

SUPPLEMENTARY INFORMATION

One Pot Synthesis of Pyrimidine-5-Carbonitrile and Pyrimidine-5-Carboxamide using Ammonium Chloride under Solvent-free Condition

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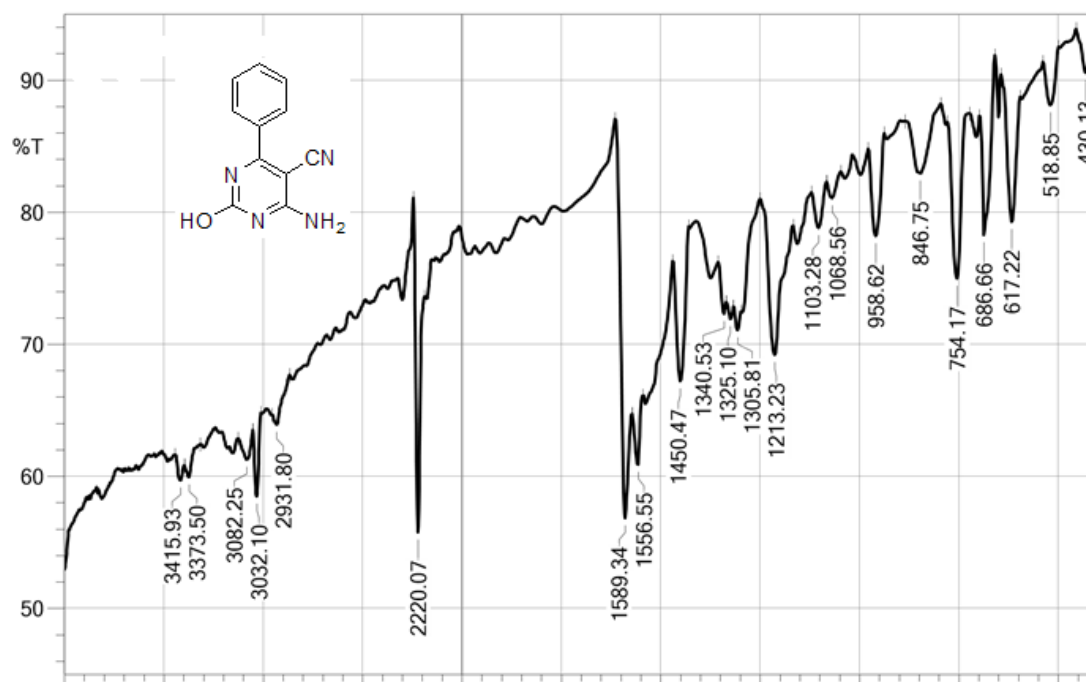
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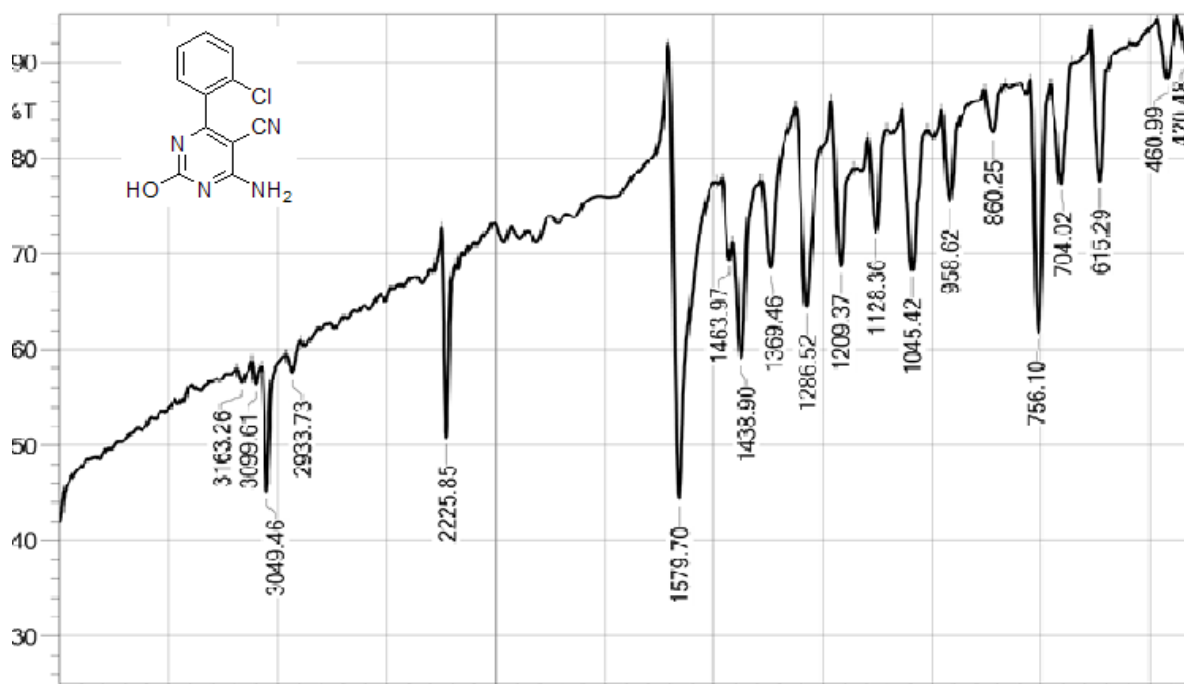
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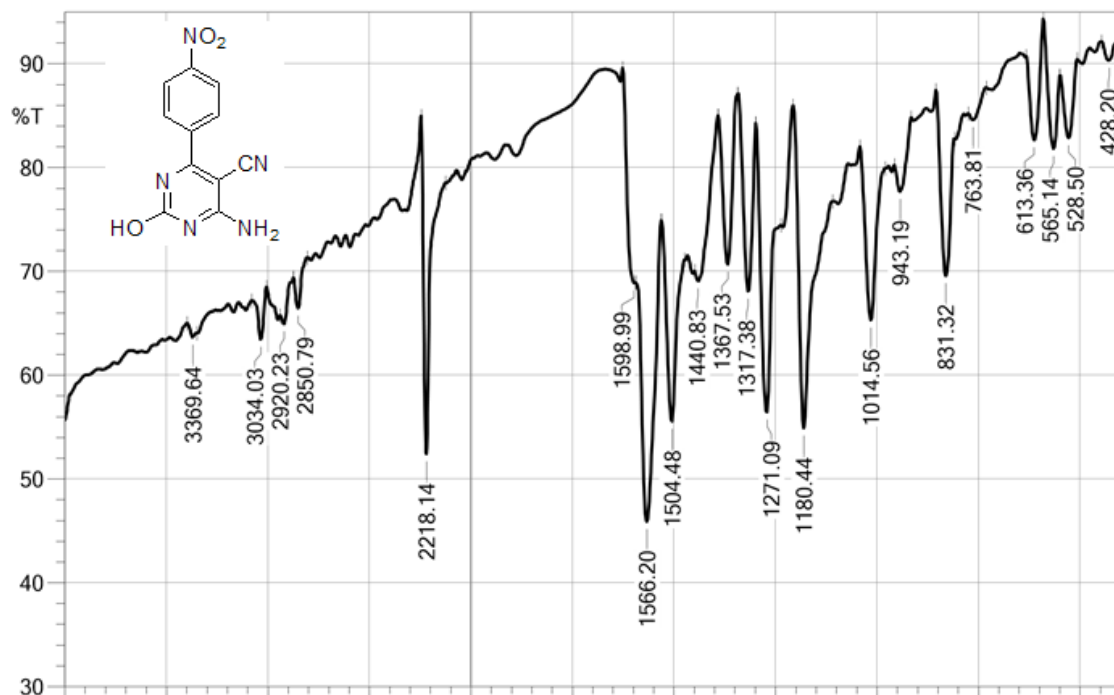
2.2.1. Entry-4a 4-Amino-2-hydroxy-6-phenylpyrimidine-5-carbonitrile



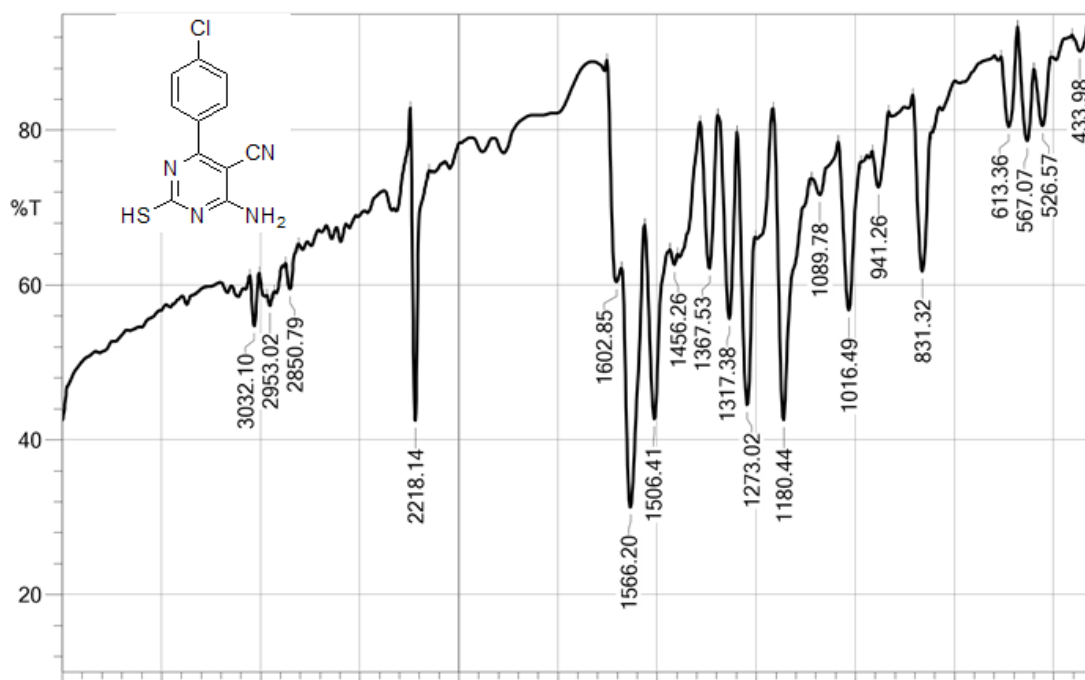
2.2.2 Entry-4b 4-Amino-6-(2-chlorophenyl)-2-hydroxypyrimidine-5-carbonitrile



2.2.3 Entry-4d 4-Amino-6-(4-nitrophenyl)-2-hydroxypyrimidine-5-carbonitrile



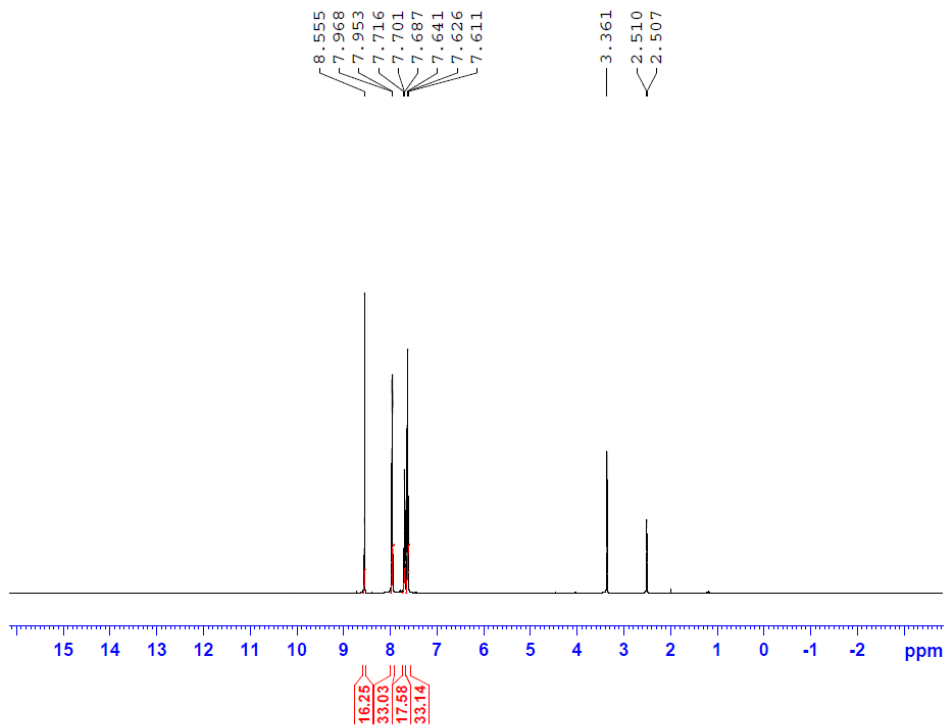
2.2.4 Entry-4h 4-Amino-6-(4-chlorophenyl)-2-mercaptopyrimidine-5-carbonitrile



The synthesized product has characterised by ¹HNMR and recorded on Bruker (500 MHz) DMSO-d₆ as a solvent in the Central Instrumentation Facility of Savitribai Phule Pune University, Pune (Formerly University of Pune).

2.2.1 Entry-4a 4-Amino-2-hydroxy-6-phenylpyrimidine-5-carbonitrile

1
PROTON DMSO {E:\KTHM} Snehal 22



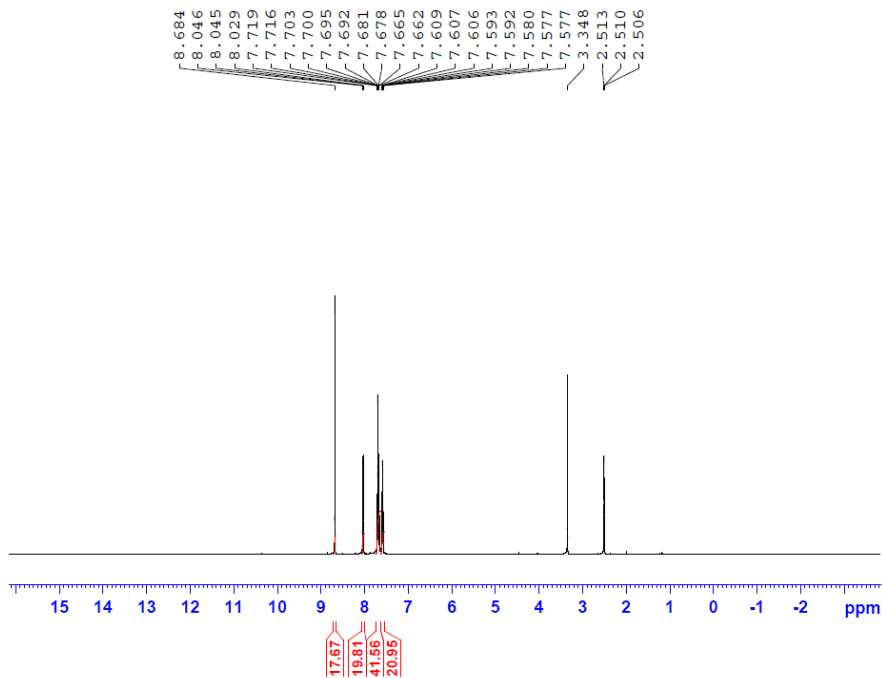
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PULPROG  zg30
TD       65536
SOLVENT  DMSO
NS       16
DS       2
SWH      10000.000 Hz
FIDRES   0.305176 Hz
AQ       3.2767999 sec
RG       77.09
DW       50.000 usec
DE       6.50 usec
TE       0 K
D1       1.00000000 sec
TD0      1
SFO1     500.1330883 MHz
NUC1     1H
P1       9.22 usec
PLW1     22.00000000 W

F2 - Processing parameters
SI       65536
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WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
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2.2.2 Entry-4b 4-Amino-6-(2-chlorophenyl)-2-hydroxypyrimidine-5-carbonitrile

2
PROTON DMSO {E:\KTHM} Snehal 23



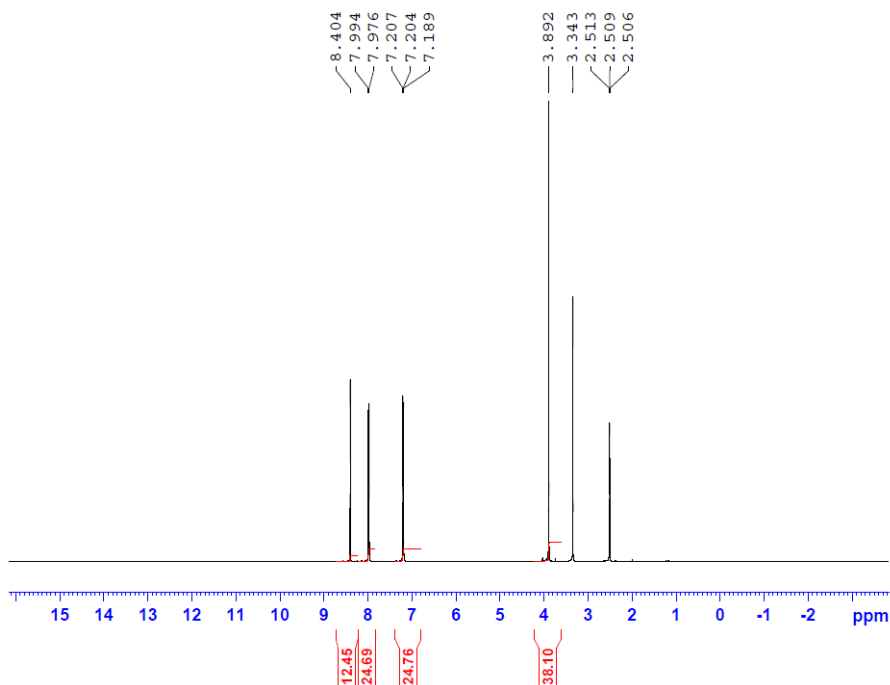
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PULPROG  zg30
TD       65536
SOLVENT  DMSO
NS       16
DS       2
SWH      10000.000 Hz
FIDRES   0.305176 Hz
AQ       3.2767999 sec
RG       109.52
DW       50.000 usec
DE       6.50 usec
TE       0 K
D1       1.00000000 sec
TD0      1
SFO1     500.1330883 MHz
NUC1     1H
P1       9.22 usec
PLW1     22.00000000 W

F2 - Processing parameters
SI       65536
SF       500.1300000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
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2.2.3 Entry-4d 4-Amino-6-(4-nitrophenyl)-2-hydroxypyrimidine-5-carbonitrile

4
PROTON DMSO {E:\KTHM} Snehal 25



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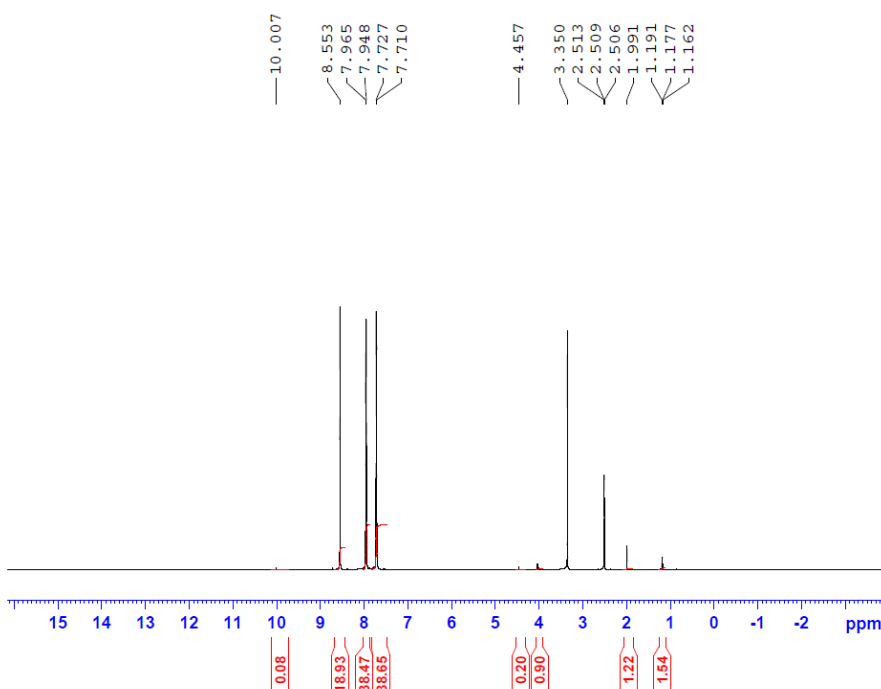
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PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            16
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FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG            139.18
DW            50.000 usec
DE            6.50 usec
TE            0 K
D1            1.00000000 sec
TDO           1
SF01          500.1330883 MHz
NUC1          1H
P1            9.22 usec
PLW1          22.00000000 W

F2 - Processing parameters
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SF           500.1300000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
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2.2.4 Entry-4h 4-Amino-6-(4-chlorophenyl)-2-mercaptopyrimidine-5-carbonitrile

8
PROTON DMSO {E:\KTHM} Snehal 29



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Current Data Parameters
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PROCNO        1

F2 - Acquisition Parameters
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Time_         18.00 h
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PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            16
DS            2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            3.2767999 sec
RG            109.52
DW            50.000 usec
DE            6.50 usec
TE            0 K
D1            1.00000000 sec
TDO           1
SF01          500.1330883 MHz
NUC1          1H
P1            9.22 usec
PLW1          22.00000000 W

F2 - Processing parameters
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SF           500.1300000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
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