Supplementary information

Synthesis and evaluation of thieno[2,3-*d*]pyrimidin-4(3*H*)-ones as potential anti-tubercular agents

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All the solvents and reagents were purchased from commercial suppliers and were used without further purification. The progress of each reaction was monitored by ascending thin layer chromatography (TLC) using TLC aluminum sheets, silica gel F254 precoated (Merck, Germany), and locating the spots using UV light or iodine vapors as the visualizing agent. Melting points were obtained by an open capillary method and are uncorrected. ^{1}H NMR spectra were recorded ($CDCl_3$/DMSO-d_6) on a Bruker Avance 200 NMR spectrometer or JEOL ECX 400 NMR spectrometer or Bruker 500 NMR spectrometer. ^{13}C NMR and DEPT 135 spectra were recorded ($CDCl_3$/DMSO-d_6) on Bruker Avance 200 NMR spectrometer or JEOL ECX 400 NMR spectrometer. Chemical shifts (δ) are reported in parts per million (ppm) using tetramethylsilane (TMS) as an internal standard. The splitting pattern abbreviations are designated as singlet (s), doublet (d), double doublet (dd), triplet (t), quartet (q) and multiplet (m).The mass spectra were recorded on a Q-TOF micromass (YA-105) spectrometer in ESI (electrospray ionization) mode.

Preparation of 6-ethyl-3-pentylthieno[2,3-d]pyrimidin-4(3H)-one (11g)

Potassium carbonate (3.44 g, 0.025 mol) was taken in a 100 mL two-necked RB flask and heated under vacuum to remove the traces of moisture and flushed with nitrogen. 6-Ethylthieno[2,3-d]pyrimidin-4(3H)-one (1.5 g, 0.008 mol) was added under nitrogen followed by dry DMF (25 mL) and stirred for 10 min. Pentyl bromide (1.55 ml, 1.88 g, 0.012 mol) was added dropwise and the reaction mixture was stirred at RT for 12 h. It was then diluted with water (100 mL) and extracted with ethyl acetate (3 x 50 mL). The combined organic layer was dried over anhydrous sodium sulphate, filtered and concentrated under reduced pressure. The residue was purified by column chromatography to afford 6-ethyl-3-pentylthieno[2,3-d]pyrimidin-4(3H)-one (**11g**) as off-white solid, 1.885 g (90%). Melting Point: 74^{0}C. ^{1}H NMR (200MHz, $CDCl_3$): δ 0.91 (t, J = 7Hz, 3H), 1.28-1.44 (m, 7H), 1.68-1.82 (m, 2H), 2.88 (q, J = 7 Hz, 2H), 3.99 (t, J = 7 Hz, 2 H), 7.17 (s, 1 H), 7.92 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.80, 15.21, 22.17, 23.91, 28.61, 29.17, 46.80, 117.44, 124.77, 145.62, 145.87, 157.22, 162.24. IR ($CHCl_3$): 1672 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{13}H_{18}ON_2S$ + H]: 251.1213, found: 251.1210; [$C_{13}H_{18}ON_2S$ + Na]: 273.1032 found: 273.1027.

Compounds **11a** to **11f** and **11h** to **11n** were prepared by above method described for **11g** using the corresponding alkyl halides and required thienopyrimidinones. In case of compounds **12a** to **12e**, same procedure was used wherein benzyl bromide was used in place of alkyl halide. Compounds **13a** and **13b** were prepared by using bromoacetonitrile while compounds **14a** to **14c** were prepared by using cyclopropylmethyl bromide. α,α'-Dibromo-p-xylene was used for preparation of compound **15a**, (1,3-dioxolan-2-yl)ethyl bromide for compounds **16a** and **16b** whereas (1,3-dioxan-2-yl)ethyl bromide was used for getting compound **16c**. Compounds **17a** to **17c** were obtained when 2-chloro-1-(2,4-difluorophenyl)ethan-1-one was reacted with the corresponding thienopyrimidinones. Allyl bromide was used in the preparation of **18a** while ethyl bromoacetate was employed for getting compounds **19a** to **19c**. Hydrolysis of **19b** and **19c** with ethanolic sodium hydroxide afforded compounds **20b** and **20c** respectively. Bromoacetaldehyde diethyl acetal was reacted with the required thienopyrimidinones to get the compounds **21a** and **21b.** Deprotection of **21a** with conc HCl in acetonitrile afforded aldehyde **22a**. The reactions of 2-bromo-1-(thiophen-2-yl)ethan-1-one with various thienopyrimidinones provided corresponding ketones **23a** to **23c**. The reactants and reagents to get compounds with general structures **24** to **38** are shown in Schemes 2-4. All the compounds screened in the present study were characterized by spectral methods and the data are given below:

6-Methyl-3-propylthieno[2,3-d]pyrimidin-4(3H)-one (11a)

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.99 (t, *J*=4 Hz, 3H), 1.75-1.85 (m, 2H), 2.54 (s, 3H), 3.96 (t, *J*= 4 Hz, 2H), 7.13 (s, 1H), 7.92 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 10.95, 15.94, 22.69, 48.30, 119.25, 124.96, 138.45, 145.63, 157.01, 162.38. IR (Neat): 1664 cm $^{-1}$. HRMS (ESI) m/z calculated for [$C_{10}H_{12}N_2OS$+H]: 209.0743, found: 209.0741; [$C_{10}H_{12}N_2OS$ +Na]:231.0563, found: 231.0559. Melting Point: 116°C.

3-Isopropyl-6-methylthieno[2,3-d]pyrimidin-4(3H)-one (11b)

^{1}H NMR (200 MHz, $CDCl_3$): δ 1.47 (d, *J*=7 Hz, 6H), 2.54 (s, 3H), 5.10-5.31 (m, 1H), 7.13 (s, 1H), 8.00 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 15.91, 22.13 (2C), 45.58, 119.33, 124.57, 138.28, 142.66, 156.65, 161.91. IR (Neat): 1666 cm $^{-1}$. HRMS (ESI) m/z calculated for [$C_{10}H_{12}N_2OS$+H]: 209.0743, found: 209.0743; [$C_{10}H_{12}N_2OS$ +Na]: 231.0563, found: 231.0561. Melting Point: 64°C.

3-Isobutyl-6-methylthieno[2,3-d]pyrimidin-4(3H)-one (11c)

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.97 (d, *J*=8 Hz, 6H), 2.12-2.25 (m, 1H), 2.54 (s, 3H), 3.80 (d, *J*=7 Hz, 2H), 7.13 (s, 1H), 7.90 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 16.02, 19.81, 28.14, 53.93, 119.43, 125.07, 138.59, 145.98, 157.24, 162.27. IR ($CHCl_3$): 1673 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{11}H_{14}N_2OS$+H]: 223.0900, found: 223.0898. Melting Point: 91°C.

3,6-Diethylthieno[2,3-d]pyrimidin-4(3H)-one (11d)

^{1}H NMR (200 MHz, $CDCl_3$): δ 1.35 (t, *J*=8 Hz, 3H), 1.41 (t, *J* =7 Hz, 3H), 2.88 (q, *J*= 8 Hz, 2H), 4.07 (q, *J*=7 Hz, 2H), 7.17 (s, 1H), 7.95 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 15.00, 15.14, 23.84, 41.87, 117.30, 124.67, 145.26, 145.88, 156.96, 162.06. IR ($CHCl_3$): 1659 cm^{-1}. HRMS (ESI) m/z calculated for

[$C_{10}H_{12}ON_2S$+H]: 209.0743, found: 209.0741; [$C_{10}H_{12}ON_2S$+Na]: 231.0563, found: 231.0560. Melting Point: 64.1^{0}C.

6-Ethyl-3-propylthieno[2,3-d]pyrimidin-4(3H)-one (11e)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.98 (t, *J*=7 Hz, 3H), 1.34 (t, *J*=8 Hz, 3H), 1.70-1.92 (m, 2H), 2.87 (q, *J*=7 Hz, 2H), 3.96 (t, *J*=8 Hz, 2H), 7.15 (s, 1H), 7.92 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 10.85, 15.08, 22.61, 23.78, 48.18, 117.32, 124.63, 145.57, 145.70, 157.09, 162.13. IR (Neat): 1659 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{11}H_{14}ON_2S$+H]: 223.0900, found: 223.0899. Melting Point: 85 ^{0}C.

6-Ethyl-3-isopropylthieno[2,3-d]pyrimidin-4(3H)-one (11f)

^{1}H NMR (200 MHz, $CDCl_3$): δ 1.29 (t, *J*=7 Hz, 3H), 1.42 (d, *J*=7 Hz, 6H), 2.82 (q, *J*=7 Hz, 2H), 5.07-5.25 (m, 1H), 7.10 (s, 1H), 7.97 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 15.20, 22.19 (2C), 23.88, 45.65, 117.54, 124.40, 142.68, 145.81, 156.82, 161.51. IR (Neat): 1649 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{11}H_{14}ON_2S$+H]: 223.0900, found: 223.0895. [$C_{11}H_{14}O\ N_2S$+Na]: 245.0719, found: 245.0713. Melting Point: 105^{0}C.

6-Ethyl-3-octylthieno[2,3-d]pyrimidin-4(3H)-one (11h)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.87 (t, *J*=7 Hz, 3H), 1.17-1.42 (m, 13H), 1.72-1.86 (m, 2H), 2.88 (q, *J*=7 Hz, 2H), 3.99 (t, *J* =7 Hz, 2H), 7.17 (s, 1H), 7.92 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 14.00, 15.25, 22.55, 23.97, 26.58, 29.06, 29.09, 29.54, 31.69, 46.89, 117.53, 124.85, 145.64, 145.94, 157.28, 162.29. IR ($CHCl_3$): 1676 cm^1. HRMS (ESI) m/z calculated for [$C_{16}H_{24}ON_2S$ + H]: 293.1682, found: 293.1677; [$C_{16}H_{24}ON_2S$ + Na]: 315.1502, found: 315.1494. Melting Point: 62^{0}C.

3,6-Dipropylthieno[2,3-d]pyrimidin-4(3H)-one (11i)

^{1}H NMR (400 MHz, $CDCl_3$) : δ 0.92-1.02 (m, 6H), 1.64-1.86 (m, 4H), 2.80 (t, *J*=8 Hz, 2H), 3.95 (t, *J*=8 Hz, 2H), 7.14 (s, 1H), 7.92 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.00, 13.74, 22.75, 24.26, 32.57, 48.36, 118.29, 124.78, 144.24, 145.62, 157.26, 162.34. IR ($CHCl_3$): 1675 cm^1. HRMS (ESI) m/z calculated for [$C_{12}H_{16}ON_2S$ + H]: 237.1056, found: 237.1055. Melting Point: 58^{0}C.

3-Isopropyl-6-propylthieno[2,3-d]pyrimidin-4(3H)-one (11*j*)

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.99 (t, *J*=8 Hz, 3H), 1.47 (d, *J*=7 Hz, 6H), 1.65-1.80 (m, 2H), 2.82 (t, *J*=7 Hz, 2H), 5.13-5.27 (m, 1H), 7.15 (s, 1H), 8.00 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.49, 22.27 (2C), 24.30, 32.61, 45.69, 118.47, 124.48, 142.68, 144.19, 156.99, 161.92. IR ($CHCl_3$): 1668 cm^1. HRMS (ESI) m/z calculated for [$C_{12}H_{16}ON_2S$ + H]: 237.1056, found: 237.1085. Melting Point: 95^{0}C.

3-Octyl-6-propylthieno[2,3-d]pyrimidin-4(3H)-one (11k)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.87 (t, *J* =7 Hz, 3H), 1.00 (t, *J* =7 Hz, 3H), 1.17-1.42 (m, 10H), 1.65-1.86 (m, 4H), 2.82 (t, *J*=8 Hz, 2H), 3.99 (t, *J*=8 Hz, 2H), 7.16 (s, 1H), 7.93 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 13.49, 14.00, 22.56, 24.30, 26.58, 29.06, 29.09, 29.55, 31.70, 32.62, 46.95, 118.37, 124.88, 144.36, 145.62, 157.22, 162.05. IR ($CHCl_3$): 1667 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{17}H_{26}ON_2S$ + H]: 307.1839, found: 307.1835; [$C_{17}H_{26}ON_2S$ + Na]: 329.1658, found: 329.1652. Melting Point: 150^{0}C.

3-Methyl-6-pentylthieno[2,3-d]pyrimidin-4(3H)-one (11l)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.89 (t, *J*=7 Hz, 3H), 1.20-1.45 (m, 4H), 1.60-1.80 (m, 2H), 2.82 (t, *J*=6 Hz, 2H), 3.58 (s, 3H), 7.14 (s, 1H), 7.95 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.91, 22.29, 30.54, 30.65, 31.03, 33.96, 118.01, 124.57, 144.74, 145.75, 157.76, 162.51. IR ($CHCl_3$): 1668 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{12}H_{16}ON_2S$ + H]: 237.1056, found: 237.1051; [$C_{12}H_{16}ON_2S$ + Na]: 259.0876, found: 259.0869. Melting Point: 88^{0}C.

6-Pentyl-3-propylthieno[2,3-d]pyrimidin-4(3H)-one (11m)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.90 (t, *J*=7 Hz , 3H), 1.00 (t, *J*=7 Hz, 3H), 1.27-1.47 (m, 4H), 1.62-1.94 (m, 4H), 2.84 (t, *J*=8 Hz, 2H), 3.98 (t, *J*=7 Hz, 2H), 7.16 (s, 1H), 8.01 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 10.93, 13.83, 22.20, 22.67, 30.44, 30.60, 30.94, 48.28, 118.08, 124.67, 144.44, 145.57, 157.13, 162.11. IR ($CHCl_3$): 1672 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{14}H_{20}ON_2S$ + H]: 265.1369, found: 265.1367; [$C_{14}H_{20}ON_2S$ + Na]: 287.1189, found: 287.1185. Melting Point: 141^{0}C.

3-Methyl-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidin-4(3H)-one (11n)

^{1}H NMR (200 MHz, $CDCl_3$): δ 1.75-1.96 (m, 4H), 2.78 (t, *J*=6 Hz, 2H), 3.02 (t, *J*=6 Hz, 2H), 3.55 (s, 3H), 7.91 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 22.18, 22.81, 25.16, 25.57, 33.67, 122.58, 131.37, 134.11, 145.61, 158.27, 162.14. IR ($CHCl_3$): 1669 cm^1. HRMS (ESI) m/z calculated for [$C_{11}H_{12}ON_2S$ + H]: 221.0743, found: 221.0740; [$C_{11}H_{12}ON_2S$ + Na]: 243.0563, found: 243.0558. Melting Point: 89^{0}C.

3-Benzyl-6-ethylthieno[2,3-d]pyrimidin-4(3H)-one (12a)

^{1}H NMR (200 MHz, $CDCl_3$): δ 1.35 (t, *J* =7 Hz, 3H), 2.88 (q, *J*=7 Hz, 2H), 5.21 (s, 2H), 7.19 (s, 1H), 7.29-7.39 (m, 5H), 8.01 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 15.19, 23.88, 49.22, 117.56, 124.74, 127.93 (2C), 128.33, 128.89 (2C), 135.69, 145.48, 146.17, 157.14, 162.05. IR (Neat): 1666 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{15}H_{14}ON_2S$+H]: 271.0900, found: 271.0896; [$C_{15}H_{14}ON_2S$+Na]: 293.0719, found: 293.0715. Melting Point: 100^{0}C.

3-Benzyl-6-propylthieno[2,3-d]pyrimidin-4(3H)-one (12b)

^{1}H NMR (200MHz, $CDCl_3$): δ 1.00 (t, *J*=7 Hz, 3H), 1.60-1.85 (m, 2H), 2.82 (t, *J*=7 Hz, 2H), 5.21 (s, 2H), 7.17 (s, 1H), 7.35 (bs, 5H), 8.02 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.54, 24.34, 32.63, 49.31, 118.51, 124.86, 128.06(2C), 128.37, 129.01(2C), 135.82, 144.57, 145.54, 157.28, 162.36. IR ($CHCl_3$): 1671 cm^1. HRMS (ESI) m/z calculated for [$C_{16}H_{16}ON_2S$ + H]: 285.1056, found: 285.1053; [$C_{16}H_{16}ON_2S$ + Na]: 307.0876, found: 307.0871. Melting Point: 93^{0}C.

3-Benzyl-6-butylthieno[2,3-d]pyrimidin-4(3H)-one (12c)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.95 (t, *J* = 7 Hz, 3H), 1.21-1.53 (m, 2H), 1.60-1.80 (m, 2H), 2.85 (dt, *J* =1, 7 Hz, 2H), 5.21 (s, 2H), 7.17 (t, *J*=1 Hz, 1H), 7.35 (bs, 5H), 8.01 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.61, 21.90, 30.17, 33.00, 49.18, 118.26, 124.72, 127.92 (2C), 128.16, 128.87 (2C), 135.71, 144.68, 145.43, 157.13, 162.19. IR ($CHCl_3$): 1674, 2403, 3018 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{17}H_{18}ON_2S$ + H]: 299.1213, found: 299.1204. Melting Point: 99^{0}C.

3-Benzyl-6-pentylthieno[2,3-d]pyrimidin-4(3H)-one (12d)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.91 (t, *J*=7 Hz, 3H), 1.30-1.43 (m, 4H), 1.64-1.79 (m, 2H), 2.84 (t, *J*=8 Hz, 2H), 5.21 (s, 2H), 7.17 (s, 1H), 7.35 (bs, 5H), 8.01 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.86, 22.24, 30.48, 30.63, 30.96, 49.21, 118.27, 124.73, 127.94(2C), 128.18, 128.89 (2C), 135.70, 144.76, 145.43, 157.16, 162.20. IR ($CHCl_3$): 1674 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{18}H_{20}ON_2S$ + H]: 313.1369, found: 313.1361; [$C_{18}H_{20}ON_2S$ + Na]: 335.1189; found: 335.1180. Melting Point: 99^{0}C.

3-Benzyl-6-hexylthieno[2,3-d]pyrimidin-4(3H)-one (12e)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.89 (t, *J*=7 Hz, 3H), 1.20-1.45 (m, 6H), 1.62-1.74 (m, 2H), 2.83 (t, *J* =8 Hz, 2H), 5.20 (s, 2H), 7.16 (s, 1H), 7.34 (bs, 5H), 8.01 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.93, 22.39, 28.45, 30.47, 30.88, 31.33, 49.15, 118.21, 124.67, 127.89 (2C), 128.11, 128.83 (2C), 135.68, 144.68, 145.41, 157.10, 162.16. IR ($CHCl_3$): 1674 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{19}H_{22}ON_2S$ + H]: 327.1526, found: 327.1519; [$C_{19}H_{22}ON_2S$ + Na]: 349.1345, found: 349.1336. Melting Point: 81^{0}C.

2-(4-Oxo-6-pentylthieno[2,3-d]pyrimidin-3(4H)-yl)acetonitrile (13a)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.91 (t, *J* =7 Hz, 3H), 1.31-1.41 (m, 4H), 1.65-1.78 (m, 2H), 2.86 (t, *J*=7 Hz, 2H), 4.92 (s, 2H), 7.18 (s, 1H), 8.05 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.85, 22.20, 30.47, 30.59, 30.96, 33.47, 113.77, 118.05, 124.10, 143.59, 146.25, 155.91, 162.18. IR ($CHCl_3$): 1674 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{13}H_{15}ON_3S$+H]: 262.1009, found: 262.1003; [$C_{13}H_{15}ON_3S$+Na]: 284.0828, found: 284.0821. Melting Point: 88^{0}C.

2-(6-Heptyl-4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)acetonitrile (13b)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.89 (t, *J*=7 Hz, 3H), 1.23-1.49 (m, 8H), 1.63-1.78 (m, 2H), 2.86 (t, *J*=8 Hz, 2H), 4.91 (s, 2H), 7.19 (s, 1H), 8.04 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.95, 22.48, 28.79 (2C), 30.51, 30.91, 31.57, 33.47, 113.82, 118.03, 124.09, 143.64, 146.23, 155.93, 162.25. IR ($CHCl_3$): 1686, 2358 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{15}H_{19}ON_3S$ + H]: 290.1322, found: 290.1318; [$C_{15}H_{19}ON_3S$ + Na]: 312.1141, found: 312.1136. Melting Point: 86^{0}C.

3-(Cyclopropylmethyl)-6-pentylthieno[2,3-d]pyrimidin-4(3H)-one (14a)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.32-0.48 (m, 2H), 0.55-0.70 (m, 2H), 0.88 (t, *J*=7 Hz, 3H), 1.17-1.44 (m, 5H), 1.63-1.75 (m, 2H), 2.82 (t, *J* =7 Hz, 2H), 3.86 (d, *J* =7 Hz , 2H), 7.14 (s, 1H), 7.99 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$) : δ 4.03 (2C), 10.88, 13.83, 22.22, 30.45, 30.60, 30.95, 50.80, 118.14, 124.66, 144.39, 145.26, 157.31, 162.28. IR ($CHCl_3$): 1671 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{15}H_{20}ON_2S$ + H]: 277.1369, found: 277.1369; [$C_{15}H_{20}ON_2S$ + Na]: 299.1189, found: 299.1186. Melting Point: 73^{0}C

3-(Cyclopropylmethyl)-6-hexylthieno[2,3-d]pyrimidin-4(3H)-one (14b)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.36-0.48 (m, 2H), 0.60-0.72 (m, 2H), 0.89 (t, *J* =7 Hz, 3H), 1.17-1.45 (m, 7H), 1.62-1.77 (m, 2H), 2.84 (t, *J* =7 Hz, 2H), 3.88 (d, *J* =7 Hz , 2H), 7.16 (s, 1H), 8.00 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 4.14 (2C), 10.98, 14.03, 22.51, 28.59, 30.62, 31.01, 31.46, 50.93, 118.26, 124.80, 144.56, 145.31, 157.45, 162.39. IR ($CHCl_3$): 1683 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{16}H_{22}ON_2S$ + H]: 291.1526, found: 291.1519; [$C_{16}H_{22}ON_2S$ + Na]: 313.1345, found: 313.1336. Melting Point: 49^{0}C

3-(Cyclopropylmethyl)-6-heptylthieno[2,3-d]pyrimidin-4(3H)-one (14c)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.35-0.48 (m, 2H), 0.58-0.69 (m, 2H), 0.87 (t, J =7 Hz, 3H), 1.14-1.47 (m, 9H), 1.68-1.76 (m, 2H), 2.83 (t, J =7 Hz, 2H), 3.86 (d, J =7 Hz , 2H), 7.15 (s, 1H), 8.00 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 4.07 (2C), 10.91, 13.98, 22.52, 28.80, 28.86, 30.53, 30.97, 31.62, 50.84, 118.18, 124.71, 144.45, 145.27, 157.35, 162.32. IR ($CHCl_3$): 1678 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{17}H_{24}ON_2S$ + H]: 305.1682, found: 305.1683; [$C_{17}H_{24}ON_2S$ + Na]: 327.1502, found: 327.1500. Melting Point: 57^{0}C.

3-(4-(Bromomethyl)benzyl)-6-propylthieno[2,3-d]pyrimidin-4(3H)-one (15a)

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.00 (t, J=7 Hz, 3H), 1.68 - 1.80 (m, 2H), 2.82 (t, J=7 Hz, 2H), 4.46 (s, 2H), 5.19 (s, 2H), 7.17(s, 1H), 7.30 - 7.35 (m, 2H), 7.35 - 7.41 (m, 2H), 8.01(s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.45, 24.24, 32.54, 32.67, 48.95, 118.38, 124.75, 128.36 (2C), 129.58 (2C), 135.96, 137.86, 144.66, 145.33, 157.12, 162.30. IR ($CHCl_3$): 1672 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{17}H_{17}ON_2{}^{79}BrS$ + H]: 377.0318, found: 377.0311. Melting Point: 150^{0}C.

3-(2-(1,3-Dioxolan-2-yl)ethyl)-6-pentylthieno[2,3-d]pyrimidin-4(3H)-one (16a)

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.90 (t, J=7 Hz, 3H), 1.20-1.47 (m, 4H), 1.60-1.85 (m, 2H), 2.19 (dt, J=5, 7 Hz, 2H), 2.83 (t, J=7 Hz, 2H), 3.86(t, J=6 Hz, 2H), 3.99(t, J=6 Hz, 2H), 4.15(t, J=7 Hz, 2H), 4.92 (t, J=5 Hz, 1H), 7.15 (s, 1H), 7.97 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.92, 22.31, 30.56, 30.70, 31.06, 32.27, 42.45, 64.95 (2C), 101.97, 118.16, 124.74, 144.55, 146.09, 157.30, 162.41. IR ($CHCl_3$): 1672, 3405 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{16}H_{22}O_3N_2S$ + H]: 323.1424, found: 323.1424; [$C_{16}H_{22}O_3N_2S$ + Na]: 345.1243, found: 345.1244. Melting Point: 60^{0}C.

3-(2-(1,3-Dioxolan-2-yl)ethyl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidin-4(3H)-one (16b)

^{1}H NMR (400 MHz, $CDCl_3$):δ 1.68-2.00 (m, 4H), 2.17 (dt, J=5 Hz, 2H), 2.77 (t, J=6 Hz, 2H), 3.02(t, J=6 Hz, 2H), 3.86 (t, J=6 Hz, 2H), 3.98(t, J=6 Hz, 2H), 4.11 (t, J=7 Hz, 2H), 4.92(t, J=5 Hz, 1H), 7.92 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 22.23, 22.86, 25.21, 25.62, 32.30, 42.19, 64.96(2C), 102.00, 122.76, 131.56, 133.99, 145.95, 157.81, 162.09. IR ($CHCl_3$): 1669, 3446 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{15}H_{18}O_3N_2S$ + H]: 307.1111, found: 307.1112; [$C_{15}H_{18}O_3N_2S$ + Na]: 329.0930, found: 329.0930. Melting Point: 77^{0}C.

3-(2-(1,3-Dioxan-2-yl)ethyl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidin-4(3H)-one (16c)

^{1}H NMR (500 MHz, $CDCl_3$): δ 1.34 (d, 2H), 1.80-1.92 (m, 4H), 2.04-2.12 (m, 3H), 2.77 (t, J=6 Hz, 2H), 3.02 (t, J=6 Hz, 2H), 3.72 (t, J=12 Hz, 2H), 4.08 (dd, J=7 Hz, 2H), 4.59 (t, J=6 Hz, 1H), 7.93 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 22.26, 22.28, 25.21, 25.64 (2C), 33.58 42.12, 66.82 (2C), 99.54, 122.77, 131.59, 133.81, 146.25, 157.86, 162.12. IR ($CHCl_3$): 1669 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{16}H_{20}O_3N_2S$ + H]: 321.1267, found: 321.1283; [$C_{16}H_{20}O_3N_2S$ + Na]: 343.1087, found: 343.1104. Melting Point: 111^{0}C.

3-(2-(2,4-Difluorophenyl)-2-oxoethyl)-6-methylthieno[2,3-d]pyrimidin-4(3H)-one (17a)

^{1}H NMR (500 MHz, $CDCl_3$): δ 2.55 (s, 3H), 5.30 (s, 2H), 6.97 (t, J=8 Hz, 1H), 7.03 (t, J=8 Hz, 1H), 7.12 (s, 1H), 7.87 (s, 1H), 8.04 (q, J=8 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 16.00, 55.01 (d), 104.89 (t), 112.98 (dd), 119.42, 119.52 (d), 124.81, 133.18 (dd), 138.93, 145.78, 156.88, 162.99, 163.26 (dd), 166.69

(dd), 188.28 (d). IR ($CHCl_3$): 1682 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{15}H_{10}O_2N_2F_2S$ + H]: 321.0504, found: 321.0507. Melting Point: 177^{0}C.

3-(2-(2,4-Difluorophenyl)-2-oxoethyl)-6-propylthieno[2,3-d]pyrimidin-4(3H)-one (17b)

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.99 (t, *J*=7 Hz, 3H), 1.68-1.81 (m, 2H), 2.81(t, *J*=8 Hz, 2H), 5.29 (d, *J*=6 Hz, 2H), 6.91-7.05 (m, 2H), 7.13 (s, 1H), 7.88 (s, 1H), 7.98-8.06 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.47, 24.27, 32.55, 55.00 (d), 104.83 (t), 112.90 (dd), 118.32, 119.39 (dd), 124.47, 133.10 (dd), 144.61, 145.73, 156.95, 162.70, 163.21 (dd), 166.62 (dd), 188.25 (d). IR ($CHCl_3$): 1679 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{17}H_{14}O_2N_2$ F_2S + H]: 349.0817, found: 349.0808; [$C_{17}H_{14}O_2N_2$ F_2S + Na]: 371.0636, found: 371.0627. Melting Point: 150^{0}C.

3-(2-(2,4-Difluorophenyl)-2-oxoethyl)-6-pentylthieno[2,3-d]pyrimidin-4(3H)-one (17c)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.91 (t, *J*=7 Hz, 3H), 1.26-1.46 (m, 4H), 1.62-1.81 (m, 2H), 2.85 (t, *J*=7 Hz, 2H), 5.31 (d, *J*=5 Hz, 2H), 6.90-7.11 (m, 2H), 7.15 (s, 1H), 7.88 (s, 1H), 7.98-8.14 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.91, 22.30, 30.54, 30.70, 31.03, 55.02(d), 104.86(t), 112.95(dd), 118.25, 119.42 (dd), 124.52, 133.15 (dd), 144.94, 145.69, 156.98, 162.69, 163.24 (dd), 166.66 (dd), 188.26(d). IR ($CHCl_3$): 1683 cm^{-1}. MS *m/z* : 377.1 [M+ H]. Melting Point: 138^{0}C.

3-Allyl-6-butylthieno[2,3-d]pyrimidin-4(3H)-one (18a)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.92 (t, *J*=8 Hz, 3H), 1.30-1.45 (m, 2H), 1.60-1.75 (m, 2H), 2.82 (t, *J*=8 Hz, 2H), 4.60 (d, *J*=7 Hz, 2H), 5.16-5.29 (m, 2H), 5.91-6.00 (m, 1H), 7.13(s, 1H), 7.91(s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.62, 21.91, 30.19, 33.01, 48.00, 118.19, 118.73, 124.62, 131.91, 144.62, 145.28, 156.89, 162.28. IR ($CHCl_3$): 1676 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{13}H_{16}ON_2S$ + H]: 249.1056, found: 249.1051. Melting Point: 45^{0}C.

Ethyl 2-(4-oxo-6-pentylthieno[2,3-d]pyrimidin-3(4H)-yl)acetate (19a)

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.90 (t, *J*=7 Hz, 3H), 1.25-1.42 (m, 7H), 1.65-1.78 (m, 2H), 2.83 (t, *J*=7 Hz, 2H), 4.27 (q, *J*=7 Hz, 2H), 4.70 (s, 2H), 7.15 (s, 1H), 7.89 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.90, 14.05, 22.29, 30.54, 30.68, 31.02, 47.12, 62.16, 118.24, 124.44, 145.08, 145.42, 156.95, 162.53, 167.21. IR ($CHCl_3$): 1666, 1743 cm^1. HRMS (ESI) m/z calculated for [$C_{15}H_{20}O_3N_2S$ + H]: 309.1267, found: 309.1263. Melting Point: 80 ^{0}C.

Ethyl 2-(6-ethyl-4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)acetate (19b)

^{1}H NMR (200 MHz, $CDCl_3$): δ 1.30 (t, *J*=7 Hz, 3H), 1.35 (t, *J*=7 Hz, 3H), 2.89 (q, *J*=7 Hz, 2H), 4.26 (q, *J*=7 Hz, 2H), 4.71 (s, 2H), 7.17 (s, 1H), 7.90 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 14.09, 15.27, 23.98, 47.21, 62.18, 117.55, 124.47, 145.65, 146.49, 156.97, 162.45, 167.27. IR (Neat): 1742, 1667 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{12}H_{14}O_3N_2S$+H]: 267.0798, found: 267.0795; [$C_{12}H_{14}O_3N_2S$+Na]: 289.0617, found: 289.0613. Melting Point: 118^{0}C.

2-(6-Ethyl-4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)acetic acid (20b)

^{1}H NMR (200 MHz, $CDCl_3$+ MeOH-d_4): δ 1.15 (t, *J*=8 Hz, 3H), 2.68 (q, *J*=8 Hz, 2H), 4.54 (s, 2H), 6.94 (s, 1H), 7.83 (s, 1H). ^{13}C NMR (50 MHz, MeOH-d_4): δ 15.88, 24.88, 50.37, 118.31, 125.41, 148.18, 148.53, 159.10, 164.15, 170.82. IR ($CHCl_3$): 1693 (broad), 2400, 3020 cm^{-1}. HRMS (ESI) m/z calculated

for [$C_{10}H_{10}O_3N_2S$+H]: 239.0485, found: 239.0481; [$C_{10}H_{10}O_3N_2S$+Na]: 261.0304, found: 261.0300. Melting Point: 206°C.

2-(6-Methyl-4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)acetic acid (20c)

^{1}H NMR (500 MHz, $CDCl_3$): δ 2.28 (s, 3H), 4.47 (s, 2H), 6.84 (s, 1H), 7.79 (s, 1H). ^{13}C NMR (125MHz, $CDCl_3$): δ 15.34, 46.37, 118.61, 123.94, 137.99, 145.81, 156.23, 162.16, 168.57. IR ($CHCl_3$): 1664 (broad), 3025 cm^1. HRMS (ESI) m/z calculated for [$C_9H_8O_3N_2S$ + H]: 225.0328, found: 225.0439; [$C_9H_8O_3N_2S$ + Na]: 247.0148, found: 247.0269. Melting Point: 225^{0}C.

3-(2,2-Diethoxyethyl)-6-methylthieno[2,3-d]pyrimidin-4(3H)-one (21b)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.96-1.22 (m, 6H), 2.44 (s, 3H), 3.31-3.53 (m, 2H), 3.57-3.80 (m, 2H), 3.97 (d, *J*=6 Hz, 2H), 4.62 (t, *J*=6 Hz, 1H), 7.01 (s, 1H), 7.89 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 15.06 (2C), 15.84, 49.03, 64.09 (2C), 99.75, 119.04, 124.33, 138.31, 146.75, 157.12, 162.73. IR ($CHCl_3$): 1062, 1676 cm^1. HRMS (ESI) m/z calculated for [$C_{13}H_{18}O_3N_2S$ + H]: 283.1111, found: 283.1104; [$C_{13}H_{18}O_3N_2S$ + Na]: 305.0930, found: 305.0923. Melting Point: 45^{0}C.

2-(6-Butyl-4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)acetaldehyde (22a)

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.91 (t, *J*=7 Hz, 3H), 1.32-1.43 (m, 2H), 1.61-1.71 (m, 2H), 2.81 (t, *J*=7 Hz, 2H), 4.80 (s, 1H), 7.09 (s, 1H), 7.85 (s, 1H), 9.68 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.63, 21.92, 30.17, 32.98, 54.84, 117.99, 124.23, 145.22, 145.31, 156.86, 162.54, 193.70. IR ($CHCl_3$): 1670, 1722, 2729 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{12}H_{14}O_2N_2S$ + H]: 251.0849, found: 251.0842. Melting Point: 90^{0}C.

3-(2-Oxo-2-(thiophen-2-yl)ethyl)-6-propylthieno[2,3-d]pyrimidin-4(3H)-one (23a)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.99 (t, *J*=7 Hz, 3H), 1.63-1.85 (m, 2H), 2.81 (t, *J*=7 Hz, 2H), 5.34 (s, 2H), 7.13 (s, 1H), 7.16-7.24 (m, 1H), 7.72-7.79 (m, 1H), 7.89-7.97 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.49, 24.29, 32.57, 50.91, 118.33, 124.41 (t), 128.49, 132.92, 135.18, 140.61, 144.65, 145.79, 156.93, 162.67, 184.46. IR ($CHCl_3$): 1676 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{15}H_{14}O_2N_2S_2$+ H]: 319.0569, found: 319.0562; [$C_{15}H_{14}O_2N_2S_2$ + Na]: 341.0389, found: 341.0381. Melting Point: 133^{0}C.

6-Hexyl-3-(2-oxo-2-(thiophen-2-yl)ethyl)thieno[2,3-d]pyrimidin-4(3H)-one (23b)

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88 (t, *J*=7 Hz, 3H), 1.25-1.40 (m, 6H), 1.60-1.80 (m, 2H), 2.82 (t, *J*=7 Hz, 2H), 5.33 (s, 2H), 7.11 (s, 1H), 7.16-7.20 (m, 1H), 7.72-7.75 (m,1H), 7.89-7.93 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.99, 22.45, 28.53, 30.54, 30.95, 31.40, 50.90, 118.16, 124.37, 128.45, 132.90, 135.12, 140.58, 144.90, 145.78, 156.89, 162.60, 184.46. IR ($CHCl_3$): 1676 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{18}H_{20}O_2N_2S_2$ + H]: 361.1039, found: 361.1028; [$C_{18}H_{20}O_2N_2S_2$ + Na]: 383.0858, found: 383.0846. Melting Point: 117^{0}C.

3-(2-Oxo-2-(thiophen-2-yl)ethyl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidin-4(3H)-one (23c)

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.71-1.94 (m, 4H), 2.79 (t, *J*=6 Hz, 2H), 2.98 (t, *J*=6 Hz, 2H), 5.29 (s, 2H), 7.21 (t, *J*=5 Hz, 1H), 7.76 (d, *J*=5 Hz, 1H), 7.89 (s, 1H), 7.94 (d, *J*=5 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 22.18, 22.82, 25.20, 25.53, 50.79, 122.55, 128.49, 131.63, 132.86, 134.47, 135.15,

140.69, 145.64, 157.46, 162.35, 184.60. IR ($CHCl_3$): 1674 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{16}H_{14}O_2N_2S_2$ + H]: 331.0569, found: 331.0561; [$C_{16}H_{14}O_2N_2S_2$ + Na]: 353.0389, found: 353.0380. Melting Point: 199^{0}C.

3-(2-Bromoethyl)-6-methylthieno[2,3-d]pyrimidin-4(3H)-one (24a)

^{1}H NMR (200 MHz, $CDCl_3$): δ 2.55 (s, 3H), 3.76 (t, *J*=6 Hz, 2H), 4.38 (t, *J* =6 Hz, 2H), 7.13 (s, 1H), 7.99 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 15.98, 29.70, 48.68, 119.15, 124.75, 138.98, 145.70, 156.86, 162.99. IR (KBr): 1660 cm^{-1}. HRMS (ESI) m/z calculated for [$C_9H_9ON_2{}^{79}BrS$ + H]: 272.9692, found: 272.9685; [$C_9H_9ON_2{}^{81}BrS$ + Na]: 274.9671, found: 274.9659. Melting Point: 137 ^{o}C.

3-(2-Bromoethyl)-6-ethylthieno[2,3-d]pyrimidin-4(3H)-one (24b)

^{1}H NMR (200 MHz $CDCl_3$): δ 1.36 (t, *J*=7Hz, 3H), 2.90 (q, *J*=7 Hz, 2H), 3.77 (t, *J*=6 Hz, 2H), 4.38 (t, *J*=6 Hz, 2H), 7.18 (s, 1H), 7.99 (s 2H). 13C NMR (50MHz $CDCl_3$): δ 15.29, 24.01, 29.82, 48.75, 117.38, 124.58, 145.80, 146.46, 157.06, 162.74. IR ($CHCl_3$): 1674 cm-1. HRMS (ESI) m/z calculated for [$C_{10}H_{11}ON_2{}^{79}BrS$ + H]: 286.9848, found: 286.9847; [$C_{10}H_{11}ON_2{}^{81}BrS$ + Na]: 288.9828, found: 288.9824. Melting Point: 123^{0}C.

3-(2-Bromoethyl)-6-propylthieno[2,3-d]pyrimidin-4(3H)-one (24c)

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.00 (t, *J*=7 Hz, 3H), 1.70-1.81 (m, 2H), 2.83 (t, *J*=8 Hz, 2H), 3.76 (t, *J*=5 Hz, 2H), 4.38 (t, *J*=5 Hz, 2H), 7.16 (s, 1H), 7.99 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.52, 24.30, 29.77, 32.62, 48.76, 118.17, 124.55, 144.81, 145.69, 157.05, 162.810. IR ($CHCl_3$): 1674 cm^1. MS *m/z* : 300, 302 [M^+]. Melting Point: 106^{0}C.

3-(2-Bromoethyl)-6-butylthieno[2,3-d]pyrimidin-4(3H)-one (24d)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.95 (t, *J*=7 Hz, 3H), 1.30-1.53 (m, 2H), 1.59-1.81 (m, 2H), 2.86 (t, *J*=8 Hz,2H), 3.77 (t, *J*=6 Hz, 2H), 4.39 (t, *J*=6 Hz, 2H), 7.16 (s, 1H), 8.03 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.67, 21.95, 29.82, 30.25, 31.12, 48.29, 118.15, 124.50, 144.57, 145.70, 157.02, 162.71. IR ($CHCl_3$): 1671 cm^1 MS *m/z* : 315.0, 317.0 [M^+]. Melting Point: 86^{0}C.

3-(2-Bromoethyl)-6-hexylthieno[2,3-d]pyrimidin-4(3H)-one (24e)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.90 (t, *J*=7 Hz, 3H), 1.23-1.47 (m, 6H), 1.66-1.78 (m, 2H), 2.85 (t, *J*=8 Hz, 2H), 3.77 (t, *J*=6 Hz, 2H), 4.39 (t, *J*=6 Hz, 2H), 7.16 (s, 1H), 8.02 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.96, 22.43, 28.51, 29.79, 30.54, 31.13, 31.38, 45.26, 118.00, 124.68, 144.92, 145.57, 157.21, 162.44. IR ($CHCl_3$): 1675 cm^1. MS *m/z* : 344.1 [M+ H] Melting Point: 60^{0}C.

3-(2-Bromoethyl)-6-heptylthieno[2,3-d]pyrimidin-4(3H)-one (24f)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.88 (t, *J*=7 Hz, 3H), 1.20-1.46 (m ,8H), 1.65-1.78 (m, 2H), 2.85 (t, *J*=7 Hz, 2H), 3.76 (t, *J*=6 Hz, 2H), 4.39 (t, *J*=6 Hz, 2H), 7.16 (s, 1H), 8.05 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.98, 22.54, 28.87(2C), 29.68, 30.57, 30.99, 31.63, 48.71, 118.03, 124.53, 145.06, 145.65, 158.97, 162.63. IR ($CHCl_3$): 1674 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{15}H_{21}ON_2{}^{79}BrS$ + H]: 357.0631, found: 357.0628: [$C_{15}H_{21}ON_2{}^{79}BrS$ + Na]: 379.0450, found: 379.0446. Melting Point: 102^{0}C.

3-(2-Bromoethyl)-6-decylthieno[2,3-d]pyrimidin-4(3H)-one (24g)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.88 (t, *J*=7 Hz, 3H), 1.19-1.45 (m, 14H), 1.72 (t, *J*=7 Hz, 2H), 2.85 (t, *J*=8 Hz, 2H), 3.77 (t, *J*=6 Hz, 2H), 4.38 (t, *J*=6 Hz, 2H), 7.16 (s, 1H), 7.99 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 14.07, 22.63, 28.91, 29.25 (2C), 29.46, 29.52, 29.76, 30.60, 31.02, 31.84, 48.73, 118.03, 124.53, 145.08, 145.66, 157.02, 162.75. IR ($CHCl_3$): 1676 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{18}H_{27}ON_2S^{79}Br$ + H]: 399.1100, found: 399.1102; [$C_{18}H_{27}ON_2S^{79}Br$ + Na]: 421.0920, found: 421.0920. Melting Point: 73^{0}C.

3-(2-Bromoethyl)-6-(non-8-en-1-yl)thieno[2,3-d]pyrimidin-4(3H)-one (24h)

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.23-1.49 (m, 8H), 1.65-1.83 (m, 2H), 1.97-2.09 (m, 2H), 2.84 (t, *J* =8 Hz, 2H), 3.76 (t, *J* =6 Hz, 2H), 4.38 (t, *J* =6 Hz, 2H), 4.90-5.07 (m, 2H), 5.73-5.90 (m, 1H), 7.15 (s, 1H), 7.99 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 28.80, 28.83, 28.90, 29.07, 29.76, 30.58, 30.98, 33.70, 48.74, 114.19, 118.05, 124.53, 139.05, 145.03, 145.67, 157.02, 162.75. IR ($CHCl_3$): 1674 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{17}H_{23}ON_2{}^{79}BrS$ + H]: 383.0787, found: 383.0786; [$C_{17}H_{23}ON_2{}^{79}BrS$ + Na]: 405.0607, found: 405.0605. Melting Point: 150^{0}C.

3-(2-Bromoethyl)-3,5,6,7-tetrahydro-4H-cyclopenta[4,5]thieno[2,3-d]pyrimidin-4-one (24i)

^{1}H NMR (200 MHz, $CDCl_3$): δ 2.40-2.57 (m, 2H), 2.93-3.13 (m, 4H), 3.77 (t, *J*=6 Hz, 2H), 4.37 (t, *J*=6 Hz, 2H), 7.94 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 28.01, 28.92, 29.59, 29.74, 48.63, 120.17, 140.00, 140.21, 145.28, 157.36, 167.29. IR ($CHCl_3$): 1667 cm^1. HRMS (ESI) m/z calculated for [$C_{11}H_{11}ON_2{}^{79}BrS$ + H]: 298.9848, found: 298.9842; [$C_{11}H_{11}ON_2{}^{81}BrS$ + Na]: 300.9828, found: 300.9820. Melting point: 176°C.

3-(2-Bromoethyl)-3,5,6,7,8,9-hexahydro-4H-cyclohepta[4,5]thieno[2,3-d]pyrimidin-4-one (24*j*)

^{1}H NMR (200 MHz, $CDCl_3$): δ 1.68-1.72 (m, 4H), 1.88-1.91 (m, 2H), 2.81-2.86 (m, 2H), 3.30-3.33 (m, 2H), 3.76 (t, *J*=5 Hz, 2H), 4.34 (t, *J*=5 Hz, 2H), 7.95 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 27.19, 27.66(2C), 27.93, 30.01, 32.55, 48.69, 123.16, 137.18, 138.93, 145.37, 157.97, 160.48. IR (KBr): 1658 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{13}H_{15}ON_2{}^{79}BrS$ + H]: 327.0161, found: 327.0153; [$C_{13}H_{15}ON_2{}^{81}BrS$ + Na]: 329.0141, found: 329.0128. Melting Point: 142^{0}C.

3-(3-Bromopropyl)-6-propylthieno[2,3-d]pyrimidin-4(3H)-one (25a)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.99 (t, *J*=7 Hz, 3H), 1.62-1.85 (m, 2H), 2.27-2.45 (m, 2H), 2.82 (t, *J*=7 Hz, 2H), 3.42 (t, *J*=7 Hz, 2H), 4.18 (t, *J*=7 Hz, 2H), 7.14 (s, 1H), 8.01 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.43, 24.22, 29.82, 31.08, 32.51, 45.24, 118.08, 124.64, 144.60, 145.58, 157.19, 162.45. IR ($CHCl_3$): 1668 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{12}H_{15}ON_2{}^{79}Br$ S + H]: 315.0161, found: 315.0157; [$C_{12}H_{15}ON_2{}^{79}Br$ S + Na]: 336.9981, found: 336.9976. Melting Point: 107^{0}C.

3-(3-Bromopropyl)-6-butylthieno[2,3-d]pyrimidin-4(3H)-one (25b)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.95 (t, *J*=7 Hz, 3H), 1.28-1.52 (m, 2H), 1.60-1.82 (m, 2H), 2.37 (quin, *J*=6 Hz, 2H), 2.85 (t, *J*=7 Hz, 2 H), 3.43 (t, *J*=6 Hz, 2 H), 4.18 (t, *J*=7 Hz, 2 H), 7.15 (s, 1 H), 8.01 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.67, 21.95, 29.82, 30.25, 31.12, 33.06, 45.29, 118.03, 124.70, 144.92, 145.59, 157.25, 162.48. IR ($CHCl_3$): 1672 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{13}H_{17}ON_2{}^{79}BrS$ + H]: 329.0318, found: 329.0320; [$C_{13}H_{17}ON_2{}^{81}BrS$ + H]: 331.0297, found: 331.0298. Melting Point: 93^{0}C.

3-(3-Bromopropyl)-6-hexylthieno[2,3-d]pyrimidin-4(3H)-one (25c)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.89 (t, *J*=7 Hz, 3H), 1.16-1.50 (m, 6H), 1.58-1.81 (m,2H), 2.26-2.46 (m, 2H), 2.84 (t, *J*=8 Hz, 2H), 3.43 (t, *J*=7 Hz, 2H), 4.18 (t, *J*=7 Hz, 2H), 7.15 (s,1H), 8.01 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.99, 22.48, 28.54, 29.82, 30.59, 30.97, 31.16, 31.42, 45.30, 118.04, 124.74, 144.99, 145.59, 157.27, 162.50. IR ($CHCl_3$): 1672 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{15}H_{21}ON_2{}^{79}BrS$ + H]: 357.0631, found: 357.0626; [$C_{15}H_{21}ON_2{}^{81}BrS$ + Na]: 359.0610, found: 359.0601. Melting Point: 70^{0}C.

3-(3-Bromopropyl)-6-heptylthieno[2,3-d]pyrimidin-4(3H)-one (25d)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.87 (t, *J* =7 Hz, 3H), 1.18-1.40 (m, 8H), 1.58-1.80 (m, 2H), 2.25-2.49 (m, 2H), 2.82 (t, *J*=7 Hz, 2H), 3.41 (t, *J*=6 Hz, 2H), 4.17 (t, *J*=6 Hz, 2H), 7.12 (s, 1H), 8.00 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.93, 22.46, 28.74, 28.79, 29.78, 30.47, 30.90, 31.06, 31.55, 45.19, 117.92, 124.59, 144.82, 145.53, 157.13, 162.36. IR ($CHCl_3$): 1670 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{16}H_{23}ON_2{}^{79}BrS$ + H]: 371.0787, found: 371.0785; [$C_{16}H_{23}ON_2{}^{79}BrS$ + Na]: 393.0607, found : 393.0605. Melting Point: 75^{0}C.

3-(3-Bromopropyl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidin-4(3H)-one (25e)

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.89-1.94 (m, 4H), 2.31-2.42 (m, 2H), 2.79 (t, *J*=6 Hz, 2H), 3.02 (t, *J*=6 Hz, 2H), 3.43 (t, *J*=7 Hz, 2H), 4.15 (t, *J*=7 Hz, 2H), 7.79 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 22.17, 22.79, 25.18, 25.58, 29.91, 31.12, 45.09, 122.72, 131.45, 134.39, 145.46, 157.79, 162.13. IR ($CHCl_3$): 1669 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{13}H_{15}O^{79}BrN_2S$+ H]: 327.0161, found: 327.0156; [$C_{13}H_{15}O^{79}BrN_2S$+Na]: 348.9981, found: 348.9974. Melting Point: 122.2°C

6-Ethyl-3-(2-hydroxyethyl)thieno[2,3-d]pyrimidin-4(3H)-one (26a)

^{1}H NMR (200 MHz, $CDCl_3$)**:** δ 1.35(t, *J*=7 Hz, 3H), 2.87 (q, *J*=7 Hz, 2H), 3.15 (bs, 1H), 3.97(t, *J*=5 Hz, 2H), 4.15 (t, *J*=5 Hz, 2H), 7.07 (s, 1H), 7.99 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 15.22, 24.01, 46.87, 48.47, 117.22, 124.39, 126.29, 144.70, 147.26, 147.85, 157.17, 162.76, 184.63. IR ($CHCl_3$): 1672, 3408 (bs) cm^{-1}. HRMS (ESI) m/z calculated for [$C_{10}H_{12}O_2N_2S$ + H]: 225.0692, found: 225.0732; [$C_{10}H_{12}O_2N_2S$ + Na]: 247.0512, found: 247.0555. Melting Point:-110°C.

6-Hexyl-3-(2-hydroxyethyl)thieno[2,3-d]pyrimidin-4(3H)-one (26b)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.90 (t, *J*=7 Hz, 3H), 1.25-1.45 (m, 6H), 1.65-1.76 (m,2H), 2.35 (bs, 1H), 2.83 (t, *J*=8 Hz, 2H), 3.97 (t, *J*=6 Hz, 2H), 4.17 (t, *J*=6 Hz, 2H), 7.10 (s, 1H), 8.01 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 13.98, 22.48, 28.62, 30.58, 30.95, 31.44, 49.40, 60.48, 117.87, 124.44, 144.84, 146.38, 157.66, 162.48. IR ($CHCl_3$): 1671, 3409 (bs) cm^{-1}. HRMS (ESI) m/z calculated for [$C_{14}H_{20}O_2N_2S$ + H]: 281.1318, found: 281.1348; [$C_{14}H_{20}O_2N_2S$ + Na]: 303.1138, found: 303.1169. Melting Point: 79^{0}C.

6-Decyl-3-(2-hydroxyethyl)thieno[2,3-d]pyrimidin-4(3H)-one (26c)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.88 (t, *J*=7 Hz, 3H), 1.18-1.43 (m, 14H), 1.62-1.78 (m, 2H), 2.82 (t, *J*=8 Hz, 2H), 2.97(t, *J*=5 Hz, 1H), 3.97 (q, *J*=5 Hz, 2H), 4.16 (t, *J*=5 Hz, 2H), 7.08 (s, 1H), 7.99 (s, 1H) . ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.08, 22.65, 28.96, 29.27 (2C), 29.49, 29.54, 30.61, 31.03, 31.85, 49.42, 60.70, 117.91, 124.48, 144.92, 146.31, 157.78, 162.56. IR ($CHCl_3$): 1675, 3408 (bs) cm^{-1}. HRMS (ESI) m/z calculated for [$C_{18}H_{28}O_2N_2S$ + H]: 337.1944, found: 337.1937; [$C_{18}H_{28}O_2N_2S$ + Na]: 359.1764 found: 359.1756. Melting Point: 62^{0}C.

3-(2-Hydroxyethyl)-3,5,6,7,8,9-hexahydro-4H-cyclohepta[4,5]thieno[2,3-d]pyrimidin-4-one (26d)

^{1}H NMR (200 MHz, $CDCl_3$): δ 1.65(m, 4H), 1.86-1.93(m, 2H), 2.81-2.89(m, 2H), 3.27-3.35(m, 2H), 3.97(t, *J*=5Hz, 2H), 4.17(t, *J*=5Hz, 2H), 8.05(s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.58, 27.04, 27.18, 29.21, 31.82, 48.24, 58.76, 122.46, 136.31, 137.06, 146.03, 157.71, 160.06. IR ($CHCl_3$): 1670, 3402 (bs) cm^{-1}. HRMS (ESI) m/z calculated for [$C_{13}H_{16}O_2N_2S$ + H]: 265.1005, found: 265.1013. Melting Point: 153^{0}C.

3-(3-Hydroxypropyl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidin-4(3H)-one (27a)

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.78-1.93 (m, 4H), 1.98 (q, *J*=6 Hz, 2H), 2.79 (t, *J*=6 Hz, 2H), 3.02(t, *J*=6 Hz, 2H), 3.59 (t, *J*=6 Hz, 2H), 4.17 (t, *J*=6 Hz, 2H), 7.94 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 22.19, 22.81, 25.25, 25.66, 32.41, 42.51, 57.85, 122.51, 131.56, 134.62, 145.43, 158.78, 162.40. IR ($CHCl_3$): 1662, 3416 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{13}H_{16}O_2N_2S$ + H]: 265.1005, found: 265.1006; [$C_{13}H_{16}O_2N_2S$ + Na]: 287.0825, found: 287.0822. Melting Point: 129^{0}C.

3-(4-Oxo-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidin-3(4H)-yl)propanal (28a)

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.77-1.91(m, 4H), 2.76 (t, *J*=6 Hz, 2H), 2.98 (t, *J*=6 Hz, 2H), 3.08 (t, *J*=6 Hz, 2H), 4.23 (t, *J*=6 Hz, 2H), 8.10 (s, 1H), 9.78 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 22.18, 22.80, 25.16, 25.55, 40.55, 42.36, 122.58, 131.31, 134.32, 146.22, 157.85, 162.16, 199.37. IR ($CHCl_3$): 1667, 1721, 2727 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{13}H_{14}O_2N_2S$ + H]: 263.0849, found: 263.0844. Melting Point: 132^{0}C.

3-(2-Azidoethyl)-6-methylthieno[2,3-d]pyrimidin-4(3H)-one (29a)

^{1}H NMR (200 MHz, $CDCl_3$): δ 2.56 (s, 3H), 3.76 (t, *J*=6 Hz, 2H), 4.13 (t, *J*=6 Hz, 2H), 7.14 (s, 1H), 7.99 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 16.04, 46.21, 49.52, 119.23, 124.82, 139.04, 145.85, 157.00, 162.93. IR (KBr): 1676, 2108 cm^{-1}. HRMS (ESI) m/z calculated for [$C_9H_9ON_5S$ + H]: 236.0601, found: 236.0598. Melting Point: 106^{0}C.

3-(2-Azidoethyl)-6-ethylthieno[2,3-d]pyrimidin-4(3H)-one (29b)

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.36 (t, *J*=8 Hz, 3H), 2.89 (q, *J*=8 Hz, 2H), 3.76 (t, *J*= 6 Hz, 2H), 4.13 (t, *J*=6 Hz, 2H), 7.17 (s, 1H), 7.94 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 15.25, 23.99, 46.20, 49.50, 117.36, 124.55, 145.76, 146.47, 157.15, 162.67. IR ($CHCl_3$): 1670, 2105 cm^{-1}. MS *m/z* :250.1 [M+ H]. Melting Point: 78^{0}C.

3-(2-Azidoethyl)-6-butylthieno[2,3-d]pyrimidin-4(3H)-one (29c)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.95 (t, *J*=7 Hz, 3H), 1.30-1.52 (m, 2H), 1.61-1.80 (m, 2H), 2.85 (t, *J*=8 Hz, 2H), 3.76 (t, *J*=7 Hz, 2H), 4.12 (t, *J*=7 Hz, 2H), 7.15 (s, 1H), 7.94 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.63, 21.93, 30.21, 33.02, 46.10, 49.43, 117.97, 124.45, 144.93, 145.71, 157.04, 162.62. IR ($CHCl_3$): 1682, 2104 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{12}H_{15}ON_5S$ + H]: 278.1070, found: 278.1064; [$C_{12}H_{15}ON_5S$ + Na]: 300.0890, found: 300.0883. Melting Point: 67^{0}C.

3-(2-Azidoethyl)-6-hexylthieno[2,3-d]pyrimidin-4(3H)-one (29d)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.88 (t, *J*=7 Hz, 3H), 1.22-1.45 (m, 6H), 1.65-1.76 (m, 2H), 2.84 (t, *J*=7 Hz, 2H), 3.76 (t, *J*=6 Hz, 2H), 4.12 (t, *J*=6 Hz, 2H), 7.14 (s, 1H), 7.94 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.99, 22.47, 28.55, 30.58, 30.96, 31.42, 46.15, 49.46, 118.01, 124.50, 145.06, 145.71,

157.11, 162.67. IR ($CHCl_3$): 1674, 2106 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{14}H_{19}ON_5S$ + H]: 306.1383, found: 306.1378; [$C_{14}H_{19}ON_5S$ + Na]: 328.1203 found: 328.1197. Melting Point: 50^0C.

3-(2-Azidoethyl)-6-heptylthieno[2,3-d]pyrimidin-4(3H)-one (29e)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.88 (t, *J*=7 Hz, 3H), 1.19-1.45 (m, 8H), 1.62-1.82 (m, 2H), 2.84 (t, *J*=7 Hz, 2H), 3.76 (t, *J*=6 Hz, 2H), 4.12 (t, *J*=6 Hz, 2H), 7.15 (s, 1H), 7.94 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.94, 22.49, 28.79, 28.83, 30.52, 30.94, 31.58, 46.09, 49.43, 117.95, 124.47, 144.99, 145.70, 157.02, 162.55. IR ($CHCl_3$): 1676, 2122 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{15}H_{21}ON_5S$ + H]: 320.1540, found: 320.1537; [$C_{15}H_{21}ON_5S$ + Na]: 342.1359 , found : 342.1354. Melting Point: 50^0C.

3-(3-Azidopropyl)-6-propylthieno[2,3-d]pyrimidin-4(3H)-one (30a)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.96(t, *J*=7 Hz, 3H), 1.60-1.84 (m,2H), 1.94-2.15 (m,2H), 2.79(t, *J*=7 Hz, 2H), 3.38 (t, *J*=7 Hz, 2H), 4.07 (t, *J*=7 Hz, 2H), 7.11 (s, 1H), 7.93 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.26, 24.05, 28.03, 32.32, 43.98, 48.01, 117.95, 124.45, 144.31, 145.42, 156.96, 162.23. IR ($CHCl_3$): 1669, 2101 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{12}H_{15}ON_5S$ + H]: 278.1070, found: 278.1066; [$C_{12}H_{15}ON_5S$ + Na]: 300.0890, found: 300.0884. Melting Point: 60^0C.

3-(3-Azidopropyl)-6-butylthieno[2,3-d]pyrimidin-4(3H)-one (30b)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.95 (t, *J* =7 Hz, 3H), 1.32-1.52 (m, 2H), 1.60-1.80 (m, 2H), 1.98-2.16 (m, 2H), 2.85 (t, *J* =7 Hz, 2H), 3.42 (t, *J*=7 Hz, 2H), 4.10 (t, *J*= 7 Hz, 2H), 7.15 (s, 1H), 7.95 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.65, 21.94, 28.20, 30.23, 33.04, 44.19, 48.16, 118.04, 124.68, 144.87, 145.48, 157.19, 162.41. IR ($CHCl_3$): 1673, 2101 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{13}H_{17}ON_5S$ + H]: 292.1227, found: 292.1224; [$C_{13}H_{17}ON_5S$ + Na]: 314.1046 found: 314.1042. Melting Point: 51^0C.

3-(3-Azidopropyl)-6-heptylthieno[2,3-d]pyrimidin-4(3H)-one (30c)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.87 (t, *J*=7 Hz, 3H), 1.15-1.38 (m, 8H), 1.60-1.79 (m, 2H), 1.98-2.13 (m, 2H), 2.82 (t, *J*=7 Hz, 2H), 3.40 (t, *J*=7 Hz, 2H), 4.08 (t, *J*=7 Hz, 2H), 7.13 (s, 1H), 7.94 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 14.00, 22.54, 28.22, 28.83, 28.88, 30.56, 30.98, 31.63, 44.20, 48.18, 118.05, 124.70, 144.95, 145.48, 157.21, 162.43. IR ($CHCl_3$): 1674, 2101 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{16}H_{23}ON_5S$ + H]: 334.1696, found: 334.1692; [$C_{16}H_{23}ON_5S$ + Na]: 356.1516, found: 356.1509. Melting Point: 52^0C.

3-(3-Azidopropyl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidin-4(3H)-one (30d)

^{1}H NMR (200 MHz, $CDCl_3$): δ 1.79-1.95 (m, 4H), 2.02-2.12 (m, 2H), 2.79 (t, *J* =6 Hz, 2H), 3.02 (t, *J*=6 Hz, 2H), 3.41 (t, *J*=6 Hz, 2H), 4.06 (t, *J*=6 Hz, 2H), 7.90 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 22.14, 22.76, 25.14, 25.54, 28.22, 43.94, 48.26, 122.67, 131.44, 134.29, 145.53, 157.69, 162.06. IR ($CHCl_3$): 1668, 2102 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{13}H_{15}ON_5S$ + H]: 290.1070, found: 290.1064; [$C_{13}H_{15}ON_5S$ + Na]: 312.0890, found: 312.0883. Melting point: 70.5 °C.

6-Ethyl-3-(2-(4-(hydroxymethyl)-1H-1,2,3-triazol-1-yl)ethyl)thieno[2,3-d]pyrimidin-4(3H)-one (31a)

^{1}H NMR (200 MHz, $CDCl_3$): δ 1.35 (t, *J*=8 Hz, 3H), 2.88 (q, *J*=8 Hz, 2H), 4.55 (t, *J*=6 Hz, 2H), 4.73 (bs, 2H), 4.79 (t, *J*=6 Hz, 2H), 7.16 (s, 1H), 7.42 (s, 1H), 7.50 (s, 1H). ^{13}C NMR (100 MHz, MeOH-d_4): δ 15.98, 24.94, 48.15, 49.79, 56.56, 118.39, 124.90, 125.55, 147.81, 148.27, 149.71, 159.13, 164.08. IR

(KBr): 1681, 3394 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{13}H_{15}N_5O_2S$+H]: 306.1019, found: 306.1016; [$C_{13}H_{15}N_5O_2S$ +Na]: 328.0839, found: 328.0835. Melting Point: 158°C.

1-(2-(6-Ethyl-4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)ethyl)-1H-1,2,3-triazole-4-carbaldehyde (31b)

^{1}H NMR (500 MHz, $CDCl_3$): δ 1.37(t, *J*=7 Hz, 3H), 2.89 (q, *J*=7 Hz, 2H), 4.60 (t, *J*=7 Hz, 2H), 4.90 (t, *J*=7 Hz, 2H), 7.17 (s, 1H), 7.54 (s, 1H), 7.97 (s, 1H), 10.11 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 15.22, 24.01, 46.87, 48.47, 117.22, 124.39, 126.29, 144.70, 147.26, 147.85, 157.17, 162.76, 184.63. IR ($CHCl_3$): 1643 (broad) cm^{-1}. MS *m/z* : 304.1 [M+ H]. Melting Point: 188°C.

6-Methyl-3-(prop-2-yn-1-yl)thieno[2,3-d]pyrimidin-4(3H)-one (32a)

^{1}H NMR (200 MHz, $CDCl_3$): δ 2.52 (t, *J*=2 Hz, 1H), 2.55 (s, 3H), 4.81 (d, *J*=2 Hz, 2H), 7.14 (s, 1H), 8.25 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 15.94, 34.94, 75.34, 76.36, 119.22, 124.45, 139.02, 144.31, 156.24, 162.50. IR (Neat): 1665, 2120 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{10}H_8ON_2S$+H]: 205.0430, found: 205.0428. Melting Point: 141^{0}C.

6-Ethyl-3-(prop-2-yn-1-yl)thieno[2,3-d]pyrimidin-4(3H)-one (32b)

^{1}H NMR (200MHz, $CDCl_3$): δ 1.35 (t, *J*=7 Hz, 3H), 2.51 (t, *J*=3 Hz, 1H), 2.80-2.97 (m, 2H), 4.81 (d, *J*=3 Hz, 2H), 7.17 (s, 1H), 8.23 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 15.10, 23.83, 34.90, 75.24, 76.37, 117.33, 124.16, 144.29, 146.35, 156.34, 162.20. IR ($CHCl_3$): 1668, 2124 cm^{-1}. MS *m/z* : 219.1 [M+ H]. Melting Point: 100 ^{0}C.

3-(Prop-2-yn-1-yl)-6-propylthieno[2,3-d]pyrimidin-4(3H)-one (32c)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.99 (t, *J* =7 Hz, 3H), 1.74 (q, *J*=7 Hz, 2H), 2.51 (t, *J*=2 Hz, 1H), 2.82 (t, *J*=7 Hz, 2H), 4.81 (d, *J*=2 Hz, 2H), 7.17 (s, 1H), 8.25 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.39, 24.16, 32.45, 34.93, 75.26, 76.57, 118.15, 124.16, 144.28, 144.71, 156.35, 162.24. IR (Neat): 1664, 2123 $cm.^{-1}$ HRMS (ESI) m/z calculated for [$C_{12}H_{12}ON_2S$+H]: 233.0743, found: 233.0740; [$C_{12}H_{12}ON_2S$+Na]: 255.0563, found: 255.0558. Melting Point: 103^{0}C.

6-Butyl-3-(prop-2-yn-1-yl)thieno[2,3-d]pyrimidin-4(3H)-one (32d)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.95 (t, *J*=7 Hz, 3H), 1.30-1.50 (m, 2H), 1.60-1.80 (m, 2H), 2.51 (t, *J*=3 Hz, 1H), 2.85 (t, *J*=8 Hz, 2H), 4.81(d, *J*=3 Hz, 2H), 7.17 (s, 1H), 8.23 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.63, 21.92, 30.21, 33.01, 34.96, 75.31, 76.37, 118.12, 124.24, 144.27, 145.03, 156.43, 162.33. IR ($CHCl_3$): 1678, 2123, 3306 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{13}H_{14}ON_2S$ + H]: 247.0900, found: 247.0898. Melting Point: 89^{0}C.

6-Pentyl-3-(prop-2-yn-1-yl)thieno[2,3-d]pyrimidin-4(3H)-one (32e)

^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.90 (t, *J*=7 Hz, 3H), 1.28-1.38 (m, 4H), 1.66-1.74 (m, 2H), 2.51 (t, *J*=2 Hz, 1H), 2.84 (t, *J*=7 Hz, 2H), 4.82 (s, 2H), 7.16 (s, 1H), 8.23 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.93, 22.31, 30.58, 30.70, 31.05, 35.02, 75.40, 76.50, 118.22, 124.33, 144.28, 145.19, 156.53, 162.41. IR ($CHCl_3$): 1677, 2124 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{14}H_{16}ON_2S$ + H]: 261.1056, found: 261.1053. Melting Point: 100^{0}C.

6-Heptyl-3-(prop-2-yn-1-yl)thieno[2,3-d]pyrimidin-4(3H)-one (32f)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.89 (t, *J*=7 Hz, 3H), 1.16-1.46 (m, 8H), 1.61-1.81 (m, 2H), 2.52 (t, *J* =3 Hz, 1H), 2.85 (t, *J* =7 Hz, 2H), 4.82 (d, *J* =3 Hz, 2H), 7.17 (s, 1H), 8.28 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.98, 22.53, 28.82, 28.86, 30.56, 30.97, 31.62, 35.01, 75.36, 76.37, 118.16, 124.29, 144.31, 145.14, 156.44, 162.29. IR (KBr): 1675, 2122, 3305 cm^{-1} MS *m/z* : 289.2 [M+ H]. Melting Point: 103°C.

3-(Prop-2-yn-1-yl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidin-4(3H)-one (32g)

^{1}H NMR (200 MHz, $CDCl_3$): δ 1.79-2.01(m, 4H), 2.49 (t, *J*=3 Hz, 1H), 2.78 (t, *J*=6 Hz, 2H) , 3.02 (t, *J*=6 Hz, 2H), 4.78 (d, *J*=3 Hz, 2H), 8.17 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 22.08, 22.72, 25.11, 25.45, 34.64, 75.08, 76.56, 122.27, 131.50, 134.48, 144.13, 156.89, 161.94. IR (KBr): 1673, 2358, 3305 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{13}H_{12}ON_2S$ + H]: 245.0743, found: 245.0739; [$C_{13}H_{12}ON_2S$ + Na]: 267.0563, found: 267.0556. Melting Point: 115.6 °C

6-Ethyl-3-((1-(2-(6-methyl-4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)ethyl)-1H-1,2,3-triazol-4-yl)methyl)thieno[2,3-d]pyrimidin-4(3H)-one (33a)

^{1}H NMR (200 MHz, $CDCl_3$+$DMSOd_6$): δ 0.91 (t, *J*=7 Hz, 3H), 2.10 (s, 1H), 2.45(q, *J*=7 Hz, 2H), 4.06(t, *J*=5Hz, 2H), 4.33(t, *J*=5Hz, 2H), 6.63(s, 1H), 6.65(s, 1H), 7.26(s, 1H), 7.51(s, 1H), 7.86(s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$+$DMSOd_6$): δ 14.23, 14.84, 22.72, 39.91, 45.24, 46.94, 116.23, 117.97, 123.26, 123.31, 123.70, 137.45, 141.33, 141.41, 144.84, 145.00, 155.57, 155.63, 161.24, 161.60. IR ($CHCl_3$): 1670 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{20}H_{19}O_2N_7S_2$ + H]: 454.1114, found: 454.1103. Melting Point: 162°C.

6-Hexyl-3-(2-(4-((4-oxo-6-propylthieno[2,3-d]pyrimidin-3(4H)-yl)methyl)-1H-1,2,3-triazol-1-yl)ethyl)thieno[2,3-d]pyrimidin-4(3H)-one (33b)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.84-1.04 (m, 6H), 1.17-1.48 (m, 6H), 1.61-1.87 (m, 4H), 2.81 (t, *J* =7 Hz, 4H), 4.52 (t, *J*=6 Hz, 2H), 4.74 (t, *J*=6Hz, 2H), 5.21 (s, 2H), 7.09 (s, 1H), 7.14 (s, 1H), 7.48 (s, 1H), 7.63 (s, 1H), 8.22 (s, 1H). ^{13}C NMR (125MHz, $CDCl_3$): δ 13.49, 14.00, 22.48, 24.27, 28.62, 30.61, 30.96, 31.44, 32.61, 41.46, 46.77, 48.18, 117.92, 118.08, 124.39, 124.51, 125.08, 142.60, 144.76, 144.91, 145.29, 145.44, 157.03, 157.08,162.67,162.73. IR ($CHCl_3$): 1673 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{26}H_{32}O_2N_7S_2$ + H]: 538.2053, found: 538.2043. Melting Point: 141°C.

6-Heptyl-3-((1-(2-(6-heptyl-4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)ethyl)-1H-1,2,3-triazol-4-yl)methyl)thieno[2,3-d]pyrimidin-4(3H)-one (33c)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.89 (t, *J*=7 Hz, 6H), 1.11-1.50 (m, 16H), 1.52-1.82 (m, 4H), 2.17(s, 1H), 2.83 (t, *J*=7 Hz, 4H), 4.52 (t, *J*=8 Hz, 2H), 4.74 (t, *J*=8 Hz, 2H), 5.21 (s, 2H), 7.09 (s, 1H), 7.14 (s, 1H), 7.48 (s, 1H), 7.64 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 14.03(2C), 22.56(2C), 28.90(4C), 30.56(2C), 30.99(2C), 31.65(2C), 41.46, 46.76, 48.15, 117.89(2C), 124.45, 125.10, 128.37, 131.13,F 144.91, 145.07, 145.25, 145.42, 157.05(2C), 162.64(2C). IR (KBr): 1667, 1679, 2359, 3433 cm.$^{-1}$ MS *m/z* : 608.3 [M+ H]. Melting point: 159 °C.

3-((1-(2-(6-Heptyl-4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)ethyl)-1H-1,2,3-triazol-4-yl)methyl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidin-4(3H)-one (33d)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.89 (t, *J* =7 Hz, 3H), 1.24-1.35 (m, 6H), 1.4-1.85 (m, 8H), 2.77-2.97 (m, 6H), 4.52 (t, *J*=6 Hz, 2H), 4.74 (t, *J*=6 Hz, 2H), 5.17 (s, 2H), 7.14 (s, 1H), 7.47 (s, 1H), 7.62 (s, 1H), 8.17 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 14.02, 22.16, 22.56, 22.77, 25.16, 25.55, 28.89(2C), 30.58, 30.98, 31.65, 41.17, 46.79, 48.15, 117.87, 122.51, 124.34, 125.07, 131.34, 134.45, 143.00(2C), 144.12,

145.43, 157.06, 157.50, 162.30, 162.63. IR (KBr): 1567, 1677, 3362 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{28}H_{33}O_2N_7S_2$ + H]: 564.2210, found: 564.2194. Melting point: 150°C

6-Butyl-3-(3-(4-((6-butyl-4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)methyl)-1H-1,2,3-triazol-1-yl)propyl)thieno[2,3-d]pyrimidin-4(3H)-one (34a)

^{1}H NMR (500 MHz, $CDCl_3$): δ 0.91-.097 (m, 6H), 1.35-1.47 (m, 4H), 1.64-1.75 (m, 4H), 2.37-2.47 (m, 2H), 2.79-2.88 (m, 4H), 4.06 (t, *J* =7 Hz, 2H), 4.39 (t, *J* =7 Hz, 2H), 5.26 (s, 2H), 7.12 (s, 1H), 7.14 (s, 1H), 7.85 (s, 1H), 7.98 (s, 1H), 8.26 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 13.68 (2C), 22.00 (2C), 29.68, 30.29 (2C), 33.09 (2C), 41.58, 43.96, 47.26, 117.98, 118.07, 124.25, 124.60, 124.69, 128.82, 145.06, 145.14, 145.41, 145.48, 157.11, 157.35, 162.58, 162.71. IR ($CHCl_3$): 1668 cm^{-1}.HRMS (ESI) m/z calculated for [$C_{26}H_{31}O_2N_7S_2$ + H]: 538.2053, found: 538.2049. Melting Point: 173 ^{0}C.

3-(3-(4-((6-Heptyl-4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)methyl)-1H-1,2,3-triazol-1-yl)propyl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidin-4(3H)-one (34b)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.87 (t, *J* =7 Hz, 3H), 1.14-1.33 (m, 8H), 1.55-1.95 (m, 6H), 2.40 (quin, *J*=8 Hz, 2H), 2.68-2.86 (m, 4H), 3.00 (t, 2H), 4.03 (t, *J*=7 Hz, 2H), 4.39 (t, *J*=7 Hz, 2H), 5.26 (s, 2H), 7.12 (s, 1H), 7.84 (s, 1H), 7.93 (s, 1H), 8.26 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 14.01, 22.16, 22.54, 22.78, 25.17, 25.58, 28.87(2C), 29.63, 30.56, 30.99, 31.63, 41.54, 43.70, 47.29, 117.88 (2C), 124.18, 124.49, 131.43, 134.55, 145.09(2C), 145.33, 145.37, 157.08, 157.83, 162.17, 162.64. IR (KBr): 1669, 3122 $cm.^{-1}$ HRMS (ESI) m/z calculated for [$C_{29}H_{35}O_2N_7S_2$ + H]: 578.2366, found: 578.2531; [$C_{29}H_{35}O_2N_7S_2$ + Na]: 600.2186, found: 600.2355. . Melting point: 157.2 °C.

3-(3-(4-((4-Oxo-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidin-3(4H)-yl)methyl)-1H-1,2,3-triazol-1-yl)propyl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidin-4(3H)-one (34c)

^{1}H NMR (200 MHz, $CDCl_3$): δ 1.71-1.95 (m, 8H), 2.25-2.60(m, 2H), 2.78 (t, *J*=6 Hz, 4H), 3.00 (t, *J*=6Hz, 4H), 4.03 (t, *J* = 6Hz, 2H), 4.40 (t, *J*=7Hz, 2H), 5.23 (s, 2H), 7.83 (s, 1H), 7.94 (s, 1H), 8.82 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 22.15(2C), 22.77(2C), 25.16(2C), 25.57(2C), 29.60, 41.22, 43.71, 47.26, 122.62, 122.67, 124.11(2C), 131.33, 131.40,134.44, 134.53, 145.30, 145.32, 157.56, 157.82, 162.16, 162.27. IR (KBr): 1668, 3017, 3422 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{26}H_{27}O_2N_7S_2$ + Na]: 556.1560, found: 556.1768. Melting point: 121.5°C.

3,3'-(Ethane-1,2-diyl)bis(6-butylthieno[2,3-d]pyrimidin-4(3H)-one) (35a)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.96 (t, *J* =8 Hz, 6H), 1.32-1.50 (m, 4H), 1.64-1.81 (m, 4H), 2.86 (t, *J*=8 Hz, 4H), 4.43 (s, 4H), 7.17 (s, 2H), 7.68 (s, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 13.69 (2C), 22.03 (2C), 30.32 (2C), 33.07 (2C), 45.51, 45.61, 117.94 (2C), 124.42 (2C), 145.16, 145.30, 145.56, 145.61, 157.30 (2C), 162.43, 162.63. IR ($CHCl_3$): 1674 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{22}H_{26}O_2N_4S_2$ + H]: 443.1570, found: 443.1571; [$C_{22}H_{26}O_2N_4S_2$ + Na]: 465.1389 found: 465.1389. Melting Point: 207^{0}C.

3,3'-(Ethane-1,2-diyl)bis(6-propylthieno[2,3-*d*]pyrimidin-4(3H)-one (35c)

^{1}H NMR (200 MHz, $CDCl_3$): δ 1.01 (t, *J*=7 Hz, 6H), 1.65-1.85 (m, 4H), 2.83 (t, *J*=7 Hz, 4H), 4.42 (s, 4H), 7.16 (s, 2H), 7.69 (s, 2H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.54 (2C), 24.27 (2C), 32.64 (2C), 45.48 (2C), 118.03 (2C), 124.40 (2C), 145.12 (2C), 145.29 (2C), 157.35 (2C), 162.86 (2C). IR ($CHCl_3$): 1660 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{20}H_{22}O_2N_4S_2$ + H]: 415.1257, found: 415.1238. Melting Point:-217^{0}C.

6-Butyl-3-(2-((6-butylthieno[2,3-d]pyrimidin-4-yl)oxy)ethyl)thieno[2,3-d]pyrimidin-4(3H)-one (36a)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.89-1.00 (m, 6H), 1.34-1.47 (m, 4H), 1.65-1.76 (m, 4H), 2.84 (t, *J*=8 Hz, 2H), 2.90 (t, *J*=8 Hz, 2H), 4.49 (t, *J*=5 Hz, 2H), 4.85 (t, *J*=5 Hz, 2H), 6.94 (s, 1H), 7.17 (s, 1H), 8.00 (s, 1H), 8.51 (s, 1H).^{13}C NMR (50 MHz, $CDCl_3$): δ 13.70, 13.74, 21.98, 22.13, 30.27, 30.67, 33.07, 33.09, 45.90, 63.79, 114.04, 118.16, 119.34, 124.70, 144.84, 145.90, 146.32, 152.04, 157.18, 161.72, 162.49, 16 8.27 IR ($CHCl_3$): 1669 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{22}H_{26}O_2N_4S_2$ + H]: 443.1570, found: 443.1588; [$C_{22}H_{26}O_2N_4S_2$ + Na]: 465.1389, found: 465.1409. Melting Point: 176^{0}C.

3-(2-Bromoethyl-6-ethylthieno[2,3-*d*]primidin-4(3*H*)-one (36b):

^{1}H NMR (200 MHz, $CDCl_3$): δ 1.36 (t, *J*=7 Hz, 3H), 2.89 (q, *J*=7 Hz, 2H), 3.77 (t, *J*=6 Hz, 2H), 4.38 (t, *J*=6 Hz, 2H), 7.18 (s, 1H), 7.99 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 15.29, 24.01, 29.82, 48.75, 117.38, 124.58, 145.80, 146.46, 157.06, 162.74. IR ($CHCl_3$): 1676 cm^{-1}. HRMS (ESI) m/z calculated for [$C_{10}H_{11}OBrN_2S$+H]: 286.9848, found: 286.9842. Melting Point: 196^{0}C.

2-(2-(6-Butyl-4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)ethyl)isoindoline-1,3-dione (37a)

^{1}H NMR (200 MHz, $CDCl_3$): δ 0.95 (t, *J*=7 Hz, 3H), 1.30-1.52 (m, 2H), 1.58-1.80 (m, 2H), 2.83 (t, *J*=7 Hz, 2H), 4.14 (t, *J*=6 Hz, 2H), 4.33 (t, *J*=6 Hz, 2H), 7.14 (s, 1H), 7.66-7.92 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.71, 22.06, 30.29, 33.02, 36.69, 45.36, 118.22, 123.58(2C), 124.62, 131.63, 131.63, 134.27(2C), 144.84, 144.98, 157.22, 162.35, 167.98(2C). IR ($CHCl_3$): 1676, 1716 cm^{-1}. MS *m/z* : 382.1 [M+ H]. Melting Point: 139^{0}C.

2-(3-(6-Butyl-4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)propyl)isoindoline-1,3-dione (38a)

^{1}H NMR (200MHz, $CDCl_3$): δ 0.94 (t, *J*=7 Hz, 3H), 1.30-1.51(m, 2H), 1.61-1.79 (m,2H), 2.11-2.29 (m, 2H), 2.84 (t, *J*=8 Hz, 2H), 3.80 (t, *J*=7 Hz, 2H), 4.06 (t, *J*=7 Hz, 2H), 7.12 (s, 1H), 7.69-7.79 (m, 2H), 7.80-7.91(m, 2H), 8.07 (s, 1H). ^{13}C NMR (50MHz, $CDCl_3$): δ 13.64, 21.92, 28.51, 30.19, 33.01, 35.10, 44.66, 118.05, 123.28 (2C), 124.64, 131.81(2C), 134.03 (2C), 144.62, 145.63, 157.11, 162.38, 168.25 (2C). IR ($CHCl_3$): 1714, 1773 cm^{-1} HRMS (ESI) m/z calculated for [$C_{21}H_{21}O_3N_3S$ + H]: 396.1376, found: 396.1373; [$C_{21}H_{21}O_3N_3S$ + Na]: 418.1196, found: 418.1190. Melting Point: 146^{0}C.

Primary antitubercular screening results against MTB H37Ra and M. bovis BCG (% inhibition)

Compound no	Mycobacterium tuberculosis H37Ra			Mycobacterium bovis BCG		
	30 µg/mL	10 µg/mL	3 µg/mL	30 µg/mL	10 µg/mL	3 µg/mL
11a	23.51	28.95	13.88	**34.0**	**12.7**	**-9.1**
11b	37.67	35.04	35.73	**13.6**	**18.1**	**11.0**
11c	57.16	50.35	50.76	**23.1**	**3.9**	**0.1**
11d	11.52	5.45	-5.71	**-5.4**	**-36.1**	**-8.0**
11e	-8.23	-1.95	-1.00	**-18.0**	**-5.0**	**-6.7**
11f	-9.04	-6.25	-5.35	**-11.9**	**-31.5**	**-9.5**
11g	88.22	84.76	71.65	**98.2**	**36.3**	**3.5**
11h	86.60	51.35	36.58	**101.1**	**95.6**	**29.4**
11i	32.75	23.74	2.78	**21.7**	**28.5**	**-5.2**
11j	-3.06	6.84	-3.35	**25.9**	**-10.4**	**-5.0**
11k	47.98	32.09	26.32	**100.4**	**99.7**	**71.1**
11l	20.47	25.34	1.62	**84.0**	**47.8**	**16.2**
11m	85.86	48.11	36.32	**91.2**	**91.6**	**77.9**
11n	24.72	9.93	0.31	**43.8**	**17.6**	**8.0**

12a	74.87	50.74	51.22	96.1	8.9	18.6
12b	26.45	11.55	17.11	17.7	23.3	-4.0
12c	-11.73	-17.29	10.37	78.2	65.5	50.6
12d	18.13	6.74	2.30	42.0	35.9	32.3
12e	36.65	35.51	38.66	99.6	100.4	101.1
13a	40.33	30.88	13.74	91.1	-7.6	-52.6
13b	96.01	99.66	93.22	98.9	98.7	99.8
14a	97.34	48.01	34.51	96.1	97.8	94.6
14b	90.94	80.98	76.78	100.9	99.7	98.2
14c	91.57	84.84	72.78	100.6	96.3	97.4
15a	98.55	62.80	23.42	59.9	34.1	0.8
16a	92.08	23.18	8.64	96.9	35.8	32.9
16b	7.57	29.70	2.35	41.8	29.0	29.1
16c	31.40	28.55	23.61	23.1	25.3	31.5
17a	-13.03	0.82	14.65	55.4	37.8	7.2
17b	27.65	22.89	20.89	47.8	56.4	45.5
17c	2.90	-1.41	1.11	65.0	62.4	67.1
18a	39.52	31.32	30.23	65.9	61.7	38.1
19a	21.16	33.23	-0.81	98.0	96.4	72.9
19b	-17.47	0.59	-8.28	-1.2	-2.2	-45.4
20b	17.85	-20.03	-4.99	7.5	-2.4	-12.5
20c	-13.34	20.73	20.20	-10.9	-11.5	-3.5
21b	27.96	22.25	16.06	37.7	18.9	23.1
22a	-16.21	3.23	8.02	22.8	-25.5	18.9
23a	31.67	31.29	11.95	86.0	88.3	54.4
23b	6.32	1.97	7.34	47.3	44.7	41.4
23c	18.12	12.39	3.87	22.4	29.1	38.8
24a	44.78	32.24	43.23	4.6	13.7	5.6
24b	11.52	-2.38	-41.06	16.6	8.0	-6.4
24c	-1.84	16.82	30.99	-3.9	6.0	-11.5
24d	-5.33	28.84	11.07	-5.8	-2.7	1.6
24e	43.51	2.52	15.11	99.8	49.4	64.1
24f	99.21	26.67	12.59	103.8	101.2	42.3
24g	93.96	81.56	34.52	99.8	100.3	101.5
24h	97.30	100.40	97.98	102.7	103.5	100.1
24i	25.78	29.55	-11.64	0.7	17.0	6.5
24j	26.05	-22.94	-43.07	-0.9	40.8	4.9
25a	4.54	-22.29	13.95	10.1	0.0	7.1
25b	4.10	6.46	11.52	45.5	45.3	-7.1
25c	48.95	35.37	23.38	102.4	53.2	38.6
25d	100.65	66.87	55.87	101.7	103.2	103.3
25e	4.05	38.18	28.54	-22.2	12.1	-50.5
26a	23.59	31.49	19.19	-6.8	-8.4	-3.7
26b	67.57	9.79	7.93	97.5	60.3	23.6
26c	93.12	89.85	91.27	98.4	96.8	99.9
26d	-1.38	-2.21	12.01	-15.4	-9.3	-12.9
27a	-6.64	-4.17	-4.99	3.6	1.0	2.6
28a	17.99	25.28	22.94	43.1	23.2	25.5
29a	30.39	14.36	-7.27	-0.4	-33.0	-4.6
29b	29.93	38.87	29.47	21.7	16.0	-3.0

29c	73.69	26.55	33.63	**97.4**	**37.0**	**22.8**
29d	97.14	94.32	73.02	**97.6**	**97.0**	**97.1**
29e	98.45	96.91	91.69	**100.4**	**100.6**	**100.2**
30a	14.77	17.51	28.98	**60.6**	**22.5**	**7.9**
30b	46.69	21.14	19.05	**100.6**	**78.8**	**92.6**
30c	82.47	74.07	70.62	**97.3**	**98.8**	**96.5**
30d	25.26	21.67	19.10	**81.4**	**27.1**	**6.0**
31a	43.83	45.76	31.05	**17.4**	**-11.9**	**11.6**
31b	26.70	-0.80	-13.65	**-13.6**	**55.8**	**13.2**
32a	-8.42	-2.19	-3.65	**-0.8**	**12.4**	**2.1**
32b	30.70	-9.33	-2.32	**26.9**	**-25.7**	**-4.9**
32c	52.13	42.80	44.58	**19.8**	**0.8**	**0.2**
32d	69.29	50.94	54.02	**92.9**	**55.7**	**39.0**
32e	51.56	64.26	28.51	**78.6**	**75.6**	**44.5**
32f	-13.98	9.74	4.26	**70.9**	**63.5**	**78.3**
32g	16.38	15.94	-9.45	**39.4**	**39.9**	**40.4**
33a	-1.13	-9.10	-6.31	**99.7**	**-79.8**	**-110.6**
33b	-4.92	-4.73	5.25	**21.6**	**29.4**	**-30.6**
33c	-4.71	6.99	-3.79	**-35.1**	**-29.7**	**-24.8**
33d	9.03	8.57	-2.64	**-16.5**	**15.5**	**8.7**
34a	-11.72	14.47	22.40	**27.4**	**24.3**	**11.3**
34b	39.25	-8.13	-2.94	**35.7**	**29.1**	**-8.4**
34c	34.23	0.79	4.67	**47.8**	**50.4**	**36.2**
35a	26.96	2.95	24.69	**98.9**	**100.2**	**99.7**
35c	22.69	39.03	9.01	**1.6**	**13.7**	**14.9**
36a	-16.41	3.58	-16.76	**15.6**	**3.4**	**27.5**
36b	-20.73	-0.21	-4.59	**6.6**	**-12.5**	**34.3**
37a	35.28	35.98	-0.42	**2.8**	**-18.1**	**-1.4**
38a	-3.47	0.37	21.72	**54.7**	**12.5**	**11.3**

Table no S1. Antimycobacterial activity data for various thienopyrimidinones

Code	**Active *M. tuberculosis* H37 Ra**		**Dormant *M. tuberculosis* H37 Ra**		**Active *M. bovis* BCG**		**Dormant *M. bovis* BCG**	
	MIC (µg/mL)	**IC_{50}** (µg/mL)	**MIC** (µg/mL)	**IC_{50}** (µg/mL)	**MIC** (µg/mL)	**IC_{50}** (µg/mL)	**MIC** (µg/mL)	**IC_{50}** (µg/mL)
11g	44.13	3.40	43.76	3.46	10.09	2.71	20.76	12.86
11m	42.89	24.61	36.32	12.78	8.51	3.04	9.82	1.76
13b	**2.51**	**1.07**	**5.20**	**1.20**	**1.89**	**1.06**	**3.02**	**1.82**
14a	38.32	11.51	>50	15.27	4.95	1.77	8.07	3.15
14b	45.86	8.76	42.70	4.51	1.37	0.71	2.34	1.26

14c	49.31	8.07	49.13	9.11	1.52	0.76	2.01	1.10
24g	24.58	12.84	35.21	7.20	2.29	1.58	3.35	1.52
24h	3.50	1.90	6.31	3.40	2.42	1.32	1.40	0.85
25d	17.51	8.11	18.49	8.84	6.30	3.66	9.37	5.02
26c	6.70	3.53	15.02	3.62	21.43	12.11	23.42	11.02
29d	8.42	5.06	11.54	5.24	4.08	2.46	4.51	3.17
29e	**2.07**	**0.91**	**8.33**	**1.20**	**1.30**	**0.69**	**2.26**	**1.55**
RIF	0.51	0.0018	0.75	0.05	0.45	0.0054	0.81	0.075

RIF indicate Rifampicin, MIC indicates Minimum Inhibitory Concentration.

Primary cytotoxic screening results against human cancer cell lines (% inhibition)

Comp no	MCF-7 cell line				A549 cell line				HCT 116 cell line		
	30 µg/mL	10 µg/mL	3 µg/mL		30 µg/mL	10 µg/mL	3 µg/mL		30 µg/mL	10 µg/mL	3 µg/mL
11a	33.39	-0.11	12.73		21.80	16.40	6.25		28.04	23.09	12.82
11b	30.73	16.84	-10.09		18.89	19.73	13.49		48.21	36.96	22.21
11c	33.09	0.92	0.00		17.87	23.61	5.09		46.63	36.11	29.58
11d	1.35	-3.06	-6.00		6.13	6.85	-7.30		8.63	5.77	-5.94
11e	10.51	6.02	-7.15		10.25	0.00	6.16		41.22	24.03	16.93
11f	-3.02	-10.70	-5.84		0.00	-10.04	-5.25		0.00	0.00	0.00
11g	33.60	17.95	9.33		30.78	18.15	19.81		14.16	12.74	2.00
11h	24.66	25.80	19.62		21.37	20.04	20.97		8.04	22.16	3.00
11i	33.77	32.06	17.56		-5.13	0.00	-19.77		-6.84	-2.72	-1.73
11j	40.86	12.22	1.25		30.74	23.39	28.15		33.54	29.89	31.97
11k	18.36	-11.15	-0.12		44.44	34.20	39.01		22.24	5.59	18.82
11m	34.65	-6.01	6.47		56.61	25.24	26.29		26.41	23.20	22.13
12a	30.28	-1.30	1.47		0.16	9.63	-2.56		13.19	9.33	18.32
12b	0.00	0.97	8.30		3.62	-1.63	10.38		0.00	-12.18	7.13
12c	0.00	0.00	0.00		12.05	0.00	0.00		11.33	27.27	1.00
12d	23.20	19.26	9.89		-23.30	0.00	0.00		39.64	30.51	13.51
12e	26.90	5.05	0.00		-12.81	0.00	0.00		36.03	9.25	11.67
13a	58.25	42.35	35.97		63.14	35.14	33.66		54.06	50.01	40.00
13b	24.49	21.50	10.92		39.49	0.00	-21.16		38.96	13.41	11.70
14a	-1.16	3.52	-7.11		9.71	14.64	13.20		11.47	3.75	1.66
14b	62.88	23.58	0.00		18.05	0.00	4.75		53.09	28.83	27.91
14c	8.89	8.22	-0.21		10.22	0.00	12.85		-1.38	-8.96	0.00
15a	51.08	33.08	32.51		11.04	9.39	3.58		-10.50	-5.80	18.73

17a	-8.86	0.00	-9.39		-17.95	0.00	0.00		8.81	-3.42	3.00
18a	0.00	-0.53	0.00		-0.35	-14.97	6.91		-6.07	0.00	3.40
19a	30.93	25.42	0.00		-12.91	6.91	-6.20		16.24	31.66	30.19
19b	25.62	8.14	5.40		-2.01	1.28	10.02		44.47	24.85	22.42
20b	-2.68	12.19	-1.75		13.08	11.28	14.73		-12.00	-9.17	2.23
20c	30.70	26.93	24.98		20.24	12.82	13.94		31.80	39.47	3.00
22a	18.55	8.41	21.41		-6.13	0.00	-6.50		-5.61	7.26	12.87
24a	31.57	3.10	9.90		19.26	18.08	9.72		38.79	28.70	22.04
24b	-9.00	12.77	7.34		-4.16	-3.06	-3.00		9.28	30.00	34.30
24c	-4.57	-14.99	5.86		10.03	9.62	5.15		21.48	16.64	5.42
24d	-2.26	-12.13	0.00		22.12	20.04	13.31		27.92	24.81	10.00
24e	6.80	-18.85	-8.21		0.00	-4.96	-17.22		47.99	41.42	34.71
24f	29.11	0.00	-10.15		-6.07	0.00	0.00		50.27	17.72	22.82
24g	53.37	-9.35	-12.05		-13.66	2.01	-6.56		0.00	0.00	2.00
24h	60.98	-3.24	9.73		34.07	0.07	0.00		86.90	17.14	11.02
24i	-7.03	4.46	-4.78		24.03	20.36	9.89		0.00	0.00	-5.14
24j	-2.42	-4.26	-5.69		26.91	16.50	17.96		-8.19	0.00	-6.38
25a	47.77	0.45	-16.58		3.75	0.67	0.00		11.55	-3.39	0.00
25b	13.63	4.38	-10.28		7.18	-9.14	0.00		36.25	31.12	35.85
25c	-10.04	0.00	-5.88		43.77	13.24	6.01		45.82	21.33	1.46
25d	50.74	17.81	14.67		16.44	-10.40	1.92		28.59	27.10	16.17
25e	0.00	0.00	0.00		0.25	1.13	-4.77		18.23	0.00	1.35
26a	37.16	32.64	28.26		29.30	23.65	24.33		50.84	48.15	32.00
26b	10.26	0.00	-16.85		-15.68	-45.62	-3.82		15.77	24.01	0.00
26c	3.79	0.00	0.00		17.15	7.21	14.62		21.68	20.95	3.00
26d	35.01	20.76	17.45		33.57	20.23	16.03		30.44	25.00	5.00
29a	26.21	20.16	8.32		22.92	14.52	15.83		28.69	36.51	1.00
29b	8.91	-10.80	2.38		-0.72	4.92	3.08		12.58	-2.62	-7.88
29d	42.77	32.57	19.39		81.88	10.34	8.11		58.07	41.28	39.41
29e	-5.28	3.99	-2.73		-11.89	-7.34	-5.22		47.38	18.69	0.87
30a	24.17	7.01	20.09		-11.42	0.00	28.02		40.57	27.77	26.15
30b	11.25	6.57	0.00		-17.29	0.00	0.00		41.27	32.94	24.00
30c	19.34	19.27	15.80		-11.62	0.00	-9.58		3.89	-0.44	-2.72
30d	0.00	0.00	0.00		3.70	-9.44	-8.18		3.80	0.00	0.00
31a	34.89	-0.94	0.00		30.34	20.33	10.71		31.99	17.58	6.35
31b	17.61	-8.13	1.71		36.77	23.95	15.68		13.94	13.30	12.62
32a	14.68	2.15	9.81		30.25	31.60	27.72		11.06	-0.46	9.95
32b	0.00	0.00	13.31		14.73	14.24	-3.78		0.00	-7.07	23.35
32c	-9.05	-1.35	-6.85		17.91	11.25	12.00		27.81	28.08	12.00
32d	10.23	6.12	5.32		9.19	0.00	-11.50		15.24	15.65	2.00
32e	46.86	16.84	36.21		19.52	-2.88	1.36		40.31	27.51	39.04
32f	0.00	0.00	-8.54		7.08	-2.54	-9.63		0.00	0.05	-8.22
32g	12.19	-0.25	-4.08		-17.61	-0.19	5.21		31.59	0.00	0.00
33a	0.00	0.00	0.00		5.71	-7.06	-8.08		4.10	-6.69	-6.37
33b	0.00	0.00	0.00		28.39	8.79	8.76		1.88	-2.82	0.00
33c	0.00	-4.09	0.00		28.24	11.80	4.28		17.28	9.17	14.89
33d	0.00	-9.10	0.00		33.11	29.71	30.89		23.61	11.64	13.27
34a	35.51	30.84	-1.58		-6.20	3.43	5.65		62.04	48.09	34.72
34b	-3.22	0.00	0.00		-5.34	0.00	0.00		26.92	29.22	12.00
34c	-1.88	0.00	0.00		10.63	0.00	0.00		4.30	0.40	3.00

35a	26.98	5.67	2.40		-54.27	-17.37	-10.21		37.87	31.80	2.54
35c	1.76	1.30	0.00		33.78	26.72	32.23		-13.30	0.00	-8.11
36a	7.33	0.00	0.00		-4.41	-6.12	-5.44		27.55	21.60	0.00
36b	21.72	-6.20	-7.62		16.79	13.68	1.02		36.96	32.40	15.00
37a	0.00	0.00	0.00		11.18	5.83	0.73		0.00	-4.74	-12.62
38a	18.49	10.66	8.98		-10.98	-5.45	4.30		41.06	17.81	-4.91

Table No S2. Cytotoxicity profile of selected compounds against human cancer cell lines

Code	In vitro cytotoxicity of selected thienopyrimidinones derivatives							
	MCF-7		A549		HCT 116		THP-1	
	GI_{50} (µg/mL)	GI_{90} (µg/mL)	GI_{50} (µg/mL)	GI_{90} (µg/mL)	GI_{50} (µg/mL)	GI_{90} (µg/mL)	GI_{50} (µg/mL)	GI_{90} (µg/mL)
11g	>100	>100	>100	>100	>100	>100	>100	>100
11m	33.8	>100	27.36	95.97	>100	>100	>100	>100
13b	>100	>100	>100	>100	>100	>100	>100	>100
14a	>100	>100	>100	>100	>100	>100	>100	>100
14b	24.83	>100	>100	>100	17.64	>100	>100	>100
14c	>100	>100	>100	>100	>100	>100	>100	>100
24g	20.52	>100	35.08	>100	>100	>100	>100	>100
24h	26.12	>100	45.44	>100	42.41	>100	>100	>100
25d	19.68	>100	34.15	>100	>100	>100	>100	>100
26c	>100	>100	>100	>100	>100	>100	>100	>100
29d	100	>100	16.17	74.66	14.7	85.56	>100	>100
29e	>100	>100	>100	>100	>100	>100	>100	>100
Rifampicin	>100	>100	>100	>100	>100	>100	>100	>100
Paclitaxel	0.0048	0.075	0.0035	0.0706	0.026	5.21	0.1374	5.8140
GI_{90} indicates the minimum concentration of compound required to inhibit the maximum (90%) growth of cells and GI_{50} indicates concentration to inhibit 50% growth of cells.								

Table No S3. Selectivity index (SI) of selected thienopyrimidinones derivatives on human cell lines against *Mycobacterium tuberculosis* H37Ra and *M. bovis* BCG.

Code	SI on MCF-7				SI on A549				SI on HCT 116				SI on THP-1			
	Against H37Ra		Against BCG		Against H37Ra		Against BCG		Against H37Ra		Against BCG		Against H37Ra		Against BCG	
	A	D	A	D	A	D	A	D	A	D	A	D	A	D	A	D
11g	2	2	10	5	2	2	10	5	2	2	10	5	2	2	10	5
11m	1	1	4	3	1	1	3	3	2	3	12	10	2	3	12	10
13b	40	19	53	33	40	19	53	33	40	19	53	33	40	19	53	33
14a	3	2	20	12	3	2	20	12	3	2	20	12	3	2	20	12

14b	1	1	18	11	2	2	73	43	0	0	13	8	2	2	73	43
14c	2	2	66	50	2	2	66	50	2	2	66	50	2	2	66	50
24g	1	1	9	6	1	1	15	10	4	3	44	30	4	3	44	30
24h	7	4	11	19	13	7	19	32	12	7	18	30	29	16	41	71
25d	1	1	3	2	2	2	5	4	6	5	16	11	6	5	16	11
26c	15	7	5	4	15	7	5	4	15	7	5	4	15	7	5	4
29d	12	9	25	22	2	1	4	4	2	1	4	3	12	9	25	22
29e	48	12	77	44	48	12	77	44	48	12	77	44	48	12	77	44
RIF	196	133	222	123	196	133	222	123	196	133	222	123	196	133	222	123

H37Ra- *Mycobacterium tuberculosis* H37Ra; BCG- *M. bovis* BCG; A- Active stage; D- Dormant stage;
Selectivity Index (SI) is calculated by using formula GI_{50} of compound against cell line /MIC of compound against H37Ra or BCG. If the SI is ≥10, then the compound is investigated further.