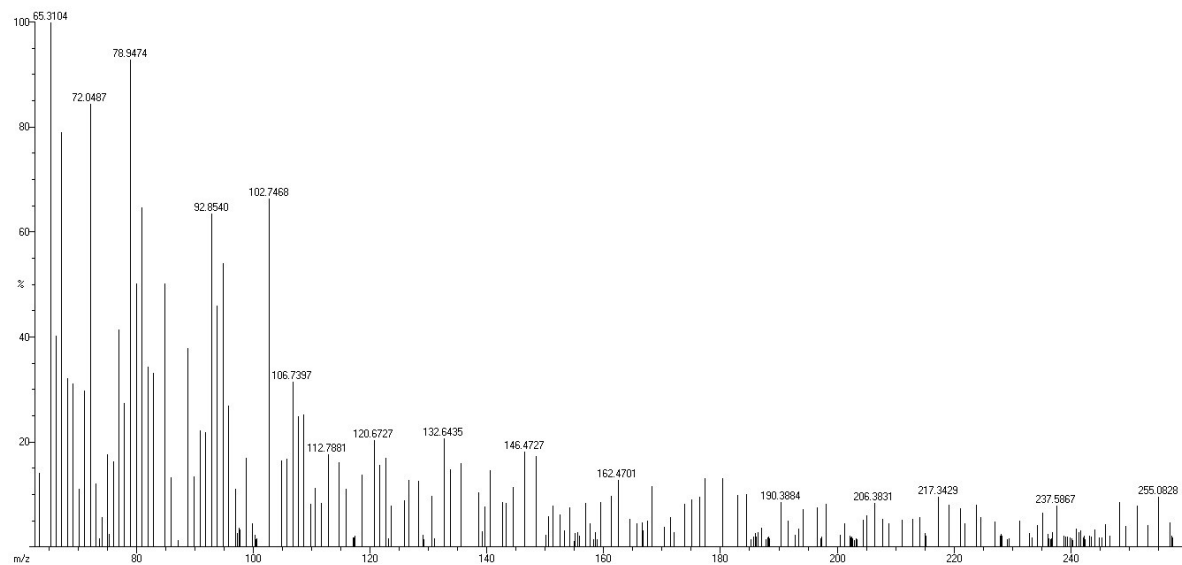
F2 - Acquisition Parameters
Date_ 20180412
Time 3.56 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 112.69
DW 20.800 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.37709999 W
PLW13 0.18968000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H and ¹³C NMR spectra of compound 4l.

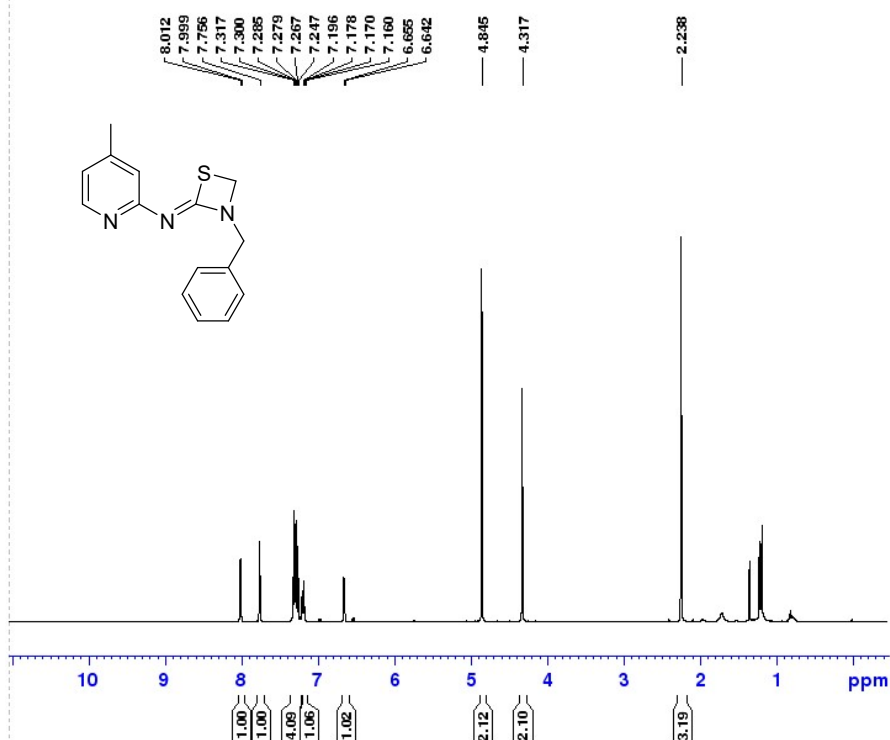
NR-TD-G

Scan: 3906 TIC=1432352 Base=3.4%FS #Ions=594 RT=18.53



HRMS and IR spectra compound 41

Signature SIF VIT VELLORE
NR-TD-418-M

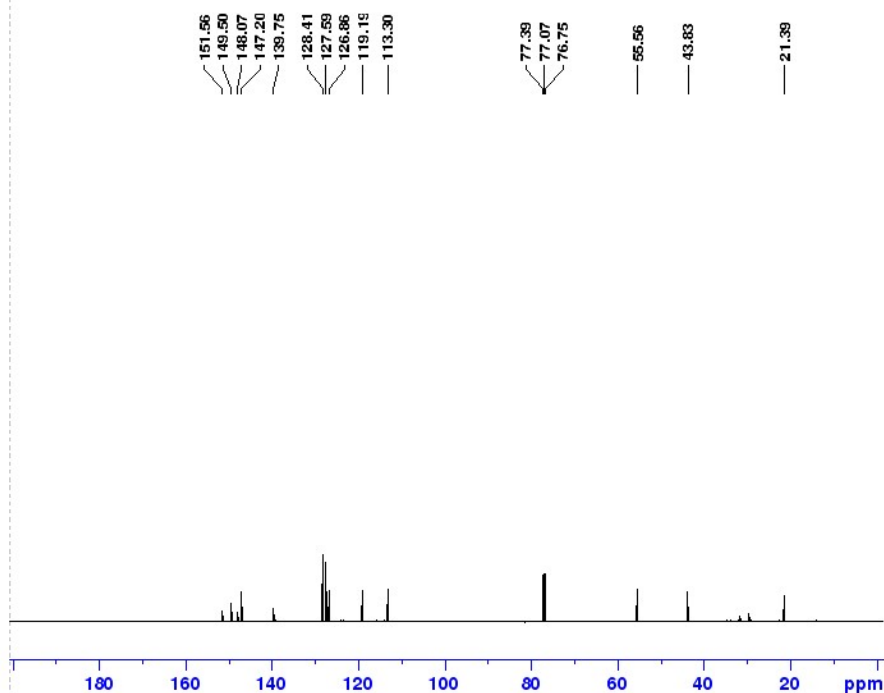


Current Data Parameters
NAME 4-Methyl Amino Pyridi
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180426
Time 2.25 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 71.13
DW 62.400 usec
DE 6.50 usec
TE 299.3 K
D1 1.0000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.27 usec
PLW1 15.0000000 W

F2 - Processing parameters
SI 65536
SF 400.2580457 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Signature SIF VIT VELLORE
NR-TD-418-M



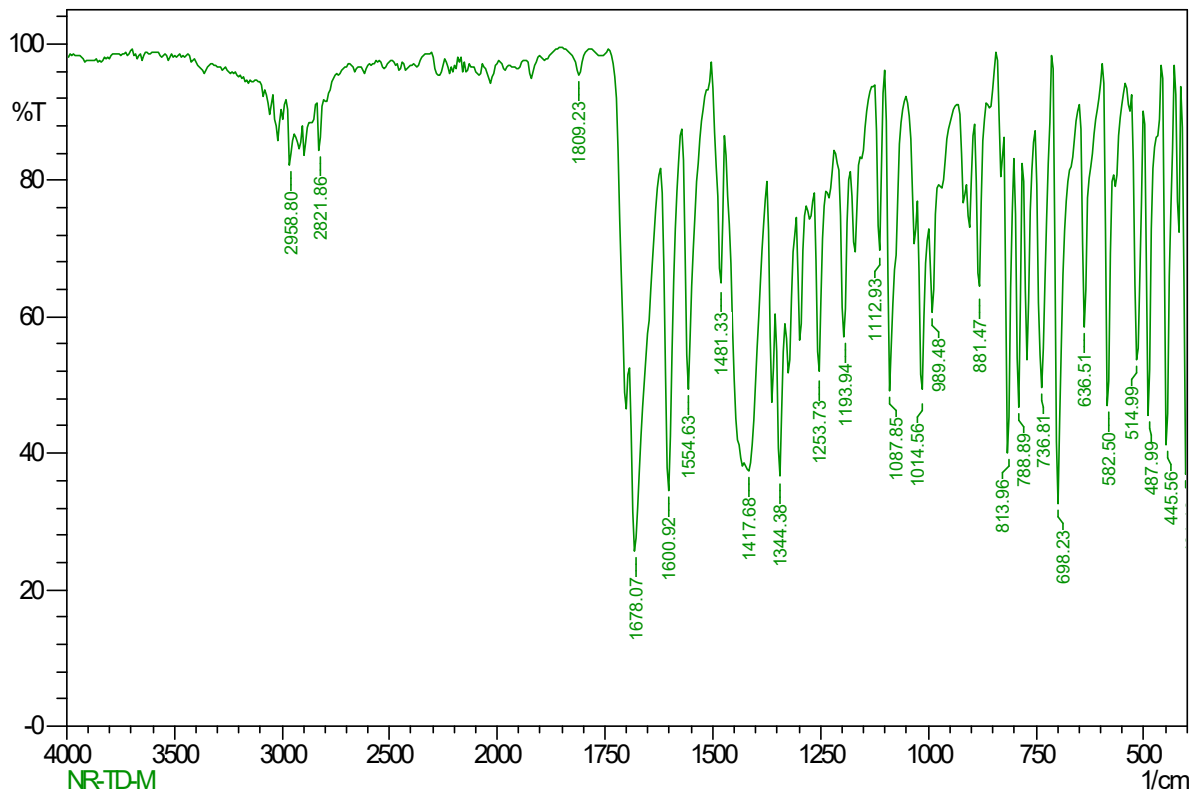
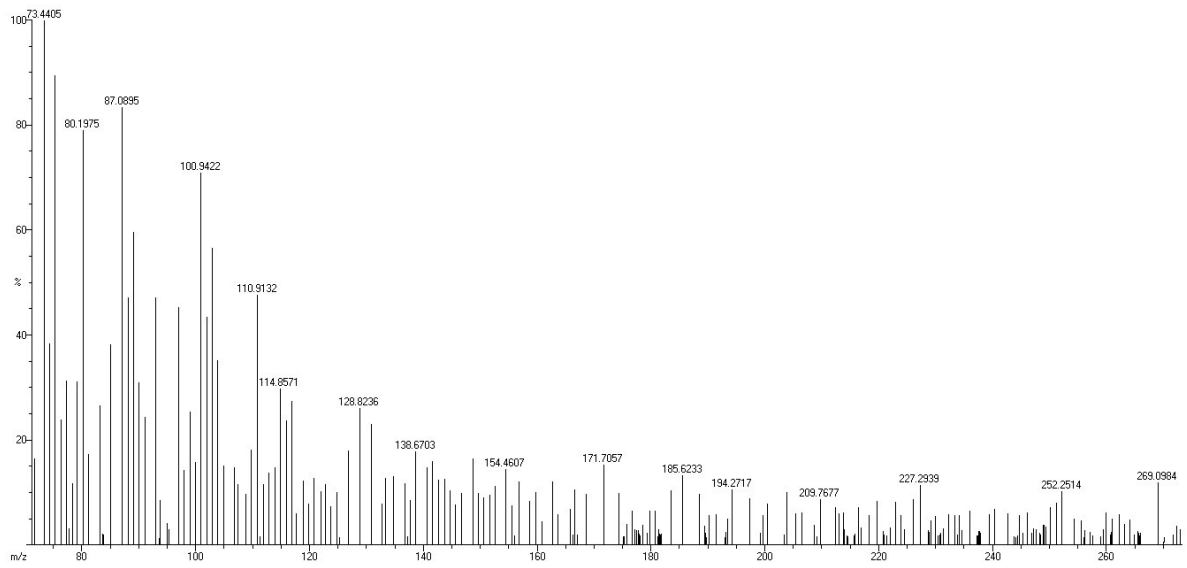
Current Data Parameters
NAME 4-Methyl Amino Pyrid
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180426
Time 2.56 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 112.69
DW 20.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.0000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.0000000 W
PLW12 0.37709999 W
PLW13 0.18968000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

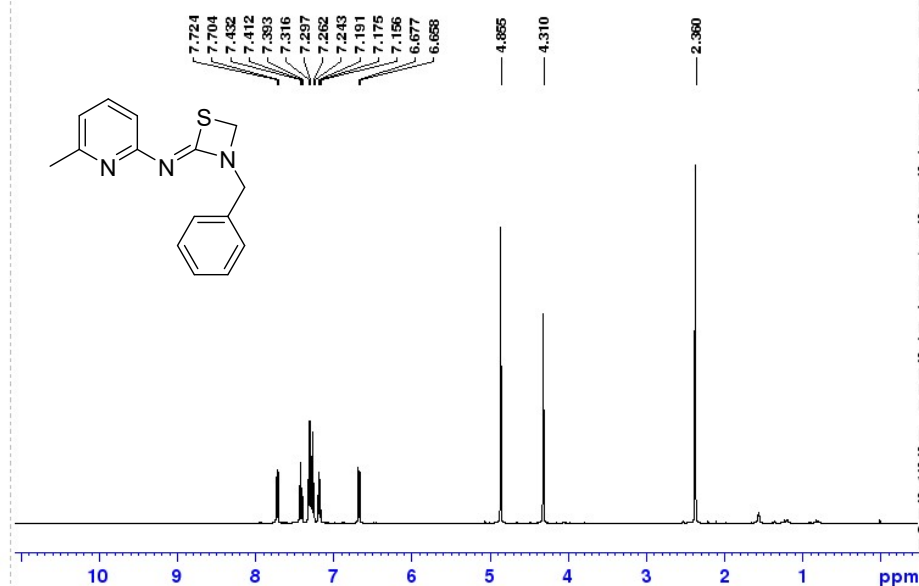
¹H and ¹³C NMR spectra of compound 4m

NR-TD-N
Scan: 3519 TIC=1374304 Base=3%FS #Ions=645 RT=18.59



HRMS and IR spectra compound 4m

Signature SIF VIT VELLORE
NR-418-TD-N

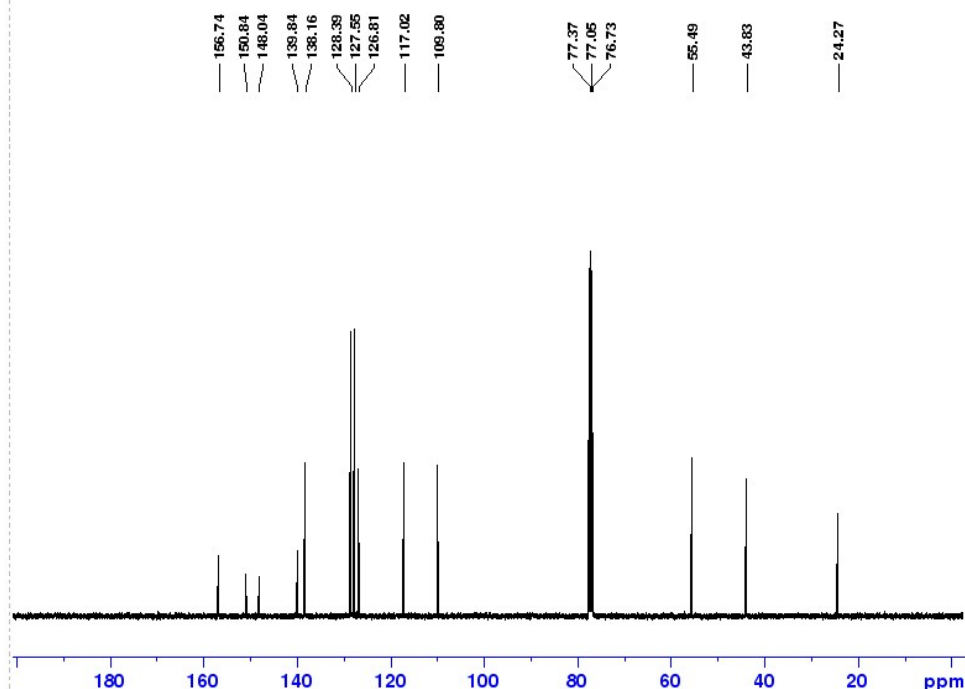


Current Data Parameters
NAME 6-Methyl Amino Pyridir
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180426
Time 7.44 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 112.69
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.27 usec
PLW1 15.0000000 W

F2 - Processing parameters
SI 65536
SF 400.2580438 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Signature SIF VIT VELLORE
NR-418-TD-N

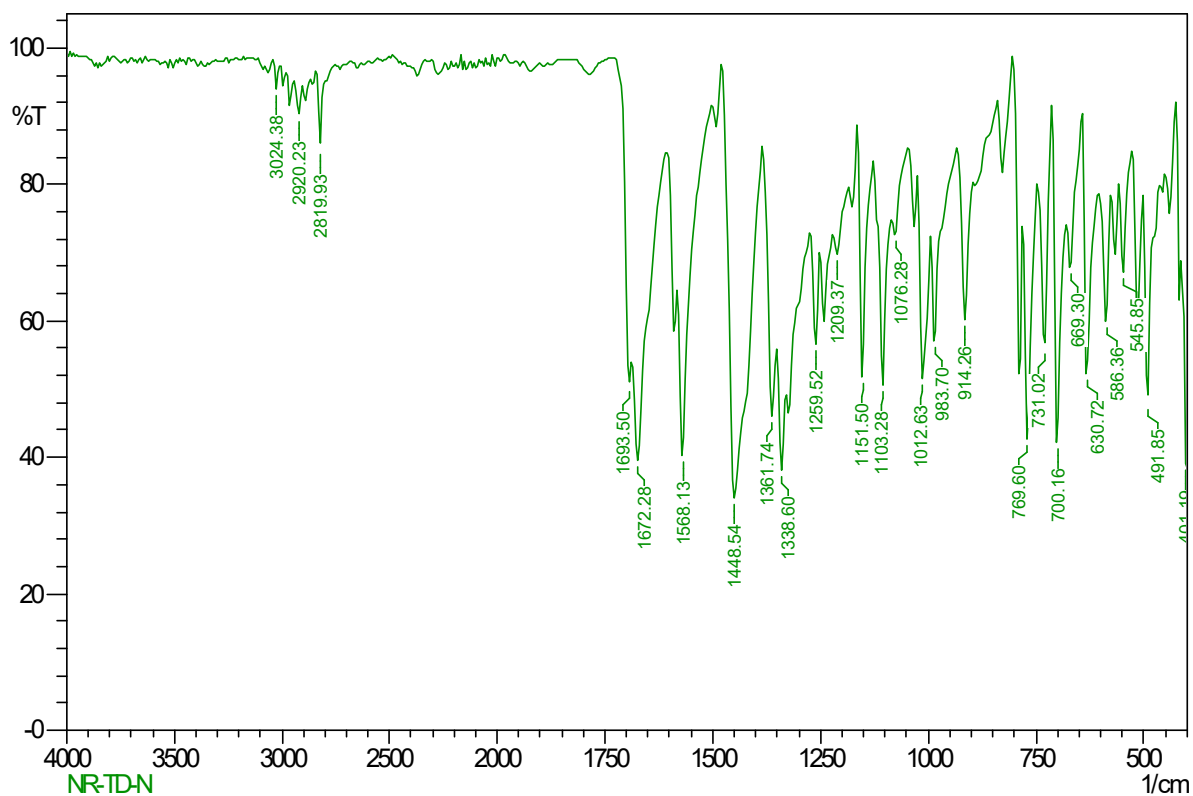
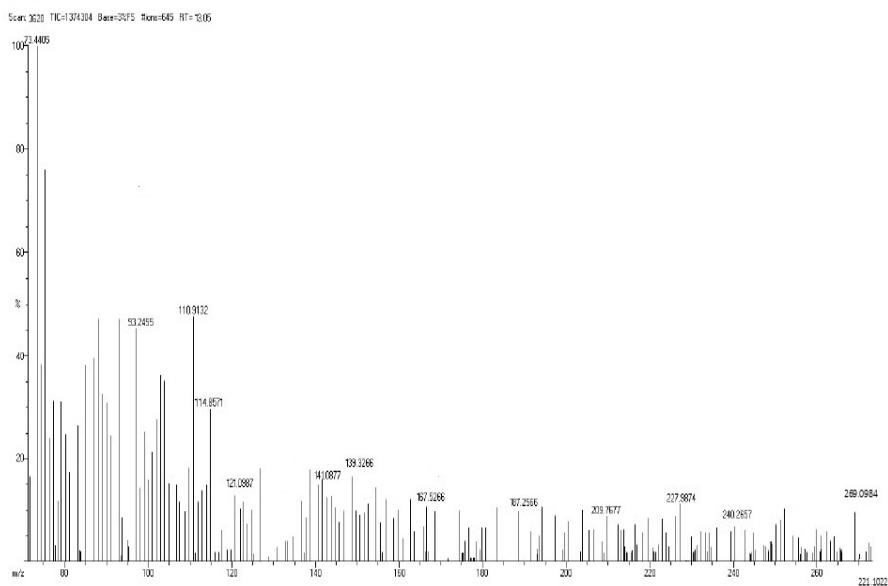


Current Data Parameters
NAME 6-Methyl Amino Pyrid
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180426
Time 8.13 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 143.73
DW 20.800 usec
DE 6.50 usec
TE 298.8 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.0000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 15.0000000 W
PLW12 0.37709999 W
PLW13 0.18968000 W

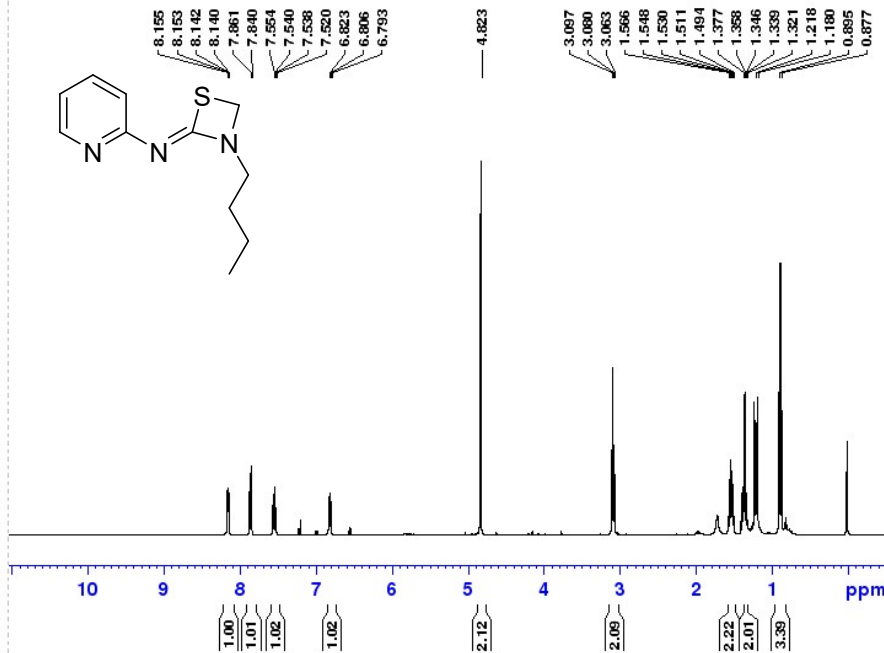
F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H and ¹³C NMR spectra of compound 4n



HRMS and IR spectra compound 4n

Signature SIF VIT VELLORE
NR-TD-518-P

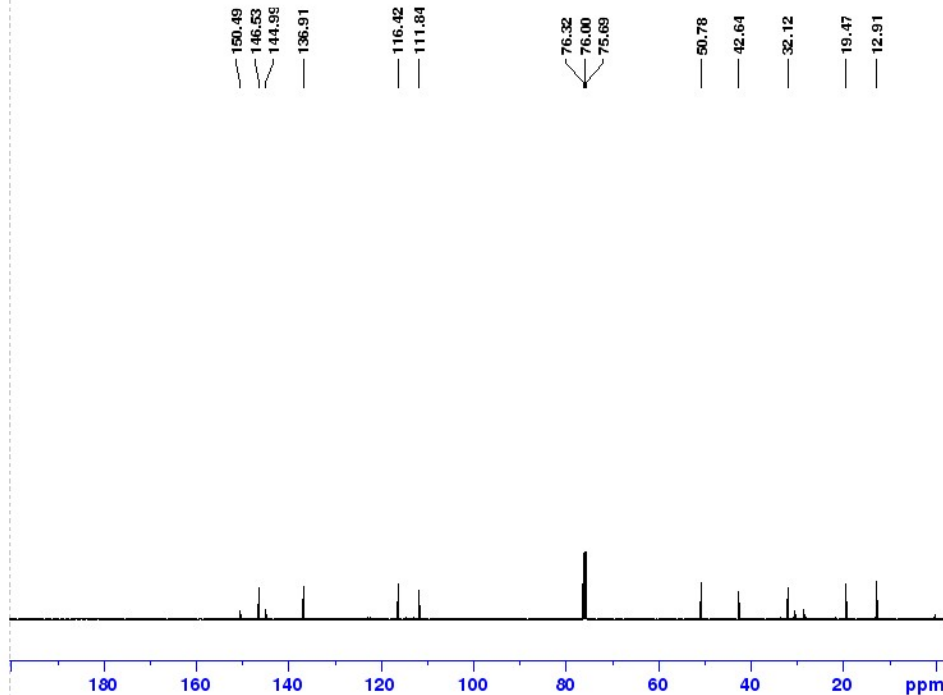


Current Data Parameters
NAME Amino pyridine
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180515
Time 20.21 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 71.13
DW 62.400 usec
DE 6.50 usec
TE 297.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.27 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2580365 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Signature SIF VIT VELLORE
NR-TD-518-P

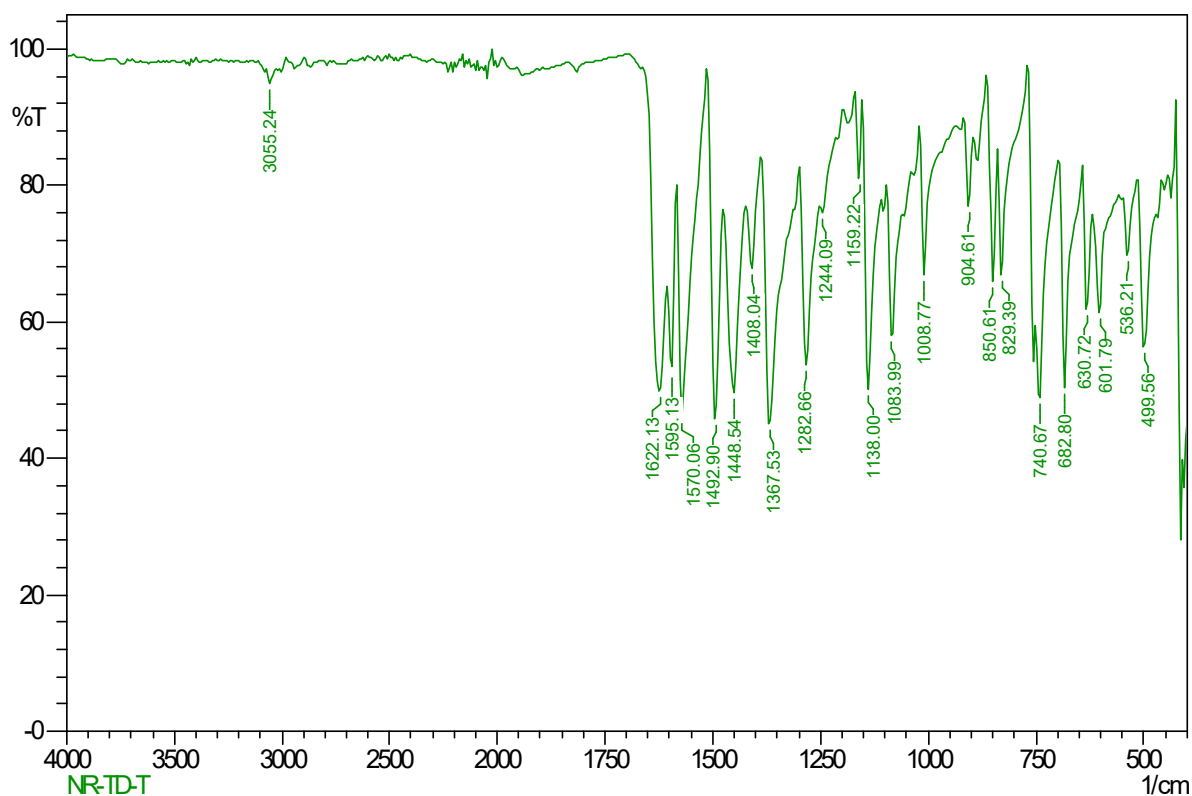
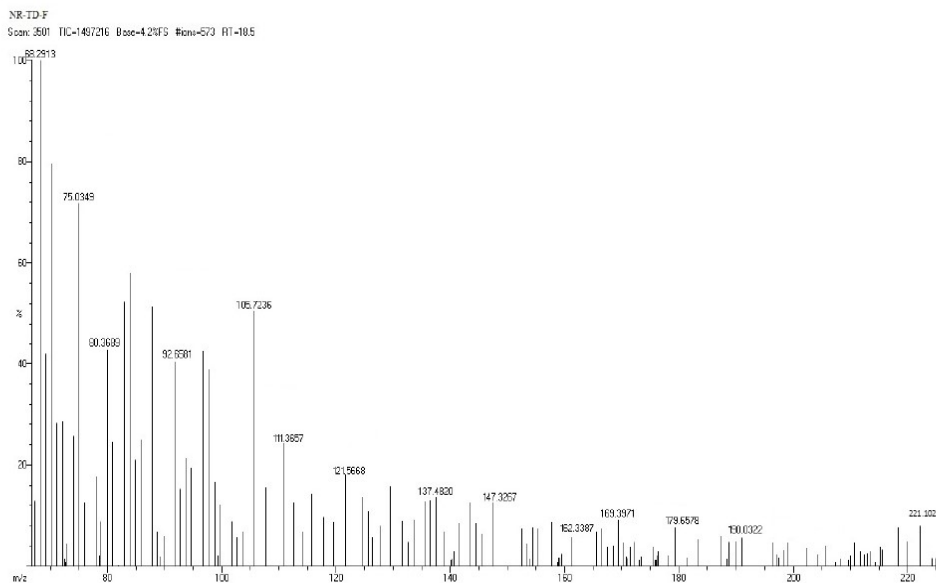


Current Data Parameters
NAME Amino pyridine
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180515
Time 20.52 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 77.73
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.37709999 W
PLW13 0.18968000 W

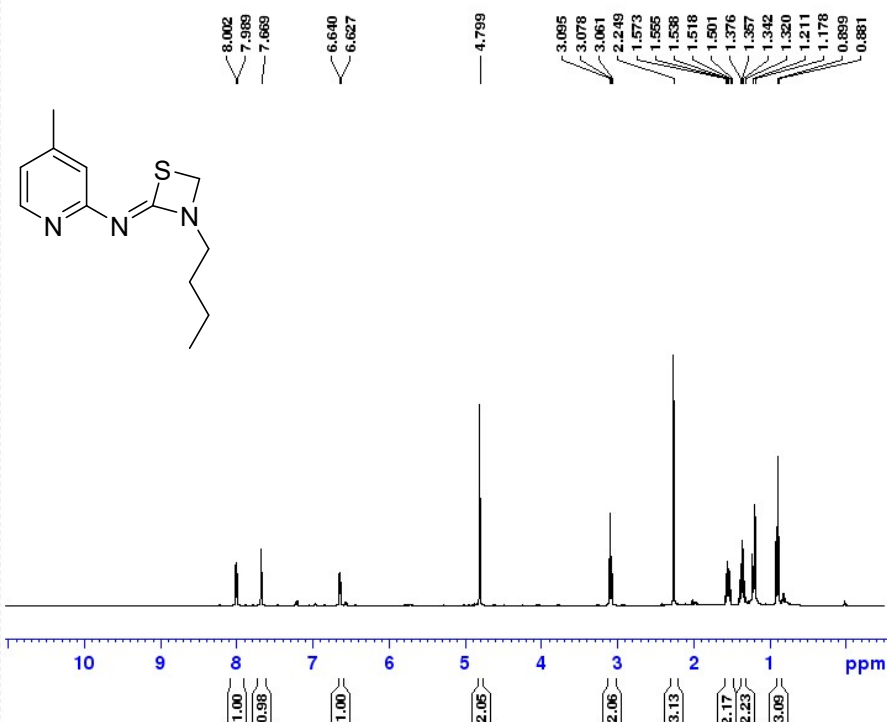
F2 - Processing parameters
SI 32768
SF 100.6450592 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H and ¹³C NMR spectra of compound 40



HRMS and IR spectra compound 4o

Signature SIF VIT VELLORE
NR-518-TD-R

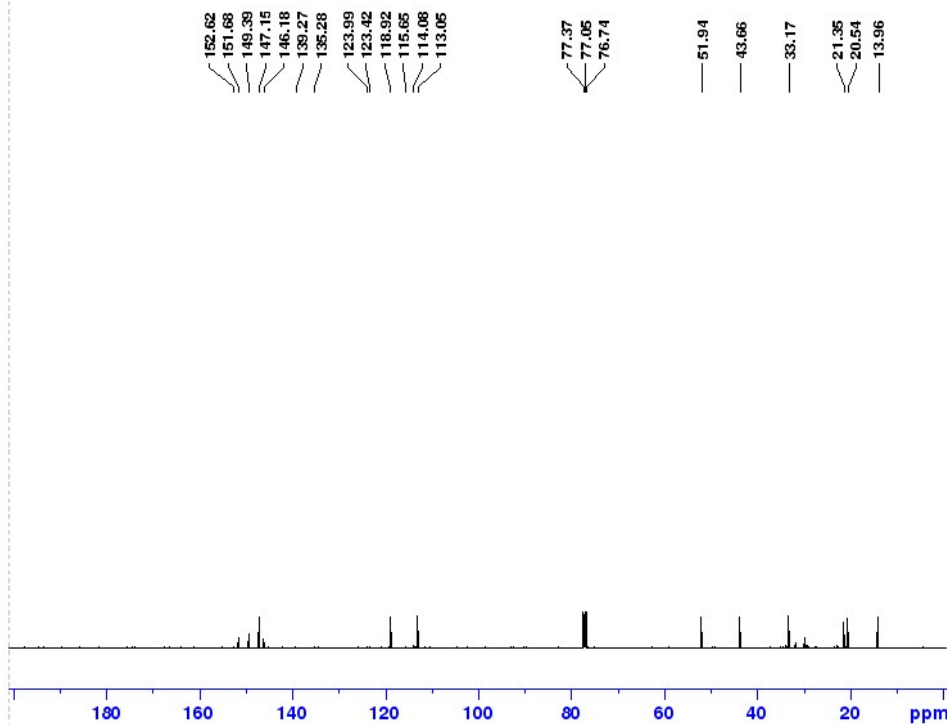


Current Data Parameters
NAME 4-Methyl Amino Pyridi
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180519
Time 10.31 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 56.08
DW 62.400 usec
DE 6.50 usec
TE 299.3 K
D1 1.0000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.27 usec
PLW1 15.0000000 W

F2 - Processing parameters
SI 65536
SF 400.2580366 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Signature SIF VIT VELLORE
NR-518-TD-R

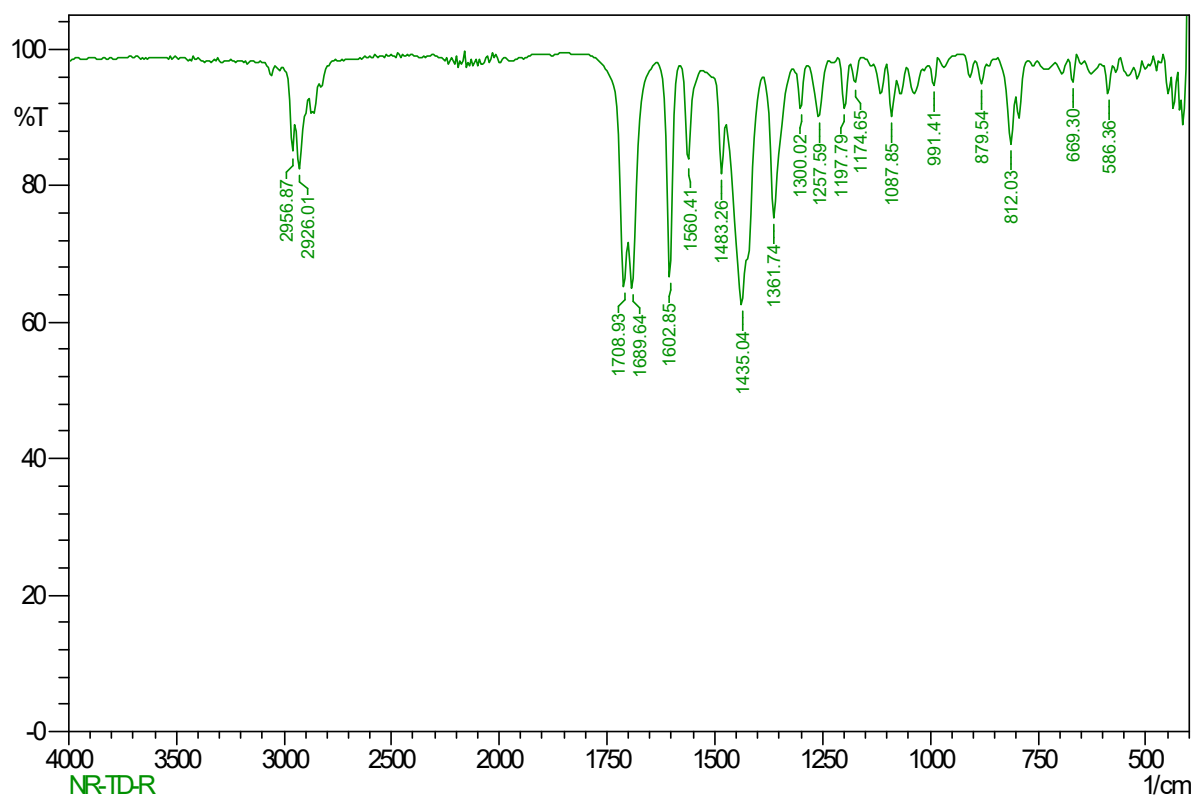
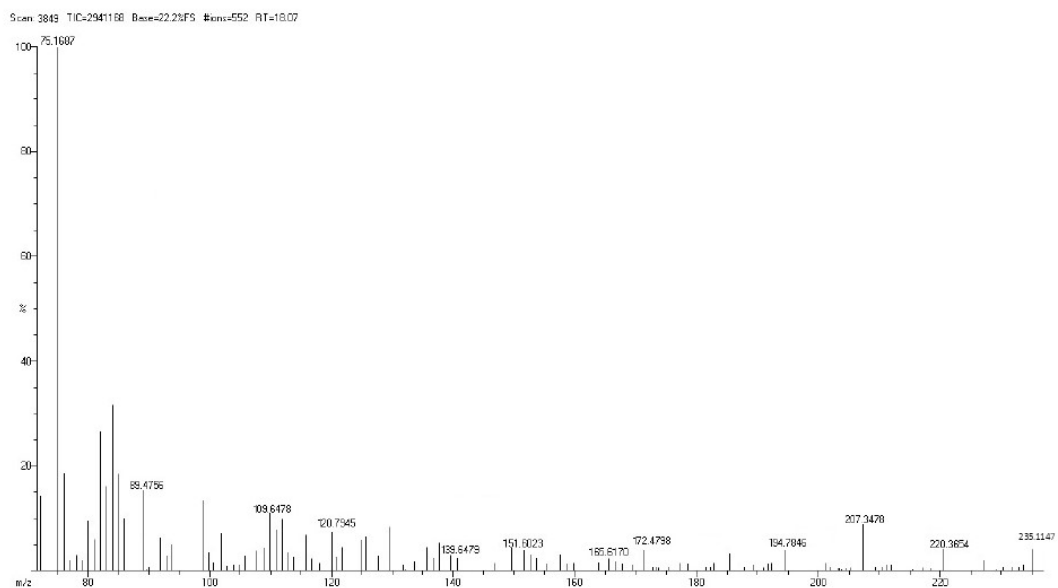


Current Data Parameters
NAME 4-Methyl Amino Pyridi
EXPNO 17
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180519
Time 13.30 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 175.97
DW 20.800 usec
DE 6.50 usec
TE 300.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.0000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.0000000 W
PLW12 0.37709999 W
PLW13 0.18968000 W

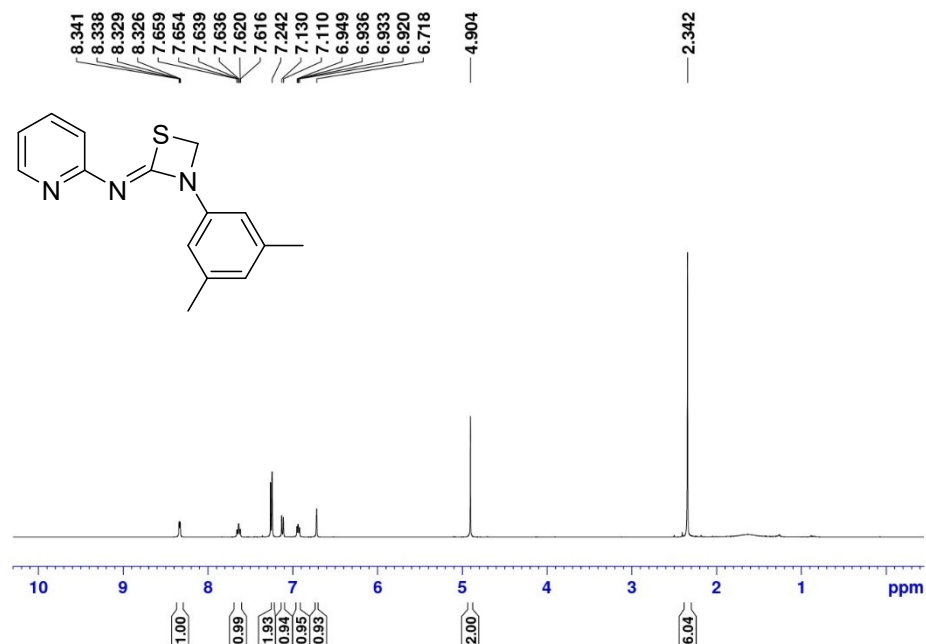
F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^1H and ^{13}C NMR spectra of compound 4p.



HRMS and IR spectra compound 4p.

Signature SIF VIT VELLORE
TD-Q

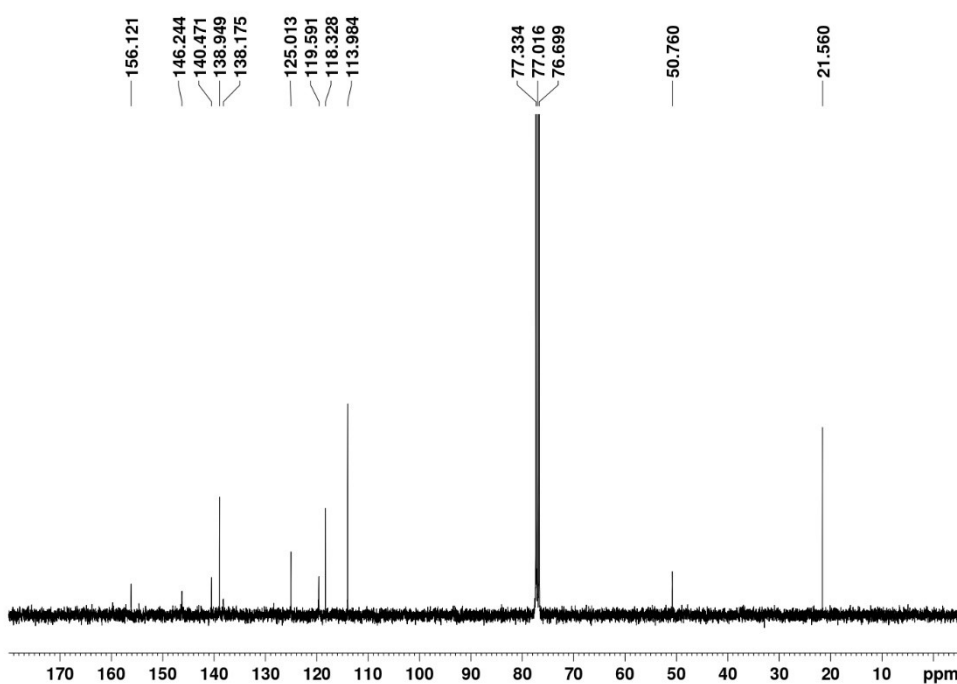


Current Data Parameters
NAME VITCBM2702224
EXPNO 39
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240227
Time 16.50 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDCI3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 175.97
DW 62.400 usec
DE 6.50 usec
TE 303.2 K
D1 1.0000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Signature SIF VIT VELLORE
TD-Q

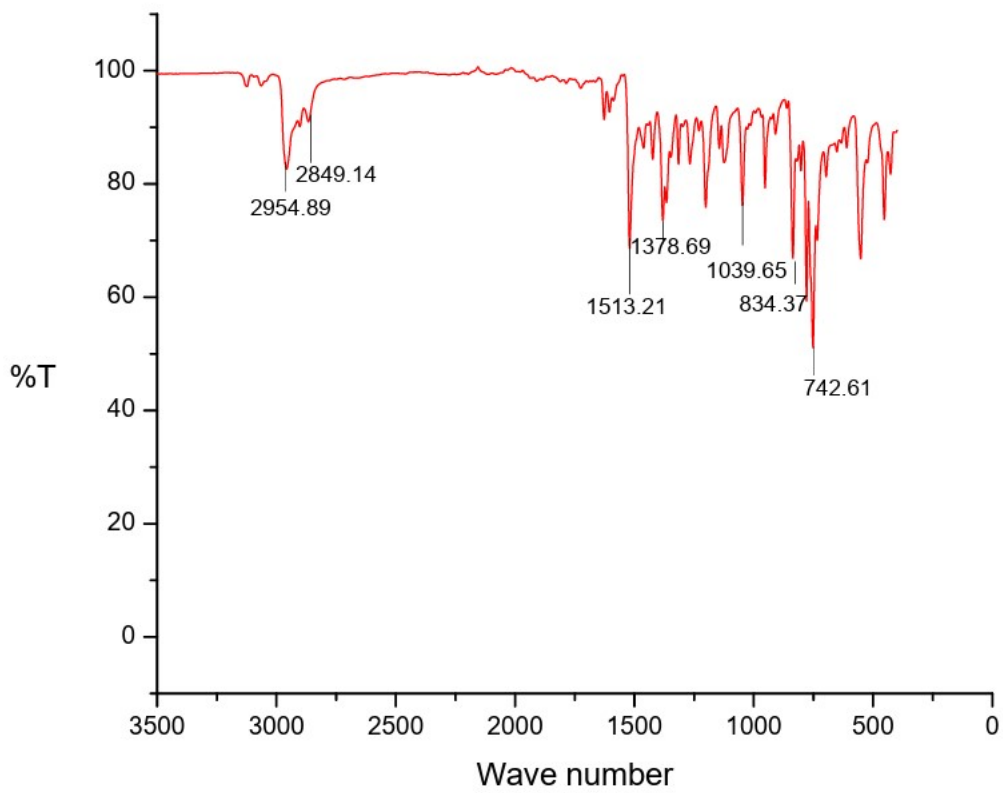
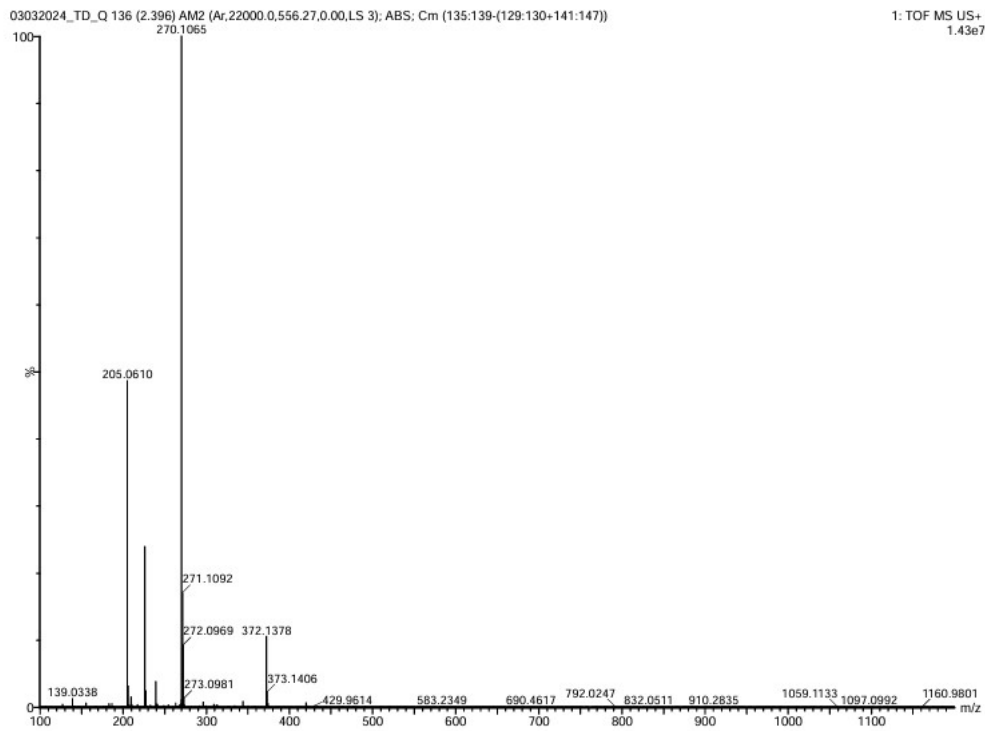


Current Data Parameters
NAME VITCBM2802224
EXPNO 43
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240229
Time 8.24 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT CDCI3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 306.8 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

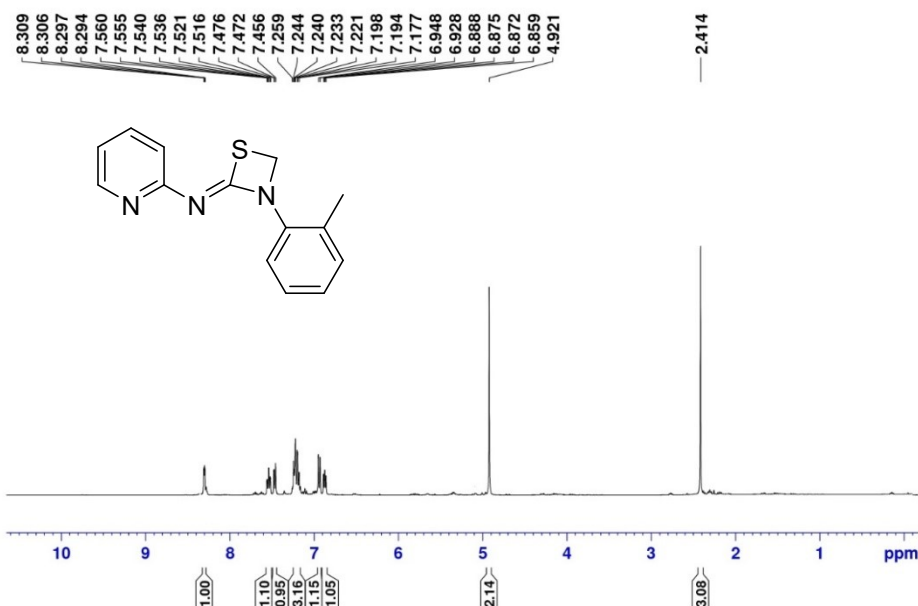
F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H and ¹³C NMR spectra of compound 4q.



HRMS and IR spectra compound 4q.

Signature SIF VIT VELLORE
TD-R

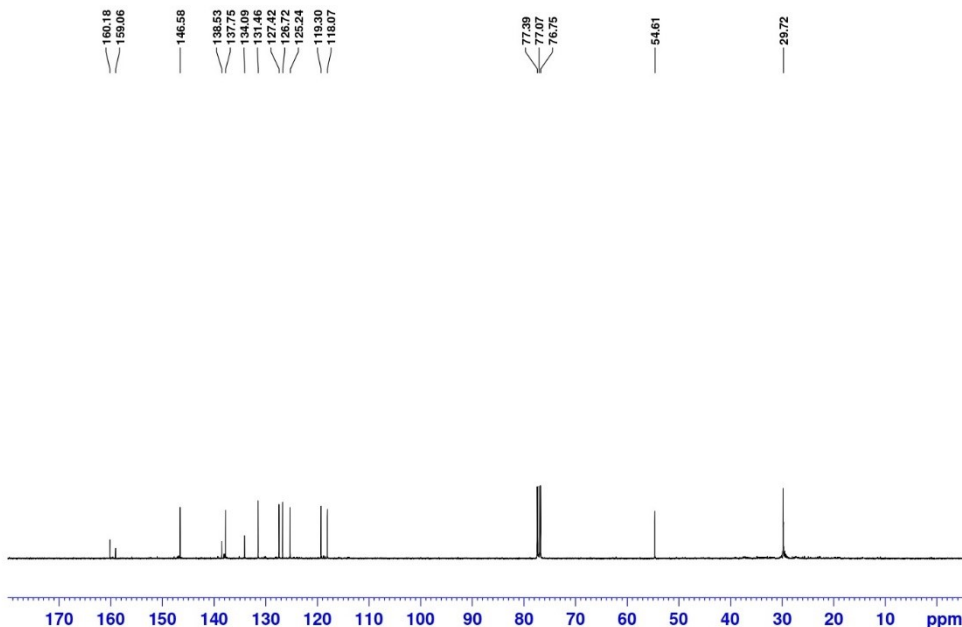


Current Data Parameters
NAME VITCBM280224
EXPNO 41
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240228
Time 17.27 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 35.49
DW 62.400 usec
DE 6.50 usec
TE 302.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580160 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Signature SIF VIT VELLORE
TD-R

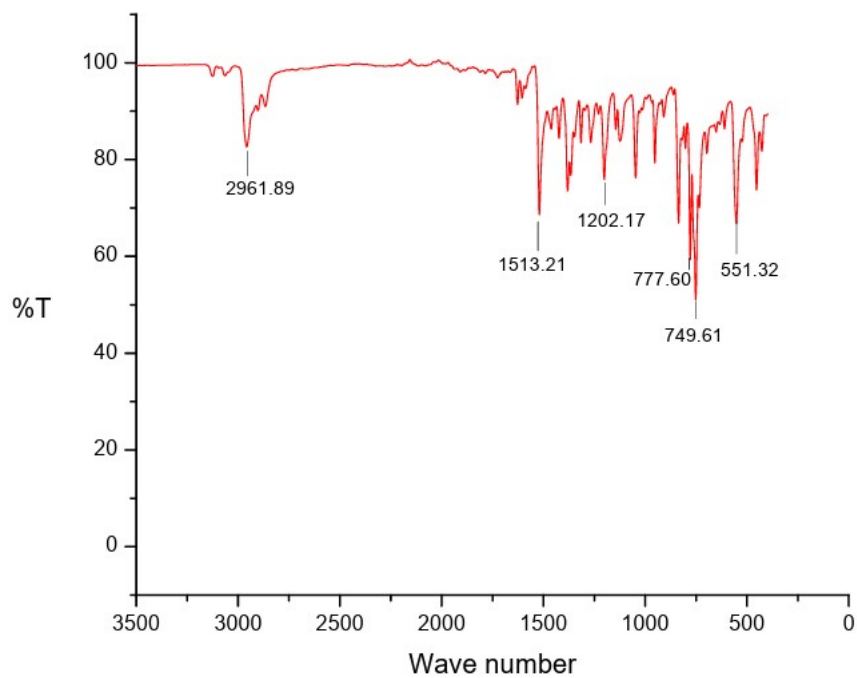
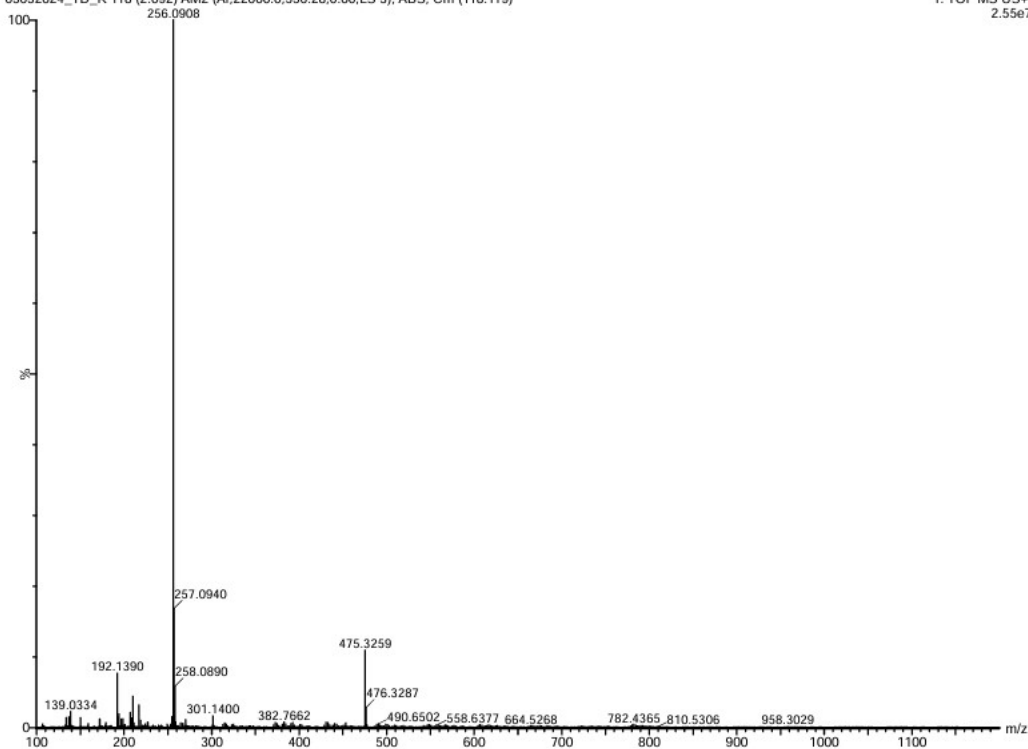


Current Data Parameters
NAME VITCBM2902224
EXPNO 44
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240301
Time 5.55 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 307.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H and ¹³C NMR spectra of compound 4r.



HRMS and IR spectra compound 4r.

Table 1. Crystal data and structure refinement of compound **4g**

| | |
|--|--|
| Chemical formula | C ₁₂ H ₁₀ N ₄ S |
| M_r | 242.30 |
| Crystal system, space group | Triclinic, <i>P</i> 1 |
| Temperature (K) | 293 |
| a, b, c (Å) | 9.7029 (7), 10.6515 (7), 11.9141 (8) |
| α, β, γ (°) | 77.212 (2), 73.407 (2), 74.174 (2) |
| V (Å ³) | 1121.49 (13) |
| Z | 4 |
| Radiation type | Mo $K\alpha$ |
| μ (mm ⁻¹) | 0.27 |
| Crystal size (mm) | 0.21 × 0.18 × 0.15 |
| Data collection | |
| Diffractometer | Bruker <i>APEX-II</i> CCD diffractometer |
| Absorption correction | Multi-scan Bruker AXS <i>SADABS</i> program |
| T_{\min}, T_{\max} | 0.944, 0.959 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 17727, 4598, 4052 |
| R_{int} | 0.020 |
| $(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹) | 0.626 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)], wR(F^2), S$ | 0.038, 0.114, 1.12 |
| No. of reflections | 4598 |
| No. of parameters | 307 |
| No. of restraints | 0 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³) | 0.25, -0.36 |

| | | | |
|-----------------------------------|------------|---------------------------------------|------------|
| a = 9.7029(0.0007) | | alpha= 77.21(0.00) | |
| b = 10.6515(0.0007) | | beta = 73.41(0.00) | |
| c = 11.9141(0.0008) | | gamma= 74.17(0.00) | |
| V = 1121.49(0.13) cubic-Angstrom | | | |
| Niggli reduced cell: | | 9.703 10.651 11.914 77.21 73.41 74.17 | |
| Niggli matrix: | | 94.1463 113.4544 141.9458 | |
| | | 28.0893 33.0124 28.1854 | |
| Transformation matrix: | | 1.00 0.00 0.00 | |
| | | 0.00 1.00 0.00 | |
| | | 0.00 0.00 1.00 | |
| Number of Atoms 54 | | | |
| Atomic coordinates | | | |
| S1 | 0.81801(0) | 0.13405(0) | 0.73670(0) |
| N1 | 1.07944(0) | -0.04469(0) | 0.65543(0) |
| N2 | 1.36149(0) | -0.11364(0) | 0.51074(0) |
| N3 | 1.04897(0) | 0.16473(0) | 0.53250(0) |
| N4 | 0.82121(0) | 0.31836(0) | 0.58773(0) |
| C1 | 1.13234(0) | 0.03965(0) | 0.56325(0) |
| C2 | 1.16812(0) | -0.16373(0) | 0.67319(0) |
| H2 | 1.13492(0) | -0.22543(0) | 0.73675(0) |
| C3 | 1.30550(0) | -0.19833(0) | 0.60175(0) |
| H3 | 1.36176(0) | -0.28335(0) | 0.61685(0) |
| C4 | 1.27500(0) | 0.00440(0) | 0.49291(0) |
| H4 | 1.31035(0) | 0.06671(0) | 0.43102(0) |
| C5 | 0.92278(0) | 0.20222(0) | 0.60032(0) |
| C6 | 0.70403(0) | 0.29664(0) | 0.69329(0) |
| H6A | 0.61369(0) | 0.29233(0) | 0.67611(0) |
| H6B | 0.68403(0) | 0.35797(0) | 0.74826(0) |
| C7 | 0.82080(0) | 0.42991(0) | 0.49964(0) |
| C8 | 0.94233(0) | 0.43993(0) | 0.40468(0) |
| H8 | 1.02602(0) | 0.37132(0) | 0.39791(0) |
| C9 | 0.93795(0) | 0.55214(0) | 0.32069(0) |
| H9 | 1.01902(0) | 0.55868(0) | 0.25701(0) |
| C10 | 0.81490(0) | 0.65482(0) | 0.32990(0) |
| H10 | 0.81277(0) | 0.73014(0) | 0.27274(0) |
| C11 | 0.69510(0) | 0.64501(0) | 0.42439(0) |
| H11 | 0.61229(0) | 0.71446(0) | 0.43116(0) |
| C12 | 0.69671(0) | 0.53328(0) | 0.50911(0) |
| H12 | 0.61503(0) | 0.52719(0) | 0.57232(0) |
| S2 | 0.68538(0) | 0.66542(0) | 0.77645(0) |
| N5 | 0.41962(0) | 0.57993(0) | 0.85778(0) |
| N6 | 0.13176(0) | 0.59322(0) | 0.99572(0) |
| N7 | 0.45077(0) | 0.71726(0) | 0.97686(0) |
| N8 | 0.68183(0) | 0.77830(0) | 0.92495(0) |

| | | | |
|--|-----------------|-----------------|----------------|
| C13 | 0.36586(0) | 0.65052(0) | 0.94630(0) |
| C14 | 0.32973(0) | 0.51388(0) | 0.84133(0) |
| H14 | 0.36403(0) | 0.46307(0) | 0.78059(0) |
| C15 | 0.18959(0) | 0.51781(0) | 0.90994(0) |
| H15 | 0.13316(0) | 0.46704(0) | 0.89679(0) |
| C16 | 0.22025(0) | 0.65890(0) | 1.01256(0) |
| H16 | 0.18392(0) | 0.71286(0) | 1.07094(0) |
| C17 | 0.57901(0) | 0.72166(0) | 0.91096(0) |
| C18 | 0.80025(0) | 0.74774(0) | 0.82097(0) |
| H18A | 0.88907(0) | 0.68874(0) | 0.83983(0) |
| H18B | 0.82297(0) | 0.82526(0) | 0.76557(0) |
| C19 | 0.68162(0) | 0.84704(0) | 1.01288(0) |
| C20 | 0.80742(0) | 0.88811(0) | 1.00808(0) |
| H20 | 0.89181(0) | 0.86893(0) | 0.94787(0) |
| C21 | 0.80630(0) | 0.95778(0) | 1.09353(0) |
| H21 | 0.89054(0) | 0.98558(0) | 1.09016(0) |
| C22 | 0.68300(0) | 0.98658(0) | 1.18327(0) |
| H22 | 0.68326(0) | 1.03392(0) | 1.24005(0) |
| C23 | 0.55870(0) | 0.94464(0) | 1.18833(0) |
| H23 | 0.47526(0) | 0.96306(0) | 1.24951(0) |
| C24 | 0.55643(0) | 0.87565(0) | 1.10380(0) |
| H24 | 0.47170(0) | 0.84844(0) | 1.10759(0) |
| Orthogonal coordinates (Angstrom) | | | |
| Orthogonalization matrix: | | | |
| a b cosgamma c cosbeta 9.70290 2.90484 3.40233 | | | |
| 0 b singamma -c sinbeta cosalpha* 0.00000 10.24775 1.77659 | | | |
| 0 0 c sinbeta sinalpha* 0.00000 0.00000 11.27890 | | | |
| Atom | X | Y | Z |
| S1 | 10.8330(0.0001) | 2.6825(0.0001) | 8.3092(0.0001) |
| N1 | 12.5739(0.0001) | 0.7065(0.0001) | 7.3925(0.0001) |
| N2 | 14.6180(0.0001) | -0.2572(0.0001) | 5.7606(0.0001) |
| N3 | 12.4683(0.0001) | 2.6341(0.0001) | 6.0060(0.0001) |
| N4 | 10.8926(0.0001) | 4.3066(0.0001) | 6.6290(0.0001) |
| C1 | 13.0185(0.0001) | 1.4070(0.0001) | 6.3528(0.0001) |
| C2 | 13.1490(0.0001) | -0.4819(0.0001) | 7.5928(0.0001) |
| H2 | 12.8638(0.0001) | -1.0012(0.0001) | 8.3097(0.0001) |
| C3 | 14.1384(0.0001) | -0.9634(0.0001) | 6.7871(0.0001) |
| H3 | 14.4887(0.0001) | -1.8078(0.0001) | 6.9574(0.0001) |
| C4 | 14.0610(0.0001) | 0.9208(0.0001) | 5.5595(0.0001) |
| H4 | 14.3744(0.0001) | 1.4494(0.0001) | 4.8614(0.0001) |
| C5 | 11.5835(0.0001) | 3.1388(0.0001) | 6.7710(0.0001) |
| C6 | 10.0516(0.0001) | 4.2716(0.0001) | 7.8196(0.0001) |
| H6A | 9.1041(0.0001) | 4.1969(0.0001) | 7.6258(0.0001) |
| H6B | 10.2227(0.0001) | 4.9977(0.0001) | 8.4396(0.0001) |
| C7 | 10.9129(0.0001) | 5.2933(0.0001) | 5.6354(0.0001) |

| | | | | | | |
|---|-----------------|-----------------|-----------------|--------|---------|--------|
| C8 | 11.7981(0.0001) | 5.2272(0.0001) | 4.5643(0.0001) | | | |
| H8 | 12.3878(0.0001) | 4.5121(0.0001) | 4.4880(0.0001) | | | |
| C9 | 11.7958(0.0001) | 6.2279(0.0001) | 3.6170(0.0001) | | | |
| H9 | 12.3848(0.0001) | 6.1818(0.0001) | 2.8988(0.0001) | | | |
| C10 | 10.9315(0.0001) | 7.2965(0.0001) | 3.7209(0.0001) | | | |
| H10 | 10.9351(0.0001) | 7.9668(0.0001) | 3.0762(0.0001) | | | |
| C11 | 10.0621(0.0001) | 7.3639(0.0001) | 4.7867(0.0001) | | | |
| H11 | 9.4833(0.0001) | 8.0876(0.0001) | 4.8630(0.0001) | | | |
| C12 | 10.0414(0.0001) | 6.3694(0.0001) | 5.7422(0.0001) | | | |
| H12 | 9.4462(0.0001) | 6.4193(0.0001) | 6.4551(0.0001) | | | |
| S2 | 11.2248(0.0001) | 8.1985(0.0001) | 8.7575(0.0001) | | | |
| N5 | 8.6746(0.0001) | 7.4669(0.0001) | 9.6748(0.0001) | | | |
| N6 | 6.3894(0.0001) | 7.8482(0.0001) | 11.2306(0.0001) | | | |
| N7 | 9.7809(0.0001) | 9.0858(0.0001) | 11.0179(0.0001) | | | |
| N8 | 12.0235(0.0001) | 9.6191(0.0001) | 10.4324(0.0001) | | | |
| C13 | 8.6592(0.0001) | 8.3476(0.0001) | 10.6732(0.0001) | | | |
| C14 | 7.5546(0.0001) | 6.7608(0.0001) | 9.4893(0.0001) | | | |
| H14 | 7.5331(0.0001) | 6.1322(0.0001) | 8.8042(0.0001) | | | |
| C15 | 6.4396(0.0001) | 6.9230(0.0001) | 10.2631(0.0001) | | | |
| H15 | 5.6999(0.0001) | 6.3793(0.0001) | 10.1148(0.0001) | | | |
| C16 | 7.4961(0.0001) | 8.5511(0.0001) | 11.4206(0.0001) | | | |
| H16 | 7.4990(0.0001) | 9.2078(0.0001) | 12.0790(0.0001) | | | |
| C17 | 10.8138(0.0001) | 9.0138(0.0001) | 10.2746(0.0001) | | | |
| C18 | 12.7300(0.0001) | 9.1212(0.0001) | 9.2596(0.0001) | | | |
| H18A | 13.4846(0.0001) | 8.5501(0.0001) | 9.4724(0.0001) | | | |
| H18B | 12.9872(0.0001) | 9.8172(0.0001) | 8.6348(0.0001) | | | |
| C19 | 12.5204(0.0001) | 10.4797(0.0001) | 11.4242(0.0001) | | | |
| C20 | 13.8440(0.0001) | 10.8921(0.0001) | 11.3700(0.0001) | | | |
| H20 | 14.4022(0.0001) | 10.5886(0.0001) | 10.6909(0.0001) | | | |
| C21 | 14.3262(0.0001) | 11.7578(0.0001) | 12.3338(0.0001) | | | |
| H21 | 15.2129(0.0001) | 12.0367(0.0001) | 12.2958(0.0001) | | | |
| C22 | 13.5188(0.0001) | 12.2124(0.0001) | 13.3460(0.0001) | | | |
| H22 | 13.8520(0.0001) | 12.7984(0.0001) | 13.9864(0.0001) | | | |
| C23 | 12.2081(0.0001) | 11.7916(0.0001) | 13.4031(0.0001) | | | |
| H23 | 11.6602(0.0001) | 12.0891(0.0001) | 14.0931(0.0001) | | | |
| C24 | 11.6981(0.0001) | 10.9344(0.0001) | 12.4497(0.0001) | | | |
| H24 | 10.8098(0.0001) | 10.6623(0.0001) | 12.4924(0.0001) | | | |
| Displacement parameters, U(I,J)x10**4 exp(-2*pi**2(U11*h**2*(a*)**2+...+2*U12*h*k*(a*)*(b*)+...) | | | | | | |
| Atom | U11 | U22 | U33 | U23 | U13 | U12 |
| S1 | 417(0) | 492(0) | 435(0) | 11(0) | -7(0) | -91(0) |
| N1 | 365(0) | 406(0) | 523(0) | -48(0) | -101(0) | -83(0) |
| N2 | 555(0) | 575(0) | 518(0) | -92(0) | 2(0) | 148(0) |
| N3 | 341(0) | 377(0) | 385(0) | -70(0) | -43(0) | -15(0) |

| | | | | | | |
|------|--------|--------|--------|---------|---------|---------|
| N4 | 290(0) | 399(0) | 403(0) | -61(0) | 13(0) | -28(0) |
| C1 | 357(0) | 381(0) | 366(0) | -114(0) | -94(0) | -36(0) |
| C2 | 487(0) | 391(0) | 609(0) | -17(0) | -172(0) | -96(0) |
| H2 | 600(0) | | | | | |
| C3 | 573(0) | 404(0) | 572(0) | -118(0) | -176(0) | 65(0) |
| H3 | 640(0) | | | | | |
| C4 | 481(0) | 520(0) | 420(0) | -42(0) | 25(0) | 60(0) |
| H4 | 650(0) | | | | | |
| C5 | 324(0) | 368(0) | 348(0) | -70(0) | -65(0) | -79(0) |
| C6 | 365(0) | 519(0) | 422(0) | -58(0) | 38(0) | -36(0) |
| H6A | 580(0) | | | | | |
| H6B | 580(0) | | | | | |
| C7 | 325(0) | 353(0) | 361(0) | -105(0) | -76(0) | -42(0) |
| C8 | 366(0) | 399(0) | 396(0) | -89(0) | -37(0) | -28(0) |
| H8 | 490(0) | | | | | |
| C9 | 492(0) | 484(0) | 398(0) | -60(0) | -42(0) | -106(0) |
| H9 | 570(0) | | | | | |
| C10 | 645(0) | 403(0) | 518(0) | -9(0) | -190(0) | -55(0) |
| H10 | 640(0) | | | | | |
| C11 | 515(0) | 423(0) | 638(0) | -110(0) | -171(0) | 77(0) |
| H11 | 660(0) | | | | | |
| C12 | 363(0) | 454(0) | 500(0) | -127(0) | -43(0) | 10(0) |
| H12 | 560(0) | | | | | |
| S2 | 410(0) | 587(0) | 494(0) | -232(0) | 15(0) | -145(0) |
| N5 | 363(0) | 462(0) | 509(0) | -128(0) | -57(0) | -124(0) |
| N6 | 405(0) | 831(0) | 548(0) | -164(0) | -31(0) | -305(0) |
| N7 | 317(0) | 468(0) | 393(0) | -74(0) | -41(0) | -158(0) |
| N8 | 278(0) | 463(0) | 405(0) | -107(0) | 16(0) | -145(0) |
| C13 | 333(0) | 387(0) | 355(0) | -3(0) | -83(0) | -113(0) |
| C14 | 450(0) | 486(0) | 567(0) | -164(0) | -105(0) | -131(0) |
| H14 | 580(0) | | | | | |
| C15 | 449(0) | 535(0) | 542(0) | -41(0) | -166(0) | -228(0) |
| H15 | 580(0) | | | | | |
| C16 | 378(0) | 727(0) | 470(0) | -192(0) | -1(0) | -237(0) |
| H16 | 610(0) | | | | | |
| C17 | 313(0) | 342(0) | 362(0) | -43(0) | -66(0) | -80(0) |
| C18 | 341(0) | 575(0) | 463(0) | -156(0) | 57(0) | -176(0) |
| H18A | 560(0) | | | | | |
| H18B | 560(0) | | | | | |
| C19 | 322(0) | 335(0) | 352(0) | -9(0) | -61(0) | -111(0) |
| C20 | 371(0) | 530(0) | 490(0) | -54(0) | -51(0) | -204(0) |
| H20 | 550(0) | | | | | |
| C21 | 538(0) | 600(0) | 619(0) | -73(0) | -173(0) | -290(0) |
| H21 | 660(0) | | | | | |
| C22 | 674(0) | 488(0) | 493(0) | -91(0) | -217(0) | -183(0) |

| H22 | 630(0) | | | | | |
|--|---------|-------------|--------|---------|------------|----------------|
| C23 | 498(0) | 544(0) | 420(0) | -127(0) | -48(0) | -118(0) |
| H23 | 590(0) | | | | | |
| C24 | 366(0) | 509(0) | 413(0) | -107(0) | -24(0) | -157(0) |
| H24 | 510(0) | | | | | |
| Principal axes of the thermal ellipsoids, Uequiv. ($\times 10^4 \text{ \AA}^2$) and Bequiv. (\AA^2) | | | | | | |
| Atom | R1 | R2 | R3 | Uequiv. | Bequiv. | Rmax/Rmin |
| S1 | 668(0) | 451(0) | 334(0) | 484(0) | 3.82(0.00) | 2 |
| N1 | 542(0) | 406(0) | 364(0) | 437(0) | 3.45(0.00) | 1.49 |
| N2 | 1051(0) | 536(0) | 311(0) | 633(0) | 4.99(0.00) | 3.37 |
| N3 | 484(0) | 391(0) | 291(0) | 389(0) | 3.07(0.00) | 1.66 |
| N4 | 539(0) | 399(0) | 247(0) | 395(0) | 3.12(0.00) | 2.18 |
| C1 | 444(0) | 351(0) | 306(0) | 367(0) | 2.90(0.00) | 1.45 |
| C2 | 637(0) | 473(0) | 383(0) | 497(0) | 3.93(0.00) | 1.66 |
| C3 | 733(0) | 552(0) | 326(0) | 537(0) | 4.24(0.00) | 2.25 |
| C4 | 878(0) | 437(0) | 313(0) | 543(0) | 4.29(0.00) | 2.81 |
| C5 | 375(0) | 348(0) | 319(0) | 347(0) | 2.74(0.00) | 1.17 |
| C6 | 678(0) | 479(0) | 281(0) | 479(0) | 3.78(0.00) | 2.42 |
| C7 | 405(0) | 343(0) | 292(0) | 347(0) | 2.74(0.00) | 1.39 |
| C8 | 491(0) | 421(0) | 306(0) | 406(0) | 3.21(0.00) | 1.6 |
| C9 | 562(0) | 483(0) | 377(0) | 474(0) | 3.74(0.00) | 1.49 |
| C10 | 680(0) | 554(0) | 369(0) | 534(0) | 4.22(0.00) | 1.84 |
| C11 | 709(0) | 630(0) | 314(0) | 551(0) | 4.35(0.00) | 2.26 |
| C12 | 568(0) | 527(0) | 297(0) | 464(0) | 3.67(0.00) | 1.91 |
| S2 | 711(0) | 435(0) | 332(0) | 493(0) | 3.89(0.00) | 2.14 |
| N5 | 557(0) | 418(0) | 344(0) | 440(0) | 3.47(0.00) | 1.62 |
| N6 | 875(0) | 535(0) | 298(0) | 569(0) | 4.49(0.00) | 2.94 |
| N7 | 488(0) | 403(0) | 269(0) | 387(0) | 3.05(0.00) | 1.82 |
| N8 | 520(0) | 403(0) | 229(0) | 384(0) | 3.03(0.00) | 2.27 |
| C13 | 438(0) | 341(0) | 303(0) | 361(0) | 2.85(0.00) | 1.45 |
| C14 | 613(0) | 460(0) | 385(0) | 486(0) | 3.84(0.00) | 1.59 |
| C15 | 627(0) | 512(0) | 305(0) | 481(0) | 3.80(0.00) | 2.05 |
| C16 | 781(0) | 433(0) | 309(0) | 507(0) | 4.01(0.00) | 2.53 |
| C17 | 380(0) | 340(0) | 308(0) | 343(0) | 2.71(0.00) | 1.24 |
| C18 | 665(0) | 471(0) | 261(0) | 465(0) | 3.67(0.00) | 2.55 |
| C19 | 400(0) | 351(0) | 270(0) | 340(0) | 2.69(0.00) | 1.48 |
| C20 | 562(0) | 522(0) | 290(0) | 458(0) | 3.62(0.00) | 1.94 |
| C21 | 713(0) | 609(0) | 323(0) | 549(0) | 4.33(0.00) | 2.21 |
| C22 | 692(0) | 502(0) | 371(0) | 522(0) | 4.12(0.00) | 1.86 |
| C23 | 567(0) | 526(0) | 383(0) | 492(0) | 3.88(0.00) | 1.48 |
| C24 | 544(0) | 417(0) | 318(0) | 426(0) | 3.37(0.00) | 1.71 |
| Bond distances (Angstrom) | | | | | | |
| (Corrections following Busing & Levy, Acta Cryst.(1964).17,142) | | | | | | |
| | | Uncorrected | Lower | Upper | Riding | Non-correlated |

| | | Distance | bound | bound | motion | motion |
|-----|------|-----------|--------|--------|--------|--------|
| S1 | -C5 | 1.7714(1) | 1.7727 | 1.8724 | 1.7831 | 1.8226 |
| S1 | -C6 | 1.8372(1) | 1.8372 | 1.9452 | 1.8377 | 1.8912 |
| N1 | -C1 | 1.3302(1) | 1.3307 | 1.4453 | 1.3382 | 1.388 |
| N1 | -C2 | 1.3353(1) | 1.3356 | 1.4857 | 1.3416 | 1.4106 |
| N2 | -C3 | 1.3351(1) | 1.3358 | 1.5023 | 1.3462 | 1.4191 |
| N2 | -C4 | 1.3184(1) | 1.319 | 1.5257 | 1.3288 | 1.4223 |
| N3 | -C1 | 1.3889(1) | 1.389 | 1.5016 | 1.3921 | 1.4453 |
| N3 | -C5 | 1.2738(1) | 1.2741 | 1.398 | 1.2794 | 1.336 |
| N4 | -C5 | 1.3643(1) | 1.3647 | 1.4766 | 1.3705 | 1.4207 |
| N4 | -C6 | 1.4581(1) | 1.4585 | 1.5968 | 1.4661 | 1.5277 |
| N4 | -C7 | 1.4004(1) | 1.4006 | 1.502 | 1.4056 | 1.4513 |
| C1 | -C4 | 1.3974(1) | 1.3998 | 1.5402 | 1.4162 | 1.47 |
| C2 | -H2 | 0.9300(0) | | | | |
| C2 | -C3 | 1.3638(1) | 1.364 | 1.511 | 1.3682 | 1.4375 |
| C3 | -H3 | 0.9299(1) | | | | |
| C4 | -H4 | 0.9300(0) | | | | |
| C6 | -H6A | 0.9700(1) | | | | |
| C6 | -H6B | 0.9700(0) | | | | |
| C7 | -C8 | 1.3911(1) | 1.3914 | 1.5026 | 1.3975 | 1.447 |
| C7 | -C12 | 1.3889(1) | 1.3901 | 1.5175 | 1.4012 | 1.4538 |
| C8 | -H8 | 0.9300(1) | | | | |
| C8 | -C9 | 1.3780(1) | 1.3783 | 1.5066 | 1.3846 | 1.4424 |
| C9 | -H9 | 0.9300(1) | | | | |
| C9 | -C10 | 1.3783(1) | 1.3786 | 1.5271 | 1.3849 | 1.4529 |
| C10 | -H10 | 0.9300(0) | | | | |
| C10 | -C11 | 1.3770(1) | 1.3771 | 1.522 | 1.3786 | 1.4495 |
| C11 | -H11 | 0.9298(1) | | | | |
| C11 | -C12 | 1.3793(1) | 1.3798 | 1.5231 | 1.3881 | 1.4515 |
| C12 | -H12 | 0.9300(1) | | | | |
| S2 | -C17 | 1.7707(1) | 1.7724 | 1.8709 | 1.7836 | 1.8216 |
| S2 | -C18 | 1.8355(1) | 1.8355 | 1.9442 | 1.8377 | 1.8899 |
| N5 | -C13 | 1.3314(1) | 1.3321 | 1.4465 | 1.3402 | 1.3893 |
| N5 | -C14 | 1.3370(1) | 1.3371 | 1.4878 | 1.3414 | 1.4124 |
| N6 | -C15 | 1.3396(1) | 1.3403 | 1.4852 | 1.3494 | 1.4128 |
| N6 | -C16 | 1.3248(1) | 1.325 | 1.5113 | 1.3317 | 1.4182 |
| N7 | -C13 | 1.3864(1) | 1.3865 | 1.4981 | 1.3904 | 1.4423 |
| N7 | -C17 | 1.2745(1) | 1.2748 | 1.3991 | 1.2807 | 1.337 |
| N8 | -C17 | 1.3619(1) | 1.3622 | 1.4739 | 1.3672 | 1.418 |
| N8 | -C18 | 1.4569(1) | 1.4573 | 1.5908 | 1.4648 | 1.5241 |
| N8 | -C19 | 1.4040(1) | 1.4042 | 1.5012 | 1.4083 | 1.4527 |
| C13 | -C16 | 1.3974(1) | 1.3992 | 1.5353 | 1.4133 | 1.4672 |
| C14 | -H14 | 0.9300(0) | | | | |
| C14 | -C15 | 1.3668(1) | 1.3668 | 1.511 | 1.3675 | 1.4389 |
| C15 | -H15 | 0.9299(0) | | | | |

| | | | | | | |
|------------------------------|-------|-----------|--------|--------|--------|--------|
| C16 | -H16 | 0.9300(0) | | | | |
| C18 | -H18A | 0.9700(1) | | | | |
| C18 | -H18B | 0.9700(1) | | | | |
| C19 | -C20 | 1.3874(1) | 1.3886 | 1.5139 | 1.3998 | 1.4512 |
| C19 | -C24 | 1.3909(1) | 1.3916 | 1.5066 | 1.3999 | 1.4491 |
| C20 | -H20 | 0.9300(1) | | | | |
| C20 | -C21 | 1.3824(1) | 1.383 | 1.5245 | 1.3918 | 1.4538 |
| C21 | -H21 | 0.9303(1) | | | | |
| C21 | -C22 | 1.3722(1) | 1.3723 | 1.5118 | 1.3756 | 1.4421 |
| C22 | -H22 | 0.9298(0) | | | | |
| C22 | -C23 | 1.3778(1) | 1.3778 | 1.5219 | 1.3809 | 1.4499 |
| C23 | -H23 | 0.9300(1) | | | | |
| C23 | -C24 | 1.3798(1) | 1.3801 | 1.517 | 1.386 | 1.4485 |
| C24 | -H24 | 0.9300(1) | | | | |
| Number of bond distances: 58 | | | | | | |
| Bond angles (deg) | | | | | | |
| | | | Angle | S.U. | | |
| C5 | -S1 | -C6 | 74.1 | 0 | | |
| C1 | -N1 | -C2 | 116.23 | 0.01 | | |
| C3 | -N2 | -C4 | 115.98 | 0.01 | | |
| C1 | -N3 | -C5 | 118.38 | 0.01 | | |
| C5 | -N4 | -C6 | 100.75 | 0.01 | | |
| C5 | -N4 | -C7 | 132.03 | 0.01 | | |
| C6 | -N4 | -C7 | 127.21 | 0.01 | | |
| N1 | -C1 | -N3 | 121.88 | 0.01 | | |
| N1 | -C1 | -C4 | 120.66 | 0.01 | | |
| N3 | -C1 | -C4 | 117.47 | 0.01 | | |
| N1 | -C2 | -H2 | 118.72 | 0.01 | | |
| N1 | -C2 | -C3 | 122.55 | 0.01 | | |
| H2 | -C2 | -C3 | 118.73 | 0.01 | | |
| N2 | -C3 | -C2 | 121.88 | 0.01 | | |
| N2 | -C3 | -H3 | 119.07 | 0.01 | | |
| C2 | -C3 | -H3 | 119.06 | 0.01 | | |
| N2 | -C4 | -C1 | 122.65 | 0.01 | | |
| N2 | -C4 | -H4 | 118.68 | 0.01 | | |
| C1 | -C4 | -H4 | 118.67 | 0.01 | | |
| S1 | -C5 | -N3 | 135.54 | 0.01 | | |
| S1 | -C5 | -N4 | 95.52 | 0 | | |
| N3 | -C5 | -N4 | 128.93 | 0.01 | | |
| S1 | -C6 | -N4 | 89.61 | 0 | | |
| S1 | -C6 | -H6A | 113.71 | 0.01 | | |
| S1 | -C6 | -H6B | 113.71 | 0.01 | | |
| N4 | -C6 | -H6A | 113.71 | 0.01 | | |
| N4 | -C6 | -H6B | 113.71 | 0.01 | | |

| | | | | |
|-----|------|-------|--------|------|
| H6A | -C6 | -H6B | 110.95 | 0.01 |
| N4 | -C7 | -C8 | 121.47 | 0.01 |
| N4 | -C7 | -C12 | 118.83 | 0.01 |
| C8 | -C7 | -C12 | 119.69 | 0.01 |
| C7 | -C8 | -H8 | 120.21 | 0.01 |
| C7 | -C8 | -C9 | 119.59 | 0.01 |
| H8 | -C8 | -C9 | 120.2 | 0.01 |
| C8 | -C9 | -H9 | 119.6 | 0.01 |
| C8 | -C9 | -C10 | 120.81 | 0.01 |
| H9 | -C9 | -C10 | 119.59 | 0.01 |
| C9 | -C10 | -H10 | 120.27 | 0.01 |
| C9 | -C10 | -C11 | 119.48 | 0.01 |
| H10 | -C10 | -C11 | 120.25 | 0.01 |
| C10 | -C11 | -H11 | 119.64 | 0.01 |
| C10 | -C11 | -C12 | 120.69 | 0.01 |
| H11 | -C11 | -C12 | 119.67 | 0.01 |
| C7 | -C12 | -C11 | 119.73 | 0.01 |
| C7 | -C12 | -H12 | 120.14 | 0.01 |
| C11 | -C12 | -H12 | 120.13 | 0.01 |
| C17 | -S2 | -C18 | 74.01 | 0 |
| C13 | -N5 | -C14 | 116.34 | 0.01 |
| C15 | -N6 | -C16 | 116.02 | 0.01 |
| C13 | -N7 | -C17 | 118.73 | 0.01 |
| C17 | -N8 | -C18 | 100.7 | 0.01 |
| C17 | -N8 | -C19 | 131.96 | 0.01 |
| C18 | -N8 | -C19 | 127.34 | 0.01 |
| N5 | -C13 | -N7 | 121.96 | 0.01 |
| N5 | -C13 | -C16 | 120.47 | 0.01 |
| N7 | -C13 | -C16 | 117.57 | 0.01 |
| N5 | -C14 | -H14 | 118.59 | 0.01 |
| N5 | -C14 | -C15 | 122.83 | 0.01 |
| H14 | -C14 | -C15 | 118.58 | 0.01 |
| N6 | -C15 | -C14 | 121.43 | 0.01 |
| N6 | -C15 | -H15 | 119.28 | 0.01 |
| C14 | -C15 | -H15 | 119.29 | 0.01 |
| N6 | -C16 | -C13 | 122.77 | 0.01 |
| N6 | -C16 | -H16 | 118.61 | 0.01 |
| C13 | -C16 | -H16 | 118.62 | 0.01 |
| S2 | -C17 | -N7 | 135.55 | 0.01 |
| S2 | -C17 | -N8 | 95.61 | 0 |
| N7 | -C17 | -N8 | 128.84 | 0.01 |
| S2 | -C18 | -N8 | 89.68 | 0 |
| S2 | -C18 | -H18A | 113.7 | 0.01 |
| S2 | -C18 | -H18B | 113.69 | 0.01 |
| N8 | -C18 | -H18A | 113.7 | 0.01 |

| | | | | | |
|----------------------|------|-------|--------|--------|------|
| N8 | -C18 | -H18B | 113.7 | 0.01 | |
| H18A | -C18 | -H18B | 110.95 | 0.01 | |
| N8 | -C19 | -C20 | 119.49 | 0.01 | |
| N8 | -C19 | -C24 | 120.8 | 0.01 | |
| C20 | -C19 | -C24 | 119.71 | 0.01 | |
| C19 | -C20 | -H20 | 120.28 | 0.01 | |
| C19 | -C20 | -C21 | 119.45 | 0.01 | |
| H20 | -C20 | -C21 | 120.27 | 0.01 | |
| C20 | -C21 | -H21 | 119.46 | 0.01 | |
| C20 | -C21 | -C22 | 121.1 | 0.01 | |
| H21 | -C21 | -C22 | 119.45 | 0.01 | |
| C21 | -C22 | -H22 | 120.39 | 0.01 | |
| C21 | -C22 | -C23 | 119.28 | 0.01 | |
| H22 | -C22 | -C23 | 120.32 | 0.01 | |
| C22 | -C23 | -H23 | 119.57 | 0.01 | |
| C22 | -C23 | -C24 | 120.85 | 0.01 | |
| H23 | -C23 | -C24 | 119.58 | 0.01 | |
| C19 | -C24 | -C23 | 119.61 | 0.01 | |
| C19 | -C24 | -H24 | 120.19 | 0.01 | |
| C23 | -C24 | -H24 | 120.2 | 0.01 | |
| Number of angles: 92 | | | | | |
| Torsion angles (deg) | | | | | |
| Angle | | | | | |
| S.U. | | | | | |
| C6 | S1 | C5 | N3 | 179.75 | 0.01 |
| C6 | S1 | C5 | N4 | 1.05 | 0 |
| C5 | S1 | C6 | N4 | 0.98 | 0 |
| C5 | S1 | C6 | H6A | 114.88 | 0.01 |
| C5 | S1 | C6 | H6B | 116.84 | 0.01 |
| C2 | N1 | C1 | N3 | 177.48 | 0.01 |
| C2 | N1 | C1 | C4 | 2.06 | 0.01 |
| C1 | N1 | C2 | H2 | 179.94 | 0.01 |
| C1 | N1 | C2 | C3 | 0.08 | 0.01 |
| C4 | N2 | C3 | C2 | 1.19 | 0.01 |
| C4 | N2 | C3 | H3 | 178.79 | 0.01 |
| C3 | N2 | C4 | C1 | 0.84 | 0.01 |
| C3 | N2 | C4 | H4 | 179.17 | 0.01 |
| C5 | N3 | C1 | N1 | 5.38 | 0.01 |
| C5 | N3 | C1 | C4 | 175.06 | 0.01 |
| C1 | N3 | C5 | S1 | 2.22 | 0.01 |
| C1 | N3 | C5 | N4 | 178.8 | 0.01 |
| C6 | N4 | C5 | S1 | 1.3 | 0.01 |
| C6 | N4 | C5 | N3 | 179.43 | 0.01 |
| C7 | N4 | C5 | S1 | 179.89 | 0.01 |
| C7 | N4 | C5 | N3 | 0.61 | 0.01 |

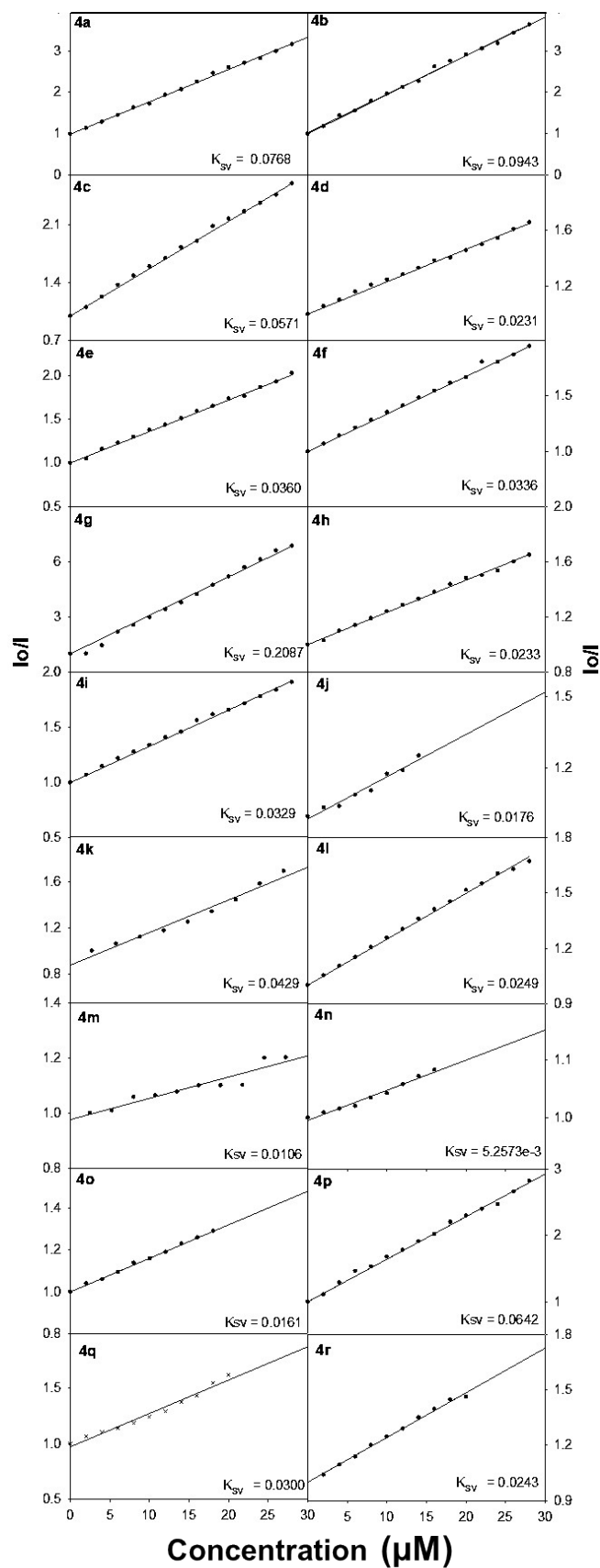
| | | | | | |
|-----|-----|-----|-----|--------|------|
| C5 | N4 | C6 | S1 | 1.25 | 0.01 |
| C5 | N4 | C6 | H6A | 114.61 | 0.01 |
| C5 | N4 | C6 | H6B | 117.11 | 0.01 |
| C7 | N4 | C6 | S1 | 179.86 | 0.01 |
| C7 | N4 | C6 | H6A | 64.28 | 0.01 |
| C7 | N4 | C6 | H6B | 64 | 0.01 |
| C5 | N4 | C7 | C8 | 3.47 | 0.01 |
| C5 | N4 | C7 | C12 | 177.62 | 0.01 |
| C6 | N4 | C7 | C8 | 177.99 | 0.01 |
| C6 | N4 | C7 | C12 | 0.92 | 0.01 |
| N1 | C1 | C4 | N2 | 2.58 | 0.01 |
| N1 | C1 | C4 | H4 | 177.44 | 0.01 |
| N3 | C1 | C4 | N2 | 176.99 | 0.01 |
| N3 | C1 | C4 | H4 | 3 | 0.01 |
| N1 | C2 | C3 | N2 | 1.65 | 0.01 |
| N1 | C2 | C3 | H3 | 178.33 | 0.01 |
| H2 | C2 | C3 | N2 | 178.34 | 0.01 |
| H2 | C2 | C3 | H3 | 1.68 | 0.01 |
| N4 | C7 | C8 | H8 | 0.79 | 0.01 |
| N4 | C7 | C8 | C9 | 179.22 | 0.01 |
| C12 | C7 | C8 | H8 | 179.69 | 0.01 |
| C12 | C7 | C8 | C9 | 0.32 | 0.01 |
| N4 | C7 | C12 | C11 | 178.86 | 0.01 |
| N4 | C7 | C12 | H12 | 1.14 | 0.01 |
| C8 | C7 | C12 | C11 | 0.08 | 0.01 |
| C8 | C7 | C12 | H12 | 179.92 | 0.01 |
| C7 | C8 | C9 | H9 | 179.71 | 0.01 |
| C7 | C8 | C9 | C10 | 0.3 | 0.01 |
| H8 | C8 | C9 | H9 | 0.28 | 0.01 |
| H8 | C8 | C9 | C10 | 179.71 | 0.01 |
| C8 | C9 | C10 | H10 | 179.87 | 0.01 |
| C8 | C9 | C10 | C11 | 0.11 | 0.01 |
| H9 | C9 | C10 | H10 | 0.14 | 0.01 |
| H9 | C9 | C10 | C11 | 179.88 | 0.01 |
| C9 | C10 | C11 | H11 | 179.45 | 0.01 |
| C9 | C10 | C11 | C12 | 0.51 | 0.01 |
| H10 | C10 | C11 | H11 | 0.57 | 0.01 |
| H10 | C10 | C11 | C12 | 179.47 | 0.01 |
| C10 | C11 | C12 | C7 | 0.49 | 0.01 |
| C10 | C11 | C12 | H12 | 179.51 | 0.01 |
| H11 | C11 | C12 | C7 | 179.47 | 0.01 |
| H11 | C11 | C12 | H12 | 0.53 | 0.01 |
| C18 | S2 | C17 | N7 | 179.83 | 0.01 |
| C18 | S2 | C17 | N8 | 0.75 | 0 |
| C17 | S2 | C18 | N8 | 0.7 | 0 |

| | | | | | |
|-----|-----|-----|------|--------|------|
| C17 | S2 | C18 | H18A | 115.18 | 0.01 |
| C17 | S2 | C18 | H18B | 116.57 | 0.01 |
| C14 | N5 | C13 | N7 | 176.22 | 0.01 |
| C14 | N5 | C13 | C16 | 3.37 | 0.01 |
| C13 | N5 | C14 | H14 | 179.56 | 0.01 |
| C13 | N5 | C14 | C15 | 0.43 | 0.01 |
| C16 | N6 | C15 | C14 | 2.53 | 0.01 |
| C16 | N6 | C15 | H15 | 177.47 | 0.01 |
| C15 | N6 | C16 | C13 | 0.46 | 0.01 |
| C15 | N6 | C16 | H16 | 179.54 | 0.01 |
| C17 | N7 | C13 | N5 | 7.02 | 0.01 |
| C17 | N7 | C13 | C16 | 173.38 | 0.01 |
| C13 | N7 | C17 | S2 | 2.8 | 0.01 |
| C13 | N7 | C17 | N8 | 178.37 | 0.01 |
| C18 | N8 | C17 | S2 | 0.92 | 0.01 |
| C18 | N8 | C17 | N7 | 179.9 | 0.01 |
| C19 | N8 | C17 | S2 | 179.58 | 0.01 |
| C19 | N8 | C17 | N7 | 0.41 | 0.01 |
| C17 | N8 | C18 | S2 | 0.89 | 0.01 |
| C17 | N8 | C18 | H18A | 114.99 | 0.01 |
| C17 | N8 | C18 | H18B | 116.76 | 0.01 |
| C19 | N8 | C18 | S2 | 179.59 | 0.01 |
| C19 | N8 | C18 | H18A | 64.53 | 0.01 |
| C19 | N8 | C18 | H18B | 63.72 | 0.01 |
| C17 | N8 | C19 | C20 | 176.25 | 0.01 |
| C17 | N8 | C19 | C24 | 4.47 | 0.01 |
| C18 | N8 | C19 | C20 | 3.12 | 0.01 |
| C18 | N8 | C19 | C24 | 176.15 | 0.01 |
| N5 | C13 | C16 | N6 | 3.56 | 0.01 |
| N5 | C13 | C16 | H16 | 176.44 | 0.01 |
| N7 | C13 | C16 | N6 | 176.05 | 0.01 |
| N7 | C13 | C16 | H16 | 3.95 | 0.01 |
| N5 | C14 | C15 | N6 | 2.67 | 0.01 |
| N5 | C14 | C15 | H15 | 177.33 | 0.01 |
| H14 | C14 | C15 | N6 | 177.33 | 0.01 |
| H14 | C14 | C15 | H15 | 2.67 | 0.01 |
| N8 | C19 | C20 | H20 | 1.11 | 0.01 |
| N8 | C19 | C20 | C21 | 178.89 | 0.01 |
| C24 | C19 | C20 | H20 | 179.6 | 0.01 |
| C24 | C19 | C20 | C21 | 0.4 | 0.01 |
| N8 | C19 | C24 | C23 | 179.27 | 0.01 |
| N8 | C19 | C24 | H24 | 0.72 | 0.01 |
| C20 | C19 | C24 | C23 | 0 | 0.01 |
| C20 | C19 | C24 | H24 | 180 | 0.01 |
| C19 | C20 | C21 | H21 | 179.78 | 0.01 |

| | | | | | |
|----------------------------------|------------------------------|---------------------------------------|--|--------|------|
| C19 | C20 | C21 | C22 | 0.24 | 0.01 |
| H20 | C20 | C21 | H21 | 0.22 | 0.01 |
| H20 | C20 | C21 | C22 | 179.76 | 0.01 |
| C20 | C21 | C22 | H22 | 179.65 | 0.01 |
| C20 | C21 | C22 | C23 | 0.32 | 0.01 |
| H21 | C21 | C22 | H22 | 0.37 | 0.01 |
| H21 | C21 | C22 | C23 | 179.66 | 0.01 |
| C21 | C22 | C23 | H23 | 179.27 | 0.01 |
| C21 | C22 | C23 | C24 | 0.73 | 0.01 |
| H22 | C22 | C23 | H23 | 0.76 | 0.01 |
| H22 | C22 | C23 | C24 | 179.24 | 0.01 |
| C22 | C23 | C24 | C19 | 0.57 | 0.01 |
| C22 | C23 | C24 | H24 | 179.43 | 0.01 |
| H23 | C23 | C24 | C19 | 179.43 | 0.01 |
| H23 | C23 | C24 | H24 | 0.58 | 0.01 |
| Number of torsion angles: 126 | | | | | |
| Possible hydrogen bonds | | | | | |
| Donor-H | Donor...Acceptor | H...Acceptor | Donor-H.....Acceptor | | |
| C8 -H8 0.930(.000) 1.080 | C8 ...N3 3.042(.000) (0) | H8 ...N3 2.416(.000) (0) 2.334 | C8 -H8 ...N3 (0) 124.55(0.01) 121.52 (**) | | |
| C8 -H8 0.930(.000) 1.080 | C8 ...S2 (1) 3.657(.000) | H8 ...S2 (1) 2.958(.000) 2.858 | C8 -H8 ...S2 (1) 133.09(0.01) 130.90 (**) | | |
| C9 -H9 0.930(.000) 1.080 | C9 ...N6 (2) 3.776(.000) | H9 ...N6 (2) 2.965(.000) 2.841 | C9 -H9 ...N6 (2) 146.59(0.01) 144.92 (**) | | |
| C11 -H11 0.930(.000) 1.080 | C11 ...N2 (3) 3.588(.000) | H11 ...N2 (3) 2.682(.000) 2.537 | C11 -H11 ...N2 (3) 164.96(0.01) 164.08 (**) | | |
| C15 -H15 0.930(.000) 1.080 | C15 ...N6 (4) 3.436(.000) | H15 ...N6 (4) 2.705(.000) 2.599 | C15 -H15 ...N6 (4) 136.11(0.01) 133.81 (**) | | |
| C22 -H22 0.930(.000) 1.080 | C22 ...N1 (5) 3.636(.000) | H22 ...N1 (5) 2.951(.000) 2.854 | C22 -H22 ...N1 (5) 131.67(0.01) 129.42 (**) | | |
| C23 -H23 0.930(.000) 1.080 | C23 ...N2 (6) 3.768(.000) | H23 ...N2 (6) 2.996(.000) 2.880 | C23 -H23 ...N2 (6) 141.39(0.01) 139.53 (**) | | |
| C24 -H24 0.930(.000) 1.080 | C24 ...S1 (7) 3.605(.000) | H24 ...S1 (6) 2.875(.000) 2.769 | C24 -H24 ...S1 (7) 136.27(0.01) 134.12 (**) | | |

Table 2. Comparison of structural parameters obtained from crystal structure and computed data

| Parameter | | Crystal structure | Computed Data |
|----------------------|--|-------------------|---------------|
| Bond length (nm) | C ₆ -N ₄ | 1.39 | 1.36 |
| | N ₄ -C ₁₃ | 1.27 | 1.27 |
| | C ₁₃ -S ₁ | 1.77 | 1.82 |
| | S ₁ -C ₁₄ | 1.84 | 1.85 |
| | C ₁₄ -N ₅ | 1.46 | 1.46 |
| | N ₅ -C ₁₃ | 1.36 | 1.36 |
| | N ₅ -C ₁₇ | 1.40 | 1.42 |
| Bond angle (deg) | C ₆ -N ₄ -C ₁₃ | 118.73 | 127.19 |
| | N ₄ -C ₁₃ -S ₁ | 135.54 | 136.75 |
| | C ₁₃ -S ₁ -C ₁₄ | 74.00 | 72.79 |
| | S ₁ -C ₁₄ -N ₅ | 89.700 | 90.67 |
| | C ₁₄ -N ₅ -C ₁₃ | 100.68 | 101.27 |
| | N ₅ -C ₁₃ -S ₁ | 95.60 | 95.27 |
| Dihedral angle (deg) | N ₄ -C ₁₃ -S ₁ -C ₁₄ | 179.83 | 177.79 |



S1: Stern-Volmer plot for various 1,3 – thiazetidine derivatives.

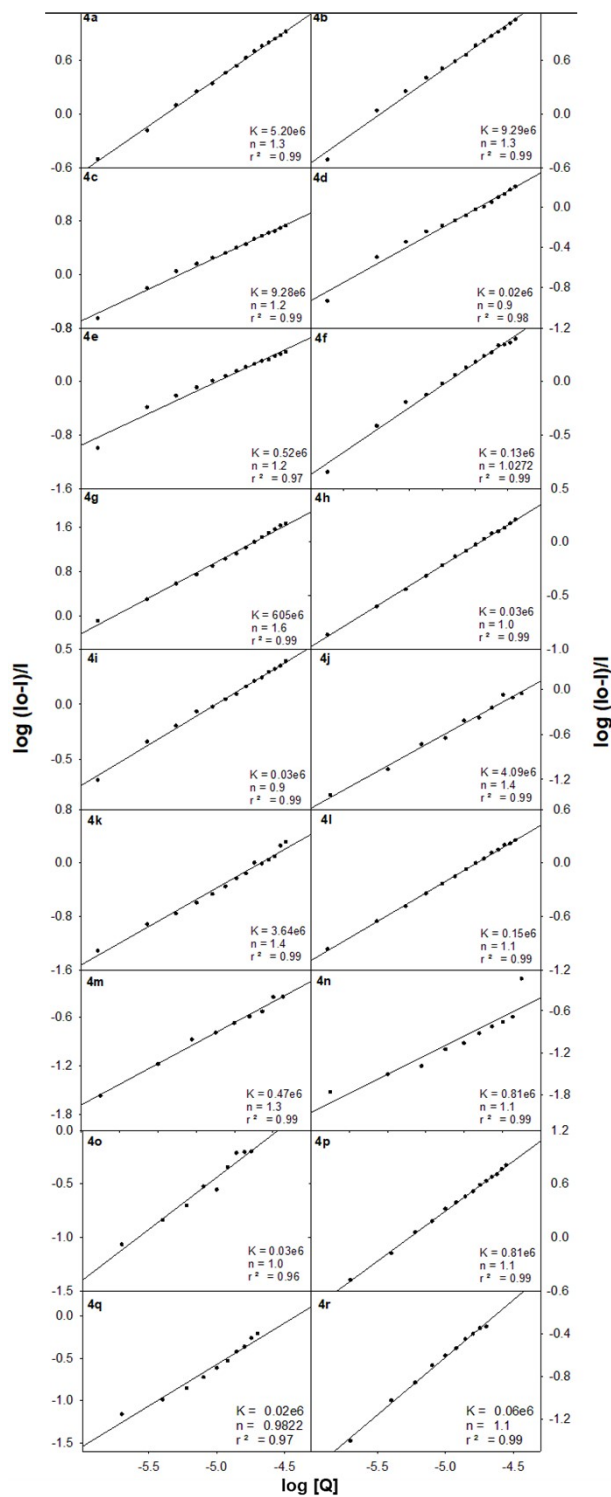


Figure S2: The plot of $\log (I_0 - I)/I$ against $\log [Q]$ for various thiazetidine derivatives (4a-r).

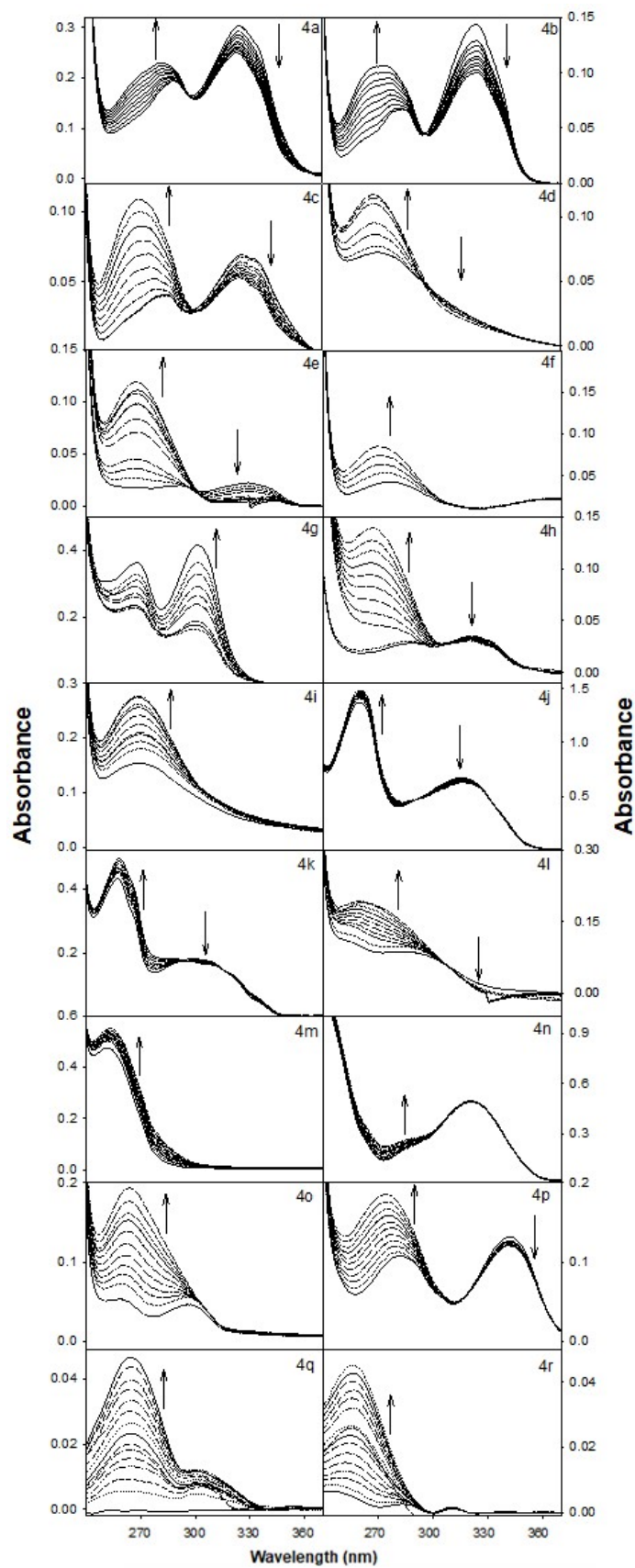


Figure S3. UV-Vis absorption spectra depicting the interaction of calf thymus DNA with various 1,3-thiazetidine derivatives **4a-r**.

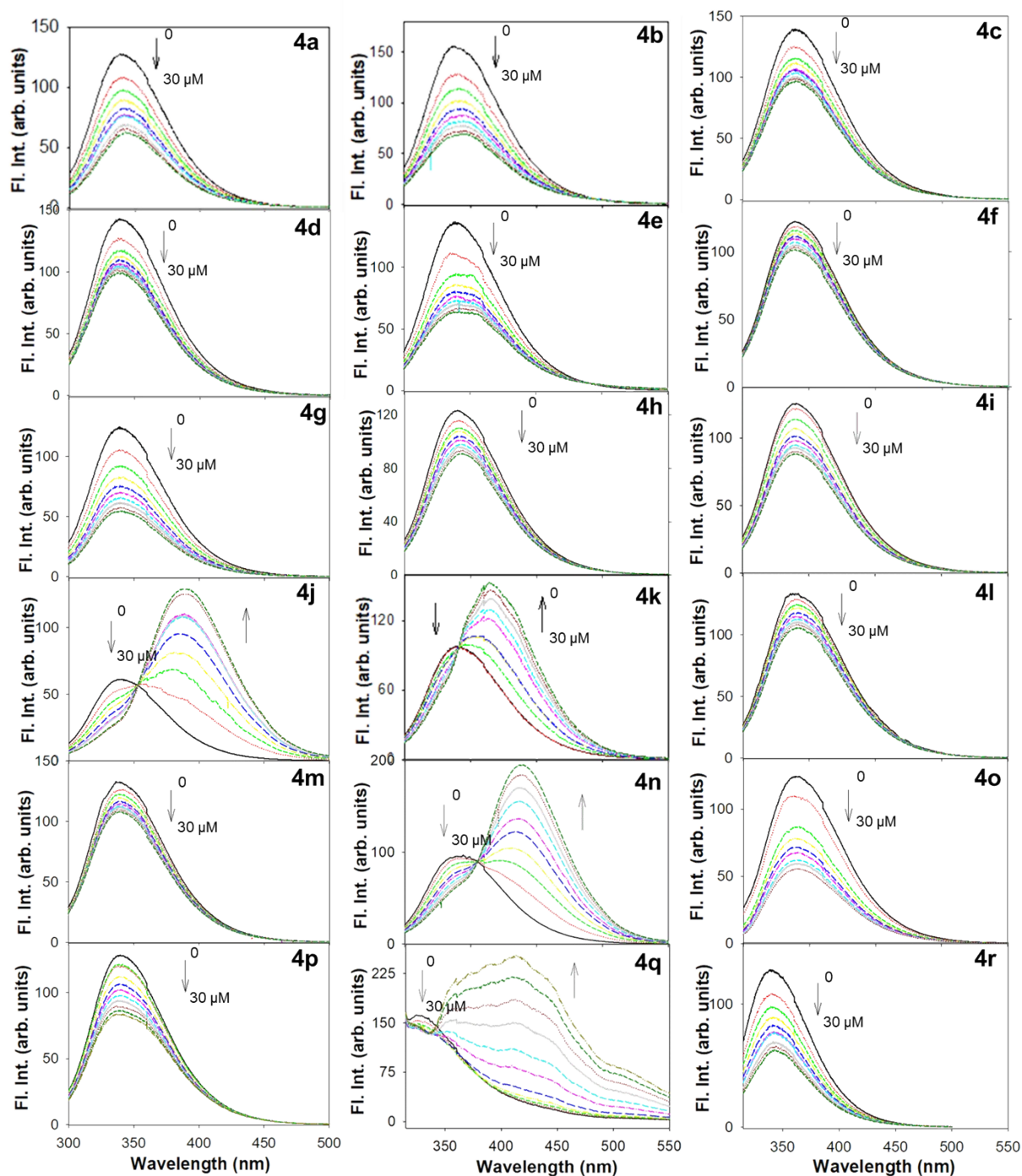


Figure S4: Fluorescence quenching plots. Fluorescence emission spectra (λ_{ex} : 280 nm) of BSA depicting the decrease in fluorescence intensity upon interaction with various thiazetidine derivatives

Experimental procedures for the binding of 1,3-thiazetidines with biomolecules.

A 10 mM stock solution of BSA was prepared in 50 mM phosphate buffer (pH 7.2) and stored at 4 °C until used. The quenching interactions of thiazetidines with BSA were monitored by change in their intrinsic fluorescence at a fixed excitation wave length of 285 nm and emission value at 345 nm. The same emission and excitation scan rates and slit widths were maintained throughout the experiments. Fixed protein concentration (1 μM) was used to titrate against different concentrations of various thiazetidine derivatives (0 - 30 μM).

In order to determine the binding interactions of the newly synthesized thiazetidine derivatives with ct-DNA, absorption spectral titration was carried out in 5 mM Tris-HCl buffer, pH-7.2. The protein free form of ct-DNA was confirmed by the ratio of UV absorbance at 260 and 280 nm (A_{260}/A_{280}) of *ca.* 1.8. The concentration of ct-DNA per nucleotide was determined by its molar absorption coefficient (6600 m^{-1}) at 260 nm.³³ Stock solutions of samples were prepared in DMSO and further dilutions were made in 5 mM Tris-HCl buffer. The binding experiments were carried out with fixed concentration of the samples (20 μM) and increasing concentrations of ct-DNA (0 – 30 μM) in both reference and sample solution to nullify the absorbance peak of ct-DNA.