***Supplementary Information***

# Synthesis, characterization and biological screening of various pharmacophoric derivatives of 4-alkylpyrimidine-5-carbonitrile

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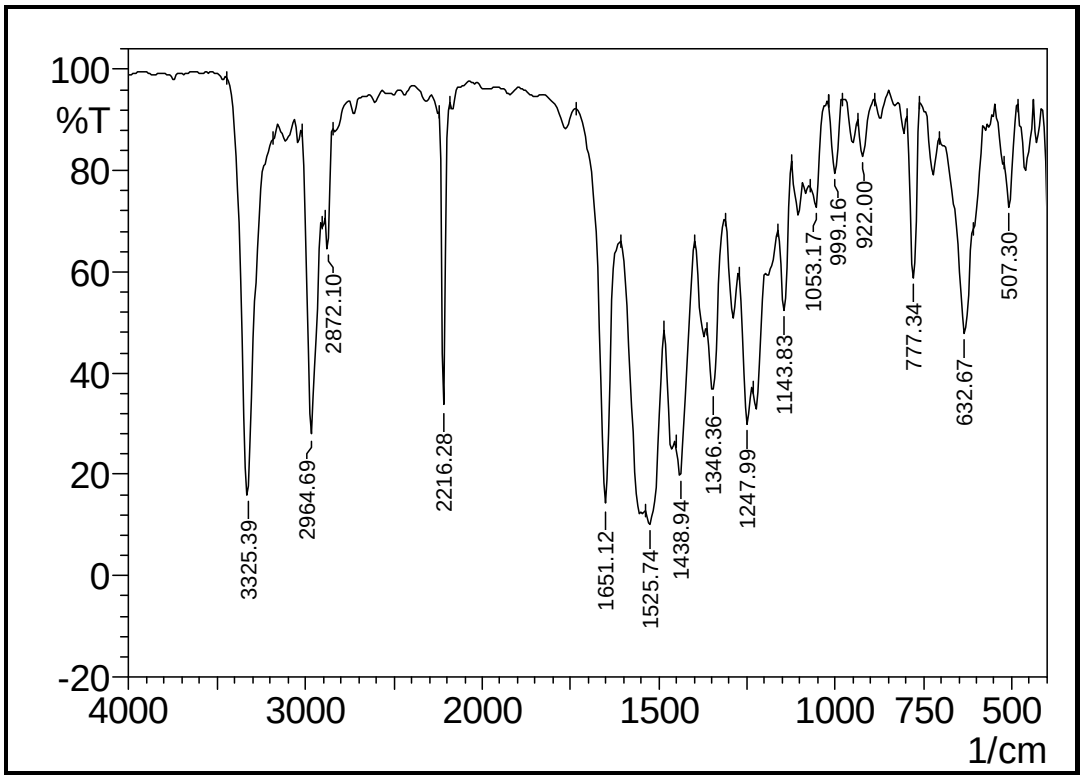
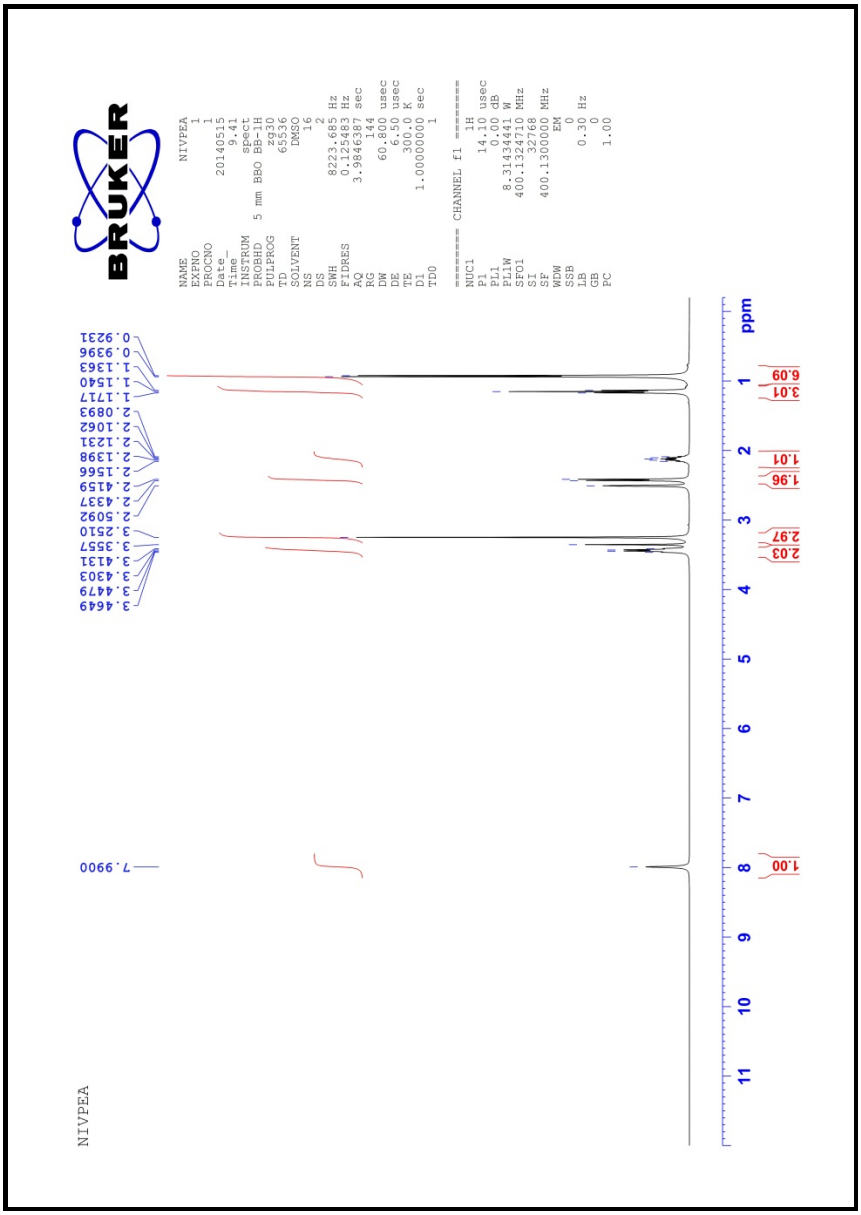
**IR spectrum of 1,6-dihydro-4-isobutyl-1-methyl-2-(methylthio)-6-oxopyrimidine-5-carbonitrile**




| System | Vibration Mode | Band Position ($cm^{-1}$) | |
|---|---|---|---|
| | | Observed | Reported |
| Secondary Amine | N – H str. | 3325 | 3500-3300 |
| | C – N vib. | 1346 | 1350-1280 |
| | N – H wag. | 777 | 750-700 |
| Alkane | C-H str. (asy.) | 2964 | 2280-2860 |
| | C-H str. (sym.) | 2872 | 2880-2860 |
| Nitrile | C=N str. | 2216 | 2260-2200 |
| Carbonyl | C=O str. | 1651 | 1760-1665 |

**NMR spectrum of 1,6-dihydro-4-isobutyl-1-methyl-2-(methylthio)-6-oxopyrimidine-5-carbonitrile**




| Signal No. | Signal Position (δ ppm) | Relative No. of Proton | Multiplicity | Inference |
|---|---|---|---|---|
| 1 | 0.92 | 6H | doublet | -CH-(C<u>H</u>$_3$)$_2$ |
| 2 | 1.15 | 3H | triplet | -CH$_2$-C<u>H</u>$_3$ |
| 3 | 2.12 | 1H | multiplet | -C<u>H</u>-(-CH$_3$)$_2$ |
| 4 | 2.41 | 2H | doublet | -CH-C<u>H</u>$_2$ |
| 5 | 3.25 | 3H | singlet | -N-C<u>H</u>$_3$ |
| 6 | 3.41 | 2H | quintet | -NH-C<u>H</u>$_2$-CH$_3$ |
| 7 | 7.99 | 1H | singlet | -N<u>H</u> |

**Mass spectrum of 1,6-dihydro-4-isobutyl-1-methyl-2-(methylthio)-6-oxopyrimidine-5-carbonitrile**