Supplementary data


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General Experimental Considerations

All commercially available reagents used in this study bought from local suppliers, Sigma-Aldrich and Alfa Aesar and were used as such. Thin-layer chromatography was performed on pre-coated TLC silica gel 60 F254 plates on aluminium (Merck). TLC was visualized in UV-254 and 360nm, iodine on silica gel. Column chromatography was performed using 230-400 mesh silica gel. Automated purifications were done using Teledyne ISCO Combitflash companion. Unless otherwise noted, all reactions were carried out under atmosphere of argon in dried glassware using standard techniques. THF was distilled from Na/ benzophenone, Analytical grade DCM, Acetonitrile and DMF were used without further drying/purification. $^1$H and $^{13}$C NMR spectra were recorded on Varian 400 and Varian 300 spectrometers. Chemical shifts are reported in ppm with TMS as reference. Data are reported as follows: chemical shift, multiplicity, (s = singlet, d = doublet, t = triplet, q = quartet, br = broad, m = multiplet), coupling constants and number of protons. HRMS data was recorded using Q-Tof micro under electrospray ionization mode. IR spectra were taken on a FT-IR Perkin Elmer Spectrum 2000 in KBr pellets. Melting points were uncorrected.
Cheminformatic Analysis:

In silico and PMI analysis were carried out on 1100 FDA-approved drugs (randomly taken from our GOSTAR proprietary database and our compounds. Each molecule was analyzed for a set of six physiochemical properties by using online cheminformatics tools, ChemDraw, or manual inspection. The data were collected on an Excel spreadsheet. (Included in the Supporting Information). These results were used to generate the plot shown in Figure 5a. The PMI calculations involved aligning each molecule to the principal moment axes in SYBYL and the normalized PMI values were calculated by using in-house software. The 2D chemical structures of the compounds were drawn in Discovery studio 3.5 (DS 3.5), whereas those of the FDA-approved drugs were collected from the GOSTAR (Gvkbio Online Structure Activity Relationship) database. These compounds were imported into DS 3.5 and converted into 3D structures. Energy minimization was performed for all of these 3D structures to identify global/local minima by applying the CHARMm force field. The resulting 3D structures were used to calculate the three principal moments of inertia; the PMI values are sorted in ascending magnitude, that is, I1, I2, and I3. Normalized PMI ratios (NPR) were calculated by dividing the two smaller PMI values (I1 and I2) by the largest PMI value (I3) and generated two characteristic values for each compound (I1/I3 and I2/I3). These values were plotted against each other and the resulting graph formed an isosceles triangle that was defined by its three corners, wherein the vector [I1/I3, I2/I3] was equal to [1,1], [0.5,0.5], and [0,1] (Figure 2c)

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Surface electrostatic potential for representative set compounds were calculated. These were calculated by projecting the Gasteiger–Marsili charge distribution onto a Connolly surface that was generated by using the MOLCAD tool in SYBYL (Figure 2b).

In addition, our molecules were plotted according to the normalized principal moment of inertia (PMI) formalism of Sauer and Schwartz. Since molecular shape and biological activity are intricately related, the screening of molecules that have a higher degree of built-in molecular-shape diversity translates into a greater probability of discovering compounds with biological activity. The three corners of the isosceles triangle of the PMI plot are dominated by rods, spheres, and discs, respectively (the shapes are representations of the overall shape of the constituent molecules). From the graph it is clear that FDA approved drugs cover the

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left edge of the PMI space taking shapes intermediate between rods and discs, our compounds are falling under the same area where the drug compounds fall in the graph, These compounds are falling at the top of the left edge of the PMI space (Figure 2c).29 The bioactivity track record of drug compounds is well-established. We hope that the similar shapes of our molecules to those of drug compounds will increase the likelihood of discovering biologically relevant molecules by using this method.

References:
a)

Molecular Weights vs ALogP vs HBA

Molecular Weights vs ALogP vs HBD

Molecular Weights vs ALogP vs LogD

Molecular Weights vs ALogP vs PSA
Figure 2 Cheminformatics analysis of our library of privileged scaffolds; in silico analysis, polar surface area, and polar moment of inertia (PMI) plots of a representative set of molecules are shown. 

a) In silico analysis of molecules (dark-blue spots) in a chemical-space plot that corresponds to a set of six drug-like properties (PSA, solubility, HBA, HBD, log A and log D), relative to 1011 FDA-approved drugs (light-blue dots), as reported in the GOSTAR database (GVKBioscience proprietary database). 

b) Surface electrostatic potential of a representative set of our compounds, that is, compounds 14a, 15a, 15d, 17e and 17k. 

c) PMI plot of our group of molecules relative to 1011 FDA-approved drugs. The PMI calculations involved aligning each molecule to principal moment axes by using SYBYL and the normalized PMI values were calculated by using in-house software.
$^1$H NMR (300 MHz, DMSO-$d_6$) Spectrum of 7-methoxy-2-0-tolylthieno[3,2-$b$]pyridin-3-ol (14g)
$^13$C NMR (75 MHz, DMSO-$d_6$) Spectrum of 7-methoxy-2-o-tolylthieno[3,2-$b$]pyridin-3-ol (14g)
**Elemental Composition Report**

**Single Mass Analysis**
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Selected filters: None

Monoisotopic Mass, Even Electron Ions
10 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
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C: 0-15   H: 0-14   N: 0-1   O: 0-2   S: 0-1

G/K=SG-3M

05-03-066 30 (0.444) AM (Cen,4, 80.00, Ar,5000,0,195.08,0.10,LS 5); Sm (SG, 2x2.00); Sb (1.46.00 )

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**HRMS Spectrum of 7-methoxy-2-o-tolylthieno[3,2-b]pyridin-3-ol (14g)**
FT-IR Spectrum of 7-methoxy-2-o-tolylthieno[3,2-b]pyridin-3-ol (14g)
$^1$H NMR (300 MHz, DMSO-$d_6$) Spectrum of 2-(2-chlorophenyl)-7-methoxythieno[3,2-$b$]pyridin-3-ol (14j).
$\delta$ ρνρNMR (75 MHz, DMSO-$d_6$) Spectrum of 2-(2-chlorophenyl)-7-methoxythieno[3,2-b]pyridin-3-ol (14j).

13C NMR (75 MHz, DMSO-$d_6$) Spectrum of 2-(2-chlorophenyl)-7-methoxythieno[3,2-b]pyridin-3-ol (14j).
HRMS Spectrum of 2-(2-chlorophenyl)-7-methoxythieno[3,2-b]pyridin-3-ol (14j).
FT-IR Spectrum of 2-(2-chlorophenyl)-7-methoxythieno[3,2-b]pyridin-3-ol (14j).
$\text{H NMR (300 MHz, DMSO-$d_6$) Spectrum of 3-hydroxy-2-phenylthieno[3,2-$b$]pyridin-7(4H)-one (15a)}$
$^{13}$C NMR (75 MHz, DMSO-$_d_6$+CF$_3$CO$_2$D) Spectrum of 3-hydroxy-2-phenylthieno[3,2-$b$]pyridin-7(4H)-one (15a)
Single Mass Analysis
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
10 formula(e) evaluated with 1 results within limits (up to 2 best isotopic matches for each mass)
Elements Used:
C: 0-13  H: 0-10  N: 0-1  O: 0-2  S: 0-1

SAMPLE ID: GVK-TP-4A
Acq. Method: GVCE-FA-11-MIN
12112013-GVK-TP-4A 15 (0.230) AM (Cen,4, 80.00, Ar,5000.0,556.24,0.00,LS 5); Sm (Mn, 3x2.00); Sb (1,40.00 )

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Maximum:  1000.0  -1.5  50.0

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HRMS Spectrum of 3-hydroxy-2-phenylthieno[3,2-b]pyridin-7(4H)-one (15a)
FT-IR Spectrum of 3-hydroxy-2-phenylthieno[3,2-b]pyridin-7(4H)-one (15a)
\(^1\)H NMR (400 MHz, DMSO-\(d_6\)) Spectrum of 3-hydroxy-2-(4-methoxyphenyl)thieno[3,2-b]pyridin-7(4H)-one (15b)
$^{13}$C NMR (100 MHz, DMSO-$d_6$+CF$_3$CO$_2$D) Spectrum of 3-hydroxy-2-(4-methoxyphenyl)thieno[3,2-b]pyridin-7(4H)-one (15b)
HRMS Spectrum of 3-hydroxy-2-(4-methoxyphenyl)thieno[3,2-b]pyridin-7(4H)-one (15b)
FT-IR Spectrum of 3-hydroxy-2-(4-methoxyphenyl)thieno[3,2-b]pyridin-7(4H)-one (15b)
$^1$H NMR (400 MHz, DMSO-$d_6$) Spectrum of 3-hydroxy-2-p-tolylthieno[3,2-$b$]pyridin-7(4H)-one (15c)
\[ ^{13} \text{C NMR (75 MHz, DMSO-}\text{d}_6+\text{CF}_3\text{CO}_2\text{D)} Spectrum of 3-hydroxy-2-p-tolylthieno[3,2-b]pyridin-7(4H)-one (15c) \]
Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
10 formula(e) evaluated with 1 results within limits (up to 2 best isotopic matches for each mass)
Elements Used:
C: 0-14  H: 0-12  N: 0-1  O: 0-2  S: 0-1

SAMPLE ID: GVK-TP-4F
Acq. Method: GVCE-FA-11-MIN
12112013-GVK-TP-4F 16 (0.239) AM (Can,4, 80.00, Ar,5000.0,556.18,0.00,LS 5); Sm (Mn, 3x2.00); Sb (1.40.00)

Date of Analysis: 12-Nov-2013:19:29:23
Instrument ID: ANL-MCLS-LCMS-001
1: TOF MS ES+
3.16e3

Minimum: -1.5
Maximum: 5.0  1000.0  50.0

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HRMS Spectrum of 3-hydroxy-2-p-tolylthieno[3,2-b]pyridin-7(4H)-one (15c)
FT-IR Spectrum of 3-hydroxy-2-p-tolylthieno[3,2-b]pyridin-7(4H)-one (15c)
$^1$H NMR (300 MHz, DMSO-$d_6$) Spectrum of 2-(15-tert-butylphenyl)-3-hydroxythieno[3,2-$b$]pyridin-7(4H)-one (15d)
$^{13}$C NMR (100 MHz, DMSO-$d_6$+CF$_3$CO$_2$D) Spectrum of 2-(4-tert-butylphenyl)-3-hydroxythieno[3,2-$b$]pyridin-7(4H)-one (15d)
Elemental Composition Report

Single Mass Analysis
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
10 formula(e) evaluated with 1 results within limits (up to 2 best isotopic matches for each mass)

Elements Used:
C: 0-17  H: 0-18  N: 0-1  O: 0-2  S: 0-1

SAMPLE ID : GVK-TP-4L
Acq. Method: GVCE-FA-11-MIN
12112013-GVK-TP-4L 15 (0.230) AM (Cen, 4, 80.00, Ar, 5000.0, 556.20, 0.00, LS 5); Sm (Mn, 3x2.0); Sb (1,40.00)

Minimum:  5.0
Maximum: 1000.0  50.0

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HRMS Spectrum of 2-(4-tert-butylyphenyl)-3-hydroxythieno[3,2-b]pyridin-7(4H)-one (15d)
FT-IR Spectrum of 2-(4-tert-butylphenyl)-3-hydroxythieno[3,2-b]pyridin-7(4H)-one (15d)
$^1$H NMR (300 MHz, DMSO-$d_6$) Spectrum of 2-(4-fluorophenyl)-3-hydroxythieno[3,2-$b$]pyridin-7(4H)-one (15e)
$^{13}$C NMR (100 MHz, DMSO-$d_6$+CF$_3$CO$_2$D) Spectrum 2-(4-fluorophenyl)-3-hydroxythieno[3,2-$b$]pyridin-7(4H)-one (15e).
**Elemental Composition Report**

**Single Mass Analysis**
Tolerance = 1000.0 PPM  /  DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 2 best isotopic matches for each mass)
Elements Used:
C: 0-14  H: 0-9  N: 0-1  O: 0-2  F: 0-1  S: 0-1

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**HRMS Spectrum of 2-(4-fluorophenyl)-3-hydroxythieno[3,2-b]pyridin-7(4H)-one (15e).**

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**DATE OF ANALYSIS:** 12-Nov-2013 19:27:47
**INSTRUMENT ID:** ANL-MCL3-LCMS-001
**SAMPLE ID:** GVKT-TP-4D
**ACQ. METHOD:** GVCE-FA-11-MIN
**12112013-GVKT-TP-4D 11 (0.157) AM** (Cen,A, 80.00, Ar,5000.0,656.24,0.00,LS 5); Sm (Mn, 3x2.00); Sb (1.40.00)

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GVK Biosciences Pvt. Ltd.
Medicinal Chemistry Laboratory - Analytical Research
FT-IR Spectrum of 2-(4-fluorophenyl)-3-hydroxythieno[3,2-b]pyridin-7(4H)-one (15e).
$^1$H NMR (300 MHz, DMSO-d$_6$) Spectrum of 2-(2-fluorophenyl)-3-hydroxythieno[3,2-b]pyridin-7(4H)-one (15f)
$^{13}$C NMR (100 MHz, DMSO-$d_6$+CF$_3$CO$_2$D) Spectrum of 2-(2-fluorophenyl)-3-hydroxythieno[3,2-$b$]pyridin-7(4H)-one (15f)
HRMS Spectrum of 2-(2-fluorophenyl)-3-hydroxythieno[3,2-b]pyridin-7(4H)-one (15f)
FT-IR Spectrum of 2-(2-fluorophenyl)-3-hydroxythieno[3,2-b]pyridin-7(4H)-one (15f)
$^1$H NMR (400 MHz, DMSO-$d_6$) Spectrum of 3-hydroxy-2-o-tolylthieno[3,2-b]pyridin-7(4H)-one (15g)
$^{13}$C NMR (75 MHz, DMSO-d$_6$+CF$_3$CO$_2$D) Spectrum of 3-hydroxy-2-o-tolylthieno[3,2-b]pyridin-7(4H)-one (15g)
Elemental Composition Report

**Single Mass Analysis**
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
10 formula(e) evaluated with 1 results within limits (up to 2 best isotopic matches for each mass)
Elements Used:
C: 0-14  H: 0-12  N: 0-1  O: 0-2  S: 0-1

---

**HRMS Spectrum of 3-hydroxy-2-o-tolylthieno[3,2-b]pyridin-7(4H)-one (15g)**

---

Data of Analysis: 12-Nov-2013 10:37:18
Instrument ID: ANL-MCL3-LCMS-001
1: TOF MS ES+
   4.73e3
FT-IR Spectrum of 3-hydroxy-2-o-tolythieno[3,2-b]pyridin-7(4H)-one (15g)
$^1$H NMR (400 MHz, DMSO-$d_6$) Spectrum of 3-hydroxy-2-(3-(trifluoromethyl)phenyl)thieno[3,2-$b$]pyridin-7(4H)-one (15h)
$^{13}$C NMR (75 MHz, DMSO-$d_6$+CF$_3$CO$_2$D) Spectrum of 3-hydroxy-2-(3-(trifluoromethyl)phenyl)thieno[3,2-$b$]pyridin-7(4H)-one (15h)
Single Mass Analysis
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
45 formula(e) evaluated with 1 results within limits (up to 2 best isotopic matches for each mass)
Elements Used:
C: 0-14  H: 0-9  N: 0-1  O: 0-2  F: 0-2  S: 0-1

SAMPLE ID : GVK-TP-41
Acq. Method: GTOE-FA-11-MIN
12112013: GVK-TP-41 13 (0.176) AM (Can, 4, 80.00, Ar, 5000.0, 586.20, 0.00, LS 5); Sm (Mn, 3x2.00); Sb (1, 40.00)

Minimum:  5.0  -1.5
Maximum:  1000.0  50.0

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
312.0111  312.0306  -19.5  -62.5  9.5  401.6  C14 H9 N O2 F3 S

HRMS Spectrum of 3-hydroxy-2-(3-(trifluoromethyl)phenyl)thieno[3,2-b]pyridin-7(4H)-one (15h)
FT-IR Spectrum of 3-hydroxy-2-(3-(trifluoromethyl)phenyl)thieno[3,2-b]pyridin-7(4H)-one (15h)
$^1$H NMR (400 MHz, DMSO-$d_6$) Spectrum of 2-(4-chlorophenyl)-3-hydroxythieno[3,2-$b$]pyridin-7(4H)-one (15i)
$^{13}$C NMR (75 MHz, DMSO-$d_6$+CF$_3$CO$_2$D) Spectrum of 2-(4-chlorophenyl)-3-hydroxythieno[3,2-$b$]pyridin-7(4H)-one (15i)
Elemental Composition Report

Single Mass Analysis
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
18 formula(e) evaluated with 1 results within limits (up to 2 best isotopic matches for each mass)
Elements Used:
C: 0-14  H: 0-9  N: 0-1  O: 0-2  S: 0-1  Cl: 0-1

SAMPLE ID: GVK-TP-4C
Acq. Method: GVCE-FA 11-MIN
12112013-GVK-TP-4C 16 (0.237) AM (Cen, 4, 80.00, Ar, 5000, 0.556, 28, 0.00, LS 5); Sm (Mn, 3x2.00); Sb (1, 40.00)

278.0565

Minimum:      Maximum:        PPM      DBE      i-FIT
Mass  Calc. Mass  mDa         5.0      1000.0     50.0
278.0565  278.0043   52.2  187.7   9.5        171.2  Cl3 H9 N O2 S Cl

HRMS Spectrum of 2-(4-chlorophenyl)-3-hydroxythieno[3,2-b]pyridin-7(4H)-one (15i)
FT-IR Spectrum of 2-(4-chlorophenyl)-3-hydroxothieno[3,2-b]pyridin-7(4H)-one (15i)
$^1$H NMR (300 MHz, DMSO-$d_6$) Spectrum of 2-(2-chlorophenyl)-3-hydroxythieno[3,2-$b$]pyridin-7(4H)-one (15j)
$^\text{13}$C NMR (75 MHz, DMSO-$_d_6$+CF$_3$CO$_2$D) Spectrum of 2-(2-chlorophenyl)-3-hydroxythieno[3,2-$b$]pyridin-7(4H)-one (15j).
HRMS Spectrum of 2-(2-chlorophenyl)-3-hydroxythieno[3,2-b]pyridin-7(4H)-one (15j).
FT-IR Spectrum of 2-(2-chlorophenyl)-3-hydroxythieno[3,2-\textit{b}]pyridin-7(4H)-one (15j).
$^1$H NMR (300 MHz, DMSO-$d_6$) Spectrum of 2-(furan-2-yl)-3-hydroxythieno[3,2-b]pyridin-7(4H)-one (15k)
$\text{\textsuperscript{13}C NMR (100 MHz, DMSO-\textit{d}_6+CF_3CO_2D) Spectrum of 2-(furan-2-yl)-3-hydroxythieno[3,2-\textit{b}]pyridin-7(4H)-one (15k)}$
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
14 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0.11  H: 0.8  N: 0.1  O: 0.3  S: 0.1
Sample ID: GVK-B1192-4K
20002027-GVK-B1192-4K-2 14 (0.186)

HRMS Spectrum of 2-(furan-2-yl)-3-hydroxythieno[3,2-b]pyridin-7(4H)-one (15k)
FT-IR Spectrum of 2-(furan-2-yl)-3-hydroxythieno[3,2-b]pyridin-7(4H)-one (15k)
$^1$H NMR (300 MHz, CDCl$_3$) Spectrum of 7-methoxy-2-phenylthieno[3,2-}b]pyridin-3-yl trifluoromethanesulfonate (16a)
$^{13}$C NMR (75 MHz, CDCl$_3$) Spectrum of 7-methoxy-2-phenylthieno[3,2-$b$]pyridin-3-yl trifluoromethanesulfonate(16a)
Elemental Composition Report

Single Mass Analysis
Tolerance = 2500.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
117 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-15  H: 0-11  N: 0-1  O: 0-4  S: 0-2  F: 0-3

SAMPLE CODE: GVK-B1192-OTF
21022014-GVK-B1192-OTF 343 (10.876)

HRMS Spectrum of 7-methoxy-2-phenylthieno[3,2-b]pyridin-3-yl trifluoromethanesulfonate (16a).
FT-IR Spectrum of 7-methoxy-2-phenylthieno[3,2-b]pyridin-3-yl trifluoromethanesulfonate (16a).
$^1$H NMR (300 MHz, CDCl$_3$) Spectrum of 2-(4-chlorophenyl)-7-methoxythieno[3,2-b]pyridin-3-yl trifluoromethanesulfonate (16i)
$^{13}$C NMR (75 MHz, CDCl$_3$) Spectrum of 2-(4-chlorophenyl)-7-methoxythieno[3,2-b]pyridin-3-yl trifluoromethanesulfonate (16i)
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
237 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-15  H: 0-10  N: 0-1  O: 0-4  F: 0-3  S: 0-2  Cl: 0-1
Sample ID:GVK-B1192-24
26062014-20-GVK-B1192-24 16 (0.239) AM (Top,4, Ar,5000.0,195.10,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

Minimum:
Maximum:
Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
423.9806  423.9692  11.4  26.9  9.5  132223.4  C15 H10 N O4 F3 S2 Cl

HRMS Spectrum of 2-(4-chlorophenyl)-7-methoxythieno[3,2-b]pyridin-3-yl trifluoromethanesulfonate (16i)
FT-IR Spectrum of 2-(4-chlorophenyl)-7-methoxythieno[3,2-\textit{b}]pyrid-3-yl trifluoromethanesulfonate (16i)
$^1$H NMR (300 MHz, CDCl$_3$) Spectrum of 2-(furan-2-yl)-7-methoxythieno[3,2-b]pyridin-3-yl trifluoromethanesulfonate (16k)
$^{15}$C NMR (100 MHz, CDCl$_3$) Spectrum of 2-(furan-2-yl)-7-methoxythieno[3,2-\textit{b}]pyridin-3-yl trifluoromethanesulfonate (16k)
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
141 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0.13  H: 0.9  N: 0.1  O: 0.5  F: 0.3  S: 0.2
Sample ID: GVK-B1192-27
26062024-GVK-B1192-27 17 (0.248) AM (Top,4, Ar, 5000.0, 556.35, 1.00, LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

Minimum:                  -1.5
Maximum:                  5.0  5000.0  50.0
Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
379.9897  379.9874  2.3  6.1  8.5  157148.0  C13  H9  N  O5  F3  S2

HRMS Spectrum of of 2-(furan-2-yl)-7-methoxythieno[3,2-b]pyridin-3-yl trifluoromethanesulfonate (16k)
FT-IR Spectrum of 2-(furan-2-yl)-7-methoxythieno[3,2-b]pyridin-3-yl trifluoromethanesulfonate (16k)
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 7-methoxy-2,3-diphenylthieno[3,2-b]pyridine (17a)
$^{13}$C NMR (75 MHz, CDCl$_3$) Spectrum of 7-methoxy-2,3-diphenythieno[3,2-$b$]pyridine (17a)
Elemental Composition Report

Single Mass Analysis
Tolerance = 200000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
4 formula(e) evaluated with 1 results within limits (up to 2 closest results for each mass)
Elements Used:
C: 0-20  H: 0-16  N: 0-1  O: 0-1  S: 0-1

SAMPLE ID: GVK-B1182-01
Age: Method: GVCE-FA-11-MIN
13130113-GVK-B1182-01 10 (0.146)

Date of Analysis: 13-Nov-2013 14:39:56
Instrument ID: ANL-MCL3-02-01
1: TOF MS ES+ 2:17e3

Minimum: -1.5
Maximum: 5.0  200000.0  50.0

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HRMS Spectrum of 7-methoxy-2,3-diphenylthieno[3,2-b]pyridine (17a)
FT-IR Spectrum of 7-methoxy-2,3-diphenylthieno[3,2-b]pyridine (17a)
$^1$H NMR (300 MHz, CDCl$_3$) Spectrum of 7-methoxy-3-(4-methoxyphenyl)-2-phenylthieno[3,2-b]pyridine (17b)
$\text{C NMR (100 MHz, CDCl}_3\text{)}$ Spectrum of 7-methoxy-3-(4-methoxyphenyl)-2-phenylthieno[3,2-\text{b}]pyridine (17b)
Elemental Composition Report

Single Mass Analysis
Tolerance = 200000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 2 closest results for each mass)
Elements Used:
C: 0-21 H: 0-18 N: 0-1 O: 0-2 S: 0-1

HRMS Spectrum of 7-methoxy-3-(4-methoxyphenyl)-2-phenylthieno[3,2-b]pyridine (17b)
FT-IR Spectrum of 7-methoxy-3-(4-methoxyphenyl)-2-phenylthieno[3,2-b]pyridine (17b)
$^1$H NMR (300 MHz, CDCl$_3$) Spectrum of 3-(4-chlorophenyl)-7-methoxy-2-phenylthieno[3,2-b]pyridine (17c)
$^{13}$C NMR (75 MHz, CDCl$_3$) Spectrum of $3'$-(4-chlorophenyl)-7-methoxy-2-phenylthieno[3,2-$b$]pyridine (17c)
Elemental Composition Report

Single Mass Analysis
Tolerance = 200000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 3 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-21  H: 0-15  N: 0-1  O: 0-2  S: 0-1  CI: 0-1

HRMS Spectrum of 3-(4-chlorophenyl)-7-methoxy-2-phenylthieno[3,2-b]pyridine (17c)
FT-IR Spectrum of 3-(4-chlorophenyl)-7-methoxy-2-phenylthieno[3,2-b]pyridine (17c)
$^1$H NMR (300 MHz, CDCl$_3$) Spectrum of 3-(4-fluorophenyl)-7-methoxy-2-phenylthieno[3,2-b]pyridine (17d)
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 3-(4-fluorophenyl)-7-methoxy-2-phenylthieno[3,2-b]pyridine (17d)
Elemental Composition Report

Single Mass Analysis
Tolerance = 200000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 4 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-21  H: 0-15  N: 0-1  O: 0-2  F: 0-1  S: 0-1

GVK Biosciences Pvt. Ltd.
Medicinal Chemistry Laboratory - Analytical Research

SAMPLE ID : GVK-B1192-04
Acc. Method : GVCE-FA-11-MIN
13112013-GVK-B1192-04 12 (0.167)

HRMS Spectrum of 3-(4-fluorophenyl)-7-methoxy-2-phenylthieno[3,2-b]pyridine (17d)

Minimum: -1.5
Maximum: 5.0  2000000.0  50.0

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FT-IR Spectrum of 3-(4-fluorophenyl)-7-methoxy-2-phenylthieno[3,2-b]pyridine (17d)
$^1$H NMR (300 MHz, CDCl$_3$) Spectrum of 4-(7-methoxy-2-phenylthieno[3,2-b]pyridin-3-yl)benzonitrile (17e)
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 4-(7-methoxy-2-phenylthieno[3,2-$b$]pyridin-3-yl)benzonitrile (17e)
Elemental Composition Report

Single Mass Analysis
Tolerance = 200000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 2 results within limits (up to 1 closest results for each mass)

Elements Used:
C: 0.21  H: 0.15  N: 0.2  O: 0.2  S: 0.1

HRMS Spectrum of 4-(7-methoxy-2-phenylthieno[3,2-b]pyridin-3-yl)benzonitrile (17e)
FT-IR Spectrum of 4-(7-methoxy-2-phenylthieno[3,2-b]pyridin-3-yl)benzonitrile (17e)
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 7-methoxy-2-phenyl-3-(4-(trifluoromethyl)phenyl)thieno[3,2-\textit{b}]pyridine (17f)
$^1$C NMR (100 MHz, CDCl$_3$) Spectrum of 7-methoxy-2-phenyl-3-(4-(trifluoromethyl)phenyl)thieno[3,2-b]pyridine (17f)
Elemental Composition Report

Single Mass Analysis

Tolerance = 200000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
49 formula(e) evaluated with 5 results within limits (up to 1 closest results for each mass)

Elements Used:
C: 0-22  H: 0-18  N: 0-2  O: 0-2  F: 0-3  S: 0-1

HRMS Spectrum of 7-methoxy-2-phenyl-3-(4-(trifluoromethyl)phenyl)thieno[3,2-b]pyridine (17f)
FT-IR Spectrum of 7-methoxy-2-phenyl-3-(4-(trifluoromethyl)phenyl)thieno[3,2-b]pyridine (17f)
$^1$H NMR (300 MHz, CDCl$_3$) Spectrum of 7-methoxy-2-phenyl-3-(4-(trifluoromethoxy)phenyl)thieno[3,2-b]pyridine (17g)
$^{13}$C NMR (75 MHz, CDCl$_3$) Spectrum of 7-methoxy-2-phenyl-3-(4-(trifluoromethoxy)phenyl)thieno[3,2-$b$]pyridine (17g)
Elemental Composition Report

Single Mass Analysis
Tolerance = 200000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
49 formula(e) evaluated with 2 results within limits (up to 1 closest results for each mass)

Elements Used:
C: 0-22   H: 0-18   N: 0-2   O: 0-2   F: 0-3   S: 0-1

SAMPLE ID : GVK-B1192-09
Acq. Method : GVCE-FA-11-MIN
13112013-GVK-B1192-09 12 (0.167) AM (Ben,4, 80.00, Ar,5000.0,566.28,0.00,LS 5); Sm (Mn, 3x2.00); Sb (1,40.00)

Minimum: -1.5
Maximum: 5.0  200000.0  50.0

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HRMS Spectrum of 7-methoxy-2-phenyl-3-(4-(trifluoromethoxy)phenyl)thieno[3,2-b]pyridine (17g)
FT-IR Spectrum of 7-methoxy-2-phenyl-3-(4-(trifluoromethoxy)phenyl)thieno[3,2-\textit{b}]pyridine (17g)

GVK BIO
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 1-(4-(7-methoxy-2-phenylthieno[3,2-b]pyridin-3-yl)phenyl)ethanone (17h)
$^{13}$C NMR (75 MHz, CDCl$_3$) Spectrum of 1-(4-(7-methoxy-2-phenylthieno[3,2-b]pyridin-3-yl)phenyl)ethanone (17h)
Elemental Composition Report

Single Mass Analysis
Tolerance = 200000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
10 formula(e) evaluated with 1 results within limits (up to 2 closest results for each mass)
Elements Used:
C: 0.22  H: 0.18  N: 0.2  O: 0.2  S: 0.1

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HRMS Spectrum of 1-(4-(7-methoxy-2-phenylthieno[3,2-b]pyridin-3-yl)phenyl)ethanone (17h)
FT-IR Spectrum of 1-(4-(7-methoxy-2-phenylthieno[3,2-b]pyridin-3-yl)phenyl)ethanone (17h)

¹H NMR (300 MHz, CDCl₃) Spectrum of 3-(furan-3-yl)-7-methoxy-2-phenylthieno[3,2-b]pyridine (17i)
$^{13}$C NMR (75 MHz, CDCl$_3$) Spectrum of 3-(furan-3-yl)-7-methoxy-2-phenylthieno[3,2-b]pyridine (17i)
Elemental Composition Report

Single Mass Analysis
Tolerance = 200000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Evon Electron Ions
19 formula(e) evaluated with 4 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-18  H: 0-14  N: 0-2  O: 0-2  S: 0-2

GVK Biosciences Pvt. Ltd.
Medicinal Chemistry Laboratory - Analytical Research

SAMPLE ID : GVKB1192-11
Acq. Method : GVCE-FA-11-MIN
13112013-GVKB1192-113 (0.044)

Date of Analysis : 13-Nov-2013 14:58:47
Instrument ID : ANL-MCL3-LCMS-001
1: TOF MS ES+
2:5263

Minimum: 308.0829
Maximum: 308.0745 8.4 27.3 12.5 C18 H14 N O2 S

Mass    Calc. Mass   mDa   PPM   DBE   Formula
308.0829  308.0745   8.4  27.3  12.5  C18 H14 N O2 S
HRMS spectrum of 3-(furan-3-yl)-7-methoxy-2-phenylthieno[3,2-b]pyridine (17i)
FT-IR spectrum of 3-(furan-3-yl)-7-methoxy-2-phenylthieno[3,2-b]pyridine (17i)
$^1$H NMR (300 MHz, CDCl$_3$) Spectrum of 7-methoxy-2-phenyl-3-(thiophen-3-yl)thieno[3,2-\textit{b}]pyridine (17j)
$^{13}$C NMR (75 MHz, CDCl$_3$) Spectrum of 7-methoxy-2-phenyl-3-(thiophen-3-yl)thieno[3,2-b]pyridine (17J)
Elemental Composition Report

Single Mass Analysis
Tolerance = 200000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
17 formula(s) evaluated with 2 results within limits (up to 1 closest results for each mass)

Elements Used:
C: 0.18  H: 0.14  N: 0.2  O: 0.2  S: 0.2

HRMS spectrum of 7-methoxy-2-phenyl-3-(thiophen-3-yl)thieno[3,2-b]pyridine (17J)
FT-IR spectrum of 7-methoxy-2-phenyl-3-(thiophen-3-yl)thieno[3,2-\text{b}]pyridine (17J)
$^1$H NMR (300 MHz, CDCl$_3$) Spectrum of 7-methoxy-2-phenyl-3-(pyridin-4-yl)thieno[3,2-$b$]pyridine (17K)
$^{13}$C NMR (75 MHz, CDCl$_3$) Spectrum of 7-methoxy-2-phenyl-3-(pyridin-4-yl)thieno[3,2-b]pyridine (17K)
Elemental Composition Report

Single Mass Analysis
Tolerance = 200000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-19 H: 0-15 N: 0-2 O: 0-1 S: 0-1

Sample ID: GVKB1119212
Acq. Method: GVCE-FA-11-MIN

HRMS spectrum of 7-methoxy-2-phenyl-3-(pyridin-4-yl)thieno[3,2-b]pyridine (17K)
FT-IR spectrum of 7-methoxy-2-phenyl-3-(pyridin-4-yl)thieno[3,2-b]pyridine (17K)
$^1$H NMR (300 MHz, CDCl$_3$) Spectrum of 2-(4-chlorophenyl)-7-methoxy-3-(4-methoxyphenyl)thieno[3,2-b]pyridine (17l)
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 2-(4-chlorophenyl)-7-methoxy-3-(4-methoxyphenyl)thieno[3,2-$b$]pyridine (17l)
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
18 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0.21  H: 0.17  N: 0.1  O: 0.2  S: 0.1  Cl: 0.1
Sample ID: GVK-B1192-25
24062014-GVK-B1192-25 22 (0.330) AM (Top,4, Ar5000.0, 556.26, 1.00, LS 10); Sm (Mn, 2x1.00); Sb (1.40.00)

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HRMS spectrum of 2-(4-chlorophenyl)-7-methoxy-3-(4-methoxyphenyl)thieno[3,2-b]pyridine (171)
FT-IR spectrum of 2-(4-chlorophenyl)-7-methoxy-3-(4-methoxyphenyl)thieno[3,2-b]pyridine (17I)
$^1$H NMR (300 MHz, CDCl$_3$) Spectrum of 4-(2-(4-chlorophenyl)-7-methoxythieno[3,2-$b$]pyridin-3-yl)benzonitrile (17m)
$^{13}$C NMR (75 MHz, CDCl$_3$) Spectrum of 4-(2-(4-chlorophenyl)-7-methoxythieno[3,2-$b$]pyridin-3-yl)benzonitrile (17m)
HRMS spectrum of 4-(2-(4-chlorophenyl)-7-methoxythieno[3,2-b]pyridin-3-yl)benzonitrile (17m)
FT-IR spectrum of 4-(2-(4-chlorophenyl)-7-methoxythieno[3,2-b]pyridin-3-yl)benzonitrile (17m)
$^{1}$H NMR (400 MHz, CDCl$_3$) Spectrum of 2-(furan-2-yl)-7-methoxy-3-(4-methoxyphenyl)thieno[3,2-b]pyridine (17n)
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 2-(furan-2-yl)-7-methoxy-3-(4-methoxyphenyl)thieno[3,2-b]pyridine (17n)
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-19 H: 0-16 N: 0-1 O: 0-3 S: 0-1
Sample ID:GVK-B1192-28
20032025-GVK-B1192-28 15 (0.229) AM (Top, 4, Ar,5000.0,550.35,1.00,LS 10); Sm (Mn, 2*1.00); Sb (1.40.00)

HRMS spectrum of 2-(furan-2-yl)-7-methoxy-3-(4-methoxyphenyl)thieno[3,2-b]pyridine (17n)
FT-IR spectrum of 2-(furan-2-yl)-7-methoxy-3-(4-methoxyphenyl)thieno[3,2-b]pyridine (17n)
$^1$H NMR (400 MHz, CDCl$_3$) Spectrum of 4-(2-(furan-2-yl)-7-methoxythieno[3,2-b]pyridin-3-yl)benzonitrile (17o)
$^\text{13}$C NMR (100 MHz, CDCl$_3$) Spectrum of 4-(2-(furan-2-yl)-7-methoxythieno[3,2-\textit{b}]pyridin-3-yl)benzonitrile (17o)
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-19  H: 0-13  N: 0-2  O: 0-2  S: 0-1
Sample ID: GVK-B1192-29
266506726 GVK-B1192 29 15 (0.229) AM (Top, 4, Ar, 500.0, 558.35, 1.00, LS 10); Sm (Mn, 2x1.00); Sb (1, 40.00)

HRMS spectrum of 4-(2-(furan-2-yl)-7-methoxythieno[3,2-b]pyridin-3-yl)benzonitrile (17o)
FT-IR spectrum of 4-(2-(furan-2-yl)-7-methoxythieno[3,2-b]pyridin-3-yl)benzonitrile (17o)
$^1$H NMR (300 MHz, CD$_3$OD) Spectrum of 2,3-diphenylthieno[3,2-b]pyridin-7(4H)-one (18a)
$^{13}$C NMR (75 MHz, DMSO-$d_6$+CF$_3$CO$_2$D) Spectrum of 2,3-diphenylthieno[3,2-b]pyridin-7(4H)-one (18a)
Elemental Composition Report

Single Mass Analysis
Tolerance = 200000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 2 closest results for each mass)
Elements Used:
C: 0-19  H: 0-16  N: 0-2  O: 0-1  S: 0-1

HRMS spectrum of 2,3-diphenylthieno[3,2-b]pyridin-7(4H)-one (18a)
FT-IR spectrum of 2,3-diphenylthieno[3,2-b]pyridin-7(4H)-one (18a)
$^{1}$H NMR (300 MHz, CD$_3$OD) Spectrum of 3-(4-methoxyphenyl)-2-phenylthieno[3,2-$b$]pyridin-7(4H)-one (18b)
$^{13}$C NMR (75 MHz, DMSO-$d_6$+CF$_3$CO$_2$D) Spectrum of 3-(4-methoxyphenyl)-2-phenylthieno[3,2-b]pyridin-7(4H)-one (18b)
### Elemental Composition Report

**Single Mass Analysis**
- **Tolerance** = 200000.0 PPM
- **DBE**: min = -1.5, max = 50.0
- **Selected filters**: None

Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 2 closest results for each mass)

**Elements Used:**
- C: 0-20
- H: 0-18
- N: 0-2
- O: 0-2
- S: 0-1

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**SAMPLE ID**: GVKB1192-14
- **Acq. Method**: GVCE-FA-11-MIN
- **Date of Analysis**: 13-Nov-2013:15:09:40
- **Instrument ID**: ANL-MCL3-LCMS-001
- **Instrument**: TOF MS ES+
- **Instrument Version**: 1.14e3

**HRMS spectrum of 3-(4-methoxyphenyl)-2-phenylthieno[3,2-b]pyridin-7(4H)-one (18b)**

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FT-IR spectrum of 3-(4-methoxyphenyl)-2-phenylthieno[3,2-b]pyridin-7(4H)-one (18b)
$^{1}$H NMR (400 MHz, CD$_3$OD) Spectrum of 3-(4-chlorophenyl)-2-phenylthieno[3,2-b]pyridin-7(4H)-one (18c)
$^{13}$C NMR (100 MHz, DMSO-$d_6$+CF$_3$CO$_2$D) Spectrum of 3-(4-chlorophenyl)-2-phenylthieno[3,2-$b$]pyridin-7(4H)-one (18c)
HRMS spectrum of 3-(4-chlorophenyl)-2-phenylthieno[3,2-b]pyridin-7(4H)-one (18c)
FT-IR spectrum of 3-(4-chlorophenyl)-2-phenylthieno[3,2-b]pyridin-7(4H)-one (18c)
$^1$H NMR (300 MHz, CD$_3$OD) Spectrum of 3-(4-fluorophenyl)-2-phenylthieno[3,2-$b$]pyridin-7(4H)-one (18d)
$13^\text{C}$ NMR (75 MHz, DMSO-$d_6$+CF$_3$CO$_2$D) Spectrum of 3-(4-fluorophenyl)-2-phenylthieno[3,2-$b$]pyridin-7(4H)-one (18d)
Elemental Composition Report

Single Mass Analysis
Tolerance = 200000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 2 closest results for each mass)
Elements Used:
C: 0-19   H: 0-16   N: 0-1   O: 0-1   S: 0-1   F: 0-1

HRMS Spectrum of 3-(4-fluorophenyl)-2-phenylthieno[3,2-b]pyridin-7(4H)-one (18d)
FT-IR spectrum of 3-(4-fluorophenyl)-2-phenylthieno[3,2-b]pyridin-7(4H)-one (18d)
$^1$H NMR (300 MHz, CD$_3$OD) Spectrum of 4-(7-oxo-2-phenyl-4,7-dihydrothieno[3,2-b]pyridin-3-yl)benzonitrile (18e)
\(^{13}\)C NMR (75 MHz, DMSO-\(d_6\)+CF\(_3\)CO\(_2\)D) Spectrum of 4-(7-oxo-2-phenyl-4,7-dihydrothieno[3,2-\(b\)]pyridin-3-yl)benzonitrile (18e)
Elemental Composition Report

Single Mass Analysis
Tolerance = 200000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 6 results within limits (up to 1 closest results for each mass)

Elements Used:
C: 0-20  H: 0-16  N: 0-2  O: 0-1  S: 0-1  Cl: 0-1

Date of Analysis : 13-Nov-201315:14:26
Instrument ID : ANL-MCL3-LCMS-001
1: TOF MS ES+
5.83e3

SAMPLE ID : GV-K192-17
Acq. Method : GVCE-FA-11-MIN
1312013-GVK-BK192-17 11 (0.157) AM (Gen, 4, 80.00, Ar, 5000.0, 556.23, 0.00, LS 5); Sm (Mn, 3x2.00); Sb (14.00)

Minimum: 5.0  200000.0  50.0
Maximum: -1.5

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HRMS spectrum of 4-(7-oxo-2-phenyl-4,7-dihydrothieno[3,2-b]pyridin-3-yl)benzonitrile (18e)

S153
FT-IR spectrum of 4-(7-oxo-2-phenyl-4,7-dihydrothieno[3,2-\textbf{b}]pyridin-3-yl)benzonitrile (18e)
$^1$H NMR (300 MHz, CD$_3$OD) Spectrum of 2-phenyl-3-(4-(trifluoromethyl)phenyl)thieno[3,2-$b$]pyridin-7(4H)-one (18f)
$^{13}$C NMR (75 MHz, DMSO-$d_6$+CF$_3$CO$_2$D) Spectrum of 2-phenyl-3-(4-(trifluoromethyl)phenyl)thieno[3,2-$b$]pyridin-7(4H)-one (18f)
Single Mass Analysis
Tolerance = 200000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
51 formula(e) evaluated with 4 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-20  H: 0-20  N: 0-2  O: 0-2  F: 0-3  S: 0-1

HRMS spectrum of 2-phenyl-3-(4-(trifluoromethyl)phenyl)thieno[3,2-b]pyridin-7(4H)-one (18f)
FT-IR-spectrum of 2-phenyl-3-(4-(trifluoromethyl)phenyl)thieno[3,2-b]pyridin-7(4H)-one (18f)
\(^1\)H NMR (300 MHz, CD\(_3\)OD) Spectrum of 2-phenyl-3-(4-(trifluoromethoxy)phenyl)thieno[3,2-\(b\)]pyridin-7(4H)-one (18g)
$^{13}$C NMR (75 MHz, DMSO-$d_6$+CF$_3$CO$_2$D) Spectrum of 2-phenyl-3-(4-(trifluoromethoxy)phenyl)thieno[3,2-$b$]pyridin-7(4H)-one (18g)
HRMS spectrum of 2-phenyl-3-(4-(trifluoromethoxy)phenyl)thieno[3,2-b]pyridin-7(4H)-one (18g)
FT-IR spectrum of 2-phenyl-3-(4-(trifluoromethoxy)phenyl)thieno[3,2-b]pyridin-7(4H)-one (18g)
1H NMR (300 MHz, CD3OD) Spectrum of 3-(4-acetylphenyl)-2-phenylthieno[3,2-b]pyridin-7(4H)-one (18h)
$^{13}$C NMR (75 MHz, DMSO-$d_6$+CF3CO2D) Spectrum of 3-(4-acetylphenyl)-2-phenylthieno[3,2-$b$]pyridin-7(4H)-one (18h)
Elemental Composition Report

Single Mass Analysis
Tolerance = 250.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-21 H: 0-17 N: 0-1 O: 0-2 S: 0-1

GWK-B1192-16
13112013-GVK-B1192-16 8 (0.125) AM (Gen,4, 80.00, Ar,5000,0.556,28,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

Minimum:
0.0  250.0  50.0

Mass Calc. Mass mDa PPM DBE 1-FIT Formula
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HRMS spectrum of 3-(4-acetylphenyl)-2-phenylthieno[3,2-b]pyridin-7(4H)-one (18h)
FT-IR spectrum of 3-(4-acetylphenyl)-2-phenylthieno[3,2-b]pyridin-7(4H)-one (18h)
$^1$H NMR (400 MHz, CD$_3$OD) Spectrum of 3-(furan-3-yl)-2-phenylthieno[3,2-b]pyridin-7(4H)-one (18i)
$^{13}$C NMR (100 MHz, DMSO-$d_6$+CF$_3$CO$_2$D) Spectrum of 3-(furan-3-yl)-2-phenylthieno[3,2-$b$]pyridin-7(4H)-one (18i)
**Elemental Composition Report**

**Single Mass Analysis**
Tolerance = 200000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 2 closest results for each mass)
Elements Used:
* C: 0-17  H: 0-14  N: 0-1  O: 0-2  S: 0-1

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**SAMPLE ID:** GVK-B1192-22  
**Acq. Method:** GVCE-FA-11-MIN
13112013-GVK-B1192-22 12 (0.165) AM (Cen,4, 80.00, Ar,5000.0,556.28,0.00,LS 5); Sm (Mr, 3x2.00); Sb (1,40.00 )

**Date of Analysis:** 13-Nov-201315:22:21
**Instrument ID:** ANL-MCL3-LCMS-001
1: TOF MS ES+ 5.85e3

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**Minimum:** -1.5  
**Maximum:** 5.0 200000.0 50.0

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HRMS spectrum of 3-(furan-3-yl)-2-phenylthieno[3,2-b]pyridin-7(4H)-one (18i)

---

S169
FT-IR spectrum of 3-(furan-3-yl)-2-phenylthieno[3,2-b]pyridin-7(4H)-one (18i)
$^{1}$H NMR (400 MHz, CD$_3$OD) Spectrum of 2-phenyl-3-((thiophen-3-yl)thieno[3,2-$b$]pyridin-7(4H)-one (18J)
$^{13}$C NMR (100 MHz, DMSO-$d_6$+CF3CO2D) Spectrum of 2-phenyl-3-(thiophen-3-yl)thieno[3,2-b]pyridin-7(4H)-one (18j)
Elemental Composition Report

Single Mass Analysis
Tolerance = 200000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
8 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-17  H: 0-14  N: 0-1  O: 0-1  S: 0-2

GVK Biosciences Pvt. Ltd.
Medicinal Chemistry Laboratory - Analytical Research

SAMPLE ID : GVK-B1192-21
Acq. Method: GVCE-FA-11-MIN
13112013-GVK-B1192-21 10 (0.147) AM (Cen,4, 80.00, Ar, 5000.0, 556.28, 0.00, LS 5); Sm (Mn, 3x2.00); Sb (1,40.00 )

310.0438

102.1338
179.0341 121.1570 276.1542
100%
300 311.0638
310.0438

Minimum:
5.0
200000.0
-1.5
50.0

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
310.0430  310.0360  7.8  25.2  12.5  1411726.0  C17 H12 N O S2

HRMS Spectrum of 2-phenyl-3-(thiophen-3-yl)thieno[3,2-b]pyridin-7(4H)-one (18j)
FT-IR spectrum of 2-phenyl-3-(thiophen-3-yl)thieno[3,2-b]pyridin-7(4H)-one (18j)
$^1$H NMR (400 MHz, CD$_3$OD) Spectrum of 2-phenyl-3-(pyridin-4-yl)thieno[3,2-b]pyridin-7(4H)-one (18k)
$^{13}$C NMR (75 MHz, DMSO-$d_6$+CF$_3$CO$_2$D) Spectrum of 2-phenyl-3-(pyridin-4-yl)thieno[3,2-\textit{b}]pyridin-7(4H)-one (18k)
Elemental Composition Report

Single Mass Analysis
Tolerance = 2500.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-18  H: 0-13  N: 0-2  O: 0-1  S: 0-1
SAMPLE CODE : GVK-B1192-23
7042014-GVK-B1192-23 9 (0.222) AM (Top,4, Ar,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Sb (1.40.00)

Minimum:  5.0	-1.5
Maximum:  2500.0	50.0

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HRMS spectrum of 2-phenyl-3-(pyridin-4-yl)thieno[3,2-b]pyridin-7(4H)-one (18k)
FT-IR spectrum of 2-phenyl-3-(pyridin-4-yl)thieno[3,2-b]pyridin-7(4H)-one (18k)
$^1$H NMR (300 MHz, CD$_3$OD) Spectrum of 2-(4-chlorophenyl)-3-(4-methoxyphenyl)thieno[3,2-$b$]pyridin-7(4H)-one (18l)
$^{13}$C NMR (100 MHz, DMSO-$d_6$+CF$_3$CO$_2$D) Spectrum of 2-(4-chlorophenyl)-3-(4-methoxyphenyl)thieno[3,2-$b$]pyridin-7(4H)-one (18l)
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
18 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-20  H: 0-15  N: 0-1  O: 0-2  S: 0-1  Cl: 0-1
Sample ID: GVK-B1192-25A
29061201-19-GVK-B1192-25A 16 (0.240) AM (Top, 4, Ar, 5000.0, 195.11, 1.00, LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

HRMS spectrum of 2-(4-chlorophenyl)-3-(4-methoxyphenyl)thieno[3,2-b]pyridin-7(4H)-one (7I)

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FT-IR spectrum of 2-(4-chlorophenyl)-3-(4-methoxyphenyl)thieno[3,2-b]pyridin-7(4H)-one (181)
$^1$H NMR (300 MHz, DMSO-$d_6$) Spectrum of 4-(2-(4-chlorophenyl)-7-oxo-4,7-dihydrothieno[3,2-$b$]pyridin-3-yl)benzonitrile (18m)
$^{13}$C NMR (100 MHz, DMSO-$d_6$+CF$_3$CO$_2$D) Spectrum of 4-(2-(4-chlorophenyl)-7-oxo-4,7-dihydrothieno[3,2-$b$]pyridin-3-yl)benzonitrile (18m)
**Elemental Composition Report**

**Single Mass Analysis (displaying only valid results)**

Tolerance = 5000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

**Monoisotopic Mass, Even Electron Ions**
18 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

**Elements Used:**
C: 0-20  H: 0-12  N: 0-2  O: 0-1  S: 0-1  Cl: 0-1

Sample ID: GVK-B1192-26A
26062014-17-GVK-B1192-26A 15 (0.228) AM (Top, 4, Ar, 5000.0, 195, 13, 1.00, LS 10); Sm (Mn, 2x1.00); Sb (1, 40.00)

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<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
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HRMS spectrum of 4-(2-(4-chlorophenyl)-7-oxo-4,7-dihydrothieno[3,2-b]pyridin-3-yl)benzonitrile (18m)
FT-IR spectrum of 4-(2-(4-chlorophenyl)-7-oxo-4,7-dihydrothieno[3,2-b]pyridin-3-yl)benzonitrile (18m)
\( ^1 \text{H NMR (300 MHz, DMSO-}\text{d}_6) \text{ Spectrum of 2-(furan-2-yl)-3-(4-methoxyphenyl)thieno[3,2-}\text{b}\text{pyridin-7(4H)-one (18n)} \)
$^{13}$C NMR (75 MHz, DMSO-$d_6$+CF$_3$CO$_2$D) Spectrum of 2-(furan-2-yl)-3-(4-methoxyphenyl)thieno[3,2-$b$]pyridin-7(4H)-one (18n)
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:
C: 0-18 H: 0-14 N: 0-1 O: 0-3 S: 0-1

Sample ID: GVK-B1192-28A
26062014-16-GVK-B1192-28A 15 (0.229) AM (Top, 4, Ar, 5000.0, 165.14, 1.00, LS 10); Sm (Mn, 2x1.00); Sb (1.40.00)

HRMS spectrum of 2-(furan-2-yl)-3-(4-methoxyphenyl)thieno[3,2-b]pyridin-7(4H)-one (18n)
FT-IR spectrum of 2-(furan-2-yl)-3-(4-methoxyphenyl)thieno[3,2-b]pyridin-7(4H)-one (18n)
\(^1\)H NMR (300 MHz, DMSO-\(d_6\)) Spectrum of 4-(2-(furan-2-yl)-7-oxo-4,7-dihydrothieno[3,2-\(b\)]pyridin-3-yl)benzonitrile (18o)
$^{13}$C NMR (100 MHz, DMSO-$d_6$+CF$_3$CO$_2$D) Spectrum of 4-(2-(furan-2-yl)-7-oxo-4,7-dihydrothieno[3,2-b]pyridin-3-yl)benzonitrile (18o)
HRMS spectrum of 4-(2-(furan-2-yl)-7-oxo-4,7-dihydrothieno[3,2-b]pyridin-3-yl)benzonitrile (18o)
FT-IR spectrum of 4-(2-(furan-2-yl)-7-oxo-4,7-dihydrothieno[3,2-\textit{b}]pyridin-3-yl)benzonitrile (18o)